Full wwPDB EM Validation Report ⓘ

Sep 9, 2026 – 07:37 pm BST

PDB ID	:	7PNK / pdb_00007pnk
EMDB ID	:	EMD-13548
Title	:	Unstacked compact Dunaliella PSII
Authors	:	Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on	:	2021-09-07
Resolution	:	3.61 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:

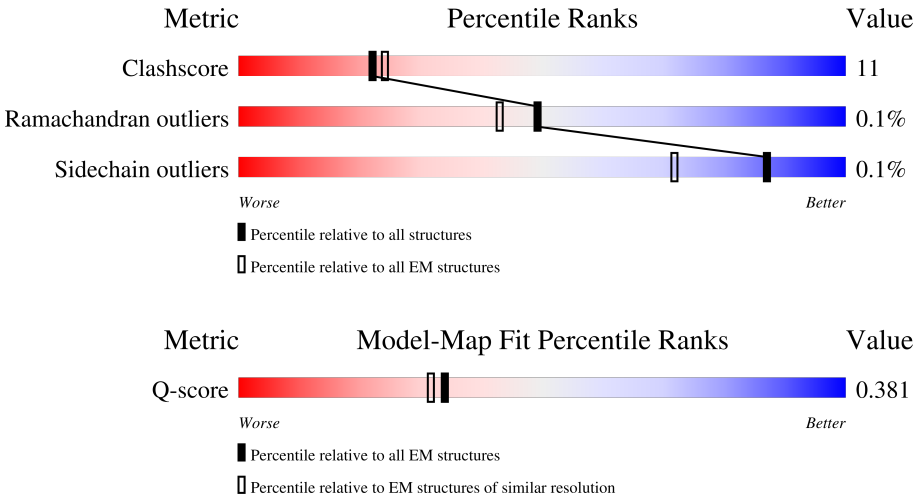
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.61 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	11801 (3.11 - 4.10)

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	8% 76% 24%
1	a	336	61% 39%
2	B	484	79% 21%
2	b	484	69% 31%

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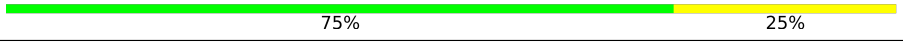
Mol	Chain	Length	Quality of chain
3	V	32	
3	v	32	
4	C	449	
4	c	449	
5	D	348	
5	d	348	
6	E	76	
6	e	76	
7	F	31	
7	f	31	
8	H	67	
8	h	67	
9	I	35	
9	i	35	
10	J	36	
10	j	36	
11	K	37	
11	k	37	
12	L	38	
12	l	38	
13	M	31	
13	m	31	
14	O	238	
14	o	238	
15	P	187	

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Mol	Chain	Length	Quality of chain
15	p	187	58% 76% 24%
16	T	30	17% 77% 23%
16	t	30	27% 77% 23%
17	W	44	9% 89% 11%
17	w	44	11% 82% 18%
18	X	30	7% 90% 10%
18	x	30	90% 10%
19	Z	61	95% 5%
19	z	61	87% 13%
20	N	222	83% 17%
21	G	221	81% 19%
22	S	243	80% 19%
23	Y	222	85% 15%
24	U	27	7% 70% 30%
24	u	27	85% 15%

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
34	C7Z	B	620	X	-	-	-
34	C7Z	b	620	X	-	-	-
39	LMK	C	527	X	-	-	-
39	LMK	c	527	X	-	-	-
43	RRX	H	101	X	-	-	-
43	RRX	h	101	X	-	-	-
46	CHL	G	601	X	-	-	-
46	CHL	G	605	X	-	-	-
46	CHL	G	607	X	-	-	-
46	CHL	G	609	X	-	-	-
46	CHL	N	601	X	-	-	-
46	CHL	N	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	CHL	N	606	X	-	-	-
46	CHL	N	607	X	-	-	-
46	CHL	N	609	X	-	-	-
46	CHL	S	608	X	-	-	-
46	CHL	Y	601	X	-	-	-
46	CHL	Y	606	X	-	-	-
46	CHL	Y	607	X	-	-	-
46	CHL	Y	609	X	-	-	-
48	XAT	G	622	X	-	-	-
48	XAT	N	622	X	-	-	-

2 Entry composition (i)

There are 51 unique types of molecules in this entry. The entry contains 60673 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
			3785	2480	630	665	10		
2	b	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- 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		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
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	31	Total 234	C 159	N 33	O 42	0	0
13	m	31	Total 234	C 159	N 33	O 42	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	conflict	UNP D0FXZ3
m	9	THR	ILE	conflict	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
			1822	1153	296	367	6		
14	o	238	Total	C	N	O	S	0	0
			1822	1153	296	367	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 PsbW.

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		

- Molecule 18 is a protein called PsbX.

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

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

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

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

- Molecule 20 is a protein called Chlorophyll a-b binding protein of LHCII type I, chloroplastic.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 22 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

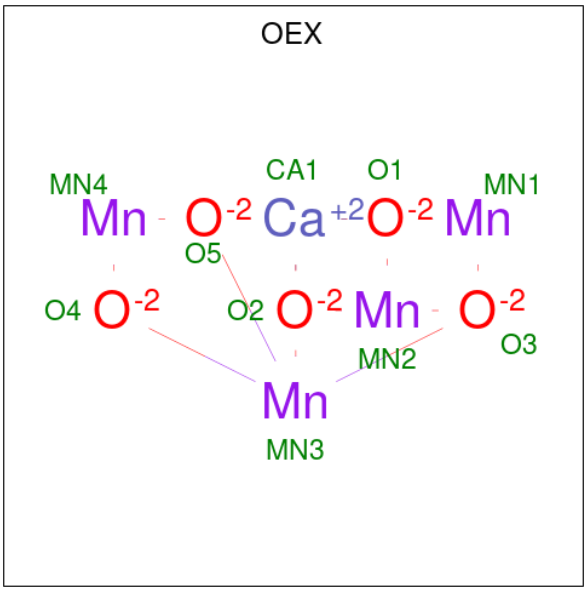
- Molecule 23 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	222	Total	C	N	O	S	0	0
			1670	1083	272	312	3		

- Molecule 24 is a protein called PsbU.

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

- Molecule 25 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

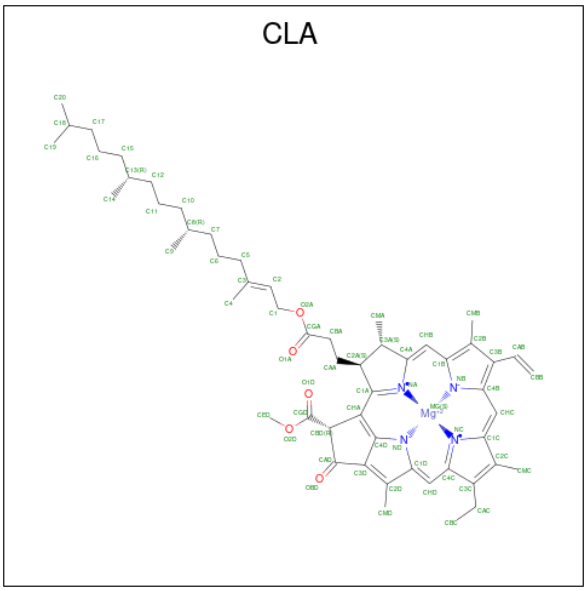
- Molecule 26 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	N	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
28	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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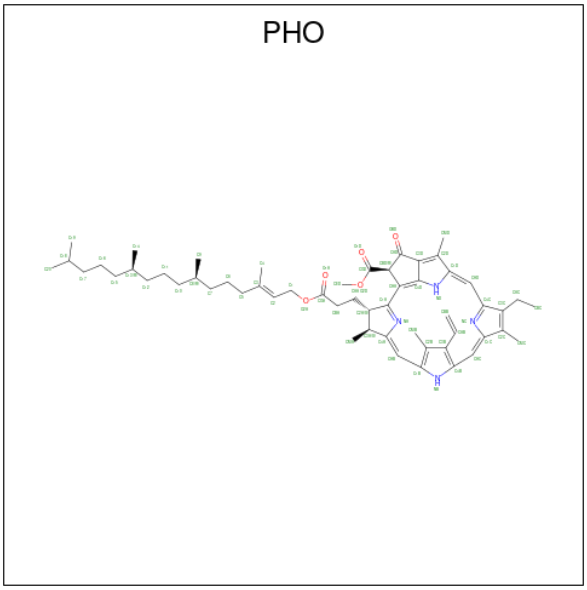
Mol	Chain	Residues	Atoms					AltConf
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	d	1	Total	C	Mg	N	O	0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

- Molecule 29 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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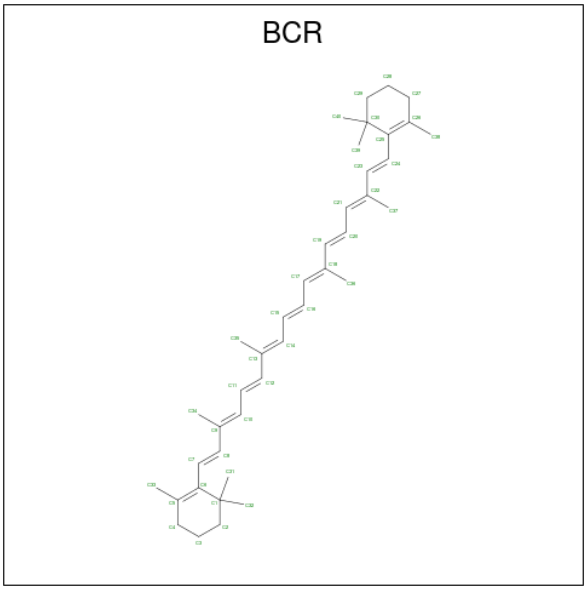
Mol	Chain	Residues	Atoms				AltConf
29	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 30 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	C	0
			40	40	
30	B	1	Total	C	0
			40	40	
30	B	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	C	1	Total	C	0
			40	40	
30	D	1	Total	C	0
			40	40	
30	a	1	Total	C	0
			40	40	
30	b	1	Total	C	0
			40	40	

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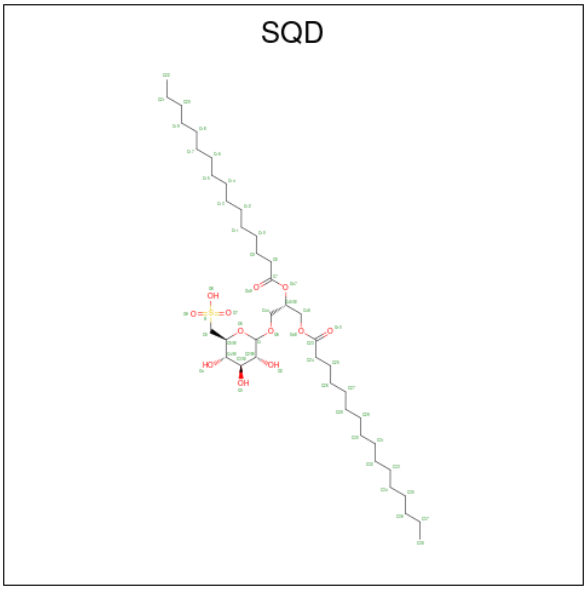
Mol	Chain	Residues	Atoms	AltConf
30	b	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	c	1	Total C 40 40	0
30	d	1	Total C 40 40	0

- Molecule 31 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
31	A	1	Total C O S 51 38 12 1	0
31	B	1	Total C O S 42 29 12 1	0
31	B	1	Total C O S 54 41 12 1	0
31	C	1	Total C O S 54 41 12 1	0
31	M	1	Total C O S 42 29 12 1	0

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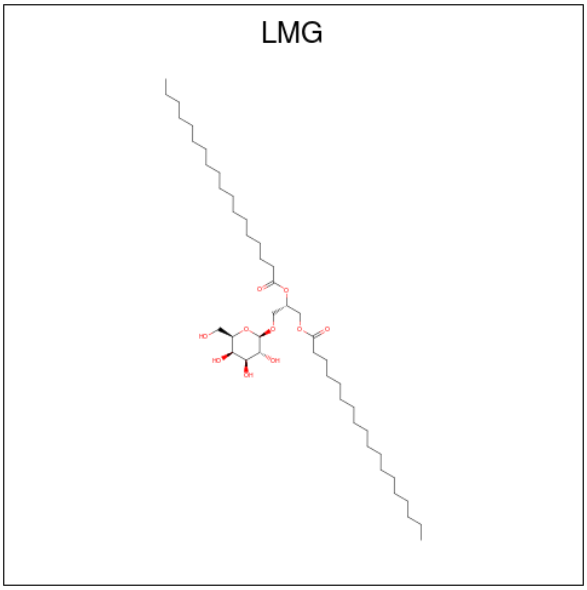
Mol	Chain	Residues	Atoms				AltConf
31	a	1	Total	C	O	S	0
			51	38	12	1	
31	b	1	Total	C	O	S	0
			42	29	12	1	
31	b	1	Total	C	O	S	0
			54	41	12	1	
31	c	1	Total	C	O	S	0
			54	41	12	1	
31	m	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			48	38	10	
32	B	1	Total	C	O	0
			44	34	10	
32	C	1	Total	C	O	0
			51	41	10	
32	C	1	Total	C	O	0
			55	45	10	
32	D	1	Total	C	O	0
			46	36	10	
32	H	1	Total	C	O	0
			48	38	10	

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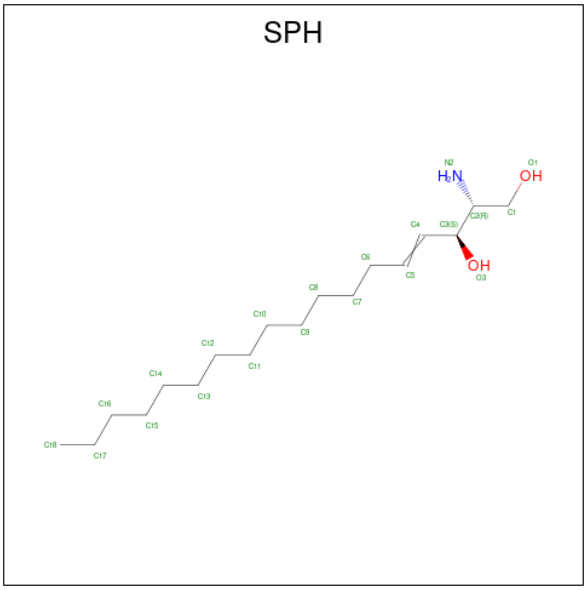
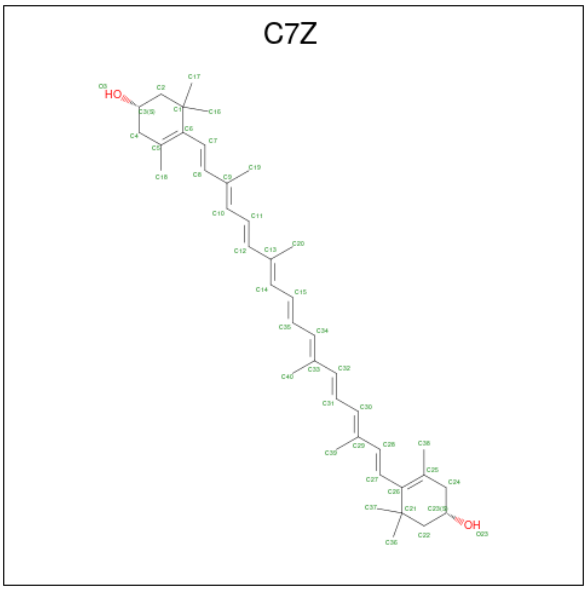
Mol	Chain	Residues	Atoms	AltConf
32	W	1	Total C O 39 29 10	0
32	a	1	Total C O 48 38 10	0
32	b	1	Total C O 44 34 10	0
32	c	1	Total C O 51 41 10	0
32	c	1	Total C O 55 45 10	0
32	d	1	Total C O 46 36 10	0
32	h	1	Total C O 48 38 10	0
32	w	1	Total C O 39 29 10	0

- Molecule 33 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



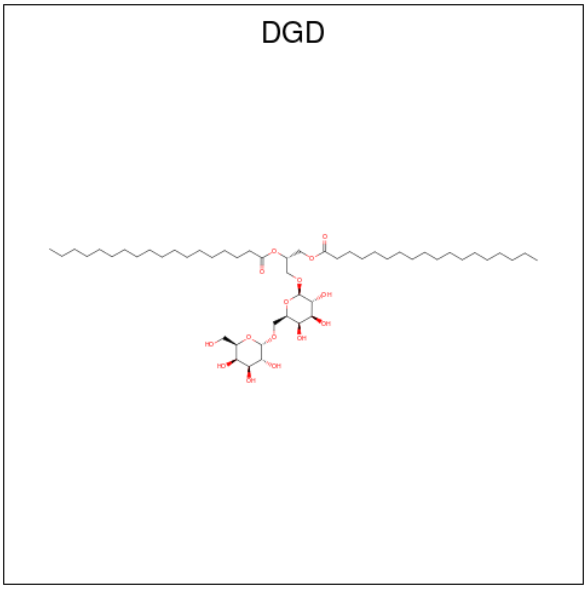
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C N O 21 18 1 2	0
33	Y	1	Total C N O 21 18 1 2	0
33	a	1	Total C N O 21 18 1 2	0

- Molecule 34 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: $C_{40}H_{56}O_2$).



