Full wwPDB EM Validation Report ⓘ

Sep 20, 2026 – 03:20 am BST

PDB ID	:	7PI5 / pdb_00007pi5
EMDB ID	:	EMD-13430
Title	:	Unstacked stretched Dunaliella PSII
Authors	:	Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on	:	2021-08-19
Resolution	:	2.78 Å(reported)
Based on initial model	:	6KAC

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

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

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

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

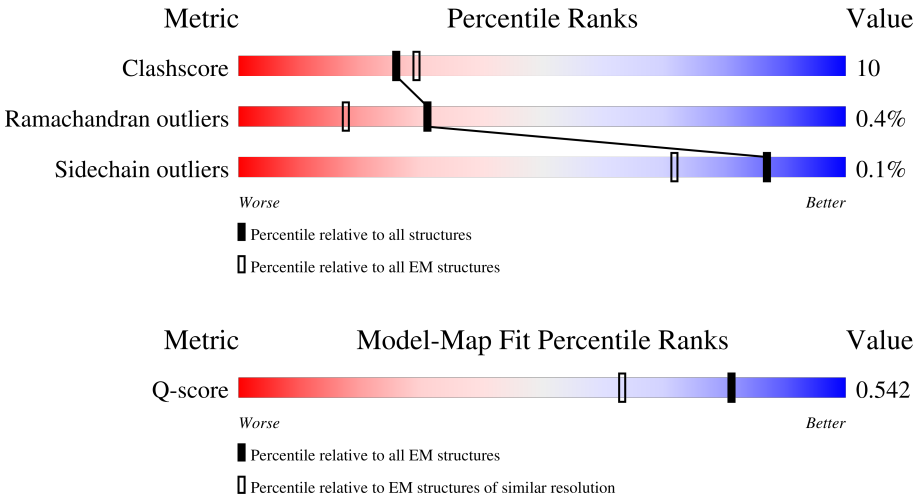
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	9% 72% 28%
1	a	336	8% 71% 29%
2	B	484	81% 19%
2	b	484	81% 19%

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Mol	Chain	Length	Quality of chain
3	V	32	97%
3	v	32	75% 25%
4	C	449	75% 25%
4	c	449	74% 26%
5	D	348	78% 22%
5	d	348	80% 20%
6	E	76	84% 16%
6	e	76	88% 12%
7	F	31	84% 16%
7	f	31	90% 10%
8	H	67	82% 18%
8	h	67	78% 22%
9	I	35	6% 86% 14%
9	i	35	94% 6%
10	J	36	6% 92% 8%
10	j	36	83% 17%
11	K	37	73% 27%
11	k	37	78% 22%
12	L	38	87% 13%
12	l	38	89% 11%
13	M	32	88% 12%
13	m	32	91% 9%
14	O	238	5% 74% 25%
14	o	238	74% 26%
15	P	187	15% 81% 19%

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Mol	Chain	Length	Quality of chain
15	p	187	20% 86% 14%
16	T	30	87% 13%
16	t	30	83% 17%
17	W	44	7% 86% 14%
17	w	44	84% 16%
18	X	30	97%
18	x	30	90% 10%
19	Z	61	90% 10%
19	z	61	90% 10%
20	N	222	80% 20%
20	n	222	83% 17%
21	G	221	82% 18%
21	g	221	83% 17%
22	R	202	24% 83% 17%
22	r	202	26% 82% 18%
23	S	243	83% 17%
23	s	243	78% 22%
24	Y	222	85% 15%
24	y	222	87% 12%
25	U	27	7% 81% 19%
25	u	27	52% 48%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	C7Z	B	620	X	-	-	-
35	C7Z	b	620	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	LMK	C	527	X	-	-	-
40	LMK	c	627	X	-	-	-
44	RRX	H	101	X	-	-	-
44	RRX	h	101	X	-	-	-
45	CHL	G	601	X	-	-	-
45	CHL	G	606	X	-	-	-
45	CHL	G	609	X	-	-	-
45	CHL	N	601	X	-	-	-
45	CHL	N	605	X	-	-	-
45	CHL	N	606	X	-	-	-
45	CHL	N	607	X	-	-	-
45	CHL	N	609	X	-	-	-
45	CHL	S	607	X	-	-	-
45	CHL	S	608	X	-	-	-
45	CHL	Y	601	X	-	-	-
45	CHL	Y	606	X	-	-	-
45	CHL	Y	607	X	-	-	-
45	CHL	Y	609	X	-	-	-
45	CHL	g	601	X	-	-	-
45	CHL	g	609	X	-	-	-
45	CHL	n	601	X	-	-	-
45	CHL	n	605	X	-	-	-
45	CHL	n	606	X	-	-	-
45	CHL	n	607	X	-	-	-
45	CHL	n	609	X	-	-	-
45	CHL	s	607	X	-	-	-
45	CHL	s	608	X	-	-	-
45	CHL	y	601	X	-	-	-
45	CHL	y	606	X	-	-	-
45	CHL	y	607	X	-	-	-
45	CHL	y	609	X	-	-	-
46	LUT	S	620	X	-	-	-
46	LUT	s	620	X	-	-	-
47	XAT	G	622	X	-	-	-
47	XAT	N	622	X	-	-	-
47	XAT	R	621	X	-	-	-
47	XAT	Y	622	X	-	-	-
47	XAT	g	622	X	-	-	-
47	XAT	n	622	X	-	-	-
47	XAT	r	622	X	-	-	-
47	XAT	y	622	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 76287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	VAL	LEU	variant	UNP D0FY05
B	415	SER	LEU	variant	UNP D0FY05
b	298	VAL	LEU	variant	UNP D0FY05
b	415	SER	LEU	variant	UNP D0FY05

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total	C	N	O	0	0
			227	152	37	38		
3	v	32	Total	C	N	O	0	0
			227	152	37	38		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		
4	c	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		
5	d	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		
6	e	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		
8	h	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	35	Total 279	C 190	N 42	O 46	S 1	0	0

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total 266	C 183	N 40	O 43	0	0
10	j	36	Total 266	C 183	N 40	O 43	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	conflict	UNP A0A1C8XRM8
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8
j	7	ILE	THR	conflict	UNP A0A1C8XRM8
j	42	LEU	GLN	conflict	UNP A0A1C8XRM8

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total 297	C 207	N 43	O 47	0	0
11	k	37	Total 297	C 207	N 43	O 47	0	0

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total 313	C 209	N 51	O 52	S 1	0	0
12	l	38	Total 313	C 209	N 51	O 52	S 1	0	0

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total 243	C 164	N 34	O 45	0	0
13	m	32	Total 243	C 164	N 34	O 45	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	variant	UNP D0FXZ3
m	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		
14	o	238	Total	C	N	O	S	0	0
			1820	1149	295	370	6		

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	65	MET	LEU	conflict	UNP A0A7S3QU88
W	96	TYR	PHE	conflict	UNP A0A7S3QU88
w	65	MET	LEU	conflict	UNP A0A7S3QU88

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Chain	Residue	Modelled	Actual	Comment	Reference
w	96	TYR	PHE	conflict	UNP A0A7S3QU88

- Molecule 18 is a protein called Hypothetical protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total 201	C 132	N 32	O 37	0	0
18	x	30	Total 201	C 132	N 32	O 37	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	81	VAL	THR	conflict	UNP A0A7S3VKF3
x	81	VAL	THR	conflict	UNP A0A7S3VKF3

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total 457	C 312	N 68	O 76	S 1	0	0
19	z	61	Total 457	C 312	N 68	O 76	S 1	0	0

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total 1703	C 1100	N 277	O 321	S 5	0	0
20	n	222	Total 1703	C 1100	N 277	O 321	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total 1680	C 1085	N 271	O 321	S 3	0	0
21	g	221	Total 1680	C 1085	N 271	O 321	S 3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		
22	r	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	242	Total	C	N	O	S	0	0
			1849	1195	297	354	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	56	ASP	GLU	conflict	UNP A0A7S3VRZ8
S	119	ILE	LEU	conflict	UNP A0A7S3VRZ8
S	209	LYS	GLN	conflict	UNP A0A7S3VRZ8
S	244	ILE	VAL	conflict	UNP A0A7S3VRZ8
S	245	ALA	GLY	conflict	UNP A0A7S3VRZ8
S	264	ILE	PHE	conflict	UNP A0A7S3VRZ8
S	268	LEU	ILE	conflict	UNP A0A7S3VRZ8
s	56	ASP	GLU	conflict	UNP A0A7S3VRZ8
s	119	ILE	LEU	conflict	UNP A0A7S3VRZ8
s	209	LYS	GLN	conflict	UNP A0A7S3VRZ8
s	244	ILE	VAL	conflict	UNP A0A7S3VRZ8
s	245	ALA	GLY	conflict	UNP A0A7S3VRZ8
s	264	ILE	PHE	conflict	UNP A0A7S3VRZ8
s	268	LEU	ILE	conflict	UNP A0A7S3VRZ8

- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

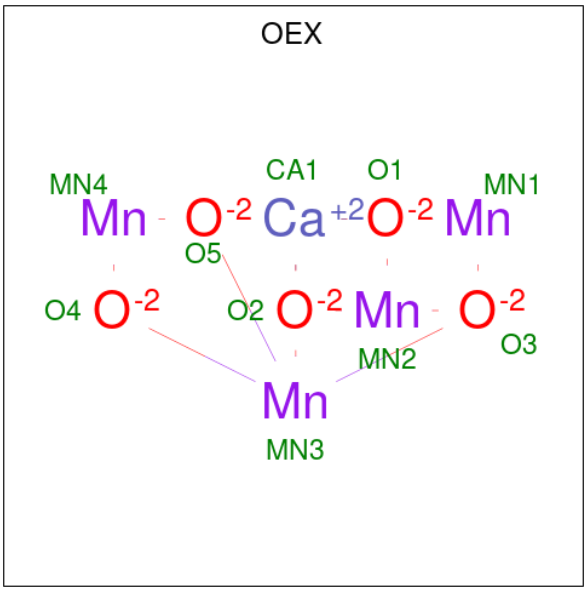
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	49	PHE	TYR	conflict	UNP A0A6S8N9J6
Y	52	SER	ALA	conflict	UNP A0A6S8N9J6
Y	73	THR	SER	conflict	UNP A0A6S8N9J6
Y	81	THR	ASN	conflict	UNP A0A6S8N9J6
Y	123	ILE	VAL	conflict	UNP A0A6S8N9J6
Y	220	LEU	PHE	conflict	UNP A0A6S8N9J6
Y	235	GLN	THR	conflict	UNP A0A6S8N9J6
Y	259	THR	SER	conflict	UNP A0A6S8N9J6
y	49	PHE	TYR	conflict	UNP A0A6S8N9J6
y	52	SER	ALA	conflict	UNP A0A6S8N9J6
y	73	THR	SER	conflict	UNP A0A6S8N9J6
y	81	THR	ASN	conflict	UNP A0A6S8N9J6
y	123	ILE	VAL	conflict	UNP A0A6S8N9J6
y	220	LEU	PHE	conflict	UNP A0A6S8N9J6
y	235	GLN	THR	conflict	UNP A0A6S8N9J6
y	259	THR	SER	conflict	UNP A0A6S8N9J6

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

- Molecule 26 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
26	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

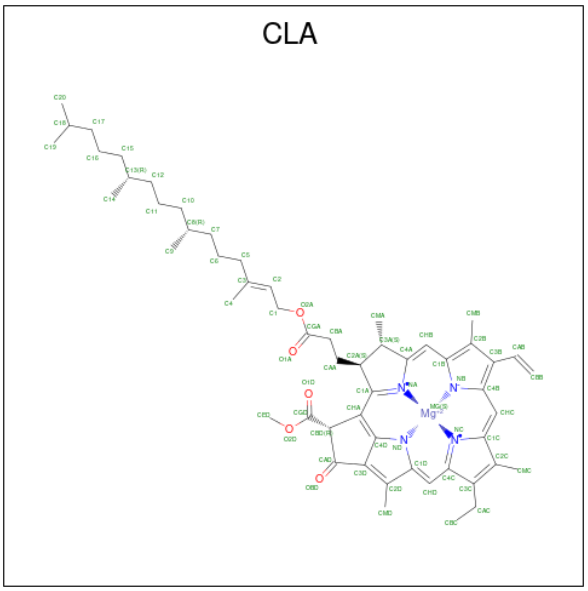
- Molecule 27 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Fe	0
			1	1	
27	a	1	Total	Fe	0
			1	1	

- Molecule 28 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
28	A	2	Total	Cl	0
			2	2	
28	a	2	Total	Cl	0
			2	2	

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	R	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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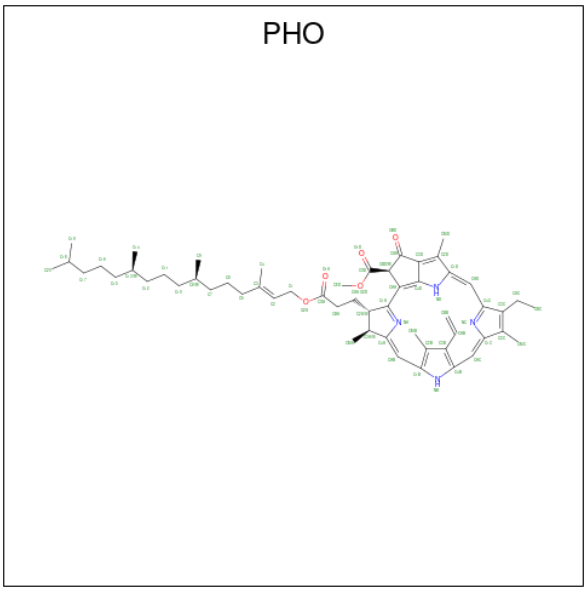
Mol	Chain	Residues	Atoms					AltConf
29	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	n	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
29	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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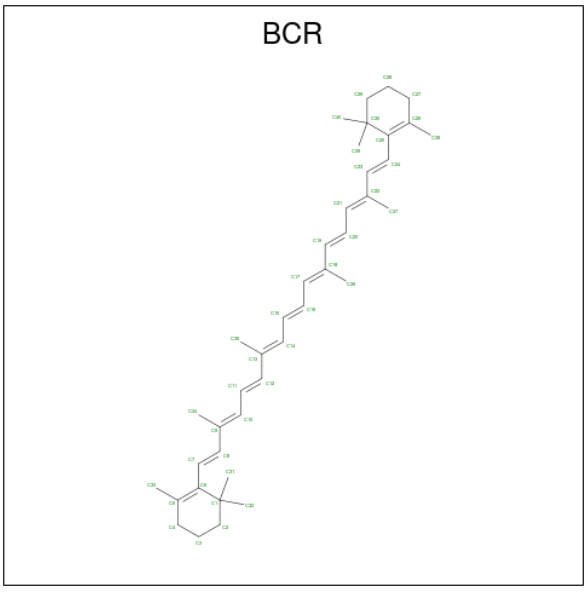
Mol	Chain	Residues	Atoms					AltConf
29	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	s	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	y	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



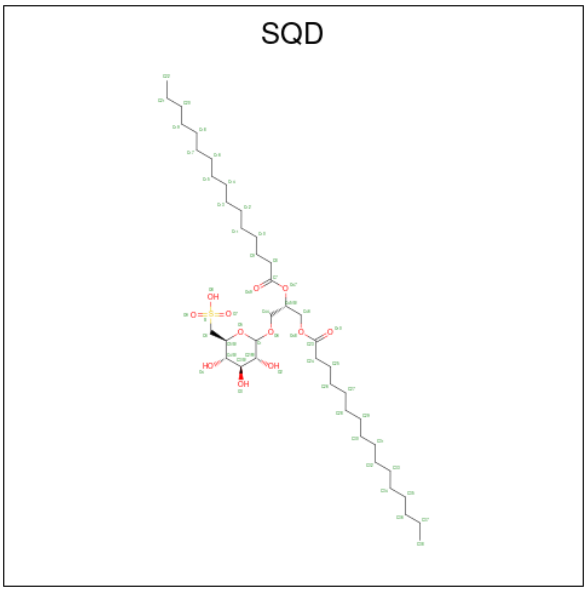
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	A	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	
30	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



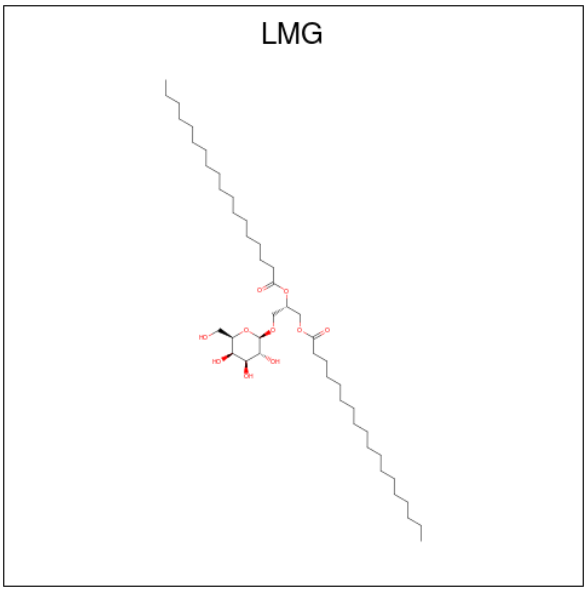
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	d	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			51	38	12	1	
32	B	1	Total	C	O	S	0
			54	41	12	1	
32	C	1	Total	C	O	S	0
			54	41	12	1	
32	a	1	Total	C	O	S	0
			51	38	12	1	
32	b	1	Total	C	O	S	0
			54	41	12	1	
32	c	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

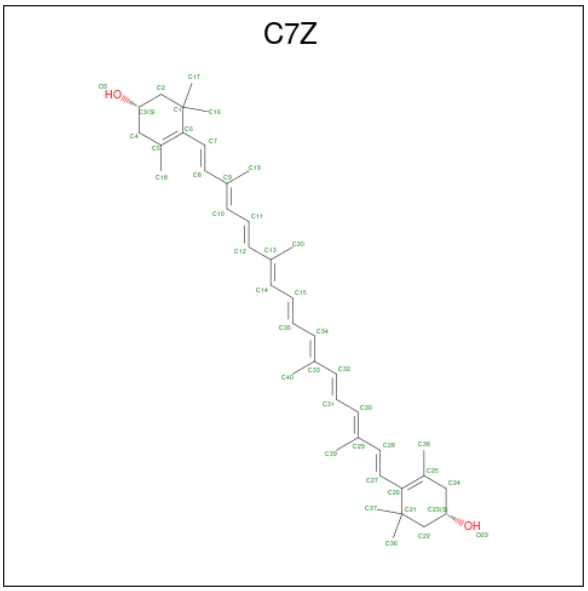


Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O 48 38 10	0
33	B	1	Total C O 44 34 10	0
33	C	1	Total C O 51 41 10	0
33	D	1	Total C O 46 36 10	0
33	H	1	Total C O 48 38 10	0
33	J	1	Total C O 45 35 10	0
33	a	1	Total C O 48 38 10	0
33	b	1	Total C O 44 34 10	0
33	c	1	Total C O 51 41 10	0
33	d	1	Total C O 46 36 10	0
33	h	1	Total C O 48 38 10	0
33	j	1	Total C O 45 35 10	0

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

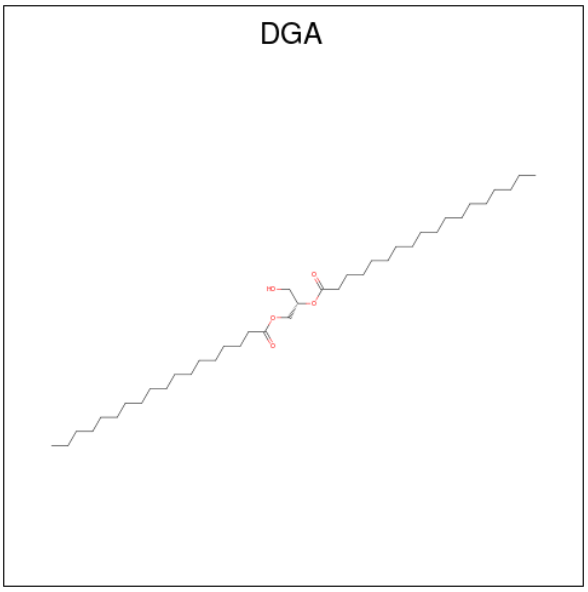
Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total Na 1 1	0
34	a	1	Total Na 1 1	0

- Molecule 35 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



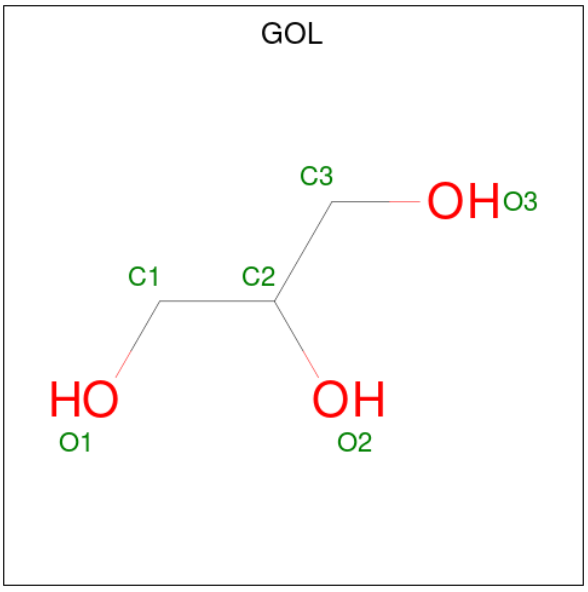
Mol	Chain	Residues	Atoms	AltConf
35	B	1	Total C O 42 40 2	0
35	b	1	Total C O 42 40 2	0

- Molecule 36 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



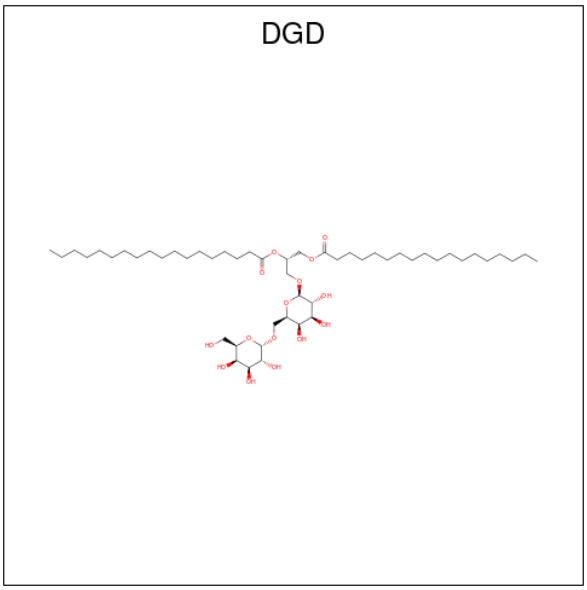
Mol	Chain	Residues	Atoms	AltConf
36	B	1	Total C O 44 39 5	0
36	C	1	Total C O 44 39 5	0
36	b	1	Total C O 44 39 5	0
36	c	1	Total C O 44 39 5	0

- Molecule 37 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	AltConf
37	B	1	Total C O 6 3 3	0
37	b	1	Total C O 6 3 3	0
37	b	1	Total C O 6 3 3	0
37	y	1	Total C O 6 3 3	0

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



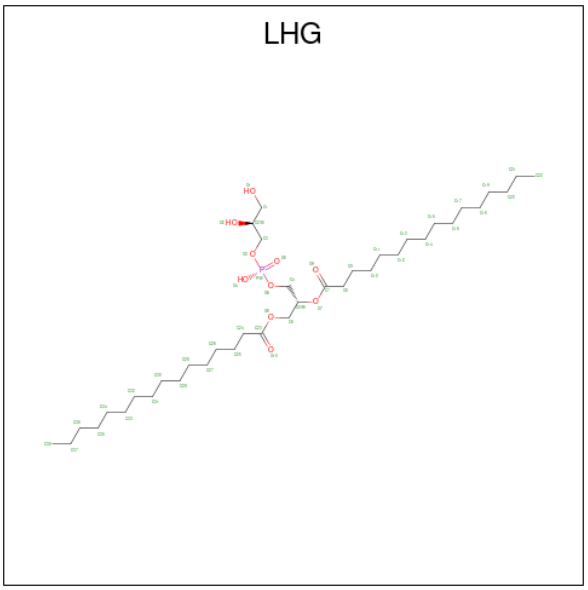
Mol	Chain	Residues	Atoms	AltConf
38	C	1	Total C O 55 40 15	0
38	C	1	Total C O 62 47 15	0
38	C	1	Total C O 59 44 15	0
38	C	1	Total C O 66 51 15	0
38	c	1	Total C O 55 40 15	0
38	c	1	Total C O 62 47 15	0
38	c	1	Total C O 59 44 15	0

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Mol	Chain	Residues	Atoms			AltConf
38	c	1	Total	C	O	0
			66	51	15	

- Molecule 39 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



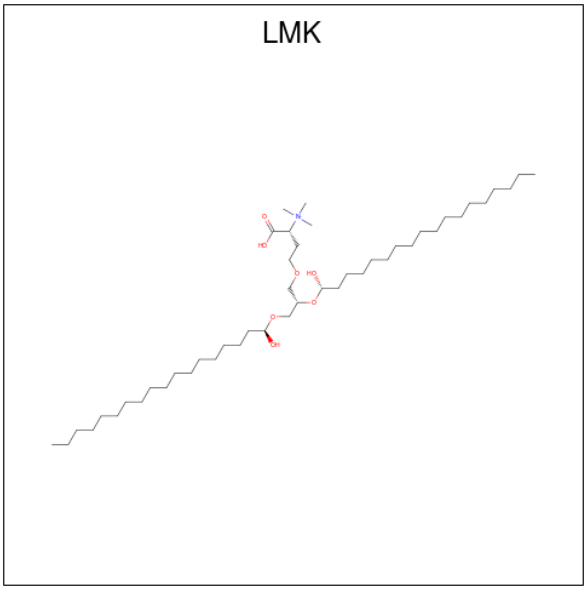
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	O	P	0
			47	36	10	1	
39	D	1	Total	C	O	P	0
			44	33	10	1	
39	D	1	Total	C	O	P	0
			49	38	10	1	
39	D	1	Total	C	O	P	0
			39	28	10	1	
39	L	1	Total	C	O	P	0
			49	38	10	1	
39	N	1	Total	C	O	P	0
			49	38	10	1	
39	G	1	Total	C	O	P	0
			49	38	10	1	
39	S	1	Total	C	O	P	0
			45	34	10	1	
39	Y	1	Total	C	O	P	0
			49	38	10	1	
39	c	1	Total	C	O	P	0
			47	36	10	1	

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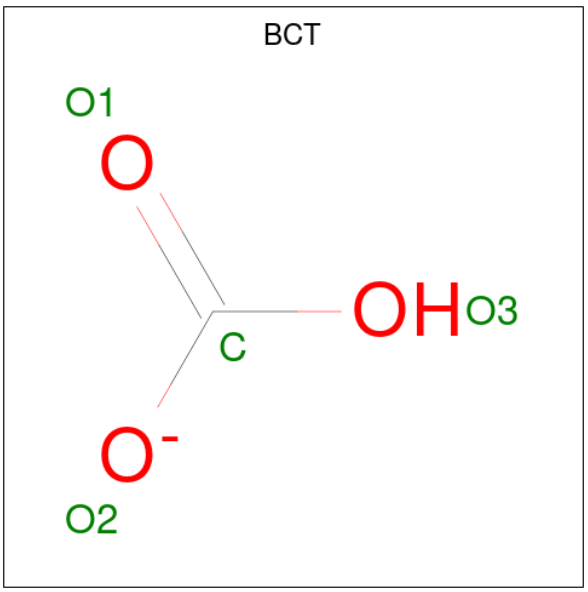
Mol	Chain	Residues	Atoms				AltConf
39	d	1	Total	C	O	P	0
			44	33	10	1	
39	d	1	Total	C	O	P	0
			49	38	10	1	
39	d	1	Total	C	O	P	0
			39	28	10	1	
39	l	1	Total	C	O	P	0
			49	38	10	1	
39	n	1	Total	C	O	P	0
			49	38	10	1	
39	g	1	Total	C	O	P	0
			49	38	10	1	
39	s	1	Total	C	O	P	0
			45	34	10	1	
39	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 40 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



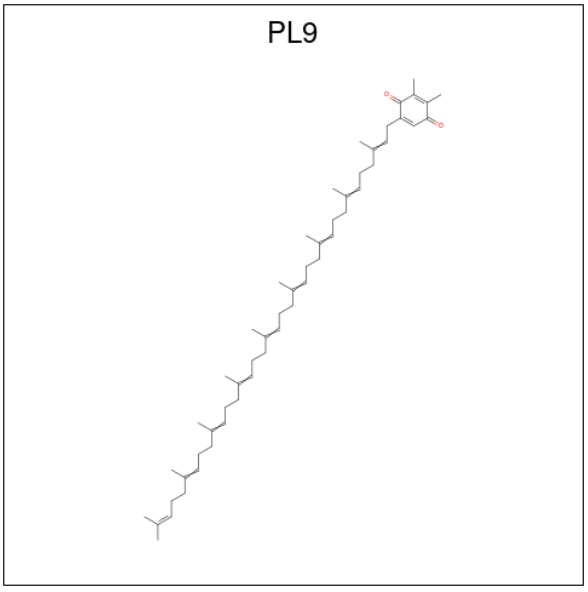
Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	N	O	0
			40	32	1	7	
40	c	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 41 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



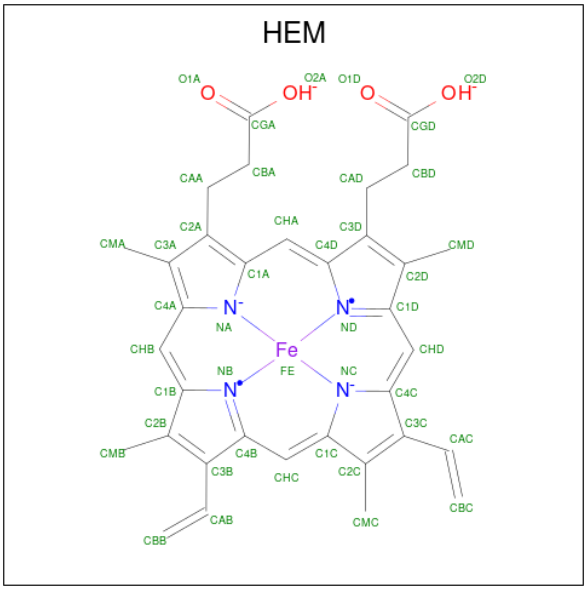
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			4	1	3	
41	d	1	Total	C	O	0
			4	1	3	

- Molecule 42 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



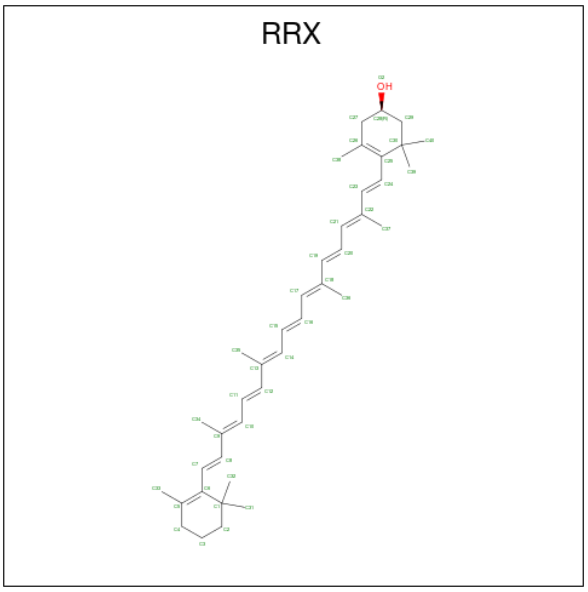
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			55	53	2	
42	d	1	Total	C	O	0
			55	53	2	

- Molecule 43 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



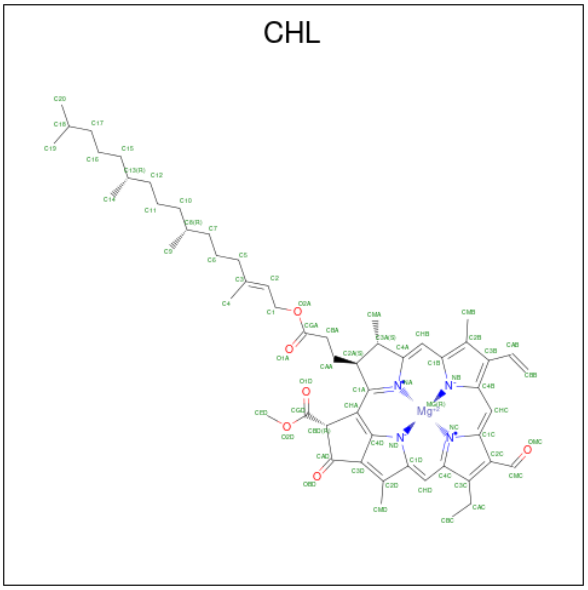
Mol	Chain	Residues	Atoms					AltConf
43	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
43	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 44 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms			AltConf
44	H	1	Total	C	O	0
			41	40	1	
44	h	1	Total	C	O	0
			41	40	1	

- Molecule 45 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
45	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
45	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
45	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
45	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
45	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
45	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
45	S	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
45	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
45	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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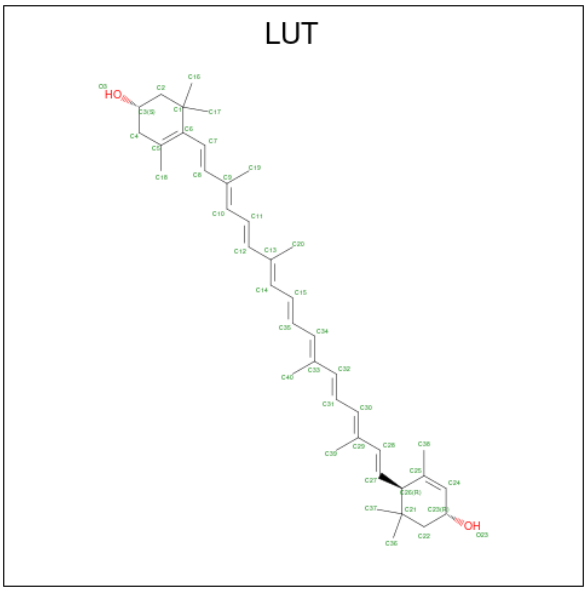
Mol	Chain	Residues	Atoms					AltConf
45	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
45	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	g	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
45	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	r	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
45	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
45	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
45	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
45	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
45	s	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
45	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
45	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
45	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
45	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 46 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



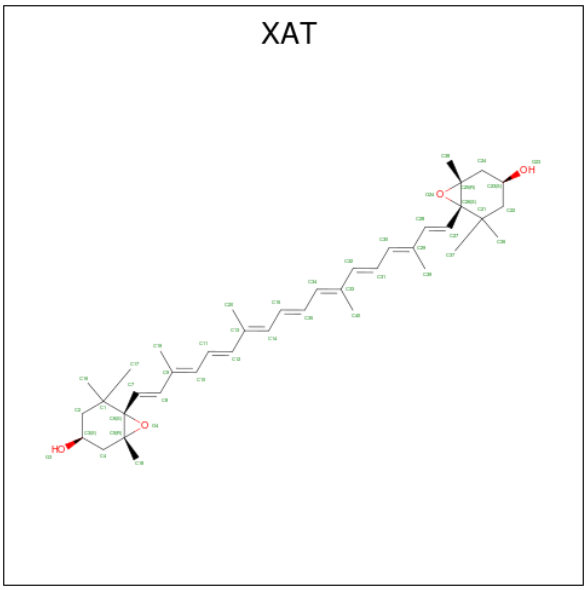
Mol	Chain	Residues	Atoms			AltConf
46	N	1	Total	C	O	0
			42	40	2	
46	N	1	Total	C	O	0
			42	40	2	
46	G	1	Total	C	O	0
			42	40	2	
46	G	1	Total	C	O	0
			42	40	2	
46	R	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			42	40	2	
46	S	1	Total	C	O	0
			42	40	2	
46	Y	1	Total	C	O	0
			42	40	2	
46	Y	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
46	n	1	Total C O 42 40 2	0
46	n	1	Total C O 42 40 2	0
46	g	1	Total C O 42 40 2	0
46	g	1	Total C O 42 40 2	0
46	r	1	Total C O 42 40 2	0
46	s	1	Total C O 42 40 2	0
46	s	1	Total C O 42 40 2	0
46	y	1	Total C O 42 40 2	0
46	y	1	Total C O 42 40 2	0

- Molecule 47 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



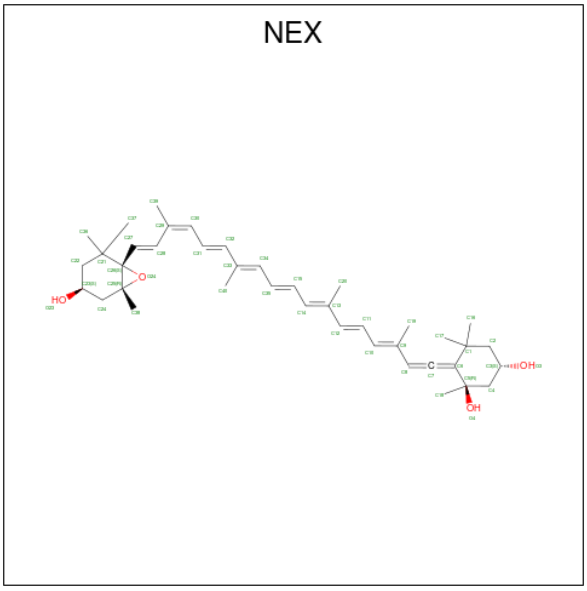
Mol	Chain	Residues	Atoms	AltConf
47	N	1	Total C O 44 40 4	0
47	G	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
47	R	1	Total C O 44 40 4	0
47	Y	1	Total C O 44 40 4	0
47	n	1	Total C O 44 40 4	0
47	g	1	Total C O 44 40 4	0
47	r	1	Total C O 44 40 4	0
47	y	1	Total C O 44 40 4	0

- Molecule 48 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



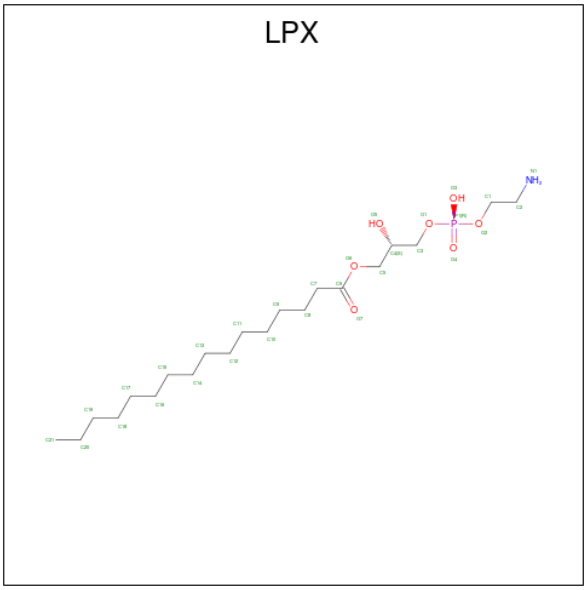
Mol	Chain	Residues	Atoms	AltConf
48	N	1	Total C O 44 40 4	0
48	G	1	Total C O 44 40 4	0
48	R	1	Total C O 44 40 4	0
48	S	1	Total C O 44 40 4	0

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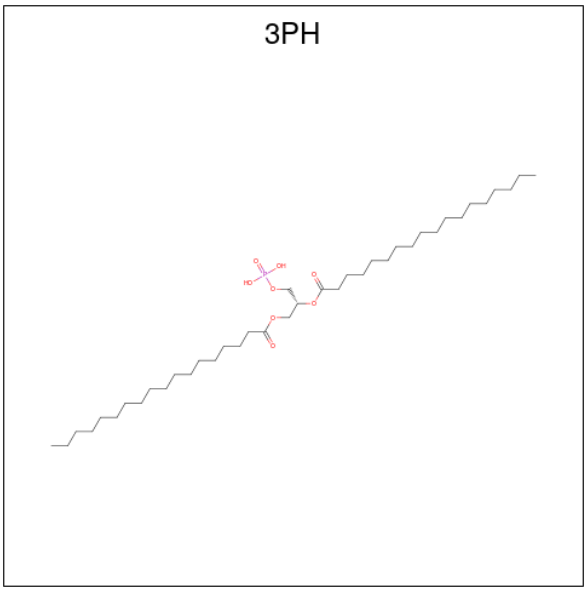
Mol	Chain	Residues	Atoms				AltConf
48	Y	1	Total	C	O		0
			44	40	4		
48	n	1	Total	C	O		0
			44	40	4		
48	g	1	Total	C	O		0
			44	40	4		
48	r	1	Total	C	O		0
			44	40	4		
48	s	1	Total	C	O		0
			44	40	4		
48	y	1	Total	C	O		0
			44	40	4		

- Molecule 49 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



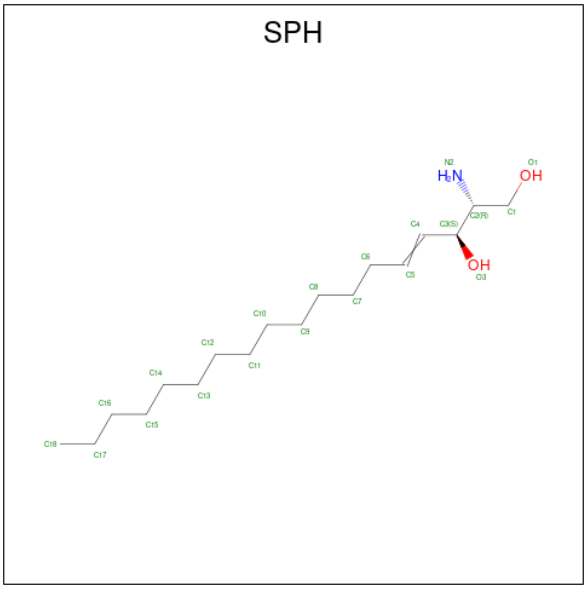
Mol	Chain	Residues	Atoms					AltConf
49	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
49	s	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 50 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
50	S	1	Total	C	O	P	0
			48	39	8	1	
50	i	1	Total	C	O	P	0
			48	39	8	1	
50	s	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 51 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
51	Y	1	Total	C	N	O	0
			21	18	1	2	

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Mol	Chain	Residues	Atoms				AltConf
51	y	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	A	43	Total	O	0
			43	43	
52	B	57	Total	O	0
			57	57	
52	C	55	Total	O	0
			55	55	
52	D	42	Total	O	0
			42	42	
52	E	7	Total	O	0
			7	7	
52	H	8	Total	O	0
			8	8	
52	I	4	Total	O	0
			4	4	
52	J	3	Total	O	0
			3	3	
52	K	2	Total	O	0
			2	2	
52	L	5	Total	O	0
			5	5	
52	M	4	Total	O	0
			4	4	
52	O	28	Total	O	0
			28	28	
52	P	10	Total	O	0
			10	10	
52	T	7	Total	O	0
			7	7	
52	W	5	Total	O	0
			5	5	
52	X	9	Total	O	0
			9	9	
52	Z	1	Total	O	0
			1	1	
52	N	5	Total	O	0
			5	5	

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Mol	Chain	Residues	Atoms	AltConf
52	G	4	Total O 4 4	0
52	R	10	Total O 10 10	0
52	S	8	Total O 8 8	0
52	Y	14	Total O 14 14	0
52	U	1	Total O 1 1	0
52	a	59	Total O 59 59	0
52	b	70	Total O 70 70	0
52	v	3	Total O 3 3	0
52	c	50	Total O 50 50	0
52	d	41	Total O 41 41	0
52	e	7	Total O 7 7	0
52	f	1	Total O 1 1	0
52	h	9	Total O 9 9	0
52	i	3	Total O 3 3	0
52	j	2	Total O 2 2	0
52	k	1	Total O 1 1	0
52	l	8	Total O 8 8	0
52	m	4	Total O 4 4	0
52	o	20	Total O 20 20	0
52	p	15	Total O 15 15	0
52	t	5	Total O 5 5	0

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Mol	Chain	Residues	Atoms	AltConf
52	w	3	Total O 3 3	0
52	x	2	Total O 2 2	0
52	n	13	Total O 13 13	0
52	g	12	Total O 12 12	0
52	r	15	Total O 15 15	0
52	s	21	Total O 21 21	0
52	y	22	Total O 22 22	0

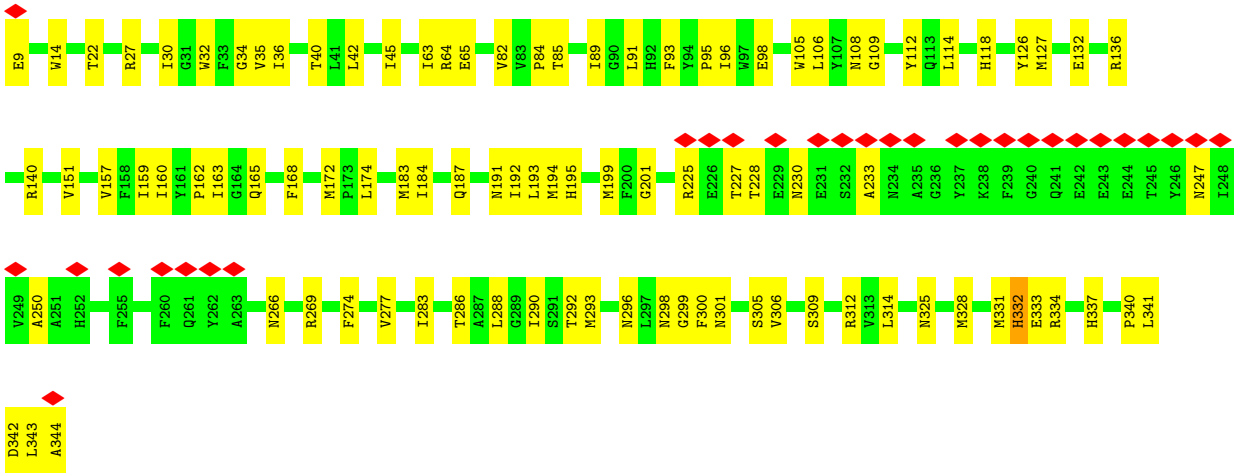
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem II protein D1

Chain A:

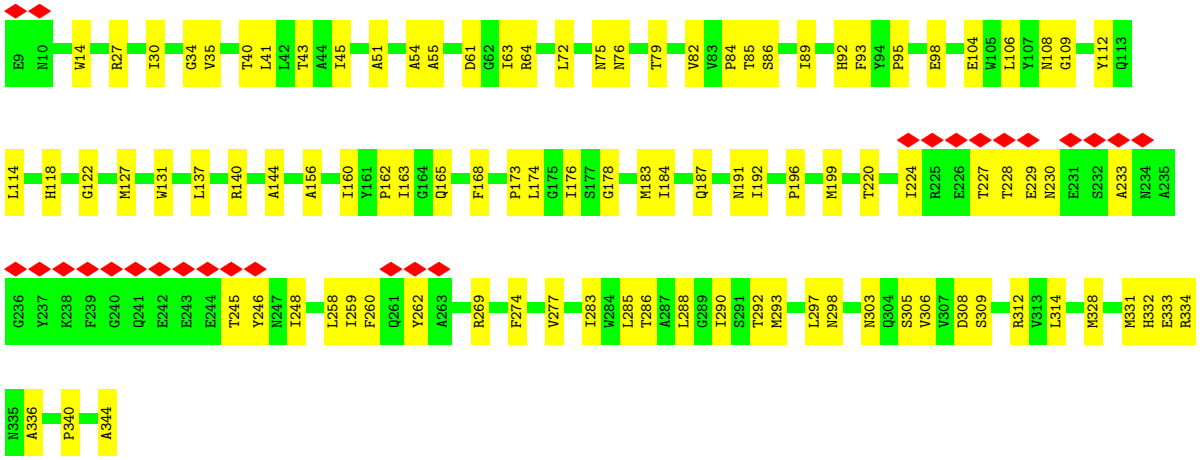




• Molecule 1: Photosystem II protein D1

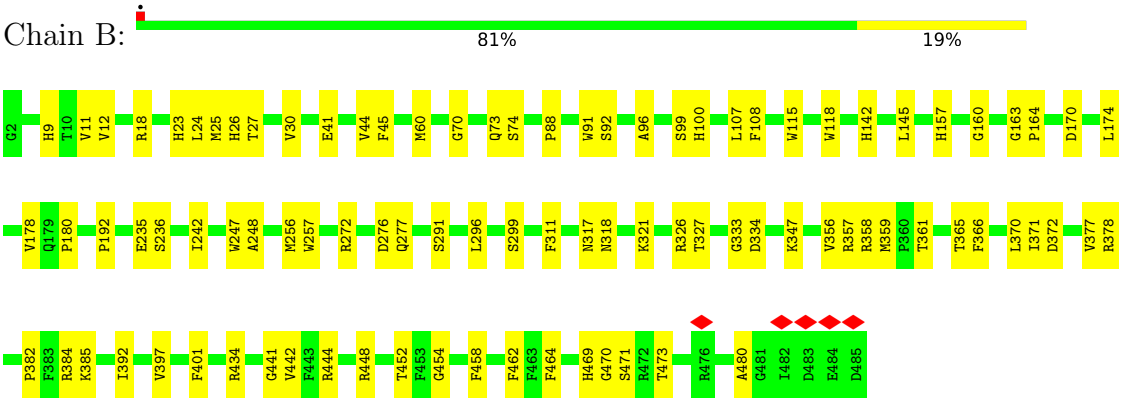
Chain a:





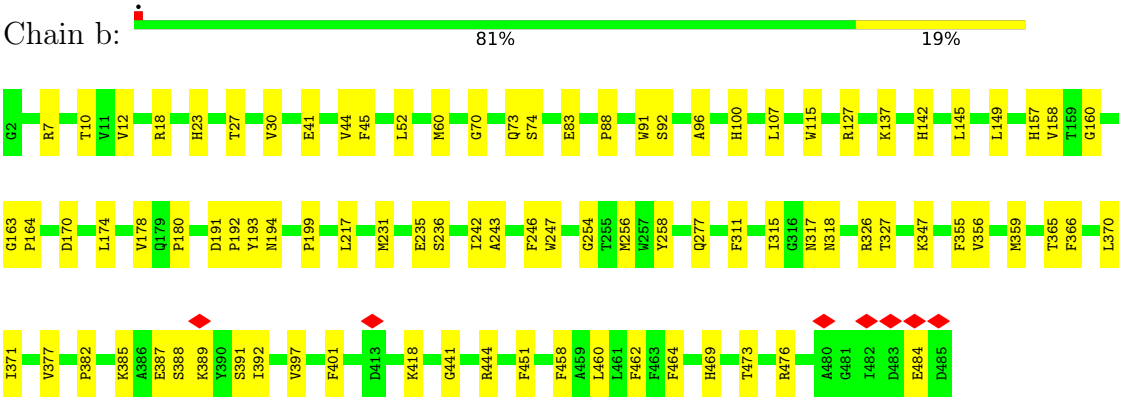
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



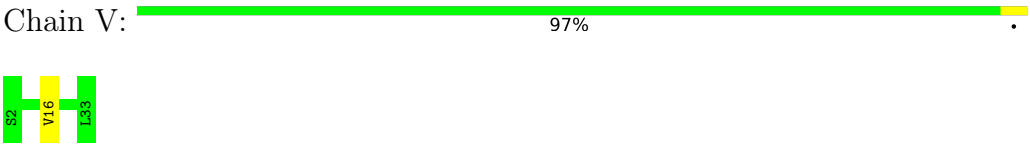
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



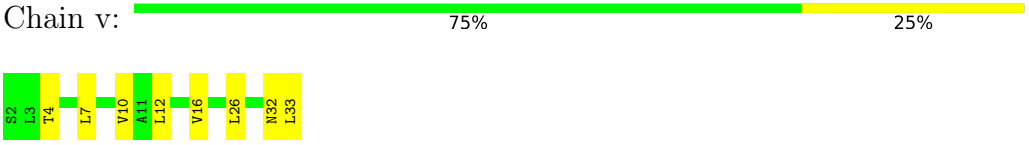
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:



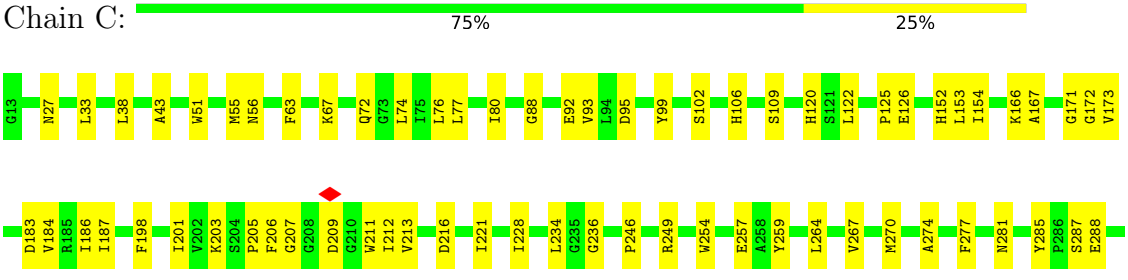
• Molecule 3: Photosystem II reaction center protein Ycf12

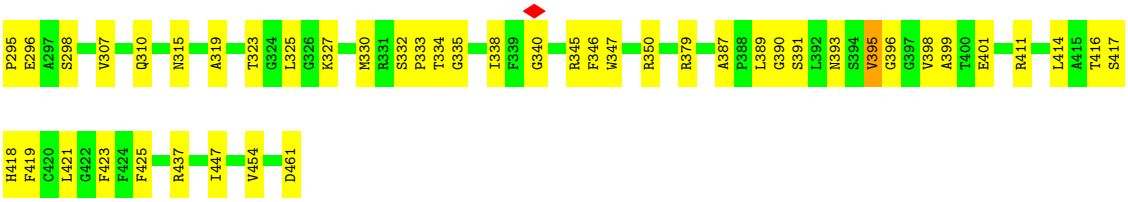
Chain v:



• Molecule 4: Photosystem II CP43 reaction center protein

Chain C:

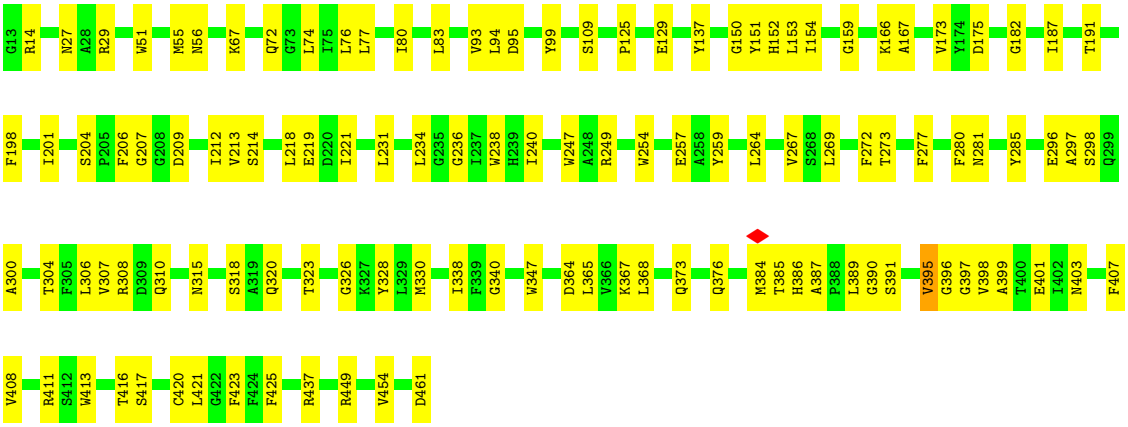




• Molecule 4: Photosystem II CP43 reaction center protein

Chain c:

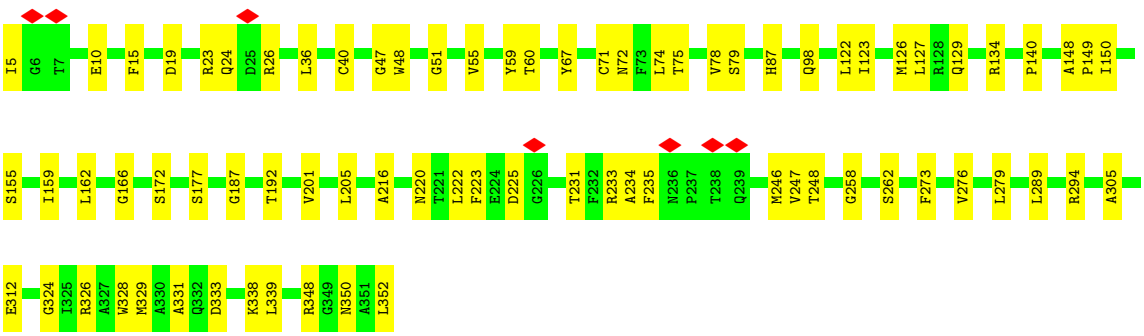




• Molecule 5: Photosystem II D2 protein

Chain D:

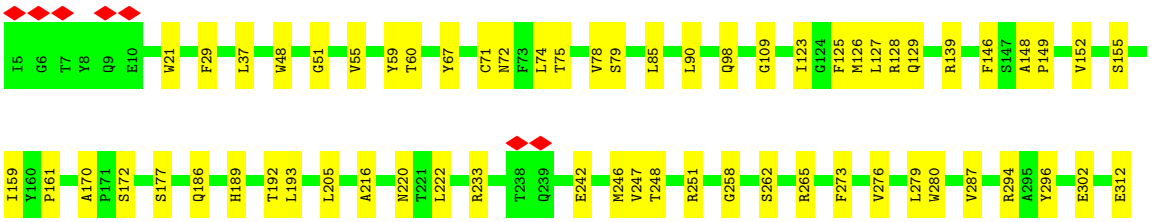




• Molecule 5: Photosystem II D2 protein

Chain d:



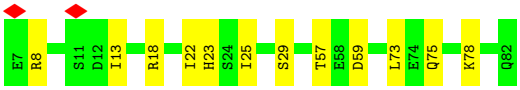




• Molecule 6: Cytochrome b559 subunit alpha

Chain E:

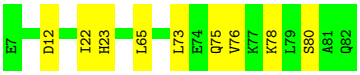




• Molecule 6: Cytochrome b559 subunit alpha

Chain e:

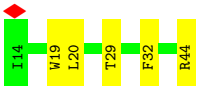




• Molecule 7: Cytochrome b559 subunit beta

Chain F:

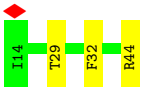




• Molecule 7: Cytochrome b559 subunit beta

Chain f:

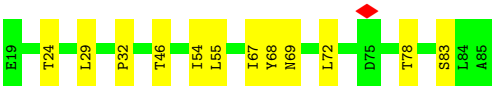




• Molecule 8: Photosystem II reaction center protein H

Chain H:

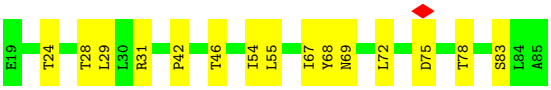




• Molecule 8: Photosystem II reaction center protein H

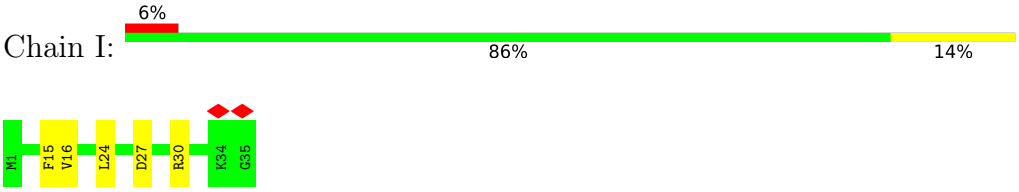
Chain h:





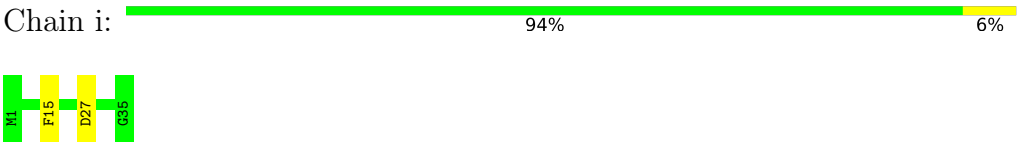
• Molecule 9: Photosystem II reaction center protein I

Chain I:



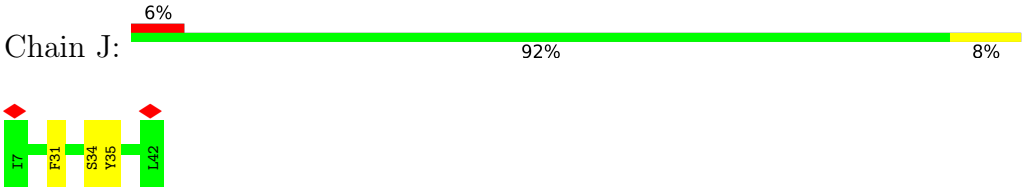
• Molecule 9: Photosystem II reaction center protein I

Chain i:



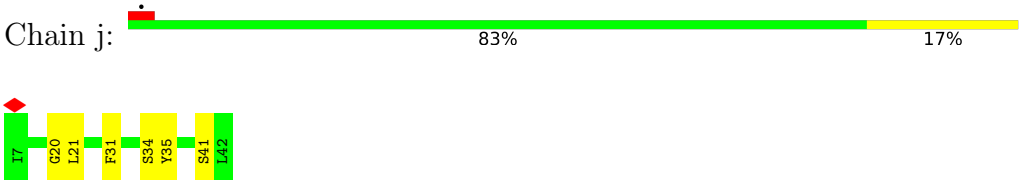
• Molecule 10: Photosystem II reaction center protein J

Chain J:



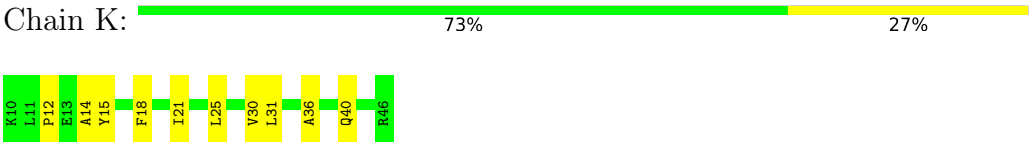
• Molecule 10: Photosystem II reaction center protein J

Chain j:



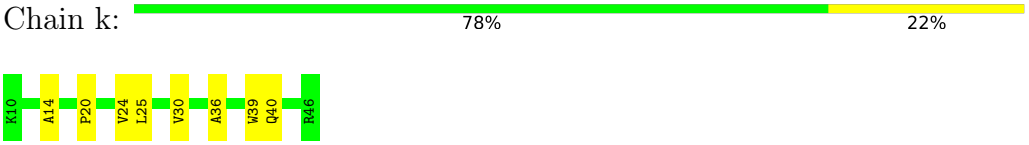
• Molecule 11: Photosystem II reaction center protein K

Chain K:



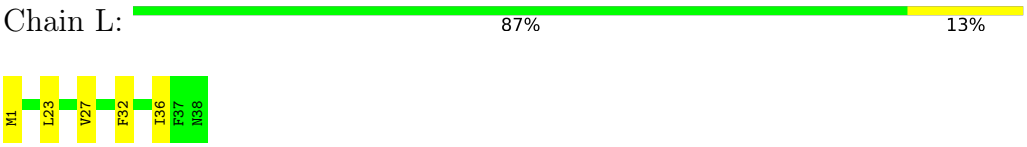
• Molecule 11: Photosystem II reaction center protein K

Chain k:



• Molecule 12: Photosystem II reaction center protein L

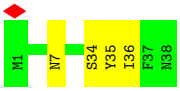
Chain L:



• Molecule 12: Photosystem II reaction center protein L

Chain l:

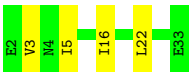




• Molecule 13: Photosystem II reaction center protein M

Chain M:

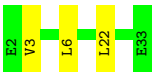




• Molecule 13: Photosystem II reaction center protein M

Chain m:

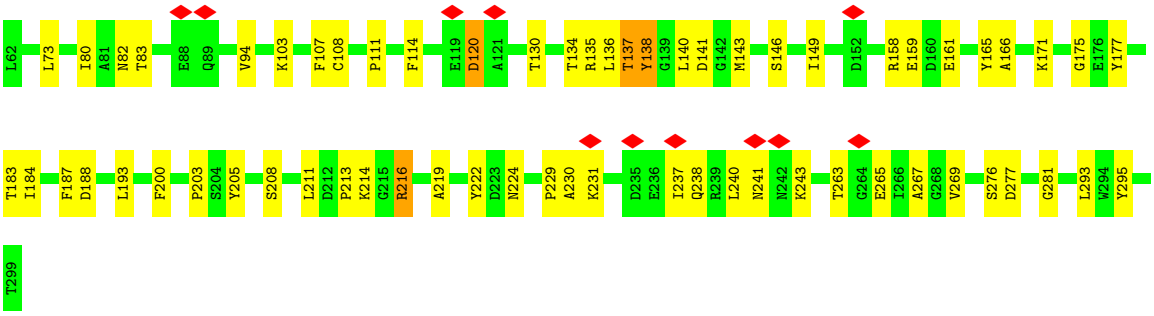




• Molecule 14: PsbO

Chain O:

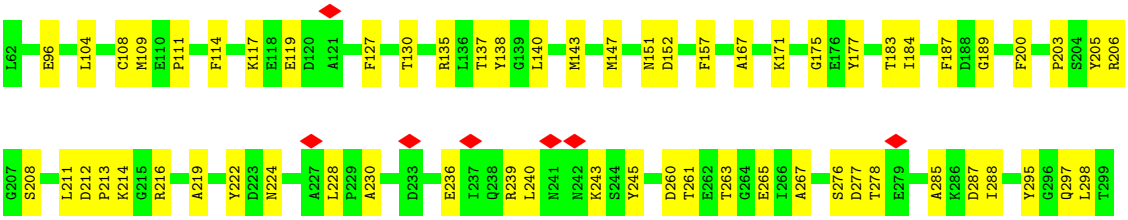




• Molecule 14: PsbO

Chain o:

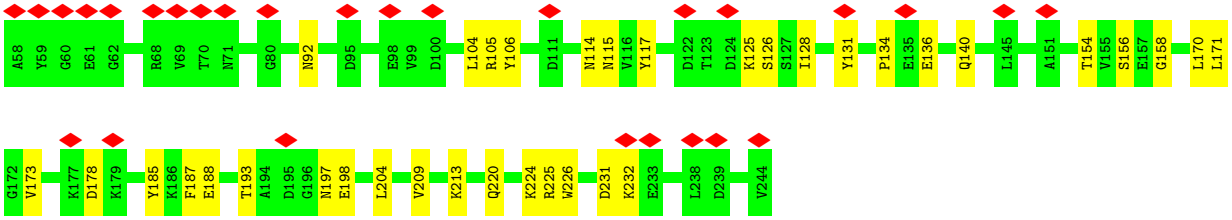




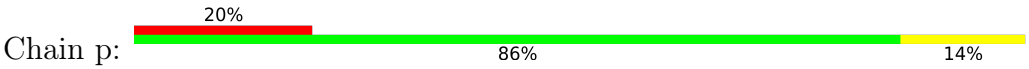
• Molecule 15: PsbP

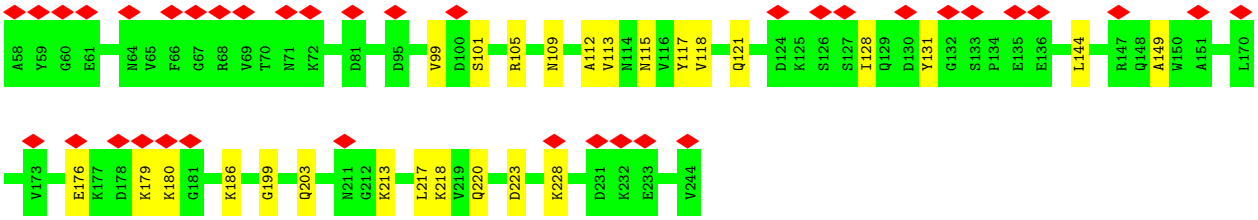
Chain P:



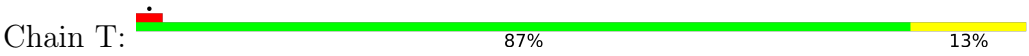


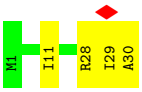
• Molecule 15: PsbP



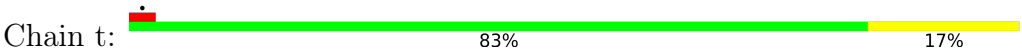


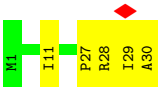
• Molecule 16: Photosystem II reaction center protein T



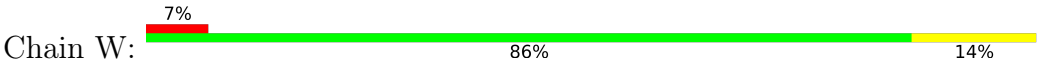


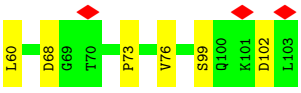
• Molecule 16: Photosystem II reaction center protein T



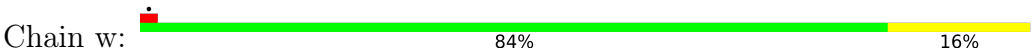


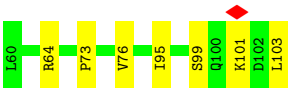
• Molecule 17: PSII 6.1 kDa protein





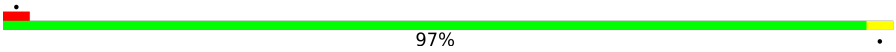
• Molecule 17: PSII 6.1 kDa protein

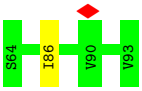




• Molecule 18: Hypothetical protein

Chain X:

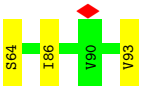




• Molecule 18: Hypothetical protein

Chain x:

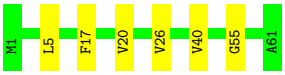




• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

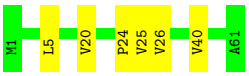




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

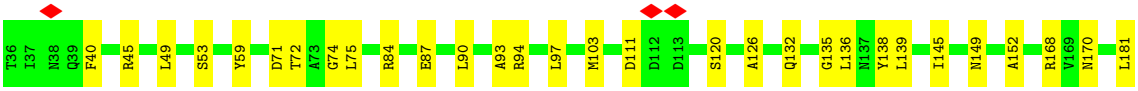


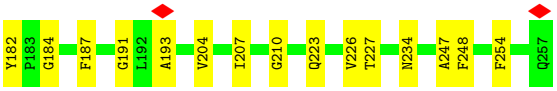


• Molecule 20: LHCII M3

Chain N:



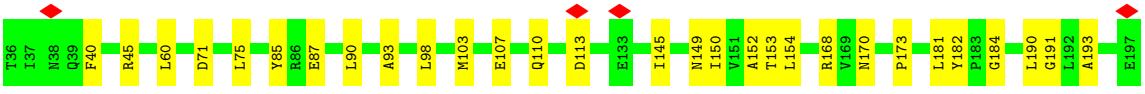


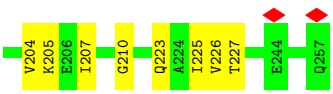


• Molecule 20: LHCII M3

Chain n:

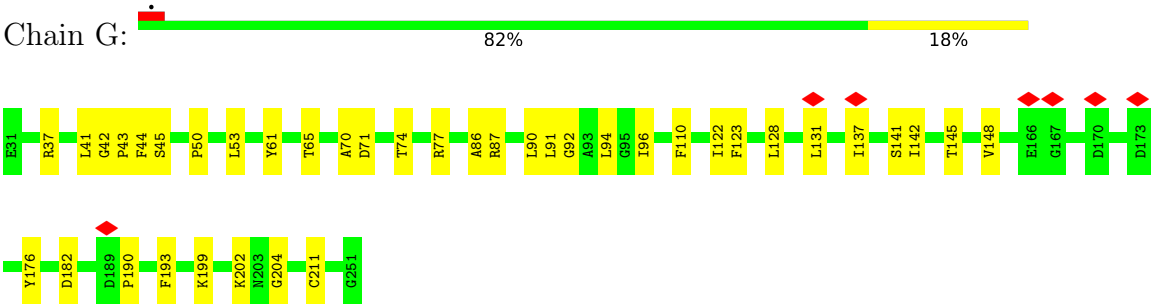






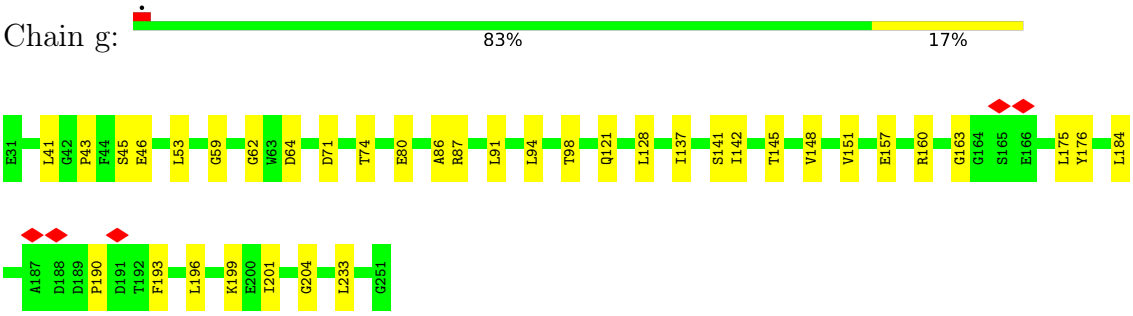
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain G:



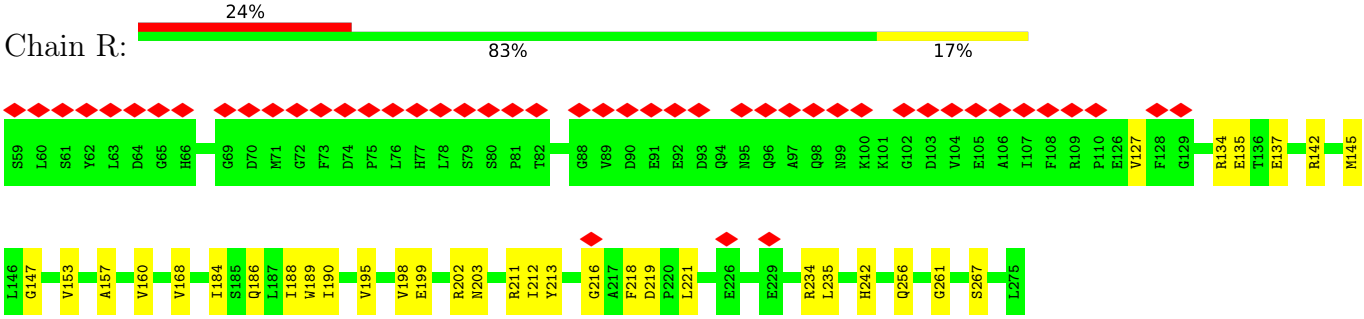
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain g:



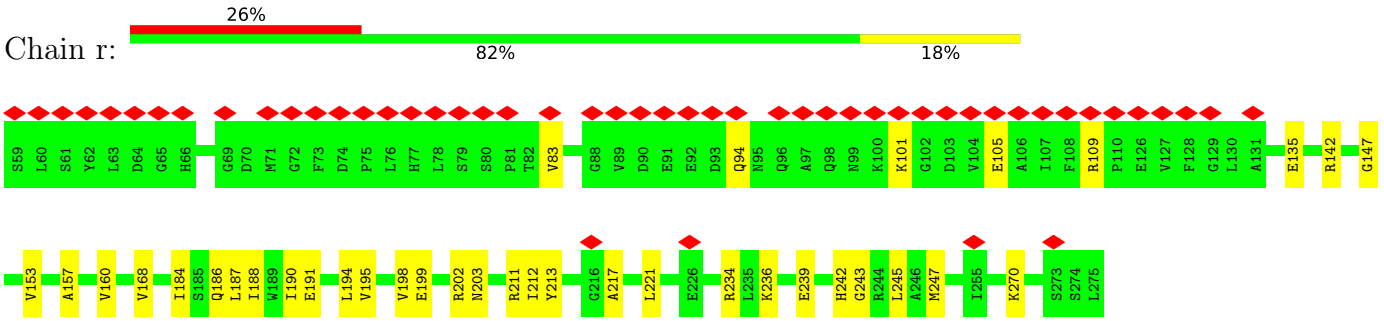
• Molecule 22: CP29

Chain R:



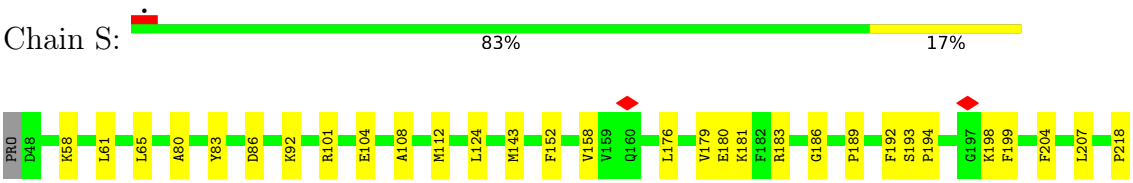
• Molecule 22: CP29

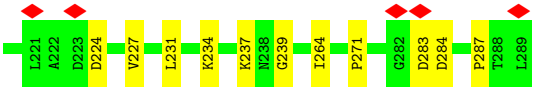
Chain r:



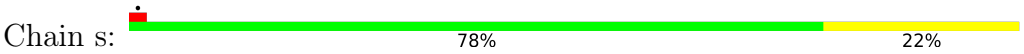
• Molecule 23: CP26

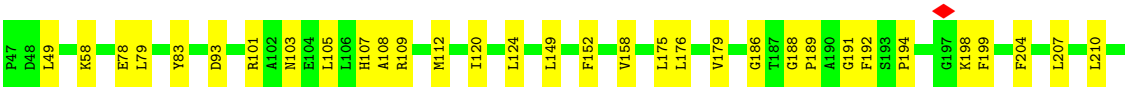
Chain S:

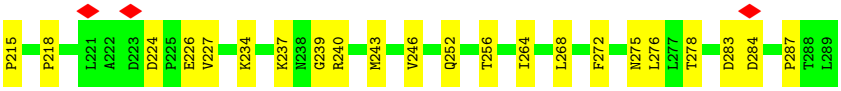




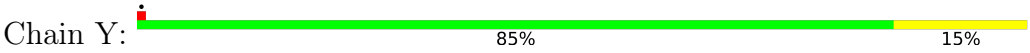
• Molecule 23: CP26

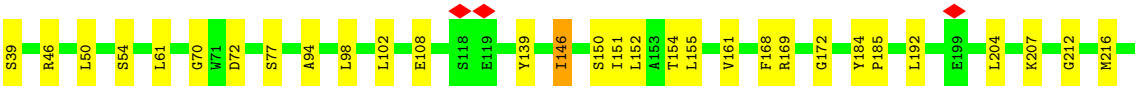


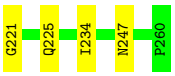




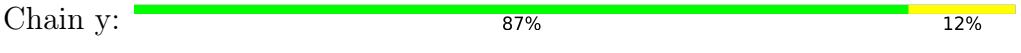
• Molecule 24: LHCII M1

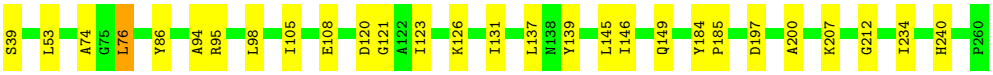




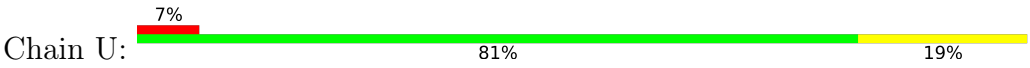


• Molecule 24: LHCII M1





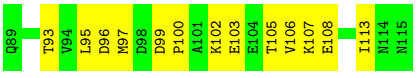
• Molecule 25: PsbU





• Molecule 25: PsbU





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23014	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	40.024	Depositor
Minimum map value	-28.419	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	448.0, 448.0, 448.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.896, 0.896, 0.896	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, NA, FE2, LMK, HEM, DGA, CL, BCR, LMG, PHO, GOL, LUT, XAT, NEX, 3PH, C7Z, SPH, LHG, CHL, CLA, SQD, LPX, BCT, PL9, OEX, RRX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.23	0/2723	0.50	1/3715 (0.0%)
1	a	0.24	0/2723	0.54	1/3715 (0.0%)
2	B	0.18	0/3912	0.41	1/5327 (0.0%)
2	b	0.19	0/3912	0.41	0/5327
3	V	0.15	0/228	0.40	0/311
3	v	0.16	0/228	0.46	0/311
4	C	0.20	0/3602	0.51	1/4913 (0.0%)
4	c	0.20	0/3602	0.52	0/4913
5	D	0.21	0/2860	0.48	2/3899 (0.1%)
5	d	0.19	0/2860	0.44	2/3899 (0.1%)
6	E	0.17	0/639	0.48	0/870
6	e	0.19	0/639	0.51	0/870
7	F	0.18	0/259	0.41	0/351
7	f	0.18	0/259	0.38	0/351
8	H	0.18	0/513	0.41	0/703
8	h	0.20	0/513	0.42	0/703
9	I	0.19	0/287	0.41	0/386
9	i	0.17	0/287	0.40	0/386
10	J	0.12	0/272	0.30	0/369
10	j	0.14	0/272	0.36	0/369
11	K	0.23	0/308	0.48	0/423
11	k	0.26	0/308	0.52	0/423
12	L	0.16	0/321	0.32	0/435
12	l	0.16	0/321	0.33	0/435
13	M	0.19	0/246	0.42	0/335
13	m	0.18	0/246	0.41	0/335
14	O	0.26	0/1855	0.55	2/2505 (0.1%)
14	o	0.20	0/1855	0.50	0/2505
15	P	0.20	0/1473	0.53	2/1988 (0.1%)
15	p	0.18	0/1473	0.51	0/1988
16	T	0.18	0/254	0.47	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	t	0.19	0/254	0.48	0/342
17	W	0.17	0/339	0.48	0/460
17	w	0.17	0/339	0.43	0/460
18	X	0.15	0/202	0.35	0/276
18	x	0.15	0/202	0.39	0/276
19	Z	0.16	0/469	0.39	0/641
19	z	0.15	0/469	0.37	0/641
20	N	0.17	0/1751	0.42	0/2386
20	n	0.16	0/1751	0.40	0/2386
21	G	0.18	0/1725	0.52	2/2348 (0.1%)
21	g	0.16	0/1725	0.40	0/2348
22	R	0.17	0/1561	0.43	0/2110
22	r	0.17	0/1561	0.43	0/2110
23	S	0.17	0/1895	0.42	0/2579
23	s	0.16	0/1902	0.38	0/2587
24	Y	0.21	0/1715	0.46	1/2338 (0.0%)
24	y	0.19	0/1715	0.43	0/2338
25	U	0.21	0/224	0.58	0/298
25	u	0.24	0/224	0.56	0/298
All	All	0.19	0/59273	0.46	15/80624 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
14	O	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	299	SER	N-CA-C	-6.96	105.98	114.75
5	D	59	TYR	CA-C-N	6.72	134.38	121.54
5	D	59	TYR	C-N-CA	6.72	134.38	121.54
5	d	59	TYR	CA-C-N	6.52	134.00	121.54
5	d	59	TYR	C-N-CA	6.52	134.00	121.54
4	C	345	ARG	N-CA-C	-5.83	105.26	112.90
14	O	138	TYR	N-CA-C	-5.70	102.33	110.59
1	a	248	ILE	N-CA-C	-5.64	107.78	113.20
14	O	140	LEU	CA-C-O	-5.30	114.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	G	70	ALA	CA-C-N	5.25	128.55	121.20
21	G	70	ALA	C-N-CA	5.25	128.55	121.20
15	P	125	LYS	CA-C-N	5.23	131.53	121.54
15	P	125	LYS	C-N-CA	5.23	131.53	121.54
24	Y	98	LEU	CA-CB-CG	5.18	134.44	116.30
1	A	332	HIS	CA-CB-CG	5.17	118.97	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	O	136	LEU	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2638	0	2541	81	0
1	a	2638	0	2541	83	0
2	B	3783	0	3663	74	0
2	b	3783	0	3663	77	0
3	V	227	0	261	1	0
3	v	227	0	261	7	0
4	C	3483	0	3376	90	0
4	c	3483	0	3376	88	0
5	D	2766	0	2655	63	0
5	d	2766	0	2654	61	0
6	E	621	0	605	10	0
6	e	621	0	605	8	0
7	F	252	0	265	4	0
7	f	252	0	265	3	0
8	H	503	0	532	13	0
8	h	503	0	532	15	0
9	I	279	0	288	5	0
9	i	279	0	288	2	0
10	J	266	0	286	2	0
10	j	266	0	286	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	297	0	312	8	0
11	k	297	0	312	8	0
12	L	313	0	325	5	0
12	l	313	0	325	4	0
13	M	243	0	264	3	0
13	m	243	0	264	2	0
14	O	1820	0	1776	48	0
14	o	1820	0	1776	45	0
15	P	1444	0	1403	26	0
15	p	1444	0	1403	21	0
16	T	247	0	260	4	0
16	t	247	0	260	5	0
17	W	332	0	323	5	0
17	w	332	0	323	5	0
18	X	201	0	224	1	0
18	x	201	0	224	3	0
19	Z	457	0	478	5	0
19	z	457	0	478	6	0
20	N	1703	0	1641	33	0
20	n	1703	0	1641	28	0
21	G	1680	0	1614	31	0
21	g	1680	0	1614	26	0
22	R	1533	0	1506	25	0
22	r	1533	0	1506	28	0
23	S	1849	0	1808	27	0
23	s	1856	0	1815	38	0
24	Y	1667	0	1624	29	0
24	y	1667	0	1624	23	0
25	U	224	0	226	5	0
25	u	224	0	226	12	0
26	A	10	0	0	0	0
26	a	10	0	0	1	0
27	A	1	0	0	0	0
27	a	1	0	0	0	0
28	A	2	0	0	0	0
28	a	2	0	0	0	0
29	A	239	0	240	18	0
29	B	1040	0	1149	68	0
29	C	845	0	932	60	0
29	D	130	0	144	10	0
29	G	446	0	428	15	0
29	N	468	0	467	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	R	501	0	455	18	0
29	S	625	0	586	19	0
29	Y	570	0	613	26	0
29	a	239	0	241	17	0
29	b	1040	0	1151	50	0
29	c	845	0	933	46	0
29	d	130	0	144	7	0
29	g	446	0	429	10	0
29	n	468	0	468	20	0
29	r	501	0	457	19	0
29	s	625	0	587	20	0
29	y	570	0	614	24	0
30	A	128	0	148	11	0
30	a	128	0	148	9	0
31	A	40	0	53	3	0
31	B	80	0	106	6	0
31	C	160	0	211	19	0
31	D	40	0	53	3	0
31	a	40	0	53	3	0
31	b	80	0	106	3	0
31	c	160	0	212	15	0
31	d	40	0	53	3	0
32	A	51	0	68	2	0
32	B	54	0	77	5	0
32	C	54	0	77	2	0
32	a	51	0	68	0	0
32	b	54	0	77	3	0
32	c	54	0	77	4	0
33	A	48	0	66	6	0
33	B	44	0	58	3	0
33	C	51	0	72	4	0
33	D	46	0	62	5	0
33	H	48	0	66	6	0
33	J	45	0	60	0	0
33	a	48	0	66	5	0
33	b	44	0	58	1	0
33	c	51	0	72	6	0
33	d	46	0	62	3	0
33	h	48	0	66	8	0
33	j	45	0	60	2	0
34	A	1	0	0	0	0
34	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	42	0	0	0	0
35	b	42	0	0	0	0
36	B	44	0	76	2	0
36	C	44	0	76	3	0
36	b	44	0	76	1	0
36	c	44	0	76	1	0
37	B	6	0	8	0	0
37	b	12	0	16	1	0
37	y	6	0	8	0	0
38	C	242	0	322	21	0
38	c	242	0	322	18	0
39	C	47	0	67	7	0
39	D	132	0	183	7	0
39	G	49	0	74	4	0
39	L	49	0	74	6	0
39	N	49	0	74	2	0
39	S	45	0	63	8	0
39	Y	49	0	74	3	0
39	c	47	0	67	2	0
39	d	132	0	183	6	0
39	g	49	0	74	4	0
39	l	49	0	74	4	0
39	n	49	0	74	2	0
39	s	45	0	63	6	0
39	y	49	0	74	2	0
40	C	40	0	0	0	0
40	c	40	0	0	0	0
41	D	4	0	0	0	0
41	d	4	0	0	0	0
42	D	55	0	80	3	0
42	d	55	0	80	2	0
43	F	43	0	30	3	0
43	f	43	0	30	3	0
44	H	41	0	56	2	0
44	h	41	0	56	1	0
45	G	324	0	273	14	0
45	N	380	0	382	14	0
45	R	94	0	66	2	0
45	S	194	0	144	12	0
45	Y	310	0	306	15	0
45	g	324	0	272	15	0
45	n	380	0	382	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	r	94	0	66	3	0
45	s	194	0	144	8	0
45	y	310	0	306	13	0
46	G	84	0	110	6	0
46	N	84	0	110	12	0
46	R	42	0	55	4	0
46	S	84	0	110	12	0
46	Y	84	0	110	5	0
46	g	84	0	110	9	0
46	n	84	0	110	6	0
46	r	42	0	55	4	0
46	s	84	0	110	9	0
46	y	84	0	110	2	0
47	G	44	0	56	4	0
47	N	44	0	56	3	0
47	R	44	0	56	5	0
47	Y	44	0	56	1	0
47	g	44	0	56	2	0
47	n	44	0	56	3	0
47	r	44	0	56	5	0
47	y	44	0	56	2	0
48	G	44	0	54	0	0
48	N	44	0	54	2	0
48	R	44	0	54	2	0
48	S	44	0	54	2	0
48	Y	44	0	54	1	0
48	g	44	0	54	0	0
48	n	44	0	54	2	0
48	r	44	0	54	3	0
48	s	44	0	54	1	0
48	y	44	0	54	0	0
49	S	30	0	43	0	0
49	s	30	0	43	0	0
50	S	48	0	75	4	0
50	i	48	0	75	1	0
50	s	48	0	75	1	0
51	Y	21	0	37	2	0
51	y	21	0	37	3	0
52	A	43	0	0	5	0
52	B	57	0	0	3	0
52	C	55	0	0	4	0
52	D	42	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	E	7	0	0	0	0
52	G	4	0	0	0	0
52	H	8	0	0	0	0
52	I	4	0	0	0	0
52	J	3	0	0	0	0
52	K	2	0	0	0	0
52	L	5	0	0	0	0
52	M	4	0	0	0	0
52	N	5	0	0	0	0
52	O	28	0	0	2	0
52	P	10	0	0	1	0
52	R	10	0	0	0	0
52	S	8	0	0	0	0
52	T	7	0	0	0	0
52	U	1	0	0	0	0
52	W	5	0	0	0	0
52	X	9	0	0	0	0
52	Y	14	0	0	1	0
52	Z	1	0	0	0	0
52	a	59	0	0	2	0
52	b	70	0	0	4	0
52	c	50	0	0	4	0
52	d	41	0	0	11	0
52	e	7	0	0	0	0
52	f	1	0	0	0	0
52	g	12	0	0	1	0
52	h	9	0	0	0	0
52	i	3	0	0	0	0
52	j	2	0	0	0	0
52	k	1	0	0	0	0
52	l	8	0	0	0	0
52	m	4	0	0	0	0
52	n	13	0	0	1	0
52	o	20	0	0	0	0
52	p	15	0	0	4	0
52	r	15	0	0	1	0
52	s	21	0	0	1	0
52	t	5	0	0	0	0
52	v	3	0	0	1	0
52	w	3	0	0	0	0
52	x	2	0	0	0	0
52	y	22	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	76287	0	76145	1540	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1540) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:80:ILE:HD12	52:O:1027:HOH:O	1.42	1.20
15:p:109:ASN:ND2	52:p:1003:HOH:O	1.75	1.18
1:A:65:GLU:OE2	52:A:1026:HOH:O	1.63	1.16
14:O:80:ILE:CD1	52:O:1027:HOH:O	1.92	1.16
5:d:348:ARG:NH1	52:d:1031:HOH:O	1.74	1.13
24:y:120:ASP:OD2	52:y:1020:HOH:O	1.70	1.06
1:A:165:GLN:NE2	52:A:1041:HOH:O	1.88	1.04
4:C:55:MET:HE2	52:C:1043:HOH:O	1.57	1.02
4:c:55:MET:HE2	52:c:1015:HOH:O	1.61	1.01
15:P:178:ASP:OD2	52:P:1009:HOH:O	1.82	0.96
24:y:120:ASP:CG	52:y:1020:HOH:O	2.12	0.87
4:c:153:LEU:HD21	29:c:506:CLA:HAB	1.55	0.86
23:s:175:LEU:HD22	48:s:623:NEX:H14	1.60	0.84
4:C:153:LEU:HD21	29:C:506:CLA:HAB	1.60	0.82
1:A:344:ALA:HB2	52:A:1040:HOH:O	1.79	0.81
22:r:195:VAL:HG23	29:r:609:CLA:HAB	1.59	0.81
5:D:71:CYS:N	52:D:1040:HOH:O	2.17	0.77
23:s:246:VAL:HG11	46:s:621:LUT:H12	1.67	0.76
24:Y:216:MET:HE1	29:Y:602:CLA:HAB	1.67	0.76
29:B:616:CLA:H2	29:B:617:CLA:HBB2	1.66	0.75
5:d:343:GLU:HB3	5:d:348:ARG:HH22	1.51	0.75
5:D:348:ARG:HH11	15:P:197:ASN:HD21	1.34	0.75
15:p:112:ALA:HB2	52:p:1006:HOH:O	1.89	0.73
2:B:247:TRP:HB2	29:B:609:CLA:HBC1	1.71	0.73
2:B:26:HIS:HD2	52:B:1008:HOH:O	1.72	0.72
15:p:109:ASN:ND2	52:p:1010:HOH:O	2.22	0.71
22:r:147:GLY:HA3	47:r:622:XAT:H193	1.72	0.71
2:b:441:GLY:HA3	14:o:228:LEU:HD12	1.71	0.71
52:d:1023:HOH:O	14:o:214:LYS:NZ	2.24	0.71
22:R:145:MET:HE1	29:R:610:CLA:HAB	1.71	0.71
2:b:387:GLU:HB2	52:b:1019:HOH:O	1.90	0.71
38:C:520:DGD:HBN1	33:D:411:LMG:H192	1.72	0.71
14:o:108:CYS:HB2	14:o:295:TYR:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:103:MET:HE3	46:n:621:LUT:H8	1.73	0.70
29:B:617:CLA:H2	48:R:622:NEX:H42	1.74	0.69
22:R:147:GLY:HA3	47:R:621:XAT:H193	1.74	0.69
14:o:109:MET:HB3	14:o:140:LEU:HB2	1.75	0.69
1:a:165:GLN:OE1	52:a:1029:HOH:O	2.11	0.68
24:y:120:ASP:OD1	52:y:1020:HOH:O	2.09	0.68
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.75	0.67
2:B:347:LYS:O	2:B:397:VAL:HA	1.95	0.67
33:d:411:LMG:HC5	52:d:1041:HOH:O	1.93	0.67
5:d:71:CYS:N	52:d:1041:HOH:O	2.27	0.67
21:g:41:LEU:HB2	21:g:45:SER:HB2	1.76	0.67
2:b:10:THR:HG23	29:b:612:CLA:HAA1	1.77	0.67
2:b:18:ARG:HH22	32:b:621:SQD:H3	1.60	0.67
2:b:247:TRP:HB2	29:b:609:CLA:HBC1	1.75	0.67
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.76	0.67
29:Y:602:CLA:H52	46:Y:621:LUT:H28	1.76	0.67
1:a:61:ASP:OD2	52:a:1048:HOH:O	2.13	0.66
29:c:513:CLA:H101	31:c:514:BCR:H21C	1.76	0.66
4:C:56:ASN:ND2	4:C:99:TYR:O	2.29	0.66
21:g:233:LEU:HD22	29:g:614:CLA:HBB1	1.78	0.66
1:a:89:ILE:HD11	1:a:108:ASN:HB3	1.77	0.66
4:C:74:LEU:HD13	4:C:77:LEU:HD12	1.77	0.66
1:A:225:ARG:NH1	1:A:227:THR:O	2.29	0.66
29:A:410:CLA:H12	33:A:413:LMG:H111	1.77	0.65
33:A:413:LMG:H191	29:C:505:CLA:H8	1.79	0.65
1:a:183:MET:HB3	29:a:405:CLA:HBC2	1.78	0.65
2:b:311:PHE:O	2:b:317:ASN:ND2	2.30	0.65
4:c:395:VAL:HG12	4:c:396:GLY:H	1.62	0.65
14:o:263:THR:HG23	14:o:265:GLU:HG3	1.77	0.65
29:b:609:CLA:HAB	5:d:123:ILE:HG12	1.79	0.64
23:s:108:ALA:HB1	23:s:239:GLY:HA3	1.80	0.64
2:b:347:LYS:O	2:b:397:VAL:HA	1.98	0.64
23:S:264:ILE:HD12	46:S:620:LUT:H163	1.79	0.64
20:n:182:TYR:HB3	29:n:610:CLA:HED3	1.78	0.64
29:A:405:CLA:H112	29:A:406:CLA:HBB1	1.79	0.63
2:b:277:GLN:HB3	25:u:106:VAL:HG23	1.80	0.63
1:a:298:ASN:HB2	4:c:391:SER:HA	1.80	0.63
52:d:1023:HOH:O	14:o:214:LYS:HE2	1.98	0.63
23:s:79:LEU:HD23	23:s:101:ARG:HE	1.62	0.63
31:C:517:BCR:H391	11:K:36:ALA:HB2	1.81	0.63
1:A:22:THR:HG21	9:I:30:ARG:HG2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:234:ARG:NH1	29:R:612:CLA:O1A	2.32	0.63
1:a:333:GLU:HB3	1:a:336:ALA:HB3	1.81	0.63
21:G:190:PRO:HA	21:G:193:PHE:HB3	1.79	0.63
30:a:409:PHO:HBC3	5:d:279:LEU:HD22	1.81	0.63
1:A:228:THR:HG23	1:A:230:ASN:H	1.63	0.62
1:A:296:ASN:ND2	52:A:1040:HOH:O	2.18	0.62
2:B:24:LEU:HD21	29:B:617:CLA:HAB	1.81	0.62
38:C:523:DGD:HBW1	29:Y:614:CLA:HBC1	1.82	0.62
23:S:224:ASP:HB3	23:S:227:VAL:HG12	1.82	0.62
5:D:19:ASP:OD2	5:D:23:ARG:NH2	2.32	0.62
15:P:128:ILE:HG23	15:P:209:VAL:HG12	1.82	0.62
2:B:30:VAL:HG12	29:B:606:CLA:HHD	1.81	0.62
14:o:265:GLU:HG2	14:o:297:GLN:HG3	1.82	0.62
23:S:108:ALA:HB1	23:S:239:GLY:HA3	1.82	0.61
29:C:513:CLA:H101	31:C:514:BCR:H21C	1.82	0.61
29:b:616:CLA:H2	29:b:617:CLA:HBB2	1.81	0.61
2:B:311:PHE:O	2:B:317:ASN:ND2	2.33	0.61
21:g:80:GLU:HG3	21:g:175:LEU:HD13	1.83	0.61
2:B:441:GLY:HA2	14:O:230:ALA:HB3	1.82	0.61
14:o:117:LYS:HE2	14:o:287:ASP:HB2	1.82	0.61
14:o:216:ARG:HA	14:o:222:TYR:H	1.65	0.61
29:r:608:CLA:HBB1	29:r:608:CLA:H8	1.82	0.61
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.83	0.61
14:O:134:THR:HG22	14:O:137:THR:HG23	1.83	0.61
1:a:245:THR:HG21	5:d:265:ARG:HH22	1.65	0.61
4:c:56:ASN:ND2	4:c:99:TYR:O	2.32	0.61
29:a:410:CLA:H12	33:a:413:LMG:H112	1.82	0.61
4:c:417:SER:HB3	38:c:519:DGD:HBT2	1.82	0.60
22:r:199:GLU:OE1	22:r:202:ARG:NH2	2.34	0.60
2:b:382:PRO:HG2	2:b:385:LYS:HG2	1.82	0.60
29:b:606:CLA:HBB1	29:b:607:CLA:H51	1.82	0.60
22:R:134:ARG:NH2	22:R:137:GLU:OE1	2.34	0.60
8:h:69:ASN:ND2	33:h:102:LMG:O10	2.34	0.60
1:A:140:ARG:HH22	39:D:410:LHG:HC41	1.67	0.60
43:f:101:HEM:HHD	43:f:101:HEM:HBC2	1.83	0.60
47:r:622:XAT:H32	29:r:602:CLA:HAB	1.82	0.60
39:C:525:LHG:H262	29:S:611:CLA:HAB	1.83	0.60
4:C:109:SER:HA	31:C:514:BCR:H16C	1.84	0.60
20:N:182:TYR:HB3	29:N:610:CLA:HED3	1.83	0.60
45:N:606:CHL:H192	50:S:626:3PH:H2A1	1.84	0.60
24:Y:108:GLU:HB3	24:Y:234:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:83:LEU:O	4:c:166:LYS:NZ	2.35	0.60
38:c:520:DGD:HBN1	33:d:411:LMG:H192	1.83	0.60
52:d:1023:HOH:O	14:o:214:LYS:CE	2.49	0.60
45:n:605:CHL:H92	29:s:611:CLA:H201	1.83	0.60
24:y:207:LYS:HD3	29:y:612:CLA:HBD	1.82	0.60
2:B:145:LEU:HD22	29:B:605:CLA:H162	1.84	0.59
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.84	0.59
29:C:513:CLA:HAB	31:C:514:BCR:H24C	1.83	0.59
4:c:437:ARG:NH2	9:i:27:ASP:OD2	2.35	0.59
2:B:235:GLU:OE2	2:B:469:HIS:ND1	2.35	0.59
4:C:167:ALA:HB1	4:C:187:ILE:HD12	1.85	0.59
31:B:618:BCR:H383	32:B:621:SQD:H252	1.85	0.59
1:a:331:MET:HB2	5:d:321:LEU:HD23	1.85	0.59
4:C:395:VAL:HG12	4:C:396:GLY:H	1.65	0.59
5:D:192:THR:HG23	29:D:402:CLA:HBC2	1.84	0.59
2:b:371:ILE:HG13	25:u:100:PRO:HB3	1.85	0.59
5:d:192:THR:HG23	29:d:402:CLA:HBC2	1.83	0.59
43:f:101:HEM:HHC	43:f:101:HEM:HBB2	1.83	0.59
23:s:234:LYS:HG3	29:s:611:CLA:HED2	1.85	0.59
29:s:603:CLA:HAB	29:s:609:CLA:HBC2	1.84	0.59
38:C:519:DGD:HB71	33:C:521:LMG:H401	1.85	0.59
2:b:30:VAL:HG12	29:b:606:CLA:HHD	1.83	0.59
1:A:40:THR:HG23	29:A:410:CLA:HBB1	1.85	0.59
4:C:95:ASP:HB3	23:S:287:PRO:HB3	1.85	0.59
4:C:152:HIS:ND1	29:C:507:CLA:OBD	2.30	0.59
30:A:409:PHO:HBC3	5:D:279:LEU:HD22	1.85	0.58
20:N:72:THR:HA	21:G:77:ARG:HH21	1.68	0.58
1:A:45:ILE:HD11	30:A:408:PHO:H51	1.84	0.58
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.83	0.58
43:F:101:HEM:HHC	43:F:101:HEM:HBB2	1.85	0.58
2:b:458:PHE:HB3	29:b:605:CLA:HBC2	1.86	0.58
1:a:344:ALA:O	26:a:401:OEX:O2	2.22	0.58
2:b:359:MET:HG3	2:b:366:PHE:HB2	1.86	0.58
14:o:171:LYS:HE2	14:o:175:GLY:HA2	1.84	0.58
23:s:224:ASP:HB3	23:s:227:VAL:HG22	1.85	0.58
1:a:269:ARG:NH2	5:d:222:LEU:O	2.36	0.58
2:b:365:THR:HG22	5:d:326:ARG:HH21	1.68	0.58
20:n:107:GLU:HA	20:n:110:GLN:HG3	1.86	0.58
1:A:159:ILE:HG13	1:A:160:ILE:HD12	1.86	0.58
29:B:604:CLA:HAB	29:B:606:CLA:H152	1.86	0.58
29:C:513:CLA:H111	39:C:525:LHG:H161	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:89:ILE:HG12	14:o:135:ARG:NH2	2.18	0.58
24:y:94:ALA:HB1	24:y:212:GLY:HA3	1.85	0.58
1:A:325:ASN:HA	1:A:328:MET:HE3	1.84	0.57
22:R:142:ARG:NH2	22:R:212:ILE:O	2.35	0.57
23:S:186:GLY:HA2	45:S:608:CHL:HAC1	1.86	0.57
4:C:267:VAL:HG22	29:C:502:CLA:HAC1	1.87	0.57
2:b:476:ARG:HH12	22:r:101:LYS:HD3	1.69	0.57
1:A:22:THR:HG23	1:A:136:ARG:HE	1.68	0.57
1:A:199:MET:HE1	5:D:74:LEU:HD13	1.85	0.57
2:B:357:ARG:NH1	2:B:358:ARG:O	2.38	0.57
29:B:609:CLA:HBB1	5:D:126:MET:HE3	1.86	0.57
21:g:86:ALA:HB1	21:g:204:GLY:HA3	1.84	0.57
22:r:213:TYR:HB3	29:r:610:CLA:HED3	1.87	0.57
1:A:30:ILE:O	1:A:34:GLY:HA3	2.04	0.57
20:N:59:TYR:OH	20:N:71:ASP:OD2	2.21	0.57
21:G:65:THR:HG21	45:Y:609:CHL:HAA2	1.86	0.57
2:b:142:HIS:ND1	29:b:611:CLA:OBD	2.30	0.57
31:c:517:BCR:H391	11:k:36:ALA:HB2	1.85	0.57
14:o:239:ARG:O	14:o:243:LYS:NZ	2.38	0.57
14:O:183:THR:HG21	14:O:203:PRO:HD2	1.86	0.57
1:a:30:ILE:O	1:a:34:GLY:HA3	2.04	0.57
14:o:187:PHE:HB2	14:o:200:PHE:HB3	1.85	0.57
22:R:153:VAL:O	22:R:157:ALA:CB	2.53	0.57
29:a:405:CLA:H112	29:a:406:CLA:HBB1	1.85	0.57
31:d:404:BCR:H17C	7:f:29:THR:HG22	1.86	0.57
2:B:365:THR:HG22	5:D:326:ARG:HH21	1.70	0.57
29:B:606:CLA:HBB1	29:B:607:CLA:H51	1.85	0.57
29:a:406:CLA:HBA1	39:l:101:LHG:H221	1.87	0.57
23:S:237:LYS:HE3	39:S:624:LHG:HC62	1.86	0.57
1:a:245:THR:HG22	1:a:246:TYR:H	1.69	0.57
4:c:14:ARG:O	4:c:29:ARG:NH1	2.38	0.57
6:e:75:GLN:HB2	25:u:113:ILE:HG22	1.86	0.57
48:r:623:NEX:H14	29:r:608:CLA:HMB2	1.86	0.57
30:A:409:PHO:OBD	5:D:129:GLN:NE2	2.38	0.56
2:B:382:PRO:HG2	2:B:385:LYS:HG2	1.87	0.56
14:O:269:VAL:HG12	14:O:293:LEU:HD23	1.87	0.56
23:S:58:LYS:HE2	39:S:624:LHG:HC12	1.86	0.56
29:Y:602:CLA:H51	29:Y:602:CLA:HBB1	1.86	0.56
29:D:402:CLA:H201	33:D:411:LMG:H332	1.88	0.56
6:E:22:ILE:HG13	6:E:23:HIS:HD1	1.68	0.56
29:s:613:CLA:H93	39:s:624:LHG:H142	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:SER:HA	7:F:44:ARG:HB2	1.87	0.56
4:c:167:ALA:HB1	4:c:187:ILE:HD12	1.86	0.56
4:c:398:VAL:CG1	52:c:1007:HOH:O	2.54	0.56
20:n:205:LYS:HE2	29:n:612:CLA:HBD	1.87	0.56
23:s:186:GLY:HA2	45:s:608:CHL:HAC1	1.87	0.56
22:r:221:LEU:HD13	46:r:620:LUT:H222	1.88	0.56
5:D:247:VAL:HG22	16:T:30:ALA:HA	1.88	0.56
14:O:158:ARG:NH1	14:O:159:GLU:O	2.38	0.56
21:G:96:ILE:HD13	46:G:621:LUT:H41	1.87	0.56
23:S:194:PRO:HG2	23:S:218:PRO:HB3	1.86	0.56
5:d:312:GLU:HB2	14:o:213:PRO:HG3	1.88	0.56
23:s:237:LYS:HE3	39:s:624:LHG:HC62	1.88	0.56
20:N:184:GLY:HA3	29:N:610:CLA:HED2	1.87	0.56
1:a:95:PRO:HD2	1:a:98:GLU:HB2	1.88	0.56
2:b:23:HIS:ND1	29:b:616:CLA:OBD	2.39	0.56
15:p:105:ARG:HG3	15:p:117:TYR:HB3	1.87	0.56
4:C:67:LYS:HB3	4:C:72:GLN:HE21	1.71	0.56
23:S:112:MET:SD	29:S:610:CLA:HAB	2.46	0.56
1:a:45:ILE:HD11	30:a:408:PHO:H51	1.88	0.56
29:A:405:CLA:H102	30:A:408:PHO:HAA1	1.88	0.56
31:C:516:BCR:H363	11:K:31:LEU:HD22	1.86	0.56
4:c:212:ILE:HG21	4:c:273:THR:HG23	1.88	0.56
29:A:406:CLA:HBA1	39:L:101:LHG:H221	1.88	0.55
8:H:69:ASN:ND2	33:H:102:LMG:O10	2.39	0.55
22:R:195:VAL:HA	22:R:198:VAL:HG12	1.88	0.55
23:S:189:PRO:HG2	48:S:622:NEX:H192	1.88	0.55
45:S:608:CHL:H12	46:S:620:LUT:H373	1.87	0.55
29:a:410:CLA:HAB	9:i:15:PHE:CD2	2.41	0.55
45:n:609:CHL:H43	45:y:601:CHL:H12	1.88	0.55
23:s:103:ASN:O	23:s:107:HIS:ND1	2.36	0.55
1:A:27:ARG:NH2	5:D:258:GLY:O	2.36	0.55
4:C:120:HIS:O	52:C:1020:HOH:O	2.18	0.55
29:C:511:CLA:HBC2	11:K:40:GLN:HG3	1.88	0.55
24:Y:172:GLY:HA2	29:Y:608:CLA:HAC1	1.88	0.55
1:a:183:MET:HE3	29:a:406:CLA:HHD	1.89	0.55
4:c:234:LEU:HB3	51:y:625:SPH:H151	1.86	0.55
29:c:513:CLA:HAB	31:c:514:BCR:H24C	1.87	0.55
2:B:357:ARG:NH2	25:U:103:GLU:OE2	2.38	0.55
29:R:609:CLA:H12	29:R:609:CLA:H3A	1.87	0.55
29:Y:602:CLA:H72	46:Y:621:LUT:H30	1.89	0.55
2:b:235:GLU:HB3	52:b:1043:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:190:LEU:HD12	46:n:620:LUT:H222	1.88	0.55
1:A:334:ARG:HG3	14:O:211:LEU:HD12	1.88	0.55
2:B:41:GLU:O	2:B:45:PHE:HB2	2.07	0.55
4:C:234:LEU:HB3	51:Y:625:SPH:H151	1.88	0.55
29:C:504:CLA:H71	38:C:519:DGD:HB72	1.88	0.55
5:d:247:VAL:HG22	16:t:30:ALA:HA	1.89	0.55
45:n:601:CHL:HED2	39:n:624:LHG:H141	1.87	0.55
23:s:78:GLU:HG2	23:s:79:LEU:HD12	1.88	0.55
24:y:74:ALA:HB3	24:y:76:LEU:HD22	1.87	0.55
14:O:83:THR:HG22	17:W:60:LEU:HD11	1.88	0.55
3:v:32:ASN:ND2	52:v:1002:HOH:O	2.40	0.55
4:c:386:HIS:HA	4:c:407:PHE:CE2	2.42	0.55
29:B:611:CLA:HHC	29:B:611:CLA:HBB1	1.89	0.55
4:C:205:PRO:HB2	38:C:518:DGD:HA21	1.89	0.55
31:C:516:BCR:HC41	11:K:25:LEU:HD21	1.88	0.55
43:F:101:HEM:HBC2	43:F:101:HEM:HHD	1.87	0.55
4:C:221:ILE:HG21	29:C:501:CLA:HED1	1.87	0.55
8:H:78:THR:HG1	8:H:83:SER:HG	1.55	0.55
2:b:7:ARG:O	2:b:10:THR:OG1	2.25	0.55
29:b:611:CLA:HHC	29:b:611:CLA:HBB1	1.88	0.55
4:c:398:VAL:HG11	52:c:1007:HOH:O	2.06	0.55
4:C:51:TRP:HB2	29:C:510:CLA:HAC2	1.89	0.55
20:N:49:LEU:HB2	20:N:53:SER:HB3	1.88	0.55
29:N:610:CLA:H92	46:N:620:LUT:H371	1.87	0.55
4:c:207:GLY:HA2	38:c:518:DGD:HD2	1.88	0.55
24:y:123:ILE:HD11	24:y:126:LYS:HE2	1.88	0.55
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.89	0.55
29:B:616:CLA:H8	29:B:617:CLA:HBB1	1.88	0.55
22:R:153:VAL:O	22:R:157:ALA:HB2	2.07	0.55
5:d:343:GLU:O	5:d:348:ARG:NH1	2.39	0.55
2:B:371:ILE:HG22	2:B:377:VAL:HA	1.89	0.55
2:B:464:PHE:HD2	29:B:612:CLA:HAC2	1.71	0.55
23:s:49:LEU:HD11	23:s:226:GLU:HA	1.89	0.55
29:B:608:CLA:H203	12:L:36:ILE:HG13	1.87	0.54
20:N:132:GLN:NE2	20:N:135:GLY:O	2.33	0.54
4:c:306:LEU:HD12	4:c:328:TYR:HB3	1.88	0.54
14:O:111:PRO:HD2	14:O:138:TYR:CE1	2.43	0.54
4:c:154:ILE:HD13	32:c:626:SQD:H121	1.90	0.54
4:c:209:ASP:O	4:c:214:SER:OG	2.25	0.54
31:c:516:BCR:HC41	11:k:25:LEU:HD21	1.89	0.54
21:g:160:ARG:NH2	45:g:609:CHL:O1D	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:r:620:LUT:H28	29:r:610:CLA:H11	1.90	0.54
1:a:104:GLU:OE2	17:w:64:ARG:NH1	2.39	0.54
1:a:303:ASN:O	4:c:403:ASN:ND2	2.40	0.54
14:o:104:LEU:HD22	14:o:147:MET:HG3	1.89	0.54
14:o:109:MET:SD	14:o:140:LEU:HD12	2.47	0.54
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.88	0.54
45:G:601:CHL:H12	45:Y:609:CHL:H43	1.89	0.54
45:y:606:CHL:HBB2	45:y:607:CHL:HAB	1.89	0.54
5:D:305:ALA:O	14:O:216:ARG:NH2	2.40	0.54
21:G:91:LEU:HB3	29:G:604:CLA:HAB	1.89	0.54
2:b:327:THR:HB	33:b:622:LMG:HC8	1.90	0.54
29:b:604:CLA:HAB	29:b:606:CLA:H152	1.89	0.54
38:c:519:DGD:HA71	33:c:521:LMG:H362	1.89	0.54
20:N:204:VAL:HA	20:N:207:ILE:HG22	1.89	0.54
24:Y:46:ARG:NH2	24:Y:61:LEU:O	2.41	0.54
1:a:35:VAL:HG12	31:a:411:BCR:HC21	1.90	0.54
1:a:140:ARG:HH22	39:d:410:LHG:HC42	1.72	0.54
1:a:297:LEU:HB2	4:c:416:THR:HG21	1.90	0.54
2:B:115:TRP:HE1	32:B:621:SQD:H1	1.73	0.54
20:N:84:ARG:NH1	24:Y:72:ASP:O	2.41	0.54
29:r:609:CLA:H12	29:r:609:CLA:H3A	1.89	0.54
2:B:327:THR:HB	33:B:622:LMG:HC8	1.91	0.54
4:C:125:PRO:HD3	29:C:513:CLA:HED3	1.90	0.54
1:a:184:ILE:HG23	1:a:328:MET:HE2	1.90	0.54
1:a:283:ILE:HA	1:a:286:THR:HG22	1.90	0.54
1:A:283:ILE:HA	1:A:286:THR:HG22	1.90	0.53
21:G:176:TYR:HB3	29:G:610:CLA:HED3	1.90	0.53
2:B:359:MET:HG3	2:B:366:PHE:HB2	1.89	0.53
39:C:525:LHG:HC62	39:S:624:LHG:HC11	1.90	0.53
14:O:108:CYS:HB2	14:O:141:ASP:OD1	2.08	0.53
29:S:613:CLA:H93	39:S:624:LHG:H142	1.90	0.53
38:c:523:DGD:HB91	29:y:611:CLA:HBC3	1.90	0.53
14:o:212:ASP:OD1	14:o:216:ARG:N	2.41	0.53
4:C:285:TYR:O	4:C:411:ARG:NH2	2.38	0.53
29:C:503:CLA:H172	29:C:510:CLA:HBB2	1.91	0.53
12:L:27:VAL:HG11	39:L:101:LHG:H201	1.89	0.53
2:b:243:ALA:HA	2:b:246:PHE:CE1	2.44	0.53
2:b:441:GLY:HA2	14:o:230:ALA:HB3	1.90	0.53
29:b:617:CLA:H12	29:b:617:CLA:H2A	1.90	0.53
4:c:67:LYS:HB2	4:c:72:GLN:HE21	1.72	0.53
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:n:603:CLA:HAC1	45:n:607:CHL:HBB2	1.90	0.53
29:n:603:CLA:HED2	45:n:609:CHL:H93	1.91	0.53
29:s:602:CLA:H72	46:s:621:LUT:H28	1.89	0.53
1:A:290:ILE:HG13	29:A:405:CLA:HED3	1.90	0.53
1:A:298:ASN:HB2	4:C:391:SER:HA	1.90	0.53
29:A:410:CLA:HAB	9:I:15:PHE:CD2	2.44	0.53
29:C:511:CLA:H13	31:C:517:BCR:H21C	1.90	0.53
39:D:408:LHG:H352	39:D:408:LHG:H111	1.91	0.53
45:R:606:CHL:HHC	45:R:606:CHL:HBB1	1.91	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
38:c:523:DGD:HAH1	51:y:625:SPH:H102	1.91	0.53
45:S:606:CHL:HHC	45:S:606:CHL:HBB1	1.90	0.53
4:c:109:SER:HA	31:c:514:BCR:H16C	1.90	0.53
4:c:221:ILE:HG21	29:c:501:CLA:HED1	1.91	0.53
21:g:53:LEU:HD11	21:g:64:ASP:HB2	1.90	0.53
4:C:281:ASN:O	4:C:411:ARG:NH1	2.42	0.53
31:D:404:BCR:H17C	7:F:29:THR:HG22	1.90	0.53
20:N:226:VAL:HG23	20:N:227:THR:HG23	1.89	0.53
22:R:235:LEU:HD11	29:R:610:CLA:HMA1	1.90	0.53
21:g:163:GLY:HA2	45:g:608:CHL:HAC1	1.91	0.53
1:a:220:THR:O	5:d:139:ARG:NH2	2.42	0.53
1:A:340:PRO:HB2	15:P:224:LYS:HG3	1.90	0.53
33:A:413:LMG:O5	4:C:209:ASP:OD2	2.27	0.53
21:G:61:TYR:OH	21:G:202:LYS:NZ	2.37	0.53
24:Y:150:SER:OG	45:Y:605:CHL:OMC	2.22	0.53
1:A:292:THR:HG22	4:C:416:THR:HB	1.91	0.52
29:C:512:CLA:H193	32:C:526:SQD:H281	1.89	0.52
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.91	0.52
2:b:91:TRP:CD2	29:b:607:CLA:HBA2	2.44	0.52
2:b:371:ILE:HG22	2:b:377:VAL:HA	1.90	0.52
29:b:608:CLA:H203	12:l:36:ILE:HG13	1.91	0.52
14:o:276:SER:OG	14:o:277:ASP:N	2.42	0.52
4:C:27:ASN:ND2	29:C:510:CLA:O1A	2.42	0.52
29:C:511:CLA:H101	31:C:517:BCR:H23C	1.91	0.52
8:H:78:THR:OG1	8:H:83:SER:OG	2.27	0.52
29:S:613:CLA:HAB	39:S:624:LHG:H301	1.90	0.52
1:a:290:ILE:HG13	29:a:405:CLA:HED3	1.90	0.52
2:b:235:GLU:OE2	2:b:469:HIS:ND1	2.42	0.52
23:s:149:LEU:HD22	29:s:604:CLA:HED1	1.91	0.52
29:B:606:CLA:HMA3	29:B:607:CLA:H3A	1.91	0.52
4:C:259:TYR:O	52:C:1002:HOH:O	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D:411:LMG:HC5	52:D:1040:HOH:O	2.08	0.52
14:O:111:PRO:HD2	14:O:138:TYR:HE1	1.74	0.52
29:N:610:CLA:H61	46:N:620:LUT:H30	1.91	0.52
30:a:408:PHO:HAB	5:d:205:LEU:HD13	1.92	0.52
2:b:41:GLU:O	2:b:45:PHE:HB2	2.09	0.52
2:B:458:PHE:HB3	29:B:605:CLA:HBC2	1.90	0.52
4:C:213:VAL:HG13	4:C:277:PHE:HA	1.92	0.52
14:O:171:LYS:HE2	14:O:175:GLY:HA2	1.92	0.52
29:y:602:CLA:CAB	46:y:621:LUT:H32	2.39	0.52
1:A:341:LEU:HG	1:A:343:LEU:HD11	1.91	0.52
29:A:406:CLA:HAA2	42:D:405:PL9:H371	1.91	0.52
45:g:609:CHL:HHC	45:g:609:CHL:HBB1	1.91	0.52
5:D:149:PRO:HB3	29:D:402:CLA:H41	1.91	0.52
21:G:41:LEU:HB2	21:G:45:SER:HB2	1.91	0.52
4:c:308:ARG:NH1	15:p:223:ASP:OD2	2.42	0.52
21:g:196:LEU:HD12	21:g:199:LYS:HD2	1.90	0.52
45:s:606:CHL:HHC	45:s:606:CHL:HBB1	1.90	0.52
2:B:91:TRP:CD2	29:B:607:CLA:HBA2	2.44	0.52
4:C:417:SER:HB3	38:C:519:DGD:HBT2	1.92	0.52
29:N:603:CLA:HAC1	45:N:607:CHL:HBB2	1.92	0.52
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.92	0.52
4:c:152:HIS:ND1	29:c:507:CLA:OBD	2.30	0.52
14:o:171:LYS:HE3	14:o:177:TYR:HE1	1.74	0.52
29:g:613:CLA:H72	39:g:624:LHG:H152	1.92	0.52
23:s:204:PHE:HA	23:s:207:LEU:HD12	1.92	0.52
2:B:142:HIS:ND1	29:B:611:CLA:OBD	2.30	0.52
29:C:513:CLA:H92	39:C:525:LHG:H271	1.92	0.52
14:O:187:PHE:HB2	14:O:200:PHE:HB3	1.92	0.52
22:R:221:LEU:HD13	46:R:620:LUT:H222	1.92	0.52
1:A:247:ASN:HD21	1:A:250:ALA:HB3	1.75	0.52
21:G:87:ARG:HA	21:G:90:LEU:HD12	1.92	0.52
23:s:58:LYS:HD2	39:s:624:LHG:HC11	1.91	0.52
15:P:136:GLU:O	15:P:140:GLN:NE2	2.43	0.52
21:G:122:ILE:HG21	21:G:142:ILE:HD13	1.91	0.52
23:S:61:LEU:HD22	23:S:65:LEU:HD23	1.92	0.52
23:S:271:PRO:HB2	29:S:614:CLA:HMA2	1.91	0.52
29:b:609:CLA:H201	33:h:102:LMG:H342	1.92	0.52
23:s:109:ARG:NH1	52:s:1016:HOH:O	2.43	0.52
4:C:437:ARG:NH2	9:I:27:ASP:OD2	2.37	0.51
5:D:187:GLY:O	5:D:326:ARG:NH1	2.43	0.51
24:Y:94:ALA:HB1	24:Y:212:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:476:ARG:NH2	52:b:1046:HOH:O	2.42	0.51
4:c:27:ASN:ND2	29:c:510:CLA:O1A	2.43	0.51
4:c:267:VAL:HG22	29:c:502:CLA:HAC1	1.92	0.51
29:c:504:CLA:H43	38:c:519:DGD:HBE1	1.91	0.51
29:B:617:CLA:H12	29:B:617:CLA:H2A	1.90	0.51
29:C:504:CLA:H2	38:C:519:DGD:HB31	1.92	0.51
15:p:179:LYS:HG3	15:p:180:LYS:HG3	1.92	0.51
45:n:601:CHL:HHC	45:n:601:CHL:HBB1	1.93	0.51
4:C:264:LEU:HD21	29:C:508:CLA:HAB	1.92	0.51
8:H:32:PRO:HB3	22:R:127:VAL:HG13	1.91	0.51
8:H:54:ILE:HG12	44:H:101:RRX:H9	1.92	0.51
21:G:128:LEU:HD21	29:G:604:CLA:HAA2	1.92	0.51
45:G:609:CHL:HHC	45:G:609:CHL:HBB1	1.91	0.51
33:a:413:LMG:H391	4:c:269:LEU:HG	1.93	0.51
29:b:603:CLA:H2	29:b:603:CLA:HBD	1.92	0.51
8:h:78:THR:HG1	8:h:83:SER:HG	1.58	0.51
50:i:101:3PH:H222	50:i:101:3PH:H322	1.91	0.51
15:p:144:LEU:HD13	15:p:218:LYS:HD2	1.93	0.51
45:g:608:CHL:HHC	45:g:608:CHL:HBB1	1.93	0.51
22:r:135:GLU:OE2	22:r:211:ARG:NH1	2.43	0.51
45:r:606:CHL:HBB1	45:r:606:CHL:HHC	1.93	0.51
29:C:501:CLA:H161	29:C:507:CLA:H93	1.92	0.51
2:b:115:TRP:HE1	32:b:621:SQD:H1	1.75	0.51
2:b:464:PHE:HD2	29:b:612:CLA:HAC2	1.75	0.51
29:b:612:CLA:HBC1	39:d:408:LHG:H301	1.92	0.51
5:D:15:PHE:O	5:D:19:ASP:HB2	2.09	0.51
5:d:338:LYS:HB2	25:u:103:GLU:HG2	1.92	0.51
29:s:602:CLA:H112	46:s:621:LUT:H371	1.92	0.51
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.92	0.51
29:B:612:CLA:HBC1	39:D:408:LHG:H301	1.91	0.51
5:d:186:GLN:HB2	29:d:402:CLA:HBC1	1.93	0.51
6:e:22:ILE:HG13	6:e:23:HIS:HD1	1.75	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
36:B:625:DGA:HA82	5:D:127:LEU:HD13	1.92	0.51
20:N:75:LEU:HD11	29:N:602:CLA:H11	1.91	0.51
1:a:27:ARG:NH2	5:d:258:GLY:O	2.42	0.51
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.93	0.51
1:a:228:THR:HG23	1:a:230:ASN:H	1.76	0.51
29:c:507:CLA:H2	29:c:507:CLA:HMA3	1.91	0.51
29:n:602:CLA:H192	52:n:1011:HOH:O	2.11	0.51
47:r:622:XAT:H30	29:r:602:CLA:HAB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s:112:MET:SD	29:s:610:CLA:HAB	2.50	0.51
45:Y:609:CHL:HHC	45:Y:609:CHL:HBB1	1.92	0.51
5:d:72:ASN:OD1	33:d:411:LMG:O2	2.25	0.51
5:d:233:ARG:NH1	52:d:1036:HOH:O	2.44	0.51
20:n:93:ALA:HB1	20:n:210:GLY:HA3	1.93	0.51
21:g:121:GLN:HE21	21:g:128:LEU:HG	1.76	0.51
23:s:109:ARG:NH1	45:s:608:CHL:OBD	2.40	0.51
4:C:228:ILE:HD11	29:C:507:CLA:H72	1.93	0.51
21:G:148:VAL:HG11	45:G:605:CHL:HBC1	1.93	0.51
4:c:175:ASP:O	4:c:182:GLY:HA2	2.11	0.51
31:B:619:BCR:H392	16:t:11:ILE:HD12	1.94	0.50
5:D:216:ALA:O	5:D:220:ASN:ND2	2.36	0.50
20:N:103:MET:HE3	46:N:621:LUT:H8	1.93	0.50
29:n:602:CLA:CAB	46:n:621:LUT:H32	2.41	0.50
45:g:605:CHL:HBB1	45:g:605:CHL:HHC	1.92	0.50
25:u:93:THR:O	25:u:97:MET:N	2.43	0.50
29:a:406:CLA:HAA2	42:d:405:PL9:H371	1.92	0.50
31:b:618:BCR:H383	32:b:621:SQD:H252	1.92	0.50
5:d:216:ALA:O	5:d:220:ASN:ND2	2.33	0.50
29:g:602:CLA:H52	46:g:621:LUT:H28	1.93	0.50
50:s:626:3PH:H351	50:s:626:3PH:H221	1.93	0.50
24:y:105:ILE:HG23	24:y:234:ILE:HD11	1.93	0.50
45:G:601:CHL:HHC	45:G:601:CHL:HBB1	1.94	0.50
45:G:608:CHL:HHC	45:G:608:CHL:HBB1	1.93	0.50
45:S:608:CHL:HHC	45:S:608:CHL:HBB1	1.93	0.50
29:a:405:CLA:H152	30:a:408:PHO:H3A	1.93	0.50
45:y:609:CHL:HHC	45:y:609:CHL:HBB1	1.93	0.50
2:B:277:GLN:HB3	25:U:106:VAL:HG23	1.94	0.50
20:n:154:LEU:HD23	29:y:613:CLA:H192	1.93	0.50
33:A:413:LMG:HC62	17:W:68:ASP:HA	1.94	0.50
4:C:249:ARG:HA	4:C:254:TRP:HE1	1.76	0.50
1:a:334:ARG:HB2	14:o:211:LEU:HD12	1.92	0.50
8:h:54:ILE:HG12	44:h:101:RRX:H9	1.92	0.50
21:g:190:PRO:HA	21:g:193:PHE:HB3	1.94	0.50
29:C:507:CLA:H2	29:C:507:CLA:HMA3	1.93	0.50
23:S:204:PHE:HA	23:S:207:LEU:HD12	1.92	0.50
2:b:73:GLN:HE21	2:b:88:PRO:HA	1.77	0.50
4:c:95:ASP:HB3	23:s:287:PRO:HB3	1.93	0.50
4:c:159:GLY:HA3	29:c:512:CLA:H41	1.92	0.50
39:l:101:LHG:H262	13:m:22:LEU:HD21	1.93	0.50
45:n:606:CHL:HBB2	45:n:607:CHL:HAB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:CD2	52:B:1008:HOH:O	2.52	0.50
4:C:414:LEU:HD13	29:C:502:CLA:HED3	1.93	0.50
6:E:57:THR:OG1	6:E:59:ASP:OD1	2.26	0.50
6:E:78:LYS:NZ	25:U:113:ILE:O	2.45	0.50
29:N:602:CLA:CAB	46:N:621:LUT:H32	2.41	0.50
3:v:7:LEU:HA	3:v:10:VAL:HG12	1.94	0.50
22:r:83:VAL:HG23	22:r:109:ARG:HA	1.93	0.50
31:B:619:BCR:H371	16:t:11:ILE:HD11	1.94	0.50
14:O:216:ARG:H	14:O:222:TYR:HB2	1.75	0.50
45:N:601:CHL:HHC	45:N:601:CHL:HBB1	1.94	0.50
22:R:213:TYR:HB3	29:R:610:CLA:HED3	1.92	0.50
25:U:105:THR:HG21	25:U:107:LYS:HZ2	1.77	0.50
1:a:199:MET:HE1	5:d:74:LEU:HD13	1.93	0.50
31:c:514:BCR:H281	39:c:625:LHG:HC82	1.94	0.50
38:c:519:DGD:HB71	33:c:521:LMG:H401	1.94	0.50
22:r:153:VAL:O	22:r:157:ALA:CB	2.58	0.50
2:B:384:ARG:HH21	15:P:193:THR:HG21	1.76	0.50
4:C:287:SER:OG	4:C:296:GLU:OE2	2.27	0.50
4:C:414:LEU:O	4:C:418:HIS:ND1	2.45	0.50
1:a:63:ILE:HB	4:c:323:THR:HG21	1.94	0.50
2:b:170:ASP:HB3	2:b:174:LEU:H	1.77	0.50
4:c:281:ASN:O	4:c:411:ARG:NH1	2.42	0.50
1:A:160:ILE:HG12	4:C:419:PHE:CZ	2.47	0.49
1:A:296:ASN:HB3	4:C:389:LEU:HD13	1.93	0.49
2:B:18:ARG:HH22	32:B:621:SQD:H3	1.77	0.49
4:C:332:SER:OG	4:C:334:THR:O	2.23	0.49
5:D:312:GLU:HB3	14:O:213:PRO:HB3	1.93	0.49
29:G:602:CLA:CAB	46:G:621:LUT:H32	2.42	0.49
45:G:605:CHL:HHC	45:G:605:CHL:HBB1	1.93	0.49
29:b:609:CLA:HBB1	5:d:126:MET:HE2	1.94	0.49
31:c:516:BCR:H372	10:j:21:LEU:HD12	1.93	0.49
45:N:605:CHL:HHC	45:N:605:CHL:HBB1	1.94	0.49
2:b:145:LEU:HD22	29:b:605:CLA:H162	1.93	0.49
8:h:69:ASN:HD22	33:h:102:LMG:HC8	1.77	0.49
2:B:24:LEU:HD21	29:B:617:CLA:CAB	2.41	0.49
5:D:155:SER:HA	5:D:159:ILE:HB	1.95	0.49
4:c:264:LEU:HD21	29:c:508:CLA:HAB	1.93	0.49
21:g:184:LEU:HD13	46:g:620:LUT:H222	1.94	0.49
22:r:187:LEU:O	22:r:191:GLU:HB3	2.12	0.49
23:s:275:ASN:H	23:s:278:THR:HB	1.77	0.49
24:y:95:ARG:HA	24:y:98:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:y:184:TYR:HB3	29:y:610:CLA:HED3	1.94	0.49
29:B:603:CLA:H172	33:H:102:LMG:H331	1.94	0.49
5:D:289:LEU:HD22	5:D:294:ARG:HG2	1.94	0.49
24:Y:221:GLY:O	24:Y:225:GLN:HB2	2.13	0.49
30:a:409:PHO:OBD	5:d:129:GLN:NE2	2.45	0.49
29:C:502:CLA:H61	29:C:512:CLA:H11	1.95	0.49
14:O:276:SER:OG	14:O:277:ASP:N	2.44	0.49
45:G:606:CHL:HHC	45:G:606:CHL:HBB1	1.94	0.49
23:S:143:MET:HE1	45:S:606:CHL:HMD3	1.95	0.49
29:b:617:CLA:HMD3	8:h:24:THR:HG21	1.93	0.49
38:c:518:DGD:O4E	38:c:518:DGD:O5E	2.29	0.49
14:o:96:GLU:OE1	14:o:261:THR:OG1	2.28	0.49
29:B:603:CLA:H2	29:B:603:CLA:HBD	1.93	0.49
5:D:24:GLN:HB3	5:D:26:ARG:HE	1.77	0.49
5:D:72:ASN:H	5:D:75:THR:HB	1.78	0.49
5:d:251:ARG:HB3	52:d:1039:HOH:O	2.11	0.49
5:d:329:MET:O	5:d:333:ASP:HB2	2.13	0.49
45:g:601:CHL:HHC	45:g:601:CHL:HBB1	1.94	0.49
29:A:410:CLA:H8	9:I:16:VAL:HG11	1.94	0.49
4:C:122:LEU:HD11	29:C:511:CLA:H92	1.95	0.49
29:C:501:CLA:HMB2	31:C:515:BCR:H23C	1.94	0.49
14:O:238:GLN:NE2	14:O:281:GLY:O	2.46	0.49
22:R:135:GLU:OE2	22:R:211:ARG:NH1	2.45	0.49
24:Y:192:LEU:HD12	46:Y:620:LUT:H222	1.95	0.49
4:c:249:ARG:HH22	38:c:523:DGD:HE62	1.77	0.49
45:g:601:CHL:H12	45:y:609:CHL:H43	1.95	0.49
1:A:174:LEU:HD22	30:A:408:PHO:H151	1.95	0.49
21:G:211:CYS:SG	46:G:621:LUT:H12	2.53	0.49
2:b:385:LYS:HB3	15:p:149:ALA:HB3	1.94	0.49
52:b:1040:HOH:O	33:h:102:LMG:O5	2.02	0.49
33:c:521:LMG:H221	33:j:101:LMG:H372	1.93	0.49
45:g:601:CHL:HED3	39:g:624:LHG:H142	1.94	0.49
38:C:518:DGD:HO4E	38:C:518:DGD:HO5E	1.60	0.49
21:G:50:PRO:HB2	21:G:53:LEU:HD23	1.94	0.49
29:n:603:CLA:H71	29:g:603:CLA:H71	1.94	0.49
29:g:602:CLA:CAB	46:g:621:LUT:H32	2.43	0.49
1:A:269:ARG:NH2	5:D:222:LEU:O	2.46	0.49
29:B:612:CLA:H71	39:L:101:LHG:H321	1.94	0.49
14:O:263:THR:HG23	14:O:265:GLU:HG3	1.95	0.49
29:d:403:CLA:H101	8:h:55:LEU:HD11	1.95	0.49
15:p:115:ASN:ND2	15:p:220:GLN:OE1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ALA:HB2	29:B:604:CLA:H61	1.95	0.48
4:C:249:ARG:HH12	38:C:523:DGD:HE62	1.78	0.48
29:R:602:CLA:H71	47:R:621:XAT:H363	1.95	0.48
29:R:608:CLA:HMB2	48:R:622:NEX:H14	1.95	0.48
2:b:231:MET:HG2	29:b:611:CLA:HAC1	1.95	0.48
29:b:608:CLA:H3A	29:b:608:CLA:HBA2	1.57	0.48
4:c:315:ASN:ND2	4:c:318:SER:OG	2.45	0.48
5:d:343:GLU:OE1	5:d:348:ARG:NH2	2.45	0.48
47:n:622:XAT:H10	39:y:624:LHG:H211	1.94	0.48
22:r:186:GLN:O	22:r:190:ILE:HG12	2.13	0.48
24:y:120:ASP:OD1	24:y:121:GLY:N	2.46	0.48
3:v:33:LEU:OXT	11:k:39:TRP:NE1	2.39	0.48
29:r:610:CLA:H13	29:r:610:CLA:H102	1.67	0.48
11:K:14:ALA:HB1	19:Z:5:LEU:HD22	1.94	0.48
39:L:101:LHG:H262	13:M:22:LEU:HD21	1.94	0.48
14:O:237:ILE:HG23	14:O:241:ASN:HB3	1.94	0.48
4:c:272:PHE:HB3	38:c:518:DGD:HB62	1.95	0.48
5:d:159:ILE:HG21	5:d:287:VAL:HG22	1.95	0.48
29:C:513:CLA:HBA2	29:C:513:CLA:H3A	1.68	0.48
6:E:13:ILE:HG21	43:F:101:HEM:HAD2	1.95	0.48
15:P:104:LEU:HD11	15:P:106:TYR:HE1	1.79	0.48
21:G:141:SER:OG	45:G:605:CHL:OMC	2.31	0.48
45:s:608:CHL:HHC	45:s:608:CHL:HBB1	1.94	0.48
2:B:442:VAL:HA	14:O:229:PRO:HD2	1.94	0.48
45:S:606:CHL:HBB2	45:S:607:CHL:CBB	2.44	0.48
1:a:64:ARG:NH1	14:o:167:ALA:O	2.47	0.48
10:j:31:PHE:O	10:j:34:SER:OG	2.32	0.48
20:n:225:ILE:HD11	45:n:607:CHL:H41	1.95	0.48
23:s:264:ILE:HD12	46:s:620:LUT:H163	1.94	0.48
2:B:242:ILE:HG23	2:B:462:PHE:HD2	1.78	0.48
4:C:212:ILE:HD11	31:C:515:BCR:H392	1.95	0.48
23:s:240:ARG:HA	23:s:243:MET:HE3	1.96	0.48
2:B:318:ASN:HB3	2:B:321:LYS:HB2	1.96	0.48
2:b:74:SER:HA	2:b:92:SER:HB2	1.96	0.48
29:b:610:CLA:OBD	8:h:46:THR:OG1	2.30	0.48
38:c:520:DGD:O1B	10:j:35:TYR:OH	2.32	0.48
5:d:149:PRO:HB3	29:d:402:CLA:H41	1.96	0.48
5:d:296:TYR:OH	5:d:326:ARG:NH1	2.39	0.48
45:y:605:CHL:HHC	45:y:605:CHL:HBB1	1.95	0.48
4:C:330:MET:HG2	4:C:340:GLY:HA2	1.94	0.48
5:D:79:SER:HA	5:D:172:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N:605:CHL:H101	29:S:612:CLA:HBB1	1.96	0.48
4:c:198:PHE:HA	4:c:201:ILE:HG22	1.96	0.48
45:r:607:CHL:HHC	45:r:607:CHL:HBB1	1.95	0.48
2:B:9:HIS:ND1	29:B:612:CLA:O1A	2.47	0.48
29:B:607:CLA:H102	22:R:189:TRP:HZ2	1.79	0.48
29:B:610:CLA:H3A	29:B:610:CLA:HBA2	1.63	0.48
4:C:295:PRO:HB3	4:C:346:PHE:HB3	1.95	0.48
33:a:413:LMG:HC72	4:c:204:SER:HB2	1.96	0.48
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.96	0.48
39:d:408:LHG:HC81	39:l:101:LHG:HC82	1.96	0.48
14:o:260:ASP:HB3	14:o:265:GLU:H	1.79	0.48
1:A:35:VAL:HG12	31:A:411:BCR:HC21	1.95	0.48
4:C:425:PHE:HA	29:C:508:CLA:HMC2	1.95	0.48
6:E:75:GLN:HB2	25:U:113:ILE:HG22	1.96	0.48
14:O:171:LYS:HE3	14:O:177:TYR:HE1	1.78	0.48
1:a:41:LEU:HG	1:a:122:GLY:HA3	1.95	0.48
1:a:288:LEU:HD11	4:c:423:PHE:HD2	1.78	0.48
20:n:45:ARG:NH2	20:n:60:LEU:O	2.47	0.48
20:n:204:VAL:HA	20:n:207:ILE:HG22	1.96	0.48
45:g:606:CHL:HBB2	45:g:607:CHL:HAB	1.96	0.48
29:s:603:CLA:HAB	29:s:609:CLA:CBC	2.43	0.48
21:G:41:LEU:HB3	21:G:44:PHE:HB2	1.95	0.47
45:R:607:CHL:HHC	45:R:607:CHL:HBB1	1.94	0.47
5:d:51:GLY:HA2	5:d:55:VAL:HB	1.96	0.47
1:A:157:VAL:HG22	1:A:172:MET:HB2	1.96	0.47
47:G:622:XAT:H31	47:G:622:XAT:H391	1.71	0.47
23:S:192:PHE:H	23:S:198:LYS:HA	1.78	0.47
4:c:129:GLU:OE2	4:c:137:TYR:N	2.48	0.47
29:c:513:CLA:H111	39:c:625:LHG:H142	1.96	0.47
23:s:194:PRO:HB2	23:s:218:PRO:HB3	1.96	0.47
45:s:601:CHL:HED2	39:s:624:LHG:H152	1.96	0.47
38:C:523:DGD:HG11	29:Y:611:CLA:H11	1.97	0.47
14:O:143:MET:HE1	14:O:184:ILE:HG21	1.96	0.47
45:G:606:CHL:HBA2	45:G:606:CHL:HBD	1.96	0.47
22:R:216:GLY:HA2	22:R:219:ASP:HB3	1.96	0.47
24:Y:155:LEU:HD13	45:Y:607:CHL:HAC2	1.97	0.47
45:Y:605:CHL:HHC	45:Y:605:CHL:HBB1	1.97	0.47
22:r:153:VAL:O	22:r:157:ALA:HB2	2.14	0.47
29:s:602:CLA:HBA2	29:s:602:CLA:H3A	1.56	0.47
1:A:187:GLN:HE21	29:A:405:CLA:HAC1	1.79	0.47
29:D:403:CLA:HBB2	18:X:86:ILE:HG13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:67:ILE:HG13	8:H:72:LEU:HD23	1.95	0.47
29:b:604:CLA:H192	29:b:610:CLA:H91	1.95	0.47
20:n:184:GLY:HA3	29:n:610:CLA:HED2	1.96	0.47
29:S:603:CLA:HBB2	45:S:607:CHL:CAB	2.44	0.47
4:c:51:TRP:HB2	29:c:510:CLA:HAC2	1.97	0.47
5:d:72:ASN:H	5:d:75:THR:HB	1.79	0.47
45:g:606:CHL:HBB1	45:g:609:CHL:HBC1	1.95	0.47
38:C:519:DGD:HA71	33:C:521:LMG:H362	1.95	0.47
29:S:610:CLA:H52	46:S:620:LUT:H30	1.96	0.47
45:n:605:CHL:H101	23:s:120:ILE:HD11	1.97	0.47
29:C:511:CLA:H171	19:Z:20:VAL:HG22	1.96	0.47
39:D:409:LHG:H112	39:D:409:LHG:H262	1.96	0.47
11:K:12:PRO:HB2	11:K:15:TYR:HD2	1.79	0.47
29:N:614:CLA:HBC1	46:N:620:LUT:H162	1.96	0.47
23:S:101:ARG:NH1	23:S:104:GLU:OE1	2.48	0.47
23:S:231:LEU:HD23	23:S:234:LYS:HD2	1.97	0.47
29:Y:603:CLA:HAC1	45:Y:607:CHL:HBB2	1.96	0.47
45:Y:607:CHL:H91	45:Y:609:CHL:H192	1.96	0.47
1:a:229:GLU:HB2	22:r:94:GLN:HB2	1.97	0.47
1:a:260:PHE:CE2	1:a:262:TYR:HB3	2.49	0.47
2:b:137:LYS:HD2	2:b:217:LEU:HD23	1.96	0.47
2:b:242:ILE:HG23	2:b:462:PHE:HD2	1.78	0.47
29:c:511:CLA:H122	19:z:24:PRO:HG3	1.97	0.47
6:e:76:VAL:O	6:e:80:SER:HB2	2.15	0.47
14:o:224:ASN:HA	14:o:240:LEU:HD13	1.96	0.47
15:p:176:GLU:HG3	15:p:186:LYS:HD3	1.97	0.47
29:n:604:CLA:H121	48:n:623:NEX:H402	1.95	0.47
45:n:605:CHL:HHC	45:n:605:CHL:HBB1	1.95	0.47
29:g:613:CLA:H143	39:g:624:LHG:H332	1.97	0.47
29:r:608:CLA:H3A	29:r:608:CLA:HBA2	1.53	0.47
4:C:38:LEU:HD11	29:C:513:CLA:HBB1	1.96	0.47
4:C:270:MET:HE3	29:C:501:CLA:H122	1.97	0.47
14:O:165:TYR:HB2	14:O:183:THR:HG22	1.96	0.47
16:T:11:ILE:HD12	31:b:619:BCR:H392	1.97	0.47
4:c:461:ASP:OD1	4:c:461:ASP:N	2.47	0.47
45:g:601:CHL:H41	45:g:601:CHL:H62	1.63	0.47
2:B:356:VAL:HG22	2:B:370:LEU:HG	1.96	0.47
29:C:506:CLA:H93	29:C:506:CLA:H61	1.80	0.47
31:C:515:BCR:HC31	9:I:24:LEU:HG	1.96	0.47
5:D:72:ASN:OD1	33:D:411:LMG:O2	2.24	0.47
21:G:37:ARG:NH2	21:G:53:LEU:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:195:VAL:HG23	29:R:609:CLA:CAB	2.45	0.47
1:a:228:THR:OG1	1:a:229:GLU:N	2.48	0.47
29:B:615:CLA:HBD	29:B:615:CLA:HBA1	1.97	0.47
4:C:461:ASP:OD1	4:C:461:ASP:N	2.47	0.47
38:C:520:DGD:O1B	10:J:35:TYR:OH	2.33	0.47
47:N:622:XAT:H391	47:N:622:XAT:H31	1.67	0.47
21:G:199:LYS:HD3	29:G:612:CLA:HBD	1.96	0.47
29:Y:612:CLA:H152	29:Y:612:CLA:HBB1	1.97	0.47
29:b:602:CLA:H62	29:b:602:CLA:H2	1.63	0.47
4:c:408:VAL:HB	4:c:413:TRP:NE1	2.30	0.47
5:d:67:TYR:HA	52:d:1041:HOH:O	2.15	0.47
20:n:226:VAL:HG23	20:n:227:THR:HG23	1.97	0.47
1:A:195:HIS:CD2	1:A:293:MET:HE2	2.50	0.46
29:B:609:CLA:HAB	5:D:123:ILE:HG12	1.98	0.46
29:C:513:CLA:H72	31:C:514:BCR:H23C	1.97	0.46
21:G:71:ASP:HB3	21:G:74:THR:HG22	1.98	0.46
45:G:601:CHL:H62	45:G:601:CHL:H41	1.57	0.46
1:a:93:PHE:HB2	4:c:206:PHE:CG	2.50	0.46
2:b:12:VAL:HG23	29:b:613:CLA:HMC2	1.97	0.46
36:b:623:DGA:HA52	5:d:127:LEU:HD22	1.96	0.46
21:g:59:GLY:HA3	21:g:201:ILE:HG21	1.97	0.46
47:g:622:XAT:H201	47:g:622:XAT:H15	1.68	0.46
24:y:76:LEU:O	24:y:86:TYR:CE2	2.68	0.46
2:B:44:VAL:HG23	2:B:60:MET:HE1	1.97	0.46
21:G:110:PHE:HE1	21:G:131:LEU:HA	1.80	0.46
1:a:93:PHE:HZ	29:a:410:CLA:HAA1	1.80	0.46
23:s:105:LEU:HB3	23:s:210:LEU:HD11	1.97	0.46
39:s:624:LHG:H271	39:s:624:LHG:HC91	1.97	0.46
1:A:91:LEU:HD22	1:A:163:ILE:HA	1.97	0.46
29:A:405:CLA:H152	30:A:408:PHO:H3A	1.98	0.46
2:B:333:GLY:O	2:B:441:GLY:N	2.37	0.46
4:C:333:PRO:HB3	14:O:135:ARG:HD3	1.97	0.46
15:P:115:ASN:ND2	15:P:220:GLN:OE1	2.43	0.46
29:d:403:CLA:HBB2	18:x:86:ILE:HG13	1.97	0.46
8:h:67:ILE:HG13	8:h:72:LEU:HD23	1.97	0.46
21:g:91:LEU:HG	29:g:610:CLA:HMC3	1.98	0.46
14:O:214:LYS:HD2	14:O:214:LYS:HA	1.77	0.46
15:P:105:ARG:HG3	15:P:117:TYR:HB3	1.98	0.46
1:a:137:LEU:HD13	52:d:1039:HOH:O	2.13	0.46
4:c:191:THR:HG23	4:c:219:GLU:HB3	1.98	0.46
11:k:14:ALA:HB1	19:z:5:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:160:VAL:HG21	22:r:168:VAL:HG21	1.97	0.46
23:s:176:LEU:HA	23:s:179:VAL:HG12	1.96	0.46
45:y:601:CHL:H51	39:y:624:LHG:H181	1.98	0.46
1:A:269:ARG:HG3	5:D:235:PHE:HB2	1.97	0.46
1:A:301:ASN:H	4:C:393:ASN:HD21	1.63	0.46
4:C:274:ALA:HA	4:C:277:PHE:HD2	1.81	0.46
29:S:604:CLA:H52	45:S:606:CHL:HAA2	1.98	0.46
45:Y:607:CHL:H151	45:Y:609:CHL:H101	1.98	0.46
29:Y:613:CLA:H8	29:Y:613:CLA:H51	1.70	0.46
2:b:44:VAL:HG23	2:b:60:MET:HE1	1.96	0.46
5:d:155:SER:HA	5:d:159:ILE:HB	1.97	0.46
22:r:194:LEU:HD22	48:r:623:NEX:H15	1.96	0.46
22:r:243:GLY:O	22:r:247:MET:HG2	2.14	0.46
23:s:276:LEU:HD13	29:s:613:CLA:HMD3	1.97	0.46
2:B:26:HIS:CE1	29:B:613:CLA:HMA3	2.51	0.46
4:C:207:GLY:HA2	38:C:518:DGD:HD2	1.96	0.46
29:S:602:CLA:H72	46:S:621:LUT:H28	1.97	0.46
45:S:607:CHL:HHC	45:S:607:CHL:HBB1	1.98	0.46
2:b:127:ARG:NH1	22:r:105:GLU:OE1	2.40	0.46
4:c:385:THR:HG22	4:c:386:HIS:H	1.80	0.46
38:c:519:DGD:HB71	33:c:521:LMG:H421	1.98	0.46
29:s:604:CLA:HBB1	46:s:621:LUT:H181	1.96	0.46
33:A:413:LMG:H402	38:C:518:DGD:HB92	1.96	0.46
2:B:192:PRO:HG3	8:H:68:TYR:HD1	1.80	0.46
10:J:31:PHE:O	10:J:34:SER:OG	2.34	0.46
29:S:602:CLA:H3A	29:S:602:CLA:HBA2	1.59	0.46
5:d:172:SER:HB2	5:d:177:SER:HB3	1.98	0.46
47:y:622:XAT:H15	47:y:622:XAT:H201	1.71	0.46
1:A:225:ARG:NE	2:B:480:ALA:O	2.31	0.46
39:C:525:LHG:H302	39:S:624:LHG:H101	1.97	0.46
1:a:163:ILE:HD11	38:c:518:DGD:HA32	1.96	0.46
1:a:292:THR:HG22	4:c:416:THR:HB	1.97	0.46
29:c:511:CLA:HBC2	11:k:40:GLN:HG3	1.98	0.46
20:n:75:LEU:HD13	29:n:602:CLA:H42	1.98	0.46
47:g:622:XAT:H31	47:g:622:XAT:H391	1.72	0.46
23:s:124:LEU:HD13	23:s:152:PHE:HD2	1.81	0.46
45:y:606:CHL:HHC	45:y:606:CHL:HBB1	1.97	0.46
45:N:606:CHL:HHC	45:N:606:CHL:HBB1	1.98	0.46
29:G:613:CLA:H72	39:G:630:LHG:H152	1.97	0.46
2:b:382:PRO:HG3	2:b:391:SER:HB3	1.97	0.46
1:A:63:ILE:HB	4:C:323:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:PHE:HZ	32:B:621:SQD:H142	1.81	0.46
2:B:326:ARG:HB3	2:B:444:ARG:HD3	1.98	0.46
29:C:505:CLA:H111	29:C:505:CLA:H72	1.78	0.46
39:D:409:LHG:H162	12:L:23:LEU:HD21	1.98	0.46
29:S:613:CLA:H11	29:S:613:CLA:H52	1.70	0.46
1:a:127:MET:HG3	1:a:144:ALA:HB1	1.98	0.46
33:a:413:LMG:H372	38:c:518:DGD:HB41	1.98	0.46
46:y:621:LUT:H35	46:y:621:LUT:H401	1.80	0.46
29:B:612:CLA:H72	29:B:612:CLA:H112	1.80	0.45
29:N:603:CLA:H91	45:N:609:CHL:H122	1.98	0.45
1:a:156:ALA:HA	1:a:160:ILE:HB	1.97	0.45
29:b:615:CLA:HBD	29:b:615:CLA:HBA1	1.99	0.45
14:o:183:THR:HG21	14:o:203:PRO:HD2	1.98	0.45
14:o:278:THR:HG22	14:o:285:ALA:HB2	1.98	0.45
1:A:36:ILE:HA	29:A:410:CLA:HBB2	1.98	0.45
1:A:93:PHE:HB2	4:C:206:PHE:CG	2.51	0.45
1:A:227:THR:HA	1:A:233:ALA:H	1.81	0.45
2:B:73:GLN:HE21	2:B:88:PRO:HA	1.82	0.45
29:B:602:CLA:H122	44:H:101:RRX:H42	1.97	0.45
29:C:504:CLA:H91	29:C:504:CLA:H112	1.85	0.45
20:N:248:PHE:HB3	21:G:123:PHE:HZ	1.82	0.45
22:R:256:GLN:O	22:R:261:GLY:N	2.46	0.45
23:S:180:GLU:OE1	23:S:183:ARG:NH2	2.37	0.45
29:S:603:CLA:HAB	29:S:609:CLA:HBC2	1.97	0.45
29:a:405:CLA:H141	29:a:405:CLA:H162	1.79	0.45
3:v:12:LEU:HA	11:k:24:VAL:HG11	1.98	0.45
4:c:93:VAL:O	4:c:95:ASP:N	2.48	0.45
29:y:604:CLA:H111	29:y:604:CLA:H71	1.70	0.45
31:B:618:BCR:H15C	31:B:618:BCR:H351	1.77	0.45
31:C:516:BCR:H313	19:Z:17:PHE:HA	1.99	0.45
14:O:267:ALA:HB2	14:O:295:TYR:HD1	1.81	0.45
20:N:247:ALA:HB3	47:G:622:XAT:H193	1.96	0.45
1:a:306:VAL:HG12	1:a:314:LEU:HD12	1.98	0.45
2:b:192:PRO:HG3	8:h:68:TYR:HD1	1.82	0.45
2:b:315:ILE:O	2:b:318:ASN:HB2	2.16	0.45
4:c:277:PHE:HB3	4:c:285:TYR:CE1	2.50	0.45
15:p:105:ARG:HG3	52:p:1015:HOH:O	2.16	0.45
29:n:603:CLA:H12	29:n:603:CLA:HBA2	1.59	0.45
25:u:102:LYS:HE3	25:u:102:LYS:HB2	1.63	0.45
2:B:392:ILE:HG23	2:B:397:VAL:HB	1.99	0.45
4:C:398:VAL:HG12	4:C:401:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:48:TRP:HA	5:D:78:VAL:HG21	1.96	0.45
14:O:120:ASP:OD1	2:b:83:GLU:HA	2.16	0.45
20:N:223:GLN:HE21	20:N:234:ASN:HD22	1.62	0.45
39:Y:624:LHG:H272	39:Y:624:LHG:H242	1.76	0.45
29:b:609:CLA:H3A	29:b:609:CLA:HBA2	1.68	0.45
4:c:387:ALA:O	4:c:389:LEU:N	2.40	0.45
29:A:407:CLA:HMA2	33:D:411:LMG:H372	1.99	0.45
20:N:226:VAL:HG12	20:N:254:PHE:HE2	1.80	0.45
23:S:80:ALA:O	23:S:101:ARG:NH2	2.50	0.45
45:S:601:CHL:HBB1	45:S:601:CHL:HHC	1.98	0.45
24:Y:184:TYR:HB3	29:Y:610:CLA:HED3	1.99	0.45
29:b:609:CLA:H143	29:b:609:CLA:H161	1.81	0.45
29:c:501:CLA:H92	29:c:501:CLA:H62	1.83	0.45
47:n:622:XAT:H391	47:n:622:XAT:H31	1.68	0.45
47:r:622:XAT:H12	29:r:603:CLA:CBB	2.46	0.45
23:s:283:ASP:N	23:s:283:ASP:OD1	2.47	0.45
29:y:603:CLA:HHC	29:y:603:CLA:HBB1	1.97	0.45
25:u:95:LEU:HD13	25:u:107:LYS:HG2	1.98	0.45
30:A:409:PHO:HBA1	30:A:409:PHO:H3A	1.50	0.45
32:A:412:SQD:H4	5:D:233:ARG:HH22	1.81	0.45
20:N:87:GLU:HG3	20:N:181:LEU:HD13	1.98	0.45
29:R:609:CLA:H8	29:R:609:CLA:H121	1.77	0.45
15:p:113:VAL:O	15:p:115:ASN:ND2	2.50	0.45
29:n:603:CLA:H62	29:n:603:CLA:H41	1.50	0.45
45:s:606:CHL:HBB2	45:s:607:CHL:CBB	2.46	0.45
1:A:305:SER:OG	38:C:520:DGD:O3D	2.33	0.45
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.99	0.45
29:B:610:CLA:OBD	8:H:46:THR:OG1	2.30	0.45
4:C:288:GLU:OE2	4:C:379:ARG:NH1	2.49	0.45
29:C:505:CLA:HBB1	29:C:505:CLA:H93	1.99	0.45
8:H:29:LEU:HD22	22:R:203:ASN:HD22	1.82	0.45
29:G:614:CLA:H2A	24:Y:152:LEU:HD11	1.99	0.45
47:R:621:XAT:H371	47:R:621:XAT:H28	1.99	0.45
1:a:229:GLU:OE1	37:b:625:GOL:O2	2.30	0.45
4:c:421:LEU:HD13	29:c:502:CLA:C2C	2.46	0.45
29:c:502:CLA:H18	23:s:272:PHE:HE2	1.80	0.45
1:A:228:THR:HB	1:A:233:ALA:HB2	1.99	0.45
5:D:148:ALA:HB2	5:D:276:VAL:HG13	1.99	0.45
20:N:94:ARG:HA	20:N:97:LEU:HD12	1.98	0.45
20:N:120:SER:HB2	20:N:126:ALA:HA	1.99	0.45
29:N:610:CLA:H72	29:N:612:CLA:HMD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N:622:XAT:H10	39:Y:624:LHG:H211	1.98	0.45
1:a:51:ALA:O	1:a:55:ALA:HB2	2.17	0.45
2:b:388:SER:OG	2:b:389:LYS:N	2.49	0.45
5:d:21:TRP:NE1	18:x:93:VAL:O	2.50	0.45
29:r:610:CLA:H62	29:r:610:CLA:H41	1.56	0.45
29:y:604:CLA:H71	29:y:604:CLA:H162	1.99	0.45
29:y:613:CLA:H172	29:y:614:CLA:HBD	1.99	0.45
32:A:412:SQD:H362	29:C:508:CLA:H142	1.99	0.45
29:B:612:CLA:H151	31:B:619:BCR:H342	1.98	0.45
38:C:520:DGD:HBN2	38:C:520:DGD:HBT1	1.98	0.45
5:D:329:MET:O	5:D:333:ASP:CB	2.64	0.45
6:E:25:ILE:O	6:E:29:SER:HB2	2.17	0.45
21:G:182:ASP:OD1	46:G:620:LUT:O23	2.30	0.45
50:S:626:3PH:H362	50:S:626:3PH:H391	1.75	0.45
24:Y:185:PRO:HB3	29:Y:608:CLA:HBC2	1.99	0.45
51:Y:625:SPH:H131	51:Y:625:SPH:H162	1.76	0.45
1:a:227:THR:HA	1:a:233:ALA:H	1.81	0.45
14:o:276:SER:HB2	14:o:288:ILE:HD11	1.99	0.45
29:n:603:CLA:H72	29:y:603:CLA:H71	1.98	0.45
45:n:606:CHL:HHC	45:n:606:CHL:HBB1	1.99	0.45
30:A:409:PHO:HBA1	29:D:402:CLA:H142	1.99	0.45
20:N:93:ALA:HB1	20:N:210:GLY:HA3	1.98	0.45
29:R:604:CLA:HBA2	29:R:604:CLA:H3A	1.68	0.45
1:a:196:PRO:HA	1:a:199:MET:HG3	1.99	0.45
2:b:149:LEU:HD21	29:b:605:CLA:H171	1.99	0.45
3:v:4:THR:HG23	11:k:20:PRO:HG3	1.97	0.45
14:o:208:SER:HA	14:o:245:TYR:CZ	2.52	0.45
20:n:173:PRO:HG2	45:n:608:CHL:HBB2	1.98	0.45
24:y:137:LEU:HD11	45:y:606:CHL:HAC1	1.99	0.45
2:B:30:VAL:HG13	29:B:614:CLA:HMC2	1.99	0.44
29:B:616:CLA:H101	29:B:616:CLA:H13	1.70	0.44
29:C:508:CLA:CAB	29:C:510:CLA:HMA3	2.47	0.44
22:R:184:ILE:O	22:R:188:ILE:HG12	2.17	0.44
29:Y:604:CLA:H92	29:Y:604:CLA:H61	1.87	0.44
4:c:151:TYR:OH	32:c:626:SQD:O2	2.30	0.44
4:c:338:ILE:HG21	4:c:347:TRP:HB2	1.98	0.44
29:c:502:CLA:H92	29:c:502:CLA:H61	1.75	0.44
29:s:613:CLA:H11	29:s:613:CLA:H52	1.69	0.44
29:y:602:CLA:H143	29:y:602:CLA:H161	1.81	0.44
1:A:191:ASN:HB2	4:C:399:ALA:HB1	2.00	0.44
15:P:128:ILE:HG22	15:P:131:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:240:ILE:HD13	32:c:626:SQD:H82	1.99	0.44
15:p:99:VAL:HG12	15:p:101:SER:H	1.83	0.44
46:g:620:LUT:H35	46:g:620:LUT:H401	1.85	0.44
23:s:268:LEU:CD1	29:s:614:CLA:HAB	2.47	0.44
29:s:603:CLA:H193	29:s:603:CLA:H162	1.81	0.44
29:s:614:CLA:HBA2	29:s:614:CLA:H3A	1.57	0.44
24:y:240:HIS:CG	29:y:613:CLA:HAA2	2.52	0.44
1:A:32:TRP:NE1	52:A:1018:HOH:O	2.42	0.44
29:B:605:CLA:CMB	29:B:608:CLA:HAB	2.48	0.44
4:C:43:ALA:HB1	31:C:517:BCR:H373	1.98	0.44
36:C:524:DGA:HB52	29:Y:611:CLA:H52	1.99	0.44
24:Y:50:LEU:HD23	24:Y:54:SER:HA	2.00	0.44
1:a:40:THR:HG23	29:a:410:CLA:HBB1	1.99	0.44
5:d:98:GLN:HB2	6:e:73:LEU:HD22	1.99	0.44
14:o:236:GLU:HB3	14:o:240:LEU:HG	1.99	0.44
20:n:87:GLU:HG3	20:n:181:LEU:HD13	2.00	0.44
22:r:142:ARG:NH2	22:r:212:ILE:O	2.48	0.44
25:u:99:ASP:HA	25:u:108:GLU:OE2	2.17	0.44
14:O:135:ARG:O	14:O:137:THR:N	2.43	0.44
46:N:621:LUT:H15	46:N:621:LUT:H201	1.84	0.44
29:c:501:CLA:H41	29:c:501:CLA:H61	1.65	0.44
31:c:517:BCR:H351	31:c:517:BCR:H15C	1.71	0.44
39:d:408:LHG:H352	39:d:408:LHG:H111	2.00	0.44
20:n:168:ARG:NH2	45:n:609:CHL:O1D	2.45	0.44
21:g:141:SER:OG	45:g:605:CHL:OMC	2.29	0.44
21:g:148:VAL:HG11	45:g:605:CHL:HBC1	1.98	0.44
29:r:609:CLA:HBB1	29:r:609:CLA:H111	1.99	0.44
1:A:64:ARG:HG2	4:C:325:LEU:HD11	2.00	0.44
29:C:501:CLA:H92	29:C:501:CLA:H62	1.79	0.44
14:O:114:PHE:O	14:O:130:THR:OG1	2.35	0.44
20:N:132:GLN:HG3	20:N:135:GLY:H	1.83	0.44
22:R:186:GLN:O	22:R:190:ILE:HG12	2.18	0.44
23:S:176:LEU:HA	23:S:179:VAL:HG12	1.99	0.44
29:c:505:CLA:H152	29:c:505:CLA:H112	1.73	0.44
12:l:7:ASN:ND2	52:r:1007:HOH:O	2.48	0.44
21:g:157:GLU:OE1	21:g:160:ARG:NH1	2.50	0.44
45:s:607:CHL:HHC	45:s:607:CHL:HBB1	1.99	0.44
24:y:76:LEU:O	24:y:86:TYR:HE2	2.00	0.44
29:B:608:CLA:H41	29:B:608:CLA:H62	1.54	0.44
29:B:616:CLA:H92	29:B:616:CLA:H61	1.82	0.44
4:C:338:ILE:HG21	4:C:347:TRP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:C:521:LMG:H141	33:C:521:LMG:H111	1.88	0.44
20:N:149:ASN:HB3	20:N:152:ALA:HB3	2.00	0.44
45:N:601:CHL:HED2	39:N:624:LHG:H141	1.99	0.44
29:R:610:CLA:H13	29:R:610:CLA:H102	1.78	0.44
4:c:320:GLN:HA	4:c:326:GLY:HA2	1.99	0.44
29:c:511:CLA:H13	31:c:517:BCR:H21C	1.99	0.44
5:d:29:PHE:HB3	5:d:128:ARG:HH21	1.82	0.44
5:d:317:LYS:NZ	52:d:1027:HOH:O	2.49	0.44
22:r:195:VAL:HA	22:r:198:VAL:HG22	1.99	0.44
2:B:236:SER:HA	2:B:473:THR:HG21	2.00	0.44
29:C:511:CLA:H122	29:C:511:CLA:H8	1.75	0.44
20:N:111:ASP:OD1	20:N:111:ASP:N	2.42	0.44
22:R:199:GLU:OE1	22:R:202:ARG:NH2	2.36	0.44
23:S:193:SER:HB2	23:S:199:PHE:HE1	1.82	0.44
24:Y:77:SER:OG	29:Y:602:CLA:O1A	2.34	0.44
1:a:86:SER:HB3	1:a:89:ILE:HG13	1.98	0.44
1:a:309:SER:HA	7:f:44:ARG:HB2	1.99	0.44
33:a:413:LMG:H341	29:c:505:CLA:H192	2.00	0.44
2:b:235:GLU:HG3	2:b:473:THR:HB	2.00	0.44
4:c:364:ASP:HB3	4:c:367:LYS:HB2	1.99	0.44
29:c:506:CLA:H93	29:c:506:CLA:H61	1.78	0.44
8:h:75:ASP:OD2	18:x:64:SER:N	2.51	0.44
21:g:94:LEU:O	21:g:98:THR:OG1	2.28	0.44
4:C:88:GLY:N	4:C:92:GLU:O	2.50	0.44
4:C:198:PHE:HA	4:C:201:ILE:HG22	2.00	0.44
15:P:231:ASP:OD1	15:P:232:LYS:N	2.50	0.44
20:N:40:PHE:HA	20:N:45:ARG:HB2	1.99	0.44
21:G:92:GLY:O	21:G:96:ILE:HG12	2.17	0.44
23:S:181:LYS:HA	23:S:181:LYS:HD3	1.82	0.44
24:Y:102:LEU:HB2	46:Y:620:LUT:H35	2.00	0.44
29:b:613:CLA:H61	29:b:613:CLA:H102	1.66	0.44
29:c:510:CLA:H8	29:c:510:CLA:H122	1.78	0.44
29:c:513:CLA:NB	31:c:514:BCR:H383	2.33	0.44
5:d:148:ALA:HB2	5:d:276:VAL:HG13	1.99	0.44
16:t:27:PRO:O	16:t:28:ARG:NH1	2.44	0.44
22:r:217:ALA:HB3	29:r:608:CLA:H93	1.99	0.44
23:s:83:TYR:OH	39:s:624:LHG:O5	2.32	0.44
14:O:216:ARG:HD3	14:O:240:LEU:HD23	2.00	0.44
15:P:114:ASN:HD21	15:P:225:ARG:HG3	1.83	0.44
15:P:170:LEU:HD21	15:P:173:VAL:HG13	1.99	0.44
3:v:16:VAL:HG13	31:c:516:BCR:H363	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:213:VAL:HG11	4:c:280:PHE:HB2	2.00	0.44
4:c:247:TRP:HB3	36:c:524:DGA:HG31	2.00	0.44
29:c:504:CLA:H41	29:c:504:CLA:H62	1.59	0.44
38:c:520:DGD:HA52	38:c:520:DGD:HA21	1.82	0.44
46:r:620:LUT:H35	46:r:620:LUT:H401	1.69	0.44
29:r:612:CLA:H52	29:r:612:CLA:H11	1.87	0.44
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.88	0.43
29:C:503:CLA:H61	29:C:503:CLA:H41	1.71	0.43
5:D:51:GLY:HA3	5:D:78:VAL:HG22	1.99	0.43
5:D:172:SER:HB2	5:D:177:SER:HB3	1.99	0.43
14:O:149:ILE:HD11	14:O:193:LEU:HD21	2.00	0.43
29:G:603:CLA:H152	45:G:609:CHL:H102	2.00	0.43
24:Y:204:LEU:HB3	29:Y:610:CLA:HMA2	2.00	0.43
47:Y:622:XAT:H15	47:Y:622:XAT:H201	1.68	0.43
29:a:405:CLA:H203	29:a:405:CLA:H161	1.85	0.43
29:b:605:CLA:H62	29:b:605:CLA:H41	1.58	0.43
29:b:610:CLA:C2	29:b:611:CLA:HBB2	2.48	0.43
29:b:612:CLA:H62	29:b:612:CLA:H41	1.47	0.43
31:b:618:BCR:H351	31:b:618:BCR:H15C	1.78	0.43
14:o:157:PHE:O	14:o:189:GLY:N	2.50	0.43
15:p:117:TYR:CZ	15:p:218:LYS:HD3	2.53	0.43
46:g:621:LUT:H15	46:g:621:LUT:H201	1.85	0.43
23:s:188:GLY:HA2	23:s:189:PRO:HD3	1.88	0.43
29:y:613:CLA:H102	29:y:614:CLA:HMD3	1.99	0.43
1:A:106:LEU:HD11	31:A:411:BCR:H402	2.00	0.43
1:A:332:HIS:O	1:A:333:GLU:C	2.61	0.43
29:A:406:CLA:H141	42:D:405:PL9:H471	1.99	0.43
2:B:74:SER:HA	2:B:92:SER:HB2	2.00	0.43
5:D:338:LYS:NZ	52:D:1042:HOH:O	2.50	0.43
45:N:606:CHL:HBB2	45:N:607:CHL:HAB	2.01	0.43
29:b:609:CLA:H141	29:d:403:CLA:H12	2.00	0.43
4:c:395:VAL:HG13	4:c:403:ASN:HA	2.00	0.43
29:c:503:CLA:H193	29:c:503:CLA:H161	1.81	0.43
38:c:523:DGD:HBW1	29:y:614:CLA:HBC1	1.99	0.43
5:d:48:TRP:HA	5:d:78:VAL:HG21	1.99	0.43
6:e:78:LYS:NZ	25:u:113:ILE:O	2.50	0.43
8:h:68:TYR:HE2	33:h:102:LMG:H121	1.82	0.43
20:n:191:GLY:O	20:n:193:ALA:N	2.49	0.43
45:n:601:CHL:H41	45:n:601:CHL:H62	1.54	0.43
46:n:620:LUT:H35	46:n:620:LUT:H401	1.90	0.43
45:y:607:CHL:H2	45:y:607:CHL:H61	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:y:611:CLA:H92	29:y:611:CLA:H62	1.81	0.43
30:A:409:PHO:HMC2	5:D:279:LEU:HD21	2.01	0.43
29:B:615:CLA:H12	32:B:621:SQD:H262	1.99	0.43
4:C:390:GLY:HA2	4:C:396:GLY:O	2.18	0.43
5:D:225:ASP:HB2	5:D:234:ALA:HB1	2.00	0.43
29:D:403:CLA:H141	29:D:403:CLA:H161	1.76	0.43
2:b:460:LEU:HB3	5:d:280:TRP:HZ3	1.83	0.43
4:c:449:ARG:NH2	5:d:242:GLU:O	2.45	0.43
29:c:509:CLA:H111	29:c:509:CLA:H142	1.71	0.43
46:g:620:LUT:H15	46:g:620:LUT:H201	1.86	0.43
1:A:127:MET:HE2	1:A:151:VAL:HG11	2.00	0.43
1:A:299:GLY:O	4:C:391:SER:OG	2.36	0.43
2:B:276:ASP:OD1	2:B:361:THR:OG1	2.29	0.43
29:B:609:CLA:H111	29:B:609:CLA:H91	1.82	0.43
29:B:612:CLA:H41	29:B:612:CLA:H62	1.53	0.43
4:C:387:ALA:HB3	52:C:1037:HOH:O	2.17	0.43
20:N:136:LEU:HD22	45:N:606:CHL:HMD2	2.01	0.43
29:Y:613:CLA:H102	29:Y:614:CLA:HMD3	1.99	0.43
2:b:96:ALA:O	2:b:100:HIS:ND1	2.46	0.43
2:b:392:ILE:HG13	2:b:418:LYS:HG2	1.99	0.43
4:c:296:GLU:C	4:c:298:SER:H	2.26	0.43
21:g:71:ASP:HB3	21:g:74:THR:HG22	2.00	0.43
24:y:139:TYR:CE2	29:y:604:CLA:H2	2.53	0.43
1:A:89:ILE:HD11	1:A:108:ASN:HB3	2.00	0.43
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.54	0.43
3:V:16:VAL:HG13	31:C:516:BCR:H362	2.00	0.43
31:C:515:BCR:H351	31:C:515:BCR:H15C	1.62	0.43
5:D:331:ALA:HA	5:D:339:LEU:HB2	2.00	0.43
20:N:74:GLY:HA3	21:G:77:ARG:HG3	2.00	0.43
15:p:101:SER:OG	15:p:121:GLN:OE1	2.26	0.43
20:n:170:ASN:HD22	24:y:53:LEU:HA	1.84	0.43
29:s:610:CLA:H152	29:s:610:CLA:H111	1.74	0.43
29:C:507:CLA:H141	29:C:507:CLA:H161	1.79	0.43
29:C:513:CLA:H41	29:C:513:CLA:H62	1.52	0.43
5:D:51:GLY:HA2	5:D:55:VAL:HB	1.99	0.43
5:D:122:LEU:HB3	5:D:150:ILE:HG12	2.00	0.43
29:D:402:CLA:H41	29:D:402:CLA:H62	1.82	0.43
33:H:102:LMG:H182	33:H:102:LMG:H151	1.54	0.43
29:N:602:CLA:H62	46:N:621:LUT:H371	2.00	0.43
2:b:157:HIS:CD2	2:b:164:PRO:HD2	2.53	0.43
29:c:512:CLA:H143	32:c:626:SQD:H332	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:e:23:HIS:NE2	43:f:101:HEM:ND	2.66	0.43
46:n:621:LUT:H35	46:n:621:LUT:H401	1.83	0.43
2:B:12:VAL:HG23	29:B:613:CLA:HMC2	1.99	0.43
29:B:608:CLA:HBA2	29:B:608:CLA:H3A	1.58	0.43
4:C:454:VAL:HG21	5:D:248:THR:HA	2.00	0.43
29:C:509:CLA:H111	29:C:509:CLA:H142	1.72	0.43
6:E:18:ARG:HD3	6:E:18:ARG:HA	1.86	0.43
14:O:224:ASN:HA	14:O:240:LEU:HD22	2.01	0.43
22:R:218:PHE:HE1	29:R:608:CLA:H2	1.84	0.43
3:v:26:LEU:HD21	19:z:25:VAL:HA	2.00	0.43
5:d:262:SER:N	39:d:409:LHG:O5	2.36	0.43
2:B:272:ARG:NH2	2:B:276:ASP:OD2	2.42	0.43
2:B:372:ASP:HB2	2:B:378:ARG:HG3	2.00	0.43
29:B:607:CLA:H151	29:B:607:CLA:H111	1.77	0.43
29:C:511:CLA:H93	29:C:511:CLA:H61	1.84	0.43
29:C:513:CLA:CAB	31:C:514:BCR:H24C	2.48	0.43
6:E:8:ARG:HB3	6:E:13:ILE:HD11	2.00	0.43
20:N:138:TYR:HD1	20:N:139:LEU:HG	1.83	0.43
29:S:602:CLA:H112	46:S:621:LUT:H371	2.00	0.43
24:Y:168:PHE:CD2	29:Y:608:CLA:HAB	2.53	0.43
29:Y:612:CLA:H12	29:Y:612:CLA:HED2	2.00	0.43
1:a:54:ALA:HB2	1:a:72:LEU:HD12	1.99	0.43
1:a:64:ARG:O	14:o:206:ARG:NH2	2.48	0.43
2:b:326:ARG:HB3	2:b:444:ARG:HD3	1.99	0.43
2:b:355:PHE:HB2	25:u:100:PRO:HB2	2.01	0.43
29:g:602:CLA:H72	46:g:621:LUT:H30	2.00	0.43
22:r:236:LYS:HA	22:r:239:GLU:HG2	2.01	0.43
1:A:85:THR:HA	1:A:109:GLY:HA3	2.00	0.43
1:A:114:LEU:O	1:A:118:HIS:ND1	2.46	0.43
29:B:605:CLA:HBB1	29:B:614:CLA:C1C	2.49	0.43
4:C:335:GLY:HA3	14:O:82:ASN:HB2	2.01	0.43
5:D:262:SER:N	39:D:409:LHG:O5	2.37	0.43
29:G:602:CLA:H202	39:G:630:LHG:H191	2.01	0.43
29:R:612:CLA:H52	29:R:612:CLA:H11	1.76	0.43
46:R:620:LUT:H35	46:R:620:LUT:H401	1.71	0.43
50:S:626:3PH:H3C1	50:S:626:3PH:H392	1.82	0.43
24:Y:161:VAL:HG13	48:Y:623:NEX:H15	2.01	0.43
45:Y:607:CHL:H121	45:Y:609:CHL:H121	1.99	0.43
1:a:274:PHE:HA	1:a:277:VAL:HG12	2.00	0.43
4:c:297:ALA:HA	4:c:300:ALA:HB3	1.99	0.43
4:c:330:MET:HG2	4:c:340:GLY:HA2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:511:CLA:H8	19:z:24:PRO:HB3	2.00	0.43
1:A:184:ILE:HG23	1:A:328:MET:SD	2.58	0.43
2:B:256:MET:O	2:B:448:ARG:NH1	2.52	0.43
29:B:602:CLA:H141	29:B:602:CLA:H162	1.89	0.43
8:H:68:TYR:HE2	33:H:102:LMG:H121	1.84	0.43
20:N:191:GLY:O	20:N:193:ALA:N	2.51	0.43
29:R:608:CLA:HBA2	29:R:608:CLA:H3A	1.61	0.43
45:Y:601:CHL:H51	39:Y:624:LHG:H181	2.00	0.43
29:b:610:CLA:H92	29:b:610:CLA:H41	2.00	0.43
29:c:504:CLA:H91	29:c:504:CLA:H111	1.80	0.43
33:c:521:LMG:HC71	33:j:101:LMG:HC92	2.01	0.43
47:n:622:XAT:H201	47:n:622:XAT:H15	1.69	0.43
29:y:603:CLA:HAC1	45:y:607:CHL:HBB2	2.01	0.43
1:A:93:PHE:HZ	29:A:410:CLA:HAA1	1.84	0.42
1:A:126:TYR:CZ	30:A:408:PHO:HBA1	2.54	0.42
29:C:509:CLA:H11	29:C:509:CLA:H51	1.67	0.42
8:H:69:ASN:HD22	33:H:102:LMG:HC8	1.83	0.42
29:N:603:CLA:H12	29:N:603:CLA:HED2	2.01	0.42
21:G:94:LEU:HD23	29:G:604:CLA:HMC1	2.01	0.42
23:S:86:ASP:OD1	46:S:621:LUT:O23	2.33	0.42
45:Y:606:CHL:HHC	45:Y:606:CHL:HBB1	2.01	0.42
29:Y:612:CLA:H62	29:Y:612:CLA:H101	1.77	0.42
1:a:114:LEU:O	1:a:118:HIS:ND1	2.45	0.42
1:a:191:ASN:HB2	4:c:399:ALA:HB1	2.00	0.42
1:a:305:SER:HA	10:j:41:SER:HB3	2.01	0.42
1:a:308:ASP:OD1	1:a:312:ARG:N	2.52	0.42
4:c:213:VAL:HG13	4:c:281:ASN:HB2	2.01	0.42
4:c:384:MET:O	15:p:228:LYS:NZ	2.43	0.42
29:c:513:CLA:CAB	31:c:514:BCR:H24C	2.49	0.42
31:d:404:BCR:H363	7:f:32:PHE:HB3	2.01	0.42
21:g:43:PRO:HA	21:g:46:GLU:HG3	2.01	0.42
46:r:620:LUT:H31	46:r:620:LUT:H391	1.85	0.42
1:A:312:ARG:NH2	15:P:92:ASN:OD1	2.52	0.42
2:B:471:SER:HB3	5:D:140:PRO:HG2	2.00	0.42
4:C:203:LYS:HG3	4:C:211:TRP:HA	2.01	0.42
4:C:319:ALA:O	15:P:158:GLY:HA3	2.19	0.42
6:E:59:ASP:OD1	6:E:59:ASP:N	2.51	0.42
14:O:224:ASN:HB2	14:O:231:LYS:HD2	2.00	0.42
15:P:204:LEU:HD11	15:P:226:TRP:HH2	1.83	0.42
24:Y:61:LEU:HD13	24:Y:70:GLY:HA2	2.01	0.42
2:b:356:VAL:HG22	2:b:370:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:505:CLA:H42	31:c:515:BCR:HC7	2.01	0.42
38:c:520:DGD:HBN2	38:c:520:DGD:HBT1	2.01	0.42
24:y:145:LEU:HD23	24:y:145:LEU:HA	1.90	0.42
29:y:612:CLA:H152	29:y:612:CLA:HBB1	2.01	0.42
1:A:274:PHE:HA	1:A:277:VAL:HG12	2.01	0.42
2:B:96:ALA:O	2:B:100:HIS:ND1	2.47	0.42
29:B:613:CLA:HBB1	29:B:615:CLA:HMB2	2.00	0.42
31:D:404:BCR:H363	7:F:32:PHE:HB3	2.01	0.42
14:O:107:PHE:CD2	14:O:143:MET:HE3	2.54	0.42
19:Z:26:VAL:HG11	19:Z:40:VAL:HG21	2.01	0.42
20:N:168:ARG:NH2	45:N:609:CHL:O1D	2.44	0.42
29:G:602:CLA:H141	29:G:602:CLA:H162	1.78	0.42
29:G:610:CLA:H143	29:G:610:CLA:H161	1.88	0.42
4:c:125:PRO:HD3	29:c:513:CLA:HED3	2.01	0.42
1:A:9:GLU:N	17:W:102:ASP:O	2.53	0.42
1:A:201:GLY:HA3	1:A:286:THR:HB	2.02	0.42
1:A:331:MET:HG3	5:D:324:GLY:HA3	2.00	0.42
29:B:604:CLA:H62	29:B:604:CLA:H41	1.85	0.42
29:C:501:CLA:H61	29:C:501:CLA:H41	1.61	0.42
21:G:86:ALA:HB1	21:G:204:GLY:HA3	2.00	0.42
1:a:131:TRP:CZ3	29:c:505:CLA:HAA2	2.54	0.42
29:c:511:CLA:H93	29:c:511:CLA:H61	1.84	0.42
5:d:79:SER:HA	5:d:172:SER:HB3	2.01	0.42
5:d:90:LEU:HD13	5:d:109:GLY:HA2	2.02	0.42
39:g:624:LHG:HC81	47:y:622:XAT:H371	2.00	0.42
29:y:613:CLA:H12	29:y:614:CLA:HED2	2.01	0.42
1:A:14:TRP:HB3	17:W:99:SER:HB2	2.01	0.42
2:B:157:HIS:CD2	2:B:164:PRO:HD2	2.55	0.42
2:B:454:GLY:HA2	33:B:622:LMG:H202	2.02	0.42
38:C:523:DGD:HBH2	38:C:523:DGD:HBT1	1.87	0.42
5:D:47:GLY:HA2	31:D:404:BCR:H332	2.01	0.42
29:N:602:CLA:H122	29:N:602:CLA:H8	1.85	0.42
29:N:602:CLA:H61	46:N:621:LUT:H30	2.01	0.42
1:a:43:THR:HG23	31:a:411:BCR:H362	2.00	0.42
1:a:76:ASN:ND2	12:l:34:SER:HB3	2.34	0.42
2:b:52:LEU:HD12	2:b:52:LEU:HA	1.92	0.42
4:c:74:LEU:HD13	4:c:77:LEU:HD12	2.01	0.42
4:c:425:PHE:HA	29:c:508:CLA:HMC2	2.00	0.42
20:n:40:PHE:HA	20:n:45:ARG:HB2	2.01	0.42
20:n:149:ASN:HB3	20:n:152:ALA:HB3	2.01	0.42
1:A:187:GLN:HE22	1:A:193:LEU:HG	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:102:SER:O	4:C:106:HIS:ND1	2.49	0.42
29:C:505:CLA:H112	29:C:505:CLA:H152	1.78	0.42
38:C:518:DGD:HB92	38:C:518:DGD:HB61	1.78	0.42
5:D:201:VAL:HG22	29:D:402:CLA:C2B	2.49	0.42
7:F:19:TRP:HE3	7:F:20:LEU:HD22	1.83	0.42
20:N:187:PHE:HB3	45:N:608:CHL:H11	2.00	0.42
47:N:622:XAT:H15	47:N:622:XAT:H201	1.69	0.42
24:Y:169:ARG:NH2	45:Y:609:CHL:O1D	2.43	0.42
1:a:41:LEU:HD23	1:a:41:LEU:HA	1.84	0.42
4:c:238:TRP:NE1	29:c:506:CLA:O1D	2.40	0.42
29:c:502:CLA:H13	29:c:502:CLA:H171	1.78	0.42
5:d:152:VAL:HG22	29:d:402:CLA:HED1	2.01	0.42
14:o:267:ALA:HB2	14:o:295:TYR:HD1	1.85	0.42
45:n:609:CHL:HBA1	45:n:609:CHL:HBD	2.00	0.42
1:A:306:VAL:HG12	1:A:314:LEU:HD12	2.01	0.42
29:B:606:CLA:H8	29:B:613:CLA:H192	2.01	0.42
29:C:506:CLA:H143	29:C:506:CLA:H112	1.83	0.42
5:D:162:LEU:HD11	33:H:102:LMG:H292	2.01	0.42
14:O:216:ARG:HB3	14:O:243:LYS:HE2	2.02	0.42
15:P:128:ILE:O	15:P:131:TYR:HB2	2.18	0.42
46:R:620:LUT:H11	46:R:620:LUT:H191	1.80	0.42
8:h:28:THR:HA	8:h:31:ARG:HB2	2.02	0.42
14:o:151:ASN:OD1	14:o:152:ASP:N	2.53	0.42
29:n:613:CLA:H2	29:n:613:CLA:H62	1.78	0.42
46:g:620:LUT:H11	46:g:620:LUT:H191	1.91	0.42
25:u:105:THR:HG22	25:u:107:LYS:H	1.85	0.42
29:B:617:CLA:HMD3	8:H:24:THR:HG21	2.02	0.42
38:C:523:DGD:HD5	29:Y:611:CLA:HAA2	2.01	0.42
39:C:525:LHG:H172	32:C:526:SQD:H371	2.02	0.42
29:D:403:CLA:H101	8:H:55:LEU:HD11	2.01	0.42
14:O:138:TYR:HA	14:O:166:ALA:HB1	2.01	0.42
45:G:601:CHL:HED3	39:G:630:LHG:H142	2.01	0.42
29:G:602:CLA:H3A	29:G:602:CLA:HBA2	1.57	0.42
23:S:283:ASP:OD1	23:S:284:ASP:N	2.45	0.42
24:Y:50:LEU:HB3	24:Y:54:SER:HB3	2.02	0.42
1:a:174:LEU:HD22	30:a:408:PHO:H151	2.02	0.42
29:a:405:CLA:H102	30:a:408:PHO:HAA1	2.02	0.42
29:b:616:CLA:H2	29:b:617:CLA:CBB	2.48	0.42
20:n:75:LEU:HB3	20:n:85:TYR:HE2	1.84	0.42
47:r:622:XAT:H28	47:r:622:XAT:H371	2.01	0.42
1:A:337:HIS:CG	5:D:352:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:605:CLA:H62	29:B:605:CLA:H41	1.69	0.42
4:C:80:ILE:HD11	29:C:503:CLA:HED3	2.02	0.42
4:C:319:ALA:HB1	4:C:327:LYS:H	1.84	0.42
4:C:421:LEU:HD22	29:C:502:CLA:HMC3	2.02	0.42
5:D:201:VAL:HG13	29:D:402:CLA:HMB1	2.02	0.42
20:N:90:LEU:HD23	20:N:181:LEU:HG	2.02	0.42
29:S:610:CLA:H143	29:S:610:CLA:H161	1.89	0.42
24:Y:247:ASN:ND2	52:Y:1004:HOH:O	2.51	0.42
30:a:409:PHO:H142	30:a:409:PHO:H112	1.86	0.42
2:b:258:TYR:HB3	33:h:102:LMG:HC61	2.02	0.42
4:c:218:LEU:HA	4:c:221:ILE:HB	2.02	0.42
4:c:259:TYR:O	52:c:1001:HOH:O	2.22	0.42
4:c:390:GLY:HA2	4:c:396:GLY:O	2.19	0.42
5:d:37:LEU:HD22	5:d:125:PHE:HA	2.02	0.42
14:o:114:PHE:O	14:o:130:THR:OG1	2.35	0.42
20:n:225:ILE:HD13	20:n:225:ILE:HA	1.90	0.42
21:g:87:ARG:NH1	45:g:608:CHL:OBD	2.53	0.42
22:r:270:LYS:NZ	29:r:613:CLA:O1D	2.37	0.42
4:C:171:GLY:HA2	4:C:186:ILE:HB	2.02	0.42
14:O:120:ASP:OD2	2:b:83:GLU:HA	2.20	0.42
15:P:134:PRO:HB3	15:P:187:PHE:HE1	1.85	0.42
21:G:142:ILE:HA	21:G:145:THR:HG22	2.02	0.42
46:S:620:LUT:H11	46:S:620:LUT:H191	1.86	0.42
1:a:176:ILE:HD13	29:a:406:CLA:HED3	2.01	0.42
1:a:187:GLN:NE2	1:a:191:ASN:HA	2.34	0.42
2:b:385:LYS:HB2	14:o:219:ALA:O	2.19	0.42
29:b:606:CLA:H61	29:b:606:CLA:H41	1.66	0.42
29:c:509:CLA:H11	29:c:509:CLA:H51	1.67	0.42
46:g:621:LUT:H363	29:y:603:CLA:HED3	2.02	0.42
24:y:197:ASP:HB3	24:y:200:ALA:HB3	2.02	0.42
1:A:194:MET:HB3	1:A:300:PHE:HB2	2.01	0.41
29:A:405:CLA:H141	29:A:405:CLA:H162	1.83	0.41
4:C:216:ASP:OD1	4:C:216:ASP:N	2.51	0.41
12:L:32:PHE:O	12:L:36:ILE:HG12	2.20	0.41
14:O:120:ASP:CG	2:b:83:GLU:HA	2.44	0.41
29:R:602:CLA:H61	29:R:602:CLA:H41	1.64	0.41
45:S:601:CHL:HED2	39:S:624:LHG:H152	2.01	0.41
1:a:224:ILE:HD11	2:b:484:GLU:H	1.85	0.41
29:a:406:CLA:H92	29:a:406:CLA:H62	1.88	0.41
30:a:409:PHO:H3A	30:a:409:PHO:HBA1	1.68	0.41
5:d:51:GLY:HA3	5:d:78:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:265:GLU:OE1	14:o:295:TYR:OH	2.36	0.41
21:g:176:TYR:HB3	29:g:610:CLA:HED3	2.01	0.41
29:s:610:CLA:HBA1	46:s:620:LUT:H363	2.02	0.41
24:y:108:GLU:HG3	24:y:234:ILE:HD13	2.02	0.41
4:C:315:ASN:HD21	14:O:161:GLU:HB2	1.84	0.41
31:C:517:BCR:H15C	31:C:517:BCR:H351	1.75	0.41
39:C:525:LHG:H262	29:S:611:CLA:CAB	2.50	0.41
29:G:603:CLA:HMD3	45:G:609:CHL:HBA2	2.01	0.41
46:G:620:LUT:H11	46:G:620:LUT:H191	1.87	0.41
45:Y:606:CHL:HBB2	45:Y:607:CHL:HAB	2.02	0.41
1:a:14:TRP:HB3	17:w:99:SER:HB2	2.01	0.41
29:b:617:CLA:H62	29:b:617:CLA:H93	1.81	0.41
4:c:150:GLY:HA2	4:c:236:GLY:HA2	2.01	0.41
31:c:516:BCR:H371	10:j:20:GLY:HA3	2.02	0.41
33:c:521:LMG:H352	11:k:30:VAL:HG21	2.03	0.41
5:d:302:GLU:OE2	14:o:214:LYS:NZ	2.53	0.41
33:h:102:LMG:H182	33:h:102:LMG:H151	1.57	0.41
15:p:213:LYS:HE3	15:p:213:LYS:HB2	1.77	0.41
17:w:101:LYS:O	17:w:103:LEU:N	2.53	0.41
24:y:185:PRO:HB3	29:y:608:CLA:HBC2	2.02	0.41
25:u:96:ASP:O	25:u:100:PRO:HD3	2.21	0.41
29:B:613:CLA:H122	29:B:613:CLA:H162	1.67	0.41
4:C:350:ARG:HD2	14:O:73:LEU:HD21	2.03	0.41
4:C:447:ILE:H	5:D:223:PHE:HA	1.84	0.41
29:C:512:CLA:H3A	29:C:512:CLA:HBA1	1.86	0.41
13:M:5:ILE:HD13	13:m:6:LEU:HD21	2.02	0.41
15:P:171:LEU:HB2	15:P:188:GLU:HG2	2.03	0.41
22:R:267:SER:OG	46:R:620:LUT:O3	2.38	0.41
23:S:124:LEU:HD13	23:S:152:PHE:HD2	1.85	0.41
2:b:236:SER:HA	2:b:473:THR:HG21	2.02	0.41
4:c:231:LEU:HD22	29:c:506:CLA:HBC1	2.02	0.41
4:c:373:GLN:HB2	4:c:376:GLN:HG3	2.02	0.41
4:c:397:GLY:H	4:c:401:GLU:HG2	1.86	0.41
29:c:503:CLA:H172	29:c:510:CLA:HBB2	2.02	0.41
29:c:511:CLA:H143	19:z:20:VAL:HG13	2.03	0.41
39:d:410:LHG:H252	39:d:410:LHG:H282	1.74	0.41
8:h:29:LEU:HD22	22:r:203:ASN:HD22	1.85	0.41
15:p:128:ILE:HA	15:p:131:TYR:HD1	1.85	0.41
48:n:623:NEX:H15	48:n:623:NEX:H201	1.92	0.41
29:r:610:CLA:H2	29:r:610:CLA:C1B	2.50	0.41
45:y:601:CHL:H62	45:y:601:CHL:H41	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASP:HB2	5:D:352:LEU:HD11	2.01	0.41
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.55	0.41
2:B:91:TRP:CG	29:B:607:CLA:HBA2	2.56	0.41
2:B:99:SER:HB2	29:B:607:CLA:H61	2.02	0.41
29:B:606:CLA:H41	29:B:606:CLA:H61	1.70	0.41
4:C:63:PHE:HZ	4:C:93:VAL:HG21	1.86	0.41
38:C:520:DGD:HA21	38:C:520:DGD:HA52	1.84	0.41
5:D:98:GLN:HB2	6:E:73:LEU:HD22	2.02	0.41
15:P:185:TYR:HB3	15:P:187:PHE:CZ	2.55	0.41
20:N:170:ASN:C	20:N:170:ASN:HD22	2.28	0.41
29:N:610:CLA:HBB2	46:N:620:LUT:H34	2.02	0.41
39:N:624:LHG:HC82	47:G:622:XAT:H361	2.01	0.41
29:S:603:CLA:H161	29:S:603:CLA:H141	1.74	0.41
46:S:621:LUT:H35	46:S:621:LUT:H401	1.75	0.41
24:Y:234:ILE:HD12	24:Y:234:ILE:H	1.85	0.41
1:a:340:PRO:HG3	15:p:199:GLY:HA3	2.03	0.41
4:c:307:VAL:HA	4:c:310:GLN:HG2	2.02	0.41
14:o:111:PRO:HD2	14:o:138:TYR:HD1	1.86	0.41
14:o:135:ARG:O	14:o:137:THR:N	2.51	0.41
22:r:242:HIS:HA	22:r:245:LEU:HG	2.01	0.41
46:s:621:LUT:H35	46:s:621:LUT:H401	1.76	0.41
24:y:39:SER:O	24:y:39:SER:OG	2.33	0.41
45:y:601:CHL:H62	45:y:601:CHL:H102	1.91	0.41
1:A:340:PRO:HB3	15:P:198:GLU:C	2.45	0.41
29:A:406:CLA:H3A	29:A:406:CLA:HBA2	1.54	0.41
2:B:25:MET:HG2	31:B:618:BCR:H23C	2.03	0.41
2:B:334:ASP:N	2:B:334:ASP:OD1	2.53	0.41
29:B:610:CLA:H141	29:B:610:CLA:H161	1.83	0.41
4:C:154:ILE:HG13	4:C:236:GLY:HA3	2.02	0.41
36:C:524:DGA:HB82	29:Y:611:CLA:H71	2.02	0.41
5:D:5:ILE:HD11	5:D:10:GLU:HB3	2.02	0.41
5:D:231:THR:O	5:D:234:ALA:HB3	2.20	0.41
5:D:328:TRP:HH2	5:D:348:ARG:HH21	1.68	0.41
15:P:213:LYS:HE3	15:P:213:LYS:HB2	1.93	0.41
29:b:605:CLA:H141	29:b:605:CLA:H161	1.87	0.41
15:p:118:VAL:HG12	15:p:217:LEU:HA	2.02	0.41
17:w:73:PRO:O	17:w:76:VAL:HG22	2.20	0.41
20:n:113:ASP:OD1	20:n:113:ASP:N	2.51	0.41
23:s:93:ASP:OD1	23:s:93:ASP:N	2.52	0.41
29:B:609:CLA:H61	29:B:609:CLA:H41	1.81	0.41
20:N:103:MET:HG2	46:N:621:LUT:H41	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:N:608:CHL:H42	46:N:620:LUT:H27	2.02	0.41
48:N:623:NEX:H35	48:N:623:NEX:H401	1.86	0.41
47:G:622:XAT:H15	47:G:622:XAT:H201	1.72	0.41
29:Y:604:CLA:H162	29:Y:604:CLA:H71	2.03	0.41
2:b:30:VAL:HG22	29:b:614:CLA:C3C	2.50	0.41
2:b:464:PHE:HB2	5:d:280:TRP:CZ2	2.56	0.41
4:c:315:ASN:OD1	4:c:315:ASN:N	2.52	0.41
29:c:513:CLA:H3A	29:c:513:CLA:HBA2	1.68	0.41
15:p:203:GLN:HE22	15:p:220:GLN:HG3	1.86	0.41
20:n:98:LEU:HG	29:n:610:CLA:HMC3	2.03	0.41
46:n:620:LUT:H15	46:n:620:LUT:H201	1.88	0.41
21:g:53:LEU:HD13	21:g:62:GLY:HA2	2.02	0.41
29:r:604:CLA:H3A	29:r:604:CLA:HBA2	1.69	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41
2:B:118:TRP:HH2	12:L:1:MET:H2	1.68	0.41
2:B:434:ARG:NH1	14:O:230:ALA:O	2.52	0.41
4:C:72:GLN:HA	38:C:519:DGD:HE61	2.03	0.41
36:C:524:DGA:HA22	36:C:524:DGA:HA51	1.87	0.41
14:O:208:SER:HB3	15:P:154:THR:HG21	2.01	0.41
45:G:601:CHL:H101	39:G:630:LHG:H212	2.02	0.41
22:R:160:VAL:HG21	22:R:168:VAL:HG21	2.02	0.41
29:Y:603:CLA:HAC1	45:Y:607:CHL:CBB	2.51	0.41
1:a:224:ILE:HD12	1:a:224:ILE:HA	1.96	0.41
1:a:258:LEU:HB3	1:a:259:ILE:HD12	2.03	0.41
1:a:288:LEU:HD23	1:a:288:LEU:HA	1.92	0.41
8:h:42:PRO:HG3	22:r:83:VAL:HG13	2.02	0.41
14:o:104:LEU:HB3	14:o:298:LEU:HD23	2.01	0.41
20:n:60:LEU:HD11	20:n:71:ASP:HB2	2.03	0.41
29:n:603:CLA:HAC1	45:n:607:CHL:CBB	2.50	0.41
21:g:142:ILE:HA	21:g:145:THR:HG22	2.03	0.41
45:g:601:CHL:H93	45:g:601:CHL:H61	1.89	0.41
29:s:611:CLA:H61	29:s:611:CLA:H41	1.76	0.41
1:A:266:ASN:OD1	1:A:266:ASN:N	2.54	0.41
30:A:408:PHO:HAB	5:D:205:LEU:HD13	2.02	0.41
2:B:291:SER:HB3	2:B:296:LEU:HD23	2.03	0.41
29:B:607:CLA:H203	29:B:607:CLA:H161	1.91	0.41
4:C:166:LYS:HZ2	4:C:172:GLY:HA3	1.86	0.41
4:C:307:VAL:HA	4:C:310:GLN:HG2	2.01	0.41
14:O:103:LYS:HA	14:O:146:SER:HA	2.03	0.41
29:N:604:CLA:H61	48:N:623:NEX:H373	2.02	0.41
46:N:620:LUT:H35	46:N:620:LUT:H401	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R:609:CLA:H101	29:R:609:CLA:H62	1.96	0.41
45:S:608:CHL:HMB3	48:S:622:NEX:H15	2.01	0.41
50:S:626:3PH:H362	50:S:626:3PH:H241	2.03	0.41
24:Y:204:LEU:HD23	24:Y:204:LEU:HA	1.95	0.41
2:b:193:TYR:HB2	8:h:83:SER:HB2	2.03	0.41
5:d:161:PRO:HB3	5:d:170:ALA:HB2	2.03	0.41
5:d:336:HIS:HA	6:e:65:LEU:HD21	2.03	0.41
14:o:184:ILE:HD12	14:o:184:ILE:HA	1.94	0.41
23:s:215:PRO:HB2	29:s:617:CLA:HBC2	2.02	0.41
29:y:603:CLA:HAC1	45:y:607:CHL:CBB	2.50	0.41
29:y:612:CLA:H62	29:y:612:CLA:H101	1.81	0.41
1:A:288:LEU:HD11	4:C:423:PHE:HD2	1.86	0.41
2:B:23:HIS:ND1	29:B:616:CLA:OBD	2.54	0.41
29:B:608:CLA:HED2	52:B:1003:HOH:O	2.21	0.41
29:C:501:CLA:H193	29:C:507:CLA:HBB1	2.02	0.41
5:D:87:HIS:CD2	5:D:166:GLY:HA2	2.56	0.41
11:K:18:PHE:HD1	11:K:21:ILE:HD12	1.86	0.41
13:M:16:ILE:HD13	13:M:16:ILE:HA	1.97	0.41
29:N:602:CLA:H141	29:N:602:CLA:H161	1.84	0.41
21:G:41:LEU:O	21:G:44:PHE:HB2	2.20	0.41
46:G:620:LUT:H15	46:G:620:LUT:H201	1.82	0.41
29:R:602:CLA:H52	47:R:621:XAT:H372	2.02	0.41
29:S:610:CLA:H102	46:S:620:LUT:H381	2.03	0.41
46:S:621:LUT:H11	46:S:621:LUT:H191	1.95	0.41
24:Y:39:SER:O	24:Y:39:SER:OG	2.33	0.41
24:Y:139:TYR:HB2	24:Y:146:ILE:HG12	2.03	0.41
1:a:14:TRP:HB2	17:w:95:ILE:HG22	2.02	0.41
1:a:85:THR:HA	1:a:109:GLY:HA3	2.03	0.41
2:b:30:VAL:HG13	29:b:614:CLA:HMC2	2.02	0.41
29:b:616:CLA:H101	29:b:616:CLA:H13	1.80	0.41
4:c:249:ARG:HA	4:c:254:TRP:HE1	1.85	0.41
4:c:365:LEU:HA	4:c:368:LEU:HD12	2.02	0.41
5:d:189:HIS:CE1	5:d:294:ARG:HH21	2.39	0.41
5:d:193:LEU:O	12:l:35:TYR:OH	2.33	0.41
5:d:246:MET:HB3	16:t:30:ALA:HB1	2.02	0.41
14:o:117:LYS:HB2	14:o:127:PHE:CE2	2.56	0.41
20:n:150:ILE:HA	20:n:153:THR:HG22	2.03	0.41
20:n:223:GLN:O	20:n:227:THR:OG1	2.27	0.41
45:n:605:CHL:H111	45:n:605:CHL:H151	1.92	0.41
29:n:613:CLA:H93	29:n:613:CLA:H61	1.86	0.41
29:n:613:CLA:H91	29:n:613:CLA:H112	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:199:LYS:NZ	52:g:1005:HOH:O	2.44	0.41
29:g:602:CLA:HBA2	29:g:602:CLA:H3A	1.53	0.41
22:r:184:ILE:O	22:r:188:ILE:HG12	2.21	0.41
22:r:234:ARG:NH2	29:r:612:CLA:H111	2.36	0.41
48:r:623:NEX:C31	45:r:606:CHL:HBA2	2.50	0.41
23:s:191:GLY:HA2	23:s:199:PHE:CZ	2.56	0.41
23:s:192:PHE:H	23:s:198:LYS:HA	1.85	0.41
45:s:601:CHL:HHC	45:s:601:CHL:HBB1	2.02	0.41
1:A:132:GLU:O	1:A:136:ARG:HG2	2.21	0.41
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.03	0.41
4:C:205:PRO:HA	4:C:211:TRP:HB2	2.02	0.41
4:C:246:PRO:HA	4:C:249:ARG:HD2	2.03	0.41
4:C:296:GLU:C	4:C:298:SER:H	2.29	0.41
4:C:330:MET:HE3	4:C:330:MET:HB2	1.98	0.41
31:C:514:BCR:HC7	19:Z:55:GLY:HA3	2.03	0.41
33:C:521:LMG:H352	11:K:30:VAL:HG21	2.03	0.41
14:O:208:SER:O	14:O:219:ALA:N	2.53	0.41
17:W:73:PRO:O	17:W:76:VAL:HG22	2.21	0.41
21:G:193:PHE:HE1	29:G:610:CLA:H2A	1.86	0.41
22:R:145:MET:SD	22:R:242:HIS:HB3	2.61	0.41
23:S:108:ALA:O	23:S:112:MET:HG3	2.21	0.41
29:Y:613:CLA:H12	29:Y:614:CLA:HED2	2.03	0.41
46:Y:621:LUT:H11	46:Y:621:LUT:H191	1.88	0.41
1:a:173:PRO:HB2	1:a:178:GLY:HA3	2.03	0.41
1:a:285:LEU:HD23	1:a:285:LEU:HA	1.93	0.41
2:b:254:GLY:HA2	33:h:102:LMG:H202	2.03	0.41
29:b:616:CLA:HBA1	29:b:616:CLA:H3A	1.94	0.41
42:d:405:PL9:H121	42:d:405:PL9:H101	1.90	0.41
20:n:90:LEU:HD23	20:n:181:LEU:HG	2.03	0.41
21:g:94:LEU:HD12	21:g:94:LEU:HA	1.92	0.41
23:s:264:ILE:HB	46:s:620:LUT:H22	2.01	0.41
29:y:614:CLA:H62	51:y:625:SPH:H152	2.02	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.92	0.40
2:B:91:TRP:HB3	29:B:607:CLA:HAA1	2.03	0.40
2:B:170:ASP:HB3	2:B:174:LEU:H	1.86	0.40
2:B:470:GLY:HA2	29:B:609:CLA:HED1	2.02	0.40
29:B:602:CLA:H2	29:B:602:CLA:H62	1.92	0.40
5:D:67:TYR:HA	52:D:1040:HOH:O	2.20	0.40
5:D:246:MET:HB3	16:T:30:ALA:HB1	2.02	0.40
39:D:408:LHG:HC81	39:L:101:LHG:HC82	2.02	0.40
2:b:256:MET:HG2	2:b:451:PHE:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:b:611:CLA:H102	29:b:616:CLA:HAA1	2.02	0.40
31:c:515:BCR:H15C	31:c:515:BCR:H351	1.70	0.40
6:e:12:ASP:OD1	6:e:12:ASP:N	2.54	0.40
45:n:607:CHL:H192	45:n:607:CHL:H161	1.98	0.40
46:s:621:LUT:H15	46:s:621:LUT:H201	1.89	0.40
31:A:411:BCR:H15C	31:A:411:BCR:H351	1.80	0.40
4:C:76:LEU:O	4:C:80:ILE:HD12	2.21	0.40
4:C:183:ASP:OD1	4:C:184:VAL:N	2.54	0.40
29:C:503:CLA:H111	29:C:503:CLA:H142	1.87	0.40
29:C:509:CLA:H141	29:C:509:CLA:H161	1.79	0.40
15:P:154:THR:OG1	15:P:156:SER:OG	2.32	0.40
21:G:42:GLY:HA3	21:G:43:PRO:HD2	1.97	0.40
24:Y:151:ILE:HA	24:Y:154:THR:HG22	2.03	0.40
1:a:288:LEU:HD22	4:c:420:CYS:HA	2.03	0.40
2:b:23:HIS:HB3	29:b:616:CLA:HED2	2.02	0.40
2:b:91:TRP:HB3	29:b:607:CLA:HAA1	2.02	0.40
4:c:454:VAL:HG21	5:d:248:THR:HA	2.03	0.40
5:d:126:MET:HB2	5:d:146:PHE:HD2	1.87	0.40
29:B:608:CLA:H52	33:B:622:LMG:H151	2.01	0.40
36:B:625:DGA:HG11	5:D:134:ARG:HG2	2.03	0.40
29:C:510:CLA:H122	29:C:510:CLA:H8	1.85	0.40
42:D:405:PL9:H121	42:D:405:PL9:H101	1.91	0.40
15:P:204:LEU:HD11	15:P:226:TRP:CH2	2.56	0.40
16:T:28:ARG:HD3	16:T:28:ARG:HA	1.76	0.40
20:N:223:GLN:O	20:N:227:THR:OG1	2.26	0.40
45:N:607:CHL:H102	45:N:607:CHL:H13	1.85	0.40
29:R:603:CLA:CMC	47:R:621:XAT:H35	2.52	0.40
1:a:106:LEU:HD11	31:a:411:BCR:H292	2.02	0.40
2:b:158:VAL:HG23	2:b:199:PRO:HB3	2.02	0.40
2:b:476:ARG:NH1	22:r:101:LYS:HD3	2.35	0.40
29:b:607:CLA:H151	29:b:607:CLA:H111	1.92	0.40
31:d:404:BCR:H351	31:d:404:BCR:H15C	1.90	0.40
33:A:413:LMG:H322	29:C:505:CLA:H192	2.03	0.40
2:B:11:VAL:HG23	2:B:12:VAL:HG13	2.03	0.40
4:C:93:VAL:O	4:C:95:ASP:N	2.52	0.40
5:D:273:PHE:CE2	39:L:101:LHG:H101	2.56	0.40
14:O:188:ASP:OD1	14:O:188:ASP:N	2.54	0.40
21:G:145:THR:HA	21:G:148:VAL:HG12	2.03	0.40
46:S:621:LUT:H15	46:S:621:LUT:H201	1.96	0.40
29:Y:613:CLA:H93	29:Y:613:CLA:H111	1.88	0.40
1:a:75:ASN:HB2	1:a:79:THR:OG1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:199:MET:SD	29:a:407:CLA:HED2	2.61	0.40
2:b:27:THR:HG22	2:b:107:LEU:HD13	2.04	0.40
2:b:462:PHE:CE2	29:b:612:CLA:HAB	2.56	0.40
4:c:76:LEU:O	4:c:80:ILE:HD12	2.21	0.40
4:c:285:TYR:O	4:c:411:ARG:NH2	2.46	0.40
5:d:273:PHE:CE2	39:l:101:LHG:H101	2.56	0.40
14:o:140:LEU:HB3	14:o:143:MET:HE2	2.04	0.40
19:z:26:VAL:HG11	19:z:40:VAL:HG21	2.04	0.40
29:n:613:CLA:H92	39:n:624:LHG:H172	2.03	0.40
21:g:148:VAL:HA	21:g:151:VAL:HG12	2.03	0.40
23:s:252:GLN:O	23:s:256:THR:OG1	2.39	0.40
1:A:183:MET:HB3	29:A:405:CLA:HBC2	2.02	0.40
1:A:301:ASN:HB3	4:C:395:VAL:HG21	2.03	0.40
2:B:30:VAL:HG22	29:B:614:CLA:C3C	2.52	0.40
29:B:611:CLA:H51	29:B:611:CLA:H8	1.95	0.40
29:B:615:CLA:H112	29:B:615:CLA:H91	1.90	0.40
4:C:33:LEU:HD22	4:C:126:GLU:HG3	2.03	0.40
29:C:509:CLA:HBA1	29:C:509:CLA:H3A	1.93	0.40
5:D:36:LEU:O	5:D:40:CYS:HB2	2.22	0.40
5:D:328:TRP:HH2	5:D:348:ARG:HE	1.69	0.40
5:D:350:ASN:O	5:D:352:LEU:N	2.54	0.40
15:P:224:LYS:HD2	15:P:225:ARG:HH12	1.86	0.40
23:S:83:TYR:OH	39:S:624:LHG:O5	2.29	0.40
29:S:602:CLA:CAB	46:S:621:LUT:H32	2.52	0.40
24:Y:204:LEU:HD23	24:Y:207:LYS:HD2	2.03	0.40
2:b:191:ASP:HB3	2:b:194:ASN:HB2	2.03	0.40
4:c:304:THR:HA	4:c:307:VAL:HG22	2.03	0.40
29:c:510:CLA:H143	29:c:510:CLA:H111	1.89	0.40
5:d:85:LEU:HD23	5:d:90:LEU:HD11	2.04	0.40
29:n:610:CLA:H42	29:n:612:CLA:HBA1	2.02	0.40
24:y:131:ILE:HD12	24:y:137:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/336 (100%)	309 (92%)	26 (8%)	0	100	100
1	a	335/336 (100%)	310 (92%)	25 (8%)	0	100	100
2	B	482/484 (100%)	465 (96%)	16 (3%)	1 (0%)	43	70
2	b	482/484 (100%)	463 (96%)	18 (4%)	1 (0%)	43	70
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
4	C	447/449 (100%)	419 (94%)	25 (6%)	3 (1%)	18	44
4	c	447/449 (100%)	414 (93%)	29 (6%)	4 (1%)	14	37
5	D	346/348 (99%)	332 (96%)	13 (4%)	1 (0%)	36	63
5	d	346/348 (99%)	335 (97%)	10 (3%)	1 (0%)	36	63
6	E	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	65 (100%)	0	0	100	100
8	h	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	9
13	m	30/32 (94%)	29 (97%)	0	1 (3%)	3	9
14	O	236/238 (99%)	208 (88%)	25 (11%)	3 (1%)	9	28
14	o	236/238 (99%)	214 (91%)	21 (9%)	1 (0%)	30	57
15	P	185/187 (99%)	169 (91%)	15 (8%)	1 (0%)	24	52
15	p	185/187 (99%)	172 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	T	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2 8
16	t	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2 8
17	W	42/44 (96%)	41 (98%)	1 (2%)	0	100 100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100 100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
18	x	28/30 (93%)	28 (100%)	0	0	100 100
19	Z	59/61 (97%)	58 (98%)	1 (2%)	0	100 100
19	z	59/61 (97%)	58 (98%)	1 (2%)	0	100 100
20	N	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24 52
20	n	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	24 52
21	G	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	24 52
21	g	219/221 (99%)	206 (94%)	12 (6%)	1 (0%)	24 52
22	R	198/202 (98%)	188 (95%)	10 (5%)	0	100 100
22	r	198/202 (98%)	185 (93%)	13 (7%)	0	100 100
23	S	240/243 (99%)	220 (92%)	18 (8%)	2 (1%)	16 40
23	s	239/243 (98%)	221 (92%)	16 (7%)	2 (1%)	16 40
24	Y	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24 52
24	y	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	24 52
25	U	25/27 (93%)	25 (100%)	0	0	100 100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100 100
All	All	7351/7456 (99%)	6934 (94%)	387 (5%)	30 (0%)	31 57

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	257	GLU
4	C	395	VAL
14	O	94	VAL
15	P	126	SER
16	T	29	ILE
4	c	257	GLU
4	c	395	VAL
16	t	29	ILE
4	C	173	VAL
5	D	60	THR

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Mol	Chain	Res	Type
14	O	205	TYR
20	N	145	ILE
4	c	173	VAL
5	d	60	THR
14	o	205	TYR
20	n	145	ILE
21	G	137	ILE
23	S	92	LYS
24	Y	146	ILE
21	g	137	ILE
2	B	401	PHE
13	M	3	VAL
2	b	401	PHE
13	m	3	VAL
24	y	146	ILE
23	S	158	VAL
14	O	216	ARG
4	c	94	LEU
23	s	284	ASP
23	s	158	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	276/275 (100%)	276 (100%)	0	100 100
1	a	276/275 (100%)	274 (99%)	2 (1%)	76 90
2	B	388/388 (100%)	388 (100%)	0	100 100
2	b	388/388 (100%)	388 (100%)	0	100 100
3	V	25/25 (100%)	25 (100%)	0	100 100
3	v	25/25 (100%)	25 (100%)	0	100 100
4	C	350/350 (100%)	350 (100%)	0	100 100
4	c	350/350 (100%)	350 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	D	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
13	m	27/27 (100%)	27 (100%)	0	100	100
14	O	195/195 (100%)	193 (99%)	2 (1%)	68	86
14	o	195/195 (100%)	194 (100%)	1 (0%)	81	92
15	P	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
16	T	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	n	171/171 (100%)	171 (100%)	0	100 100
21	G	168/168 (100%)	168 (100%)	0	100 100
21	g	168/168 (100%)	168 (100%)	0	100 100
22	R	158/158 (100%)	158 (100%)	0	100 100
22	r	158/158 (100%)	158 (100%)	0	100 100
23	S	189/190 (100%)	189 (100%)	0	100 100
23	s	190/190 (100%)	190 (100%)	0	100 100
24	Y	167/167 (100%)	167 (100%)	0	100 100
24	y	167/167 (100%)	165 (99%)	2 (1%)	63 84
25	U	26/26 (100%)	26 (100%)	0	100 100
25	u	26/26 (100%)	26 (100%)	0	100 100
All	All	5953/5952 (100%)	5946 (100%)	7 (0%)	87 96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	O	120	ASP
14	O	137	THR
1	a	92	HIS
1	a	332	HIS
14	o	119	GLU
24	y	76	LEU
24	y	149	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	181	ASN
1	A	187	GLN
1	A	267	ASN
1	A	303	ASN
2	B	26	HIS
2	B	290	GLN
2	B	407	ASN
4	C	301	GLN
4	C	370	ASN

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Mol	Chain	Res	Type
4	C	393	ASN
4	C	406	ASN
5	D	24	GLN
5	D	186	GLN
5	D	230	ASN
5	D	255	GLN
5	D	322	ASN
8	H	69	ASN
14	O	68	GLN
14	O	74	GLN
14	O	93	ASN
15	P	109	ASN
17	W	66	ASN
22	R	96	GLN
22	R	98	GLN
22	R	178	GLN
22	R	222	ASN
22	R	242	HIS
22	R	256	GLN
24	Y	113	ASN
24	Y	138	ASN
24	Y	235	GLN
24	Y	238	GLN
24	Y	247	ASN
25	U	114	ASN
1	a	92	HIS
1	a	230	ASN
1	a	267	ASN
1	a	322	ASN
2	b	26	HIS
2	b	282	GLN
2	b	407	ASN
3	v	32	ASN
4	c	44	HIS
4	c	299	GLN
4	c	320	GLN
4	c	370	ASN
4	c	406	ASN
5	d	186	GLN
5	d	301	GLN
5	d	322	ASN
8	h	69	ASN