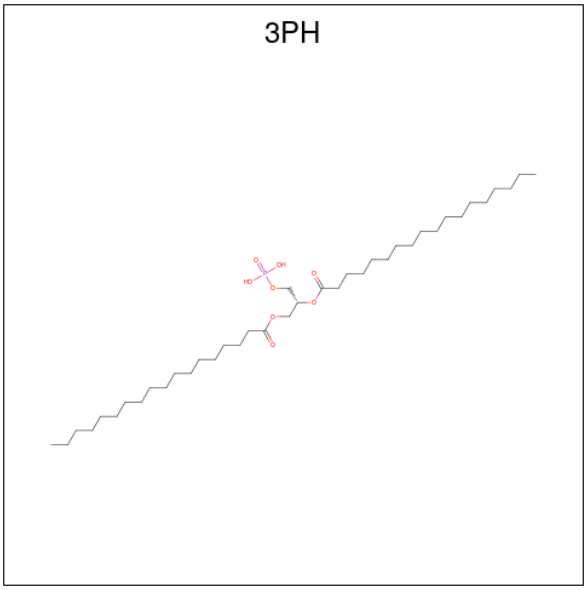
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			42	40	2	
34	b	1	Total	C	O	0
			42	40	2	

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total 43	C 28	O 15	0
35	C	1	Total 55	C 40	O 15	0
35	C	1	Total 62	C 47	O 15	0
35	C	1	Total 59	C 44	O 15	0
35	b	1	Total 43	C 28	O 15	0
35	c	1	Total 55	C 40	O 15	0
35	c	1	Total 62	C 47	O 15	0
35	c	1	Total 59	C 44	O 15	0

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
36	B	1	Total 48	C 39	O 8	P 1	0
36	T	1	Total 48	C 39	O 8	P 1	0
36	S	1	Total 48	C 39	O 8	P 1	0

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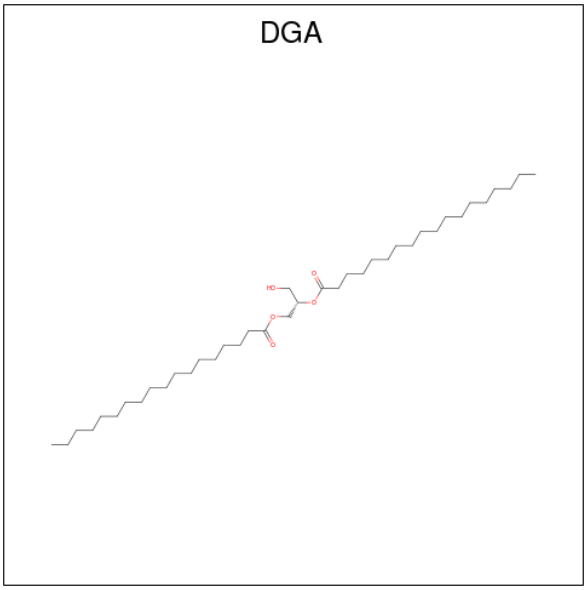
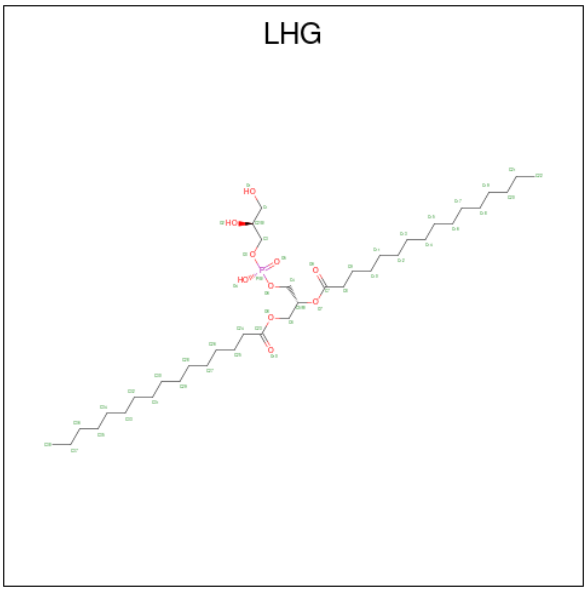
Mol	Chain	Residues	Atoms				AltConf
36	b	1	Total	C	O	P	0
			48	39	8	1	
36	t	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 37 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



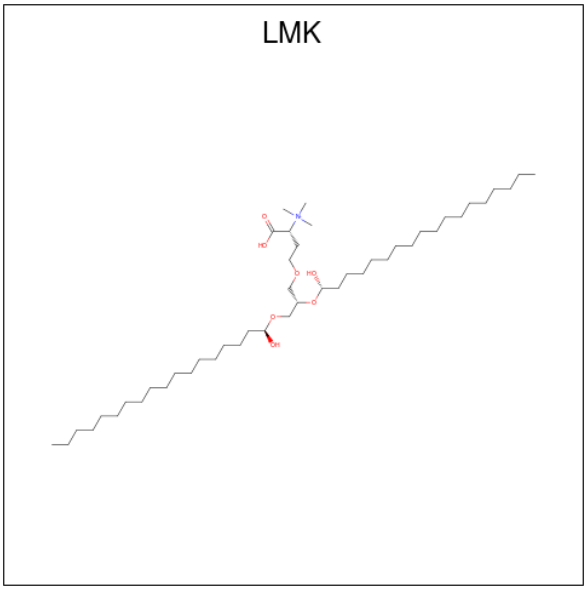
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			44	39	5	
37	C	1	Total	C	O	0
			44	39	5	
37	J	1	Total	C	O	0
			29	24	5	
37	b	1	Total	C	O	0
			44	39	5	
37	c	1	Total	C	O	0
			44	39	5	
37	j	1	Total	C	O	0
			29	24	5	

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



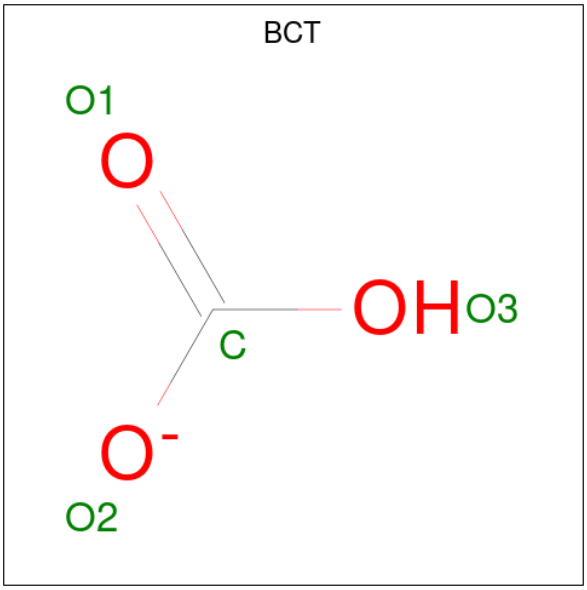
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	C	O	P	0
			47	36	10	1	
38	D	1	Total	C	O	P	0
			44	33	10	1	
38	D	1	Total	C	O	P	0
			49	38	10	1	
38	D	1	Total	C	O	P	0
			39	28	10	1	
38	L	1	Total	C	O	P	0
			49	38	10	1	
38	N	1	Total	C	O	P	0
			49	38	10	1	
38	G	1	Total	C	O	P	0
			49	38	10	1	
38	S	1	Total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

- Molecule 39 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: $C_{46}H_{94}NO_7$).



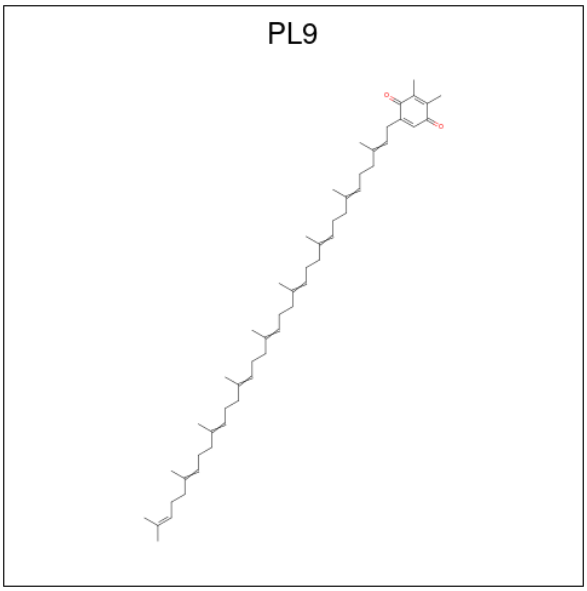
Mol	Chain	Residues	Atoms				AltConf
39	C	1	Total	C	N	O	0
			40	32	1	7	
39	c	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 40 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



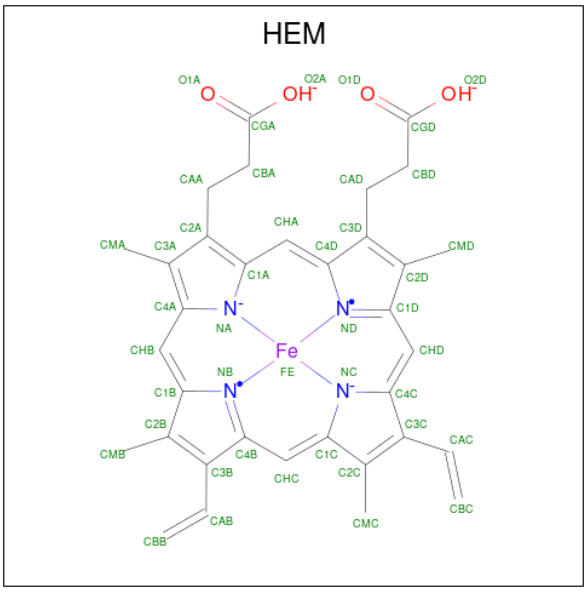
Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			4	1	3	
40	d	1	Total	C	O	0
			4	1	3	

- Molecule 41 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: $C_{53}H_{80}O_2$).



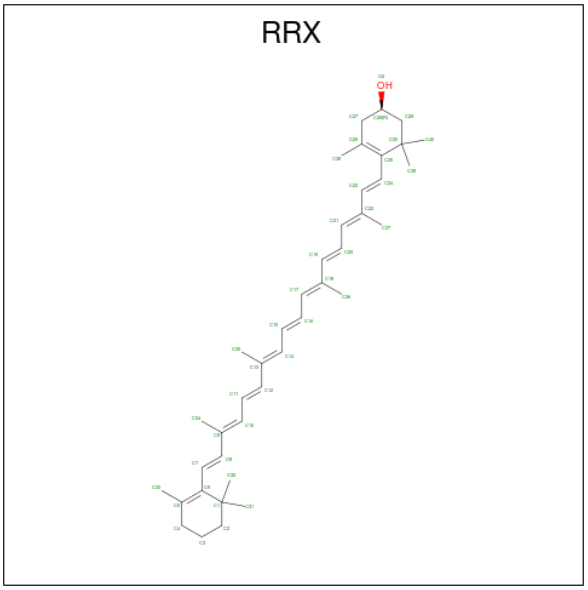
Mol	Chain	Residues	Atoms			AltConf
41	D	1	Total	C	O	0
			55	53	2	
41	d	1	Total	C	O	0
			55	53	2	

- Molecule 42 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



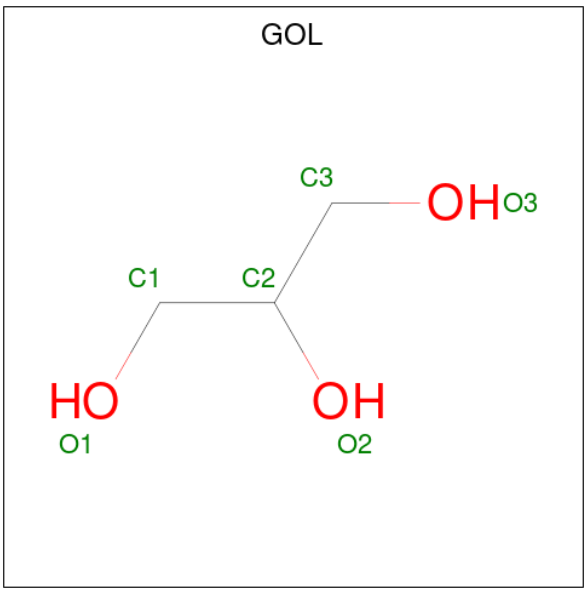
Mol	Chain	Residues	Atoms					AltConf
42	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
42	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 43 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



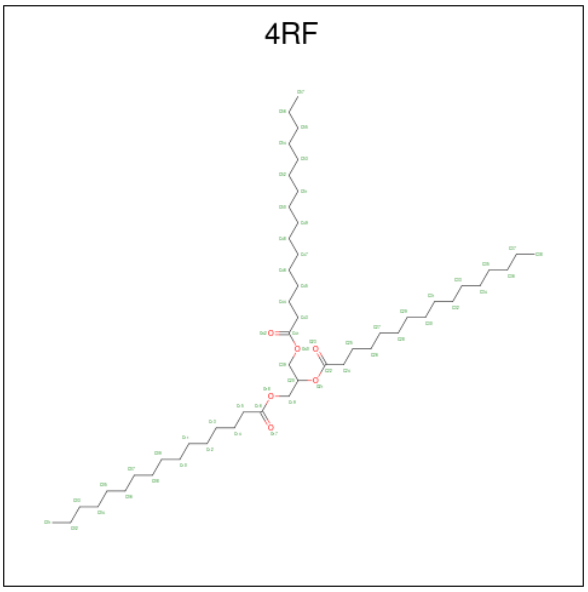
Mol	Chain	Residues	Atoms			AltConf
43	H	1	Total	C	O	0
			41	40	1	
43	h	1	Total	C	O	0
			41	40	1	

- Molecule 44 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			AltConf
44	I	1	Total	C	O	0
			6	3	3	

- Molecule 45 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



Mol	Chain	Residues	Atoms			AltConf
45	I	1	Total	C	O	0
			57	51	6	
45	K	1	Total	C	O	0
			57	51	6	

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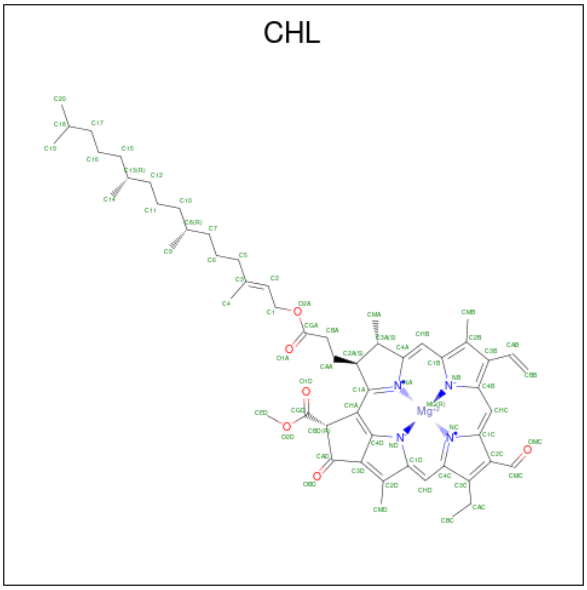
Mol	Chain	Residues	Atoms	AltConf
45	i	1	Total C O 57 51 6	0
45	k	1	Total C O 57 51 6	0

- Molecule 46 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
46	N	1	Total C Mg N O 66 55 1 4 6	0
46	N	1	Total C Mg N O 66 55 1 4 6	0
46	N	1	Total C Mg N O 66 55 1 4 6	0
46	N	1	Total C Mg N O 66 55 1 4 6	0
46	N	1	Total C Mg N O 50 39 1 4 6	0
46	N	1	Total C Mg N O 66 55 1 4 6	0
46	G	1	Total C Mg N O 66 55 1 4 6	0
46	G	1	Total C Mg N O 48 37 1 4 6	0
46	G	1	Total C Mg N O 50 39 1 4 6	0

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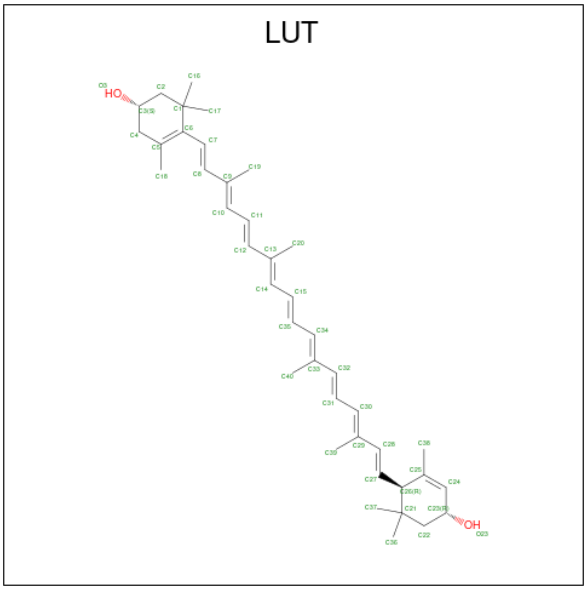
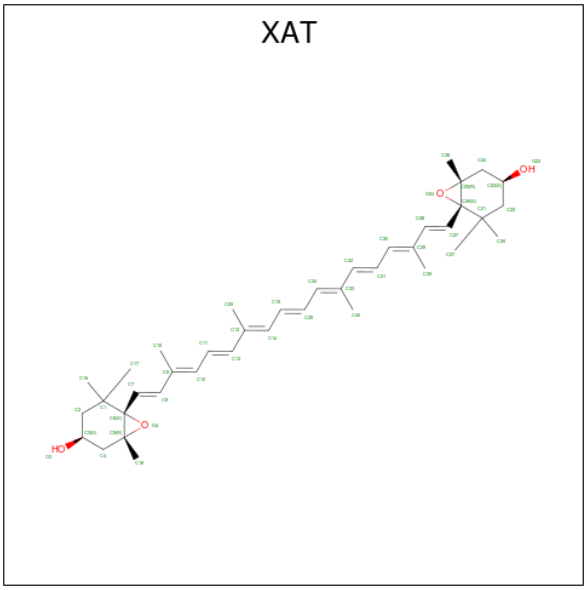
Mol	Chain	Residues	Atoms					AltConf
46	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
46	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
46	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
46	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
46	S	1	Total	C	Mg	N	O	0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

- Molecule 47 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



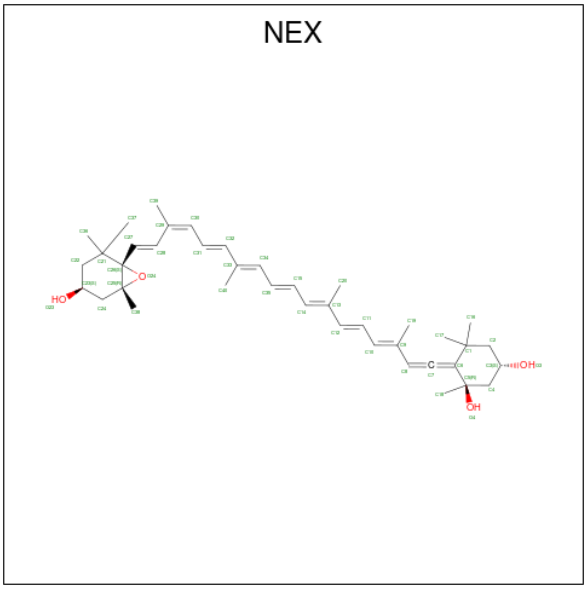
Mol	Chain	Residues	Atoms	AltConf
47	N	1	Total C O 42 40 2	0
47	N	1	Total C O 42 40 2	0
47	G	1	Total C O 42 40 2	0
47	G	1	Total C O 42 40 2	0
47	S	1	Total C O 42 40 2	0
47	S	1	Total C O 42 40 2	0
47	Y	1	Total C O 42 40 2	0
47	Y	1	Total C O 42 40 2	0

- Molecule 48 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: $C_{40}H_{56}O_4$).



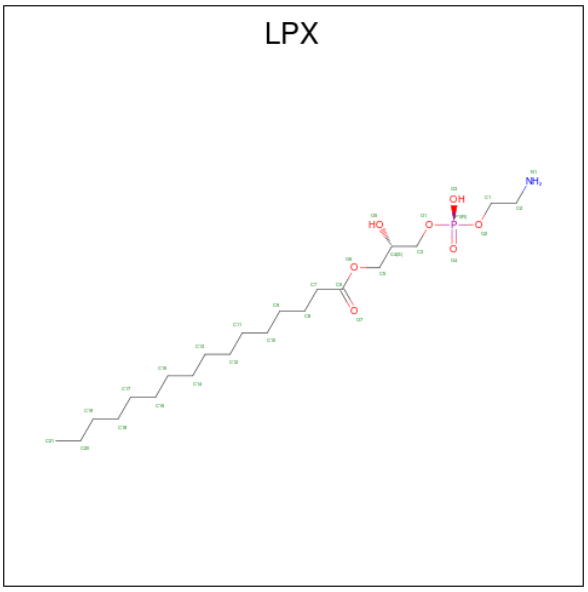
Mol	Chain	Residues	Atoms	AltConf
48	N	1	Total C O 44 40 4	0
48	G	1	Total C O 44 40 4	0
48	Y	1	Total C O 44 40 4	0

- Molecule 49 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: $C_{40}H_{56}O_4$).



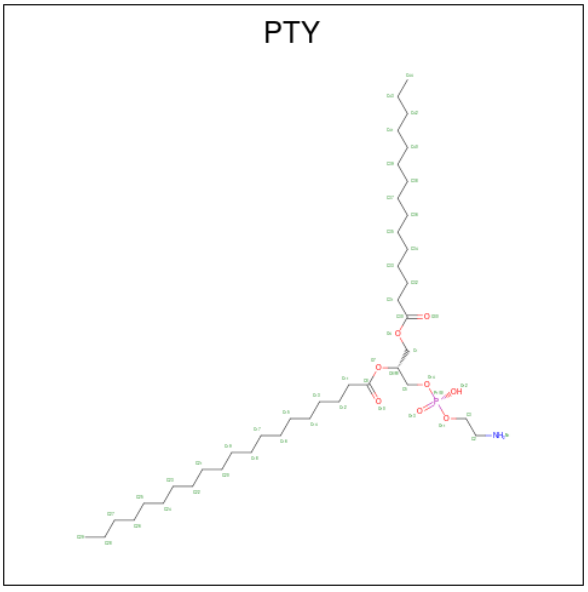
Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	S	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	

- Molecule 50 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
50	S	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



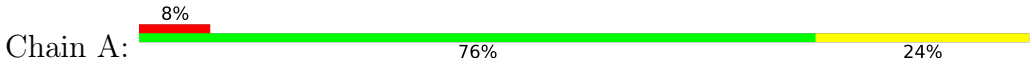
Mol	Chain	Residues	Atoms					AltConf
51	Y	1	Total	C	N	O	P	0
			50	40	1	8	1	
51	Y	1	Total	C	N	O	P	0
			19	9	1	8	1	

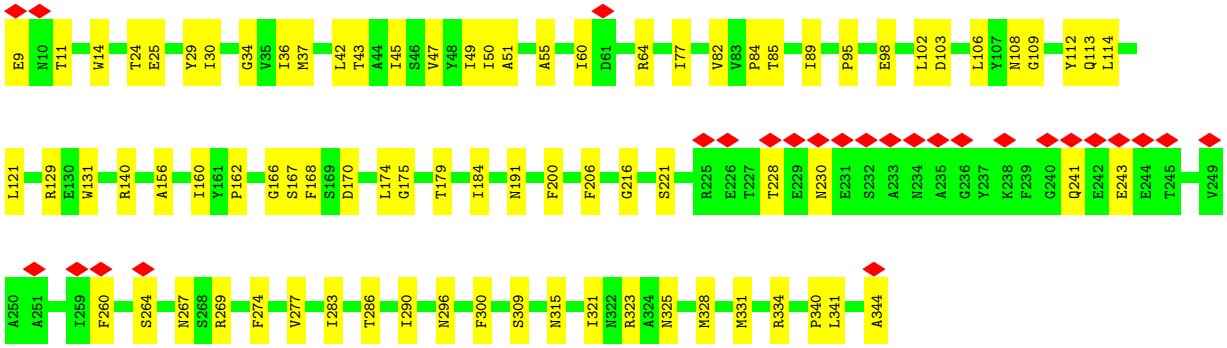
3 Residue-property plots (i)

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

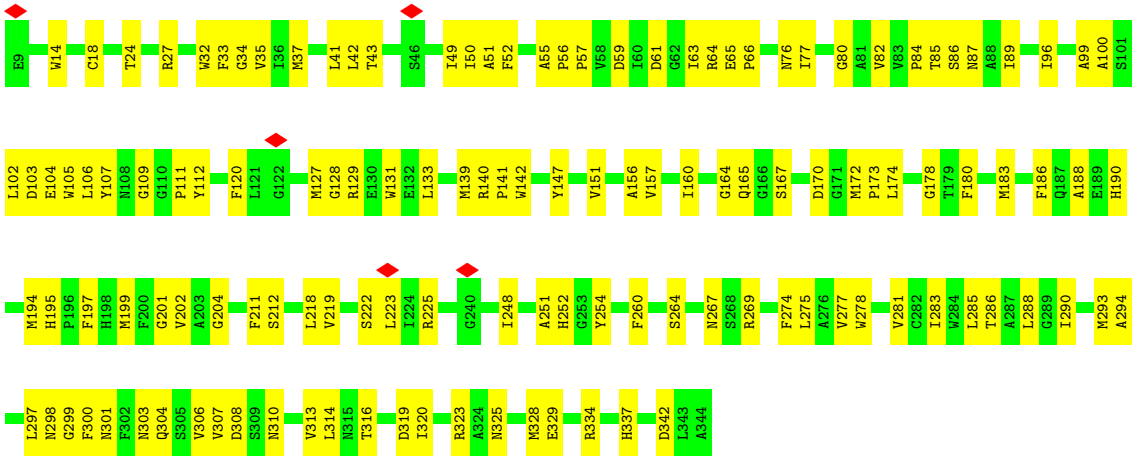
Chain A:





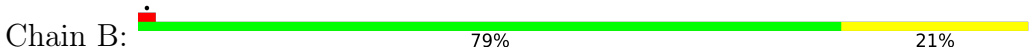
• Molecule 1: Photosystem II protein D1

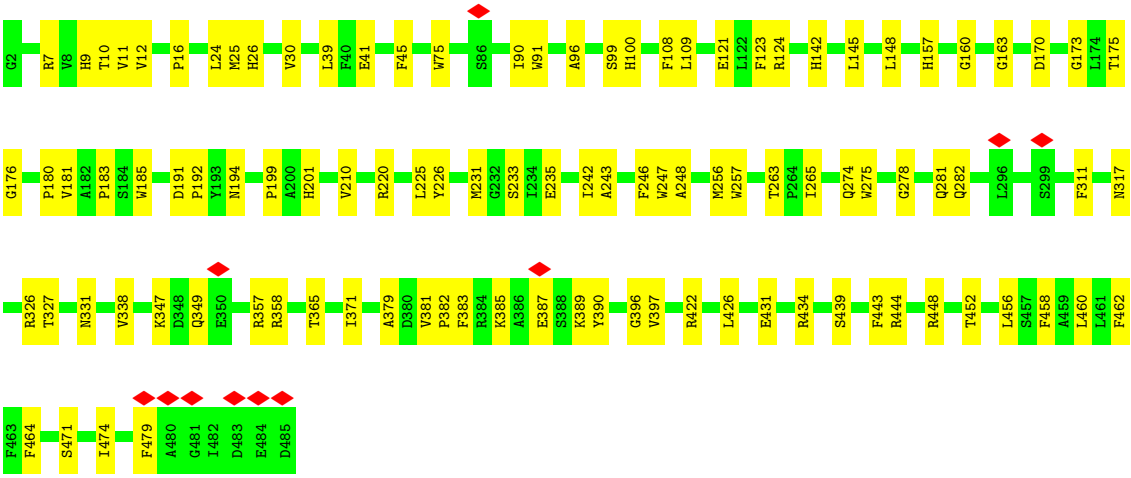
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

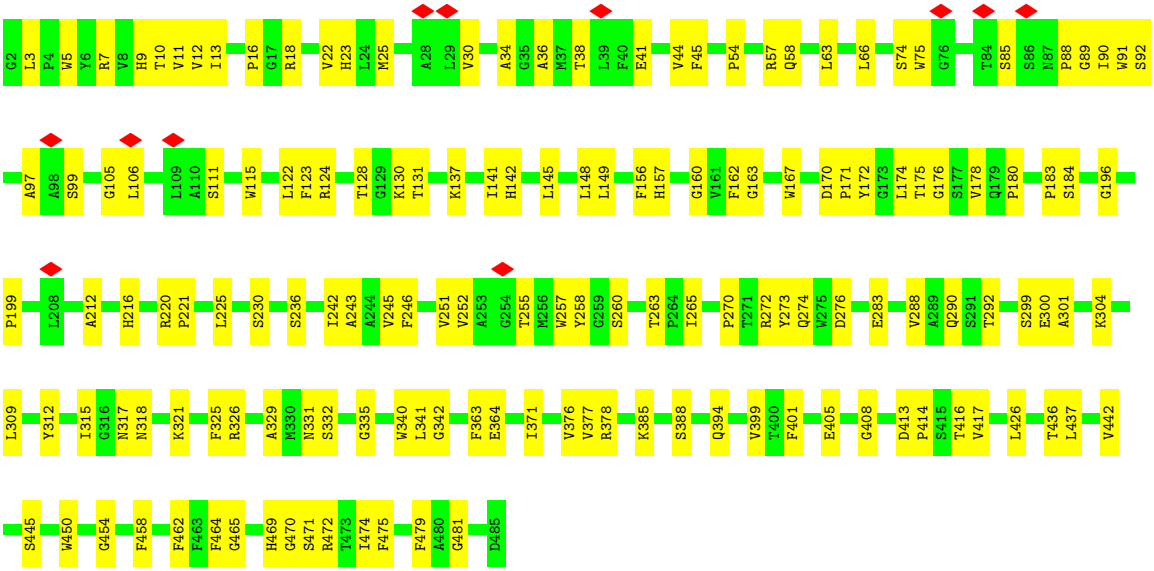
Chain B:





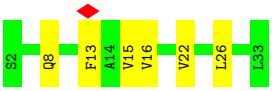
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:

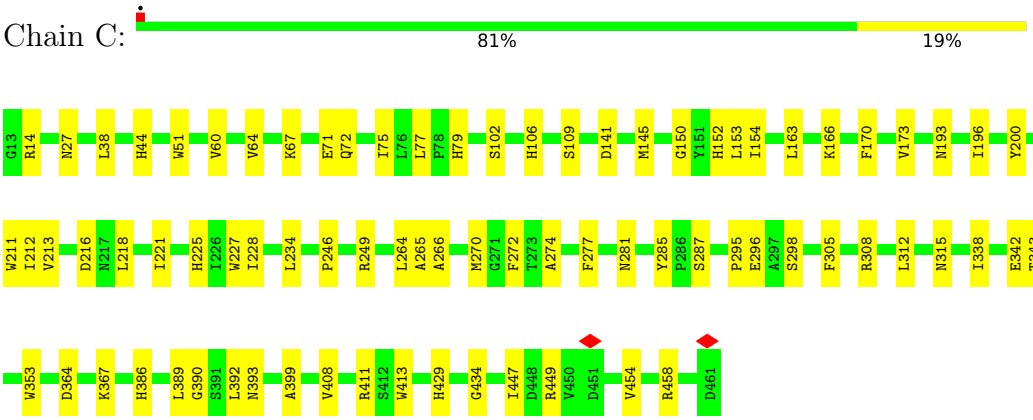


• Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:

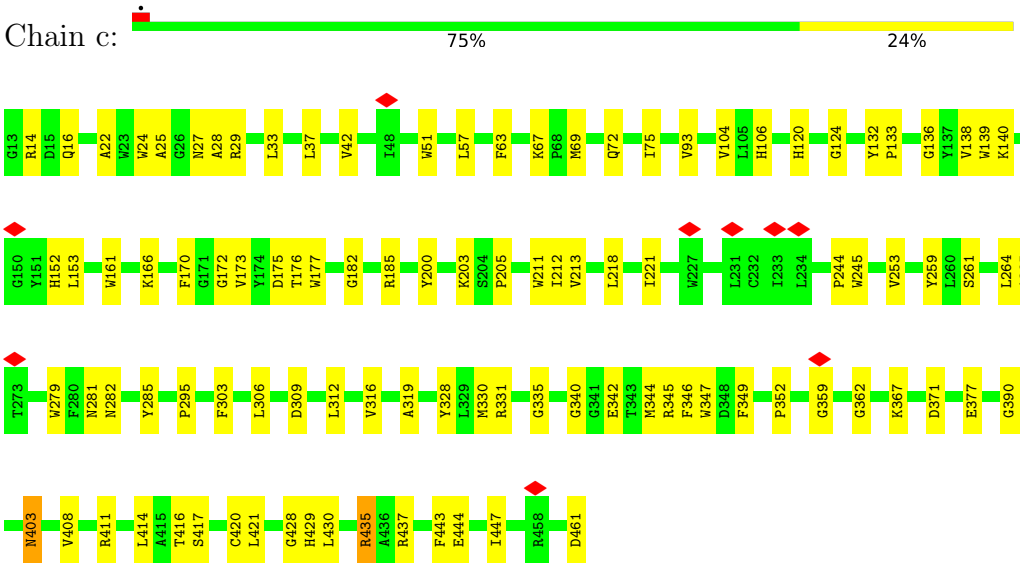
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C:



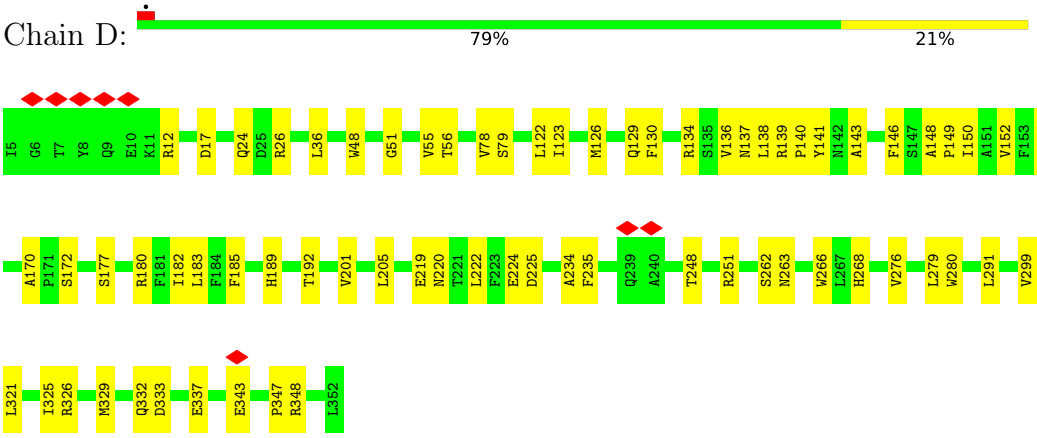
• Molecule 4: Photosystem II CP43 reaction center protein

Chain c:



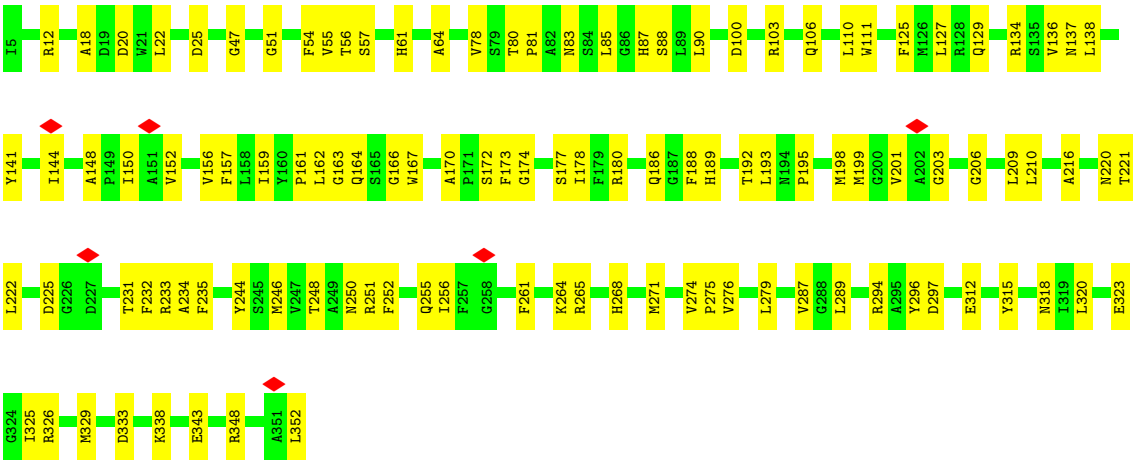
• Molecule 5: Photosystem II D2 protein

Chain D:



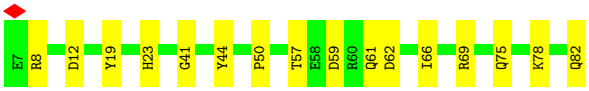
• Molecule 5: Photosystem II D2 protein

Chain d:



• Molecule 6: Cytochrome b559 subunit alpha

Chain E:



• Molecule 6: Cytochrome b559 subunit alpha

Chain e:

• Molecule 7: Cytochrome b559 subunit beta

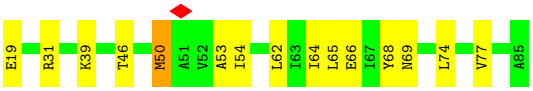
Chain F:

• Molecule 7: Cytochrome b559 subunit beta

Chain f:

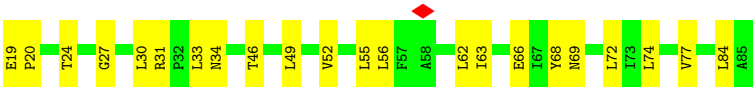
• Molecule 8: Photosystem II reaction center protein H

Chain H:



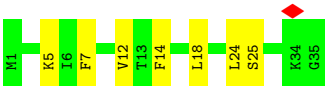
• Molecule 8: Photosystem II reaction center protein H

Chain h:



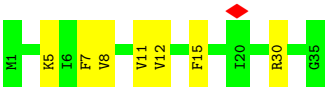
• Molecule 9: Photosystem II reaction center protein I

Chain I:



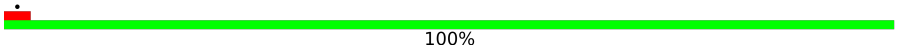
• Molecule 9: Photosystem II reaction center protein I

Chain i:



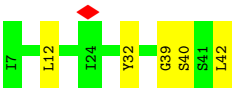
• Molecule 10: Photosystem II reaction center protein J

Chain J:



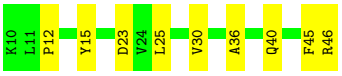
• Molecule 10: Photosystem II reaction center protein J

Chain j:



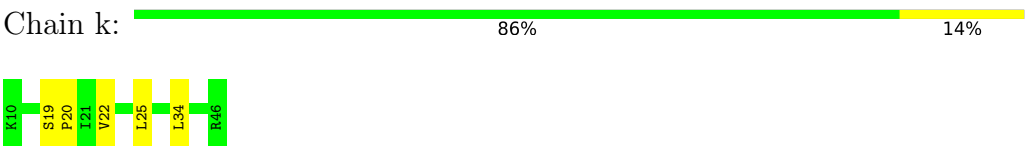
• Molecule 11: Photosystem II reaction center protein K

Chain K:



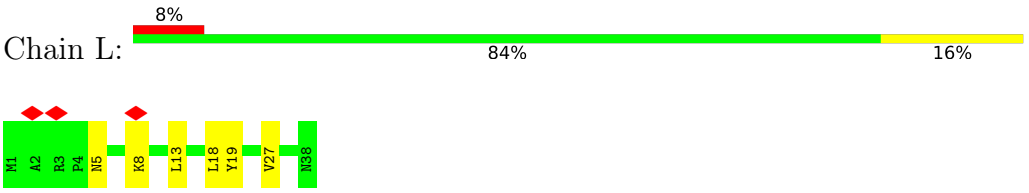
• Molecule 11: Photosystem II reaction center protein K

Chain k:



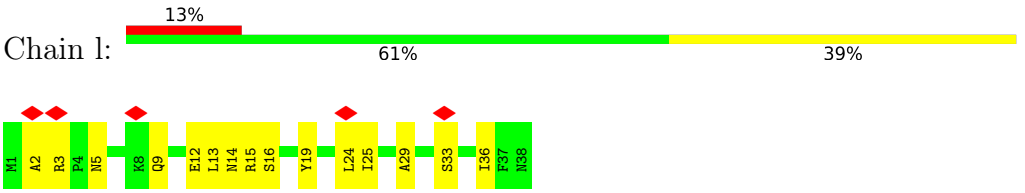
• Molecule 12: Photosystem II reaction center protein L

Chain L:



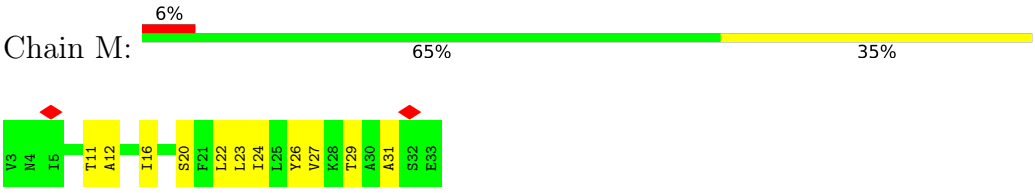
• Molecule 12: Photosystem II reaction center protein L

Chain l:



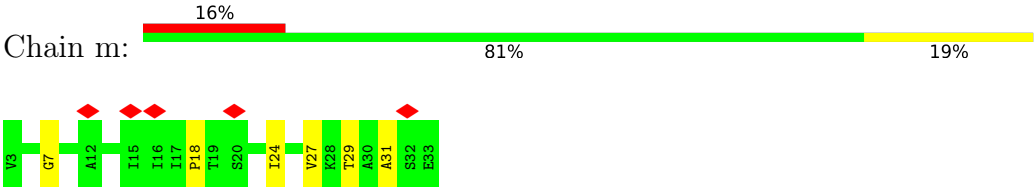
• Molecule 13: Photosystem II reaction center protein M

Chain M:



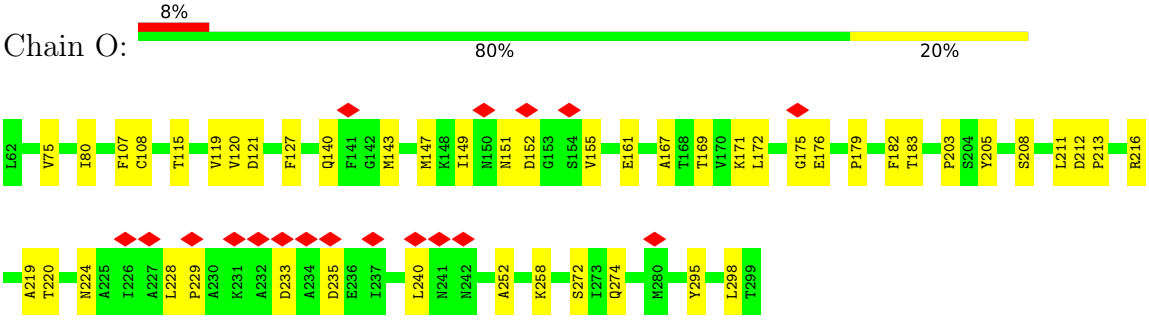
• Molecule 13: Photosystem II reaction center protein M

Chain m:



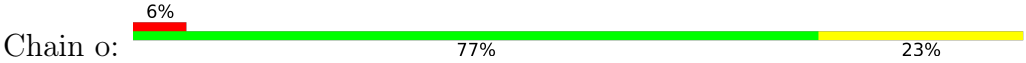
• Molecule 14: PsbO

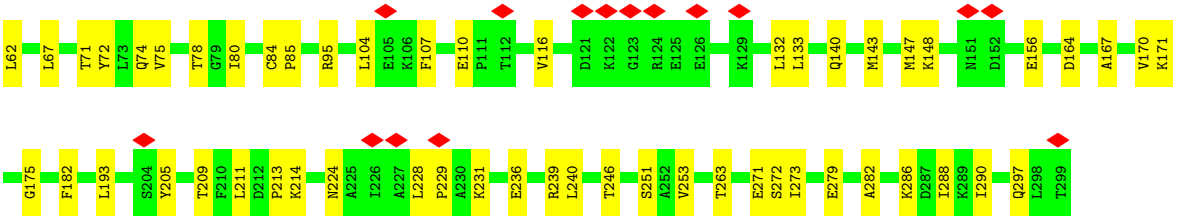
Chain O:



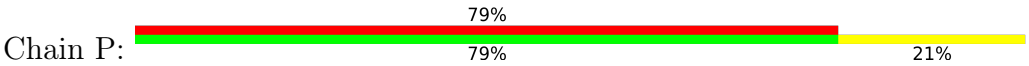
• Molecule 14: PsbO

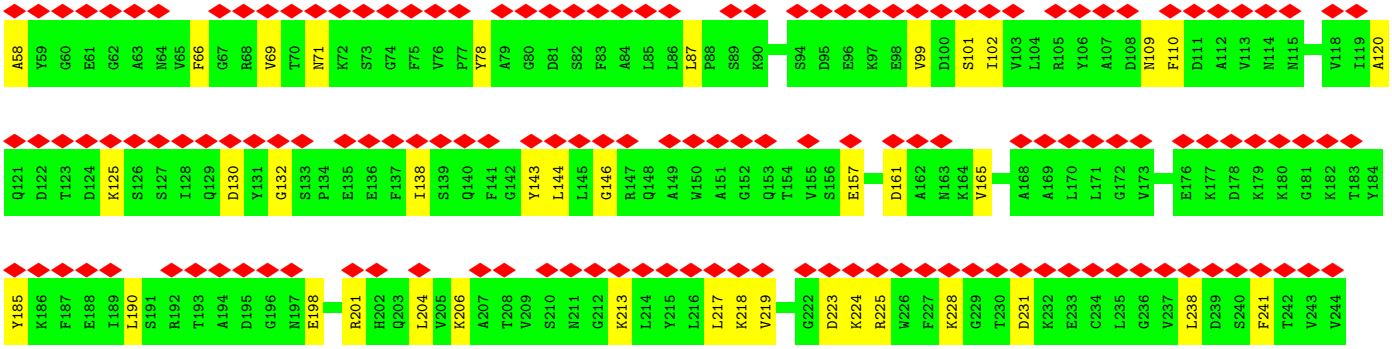
Chain o:



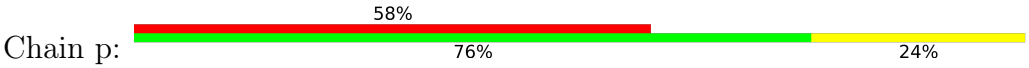


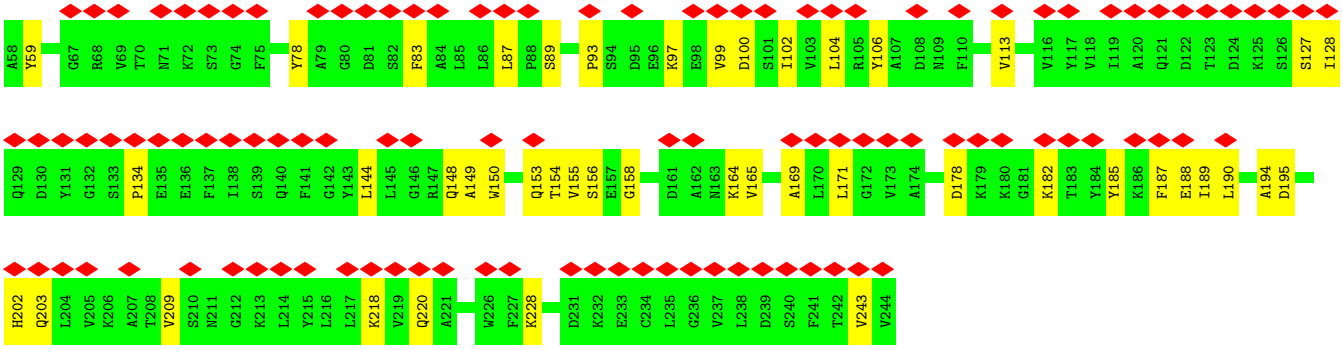
• Molecule 15: PsbP



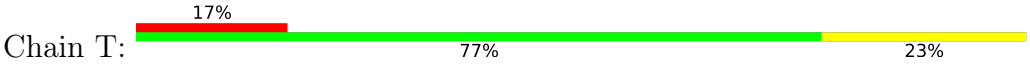


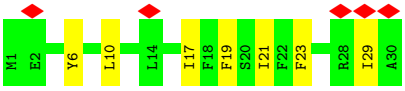
• Molecule 15: PsbP



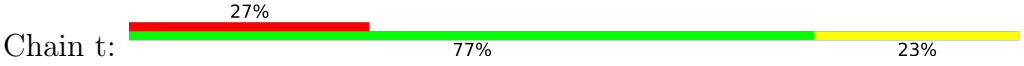


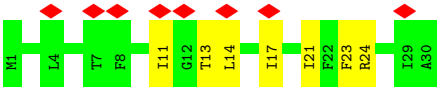
• Molecule 16: Photosystem II reaction center protein T



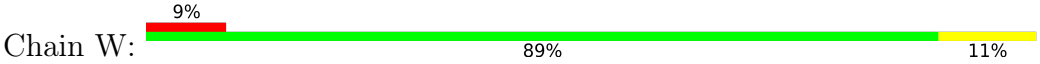


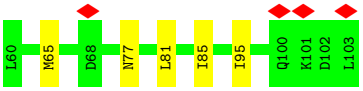
• Molecule 16: Photosystem II reaction center protein T



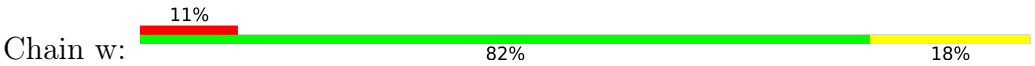


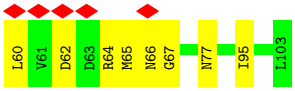
• Molecule 17: PsbW



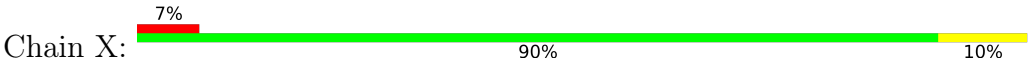


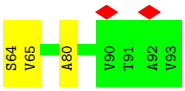
• Molecule 17: PsbW



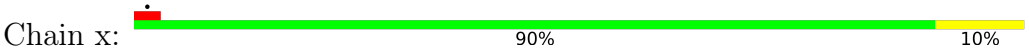


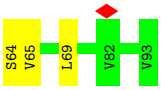
• Molecule 18: PsbX



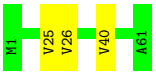


• Molecule 18: PsbX

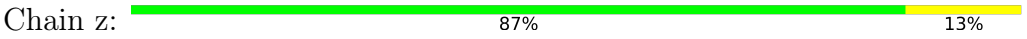


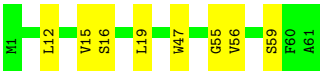


• Molecule 19: Photosystem II reaction center protein Z

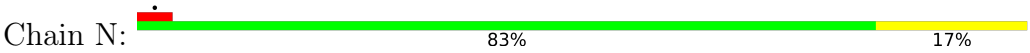


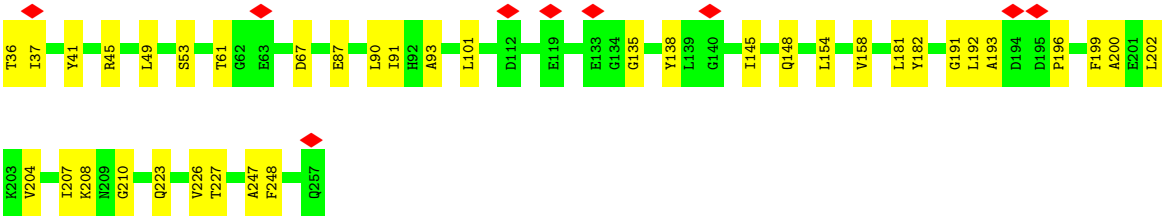
• Molecule 19: Photosystem II reaction center protein Z