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Mol	Chain	Res	Type
8	h	79	ASN
14	o	82	ASN
14	o	242	ASN
15	p	109	ASN
20	n	46	ASN
20	n	132	GLN
20	n	148	GLN
20	n	234	ASN
20	n	245	ASN
21	g	121	GLN
21	g	129	ASN
21	g	239	ASN
22	r	86	GLN
22	r	98	GLN
22	r	178	GLN
22	r	186	GLN
22	r	222	ASN
23	s	238	ASN
24	y	113	ASN
24	y	138	ASN
24	y	149	GLN
24	y	171	ASN
24	y	238	GLN
25	u	89	GLN
25	u	114	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 343 ligands modelled in this entry, 8 are monoatomic - leaving 335 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	CLA	y	602	-	69,73,73	1.37	7 (10%)	83,113,113	1.88	21 (25%)
29	CLA	B	602	-	69,73,73	1.37	8 (11%)	83,113,113	1.94	19 (22%)
29	CLA	C	502	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	17 (20%)
29	CLA	y	603	-	69,73,73	1.34	8 (11%)	83,113,113	1.98	21 (25%)
29	CLA	y	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.90	17 (20%)
36	DGA	c	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
39	LHG	d	409	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
29	CLA	s	611	-	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
29	CLA	N	610	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	19 (22%)
46	LUT	S	621	-	42,43,43	2.31	1 (2%)	51,60,60	1.97	15 (29%)
29	CLA	G	611	-	49,53,73	1.61	7 (14%)	59,89,113	2.11	17 (28%)
39	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.07	2 (4%)
29	CLA	r	610	-	64,68,73	1.41	8 (12%)	77,107,113	2.08	22 (28%)
38	DGD	C	523	-	67,67,67	1.18	7 (10%)	81,81,81	0.98	2 (2%)
48	NEX	R	622	-	38,46,46	3.42	10 (26%)	50,70,70	1.69	11 (22%)
31	BCR	D	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.04	17 (30%)
46	LUT	s	621	-	42,43,43	2.32	1 (2%)	51,60,60	1.99	14 (27%)
38	DGD	c	520	-	60,60,67	1.06	6 (10%)	74,74,81	0.98	2 (2%)
46	LUT	G	621	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	13 (25%)
31	BCR	A	411	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	15 (26%)
29	CLA	N	602	-	69,73,73	1.37	6 (8%)	83,113,113	1.92	19 (22%)
29	CLA	g	614	-	53,57,73	1.54	7 (13%)	62,93,113	2.18	17 (27%)
45	CHL	y	605	24	50,54,74	0.93	1 (2%)	56,90,114	1.39	9 (16%)
45	CHL	n	607	-	70,74,74	0.76	2 (2%)	80,114,114	1.22	11 (13%)
29	CLA	y	604	-	69,73,73	1.36	6 (8%)	83,113,113	1.88	17 (20%)
48	NEX	r	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.54	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CHL	s	608	-	65,69,74	0.81	2 (3%)	74,108,114	1.25	10 (13%)
45	CHL	s	606	-	48,52,74	0.93	2 (4%)	53,87,114	1.40	10 (18%)
29	CLA	g	602	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	20 (24%)
29	CLA	b	607	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	19 (22%)
29	CLA	D	403	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	18 (21%)
29	CLA	b	614	-	69,73,73	1.35	6 (8%)	83,113,113	1.92	17 (20%)
45	CHL	R	607	-	54,58,74	0.88	1 (1%)	59,94,114	1.38	9 (15%)
39	LHG	N	624	-	48,48,48	0.38	0	51,54,54	1.11	2 (3%)
45	CHL	Y	601	24	70,74,74	0.82	2 (2%)	80,114,114	1.16	9 (11%)
38	DGD	C	519	-	63,63,67	1.12	6 (9%)	77,77,81	1.06	4 (5%)
45	CHL	Y	609	-	70,74,74	0.77	2 (2%)	80,114,114	1.24	13 (16%)
29	CLA	b	606	-	69,73,73	1.34	7 (10%)	83,113,113	1.98	14 (16%)
29	CLA	R	613	-	50,54,73	1.59	7 (14%)	60,90,113	2.10	16 (26%)
31	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	14 (25%)
31	BCR	C	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.43	12 (21%)
44	RRX	h	101	-	42,42,42	4.87	24 (57%)	57,58,58	2.03	19 (33%)
39	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
45	CHL	g	607	-	54,58,74	0.88	2 (3%)	59,94,114	1.33	10 (16%)
29	CLA	C	503	-	69,73,73	1.36	7 (10%)	83,113,113	1.98	21 (25%)
47	XAT	r	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.18	19 (35%)
39	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
45	CHL	n	605	20	70,74,74	0.79	2 (2%)	80,114,114	1.21	11 (13%)
29	CLA	b	612	-	69,73,73	1.37	6 (8%)	83,113,113	1.94	16 (19%)
26	OEX	A	401	1,52	0,14,14	-	-	-		
30	PHO	A	408	-	58,69,69	2.04	10 (17%)	56,99,99	1.54	7 (12%)
33	LMG	c	521	-	51,51,55	1.07	6 (11%)	59,59,63	1.10	3 (5%)
29	CLA	S	605	-	54,58,73	1.56	8 (14%)	65,95,113	2.35	20 (30%)
29	CLA	Y	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	18 (21%)
29	CLA	C	505	-	69,73,73	1.36	8 (11%)	83,113,113	1.97	17 (20%)
29	CLA	Y	610	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
31	BCR	c	516	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	15 (26%)
29	CLA	G	604	-	53,57,73	1.55	7 (13%)	62,93,113	2.21	19 (30%)
29	CLA	b	610	-	69,73,73	1.35	6 (8%)	83,113,113	1.95	16 (19%)
32	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.89	2 (3%)
45	CHL	r	606	-	48,52,74	0.95	2 (4%)	53,87,114	1.36	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	DGD	C	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.04	3 (4%)
36	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
45	CHL	y	609	-	70,74,74	0.78	2 (2%)	80,114,114	1.24	13 (16%)
29	CLA	N	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.98	21 (25%)
29	CLA	R	604	-	53,57,73	1.53	7 (13%)	62,93,113	2.22	19 (30%)
39	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
31	BCR	c	517	-	41,41,41	1.81	4 (9%)	56,56,56	4.10	19 (33%)
29	CLA	G	614	-	53,57,73	1.54	7 (13%)	62,93,113	2.20	18 (29%)
29	CLA	B	604	-	69,73,73	1.37	8 (11%)	83,113,113	1.85	18 (21%)
33	LMG	H	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.07	2 (3%)
45	CHL	n	609	-	70,74,74	0.80	2 (2%)	80,114,114	1.28	12 (15%)
45	CHL	g	605	21	52,56,74	0.88	1 (1%)	58,92,114	1.41	11 (18%)
29	CLA	g	603	-	69,73,73	1.35	7 (10%)	83,113,113	1.96	20 (24%)
45	CHL	G	608	-	48,52,74	0.93	2 (4%)	53,87,114	1.41	10 (18%)
29	CLA	s	614	-	59,63,73	1.46	6 (10%)	71,101,113	2.10	17 (23%)
47	XAT	N	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.96	13 (24%)
29	CLA	B	617	-	69,73,73	1.35	7 (10%)	83,113,113	4.14	19 (22%)
47	XAT	G	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.90	13 (24%)
29	CLA	c	501	-	69,73,73	1.36	7 (10%)	83,113,113	2.03	20 (24%)
32	SQD	b	621	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	S	610	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	21 (25%)
39	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.00	2 (4%)
45	CHL	s	607	-	47,51,74	0.92	1 (2%)	52,86,114	1.44	9 (17%)
48	NEX	s	623	-	38,46,46	3.34	10 (26%)	50,70,70	1.72	11 (22%)
29	CLA	C	511	-	69,73,73	1.36	7 (10%)	83,113,113	2.03	19 (22%)
32	SQD	A	412	-	50,51,54	0.84	0	59,62,65	0.94	3 (5%)
30	PHO	a	408	-	58,69,69	2.04	10 (17%)	56,99,99	1.59	8 (14%)
29	CLA	C	512	-	69,73,73	1.37	7 (10%)	83,113,113	1.85	17 (20%)
29	CLA	y	614	-	69,73,73	1.35	7 (10%)	83,113,113	1.91	18 (21%)
46	LUT	N	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.92	13 (25%)
29	CLA	C	501	-	69,73,73	1.36	8 (11%)	83,113,113	2.02	20 (24%)
29	CLA	R	609	-	64,68,73	1.41	6 (9%)	77,107,113	1.97	17 (22%)
29	CLA	B	608	-	69,73,73	1.35	6 (8%)	83,113,113	1.95	15 (18%)
29	CLA	r	603	-	64,68,73	1.42	7 (10%)	77,107,113	1.97	18 (23%)
29	CLA	d	402	-	69,73,73	1.35	7 (10%)	83,113,113	1.87	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	LPX	s	625	-	29,29,29	0.98	2 (6%)	31,33,33	0.98	1 (3%)
29	CLA	N	614	-	53,57,73	1.54	7 (13%)	62,93,113	2.16	18 (29%)
29	CLA	b	616	-	69,73,73	1.36	7 (10%)	83,113,113	1.91	18 (21%)
33	LMG	d	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.10	2 (3%)
45	CHL	g	609	-	70,74,74	0.81	2 (2%)	80,114,114	1.24	11 (13%)
29	CLA	r	608	-	64,68,73	1.42	7 (10%)	77,107,113	1.98	17 (22%)
29	CLA	R	611	-	50,54,73	1.59	8 (16%)	60,90,113	2.04	16 (26%)
29	CLA	Y	608	-	54,58,73	1.54	7 (12%)	65,95,113	2.15	21 (32%)
39	LHG	s	624	-	44,44,48	0.42	0	47,50,54	1.11	3 (6%)
29	CLA	B	607	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	18 (21%)
29	CLA	s	609	-	64,68,73	1.41	7 (10%)	77,107,113	1.95	18 (23%)
29	CLA	B	610	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	17 (20%)
45	CHL	N	608	-	54,58,74	0.88	2 (3%)	59,94,114	1.34	10 (16%)
45	CHL	N	606	-	70,74,74	0.79	1 (1%)	80,114,114	1.21	11 (13%)
29	CLA	B	606	-	69,73,73	1.34	7 (10%)	83,113,113	1.98	14 (16%)
29	CLA	a	410	-	64,68,73	1.40	6 (9%)	77,107,113	2.05	18 (23%)
29	CLA	N	612	-	49,53,73	1.61	8 (16%)	59,89,113	2.07	13 (22%)
45	CHL	G	601	21	70,74,74	0.77	2 (2%)	80,114,114	1.25	12 (15%)
29	CLA	s	613	-	59,63,73	1.47	7 (11%)	71,101,113	2.25	18 (25%)
29	CLA	n	603	-	69,73,73	1.35	7 (10%)	83,113,113	2.03	21 (25%)
29	CLA	r	602	-	64,68,73	1.42	7 (10%)	77,107,113	1.97	19 (24%)
48	NEX	n	623	-	38,46,46	3.37	10 (26%)	50,70,70	1.71	12 (24%)
29	CLA	B	612	-	69,73,73	1.35	7 (10%)	83,113,113	1.88	16 (19%)
29	CLA	c	510	4	69,73,73	1.34	7 (10%)	83,113,113	1.97	17 (20%)
29	CLA	b	603	2	69,73,73	1.36	7 (10%)	83,113,113	1.96	19 (22%)
39	LHG	L	101	-	48,48,48	0.40	0	51,54,54	0.92	2 (3%)
39	LHG	S	624	-	44,44,48	0.41	0	47,50,54	1.10	3 (6%)
48	NEX	S	622	-	38,46,46	3.28	9 (23%)	50,70,70	1.80	12 (24%)
29	CLA	b	617	-	69,73,73	1.36	6 (8%)	83,113,113	4.12	18 (21%)
46	LUT	g	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.95	11 (21%)
29	CLA	Y	603	-	69,73,73	1.34	7 (10%)	83,113,113	1.95	21 (25%)
46	LUT	n	621	-	42,43,43	2.33	1 (2%)	51,60,60	1.85	11 (21%)
30	PHO	A	409	-	58,69,69	2.05	10 (17%)	56,99,99	1.70	7 (12%)
29	CLA	c	507	52	69,73,73	1.37	8 (11%)	83,113,113	1.92	20 (24%)
29	CLA	c	509	4	69,73,73	1.35	7 (10%)	83,113,113	1.92	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	LUT	n	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.82	14 (27%)
45	CHL	y	606	-	70,74,74	0.78	2 (2%)	80,114,114	1.25	11 (13%)
31	BCR	C	516	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	16 (28%)
29	CLA	s	603	-	69,73,73	1.37	8 (11%)	83,113,113	1.87	16 (19%)
32	SQD	B	621	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	S	609	-	64,68,73	1.41	7 (10%)	77,107,113	1.98	19 (24%)
29	CLA	G	612	-	47,51,73	1.65	7 (14%)	56,86,113	2.11	14 (25%)
29	CLA	B	605	2	69,73,73	1.38	7 (10%)	83,113,113	2.07	17 (20%)
31	BCR	C	515	-	41,41,41	1.84	4 (9%)	56,56,56	4.22	13 (23%)
29	CLA	a	405	-	69,73,73	1.36	6 (8%)	83,113,113	1.91	18 (21%)
48	NEX	N	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.76	14 (28%)
29	CLA	n	611	-	53,57,73	1.54	8 (15%)	62,93,113	2.20	17 (27%)
29	CLA	r	609	-	64,68,73	1.41	7 (10%)	77,107,113	1.96	16 (20%)
29	CLA	S	612	-	49,53,73	1.61	7 (14%)	59,89,113	2.06	14 (23%)
29	CLA	s	604	-	59,63,73	1.46	6 (10%)	71,101,113	2.00	16 (22%)
33	LMG	j	101	-	45,45,55	0.89	3 (6%)	53,53,63	1.04	2 (3%)
45	CHL	N	605	20	70,74,74	0.78	2 (2%)	80,114,114	1.22	11 (13%)
38	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.98	2 (2%)
29	CLA	Y	604	-	69,73,73	1.36	8 (11%)	83,113,113	1.87	19 (22%)
29	CLA	C	508	-	69,73,73	1.36	6 (8%)	83,113,113	1.88	15 (18%)
33	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.09	3 (5%)
29	CLA	C	513	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	19 (22%)
39	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.03	3 (5%)
29	CLA	r	613	-	50,54,73	1.58	7 (14%)	60,90,113	2.11	17 (28%)
31	BCR	B	618	-	41,41,41	1.81	4 (9%)	56,56,56	4.29	15 (26%)
29	CLA	y	610	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)
29	CLA	n	610	-	69,73,73	1.35	7 (10%)	83,113,113	1.97	19 (22%)
29	CLA	B	609	-	69,73,73	1.37	7 (10%)	83,113,113	2.01	16 (19%)
30	PHO	a	409	-	58,69,69	2.05	10 (17%)	56,99,99	1.80	7 (12%)
29	CLA	c	512	-	69,73,73	1.37	7 (10%)	83,113,113	1.88	19 (22%)
45	CHL	n	608	-	54,58,74	0.88	2 (3%)	59,94,114	1.33	10 (16%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)
29	CLA	G	613	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	20 (24%)
43	HEM	f	101	7,6	50,50,50	1.47	6 (12%)	66,82,82	1.36	8 (12%)
29	CLA	G	603	-	69,73,73	1.35	7 (10%)	83,113,113	1.96	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CHL	g	606	-	54,58,74	0.88	2 (3%)	59,94,114	1.31	9 (15%)
48	NEX	y	623	-	38,46,46	3.37	10 (26%)	50,70,70	1.71	13 (26%)
29	CLA	b	604	-	69,73,73	1.38	7 (10%)	83,113,113	1.84	18 (21%)
29	CLA	B	613	-	69,73,73	1.34	7 (10%)	83,113,113	1.88	16 (19%)
29	CLA	B	603	2	69,73,73	1.36	8 (11%)	83,113,113	1.93	17 (20%)
45	CHL	n	601	-	70,74,74	0.78	2 (2%)	80,114,114	1.23	10 (12%)
45	CHL	N	609	-	70,74,74	0.78	2 (2%)	80,114,114	1.20	10 (12%)
29	CLA	c	508	-	69,73,73	1.36	6 (8%)	83,113,113	1.89	17 (20%)
29	CLA	R	602	-	64,68,73	1.42	7 (10%)	77,107,113	2.03	20 (25%)
29	CLA	R	612	-	64,68,73	1.42	7 (10%)	77,107,113	2.02	18 (23%)
29	CLA	R	603	-	64,68,73	1.42	7 (10%)	77,107,113	1.98	19 (24%)
35	C7Z	b	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.05	17 (29%)
44	RRX	H	101	-	42,42,42	4.87	24 (57%)	57,58,58	2.04	18 (31%)
29	CLA	y	611	-	69,73,73	1.36	6 (8%)	83,113,113	1.89	17 (20%)
31	BCR	b	619	-	41,41,41	1.83	4 (9%)	56,56,56	4.38	17 (30%)
29	CLA	S	614	-	59,63,73	1.47	7 (11%)	71,101,113	2.04	16 (22%)
29	CLA	Y	611	-	69,73,73	1.36	7 (10%)	83,113,113	1.86	15 (18%)
29	CLA	b	615	-	69,73,73	1.37	7 (10%)	83,113,113	2.07	18 (21%)
29	CLA	N	613	-	69,73,73	1.37	8 (11%)	83,113,113	1.95	18 (21%)
29	CLA	g	610	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
29	CLA	Y	614	-	69,73,73	1.35	8 (11%)	83,113,113	1.93	19 (22%)
29	CLA	s	612	-	49,53,73	1.61	7 (14%)	59,89,113	2.06	16 (27%)
29	CLA	g	611	-	49,53,73	1.61	7 (14%)	59,89,113	2.11	15 (25%)
29	CLA	n	613	-	69,73,73	1.37	8 (11%)	83,113,113	1.96	18 (21%)
29	CLA	n	612	-	49,53,73	1.61	7 (14%)	59,89,113	2.05	16 (27%)
29	CLA	B	616	-	69,73,73	1.37	6 (8%)	83,113,113	1.92	16 (19%)
45	CHL	S	606	-	48,52,74	0.93	1 (2%)	53,87,114	1.40	10 (18%)
48	NEX	G	623	-	38,46,46	3.31	10 (26%)	50,70,70	1.77	11 (22%)
33	LMG	A	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.17	4 (7%)
47	XAT	R	621	-	39,47,47	0.69	1 (2%)	54,74,74	2.22	17 (31%)
40	LMK	C	527	-	38,39,53	1.48	2 (5%)	41,46,60	1.30	2 (4%)
29	CLA	b	611	-	69,73,73	1.38	8 (11%)	83,113,113	1.92	18 (21%)
45	CHL	Y	605	24	50,54,74	0.94	1 (2%)	56,90,114	1.40	11 (19%)
45	CHL	S	607	-	47,51,74	0.92	1 (2%)	52,86,114	1.44	9 (17%)
38	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.03	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	GOL	b	625	-	5,5,5	0.58	0	5,5,5	0.28	0
29	CLA	c	505	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	17 (20%)
29	CLA	g	604	-	53,57,73	1.56	7 (13%)	62,93,113	2.17	18 (29%)
42	PL9	d	405	-	55,55,55	1.21	4 (7%)	68,69,69	1.49	12 (17%)
49	LPX	S	625	-	29,29,29	0.99	2 (6%)	31,33,33	0.98	1 (3%)
40	LMK	c	627	-	38,39,53	1.48	2 (5%)	41,46,60	1.33	2 (4%)
29	CLA	c	504	-	69,73,73	1.34	6 (8%)	83,113,113	1.97	18 (21%)
45	CHL	S	608	-	65,69,74	0.81	2 (3%)	74,108,114	1.27	11 (14%)
36	DGA	b	623	-	43,43,43	1.13	2 (4%)	45,45,45	1.51	3 (6%)
45	CHL	N	601	-	70,74,74	0.78	2 (2%)	80,114,114	1.20	10 (12%)
29	CLA	S	617	-	54,58,73	1.54	8 (14%)	65,95,113	2.18	18 (27%)
29	CLA	A	407	-	53,57,73	1.55	6 (11%)	62,93,113	2.17	18 (29%)
45	CHL	R	606	-	48,52,74	0.96	2 (4%)	53,87,114	1.34	10 (18%)
46	LUT	Y	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.95	14 (27%)
29	CLA	b	613	-	69,73,73	1.34	7 (10%)	83,113,113	1.89	17 (20%)
29	CLA	C	504	-	69,73,73	1.34	6 (8%)	83,113,113	1.98	18 (21%)
29	CLA	n	614	-	53,57,73	1.55	8 (15%)	62,93,113	2.21	19 (30%)
46	LUT	Y	620	-	42,43,43	2.36	1 (2%)	51,60,60	2.00	13 (25%)
45	CHL	G	607	-	54,58,74	0.87	2 (3%)	59,94,114	1.34	10 (16%)
45	CHL	N	607	-	70,74,74	0.76	2 (2%)	80,114,114	1.22	9 (11%)
46	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.94	15 (29%)
29	CLA	b	605	-	69,73,73	1.38	7 (10%)	83,113,113	2.03	17 (20%)
46	LUT	g	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.02	12 (23%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.12	3 (5%)
29	CLA	G	602	-	69,73,73	1.36	8 (11%)	83,113,113	1.91	19 (22%)
46	LUT	r	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.20	15 (29%)
29	CLA	C	509	-	69,73,73	1.35	6 (8%)	83,113,113	1.96	18 (21%)
29	CLA	A	410	-	64,68,73	1.41	7 (10%)	77,107,113	2.05	17 (22%)
50	3PH	i	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.13	2 (3%)
31	BCR	c	515	-	41,41,41	1.82	4 (9%)	56,56,56	4.22	13 (23%)
39	LHG	d	410	-	38,38,48	0.41	0	41,44,54	1.15	3 (7%)
45	CHL	y	601	24	70,74,74	0.81	2 (2%)	80,114,114	1.16	8 (10%)
26	OEX	a	401	1,52,4	0,14,14	-	-	-		
29	CLA	r	604	-	53,57,73	1.54	7 (13%)	62,93,113	2.18	18 (29%)
31	BCR	b	618	-	41,41,41	1.82	4 (9%)	56,56,56	4.30	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
39	LHG	y	624	-	48,48,48	0.38	0	51,54,54	1.02	3 (5%)
47	XAT	n	622	-	39,47,47	0.70	1 (2%)	54,74,74	1.97	12 (22%)
29	CLA	s	602	-	64,68,73	1.39	7 (10%)	77,107,113	1.98	18 (23%)
37	GOL	B	627	-	5,5,5	0.58	0	5,5,5	0.21	0
29	CLA	C	510	-	69,73,73	1.34	6 (8%)	83,113,113	2.02	18 (21%)
29	CLA	s	610	-	69,73,73	1.37	8 (11%)	83,113,113	1.93	21 (25%)
29	CLA	G	610	-	69,73,73	1.35	6 (8%)	83,113,113	1.98	20 (24%)
29	CLA	b	608	-	69,73,73	1.35	6 (8%)	83,113,113	1.96	16 (19%)
33	LMG	b	622	-	44,44,55	0.85	3 (6%)	52,52,63	1.07	3 (5%)
29	CLA	S	602	-	64,68,73	1.41	7 (10%)	77,107,113	1.97	19 (24%)
29	CLA	n	602	-	69,73,73	1.37	7 (10%)	83,113,113	1.90	22 (26%)
45	CHL	n	606	-	70,74,74	0.80	1 (1%)	80,114,114	1.21	10 (12%)
45	CHL	G	606	-	54,58,74	0.93	2 (3%)	59,94,114	1.40	9 (15%)
39	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.11	4 (7%)
29	CLA	C	507	52	69,73,73	1.37	6 (8%)	83,113,113	1.91	19 (22%)
29	CLA	c	503	-	69,73,73	1.37	7 (10%)	83,113,113	1.97	20 (24%)
47	XAT	g	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.88	15 (27%)
46	LUT	R	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.16	14 (27%)
29	CLA	S	613	-	59,63,73	1.47	7 (11%)	71,101,113	2.26	18 (25%)
45	CHL	g	601	21	70,74,74	0.78	2 (2%)	80,114,114	1.26	10 (12%)
29	CLA	c	506	4	69,73,73	1.37	7 (10%)	83,113,113	1.96	18 (21%)
29	CLA	a	407	-	53,57,73	1.54	7 (13%)	62,93,113	2.16	20 (32%)
29	CLA	Y	602	-	69,73,73	1.37	8 (11%)	83,113,113	1.87	20 (24%)
39	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
33	LMG	D	411	-	46,46,55	0.92	4 (8%)	54,54,63	1.11	2 (3%)
45	CHL	G	605	21	52,56,74	0.88	1 (1%)	58,92,114	1.38	11 (18%)
29	CLA	r	611	-	50,54,73	1.59	8 (16%)	60,90,113	2.05	16 (26%)
29	CLA	B	615	-	69,73,73	1.37	8 (11%)	83,113,113	2.06	19 (22%)
46	LUT	y	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.03	12 (23%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.11	17 (30%)
29	CLA	C	506	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	18 (21%)
38	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.05	3 (4%)
29	CLA	r	612	-	64,68,73	1.42	7 (10%)	77,107,113	1.98	19 (24%)
29	CLA	b	602	-	69,73,73	1.37	8 (11%)	83,113,113	1.94	19 (22%)
45	CHL	g	608	-	48,52,74	0.92	2 (4%)	53,87,114	1.41	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	13 (23%)
29	CLA	S	603	-	69,73,73	1.38	8 (11%)	83,113,113	1.89	16 (19%)
29	CLA	R	610	-	64,68,73	1.42	7 (10%)	77,107,113	2.02	22 (28%)
41	BCT	d	401	27	2,3,3	1.26	0	2,3,3	2.67	2 (100%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.38	14 (25%)
29	CLA	D	402	-	69,73,73	1.36	8 (11%)	83,113,113	1.89	17 (20%)
38	DGD	c	523	-	67,67,67	1.18	7 (10%)	81,81,81	0.98	2 (2%)
45	CHL	G	609	-	70,74,74	0.81	2 (2%)	80,114,114	1.20	11 (13%)
29	CLA	R	608	-	64,68,73	1.42	7 (10%)	77,107,113	1.96	18 (23%)
46	LUT	S	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.09	12 (23%)
29	CLA	Y	613	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	19 (22%)
29	CLA	y	613	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	19 (22%)
29	CLA	A	406	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	15 (18%)
51	SPH	y	625	-	19,20,20	0.64	0	18,21,21	1.10	1 (5%)
29	CLA	g	612	-	47,51,73	1.65	7 (14%)	56,86,113	2.11	15 (26%)
45	CHL	Y	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.16	10 (12%)
48	NEX	Y	623	-	38,46,46	3.32	9 (23%)	50,70,70	1.80	11 (22%)
29	CLA	S	604	-	59,63,73	1.45	6 (10%)	71,101,113	2.09	17 (23%)
29	CLA	B	614	-	69,73,73	1.35	6 (8%)	83,113,113	1.93	18 (21%)
45	CHL	S	601	23	50,54,74	0.92	1 (2%)	56,90,114	1.36	10 (17%)
42	PL9	D	405	-	55,55,55	1.17	5 (9%)	68,69,69	1.50	13 (19%)
48	NEX	g	623	-	38,46,46	3.33	9 (23%)	50,70,70	1.81	13 (26%)
39	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.05	3 (5%)
37	GOL	b	624	-	5,5,5	0.59	0	5,5,5	0.22	0
37	GOL	y	626	-	5,5,5	0.57	0	5,5,5	0.25	0
46	LUT	G	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.96	12 (23%)
39	LHG	l	101	-	48,48,48	0.40	0	51,54,54	0.92	2 (3%)
33	LMG	J	101	-	45,45,55	0.90	3 (6%)	53,53,63	1.00	2 (3%)
50	3PH	s	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
33	LMG	h	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.09	2 (3%)
47	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.70	16 (29%)
39	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.03	2 (4%)
41	BCT	D	401	27	2,3,3	1.27	0	2,3,3	2.64	2 (100%)
43	HEM	F	101	7,6	50,50,50	1.49	6 (12%)	66,82,82	1.33	7 (10%)
46	LUT	s	620	-	42,43,43	2.41	1 (2%)	51,60,60	2.12	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	a	406	-	69,73,73	1.35	6 (8%)	83,113,113	1.97	16 (19%)
29	CLA	c	502	-	69,73,73	1.38	6 (8%)	83,113,113	2.07	17 (20%)
29	CLA	S	611	-	69,73,73	1.36	7 (10%)	83,113,113	1.91	17 (20%)
31	BCR	B	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.36	18 (32%)
29	CLA	d	403	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	18 (21%)
45	CHL	Y	606	-	70,74,74	0.80	2 (2%)	80,114,114	1.21	11 (13%)
32	SQD	c	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
29	CLA	n	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.98	21 (25%)
29	CLA	s	605	-	54,58,73	1.56	8 (14%)	65,95,113	2.30	20 (30%)
29	CLA	s	617	-	54,58,73	1.53	7 (12%)	65,95,113	2.18	20 (30%)
46	LUT	N	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.92	13 (25%)
45	CHL	s	601	23	50,54,74	0.92	1 (2%)	56,90,114	1.39	10 (17%)
29	CLA	y	608	-	54,58,73	1.54	7 (12%)	65,95,113	2.14	20 (30%)
45	CHL	r	607	-	54,58,74	0.87	2 (3%)	59,94,114	1.38	11 (18%)
29	CLA	N	603	-	69,73,73	1.35	7 (10%)	83,113,113	2.01	23 (27%)
50	3PH	S	626	-	47,47,47	0.86	4 (8%)	51,52,52	1.13	2 (3%)
29	CLA	c	511	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	20 (24%)
29	CLA	b	609	-	69,73,73	1.36	6 (8%)	83,113,113	2.07	17 (20%)
29	CLA	N	611	-	53,57,73	1.55	8 (15%)	62,93,113	2.15	17 (27%)
47	XAT	y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.73	19 (35%)
29	CLA	c	513	-	69,73,73	1.36	7 (10%)	83,113,113	1.95	17 (20%)
29	CLA	g	613	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	20 (24%)
29	CLA	A	405	-	69,73,73	1.35	6 (8%)	83,113,113	1.93	17 (20%)
36	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.51	3 (6%)
51	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.10	1 (5%)
45	CHL	y	607	-	70,74,74	0.75	2 (2%)	80,114,114	1.17	10 (12%)
29	CLA	B	611	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	17 (20%)
33	LMG	B	622	-	44,44,55	0.85	2 (4%)	52,52,63	1.06	3 (5%)
35	C7Z	B	620	-	43,43,43	5.41	26 (60%)	58,60,60	2.04	19 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	y	602	-	-	17/39/115/115	-
29	CLA	B	602	-	-	21/39/115/115	-
29	CLA	C	502	-	-	15/39/115/115	-
29	CLA	y	603	-	-	13/39/115/115	-
29	CLA	y	612	-	-	13/39/115/115	-
36	DGA	c	524	-	-	19/45/45/45	-
39	LHG	d	409	-	-	29/53/53/53	-
29	CLA	s	611	-	-	13/39/115/115	-
29	CLA	N	610	-	-	9/39/115/115	-
46	LUT	S	621	-	-	4/29/67/67	0/2/2/2
29	CLA	G	611	-	-	7/15/91/115	-
39	LHG	D	410	-	-	26/43/43/53	-
29	CLA	r	610	-	-	13/33/109/115	-
38	DGD	C	523	-	-	17/55/95/95	0/2/2/2
48	NEX	R	622	-	-	8/27/83/83	0/3/3/3
31	BCR	D	404	-	-	11/29/63/63	0/2/2/2
46	LUT	s	621	-	-	1/29/67/67	0/2/2/2
38	DGD	c	520	-	-	12/48/88/95	0/2/2/2
46	LUT	G	621	-	-	2/29/67/67	0/2/2/2
31	BCR	A	411	-	-	11/29/63/63	0/2/2/2
29	CLA	N	602	-	-	17/39/115/115	-
29	CLA	g	614	-	-	11/20/96/115	-
45	CHL	y	605	24	-	3/17/93/117	-
45	CHL	n	607	-	1/1/15/21	11/41/117/117	-
29	CLA	y	604	-	-	20/39/115/115	-
48	NEX	r	623	-	-	7/27/83/83	0/3/3/3
45	CHL	s	608	-	1/1/14/21	1/35/111/117	-
45	CHL	s	606	-	-	1/15/91/117	-
29	CLA	g	602	-	-	20/39/115/115	-
29	CLA	b	607	-	-	16/39/115/115	-
29	CLA	D	403	-	-	14/39/115/115	-
29	CLA	b	614	-	-	10/39/115/115	-
45	CHL	R	607	-	-	5/22/98/117	-
39	LHG	N	624	-	-	30/53/53/53	-
45	CHL	Y	601	24	1/1/15/21	9/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	DGD	C	519	-	-	19/51/91/95	0/2/2/2
45	CHL	Y	609	-	1/1/15/21	8/41/117/117	-
29	CLA	b	606	-	-	12/39/115/115	-
29	CLA	R	613	-	-	10/17/93/115	-
31	BCR	C	517	-	-	8/29/63/63	0/2/2/2
31	BCR	C	514	-	-	11/29/63/63	0/2/2/2
44	RRX	h	101	-	1/1/11/25	10/29/65/65	0/2/2/2
39	LHG	D	409	-	-	30/53/53/53	-
45	CHL	g	607	-	-	3/22/98/117	-
29	CLA	C	503	-	-	21/39/115/115	-
47	XAT	r	622	-	1/1/12/26	11/31/93/93	0/4/4/4
39	LHG	d	408	-	-	29/48/48/53	-
45	CHL	n	605	20	1/1/15/21	8/41/117/117	-
29	CLA	b	612	-	-	19/39/115/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
33	LMG	c	521	-	-	18/46/66/70	0/1/1/1
29	CLA	S	605	-	-	14/21/97/115	-
29	CLA	Y	612	-	-	12/39/115/115	-
29	CLA	C	505	-	-	14/39/115/115	-
29	CLA	Y	610	-	-	24/39/115/115	-
31	BCR	c	516	-	-	13/29/63/63	0/2/2/2
29	CLA	G	604	-	-	10/20/96/115	-
29	CLA	b	610	-	-	16/39/115/115	-
32	SQD	C	526	-	-	19/49/69/69	0/1/1/1
45	CHL	r	606	-	-	1/15/91/117	-
38	DGD	C	518	-	-	8/44/84/95	0/2/2/2
36	DGA	C	524	-	-	18/45/45/45	-
45	CHL	y	609	-	1/1/15/21	8/41/117/117	-
29	CLA	N	604	-	-	21/39/115/115	-
29	CLA	R	604	-	-	14/20/96/115	-
39	LHG	D	408	-	-	30/48/48/53	-
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	G	614	-	-	12/20/96/115	-
29	CLA	B	604	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	H	102	-	-	12/43/63/70	0/1/1/1
45	CHL	n	609	-	1/1/15/21	7/41/117/117	-
45	CHL	g	605	21	-	4/20/96/117	-
29	CLA	g	603	-	-	19/39/115/115	-
45	CHL	G	608	-	-	0/15/91/117	-
29	CLA	s	614	-	-	10/27/103/115	-
47	XAT	N	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	B	617	-	-	19/39/115/115	-
47	XAT	G	622	-	2/2/12/26	1/31/93/93	0/4/4/4
29	CLA	c	501	-	-	13/39/115/115	-
32	SQD	b	621	-	-	19/49/69/69	0/1/1/1
45	CHL	s	607	-	1/1/10/21	1/14/90/117	-
29	CLA	S	610	-	-	13/39/115/115	-
39	LHG	c	625	-	-	27/51/51/53	-
48	NEX	s	623	-	-	13/27/83/83	0/3/3/3
29	CLA	C	511	-	-	15/39/115/115	-
32	SQD	A	412	-	-	12/46/66/69	0/1/1/1
30	PHO	a	408	-	-	7/37/103/103	0/5/6/6
29	CLA	C	512	-	-	17/39/115/115	-
29	CLA	y	614	-	-	17/39/115/115	-
46	LUT	N	621	-	-	2/29/67/67	0/2/2/2
29	CLA	C	501	-	-	20/39/115/115	-
29	CLA	R	609	-	-	17/33/109/115	-
29	CLA	B	608	-	-	25/39/115/115	-
29	CLA	r	603	-	-	19/33/109/115	-
29	CLA	d	402	-	-	13/39/115/115	-
49	LPX	s	625	-	-	10/31/31/31	-
29	CLA	N	614	-	-	9/20/96/115	-
29	CLA	b	616	-	-	12/39/115/115	-
45	CHL	g	609	-	1/1/15/21	6/41/117/117	-
33	LMG	d	411	-	-	12/41/61/70	0/1/1/1
29	CLA	r	608	-	-	15/33/109/115	-
29	CLA	R	611	-	-	7/17/93/115	-
29	CLA	Y	608	-	-	8/21/97/115	-
39	LHG	s	624	-	-	31/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	607	-	-	14/39/115/115	-
29	CLA	s	609	-	-	16/33/109/115	-
29	CLA	B	610	-	-	17/39/115/115	-
45	CHL	N	608	-	-	4/22/98/117	-
45	CHL	N	606	-	1/1/15/21	4/41/117/117	-
29	CLA	B	606	-	-	12/39/115/115	-
29	CLA	a	410	-	-	10/33/109/115	-
29	CLA	N	612	-	-	7/15/91/115	-
45	CHL	G	601	21	1/1/15/21	8/41/117/117	-
29	CLA	s	613	-	-	12/27/103/115	-
29	CLA	n	603	-	-	24/39/115/115	-
29	CLA	r	602	-	-	11/33/109/115	-
48	NEX	n	623	-	-	2/27/83/83	0/3/3/3
29	CLA	B	612	-	-	21/39/115/115	-
29	CLA	c	510	4	-	12/39/115/115	-
29	CLA	b	603	2	-	18/39/115/115	-
39	LHG	L	101	-	-	30/53/53/53	-
39	LHG	S	624	-	-	28/49/49/53	-
48	NEX	S	622	-	-	11/27/83/83	0/3/3/3
29	CLA	b	617	-	-	18/39/115/115	-
46	LUT	g	620	-	-	3/29/67/67	0/2/2/2
29	CLA	Y	603	-	-	17/39/115/115	-
46	LUT	n	621	-	-	4/29/67/67	0/2/2/2
30	PHO	A	409	-	-	10/37/103/103	0/5/6/6
29	CLA	c	507	52	-	21/39/115/115	-
29	CLA	c	509	4	-	11/39/115/115	-
46	LUT	n	620	-	-	6/29/67/67	0/2/2/2
45	CHL	y	606	-	1/1/15/21	8/41/117/117	-
31	BCR	C	516	-	-	15/29/63/63	0/2/2/2
29	CLA	s	603	-	-	17/39/115/115	-
32	SQD	B	621	-	-	19/49/69/69	0/1/1/1
29	CLA	S	609	-	-	10/33/109/115	-
29	CLA	G	612	-	-	6/13/89/115	-
29	CLA	B	605	2	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	C	515	-	-	11/29/63/63	0/2/2/2
29	CLA	a	405	-	-	14/39/115/115	-
48	NEX	N	623	-	-	2/27/83/83	0/3/3/3
29	CLA	n	611	-	-	12/20/96/115	-
29	CLA	r	609	-	-	20/33/109/115	-
29	CLA	S	612	-	-	7/15/91/115	-
29	CLA	s	604	-	-	14/27/103/115	-
33	LMG	j	101	-	-	12/40/60/70	0/1/1/1
45	CHL	N	605	20	1/1/15/21	10/41/117/117	-
38	DGD	C	520	-	-	12/48/88/95	0/2/2/2
29	CLA	Y	604	-	-	20/39/115/115	-
29	CLA	C	508	-	-	12/39/115/115	-
33	LMG	C	521	-	-	18/46/66/70	0/1/1/1
29	CLA	C	513	-	-	19/39/115/115	-
39	LHG	Y	624	-	-	31/53/53/53	-
29	CLA	r	613	-	-	11/17/93/115	-
31	BCR	B	618	-	-	13/29/63/63	0/2/2/2
29	CLA	y	610	-	-	26/39/115/115	-
29	CLA	n	610	-	-	14/39/115/115	-
29	CLA	B	609	-	-	14/39/115/115	-
30	PHO	a	409	-	-	9/37/103/103	0/5/6/6
29	CLA	c	512	-	-	19/39/115/115	-
45	CHL	n	608	-	-	4/22/98/117	-
32	SQD	a	412	-	-	13/46/66/69	0/1/1/1
29	CLA	G	613	-	-	22/39/115/115	-
43	HEM	f	101	7,6	-	3/14/54/54	-
29	CLA	G	603	-	-	20/39/115/115	-
45	CHL	g	606	-	-	5/22/98/117	-
48	NEX	y	623	-	-	3/27/83/83	0/3/3/3
29	CLA	b	604	-	-	16/39/115/115	-
29	CLA	B	613	-	-	15/39/115/115	-
29	CLA	B	603	2	-	16/39/115/115	-
45	CHL	n	601	-	1/1/15/21	10/41/117/117	-
45	CHL	N	609	-	1/1/15/21	7/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	c	508	-	-	12/39/115/115	-
29	CLA	R	602	-	-	15/33/109/115	-
29	CLA	R	612	-	-	15/33/109/115	-
29	CLA	R	603	-	-	16/33/109/115	-
35	C7Z	b	620	-	1/1/12/26	9/29/67/67	0/2/2/2
44	RRX	H	101	-	1/1/11/25	9/29/65/65	0/2/2/2
29	CLA	y	611	-	-	17/39/115/115	-
31	BCR	b	619	-	-	8/29/63/63	0/2/2/2
29	CLA	S	614	-	-	10/27/103/115	-
29	CLA	Y	611	-	-	19/39/115/115	-
29	CLA	b	615	-	-	12/39/115/115	-
29	CLA	N	613	-	-	21/39/115/115	-
29	CLA	g	610	-	-	13/39/115/115	-
29	CLA	Y	614	-	-	15/39/115/115	-
29	CLA	s	612	-	-	8/15/91/115	-
29	CLA	g	611	-	-	6/15/91/115	-
29	CLA	n	613	-	-	16/39/115/115	-
29	CLA	n	612	-	-	8/15/91/115	-
29	CLA	B	616	-	-	12/39/115/115	-
45	CHL	S	606	-	-	0/15/91/117	-
48	NEX	G	623	-	-	3/27/83/83	0/3/3/3
33	LMG	A	413	-	-	14/43/63/70	0/1/1/1
47	XAT	R	621	-	1/1/12/26	11/31/93/93	0/4/4/4
40	LMK	C	527	-	1/1/6/6	10/46/46/60	-
29	CLA	b	611	-	-	9/39/115/115	-
45	CHL	Y	605	24	-	1/17/93/117	-
45	CHL	S	607	-	1/1/10/21	1/14/90/117	-
38	DGD	c	519	-	-	21/51/91/95	0/2/2/2
37	GOL	b	625	-	-	1/4/4/4	-
29	CLA	c	505	-	-	17/39/115/115	-
29	CLA	g	604	-	-	14/20/96/115	-
42	PL9	d	405	-	-	10/53/73/73	0/1/1/1
49	LPX	S	625	-	-	10/31/31/31	-
40	LMK	c	627	-	1/1/6/6	9/46/46/60	-
29	CLA	c	504	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CHL	S	608	-	1/1/14/21	3/35/111/117	-
36	DGA	b	623	-	-	26/45/45/45	-
45	CHL	N	601	-	1/1/15/21	5/41/117/117	-
29	CLA	S	617	-	-	12/21/97/115	-
29	CLA	A	407	-	-	6/20/96/115	-
45	CHL	R	606	-	-	4/15/91/117	-
46	LUT	Y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	b	613	-	-	17/39/115/115	-
29	CLA	C	504	-	-	16/39/115/115	-
29	CLA	n	614	-	-	7/20/96/115	-
46	LUT	Y	620	-	-	4/29/67/67	0/2/2/2
45	CHL	G	607	-	-	4/22/98/117	-
45	CHL	N	607	-	1/1/15/21	8/41/117/117	-
46	LUT	y	620	-	-	4/29/67/67	0/2/2/2
29	CLA	b	605	-	-	22/39/115/115	-
46	LUT	g	621	-	-	2/29/67/67	0/2/2/2
33	LMG	a	413	-	-	13/43/63/70	0/1/1/1
29	CLA	G	602	-	-	23/39/115/115	-
46	LUT	r	620	-	-	9/29/67/67	0/2/2/2
29	CLA	C	509	-	-	10/39/115/115	-
29	CLA	A	410	-	-	12/33/109/115	-
50	3PH	i	101	-	-	20/49/49/49	-
31	BCR	c	515	-	-	11/29/63/63	0/2/2/2
39	LHG	d	410	-	-	33/43/43/53	-
45	CHL	y	601	24	1/1/15/21	8/41/117/117	-
29	CLA	r	604	-	-	14/20/96/115	-
31	BCR	b	618	-	-	13/29/63/63	0/2/2/2
39	LHG	y	624	-	-	30/53/53/53	-
47	XAT	n	622	-	1/1/12/26	0/31/93/93	0/4/4/4
29	CLA	s	602	-	-	12/33/109/115	-
37	GOL	B	627	-	-	0/4/4/4	-
29	CLA	C	510	-	-	16/39/115/115	-
29	CLA	s	610	-	-	22/39/115/115	-
29	CLA	G	610	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	608	-	-	25/39/115/115	-
33	LMG	b	622	-	-	11/39/59/70	0/1/1/1
29	CLA	S	602	-	-	14/33/109/115	-
29	CLA	n	602	-	-	17/39/115/115	-
45	CHL	n	606	-	1/1/15/21	5/41/117/117	-
45	CHL	G	606	-	1/1/11/21	5/22/98/117	-
39	LHG	n	624	-	-	27/53/53/53	-
29	CLA	C	507	52	-	19/39/115/115	-
29	CLA	c	503	-	-	22/39/115/115	-
47	XAT	g	622	-	2/2/12/26	0/31/93/93	0/4/4/4
46	LUT	R	620	-	-	8/29/67/67	0/2/2/2
29	CLA	S	613	-	-	12/27/103/115	-
45	CHL	g	601	21	1/1/15/21	12/41/117/117	-
29	CLA	c	506	4	-	22/39/115/115	-
29	CLA	a	407	-	-	6/20/96/115	-
29	CLA	Y	602	-	-	17/39/115/115	-
39	LHG	g	624	-	-	28/53/53/53	-
33	LMG	D	411	-	-	8/41/61/70	0/1/1/1
45	CHL	G	605	21	-	2/20/96/117	-
29	CLA	r	611	-	-	7/17/93/115	-
29	CLA	B	615	-	-	8/39/115/115	-
46	LUT	y	621	-	-	2/29/67/67	0/2/2/2
31	BCR	d	404	-	-	12/29/63/63	0/2/2/2
29	CLA	C	506	-	-	21/39/115/115	-
38	DGD	c	518	-	-	11/44/84/95	0/2/2/2
29	CLA	r	612	-	-	14/33/109/115	-
29	CLA	b	602	-	-	23/39/115/115	-
45	CHL	g	608	-	-	1/15/91/117	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
29	CLA	S	603	-	-	17/39/115/115	-
29	CLA	R	610	-	-	12/33/109/115	-
31	BCR	c	514	-	-	12/29/63/63	0/2/2/2
29	CLA	D	402	-	-	11/39/115/115	-
38	DGD	c	523	-	-	18/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CHL	G	609	-	1/1/15/21	10/41/117/117	-
29	CLA	R	608	-	-	18/33/109/115	-
46	LUT	S	620	-	1/1/12/27	4/29/67/67	0/2/2/2
29	CLA	Y	613	-	-	21/39/115/115	-
29	CLA	y	613	-	-	19/39/115/115	-
29	CLA	A	406	-	-	13/39/115/115	-
51	SPH	y	625	-	-	11/21/21/21	-
29	CLA	g	612	-	-	6/13/89/115	-
45	CHL	Y	607	-	1/1/15/21	4/41/117/117	-
48	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
29	CLA	S	604	-	-	11/27/103/115	-
29	CLA	B	614	-	-	12/39/115/115	-
45	CHL	S	601	23	-	3/17/93/117	-
42	PL9	D	405	-	-	12/53/73/73	0/1/1/1
48	NEX	g	623	-	-	3/27/83/83	0/3/3/3
39	LHG	G	630	-	-	31/53/53/53	-
37	GOL	b	624	-	-	0/4/4/4	-
37	GOL	y	626	-	-	0/4/4/4	-
46	LUT	G	620	-	-	6/29/67/67	0/2/2/2
39	LHG	l	101	-	-	29/53/53/53	-
33	LMG	J	101	-	-	12/40/60/70	0/1/1/1
50	3PH	s	626	-	-	27/49/49/49	-
33	LMG	h	102	-	-	14/43/63/70	0/1/1/1
47	XAT	Y	622	-	1/1/12/26	3/31/93/93	0/4/4/4
39	LHG	C	525	-	-	28/51/51/53	-
43	HEM	F	101	7,6	-	3/14/54/54	-
46	LUT	s	620	-	1/1/12/27	3/29/67/67	0/2/2/2
29	CLA	a	406	-	-	13/39/115/115	-
29	CLA	c	502	-	-	21/39/115/115	-
29	CLA	S	611	-	-	14/39/115/115	-
31	BCR	B	619	-	-	11/29/63/63	0/2/2/2
45	CHL	Y	606	-	1/1/15/21	6/41/117/117	-
29	CLA	d	403	-	-	15/39/115/115	-
32	SQD	c	626	-	-	16/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	n	604	-	-	18/39/115/115	-
29	CLA	s	605	-	-	10/21/97/115	-
29	CLA	s	617	-	-	11/21/97/115	-
46	LUT	N	620	-	-	3/29/67/67	0/2/2/2
45	CHL	s	601	23	-	7/17/93/117	-
29	CLA	y	608	-	-	10/21/97/115	-
45	CHL	r	607	-	-	8/22/98/117	-
29	CLA	N	603	-	-	16/39/115/115	-
50	3PH	S	626	-	-	19/49/49/49	-
29	CLA	c	511	-	-	13/39/115/115	-
29	CLA	b	609	-	-	17/39/115/115	-
29	CLA	N	611	-	-	12/20/96/115	-
47	XAT	y	622	-	1/1/12/26	1/31/93/93	0/4/4/4
29	CLA	c	513	-	-	19/39/115/115	-
29	CLA	g	613	-	-	23/39/115/115	-
29	CLA	A	405	-	-	16/39/115/115	-
36	DGA	B	625	-	-	24/45/45/45	-
51	SPH	Y	625	-	-	10/21/21/21	-
45	CHL	y	607	-	1/1/15/21	5/41/117/117	-
29	CLA	B	611	-	-	9/39/115/115	-
33	LMG	B	622	-	-	11/39/59/70	0/1/1/1
35	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2

All (1666) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	620	C7Z	C25-C26	16.16	1.62	1.34
35	b	620	C7Z	C25-C26	16.13	1.62	1.34
44	h	101	RRX	C26-C25	15.49	1.61	1.34
44	H	101	RRX	C26-C25	15.48	1.61	1.34
35	b	620	C7Z	C5-C6	15.32	1.61	1.34
35	B	620	C7Z	C5-C6	15.20	1.60	1.34
46	s	620	LUT	C24-C25	14.79	1.51	1.33
44	h	101	RRX	C5-C6	14.75	1.60	1.34
44	H	101	RRX	C5-C6	14.75	1.60	1.34
46	n	620	LUT	C24-C25	14.61	1.51	1.33
46	S	620	LUT	C24-C25	14.60	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	G	621	LUT	C24-C25	14.56	1.51	1.33
46	g	621	LUT	C24-C25	14.53	1.51	1.33
46	N	621	LUT	C24-C25	14.51	1.51	1.33
46	g	620	LUT	C24-C25	14.50	1.51	1.33
46	y	621	LUT	C24-C25	14.44	1.51	1.33
46	Y	620	LUT	C24-C25	14.43	1.51	1.33
46	R	620	LUT	C24-C25	14.42	1.51	1.33
46	N	620	LUT	C24-C25	14.41	1.51	1.33
46	r	620	LUT	C24-C25	14.39	1.51	1.33
46	G	620	LUT	C24-C25	14.37	1.51	1.33
46	y	620	LUT	C24-C25	14.32	1.51	1.33
46	Y	621	LUT	C24-C25	14.32	1.51	1.33
46	n	621	LUT	C24-C25	14.28	1.50	1.33
46	s	621	LUT	C24-C25	14.21	1.50	1.33
46	S	621	LUT	C24-C25	14.17	1.50	1.33
35	B	620	C7Z	C24-C23	11.64	1.72	1.52
35	b	620	C7Z	C24-C23	11.61	1.72	1.52
35	B	620	C7Z	C22-C23	-10.94	1.36	1.52
35	b	620	C7Z	C22-C23	-10.87	1.36	1.52
35	B	620	C7Z	C2-C3	-10.53	1.37	1.52
35	b	620	C7Z	C2-C3	-10.31	1.37	1.52
44	h	101	RRX	C29-C28	-10.10	1.37	1.52
44	H	101	RRX	C29-C28	-10.03	1.37	1.52
30	A	409	PHO	C1B-C2B	9.29	1.49	1.39
30	a	409	PHO	C1B-C2B	9.22	1.49	1.39
30	a	408	PHO	C1B-C2B	9.14	1.49	1.39
30	A	408	PHO	C1B-C2B	9.13	1.49	1.39
35	b	620	C7Z	C4-C3	8.49	1.67	1.52
35	B	620	C7Z	C4-C3	8.37	1.66	1.52
44	h	101	RRX	C27-C28	8.11	1.66	1.52
44	H	101	RRX	C27-C28	8.11	1.66	1.52
48	R	622	NEX	C10-C9	-8.03	1.25	1.35
30	a	409	PHO	C3B-C4B	7.79	1.50	1.41
30	A	408	PHO	C3B-C4B	7.79	1.50	1.41
30	a	408	PHO	C3B-C4B	7.71	1.50	1.41
30	A	409	PHO	C3B-C4B	7.69	1.50	1.41
48	R	622	NEX	C30-C29	-7.66	1.25	1.35
48	R	622	NEX	C14-C13	-7.62	1.25	1.35
48	y	623	NEX	C30-C29	-7.59	1.25	1.35
48	y	623	NEX	C10-C9	-7.55	1.25	1.35
48	n	623	NEX	C10-C9	-7.55	1.25	1.35
48	g	623	NEX	C34-C33	-7.54	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	g	623	NEX	C14-C13	-7.54	1.25	1.35
48	n	623	NEX	C14-C13	-7.53	1.25	1.35
48	n	623	NEX	C34-C33	-7.52	1.25	1.35
48	y	623	NEX	C14-C13	-7.51	1.25	1.35
48	R	622	NEX	C34-C33	-7.49	1.25	1.35
48	y	623	NEX	C34-C33	-7.48	1.25	1.35
48	Y	623	NEX	C30-C29	-7.48	1.25	1.35
48	s	623	NEX	C10-C9	-7.48	1.25	1.35
48	r	623	NEX	C14-C13	-7.47	1.25	1.35
48	r	623	NEX	C30-C29	-7.47	1.25	1.35
48	Y	623	NEX	C14-C13	-7.47	1.25	1.35
48	N	623	NEX	C34-C33	-7.46	1.25	1.35
48	N	623	NEX	C10-C9	-7.45	1.25	1.35
48	Y	623	NEX	C34-C33	-7.45	1.25	1.35
48	G	623	NEX	C34-C33	-7.44	1.25	1.35
48	S	622	NEX	C10-C9	-7.43	1.25	1.35
48	g	623	NEX	C30-C29	-7.42	1.25	1.35
48	G	623	NEX	C30-C29	-7.42	1.25	1.35
48	N	623	NEX	C30-C29	-7.42	1.25	1.35
48	n	623	NEX	C30-C29	-7.41	1.26	1.35
48	N	623	NEX	C14-C13	-7.41	1.26	1.35
48	r	623	NEX	C34-C33	-7.40	1.26	1.35
48	g	623	NEX	C10-C9	-7.39	1.26	1.35
48	G	623	NEX	C14-C13	-7.38	1.26	1.35
48	s	623	NEX	C14-C13	-7.38	1.26	1.35
48	s	623	NEX	C30-C29	-7.35	1.26	1.35
48	Y	623	NEX	C10-C9	-7.35	1.26	1.35
31	c	516	BCR	C10-C9	7.34	1.45	1.35
48	S	622	NEX	C14-C13	-7.31	1.26	1.35
48	s	623	NEX	C34-C33	-7.28	1.26	1.35
31	C	516	BCR	C10-C9	7.27	1.45	1.35
31	D	404	BCR	C10-C9	7.26	1.45	1.35
48	S	622	NEX	C34-C33	-7.25	1.26	1.35
48	S	622	NEX	C30-C29	-7.24	1.26	1.35
48	r	623	NEX	C10-C9	-7.23	1.26	1.35
48	G	623	NEX	C10-C9	-7.16	1.26	1.35
31	C	514	BCR	C10-C9	7.13	1.45	1.35
31	d	404	BCR	C10-C9	7.11	1.45	1.35
40	C	527	LMK	O3-C4	7.09	1.43	1.22
40	c	627	LMK	O3-C4	7.07	1.43	1.22
31	c	514	BCR	C10-C9	7.05	1.45	1.35
31	C	515	BCR	C10-C9	6.99	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	619	BCR	C10-C9	6.91	1.44	1.35
31	b	618	BCR	C10-C9	6.89	1.44	1.35
31	C	517	BCR	C10-C9	6.84	1.44	1.35
48	y	623	NEX	C35-C15	-6.81	1.18	1.36
31	c	515	BCR	C10-C9	6.81	1.44	1.35
31	A	411	BCR	C10-C9	6.81	1.44	1.35
48	R	622	NEX	C35-C15	-6.80	1.18	1.36
48	n	623	NEX	C35-C15	-6.80	1.18	1.36
31	b	619	BCR	C10-C9	6.80	1.44	1.35
31	B	618	BCR	C10-C9	6.79	1.44	1.35
48	g	623	NEX	C35-C15	-6.79	1.18	1.36
31	a	411	BCR	C10-C9	6.78	1.44	1.35
48	N	623	NEX	C35-C15	-6.75	1.18	1.36
48	Y	623	NEX	C35-C15	-6.75	1.18	1.36
48	r	623	NEX	C35-C15	-6.72	1.18	1.36
48	G	623	NEX	C35-C15	-6.72	1.18	1.36
48	s	623	NEX	C35-C15	-6.68	1.18	1.36
48	S	622	NEX	C35-C15	-6.67	1.18	1.36
31	c	517	BCR	C10-C9	6.53	1.44	1.35
29	B	616	CLA	MG-NA	6.47	2.21	2.06
29	S	605	CLA	MG-NA	6.46	2.21	2.06
29	s	605	CLA	MG-NA	6.46	2.21	2.06
29	s	603	CLA	MG-NA	6.45	2.21	2.06
29	r	612	CLA	MG-NA	6.45	2.21	2.06
29	b	616	CLA	MG-NA	6.44	2.21	2.06
44	h	101	RRX	C2-C3	-6.43	1.36	1.52
44	H	101	RRX	C2-C3	-6.43	1.36	1.52
29	r	611	CLA	MG-NA	6.42	2.21	2.06
29	N	613	CLA	MG-NA	6.42	2.21	2.06
29	B	605	CLA	MG-NA	6.41	2.21	2.06
29	G	612	CLA	MG-NA	6.41	2.21	2.06
29	s	609	CLA	MG-NA	6.41	2.21	2.06
29	n	611	CLA	MG-NA	6.41	2.21	2.06
29	R	611	CLA	MG-NA	6.40	2.21	2.06
29	R	603	CLA	MG-NA	6.40	2.21	2.06
29	b	602	CLA	MG-NA	6.40	2.21	2.06
29	R	612	CLA	MG-NA	6.39	2.21	2.06
29	b	605	CLA	MG-NA	6.39	2.21	2.06
29	S	603	CLA	MG-NA	6.39	2.21	2.06
29	Y	608	CLA	MG-NA	6.39	2.21	2.06
29	G	613	CLA	MG-NA	6.39	2.21	2.06
29	C	503	CLA	MG-NA	6.39	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	512	CLA	MG-NA	6.39	2.21	2.06
29	g	611	CLA	MG-NA	6.39	2.21	2.06
29	r	603	CLA	MG-NA	6.39	2.21	2.06
29	B	611	CLA	MG-NA	6.39	2.21	2.06
29	n	614	CLA	MG-NA	6.39	2.21	2.06
29	n	612	CLA	MG-NA	6.39	2.21	2.06
29	g	612	CLA	MG-NA	6.38	2.21	2.06
29	c	503	CLA	MG-NA	6.38	2.21	2.06
29	S	612	CLA	MG-NA	6.38	2.21	2.06
29	Y	612	CLA	MG-NA	6.38	2.21	2.06
29	s	613	CLA	MG-NA	6.38	2.21	2.06
29	S	611	CLA	MG-NA	6.38	2.21	2.06
29	n	613	CLA	MG-NA	6.38	2.21	2.06
29	r	608	CLA	MG-NA	6.37	2.21	2.06
29	b	611	CLA	MG-NA	6.37	2.21	2.06
29	C	501	CLA	MG-NA	6.37	2.21	2.06
29	s	612	CLA	MG-NA	6.37	2.21	2.06
29	S	617	CLA	MG-NA	6.37	2.21	2.06
29	G	611	CLA	MG-NA	6.37	2.21	2.06
29	d	403	CLA	MG-NA	6.37	2.21	2.06
29	R	610	CLA	MG-NA	6.37	2.21	2.06
29	R	602	CLA	MG-NA	6.36	2.21	2.06
29	B	602	CLA	MG-NA	6.36	2.21	2.06
29	R	613	CLA	MG-NA	6.36	2.21	2.06
29	S	609	CLA	MG-NA	6.36	2.21	2.06
29	g	613	CLA	MG-NA	6.36	2.21	2.06
29	N	611	CLA	MG-NA	6.36	2.21	2.06
29	C	513	CLA	MG-NA	6.36	2.21	2.06
29	N	612	CLA	MG-NA	6.36	2.21	2.06
29	c	507	CLA	MG-NA	6.35	2.21	2.06
29	c	501	CLA	MG-NA	6.35	2.21	2.06
29	D	403	CLA	MG-NA	6.35	2.21	2.06
29	G	604	CLA	MG-NA	6.35	2.21	2.06
29	r	602	CLA	MG-NA	6.35	2.21	2.06
29	g	614	CLA	MG-NA	6.35	2.21	2.06
29	y	611	CLA	MG-NA	6.35	2.21	2.06
29	y	612	CLA	MG-NA	6.34	2.21	2.06
29	c	511	CLA	MG-NA	6.34	2.21	2.06
29	y	613	CLA	MG-NA	6.34	2.21	2.06
29	c	502	CLA	MG-NA	6.34	2.21	2.06
29	g	604	CLA	MG-NA	6.34	2.21	2.06
29	C	511	CLA	MG-NA	6.34	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	614	CLA	MG-NA	6.33	2.21	2.06
29	C	507	CLA	MG-NA	6.33	2.21	2.06
29	N	614	CLA	MG-NA	6.33	2.21	2.06
29	c	512	CLA	MG-NA	6.33	2.21	2.06
29	s	617	CLA	MG-NA	6.33	2.21	2.06
29	B	609	CLA	MG-NA	6.32	2.21	2.06
29	S	613	CLA	MG-NA	6.32	2.21	2.06
29	G	614	CLA	MG-NA	6.32	2.21	2.06
29	S	610	CLA	MG-NA	6.32	2.21	2.06
29	A	407	CLA	MG-NA	6.32	2.21	2.06
29	r	610	CLA	MG-NA	6.31	2.21	2.06
48	Y	623	NEX	C31-C32	-6.31	1.18	1.34
29	R	608	CLA	MG-NA	6.31	2.21	2.06
48	G	623	NEX	C11-C12	-6.31	1.18	1.34
29	s	610	CLA	MG-NA	6.31	2.21	2.06
29	Y	611	CLA	MG-NA	6.30	2.21	2.06
29	n	602	CLA	MG-NA	6.30	2.21	2.06
29	b	604	CLA	MG-NA	6.30	2.21	2.06
29	Y	613	CLA	MG-NA	6.30	2.21	2.06
29	c	506	CLA	MG-NA	6.30	2.21	2.06
29	g	602	CLA	MG-NA	6.30	2.21	2.06
29	s	611	CLA	MG-NA	6.30	2.21	2.06
29	y	614	CLA	MG-NA	6.30	2.21	2.06
29	y	602	CLA	MG-NA	6.30	2.21	2.06
48	s	623	NEX	C11-C12	-6.30	1.18	1.34
29	b	603	CLA	MG-NA	6.30	2.21	2.06
29	g	603	CLA	MG-NA	6.30	2.21	2.06
29	y	608	CLA	MG-NA	6.30	2.21	2.06
29	N	603	CLA	MG-NA	6.30	2.21	2.06
29	B	604	CLA	MG-NA	6.29	2.21	2.06
48	n	623	NEX	C11-C12	-6.29	1.18	1.34
29	Y	603	CLA	MG-NA	6.29	2.21	2.06
29	y	603	CLA	MG-NA	6.28	2.21	2.06
29	n	604	CLA	MG-NA	6.28	2.21	2.06
48	Y	623	NEX	C11-C12	-6.28	1.18	1.34
29	S	602	CLA	MG-NA	6.28	2.21	2.06
29	b	609	CLA	MG-NA	6.28	2.21	2.06
29	C	506	CLA	MG-NA	6.28	2.21	2.06
29	N	610	CLA	MG-NA	6.28	2.21	2.06
29	a	407	CLA	MG-NA	6.27	2.21	2.06
29	G	603	CLA	MG-NA	6.27	2.21	2.06
29	G	602	CLA	MG-NA	6.27	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	y	623	NEX	C11-C12	-6.27	1.18	1.34
29	N	604	CLA	MG-NA	6.26	2.21	2.06
29	N	602	CLA	MG-NA	6.26	2.21	2.06
48	y	623	NEX	C31-C32	-6.26	1.18	1.34
29	C	502	CLA	MG-NA	6.26	2.21	2.06
48	n	623	NEX	C31-C32	-6.26	1.18	1.34
29	c	513	CLA	MG-NA	6.25	2.21	2.06
29	r	613	CLA	MG-NA	6.25	2.21	2.06
48	s	623	NEX	C31-C32	-6.25	1.18	1.34
48	r	623	NEX	C31-C32	-6.25	1.18	1.34
29	B	603	CLA	MG-NA	6.25	2.21	2.06
29	C	509	CLA	MG-NA	6.25	2.21	2.06
29	B	607	CLA	MG-NA	6.25	2.21	2.06
29	g	610	CLA	MG-NA	6.24	2.21	2.06
48	N	623	NEX	C31-C32	-6.24	1.18	1.34
48	R	622	NEX	C31-C32	-6.24	1.18	1.34
29	r	604	CLA	MG-NA	6.24	2.21	2.06
29	s	604	CLA	MG-NA	6.24	2.21	2.06
29	Y	602	CLA	MG-NA	6.24	2.21	2.06
29	Y	604	CLA	MG-NA	6.23	2.21	2.06
29	S	614	CLA	MG-NA	6.23	2.21	2.06
29	C	505	CLA	MG-NA	6.23	2.21	2.06
48	g	623	NEX	C31-C32	-6.23	1.18	1.34
29	B	614	CLA	MG-NA	6.22	2.21	2.06
48	N	623	NEX	C11-C12	-6.22	1.18	1.34
29	A	406	CLA	MG-NA	6.22	2.21	2.06
48	G	623	NEX	C31-C32	-6.22	1.18	1.34
48	g	623	NEX	C11-C12	-6.22	1.18	1.34
29	n	603	CLA	MG-NA	6.21	2.21	2.06
48	S	622	NEX	C11-C12	-6.21	1.18	1.34
29	R	609	CLA	MG-NA	6.21	2.21	2.06
29	b	607	CLA	MG-NA	6.21	2.21	2.06
29	B	608	CLA	MG-NA	6.21	2.21	2.06
29	d	402	CLA	MG-NA	6.20	2.21	2.06
29	n	610	CLA	MG-NA	6.20	2.21	2.06
29	y	604	CLA	MG-NA	6.20	2.21	2.06
29	b	614	CLA	MG-NA	6.20	2.21	2.06
29	b	608	CLA	MG-NA	6.20	2.21	2.06
48	r	623	NEX	C11-C12	-6.20	1.18	1.34
29	Y	610	CLA	MG-NA	6.20	2.21	2.06
29	y	610	CLA	MG-NA	6.19	2.21	2.06
29	c	505	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	410	CLA	MG-NA	6.19	2.21	2.06
29	s	614	CLA	MG-NA	6.18	2.21	2.06
29	D	402	CLA	MG-NA	6.18	2.21	2.06
29	C	508	CLA	MG-NA	6.18	2.21	2.06
29	r	609	CLA	MG-NA	6.18	2.21	2.06
29	s	602	CLA	MG-NA	6.18	2.20	2.06
29	b	612	CLA	MG-NA	6.17	2.20	2.06
29	R	604	CLA	MG-NA	6.17	2.20	2.06
29	a	406	CLA	MG-NA	6.17	2.20	2.06
48	S	622	NEX	C31-C32	-6.17	1.18	1.34
29	b	615	CLA	MG-NA	6.16	2.20	2.06
29	C	510	CLA	MG-NA	6.16	2.20	2.06
29	c	509	CLA	MG-NA	6.16	2.20	2.06
29	a	410	CLA	MG-NA	6.15	2.20	2.06
29	S	604	CLA	MG-NA	6.15	2.20	2.06
29	B	612	CLA	MG-NA	6.14	2.20	2.06
29	c	510	CLA	MG-NA	6.13	2.20	2.06
29	B	610	CLA	MG-NA	6.13	2.20	2.06
29	B	615	CLA	MG-NA	6.13	2.20	2.06
29	c	508	CLA	MG-NA	6.08	2.20	2.06
29	b	617	CLA	MG-NA	6.08	2.20	2.06
29	B	617	CLA	MG-NA	6.06	2.20	2.06
29	C	504	CLA	MG-NA	6.06	2.20	2.06
29	b	610	CLA	MG-NA	6.06	2.20	2.06
29	a	405	CLA	MG-NA	6.05	2.20	2.06
29	b	613	CLA	MG-NA	6.05	2.20	2.06
29	A	405	CLA	MG-NA	6.04	2.20	2.06
29	G	610	CLA	MG-NA	6.04	2.20	2.06
29	c	504	CLA	MG-NA	6.03	2.20	2.06
48	R	622	NEX	C11-C12	-6.03	1.19	1.34
29	B	613	CLA	MG-NA	6.02	2.20	2.06
29	b	606	CLA	MG-NA	6.00	2.20	2.06
29	B	606	CLA	MG-NA	5.98	2.20	2.06
44	h	101	RRX	C1-C6	-5.88	1.45	1.53
48	R	622	NEX	C7-C8	5.83	1.41	1.32
31	D	404	BCR	C24-C23	5.79	1.50	1.33
31	d	404	BCR	C24-C23	5.78	1.50	1.33
44	H	101	RRX	C1-C6	-5.76	1.45	1.53
31	c	516	BCR	C24-C23	5.75	1.50	1.33
31	B	619	BCR	C24-C23	5.73	1.50	1.33
31	C	516	BCR	C24-C23	5.70	1.50	1.33
35	b	620	C7Z	C12-C13	5.70	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	517	BCR	C24-C23	5.66	1.50	1.33
31	C	517	BCR	C24-C23	5.65	1.50	1.33
35	B	620	C7Z	C12-C13	5.65	1.58	1.45
31	A	411	BCR	C24-C23	5.65	1.50	1.33
31	b	619	BCR	C24-C23	5.61	1.50	1.33
31	C	514	BCR	C24-C23	5.60	1.50	1.33
31	a	411	BCR	C24-C23	5.60	1.50	1.33
44	h	101	RRX	C30-C25	-5.58	1.46	1.53
31	C	515	BCR	C24-C23	5.58	1.49	1.33
44	H	101	RRX	C30-C25	-5.57	1.46	1.53
31	c	514	BCR	C24-C23	5.56	1.49	1.33
48	s	623	NEX	C7-C8	5.56	1.41	1.32
31	b	618	BCR	C24-C23	5.53	1.49	1.33
31	c	515	BCR	C24-C23	5.52	1.49	1.33
48	n	623	NEX	C7-C8	5.51	1.41	1.32
48	r	623	NEX	C7-C8	5.49	1.41	1.32
31	B	618	BCR	C24-C23	5.45	1.49	1.33
48	y	623	NEX	C7-C8	5.44	1.41	1.32
48	R	622	NEX	C28-C29	-5.32	1.34	1.45
31	c	517	BCR	C11-C12	-5.31	1.20	1.34
48	r	623	NEX	C28-C29	-5.30	1.34	1.45
31	C	517	BCR	C11-C12	-5.30	1.20	1.34
31	A	411	BCR	C11-C12	-5.29	1.20	1.34
48	N	623	NEX	C7-C8	5.29	1.40	1.32
31	B	618	BCR	C11-C12	-5.29	1.21	1.34
31	a	411	BCR	C11-C12	-5.28	1.21	1.34
31	b	619	BCR	C11-C12	-5.28	1.21	1.34
31	B	619	BCR	C11-C12	-5.27	1.21	1.34
31	b	618	BCR	C11-C12	-5.27	1.21	1.34
48	s	623	NEX	C28-C29	-5.27	1.34	1.45
31	c	515	BCR	C11-C12	-5.25	1.21	1.34
48	n	623	NEX	C28-C29	-5.25	1.34	1.45
48	N	623	NEX	C28-C29	-5.24	1.34	1.45
48	G	623	NEX	C7-C8	5.23	1.40	1.32
48	g	623	NEX	C7-C8	5.23	1.40	1.32
31	c	514	BCR	C11-C12	-5.22	1.21	1.34
48	Y	623	NEX	C28-C29	-5.22	1.34	1.45
48	y	623	NEX	C28-C29	-5.22	1.34	1.45
31	C	515	BCR	C11-C12	-5.21	1.21	1.34
48	g	623	NEX	C28-C29	-5.20	1.34	1.45
48	G	623	NEX	C28-C29	-5.19	1.34	1.45
48	S	622	NEX	C28-C29	-5.16	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S	622	NEX	C7-C8	5.16	1.40	1.32
35	B	620	C7Z	C1-C6	-5.16	1.46	1.53
31	C	514	BCR	C11-C12	-5.15	1.21	1.34
31	d	404	BCR	C11-C12	-5.13	1.21	1.34
44	H	101	RRX	C2-C1	5.12	1.65	1.54
31	C	516	BCR	C11-C12	-5.09	1.21	1.34
44	h	101	RRX	C2-C1	5.09	1.65	1.54
31	c	516	BCR	C11-C12	-5.08	1.21	1.34
31	D	404	BCR	C11-C12	-5.00	1.21	1.34
35	b	620	C7Z	C28-C29	4.97	1.56	1.45
35	B	620	C7Z	C28-C29	4.96	1.56	1.45
35	b	620	C7Z	C1-C6	-4.94	1.47	1.53
48	Y	623	NEX	C7-C8	4.91	1.40	1.32
44	H	101	RRX	C19-C18	4.90	1.56	1.45
44	h	101	RRX	C19-C18	4.89	1.56	1.45
44	H	101	RRX	C8-C9	4.82	1.56	1.45
44	h	101	RRX	C8-C9	4.73	1.56	1.45
35	B	620	C7Z	C24-C25	-4.69	1.43	1.51
35	b	620	C7Z	C24-C25	-4.63	1.43	1.51
35	B	620	C7Z	C32-C33	4.61	1.55	1.45
35	b	620	C7Z	C32-C33	4.61	1.55	1.45
31	A	411	BCR	C16-C17	-4.46	1.29	1.43
31	a	411	BCR	C16-C17	-4.45	1.29	1.43
44	h	101	RRX	C27-C26	-4.43	1.44	1.51
31	c	517	BCR	C16-C17	-4.42	1.29	1.43
35	b	620	C7Z	C8-C9	4.41	1.55	1.45
45	N	608	CHL	CBB-CAB	4.40	1.52	1.30
44	H	101	RRX	C27-C26	-4.40	1.44	1.51
35	b	620	C7Z	C31-C30	4.39	1.57	1.43
31	c	515	BCR	C16-C17	-4.39	1.29	1.43
31	C	517	BCR	C16-C17	-4.38	1.29	1.43
45	Y	601	CHL	CBB-CAB	4.38	1.52	1.30
45	n	608	CHL	CBB-CAB	4.38	1.52	1.30
45	y	601	CHL	CBB-CAB	4.38	1.52	1.30
45	n	609	CHL	CBB-CAB	4.37	1.52	1.30
35	B	620	C7Z	C8-C9	4.37	1.55	1.45
35	B	620	C7Z	C31-C30	4.37	1.57	1.43
35	B	620	C7Z	C4-C5	-4.36	1.44	1.51
29	B	614	CLA	CBB-CAB	4.35	1.51	1.30
45	N	609	CHL	CBB-CAB	4.35	1.51	1.30
31	B	618	BCR	C16-C17	-4.34	1.30	1.43
29	b	614	CLA	CBB-CAB	4.33	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Y	605	CHL	CBB-CAB	4.33	1.51	1.30
45	y	605	CHL	CBB-CAB	4.33	1.51	1.30
38	c	518	DGD	O1G-C1A	4.33	1.46	1.33
38	C	523	DGD	O1G-C1A	4.33	1.46	1.33
31	b	618	BCR	C16-C17	-4.33	1.30	1.43
38	c	523	DGD	O1G-C1A	4.33	1.46	1.33
45	n	601	CHL	CBB-CAB	4.32	1.51	1.30
45	N	601	CHL	CBB-CAB	4.32	1.51	1.30
31	C	515	BCR	C16-C17	-4.32	1.30	1.43
29	n	602	CLA	CBB-CAB	4.32	1.51	1.30
45	G	605	CHL	CBB-CAB	4.32	1.51	1.30
45	G	609	CHL	CBB-CAB	4.32	1.51	1.30
29	R	602	CLA	CBB-CAB	4.32	1.51	1.30
29	C	509	CLA	CBB-CAB	4.31	1.51	1.30
31	b	619	BCR	C16-C17	-4.31	1.30	1.43
45	y	609	CHL	CBB-CAB	4.31	1.51	1.30
29	r	610	CLA	CBB-CAB	4.31	1.51	1.30
29	N	602	CLA	CBB-CAB	4.31	1.51	1.30
29	y	602	CLA	CBB-CAB	4.31	1.51	1.30
29	r	602	CLA	CBB-CAB	4.31	1.51	1.30
29	g	604	CLA	CBB-CAB	4.31	1.51	1.30
29	A	405	CLA	CBB-CAB	4.30	1.51	1.30
45	G	601	CHL	CBB-CAB	4.30	1.51	1.30
29	R	613	CLA	CBB-CAB	4.30	1.51	1.30
29	y	603	CLA	CBB-CAB	4.30	1.51	1.30
29	g	610	CLA	CBB-CAB	4.30	1.51	1.30
29	B	602	CLA	CBB-CAB	4.30	1.51	1.30
29	C	508	CLA	CBB-CAB	4.30	1.51	1.30
38	C	518	DGD	O1G-C1A	4.30	1.45	1.33
29	b	608	CLA	CBB-CAB	4.30	1.51	1.30
29	n	610	CLA	CBB-CAB	4.30	1.51	1.30
29	a	405	CLA	CBB-CAB	4.30	1.51	1.30
29	B	604	CLA	CBB-CAB	4.30	1.51	1.30
45	g	608	CHL	CBB-CAB	4.30	1.51	1.30
29	G	603	CLA	CBB-CAB	4.30	1.51	1.30
31	c	514	BCR	C16-C17	-4.30	1.30	1.43
29	N	604	CLA	CBB-CAB	4.30	1.51	1.30
29	s	605	CLA	CBB-CAB	4.30	1.51	1.30
29	s	614	CLA	CBB-CAB	4.30	1.51	1.30
29	r	613	CLA	CBB-CAB	4.30	1.51	1.30
45	G	608	CHL	CBB-CAB	4.30	1.51	1.30
29	s	604	CLA	CBB-CAB	4.29	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	509	CLA	CBB-CAB	4.29	1.51	1.30
29	r	612	CLA	CBB-CAB	4.29	1.51	1.30
29	n	612	CLA	CBB-CAB	4.29	1.51	1.30
29	R	612	CLA	CBB-CAB	4.29	1.51	1.30
45	g	609	CHL	CBB-CAB	4.29	1.51	1.30
29	R	603	CLA	CBB-CAB	4.29	1.51	1.30
29	b	610	CLA	CBB-CAB	4.29	1.51	1.30
45	Y	609	CHL	CBB-CAB	4.29	1.51	1.30
29	B	611	CLA	CBB-CAB	4.29	1.51	1.30
29	c	508	CLA	CBB-CAB	4.29	1.51	1.30
29	S	605	CLA	CBB-CAB	4.29	1.51	1.30
29	B	615	CLA	CBB-CAB	4.29	1.51	1.30
29	B	603	CLA	CBB-CAB	4.29	1.51	1.30
29	d	403	CLA	CBB-CAB	4.29	1.51	1.30
29	R	611	CLA	CBB-CAB	4.29	1.51	1.30
29	g	613	CLA	CBB-CAB	4.29	1.51	1.30
29	G	602	CLA	CBB-CAB	4.29	1.51	1.30
29	s	617	CLA	CBB-CAB	4.29	1.51	1.30
29	N	614	CLA	CBB-CAB	4.29	1.51	1.30
45	g	605	CHL	CBB-CAB	4.29	1.51	1.30
44	H	101	RRX	C12-C13	4.29	1.55	1.45
35	b	620	C7Z	C4-C5	-4.29	1.44	1.51
29	B	612	CLA	CBB-CAB	4.29	1.51	1.30
29	G	612	CLA	CBB-CAB	4.29	1.51	1.30
29	S	614	CLA	CBB-CAB	4.29	1.51	1.30
29	b	604	CLA	CBB-CAB	4.29	1.51	1.30
29	c	507	CLA	CBB-CAB	4.29	1.51	1.30
29	n	604	CLA	CBB-CAB	4.29	1.51	1.30
29	y	608	CLA	CBB-CAB	4.28	1.51	1.30
45	n	605	CHL	CBB-CAB	4.28	1.51	1.30
29	c	512	CLA	CBB-CAB	4.28	1.51	1.30
29	B	608	CLA	CBB-CAB	4.28	1.51	1.30
29	N	603	CLA	CBB-CAB	4.28	1.51	1.30
29	N	610	CLA	CBB-CAB	4.28	1.51	1.30
29	G	611	CLA	CBB-CAB	4.28	1.51	1.30
29	N	612	CLA	CBB-CAB	4.28	1.51	1.30
29	b	615	CLA	CBB-CAB	4.28	1.51	1.30
29	n	614	CLA	CBB-CAB	4.28	1.51	1.30
29	S	613	CLA	CBB-CAB	4.28	1.51	1.30
29	g	602	CLA	CBB-CAB	4.28	1.51	1.30
29	c	506	CLA	CBB-CAB	4.28	1.51	1.30
29	R	610	CLA	CBB-CAB	4.28	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	610	CLA	CBB-CAB	4.28	1.51	1.30
29	r	611	CLA	CBB-CAB	4.28	1.51	1.30
29	Y	604	CLA	CBB-CAB	4.28	1.51	1.30
29	C	506	CLA	CBB-CAB	4.28	1.51	1.30
29	S	617	CLA	CBB-CAB	4.28	1.51	1.30
29	c	510	CLA	CBB-CAB	4.28	1.51	1.30
29	S	609	CLA	CBB-CAB	4.28	1.51	1.30
29	Y	602	CLA	CBB-CAB	4.28	1.51	1.30
29	Y	614	CLA	CBB-CAB	4.28	1.51	1.30
29	Y	603	CLA	CBB-CAB	4.28	1.51	1.30
29	g	614	CLA	CBB-CAB	4.28	1.51	1.30
29	S	604	CLA	CBB-CAB	4.28	1.51	1.30
29	S	602	CLA	CBB-CAB	4.28	1.51	1.30
29	C	510	CLA	CBB-CAB	4.27	1.51	1.30
29	g	603	CLA	CBB-CAB	4.27	1.51	1.30
29	b	607	CLA	CBB-CAB	4.27	1.51	1.30
29	C	512	CLA	CBB-CAB	4.27	1.51	1.30
29	R	609	CLA	CBB-CAB	4.27	1.51	1.30
29	n	611	CLA	CBB-CAB	4.27	1.51	1.30
29	g	611	CLA	CBB-CAB	4.27	1.51	1.30
29	Y	610	CLA	CBB-CAB	4.27	1.51	1.30
29	y	604	CLA	CBB-CAB	4.27	1.51	1.30
29	C	502	CLA	CBB-CAB	4.27	1.51	1.30
29	s	609	CLA	CBB-CAB	4.27	1.51	1.30
29	r	604	CLA	CBB-CAB	4.27	1.51	1.30
29	b	616	CLA	CBB-CAB	4.27	1.51	1.30
29	R	608	CLA	CBB-CAB	4.27	1.51	1.30
31	C	514	BCR	C16-C17	-4.27	1.30	1.43
45	N	605	CHL	CBB-CAB	4.27	1.51	1.30
29	b	612	CLA	CBB-CAB	4.27	1.51	1.30
29	r	609	CLA	CBB-CAB	4.27	1.51	1.30
29	y	614	CLA	CBB-CAB	4.27	1.51	1.30
29	y	613	CLA	CBB-CAB	4.27	1.51	1.30
29	G	604	CLA	CBB-CAB	4.27	1.51	1.30
29	Y	608	CLA	CBB-CAB	4.27	1.51	1.30
29	B	616	CLA	CBB-CAB	4.27	1.51	1.30
29	n	613	CLA	CBB-CAB	4.27	1.51	1.30
29	B	607	CLA	CBB-CAB	4.27	1.51	1.30
29	y	610	CLA	CBB-CAB	4.27	1.51	1.30
29	R	604	CLA	CBB-CAB	4.26	1.51	1.30
29	g	612	CLA	CBB-CAB	4.26	1.51	1.30
29	r	603	CLA	CBB-CAB	4.26	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	602	CLA	CBB-CAB	4.26	1.51	1.30
29	N	613	CLA	CBB-CAB	4.26	1.51	1.30
29	C	507	CLA	CBB-CAB	4.26	1.51	1.30
29	D	403	CLA	CBB-CAB	4.26	1.51	1.30
29	C	504	CLA	CBB-CAB	4.26	1.51	1.30
29	s	602	CLA	CBB-CAB	4.26	1.51	1.30
45	G	607	CHL	CBB-CAB	4.26	1.51	1.30
45	r	606	CHL	CBB-CAB	4.26	1.51	1.30
29	G	614	CLA	CBB-CAB	4.26	1.51	1.30
29	s	612	CLA	CBB-CAB	4.26	1.51	1.30
29	b	611	CLA	CBB-CAB	4.26	1.51	1.30
29	b	603	CLA	CBB-CAB	4.26	1.51	1.30
29	b	605	CLA	CBB-CAB	4.26	1.51	1.30
29	c	504	CLA	CBB-CAB	4.26	1.51	1.30
45	N	607	CHL	CBB-CAB	4.26	1.51	1.30
29	r	608	CLA	CBB-CAB	4.26	1.51	1.30
29	s	613	CLA	CBB-CAB	4.26	1.51	1.30
29	c	501	CLA	CBB-CAB	4.26	1.51	1.30
31	B	619	BCR	C16-C17	-4.26	1.30	1.43
29	G	610	CLA	CBB-CAB	4.26	1.51	1.30
29	y	611	CLA	CBB-CAB	4.26	1.51	1.30
29	N	611	CLA	CBB-CAB	4.26	1.51	1.30
45	g	601	CHL	CBB-CAB	4.26	1.51	1.30
29	c	511	CLA	CBB-CAB	4.26	1.51	1.30
29	c	503	CLA	CBB-CAB	4.25	1.51	1.30
29	Y	612	CLA	CBB-CAB	4.25	1.51	1.30
29	S	610	CLA	CBB-CAB	4.25	1.51	1.30
29	Y	613	CLA	CBB-CAB	4.25	1.51	1.30
44	h	101	RRX	C3-C4	4.25	1.65	1.52
29	C	501	CLA	CBB-CAB	4.25	1.51	1.30
29	C	511	CLA	CBB-CAB	4.25	1.51	1.30
29	s	603	CLA	CBB-CAB	4.25	1.51	1.30
29	y	612	CLA	CBB-CAB	4.25	1.51	1.30
42	d	405	PL9	C7-C3	-4.25	1.47	1.51
45	S	607	CHL	CBB-CAB	4.25	1.51	1.30
29	S	612	CLA	CBB-CAB	4.25	1.51	1.30
29	S	603	CLA	CBB-CAB	4.25	1.51	1.30
29	s	611	CLA	CBB-CAB	4.25	1.51	1.30
29	c	502	CLA	CBB-CAB	4.24	1.51	1.30
45	R	606	CHL	CBB-CAB	4.24	1.51	1.30
29	A	407	CLA	CBB-CAB	4.24	1.51	1.30
29	G	613	CLA	CBB-CAB	4.24	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	406	CLA	CBB-CAB	4.24	1.51	1.30
29	s	610	CLA	CBB-CAB	4.24	1.51	1.30
29	B	613	CLA	CBB-CAB	4.24	1.51	1.30
29	a	407	CLA	CBB-CAB	4.24	1.51	1.30
29	S	611	CLA	CBB-CAB	4.24	1.51	1.30
29	b	613	CLA	CBB-CAB	4.24	1.51	1.30
29	D	402	CLA	CBB-CAB	4.24	1.51	1.30
29	n	603	CLA	CBB-CAB	4.23	1.51	1.30
29	b	606	CLA	CBB-CAB	4.23	1.51	1.30
29	C	503	CLA	CBB-CAB	4.23	1.51	1.30
44	H	101	RRX	C3-C4	4.23	1.65	1.52
29	C	513	CLA	CBB-CAB	4.23	1.51	1.30
45	s	606	CHL	CBB-CAB	4.23	1.51	1.30
29	B	609	CLA	CBB-CAB	4.22	1.51	1.30
45	s	607	CHL	CBB-CAB	4.22	1.51	1.30
29	a	406	CLA	CBB-CAB	4.22	1.51	1.30
45	g	607	CHL	CBB-CAB	4.22	1.51	1.30
38	C	520	DGD	O1G-C1A	4.22	1.45	1.33
45	s	608	CHL	CBB-CAB	4.21	1.51	1.30
29	B	605	CLA	CBB-CAB	4.21	1.51	1.30
31	d	404	BCR	C16-C17	-4.21	1.30	1.43
45	S	606	CHL	CBB-CAB	4.21	1.51	1.30
29	B	606	CLA	CBB-CAB	4.21	1.51	1.30
29	c	513	CLA	CBB-CAB	4.21	1.51	1.30
45	r	607	CHL	CBB-CAB	4.20	1.51	1.30
29	c	505	CLA	CBB-CAB	4.20	1.51	1.30
45	S	608	CHL	CBB-CAB	4.20	1.51	1.30
29	b	617	CLA	CBB-CAB	4.20	1.51	1.30
29	Y	611	CLA	CBB-CAB	4.20	1.51	1.30
31	C	516	BCR	C16-C17	-4.20	1.30	1.43
31	c	516	BCR	C16-C17	-4.20	1.30	1.43
45	Y	607	CHL	CBB-CAB	4.19	1.51	1.30
29	d	402	CLA	CBB-CAB	4.19	1.51	1.30
45	R	607	CHL	CBB-CAB	4.19	1.51	1.30
29	b	609	CLA	CBB-CAB	4.19	1.51	1.30
29	C	505	CLA	CBB-CAB	4.19	1.51	1.30
35	B	620	C7Z	C11-C10	4.19	1.56	1.43
38	C	519	DGD	O1G-C1A	4.19	1.45	1.33
44	h	101	RRX	C12-C13	4.18	1.54	1.45
45	G	606	CHL	CBB-CAB	4.18	1.51	1.30
29	B	617	CLA	CBB-CAB	4.17	1.51	1.30
31	D	404	BCR	C16-C17	-4.17	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	g	606	CHL	CBB-CAB	4.17	1.51	1.30
38	c	520	DGD	O1G-C1A	4.17	1.45	1.33
38	c	519	DGD	O1G-C1A	4.16	1.45	1.33
30	A	408	PHO	C1D-C2D	4.16	1.44	1.39
45	n	607	CHL	CBB-CAB	4.15	1.50	1.30
35	b	620	C7Z	C11-C10	4.15	1.56	1.43
45	y	606	CHL	CBB-CAB	4.15	1.50	1.30
45	S	601	CHL	CBB-CAB	4.15	1.50	1.30
45	y	607	CHL	CBB-CAB	4.13	1.50	1.30
29	c	506	CLA	MG-ND	-4.12	1.97	2.05
29	a	410	CLA	CBB-CAB	4.11	1.50	1.30
45	Y	606	CHL	CBB-CAB	4.11	1.50	1.30
29	b	609	CLA	MG-ND	-4.10	1.97	2.05
29	b	612	CLA	MG-ND	-4.10	1.97	2.05
29	b	604	CLA	MG-ND	-4.09	1.97	2.05
29	A	410	CLA	CBB-CAB	4.08	1.50	1.30
45	N	606	CHL	CBB-CAB	4.08	1.50	1.30
29	C	506	CLA	MG-ND	-4.07	1.97	2.05
45	s	601	CHL	CBB-CAB	4.06	1.50	1.30
29	B	609	CLA	MG-ND	-4.05	1.97	2.05
29	S	603	CLA	MG-ND	-4.02	1.97	2.05
42	D	405	PL9	C7-C3	-4.02	1.47	1.51
29	B	604	CLA	MG-ND	-4.02	1.97	2.05
40	C	527	LMK	O2-C4	4.01	1.43	1.30
30	a	408	PHO	C1D-C2D	4.00	1.44	1.39
29	B	612	CLA	MG-ND	-3.99	1.97	2.05
43	f	101	HEM	FE-ND	3.99	2.07	1.94
29	c	507	CLA	MG-ND	-3.98	1.97	2.05
29	C	508	CLA	MG-ND	-3.98	1.97	2.05
29	B	615	CLA	MG-ND	-3.96	1.97	2.05
45	n	606	CHL	CBB-CAB	3.96	1.49	1.30
29	s	603	CLA	MG-ND	-3.95	1.98	2.05
29	C	505	CLA	MG-ND	-3.95	1.98	2.05
29	b	617	CLA	MG-ND	-3.95	1.98	2.05
29	C	507	CLA	MG-ND	-3.94	1.98	2.05
40	c	627	LMK	O2-C4	3.94	1.43	1.30
29	c	505	CLA	MG-ND	-3.94	1.98	2.05
29	B	607	CLA	MG-ND	-3.93	1.98	2.05
29	B	617	CLA	MG-ND	-3.93	1.98	2.05
29	b	615	CLA	MG-ND	-3.92	1.98	2.05
29	c	508	CLA	MG-ND	-3.92	1.98	2.05
44	h	101	RRX	C20-C21	3.92	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	605	CLA	MG-ND	-3.91	1.98	2.05
29	Y	611	CLA	MG-ND	-3.90	1.98	2.05
29	A	410	CLA	MG-ND	-3.90	1.98	2.05
29	B	613	CLA	MG-ND	-3.90	1.98	2.05
29	B	605	CLA	MG-ND	-3.90	1.98	2.05
29	B	603	CLA	MG-ND	-3.90	1.98	2.05
29	s	611	CLA	MG-ND	-3.88	1.98	2.05
30	A	409	PHO	C1D-C2D	3.88	1.43	1.39
29	y	608	CLA	MG-ND	-3.88	1.98	2.05
44	H	101	RRX	C20-C21	3.87	1.55	1.43
29	C	502	CLA	MG-ND	-3.87	1.98	2.05
44	H	101	RRX	C23-C22	3.87	1.54	1.45
29	D	402	CLA	MG-ND	-3.87	1.98	2.05
29	N	612	CLA	MG-ND	-3.87	1.98	2.05
29	b	613	CLA	MG-ND	-3.87	1.98	2.05
29	b	603	CLA	MG-ND	-3.87	1.98	2.05
29	a	410	CLA	MG-ND	-3.86	1.98	2.05
29	b	607	CLA	MG-ND	-3.86	1.98	2.05
29	Y	612	CLA	MG-ND	-3.86	1.98	2.05
29	S	611	CLA	MG-ND	-3.86	1.98	2.05
29	a	405	CLA	MG-ND	-3.86	1.98	2.05
44	h	101	RRX	C23-C22	3.85	1.54	1.45
29	g	604	CLA	MG-ND	-3.85	1.98	2.05
29	b	605	CLA	MG-ND	-3.85	1.98	2.05
29	d	403	CLA	MG-ND	-3.85	1.98	2.05
29	c	513	CLA	MG-ND	-3.85	1.98	2.05
29	N	604	CLA	MG-ND	-3.85	1.98	2.05
29	r	609	CLA	MG-ND	-3.85	1.98	2.05
29	R	604	CLA	MG-ND	-3.84	1.98	2.05
29	r	604	CLA	MG-ND	-3.84	1.98	2.05
29	s	605	CLA	MG-ND	-3.84	1.98	2.05
29	D	403	CLA	MG-ND	-3.84	1.98	2.05
29	c	502	CLA	MG-ND	-3.84	1.98	2.05
29	d	402	CLA	MG-ND	-3.84	1.98	2.05
29	B	606	CLA	MG-ND	-3.84	1.98	2.05
29	b	606	CLA	MG-ND	-3.84	1.98	2.05
29	s	610	CLA	MG-ND	-3.83	1.98	2.05
29	y	614	CLA	MG-ND	-3.83	1.98	2.05
29	c	509	CLA	MG-ND	-3.83	1.98	2.05
29	y	612	CLA	MG-ND	-3.83	1.98	2.05
29	c	501	CLA	MG-ND	-3.83	1.98	2.05
29	S	613	CLA	MG-ND	-3.83	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	603	CLA	MG-ND	-3.83	1.98	2.05
29	b	611	CLA	MG-ND	-3.83	1.98	2.05
29	C	509	CLA	MG-ND	-3.83	1.98	2.05
29	n	613	CLA	MG-ND	-3.83	1.98	2.05
29	S	610	CLA	MG-ND	-3.83	1.98	2.05
29	b	608	CLA	MG-ND	-3.83	1.98	2.05
29	C	512	CLA	MG-ND	-3.83	1.98	2.05
29	A	407	CLA	MG-ND	-3.83	1.98	2.05
29	C	513	CLA	MG-ND	-3.83	1.98	2.05
29	c	512	CLA	MG-ND	-3.83	1.98	2.05
29	G	612	CLA	MG-ND	-3.82	1.98	2.05
29	A	405	CLA	MG-ND	-3.82	1.98	2.05
29	r	612	CLA	MG-ND	-3.82	1.98	2.05
29	Y	608	CLA	MG-ND	-3.82	1.98	2.05
29	A	406	CLA	MG-ND	-3.82	1.98	2.05
29	b	614	CLA	MG-ND	-3.82	1.98	2.05
29	R	609	CLA	MG-ND	-3.82	1.98	2.05
29	N	613	CLA	MG-ND	-3.81	1.98	2.05
29	n	602	CLA	MG-ND	-3.81	1.98	2.05
29	N	610	CLA	MG-ND	-3.81	1.98	2.05
29	N	602	CLA	MG-ND	-3.81	1.98	2.05
29	S	614	CLA	MG-ND	-3.81	1.98	2.05
29	g	612	CLA	MG-ND	-3.81	1.98	2.05
29	G	604	CLA	MG-ND	-3.80	1.98	2.05
29	Y	602	CLA	MG-ND	-3.80	1.98	2.05
29	Y	610	CLA	MG-ND	-3.80	1.98	2.05
29	s	614	CLA	MG-ND	-3.80	1.98	2.05
29	S	612	CLA	MG-ND	-3.80	1.98	2.05
29	r	608	CLA	MG-ND	-3.80	1.98	2.05
29	a	406	CLA	MG-ND	-3.80	1.98	2.05
29	n	604	CLA	MG-ND	-3.80	1.98	2.05
29	B	611	CLA	MG-ND	-3.79	1.98	2.05
29	C	501	CLA	MG-ND	-3.79	1.98	2.05
29	s	612	CLA	MG-ND	-3.78	1.98	2.05
29	a	407	CLA	MG-ND	-3.78	1.98	2.05
29	b	610	CLA	MG-ND	-3.78	1.98	2.05
29	B	610	CLA	MG-ND	-3.78	1.98	2.05
29	S	604	CLA	MG-ND	-3.78	1.98	2.05
29	C	504	CLA	MG-ND	-3.78	1.98	2.05
29	s	613	CLA	MG-ND	-3.78	1.98	2.05
35	B	620	C7Z	C27-C26	3.78	1.58	1.45
29	y	604	CLA	MG-ND	-3.78	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	612	CLA	MG-ND	-3.78	1.98	2.05
29	B	608	CLA	MG-ND	-3.78	1.98	2.05
29	S	617	CLA	MG-ND	-3.78	1.98	2.05
29	r	603	CLA	MG-ND	-3.78	1.98	2.05
29	C	503	CLA	MG-ND	-3.78	1.98	2.05
29	R	613	CLA	MG-ND	-3.78	1.98	2.05
29	c	504	CLA	MG-ND	-3.77	1.98	2.05
29	R	611	CLA	MG-ND	-3.77	1.98	2.05
29	y	611	CLA	MG-ND	-3.77	1.98	2.05
29	c	510	CLA	MG-ND	-3.77	1.98	2.05
44	h	101	RRX	C15-C14	3.77	1.55	1.43
29	S	602	CLA	MG-ND	-3.77	1.98	2.05
29	y	610	CLA	MG-ND	-3.77	1.98	2.05
29	g	602	CLA	MG-ND	-3.77	1.98	2.05
29	N	614	CLA	MG-ND	-3.77	1.98	2.05
29	r	611	CLA	MG-ND	-3.77	1.98	2.05
29	c	503	CLA	MG-ND	-3.76	1.98	2.05
35	b	620	C7Z	C15-C14	3.76	1.55	1.43
29	G	613	CLA	MG-ND	-3.76	1.98	2.05
29	n	614	CLA	MG-ND	-3.76	1.98	2.05
29	g	610	CLA	MG-ND	-3.76	1.98	2.05
29	C	511	CLA	MG-ND	-3.76	1.98	2.05
29	R	608	CLA	MG-ND	-3.76	1.98	2.05
35	b	620	C7Z	C22-C21	3.76	1.66	1.54
43	F	101	HEM	FE-ND	3.76	2.06	1.94
29	R	612	CLA	MG-ND	-3.75	1.98	2.05
29	N	611	CLA	MG-ND	-3.75	1.98	2.05
29	Y	604	CLA	MG-ND	-3.75	1.98	2.05
29	r	602	CLA	MG-ND	-3.75	1.98	2.05
29	B	614	CLA	MG-ND	-3.75	1.98	2.05
29	N	603	CLA	MG-ND	-3.75	1.98	2.05
29	g	611	CLA	MG-ND	-3.75	1.98	2.05
29	r	613	CLA	MG-ND	-3.75	1.98	2.05
35	b	620	C7Z	C27-C26	3.75	1.58	1.45
35	B	620	C7Z	C22-C21	3.75	1.66	1.54
29	g	613	CLA	MG-ND	-3.75	1.98	2.05
44	H	101	RRX	C15-C14	3.74	1.55	1.43
29	R	610	CLA	MG-ND	-3.74	1.98	2.05
29	G	611	CLA	MG-ND	-3.74	1.98	2.05
29	y	602	CLA	MG-ND	-3.74	1.98	2.05
29	c	508	CLA	C1C-NC	-3.74	1.32	1.37
29	r	610	CLA	MG-ND	-3.74	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	604	CLA	MG-ND	-3.74	1.98	2.05
29	n	611	CLA	MG-ND	-3.74	1.98	2.05
29	s	617	CLA	MG-ND	-3.74	1.98	2.05
29	n	603	CLA	MG-ND	-3.73	1.98	2.05
29	Y	614	CLA	MG-ND	-3.73	1.98	2.05
29	Y	613	CLA	MG-ND	-3.73	1.98	2.05
43	F	101	HEM	FE-NB	3.73	2.06	1.94
29	G	602	CLA	MG-ND	-3.73	1.98	2.05
29	G	610	CLA	MG-ND	-3.73	1.98	2.05
29	B	602	CLA	MG-ND	-3.73	1.98	2.05
29	B	616	CLA	MG-ND	-3.72	1.98	2.05
29	s	609	CLA	MG-ND	-3.72	1.98	2.05
29	y	613	CLA	MG-ND	-3.72	1.98	2.05
29	R	602	CLA	MG-ND	-3.72	1.98	2.05
30	a	409	PHO	C1D-C2D	3.72	1.43	1.39
29	S	609	CLA	MG-ND	-3.72	1.98	2.05
35	B	620	C7Z	C15-C14	3.72	1.55	1.43
30	a	409	PHO	C4D-CHA	3.72	1.45	1.39
29	C	508	CLA	C1C-NC	-3.72	1.32	1.37
29	g	614	CLA	MG-ND	-3.71	1.98	2.05
29	G	614	CLA	MG-ND	-3.71	1.98	2.05
29	s	602	CLA	MG-ND	-3.71	1.98	2.05
29	b	602	CLA	MG-ND	-3.70	1.98	2.05
29	b	617	CLA	C1C-NC	-3.70	1.32	1.37
29	G	603	CLA	MG-ND	-3.70	1.98	2.05
30	A	409	PHO	C4D-CHA	3.69	1.45	1.39
29	n	610	CLA	MG-ND	-3.68	1.98	2.05
29	c	511	CLA	MG-ND	-3.68	1.98	2.05
29	B	617	CLA	C1C-NC	-3.67	1.32	1.37
29	b	616	CLA	MG-ND	-3.65	1.98	2.05
29	g	603	CLA	MG-ND	-3.65	1.98	2.05
36	b	623	DGA	OG2-CB1	3.64	1.44	1.34
36	B	625	DGA	OG2-CB1	3.63	1.44	1.34
29	Y	603	CLA	MG-ND	-3.63	1.98	2.05
29	c	502	CLA	C1C-NC	-3.62	1.32	1.37
29	b	612	CLA	C1C-NC	-3.61	1.32	1.37
35	B	620	C7Z	C2-C1	3.60	1.66	1.54
29	b	610	CLA	C1C-NC	-3.60	1.32	1.37
29	G	610	CLA	C1C-NC	-3.60	1.32	1.37
29	B	605	CLA	C1C-NC	-3.59	1.32	1.37
35	b	620	C7Z	C2-C1	3.59	1.66	1.54
29	A	406	CLA	C1C-NC	-3.58	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	611	CLA	C1C-NC	-3.58	1.32	1.37
35	B	620	C7Z	C35-C34	3.57	1.54	1.43
35	b	620	C7Z	C35-C34	3.57	1.54	1.43
43	f	101	HEM	FE-NA	3.55	2.07	1.95
29	y	603	CLA	MG-ND	-3.55	1.98	2.05
29	C	510	CLA	MG-ND	-3.55	1.98	2.05
29	B	606	CLA	C1C-NC	-3.54	1.32	1.37
35	b	620	C7Z	C7-C6	3.54	1.57	1.45
29	N	602	CLA	C1C-NC	-3.51	1.32	1.37
29	c	506	CLA	C1C-NC	-3.50	1.32	1.37
29	B	611	CLA	C1C-NC	-3.49	1.32	1.37
35	B	620	C7Z	C7-C6	3.49	1.57	1.45
29	c	504	CLA	C1C-NC	-3.48	1.32	1.37
29	b	606	CLA	C1C-NC	-3.48	1.32	1.37
35	B	620	C7Z	C38-C25	3.47	1.56	1.50
29	b	605	CLA	C1C-NC	-3.47	1.32	1.37
42	d	405	PL9	C3-C4	-3.46	1.43	1.49
29	B	612	CLA	C1C-NC	-3.46	1.32	1.37
29	a	405	CLA	C1C-NC	-3.46	1.32	1.37
29	C	506	CLA	C1C-NC	-3.45	1.32	1.37
35	b	620	C7Z	C38-C25	3.44	1.56	1.50
29	C	504	CLA	C1C-NC	-3.42	1.32	1.37
29	a	410	CLA	C1C-NC	-3.42	1.32	1.37
29	B	610	CLA	C1C-NC	-3.41	1.32	1.37
29	a	407	CLA	C1C-NC	-3.41	1.32	1.37
36	C	524	DGA	OG2-CB1	3.41	1.43	1.34
29	C	502	CLA	C1C-NC	-3.41	1.32	1.37
29	a	406	CLA	C1C-NC	-3.40	1.32	1.37
36	c	524	DGA	OG2-CB1	3.40	1.43	1.34
29	r	608	CLA	C1C-NC	-3.40	1.32	1.37
29	b	608	CLA	C1C-NC	-3.40	1.32	1.37
30	a	408	PHO	C4D-CHA	3.39	1.45	1.39
29	c	503	CLA	C1C-NC	-3.38	1.32	1.37
30	A	408	PHO	C4D-CHA	3.38	1.45	1.39
29	N	610	CLA	C1C-NC	-3.37	1.32	1.37
29	R	608	CLA	C1C-NC	-3.37	1.32	1.37
29	C	507	CLA	C1C-NC	-3.37	1.32	1.37
29	A	405	CLA	C1C-NC	-3.37	1.32	1.37
29	n	602	CLA	C1C-NC	-3.37	1.32	1.37
29	B	602	CLA	C1C-NC	-3.36	1.32	1.37
44	h	101	RRX	C11-C10	3.36	1.53	1.43
44	H	101	RRX	C11-C10	3.36	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	608	CLA	C1C-NC	-3.36	1.32	1.37
29	Y	611	CLA	C1C-NC	-3.36	1.32	1.37
29	c	509	CLA	C1C-NC	-3.36	1.32	1.37
29	A	410	CLA	C1C-NC	-3.35	1.32	1.37
29	B	613	CLA	C1C-NC	-3.35	1.32	1.37
36	B	625	DGA	OG1-CA1	3.35	1.43	1.33
29	A	407	CLA	C1C-NC	-3.35	1.32	1.37
29	d	402	CLA	C1C-NC	-3.35	1.32	1.37
29	n	610	CLA	C1C-NC	-3.34	1.32	1.37
29	Y	602	CLA	C1C-NC	-3.34	1.32	1.37
29	g	610	CLA	C1C-NC	-3.34	1.32	1.37
29	n	612	CLA	C1C-NC	-3.33	1.32	1.37
36	b	623	DGA	OG1-CA1	3.33	1.43	1.33
29	b	615	CLA	C1C-NC	-3.33	1.32	1.37
29	C	509	CLA	C1C-NC	-3.33	1.32	1.37
29	y	603	CLA	C1C-NC	-3.32	1.32	1.37
29	y	604	CLA	C1C-NC	-3.32	1.32	1.37
29	Y	610	CLA	C1C-NC	-3.32	1.32	1.37
29	n	603	CLA	C1C-NC	-3.32	1.32	1.37
29	c	513	CLA	C1C-NC	-3.31	1.32	1.37
29	y	610	CLA	C1C-NC	-3.31	1.32	1.37
29	c	507	CLA	C1C-NC	-3.31	1.32	1.37
29	b	613	CLA	C1C-NC	-3.31	1.32	1.37
29	C	510	CLA	C1C-NC	-3.31	1.32	1.37
29	D	402	CLA	C1C-NC	-3.31	1.32	1.37
29	c	505	CLA	C1C-NC	-3.30	1.32	1.37
29	s	604	CLA	C1C-NC	-3.30	1.32	1.37
29	y	602	CLA	C1C-NC	-3.30	1.32	1.37
36	C	524	DGA	OG1-CA1	3.30	1.43	1.33
29	S	604	CLA	C1C-NC	-3.30	1.32	1.37
29	B	604	CLA	C1C-NC	-3.30	1.32	1.37
29	C	505	CLA	C1C-NC	-3.30	1.32	1.37
29	G	602	CLA	C1C-NC	-3.29	1.32	1.37
29	B	615	CLA	C1C-NC	-3.29	1.32	1.37
29	r	609	CLA	C1C-NC	-3.29	1.32	1.37
36	c	524	DGA	OG1-CA1	3.29	1.42	1.33
29	g	602	CLA	C1C-NC	-3.28	1.32	1.37
29	g	612	CLA	C1C-NC	-3.28	1.32	1.37
29	C	503	CLA	C1C-NC	-3.28	1.32	1.37
29	c	501	CLA	C1C-NC	-3.28	1.32	1.37
29	n	604	CLA	C1C-NC	-3.28	1.32	1.37
29	b	604	CLA	C1C-NC	-3.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	c	519	DGD	CDB-CCB	-3.27	1.33	1.51
29	S	603	CLA	C1C-NC	-3.27	1.32	1.37
44	H	101	RRX	C24-C25	3.27	1.56	1.45
29	C	513	CLA	C1C-NC	-3.27	1.32	1.37
29	s	603	CLA	C1C-NC	-3.27	1.32	1.37
29	b	602	CLA	C1C-NC	-3.27	1.32	1.37
29	r	610	CLA	C1C-NC	-3.26	1.32	1.37
29	B	607	CLA	C1C-NC	-3.26	1.32	1.37
42	D	405	PL9	C3-C4	-3.26	1.44	1.49
29	N	603	CLA	C1C-NC	-3.26	1.32	1.37
29	r	613	CLA	C1C-NC	-3.26	1.32	1.37
29	C	511	CLA	C1C-NC	-3.26	1.32	1.37
29	G	603	CLA	C1C-NC	-3.26	1.32	1.37
38	c	518	DGD	CDB-CCB	-3.26	1.33	1.51
29	R	613	CLA	C1C-NC	-3.26	1.32	1.37
29	b	614	CLA	C1C-NC	-3.26	1.32	1.37
33	b	622	LMG	C22-C21	-3.26	1.33	1.51
38	C	523	DGD	CAA-C9A	-3.25	1.33	1.51
29	y	608	CLA	C1C-NC	-3.25	1.32	1.37
38	C	519	DGD	CDB-CCB	-3.25	1.33	1.51
29	D	403	CLA	C1C-NC	-3.25	1.33	1.37
38	c	520	DGD	CAA-C9A	-3.25	1.33	1.51
38	C	523	DGD	CGA-CFA	-3.25	1.33	1.51
33	h	102	LMG	C37-C36	-3.25	1.33	1.51
38	C	520	DGD	CAB-C9B	-3.25	1.33	1.51
29	R	609	CLA	C1C-NC	-3.25	1.33	1.37
38	c	523	DGD	CAA-C9A	-3.25	1.33	1.51
33	B	622	LMG	C22-C21	-3.25	1.33	1.51
29	N	612	CLA	C1C-NC	-3.25	1.33	1.37
29	Y	612	CLA	C1C-NC	-3.25	1.33	1.37
38	c	523	DGD	CDB-CCB	-3.25	1.33	1.51
44	h	101	RRX	C24-C25	3.25	1.56	1.45
38	C	520	DGD	CAA-C9A	-3.25	1.33	1.51
33	H	102	LMG	C19-C18	-3.24	1.33	1.51
38	c	520	DGD	CAB-C9B	-3.24	1.33	1.51
29	y	611	CLA	C1C-NC	-3.24	1.33	1.37
33	c	521	LMG	C22-C21	-3.24	1.33	1.51
33	c	521	LMG	C40-C39	-3.24	1.33	1.51
29	s	609	CLA	C1C-NC	-3.24	1.33	1.37
38	c	523	DGD	CGA-CFA	-3.24	1.33	1.51
29	b	616	CLA	C1C-NC	-3.24	1.33	1.37
38	C	519	DGD	CDA-CCA	-3.24	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	609	CLA	C1C-NC	-3.24	1.33	1.37
29	S	602	CLA	C1C-NC	-3.24	1.33	1.37
43	F	101	HEM	FE-NC	3.24	2.06	1.95
29	Y	604	CLA	C1C-NC	-3.24	1.33	1.37
33	h	102	LMG	C19-C18	-3.24	1.33	1.51
29	d	403	CLA	C1C-NC	-3.24	1.33	1.37
38	c	519	DGD	CDA-CCA	-3.23	1.33	1.51
29	b	607	CLA	C1C-NC	-3.23	1.33	1.37
33	C	521	LMG	C22-C21	-3.23	1.33	1.51
29	s	611	CLA	C1C-NC	-3.23	1.33	1.37
29	G	604	CLA	C1C-NC	-3.23	1.33	1.37
33	C	521	LMG	C40-C39	-3.23	1.33	1.51
33	H	102	LMG	C40-C39	-3.23	1.33	1.51
38	C	518	DGD	CDB-CCB	-3.23	1.33	1.51
38	C	523	DGD	CDB-CCB	-3.23	1.33	1.51
29	g	611	CLA	C1C-NC	-3.23	1.33	1.37
29	g	613	CLA	C1C-NC	-3.23	1.33	1.37
29	g	603	CLA	C1C-NC	-3.23	1.33	1.37
29	s	610	CLA	C1C-NC	-3.23	1.33	1.37
33	b	622	LMG	C19-C18	-3.22	1.33	1.51
29	C	512	CLA	C1C-NC	-3.22	1.33	1.37
29	N	613	CLA	C1C-NC	-3.22	1.33	1.37
44	h	101	RRX	C16-C17	3.22	1.53	1.43
38	c	523	DGD	CAB-C9B	-3.22	1.33	1.51
29	r	603	CLA	C1C-NC	-3.22	1.33	1.37
38	c	519	DGD	CAB-C9B	-3.22	1.33	1.51
29	G	612	CLA	C1C-NC	-3.22	1.33	1.37
33	B	622	LMG	C19-C18	-3.21	1.33	1.51
29	c	512	CLA	C1C-NC	-3.21	1.33	1.37
33	H	102	LMG	C37-C36	-3.21	1.33	1.51
29	Y	603	CLA	C1C-NC	-3.21	1.33	1.37
38	C	518	DGD	CAB-C9B	-3.21	1.33	1.51
38	c	518	DGD	CAB-C9B	-3.21	1.33	1.51
33	J	101	LMG	C19-C18	-3.21	1.33	1.51
38	C	523	DGD	CDA-CCA	-3.21	1.33	1.51
38	C	523	DGD	CAB-C9B	-3.21	1.33	1.51
29	y	613	CLA	C1C-NC	-3.21	1.33	1.37
29	s	613	CLA	C1C-NC	-3.21	1.33	1.37
29	B	616	CLA	C1C-NC	-3.21	1.33	1.37
38	C	523	DGD	CGB-CFB	-3.21	1.33	1.51
33	h	102	LMG	C40-C39	-3.21	1.33	1.51
38	C	519	DGD	CAB-C9B	-3.21	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	411	LMG	C19-C18	-3.21	1.33	1.51
33	c	521	LMG	C19-C18	-3.20	1.33	1.51
33	A	413	LMG	C40-C39	-3.20	1.33	1.51
33	J	101	LMG	C22-C21	-3.20	1.33	1.51
33	c	521	LMG	C37-C36	-3.20	1.33	1.51
29	S	610	CLA	C1C-NC	-3.20	1.33	1.37
29	S	614	CLA	C1C-NC	-3.20	1.33	1.37
33	j	101	LMG	C19-C18	-3.20	1.33	1.51
29	N	604	CLA	C1C-NC	-3.20	1.33	1.37
29	a	410	CLA	C4B-NB	-3.20	1.33	1.37
29	g	604	CLA	C1C-NC	-3.20	1.33	1.37
33	D	411	LMG	C19-C18	-3.20	1.33	1.51
33	d	411	LMG	C22-C21	-3.20	1.33	1.51
44	H	101	RRX	C16-C17	3.20	1.53	1.43
33	D	411	LMG	C22-C21	-3.20	1.33	1.51
33	a	413	LMG	C37-C36	-3.20	1.33	1.51
33	A	413	LMG	C37-C36	-3.20	1.33	1.51
44	h	101	RRX	C29-C30	3.20	1.64	1.54
29	Y	613	CLA	C1C-NC	-3.20	1.33	1.37
33	j	101	LMG	C22-C21	-3.20	1.33	1.51
33	C	521	LMG	C37-C36	-3.20	1.33	1.51
29	S	613	CLA	C1C-NC	-3.20	1.33	1.37
33	C	521	LMG	C19-C18	-3.20	1.33	1.51
38	c	523	DGD	CDA-CCA	-3.20	1.33	1.51
38	c	523	DGD	CGB-CFB	-3.20	1.33	1.51
29	r	604	CLA	C1C-NC	-3.19	1.33	1.37
29	R	602	CLA	C1C-NC	-3.19	1.33	1.37
29	c	510	CLA	C1C-NC	-3.19	1.33	1.37
38	c	519	DGD	CAA-C9A	-3.19	1.33	1.51
29	R	610	CLA	C1C-NC	-3.19	1.33	1.37
33	a	413	LMG	C40-C39	-3.19	1.33	1.51
29	R	604	CLA	C1C-NC	-3.18	1.33	1.37
29	S	605	CLA	C1C-NC	-3.18	1.33	1.37
29	s	605	CLA	C1C-NC	-3.18	1.33	1.37
44	H	101	RRX	C4-C5	-3.18	1.44	1.51
29	c	502	CLA	C4B-NB	-3.18	1.33	1.37
29	g	614	CLA	C1C-NC	-3.18	1.33	1.37
29	c	511	CLA	C1C-NC	-3.18	1.33	1.37
43	F	101	HEM	FE-NA	3.18	2.05	1.95
29	S	611	CLA	C1C-NC	-3.18	1.33	1.37
29	b	603	CLA	C1C-NC	-3.18	1.33	1.37
29	B	603	CLA	C1C-NC	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	612	CLA	C1C-NC	-3.18	1.33	1.37
29	G	613	CLA	C1C-NC	-3.18	1.33	1.37
29	s	617	CLA	C1C-NC	-3.18	1.33	1.37
29	B	609	CLA	C1C-NC	-3.18	1.33	1.37
33	A	413	LMG	C19-C18	-3.18	1.33	1.51
29	y	614	CLA	C1C-NC	-3.17	1.33	1.37
44	h	101	RRX	C4-C5	-3.17	1.44	1.51
29	C	501	CLA	C1C-NC	-3.17	1.33	1.37
29	G	611	CLA	C1C-NC	-3.17	1.33	1.37
29	n	614	CLA	C1C-NC	-3.17	1.33	1.37
38	C	519	DGD	CAA-C9A	-3.17	1.33	1.51
29	R	603	CLA	C1C-NC	-3.17	1.33	1.37
44	H	101	RRX	C29-C30	3.17	1.64	1.54
29	G	614	CLA	C1C-NC	-3.17	1.33	1.37
29	r	602	CLA	C1C-NC	-3.17	1.33	1.37
29	n	613	CLA	C1C-NC	-3.16	1.33	1.37
29	y	612	CLA	C1C-NC	-3.16	1.33	1.37
33	a	413	LMG	C19-C18	-3.16	1.33	1.51
38	c	520	DGD	CDB-CCB	-3.16	1.33	1.51
29	S	612	CLA	C1C-NC	-3.16	1.33	1.37
29	s	612	CLA	C1C-NC	-3.16	1.33	1.37
29	S	609	CLA	C1C-NC	-3.16	1.33	1.37
29	S	617	CLA	C1C-NC	-3.16	1.33	1.37
29	r	612	CLA	C1C-NC	-3.16	1.33	1.37
38	C	520	DGD	CDB-CCB	-3.15	1.33	1.51
29	B	614	CLA	C1C-NC	-3.15	1.33	1.37
29	Y	614	CLA	C1C-NC	-3.14	1.33	1.37
29	N	611	CLA	C1C-NC	-3.14	1.33	1.37
29	b	606	CLA	C4B-NB	-3.14	1.33	1.37
29	B	606	CLA	C4B-NB	-3.13	1.33	1.37
29	s	602	CLA	C1C-NC	-3.13	1.33	1.37
29	A	410	CLA	C4B-NB	-3.13	1.33	1.37
29	N	602	CLA	C4B-NB	-3.13	1.33	1.37
29	b	617	CLA	C4B-NB	-3.13	1.33	1.37
29	r	611	CLA	C1C-NC	-3.13	1.33	1.37
29	N	614	CLA	C1C-NC	-3.12	1.33	1.37
29	A	406	CLA	C4B-NB	-3.12	1.33	1.37
29	a	405	CLA	C4B-NB	-3.12	1.33	1.37
29	a	406	CLA	C4B-NB	-3.12	1.33	1.37
29	Y	608	CLA	C1C-NC	-3.12	1.33	1.37
29	n	611	CLA	C1C-NC	-3.12	1.33	1.37
29	s	614	CLA	C1C-NC	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	617	CLA	C4B-NB	-3.11	1.34	1.37
29	R	611	CLA	C1C-NC	-3.10	1.33	1.37
29	A	405	CLA	C4B-NB	-3.09	1.34	1.37
43	f	101	HEM	FE-NB	3.07	2.04	1.94
29	C	502	CLA	C4B-NB	-3.06	1.34	1.37
43	f	101	HEM	CAC-C3C	3.06	1.55	1.47
29	c	508	CLA	C4B-NB	-3.05	1.34	1.37
44	H	101	RRX	C7-C6	3.03	1.55	1.45
43	F	101	HEM	CAC-C3C	3.03	1.55	1.47
29	c	507	CLA	C4B-NB	-3.03	1.34	1.37
29	C	507	CLA	C4B-NB	-3.03	1.34	1.37
29	c	506	CLA	C4B-NB	-3.03	1.34	1.37
29	c	509	CLA	C4B-NB	-3.01	1.34	1.37
44	h	101	RRX	C7-C6	3.00	1.55	1.45
29	b	612	CLA	C4B-NB	-3.00	1.34	1.37
29	b	615	CLA	C4B-NB	-2.98	1.34	1.37
43	f	101	HEM	CAB-C3B	2.97	1.55	1.47
43	F	101	HEM	CAB-C3B	2.97	1.55	1.47
29	b	610	CLA	C4B-NB	-2.96	1.34	1.37
29	y	604	CLA	C4B-NB	-2.96	1.34	1.37
29	B	615	CLA	C4B-NB	-2.96	1.34	1.37
29	c	504	CLA	C4B-NB	-2.95	1.34	1.37
29	s	612	CLA	C4B-NB	-2.95	1.34	1.37
29	C	506	CLA	C4B-NB	-2.95	1.34	1.37
29	C	510	CLA	C4B-NB	-2.94	1.34	1.37
29	b	616	CLA	C4B-NB	-2.94	1.34	1.37
29	B	610	CLA	C4B-NB	-2.94	1.34	1.37
29	C	508	CLA	C4B-NB	-2.94	1.34	1.37
29	B	616	CLA	C4B-NB	-2.94	1.34	1.37
29	S	603	CLA	C4B-NB	-2.94	1.34	1.37
29	n	602	CLA	C4B-NB	-2.94	1.34	1.37
29	s	610	CLA	C4B-NB	-2.93	1.34	1.37
29	G	610	CLA	C4B-NB	-2.93	1.34	1.37
29	b	613	CLA	C4B-NB	-2.93	1.34	1.37
43	f	101	HEM	FE-NC	2.92	2.05	1.95
29	C	504	CLA	C4B-NB	-2.91	1.34	1.37
29	C	509	CLA	C4B-NB	-2.91	1.34	1.37
29	B	609	CLA	C4B-NB	-2.90	1.34	1.37
29	b	605	CLA	C4B-NB	-2.90	1.34	1.37
29	b	608	CLA	C4B-NB	-2.90	1.34	1.37
29	c	510	CLA	C4B-NB	-2.90	1.34	1.37
29	Y	611	CLA	C4B-NB	-2.89	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	407	CLA	C4B-NB	-2.89	1.34	1.37
29	S	612	CLA	C4B-NB	-2.89	1.34	1.37
29	y	612	CLA	C4B-NB	-2.89	1.34	1.37
29	b	609	CLA	C4B-NB	-2.88	1.34	1.37
29	S	610	CLA	C4B-NB	-2.88	1.34	1.37
29	A	407	CLA	C4B-NB	-2.88	1.34	1.37
29	C	511	CLA	C4B-NB	-2.87	1.34	1.37
29	g	610	CLA	C4B-NB	-2.87	1.34	1.37
29	c	511	CLA	C4B-NB	-2.87	1.34	1.37
29	B	608	CLA	C4B-NB	-2.87	1.34	1.37
29	C	512	CLA	C4B-NB	-2.86	1.34	1.37
29	r	609	CLA	C4B-NB	-2.86	1.34	1.37
29	Y	610	CLA	C4B-NB	-2.86	1.34	1.37
29	Y	612	CLA	C4B-NB	-2.86	1.34	1.37
29	c	513	CLA	C4B-NB	-2.86	1.34	1.37
29	Y	613	CLA	C4B-NB	-2.86	1.34	1.37
29	B	603	CLA	C4B-NB	-2.86	1.34	1.37
29	Y	602	CLA	C4B-NB	-2.85	1.34	1.37
29	C	513	CLA	C4B-NB	-2.85	1.34	1.37
29	y	611	CLA	C4B-NB	-2.85	1.34	1.37
29	c	505	CLA	C4B-NB	-2.85	1.34	1.37
29	C	505	CLA	C4B-NB	-2.84	1.34	1.37
29	B	613	CLA	C4B-NB	-2.83	1.34	1.37
29	n	610	CLA	C4B-NB	-2.82	1.34	1.37
29	B	612	CLA	C4B-NB	-2.82	1.34	1.37
29	c	512	CLA	C4B-NB	-2.82	1.34	1.37
29	s	604	CLA	C4B-NB	-2.82	1.34	1.37
29	Y	608	CLA	C4B-NB	-2.81	1.34	1.37
49	S	625	LPX	P1-O1	2.81	1.70	1.59
29	S	614	CLA	C4B-NB	-2.81	1.34	1.37
29	g	613	CLA	C4B-NB	-2.81	1.34	1.37
29	S	604	CLA	C4B-NB	-2.81	1.34	1.37
29	B	614	CLA	C4B-NB	-2.80	1.34	1.37
29	B	607	CLA	C4B-NB	-2.80	1.34	1.37
29	n	604	CLA	C4B-NB	-2.80	1.34	1.37
29	r	603	CLA	C4B-NB	-2.80	1.34	1.37
29	s	614	CLA	C4B-NB	-2.80	1.34	1.37
29	S	617	CLA	C4B-NB	-2.80	1.34	1.37
29	N	610	CLA	C4B-NB	-2.79	1.34	1.37
29	y	602	CLA	C4B-NB	-2.79	1.34	1.37
29	s	603	CLA	C4B-NB	-2.79	1.34	1.37
29	Y	604	CLA	C4B-NB	-2.79	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g	611	CLA	C4B-NB	-2.79	1.34	1.37
29	s	617	CLA	C4B-NB	-2.79	1.34	1.37
29	R	609	CLA	C4B-NB	-2.78	1.34	1.37
29	y	610	CLA	C4B-NB	-2.78	1.34	1.37
29	G	604	CLA	C4B-NB	-2.78	1.34	1.37
29	s	605	CLA	C4B-NB	-2.78	1.34	1.37
29	R	612	CLA	C4B-NB	-2.78	1.34	1.37
29	B	604	CLA	C4B-NB	-2.78	1.34	1.37
29	S	602	CLA	C4B-NB	-2.78	1.34	1.37
29	r	602	CLA	C4B-NB	-2.77	1.34	1.37
29	y	608	CLA	C4B-NB	-2.77	1.34	1.37
29	b	614	CLA	C4B-NB	-2.77	1.34	1.37
29	G	602	CLA	C4B-NB	-2.77	1.34	1.37
29	N	613	CLA	C4B-NB	-2.77	1.34	1.37
45	n	609	CHL	C1B-NB	-2.77	1.34	1.37
29	b	604	CLA	C4B-NB	-2.76	1.34	1.37
29	G	611	CLA	C4B-NB	-2.75	1.34	1.37
29	b	607	CLA	C4B-NB	-2.75	1.34	1.37
49	s	625	LPX	P1-O1	2.75	1.70	1.59
29	S	611	CLA	C4B-NB	-2.75	1.34	1.37
29	N	614	CLA	C4B-NB	-2.75	1.34	1.37
29	R	604	CLA	C4B-NB	-2.74	1.34	1.37
29	R	602	CLA	C4B-NB	-2.74	1.34	1.37
29	r	610	CLA	C4B-NB	-2.74	1.34	1.37
29	R	603	CLA	C4B-NB	-2.74	1.34	1.37
29	b	603	CLA	C4B-NB	-2.74	1.34	1.37
29	G	613	CLA	C4B-NB	-2.73	1.34	1.37
29	c	503	CLA	C4B-NB	-2.73	1.34	1.37
29	B	605	CLA	C4B-NB	-2.73	1.34	1.37
29	g	602	CLA	C4B-NB	-2.73	1.34	1.37
29	r	604	CLA	C4B-NB	-2.73	1.34	1.37
29	n	613	CLA	C4B-NB	-2.73	1.34	1.37
29	g	612	CLA	C4B-NB	-2.72	1.34	1.37
29	R	613	CLA	C4B-NB	-2.71	1.34	1.37
29	S	609	CLA	C4B-NB	-2.71	1.34	1.37
29	g	604	CLA	C4B-NB	-2.71	1.34	1.37
29	N	604	CLA	C4B-NB	-2.71	1.34	1.37
29	s	602	CLA	C4B-NB	-2.71	1.34	1.37
44	H	101	RRX	C32-C1	2.71	1.59	1.53
29	N	611	CLA	C4B-NB	-2.71	1.34	1.37
29	R	610	CLA	C4B-NB	-2.71	1.34	1.37
29	r	613	CLA	C4B-NB	-2.70	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	612	CLA	C4B-NB	-2.70	1.34	1.37
29	Y	614	CLA	C4B-NB	-2.70	1.34	1.37
29	n	603	CLA	C4B-NB	-2.70	1.34	1.37
44	h	101	RRX	C32-C1	2.70	1.59	1.53
45	Y	601	CHL	C1B-NB	-2.69	1.34	1.37
29	G	614	CLA	C4B-NB	-2.68	1.34	1.37
29	C	503	CLA	C4B-NB	-2.67	1.34	1.37
29	r	612	CLA	C4B-NB	-2.67	1.34	1.37
30	A	409	PHO	CMD-C2D	-2.66	1.46	1.51
29	s	613	CLA	C4B-NB	-2.66	1.34	1.37
29	R	611	CLA	C4B-NB	-2.65	1.34	1.37
29	n	614	CLA	C4B-NB	-2.65	1.34	1.37
29	y	613	CLA	C4B-NB	-2.65	1.34	1.37
29	S	605	CLA	C4B-NB	-2.65	1.34	1.37
45	Y	607	CHL	C1B-NB	-2.65	1.34	1.37
29	s	611	CLA	C4B-NB	-2.65	1.34	1.37
29	N	603	CLA	C4B-NB	-2.64	1.34	1.37
29	g	603	CLA	C4B-NB	-2.63	1.34	1.37
29	c	501	CLA	C4B-NB	-2.62	1.34	1.37
29	s	609	CLA	C4B-NB	-2.62	1.34	1.37
29	C	501	CLA	C4B-NB	-2.62	1.34	1.37
29	Y	603	CLA	C4B-NB	-2.62	1.34	1.37
29	D	403	CLA	C4B-NB	-2.62	1.34	1.37
29	S	613	CLA	C4B-NB	-2.62	1.34	1.37
29	g	614	CLA	C4B-NB	-2.61	1.34	1.37
29	d	403	CLA	C4B-NB	-2.61	1.34	1.37
29	n	611	CLA	C4B-NB	-2.61	1.34	1.37
42	d	405	PL9	C6-C1	-2.61	1.43	1.48
29	b	602	CLA	C4B-NB	-2.61	1.34	1.37
30	a	409	PHO	CMC-C2C	-2.60	1.46	1.50
29	y	614	CLA	C4B-NB	-2.60	1.34	1.37
33	J	101	LMG	C37-C36	-2.60	1.33	1.51
29	n	612	CLA	C4B-NB	-2.60	1.34	1.37
33	j	101	LMG	C37-C36	-2.59	1.33	1.51
45	y	601	CHL	C1B-NB	-2.58	1.34	1.37
42	D	405	PL9	C6-C1	-2.57	1.44	1.48
45	n	607	CHL	C1B-NB	-2.56	1.34	1.37
48	s	623	NEX	C1-C6	-2.55	1.50	1.54
29	r	611	CLA	C4B-NB	-2.55	1.34	1.37
33	d	411	LMG	C37-C36	-2.55	1.33	1.51
29	R	608	CLA	C4B-NB	-2.55	1.34	1.37
29	B	602	CLA	C4B-NB	-2.55	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	612	CLA	C4B-NB	-2.55	1.34	1.37
35	b	620	C7Z	C18-C5	2.54	1.55	1.50
29	G	603	CLA	C4B-NB	-2.54	1.34	1.37
33	D	411	LMG	C37-C36	-2.53	1.33	1.51
50	s	626	3PH	O21-C2	-2.53	1.40	1.46
45	G	607	CHL	C1B-NB	-2.52	1.34	1.37
30	A	409	PHO	CMC-C2C	-2.52	1.46	1.50
29	r	608	CLA	C4B-NB	-2.52	1.34	1.37
30	a	408	PHO	CMC-C2C	-2.52	1.46	1.50
29	b	611	CLA	C4B-NB	-2.52	1.34	1.37
35	B	620	C7Z	C18-C5	2.51	1.55	1.50
45	g	607	CHL	C1B-NB	-2.51	1.34	1.37
50	S	626	3PH	O21-C2	-2.51	1.40	1.46
29	B	611	CLA	C4B-NB	-2.50	1.34	1.37
45	N	607	CHL	C1B-NB	-2.50	1.34	1.37
30	A	408	PHO	C4D-ND	-2.49	1.35	1.38
35	b	620	C7Z	C21-C26	-2.49	1.50	1.53
35	B	620	C7Z	C21-C26	-2.49	1.50	1.53
30	a	408	PHO	C4D-ND	-2.48	1.35	1.38
30	a	409	PHO	CMD-C2D	-2.46	1.46	1.51
50	i	101	3PH	O21-C2	-2.46	1.40	1.46
50	S	626	3PH	O31-C31	2.45	1.40	1.33
30	A	408	PHO	CMC-C2C	-2.45	1.46	1.50
30	a	409	PHO	C3D-C4D	2.44	1.44	1.41
45	N	609	CHL	C1B-NB	-2.44	1.34	1.37
30	A	408	PHO	CMD-C2D	-2.44	1.46	1.51
44	h	101	RRX	C35-C13	2.44	1.55	1.50
29	d	402	CLA	C4B-NB	-2.44	1.34	1.37
47	r	622	XAT	O24-C25	-2.43	1.42	1.46
44	H	101	RRX	C35-C13	2.43	1.55	1.50
45	y	607	CHL	C1B-NB	-2.42	1.34	1.37
50	i	101	3PH	O31-C31	2.42	1.40	1.33
30	a	408	PHO	CMD-C2D	-2.42	1.46	1.51
47	g	622	XAT	O24-C25	-2.41	1.42	1.46
35	B	620	C7Z	C20-C13	2.41	1.55	1.50
35	b	620	C7Z	C20-C13	2.41	1.55	1.50
50	s	626	3PH	O31-C31	2.39	1.40	1.33
45	g	606	CHL	C1B-NB	-2.39	1.34	1.37
29	S	613	CLA	C1A-CHA	2.39	1.53	1.43
29	s	613	CLA	C1A-CHA	2.38	1.53	1.43
29	S	605	CLA	C1A-CHA	2.36	1.52	1.43
29	b	609	CLA	C1A-CHA	2.36	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	N	608	CHL	C1B-NB	-2.35	1.34	1.37
29	R	610	CLA	C1C-C2C	2.35	1.49	1.44
30	A	408	PHO	CMB-C2B	-2.34	1.46	1.51
47	G	622	XAT	O24-C25	-2.34	1.42	1.46
30	a	408	PHO	CMB-C2B	-2.33	1.46	1.51
29	D	402	CLA	C4B-NB	-2.33	1.34	1.37
29	s	605	CLA	C1A-CHA	2.33	1.52	1.43
29	d	403	CLA	C1C-C2C	2.32	1.49	1.44
29	B	609	CLA	C1A-CHA	2.32	1.52	1.43
29	B	616	CLA	C1A-CHA	2.32	1.52	1.43
45	N	601	CHL	C1B-NB	-2.31	1.34	1.37
29	B	608	CLA	C1A-CHA	2.30	1.52	1.43
29	b	605	CLA	C1A-CHA	2.30	1.52	1.43
47	Y	622	XAT	O24-C25	-2.30	1.42	1.46
29	y	603	CLA	C4B-NB	-2.30	1.35	1.37
30	A	409	PHO	CMB-C2B	-2.29	1.46	1.51
48	n	623	NEX	C1-C6	-2.29	1.50	1.54
29	c	505	CLA	C1A-CHA	2.29	1.52	1.43
49	S	625	LPX	P1-O2	2.28	1.68	1.59
29	C	505	CLA	C1A-CHA	2.28	1.52	1.43
29	B	605	CLA	C1A-CHA	2.28	1.52	1.43
29	b	615	CLA	C1A-CHA	2.28	1.52	1.43
47	R	621	XAT	O24-C25	-2.28	1.43	1.46
29	c	512	CLA	C1C-C2C	2.28	1.49	1.44
49	s	625	LPX	P1-O2	2.27	1.68	1.59
29	b	616	CLA	C1A-CHA	2.27	1.52	1.43
29	B	611	CLA	C3B-C4B	2.27	1.48	1.42
30	A	408	PHO	CAC-C3C	-2.26	1.47	1.51
29	b	608	CLA	C1A-CHA	2.26	1.52	1.43
45	n	608	CHL	C1B-NB	-2.25	1.35	1.37
45	G	609	CHL	C1B-NB	-2.25	1.35	1.37
29	b	612	CLA	C1A-CHA	2.25	1.52	1.43
29	n	613	CLA	C1C-C2C	2.25	1.48	1.44
30	A	409	PHO	CAC-C3C	-2.25	1.47	1.51
30	a	409	PHO	CMB-C2B	-2.25	1.47	1.51
45	R	606	CHL	C1B-NB	-2.24	1.35	1.37
29	c	501	CLA	C1A-CHA	2.24	1.52	1.43
29	R	603	CLA	C1C-C2C	2.24	1.48	1.44
45	r	606	CHL	C1B-NB	-2.24	1.35	1.37
29	C	512	CLA	C1C-C2C	2.24	1.48	1.44
29	b	611	CLA	C3B-C4B	2.24	1.48	1.42
29	a	407	CLA	C1A-CHA	2.24	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	r	608	CLA	C1A-CHA	2.24	1.52	1.43
29	C	501	CLA	C1A-CHA	2.24	1.52	1.43
30	A	409	PHO	C3D-C4D	2.24	1.44	1.41
29	S	602	CLA	C1C-C2C	2.24	1.48	1.44
29	D	403	CLA	C1C-C2C	2.23	1.48	1.44
29	r	603	CLA	C1C-C2C	2.23	1.48	1.44
29	N	604	CLA	C1C-C2C	2.23	1.48	1.44
29	C	507	CLA	C1A-CHA	2.23	1.52	1.43
47	N	622	XAT	O24-C25	-2.22	1.43	1.46
29	R	608	CLA	C1A-CHA	2.22	1.52	1.43
29	n	611	CLA	C1A-CHA	2.22	1.52	1.43
29	r	610	CLA	C1A-CHA	2.22	1.52	1.43
29	y	611	CLA	C1A-CHA	2.22	1.52	1.43
29	N	613	CLA	C1A-CHA	2.22	1.52	1.43
29	n	614	CLA	C1C-C2C	2.22	1.48	1.44
29	B	615	CLA	C1A-CHA	2.22	1.52	1.43
29	B	614	CLA	C1A-CHA	2.22	1.52	1.43
29	y	613	CLA	C1C-C2C	2.22	1.48	1.44
29	R	613	CLA	C1A-CHA	2.22	1.52	1.43
29	c	512	CLA	C1A-CHA	2.22	1.52	1.43
29	R	612	CLA	C1A-CHA	2.22	1.52	1.43
30	a	408	PHO	CAC-C3C	-2.22	1.47	1.51
29	A	406	CLA	C1A-CHA	2.21	1.52	1.43
29	C	512	CLA	C1A-CHA	2.21	1.52	1.43
29	s	609	CLA	C1A-CHA	2.21	1.52	1.43
29	A	407	CLA	C1A-CHA	2.21	1.52	1.43
29	N	604	CLA	C1A-CHA	2.21	1.52	1.43
29	y	613	CLA	C1A-CHA	2.21	1.52	1.43
47	n	622	XAT	O24-C25	-2.21	1.43	1.46
29	g	611	CLA	C1A-CHA	2.21	1.52	1.43
29	G	614	CLA	C1C-C2C	2.20	1.48	1.44
29	Y	612	CLA	C1A-CHA	2.20	1.52	1.43
29	G	611	CLA	C1A-CHA	2.20	1.52	1.43
29	Y	613	CLA	C1A-CHA	2.20	1.52	1.43
29	S	611	CLA	C1A-CHA	2.20	1.52	1.43
42	d	405	PL9	C53-C6	-2.20	1.46	1.50
45	s	606	CHL	C1B-NB	-2.20	1.35	1.37
29	y	612	CLA	C1A-CHA	2.20	1.52	1.43
29	R	602	CLA	C1C-C2C	2.20	1.48	1.44
29	Y	611	CLA	C1A-CHA	2.20	1.52	1.43
29	g	610	CLA	C1A-CHA	2.20	1.52	1.43
29	N	614	CLA	C1C-C2C	2.20	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	604	CLA	C1A-CHA	2.20	1.52	1.43
29	b	603	CLA	C1A-CHA	2.20	1.52	1.43
29	G	613	CLA	C1A-CHA	2.20	1.52	1.43
47	y	622	XAT	O24-C25	-2.19	1.43	1.46
29	d	402	CLA	C1C-C2C	2.19	1.48	1.44
29	S	603	CLA	C1A-CHA	2.19	1.52	1.43
29	b	614	CLA	C1A-CHA	2.19	1.52	1.43
29	S	603	CLA	C1C-C2C	2.19	1.48	1.44
29	Y	603	CLA	C1A-CHA	2.19	1.52	1.43
29	r	612	CLA	C1A-CHA	2.19	1.52	1.43
29	C	502	CLA	C1A-CHA	2.19	1.52	1.43
29	n	614	CLA	C1A-CHA	2.19	1.52	1.43
29	C	513	CLA	C1C-C2C	2.19	1.48	1.44
30	a	409	PHO	C4D-ND	-2.19	1.35	1.38
29	c	502	CLA	C1A-CHA	2.19	1.52	1.43
29	S	617	CLA	C1C-C2C	2.19	1.48	1.44
29	s	610	CLA	C1C-C2C	2.19	1.48	1.44
29	s	605	CLA	C1C-C2C	2.18	1.48	1.44
29	y	603	CLA	C1A-CHA	2.18	1.52	1.43
29	C	501	CLA	C1C-C2C	2.18	1.48	1.44
29	N	611	CLA	C1A-CHA	2.18	1.52	1.43
29	B	612	CLA	C1A-CHA	2.18	1.52	1.43
29	s	611	CLA	C1A-CHA	2.18	1.52	1.43
29	N	612	CLA	C1A-CHA	2.18	1.52	1.43
29	N	614	CLA	C1A-CHA	2.18	1.52	1.43
29	g	613	CLA	C1A-CHA	2.18	1.52	1.43
29	R	611	CLA	C1A-CHA	2.18	1.52	1.43
29	b	602	CLA	C1C-C2C	2.18	1.48	1.44
29	S	612	CLA	C1A-CHA	2.18	1.52	1.43
29	a	406	CLA	C1A-CHA	2.18	1.52	1.43
29	s	617	CLA	C1A-CHA	2.18	1.52	1.43
29	R	611	CLA	C1C-C2C	2.18	1.48	1.44
29	y	602	CLA	C1C-C2C	2.18	1.48	1.44
29	S	609	CLA	C1A-CHA	2.18	1.52	1.43
29	n	613	CLA	C1A-CHA	2.17	1.52	1.43
29	G	604	CLA	C1A-CHA	2.17	1.52	1.43
29	g	614	CLA	C1A-CHA	2.17	1.52	1.43
29	b	604	CLA	C1A-CHA	2.17	1.52	1.43
29	r	603	CLA	C1A-CHA	2.17	1.52	1.43
29	r	611	CLA	C1A-CHA	2.17	1.52	1.43
29	r	613	CLA	C1A-CHA	2.17	1.52	1.43
29	s	612	CLA	C1A-CHA	2.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	613	CLA	C1C-C2C	2.17	1.48	1.44
29	Y	602	CLA	C1C-C2C	2.17	1.48	1.44
29	s	604	CLA	C1A-CHA	2.17	1.52	1.43
29	B	611	CLA	C1C-C2C	2.17	1.48	1.44
42	D	405	PL9	C53-C6	-2.17	1.46	1.50
30	a	408	PHO	C3D-C4D	2.17	1.44	1.41
30	a	409	PHO	CAC-C3C	-2.17	1.47	1.51
29	n	610	CLA	C1A-CHA	2.17	1.52	1.43
29	b	610	CLA	C1A-CHA	2.17	1.52	1.43
29	y	612	CLA	C1C-C2C	2.17	1.48	1.44
29	C	509	CLA	C1A-CHA	2.17	1.52	1.43
29	y	614	CLA	C1A-CHA	2.17	1.52	1.43
29	c	507	CLA	C1A-CHA	2.16	1.52	1.43
29	y	608	CLA	C1A-CHA	2.16	1.52	1.43
50	s	626	3PH	O21-C21	2.16	1.40	1.34
29	g	612	CLA	C1A-CHA	2.16	1.52	1.43
29	G	612	CLA	C1A-CHA	2.16	1.52	1.43
29	D	402	CLA	C1C-C2C	2.16	1.48	1.44
29	N	611	CLA	C1C-C2C	2.16	1.48	1.44
29	G	614	CLA	C1A-CHA	2.16	1.52	1.43
29	R	603	CLA	C1A-CHA	2.16	1.52	1.43
50	i	101	3PH	O21-C21	2.16	1.40	1.34
29	C	513	CLA	C1A-CHA	2.16	1.52	1.43
29	a	410	CLA	C1A-CHA	2.16	1.52	1.43
29	S	617	CLA	C1A-CHA	2.15	1.52	1.43
29	y	603	CLA	C3B-C4B	2.15	1.47	1.42
36	c	524	DGA	OG2-CG2	-2.15	1.41	1.46
29	s	603	CLA	C1A-CHA	2.15	1.52	1.43
36	C	524	DGA	OG2-CG2	-2.15	1.41	1.46
29	C	503	CLA	C1A-CHA	2.15	1.52	1.43
29	n	602	CLA	C1C-C2C	2.15	1.48	1.44
29	A	410	CLA	C1A-CHA	2.15	1.52	1.43
29	S	602	CLA	C1A-CHA	2.15	1.52	1.43
29	g	604	CLA	C1A-CHA	2.15	1.52	1.43
29	Y	608	CLA	C1A-CHA	2.15	1.52	1.43
29	Y	610	CLA	C1A-CHA	2.15	1.52	1.43
29	C	511	CLA	C1A-CHA	2.15	1.52	1.43
29	R	610	CLA	C1A-CHA	2.15	1.52	1.43
29	B	610	CLA	C1A-CHA	2.14	1.52	1.43
29	n	612	CLA	C1A-CHA	2.14	1.52	1.43
29	r	611	CLA	C1C-C2C	2.14	1.48	1.44
29	B	602	CLA	C1A-CHA	2.14	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	614	CLA	C1A-CHA	2.14	1.52	1.43
29	S	610	CLA	C1C-C2C	2.14	1.48	1.44
29	Y	608	CLA	C1C-C2C	2.14	1.48	1.44
45	Y	609	CHL	C1B-NB	-2.14	1.35	1.37
29	B	607	CLA	C1A-CHA	2.14	1.52	1.43
29	c	501	CLA	C1C-C2C	2.14	1.48	1.44
29	c	513	CLA	C1A-CHA	2.14	1.52	1.43
29	s	603	CLA	C1C-C2C	2.14	1.48	1.44
45	n	601	CHL	C1B-NB	-2.14	1.35	1.37
45	y	609	CHL	C1B-NB	-2.14	1.35	1.37
29	G	612	CLA	C1C-C2C	2.14	1.48	1.44
29	S	610	CLA	C1A-CHA	2.14	1.52	1.43
29	c	511	CLA	C1A-CHA	2.14	1.52	1.43
45	G	606	CHL	C1B-NB	-2.14	1.35	1.37
45	g	609	CHL	C1B-NB	-2.14	1.35	1.37
29	c	513	CLA	C1C-C2C	2.14	1.48	1.44
29	y	610	CLA	C1A-CHA	2.14	1.52	1.43
45	g	601	CHL	C1B-NB	-2.14	1.35	1.37
50	S	626	3PH	O21-C21	2.13	1.40	1.34
29	N	603	CLA	C1A-CHA	2.13	1.52	1.43
29	b	611	CLA	C1C-C2C	2.13	1.48	1.44
29	d	403	CLA	C1A-CHA	2.13	1.52	1.43
29	r	602	CLA	C1C-C2C	2.13	1.48	1.44
29	s	613	CLA	C1C-C2C	2.13	1.48	1.44
29	G	602	CLA	C1C-C2C	2.13	1.48	1.44
29	g	603	CLA	C1C-C2C	2.13	1.48	1.44
29	g	612	CLA	C1C-C2C	2.13	1.48	1.44
29	b	602	CLA	C1A-CHA	2.13	1.52	1.43
29	G	603	CLA	C1C-C2C	2.13	1.48	1.44
29	N	612	CLA	C1C-C2C	2.13	1.48	1.44
29	D	402	CLA	C3D-C4D	-2.13	1.39	1.44
29	s	614	CLA	C1A-CHA	2.13	1.51	1.43
29	B	603	CLA	C1A-CHA	2.13	1.51	1.43
29	B	611	CLA	C1A-CHA	2.13	1.51	1.43
29	b	603	CLA	C1C-C2C	2.13	1.48	1.44
50	s	626	3PH	O31-C3	-2.13	1.40	1.45
29	s	602	CLA	C1C-C2C	2.13	1.48	1.44
29	s	617	CLA	C1C-C2C	2.13	1.48	1.44
29	y	603	CLA	C1C-C2C	2.13	1.48	1.44
29	D	403	CLA	C1A-CHA	2.13	1.51	1.43
29	b	607	CLA	C1A-CHA	2.13	1.51	1.43
29	R	609	CLA	C1A-CHA	2.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	610	CLA	C1A-CHA	2.13	1.51	1.43
29	c	503	CLA	C1A-CHA	2.12	1.51	1.43
29	B	604	CLA	C1A-CHA	2.12	1.51	1.43
29	N	610	CLA	C1A-CHA	2.12	1.51	1.43
29	r	604	CLA	C1A-CHA	2.12	1.51	1.43
29	R	602	CLA	C1A-CHA	2.12	1.51	1.43
29	r	612	CLA	C1C-C2C	2.12	1.48	1.44
45	r	607	CHL	C1B-NB	-2.12	1.35	1.37
29	r	602	CLA	C1A-CHA	2.12	1.51	1.43
29	g	604	CLA	C1C-C2C	2.12	1.48	1.44
29	Y	604	CLA	C1A-CHA	2.12	1.51	1.43
29	g	602	CLA	C1A-CHA	2.12	1.51	1.43
29	C	504	CLA	C1A-CHA	2.12	1.51	1.43
29	S	605	CLA	C1C-C2C	2.12	1.48	1.44
29	B	604	CLA	C3D-C4D	-2.11	1.39	1.44
29	y	604	CLA	C1A-CHA	2.11	1.51	1.43
35	b	620	C7Z	C40-C33	2.11	1.55	1.50
29	G	611	CLA	C1C-C2C	2.11	1.48	1.44
48	G	623	NEX	C1-C6	-2.11	1.51	1.54
29	c	504	CLA	C1A-CHA	2.11	1.51	1.43
29	r	604	CLA	C1C-C2C	2.11	1.48	1.44
45	Y	606	CHL	C1B-NB	-2.11	1.35	1.37
29	R	604	CLA	C1A-CHA	2.11	1.51	1.43
29	G	613	CLA	C1C-C2C	2.11	1.48	1.44
29	N	610	CLA	C1C-C2C	2.11	1.48	1.44
29	R	608	CLA	C1C-C2C	2.11	1.48	1.44
29	G	610	CLA	C1A-CHA	2.10	1.51	1.43
29	n	603	CLA	C1C-C2C	2.10	1.48	1.44
35	B	620	C7Z	C40-C33	2.10	1.55	1.50
29	b	611	CLA	C1A-CHA	2.10	1.51	1.43
50	S	626	3PH	O31-C3	-2.10	1.40	1.45
45	G	608	CHL	C1B-NB	-2.10	1.35	1.37
29	S	604	CLA	C1A-CHA	2.10	1.51	1.43
29	b	617	CLA	C3D-C4D	-2.10	1.39	1.44
29	Y	613	CLA	C1C-C2C	2.10	1.48	1.44
29	A	410	CLA	C1C-C2C	2.10	1.48	1.44
29	g	613	CLA	C1C-C2C	2.10	1.48	1.44
29	B	606	CLA	C3D-C4D	-2.09	1.39	1.44
29	r	609	CLA	C1A-CHA	2.09	1.51	1.43
29	n	603	CLA	C1A-CHA	2.09	1.51	1.43
29	g	603	CLA	C1A-CHA	2.09	1.51	1.43
29	s	602	CLA	C1A-CHA	2.09	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	609	CLA	C1C-C2C	2.09	1.48	1.44
29	n	611	CLA	C1C-C2C	2.09	1.48	1.44
29	c	508	CLA	C1A-CHA	2.09	1.51	1.43
29	N	602	CLA	C1A-CHA	2.09	1.51	1.43
29	Y	603	CLA	C1C-C2C	2.09	1.48	1.44
30	A	408	PHO	C3D-C4D	2.09	1.44	1.41
29	N	603	CLA	C1C-C2C	2.09	1.48	1.44
29	G	603	CLA	C1A-CHA	2.08	1.51	1.43
29	R	612	CLA	C1C-C2C	2.08	1.48	1.44
29	g	614	CLA	C1C-C2C	2.08	1.48	1.44
29	S	612	CLA	C1C-C2C	2.08	1.48	1.44
29	s	609	CLA	C1C-C2C	2.08	1.48	1.44
29	Y	612	CLA	C1C-C2C	2.08	1.48	1.44
29	r	610	CLA	C1C-C2C	2.08	1.48	1.44
45	s	608	CHL	C1B-NB	-2.08	1.35	1.37
29	n	602	CLA	C1A-CHA	2.08	1.51	1.43
29	S	614	CLA	C1A-CHA	2.08	1.51	1.43
29	D	402	CLA	C3B-C4B	2.08	1.47	1.42
29	C	506	CLA	C1A-CHA	2.08	1.51	1.43
29	Y	604	CLA	C1C-C2C	2.08	1.48	1.44
29	B	602	CLA	C1C-C2C	2.08	1.48	1.44
29	y	610	CLA	C1C-C2C	2.07	1.48	1.44
29	G	604	CLA	C1C-C2C	2.07	1.48	1.44
29	B	606	CLA	C1A-CHA	2.07	1.51	1.43
29	B	603	CLA	C1C-C2C	2.07	1.48	1.44
29	c	506	CLA	C1A-CHA	2.07	1.51	1.43
29	b	604	CLA	C3D-C4D	-2.07	1.39	1.44
29	S	611	CLA	C1C-C2C	2.07	1.48	1.44
29	g	611	CLA	C1C-C2C	2.07	1.48	1.44
29	C	508	CLA	C1A-CHA	2.07	1.51	1.43
29	g	602	CLA	C1C-C2C	2.07	1.48	1.44
29	b	606	CLA	C1A-CHA	2.07	1.51	1.43
45	G	601	CHL	C1B-NB	-2.07	1.35	1.37
29	c	509	CLA	C1A-CHA	2.06	1.51	1.43
29	b	613	CLA	C1A-CHA	2.06	1.51	1.43
29	y	608	CLA	C1C-C2C	2.06	1.48	1.44
29	S	614	CLA	C1C-C2C	2.06	1.48	1.44
29	n	612	CLA	C1C-C2C	2.06	1.48	1.44
29	A	405	CLA	C1A-CHA	2.06	1.51	1.43
42	D	405	PL9	C52-C5	-2.06	1.46	1.50
29	B	617	CLA	C1A-CHA	2.06	1.51	1.43
29	C	510	CLA	C1A-CHA	2.06	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	r	613	CLA	C1C-C2C	2.06	1.48	1.44
29	S	603	CLA	MG-NC	2.06	2.11	2.06
45	n	605	CHL	C1B-NB	-2.05	1.35	1.37
29	b	606	CLA	C3D-C4D	-2.05	1.39	1.44
29	a	405	CLA	C1A-CHA	2.05	1.51	1.43
29	n	610	CLA	C1C-C2C	2.05	1.48	1.44
29	c	510	CLA	C3D-C4D	-2.05	1.39	1.44
29	c	511	CLA	C1C-C2C	2.05	1.48	1.44
29	C	503	CLA	C1C-C2C	2.05	1.48	1.44
29	B	612	CLA	C3D-C4D	-2.05	1.39	1.44
29	n	604	CLA	C1C-C2C	2.05	1.48	1.44
29	r	608	CLA	C1C-C2C	2.05	1.48	1.44
29	b	616	CLA	C1C-C2C	2.05	1.48	1.44
29	y	614	CLA	C1C-C2C	2.05	1.48	1.44
29	B	607	CLA	C3D-C4D	-2.05	1.39	1.44
29	s	605	CLA	MG-NC	2.05	2.11	2.06
29	R	613	CLA	C1C-C2C	2.05	1.48	1.44
45	g	608	CHL	C1B-NB	-2.05	1.35	1.37
29	b	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	b	613	CLA	C3D-C4D	-2.05	1.39	1.44
29	b	605	CLA	MG-NC	2.05	2.11	2.06
50	i	101	3PH	O31-C3	-2.05	1.40	1.45
29	S	605	CLA	MG-NC	2.04	2.11	2.06
45	N	605	CHL	C1B-NB	-2.04	1.35	1.37
29	r	609	CLA	C3D-C4D	-2.04	1.39	1.44
45	S	608	CHL	C1B-NB	-2.04	1.35	1.37
29	B	615	CLA	C1C-C2C	2.04	1.48	1.44
29	R	604	CLA	C1C-C2C	2.04	1.48	1.44
29	Y	604	CLA	C3D-C4D	-2.04	1.39	1.44
29	B	604	CLA	C1C-C2C	2.04	1.48	1.44
29	Y	614	CLA	C1C-C2C	2.04	1.48	1.44
48	y	623	NEX	C1-C6	-2.04	1.51	1.54
29	n	613	CLA	MG-NC	2.04	2.11	2.06
29	c	503	CLA	C1C-C2C	2.04	1.48	1.44
33	H	102	LMG	C22-C21	-2.04	1.33	1.49
29	B	602	CLA	C3D-C4D	-2.03	1.39	1.44
29	B	609	CLA	C1C-C2C	2.03	1.48	1.44
29	b	607	CLA	C3D-C4D	-2.03	1.39	1.44
29	s	612	CLA	C1C-C2C	2.03	1.48	1.44
29	B	615	CLA	C3D-C4D	-2.03	1.39	1.44
33	h	102	LMG	C22-C21	-2.03	1.33	1.49
29	R	611	CLA	MG-NC	2.03	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	613	CLA	C1A-CHA	2.03	1.51	1.43
29	n	611	CLA	MG-NC	2.03	2.11	2.06
29	B	603	CLA	CHD-C1D	2.03	1.42	1.38
29	s	610	CLA	C3D-C4D	-2.03	1.39	1.44
29	C	511	CLA	C1C-C2C	2.03	1.48	1.44
29	C	505	CLA	C3D-C4D	-2.03	1.39	1.44
29	r	610	CLA	C3D-C4D	-2.03	1.39	1.44
29	c	510	CLA	C1A-CHA	2.02	1.51	1.43
38	c	520	DGD	CDA-CCA	-2.02	1.33	1.49
29	C	506	CLA	C3D-C4D	-2.02	1.39	1.44
29	S	613	CLA	C1C-C2C	2.02	1.48	1.44
29	G	602	CLA	C1A-CHA	2.02	1.51	1.43
33	A	413	LMG	C22-C21	-2.02	1.33	1.49
29	B	605	CLA	MG-NC	2.02	2.11	2.06
29	C	505	CLA	C1C-C2C	2.02	1.48	1.44
38	c	518	DGD	CGB-CFB	-2.02	1.33	1.49
29	d	402	CLA	C3D-C4D	-2.02	1.39	1.44
29	S	617	CLA	MG-NC	2.02	2.11	2.06
29	G	602	CLA	C3D-C4D	-2.02	1.39	1.44
29	c	507	CLA	C1C-C2C	2.02	1.48	1.44
29	Y	602	CLA	C1A-CHA	2.02	1.51	1.43
30	A	409	PHO	C4D-ND	-2.02	1.35	1.38
29	N	611	CLA	MG-NC	2.02	2.11	2.06
29	A	406	CLA	CHD-C1D	2.02	1.42	1.38
29	C	501	CLA	C3D-C4D	-2.01	1.39	1.44
29	c	507	CLA	C3D-C4D	-2.01	1.39	1.44
33	a	413	LMG	C22-C21	-2.01	1.33	1.49
29	b	615	CLA	C1C-C2C	2.01	1.48	1.44
38	C	520	DGD	CDA-CCA	-2.01	1.33	1.49
38	C	518	DGD	CGB-CFB	-2.01	1.33	1.49
38	C	520	DGD	CGB-CFB	-2.01	1.33	1.49
29	Y	614	CLA	C3D-C4D	-2.01	1.39	1.44
33	H	102	LMG	C43-C42	-2.01	1.33	1.49
33	c	521	LMG	C25-C24	-2.01	1.33	1.49
38	c	520	DGD	CGB-CFB	-2.01	1.33	1.49
29	Y	611	CLA	C1C-C2C	2.01	1.48	1.44
33	c	521	LMG	C43-C42	-2.01	1.33	1.49
33	A	413	LMG	C43-C42	-2.01	1.33	1.49
33	C	521	LMG	C43-C42	-2.01	1.33	1.49
29	y	602	CLA	C1A-CHA	2.01	1.51	1.43
29	Y	610	CLA	C1C-C2C	2.01	1.48	1.44
48	R	622	NEX	O24-C25	-2.01	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	411	LMG	C25-C24	-2.01	1.33	1.49
45	y	606	CHL	C1B-NB	-2.01	1.35	1.37
29	n	614	CLA	MG-NC	2.01	2.11	2.06
38	C	519	DGD	CGB-CFB	-2.00	1.33	1.49
29	B	617	CLA	C3D-C4D	-2.00	1.39	1.44
29	B	613	CLA	C3D-C4D	-2.00	1.39	1.44
29	N	612	CLA	MG-NC	2.00	2.11	2.06
29	c	509	CLA	C3D-C4D	-2.00	1.39	1.44
29	N	613	CLA	MG-NC	2.00	2.11	2.06
33	a	413	LMG	C43-C42	-2.00	1.33	1.49
33	C	521	LMG	C25-C24	-2.00	1.33	1.49
29	Y	602	CLA	C3D-C4D	-2.00	1.39	1.44
29	c	506	CLA	C3D-C4D	-2.00	1.39	1.44
29	a	407	CLA	C1C-C2C	2.00	1.48	1.44
29	r	611	CLA	MG-NC	2.00	2.11	2.06
29	s	603	CLA	MG-NC	2.00	2.11	2.06
33	b	622	LMG	C25-C24	-2.00	1.33	1.49