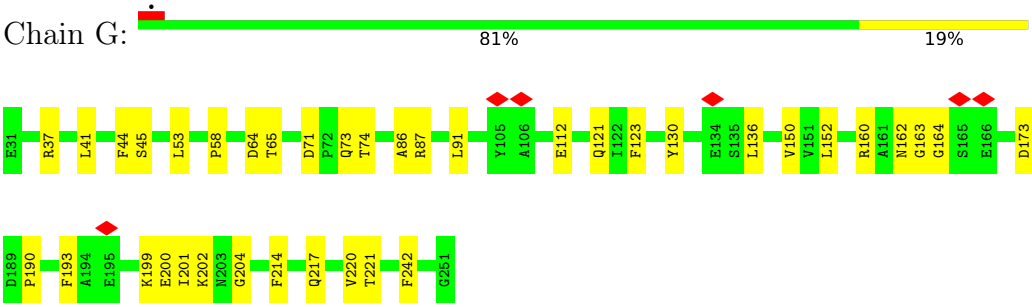


• Molecule 20: Chlorophyll a-b binding protein of LHCII type I, chloroplastic

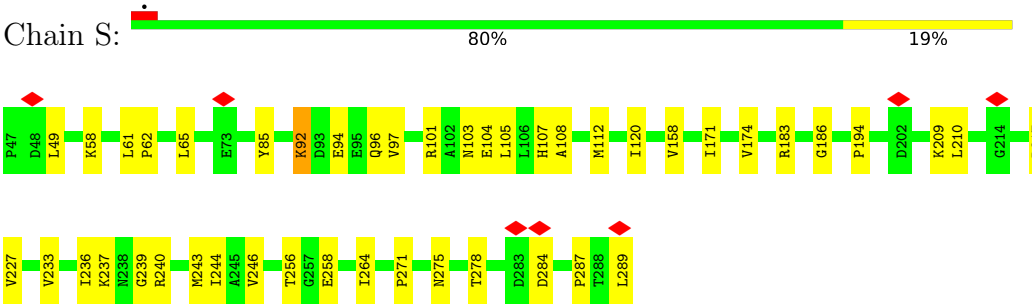




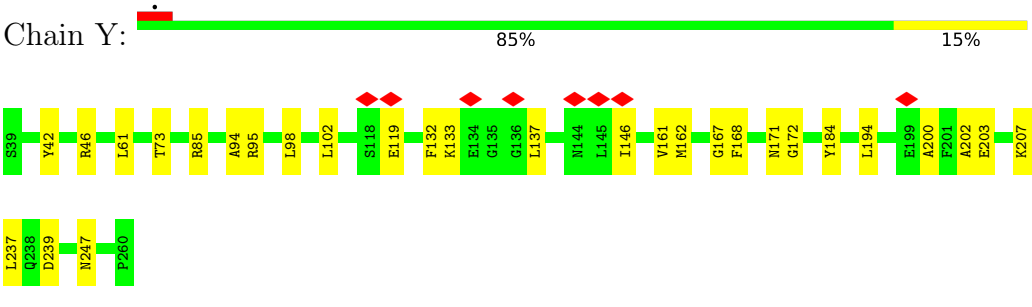
• Molecule 21: Chlorophyll a-b binding protein, chloroplastic



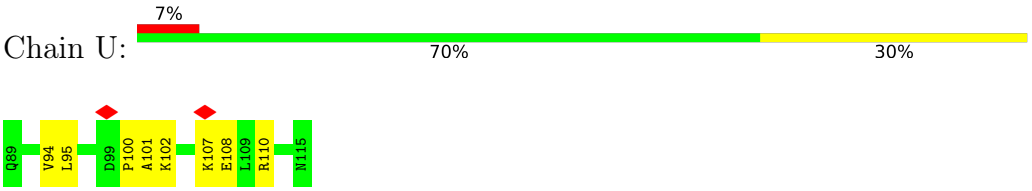
• Molecule 22: CP26



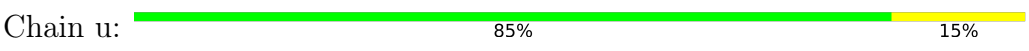
• Molecule 23: LHCII M1

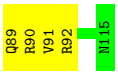


• Molecule 24: PsbU



• Molecule 24: PsbU




Q89
R90
V91
R92
N115

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21066	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	22.262	Depositor
Minimum map value	-13.270	Depositor
Average map value	0.035	Depositor
Map value standard deviation	1.121	Depositor
Recommended contour level	3.5	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: C7Z, OEX, CHL, PL9, LMK, RRX, DGA, GOL, LMG, HEM, LUT, BCR, SPH, 4RF, CLA, SQD, XAT, LHG, NEX, FE2, 3PH, DGD, BCT, PTY, CSD, LPX, CL, PHO

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	0.20	0/2723	0.44	0/3715
1	a	0.24	0/2723	0.58	1/3715 (0.0%)
2	B	0.16	0/3906	0.41	0/5319
2	b	0.18	0/3906	0.45	0/5319
3	V	0.16	0/228	0.40	0/311
3	v	0.19	0/228	0.56	0/311
4	C	0.17	0/3602	0.38	0/4913
4	c	0.19	0/3602	0.45	0/4913
5	D	0.18	0/2860	0.44	0/3899
5	d	0.21	0/2860	0.52	0/3899
6	E	0.17	0/639	0.46	0/870
6	e	0.19	0/639	0.44	0/870
7	F	0.17	0/259	0.36	0/351
7	f	0.23	0/259	0.66	1/351 (0.3%)
8	H	0.22	0/513	0.54	1/703 (0.1%)
8	h	0.22	0/513	0.53	0/703
9	I	0.20	0/287	0.51	0/386
9	i	0.25	0/287	0.54	0/386
10	J	0.13	0/272	0.32	0/369
10	j	0.14	0/272	0.38	0/369
11	K	0.24	0/308	0.53	0/423
11	k	0.29	0/308	0.61	0/423
12	L	0.15	0/321	0.35	0/435
12	l	0.23	0/321	0.47	0/435
13	M	0.26	0/237	0.59	0/323
13	m	0.25	0/237	0.60	0/323
14	O	0.17	0/1857	0.50	1/2508 (0.0%)
14	o	0.17	0/1857	0.45	0/2508
15	P	0.15	0/1473	0.44	1/1988 (0.1%)
15	p	0.15	0/1473	0.48	1/1988 (0.1%)
16	T	0.21	0/254	0.58	0/342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	t	0.16	0/254	0.42	0/342
17	W	0.20	0/339	0.53	0/460
17	w	0.18	0/339	0.51	0/460
18	X	0.18	0/202	0.45	0/276
18	x	0.20	0/202	0.49	0/276
19	Z	0.14	0/469	0.35	0/641
19	z	0.22	0/469	0.49	0/641
20	N	0.18	0/1751	0.46	0/2386
21	G	0.17	0/1725	0.44	0/2348
22	S	0.18	0/1903	0.50	0/2590
23	Y	0.15	0/1719	0.35	0/2343
24	U	0.19	0/224	0.51	0/298
24	u	0.17	0/224	0.43	0/298
All	All	0.19	0/49044	0.46	6/66727 (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
4	c	0	1
5	d	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	199	MET	CB-CG-SD	6.32	131.66	112.70
15	p	155	VAL	N-CA-C	-6.30	106.99	113.10
7	f	39	MET	CB-CG-SD	-6.16	94.23	112.70
8	H	50	MET	CB-CG-SD	-6.05	94.54	112.70
14	O	120	VAL	N-CA-C	-5.59	107.83	113.47
15	P	161	ASP	CB-CA-C	-5.15	110.22	117.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	c	435	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	d	136	VAL	Peptide

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	70	0
1	a	2638	0	2541	118	0
2	B	3785	0	3663	80	0
2	b	3785	0	3663	116	0
3	V	227	0	261	6	0
3	v	227	0	261	6	0
4	C	3483	0	3376	70	0
4	c	3483	0	3376	95	0
5	D	2766	0	2655	66	0
5	d	2766	0	2655	101	0
6	E	621	0	605	12	0
6	e	621	0	605	19	0
7	F	252	0	265	9	0
7	f	252	0	265	10	0
8	H	503	0	532	16	0
8	h	503	0	532	18	0
9	I	279	0	288	7	0
9	i	279	0	288	6	0
10	J	266	0	286	0	0
10	j	266	0	286	6	0
11	K	297	0	312	8	0
11	k	297	0	312	5	0
12	L	313	0	325	7	0
12	l	313	0	325	15	0
13	M	234	0	258	11	0
13	m	234	0	258	8	0
14	O	1822	0	1789	29	0
14	o	1822	0	1789	35	0
15	P	1444	0	1403	30	0
15	p	1444	0	1403	29	0
16	T	247	0	260	7	0
16	t	247	0	260	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	W	332	0	323	4	0
17	w	332	0	323	6	0
18	X	201	0	224	2	0
18	x	201	0	224	2	0
19	Z	457	0	478	3	0
19	z	457	0	478	5	0
20	N	1703	0	1641	26	0
21	G	1680	0	1614	34	0
22	S	1856	0	1816	33	0
23	Y	1670	0	1622	23	0
24	U	224	0	226	7	0
24	u	224	0	226	3	0
25	A	10	0	0	1	0
25	a	10	0	0	0	0
26	A	1	0	0	0	0
26	a	1	0	0	0	0
27	A	2	0	0	1	0
27	a	2	0	0	0	0
28	A	240	0	240	16	0
28	B	1040	0	1149	65	0
28	C	845	0	932	43	0
28	D	130	0	144	12	0
28	G	466	0	468	19	0
28	N	468	0	468	15	0
28	S	625	0	586	18	0
28	Y	570	0	613	34	0
28	a	239	0	239	18	0
28	b	1040	0	1148	67	0
28	c	845	0	926	58	0
28	d	130	0	143	10	0
29	A	128	0	148	8	0
29	a	128	0	148	14	0
30	A	40	0	53	3	0
30	B	80	0	106	5	0
30	C	160	0	211	17	0
30	D	40	0	53	1	0
30	a	40	0	53	6	0
30	b	80	0	106	8	0
30	c	160	0	211	19	0
30	d	40	0	53	3	0
31	A	51	0	68	3	0
31	B	96	0	124	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	C	54	0	77	2	0
31	M	42	0	47	1	0
31	a	51	0	68	4	0
31	b	96	0	124	10	0
31	c	54	0	77	2	0
31	m	42	0	47	1	0
32	A	48	0	66	6	0
32	B	44	0	58	6	0
32	C	106	0	158	6	0
32	D	46	0	62	1	0
32	H	48	0	66	8	0
32	W	39	0	48	2	0
32	a	48	0	66	4	0
32	b	44	0	58	3	0
32	c	106	0	158	2	0
32	d	46	0	62	5	0
32	h	48	0	66	7	0
32	w	39	0	48	0	0
33	A	21	0	37	2	0
33	Y	21	0	37	2	0
33	a	21	0	37	2	0
34	B	42	0	0	0	0
34	b	42	0	0	0	0
35	B	43	0	44	1	0
35	C	176	0	226	14	0
35	b	43	0	44	2	0
35	c	176	0	226	20	0
36	B	48	0	75	1	0
36	S	48	0	75	4	0
36	T	48	0	75	1	0
36	b	48	0	75	2	0
36	t	48	0	75	2	0
37	B	44	0	76	4	0
37	C	44	0	76	3	0
37	J	29	0	40	1	0
37	b	44	0	76	4	0
37	c	44	0	76	2	0
37	j	29	0	40	3	0
38	C	47	0	67	5	0
38	D	132	0	183	14	0
38	G	49	0	74	4	0
38	L	49	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	N	49	0	74	4	0
38	S	45	0	63	4	0
38	Y	49	0	74	6	0
38	c	47	0	67	4	0
38	d	132	0	183	13	0
38	l	49	0	74	3	0
39	C	40	0	0	0	0
39	c	40	0	0	0	0
40	D	4	0	1	0	0
40	d	4	0	1	0	0
41	D	55	0	80	3	0
41	d	55	0	80	9	0
42	F	43	0	30	2	0
42	f	43	0	30	1	0
43	H	41	0	56	3	0
43	h	41	0	56	4	0
44	I	6	0	8	0	0
45	I	57	0	98	4	0
45	K	57	0	98	3	0
45	i	57	0	98	3	0
45	k	57	0	98	2	0
46	G	340	0	305	21	0
46	N	380	0	382	23	0
46	S	194	0	144	7	0
46	Y	310	0	306	14	0
47	G	84	0	110	5	0
47	N	84	0	110	9	0
47	S	84	0	110	8	0
47	Y	84	0	110	7	0
48	G	44	0	56	7	0
48	N	44	0	56	1	0
48	Y	44	0	56	3	0
49	G	44	0	54	2	0
49	N	44	0	54	3	0
49	S	44	0	54	1	0
49	Y	44	0	54	2	0
50	S	30	0	43	1	0
51	Y	69	0	90	7	0
All	All	60673	0	61750	1404	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 11.

All (1404) 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)
4:c:153:LEU:HD21	28:c:506:CLA:HAB	1.53	0.91
1:a:141:PRO:HD2	4:c:435:ARG:HH22	1.42	0.82
1:A:328:MET:HG3	5:D:325:ILE:HD11	1.61	0.82
8:h:56:LEU:HB3	43:h:101:RRX:H31	1.63	0.80
22:S:246:VAL:HG11	47:S:621:LUT:H12	1.62	0.80
4:C:153:LEU:HD21	28:C:506:CLA:HAB	1.64	0.79
14:O:182:PHE:HA	14:O:274:GLN:HE22	1.48	0.77
12:L:13:LEU:H	13:M:29:THR:HG21	1.51	0.75
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.67	0.75
4:c:104:VAL:HG22	30:c:517:BCR:HC42	1.66	0.75
5:D:152:VAL:HG21	5:D:279:LEU:HD12	1.69	0.74
2:B:282:GLN:HE21	24:U:107:LYS:HD2	1.52	0.72
5:d:188:PHE:HA	5:d:326:ARG:HD3	1.71	0.72
14:o:209:THR:HG21	15:p:195:ASP:HB3	1.71	0.72
32:A:413:LMG:H392	35:C:518:DGD:HB92	1.71	0.72
28:B:608:CLA:HBB1	32:B:622:LMG:H182	1.72	0.72
35:C:519:DGD:HB72	32:C:521:LMG:H401	1.72	0.72
4:c:175:ASP:O	4:c:182:GLY:HA2	1.89	0.71
1:a:194:MET:HB3	1:a:300:PHE:HB2	1.72	0.71
1:a:325:ASN:HB3	4:c:400:THR:HG22	1.71	0.70
4:c:138:VAL:HG23	4:c:140:LYS:H	1.56	0.70
2:B:25:MET:HE3	30:B:618:BCR:H23C	1.74	0.70
28:b:602:CLA:H162	43:h:101:RRX:H42	1.74	0.69
4:c:172:GLY:HA3	4:c:185:ARG:O	1.91	0.69
28:Y:614:CLA:H2	51:Y:626:PTY:H372	1.73	0.69
20:N:93:ALA:HB1	20:N:210:GLY:HA3	1.75	0.69
1:a:165:GLN:NE2	1:a:294:ALA:O	2.25	0.69
23:Y:167:GLY:O	23:Y:171:ASN:ND2	2.26	0.68
1:a:18:CYS:SG	9:i:30:ARG:NH2	2.66	0.68
4:C:264:LEU:HD21	28:C:508:CLA:HAB	1.75	0.68
32:A:413:LMG:H402	35:C:518:DGD:HBT2	1.75	0.68
5:D:126:MET:HG3	5:D:143:ALA:HB1	1.76	0.68
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.76	0.67
2:B:278:GLY:O	2:B:282:GLN:HB2	1.94	0.67
2:b:474:ILE:O	5:d:134:ARG:NH2	2.28	0.67
28:c:511:CLA:HBA1	30:c:517:BCR:H282	1.74	0.67
13:M:24:ILE:HG23	13:m:27:VAL:HG11	1.77	0.67
15:p:144:LEU:O	15:p:218:LYS:NZ	2.28	0.67
28:Y:602:CLA:H52	47:Y:621:LUT:H28	1.75	0.67
37:B:625:DGA:HBV2	37:B:625:DGA:HAG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:298:ASN:HB3	4:c:391:SER:HA	1.78	0.66
29:a:409:PHO:HBC3	5:d:279:LEU:HD22	1.76	0.66
28:N:602:CLA:H72	47:N:621:LUT:H30	1.78	0.66
28:C:505:CLA:H42	30:C:515:BCR:HC7	1.76	0.66
23:Y:172:GLY:HA2	28:Y:608:CLA:HAC1	1.77	0.66
28:c:511:CLA:H112	30:c:517:BCR:H24C	1.78	0.66
32:c:521:LMG:H112	37:j:101:DGA:HB31	1.77	0.66
1:A:36:ILE:HG23	28:A:410:CLA:HBB1	1.77	0.65
2:b:321:LYS:NZ	2:b:363:PHE:O	2.28	0.65
14:O:216:ARG:HH11	14:O:240:LEU:HB3	1.61	0.65
12:l:15:ARG:NH1	16:t:23:PHE:O	2.30	0.65
2:B:41:GLU:O	2:B:45:PHE:HB2	1.95	0.65
6:e:43:ALA:O	6:e:47:PHE:HB2	1.96	0.65
1:a:288:LEU:HD11	4:c:420:CYS:HA	1.76	0.65
4:c:152:HIS:ND1	28:c:507:CLA:OBD	2.29	0.65
28:A:406:CLA:HAA2	41:D:405:PL9:H371	1.78	0.65
28:C:502:CLA:H61	28:C:512:CLA:H42	1.79	0.65
1:A:277:VAL:HG23	38:D:410:LHG:H292	1.77	0.65
14:O:115:THR:HB	14:O:127:PHE:HB3	1.78	0.64
21:G:87:ARG:NH1	21:G:200:GLU:OE2	2.31	0.64
22:S:108:ALA:HB1	22:S:239:GLY:HA3	1.79	0.64
38:L:101:LHG:H271	13:M:22:LEU:HD21	1.78	0.64
4:c:67:LYS:HB2	4:c:72:GLN:HE21	1.63	0.64
2:B:11:VAL:HG23	2:B:12:VAL:HG13	1.79	0.64
2:B:311:PHE:O	2:B:317:ASN:ND2	2.31	0.64
20:N:182:TYR:HB3	28:N:610:CLA:HED3	1.80	0.64
4:c:403:ASN:N	4:c:403:ASN:HD22	1.94	0.64
28:c:513:CLA:H101	30:c:514:BCR:H23C	1.78	0.64
4:C:166:LYS:HA	4:C:170:PHE:HB2	1.77	0.64
7:F:43:GLN:HE22	15:P:66:PHE:H	1.45	0.64
1:a:140:ARG:NH1	4:c:443:PHE:O	2.30	0.64
8:h:74:LEU:HB2	8:h:77:VAL:HG12	1.80	0.64
22:S:186:GLY:HA2	46:S:608:CHL:HAC1	1.79	0.64
1:a:85:THR:HA	1:a:109:GLY:HA3	1.78	0.64
28:c:508:CLA:H2	28:c:510:CLA:H12	1.81	0.64
2:b:301:ALA:O	2:b:304:LYS:HB2	1.98	0.63
13:M:27:VAL:HG21	13:m:24:ILE:HG23	1.79	0.63
28:a:405:CLA:H18	38:d:409:LHG:H332	1.80	0.63
14:o:107:PHE:HB3	14:o:143:MET:HB2	1.80	0.63
2:B:389:LYS:NZ	15:P:143:TYR:O	2.31	0.63
2:B:434:ARG:HG2	2:B:439:SER:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:107:PHE:HB3	14:O:143:MET:HB2	1.81	0.63
4:c:403:ASN:H	4:c:403:ASN:ND2	1.95	0.63
8:h:49:LEU:HA	8:h:52:VAL:HG12	1.81	0.62
1:a:51:ALA:O	1:a:55:ALA:HB2	1.99	0.62
5:d:85:LEU:HD13	5:d:90:LEU:HD21	1.80	0.62
23:Y:94:ALA:HB1	23:Y:212:GLY:HA3	1.81	0.62
2:B:99:SER:HB2	28:B:607:CLA:H62	1.82	0.62
2:B:247:TRP:HB2	28:B:609:CLA:HBC1	1.79	0.62
2:b:399:VAL:HG12	2:b:417:VAL:HG12	1.81	0.62
20:N:49:LEU:HB2	20:N:53:SER:HB3	1.82	0.62
1:a:133:LEU:HD22	5:d:252:PHE:HD1	1.64	0.62
4:c:264:LEU:HD11	28:c:508:CLA:HAB	1.80	0.62
6:e:43:ALA:O	6:e:47:PHE:CB	2.47	0.62
7:F:44:ARG:NH2	15:P:71:ASN:O	2.33	0.62
28:a:405:CLA:H152	29:a:408:PHO:H3A	1.81	0.62
4:c:145:MET:HA	4:c:148:ILE:HD12	1.82	0.62
35:c:520:DGD:HA62	32:d:411:LMG:H141	1.82	0.62
5:d:78:VAL:HB	5:d:173:PHE:HB2	1.82	0.62
14:O:147:MET:HE3	14:O:149:ILE:HD11	1.82	0.61
23:Y:207:LYS:HG3	28:Y:611:CLA:HED2	1.81	0.61
1:a:96:ILE:O	1:a:99:ALA:HB3	2.00	0.61
2:b:472:ARG:HA	2:b:479:PHE:HZ	1.65	0.61
2:b:242:ILE:HA	2:b:245:VAL:HG12	1.81	0.61
8:H:50:MET:HE1	43:H:101:RRX:H16	1.82	0.61
28:A:405:CLA:H201	38:D:409:LHG:H161	1.82	0.61
21:G:163:GLY:HA2	46:G:608:CHL:HAC1	1.82	0.61
22:S:103:ASN:O	22:S:107:HIS:ND1	2.33	0.61
5:d:159:ILE:HG21	5:d:287:VAL:HG22	1.82	0.61
14:O:171:LYS:HE3	14:O:175:GLY:HA2	1.82	0.61
21:G:130:TYR:HB3	21:G:136:LEU:HD13	1.82	0.61
4:c:166:LYS:HA	4:c:170:PHE:HB2	1.81	0.61
41:d:405:PL9:H111	38:d:409:LHG:H102	1.83	0.61
6:e:66:ILE:O	6:e:75:GLN:NE2	2.34	0.61
8:h:24:THR:HG23	8:h:27:GLY:H	1.65	0.61
28:S:604:CLA:H43	46:S:606:CHL:HAA2	1.83	0.61
1:A:170:ASP:OD2	4:C:345:ARG:NH1	2.33	0.61
1:a:267:ASN:ND2	5:d:232:PHE:O	2.33	0.61
28:b:608:CLA:H203	12:l:36:ILE:HG13	1.81	0.61
14:o:140:GLN:NE2	14:o:182:PHE:O	2.34	0.61
4:c:14:ARG:O	4:c:29:ARG:NH1	2.33	0.60
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:364:ASP:HB3	4:C:367:LYS:HB2	1.82	0.60
2:b:105:GLY:HA3	30:b:619:BCR:H402	1.83	0.60
37:b:625:DGA:HG11	5:d:134:ARG:HG2	1.83	0.60
8:h:69:ASN:ND2	32:h:102:LMG:O10	2.34	0.60
4:C:234:LEU:HB3	33:Y:625:SPH:H151	1.83	0.60
21:G:242:PHE:HB3	23:Y:132:PHE:HZ	1.65	0.60
28:G:603:CLA:H52	28:Y:603:CLA:H52	1.84	0.60
1:a:131:TRP:HZ2	4:c:437:ARG:HG3	1.67	0.60
32:a:413:LMG:H371	35:c:518:DGD:HB41	1.82	0.60
4:c:345:ARG:HG3	4:c:346:PHE:HD1	1.67	0.60
2:B:226:TYR:HA	2:B:231:MET:HG3	1.83	0.60
4:C:71:GLU:OE2	4:C:386:HIS:NE2	2.34	0.60
28:D:403:CLA:H102	18:X:80:ALA:HB2	1.84	0.60
1:a:323:ARG:HH12	5:d:329:MET:HE2	1.66	0.60
2:b:265:ILE:HD12	2:b:270:PRO:HA	1.84	0.60
19:z:19:LEU:HD22	19:z:47:TRP:HE1	1.66	0.60
24:u:90:ARG:HH21	24:u:91:VAL:HG22	1.66	0.60
7:f:35:ALA:O	7:f:39:MET:HB2	2.01	0.59
37:C:524:DGA:HAS1	32:W:201:LMG:H361	1.84	0.59
15:p:148:GLN:NE2	15:p:150:TRP:O	2.34	0.59
1:A:77:ILE:HD11	16:T:6:TYR:HB3	1.85	0.59
1:a:106:LEU:HD11	30:a:411:BCR:H402	1.84	0.59
2:b:7:ARG:O	2:b:10:THR:OG1	2.18	0.59
28:b:609:CLA:HBB2	5:d:150:ILE:HD13	1.83	0.59
4:c:403:ASN:N	4:c:403:ASN:ND2	2.49	0.59
4:C:152:HIS:ND1	28:C:507:CLA:OBD	2.29	0.59
5:D:122:LEU:HB3	5:D:150:ILE:HG12	1.83	0.59
22:S:62:PRO:HG2	22:S:65:LEU:HD23	1.85	0.59
2:b:167:TRP:HE3	2:b:178:VAL:HG23	1.67	0.59
2:B:479:PHE:O	5:D:139:ARG:NH2	2.36	0.59
28:b:609:CLA:H171	28:b:610:CLA:H192	1.85	0.59
1:A:85:THR:HA	1:A:109:GLY:HA3	1.84	0.59
28:C:507:CLA:H142	30:C:515:BCR:H16C	1.83	0.59
21:G:41:LEU:HB2	21:G:45:SER:HB3	1.84	0.59
1:a:334:ARG:HH21	14:o:211:LEU:HD13	1.68	0.59
28:C:506:CLA:HBB2	28:C:507:CLA:H52	1.84	0.59
21:G:220:VAL:HG23	21:G:221:THR:HG23	1.84	0.59
2:b:230:SER:OG	2:b:236:SER:OG	2.20	0.59
4:c:331:ARG:NH1	4:c:335:GLY:O	2.36	0.59
2:B:145:LEU:HD11	28:B:605:CLA:H151	1.84	0.58
38:C:525:LHG:H251	28:S:611:CLA:HAB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:211:PHE:HB3	1:a:275:LEU:HD22	1.84	0.58
37:b:625:DGA:HA62	5:d:127:LEU:HD22	1.85	0.58
2:B:275:TRP:O	24:U:102:LYS:NZ	2.35	0.58
14:O:140:GLN:NE2	14:O:182:PHE:O	2.36	0.58
28:G:603:CLA:H91	46:G:609:CHL:H121	1.85	0.58
7:F:41:PHE:O	7:F:43:GLN:NE2	2.36	0.58
2:B:365:THR:OG1	5:D:326:ARG:NH2	2.37	0.58
2:B:371:ILE:HG23	24:U:100:PRO:HB2	1.86	0.58
14:O:75:VAL:HG13	14:O:80:ILE:HB	1.84	0.58
4:c:461:ASP:OD2	16:t:24:ARG:NH2	2.37	0.58
28:c:503:CLA:H172	28:c:510:CLA:HBB2	1.86	0.58
1:A:47:VAL:HG11	1:A:114:LEU:HD22	1.86	0.58
15:P:144:LEU:O	15:P:218:LYS:NZ	2.37	0.58
5:d:199:MET:HE3	41:d:405:PL9:H272	1.86	0.58
14:o:263:THR:O	14:o:297:GLN:NE2	2.35	0.58
28:D:403:CLA:H42	8:H:62:LEU:HD22	1.85	0.58
1:a:195:HIS:HD2	1:a:197:PHE:H	1.51	0.58
4:c:342:GLU:OE2	4:c:345:ARG:NH2	2.37	0.58
28:B:604:CLA:HAB	28:B:606:CLA:H152	1.84	0.58
51:Y:626:PTY:H182	51:Y:626:PTY:H381	1.86	0.58
6:E:19:TYR:O	6:E:23:HIS:ND1	2.37	0.58
23:Y:95:ARG:HA	23:Y:98:LEU:HD12	1.84	0.58
1:a:100:ALA:N	1:a:104:GLU:OE2	2.37	0.58
4:c:200:TYR:HB3	4:c:212:ILE:HG22	1.86	0.57
4:C:109:SER:HA	30:C:514:BCR:H16C	1.86	0.57
23:Y:200:ALA:HA	23:Y:203:GLU:HG2	1.87	0.57
21:G:112:GLU:O	21:G:121:GLN:NE2	2.37	0.57
1:a:316:THR:HG22	5:d:64:ALA:HB3	1.85	0.57
5:d:216:ALA:O	5:d:220:ASN:ND2	2.36	0.57
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.87	0.57
2:B:452:THR:HB	5:D:291:LEU:HD21	1.85	0.57
7:F:36:ILE:HA	7:F:39:MET:HG2	1.86	0.57
2:B:39:LEU:HD12	36:B:624:3PH:H3D2	1.84	0.57
5:D:263:ASN:HB3	5:D:266:TRP:HB3	1.86	0.57
2:B:96:ALA:O	2:B:100:HIS:ND1	2.35	0.57
5:d:106:GLN:NE2	6:e:48:GLY:O	2.38	0.57
7:f:44:ARG:NH1	10:j:42:LEU:O	2.37	0.57
8:H:69:ASN:ND2	32:H:102:LMG:O10	2.37	0.57
20:N:191:GLY:O	20:N:193:ALA:N	2.38	0.57
21:G:176:TYR:HB3	28:G:610:CLA:HED3	1.85	0.57
4:c:309:ASP:HA	4:c:312:LEU:HG	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:504:CLA:H43	35:C:520:DGD:HB32	1.86	0.57
22:S:209:LYS:HG3	22:S:210:LEU:HG	1.85	0.57
51:Y:626:PTY:H182	51:Y:626:PTY:H362	1.86	0.57
1:a:14:TRP:HB2	17:w:95:ILE:HG22	1.86	0.57
28:A:405:CLA:H102	29:A:408:PHO:HAA1	1.86	0.57
2:B:233:SER:OG	2:B:235:GLU:OE2	2.23	0.57
3:V:22:VAL:HG23	19:Z:25:VAL:HG23	1.87	0.57
4:c:16:GLN:OE1	5:d:233:ARG:NH2	2.38	0.57
5:D:51:GLY:HA2	5:D:55:VAL:HB	1.86	0.57
1:a:41:LEU:HD11	29:a:408:PHO:H62	1.85	0.57
4:c:25:ALA:HA	28:c:508:CLA:HAA1	1.87	0.57
21:G:162:ASN:ND2	21:G:164:GLY:O	2.38	0.56
28:Y:610:CLA:H52	47:Y:620:LUT:H30	1.87	0.56
2:b:288:VAL:O	2:b:292:THR:OG1	2.22	0.56