All (4364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	617	CLA	C4-C3-C5	-22.25	77.84	115.27
29	b	617	CLA	C4-C3-C5	-22.23	77.87	115.27
29	b	617	CLA	C5-C3-C2	18.79	159.15	121.12
29	B	617	CLA	C5-C3-C2	18.73	159.01	121.12
31	C	517	BCR	C10-C11-C12	17.71	178.49	123.22
31	c	516	BCR	C10-C11-C12	17.71	178.47	123.22
31	C	516	BCR	C10-C11-C12	17.55	177.99	123.22
31	c	515	BCR	C10-C11-C12	17.52	177.89	123.22
31	d	404	BCR	C10-C11-C12	17.51	177.87	123.22
31	B	619	BCR	C10-C11-C12	17.49	177.80	123.22
31	b	618	BCR	C10-C11-C12	17.48	177.75	123.22
31	B	618	BCR	C10-C11-C12	17.47	177.73	123.22
31	b	619	BCR	C10-C11-C12	17.41	177.54	123.22
31	C	514	BCR	C10-C11-C12	17.25	177.05	123.22
31	c	514	BCR	C10-C11-C12	17.20	176.90	123.22
31	A	411	BCR	C10-C11-C12	17.15	176.75	123.22
31	a	411	BCR	C10-C11-C12	17.07	176.49	123.22
47	y	622	XAT	C37-C21-C36	-16.87	82.48	107.37
31	D	404	BCR	C10-C11-C12	16.82	175.70	123.22
31	c	517	BCR	C10-C11-C12	16.59	174.99	123.22
47	Y	622	XAT	C37-C21-C36	-16.58	82.91	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	617	CLA	C4-C3-C2	-16.55	81.23	123.68
29	b	617	CLA	C4-C3-C2	-16.50	81.35	123.68
31	C	515	BCR	C10-C11-C12	16.43	174.48	123.22
31	C	514	BCR	C16-C15-C14	14.95	154.10	123.47
31	C	515	BCR	C16-C15-C14	14.26	152.69	123.47
31	c	514	BCR	C16-C15-C14	14.21	152.59	123.47
31	c	514	BCR	C11-C10-C9	13.76	146.95	127.31
31	C	516	BCR	C11-C10-C9	13.63	146.76	127.31
31	C	514	BCR	C11-C10-C9	13.60	146.72	127.31
31	b	619	BCR	C16-C15-C14	13.44	151.00	123.47
31	c	516	BCR	C11-C10-C9	13.21	146.16	127.31
31	c	515	BCR	C16-C15-C14	13.06	150.23	123.47
31	b	618	BCR	C11-C10-C9	13.02	145.90	127.31
31	B	618	BCR	C11-C10-C9	12.97	145.82	127.31
31	B	619	BCR	C16-C15-C14	12.93	149.96	123.47
31	b	618	BCR	C16-C15-C14	12.90	149.90	123.47
31	B	618	BCR	C16-C15-C14	12.82	149.73	123.47
31	b	619	BCR	C21-C20-C19	12.80	163.15	123.22
31	C	516	BCR	C16-C15-C14	12.77	149.64	123.47
31	a	411	BCR	C11-C10-C9	12.73	145.48	127.31
31	B	619	BCR	C21-C20-C19	12.65	162.68	123.22
31	A	411	BCR	C11-C10-C9	12.64	145.35	127.31
47	Y	622	XAT	C37-C21-C22	-12.62	87.06	108.98
47	y	622	XAT	C37-C21-C22	-12.60	87.09	108.98
31	c	517	BCR	C21-C20-C19	12.54	162.35	123.22
31	a	411	BCR	C21-C20-C19	12.41	161.95	123.22
31	c	517	BCR	C16-C15-C14	12.33	148.73	123.47
31	A	411	BCR	C21-C20-C19	12.31	161.62	123.22
31	B	619	BCR	C11-C10-C9	12.18	144.70	127.31
31	C	517	BCR	C21-C20-C19	12.09	160.96	123.22
31	b	619	BCR	C11-C10-C9	12.03	144.47	127.31
31	c	516	BCR	C16-C15-C14	12.02	148.10	123.47
31	C	517	BCR	C16-C15-C14	11.97	147.99	123.47
31	d	404	BCR	C11-C10-C9	11.72	144.04	127.31
31	a	411	BCR	C16-C15-C14	11.66	147.36	123.47
31	C	515	BCR	C21-C20-C19	11.61	159.45	123.22
31	c	514	BCR	C21-C20-C19	11.59	159.38	123.22
31	A	411	BCR	C16-C15-C14	11.53	147.08	123.47
31	D	404	BCR	C16-C15-C14	11.49	147.02	123.47
31	c	515	BCR	C11-C10-C9	11.40	143.59	127.31
31	d	404	BCR	C16-C15-C14	11.38	146.78	123.47
31	D	404	BCR	C11-C10-C9	11.38	143.55	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	514	BCR	C21-C20-C19	11.37	158.69	123.22
31	C	517	BCR	C11-C10-C9	11.36	143.52	127.31
31	b	618	BCR	C21-C20-C19	11.11	157.89	123.22
31	c	516	BCR	C21-C20-C19	11.02	157.60	123.22
31	D	404	BCR	C11-C12-C13	10.97	157.24	126.42
31	B	618	BCR	C21-C20-C19	10.97	157.45	123.22
31	c	515	BCR	C21-C20-C19	10.78	156.86	123.22
31	a	411	BCR	C11-C12-C13	10.75	156.61	126.42
31	d	404	BCR	C11-C12-C13	10.74	156.60	126.42
31	C	515	BCR	C11-C10-C9	10.73	142.62	127.31
29	b	609	CLA	C4A-NA-C1A	10.65	111.49	106.71
31	c	515	BCR	C11-C12-C13	10.58	156.15	126.42
31	C	517	BCR	C11-C12-C13	10.51	155.95	126.42
31	A	411	BCR	C11-C12-C13	10.49	155.89	126.42
31	c	517	BCR	C11-C10-C9	10.39	142.14	127.31
31	C	516	BCR	C11-C12-C13	10.32	155.41	126.42
31	b	619	BCR	C11-C12-C13	10.25	155.20	126.42
31	C	515	BCR	C11-C12-C13	10.21	155.10	126.42
31	c	516	BCR	C11-C12-C13	10.20	155.06	126.42
31	C	516	BCR	C21-C20-C19	10.15	154.91	123.22
31	b	618	BCR	C11-C12-C13	10.12	154.85	126.42
31	B	619	BCR	C11-C12-C13	10.10	154.78	126.42
31	B	618	BCR	C11-C12-C13	9.92	154.29	126.42
29	S	613	CLA	C4A-NA-C1A	9.87	111.14	106.71
29	B	609	CLA	C4A-NA-C1A	9.86	111.14	106.71
29	B	608	CLA	C4A-NA-C1A	9.85	111.13	106.71
29	b	608	CLA	C4A-NA-C1A	9.82	111.12	106.71
29	b	605	CLA	C4A-NA-C1A	9.76	111.10	106.71
29	b	615	CLA	C4A-NA-C1A	9.75	111.09	106.71
29	b	610	CLA	C4A-NA-C1A	9.69	111.06	106.71
29	B	605	CLA	C4A-NA-C1A	9.69	111.06	106.71
29	c	505	CLA	C4A-NA-C1A	9.68	111.06	106.71
29	s	613	CLA	C4A-NA-C1A	9.68	111.06	106.71
31	c	517	BCR	C11-C12-C13	9.67	153.58	126.42
31	d	404	BCR	C21-C20-C19	9.65	153.34	123.22
29	B	617	CLA	C4A-NA-C1A	9.62	111.03	106.71
31	c	514	BCR	C11-C12-C13	9.62	153.45	126.42
29	b	613	CLA	C4A-NA-C1A	9.62	111.03	106.71
31	C	514	BCR	C11-C12-C13	9.61	153.42	126.42
29	C	505	CLA	C4A-NA-C1A	9.58	111.01	106.71
29	B	613	CLA	C4A-NA-C1A	9.54	111.00	106.71
29	c	502	CLA	C4A-NA-C1A	9.54	110.99	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	406	CLA	C4A-NA-C1A	9.53	110.99	106.71
29	b	606	CLA	C4A-NA-C1A	9.53	110.99	106.71
29	A	406	CLA	C4A-NA-C1A	9.52	110.99	106.71
29	B	610	CLA	C4A-NA-C1A	9.51	110.98	106.71
29	B	614	CLA	C4A-NA-C1A	9.49	110.97	106.71
29	b	612	CLA	C4A-NA-C1A	9.46	110.96	106.71
29	C	509	CLA	C4A-NA-C1A	9.45	110.95	106.71
29	C	502	CLA	C4A-NA-C1A	9.45	110.95	106.71
29	B	606	CLA	C4A-NA-C1A	9.44	110.95	106.71
29	s	605	CLA	C4A-NA-C1A	9.43	110.95	106.71
31	D	404	BCR	C21-C20-C19	9.42	152.62	123.22
29	R	604	CLA	C4A-NA-C1A	9.40	110.93	106.71
29	c	513	CLA	C4A-NA-C1A	9.38	110.92	106.71
29	G	610	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	c	504	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	c	509	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	n	604	CLA	C4A-NA-C1A	9.34	110.90	106.71
29	y	613	CLA	C4A-NA-C1A	9.34	110.90	106.71
29	b	614	CLA	C4A-NA-C1A	9.33	110.90	106.71
29	B	615	CLA	C4A-NA-C1A	9.32	110.90	106.71
29	S	605	CLA	C4A-NA-C1A	9.32	110.89	106.71
30	a	409	PHO	C4D-CHA-CBD	-9.30	104.31	108.52
29	y	603	CLA	C4A-NA-C1A	9.29	110.88	106.71
31	C	516	BCR	C20-C19-C18	9.28	152.47	126.42
29	n	613	CLA	C4A-NA-C1A	9.28	110.88	106.71
29	c	511	CLA	C4A-NA-C1A	9.25	110.86	106.71
29	N	604	CLA	C4A-NA-C1A	9.24	110.86	106.71
29	Y	613	CLA	C4A-NA-C1A	9.24	110.86	106.71
29	c	501	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	N	613	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	n	610	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	a	410	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	S	604	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	r	604	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	C	511	CLA	C4A-NA-C1A	9.19	110.84	106.71
29	r	610	CLA	C4A-NA-C1A	9.16	110.83	106.71
29	N	603	CLA	C4A-NA-C1A	9.16	110.82	106.71
29	A	410	CLA	C4A-NA-C1A	9.15	110.82	106.71
29	n	603	CLA	C4A-NA-C1A	9.14	110.81	106.71
29	N	612	CLA	C4A-NA-C1A	9.13	110.81	106.71
29	s	602	CLA	C4A-NA-C1A	9.12	110.81	106.71
29	a	405	CLA	C4A-NA-C1A	9.12	110.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	614	CLA	C4A-NA-C1A	9.12	110.80	106.71
29	B	616	CLA	C4A-NA-C1A	9.11	110.80	106.71
29	G	613	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	C	510	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	S	617	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	Y	603	CLA	C4A-NA-C1A	9.08	110.79	106.71
29	C	501	CLA	C4A-NA-C1A	9.08	110.79	106.71
29	R	603	CLA	C4A-NA-C1A	9.07	110.78	106.71
29	C	504	CLA	C4A-NA-C1A	9.06	110.78	106.71
29	g	610	CLA	C4A-NA-C1A	9.06	110.78	106.71
29	A	407	CLA	C4A-NA-C1A	9.06	110.78	106.71
29	Y	611	CLA	C4A-NA-C1A	9.06	110.78	106.71
29	g	611	CLA	C4A-NA-C1A	9.05	110.78	106.71
29	G	614	CLA	C4A-NA-C1A	9.05	110.78	106.71
29	g	613	CLA	C4A-NA-C1A	9.04	110.77	106.71
29	C	507	CLA	C4A-NA-C1A	9.02	110.76	106.71
29	Y	610	CLA	C4A-NA-C1A	9.01	110.75	106.71
29	Y	612	CLA	C4A-NA-C1A	9.01	110.75	106.71
29	N	614	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	A	405	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	G	604	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	b	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	b	616	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	s	617	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	r	608	CLA	C4A-NA-C1A	8.98	110.74	106.71
29	B	612	CLA	C4A-NA-C1A	8.98	110.74	106.71
29	G	603	CLA	C4A-NA-C1A	8.97	110.74	106.71
29	c	512	CLA	C4A-NA-C1A	8.96	110.73	106.71
29	g	603	CLA	C4A-NA-C1A	8.95	110.73	106.71
29	c	507	CLA	C4A-NA-C1A	8.94	110.73	106.71
29	S	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
29	c	508	CLA	C4A-NA-C1A	8.93	110.72	106.71
29	R	613	CLA	C4A-NA-C1A	8.92	110.72	106.71
29	n	611	CLA	C4A-NA-C1A	8.91	110.71	106.71
29	y	611	CLA	C4A-NA-C1A	8.91	110.71	106.71
29	G	611	CLA	C4A-NA-C1A	8.90	110.71	106.71
29	B	604	CLA	C4A-NA-C1A	8.89	110.70	106.71
29	R	608	CLA	C4A-NA-C1A	8.89	110.70	106.71
29	r	613	CLA	C4A-NA-C1A	8.89	110.70	106.71
29	y	610	CLA	C4A-NA-C1A	8.89	110.70	106.71
29	N	610	CLA	C4A-NA-C1A	8.88	110.70	106.71
29	c	510	CLA	C4A-NA-C1A	8.86	110.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	602	CLA	C4A-NA-C1A	8.86	110.69	106.71
29	r	603	CLA	C4A-NA-C1A	8.85	110.69	106.71
29	g	614	CLA	C4A-NA-C1A	8.84	110.68	106.71
29	C	508	CLA	C4A-NA-C1A	8.84	110.68	106.71
29	a	407	CLA	C4A-NA-C1A	8.82	110.67	106.71
29	g	612	CLA	C4A-NA-C1A	8.82	110.67	106.71
29	Y	614	CLA	C4A-NA-C1A	8.81	110.67	106.71
29	R	602	CLA	C4A-NA-C1A	8.80	110.66	106.71
29	B	602	CLA	C4A-NA-C1A	8.80	110.66	106.71
29	r	611	CLA	C4A-NA-C1A	8.79	110.66	106.71
29	s	609	CLA	C4A-NA-C1A	8.78	110.65	106.71
29	r	602	CLA	C4A-NA-C1A	8.78	110.65	106.71
29	y	608	CLA	C4A-NA-C1A	8.78	110.65	106.71
29	S	609	CLA	C4A-NA-C1A	8.77	110.65	106.71
29	s	604	CLA	C4A-NA-C1A	8.77	110.65	106.71
29	C	513	CLA	C4A-NA-C1A	8.77	110.65	106.71
29	g	602	CLA	C4A-NA-C1A	8.75	110.64	106.71
29	S	611	CLA	C4A-NA-C1A	8.74	110.64	106.71
29	s	612	CLA	C4A-NA-C1A	8.74	110.64	106.71
29	S	603	CLA	C4A-NA-C1A	8.73	110.63	106.71
29	y	614	CLA	C4A-NA-C1A	8.73	110.63	106.71
29	y	604	CLA	C4A-NA-C1A	8.73	110.63	106.71
29	c	506	CLA	C4A-NA-C1A	8.71	110.62	106.71
29	b	602	CLA	C4A-NA-C1A	8.71	110.62	106.71
29	Y	604	CLA	C4A-NA-C1A	8.71	110.62	106.71
29	C	503	CLA	C4A-NA-C1A	8.69	110.61	106.71
29	y	612	CLA	C4A-NA-C1A	8.69	110.61	106.71
29	R	612	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	G	612	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	B	603	CLA	C4A-NA-C1A	8.67	110.61	106.71
29	R	611	CLA	C4A-NA-C1A	8.64	110.59	106.71
29	C	512	CLA	C4A-NA-C1A	8.63	110.59	106.71
29	s	611	CLA	C4A-NA-C1A	8.63	110.59	106.71
29	Y	608	CLA	C4A-NA-C1A	8.61	110.58	106.71
29	b	607	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	b	618	BCR	C20-C19-C18	8.60	150.58	126.42
29	R	609	CLA	C4A-NA-C1A	8.60	110.57	106.71
29	s	614	CLA	C4A-NA-C1A	8.60	110.57	106.71
29	b	617	CLA	C4A-NA-C1A	8.59	110.57	106.71
29	C	506	CLA	C4A-NA-C1A	8.59	110.57	106.71
29	g	604	CLA	C4A-NA-C1A	8.58	110.56	106.71
31	B	618	BCR	C20-C19-C18	8.58	150.52	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	604	CLA	C4A-NA-C1A	8.55	110.55	106.71
31	c	515	BCR	C20-C19-C18	8.55	150.44	126.42
29	B	607	CLA	C4A-NA-C1A	8.53	110.54	106.71
29	N	602	CLA	C4A-NA-C1A	8.53	110.54	106.71
29	S	614	CLA	C4A-NA-C1A	8.52	110.54	106.71
29	r	612	CLA	C4A-NA-C1A	8.51	110.53	106.71
29	N	611	CLA	C4A-NA-C1A	8.51	110.53	106.71
31	c	516	BCR	C20-C19-C18	8.50	150.28	126.42
29	S	610	CLA	C4A-NA-C1A	8.46	110.51	106.71
29	n	612	CLA	C4A-NA-C1A	8.45	110.50	106.71
29	c	503	CLA	C4A-NA-C1A	8.44	110.50	106.71
29	d	403	CLA	C4A-NA-C1A	8.44	110.50	106.71
29	G	602	CLA	C4A-NA-C1A	8.44	110.50	106.71
29	r	609	CLA	C4A-NA-C1A	8.42	110.49	106.71
29	s	603	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	C	514	BCR	C20-C19-C18	8.35	149.89	126.42
29	D	402	CLA	C4A-NA-C1A	8.35	110.46	106.71
29	D	403	CLA	C4A-NA-C1A	8.28	110.43	106.71
29	s	610	CLA	C4A-NA-C1A	8.27	110.43	106.71
31	C	515	BCR	C20-C19-C18	8.26	149.62	126.42
30	A	409	PHO	C4D-CHA-CBD	-8.19	104.81	108.52
29	d	402	CLA	C4A-NA-C1A	8.16	110.37	106.71
29	R	610	CLA	C4A-NA-C1A	8.13	110.36	106.71
29	b	611	CLA	C4A-NA-C1A	8.12	110.36	106.71
29	n	602	CLA	C4A-NA-C1A	8.10	110.35	106.71
29	y	602	CLA	C4A-NA-C1A	8.05	110.33	106.71
29	Y	602	CLA	C4A-NA-C1A	7.99	110.30	106.71
29	B	611	CLA	C4A-NA-C1A	7.98	110.29	106.71
31	c	514	BCR	C20-C19-C18	7.97	148.80	126.42
31	C	517	BCR	C20-C19-C18	7.65	147.92	126.42
30	a	408	PHO	C4D-CHA-CBD	-7.39	105.18	108.52
31	B	619	BCR	C20-C19-C18	7.34	147.04	126.42
29	s	613	CLA	O2D-CGD-CBD	7.34	124.31	111.27
47	y	622	XAT	C36-C21-C22	7.34	121.73	108.98
29	S	613	CLA	O2D-CGD-CBD	7.28	124.20	111.27
31	b	619	BCR	C20-C19-C18	7.26	146.82	126.42
31	A	411	BCR	C20-C19-C18	7.18	146.58	126.42
29	c	502	CLA	O2A-C1-C2	7.17	127.49	108.64
47	Y	622	XAT	C36-C21-C22	7.13	121.38	108.98
31	c	517	BCR	C20-C19-C18	7.09	146.33	126.42
31	a	411	BCR	C20-C19-C18	7.09	146.32	126.42
47	y	622	XAT	C37-C21-C26	-7.05	91.02	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Y	622	XAT	C37-C21-C26	-7.04	91.04	110.05
30	A	408	PHO	C4D-CHA-CBD	-6.96	105.37	108.52
47	R	621	XAT	C15-C14-C13	-6.91	117.45	127.31
36	B	625	DGA	CDB-CCB-CBB	-6.76	80.12	114.42
29	s	605	CLA	O2D-CGD-CBD	6.75	123.27	111.27
36	b	623	DGA	CDB-CCB-CBB	-6.73	80.25	114.42
29	S	605	CLA	O2D-CGD-CBD	6.72	123.20	111.27
36	c	524	DGA	CDB-CCB-CBB	-6.67	80.55	114.42
36	C	524	DGA	CDB-CCB-CBB	-6.66	80.64	114.42
47	r	622	XAT	C15-C14-C13	-6.60	117.89	127.31
40	c	627	LMK	O2-C4-O3	-6.60	109.11	124.09
40	C	527	LMK	O2-C4-O3	-6.54	109.23	124.09
29	S	605	CLA	O2A-C1-C2	6.36	125.34	108.64
29	B	609	CLA	O2D-CGD-CBD	6.24	122.36	111.27
29	C	506	CLA	O2D-CGD-CBD	6.24	122.35	111.27
29	c	506	CLA	O2D-CGD-CBD	6.21	122.31	111.27
29	c	501	CLA	O2D-CGD-CBD	6.20	122.28	111.27
29	b	609	CLA	O2D-CGD-CBD	6.13	122.16	111.27
29	R	602	CLA	O2D-CGD-CBD	6.06	122.03	111.27
29	C	501	CLA	O2D-CGD-CBD	6.05	122.03	111.27
29	C	504	CLA	O2A-C1-C2	5.99	124.37	108.64
29	B	605	CLA	O2A-C1-C2	5.97	124.32	108.64
47	n	622	XAT	C31-C30-C29	-5.96	118.81	127.31
29	R	604	CLA	O2A-C1-C2	5.93	122.84	108.97
29	c	504	CLA	O2A-C1-C2	5.93	124.22	108.64
29	G	604	CLA	O2A-C1-C2	5.91	122.80	108.97
29	B	602	CLA	CMD-C2D-C1D	5.90	135.12	124.71
29	b	606	CLA	CMD-C2D-C1D	5.90	135.11	124.71
31	d	404	BCR	C20-C19-C18	5.90	142.98	126.42
29	A	405	CLA	O2A-C1-C2	5.89	124.12	108.64
29	s	614	CLA	O2A-C1-C2	5.89	124.11	108.64
29	c	503	CLA	CMD-C2D-C1D	5.88	135.07	124.71
29	C	513	CLA	O2A-C1-C2	5.87	124.06	108.64
29	b	602	CLA	CMD-C2D-C1D	5.87	135.05	124.71
29	C	511	CLA	CMD-C2D-C1D	5.87	135.05	124.71
29	s	610	CLA	O2A-C1-C2	5.86	124.05	108.64
29	B	606	CLA	CMD-C2D-C1D	5.85	135.03	124.71
29	c	510	CLA	CMD-C2D-C1D	5.85	135.02	124.71
29	c	513	CLA	O2A-C1-C2	5.83	123.95	108.64
29	n	613	CLA	O2A-C1-C2	5.82	123.94	108.64
47	r	622	XAT	C7-C8-C9	-5.81	116.52	125.53
29	c	511	CLA	CMD-C2D-C1D	5.80	134.94	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	501	CLA	CMD-C2D-C1D	5.80	134.93	124.71
29	b	605	CLA	O2A-C1-C2	5.78	123.83	108.64
29	C	510	CLA	CMD-C2D-C1D	5.76	134.87	124.71
29	S	614	CLA	CMD-C2D-C1D	5.76	134.86	124.71
29	G	614	CLA	CMD-C2D-C1D	5.76	134.86	124.71
29	r	613	CLA	O2D-CGD-CBD	5.76	121.50	111.27
29	C	503	CLA	CMD-C2D-C1D	5.75	134.84	124.71
46	y	620	LUT	C21-C26-C25	5.74	121.71	111.42
29	y	603	CLA	O2D-CGD-CBD	5.73	121.45	111.27
31	D	404	BCR	C20-C19-C18	5.73	142.50	126.42
46	s	620	LUT	C21-C26-C27	5.73	119.94	112.70
29	r	604	CLA	O2A-C1-C2	5.73	122.36	108.97
29	R	609	CLA	CMD-C2D-C1D	5.72	134.79	124.71
44	H	101	RRX	C15-C14-C13	-5.72	119.15	127.31
29	g	604	CLA	O2D-CGD-CBD	5.72	121.43	111.27
29	n	611	CLA	O2A-C1-C2	5.72	122.34	108.97
29	r	608	CLA	CMD-C2D-C1D	5.70	134.76	124.71
29	N	611	CLA	O2D-CGD-CBD	5.69	121.38	111.27
29	B	603	CLA	CMD-C2D-C1D	5.69	134.73	124.71
29	n	604	CLA	CMD-C2D-C1D	5.68	134.72	124.71
29	b	617	CLA	O2A-C1-C2	5.68	123.56	108.64
29	a	405	CLA	O2A-C1-C2	5.68	123.55	108.64
46	Y	620	LUT	C21-C26-C25	5.67	121.58	111.42
35	B	620	C7Z	C11-C10-C9	-5.67	119.22	127.31
47	y	622	XAT	C31-C30-C29	-5.67	119.22	127.31
29	R	612	CLA	CMD-C2D-C1D	5.67	134.71	124.71
29	r	609	CLA	CMD-C2D-C1D	5.67	134.70	124.71
47	R	621	XAT	C7-C8-C9	-5.66	116.74	125.53
29	s	604	CLA	CMD-C2D-C1D	5.66	134.69	124.71
29	S	604	CLA	CMD-C2D-C1D	5.66	134.69	124.71
29	g	613	CLA	CMD-C2D-C1D	5.64	134.66	124.71
29	s	614	CLA	CMD-C2D-C1D	5.64	134.66	124.71
29	B	613	CLA	O2D-CGD-CBD	5.64	121.29	111.27
29	n	611	CLA	O2D-CGD-CBD	5.64	121.29	111.27
29	c	503	CLA	O2D-CGD-CBD	5.64	121.28	111.27
46	G	621	LUT	C21-C26-C25	5.64	121.51	111.42
29	g	614	CLA	CMD-C2D-C1D	5.63	134.64	124.71
29	c	501	CLA	CMD-C2D-C1D	5.62	134.63	124.71
29	C	502	CLA	O2A-C1-C2	5.62	123.41	108.64
29	r	613	CLA	CMD-C2D-C1D	5.61	134.61	124.71
29	R	608	CLA	CMD-C2D-C1D	5.61	134.59	124.71
29	n	614	CLA	O2A-C1-C2	5.60	122.08	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	407	CLA	O2A-C1-C2	5.60	122.07	108.97
29	Y	603	CLA	O2D-CGD-CBD	5.60	121.22	111.27
29	b	608	CLA	O2A-C1-C2	5.60	123.35	108.64
29	s	610	CLA	CMD-C2D-C1D	5.60	134.58	124.71
29	g	604	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	N	604	CLA	O2D-CGD-CBD	5.59	121.21	111.27
29	r	610	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	R	603	CLA	CMD-C2D-C1D	5.58	134.56	124.71
29	B	607	CLA	O2D-CGD-CBD	5.58	121.19	111.27
29	g	603	CLA	CMD-C2D-C1D	5.58	134.55	124.71
29	G	604	CLA	CMD-C2D-C1D	5.58	134.54	124.71
29	a	406	CLA	CMD-C2D-C1D	5.57	134.54	124.71
29	G	613	CLA	CMD-C2D-C1D	5.57	134.53	124.71
47	N	622	XAT	C31-C30-C29	-5.57	119.36	127.31
29	C	509	CLA	CMD-C2D-C1D	5.57	134.53	124.71
29	R	602	CLA	CMD-C2D-C1D	5.57	134.53	124.71
29	b	613	CLA	O2D-CGD-CBD	5.57	121.16	111.27
29	Y	608	CLA	CMD-C2D-C1D	5.56	134.52	124.71
29	R	613	CLA	O2D-CGD-CBD	5.56	121.15	111.27
29	c	502	CLA	CMD-C2D-C1D	5.56	134.50	124.71
46	y	621	LUT	C21-C26-C25	5.55	121.37	111.42
29	r	603	CLA	CMD-C2D-C1D	5.55	134.50	124.71
29	B	608	CLA	O2A-C1-C2	5.55	123.23	108.64
29	y	604	CLA	CMD-C2D-C1D	5.55	134.49	124.71
29	c	509	CLA	O2D-CGD-CBD	5.55	121.13	111.27
29	R	604	CLA	CMD-C2D-C1D	5.54	134.48	124.71
29	B	605	CLA	CMD-C2D-C1D	5.54	134.48	124.71
29	B	607	CLA	CMD-C2D-C1D	5.54	134.48	124.71
29	C	513	CLA	CMD-C2D-C1D	5.54	134.48	124.71
29	G	604	CLA	O2D-CGD-CBD	5.53	121.10	111.27
46	g	621	LUT	C21-C26-C25	5.53	121.33	111.42
29	b	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
46	s	621	LUT	C21-C26-C25	5.53	121.33	111.42
29	Y	604	CLA	CMD-C2D-C1D	5.53	134.46	124.71
29	g	610	CLA	CMD-C2D-C1D	5.53	134.45	124.71
29	N	604	CLA	CMD-C2D-C1D	5.52	134.45	124.71
29	b	607	CLA	O2D-CGD-CBD	5.52	121.08	111.27
29	R	613	CLA	CMD-C2D-C1D	5.52	134.45	124.71
29	c	509	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	Y	614	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	S	610	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	r	612	CLA	CMD-C2D-C1D	5.52	134.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	407	CLA	O2A-C1-C2	5.52	121.88	108.97
29	n	604	CLA	O2D-CGD-CBD	5.52	121.07	111.27
44	h	101	RRX	C15-C14-C13	-5.52	119.44	127.31
29	r	602	CLA	CMD-C2D-C1D	5.51	134.43	124.71
29	A	406	CLA	CMD-C2D-C1D	5.51	134.43	124.71
29	y	608	CLA	CMD-C2D-C1D	5.51	134.42	124.71
29	r	611	CLA	CMD-C2D-C1D	5.51	134.42	124.71
29	c	507	CLA	CMD-C2D-C1D	5.51	134.42	124.71
29	b	615	CLA	O2A-C1-C2	5.50	123.10	108.64
29	g	602	CLA	O2A-C1-C2	5.50	123.09	108.64
29	A	405	CLA	CMD-C2D-C1D	5.50	134.40	124.71
29	g	602	CLA	O2D-CGD-CBD	5.50	121.03	111.27
29	d	403	CLA	O2D-CGD-CBD	5.49	121.03	111.27
29	C	506	CLA	CMD-C2D-C1D	5.49	134.39	124.71
29	r	609	CLA	O2A-C1-C2	5.49	123.07	108.64
29	N	604	CLA	O2A-C1-C2	5.49	123.06	108.64
29	B	615	CLA	O2A-C1-C2	5.48	123.04	108.64
29	D	402	CLA	O2A-C1-C2	5.47	123.02	108.64
29	n	603	CLA	O2A-C1-C2	5.47	123.02	108.64
29	G	610	CLA	CMD-C2D-C1D	5.47	134.35	124.71
29	G	602	CLA	O2A-C1-C2	5.47	123.01	108.64
29	G	602	CLA	CMD-C2D-C1D	5.47	134.35	124.71
46	n	621	LUT	C21-C26-C25	5.47	121.21	111.42
47	Y	622	XAT	C15-C14-C13	-5.47	119.51	127.31
46	Y	621	LUT	C21-C26-C25	5.46	121.20	111.42
29	B	617	CLA	O2A-C1-C2	5.46	122.98	108.64
29	b	607	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	C	503	CLA	O2D-CGD-CBD	5.46	120.97	111.27
35	b	620	C7Z	C11-C10-C9	-5.46	119.52	127.31
29	y	614	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	n	612	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	S	609	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	Y	613	CLA	CMD-C2D-C1D	5.45	134.33	124.71
29	n	604	CLA	O2A-C1-C2	5.45	122.97	108.64
29	R	610	CLA	CMD-C2D-C1D	5.45	134.32	124.71
29	S	613	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	G	603	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	c	506	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	s	613	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	C	507	CLA	CMD-C2D-C1D	5.44	134.30	124.71
29	R	604	CLA	O2D-CGD-CBD	5.44	120.94	111.27
29	y	613	CLA	CMD-C2D-C1D	5.44	134.30	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	509	CLA	O2D-CGD-CBD	5.44	120.93	111.27
29	G	611	CLA	O2D-CGD-CBD	5.43	120.92	111.27
29	b	603	CLA	O2A-C1-C2	5.43	122.91	108.64
29	G	610	CLA	O2A-C1-C2	5.43	122.90	108.64
29	A	410	CLA	O2D-CGD-CBD	5.43	120.91	111.27
29	N	603	CLA	O2D-CGD-CBD	5.43	120.91	111.27
29	n	603	CLA	O2D-CGD-CBD	5.43	120.91	111.27
29	R	609	CLA	O2A-C1-C2	5.42	122.89	108.64
29	B	614	CLA	CMD-C2D-C1D	5.42	134.27	124.71
29	B	603	CLA	O2A-C1-C2	5.42	122.89	108.64
29	Y	612	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	d	402	CLA	O2A-C1-C2	5.42	122.88	108.64
29	s	617	CLA	CMD-C2D-C1D	5.42	134.26	124.71
29	b	605	CLA	CMD-C2D-C1D	5.41	134.26	124.71
29	a	410	CLA	O2D-CGD-CBD	5.41	120.89	111.27
29	C	504	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	a	405	CLA	CMD-C2D-C1D	5.41	134.24	124.71
29	b	616	CLA	CMD-C2D-C1D	5.41	134.24	124.71
29	y	603	CLA	CMD-C2D-C1D	5.41	134.24	124.71
29	Y	603	CLA	CMD-C2D-C1D	5.41	134.24	124.71
29	g	610	CLA	O2A-C1-C2	5.40	122.84	108.64
46	r	620	LUT	C15-C14-C13	-5.40	119.60	127.31
29	g	604	CLA	O2A-C1-C2	5.40	121.59	108.97
29	y	602	CLA	O2D-CGD-CBD	5.39	120.85	111.27
29	b	614	CLA	CMD-C2D-C1D	5.39	134.22	124.71
29	r	604	CLA	CMD-C2D-C1D	5.39	134.22	124.71
29	G	611	CLA	CMD-C2D-C1D	5.39	134.21	124.71
46	r	620	LUT	C21-C26-C27	5.39	119.51	112.70
29	g	614	CLA	O2A-C1-C2	5.38	121.56	108.97
29	B	616	CLA	CMD-C2D-C1D	5.38	134.19	124.71
29	n	602	CLA	CMD-C2D-C1D	5.38	134.19	124.71
29	b	611	CLA	O2D-CGD-CBD	5.38	120.82	111.27
29	C	505	CLA	O2A-C1-C2	5.38	122.77	108.64
29	C	504	CLA	O2D-CGD-CBD	5.38	120.82	111.27
46	r	620	LUT	C35-C34-C33	-5.37	119.64	127.31
29	y	610	CLA	CMD-C2D-C1D	5.37	134.18	124.71
29	C	513	CLA	O2D-CGD-CBD	5.37	120.81	111.27
29	D	402	CLA	CMD-C2D-C1D	5.37	134.18	124.71
46	N	621	LUT	C21-C26-C25	5.37	121.04	111.42
29	N	603	CLA	CMD-C2D-C1D	5.37	134.17	124.71
46	S	620	LUT	C21-C26-C27	5.37	119.48	112.70
29	N	610	CLA	CMD-C2D-C1D	5.37	134.17	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	510	CLA	O2D-CGD-CBD	5.37	120.80	111.27
29	g	611	CLA	O2D-CGD-CBD	5.36	120.80	111.27
47	g	622	XAT	C31-C30-C29	-5.36	119.66	127.31
29	y	612	CLA	O2D-CGD-CBD	5.36	120.80	111.27
46	R	620	LUT	C15-C14-C13	-5.36	119.66	127.31
29	b	611	CLA	CMD-C2D-C1D	5.36	134.16	124.71
29	R	612	CLA	O2D-CGD-CBD	5.36	120.78	111.27
29	B	615	CLA	CMD-C2D-C1D	5.35	134.15	124.71
29	N	614	CLA	CMD-C2D-C1D	5.35	134.14	124.71
29	n	614	CLA	CMD-C2D-C1D	5.35	134.14	124.71
29	D	403	CLA	O2A-C1-C2	5.35	122.69	108.64
29	s	602	CLA	O2A-C1-C2	5.35	122.69	108.64
29	s	605	CLA	O2A-C1-C2	5.35	122.69	108.64
29	C	505	CLA	O2D-CGD-CBD	5.35	120.77	111.27
29	R	610	CLA	O2A-C1-C2	5.35	122.69	108.64
29	a	407	CLA	CMD-C2D-C1D	5.35	134.13	124.71
29	g	611	CLA	CMD-C2D-C1D	5.35	134.13	124.71
29	y	602	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	Y	608	CLA	O2A-C1-C2	5.34	122.68	108.64
29	b	610	CLA	CMD-C2D-C1D	5.34	134.12	124.71
29	b	608	CLA	CMD-C2D-C1D	5.34	134.12	124.71
29	n	610	CLA	CMD-C2D-C1D	5.34	134.12	124.71
29	n	611	CLA	CMD-C2D-C1D	5.34	134.12	124.71
47	N	622	XAT	C15-C14-C13	-5.34	119.70	127.31
29	C	510	CLA	O2A-C1-C2	5.33	122.65	108.64
29	g	612	CLA	O2D-CGD-CBD	5.33	120.75	111.27
29	y	611	CLA	O2D-CGD-CBD	5.33	120.74	111.27
29	D	403	CLA	O2D-CGD-CBD	5.32	120.73	111.27
29	c	510	CLA	O2D-CGD-CBD	5.32	120.73	111.27
29	b	606	CLA	O2D-CGD-CBD	5.32	120.73	111.27
29	s	605	CLA	CMD-C2D-C1D	5.32	134.09	124.71
29	Y	602	CLA	O2D-CGD-CBD	5.32	120.72	111.27
29	n	610	CLA	O2A-C1-C2	5.32	122.62	108.64
29	G	614	CLA	O2A-C1-C2	5.31	121.40	108.97
46	g	620	LUT	C21-C26-C25	5.31	120.94	111.42
29	g	603	CLA	O2D-CGD-CBD	5.31	120.71	111.27
29	c	513	CLA	O2D-CGD-CBD	5.31	120.70	111.27
29	R	611	CLA	CMD-C2D-C1D	5.31	134.06	124.71
29	S	611	CLA	CMD-C2D-C1D	5.31	134.06	124.71
29	C	511	CLA	O2D-CGD-CBD	5.30	120.69	111.27
29	G	602	CLA	O2D-CGD-CBD	5.30	120.69	111.27
29	N	602	CLA	O2D-CGD-CBD	5.30	120.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	606	CLA	O2D-CGD-CBD	5.30	120.68	111.27
47	n	622	XAT	C15-C14-C13	-5.30	119.75	127.31
29	B	610	CLA	CMD-C2D-C1D	5.30	134.04	124.71
29	c	507	CLA	O2D-CGD-CBD	5.29	120.68	111.27
29	C	511	CLA	O2A-C1-C2	5.29	122.55	108.64
29	B	611	CLA	O2D-CGD-CBD	5.29	120.67	111.27
29	c	504	CLA	CMD-C2D-C1D	5.29	134.04	124.71
29	n	603	CLA	CMD-C2D-C1D	5.29	134.03	124.71
29	N	614	CLA	O2D-CGD-CBD	5.29	120.67	111.27
29	N	613	CLA	CMD-C2D-C1D	5.28	134.03	124.71
29	d	402	CLA	CMD-C2D-C1D	5.28	134.03	124.71
29	b	610	CLA	O2D-CGD-CBD	5.28	120.66	111.27
29	r	604	CLA	O2D-CGD-CBD	5.28	120.66	111.27
29	a	410	CLA	CMD-C2D-C1D	5.28	134.01	124.71
29	b	615	CLA	CMD-C2D-C1D	5.28	134.01	124.71
29	N	613	CLA	O2A-C1-C2	5.27	122.49	108.64
29	B	608	CLA	CMD-C2D-C1D	5.27	134.00	124.71
29	c	511	CLA	O2A-C1-C2	5.27	122.48	108.64
29	S	610	CLA	O2A-C1-C2	5.27	122.48	108.64
29	B	611	CLA	CMD-C2D-C1D	5.27	134.00	124.71
46	N	620	LUT	C21-C26-C25	5.27	120.85	111.42
29	s	614	CLA	O2D-CGD-CBD	5.26	120.62	111.27
29	y	608	CLA	O2A-C1-C2	5.26	122.47	108.64
47	G	622	XAT	C31-C30-C29	-5.26	119.80	127.31
29	B	613	CLA	CMD-C2D-C1D	5.25	133.97	124.71
29	n	613	CLA	CMD-C2D-C1D	5.25	133.97	124.71
29	s	612	CLA	CMD-C2D-C1D	5.25	133.97	124.71
29	n	612	CLA	O2D-CGD-CBD	5.25	120.60	111.27
46	s	620	LUT	C21-C26-C25	5.25	120.82	111.42
29	r	610	CLA	O2A-C1-C2	5.25	122.43	108.64
29	N	611	CLA	CMD-C2D-C1D	5.25	133.96	124.71
29	B	602	CLA	O2D-CGD-CBD	5.25	120.59	111.27
29	Y	610	CLA	CMD-C2D-C1D	5.25	133.96	124.71
29	b	611	CLA	O2A-C1-C2	5.25	122.42	108.64
29	b	610	CLA	O2A-C1-C2	5.24	122.42	108.64
29	g	602	CLA	CMD-C2D-C1D	5.24	133.95	124.71
29	n	614	CLA	O2D-CGD-CBD	5.24	120.58	111.27
29	c	513	CLA	CMD-C2D-C1D	5.23	133.94	124.71
29	g	612	CLA	CMD-C2D-C1D	5.23	133.94	124.71
29	C	512	CLA	O2A-C1-C2	5.23	122.39	108.64
29	Y	610	CLA	O2D-CGD-CBD	5.23	120.57	111.27
29	G	612	CLA	O2D-CGD-CBD	5.23	120.56	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	602	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	b	602	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	s	609	CLA	CMD-C2D-C1D	5.23	133.93	124.71
29	c	501	CLA	O2A-C1-C2	5.23	122.38	108.64
29	s	612	CLA	O2D-CGD-CBD	5.23	120.55	111.27
29	b	613	CLA	CMD-C2D-C1D	5.22	133.91	124.71
29	B	610	CLA	O2A-C1-C2	5.22	122.35	108.64
29	s	602	CLA	CMD-C2D-C1D	5.22	133.91	124.71
29	c	510	CLA	O2A-C1-C2	5.22	122.35	108.64
29	G	603	CLA	O2D-CGD-CBD	5.22	120.54	111.27
29	b	612	CLA	O2A-C1-C2	5.21	122.34	108.64
29	d	403	CLA	O2A-C1-C2	5.21	122.34	108.64
29	s	611	CLA	CMD-C2D-C1D	5.21	133.90	124.71
29	r	612	CLA	O2D-CGD-CBD	5.21	120.52	111.27
29	b	608	CLA	O2D-CGD-CBD	5.21	120.52	111.27
29	R	610	CLA	O2D-CGD-CBD	5.21	120.52	111.27
29	N	602	CLA	CMD-C2D-C1D	5.20	133.89	124.71
29	C	501	CLA	O2A-C1-C2	5.20	122.31	108.64
29	B	608	CLA	O2D-CGD-CBD	5.20	120.51	111.27
29	b	604	CLA	CMD-C2D-C1D	5.20	133.88	124.71
29	r	608	CLA	O2A-C1-C2	5.20	122.31	108.64
29	R	602	CLA	O2A-C1-C2	5.20	122.30	108.64
29	r	602	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	B	610	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	C	507	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	c	508	CLA	CMD-C2D-C1D	5.20	133.87	124.71
29	R	603	CLA	O2D-CGD-CBD	5.19	120.49	111.27
29	b	603	CLA	O2D-CGD-CBD	5.19	120.49	111.27
29	c	505	CLA	O2D-CGD-CBD	5.18	120.48	111.27
29	y	611	CLA	CMD-C2D-C1D	5.18	133.85	124.71
29	c	504	CLA	O2D-CGD-CBD	5.18	120.48	111.27
29	c	511	CLA	O2D-CGD-CBD	5.18	120.48	111.27
29	S	602	CLA	O2A-C1-C2	5.18	122.25	108.64
29	S	617	CLA	CMD-C2D-C1D	5.18	133.84	124.71
29	c	512	CLA	O2A-C1-C2	5.18	122.25	108.64
46	N	621	LUT	C21-C26-C27	5.18	119.25	112.70
29	Y	614	CLA	O2D-CGD-CBD	5.18	120.47	111.27
29	N	614	CLA	O2A-C1-C2	5.17	121.07	108.97
29	B	605	CLA	O2D-CGD-CBD	5.17	120.45	111.27
29	g	613	CLA	O2A-C1-C2	5.17	122.22	108.64
29	B	614	CLA	O2A-C1-C2	5.17	122.22	108.64
29	S	602	CLA	CMD-C2D-C1D	5.16	133.81	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	502	CLA	CMD-C2D-C1D	5.16	133.81	124.71
29	c	505	CLA	O2A-C1-C2	5.16	122.19	108.64
29	y	614	CLA	O2D-CGD-CBD	5.16	120.43	111.27
29	A	410	CLA	CMD-C2D-C1D	5.16	133.80	124.71
29	S	617	CLA	O2D-CGD-CBD	5.15	120.43	111.27
29	D	403	CLA	CMD-C2D-C1D	5.15	133.79	124.71
29	c	503	CLA	O2A-C1-C2	5.15	122.17	108.64
29	G	612	CLA	CMD-C2D-C1D	5.14	133.78	124.71
29	B	604	CLA	CMD-C2D-C1D	5.14	133.78	124.71
29	G	610	CLA	O2D-CGD-CBD	5.14	120.41	111.27
29	c	508	CLA	O2A-C1-C2	5.14	122.14	108.64
29	B	616	CLA	O2D-CGD-CBD	5.14	120.39	111.27
29	B	611	CLA	O2A-C1-C2	5.13	122.13	108.64
29	y	612	CLA	CMD-C2D-C1D	5.13	133.76	124.71
29	S	609	CLA	O2D-CGD-CBD	5.13	120.39	111.27
29	G	613	CLA	O2A-C1-C2	5.13	122.11	108.64
29	S	604	CLA	O2D-CGD-CBD	5.13	120.38	111.27
29	Y	610	CLA	O2A-C1-C2	5.12	122.10	108.64
29	C	505	CLA	CMD-C2D-C1D	5.12	133.74	124.71
29	R	608	CLA	O2A-C1-C2	5.12	122.08	108.64
29	g	614	CLA	O2D-CGD-CBD	5.12	120.36	111.27
29	Y	602	CLA	CMD-C2D-C1D	5.12	133.73	124.71
29	C	508	CLA	O2A-C1-C2	5.12	122.08	108.64
29	a	410	CLA	O2A-C1-C2	5.11	122.07	108.64
47	g	622	XAT	C15-C14-C13	-5.11	120.02	127.31
29	S	617	CLA	O2A-C1-C2	5.11	122.06	108.64
29	A	410	CLA	O2A-C1-C2	5.11	122.06	108.64
29	S	613	CLA	O2A-C1-C2	5.11	122.06	108.64
29	r	612	CLA	O2A-C1-C2	5.11	122.06	108.64
29	Y	612	CLA	CMD-C2D-C1D	5.11	133.71	124.71
46	r	620	LUT	C31-C30-C29	-5.11	120.02	127.31
29	B	617	CLA	O2D-CGD-CBD	5.10	120.33	111.27
29	b	605	CLA	O2D-CGD-CBD	5.10	120.33	111.27
46	S	621	LUT	C21-C26-C25	5.10	120.55	111.42
29	y	610	CLA	O2A-C1-C2	5.10	122.04	108.64
29	b	606	CLA	O2A-C1-C2	5.10	122.03	108.64
29	C	508	CLA	CMD-C2D-C1D	5.09	133.69	124.71
29	S	604	CLA	O2A-C1-C2	5.09	122.02	108.64
29	b	614	CLA	O2A-C1-C2	5.09	122.01	108.64
29	b	616	CLA	O2D-CGD-CBD	5.09	120.31	111.27
29	N	602	CLA	O2A-C1-C2	5.09	122.01	108.64
29	s	611	CLA	O2D-CGD-CBD	5.09	120.31	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	609	CLA	CMD-C2D-C1D	5.09	133.68	124.71
29	S	605	CLA	CMD-C2D-C1D	5.08	133.67	124.71
29	S	612	CLA	CMD-C2D-C1D	5.08	133.67	124.71
29	c	505	CLA	CMD-C2D-C1D	5.08	133.67	124.71
46	G	621	LUT	C21-C26-C27	5.08	119.12	112.70
29	A	407	CLA	CMD-C2D-C1D	5.08	133.66	124.71
29	S	614	CLA	O2D-CGD-CBD	5.07	120.29	111.27
29	Y	613	CLA	O2A-C1-C2	5.07	121.96	108.64
46	R	620	LUT	C35-C34-C33	-5.07	120.08	127.31
29	B	606	CLA	O2A-C1-C2	5.06	121.94	108.64
46	g	621	LUT	C21-C26-C27	5.06	119.10	112.70
29	n	602	CLA	O2A-C1-C2	5.06	121.93	108.64
29	s	617	CLA	O2D-CGD-CBD	5.06	120.26	111.27
29	N	611	CLA	O2A-C1-C2	5.05	120.79	108.97
47	G	622	XAT	C15-C14-C13	-5.05	120.10	127.31
29	S	614	CLA	O2A-C1-C2	5.05	121.92	108.64
29	a	406	CLA	O2A-C1-C2	5.04	121.89	108.64
29	B	615	CLA	O2D-CGD-CBD	5.04	120.22	111.27
29	s	613	CLA	O2A-C1-C2	5.04	121.87	108.64
29	S	611	CLA	O2D-CGD-CBD	5.03	120.21	111.27
29	S	602	CLA	O2D-CGD-CBD	5.03	120.21	111.27
29	R	612	CLA	O2A-C1-C2	5.02	121.84	108.64
29	b	616	CLA	O2A-C1-C2	5.02	121.82	108.64
29	s	617	CLA	O2A-C1-C2	5.01	121.81	108.64
29	d	403	CLA	CMD-C2D-C1D	5.01	133.54	124.71
29	N	612	CLA	CMD-C2D-C1D	5.01	133.53	124.71
29	y	613	CLA	O2A-C1-C2	4.99	121.76	108.64
29	s	610	CLA	O2D-CGD-CBD	4.99	120.14	111.27
29	N	603	CLA	O2A-C1-C2	4.99	121.75	108.64
29	S	610	CLA	O2D-CGD-CBD	4.99	120.14	111.27
29	S	612	CLA	O2D-CGD-CBD	4.99	120.14	111.27
29	s	609	CLA	O2D-CGD-CBD	4.98	120.11	111.27
29	B	612	CLA	CMD-C2D-C1D	4.98	133.49	124.71
29	c	507	CLA	O2A-C1-C2	4.98	121.72	108.64
29	C	502	CLA	O2D-CGD-CBD	4.98	120.11	111.27
29	A	406	CLA	O2A-C1-C2	4.97	121.71	108.64
47	Y	622	XAT	C31-C30-C29	-4.97	120.22	127.31
29	N	610	CLA	O2D-CGD-CBD	4.97	120.09	111.27
29	y	610	CLA	O2D-CGD-CBD	4.96	120.09	111.27
35	b	620	C7Z	C15-C14-C13	-4.96	120.24	127.31
46	G	620	LUT	C21-C26-C25	4.95	120.29	111.42
29	G	614	CLA	O2D-CGD-CBD	4.95	120.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	609	CLA	O2D-CGD-CBD	4.94	120.05	111.27
29	r	603	CLA	O2D-CGD-CBD	4.94	120.05	111.27
29	r	609	CLA	O2D-CGD-CBD	4.94	120.05	111.27
29	b	604	CLA	O2D-CGD-CBD	4.94	120.05	111.27
29	Y	612	CLA	O2A-C1-C2	4.94	121.61	108.64
29	b	602	CLA	O2A-C1-C2	4.93	121.60	108.64
29	b	609	CLA	CMD-C2D-C1D	4.93	133.40	124.71
29	s	603	CLA	O2D-CGD-CBD	4.93	120.03	111.27
29	c	506	CLA	O2A-C1-C2	4.93	121.58	108.64
29	S	603	CLA	CMD-C2D-C1D	4.92	133.39	124.71
29	B	604	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	C	507	CLA	O2A-C1-C2	4.92	121.56	108.64
29	Y	608	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	b	617	CLA	O2D-CGD-CBD	4.91	120.00	111.27
29	D	402	CLA	O2D-CGD-CBD	4.91	120.00	111.27
29	c	512	CLA	O2D-CGD-CBD	4.91	120.00	111.27
29	b	615	CLA	O2D-CGD-CBD	4.91	120.00	111.27
29	B	616	CLA	O2A-C1-C2	4.91	121.54	108.64
29	n	610	CLA	O2D-CGD-CBD	4.91	119.99	111.27
29	d	402	CLA	O2D-CGD-CBD	4.91	119.98	111.27
29	N	612	CLA	O2D-CGD-CBD	4.90	119.98	111.27
29	B	603	CLA	O2D-CGD-CBD	4.90	119.98	111.27
29	b	612	CLA	CMD-C2D-C1D	4.90	133.35	124.71
48	R	622	NEX	C38-C25-C24	4.90	119.79	114.28
29	B	609	CLA	O2A-C1-C2	4.89	121.50	108.64
29	G	613	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	A	407	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	r	610	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	s	602	CLA	O2D-CGD-CBD	4.88	119.94	111.27
29	b	607	CLA	O2A-C1-C2	4.88	121.46	108.64
29	y	612	CLA	O2A-C1-C2	4.88	121.45	108.64
29	S	603	CLA	O2A-C1-C2	4.88	121.45	108.64
29	y	608	CLA	O2D-CGD-CBD	4.87	119.92	111.27
29	Y	604	CLA	O2D-CGD-CBD	4.87	119.92	111.27
29	y	613	CLA	O2D-CGD-CBD	4.87	119.92	111.27
29	B	612	CLA	O2A-C1-C2	4.87	121.43	108.64
48	r	623	NEX	C38-C25-C24	4.86	119.75	114.28
46	R	620	LUT	C11-C10-C9	-4.86	120.37	127.31
29	s	603	CLA	CMD-C2D-C1D	4.86	133.28	124.71
46	n	620	LUT	C21-C26-C25	4.86	120.12	111.42
29	B	612	CLA	O2D-CGD-CBD	4.85	119.89	111.27
29	a	406	CLA	O2D-CGD-CBD	4.85	119.88	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	604	CLA	O2A-C1-C2	4.85	121.37	108.64
29	r	602	CLA	O2A-C1-C2	4.85	121.37	108.64
47	y	622	XAT	C15-C14-C13	-4.85	120.39	127.31
29	R	611	CLA	O2D-CGD-CBD	4.84	119.87	111.27
29	s	603	CLA	O2A-C1-C2	4.84	121.35	108.64
29	b	612	CLA	O2D-CGD-CBD	4.83	119.85	111.27
29	Y	613	CLA	O2D-CGD-CBD	4.83	119.85	111.27
39	n	624	LHG	O7-C7-C8	4.83	121.91	111.50
29	S	609	CLA	O2A-C1-C2	4.83	121.32	108.64
29	c	502	CLA	C1-C2-C3	-4.83	117.70	126.04
29	s	609	CLA	O2A-C1-C2	4.82	121.31	108.64
29	y	604	CLA	O2A-C1-C2	4.82	121.30	108.64
46	R	620	LUT	C21-C26-C27	4.82	118.79	112.70
29	N	613	CLA	O2D-CGD-CBD	4.81	119.82	111.27
29	y	602	CLA	O2A-C1-C2	4.81	121.28	108.64
29	B	607	CLA	O2A-C1-C2	4.81	121.28	108.64
46	S	620	LUT	C21-C26-C25	4.81	120.03	111.42
29	Y	611	CLA	O2A-C1-C2	4.81	121.26	108.64
29	S	611	CLA	O2A-C1-C2	4.80	121.26	108.64
29	r	608	CLA	O2D-CGD-CBD	4.80	119.80	111.27
29	N	610	CLA	O2A-C1-C2	4.80	121.25	108.64
35	B	620	C7Z	C18-C5-C6	-4.80	119.14	124.53
29	c	508	CLA	O2D-CGD-CBD	4.80	119.79	111.27
29	R	608	CLA	O2D-CGD-CBD	4.79	119.79	111.27
29	b	614	CLA	O2D-CGD-CBD	4.78	119.77	111.27
29	C	503	CLA	O2A-C1-C2	4.78	121.20	108.64
29	g	613	CLA	O2D-CGD-CBD	4.78	119.76	111.27
29	Y	611	CLA	O2D-CGD-CBD	4.77	119.75	111.27
29	s	604	CLA	O2D-CGD-CBD	4.77	119.75	111.27
29	B	602	CLA	O2A-C1-C2	4.77	121.17	108.64
39	N	624	LHG	O7-C7-C8	4.77	121.78	111.50
29	g	610	CLA	O2D-CGD-CBD	4.76	119.73	111.27
46	r	620	LUT	C11-C10-C9	-4.76	120.52	127.31
29	n	613	CLA	O2D-CGD-CBD	4.75	119.71	111.27
29	C	512	CLA	O2D-CGD-CBD	4.75	119.71	111.27
29	a	407	CLA	O2D-CGD-CBD	4.75	119.71	111.27
35	B	620	C7Z	C15-C14-C13	-4.75	120.53	127.31
48	N	623	NEX	C17-C1-C6	-4.75	106.22	110.47
29	s	611	CLA	O2A-C1-C2	4.75	121.11	108.64
29	b	613	CLA	O2A-C1-C2	4.74	121.09	108.64
42	D	405	PL9	C7-C3-C4	4.73	120.72	116.88
46	S	621	LUT	C35-C34-C33	-4.73	120.56	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	614	CLA	O2A-C1-C2	4.73	121.07	108.64
29	C	508	CLA	O2D-CGD-CBD	4.72	119.66	111.27
48	N	623	NEX	C2-C1-C6	4.71	113.79	109.21
29	Y	611	CLA	CMD-C2D-C1D	4.71	133.01	124.71
29	C	506	CLA	O2A-C1-C2	4.70	120.99	108.64
29	r	611	CLA	O2D-CGD-CBD	4.69	119.60	111.27
48	s	623	NEX	C38-C25-C24	4.69	119.56	114.28
29	Y	602	CLA	O2A-C1-C2	4.69	120.95	108.64
29	b	617	CLA	CMD-C2D-C1D	4.68	132.96	124.71
48	S	622	NEX	C38-C25-C24	4.68	119.54	114.28
48	g	623	NEX	C38-C25-C24	4.67	119.54	114.28
29	y	604	CLA	O2D-CGD-CBD	4.67	119.57	111.27
29	C	509	CLA	O2A-C1-C2	4.67	120.91	108.64
29	y	611	CLA	O2A-C1-C2	4.66	120.89	108.64
47	N	622	XAT	C18-C5-C4	4.66	119.53	114.28
29	S	603	CLA	O2D-CGD-CBD	4.66	119.55	111.27
48	s	623	NEX	C2-C1-C6	4.66	113.74	109.21
48	n	623	NEX	C2-C1-C6	4.66	113.74	109.21
47	R	621	XAT	C38-C25-C24	4.65	119.51	114.28
29	B	617	CLA	CMD-C2D-C1D	4.65	132.90	124.71
29	B	614	CLA	O2D-CGD-CBD	4.64	119.51	111.27
48	Y	623	NEX	C2-C1-C6	4.63	113.71	109.21
29	b	609	CLA	O2A-C1-C2	4.63	120.80	108.64
47	N	622	XAT	C38-C25-C24	4.62	119.48	114.28
29	y	614	CLA	O2A-C1-C2	4.61	120.74	108.64
47	n	622	XAT	C38-C25-C24	4.60	119.46	114.28
29	C	512	CLA	CMD-C2D-C1D	4.60	132.82	124.71
29	c	512	CLA	CMD-C2D-C1D	4.59	132.80	124.71
47	n	622	XAT	C18-C5-C4	4.58	119.43	114.28
48	N	623	NEX	C38-C25-C24	4.58	119.43	114.28
46	Y	621	LUT	C21-C26-C27	4.58	118.48	112.70
48	S	622	NEX	C17-C1-C6	-4.57	106.38	110.47
47	G	622	XAT	C18-C5-C4	4.57	119.42	114.28
48	G	623	NEX	C38-C25-C24	4.57	119.42	114.28
29	r	603	CLA	O2A-C1-C2	4.55	120.60	108.64
29	A	406	CLA	O2D-CGD-CBD	4.55	119.35	111.27
46	S	621	LUT	C21-C26-C27	4.54	118.44	112.70
48	S	622	NEX	C2-C1-C6	4.54	113.62	109.21
29	B	604	CLA	O2A-C1-C2	4.53	120.54	108.64
46	s	621	LUT	C35-C34-C33	-4.53	120.85	127.31
48	G	623	NEX	C2-C1-C6	4.52	113.61	109.21
29	g	603	CLA	O2A-C1-C2	4.52	120.52	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	R	620	LUT	C31-C30-C29	-4.52	120.86	127.31
46	y	621	LUT	C35-C34-C33	-4.52	120.86	127.31
29	a	405	CLA	O2D-CGD-CBD	4.51	119.29	111.27
29	G	603	CLA	O2A-C1-C2	4.51	120.50	108.64
46	G	620	LUT	C21-C26-C27	4.51	118.40	112.70
46	Y	620	LUT	C21-C26-C27	4.50	118.39	112.70
48	Y	623	NEX	C38-C25-C24	4.49	119.33	114.28
29	b	604	CLA	O2A-C1-C2	4.48	120.42	108.64
42	d	405	PL9	C7-C3-C4	4.48	120.52	116.88
29	A	405	CLA	O2D-CGD-CBD	4.47	119.21	111.27
47	y	622	XAT	C18-C5-C4	4.46	119.30	114.28
48	y	623	NEX	C38-C25-C24	4.45	119.29	114.28
31	c	516	BCR	C33-C5-C6	-4.43	119.56	124.53
29	B	613	CLA	O2A-C1-C2	4.42	120.26	108.64
31	C	516	BCR	C33-C5-C6	-4.42	119.56	124.53
38	C	519	DGD	O2G-C1B-C2B	4.42	121.03	111.50
48	n	623	NEX	C38-C25-C24	4.42	119.25	114.28
46	S	620	LUT	C35-C34-C33	-4.41	121.02	127.31
48	g	623	NEX	C2-C1-C6	4.41	113.50	109.21
46	R	620	LUT	C7-C8-C9	-4.39	119.59	126.23
39	D	408	LHG	O7-C7-C8	4.38	120.94	111.50
46	n	621	LUT	C21-C26-C27	4.37	118.23	112.70
29	s	604	CLA	O2A-C1-C2	4.37	120.13	108.64
47	Y	622	XAT	C18-C5-C4	4.37	119.19	114.28
29	c	509	CLA	O2A-C1-C2	4.35	120.06	108.64
29	B	615	CLA	CAA-C2A-C3A	-4.33	100.91	112.78
47	y	622	XAT	C38-C25-C24	4.33	119.15	114.28
46	N	620	LUT	C21-C26-C27	4.33	118.17	112.70
39	d	408	LHG	O7-C7-C8	4.32	120.82	111.50
39	S	624	LHG	O7-C7-C8	4.32	120.81	111.50
29	Y	603	CLA	O2A-C1-C2	4.32	119.98	108.64
35	b	620	C7Z	C18-C5-C6	-4.31	119.68	124.53
29	R	603	CLA	O2A-C1-C2	4.30	119.94	108.64
46	g	620	LUT	C7-C8-C9	-4.29	119.75	126.23
46	N	621	LUT	C22-C23-C24	-4.29	106.86	111.74
46	y	620	LUT	C21-C26-C27	4.29	118.12	112.70
30	a	408	PHO	C2B-C1B-NB	-4.28	106.57	109.53
31	C	515	BCR	C15-C14-C13	-4.27	121.22	127.31
46	r	620	LUT	C7-C8-C9	-4.27	119.78	126.23
47	g	622	XAT	C18-C5-C4	4.27	119.08	114.28
39	G	630	LHG	O7-C7-C8	4.26	120.69	111.50
47	r	622	XAT	C38-C25-C24	4.26	119.08	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	g	621	LUT	C22-C23-C24	-4.25	106.90	111.74
46	s	620	LUT	C22-C23-C24	-4.25	106.91	111.74
45	g	609	CHL	CHD-C1D-ND	-4.24	120.56	124.45
38	C	520	DGD	O2G-C1B-C2B	4.23	120.61	111.50
39	s	624	LHG	O7-C7-C8	4.23	120.61	111.50
47	Y	622	XAT	C38-C25-C24	4.22	119.03	114.28
29	b	612	CLA	CAA-C2A-C3A	-4.22	101.22	112.78
33	a	413	LMG	O7-C10-C11	4.22	120.59	111.50
46	R	620	LUT	C21-C26-C25	4.22	118.97	111.42
38	c	519	DGD	O2G-C1B-C2B	4.21	120.58	111.50
48	Y	623	NEX	C17-C1-C6	-4.20	106.71	110.47
33	A	413	LMG	O7-C10-C11	4.20	120.55	111.50
38	C	523	DGD	O2G-C1B-C2B	4.18	120.51	111.50
29	b	615	CLA	CAA-C2A-C3A	-4.17	101.35	112.78
46	Y	620	LUT	C15-C14-C13	-4.17	121.36	127.31
44	H	101	RRX	C11-C10-C9	-4.17	121.36	127.31
47	G	622	XAT	C38-C25-C24	4.16	118.96	114.28
38	c	520	DGD	O2G-C1B-C2B	4.16	120.47	111.50
46	n	620	LUT	C21-C26-C27	4.14	117.94	112.70
46	y	621	LUT	C7-C8-C9	-4.14	119.97	126.23
47	n	622	XAT	C7-C8-C9	-4.13	119.11	125.53
46	y	621	LUT	C21-C26-C27	4.13	117.92	112.70
47	R	621	XAT	C18-C5-C4	4.13	118.92	114.28
48	y	623	NEX	C2-C1-C6	4.13	113.22	109.21
46	G	620	LUT	C7-C8-C9	-4.12	120.00	126.23
48	s	623	NEX	C17-C1-C6	-4.12	106.78	110.47
33	h	102	LMG	O7-C10-C11	4.12	120.38	111.50
29	y	603	CLA	O2A-C1-C2	4.12	119.46	108.64
48	R	622	NEX	C2-C1-C6	4.11	113.21	109.21
46	y	621	LUT	C22-C23-C24	-4.11	107.06	111.74
47	g	622	XAT	C38-C25-C24	4.11	118.90	114.28
46	s	620	LUT	C35-C34-C33	-4.11	121.45	127.31
39	g	624	LHG	O7-C7-C8	4.10	120.34	111.50
46	Y	620	LUT	C22-C23-C24	-4.10	107.08	111.74
50	i	101	3PH	O21-C21-C22	4.09	120.33	111.50
35	b	620	C7Z	C38-C25-C26	-4.09	119.93	124.53
46	Y	621	LUT	C7-C8-C9	-4.09	120.05	126.23
33	C	521	LMG	O7-C10-C11	4.09	120.31	111.50
47	Y	622	XAT	C36-C21-C26	4.08	121.06	110.05
38	c	523	DGD	O2G-C1B-C2B	4.08	120.30	111.50
39	d	410	LHG	O7-C7-C8	4.07	120.28	111.50
45	N	609	CHL	CHD-C1D-ND	-4.07	120.71	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	H	102	LMG	O7-C10-C11	4.07	120.26	111.50
29	c	502	CLA	O2D-CGD-CBD	4.06	118.48	111.27
33	c	521	LMG	O7-C10-C11	4.05	120.22	111.50
31	D	404	BCR	C19-C18-C17	4.03	125.13	118.94
44	h	101	RRX	C11-C10-C9	-4.01	121.58	127.31
50	S	626	3PH	O21-C21-C22	4.01	120.15	111.50
30	a	409	PHO	C2B-C1B-NB	-4.01	106.76	109.53
32	A	412	SQD	O7-S-C6	-4.00	102.18	106.94
46	Y	621	LUT	C22-C23-C24	-3.98	107.21	111.74
50	s	626	3PH	O21-C21-C22	3.98	120.08	111.50
36	C	524	DGA	OG2-CB1-CB2	3.98	120.07	111.50
31	d	404	BCR	C19-C18-C17	3.97	125.04	118.94
30	A	409	PHO	C2B-C1B-NB	-3.97	106.78	109.53
48	g	623	NEX	C27-C28-C29	-3.97	119.36	125.53
46	G	621	LUT	C22-C23-C24	-3.97	107.23	111.74
39	C	525	LHG	O7-C7-C8	3.96	120.05	111.50
36	b	623	DGA	OG2-CB1-CB2	3.96	120.03	111.50
45	g	601	CHL	CHD-C1D-ND	-3.96	120.82	124.45
46	g	621	LUT	C7-C8-C9	-3.96	120.26	126.23
46	S	620	LUT	C7-C8-C9	-3.95	120.27	126.23
46	G	620	LUT	C15-C14-C13	-3.95	121.68	127.31
47	y	622	XAT	C36-C21-C26	3.94	120.68	110.05
36	c	524	DGA	OG2-CB1-CB2	3.94	119.99	111.50
38	c	518	DGD	O2G-C1B-C2B	3.94	119.98	111.50
46	N	620	LUT	C35-C34-C33	-3.92	121.71	127.31
29	B	605	CLA	C2C-C1C-NC	3.91	113.63	109.97
39	c	625	LHG	O7-C7-C8	3.90	119.91	111.50
30	a	409	PHO	CMB-C2B-C3B	3.90	131.97	124.68
46	n	621	LUT	C35-C34-C33	-3.90	121.75	127.31
46	r	620	LUT	C21-C26-C25	3.90	118.40	111.42
45	y	601	CHL	CHD-C1D-ND	-3.90	120.87	124.45
45	Y	605	CHL	CHD-C1D-ND	-3.89	120.88	124.45
46	g	621	LUT	C35-C34-C33	-3.89	121.77	127.31
29	C	502	CLA	C1-C2-C3	-3.88	119.33	126.04
29	B	606	CLA	CHD-C1D-ND	-3.87	120.90	124.45
46	y	620	LUT	C22-C23-C24	-3.87	107.34	111.74
29	b	605	CLA	C2C-C1C-NC	3.87	113.60	109.97
36	B	625	DGA	OG2-CB1-CB2	3.86	119.81	111.50
35	B	620	C7Z	C38-C25-C26	-3.86	120.20	124.53
33	B	622	LMG	O7-C10-C11	3.85	119.79	111.50
33	j	101	LMG	O7-C10-C11	3.85	119.79	111.50
46	g	620	LUT	C21-C26-C27	3.84	117.55	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	408	PHO	C2B-C1B-NB	-3.84	106.88	109.53
45	n	605	CHL	CHD-C1D-ND	-3.83	120.93	124.45
45	N	605	CHL	CHD-C1D-ND	-3.82	120.94	124.45
39	D	409	LHG	O7-C7-C8	3.82	119.74	111.50
46	N	620	LUT	C15-C14-C13	-3.82	121.85	127.31
46	G	621	LUT	C7-C8-C9	-3.82	120.47	126.23
48	Y	623	NEX	C27-C28-C29	-3.81	119.61	125.53
39	Y	624	LHG	O7-C7-C8	3.81	119.72	111.50
29	S	617	CLA	C1-C2-C3	-3.81	120.59	126.75
46	S	620	LUT	C22-C23-C24	-3.80	107.41	111.74
45	Y	601	CHL	CHD-C1D-ND	-3.80	120.96	124.45
46	G	621	LUT	C35-C34-C33	-3.80	121.89	127.31
45	y	605	CHL	CHD-C1D-ND	-3.80	120.96	124.45
46	s	621	LUT	C21-C26-C27	3.79	117.50	112.70
33	b	622	LMG	O7-C10-C11	3.79	119.67	111.50
30	A	409	PHO	CMB-C2B-C3B	3.79	131.76	124.68
39	d	409	LHG	O7-C7-C8	3.78	119.65	111.50
44	H	101	RRX	C7-C8-C9	-3.78	120.53	126.23
33	d	411	LMG	O7-C10-C11	3.78	119.64	111.50
29	C	509	CLA	C2C-C1C-NC	3.77	113.50	109.97
35	b	620	C7Z	C1-C6-C5	-3.77	117.31	122.61
47	r	622	XAT	C18-C5-C4	3.77	118.52	114.28
29	S	613	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
33	D	411	LMG	O7-C10-C11	3.77	119.62	111.50
29	s	617	CLA	C1-C2-C3	-3.76	120.66	126.75
29	A	406	CLA	C2C-C1C-NC	3.76	113.50	109.97
39	D	410	LHG	O7-C7-C8	3.76	119.60	111.50
46	N	621	LUT	C35-C34-C33	-3.75	121.96	127.31
29	s	613	CLA	C1-C2-C3	-3.74	119.57	126.04
33	J	101	LMG	O7-C10-C11	3.74	119.57	111.50
48	n	623	NEX	C27-C28-C29	-3.74	119.72	125.53
47	N	622	XAT	C7-C8-C9	-3.74	119.73	125.53
46	g	620	LUT	C35-C34-C33	-3.73	121.98	127.31
29	B	605	CLA	C1-C2-C3	-3.73	119.59	126.04
32	a	412	SQD	O7-S-C6	-3.72	102.51	106.94
29	b	606	CLA	CHD-C1D-ND	-3.72	121.03	124.45
45	S	608	CHL	CHD-C1D-ND	-3.72	121.04	124.45
46	g	621	LUT	C15-C14-C13	-3.72	122.01	127.31
46	n	621	LUT	C22-C23-C24	-3.71	107.52	111.74
45	G	601	CHL	CHD-C1D-ND	-3.71	121.04	124.45
40	c	627	LMK	O3-C4-C3	-3.71	110.25	122.98
45	s	608	CHL	CHD-C1D-ND	-3.70	121.05	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	613	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
32	B	621	SQD	O7-S-C6	-3.70	102.54	106.94
32	b	621	SQD	O7-S-C6	-3.70	102.55	106.94
45	R	607	CHL	CHD-C1D-ND	-3.70	121.06	124.45
46	n	621	LUT	C15-C14-C13	-3.69	122.04	127.31
31	d	404	BCR	C36-C18-C17	-3.69	117.75	122.92
47	R	621	XAT	C19-C9-C10	-3.69	117.75	122.92
35	B	620	C7Z	C35-C34-C33	-3.69	122.05	127.31
29	S	613	CLA	C1-C2-C3	-3.69	119.67	126.04
46	N	620	LUT	C22-C23-C24	-3.69	107.55	111.74
46	s	621	LUT	C15-C14-C13	-3.68	122.05	127.31
46	y	621	LUT	C11-C10-C9	-3.68	122.05	127.31
45	r	606	CHL	CHD-C1D-ND	-3.68	121.07	124.45
45	y	609	CHL	CHD-C1D-ND	-3.68	121.07	124.45
31	B	619	BCR	C37-C22-C21	-3.67	117.78	122.92
45	G	609	CHL	CHD-C1D-ND	-3.67	121.08	124.45
45	g	605	CHL	CHD-C1D-ND	-3.67	121.08	124.45
39	y	624	LHG	O7-C7-C8	3.67	119.41	111.50
46	S	620	LUT	C18-C5-C6	-3.66	120.41	124.53
45	n	608	CHL	CHD-C1D-ND	-3.66	121.09	124.45
48	G	623	NEX	C27-C28-C29	-3.66	119.86	125.53
45	n	606	CHL	CHD-C1D-ND	-3.65	121.10	124.45
44	h	101	RRX	C33-C5-C4	3.64	120.61	113.62
46	g	621	LUT	C11-C10-C9	-3.64	122.12	127.31
38	C	518	DGD	O2G-C1B-C2B	3.64	119.34	111.50
46	s	621	LUT	C7-C8-C9	-3.63	120.75	126.23
45	s	607	CHL	CHD-C1D-ND	-3.62	121.12	124.45
46	S	620	LUT	C15-C14-C13	-3.62	122.14	127.31
47	R	621	XAT	C26-C27-C28	-3.62	118.35	125.99
47	r	622	XAT	C38-C25-C26	-3.61	116.20	122.26
45	n	606	CHL	C3B-C4B-NB	-3.61	107.17	110.52
45	Y	609	CHL	CHD-C1D-ND	-3.61	121.14	124.45
48	S	622	NEX	C27-C28-C29	-3.61	119.93	125.53
32	c	626	SQD	O7-S-C6	-3.61	102.65	106.94
46	Y	620	LUT	C7-C8-C9	-3.60	120.79	126.23
45	G	605	CHL	CHD-C1D-ND	-3.60	121.14	124.45
46	g	620	LUT	C15-C14-C13	-3.60	122.17	127.31
29	B	603	CLA	CHD-C1D-ND	-3.60	121.14	124.45
45	n	601	CHL	CHD-C1D-ND	-3.60	121.14	124.45
48	y	623	NEX	C27-C28-C29	-3.58	119.98	125.53
31	D	404	BCR	C36-C18-C17	-3.58	117.91	122.92
31	b	619	BCR	C33-C5-C4	3.57	120.47	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	C	527	LMK	O3-C4-C3	-3.57	110.73	122.98
31	c	517	BCR	C28-C27-C26	-3.57	107.70	114.08
48	g	623	NEX	C17-C1-C6	-3.57	107.28	110.47
31	D	404	BCR	C37-C22-C21	-3.57	117.93	122.92
32	C	526	SQD	O7-S-C6	-3.57	102.70	106.94
45	s	601	CHL	CHD-C1D-ND	-3.56	121.18	124.45
46	s	620	LUT	C35-C15-C14	-3.56	116.18	123.47
45	g	608	CHL	CHD-C1D-ND	-3.56	121.18	124.45
31	A	411	BCR	C33-C5-C6	-3.55	120.54	124.53
48	s	623	NEX	C27-C28-C29	-3.55	120.02	125.53
47	N	622	XAT	O24-C25-C24	3.55	116.05	113.38
45	N	608	CHL	CHD-C1D-ND	-3.55	121.19	124.45
31	B	619	BCR	C33-C5-C4	3.54	120.43	113.62
29	B	605	CLA	CMA-C3A-C4A	3.54	121.30	111.77
29	g	613	CLA	CMA-C3A-C4A	3.54	121.30	111.77
35	b	620	C7Z	C35-C34-C33	-3.54	122.25	127.31
45	y	606	CHL	C2C-C3C-C4C	3.54	109.01	106.49
46	g	620	LUT	C22-C23-C24	-3.54	107.71	111.74
44	H	101	RRX	C33-C5-C4	3.54	120.41	113.62
29	N	610	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
29	S	604	CLA	CHD-C1D-ND	-3.54	121.20	124.45
46	G	620	LUT	C11-C10-C9	-3.53	122.27	127.31
29	c	506	CLA	CHD-C1D-ND	-3.53	121.21	124.45
29	c	506	CLA	C2C-C1C-NC	3.53	113.28	109.97
45	G	608	CHL	CHD-C1D-ND	-3.53	121.21	124.45
29	C	508	CLA	C1-C2-C3	-3.52	119.95	126.04
46	s	620	LUT	C7-C8-C9	-3.52	120.91	126.23
29	c	512	CLA	C2D-C1D-ND	3.52	112.70	110.10
31	a	411	BCR	C33-C5-C6	-3.51	120.58	124.53
45	S	607	CHL	CHD-C1D-ND	-3.51	121.22	124.45
29	C	510	CLA	CHD-C1D-ND	-3.51	121.23	124.45
46	N	621	LUT	C15-C14-C13	-3.51	122.30	127.31
29	B	610	CLA	C1-C2-C3	-3.50	119.99	126.04
47	y	622	XAT	C7-C8-C9	-3.50	120.10	125.53
46	y	620	LUT	C35-C34-C33	-3.50	122.32	127.31
47	G	622	XAT	C7-C8-C9	-3.49	120.11	125.53
35	B	620	C7Z	C1-C6-C5	-3.49	117.69	122.61
44	h	101	RRX	C30-C25-C26	-3.49	117.69	122.61
47	R	621	XAT	C11-C10-C9	-3.49	122.33	127.31
29	G	613	CLA	CMA-C3A-C4A	3.49	121.16	111.77
29	C	505	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
44	H	101	RRX	C30-C25-C26	-3.49	117.70	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	604	CLA	C1-C2-C3	-3.49	120.01	126.04
47	r	622	XAT	C19-C9-C10	-3.49	118.04	122.92
29	s	614	CLA	CHD-C1D-ND	-3.48	121.25	124.45
29	C	506	CLA	C2C-C1C-NC	3.48	113.23	109.97
29	r	610	CLA	CMA-C3A-C4A	3.48	121.12	111.77
46	y	620	LUT	C15-C14-C13	-3.47	122.35	127.31
29	c	502	CLA	C2C-C1C-NC	3.47	113.22	109.97
48	N	623	NEX	C27-C28-C29	-3.47	120.14	125.53
29	C	511	CLA	CHD-C1D-ND	-3.47	121.27	124.45
29	C	504	CLA	C1-C2-C3	-3.47	120.05	126.04
29	a	406	CLA	C2C-C1C-NC	3.46	113.22	109.97
46	S	621	LUT	C35-C15-C14	-3.46	116.38	123.47
47	r	622	XAT	C20-C13-C14	-3.46	118.07	122.92
29	N	603	CLA	C1-C2-C3	-3.46	120.05	126.04
45	s	606	CHL	CHD-C1D-ND	-3.46	121.27	124.45
29	N	604	CLA	C1-C2-C3	-3.45	120.07	126.04
29	B	602	CLA	C2C-C1C-NC	3.45	113.21	109.97
31	C	514	BCR	C15-C14-C13	-3.45	122.38	127.31
31	d	404	BCR	C37-C22-C21	-3.45	118.09	122.92
31	D	404	BCR	C23-C22-C21	3.45	124.24	118.94
45	S	606	CHL	CHD-C1D-ND	-3.45	121.28	124.45
29	C	511	CLA	C1-C2-C3	-3.44	120.09	126.04
29	c	508	CLA	C1-C2-C3	-3.44	120.09	126.04
44	h	101	RRX	C7-C8-C9	-3.44	121.03	126.23
29	s	605	CLA	C1-C2-C3	-3.44	121.19	126.75
29	c	503	CLA	CHD-C1D-ND	-3.44	121.30	124.45
29	b	605	CLA	CMA-C3A-C4A	3.44	121.01	111.77
46	G	620	LUT	C35-C34-C33	-3.43	122.41	127.31
29	C	510	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
47	R	621	XAT	C38-C25-C26	-3.43	116.51	122.26
29	g	610	CLA	C1-C2-C3	-3.43	120.11	126.04
46	S	620	LUT	C11-C10-C9	-3.43	122.42	127.31
29	S	614	CLA	CHD-C1D-ND	-3.43	121.31	124.45
29	b	610	CLA	C1-C2-C3	-3.43	120.12	126.04
29	a	406	CLA	CHD-C1D-ND	-3.42	121.31	124.45
29	c	511	CLA	CHD-C1D-ND	-3.42	121.31	124.45
29	c	510	CLA	C1-C2-C3	-3.42	120.12	126.04
29	c	501	CLA	C1-C2-C3	-3.42	120.12	126.04
29	C	507	CLA	C2C-C1C-NC	3.42	113.18	109.97
29	d	402	CLA	C2D-C1D-ND	3.42	112.62	110.10
29	C	503	CLA	CHD-C1D-ND	-3.42	121.31	124.45
29	B	603	CLA	C1-C2-C3	-3.41	120.14	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	510	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
29	s	611	CLA	C2C-C1C-NC	3.41	113.17	109.97
29	R	610	CLA	CMA-C3A-C4A	3.41	120.95	111.77
29	N	613	CLA	CMA-C3A-C4A	3.41	120.95	111.77
29	b	617	CLA	C1-C2-C3	-3.41	120.14	126.04
29	Y	613	CLA	C1-C2-C3	-3.41	120.14	126.04
48	G	623	NEX	C17-C1-C6	-3.41	107.42	110.47
46	S	621	LUT	C22-C23-C24	-3.41	107.86	111.74
45	N	606	CHL	C3B-C4B-NB	-3.41	107.35	110.52
29	c	505	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
29	G	610	CLA	C1-C2-C3	-3.41	120.15	126.04
46	r	620	LUT	C31-C32-C33	-3.41	116.85	126.42
31	b	619	BCR	C37-C22-C21	-3.41	118.15	122.92
46	s	621	LUT	C18-C5-C6	-3.40	120.71	124.53
29	c	505	CLA	C1-C2-C3	-3.40	120.16	126.04
29	c	510	CLA	CHD-C1D-ND	-3.40	121.33	124.45
29	s	604	CLA	CHD-C1D-ND	-3.40	121.33	124.45
46	n	620	LUT	C22-C23-C24	-3.40	107.88	111.74
29	C	513	CLA	CHD-C1D-ND	-3.40	121.33	124.45
47	n	622	XAT	O24-C25-C24	3.40	115.93	113.38
29	C	510	CLA	C1-C2-C3	-3.39	120.18	126.04
29	C	506	CLA	CHD-C1D-ND	-3.39	121.34	124.45
48	Y	623	NEX	C39-C29-C30	-3.39	118.17	122.92
46	g	620	LUT	C11-C10-C9	-3.39	122.47	127.31
29	N	612	CLA	CMA-C3A-C4A	3.39	120.89	111.77
29	c	509	CLA	C2C-C1C-NC	3.39	113.15	109.97
29	b	603	CLA	C1-C2-C3	-3.39	120.18	126.04
46	n	620	LUT	C15-C14-C13	-3.39	122.48	127.31
45	G	606	CHL	C3B-C4B-NB	-3.38	107.38	110.52
47	r	622	XAT	O24-C25-C24	3.38	115.92	113.38
29	n	613	CLA	CMA-C3A-C4A	3.38	120.86	111.77
29	b	606	CLA	C1-C2-C3	-3.38	120.20	126.04
46	Y	621	LUT	C11-C10-C9	-3.38	122.49	127.31
29	b	616	CLA	C2C-C1C-NC	3.38	113.14	109.97
29	c	504	CLA	CHD-C1D-ND	-3.38	121.35	124.45
29	S	605	CLA	C2C-C1C-NC	3.38	113.13	109.97
29	C	512	CLA	C2D-C1D-ND	3.37	112.59	110.10
45	y	606	CHL	CHD-C1D-ND	-3.37	121.35	124.45
29	B	606	CLA	C2C-C1C-NC	3.37	113.13	109.97
29	B	609	CLA	C2C-C1C-NC	3.37	113.13	109.97
45	G	601	CHL	C2C-C3C-C4C	3.37	108.89	106.49
45	Y	606	CHL	CHD-C1D-ND	-3.37	121.36	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	r	622	XAT	C27-C28-C29	3.37	130.76	125.53
46	y	621	LUT	C15-C14-C13	-3.37	122.50	127.31
45	g	601	CHL	C3C-C4C-NC	-3.37	106.80	110.57
47	r	622	XAT	C26-C27-C28	-3.37	118.88	125.99
45	Y	606	CHL	C3B-C4B-NB	-3.37	107.39	110.52
29	b	603	CLA	CHD-C1D-ND	-3.36	121.36	124.45
29	b	609	CLA	C2C-C1C-NC	3.36	113.12	109.97
45	S	601	CHL	CHD-C1D-ND	-3.36	121.36	124.45
29	C	504	CLA	CHD-C1D-ND	-3.36	121.37	124.45
45	y	606	CHL	C3C-C4C-NC	-3.36	106.81	110.57
29	b	605	CLA	C1-C2-C3	-3.36	120.24	126.04
45	G	607	CHL	CHD-C1D-ND	-3.35	121.37	124.45
29	r	610	CLA	C2D-C1D-ND	3.35	112.58	110.10
45	g	609	CHL	C4B-CHC-C1C	3.35	134.29	126.34
29	n	603	CLA	CHD-C1D-ND	-3.35	121.38	124.45
29	A	407	CLA	C2C-C1C-NC	3.35	113.11	109.97
29	y	613	CLA	CMA-C3A-C4A	3.35	120.76	111.77
45	s	601	CHL	C3B-C4B-NB	-3.34	107.41	110.52
47	y	622	XAT	O4-C5-C4	-3.34	110.87	113.38
29	r	608	CLA	C2C-C1C-NC	3.34	113.10	109.97
29	B	615	CLA	CBA-CAA-C2A	3.34	123.72	113.86
48	r	623	NEX	C2-C1-C6	3.34	112.45	109.21
29	y	603	CLA	C2D-C1D-ND	3.34	112.56	110.10
45	y	607	CHL	CHD-C1D-ND	-3.33	121.39	124.45
45	G	601	CHL	C3C-C4C-NC	-3.33	106.83	110.57
29	g	610	CLA	CHD-C1D-ND	-3.33	121.39	124.45
31	B	618	BCR	C23-C24-C25	-3.33	117.85	127.20
29	s	605	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
44	h	101	RRX	C1-C6-C5	-3.33	117.93	122.61
29	b	609	CLA	CMA-C3A-C4A	3.33	120.71	111.77
29	R	610	CLA	C1-C2-C3	-3.32	120.30	126.04
29	A	405	CLA	CHD-C1D-ND	-3.32	121.40	124.45
29	c	505	CLA	C2C-C1C-NC	3.32	113.08	109.97
46	G	620	LUT	C31-C30-C29	-3.32	122.58	127.31
29	D	403	CLA	C1-C2-C3	-3.31	120.31	126.04
29	b	607	CLA	CHD-C1D-ND	-3.31	121.41	124.45
29	S	605	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
45	s	607	CHL	C2C-C3C-C4C	3.31	108.85	106.49
47	R	621	XAT	C27-C28-C29	3.31	130.67	125.53
29	a	407	CLA	C2C-C1C-NC	3.31	113.07	109.97
29	B	612	CLA	CHD-C1D-ND	-3.31	121.41	124.45
29	G	612	CLA	C2C-C1C-NC	3.31	113.07	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	616	CLA	C2C-C1C-NC	3.31	113.07	109.97
29	c	503	CLA	CMA-C3A-C4A	3.31	120.66	111.77
29	C	502	CLA	C2C-C1C-NC	3.30	113.07	109.97
45	N	606	CHL	CHD-C1D-ND	-3.30	121.42	124.45
45	g	607	CHL	CHD-C1D-ND	-3.30	121.42	124.45
47	G	622	XAT	C38-C25-C26	-3.30	116.72	122.26
29	B	606	CLA	C1-C2-C3	-3.30	120.33	126.04
29	S	603	CLA	C2C-C1C-NC	3.30	113.06	109.97
29	s	602	CLA	CHD-C1D-ND	-3.30	121.42	124.45
44	H	101	RRX	C16-C17-C18	-3.30	122.60	127.31
29	g	603	CLA	C1-C2-C3	-3.30	120.33	126.04
45	G	606	CHL	CHD-C1D-ND	-3.30	121.42	124.45
29	S	605	CLA	C1-O2A-CGA	3.30	125.10	116.44
45	g	601	CHL	C2C-C3C-C4C	3.30	108.84	106.49
44	h	101	RRX	C20-C21-C22	-3.30	122.61	127.31
29	S	613	CLA	C2C-C1C-NC	3.29	113.06	109.97
45	s	607	CHL	CMA-C3A-C4A	3.29	120.62	111.77
45	y	605	CHL	C3C-C4C-NC	-3.29	106.88	110.57
29	a	406	CLA	C1-C2-C3	-3.29	120.35	126.04
29	y	608	CLA	C1-C2-C3	-3.29	121.44	126.75
45	Y	605	CHL	C3C-C4C-NC	-3.28	106.89	110.57
29	B	607	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	n	612	CLA	C2C-C1C-NC	3.28	113.05	109.97
29	G	610	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	N	602	CLA	C2C-C1C-NC	3.28	113.04	109.97
29	r	612	CLA	C2C-C1C-NC	3.27	113.04	109.97
45	G	606	CHL	CMA-C3A-C4A	3.27	120.57	111.77
45	g	606	CHL	C2C-C3C-C4C	3.27	108.82	106.49
45	r	607	CHL	C2C-C3C-C4C	3.27	108.82	106.49
29	C	505	CLA	C2C-C1C-NC	3.27	113.03	109.97
29	G	603	CLA	C2C-C1C-NC	3.27	113.03	109.97
45	N	609	CHL	C3C-C4C-NC	-3.27	106.91	110.57
47	Y	622	XAT	C6-C7-C8	-3.27	119.08	125.99
45	R	607	CHL	C3C-C4C-NC	-3.27	106.91	110.57
29	C	501	CLA	C1-C2-C3	-3.27	120.39	126.04
46	s	621	LUT	C22-C23-C24	-3.26	108.03	111.74
29	r	613	CLA	CHD-C1D-ND	-3.26	121.45	124.45
29	y	610	CLA	C1-C2-C3	-3.26	120.40	126.04
29	s	604	CLA	C2C-C1C-NC	3.26	113.03	109.97
29	c	506	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
45	N	601	CHL	CHD-C1D-ND	-3.26	121.46	124.45
29	s	602	CLA	C2D-C1D-ND	3.26	112.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S	607	CHL	C2C-C3C-C4C	3.26	108.81	106.49
29	Y	611	CLA	C2C-C1C-NC	3.26	113.02	109.97
31	C	516	BCR	C34-C9-C10	-3.26	118.36	122.92
45	S	607	CHL	CMA-C3A-C4A	3.25	120.52	111.77
35	b	620	C7Z	C2-C3-C4	3.25	114.76	110.30
29	G	611	CLA	C2C-C1C-NC	3.25	113.02	109.97
29	b	606	CLA	C2C-C1C-NC	3.25	113.02	109.97
29	b	609	CLA	C2D-C1D-ND	3.25	112.50	110.10
29	R	612	CLA	C2C-C1C-NC	3.25	113.02	109.97
29	G	614	CLA	CHD-C1D-ND	-3.25	121.47	124.45
29	c	507	CLA	C2C-C1C-NC	3.25	113.01	109.97
45	n	609	CHL	CHD-C1D-ND	-3.25	121.47	124.45
29	y	604	CLA	CHD-C1D-ND	-3.25	121.47	124.45
46	G	621	LUT	C18-C5-C6	-3.25	120.88	124.53
45	n	601	CHL	C2C-C3C-C4C	3.24	108.80	106.49
29	R	610	CLA	CHD-C1D-ND	-3.24	121.47	124.45
29	s	617	CLA	CHD-C1D-ND	-3.24	121.47	124.45
29	g	611	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	y	610	CLA	CHD-C1D-ND	-3.24	121.47	124.45
46	s	620	LUT	C15-C14-C13	-3.24	122.69	127.31
45	r	607	CHL	C3C-C4C-NC	-3.24	106.94	110.57
30	A	408	PHO	CMB-C2B-C3B	3.24	130.74	124.68
29	S	612	CLA	C2C-C1C-NC	3.24	113.00	109.97
29	C	503	CLA	CMA-C3A-C4A	3.23	120.47	111.77
29	b	615	CLA	C1-C2-C3	-3.23	120.45	126.04
31	C	514	BCR	C33-C5-C6	-3.23	120.90	124.53
46	G	620	LUT	C18-C5-C6	-3.23	120.90	124.53
45	R	607	CHL	C2C-C3C-C4C	3.23	108.79	106.49
29	B	611	CLA	C2C-C1C-NC	3.23	113.00	109.97
29	D	402	CLA	C2D-C1D-ND	3.23	112.48	110.10
47	g	622	XAT	C7-C8-C9	-3.23	120.52	125.53
29	a	405	CLA	CHD-C1D-ND	-3.23	121.49	124.45
29	b	611	CLA	C2C-C1C-NC	3.23	112.99	109.97
29	a	410	CLA	CHD-C1D-ND	-3.22	121.49	124.45
29	b	614	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	s	610	CLA	CHD-C1D-ND	-3.22	121.49	124.45
29	S	611	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	g	613	CLA	CHD-C1D-ND	-3.22	121.50	124.45
31	c	514	BCR	C15-C14-C13	-3.22	122.72	127.31
29	c	511	CLA	C1-C2-C3	-3.22	120.48	126.04
29	S	604	CLA	C1-C2-C3	-3.22	120.48	126.04
29	s	612	CLA	C2C-C1C-NC	3.22	112.98	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	N	607	CHL	CHD-C1D-ND	-3.22	121.50	124.45
43	f	101	HEM	C1B-NB-C4B	3.22	108.39	105.07
29	R	608	CLA	C2C-C1C-NC	3.22	112.98	109.97
29	N	603	CLA	CHD-C1D-ND	-3.21	121.50	124.45
45	g	606	CHL	CHD-C1D-ND	-3.21	121.50	124.45
29	n	603	CLA	C2D-C1D-ND	3.21	112.47	110.10
29	n	610	CLA	CHD-C1D-ND	-3.21	121.50	124.45
29	Y	608	CLA	C1-C2-C3	-3.21	121.56	126.75
29	B	609	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
29	b	609	CLA	C1-C2-C3	-3.21	120.50	126.04
29	S	617	CLA	CMA-C3A-C4A	3.21	120.39	111.77
29	c	501	CLA	CHD-C1D-ND	-3.21	121.51	124.45
29	c	508	CLA	CHD-C1D-ND	-3.20	121.51	124.45
29	g	614	CLA	CHD-C1D-ND	-3.20	121.51	124.45
29	B	614	CLA	C2D-C1D-ND	3.20	112.46	110.10
45	n	609	CHL	C1-O2A-CGA	3.20	124.85	116.44
45	n	601	CHL	C3C-C4C-NC	-3.20	106.98	110.57
48	G	623	NEX	C39-C29-C30	-3.20	118.44	122.92
29	A	406	CLA	C1-C2-C3	-3.20	120.51	126.04
29	B	614	CLA	C2C-C1C-NC	3.20	112.97	109.97
45	n	607	CHL	CHB-C4A-NA	3.20	128.93	124.51
29	c	504	CLA	C1-C2-C3	-3.20	120.51	126.04
42	D	405	PL9	C7-C3-C2	-3.20	119.10	123.30
47	g	622	XAT	C38-C25-C26	-3.20	116.90	122.26
46	R	620	LUT	C31-C32-C33	-3.19	117.44	126.42
29	Y	614	CLA	C2C-C1C-NC	3.19	112.96	109.97
29	n	610	CLA	C1-C2-C3	-3.19	120.53	126.04
29	s	605	CLA	C2C-C1C-NC	3.19	112.96	109.97
29	B	615	CLA	CHD-C1D-ND	-3.19	121.52	124.45
29	Y	614	CLA	CHD-C1D-ND	-3.19	121.52	124.45
29	y	603	CLA	CHD-C1D-ND	-3.19	121.52	124.45
45	Y	609	CHL	CMA-C3A-C4A	3.19	120.34	111.77
29	b	602	CLA	C2C-C1C-NC	3.19	112.96	109.97
29	g	614	CLA	C2C-C1C-NC	3.19	112.96	109.97
29	Y	604	CLA	CHD-C1D-ND	-3.19	121.53	124.45
29	b	609	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
48	R	622	NEX	C17-C1-C6	-3.18	107.62	110.47
46	s	620	LUT	C18-C5-C6	-3.18	120.95	124.53
46	n	620	LUT	C35-C34-C33	-3.18	122.77	127.31
29	g	603	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	y	613	CLA	CHD-C1D-ND	-3.18	121.53	124.45
45	G	607	CHL	C3C-C4C-NC	-3.18	107.01	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	y	606	CHL	C3B-C4B-NB	-3.18	107.57	110.52
29	n	614	CLA	CHD-C1D-ND	-3.18	121.53	124.45
48	G	623	NEX	C31-C30-C29	3.18	131.84	127.31
45	y	607	CHL	C2C-C3C-C4C	3.18	108.75	106.49
44	h	101	RRX	C4-C5-C6	-3.18	118.12	122.73
45	g	605	CHL	C2C-C3C-C4C	3.17	108.75	106.49
29	y	614	CLA	C2C-C1C-NC	3.17	112.95	109.97
29	r	611	CLA	C2C-C1C-NC	3.17	112.94	109.97
45	S	601	CHL	C3B-C4B-NB	-3.17	107.57	110.52
45	Y	609	CHL	C3C-C4C-NC	-3.17	107.01	110.57
29	B	615	CLA	C1-C2-C3	-3.17	120.56	126.04
29	y	602	CLA	CHD-C1D-ND	-3.17	121.54	124.45
29	N	603	CLA	C2C-C1C-NC	3.17	112.94	109.97
29	b	611	CLA	C1-C2-C3	-3.17	120.56	126.04
45	N	606	CHL	C2C-C3C-C4C	3.17	108.75	106.49
29	R	604	CLA	CHD-C1D-ND	-3.17	121.54	124.45
29	C	506	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
45	G	606	CHL	C3C-C4C-NC	-3.17	107.02	110.57
31	C	516	BCR	C23-C24-C25	-3.17	118.31	127.20
46	g	621	LUT	C18-C5-C6	-3.17	120.97	124.53
29	b	602	CLA	CHD-C1D-ND	-3.17	121.55	124.45
29	s	613	CLA	C2C-C1C-NC	3.16	112.94	109.97
29	y	611	CLA	C2C-C1C-NC	3.16	112.94	109.97
29	r	603	CLA	CMA-C3A-C4A	3.16	120.28	111.77
29	A	410	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	C	501	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	R	613	CLA	C2C-C1C-NC	3.16	112.94	109.97
31	a	411	BCR	C23-C24-C25	-3.16	118.32	127.20
31	c	514	BCR	C33-C5-C6	-3.16	120.98	124.53
29	s	617	CLA	C2C-C1C-NC	3.16	112.93	109.97
41	d	401	BCT	O2-C-O1	-3.16	111.34	119.55
45	s	607	CHL	C3C-C4C-NC	-3.16	107.03	110.57
29	Y	610	CLA	CHD-C1D-ND	-3.16	121.55	124.45
44	H	101	RRX	C4-C5-C6	-3.16	118.14	122.73
45	s	608	CHL	C2C-C3C-C4C	3.16	108.74	106.49
45	N	608	CHL	CMA-C3A-C4A	3.16	120.26	111.77
45	N	609	CHL	CMA-C3A-C4A	3.16	120.26	111.77
29	c	501	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
29	C	510	CLA	C2D-C1D-ND	3.16	112.43	110.10
29	n	611	CLA	C2C-C1C-NC	3.16	112.93	109.97
29	N	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	y	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	H	101	RRX	C20-C21-C22	-3.16	122.81	127.31
47	Y	622	XAT	O4-C5-C4	-3.16	111.01	113.38
29	n	602	CLA	CHD-C1D-ND	-3.16	121.55	124.45
45	r	607	CHL	CHD-C1D-ND	-3.16	121.55	124.45
46	G	621	LUT	C15-C14-C13	-3.16	122.81	127.31
29	S	609	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	D	402	CLA	C3B-C4B-NB	-3.15	107.59	110.52
47	n	622	XAT	C38-C25-C26	-3.15	116.98	122.26
29	g	602	CLA	C1-C2-C3	-3.15	120.59	126.04
29	C	511	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	G	613	CLA	CHD-C1D-ND	-3.15	121.56	124.45
47	N	622	XAT	C38-C25-C26	-3.15	116.98	122.26
29	S	617	CLA	C2C-C1C-NC	3.15	112.92	109.97
45	G	609	CHL	C4B-CHC-C1C	3.15	133.81	126.34
45	G	608	CHL	C2C-C3C-C4C	3.15	108.73	106.49
29	g	612	CLA	C2C-C1C-NC	3.15	112.92	109.97
45	g	605	CHL	C3C-C4C-NC	-3.15	107.04	110.57
29	S	610	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	C	503	CLA	C2C-C1C-NC	3.15	112.92	109.97
48	y	623	NEX	C39-C29-C30	-3.15	118.52	122.92
31	B	619	BCR	C33-C5-C6	-3.15	121.00	124.53
29	c	510	CLA	C2C-C1C-NC	3.14	112.92	109.97
29	S	604	CLA	C2C-C1C-NC	3.14	112.92	109.97
29	S	605	CLA	C1-C2-C3	-3.14	121.67	126.75
29	s	603	CLA	C2C-C1C-NC	3.14	112.92	109.97
29	R	603	CLA	CMA-C3A-C4A	3.14	120.22	111.77
29	N	610	CLA	CHD-C1D-ND	-3.14	121.57	124.45
29	R	603	CLA	CHD-C1D-ND	-3.14	121.57	124.45
29	r	602	CLA	CHD-C1D-ND	-3.14	121.57	124.45
45	y	609	CHL	CMA-C3A-C4A	3.14	120.22	111.77
29	N	614	CLA	C2C-C1C-NC	3.14	112.91	109.97
29	B	611	CLA	CHD-C1D-ND	-3.14	121.57	124.45
29	c	502	CLA	C1-O2A-CGA	3.14	124.67	116.44
29	r	609	CLA	C1-C2-C3	-3.14	120.62	126.04
29	G	602	CLA	CHD-C1D-ND	-3.14	121.57	124.45
48	g	623	NEX	C39-C29-C30	-3.14	118.53	122.92
41	D	401	BCT	O2-C-O1	-3.13	111.42	119.55
29	r	603	CLA	C2C-C1C-NC	3.13	112.91	109.97
29	b	615	CLA	CBA-CAA-C2A	3.13	123.11	113.86
29	Y	608	CLA	CHD-C1D-ND	-3.13	121.58	124.45
29	n	603	CLA	C1-C2-C3	-3.13	120.63	126.04
29	C	509	CLA	C1-C2-C3	-3.13	120.63	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	609	CLA	CHD-C1D-ND	-3.13	121.58	124.45
45	s	606	CHL	C4B-CHC-C1C	3.13	133.76	126.34
29	b	614	CLA	C2D-C1D-ND	3.13	112.41	110.10
29	r	602	CLA	C2C-C1C-NC	3.13	112.90	109.97
45	n	605	CHL	C3C-C4C-NC	-3.13	107.06	110.57
44	h	101	RRX	C16-C17-C18	-3.13	122.85	127.31
29	C	509	CLA	CHD-C1D-ND	-3.13	121.58	124.45
29	n	604	CLA	CHD-C1D-ND	-3.13	121.58	124.45
29	C	502	CLA	C2D-C1D-ND	3.13	112.41	110.10
46	S	620	LUT	C35-C15-C14	-3.12	117.07	123.47
29	a	410	CLA	C2C-C1C-NC	3.12	112.90	109.97
29	B	611	CLA	C1-C2-C3	-3.12	120.64	126.04
29	b	604	CLA	C2C-C1C-NC	3.12	112.90	109.97
48	S	622	NEX	C39-C29-C30	-3.12	118.55	122.92
29	N	611	CLA	C2C-C1C-NC	3.12	112.90	109.97
45	g	606	CHL	CMA-C3A-C4A	3.12	120.16	111.77
45	g	607	CHL	C3C-C4C-NC	-3.12	107.07	110.57
29	y	612	CLA	C2C-C1C-NC	3.12	112.89	109.97
45	G	607	CHL	CHB-C4A-NA	3.12	128.82	124.51
45	y	605	CHL	C2C-C3C-C4C	3.12	108.71	106.49
45	y	609	CHL	C3C-C4C-NC	-3.12	107.07	110.57
43	F	101	HEM	C3B-C2B-C1B	3.12	108.80	106.49
29	A	406	CLA	CHD-C1D-ND	-3.12	121.59	124.45
29	R	613	CLA	CHD-C1D-ND	-3.12	121.59	124.45
45	s	601	CHL	C3C-C4C-NC	-3.12	107.08	110.57
29	Y	613	CLA	CMA-C3A-C4A	3.12	120.15	111.77
46	y	621	LUT	C35-C15-C14	-3.12	117.09	123.47
29	R	611	CLA	C2C-C1C-NC	3.12	112.89	109.97
45	g	608	CHL	C2C-C3C-C4C	3.12	108.71	106.49
29	b	611	CLA	CHD-C1D-ND	-3.12	121.59	124.45
29	b	610	CLA	C2D-C1D-ND	3.11	112.40	110.10
31	C	515	BCR	C33-C5-C6	-3.11	121.03	124.53
45	N	605	CHL	C3C-C4C-NC	-3.11	107.08	110.57
46	Y	621	LUT	C18-C5-C6	-3.11	121.03	124.53
29	b	603	CLA	C2C-C1C-NC	3.11	112.89	109.97
29	n	603	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
29	Y	612	CLA	C2C-C1C-NC	3.11	112.89	109.97
29	A	410	CLA	C1-C2-C3	-3.11	120.66	126.04
31	C	517	BCR	C28-C27-C26	-3.11	108.52	114.08
45	n	608	CHL	CMA-C3A-C4A	3.11	120.13	111.77
29	r	603	CLA	CHD-C1D-ND	-3.11	121.60	124.45
43	f	101	HEM	C3B-C2B-C1B	3.11	108.79	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	604	CLA	C2C-C1C-NC	3.11	112.89	109.97
29	R	602	CLA	CHD-C1D-ND	-3.11	121.60	124.45
29	g	603	CLA	C2C-C1C-NC	3.11	112.88	109.97
29	Y	613	CLA	CHD-C1D-ND	-3.11	121.60	124.45
31	b	619	BCR	C33-C5-C6	-3.11	121.04	124.53
29	r	610	CLA	CHD-C1D-ND	-3.10	121.60	124.45
29	N	613	CLA	C2C-C1C-NC	3.10	112.88	109.97
29	b	614	CLA	CHD-C1D-ND	-3.10	121.60	124.45
45	Y	606	CHL	C2C-C3C-C4C	3.10	108.70	106.49
29	c	503	CLA	C2C-C1C-NC	3.10	112.88	109.97
29	B	614	CLA	CHD-C1D-ND	-3.10	121.61	124.45
45	S	608	CHL	C2C-C3C-C4C	3.10	108.70	106.49
29	Y	603	CLA	CHD-C1D-ND	-3.10	121.61	124.45
46	S	621	LUT	C7-C8-C9	-3.10	121.55	126.23
45	n	609	CHL	C3C-C4C-NC	-3.10	107.10	110.57
29	S	609	CLA	C2C-C1C-NC	3.10	112.87	109.97
29	C	510	CLA	C2C-C1C-NC	3.09	112.87	109.97
46	s	620	LUT	C38-C25-C24	-3.09	116.94	123.56
29	G	603	CLA	CHD-C1D-ND	-3.09	121.61	124.45
29	b	615	CLA	C2C-C1C-NC	3.09	112.87	109.97
45	s	608	CHL	C3C-C4C-NC	-3.09	107.10	110.57
45	y	609	CHL	C4B-CHC-C1C	3.09	133.67	126.34
29	d	403	CLA	C1-C2-C3	-3.09	120.69	126.04
45	S	607	CHL	C3C-C4C-NC	-3.09	107.10	110.57
45	g	605	CHL	CMA-C3A-C4A	3.09	120.08	111.77
29	R	612	CLA	CHD-C1D-ND	-3.09	121.61	124.45
45	N	601	CHL	C2C-C3C-C4C	3.09	108.69	106.49
45	Y	607	CHL	CHB-C4A-NA	3.09	128.78	124.51
45	R	606	CHL	CMA-C3A-C4A	3.09	120.07	111.77
45	N	608	CHL	C3C-C4C-NC	-3.09	107.11	110.57
39	L	101	LHG	O7-C7-C8	3.09	118.15	111.50
29	b	610	CLA	CHD-C1D-ND	-3.08	121.62	124.45
29	Y	603	CLA	C2D-C1D-ND	3.08	112.38	110.10
45	S	606	CHL	C4B-CHC-C1C	3.08	133.65	126.34
29	B	609	CLA	C1-C2-C3	-3.08	120.71	126.04
29	G	613	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	N	612	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	y	608	CLA	CHD-C1D-ND	-3.08	121.62	124.45
45	S	608	CHL	C3C-C4C-NC	-3.08	107.12	110.57
45	n	608	CHL	C3C-C4C-NC	-3.08	107.12	110.57
29	Y	602	CLA	CHD-C1D-ND	-3.08	121.62	124.45
29	r	604	CLA	CHD-C1D-ND	-3.08	121.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	G	608	CHL	C3C-C4C-NC	-3.08	107.12	110.57
29	b	614	CLA	C1-C2-C3	-3.08	120.72	126.04
29	B	609	CLA	CMA-C3A-C4A	3.08	120.04	111.77
45	G	605	CHL	CMA-C3A-C4A	3.08	120.04	111.77
29	s	617	CLA	CMA-C3A-C4A	3.07	120.04	111.77
29	N	610	CLA	O2A-CGA-CBA	3.07	121.55	111.91
46	g	620	LUT	C18-C5-C6	-3.07	121.08	124.53
29	B	615	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
29	C	501	CLA	CMA-C3A-C4A	3.07	120.03	111.77
29	n	614	CLA	C2C-C1C-NC	3.07	112.85	109.97
44	h	101	RRX	C23-C24-C25	-3.07	118.58	127.20
39	l	101	LHG	O7-C7-C8	3.07	118.12	111.50
29	B	610	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	d	402	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	S	603	CLA	C1-C2-C3	-3.07	120.73	126.04
29	B	617	CLA	C2C-C1C-NC	3.07	112.85	109.97
29	A	407	CLA	CMA-C3A-C4A	3.07	120.02	111.77
29	C	508	CLA	C2C-C1C-NC	3.07	112.85	109.97
45	Y	609	CHL	C4B-CHC-C1C	3.07	133.61	126.34
45	Y	609	CHL	C2C-C3C-C4C	3.07	108.67	106.49
29	S	602	CLA	C1-C2-C3	-3.07	120.74	126.04
45	n	607	CHL	C1-C2-C3	-3.07	120.74	126.04
29	G	602	CLA	CMA-C3A-C4A	3.07	120.01	111.77
45	g	609	CHL	C4D-CHA-C1A	3.06	124.98	121.25
45	n	607	CHL	C1-O2A-CGA	3.06	124.48	116.44
29	g	613	CLA	C2C-C1C-NC	3.06	112.84	109.97
45	N	607	CHL	CHB-C4A-NA	3.06	128.75	124.51
29	n	603	CLA	C2C-C1C-NC	3.06	112.84	109.97
29	B	614	CLA	C1-C2-C3	-3.06	120.75	126.04
45	G	605	CHL	C2C-C3C-C4C	3.06	108.67	106.49
47	Y	622	XAT	C7-C8-C9	-3.06	120.78	125.53
42	d	405	PL9	C7-C3-C2	-3.06	119.28	123.30
29	s	602	CLA	C1-C2-C3	-3.06	120.75	126.04
29	b	615	CLA	CHD-C1D-ND	-3.06	121.64	124.45
29	d	402	CLA	C3B-C4B-NB	-3.06	107.68	110.52
29	g	613	CLA	C1-C2-C3	-3.06	120.76	126.04
29	G	613	CLA	C1-C2-C3	-3.06	120.76	126.04
29	c	503	CLA	C1-C2-C3	-3.06	120.76	126.04
31	c	515	BCR	C33-C5-C6	-3.05	121.10	124.53
29	B	615	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	G	614	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	b	615	CLA	O2D-CGD-O1D	-3.05	117.87	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	608	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	R	612	CLA	C1-C2-C3	-3.05	120.77	126.04
29	n	604	CLA	C2C-C1C-NC	3.05	112.83	109.97
45	S	601	CHL	C3C-C4C-NC	-3.05	107.15	110.57
29	S	610	CLA	C1-C2-C3	-3.05	120.77	126.04
29	c	507	CLA	CHD-C1D-ND	-3.05	121.65	124.45
45	Y	606	CHL	C3C-C4C-NC	-3.05	107.15	110.57
45	G	606	CHL	C2C-C3C-C4C	3.05	108.66	106.49
42	d	405	PL9	C7-C8-C9	-3.05	121.72	126.79
29	C	508	CLA	CHD-C1D-ND	-3.05	121.65	124.45
29	c	509	CLA	C1-C2-C3	-3.05	120.77	126.04
45	g	608	CHL	CMA-C3A-C4A	3.05	119.96	111.77
29	N	614	CLA	CMA-C3A-C4A	3.04	119.95	111.77
46	Y	620	LUT	C18-C5-C6	-3.04	121.11	124.53
29	G	614	CLA	CMA-C3A-C4A	3.04	119.95	111.77
45	g	608	CHL	C3C-C4C-NC	-3.04	107.16	110.57
29	a	407	CLA	CMA-C3A-C4A	3.04	119.95	111.77
29	D	403	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	c	513	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	G	602	CLA	C1-C2-C3	-3.04	120.78	126.04
29	N	604	CLA	C2D-C1D-ND	3.04	112.34	110.10
29	Y	610	CLA	C1-C2-C3	-3.04	120.79	126.04
45	G	607	CHL	C2C-C3C-C4C	3.04	108.66	106.49
29	b	607	CLA	CAA-C2A-C3A	-3.04	104.46	112.78
29	G	603	CLA	C2D-C1D-ND	3.04	112.34	110.10
29	A	410	CLA	CMA-C3A-C4A	3.04	119.94	111.77
47	R	621	XAT	O4-C5-C4	-3.04	111.10	113.38
46	G	620	LUT	C22-C23-C24	-3.04	108.28	111.74
45	N	609	CHL	C2C-C3C-C4C	3.04	108.65	106.49
29	N	604	CLA	CHD-C1D-ND	-3.04	121.66	124.45
45	N	601	CHL	C3C-C4C-NC	-3.04	107.17	110.57
29	r	611	CLA	CMA-C3A-C4A	3.04	119.93	111.77
29	s	610	CLA	C1-O2A-CGA	3.04	124.41	116.44
29	R	603	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	Y	613	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	c	511	CLA	C2C-C1C-NC	3.03	112.81	109.97
45	N	605	CHL	C2C-C3C-C4C	3.03	108.65	106.49
29	a	405	CLA	C2D-C1D-ND	3.03	112.34	110.10
29	a	407	CLA	CHD-C1D-ND	-3.03	121.67	124.45
29	A	406	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
45	G	601	CHL	CMA-C3A-C4A	3.03	119.92	111.77
29	c	509	CLA	CHD-C1D-ND	-3.03	121.67	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	y	605	CHL	CMA-C3A-C4A	3.03	119.92	111.77
29	r	608	CLA	CHD-C1D-ND	-3.03	121.67	124.45
29	g	604	CLA	C2C-C1C-NC	3.03	112.81	109.97
45	y	607	CHL	C3C-C4C-NC	-3.03	107.17	110.57
45	Y	605	CHL	CMA-C3A-C4A	3.03	119.92	111.77
29	C	509	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
29	y	613	CLA	C2D-C1D-ND	3.03	112.34	110.10
29	R	608	CLA	CHD-C1D-ND	-3.03	121.67	124.45
29	A	410	CLA	C2C-C1C-NC	3.03	112.81	109.97
43	F	101	HEM	C1B-NB-C4B	3.03	108.20	105.07
33	d	411	LMG	O8-C28-C29	3.02	121.40	111.91
29	y	613	CLA	C1-C2-C3	-3.02	120.81	126.04
45	n	609	CHL	CMA-C3A-C4A	3.02	119.90	111.77
29	B	608	CLA	C2C-C1C-NC	3.02	112.81	109.97
29	s	614	CLA	C2C-C1C-NC	3.02	112.81	109.97
46	s	621	LUT	C35-C15-C14	-3.02	117.28	123.47
29	b	611	CLA	C4B-CHC-C1C	3.02	133.51	126.34
45	S	608	CHL	CMA-C3A-C4A	3.02	119.89	111.77
45	N	607	CHL	C3C-C4C-NC	-3.02	107.18	110.57
29	g	604	CLA	CHD-C1D-ND	-3.02	121.68	124.45
30	a	409	PHO	O2D-CGD-O1D	-3.02	117.94	123.84
29	S	604	CLA	C1C-C2C-C3C	-3.02	103.79	106.96
29	G	611	CLA	CHD-C1D-ND	-3.02	121.68	124.45
45	R	607	CHL	CMA-C3A-C4A	3.01	119.88	111.77
48	y	623	NEX	C17-C1-C6	-3.01	107.77	110.47
29	r	612	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	r	610	CLA	C1-C2-C3	-3.01	120.83	126.04
31	d	404	BCR	C23-C22-C21	3.01	123.56	118.94
29	B	607	CLA	CMA-C3A-C4A	3.01	119.87	111.77
45	N	605	CHL	CMA-C3A-C4A	3.01	119.87	111.77
29	S	614	CLA	C2C-C1C-NC	3.01	112.79	109.97
29	R	602	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	y	603	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
29	S	611	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	a	406	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
29	b	614	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
29	c	504	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	G	603	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
45	n	607	CHL	C3C-C4C-NC	-3.01	107.20	110.57
47	y	622	XAT	C6-C7-C8	-3.01	119.63	125.99
29	n	614	CLA	CMA-C3A-C4A	3.01	119.86	111.77
47	Y	622	XAT	C38-C25-C26	-3.01	117.22	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	H	101	RRX	C1-C6-C5	-3.01	118.38	122.61
44	H	101	RRX	C23-C24-C25	-3.01	118.76	127.20
29	B	607	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
45	n	609	CHL	C2C-C3C-C4C	3.00	108.63	106.49
48	g	623	NEX	C20-C13-C14	-3.00	118.71	122.92
29	Y	610	CLA	C2D-C1D-ND	3.00	112.32	110.10
29	B	604	CLA	C2C-C1C-NC	3.00	112.79	109.97
29	Y	603	CLA	C2C-C1C-NC	3.00	112.79	109.97
45	r	606	CHL	CMA-C3A-C4A	3.00	119.84	111.77
29	s	613	CLA	C2D-C1D-ND	3.00	112.32	110.10
29	b	612	CLA	C2C-C1C-NC	3.00	112.78	109.97
43	f	101	HEM	C4C-NC-C1C	3.00	108.29	105.35
29	s	609	CLA	C2C-C1C-NC	3.00	112.78	109.97
45	N	608	CHL	C2C-C3C-C4C	3.00	108.63	106.49
29	b	607	CLA	O2A-CGA-CBA	3.00	121.32	111.91
29	c	502	CLA	CHD-C1D-ND	-3.00	121.70	124.45
29	B	607	CLA	O2A-CGA-CBA	3.00	121.32	111.91
45	s	601	CHL	C2C-C3C-C4C	3.00	108.63	106.49
45	n	607	CHL	CHD-C1D-ND	-3.00	121.70	124.45
29	D	403	CLA	C2C-C1C-NC	3.00	112.78	109.97
44	h	101	RRX	C33-C5-C6	-3.00	121.16	124.53
29	B	610	CLA	C2D-C1D-ND	3.00	112.31	110.10
45	n	606	CHL	C3C-C4C-NC	-3.00	107.21	110.57
29	N	602	CLA	CHD-C1D-ND	-2.99	121.70	124.45
45	g	607	CHL	C2C-C3C-C4C	2.99	108.62	106.49
29	s	611	CLA	CHD-C1D-ND	-2.99	121.70	124.45
29	R	604	CLA	C2D-C1D-ND	2.99	112.31	110.10
29	R	610	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
44	H	101	RRX	C38-C26-C27	2.99	119.90	114.36
29	C	512	CLA	C2C-C1C-NC	2.99	112.77	109.97
29	N	611	CLA	CMA-C3A-C4A	2.99	119.81	111.77
29	B	614	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
47	r	622	XAT	C11-C10-C9	-2.99	123.05	127.31
29	S	617	CLA	CHD-C1D-ND	-2.99	121.71	124.45
45	s	607	CHL	C3B-C4B-NB	-2.99	107.75	110.52
44	H	101	RRX	C21-C20-C19	-2.99	113.90	123.22
29	N	613	CLA	O2A-CGA-CBA	2.98	121.28	111.91
45	g	606	CHL	C3C-C4C-NC	-2.98	107.22	110.57
29	g	610	CLA	C2C-C1C-NC	2.98	112.77	109.97
45	s	608	CHL	CMA-C3A-C4A	2.98	119.79	111.77
29	r	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
29	c	501	CLA	CMA-C3A-C4A	2.98	119.78	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	611	CLA	C4B-CHC-C1C	2.98	133.41	126.34
29	G	604	CLA	CHD-C1D-ND	-2.98	121.72	124.45
45	N	607	CHL	CMA-C3A-C4A	2.98	119.78	111.77
45	G	605	CHL	C3C-C4C-NC	-2.98	107.23	110.57
29	n	611	CLA	CMA-C3A-C4A	2.98	119.78	111.77
29	s	612	CLA	CHD-C1D-ND	-2.98	121.72	124.45
29	S	614	CLA	C1-C2-C3	-2.98	120.89	126.04
45	S	606	CHL	CMA-C3A-C4A	2.98	119.78	111.77
29	n	612	CLA	CHD-C1D-ND	-2.98	121.72	124.45
48	n	623	NEX	C39-C29-C30	-2.98	118.75	122.92
29	y	608	CLA	C2C-C1C-NC	2.98	112.76	109.97
29	s	609	CLA	CMA-C3A-C4A	2.98	119.77	111.77
29	R	611	CLA	CMA-C3A-C4A	2.97	119.77	111.77
46	y	620	LUT	C10-C11-C12	-2.97	113.94	123.22
48	R	622	NEX	C27-C28-C29	-2.97	120.92	125.53
45	y	606	CHL	CMA-C3A-C4A	2.97	119.75	111.77
43	F	101	HEM	C4C-NC-C1C	2.97	108.26	105.35
29	s	612	CLA	C2D-C1D-ND	2.97	112.29	110.10
45	S	606	CHL	C3B-C4B-NB	-2.97	107.76	110.52
45	N	607	CHL	C2C-C3C-C4C	2.97	108.61	106.49
29	y	604	CLA	C2C-C1C-NC	2.97	112.75	109.97
29	N	610	CLA	CMA-C3A-C4A	2.97	119.75	111.77
29	B	613	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	A	410	CLA	C2D-C1D-ND	2.96	112.29	110.10
29	C	502	CLA	CMA-C3A-C4A	2.96	119.74	111.77
29	y	602	CLA	C2D-C1D-ND	2.96	112.29	110.10
29	C	507	CLA	CHD-C1D-ND	-2.96	121.73	124.45
45	g	609	CHL	C1-O2A-CGA	2.96	124.21	116.44
29	n	613	CLA	C2C-C1C-NC	2.96	112.75	109.97
30	a	408	PHO	CMB-C2B-C3B	2.96	130.22	124.68
29	G	610	CLA	C2D-C1D-ND	2.96	112.29	110.10
29	S	612	CLA	C2D-C1D-ND	2.96	112.29	110.10
45	N	606	CHL	C3C-C4C-NC	-2.96	107.25	110.57
29	B	609	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
45	n	607	CHL	C2C-C3C-C4C	2.96	108.60	106.49
45	G	608	CHL	CMA-C3A-C4A	2.96	119.73	111.77
29	r	609	CLA	C2C-C1C-NC	2.96	112.74	109.97
45	Y	601	CHL	CMA-C3A-C4A	2.96	119.72	111.77
48	r	623	NEX	C27-C28-C29	-2.96	120.94	125.53
45	s	606	CHL	C3C-C4C-NC	-2.96	107.25	110.57
29	d	403	CLA	CHD-C1D-ND	-2.96	121.74	124.45
29	s	609	CLA	CHD-C1D-ND	-2.96	121.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	g	607	CHL	CHB-C4A-NA	2.96	128.60	124.51
45	Y	605	CHL	C4B-CHC-C1C	2.96	133.35	126.34
29	r	609	CLA	CHD-C1D-ND	-2.95	121.74	124.45
29	N	603	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
29	n	602	CLA	CMA-C3A-C4A	2.95	119.70	111.77
29	a	410	CLA	C1-C2-C3	-2.95	120.94	126.04
45	n	606	CHL	C2C-C3C-C4C	2.95	108.59	106.49
29	d	403	CLA	C2C-C1C-NC	2.95	112.73	109.97
29	y	602	CLA	C1-C2-C3	-2.95	120.94	126.04
45	R	606	CHL	CHD-C1D-ND	-2.95	121.75	124.45
29	R	602	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	R	611	CLA	CHD-C1D-ND	-2.95	121.75	124.45
29	B	608	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
46	y	620	LUT	C7-C8-C9	-2.94	121.78	126.23
29	S	605	CLA	O2A-CGA-CBA	2.94	121.15	111.91
29	S	613	CLA	C2D-C1D-ND	2.94	112.27	110.10
45	n	608	CHL	C2C-C3C-C4C	2.94	108.59	106.49
45	N	609	CHL	C4B-CHC-C1C	2.94	133.32	126.34
29	S	605	CLA	CMA-C3A-C4A	2.94	119.69	111.77
48	S	622	NEX	C31-C30-C29	2.94	131.51	127.31
31	A	411	BCR	C23-C24-C25	-2.94	118.94	127.20
39	d	408	LHG	O8-C23-C24	2.94	121.14	111.91
29	B	603	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	y	603	CLA	C2C-C1C-NC	2.94	112.73	109.97
45	g	609	CHL	C3B-C4B-NB	-2.94	107.79	110.52
45	r	607	CHL	CMA-C3A-C4A	2.94	119.68	111.77
29	a	410	CLA	CMA-C3A-C4A	2.94	119.67	111.77
45	n	601	CHL	CMA-C3A-C4A	2.94	119.67	111.77
45	n	605	CHL	C2C-C3C-C4C	2.94	108.58	106.49
48	R	622	NEX	C26-C27-C28	-2.94	119.78	125.99
48	r	623	NEX	C26-C27-C28	-2.94	119.78	125.99
45	g	601	CHL	CMA-C3A-C4A	2.94	119.67	111.77
47	g	622	XAT	O4-C5-C4	-2.94	111.17	113.38
29	c	504	CLA	C2C-C1C-NC	2.94	112.72	109.97
29	s	603	CLA	C1-C2-C3	-2.94	120.97	126.04
29	Y	604	CLA	C2C-C1C-NC	2.94	112.72	109.97
29	c	512	CLA	C2C-C1C-NC	2.94	112.72	109.97
29	c	502	CLA	CMA-C3A-C4A	2.93	119.66	111.77
46	r	620	LUT	C2-C3-C4	-2.93	106.29	110.30
29	s	605	CLA	CMA-C3A-C4A	2.93	119.65	111.77
29	r	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
45	n	606	CHL	CMA-C3A-C4A	2.93	119.65	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	h	101	RRX	C21-C20-C19	-2.93	114.07	123.22
29	n	614	CLA	C2D-C1D-ND	2.93	112.26	110.10
29	g	603	CLA	C2D-C1D-ND	2.93	112.26	110.10
29	N	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	S	609	CLA	CMA-C3A-C4A	2.93	119.64	111.77
29	n	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	A	407	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	g	614	CLA	CMA-C3A-C4A	2.93	119.64	111.77
45	n	608	CHL	C4B-CHC-C1C	2.93	133.28	126.34
31	b	619	BCR	C4-C5-C6	-2.92	118.48	122.73
29	S	613	CLA	CMA-C3A-C4A	2.92	119.63	111.77
35	b	620	C7Z	C8-C7-C6	-2.92	118.99	127.20
45	S	608	CHL	C3B-C4B-NB	-2.92	107.80	110.52
29	g	611	CLA	C2D-C1D-ND	2.92	112.26	110.10
46	Y	621	LUT	C15-C14-C13	-2.92	123.14	127.31
45	N	606	CHL	CMA-C3A-C4A	2.92	119.63	111.77
29	B	602	CLA	CHD-C1D-ND	-2.92	121.77	124.45
29	n	610	CLA	C2D-C1D-ND	2.92	112.26	110.10
29	n	612	CLA	C2D-C1D-ND	2.92	112.26	110.10
29	D	403	CLA	CMA-C3A-C4A	2.92	119.62	111.77
29	c	501	CLA	C2C-C1C-NC	2.92	112.71	109.97
45	g	609	CHL	CMA-C3A-C4A	2.92	119.62	111.77
29	g	602	CLA	CHD-C1D-ND	-2.92	121.77	124.45
29	R	602	CLA	C2C-C1C-NC	2.92	112.71	109.97
46	S	620	LUT	C38-C25-C24	-2.92	117.31	123.56
29	A	407	CLA	C2D-C1D-ND	2.92	112.25	110.10
29	B	610	CLA	C2C-C1C-NC	2.92	112.70	109.97
29	R	610	CLA	C2D-C1D-ND	2.92	112.25	110.10
29	b	613	CLA	CHD-C1D-ND	-2.92	121.78	124.45
29	C	504	CLA	C2D-C1D-ND	2.91	112.25	110.10
29	C	501	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
29	G	610	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	B	608	CLA	CHD-C1D-ND	-2.91	121.78	124.45
45	g	607	CHL	CMA-C3A-C4A	2.91	119.60	111.77
29	Y	608	CLA	CMA-C3A-C4A	2.91	119.60	111.77
29	s	613	CLA	CMA-C3A-C4A	2.91	119.60	111.77
29	Y	612	CLA	C2D-C1D-ND	2.91	112.25	110.10
29	S	602	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	Y	603	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
29	g	603	CLA	CMA-C3A-C4A	2.91	119.60	111.77
45	n	609	CHL	CHB-C4A-NA	2.91	128.54	124.51
29	s	610	CLA	CAA-C2A-C3A	-2.91	104.81	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	602	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
29	y	613	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	G	610	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
31	d	404	BCR	C34-C9-C10	-2.91	118.85	122.92
29	y	611	CLA	C1-C2-C3	-2.91	121.02	126.04
29	G	612	CLA	CMA-C3A-C4A	2.91	119.58	111.77
47	R	621	XAT	C20-C13-C14	-2.91	118.85	122.92
29	C	501	CLA	C2C-C1C-NC	2.90	112.69	109.97
29	N	602	CLA	C1-C2-C3	-2.90	121.02	126.04
29	S	602	CLA	C2D-C1D-ND	2.90	112.24	110.10
29	y	610	CLA	C2D-C1D-ND	2.90	112.24	110.10
29	N	610	CLA	C2C-C1C-NC	2.90	112.69	109.97
29	Y	608	CLA	C2C-C1C-NC	2.90	112.69	109.97
29	C	503	CLA	C1-C2-C3	-2.90	121.02	126.04
29	S	617	CLA	C2D-C1D-ND	2.90	112.24	110.10
39	D	408	LHG	O8-C23-C24	2.90	121.00	111.91
29	C	503	CLA	C2D-C1D-ND	2.90	112.24	110.10
48	n	623	NEX	C17-C1-C6	-2.90	107.88	110.47
29	G	611	CLA	C2D-C1D-ND	2.90	112.24	110.10
29	c	513	CLA	C2D-C1D-ND	2.90	112.24	110.10
29	G	611	CLA	CMA-C3A-C4A	2.90	119.56	111.77
29	S	612	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	s	602	CLA	C2C-C1C-NC	2.90	112.69	109.97
29	b	602	CLA	C1-C2-C3	-2.89	121.04	126.04
29	b	608	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
45	S	607	CHL	C3B-C4B-NB	-2.89	107.83	110.52
45	S	606	CHL	C3C-C4C-NC	-2.89	107.33	110.57
29	B	612	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
29	R	609	CLA	C2C-C1C-NC	2.89	112.68	109.97
29	n	610	CLA	C2C-C1C-NC	2.89	112.68	109.97
29	B	616	CLA	C2D-C1D-ND	2.89	112.23	110.10
29	D	402	CLA	CHD-C1D-ND	-2.89	121.80	124.45
29	b	608	CLA	CHD-C1D-ND	-2.89	121.80	124.45
29	a	407	CLA	C2D-C1D-ND	2.89	112.23	110.10
29	s	617	CLA	C2D-C1D-ND	2.89	112.23	110.10
48	Y	623	NEX	C31-C30-C29	2.89	131.43	127.31
29	y	614	CLA	CMA-C3A-C4A	2.89	119.53	111.77
45	n	607	CHL	CMA-C3A-C4A	2.89	119.53	111.77
45	g	605	CHL	C4B-CHC-C1C	2.88	133.18	126.34
29	Y	614	CLA	CMA-C3A-C4A	2.88	119.52	111.77
45	Y	607	CHL	C3C-C4C-NC	-2.88	107.34	110.57
29	N	602	CLA	CMA-C3A-C4A	2.88	119.52	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	502	CLA	CHD-C1D-ND	-2.88	121.81	124.45
45	R	607	CHL	C3B-C4B-NB	-2.88	107.84	110.52
29	N	604	CLA	C2C-C1C-NC	2.88	112.67	109.97
35	b	620	C7Z	C22-C23-C24	2.88	114.25	110.30
45	s	608	CHL	C3B-C4B-NB	-2.88	107.84	110.52
29	n	611	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
47	G	622	XAT	C26-C27-C28	-2.88	119.91	125.99
29	C	504	CLA	C2C-C1C-NC	2.88	112.67	109.97
29	n	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	b	607	CLA	CMA-C3A-C4A	2.88	119.50	111.77
29	s	609	CLA	C2D-C1D-ND	2.88	112.22	110.10
29	d	403	CLA	CMA-C3A-C4A	2.88	119.50	111.77
45	S	601	CHL	CMA-C3A-C4A	2.88	119.50	111.77
45	y	601	CHL	CMA-C3A-C4A	2.88	119.50	111.77
45	y	607	CHL	CMA-C3A-C4A	2.87	119.50	111.77
29	S	602	CLA	CHD-C1D-ND	-2.87	121.81	124.45
29	g	611	CLA	CHD-C1D-ND	-2.87	121.81	124.45
29	C	507	CLA	C1C-C2C-C3C	-2.87	103.93	106.96
29	c	508	CLA	C2C-C1C-NC	2.87	112.67	109.97
29	N	603	CLA	C2D-C1D-ND	2.87	112.22	110.10
29	N	613	CLA	C2D-C1D-ND	2.87	112.22	110.10
33	D	411	LMG	O8-C28-C29	2.87	120.92	111.91
29	C	510	CLA	C1D-ND-C4D	-2.87	104.30	106.33
29	s	611	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
29	B	602	CLA	C1-C2-C3	-2.87	121.08	126.04
29	a	410	CLA	C2D-C1D-ND	2.87	112.22	110.10
45	N	607	CHL	C1-O2A-CGA	2.87	123.97	116.44
29	B	617	CLA	C1-C2-C3	-2.87	121.08	126.04
29	B	612	CLA	C2C-C1C-NC	2.87	112.66	109.97
38	C	523	DGD	O1G-C1A-C2A	2.87	120.91	111.91
29	G	603	CLA	C1-C2-C3	-2.87	121.08	126.04
46	Y	621	LUT	C35-C15-C14	-2.87	117.60	123.47
45	Y	607	CHL	C2C-C3C-C4C	2.87	108.53	106.49
29	r	613	CLA	C2C-C1C-NC	2.87	112.66	109.97
29	N	603	CLA	CMA-C3A-C4A	2.87	119.48	111.77
29	n	602	CLA	C1-C2-C3	-2.87	121.08	126.04
29	n	602	CLA	C2C-C1C-NC	2.87	112.66	109.97
29	G	612	CLA	C2D-C1D-ND	2.87	112.22	110.10
29	C	513	CLA	C1-C2-C3	-2.86	121.09	126.04
29	B	611	CLA	C2D-C1D-ND	2.86	112.22	110.10
33	A	413	LMG	C8-O7-C10	-2.86	110.74	117.79
29	b	616	CLA	CHD-C1D-ND	-2.86	121.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	c	518	DGD	O1G-C1A-C2A	2.86	120.89	111.91
29	n	603	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
46	S	621	LUT	C18-C5-C6	-2.86	121.31	124.53
31	B	619	BCR	C4-C5-C6	-2.86	118.58	122.73
29	r	610	CLA	C1D-ND-C4D	-2.86	104.30	106.33
35	b	620	C7Z	C31-C30-C29	-2.86	123.23	127.31
29	s	603	CLA	C2D-C1D-ND	2.86	112.21	110.10
47	g	622	XAT	C6-C7-C8	-2.86	119.95	125.99
29	R	609	CLA	C1-C2-C3	-2.86	121.10	126.04
29	g	602	CLA	C2D-C1D-ND	2.86	112.21	110.10
45	y	601	CHL	CHB-C4A-NA	2.86	128.46	124.51
45	y	605	CHL	C3B-C4B-NB	-2.86	107.87	110.52
29	r	608	CLA	C1-C2-C3	-2.86	121.11	126.04
29	a	405	CLA	CAA-C2A-C3A	-2.85	104.96	112.78
31	B	619	BCR	C36-C18-C17	-2.85	118.92	122.92
47	N	622	XAT	C6-C7-C8	-2.85	119.96	125.99
30	A	409	PHO	O1D-CGD-CBD	2.85	129.48	124.74
29	y	612	CLA	C2D-C1D-ND	2.85	112.20	110.10
29	a	407	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
29	B	607	CLA	C2C-C1C-NC	2.85	112.64	109.97
42	D	405	PL9	C7-C8-C9	-2.85	122.05	126.79
45	Y	605	CHL	C2C-C3C-C4C	2.85	108.52	106.49
29	y	610	CLA	C2C-C1C-NC	2.85	112.64	109.97
29	c	509	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
29	b	609	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
29	g	603	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
29	B	608	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	Y	602	CLA	CMA-C3A-C4A	2.84	119.40	111.77
29	b	608	CLA	C2D-C1D-ND	2.84	112.19	110.10
45	N	608	CHL	C4B-CHC-C1C	2.84	133.07	126.34
29	S	610	CLA	C2D-C1D-ND	2.84	112.19	110.10
29	d	402	CLA	C1D-ND-C4D	-2.83	104.32	106.33
31	c	515	BCR	C23-C24-C25	-2.83	119.25	127.20
29	S	609	CLA	C2D-C1D-ND	2.83	112.19	110.10
29	A	407	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
29	b	605	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
29	c	507	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
29	G	603	CLA	CMA-C3A-C4A	2.83	119.38	111.77
45	r	607	CHL	C3B-C4B-NB	-2.83	107.89	110.52
38	c	523	DGD	O1G-C1A-C2A	2.83	120.79	111.91
29	G	614	CLA	C2D-C1D-ND	2.83	112.19	110.10
29	B	602	CLA	C4B-CHC-C1C	2.83	133.04	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	y	622	XAT	C38-C25-C26	-2.83	117.52	122.26
29	r	610	CLA	OBD-CAD-C3D	-2.83	121.72	128.52
29	N	613	CLA	C1-C2-C3	-2.83	121.15	126.04
29	Y	614	CLA	C1-C2-C3	-2.83	121.16	126.04
44	h	101	RRX	C15-C16-C17	-2.83	117.69	123.47
29	g	611	CLA	CMA-C3A-C4A	2.82	119.36	111.77
29	B	606	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
29	b	602	CLA	CMA-C3A-C4A	2.82	119.36	111.77
46	y	621	LUT	C38-C25-C24	-2.82	117.52	123.56
29	N	614	CLA	C2D-C1D-ND	2.82	112.18	110.10
29	B	615	CLA	C1-O2A-CGA	2.82	123.85	116.44
48	N	623	NEX	C39-C29-C30	-2.82	118.97	122.92
29	n	604	CLA	C2D-C1D-ND	2.82	112.18	110.10
31	b	618	BCR	C23-C24-C25	-2.82	119.28	127.20
29	B	602	CLA	CMA-C3A-C4A	2.82	119.35	111.77
29	r	602	CLA	C2D-C1D-ND	2.82	112.18	110.10
44	H	101	RRX	C15-C16-C17	-2.82	117.70	123.47
38	C	518	DGD	O1G-C1A-C2A	2.82	120.75	111.91
30	A	409	PHO	O2D-CGD-O1D	-2.82	118.33	123.84
29	b	607	CLA	C2C-C1C-NC	2.82	112.61	109.97
29	S	603	CLA	C2D-C1D-ND	2.82	112.18	110.10
46	G	621	LUT	C11-C10-C9	-2.82	123.29	127.31
29	d	403	CLA	C2D-C1D-ND	2.81	112.18	110.10
29	C	513	CLA	C2D-C1D-ND	2.81	112.18	110.10
48	G	623	NEX	C38-C25-C26	-2.81	117.55	122.26
29	n	602	CLA	C2D-C1D-ND	2.81	112.18	110.10
29	g	612	CLA	C2D-C1D-ND	2.81	112.18	110.10
29	b	612	CLA	C1-C2-C3	-2.81	121.18	126.04
29	r	608	CLA	CMA-C3A-C4A	2.81	119.33	111.77
46	y	620	LUT	C38-C25-C24	-2.81	117.55	123.56
45	r	606	CHL	C4B-CHC-C1C	2.81	133.00	126.34
45	s	601	CHL	CMA-C3A-C4A	2.81	119.32	111.77
47	R	621	XAT	C31-C30-C29	-2.81	123.30	127.31
46	g	620	LUT	C31-C30-C29	-2.81	123.31	127.31
29	Y	602	CLA	C2D-C1D-ND	2.81	112.17	110.10
29	r	604	CLA	C2C-C1C-NC	2.81	112.60	109.97
45	y	601	CHL	C1-C2-C3	-2.80	121.19	126.04
29	G	612	CLA	CHD-C1D-ND	-2.80	121.88	124.45
48	s	623	NEX	C39-C29-C30	-2.80	119.00	122.92
29	r	610	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
35	B	620	C7Z	C22-C23-C24	2.80	114.14	110.30
45	N	601	CHL	CMA-C3A-C4A	2.80	119.31	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	613	CLA	CHD-C1D-ND	-2.80	121.88	124.45
45	s	606	CHL	CMA-C3A-C4A	2.80	119.30	111.77
29	D	402	CLA	C1D-ND-C4D	-2.80	104.34	106.33
45	g	601	CHL	C4B-CHC-C1C	2.80	132.98	126.34
29	b	612	CLA	CHD-C1D-ND	-2.80	121.88	124.45
30	A	408	PHO	O2D-CGD-O1D	-2.80	118.36	123.84
29	b	611	CLA	C3B-C4B-NB	-2.80	107.92	110.52
29	n	610	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
29	C	501	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	D	403	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	B	612	CLA	C1-C2-C3	-2.80	121.20	126.04
31	D	404	BCR	C34-C9-C10	-2.80	119.00	122.92
29	b	606	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
29	N	610	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	Y	613	CLA	C2D-C1D-ND	2.80	112.17	110.10
45	Y	607	CHL	C1-O2A-CGA	2.80	123.78	116.44
29	y	611	CLA	CHD-C1D-ND	-2.80	121.89	124.45
45	S	601	CHL	C2C-C3C-C4C	2.79	108.48	106.49
29	C	504	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
35	B	620	C7Z	C8-C7-C6	-2.79	119.36	127.20
29	C	511	CLA	O2A-CGA-CBA	2.79	120.67	111.91
29	R	604	CLA	C2C-C1C-NC	2.79	112.59	109.97
45	Y	606	CHL	CMA-C3A-C4A	2.79	119.28	111.77
29	R	602	CLA	C1-C2-C3	-2.79	121.22	126.04
29	s	610	CLA	C2D-C1D-ND	2.79	112.16	110.10
46	Y	620	LUT	C38-C25-C24	-2.79	117.59	123.56
29	G	613	CLA	C2D-C1D-ND	2.79	112.16	110.10
29	R	611	CLA	C2D-C1D-ND	2.79	112.16	110.10
29	s	614	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
29	b	604	CLA	CHD-C1D-ND	-2.79	121.89	124.45
29	r	613	CLA	C2D-C1D-ND	2.79	112.16	110.10
47	g	622	XAT	C26-C27-C28	-2.79	120.10	125.99
29	b	617	CLA	C2C-C1C-NC	2.79	112.58	109.97
29	S	614	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
33	c	521	LMG	O8-C28-C29	2.79	120.65	111.91
46	g	621	LUT	C31-C30-C29	-2.79	123.33	127.31
45	G	609	CHL	C1-O2A-CGA	2.79	123.75	116.44
45	G	608	CHL	C3B-C4B-NB	-2.78	107.93	110.52
45	g	606	CHL	C1-O2A-CGA	2.78	123.75	116.44
29	c	509	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
45	G	605	CHL	C4B-CHC-C1C	2.78	132.94	126.34
29	C	513	CLA	CMA-C3A-C4A	2.78	119.25	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	617	CLA	O2A-CGA-CBA	2.78	120.64	111.91
29	A	405	CLA	C2D-C1D-ND	2.78	112.16	110.10
29	N	613	CLA	CHD-C1D-ND	-2.78	121.90	124.45
29	c	504	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	y	604	CLA	C1-C2-C3	-2.78	121.23	126.04
45	G	601	CHL	C4B-CHC-C1C	2.78	132.93	126.34
29	B	617	CLA	C2D-C1D-ND	2.78	112.15	110.10
29	c	511	CLA	O2A-CGA-CBA	2.78	120.63	111.91
29	y	608	CLA	CMA-C3A-C4A	2.78	119.24	111.77
29	g	613	CLA	C2D-C1D-ND	2.78	112.15	110.10
31	B	619	BCR	C23-C22-C21	2.78	123.20	118.94
29	r	602	CLA	C1-C2-C3	-2.78	121.24	126.04
31	c	514	BCR	C23-C24-C25	-2.78	119.40	127.20
45	y	609	CHL	C2C-C3C-C4C	2.78	108.47	106.49
29	a	410	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
47	G	622	XAT	C6-C7-C8	-2.77	120.13	125.99
47	G	622	XAT	O24-C25-C24	2.77	115.47	113.38
29	g	612	CLA	CMA-C3A-C4A	2.77	119.23	111.77
39	D	409	LHG	O8-C23-C24	2.77	120.61	111.91
29	G	604	CLA	C2D-C1D-ND	2.77	112.15	110.10
29	y	603	CLA	C4B-CHC-C1C	2.77	132.91	126.34
29	Y	611	CLA	C1-C2-C3	-2.77	121.25	126.04
45	n	605	CHL	C3B-C4B-NB	-2.77	107.94	110.52
29	n	613	CLA	O2A-CGA-CBA	2.77	120.61	111.91
49	s	625	LPX	O3-P1-O4	2.77	125.95	112.24
29	r	603	CLA	C1-C2-C3	-2.77	121.25	126.04
29	b	616	CLA	C2D-C1D-ND	2.77	112.15	110.10
45	y	601	CHL	C3C-C4C-NC	-2.77	107.47	110.57
31	c	515	BCR	C33-C5-C4	2.77	118.94	113.62
45	R	606	CHL	CHB-C4A-NA	2.77	128.34	124.51
29	B	605	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
29	s	604	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
49	S	625	LPX	O3-P1-O4	2.77	125.92	112.24
38	C	519	DGD	O1G-C1A-C2A	2.77	120.59	111.91
29	G	602	CLA	C2D-C1D-ND	2.77	112.14	110.10
29	c	507	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
29	g	612	CLA	CHD-C1D-ND	-2.77	121.91	124.45
45	Y	605	CHL	C3B-C4B-NB	-2.77	107.95	110.52
29	Y	611	CLA	C2D-C1D-ND	2.77	112.14	110.10
45	Y	607	CHL	CMA-C3A-C4A	2.77	119.20	111.77
29	R	602	CLA	CMA-C3A-C4A	2.76	119.20	111.77
31	c	516	BCR	C34-C9-C10	-2.76	119.05	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	611	CLA	C1-C2-C3	-2.76	121.27	126.04
39	d	410	LHG	O8-C23-C24	2.76	120.57	111.91
29	n	613	CLA	C2D-C1D-ND	2.76	112.14	110.10
29	y	608	CLA	C2D-C1D-ND	2.76	112.14	110.10
29	b	616	CLA	C1-C2-C3	-2.76	121.27	126.04
29	c	511	CLA	CMA-C3A-C4A	2.76	119.19	111.77
29	S	610	CLA	C2C-C1C-NC	2.76	112.56	109.97
29	s	617	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
45	y	605	CHL	C4B-CHC-C1C	2.76	132.87	126.34
29	s	603	CLA	C3B-C4B-NB	-2.76	107.96	110.52
29	B	615	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
29	C	512	CLA	CHD-C1D-ND	-2.75	121.92	124.45
29	y	612	CLA	CHD-C1D-ND	-2.75	121.92	124.45
29	B	613	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
31	b	619	BCR	C28-C27-C26	-2.75	109.16	114.08
29	b	616	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
29	Y	608	CLA	C2D-C1D-ND	2.75	112.13	110.10
29	b	611	CLA	C2D-C1D-ND	2.75	112.13	110.10
29	n	603	CLA	CMA-C3A-C4A	2.75	119.17	111.77
29	a	410	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
29	b	603	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
45	S	606	CHL	C2C-C3C-C4C	2.75	108.45	106.49
29	c	501	CLA	C2D-C1D-ND	2.75	112.13	110.10
29	N	602	CLA	C4B-CHC-C1C	2.75	132.86	126.34
46	n	620	LUT	C10-C11-C12	-2.75	114.64	123.22
29	c	512	CLA	C1-C2-C3	-2.75	121.29	126.04
29	s	614	CLA	C1-O2A-CGA	2.75	123.66	116.44
29	s	610	CLA	C2C-C1C-NC	2.75	112.55	109.97
29	B	602	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
45	S	608	CHL	C4B-CHC-C1C	2.75	132.86	126.34
45	N	605	CHL	C3B-C4B-NB	-2.75	107.97	110.52
44	H	101	RRX	C33-C5-C6	-2.75	121.44	124.53
45	N	607	CHL	C1-C2-C3	-2.75	121.29	126.04
29	c	505	CLA	CHD-C1D-ND	-2.75	121.93	124.45
29	g	604	CLA	C2D-C1D-ND	2.75	112.13	110.10
46	Y	621	LUT	C38-C25-C24	-2.75	117.68	123.56
31	C	515	BCR	C33-C5-C4	2.75	118.89	113.62
29	B	611	CLA	C3B-C4B-NB	-2.75	107.97	110.52
42	d	405	PL9	C40-C39-C41	2.74	119.89	115.27
29	d	403	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
29	b	615	CLA	C1-O2A-CGA	2.74	123.64	116.44
45	r	607	CHL	CHB-C4A-NA	2.74	128.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	y	607	CHL	CHB-C4A-NA	2.74	128.31	124.51
29	Y	614	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
29	c	513	CLA	C2C-C1C-NC	2.74	112.54	109.97
46	Y	620	LUT	C15-C35-C34	-2.74	117.86	123.47
46	y	621	LUT	C18-C5-C6	-2.74	121.45	124.53
46	Y	620	LUT	C11-C10-C9	-2.74	123.40	127.31
29	g	602	CLA	CMA-C3A-C4A	2.74	119.14	111.77
35	B	620	C7Z	C31-C30-C29	-2.74	123.40	127.31
46	N	621	LUT	C11-C10-C9	-2.74	123.40	127.31
29	s	603	CLA	CMA-C3A-C4A	2.74	119.14	111.77
29	d	403	CLA	C3B-C4B-NB	-2.74	107.97	110.52
29	y	612	CLA	C1-C2-C3	-2.74	121.30	126.04
31	A	411	BCR	C38-C26-C25	-2.74	121.45	124.53
45	G	601	CHL	CHB-C4A-NA	2.74	128.30	124.51
29	R	613	CLA	C2D-C1D-ND	2.74	112.12	110.10
45	N	607	CHL	C4A-NA-C1A	2.74	107.94	106.71
29	A	406	CLA	CMA-C3A-C4A	2.74	119.13	111.77
29	c	513	CLA	C1-C2-C3	-2.74	121.31	126.04
30	A	409	PHO	C2D-C1D-ND	-2.74	107.64	109.53
29	N	602	CLA	O2A-CGA-CBA	2.74	120.49	111.91
46	Y	620	LUT	C10-C11-C12	-2.73	114.68	123.22
29	n	610	CLA	O2A-CGA-CBA	2.73	120.49	111.91
33	C	521	LMG	O8-C28-C29	2.73	120.49	111.91
46	Y	621	LUT	C31-C30-C29	-2.73	123.41	127.31
45	Y	601	CHL	CHB-C4A-NA	2.73	128.29	124.51
29	b	613	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	a	410	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
47	n	622	XAT	C6-C7-C8	-2.73	120.22	125.99
29	g	604	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	R	608	CLA	C2D-C1D-ND	2.73	112.11	110.10
29	S	611	CLA	CMA-C3A-C4A	2.73	119.11	111.77
29	S	610	CLA	O2A-CGA-CBA	2.73	120.47	111.91
29	y	614	CLA	C2D-C1D-ND	2.73	112.11	110.10
45	Y	601	CHL	C1-C2-C3	-2.73	121.33	126.04
39	D	410	LHG	O8-C23-C24	2.73	120.46	111.91
29	N	611	CLA	C2D-C1D-ND	2.73	112.11	110.10
38	C	520	DGD	O1G-C1A-C2A	2.73	120.46	111.91
29	c	505	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
29	S	605	CLA	C2D-C1D-ND	2.72	112.11	110.10
29	N	611	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
29	B	609	CLA	C2D-C1D-ND	2.72	112.11	110.10
45	N	605	CHL	C4B-CHC-C1C	2.72	132.79	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	R	620	LUT	C2-C3-C4	-2.72	106.58	110.30
29	r	609	CLA	O2A-CGA-CBA	2.72	120.45	111.91
29	r	612	CLA	C2D-C1D-ND	2.72	112.11	110.10
29	B	604	CLA	CHD-C1D-ND	-2.72	121.95	124.45
31	A	411	BCR	C33-C5-C4	2.72	118.84	113.62
29	g	610	CLA	CMA-C3A-C4A	2.72	119.08	111.77
29	n	602	CLA	C4B-CHC-C1C	2.72	132.79	126.34
29	C	507	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	b	619	BCR	C27-C26-C25	-2.72	118.78	122.73
45	Y	609	CHL	C1-O2A-CGA	2.72	123.57	116.44
45	s	606	CHL	C2C-C3C-C4C	2.72	108.43	106.49
29	A	410	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
48	g	623	NEX	C31-C30-C29	2.72	131.19	127.31
29	B	616	CLA	CHD-C1D-ND	-2.72	121.96	124.45
48	s	623	NEX	C38-C25-C26	-2.72	117.71	122.26
30	a	408	PHO	O2D-CGD-O1D	-2.71	118.53	123.84
29	C	506	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
29	R	608	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
29	A	410	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
48	g	623	NEX	C38-C25-C26	-2.71	117.71	122.26
39	L	101	LHG	O8-C23-C24	2.71	120.41	111.91
29	N	604	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	c	501	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
46	s	621	LUT	C38-C25-C24	-2.71	117.76	123.56
31	B	618	BCR	C15-C14-C13	-2.71	123.44	127.31
29	g	610	CLA	C2D-C1D-ND	2.71	112.10	110.10
45	n	605	CHL	C4B-CHC-C1C	2.71	132.76	126.34
29	N	614	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	c	506	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	b	619	BCR	C36-C18-C17	-2.71	119.13	122.92
29	s	614	CLA	O2A-CGA-CBA	2.71	120.40	111.91
29	y	614	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	B	616	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
29	r	610	CLA	O2A-CGA-CBA	2.70	120.39	111.91
29	C	513	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	b	615	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
33	j	101	LMG	O8-C28-C29	2.70	120.39	111.91
29	y	611	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
45	G	609	CHL	CMA-C3A-C4A	2.70	119.04	111.77
29	C	505	CLA	C1-C2-C3	-2.70	121.37	126.04
29	g	602	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	N	602	CLA	C1C-C2C-C3C	-2.70	104.12	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	503	CLA	C2D-C1D-ND	2.70	112.09	110.10
29	B	615	CLA	OBD-CAD-C3D	-2.70	122.02	128.52
31	c	514	BCR	C36-C18-C17	-2.70	119.14	122.92
29	n	614	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
39	S	624	LHG	O8-C23-C24	2.70	120.38	111.91
29	n	611	CLA	C2D-C1D-ND	2.70	112.09	110.10
29	b	602	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
29	Y	602	CLA	C2C-C1C-NC	2.70	112.50	109.97
38	c	519	DGD	O1G-C1A-C2A	2.70	120.38	111.91
46	N	620	LUT	C7-C8-C9	-2.70	122.16	126.23
45	g	608	CHL	C3B-C4B-NB	-2.70	108.01	110.52
29	b	610	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
29	C	511	CLA	C2D-C1D-ND	2.70	112.09	110.10
29	S	611	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
45	n	601	CHL	C4B-CHC-C1C	2.70	132.73	126.34
29	b	605	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
46	n	621	LUT	C38-C25-C24	-2.69	117.80	123.56
29	a	406	CLA	C2D-C1D-ND	2.69	112.09	110.10
46	N	620	LUT	C31-C30-C29	-2.69	123.47	127.31
29	D	403	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
29	Y	602	CLA	C4B-CHC-C1C	2.69	132.72	126.34
46	N	620	LUT	C10-C11-C12	-2.69	114.82	123.22
29	r	603	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	S	604	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	y	602	CLA	CMA-C3A-C4A	2.69	119.00	111.77
39	l	101	LHG	O8-C23-C24	2.69	120.35	111.91
29	G	602	CLA	C2C-C1C-NC	2.69	112.49	109.97
29	R	610	CLA	C3B-C4B-NB	-2.69	108.02	110.52
29	g	614	CLA	C2D-C1D-ND	2.69	112.08	110.10
45	G	608	CHL	C4B-CHC-C1C	2.69	132.71	126.34
29	S	603	CLA	C3B-C4B-NB	-2.69	108.02	110.52
45	G	609	CHL	C3C-C4C-NC	-2.68	107.56	110.57
29	R	603	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
29	A	410	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
29	y	614	CLA	C1-C2-C3	-2.68	121.40	126.04
29	S	611	CLA	C2D-C1D-ND	2.68	112.08	110.10
29	g	614	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
48	n	623	NEX	C16-C1-C6	-2.68	108.07	110.47
44	h	101	RRX	C38-C26-C27	2.68	119.32	114.36
33	a	413	LMG	C8-O7-C10	-2.68	111.19	117.79
29	R	612	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
29	n	612	CLA	C1C-C2C-C3C	-2.68	104.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	N	620	LUT	C11-C10-C9	-2.68	123.49	127.31
29	G	612	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
29	s	611	CLA	CMA-C3A-C4A	2.68	118.97	111.77
29	S	613	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	B	619	BCR	C28-C27-C26	-2.68	109.30	114.08
29	S	617	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
38	C	519	DGD	C2G-O2G-C1B	-2.68	111.20	117.79
29	C	511	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
29	n	602	CLA	O2A-CGA-CBA	2.67	120.30	111.91
29	s	610	CLA	C3B-C4B-NB	-2.67	108.03	110.52
30	a	408	PHO	O1D-CGD-CBD	2.67	129.19	124.74
29	G	613	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
29	b	602	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
29	b	617	CLA	O2A-CGA-CBA	2.67	120.30	111.91
29	B	605	CLA	CHA-C4D-ND	2.67	138.09	132.50
29	G	611	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
45	g	601	CHL	CHB-C4A-NA	2.67	128.21	124.51
31	B	618	BCR	C3-C4-C5	-2.67	109.31	114.08
45	Y	601	CHL	C3C-C4C-NC	-2.67	107.58	110.57
29	c	511	CLA	C2D-C1D-ND	2.67	112.07	110.10
29	R	613	CLA	CMA-C3A-C4A	2.67	118.95	111.77
29	B	616	CLA	C1-C2-C3	-2.67	121.43	126.04
29	r	603	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
47	G	622	XAT	O4-C5-C4	-2.67	111.38	113.38
45	R	607	CHL	C4B-CHC-C1C	2.67	132.67	126.34
29	G	614	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	C	511	CLA	CMA-C3A-C4A	2.67	118.94	111.77
45	g	601	CHL	C3B-C4B-NB	-2.67	108.04	110.52
29	C	513	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	r	613	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
45	n	607	CHL	C4A-NA-C1A	2.67	107.91	106.71
29	B	613	CLA	C2D-C1D-ND	2.67	112.07	110.10
29	g	611	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	Y	603	CLA	CMA-C3A-C4A	2.67	118.94	111.77
29	Y	602	CLA	O2A-CGA-CBA	2.67	120.27	111.91
29	R	612	CLA	C2D-C1D-ND	2.67	112.07	110.10
45	N	601	CHL	CHB-C4A-NA	2.66	128.20	124.51
29	b	611	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
45	G	605	CHL	C3B-C4B-NB	-2.66	108.04	110.52
29	B	616	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	S	602	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	r	612	CLA	C1C-C2C-C3C	-2.66	104.16	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	619	BCR	C23-C22-C21	2.66	123.03	118.94
29	B	611	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
38	c	518	DGD	O6D-C5D-C6D	2.66	112.04	106.67
39	s	624	LHG	C5-O7-C7	-2.66	111.24	117.79
29	b	603	CLA	CMA-C3A-C4A	2.66	118.93	111.77
31	a	411	BCR	C35-C13-C12	2.66	122.27	118.08
39	c	625	LHG	O8-C23-C24	2.66	120.26	111.91
39	s	624	LHG	O8-C23-C24	2.66	120.26	111.91
29	C	505	CLA	CHD-C1D-ND	-2.66	122.01	124.45
29	S	612	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	S	603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	c	511	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
48	Y	623	NEX	C38-C25-C26	-2.66	117.81	122.26
45	G	607	CHL	C4B-CHC-C1C	2.66	132.64	126.34
45	R	606	CHL	C4B-CHC-C1C	2.66	132.64	126.34
29	S	609	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	G	610	CLA	CMA-C3A-C4A	2.66	118.91	111.77
43	F	101	HEM	C4D-ND-C1D	2.66	107.82	105.07
35	b	620	C7Z	C27-C28-C29	-2.66	122.22	126.23
45	Y	607	CHL	CHD-C1D-ND	-2.66	122.01	124.45
29	A	410	CLA	C3B-C4B-NB	-2.65	108.05	110.52
31	c	517	BCR	C36-C18-C17	-2.65	119.20	122.92
36	C	524	DGA	OG1-CA1-CA2	2.65	120.24	111.91
31	C	517	BCR	C31-C1-C6	-2.65	105.99	110.30
45	n	609	CHL	C4B-CHC-C1C	2.65	132.63	126.34
47	R	621	XAT	C8-C9-C10	2.65	123.01	118.94
29	c	512	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	s	605	CLA	O2A-CGA-CBA	2.65	120.22	111.91
29	s	613	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
36	c	524	DGA	OG1-CA1-CA2	2.65	120.22	111.91
45	G	607	CHL	CMA-C3A-C4A	2.65	118.89	111.77
31	b	619	BCR	C1-C6-C5	-2.65	118.88	122.61
29	g	603	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
45	s	606	CHL	C4D-CHA-C1A	2.65	124.47	121.25
45	G	606	CHL	C4B-CHC-C1C	2.65	132.62	126.34
35	b	620	C7Z	C28-C27-C26	-2.65	119.77	127.20
31	a	411	BCR	C38-C26-C25	-2.65	121.56	124.53
48	S	622	NEX	C38-C25-C26	-2.65	117.83	122.26
29	C	503	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	Y	612	CLA	CHD-C1D-ND	-2.65	122.02	124.45
29	b	607	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
29	b	614	CLA	O2D-CGD-O1D	-2.64	118.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	512	CLA	CHD-C1D-ND	-2.64	122.02	124.45
29	N	612	CLA	C2D-C1D-ND	2.64	112.05	110.10
29	R	609	CLA	O2A-CGA-CBA	2.64	120.20	111.91
31	C	517	BCR	C23-C24-C25	-2.64	119.78	127.20
29	B	602	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
29	b	610	CLA	C2C-C1C-NC	2.64	112.45	109.97
29	y	602	CLA	O2A-CGA-CBA	2.64	120.20	111.91
29	B	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
29	b	602	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
45	y	609	CHL	C3B-C4B-NB	-2.64	108.06	110.52
29	g	613	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
29	r	608	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
29	r	608	CLA	C2D-C1D-ND	2.64	112.05	110.10
31	c	516	BCR	C37-C22-C23	2.64	122.23	118.08
48	y	623	NEX	C38-C25-C26	-2.64	117.84	122.26
46	n	620	LUT	C31-C30-C29	-2.64	123.55	127.31
29	B	610	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
29	R	608	CLA	CMA-C3A-C4A	2.64	118.86	111.77
29	C	509	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
29	s	611	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
38	c	520	DGD	O1G-C1A-C2A	2.64	120.18	111.91
45	N	601	CHL	C1-O2A-CGA	2.64	123.36	116.44
29	Y	604	CLA	C1-C2-C3	-2.64	121.48	126.04
45	y	609	CHL	C1-O2A-CGA	2.64	123.36	116.44
29	Y	613	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	s	605	CLA	C2D-C1D-ND	2.63	112.05	110.10
29	G	603	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
29	s	605	CLA	CHA-C4D-ND	2.63	138.01	132.50
29	c	506	CLA	CMA-C3A-C4A	2.63	118.85	111.77
46	S	621	LUT	C38-C25-C24	-2.63	117.93	123.56
45	y	607	CHL	C1-O2A-CGA	2.63	123.35	116.44
29	B	613	CLA	C2C-C1C-NC	2.63	112.44	109.97
29	y	603	CLA	C3B-C4B-NB	-2.63	108.07	110.52
39	d	409	LHG	O8-C23-C24	2.63	120.17	111.91
29	R	610	CLA	C4B-CHC-C1C	2.63	132.58	126.34
29	C	505	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	S	611	CLA	C1-C2-C3	-2.63	121.50	126.04
29	s	614	CLA	C1-C2-C3	-2.63	121.50	126.04
29	n	610	CLA	CMA-C3A-C4A	2.63	118.84	111.77
29	b	611	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	b	618	BCR	C15-C14-C13	-2.63	123.56	127.31
29	R	609	CLA	C3B-C4B-NB	-2.63	108.08	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	S	610	CLA	C3B-C4B-NB	-2.63	108.08	110.52
47	N	622	XAT	C18-C5-C6	-2.63	117.86	122.26
29	d	403	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	r	609	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	C	501	CLA	C3B-C4B-NB	-2.63	108.08	110.52
50	s	626	3PH	O31-C31-C32	2.63	120.15	111.91
29	Y	604	CLA	C2D-C1D-ND	2.63	112.04	110.10
29	Y	614	CLA	C2D-C1D-ND	2.63	112.04	110.10
39	S	624	LHG	C5-O7-C7	-2.62	111.33	117.79
48	n	623	NEX	C1-C2-C3	2.62	119.57	113.64
29	S	602	CLA	CMA-C3A-C4A	2.62	118.82	111.77
47	n	622	XAT	C18-C5-C6	-2.62	117.86	122.26
29	s	612	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
45	G	601	CHL	C3B-C4B-NB	-2.62	108.08	110.52
45	n	601	CHL	C3B-C4B-NB	-2.62	108.08	110.52
29	s	603	CLA	CHD-C1D-ND	-2.62	122.04	124.45
29	S	613	CLA	CHA-C4D-ND	2.62	137.98	132.50
29	C	501	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
29	r	611	CLA	C2D-C1D-ND	2.62	112.04	110.10
45	r	606	CHL	C3B-C4B-NB	-2.62	108.08	110.52
38	C	518	DGD	O6D-C5D-C6D	2.62	111.96	106.67
29	C	505	CLA	C1-O2A-CGA	2.62	123.32	116.44
29	c	513	CLA	CMA-C3A-C4A	2.62	118.82	111.77
29	c	510	CLA	CMD-C2D-C3D	-2.62	121.59	127.61
29	Y	612	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
48	Y	623	NEX	C4-C3-C2	2.62	115.83	110.77
29	y	612	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
29	C	505	CLA	O2A-CGA-CBA	2.62	120.13	111.91
29	A	405	CLA	C6-C5-C3	-2.62	106.59	113.45
45	y	606	CHL	C4B-CHC-C1C	2.62	132.55	126.34
29	C	512	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
29	y	613	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
46	N	621	LUT	C38-C25-C24	-2.62	117.96	123.56
29	Y	610	CLA	C2C-C1C-NC	2.62	112.42	109.97
29	N	614	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
45	Y	607	CHL	C4A-NA-C1A	2.62	107.88	106.71
29	B	605	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
29	c	507	CLA	C2D-C1D-ND	2.62	112.03	110.10
42	D	405	PL9	C40-C39-C41	2.62	119.67	115.27
29	B	609	CLA	CHA-C4D-ND	2.62	137.97	132.50
31	a	411	BCR	C33-C5-C4	2.62	118.64	113.62
48	G	623	NEX	C1-C2-C3	2.62	119.55	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S	601	CHL	C4B-CHC-C1C	2.62	132.54	126.34
29	b	613	CLA	C2C-C1C-NC	2.62	112.42	109.97
31	C	514	BCR	C36-C18-C17	-2.61	119.26	122.92
29	g	602	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
29	b	616	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
29	y	614	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
45	g	608	CHL	C4B-CHC-C1C	2.61	132.54	126.34
29	y	613	CLA	O2A-CGA-CBA	2.61	120.11	111.91
29	c	513	CLA	O2A-CGA-CBA	2.61	120.11	111.91
35	B	620	C7Z	C28-C27-C26	-2.61	119.87	127.20
42	D	405	PL9	C22-C23-C24	-2.61	121.37	127.66
50	i	101	3PH	O31-C31-C32	2.61	120.10	111.91
45	n	606	CHL	C4B-CHC-C1C	2.61	132.53	126.34
31	c	514	BCR	C38-C26-C25	-2.61	121.60	124.53
29	G	604	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
29	b	604	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
29	b	604	CLA	CMA-C3A-C4A	2.61	118.78	111.77
29	r	602	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
31	c	515	BCR	C34-C9-C10	-2.61	119.27	122.92
29	B	606	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
29	r	609	CLA	CHA-C4D-ND	2.61	137.95	132.50
29	s	613	CLA	CHA-C4D-ND	2.61	137.95	132.50
29	S	604	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
29	y	603	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
29	g	603	CLA	C3B-C4B-NB	-2.60	108.10	110.52
48	R	622	NEX	C20-C13-C14	-2.60	119.28	122.92
29	g	604	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
45	G	608	CHL	CHB-C4A-NA	2.60	128.11	124.51
29	S	605	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
29	b	608	CLA	CMA-C3A-C4A	2.60	118.77	111.77
29	b	605	CLA	CHA-C4D-ND	2.60	137.94	132.50
29	D	403	CLA	C3B-C4B-NB	-2.60	108.10	110.52
29	Y	603	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
46	S	620	LUT	C31-C30-C29	-2.60	123.60	127.31
31	A	411	BCR	C35-C13-C12	2.60	122.17	118.08
31	B	619	BCR	C1-C6-C5	-2.60	118.95	122.61
29	S	605	CLA	CHA-C4D-ND	2.60	137.94	132.50
29	g	611	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
45	s	601	CHL	CHB-C4A-NA	2.60	128.11	124.51
29	a	406	CLA	CMA-C3A-C4A	2.60	118.76	111.77
29	R	613	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
29	C	502	CLA	O2D-CGD-O1D	-2.60	118.76	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	g	606	CHL	C4B-CHC-C1C	2.60	132.50	126.34
29	y	603	CLA	CMA-C3A-C4A	2.60	118.75	111.77
29	Y	602	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
29	R	610	CLA	C2C-C1C-NC	2.60	112.40	109.97
29	n	603	CLA	C3B-C4B-NB	-2.60	108.11	110.52
29	B	611	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
29	b	602	CLA	C4B-CHC-C1C	2.60	132.49	126.34
29	r	610	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	R	608	CLA	C1-C2-C3	-2.59	121.56	126.04
29	R	603	CLA	C2D-C1D-ND	2.59	112.02	110.10
29	b	615	CLA	C2D-C1D-ND	2.59	112.02	110.10
29	c	503	CLA	C3B-C4B-NB	-2.59	108.11	110.52
29	C	505	CLA	CHA-C4D-ND	2.59	137.92	132.50
45	G	609	CHL	CHC-C1C-NC	2.59	128.13	124.20
45	g	605	CHL	C3B-C4B-NB	-2.59	108.11	110.52
29	B	607	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
33	c	521	LMG	C8-O7-C10	-2.59	111.41	117.79
46	g	620	LUT	C38-C25-C24	-2.59	118.02	123.56
45	y	601	CHL	C1-O2A-CGA	2.59	123.24	116.44
45	s	608	CHL	C4B-CHC-C1C	2.59	132.48	126.34
29	B	612	CLA	C2D-C1D-ND	2.59	112.01	110.10
29	y	612	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	B	603	CLA	CMA-C3A-C4A	2.59	118.73	111.77
29	N	610	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	n	602	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	s	613	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
31	c	517	BCR	C23-C24-C25	-2.59	119.94	127.20
29	s	611	CLA	C2D-C1D-ND	2.59	112.01	110.10
29	R	609	CLA	CHA-C4D-ND	2.59	137.91	132.50
29	s	605	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
46	r	620	LUT	C3-C4-C5	-2.59	106.70	111.85
46	r	620	LUT	C11-C12-C13	-2.59	119.15	126.42
31	B	619	BCR	C19-C18-C17	2.58	122.91	118.94
45	s	606	CHL	C3B-C4B-NB	-2.58	108.12	110.52
29	b	603	CLA	C2D-C1D-ND	2.58	112.01	110.10
29	G	611	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
29	S	603	CLA	CHD-C1D-ND	-2.58	122.08	124.45
33	J	101	LMG	O8-C28-C29	2.58	120.00	111.91
29	c	505	CLA	CHA-C4D-ND	2.58	137.90	132.50
29	D	403	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
29	G	604	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
29	c	501	CLA	C3B-C4B-NB	-2.58	108.12	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	608	CLA	CMA-C3A-C4A	2.58	118.70	111.77
29	b	617	CLA	CHD-C1D-ND	-2.58	122.08	124.45
29	B	604	CLA	CMA-C3A-C4A	2.58	118.70	111.77
29	Y	610	CLA	O2A-CGA-CBA	2.58	120.00	111.91
29	y	611	CLA	C2D-C1D-ND	2.58	112.00	110.10
31	C	514	BCR	C23-C24-C25	-2.58	119.97	127.20
29	Y	611	CLA	CMA-C3A-C4A	2.57	118.69	111.77
29	B	615	CLA	CHA-C4D-ND	2.57	137.88	132.50
31	c	515	BCR	C15-C14-C13	-2.57	123.64	127.31
29	B	602	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	b	606	CLA	CMD-C2D-C3D	-2.57	121.69	127.61
29	C	507	CLA	C2D-C1D-ND	2.57	112.00	110.10
29	n	612	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
33	C	521	LMG	C8-O7-C10	-2.57	111.46	117.79
47	r	622	XAT	C8-C9-C10	2.57	122.89	118.94
29	Y	612	CLA	C1-C2-C3	-2.57	121.59	126.04
29	b	606	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
45	N	606	CHL	C2B-C1B-NB	-2.57	108.51	110.23
29	s	613	CLA	CHD-C1D-ND	-2.57	122.09	124.45
29	Y	604	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	g	612	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	C	511	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
29	y	602	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
45	g	607	CHL	C4B-CHC-C1C	2.57	132.44	126.34
50	S	626	3PH	O31-C31-C32	2.57	119.97	111.91
45	N	601	CHL	C4B-CHC-C1C	2.57	132.43	126.34
29	N	602	CLA	C2D-C1D-ND	2.57	112.00	110.10
31	B	618	BCR	C36-C18-C17	-2.57	119.32	122.92
29	Y	603	CLA	C3B-C4B-NB	-2.57	108.13	110.52
45	Y	609	CHL	C3B-C4B-NB	-2.57	108.13	110.52
29	C	501	CLA	CHA-C4D-ND	2.57	137.87	132.50
29	r	609	CLA	CMD-C2D-C3D	-2.57	121.71	127.61
45	Y	601	CHL	C4B-CHC-C1C	2.57	132.42	126.34
29	g	612	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
29	s	609	CLA	C1-C2-C3	-2.56	121.61	126.04
29	Y	611	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
29	g	604	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	b	613	CLA	C2D-C1D-ND	2.56	111.99	110.10
45	g	609	CHL	C3C-C4C-NC	-2.56	107.70	110.57
46	Y	620	LUT	C31-C30-C29	-2.56	123.66	127.31
29	B	603	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
29	c	506	CLA	C1-C2-C3	-2.56	121.62	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	516	BCR	C36-C18-C17	-2.56	119.34	122.92
29	c	512	CLA	C1D-ND-C4D	-2.56	104.52	106.33
29	S	609	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
45	N	607	CHL	C4B-CHC-C1C	2.56	132.41	126.34
29	n	604	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
29	c	501	CLA	CHA-C4D-ND	2.56	137.85	132.50
45	R	607	CHL	C1-O2A-CGA	2.56	123.15	116.44
31	d	404	BCR	C33-C5-C4	2.56	118.53	113.62
39	y	624	LHG	O8-C23-C24	2.55	119.92	111.91
29	c	513	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
29	Y	612	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
29	b	609	CLA	CHA-C4D-ND	2.55	137.84	132.50
31	C	515	BCR	C23-C24-C25	-2.55	120.03	127.20
29	C	506	CLA	C1-C2-C3	-2.55	121.63	126.04
29	y	604	CLA	C2D-C1D-ND	2.55	111.99	110.10
29	B	604	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	b	604	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	C	513	CLA	O2A-CGA-CBA	2.55	119.92	111.91
45	R	606	CHL	C3B-C4B-NB	-2.55	108.15	110.52
29	c	502	CLA	C2D-C1D-ND	2.55	111.98	110.10
45	S	607	CHL	CHB-C4A-NA	2.55	128.04	124.51
29	y	611	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	R	612	CLA	CHA-C4D-ND	2.55	137.83	132.50
29	B	606	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
45	R	606	CHL	C4A-NA-C1A	2.55	107.85	106.71
31	C	517	BCR	C36-C18-C17	-2.55	119.35	122.92
31	c	517	BCR	C31-C1-C6	-2.55	106.17	110.30
29	s	602	CLA	C1D-ND-C4D	-2.55	104.53	106.33
29	y	603	CLA	C1D-ND-C4D	-2.55	104.53	106.33
45	g	609	CHL	CHD-C4C-C3C	2.55	128.59	124.84
29	b	603	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
44	h	101	RRX	C8-C7-C6	-2.55	120.05	127.20
45	r	607	CHL	C1-O2A-CGA	2.55	123.13	116.44
29	c	503	CLA	C4B-CHC-C1C	2.55	132.38	126.34
29	C	503	CLA	C4B-CHC-C1C	2.55	132.38	126.34
29	R	613	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
33	a	413	LMG	O8-C28-C29	2.55	119.90	111.91
45	N	601	CHL	C3B-C4B-NB	-2.54	108.15	110.52
29	D	402	CLA	CMC-C2C-C1C	2.54	128.91	125.04
29	N	612	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	N	604	CLA	CHA-C4D-ND	2.54	137.82	132.50
29	N	604	CLA	O2D-CGD-O1D	-2.54	118.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	503	CLA	C3B-C4B-NB	-2.54	108.16	110.52
45	r	606	CHL	C3C-C4C-NC	-2.54	107.72	110.57
29	N	612	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
47	r	622	XAT	O4-C5-C4	-2.54	111.47	113.38
29	C	508	CLA	CMA-C3A-C4A	2.54	118.61	111.77
45	n	605	CHL	CHB-C4A-NA	2.54	128.03	124.51
29	r	611	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
29	Y	608	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	s	611	CLA	C3B-C4B-NB	-2.54	108.16	110.52
29	n	604	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
29	n	604	CLA	CHA-C4D-ND	2.54	137.81	132.50
29	d	403	CLA	O2A-CGA-CBA	2.54	119.88	111.91
29	c	507	CLA	C1-C2-C3	-2.54	121.65	126.04
29	r	612	CLA	O2A-CGA-CBA	2.54	119.88	111.91
29	N	613	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
29	s	610	CLA	CHA-C4D-ND	2.54	137.81	132.50
29	b	602	CLA	CHA-C4D-ND	2.54	137.81	132.50
31	a	411	BCR	C36-C18-C17	-2.54	119.37	122.92
44	h	101	RRX	C24-C23-C22	-2.54	122.40	126.23
29	C	507	CLA	CHA-C4D-ND	2.54	137.80	132.50
29	y	602	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	C	506	CLA	CMA-C3A-C4A	2.53	118.59	111.77
45	G	606	CHL	CHB-C4A-NA	2.53	128.02	124.51
45	S	601	CHL	CHB-C4A-NA	2.53	128.02	124.51
29	n	614	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
29	S	613	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
29	c	511	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	A	408	PHO	C2D-C1D-ND	-2.53	107.78	109.53
29	b	615	CLA	CHA-C4D-ND	2.53	137.80	132.50
29	Y	614	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
45	G	606	CHL	C1-O2A-CGA	2.53	123.09	116.44
29	y	604	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
29	Y	612	CLA	CHA-C4D-ND	2.53	137.80	132.50
29	S	612	CLA	CMA-C3A-C4A	2.53	118.57	111.77
29	R	609	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
29	d	402	CLA	O2A-CGA-CBA	2.53	119.84	111.91
42	d	405	PL9	C22-C23-C24	-2.53	121.57	127.66
29	R	611	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
45	Y	607	CHL	C4B-CHC-C1C	2.53	132.33	126.34
29	R	612	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
29	Y	602	CLA	C3B-C4B-NB	-2.53	108.17	110.52
29	Y	608	CLA	C1C-C2C-C3C	-2.53	104.30	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	R	621	XAT	C18-C5-C6	-2.53	118.03	122.26
46	s	620	LUT	C11-C10-C9	-2.53	123.71	127.31
29	C	512	CLA	C1-C2-C3	-2.52	121.68	126.04
45	G	607	CHL	C4A-NA-C1A	2.52	107.84	106.71
29	n	612	CLA	CMA-C3A-C4A	2.52	118.56	111.77
43	f	101	HEM	C4A-NA-C1A	2.52	107.82	105.35
29	G	603	CLA	C4B-CHC-C1C	2.52	132.32	126.34
48	G	623	NEX	C16-C1-C6	-2.52	108.21	110.47
29	B	603	CLA	CHA-C4D-ND	2.52	137.78	132.50
29	s	605	CLA	CHD-C1D-ND	-2.52	122.14	124.45
29	y	602	CLA	C4B-CHC-C1C	2.52	132.32	126.34
29	s	604	CLA	C1-C2-C3	-2.52	121.68	126.04
29	s	614	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
45	S	607	CHL	C4B-CHC-C1C	2.52	132.32	126.34
29	b	606	CLA	C2D-C1D-ND	2.52	111.96	110.10
45	g	608	CHL	CHB-C4A-NA	2.52	128.00	124.51
45	g	605	CHL	C4A-NA-C1A	2.52	107.84	106.71
29	b	602	CLA	C3B-C4B-NB	-2.52	108.17	110.52
29	r	611	CLA	C3B-C4B-NB	-2.52	108.17	110.52
29	N	611	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
29	b	617	CLA	C2D-C1D-ND	2.52	111.96	110.10
29	g	603	CLA	C1D-ND-C4D	-2.52	104.54	106.33
45	G	609	CHL	CHD-C4C-C3C	2.52	128.54	124.84
39	G	630	LHG	O8-C23-C24	2.52	119.82	111.91
29	N	602	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
29	Y	608	CLA	CHA-C4D-ND	2.52	137.77	132.50
29	D	402	CLA	C4B-CHC-C1C	2.52	132.31	126.34
33	A	413	LMG	O8-C28-C29	2.52	119.81	111.91
29	n	613	CLA	C1-O2A-CGA	2.52	123.05	116.44
48	S	622	NEX	C1-C2-C3	2.52	119.33	113.64
29	n	611	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
29	G	604	CLA	CMA-C3A-C4A	2.52	118.53	111.77
29	G	612	CLA	C3B-C4B-NB	-2.52	108.18	110.52
29	S	603	CLA	CMA-C3A-C4A	2.51	118.53	111.77
29	C	509	CLA	C2D-C1D-ND	2.51	111.96	110.10
45	n	605	CHL	C1-O2A-CGA	2.51	123.04	116.44
29	y	608	CLA	CHA-C4D-ND	2.51	137.76	132.50
29	S	609	CLA	C1-C2-C3	-2.51	121.70	126.04
29	S	610	CLA	CHA-C4D-ND	2.51	137.76	132.50
29	y	610	CLA	O2A-CGA-CBA	2.51	119.79	111.91
29	n	610	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
29	b	617	CLA	OBD-CAD-C3D	-2.51	122.48	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	N	609	CHL	C1-O2A-CGA	2.51	123.03	116.44
35	B	620	C7Z	C21-C26-C25	-2.51	119.08	122.61
31	b	619	BCR	C8-C7-C6	-2.51	120.16	127.20
45	y	607	CHL	C4B-CHC-C1C	2.51	132.29	126.34
29	n	613	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
29	B	613	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	n	611	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	s	611	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	B	604	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
29	N	603	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
29	y	612	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	Y	612	CLA	O2A-CGA-CBA	2.51	119.78	111.91
45	n	601	CHL	CHB-C4A-NA	2.51	127.98	124.51
39	g	624	LHG	O8-C23-C24	2.51	119.78	111.91
29	d	402	CLA	C4B-CHC-C1C	2.51	132.28	126.34
29	R	604	CLA	CHA-C4D-ND	2.51	137.74	132.50
45	Y	601	CHL	C4A-NA-C1A	2.51	107.83	106.71
29	C	503	CLA	O1D-CGD-CBD	-2.51	119.36	124.48
46	R	620	LUT	C22-C23-C24	-2.51	108.89	111.74
29	c	510	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
29	s	612	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
46	n	620	LUT	C18-C5-C6	-2.50	121.72	124.53
29	g	612	CLA	C3B-C4B-NB	-2.50	108.19	110.52
29	r	602	CLA	CMA-C3A-C4A	2.50	118.50	111.77
29	c	510	CLA	C2D-C1D-ND	2.50	111.95	110.10
29	B	612	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
29	Y	611	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
29	B	607	CLA	CHA-C4D-ND	2.50	137.73	132.50
45	S	608	CHL	C1-O2A-CGA	2.50	123.00	116.44
29	R	613	CLA	CHA-C4D-ND	2.50	137.73	132.50
46	G	621	LUT	C10-C11-C12	-2.50	115.42	123.22
29	r	608	CLA	CHA-C4D-ND	2.50	137.73	132.50
29	C	501	CLA	CMD-C2D-C3D	-2.50	121.87	127.61
29	S	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
29	c	507	CLA	CHA-C4D-ND	2.50	137.72	132.50
46	N	620	LUT	C38-C25-C24	-2.50	118.21	123.56
29	S	612	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
45	S	607	CHL	C4A-NA-C1A	2.50	107.83	106.71
35	B	620	C7Z	C27-C28-C29	-2.50	122.46	126.23
29	G	602	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
29	g	603	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
29	B	617	CLA	O2D-CGD-O1D	-2.50	118.96	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	611	CLA	CHA-C4D-ND	2.50	137.72	132.50
29	c	510	CLA	CHA-C4D-ND	2.50	137.72	132.50
29	r	612	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	b	618	BCR	C36-C18-C17	-2.49	119.43	122.92
29	R	609	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
45	y	601	CHL	C4A-NA-C1A	2.49	107.83	106.71
29	b	606	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	G	612	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
45	N	609	CHL	CHD-C4C-C3C	2.49	128.50	124.84
29	c	503	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
45	n	605	CHL	CMA-C3A-C4A	2.49	118.47	111.77
29	G	604	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	B	619	BCR	C27-C26-C25	-2.49	119.11	122.73
45	g	601	CHL	C1-O2A-CGA	2.49	122.98	116.44
29	C	504	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
43	f	101	HEM	C4D-ND-C1D	2.49	107.65	105.07
29	b	607	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	b	608	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	b	614	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	b	613	CLA	C1-C2-C3	-2.49	121.74	126.04
29	g	613	CLA	O2A-CGA-CBA	2.49	119.72	111.91
29	s	605	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
29	B	604	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
31	c	516	BCR	C23-C24-C25	-2.49	120.21	127.20
29	Y	610	CLA	CMA-C3A-C4A	2.49	118.46	111.77
29	S	614	CLA	CMD-C2D-C3D	-2.49	121.89	127.61
29	c	505	CLA	CMA-C3A-C4A	2.49	118.46	111.77
29	R	608	CLA	C3B-C4B-NB	-2.49	108.21	110.52
29	Y	603	CLA	CHA-C4D-ND	2.49	137.70	132.50
29	R	604	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
29	c	503	CLA	CMD-C2D-C3D	-2.49	121.90	127.61
29	b	613	CLA	CHA-C4D-ND	2.48	137.70	132.50
29	y	608	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
31	d	404	BCR	C38-C26-C27	2.48	118.39	113.62
48	R	622	NEX	C19-C9-C10	-2.48	119.44	122.92
29	y	614	CLA	C3B-C4B-NB	-2.48	108.21	110.52
44	H	101	RRX	C24-C23-C22	-2.48	122.48	126.23
45	s	607	CHL	CHB-C4A-NA	2.48	127.94	124.51
29	c	511	CLA	CHA-C4D-ND	2.48	137.69	132.50
29	R	602	CLA	O2A-CGA-CBA	2.48	119.69	111.91
45	N	608	CHL	CHB-C4A-NA	2.48	127.94	124.51
29	C	511	CLA	CHA-C4D-ND	2.48	137.69	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	r	606	CHL	C4A-NA-C1A	2.48	107.82	106.71
29	D	402	CLA	CHA-C4D-ND	2.48	137.69	132.50
45	G	609	CHL	C3B-C4B-NB	-2.48	108.22	110.52
29	s	614	CLA	CHA-C4D-ND	2.48	137.69	132.50
29	N	611	CLA	C3B-C4B-NB	-2.48	108.22	110.52
29	R	602	CLA	CHA-C4D-ND	2.48	137.68	132.50
29	y	610	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
29	s	612	CLA	CMA-C3A-C4A	2.48	118.43	111.77
29	G	602	CLA	O2A-CGA-CBA	2.48	119.68	111.91
29	B	614	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
46	G	621	LUT	C35-C15-C14	-2.48	118.40	123.47
29	S	614	CLA	C2D-C1D-ND	2.48	111.93	110.10
45	n	601	CHL	C1-C2-C3	-2.48	121.76	126.04
29	r	604	CLA	CHA-C4D-ND	2.48	137.68	132.50
48	G	623	NEX	C20-C13-C14	-2.48	119.45	122.92
45	R	606	CHL	C3C-C4C-NC	-2.48	107.80	110.57
29	C	505	CLA	CMA-C3A-C4A	2.47	118.42	111.77
29	b	612	CLA	C2A-C1A-CHA	2.47	128.19	123.86
29	N	603	CLA	CHA-C4D-ND	2.47	137.68	132.50
29	N	612	CLA	CHA-C4D-ND	2.47	137.68	132.50
29	S	611	CLA	CHA-C4D-ND	2.47	137.68	132.50
45	Y	606	CHL	C2B-C1B-NB	-2.47	108.57	110.23
31	C	515	BCR	C34-C9-C10	-2.47	119.46	122.92
29	c	503	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
45	s	607	CHL	C4B-CHC-C1C	2.47	132.20	126.34
29	c	509	CLA	CHA-C4D-ND	2.47	137.67	132.50
39	D	409	LHG	C5-O7-C7	-2.47	111.71	117.79
29	S	605	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
29	g	603	CLA	C4B-CHC-C1C	2.47	132.19	126.34
29	g	611	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	n	612	CLA	C4B-CHC-C1C	2.47	132.19	126.34
29	d	402	CLA	C1-C2-C3	-2.47	121.77	126.04
39	C	525	LHG	O8-C23-C24	2.47	119.65	111.91
31	A	411	BCR	C36-C18-C17	-2.47	119.47	122.92
48	N	623	NEX	C38-C25-C26	-2.47	118.12	122.26
29	y	608	CLA	C1-O2A-CGA	2.47	122.92	116.44
29	G	603	CLA	C3B-C4B-NB	-2.47	108.23	110.52
29	c	508	CLA	C2D-C1D-ND	2.47	111.92	110.10
29	b	607	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
29	r	611	CLA	CHA-C4D-ND	2.47	137.66	132.50
36	B	625	DGA	OG1-CA1-CA2	2.47	119.64	111.91
46	S	621	LUT	C10-C11-C12	-2.47	115.52	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	g	613	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	Y	613	CLA	O2A-CGA-CBA	2.47	119.64	111.91
45	S	606	CHL	C4D-CHA-C1A	2.47	124.25	121.25
29	g	610	CLA	O2A-CGA-CBA	2.46	119.64	111.91
29	n	610	CLA	C4B-CHC-C1C	2.46	132.18	126.34
29	G	613	CLA	CHA-C4D-ND	2.46	137.66	132.50
29	B	607	CLA	C1C-C2C-C3C	-2.46	104.36	106.96
29	b	612	CLA	CHA-C1A-NA	-2.46	120.75	126.40
46	s	620	LUT	C10-C11-C12	-2.46	115.53	123.22
29	C	510	CLA	CMD-C2D-C3D	-2.46	121.94	127.61
29	S	603	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	S	611	CLA	C3B-C4B-NB	-2.46	108.23	110.52
29	G	613	CLA	O2A-CGA-CBA	2.46	119.64	111.91
47	r	622	XAT	C18-C5-C6	-2.46	118.13	122.26
29	B	608	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	S	602	CLA	C4B-CHC-C1C	2.46	132.18	126.34
29	b	603	CLA	O2A-CGA-CBA	2.46	119.63	111.91
29	C	512	CLA	C1D-ND-C4D	-2.46	104.59	106.33
29	N	612	CLA	C3B-C4B-NB	-2.46	108.23	110.52
29	C	510	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
29	s	617	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
45	s	606	CHL	CHB-C4A-NA	2.46	127.92	124.51
45	N	606	CHL	C1-O2A-CGA	2.46	122.90	116.44
29	R	608	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	y	614	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	c	509	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
29	n	611	CLA	C3B-C4B-NB	-2.46	108.23	110.52
39	Y	624	LHG	O8-C23-C24	2.46	119.62	111.91
29	R	603	CLA	C1-C2-C3	-2.46	121.79	126.04
39	N	624	LHG	O8-C23-C24	2.46	119.62	111.91
45	Y	601	CHL	C1-O2A-CGA	2.46	122.89	116.44
29	s	603	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
29	b	612	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
29	D	403	CLA	O2A-CGA-CBA	2.46	119.61	111.91
29	B	606	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	S	612	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	r	613	CLA	C3B-C4B-NB	-2.46	108.24	110.52
46	N	620	LUT	C18-C5-C6	-2.46	121.77	124.53
29	S	617	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
29	s	612	CLA	CHA-C4D-ND	2.45	137.63	132.50
29	c	508	CLA	CMA-C3A-C4A	2.45	118.37	111.77
29	C	509	CLA	CHA-C4D-ND	2.45	137.63	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	506	CLA	C2D-C1D-ND	2.45	111.91	110.10
29	y	611	CLA	CHA-C4D-ND	2.45	137.63	132.50
29	G	602	CLA	C4B-CHC-C1C	2.45	132.16	126.34
29	b	613	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
29	c	504	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
29	s	605	CLA	C1-O2A-CGA	2.45	122.88	116.44
29	B	611	CLA	CHA-C4D-ND	2.45	137.63	132.50
29	R	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
29	r	612	CLA	C3B-C4B-NB	-2.45	108.24	110.52
45	n	605	CHL	C1-C2-C3	-2.45	121.80	126.04
29	S	611	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
29	g	612	CLA	CHA-C4D-ND	2.45	137.63	132.50
29	s	604	CLA	CHA-C4D-ND	2.45	137.63	132.50
29	B	603	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
29	S	613	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	r	608	CLA	C3B-C4B-NB	-2.45	108.24	110.52
29	N	611	CLA	CHA-C4D-ND	2.45	137.62	132.50
29	B	614	CLA	CHA-C4D-ND	2.45	137.62	132.50
29	y	602	CLA	CHA-C4D-ND	2.45	137.62	132.50
29	r	612	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	c	516	BCR	C38-C26-C25	-2.45	121.78	124.53
29	y	612	CLA	C3B-C4B-NB	-2.45	108.25	110.52
29	R	602	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
29	G	614	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	C	517	BCR	C33-C5-C6	-2.45	121.78	124.53
29	y	603	CLA	CHA-C4D-ND	2.45	137.62	132.50
46	G	621	LUT	C31-C30-C29	-2.45	123.82	127.31
29	N	610	CLA	C4B-CHC-C1C	2.44	132.13	126.34
47	N	622	XAT	O4-C5-C4	-2.44	111.55	113.38
29	n	613	CLA	CHA-C4D-ND	2.44	137.61	132.50
48	r	623	NEX	C39-C29-C30	-2.44	119.50	122.92
33	b	622	LMG	O8-C28-C29	2.44	119.58	111.91
29	C	511	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
47	r	622	XAT	C31-C30-C29	-2.44	123.82	127.31
29	s	610	CLA	C4B-CHC-C1C	2.44	132.13	126.34
29	R	612	CLA	O2A-CGA-CBA	2.44	119.57	111.91
45	y	609	CHL	C4D-CHA-C1A	2.44	124.22	121.25
29	G	612	CLA	C4B-CHC-C1C	2.44	132.13	126.34
29	R	611	CLA	C3B-C4B-NB	-2.44	108.25	110.52
31	c	514	BCR	C34-C9-C10	-2.44	119.50	122.92
29	Y	611	CLA	CHA-C4D-ND	2.44	137.61	132.50
29	r	612	CLA	C1-C2-C3	-2.44	121.82	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	n	621	LUT	C10-C11-C12	-2.44	115.60	123.22
29	B	604	CLA	O2A-CGA-CBA	2.44	119.57	111.91
46	S	621	LUT	C3-C4-C5	-2.44	106.99	111.85
46	G	621	LUT	C38-C25-C24	-2.44	118.34	123.56
33	B	622	LMG	O8-C28-C29	2.44	119.56	111.91
29	B	616	CLA	CHA-C4D-ND	2.44	137.60	132.50
29	G	611	CLA	CHA-C4D-ND	2.44	137.60	132.50
45	y	601	CHL	C4B-CHC-C1C	2.44	132.12	126.34
48	n	623	NEX	C31-C30-C29	2.44	130.79	127.31
29	G	612	CLA	CHA-C4D-ND	2.44	137.60	132.50
29	S	609	CLA	CHA-C4D-ND	2.44	137.60	132.50
45	Y	606	CHL	C4B-CHC-C1C	2.44	132.12	126.34
45	r	607	CHL	C4B-CHC-C1C	2.44	132.12	126.34
29	N	602	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	S	614	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	g	612	CLA	C4B-CHC-C1C	2.44	132.12	126.34
29	D	402	CLA	O2A-CGA-CBA	2.44	119.56	111.91
29	S	609	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	Y	613	CLA	CHA-C4D-ND	2.44	137.60	132.50
29	Y	604	CLA	CMA-C3A-C4A	2.44	118.32	111.77
29	R	610	CLA	CMC-C2C-C1C	2.44	128.75	125.04
39	d	409	LHG	C5-O7-C7	-2.44	111.79	117.79
29	g	602	CLA	C4B-CHC-C1C	2.44	132.12	126.34
30	A	408	PHO	C1C-C2C-C3C	-2.44	106.58	108.61
29	b	605	CLA	CHD-C1D-ND	-2.44	122.22	124.45
29	S	610	CLA	CMA-C3A-C4A	2.44	118.32	111.77
29	d	403	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	r	602	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
29	s	614	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
29	B	606	CLA	O2A-CGA-CBA	2.43	119.54	111.91
29	C	510	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	r	613	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	g	614	CLA	C3B-C4B-NB	-2.43	108.26	110.52
48	R	622	NEX	C40-C33-C34	-2.43	119.52	122.92
29	R	610	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
45	N	605	CHL	CHB-C4A-NA	2.43	127.87	124.51
29	y	612	CLA	O2A-CGA-CBA	2.43	119.54	111.91
44	H	101	RRX	C8-C7-C6	-2.43	120.38	127.20
48	y	623	NEX	C4-C3-C2	2.43	115.47	110.77
29	N	603	CLA	OBD-CAD-C3D	-2.43	122.67	128.52
31	c	516	BCR	C38-C26-C27	2.43	118.28	113.62
29	N	613	CLA	CHA-C4D-ND	2.43	137.58	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	509	CLA	C2D-C1D-ND	2.43	111.89	110.10
46	R	620	LUT	C3-C4-C5	-2.43	107.01	111.85
29	Y	602	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
29	s	611	CLA	C4B-CHC-C1C	2.43	132.10	126.34
29	r	604	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	s	614	CLA	C2D-C1D-ND	2.43	111.89	110.10
29	n	603	CLA	CHA-C4D-ND	2.43	137.58	132.50
45	Y	609	CHL	CHB-C4A-NA	2.43	127.87	124.51
45	g	605	CHL	C4D-CHA-C1A	2.43	124.20	121.25
29	r	602	CLA	CHA-C4D-ND	2.43	137.58	132.50
29	y	613	CLA	C1-O2A-CGA	2.43	122.81	116.44
29	S	614	CLA	O2A-CGA-CBA	2.43	119.53	111.91
45	G	609	CHL	C4D-CHA-C1A	2.43	124.20	121.25
29	D	403	CLA	C4B-CHC-C1C	2.43	132.09	126.34
29	S	605	CLA	CHD-C1D-ND	-2.43	122.22	124.45
29	Y	610	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
29	N	603	CLA	C3B-C4B-NB	-2.43	108.26	110.52
29	Y	610	CLA	C3B-C4B-NB	-2.43	108.26	110.52
29	y	602	CLA	C3B-C4B-NB	-2.43	108.26	110.52
29	s	604	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
29	r	612	CLA	CMA-C3A-C4A	2.42	118.29	111.77
29	r	602	CLA	C4B-CHC-C1C	2.42	132.09	126.34
29	b	603	CLA	CHA-C4D-ND	2.42	137.57	132.50
29	s	609	CLA	C3B-C4B-NB	-2.42	108.27	110.52
29	Y	604	CLA	CHA-C4D-ND	2.42	137.56	132.50
47	g	622	XAT	C19-C9-C10	-2.42	119.53	122.92
39	Y	624	LHG	C6-C5-C4	-2.42	106.06	111.79
29	B	605	CLA	C4B-CHC-C1C	2.42	132.08	126.34
29	B	605	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
29	a	410	CLA	CHA-C4D-ND	2.42	137.56	132.50
33	b	622	LMG	O1-C7-C8	-2.42	105.06	110.90
29	N	611	CLA	C4B-CHC-C1C	2.42	132.08	126.34
29	n	602	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	g	603	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	n	614	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	s	610	CLA	CMA-C3A-C4A	2.42	118.28	111.77
45	r	606	CHL	CHB-C4A-NA	2.42	127.86	124.51
29	r	603	CLA	CHA-C4D-ND	2.42	137.56	132.50
45	n	609	CHL	CAA-C2A-C1A	2.42	119.90	111.97
47	G	622	XAT	C19-C9-C10	-2.42	119.53	122.92
35	b	620	C7Z	C21-C26-C25	-2.42	119.21	122.61
29	b	604	CLA	O2A-CGA-CBA	2.42	119.50	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	y	606	CHL	C2B-C1B-NB	-2.42	108.61	110.23
29	g	610	CLA	C4B-CHC-C1C	2.42	132.07	126.34
45	s	601	CHL	C4B-CHC-C1C	2.42	132.07	126.34
29	R	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	r	604	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
46	n	621	LUT	C35-C15-C14	-2.42	118.52	123.47
29	n	612	CLA	C3B-C4B-NB	-2.42	108.27	110.52
48	R	622	NEX	C38-C25-C26	-2.42	118.21	122.26
29	c	502	CLA	CHA-C4D-ND	2.42	137.55	132.50
29	g	614	CLA	CHA-C4D-ND	2.42	137.55	132.50
29	G	602	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	y	610	CLA	CHA-C4D-ND	2.41	137.55	132.50
33	h	102	LMG	O8-C28-C29	2.41	119.48	111.91
31	D	404	BCR	C38-C26-C27	2.41	118.25	113.62
29	c	503	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	C	513	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
29	s	609	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
29	N	614	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	n	613	CLA	C3B-C4B-NB	-2.41	108.28	110.52
29	S	617	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	g	614	CLA	C4B-CHC-C1C	2.41	132.06	126.34
29	G	603	CLA	C1D-ND-C4D	-2.41	104.62	106.33
29	g	602	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	c	509	CLA	O2A-CGA-CBA	2.41	119.47	111.91
29	C	508	CLA	C2D-C1D-ND	2.41	111.88	110.10
29	y	604	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
45	n	608	CHL	CHB-C4A-NA	2.41	127.84	124.51
29	B	605	CLA	CHD-C1D-ND	-2.41	122.24	124.45
31	C	515	BCR	C38-C26-C25	-2.41	121.82	124.53
29	a	407	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	r	610	CLA	C3B-C4B-NB	-2.41	108.28	110.52
29	g	610	CLA	C1C-C2C-C3C	-2.41	104.43	106.96
46	g	621	LUT	C35-C15-C14	-2.41	118.54	123.47
29	b	604	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
29	s	603	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	D	403	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	Y	614	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	b	616	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	b	617	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
29	s	604	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
29	R	602	CLA	C3B-C4B-NB	-2.41	108.28	110.52
29	B	602	CLA	C2D-C1D-ND	2.41	111.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	R	622	NEX	C39-C29-C30	-2.41	119.55	122.92
29	A	406	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	c	501	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
29	r	608	CLA	CMD-C2D-C3D	-2.40	122.08	127.61
45	G	601	CHL	C1-O2A-CGA	2.40	122.75	116.44
29	c	511	CLA	CMD-C2D-C3D	-2.40	122.08	127.61
29	y	611	CLA	CMA-C3A-C4A	2.40	118.23	111.77
29	s	610	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
43	F	101	HEM	C4A-NA-C1A	2.40	107.70	105.35
29	G	614	CLA	C3B-C4B-NB	-2.40	108.28	110.52
29	R	612	CLA	C3B-C4B-NB	-2.40	108.28	110.52
29	a	410	CLA	O2A-CGA-CBA	2.40	119.45	111.91
31	C	516	BCR	C38-C26-C27	2.40	118.23	113.62
29	y	610	CLA	C4B-CHC-C1C	2.40	132.04	126.34
29	N	610	CLA	CHA-C4D-ND	2.40	137.53	132.50
29	y	604	CLA	CHA-C4D-ND	2.40	137.53	132.50
29	A	407	CLA	CHA-C4D-ND	2.40	137.53	132.50
29	b	608	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
29	a	407	CLA	C4B-CHC-C1C	2.40	132.03	126.34
45	N	606	CHL	C4B-CHC-C1C	2.40	132.03	126.34
29	Y	611	CLA	CHD-C1D-ND	-2.40	122.25	124.45
29	C	506	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	N	602	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	B	603	CLA	O2A-CGA-CBA	2.40	119.44	111.91
46	N	621	LUT	C18-C5-C6	-2.40	121.83	124.53
29	d	403	CLA	C4B-CHC-C1C	2.40	132.03	126.34
45	s	608	CHL	CHB-C4A-NA	2.40	127.83	124.51
29	B	610	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	b	606	CLA	O2A-CGA-CBA	2.40	119.44	111.91
45	y	606	CHL	C1-O2A-CGA	2.40	122.74	116.44
29	C	513	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	Y	610	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	a	406	CLA	O2A-CGA-CBA	2.40	119.43	111.91
45	g	606	CHL	CHB-C4A-NA	2.40	127.83	124.51
29	g	614	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
29	B	606	CLA	C2D-C1D-ND	2.40	111.87	110.10
31	d	404	BCR	C4-C5-C6	-2.40	119.25	122.73
29	S	602	CLA	CHA-C4D-ND	2.40	137.51	132.50
48	S	622	NEX	C40-C33-C34	-2.40	119.56	122.92
29	C	502	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
29	y	614	CLA	C4B-CHC-C1C	2.40	132.02	126.34
29	c	513	CLA	C3B-C4B-NB	-2.40	108.29	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	513	CLA	CHA-C4D-ND	2.40	137.51	132.50
45	n	608	CHL	C1-O2A-CGA	2.40	122.73	116.44
29	r	603	CLA	C4B-CHC-C1C	2.40	132.02	126.34
29	c	506	CLA	CHA-C4D-ND	2.40	137.51	132.50
29	S	605	CLA	C3B-C4B-NB	-2.40	108.29	110.52
29	s	609	CLA	CHA-C4D-ND	2.39	137.51	132.50
29	s	617	CLA	O2A-CGA-CBA	2.39	119.42	111.91
48	Y	623	NEX	C16-C1-C6	-2.39	108.33	110.47
29	C	503	CLA	CHA-C4D-ND	2.39	137.51	132.50
45	G	605	CHL	CHB-C4A-NA	2.39	127.82	124.51
29	D	402	CLA	C1-C2-C3	-2.39	121.90	126.04
29	C	512	CLA	C4B-CHC-C1C	2.39	132.01	126.34
29	C	512	CLA	CMA-C3A-C4A	2.39	118.20	111.77
29	A	407	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
29	s	602	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
29	G	614	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
29	C	502	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	n	612	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	s	617	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	a	406	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	r	608	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
29	y	613	CLA	CHA-C4D-ND	2.39	137.50	132.50
45	y	606	CHL	CHB-C4A-NA	2.39	127.82	124.51
29	Y	604	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	S	610	CLA	C4B-CHC-C1C	2.39	132.00	126.34
29	S	604	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	G	610	CLA	C1D-ND-C4D	-2.39	104.64	106.33
29	y	608	CLA	C3B-C4B-NB	-2.39	108.30	110.52
29	g	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	Y	614	CLA	C3B-C4B-NB	-2.39	108.30	110.52
31	C	516	BCR	C31-C1-C6	-2.39	106.43	110.30
29	B	612	CLA	CMA-C3A-C4A	2.39	118.19	111.77
29	b	610	CLA	CHA-C4D-ND	2.38	137.49	132.50
29	R	604	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
29	C	511	CLA	CHA-C1A-NA	-2.38	120.94	126.40
29	Y	603	CLA	C1-C2-C3	-2.38	121.92	126.04
29	C	503	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
46	R	620	LUT	C11-C12-C13	-2.38	119.72	126.42
31	b	618	BCR	C33-C5-C6	-2.38	121.85	124.53
45	G	606	CHL	C2B-C1B-NB	-2.38	108.63	110.23
29	a	405	CLA	CHA-C4D-ND	2.38	137.49	132.50
29	d	402	CLA	CHA-C4D-ND	2.38	137.49	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	619	BCR	C8-C7-C6	-2.38	120.51	127.20
45	G	609	CHL	CHB-C4A-NA	2.38	127.81	124.51
29	g	602	CLA	O2A-CGA-CBA	2.38	119.38	111.91
29	y	610	CLA	CMA-C3A-C4A	2.38	118.17	111.77
29	R	610	CLA	C1D-ND-C4D	-2.38	104.64	106.33
29	G	603	CLA	CHA-C4D-ND	2.38	137.48	132.50
29	s	609	CLA	C4B-CHC-C1C	2.38	131.99	126.34
29	C	509	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
29	Y	602	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
31	c	517	BCR	C3-C4-C5	-2.38	109.83	114.08
36	b	623	DGA	OG1-CA1-CA2	2.38	119.38	111.91
29	C	506	CLA	C4B-CHC-C1C	2.38	131.98	126.34
45	N	608	CHL	C4A-NA-C1A	2.38	107.78	106.71
29	R	602	CLA	C4B-CHC-C1C	2.38	131.98	126.34
29	s	609	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
30	a	408	PHO	C1C-C2C-C3C	-2.38	106.63	108.61
45	S	608	CHL	C1-C2-C3	-2.38	121.93	126.04
31	b	618	BCR	C3-C4-C5	-2.38	109.83	114.08
31	C	514	BCR	C33-C5-C4	2.38	118.19	113.62
29	S	610	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
46	S	621	LUT	C15-C14-C13	-2.38	123.92	127.31
29	b	608	CLA	O2A-CGA-CBA	2.38	119.37	111.91
45	n	606	CHL	C1-O2A-CGA	2.38	122.68	116.44
29	n	603	CLA	C4B-CHC-C1C	2.38	131.97	126.34
45	G	607	CHL	C1-O2A-CGA	2.38	122.68	116.44
29	B	610	CLA	O2A-CGA-CBA	2.37	119.36	111.91
29	Y	608	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
29	b	612	CLA	CHA-C4D-ND	2.37	137.47	132.50
29	b	612	CLA	C2D-C1D-ND	2.37	111.85	110.10
29	c	512	CLA	C4B-CHC-C1C	2.37	131.97	126.34
42	D	405	PL9	C20-C19-C21	2.37	119.26	115.27
45	n	608	CHL	C4D-CHA-C1A	2.37	124.14	121.25
48	y	623	NEX	C19-C9-C10	-2.37	119.60	122.92
45	S	608	CHL	CHB-C4A-NA	2.37	127.79	124.51
29	c	513	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
29	A	407	CLA	C4B-CHC-C1C	2.37	131.96	126.34
29	C	501	CLA	C4B-CHC-C1C	2.37	131.96	126.34
29	S	604	CLA	O2A-CGA-CBA	2.37	119.35	111.91
29	g	602	CLA	C3B-C4B-NB	-2.37	108.31	110.52
45	s	608	CHL	C1-O2A-CGA	2.37	122.67	116.44
45	Y	606	CHL	CHB-C4A-NA	2.37	127.79	124.51
29	A	410	CLA	CHA-C4D-ND	2.37	137.46	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	506	CLA	C2D-C1D-ND	2.37	111.85	110.10
29	s	604	CLA	C2D-C1D-ND	2.37	111.85	110.10
45	Y	606	CHL	C1-C2-C3	-2.37	121.95	126.04
29	C	504	CLA	CHA-C4D-ND	2.37	137.45	132.50
29	y	604	CLA	C4B-CHC-C1C	2.37	131.95	126.34
29	n	610	CLA	CHA-C4D-ND	2.37	137.45	132.50
39	d	408	LHG	C6-C5-C4	-2.37	106.19	111.79
29	S	602	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
45	n	601	CHL	C1-O2A-CGA	2.37	122.65	116.44
29	r	611	CLA	C4B-CHC-C1C	2.36	131.95	126.34
29	Y	614	CLA	C4B-CHC-C1C	2.36	131.94	126.34
46	N	621	LUT	C2-C3-C4	-2.36	107.07	110.30
29	r	610	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	R	603	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
29	G	603	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
29	N	603	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
31	d	404	BCR	C27-C26-C25	-2.36	119.30	122.73
29	R	610	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	G	614	CLA	C4B-CHC-C1C	2.36	131.94	126.34
46	Y	621	LUT	C10-C11-C12	-2.36	115.85	123.22
29	a	405	CLA	C2C-C1C-NC	2.36	112.18	109.97
29	B	613	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
29	b	617	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	r	610	CLA	C4B-CHC-C1C	2.36	131.94	126.34
29	n	614	CLA	C4B-CHC-C1C	2.36	131.94	126.34
29	r	612	CLA	C4B-CHC-C1C	2.36	131.94	126.34
29	y	603	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
47	n	622	XAT	C39-C29-C30	-2.36	119.62	122.92
48	n	623	NEX	C40-C33-C34	-2.36	119.62	122.92
29	B	610	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
29	A	405	CLA	CHA-C4D-ND	2.36	137.43	132.50
29	R	612	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
29	y	613	CLA	C4B-CHC-C1C	2.36	131.93	126.34
29	c	505	CLA	O2A-CGA-CBA	2.36	119.31	111.91
47	r	622	XAT	C31-C32-C33	2.36	133.04	126.42
29	Y	603	CLA	O2A-CGA-CBA	2.36	119.31	111.91
29	C	501	CLA	C1D-ND-C4D	-2.36	104.66	106.33
29	s	613	CLA	C4B-CHC-C1C	2.36	131.93	126.34
46	S	621	LUT	C16-C1-C6	-2.36	106.48	110.30
29	s	609	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
29	R	609	CLA	C2D-C1D-ND	2.36	111.84	110.10
29	Y	611	CLA	C4B-CHC-C1C	2.36	131.93	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	r	607	CHL	C4A-NA-C1A	2.36	107.77	106.71
29	S	617	CLA	O2A-CGA-CBA	2.36	119.30	111.91
29	Y	613	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
29	S	604	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
29	b	602	CLA	C2D-C1D-ND	2.35	111.84	110.10
29	c	507	CLA	C3B-C4B-NB	-2.35	108.33	110.52
45	n	607	CHL	C4B-CHC-C1C	2.35	131.92	126.34
29	r	613	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
29	Y	602	CLA	CHA-C4D-ND	2.35	137.42	132.50
47	r	622	XAT	C30-C31-C32	-2.35	115.87	123.22
29	G	614	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
29	c	508	CLA	C4B-CHC-C1C	2.35	131.92	126.34
29	g	614	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
29	c	505	CLA	C2D-C1D-ND	2.35	111.84	110.10
29	R	610	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
29	c	504	CLA	CHA-C4D-ND	2.35	137.42	132.50
29	b	610	CLA	O2A-CGA-CBA	2.35	119.28	111.91
48	N	623	NEX	C1-C2-C3	2.35	118.95	113.64
29	G	602	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
29	B	617	CLA	CHA-C4D-ND	2.35	137.41	132.50
29	B	617	CLA	CHD-C1D-ND	-2.35	122.30	124.45
29	y	608	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
45	Y	609	CHL	CHD-C4C-C3C	2.35	128.29	124.84
45	n	609	CHL	C4A-NA-C1A	2.35	107.76	106.71
29	y	604	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
29	n	602	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	c	506	CLA	CHA-C1A-NA	-2.35	121.02	126.40
29	b	603	CLA	C1-O2A-CGA	2.35	122.60	116.44
29	G	610	CLA	O2A-CGA-CBA	2.35	119.27	111.91
48	y	623	NEX	C5-C4-C3	2.35	114.52	111.75
29	C	503	CLA	O2A-CGA-CBA	2.35	119.27	111.91
29	c	501	CLA	C4B-CHC-C1C	2.35	131.90	126.34
29	b	605	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
29	R	611	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	B	608	CLA	O2A-CGA-CBA	2.34	119.27	111.91
45	S	606	CHL	CHB-C4A-NA	2.34	127.75	124.51
47	y	622	XAT	C18-C5-C6	-2.34	118.33	122.26
29	A	406	CLA	C2D-C1D-ND	2.34	111.83	110.10
29	r	608	CLA	C4B-CHC-C1C	2.34	131.90	126.34
46	y	621	LUT	C10-C11-C12	-2.34	115.91	123.22
45	y	609	CHL	CHB-C4A-NA	2.34	127.75	124.51
29	r	609	CLA	C3B-C4B-NB	-2.34	108.34	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	g	605	CHL	CHB-C4A-NA	2.34	127.75	124.51
29	B	611	CLA	O2A-CGA-CBA	2.34	119.26	111.91
29	C	506	CLA	CHA-C1A-NA	-2.34	121.03	126.40
29	B	607	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
29	R	611	CLA	C4B-CHC-C1C	2.34	131.89	126.34
29	B	608	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
29	s	602	CLA	CHA-C4D-ND	2.34	137.40	132.50
45	N	606	CHL	CHB-C4A-NA	2.34	127.75	124.51
46	n	620	LUT	C38-C25-C24	-2.34	118.55	123.56
29	c	511	CLA	C4B-CHC-C1C	2.34	131.89	126.34
29	n	611	CLA	C4B-CHC-C1C	2.34	131.89	126.34
29	S	617	CLA	C3B-C4B-NB	-2.34	108.34	110.52
29	R	609	CLA	CHA-C1A-NA	-2.34	121.04	126.40
29	g	613	CLA	C4B-CHC-C1C	2.34	131.89	126.34
29	r	609	CLA	CHA-C1A-NA	-2.34	121.04	126.40
29	c	509	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
29	g	613	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
47	N	622	XAT	C19-C9-C10	-2.34	119.65	122.92
29	B	612	CLA	O2A-CGA-CBA	2.34	119.25	111.91
45	N	608	CHL	C4D-CHA-C1A	2.34	124.09	121.25
47	y	622	XAT	O24-C25-C38	-2.34	112.25	115.06
29	c	507	CLA	C4B-CHC-C1C	2.34	131.88	126.34
33	B	622	LMG	O1-C7-C8	-2.34	105.26	110.90
31	B	618	BCR	C2-C1-C6	2.34	114.08	110.48
29	C	508	CLA	CHA-C4D-ND	2.34	137.39	132.50
29	C	501	CLA	O2A-CGA-CBA	2.34	119.24	111.91
29	Y	603	CLA	C1D-ND-C4D	-2.34	104.68	106.33
29	n	613	CLA	C4B-CHC-C1C	2.34	131.88	126.34
29	B	612	CLA	C1C-C2C-C3C	-2.33	104.50	106.96
46	g	620	LUT	C10-C11-C12	-2.33	115.93	123.22
46	y	620	LUT	C30-C31-C32	-2.33	115.93	123.22
46	s	620	LUT	C31-C30-C29	-2.33	123.98	127.31
30	a	409	PHO	O1D-CGD-CBD	2.33	128.62	124.74
29	y	612	CLA	CMA-C3A-C4A	2.33	118.04	111.77
29	C	508	CLA	C4B-CHC-C1C	2.33	131.87	126.34
33	H	102	LMG	O8-C28-C29	2.33	119.23	111.91
29	C	507	CLA	CHA-C1A-NA	-2.33	121.06	126.40
29	a	407	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
29	C	513	CLA	C3B-C4B-NB	-2.33	108.35	110.52
29	c	507	CLA	CHA-C1A-NA	-2.33	121.06	126.40
29	R	603	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
29	s	603	CLA	CHA-C1A-NA	-2.33	121.07	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	608	CLA	C4B-CHC-C1C	2.33	131.86	126.34
29	n	604	CLA	C4B-CHC-C1C	2.33	131.86	126.34
29	N	614	CLA	C4B-CHC-C1C	2.33	131.86	126.34
29	y	613	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
29	B	604	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	N	604	CLA	CMA-C3A-C4A	2.33	118.02	111.77
29	c	503	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
29	y	602	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
29	C	507	CLA	C4B-CHC-C1C	2.32	131.85	126.34
29	R	609	CLA	C4B-CHC-C1C	2.32	131.85	126.34
46	g	621	LUT	C38-C25-C24	-2.32	118.59	123.56
45	s	606	CHL	CHD-C4C-C3C	2.32	128.26	124.84
31	D	404	BCR	C1-C6-C5	-2.32	119.34	122.61
29	r	609	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	S	602	CLA	C3B-C4B-NB	-2.32	108.36	110.52
29	G	611	CLA	C4B-CHC-C1C	2.32	131.85	126.34
29	B	605	CLA	CMB-C2B-C1B	2.32	128.90	125.37
48	r	623	NEX	C38-C25-C26	-2.32	118.37	122.26
47	y	622	XAT	C40-C33-C34	-2.32	119.67	122.92
29	d	402	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	S	605	CLA	C4B-CHC-C1C	2.32	131.84	126.34
29	S	612	CLA	C4B-CHC-C1C	2.32	131.84	126.34
29	A	410	CLA	O2A-CGA-CBA	2.32	119.19	111.91
29	C	511	CLA	C4B-CHC-C1C	2.32	131.84	126.34
29	r	604	CLA	C1D-ND-C4D	-2.32	104.69	106.33
29	c	512	CLA	CHA-C4D-ND	2.32	137.35	132.50
29	N	612	CLA	C4B-CHC-C1C	2.32	131.84	126.34
29	s	612	CLA	C4B-CHC-C1C	2.32	131.84	126.34
31	D	404	BCR	C33-C5-C4	2.32	118.07	113.62
29	b	607	CLA	C2D-C1D-ND	2.32	111.81	110.10
29	s	603	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
29	Y	610	CLA	C4B-CHC-C1C	2.32	131.83	126.34
35	B	620	C7Z	C30-C31-C32	-2.32	115.99	123.22
29	S	611	CLA	O2A-CGA-CBA	2.32	119.17	111.91
29	R	612	CLA	C4B-CHC-C1C	2.32	131.83	126.34
31	B	618	BCR	C33-C5-C6	-2.31	121.93	124.53
29	y	611	CLA	C4B-CHC-C1C	2.31	131.83	126.34
45	R	607	CHL	CHB-C4A-NA	2.31	127.71	124.51
45	G	601	CHL	C1-C2-C3	-2.31	122.04	126.04
29	r	602	CLA	O2A-CGA-CBA	2.31	119.17	111.91
29	c	511	CLA	CHA-C1A-NA	-2.31	121.10	126.40
29	b	617	CLA	C4B-CHC-C1C	2.31	131.83	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	N	621	LUT	C35-C15-C14	-2.31	118.73	123.47
46	y	620	LUT	C39-C29-C28	2.31	121.72	118.08
29	B	603	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	B	611	CLA	CHA-C1A-NA	-2.31	121.10	126.40
29	Y	612	CLA	C3B-C4B-NB	-2.31	108.37	110.52
29	S	613	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	Y	604	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
29	Y	613	CLA	C4B-CHC-C1C	2.31	131.82	126.34
31	c	514	BCR	C33-C5-C4	2.31	118.06	113.62
29	Y	608	CLA	O2A-CGA-CBA	2.31	119.16	111.91
30	A	408	PHO	O1D-CGD-CBD	2.31	128.59	124.74
32	C	526	SQD	O3-C3-C2	-2.31	105.01	110.35
29	c	507	CLA	CMA-C3A-C4A	2.31	117.98	111.77
29	S	609	CLA	C4B-CHC-C1C	2.31	131.82	126.34
29	r	611	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
29	B	615	CLA	C2D-C1D-ND	2.31	111.81	110.10
29	A	406	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
29	C	510	CLA	O2A-CGA-CBA	2.31	119.15	111.91
29	r	611	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
29	G	610	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
29	c	510	CLA	O2A-CGA-CBA	2.31	119.15	111.91
29	c	508	CLA	CHA-C4D-ND	2.31	137.32	132.50
48	s	623	NEX	C26-C27-C28	-2.31	121.12	125.99
29	C	513	CLA	C4B-CHC-C1C	2.31	131.81	126.34
29	N	613	CLA	C4B-CHC-C1C	2.31	131.81	126.34
29	S	617	CLA	C4B-CHC-C1C	2.31	131.81	126.34
29	G	610	CLA	CHA-C4D-ND	2.31	137.32	132.50
29	g	603	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
29	c	505	CLA	C3B-C4B-NB	-2.30	108.38	110.52
29	r	609	CLA	C4B-CHC-C1C	2.30	131.80	126.34
45	s	608	CHL	C1-C2-C3	-2.30	122.06	126.04
29	C	505	CLA	C3B-C4B-NB	-2.30	108.38	110.52
29	Y	604	CLA	C4B-CHC-C1C	2.30	131.80	126.34
31	b	619	BCR	C19-C18-C17	2.30	122.47	118.94
29	G	602	CLA	C3B-C4B-NB	-2.30	108.38	110.52
29	R	608	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
29	Y	603	CLA	C4B-CHC-C1C	2.30	131.80	126.34
44	h	101	RRX	C38-C26-C25	-2.30	121.94	124.53
31	C	514	BCR	C34-C9-C10	-2.30	119.70	122.92
46	s	620	LUT	C39-C29-C28	2.30	121.70	118.08
29	g	613	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
29	s	617	CLA	C4B-CHC-C1C	2.30	131.79	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	604	CLA	C1D-ND-C4D	-2.30	104.70	106.33
42	d	405	PL9	C20-C19-C21	2.30	119.14	115.27
42	d	405	PL9	C27-C28-C29	-2.30	122.12	127.66
29	A	405	CLA	C2C-C1C-NC	2.30	112.13	109.97
29	n	604	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
48	N	623	NEX	C4-C3-C2	2.30	115.21	110.77
45	n	605	CHL	C2B-C1B-NB	-2.30	108.69	110.23
45	r	606	CHL	C2B-C1B-NB	-2.30	108.69	110.23
29	B	602	CLA	C3B-C4B-NB	-2.30	108.38	110.52
29	c	502	CLA	C4B-CHC-C1C	2.30	131.79	126.34
46	s	620	LUT	C31-C32-C33	-2.30	119.96	126.42
29	a	405	CLA	CMA-C3A-C4A	2.30	117.95	111.77
29	s	613	CLA	C3B-C4B-NB	-2.30	108.38	110.52
29	S	603	CLA	CHA-C1A-NA	-2.30	121.14	126.40
29	d	402	CLA	CAC-C3C-C4C	2.30	127.79	124.81
29	B	616	CLA	C4B-CHC-C1C	2.30	131.78	126.34
29	N	613	CLA	C3B-C4B-NB	-2.29	108.39	110.52
29	R	603	CLA	C4B-CHC-C1C	2.29	131.78	126.34
29	N	604	CLA	C3B-C4B-NB	-2.29	108.39	110.52
32	A	412	SQD	O3-C3-C2	-2.29	105.05	110.35
29	b	616	CLA	C4B-CHC-C1C	2.29	131.78	126.34
29	s	603	CLA	C4B-CHC-C1C	2.29	131.78	126.34
29	y	612	CLA	C4B-CHC-C1C	2.29	131.78	126.34
30	A	409	PHO	C1C-C2C-C3C	-2.29	106.70	108.61
29	c	513	CLA	C4B-CHC-C1C	2.29	131.77	126.34
45	y	605	CHL	C2B-C1B-NB	-2.29	108.70	110.23
46	G	620	LUT	C38-C25-C24	-2.29	118.66	123.56
29	b	603	CLA	C4B-CHC-C1C	2.29	131.77	126.34
29	c	502	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
29	a	405	CLA	C4B-CHC-C1C	2.29	131.77	126.34
29	a	410	CLA	C4B-CHC-C1C	2.29	131.77	126.34
29	r	613	CLA	C4B-CHC-C1C	2.29	131.76	126.34
45	y	605	CHL	CHB-C4A-NA	2.29	127.68	124.51
29	r	613	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
45	y	607	CHL	C3B-C4B-NB	-2.29	108.39	110.52
29	S	603	CLA	C4B-CHC-C1C	2.29	131.76	126.34
45	g	606	CHL	C4D-CHA-C1A	2.29	124.03	121.25
46	Y	620	LUT	C35-C34-C33	-2.29	124.05	127.31
29	G	613	CLA	C4B-CHC-C1C	2.29	131.76	126.34
29	y	603	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
29	N	603	CLA	C4B-CHC-C1C	2.29	131.76	126.34
29	C	512	CLA	CHA-C4D-ND	2.29	137.28	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	y	621	LUT	C16-C1-C6	-2.28	106.59	110.30
29	S	611	CLA	C4B-CHC-C1C	2.28	131.76	126.34
29	g	611	CLA	C4B-CHC-C1C	2.28	131.76	126.34
29	n	603	CLA	C1D-ND-C4D	-2.28	104.71	106.33
31	C	517	BCR	C34-C9-C10	-2.28	119.72	122.92
29	a	406	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
29	A	410	CLA	C4B-CHC-C1C	2.28	131.76	126.34
32	c	626	SQD	O3-C3-C2	-2.28	105.07	110.35
29	n	614	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	C	509	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
47	g	622	XAT	O24-C25-C24	2.28	115.10	113.38
29	d	402	CLA	C2C-C1C-NC	2.28	112.11	109.97
29	A	407	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	r	613	CLA	CMA-C3A-C4A	2.28	117.91	111.77
29	G	602	CLA	C1D-ND-C4D	-2.28	104.71	106.33
29	B	610	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	B	615	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	B	613	CLA	C1-C2-C3	-2.28	122.10	126.04
29	R	613	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	A	405	CLA	C1-O2A-CGA	2.28	122.43	116.44
29	G	610	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
29	Y	612	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	s	602	CLA	C3B-C4B-NB	-2.28	108.40	110.52
29	C	503	CLA	C1D-ND-C4D	-2.28	104.72	106.33
29	c	510	CLA	C1D-ND-C4D	-2.28	104.72	106.33
45	n	609	CHL	CHD-C4C-C3C	2.28	128.19	124.84
29	g	604	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	c	503	CLA	O2A-CGA-CBA	2.28	119.06	111.91
45	n	606	CHL	C4D-CHA-C1A	2.28	124.02	121.25
29	S	603	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
29	N	613	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
29	B	616	CLA	CHA-C1A-NA	-2.28	121.18	126.40
46	S	621	LUT	C11-C10-C9	-2.28	124.06	127.31
29	n	610	CLA	C1D-ND-C4D	-2.28	104.72	106.33
29	D	402	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
45	y	606	CHL	C1-C2-C3	-2.28	122.11	126.04
29	y	602	CLA	C1D-ND-C4D	-2.28	104.72	106.33
45	Y	606	CHL	C1-O2A-CGA	2.28	122.42	116.44
29	r	603	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
29	B	612	CLA	CHA-C1A-NA	-2.28	121.19	126.40
45	G	605	CHL	C4D-CHA-C1A	2.28	124.02	121.25
48	N	623	NEX	C19-C9-C10	-2.28	119.74	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	612	CLA	CHA-C1A-NA	-2.27	121.19	126.40
31	c	516	BCR	C31-C1-C6	-2.27	106.61	110.30
29	c	510	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
29	G	610	CLA	C4B-CHC-C1C	2.27	131.73	126.34
29	N	604	CLA	O2A-CGA-CBA	2.27	119.04	111.91
31	b	618	BCR	C34-C9-C10	-2.27	119.74	122.92
29	y	610	CLA	C3B-C4B-NB	-2.27	108.41	110.52
29	C	504	CLA	O2A-CGA-CBA	2.27	119.04	111.91
39	n	624	LHG	O8-C23-C24	2.27	119.04	111.91
29	n	612	CLA	CHA-C1A-NA	-2.27	121.19	126.40
35	B	620	C7Z	C7-C8-C9	-2.27	122.80	126.23
29	C	501	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
29	B	604	CLA	C3B-C4B-NB	-2.27	108.41	110.52
29	b	615	CLA	C4B-CHC-C1C	2.27	131.73	126.34
31	C	516	BCR	C37-C22-C23	2.27	121.66	118.08
29	s	611	CLA	O2A-CGA-CBA	2.27	119.04	111.91
45	N	608	CHL	C1-O2A-CGA	2.27	122.40	116.44
29	B	614	CLA	C1D-ND-C4D	-2.27	104.72	106.33
45	Y	605	CHL	C2B-C1B-NB	-2.27	108.71	110.23
29	b	611	CLA	CHA-C1A-NA	-2.27	121.20	126.40
29	N	604	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
29	y	613	CLA	C1D-ND-C4D	-2.27	104.72	106.33
29	a	410	CLA	C3B-C4B-NB	-2.27	108.41	110.52
42	d	405	PL9	C31-C32-C33	-2.27	104.42	111.88
29	C	507	CLA	C1-C2-C3	-2.27	122.12	126.04
29	B	604	CLA	C4B-CHC-C1C	2.27	131.72	126.34
29	y	614	CLA	O2A-CGA-CBA	2.27	119.03	111.91
29	B	611	CLA	CMA-C3A-C4A	2.27	117.87	111.77
29	b	616	CLA	CHA-C1A-NA	-2.27	121.20	126.40
48	N	623	NEX	C40-C33-C34	-2.27	119.75	122.92
45	N	609	CHL	CHB-C4A-NA	2.27	127.65	124.51
29	g	614	CLA	O2A-CGA-CBA	2.27	119.02	111.91
29	g	610	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
45	y	609	CHL	CHD-C4C-C3C	2.27	128.17	124.84
29	y	604	CLA	CMA-C3A-C4A	2.27	117.86	111.77
31	c	517	BCR	C2-C1-C6	2.27	113.97	110.48
29	R	603	CLA	O2A-CGA-CBA	2.27	119.02	111.91
42	d	405	PL9	O1-C4-C3	-2.27	118.22	120.72
29	b	607	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
29	S	614	CLA	C4B-CHC-C1C	2.27	131.71	126.34
29	R	602	CLA	C1D-ND-C4D	-2.26	104.73	106.33
29	S	602	CLA	C1D-ND-C4D	-2.26	104.73	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	602	CLA	C1D-ND-C4D	-2.26	104.73	106.33
43	f	101	HEM	CHC-C1C-NC	2.26	126.89	124.44
48	g	623	NEX	C1-C2-C3	2.26	118.76	113.64
29	c	512	CLA	O2A-CGA-CBA	2.26	119.01	111.91
29	G	604	CLA	C4B-CHC-C1C	2.26	131.71	126.34
29	r	604	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	y	610	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
32	B	621	SQD	O3-C3-C2	-2.26	105.12	110.35
39	d	410	LHG	C5-O7-C7	-2.26	112.22	117.79
45	N	605	CHL	C2B-C1B-NB	-2.26	108.72	110.23
29	B	603	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
29	G	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	b	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	s	617	CLA	C1D-ND-C4D	-2.26	104.73	106.33
29	g	602	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
31	c	517	BCR	C15-C14-C13	-2.26	124.09	127.31
45	G	609	CHL	C2B-C1B-NB	-2.26	108.72	110.23
32	a	412	SQD	O3-C3-C2	-2.26	105.13	110.35
29	s	604	CLA	C4B-CHC-C1C	2.26	131.69	126.34
29	Y	610	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
29	C	510	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
29	G	613	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	Y	614	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	c	501	CLA	C1D-ND-C4D	-2.26	104.73	106.33
47	g	622	XAT	C18-C5-C6	-2.26	118.48	122.26
29	r	610	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
29	R	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	g	604	CLA	C3B-C4B-NB	-2.26	108.42	110.52
29	a	406	CLA	C4B-CHC-C1C	2.25	131.69	126.34
29	A	406	CLA	O2A-CGA-CBA	2.25	118.98	111.91
29	d	403	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
29	R	609	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
29	c	512	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
29	r	604	CLA	C4B-CHC-C1C	2.25	131.68	126.34
45	n	606	CHL	CHB-C4A-NA	2.25	127.63	124.51
29	B	602	CLA	O2A-CGA-CBA	2.25	118.98	111.91
29	Y	604	CLA	C3B-C4B-NB	-2.25	108.42	110.52
48	Y	623	NEX	C1-C2-C3	2.25	118.73	113.64
29	r	612	CLA	CHA-C1A-NA	-2.25	121.24	126.40
29	B	603	CLA	C2D-C1D-ND	2.25	111.76	110.10
29	C	507	CLA	CMA-C3A-C4A	2.25	117.83	111.77
29	g	604	CLA	O2A-CGA-CBA	2.25	118.97	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	g	601	CHL	C1-C2-C3	-2.25	122.15	126.04
48	y	623	NEX	C31-C30-C29	2.25	130.52	127.31
29	c	503	CLA	CHA-C1A-NA	-2.25	121.24	126.40
39	D	408	LHG	C6-C5-C4	-2.25	106.47	111.79
29	C	505	CLA	C2D-C1D-ND	2.25	111.76	110.10
29	r	603	CLA	O2A-CGA-CBA	2.25	118.97	111.91
45	S	608	CHL	C4D-CHA-C1A	2.25	123.99	121.25
48	g	623	NEX	C16-C1-C6	-2.25	108.46	110.47
29	C	507	CLA	C1-O2A-CGA	2.25	122.34	116.44
29	r	613	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
45	G	608	CHL	C4A-NA-C1A	2.25	107.72	106.71
45	g	607	CHL	C4D-CHA-C1A	2.25	123.98	121.25
29	y	603	CLA	C1-C2-C3	-2.25	122.16	126.04
30	a	408	PHO	C1-C2-C3	-2.25	122.16	126.04
42	D	405	PL9	C31-C32-C33	-2.25	104.49	111.88
48	y	623	NEX	C20-C13-C14	-2.25	119.77	122.92
45	g	607	CHL	C1-O2A-CGA	2.25	122.34	116.44
29	s	602	CLA	C4B-CHC-C1C	2.25	131.67	126.34
46	s	621	LUT	C10-C11-C12	-2.25	116.20	123.22
29	A	405	CLA	C4B-CHC-C1C	2.25	131.67	126.34
46	y	620	LUT	C11-C10-C9	-2.25	124.10	127.31
29	G	614	CLA	O2A-CGA-CBA	2.25	118.96	111.91
29	Y	611	CLA	C3B-C4B-NB	-2.25	108.43	110.52
29	R	608	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
46	n	621	LUT	C8-C7-C6	-2.25	120.89	127.20
29	s	605	CLA	C4B-CHC-C1C	2.25	131.67	126.34
29	s	612	CLA	C1D-ND-C4D	-2.25	104.74	106.33
29	C	509	CLA	O2A-CGA-CBA	2.24	118.95	111.91
29	b	608	CLA	C1-C2-C3	-2.24	122.16	126.04
29	s	614	CLA	CHA-C1A-NA	-2.24	121.26	126.40
29	c	501	CLA	O2A-CGA-CBA	2.24	118.95	111.91
29	R	602	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
46	n	620	LUT	C7-C8-C9	-2.24	122.84	126.23
45	N	609	CHL	C4D-CHA-C1A	2.24	123.98	121.25
45	G	605	CHL	C4A-NA-C1A	2.24	107.71	106.71
29	n	604	CLA	O2A-CGA-CBA	2.24	118.94	111.91
29	c	512	CLA	CMA-C3A-C4A	2.24	117.80	111.77
46	s	621	LUT	C11-C10-C9	-2.24	124.11	127.31
29	c	504	CLA	O2A-CGA-CBA	2.24	118.94	111.91
29	Y	614	CLA	O2A-CGA-CBA	2.24	118.94	111.91
29	R	603	CLA	CHA-C1A-NA	-2.24	121.27	126.40
29	G	604	CLA	C3B-C4B-NB	-2.24	108.44	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	N	612	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
47	n	622	XAT	C19-C9-C10	-2.24	119.79	122.92
48	r	623	NEX	C40-C33-C34	-2.24	119.79	122.92
46	Y	621	LUT	C35-C34-C33	-2.24	124.12	127.31
29	g	613	CLA	C1-O2A-CGA	2.24	122.31	116.44
29	b	611	CLA	O2A-CGA-CBA	2.24	118.93	111.91
29	B	617	CLA	C4B-CHC-C1C	2.24	131.64	126.34
45	G	608	CHL	C2B-C1B-NB	-2.24	108.73	110.23
45	r	607	CHL	C2B-C1B-NB	-2.24	108.73	110.23
29	N	604	CLA	C4B-CHC-C1C	2.24	131.64	126.34
29	g	604	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
29	B	607	CLA	C3B-C4B-NB	-2.23	108.44	110.52
29	b	605	CLA	O2A-CGA-CBA	2.23	118.92	111.91
45	n	609	CHL	C4D-CHA-C1A	2.23	123.97	121.25
39	y	624	LHG	C6-C5-C4	-2.23	106.50	111.79
32	b	621	SQD	O3-C3-C2	-2.23	105.19	110.35
45	Y	605	CHL	CHB-C4A-NA	2.23	127.60	124.51
29	B	613	CLA	O2A-CGA-CBA	2.23	118.91	111.91
29	n	613	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
48	n	623	NEX	C38-C25-C26	-2.23	118.52	122.26
47	N	622	XAT	C39-C29-C30	-2.23	119.80	122.92
29	n	610	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
29	R	608	CLA	CHA-C1A-NA	-2.23	121.29	126.40
31	D	404	BCR	C27-C26-C25	-2.23	119.49	122.73
29	n	614	CLA	CHA-C1A-NA	-2.23	121.29	126.40
29	c	506	CLA	C4B-CHC-C1C	2.23	131.63	126.34
29	A	405	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
29	R	613	CLA	CHA-C1A-NA	-2.23	121.29	126.40
45	N	601	CHL	C2B-C1B-NB	-2.23	108.74	110.23
31	B	618	BCR	C33-C5-C4	2.23	117.90	113.62
31	b	618	BCR	C2-C1-C6	2.23	113.91	110.48
33	A	413	LMG	C7-O1-C1	-2.23	109.38	113.74
29	s	617	CLA	CHA-C1A-NA	-2.23	121.29	126.40
29	c	509	CLA	C4B-CHC-C1C	2.23	131.62	126.34
29	r	612	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
29	b	615	CLA	C2A-C1A-CHA	2.23	127.75	123.86
29	b	604	CLA	C3B-C4B-NB	-2.23	108.45	110.52
29	N	604	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
29	r	602	CLA	C3B-C4B-NB	-2.23	108.45	110.52
35	b	620	C7Z	C19-C9-C10	-2.23	119.80	122.92
29	b	603	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
29	D	403	CLA	CAA-C2A-C3A	-2.23	106.68	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	504	CLA	C4B-CHC-C1C	2.23	131.62	126.34
29	r	603	CLA	CHA-C1A-NA	-2.23	121.30	126.40
45	y	609	CHL	C1-C2-C3	-2.23	122.19	126.04
29	N	610	CLA	C3B-C4B-NB	-2.23	108.45	110.52
35	B	620	C7Z	C19-C9-C10	-2.23	119.81	122.92
35	b	620	C7Z	C30-C31-C32	-2.23	116.27	123.22
29	R	613	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
29	c	504	CLA	C1D-ND-C4D	-2.23	104.75	106.33
46	y	620	LUT	C18-C5-C6	-2.23	122.03	124.53
29	C	507	CLA	O2A-CGA-CBA	2.23	118.89	111.91
31	c	517	BCR	C35-C13-C12	2.22	121.58	118.08
29	A	406	CLA	C4B-CHC-C1C	2.22	131.61	126.34
29	b	610	CLA	C4B-CHC-C1C	2.22	131.61	126.34
29	Y	612	CLA	CMA-C3A-C4A	2.22	117.75	111.77
29	A	407	CLA	C1D-ND-C4D	-2.22	104.76	106.33
29	c	502	CLA	CHA-C1A-NA	-2.22	121.31	126.40
31	C	517	BCR	C33-C5-C4	2.22	117.88	113.62
29	C	504	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
29	S	612	CLA	C3B-C4B-NB	-2.22	108.45	110.52
29	C	510	CLA	C4B-CHC-C1C	2.22	131.61	126.34
29	s	614	CLA	C4B-CHC-C1C	2.22	131.61	126.34
42	D	405	PL9	C27-C28-C29	-2.22	122.31	127.66
45	g	608	CHL	C2B-C1B-NB	-2.22	108.74	110.23
29	B	614	CLA	C4B-CHC-C1C	2.22	131.61	126.34
29	G	613	CLA	C3B-C4B-NB	-2.22	108.45	110.52
29	g	611	CLA	C3B-C4B-NB	-2.22	108.45	110.52
29	Y	613	CLA	C1-O2A-CGA	2.22	122.27	116.44
47	g	622	XAT	C20-C13-C14	-2.22	119.81	122.92
29	B	607	CLA	C2D-C1D-ND	2.22	111.74	110.10
29	b	613	CLA	O2A-CGA-CBA	2.22	118.87	111.91
29	R	612	CLA	CMA-C3A-C4A	2.22	117.74	111.77
29	r	604	CLA	CMA-C3A-C4A	2.22	117.74	111.77
29	B	604	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
29	B	613	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
29	y	612	CLA	CHA-C1A-NA	-2.22	121.32	126.40
29	B	615	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
45	g	609	CHL	C2B-C1B-NB	-2.22	108.75	110.23
29	s	610	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
29	S	610	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
47	n	622	XAT	C40-C33-C34	-2.22	119.82	122.92
29	N	614	CLA	C3B-C4B-NB	-2.22	108.46	110.52
29	B	613	CLA	C1D-ND-C4D	-2.22	104.76	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	R	604	CLA	O2A-CGA-CBA	2.22	118.86	111.91
47	r	622	XAT	C12-C13-C14	2.22	122.34	118.94
29	Y	608	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
29	B	613	CLA	C4B-CHC-C1C	2.22	131.60	126.34
29	c	507	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
29	b	614	CLA	O2A-CGA-CBA	2.22	118.86	111.91
29	S	605	CLA	CHA-C1A-NA	-2.22	121.32	126.40
31	c	516	BCR	C33-C5-C4	2.22	117.87	113.62
29	b	604	CLA	C2D-C1D-ND	2.22	111.74	110.10
47	y	622	XAT	C19-C9-C10	-2.22	119.82	122.92
29	s	617	CLA	C3B-C4B-NB	-2.22	108.46	110.52
29	G	613	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
29	b	610	CLA	C1D-ND-C4D	-2.21	104.76	106.33
29	n	603	CLA	OBD-CAD-C3D	-2.21	123.19	128.52
29	B	614	CLA	C1-O2A-CGA	2.21	122.25	116.44
29	C	512	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
45	y	606	CHL	C4D-CHA-C1A	2.21	123.94	121.25
31	C	517	BCR	C35-C13-C12	2.21	121.56	118.08
29	c	501	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
29	y	603	CLA	O2A-CGA-CBA	2.21	118.85	111.91
29	A	407	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
45	g	609	CHL	CHC-C1C-NC	2.21	127.56	124.20
45	g	608	CHL	C4A-NA-C1A	2.21	107.70	106.71
47	G	622	XAT	C18-C5-C6	-2.21	118.56	122.26
29	R	604	CLA	CMA-C3A-C4A	2.21	117.71	111.77
29	R	604	CLA	C4B-CHC-C1C	2.21	131.58	126.34
29	b	611	CLA	CMA-C3A-C4A	2.21	117.71	111.77
45	n	606	CHL	C2B-C1B-NB	-2.21	108.75	110.23
29	b	602	CLA	O2A-CGA-CBA	2.21	118.84	111.91
29	s	612	CLA	CHA-C1A-NA	-2.21	121.34	126.40
29	B	605	CLA	O2A-CGA-CBA	2.21	118.83	111.91
29	N	610	CLA	C1D-ND-C4D	-2.21	104.77	106.33
29	C	513	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
29	S	605	CLA	C2A-C1A-CHA	2.21	127.72	123.86
29	B	612	CLA	CHA-C4D-ND	2.21	137.11	132.50
29	R	602	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
47	y	622	XAT	C39-C29-C30	-2.21	119.83	122.92
29	C	502	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
29	Y	610	CLA	C1D-ND-C4D	-2.20	104.77	106.33
29	y	614	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
45	n	608	CHL	C4A-NA-C1A	2.20	107.70	106.71
48	s	623	NEX	C4-C3-C2	2.20	115.03	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	614	CLA	C4B-CHC-C1C	2.20	131.56	126.34
44	H	101	RRX	C35-C13-C14	-2.20	119.84	122.92
29	G	602	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	C	516	BCR	C27-C26-C25	-2.20	119.53	122.73
29	a	407	CLA	C1D-ND-C4D	-2.20	104.77	106.33
29	n	603	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
42	D	405	PL9	O1-C4-C3	-2.20	118.29	120.72
46	Y	620	LUT	C30-C31-C32	-2.20	116.34	123.22
29	S	614	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	N	604	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
31	b	618	BCR	C33-C5-C4	2.20	117.85	113.62
29	c	504	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
45	y	607	CHL	C1-C2-C3	-2.20	122.24	126.04
29	b	613	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
29	S	602	CLA	O2A-CGA-CBA	2.20	118.81	111.91
45	G	605	CHL	C2B-C1B-NB	-2.20	108.76	110.23
45	R	607	CHL	C2B-C1B-NB	-2.20	108.76	110.23
29	r	602	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
29	B	603	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	n	611	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	g	604	CLA	CMA-C3A-C4A	2.20	117.68	111.77
29	s	614	CLA	C3B-C4B-NB	-2.20	108.48	110.52
45	G	601	CHL	C4A-NA-C1A	2.20	107.69	106.71
29	a	405	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	Y	604	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
29	B	606	CLA	C4B-CHC-C1C	2.20	131.55	126.34
45	R	606	CHL	C2B-C1B-NB	-2.20	108.76	110.23
29	R	612	CLA	CHA-C1A-NA	-2.20	121.37	126.40
29	g	604	CLA	CHA-C1A-NA	-2.20	121.37	126.40
38	c	519	DGD	C2G-O2G-C1B	-2.20	112.39	117.79
29	r	603	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
29	R	610	CLA	CHA-C1A-NA	-2.20	121.37	126.40
29	b	607	CLA	C3B-C4B-NB	-2.19	108.48	110.52
45	g	606	CHL	C3B-C4B-NB	-2.19	108.48	110.52
29	s	605	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	C	509	CLA	C4B-CHC-C1C	2.19	131.54	126.34
29	a	407	CLA	C3B-C4B-NB	-2.19	108.48	110.52
29	S	609	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	C	512	CLA	O2A-CGA-CBA	2.19	118.78	111.91
29	r	613	CLA	C1D-ND-C4D	-2.19	104.78	106.33
29	B	608	CLA	C4B-CHC-C1C	2.19	131.53	126.34
31	d	404	BCR	C1-C6-C5	-2.19	119.53	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	405	CLA	CAC-C3C-C4C	2.19	127.65	124.81
46	Y	621	LUT	C16-C1-C6	-2.19	106.75	110.30
46	s	621	LUT	C1-C6-C5	-2.19	119.53	122.61
29	C	506	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
29	r	610	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
29	C	504	CLA	C4B-CHC-C1C	2.19	131.53	126.34
29	C	505	CLA	C4B-CHC-C1C	2.19	131.53	126.34
29	n	603	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
29	B	610	CLA	C1D-ND-C4D	-2.19	104.78	106.33
29	s	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	c	507	CLA	C1-O2A-CGA	2.19	122.18	116.44
46	n	621	LUT	C19-C9-C8	2.19	121.52	118.08
29	G	611	CLA	C3B-C4B-NB	-2.18	108.49	110.52
43	f	101	HEM	C3C-C2C-C1C	2.18	109.16	107.08
29	c	506	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
29	b	602	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	n	614	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	g	610	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	y	608	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
29	G	612	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	N	611	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
29	b	609	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
29	B	609	CLA	CHD-C1D-ND	-2.18	122.45	124.45
29	S	611	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	r	613	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	y	608	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
29	b	612	CLA	C1C-C2C-C3C	-2.18	104.66	106.96
31	B	618	BCR	C34-C9-C10	-2.18	119.87	122.92
45	n	601	CHL	C2B-C1B-NB	-2.18	108.77	110.23
45	s	608	CHL	C2B-C1B-NB	-2.18	108.77	110.23
29	G	614	CLA	C1D-ND-C4D	-2.18	104.79	106.33
29	y	610	CLA	C1D-ND-C4D	-2.18	104.79	106.33
29	b	605	CLA	C4B-CHC-C1C	2.18	131.51	126.34
29	g	610	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
29	N	611	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	S	609	CLA	C3B-C4B-NB	-2.18	108.49	110.52
31	b	618	BCR	C38-C26-C25	-2.18	122.08	124.53
43	F	101	HEM	CAC-C3C-C4C	2.18	130.16	124.90
46	G	620	LUT	C10-C11-C12	-2.18	116.42	123.22
29	b	616	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
29	B	607	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
29	B	607	CLA	C4B-CHC-C1C	2.18	131.50	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	603	CLA	C1-O2A-CGA	2.18	122.16	116.44
29	b	614	CLA	C1D-ND-C4D	-2.18	104.79	106.33
29	c	503	CLA	C1D-ND-C4D	-2.18	104.79	106.33
29	S	610	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	r	610	CLA	C1C-C2C-C3C	-2.18	104.67	106.96
29	s	612	CLA	C3B-C4B-NB	-2.18	108.50	110.52
29	Y	603	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
29	C	506	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
45	r	607	CHL	CHD-C4C-C3C	2.18	128.04	124.84
48	g	623	NEX	C19-C9-C10	-2.18	119.88	122.92
29	b	606	CLA	C4B-CHC-C1C	2.18	131.50	126.34
29	Y	613	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
29	c	512	CLA	C1-O2A-CGA	2.17	122.15	116.44
29	R	611	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	r	608	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	S	609	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
29	S	610	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
29	n	610	CLA	C3B-C4B-NB	-2.17	108.50	110.52
29	R	610	CLA	O2A-CGA-CBA	2.17	118.73	111.91
44	H	101	RRX	C38-C26-C25	-2.17	122.09	124.53
29	N	612	CLA	CHA-C1A-NA	-2.17	121.42	126.40
29	B	617	CLA	C3B-C4B-NB	-2.17	108.50	110.52
29	B	614	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
29	Y	608	CLA	C1-O2A-CGA	2.17	122.14	116.44
29	C	502	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	Y	608	CLA	C4B-CHC-C1C	2.17	131.49	126.34
29	b	608	CLA	C4B-CHC-C1C	2.17	131.48	126.34
29	A	405	CLA	C1D-ND-C4D	-2.17	104.79	106.33
29	n	612	CLA	C1D-ND-C4D	-2.17	104.79	106.33
48	g	623	NEX	C4-C3-C2	2.17	114.96	110.77
29	C	510	CLA	C3B-C4B-NB	-2.17	108.50	110.52
29	y	608	CLA	C4B-CHC-C1C	2.17	131.48	126.34
29	c	506	CLA	O2A-CGA-CBA	2.17	118.71	111.91
48	N	623	NEX	C26-C27-C28	-2.17	121.41	125.99
29	C	503	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	s	610	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	c	501	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
29	y	608	CLA	CHA-C1A-NA	-2.17	121.44	126.40
48	s	623	NEX	C31-C30-C29	2.17	130.40	127.31
29	s	617	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
29	N	613	CLA	C1D-ND-C4D	-2.17	104.80	106.33
51	Y	625	SPH	C3-C4-C5	-2.17	119.96	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	s	620	LUT	C20-C13-C12	2.17	121.49	118.08
29	a	407	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
45	Y	605	CHL	C4D-CHA-C1A	2.17	123.89	121.25
29	s	610	CLA	C1-C2-C3	-2.17	122.30	126.04
29	y	611	CLA	CHA-C1A-NA	-2.17	121.44	126.40
29	S	604	CLA	C4B-CHC-C1C	2.17	131.47	126.34
29	n	604	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
29	N	614	CLA	O2A-CGA-CBA	2.16	118.70	111.91
29	b	609	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	b	603	CLA	CHA-C1A-NA	-2.16	121.44	126.40
29	C	505	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
46	N	621	LUT	C10-C11-C12	-2.16	116.46	123.22
29	y	603	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
43	f	101	HEM	CAC-C3C-C4C	2.16	130.12	124.90
29	Y	602	CLA	C1-C2-C3	-2.16	122.30	126.04
29	A	405	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
29	R	603	CLA	C3B-C4B-NB	-2.16	108.51	110.52
29	G	610	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
29	B	609	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
29	G	603	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
29	S	613	CLA	C3B-C4B-NB	-2.16	108.51	110.52
45	S	607	CHL	C2B-C1B-NB	-2.16	108.78	110.23
39	n	624	LHG	C6-C5-C4	-2.16	106.68	111.79
29	r	604	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
29	g	614	CLA	C1D-ND-C4D	-2.16	104.80	106.33
29	g	610	CLA	CHA-C1A-NA	-2.16	121.45	126.40
29	D	402	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
29	y	613	CLA	C3B-C4B-NB	-2.16	108.51	110.52
31	c	515	BCR	C38-C26-C25	-2.16	122.10	124.53
29	C	503	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
29	C	509	CLA	CHA-C1A-NA	-2.16	121.45	126.40
29	S	612	CLA	CHA-C1A-NA	-2.16	121.45	126.40
29	s	617	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
47	N	622	XAT	C26-C27-C28	-2.16	121.43	125.99
29	G	611	CLA	CHA-C1A-NA	-2.16	121.46	126.40
29	g	604	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
29	C	507	CLA	C3B-C4B-NB	-2.16	108.52	110.52
45	g	607	CHL	C4A-NA-C1A	2.16	107.67	106.71
29	b	613	CLA	C4B-CHC-C1C	2.16	131.45	126.34
29	g	613	CLA	C3B-C4B-NB	-2.15	108.52	110.52
29	y	604	CLA	C1D-ND-C4D	-2.15	104.81	106.33
46	G	620	LUT	C31-C32-C33	-2.15	120.37	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	y	604	CLA	O2A-CGA-CBA	2.15	118.67	111.91
29	C	512	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	Y	604	CLA	O2A-CGA-CBA	2.15	118.66	111.91
29	B	611	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
29	g	611	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	r	602	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	r	602	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	G	603	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	B	607	CLA	C1-C2-C3	-2.15	122.32	126.04
29	c	510	CLA	C4B-CHC-C1C	2.15	131.44	126.34
29	r	604	CLA	O2A-CGA-CBA	2.15	118.66	111.91
29	N	610	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
29	R	604	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
29	c	502	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
29	C	504	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	B	609	CLA	C4B-CHC-C1C	2.15	131.44	126.34
29	b	603	CLA	C3B-C4B-NB	-2.15	108.52	110.52
45	Y	601	CHL	CHC-C1C-NC	2.15	127.46	124.20
29	Y	603	CLA	CHA-C1A-NA	-2.15	121.48	126.40
45	Y	606	CHL	C4D-CHA-C1A	2.15	123.86	121.25
51	y	625	SPH	C3-C4-C5	-2.15	120.00	124.79
29	c	509	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	S	613	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
47	Y	622	XAT	C18-C5-C6	-2.15	118.66	122.26
29	b	604	CLA	C4B-CHC-C1C	2.15	131.43	126.34
31	c	517	BCR	C33-C5-C6	-2.15	122.12	124.53
29	C	508	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	r	610	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
29	s	605	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
29	R	613	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
46	n	620	LUT	C15-C35-C34	-2.15	119.08	123.47
29	b	611	CLA	C3D-C2D-C1D	-2.14	102.90	105.83
29	R	610	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
31	D	404	BCR	C4-C5-C6	-2.14	119.62	122.73
29	C	502	CLA	C4B-CHC-C1C	2.14	131.42	126.34
47	g	622	XAT	C40-C33-C34	-2.14	119.92	122.92
29	y	611	CLA	C3B-C4B-NB	-2.14	108.53	110.52
29	S	602	CLA	CMC-C2C-C1C	2.14	128.30	125.04
29	S	617	CLA	CHA-C1A-NA	-2.14	121.49	126.40
45	Y	605	CHL	C4A-NA-C1A	2.14	107.67	106.71
45	Y	609	CHL	C4D-CHA-C1A	2.14	123.86	121.25
29	S	612	CLA	C1D-ND-C4D	-2.14	104.81	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	g	622	XAT	C39-C29-C30	-2.14	119.92	122.92
29	c	505	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
29	C	507	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	s	610	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	r	611	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	b	604	CLA	C1-C2-C3	-2.14	122.34	126.04
29	b	610	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	s	613	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	N	603	CLA	C1D-ND-C4D	-2.14	104.81	106.33
29	N	611	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
29	a	405	CLA	C1D-ND-C4D	-2.14	104.82	106.33
29	n	604	CLA	CMA-C3A-C4A	2.14	117.52	111.77
29	B	614	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	B	616	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
29	S	604	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
29	Y	603	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
29	c	505	CLA	C1-O2A-CGA	2.14	122.05	116.44
29	n	613	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
29	s	605	CLA	CHA-C1A-NA	-2.14	121.51	126.40
29	y	610	CLA	CHA-C1A-NA	-2.13	121.51	126.40
29	S	614	CLA	C3B-C4B-NB	-2.13	108.53	110.52
29	B	602	CLA	C1D-ND-C4D	-2.13	104.82	106.33
29	c	507	CLA	O2A-CGA-CBA	2.13	118.60	111.91
29	B	608	CLA	C1-C2-C3	-2.13	122.35	126.04
29	n	612	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
29	Y	608	CLA	CHA-C1A-NA	-2.13	121.51	126.40
45	N	605	CHL	C1-O2A-CGA	2.13	122.04	116.44
45	s	607	CHL	C2B-C1B-NB	-2.13	108.80	110.23
29	n	602	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
45	N	609	CHL	C1-C2-C3	-2.13	122.36	126.04
31	C	516	BCR	C33-C5-C4	2.13	117.71	113.62
29	R	613	CLA	C3B-C4B-NB	-2.13	108.54	110.52
29	c	512	CLA	C3B-C4B-NB	-2.13	108.54	110.52
47	R	621	XAT	C30-C31-C32	-2.13	116.57	123.22
46	s	620	LUT	C36-C21-C26	2.13	112.77	109.55
29	D	403	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	g	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	b	609	CLA	O2A-CGA-CBA	2.13	118.59	111.91
29	C	503	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
45	g	605	CHL	C2B-C1B-NB	-2.13	108.81	110.23
29	Y	604	CLA	C1D-ND-C4D	-2.13	104.82	106.33
29	g	613	CLA	C1D-ND-C4D	-2.13	104.82	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	607	CLA	C4B-CHC-C1C	2.13	131.39	126.34
29	b	617	CLA	C3B-C4B-NB	-2.13	108.54	110.52
45	g	609	CHL	CHB-C4A-NA	2.13	127.45	124.51
46	y	620	LUT	C20-C13-C12	2.13	121.43	118.08
29	r	603	CLA	C3B-C4B-NB	-2.13	108.54	110.52
29	s	604	CLA	CHA-C1A-NA	-2.13	121.53	126.40
29	y	611	CLA	CAA-C2A-C3A	-2.13	106.96	112.78
39	g	624	LHG	C6-C5-C4	-2.13	106.76	111.79
29	N	604	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
29	g	610	CLA	C3B-C4B-NB	-2.12	108.54	110.52
29	s	610	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
29	s	609	CLA	C1D-ND-C4D	-2.12	104.83	106.33
45	g	608	CHL	C4D-CHA-C1A	2.12	123.83	121.25
45	N	606	CHL	C1-C2-C3	-2.12	122.37	126.04
29	b	609	CLA	CHD-C1D-ND	-2.12	122.50	124.45
29	b	614	CLA	CHA-C1A-NA	-2.12	121.54	126.40
29	N	610	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
29	y	613	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
45	S	606	CHL	C2B-C1B-NB	-2.12	108.81	110.23
29	R	602	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
29	n	602	CLA	C3B-C4B-NB	-2.12	108.55	110.52
45	r	606	CHL	CHC-C1C-NC	2.12	127.42	124.20
29	N	603	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
29	B	616	CLA	C2A-C1A-CHA	2.12	127.57	123.86
29	Y	611	CLA	CHA-C1A-NA	-2.12	121.54	126.40
46	n	620	LUT	C11-C10-C9	-2.12	124.28	127.31
29	s	602	CLA	O2A-CGA-CBA	2.12	118.56	111.91
29	s	603	CLA	O2A-CGA-CBA	2.12	118.56	111.91
29	B	616	CLA	C1D-ND-C4D	-2.12	104.83	106.33
29	n	613	CLA	C1D-ND-C4D	-2.12	104.83	106.33
29	b	604	CLA	CHA-C1A-NA	-2.12	121.54	126.40
29	g	612	CLA	CHA-C1A-NA	-2.12	121.54	126.40
35	B	620	C7Z	C35-C15-C14	-2.12	119.13	123.47
29	C	504	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
29	r	609	CLA	C2D-C1D-ND	2.12	111.67	110.10
45	N	605	CHL	C4D-CHA-C1A	2.12	123.83	121.25
29	S	604	CLA	C1D-ND-C4D	-2.12	104.83	106.33
29	Y	610	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	G	604	CLA	CHA-C1A-NA	-2.12	121.55	126.40
47	r	622	XAT	C39-C29-C28	2.12	121.41	118.08
29	n	602	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
29	d	403	CLA	CHA-C1A-NA	-2.12	121.55	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	n	614	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
29	B	612	CLA	C4B-CHC-C1C	2.12	131.36	126.34
29	B	610	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	G	611	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
29	C	501	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
29	B	602	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	S	610	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
29	C	506	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	a	406	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
29	Y	602	CLA	CMC-C2C-C1C	2.11	128.26	125.04
45	g	607	CHL	C3B-C4B-NB	-2.11	108.55	110.52
29	G	604	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
29	C	508	CLA	C1C-C2C-C3C	-2.11	104.73	106.96
45	y	609	CHL	C4A-NA-C1A	2.11	107.66	106.71
29	y	614	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	A	410	CLA	C1D-ND-C4D	-2.11	104.83	106.33
46	n	620	LUT	C19-C9-C8	2.11	121.41	118.08
29	y	608	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	b	617	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	N	603	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	N	614	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	Y	602	CLA	C1-O2A-CGA	2.11	121.98	116.44
48	y	623	NEX	C26-C27-C28	-2.11	121.53	125.99
29	n	604	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	s	610	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
29	s	611	CLA	CHA-C1A-NA	-2.11	121.57	126.40
29	N	603	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
46	N	621	LUT	C16-C1-C6	-2.11	106.88	110.30
46	r	620	LUT	C35-C15-C14	-2.11	119.15	123.47
29	b	605	CLA	C2D-C1D-ND	2.11	111.66	110.10
29	C	511	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
44	h	101	RRX	C1-C6-C7	2.11	121.74	115.78
29	r	610	CLA	CHA-C1A-NA	-2.11	121.57	126.40
29	C	511	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	g	604	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	C	510	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
47	G	622	XAT	C39-C29-C30	-2.11	119.97	122.92
29	n	602	CLA	C1D-ND-C4D	-2.11	104.84	106.33
29	g	602	CLA	C1D-ND-C4D	-2.11	104.84	106.33
31	c	517	BCR	C27-C26-C25	-2.11	119.67	122.73
29	y	602	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
29	y	603	CLA	CHA-C1A-NA	-2.11	121.58	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	S	601	CHL	C4A-NA-C1A	2.10	107.65	106.71
29	N	604	CLA	CHA-C1A-NA	-2.10	121.58	126.40
30	a	409	PHO	C1C-C2C-C3C	-2.10	106.86	108.61
29	c	507	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
29	s	611	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
29	y	610	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
45	Y	607	CHL	C1-C2-C3	-2.10	122.41	126.04
29	B	617	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
45	Y	605	CHL	CHD-C4C-C3C	2.10	127.93	124.84
29	s	613	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
45	Y	609	CHL	C1-C2-C3	-2.10	122.41	126.04
29	a	407	CLA	CHA-C1A-NA	-2.10	121.59	126.40
29	c	508	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
29	S	603	CLA	O2A-CGA-CBA	2.10	118.50	111.91
29	n	612	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
29	B	605	CLA	C2D-C1D-ND	2.10	111.65	110.10
45	G	605	CHL	C1-O2A-CGA	2.10	122.83	116.73
29	C	512	CLA	C3B-C4B-NB	-2.10	108.57	110.52
29	R	604	CLA	C3B-C4B-NB	-2.10	108.57	110.52
29	n	604	CLA	C3B-C4B-NB	-2.10	108.57	110.52
29	c	511	CLA	CAA-CBA-CGA	-2.10	107.12	113.25
29	b	615	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
29	C	507	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
29	b	613	CLA	C1D-ND-C4D	-2.10	104.84	106.33
29	r	603	CLA	C1D-ND-C4D	-2.10	104.84	106.33
45	S	608	CHL	C2B-C1B-NB	-2.10	108.83	110.23
29	S	613	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
29	b	614	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
29	b	605	CLA	C1-O2A-CGA	2.10	121.95	116.44
29	c	502	CLA	O2A-CGA-CBA	2.10	118.49	111.91
29	n	602	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
29	C	511	CLA	C1D-ND-C4D	-2.10	104.84	106.33
29	c	513	CLA	C1D-ND-C4D	-2.10	104.84	106.33
29	c	508	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
29	Y	608	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
29	Y	614	CLA	CHA-C1A-NA	-2.10	121.60	126.40
29	G	612	CLA	C1D-ND-C4D	-2.10	104.85	106.33
45	S	601	CHL	C2B-C1B-NB	-2.10	108.83	110.23
29	B	609	CLA	C1-O2A-CGA	2.10	121.94	116.44
29	B	617	CLA	CHA-C1A-NA	-2.10	121.60	126.40
29	R	611	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
29	a	405	CLA	CAC-C3C-C4C	2.09	127.53	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	511	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
29	y	613	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
29	S	602	CLA	CHA-C1A-NA	-2.09	121.60	126.40
29	a	407	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
29	g	611	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
29	N	614	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
31	c	515	BCR	C35-C13-C12	2.09	121.37	118.08
48	S	622	NEX	C4-C3-C2	2.09	114.81	110.77
29	n	602	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	g	610	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
29	Y	603	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
31	c	516	BCR	C30-C25-C24	2.09	121.70	115.78
29	n	611	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
29	c	505	CLA	C4B-CHC-C1C	2.09	131.30	126.34
29	b	602	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	g	614	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	S	609	CLA	C1D-ND-C4D	-2.09	104.85	106.33
45	n	607	CHL	C3B-C4B-NB	-2.09	108.58	110.52
29	n	610	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
45	G	601	CHL	CHD-C4C-C3C	2.09	127.91	124.84
48	N	623	NEX	O24-C25-C38	-2.09	112.55	115.06
29	r	610	CLA	C6-C7-C8	-2.09	109.17	115.92
29	B	614	CLA	O2A-CGA-CBA	2.09	118.46	111.91
29	S	611	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
29	r	611	CLA	C1D-ND-C4D	-2.09	104.85	106.33
29	g	603	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	y	608	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
46	N	620	LUT	C35-C15-C14	-2.09	119.20	123.47
29	b	609	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
29	C	509	CLA	CMA-C3A-C4A	2.09	117.38	111.77
29	c	502	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
29	a	410	CLA	C1D-ND-C4D	-2.09	104.85	106.33
29	A	407	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	b	614	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
29	C	508	CLA	O2A-CGA-CBA	2.08	118.45	111.91
29	g	612	CLA	C1D-ND-C4D	-2.08	104.85	106.33
29	C	513	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
45	r	606	CHL	C4D-CHA-C1A	2.08	123.79	121.25
29	N	613	CLA	CHA-C1A-NA	-2.08	121.62	126.40
29	A	407	CLA	C1-O2A-CGA	2.08	121.91	116.44
39	G	630	LHG	C6-C5-C4	-2.08	106.86	111.79
45	R	606	CHL	C3A-C2A-C1A	2.08	104.46	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	602	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	s	611	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
46	R	620	LUT	C20-C13-C14	-2.08	120.00	122.92
29	G	603	CLA	O2A-CGA-CBA	2.08	118.44	111.91
29	n	614	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	c	506	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
42	D	405	PL9	C12-C13-C14	-2.08	122.65	127.66
29	b	612	CLA	CMA-C3A-C4A	2.08	117.37	111.77
48	s	623	NEX	C40-C33-C34	-2.08	120.01	122.92
29	b	612	CLA	C4B-CHC-C1C	2.08	131.27	126.34
29	b	609	CLA	C1-O2A-CGA	2.08	121.90	116.44
48	N	623	NEX	C20-C13-C14	-2.08	120.01	122.92
45	y	607	CHL	C4D-CHA-C1A	2.08	123.78	121.25
29	c	508	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	N	602	CLA	C6-C5-C3	-2.08	108.00	113.45
29	S	610	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
29	C	513	CLA	C1D-ND-C4D	-2.08	104.86	106.33
45	n	608	CHL	CHD-C4C-C3C	2.08	127.89	124.84
29	y	604	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	R	610	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
29	G	610	CLA	C3B-C4B-NB	-2.08	108.59	110.52
29	a	405	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
29	R	611	CLA	C1D-ND-C4D	-2.08	104.86	106.33
46	R	620	LUT	C40-C33-C34	-2.08	120.02	122.92
48	N	623	NEX	C31-C30-C29	2.08	130.27	127.31
29	n	614	CLA	C1-O2A-CGA	2.08	121.89	116.44
29	b	608	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
46	r	620	LUT	C22-C23-C24	-2.08	109.38	111.74
29	C	502	CLA	C1D-ND-C4D	-2.07	104.86	106.33
29	G	604	CLA	C1D-ND-C4D	-2.07	104.86	106.33
29	b	607	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
29	g	602	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
29	G	603	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
29	C	506	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
46	r	620	LUT	C20-C13-C14	-2.07	120.02	122.92
29	N	613	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
45	y	605	CHL	C4A-NA-C1A	2.07	107.64	106.71
29	s	604	CLA	CMA-C3A-C4A	2.07	117.34	111.77
29	c	512	CLA	CHA-C1A-NA	-2.07	121.65	126.40
29	B	610	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
29	r	611	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
29	G	610	CLA	C3D-C2D-C1D	-2.07	103.00	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	s	605	CLA	C2A-C1A-CHA	2.07	127.48	123.86
29	N	602	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
45	N	601	CHL	C1-C2-C3	-2.07	122.46	126.04
42	d	405	PL9	C36-C34-C33	-2.07	116.93	121.12
46	s	621	LUT	C31-C32-C33	-2.07	120.60	126.42
46	Y	621	LUT	C2-C3-C4	-2.07	107.47	110.30
29	R	603	CLA	C1D-ND-C4D	-2.07	104.86	106.33
29	a	410	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
29	A	405	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
41	d	401	BCT	O3-C-O1	-2.07	114.18	119.55
29	R	610	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
46	N	621	LUT	C7-C8-C9	-2.07	123.11	126.23
29	Y	614	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
29	C	504	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
45	g	605	CHL	C1-O2A-CGA	2.07	122.74	116.73
29	b	607	CLA	C11-C10-C8	-2.07	109.23	115.92
29	r	604	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
29	A	406	CLA	CHA-C1A-NA	-2.07	121.66	126.40
29	n	604	CLA	CHA-C1A-NA	-2.07	121.66	126.40
29	g	613	CLA	CHA-C1A-NA	-2.07	121.66	126.40
29	N	603	CLA	O2A-CGA-CBA	2.07	118.39	111.91
48	S	622	NEX	C26-C27-C28	-2.07	121.62	125.99
35	b	620	C7Z	C18-C5-C4	2.07	118.18	114.36
29	d	402	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
29	G	613	CLA	C1D-ND-C4D	-2.07	104.87	106.33
29	B	613	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
29	B	614	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
29	c	511	CLA	C1-O2A-CGA	2.07	121.86	116.44
29	G	613	CLA	C1-O2A-CGA	2.07	121.86	116.44
29	B	604	CLA	CHA-C1A-NA	-2.06	121.67	126.40
29	C	508	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
29	S	604	CLA	CMA-C3A-C4A	2.06	117.32	111.77
45	n	605	CHL	C4D-CHA-C1A	2.06	123.76	121.25
47	Y	622	XAT	C39-C29-C30	-2.06	120.03	122.92
35	B	620	C7Z	C2-C3-C4	2.06	113.13	110.30
29	a	406	CLA	C1D-ND-C4D	-2.06	104.87	106.33
29	b	616	CLA	C1D-ND-C4D	-2.06	104.87	106.33
29	r	602	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	n	603	CLA	O2A-CGA-CBA	2.06	118.38	111.91
35	b	620	C7Z	C10-C11-C12	-2.06	116.78	123.22
45	g	601	CHL	CHD-C4C-C3C	2.06	127.87	124.84
29	n	614	CLA	CMD-C2D-C3D	-2.06	122.87	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	R	621	XAT	C39-C29-C28	2.06	121.33	118.08
29	b	610	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	Y	610	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
42	d	405	PL9	C12-C13-C14	-2.06	122.70	127.66
29	c	508	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
29	R	604	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	G	602	CLA	CHA-C1A-NA	-2.06	121.68	126.40
48	r	623	NEX	C20-C13-C14	-2.06	120.04	122.92
29	b	615	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	y	611	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
29	n	602	CLA	CMC-C2C-C1C	2.06	128.17	125.04
45	y	609	CHL	C2B-C1B-NB	-2.06	108.85	110.23
29	B	615	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	y	603	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
31	c	517	BCR	C34-C9-C10	-2.06	120.04	122.92
29	s	610	CLA	C1D-ND-C4D	-2.06	104.87	106.33
29	b	607	CLA	C1-C2-C3	-2.06	122.48	126.04
48	Y	623	NEX	C20-C13-C14	-2.06	120.04	122.92
29	s	613	CLA	O2A-CGA-CBA	2.06	118.36	111.91
45	G	607	CHL	CHD-C4C-C3C	2.06	127.86	124.84
29	N	610	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
29	R	602	CLA	CHA-C1A-NA	-2.06	121.69	126.40
29	c	508	CLA	O2A-CGA-CBA	2.06	118.36	111.91
46	S	621	LUT	C20-C13-C12	2.06	121.32	118.08
46	r	620	LUT	C40-C33-C34	-2.06	120.04	122.92
48	n	623	NEX	C20-C13-C14	-2.06	120.04	122.92
29	c	501	CLA	CHA-C1A-NA	-2.06	121.69	126.40
29	C	503	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
48	R	622	NEX	O24-C25-C38	-2.05	112.59	115.06
29	G	614	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	S	617	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	S	610	CLA	C1D-ND-C4D	-2.05	104.88	106.33
31	d	404	BCR	C33-C5-C6	-2.05	122.22	124.53
45	Y	609	CHL	C4A-NA-C1A	2.05	107.63	106.71
29	a	407	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
29	g	611	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
29	G	611	CLA	C1D-ND-C4D	-2.05	104.88	106.33
29	b	602	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
29	B	608	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
29	a	405	CLA	C6-C5-C3	-2.05	108.08	113.45
29	G	610	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
29	S	605	CLA	CAA-C2A-C3A	-2.05	107.16	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	611	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
29	c	503	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
48	y	623	NEX	C1-C2-C3	2.05	118.27	113.64
29	G	613	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	c	511	CLA	C1D-ND-C4D	-2.05	104.88	106.33
29	b	605	CLA	CHA-C1A-NA	-2.05	121.71	126.40
47	R	621	XAT	C12-C13-C14	2.05	122.08	118.94
29	C	501	CLA	CHA-C1A-NA	-2.05	121.71	126.40
46	S	621	LUT	C31-C30-C29	-2.05	124.39	127.31
29	S	617	CLA	C1D-ND-C4D	-2.05	104.88	106.33
29	y	610	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
29	N	602	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
46	y	620	LUT	C15-C35-C34	-2.05	119.28	123.47
29	C	504	CLA	CMA-C3A-C4A	2.05	117.27	111.77
29	D	402	CLA	C2C-C1C-NC	2.05	111.89	109.97
29	b	608	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
29	y	602	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
29	c	504	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
29	b	616	CLA	C3B-C4B-NB	-2.04	108.62	110.52
31	C	516	BCR	C38-C26-C25	-2.04	122.23	124.53
29	N	602	CLA	CHA-C1A-NA	-2.04	121.72	126.40
29	Y	613	CLA	CHA-C1A-NA	-2.04	121.72	126.40
45	N	605	CHL	CHD-C4C-C3C	2.04	127.84	124.84
29	R	608	CLA	O2A-CGA-CBA	2.04	118.32	111.91
45	s	607	CHL	C4A-NA-C1A	2.04	107.62	106.71
29	s	609	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
29	B	617	CLA	C1D-ND-C4D	-2.04	104.88	106.33
29	r	613	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
29	B	605	CLA	CHA-C1A-NA	-2.04	121.72	126.40
29	g	612	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
46	y	620	LUT	C35-C15-C14	-2.04	119.29	123.47
29	G	604	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
29	Y	613	CLA	C1D-ND-C4D	-2.04	104.88	106.33
48	g	623	NEX	C40-C33-C34	-2.04	120.06	122.92
29	r	604	CLA	CHA-C1A-NA	-2.04	121.72	126.40
45	Y	609	CHL	C2B-C1B-NB	-2.04	108.86	110.23
31	a	411	BCR	C19-C18-C17	2.04	122.07	118.94
29	G	603	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
29	c	513	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
29	y	602	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
46	g	621	LUT	C10-C11-C12	-2.04	116.85	123.22
45	G	607	CHL	C4D-CHA-C1A	2.04	123.73	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
29	b	603	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
45	S	601	CHL	C4D-CHA-C1A	2.04	123.73	121.25
29	N	611	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	G	613	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
43	F	101	HEM	C3C-C2C-C1C	2.04	109.02	107.08
29	a	405	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	B	604	CLA	C1-C2-C3	-2.04	122.52	126.04
29	D	403	CLA	C1D-ND-C4D	-2.04	104.89	106.33
29	N	614	CLA	C1D-ND-C4D	-2.04	104.89	106.33
30	a	408	PHO	C2D-C1D-ND	-2.04	108.12	109.53
29	b	604	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
29	R	612	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
45	N	606	CHL	C4D-CHA-C1A	2.04	123.73	121.25
29	A	405	CLA	CAA-CBA-CGA	-2.04	107.30	113.25
29	G	604	CLA	OBD-CAD-C3D	-2.04	123.62	128.52
29	n	611	CLA	C1-O2A-CGA	2.03	121.78	116.44
29	B	615	CLA	C2A-C1A-CHA	2.03	127.42	123.86
29	n	603	CLA	CHA-C1A-NA	-2.03	121.74	126.40
29	R	603	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
29	c	504	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	c	508	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
45	S	606	CHL	CHD-C4C-C3C	2.03	127.83	124.84
32	A	412	SQD	O5-C1-O6	-2.03	105.16	109.97
29	R	613	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	g	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	s	602	CLA	CHA-C1A-NA	-2.03	121.74	126.40
29	Y	603	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	b	611	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
29	r	608	CLA	O2A-CGA-CBA	2.03	118.28	111.91
48	S	622	NEX	C16-C1-C6	-2.03	108.65	110.47
29	n	604	CLA	C1D-ND-C4D	-2.03	104.89	106.33
29	S	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	N	603	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
45	s	601	CHL	C4A-NA-C1A	2.03	107.62	106.71
29	g	603	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
29	s	612	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
29	S	602	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
30	a	409	PHO	C1-C2-C3	-2.03	122.53	126.04
29	s	602	CLA	CMA-C3A-C4A	2.03	117.23	111.77
29	N	614	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	c	512	CLA	C3D-C2D-C1D	-2.03	103.06	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	407	CLA	O2A-CGA-CBA	2.03	118.28	111.91
31	c	517	BCR	C33-C5-C4	2.03	117.52	113.62
29	n	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	c	510	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
29	Y	613	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	B	618	BCR	C31-C1-C6	-2.03	107.01	110.30
29	N	604	CLA	C1D-ND-C4D	-2.03	104.89	106.33
29	D	402	CLA	CAC-C3C-C4C	2.03	127.44	124.81
29	N	603	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	y	602	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
29	c	504	CLA	CMA-C3A-C4A	2.03	117.22	111.77
29	B	610	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
29	n	613	CLA	CHA-C1A-NA	-2.03	121.76	126.40
41	D	401	BCT	O3-C-O1	-2.03	114.29	119.55
29	B	604	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
45	G	601	CHL	C2B-C1B-NB	-2.03	108.87	110.23
29	r	612	CLA	C1D-ND-C4D	-2.03	104.90	106.33
29	a	405	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	D	404	BCR	C38-C26-C25	-2.03	122.25	124.53
48	r	623	NEX	O24-C25-C38	-2.02	112.63	115.06
29	y	612	CLA	C1D-ND-C4D	-2.02	104.90	106.33
29	G	614	CLA	CHA-C1A-NA	-2.02	121.76	126.40
29	y	602	CLA	CHA-C1A-NA	-2.02	121.76	126.40
45	R	606	CHL	CHC-C1C-NC	2.02	127.27	124.20
29	Y	602	CLA	CHA-C1A-NA	-2.02	121.76	126.40
46	G	621	LUT	C20-C13-C12	2.02	121.27	118.08
45	Y	607	CHL	C3B-C4B-NB	-2.02	108.64	110.52
35	B	620	C7Z	C18-C5-C4	2.02	118.10	114.36
29	d	403	CLA	C1D-ND-C4D	-2.02	104.90	106.33
42	D	405	PL9	O2-C1-C6	2.02	124.09	120.59
29	B	602	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
29	b	613	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
29	r	612	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
29	b	616	CLA	CMA-C3A-C4A	2.02	117.20	111.77
29	n	610	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
45	s	606	CHL	CHC-C1C-NC	2.02	127.27	124.20
29	b	610	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
29	B	609	CLA	CHA-C1A-NA	-2.02	121.77	126.40
29	C	513	CLA	CHA-C1A-NA	-2.02	121.77	126.40
45	N	608	CHL	CHD-C4C-C3C	2.02	127.81	124.84
31	A	411	BCR	C37-C22-C23	2.02	121.26	118.08
29	n	611	CLA	C3D-C2D-C1D	-2.02	103.08	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	h	101	RRX	C35-C13-C14	-2.02	120.10	122.92
31	c	517	BCR	C29-C30-C25	2.02	113.59	110.48
29	Y	614	CLA	C1D-ND-C4D	-2.02	104.90	106.33
39	n	624	LHG	O7-C7-O9	-2.02	118.83	123.70
29	G	602	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
42	d	405	PL9	O2-C1-C2	-2.02	117.16	121.78
29	Y	604	CLA	CHA-C1A-NA	-2.02	121.78	126.40
48	s	623	NEX	C1-C2-C3	2.02	118.19	113.64
46	n	620	LUT	C8-C7-C6	-2.01	121.55	127.20
46	N	620	LUT	C39-C29-C28	2.01	121.25	118.08
45	n	607	CHL	CHA-C1A-NA	-2.01	121.79	126.40
29	C	502	CLA	CAC-C3C-C4C	2.01	127.42	124.81
29	y	614	CLA	C1D-ND-C4D	-2.01	104.91	106.33
29	s	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
46	S	620	LUT	C10-C11-C12	-2.01	116.94	123.22
29	R	608	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	Y	608	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
29	g	602	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
35	B	620	C7Z	C4-C5-C6	-2.01	116.37	120.85
29	Y	608	CLA	C1D-ND-C4D	-2.01	104.91	106.33
29	S	610	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
29	Y	610	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
29	s	617	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	n	604	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
29	Y	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	g	613	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
29	A	407	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
42	D	405	PL9	C36-C34-C33	-2.01	117.05	121.12
29	c	506	CLA	C1-O2A-CGA	2.01	121.71	116.44
38	C	519	DGD	O2G-C1B-O1B	-2.01	118.85	123.70
48	G	623	NEX	C26-C27-C28	-2.01	121.75	125.99
45	n	609	CHL	CHA-C1A-NA	-2.01	121.80	126.40
29	Y	612	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
29	g	603	CLA	O2A-CGA-CBA	2.01	118.20	111.91
31	C	515	BCR	C3-C4-C5	-2.01	110.50	114.08
42	D	405	PL9	O2-C1-C2	-2.01	117.18	121.78
29	S	613	CLA	C2A-C1A-CHA	2.01	127.37	123.86
29	c	507	CLA	C2A-C1A-CHA	2.01	127.37	123.86
29	s	604	CLA	C3B-C4B-NB	-2.00	108.66	110.52
31	c	514	BCR	C29-C28-C27	2.00	115.86	111.38
29	R	611	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
46	n	621	LUT	C11-C10-C9	-2.00	124.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	411	BCR	C12-C13-C14	-2.00	115.86	118.94
31	A	411	BCR	C19-C18-C17	2.00	122.02	118.94
29	a	407	CLA	C1-O2A-CGA	2.00	121.70	116.44
29	R	604	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
45	G	608	CHL	C4D-CHA-C1A	2.00	123.69	121.25
31	B	619	BCR	C30-C25-C26	-2.00	119.79	122.61
47	y	622	XAT	C26-C27-C28	-2.00	121.76	125.99
29	C	509	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
45	s	601	CHL	C2B-C1B-NB	-2.00	108.89	110.23
29	b	616	CLA	C2A-C1A-CHA	2.00	127.36	123.86
29	b	613	CLA	CHA-C1A-NA	-2.00	121.81	126.40
48	n	623	NEX	O24-C25-C38	-2.00	112.66	115.06
29	N	610	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
46	s	621	LUT	C39-C29-C28	2.00	121.23	118.08
29	R	609	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
47	Y	622	XAT	C40-C33-C34	-2.00	120.12	122.92
45	s	601	CHL	C4D-CHA-C1A	2.00	123.68	121.25

All (45) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	B	620	C7Z	C3
35	b	620	C7Z	C3
40	C	527	LMK	C3
40	c	627	LMK	C3
44	H	101	RRX	C28
44	h	101	RRX	C28
45	N	601	CHL	C8
45	N	605	CHL	C8
45	N	606	CHL	C8
45	N	607	CHL	C8
45	N	609	CHL	C8
45	G	601	CHL	C8
45	G	606	CHL	C3A
45	G	609	CHL	C8
45	S	607	CHL	C3A
45	S	608	CHL	C8
45	Y	601	CHL	C8
45	Y	606	CHL	C8
45	Y	607	CHL	C8
45	Y	609	CHL	C8
45	n	601	CHL	C8

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Mol	Chain	Res	Type	Atom
45	n	605	CHL	C8
45	n	606	CHL	C8
45	n	607	CHL	C8
45	n	609	CHL	C8
45	g	601	CHL	C8
45	g	609	CHL	C8
45	s	607	CHL	C3A
45	s	608	CHL	C8
45	y	601	CHL	C8
45	y	606	CHL	C8
45	y	607	CHL	C8
45	y	609	CHL	C8
46	S	620	LUT	C26
46	s	620	LUT	C26
47	N	622	XAT	C6
47	G	622	XAT	C26
47	G	622	XAT	C6
47	R	621	XAT	C26
47	Y	622	XAT	C6
47	n	622	XAT	C6
47	g	622	XAT	C26
47	g	622	XAT	C6
47	r	622	XAT	C26
47	y	622	XAT	C6