28:C:505:CLA:H172	35:C:518:DGD:HA71	1.87	0.56
8:H:54:ILE:HG12	43:H:101:RRX:H9	1.87	0.56
50:S:625:LPX:H10	36:S:626:3PH:H291	1.86	0.56
2:b:30:VAL:HG12	28:b:606:CLA:HHD	1.87	0.56
8:h:46:THR:HG22	8:h:49:LEU:HB2	1.86	0.56
30:C:517:BCR:H391	11:K:36:ALA:HB2	1.86	0.56
15:P:204:LEU:HB3	15:P:238:LEU:HD13	1.86	0.56
21:G:65:THR:OG1	23:Y:85:ARG:NH2	2.38	0.56
51:Y:626:PTY:H401	51:Y:626:PTY:H212	1.86	0.56
4:c:285:TYR:O	4:c:411:ARG:NH2	2.30	0.56
5:d:51:GLY:HA3	5:d:78:VAL:HG22	1.86	0.56
8:h:30:LEU:HB2	8:h:33:LEU:HD12	1.87	0.56
2:B:30:VAL:HG12	28:B:606:CLA:HHD	1.87	0.56
2:B:357:ARG:NH2	5:D:337:GLU:OE1	2.39	0.56
20:N:101:LEU:HB3	28:N:604:CLA:HMC2	1.87	0.56
2:b:11:VAL:HG23	2:b:12:VAL:HG13	1.87	0.56
1:A:64:ARG:NH1	14:O:167:ALA:O	2.39	0.56
1:a:139:MET:HE3	5:d:248:THR:HG22	1.87	0.56
1:a:170:ASP:OD2	4:c:345:ARG:NH1	2.39	0.56
14:o:104:LEU:HD22	14:o:147:MET:HE2	1.87	0.56
4:C:173:VAL:HG23	4:C:218:LEU:HD13	1.87	0.56
4:C:285:TYR:O	4:C:411:ARG:NH2	2.38	0.56
22:S:240:ARG:HA	22:S:243:MET:HE3	1.87	0.56
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.86	0.56
4:C:308:ARG:NH1	15:P:223:ASP:OD2	2.38	0.56
28:c:513:CLA:HAB	30:c:514:BCR:H24C	1.86	0.56
2:b:174:LEU:HD21	2:b:309:LEU:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:258:TYR:HB3	32:h:102:LMG:HC61	1.88	0.56
38:d:409:LHG:HC62	12:l:16:SER:HB3	1.88	0.56
28:B:610:CLA:OBD	8:H:46:THR:OG1	2.24	0.56
38:G:624:LHG:H312	38:G:624:LHG:HC91	1.88	0.56
1:a:223:LEU:HD13	5:d:265:ARG:HD2	1.88	0.56
23:Y:46:ARG:NH2	23:Y:61:LEU:O	2.39	0.55
32:C:523:LMG:H131	32:C:523:LMG:H332	1.88	0.55
14:O:149:ILE:HA	14:O:155:VAL:HG12	1.88	0.55
1:a:201:GLY:HA3	1:a:286:THR:HB	1.87	0.55
28:c:504:CLA:H42	35:c:519:DGD:HB32	1.88	0.55
7:f:19:TRP:O	7:f:23:HIS:ND1	2.39	0.55
9:i:5:LYS:NZ	17:w:77:ASN:OD1	2.38	0.55
31:B:621:SQD:H122	16:t:23:PHE:HB3	1.88	0.55
5:D:192:THR:HG23	28:D:402:CLA:HBC2	1.88	0.55
2:b:312:TYR:HA	2:b:317:ASN:HD22	1.70	0.55
1:A:30:ILE:O	1:A:34:GLY:HA3	2.06	0.55
1:A:340:PRO:HB3	15:P:198:GLU:HA	1.87	0.55
30:D:404:BCR:H373	7:F:33:LEU:HD21	1.87	0.55
28:a:410:CLA:H12	32:a:413:LMG:H112	1.89	0.55
2:b:9:HIS:CD2	28:b:613:CLA:HAB	2.41	0.55
28:b:612:CLA:H93	38:l:101:LHG:H322	1.89	0.55
28:c:502:CLA:H11	28:c:503:CLA:H161	1.87	0.55
15:p:169:ALA:HB3	15:p:190:LEU:HB3	1.89	0.55
14:O:183:THR:HG21	14:O:203:PRO:HD2	1.87	0.55
15:P:204:LEU:HB2	15:P:219:VAL:HB	1.88	0.55
1:a:129:ARG:NH2	5:d:255:GLN:O	2.40	0.55
2:b:388:SER:O	2:b:394:GLN:NE2	2.33	0.55
4:c:203:LYS:HB3	4:c:211:TRP:HA	1.89	0.55
15:p:93:PRO:HA	15:p:106:TYR:HA	1.88	0.55
2:B:458:PHE:HB3	28:B:605:CLA:HBC2	1.88	0.55
9:I:5:LYS:HD2	17:W:65:MET:HE1	1.88	0.55
20:N:247:ALA:HB1	48:G:622:XAT:H161	1.89	0.55
22:S:105:LEU:HD23	22:S:210:LEU:HB3	1.87	0.55
28:N:603:CLA:HAC1	46:N:607:CHL:HBB2	1.89	0.55
28:N:611:CLA:HAB	48:G:622:XAT:H221	1.87	0.55
1:a:50:ILE:HD13	30:a:411:BCR:H23C	1.89	0.55
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.89	0.55
5:D:155:SER:HA	5:D:159:ILE:HB	1.89	0.55
46:N:609:CHL:H43	46:Y:601:CHL:H12	1.88	0.55
21:G:86:ALA:HB1	21:G:204:GLY:HA3	1.89	0.55
2:b:413:ASP:HB3	2:b:416:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:510:CLA:HED2	28:c:510:CLA:H121	1.89	0.55
5:d:206:GLY:HA2	5:d:209:LEU:HD12	1.89	0.55
1:A:309:SER:HA	7:F:44:ARG:HG2	1.89	0.54
28:B:614:CLA:H43	38:D:408:LHG:H383	1.89	0.54
28:B:615:CLA:H52	31:B:621:SQD:H282	1.88	0.54
1:a:24:THR:O	5:d:251:ARG:NH2	2.37	0.54
28:a:407:CLA:HMB2	29:a:409:PHO:H152	1.88	0.54
4:c:161:TRP:HB3	31:c:526:SQD:H202	1.89	0.54
2:B:148:LEU:HD12	2:B:210:VAL:HG22	1.88	0.54
2:b:75:TRP:NE1	2:b:89:GLY:O	2.40	0.54
5:d:55:VAL:HG21	5:d:110:LEU:HD11	1.89	0.54
20:N:202:LEU:HB3	28:N:610:CLA:HMA2	1.88	0.54
46:N:601:CHL:HED1	38:N:624:LHG:H271	1.88	0.54
1:a:76:ASN:O	1:a:80:GLY:N	2.40	0.54
15:p:78:TYR:HB3	15:p:87:LEU:HD23	1.89	0.54
1:a:283:ILE:HA	1:a:286:THR:HG22	1.90	0.54
2:B:338:VAL:HB	2:B:431:GLU:HG3	1.90	0.54
28:C:506:CLA:H102	37:C:524:DGA:HA91	1.89	0.54
2:b:471:SER:O	2:b:475:PHE:HB2	2.07	0.54
5:d:47:GLY:HA2	30:d:404:BCR:H332	1.90	0.54
5:d:203:GLY:HA2	41:d:405:PL9:H23	1.88	0.54
1:A:51:ALA:O	1:A:55:ALA:HB2	2.06	0.54
28:C:501:CLA:HMB2	30:C:515:BCR:H23C	1.90	0.54
23:Y:239:ASP:HB3	23:Y:247:ASN:HD21	1.72	0.54
28:b:602:CLA:H122	43:h:101:RRX:H46	1.89	0.54
4:c:218:LEU:HD23	4:c:221:ILE:HD12	1.89	0.54
4:C:203:LYS:HG2	4:C:209:ASP:HB3	1.89	0.54
38:C:525:LHG:H142	28:S:611:CLA:HBB2	1.89	0.54
1:a:167:SER:HB3	4:c:345:ARG:HD3	1.88	0.54
15:p:113:VAL:HG13	15:p:220:GLN:HE22	1.73	0.54
2:B:256:MET:O	2:B:448:ARG:NH1	2.36	0.54
28:B:608:CLA:H2	32:B:622:LMG:H151	1.89	0.54
1:a:106:LEU:HD21	30:a:411:BCR:H383	1.90	0.54
1:a:167:SER:OG	4:c:345:ARG:NH1	2.41	0.54
2:b:371:ILE:HG12	2:b:377:VAL:HG22	1.89	0.54
14:o:71:THR:OG1	14:o:74:GLN:OE1	2.25	0.54
14:o:253:VAL:HB	14:o:271:GLU:HB3	1.90	0.54
5:D:134:ARG:NH2	5:D:137:ASN:OD1	2.41	0.53
4:c:359:GLY:N	4:c:362:GLY:O	2.38	0.53
14:o:272:SER:HB3	14:o:290:ILE:HB	1.89	0.53
1:A:14:TRP:HB2	17:W:95:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:183:MET:HB3	28:a:405:CLA:HBC2	1.91	0.53
1:a:212:SER:OG	5:d:271:MET:O	2.25	0.53
28:b:613:CLA:H171	28:b:614:CLA:HBB2	1.89	0.53
5:d:161:PRO:HB3	5:d:170:ALA:HB2	1.89	0.53
46:N:601:CHL:H202	46:G:607:CHL:H13	1.91	0.53
46:G:609:CHL:HHC	46:G:609:CHL:HBB1	1.90	0.53
31:a:412:SQD:H341	35:c:519:DGD:HAF2	1.89	0.53
2:b:122:LEU:O	8:h:34:ASN:ND2	2.40	0.53
3:v:20:PRO:HA	3:v:23:VAL:HG12	1.91	0.53
1:a:298:ASN:OD1	1:a:299:GLY:N	2.41	0.53
2:b:57:ARG:NH2	2:b:335:GLY:O	2.41	0.53
15:p:178:ASP:OD1	15:p:182:LYS:N	2.39	0.53
1:a:127:MET:HE1	4:c:430:LEU:HD11	1.90	0.53
1:a:194:MET:O	1:a:300:PHE:N	2.36	0.53
1:A:166:GLY:HA3	4:C:346:PHE:HE1	1.74	0.53
2:B:124:ARG:NH1	8:H:19:GLU:O	2.41	0.53
4:C:227:TRP:HH2	28:Y:614:CLA:HAB	1.72	0.53
4:C:296:GLU:HG3	4:C:353:TRP:HZ2	1.74	0.53
13:M:20:SER:O	13:M:24:ILE:HG12	2.08	0.53
28:N:603:CLA:HED1	28:Y:602:CLA:H121	1.91	0.53
21:G:71:ASP:HB3	21:G:74:THR:HG22	1.90	0.53
2:B:464:PHE:HD2	28:B:612:CLA:HAC2	1.74	0.53
2:b:74:SER:HA	2:b:92:SER:HB2	1.90	0.53
1:A:43:THR:HG23	30:A:411:BCR:H362	1.91	0.53
28:B:613:CLA:H171	28:B:614:CLA:HBB2	1.89	0.53
4:C:166:LYS:HB2	28:C:502:CLA:H203	1.91	0.53
2:b:41:GLU:O	2:b:45:PHE:HB2	2.09	0.53
3:V:26:LEU:HD21	19:Z:25:VAL:HA	1.90	0.53
1:a:64:ARG:NH1	14:o:167:ALA:O	2.41	0.53
5:d:56:THR:HG21	6:e:50:PRO:HD2	1.91	0.53
5:d:274:VAL:HG23	5:d:275:PRO:HD3	1.91	0.53
5:d:296:TYR:O	5:d:315:TYR:OH	2.23	0.53
14:o:224:ASN:HA	14:o:240:LEU:HB2	1.89	0.53
1:A:167:SER:O	1:A:170:ASP:HB2	2.09	0.53
14:O:172:LEU:HB2	14:O:176:GLU:HB2	1.91	0.53
15:P:224:LYS:HE3	15:P:225:ARG:HH12	1.72	0.53
46:N:605:CHL:H51	28:S:611:CLA:H193	1.91	0.53
22:S:224:ASP:HB3	22:S:227:VAL:HG22	1.90	0.53
4:c:213:VAL:O	4:c:281:ASN:ND2	2.42	0.53
35:c:520:DGD:HA71	32:d:411:LMG:H161	1.90	0.53
5:d:192:THR:HG23	28:d:402:CLA:HBC2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:C:523:LMG:H382	28:Y:614:CLA:H92	1.91	0.52
15:P:144:LEU:HD13	15:P:218:LYS:HD2	1.91	0.52
2:b:341:LEU:HD23	2:b:405:GLU:HB2	1.92	0.52
4:c:25:ALA:O	4:c:28:ALA:HB3	2.09	0.52
4:c:57:LEU:HB3	11:k:22:VAL:HG21	1.92	0.52
5:D:24:GLN:OE1	5:D:26:ARG:NH2	2.42	0.52
28:G:613:CLA:H2	28:G:614:CLA:HMD1	1.92	0.52
2:B:7:ARG:O	2:B:10:THR:OG1	2.20	0.52
4:C:200:TYR:HB3	4:C:212:ILE:HG22	1.91	0.52
8:H:62:LEU:O	8:H:66:GLU:HG2	2.08	0.52
46:N:601:CHL:HHC	46:N:601:CHL:HBB1	1.92	0.52
1:a:41:LEU:HD21	29:a:408:PHO:H42	1.90	0.52
1:a:87:ASN:OD1	4:c:345:ARG:NE	2.42	0.52
1:a:112:TYR:OH	1:a:172:MET:O	2.20	0.52
5:d:81:PRO:HD3	5:d:111:TRP:HB3	1.92	0.52
38:d:410:LHG:O3	38:d:410:LHG:O1	2.27	0.52
28:B:606:CLA:HMA3	28:B:607:CLA:H3A	1.91	0.52
41:D:405:PL9:H403	12:L:27:VAL:HG13	1.92	0.52
21:G:217:GLN:O	21:G:221:THR:OG1	2.26	0.52
23:Y:184:TYR:HB3	28:Y:610:CLA:HED3	1.91	0.52
12:l:12:GLU:HB2	13:m:29:THR:HG23	1.91	0.52
15:p:128:ILE:HG23	15:p:209:VAL:HG23	1.90	0.52
46:G:607:CHL:H91	46:G:609:CHL:H171	1.92	0.52
1:a:57:PRO:HB2	1:a:66:PRO:HB2	1.91	0.52
1:a:102:LEU:HD11	33:a:414:SPH:H5	1.91	0.52
2:b:299:SER:OG	2:b:300:GLU:OE2	2.28	0.52
3:v:7:LEU:HA	3:v:10:VAL:HG22	1.90	0.52
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.44	0.52
4:C:287:SER:OG	4:C:296:GLU:OE2	2.24	0.52
46:G:607:CHL:H143	46:G:609:CHL:H92	1.91	0.52
23:Y:161:VAL:HG13	49:Y:623:NEX:H15	1.91	0.52
2:b:464:PHE:HD2	28:b:612:CLA:HAC2	1.73	0.52
4:c:345:ARG:HG3	4:c:346:PHE:CD1	2.43	0.52
14:o:110:GLU:OE2	17:w:60:LEU:N	2.42	0.52
1:a:140:ARG:NH2	4:c:444:GLU:HA	2.24	0.52
2:b:124:ARG:HH21	2:b:131:THR:HA	1.74	0.52
5:d:222:LEU:HA	5:d:244:TYR:HA	1.92	0.52
30:B:619:BCR:HC21	32:B:622:LMG:H201	1.92	0.52
41:D:405:PL9:H461	16:T:10:LEU:HD21	1.92	0.52
22:S:237:LYS:NZ	38:S:624:LHG:O5	2.43	0.52
1:A:24:THR:O	5:D:251:ARG:NH2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:513:CLA:H101	30:C:514:BCR:H23C	1.92	0.52
2:b:22:VAL:HA	2:b:25:MET:HG2	1.91	0.52
2:b:243:ALA:HA	2:b:246:PHE:CE1	2.45	0.52
28:b:611:CLA:HHC	28:b:611:CLA:HBB1	1.91	0.52
1:a:131:TRP:CH2	28:c:505:CLA:HAA2	2.45	0.51
14:o:67:LEU:HD22	14:o:85:PRO:HG3	1.92	0.51
15:p:97:LYS:NZ	15:p:100:ASP:OD1	2.42	0.51
36:t:101:3PH:H2I3	36:t:101:3PH:H2A2	1.91	0.51
22:S:49:LEU:HD11	22:S:226:GLU:HA	1.92	0.51
1:a:248:ILE:HG21	5:d:235:PHE:HZ	1.75	0.51
1:a:329:GLU:HG2	5:d:352:LEU:HD21	1.92	0.51
1:a:337:HIS:NE2	1:a:342:ASP:OD2	2.41	0.51
2:b:252:VAL:HA	2:b:255:THR:HG22	1.93	0.51
4:c:367:LYS:HD2	4:c:371:ASP:HB2	1.92	0.51
5:d:25:ASP:OD2	5:d:25:ASP:N	2.44	0.51
5:D:136:VAL:HG23	5:D:138:LEU:HD23	1.91	0.51
2:b:436:THR:HG23	2:b:437:LEU:HG	1.93	0.51
7:f:14:ILE:HD13	42:f:101:HEM:HAA1	1.93	0.51
1:A:175:GLY:O	1:A:179:THR:OG1	2.27	0.51
1:A:191:ASN:HB2	4:C:399:ALA:HB1	1.92	0.51
32:A:413:LMG:H371	35:C:518:DGD:HB41	1.93	0.51
1:a:82:VAL:HB	1:a:174:LEU:HB2	1.92	0.51
6:e:74:GLU:HA	6:e:77:LYS:HD2	1.92	0.51
2:B:90:ILE:HD13	45:i:101:4RF:H52	1.93	0.51
5:d:85:LEU:HD23	6:e:69:ARG:HA	1.93	0.51
5:d:198:MET:HA	5:d:201:VAL:HG12	1.93	0.51
6:e:78:LYS:HG3	6:e:79:LEU:HD12	1.93	0.51
37:B:625:DGA:HAN2	5:D:36:LEU:HD12	1.93	0.51
9:I:5:LYS:NZ	17:W:77:ASN:OD1	2.40	0.51