All (4161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	CBD-CGD-O2D-CED
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	CHA-CBD-CGD-O1D
29	A	406	CLA	CHA-CBD-CGD-O2D
29	A	407	CLA	CHA-CBD-CGD-O1D
29	A	407	CLA	CHA-CBD-CGD-O2D
29	B	602	CLA	CHA-CBD-CGD-O1D
29	B	602	CLA	CHA-CBD-CGD-O2D
29	B	602	CLA	CBD-CGD-O2D-CED
29	B	603	CLA	CHA-CBD-CGD-O1D
29	B	603	CLA	CHA-CBD-CGD-O2D
29	B	603	CLA	CBD-CGD-O2D-CED
29	B	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	604	CLA	C2-C3-C5-C6
29	B	604	CLA	C4-C3-C5-C6
29	B	605	CLA	C2-C1-O2A-CGA
29	B	605	CLA	CHA-CBD-CGD-O1D
29	B	605	CLA	CHA-CBD-CGD-O2D
29	B	605	CLA	CAD-CBD-CGD-O1D
29	B	605	CLA	CAD-CBD-CGD-O2D
29	B	605	CLA	C2-C3-C5-C6
29	B	605	CLA	C4-C3-C5-C6
29	B	606	CLA	C2-C3-C5-C6
29	B	606	CLA	C4-C3-C5-C6
29	B	607	CLA	CHA-CBD-CGD-O1D
29	B	607	CLA	CHA-CBD-CGD-O2D
29	B	607	CLA	CBD-CGD-O2D-CED
29	B	608	CLA	C1A-C2A-CAA-CBA
29	B	608	CLA	C3A-C2A-CAA-CBA
29	B	608	CLA	CHA-CBD-CGD-O1D
29	B	608	CLA	CHA-CBD-CGD-O2D
29	B	608	CLA	CAD-CBD-CGD-O1D
29	B	608	CLA	CAD-CBD-CGD-O2D
29	B	608	CLA	CBD-CGD-O2D-CED
29	B	608	CLA	C2-C3-C5-C6
29	B	608	CLA	C4-C3-C5-C6
29	B	609	CLA	C1A-C2A-CAA-CBA
29	B	609	CLA	CHA-CBD-CGD-O1D
29	B	609	CLA	CHA-CBD-CGD-O2D
29	B	610	CLA	C1A-C2A-CAA-CBA
29	B	610	CLA	C3A-C2A-CAA-CBA
29	B	610	CLA	CHA-CBD-CGD-O1D
29	B	610	CLA	CHA-CBD-CGD-O2D
29	B	610	CLA	CAD-CBD-CGD-O1D
29	B	610	CLA	CBD-CGD-O2D-CED
29	B	612	CLA	C1A-C2A-CAA-CBA
29	B	612	CLA	CHA-CBD-CGD-O1D
29	B	612	CLA	CHA-CBD-CGD-O2D
29	B	612	CLA	CBD-CGD-O2D-CED
29	B	612	CLA	C2-C3-C5-C6
29	B	612	CLA	C4-C3-C5-C6
29	B	613	CLA	C1A-C2A-CAA-CBA
29	B	613	CLA	C2-C1-O2A-CGA
29	B	614	CLA	C2-C1-O2A-CGA
29	B	614	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	615	CLA	C1A-C2A-CAA-CBA
29	B	615	CLA	CAD-CBD-CGD-O1D
29	B	615	CLA	CAD-CBD-CGD-O2D
29	B	617	CLA	O1A-CGA-O2A-C1
29	B	617	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	CHA-CBD-CGD-O1D
29	C	501	CLA	CHA-CBD-CGD-O2D
29	C	501	CLA	C2-C3-C5-C6
29	C	501	CLA	C4-C3-C5-C6
29	C	502	CLA	CHA-CBD-CGD-O1D
29	C	502	CLA	CHA-CBD-CGD-O2D
29	C	502	CLA	CAD-CBD-CGD-O1D
29	C	503	CLA	CBD-CGD-O2D-CED
29	C	503	CLA	C2-C3-C5-C6
29	C	503	CLA	C4-C3-C5-C6
29	C	504	CLA	CHA-CBD-CGD-O1D
29	C	504	CLA	CHA-CBD-CGD-O2D
29	C	504	CLA	C2-C3-C5-C6
29	C	504	CLA	C4-C3-C5-C6
29	C	505	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	CAD-CBD-CGD-O2D
29	C	506	CLA	C1A-C2A-CAA-CBA
29	C	507	CLA	CBD-CGD-O2D-CED
29	C	508	CLA	CHA-CBD-CGD-O1D
29	C	508	CLA	CHA-CBD-CGD-O2D
29	C	509	CLA	C2-C1-O2A-CGA
29	C	511	CLA	C1A-C2A-CAA-CBA
29	C	511	CLA	CBD-CGD-O2D-CED
29	C	512	CLA	CHA-CBD-CGD-O1D
29	C	512	CLA	CHA-CBD-CGD-O2D
29	C	513	CLA	C1A-C2A-CAA-CBA
29	C	513	CLA	C2-C3-C5-C6
29	C	513	CLA	C4-C3-C5-C6
29	D	403	CLA	CBD-CGD-O2D-CED
29	N	610	CLA	C1A-C2A-CAA-CBA
29	N	610	CLA	CHA-CBD-CGD-O1D
29	N	610	CLA	CHA-CBD-CGD-O2D
29	N	610	CLA	CBD-CGD-O2D-CED
29	N	611	CLA	CHA-CBD-CGD-O1D
29	N	611	CLA	CHA-CBD-CGD-O2D
29	N	612	CLA	C1A-C2A-CAA-CBA
29	N	612	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	N	613	CLA	CHA-CBD-CGD-O1D
29	N	613	CLA	CHA-CBD-CGD-O2D
29	G	602	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	CBD-CGD-O2D-CED
29	G	604	CLA	C1A-C2A-CAA-CBA
29	G	610	CLA	CBD-CGD-O2D-CED
29	G	614	CLA	C2B-C3B-CAB-CBB
29	G	614	CLA	C4B-C3B-CAB-CBB
29	G	614	CLA	CBD-CGD-O2D-CED
29	R	603	CLA	C2-C1-O2A-CGA
29	R	604	CLA	C1A-C2A-CAA-CBA
29	R	608	CLA	C3A-C2A-CAA-CBA
29	R	608	CLA	CHA-CBD-CGD-O1D
29	R	608	CLA	CHA-CBD-CGD-O2D
29	R	609	CLA	C4B-C3B-CAB-CBB
29	R	609	CLA	CBD-CGD-O2D-CED
29	R	610	CLA	C1A-C2A-CAA-CBA
29	R	610	CLA	CHA-CBD-CGD-O1D
29	R	610	CLA	CHA-CBD-CGD-O2D
29	R	611	CLA	CBA-CGA-O2A-C1
29	R	611	CLA	O1A-CGA-O2A-C1
29	R	612	CLA	C2-C1-O2A-CGA
29	R	613	CLA	CBA-CGA-O2A-C1
29	R	613	CLA	CHA-CBD-CGD-O1D
29	R	613	CLA	CHA-CBD-CGD-O2D
29	S	602	CLA	C3A-C2A-CAA-CBA
29	S	602	CLA	CHA-CBD-CGD-O1D
29	S	602	CLA	CHA-CBD-CGD-O2D
29	S	603	CLA	C2B-C3B-CAB-CBB
29	S	603	CLA	C4B-C3B-CAB-CBB
29	S	603	CLA	CBD-CGD-O2D-CED
29	S	604	CLA	CHA-CBD-CGD-O1D
29	S	604	CLA	CHA-CBD-CGD-O2D
29	S	605	CLA	C1A-C2A-CAA-CBA
29	S	605	CLA	C2-C1-O2A-CGA
29	S	605	CLA	CHA-CBD-CGD-O1D
29	S	605	CLA	CHA-CBD-CGD-O2D
29	S	609	CLA	CBD-CGD-O2D-CED
29	S	610	CLA	CHA-CBD-CGD-O1D
29	S	610	CLA	CHA-CBD-CGD-O2D
29	S	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	S	611	CLA	CHA-CBD-CGD-O1D
29	S	611	CLA	CHA-CBD-CGD-O2D
29	S	612	CLA	CBD-CGD-O2D-CED
29	S	613	CLA	CHA-CBD-CGD-O1D
29	S	613	CLA	CHA-CBD-CGD-O2D
29	S	617	CLA	CBD-CGD-O2D-CED
29	Y	603	CLA	C2-C1-O2A-CGA
29	Y	604	CLA	CBD-CGD-O2D-CED
29	Y	610	CLA	CBD-CGD-O2D-CED
29	Y	611	CLA	CHA-CBD-CGD-O1D
29	Y	611	CLA	CHA-CBD-CGD-O2D
29	Y	613	CLA	CHA-CBD-CGD-O1D
29	Y	613	CLA	CHA-CBD-CGD-O2D
29	Y	614	CLA	CBD-CGD-O2D-CED
29	a	405	CLA	CBD-CGD-O2D-CED
29	a	406	CLA	C1A-C2A-CAA-CBA
29	a	406	CLA	C3A-C2A-CAA-CBA
29	a	406	CLA	CHA-CBD-CGD-O1D
29	a	406	CLA	CHA-CBD-CGD-O2D
29	a	407	CLA	CHA-CBD-CGD-O1D
29	a	407	CLA	CHA-CBD-CGD-O2D
29	b	602	CLA	CHA-CBD-CGD-O1D
29	b	602	CLA	CHA-CBD-CGD-O2D
29	b	602	CLA	CBD-CGD-O2D-CED
29	b	603	CLA	CHA-CBD-CGD-O1D
29	b	603	CLA	CHA-CBD-CGD-O2D
29	b	604	CLA	CBD-CGD-O2D-CED
29	b	604	CLA	C4-C3-C5-C6
29	b	605	CLA	CHA-CBD-CGD-O1D
29	b	605	CLA	CHA-CBD-CGD-O2D
29	b	605	CLA	CAD-CBD-CGD-O1D
29	b	605	CLA	CAD-CBD-CGD-O2D
29	b	605	CLA	C2-C3-C5-C6
29	b	605	CLA	C4-C3-C5-C6
29	b	606	CLA	C2-C3-C5-C6
29	b	606	CLA	C4-C3-C5-C6
29	b	607	CLA	CHA-CBD-CGD-O1D
29	b	607	CLA	CHA-CBD-CGD-O2D
29	b	607	CLA	CBD-CGD-O2D-CED
29	b	608	CLA	C1A-C2A-CAA-CBA
29	b	608	CLA	C3A-C2A-CAA-CBA
29	b	608	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	b	608	CLA	CHA-CBD-CGD-O2D
29	b	608	CLA	CAD-CBD-CGD-O1D
29	b	608	CLA	CAD-CBD-CGD-O2D
29	b	608	CLA	CBD-CGD-O2D-CED
29	b	608	CLA	C2-C3-C5-C6
29	b	608	CLA	C4-C3-C5-C6
29	b	609	CLA	C1A-C2A-CAA-CBA
29	b	609	CLA	C3A-C2A-CAA-CBA
29	b	609	CLA	CBD-CGD-O2D-CED
29	b	610	CLA	C3A-C2A-CAA-CBA
29	b	610	CLA	CHA-CBD-CGD-O1D
29	b	610	CLA	CHA-CBD-CGD-O2D
29	b	610	CLA	CAD-CBD-CGD-O1D
29	b	610	CLA	CBD-CGD-O2D-CED
29	b	612	CLA	C1A-C2A-CAA-CBA
29	b	612	CLA	CHA-CBD-CGD-O1D
29	b	612	CLA	CHA-CBD-CGD-O2D
29	b	613	CLA	C2-C1-O2A-CGA
29	b	615	CLA	C1A-C2A-CAA-CBA
29	b	615	CLA	CAD-CBD-CGD-O1D
29	b	615	CLA	CAD-CBD-CGD-O2D
29	b	616	CLA	CHA-CBD-CGD-O1D
29	b	616	CLA	CHA-CBD-CGD-O2D
29	b	617	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	C1A-C2A-CAA-CBA
29	c	501	CLA	CHA-CBD-CGD-O1D
29	c	501	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CBD-CGD-O2D-CED
29	c	503	CLA	C4-C3-C5-C6
29	c	504	CLA	CHA-CBD-CGD-O1D
29	c	504	CLA	CHA-CBD-CGD-O2D
29	c	504	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	C2-C3-C5-C6
29	c	504	CLA	C4-C3-C5-C6
29	c	505	CLA	CAD-CBD-CGD-O1D
29	c	505	CLA	CAD-CBD-CGD-O2D
29	c	506	CLA	C1A-C2A-CAA-CBA
29	c	508	CLA	CHA-CBD-CGD-O1D
29	c	508	CLA	CHA-CBD-CGD-O2D
29	c	509	CLA	C2-C1-O2A-CGA
29	c	511	CLA	C1A-C2A-CAA-CBA
29	c	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	c	512	CLA	CHA-CBD-CGD-O1D
29	c	513	CLA	C1A-C2A-CAA-CBA
29	c	513	CLA	C2-C3-C5-C6
29	c	513	CLA	C4-C3-C5-C6
29	d	403	CLA	CBD-CGD-O2D-CED
29	n	603	CLA	C3A-C2A-CAA-CBA
29	n	603	CLA	CBA-CGA-O2A-C1
29	n	603	CLA	O1A-CGA-O2A-C1
29	n	603	CLA	CHA-CBD-CGD-O1D
29	n	603	CLA	CHA-CBD-CGD-O2D
29	n	603	CLA	CAD-CBD-CGD-O1D
29	n	603	CLA	C2-C3-C5-C6
29	n	603	CLA	C4-C3-C5-C6
29	n	604	CLA	C1A-C2A-CAA-CBA
29	n	610	CLA	C1A-C2A-CAA-CBA
29	n	610	CLA	CHA-CBD-CGD-O1D
29	n	610	CLA	CHA-CBD-CGD-O2D
29	n	610	CLA	CBD-CGD-O2D-CED
29	n	611	CLA	C1A-C2A-CAA-CBA
29	n	611	CLA	C3A-C2A-CAA-CBA
29	n	611	CLA	CHA-CBD-CGD-O1D
29	n	611	CLA	CHA-CBD-CGD-O2D
29	n	612	CLA	CBD-CGD-O2D-CED
29	n	613	CLA	CHA-CBD-CGD-O1D
29	n	613	CLA	CHA-CBD-CGD-O2D
29	n	613	CLA	CBD-CGD-O2D-CED
29	n	614	CLA	C1A-C2A-CAA-CBA
29	n	614	CLA	CBD-CGD-O2D-CED
29	g	602	CLA	C1A-C2A-CAA-CBA
29	g	602	CLA	C3A-C2A-CAA-CBA
29	g	610	CLA	CHA-CBD-CGD-O2D
29	g	610	CLA	CBD-CGD-O2D-CED
29	g	613	CLA	CHA-CBD-CGD-O1D
29	g	613	CLA	CHA-CBD-CGD-O2D
29	g	614	CLA	C2A-CAA-CBA-CGA
29	g	614	CLA	CBD-CGD-O2D-CED
29	r	608	CLA	C3A-C2A-CAA-CBA
29	r	608	CLA	CHA-CBD-CGD-O1D
29	r	608	CLA	CHA-CBD-CGD-O2D
29	r	609	CLA	CBD-CGD-O2D-CED
29	r	610	CLA	C1A-C2A-CAA-CBA
29	r	610	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	r	610	CLA	C4-C3-C5-C6
29	r	612	CLA	C2-C1-O2A-CGA
29	r	613	CLA	CBA-CGA-O2A-C1
29	r	613	CLA	CBD-CGD-O2D-CED
29	s	602	CLA	C1A-C2A-CAA-CBA
29	s	602	CLA	C3A-C2A-CAA-CBA
29	s	602	CLA	CHA-CBD-CGD-O1D
29	s	602	CLA	CHA-CBD-CGD-O2D
29	s	603	CLA	C2B-C3B-CAB-CBB
29	s	603	CLA	C4B-C3B-CAB-CBB
29	s	604	CLA	CHA-CBD-CGD-O1D
29	s	604	CLA	CHA-CBD-CGD-O2D
29	s	605	CLA	C1A-C2A-CAA-CBA
29	s	605	CLA	CHA-CBD-CGD-O1D
29	s	605	CLA	CHA-CBD-CGD-O2D
29	s	609	CLA	C2-C3-C5-C6
29	s	609	CLA	C4-C3-C5-C6
29	s	610	CLA	CHA-CBD-CGD-O1D
29	s	610	CLA	CHA-CBD-CGD-O2D
29	s	610	CLA	CBD-CGD-O2D-CED
29	s	611	CLA	CHA-CBD-CGD-O1D
29	s	611	CLA	CHA-CBD-CGD-O2D
29	s	613	CLA	CHA-CBD-CGD-O1D
29	s	613	CLA	CHA-CBD-CGD-O2D
29	s	614	CLA	C1A-C2A-CAA-CBA
29	s	617	CLA	CBD-CGD-O2D-CED
29	y	603	CLA	C3A-C2A-CAA-CBA
29	y	604	CLA	CHA-CBD-CGD-O1D
29	y	604	CLA	CHA-CBD-CGD-O2D
29	y	610	CLA	CBD-CGD-O2D-CED
29	y	614	CLA	C2-C1-O2A-CGA
30	A	409	PHO	C3A-C2A-CAA-CBA
31	A	411	BCR	C11-C10-C9-C8
31	A	411	BCR	C11-C10-C9-C34
31	A	411	BCR	C10-C11-C12-C13
31	A	411	BCR	C11-C12-C13-C35
31	A	411	BCR	C17-C18-C19-C20
31	A	411	BCR	C36-C18-C19-C20
31	A	411	BCR	C23-C24-C25-C30
31	B	618	BCR	C1-C6-C7-C8
31	B	618	BCR	C7-C8-C9-C10
31	B	618	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
31	B	618	BCR	C11-C10-C9-C8
31	B	618	BCR	C11-C10-C9-C34
31	B	618	BCR	C10-C11-C12-C13
31	B	618	BCR	C17-C18-C19-C20
31	B	618	BCR	C36-C18-C19-C20
31	B	618	BCR	C37-C22-C23-C24
31	B	619	BCR	C11-C10-C9-C8
31	B	619	BCR	C11-C10-C9-C34
31	B	619	BCR	C10-C11-C12-C13
31	B	619	BCR	C21-C22-C23-C24
31	B	619	BCR	C37-C22-C23-C24
31	C	514	BCR	C11-C10-C9-C8
31	C	514	BCR	C11-C10-C9-C34
31	C	514	BCR	C9-C10-C11-C12
31	C	514	BCR	C10-C11-C12-C13
31	C	514	BCR	C13-C14-C15-C16
31	C	514	BCR	C17-C18-C19-C20
31	C	514	BCR	C36-C18-C19-C20
31	C	515	BCR	C7-C8-C9-C10
31	C	515	BCR	C7-C8-C9-C34
31	C	515	BCR	C11-C10-C9-C8
31	C	515	BCR	C11-C10-C9-C34
31	C	515	BCR	C17-C18-C19-C20
31	C	515	BCR	C36-C18-C19-C20
31	C	515	BCR	C23-C24-C25-C30
31	C	516	BCR	C1-C6-C7-C8
31	C	516	BCR	C5-C6-C7-C8
31	C	516	BCR	C7-C8-C9-C10
31	C	516	BCR	C7-C8-C9-C34
31	C	516	BCR	C11-C10-C9-C8
31	C	516	BCR	C11-C10-C9-C34
31	C	516	BCR	C10-C11-C12-C13
31	C	516	BCR	C17-C18-C19-C20
31	C	516	BCR	C36-C18-C19-C20
31	C	516	BCR	C21-C22-C23-C24
31	C	516	BCR	C37-C22-C23-C24
31	C	517	BCR	C11-C10-C9-C8
31	C	517	BCR	C11-C10-C9-C34
31	C	517	BCR	C10-C11-C12-C13
31	C	517	BCR	C17-C18-C19-C20
31	C	517	BCR	C36-C18-C19-C20
31	D	404	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	D	404	BCR	C11-C10-C9-C34
31	D	404	BCR	C10-C11-C12-C13
31	a	411	BCR	C11-C10-C9-C8
31	a	411	BCR	C11-C10-C9-C34
31	a	411	BCR	C10-C11-C12-C13
31	a	411	BCR	C17-C18-C19-C20
31	a	411	BCR	C36-C18-C19-C20
31	a	411	BCR	C23-C24-C25-C30
31	b	618	BCR	C7-C8-C9-C10
31	b	618	BCR	C7-C8-C9-C34
31	b	618	BCR	C11-C10-C9-C8
31	b	618	BCR	C11-C10-C9-C34
31	b	618	BCR	C10-C11-C12-C13
31	b	618	BCR	C17-C18-C19-C20
31	b	618	BCR	C36-C18-C19-C20
31	b	619	BCR	C11-C10-C9-C8
31	b	619	BCR	C11-C10-C9-C34
31	b	619	BCR	C10-C11-C12-C13
31	b	619	BCR	C21-C22-C23-C24
31	b	619	BCR	C37-C22-C23-C24
31	c	514	BCR	C11-C10-C9-C8
31	c	514	BCR	C11-C10-C9-C34
31	c	514	BCR	C9-C10-C11-C12
31	c	514	BCR	C10-C11-C12-C13
31	c	514	BCR	C17-C18-C19-C20
31	c	514	BCR	C36-C18-C19-C20
31	c	515	BCR	C7-C8-C9-C34
31	c	515	BCR	C11-C10-C9-C8
31	c	515	BCR	C11-C10-C9-C34
31	c	515	BCR	C10-C11-C12-C13
31	c	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C36-C18-C19-C20
31	c	516	BCR	C1-C6-C7-C8
31	c	516	BCR	C5-C6-C7-C8
31	c	516	BCR	C7-C8-C9-C10
31	c	516	BCR	C7-C8-C9-C34
31	c	516	BCR	C11-C10-C9-C8
31	c	516	BCR	C11-C10-C9-C34
31	c	516	BCR	C10-C11-C12-C13
31	c	516	BCR	C21-C22-C23-C24
31	c	516	BCR	C37-C22-C23-C24
31	c	516	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
31	c	517	BCR	C11-C10-C9-C8
31	c	517	BCR	C11-C10-C9-C34
31	c	517	BCR	C17-C18-C19-C20
31	c	517	BCR	C36-C18-C19-C20
31	d	404	BCR	C11-C10-C9-C8
31	d	404	BCR	C11-C10-C9-C34
31	d	404	BCR	C10-C11-C12-C13
32	A	412	SQD	C2-C1-O6-C44
32	A	412	SQD	O5-C1-O6-C44
32	A	412	SQD	O5-C5-C6-S
32	B	621	SQD	O5-C1-O6-C44
32	B	621	SQD	C8-C7-O47-C45
32	B	621	SQD	C5-C6-S-O7
32	B	621	SQD	C5-C6-S-O8
32	B	621	SQD	C5-C6-S-O9
32	C	526	SQD	O5-C5-C6-S
32	C	526	SQD	C5-C6-S-O7
32	C	526	SQD	C5-C6-S-O8
32	C	526	SQD	C5-C6-S-O9
32	a	412	SQD	O5-C1-O6-C44
32	a	412	SQD	O5-C5-C6-S
32	b	621	SQD	O5-C1-O6-C44
32	b	621	SQD	C8-C7-O47-C45
32	b	621	SQD	C5-C6-S-O7
32	b	621	SQD	C5-C6-S-O8
32	b	621	SQD	C5-C6-S-O9
32	c	626	SQD	O5-C5-C6-S
32	c	626	SQD	C5-C6-S-O7
32	c	626	SQD	C5-C6-S-O8
32	c	626	SQD	C5-C6-S-O9
33	A	413	LMG	O9-C10-O7-C8
33	A	413	LMG	C11-C10-O7-C8
33	B	622	LMG	C9-C8-O7-C10
33	B	622	LMG	C11-C10-O7-C8
33	C	521	LMG	C2-C1-O1-C7
33	C	521	LMG	O6-C1-O1-C7
33	C	521	LMG	C11-C10-O7-C8
33	b	622	LMG	O9-C10-O7-C8
33	c	521	LMG	C2-C1-O1-C7
33	c	521	LMG	O6-C1-O1-C7
33	c	521	LMG	C11-C10-O7-C8
33	j	101	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
35	B	620	C7Z	C7-C8-C9-C19
35	B	620	C7Z	C7-C8-C9-C10
35	B	620	C7Z	C11-C12-C13-C20
35	B	620	C7Z	C11-C12-C13-C14
35	B	620	C7Z	C27-C28-C29-C30
35	B	620	C7Z	C27-C28-C29-C39
35	b	620	C7Z	C7-C8-C9-C19
35	b	620	C7Z	C7-C8-C9-C10
35	b	620	C7Z	C11-C12-C13-C20
35	b	620	C7Z	C11-C12-C13-C14
35	b	620	C7Z	C27-C28-C29-C30
35	b	620	C7Z	C27-C28-C29-C39
36	B	625	DGA	OB1-CB1-OG2-CG2
36	B	625	DGA	CG1-CG2-CG3-OXT
36	B	625	DGA	OG2-CG2-CG3-OXT
36	b	623	DGA	OB1-CB1-OG2-CG2
38	C	519	DGD	C2E-C1E-O5D-C6D
38	C	519	DGD	O6E-C1E-O5D-C6D
38	C	520	DGD	C2B-C1B-O2G-C2G
38	C	523	DGD	C2A-C1A-O1G-C1G
38	C	523	DGD	O1A-C1A-O1G-C1G
38	C	523	DGD	O1B-C1B-O2G-C2G
38	C	523	DGD	C2E-C1E-O5D-C6D
38	C	523	DGD	O6E-C1E-O5D-C6D
38	c	519	DGD	C2E-C1E-O5D-C6D
38	c	519	DGD	O6E-C1E-O5D-C6D
38	c	520	DGD	C2B-C1B-O2G-C2G
38	c	523	DGD	C2E-C1E-O5D-C6D
38	c	523	DGD	O6E-C1E-O5D-C6D
39	C	525	LHG	C1-C2-C3-O3
39	C	525	LHG	C3-O3-P-O4
39	C	525	LHG	C4-O6-P-O4
39	D	408	LHG	C1-C2-C3-O3
39	D	408	LHG	C4-O6-P-O4
39	D	409	LHG	O2-C2-C3-O3
39	D	409	LHG	C3-O3-P-O5
39	D	409	LHG	C3-O3-P-O6
39	D	409	LHG	C4-O6-P-O5
39	D	410	LHG	C1-C2-C3-O3
39	D	410	LHG	C3-O3-P-O5
39	D	410	LHG	C4-O6-P-O4
39	L	101	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
39	L	101	LHG	C1-C2-C3-O3
39	L	101	LHG	C4-O6-P-O3
39	L	101	LHG	C4-O6-P-O5
39	N	624	LHG	O9-C7-O7-C5
39	N	624	LHG	C8-C7-O7-C5
39	G	630	LHG	O1-C1-C2-C3
39	G	630	LHG	C1-C2-C3-O3
39	G	630	LHG	C4-O6-P-O4
39	S	624	LHG	C8-C7-O7-C5
39	Y	624	LHG	C1-C2-C3-O3
39	Y	624	LHG	O2-C2-C3-O3
39	Y	624	LHG	C4-O6-P-O3
39	Y	624	LHG	C4-O6-P-O4
39	Y	624	LHG	C4-O6-P-O5
39	c	625	LHG	C3-O3-P-O6
39	c	625	LHG	C4-O6-P-O3
39	c	625	LHG	C4-O6-P-O4
39	c	625	LHG	C4-O6-P-O5
39	d	408	LHG	O1-C1-C2-C3
39	d	408	LHG	C4-O6-P-O4
39	d	408	LHG	C4-O6-P-O5
39	d	409	LHG	C1-C2-C3-O3
39	d	409	LHG	C4-O6-P-O5
39	d	410	LHG	O1-C1-C2-C3
39	d	410	LHG	C3-O3-P-O4
39	d	410	LHG	C3-O3-P-O5
39	d	410	LHG	C4-O6-P-O5
39	d	410	LHG	O7-C5-C6-O8
39	l	101	LHG	O1-C1-C2-C3
39	l	101	LHG	C1-C2-C3-O3
39	l	101	LHG	C4-O6-P-O3
39	l	101	LHG	C4-O6-P-O5
39	n	624	LHG	O9-C7-O7-C5
39	n	624	LHG	C8-C7-O7-C5
39	g	624	LHG	O1-C1-C2-C3
39	g	624	LHG	C1-C2-C3-O3
39	g	624	LHG	C4-O6-P-O4
39	g	624	LHG	O7-C5-C6-O8
39	s	624	LHG	O1-C1-C2-C3
39	s	624	LHG	C8-C7-O7-C5
39	y	624	LHG	C1-C2-C3-O3
39	y	624	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
39	y	624	LHG	C4-O6-P-O5
40	C	527	LMK	O9-C10-O7-C8
40	C	527	LMK	O10-C28-O8-C9
40	c	627	LMK	O9-C10-C11-C12
40	c	627	LMK	O9-C10-O7-C8
42	D	405	PL9	C12-C13-C14-C15
42	D	405	PL9	C12-C13-C14-C16
42	d	405	PL9	C12-C13-C14-C15
44	H	101	RRX	C37-C22-C23-C24
44	H	101	RRX	C21-C22-C23-C24
44	H	101	RRX	C7-C8-C9-C34
44	h	101	RRX	C37-C22-C23-C24
44	h	101	RRX	C21-C22-C23-C24
44	h	101	RRX	C7-C8-C9-C10
44	h	101	RRX	C7-C8-C9-C34
45	G	601	CHL	CHA-CBD-CGD-O1D
45	G	601	CHL	CHA-CBD-CGD-O2D
45	G	601	CHL	C2-C3-C5-C6
45	G	601	CHL	C4-C3-C5-C6
45	G	606	CHL	C1A-C2A-CAA-CBA
45	G	607	CHL	C1A-C2A-CAA-CBA
45	R	606	CHL	CHA-CBD-CGD-O1D
45	R	606	CHL	CHA-CBD-CGD-O2D
45	R	606	CHL	CAD-CBD-CGD-O1D
45	R	606	CHL	CAD-CBD-CGD-O2D
45	R	607	CHL	CHA-CBD-CGD-O1D
45	R	607	CHL	CHA-CBD-CGD-O2D
45	S	607	CHL	C1A-C2A-CAA-CBA
45	Y	601	CHL	CHA-CBD-CGD-O1D
45	Y	601	CHL	CHA-CBD-CGD-O2D
45	n	609	CHL	C1A-C2A-CAA-CBA
45	g	601	CHL	CHA-CBD-CGD-O1D
45	g	601	CHL	CHA-CBD-CGD-O2D
45	g	601	CHL	C2-C3-C5-C6
45	g	601	CHL	C4-C3-C5-C6
45	g	605	CHL	CHA-CBD-CGD-O1D
45	g	606	CHL	C1A-C2A-CAA-CBA
45	s	607	CHL	C1A-C2A-CAA-CBA
45	y	601	CHL	CHA-CBD-CGD-O1D
45	y	601	CHL	CHA-CBD-CGD-O2D
45	y	601	CHL	C2-C3-C5-C6
45	y	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
46	N	621	LUT	C21-C26-C27-C28
46	G	620	LUT	C25-C26-C27-C28
46	G	621	LUT	C21-C26-C27-C28
46	R	620	LUT	C7-C8-C9-C10
46	S	620	LUT	C21-C26-C27-C28
46	S	620	LUT	C27-C28-C29-C30
46	S	620	LUT	C27-C28-C29-C39
46	S	621	LUT	C25-C26-C27-C28
46	Y	620	LUT	C27-C28-C29-C39
46	Y	621	LUT	C21-C26-C27-C28
46	n	620	LUT	C1-C6-C7-C8
46	n	620	LUT	C25-C26-C27-C28
46	n	621	LUT	C21-C26-C27-C28
46	g	620	LUT	C27-C28-C29-C30
46	g	620	LUT	C27-C28-C29-C39
46	g	621	LUT	C21-C26-C27-C28
46	s	620	LUT	C21-C26-C27-C28
46	s	620	LUT	C25-C26-C27-C28
47	R	621	XAT	C9-C10-C11-C12
47	R	621	XAT	C10-C11-C12-C13
47	R	621	XAT	O24-C26-C27-C28
47	R	621	XAT	C26-C27-C28-C29
47	Y	622	XAT	C27-C28-C29-C30
47	Y	622	XAT	C27-C28-C29-C39
47	r	622	XAT	C7-C8-C9-C10
47	r	622	XAT	C7-C8-C9-C19
47	r	622	XAT	C9-C10-C11-C12
47	r	622	XAT	C10-C11-C12-C13
47	r	622	XAT	C20-C13-C14-C15
47	r	622	XAT	O24-C26-C27-C28
47	r	622	XAT	C26-C27-C28-C29
48	R	622	NEX	C12-C13-C14-C15
48	R	622	NEX	C20-C13-C14-C15
48	R	622	NEX	C14-C15-C35-C34
48	S	622	NEX	C11-C10-C9-C8
48	S	622	NEX	C11-C10-C9-C19
48	S	622	NEX	C10-C11-C12-C13
48	S	622	NEX	C11-C12-C13-C14
48	S	622	NEX	C11-C12-C13-C20
48	r	623	NEX	C12-C13-C14-C15
48	r	623	NEX	C20-C13-C14-C15
48	r	623	NEX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
48	s	623	NEX	C10-C11-C12-C13
48	s	623	NEX	C11-C12-C13-C14
48	s	623	NEX	C11-C12-C13-C20
49	S	625	LPX	C3-C4-C5-O6
49	S	625	LPX	O1-C3-C4-C5
49	s	625	LPX	O1-C3-C4-O5
50	S	626	3PH	C22-C21-O21-C2
50	i	101	3PH	C1-O11-P-O13
50	i	101	3PH	C1-O11-P-O14
50	s	626	3PH	C1-O11-P-O13
50	s	626	3PH	C1-O11-P-O14
50	s	626	3PH	C1-O11-P-O12
50	s	626	3PH	O21-C2-C3-O31
50	s	626	3PH	C22-C21-O21-C2
51	Y	625	SPH	C1-C2-C3-O3
51	Y	625	SPH	C1-C2-C3-C4
51	Y	625	SPH	N2-C2-C3-O3
51	Y	625	SPH	N2-C2-C3-C4
51	y	625	SPH	O1-C1-C2-N2
51	y	625	SPH	C1-C2-C3-O3
51	y	625	SPH	C1-C2-C3-C4
51	y	625	SPH	N2-C2-C3-O3
51	y	625	SPH	N2-C2-C3-C4
29	S	603	CLA	O1D-CGD-O2D-CED
29	c	502	CLA	O1D-CGD-O2D-CED
29	r	611	CLA	O1D-CGD-O2D-CED
29	N	612	CLA	O1D-CGD-O2D-CED
29	R	603	CLA	O1D-CGD-O2D-CED
29	R	611	CLA	O1D-CGD-O2D-CED
29	b	612	CLA	O1D-CGD-O2D-CED
29	g	613	CLA	O1D-CGD-O2D-CED
29	r	603	CLA	O1D-CGD-O2D-CED
29	s	603	CLA	O1D-CGD-O2D-CED
29	y	604	CLA	O1D-CGD-O2D-CED
29	A	410	CLA	CBD-CGD-O2D-CED
29	B	606	CLA	CBD-CGD-O2D-CED
29	B	609	CLA	CBD-CGD-O2D-CED
29	B	611	CLA	CBD-CGD-O2D-CED
29	B	616	CLA	CBD-CGD-O2D-CED
29	C	502	CLA	CBD-CGD-O2D-CED
29	C	504	CLA	CBD-CGD-O2D-CED
29	C	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	C	513	CLA	CBD-CGD-O2D-CED
29	N	602	CLA	CBD-CGD-O2D-CED
29	N	612	CLA	CBD-CGD-O2D-CED
29	N	613	CLA	CBD-CGD-O2D-CED
29	N	614	CLA	CBD-CGD-O2D-CED
29	G	602	CLA	CBD-CGD-O2D-CED
29	G	604	CLA	CBD-CGD-O2D-CED
29	G	611	CLA	CBD-CGD-O2D-CED
29	G	612	CLA	CBD-CGD-O2D-CED
29	G	613	CLA	CBD-CGD-O2D-CED
29	R	602	CLA	CBD-CGD-O2D-CED
29	R	603	CLA	CBD-CGD-O2D-CED
29	R	608	CLA	CBD-CGD-O2D-CED
29	R	611	CLA	CBD-CGD-O2D-CED
29	R	612	CLA	CBD-CGD-O2D-CED
29	R	613	CLA	CBD-CGD-O2D-CED
29	S	604	CLA	CBD-CGD-O2D-CED
29	S	605	CLA	CBD-CGD-O2D-CED
29	S	613	CLA	CBD-CGD-O2D-CED
29	S	614	CLA	CBD-CGD-O2D-CED
29	Y	602	CLA	CBD-CGD-O2D-CED
29	Y	603	CLA	CBD-CGD-O2D-CED
29	Y	608	CLA	CBD-CGD-O2D-CED
29	Y	612	CLA	CBD-CGD-O2D-CED
29	Y	613	CLA	CBD-CGD-O2D-CED
29	a	410	CLA	CBD-CGD-O2D-CED
29	b	603	CLA	CBD-CGD-O2D-CED
29	b	606	CLA	CBD-CGD-O2D-CED
29	b	611	CLA	CBD-CGD-O2D-CED
29	b	612	CLA	CBD-CGD-O2D-CED
29	b	614	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	CBD-CGD-O2D-CED
29	c	503	CLA	CBD-CGD-O2D-CED
29	c	504	CLA	CBD-CGD-O2D-CED
29	c	507	CLA	CBD-CGD-O2D-CED
29	c	509	CLA	CBD-CGD-O2D-CED
29	c	510	CLA	CBD-CGD-O2D-CED
29	c	513	CLA	CBD-CGD-O2D-CED
29	d	402	CLA	CBD-CGD-O2D-CED
29	n	602	CLA	CBD-CGD-O2D-CED
29	n	611	CLA	CBD-CGD-O2D-CED
29	g	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	g	603	CLA	CBD-CGD-O2D-CED
29	g	604	CLA	CBD-CGD-O2D-CED
29	g	611	CLA	CBD-CGD-O2D-CED
29	g	612	CLA	CBD-CGD-O2D-CED
29	g	613	CLA	CBD-CGD-O2D-CED
29	r	602	CLA	CBD-CGD-O2D-CED
29	r	603	CLA	CBD-CGD-O2D-CED
29	r	604	CLA	CBD-CGD-O2D-CED
29	r	608	CLA	CBD-CGD-O2D-CED
29	r	611	CLA	CBD-CGD-O2D-CED
29	r	612	CLA	CBD-CGD-O2D-CED
29	s	603	CLA	CBD-CGD-O2D-CED
29	s	604	CLA	CBD-CGD-O2D-CED
29	s	609	CLA	CBD-CGD-O2D-CED
29	s	612	CLA	CBD-CGD-O2D-CED
29	s	613	CLA	CBD-CGD-O2D-CED
29	s	614	CLA	CBD-CGD-O2D-CED
29	y	603	CLA	CBD-CGD-O2D-CED
29	y	604	CLA	CBD-CGD-O2D-CED
29	y	608	CLA	CBD-CGD-O2D-CED
29	y	612	CLA	CBD-CGD-O2D-CED
29	y	613	CLA	CBD-CGD-O2D-CED
29	y	614	CLA	CBD-CGD-O2D-CED
30	A	409	PHO	CBD-CGD-O2D-CED
29	A	406	CLA	O1A-CGA-O2A-C1
29	C	504	CLA	O1A-CGA-O2A-C1
29	G	614	CLA	O1A-CGA-O2A-C1
29	S	605	CLA	O1A-CGA-O2A-C1
29	S	613	CLA	O1A-CGA-O2A-C1
29	S	617	CLA	O1A-CGA-O2A-C1
29	a	406	CLA	O1A-CGA-O2A-C1
29	b	603	CLA	O1A-CGA-O2A-C1
29	b	617	CLA	O1A-CGA-O2A-C1
29	c	504	CLA	O1A-CGA-O2A-C1
29	s	603	CLA	O1A-CGA-O2A-C1
29	s	605	CLA	O1A-CGA-O2A-C1
29	s	614	CLA	O1A-CGA-O2A-C1
29	y	603	CLA	O1A-CGA-O2A-C1
33	j	101	LMG	O10-C28-O8-C9
38	c	523	DGD	O1A-C1A-O1G-C1G
29	R	613	CLA	O1A-CGA-O2A-C1
29	r	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	r	613	CLA	O1A-CGA-O2A-C1
29	A	405	CLA	O1D-CGD-O2D-CED
29	B	606	CLA	O1D-CGD-O2D-CED
29	D	403	CLA	O1D-CGD-O2D-CED
29	N	610	CLA	O1D-CGD-O2D-CED
29	N	613	CLA	O1D-CGD-O2D-CED
29	G	613	CLA	O1D-CGD-O2D-CED
29	R	608	CLA	O1D-CGD-O2D-CED
29	Y	608	CLA	O1D-CGD-O2D-CED
29	a	405	CLA	O1D-CGD-O2D-CED
29	b	606	CLA	O1D-CGD-O2D-CED
29	b	617	CLA	O1D-CGD-O2D-CED
29	d	403	CLA	O1D-CGD-O2D-CED
29	r	608	CLA	O1D-CGD-O2D-CED
29	s	610	CLA	O1D-CGD-O2D-CED
29	y	608	CLA	O1D-CGD-O2D-CED
29	y	613	CLA	O1D-CGD-O2D-CED
29	r	611	CLA	CBA-CGA-O2A-C1
29	B	602	CLA	O1D-CGD-O2D-CED
29	B	604	CLA	O1D-CGD-O2D-CED
29	B	607	CLA	O1D-CGD-O2D-CED
29	B	608	CLA	O1D-CGD-O2D-CED
29	B	612	CLA	O1D-CGD-O2D-CED
29	B	614	CLA	O1D-CGD-O2D-CED
29	C	502	CLA	O1D-CGD-O2D-CED
29	C	503	CLA	O1D-CGD-O2D-CED
29	C	507	CLA	O1D-CGD-O2D-CED
29	C	511	CLA	O1D-CGD-O2D-CED
29	G	614	CLA	O1D-CGD-O2D-CED
29	R	609	CLA	O1D-CGD-O2D-CED
29	S	609	CLA	O1D-CGD-O2D-CED
29	S	612	CLA	O1D-CGD-O2D-CED
29	S	614	CLA	O1D-CGD-O2D-CED
29	Y	613	CLA	O1D-CGD-O2D-CED
29	b	604	CLA	O1D-CGD-O2D-CED
29	b	607	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	O1D-CGD-O2D-CED
29	n	612	CLA	O1D-CGD-O2D-CED
29	n	613	CLA	O1D-CGD-O2D-CED
29	n	614	CLA	O1D-CGD-O2D-CED
29	y	610	CLA	O1D-CGD-O2D-CED
29	A	406	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	C	504	CLA	CBA-CGA-O2A-C1
29	C	505	CLA	CBA-CGA-O2A-C1
29	G	614	CLA	CBA-CGA-O2A-C1
29	S	605	CLA	CBA-CGA-O2A-C1
29	S	617	CLA	CBA-CGA-O2A-C1
29	a	406	CLA	CBA-CGA-O2A-C1
29	b	617	CLA	CBA-CGA-O2A-C1
29	c	504	CLA	CBA-CGA-O2A-C1
29	s	603	CLA	CBA-CGA-O2A-C1
29	s	605	CLA	CBA-CGA-O2A-C1
29	s	614	CLA	CBA-CGA-O2A-C1
29	y	603	CLA	CBA-CGA-O2A-C1
38	c	523	DGD	C2A-C1A-O1G-C1G
29	B	613	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	CBD-CGD-O2D-CED
29	C	510	CLA	CBD-CGD-O2D-CED
29	D	402	CLA	CBD-CGD-O2D-CED
29	N	604	CLA	CBD-CGD-O2D-CED
29	N	611	CLA	CBD-CGD-O2D-CED
29	R	604	CLA	CBD-CGD-O2D-CED
29	R	610	CLA	CBD-CGD-O2D-CED
29	S	611	CLA	CBD-CGD-O2D-CED
29	Y	611	CLA	CBD-CGD-O2D-CED
29	b	613	CLA	CBD-CGD-O2D-CED
29	b	616	CLA	CBD-CGD-O2D-CED
29	n	603	CLA	CBD-CGD-O2D-CED
29	n	604	CLA	CBD-CGD-O2D-CED
29	s	605	CLA	CBD-CGD-O2D-CED
29	s	611	CLA	CBD-CGD-O2D-CED
29	y	602	CLA	CBD-CGD-O2D-CED
29	B	603	CLA	O1A-CGA-O2A-C1
29	C	505	CLA	O1A-CGA-O2A-C1
29	C	511	CLA	O1A-CGA-O2A-C1
29	N	611	CLA	O1A-CGA-O2A-C1
29	Y	603	CLA	O1A-CGA-O2A-C1
29	Y	604	CLA	O1A-CGA-O2A-C1
29	Y	611	CLA	O1A-CGA-O2A-C1
29	c	505	CLA	O1A-CGA-O2A-C1
29	c	511	CLA	O1A-CGA-O2A-C1
29	g	602	CLA	O1A-CGA-O2A-C1
29	g	614	CLA	O1A-CGA-O2A-C1
29	s	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	s	613	CLA	O1A-CGA-O2A-C1
29	y	604	CLA	O1A-CGA-O2A-C1
29	y	611	CLA	O1A-CGA-O2A-C1
33	J	101	LMG	O10-C28-O8-C9
50	S	626	3PH	O32-C31-O31-C3
50	s	626	3PH	O32-C31-O31-C3
29	B	610	CLA	O1D-CGD-O2D-CED
29	G	610	CLA	O1D-CGD-O2D-CED
29	S	610	CLA	O1D-CGD-O2D-CED
29	S	617	CLA	O1D-CGD-O2D-CED
29	Y	604	CLA	O1D-CGD-O2D-CED
29	Y	610	CLA	O1D-CGD-O2D-CED
29	b	602	CLA	O1D-CGD-O2D-CED
29	b	608	CLA	O1D-CGD-O2D-CED
29	b	609	CLA	O1D-CGD-O2D-CED
29	n	610	CLA	O1D-CGD-O2D-CED
29	g	614	CLA	O1D-CGD-O2D-CED
29	s	617	CLA	O1D-CGD-O2D-CED
29	B	603	CLA	O1D-CGD-O2D-CED
29	B	617	CLA	O1D-CGD-O2D-CED
29	G	603	CLA	O1D-CGD-O2D-CED
29	Y	614	CLA	O1D-CGD-O2D-CED
29	b	610	CLA	O1D-CGD-O2D-CED
29	g	610	CLA	O1D-CGD-O2D-CED
29	r	609	CLA	O1D-CGD-O2D-CED
29	r	613	CLA	O1D-CGD-O2D-CED
29	C	506	CLA	CBD-CGD-O2D-CED
29	N	603	CLA	CBD-CGD-O2D-CED
29	c	506	CLA	CBD-CGD-O2D-CED
29	N	614	CLA	O1D-CGD-O2D-CED
29	R	602	CLA	O1D-CGD-O2D-CED
29	b	603	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	O1D-CGD-O2D-CED
29	s	609	CLA	O1D-CGD-O2D-CED
32	B	621	SQD	O49-C7-O47-C45
32	b	621	SQD	O49-C7-O47-C45
33	B	622	LMG	O9-C10-O7-C8
33	C	521	LMG	O9-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
38	C	520	DGD	O1B-C1B-O2G-C2G
38	c	520	DGD	O1B-C1B-O2G-C2G
38	c	523	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
39	s	624	LHG	O9-C7-O7-C5
50	S	626	3PH	O22-C21-O21-C2
50	s	626	3PH	O22-C21-O21-C2
29	A	410	CLA	C3-C5-C6-C7
29	B	605	CLA	C3-C5-C6-C7
29	B	612	CLA	C3-C5-C6-C7
29	C	504	CLA	C3-C5-C6-C7
29	C	511	CLA	C3-C5-C6-C7
29	C	512	CLA	C3-C5-C6-C7
29	D	403	CLA	C3-C5-C6-C7
29	N	603	CLA	C3-C5-C6-C7
29	N	610	CLA	C3-C5-C6-C7
29	G	603	CLA	C3-C5-C6-C7
29	S	609	CLA	C3-C5-C6-C7
29	Y	613	CLA	C3-C5-C6-C7
29	b	602	CLA	C3-C5-C6-C7
29	b	605	CLA	C3-C5-C6-C7
29	b	608	CLA	C3-C5-C6-C7
29	b	610	CLA	C3-C5-C6-C7
29	b	612	CLA	C3-C5-C6-C7
29	c	504	CLA	C3-C5-C6-C7
29	c	512	CLA	C3-C5-C6-C7
29	n	602	CLA	C3-C5-C6-C7
29	r	609	CLA	C3-C5-C6-C7
29	s	609	CLA	C3-C5-C6-C7
29	y	611	CLA	C3-C5-C6-C7
30	a	409	PHO	C3-C5-C6-C7
29	B	617	CLA	CBA-CGA-O2A-C1
29	C	511	CLA	CBA-CGA-O2A-C1
29	N	603	CLA	CBA-CGA-O2A-C1
29	S	613	CLA	CBA-CGA-O2A-C1
29	Y	604	CLA	CBA-CGA-O2A-C1
29	Y	611	CLA	CBA-CGA-O2A-C1
29	Y	612	CLA	CBA-CGA-O2A-C1
29	b	603	CLA	CBA-CGA-O2A-C1
29	c	505	CLA	CBA-CGA-O2A-C1
29	c	511	CLA	CBA-CGA-O2A-C1
29	r	612	CLA	CBA-CGA-O2A-C1
29	s	613	CLA	CBA-CGA-O2A-C1
29	y	604	CLA	CBA-CGA-O2A-C1
29	y	611	CLA	CBA-CGA-O2A-C1
33	J	101	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
33	j	101	LMG	C29-C28-O8-C9
50	S	626	3PH	C32-C31-O31-C3
50	s	626	3PH	C32-C31-O31-C3
33	b	622	LMG	C11-C10-O7-C8
36	B	625	DGA	CB2-CB1-OG2-CG2
36	b	623	DGA	CB2-CB1-OG2-CG2
38	C	523	DGD	C2B-C1B-O2G-C2G
38	c	523	DGD	C2B-C1B-O2G-C2G
29	G	604	CLA	O1D-CGD-O2D-CED
29	r	602	CLA	O1D-CGD-O2D-CED
29	y	611	CLA	CBD-CGD-O2D-CED
29	s	617	CLA	O1A-CGA-O2A-C1
50	i	101	3PH	O32-C31-O31-C3
29	R	602	CLA	C4-C3-C5-C6
29	R	602	CLA	C2-C3-C5-C6
29	c	503	CLA	C2-C3-C5-C6
29	r	610	CLA	CBD-CGD-O2D-CED
29	N	612	CLA	C2A-CAA-CBA-CGA
29	N	614	CLA	C2A-CAA-CBA-CGA
29	G	604	CLA	C2A-CAA-CBA-CGA
29	G	613	CLA	C2A-CAA-CBA-CGA
29	R	609	CLA	C2A-CAA-CBA-CGA
29	S	617	CLA	C2A-CAA-CBA-CGA
29	b	612	CLA	C2A-CAA-CBA-CGA
29	n	603	CLA	C2A-CAA-CBA-CGA
29	n	611	CLA	C2A-CAA-CBA-CGA
29	g	613	CLA	C2A-CAA-CBA-CGA
29	r	602	CLA	C2A-CAA-CBA-CGA
29	r	609	CLA	C2A-CAA-CBA-CGA
29	s	617	CLA	C2A-CAA-CBA-CGA
45	G	605	CHL	C2A-CAA-CBA-CGA
45	G	606	CHL	C2A-CAA-CBA-CGA
45	Y	605	CHL	C2A-CAA-CBA-CGA
45	n	605	CHL	C2A-CAA-CBA-CGA
45	y	605	CHL	C2A-CAA-CBA-CGA
29	C	512	CLA	O1A-CGA-O2A-C1
29	S	603	CLA	O1A-CGA-O2A-C1
29	c	512	CLA	O1A-CGA-O2A-C1
29	g	613	CLA	O1A-CGA-O2A-C1
33	A	413	LMG	C17-C18-C19-C20
33	A	413	LMG	C35-C36-C37-C38
33	A	413	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
33	B	622	LMG	C17-C18-C19-C20
33	C	521	LMG	C17-C18-C19-C20
33	C	521	LMG	C35-C36-C37-C38
33	D	411	LMG	C17-C18-C19-C20
33	D	411	LMG	C20-C21-C22-C23
33	H	102	LMG	C38-C39-C40-C41
33	J	101	LMG	C17-C18-C19-C20
33	J	101	LMG	C20-C21-C22-C23
33	a	413	LMG	C17-C18-C19-C20
33	a	413	LMG	C35-C36-C37-C38
33	a	413	LMG	C38-C39-C40-C41
33	b	622	LMG	C17-C18-C19-C20
33	c	521	LMG	C17-C18-C19-C20
33	c	521	LMG	C35-C36-C37-C38
33	d	411	LMG	C17-C18-C19-C20
33	d	411	LMG	C20-C21-C22-C23
33	h	102	LMG	C38-C39-C40-C41
33	j	101	LMG	C17-C18-C19-C20
33	j	101	LMG	C20-C21-C22-C23
38	C	518	DGD	C8B-C9B-CAB-CBB
38	C	519	DGD	C8A-C9A-CAA-CBA
38	C	519	DGD	C8B-C9B-CAB-CBB
38	C	520	DGD	CBB-CCB-CDB-CEB
38	C	523	DGD	CBA-CCA-CDA-CEA
38	C	523	DGD	CEB-CFB-CGB-CHB
38	c	518	DGD	C8B-C9B-CAB-CBB
38	c	519	DGD	C8A-C9A-CAA-CBA
38	c	519	DGD	C8B-C9B-CAB-CBB
38	c	520	DGD	CBB-CCB-CDB-CEB
38	c	523	DGD	CBA-CCA-CDA-CEA
38	c	523	DGD	CEB-CFB-CGB-CHB
29	B	608	CLA	C3-C5-C6-C7
29	N	602	CLA	C3-C5-C6-C7
29	Y	610	CLA	C3-C5-C6-C7
29	c	502	CLA	C3-C5-C6-C7
29	d	403	CLA	C3-C5-C6-C7
29	y	610	CLA	C3-C5-C6-C7
30	A	409	PHO	C3-C5-C6-C7
29	B	603	CLA	CBA-CGA-O2A-C1
29	B	605	CLA	CBA-CGA-O2A-C1
29	D	403	CLA	CBA-CGA-O2A-C1
29	N	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	R	603	CLA	CBA-CGA-O2A-C1
29	R	608	CLA	CBA-CGA-O2A-C1
29	R	612	CLA	CBA-CGA-O2A-C1
29	Y	603	CLA	CBA-CGA-O2A-C1
29	a	405	CLA	CBA-CGA-O2A-C1
29	b	605	CLA	CBA-CGA-O2A-C1
29	g	602	CLA	CBA-CGA-O2A-C1
29	g	614	CLA	CBA-CGA-O2A-C1
29	r	603	CLA	CBA-CGA-O2A-C1
29	r	608	CLA	CBA-CGA-O2A-C1
29	r	609	CLA	CBA-CGA-O2A-C1
29	s	602	CLA	CBA-CGA-O2A-C1
29	s	609	CLA	CBA-CGA-O2A-C1
29	s	617	CLA	CBA-CGA-O2A-C1
29	B	611	CLA	O1D-CGD-O2D-CED
29	C	504	CLA	O1D-CGD-O2D-CED
29	N	602	CLA	O1D-CGD-O2D-CED
29	S	604	CLA	O1D-CGD-O2D-CED
29	b	614	CLA	O1D-CGD-O2D-CED
29	c	503	CLA	O1D-CGD-O2D-CED
29	c	513	CLA	O1D-CGD-O2D-CED
29	r	612	CLA	O1D-CGD-O2D-CED
29	s	604	CLA	O1D-CGD-O2D-CED
29	C	509	CLA	O1D-CGD-O2D-CED
29	G	612	CLA	O1D-CGD-O2D-CED
29	R	612	CLA	O1D-CGD-O2D-CED
29	b	611	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	O1D-CGD-O2D-CED
29	c	509	CLA	O1D-CGD-O2D-CED
29	n	602	CLA	O1D-CGD-O2D-CED
29	s	614	CLA	O1D-CGD-O2D-CED
29	y	612	CLA	O1D-CGD-O2D-CED
39	S	624	LHG	O9-C7-O7-C5
29	D	403	CLA	O1A-CGA-O2A-C1
29	N	603	CLA	O1A-CGA-O2A-C1
29	G	602	CLA	O1A-CGA-O2A-C1
29	R	612	CLA	O1A-CGA-O2A-C1
29	S	609	CLA	O1A-CGA-O2A-C1
29	Y	612	CLA	O1A-CGA-O2A-C1
29	a	405	CLA	O1A-CGA-O2A-C1
29	c	502	CLA	O1A-CGA-O2A-C1
29	d	403	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	r	612	CLA	O1A-CGA-O2A-C1
29	s	609	CLA	O1A-CGA-O2A-C1
29	S	613	CLA	O1D-CGD-O2D-CED
29	c	504	CLA	O1D-CGD-O2D-CED
29	y	614	CLA	O1D-CGD-O2D-CED
47	R	621	XAT	C13-C14-C15-C35
47	r	622	XAT	C13-C14-C15-C35
30	a	409	PHO	CBD-CGD-O2D-CED
29	B	609	CLA	O1D-CGD-O2D-CED
29	B	616	CLA	O1D-CGD-O2D-CED
29	g	612	CLA	O1D-CGD-O2D-CED
39	C	525	LHG	O2-C2-C3-O3
39	D	410	LHG	O2-C2-C3-O3
39	G	630	LHG	O2-C2-C3-O3
39	c	625	LHG	O2-C2-C3-O3
39	d	409	LHG	O2-C2-C3-O3
39	g	624	LHG	O2-C2-C3-O3
39	y	624	LHG	O2-C2-C3-O3
49	S	625	LPX	O1-C3-C4-O5
29	B	610	CLA	C3-C5-C6-C7
29	C	502	CLA	C3-C5-C6-C7
29	c	508	CLA	C3-C5-C6-C7
29	c	511	CLA	C3-C5-C6-C7
29	y	613	CLA	C3-C5-C6-C7
29	B	608	CLA	CBA-CGA-O2A-C1
29	B	613	CLA	CBA-CGA-O2A-C1
29	C	506	CLA	CBA-CGA-O2A-C1
29	C	512	CLA	CBA-CGA-O2A-C1
29	G	602	CLA	CBA-CGA-O2A-C1
29	G	603	CLA	CBA-CGA-O2A-C1
29	G	613	CLA	CBA-CGA-O2A-C1
29	S	602	CLA	CBA-CGA-O2A-C1
29	S	609	CLA	CBA-CGA-O2A-C1
29	Y	613	CLA	CBA-CGA-O2A-C1
29	b	608	CLA	CBA-CGA-O2A-C1
29	c	502	CLA	CBA-CGA-O2A-C1
29	g	604	CLA	CBA-CGA-O2A-C1
29	y	602	CLA	CBA-CGA-O2A-C1
29	y	612	CLA	CBA-CGA-O2A-C1
38	c	519	DGD	C2A-C1A-O1G-C1G
50	i	101	3PH	C32-C31-O31-C3
29	B	605	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	G	613	CLA	O1A-CGA-O2A-C1
29	R	603	CLA	O1A-CGA-O2A-C1
29	R	608	CLA	O1A-CGA-O2A-C1
29	S	602	CLA	O1A-CGA-O2A-C1
29	b	605	CLA	O1A-CGA-O2A-C1
29	r	603	CLA	O1A-CGA-O2A-C1
29	r	608	CLA	O1A-CGA-O2A-C1
29	A	410	CLA	O1D-CGD-O2D-CED
29	G	611	CLA	O1D-CGD-O2D-CED
29	Y	612	CLA	O1D-CGD-O2D-CED
29	d	402	CLA	O1D-CGD-O2D-CED
29	g	602	CLA	O1D-CGD-O2D-CED
29	g	604	CLA	O1D-CGD-O2D-CED
29	s	612	CLA	O1D-CGD-O2D-CED
29	s	613	CLA	O1D-CGD-O2D-CED
29	y	603	CLA	O1D-CGD-O2D-CED
30	A	409	PHO	O1D-CGD-O2D-CED
49	S	625	LPX	O5-C4-C5-O6
38	c	519	DGD	C2B-C1B-O2G-C2G
29	Y	602	CLA	O1D-CGD-O2D-CED
48	r	623	NEX	C14-C15-C35-C34
29	C	513	CLA	O1D-CGD-O2D-CED
29	Y	603	CLA	O1D-CGD-O2D-CED
39	l	101	LHG	C11-C10-C9-C8
29	S	603	CLA	CBA-CGA-O2A-C1
29	c	512	CLA	CBA-CGA-O2A-C1
29	d	403	CLA	CBA-CGA-O2A-C1
29	g	613	CLA	CBA-CGA-O2A-C1
29	G	603	CLA	O1A-CGA-O2A-C1
29	b	608	CLA	O1A-CGA-O2A-C1
29	r	609	CLA	O1A-CGA-O2A-C1
39	L	101	LHG	C11-C10-C9-C8
29	b	612	CLA	C4-C3-C5-C6
29	c	501	CLA	C4-C3-C5-C6
45	Y	601	CHL	C4-C3-C5-C6
45	n	601	CHL	C4-C3-C5-C6
29	b	604	CLA	C2-C3-C5-C6
29	b	612	CLA	C2-C3-C5-C6
45	Y	601	CHL	C2-C3-C5-C6
45	n	601	CHL	C2-C3-C5-C6
29	R	602	CLA	C2A-CAA-CBA-CGA
29	g	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	r	603	CLA	C2A-CAA-CBA-CGA
45	g	605	CHL	C2A-CAA-CBA-CGA
29	R	613	CLA	O1D-CGD-O2D-CED
29	a	410	CLA	O1D-CGD-O2D-CED
29	B	613	CLA	O1A-CGA-O2A-C1
29	C	506	CLA	O1A-CGA-O2A-C1
29	C	510	CLA	O1A-CGA-O2A-C1
29	R	609	CLA	O1A-CGA-O2A-C1
29	g	604	CLA	O1A-CGA-O2A-C1
29	y	602	CLA	O1A-CGA-O2A-C1
29	y	612	CLA	O1A-CGA-O2A-C1
42	d	405	PL9	C34-C36-C37-C38
29	A	405	CLA	CBA-CGA-O2A-C1
29	B	606	CLA	CBA-CGA-O2A-C1
29	C	510	CLA	CBA-CGA-O2A-C1
29	R	604	CLA	CBA-CGA-O2A-C1
29	R	609	CLA	CBA-CGA-O2A-C1
29	Y	602	CLA	CBA-CGA-O2A-C1
29	b	614	CLA	CBA-CGA-O2A-C1
29	c	506	CLA	CBA-CGA-O2A-C1
29	r	604	CLA	CBA-CGA-O2A-C1
39	d	410	LHG	C25-C26-C27-C28
29	n	611	CLA	O1D-CGD-O2D-CED
29	r	604	CLA	O1D-CGD-O2D-CED
29	D	402	CLA	O1D-CGD-O2D-CED
29	G	602	CLA	O1D-CGD-O2D-CED
29	R	610	CLA	O1D-CGD-O2D-CED
29	S	605	CLA	O1D-CGD-O2D-CED
29	b	616	CLA	O1D-CGD-O2D-CED
29	c	501	CLA	O1D-CGD-O2D-CED
29	c	510	CLA	O1D-CGD-O2D-CED
29	g	611	CLA	O1D-CGD-O2D-CED
29	B	608	CLA	O1A-CGA-O2A-C1
29	Y	613	CLA	O1A-CGA-O2A-C1
38	c	519	DGD	O1A-C1A-O1G-C1G
29	R	604	CLA	O1D-CGD-O2D-CED
29	S	611	CLA	O1D-CGD-O2D-CED
29	s	605	CLA	O1D-CGD-O2D-CED
29	C	505	CLA	CBD-CGD-O2D-CED
29	c	505	CLA	CBD-CGD-O2D-CED
39	D	409	LHG	C1-C2-C3-O3
38	c	519	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
29	B	606	CLA	O1A-CGA-O2A-C1
29	Y	602	CLA	O1A-CGA-O2A-C1
29	b	606	CLA	O1A-CGA-O2A-C1
29	b	611	CLA	O1A-CGA-O2A-C1
29	c	506	CLA	O1A-CGA-O2A-C1
29	S	604	CLA	C3-C5-C6-C7
29	n	610	CLA	C3-C5-C6-C7
29	N	611	CLA	O1D-CGD-O2D-CED
29	A	410	CLA	CBA-CGA-O2A-C1
29	B	611	CLA	CBA-CGA-O2A-C1
29	B	614	CLA	CBA-CGA-O2A-C1
29	C	509	CLA	CBA-CGA-O2A-C1
29	N	614	CLA	CBA-CGA-O2A-C1
29	b	602	CLA	CBA-CGA-O2A-C1
29	b	606	CLA	CBA-CGA-O2A-C1
29	b	611	CLA	CBA-CGA-O2A-C1
29	b	613	CLA	CBA-CGA-O2A-C1
29	c	503	CLA	CBA-CGA-O2A-C1
29	c	509	CLA	CBA-CGA-O2A-C1
29	c	510	CLA	CBA-CGA-O2A-C1
29	g	603	CLA	CBA-CGA-O2A-C1
29	s	611	CLA	CBA-CGA-O2A-C1
29	y	613	CLA	CBA-CGA-O2A-C1
38	C	519	DGD	C2A-C1A-O1G-C1G
39	c	625	LHG	C24-C23-O8-C6
31	B	618	BCR	C9-C10-C11-C12
35	b	620	C7Z	C9-C10-C11-C12
29	C	502	CLA	C5-C6-C7-C8
29	b	612	CLA	C13-C15-C16-C17
29	c	509	CLA	C10-C11-C12-C13
29	g	603	CLA	O1A-CGA-O2A-C1
49	s	625	LPX	C3-C4-C5-O6
29	C	510	CLA	O1D-CGD-O2D-CED
29	y	602	CLA	O1D-CGD-O2D-CED
39	S	624	LHG	O6-C4-C5-O7
29	A	410	CLA	C10-C11-C12-C13
29	N	602	CLA	C5-C6-C7-C8
29	G	602	CLA	C13-C15-C16-C17
29	c	502	CLA	C8-C10-C11-C12
29	c	506	CLA	C8-C10-C11-C12
29	r	612	CLA	C8-C10-C11-C12
39	S	624	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
32	b	621	SQD	C23-C24-C25-C26
36	c	524	DGA	CB1-CB2-CB3-CB4
38	c	519	DGD	C1B-C2B-C3B-C4B
39	C	525	LHG	C7-C8-C9-C10
32	C	526	SQD	C2-C1-O6-C44
32	a	412	SQD	C2-C1-O6-C44
32	c	626	SQD	C2-C1-O6-C44
38	C	519	DGD	C2D-C1D-O3G-C3G
38	c	519	DGD	C2D-C1D-O3G-C3G
39	G	630	LHG	O7-C5-C6-O8
29	B	611	CLA	O1A-CGA-O2A-C1
29	b	613	CLA	O1A-CGA-O2A-C1
29	y	613	CLA	O1A-CGA-O2A-C1
29	g	602	CLA	C4-C3-C5-C6
29	B	603	CLA	C14-C13-C15-C16
29	C	506	CLA	C11-C12-C13-C14
29	C	507	CLA	C11-C10-C8-C9
29	C	507	CLA	C14-C13-C15-C16
29	C	513	CLA	C11-C10-C8-C9
29	G	602	CLA	C14-C13-C15-C16
29	R	603	CLA	C11-C10-C8-C9
29	b	603	CLA	C14-C13-C15-C16
29	c	502	CLA	C6-C7-C8-C9
29	c	502	CLA	C11-C12-C13-C14
29	c	506	CLA	C11-C12-C13-C14
29	c	507	CLA	C11-C10-C8-C9
29	c	507	CLA	C14-C13-C15-C16
29	c	513	CLA	C11-C10-C8-C9
29	g	602	CLA	C14-C13-C15-C16
29	r	603	CLA	C11-C10-C8-C9
30	A	409	PHO	C6-C7-C8-C9
30	a	409	PHO	C6-C7-C8-C9
45	Y	601	CHL	C11-C10-C8-C9
45	Y	607	CHL	C11-C10-C8-C9
45	n	605	CHL	C14-C13-C15-C16
45	n	607	CHL	C14-C13-C15-C16
45	y	609	CHL	C11-C12-C13-C14
29	C	501	CLA	O1D-CGD-O2D-CED
29	b	613	CLA	O1D-CGD-O2D-CED
29	C	507	CLA	C5-C6-C7-C8
29	C	507	CLA	C15-C16-C17-C18
29	c	504	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	g	613	CLA	C10-C11-C12-C13
29	c	505	CLA	C2A-CAA-CBA-CGA
45	r	607	CHL	C2A-CAA-CBA-CGA
44	H	101	RRX	C36-C18-C19-C20
44	h	101	RRX	C36-C18-C19-C20
46	R	620	LUT	C7-C8-C9-C19
46	r	620	LUT	C7-C8-C9-C19
46	r	620	LUT	C31-C32-C33-C40
44	H	101	RRX	C17-C18-C19-C20
44	h	101	RRX	C17-C18-C19-C20
46	r	620	LUT	C7-C8-C9-C10
49	s	625	LPX	O5-C4-C5-O6
38	C	519	DGD	C2B-C1B-O2G-C2G
32	B	621	SQD	C23-C24-C25-C26
36	C	524	DGA	CB1-CB2-CB3-CB4
38	c	518	DGD	C1A-C2A-C3A-C4A
39	D	408	LHG	C7-C8-C9-C10
39	d	408	LHG	C7-C8-C9-C10
42	D	405	PL9	C47-C48-C49-C51
29	B	614	CLA	O1A-CGA-O2A-C1
29	b	602	CLA	O1A-CGA-O2A-C1
29	c	510	CLA	O1A-CGA-O2A-C1
38	C	519	DGD	O1A-C1A-O1G-C1G
29	C	501	CLA	C8-C10-C11-C12
29	Y	611	CLA	C10-C11-C12-C13
29	a	410	CLA	C8-C10-C11-C12
29	b	610	CLA	C15-C16-C17-C18
29	n	603	CLA	C10-C11-C12-C13
29	g	610	CLA	C8-C10-C11-C12
29	r	608	CLA	C8-C10-C11-C12
29	Y	611	CLA	O1D-CGD-O2D-CED
29	n	603	CLA	O1D-CGD-O2D-CED
29	C	508	CLA	C3-C5-C6-C7
29	R	602	CLA	CBA-CGA-O2A-C1
29	Y	614	CLA	CBA-CGA-O2A-C1
29	a	410	CLA	CBA-CGA-O2A-C1
29	y	614	CLA	CBA-CGA-O2A-C1
29	B	602	CLA	C5-C6-C7-C8
29	B	611	CLA	C15-C16-C17-C18
29	B	612	CLA	C15-C16-C17-C18
29	C	502	CLA	C8-C10-C11-C12
29	C	502	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	C	503	CLA	C10-C11-C12-C13
29	C	503	CLA	C15-C16-C17-C18
29	C	508	CLA	C10-C11-C12-C13
29	N	603	CLA	C5-C6-C7-C8
29	N	603	CLA	C13-C15-C16-C17
29	N	604	CLA	C10-C11-C12-C13
29	Y	602	CLA	C15-C16-C17-C18
29	Y	610	CLA	C5-C6-C7-C8
29	b	606	CLA	C15-C16-C17-C18
29	b	617	CLA	C5-C6-C7-C8
29	c	507	CLA	C5-C6-C7-C8
29	c	512	CLA	C13-C15-C16-C17
29	g	602	CLA	C13-C15-C16-C17
29	y	603	CLA	C13-C15-C16-C17
29	y	604	CLA	C15-C16-C17-C18
29	y	610	CLA	C13-C15-C16-C17
29	y	613	CLA	C15-C16-C17-C18
39	Y	624	LHG	C33-C34-C35-C36
39	D	408	LHG	C23-C24-C25-C26
39	N	624	LHG	C7-C8-C9-C10
39	d	408	LHG	C23-C24-C25-C26
29	n	604	CLA	O1D-CGD-O2D-CED
29	s	611	CLA	O1D-CGD-O2D-CED
29	c	509	CLA	O1A-CGA-O2A-C1
29	B	605	CLA	C8-C10-C11-C12
29	B	606	CLA	C15-C16-C17-C18
29	B	607	CLA	C8-C10-C11-C12
29	B	607	CLA	C10-C11-C12-C13
29	B	617	CLA	C5-C6-C7-C8
29	D	403	CLA	C15-C16-C17-C18
29	N	604	CLA	C13-C15-C16-C17
29	R	612	CLA	C10-C11-C12-C13
29	S	603	CLA	C13-C15-C16-C17
29	S	613	CLA	C5-C6-C7-C8
29	Y	604	CLA	C15-C16-C17-C18
29	Y	611	CLA	C5-C6-C7-C8
29	Y	613	CLA	C15-C16-C17-C18
29	b	602	CLA	C5-C6-C7-C8
29	b	602	CLA	C15-C16-C17-C18
29	b	604	CLA	C15-C16-C17-C18
29	b	607	CLA	C13-C15-C16-C17
29	b	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	c	505	CLA	C13-C15-C16-C17
29	c	507	CLA	C15-C16-C17-C18
29	n	602	CLA	C5-C6-C7-C8
29	s	613	CLA	C5-C6-C7-C8
29	y	603	CLA	C15-C16-C17-C18
29	y	604	CLA	C5-C6-C7-C8
29	y	610	CLA	C5-C6-C7-C8
29	y	611	CLA	C8-C10-C11-C12
29	y	613	CLA	C8-C10-C11-C12
39	Y	624	LHG	O1-C1-C2-O2
29	A	410	CLA	O1A-CGA-O2A-C1
38	c	518	DGD	C1B-C2B-C3B-C4B
39	C	525	LHG	C23-C24-C25-C26
39	D	410	LHG	C7-C8-C9-C10
39	c	625	LHG	C23-C24-C25-C26
39	d	410	LHG	C7-C8-C9-C10
49	s	625	LPX	C6-C7-C8-C9
29	A	410	CLA	C8-C10-C11-C12
29	B	608	CLA	C15-C16-C17-C18
29	B	616	CLA	C5-C6-C7-C8
29	B	617	CLA	C13-C15-C16-C17
29	C	501	CLA	C13-C15-C16-C17
29	R	602	CLA	C8-C10-C11-C12
29	R	612	CLA	C8-C10-C11-C12
29	Y	603	CLA	C5-C6-C7-C8
29	Y	610	CLA	C13-C15-C16-C17
29	Y	614	CLA	C8-C10-C11-C12
29	b	608	CLA	C15-C16-C17-C18
29	b	613	CLA	C15-C16-C17-C18
29	c	503	CLA	C15-C16-C17-C18
29	c	505	CLA	C5-C6-C7-C8
29	n	604	CLA	C10-C11-C12-C13
29	r	608	CLA	C5-C6-C7-C8
29	s	603	CLA	C5-C6-C7-C8
29	s	610	CLA	C5-C6-C7-C8
29	s	610	CLA	C15-C16-C17-C18
29	C	507	CLA	CBA-CGA-O2A-C1
29	S	614	CLA	CBA-CGA-O2A-C1
29	B	613	CLA	O1D-CGD-O2D-CED
29	N	603	CLA	O1D-CGD-O2D-CED
29	B	602	CLA	C2-C1-O2A-CGA
29	B	608	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	B	612	CLA	C2-C1-O2A-CGA
29	C	512	CLA	C2-C1-O2A-CGA
29	N	614	CLA	C2-C1-O2A-CGA
29	Y	614	CLA	C2-C1-O2A-CGA
29	b	602	CLA	C2-C1-O2A-CGA
29	b	605	CLA	C2-C1-O2A-CGA
29	b	608	CLA	C2-C1-O2A-CGA
29	b	614	CLA	C2-C1-O2A-CGA
29	c	506	CLA	C2-C1-O2A-CGA
29	c	512	CLA	C2-C1-O2A-CGA
29	n	613	CLA	C2-C1-O2A-CGA
29	g	614	CLA	C2-C1-O2A-CGA
29	r	602	CLA	C2-C1-O2A-CGA
29	r	603	CLA	C2-C1-O2A-CGA
29	s	610	CLA	C2-C1-O2A-CGA
29	s	614	CLA	C2-C1-O2A-CGA
29	s	617	CLA	C2-C1-O2A-CGA
29	y	603	CLA	C2-C1-O2A-CGA
42	D	405	PL9	C42-C43-C44-C46
29	B	604	CLA	C5-C6-C7-C8
29	B	613	CLA	C5-C6-C7-C8
29	B	613	CLA	C13-C15-C16-C17
29	C	504	CLA	C13-C15-C16-C17
29	C	505	CLA	C5-C6-C7-C8
29	Y	613	CLA	C8-C10-C11-C12
29	b	612	CLA	C15-C16-C17-C18
29	b	614	CLA	C10-C11-C12-C13
29	c	503	CLA	C5-C6-C7-C8
29	d	402	CLA	C15-C16-C17-C18
29	d	403	CLA	C8-C10-C11-C12
29	g	613	CLA	C15-C16-C17-C18
39	D	410	LHG	C23-C24-C25-C26
39	n	624	LHG	C7-C8-C9-C10
39	s	624	LHG	C23-C24-C25-C26
43	F	101	HEM	C3D-CAD-CBD-CGD
29	Y	614	CLA	C10-C11-C12-C13
29	n	603	CLA	C8-C10-C11-C12
29	n	613	CLA	C8-C10-C11-C12
29	y	612	CLA	C13-C15-C16-C17
29	y	612	CLA	C15-C16-C17-C18
45	n	601	CHL	C8-C10-C11-C12
29	r	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	603	CLA	C12-C13-C15-C16
29	B	604	CLA	C6-C7-C8-C10
29	c	506	CLA	C11-C12-C13-C15
29	s	609	CLA	C11-C10-C8-C7
29	A	405	CLA	O1A-CGA-O2A-C1
29	N	614	CLA	O1A-CGA-O2A-C1
31	b	618	BCR	C9-C10-C11-C12
31	c	517	BCR	C9-C10-C11-C12
44	H	101	RRX	C19-C20-C21-C22
44	h	101	RRX	C19-C20-C21-C22
46	G	621	LUT	C29-C30-C31-C32
46	n	621	LUT	C29-C30-C31-C32
29	B	612	CLA	C2A-CAA-CBA-CGA
29	R	603	CLA	C2A-CAA-CBA-CGA
29	S	613	CLA	C2A-CAA-CBA-CGA
29	S	614	CLA	C2A-CAA-CBA-CGA
29	Y	610	CLA	C2A-CAA-CBA-CGA
29	a	405	CLA	C2A-CAA-CBA-CGA
29	s	610	CLA	C2A-CAA-CBA-CGA
29	N	604	CLA	O1D-CGD-O2D-CED
29	y	611	CLA	O1D-CGD-O2D-CED
29	B	607	CLA	C13-C15-C16-C17
29	B	607	CLA	C15-C16-C17-C18
29	B	614	CLA	C10-C11-C12-C13
29	C	505	CLA	C13-C15-C16-C17
29	N	613	CLA	C5-C6-C7-C8
29	N	613	CLA	C8-C10-C11-C12
29	R	609	CLA	C5-C6-C7-C8
29	S	609	CLA	C10-C11-C12-C13
29	Y	612	CLA	C13-C15-C16-C17
29	b	608	CLA	C10-C11-C12-C13
29	b	614	CLA	C5-C6-C7-C8
29	c	506	CLA	C5-C6-C7-C8
29	n	602	CLA	C15-C16-C17-C18
29	r	602	CLA	C8-C10-C11-C12
29	y	611	CLA	C5-C6-C7-C8
29	y	614	CLA	C8-C10-C11-C12
29	y	614	CLA	C13-C15-C16-C17
29	C	507	CLA	O1A-CGA-O2A-C1
29	C	509	CLA	O1A-CGA-O2A-C1
29	c	503	CLA	O1A-CGA-O2A-C1
29	S	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	b	622	LMG	O6-C1-O1-C7
33	j	101	LMG	O6-C1-O1-C7
38	c	519	DGD	O6D-C1D-O3G-C3G
29	B	603	CLA	C10-C11-C12-C13
29	B	614	CLA	C5-C6-C7-C8
29	C	506	CLA	C5-C6-C7-C8
29	C	506	CLA	C8-C10-C11-C12
29	Y	602	CLA	C8-C10-C11-C12
31	C	515	BCR	C10-C11-C12-C13
31	c	517	BCR	C10-C11-C12-C13
48	R	622	NEX	C30-C31-C32-C33
33	D	411	LMG	C35-C36-C37-C38
33	d	411	LMG	C35-C36-C37-C38
29	c	506	CLA	O1D-CGD-O2D-CED
39	D	408	LHG	O2-C2-C3-O3
39	L	101	LHG	O2-C2-C3-O3
39	l	101	LHG	O2-C2-C3-O3
38	C	519	DGD	O1B-C1B-O2G-C2G
29	n	603	CLA	C3-C5-C6-C7
29	y	614	CLA	C3-C5-C6-C7
29	B	602	CLA	C13-C15-C16-C17
29	B	610	CLA	C13-C15-C16-C17
29	B	613	CLA	C15-C16-C17-C18
29	C	502	CLA	C15-C16-C17-C18
29	G	610	CLA	C5-C6-C7-C8
29	R	602	CLA	C5-C6-C7-C8
29	S	602	CLA	C10-C11-C12-C13
29	S	610	CLA	C8-C10-C11-C12
29	b	603	CLA	C10-C11-C12-C13
29	c	508	CLA	C10-C11-C12-C13
29	g	603	CLA	C10-C11-C12-C13
29	y	611	CLA	C10-C11-C12-C13
29	y	614	CLA	C10-C11-C12-C13
45	n	607	CHL	C8-C10-C11-C12
29	B	612	CLA	CBA-CGA-O2A-C1
29	R	602	CLA	O1A-CGA-O2A-C1
29	R	604	CLA	O1A-CGA-O2A-C1
29	Y	614	CLA	O1A-CGA-O2A-C1
29	a	410	CLA	O1A-CGA-O2A-C1
29	b	614	CLA	O1A-CGA-O2A-C1
29	r	604	CLA	O1A-CGA-O2A-C1
29	s	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	y	614	CLA	O1A-CGA-O2A-C1
39	c	625	LHG	O10-C23-O8-C6
39	s	624	LHG	C7-C8-C9-C10
29	B	604	CLA	C13-C15-C16-C17
29	C	505	CLA	C10-C11-C12-C13
29	C	506	CLA	C13-C15-C16-C17
29	C	507	CLA	C8-C10-C11-C12
29	C	513	CLA	C10-C11-C12-C13
29	R	608	CLA	C5-C6-C7-C8
29	Y	610	CLA	C15-C16-C17-C18
29	Y	613	CLA	C13-C15-C16-C17
29	b	603	CLA	C13-C15-C16-C17
29	c	507	CLA	C8-C10-C11-C12
29	c	507	CLA	C13-C15-C16-C17
29	c	513	CLA	C10-C11-C12-C13
29	g	603	CLA	C8-C10-C11-C12
45	Y	606	CHL	C15-C16-C17-C18
33	a	413	LMG	C11-C10-O7-C8
39	G	630	LHG	C8-C7-O7-C5
38	c	518	DGD	CAB-CBB-CCB-CDB
29	B	604	CLA	C8-C10-C11-C12
29	C	503	CLA	C5-C6-C7-C8
29	C	506	CLA	C15-C16-C17-C18
29	b	607	CLA	C8-C10-C11-C12
29	b	607	CLA	C10-C11-C12-C13
29	b	608	CLA	C13-C15-C16-C17
29	d	403	CLA	C15-C16-C17-C18
29	g	610	CLA	C15-C16-C17-C18
29	y	604	CLA	C8-C10-C11-C12
39	C	525	LHG	C3-O3-P-O6
39	C	525	LHG	C4-O6-P-O3
39	D	408	LHG	C3-O3-P-O6
39	D	408	LHG	C4-O6-P-O3
39	D	410	LHG	C3-O3-P-O6
39	D	410	LHG	C4-O6-P-O3
39	L	101	LHG	C3-O3-P-O6
39	N	624	LHG	C4-O6-P-O3
39	G	630	LHG	C4-O6-P-O3
39	S	624	LHG	C4-O6-P-O3
39	d	408	LHG	C4-O6-P-O3
39	d	409	LHG	C3-O3-P-O6
39	d	410	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
39	l	101	LHG	C3-O3-P-O6
39	n	624	LHG	C4-O6-P-O3
39	g	624	LHG	C4-O6-P-O3
39	s	624	LHG	C4-O6-P-O3
39	y	624	LHG	C4-O6-P-O3
49	S	625	LPX	C1-O2-P1-O1
49	s	625	LPX	C1-O2-P1-O1
39	G	630	LHG	C7-C8-C9-C10
29	C	510	CLA	C3-C5-C6-C7
29	B	602	CLA	CBA-CGA-O2A-C1
29	n	602	CLA	CBA-CGA-O2A-C1
38	c	520	DGD	C2A-C1A-O1G-C1G
39	d	410	LHG	C24-C23-O8-C6
29	B	610	CLA	C15-C16-C17-C18
29	C	509	CLA	C10-C11-C12-C13
29	b	611	CLA	C15-C16-C17-C18
29	c	506	CLA	C13-C15-C16-C17
29	S	614	CLA	O1A-CGA-O2A-C1
29	C	506	CLA	O1D-CGD-O2D-CED
39	c	625	LHG	C1-C2-C3-O3
33	a	413	LMG	O9-C10-O7-C8
39	G	630	LHG	O9-C7-O7-C5
29	n	613	CLA	C4-C3-C5-C6
45	y	607	CHL	C4-C3-C5-C6
29	C	505	CLA	C2A-CAA-CBA-CGA
29	N	602	CLA	C2A-CAA-CBA-CGA
29	Y	602	CLA	C2A-CAA-CBA-CGA
29	Y	613	CLA	C2A-CAA-CBA-CGA
29	n	602	CLA	C2A-CAA-CBA-CGA
29	s	613	CLA	C2A-CAA-CBA-CGA
29	y	602	CLA	C2A-CAA-CBA-CGA
29	y	613	CLA	C2A-CAA-CBA-CGA
29	B	612	CLA	C16-C17-C18-C20
29	c	505	CLA	C16-C17-C18-C19
29	C	503	CLA	CBA-CGA-O2A-C1
29	c	507	CLA	CBA-CGA-O2A-C1
29	s	604	CLA	CBA-CGA-O2A-C1
38	c	518	DGD	CCB-CDB-CEB-CFB
46	g	621	LUT	C29-C30-C31-C32
46	y	621	LUT	C29-C30-C31-C32
48	S	622	NEX	C13-C14-C15-C35
39	L	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
39	S	624	LHG	C23-C24-C25-C26
36	b	623	DGA	CA6-CA7-CA8-CA9
36	c	524	DGA	CB2-CB1-OG2-CG2
39	g	624	LHG	C8-C7-O7-C5
39	y	624	LHG	C8-C7-O7-C5
50	i	101	3PH	C22-C21-O21-C2
29	c	506	CLA	C15-C16-C17-C18
29	n	610	CLA	C5-C6-C7-C8
47	R	621	XAT	C20-C13-C14-C15
47	R	621	XAT	C40-C33-C34-C35
48	N	623	NEX	C39-C29-C30-C31
48	G	623	NEX	C39-C29-C30-C31
48	R	622	NEX	C39-C29-C30-C31
48	R	622	NEX	C40-C33-C34-C35
48	S	622	NEX	C40-C33-C34-C35
48	Y	623	NEX	C39-C29-C30-C31
48	n	623	NEX	C39-C29-C30-C31
48	g	623	NEX	C39-C29-C30-C31
48	r	623	NEX	C39-C29-C30-C31
48	s	623	NEX	C11-C10-C9-C19
48	s	623	NEX	C40-C33-C34-C35
48	y	623	NEX	C39-C29-C30-C31
32	A	412	SQD	C30-C31-C32-C33
33	B	622	LMG	C15-C16-C17-C18
39	G	630	LHG	C31-C32-C33-C34
39	S	624	LHG	C30-C31-C32-C33
39	c	625	LHG	C24-C25-C26-C27
39	d	410	LHG	C26-C27-C28-C29
39	g	624	LHG	C13-C14-C15-C16
29	G	602	CLA	C16-C17-C18-C19
29	R	609	CLA	C11-C12-C13-C15
29	S	602	CLA	C11-C12-C13-C15
29	S	613	CLA	C6-C7-C8-C9
29	Y	613	CLA	C16-C17-C18-C20
29	c	513	CLA	C16-C17-C18-C19
29	n	604	CLA	C16-C17-C18-C19
29	r	609	CLA	C11-C12-C13-C14
29	r	612	CLA	C11-C12-C13-C15
29	y	604	CLA	C16-C17-C18-C19
29	y	610	CLA	C16-C17-C18-C20
32	A	412	SQD	C14-C15-C16-C17
36	c	524	DGA	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
39	N	624	LHG	C15-C16-C17-C18
39	G	630	LHG	C10-C11-C12-C13
39	Y	624	LHG	C30-C31-C32-C33
39	d	408	LHG	C13-C14-C15-C16
39	d	409	LHG	C26-C27-C28-C29
39	g	624	LHG	C31-C32-C33-C34
39	s	624	LHG	C30-C31-C32-C33
50	S	626	3PH	C3E-C3F-C3G-C3H
36	c	524	DGA	OB1-CB1-OG2-CG2
39	g	624	LHG	O9-C7-O7-C5
50	i	101	3PH	O22-C21-O21-C2
29	B	609	CLA	C15-C16-C17-C18
39	g	624	LHG	C7-C8-C9-C10
50	s	626	3PH	C21-C22-C23-C24
36	B	625	DGA	CA6-CA7-CA8-CA9
36	B	625	DGA	CDA-CEA-CFA-CGA
36	C	524	DGA	CDA-CEA-CFA-CGA
39	y	624	LHG	C11-C10-C9-C8
50	s	626	3PH	C3E-C3F-C3G-C3H
51	Y	625	SPH	C10-C11-C12-C13
39	D	408	LHG	C13-C14-C15-C16
39	N	624	LHG	C13-C14-C15-C16
39	n	624	LHG	C13-C14-C15-C16
39	N	624	LHG	O2-C2-C3-O3
36	C	524	DGA	CB5-CB6-CB7-CB8
38	C	520	DGD	C3B-C4B-C5B-C6B
39	D	408	LHG	C33-C34-C35-C36
39	l	101	LHG	C33-C34-C35-C36
39	n	624	LHG	C26-C27-C28-C29
29	a	405	CLA	C3-C5-C6-C7
39	y	624	LHG	C7-C8-C9-C10
49	S	625	LPX	C6-C7-C8-C9
47	R	621	XAT	C12-C13-C14-C15
47	R	621	XAT	C32-C33-C34-C35
47	r	622	XAT	C12-C13-C14-C15
48	N	623	NEX	C28-C29-C30-C31
48	G	623	NEX	C28-C29-C30-C31
48	R	622	NEX	C28-C29-C30-C31
48	R	622	NEX	C32-C33-C34-C35
48	S	622	NEX	C32-C33-C34-C35
48	Y	623	NEX	C28-C29-C30-C31
48	n	623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
48	g	623	NEX	C28-C29-C30-C31
48	r	623	NEX	C28-C29-C30-C31
48	s	623	NEX	C11-C10-C9-C8
48	s	623	NEX	C32-C33-C34-C35
48	y	623	NEX	C28-C29-C30-C31
29	S	604	CLA	CBA-CGA-O2A-C1
29	S	610	CLA	CBA-CGA-O2A-C1
38	C	520	DGD	C2A-C1A-O1G-C1G
33	c	521	LMG	C29-C30-C31-C32
36	c	524	DGA	CDA-CEA-CFA-CGA
36	c	524	DGA	CB2-CB3-CB4-CB5
39	N	624	LHG	C26-C27-C28-C29
39	d	408	LHG	C28-C29-C30-C31
39	d	409	LHG	C29-C30-C31-C32
51	y	625	SPH	C7-C8-C9-C10
29	G	613	CLA	C8-C10-C11-C12
29	C	503	CLA	O1A-CGA-O2A-C1
29	B	617	CLA	C16-C17-C18-C19
29	C	507	CLA	C16-C17-C18-C19
29	C	507	CLA	C16-C17-C18-C20
29	G	613	CLA	C16-C17-C18-C19
29	c	507	CLA	C16-C17-C18-C19
29	s	613	CLA	C6-C7-C8-C10
29	y	611	CLA	C16-C17-C18-C19
29	y	613	CLA	C16-C17-C18-C19
29	c	510	CLA	C4-C3-C5-C6
32	a	412	SQD	C14-C15-C16-C17
36	B	625	DGA	CB7-CB8-CB9-CAB
39	L	101	LHG	C33-C34-C35-C36
39	c	625	LHG	C28-C29-C30-C31
29	c	510	CLA	C2-C3-C5-C6
45	y	607	CHL	C2-C3-C5-C6
29	A	405	CLA	C11-C12-C13-C14
29	C	511	CLA	C11-C10-C8-C9
29	Y	610	CLA	C11-C12-C13-C14
29	Y	613	CLA	C6-C7-C8-C9
29	Y	613	CLA	C11-C12-C13-C14
29	b	602	CLA	C6-C7-C8-C9
29	b	616	CLA	C11-C10-C8-C9
29	c	502	CLA	C14-C13-C15-C16
29	g	603	CLA	C14-C13-C15-C16
29	y	604	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	y	610	CLA	C11-C12-C13-C14
29	y	613	CLA	C11-C12-C13-C14
45	g	609	CHL	C11-C12-C13-C14
39	l	101	LHG	C7-C8-C9-C10
32	B	621	SQD	C30-C31-C32-C33
32	B	621	SQD	C32-C33-C34-C35
32	b	621	SQD	C32-C33-C34-C35
33	C	521	LMG	C29-C30-C31-C32
33	j	101	LMG	C31-C32-C33-C34
39	D	408	LHG	C28-C29-C30-C31
39	D	409	LHG	C26-C27-C28-C29
39	d	408	LHG	C33-C34-C35-C36
29	C	512	CLA	C8-C10-C11-C12
29	N	610	CLA	C15-C16-C17-C18
29	c	512	CLA	C15-C16-C17-C18
29	r	608	CLA	C10-C11-C12-C13
29	b	602	CLA	C2A-CAA-CBA-CGA
29	B	602	CLA	O1A-CGA-O2A-C1
29	c	507	CLA	O1A-CGA-O2A-C1
39	d	410	LHG	O10-C23-O8-C6
39	C	525	LHG	O1-C1-C2-C3
39	D	408	LHG	O1-C1-C2-C3
39	D	409	LHG	O1-C1-C2-C3
39	D	410	LHG	O1-C1-C2-C3
39	N	624	LHG	O1-C1-C2-C3
39	S	624	LHG	O1-C1-C2-C3
39	Y	624	LHG	O1-C1-C2-C3
39	d	409	LHG	O1-C1-C2-C3
39	n	624	LHG	O1-C1-C2-C3
39	y	624	LHG	O1-C1-C2-C3
31	A	411	BCR	C11-C12-C13-C14
31	c	515	BCR	C7-C8-C9-C10
44	H	101	RRX	C7-C8-C9-C10
29	Y	614	CLA	C3-C5-C6-C7
36	C	524	DGA	OB1-CB1-OG2-CG2
39	d	408	LHG	O9-C7-O7-C5
39	y	624	LHG	O9-C7-O7-C5
29	D	403	CLA	C13-C15-C16-C17
36	C	524	DGA	CB2-CB1-OG2-CG2
39	d	408	LHG	C8-C7-O7-C5
32	c	626	SQD	C31-C32-C33-C34
36	C	524	DGA	CA7-CA8-CA9-CAA

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Mol	Chain	Res	Type	Atoms
38	c	520	DGD	C3B-C4B-C5B-C6B
39	D	409	LHG	C29-C30-C31-C32
39	D	409	LHG	C31-C32-C33-C34
39	L	101	LHG	C13-C14-C15-C16
39	Y	624	LHG	C28-C29-C30-C31
38	C	518	DGD	C1B-C2B-C3B-C4B
39	G	630	LHG	C23-C24-C25-C26
39	S	624	LHG	C7-C8-C9-C10
39	d	410	LHG	C23-C24-C25-C26
33	B	622	LMG	C18-C19-C20-C21
33	c	521	LMG	C15-C16-C17-C18
33	c	521	LMG	C16-C17-C18-C19
36	B	625	DGA	CA4-CA5-CA6-CA7
36	b	623	DGA	CDB-CEB-CFB-CGB
38	C	523	DGD	C9B-CAB-CBB-CCB
39	l	101	LHG	C13-C14-C15-C16
39	y	624	LHG	C11-C12-C13-C14
50	S	626	3PH	C22-C23-C24-C25
50	S	626	3PH	C27-C28-C29-C2A
29	s	604	CLA	O1A-CGA-O2A-C1
29	A	407	CLA	C4B-C3B-CAB-CBB
29	B	617	CLA	C4B-C3B-CAB-CBB
29	C	501	CLA	C4B-C3B-CAB-CBB
29	D	403	CLA	C4B-C3B-CAB-CBB
29	N	603	CLA	C4B-C3B-CAB-CBB
29	N	611	CLA	C4B-C3B-CAB-CBB
29	N	612	CLA	C4B-C3B-CAB-CBB
29	G	610	CLA	C4B-C3B-CAB-CBB
29	G	612	CLA	C4B-C3B-CAB-CBB
29	R	611	CLA	C4B-C3B-CAB-CBB
29	R	612	CLA	C4B-C3B-CAB-CBB
29	R	613	CLA	C4B-C3B-CAB-CBB
29	S	605	CLA	C4B-C3B-CAB-CBB
29	S	610	CLA	C4B-C3B-CAB-CBB
29	S	611	CLA	C4B-C3B-CAB-CBB
29	S	612	CLA	C4B-C3B-CAB-CBB
29	S	613	CLA	C4B-C3B-CAB-CBB
29	Y	608	CLA	C4B-C3B-CAB-CBB
29	Y	614	CLA	C4B-C3B-CAB-CBB
29	c	505	CLA	C4B-C3B-CAB-CBB
29	d	403	CLA	C4B-C3B-CAB-CBB
29	n	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	g	611	CLA	C4B-C3B-CAB-CBB
29	g	612	CLA	C4B-C3B-CAB-CBB
29	g	614	CLA	C4B-C3B-CAB-CBB
29	r	608	CLA	C4B-C3B-CAB-CBB
29	r	609	CLA	C4B-C3B-CAB-CBB
29	r	611	CLA	C4B-C3B-CAB-CBB
29	r	612	CLA	C4B-C3B-CAB-CBB
29	r	613	CLA	C4B-C3B-CAB-CBB
29	s	609	CLA	C4B-C3B-CAB-CBB
29	s	610	CLA	C4B-C3B-CAB-CBB
29	s	613	CLA	C4B-C3B-CAB-CBB
29	y	612	CLA	C4B-C3B-CAB-CBB
29	y	614	CLA	C4B-C3B-CAB-CBB
29	R	608	CLA	C11-C12-C13-C15
29	R	609	CLA	C11-C12-C13-C14
29	R	612	CLA	C11-C12-C13-C15
29	S	613	CLA	C6-C7-C8-C10
29	Y	604	CLA	C16-C17-C18-C19
29	Y	604	CLA	C16-C17-C18-C20
29	b	605	CLA	C16-C17-C18-C19
29	b	617	CLA	C16-C17-C18-C19
29	r	609	CLA	C11-C12-C13-C15
29	y	602	CLA	C16-C17-C18-C19
32	C	526	SQD	O5-C1-O6-C44
29	C	506	CLA	C10-C11-C12-C13
32	b	621	SQD	C26-C27-C28-C29
39	D	409	LHG	C28-C29-C30-C31
39	Y	624	LHG	C11-C10-C9-C8
39	c	625	LHG	C11-C12-C13-C14
39	y	624	LHG	C33-C34-C35-C36
36	b	623	DGA	CEA-CFA-CGA-CHA
36	c	524	DGA	CB3-CB4-CB5-CB6
39	Y	624	LHG	C11-C12-C13-C14
39	y	624	LHG	C26-C27-C28-C29
39	g	624	LHG	C23-C24-C25-C26
50	i	101	3PH	C31-C32-C33-C34
29	B	612	CLA	C8-C10-C11-C12
29	G	610	CLA	C8-C10-C11-C12
29	G	613	CLA	C15-C16-C17-C18
29	n	610	CLA	C13-C15-C16-C17
29	n	602	CLA	O1A-CGA-O2A-C1
33	b	622	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	B	625	DGA	CB3-CB4-CB5-CB6
39	C	525	LHG	C31-C32-C33-C34
39	G	630	LHG	C11-C12-C13-C14
29	b	614	CLA	C3-C5-C6-C7
29	c	507	CLA	C3-C5-C6-C7
29	N	602	CLA	CBA-CGA-O2A-C1
36	b	623	DGA	CCA-CDA-CEA-CFA
36	b	623	DGA	CB7-CB8-CB9-CAB
39	S	624	LHG	C11-C12-C13-C14
29	c	505	CLA	O1D-CGD-O2D-CED
30	a	409	PHO	O1D-CGD-O2D-CED
29	B	609	CLA	C3A-C2A-CAA-CBA
29	B	612	CLA	C3A-C2A-CAA-CBA
29	B	615	CLA	C3A-C2A-CAA-CBA
29	C	513	CLA	C3A-C2A-CAA-CBA
29	N	603	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	C3A-C2A-CAA-CBA
29	G	611	CLA	C3A-C2A-CAA-CBA
29	Y	603	CLA	C3A-C2A-CAA-CBA
29	a	405	CLA	C3A-C2A-CAA-CBA
29	b	612	CLA	C3A-C2A-CAA-CBA
29	b	615	CLA	C3A-C2A-CAA-CBA
29	c	506	CLA	C3A-C2A-CAA-CBA
29	c	513	CLA	C3A-C2A-CAA-CBA
29	n	604	CLA	C3A-C2A-CAA-CBA
29	n	614	CLA	C3A-C2A-CAA-CBA
29	g	603	CLA	C3A-C2A-CAA-CBA
29	g	611	CLA	C3A-C2A-CAA-CBA
45	G	607	CHL	C3A-C2A-CAA-CBA
45	Y	606	CHL	C3A-C2A-CAA-CBA
45	n	609	CHL	C3A-C2A-CAA-CBA
45	g	606	CHL	C3A-C2A-CAA-CBA
45	y	606	CHL	C3A-C2A-CAA-CBA
29	b	602	CLA	C8-C10-C11-C12
29	r	603	CLA	C8-C10-C11-C12
31	c	514	BCR	C13-C14-C15-C16
32	b	621	SQD	C30-C31-C32-C33
33	C	521	LMG	C15-C16-C17-C18
36	C	524	DGA	CA6-CA7-CA8-CA9
36	C	524	DGA	CB2-CB3-CB4-CB5
36	C	524	DGA	CB3-CB4-CB5-CB6
36	b	623	DGA	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
39	D	408	LHG	C29-C30-C31-C32
39	L	101	LHG	C11-C12-C13-C14
39	n	624	LHG	C15-C16-C17-C18
38	c	520	DGD	O1A-C1A-O1G-C1G
29	G	613	CLA	C16-C17-C18-C20
29	R	608	CLA	C11-C12-C13-C14
29	R	612	CLA	C11-C12-C13-C14
29	S	602	CLA	C11-C12-C13-C14
29	n	604	CLA	C16-C17-C18-C20
29	g	602	CLA	C16-C17-C18-C19
29	g	602	CLA	C16-C17-C18-C20
29	r	612	CLA	C11-C12-C13-C14
29	s	613	CLA	C6-C7-C8-C9
29	y	604	CLA	C16-C17-C18-C20
32	C	526	SQD	C11-C12-C13-C14
33	J	101	LMG	C31-C32-C33-C34
39	S	624	LHG	C9-C10-C11-C12
39	c	625	LHG	C31-C32-C33-C34
39	d	408	LHG	C29-C30-C31-C32
39	y	624	LHG	C16-C17-C18-C19
50	S	626	3PH	C23-C24-C25-C26
29	C	505	CLA	O1D-CGD-O2D-CED
39	d	408	LHG	C4-C5-C6-O8
39	y	624	LHG	C31-C32-C33-C34
50	i	101	3PH	C23-C24-C25-C26
50	s	626	3PH	C25-C26-C27-C28
29	A	405	CLA	O2A-C1-C2-C3
45	n	601	CHL	C3-C5-C6-C7
39	n	624	LHG	C28-C29-C30-C31
29	B	614	CLA	C15-C16-C17-C18
29	b	604	CLA	CBA-CGA-O2A-C1
29	c	501	CLA	C2-C3-C5-C6
29	n	613	CLA	C2-C3-C5-C6
45	N	601	CHL	C2-C3-C5-C6
39	D	408	LHG	C8-C7-O7-C5
36	b	623	DGA	CA4-CA5-CA6-CA7
39	D	409	LHG	C11-C12-C13-C14
39	G	630	LHG	C28-C29-C30-C31
39	d	409	LHG	C11-C12-C13-C14
50	S	626	3PH	C24-C25-C26-C27
39	C	525	LHG	O1-C1-C2-O2
39	D	409	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
39	D	410	LHG	O1-C1-C2-O2
39	L	101	LHG	O1-C1-C2-O2
39	N	624	LHG	O1-C1-C2-O2
39	S	624	LHG	O1-C1-C2-O2
39	d	408	LHG	O1-C1-C2-O2
39	d	409	LHG	O1-C1-C2-O2
39	l	101	LHG	O1-C1-C2-O2
39	n	624	LHG	O1-C1-C2-O2
39	y	624	LHG	O1-C1-C2-O2
40	C	527	LMK	O9-C10-C11-C12
29	C	502	CLA	C10-C11-C12-C13
39	D	408	LHG	C25-C26-C27-C28
39	Y	624	LHG	C16-C17-C18-C19
39	d	409	LHG	C28-C29-C30-C31
39	l	101	LHG	C11-C12-C13-C14
39	y	624	LHG	C13-C14-C15-C16
50	s	626	3PH	C26-C27-C28-C29
29	B	612	CLA	O1A-CGA-O2A-C1
29	G	602	CLA	C16-C17-C18-C20
29	Y	613	CLA	C16-C17-C18-C19
29	y	602	CLA	C16-C17-C18-C20
29	y	610	CLA	C16-C17-C18-C19
39	N	624	LHG	C11-C12-C13-C14
29	A	407	CLA	C2B-C3B-CAB-CBB
29	B	617	CLA	C2B-C3B-CAB-CBB
29	C	501	CLA	C2B-C3B-CAB-CBB
29	D	403	CLA	C2B-C3B-CAB-CBB
29	N	603	CLA	C2B-C3B-CAB-CBB
29	N	611	CLA	C2B-C3B-CAB-CBB
29	N	612	CLA	C2B-C3B-CAB-CBB
29	G	610	CLA	C2B-C3B-CAB-CBB
29	G	612	CLA	C2B-C3B-CAB-CBB
29	R	609	CLA	C2B-C3B-CAB-CBB
29	R	611	CLA	C2B-C3B-CAB-CBB
29	R	612	CLA	C2B-C3B-CAB-CBB
29	R	613	CLA	C2B-C3B-CAB-CBB
29	S	605	CLA	C2B-C3B-CAB-CBB
29	S	610	CLA	C2B-C3B-CAB-CBB
29	S	611	CLA	C2B-C3B-CAB-CBB
29	S	612	CLA	C2B-C3B-CAB-CBB
29	S	613	CLA	C2B-C3B-CAB-CBB
29	Y	608	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	Y	614	CLA	C2B-C3B-CAB-CBB
29	a	407	CLA	C2B-C3B-CAB-CBB
29	d	403	CLA	C2B-C3B-CAB-CBB
29	n	611	CLA	C2B-C3B-CAB-CBB
29	g	611	CLA	C2B-C3B-CAB-CBB
29	g	612	CLA	C2B-C3B-CAB-CBB
29	g	614	CLA	C2B-C3B-CAB-CBB
29	r	608	CLA	C2B-C3B-CAB-CBB
29	r	609	CLA	C2B-C3B-CAB-CBB
29	r	611	CLA	C2B-C3B-CAB-CBB
29	r	612	CLA	C2B-C3B-CAB-CBB
29	r	613	CLA	C2B-C3B-CAB-CBB
29	s	609	CLA	C2B-C3B-CAB-CBB
29	s	610	CLA	C2B-C3B-CAB-CBB
29	s	613	CLA	C2B-C3B-CAB-CBB
29	y	612	CLA	C2B-C3B-CAB-CBB
29	y	614	CLA	C2B-C3B-CAB-CBB
29	B	603	CLA	C13-C15-C16-C17
29	c	503	CLA	C10-C11-C12-C13
29	c	505	CLA	C10-C11-C12-C13
39	c	625	LHG	C34-C35-C36-C37
39	G	630	LHG	C13-C14-C15-C16
39	l	101	LHG	C34-C35-C36-C37
29	s	603	CLA	C15-C16-C17-C18
36	c	524	DGA	CB9-CAB-CBB-CCB
39	D	409	LHG	C13-C14-C15-C16
39	d	408	LHG	C11-C12-C13-C14
39	d	409	LHG	C31-C32-C33-C34
39	n	624	LHG	C11-C12-C13-C14
39	D	408	LHG	O9-C7-O7-C5
29	A	406	CLA	C2-C1-O2A-CGA
29	B	607	CLA	C2-C1-O2A-CGA
29	C	502	CLA	C2-C1-O2A-CGA
29	C	503	CLA	C2-C1-O2A-CGA
29	C	506	CLA	C2-C1-O2A-CGA
29	N	603	CLA	C2-C1-O2A-CGA
29	G	602	CLA	C2-C1-O2A-CGA
29	G	603	CLA	C2-C1-O2A-CGA
29	G	614	CLA	C2-C1-O2A-CGA
29	R	604	CLA	C2-C1-O2A-CGA
29	R	609	CLA	C2-C1-O2A-CGA
29	S	611	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	S	617	CLA	C2-C1-O2A-CGA
29	Y	604	CLA	C2-C1-O2A-CGA
29	Y	608	CLA	C2-C1-O2A-CGA
29	a	405	CLA	C2-C1-O2A-CGA
29	a	406	CLA	C2-C1-O2A-CGA
29	a	407	CLA	C2-C1-O2A-CGA
29	b	612	CLA	C2-C1-O2A-CGA
29	b	616	CLA	C2-C1-O2A-CGA
29	c	502	CLA	C2-C1-O2A-CGA
29	g	604	CLA	C2-C1-O2A-CGA
29	r	604	CLA	C2-C1-O2A-CGA
29	r	609	CLA	C2-C1-O2A-CGA
29	s	603	CLA	C2-C1-O2A-CGA
29	s	611	CLA	C2-C1-O2A-CGA
29	y	604	CLA	C2-C1-O2A-CGA
29	y	608	CLA	C2-C1-O2A-CGA
39	C	525	LHG	C13-C14-C15-C16
29	C	507	CLA	C13-C15-C16-C17
29	N	602	CLA	C15-C16-C17-C18
29	c	506	CLA	C10-C11-C12-C13
29	N	602	CLA	O1A-CGA-O2A-C1
29	S	604	CLA	O1A-CGA-O2A-C1
33	J	101	LMG	C29-C30-C31-C32
39	g	624	LHG	C25-C26-C27-C28
39	g	624	LHG	C28-C29-C30-C31
39	d	409	LHG	C23-C24-C25-C26
29	Y	611	CLA	C3-C5-C6-C7
31	A	411	BCR	C23-C24-C25-C26
31	B	618	BCR	C5-C6-C7-C8
31	C	514	BCR	C1-C6-C7-C8
31	C	514	BCR	C5-C6-C7-C8
31	C	515	BCR	C23-C24-C25-C26
31	C	517	BCR	C23-C24-C25-C26
31	C	517	BCR	C23-C24-C25-C30
31	D	404	BCR	C1-C6-C7-C8
31	D	404	BCR	C5-C6-C7-C8
31	a	411	BCR	C23-C24-C25-C26
31	b	618	BCR	C1-C6-C7-C8
31	b	618	BCR	C5-C6-C7-C8
31	c	514	BCR	C1-C6-C7-C8
31	c	514	BCR	C5-C6-C7-C8
31	c	516	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	c	517	BCR	C23-C24-C25-C26
31	c	517	BCR	C23-C24-C25-C30
31	d	404	BCR	C1-C6-C7-C8
31	d	404	BCR	C5-C6-C7-C8
31	d	404	BCR	C23-C24-C25-C30
46	n	620	LUT	C5-C6-C7-C8
39	L	101	LHG	C34-C35-C36-C37
39	G	630	LHG	C11-C10-C9-C8
50	S	626	3PH	C25-C26-C27-C28
29	B	614	CLA	C8-C10-C11-C12
29	b	605	CLA	C8-C10-C11-C12
29	b	609	CLA	C8-C10-C11-C12
29	d	403	CLA	C10-C11-C12-C13
29	g	603	CLA	C15-C16-C17-C18
39	d	409	LHG	C8-C7-O7-C5
36	B	625	DGA	CAA-CBA-CCA-CDA
36	c	524	DGA	CA6-CA7-CA8-CA9
39	D	408	LHG	C30-C31-C32-C33
39	G	630	LHG	C25-C26-C27-C28
50	S	626	3PH	C35-C36-C37-C38
29	S	610	CLA	O1A-CGA-O2A-C1
38	C	520	DGD	O1A-C1A-O1G-C1G
36	C	524	DGA	CB4-CB5-CB6-CB7
39	Y	624	LHG	C13-C14-C15-C16
29	c	502	CLA	C4-C3-C5-C6
45	N	601	CHL	C4-C3-C5-C6
45	G	609	CHL	C4-C3-C5-C6
29	A	405	CLA	C11-C12-C13-C15
29	B	602	CLA	C6-C7-C8-C10
29	B	602	CLA	C11-C10-C8-C7
29	C	501	CLA	C12-C13-C15-C16
29	C	506	CLA	C11-C12-C13-C15
29	C	507	CLA	C11-C12-C13-C15
29	C	513	CLA	C11-C10-C8-C7
29	N	613	CLA	C2-C3-C5-C6
29	R	603	CLA	C11-C10-C8-C7
29	Y	604	CLA	C11-C10-C8-C7
29	Y	613	CLA	C11-C12-C13-C15
29	b	602	CLA	C6-C7-C8-C10
29	b	603	CLA	C12-C13-C15-C16
29	b	604	CLA	C6-C7-C8-C10
29	b	616	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	c	502	CLA	C12-C13-C15-C16
29	c	506	CLA	C11-C10-C8-C7
29	c	507	CLA	C11-C12-C13-C15
29	c	513	CLA	C11-C10-C8-C7
29	g	603	CLA	C12-C13-C15-C16
29	s	611	CLA	C6-C7-C8-C10
29	y	604	CLA	C11-C12-C13-C15
29	y	610	CLA	C11-C12-C13-C15
29	y	613	CLA	C11-C12-C13-C15
45	Y	601	CHL	C11-C10-C8-C7
45	Y	607	CHL	C11-C10-C8-C7
45	Y	609	CHL	C11-C12-C13-C15
45	n	607	CHL	C11-C12-C13-C15
29	B	614	CLA	C3-C5-C6-C7
29	b	604	CLA	O1A-CGA-O2A-C1
39	D	408	LHG	C26-C27-C28-C29
29	A	406	CLA	C5-C6-C7-C8
29	B	610	CLA	C5-C6-C7-C8
29	a	406	CLA	C5-C6-C7-C8
29	b	608	CLA	C5-C6-C7-C8
29	b	608	CLA	C8-C10-C11-C12
29	y	612	CLA	C8-C10-C11-C12
31	c	514	BCR	C15-C16-C17-C18
35	B	620	C7Z	C9-C10-C11-C12
46	S	621	LUT	C29-C30-C31-C32
46	s	621	LUT	C29-C30-C31-C32
29	B	609	CLA	C16-C17-C18-C19
29	Y	610	CLA	C16-C17-C18-C20
39	D	409	LHG	O9-C7-O7-C5
39	Y	624	LHG	O9-C7-O7-C5
39	D	409	LHG	C23-C24-C25-C26
29	B	604	CLA	CBA-CGA-O2A-C1
29	C	508	CLA	CBA-CGA-O2A-C1
29	S	611	CLA	CBA-CGA-O2A-C1
29	r	602	CLA	CBA-CGA-O2A-C1
38	C	518	DGD	C2A-C1A-O1G-C1G
38	c	518	DGD	C2A-C1A-O1G-C1G
36	c	524	DGA	CB7-CB8-CB9-CAB
38	c	523	DGD	C9B-CAB-CBB-CCB
39	D	409	LHG	C33-C34-C35-C36
29	R	613	CLA	C2A-CAA-CBA-CGA
29	S	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	r	612	CLA	C2A-CAA-CBA-CGA
29	y	610	CLA	C2A-CAA-CBA-CGA
30	A	408	PHO	C2A-CAA-CBA-CGA
29	B	615	CLA	C8-C10-C11-C12
29	c	512	CLA	C8-C10-C11-C12
29	s	609	CLA	C8-C10-C11-C12
33	d	411	LMG	C11-C12-C13-C14
36	b	623	DGA	CDA-CEA-CFA-CGA
39	n	624	LHG	C25-C26-C27-C28
50	i	101	3PH	C33-C34-C35-C36
50	i	101	3PH	C3E-C3F-C3G-C3H
39	c	625	LHG	C7-C8-C9-C10
29	B	608	CLA	C10-C11-C12-C13
29	B	616	CLA	C8-C10-C11-C12
29	c	502	CLA	C5-C6-C7-C8
29	g	610	CLA	C5-C6-C7-C8
32	A	412	SQD	C11-C12-C13-C14
39	d	409	LHG	C13-C14-C15-C16
39	y	624	LHG	C30-C31-C32-C33
32	B	621	SQD	C25-C26-C27-C28
39	L	101	LHG	C28-C29-C30-C31
39	d	408	LHG	C30-C31-C32-C33
29	c	508	CLA	CBA-CGA-O2A-C1
29	R	603	CLA	C11-C12-C13-C15
29	y	611	CLA	C16-C17-C18-C20
29	C	511	CLA	C10-C11-C12-C13
29	c	501	CLA	C5-C6-C7-C8
29	s	610	CLA	C10-C11-C12-C13
36	C	524	DGA	CA4-CA5-CA6-CA7
39	D	408	LHG	C27-C28-C29-C30
39	l	101	LHG	C9-C10-C11-C12
36	B	625	DGA	CB1-CB2-CB3-CB4
32	A	412	SQD	C8-C7-O47-C45
39	D	409	LHG	C8-C7-O7-C5
39	Y	624	LHG	C8-C7-O7-C5
39	c	625	LHG	C8-C7-O7-C5
39	d	410	LHG	C8-C7-O7-C5
39	D	410	LHG	O6-C4-C5-O7
32	b	621	SQD	C24-C25-C26-C27
39	d	408	LHG	C34-C35-C36-C37
43	f	101	HEM	C4C-C3C-CAC-CBC
47	r	622	XAT	C14-C15-C35-C34

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Mol	Chain	Res	Type	Atoms
29	A	405	CLA	C8-C10-C11-C12
29	N	610	CLA	C13-C15-C16-C17
29	Y	604	CLA	C8-C10-C11-C12
29	b	614	CLA	C15-C16-C17-C18
29	y	602	CLA	C13-C15-C16-C17
29	y	603	CLA	C8-C10-C11-C12
33	C	521	LMG	C16-C17-C18-C19
39	l	101	LHG	C28-C29-C30-C31
39	c	625	LHG	O9-C7-O7-C5
29	c	513	CLA	C3-C5-C6-C7
36	B	625	DGA	CBB-CAB-CB9-CB8
50	i	101	3PH	C2D-C2E-C2F-C2G
33	J	101	LMG	O7-C8-C9-O8
33	a	413	LMG	O1-C7-C8-O7
36	C	524	DGA	CB7-CB8-CB9-CAB
38	c	520	DGD	CAB-CBB-CCB-CDB
39	N	624	LHG	C28-C29-C30-C31
39	d	408	LHG	C26-C27-C28-C29
39	s	624	LHG	C9-C10-C11-C12
50	i	101	3PH	C22-C23-C24-C25
29	B	617	CLA	C16-C17-C18-C20
29	c	507	CLA	C16-C17-C18-C20
29	y	613	CLA	C16-C17-C18-C20
33	a	413	LMG	C16-C17-C18-C19
38	C	520	DGD	CAB-CBB-CCB-CDB
39	c	625	LHG	C11-C10-C9-C8
39	n	624	LHG	C34-C35-C36-C37
33	C	521	LMG	O6-C5-C6-O5
29	A	410	CLA	C5-C6-C7-C8
29	Y	612	CLA	C8-C10-C11-C12
29	N	613	CLA	C4-C3-C5-C6
29	c	502	CLA	C2-C3-C5-C6
29	g	602	CLA	C2-C3-C5-C6
42	D	405	PL9	C4-C3-C7-C8
42	d	405	PL9	C4-C3-C7-C8
32	B	621	SQD	C26-C27-C28-C29
29	B	602	CLA	C6-C7-C8-C9
29	B	602	CLA	C11-C10-C8-C9
29	B	604	CLA	C6-C7-C8-C9
29	C	501	CLA	C14-C13-C15-C16
29	C	503	CLA	C14-C13-C15-C16
29	C	506	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	C	507	CLA	C11-C12-C13-C14
29	G	603	CLA	C14-C13-C15-C16
29	b	604	CLA	C6-C7-C8-C9
29	c	507	CLA	C11-C12-C13-C14
29	c	512	CLA	C11-C12-C13-C14
29	g	603	CLA	C11-C12-C13-C14
29	g	613	CLA	C11-C10-C8-C9
29	s	609	CLA	C6-C7-C8-C9
29	s	609	CLA	C11-C10-C8-C9
29	s	611	CLA	C6-C7-C8-C9
45	N	607	CHL	C11-C12-C13-C14
39	C	525	LHG	C11-C12-C13-C14
29	A	405	CLA	C3-C5-C6-C7
29	C	506	CLA	C3-C5-C6-C7
29	B	604	CLA	C2A-CAA-CBA-CGA
29	R	608	CLA	C2A-CAA-CBA-CGA
29	b	604	CLA	C2A-CAA-CBA-CGA
29	r	604	CLA	C2A-CAA-CBA-CGA
45	N	606	CHL	C2A-CAA-CBA-CGA
45	N	608	CHL	C2A-CAA-CBA-CGA
45	Y	607	CHL	C2A-CAA-CBA-CGA
45	y	607	CHL	C2A-CAA-CBA-CGA
39	S	624	LHG	C12-C13-C14-C15
39	S	624	LHG	C28-C29-C30-C31
33	H	102	LMG	O6-C5-C6-O5
46	G	620	LUT	C27-C28-C29-C39
46	R	620	LUT	C31-C32-C33-C40
29	B	608	CLA	C5-C6-C7-C8
39	D	408	LHG	C11-C12-C13-C14
39	S	624	LHG	C11-C10-C9-C8
50	s	626	3PH	C32-C33-C34-C35
29	B	604	CLA	O1A-CGA-O2A-C1
29	S	611	CLA	O1A-CGA-O2A-C1
29	A	407	CLA	C1A-C2A-CAA-CBA
29	A	410	CLA	C1A-C2A-CAA-CBA
29	B	602	CLA	C1A-C2A-CAA-CBA
29	B	604	CLA	C1A-C2A-CAA-CBA
29	B	607	CLA	C1A-C2A-CAA-CBA
29	C	501	CLA	C1A-C2A-CAA-CBA
29	C	503	CLA	C1A-C2A-CAA-CBA
29	N	602	CLA	C1A-C2A-CAA-CBA
29	N	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	N	604	CLA	C1A-C2A-CAA-CBA
29	N	611	CLA	C1A-C2A-CAA-CBA
29	N	613	CLA	C1A-C2A-CAA-CBA
29	N	614	CLA	C1A-C2A-CAA-CBA
29	G	603	CLA	C1A-C2A-CAA-CBA
29	G	610	CLA	C1A-C2A-CAA-CBA
29	G	611	CLA	C1A-C2A-CAA-CBA
29	R	603	CLA	C1A-C2A-CAA-CBA
29	R	608	CLA	C1A-C2A-CAA-CBA
29	R	609	CLA	C1A-C2A-CAA-CBA
29	R	613	CLA	C1A-C2A-CAA-CBA
29	S	602	CLA	C1A-C2A-CAA-CBA
29	S	609	CLA	C1A-C2A-CAA-CBA
29	S	610	CLA	C1A-C2A-CAA-CBA
29	Y	602	CLA	C1A-C2A-CAA-CBA
29	Y	603	CLA	C1A-C2A-CAA-CBA
29	Y	610	CLA	C1A-C2A-CAA-CBA
29	Y	611	CLA	C1A-C2A-CAA-CBA
29	a	405	CLA	C1A-C2A-CAA-CBA
29	a	407	CLA	C1A-C2A-CAA-CBA
29	a	410	CLA	C1A-C2A-CAA-CBA
29	b	602	CLA	C1A-C2A-CAA-CBA
29	b	604	CLA	C1A-C2A-CAA-CBA
29	b	607	CLA	C1A-C2A-CAA-CBA
29	b	610	CLA	C1A-C2A-CAA-CBA
29	c	502	CLA	C1A-C2A-CAA-CBA
29	c	503	CLA	C1A-C2A-CAA-CBA
29	n	603	CLA	C1A-C2A-CAA-CBA
29	n	613	CLA	C1A-C2A-CAA-CBA
29	g	603	CLA	C1A-C2A-CAA-CBA
29	g	610	CLA	C1A-C2A-CAA-CBA
29	g	611	CLA	C1A-C2A-CAA-CBA
29	r	603	CLA	C1A-C2A-CAA-CBA
29	r	604	CLA	C1A-C2A-CAA-CBA
29	r	608	CLA	C1A-C2A-CAA-CBA
29	r	611	CLA	C1A-C2A-CAA-CBA
29	r	613	CLA	C1A-C2A-CAA-CBA
29	s	604	CLA	C1A-C2A-CAA-CBA
29	s	609	CLA	C1A-C2A-CAA-CBA
29	s	610	CLA	C1A-C2A-CAA-CBA
29	s	617	CLA	C1A-C2A-CAA-CBA
29	y	603	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	y	608	CLA	C1A-C2A-CAA-CBA
29	y	610	CLA	C1A-C2A-CAA-CBA
29	y	611	CLA	C1A-C2A-CAA-CBA
45	Y	606	CHL	C1A-C2A-CAA-CBA
45	y	606	CHL	C1A-C2A-CAA-CBA
29	R	603	CLA	C11-C12-C13-C14
29	b	605	CLA	C16-C17-C18-C20
29	b	617	CLA	C16-C17-C18-C20
32	A	412	SQD	O49-C7-O47-C45
39	d	409	LHG	O9-C7-O7-C5
39	d	410	LHG	O9-C7-O7-C5
39	L	101	LHG	C29-C30-C31-C32
31	C	517	BCR	C9-C10-C11-C12
46	N	621	LUT	C29-C30-C31-C32
46	S	620	LUT	C29-C30-C31-C32
46	s	620	LUT	C29-C30-C31-C32
29	B	609	CLA	C8-C10-C11-C12
29	R	603	CLA	C8-C10-C11-C12
29	Y	602	CLA	C5-C6-C7-C8
29	Y	604	CLA	C13-C15-C16-C17
29	b	613	CLA	C10-C11-C12-C13
29	R	610	CLA	C3-C5-C6-C7
39	C	525	LHG	C2-C3-O3-P
29	B	607	CLA	C5-C6-C7-C8
29	B	609	CLA	C10-C11-C12-C13
29	D	403	CLA	C8-C10-C11-C12
29	b	609	CLA	C15-C16-C17-C18
39	C	525	LHG	O6-C4-C5-C6
39	D	409	LHG	O6-C4-C5-C6
39	N	624	LHG	O6-C4-C5-C6
39	G	630	LHG	O6-C4-C5-C6
39	S	624	LHG	O6-C4-C5-C6
39	d	409	LHG	O6-C4-C5-C6
39	g	624	LHG	O6-C4-C5-C6
50	S	626	3PH	O11-C1-C2-C3
32	C	526	SQD	C30-C31-C32-C33
38	C	519	DGD	C2B-C3B-C4B-C5B
39	d	408	LHG	C25-C26-C27-C28
29	B	602	CLA	C10-C11-C12-C13
29	B	608	CLA	C13-C15-C16-C17
29	c	505	CLA	C16-C17-C18-C20
29	c	513	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
39	d	409	LHG	C33-C34-C35-C36
39	s	624	LHG	C11-C10-C9-C8
33	j	101	LMG	O6-C5-C6-O5
33	A	413	LMG	C18-C19-C20-C21
39	y	624	LHG	C32-C33-C34-C35
29	r	610	CLA	C3-C5-C6-C7
39	L	101	LHG	C9-C10-C11-C12
33	h	102	LMG	O6-C5-C6-O5
49	s	625	LPX	O1-C3-C4-C5
29	B	602	CLA	C4-C3-C5-C6
36	b	623	DGA	CB9-CAB-CBB-CCB
29	C	503	CLA	C13-C15-C16-C17
29	C	509	CLA	C8-C10-C11-C12
29	b	617	CLA	C10-C11-C12-C13
29	y	604	CLA	C10-C11-C12-C13
38	C	518	DGD	O1A-C1A-O1G-C1G
38	c	518	DGD	O1A-C1A-O1G-C1G
32	c	626	SQD	C27-C28-C29-C30
33	b	622	LMG	C18-C19-C20-C21
33	j	101	LMG	C11-C12-C13-C14
39	l	101	LHG	C29-C30-C31-C32
29	N	604	CLA	C2A-CAA-CBA-CGA
29	R	612	CLA	C2A-CAA-CBA-CGA
33	C	521	LMG	O1-C7-C8-C9
33	j	101	LMG	C7-C8-C9-O8
38	c	523	DGD	O1G-C1G-C2G-C3G
39	N	624	LHG	C34-C35-C36-C37
39	Y	624	LHG	C4-C5-C6-O8
39	c	625	LHG	C4-C5-C6-O8
39	s	624	LHG	C4-C5-C6-O8
40	c	627	LMK	O1-C7-C8-C9
50	s	626	3PH	C1-C2-C3-O31
29	B	603	CLA	C5-C6-C7-C8
29	g	602	CLA	C5-C6-C7-C8
29	s	602	CLA	C8-C10-C11-C12
29	y	613	CLA	C13-C15-C16-C17
45	n	607	CHL	C15-C16-C17-C18
36	b	623	DGA	CB5-CB6-CB7-CB8
39	C	525	LHG	C30-C31-C32-C33
29	r	602	CLA	O1A-CGA-O2A-C1
32	A	412	SQD	C45-C44-O6-C1
38	c	519	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
40	C	527	LMK	C8-C9-O8-C28
29	S	602	CLA	O1D-CGD-O2D-CED
39	D	408	LHG	C34-C35-C36-C37
29	Y	612	CLA	C10-C11-C12-C13
29	b	614	CLA	C8-C10-C11-C12
29	c	511	CLA	C15-C16-C17-C18
39	C	525	LHG	C34-C35-C36-C37
39	c	625	LHG	C13-C14-C15-C16
39	s	624	LHG	C29-C30-C31-C32
29	C	508	CLA	O1A-CGA-O2A-C1
39	s	624	LHG	C11-C12-C13-C14
39	s	624	LHG	C28-C29-C30-C31
29	C	507	CLA	C3-C5-C6-C7
29	s	610	CLA	C3-C5-C6-C7
32	c	626	SQD	O5-C1-O6-C44
33	B	622	LMG	O6-C1-O1-C7
29	b	604	CLA	C5-C6-C7-C8
29	b	612	CLA	C10-C11-C12-C13
29	n	610	CLA	C15-C16-C17-C18
42	D	405	PL9	C34-C36-C37-C38
51	y	625	SPH	C10-C11-C12-C13
33	D	411	LMG	O6-C5-C6-O5
33	c	521	LMG	O6-C5-C6-O5
39	G	630	LHG	O1-C1-C2-O2
39	d	410	LHG	O1-C1-C2-O2
39	g	624	LHG	O1-C1-C2-O2
39	s	624	LHG	O1-C1-C2-O2
38	c	519	DGD	C9A-CAA-CBA-CCA
50	S	626	3PH	C37-C38-C39-C3A
45	S	608	CHL	C5-C6-C7-C8
45	n	607	CHL	C10-C11-C12-C13
32	C	526	SQD	C7-C8-C9-C10
33	b	622	LMG	C28-C29-C30-C31
39	n	624	LHG	C31-C32-C33-C34
38	c	520	DGD	CCB-CDB-CEB-CFB
50	i	101	3PH	C34-C35-C36-C37
29	R	610	CLA	C5-C6-C7-C8
29	c	504	CLA	C8-C10-C11-C12
29	c	513	CLA	C15-C16-C17-C18
45	n	601	CHL	C10-C11-C12-C13
45	y	606	CHL	C15-C16-C17-C18
33	d	411	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
29	B	605	CLA	C16-C17-C18-C19
29	c	504	CLA	C10-C11-C12-C13
45	G	601	CHL	C10-C11-C12-C13
33	b	622	LMG	C9-C8-O7-C10
36	B	625	DGA	CG1-CG2-OG2-CB1
36	b	623	DGA	CG1-CG2-OG2-CB1
29	b	616	CLA	C13-C15-C16-C17
45	s	608	CHL	C5-C6-C7-C8
29	A	405	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C2-C1-O2A-CGA
29	B	603	CLA	C2-C1-O2A-CGA
29	B	611	CLA	C2-C1-O2A-CGA
29	B	615	CLA	C2-C1-O2A-CGA
29	N	613	CLA	C2-C1-O2A-CGA
29	b	607	CLA	C2-C1-O2A-CGA
45	n	607	CHL	C2-C1-O2A-CGA
39	S	624	LHG	C26-C27-C28-C29
39	s	624	LHG	C31-C32-C33-C34
38	C	519	DGD	C9A-CAA-CBA-CCA
29	b	607	CLA	C5-C6-C7-C8
29	y	602	CLA	C8-C10-C11-C12
36	c	524	DGA	CA4-CA5-CA6-CA7
39	N	624	LHG	C25-C26-C27-C28
39	Y	624	LHG	C32-C33-C34-C35
39	d	410	LHG	C28-C29-C30-C31
39	s	624	LHG	C34-C35-C36-C37
29	Y	610	CLA	CBA-CGA-O2A-C1
29	s	610	CLA	CBA-CGA-O2A-C1
39	C	525	LHG	C24-C23-O8-C6
29	B	609	CLA	C16-C17-C18-C20
29	Y	610	CLA	C16-C17-C18-C19
38	C	519	DGD	C9B-CAB-CBB-CCB
39	S	624	LHG	C31-C32-C33-C34
38	c	518	DGD	O6D-C5D-C6D-O5D
29	r	609	CLA	C10-C11-C12-C13
36	C	524	DGA	CAB-CBB-CCB-CDB
29	c	508	CLA	O1A-CGA-O2A-C1
29	s	610	CLA	O1A-CGA-O2A-C1
36	c	524	DGA	CB4-CB5-CB6-CB7
39	D	410	LHG	C30-C31-C32-C33
33	B	622	LMG	C28-C29-C30-C31
29	B	606	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	B	608	CLA	C8-C10-C11-C12
29	b	609	CLA	C13-C15-C16-C17
29	b	613	CLA	C13-C15-C16-C17
29	n	604	CLA	C13-C15-C16-C17
39	N	624	LHG	C31-C32-C33-C34
29	N	613	CLA	CAA-CBA-CGA-O2A
33	A	413	LMG	O1-C7-C8-O7
38	C	523	DGD	O1G-C1G-C2G-O2G
50	i	101	3PH	O21-C2-C3-O31
29	C	501	CLA	C5-C6-C7-C8
39	N	624	LHG	C23-C24-C25-C26
38	C	520	DGD	CCB-CDB-CEB-CFB
39	D	409	LHG	C34-C35-C36-C37
29	B	602	CLA	C2-C3-C5-C6
29	B	613	CLA	C6-C7-C8-C10
29	C	501	CLA	C11-C10-C8-C7
29	C	503	CLA	C12-C13-C15-C16
29	C	506	CLA	C11-C10-C8-C7
29	C	506	CLA	C12-C13-C15-C16
29	C	508	CLA	C11-C10-C8-C7
29	C	508	CLA	C12-C13-C15-C16
29	C	511	CLA	C11-C10-C8-C7
29	D	402	CLA	C11-C10-C8-C7
29	D	402	CLA	C11-C12-C13-C15
29	N	613	CLA	C12-C13-C15-C16
29	G	603	CLA	C11-C12-C13-C15
29	G	603	CLA	C12-C13-C15-C16
29	G	613	CLA	C6-C7-C8-C10
29	S	603	CLA	C6-C7-C8-C10
29	Y	610	CLA	C11-C12-C13-C15
29	Y	611	CLA	C11-C10-C8-C7
29	Y	613	CLA	C6-C7-C8-C10
29	b	602	CLA	C11-C10-C8-C7
29	b	602	CLA	C11-C12-C13-C15
29	c	506	CLA	C12-C13-C15-C16
29	c	510	CLA	C6-C7-C8-C10
29	c	511	CLA	C11-C12-C13-C15
29	c	512	CLA	C11-C12-C13-C15
29	c	513	CLA	C6-C7-C8-C10
29	c	513	CLA	C11-C12-C13-C15
29	g	603	CLA	C11-C12-C13-C15
29	g	613	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	r	603	CLA	C11-C10-C8-C7
29	s	610	CLA	C6-C7-C8-C10
29	s	610	CLA	C11-C10-C8-C7
29	y	602	CLA	C6-C7-C8-C10
29	y	604	CLA	C12-C13-C15-C16
29	y	611	CLA	C11-C10-C8-C7
29	y	611	CLA	C12-C13-C15-C16
29	y	612	CLA	C11-C12-C13-C15
42	D	405	PL9	C43-C44-C46-C47
45	N	607	CHL	C11-C10-C8-C7
45	N	609	CHL	C11-C10-C8-C7
45	G	609	CHL	C11-C12-C13-C15
45	n	605	CHL	C12-C13-C15-C16
45	n	606	CHL	C11-C10-C8-C7
45	n	607	CHL	C12-C13-C15-C16
45	g	601	CHL	C11-C12-C13-C15
45	y	606	CHL	C11-C10-C8-C7
45	y	609	CHL	C11-C12-C13-C15
29	B	608	CLA	C14-C13-C15-C16
29	B	617	CLA	C11-C12-C13-C14
29	C	501	CLA	C11-C10-C8-C9
29	C	508	CLA	C11-C10-C8-C9
29	C	512	CLA	C11-C10-C8-C9
29	C	513	CLA	C11-C12-C13-C14
29	D	402	CLA	C6-C7-C8-C9
29	N	602	CLA	C14-C13-C15-C16
29	N	613	CLA	C14-C13-C15-C16
29	G	602	CLA	C6-C7-C8-C9
29	G	603	CLA	C11-C12-C13-C14
29	G	613	CLA	C6-C7-C8-C9
29	S	611	CLA	C6-C7-C8-C9
29	Y	604	CLA	C11-C12-C13-C14
29	Y	611	CLA	C11-C10-C8-C9
29	a	405	CLA	C11-C12-C13-C14
29	b	602	CLA	C11-C10-C8-C9
29	c	506	CLA	C11-C10-C8-C9
29	c	508	CLA	C11-C10-C8-C9
29	c	508	CLA	C14-C13-C15-C16
29	c	509	CLA	C6-C7-C8-C9
29	c	510	CLA	C6-C7-C8-C9
29	c	512	CLA	C14-C13-C15-C16
29	c	513	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	C6-C7-C8-C9
29	g	613	CLA	C6-C7-C8-C9
29	g	613	CLA	C14-C13-C15-C16
29	s	610	CLA	C11-C10-C8-C9
29	y	602	CLA	C6-C7-C8-C9
29	y	604	CLA	C14-C13-C15-C16
29	y	611	CLA	C11-C10-C8-C9
45	G	609	CHL	C11-C12-C13-C14
45	Y	609	CHL	C14-C13-C15-C16
45	n	607	CHL	C11-C12-C13-C14
45	y	606	CHL	C11-C10-C8-C9
31	A	411	BCR	C9-C10-C11-C12
31	B	619	BCR	C9-C10-C11-C12
29	d	402	CLA	C13-C15-C16-C17
29	B	605	CLA	C2A-CAA-CBA-CGA
30	a	408	PHO	C2A-CAA-CBA-CGA
45	N	605	CHL	C2A-CAA-CBA-CGA
45	g	606	CHL	C2A-CAA-CBA-CGA
39	c	625	LHG	C35-C36-C37-C38
29	n	610	CLA	C16-C17-C18-C20
46	Y	620	LUT	C27-C28-C29-C30
36	c	524	DGA	CA7-CA8-CA9-CAA
29	C	513	CLA	C3-C5-C6-C7
29	b	603	CLA	C5-C6-C7-C8
39	D	410	LHG	C26-C27-C28-C29
39	L	101	LHG	C35-C36-C37-C38
42	d	405	PL9	C42-C43-C44-C46
29	b	610	CLA	C13-C15-C16-C17
45	n	609	CHL	C8-C10-C11-C12
39	l	101	LHG	C25-C26-C27-C28
29	s	602	CLA	CBD-CGD-O2D-CED
29	A	410	CLA	C4B-C3B-CAB-CBB
29	B	605	CLA	C4B-C3B-CAB-CBB
29	B	607	CLA	C4B-C3B-CAB-CBB
29	C	505	CLA	C4B-C3B-CAB-CBB
29	C	510	CLA	C4B-C3B-CAB-CBB
29	N	613	CLA	C4B-C3B-CAB-CBB
29	N	614	CLA	C4B-C3B-CAB-CBB
29	G	604	CLA	C4B-C3B-CAB-CBB
29	G	611	CLA	C4B-C3B-CAB-CBB
29	G	613	CLA	C4B-C3B-CAB-CBB
29	R	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	R	608	CLA	C4B-C3B-CAB-CBB
29	R	610	CLA	C4B-C3B-CAB-CBB
29	S	602	CLA	C4B-C3B-CAB-CBB
29	S	609	CLA	C4B-C3B-CAB-CBB
29	S	617	CLA	C4B-C3B-CAB-CBB
29	Y	602	CLA	C4B-C3B-CAB-CBB
29	Y	603	CLA	C4B-C3B-CAB-CBB
29	Y	610	CLA	C4B-C3B-CAB-CBB
29	Y	611	CLA	C4B-C3B-CAB-CBB
29	Y	612	CLA	C4B-C3B-CAB-CBB
29	a	407	CLA	C4B-C3B-CAB-CBB
29	b	605	CLA	C4B-C3B-CAB-CBB
29	b	609	CLA	C4B-C3B-CAB-CBB
29	b	617	CLA	C4B-C3B-CAB-CBB
29	c	501	CLA	C4B-C3B-CAB-CBB
29	c	507	CLA	C4B-C3B-CAB-CBB
29	n	603	CLA	C4B-C3B-CAB-CBB
29	n	604	CLA	C4B-C3B-CAB-CBB
29	n	612	CLA	C4B-C3B-CAB-CBB
29	n	613	CLA	C4B-C3B-CAB-CBB
29	g	613	CLA	C4B-C3B-CAB-CBB
29	r	602	CLA	C4B-C3B-CAB-CBB
29	r	603	CLA	C4B-C3B-CAB-CBB
29	r	610	CLA	C4B-C3B-CAB-CBB
29	s	602	CLA	C4B-C3B-CAB-CBB
29	s	604	CLA	C4B-C3B-CAB-CBB
29	s	605	CLA	C4B-C3B-CAB-CBB
29	s	614	CLA	C4B-C3B-CAB-CBB
29	s	617	CLA	C4B-C3B-CAB-CBB
29	y	608	CLA	C4B-C3B-CAB-CBB
29	y	610	CLA	C4B-C3B-CAB-CBB
29	Y	603	CLA	C15-C16-C17-C18
39	D	410	LHG	O6-C4-C5-C6
39	d	410	LHG	O6-C4-C5-C6
39	l	101	LHG	O6-C4-C5-C6
39	n	624	LHG	O6-C4-C5-C6
39	n	624	LHG	C23-C24-C25-C26
29	y	610	CLA	CBA-CGA-O2A-C1
50	s	626	3PH	C39-C3A-C3B-C3C
29	G	610	CLA	C4-C3-C5-C6
45	N	609	CHL	C4-C3-C5-C6
42	d	405	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
33	H	102	LMG	C28-C29-C30-C31
50	S	626	3PH	C3D-C3E-C3F-C3G
29	B	604	CLA	C10-C11-C12-C13
29	Y	614	CLA	C5-C6-C7-C8
32	c	626	SQD	C32-C33-C34-C35
33	D	411	LMG	C11-C12-C13-C14
39	L	101	LHG	C25-C26-C27-C28
49	s	625	LPX	C14-C15-C16-C17
29	Y	604	CLA	C5-C6-C7-C8
29	b	613	CLA	C8-C10-C11-C12
39	s	624	LHG	C24-C23-O8-C6
39	C	525	LHG	C10-C11-C12-C13
50	s	626	3PH	C3F-C3G-C3H-C3I
29	B	613	CLA	C3A-C2A-CAA-CBA
29	C	506	CLA	C3A-C2A-CAA-CBA
29	N	604	CLA	C3A-C2A-CAA-CBA
29	N	613	CLA	C3A-C2A-CAA-CBA
29	G	604	CLA	C3A-C2A-CAA-CBA
29	R	604	CLA	C3A-C2A-CAA-CBA
29	b	613	CLA	C3A-C2A-CAA-CBA
29	n	613	CLA	C3A-C2A-CAA-CBA
29	r	604	CLA	C3A-C2A-CAA-CBA
29	r	610	CLA	C3A-C2A-CAA-CBA
29	s	614	CLA	C3A-C2A-CAA-CBA
30	a	408	PHO	C3A-C2A-CAA-CBA
45	Y	601	CHL	C3A-C2A-CAA-CBA
36	C	524	DGA	CB9-CAB-CBB-CCB
39	n	624	LHG	C35-C36-C37-C38
50	S	626	3PH	C3F-C3G-C3H-C3I
31	a	411	BCR	C9-C10-C11-C12
46	Y	621	LUT	C33-C34-C35-C15
39	C	525	LHG	C35-C36-C37-C38
39	d	410	LHG	C33-C34-C35-C36
39	l	101	LHG	C35-C36-C37-C38
29	G	610	CLA	C13-C15-C16-C17
39	d	408	LHG	C27-C28-C29-C30
29	y	608	CLA	CBA-CGA-O2A-C1
36	B	625	DGA	CA8-CA9-CAA-CBA
38	c	519	DGD	C9B-CAB-CBB-CCB
32	B	621	SQD	C44-C45-C46-O48
32	b	621	SQD	C44-C45-C46-O48
33	A	413	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
33	J	101	LMG	C7-C8-C9-O8
33	a	413	LMG	O1-C7-C8-C9
39	D	410	LHG	C4-C5-C6-O8
39	G	630	LHG	C4-C5-C6-O8
39	d	410	LHG	C4-C5-C6-O8
39	l	101	LHG	C4-C5-C6-O8
40	C	527	LMK	O1-C7-C8-C9
46	y	621	LUT	C21-C26-C27-C28
36	B	625	DGA	CCB-CDB-CEB-CFB
36	b	623	DGA	CFB-CGB-CHB-CIB
39	y	624	LHG	C9-C10-C11-C12
36	C	524	DGA	CA8-CA9-CAA-CBA
51	y	625	SPH	C6-C7-C8-C9
29	C	501	CLA	C3-C5-C6-C7
29	Y	610	CLA	O1A-CGA-O2A-C1
45	N	609	CHL	C2-C3-C5-C6
39	D	410	LHG	C33-C34-C35-C36
39	S	624	LHG	C34-C35-C36-C37
50	i	101	3PH	C25-C26-C27-C28
29	N	602	CLA	C13-C15-C16-C17
40	C	527	LMK	C9-C8-O7-C10
40	c	627	LMK	C9-C8-O7-C10
36	b	623	DGA	CB1-CB2-CB3-CB4
39	C	525	LHG	O10-C23-O8-C6
29	G	614	CLA	C2A-CAA-CBA-CGA
29	b	605	CLA	C2A-CAA-CBA-CGA
39	D	408	LHG	O1-C1-C2-O2
39	d	409	LHG	C25-C26-C27-C28
39	D	408	LHG	O6-C4-C5-O7
39	D	409	LHG	O6-C4-C5-O7
39	d	410	LHG	O6-C4-C5-O7
39	l	101	LHG	O6-C4-C5-O7
39	n	624	LHG	O6-C4-C5-O7
39	g	624	LHG	O6-C4-C5-O7
39	s	624	LHG	O6-C4-C5-O7
38	c	518	DGD	C4D-C5D-C6D-O5D
39	N	624	LHG	C24-C23-O8-C6
33	h	102	LMG	C28-C29-C30-C31
29	B	612	CLA	C16-C17-C18-C19
51	y	625	SPH	C11-C10-C9-C8
29	A	410	CLA	C2B-C3B-CAB-CBB
29	B	605	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	C	505	CLA	C2B-C3B-CAB-CBB
29	N	613	CLA	C2B-C3B-CAB-CBB
29	G	604	CLA	C2B-C3B-CAB-CBB
29	G	611	CLA	C2B-C3B-CAB-CBB
29	G	613	CLA	C2B-C3B-CAB-CBB
29	R	602	CLA	C2B-C3B-CAB-CBB
29	R	608	CLA	C2B-C3B-CAB-CBB
29	R	610	CLA	C2B-C3B-CAB-CBB
29	S	609	CLA	C2B-C3B-CAB-CBB
29	S	617	CLA	C2B-C3B-CAB-CBB
29	Y	603	CLA	C2B-C3B-CAB-CBB
29	Y	611	CLA	C2B-C3B-CAB-CBB
29	b	605	CLA	C2B-C3B-CAB-CBB
29	c	501	CLA	C2B-C3B-CAB-CBB
29	c	505	CLA	C2B-C3B-CAB-CBB
29	n	603	CLA	C2B-C3B-CAB-CBB
29	n	612	CLA	C2B-C3B-CAB-CBB
29	n	613	CLA	C2B-C3B-CAB-CBB
29	s	604	CLA	C2B-C3B-CAB-CBB
29	s	605	CLA	C2B-C3B-CAB-CBB
29	y	608	CLA	C2B-C3B-CAB-CBB
39	N	624	LHG	C35-C36-C37-C38
51	Y	625	SPH	C11-C12-C13-C14
29	G	613	CLA	C3-C5-C6-C7
32	B	621	SQD	O47-C45-C46-O48
32	b	621	SQD	O47-C45-C46-O48
33	C	521	LMG	O1-C7-C8-O7
38	C	519	DGD	O1G-C1G-C2G-O2G
39	Y	624	LHG	O7-C5-C6-O8
39	c	625	LHG	O7-C5-C6-O8
39	l	101	LHG	O7-C5-C6-O8
29	C	512	CLA	C13-C15-C16-C17
29	R	602	CLA	C10-C11-C12-C13
29	y	614	CLA	C5-C6-C7-C8
29	s	602	CLA	O1D-CGD-O2D-CED
32	B	621	SQD	C10-C11-C12-C13
32	a	412	SQD	C28-C29-C30-C31
33	J	101	LMG	O6-C1-O1-C7
38	C	519	DGD	O6D-C1D-O3G-C3G
29	A	405	CLA	C13-C15-C16-C17
29	C	511	CLA	C15-C16-C17-C18
29	b	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
36	b	623	DGA	CG1-CG2-CG3-OXT
29	A	410	CLA	C2-C1-O2A-CGA
29	a	410	CLA	C2-C1-O2A-CGA
29	b	617	CLA	C2-C1-O2A-CGA
30	a	409	PHO	C2-C1-O2A-CGA
36	B	625	DGA	CB9-CAB-CBB-CCB
39	N	624	LHG	C16-C17-C18-C19
39	n	624	LHG	C16-C17-C18-C19
39	g	624	LHG	C11-C12-C13-C14
29	c	511	CLA	C13-C15-C16-C17
29	d	403	CLA	C13-C15-C16-C17
29	y	610	CLA	C10-C11-C12-C13
29	B	606	CLA	C6-C7-C8-C9
29	B	613	CLA	C6-C7-C8-C9
29	B	616	CLA	C14-C13-C15-C16
29	C	506	CLA	C14-C13-C15-C16
29	C	508	CLA	C14-C13-C15-C16
29	C	512	CLA	C14-C13-C15-C16
29	D	402	CLA	C11-C12-C13-C14
29	N	604	CLA	C6-C7-C8-C9
29	N	604	CLA	C14-C13-C15-C16
29	b	604	CLA	C14-C13-C15-C16
29	b	605	CLA	C11-C12-C13-C14
29	c	506	CLA	C14-C13-C15-C16
29	d	402	CLA	C6-C7-C8-C9
29	g	602	CLA	C6-C7-C8-C9
29	y	602	CLA	C11-C10-C8-C9
45	N	606	CHL	C11-C12-C13-C14
45	G	609	CHL	C14-C13-C15-C16
45	g	601	CHL	C11-C12-C13-C14
39	D	410	LHG	C28-C29-C30-C31
32	B	621	SQD	C24-C25-C26-C27
50	i	101	3PH	C38-C39-C3A-C3B
50	s	626	3PH	C38-C39-C3A-C3B
29	C	503	CLA	C8-C10-C11-C12
29	s	609	CLA	C10-C11-C12-C13
30	a	408	PHO	C1A-C2A-CAA-CBA
39	D	409	LHG	C2-C3-O3-P
39	d	409	LHG	C2-C3-O3-P
29	A	406	CLA	C2A-CAA-CBA-CGA
29	C	506	CLA	C2A-CAA-CBA-CGA
29	R	604	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	c	506	CLA	C2A-CAA-CBA-CGA
45	n	607	CHL	C2A-CAA-CBA-CGA
29	B	605	CLA	C16-C17-C18-C20
31	C	516	BCR	C23-C24-C25-C26
31	C	516	BCR	C23-C24-C25-C30
31	D	404	BCR	C23-C24-C25-C26
31	D	404	BCR	C23-C24-C25-C30
31	c	515	BCR	C23-C24-C25-C26
31	c	515	BCR	C23-C24-C25-C30
31	d	404	BCR	C23-C24-C25-C26
35	B	620	C7Z	C21-C26-C27-C28
35	b	620	C7Z	C21-C26-C27-C28
44	H	101	RRX	C23-C24-C25-C30
44	h	101	RRX	C23-C24-C25-C30
46	N	620	LUT	C1-C6-C7-C8
46	R	620	LUT	C1-C6-C7-C8
46	R	620	LUT	C5-C6-C7-C8
46	n	621	LUT	C1-C6-C7-C8
46	n	621	LUT	C5-C6-C7-C8
46	r	620	LUT	C1-C6-C7-C8
46	r	620	LUT	C5-C6-C7-C8
29	C	510	CLA	C15-C16-C17-C18
32	B	621	SQD	C18-C19-C20-C21
33	a	413	LMG	C30-C31-C32-C33
33	H	102	LMG	O7-C10-C11-C12
33	h	102	LMG	O7-C10-C11-C12
42	d	405	PL9	C47-C48-C49-C51
36	b	623	DGA	CBB-CAB-CB9-CB8
31	B	618	BCR	C21-C22-C23-C24
46	R	620	LUT	C31-C32-C33-C34
46	r	620	LUT	C31-C32-C33-C34
29	y	614	CLA	C15-C16-C17-C18
48	s	623	NEX	C14-C15-C35-C34
39	s	624	LHG	C13-C14-C15-C16
39	D	409	LHG	C19-C20-C21-C22
29	Y	610	CLA	C8-C10-C11-C12
29	A	405	CLA	C10-C11-C12-C13
29	C	512	CLA	C5-C6-C7-C8
29	C	512	CLA	C15-C16-C17-C18
39	D	408	LHG	O6-C4-C5-C6
39	L	101	LHG	O6-C4-C5-C6
36	B	625	DGA	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
39	D	409	LHG	C24-C25-C26-C27
29	B	603	CLA	C6-C7-C8-C10
29	B	605	CLA	C11-C12-C13-C15
29	B	608	CLA	C12-C13-C15-C16
29	B	616	CLA	C12-C13-C15-C16
29	C	507	CLA	C11-C10-C8-C7
29	C	512	CLA	C11-C10-C8-C7
29	C	512	CLA	C12-C13-C15-C16
29	C	513	CLA	C6-C7-C8-C10
29	C	513	CLA	C11-C12-C13-C15
29	D	403	CLA	C11-C12-C13-C15
29	N	602	CLA	C11-C10-C8-C7
29	N	604	CLA	C6-C7-C8-C10
29	N	613	CLA	C11-C12-C13-C15
29	G	602	CLA	C6-C7-C8-C10
29	S	611	CLA	C6-C7-C8-C10
29	Y	602	CLA	C6-C7-C8-C10
29	Y	604	CLA	C11-C12-C13-C15
29	Y	614	CLA	C11-C10-C8-C7
29	a	405	CLA	C11-C12-C13-C15
29	b	617	CLA	C11-C12-C13-C15
29	c	504	CLA	C6-C7-C8-C10
29	c	507	CLA	C12-C13-C15-C16
29	c	508	CLA	C11-C10-C8-C7
29	c	508	CLA	C12-C13-C15-C16
29	c	512	CLA	C12-C13-C15-C16
29	n	603	CLA	C6-C7-C8-C10
29	n	604	CLA	C6-C7-C8-C10
29	n	613	CLA	C12-C13-C15-C16
29	g	602	CLA	C6-C7-C8-C10
29	g	613	CLA	C6-C7-C8-C10
29	g	613	CLA	C12-C13-C15-C16
29	s	603	CLA	C11-C12-C13-C15
45	N	605	CHL	C11-C10-C8-C7
45	N	605	CHL	C12-C13-C15-C16
45	N	606	CHL	C11-C12-C13-C15
45	Y	609	CHL	C12-C13-C15-C16
45	G	601	CHL	C3-C5-C6-C7
33	B	622	LMG	C14-C15-C16-C17
31	C	514	BCR	C15-C16-C17-C18
31	C	516	BCR	C9-C10-C11-C12
31	C	516	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	b	619	BCR	C9-C10-C11-C12
31	b	619	BCR	C13-C14-C15-C16
31	c	515	BCR	C19-C20-C21-C22
44	H	101	RRX	C9-C10-C11-C12
44	h	101	RRX	C9-C10-C11-C12
46	g	620	LUT	C29-C30-C31-C32
48	s	623	NEX	C13-C14-C15-C35
39	d	409	LHG	C19-C20-C21-C22
29	B	612	CLA	C10-C11-C12-C13
29	R	609	CLA	C10-C11-C12-C13
29	r	609	CLA	CAA-CBA-CGA-O2A
29	S	604	CLA	C2A-CAA-CBA-CGA
29	c	512	CLA	C2A-CAA-CBA-CGA
29	n	604	CLA	C2A-CAA-CBA-CGA
29	r	608	CLA	C2A-CAA-CBA-CGA
29	s	614	CLA	C2A-CAA-CBA-CGA
40	C	527	LMK	O1-C1-C2-C3
29	C	509	CLA	C5-C6-C7-C8
48	r	623	NEX	C40-C33-C34-C35
48	s	623	NEX	C20-C13-C14-C15
50	s	626	3PH	C23-C24-C25-C26
38	c	523	DGD	O6D-C5D-C6D-O5D
45	g	609	CHL	C3-C5-C6-C7
29	n	610	CLA	C16-C17-C18-C19
42	D	405	PL9	C47-C48-C49-C50
36	c	524	DGA	CA8-CA9-CAA-CBA
39	s	624	LHG	C12-C13-C14-C15
50	S	626	3PH	C38-C39-C3A-C3B
50	s	626	3PH	C34-C35-C36-C37
29	B	613	CLA	CAD-CBD-CGD-O2D
29	B	616	CLA	CAD-CBD-CGD-O2D
29	B	617	CLA	CAD-CBD-CGD-O2D
29	C	502	CLA	CAD-CBD-CGD-O2D
29	N	602	CLA	CAD-CBD-CGD-O2D
29	G	603	CLA	CAD-CBD-CGD-O2D
29	G	614	CLA	CAD-CBD-CGD-O2D
29	c	509	CLA	CAD-CBD-CGD-O2D
29	n	602	CLA	CAD-CBD-CGD-O2D
38	C	523	DGD	C1G-C2G-O2G-C1B
38	c	523	DGD	C1G-C2G-O2G-C1B
45	Y	606	CHL	CAD-CBD-CGD-O2D
48	S	622	NEX	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
48	s	623	NEX	C7-C8-C9-C19
32	C	526	SQD	C32-C33-C34-C35
33	A	413	LMG	C29-C30-C31-C32
29	B	609	CLA	C5-C6-C7-C8
29	N	604	CLA	C15-C16-C17-C18
29	b	615	CLA	C8-C10-C11-C12
29	g	603	CLA	C13-C15-C16-C17
39	Y	624	LHG	C25-C26-C27-C28
29	r	603	CLA	C4-C3-C5-C6
29	r	609	CLA	C4-C3-C5-C6
33	b	622	LMG	C14-C15-C16-C17
33	a	413	LMG	O6-C1-O1-C7
29	r	609	CLA	C2-C3-C5-C6
45	n	605	CHL	C2-C3-C5-C6
33	c	521	LMG	O1-C7-C8-C9
38	c	520	DGD	O1G-C1G-C2G-C3G
39	D	408	LHG	C4-C5-C6-O8
39	L	101	LHG	C4-C5-C6-O8
39	S	624	LHG	C4-C5-C6-O8
39	g	624	LHG	C4-C5-C6-O8
29	y	610	CLA	O1A-CGA-O2A-C1
39	L	101	LHG	O6-C4-C5-O7
39	N	624	LHG	O6-C4-C5-O7
39	c	625	LHG	O6-C4-C5-O7
29	B	602	CLA	C8-C10-C11-C12
43	F	101	HEM	C4B-C3B-CAB-CBB
43	F	101	HEM	C4C-C3C-CAC-CBC
43	f	101	HEM	C4B-C3B-CAB-CBB
36	b	623	DGA	CA8-CA9-CAA-CBA
36	b	623	DGA	CCB-CDB-CEB-CFB
39	y	624	LHG	C28-C29-C30-C31
39	S	624	LHG	C1-C2-C3-O3
39	d	410	LHG	C1-C2-C3-O3
29	N	604	CLA	CHA-CBD-CGD-O1D
29	N	604	CLA	CHA-CBD-CGD-O2D
29	G	602	CLA	CHA-CBD-CGD-O1D
29	G	602	CLA	CHA-CBD-CGD-O2D
29	R	604	CLA	CHA-CBD-CGD-O1D
29	R	604	CLA	CHA-CBD-CGD-O2D
29	R	612	CLA	CHA-CBD-CGD-O1D
29	R	612	CLA	CHA-CBD-CGD-O2D
29	Y	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	Y	603	CLA	CHA-CBD-CGD-O2D
29	Y	604	CLA	CHA-CBD-CGD-O1D
29	Y	612	CLA	CHA-CBD-CGD-O1D
29	Y	612	CLA	CHA-CBD-CGD-O2D
29	c	512	CLA	CHA-CBD-CGD-O2D
29	g	604	CLA	CHA-CBD-CGD-O1D
29	g	604	CLA	CHA-CBD-CGD-O2D
29	g	610	CLA	CHA-CBD-CGD-O1D
29	r	612	CLA	CHA-CBD-CGD-O1D
29	r	612	CLA	CHA-CBD-CGD-O2D
29	r	613	CLA	CHA-CBD-CGD-O1D
29	r	613	CLA	CHA-CBD-CGD-O2D
29	y	612	CLA	CHA-CBD-CGD-O1D
29	y	612	CLA	CHA-CBD-CGD-O2D
40	C	527	LMK	C2-C3-C4-O2
40	c	627	LMK	C2-C3-C4-O2
45	N	601	CHL	CHA-CBD-CGD-O1D
45	n	601	CHL	CHA-CBD-CGD-O1D
45	g	605	CHL	CHA-CBD-CGD-O2D
39	D	409	LHG	C25-C26-C27-C28
29	y	608	CLA	O1A-CGA-O2A-C1
32	c	626	SQD	C28-C29-C30-C31
33	A	413	LMG	O7-C8-C9-O8
33	H	102	LMG	O7-C8-C9-O8
38	c	519	DGD	O1G-C1G-C2G-O2G
39	S	624	LHG	O7-C5-C6-O8
40	c	627	LMK	O1-C7-C8-O7
29	B	610	CLA	CBA-CGA-O2A-C1
39	d	410	LHG	C30-C31-C32-C33
29	G	613	CLA	C5-C6-C7-C8
29	b	606	CLA	C5-C6-C7-C8
38	c	523	DGD	CCB-CDB-CEB-CFB
39	Y	624	LHG	C31-C32-C33-C34
29	b	608	CLA	C16-C17-C18-C20
29	C	509	CLA	C13-C15-C16-C17
45	n	605	CHL	C4-C3-C5-C6
39	s	624	LHG	O10-C23-O8-C6
39	L	101	LHG	C17-C18-C19-C20
29	B	615	CLA	C11-C12-C13-C14
29	D	403	CLA	C11-C12-C13-C14
29	N	613	CLA	C11-C12-C13-C14
29	G	613	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	b	603	CLA	C6-C7-C8-C9
29	b	606	CLA	C6-C7-C8-C9
29	c	503	CLA	C11-C12-C13-C14
45	N	605	CHL	C11-C10-C8-C9
45	N	609	CHL	C14-C13-C15-C16
45	Y	606	CHL	C11-C10-C8-C9
45	n	601	CHL	C11-C10-C8-C9
39	D	410	LHG	C11-C10-C9-C8
39	N	624	LHG	O10-C23-O8-C6
39	Y	624	LHG	C9-C10-C11-C12
50	i	101	3PH	C3B-C3C-C3D-C3E
32	c	626	SQD	C4-C5-C6-S
29	n	602	CLA	C16-C17-C18-C19
29	a	406	CLA	C2A-CAA-CBA-CGA
29	b	617	CLA	C2A-CAA-CBA-CGA
45	N	607	CHL	C2A-CAA-CBA-CGA
39	n	624	LHG	O8-C23-C24-C25
39	g	624	LHG	C12-C13-C14-C15
46	G	620	LUT	C27-C28-C29-C30
32	c	626	SQD	C12-C13-C14-C15
33	H	102	LMG	C15-C16-C17-C18
29	R	611	CLA	C1A-C2A-CAA-CBA
29	Y	604	CLA	C1A-C2A-CAA-CBA
29	Y	608	CLA	C1A-C2A-CAA-CBA
29	b	613	CLA	C1A-C2A-CAA-CBA
29	n	602	CLA	C1A-C2A-CAA-CBA
29	y	604	CLA	C1A-C2A-CAA-CBA
45	R	607	CHL	C1A-C2A-CAA-CBA
45	y	605	CHL	C1A-C2A-CAA-CBA
29	n	603	CLA	C5-C6-C7-C8
29	r	603	CLA	C10-C11-C12-C13
39	l	101	LHG	C24-C25-C26-C27
29	N	611	CLA	C2-C1-O2A-CGA
29	S	603	CLA	C2-C1-O2A-CGA
29	S	614	CLA	C2-C1-O2A-CGA
29	b	611	CLA	C2-C1-O2A-CGA
29	c	503	CLA	C2-C1-O2A-CGA
29	n	614	CLA	C2-C1-O2A-CGA
29	g	603	CLA	C2-C1-O2A-CGA
39	C	525	LHG	C28-C29-C30-C31
49	S	625	LPX	C12-C13-C14-C15
31	c	515	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
46	R	620	LUT	C29-C30-C31-C32
39	D	409	LHG	C4-O6-P-O3
39	d	410	LHG	C4-O6-P-O3
49	S	625	LPX	C3-O1-P1-O2
32	C	526	SQD	C13-C14-C15-C16
39	D	410	LHG	C2-C3-O3-P
39	d	410	LHG	C2-C3-O3-P
50	s	626	3PH	C2-C1-O11-P
45	G	609	CHL	C2-C3-C5-C6
32	b	621	SQD	C10-C11-C12-C13
39	n	624	LHG	C11-C10-C9-C8
39	s	624	LHG	C33-C34-C35-C36
29	B	610	CLA	O1A-CGA-O2A-C1
29	C	503	CLA	C4B-C3B-CAB-CBB
29	G	603	CLA	C4B-C3B-CAB-CBB
29	b	602	CLA	C4B-C3B-CAB-CBB
29	c	503	CLA	C4B-C3B-CAB-CBB
29	g	603	CLA	C4B-C3B-CAB-CBB
29	s	611	CLA	C4B-C3B-CAB-CBB
39	D	408	LHG	C3-O3-P-O5
39	D	410	LHG	C3-O3-P-O4
39	L	101	LHG	C3-O3-P-O5
39	N	624	LHG	C4-O6-P-O4
39	S	624	LHG	C4-O6-P-O5
39	c	625	LHG	C3-O3-P-O4
39	d	409	LHG	C3-O3-P-O5
39	d	410	LHG	C4-O6-P-O4
39	l	101	LHG	C3-O3-P-O5
39	n	624	LHG	C4-O6-P-O4
39	s	624	LHG	C4-O6-P-O5
49	S	625	LPX	C1-O2-P1-O4
49	s	625	LPX	C1-O2-P1-O4
29	N	604	CLA	C16-C17-C18-C19
29	b	611	CLA	C16-C17-C18-C20
29	b	615	CLA	C16-C17-C18-C19
29	r	603	CLA	C11-C12-C13-C15
38	c	523	DGD	C7B-C8B-C9B-CAB
30	A	408	PHO	CBA-CGA-O2A-C1
39	c	625	LHG	O6-C4-C5-C6
39	G	630	LHG	C35-C36-C37-C38
33	a	413	LMG	C28-C29-C30-C31
29	r	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	J	101	LMG	C11-C12-C13-C14
33	A	413	LMG	C34-C35-C36-C37
29	C	504	CLA	CAD-CBD-CGD-O1D
29	G	604	CLA	CAD-CBD-CGD-O1D
29	n	612	CLA	CAD-CBD-CGD-O1D
29	g	604	CLA	CAD-CBD-CGD-O1D
45	N	601	CHL	CAD-CBD-CGD-O1D
45	n	601	CHL	CAD-CBD-CGD-O1D
45	s	601	CHL	CAD-CBD-CGD-O1D
49	S	625	LPX	C2-C1-O2-P1
49	s	625	LPX	C2-C1-O2-P1
38	C	518	DGD	C2B-C3B-C4B-C5B
45	N	605	CHL	C3-C5-C6-C7
29	R	608	CLA	C8-C10-C11-C12
39	g	624	LHG	C35-C36-C37-C38
38	c	523	DGD	C4D-C5D-C6D-O5D
29	B	604	CLA	C11-C12-C13-C15
29	B	615	CLA	C11-C12-C13-C15
29	B	617	CLA	C11-C10-C8-C7
29	C	510	CLA	C6-C7-C8-C10
29	C	510	CLA	C11-C10-C8-C7
29	G	602	CLA	C12-C13-C15-C16
29	G	603	CLA	C11-C10-C8-C7
29	G	613	CLA	C11-C10-C8-C7
29	R	608	CLA	C6-C7-C8-C10
29	S	603	CLA	C11-C10-C8-C7
29	Y	611	CLA	C12-C13-C15-C16
29	a	406	CLA	C11-C10-C8-C7
29	b	603	CLA	C6-C7-C8-C10
29	b	605	CLA	C11-C12-C13-C15
29	b	613	CLA	C11-C12-C13-C15
29	b	615	CLA	C11-C12-C13-C15
29	c	502	CLA	C6-C7-C8-C10
29	c	507	CLA	C11-C10-C8-C7
29	c	512	CLA	C6-C7-C8-C10
29	c	512	CLA	C11-C10-C8-C7
29	d	402	CLA	C11-C12-C13-C15
29	d	403	CLA	C11-C12-C13-C15
29	g	602	CLA	C12-C13-C15-C16
29	s	609	CLA	C6-C7-C8-C10
29	y	610	CLA	C11-C10-C8-C7
29	y	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
30	A	409	PHO	C6-C7-C8-C10
30	a	409	PHO	C6-C7-C8-C10
39	C	525	LHG	O6-C4-C5-O7
39	G	630	LHG	O6-C4-C5-O7
45	G	601	CHL	C11-C12-C13-C15
45	Y	606	CHL	C11-C10-C8-C7
45	n	606	CHL	C11-C12-C13-C15
46	R	620	LUT	C25-C26-C27-C28
46	r	620	LUT	C25-C26-C27-C28
50	S	626	3PH	O11-C1-C2-O21
50	s	626	3PH	O11-C1-C2-O21
36	B	625	DGA	CA5-CA6-CA7-CA8
36	B	625	DGA	CDB-CEB-CFB-CGB
45	g	601	CHL	C10-C11-C12-C13
36	c	524	DGA	CAB-CBB-CCB-CDB
38	c	519	DGD	C5A-C6A-C7A-C8A
29	g	613	CLA	C8-C10-C11-C12
33	d	411	LMG	C28-C29-C30-C31
39	d	410	LHG	O2-C2-C3-O3
39	c	625	LHG	C25-C26-C27-C28
29	B	613	CLA	C2A-CAA-CBA-CGA
29	C	501	CLA	C2A-CAA-CBA-CGA
29	b	607	CLA	C2A-CAA-CBA-CGA
45	n	607	CHL	CAA-CBA-CGA-O2A
32	A	412	SQD	C44-C45-C46-O48
33	A	413	LMG	O1-C7-C8-C9
39	Y	624	LHG	C34-C35-C36-C37
32	A	412	SQD	O47-C45-C46-O48
38	c	519	DGD	O2G-C2G-C3G-O3G
39	D	410	LHG	O7-C5-C6-O8
39	L	101	LHG	O7-C5-C6-O8
39	d	408	LHG	O7-C5-C6-O8
39	s	624	LHG	O7-C5-C6-O8
39	y	624	LHG	O7-C5-C6-O8
40	C	527	LMK	O1-C7-C8-O7
33	h	102	LMG	C15-C16-C17-C18
40	c	627	LMK	C8-C9-O8-C28
39	g	624	LHG	O8-C23-C24-C25
29	c	513	CLA	C8-C10-C11-C12
29	G	602	CLA	C3-C5-C6-C7
29	n	602	CLA	C8-C10-C11-C12
36	b	623	DGA	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
29	Y	602	CLA	C10-C11-C12-C13
29	s	610	CLA	C8-C10-C11-C12
29	B	603	CLA	C6-C7-C8-C9
29	B	605	CLA	C11-C12-C13-C14
29	C	501	CLA	C11-C12-C13-C14
29	C	513	CLA	C6-C7-C8-C9
29	N	602	CLA	C11-C10-C8-C9
29	N	603	CLA	C11-C12-C13-C14
29	Y	602	CLA	C6-C7-C8-C9
29	Y	614	CLA	C11-C10-C8-C9
29	b	606	CLA	C11-C12-C13-C14
29	b	612	CLA	C11-C12-C13-C14
29	c	504	CLA	C6-C7-C8-C9
29	c	509	CLA	C11-C12-C13-C14
29	c	512	CLA	C11-C10-C8-C9
29	d	402	CLA	C11-C12-C13-C14
29	n	604	CLA	C6-C7-C8-C9
29	n	613	CLA	C14-C13-C15-C16
29	s	603	CLA	C11-C12-C13-C14
45	N	607	CHL	C11-C10-C8-C9
45	N	609	CHL	C11-C10-C8-C9
45	Y	609	CHL	C11-C12-C13-C14
45	n	606	CHL	C11-C10-C8-C9
45	y	601	CHL	C11-C10-C8-C9
29	G	610	CLA	C3-C5-C6-C7
29	Y	610	CLA	C10-C11-C12-C13
42	D	405	PL9	C14-C16-C17-C18
42	d	405	PL9	C39-C41-C42-C43
30	A	408	PHO	O1A-CGA-O2A-C1
39	N	624	LHG	O8-C23-C24-C25
31	D	404	BCR	C18-C19-C20-C21
31	d	404	BCR	C18-C19-C20-C21
31	B	619	BCR	C11-C12-C13-C35
46	G	620	LUT	C31-C32-C33-C40
29	c	508	CLA	C8-C10-C11-C12
29	B	604	CLA	C2B-C3B-CAB-CBB
29	B	607	CLA	C2B-C3B-CAB-CBB
29	B	610	CLA	C2B-C3B-CAB-CBB
29	B	616	CLA	C2B-C3B-CAB-CBB
29	C	503	CLA	C2B-C3B-CAB-CBB
29	C	504	CLA	C2B-C3B-CAB-CBB
29	C	507	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	C	510	CLA	C2B-C3B-CAB-CBB
29	N	614	CLA	C2B-C3B-CAB-CBB
29	S	602	CLA	C2B-C3B-CAB-CBB
29	S	614	CLA	C2B-C3B-CAB-CBB
29	Y	602	CLA	C2B-C3B-CAB-CBB
29	Y	610	CLA	C2B-C3B-CAB-CBB
29	Y	612	CLA	C2B-C3B-CAB-CBB
29	b	602	CLA	C2B-C3B-CAB-CBB
29	b	603	CLA	C2B-C3B-CAB-CBB
29	b	604	CLA	C2B-C3B-CAB-CBB
29	b	607	CLA	C2B-C3B-CAB-CBB
29	b	609	CLA	C2B-C3B-CAB-CBB
29	b	616	CLA	C2B-C3B-CAB-CBB
29	b	617	CLA	C2B-C3B-CAB-CBB
29	c	507	CLA	C2B-C3B-CAB-CBB
29	n	604	CLA	C2B-C3B-CAB-CBB
29	n	610	CLA	C2B-C3B-CAB-CBB
29	n	614	CLA	C2B-C3B-CAB-CBB
29	g	602	CLA	C2B-C3B-CAB-CBB
29	g	604	CLA	C2B-C3B-CAB-CBB
29	g	610	CLA	C2B-C3B-CAB-CBB
29	g	613	CLA	C2B-C3B-CAB-CBB
29	r	602	CLA	C2B-C3B-CAB-CBB
29	r	603	CLA	C2B-C3B-CAB-CBB
29	r	610	CLA	C2B-C3B-CAB-CBB
29	s	602	CLA	C2B-C3B-CAB-CBB
29	s	612	CLA	C2B-C3B-CAB-CBB
29	s	614	CLA	C2B-C3B-CAB-CBB
29	s	617	CLA	C2B-C3B-CAB-CBB
29	y	610	CLA	C2B-C3B-CAB-CBB
29	y	611	CLA	C2B-C3B-CAB-CBB
50	s	626	3PH	C31-C32-C33-C34
36	b	623	DGA	CA7-CA8-CA9-CAA
39	d	409	LHG	C34-C35-C36-C37
36	B	625	DGA	CCA-CDA-CEA-CFA
42	D	405	PL9	C45-C44-C46-C47
29	B	617	CLA	C10-C11-C12-C13
29	C	504	CLA	C10-C11-C12-C13
29	Y	611	CLA	C8-C10-C11-C12
39	d	409	LHG	C17-C18-C19-C20
29	b	617	CLA	C15-C16-C17-C18
29	N	611	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
29	G	604	CLA	C1-C2-C3-C4
29	G	614	CLA	C1-C2-C3-C4
29	n	611	CLA	C1-C2-C3-C4
29	g	604	CLA	C1-C2-C3-C4
29	g	614	CLA	C1-C2-C3-C4
45	N	608	CHL	C1-C2-C3-C4
45	G	606	CHL	C1-C2-C3-C4
45	G	607	CHL	C1-C2-C3-C4
45	n	608	CHL	C1-C2-C3-C4
45	g	606	CHL	C1-C2-C3-C4
45	g	607	CHL	C1-C2-C3-C4
45	r	607	CHL	C1-C2-C3-C4
29	C	505	CLA	C3-C5-C6-C7
38	C	518	DGD	CAB-CBB-CCB-CDB
39	S	624	LHG	C13-C14-C15-C16
29	A	405	CLA	C5-C6-C7-C8
39	N	624	LHG	C6-C5-O7-C7
50	s	626	3PH	O11-C1-C2-C3
29	B	607	CLA	C2A-CAA-CBA-CGA
29	N	613	CLA	C2A-CAA-CBA-CGA
29	S	610	CLA	C2A-CAA-CBA-CGA
29	c	501	CLA	C2A-CAA-CBA-CGA
29	y	603	CLA	C2A-CAA-CBA-CGA
45	n	606	CHL	C2A-CAA-CBA-CGA
29	b	603	CLA	C2-C1-O2A-CGA
29	d	403	CLA	C2-C1-O2A-CGA
38	C	519	DGD	C6B-C7B-C8B-C9B
33	C	521	LMG	C10-C11-C12-C13
29	R	609	CLA	CAA-CBA-CGA-O2A
29	G	603	CLA	C15-C16-C17-C18
39	d	410	LHG	C31-C32-C33-C34
39	L	101	LHG	C2-C3-O3-P
32	b	621	SQD	C14-C15-C16-C17
44	h	101	RRX	C15-C16-C17-C18
48	g	623	NEX	C13-C14-C15-C35
29	N	604	CLA	O1A-CGA-O2A-C1
39	d	409	LHG	O6-C4-C5-O7
39	L	101	LHG	C24-C25-C26-C27
30	a	408	PHO	C16-C17-C18-C19
45	R	607	CHL	O2A-C1-C2-C3
29	R	603	CLA	C4-C3-C5-C6
29	c	506	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	c	517	BCR	C5-C6-C7-C8
35	b	620	C7Z	C1-C6-C7-C8
46	N	620	LUT	C5-C6-C7-C8
29	G	610	CLA	C2-C3-C5-C6
45	N	607	CHL	CAA-CBA-CGA-O2A
29	b	610	CLA	C5-C6-C7-C8
39	D	408	LHG	C11-C10-C9-C8
29	B	608	CLA	C16-C17-C18-C20
29	b	608	CLA	C16-C17-C18-C19
29	r	603	CLA	C11-C12-C13-C14
39	l	101	LHG	C17-C18-C19-C20
29	B	617	CLA	C2A-CAA-CBA-CGA
33	c	521	LMG	O1-C7-C8-O7
38	c	523	DGD	O1G-C1G-C2G-O2G
29	Y	613	CLA	C10-C11-C12-C13
39	d	410	LHG	C11-C10-C9-C8
29	N	604	CLA	CBA-CGA-O2A-C1
39	N	624	LHG	C3-O3-P-O6
39	G	630	LHG	C3-O3-P-O6
39	S	624	LHG	C3-O3-P-O6
39	Y	624	LHG	C3-O3-P-O6
39	d	408	LHG	C3-O3-P-O6
39	d	409	LHG	C4-O6-P-O3
39	n	624	LHG	C3-O3-P-O6
39	g	624	LHG	C3-O3-P-O6
39	s	624	LHG	C3-O3-P-O6
39	y	624	LHG	C3-O3-P-O6
49	s	625	LPX	C3-O1-P1-O2
32	C	526	SQD	C12-C13-C14-C15
29	Y	613	CLA	C5-C6-C7-C8
30	a	409	PHO	CHA-CBD-CGD-O1D
30	a	409	PHO	CHA-CBD-CGD-O2D
36	B	625	DGA	CB4-CB5-CB6-CB7
33	H	102	LMG	C7-C8-C9-O8
50	i	101	3PH	C1-C2-C3-O31
39	C	525	LHG	C33-C34-C35-C36
39	N	624	LHG	C11-C10-C9-C8
29	B	613	CLA	C12-C13-C15-C16
29	B	617	CLA	C11-C12-C13-C15
29	N	603	CLA	C11-C12-C13-C15
29	b	606	CLA	C11-C12-C13-C15
29	r	603	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	S	614	CLA	CAA-CBA-CGA-O2A
32	b	621	SQD	C25-C26-C27-C28
29	C	510	CLA	C6-C7-C8-C9
29	D	402	CLA	C11-C10-C8-C9
29	G	603	CLA	C11-C10-C8-C9
29	S	603	CLA	C6-C7-C8-C9
29	Y	604	CLA	C11-C10-C8-C9
29	Y	611	CLA	C14-C13-C15-C16
29	b	602	CLA	C11-C12-C13-C14
29	b	612	CLA	C14-C13-C15-C16
29	b	615	CLA	C11-C12-C13-C14
29	b	617	CLA	C11-C12-C13-C14
29	c	511	CLA	C11-C12-C13-C14
29	c	513	CLA	C6-C7-C8-C9
29	d	403	CLA	C11-C12-C13-C14
29	s	610	CLA	C6-C7-C8-C9
29	y	611	CLA	C14-C13-C15-C16
29	y	612	CLA	C11-C12-C13-C14
45	N	605	CHL	C14-C13-C15-C16
31	C	515	BCR	C9-C10-C11-C12
31	c	516	BCR	C9-C10-C11-C12
29	C	513	CLA	C16-C17-C18-C19
29	b	613	CLA	C16-C17-C18-C19
39	n	624	LHG	C24-C23-O8-C6
29	D	403	CLA	C10-C11-C12-C13
29	C	513	CLA	C8-C10-C11-C12
33	A	413	LMG	C30-C31-C32-C33
46	n	620	LUT	C31-C32-C33-C40
29	n	602	CLA	C16-C17-C18-C20
30	a	408	PHO	C16-C17-C18-C20
39	d	409	LHG	C24-C25-C26-C27
29	b	606	CLA	C8-C10-C11-C12
33	d	411	LMG	C12-C13-C14-C15
50	s	626	3PH	C3D-C3E-C3F-C3G
39	Y	624	LHG	C29-C30-C31-C32
39	d	408	LHG	C11-C10-C9-C8
29	N	611	CLA	O2A-C1-C2-C3
29	s	604	CLA	C4-C3-C5-C6
33	c	521	LMG	C28-C29-C30-C31
29	n	611	CLA	O1A-CGA-O2A-C1
29	N	604	CLA	C16-C17-C18-C20
29	b	611	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	n	611	CLA	CBA-CGA-O2A-C1
30	a	408	PHO	CBA-CGA-O2A-C1
29	y	610	CLA	C15-C16-C17-C18
50	s	626	3PH	C22-C23-C24-C25
29	B	604	CLA	C4B-C3B-CAB-CBB
29	B	610	CLA	C4B-C3B-CAB-CBB
29	B	616	CLA	C4B-C3B-CAB-CBB
29	C	504	CLA	C4B-C3B-CAB-CBB
29	C	507	CLA	C4B-C3B-CAB-CBB
29	N	604	CLA	C4B-C3B-CAB-CBB
29	N	610	CLA	C4B-C3B-CAB-CBB
29	G	602	CLA	C4B-C3B-CAB-CBB
29	S	614	CLA	C4B-C3B-CAB-CBB
29	Y	604	CLA	C4B-C3B-CAB-CBB
29	b	603	CLA	C4B-C3B-CAB-CBB
29	b	604	CLA	C4B-C3B-CAB-CBB
29	b	607	CLA	C4B-C3B-CAB-CBB
29	b	610	CLA	C4B-C3B-CAB-CBB
29	b	616	CLA	C4B-C3B-CAB-CBB
29	n	610	CLA	C4B-C3B-CAB-CBB
29	n	614	CLA	C4B-C3B-CAB-CBB
29	g	602	CLA	C4B-C3B-CAB-CBB
29	g	604	CLA	C4B-C3B-CAB-CBB
29	g	610	CLA	C4B-C3B-CAB-CBB
29	s	612	CLA	C4B-C3B-CAB-CBB
29	y	611	CLA	C4B-C3B-CAB-CBB
29	B	611	CLA	C2A-CAA-CBA-CGA
29	C	510	CLA	C2A-CAA-CBA-CGA
31	B	619	BCR	C13-C14-C15-C16
31	d	404	BCR	C9-C10-C11-C12
46	n	620	LUT	C29-C30-C31-C32
46	r	620	LUT	C9-C10-C11-C12
46	r	620	LUT	C29-C30-C31-C32
46	y	620	LUT	C29-C30-C31-C32
39	s	624	LHG	O6-C4-C5-C6
42	D	405	PL9	C39-C41-C42-C43
29	y	602	CLA	C10-C11-C12-C13
39	y	624	LHG	C34-C35-C36-C37
47	R	621	XAT	C30-C31-C32-C33
48	y	623	NEX	C30-C31-C32-C33
33	C	521	LMG	C28-C29-C30-C31
29	Y	611	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	G	602	CLA	C4-C3-C5-C6
29	b	607	CLA	C4-C3-C5-C6
29	n	602	CLA	C13-C15-C16-C17
39	n	624	LHG	C33-C34-C35-C36
39	n	624	LHG	O10-C23-O8-C6
36	b	623	DGA	CB2-CB3-CB4-CB5
29	B	606	CLA	C8-C10-C11-C12
29	C	504	CLA	C8-C10-C11-C12
29	S	610	CLA	C2-C1-O2A-CGA
29	Y	602	CLA	C2-C1-O2A-CGA
29	y	602	CLA	C2-C1-O2A-CGA
30	A	409	PHO	C2-C1-O2A-CGA
39	l	101	LHG	C26-C27-C28-C29
38	c	520	DGD	C4B-C5B-C6B-C7B
29	C	502	CLA	C2A-CAA-CBA-CGA
29	C	512	CLA	C2A-CAA-CBA-CGA
29	G	610	CLA	C2A-CAA-CBA-CGA
29	b	611	CLA	C2A-CAA-CBA-CGA
29	g	602	CLA	C2A-CAA-CBA-CGA
29	r	613	CLA	C2A-CAA-CBA-CGA
33	h	102	LMG	O7-C8-C9-O8
39	S	624	LHG	C2-C3-O3-P
39	l	101	LHG	C2-C3-O3-P
33	D	411	LMG	C32-C33-C34-C35
29	C	511	CLA	C3A-C2A-CAA-CBA
29	S	605	CLA	C3A-C2A-CAA-CBA
45	y	601	CHL	C3A-C2A-CAA-CBA
33	h	102	LMG	C12-C13-C14-C15
39	D	409	LHG	C17-C18-C19-C20
46	Y	620	LUT	C33-C34-C35-C15
29	C	510	CLA	C4-C3-C5-C6
39	C	525	LHG	C9-C10-C11-C12
50	i	101	3PH	C27-C28-C29-C2A
29	c	510	CLA	C5-C6-C7-C8
29	B	616	CLA	C6-C7-C8-C9
29	C	510	CLA	C11-C10-C8-C9
29	G	602	CLA	C11-C10-C8-C9
29	b	609	CLA	C11-C12-C13-C14
29	b	617	CLA	C6-C7-C8-C9
29	c	511	CLA	C6-C7-C8-C9
29	n	603	CLA	C11-C12-C13-C14
29	y	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	y	614	CLA	C11-C10-C8-C9
45	N	605	CHL	C11-C12-C13-C14
45	N	606	CHL	C14-C13-C15-C16
45	n	609	CHL	C14-C13-C15-C16
45	g	601	CHL	C11-C10-C8-C9
45	y	607	CHL	C11-C12-C13-C14
29	c	503	CLA	C16-C17-C18-C19
45	s	601	CHL	CAA-CBA-CGA-O2A
29	c	509	CLA	C8-C10-C11-C12
39	C	525	LHG	C25-C26-C27-C28
39	d	410	LHG	C34-C35-C36-C37
31	D	404	BCR	C20-C21-C22-C37
31	d	404	BCR	C20-C21-C22-C37
38	c	519	DGD	C1G-C2G-C3G-O3G
39	y	624	LHG	C4-C5-C6-O8
48	S	622	NEX	C39-C29-C30-C31
48	s	623	NEX	C39-C29-C30-C31
33	h	102	LMG	O9-C10-O7-C8
32	c	626	SQD	C9-C10-C11-C12
39	C	525	LHG	C12-C13-C14-C15
45	s	606	CHL	C2A-CAA-CBA-CGA
29	C	511	CLA	C2A-CAA-CBA-CGA
29	b	615	CLA	C16-C17-C18-C20
38	C	518	DGD	O6E-C1E-O5D-C6D
29	r	609	CLA	C8-C10-C11-C12
45	S	601	CHL	CAA-CBA-CGA-O1A
47	G	622	XAT	C14-C15-C35-C34
45	N	607	CHL	C8-C10-C11-C12
33	H	102	LMG	C12-C13-C14-C15
51	Y	625	SPH	C11-C10-C9-C8
39	n	624	LHG	C6-C5-O7-C7
51	Y	625	SPH	O3-C3-C4-C5
29	b	605	CLA	C15-C16-C17-C18
45	y	609	CHL	C4-C3-C5-C6
29	D	403	CLA	C1A-C2A-CAA-CBA
29	Y	614	CLA	C1A-C2A-CAA-CBA
29	d	403	CLA	C1A-C2A-CAA-CBA
29	g	614	CLA	C1A-C2A-CAA-CBA
29	y	602	CLA	C1A-C2A-CAA-CBA
45	N	609	CHL	C1A-C2A-CAA-CBA
45	Y	601	CHL	C1A-C2A-CAA-CBA
29	A	406	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	C	510	CLA	C2-C3-C5-C6
29	R	609	CLA	C6-C7-C8-C10
29	b	608	CLA	C12-C13-C15-C16
29	c	503	CLA	C6-C7-C8-C10
29	c	510	CLA	C11-C10-C8-C7
29	d	402	CLA	C11-C10-C8-C7
29	y	604	CLA	C11-C10-C8-C7
45	N	607	CHL	C11-C12-C13-C15
29	C	508	CLA	C8-C10-C11-C12
29	G	613	CLA	C13-C15-C16-C17
29	Y	603	CLA	C10-C11-C12-C13
29	c	501	CLA	C3-C5-C6-C7
31	C	514	BCR	C19-C20-C21-C22
31	C	515	BCR	C19-C20-C21-C22
39	L	101	LHG	C31-C32-C33-C34
30	a	408	PHO	O1A-CGA-O2A-C1
29	g	603	CLA	C3-C5-C6-C7
29	A	405	CLA	C2A-CAA-CBA-CGA
29	G	602	CLA	C2A-CAA-CBA-CGA
29	g	610	CLA	C2A-CAA-CBA-CGA
29	c	509	CLA	C13-C15-C16-C17
29	c	512	CLA	C5-C6-C7-C8
38	C	523	DGD	C6A-C7A-C8A-C9A
39	D	410	LHG	C34-C35-C36-C37
39	G	630	LHG	C33-C34-C35-C36
45	N	608	CHL	O2A-C1-C2-C3
45	n	608	CHL	O2A-C1-C2-C3
29	N	613	CLA	C10-C11-C12-C13
38	c	519	DGD	C6A-C7A-C8A-C9A
36	b	623	DGA	CA5-CA6-CA7-CA8
39	G	630	LHG	O8-C23-C24-C25
29	n	602	CLA	C4-C3-C5-C6
33	d	411	LMG	C32-C33-C34-C35
29	s	603	CLA	C8-C10-C11-C12
38	C	520	DGD	C1A-C2A-C3A-C4A
29	G	602	CLA	C2B-C3B-CAB-CBB
29	G	603	CLA	C2B-C3B-CAB-CBB
29	S	604	CLA	C2B-C3B-CAB-CBB
29	Y	604	CLA	C2B-C3B-CAB-CBB
29	c	503	CLA	C2B-C3B-CAB-CBB
29	g	603	CLA	C2B-C3B-CAB-CBB
29	r	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
29	s	611	CLA	C2B-C3B-CAB-CBB
29	y	602	CLA	C2B-C3B-CAB-CBB
32	C	526	SQD	C31-C32-C33-C34
43	f	101	HEM	C3D-CAD-CBD-CGD
45	s	601	CHL	CAA-CBA-CGA-O1A
29	g	603	CLA	C5-C6-C7-C8
39	G	630	LHG	C9-C10-C11-C12
39	l	101	LHG	C31-C32-C33-C34
29	a	406	CLA	C3-C5-C6-C7
45	g	601	CHL	C3-C5-C6-C7
31	D	404	BCR	C20-C21-C22-C23
31	d	404	BCR	C20-C21-C22-C23
48	S	622	NEX	C28-C29-C30-C31
48	s	623	NEX	C28-C29-C30-C31
29	s	602	CLA	C10-C11-C12-C13
32	a	412	SQD	C27-C28-C29-C30
38	C	519	DGD	O2G-C2G-C3G-O3G
39	D	408	LHG	O7-C5-C6-O8
29	D	402	CLA	CBA-CGA-O2A-C1
32	a	412	SQD	C32-C33-C34-C35
39	G	630	LHG	C16-C17-C18-C19
50	s	626	3PH	C33-C34-C35-C36
31	a	411	BCR	C19-C20-C21-C22
31	c	514	BCR	C19-C20-C21-C22
46	Y	620	LUT	C29-C30-C31-C32
33	h	102	LMG	C19-C20-C21-C22
29	D	402	CLA	O1A-CGA-O2A-C1
33	C	521	LMG	O10-C28-O8-C9
39	N	624	LHG	C1-C2-C3-O3
29	a	406	CLA	C15-C16-C17-C18
45	N	609	CHL	C8-C10-C11-C12
29	R	602	CLA	C3-C5-C6-C7
29	C	506	CLA	C4-C3-C5-C6
29	N	613	CLA	CAA-CBA-CGA-O1A
29	N	602	CLA	C2-C1-O2A-CGA
29	b	615	CLA	C2-C1-O2A-CGA
29	c	501	CLA	C2-C1-O2A-CGA
45	G	609	CHL	C2-C1-O2A-CGA
45	g	607	CHL	C2-C1-O2A-CGA
29	c	506	CLA	C2-C3-C5-C6
29	s	604	CLA	C2-C3-C5-C6
39	D	409	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	d	409	LHG	C18-C19-C20-C21
45	S	601	CHL	CAA-CBA-CGA-O2A
29	C	512	CLA	C11-C12-C13-C14
29	c	504	CLA	C14-C13-C15-C16
29	r	610	CLA	C10-C11-C12-C13
45	g	608	CHL	C2A-CAA-CBA-CGA
33	c	521	LMG	O10-C28-O8-C9
29	A	406	CLA	C3-C5-C6-C7
29	S	614	CLA	C5-C6-C7-C8
51	y	625	SPH	O1-C1-C2-C3
29	d	402	CLA	CAA-CBA-CGA-O2A
33	H	102	LMG	C19-C20-C21-C22
39	N	624	LHG	C33-C34-C35-C36
45	g	605	CHL	C2-C1-O2A-CGA
29	B	602	CLA	C16-C17-C18-C19
38	c	520	DGD	C9B-CAB-CBB-CCB
38	c	523	DGD	CDA-CEA-CFA-CGA
31	B	618	BCR	C23-C24-C25-C30
31	B	619	BCR	C23-C24-C25-C30
31	b	618	BCR	C23-C24-C25-C30
31	c	514	BCR	C23-C24-C25-C30
31	c	517	BCR	C1-C6-C7-C8
35	B	620	C7Z	C1-C6-C7-C8
46	S	621	LUT	C1-C6-C7-C8
46	y	620	LUT	C1-C6-C7-C8
46	y	620	LUT	C5-C6-C7-C8
29	Y	612	CLA	C5-C6-C7-C8
29	s	611	CLA	CAA-CBA-CGA-O2A
39	C	525	LHG	O8-C23-C24-C25
32	B	621	SQD	O6-C44-C45-C46
32	b	621	SQD	O6-C44-C45-C46
33	h	102	LMG	C7-C8-C9-O8
31	b	619	BCR	C15-C16-C17-C18
46	G	620	LUT	C29-C30-C31-C32
47	r	622	XAT	C33-C34-C35-C15
47	y	622	XAT	C29-C30-C31-C32
29	B	617	CLA	C4-C3-C5-C6
29	N	602	CLA	C4-C3-C5-C6
29	c	511	CLA	C4-C3-C5-C6
29	y	610	CLA	C4-C3-C5-C6
45	n	609	CHL	C4-C3-C5-C6
31	B	619	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
46	G	620	LUT	C31-C32-C33-C34
38	C	519	DGD	C5A-C6A-C7A-C8A
29	R	603	CLA	C2-C3-C5-C6
48	G	623	NEX	C14-C15-C35-C34
39	L	101	LHG	C26-C27-C28-C29
29	D	402	CLA	C15-C16-C17-C18
29	g	613	CLA	C5-C6-C7-C8
29	b	613	CLA	C2A-CAA-CBA-CGA
33	C	521	LMG	C29-C28-O8-C9
29	g	610	CLA	C3-C5-C6-C7
29	n	612	CLA	CAA-CBA-CGA-O2A
29	C	502	CLA	C4B-C3B-CAB-CBB
29	R	604	CLA	C4B-C3B-CAB-CBB
29	S	604	CLA	C4B-C3B-CAB-CBB
29	c	502	CLA	C4B-C3B-CAB-CBB
29	c	513	CLA	C4B-C3B-CAB-CBB
29	n	602	CLA	C4B-C3B-CAB-CBB
29	r	604	CLA	C4B-C3B-CAB-CBB
29	y	602	CLA	C4B-C3B-CAB-CBB
29	B	604	CLA	C15-C16-C17-C18
29	G	610	CLA	C15-C16-C17-C18
39	D	410	LHG	C29-C30-C31-C32
29	C	512	CLA	C11-C12-C13-C15
29	n	603	CLA	C11-C12-C13-C15
45	n	605	CHL	C11-C12-C13-C15
45	g	609	CHL	C11-C12-C13-C15
45	y	609	CHL	C2-C3-C5-C6
33	c	521	LMG	C29-C28-O8-C9
33	A	413	LMG	C33-C34-C35-C36
33	h	102	LMG	C11-C12-C13-C14
36	b	623	DGA	OG2-CG2-CG3-OXT
36	c	524	DGA	OG2-CG2-CG3-OXT
31	A	411	BCR	C19-C20-C21-C22
31	D	404	BCR	C13-C14-C15-C16
46	N	620	LUT	C29-C30-C31-C32
29	D	402	CLA	CAA-CBA-CGA-O2A
30	A	408	PHO	C16-C17-C18-C19
32	b	621	SQD	C18-C19-C20-C21
29	S	603	CLA	C10-C11-C12-C13
38	c	520	DGD	O1G-C1G-C2G-O2G
39	s	624	LHG	C35-C36-C37-C38
29	Y	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
45	g	606	CHL	O2A-C1-C2-C3
45	r	607	CHL	O2A-C1-C2-C3
29	b	605	CLA	CAA-CBA-CGA-O2A
29	y	613	CLA	CAA-CBA-CGA-O2A
39	d	410	LHG	O8-C23-C24-C25
45	r	607	CHL	CAA-CBA-CGA-O2A
33	d	411	LMG	C29-C30-C31-C32
39	D	408	LHG	C31-C32-C33-C34
29	y	613	CLA	C10-C11-C12-C13
29	B	608	CLA	C16-C17-C18-C19
36	c	524	DGA	CA2-CA1-OG1-CG1
38	C	520	DGD	O6D-C5D-C6D-O5D
29	S	604	CLA	C4-C3-C5-C6
29	b	609	CLA	C4-C3-C5-C6
29	b	617	CLA	C4-C3-C5-C6
29	c	505	CLA	C4-C3-C5-C6
29	s	611	CLA	C4-C3-C5-C6
42	d	405	PL9	C20-C19-C21-C22
45	Y	609	CHL	C4-C3-C5-C6
29	A	406	CLA	C15-C16-C17-C18
38	C	520	DGD	C9A-CAA-CBA-CCA
29	N	602	CLA	C2-C3-C5-C6
29	n	602	CLA	C2-C3-C5-C6
30	A	408	PHO	C2-C3-C5-C6
42	d	405	PL9	C18-C19-C21-C22
33	b	622	LMG	O7-C10-C11-C12
39	Y	624	LHG	C15-C16-C17-C18
29	B	604	CLA	C11-C12-C13-C14
29	R	608	CLA	C6-C7-C8-C9
29	S	603	CLA	C11-C10-C8-C9
29	a	406	CLA	C11-C10-C8-C9
29	b	613	CLA	C11-C12-C13-C14
29	c	506	CLA	C6-C7-C8-C9
29	c	512	CLA	C6-C7-C8-C9
29	n	604	CLA	C11-C10-C8-C9
45	y	609	CHL	C11-C10-C8-C9
51	Y	625	SPH	C2-C3-C4-C5
29	R	610	CLA	C3A-C2A-CAA-CBA
29	n	610	CLA	C3A-C2A-CAA-CBA
29	g	604	CLA	C3A-C2A-CAA-CBA
29	s	605	CLA	C3A-C2A-CAA-CBA
45	R	607	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
45	g	601	CHL	C3A-C2A-CAA-CBA
45	s	601	CHL	C3A-C2A-CAA-CBA
45	y	605	CHL	C3A-C2A-CAA-CBA
39	d	409	LHG	C16-C17-C18-C19
39	g	624	LHG	C16-C17-C18-C19
45	Y	607	CHL	C10-C11-C12-C13
29	b	610	CLA	O1A-CGA-O2A-C1
36	c	524	DGA	OA1-CA1-OG1-CG1
29	b	609	CLA	CAA-CBA-CGA-O2A
32	a	412	SQD	O47-C7-C8-C9
33	B	622	LMG	O7-C10-C11-C12
39	l	101	LHG	O7-C7-C8-C9
50	s	626	3PH	C36-C37-C38-C39
29	S	612	CLA	CAA-CBA-CGA-O2A
29	B	610	CLA	CAD-CBD-CGD-O2D
29	C	509	CLA	CAD-CBD-CGD-O2D
29	C	510	CLA	CAD-CBD-CGD-O2D
29	N	603	CLA	CAD-CBD-CGD-O2D
29	G	611	CLA	CAD-CBD-CGD-O2D
29	S	612	CLA	CAD-CBD-CGD-O2D
29	b	610	CLA	CAD-CBD-CGD-O2D
29	b	617	CLA	CAD-CBD-CGD-O2D
29	c	503	CLA	CAD-CBD-CGD-O2D
29	c	504	CLA	CAD-CBD-CGD-O2D
29	n	603	CLA	CAD-CBD-CGD-O2D
29	y	614	CLA	CAD-CBD-CGD-O2D
30	A	408	PHO	CAD-CBD-CGD-O2D
40	c	627	LMK	C1-C2-C3-N4
45	S	601	CHL	CAD-CBD-CGD-O2D
45	r	606	CHL	CAD-CBD-CGD-O2D
45	y	606	CHL	CAD-CBD-CGD-O2D
29	C	513	CLA	C16-C17-C18-C20
29	y	610	CLA	C8-C10-C11-C12
29	B	617	CLA	C2-C1-O2A-CGA
38	c	519	DGD	O6D-C5D-C6D-O5D
39	D	410	LHG	O8-C23-C24-C25
33	d	411	LMG	C15-C16-C17-C18
39	D	410	LHG	C31-C32-C33-C34
39	G	630	LHG	C34-C35-C36-C37
42	D	405	PL9	C20-C19-C21-C22
29	b	609	CLA	C16-C17-C18-C19
39	g	624	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	b	602	CLA	C2-C3-C5-C6
29	S	617	CLA	CAA-CBA-CGA-O2A
29	Y	613	CLA	CAA-CBA-CGA-O2A
33	c	521	LMG	O7-C10-C11-C12
32	C	526	SQD	C27-C28-C29-C30
38	C	520	DGD	C9B-CAB-CBB-CCB
46	n	620	LUT	C31-C32-C33-C34
38	C	519	DGD	O1G-C1G-C2G-C3G
38	C	523	DGD	O1G-C1G-C2G-C3G
39	c	625	LHG	C5-C4-O6-P
40	C	527	LMK	C11-C10-O7-C8
47	N	622	XAT	O24-C26-C27-C28
47	Y	622	XAT	O24-C26-C27-C28
29	n	612	CLA	CAA-CBA-CGA-O1A
39	Y	624	LHG	O6-C4-C5-O7
29	C	503	CLA	CAA-CBA-CGA-O2A
29	G	613	CLA	CAA-CBA-CGA-O2A
36	B	625	DGA	OG2-CB1-CB2-CB3
29	n	613	CLA	C16-C17-C18-C19
39	S	624	LHG	C35-C36-C37-C38
36	C	524	DGA	CA5-CA6-CA7-CA8
29	S	605	CLA	C2A-CAA-CBA-CGA
29	b	605	CLA	C13-C15-C16-C17
39	G	630	LHG	C32-C33-C34-C35
29	a	410	CLA	C3-C5-C6-C7
39	D	409	LHG	C27-C28-C29-C30
29	B	611	CLA	CHA-CBD-CGD-O1D
29	B	611	CLA	CHA-CBD-CGD-O2D
29	C	507	CLA	CHA-CBD-CGD-O2D
29	G	604	CLA	CHA-CBD-CGD-O1D
29	G	610	CLA	CHA-CBD-CGD-O1D
29	G	610	CLA	CHA-CBD-CGD-O2D
29	G	612	CLA	CHA-CBD-CGD-O1D
29	G	612	CLA	CHA-CBD-CGD-O2D
29	G	613	CLA	CHA-CBD-CGD-O1D
29	G	613	CLA	CHA-CBD-CGD-O2D
29	R	602	CLA	CHA-CBD-CGD-O1D
29	R	602	CLA	CHA-CBD-CGD-O2D
29	R	603	CLA	CHA-CBD-CGD-O1D
29	R	603	CLA	CHA-CBD-CGD-O2D
29	R	609	CLA	CHA-CBD-CGD-O1D
29	R	609	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	S	603	CLA	CHA-CBD-CGD-O1D
29	S	603	CLA	CHA-CBD-CGD-O2D
29	S	617	CLA	CHA-CBD-CGD-O1D
29	S	617	CLA	CHA-CBD-CGD-O2D
29	Y	602	CLA	CHA-CBD-CGD-O1D
29	Y	604	CLA	CHA-CBD-CGD-O2D
29	Y	608	CLA	CHA-CBD-CGD-O1D
29	Y	608	CLA	CHA-CBD-CGD-O2D
29	Y	610	CLA	CHA-CBD-CGD-O1D
29	Y	610	CLA	CHA-CBD-CGD-O2D
29	b	609	CLA	CHA-CBD-CGD-O1D
29	b	609	CLA	CHA-CBD-CGD-O2D
29	b	615	CLA	CHA-CBD-CGD-O1D
29	b	615	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CHA-CBD-CGD-O1D
29	c	502	CLA	CHA-CBD-CGD-O2D
29	c	507	CLA	CHA-CBD-CGD-O1D
29	c	507	CLA	CHA-CBD-CGD-O2D
29	d	402	CLA	CHA-CBD-CGD-O2D
29	n	604	CLA	CHA-CBD-CGD-O1D
29	n	604	CLA	CHA-CBD-CGD-O2D
29	n	612	CLA	CHA-CBD-CGD-O1D
29	g	602	CLA	CHA-CBD-CGD-O2D
29	g	612	CLA	CHA-CBD-CGD-O1D
29	g	612	CLA	CHA-CBD-CGD-O2D
29	r	602	CLA	CHA-CBD-CGD-O1D
29	r	602	CLA	CHA-CBD-CGD-O2D
29	r	603	CLA	CHA-CBD-CGD-O2D
29	r	604	CLA	CHA-CBD-CGD-O1D
29	r	604	CLA	CHA-CBD-CGD-O2D
29	r	609	CLA	CHA-CBD-CGD-O1D
29	r	609	CLA	CHA-CBD-CGD-O2D
29	r	610	CLA	CHA-CBD-CGD-O1D
29	r	610	CLA	CHA-CBD-CGD-O2D
29	s	603	CLA	CHA-CBD-CGD-O2D
29	s	612	CLA	CHA-CBD-CGD-O1D
29	s	612	CLA	CHA-CBD-CGD-O2D
29	s	617	CLA	CHA-CBD-CGD-O1D
29	s	617	CLA	CHA-CBD-CGD-O2D
29	y	603	CLA	CHA-CBD-CGD-O1D
29	y	603	CLA	CHA-CBD-CGD-O2D
29	y	608	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	y	608	CLA	CHA-CBD-CGD-O2D
29	y	610	CLA	CHA-CBD-CGD-O1D
29	y	610	CLA	CHA-CBD-CGD-O2D
29	y	613	CLA	CHA-CBD-CGD-O1D
29	y	613	CLA	CHA-CBD-CGD-O2D
31	d	404	BCR	C13-C14-C15-C16
45	N	601	CHL	CHA-CBD-CGD-O2D
45	G	606	CHL	CHA-CBD-CGD-O1D
45	G	606	CHL	CHA-CBD-CGD-O2D
45	G	609	CHL	CHA-CBD-CGD-O1D
45	G	609	CHL	CHA-CBD-CGD-O2D
45	Y	609	CHL	CHA-CBD-CGD-O2D
45	n	601	CHL	CHA-CBD-CGD-O2D
45	g	609	CHL	CHA-CBD-CGD-O1D
45	g	609	CHL	CHA-CBD-CGD-O2D
45	r	607	CHL	CHA-CBD-CGD-O1D
45	r	607	CHL	CHA-CBD-CGD-O2D
45	s	601	CHL	CHA-CBD-CGD-O1D
45	y	609	CHL	CHA-CBD-CGD-O1D
45	y	609	CHL	CHA-CBD-CGD-O2D
29	s	612	CLA	CAA-CBA-CGA-O2A
29	B	608	CLA	CAA-CBA-CGA-O2A
29	g	613	CLA	CAA-CBA-CGA-O2A
29	c	505	CLA	C2-C3-C5-C6
45	n	609	CHL	C2-C3-C5-C6
29	s	604	CLA	C3-C5-C6-C7
39	Y	624	LHG	O6-C4-C5-C6
39	d	408	LHG	O6-C4-C5-C6
29	S	612	CLA	CAA-CBA-CGA-O1A
39	d	408	LHG	C31-C32-C33-C34
29	s	604	CLA	C6-C7-C8-C9
42	d	405	PL9	C2-C3-C7-C8
29	B	605	CLA	CAA-CBA-CGA-O2A
29	B	612	CLA	CAA-CBA-CGA-O2A
29	S	611	CLA	CAA-CBA-CGA-O2A
29	b	608	CLA	CAA-CBA-CGA-O2A
29	n	604	CLA	CAA-CBA-CGA-O2A
32	C	526	SQD	O47-C7-C8-C9
33	C	521	LMG	O7-C10-C11-C12
33	J	101	LMG	O7-C10-C11-C12
32	a	412	SQD	O6-C44-C45-O47
40	c	627	LMK	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	C15-C16-C17-C18
29	A	405	CLA	CAA-CBA-CGA-O2A
29	B	603	CLA	CAA-CBA-CGA-O2A
29	B	609	CLA	CAA-CBA-CGA-O2A
29	R	604	CLA	CAA-CBA-CGA-O2A
36	b	623	DGA	OG2-CB1-CB2-CB3
39	D	408	LHG	O7-C7-C8-C9
45	n	605	CHL	CAA-CBA-CGA-O2A
30	A	409	PHO	CHA-CBD-CGD-O1D
30	A	409	PHO	CHA-CBD-CGD-O2D
29	a	405	CLA	C8-C10-C11-C12
29	a	405	CLA	C15-C16-C17-C18
29	b	610	CLA	CBA-CGA-O2A-C1
32	C	526	SQD	O48-C23-C24-C25
36	C	524	DGA	OG1-CA1-CA2-CA3
32	a	412	SQD	C11-C12-C13-C14
39	g	624	LHG	C34-C35-C36-C37
39	s	624	LHG	C25-C26-C27-C28
29	r	610	CLA	C8-C10-C11-C12
29	G	602	CLA	C2-C3-C5-C6
29	S	610	CLA	C11-C12-C13-C15
29	S	611	CLA	C11-C12-C13-C15
29	Y	603	CLA	C11-C12-C13-C15
29	b	607	CLA	C2-C3-C5-C6
29	s	603	CLA	C12-C13-C15-C16
29	y	610	CLA	C6-C7-C8-C10
45	Y	609	CHL	C2-C3-C5-C6
29	Y	611	CLA	C16-C17-C18-C20
38	c	523	DGD	C6A-C7A-C8A-C9A
29	b	603	CLA	CAA-CBA-CGA-O2A
32	A	412	SQD	C10-C11-C12-C13
29	A	406	CLA	C11-C10-C8-C9
29	B	606	CLA	C11-C12-C13-C14
29	B	617	CLA	C11-C10-C8-C9
29	Y	610	CLA	C11-C10-C8-C9
29	b	608	CLA	C14-C13-C15-C16
29	c	503	CLA	C6-C7-C8-C9
31	B	619	BCR	C19-C20-C21-C22
31	b	618	BCR	C13-C14-C15-C16
31	c	516	BCR	C19-C20-C21-C22
29	N	604	CLA	C2B-C3B-CAB-CBB
29	R	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
45	N	607	CHL	C2B-C3B-CAB-CBB
45	N	608	CHL	C2B-C3B-CAB-CBB
45	G	607	CHL	C2B-C3B-CAB-CBB
45	Y	601	CHL	C2B-C3B-CAB-CBB
45	n	607	CHL	C2B-C3B-CAB-CBB
45	n	608	CHL	C2B-C3B-CAB-CBB
45	y	601	CHL	C2B-C3B-CAB-CBB
39	D	409	LHG	C11-C10-C9-C8
50	S	626	3PH	C2E-C2F-C2G-C2H
29	R	612	CLA	CAA-CBA-CGA-O2A
29	S	603	CLA	CAA-CBA-CGA-O2A
32	a	412	SQD	C4-C5-C6-S
39	G	630	LHG	C19-C20-C21-C22
33	h	102	LMG	C11-C10-O7-C8
29	B	610	CLA	C2A-CAA-CBA-CGA
29	B	614	CLA	C2A-CAA-CBA-CGA
29	G	613	CLA	CAA-CBA-CGA-O1A
29	r	609	CLA	CAA-CBA-CGA-O1A
45	N	605	CHL	CAA-CBA-CGA-O2A
39	y	624	LHG	C14-C15-C16-C17
32	C	526	SQD	C9-C10-C11-C12
29	B	602	CLA	CAA-CBA-CGA-O2A
39	d	408	LHG	C10-C11-C12-C13
39	d	410	LHG	C27-C28-C29-C30
31	a	411	BCR	C7-C8-C9-C10
31	a	411	BCR	C11-C12-C13-C14
47	R	621	XAT	C7-C8-C9-C10
29	g	604	CLA	C1A-C2A-CAA-CBA
29	r	609	CLA	C1A-C2A-CAA-CBA
45	N	605	CHL	C1A-C2A-CAA-CBA
45	G	601	CHL	C1A-C2A-CAA-CBA
45	g	601	CHL	C1A-C2A-CAA-CBA
45	g	607	CHL	C1A-C2A-CAA-CBA
45	r	607	CHL	C1A-C2A-CAA-CBA
45	s	601	CHL	C1A-C2A-CAA-CBA
45	y	601	CHL	C1A-C2A-CAA-CBA
29	b	605	CLA	CAA-CBA-CGA-O1A
45	r	607	CHL	CAA-CBA-CGA-O1A
29	c	503	CLA	CAA-CBA-CGA-O2A
29	S	609	CLA	C8-C10-C11-C12
33	H	102	LMG	C29-C30-C31-C32
33	d	411	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
29	S	617	CLA	CAA-CBA-CGA-O1A
33	B	622	LMG	O9-C10-C11-C12
39	d	410	LHG	O10-C23-C24-C25
45	N	605	CHL	CAA-CBA-CGA-O1A
32	a	412	SQD	C12-C13-C14-C15
39	d	408	LHG	C12-C13-C14-C15
38	c	519	DGD	O1G-C1G-C2G-C3G
29	s	610	CLA	CAA-CBA-CGA-O2A
39	y	624	LHG	O8-C23-C24-C25
29	B	603	CLA	CAA-CBA-CGA-O1A
29	y	613	CLA	CAA-CBA-CGA-O1A
32	C	526	SQD	O49-C7-C8-C9
33	a	413	LMG	C29-C30-C31-C32
30	A	408	PHO	C4-C3-C5-C6
39	g	624	LHG	C10-C11-C12-C13
51	y	625	SPH	C12-C13-C14-C15
29	B	605	CLA	CAA-CBA-CGA-O1A
29	B	608	CLA	CAA-CBA-CGA-O1A
33	C	521	LMG	O9-C10-C11-C12
33	b	622	LMG	O9-C10-C11-C12
50	S	626	3PH	C29-C2A-C2B-C2C
29	C	511	CLA	C13-C15-C16-C17
29	R	608	CLA	C10-C11-C12-C13
29	a	410	CLA	C4B-C3B-CAB-CBB
39	N	624	LHG	C3-O3-P-O5
39	G	630	LHG	C3-O3-P-O5
39	Y	624	LHG	C3-O3-P-O5
39	d	408	LHG	C3-O3-P-O5
39	g	624	LHG	C3-O3-P-O5
39	y	624	LHG	C3-O3-P-O5
45	G	605	CHL	C4B-C3B-CAB-CBB
45	G	609	CHL	C4B-C3B-CAB-CBB
45	S	608	CHL	C4B-C3B-CAB-CBB
45	Y	609	CHL	C4B-C3B-CAB-CBB
45	y	609	CHL	C4B-C3B-CAB-CBB
29	B	609	CLA	CAA-CBA-CGA-O1A
29	C	503	CLA	CAA-CBA-CGA-O1A
29	b	603	CLA	CAA-CBA-CGA-O1A
29	b	609	CLA	CAA-CBA-CGA-O1A
36	B	625	DGA	OB1-CB1-CB2-CB3
29	C	508	CLA	CAA-CBA-CGA-O2A
29	s	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
46	S	621	LUT	C5-C6-C7-C8
33	j	101	LMG	C30-C31-C32-C33
29	B	616	CLA	C10-C11-C12-C13
29	B	612	CLA	CAA-CBA-CGA-O1A
29	b	608	CLA	CAA-CBA-CGA-O1A
33	c	521	LMG	O9-C10-C11-C12
29	c	503	CLA	C8-C10-C11-C12
39	D	409	LHG	C18-C19-C20-C21
45	s	601	CHL	C2A-CAA-CBA-CGA
29	g	613	CLA	CAA-CBA-CGA-O1A
39	D	410	LHG	O10-C23-C24-C25
39	L	101	LHG	C19-C20-C21-C22
39	Y	624	LHG	C23-C24-C25-C26
39	y	624	LHG	C23-C24-C25-C26
29	Y	613	CLA	CAA-CBA-CGA-O1A
33	J	101	LMG	O9-C10-C11-C12
29	b	610	CLA	C4-C3-C5-C6
30	a	409	PHO	C4-C3-C5-C6
32	a	412	SQD	C10-C11-C12-C13
29	B	614	CLA	CAD-CBD-CGD-O1D
29	C	511	CLA	CAD-CBD-CGD-O1D
29	a	410	CLA	CAD-CBD-CGD-O1D
29	b	613	CLA	CAD-CBD-CGD-O1D
29	c	502	CLA	CAD-CBD-CGD-O1D
29	c	510	CLA	CAD-CBD-CGD-O1D
29	d	402	CLA	CAD-CBD-CGD-O1D
29	r	603	CLA	CAD-CBD-CGD-O1D
29	r	613	CLA	CAD-CBD-CGD-O1D
29	s	603	CLA	CAD-CBD-CGD-O1D
29	y	610	CLA	CAD-CBD-CGD-O1D
32	B	621	SQD	O5-C5-C6-S
32	b	621	SQD	O5-C5-C6-S
45	G	609	CHL	CAD-CBD-CGD-O1D
29	R	604	CLA	CAA-CBA-CGA-O1A
29	n	604	CLA	CAA-CBA-CGA-O1A
36	b	623	DGA	OB1-CB1-CB2-CB3
39	D	408	LHG	O9-C7-C8-C9
29	S	605	CLA	CAA-CBA-CGA-O2A
29	g	614	CLA	CAA-CBA-CGA-O2A
29	B	612	CLA	C11-C12-C13-C14
29	C	503	CLA	C6-C7-C8-C9
29	C	504	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	S	611	CLA	C11-C12-C13-C14
29	Y	603	CLA	C11-C12-C13-C14
29	c	510	CLA	C11-C10-C8-C9
29	d	402	CLA	C11-C10-C8-C9
29	n	613	CLA	C11-C12-C13-C14
29	y	604	CLA	C11-C10-C8-C9
29	y	610	CLA	C6-C7-C8-C9
29	y	613	CLA	C6-C7-C8-C9
45	n	606	CHL	C11-C12-C13-C14
45	n	609	CHL	C11-C10-C8-C9
45	g	609	CHL	C14-C13-C15-C16
32	B	621	SQD	C14-C15-C16-C17
37	b	625	GOL	O2-C2-C3-O3
33	a	413	LMG	C11-C12-C13-C14
33	H	102	LMG	O9-C10-C11-C12
33	h	102	LMG	O9-C10-C11-C12
36	C	524	DGA	OA1-CA1-CA2-CA3
29	C	505	CLA	CAA-CBA-CGA-O2A
29	R	610	CLA	CAA-CBA-CGA-O2A
29	r	604	CLA	CAA-CBA-CGA-O2A
29	s	603	CLA	CAA-CBA-CGA-O2A
45	y	606	CHL	CAA-CBA-CGA-O2A
39	s	624	LHG	C10-C11-C12-C13
29	s	610	CLA	CAA-CBA-CGA-O1A
45	n	605	CHL	CAA-CBA-CGA-O1A
29	C	513	CLA	C15-C16-C17-C18
29	Y	602	CLA	C13-C15-C16-C17
29	N	604	CLA	CAA-CBA-CGA-O2A
29	G	614	CLA	CAA-CBA-CGA-O2A
33	D	411	LMG	O7-C10-C11-C12
33	d	411	LMG	O7-C10-C11-C12
33	j	101	LMG	O7-C10-C11-C12
38	c	518	DGD	O1G-C1A-C2A-C3A
29	N	603	CLA	C10-C11-C12-C13
29	b	612	CLA	C5-C6-C7-C8
29	g	613	CLA	C3-C5-C6-C7
29	A	405	CLA	CAA-CBA-CGA-O1A
36	B	625	DGA	CA7-CA8-CA9-CAA
29	R	610	CLA	C4-C3-C5-C6
29	Y	610	CLA	C4-C3-C5-C6
29	b	602	CLA	C4-C3-C5-C6
29	b	616	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	g	610	CLA	C4-C3-C5-C6
30	A	409	PHO	C4-C3-C5-C6
29	B	616	CLA	C15-C16-C17-C18
36	c	524	DGA	CA2-CA3-CA4-CA5
29	B	606	CLA	C11-C12-C13-C15
29	C	501	CLA	C11-C12-C13-C15
29	C	503	CLA	C6-C7-C8-C10
29	Y	610	CLA	C6-C7-C8-C10
29	Y	610	CLA	C11-C10-C8-C7
29	b	607	CLA	C11-C12-C13-C15
29	b	609	CLA	C11-C12-C13-C15
29	b	612	CLA	C11-C12-C13-C15
29	b	612	CLA	C12-C13-C15-C16
29	b	613	CLA	C6-C7-C8-C10
29	c	503	CLA	C11-C10-C8-C7
29	c	511	CLA	C3A-C2A-CAA-CBA
29	g	613	CLA	C11-C12-C13-C15
45	S	608	CHL	C11-C10-C8-C7
45	n	601	CHL	C11-C10-C8-C7
29	S	603	CLA	CAA-CBA-CGA-O1A
39	y	624	LHG	O10-C23-C24-C25
38	C	523	DGD	C4D-C5D-C6D-O5D
38	C	523	DGD	O6D-C5D-C6D-O5D
29	Y	614	CLA	CAA-CBA-CGA-O2A
29	c	505	CLA	CAA-CBA-CGA-O2A
29	y	614	CLA	CAA-CBA-CGA-O2A
38	C	523	DGD	O1G-C1A-C2A-C3A
39	Y	624	LHG	O8-C23-C24-C25
39	d	408	LHG	O7-C7-C8-C9
39	s	624	LHG	O8-C23-C24-C25
29	C	511	CLA	C8-C10-C11-C12
51	Y	625	SPH	C4-C5-C6-C7
33	c	521	LMG	C30-C31-C32-C33
38	C	519	DGD	C1B-C2B-C3B-C4B
31	b	618	BCR	C21-C22-C23-C24
46	y	620	LUT	C27-C28-C29-C30
29	c	503	CLA	CAA-CBA-CGA-O1A
32	c	626	SQD	O49-C7-C8-C9
45	y	606	CHL	CAA-CBA-CGA-O1A
29	s	604	CLA	C6-C7-C8-C10
30	A	408	PHO	C16-C17-C18-C20
29	G	603	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
39	L	101	LHG	O7-C7-C8-C9
33	H	102	LMG	C16-C17-C18-C19
38	C	518	DGD	C6A-C7A-C8A-C9A
29	a	405	CLA	C13-C15-C16-C17
29	B	602	CLA	CAA-CBA-CGA-O1A
29	N	604	CLA	CAA-CBA-CGA-O1A
29	G	603	CLA	CAA-CBA-CGA-O1A
29	G	614	CLA	CAA-CBA-CGA-O1A
29	S	605	CLA	CAA-CBA-CGA-O1A
29	s	603	CLA	CAA-CBA-CGA-O1A
32	C	526	SQD	O10-C23-C24-C25
33	D	411	LMG	O9-C10-C11-C12
38	C	523	DGD	O1A-C1A-C2A-C3A
38	c	518	DGD	O1A-C1A-C2A-C3A
29	r	612	CLA	C5-C6-C7-C8
45	g	601	CHL	C8-C10-C11-C12
45	y	607	CHL	C10-C11-C12-C13
33	h	102	LMG	C16-C17-C18-C19
50	i	101	3PH	C2C-C2D-C2E-C2F
29	c	502	CLA	CAA-CBA-CGA-O2A
29	c	508	CLA	CAA-CBA-CGA-O2A
32	c	626	SQD	O47-C7-C8-C9
39	S	624	LHG	O8-C23-C24-C25
39	d	409	LHG	C35-C36-C37-C38
29	r	604	CLA	CAA-CBA-CGA-O1A
45	n	608	CHL	C2A-CAA-CBA-CGA
29	d	402	CLA	O1A-CGA-O2A-C1
32	c	626	SQD	C11-C12-C13-C14
39	s	624	LHG	O10-C23-C24-C25
39	d	410	LHG	C10-C11-C12-C13
29	C	513	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

301 monomers are involved in 799 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	y	602	CLA	2	0
29	B	602	CLA	3	0
29	C	502	CLA	4	0
29	y	603	CLA	5	0
29	y	612	CLA	3	0
36	c	524	DGA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	d	409	LHG	1	0
29	s	611	CLA	3	0
29	N	610	CLA	6	0
46	S	621	LUT	7	0
39	D	410	LHG	1	0
29	r	610	CLA	5	0
38	C	523	DGD	5	0
48	R	622	NEX	2	0
31	D	404	BCR	3	0
46	s	621	LUT	6	0
38	c	520	DGD	4	0
46	G	621	LUT	3	0
31	A	411	BCR	3	0
29	N	602	CLA	6	0
29	g	614	CLA	1	0
45	y	605	CHL	1	0
45	n	607	CHL	5	0
29	y	604	CLA	3	0
48	r	623	NEX	3	0
45	s	608	CHL	3	0
45	s	606	CHL	2	0
29	g	602	CLA	4	0
29	b	607	CLA	4	0
29	D	403	CLA	3	0
29	b	614	CLA	2	0
45	R	607	CHL	1	0
39	N	624	LHG	2	0
45	Y	601	CHL	1	0
38	C	519	DGD	6	0
45	Y	609	CHL	7	0
29	b	606	CLA	4	0
31	C	517	BCR	5	0
31	C	514	BCR	6	0
44	h	101	RRX	1	0
39	D	409	LHG	3	0
45	g	607	CHL	1	0
29	C	503	CLA	4	0
47	r	622	XAT	5	0
39	d	408	LHG	3	0
45	n	605	CHL	4	0
29	b	612	CLA	5	0
30	A	408	PHO	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	c	521	LMG	6	0
29	Y	612	CLA	3	0
29	C	505	CLA	5	0
29	Y	610	CLA	2	0
31	c	516	BCR	4	0
29	G	604	CLA	3	0
29	b	610	CLA	4	0
32	C	526	SQD	2	0
45	r	606	CHL	2	0
38	C	518	DGD	5	0
36	C	524	DGA	3	0
45	y	609	CHL	2	0
29	N	604	CLA	1	0
29	R	604	CLA	1	0
39	D	408	LHG	3	0
31	c	517	BCR	3	0
29	G	614	CLA	1	0
29	B	604	CLA	3	0
33	H	102	LMG	6	0
45	n	609	CHL	4	0
45	g	605	CHL	3	0
29	g	603	CLA	1	0
45	G	608	CHL	1	0
29	s	614	CLA	2	0
47	N	622	XAT	3	0
29	B	617	CLA	7	0
47	G	622	XAT	4	0
29	c	501	CLA	3	0
32	b	621	SQD	3	0
29	S	610	CLA	4	0
39	c	625	LHG	2	0
45	s	607	CHL	2	0
48	s	623	NEX	1	0
29	C	511	CLA	7	0
32	A	412	SQD	2	0
30	a	408	PHO	5	0
29	C	512	CLA	3	0
29	y	614	CLA	5	0
46	N	621	LUT	6	0
29	C	501	CLA	7	0
29	R	609	CLA	4	0
29	B	608	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	r	603	CLA	1	0
29	d	402	CLA	4	0
29	N	614	CLA	1	0
29	b	616	CLA	7	0
33	d	411	LMG	3	0
45	g	609	CHL	3	0
29	r	608	CLA	4	0
29	Y	608	CLA	3	0
39	s	624	LHG	6	0
29	B	607	CLA	9	0
29	s	609	CLA	2	0
29	B	610	CLA	3	0
45	N	608	CHL	2	0
45	N	606	CHL	4	0
29	B	606	CLA	6	0
29	a	410	CLA	4	0
29	N	612	CLA	1	0
45	G	601	CHL	5	0
29	s	613	CLA	3	0
29	n	603	CLA	7	0
29	r	602	CLA	2	0
48	n	623	NEX	2	0
29	B	612	CLA	7	0
29	c	510	CLA	5	0
29	b	603	CLA	1	0
39	L	101	LHG	6	0
39	S	624	LHG	8	0
48	S	622	NEX	2	0
29	b	617	CLA	5	0
46	g	620	LUT	4	0
29	Y	603	CLA	2	0
46	n	621	LUT	3	0
30	A	409	PHO	5	0
29	c	507	CLA	2	0
29	c	509	CLA	2	0
46	n	620	LUT	3	0
45	y	606	CHL	3	0
31	C	516	BCR	4	0
29	s	603	CLA	3	0
32	B	621	SQD	5	0
29	S	609	CLA	1	0
29	G	612	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	605	CLA	5	0
31	C	515	BCR	4	0
29	a	405	CLA	7	0
48	N	623	NEX	2	0
29	r	609	CLA	3	0
29	S	612	CLA	1	0
29	s	604	CLA	2	0
33	j	101	LMG	2	0
45	N	605	CHL	2	0
38	C	520	DGD	5	0
29	Y	604	CLA	2	0
29	C	508	CLA	4	0
33	C	521	LMG	4	0
29	C	513	CLA	10	0
39	Y	624	LHG	3	0
29	r	613	CLA	1	0
31	B	618	BCR	3	0
29	y	610	CLA	1	0
29	n	610	CLA	4	0
29	B	609	CLA	6	0
30	a	409	PHO	4	0
29	c	512	CLA	2	0
45	n	608	CHL	1	0
29	G	613	CLA	1	0
43	f	101	HEM	3	0
29	G	603	CLA	2	0
45	g	606	CHL	2	0
29	b	604	CLA	2	0
29	B	613	CLA	5	0
29	B	603	CLA	2	0
45	n	601	CHL	3	0
45	N	609	CHL	2	0
29	c	508	CLA	2	0
29	R	602	CLA	3	0
29	R	612	CLA	2	0
29	R	603	CLA	1	0
44	H	101	RRX	2	0
29	y	611	CLA	2	0
31	b	619	BCR	1	0
29	S	614	CLA	1	0
29	Y	611	CLA	4	0
29	b	615	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	g	610	CLA	2	0
29	Y	614	CLA	3	0
29	n	613	CLA	4	0
29	n	612	CLA	2	0
29	B	616	CLA	5	0
45	S	606	CHL	4	0
33	A	413	LMG	6	0
47	R	621	XAT	5	0
29	b	611	CLA	5	0
45	Y	605	CHL	2	0
45	S	607	CHL	3	0
38	c	519	DGD	5	0
37	b	625	GOL	1	0
29	c	505	CLA	4	0
42	d	405	PL9	2	0
29	c	504	CLA	3	0
45	S	608	CHL	4	0
36	b	623	DGA	1	0
45	N	601	CHL	2	0
29	A	407	CLA	1	0
45	R	606	CHL	1	0
46	Y	621	LUT	3	0
29	b	613	CLA	2	0
29	C	504	CLA	3	0
46	Y	620	LUT	2	0
45	N	607	CHL	3	0
29	b	605	CLA	5	0
46	g	621	LUT	5	0
33	a	413	LMG	5	0
29	G	602	CLA	4	0
46	r	620	LUT	4	0
29	C	509	CLA	4	0
29	A	410	CLA	6	0
50	i	101	3PH	1	0
31	c	515	BCR	2	0
39	d	410	LHG	2	0
45	y	601	CHL	4	0
26	a	401	OEX	1	0
29	r	604	CLA	1	0
31	b	618	BCR	2	0
39	y	624	LHG	2	0
47	n	622	XAT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	s	602	CLA	3	0
29	C	510	CLA	5	0
29	s	610	CLA	3	0
29	G	610	CLA	3	0
29	b	608	CLA	2	0
33	b	622	LMG	1	0
29	S	602	CLA	4	0
29	n	602	CLA	3	0
45	n	606	CHL	2	0
45	G	606	CHL	2	0
39	n	624	LHG	2	0
29	C	507	CLA	6	0
29	c	503	CLA	2	0
47	g	622	XAT	2	0
46	R	620	LUT	4	0
29	S	613	CLA	3	0
45	g	601	CHL	5	0
29	c	506	CLA	4	0
29	a	407	CLA	1	0
29	Y	602	CLA	5	0
39	g	624	LHG	4	0
33	D	411	LMG	5	0
45	G	605	CHL	3	0
29	B	615	CLA	4	0
46	y	621	LUT	2	0
31	d	404	BCR	3	0
29	C	506	CLA	3	0
38	c	518	DGD	5	0
29	r	612	CLA	2	0
29	b	602	CLA	1	0
45	g	608	CHL	3	0
31	a	411	BCR	3	0
29	S	603	CLA	3	0
29	R	610	CLA	4	0
31	c	514	BCR	6	0
29	D	402	CLA	7	0
38	c	523	DGD	4	0
45	G	609	CHL	3	0
29	R	608	CLA	3	0
46	S	620	LUT	5	0
29	Y	613	CLA	4	0
29	y	613	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	406	CLA	5	0
51	y	625	SPH	3	0
45	Y	607	CHL	7	0
48	Y	623	NEX	1	0
29	S	604	CLA	1	0
29	B	614	CLA	3	0
45	S	601	CHL	2	0
42	D	405	PL9	3	0
39	G	630	LHG	4	0
46	G	620	LUT	3	0
39	l	101	LHG	4	0
50	s	626	3PH	1	0
33	h	102	LMG	8	0
47	Y	622	XAT	1	0
39	C	525	LHG	7	0
43	F	101	HEM	3	0
46	s	620	LUT	3	0
29	a	406	CLA	6	0
29	c	502	CLA	5	0
29	S	611	CLA	2	0
31	B	619	BCR	3	0
29	d	403	CLA	3	0
45	Y	606	CHL	2	0
32	c	626	SQD	4	0
29	n	604	CLA	1	0
29	s	617	CLA	1	0
46	N	620	LUT	6	0
45	s	601	CHL	2	0
29	y	608	CLA	1	0
45	r	607	CHL	1	0
29	N	603	CLA	3	0
50	S	626	3PH	4	0
29	c	511	CLA	6	0
29	b	609	CLA	7	0
47	y	622	XAT	2	0
29	c	513	CLA	7	0
29	g	613	CLA	2	0
29	A	405	CLA	7	0
36	B	625	DGA	2	0
51	Y	625	SPH	2	0
45	y	607	CHL	4	0
29	B	611	CLA	3	0

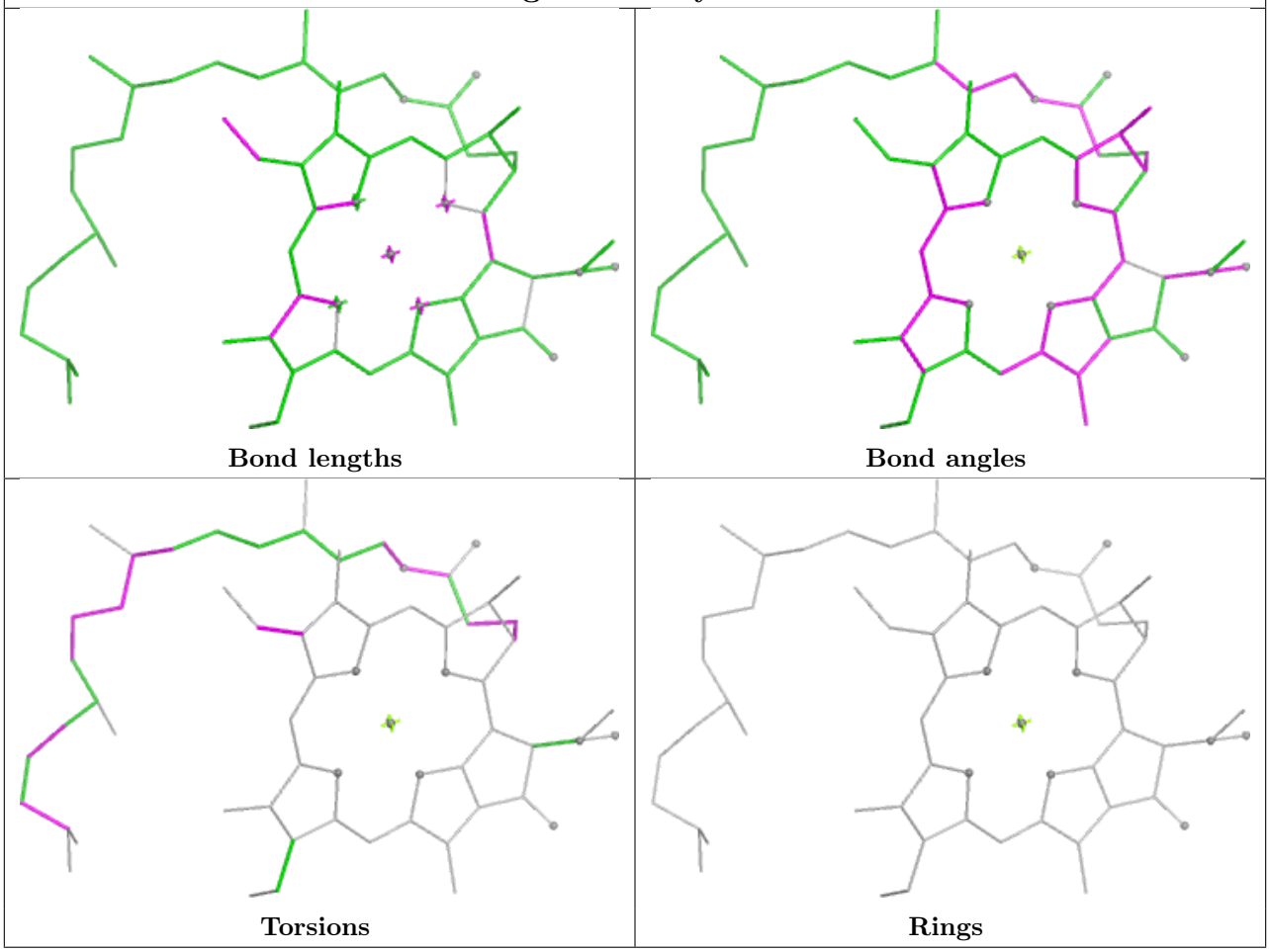
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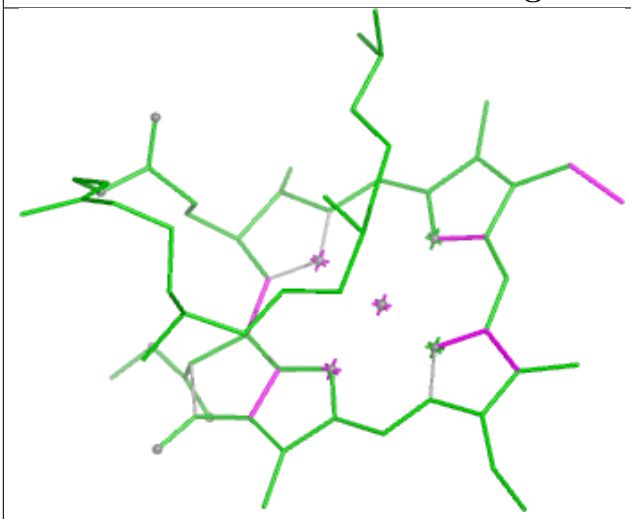
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	B	622	LMG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

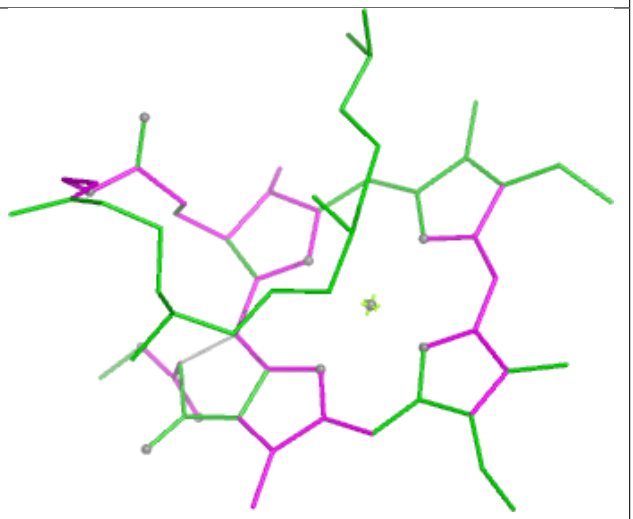
Ligand CLA y 602



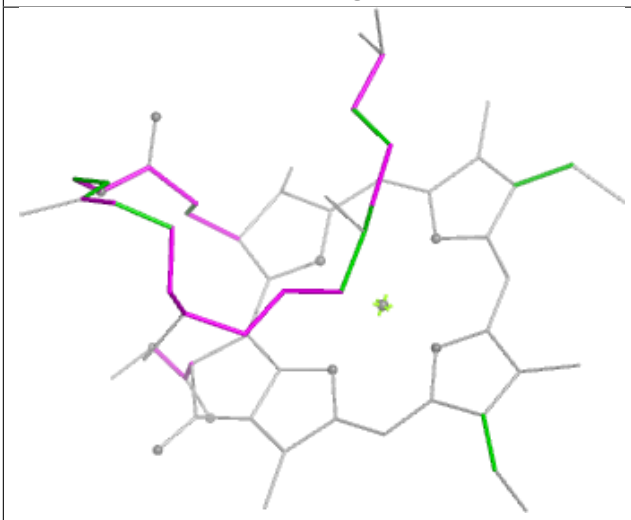
Ligand CLA B 602



Bond lengths



Bond angles

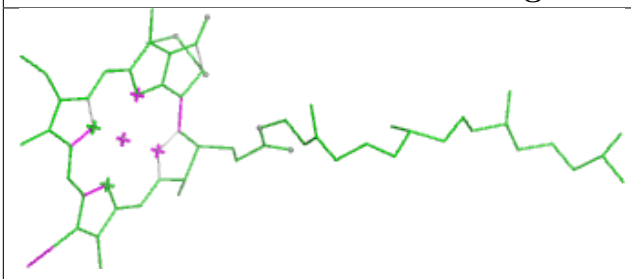


Torsions

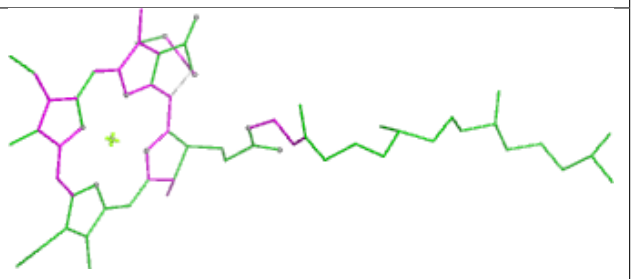


Rings

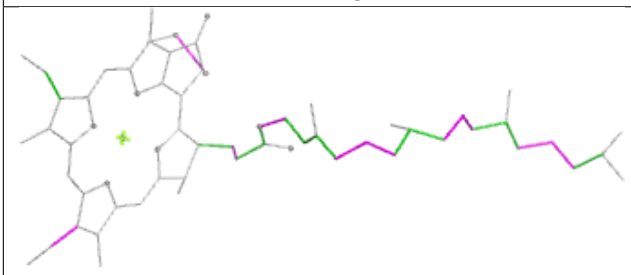
Ligand CLA C 502



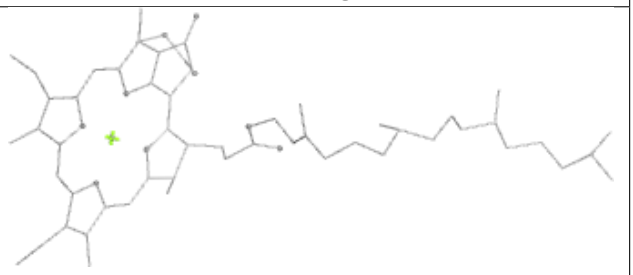
Bond lengths



Bond angles

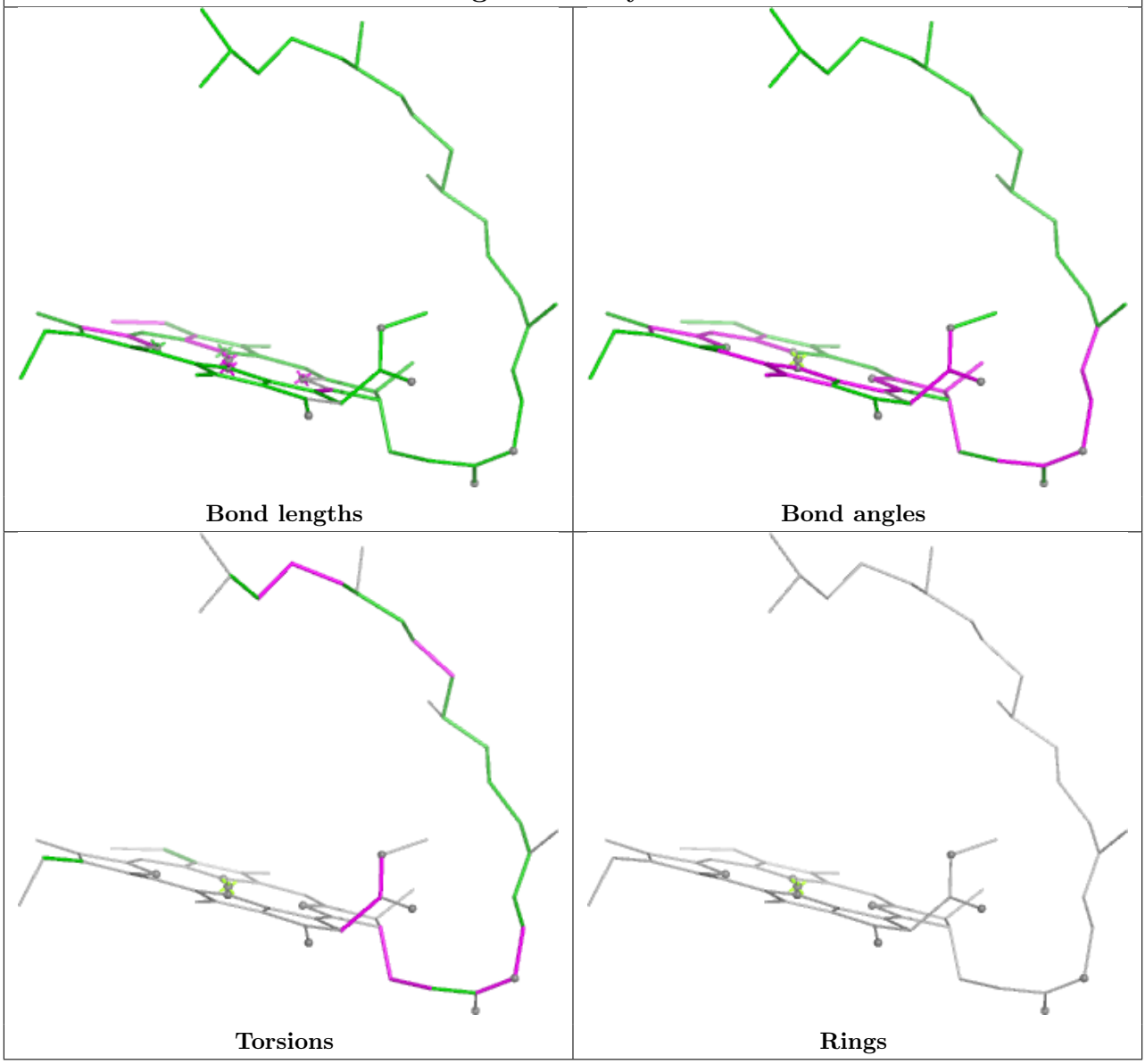


Torsions

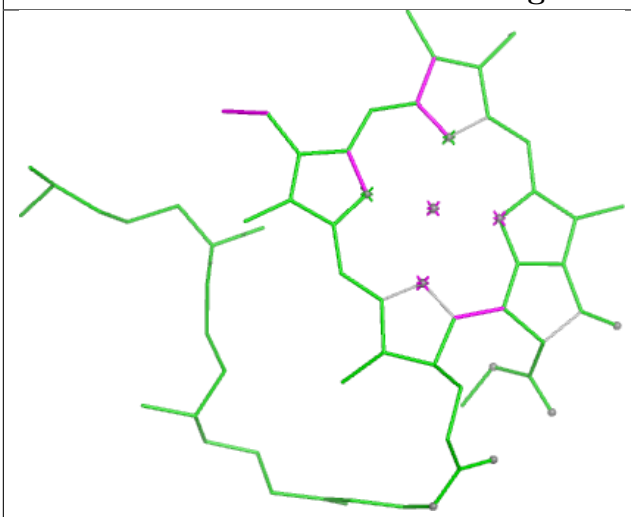


Rings

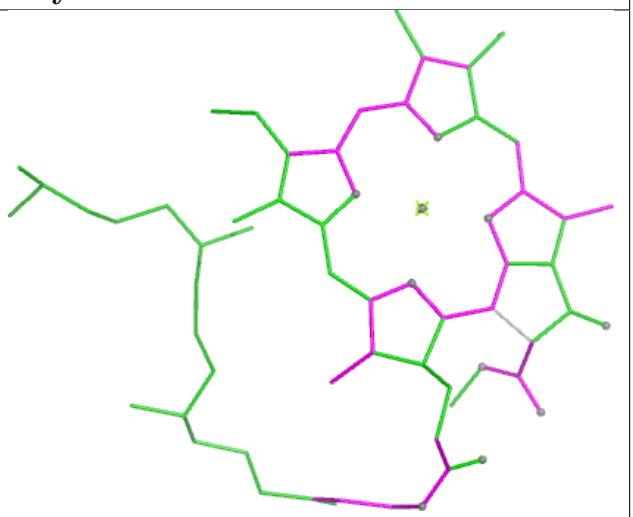
Ligand CLA y 603



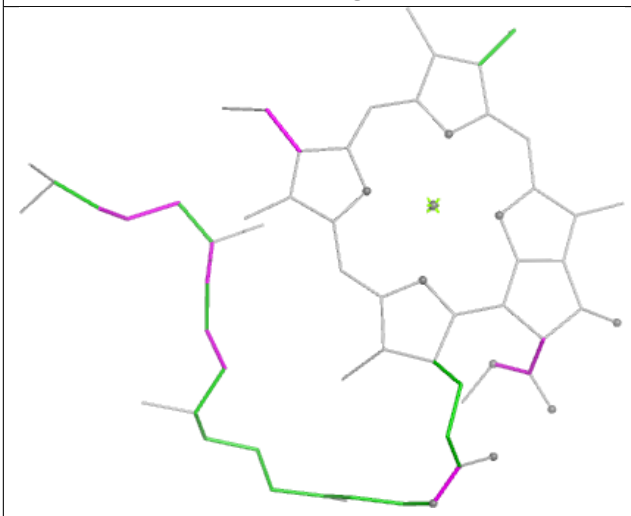
Ligand CLA y 612



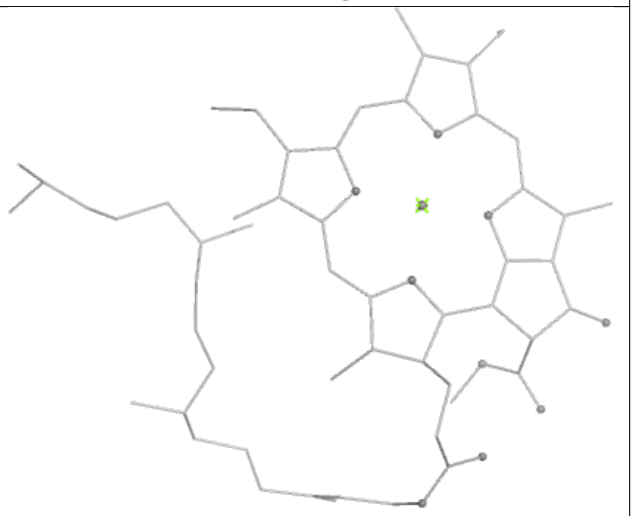
Bond lengths



Bond angles

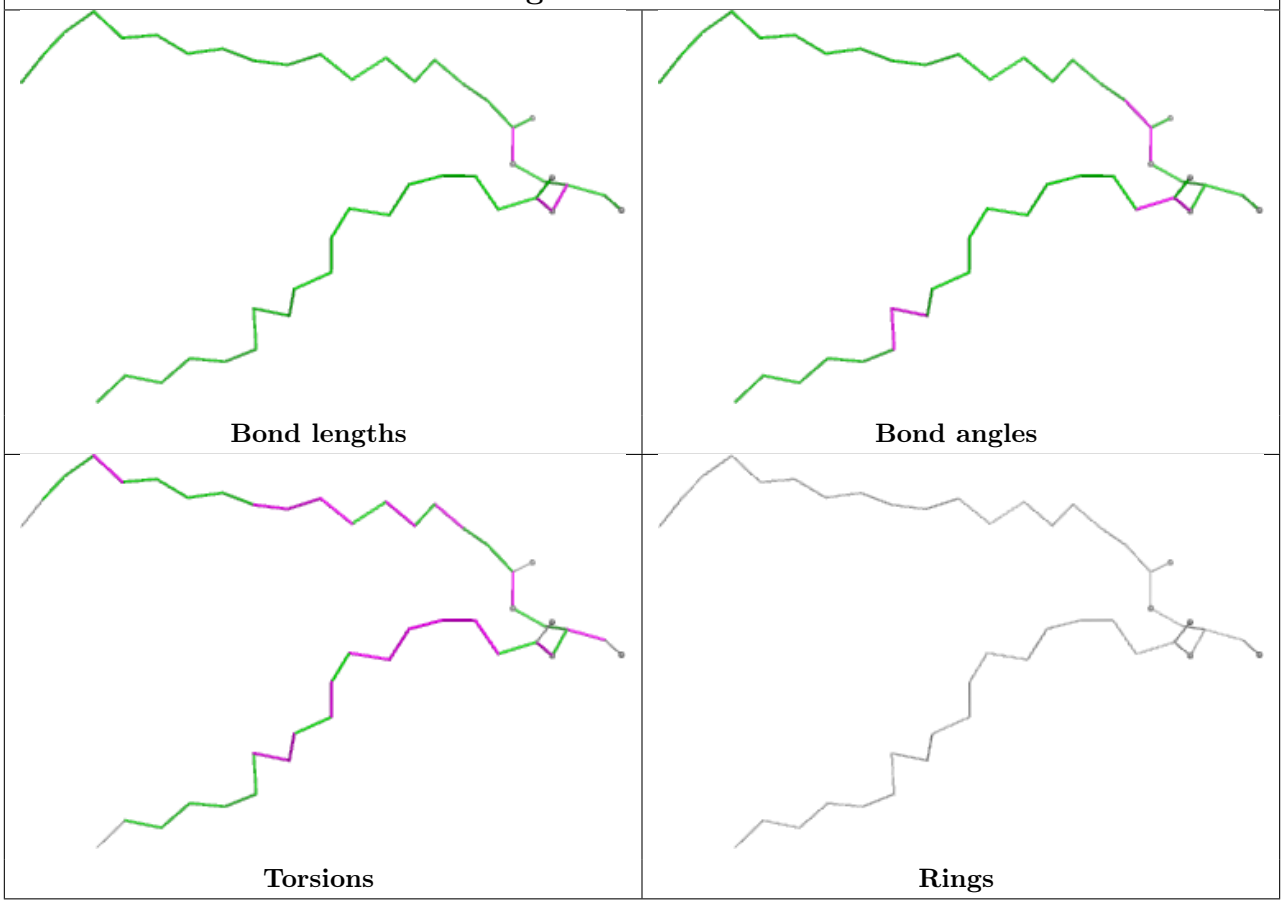


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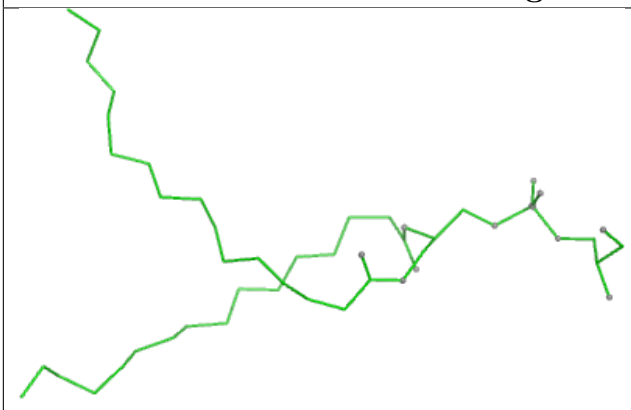


Rings

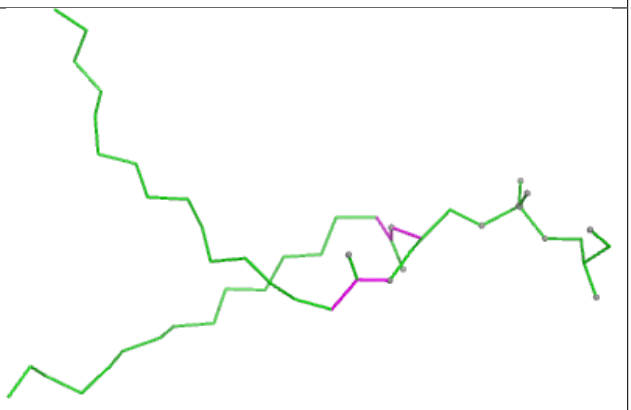
Ligand DGA c 524



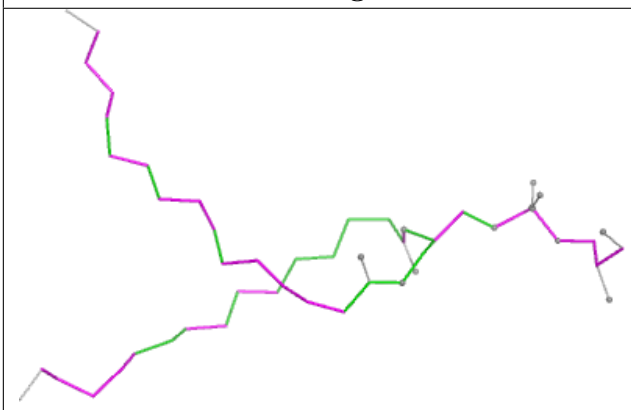
Ligand LHG d 409



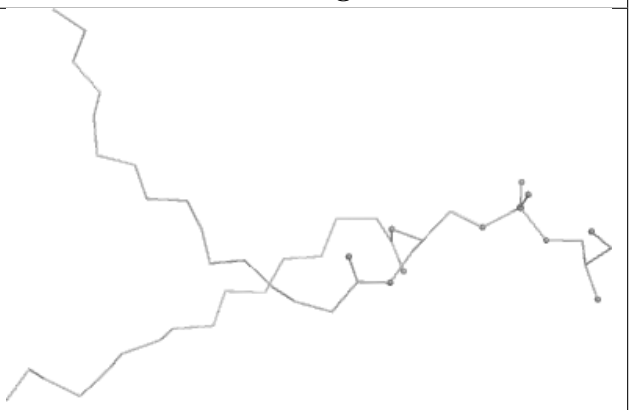
Bond lengths



Bond angles

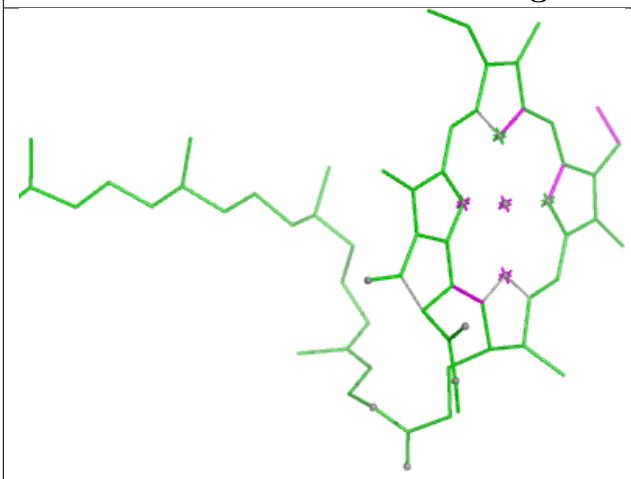


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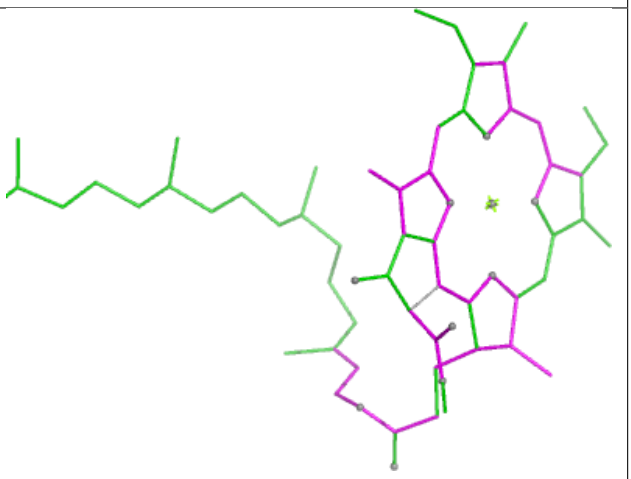


Rings

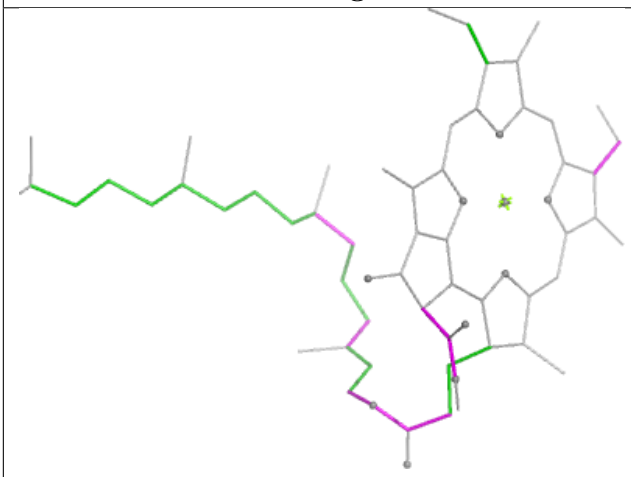
Ligand CLA s 611



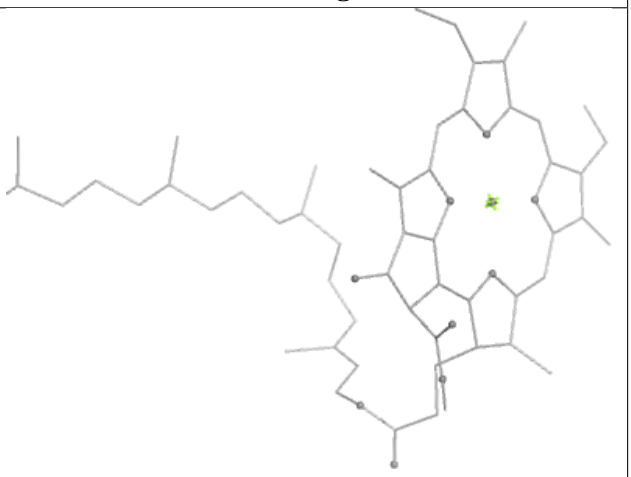
Bond lengths



Bond angles

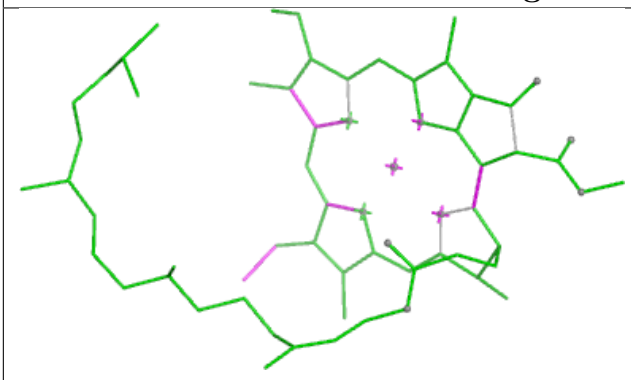


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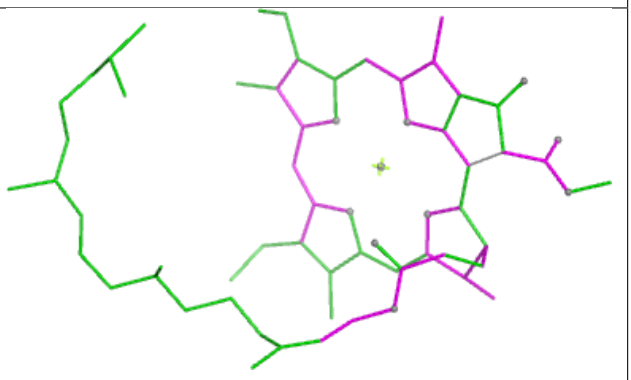


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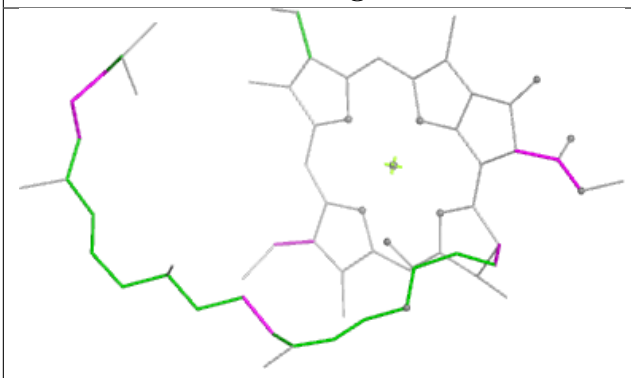
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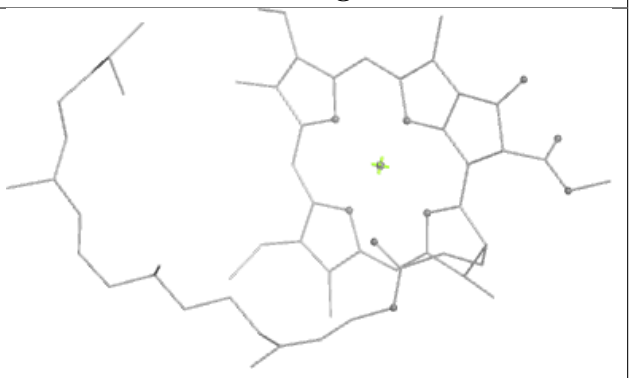
Bond lengths



Bond angles

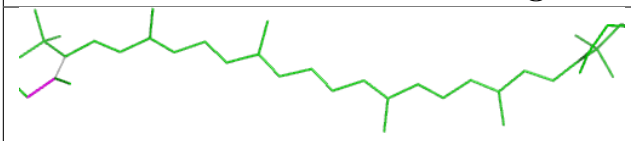


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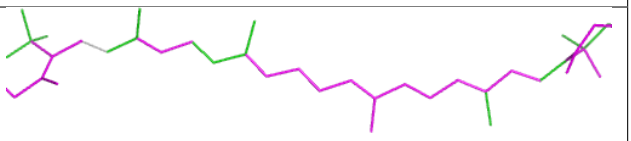


Rings

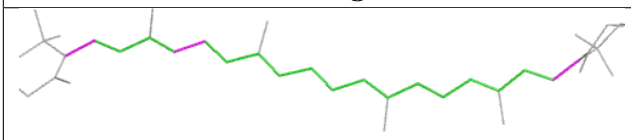
Ligand LUT S 621



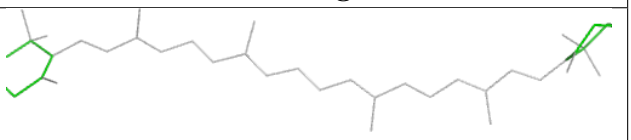
Bond lengths



Bond angles

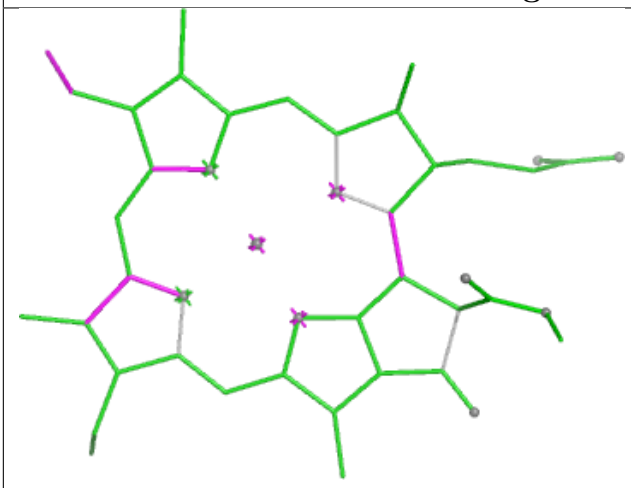


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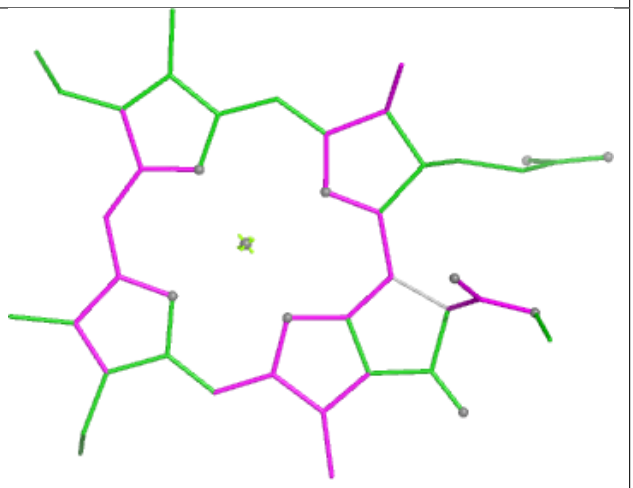


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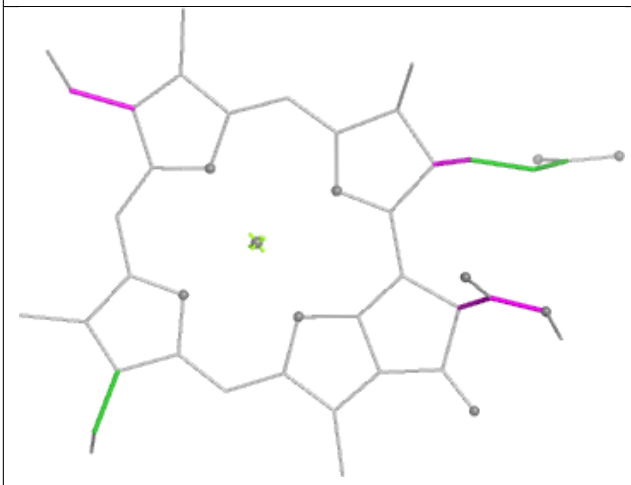
Ligand CLA G 611



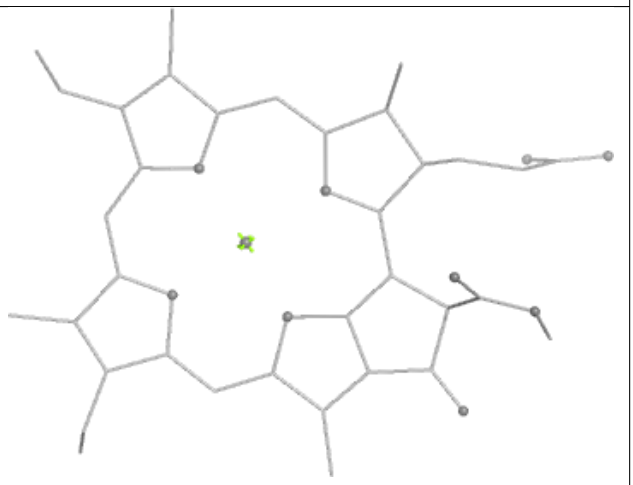
Bond lengths



Bond angles

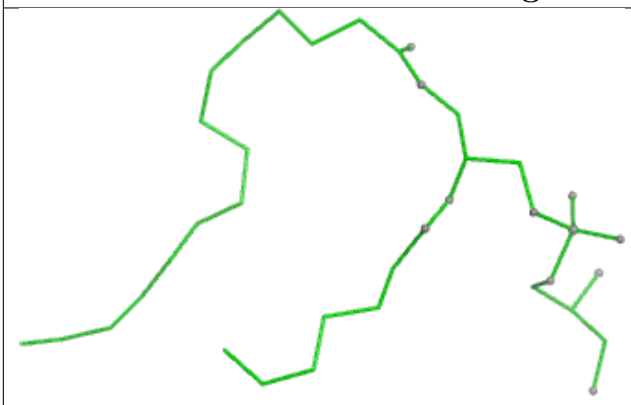


Torsions

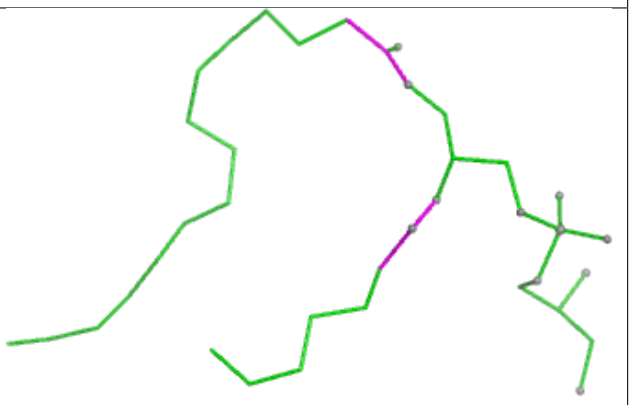


Rings

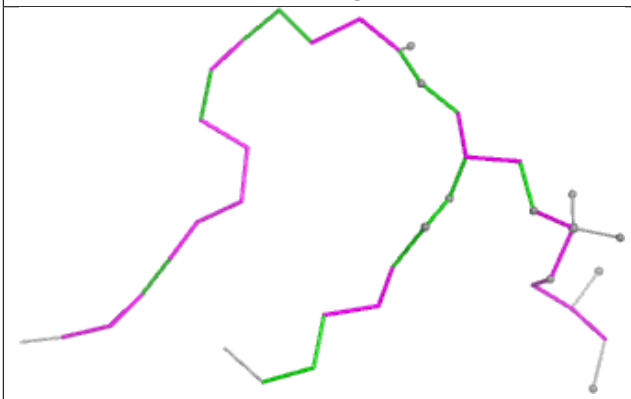
Ligand LHG D 410



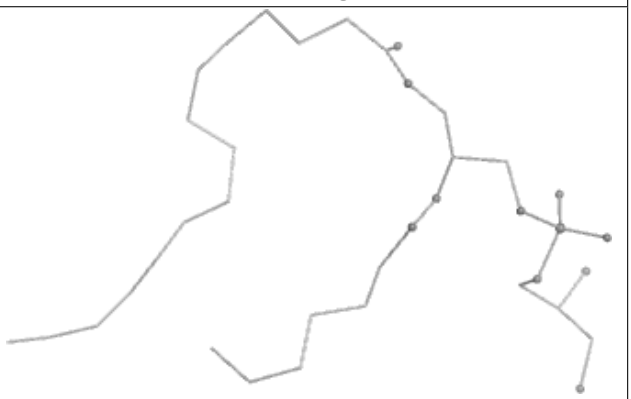
Bond lengths



Bond angles

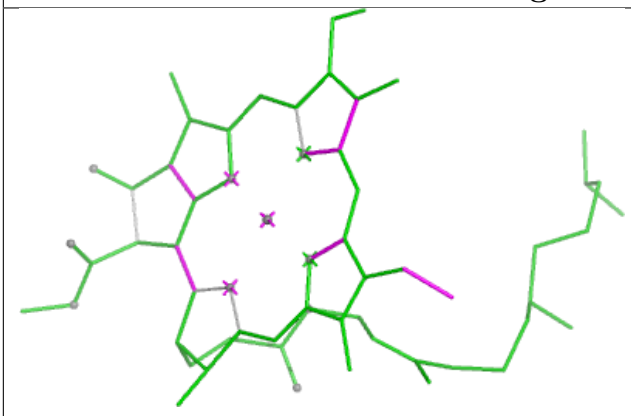


Torsions

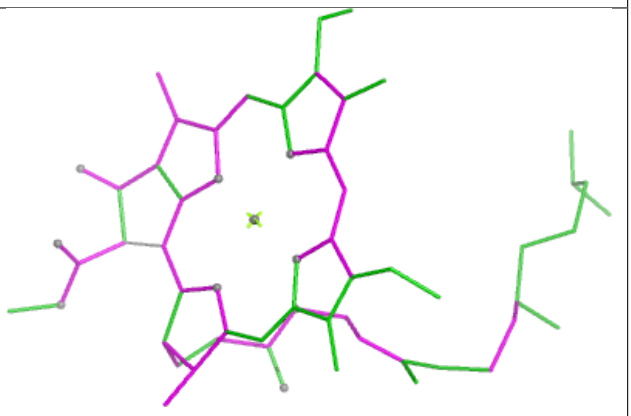


Rings

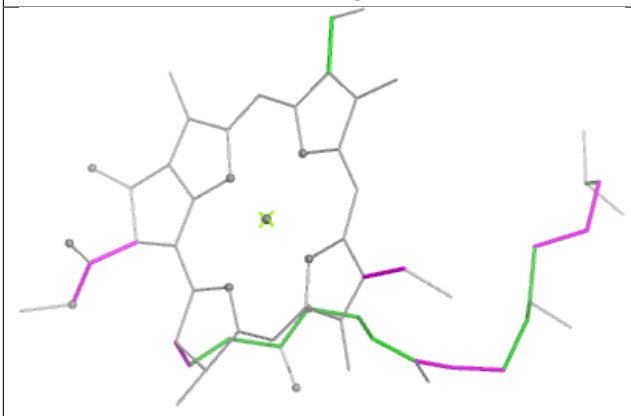
Ligand CLA r 610



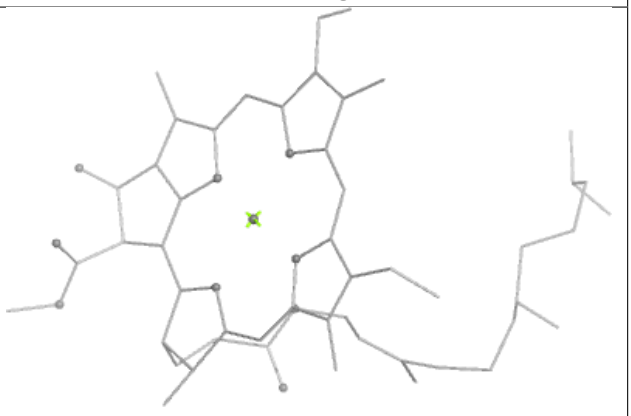
Bond lengths



Bond angles

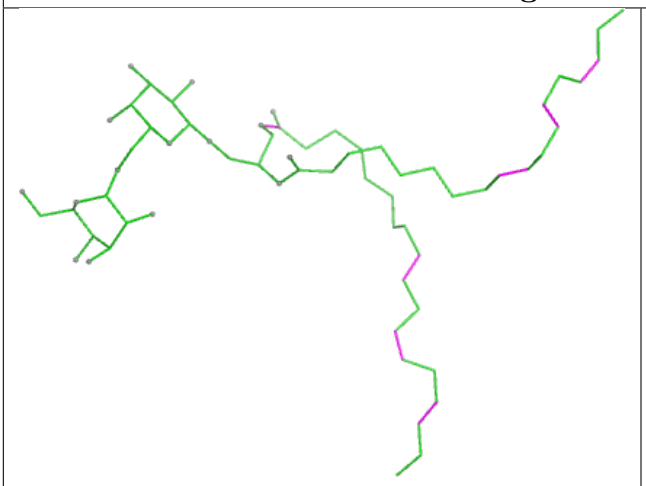


Torsions



Rings

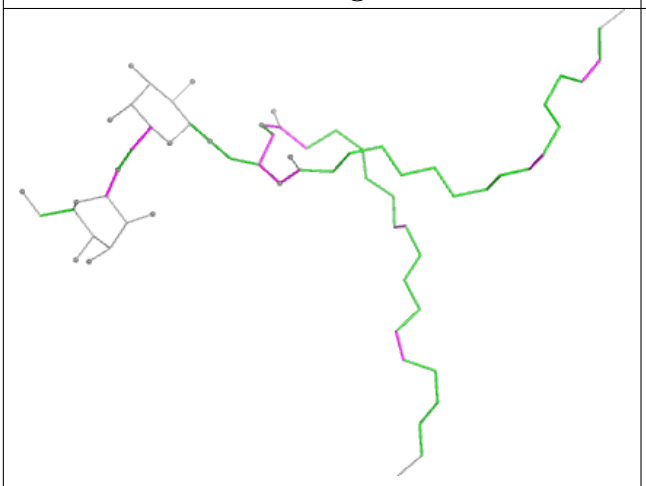
Ligand DGD C 523



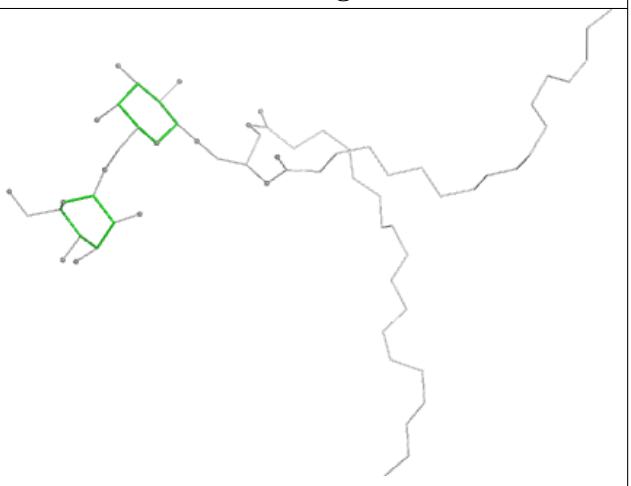
Bond lengths



Bond angles

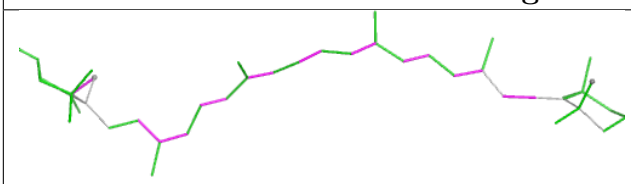


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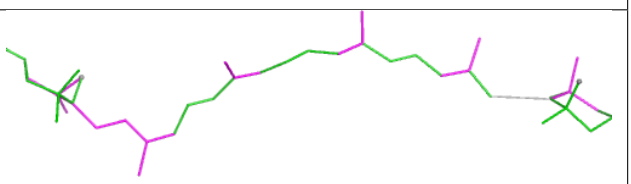


Rings

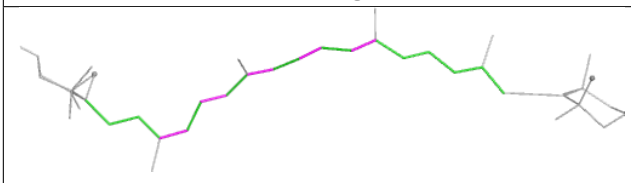
Ligand NEX R 622



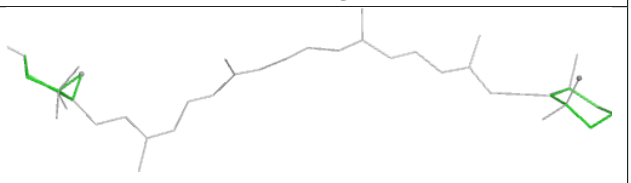
Bond lengths



Bond angles

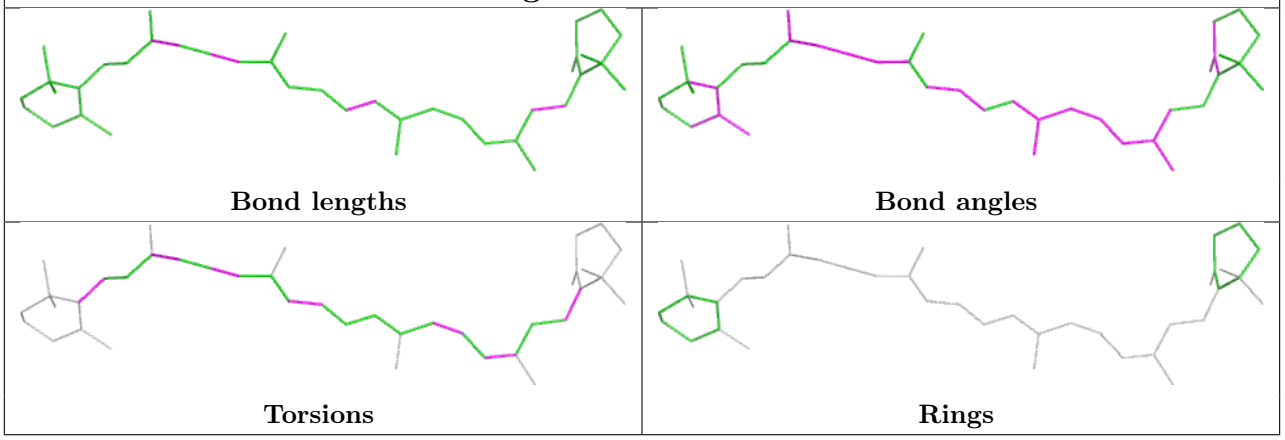


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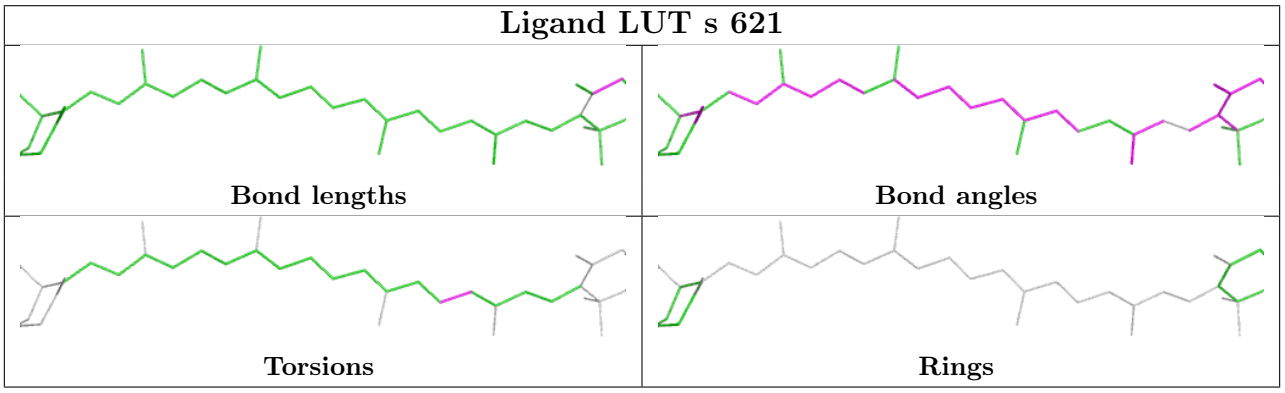


Rings

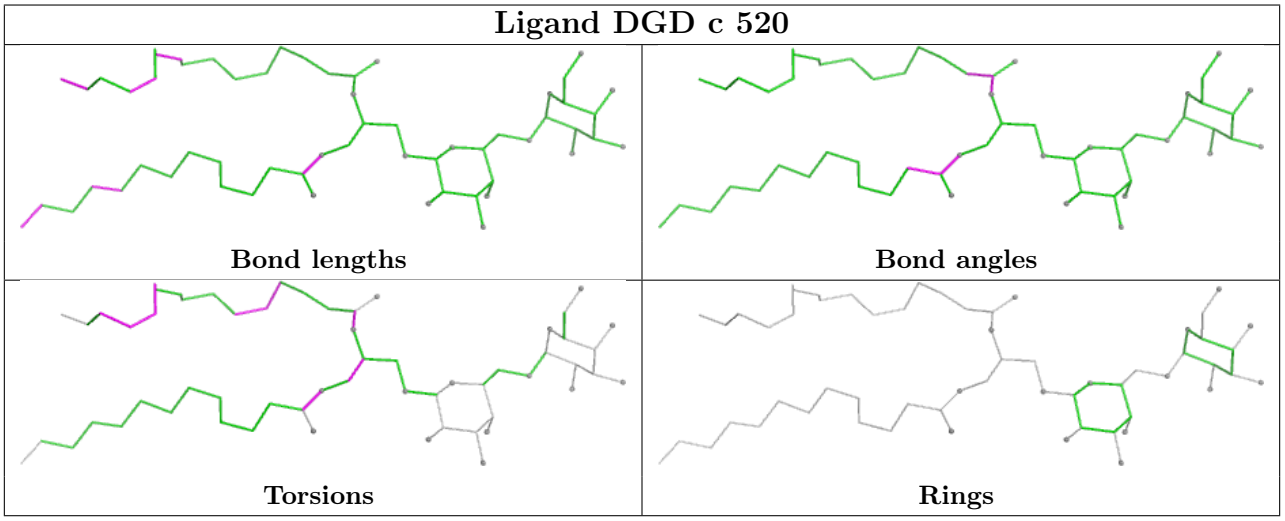
Ligand BCR D 404



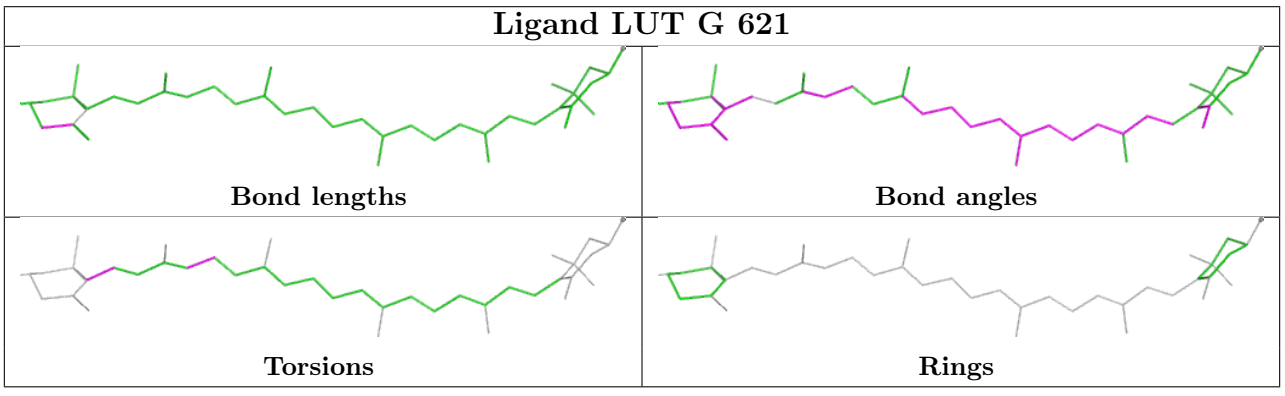
Ligand LUT s 621



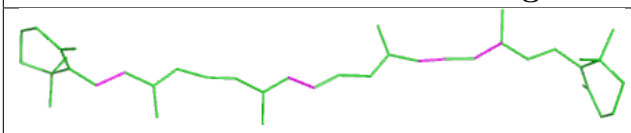
Ligand DGD c 520



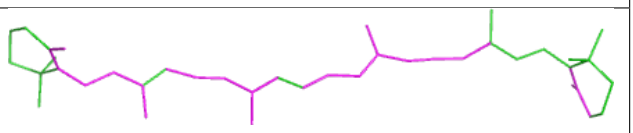
Ligand LUT G 621



Ligand BCR A 411



Bond lengths



Bond angles

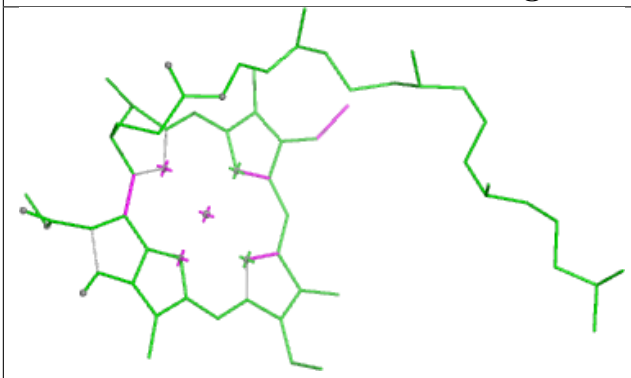


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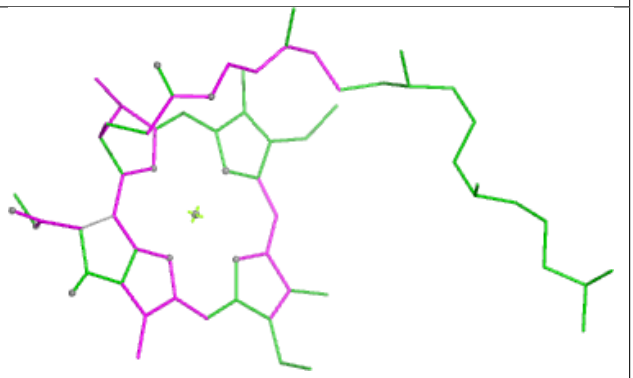


Rings

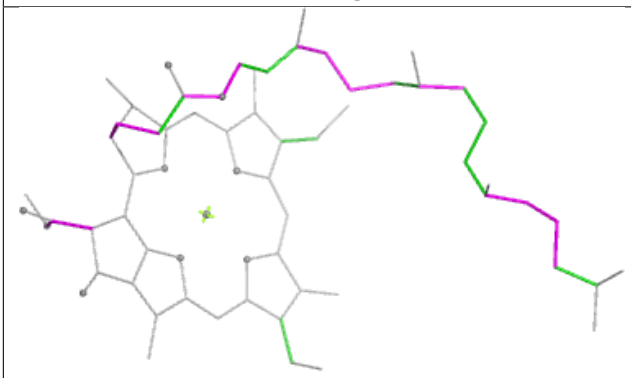
Ligand CLA N 602



Bond lengths



Bond angles

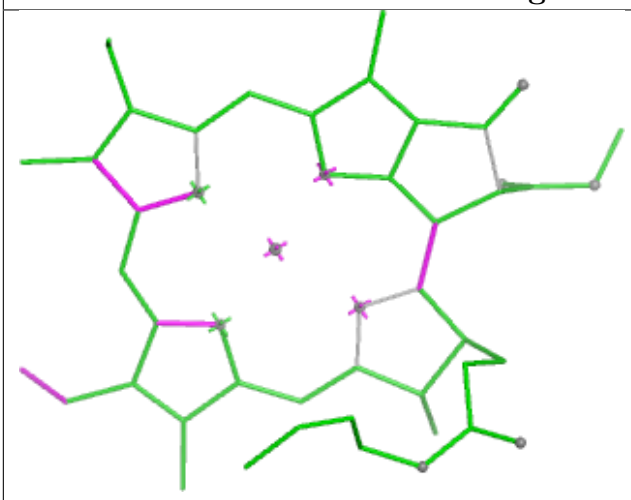


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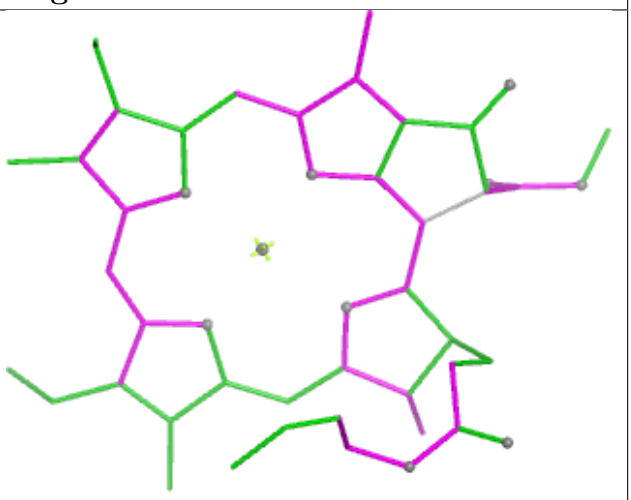


Rings

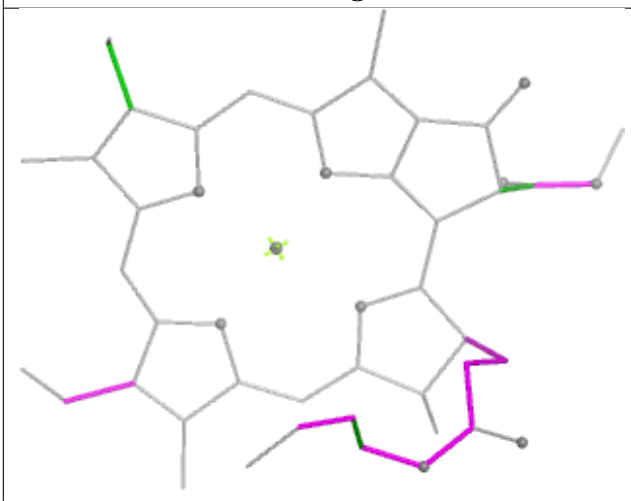
Ligand CLA g 614



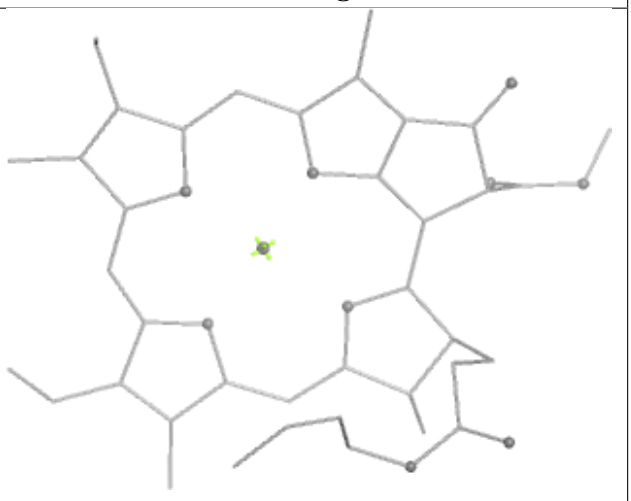
Bond lengths



Bond angles

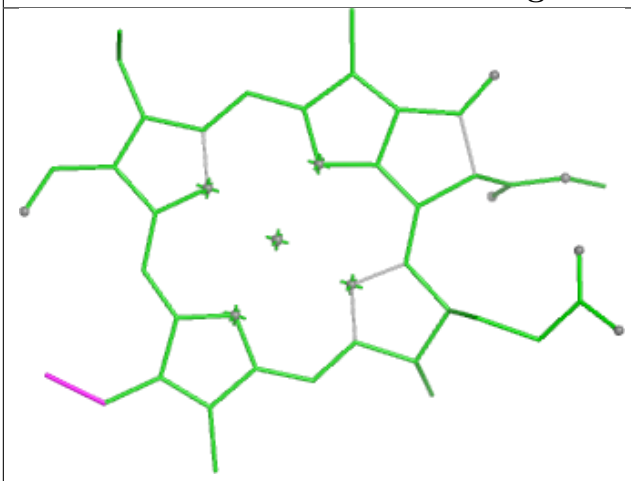


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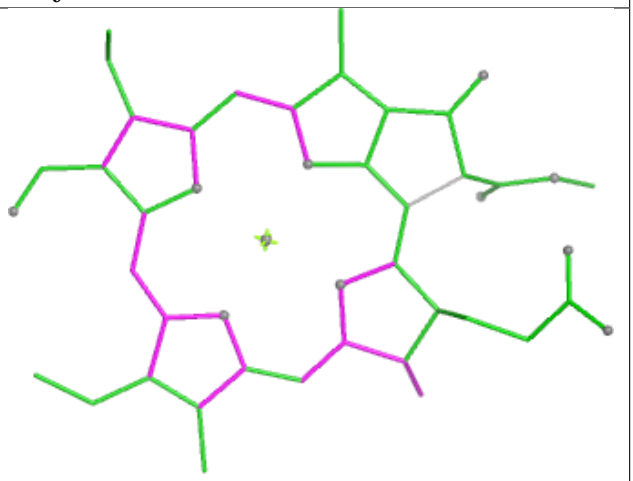


Rings

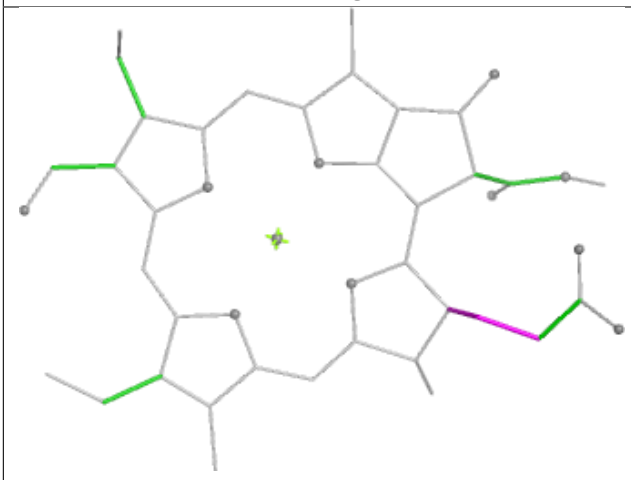
Ligand CHL y 605



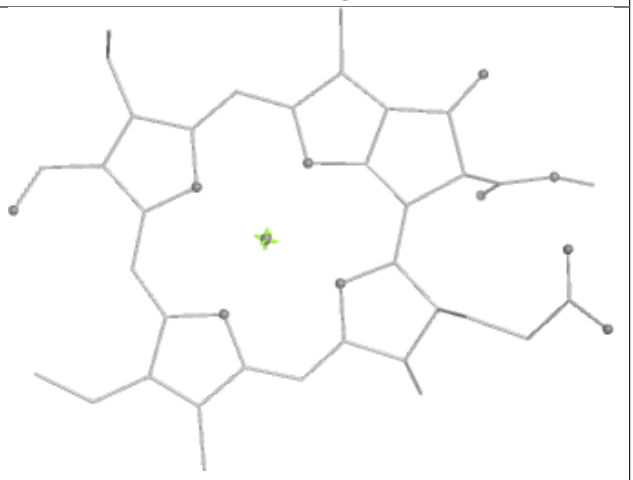
Bond lengths



Bond angles

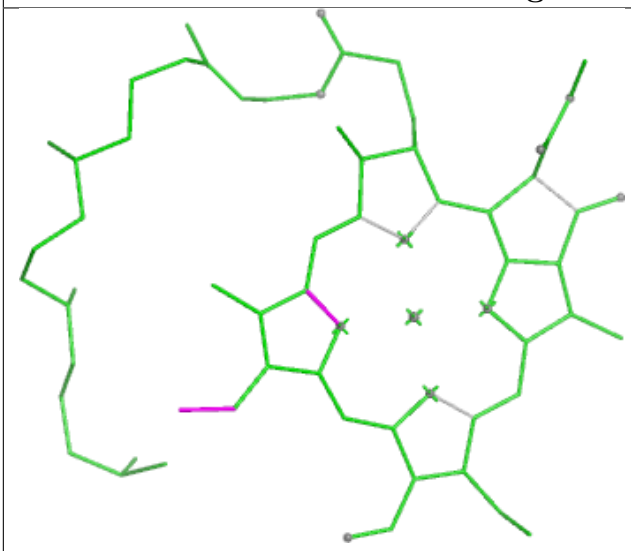


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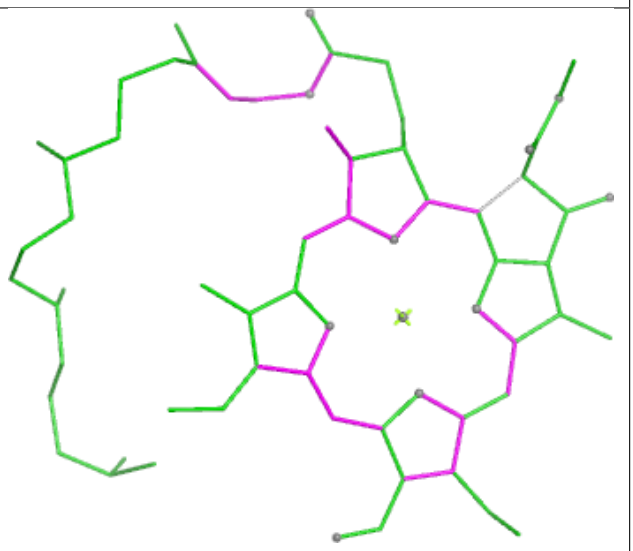


Rings

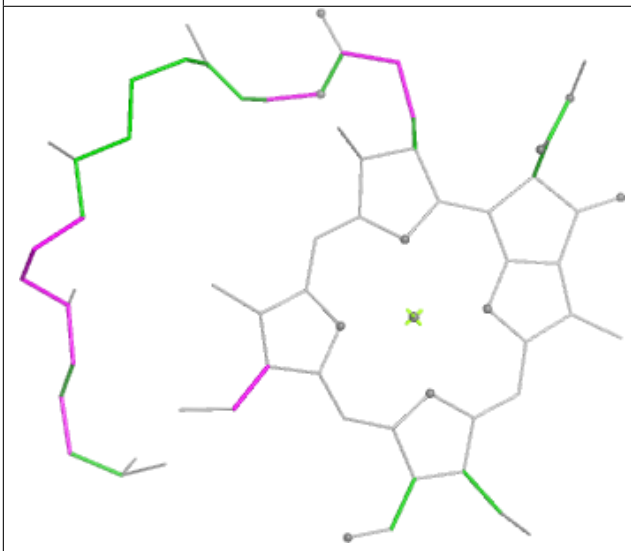
Ligand CHL n 607



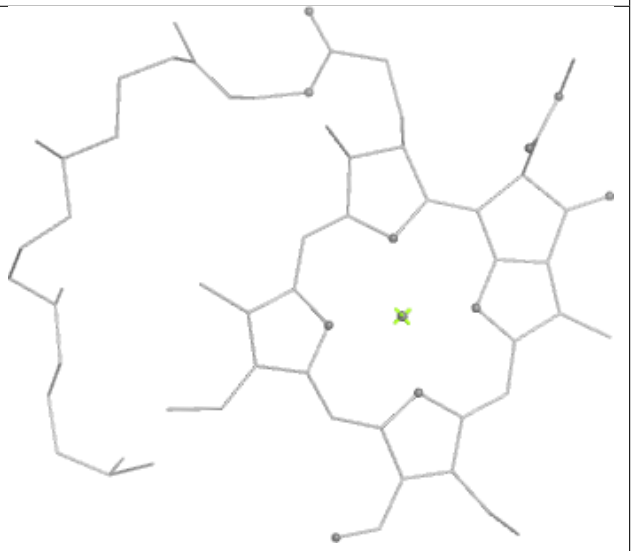
Bond lengths



Bond angles

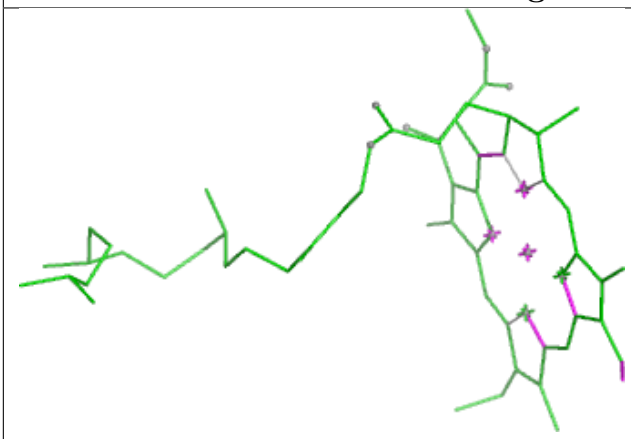


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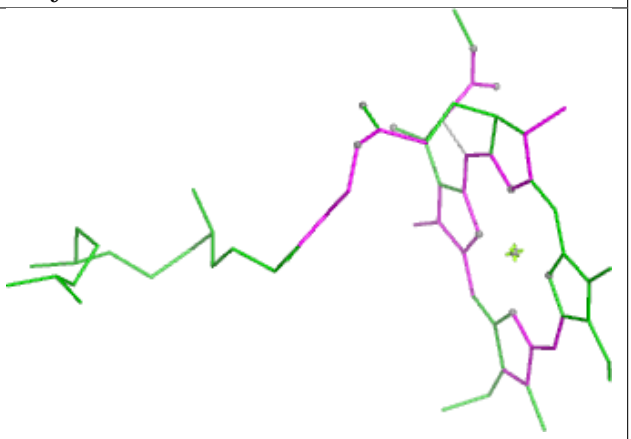


Rings

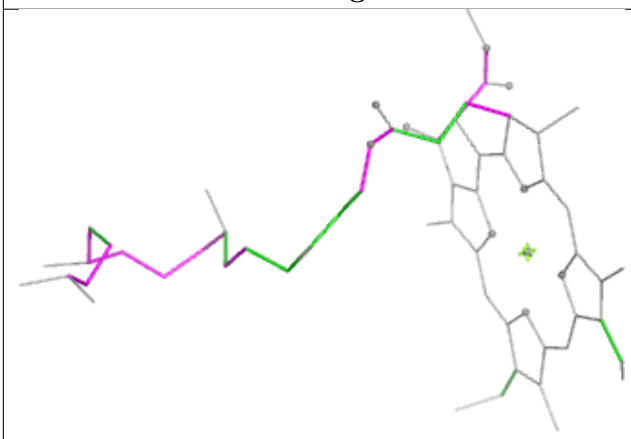
Ligand CLA y 604



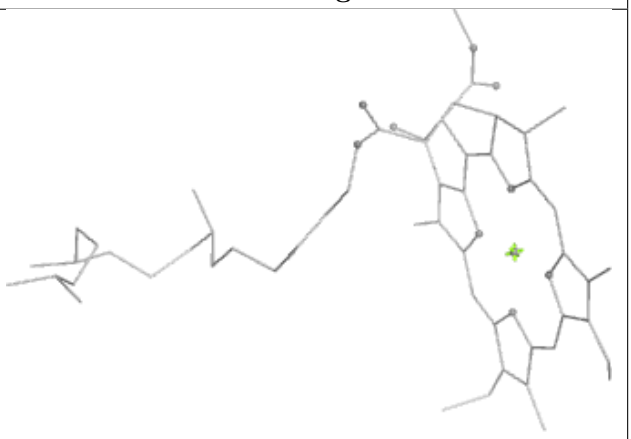
Bond lengths



Bond angles

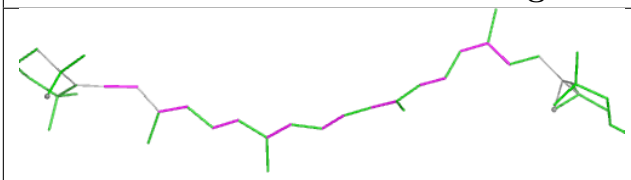


Torsions

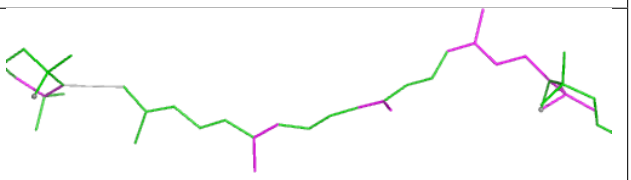


Rings

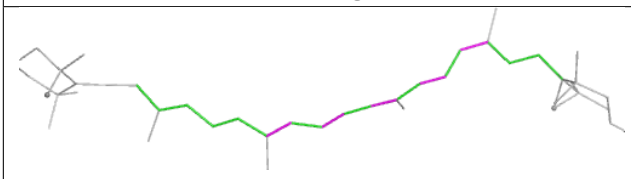
Ligand NEX r 623



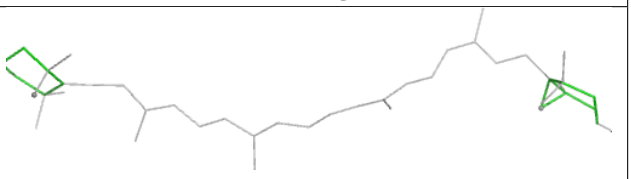
Bond lengths



Bond angles

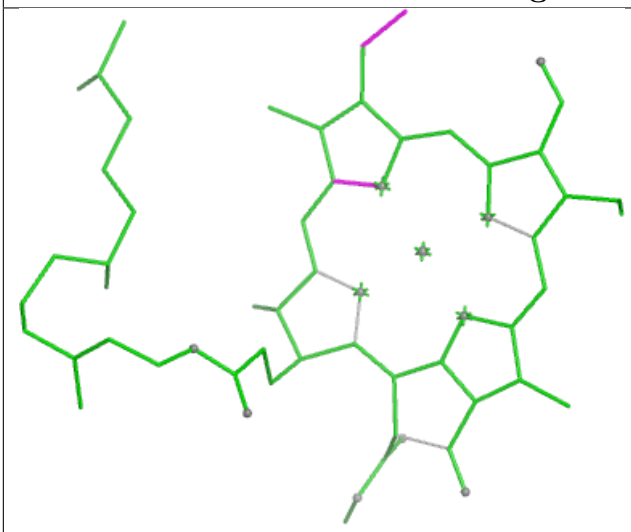


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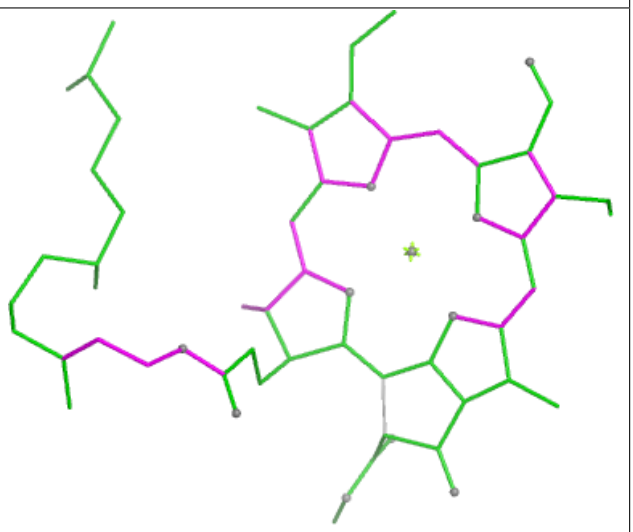


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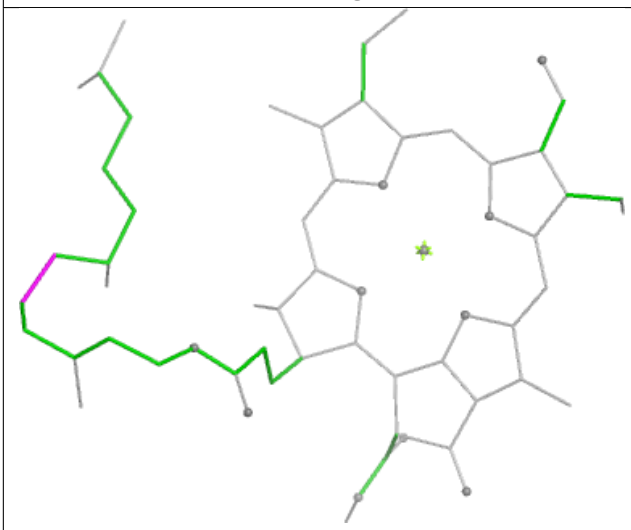
Ligand CHL s 608



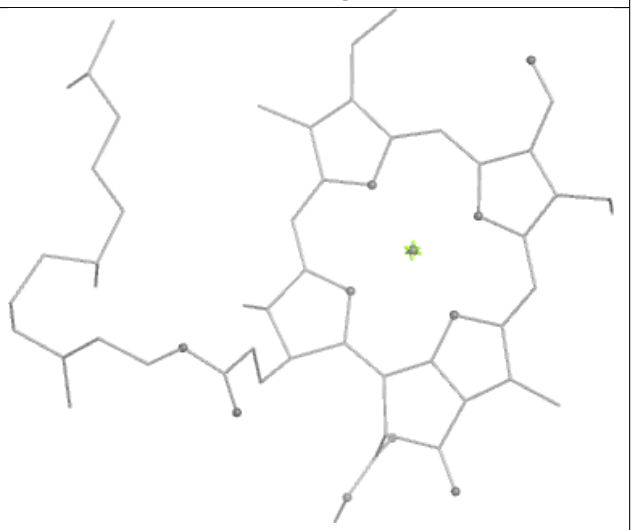
Bond lengths



Bond angles

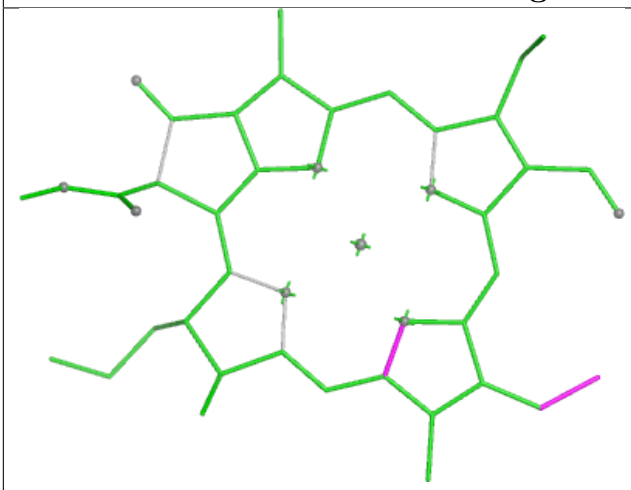


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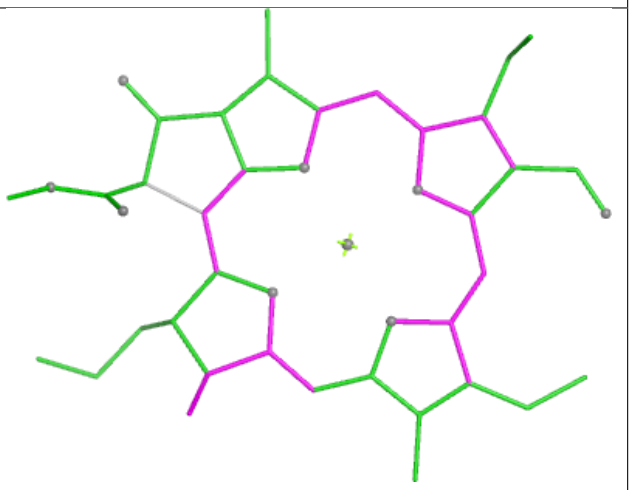


Rings

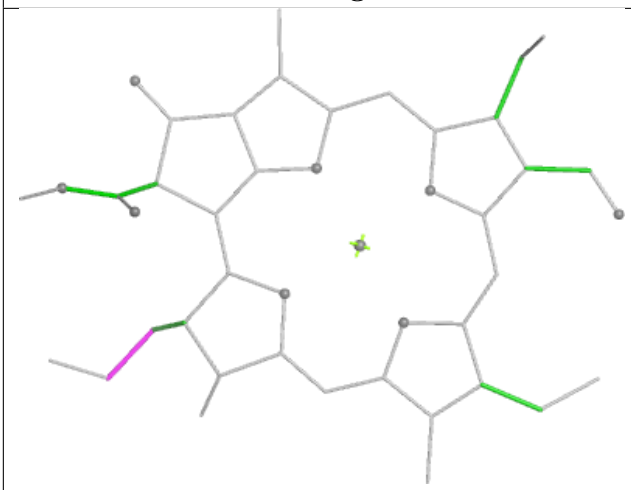
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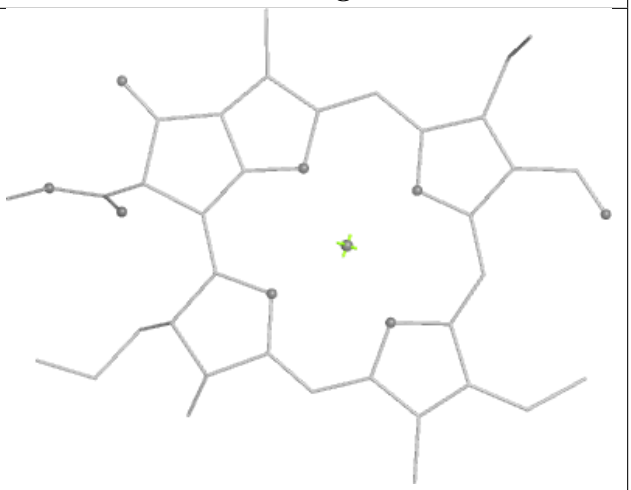
Bond lengths



Bond angles

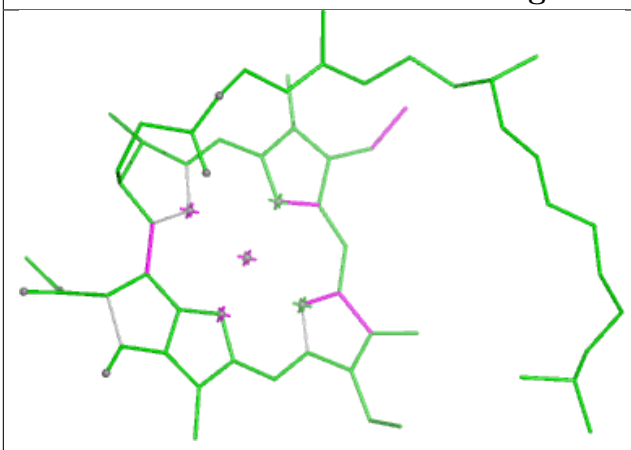


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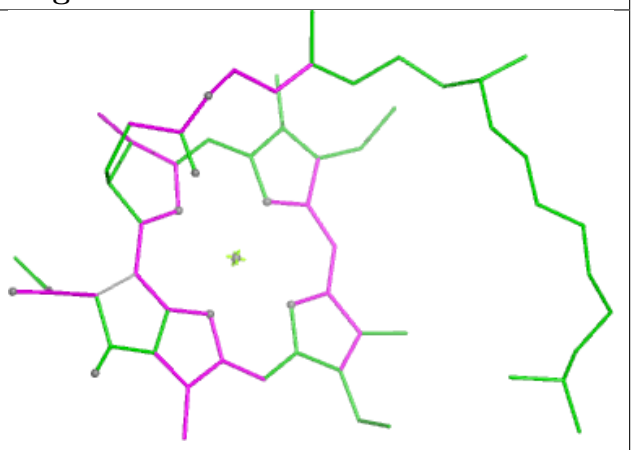


Rings

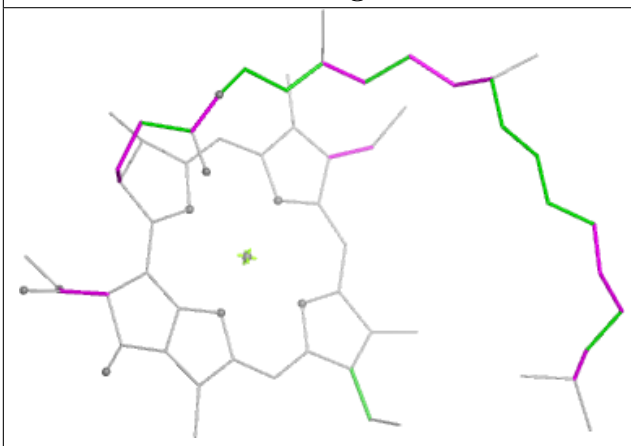
Ligand CLA g 602



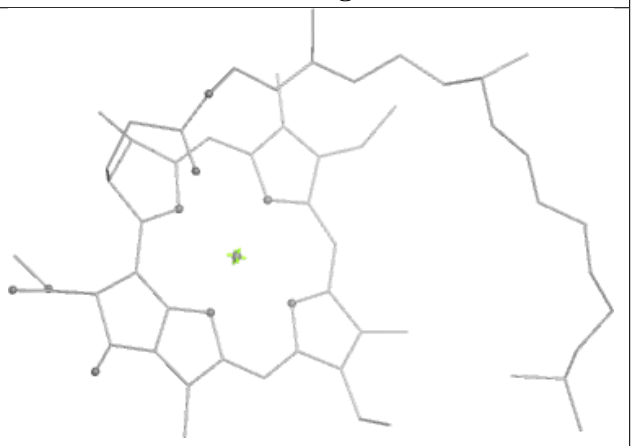
Bond lengths



Bond angles

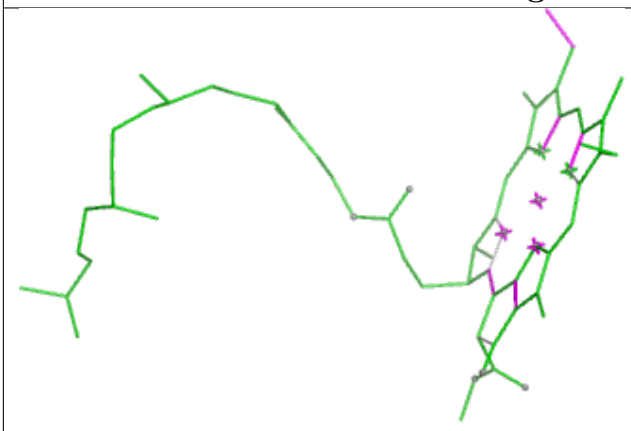


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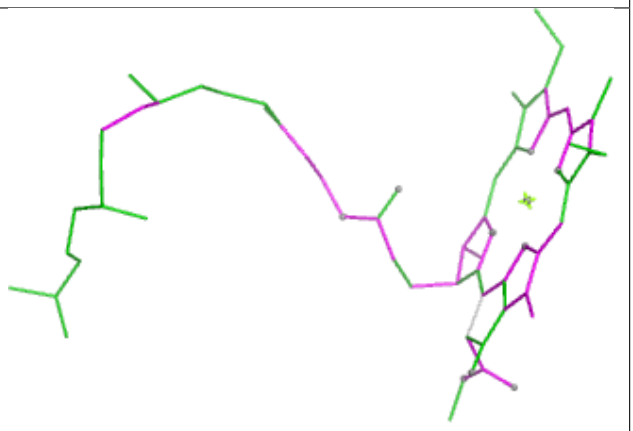


Rings

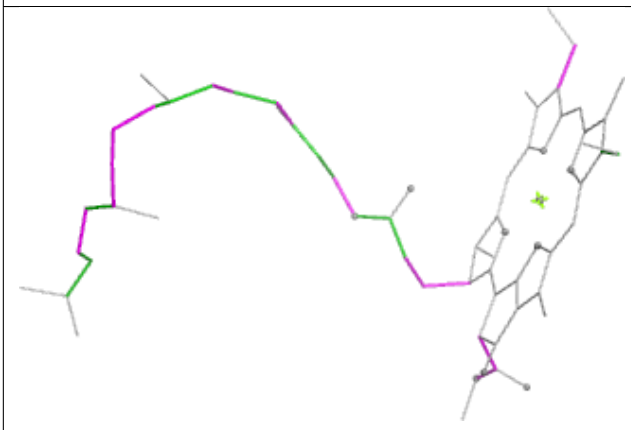
Ligand CLA b 607



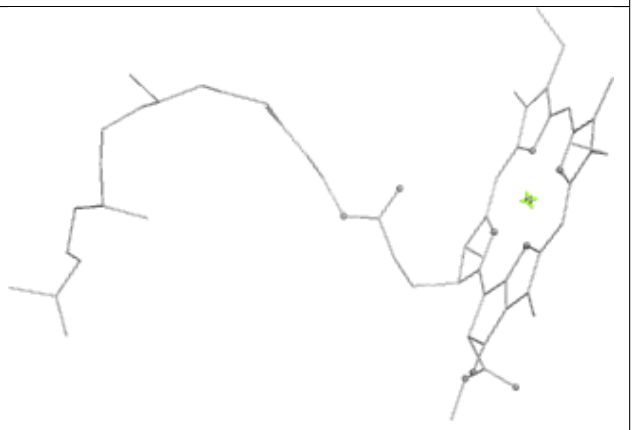
Bond lengths



Bond angles

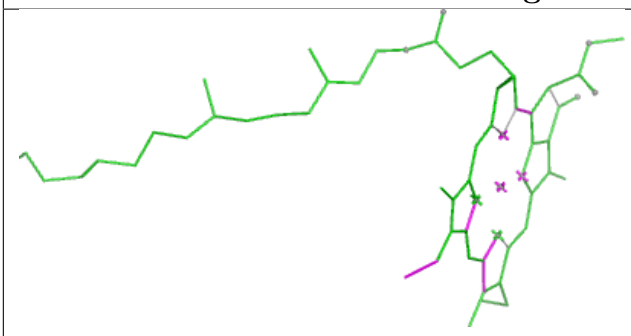


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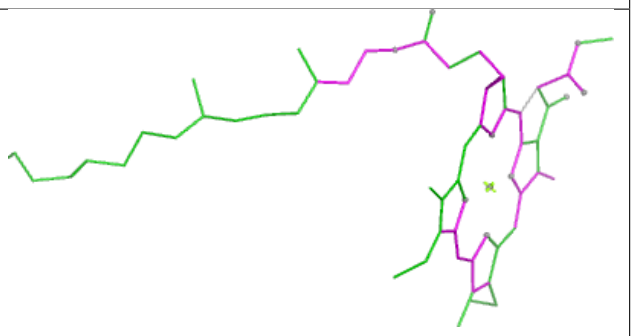


Rings

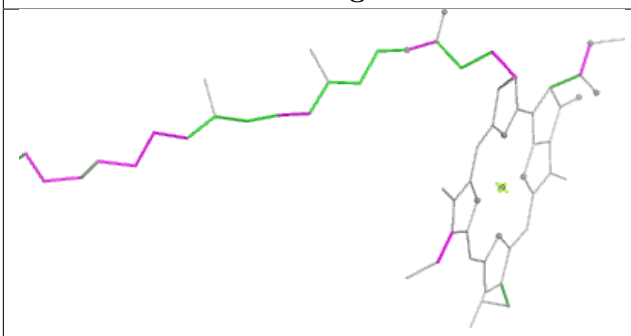
Ligand CLA D 403



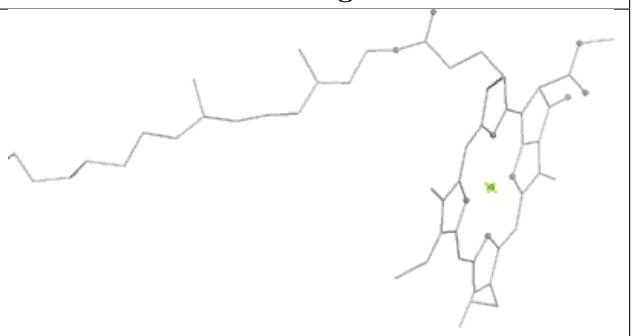
Bond lengths



Bond angles

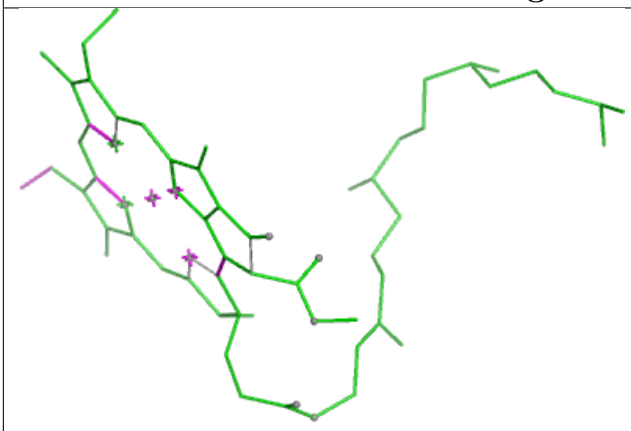


Torsions

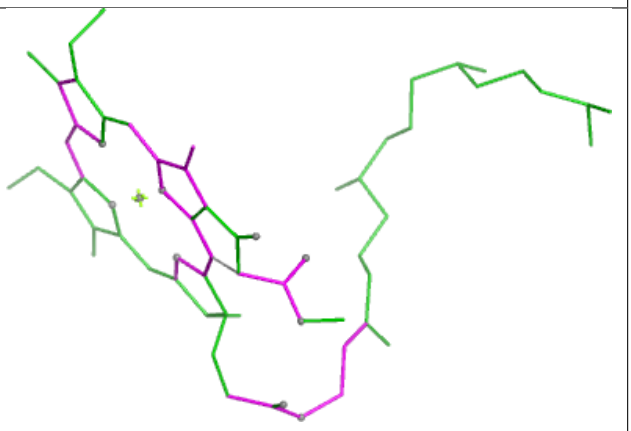


Rings

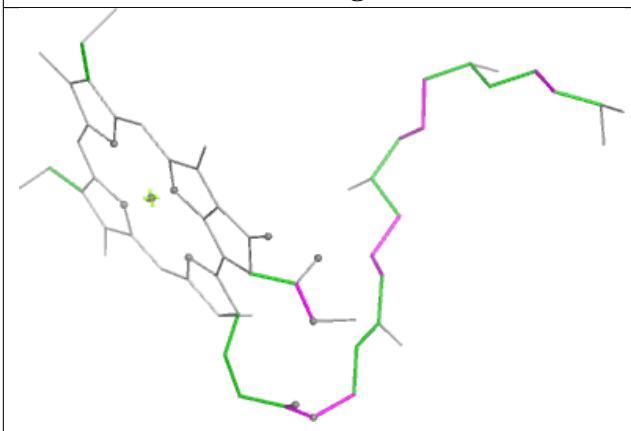
Ligand CLA b 614



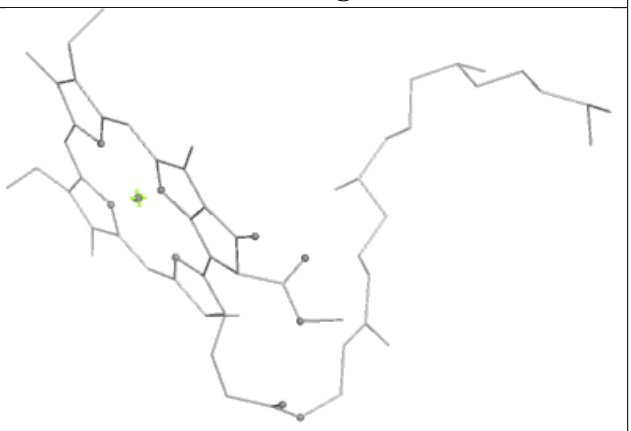
Bond lengths



Bond angles

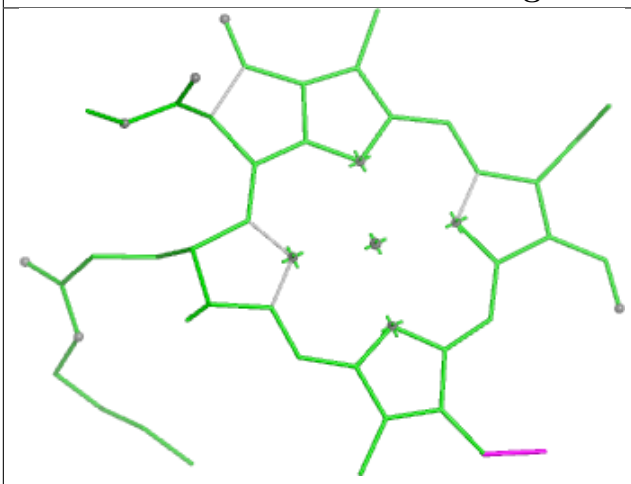


Torsions

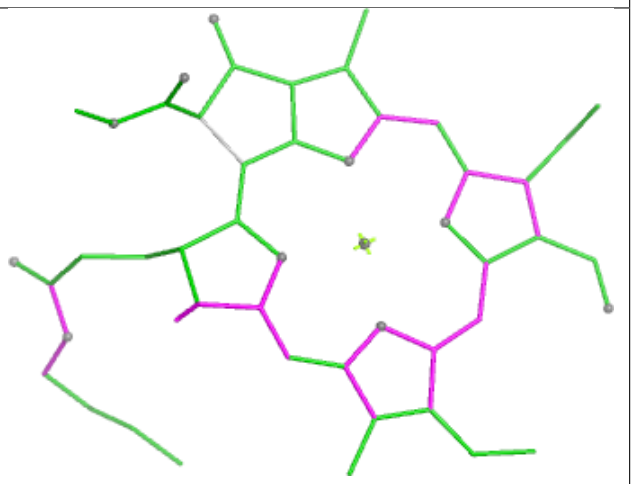


Rings

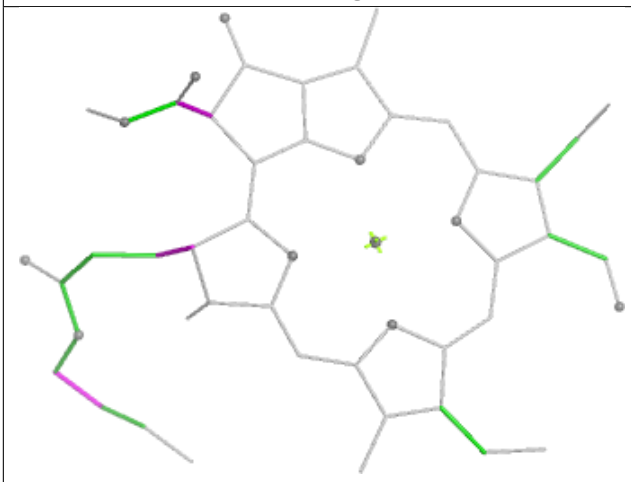
Ligand CHL R 607



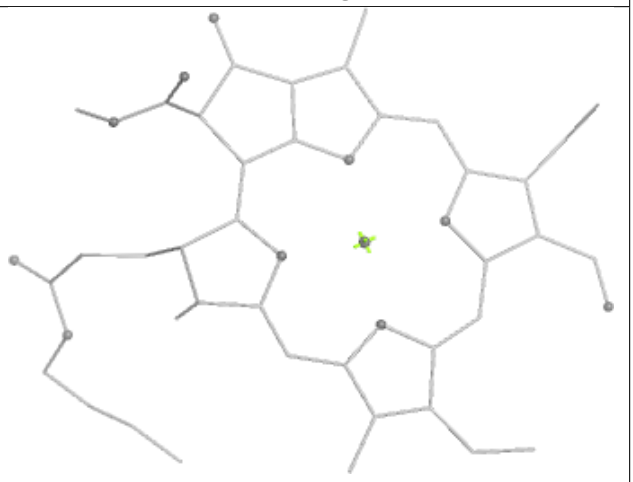
Bond lengths



Bond angles

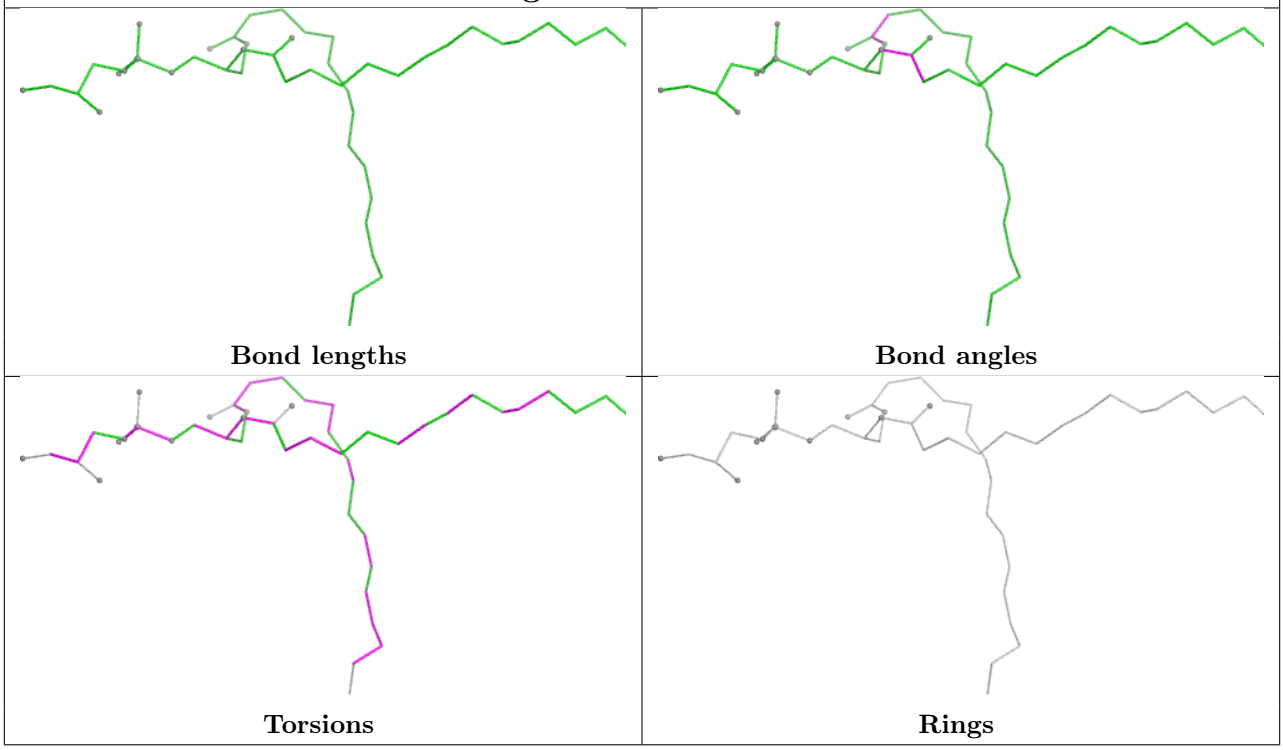


Torsions

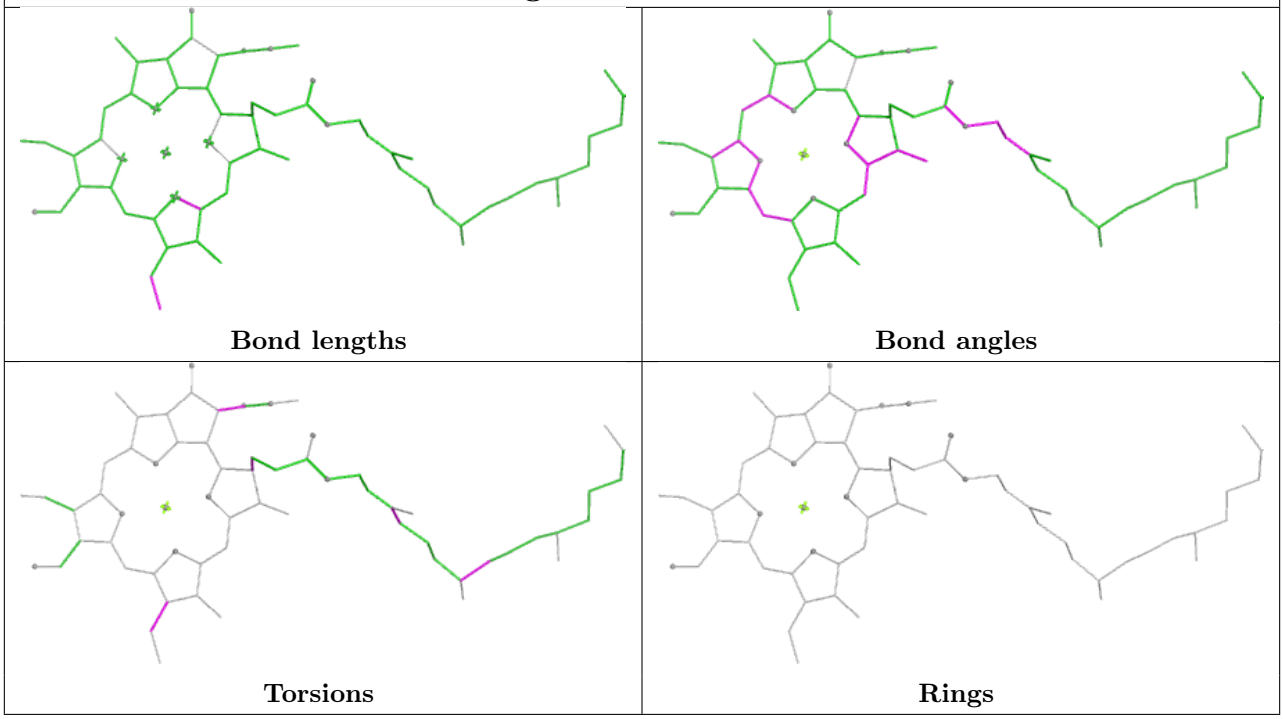


Rings

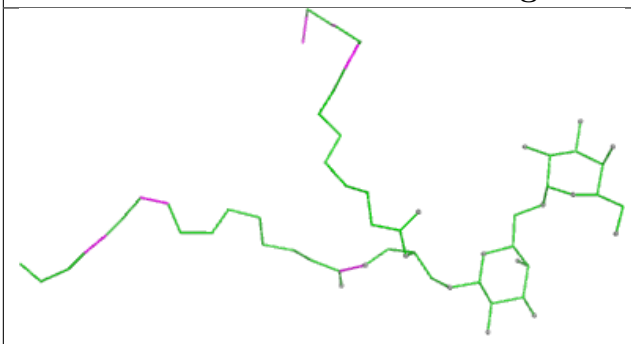
Ligand LHG N 624



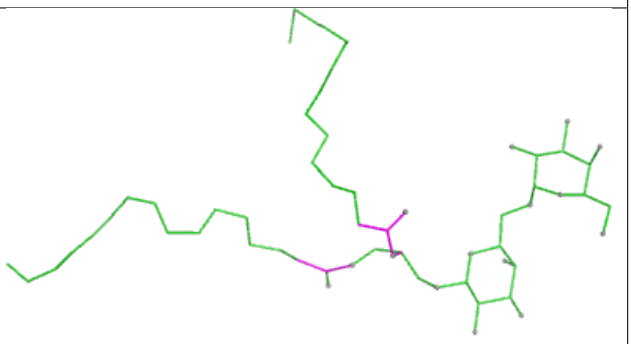
Ligand CHL Y 601



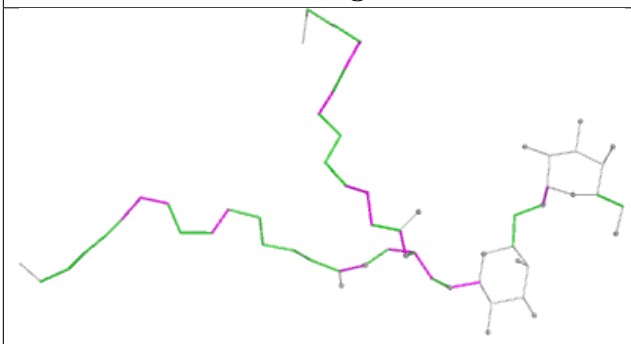
Ligand DGD C 519



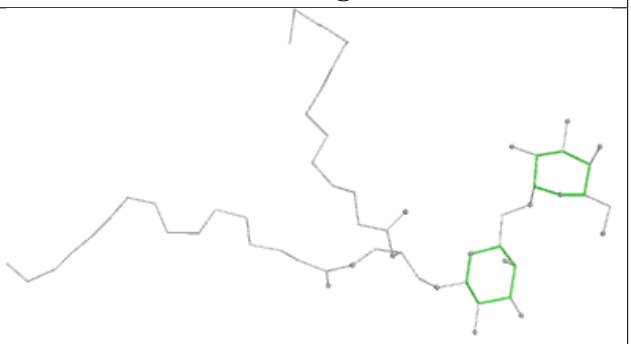
Bond lengths



Bond angles

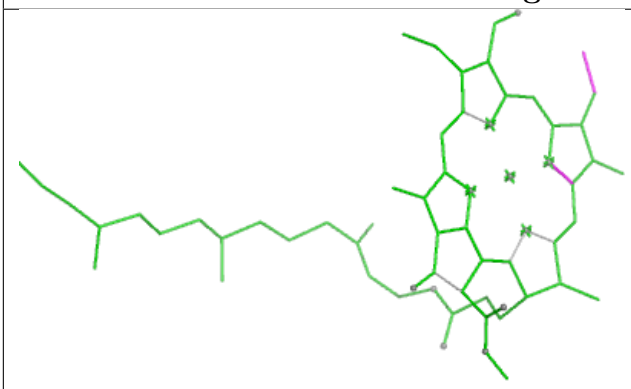


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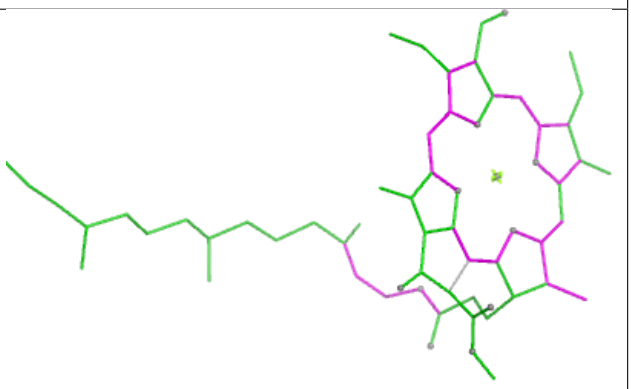


Rings

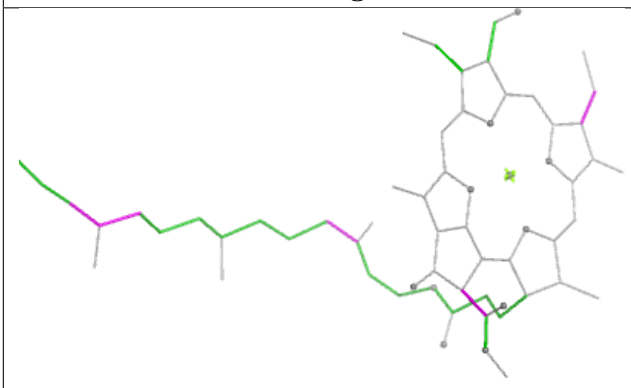
Ligand CHL Y 609



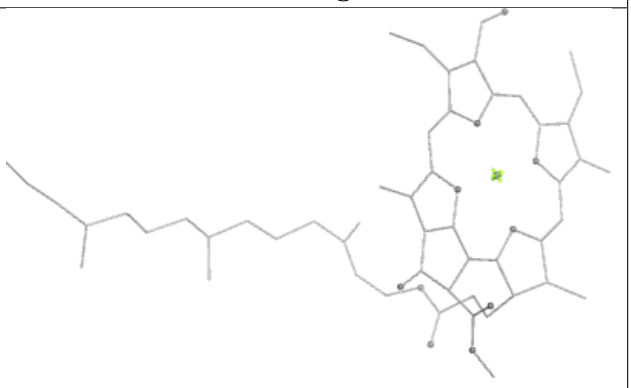
Bond lengths



Bond angles

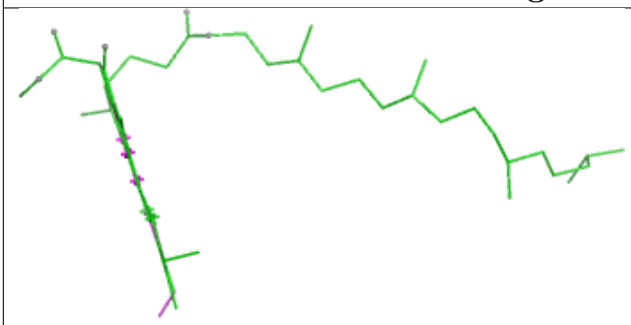


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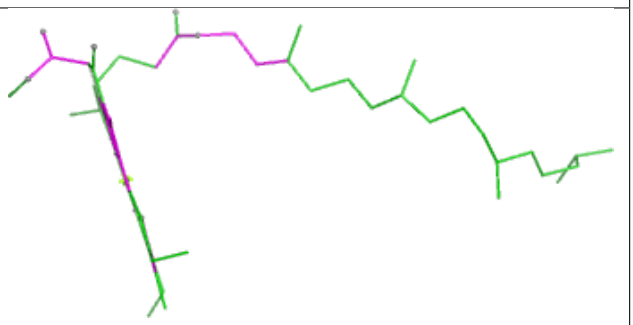


Rings

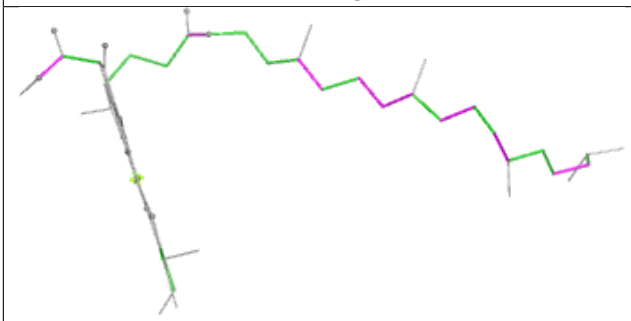
Ligand CLA b 606



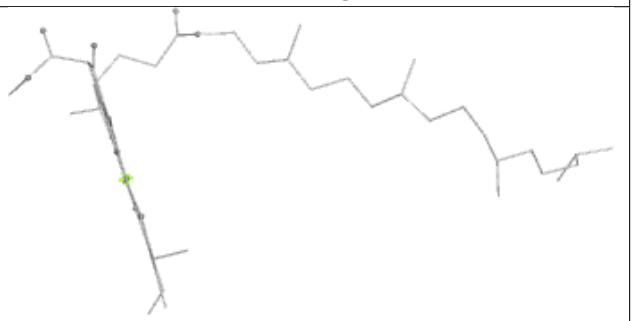
Bond lengths



Bond angles

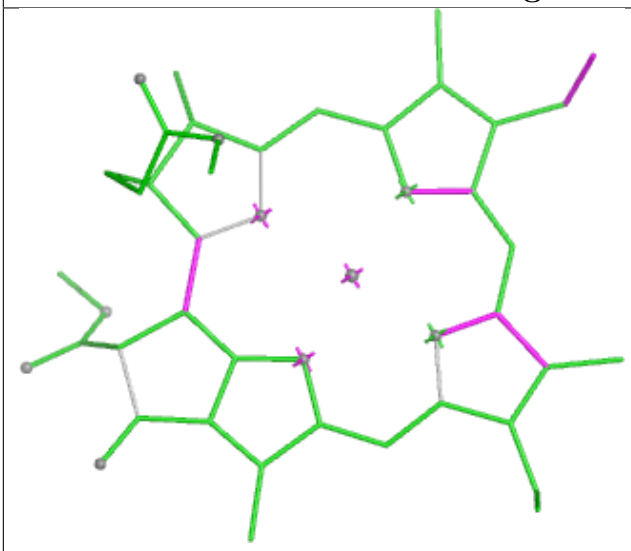


Torsions

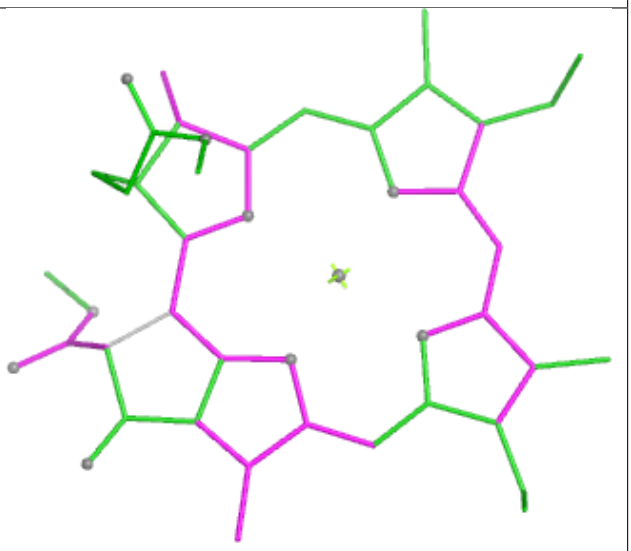


Rings

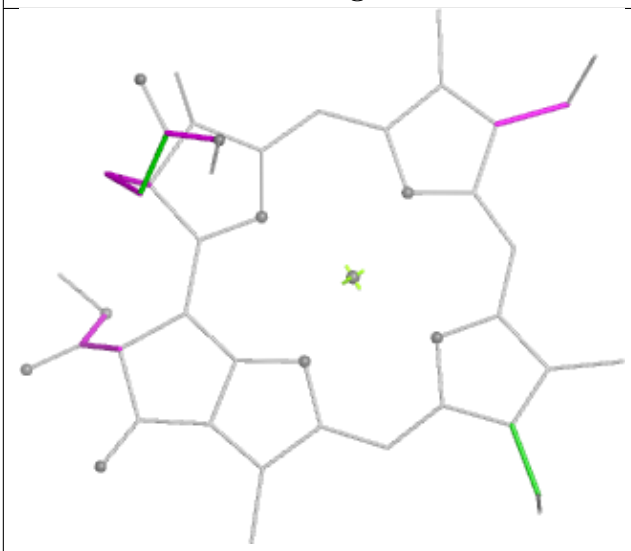
Ligand CLA R 613



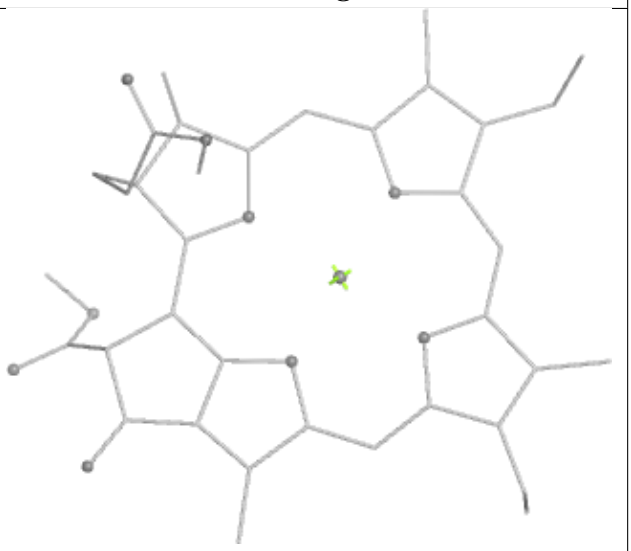
Bond lengths



Bond angles

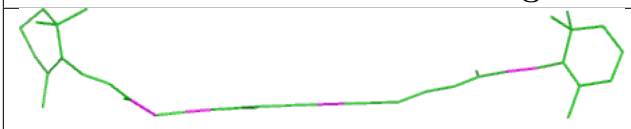


Torsions



Rings

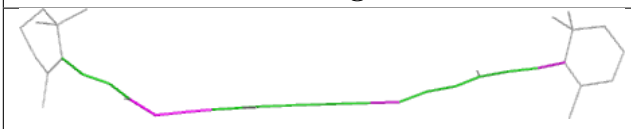
Ligand BCR C 517



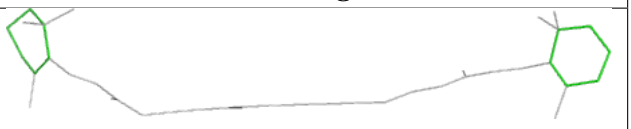
Bond lengths



Bond angles



Torsions

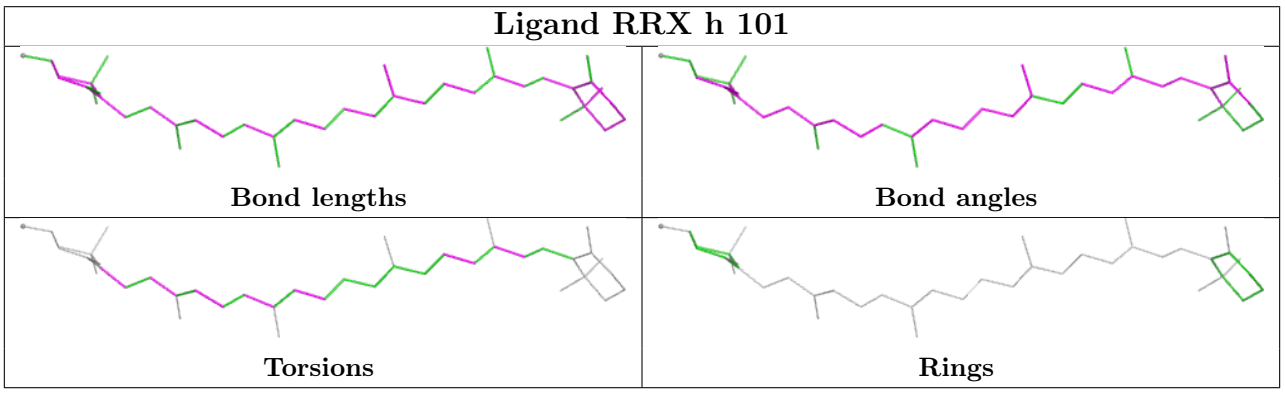


Rings

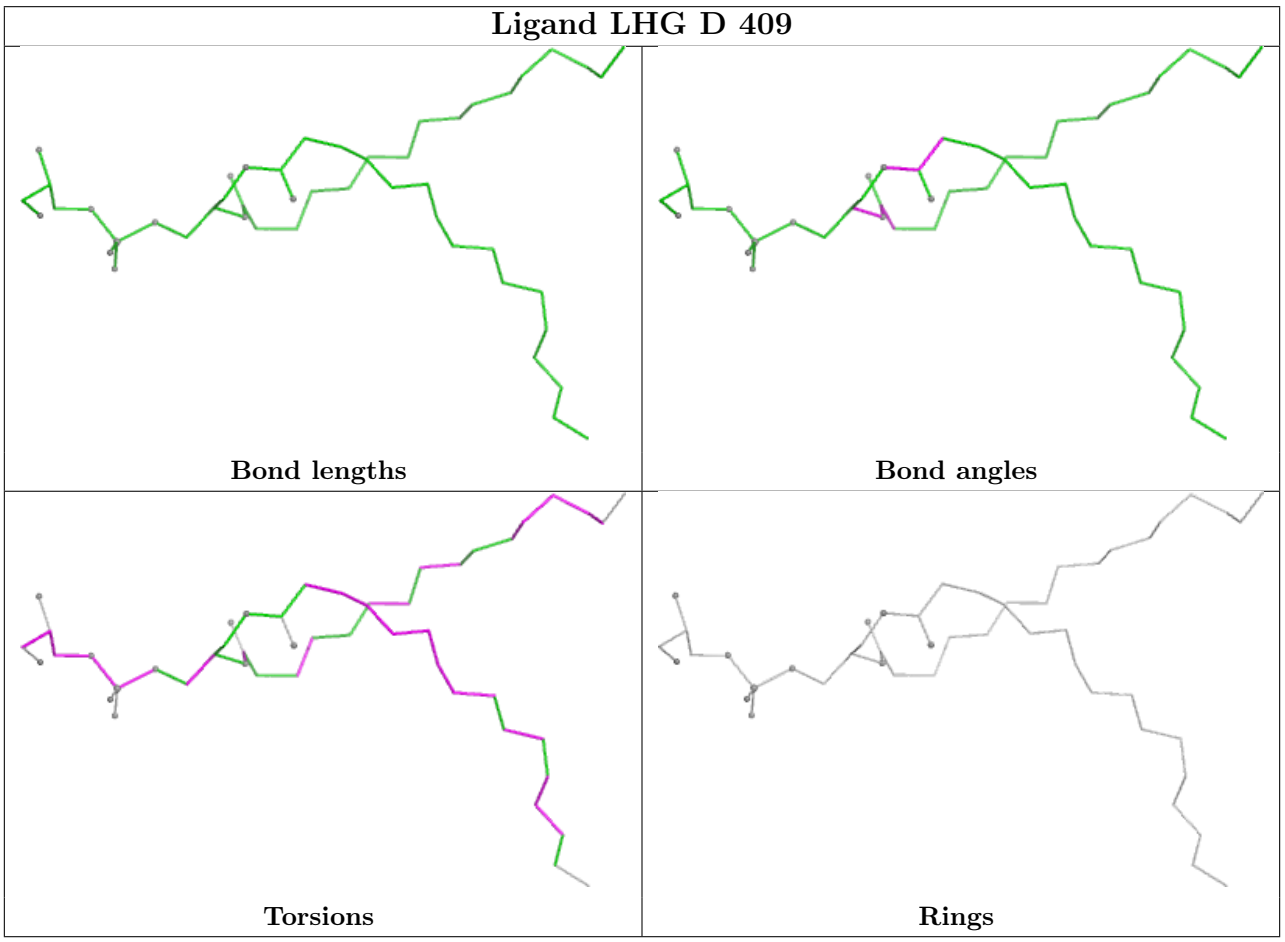
Ligand BCR C 514



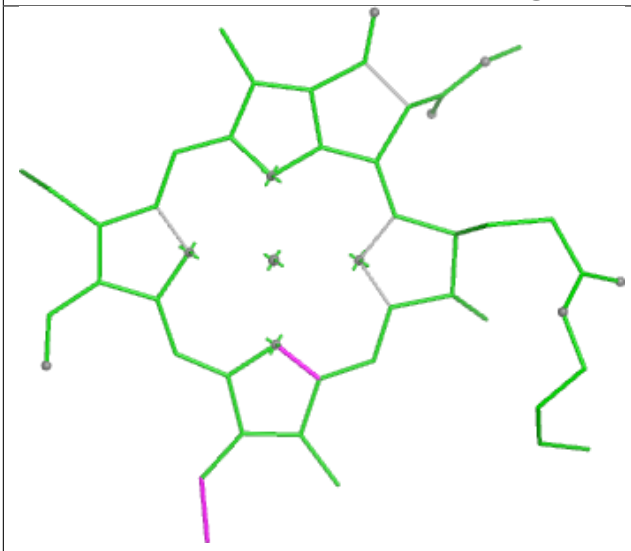
Ligand RRX h 101



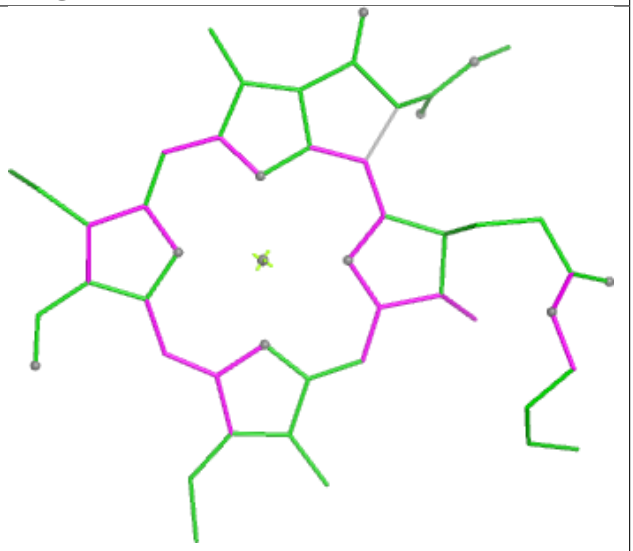
Ligand LHG D 409



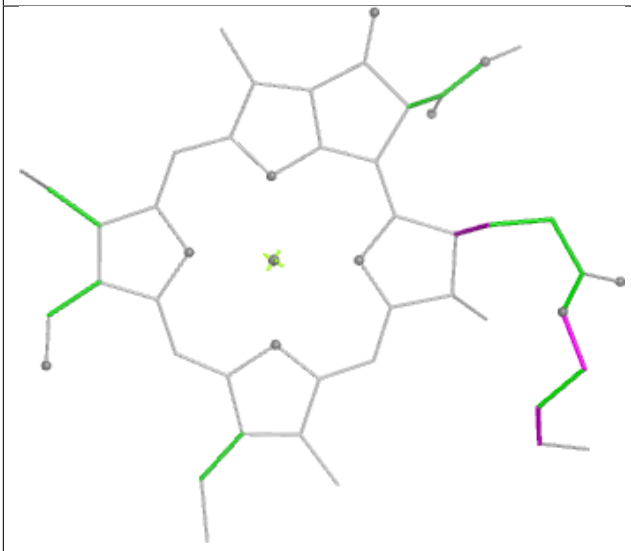
Ligand CHL g 607



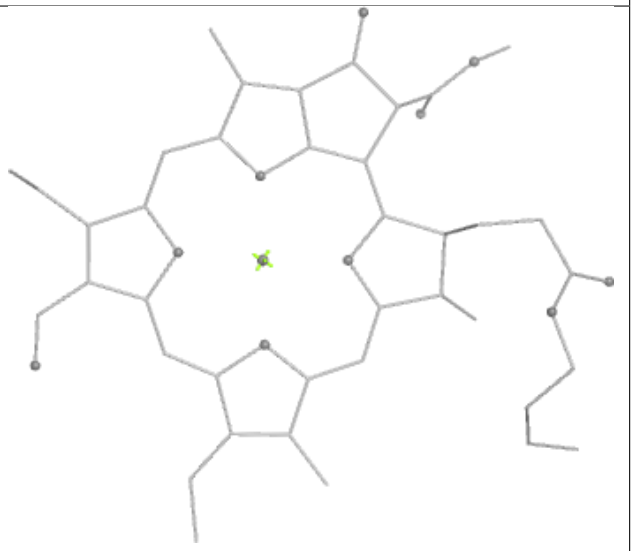
Bond lengths



Bond angles

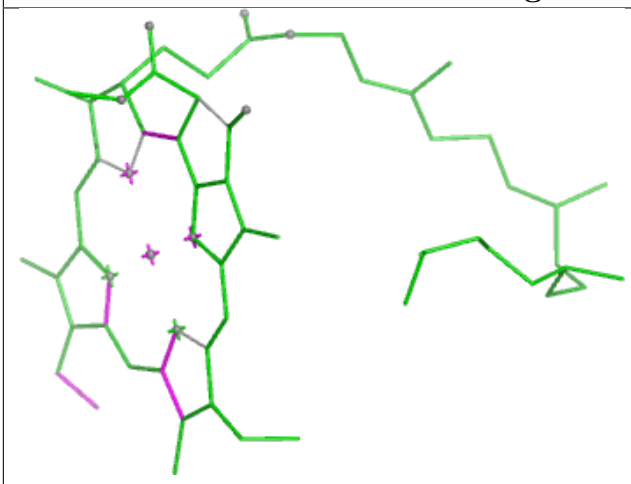


Torsions

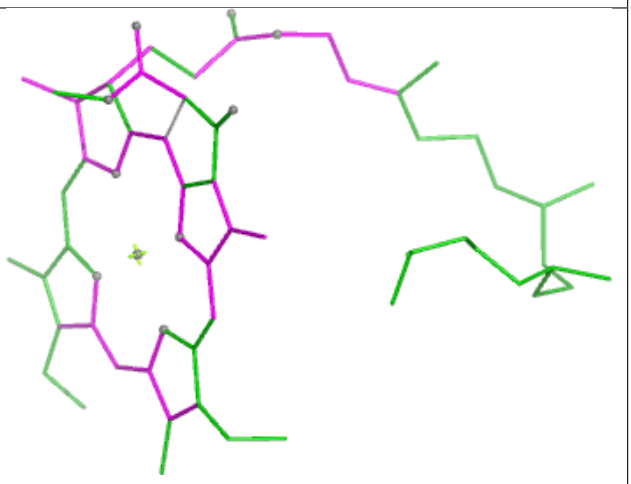


Rings

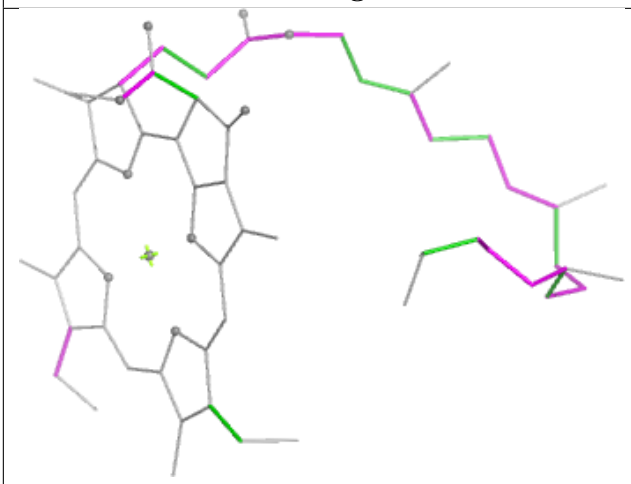
Ligand CLA C 503



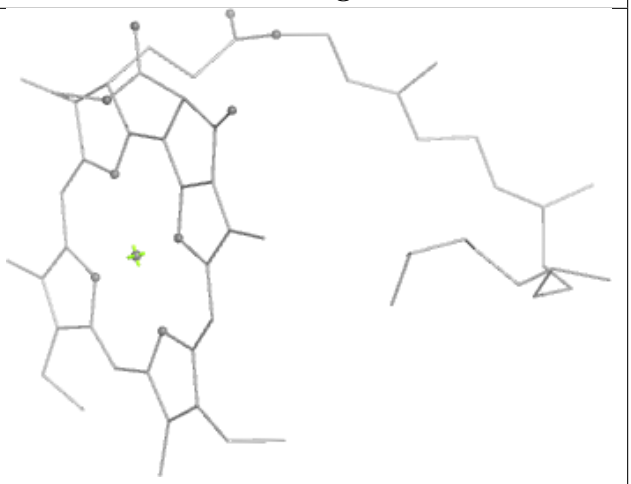
Bond lengths



Bond angles

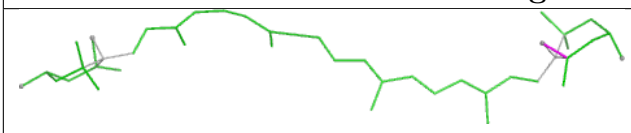


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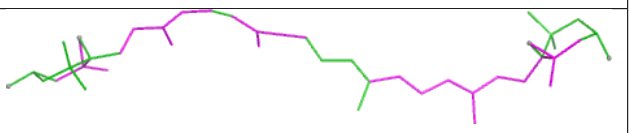


Rings

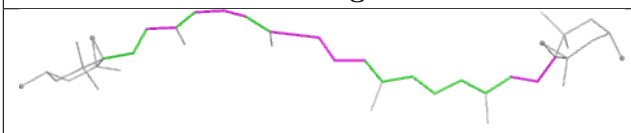
Ligand XAT r 622



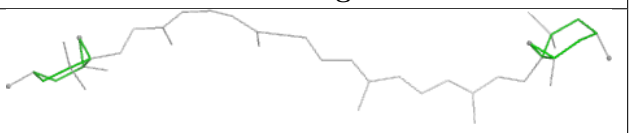
Bond lengths



Bond angles

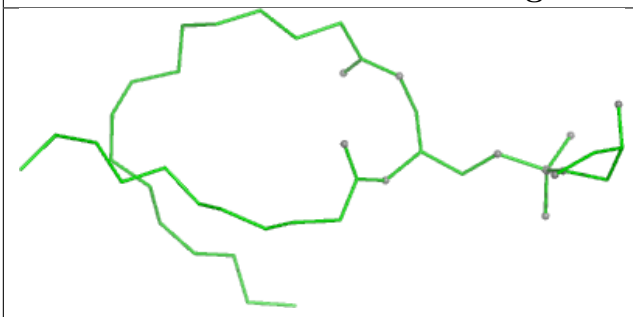


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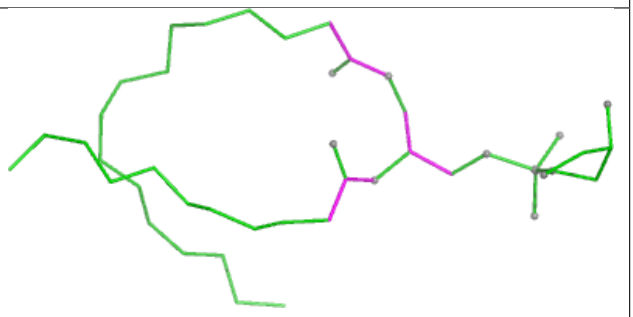


Rings

Ligand LHG d 408



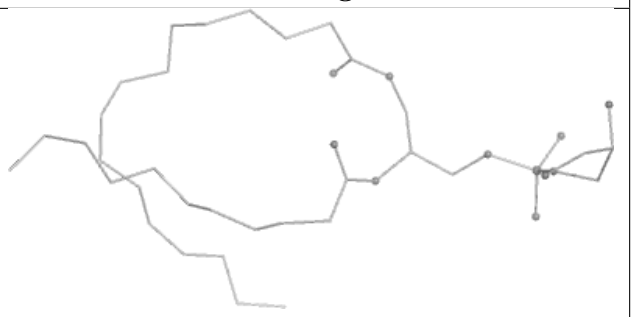
Bond lengths



Bond angles

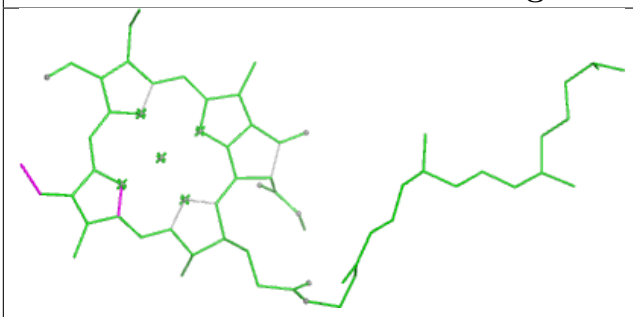


Torsions

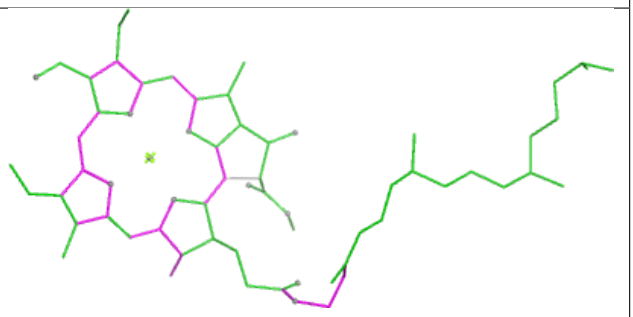


Rings

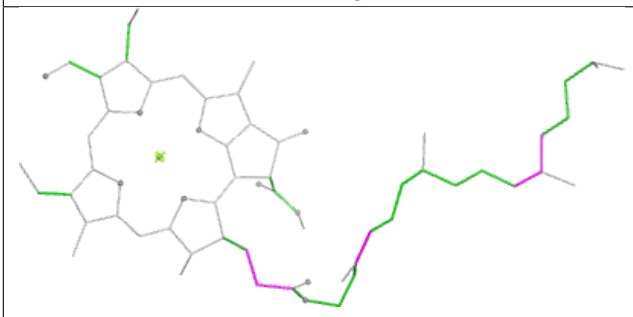
Ligand CHL n 605



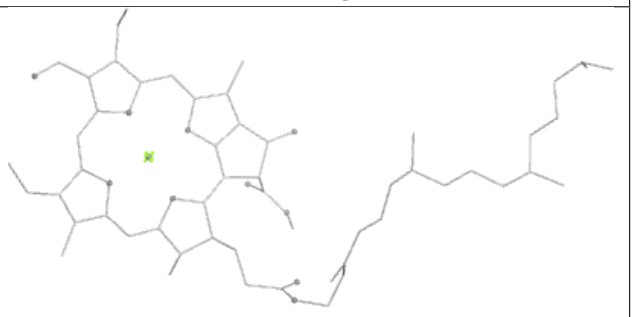
Bond lengths



Bond angles

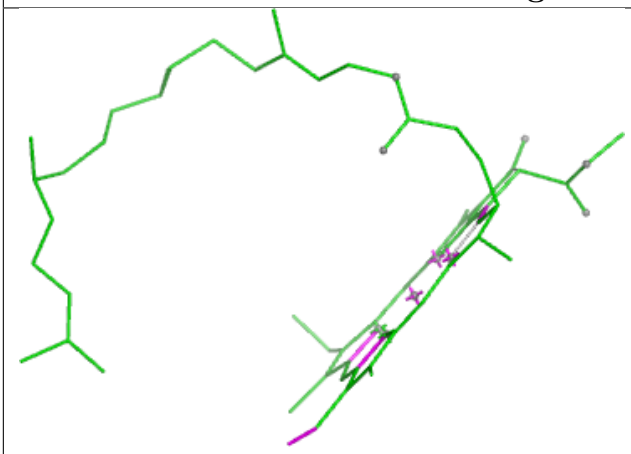


Torsions

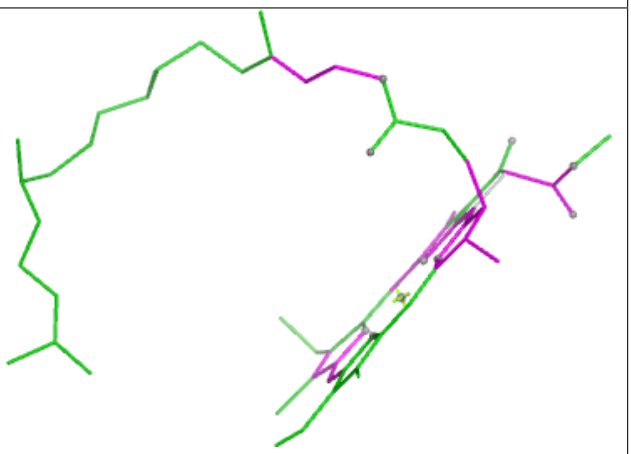


Rings

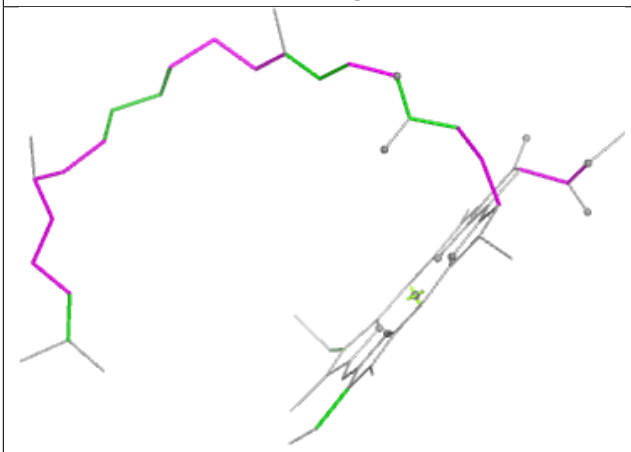
Ligand CLA b 612



Bond lengths



Bond angles

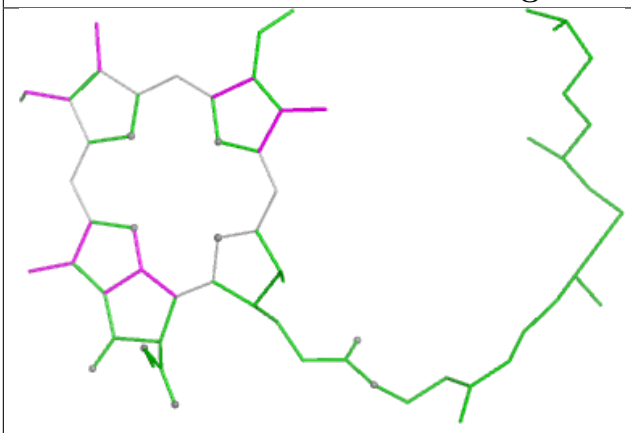


Torsions

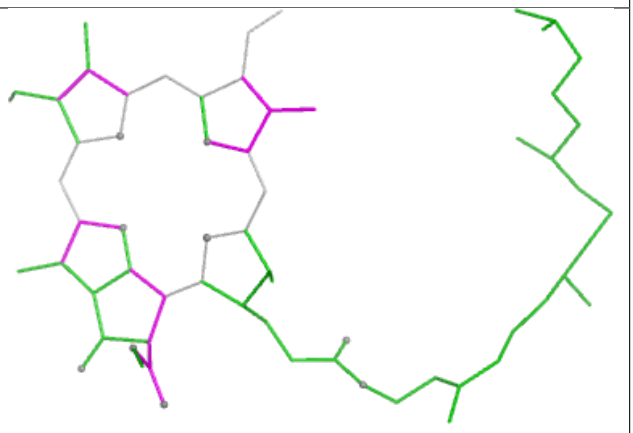


Rings

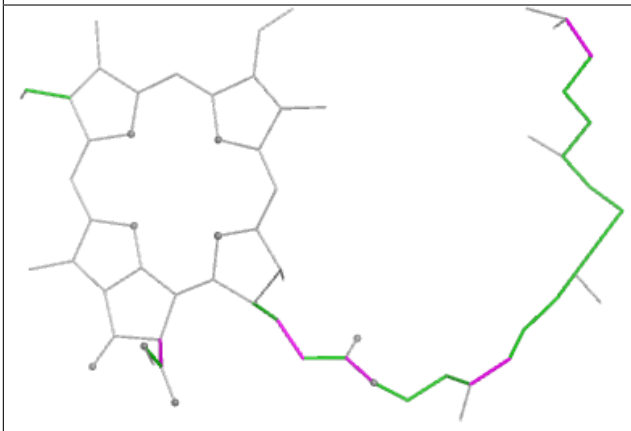
Ligand PHO A 408



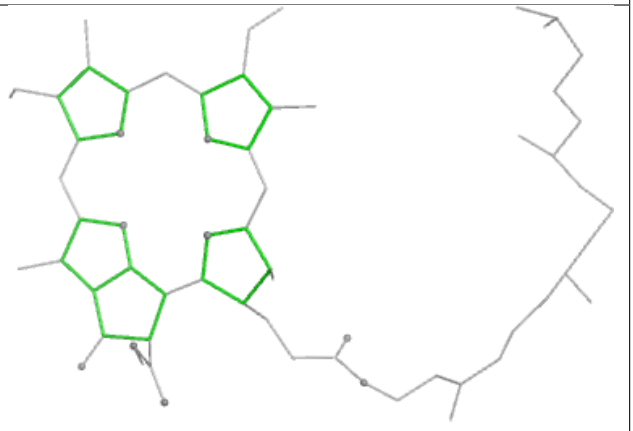
Bond lengths



Bond angles

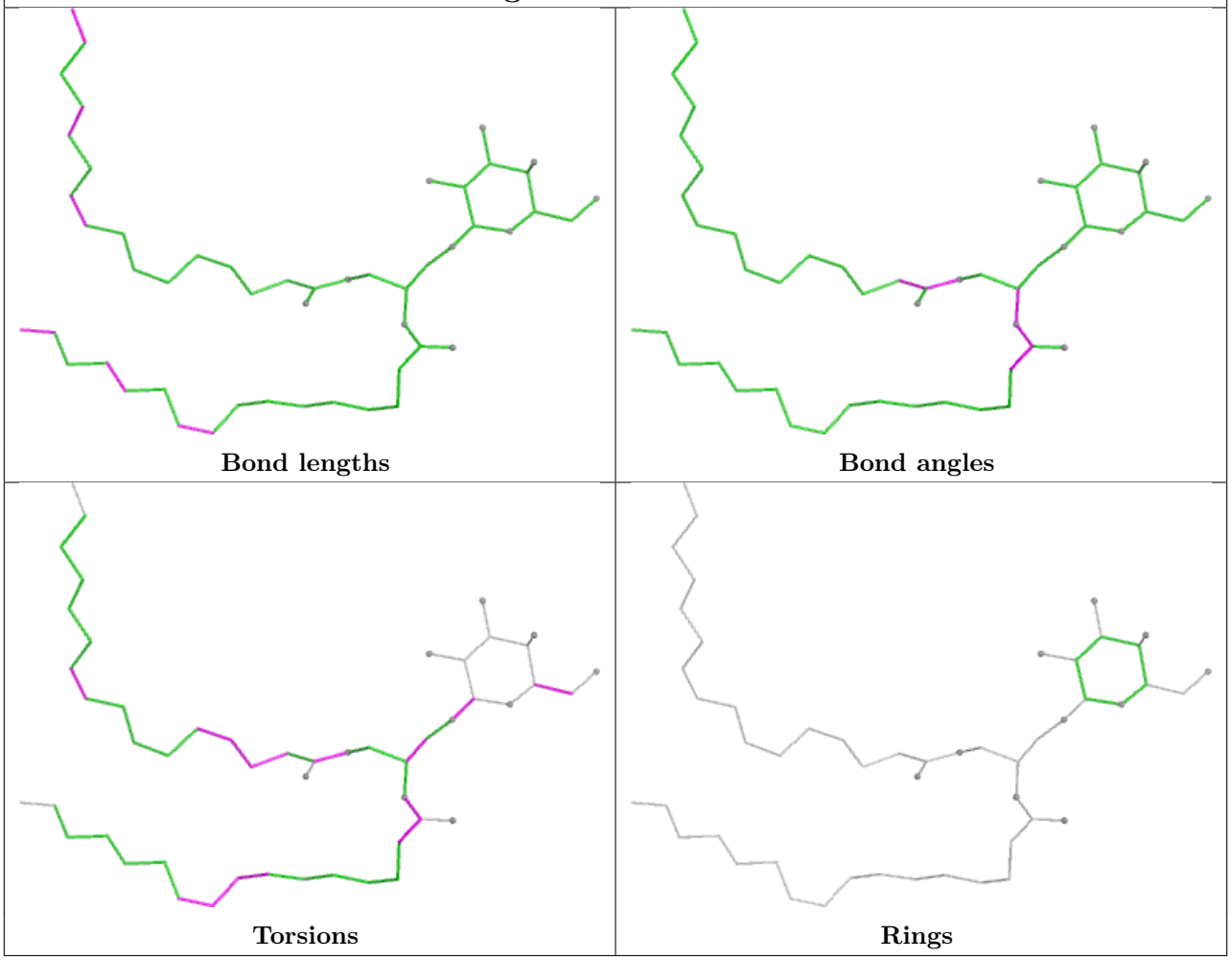


Torsions

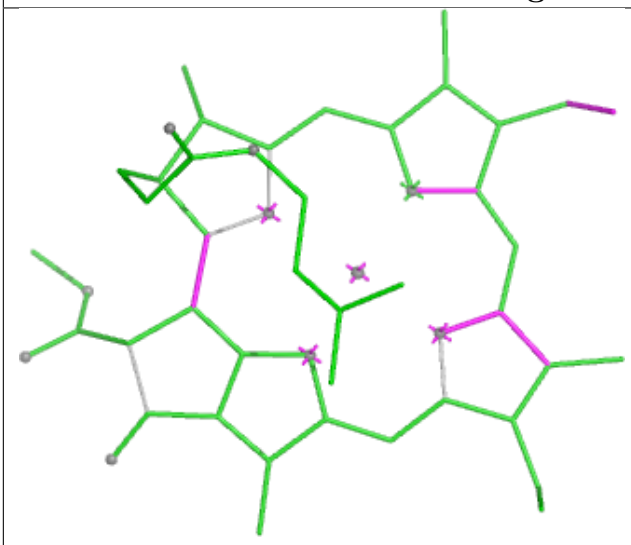


Rings

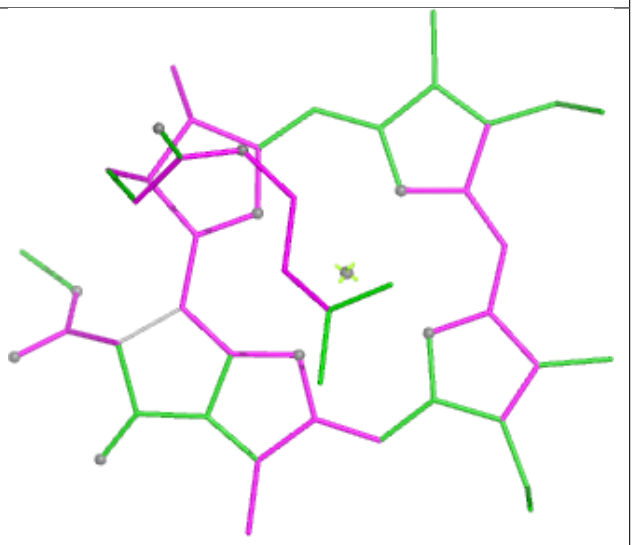
Ligand LMG c 521



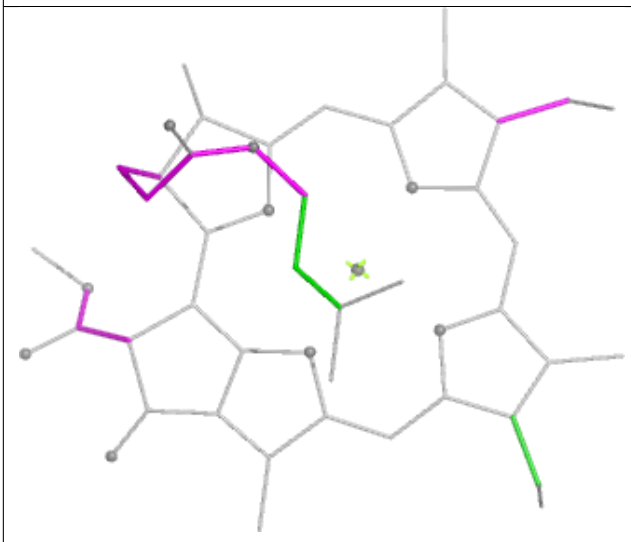
Ligand CLA S 605



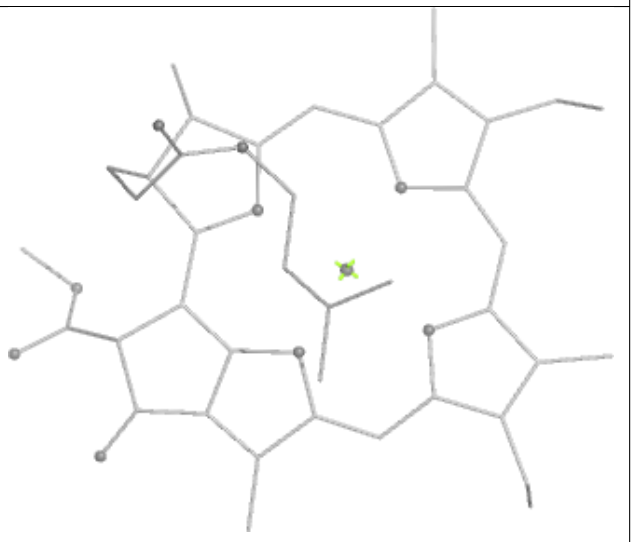
Bond lengths



Bond angles

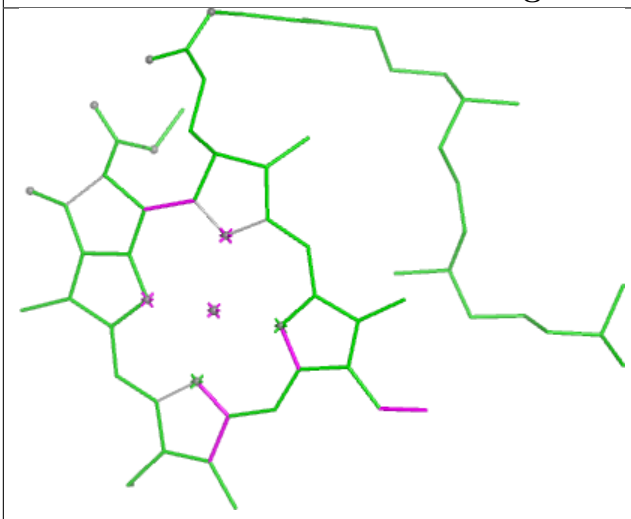


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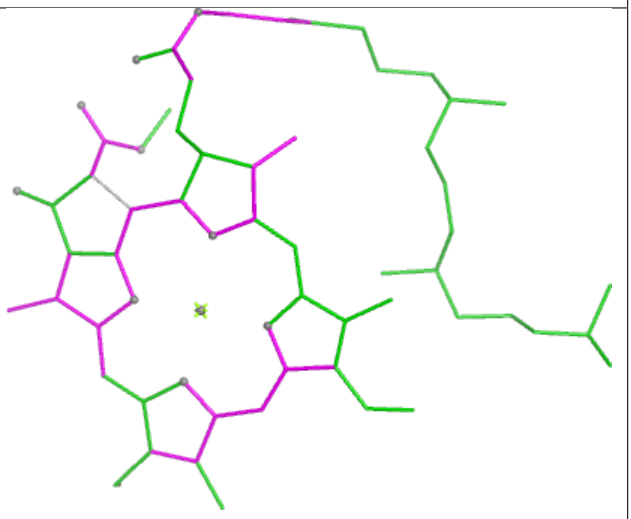


Rings

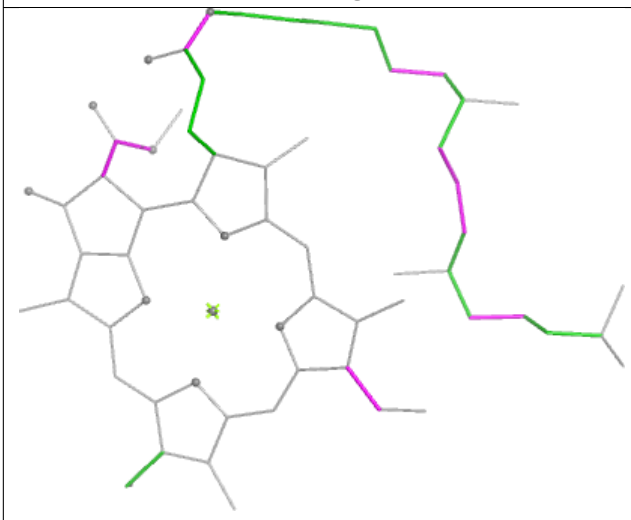
Ligand CLA Y 612



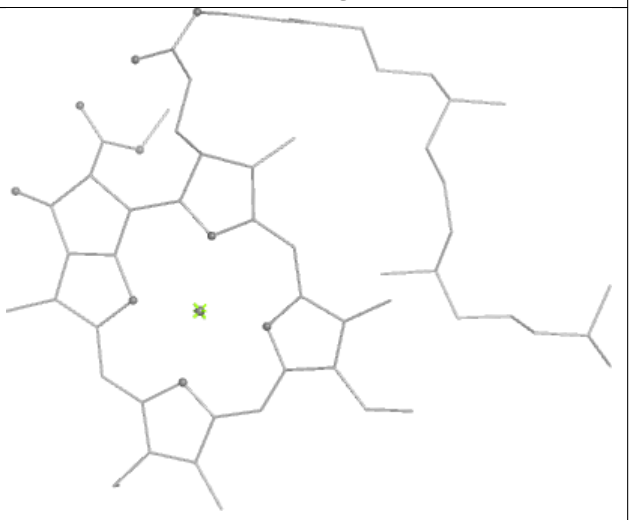
Bond lengths



Bond angles

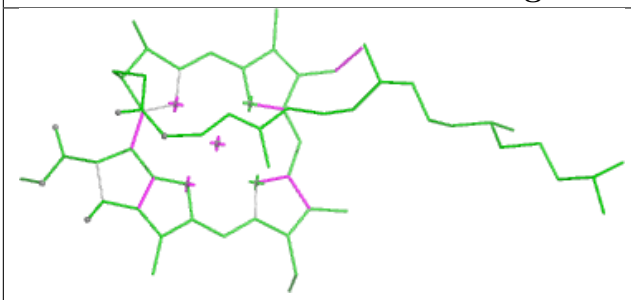


Torsions



Rings

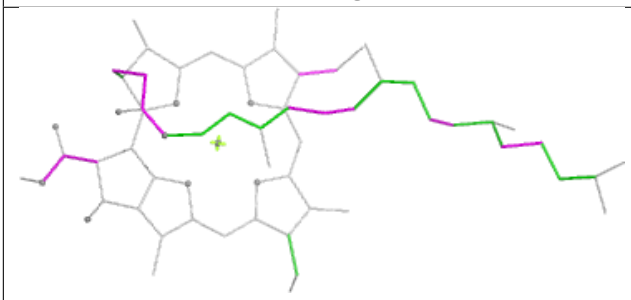
Ligand CLA C 505



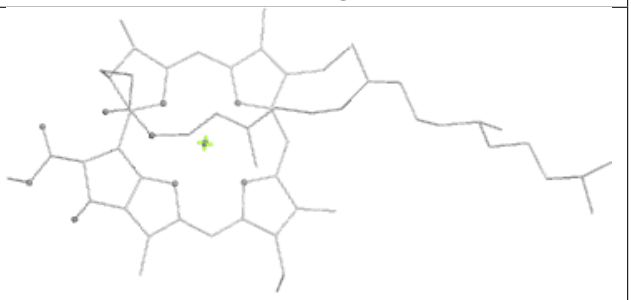
Bond lengths



Bond angles

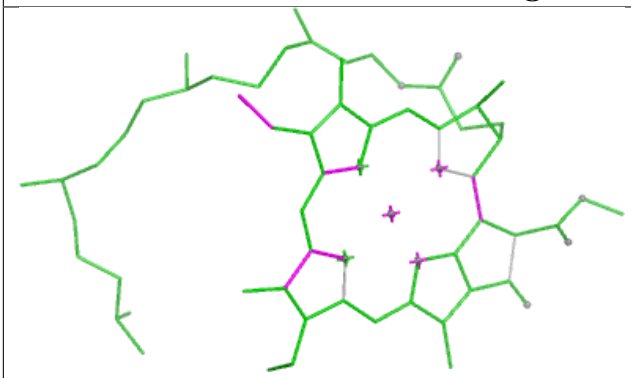


Torsions

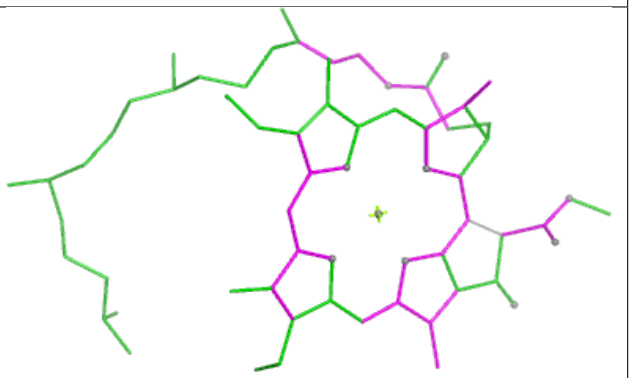


Rings

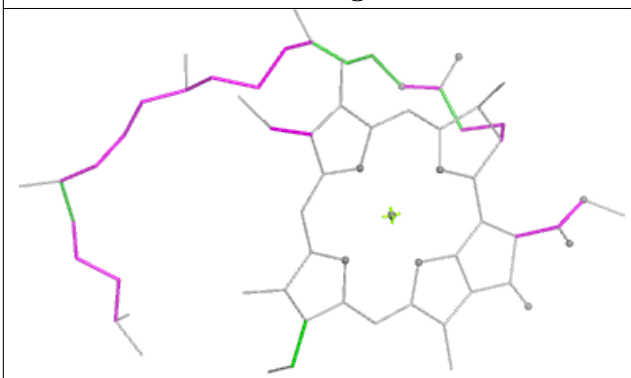
Ligand CLA Y 610



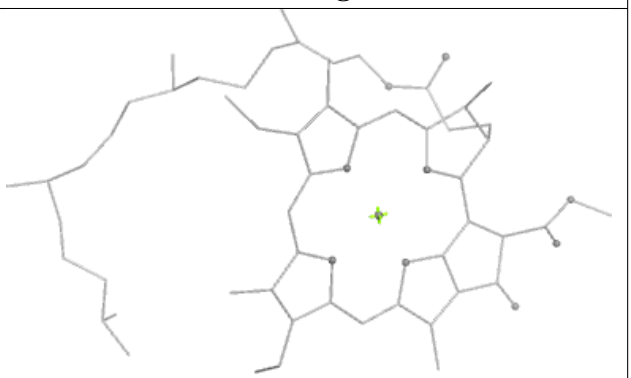
Bond lengths



Bond angles

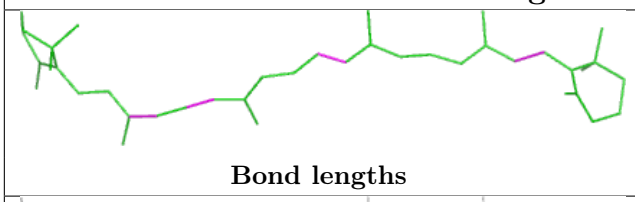


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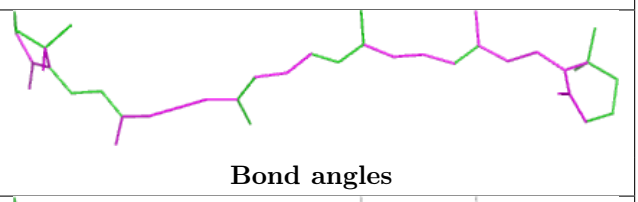


Rings

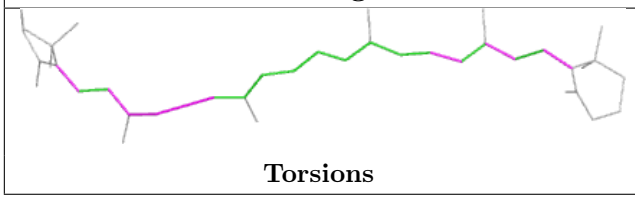
Ligand BCR c 516



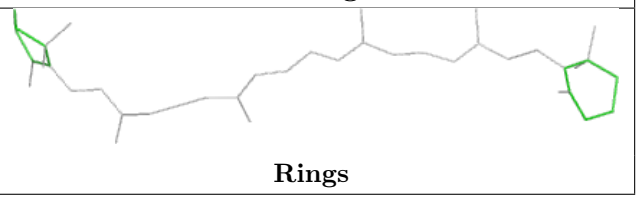
Bond lengths



Bond angles

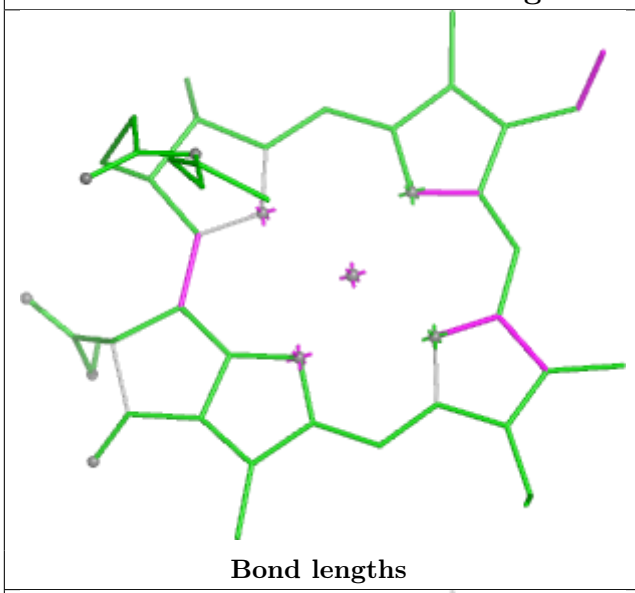


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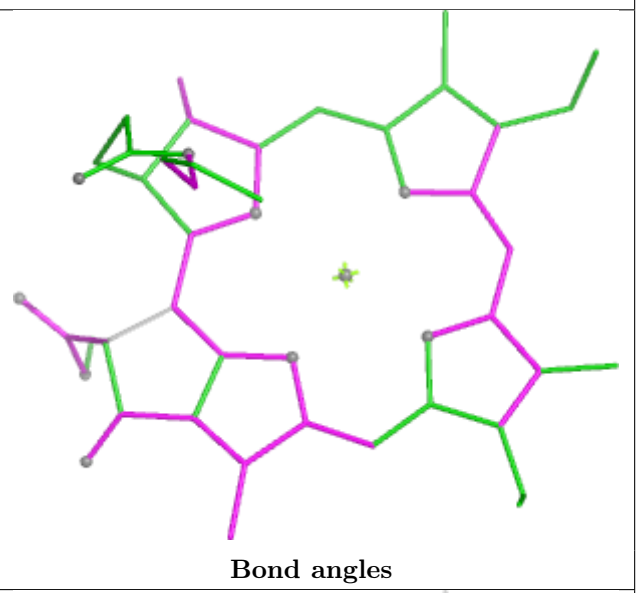


Rings

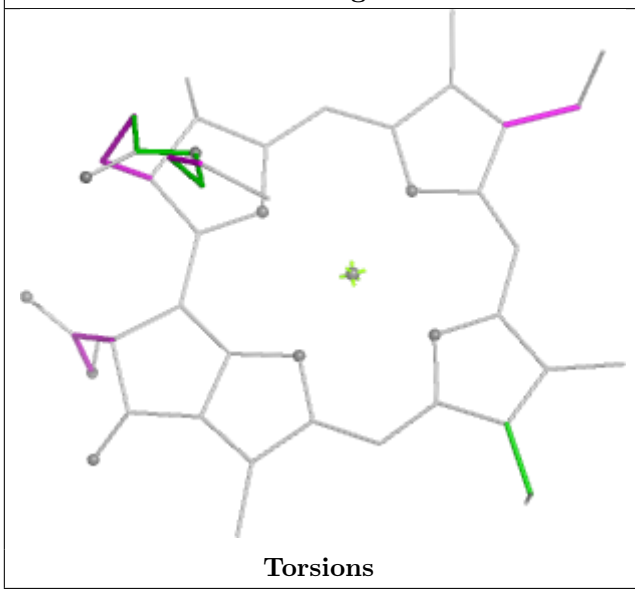
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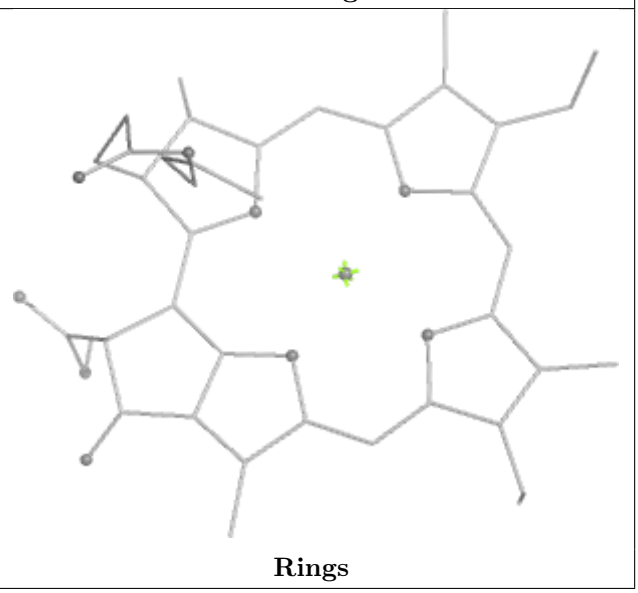
Bond lengths



Bond angles

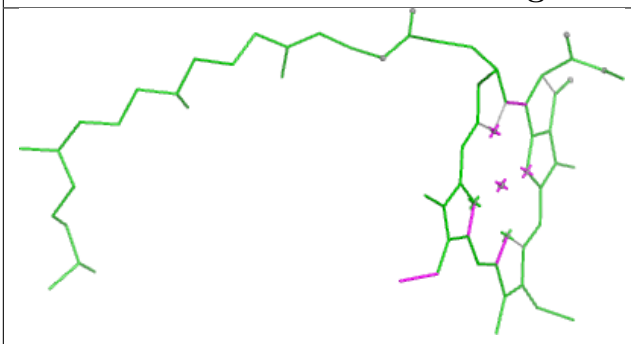


Torsions

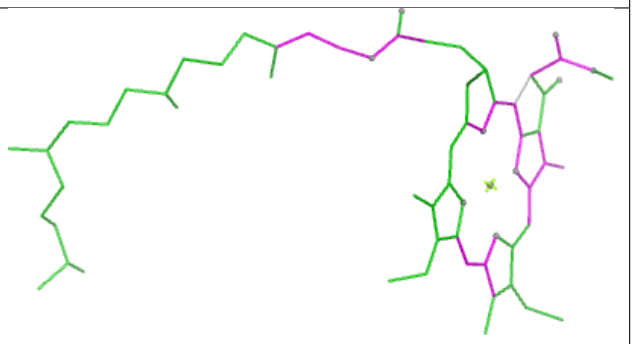


Rings

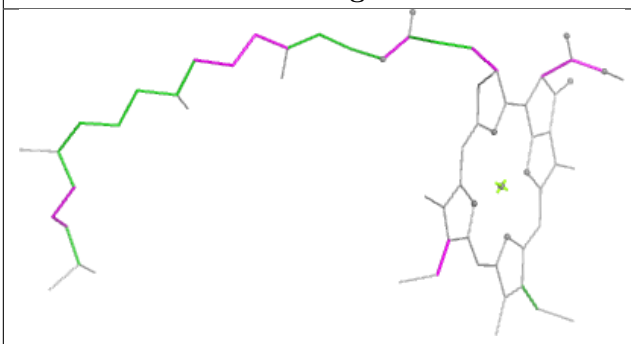
Ligand CLA b 610



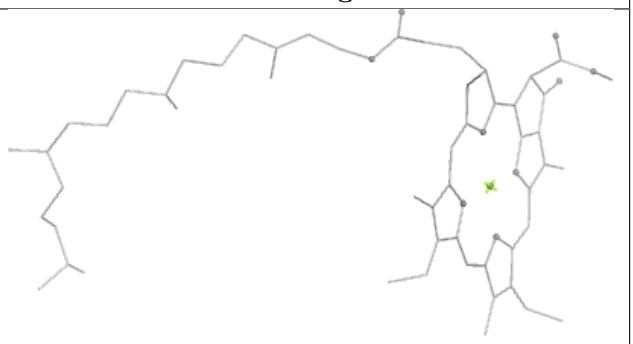
Bond lengths



Bond angles

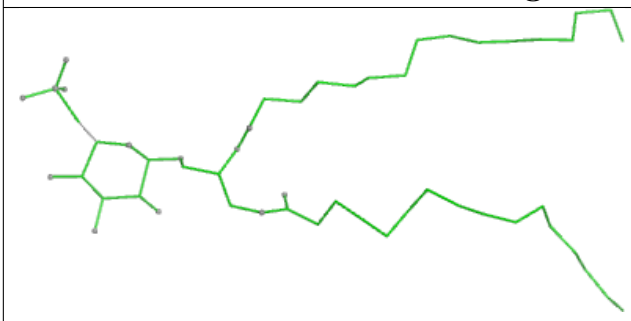


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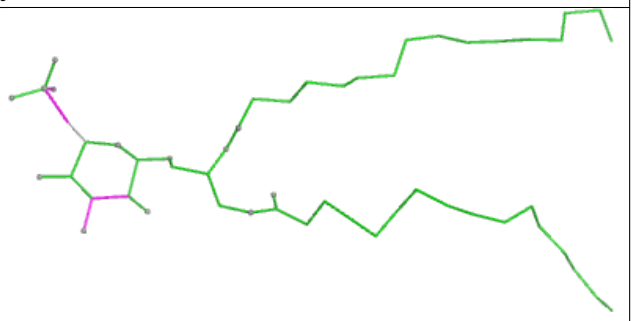


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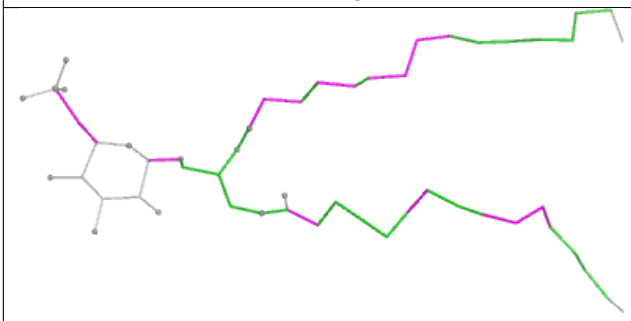
Ligand SQD C 526



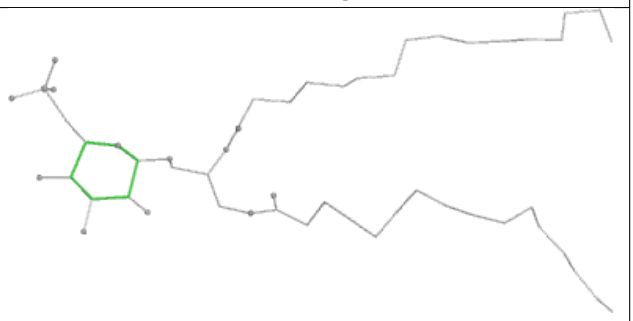
Bond lengths



Bond angles

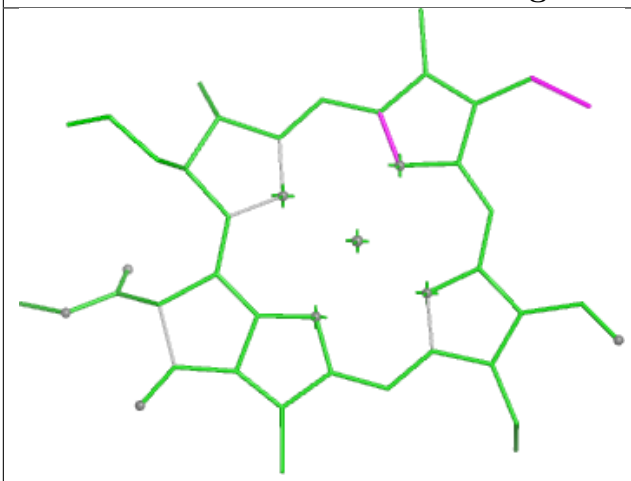


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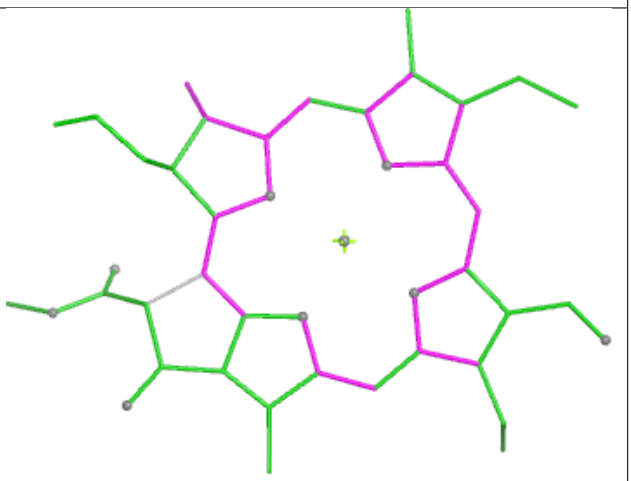


Rings

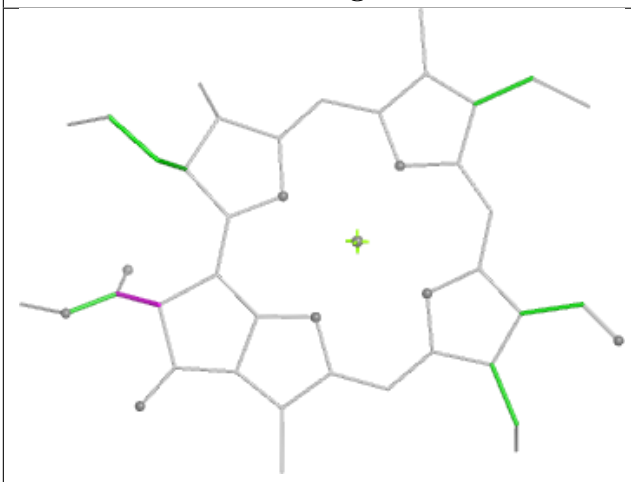
Ligand CHL r 606



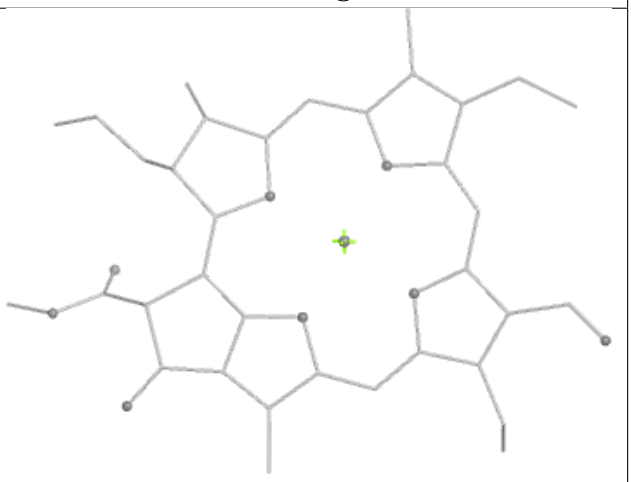
Bond lengths



Bond angles

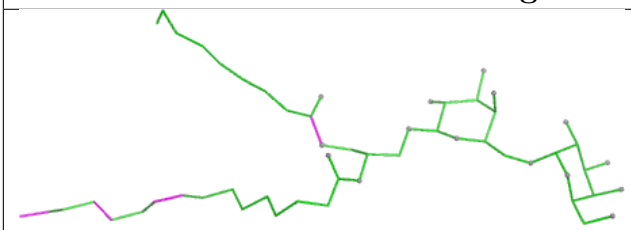


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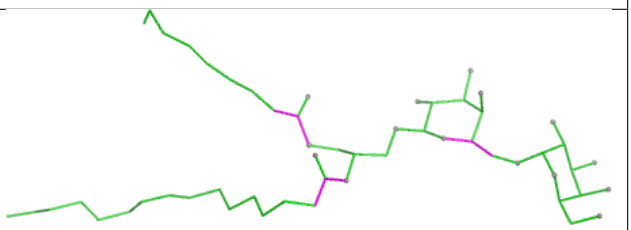


Rings

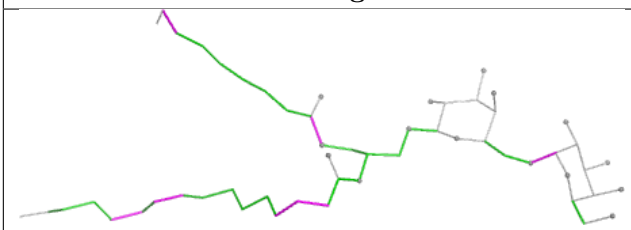
Ligand DGD C 518



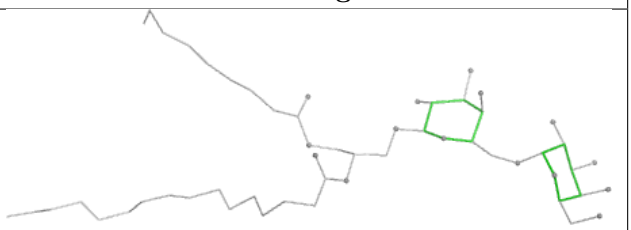
Bond lengths



Bond angles

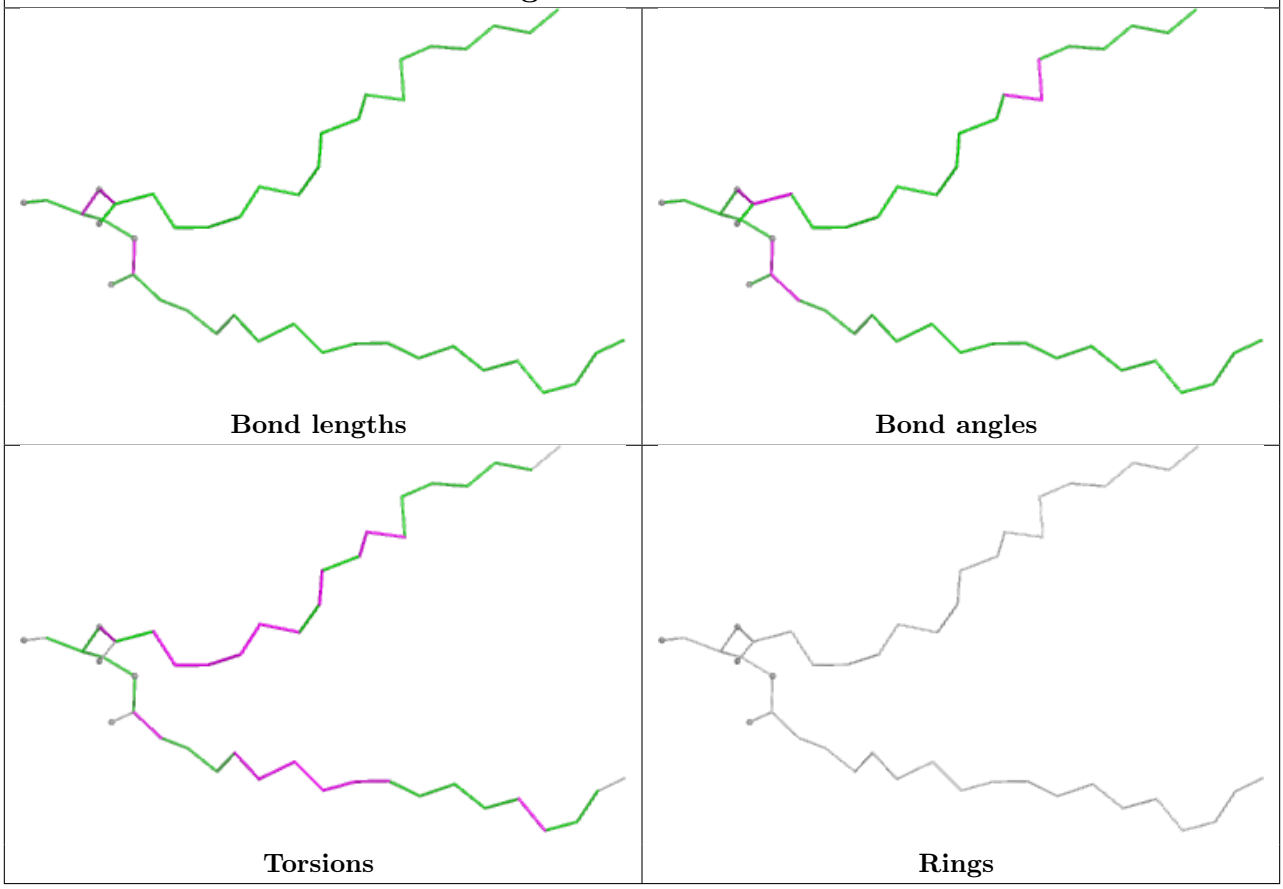


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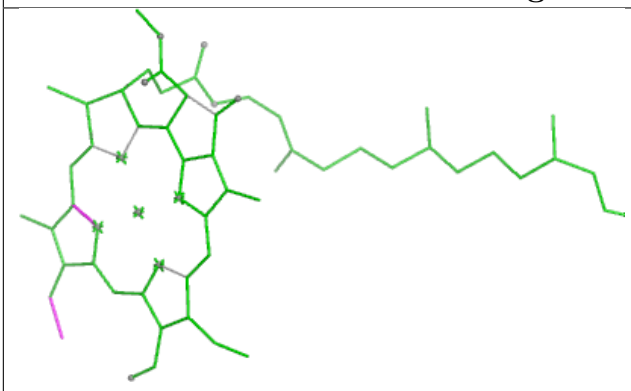


Rings

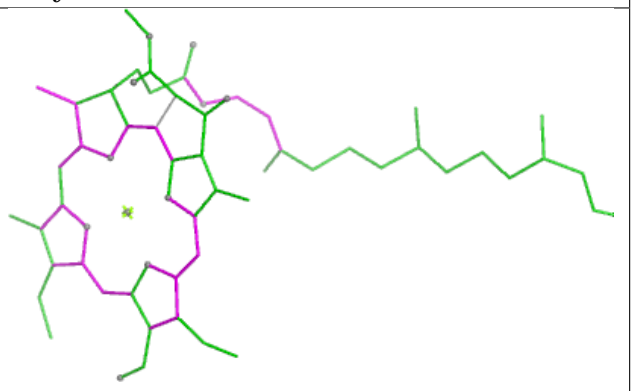
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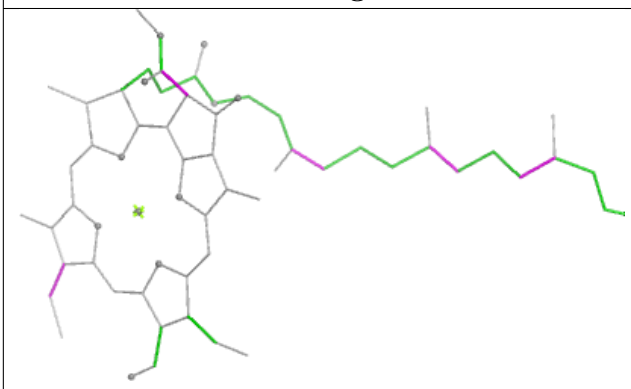
Ligand CHL y 609



Bond lengths



Bond angles

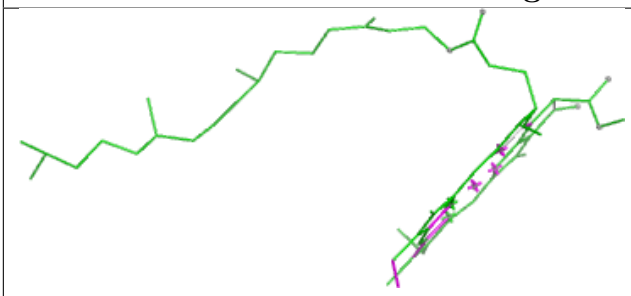


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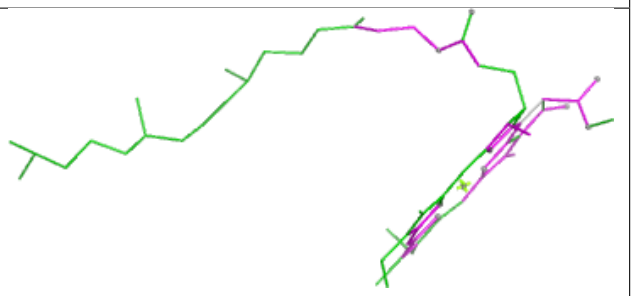


Rings

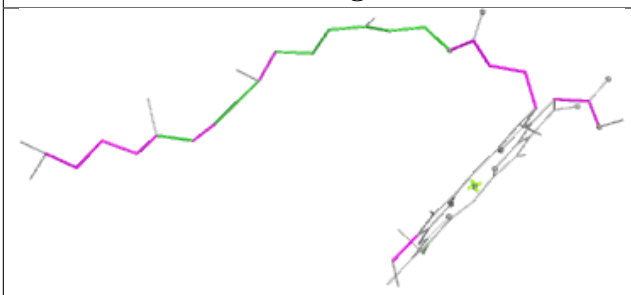
Ligand CLA N 604



Bond lengths



Bond angles

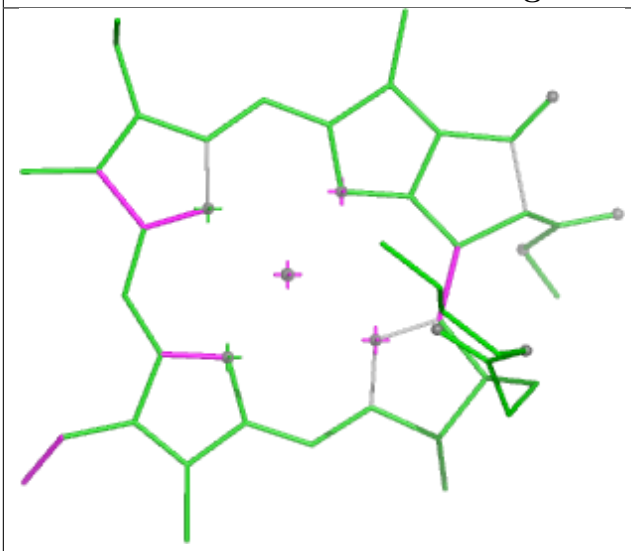


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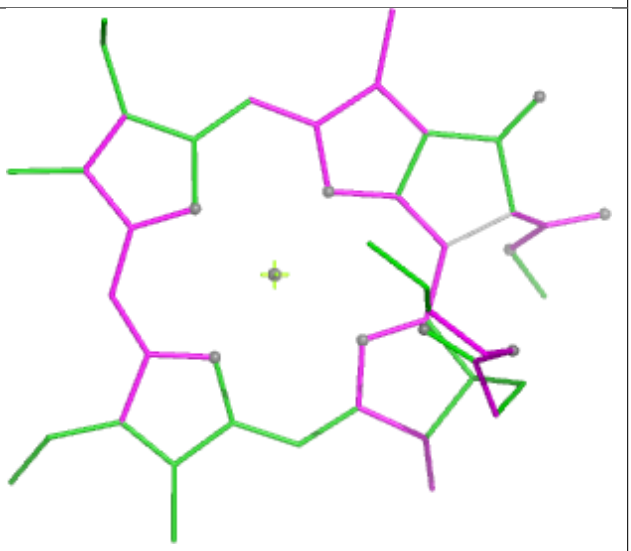


Rings

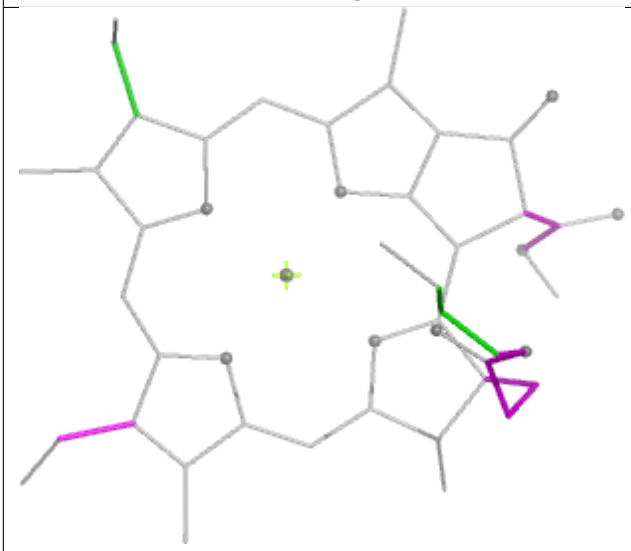
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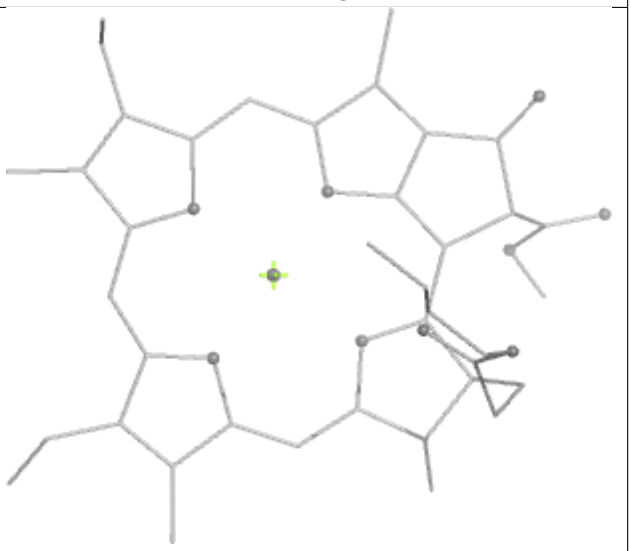
Bond lengths



Bond angles

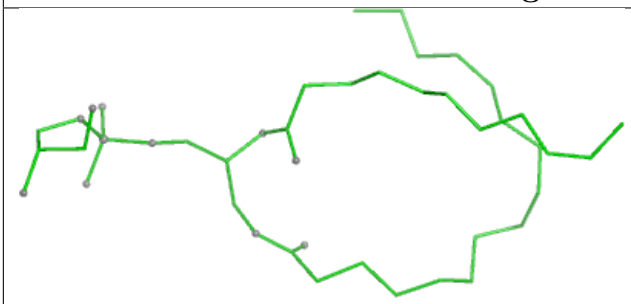


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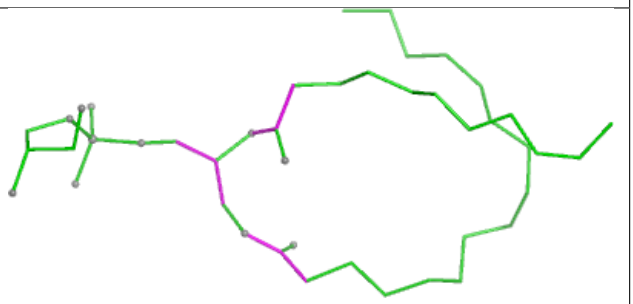


Rings

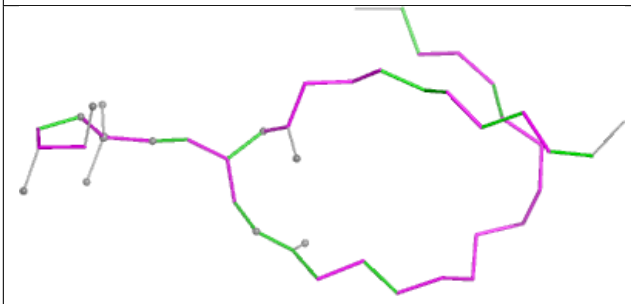
Ligand LHG D 408



Bond lengths



Bond angles

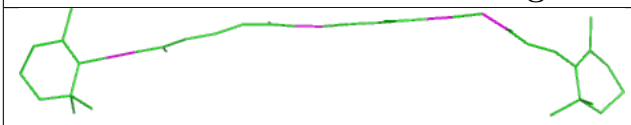


Torsions

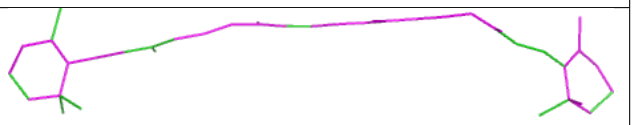


Rings

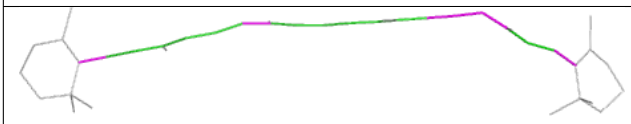
Ligand BCR c 517



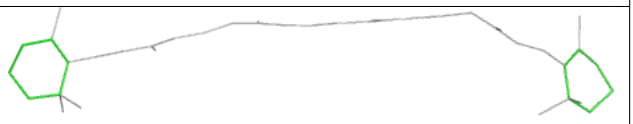
Bond lengths



Bond angles

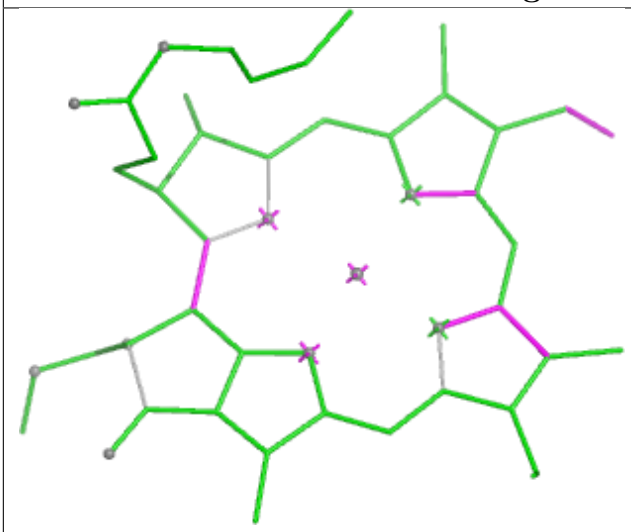


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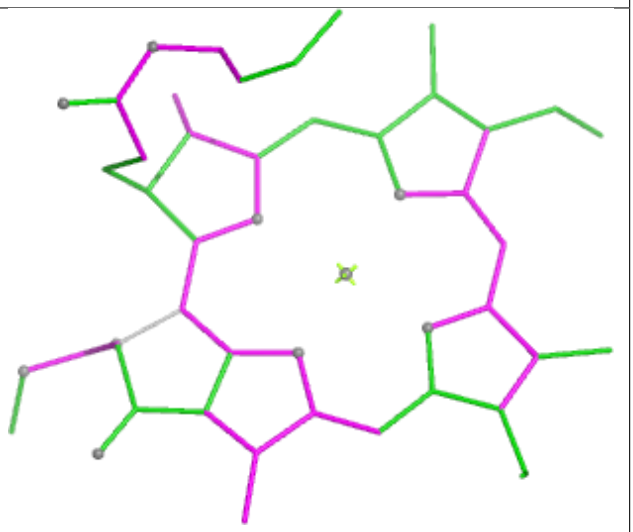


Rings

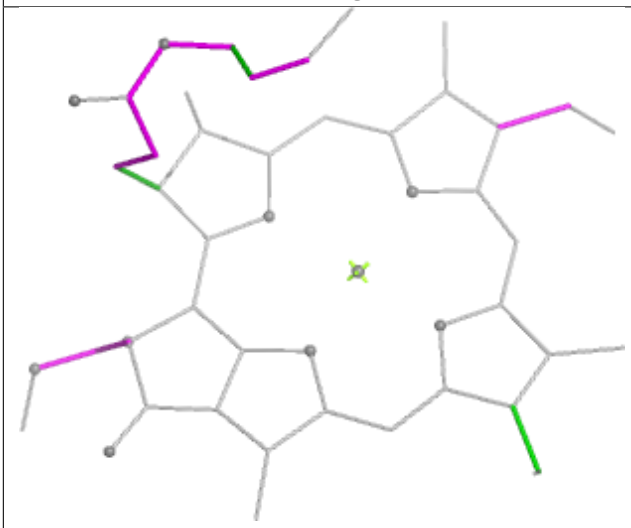
Ligand CLA G 614



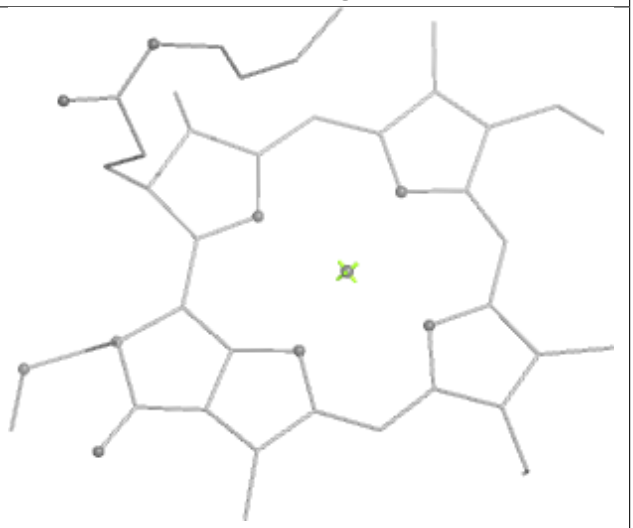
Bond lengths



Bond angles

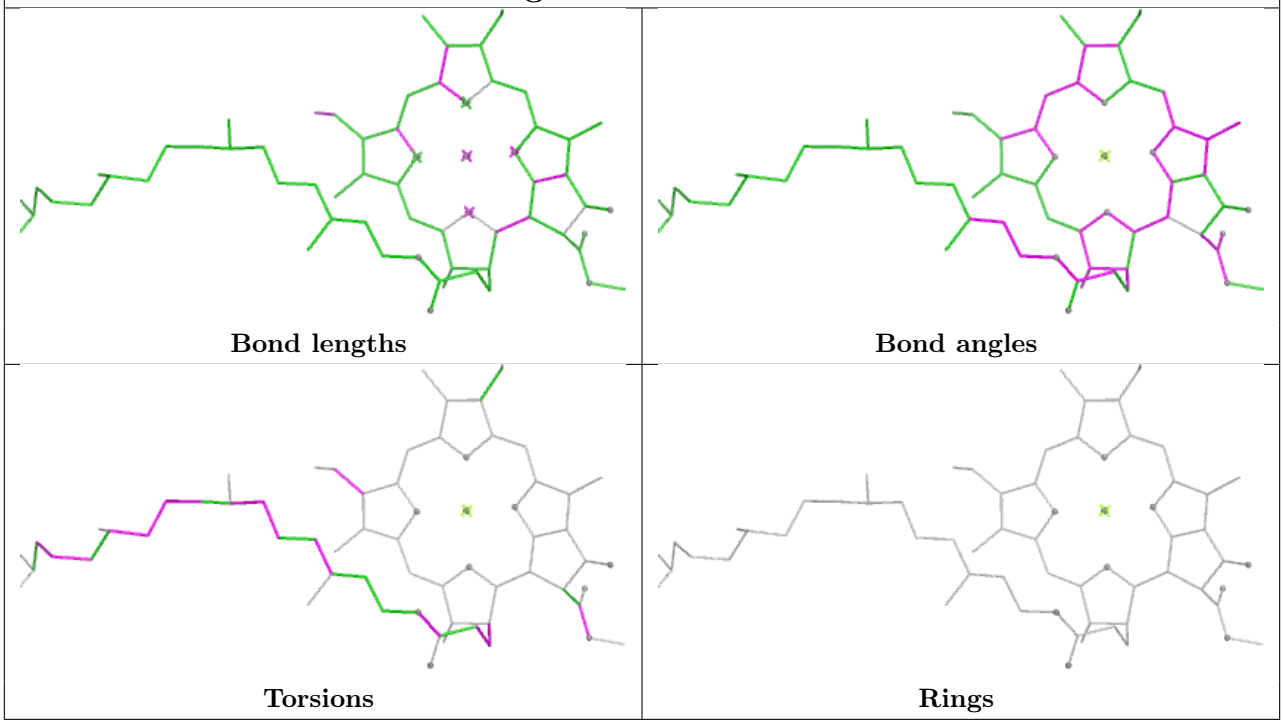


Torsions

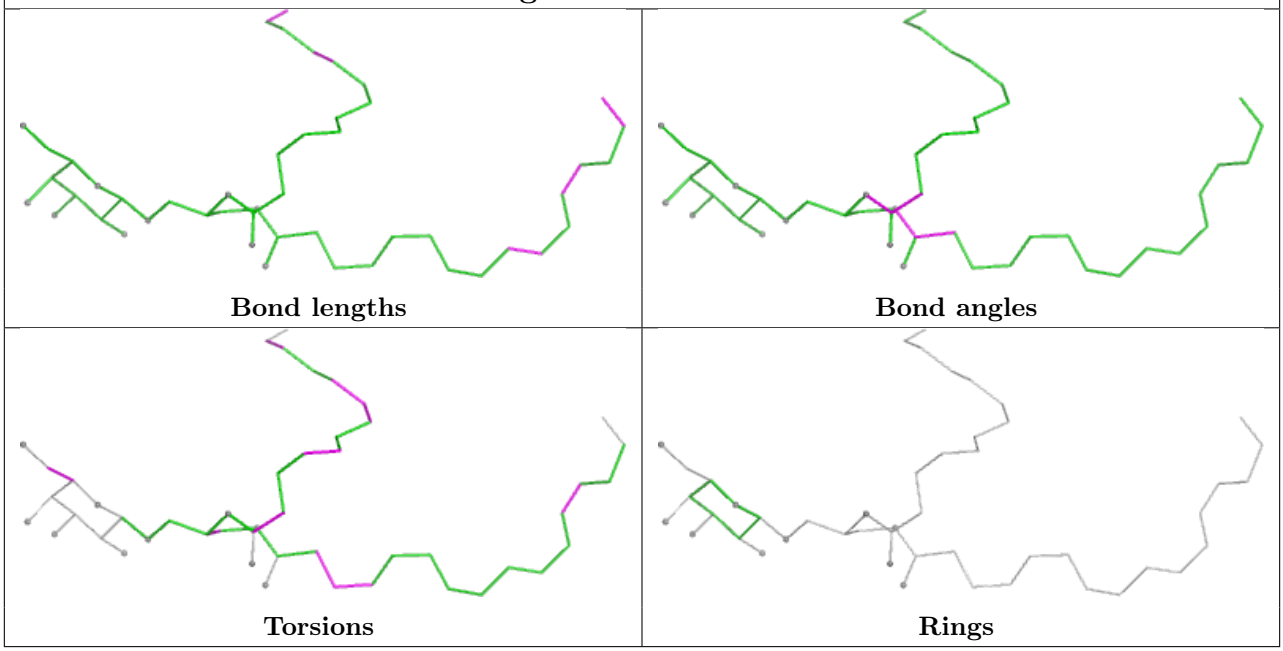


Rings

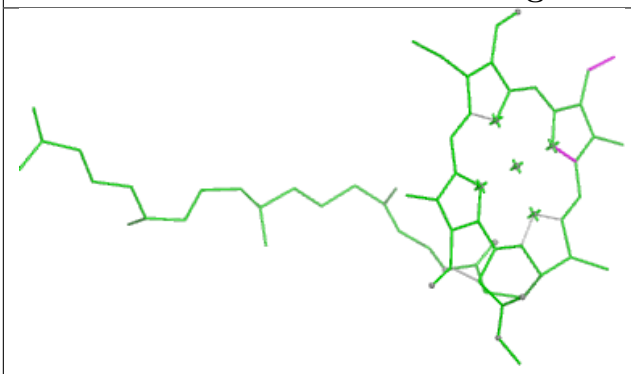
Ligand CLA B 604



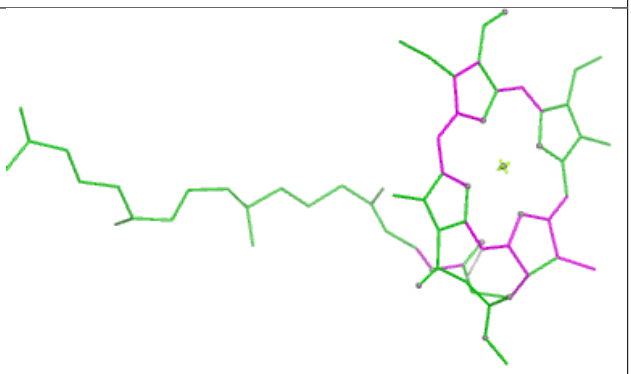
Ligand LMG H 102



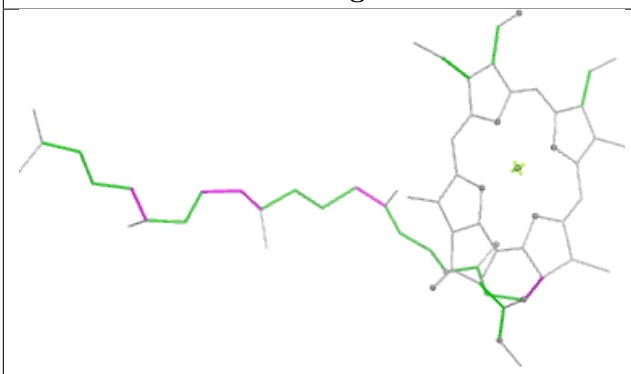
Ligand CHL n 609



Bond lengths



Bond angles

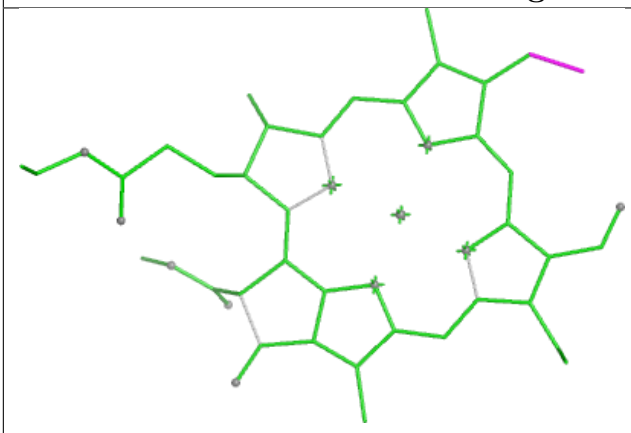


Torsions

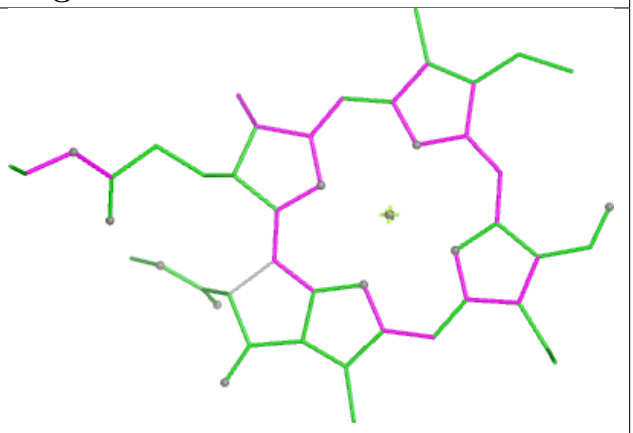


Rings

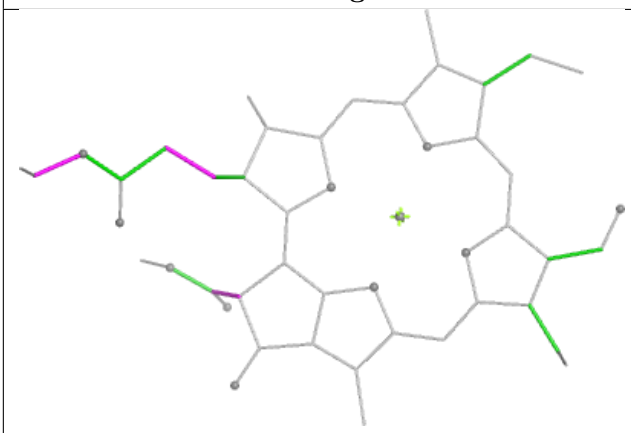
Ligand CHL g 605



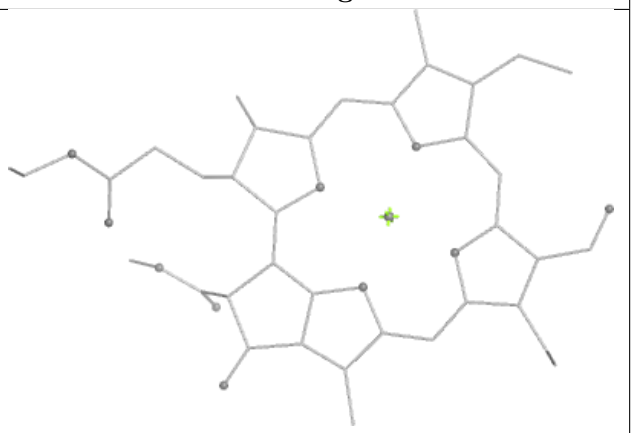
Bond lengths



Bond angles

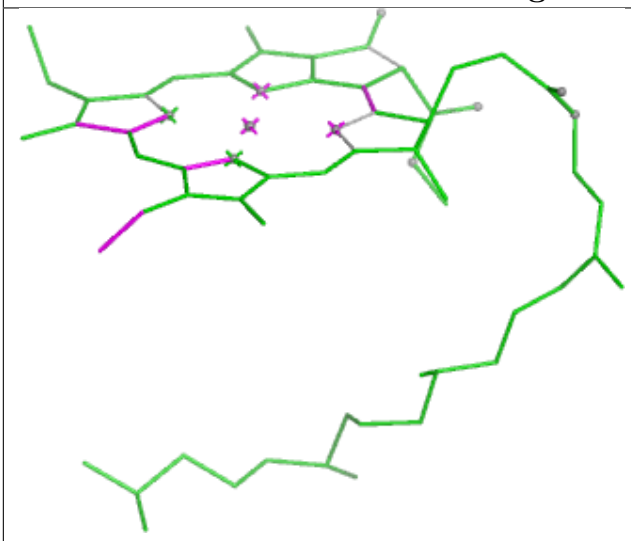


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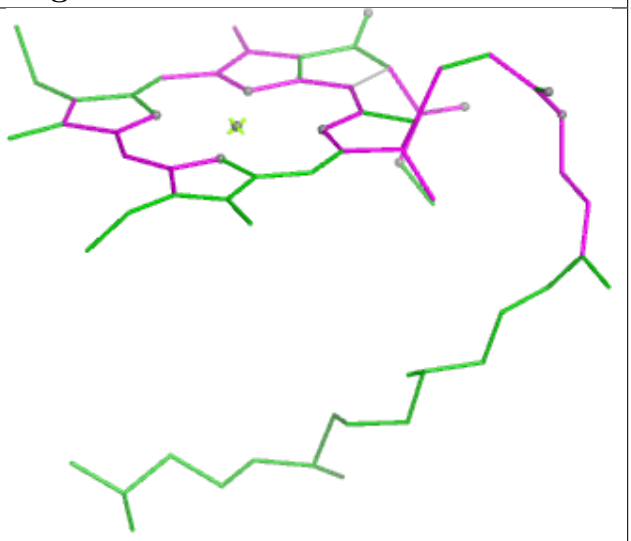


Rings

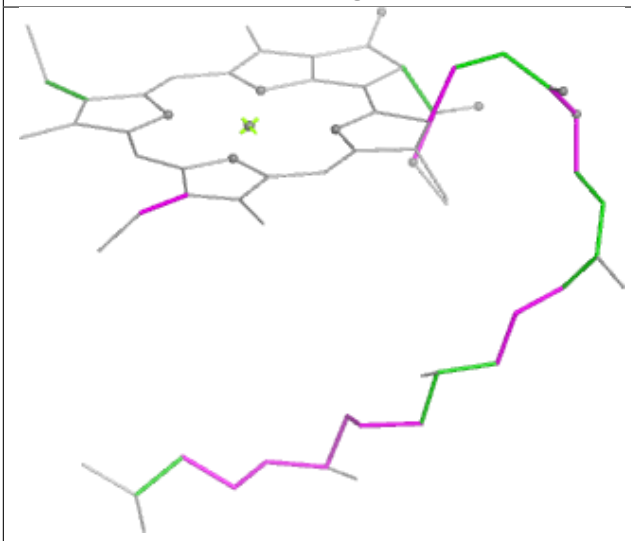
Ligand CLA g 603



Bond lengths



Bond angles

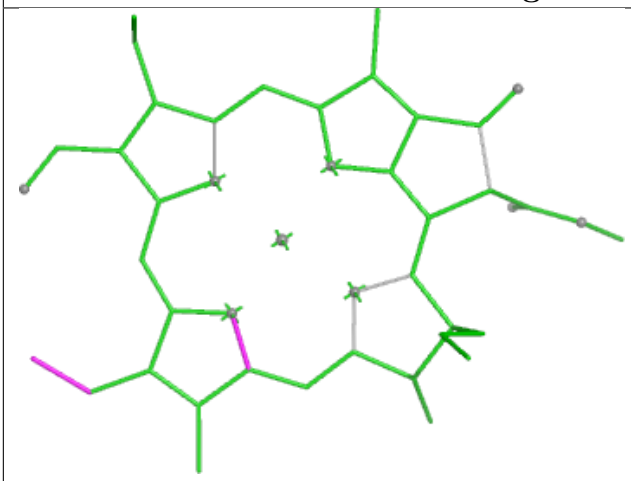


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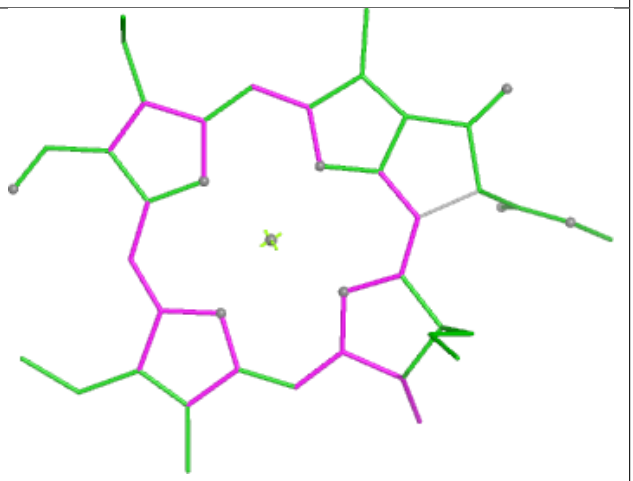


Rings

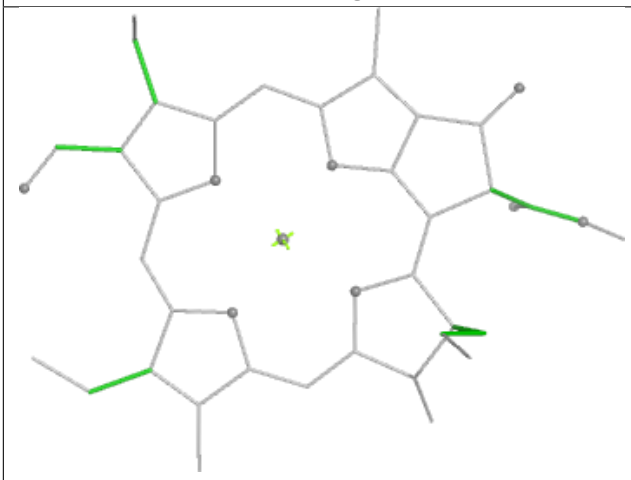
Ligand CHL G 608



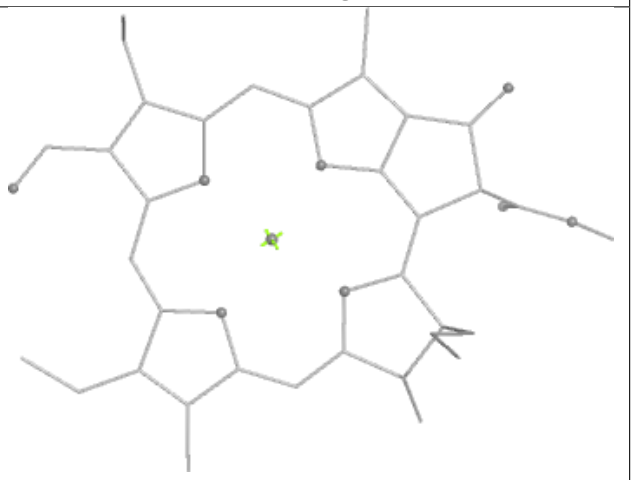
Bond lengths



Bond angles

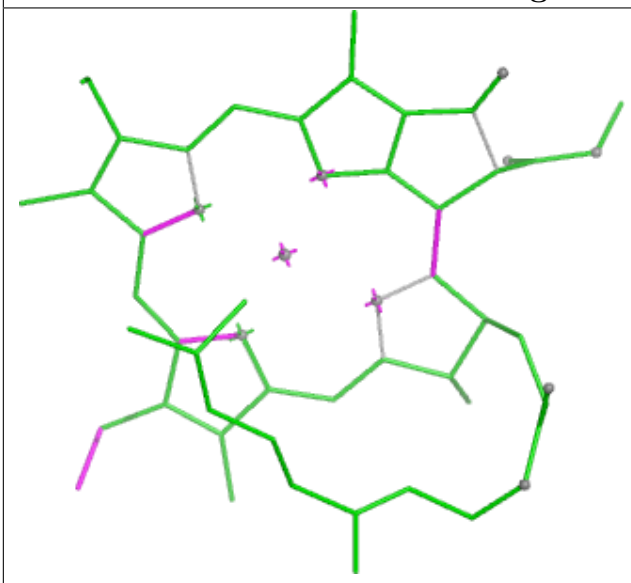


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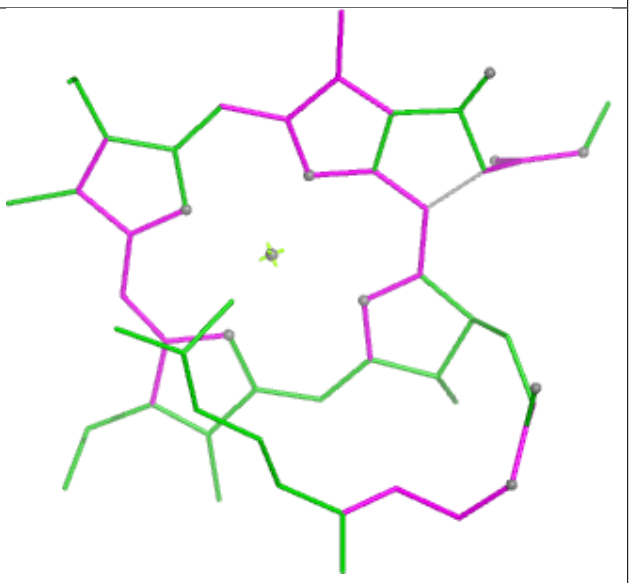


Rings

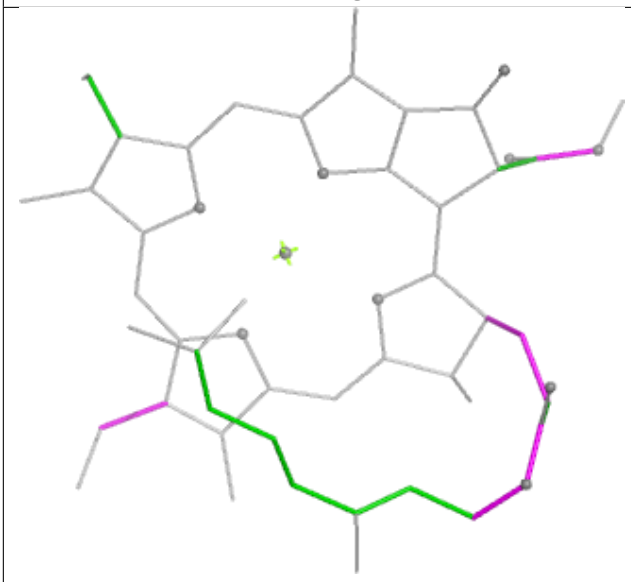
Ligand CLA s 614



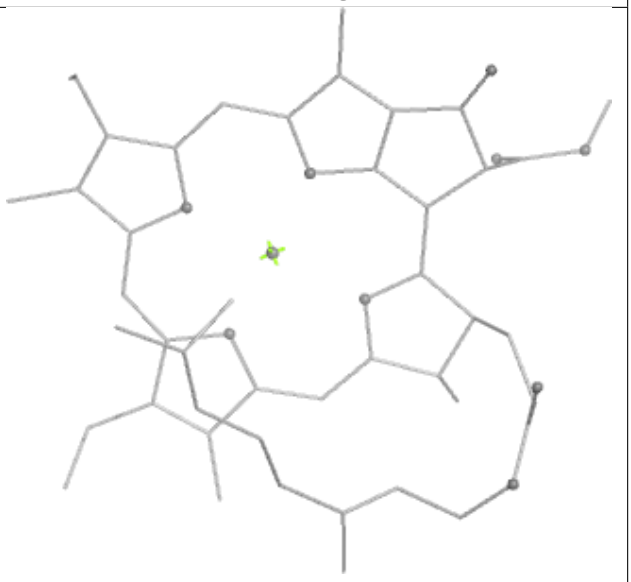
Bond lengths



Bond angles



Torsions

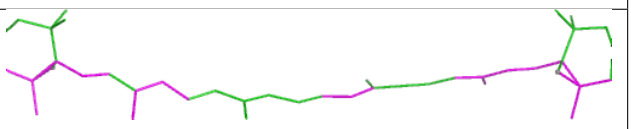


Rings

Ligand XAT N 622



Bond lengths



Bond angles

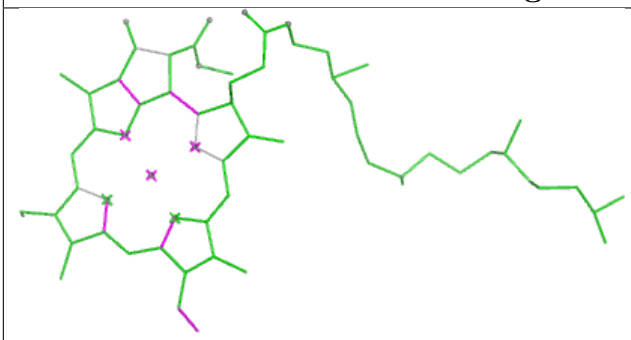


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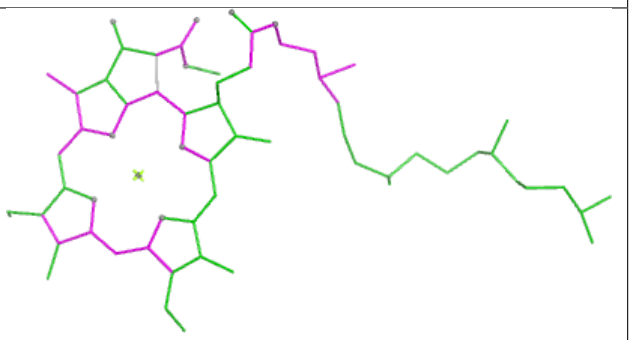


Rings

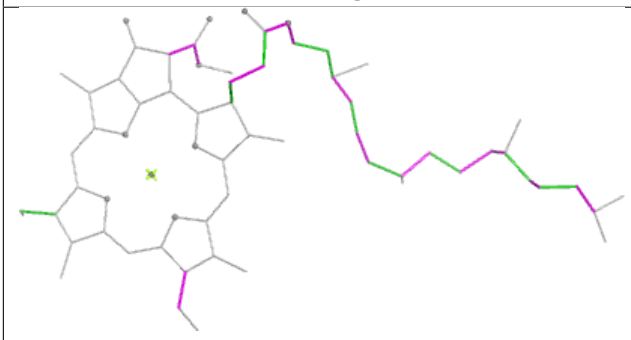
Ligand CLA B 617



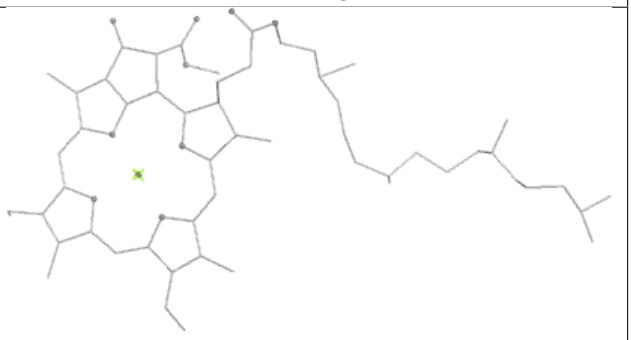
Bond lengths



Bond angles



Torsions

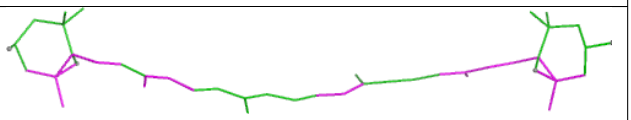


Rings

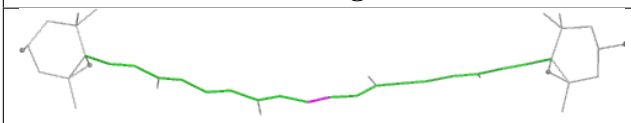
Ligand XAT G 622



Bond lengths



Bond angles

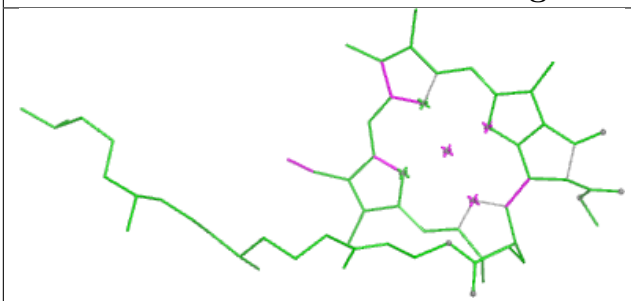


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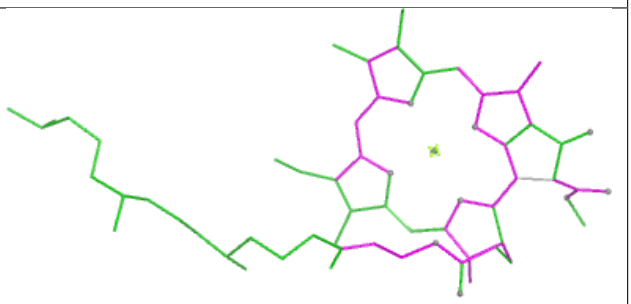


Rings

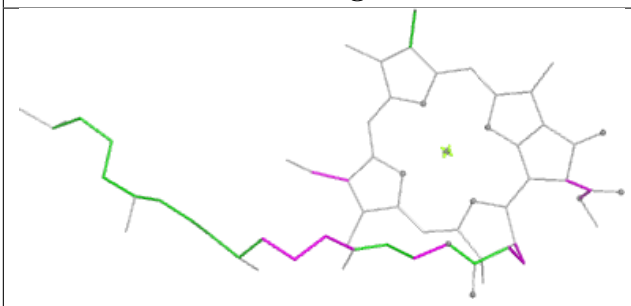
Ligand CLA c 501



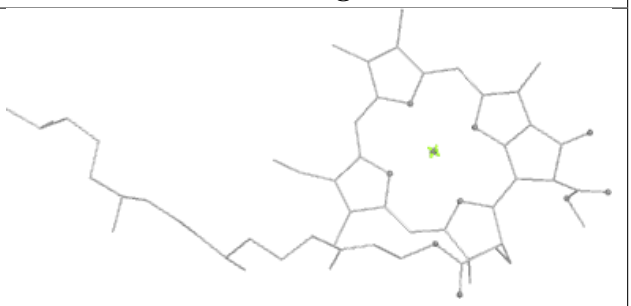
Bond lengths



Bond angles

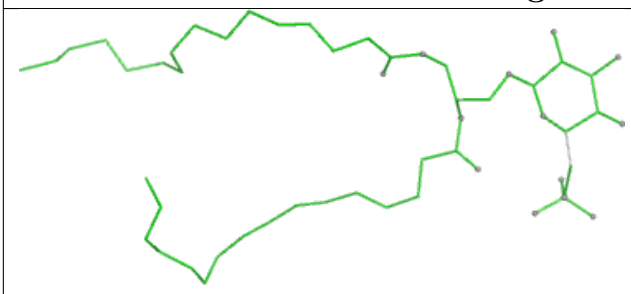


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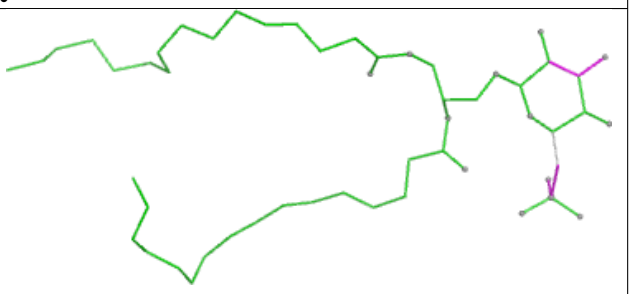


Rings

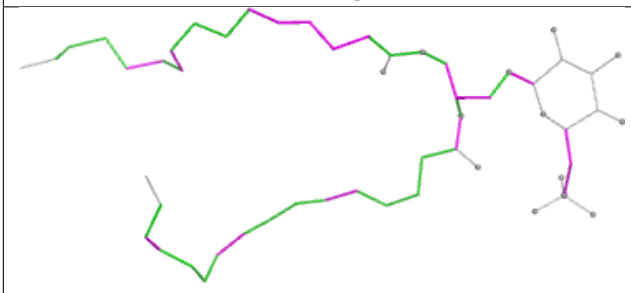
Ligand SQD b 621



Bond lengths



Bond angles

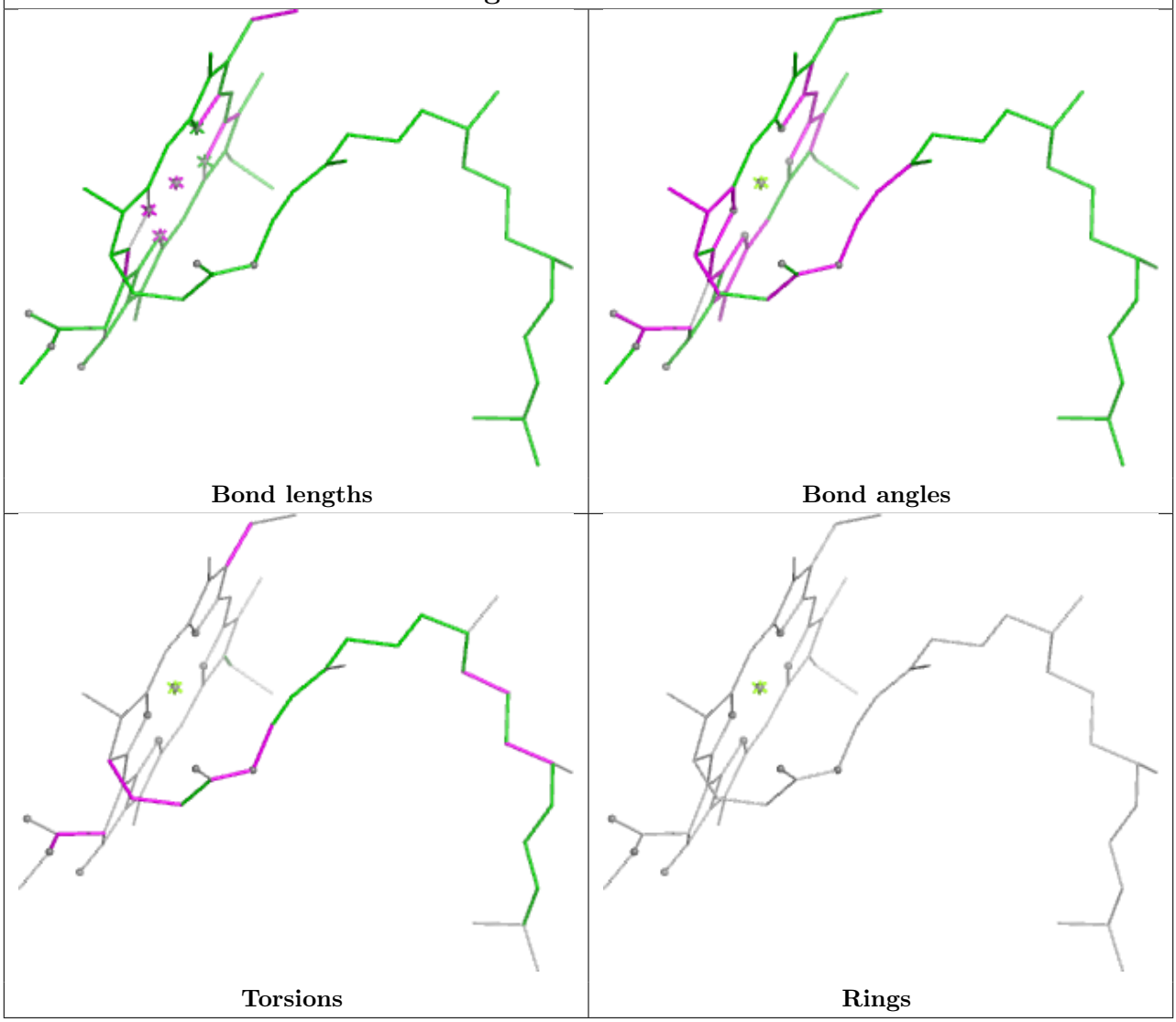


Torsions

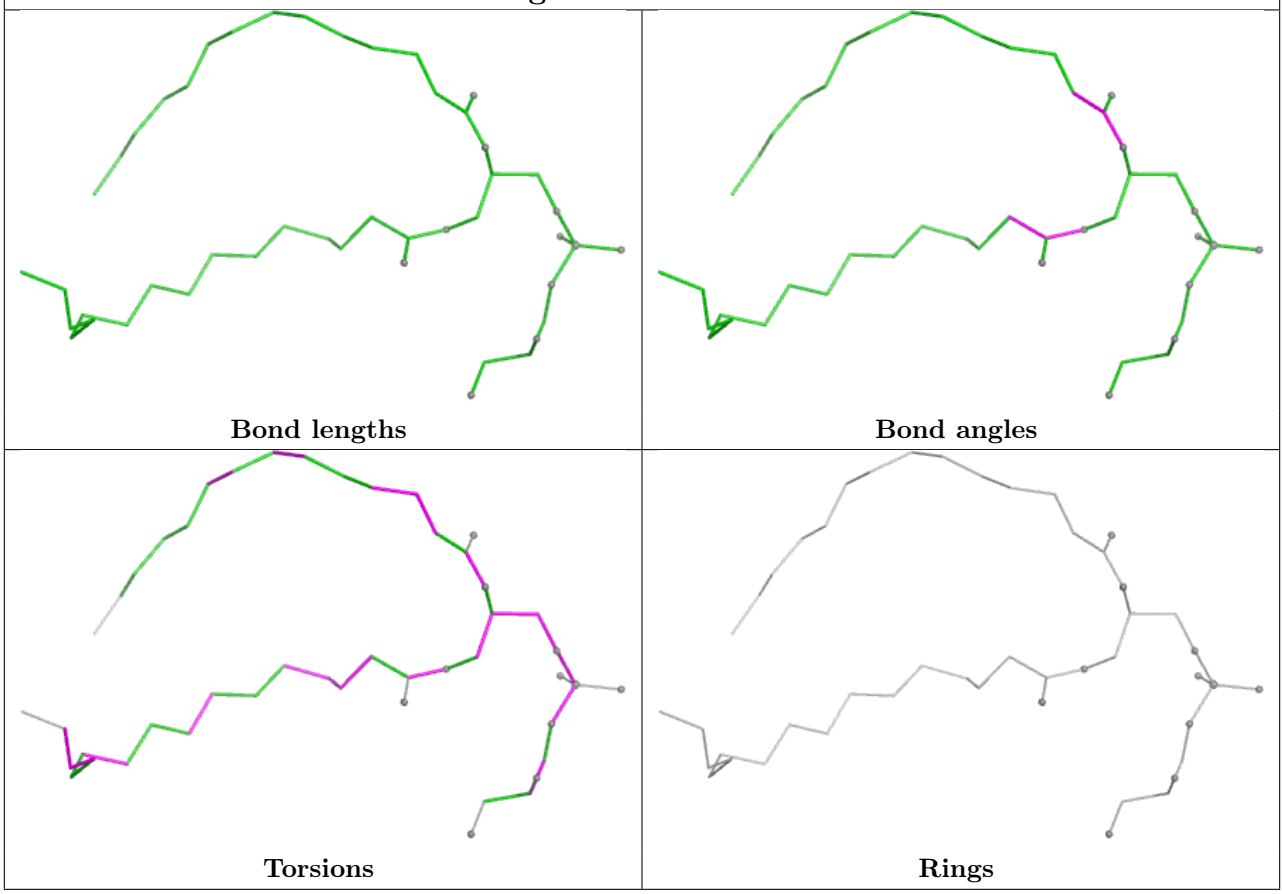


Rings

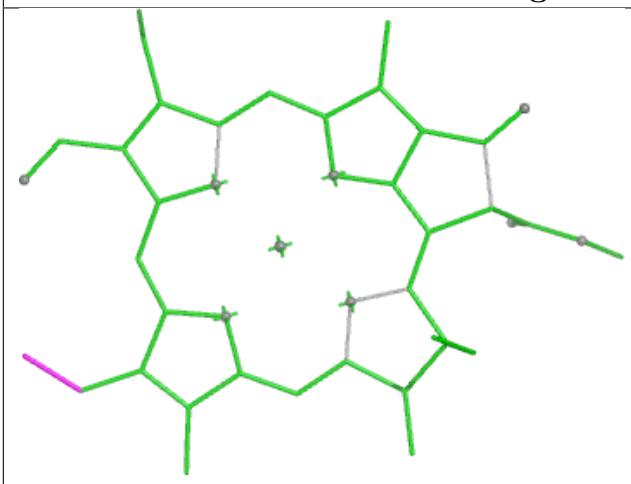
Ligand CLA S 610



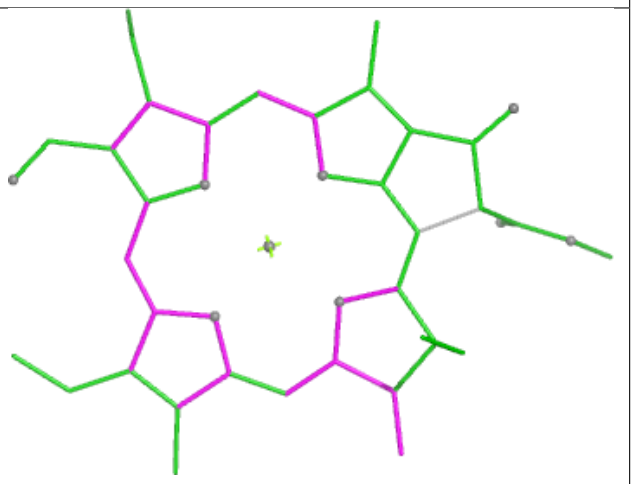
Ligand LHG c 625



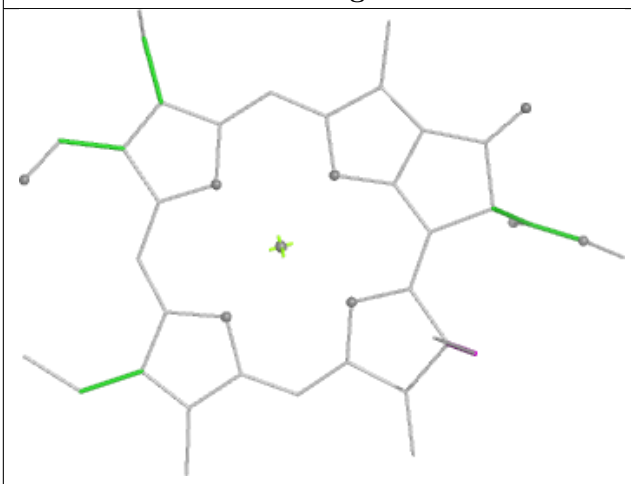
Ligand CHL s 607



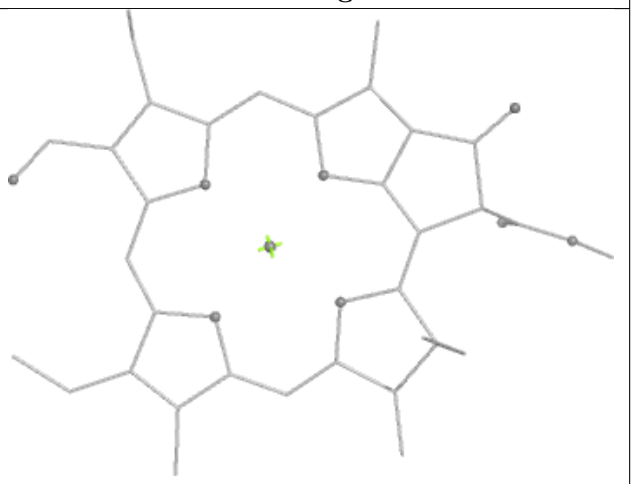
Bond lengths



Bond angles

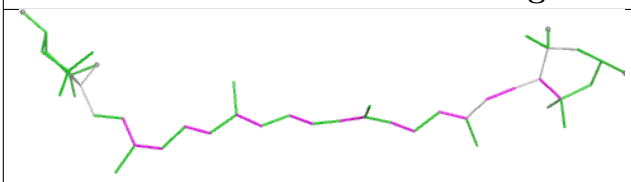


Torsions

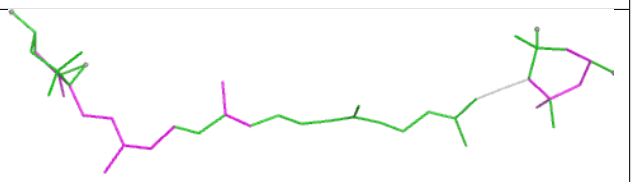


Rings

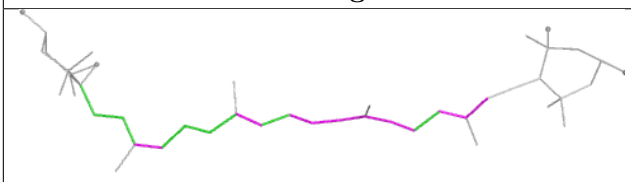
Ligand NEX s 623



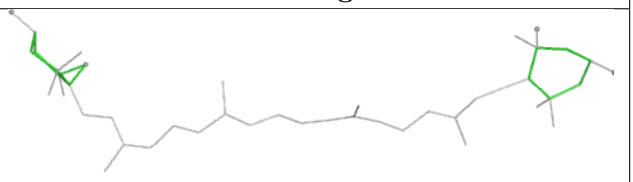
Bond lengths



Bond angles

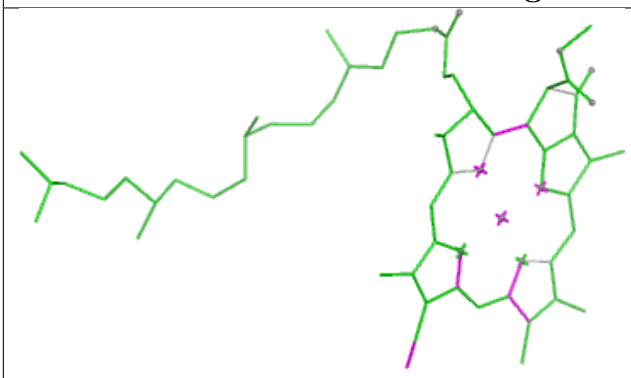


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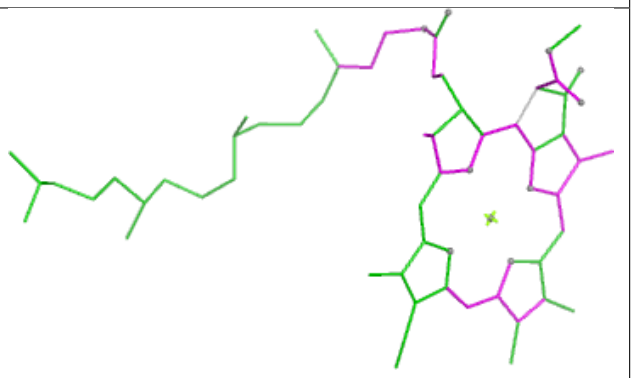


Rings

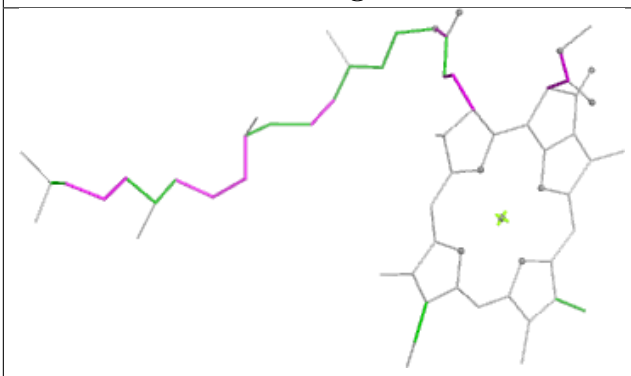
Ligand CLA C 511



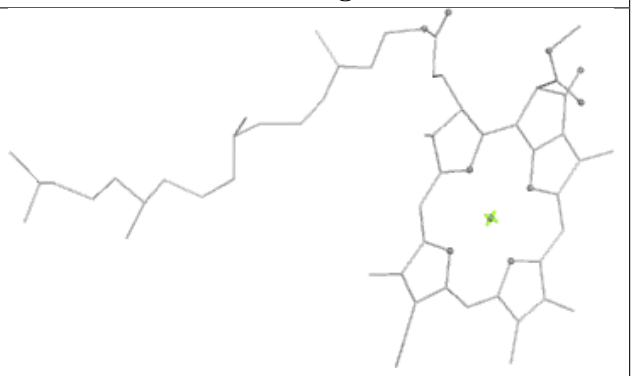
Bond lengths



Bond angles

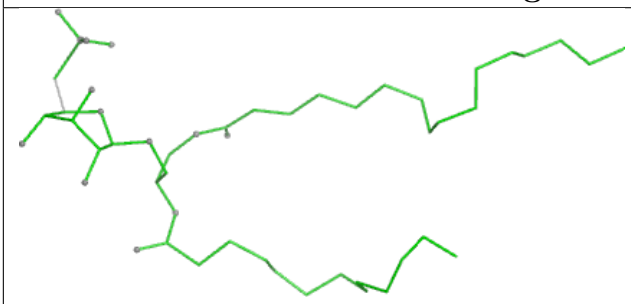


Torsions

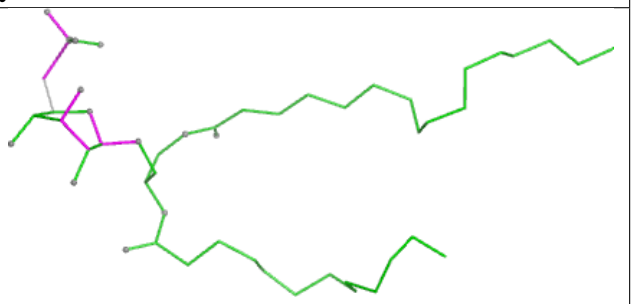


Rings

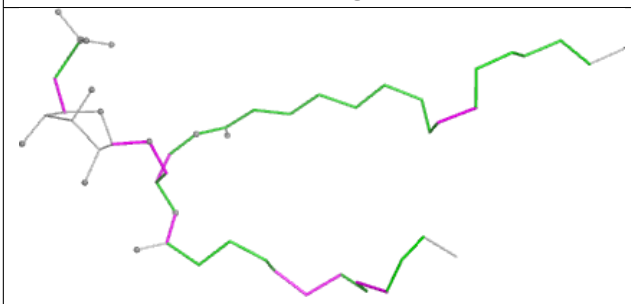
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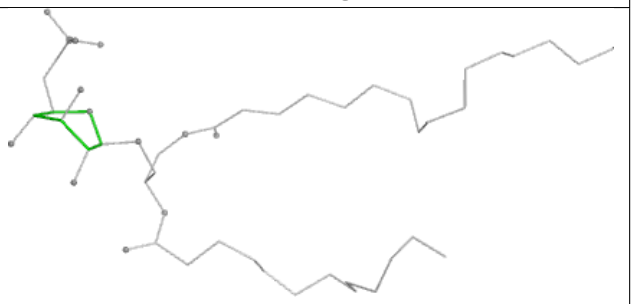
Bond lengths



Bond angles

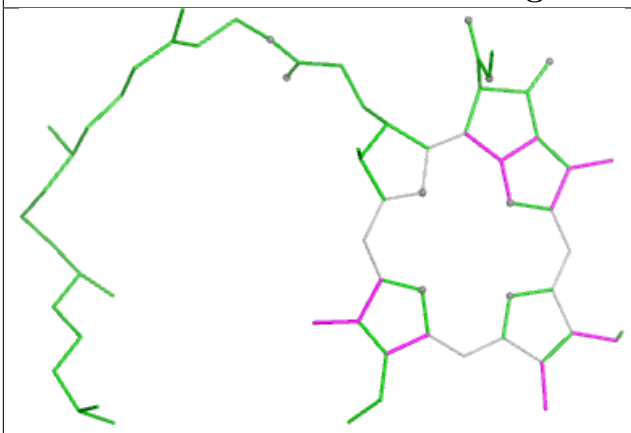


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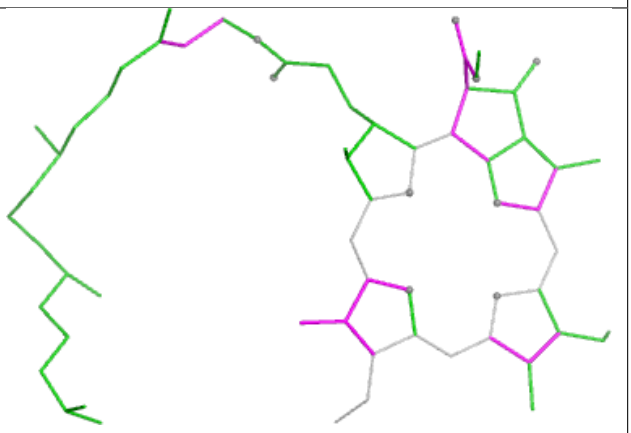


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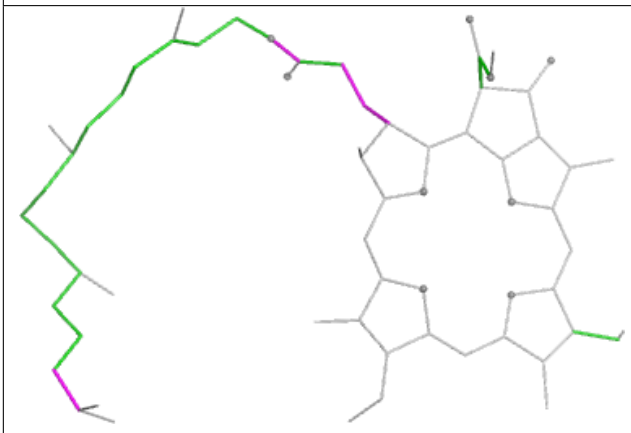
Ligand PHO a 408



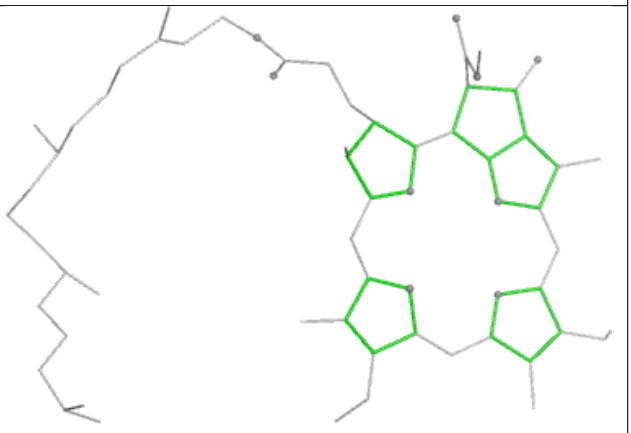
Bond lengths



Bond angles

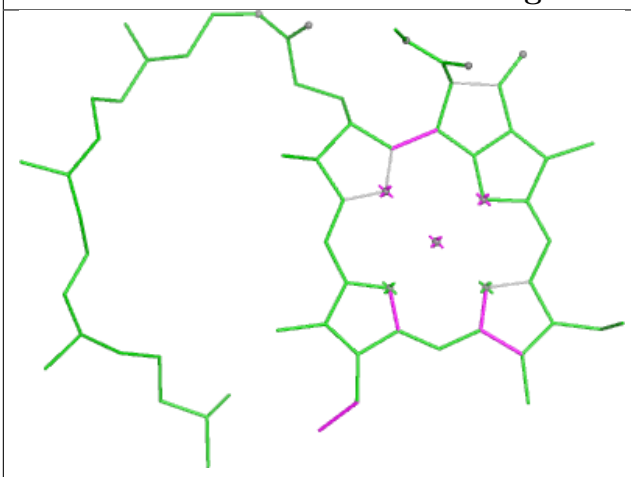


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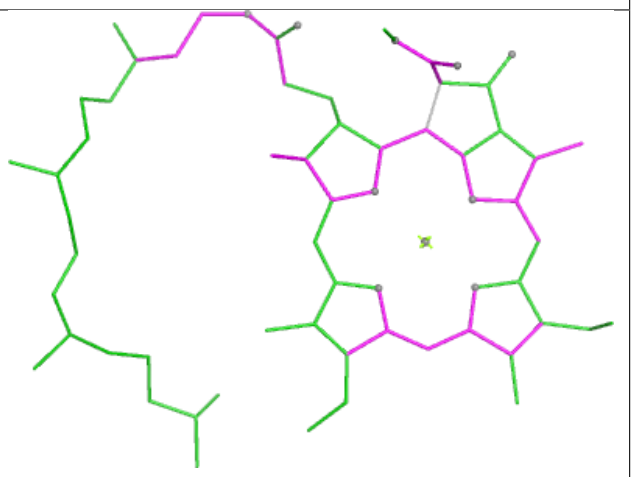


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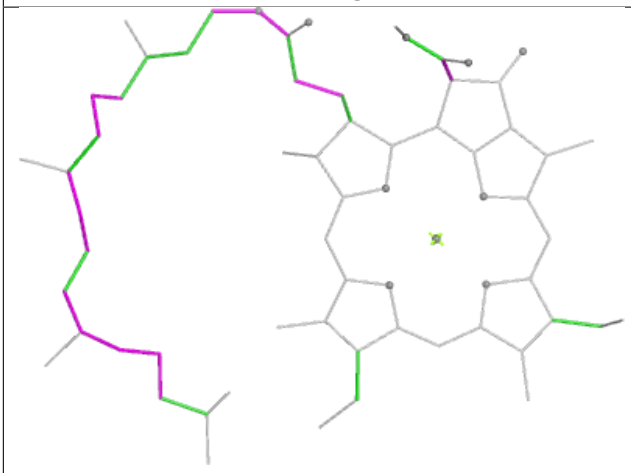
Ligand CLA C 512



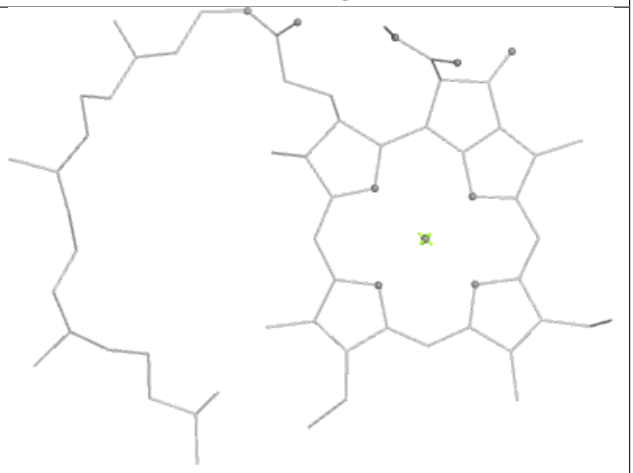
Bond lengths



Bond angles

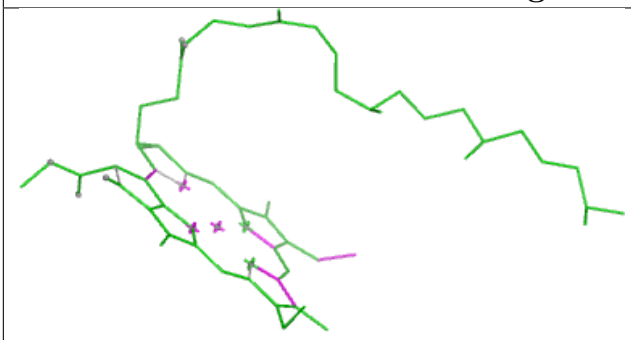


Torsions



Rings

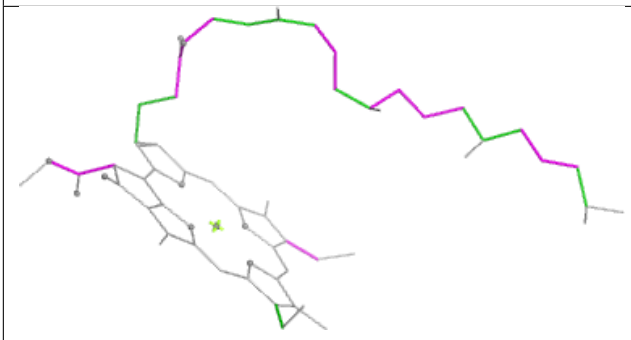
Ligand CLA y 614



Bond lengths



Bond angles



Torsions

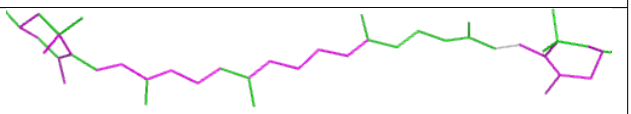


Rings

Ligand LUT N 621



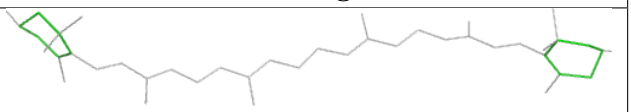
Bond lengths



Bond angles

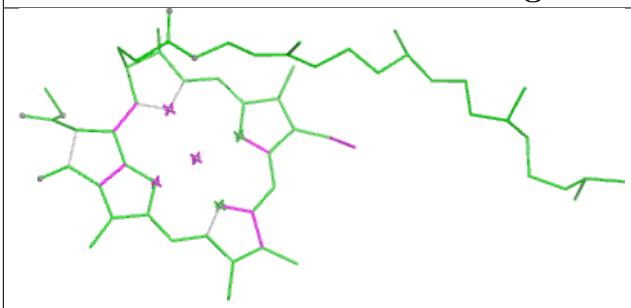


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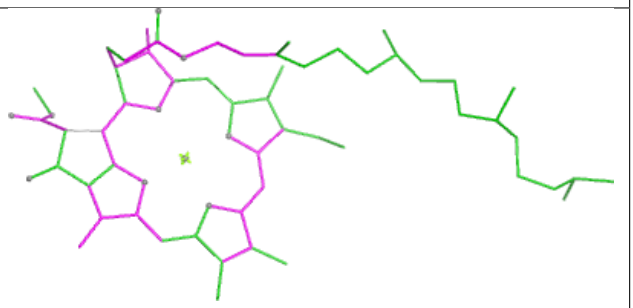


Rings

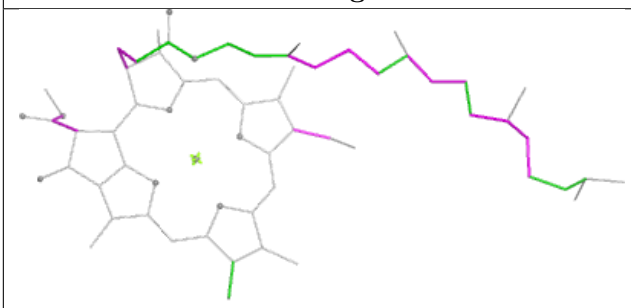
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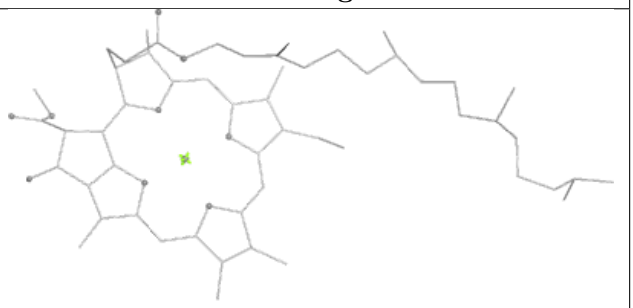
Bond lengths



Bond angles

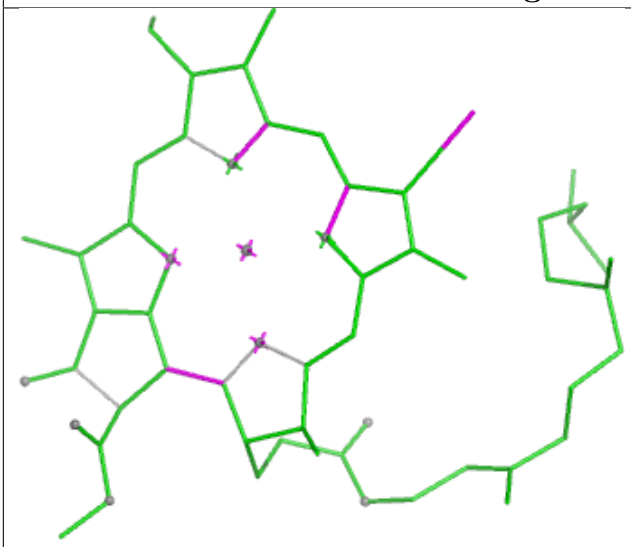


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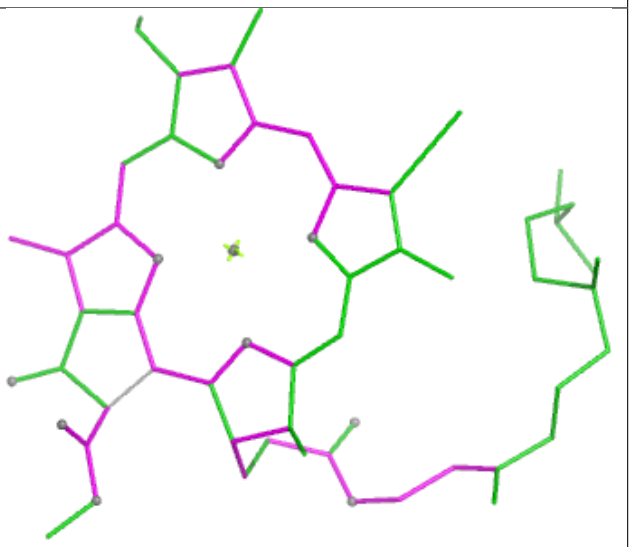


Rings

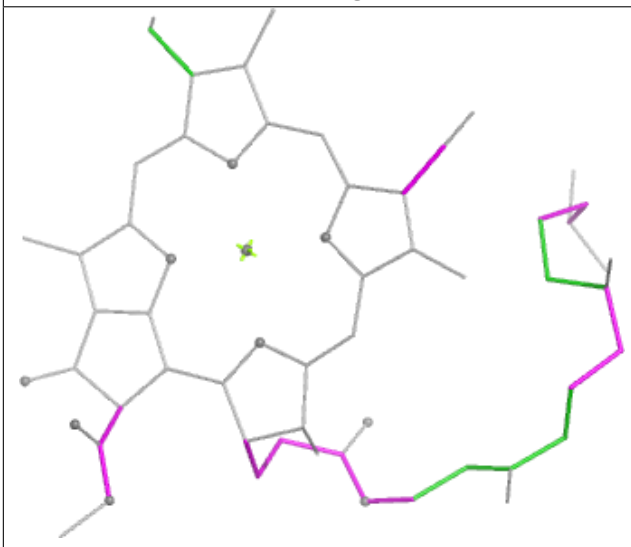
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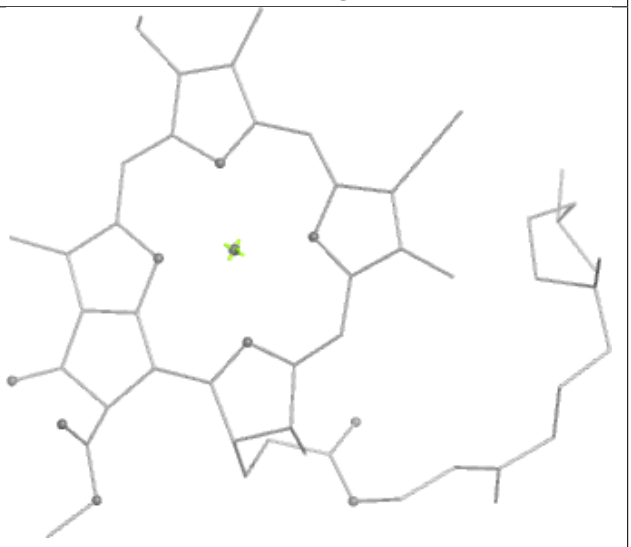
Bond lengths



Bond angles

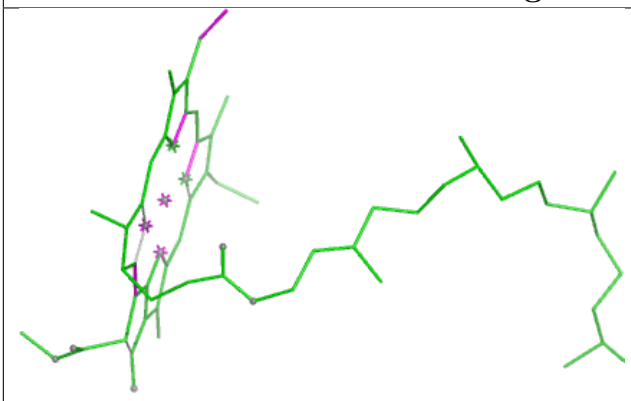


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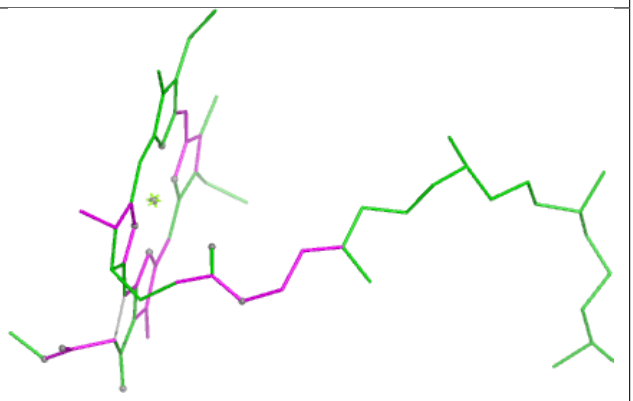


Rings

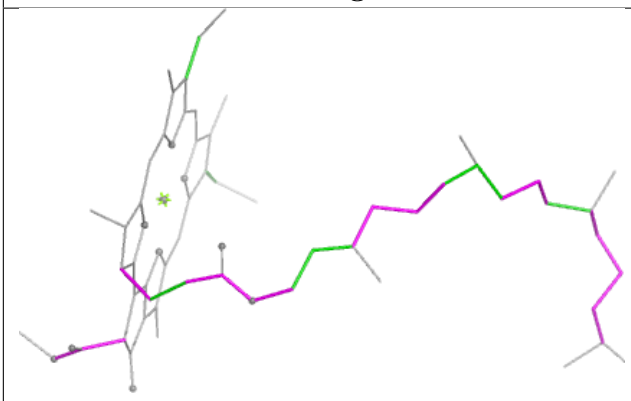
Ligand CLA B 608



Bond lengths



Bond angles

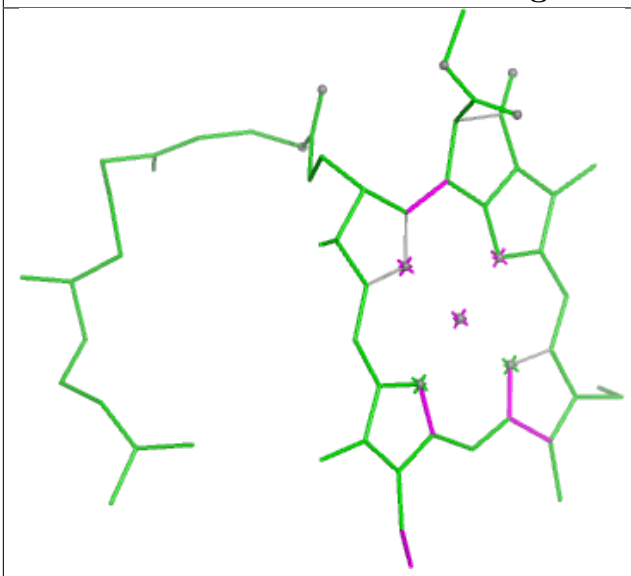


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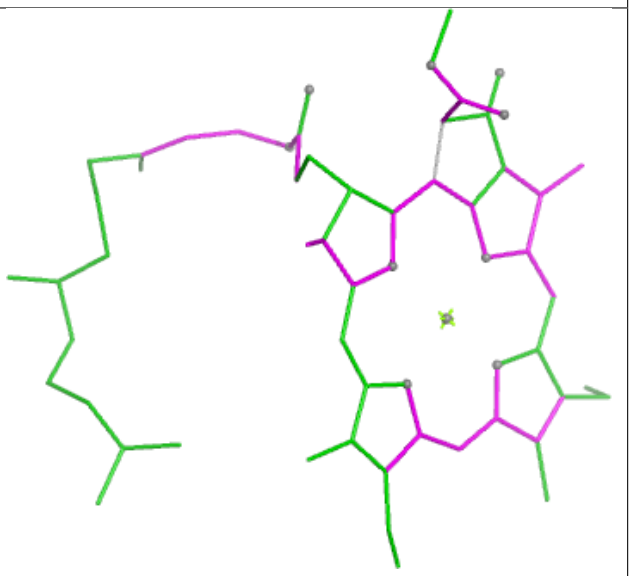


Rings

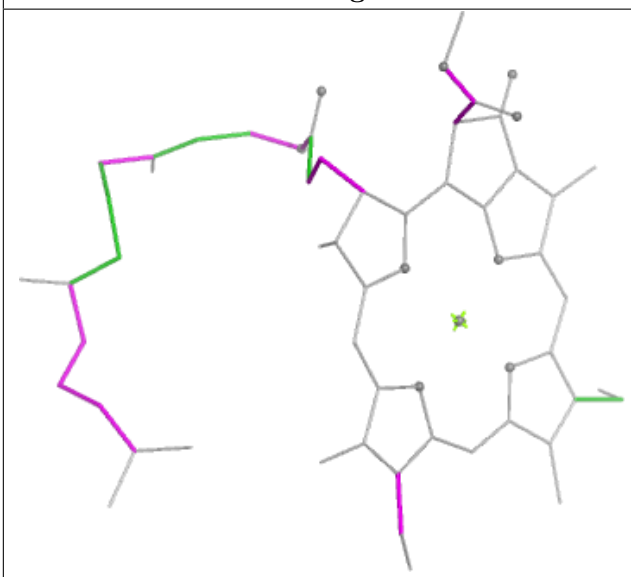
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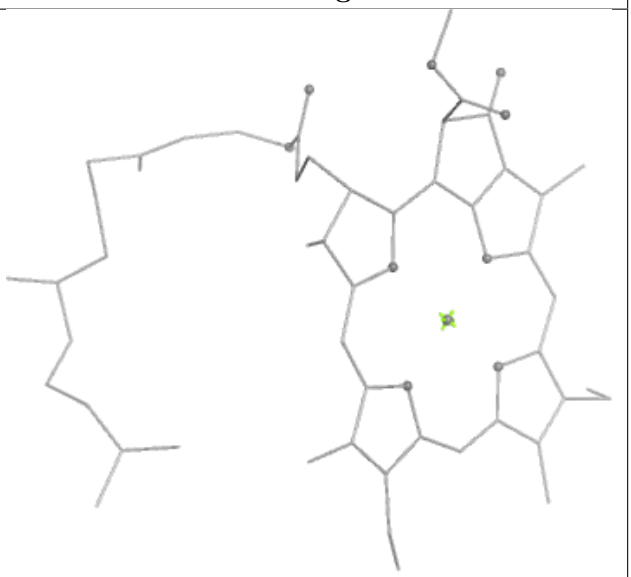
Bond lengths



Bond angles

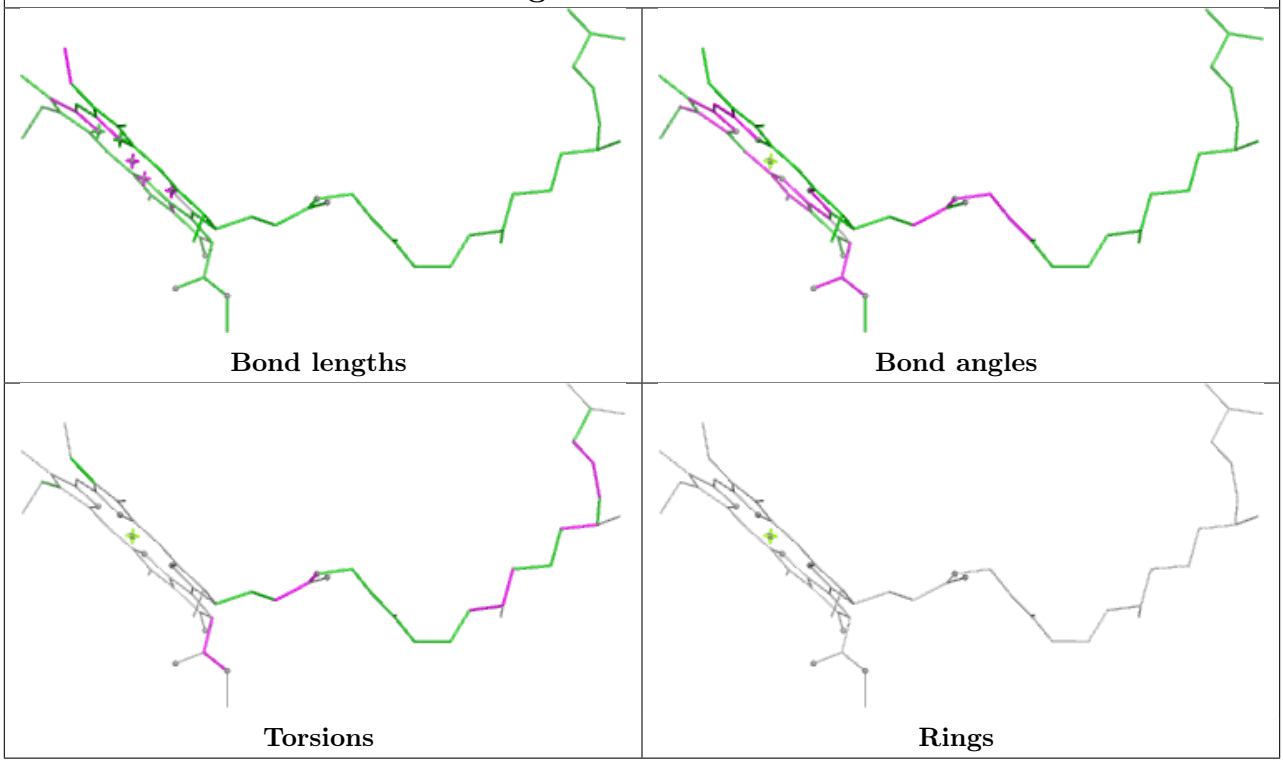


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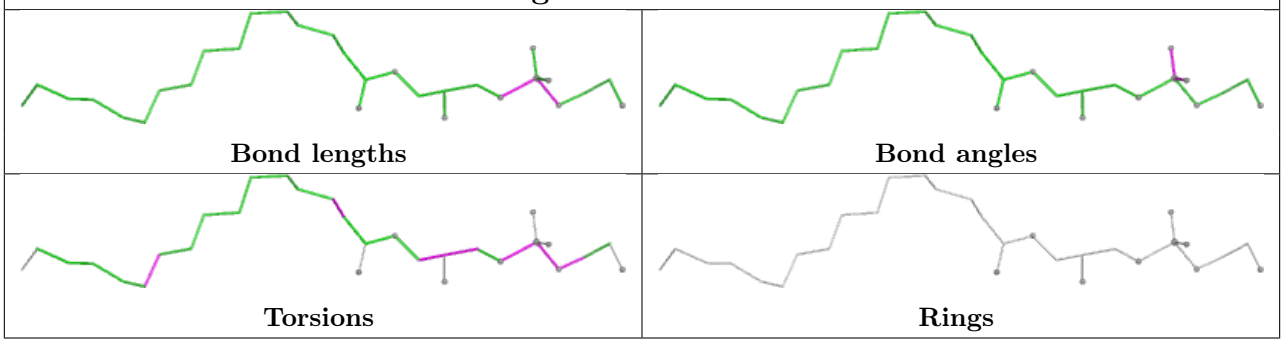


Rings

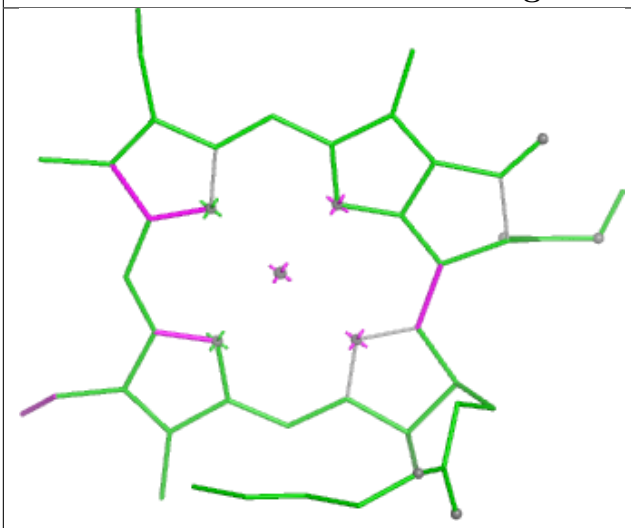
Ligand CLA d 402



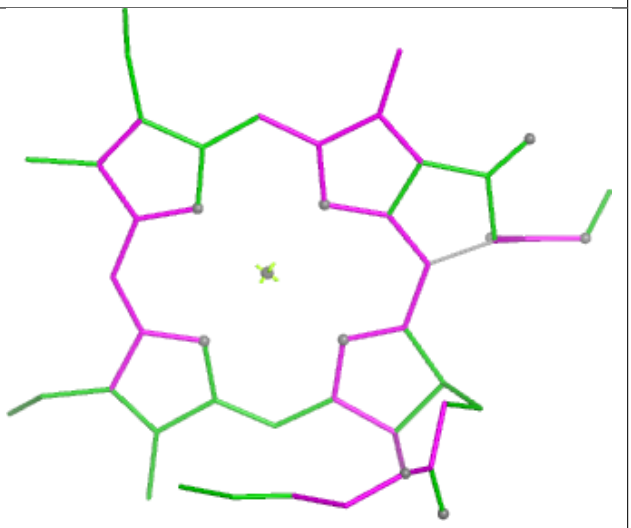
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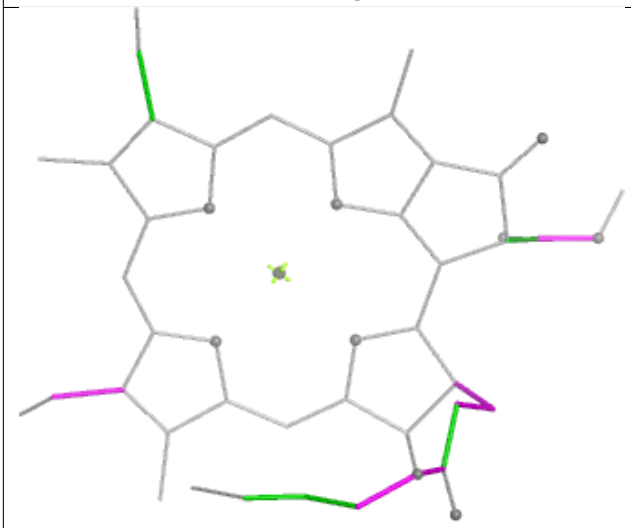
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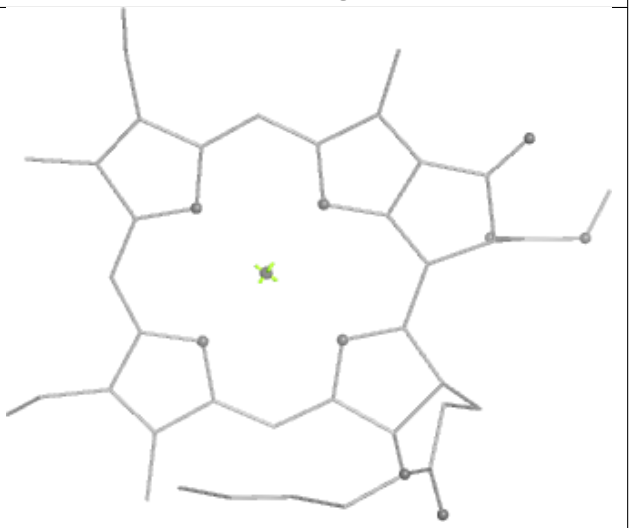
Bond lengths



Bond angles

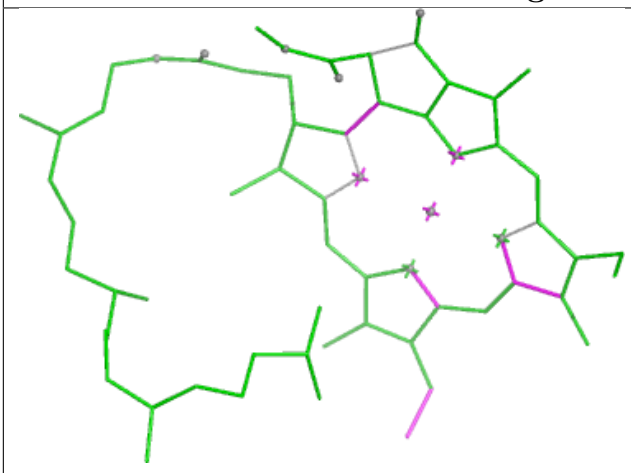


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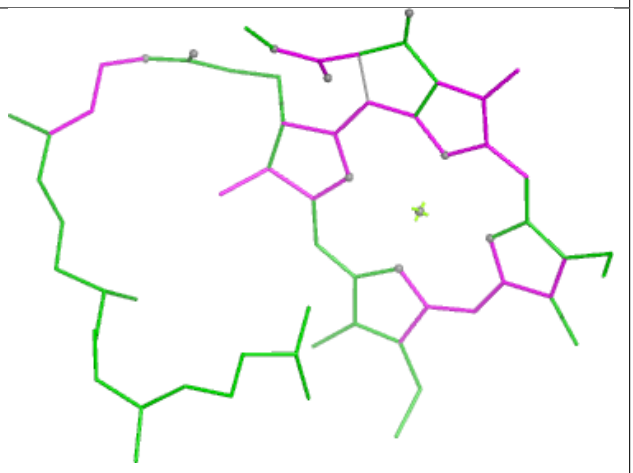


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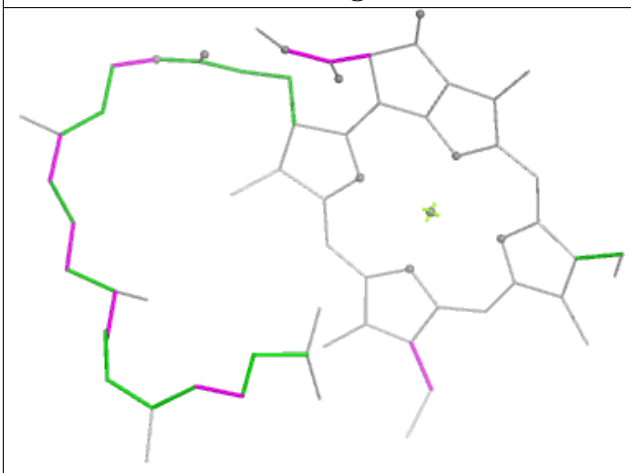
Ligand CLA b 616



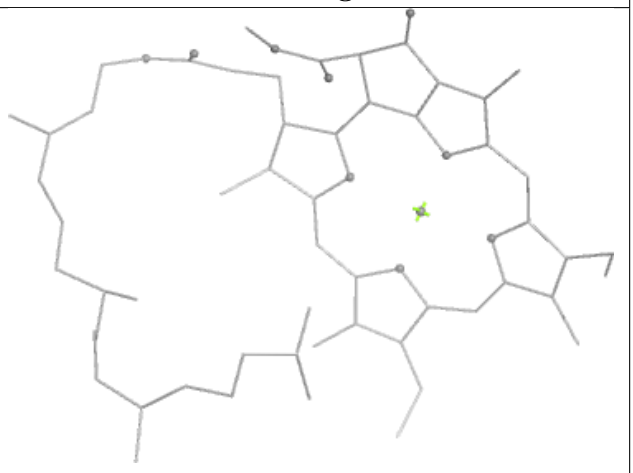
Bond lengths



Bond angles

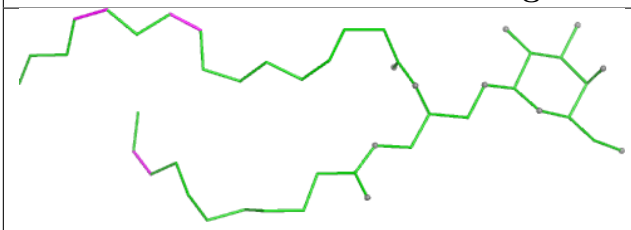


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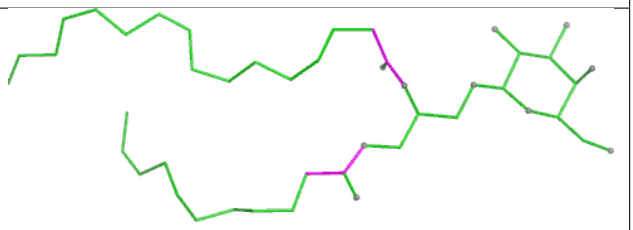


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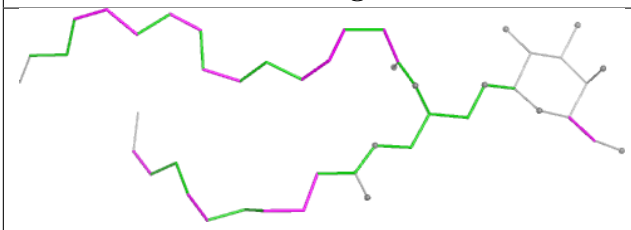
Ligand LMG d 411



Bond lengths



Bond angles

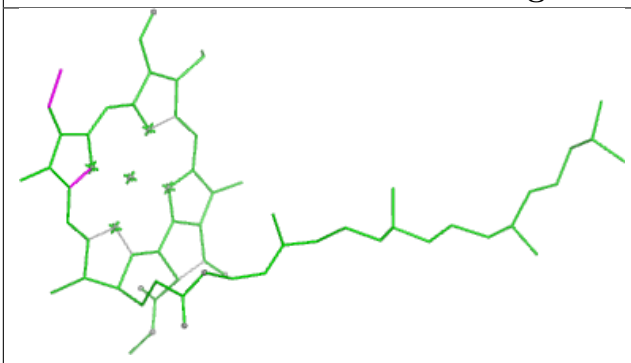


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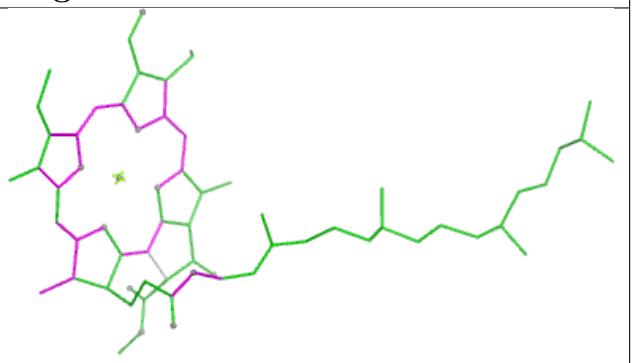


Rings

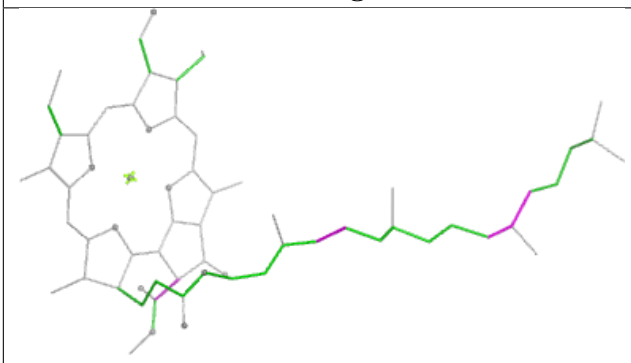
Ligand CHL g 609



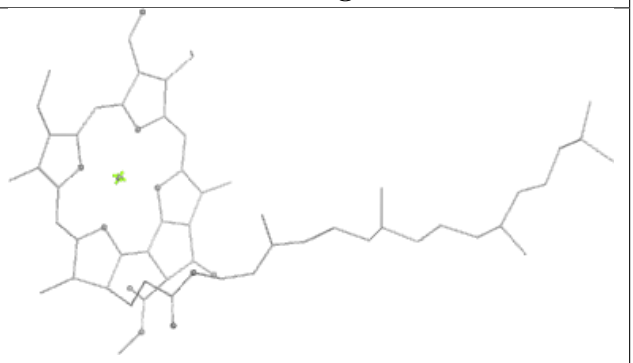
Bond lengths



Bond angles

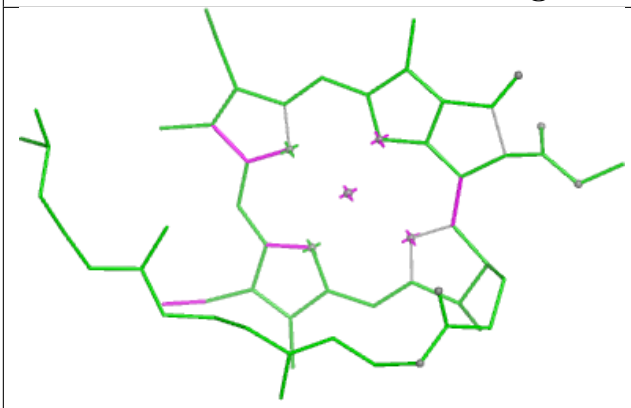


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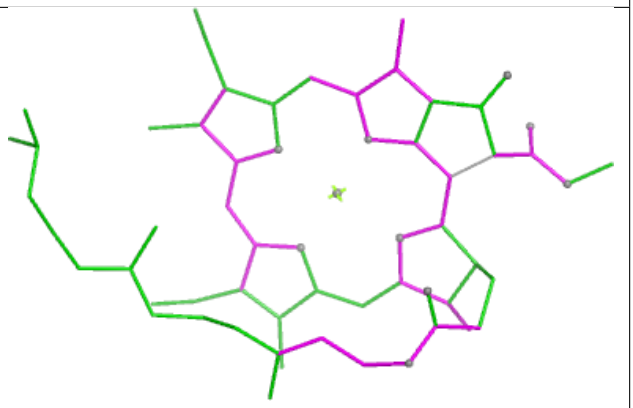


Rings

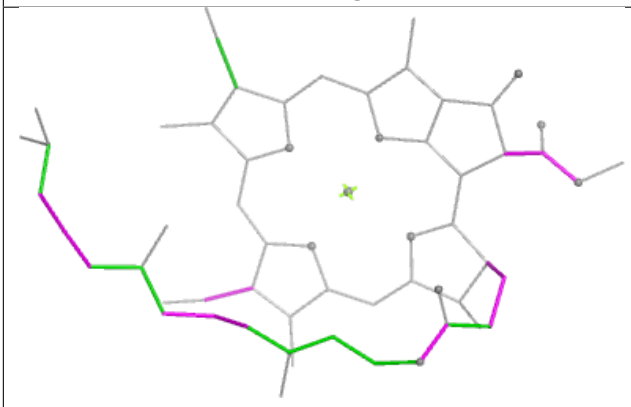
Ligand CLA r 608



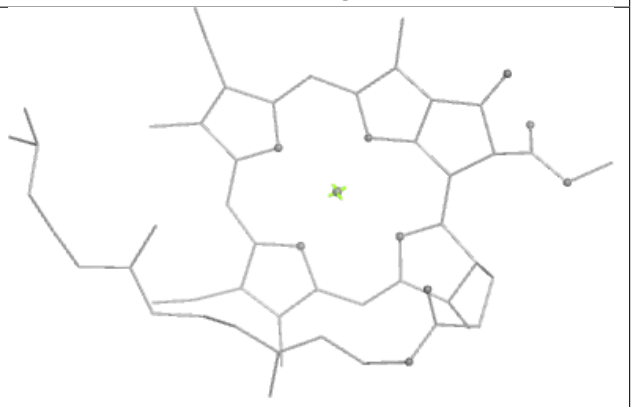
Bond lengths



Bond angles

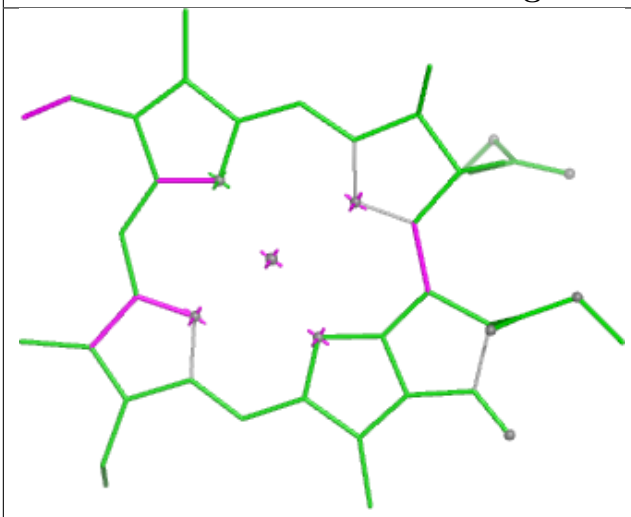


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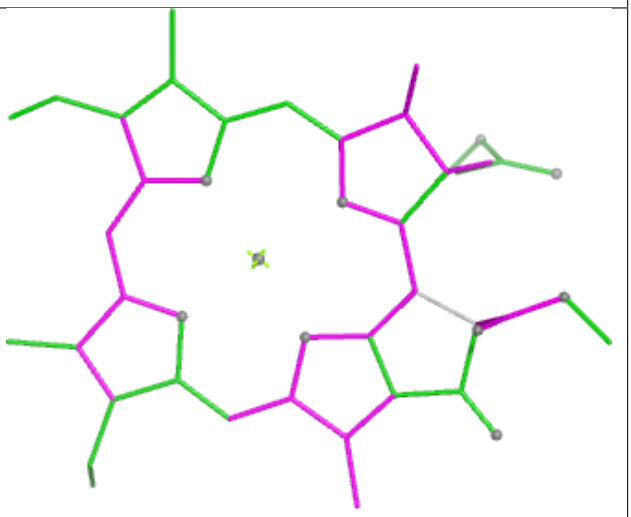


Rings

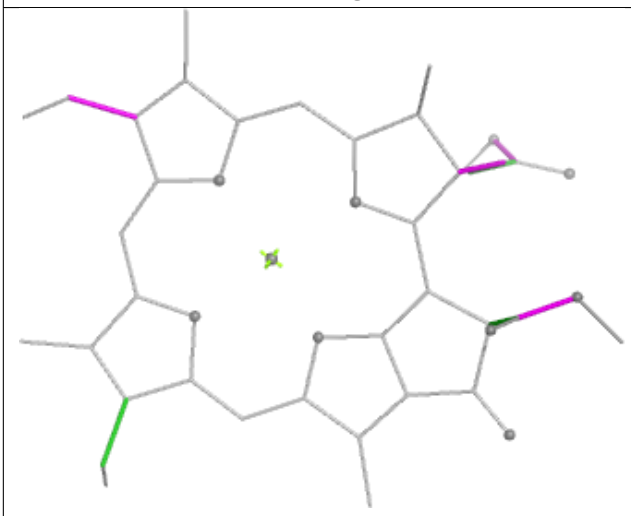
Ligand CLA R 611



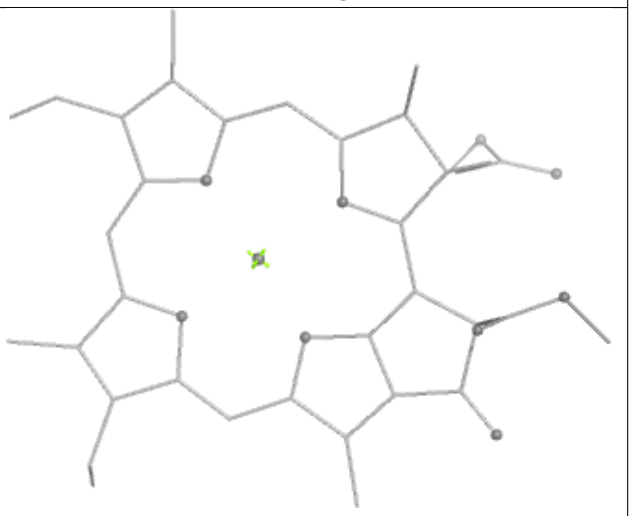
Bond lengths



Bond angles

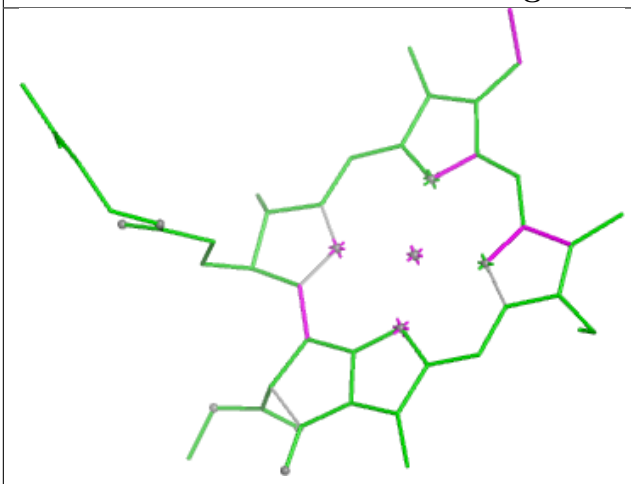


Torsions

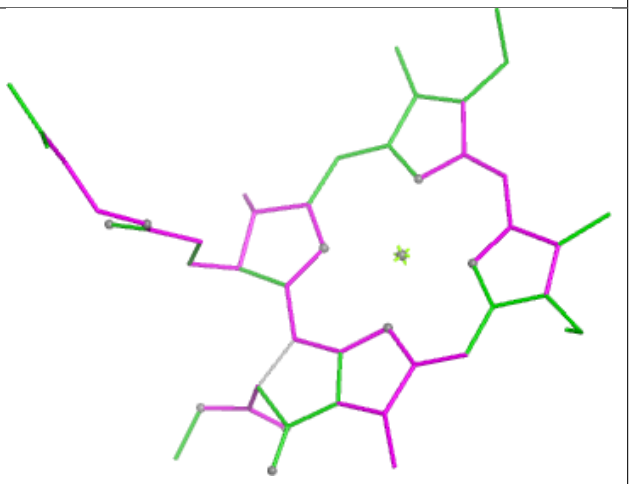


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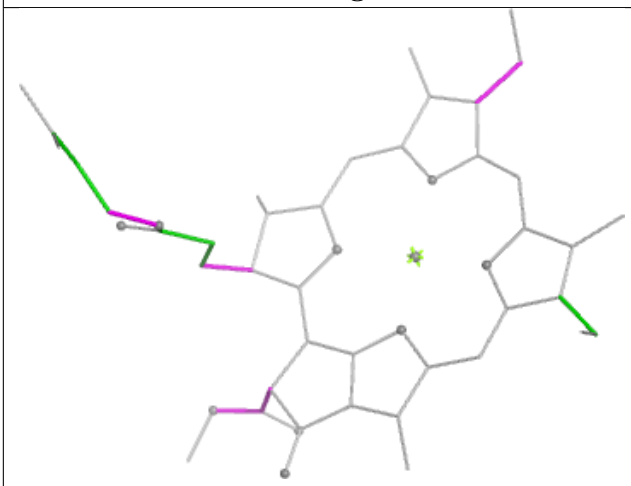
Ligand CLA Y 608



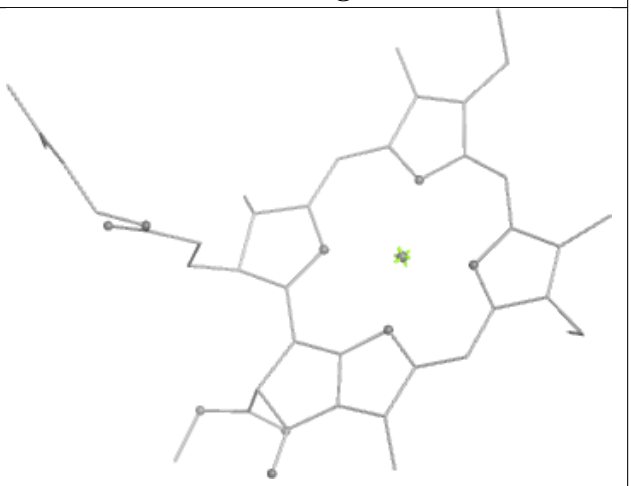
Bond lengths



Bond angles

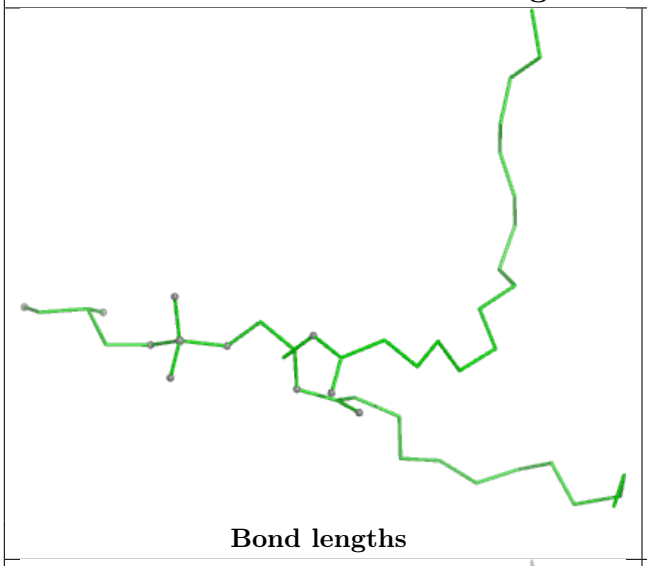


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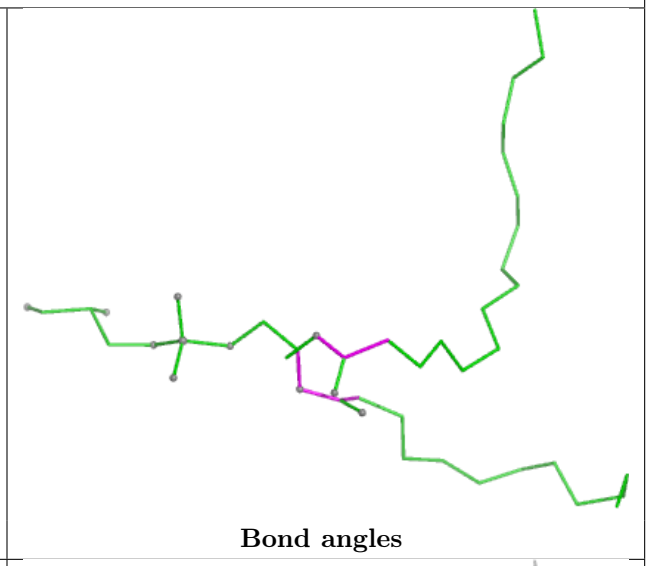


Rings

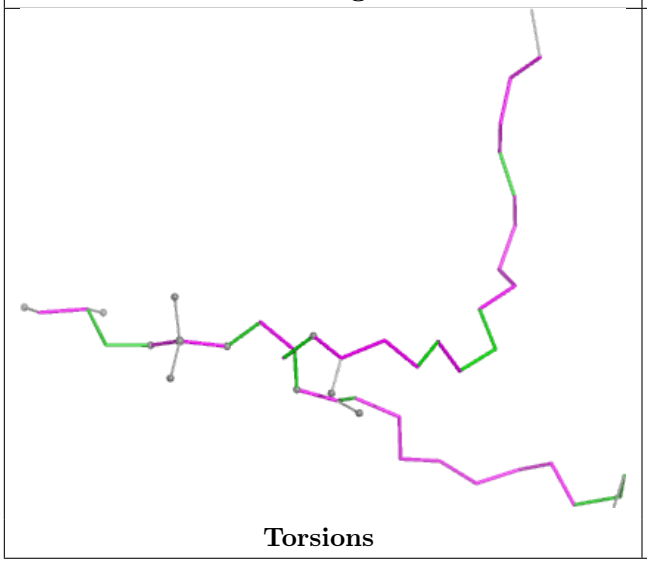
Ligand LHG s 624



Bond lengths



Bond angles

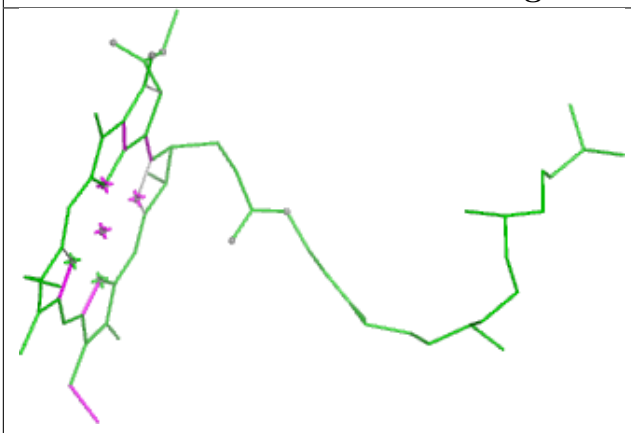


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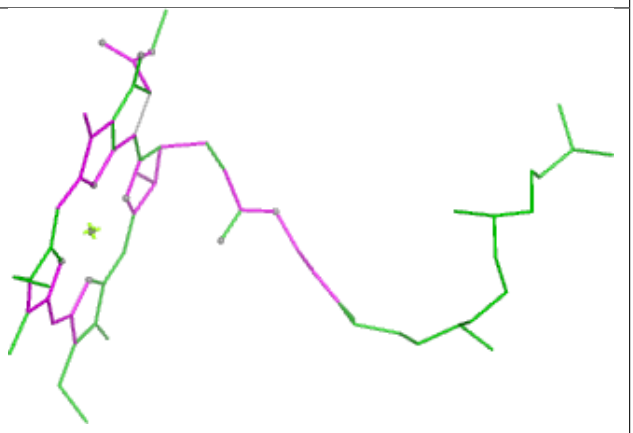


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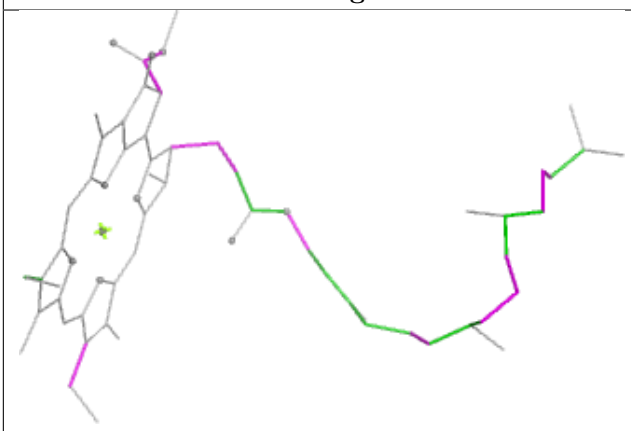
Ligand CLA B 607



Bond lengths



Bond angles

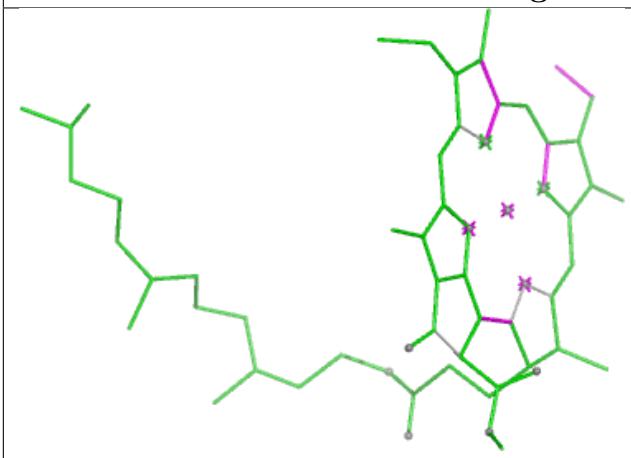


Torsions

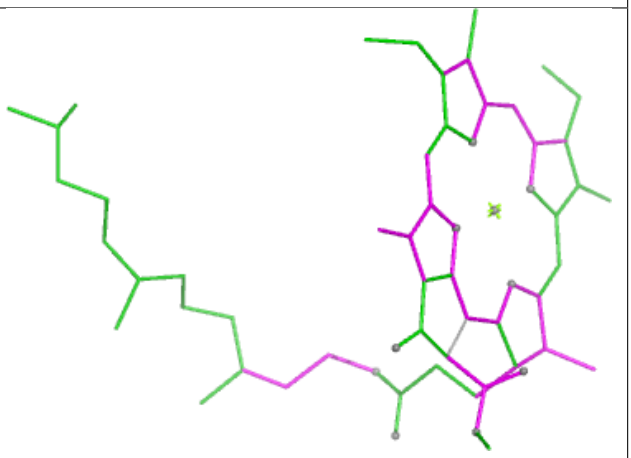


Rings

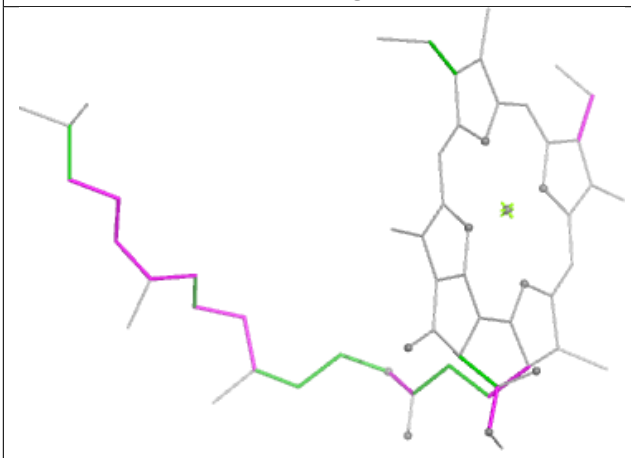
Ligand CLA s 609



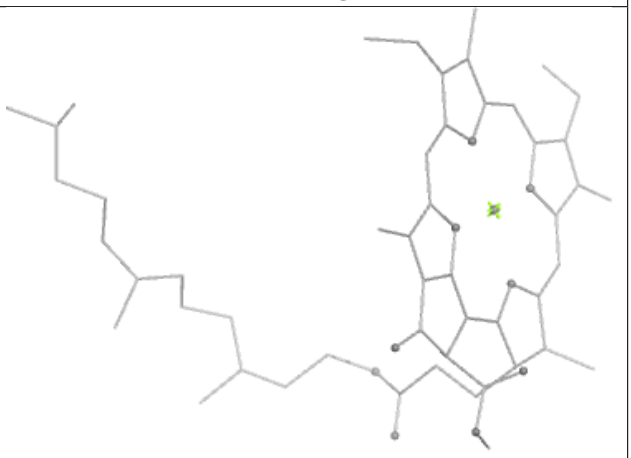
Bond lengths



Bond angles

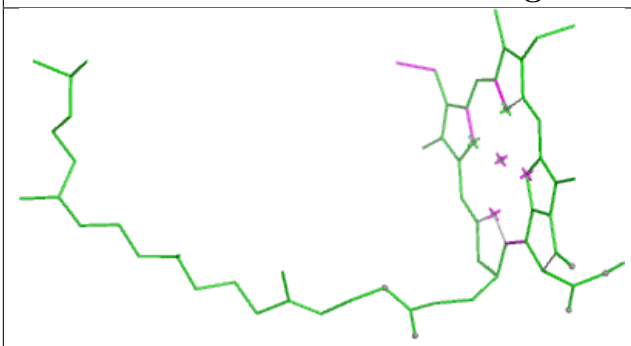


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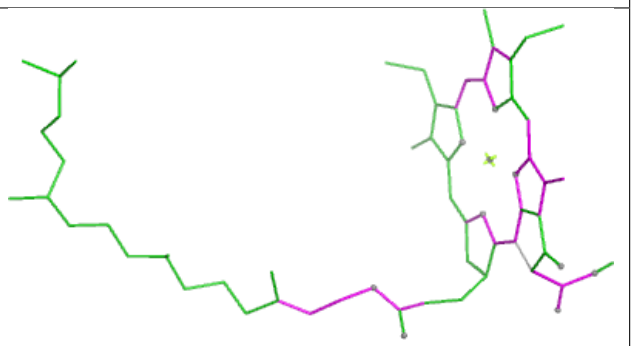


Rings

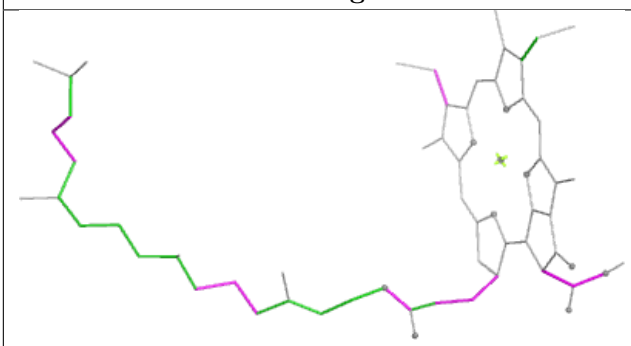
Ligand CLA B 610



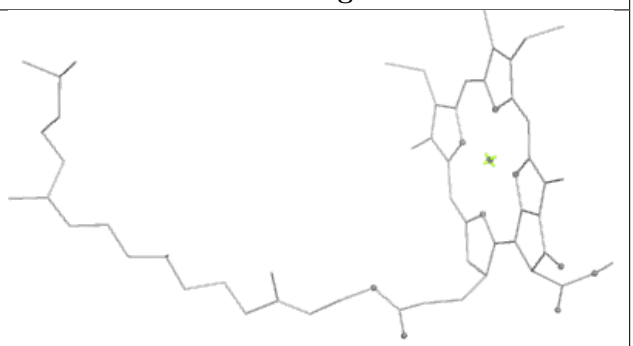
Bond lengths



Bond angles

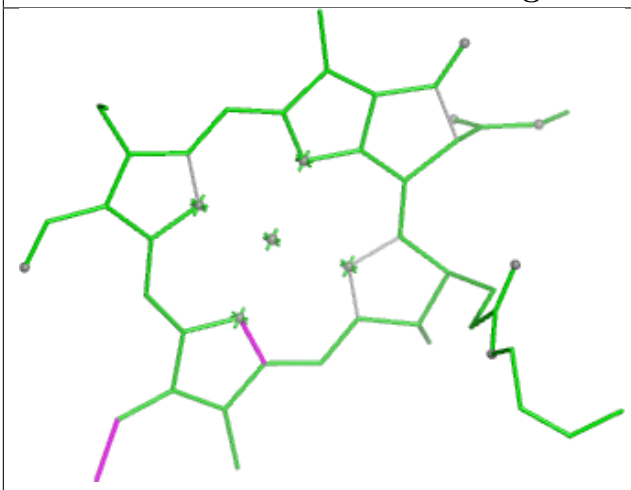


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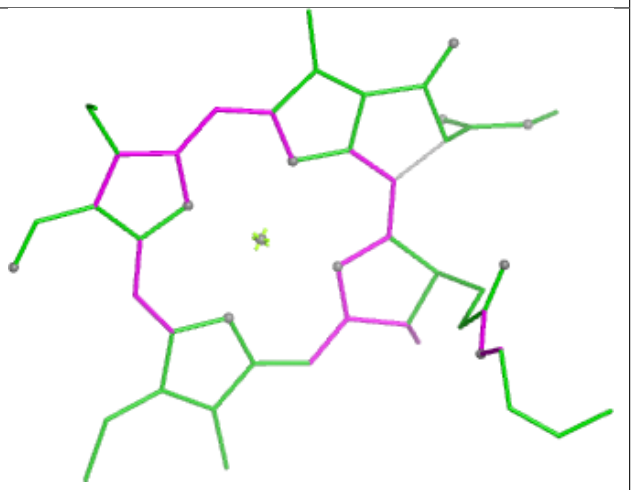


Rings

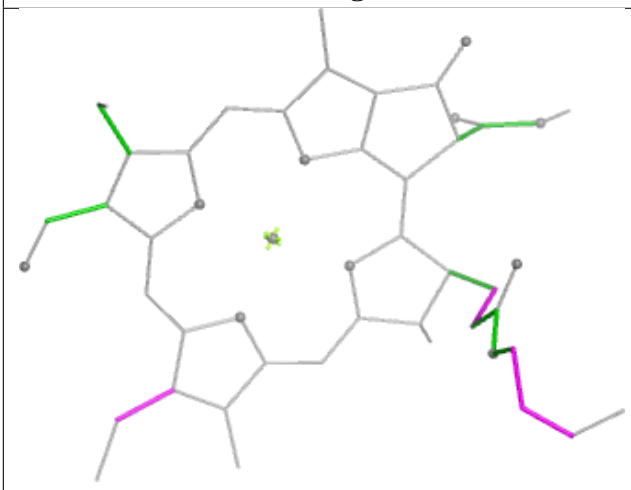
Ligand CHL N 608



Bond lengths



Bond angles

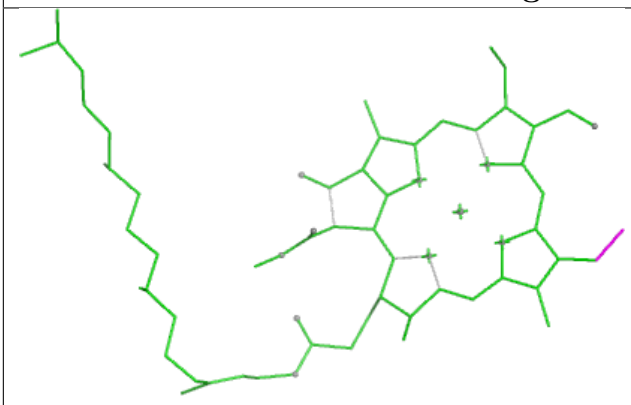


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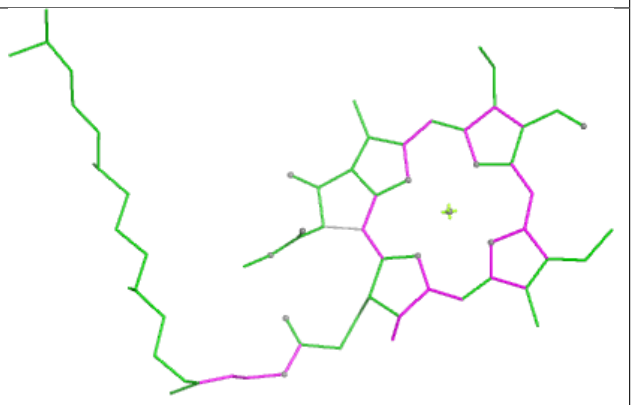


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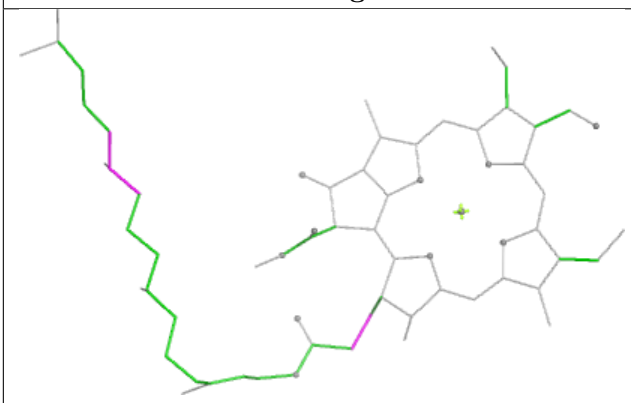
Ligand CHL N 606



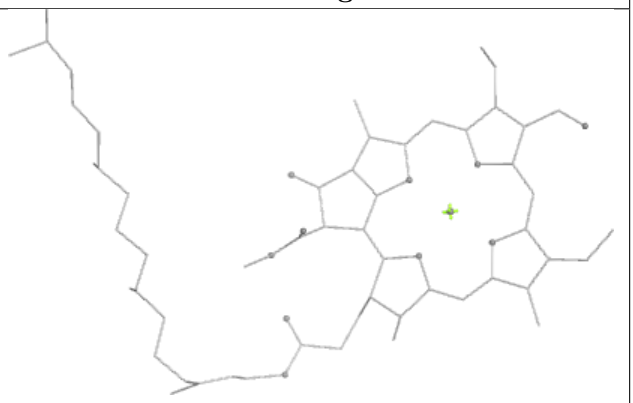
Bond lengths



Bond angles

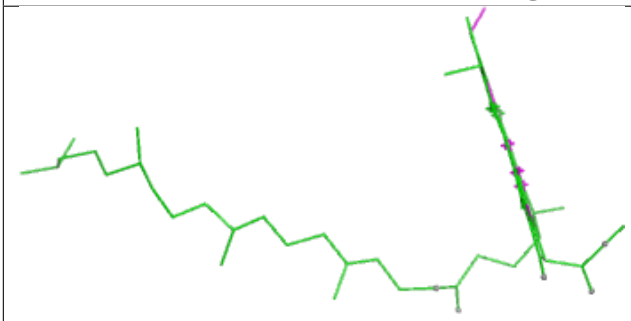


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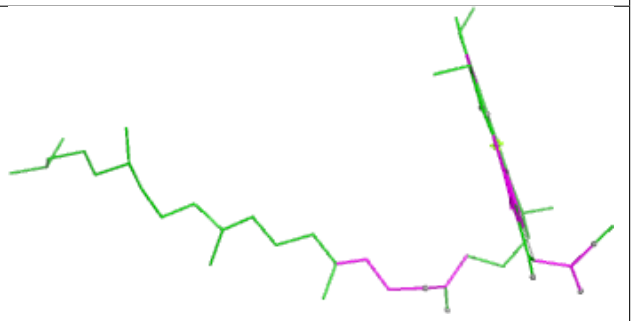


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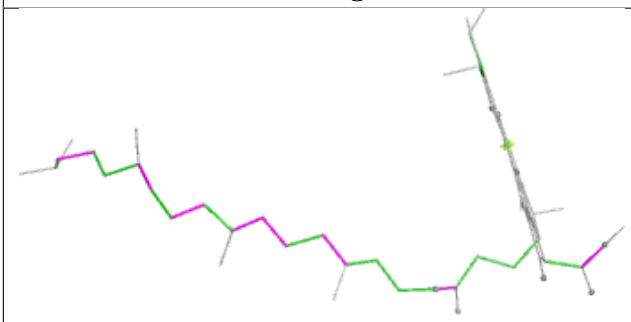
Ligand CLA B 606



Bond lengths



Bond angles

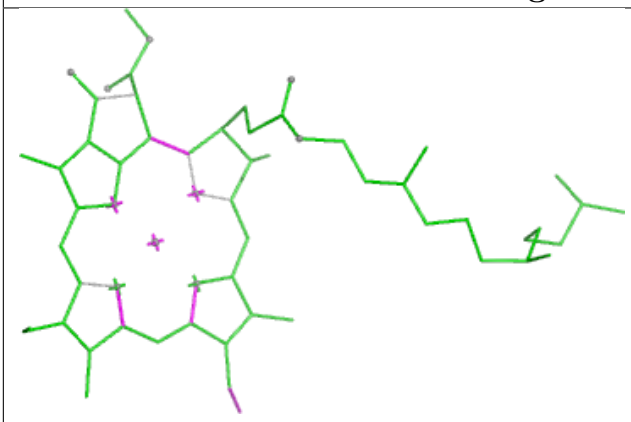


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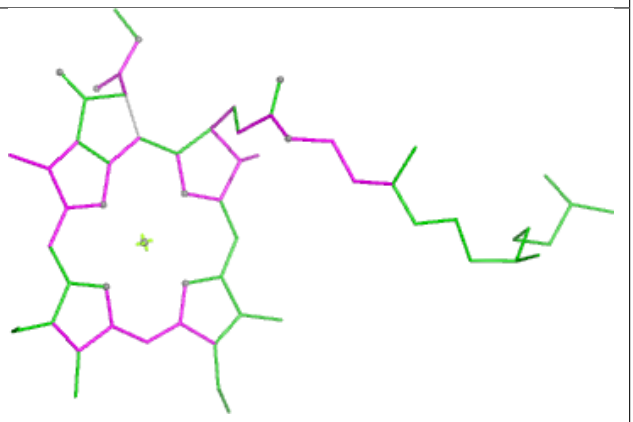


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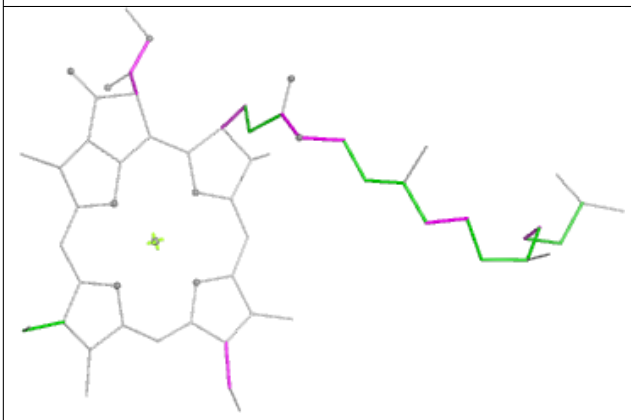
Ligand CLA a 410



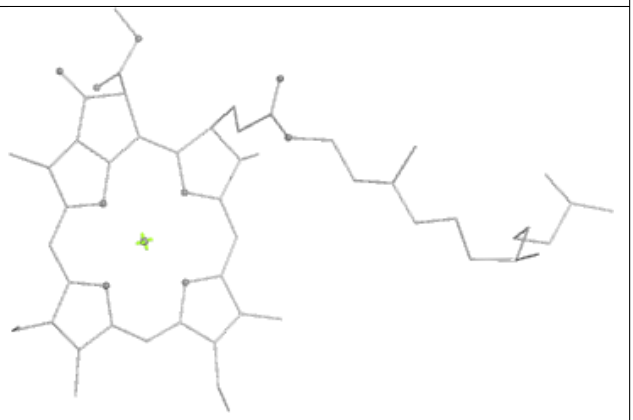
Bond lengths



Bond angles

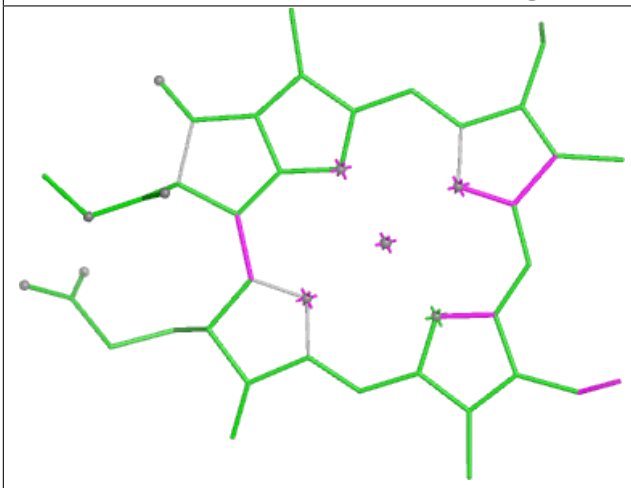


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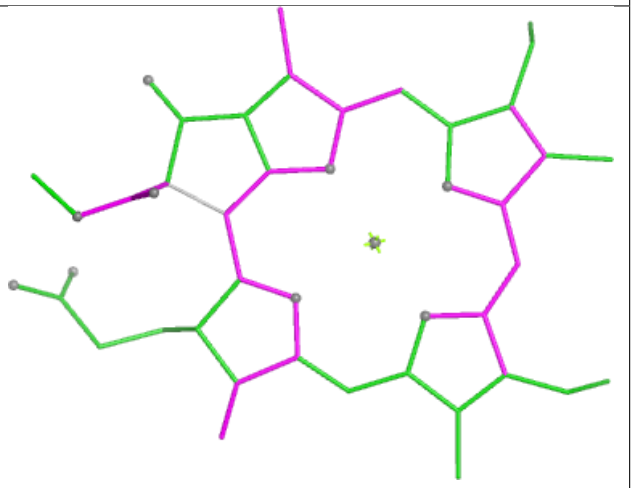


Rings

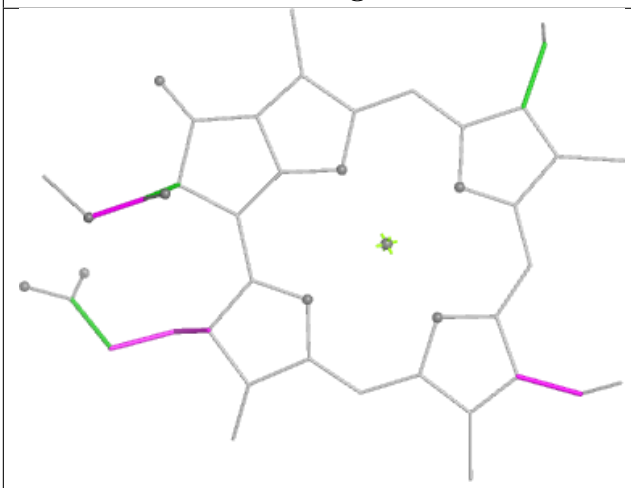
Ligand CLA N 612



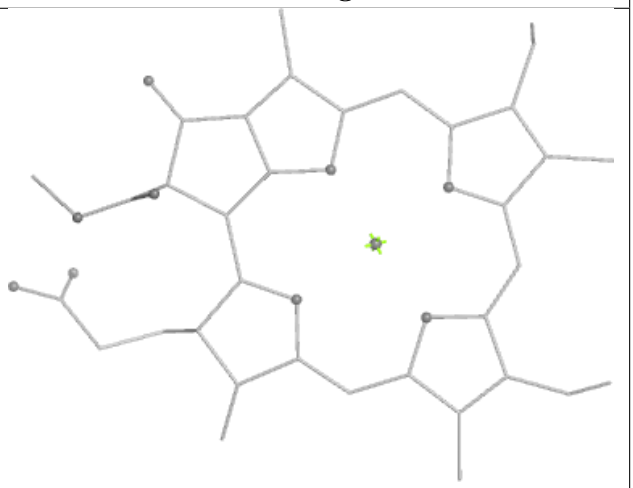
Bond lengths



Bond angles

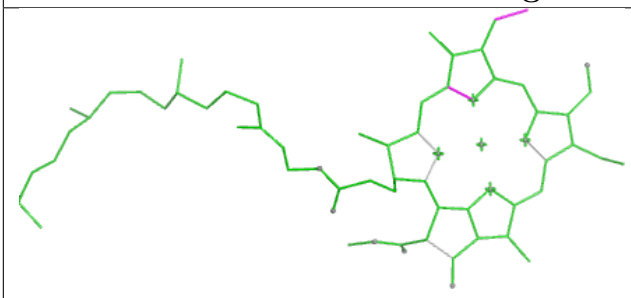


Torsions



Rings

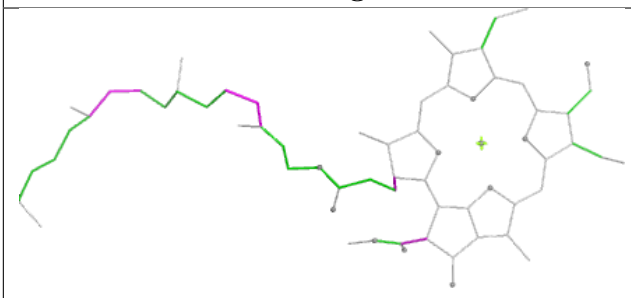
Ligand CHL G 601



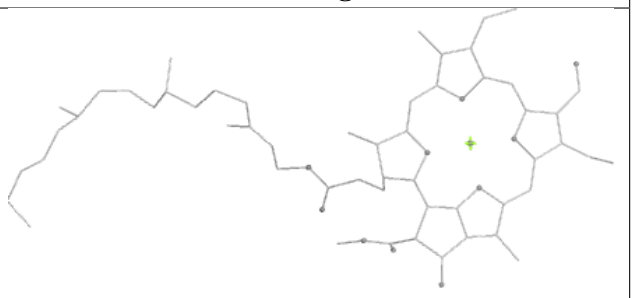
Bond lengths



Bond angles

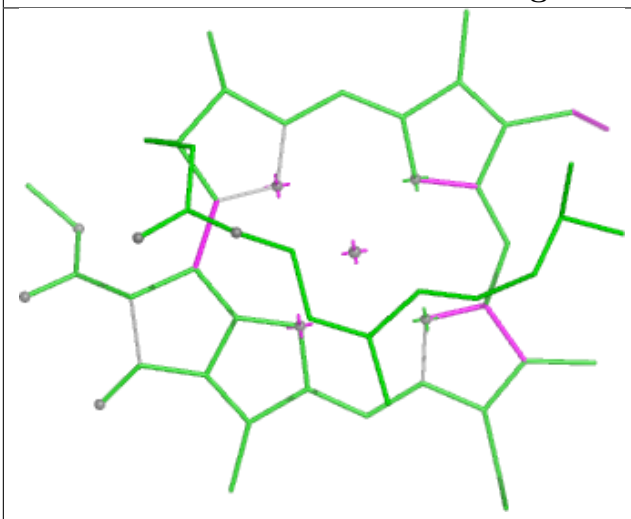


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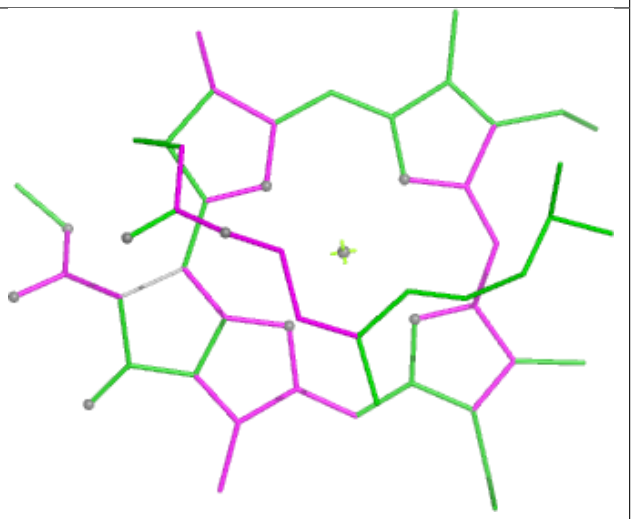


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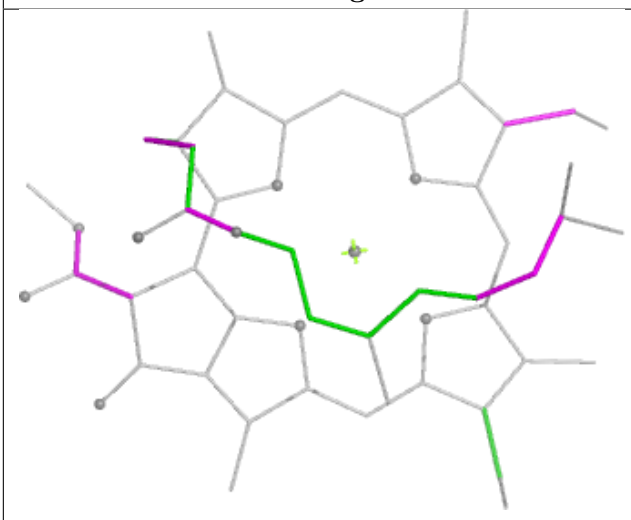
Ligand CLA s 613



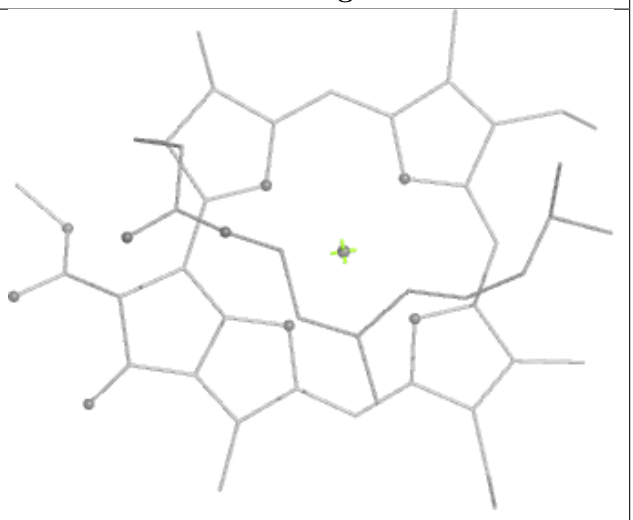
Bond lengths



Bond angles

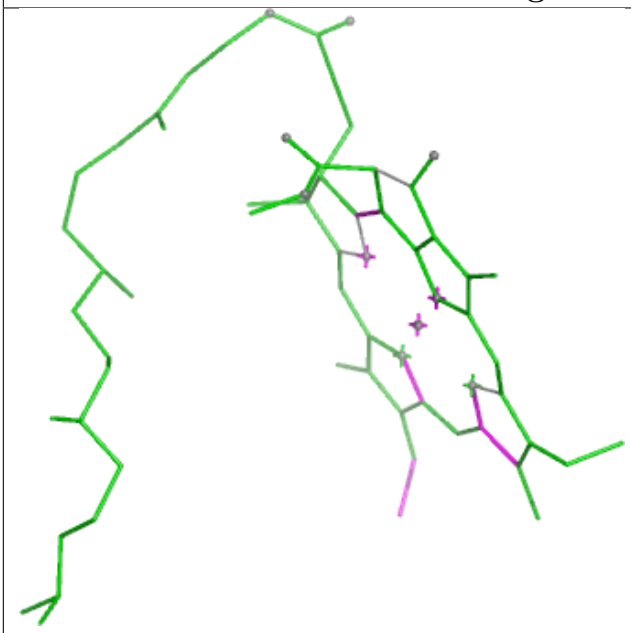


Torsions

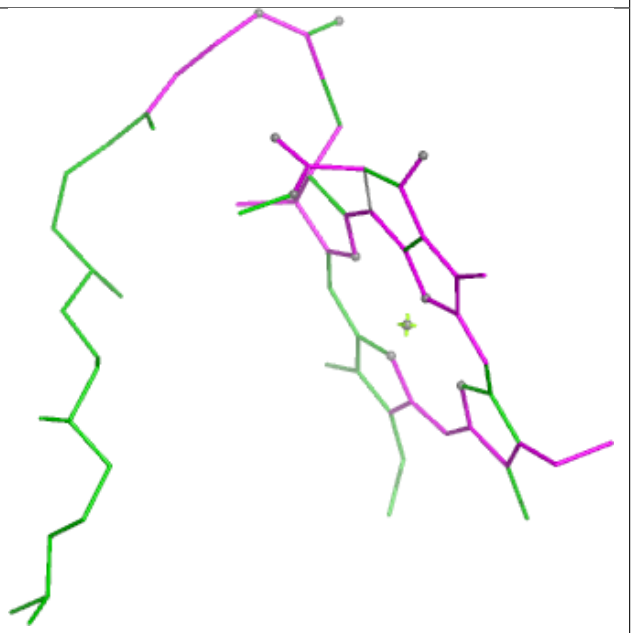


Rings

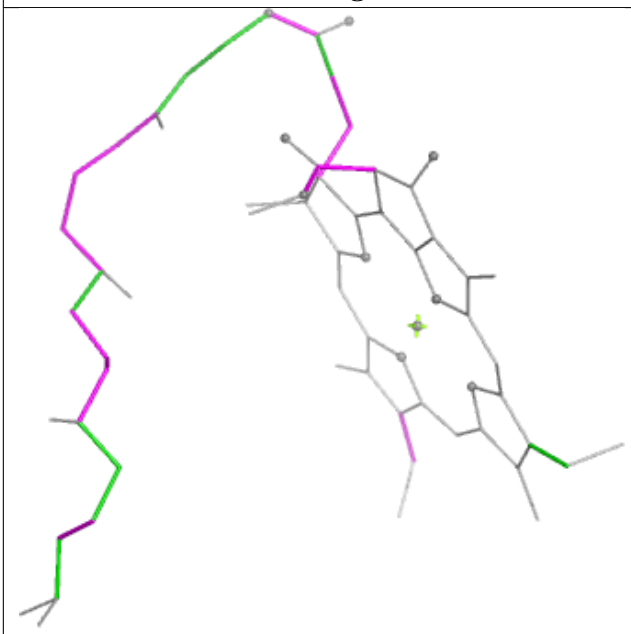
Ligand CLA n 603



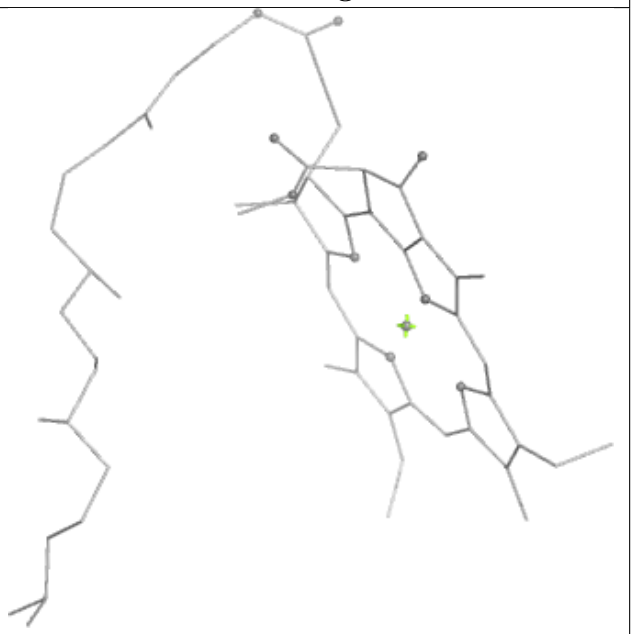
Bond lengths



Bond angles

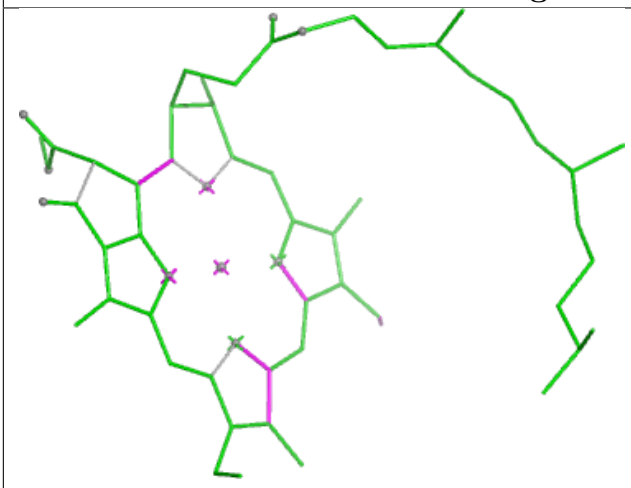


Torsions

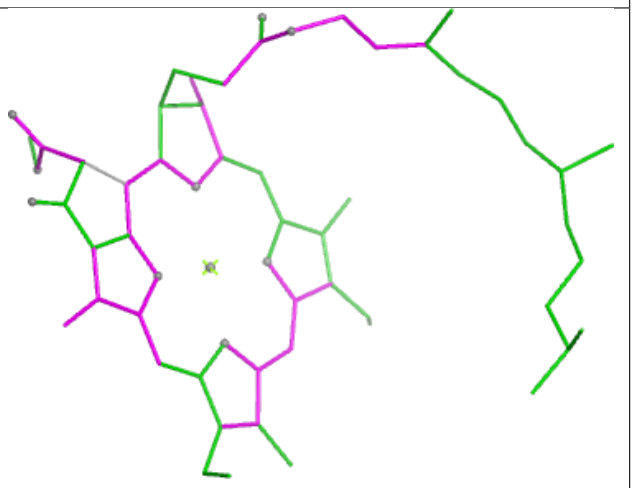


Rings

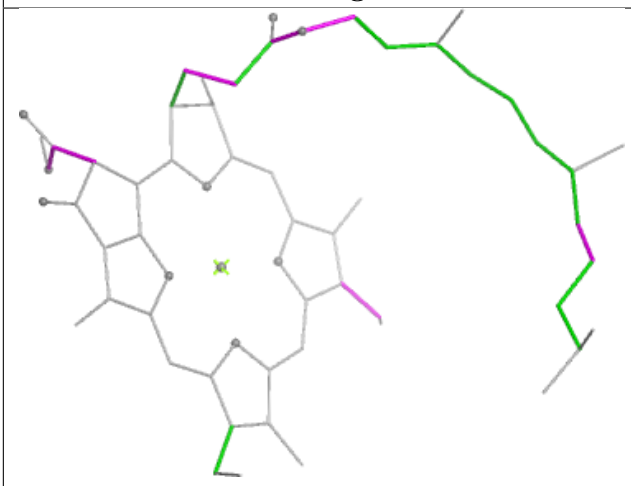
Ligand CLA r 602



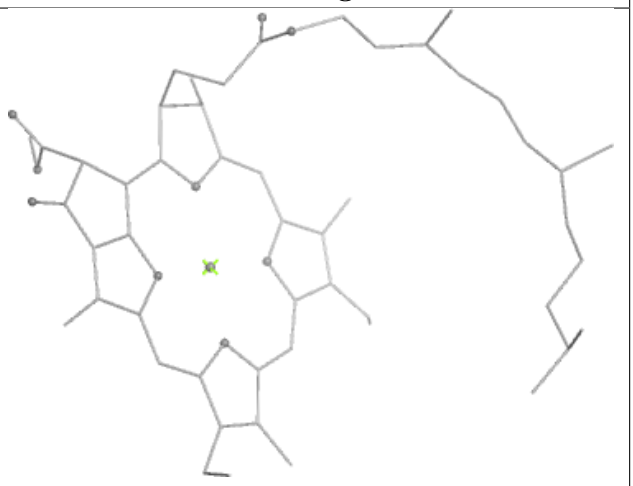
Bond lengths



Bond angles

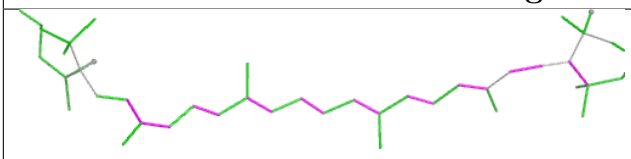


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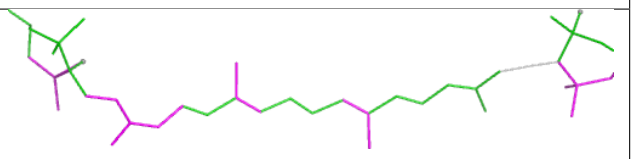


Rings

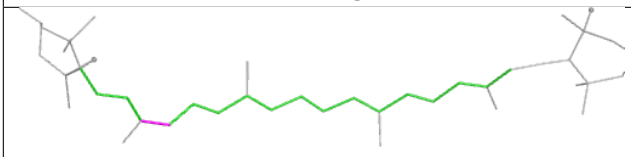
Ligand NEX n 623



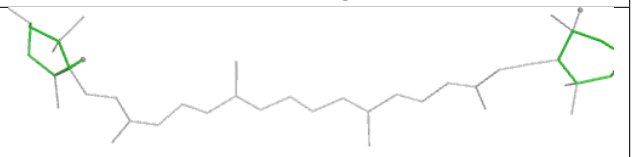
Bond lengths



Bond angles

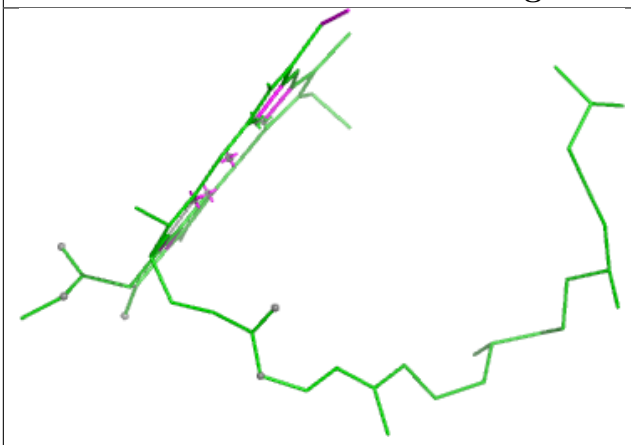


Torsions

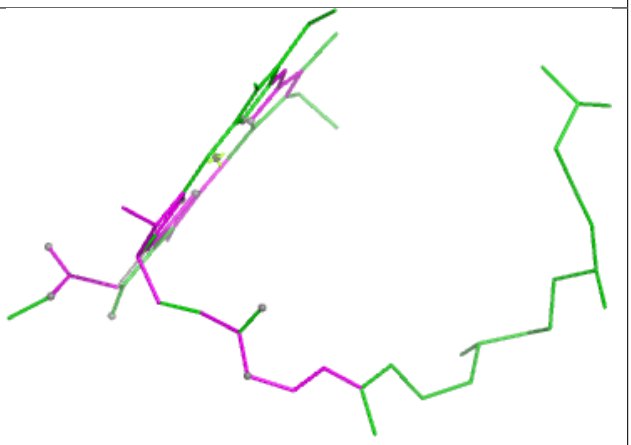


Rings

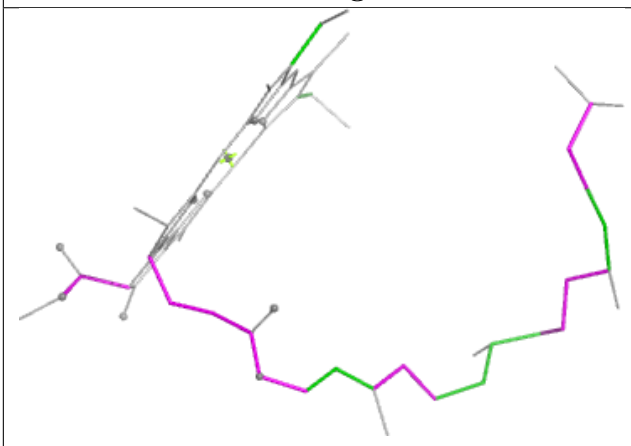
Ligand CLA B 612



Bond lengths



Bond angles

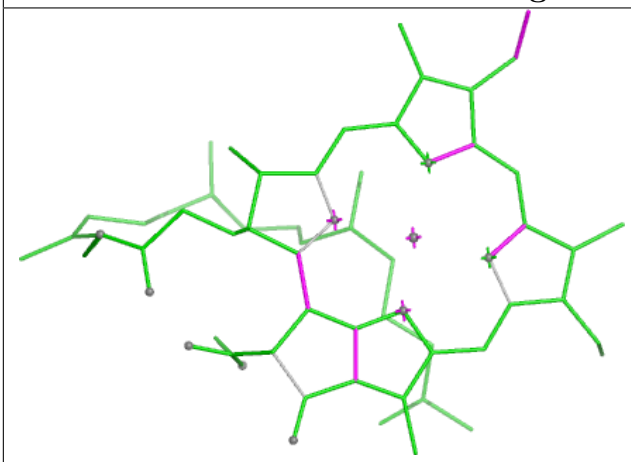


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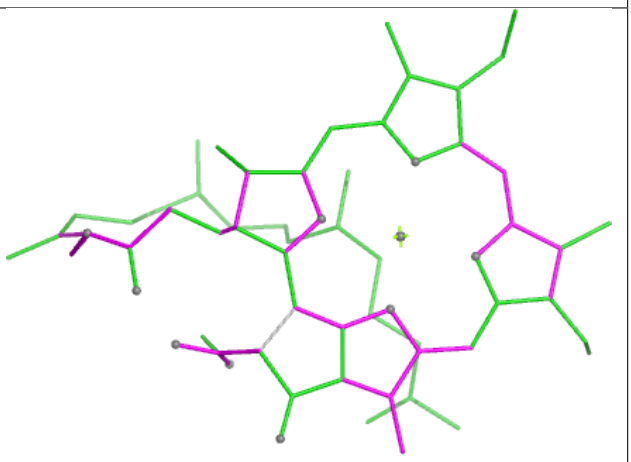


Rings

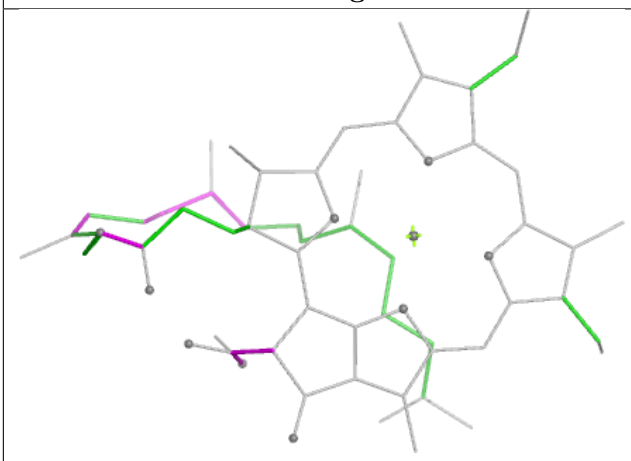
Ligand CLA c 510



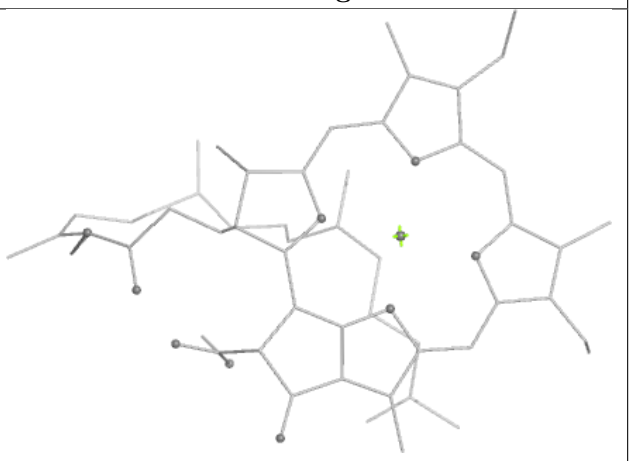
Bond lengths



Bond angles

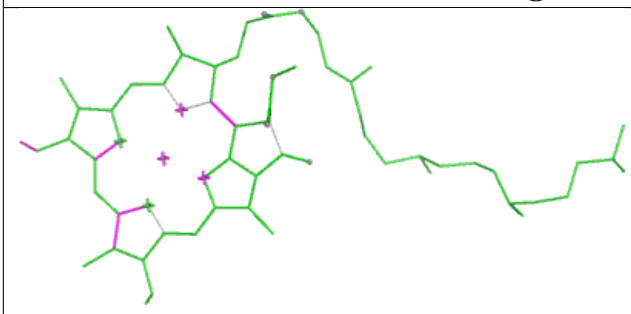


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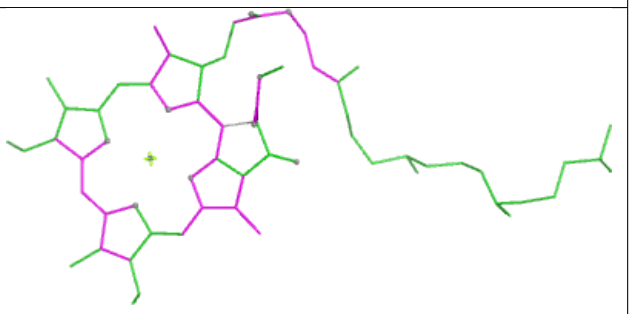


Rings

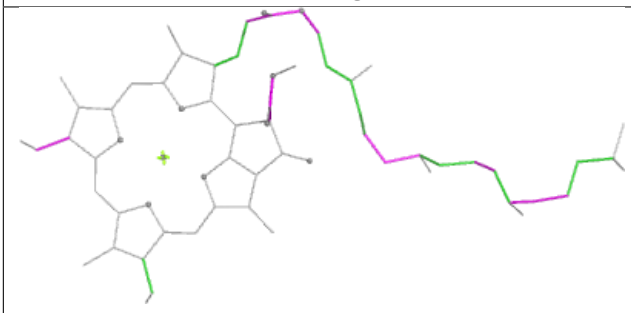
Ligand CLA b 603



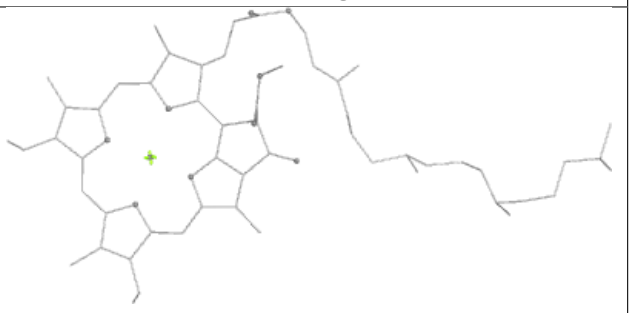
Bond lengths



Bond angles



Torsions



Rings

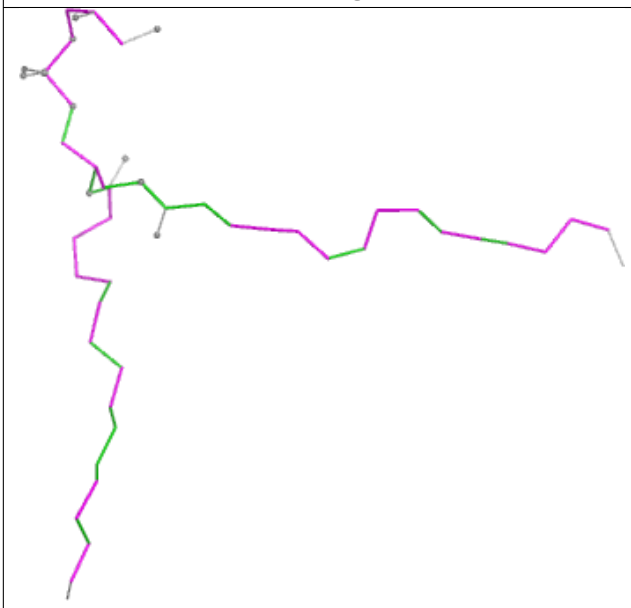
Ligand LHG L 101



Bond lengths



Bond angles



Torsions

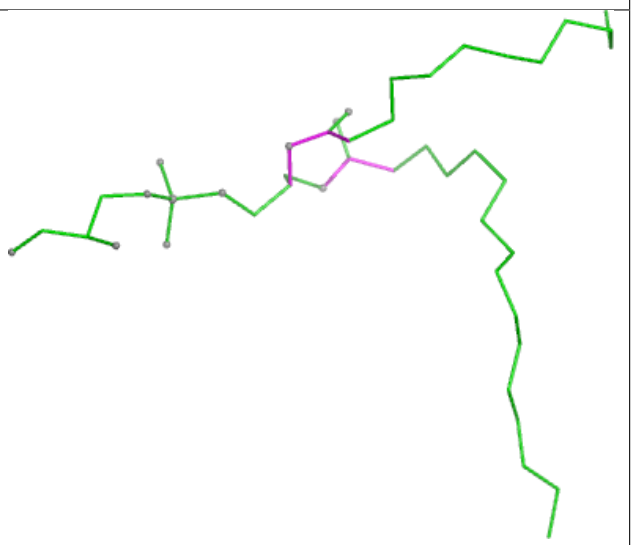


Rings

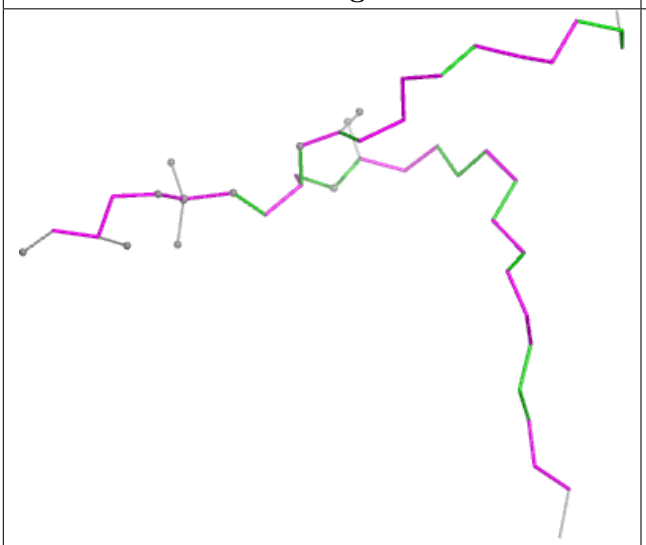
Ligand LHG S 624



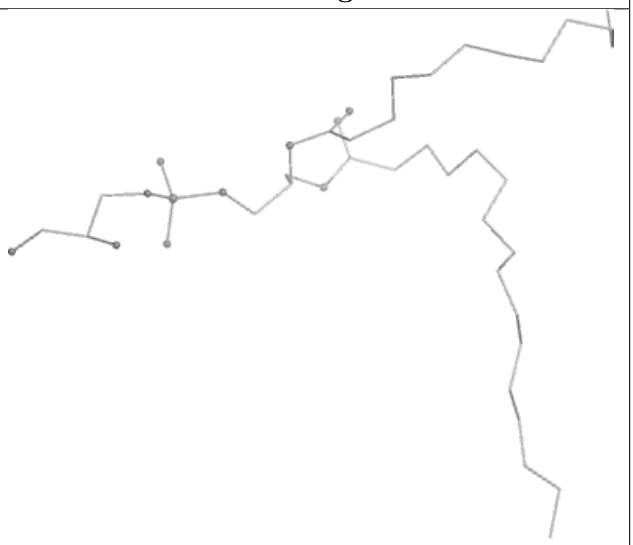
Bond lengths



Bond angles

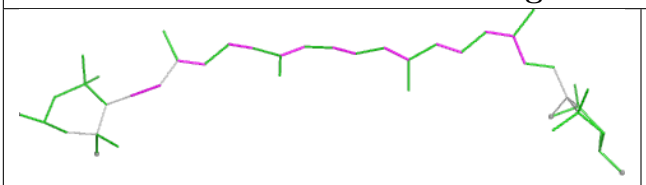


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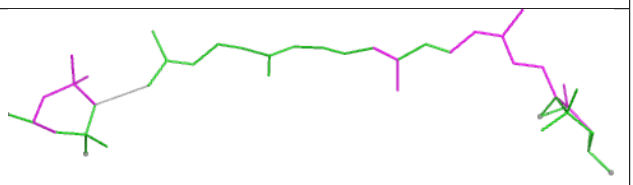


Rings

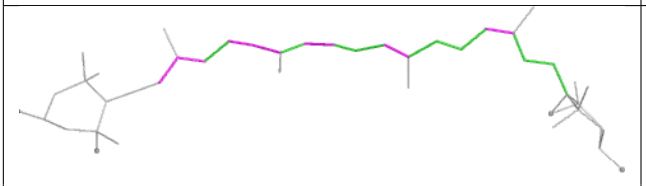
Ligand NEX S 622



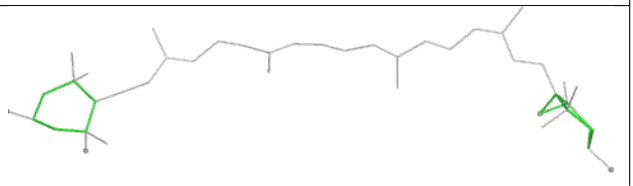
Bond lengths



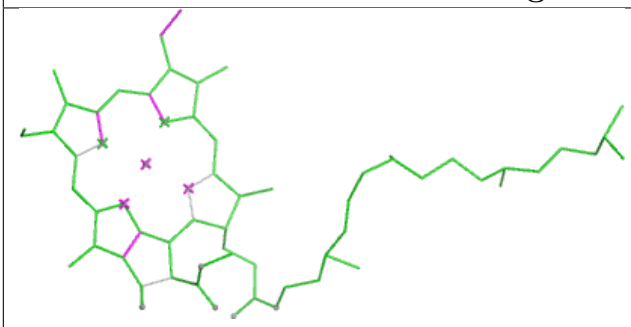
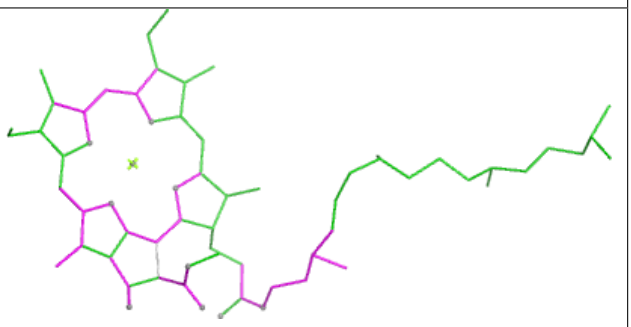
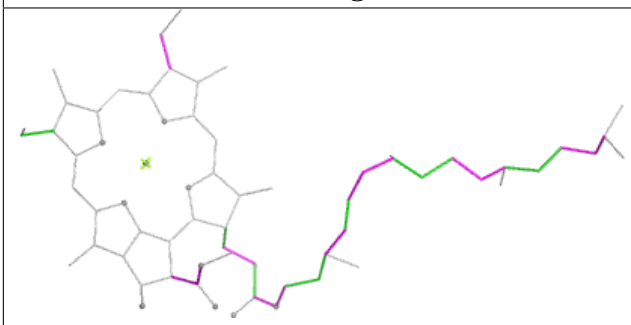
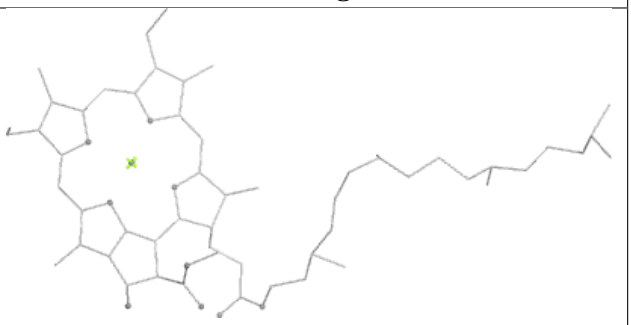
Bond angles

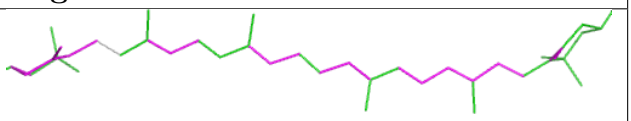
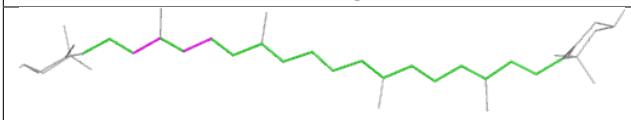
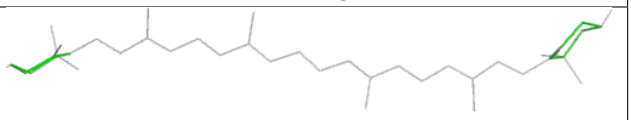


Torsions

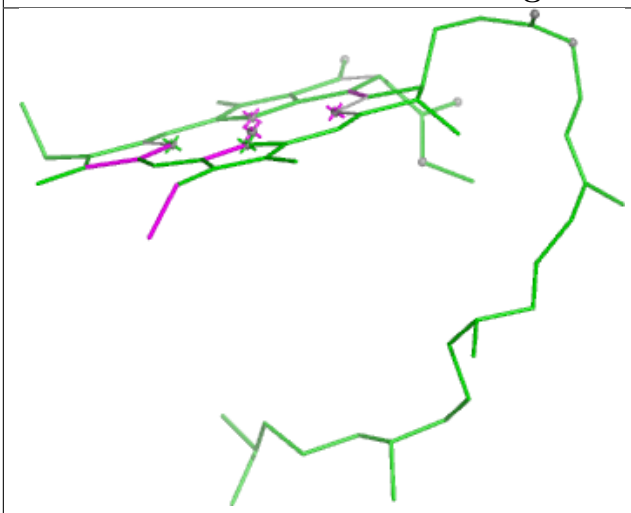


Rings

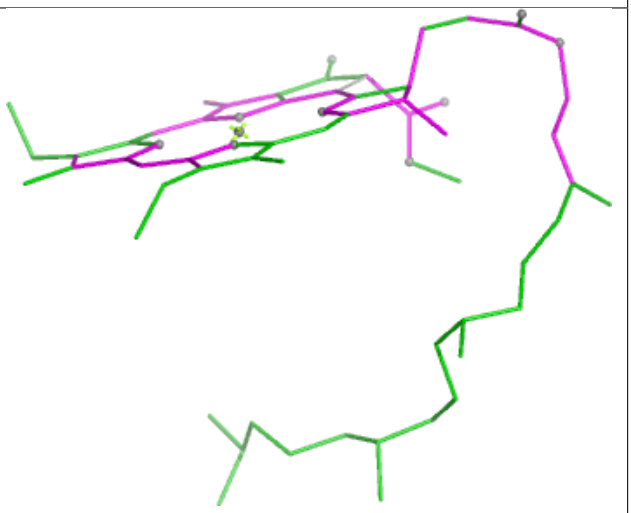
Ligand CLA b 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT g 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 603



Bond lengths



Bond angles

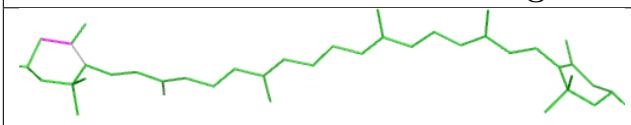


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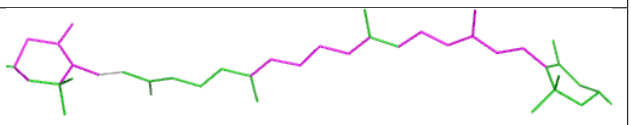


Rings

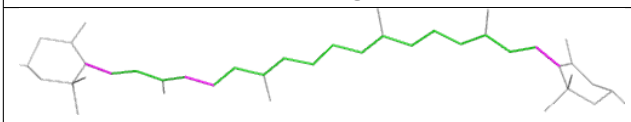
Ligand LUT n 621



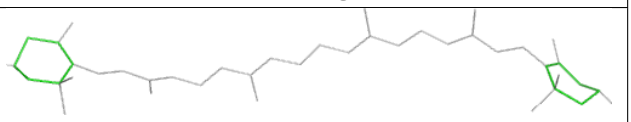
Bond lengths



Bond angles

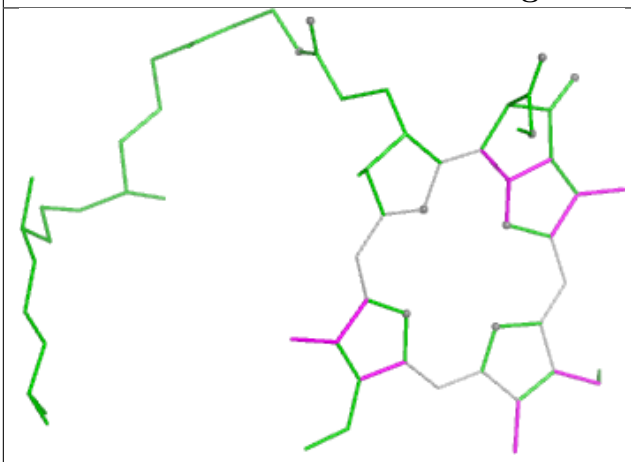


Torsions

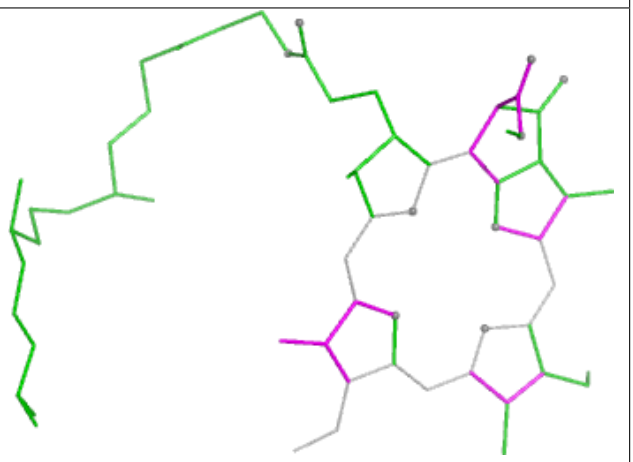


Rings

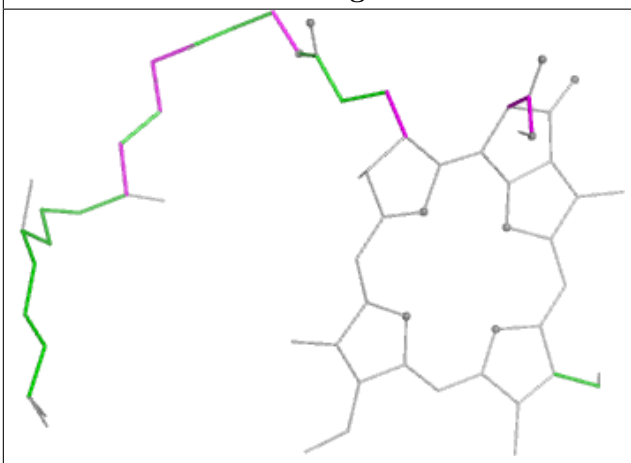
Ligand PHO A 409



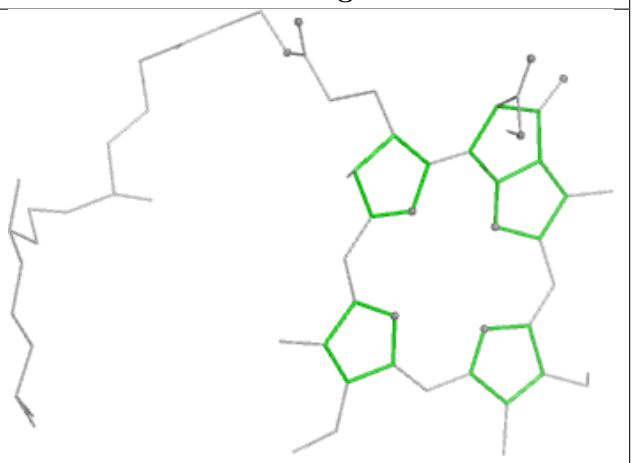
Bond lengths



Bond angles

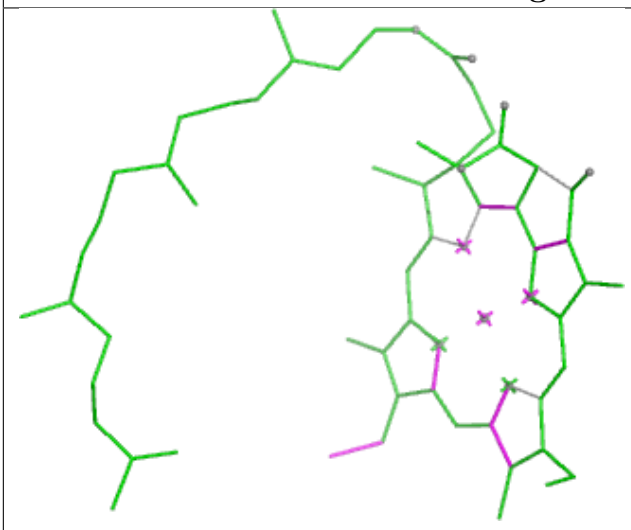


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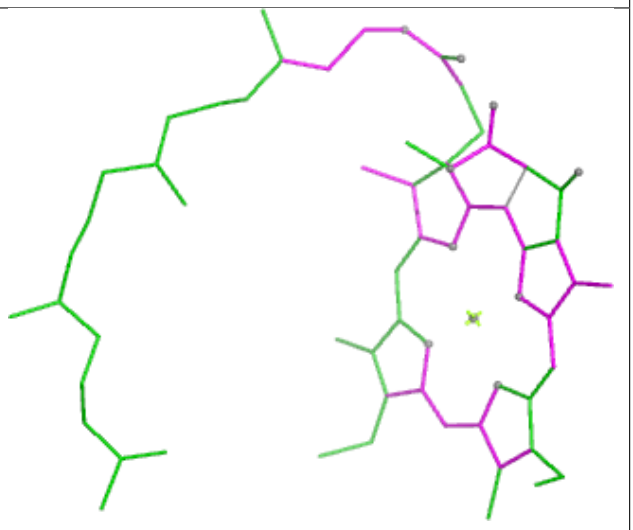


Rings

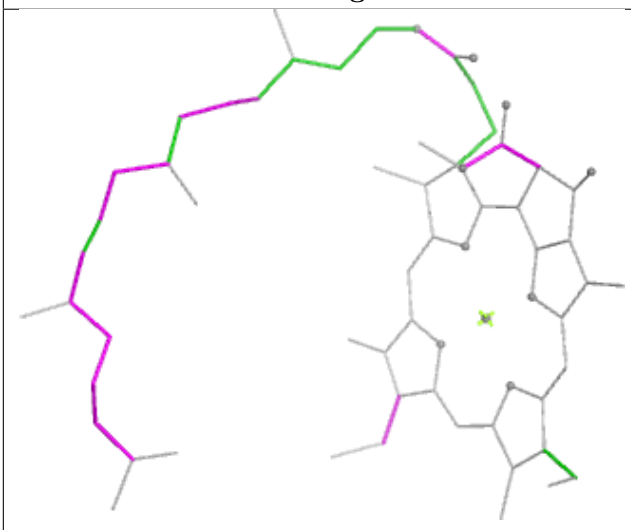
Ligand CLA c 507



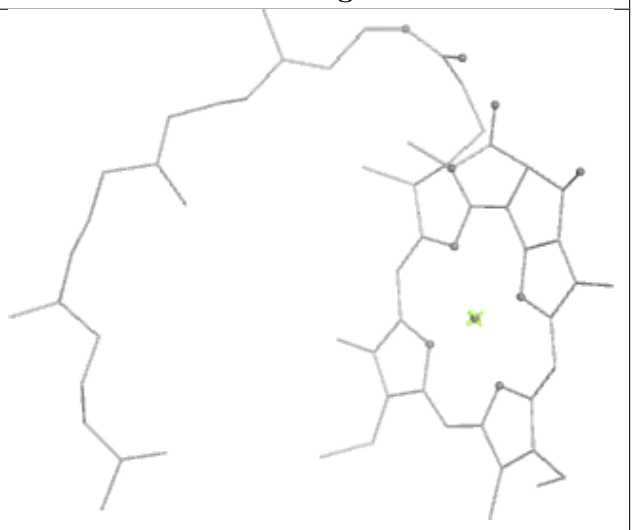
Bond lengths



Bond angles

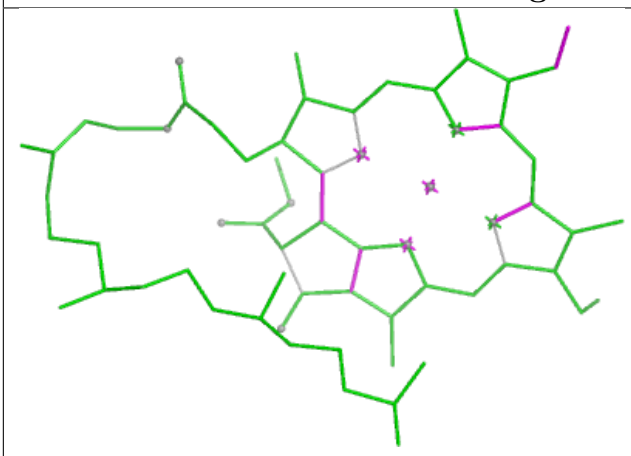


Torsions

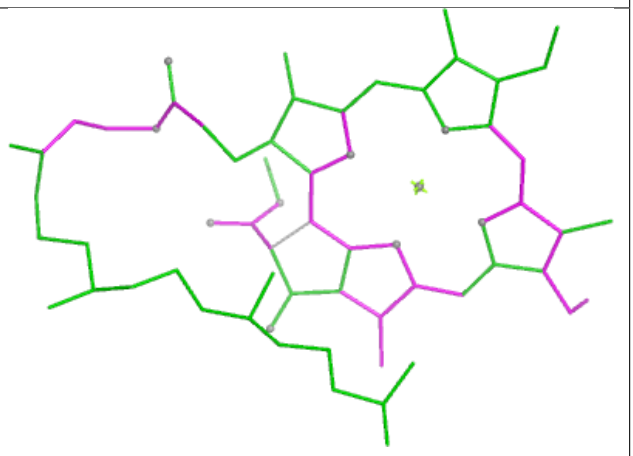


Rings

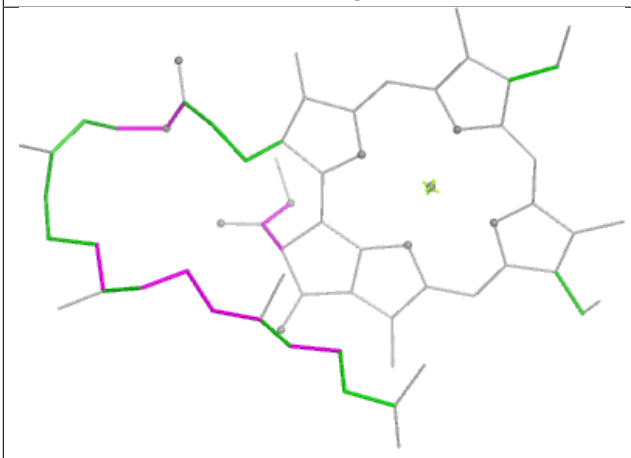
Ligand CLA c 509



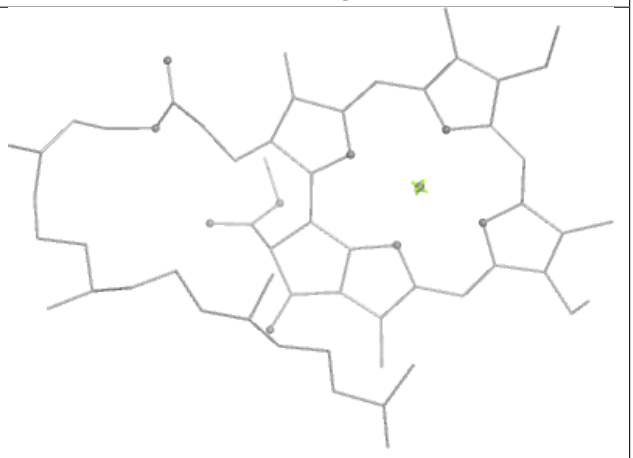
Bond lengths



Bond angles



Torsions

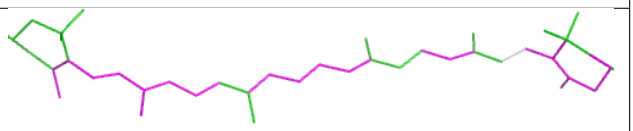


Rings

Ligand LUT n 620



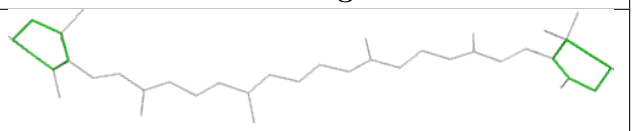
Bond lengths



Bond angles

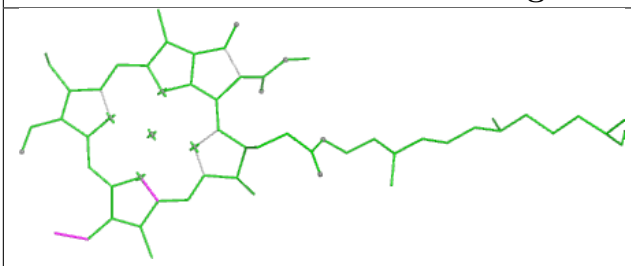


Torsions

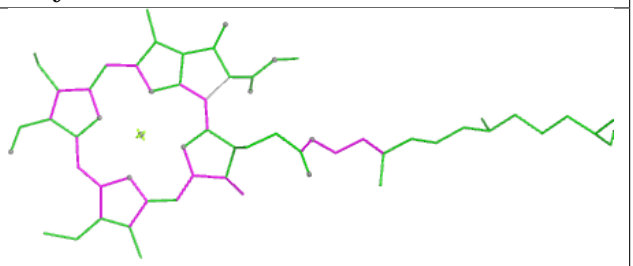


Rings

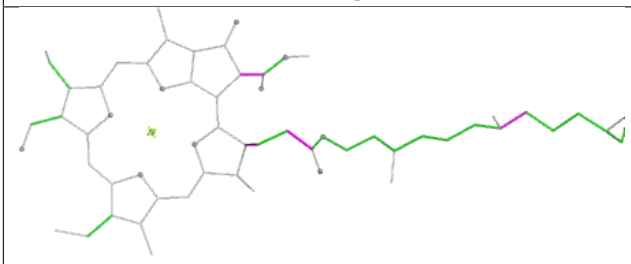
Ligand CHL y 606



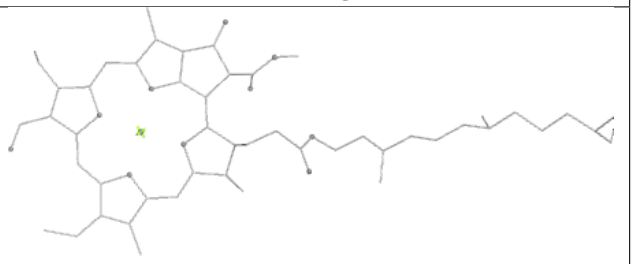
Bond lengths



Bond angles

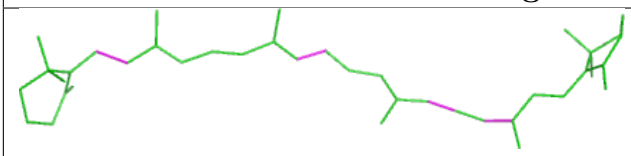


Torsions

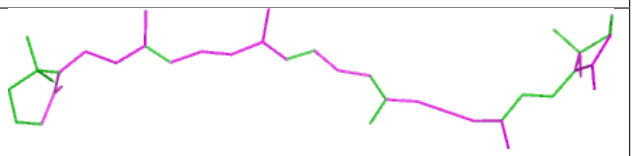


Rings

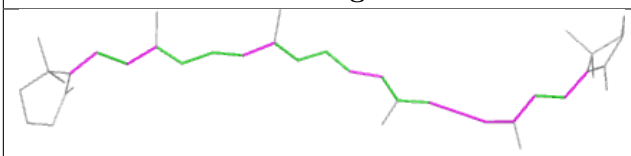
Ligand BCR C 516



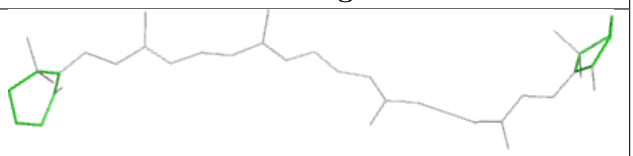
Bond lengths



Bond angles

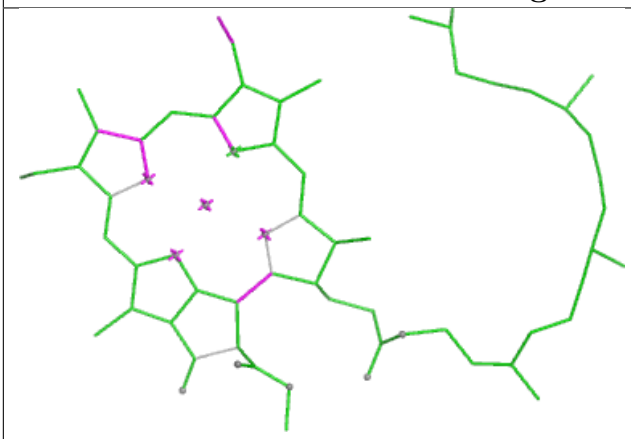


Torsions

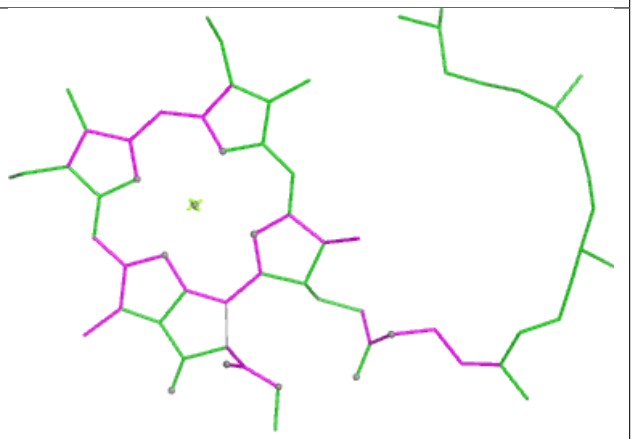


Rings

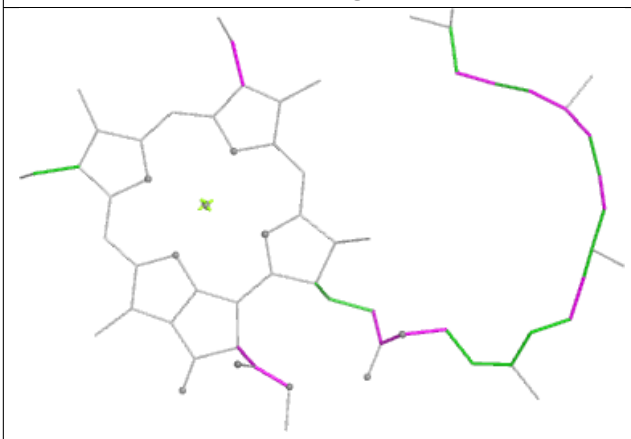
Ligand CLA s 603



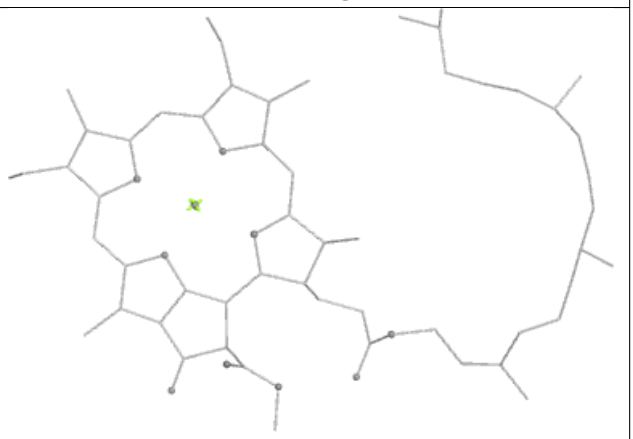
Bond lengths



Bond angles

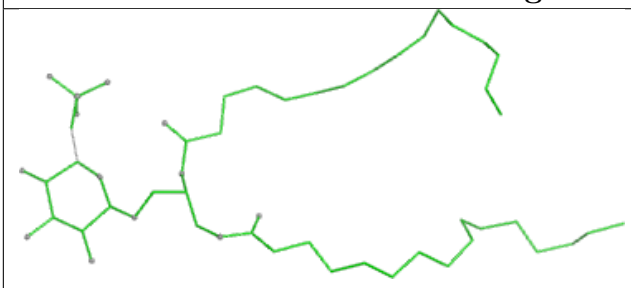


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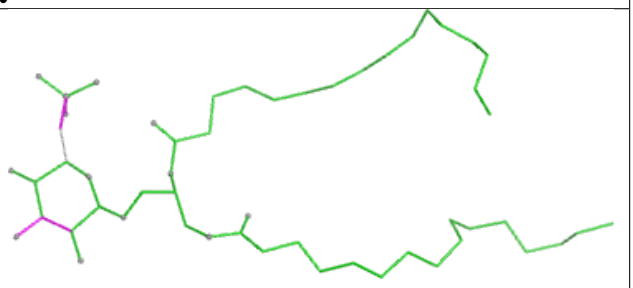


Rings

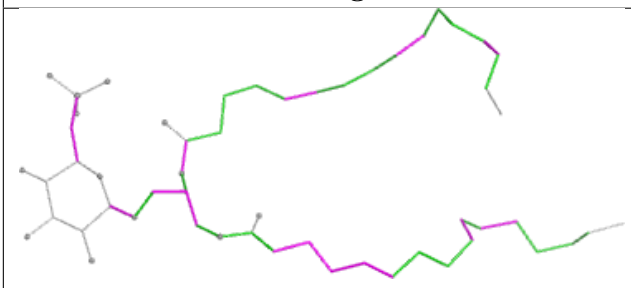
Ligand SQD B 621



Bond lengths



Bond angles

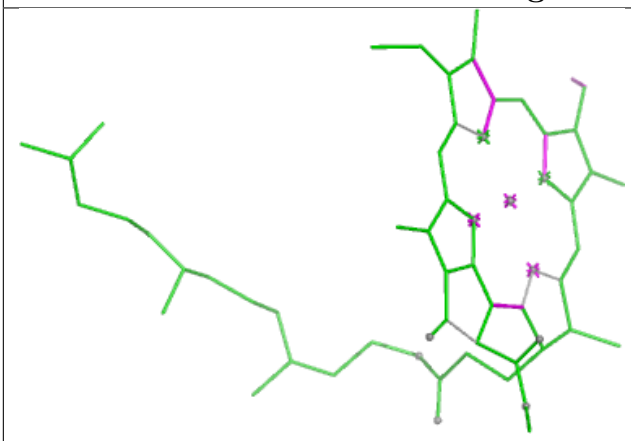


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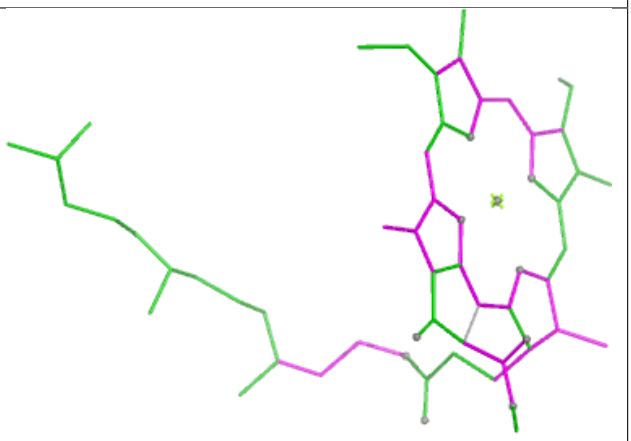


Rings

Ligand CLA S 609



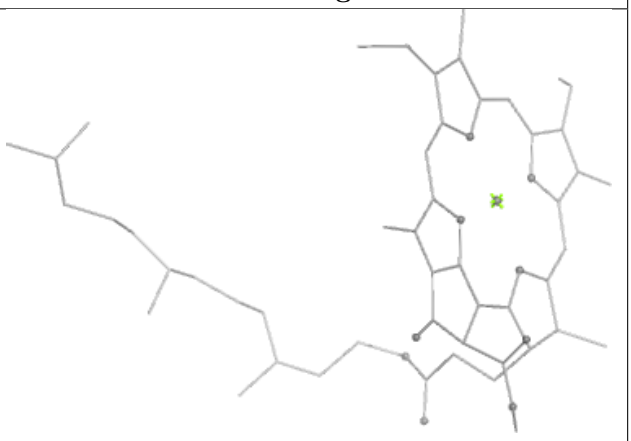
Bond lengths



Bond angles

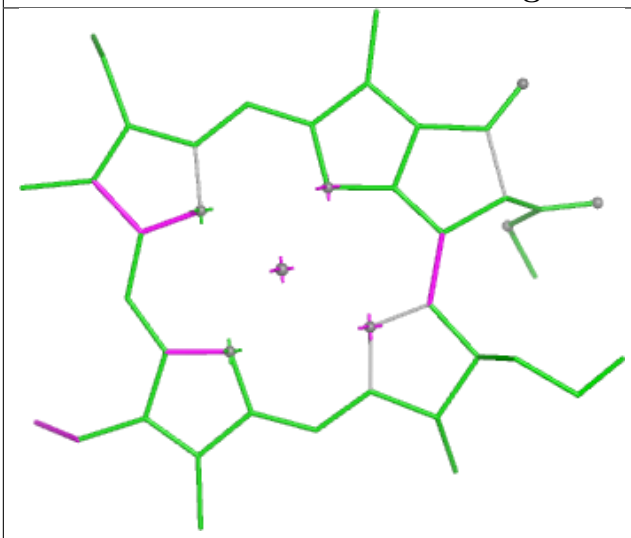


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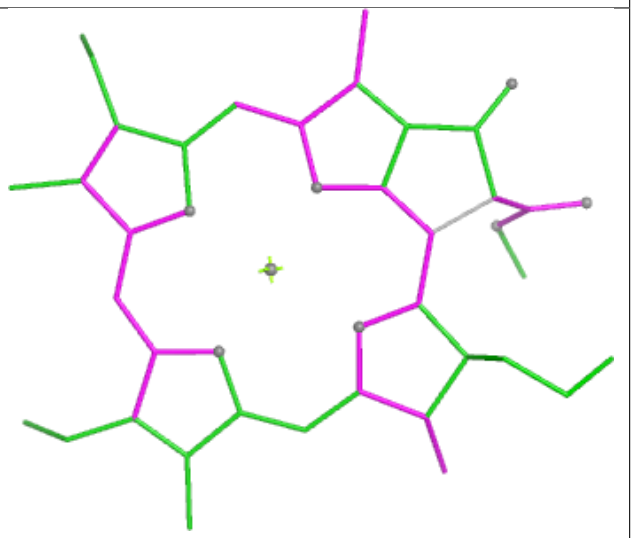


Rings

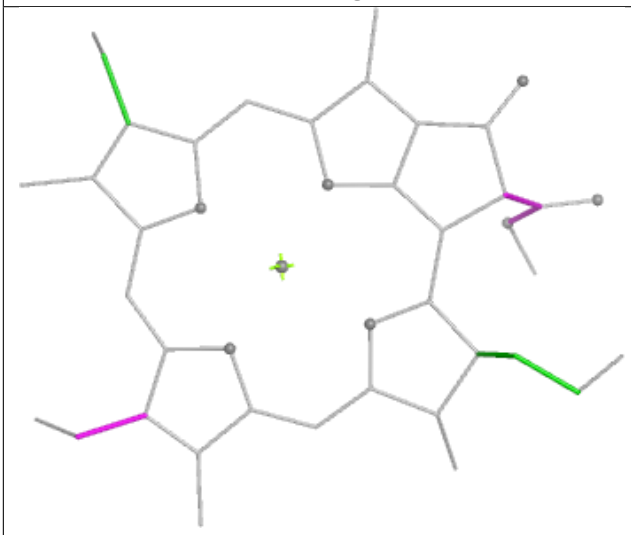
Ligand CLA G 612



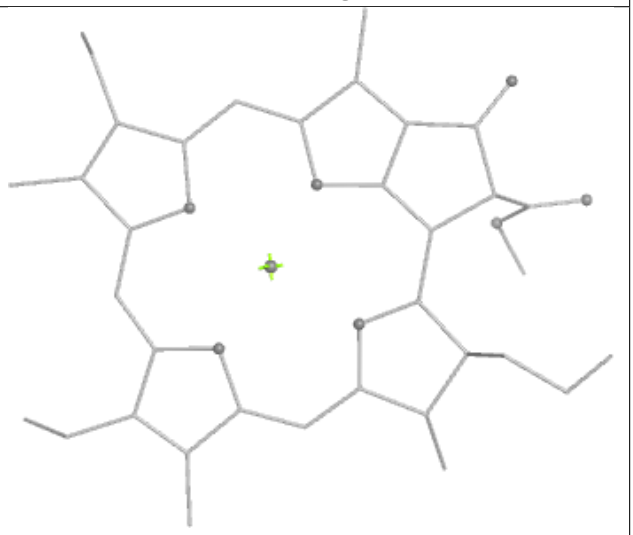
Bond lengths



Bond angles

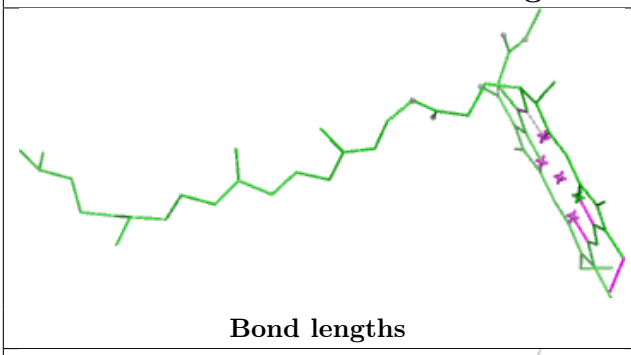


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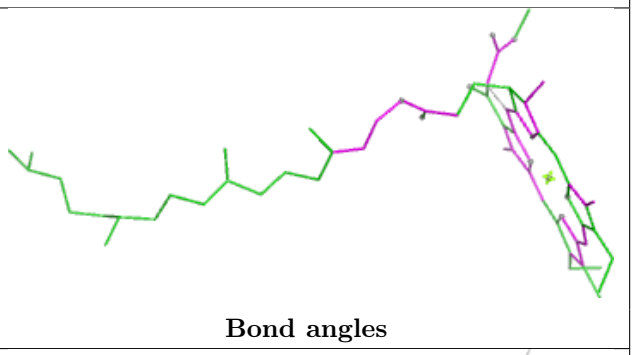


Rings

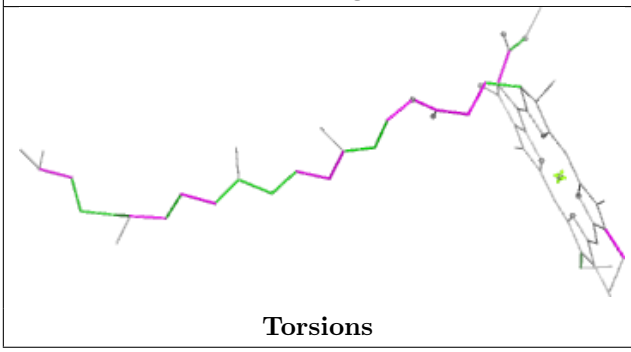
Ligand CLA B 605



Bond lengths



Bond angles

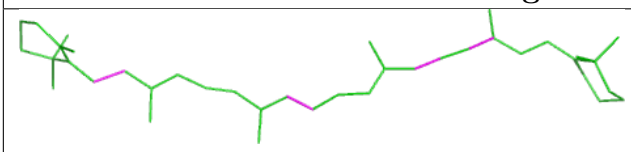


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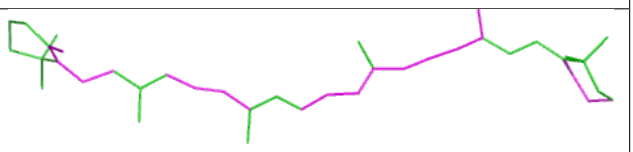


Rings

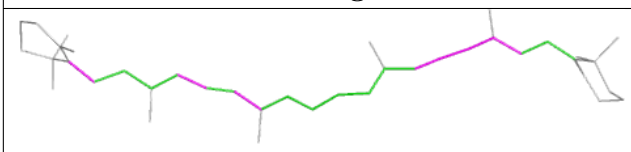
Ligand BCR C 515



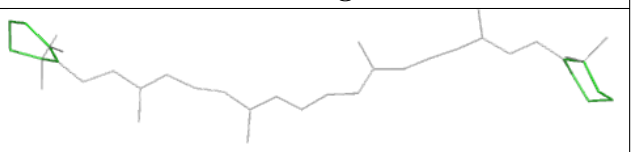
Bond lengths



Bond angles

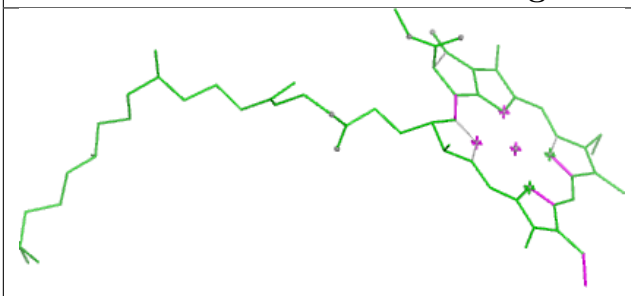


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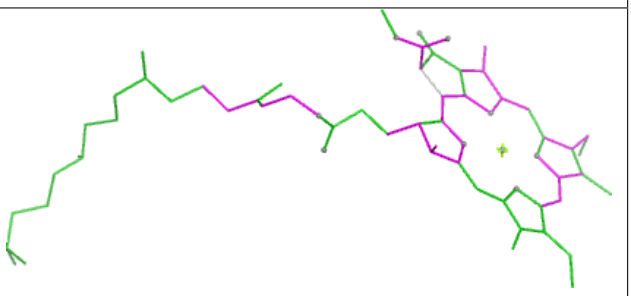


Rings

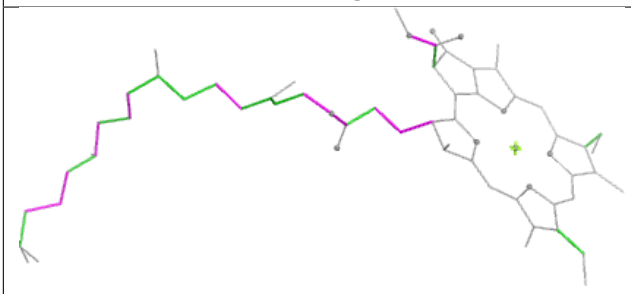
Ligand CLA a 405



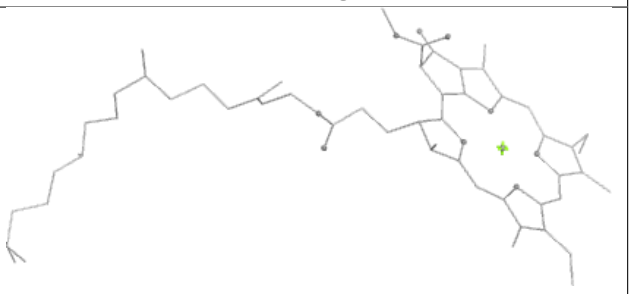
Bond lengths



Bond angles

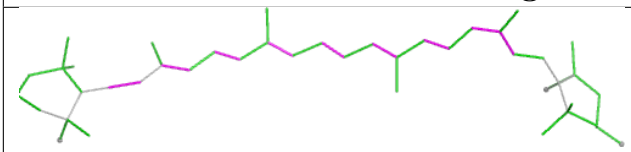


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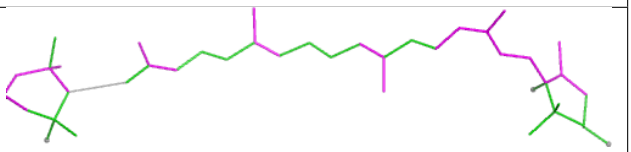


Rings

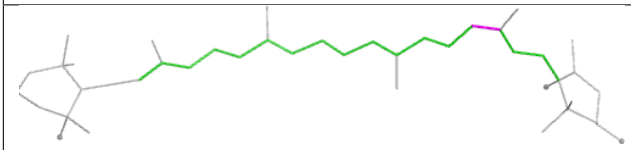
Ligand NEX N 623



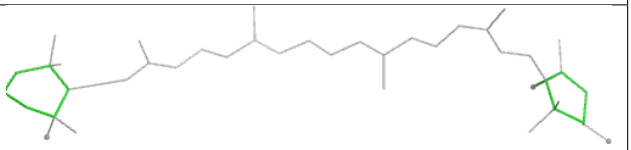
Bond lengths



Bond angles

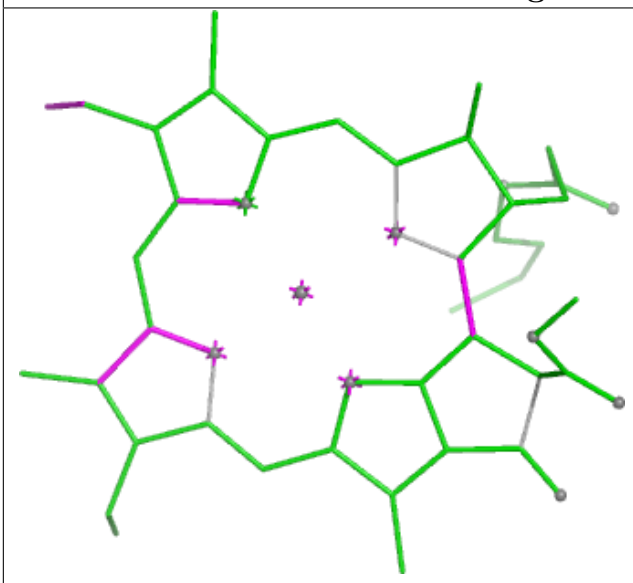


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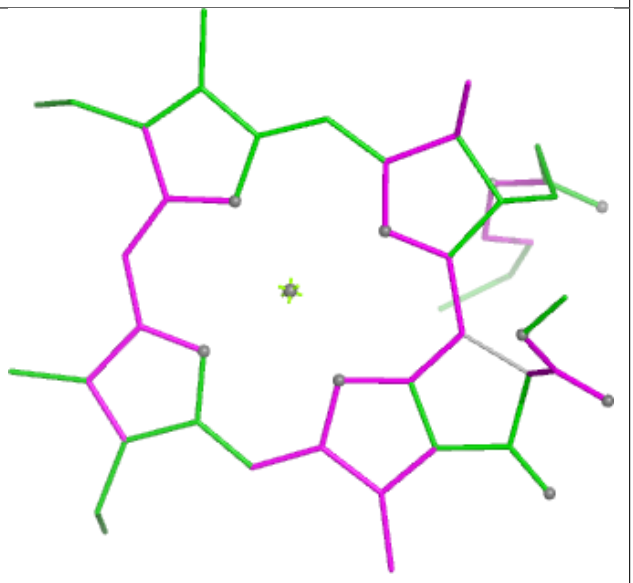


Rings

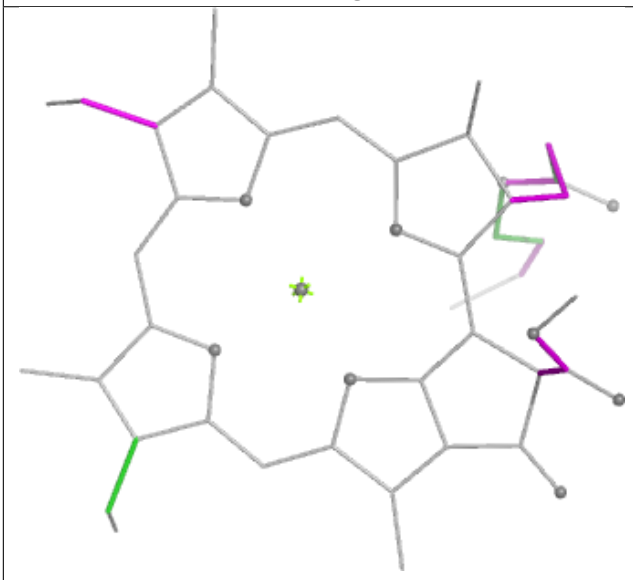
Ligand CLA n 611



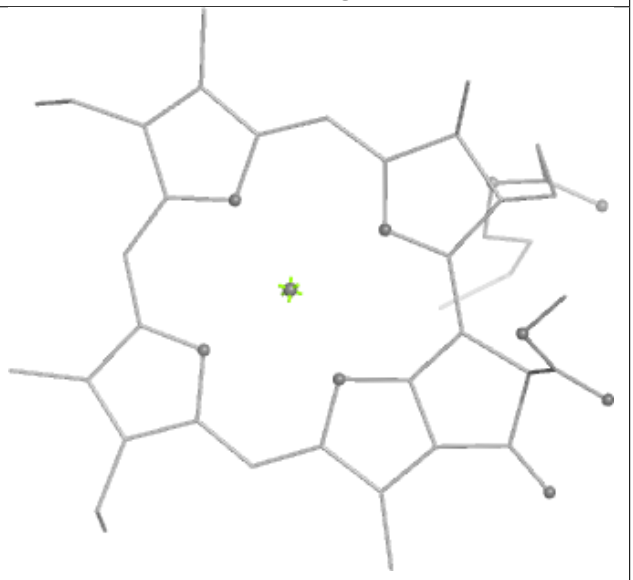
Bond lengths



Bond angles

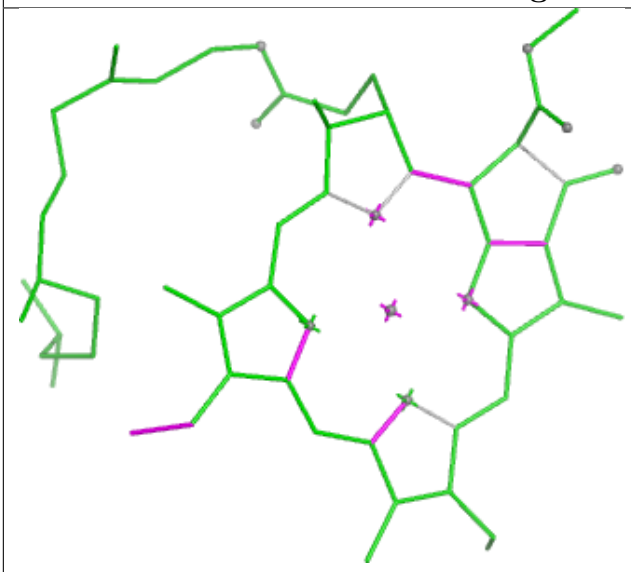


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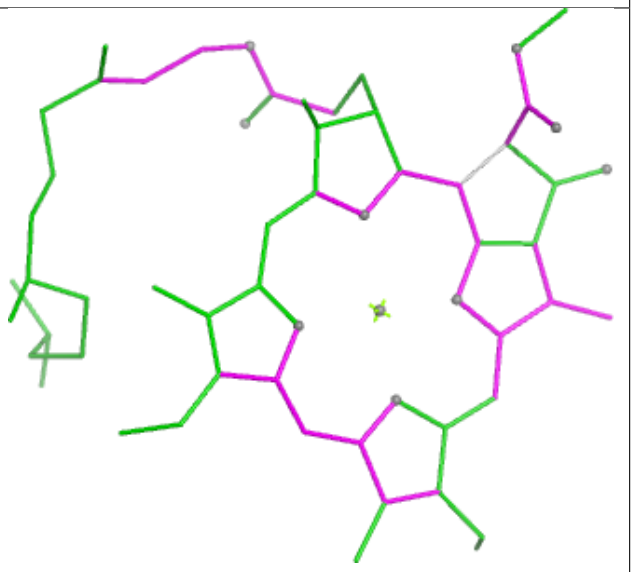


Rings

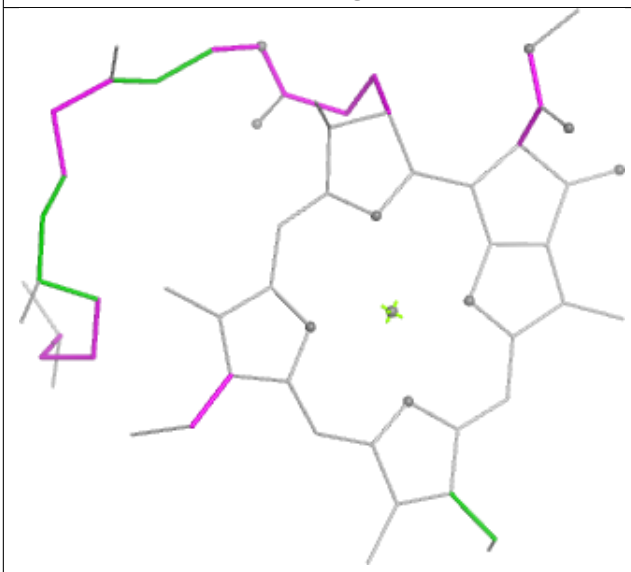
Ligand CLA r 609



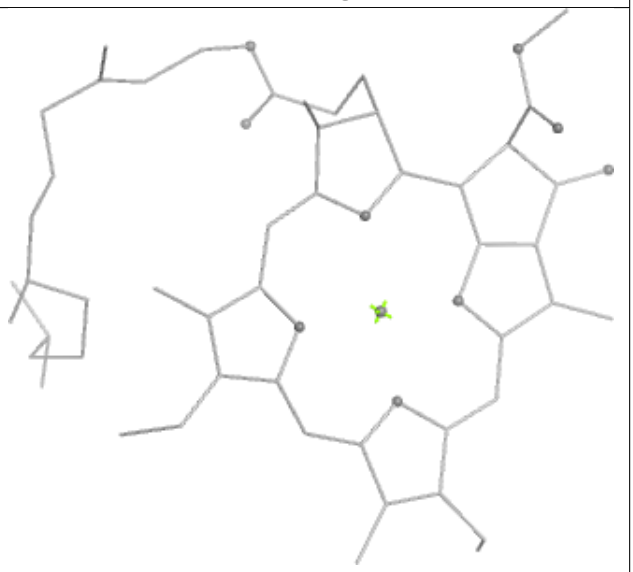
Bond lengths



Bond angles

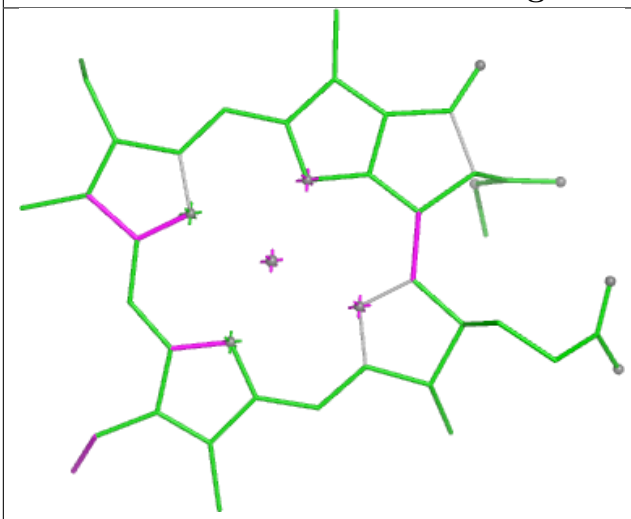


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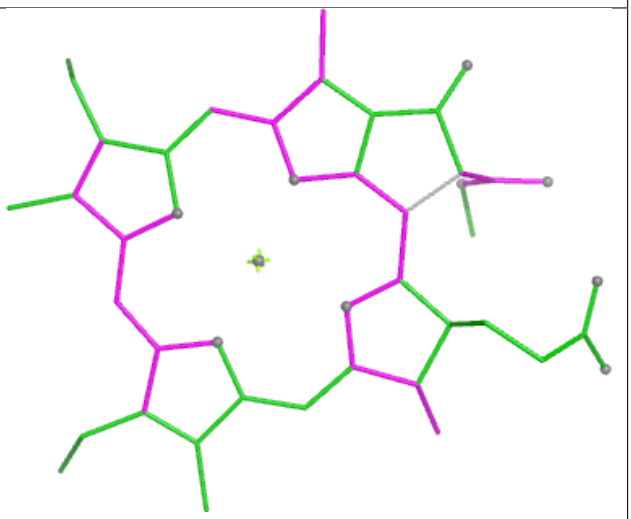


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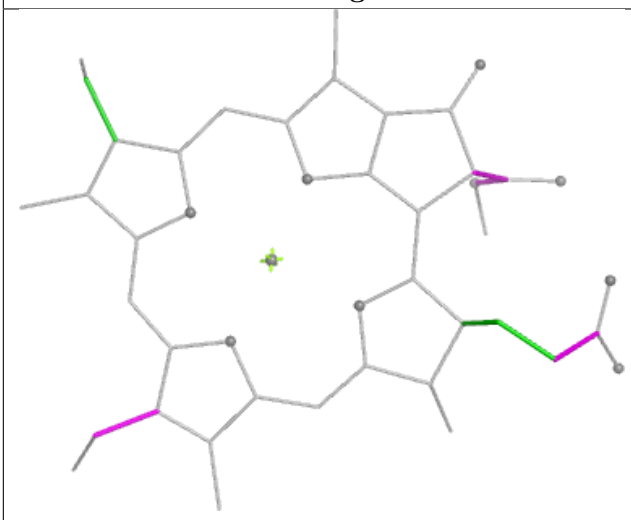
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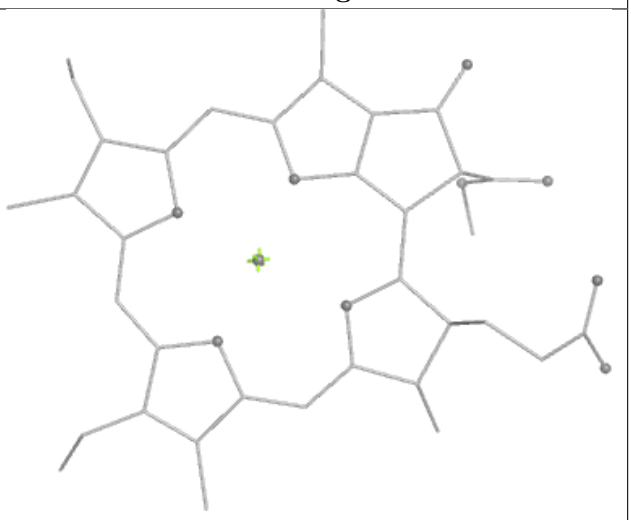
Bond lengths



Bond angles



Torsions

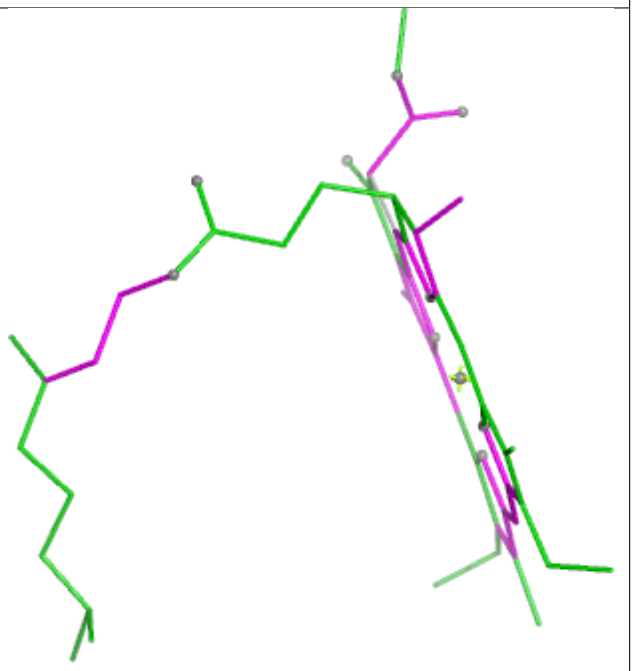


Rings

Ligand CLA s 604



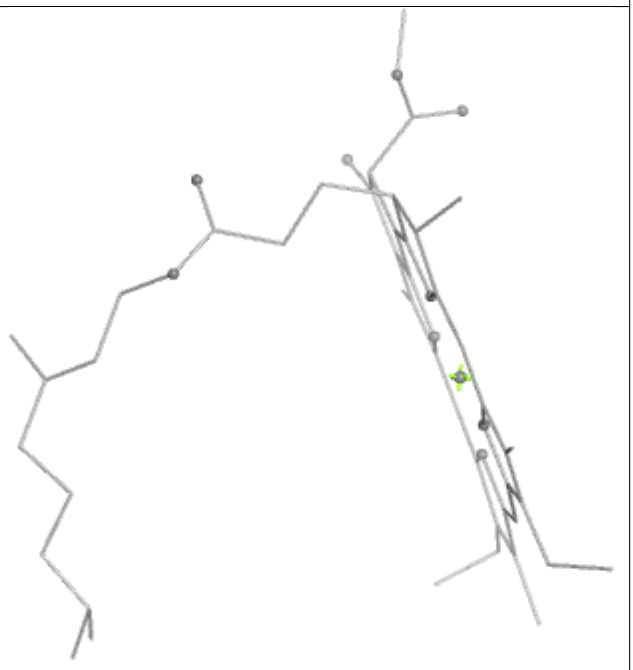
Bond lengths



Bond angles

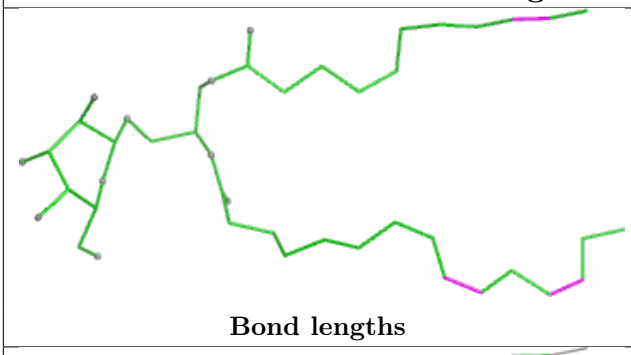


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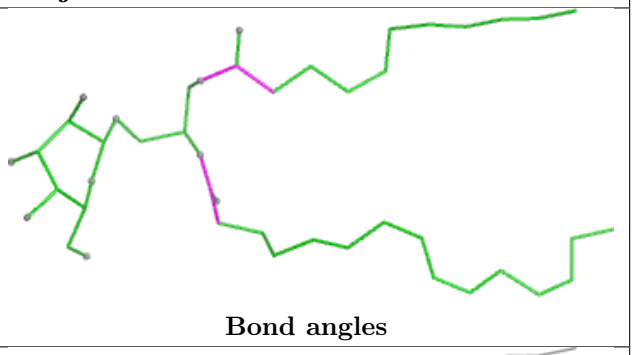


Rings

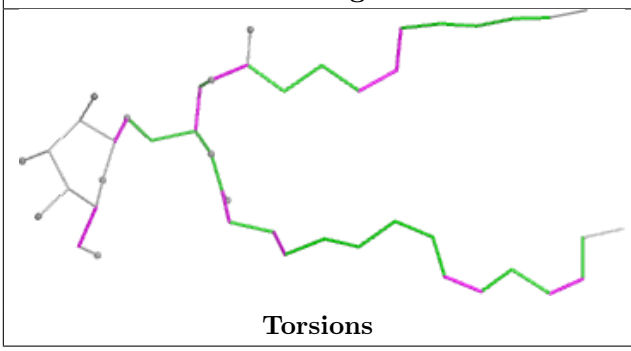
Ligand LMG j 101



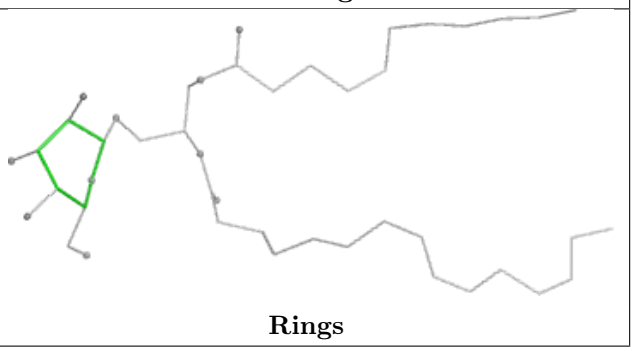
Bond lengths



Bond angles

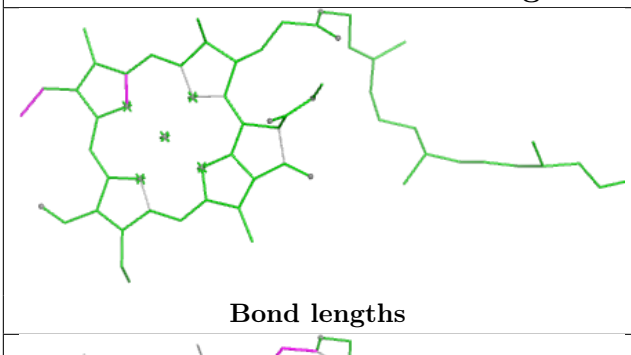


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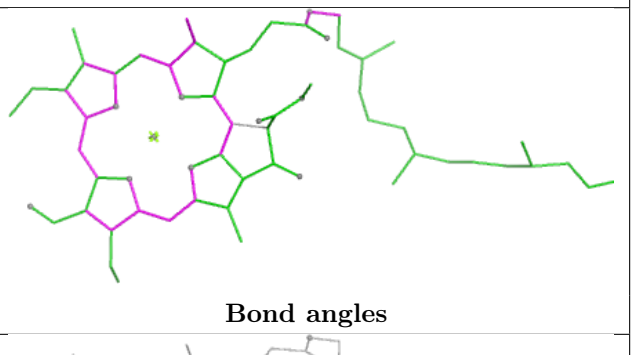


Rings

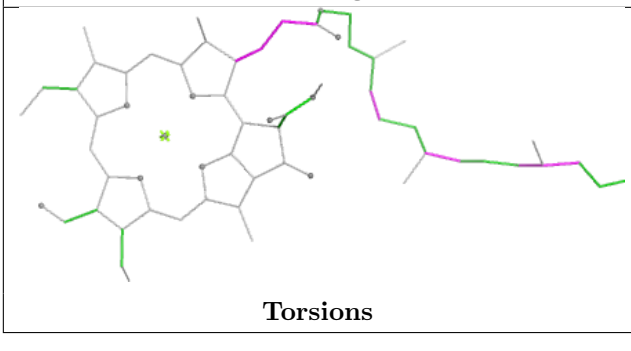
Ligand CHL N 605



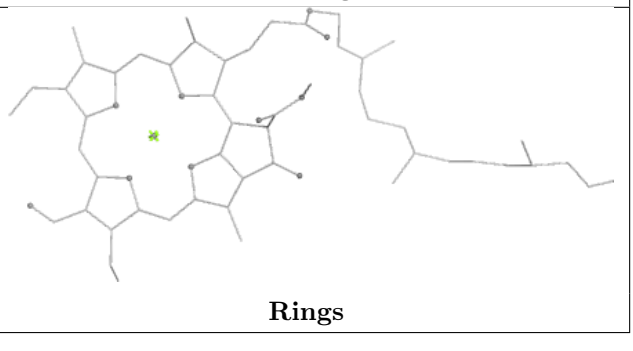
Bond lengths



Bond angles

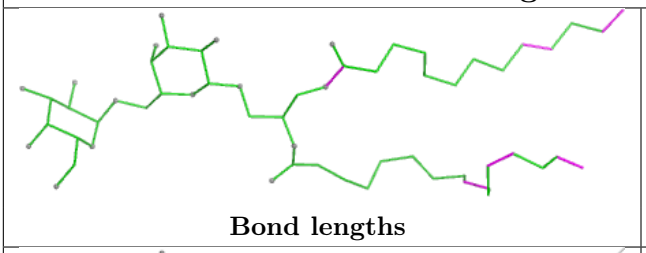


Torsions

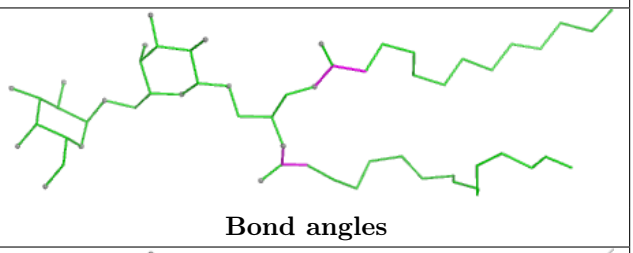


Rings

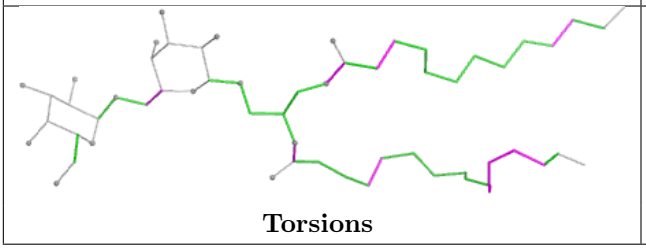
Ligand DGD C 520



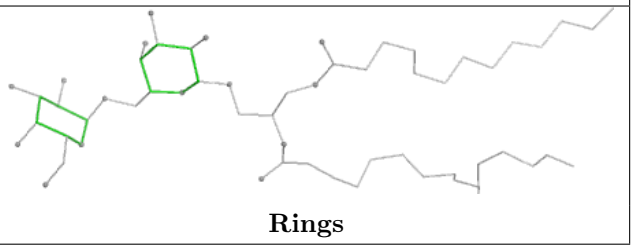
Bond lengths



Bond angles

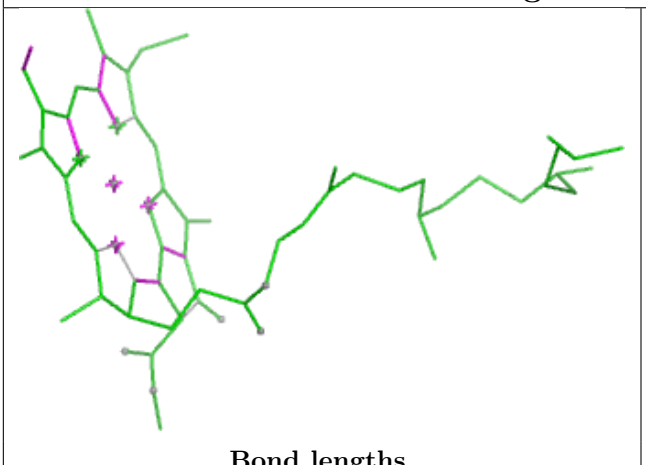


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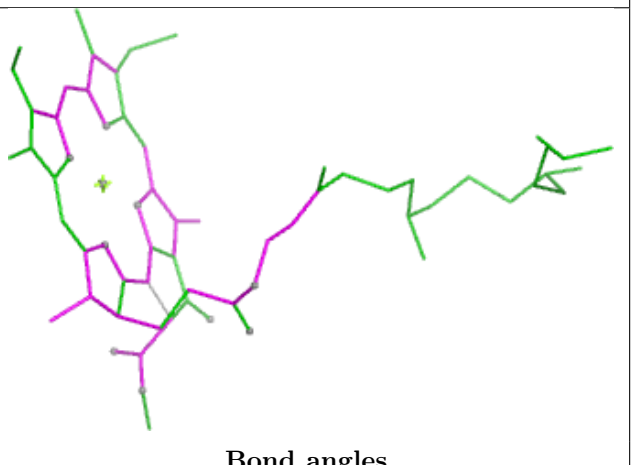


Rings

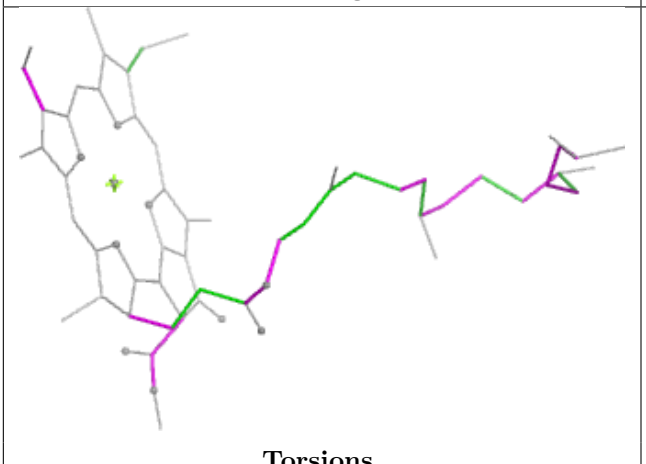
Ligand CLA Y 604



Bond lengths



Bond angles

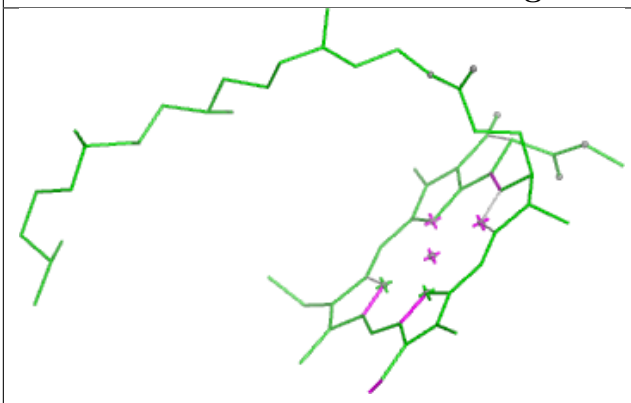


Torsions

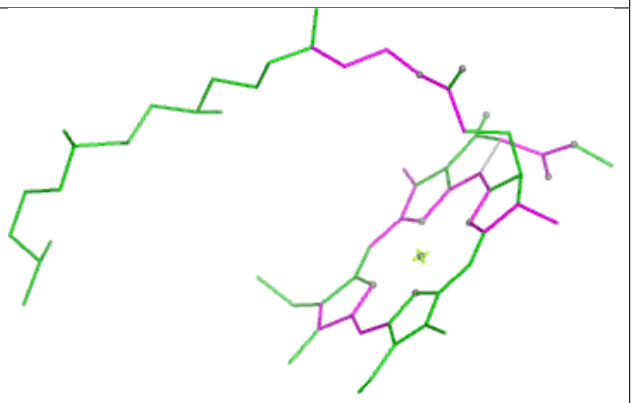


Rings

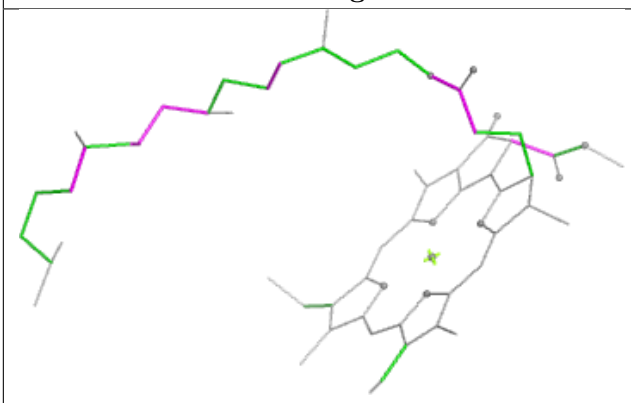
Ligand CLA C 508



Bond lengths



Bond angles

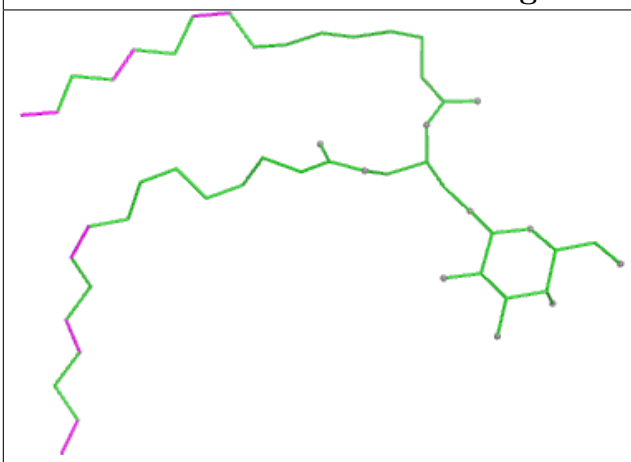


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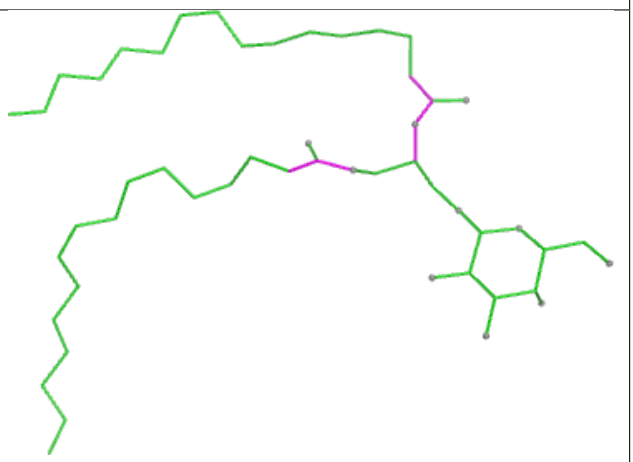


Rings

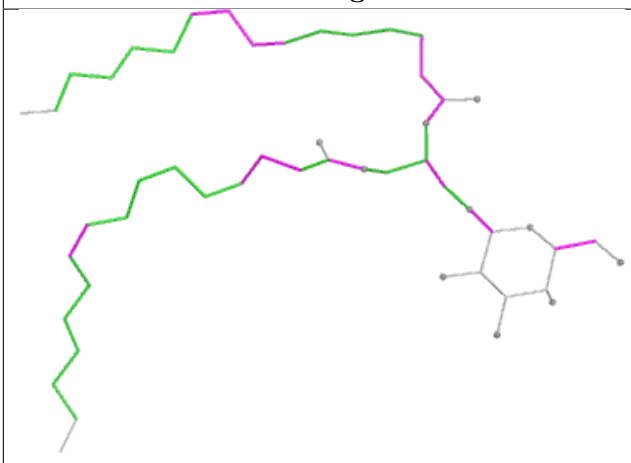
Ligand LMG C 521



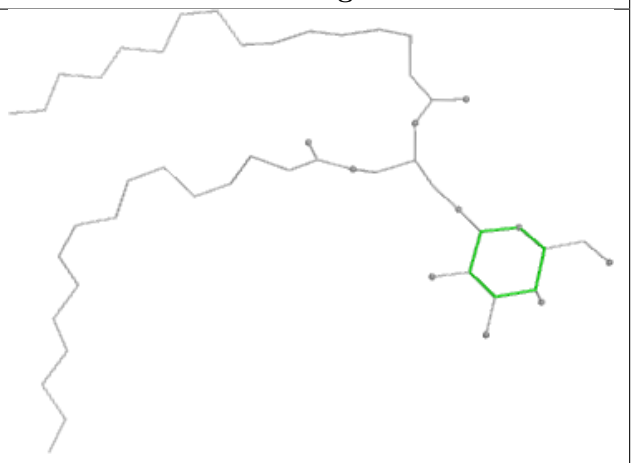
Bond lengths



Bond angles

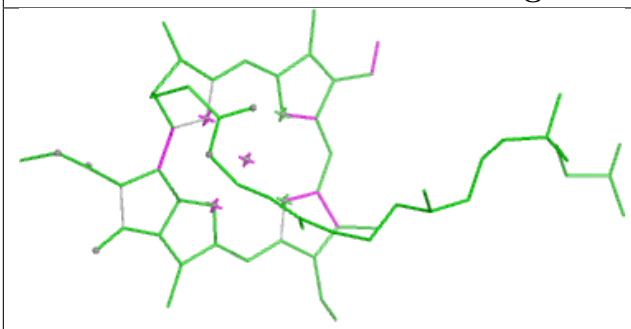


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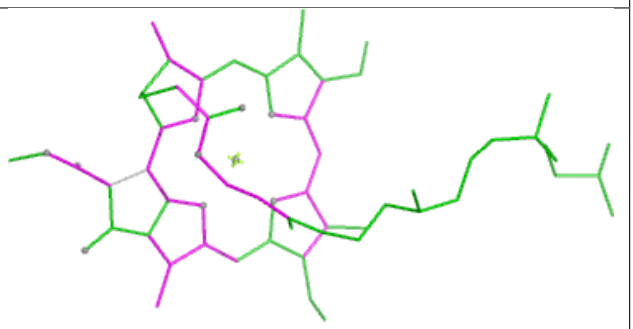


Rings

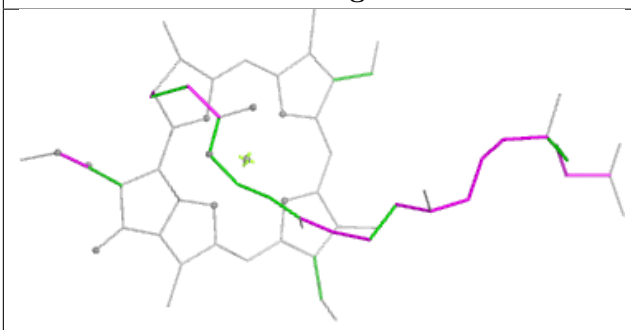
Ligand CLA C 513



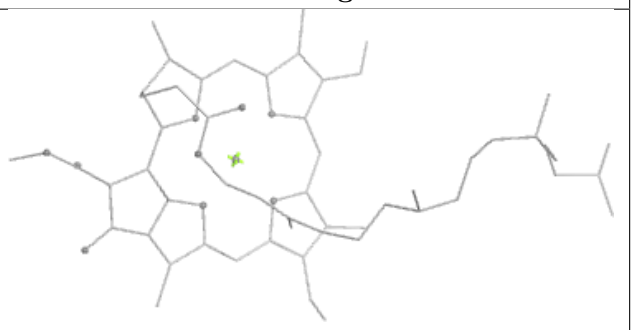
Bond lengths



Bond angles



Torsions

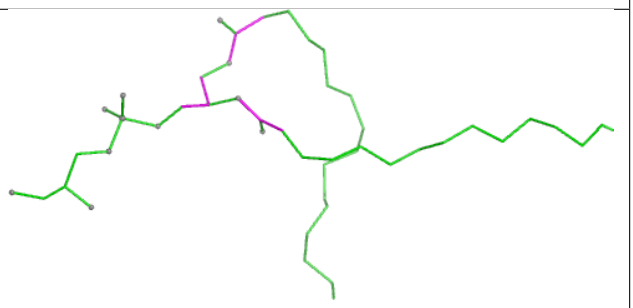


Rings

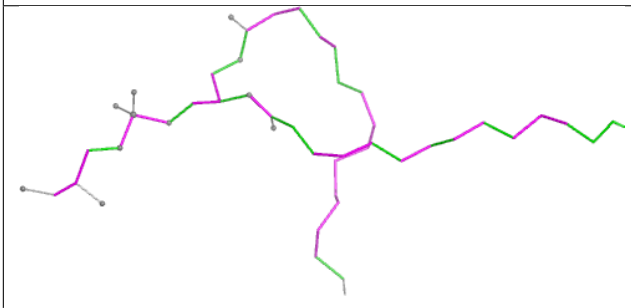
Ligand LHG Y 624



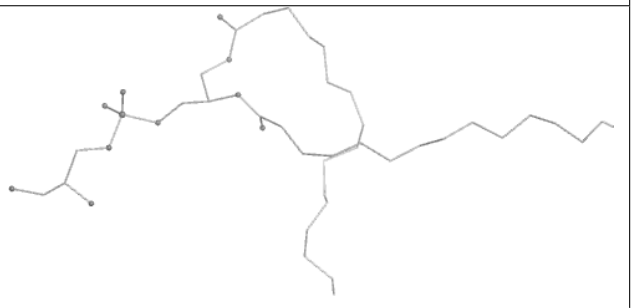
Bond lengths



Bond angles

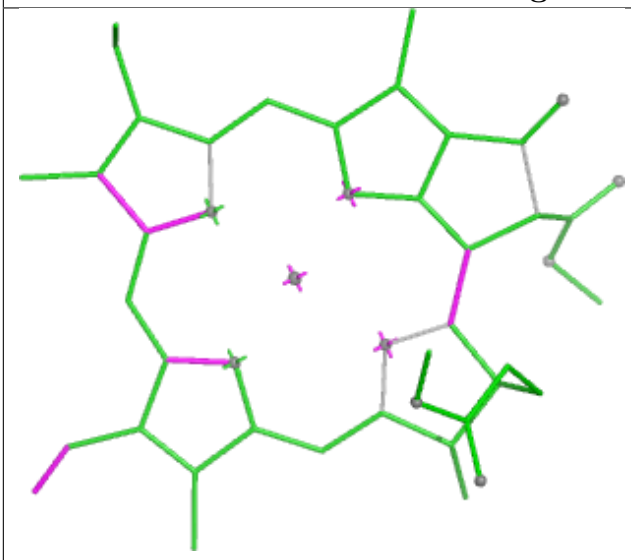


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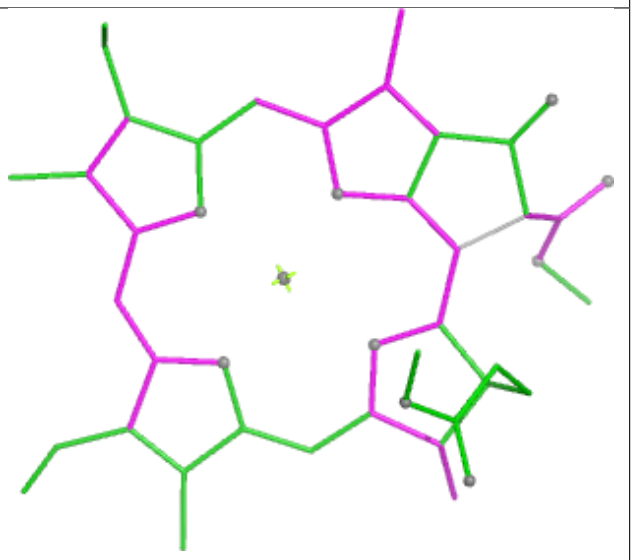


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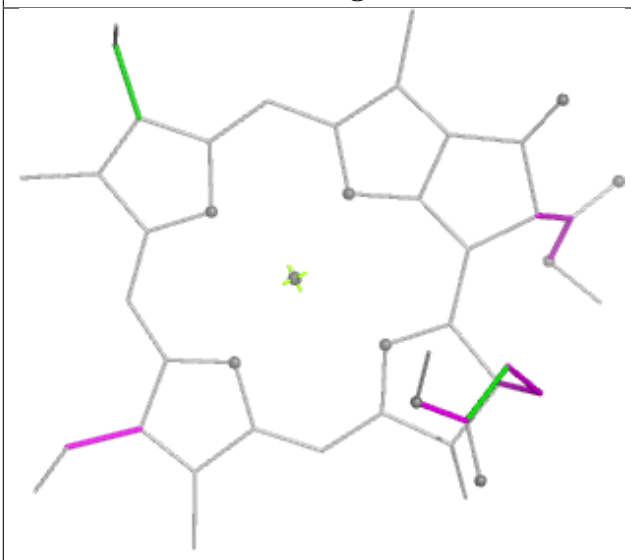
Ligand CLA r 613



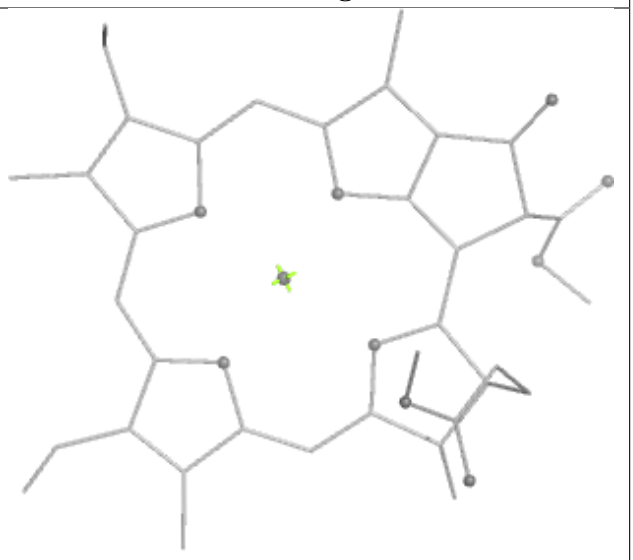
Bond lengths



Bond angles

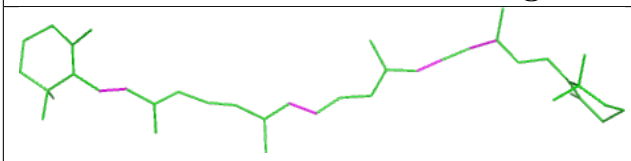


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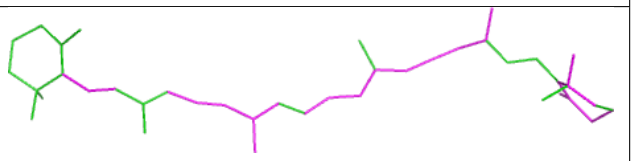


Rings

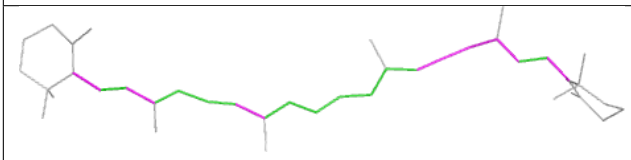
Ligand BCR B 618



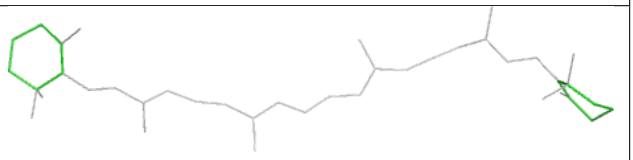
Bond lengths



Bond angles

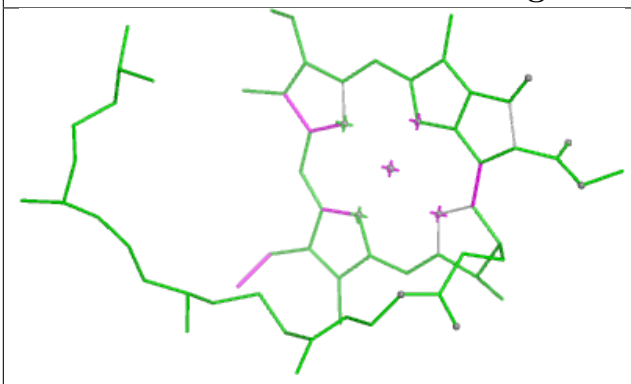


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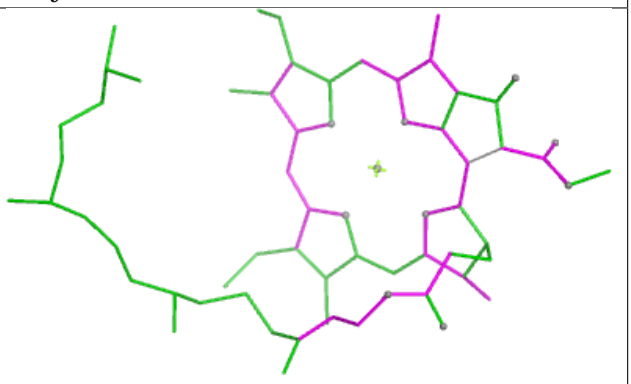


Rings

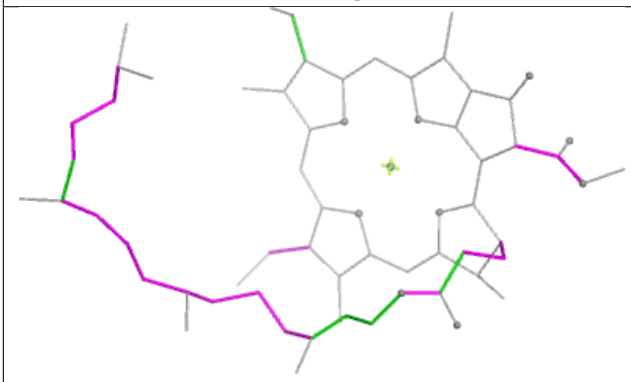
Ligand CLA y 610



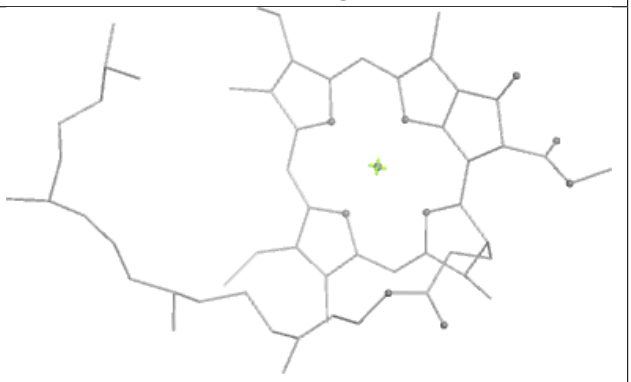
Bond lengths



Bond angles

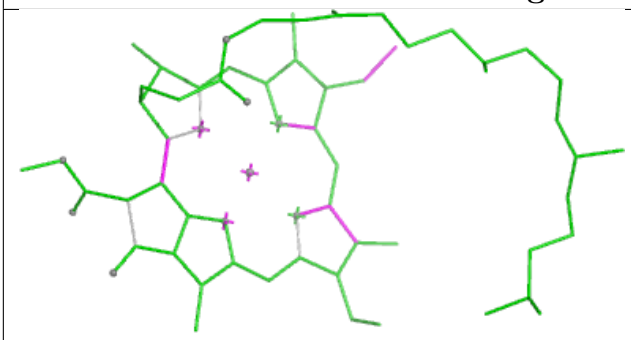


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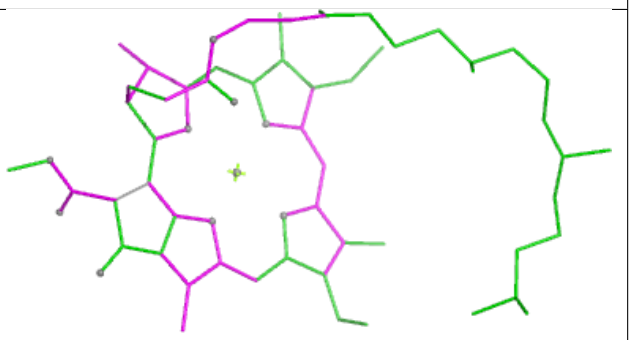


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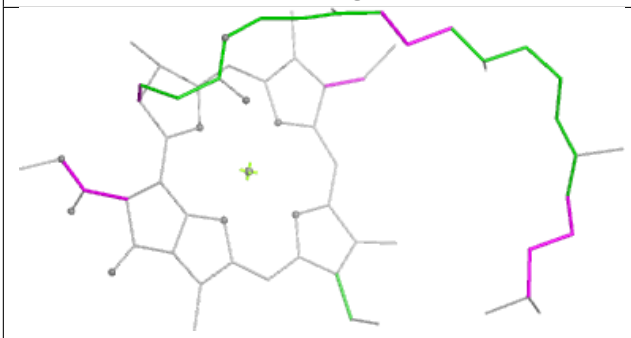
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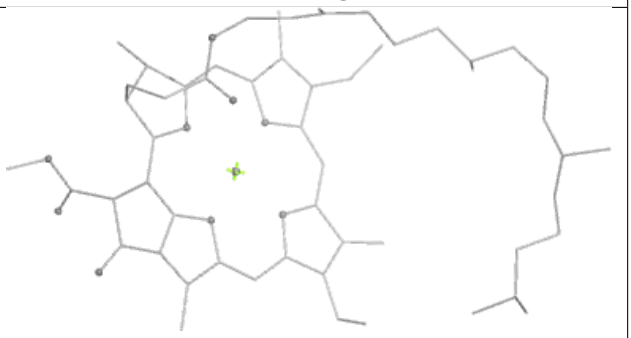
Bond lengths



Bond angles

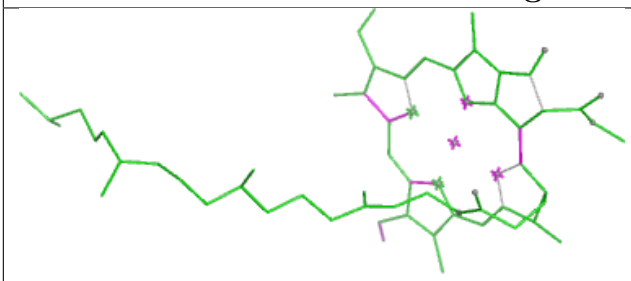


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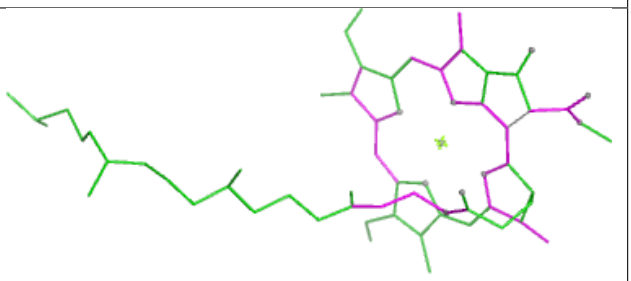


Rings

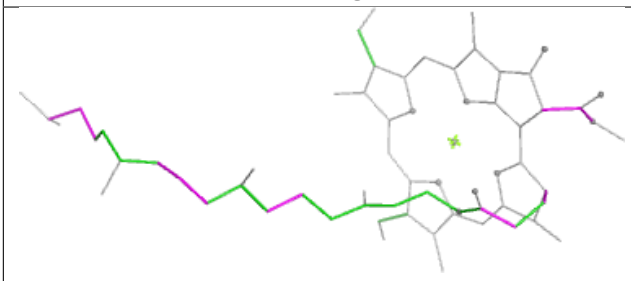
Ligand CLA B 609



Bond lengths



Bond angles

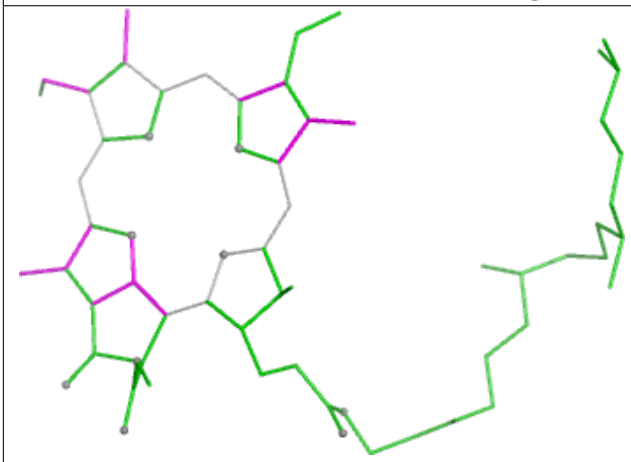


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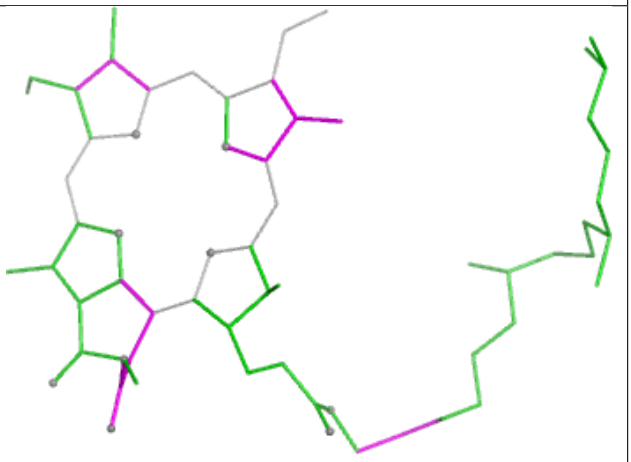


Rings

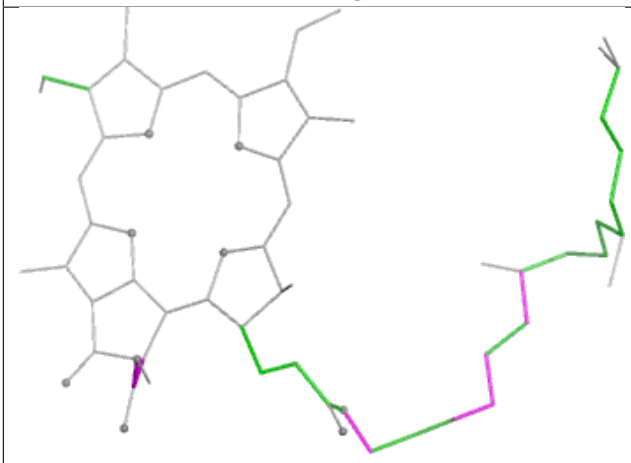
Ligand PHO a 409



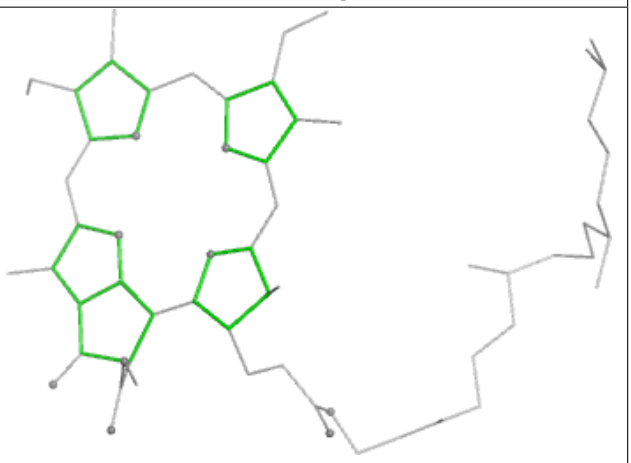
Bond lengths



Bond angles

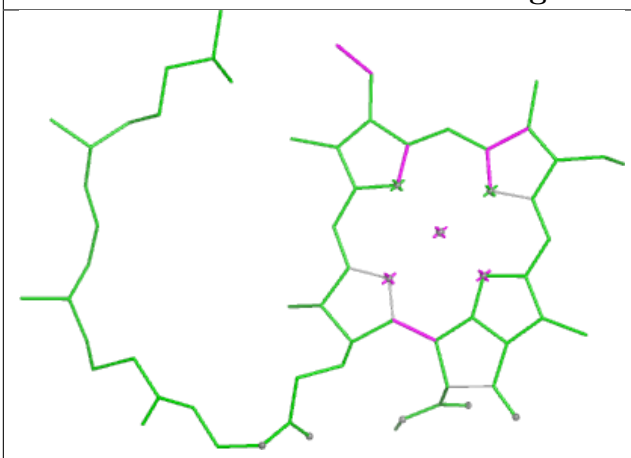


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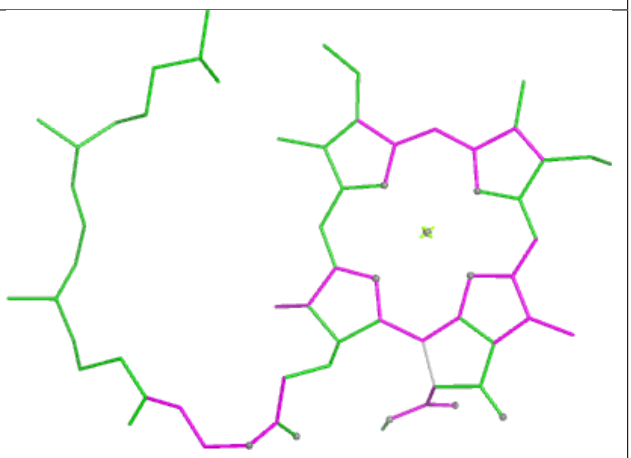


Rings

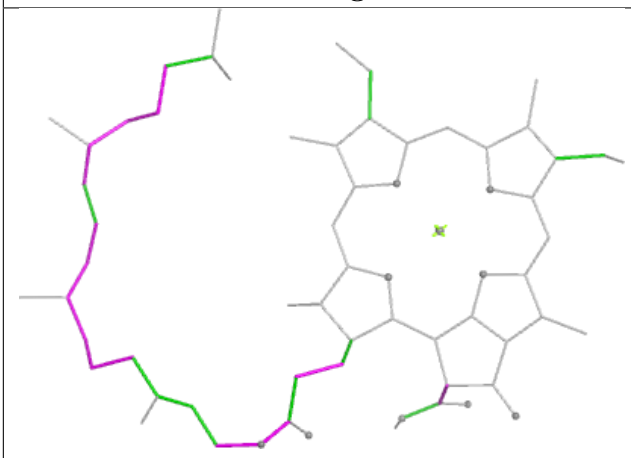
Ligand CLA c 512



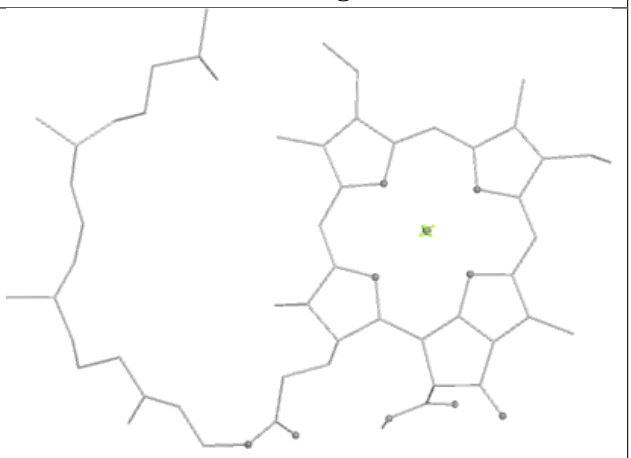
Bond lengths



Bond angles

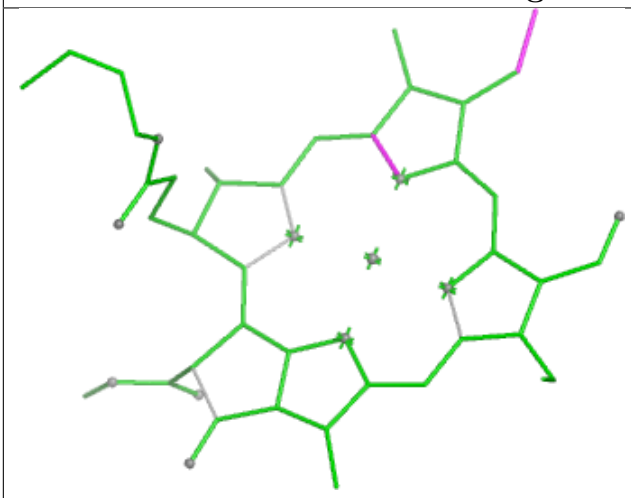


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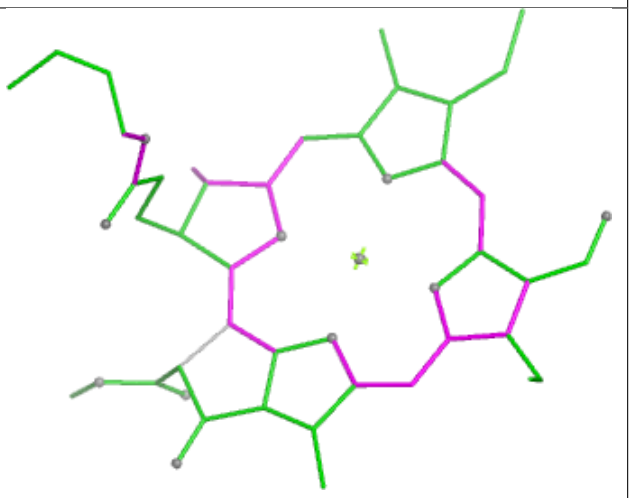


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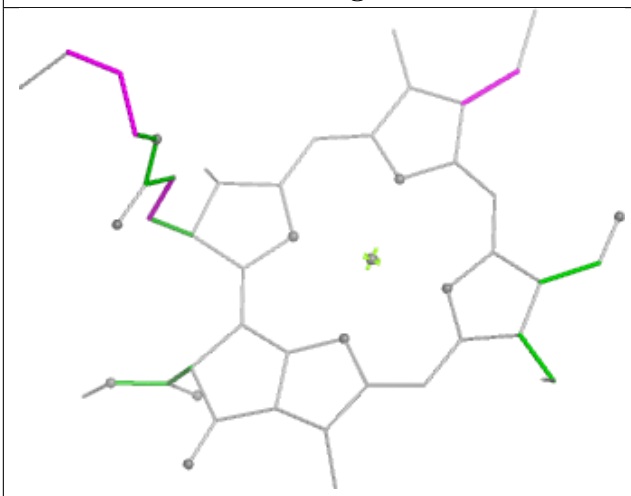
Ligand CHL n 608



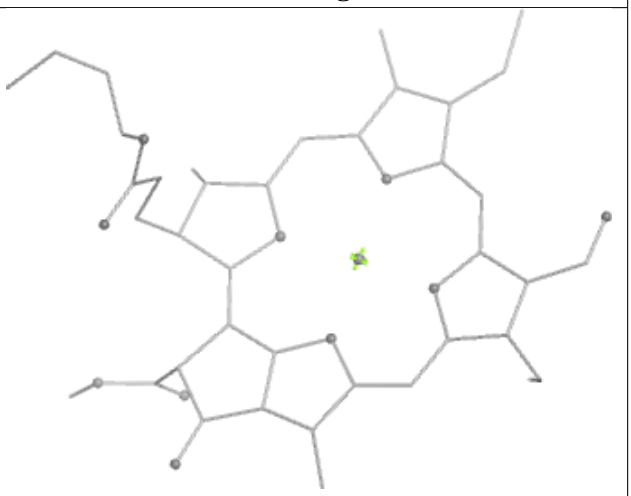
Bond lengths



Bond angles

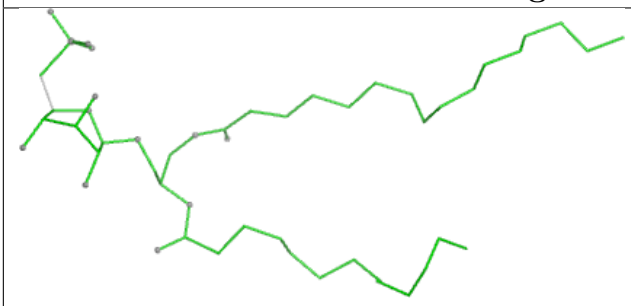


Torsions

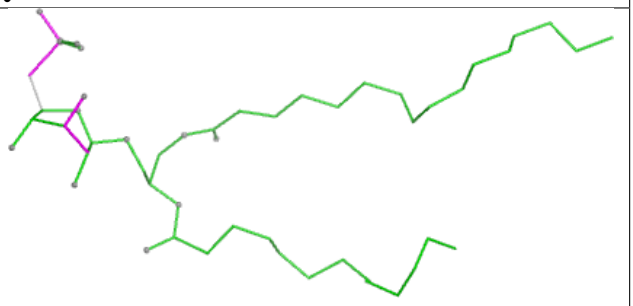


Rings

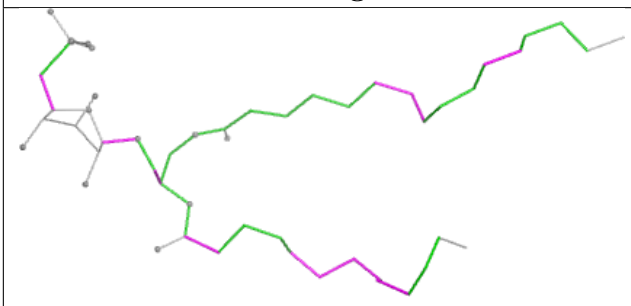
Ligand SQD a 412



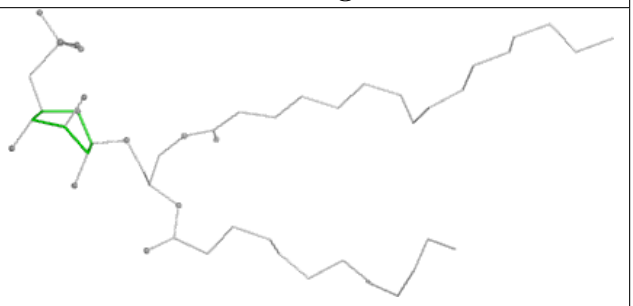
Bond lengths



Bond angles

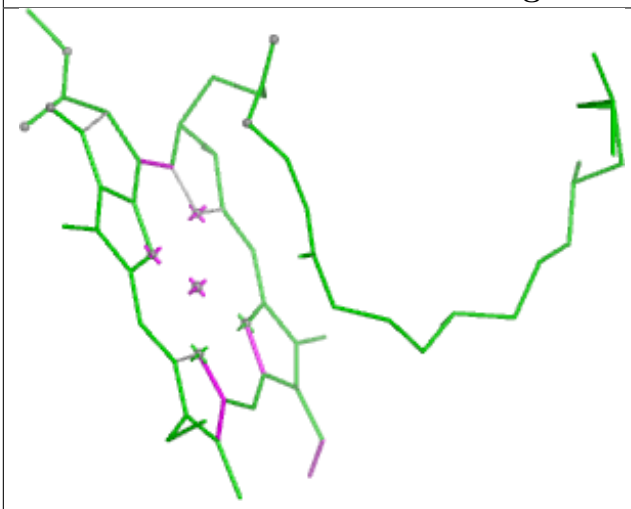


Torsions

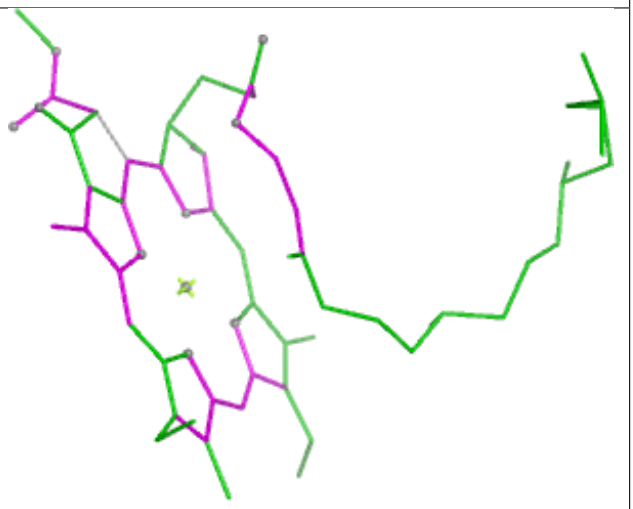


Rings

Ligand CLA G 613



Bond lengths



Bond angles

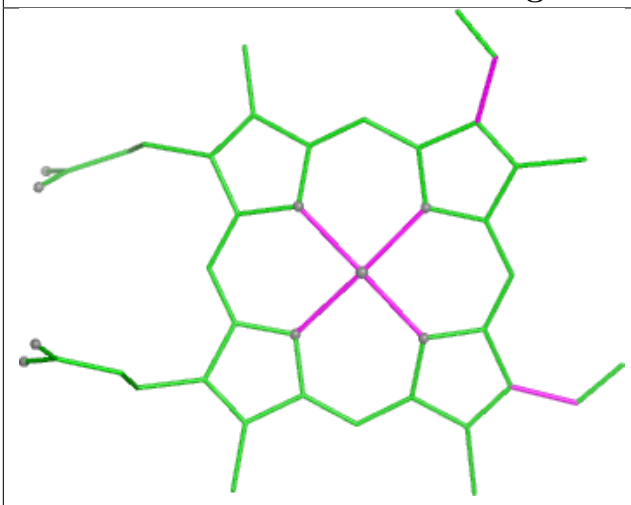


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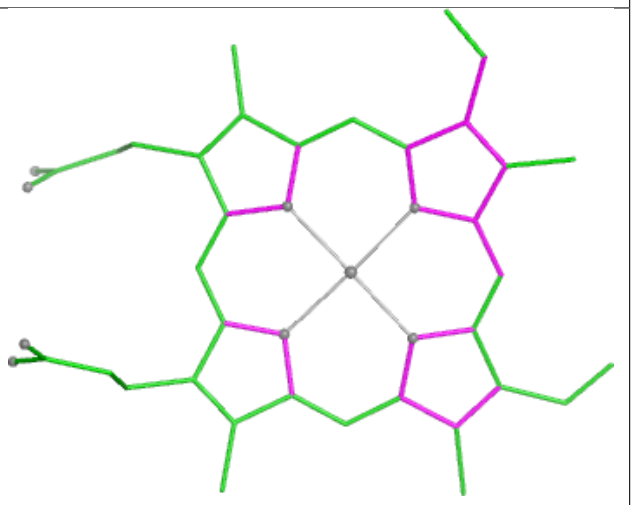


Rings

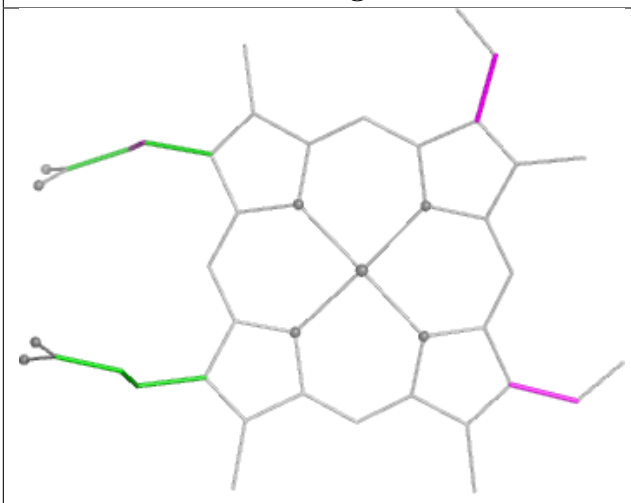
Ligand HEM f 101



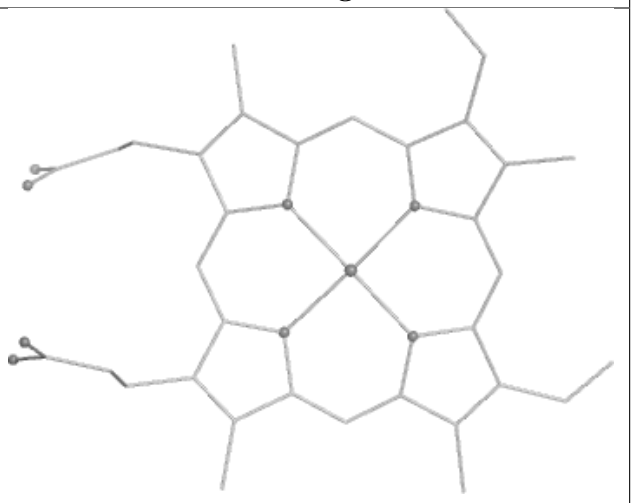
Bond lengths



Bond angles

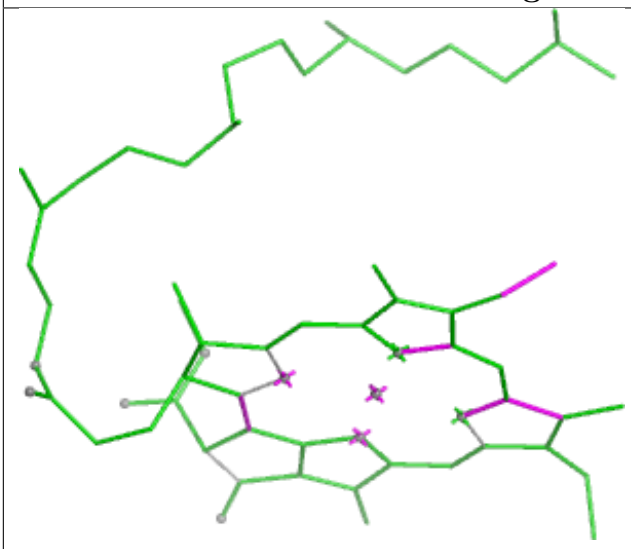


Torsions

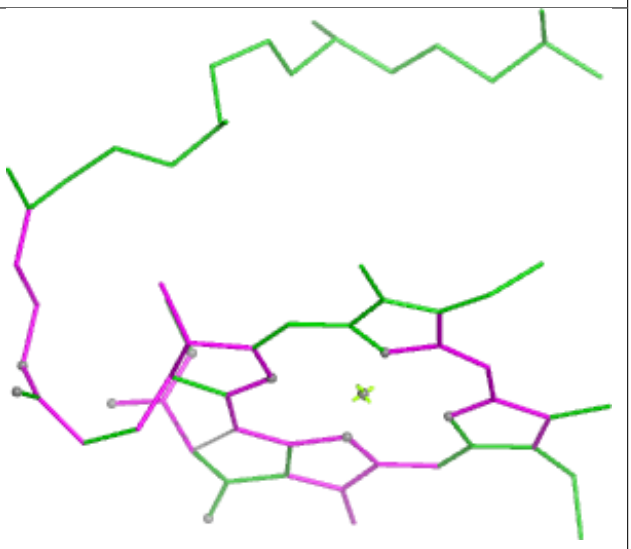


Rings

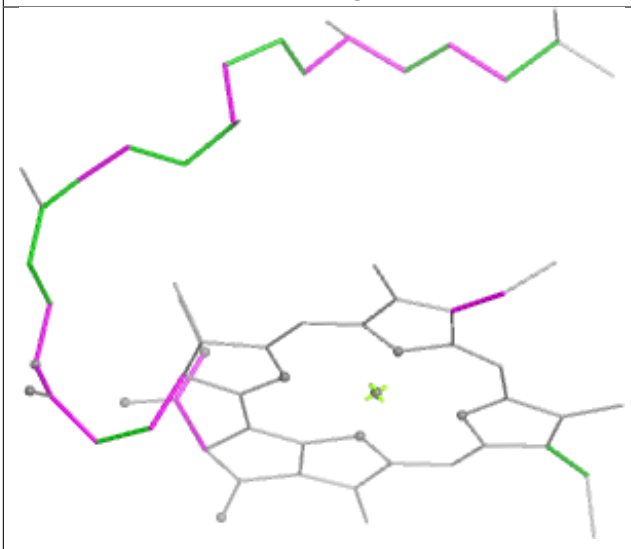
Ligand CLA G 603



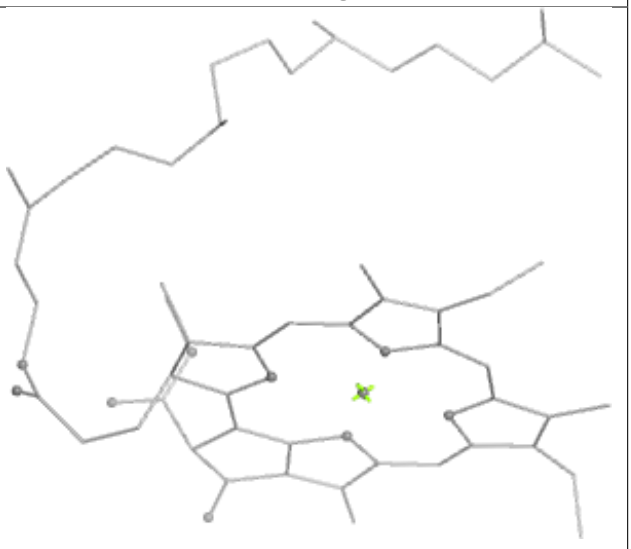
Bond lengths



Bond angles

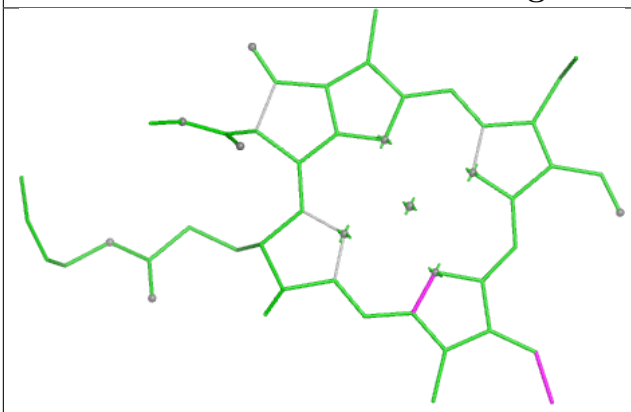


Torsions

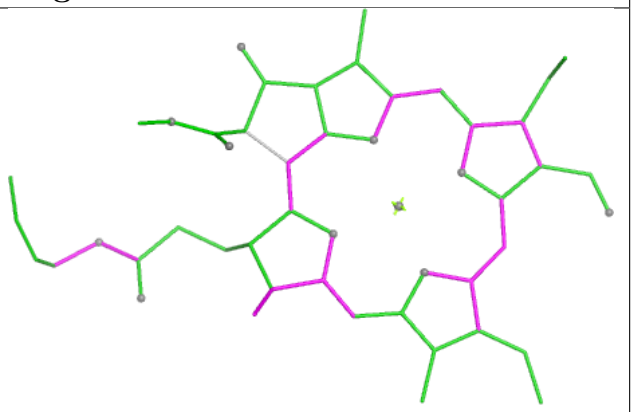


Rings

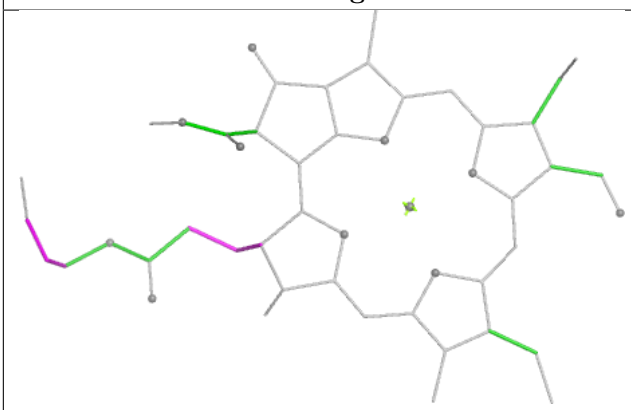
Ligand CHL g 606



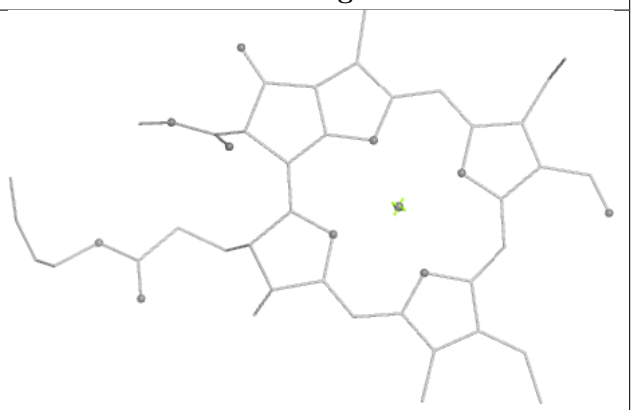
Bond lengths



Bond angles

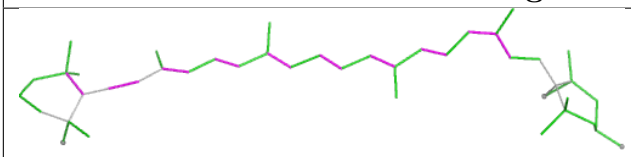


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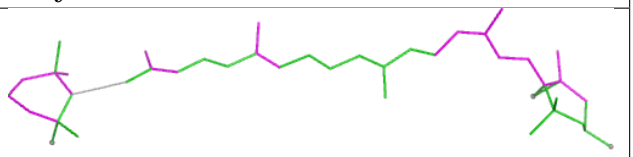


Rings

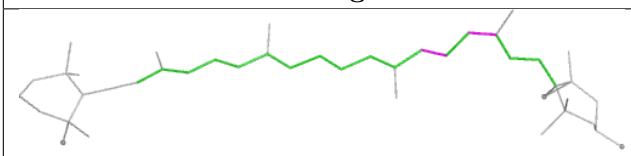
Ligand NEX y 623



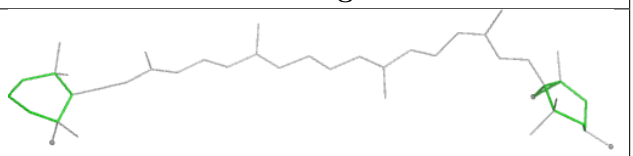
Bond lengths



Bond angles

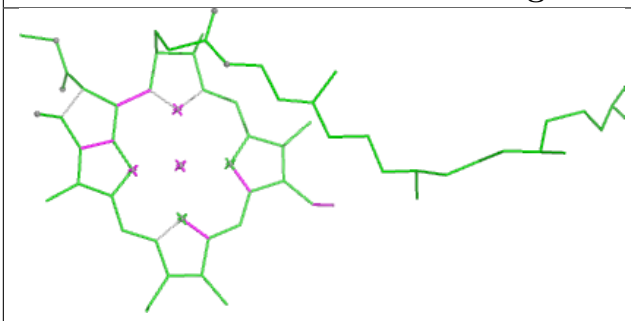


Torsions

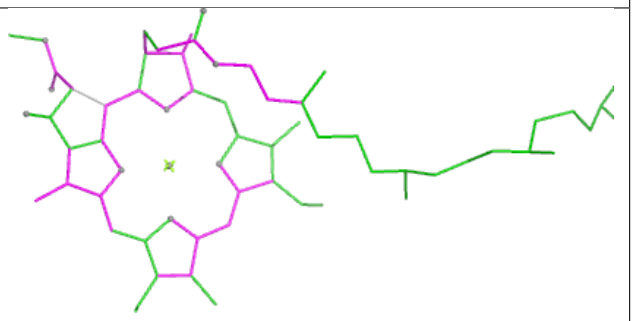


Rings

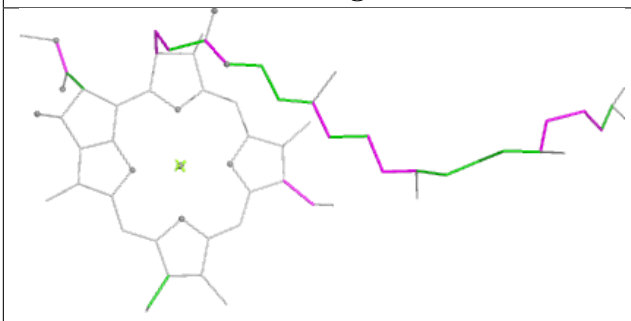
Ligand CLA b 604



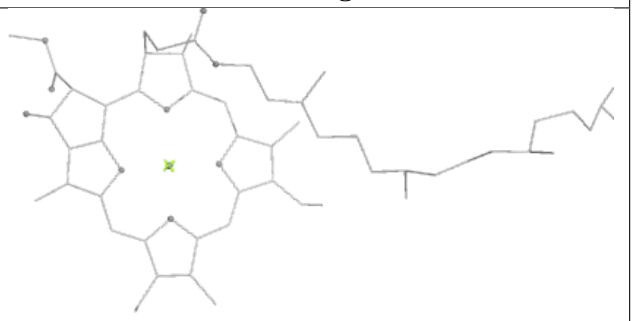
Bond lengths



Bond angles

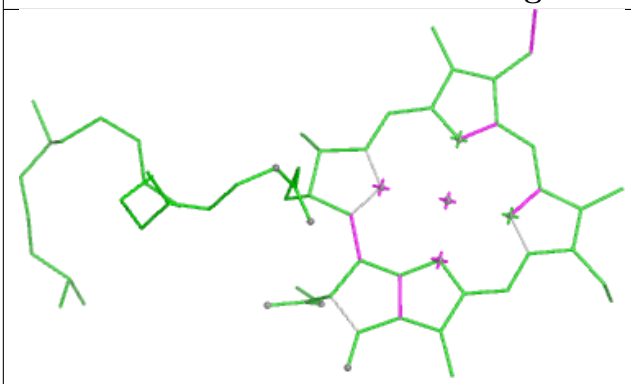


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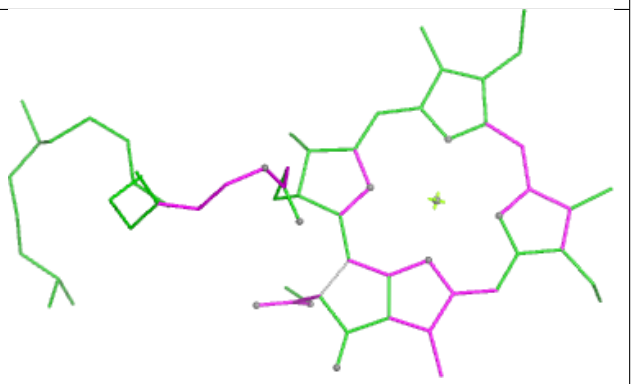


Rings

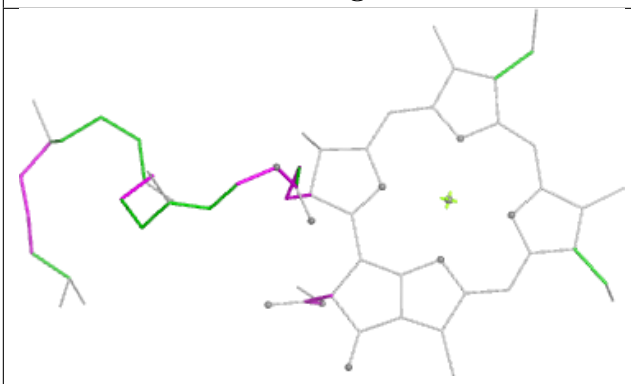
Ligand CLA B 613



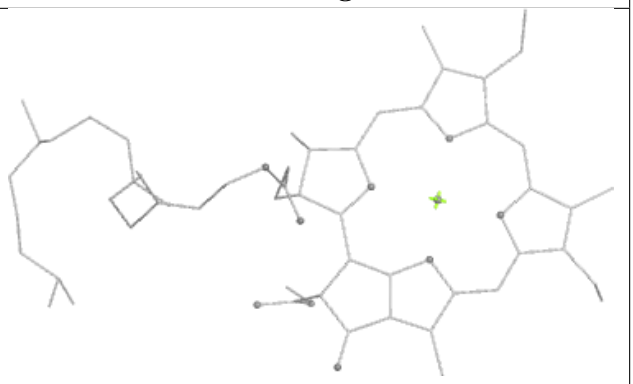
Bond lengths



Bond angles

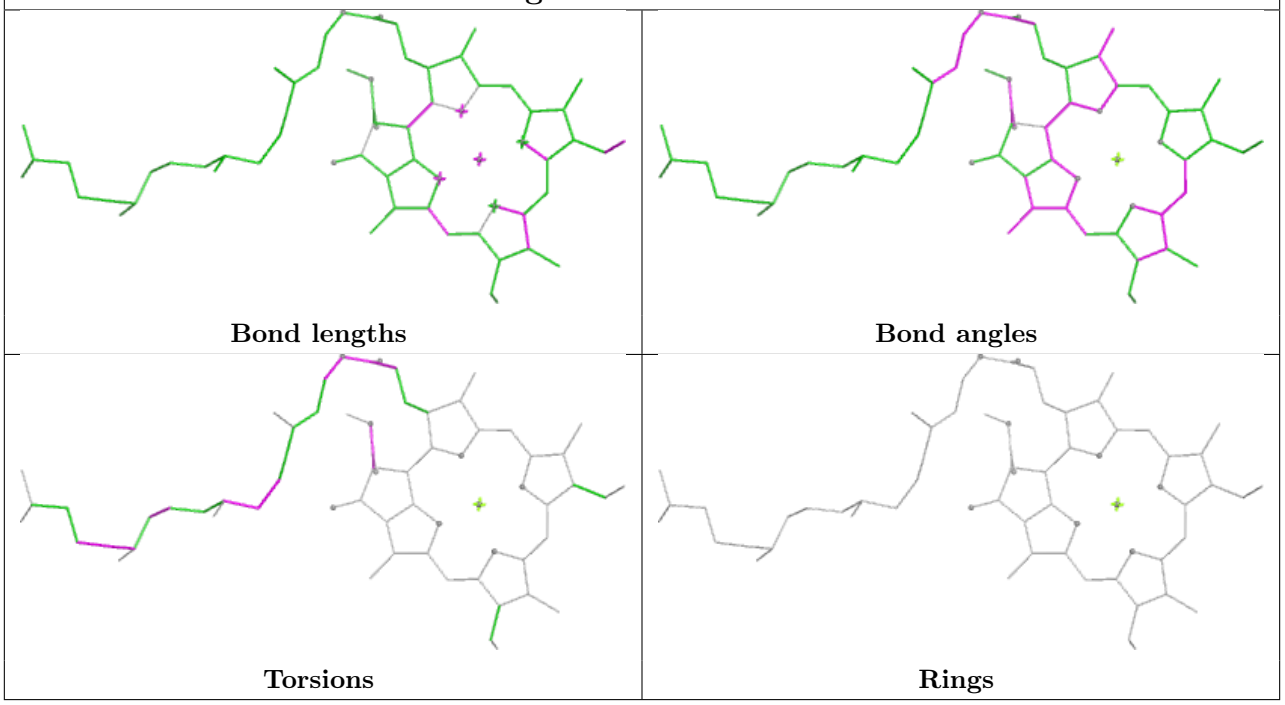


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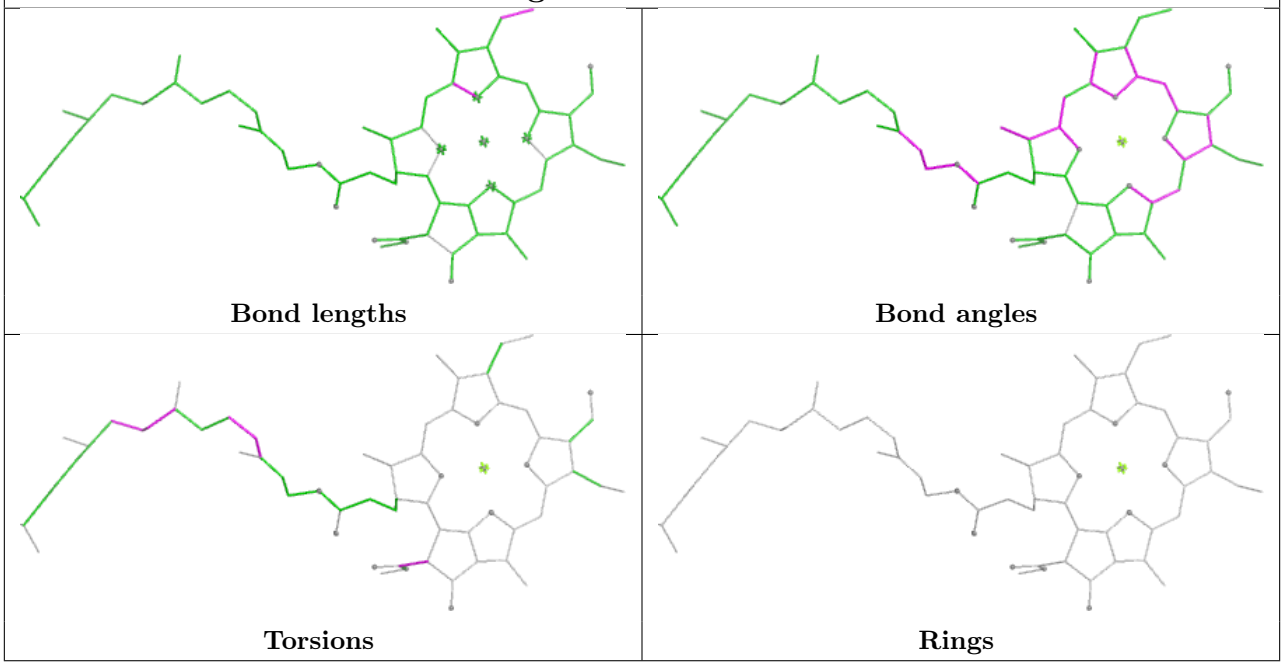


Rings

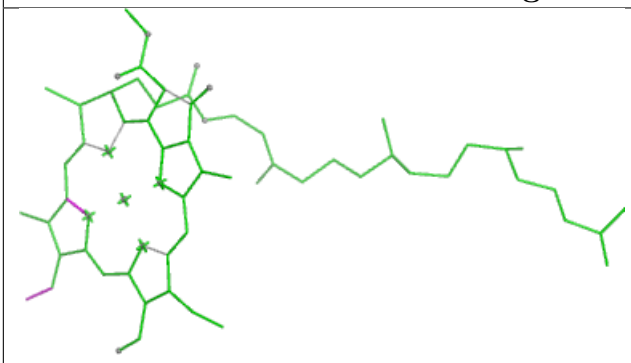
Ligand CLA B 603



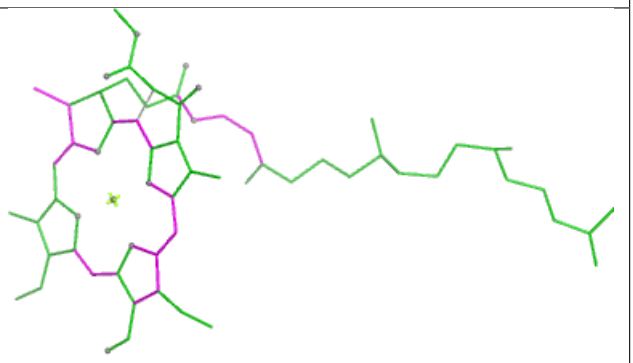
Ligand CHL n 601



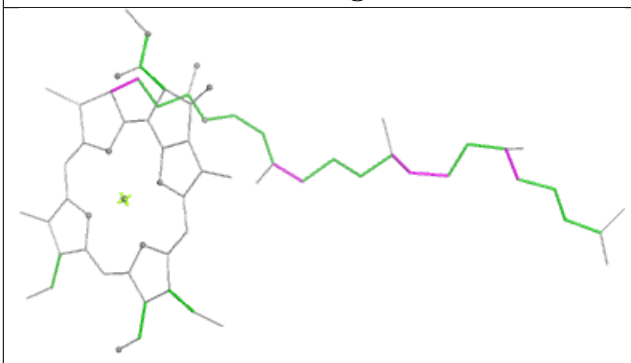
Ligand CHL N 609



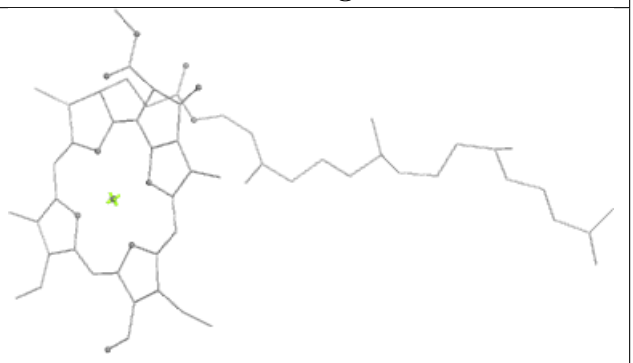
Bond lengths



Bond angles

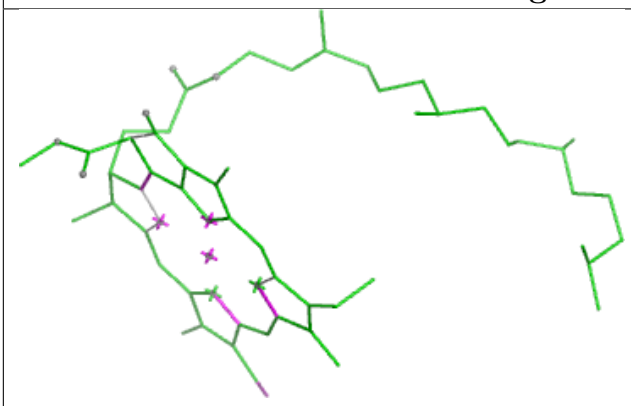


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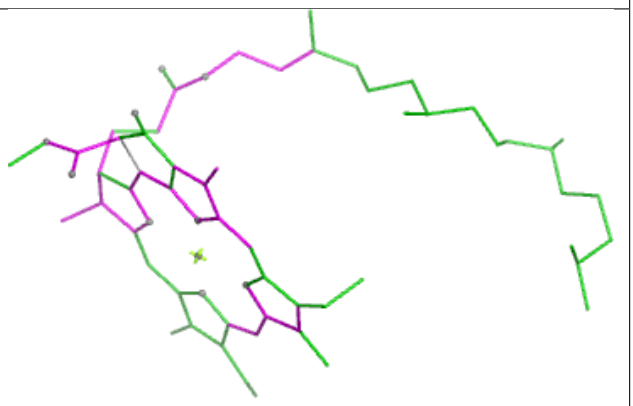


Rings

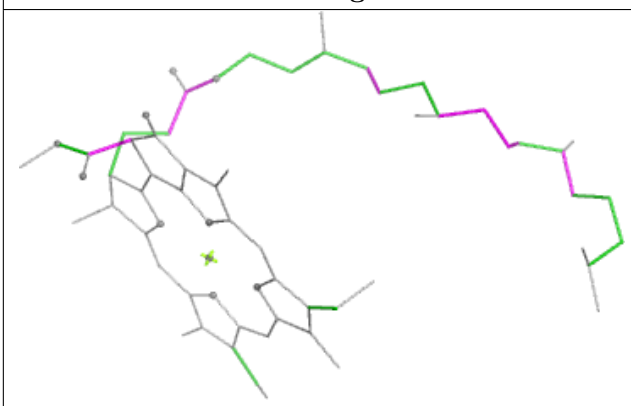
Ligand CLA c 508



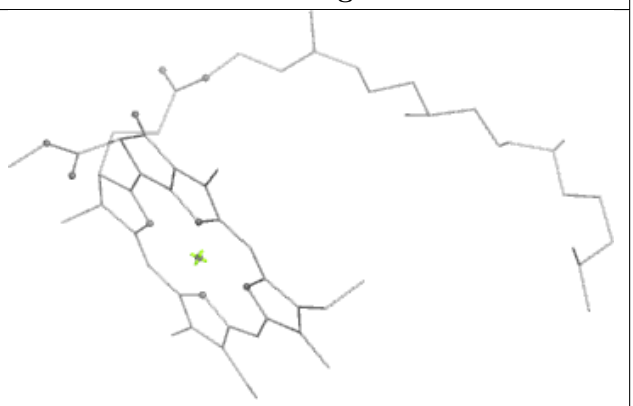
Bond lengths



Bond angles

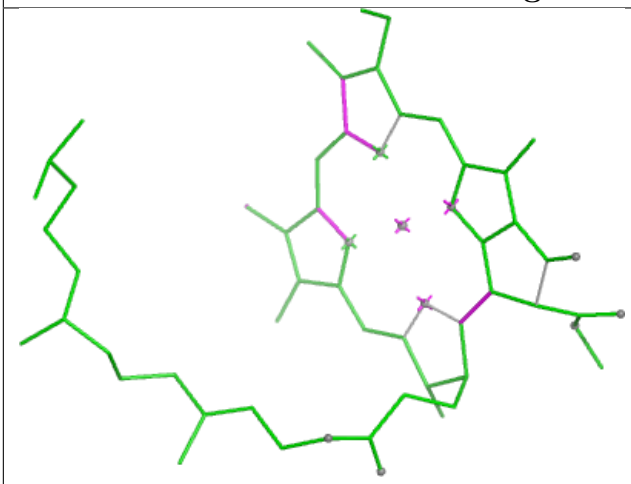


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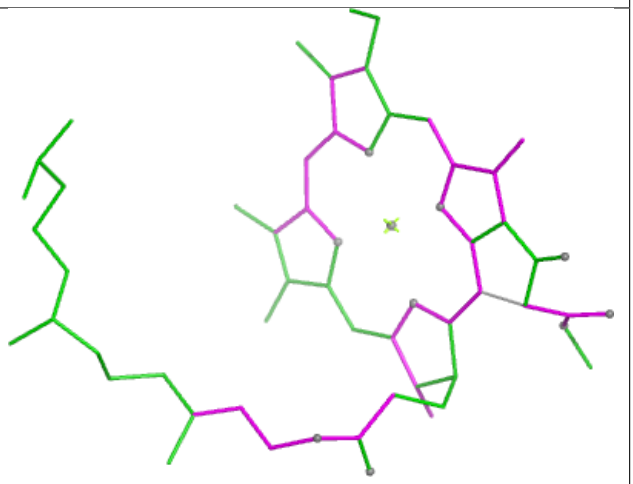


Rings

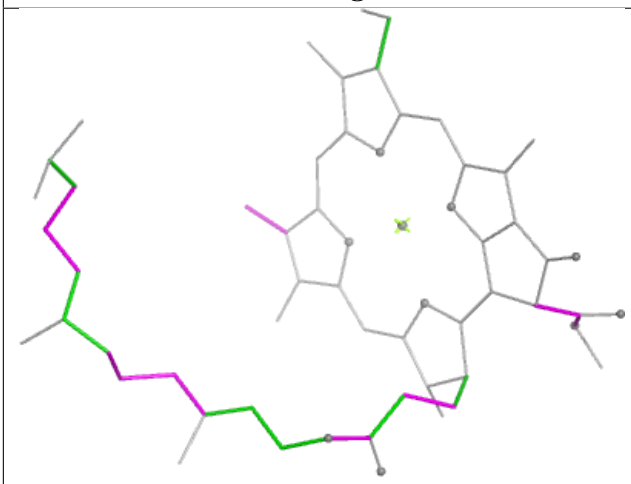
Ligand CLA R 602



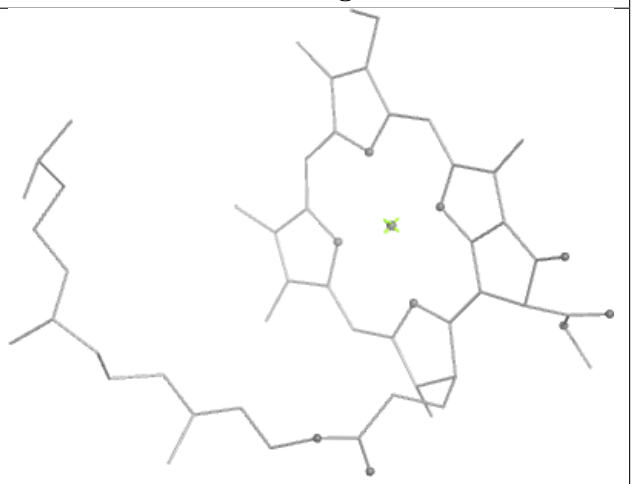
Bond lengths



Bond angles

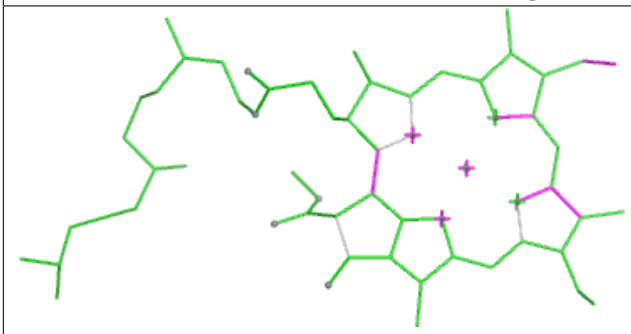


Torsions

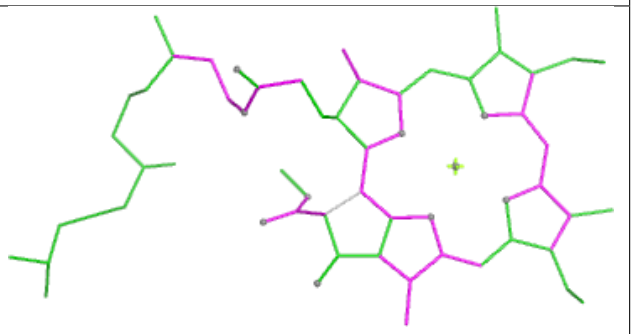


Rings

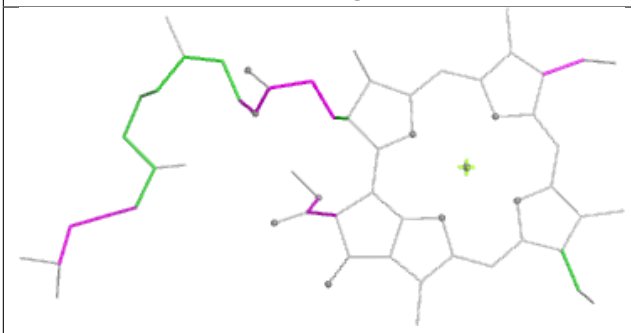
Ligand CLA R 612



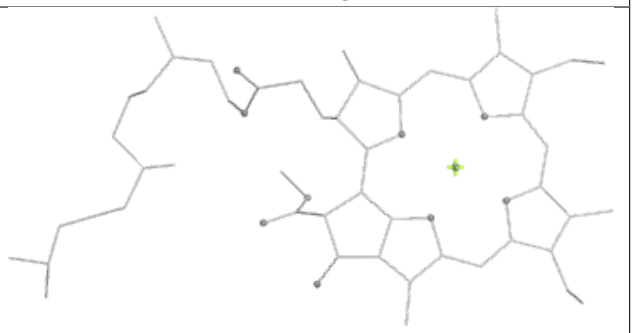
Bond lengths



Bond angles

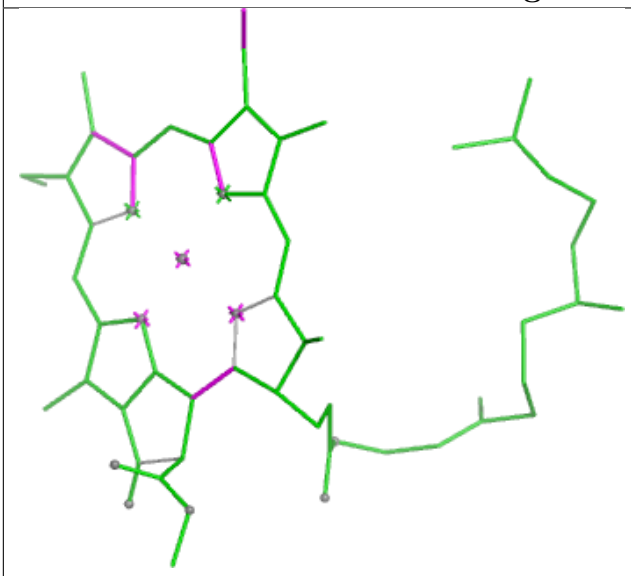


Torsions

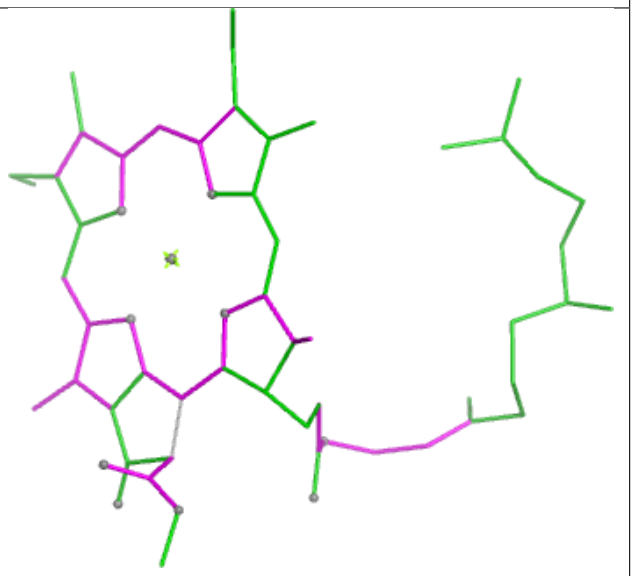


Rings

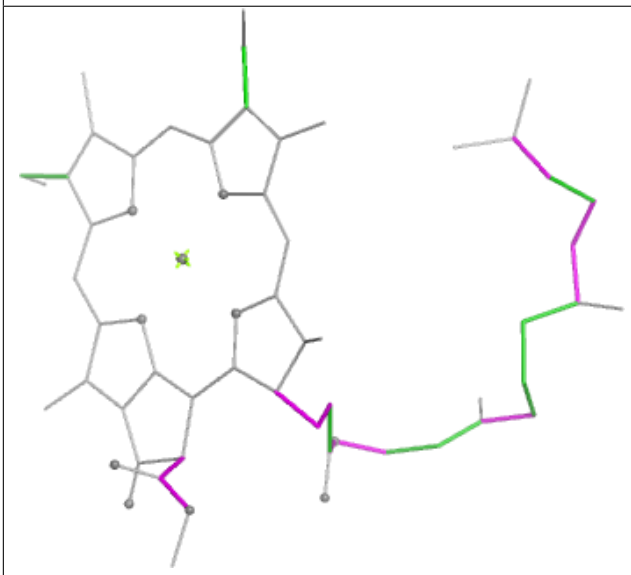
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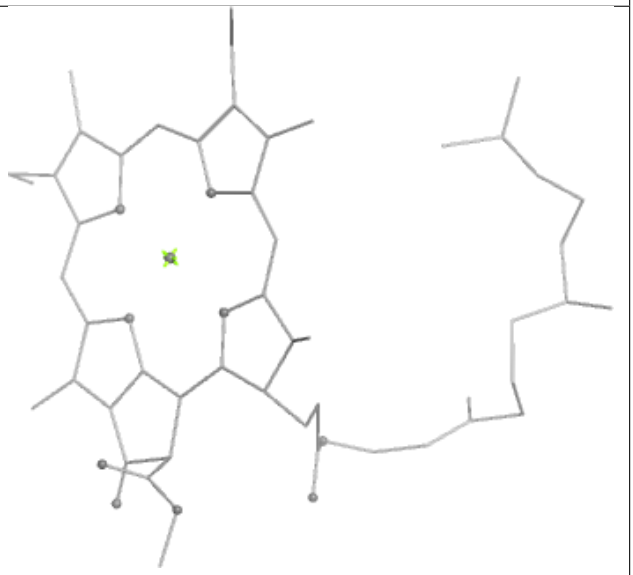
Bond lengths



Bond angles

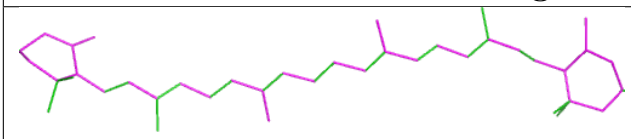


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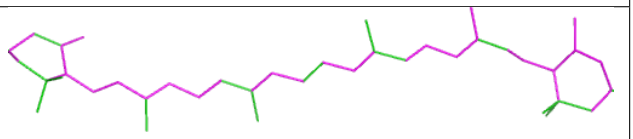


Rings

Ligand C7Z b 620



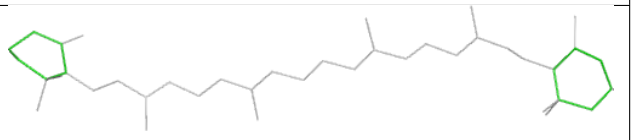
Bond lengths



Bond angles

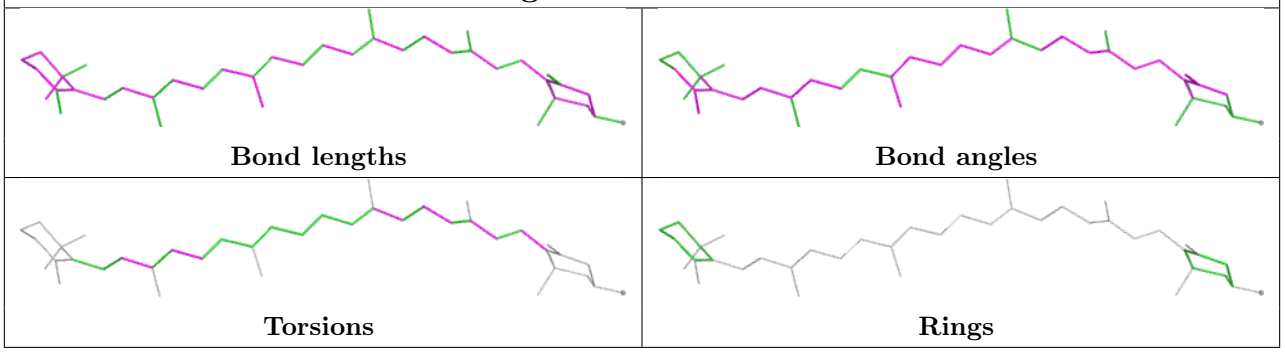


Torsions

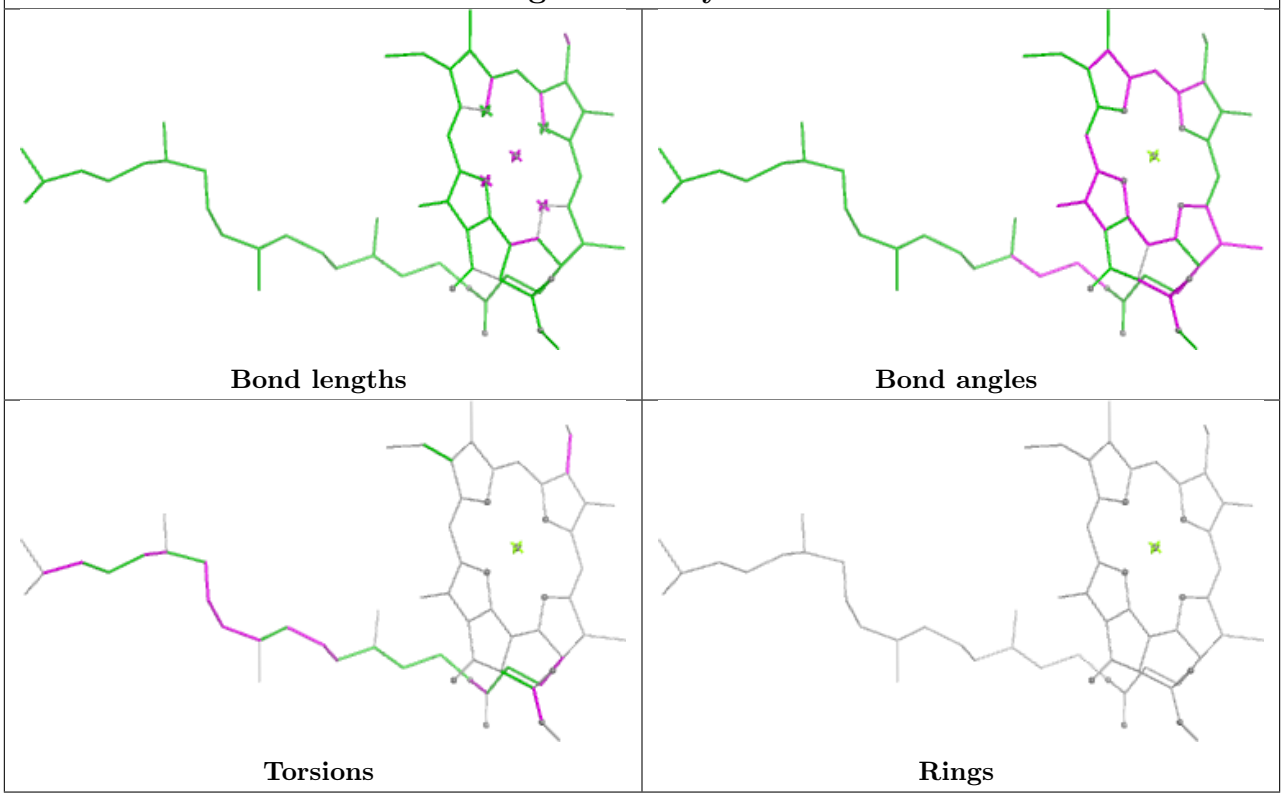


Rings

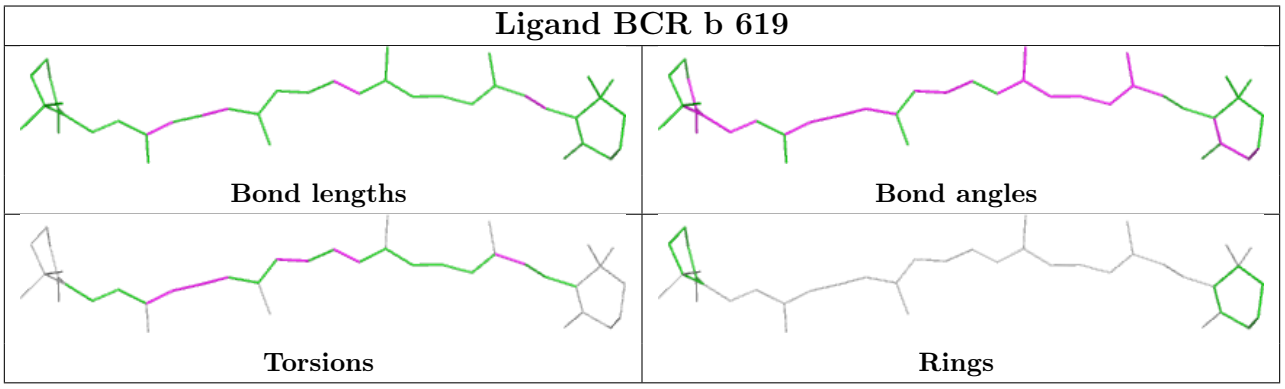
Ligand RRX H 101



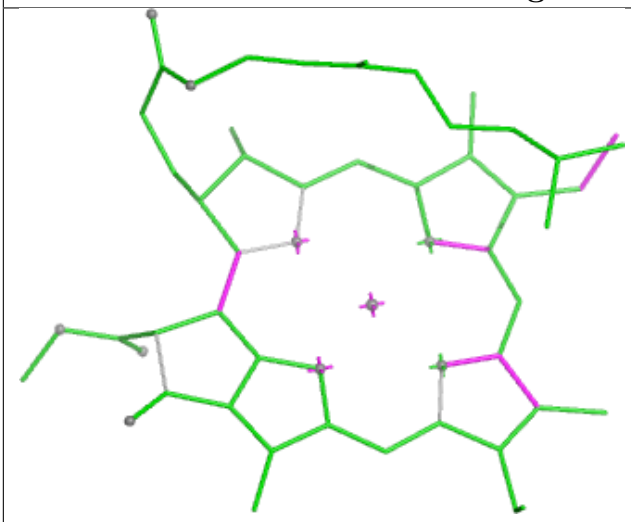
Ligand CLA y 611



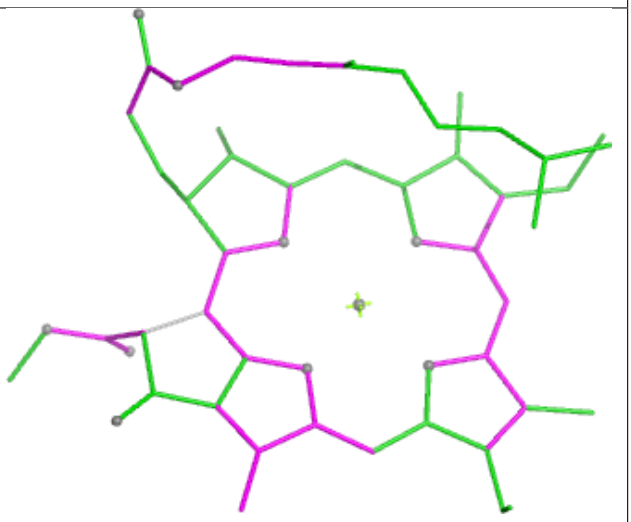
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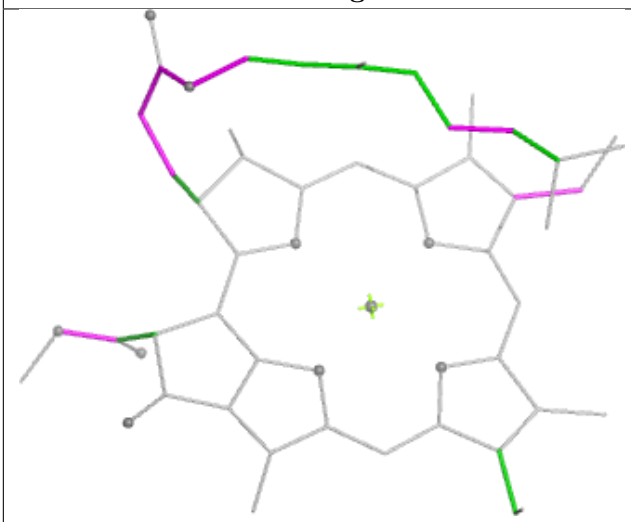
Ligand CLA S 614



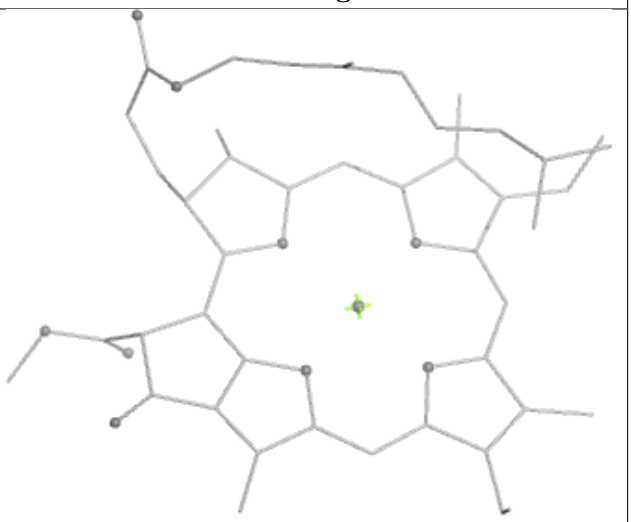
Bond lengths



Bond angles

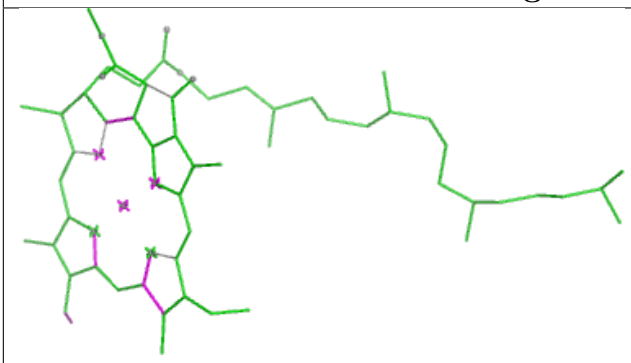


Torsions

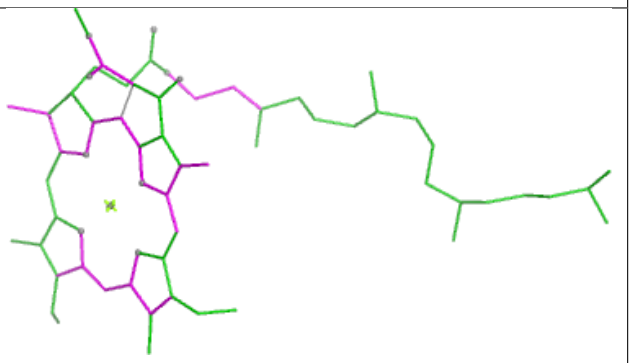


Rings

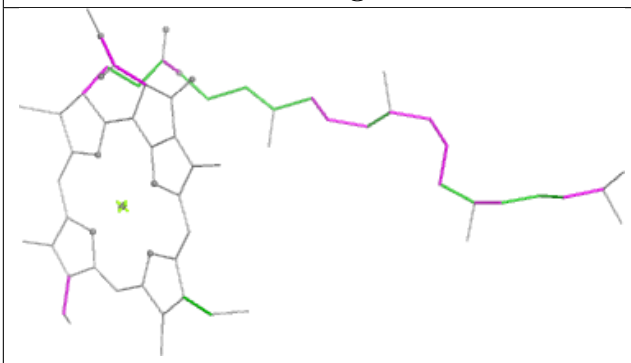
Ligand CLA Y 611



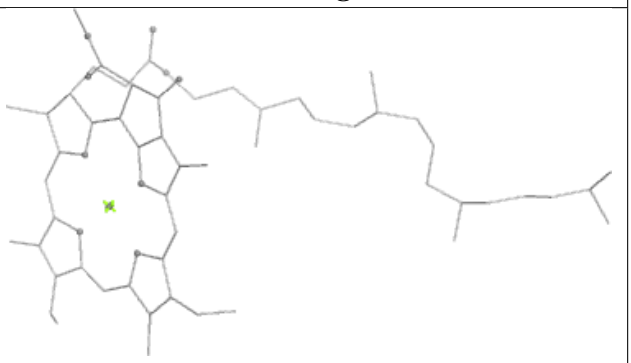
Bond lengths



Bond angles

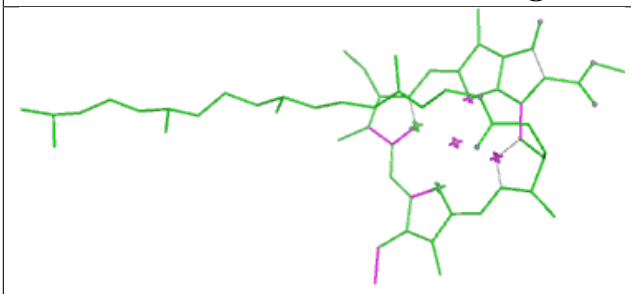


Torsions

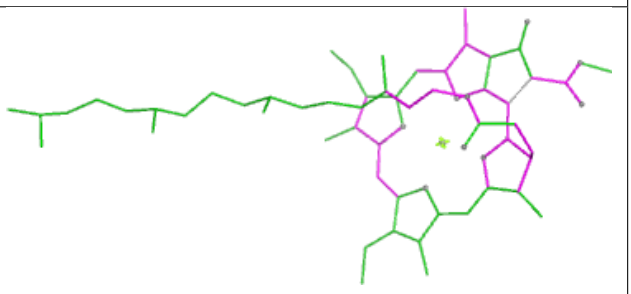


Rings

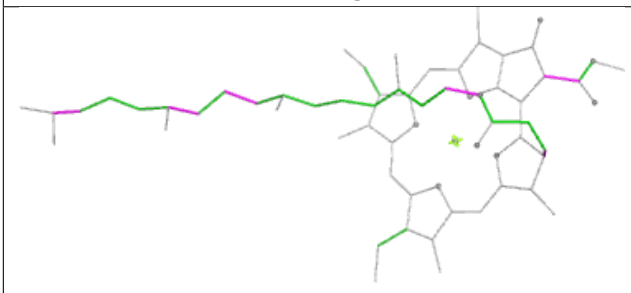
Ligand CLA b 615



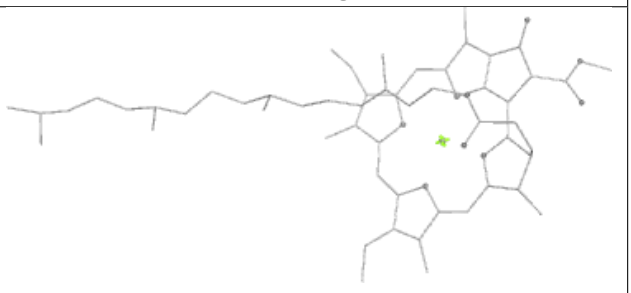
Bond lengths



Bond angles

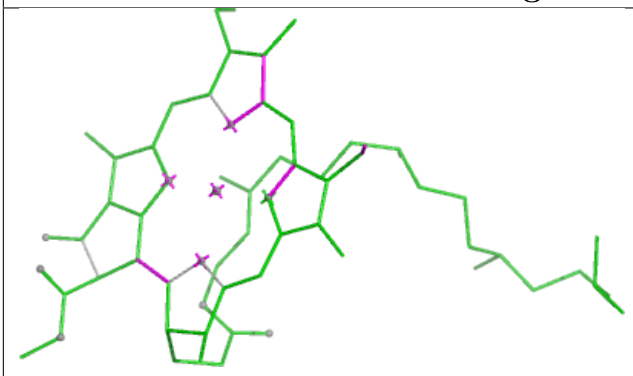


Torsions

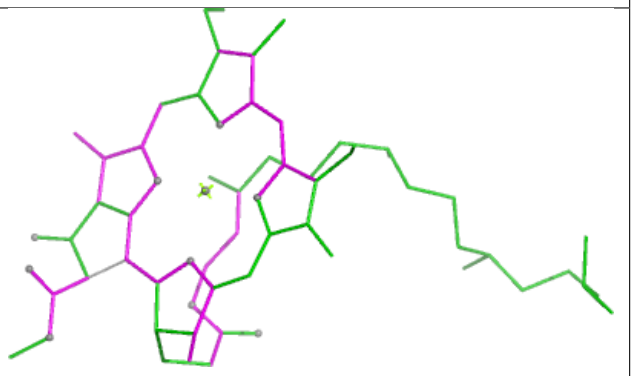


Rings

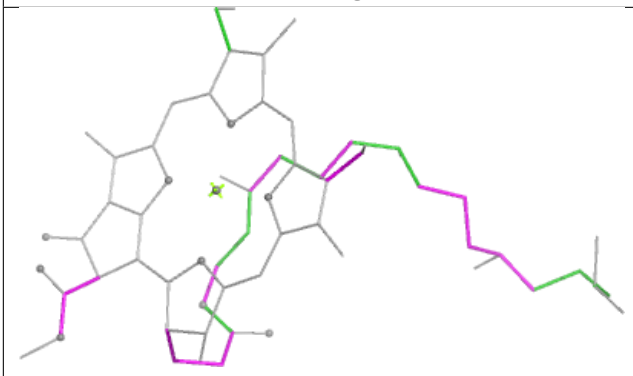
Ligand CLA N 613



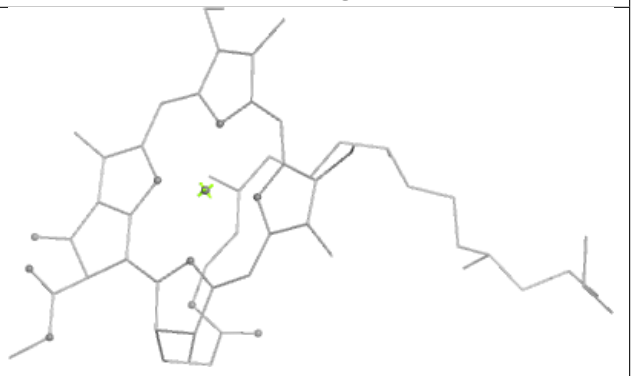
Bond lengths



Bond angles

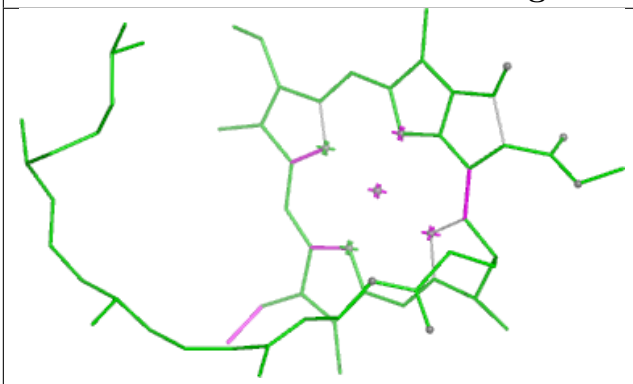


Torsions

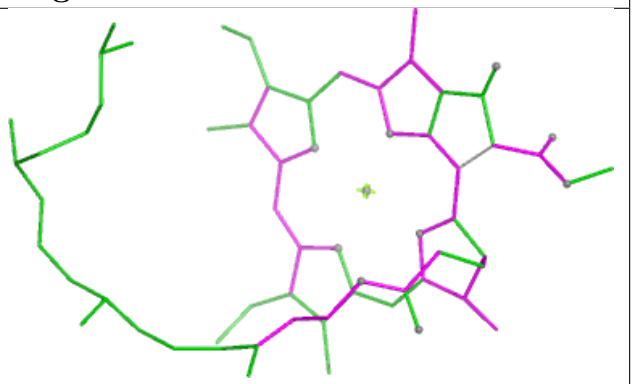


Rings

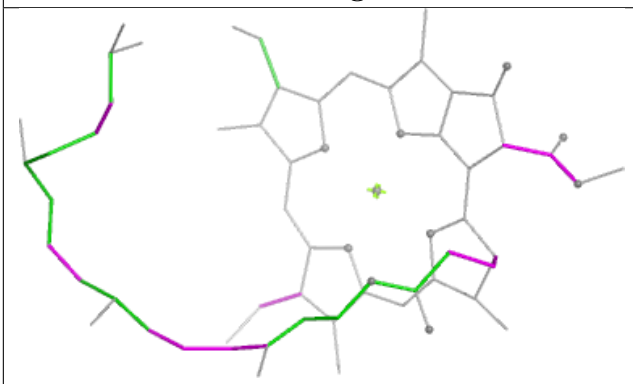
Ligand CLA g 610



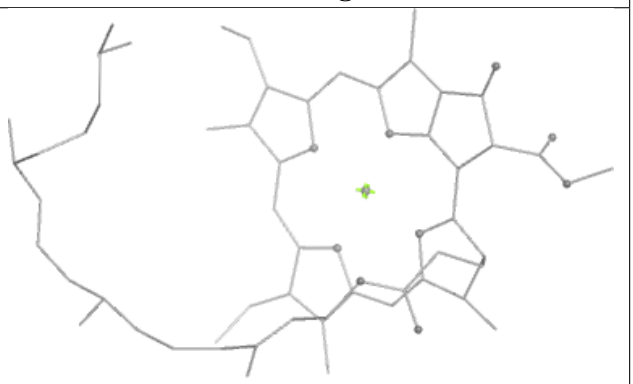
Bond lengths



Bond angles

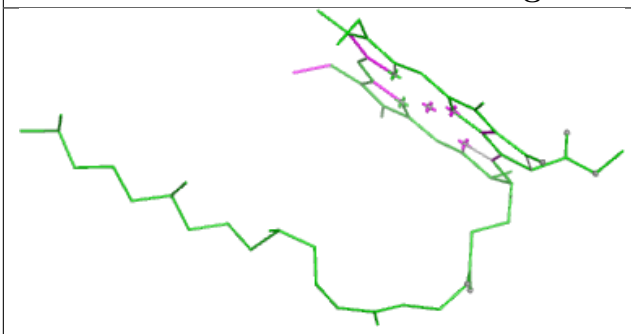


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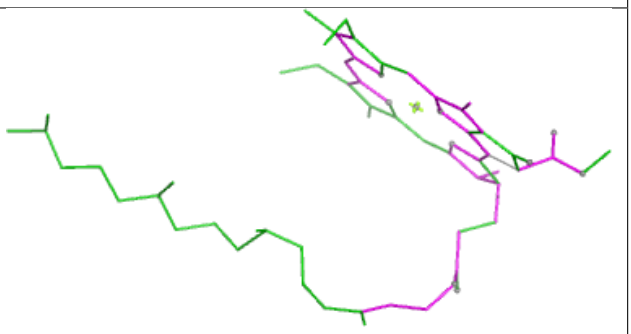


Rings

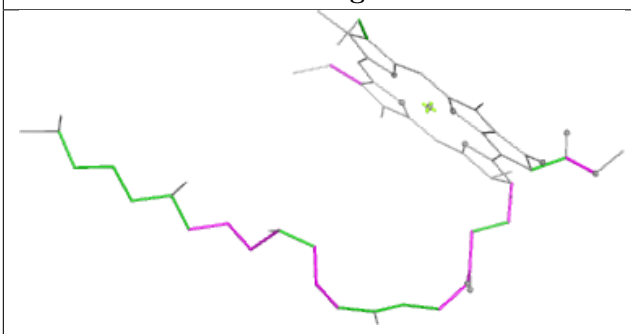
Ligand CLA Y 614



Bond lengths



Bond angles

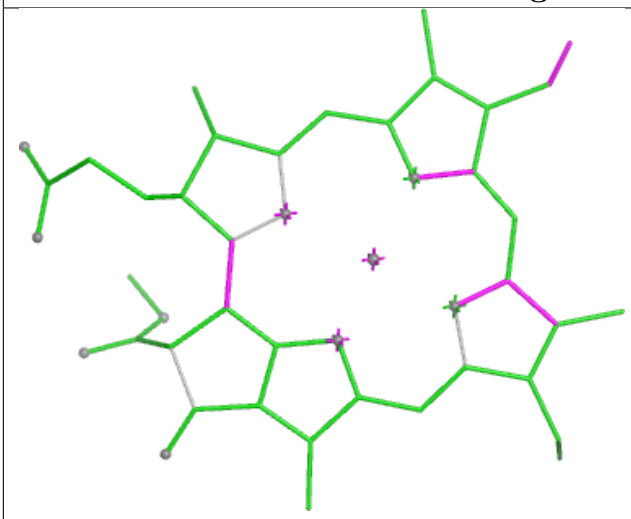


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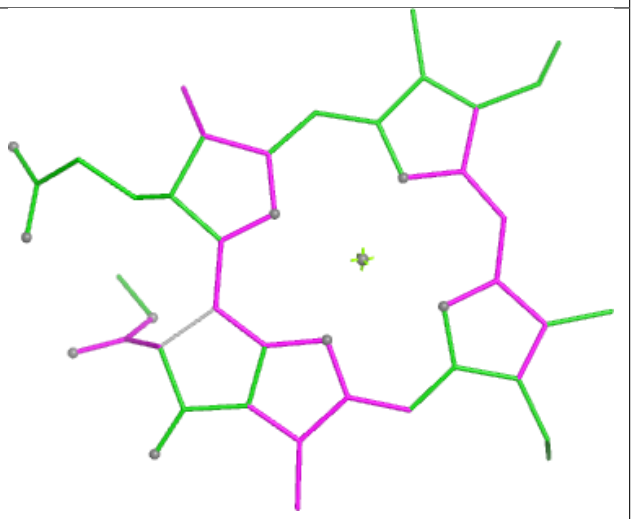


Rings

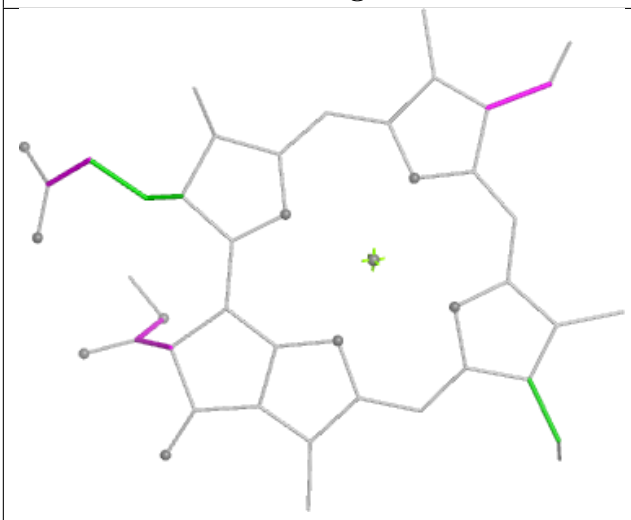
Ligand CLA s 612



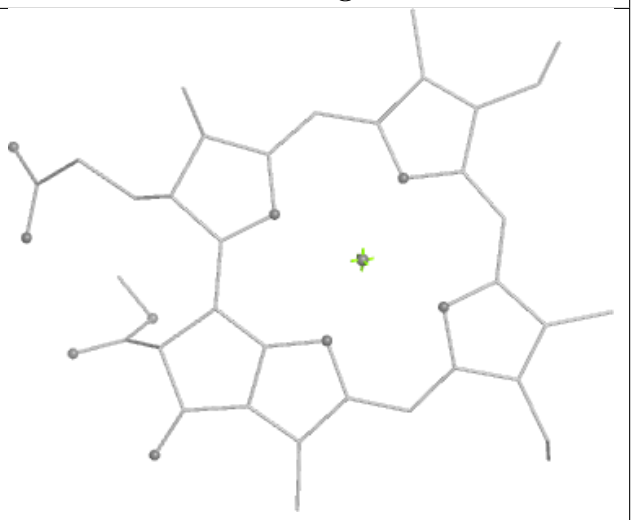
Bond lengths



Bond angles

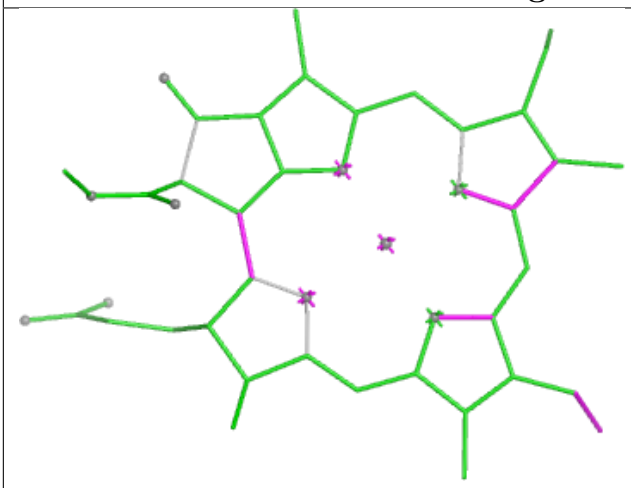


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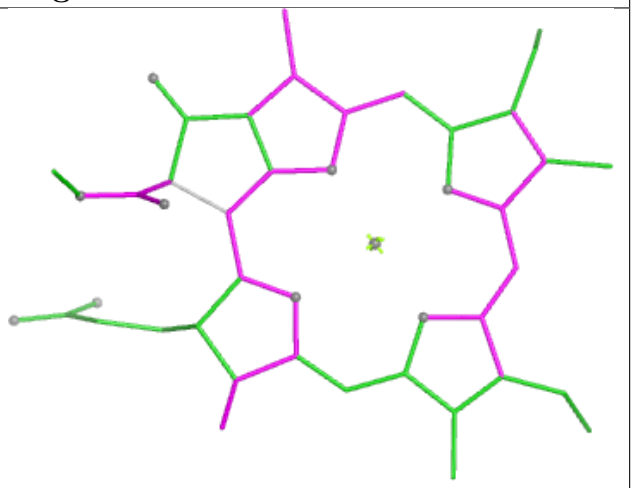


Rings

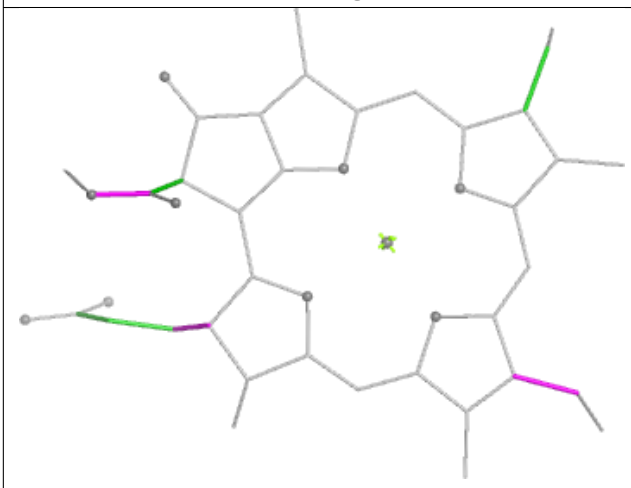
Ligand CLA g 611



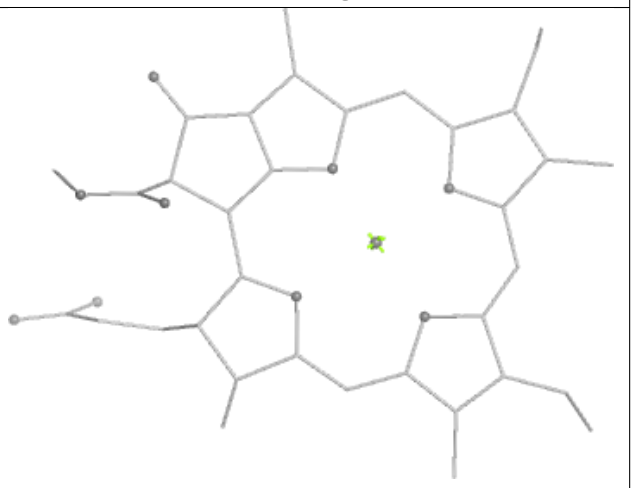
Bond lengths



Bond angles

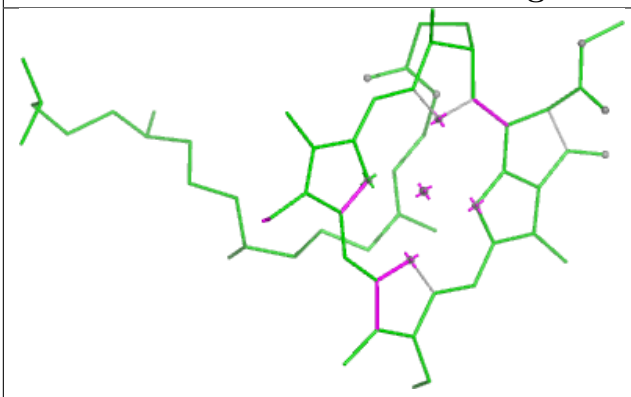


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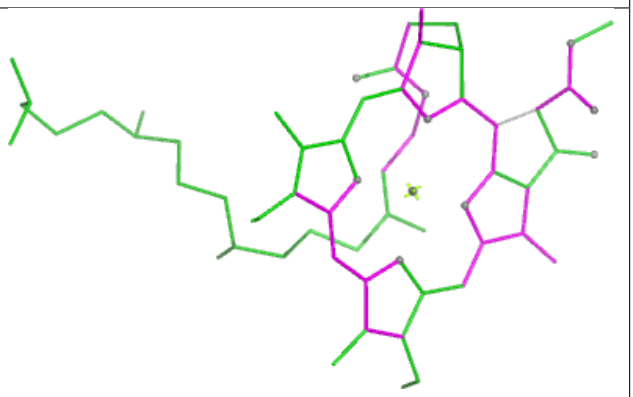


Rings

Ligand CLA n 613



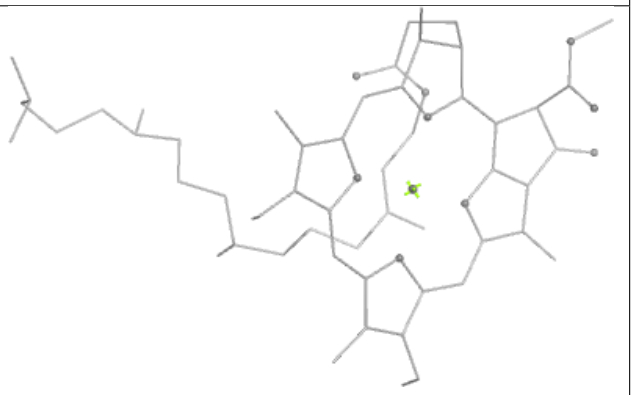
Bond lengths



Bond angles

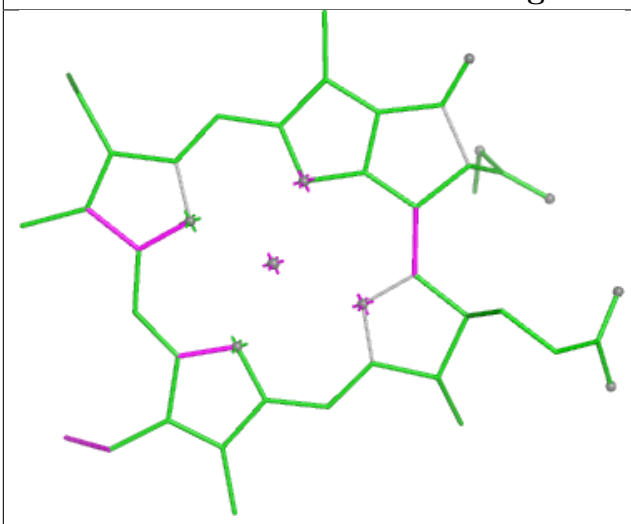


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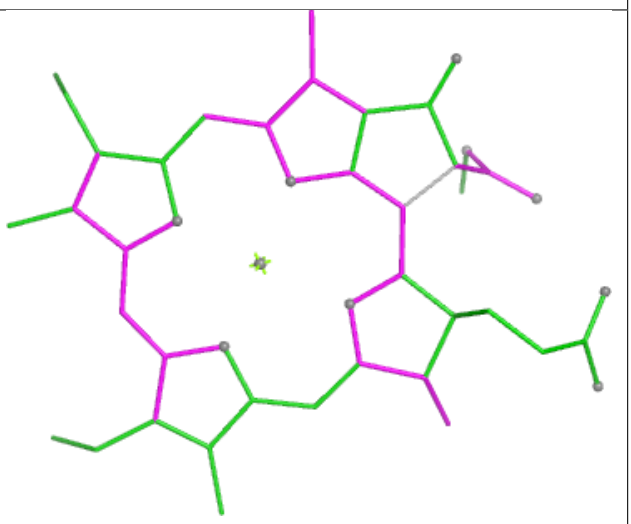


Rings

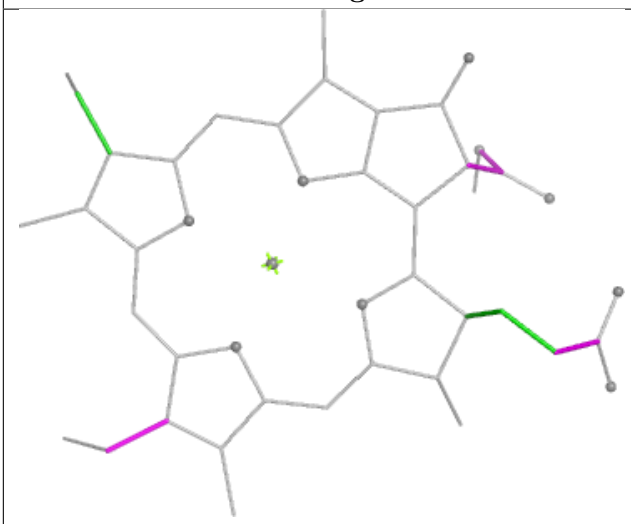
Ligand CLA n 612



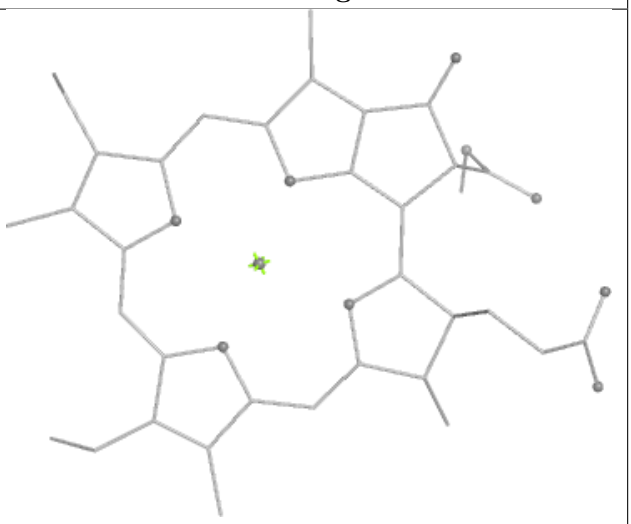
Bond lengths



Bond angles

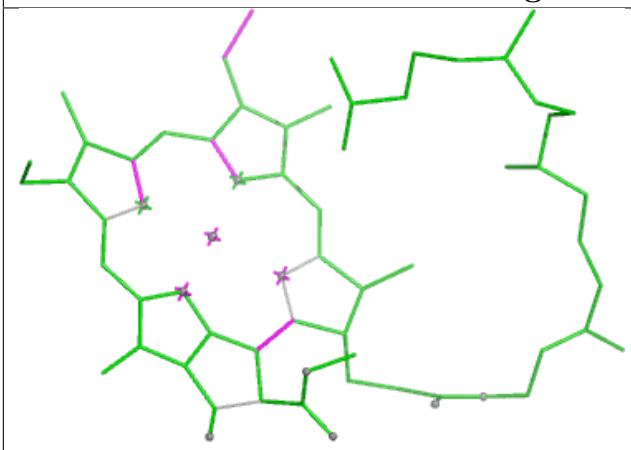


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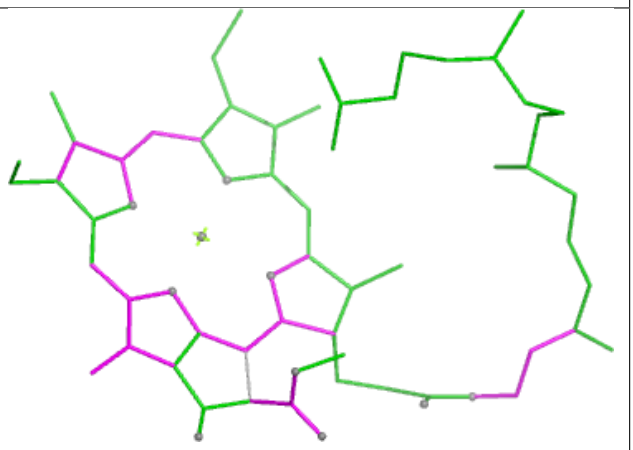


Rings

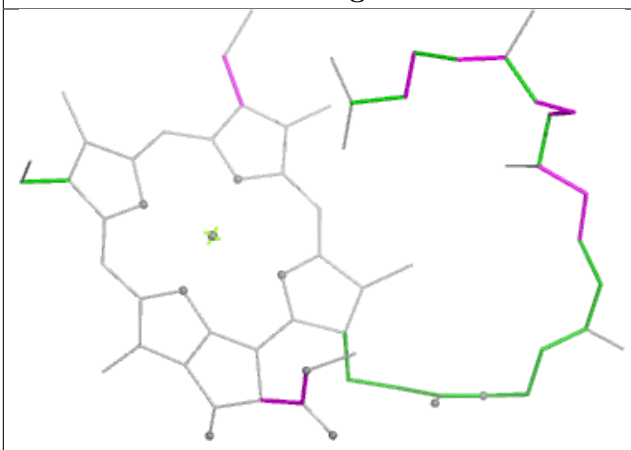
Ligand CLA B 616



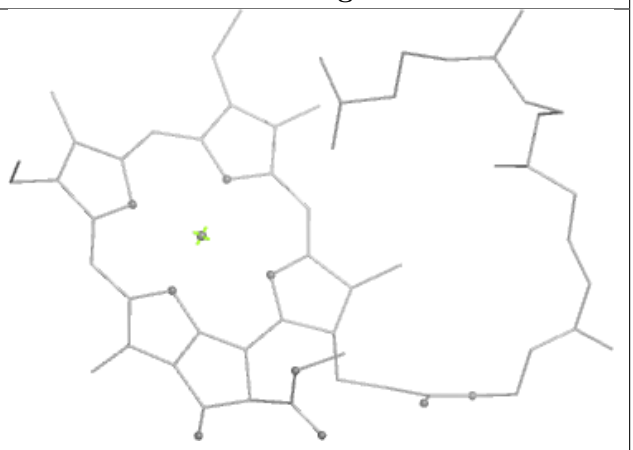
Bond lengths



Bond angles

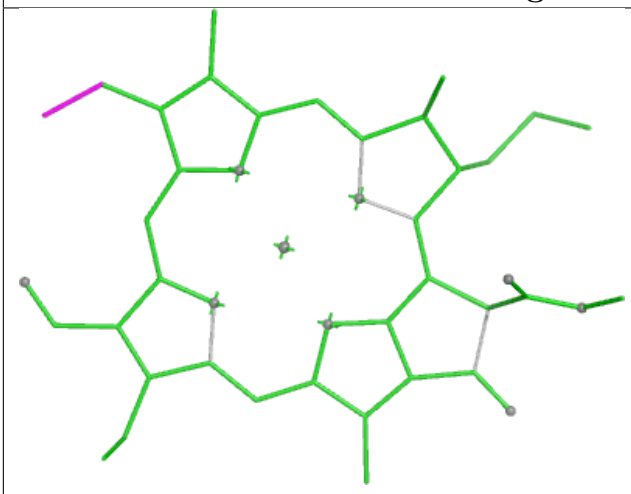


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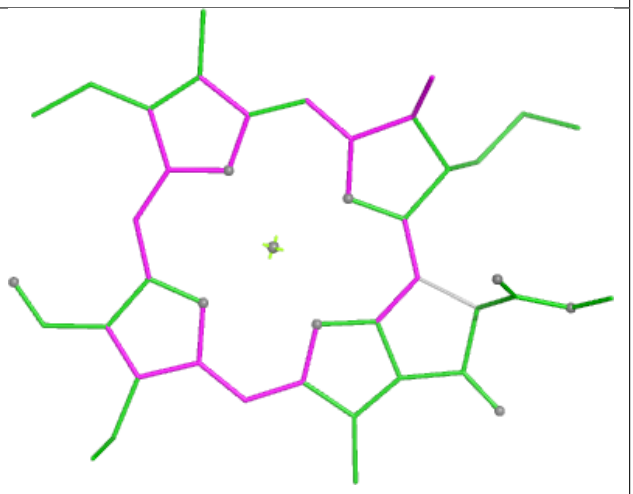


Rings

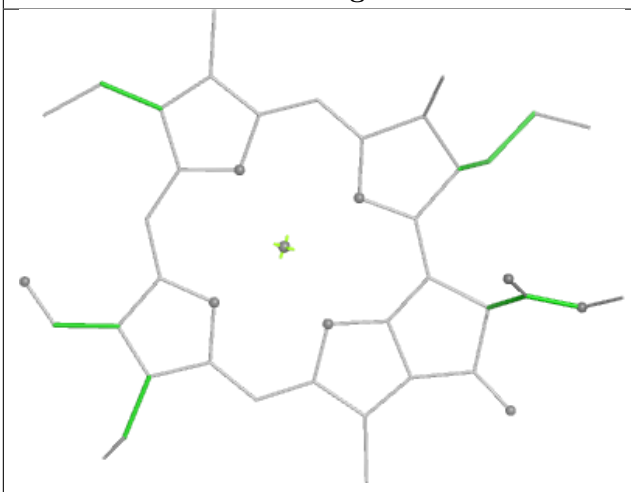
Ligand CHL S 606



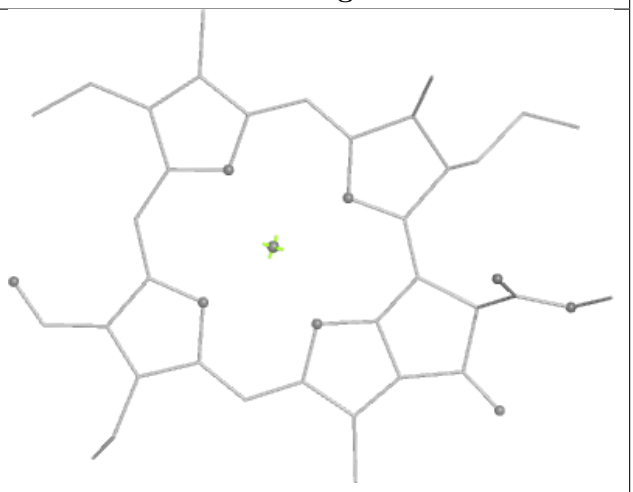
Bond lengths



Bond angles

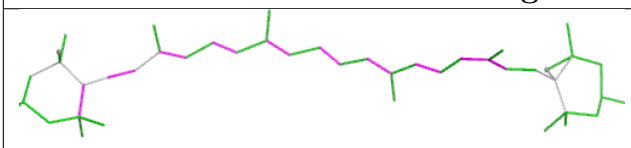


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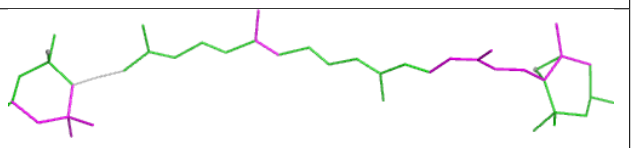


Rings

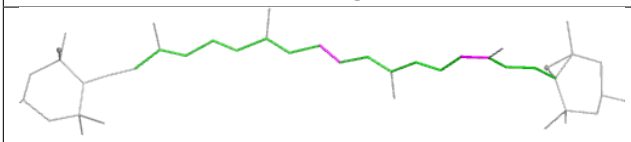
Ligand NEX G 623



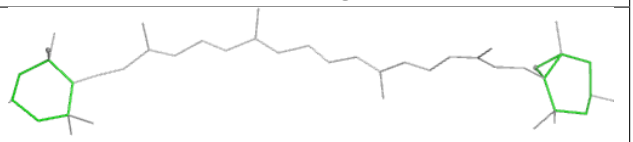
Bond lengths



Bond angles

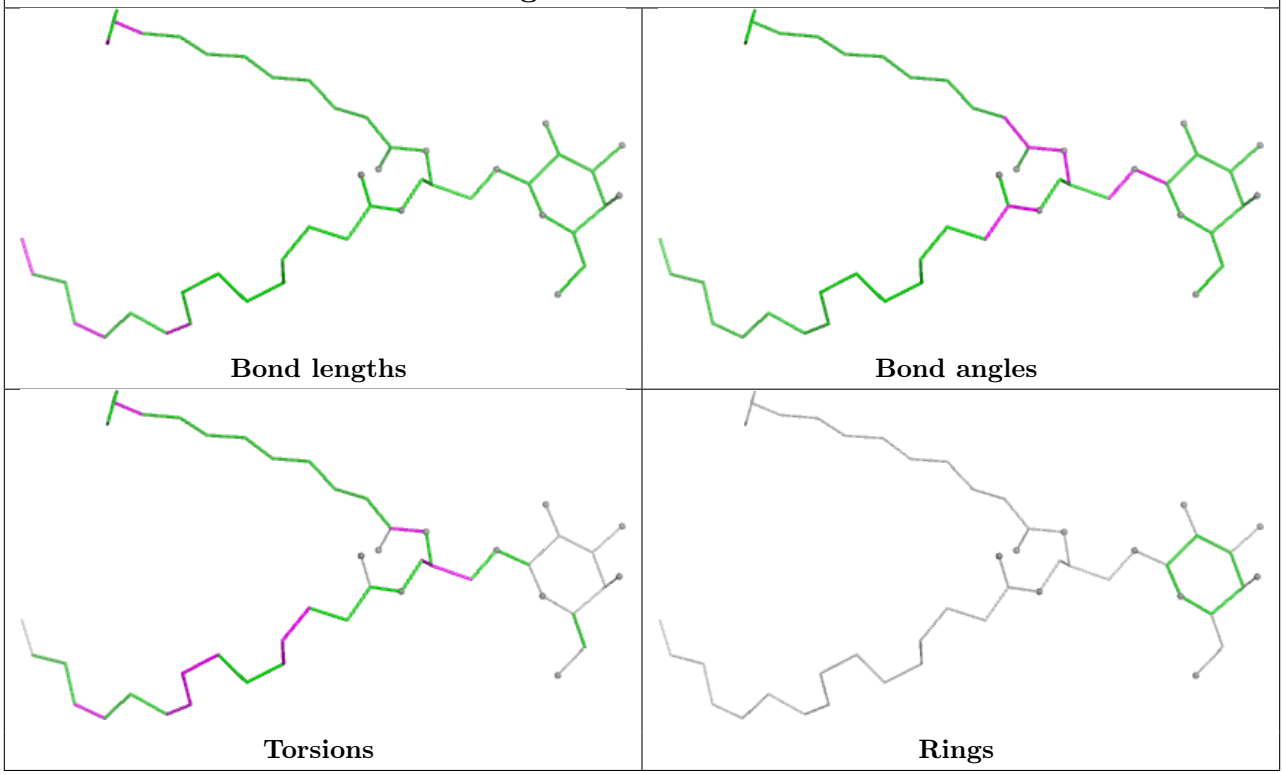


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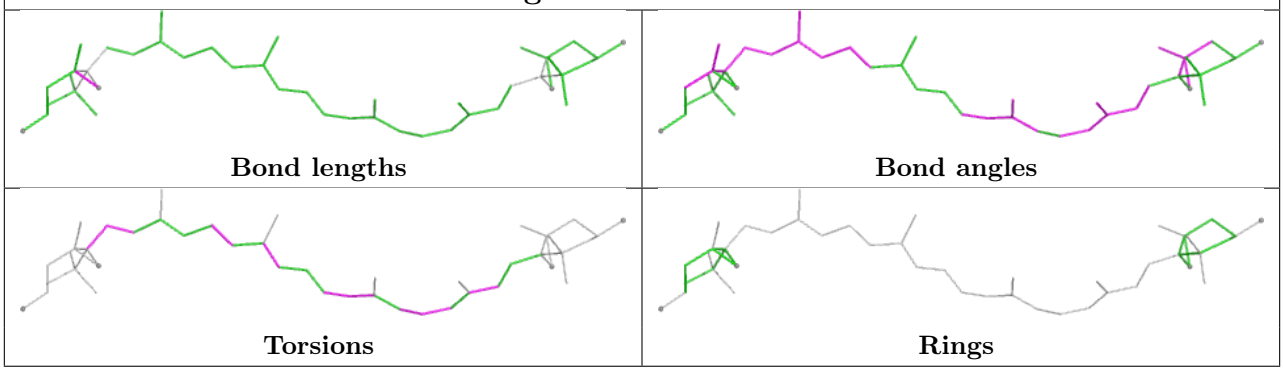


Rings

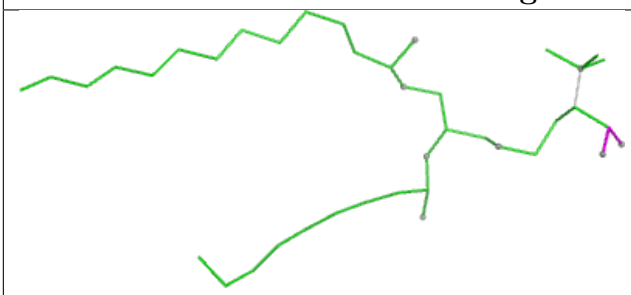
Ligand LMG A 413



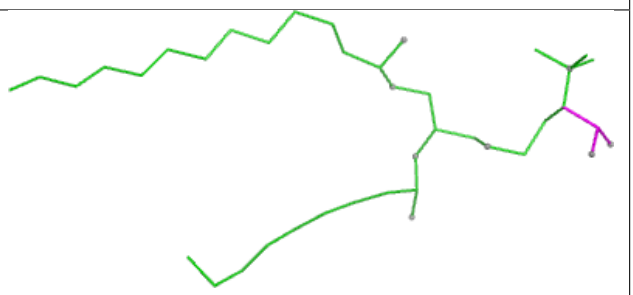
Ligand XAT R 621



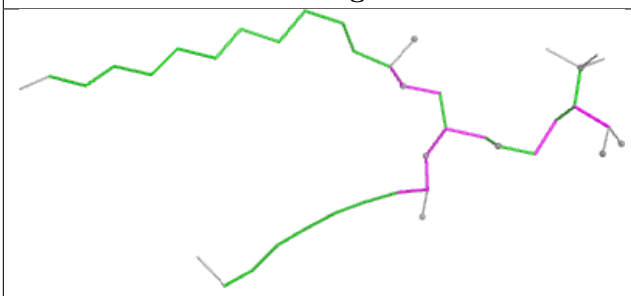
Ligand LMK C 527



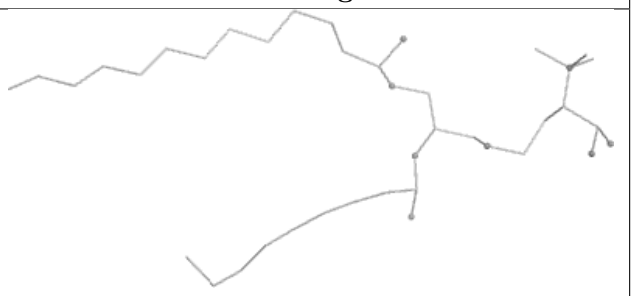
Bond lengths



Bond angles

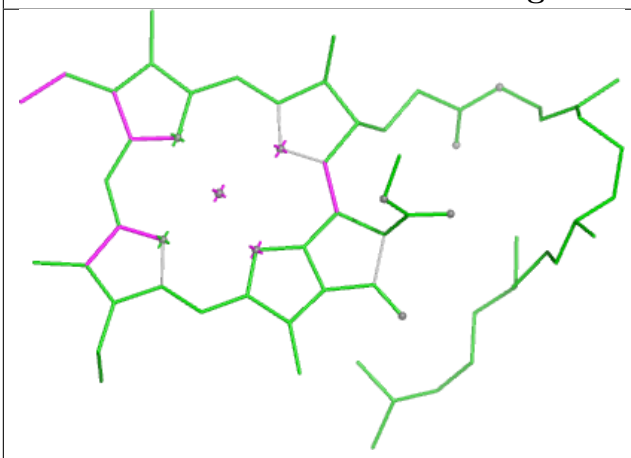


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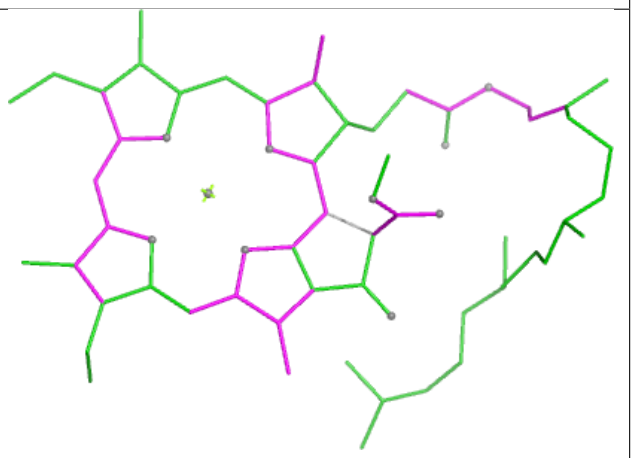


Rings

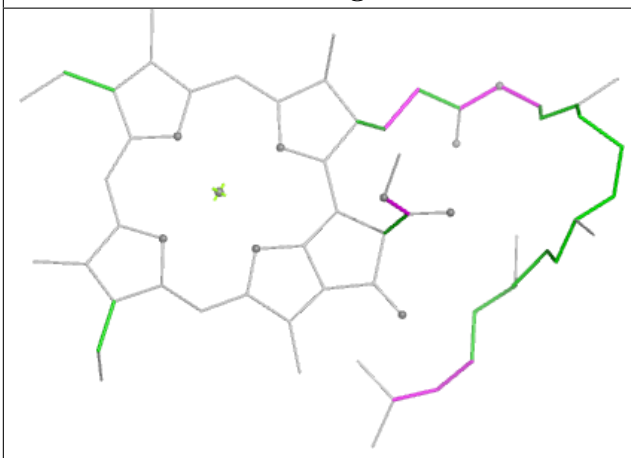
Ligand CLA b 611



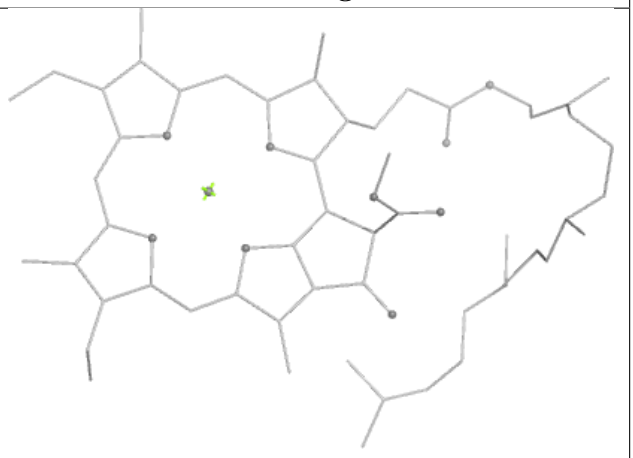
Bond lengths



Bond angles

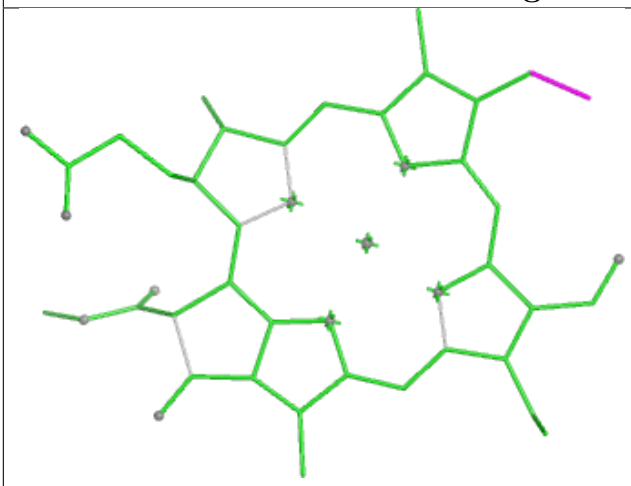


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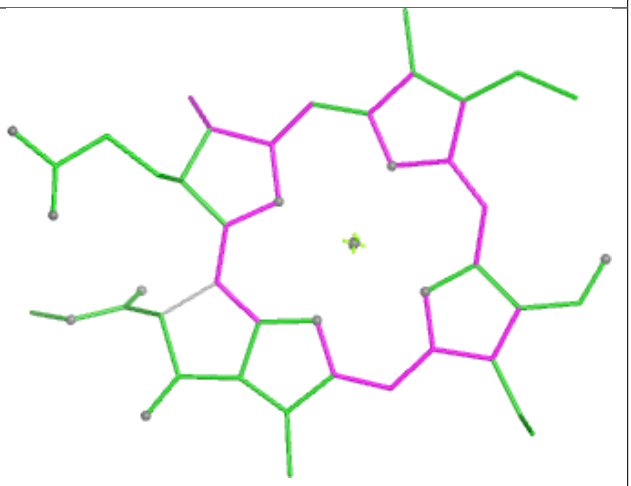


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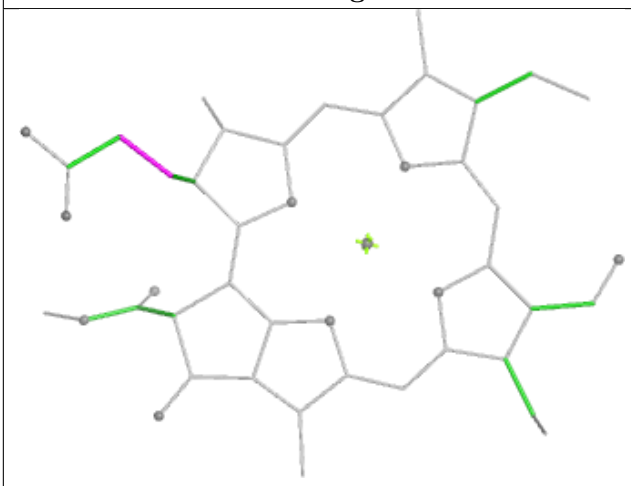
Ligand CHL Y 605



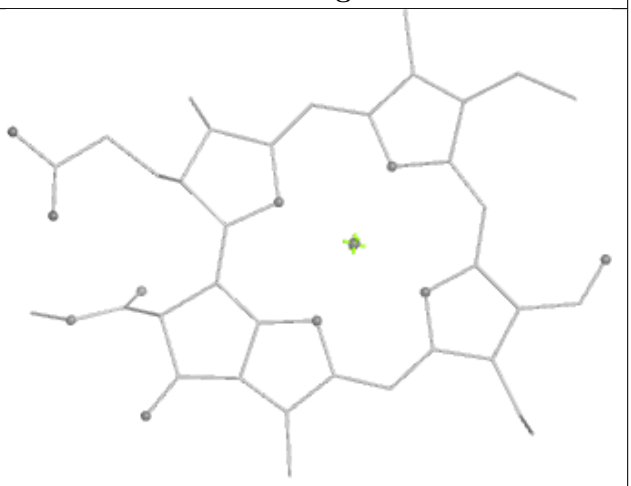
Bond lengths



Bond angles

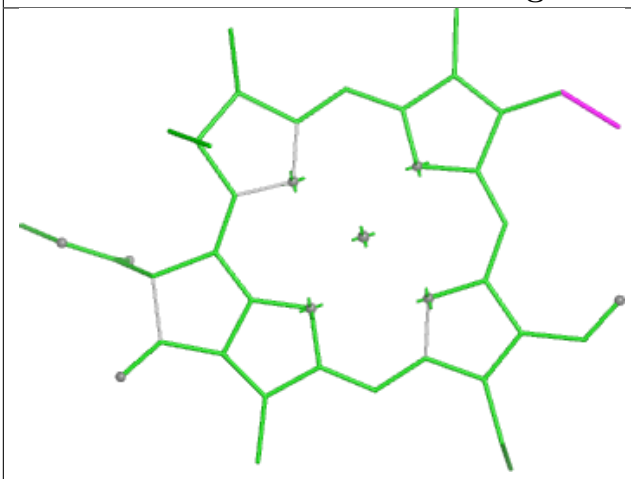


Torsions

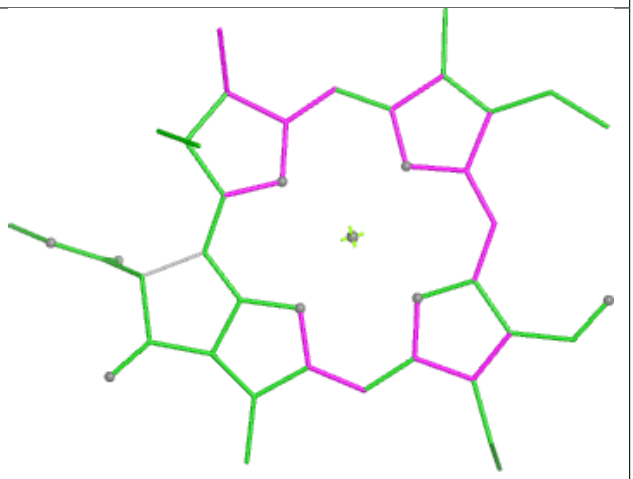


Rings

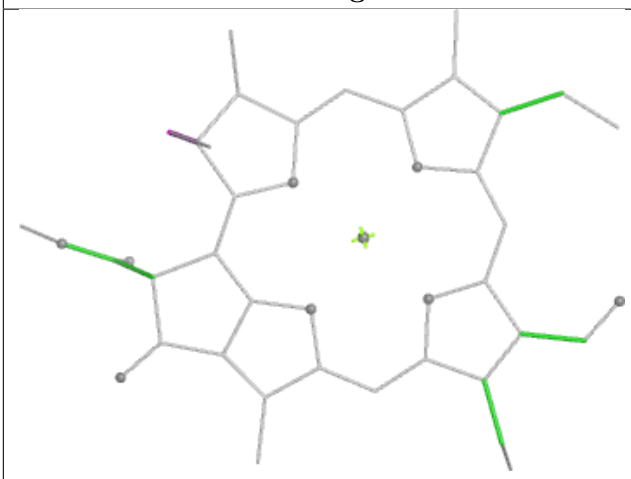
Ligand CHL S 607



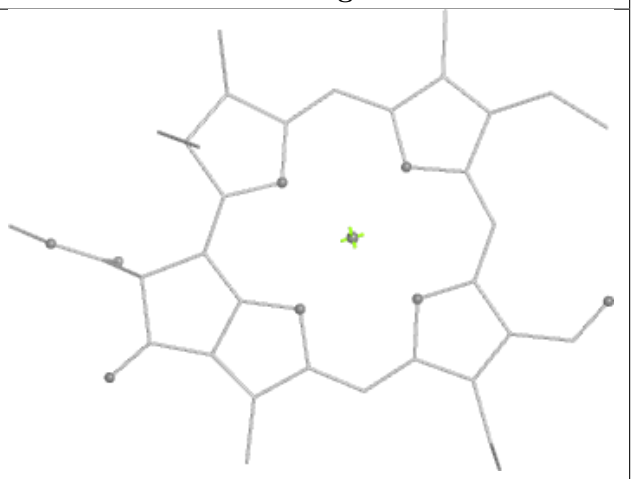
Bond lengths



Bond angles



Torsions



Rings

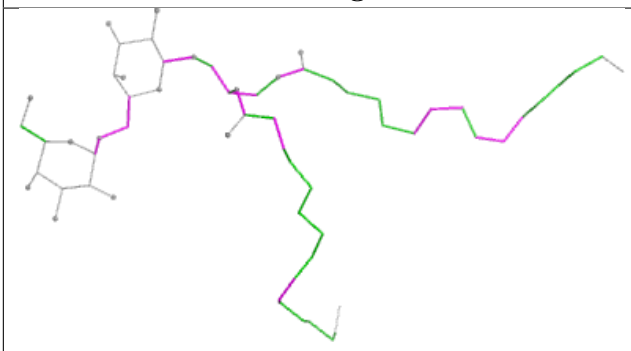
Ligand DGD c 519



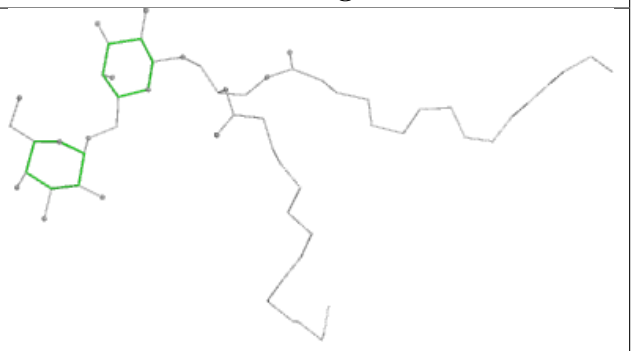
Bond lengths



Bond angles

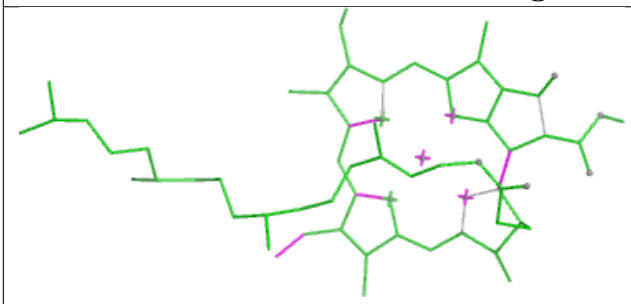


Torsions

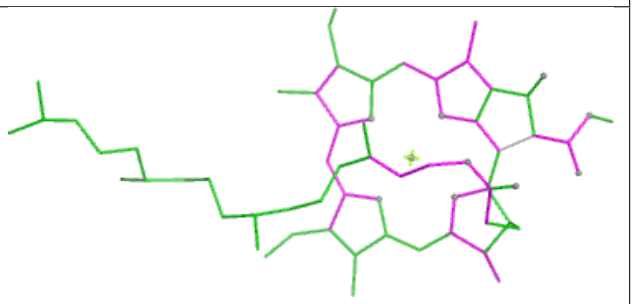


Rings

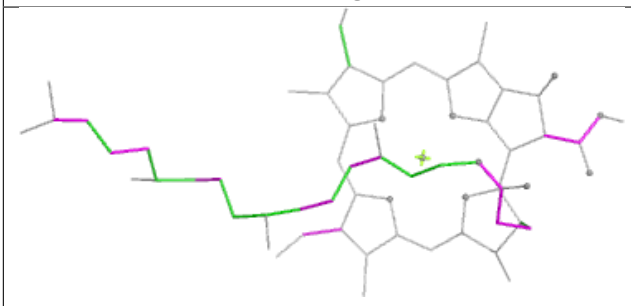
Ligand CLA c 505



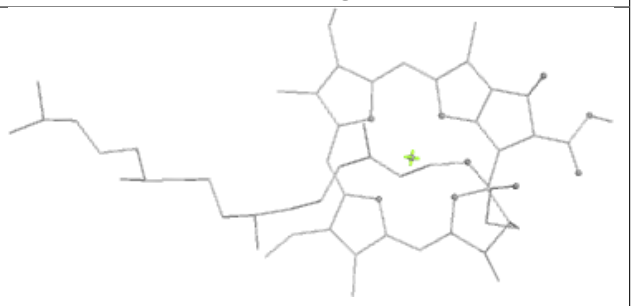
Bond lengths



Bond angles

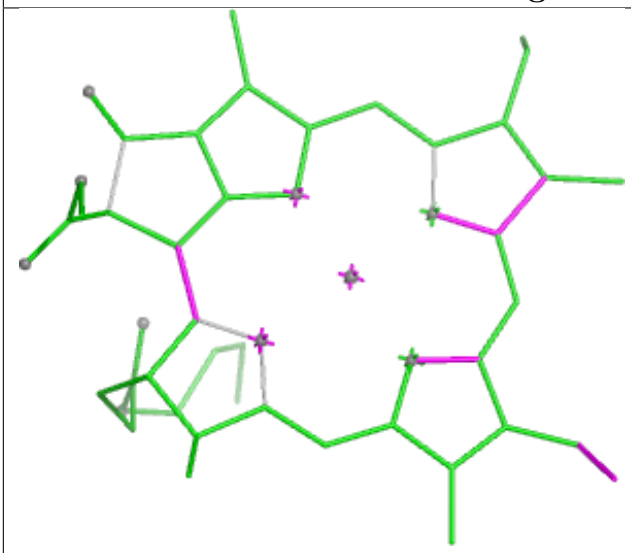


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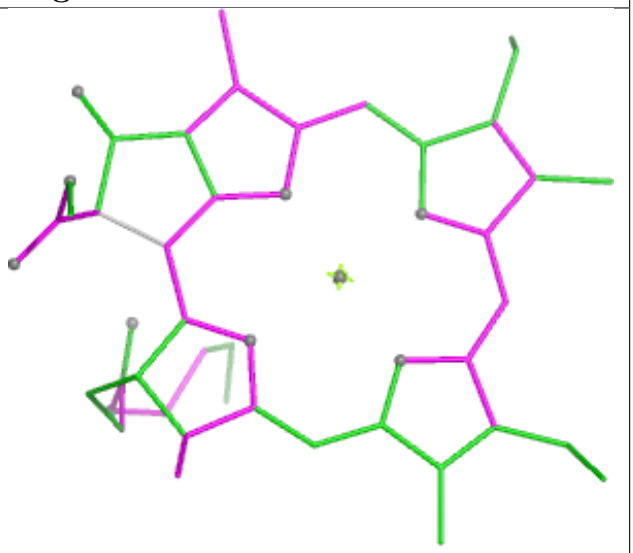


Rings

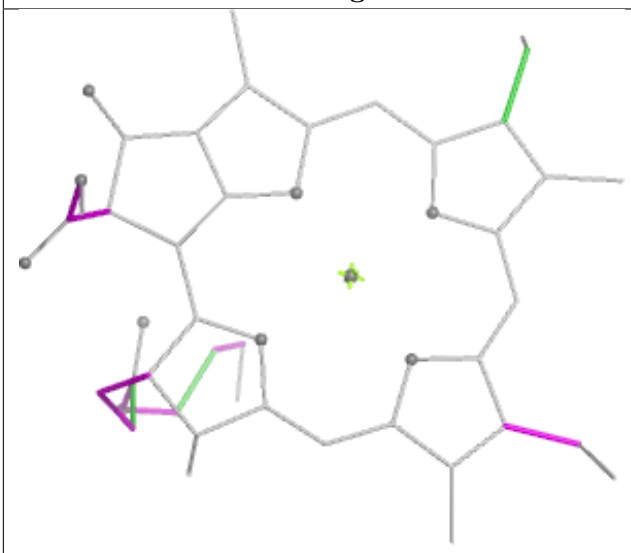
Ligand CLA g 604



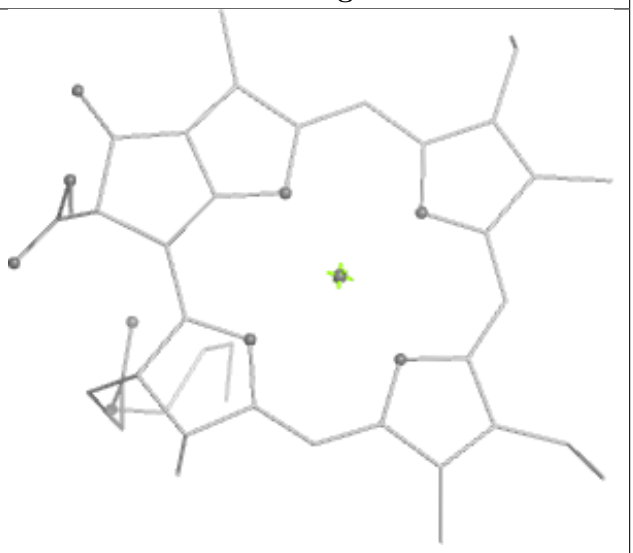
Bond lengths



Bond angles

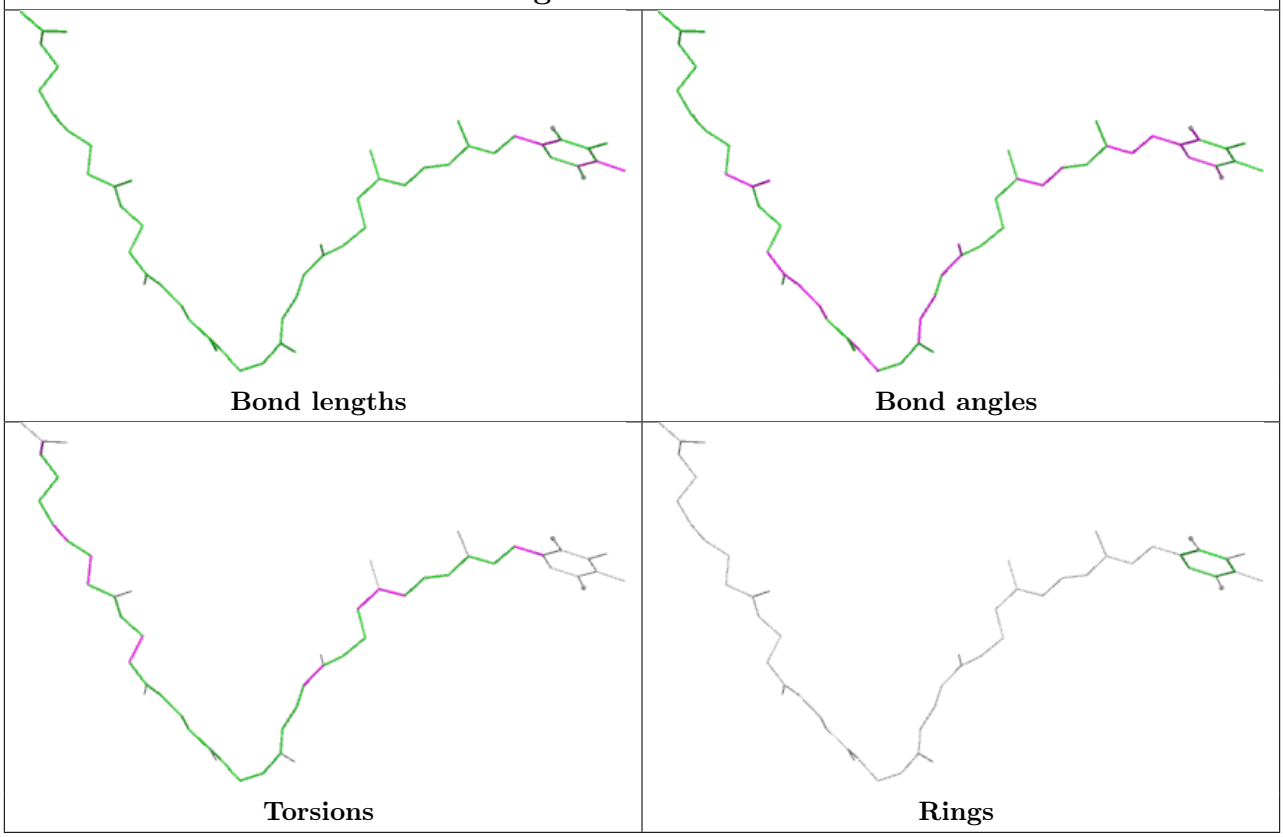


Torsions

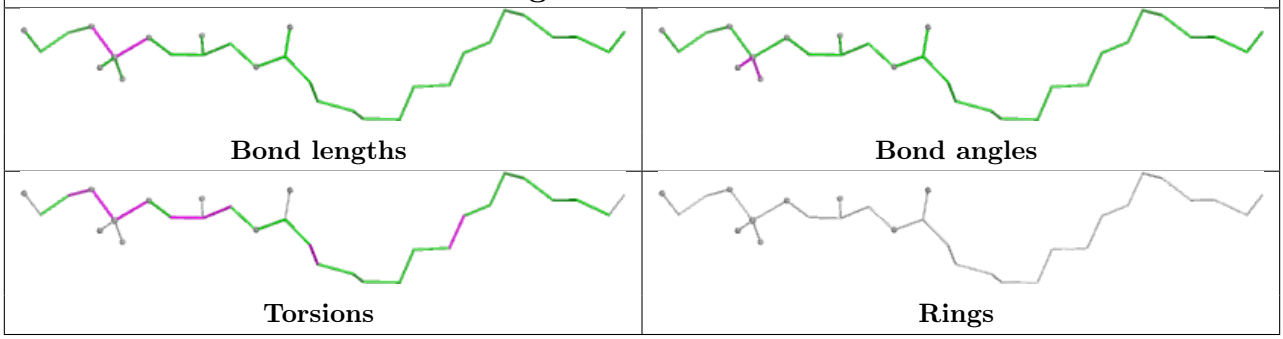


Rings

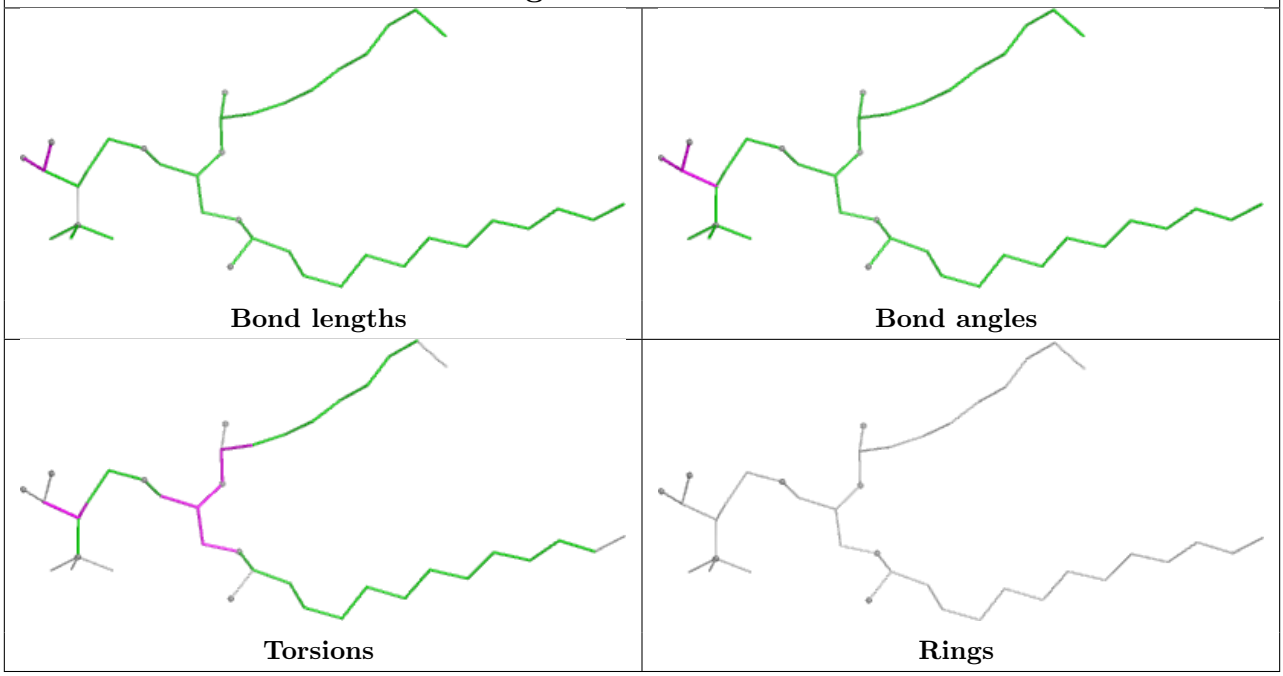
Ligand PL9 d 405



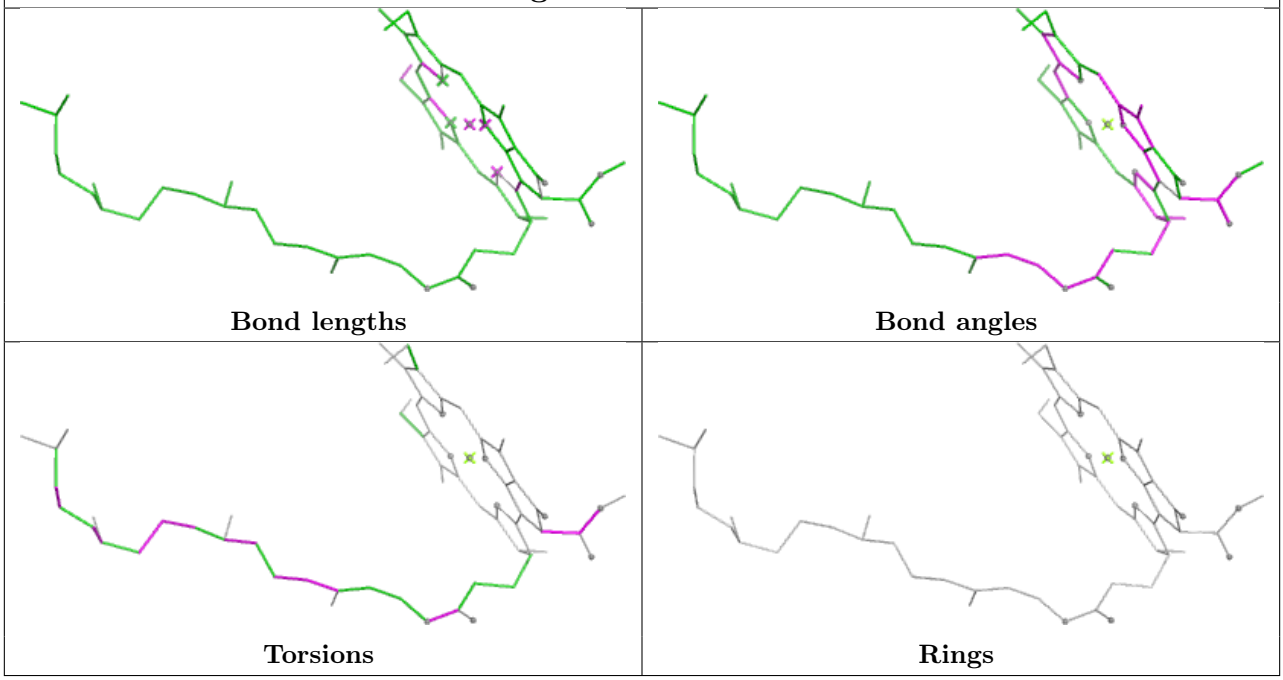
Ligand LPX S 625



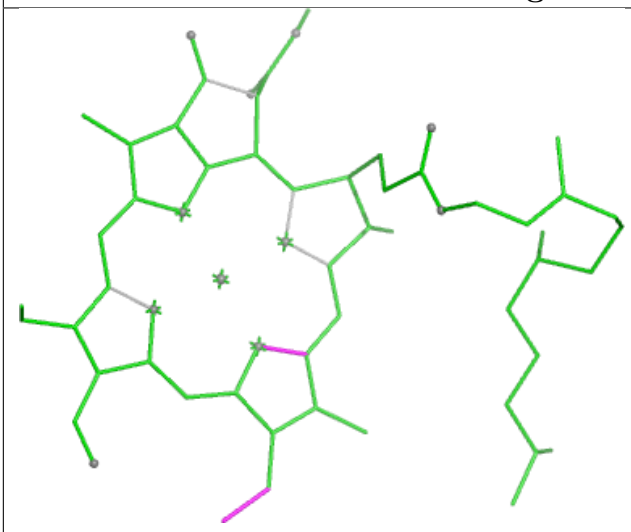
Ligand LMK c 627



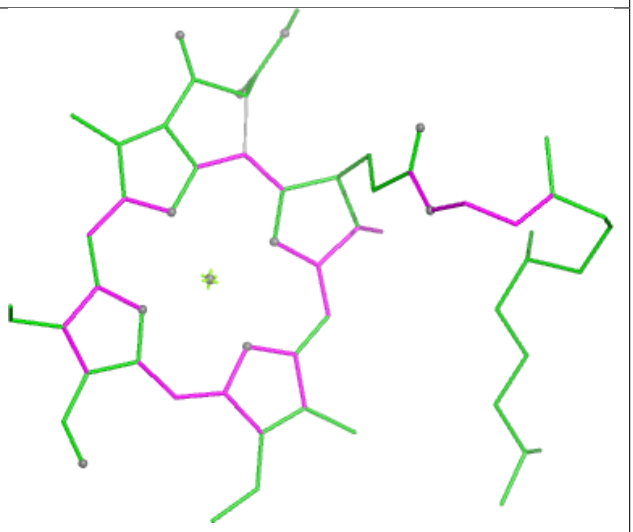
Ligand CLA c 504



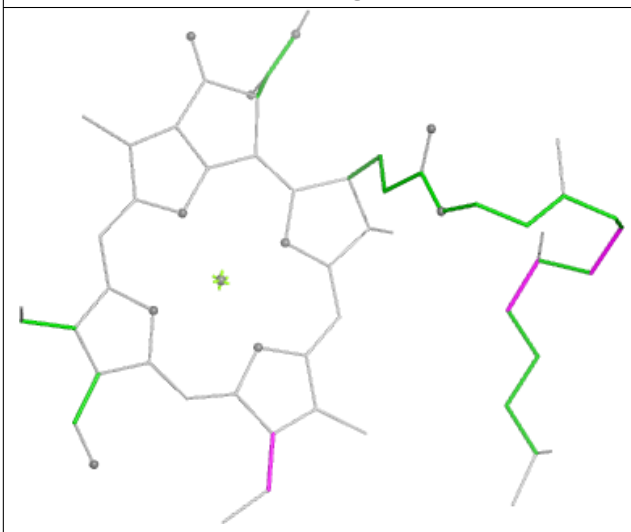
Ligand CHL S 608



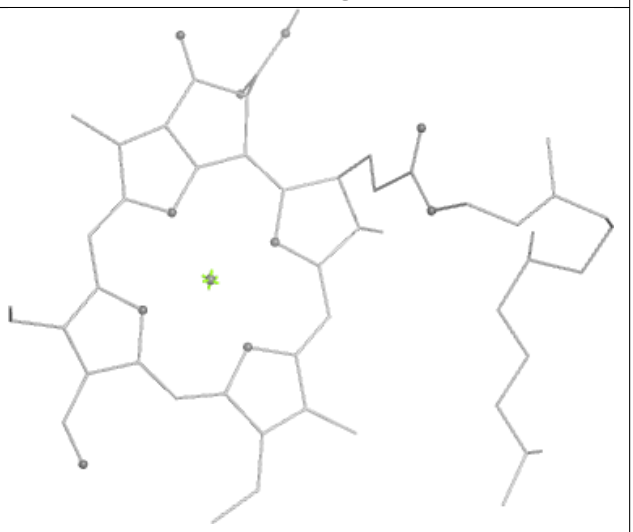
Bond lengths



Bond angles

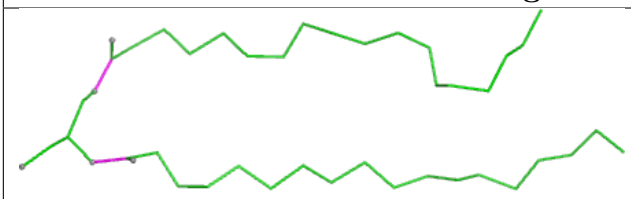


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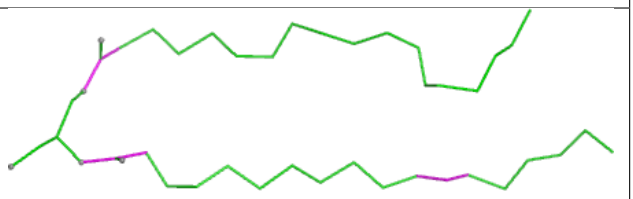


Rings

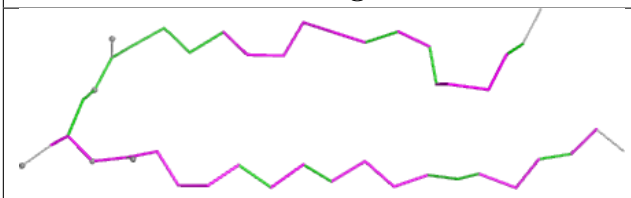
Ligand DGA b 623



Bond lengths



Bond angles

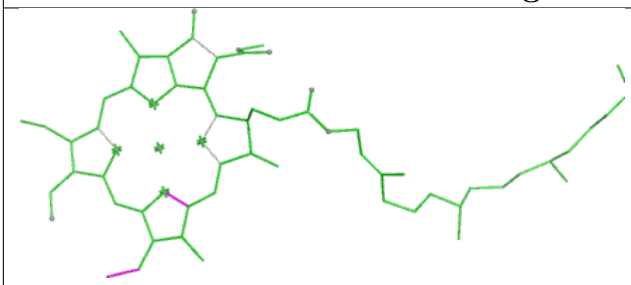


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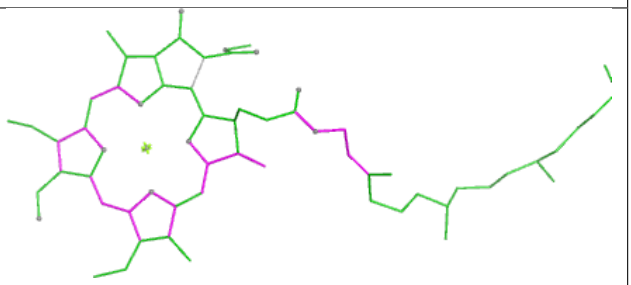


Rings

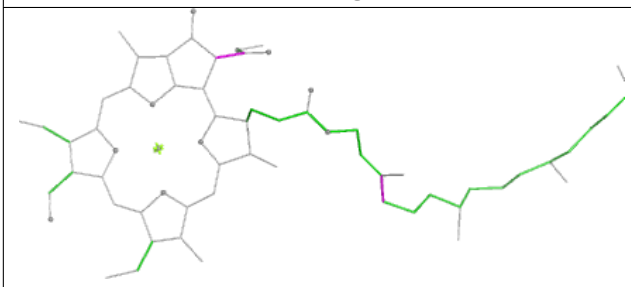
Ligand CHL N 601



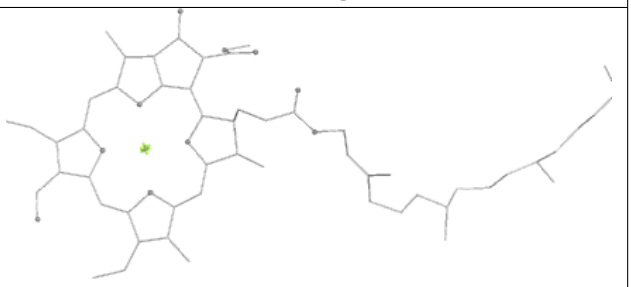
Bond lengths



Bond angles

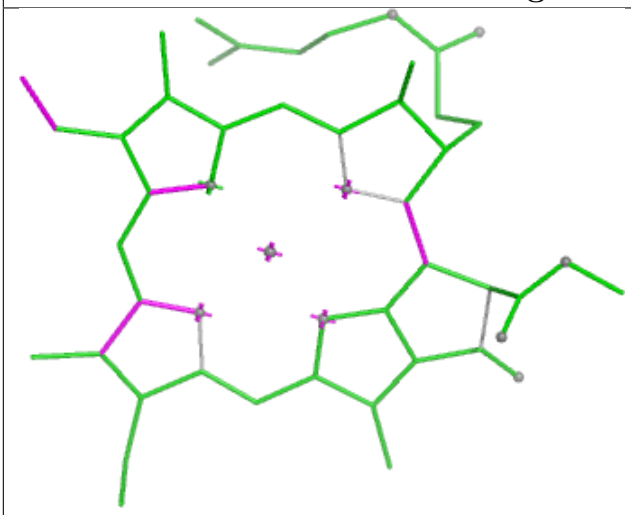


Torsions

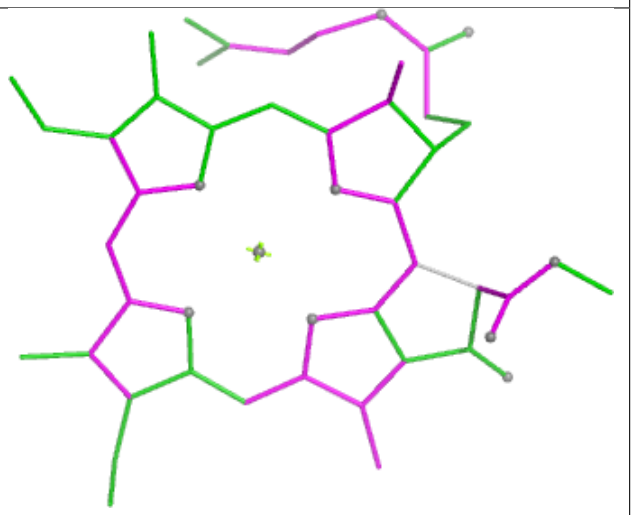


Rings

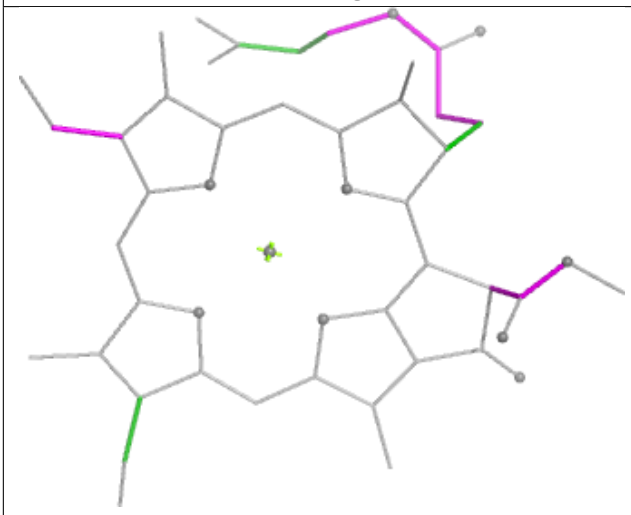
Ligand CLA S 617



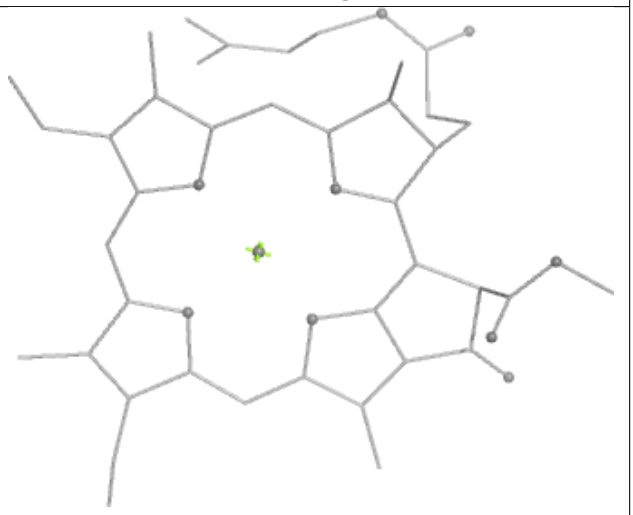
Bond lengths



Bond angles

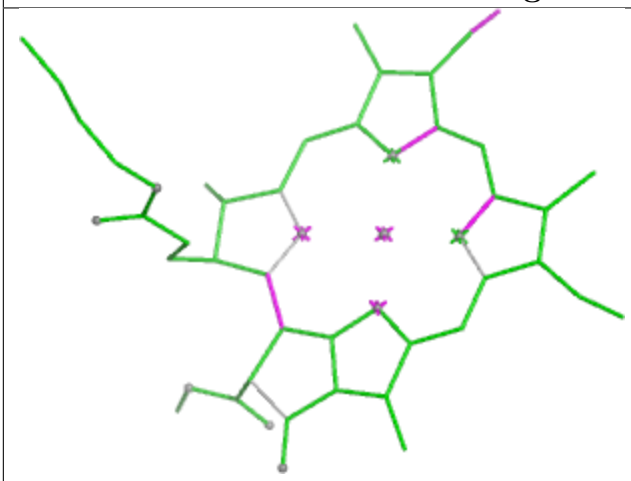


Torsions

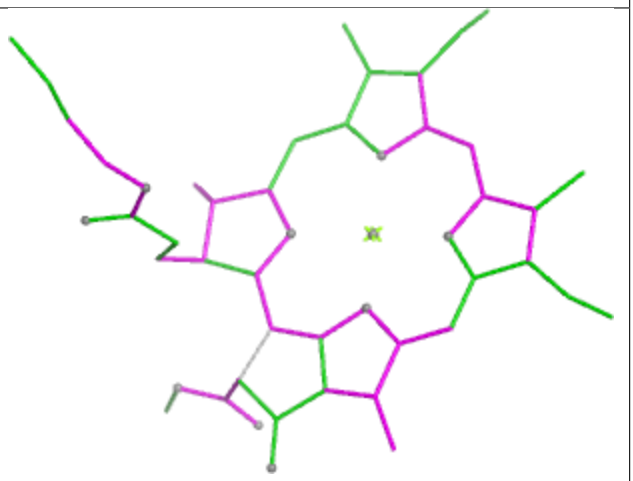


Rings

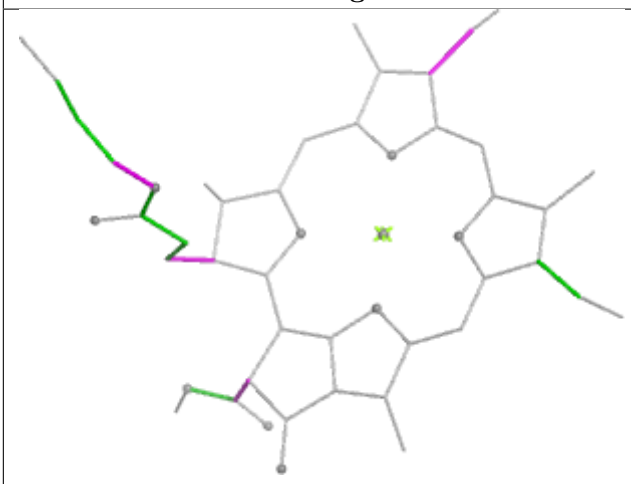
Ligand CLA A 407



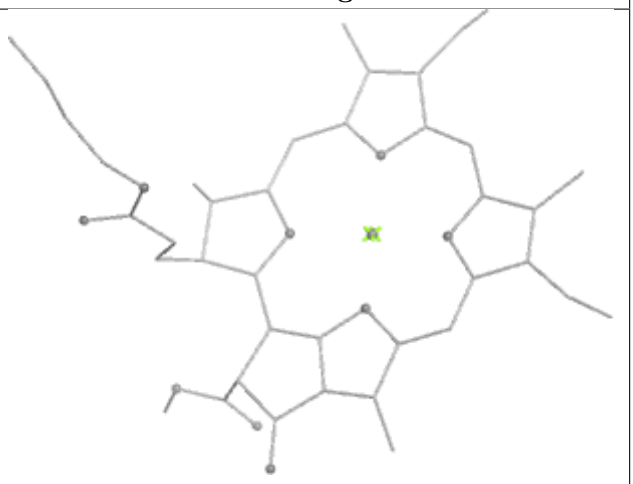
Bond lengths



Bond angles

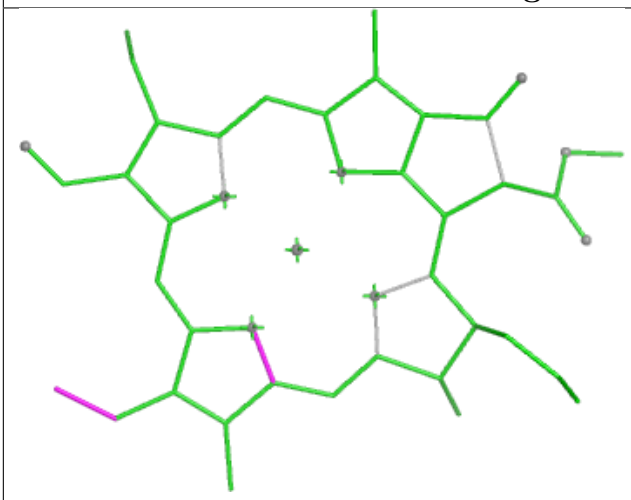


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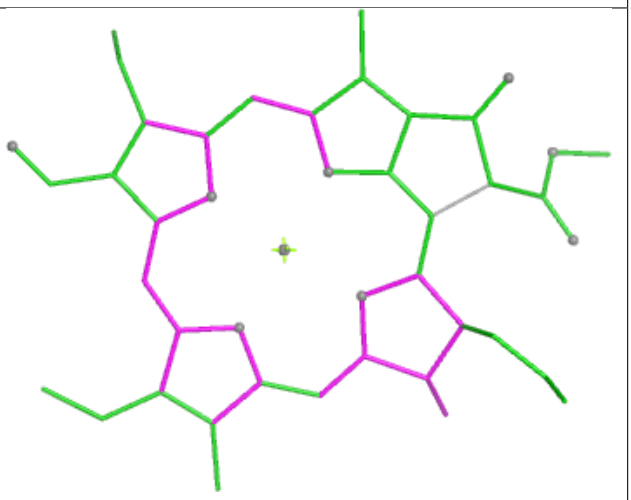


Rings

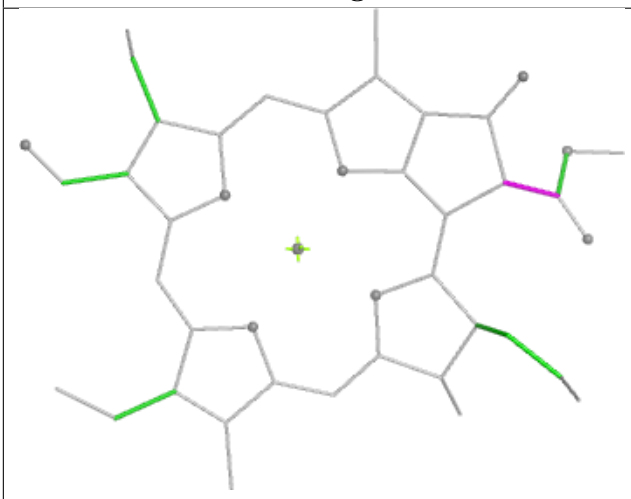
Ligand CHL R 606



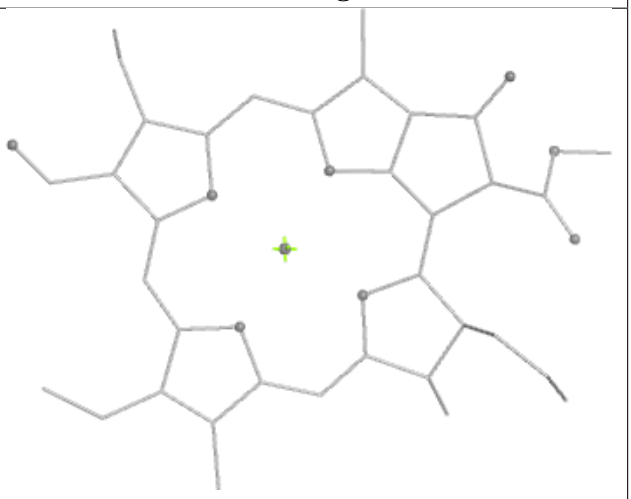
Bond lengths



Bond angles

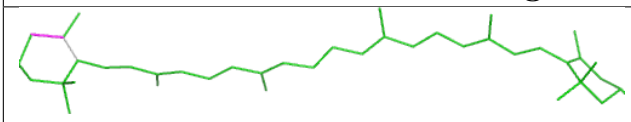


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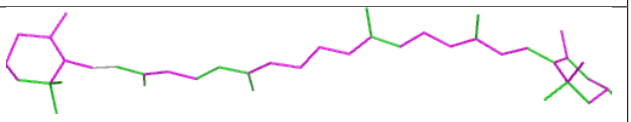


Rings

Ligand LUT Y 621



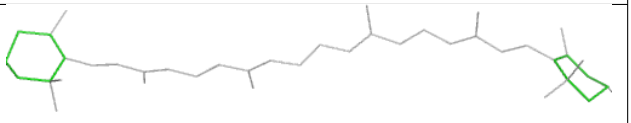
Bond lengths



Bond angles

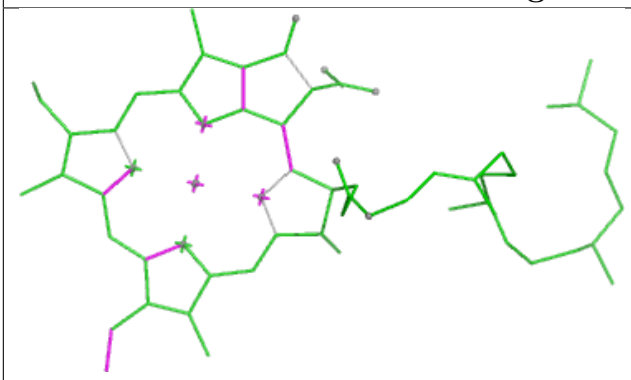


Torsions

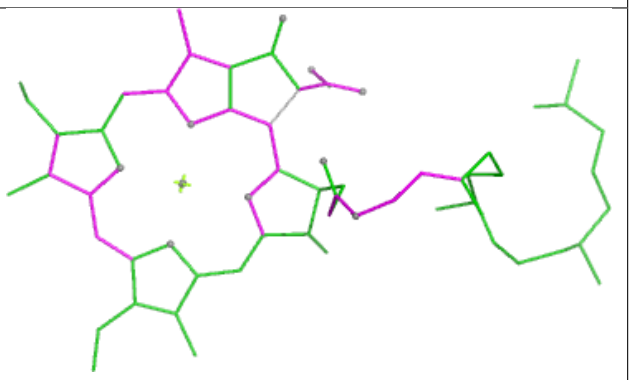


Rings

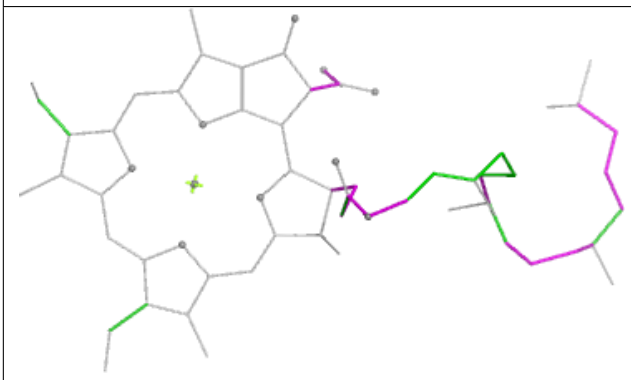
Ligand CLA b 613



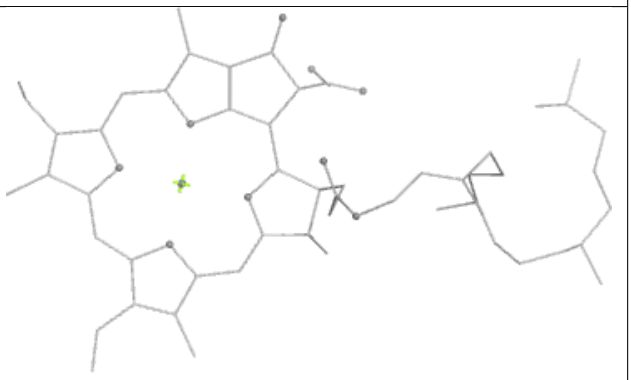
Bond lengths



Bond angles



Torsions

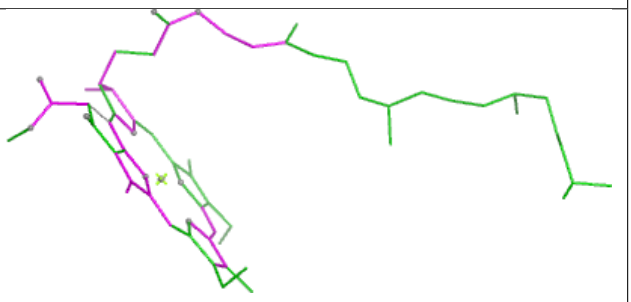


Rings

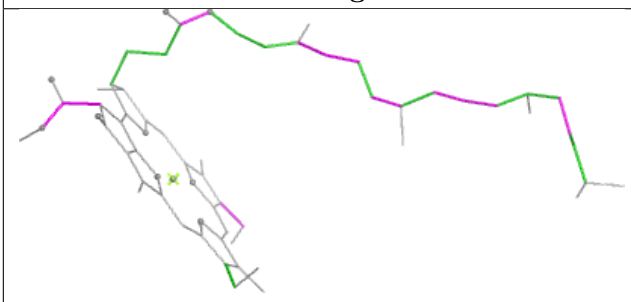
Ligand CLA C 504



Bond lengths



Bond angles

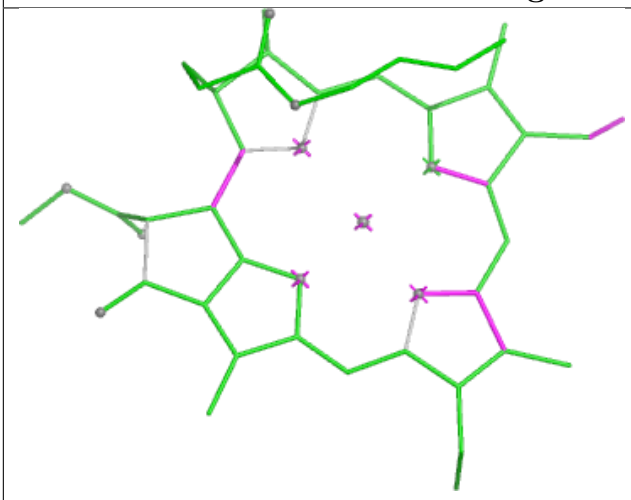


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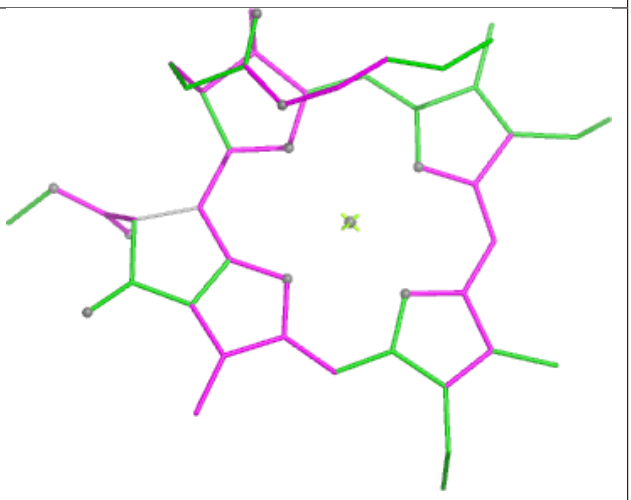


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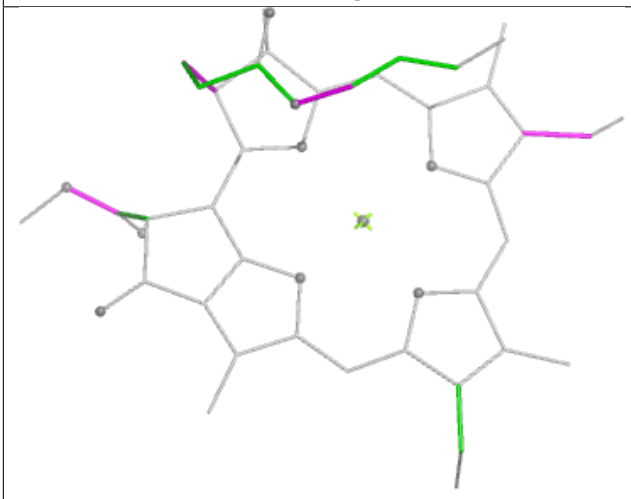
Ligand CLA n 614



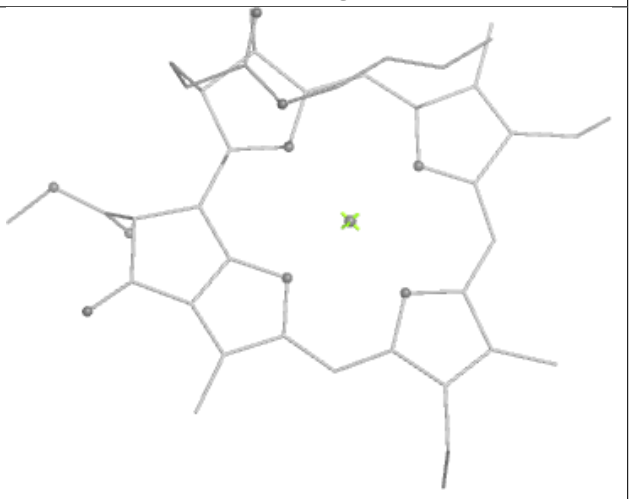
Bond lengths



Bond angles



Torsions

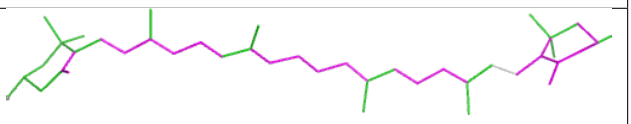


Rings

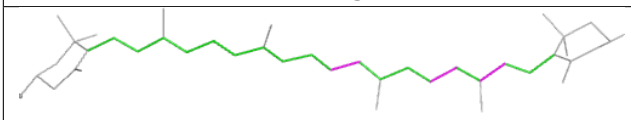
Ligand LUT Y 620



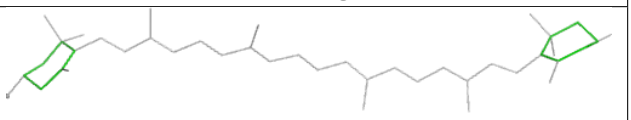
Bond lengths



Bond angles

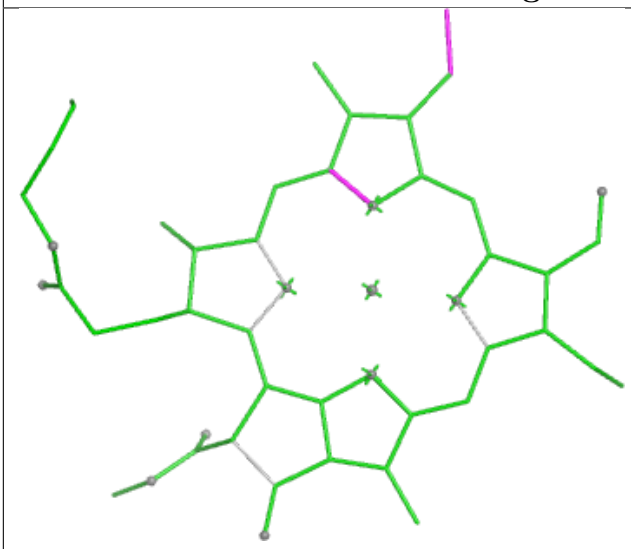


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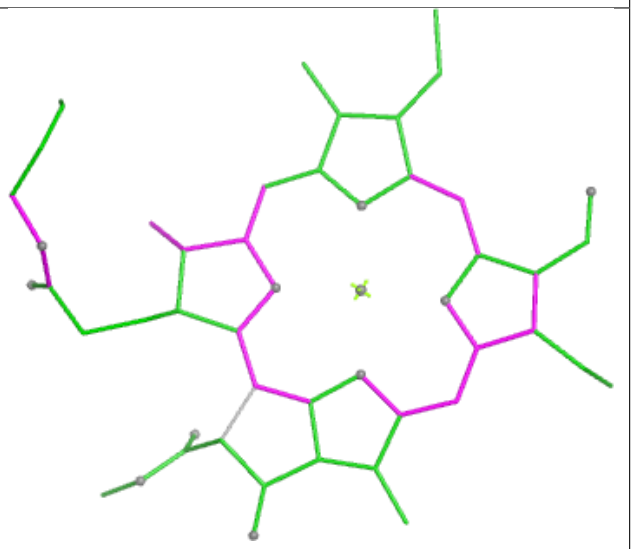


Rings

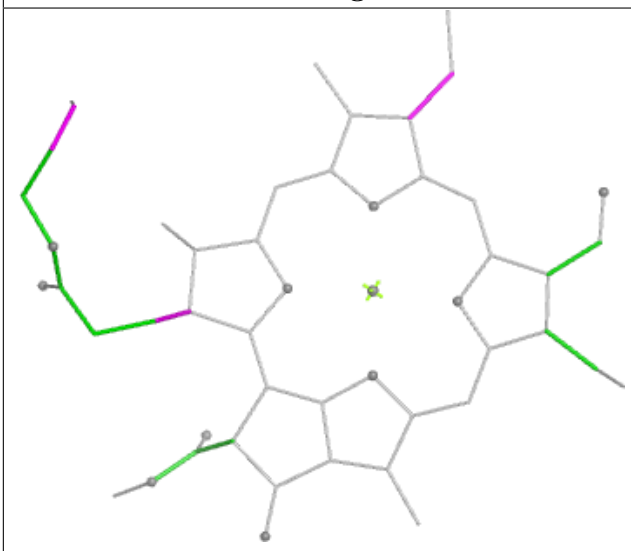
Ligand CHL G 607



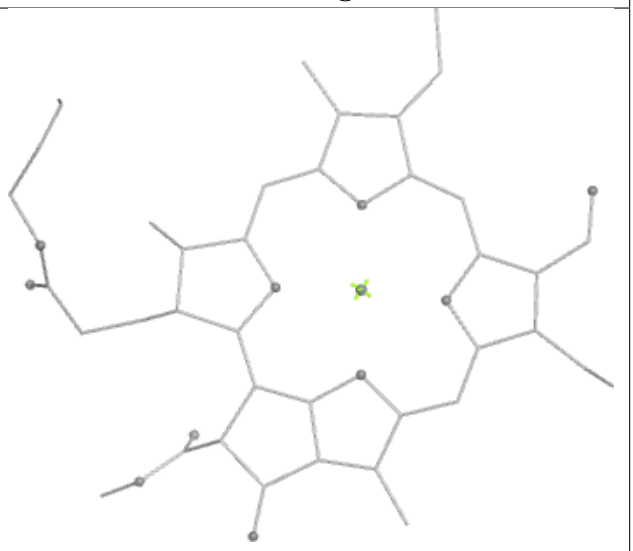
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Bond angles

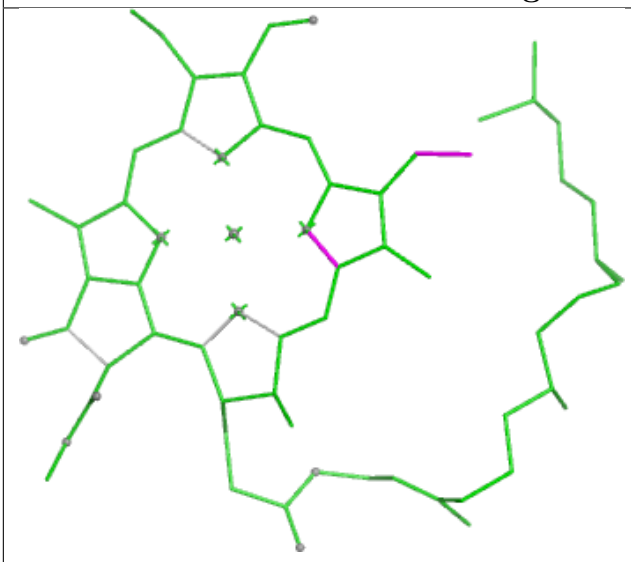


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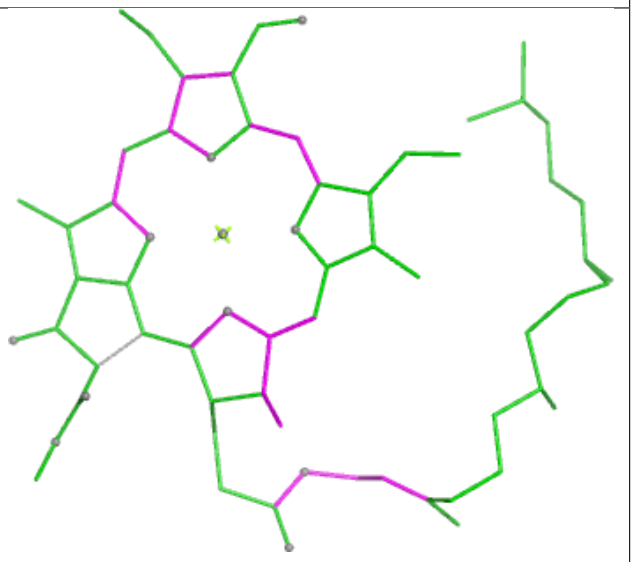


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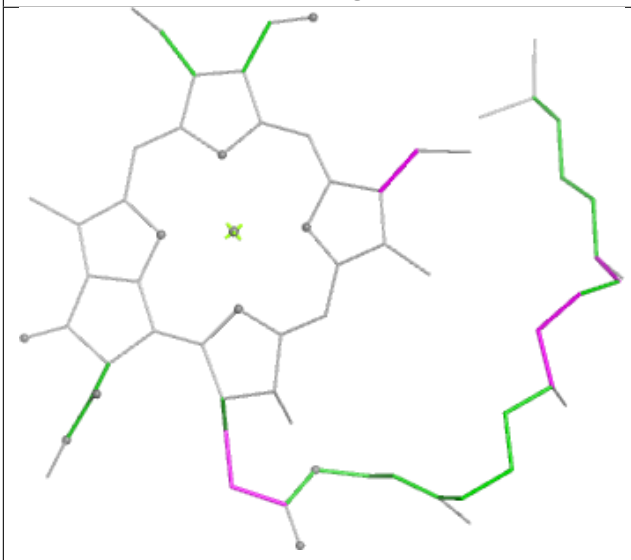
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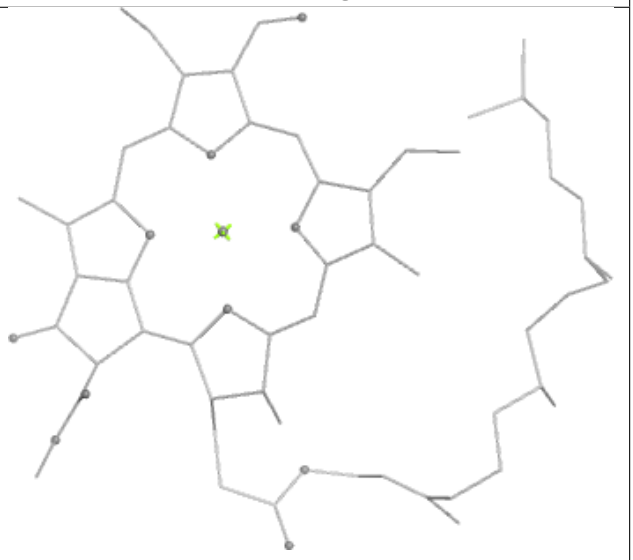
Bond lengths



Bond angles



Torsions

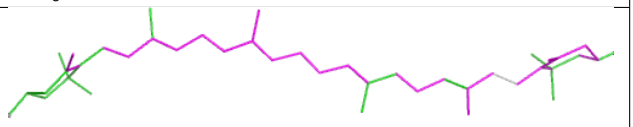


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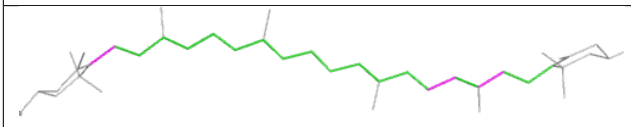
Ligand LUT y 620



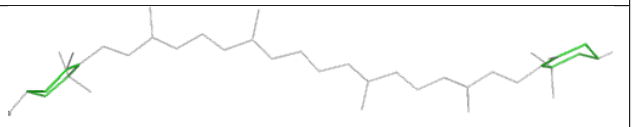
Bond lengths



Bond angles

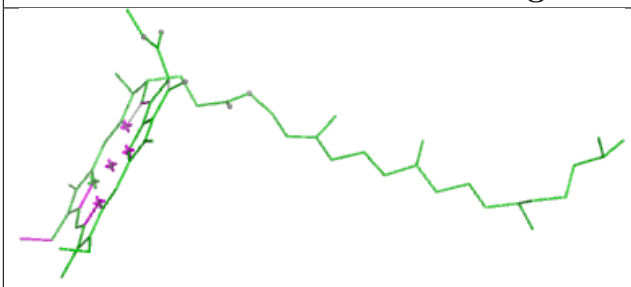


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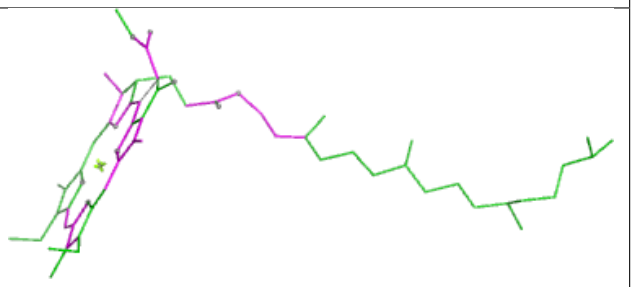


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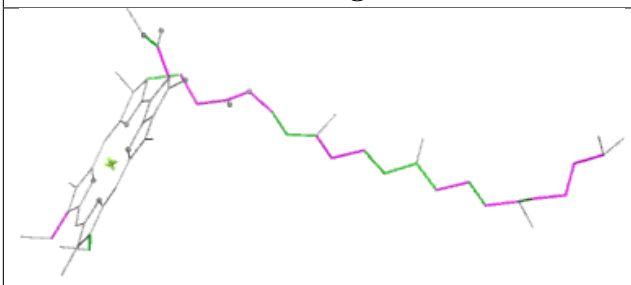
Ligand CLA b 605



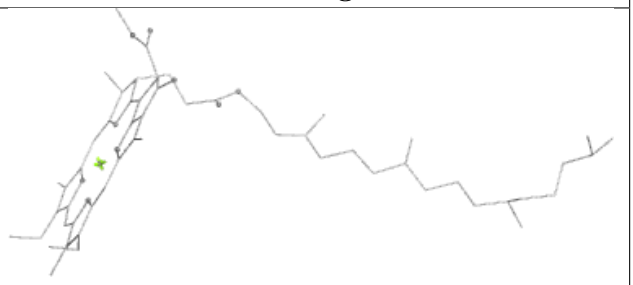
Bond lengths



Bond angles

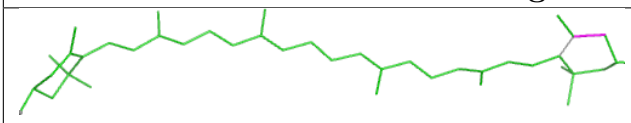


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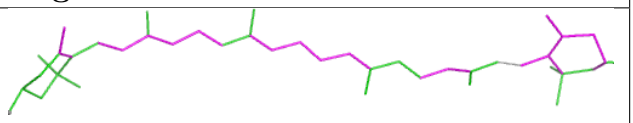


Rings

Ligand LUT g 621



Bond lengths



Bond angles

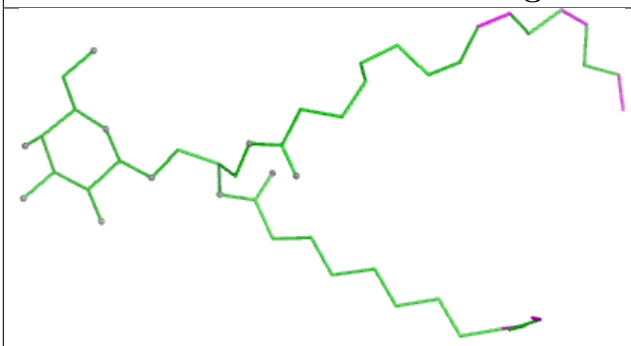


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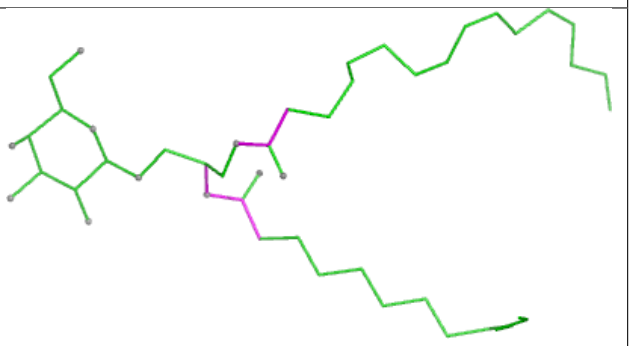


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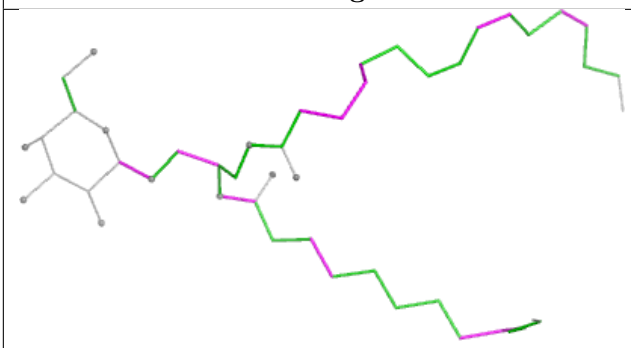
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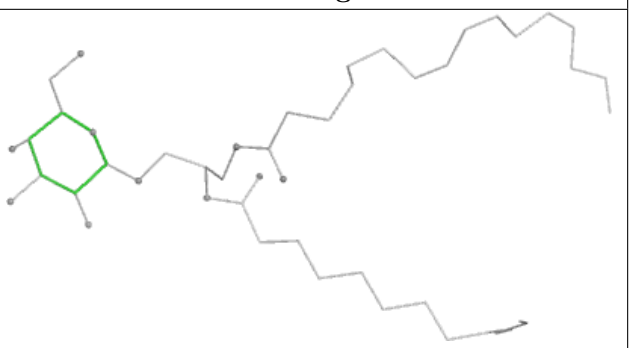
Bond lengths



Bond angles

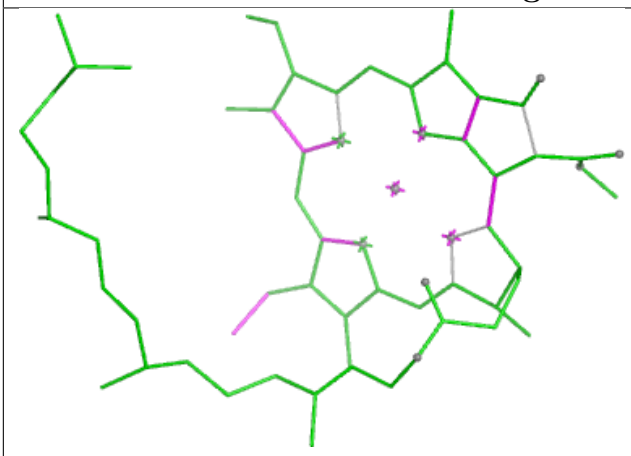


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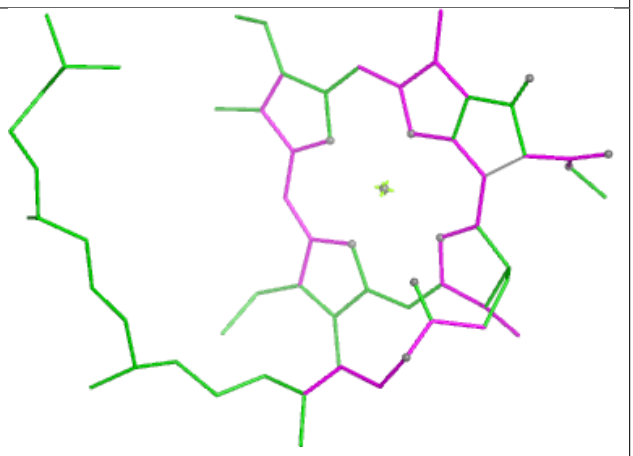


Rings

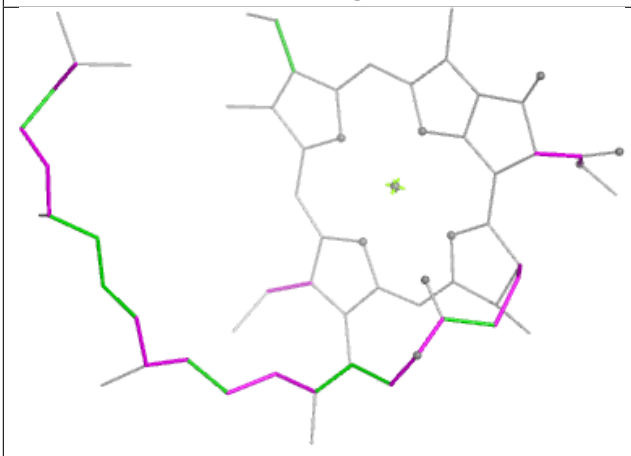
Ligand CLA G 602



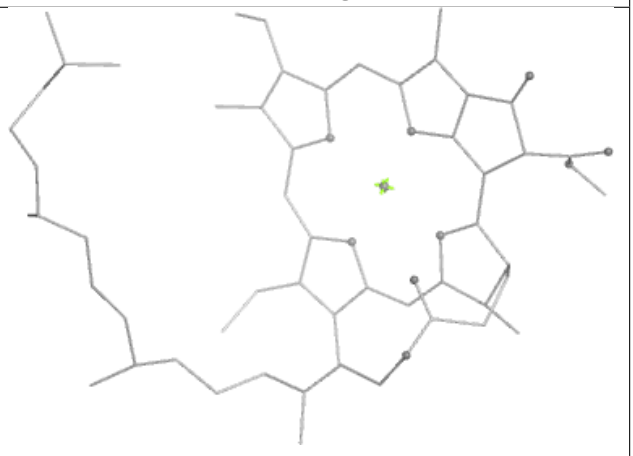
Bond lengths



Bond angles

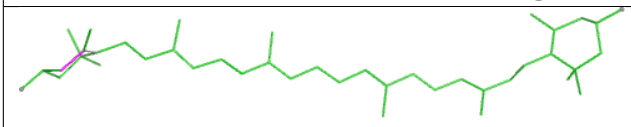


Torsions



Rings

Ligand LUT r 620



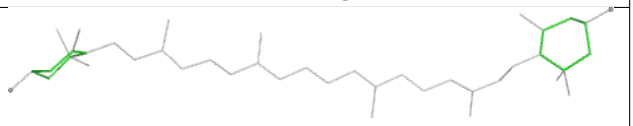
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Bond angles

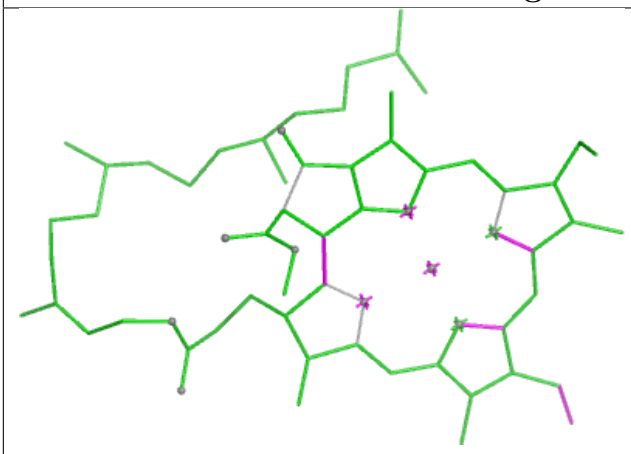


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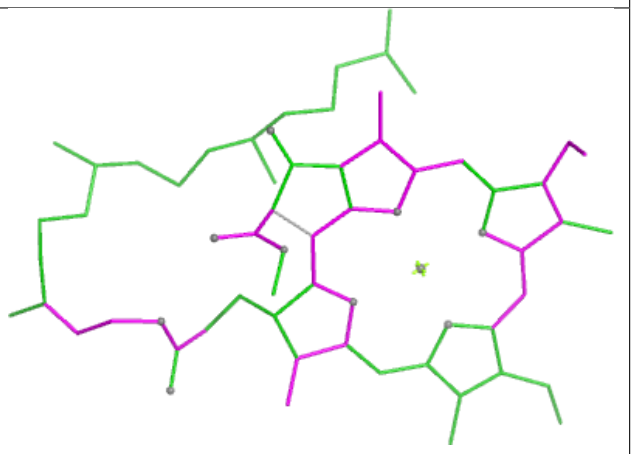


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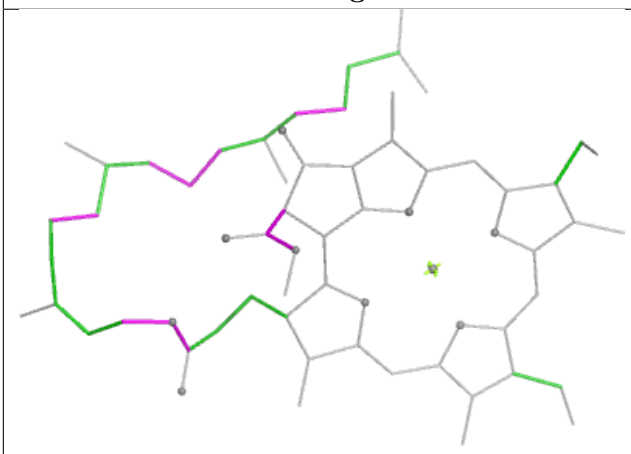
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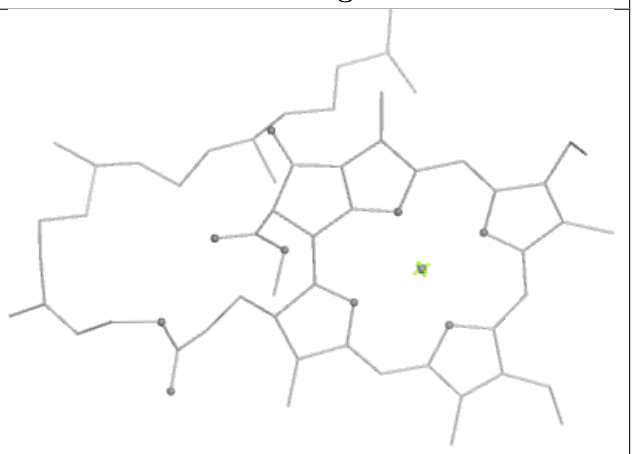
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Bond angles

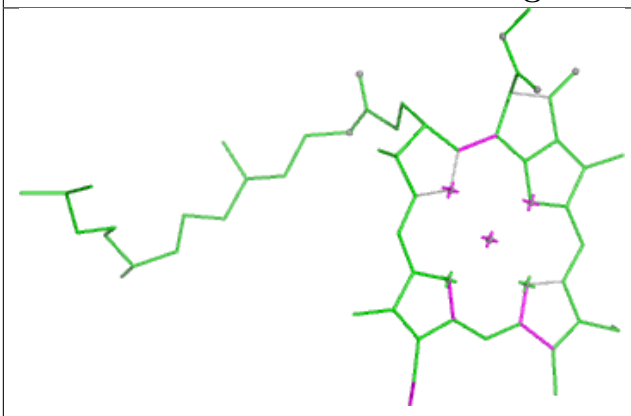


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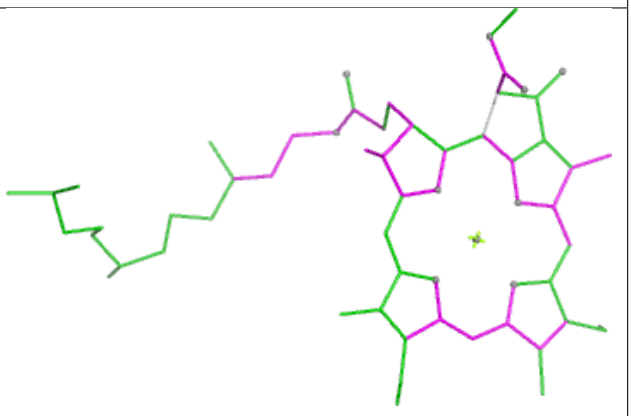


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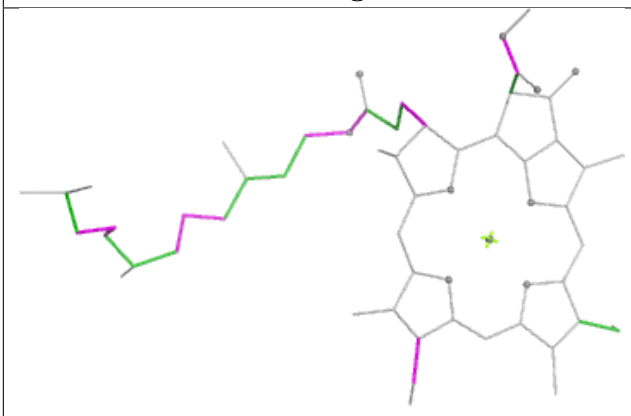
Ligand CLA A 410



Bond lengths



Bond angles

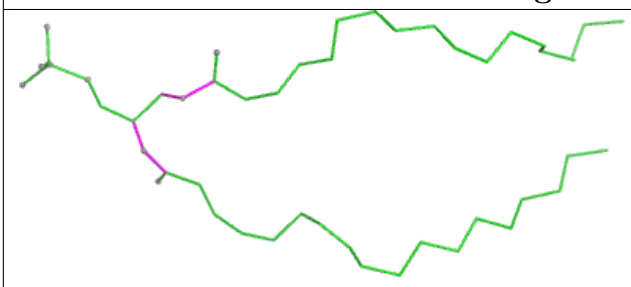


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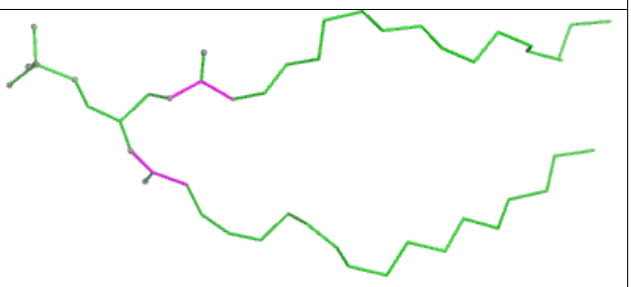


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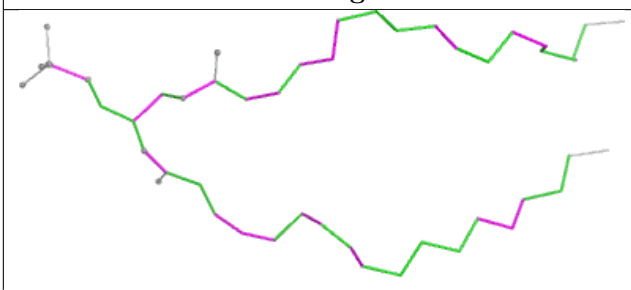
Ligand 3PH i 101



Bond lengths



Bond angles

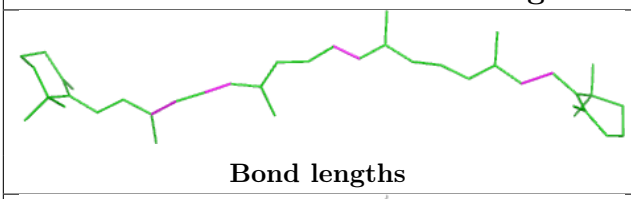


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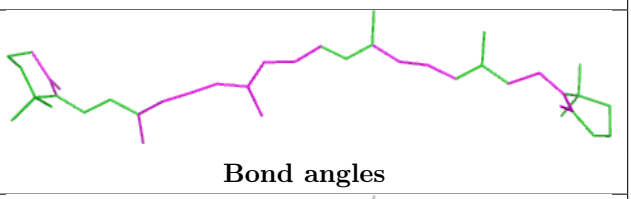


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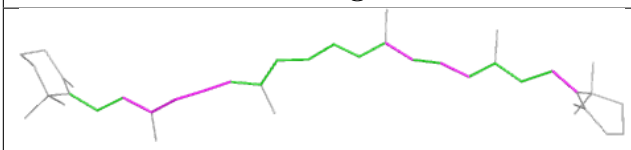
Ligand BCR c 515



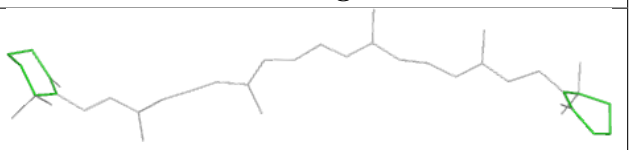
Bond lengths



Bond angles

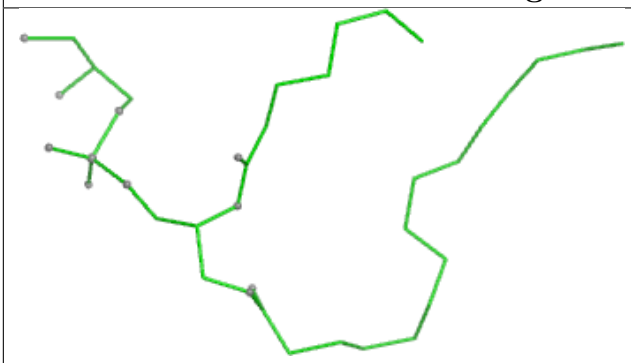


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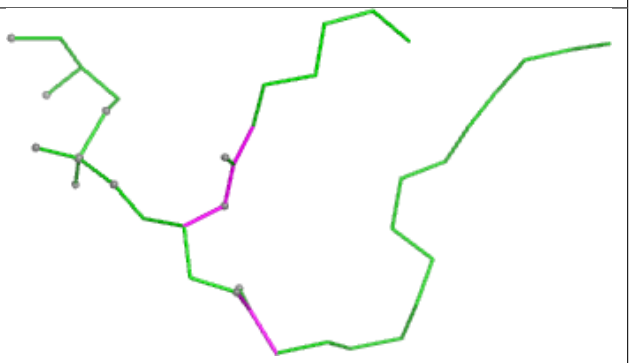


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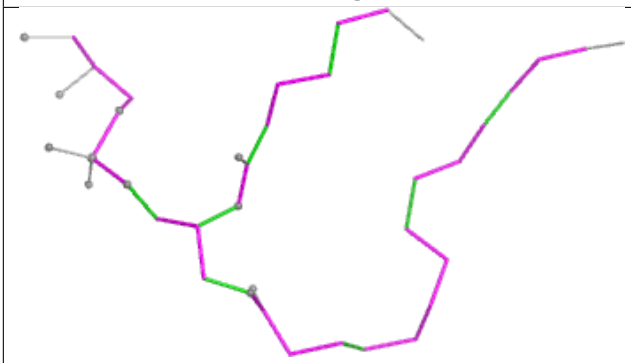
Ligand LHG d 410



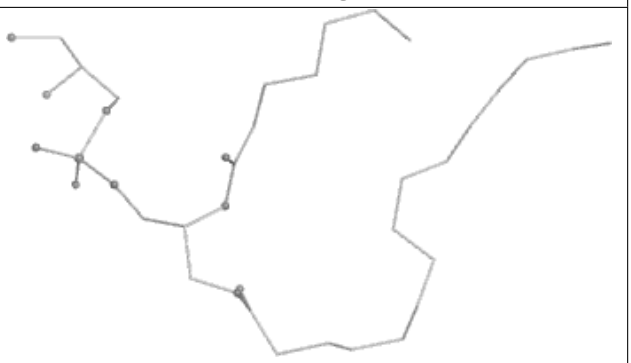
Bond lengths



Bond angles

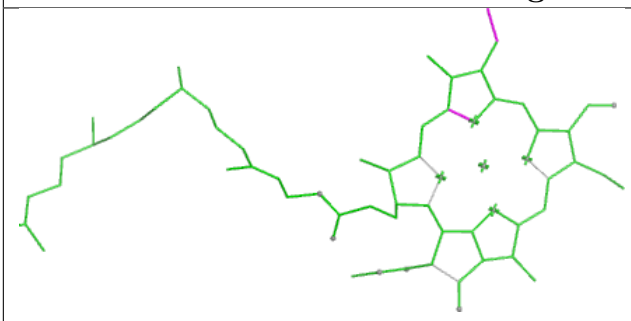


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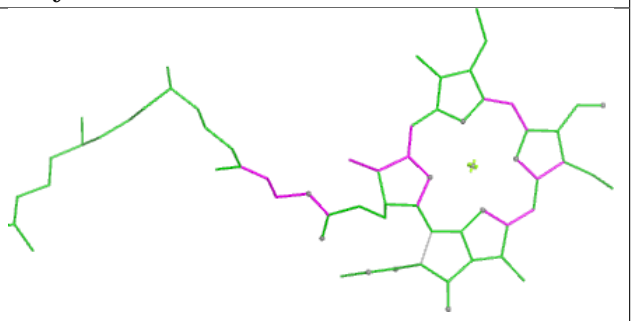


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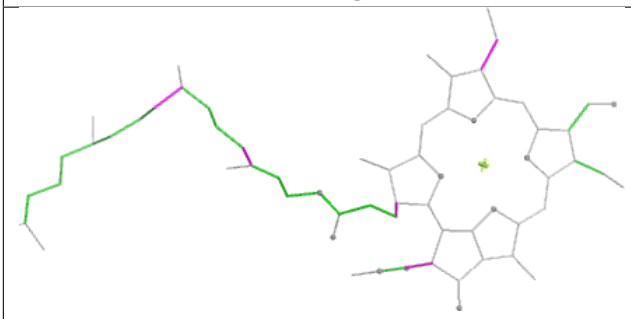
Ligand CHL y 601



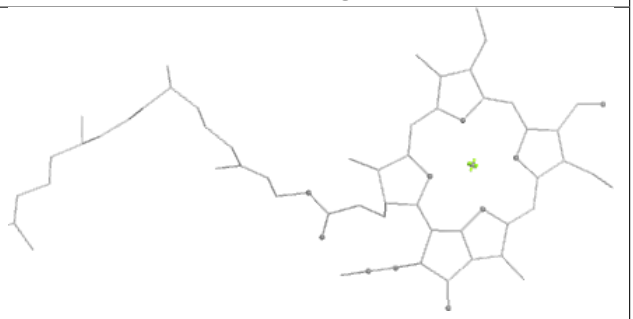
Bond lengths



Bond angles

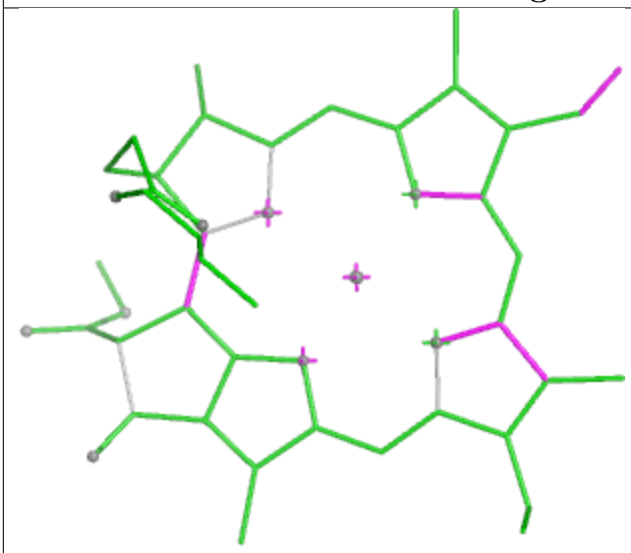


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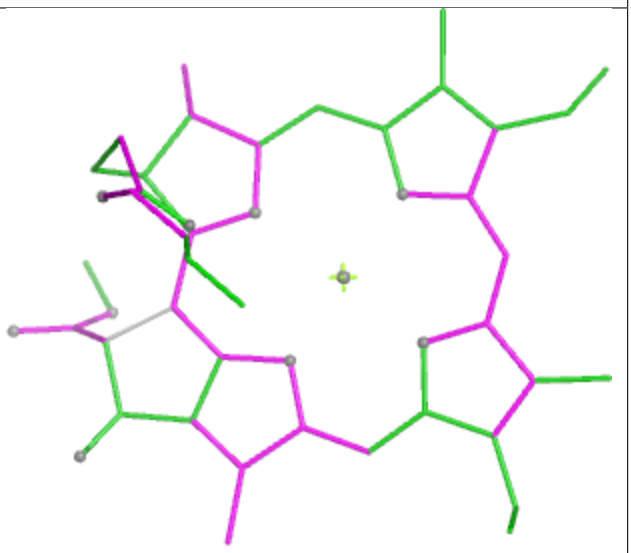


Rings

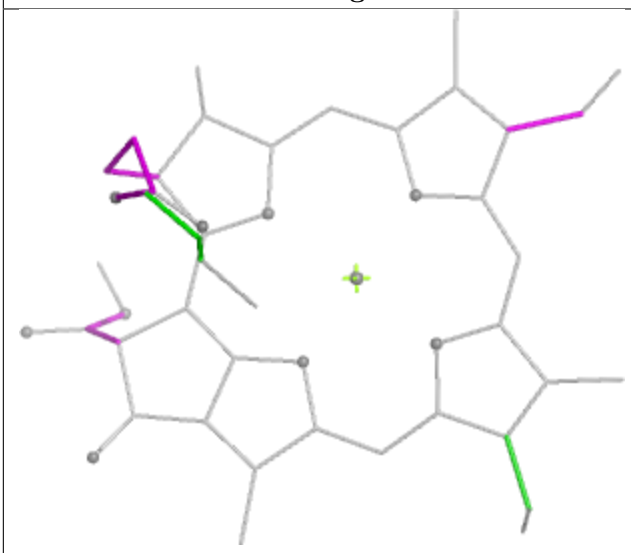
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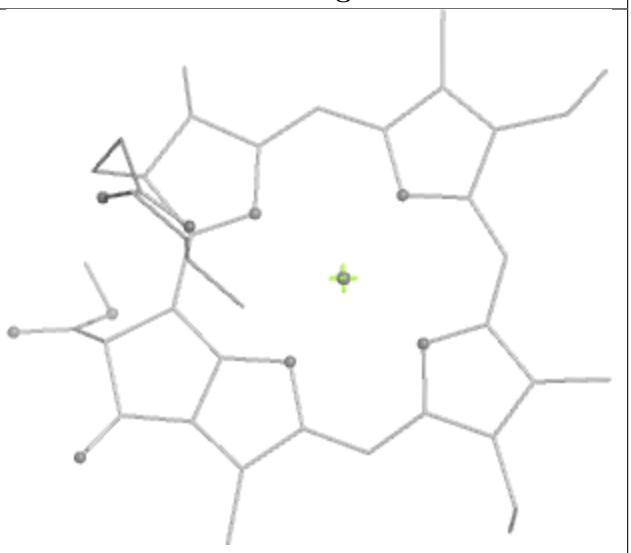
Bond lengths



Bond angles

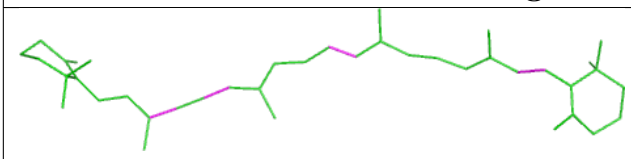


Torsions

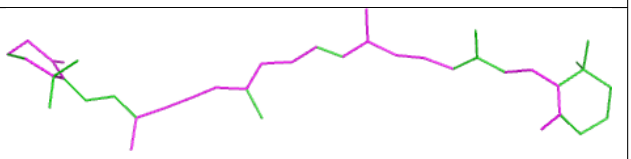


Rings

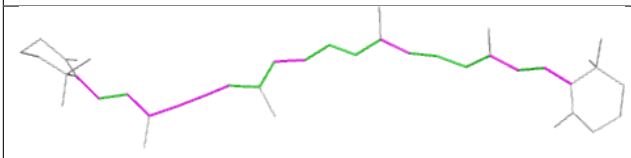
Ligand BCR b 618



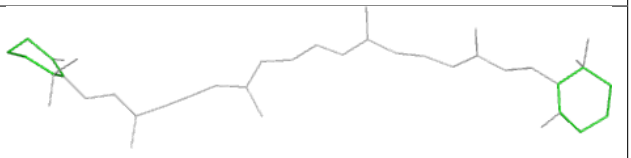
Bond lengths



Bond angles

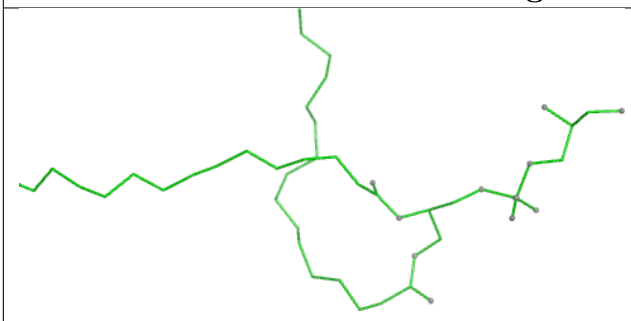


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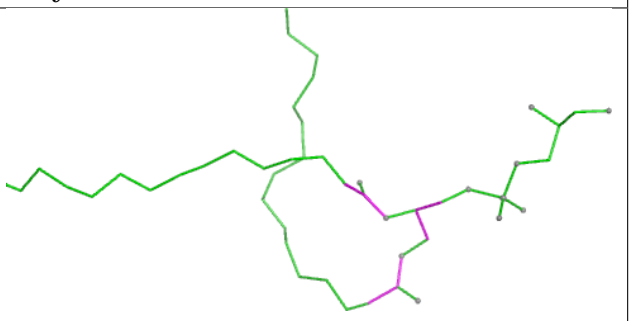


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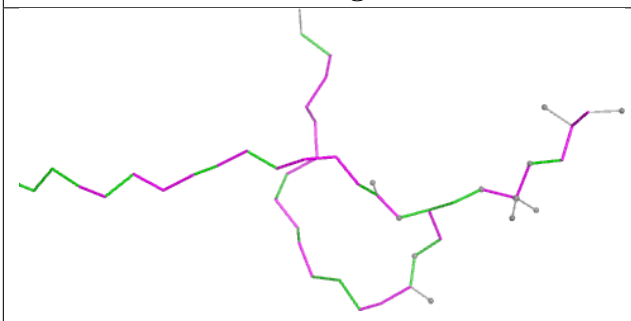
Ligand LHG y 624



Bond lengths



Bond angles

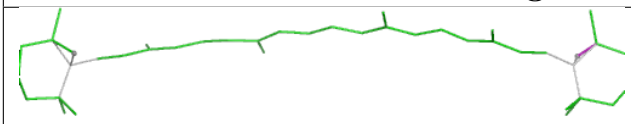


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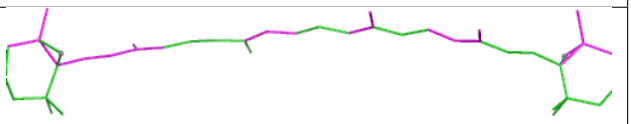


Rings

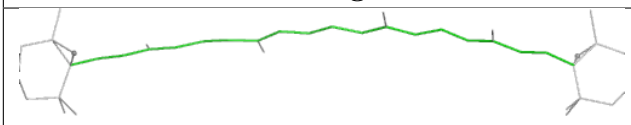
Ligand XAT n 622



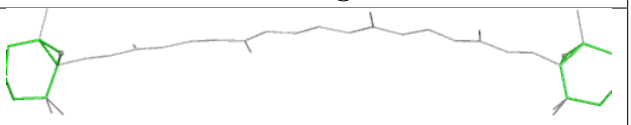
Bond lengths



Bond angles

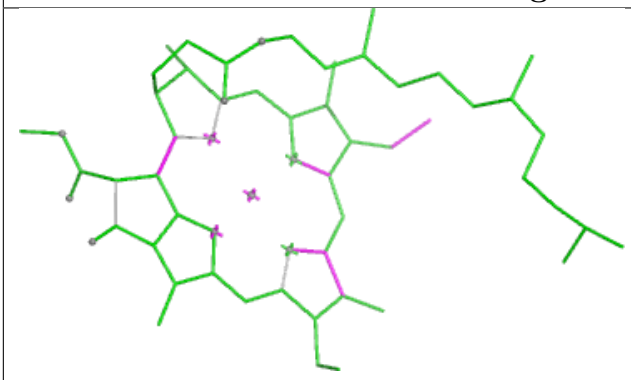


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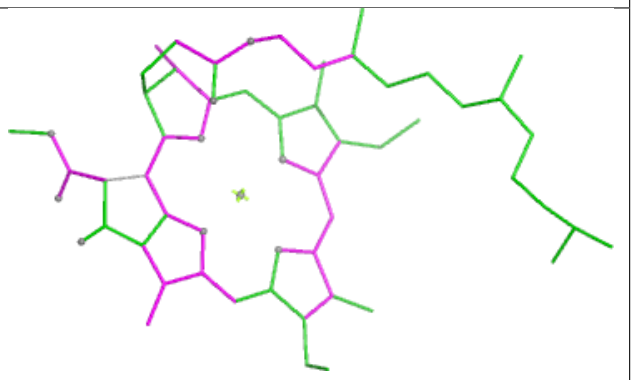


Rings

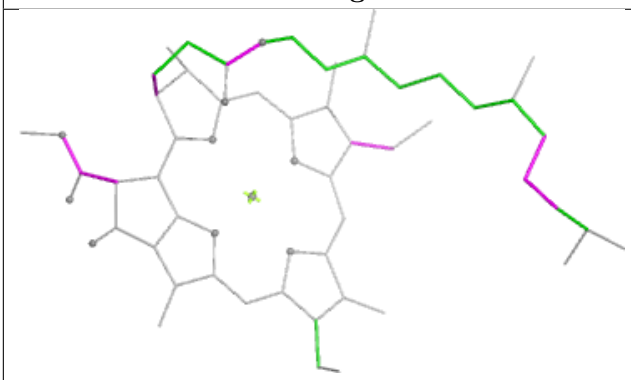
Ligand CLA s 602



Bond lengths



Bond angles

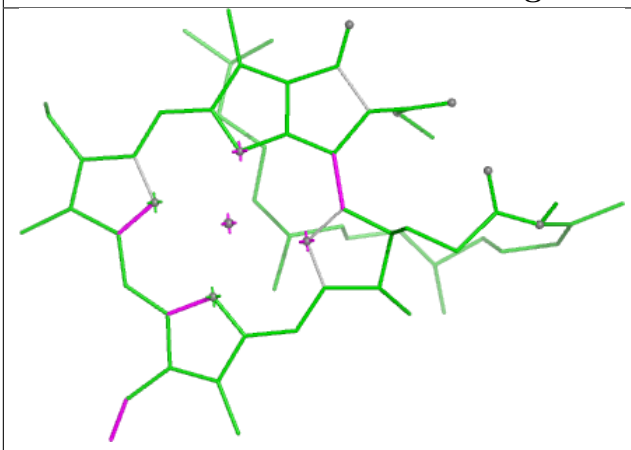


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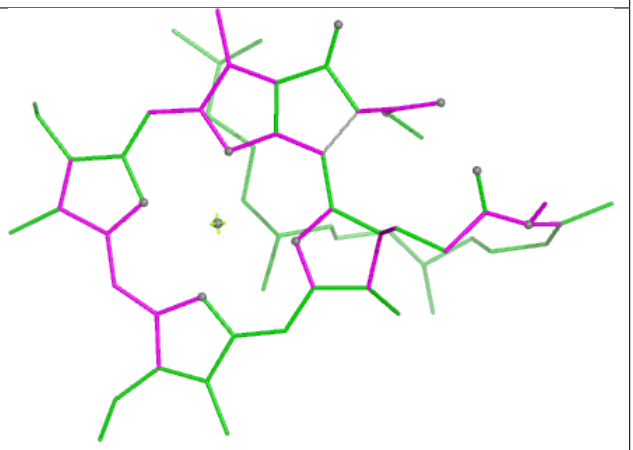


Rings

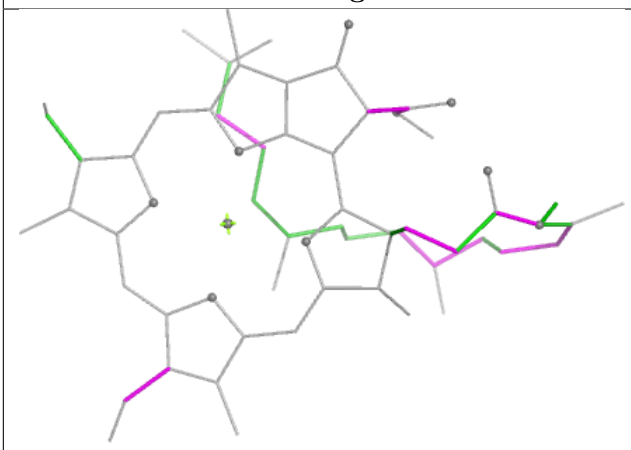
Ligand CLA C 510



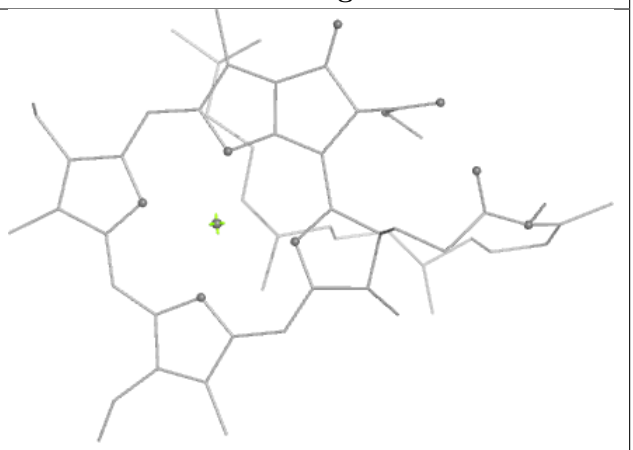
Bond lengths



Bond angles

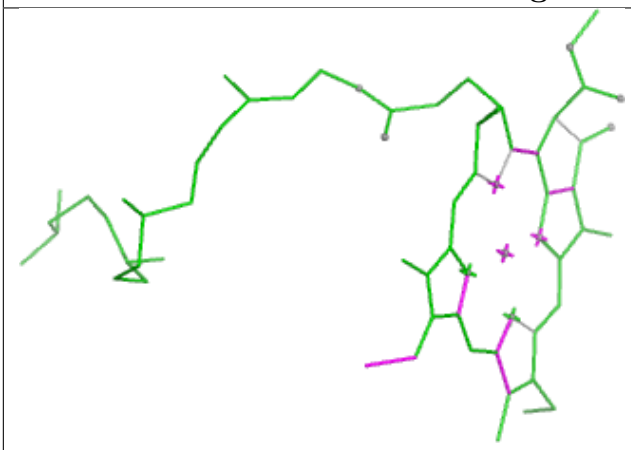


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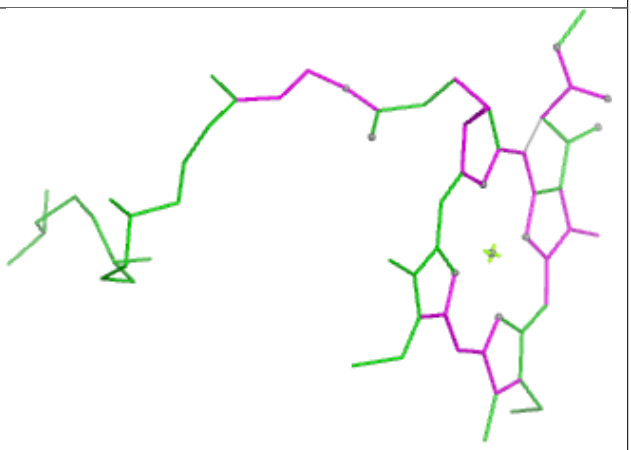


Rings

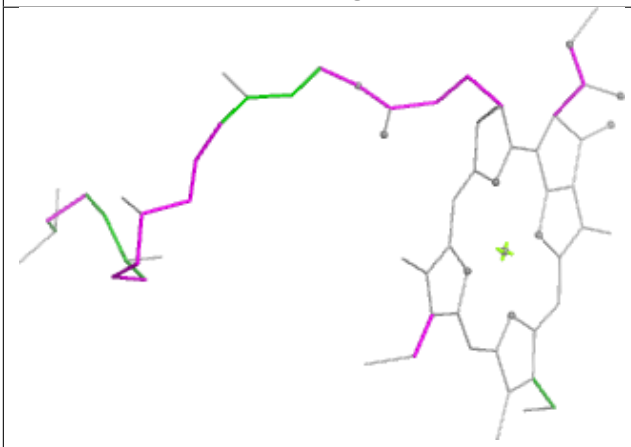
Ligand CLA s 610



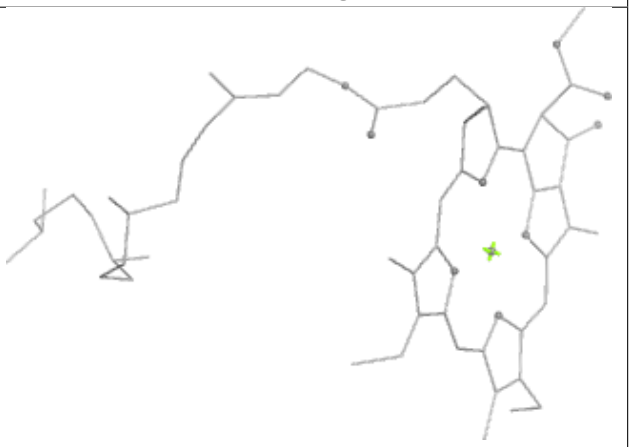
Bond lengths



Bond angles

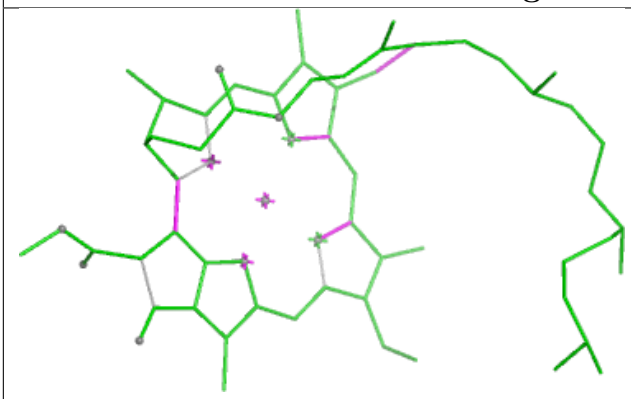


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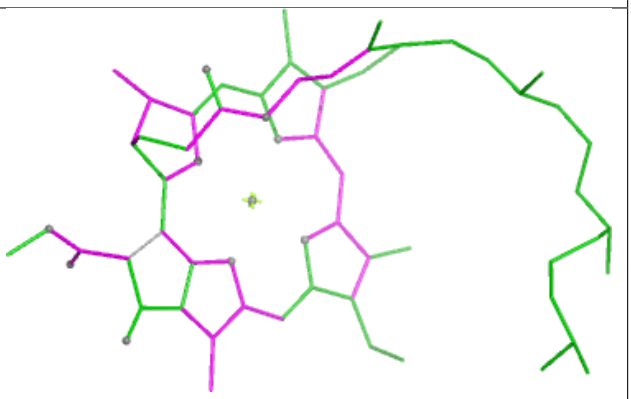


Rings

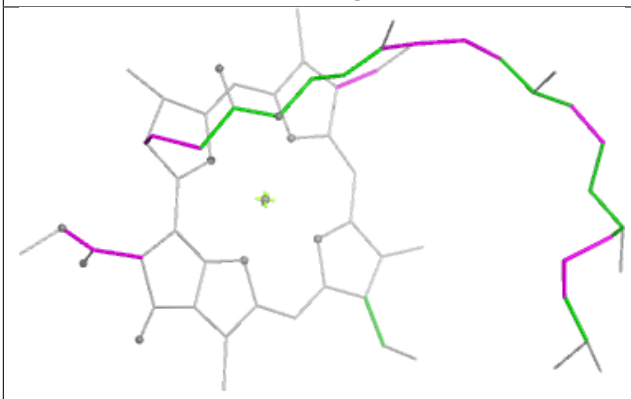
Ligand CLA G 610



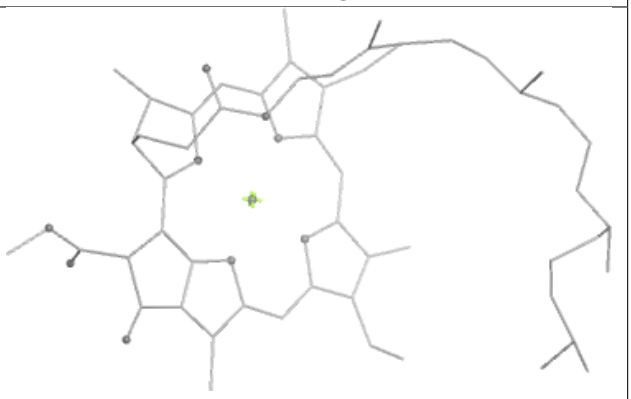
Bond lengths



Bond angles

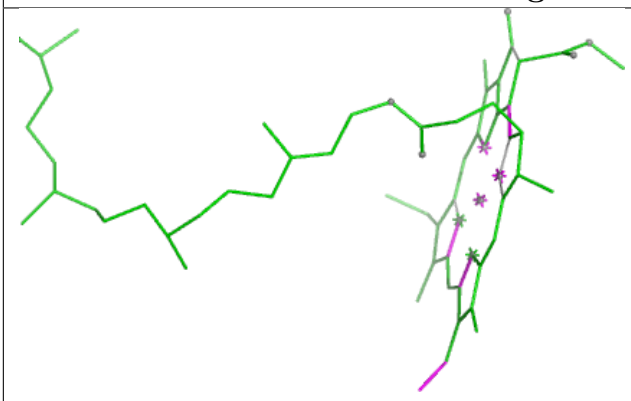


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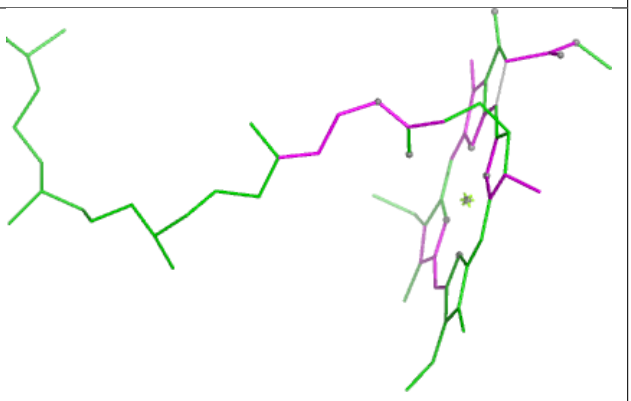


Rings

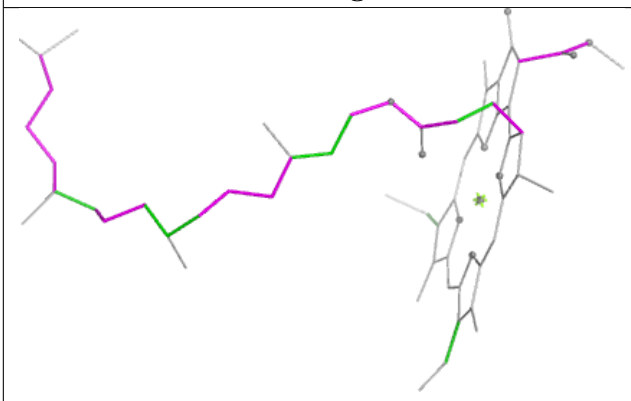
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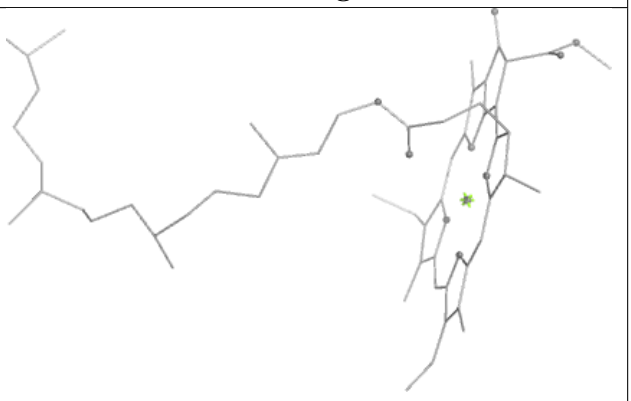
Bond lengths



Bond angles

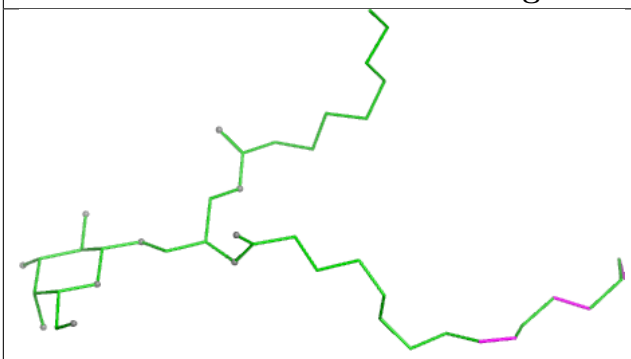


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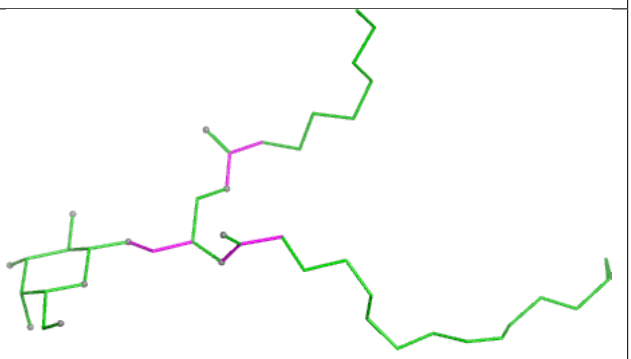


Rings

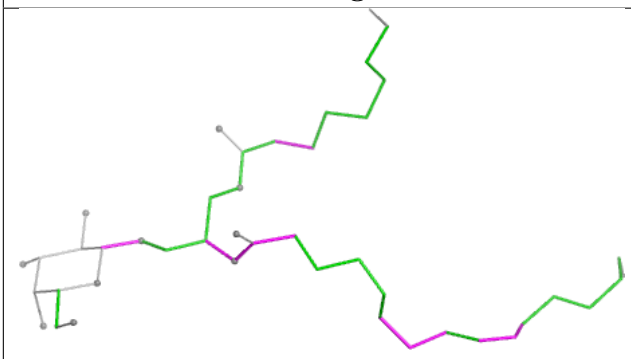
Ligand LMG b 622



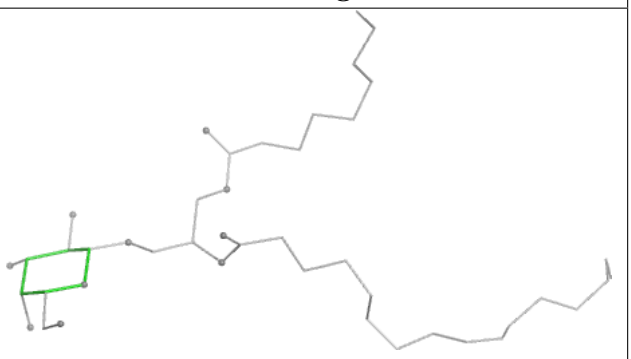
Bond lengths



Bond angles

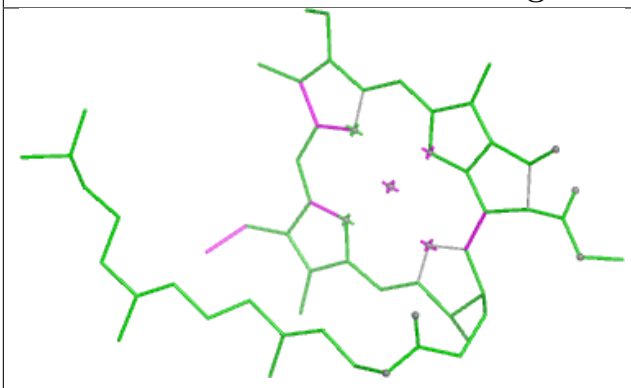


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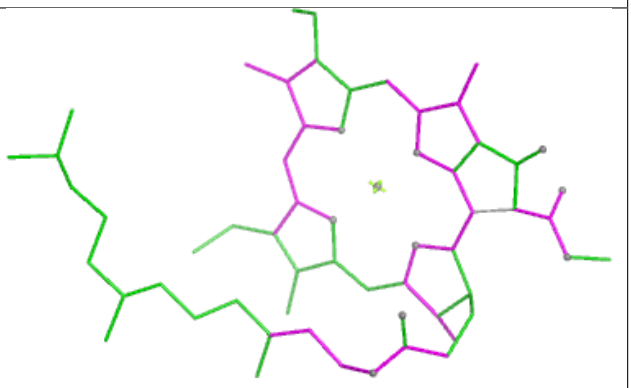


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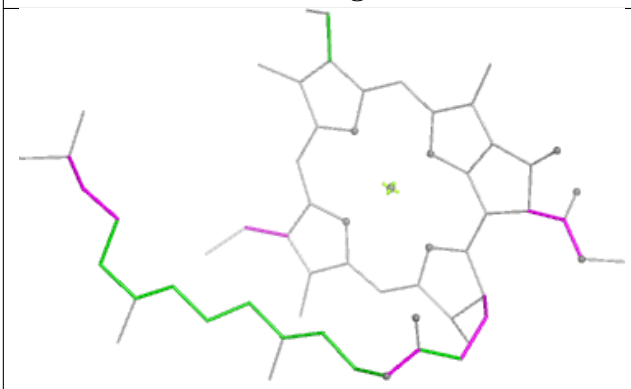
Ligand CLA S 602



Bond lengths



Bond angles

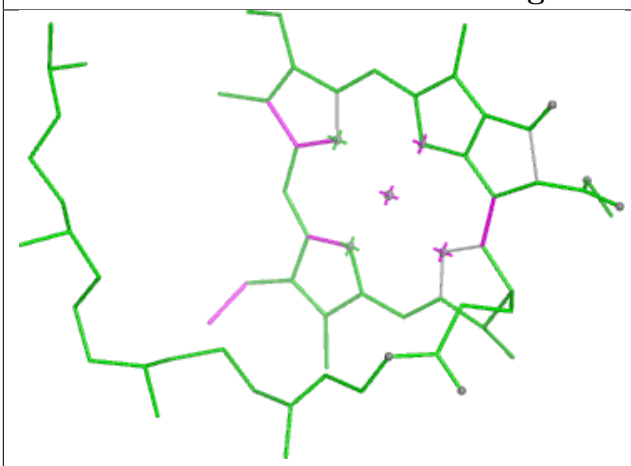


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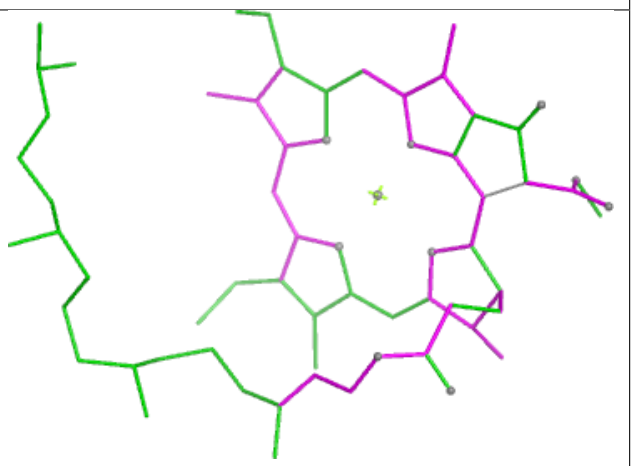


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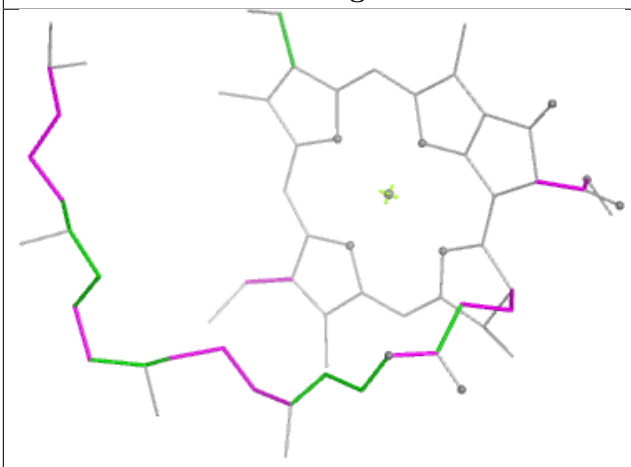
Ligand CLA n 602



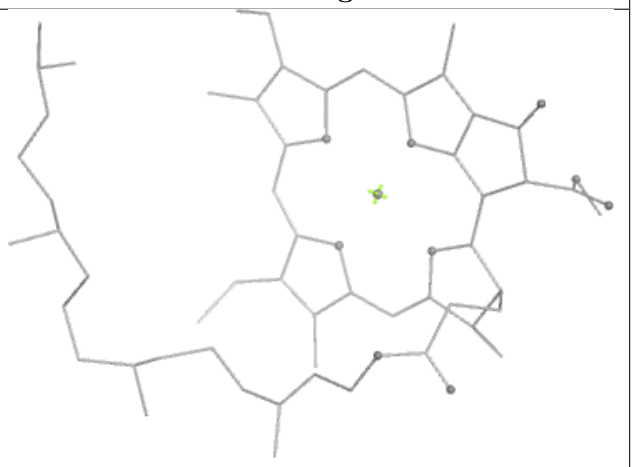
Bond lengths



Bond angles

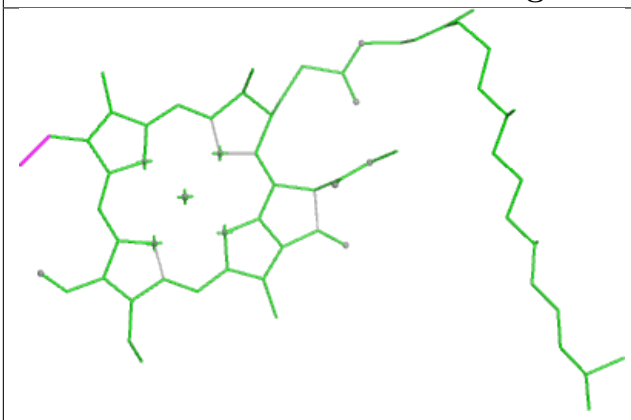


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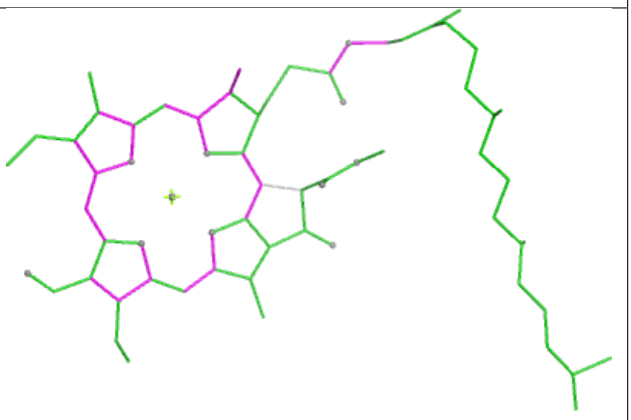


Rings

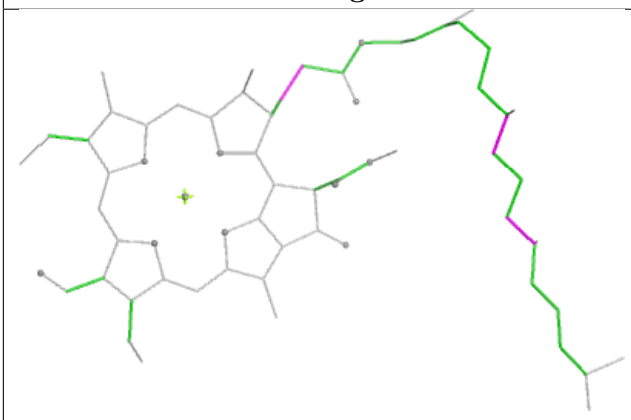
Ligand CHL n 606



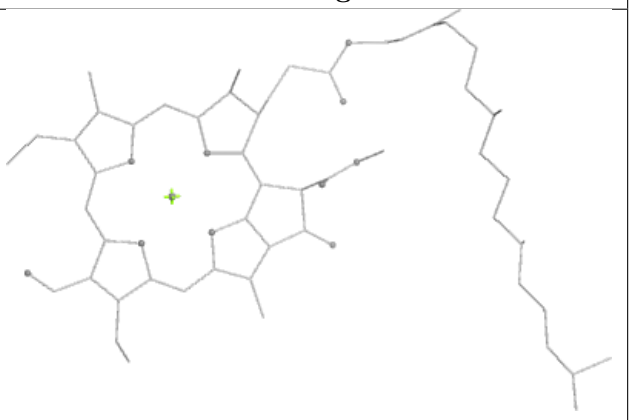
Bond lengths



Bond angles

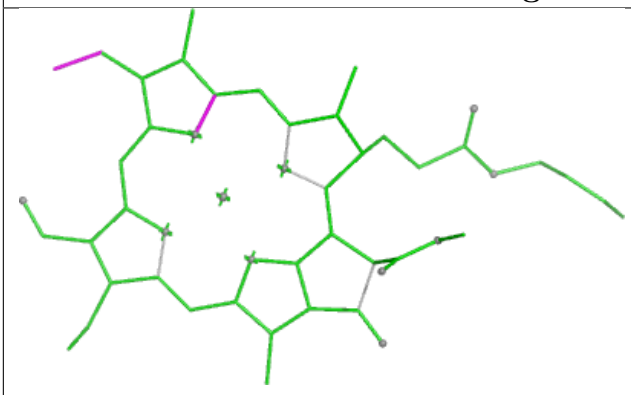


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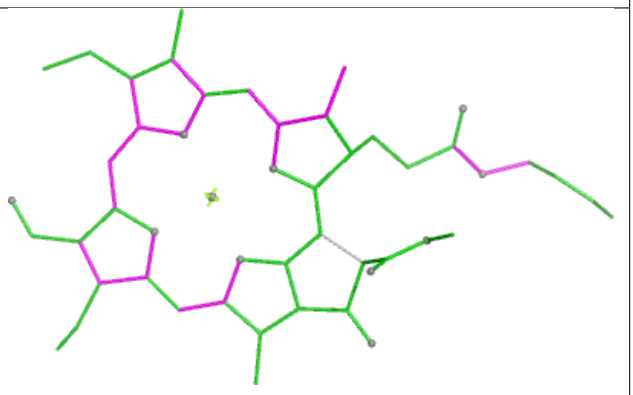


Rings

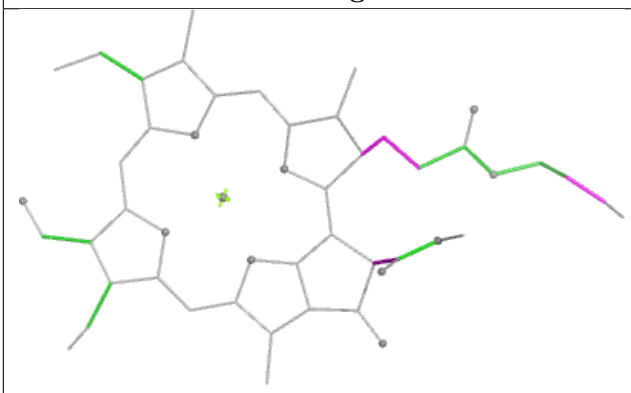
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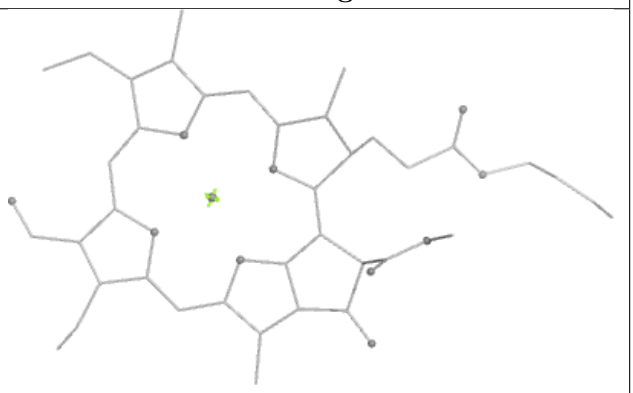
Bond lengths



Bond angles

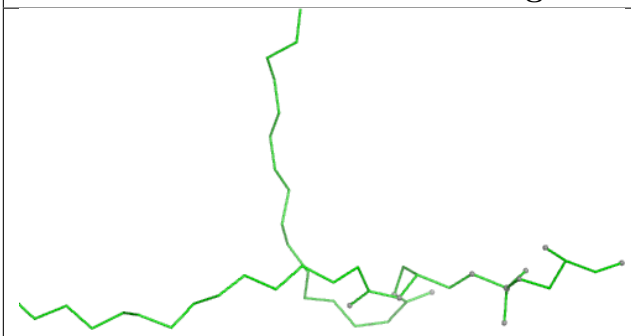


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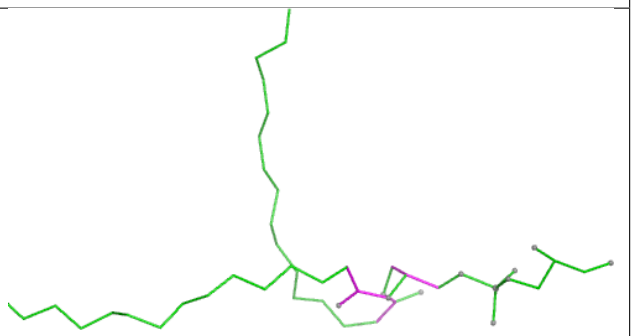


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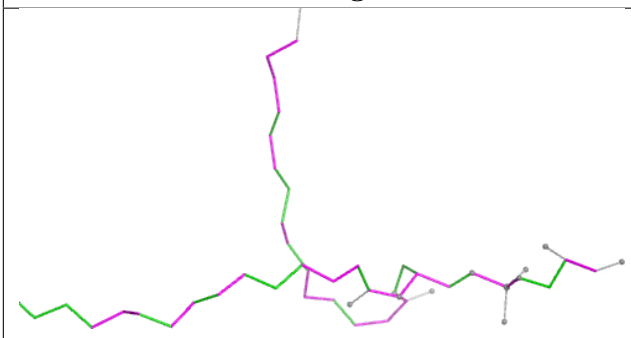
Ligand LHG n 624



Bond lengths



Bond angles

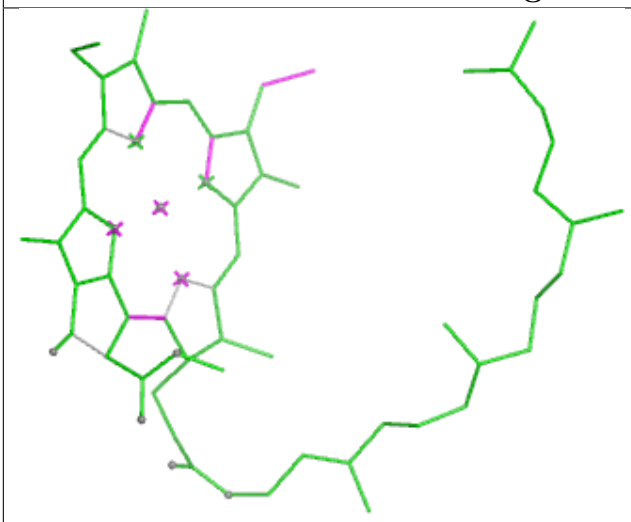


Torsions

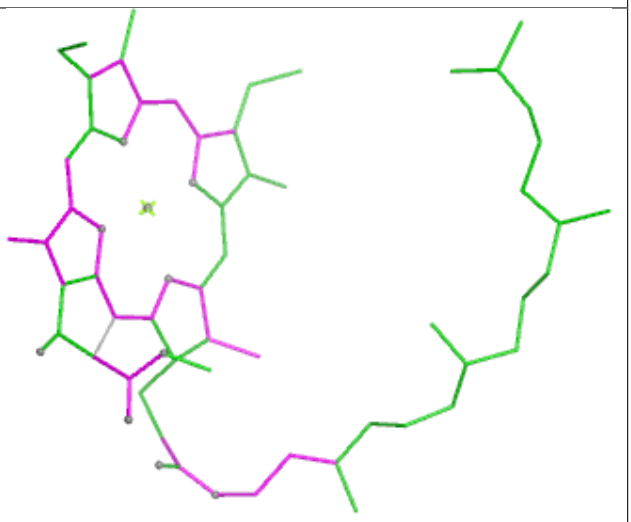


Rings

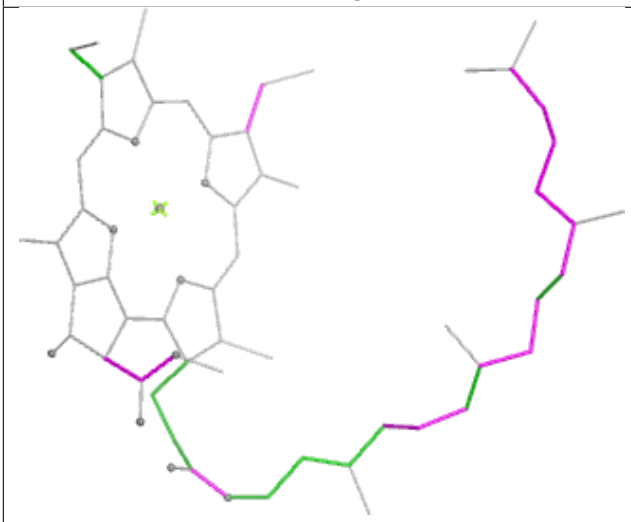
Ligand CLA C 507



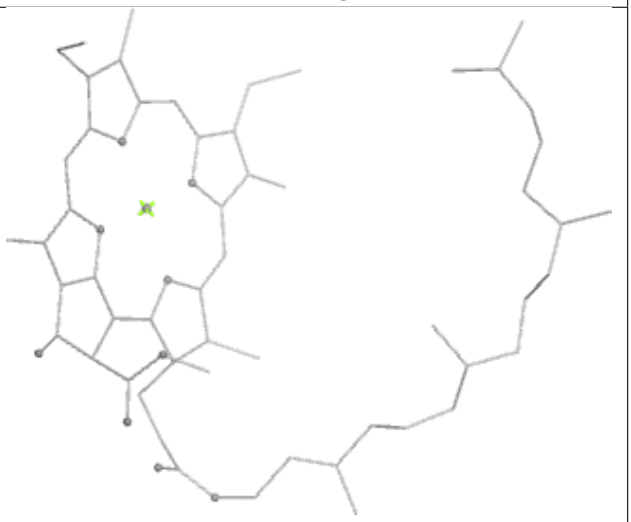
Bond lengths



Bond angles

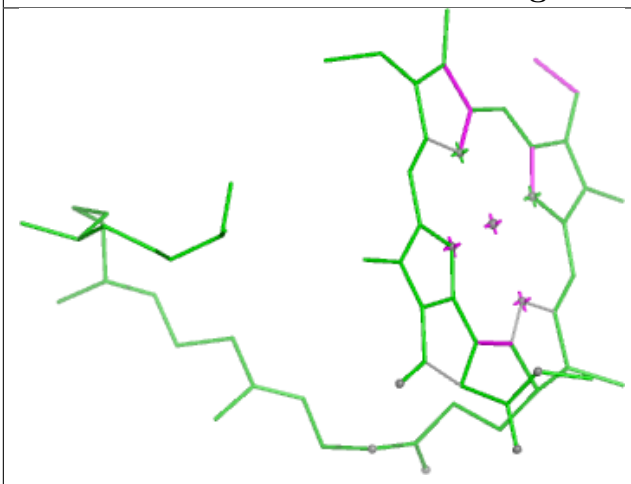


Torsions

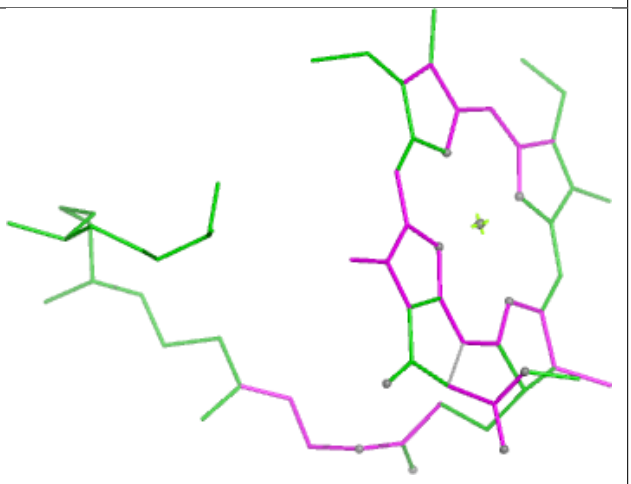


Rings

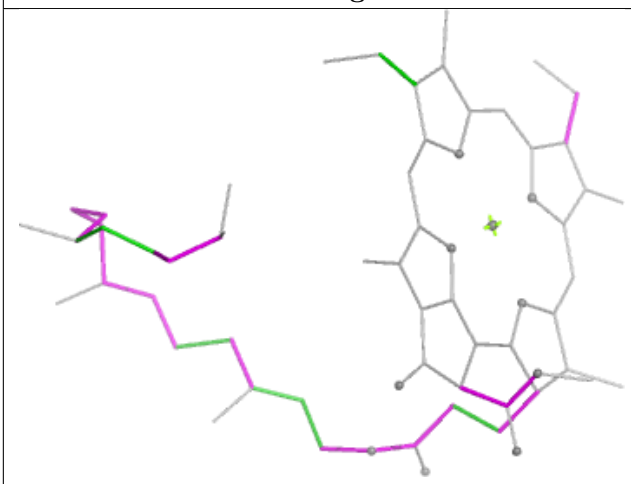
Ligand CLA c 503



Bond lengths



Bond angles

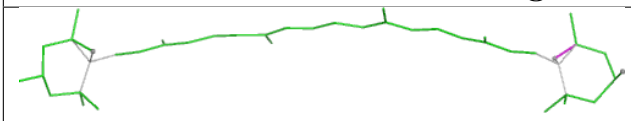


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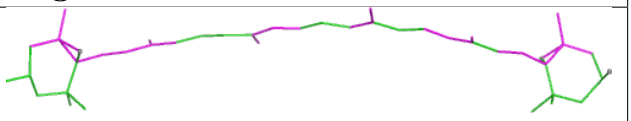


Rings

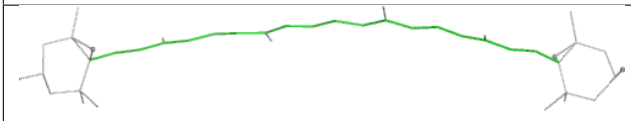
Ligand XAT g 622



Bond lengths



Bond angles

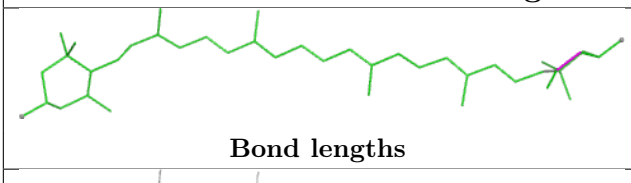


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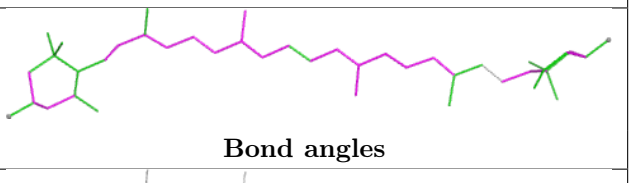


Rings

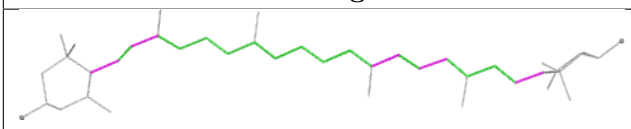
Ligand LUT R 620



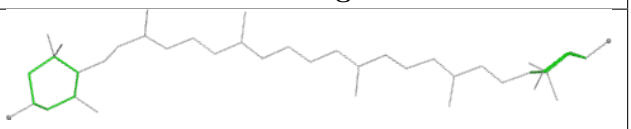
Bond lengths



Bond angles

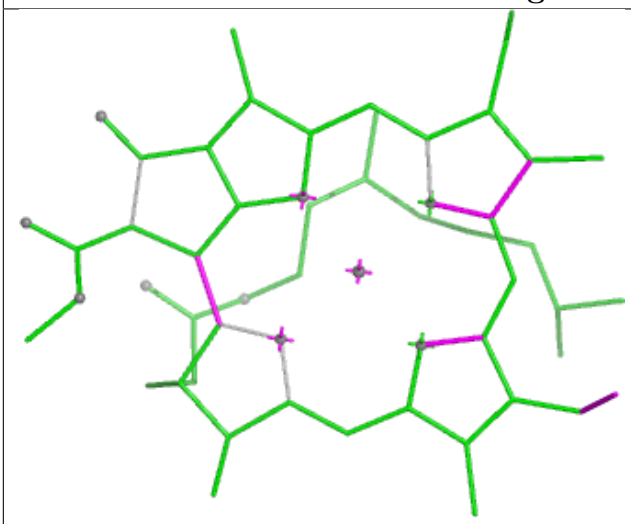


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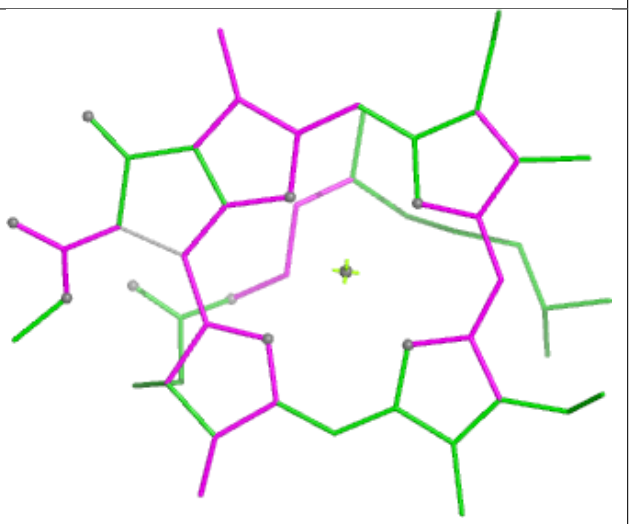


Rings

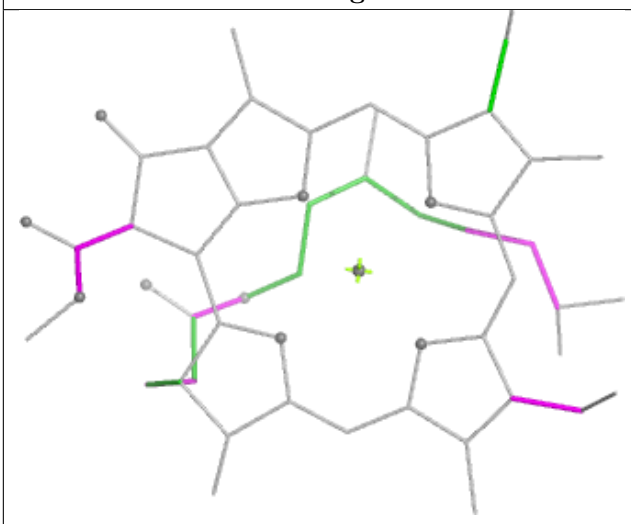
Ligand CLA S 613



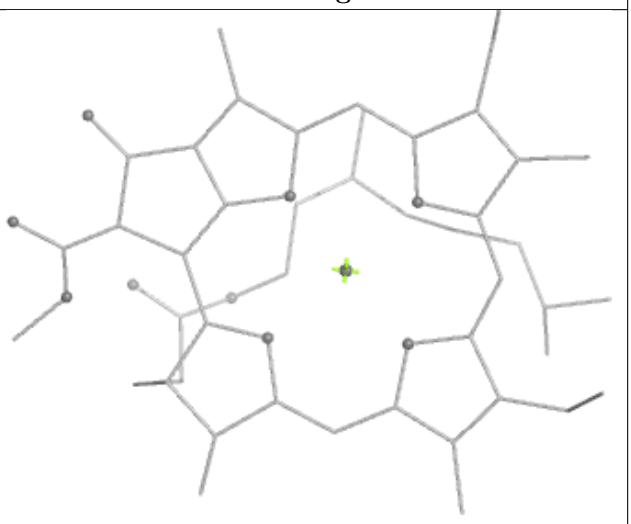
Bond lengths



Bond angles

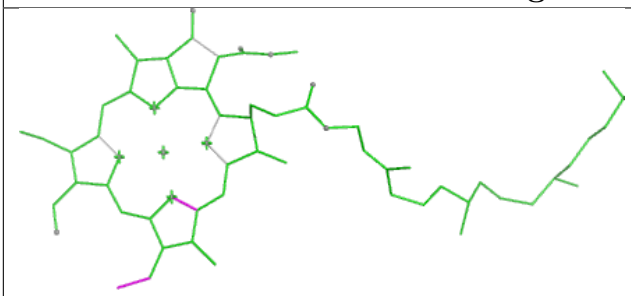


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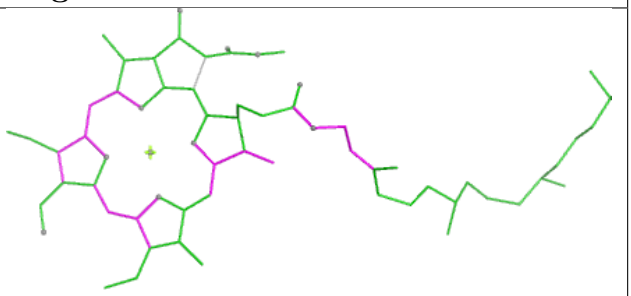


Rings

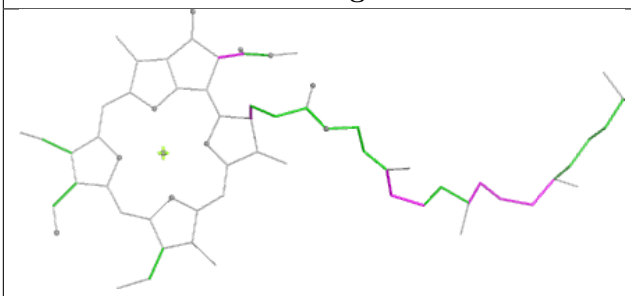
Ligand CHL g 601



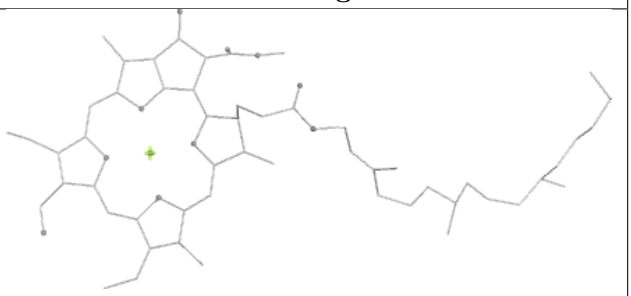
Bond lengths



Bond angles

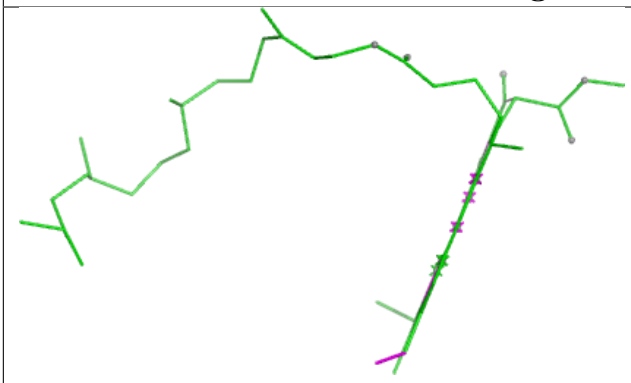


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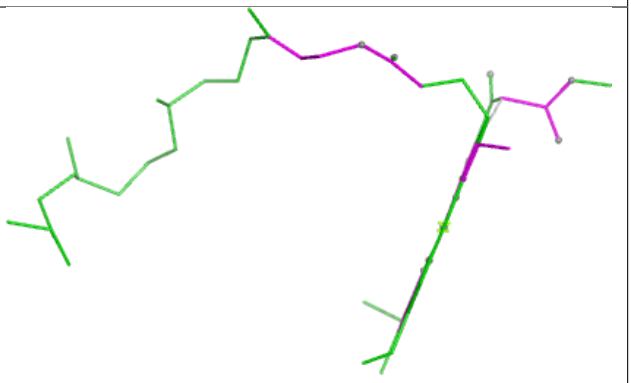


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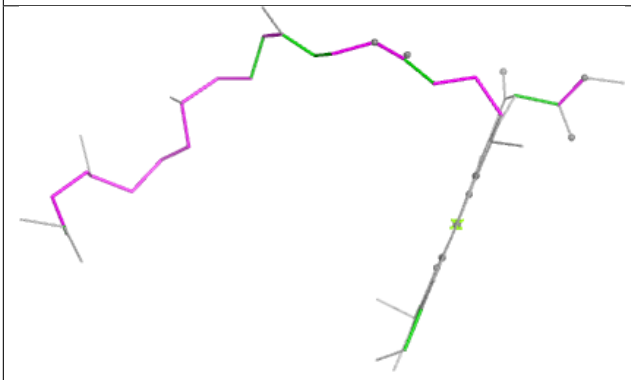
Ligand CLA c 506



Bond lengths



Bond angles

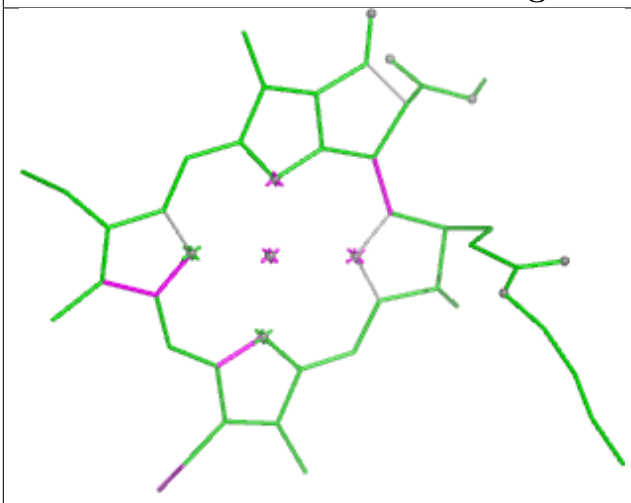


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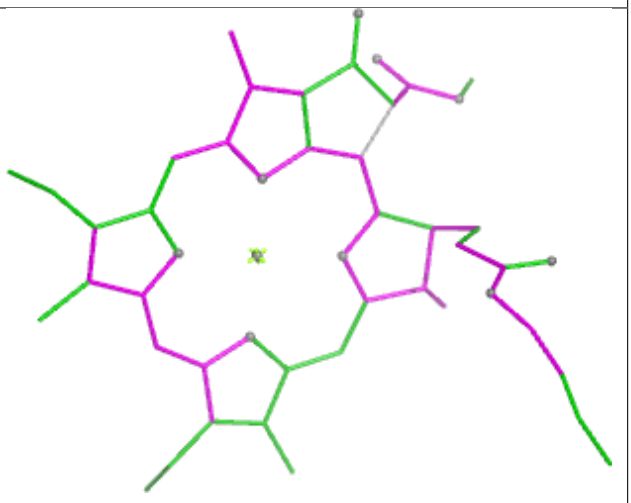


Rings

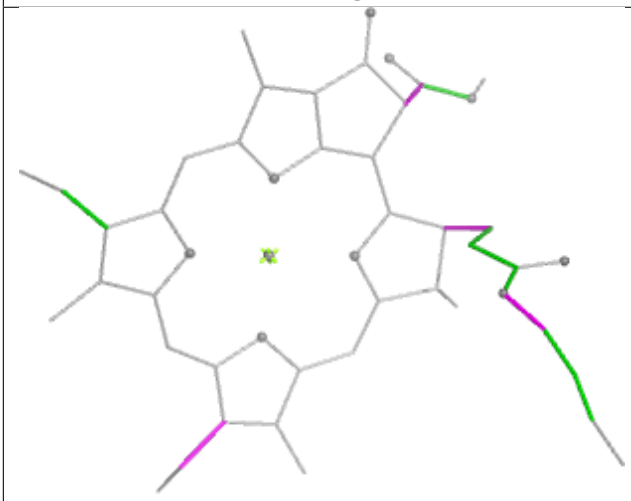
Ligand CLA a 407



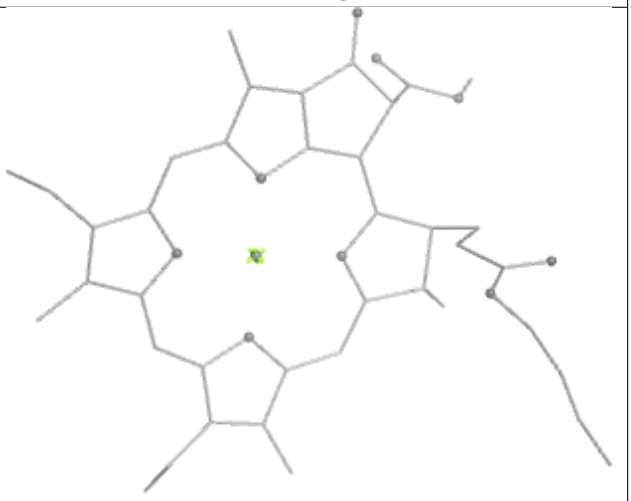
Bond lengths



Bond angles

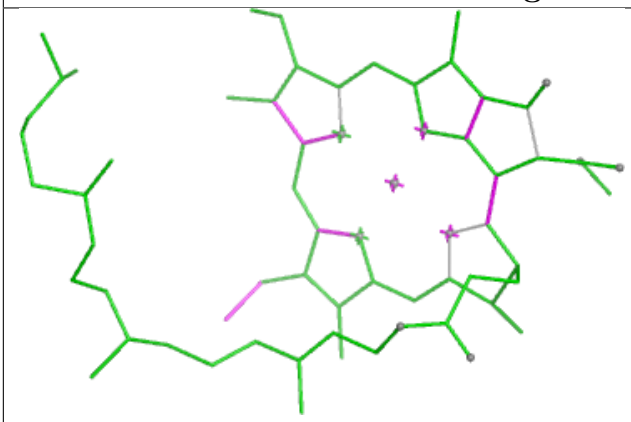


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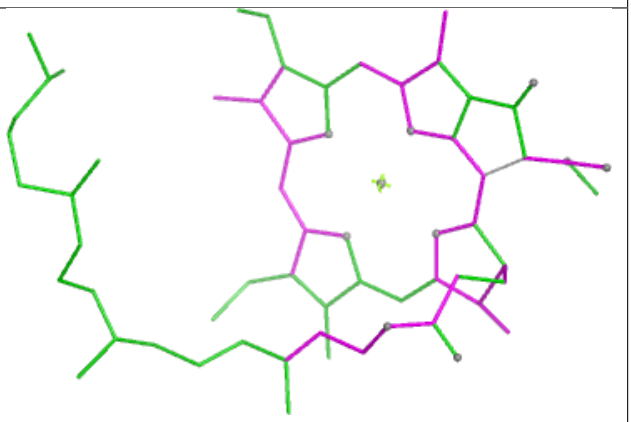


Rings

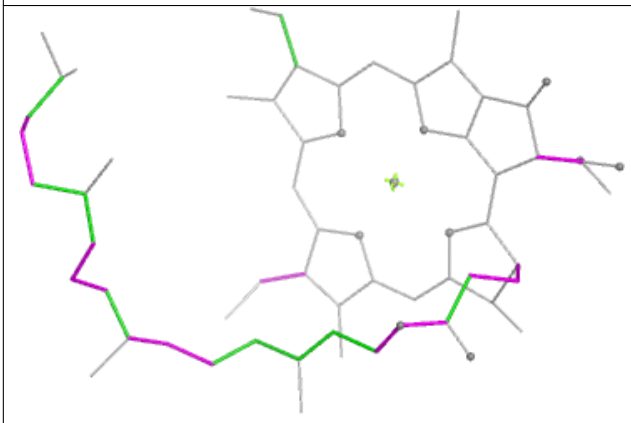
Ligand CLA Y 602



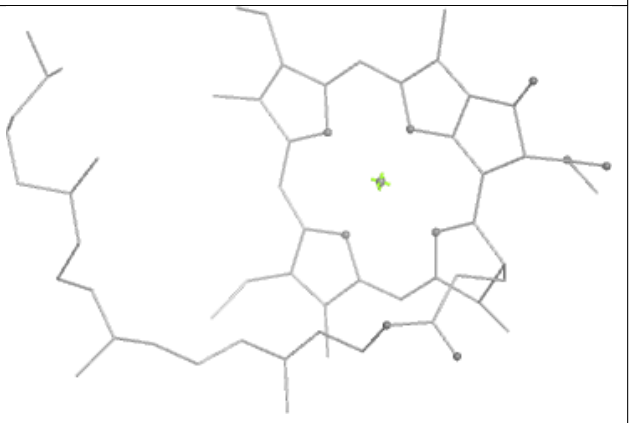
Bond lengths



Bond angles

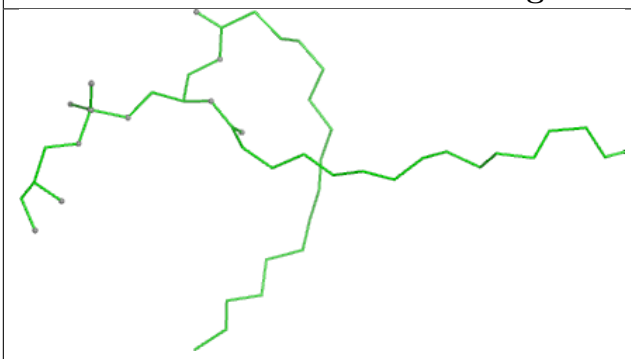


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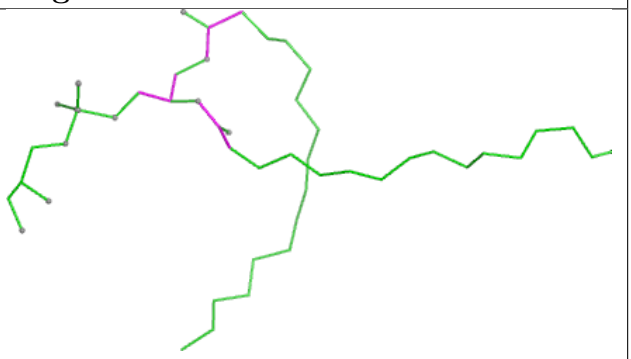


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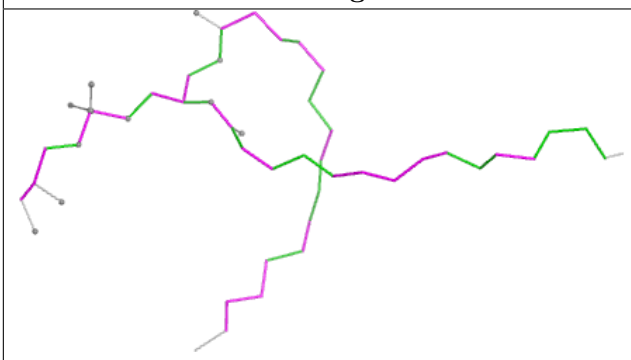
Ligand LHG g 624



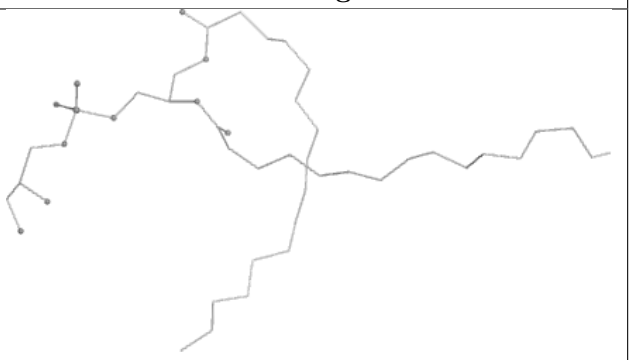
Bond lengths



Bond angles

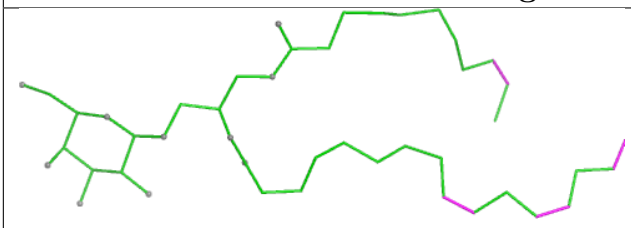


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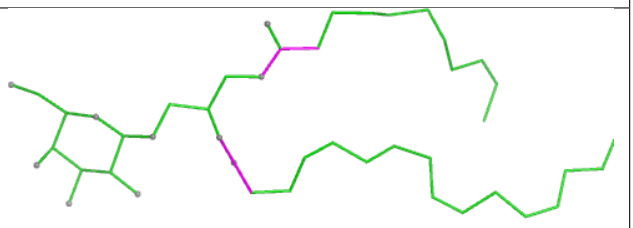


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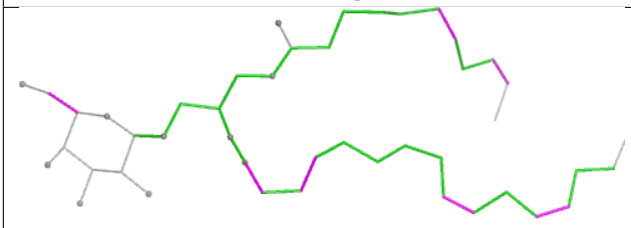
Ligand LMG D 411



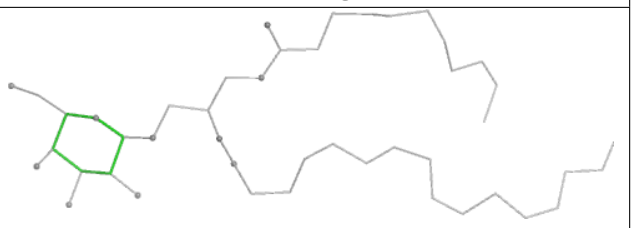
Bond lengths



Bond angles

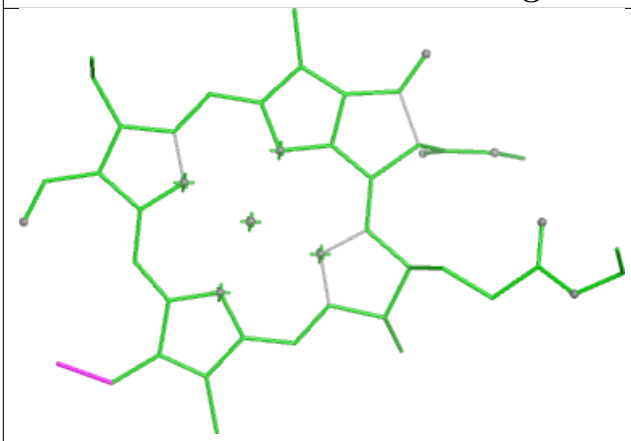


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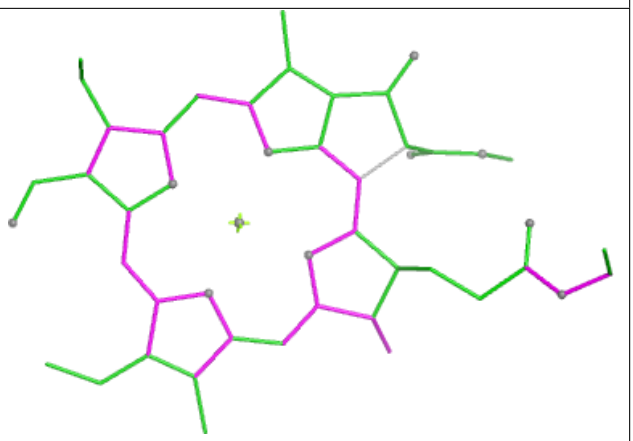


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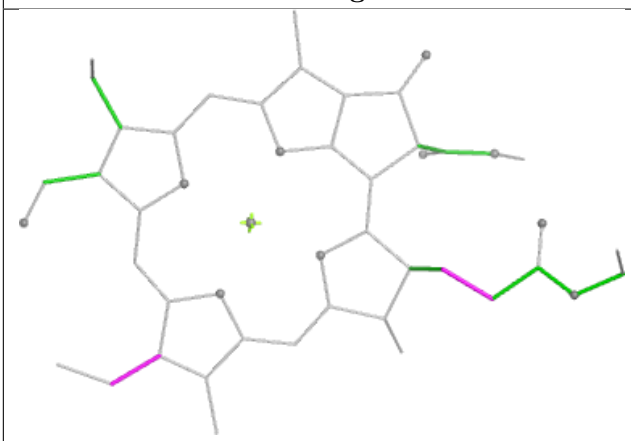
Ligand CHL G 605



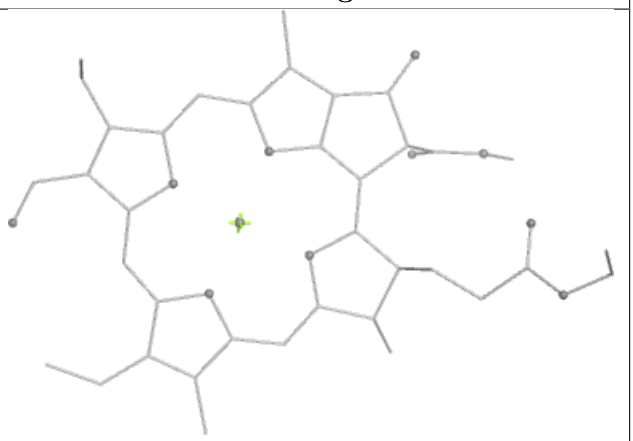
Bond lengths



Bond angles

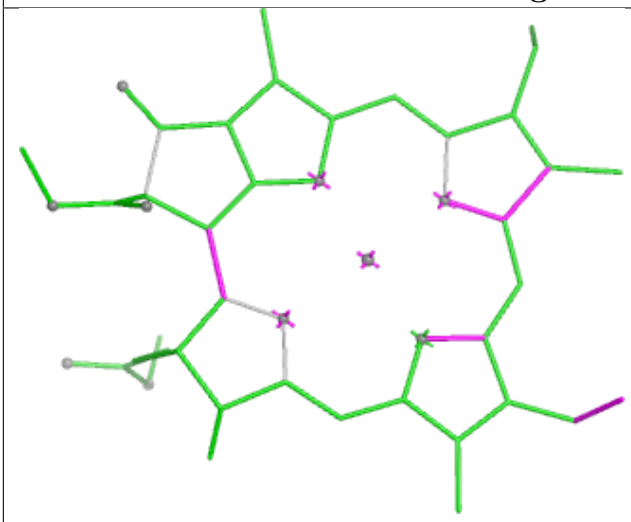


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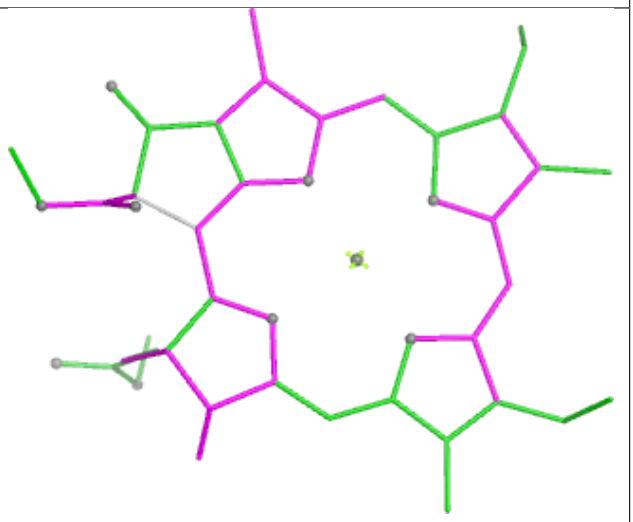


Rings

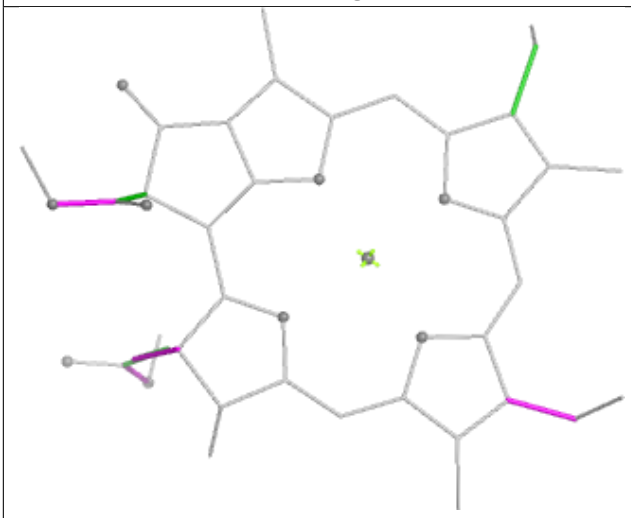
Ligand CLA r 611



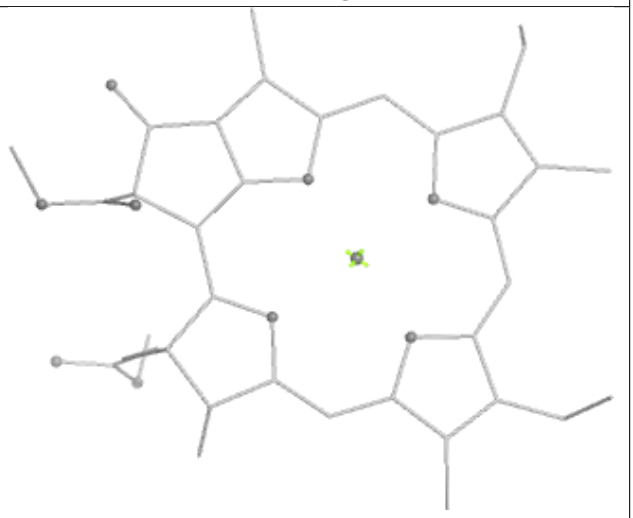
Bond lengths



Bond angles

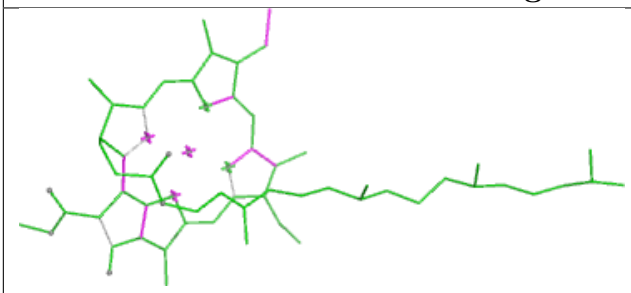


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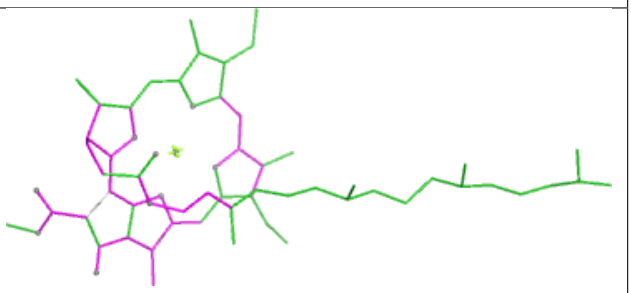


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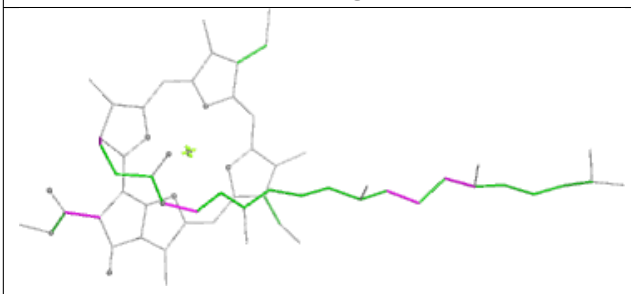
Ligand CLA B 615



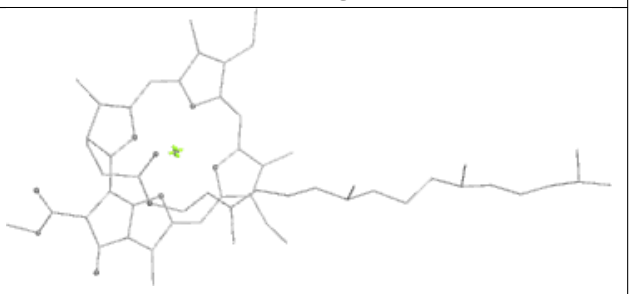
Bond lengths



Bond angles



Torsions

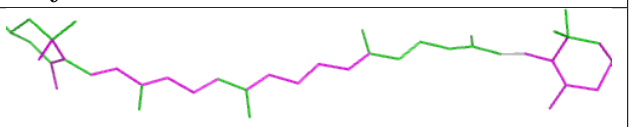


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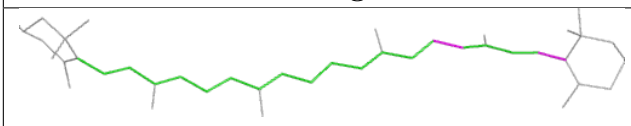
Ligand LUT y 621



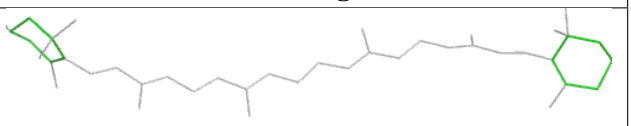
Bond lengths



Bond angles

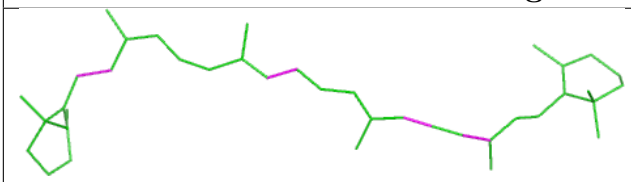


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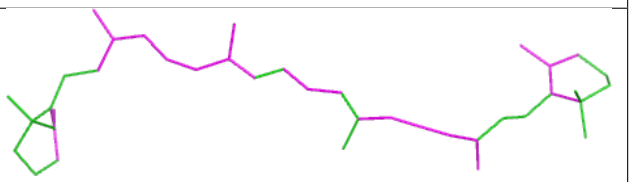


Rings

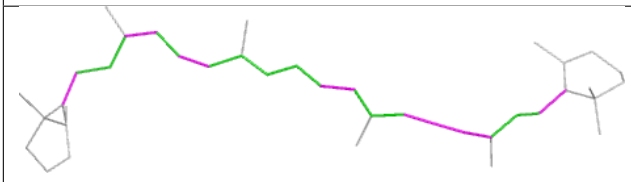
Ligand BCR d 404



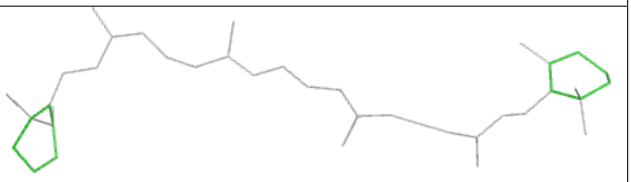
Bond lengths



Bond angles

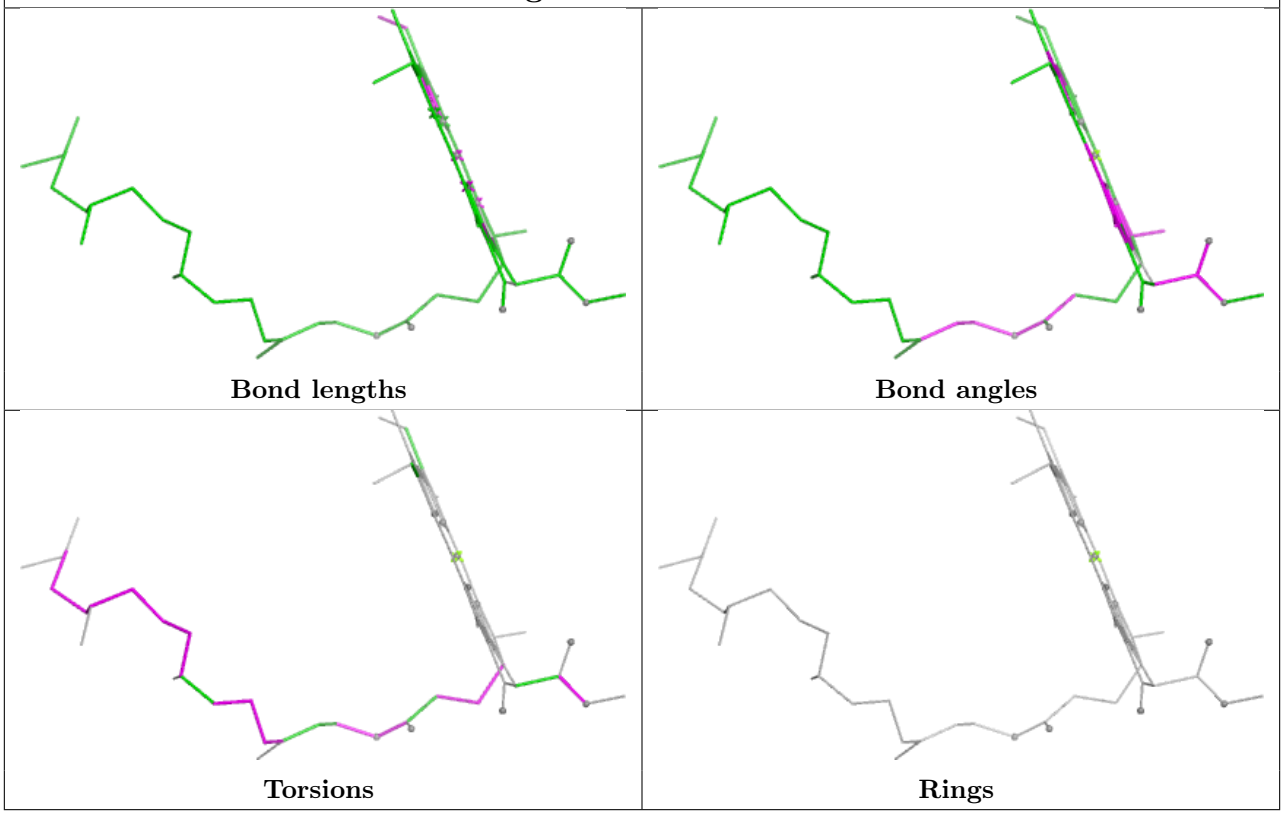


Torsions

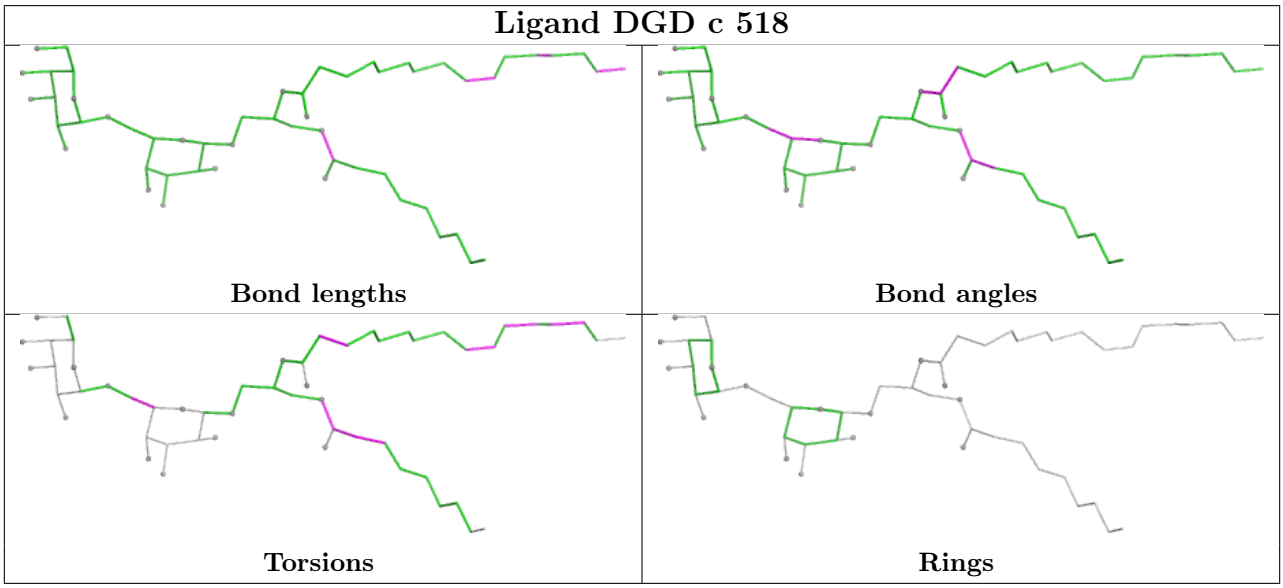


Rings

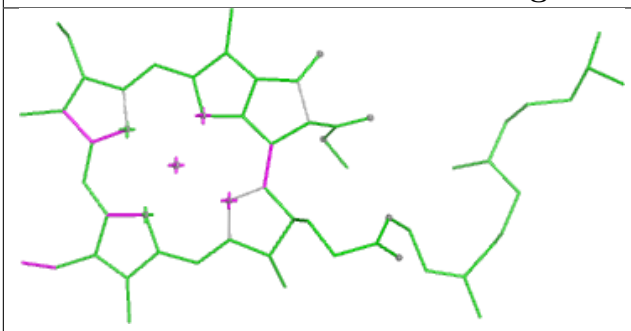
Ligand CLA C 506



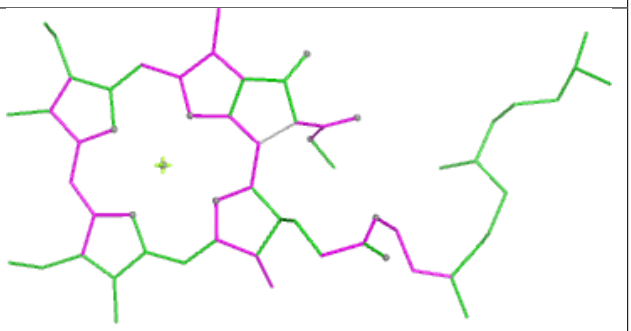
Ligand DGD c 518



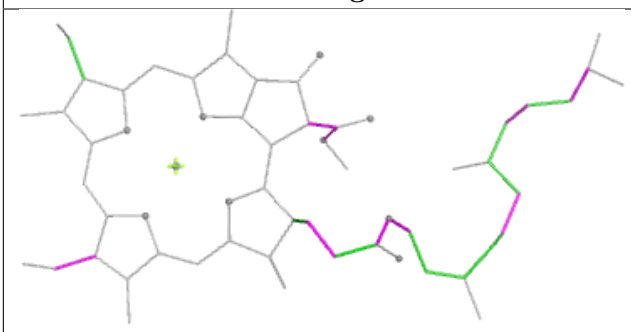
Ligand CLA r 612



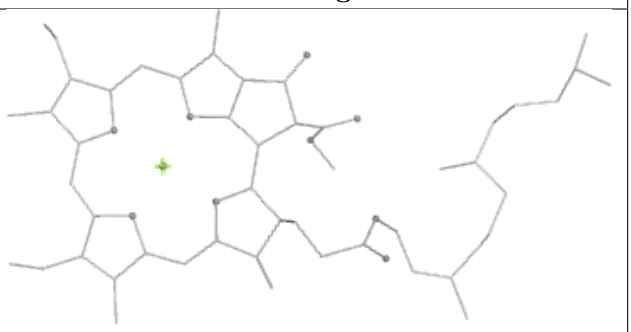
Bond lengths



Bond angles

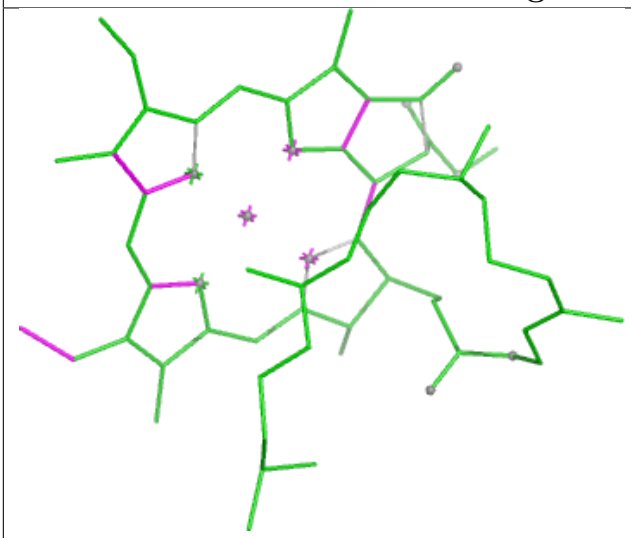


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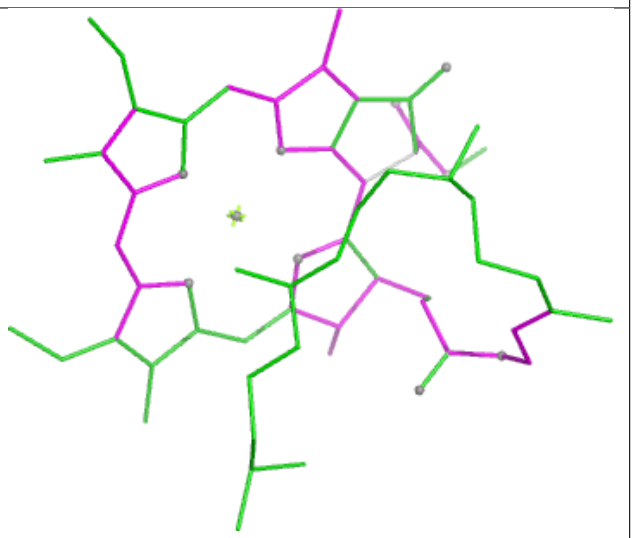


Rings

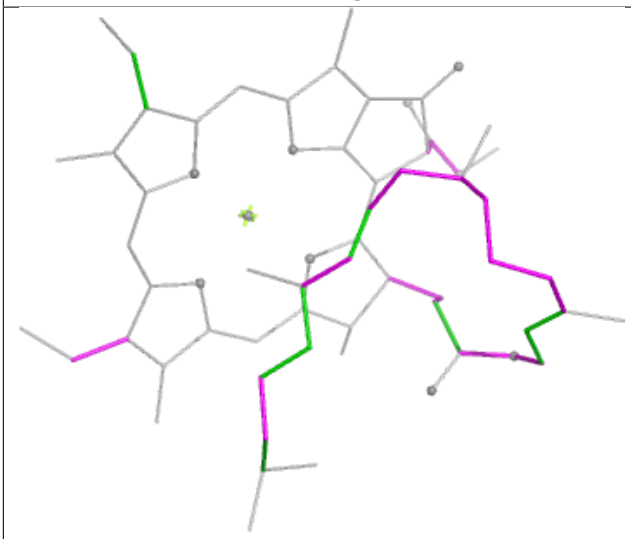
Ligand CLA b 602



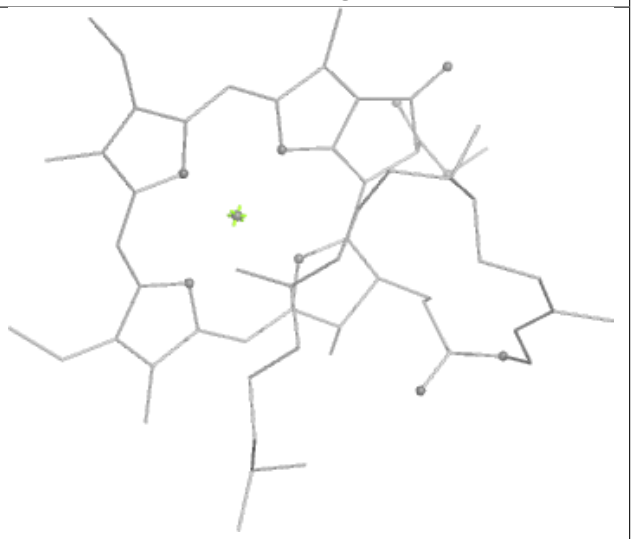
Bond lengths



Bond angles

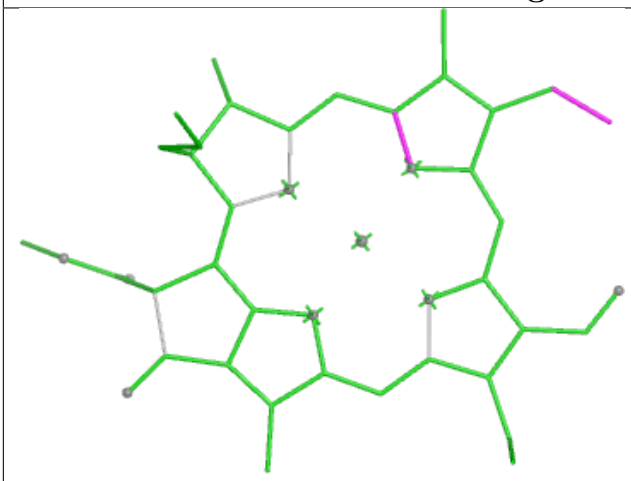


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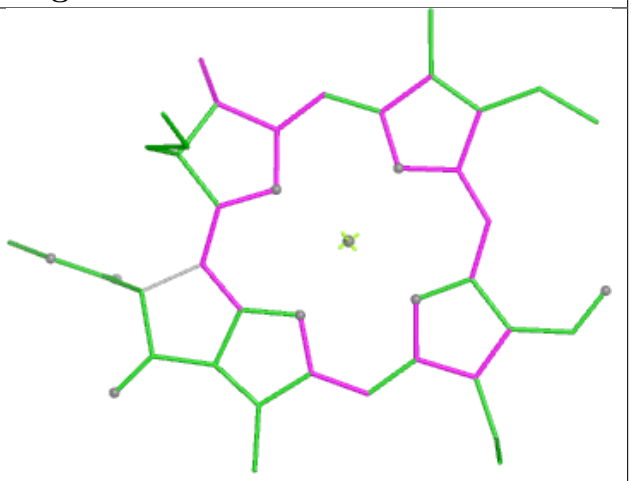


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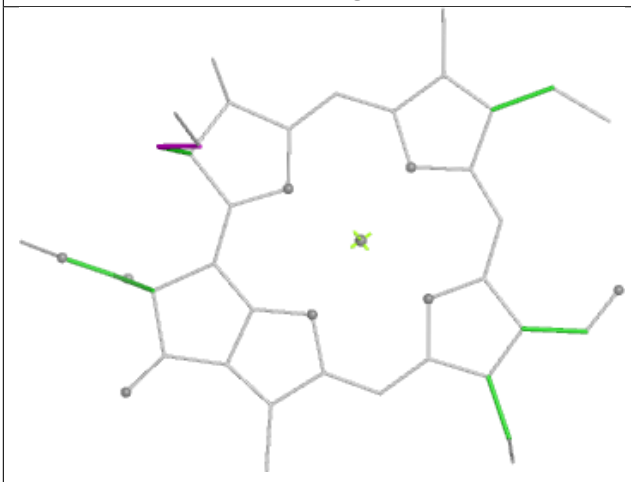
Ligand CHL g 608



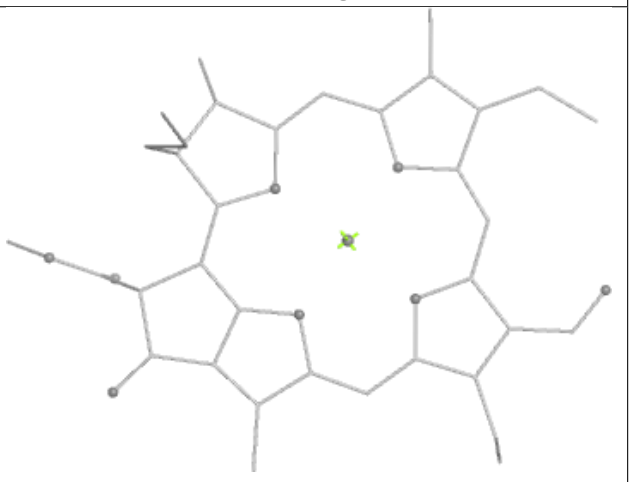
Bond lengths



Bond angles

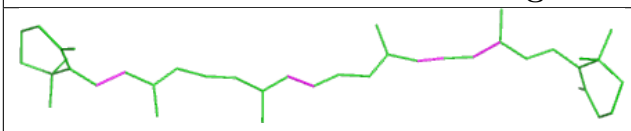


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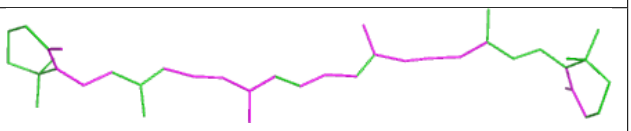


Rings

Ligand BCR a 411



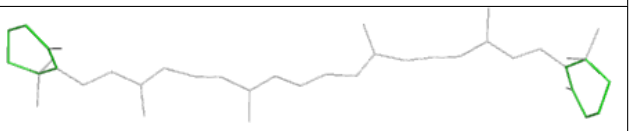
Bond lengths



Bond angles

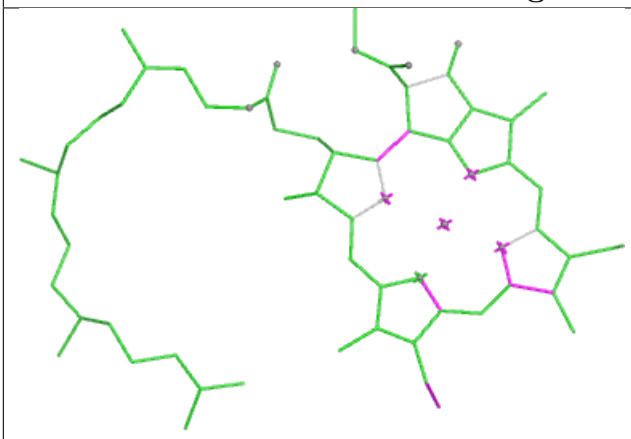


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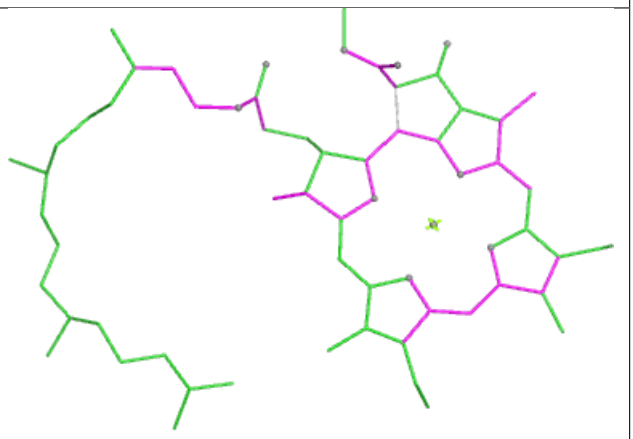


Rings

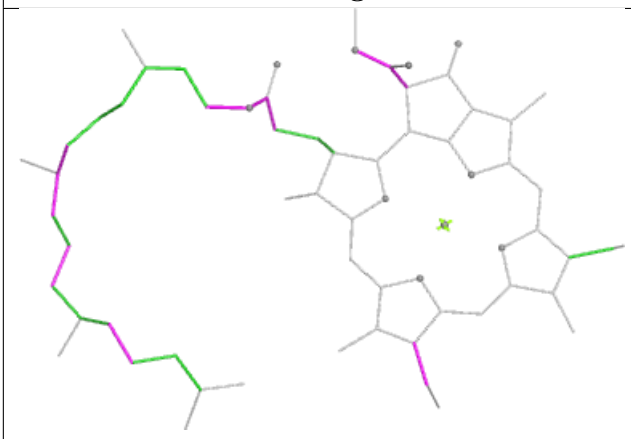
Ligand CLA S 603



Bond lengths



Bond angles

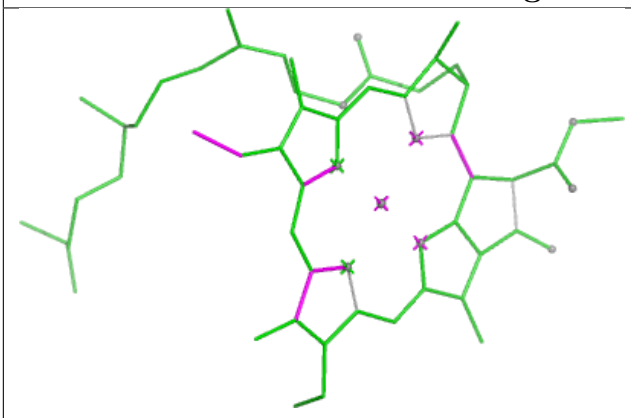


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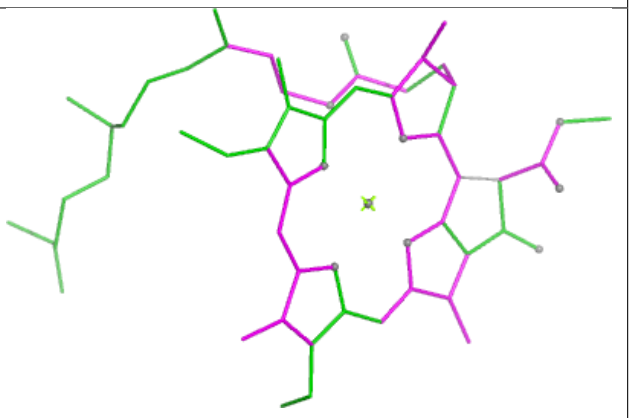


Rings

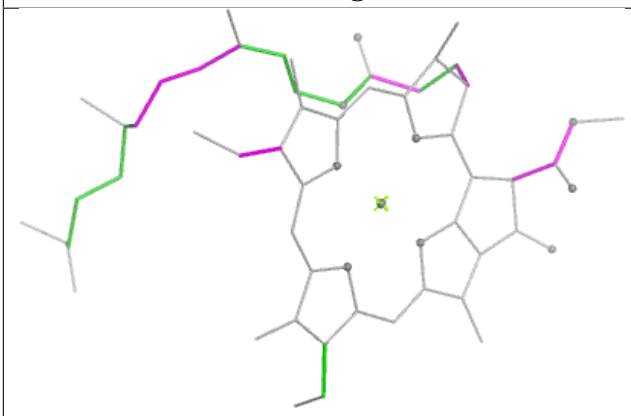
Ligand CLA R 610



Bond lengths



Bond angles

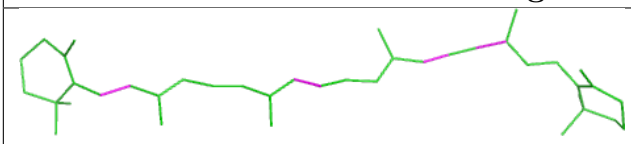


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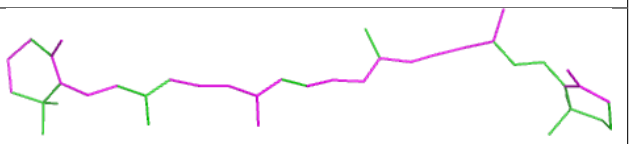


Rings

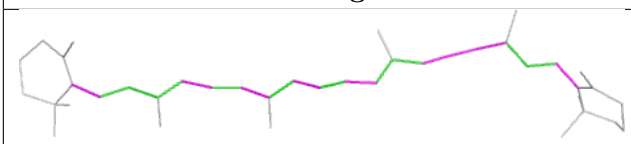
Ligand BCR c 514



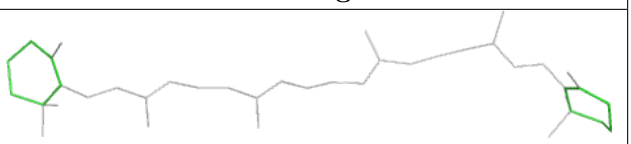
Bond lengths



Bond angles

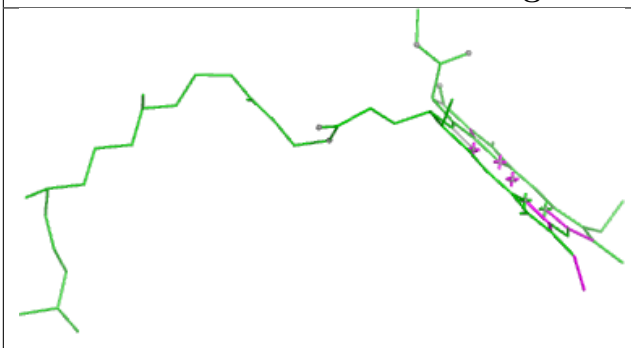


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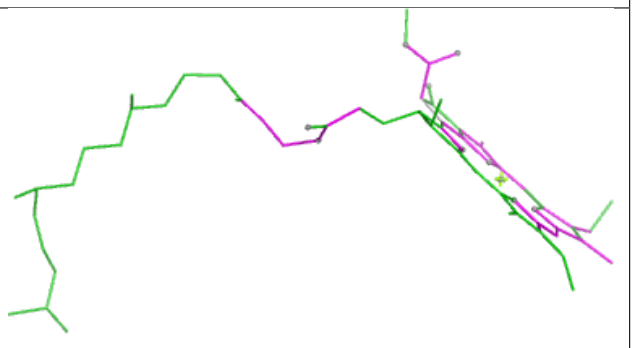


Rings

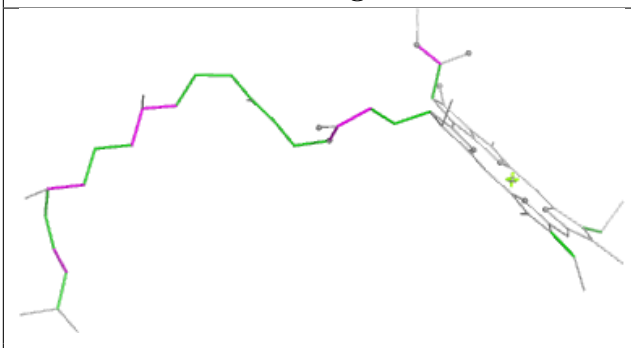
Ligand CLA D 402



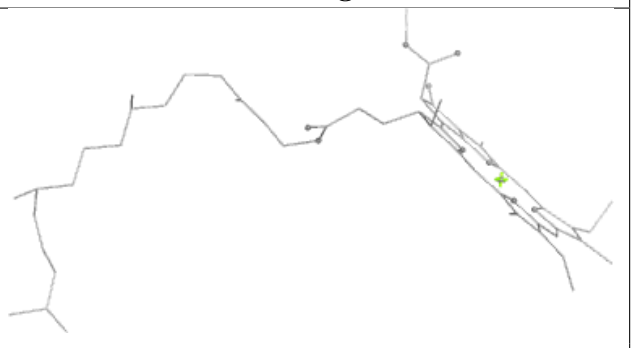
Bond lengths



Bond angles

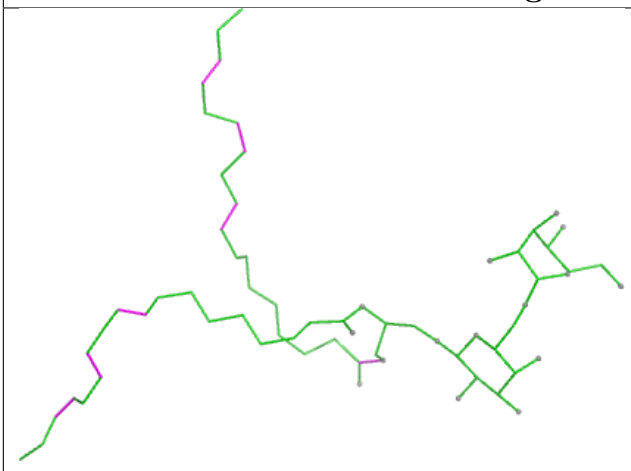


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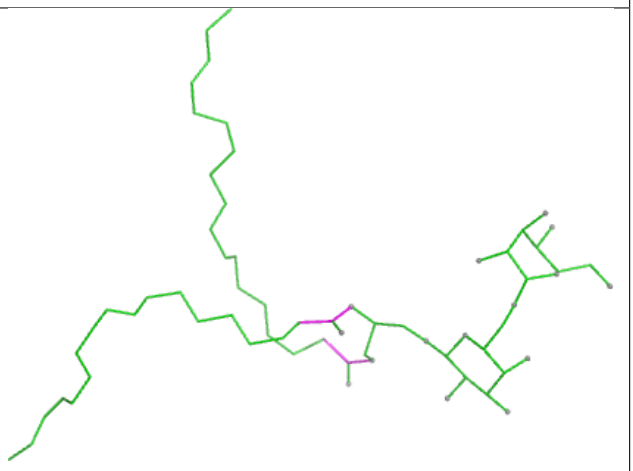


Rings

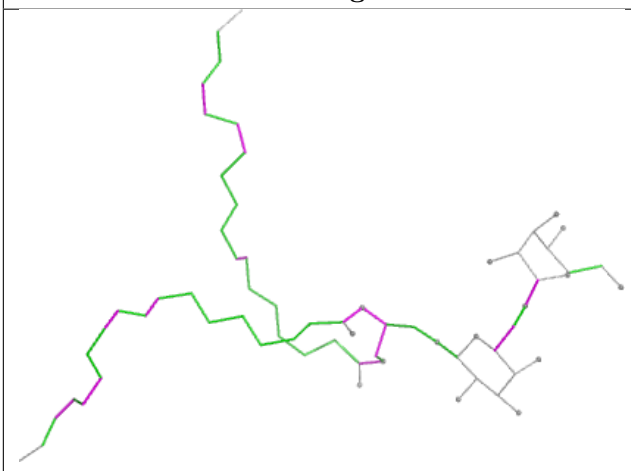
Ligand DGD c 523



Bond lengths



Bond angles

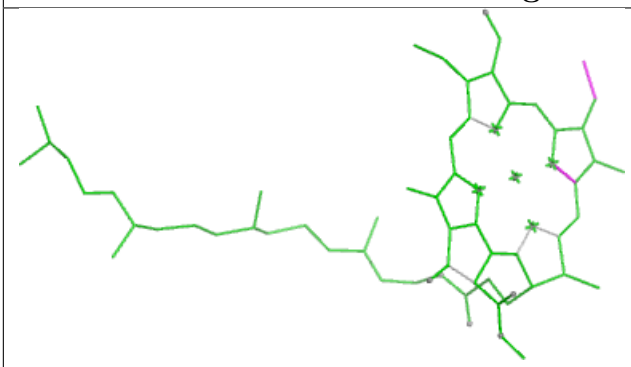


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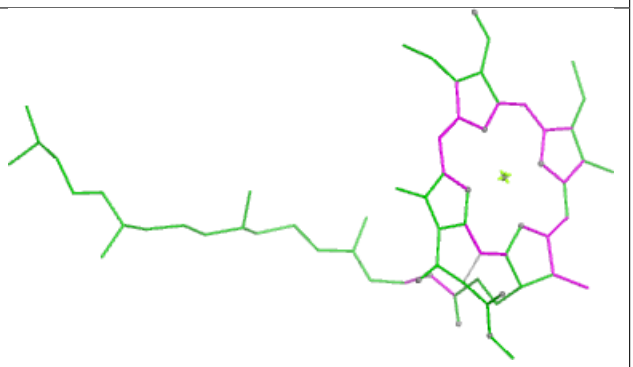


Rings

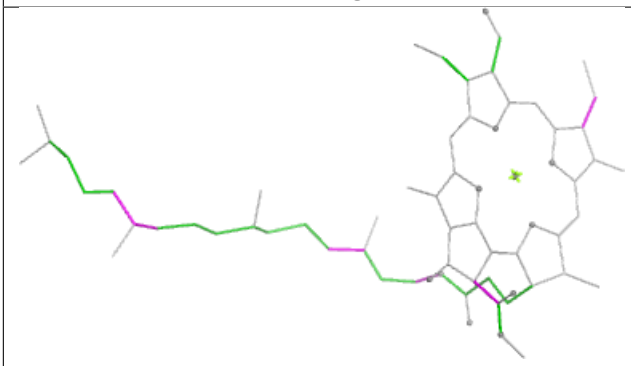
Ligand CHL G 609



Bond lengths



Bond angles

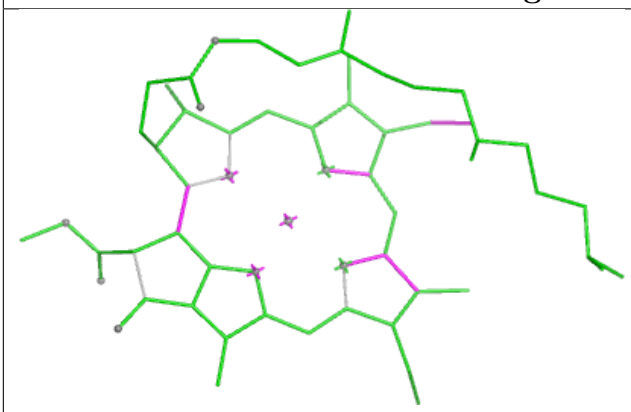


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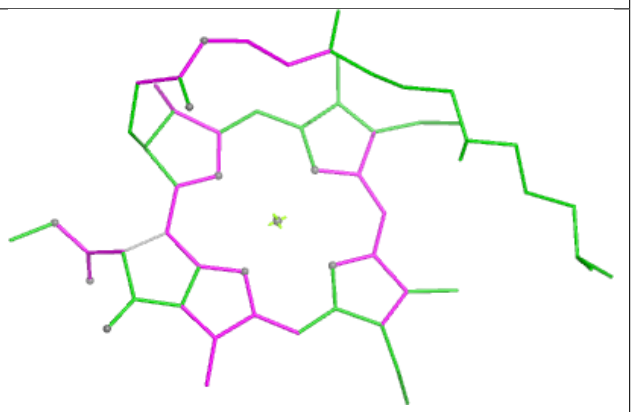


Rings

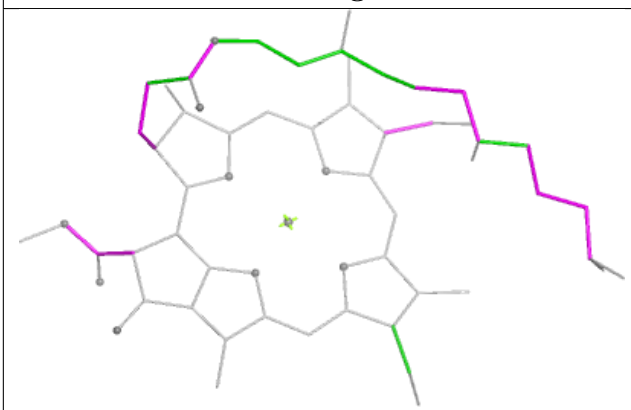
Ligand CLA R 608



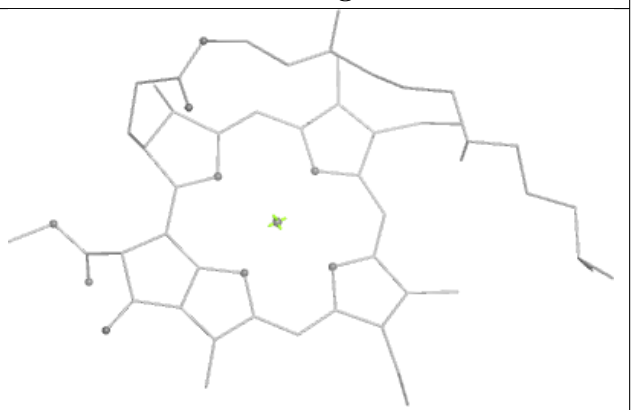
Bond lengths



Bond angles

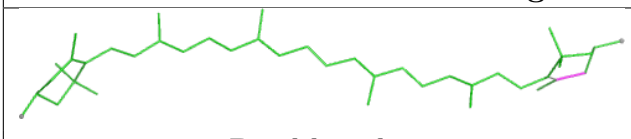


Torsions



Rings

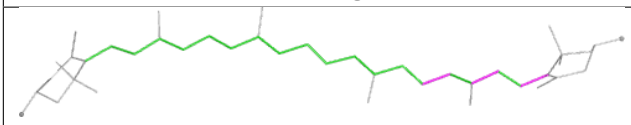
Ligand LUT S 620



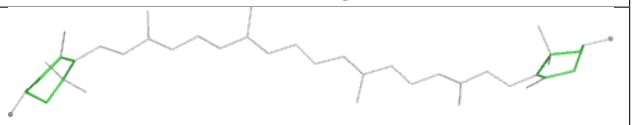
Bond lengths



Bond angles

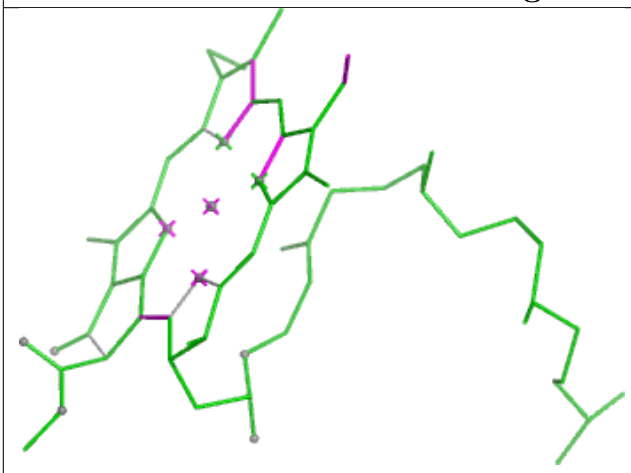


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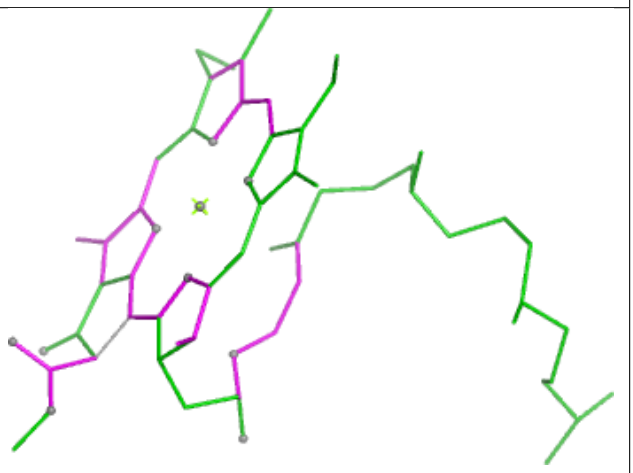


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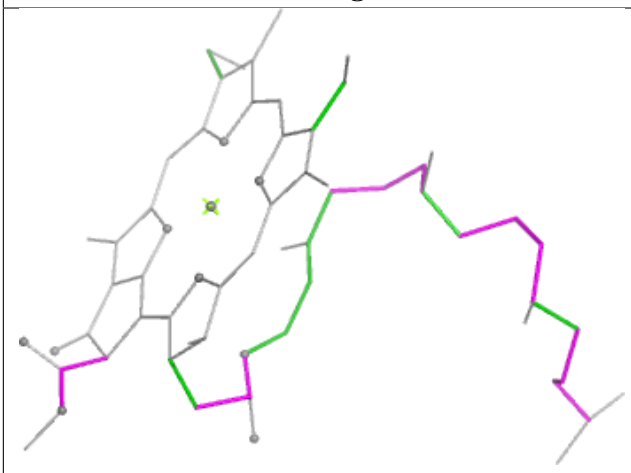
Ligand CLA Y 613



Bond lengths



Bond angles



Torsions

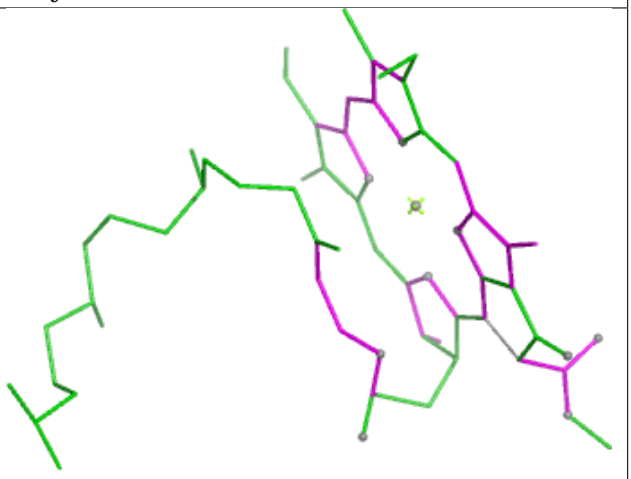


Rings

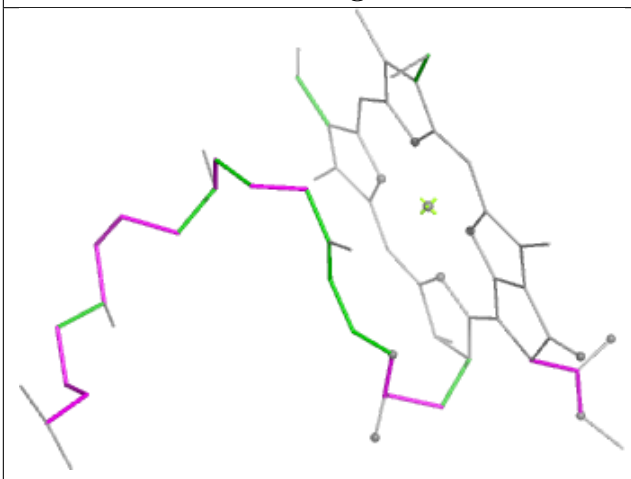
Ligand CLA y 613



Bond lengths



Bond angles

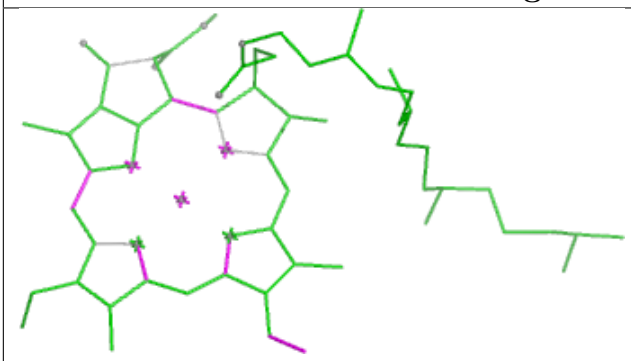


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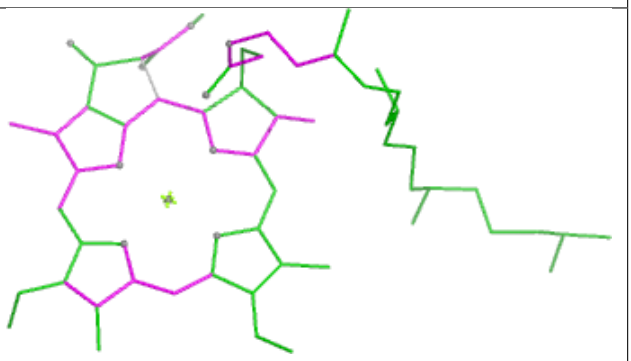


Rings

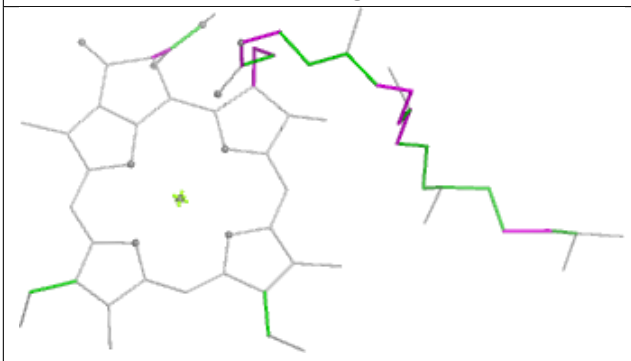
Ligand CLA A 406



Bond lengths



Bond angles



Torsions

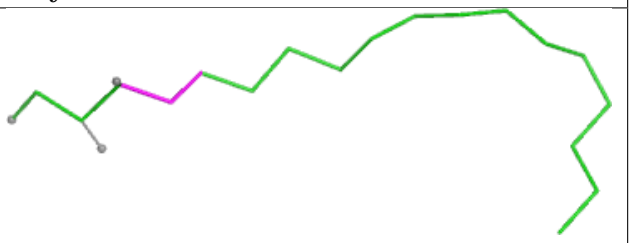


Rings

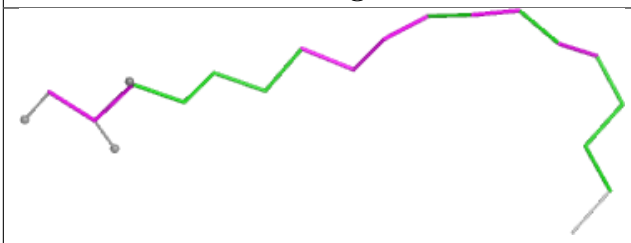
Ligand SPH y 625



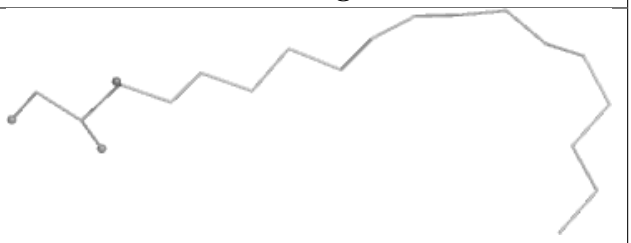
Bond lengths



Bond angles

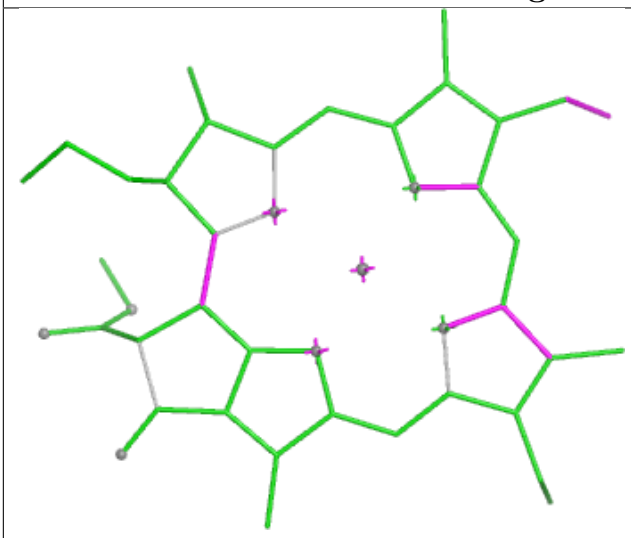


Torsions

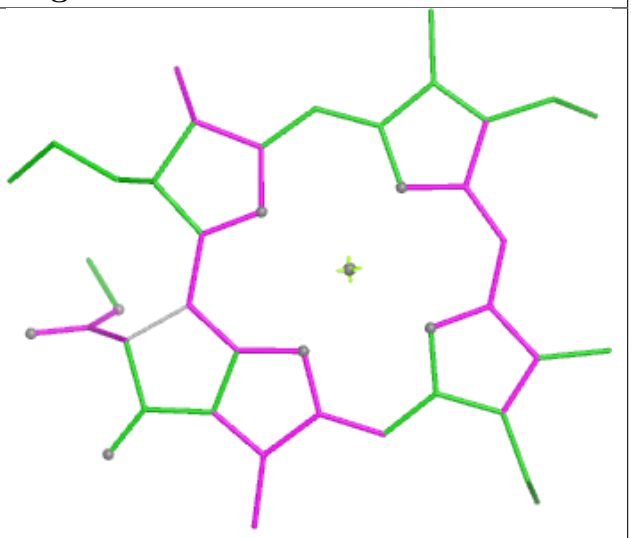


Rings

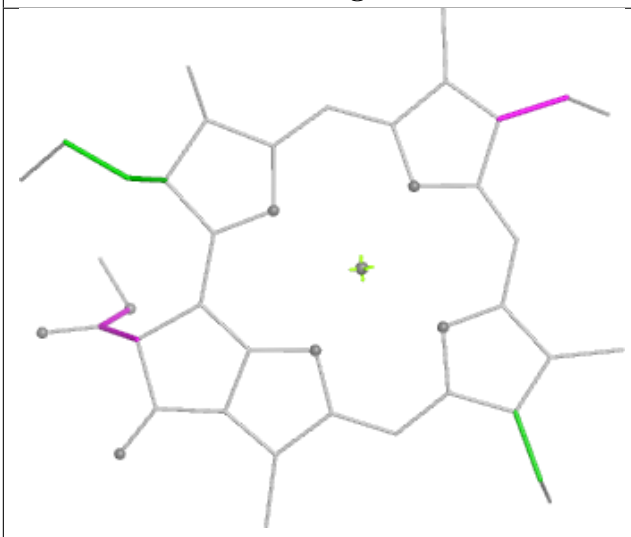
Ligand CLA g 612



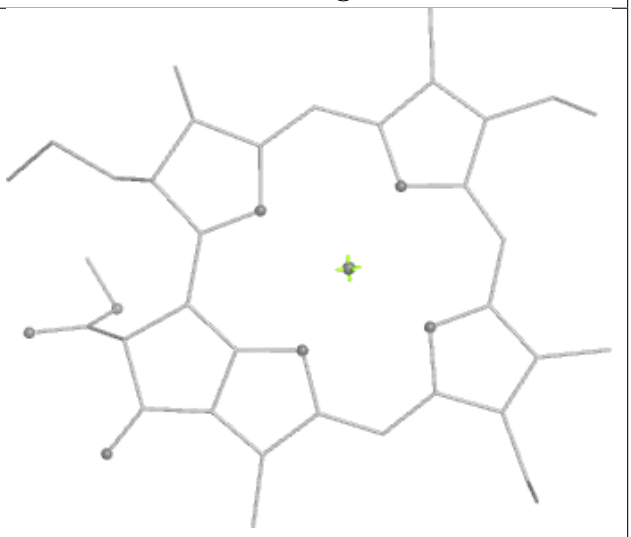
Bond lengths



Bond angles

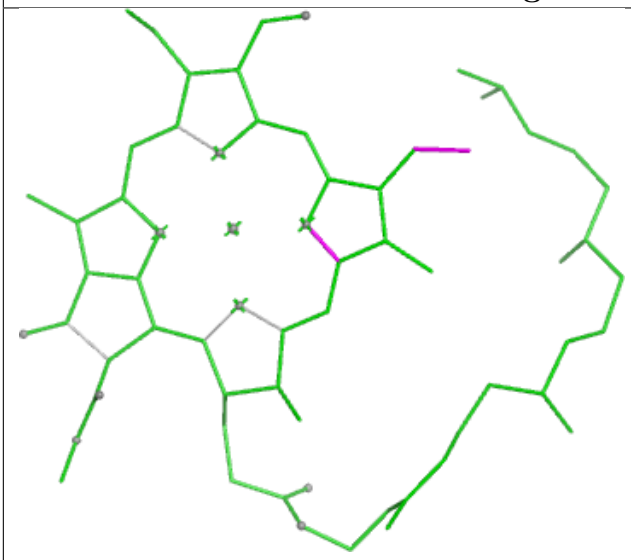


Torsions

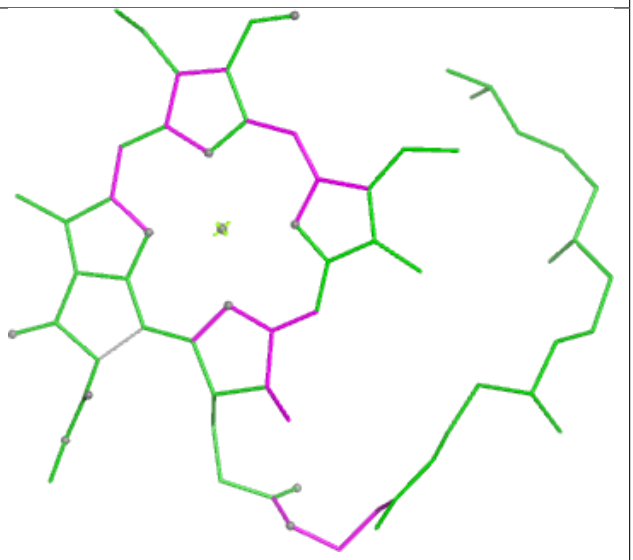


Rings

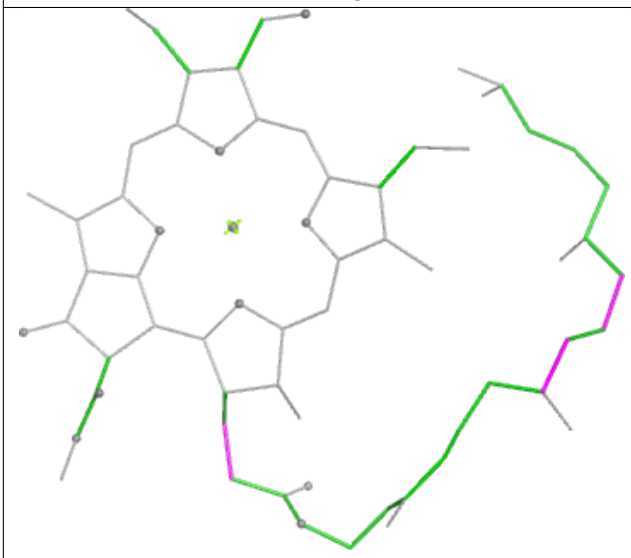
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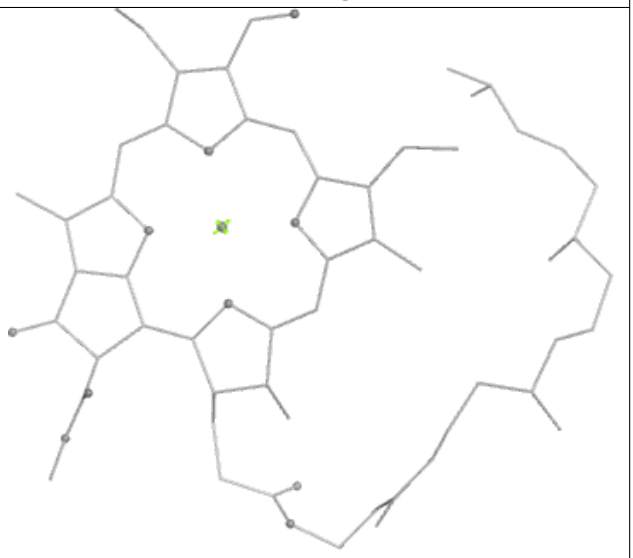
Bond lengths



Bond angles

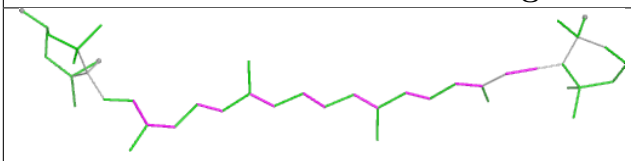


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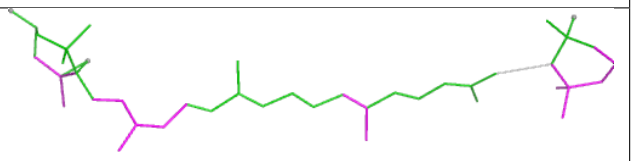


Rings

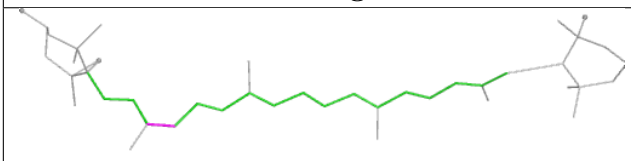
Ligand NEX Y 623



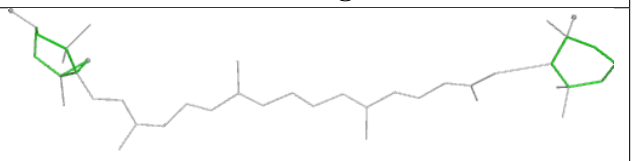
Bond lengths



Bond angles

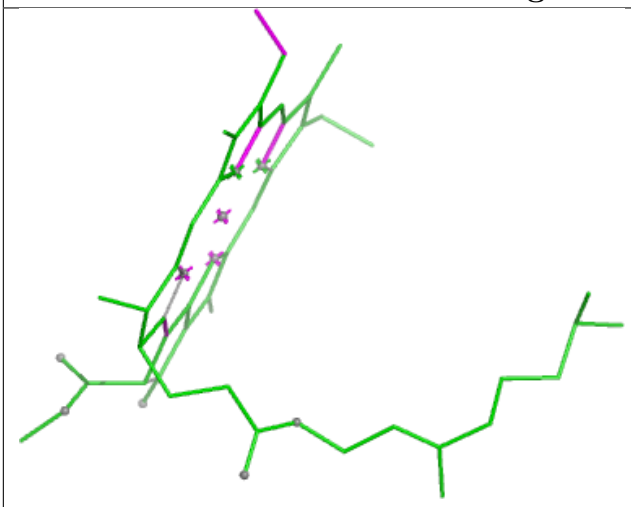


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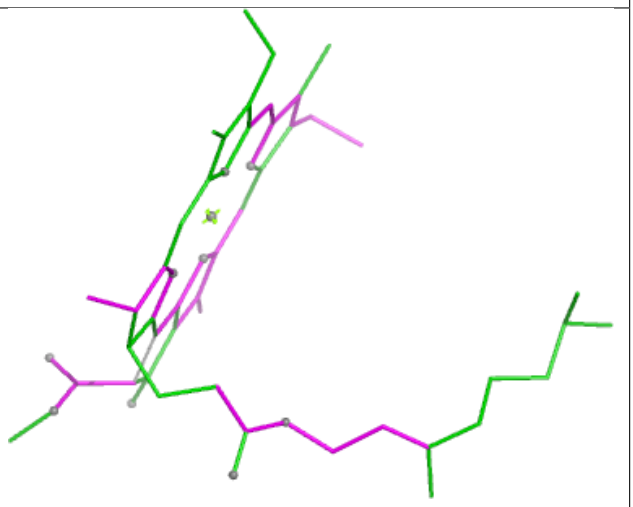


Rings

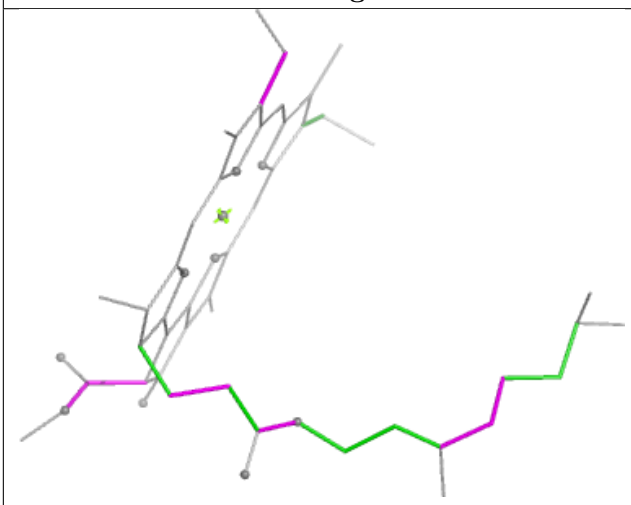
Ligand CLA S 604



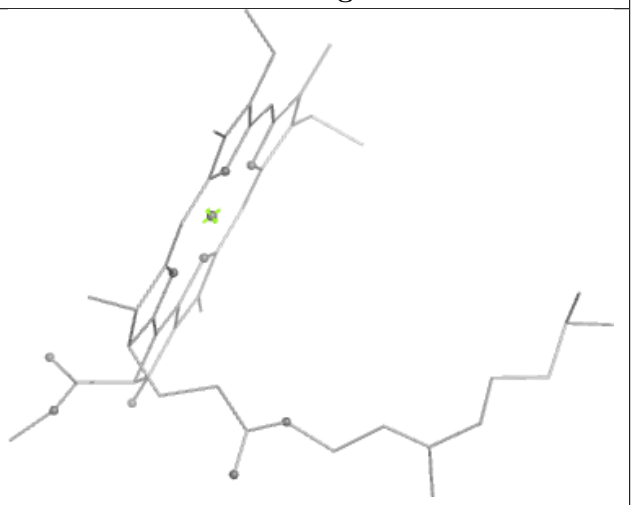
Bond lengths



Bond angles



Torsions

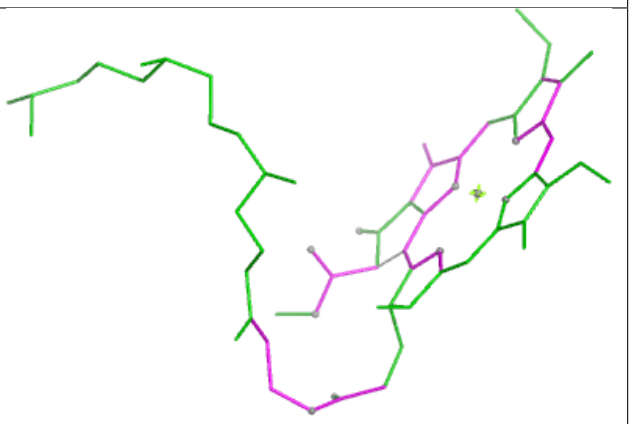


Rings

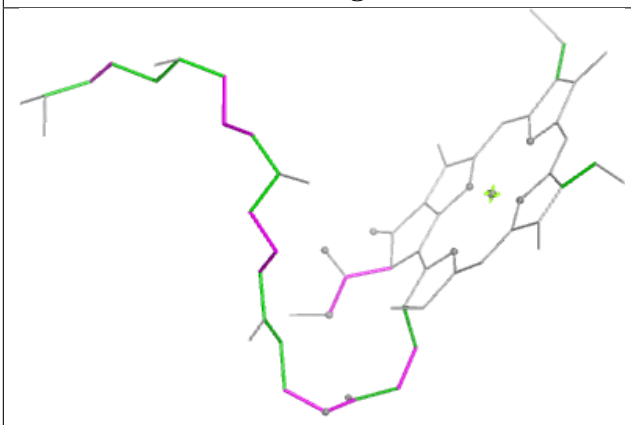
Ligand CLA B 614



Bond lengths



Bond angles

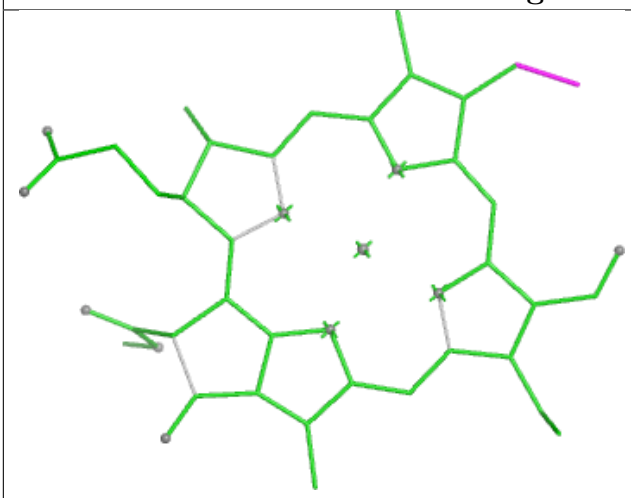


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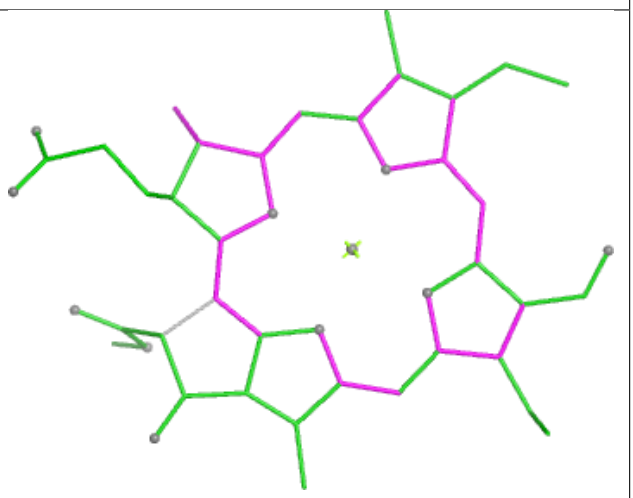


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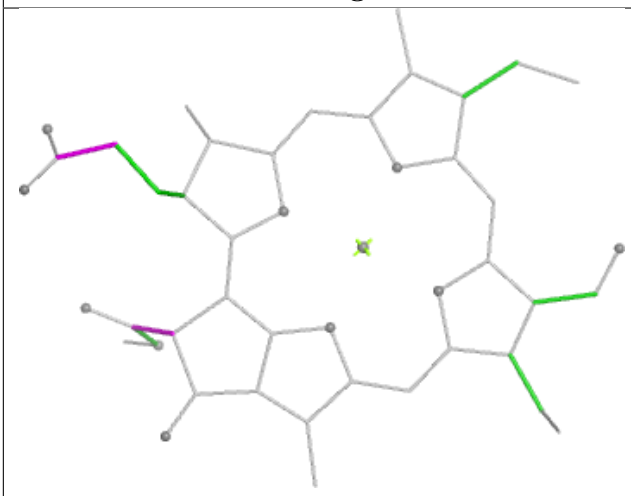
Ligand CHL S 601



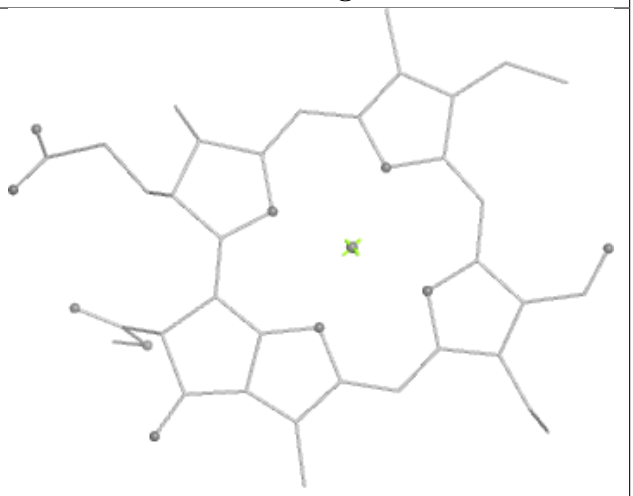
Bond lengths



Bond angles

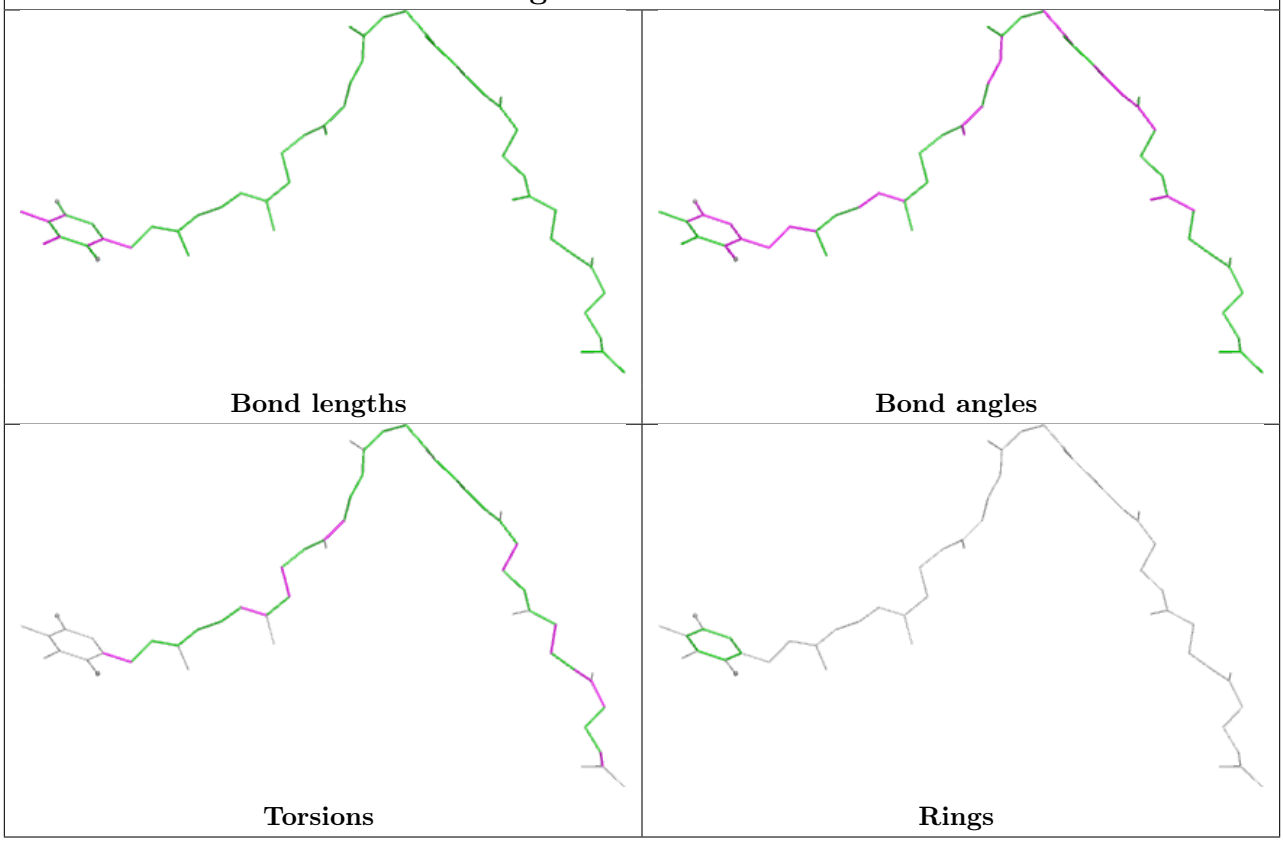


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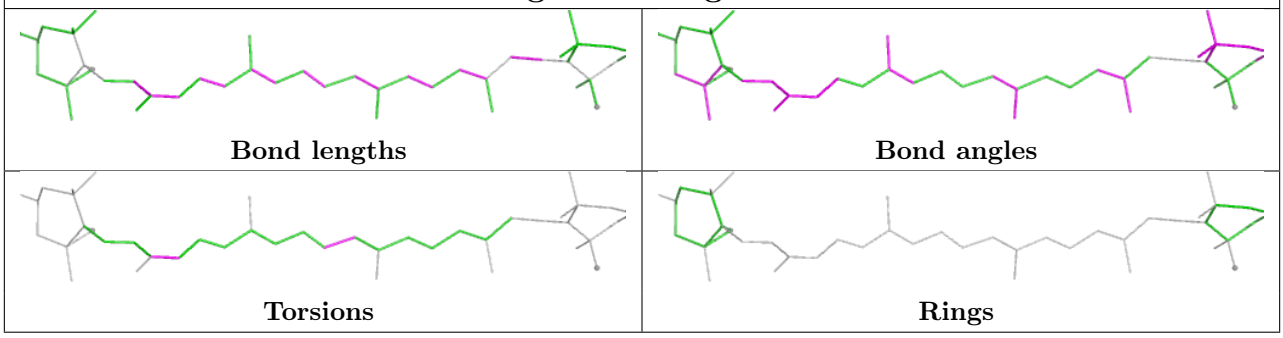


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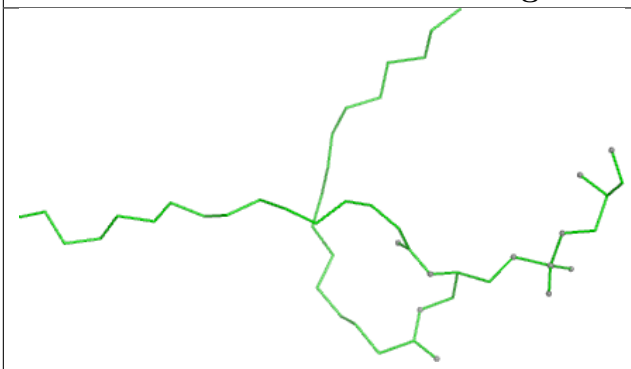
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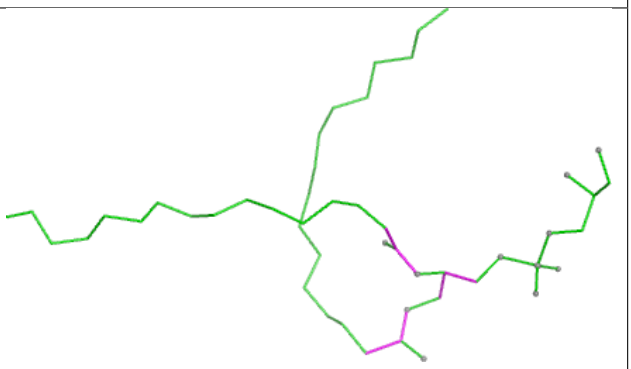
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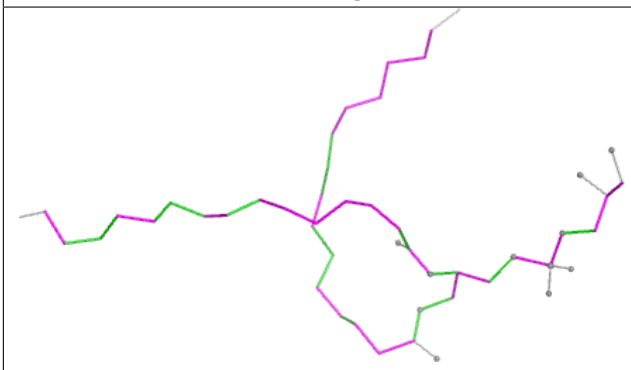
Ligand LHG G 630



Bond lengths



Bond angles

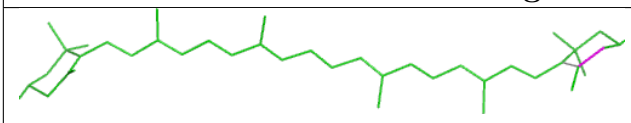


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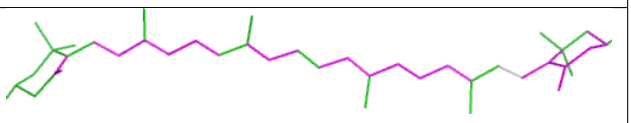


Rings

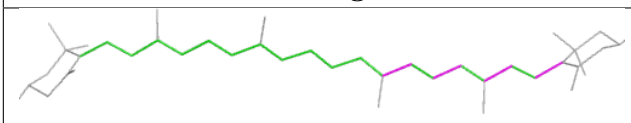
Ligand LUT G 620



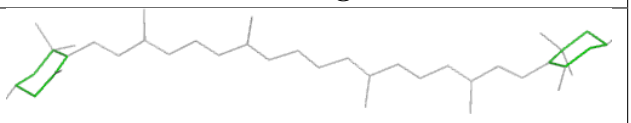
Bond lengths



Bond angles

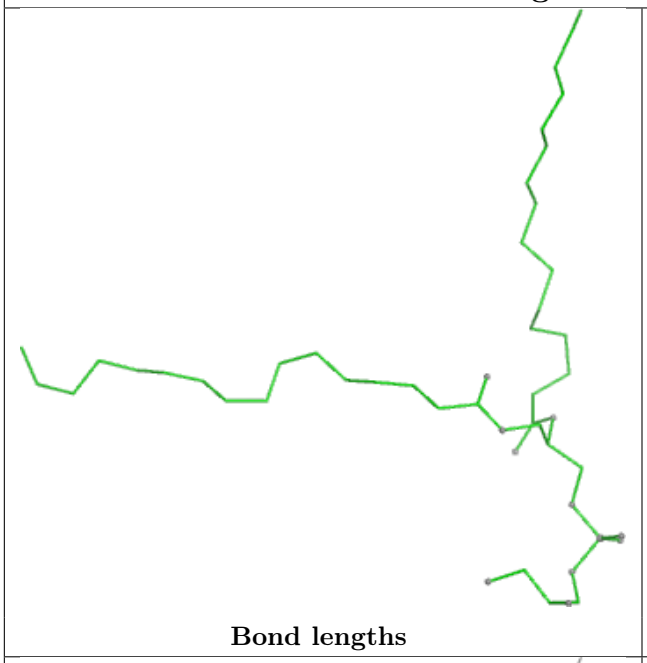


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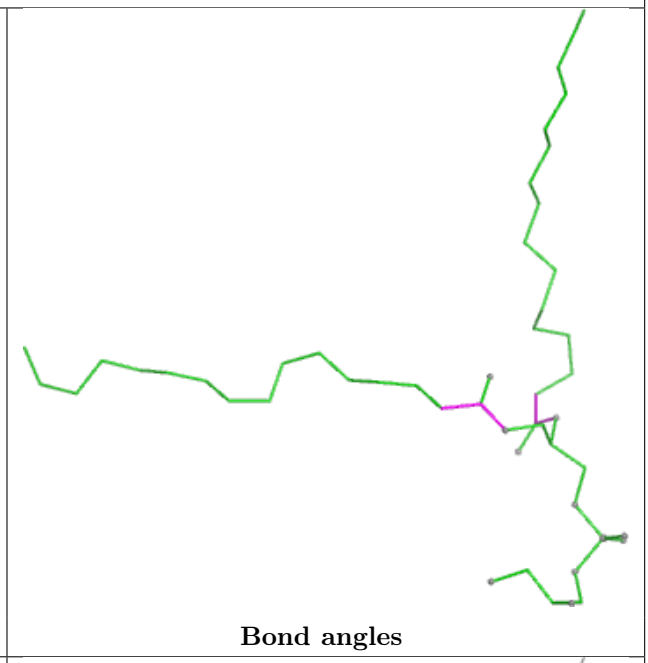


Rings

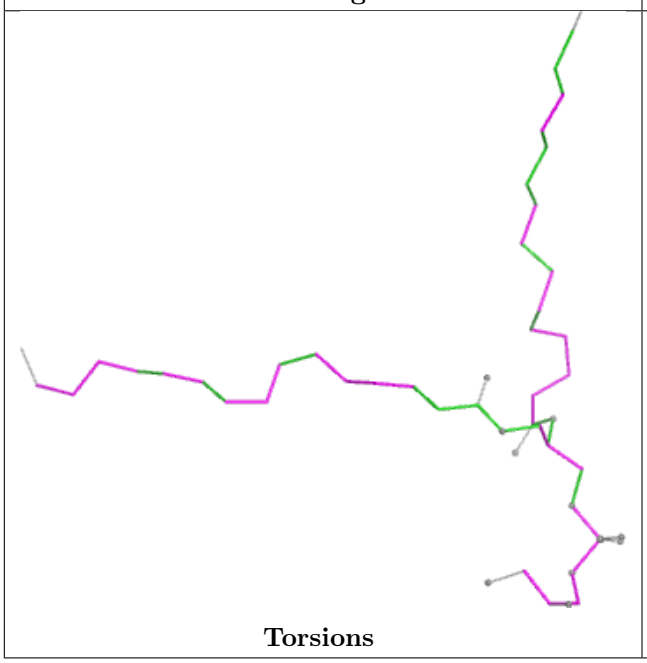
Ligand LHG l 101



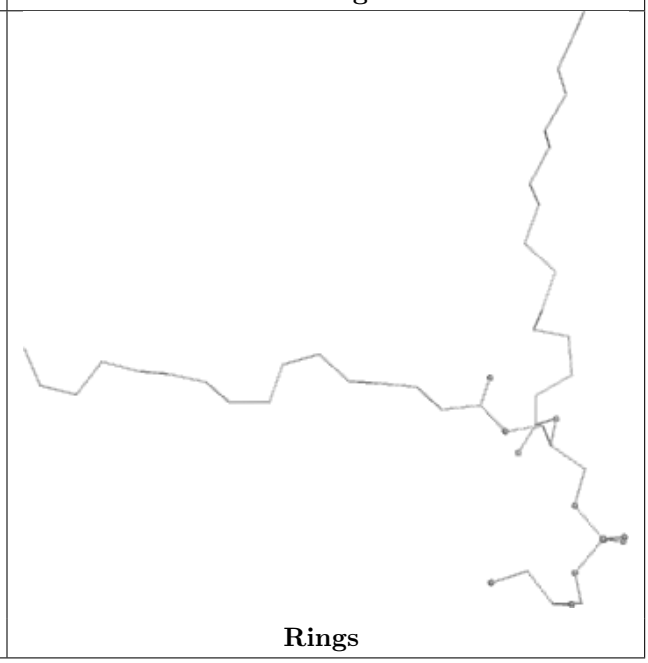
Bond lengths



Bond angles

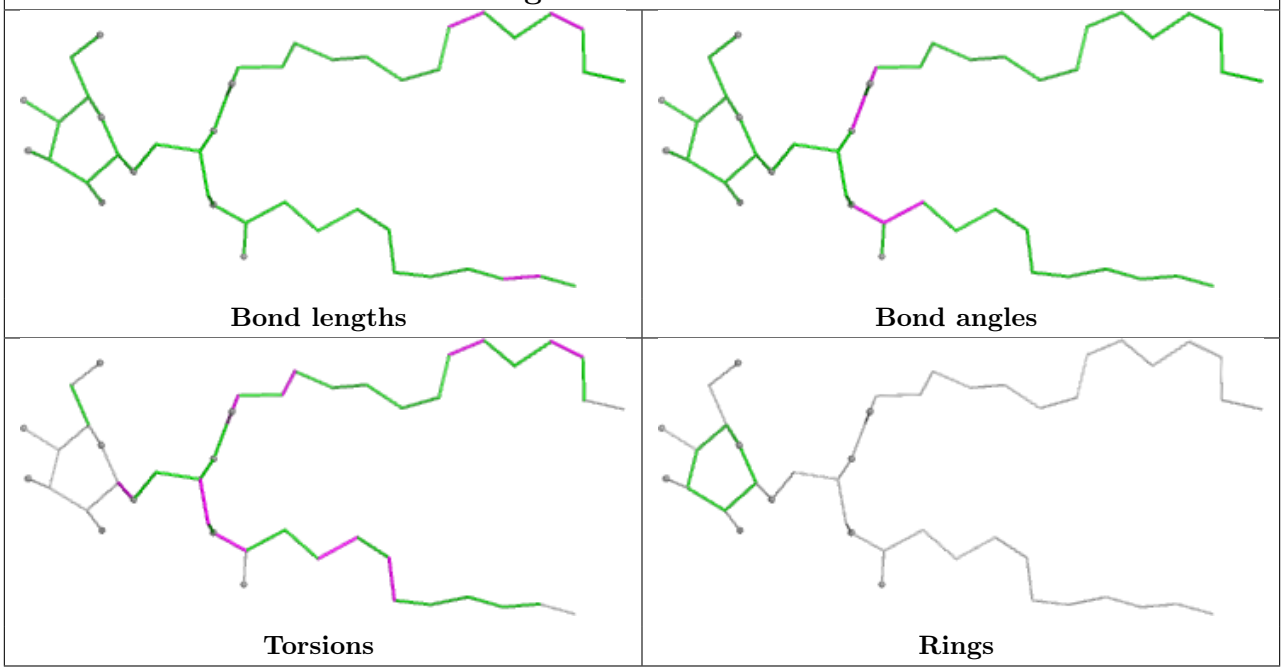


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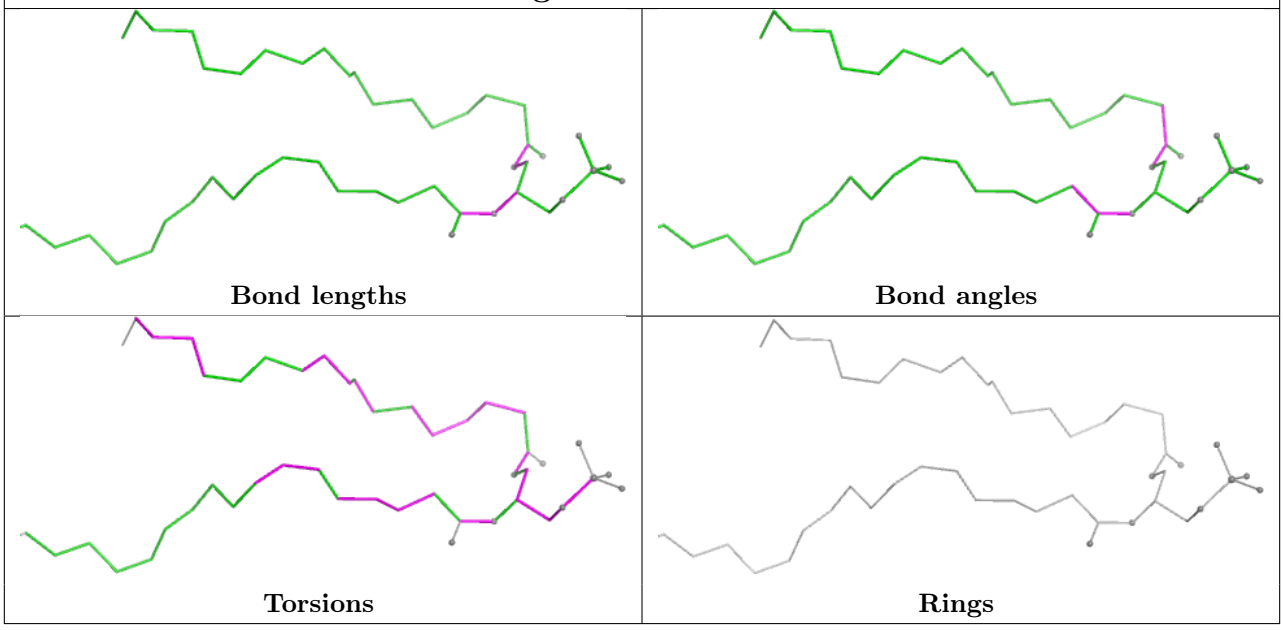


Rings

Ligand LMG J 101



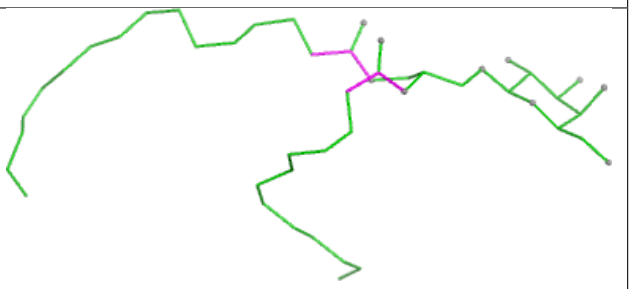
Ligand 3PH s 626



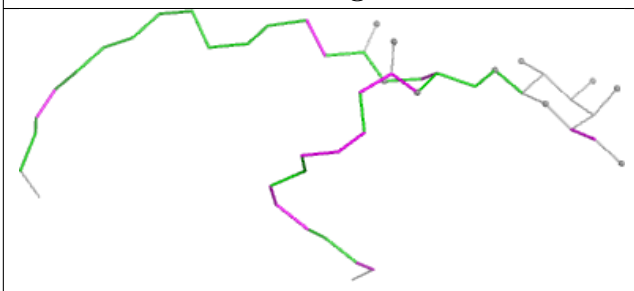
Ligand LMG h 102



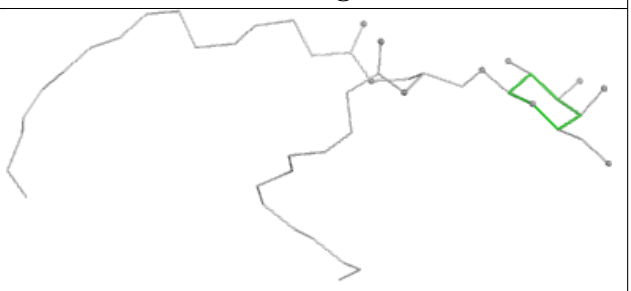
Bond lengths



Bond angles

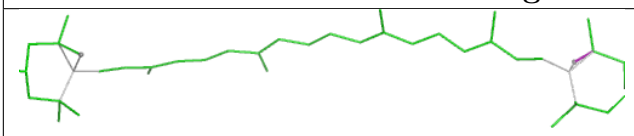


Torsions

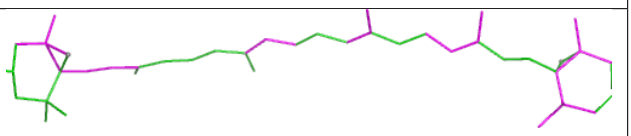


Rings

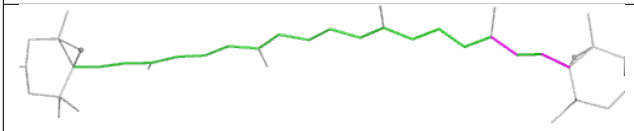
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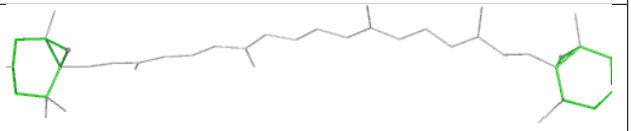
Bond lengths



Bond angles

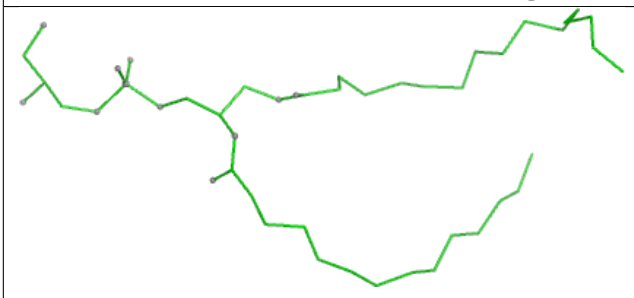


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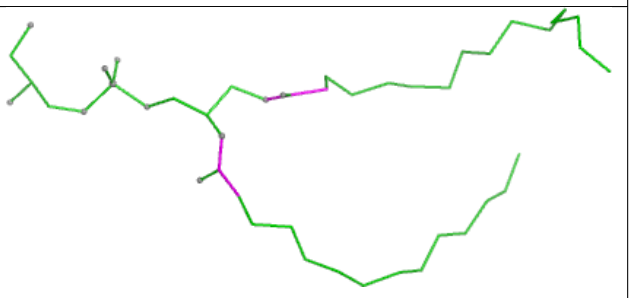


Rings

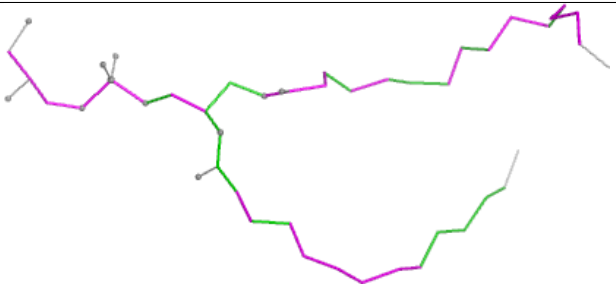
Ligand LHG C 525



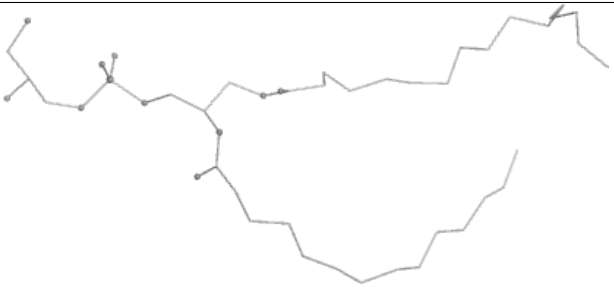
Bond lengths



Bond angles

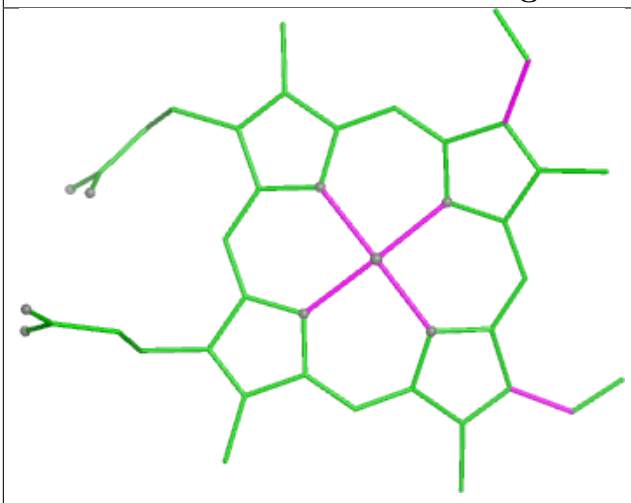


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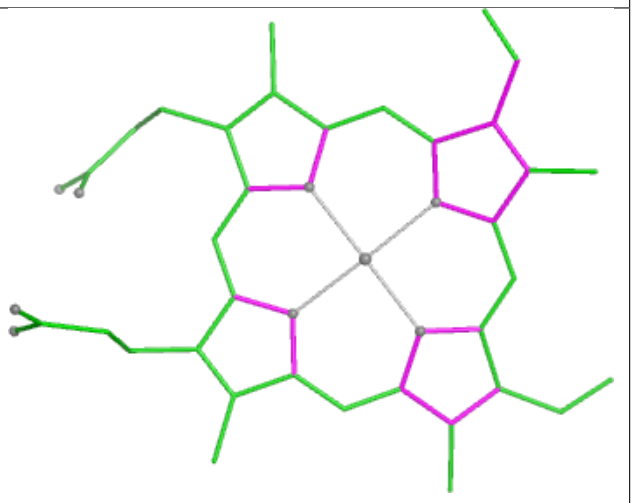


Rings

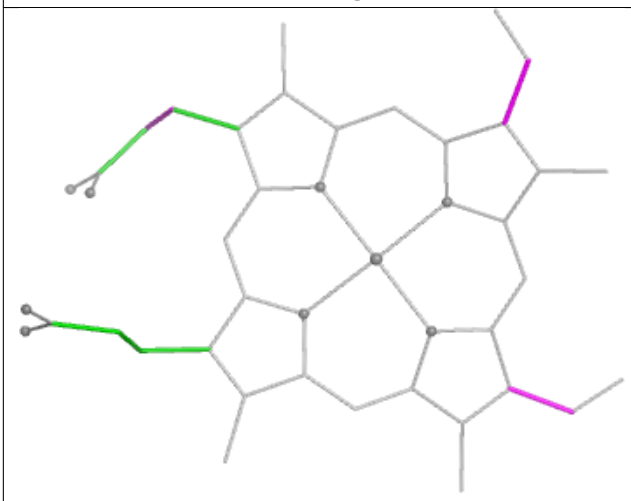
Ligand HEM F 101



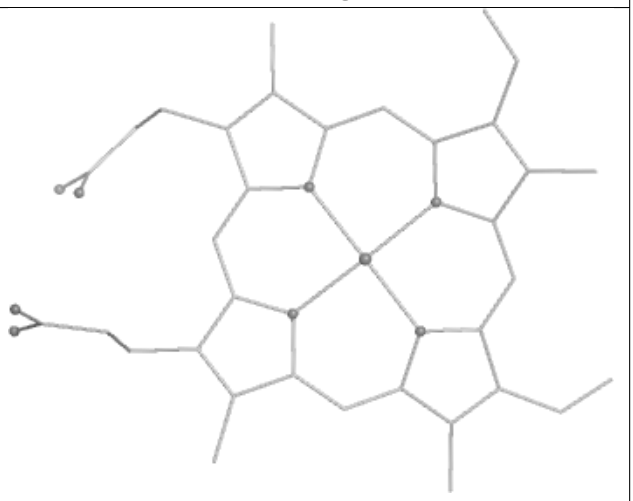
Bond lengths



Bond angles

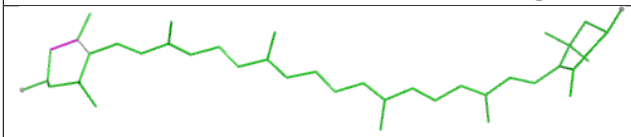


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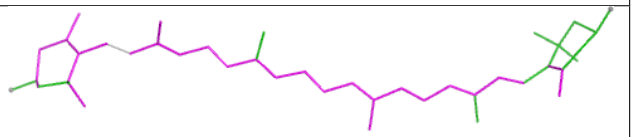


Rings

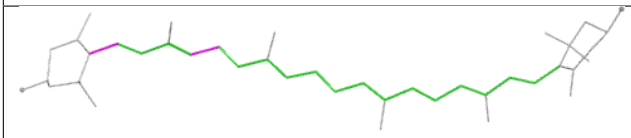
Ligand LUT s 620



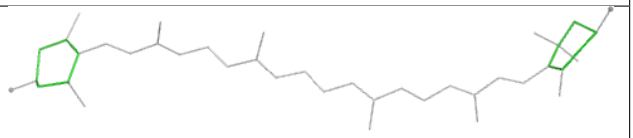
Bond lengths



Bond angles

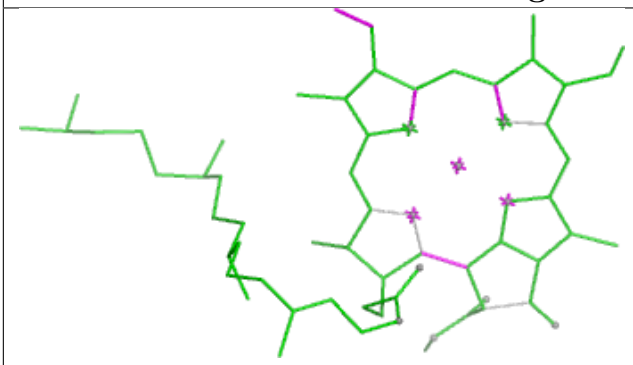


Torsions

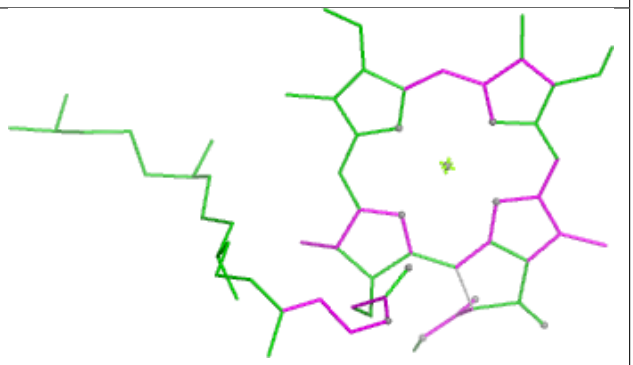


Rings

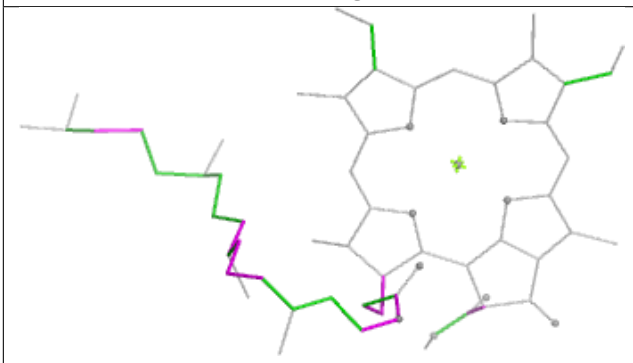
Ligand CLA a 406



Bond lengths



Bond angles

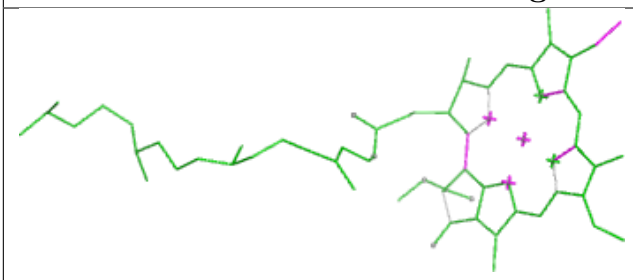


Torsions

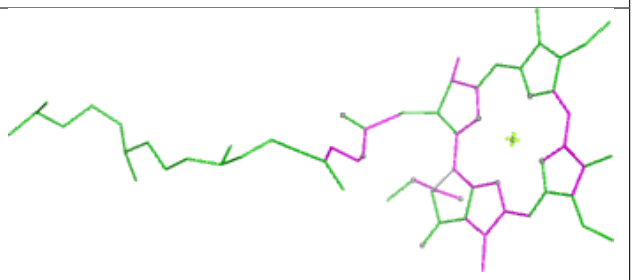


Rings

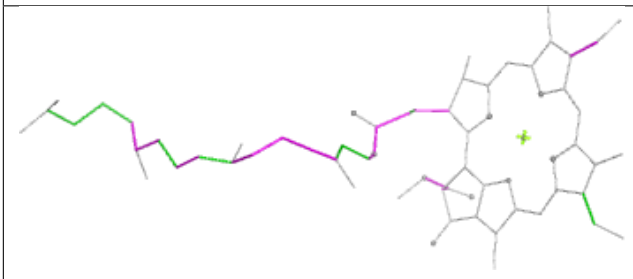
Ligand CLA c 502



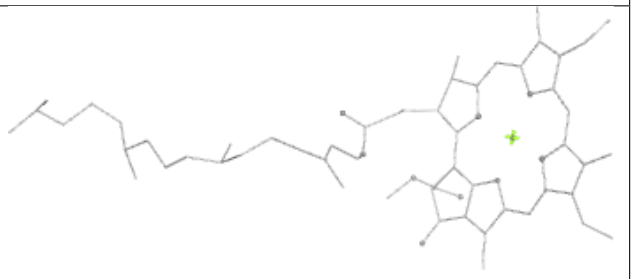
Bond lengths



Bond angles

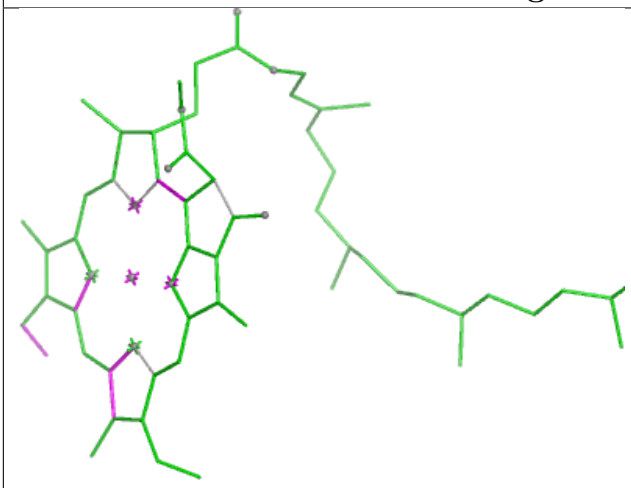


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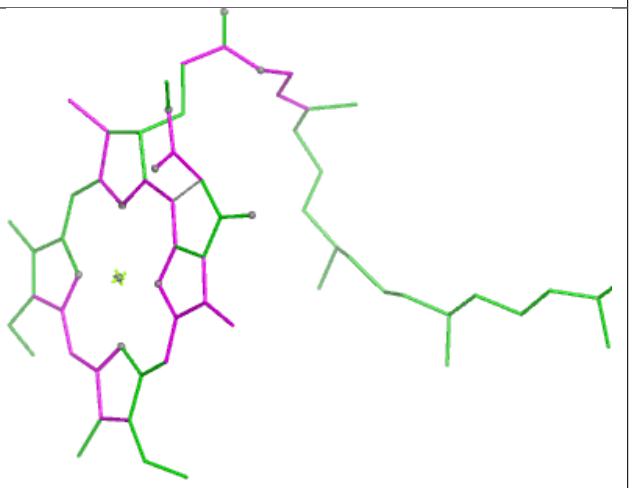


Rings

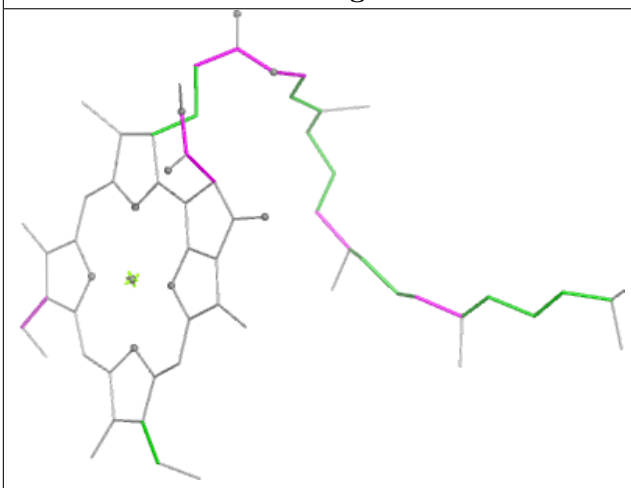
Ligand CLA S 611



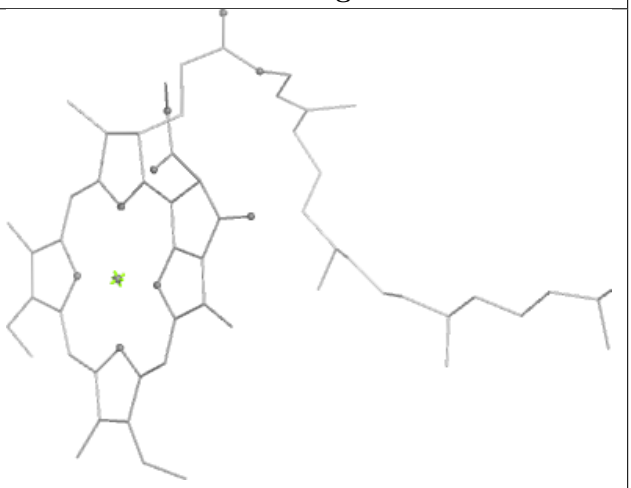
Bond lengths



Bond angles

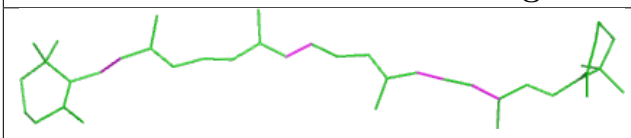


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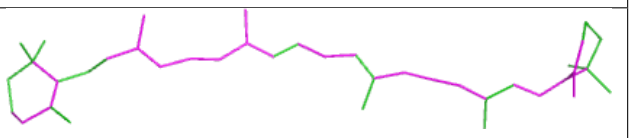


Rings

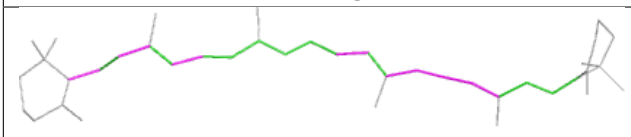
Ligand BCR B 619



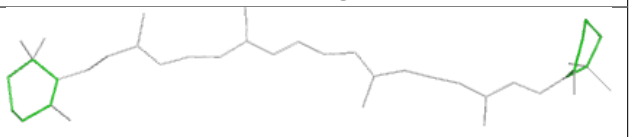
Bond lengths



Bond angles

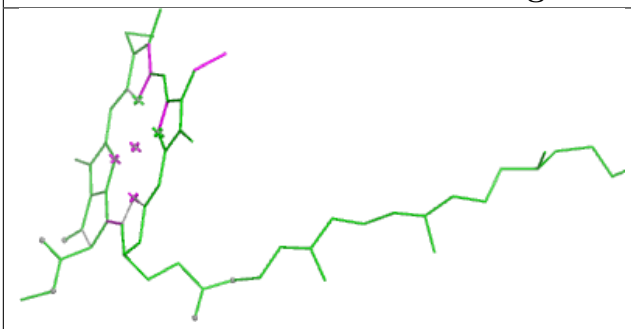


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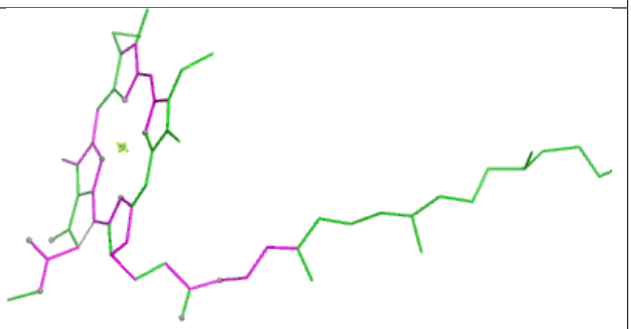


Rings

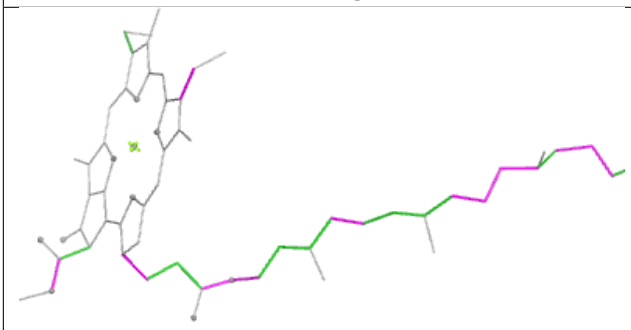
Ligand CLA d 403



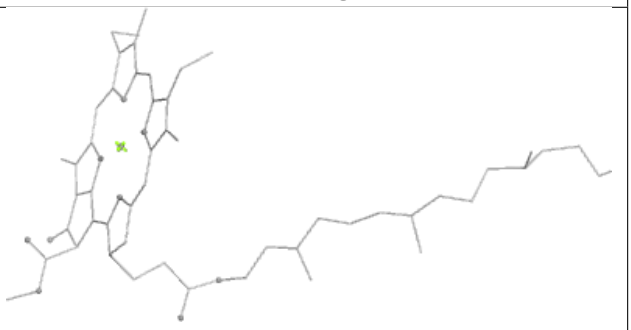
Bond lengths



Bond angles

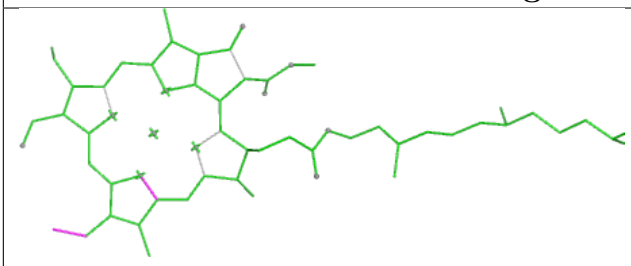


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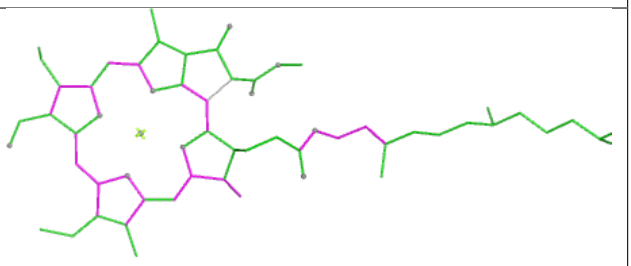


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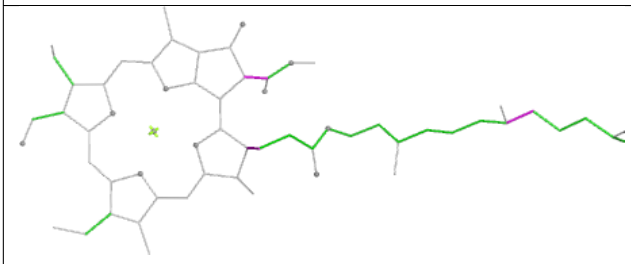
Ligand CHL Y 606



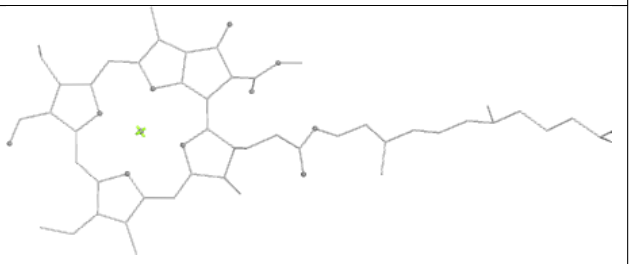
Bond lengths



Bond angles

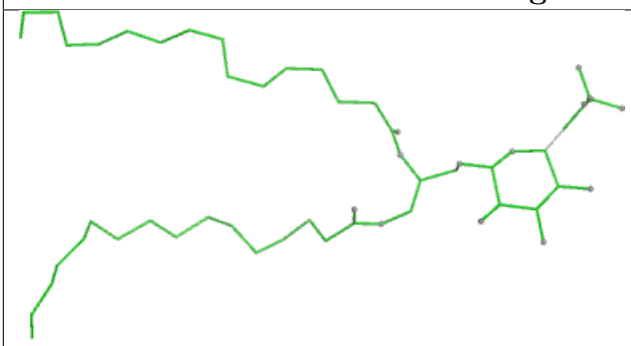


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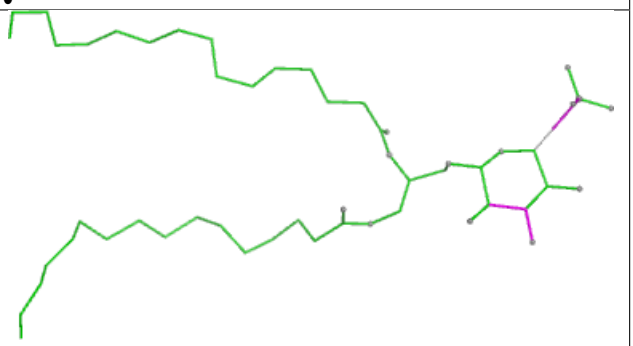


Rings

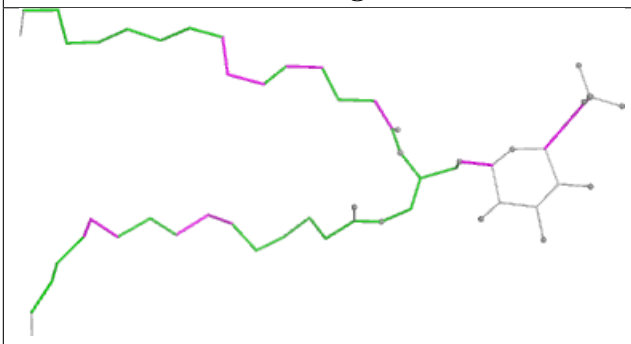
Ligand SQD c 626



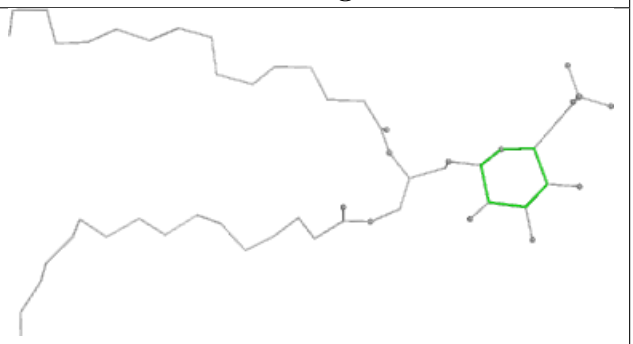
Bond lengths



Bond angles

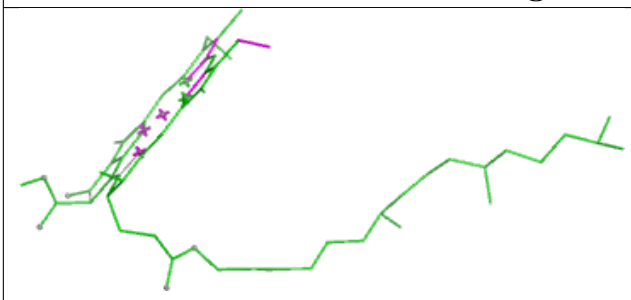


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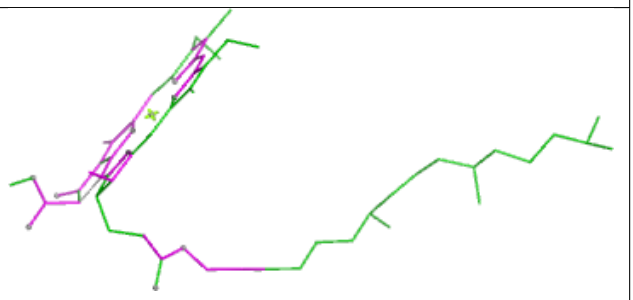


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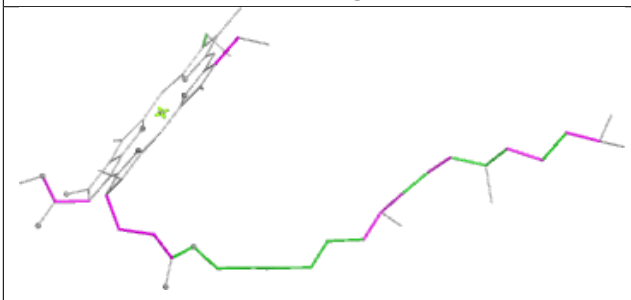
Ligand CLA n 604



Bond lengths



Bond angles

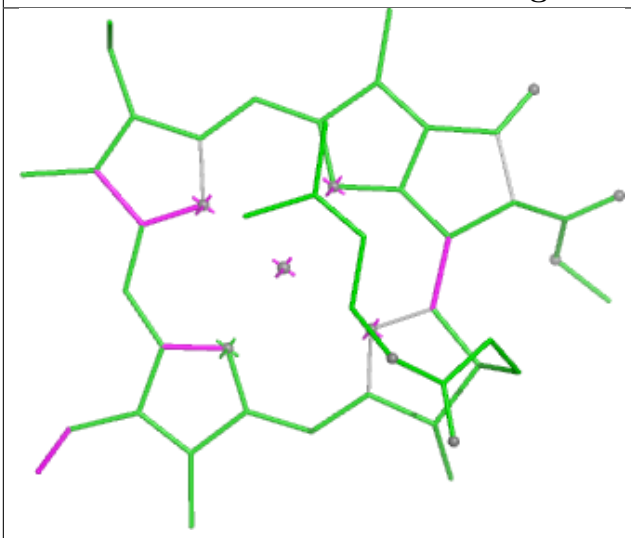


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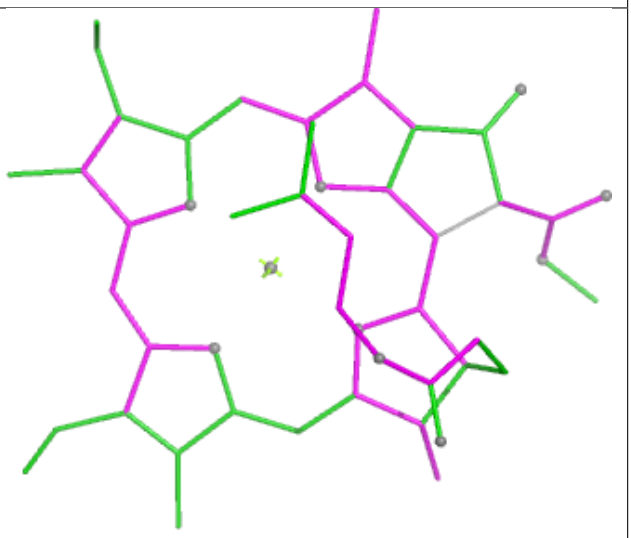


Rings

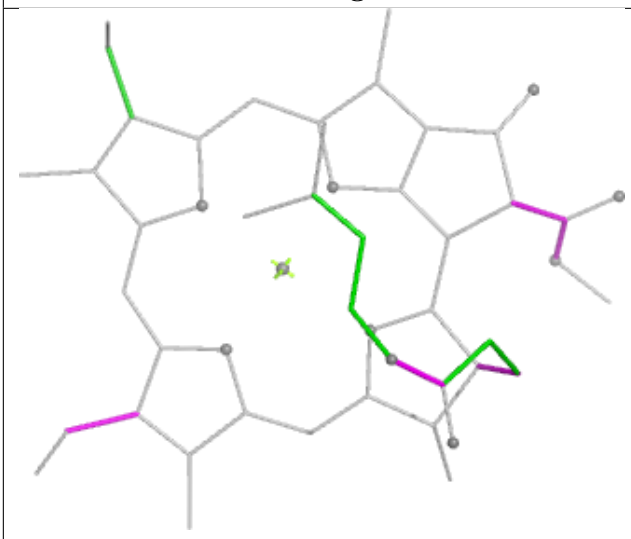
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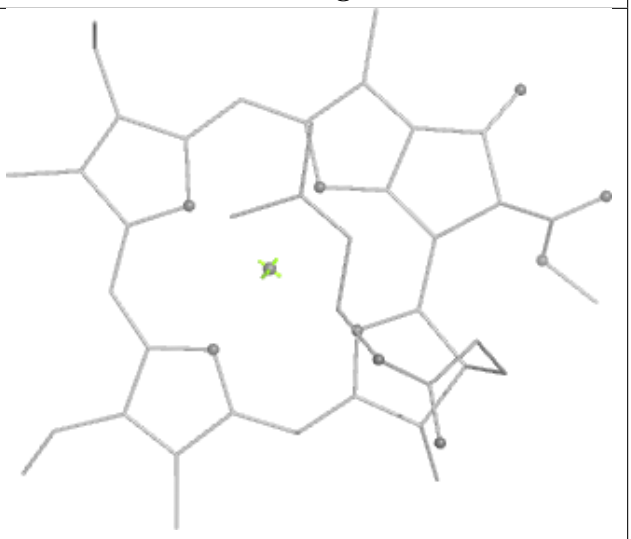
Bond lengths



Bond angles

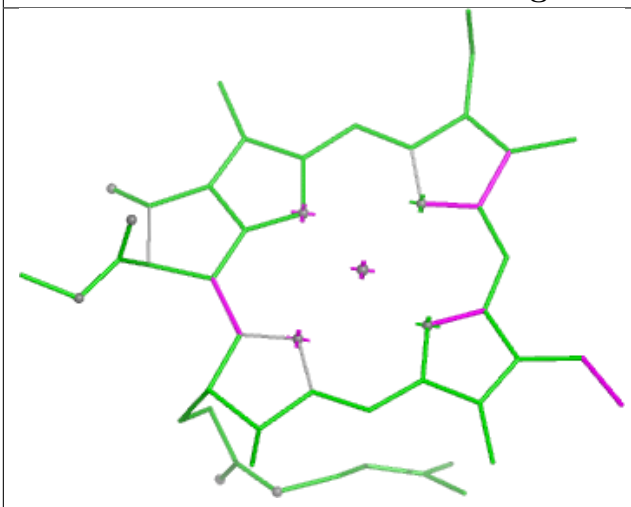


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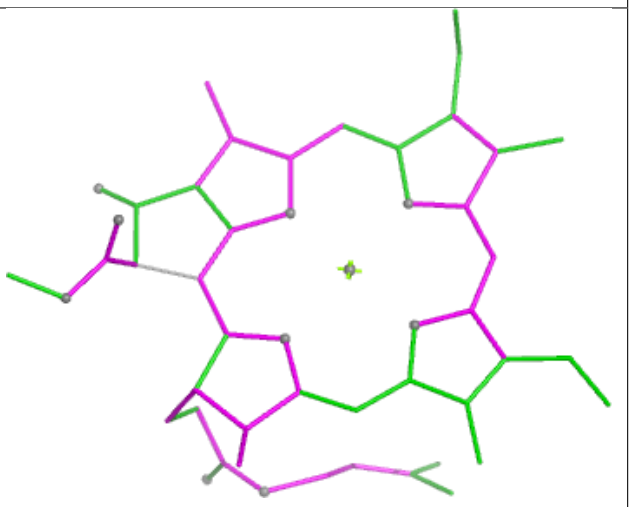


Rings

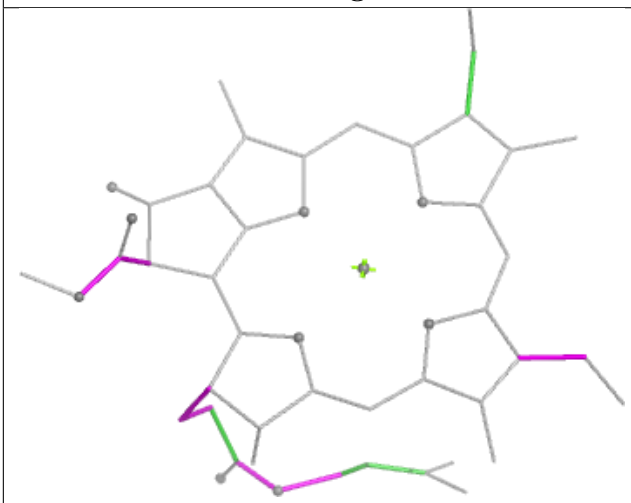
Ligand CLA s 617



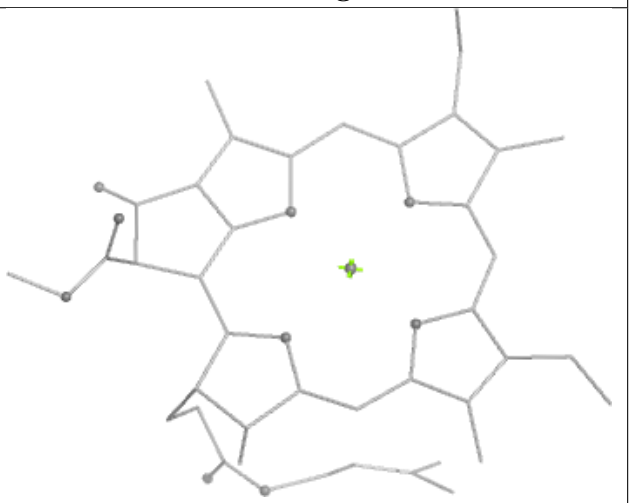
Bond lengths



Bond angles

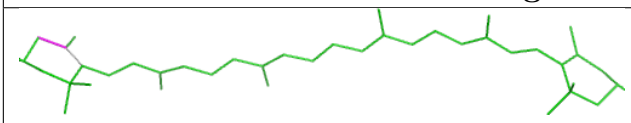


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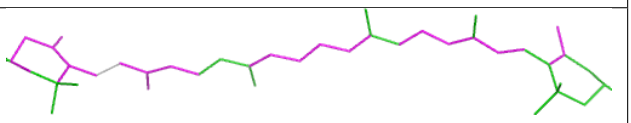


Rings

Ligand LUT N 620



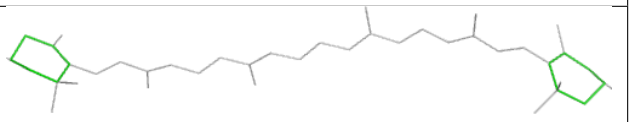
Bond lengths



Bond angles

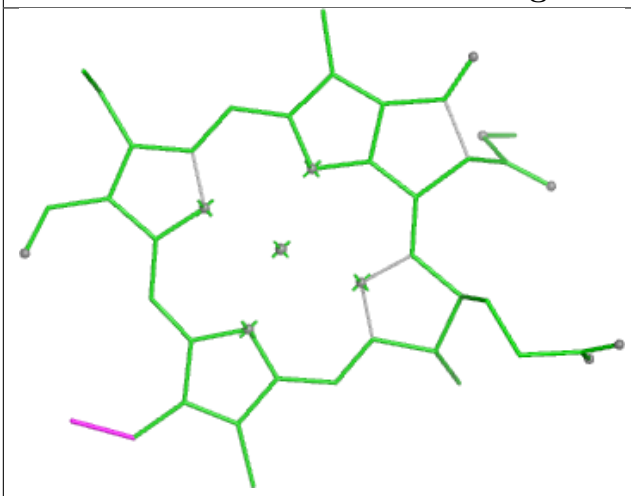


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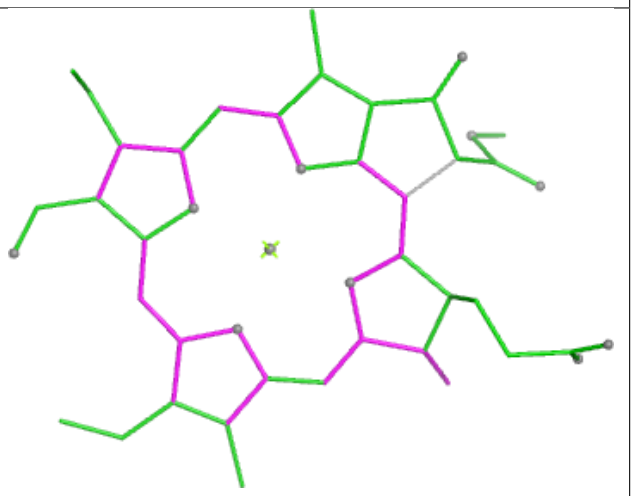


Rings

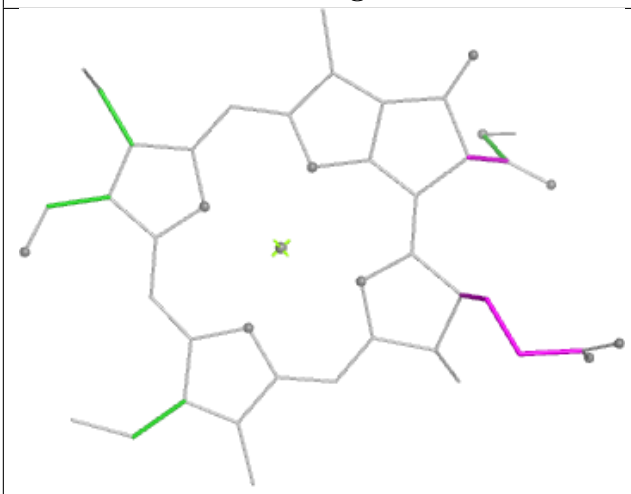
Ligand CHL s 601



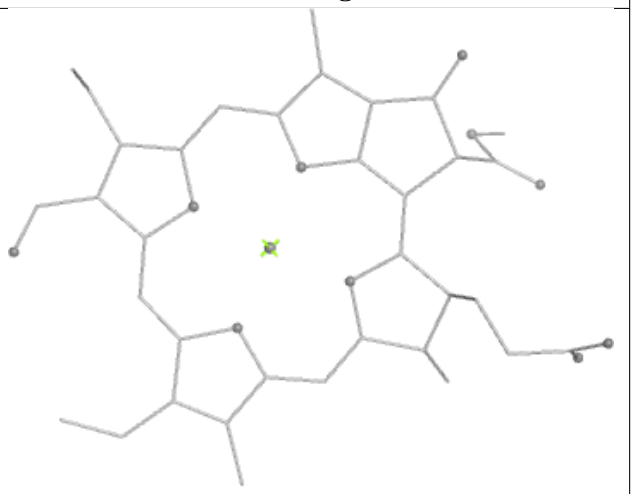
Bond lengths



Bond angles

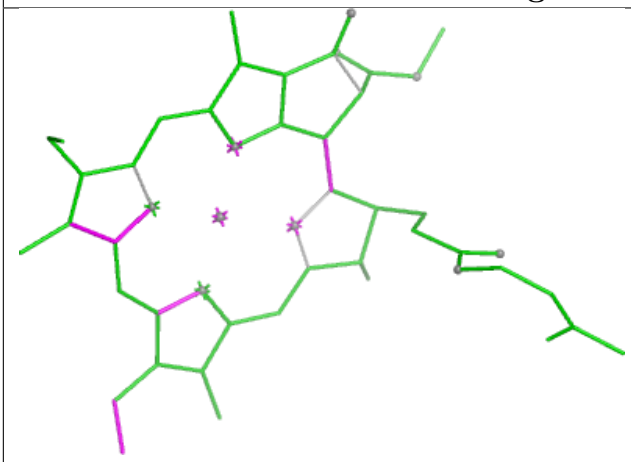


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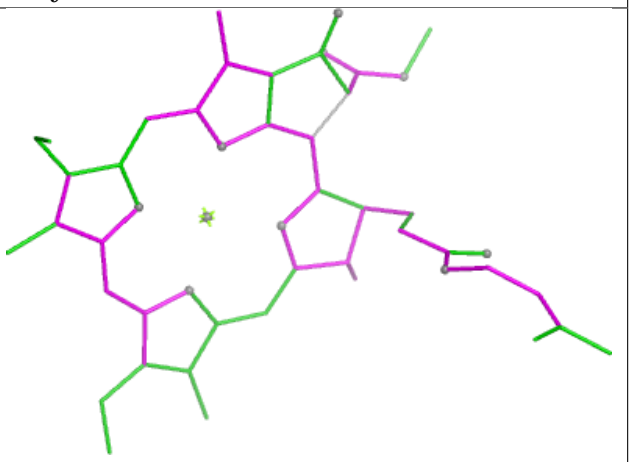


Rings

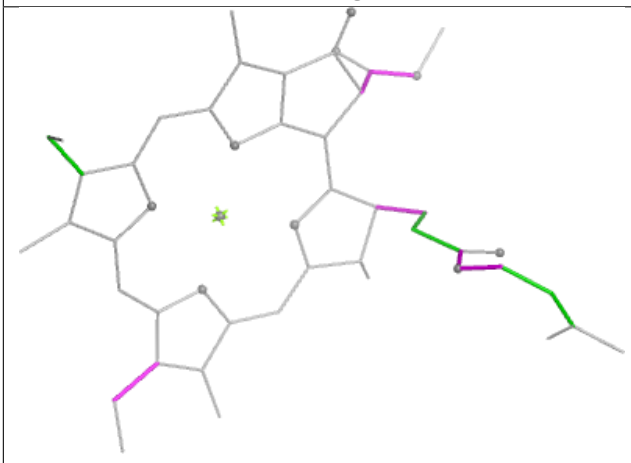
Ligand CLA y 608



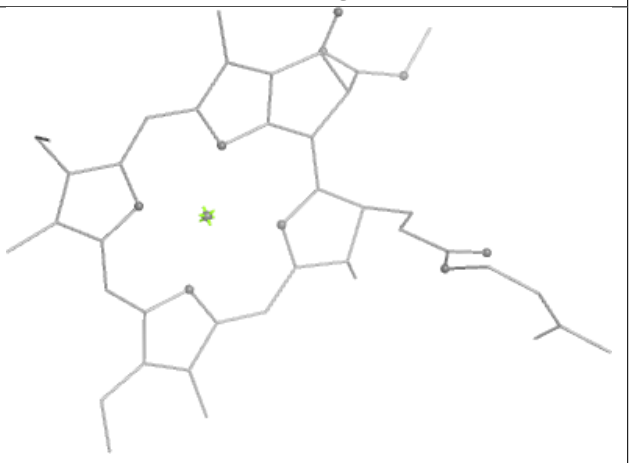
Bond lengths



Bond angles

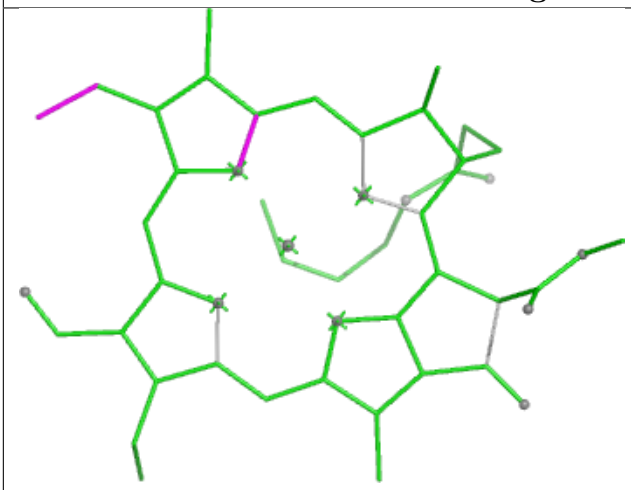


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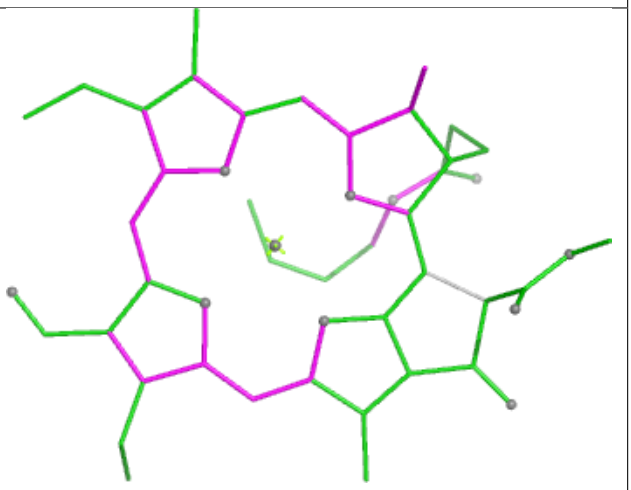


Rings

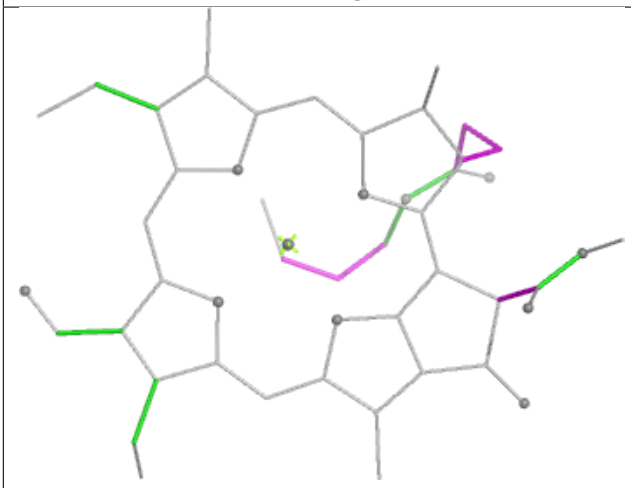
Ligand CHL r 607



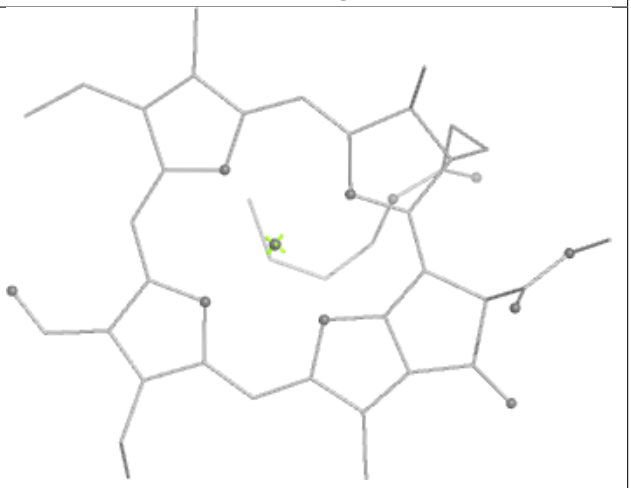
Bond lengths



Bond angles

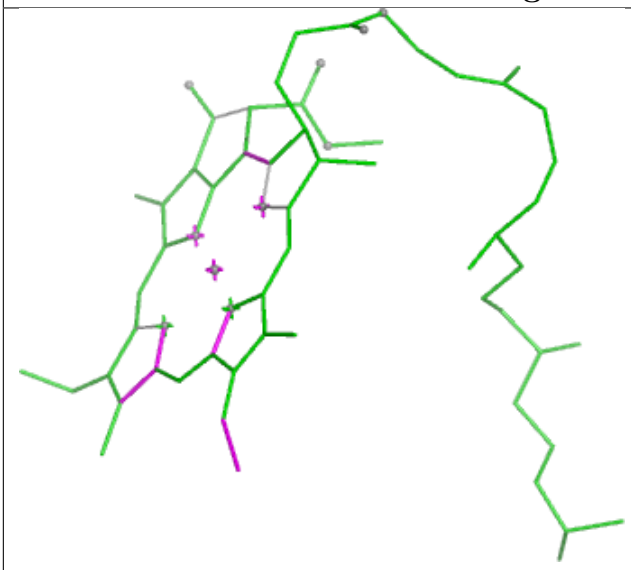


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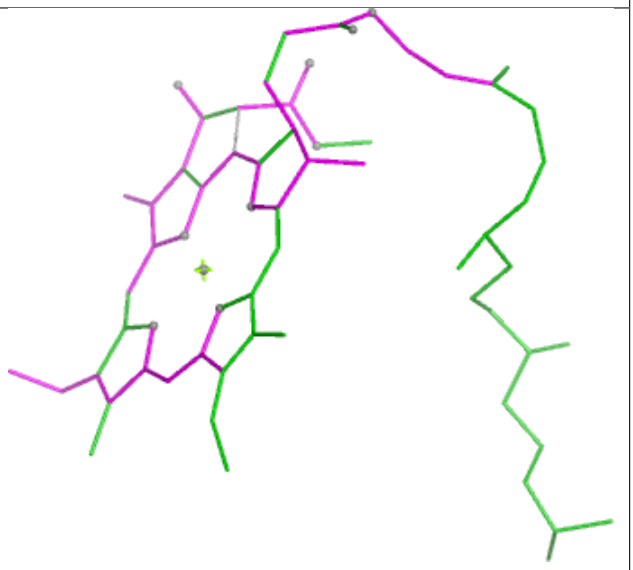


Rings

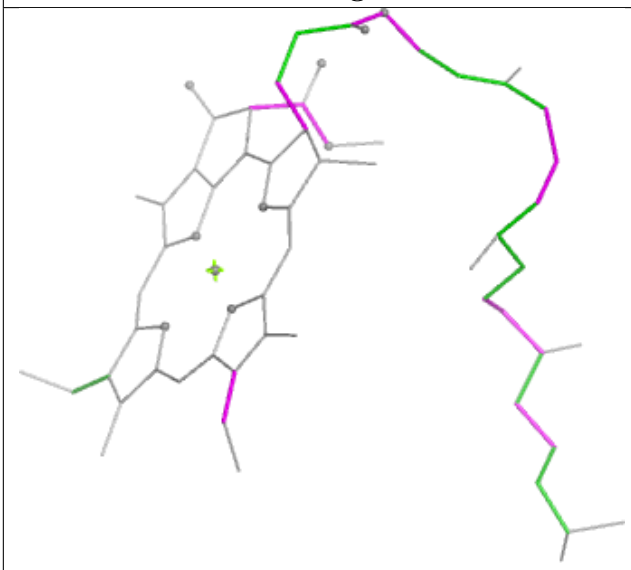
Ligand CLA N 603



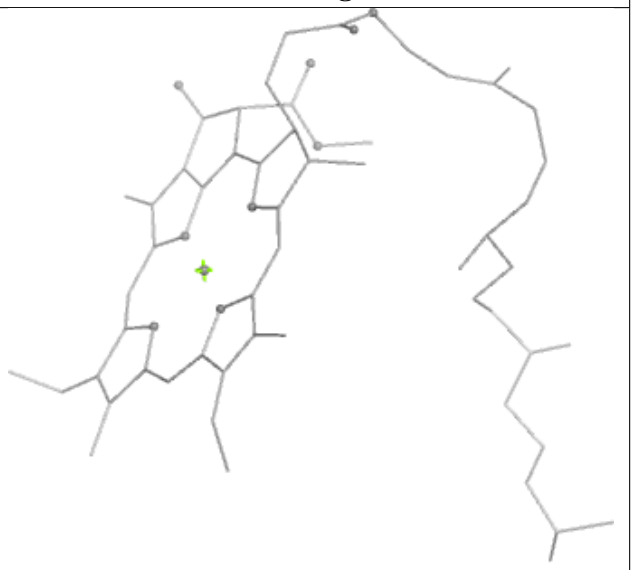
Bond lengths



Bond angles

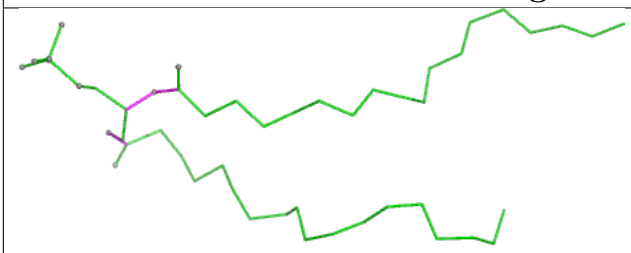


Torsions

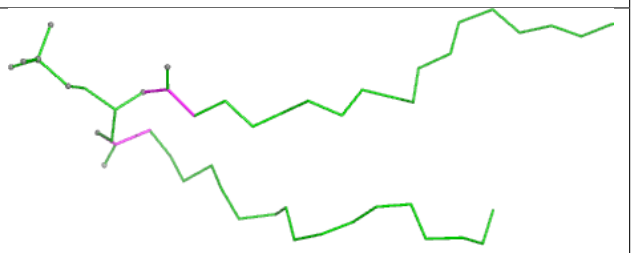


Rings

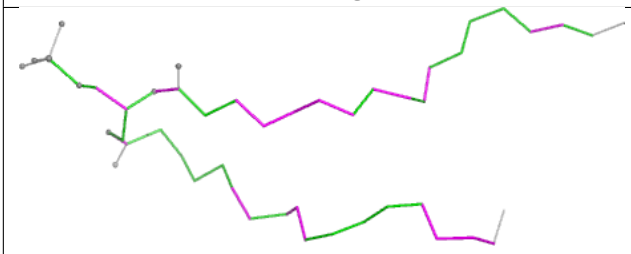
Ligand 3PH S 626



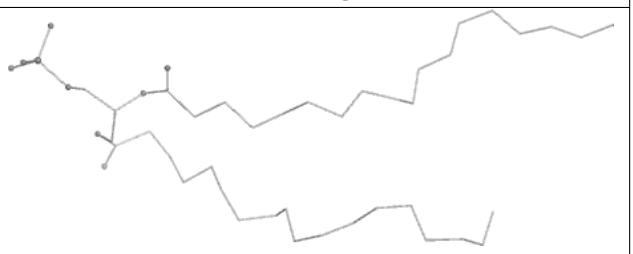
Bond lengths



Bond angles

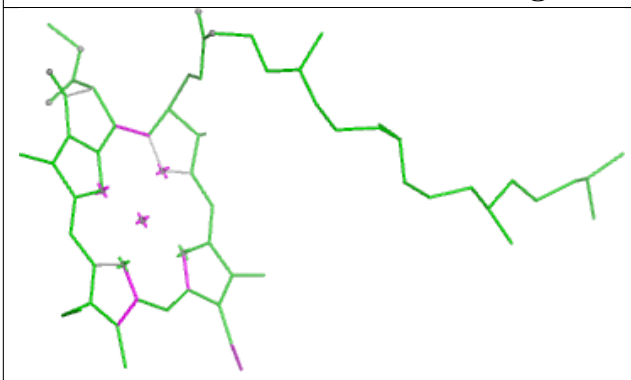


Torsions

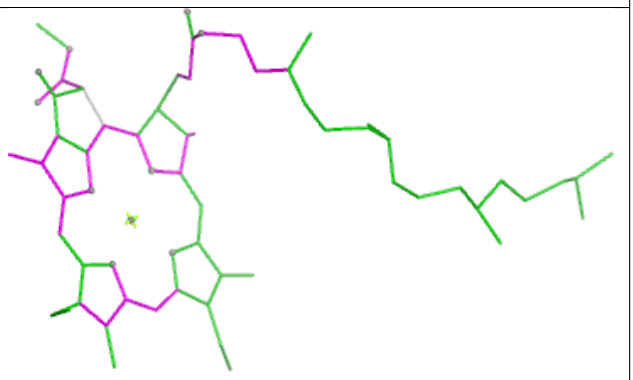


Rings

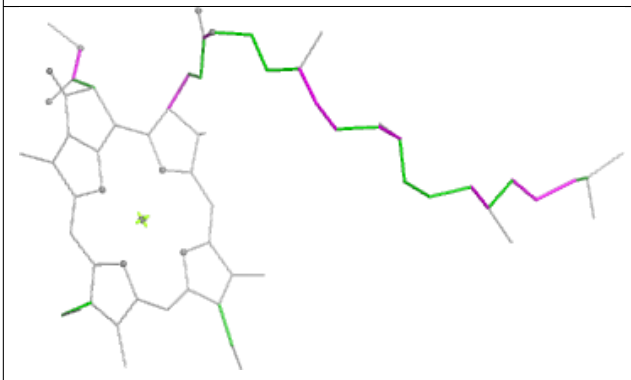
Ligand CLA c 511



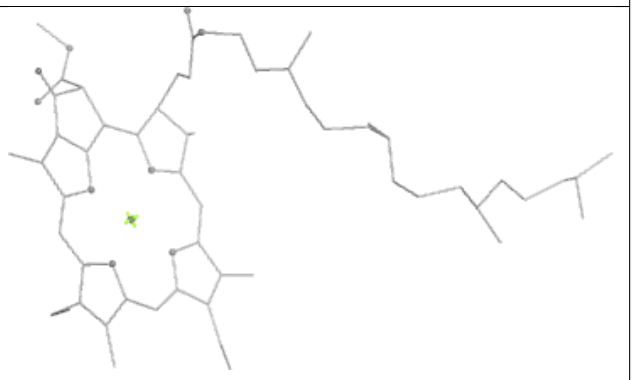
Bond lengths



Bond angles

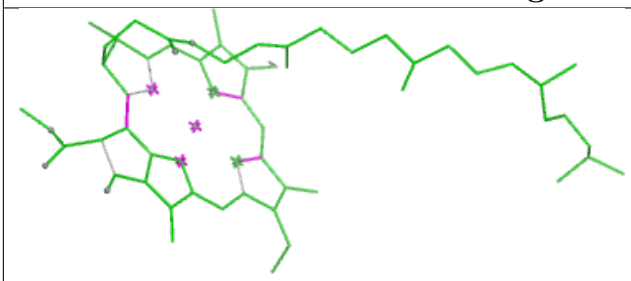


Torsions

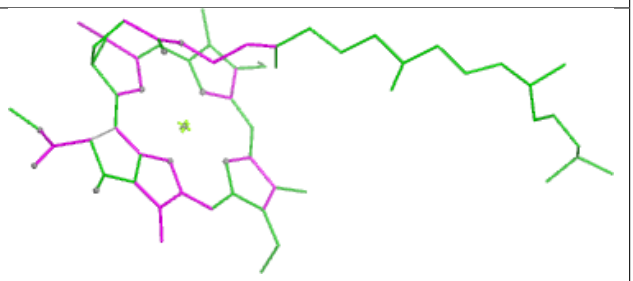


Rings

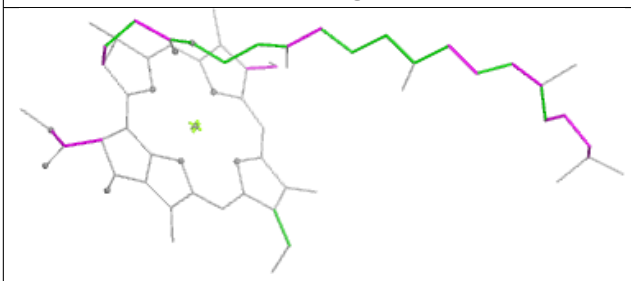
Ligand CLA b 609



Bond lengths



Bond angles

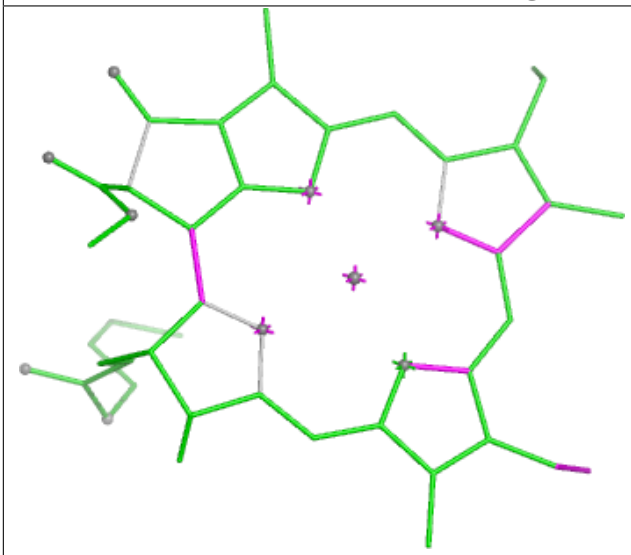


Torsions

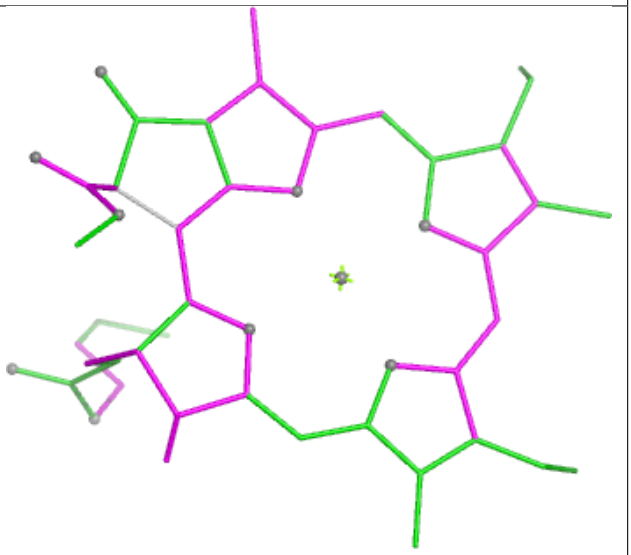


Rings

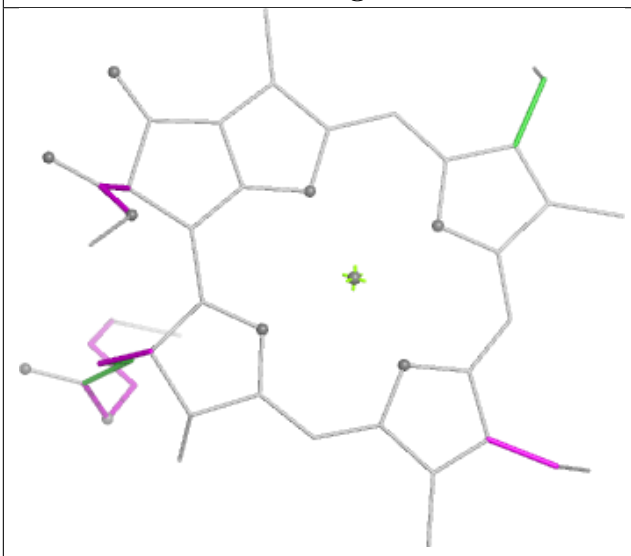
Ligand CLA N 611



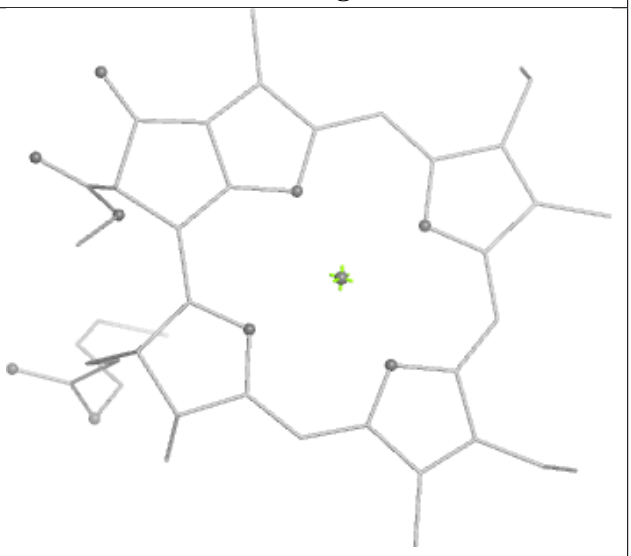
Bond lengths



Bond angles

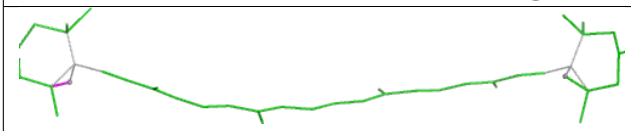


Torsions

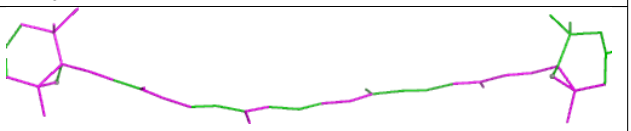


Rings

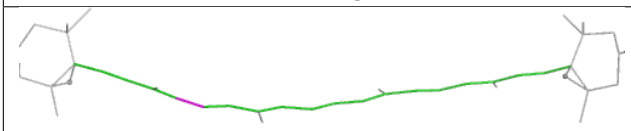
Ligand XAT y 622



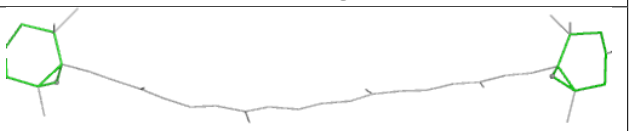
Bond lengths



Bond angles

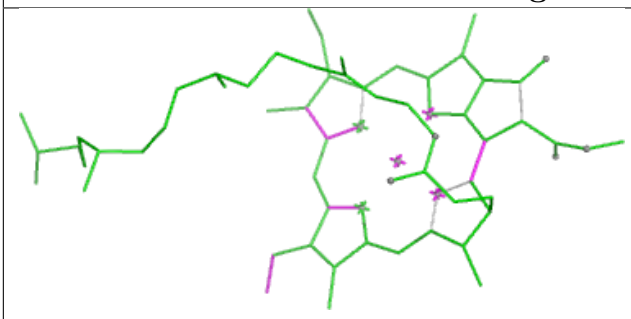


Torsions

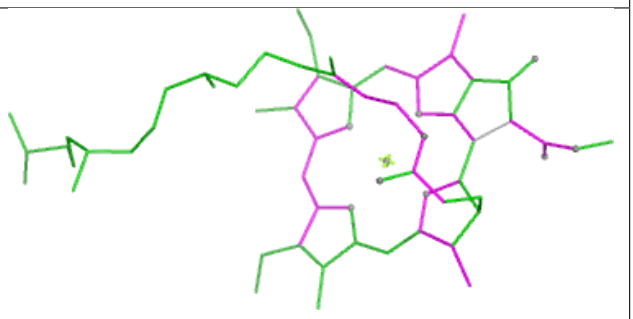


Rings

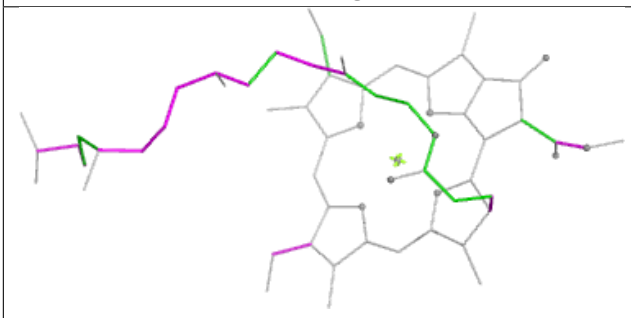
Ligand CLA c 513



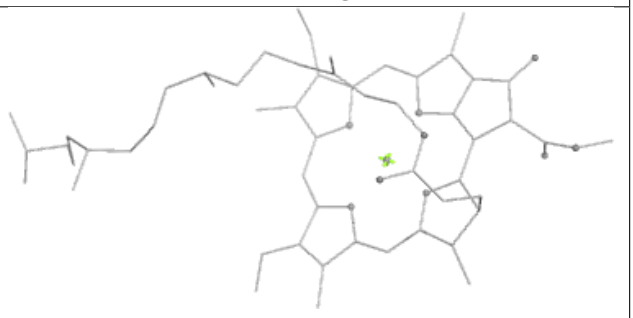
Bond lengths



Bond angles

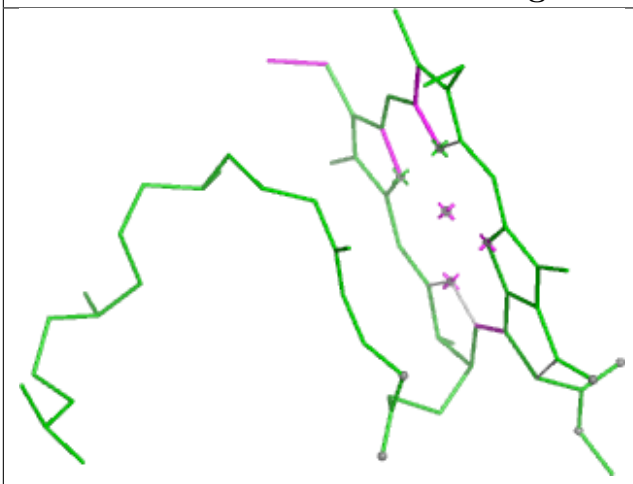


Torsions

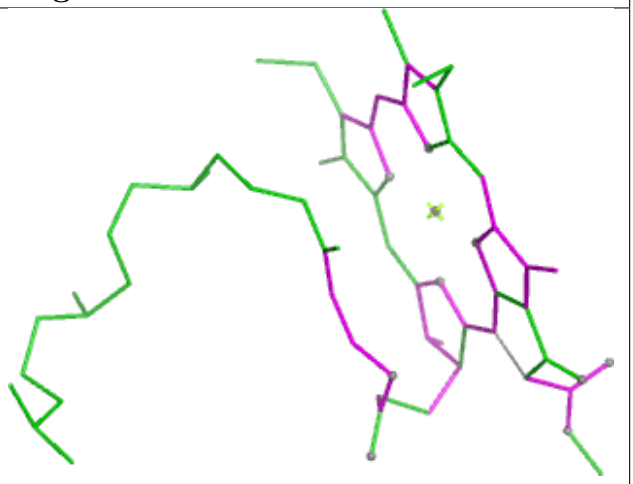


Rings

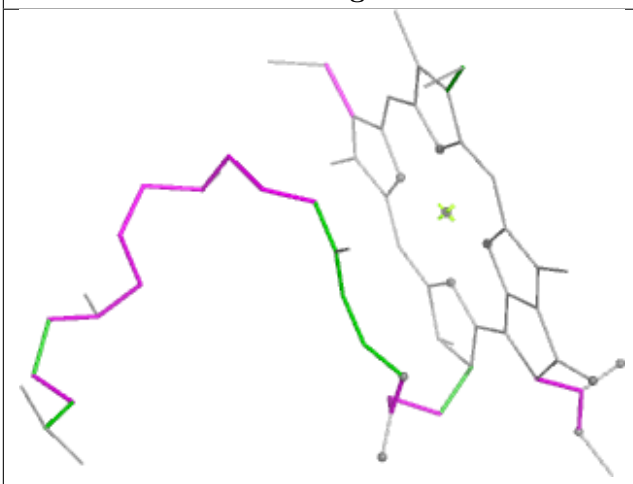
Ligand CLA g 613



Bond lengths



Bond angles

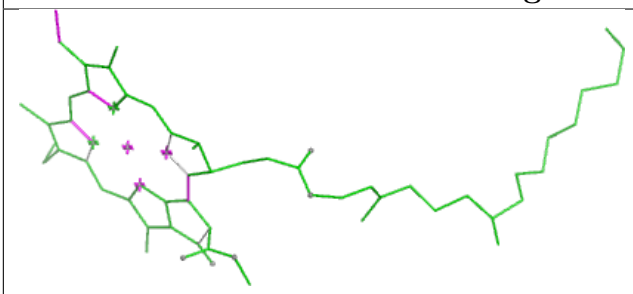


Torsions

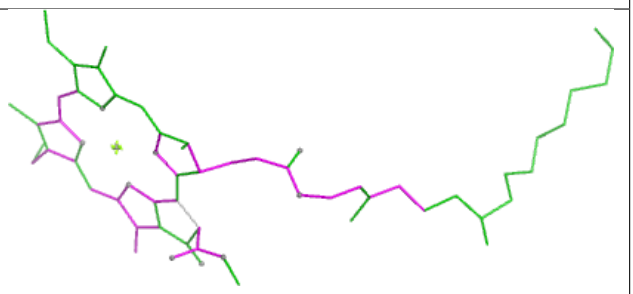


Rings

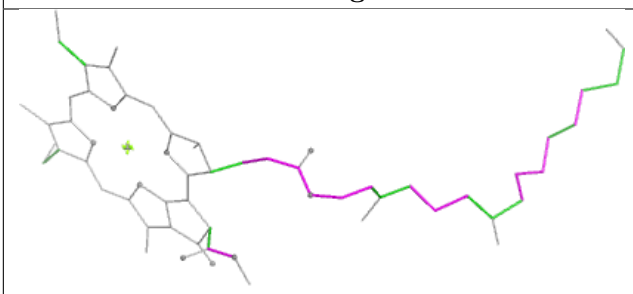
Ligand CLA A 405



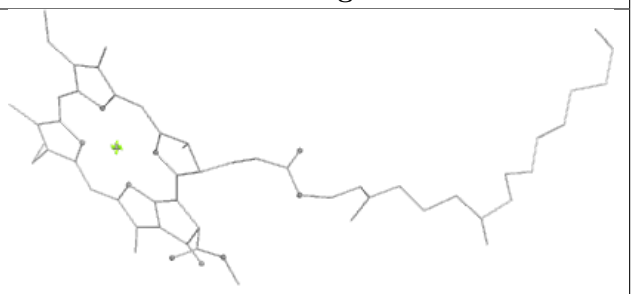
Bond lengths



Bond angles

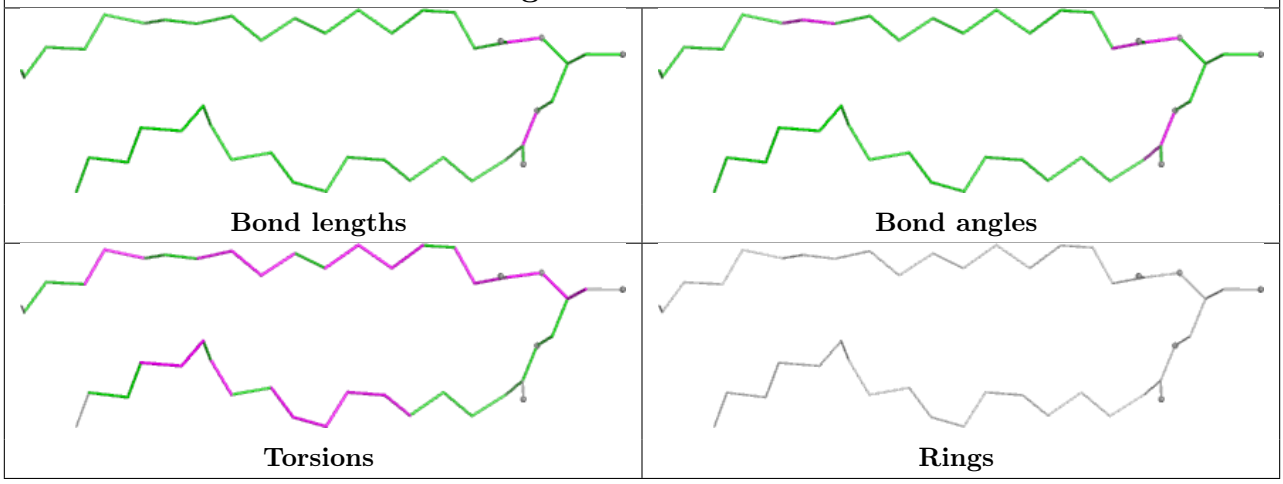


Torsions

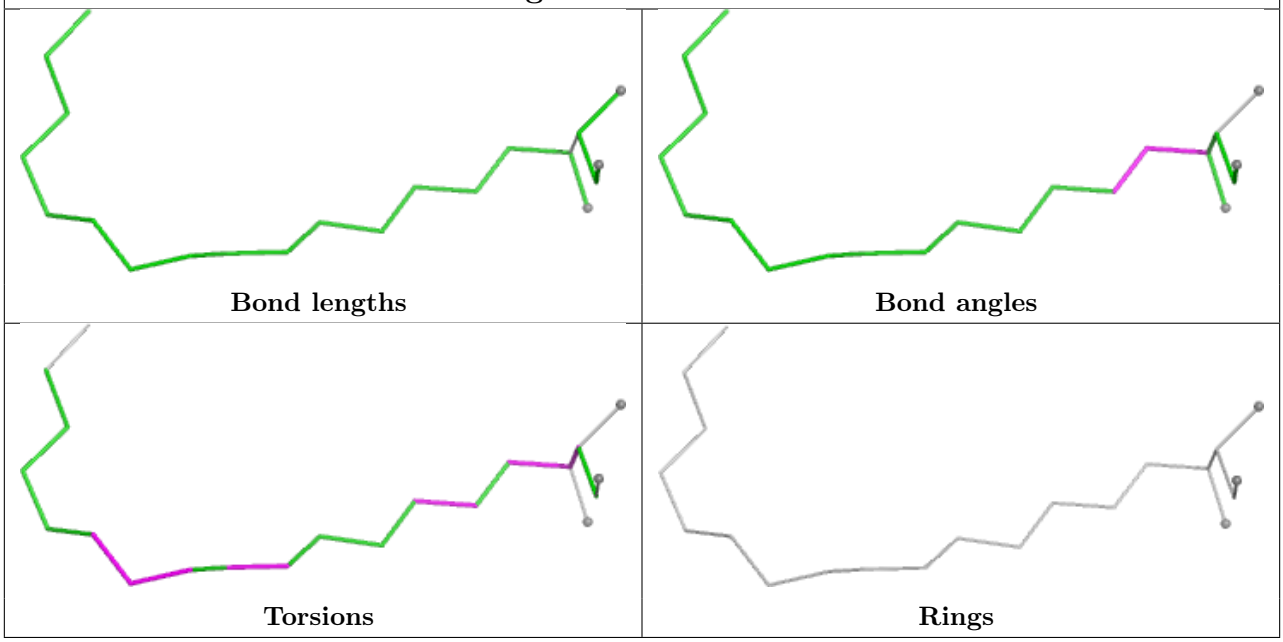


Rings

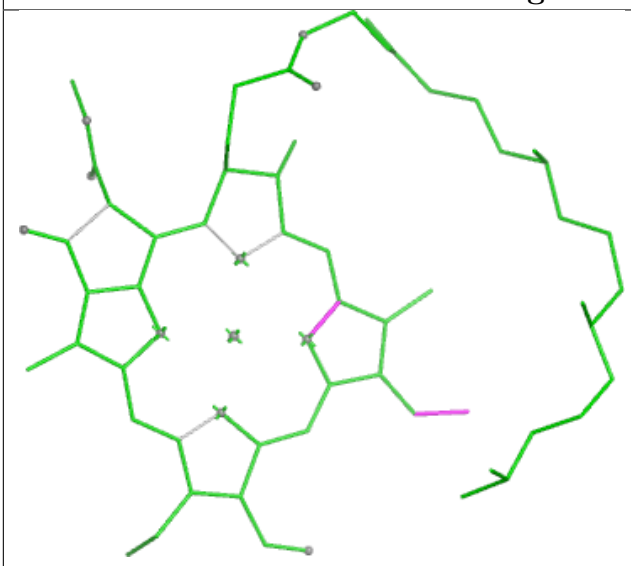
Ligand DGA B 625



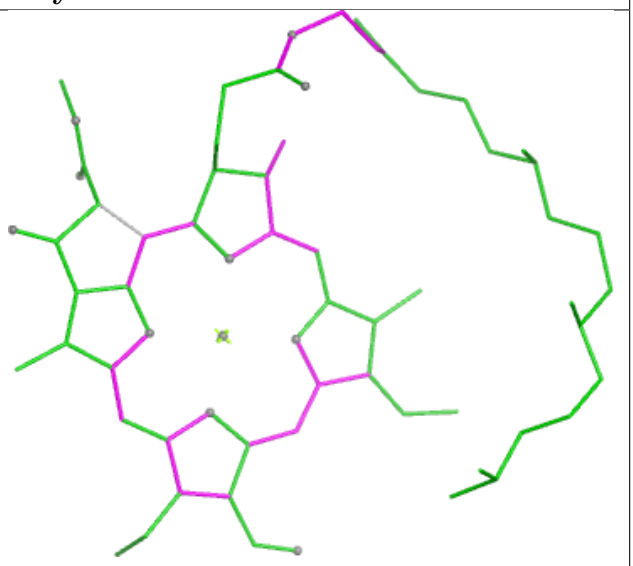
Ligand SPH Y 625



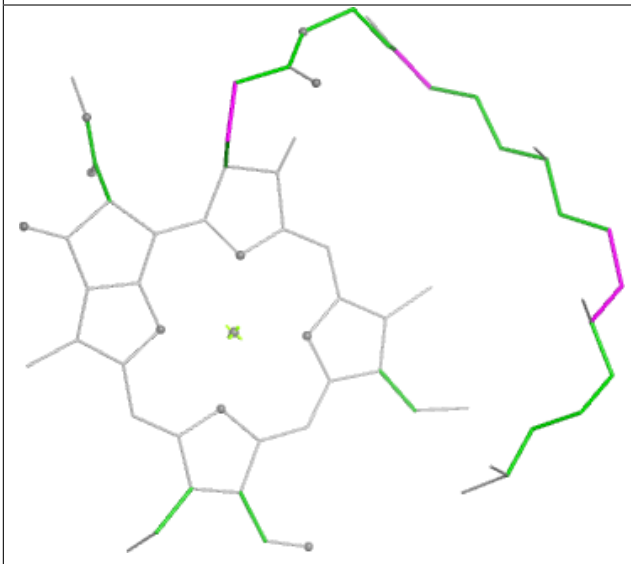
Ligand CHL y 607



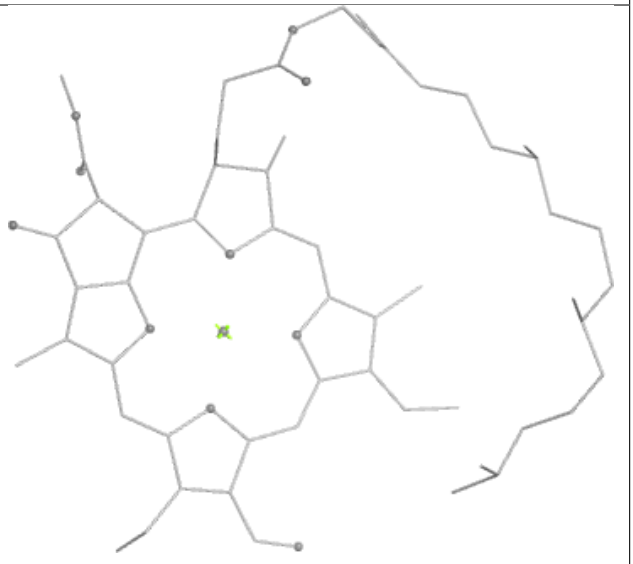
Bond lengths



Bond angles

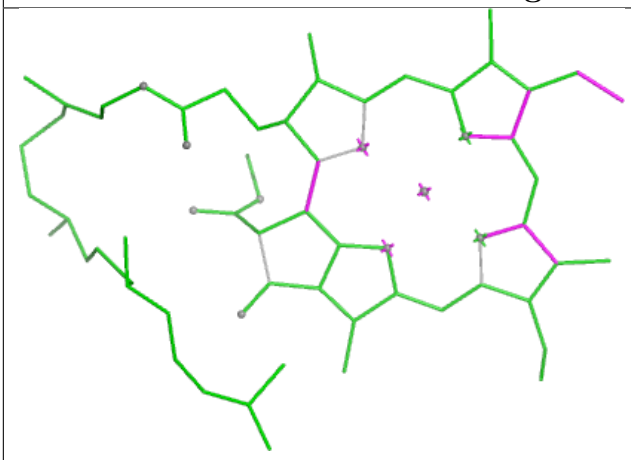


Torsions

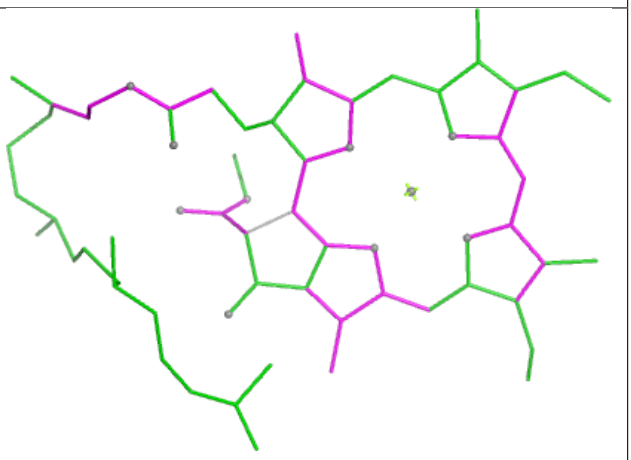


Rings

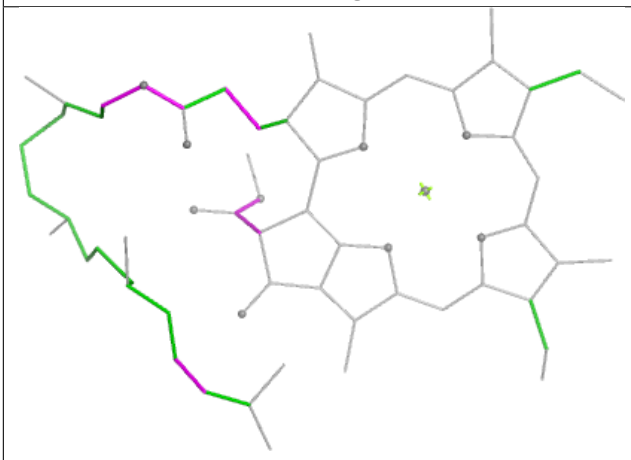
Ligand CLA B 611



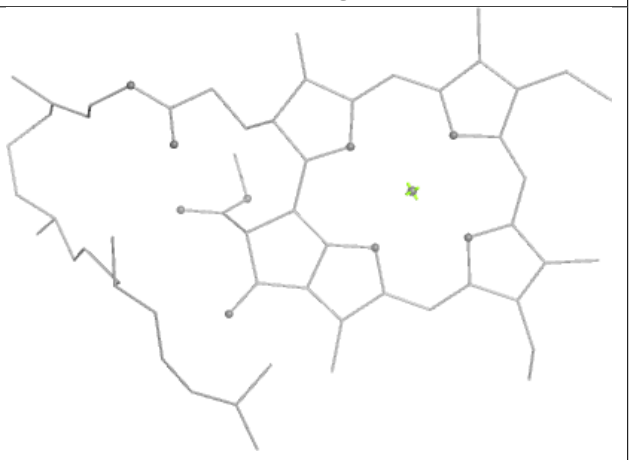
Bond lengths



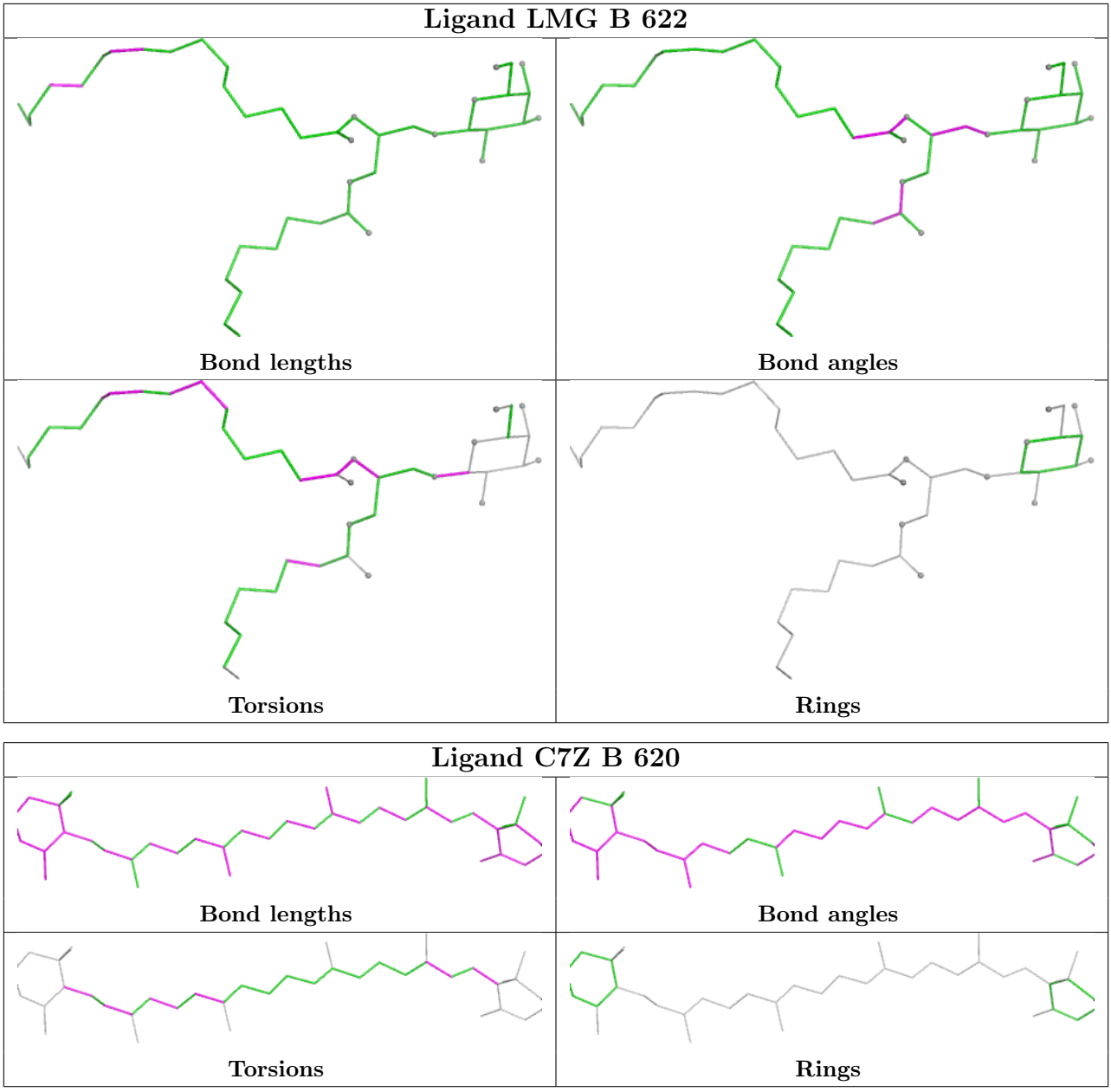
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	R	1
22	r	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
23	s	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	110:PRO	C	126:GLU	N	17.87
1	r	110:PRO	C	126:GLU	N	17.80
1	s	285:ARG	C	286:VAL	N	3.20

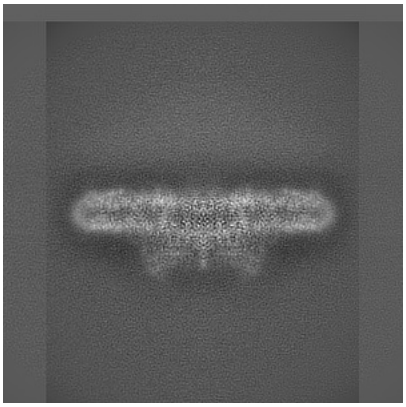
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13430. These allow visual inspection of the internal detail of the map and identification of artifacts.

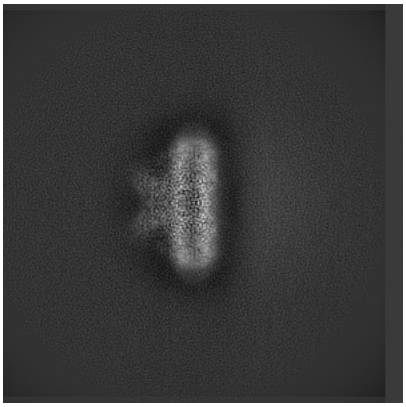
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

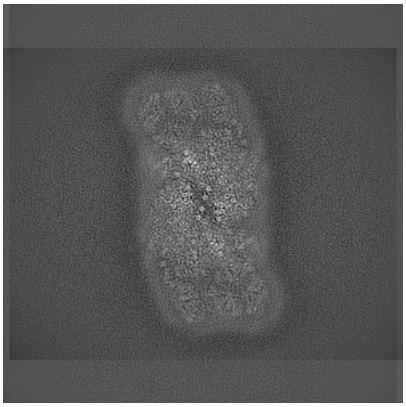
6.1.1 Primary map



X



Y

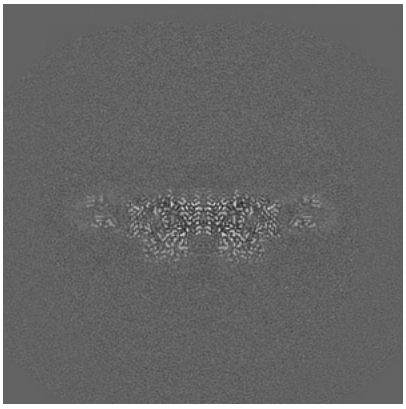


Z

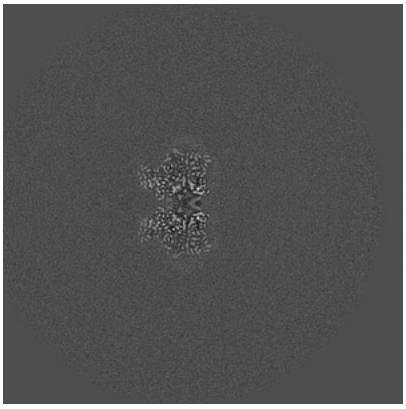
The images above show the map projected in three orthogonal directions.

6.2 Central slices

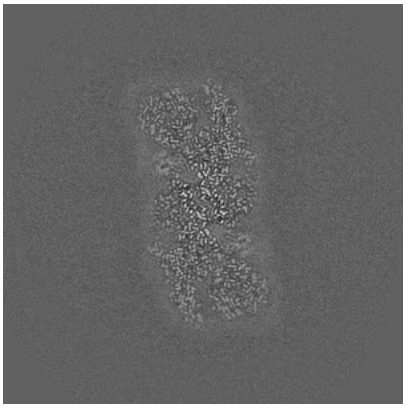
6.2.1 Primary map



X Index: 250



Y Index: 250

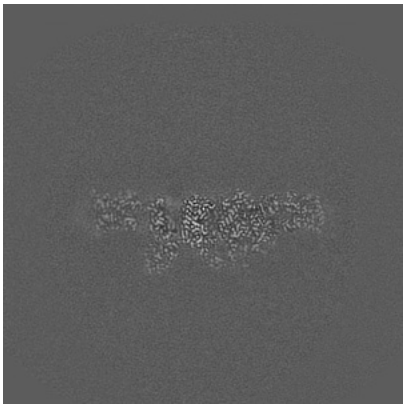


Z Index: 250

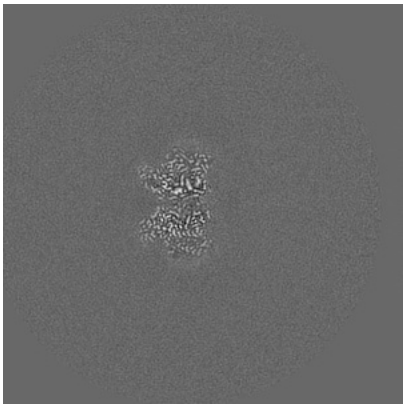
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

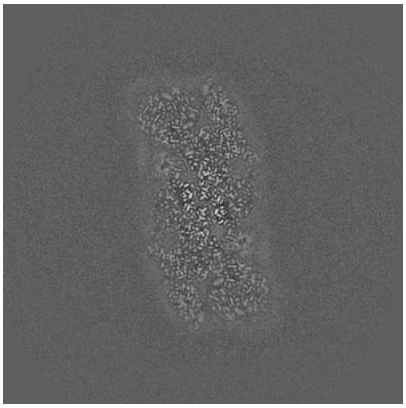
6.3.1 Primary map



X Index: 268



Y Index: 248

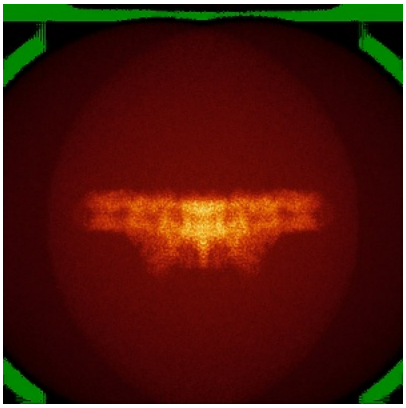


Z Index: 249

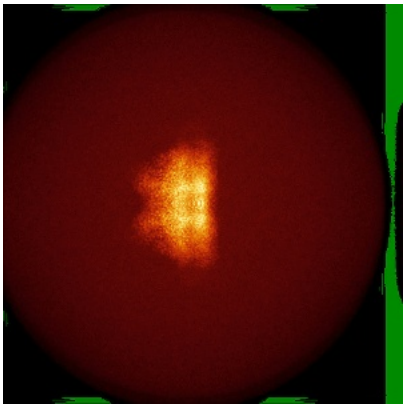
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

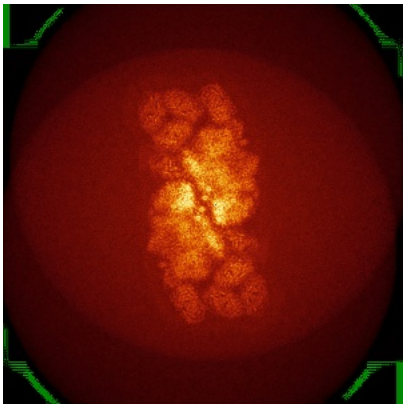
6.4.1 Primary map



X



Y

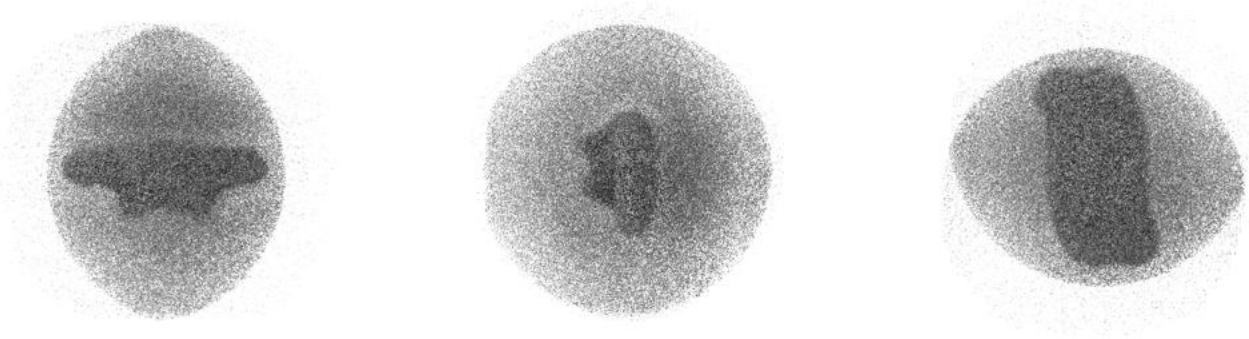


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

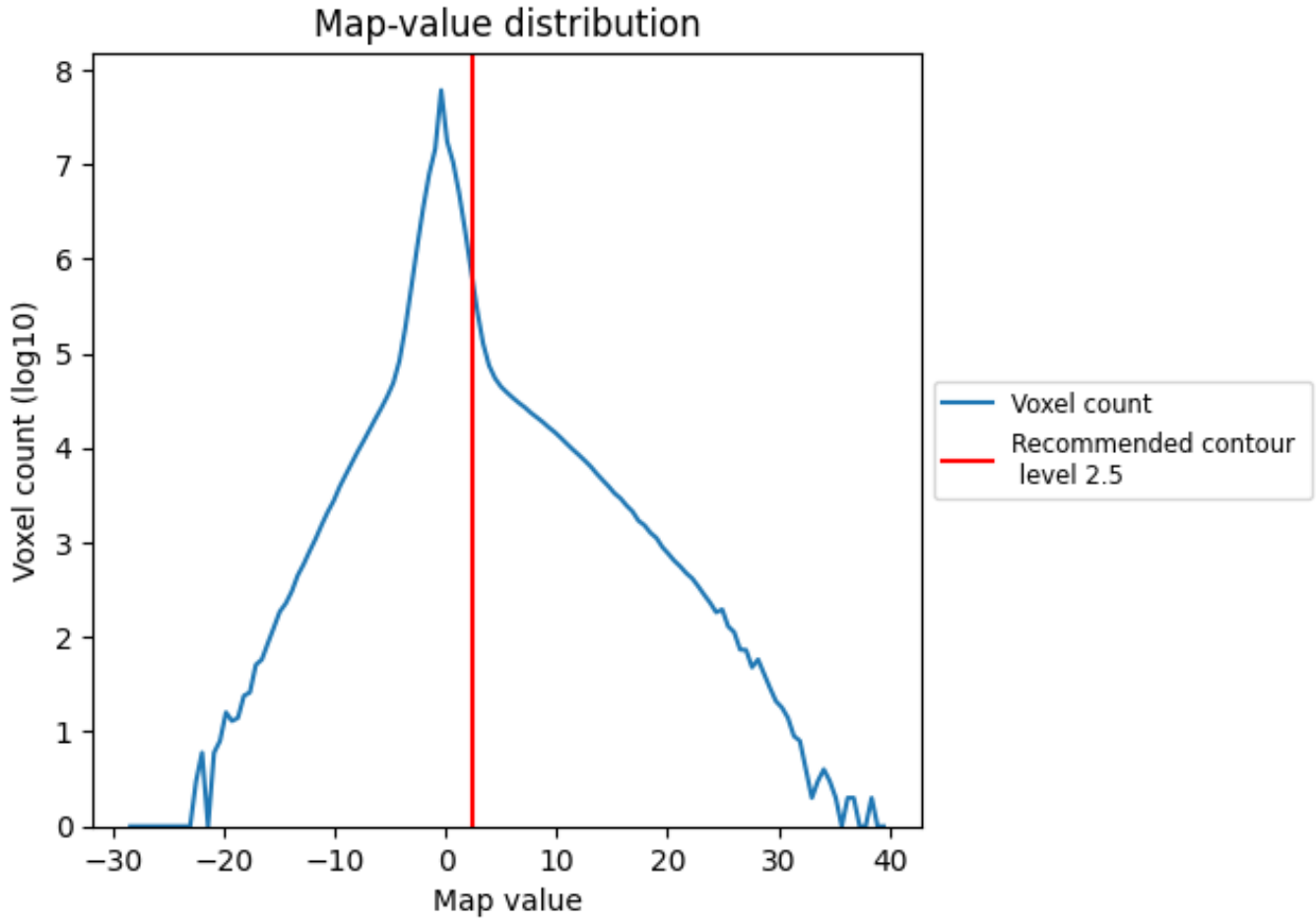
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

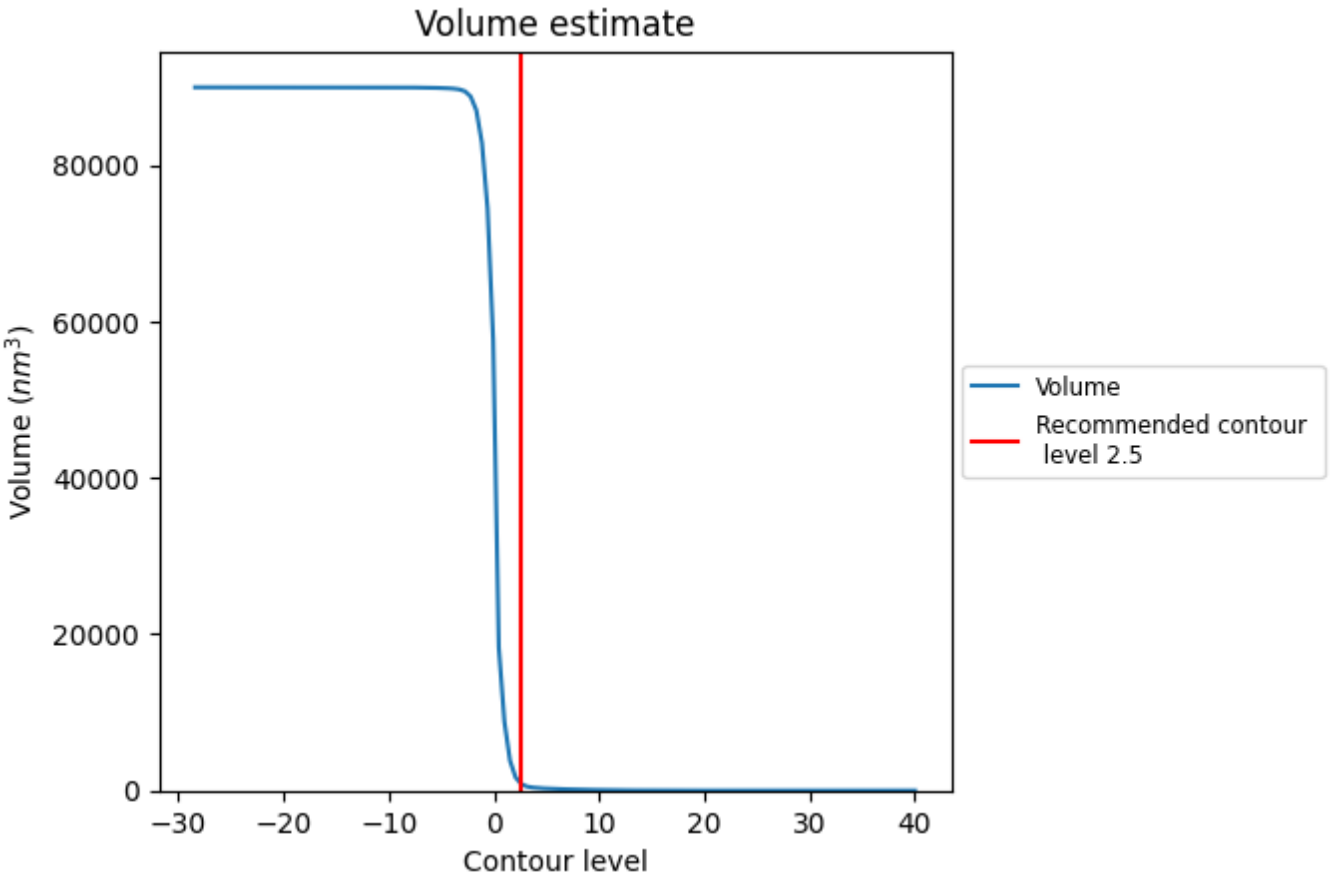
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

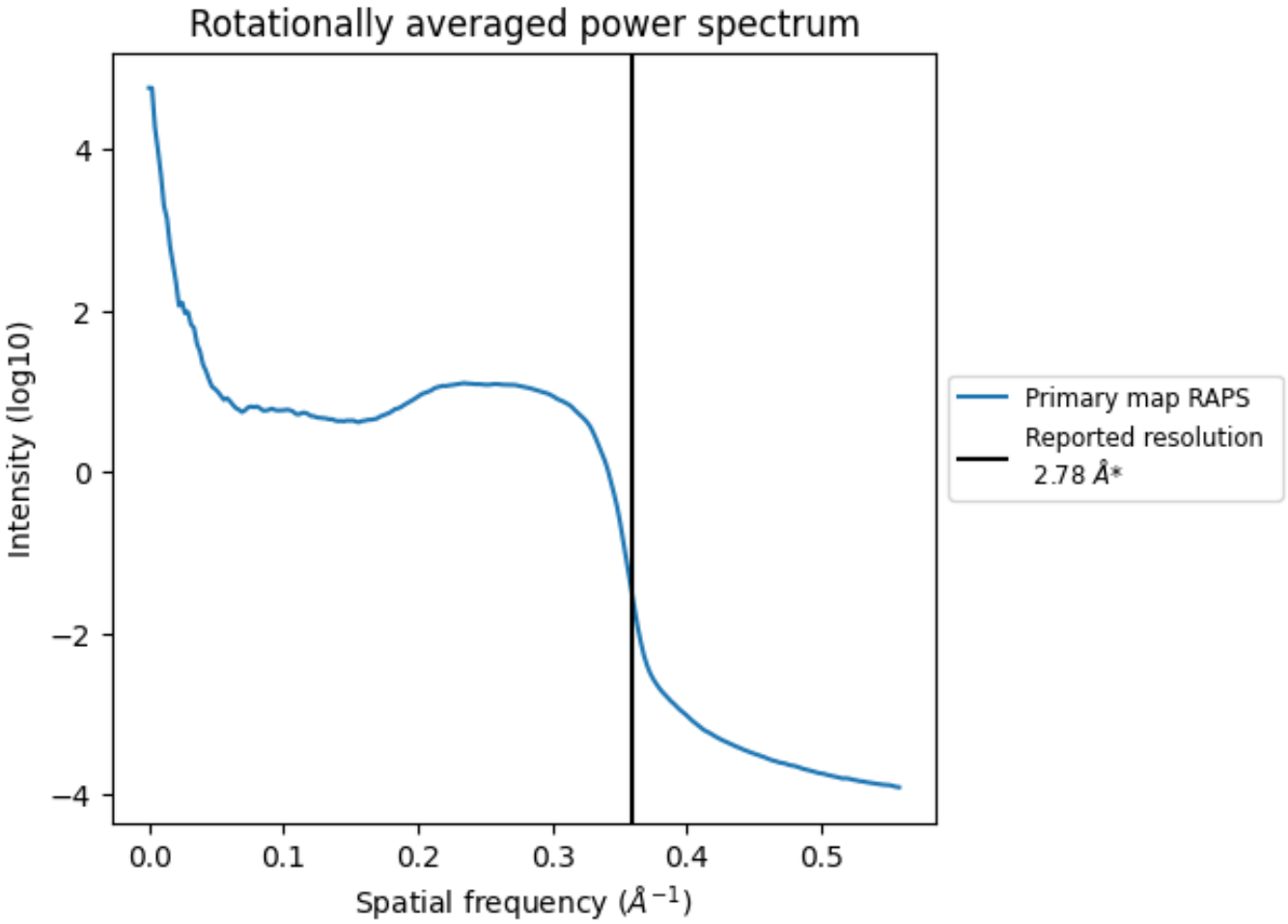
7.2 Volume estimate



The volume at the recommended contour level is 980 nm^3; this corresponds to an approximate mass of 885 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

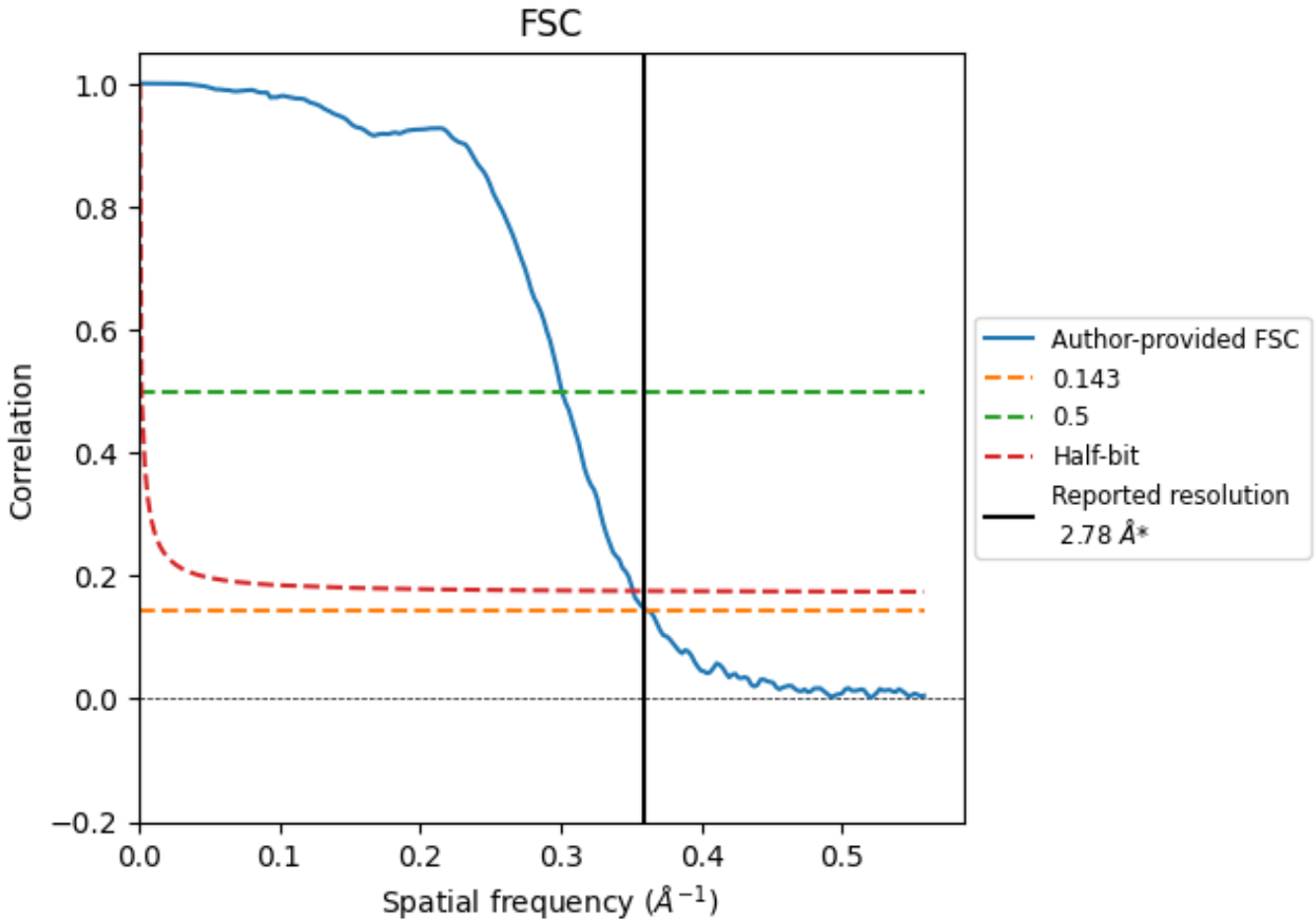


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

8.2 Resolution estimates (i)

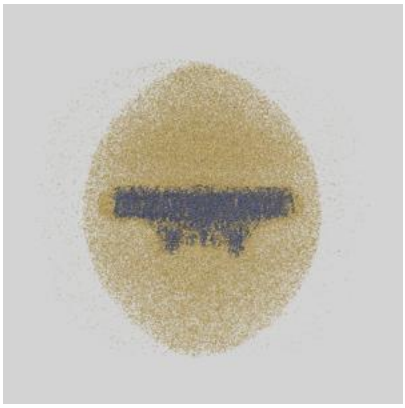
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.77	3.32	2.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

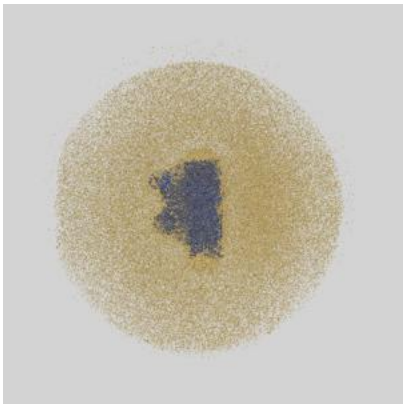
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13430 and PDB model 7PI5. Per-residue inclusion information can be found in section 3 on page 44.

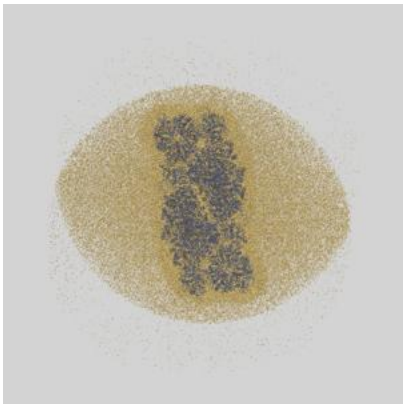
9.1 Map-model overlay



X



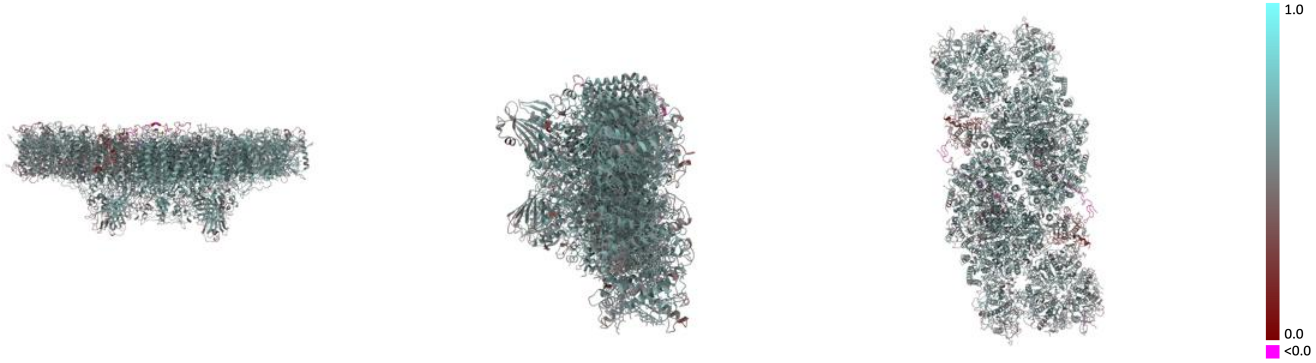
Y



Z

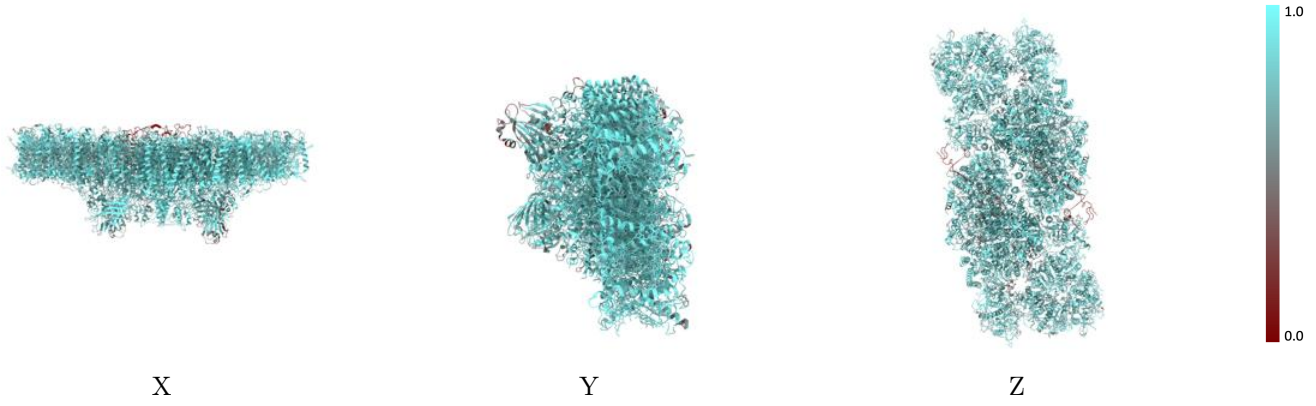
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



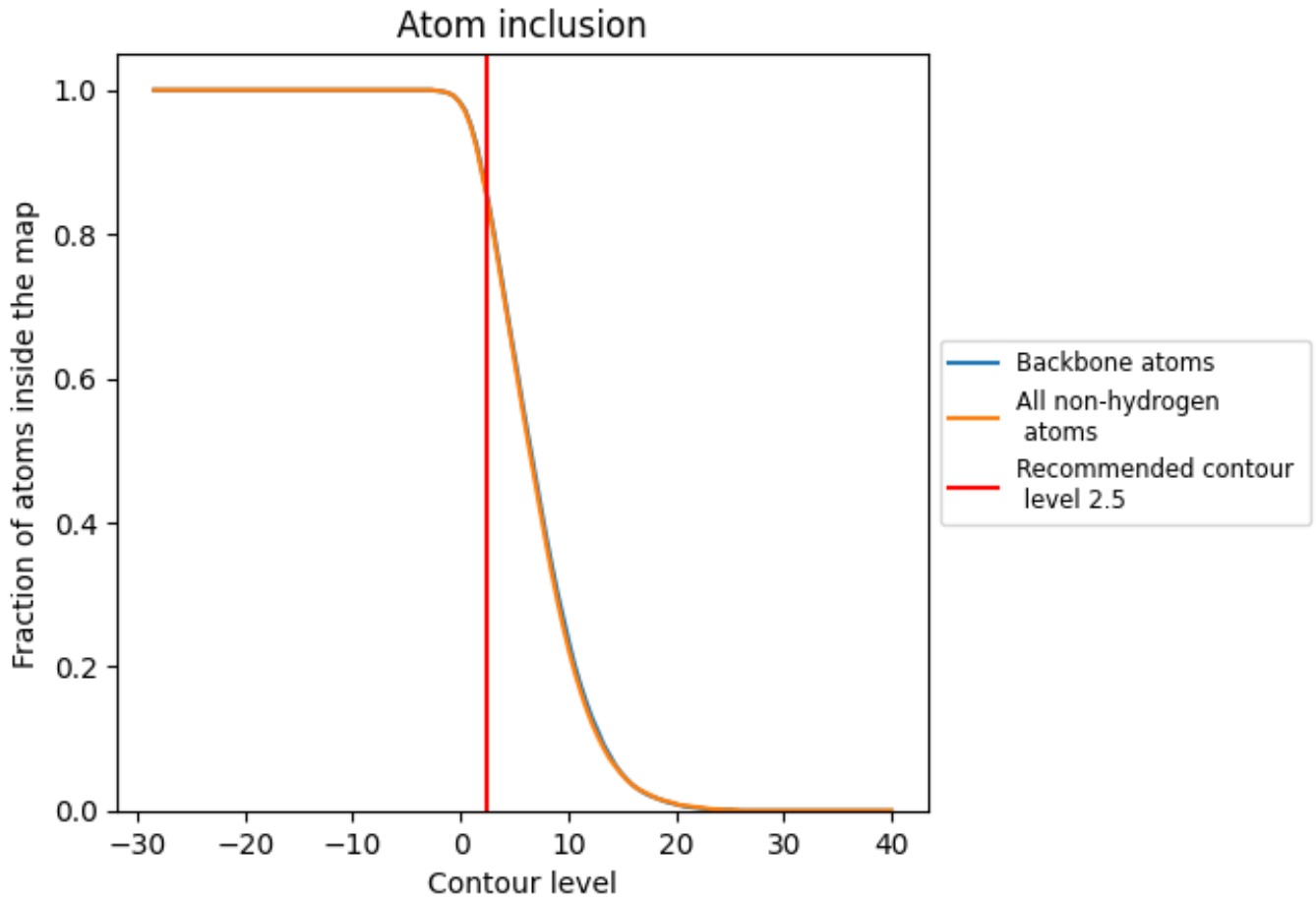
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5420
A	0.8520	0.5510
B	0.9210	0.5880
C	0.8770	0.5650
D	0.8960	0.5800
E	0.8730	0.5320
F	0.8500	0.5380
G	0.7990	0.4950
H	0.8770	0.5610
I	0.8800	0.5740
J	0.8170	0.5330
K	0.8700	0.5590
L	0.9350	0.5800
M	0.9130	0.5710
N	0.8080	0.5170
O	0.8090	0.4940
P	0.6310	0.4770
R	0.6810	0.3480
S	0.8070	0.5130
T	0.9300	0.5740
U	0.6610	0.4280
V	0.8400	0.5450
W	0.8200	0.5230
X	0.7860	0.5080
Y	0.8590	0.5380
Z	0.8700	0.5380
a	0.8720	0.5630
b	0.9230	0.5900
c	0.8990	0.5810
d	0.9150	0.5920
e	0.8760	0.5540
f	0.8990	0.5730
g	0.8360	0.5390
h	0.8910	0.5730
i	0.9470	0.5810



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Chain	Atom inclusion	Q-score
j	0.8460	0.5670
k	0.8770	0.5850
l	0.9320	0.5910
m	0.9050	0.5660
n	0.8520	0.5550
o	0.8460	0.5340
p	0.6150	0.4980
r	0.6650	0.3580
s	0.8420	0.5460
t	0.9170	0.5760
u	0.7480	0.4740
v	0.8760	0.5630
w	0.8590	0.5380
x	0.8260	0.5260
y	0.8810	0.5690
z	0.9010	0.5730