13:M:31:ALA:HB3	13:m:31:ALA:HB3	1.93	0.51
22:S:112:MET:SD	28:S:610:CLA:HAB	2.51	0.51
1:A:42:LEU:HD21	36:T:101:3PH:H292	1.93	0.51
1:A:344:ALA:OXT	4:C:345:ARG:NH1	2.43	0.51
28:B:615:CLA:H71	31:B:621:SQD:H302	1.92	0.51
9:I:7:PHE:HB2	45:I:102:4RF:H71	1.93	0.51
21:G:58:PRO:HB2	21:G:201:ILE:HD12	1.93	0.51
46:G:601:CHL:H11	46:Y:609:CHL:H43	1.92	0.51
2:b:22:VAL:HG21	28:b:613:CLA:HBB1	1.92	0.51
2:b:170:ASP:OD1	2:b:174:LEU:N	2.43	0.51
28:c:513:CLA:HMB2	30:c:514:BCR:H292	1.93	0.51
5:d:325:ILE:HG23	5:d:329:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:189:ILE:HB	15:p:203:GLN:HB2	1.92	0.51
1:A:221:SER:OG	5:D:139:ARG:O	2.26	0.51
7:F:30:ILE:HG13	42:F:101:HEM:HMC2	1.93	0.51
21:G:65:THR:HG21	46:Y:609:CHL:HAA2	1.93	0.51
1:a:127:MET:HG2	1:a:151:VAL:HG21	1.92	0.51
1:a:190:HIS:HB3	1:a:293:MET:HE2	1.92	0.51
28:b:607:CLA:OBD	35:b:623:DGD:O3D	2.29	0.51
28:b:613:CLA:H142	28:b:614:CLA:HAB	1.93	0.51
4:c:173:VAL:HG23	4:c:218:LEU:HD13	1.92	0.51
8:h:20:PRO:O	12:l:3:ARG:NH2	2.44	0.51
14:O:224:ASN:HA	14:O:240:LEU:HB2	1.93	0.51
28:N:610:CLA:H51	47:N:620:LUT:H30	1.93	0.51
1:A:283:ILE:HA	1:A:286:THR:HG22	1.93	0.51
4:C:27:ASN:HB3	28:C:509:CLA:HAB	1.93	0.51
28:C:513:CLA:HAB	30:C:514:BCR:H24C	1.93	0.51
1:a:51:ALA:O	1:a:55:ALA:CB	2.58	0.51
46:G:608:CHL:HHC	46:G:608:CHL:HBB1	1.93	0.50
28:c:504:CLA:H61	35:c:519:DGD:HB92	1.92	0.50
28:c:513:CLA:CAB	30:c:514:BCR:H24C	2.41	0.50
14:o:143:MET:HE1	14:o:164:ASP:HA	1.92	0.50
6:E:23:HIS:NE2	42:F:101:HEM:ND	2.59	0.50
46:G:605:CHL:HHC	46:G:605:CHL:HBB1	1.92	0.50
2:b:376:VAL:HB	2:b:378:ARG:HH12	1.75	0.50
1:A:340:PRO:HD2	4:C:305:PHE:HE2	1.75	0.50
31:A:412:SQD:H322	45:K:101:4RF:H96	1.94	0.50
2:B:256:MET:HA	2:B:263:THR:HG21	1.93	0.50
4:C:51:TRP:HB2	28:C:510:CLA:HAC2	1.93	0.50
30:C:516:BCR:HC41	11:K:25:LEU:HD21	1.94	0.50
8:H:65:LEU:HD11	32:H:102:LMG:H302	1.93	0.50
15:P:157:GLU:HG3	15:P:165:VAL:HG12	1.93	0.50
28:N:614:CLA:HBC1	47:N:620:LUT:H162	1.94	0.50
1:a:56:PRO:HD2	1:a:106:LEU:HD22	1.92	0.50
1:a:269:ARG:NH2	5:d:225:ASP:OD2	2.43	0.50
4:c:267:VAL:HA	4:c:270:MET:HB2	1.93	0.50
4:C:193:ASN:HB3	4:C:196:ILE:HG22	1.93	0.50
4:C:390:GLY:HA3	4:C:408:VAL:HG22	1.94	0.50
46:Y:601:CHL:HHD	38:Y:624:LHG:HC41	1.94	0.50
28:c:513:CLA:H62	38:c:525:LHG:H292	1.94	0.50
32:A:413:LMG:H362	35:C:518:DGD:HA81	1.93	0.50
46:N:605:CHL:HHC	46:N:605:CHL:HBB1	1.94	0.50
2:b:38:THR:HG23	2:b:97:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:69:MET:SD	4:c:69:MET:N	2.84	0.50
5:d:186:GLN:HB2	28:d:402:CLA:HBC1	1.93	0.50
8:h:19:GLU:HG2	12:l:2:ALA:HA	1.93	0.50
1:A:121:LEU:HD21	28:C:505:CLA:H162	1.94	0.50
32:A:413:LMG:H191	28:C:505:CLA:H8	1.94	0.50
2:B:121:GLU:O	8:H:31:ARG:NH1	2.44	0.50
28:C:513:CLA:H43	38:C:525:LHG:H241	1.93	0.50
1:a:133:LEU:HD13	5:d:256:ILE:HG12	1.92	0.50
1:a:204:GLY:HA2	1:a:278:TRP:HE1	1.77	0.50
28:c:512:CLA:H192	31:c:526:SQD:H91	1.92	0.50
2:B:357:ARG:NH1	2:B:358:ARG:O	2.44	0.50
2:b:63:LEU:HD12	2:b:66:LEU:HD12	1.93	0.50
6:e:51:ARG:NH2	15:p:59:TYR:O	2.45	0.50
15:p:154:THR:HG22	15:p:156:SER:H	1.76	0.50
25:A:401:OEX:O4	4:C:345:ARG:NH2	2.37	0.50
46:G:601:CHL:HHC	46:G:601:CHL:HBB1	1.93	0.50
46:G:601:CHL:H152	38:G:624:LHG:H223	1.93	0.50
51:Y:626:PTY:H341	51:Y:626:PTY:H162	1.94	0.50
28:c:511:CLA:H62	30:c:517:BCR:H402	1.94	0.50
8:H:74:LEU:HB2	8:H:77:VAL:HG22	1.94	0.50
28:Y:603:CLA:H152	46:Y:609:CHL:H8	1.94	0.50
1:a:34:GLY:HA2	1:a:37:MET:HE2	1.94	0.50
1:a:103:ASP:HB3	14:o:171:LYS:HD3	1.94	0.50
28:a:410:CLA:HAB	9:i:15:PHE:CD2	2.45	0.50
2:b:212:ALA:O	2:b:216:HIS:ND1	2.44	0.50
2:b:401:PHE:O	2:b:408:GLY:N	2.40	0.50
5:d:148:ALA:HB2	5:d:276:VAL:HG23	1.93	0.50
5:d:289:LEU:HD22	5:d:294:ARG:HG3	1.93	0.50
4:C:38:LEU:HD11	28:C:513:CLA:HBB1	1.93	0.49
21:G:91:LEU:HD13	28:G:604:CLA:HBB2	1.94	0.49
2:b:124:ARG:O	8:h:31:ARG:NH2	2.44	0.49
4:c:295:PRO:HB3	4:c:349:PHE:HB2	1.93	0.49
1:A:140:ARG:HB2	5:D:220:ASN:HA	1.95	0.49
4:C:264:LEU:HD21	28:C:508:CLA:CAB	2.43	0.49
4:c:245:TRP:NE1	28:c:506:CLA:OBD	2.40	0.49
30:c:516:BCR:H19C	11:k:34:LEU:HB3	1.93	0.49
2:B:75:TRP:O	31:B:626:SQD:O3	2.30	0.49
20:N:90:LEU:HD23	20:N:181:LEU:HD22	1.93	0.49
46:S:608:CHL:HHC	46:S:608:CHL:HBB1	1.94	0.49
2:b:442:VAL:HA	14:o:229:PRO:HD2	1.94	0.49
38:C:525:LHG:H131	31:C:526:SQD:H291	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:41:GLY:HA2	6:E:44:TYR:HD2	1.78	0.49
46:N:601:CHL:H102	48:G:622:XAT:H14	1.94	0.49
1:a:133:LEU:HD22	5:d:252:PHE:CD1	2.44	0.49
2:b:137:LYS:HB2	2:b:220:ARG:HH12	1.76	0.49
4:c:75:ILE:HG21	4:c:414:LEU:HD21	1.94	0.49
4:c:253:VAL:HG21	4:c:437:ARG:HD2	1.94	0.49
35:c:519:DGD:HA21	37:j:101:DGA:HA72	1.94	0.49
38:C:525:LHG:H152	31:C:526:SQD:H372	1.94	0.49
22:S:256:THR:HG23	22:S:258:GLU:H	1.78	0.49
28:Y:603:CLA:HAC2	46:Y:607:CHL:H202	1.95	0.49
46:Y:606:CHL:HHC	46:Y:606:CHL:HBB1	1.95	0.49
1:a:260:PHE:O	1:a:264:SER:OG	2.30	0.49
1:a:323:ARG:NH2	5:d:333:ASP:OD1	2.45	0.49
38:d:409:LHG:H121	38:d:409:LHG:H281	1.94	0.49
1:A:269:ARG:HE	5:D:222:LEU:HD13	1.77	0.49
15:P:231:ASP:OD1	15:P:231:ASP:N	2.46	0.49
1:a:84:PRO:HA	1:a:112:TYR:CG	2.48	0.49
1:a:107:TYR:HB2	14:o:133:LEU:HD22	1.95	0.49
4:c:264:LEU:HA	4:c:267:VAL:HG22	1.94	0.49
5:d:325:ILE:O	5:d:329:MET:HG2	2.13	0.49
28:B:605:CLA:H142	28:B:616:CLA:H61	1.93	0.49
4:C:266:ALA:O	4:C:270:MET:HG3	2.12	0.49
5:D:279:LEU:HD11	28:D:402:CLA:HBA1	1.94	0.49
6:E:57:THR:O	6:E:61:GLN:NE2	2.46	0.49
14:O:108:CYS:HB2	14:O:295:TYR:HB3	1.94	0.49
20:N:204:VAL:HA	20:N:207:ILE:HG22	1.95	0.49
46:Y:605:CHL:HHC	46:Y:605:CHL:HBB1	1.93	0.49
1:a:186:PHE:O	1:a:190:HIS:HB2	2.13	0.49
28:b:609:CLA:H143	28:d:403:CLA:HMA3	1.94	0.49
1:A:241:GLN:NE2	1:A:243:GLU:O	2.42	0.49
28:A:406:CLA:H3A	28:A:406:CLA:HBA2	1.56	0.49
1:a:310:ASN:O	15:p:89:SER:OG	2.31	0.49
2:B:91:TRP:CD2	28:B:607:CLA:HBA2	2.48	0.48
20:N:91:ILE:HG13	46:N:609:CHL:HED1	1.95	0.48
22:S:171:ILE:HA	22:S:174:VAL:HG22	1.93	0.48
46:S:601:CHL:HBB1	46:S:601:CHL:HHC	1.94	0.48
28:Y:613:CLA:H72	28:Y:614:CLA:HMD3	1.95	0.48
2:b:58:GLN:HG2	2:b:331:ASN:HD21	1.77	0.48
5:D:299:VAL:O	5:D:303:ILE:HG13	2.13	0.48
5:D:325:ILE:O	5:D:329:MET:HB2	2.13	0.48
28:b:613:CLA:H111	28:b:614:CLA:HAB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:33:LEU:O	4:c:37:LEU:HB2	2.13	0.48
28:c:513:CLA:H2	30:c:514:BCR:H381	1.94	0.48
9:i:7:PHE:HB2	45:i:101:4RF:H71	1.95	0.48
18:x:64:SER:OG	18:x:65:VAL:N	2.45	0.48
5:D:12:ARG:HH12	5:D:17:ASP:HB2	1.78	0.48
28:Y:612:CLA:H12	28:Y:612:CLA:HED2	1.95	0.48
4:c:319:ALA:HA	15:p:158:GLY:HA3	1.95	0.48
21:G:37:ARG:NH2	21:G:53:LEU:O	2.46	0.48
1:a:106:LEU:HD23	1:a:111:PRO:HG2	1.95	0.48
1:a:325:ASN:O	1:a:329:GLU:HB2	2.13	0.48
30:b:618:BCR:H382	31:b:621:SQD:H281	1.95	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.48
28:B:603:CLA:H61	28:B:603:CLA:H41	1.54	0.48
4:C:454:VAL:HG21	5:D:248:THR:HA	1.95	0.48
46:N:601:CHL:H171	46:G:607:CHL:H161	1.96	0.48
46:N:606:CHL:H41	46:N:606:CHL:H62	1.64	0.48
2:b:54:PRO:HD2	2:b:57:ARG:HG3	1.95	0.48
12:l:13:LEU:N	13:m:29:THR:OG1	2.36	0.48
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.96	0.48
15:P:125:LYS:HE2	15:P:130:ASP:HB3	1.95	0.48
1:a:180:PHE:HB2	5:d:318:ASN:HD21	1.78	0.48
2:b:3:LEU:HD13	12:l:9:GLN:HG2	1.95	0.48
2:b:99:SER:HB2	28:b:607:CLA:H62	1.95	0.48
4:c:261:SER:O	4:c:429:HIS:ND1	2.43	0.48
4:c:390:GLY:HA3	4:c:408:VAL:HG22	1.94	0.48
28:c:508:CLA:HED2	38:d:410:LHG:HC2	1.96	0.48
11:k:19:SER:HA	11:k:22:VAL:HG12	1.95	0.48
1:A:274:PHE:HA	1:A:277:VAL:HG12	1.96	0.48
28:B:608:CLA:H92	32:B:622:LMG:H202	1.96	0.48
2:b:318:ASN:HB3	2:b:321:LYS:HG2	1.94	0.48
2:B:16:PRO:HG2	2:B:123:PHE:HB3	1.96	0.48
2:B:25:MET:HE1	2:B:108:PHE:HD1	1.77	0.48
28:B:605:CLA:HBB1	28:B:614:CLA:HBC2	1.95	0.48
12:L:19:TYR:OH	16:T:23:PHE:O	2.32	0.48
46:N:601:CHL:HED2	38:N:624:LHG:H141	1.95	0.48
46:G:607:CHL:H62	46:G:607:CHL:HMA3	1.95	0.48
28:d:403:CLA:H91	8:h:55:LEU:HB2	1.94	0.48
27:A:404:CL:CL	4:C:342:GLU:N	2.84	0.48
2:B:265:ILE:HG21	2:B:274:GLN:HE22	1.79	0.48
28:B:615:CLA:H92	31:M:101:SQD:H161	1.96	0.48
28:B:616:CLA:H8	28:B:617:CLA:HBB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:513:CLA:H101	30:C:514:BCR:H21C	1.96	0.48
5:D:185:PHE:CD1	5:D:189:HIS:HD2	2.32	0.48
13:M:23:LEU:HD13	13:m:24:ILE:HD11	1.96	0.48
20:N:45:ARG:NH1	20:N:61:THR:O	2.46	0.48
2:b:458:PHE:HB3	28:b:605:CLA:HBC2	1.96	0.48
1:A:156:ALA:HA	1:A:160:ILE:HB	1.96	0.48
1:A:328:MET:HE1	5:D:183:LEU:HD22	1.95	0.48
28:B:616:CLA:H2	28:B:617:CLA:HBB2	1.96	0.48
20:N:196:PRO:HA	20:N:199:PHE:HB3	1.96	0.48
22:S:194:PRO:HB2	22:S:218:PRO:HB3	1.95	0.48
46:Y:609:CHL:HHC	46:Y:609:CHL:HBB1	1.95	0.48
1:a:61:ASP:HB2	1:a:63:ILE:HG12	1.96	0.48
31:b:621:SQD:H142	31:b:621:SQD:H251	1.96	0.48
30:c:516:BCR:H15C	30:c:516:BCR:H351	1.58	0.48
14:o:78:THR:HA	17:w:66:ASN:HB3	1.96	0.48
14:o:279:GLU:HG2	14:o:282:ALA:HB3	1.96	0.48
28:A:405:CLA:H122	29:A:408:PHO:H3A	1.96	0.47
28:A:405:CLA:H18	38:D:409:LHG:H332	1.96	0.47
15:P:217:LEU:HD22	15:P:241:PHE:HB2	1.94	0.47
22:S:101:ARG:NE	22:S:104:GLU:OE1	2.46	0.47
28:a:405:CLA:H2	29:a:408:PHO:CHC	2.44	0.47
2:b:142:HIS:ND1	28:b:611:CLA:OBD	2.37	0.47
2:b:221:PRO:HB2	2:b:225:LEU:HD11	1.96	0.47
4:c:306:LEU:HG	4:c:316:VAL:HG11	1.96	0.47
4:C:102:SER:O	4:C:106:HIS:ND1	2.44	0.47
20:N:87:GLU:HG2	20:N:181:LEU:HD21	1.95	0.47
28:Y:613:CLA:H112	28:Y:613:CLA:H71	1.65	0.47
1:a:59:ASP:HA	1:a:66:PRO:HA	1.95	0.47
2:b:290:GLN:NE2	24:u:89:GLN:OE1	2.47	0.47
3:v:33:LEU:HB2	28:c:511:CLA:H42	1.96	0.47
14:o:116:VAL:HG22	14:o:288:ILE:HD12	1.96	0.47
4:C:67:LYS:NZ	4:C:71:GLU:OE1	2.47	0.47
5:D:154:VAL:HG21	32:H:102:LMG:H401	1.95	0.47
5:D:172:SER:HB2	5:D:177:SER:HB2	1.95	0.47
32:d:411:LMG:HC62	7:f:40:GLN:HE22	1.79	0.47
1:A:315:ASN:OD1	15:P:109:ASN:ND2	2.40	0.47
38:D:410:LHG:O3	38:D:410:LHG:O1	2.31	0.47
28:N:610:CLA:HBA2	28:N:610:CLA:H3A	1.64	0.47
28:Y:603:CLA:HAC1	46:Y:607:CHL:HBB2	1.97	0.47
4:C:312:LEU:HD11	15:P:190:LEU:HD23	1.97	0.47
5:D:122:LEU:HD21	28:D:402:CLA:H8	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:53:ALA:O	43:H:101:RRX:H21	2.14	0.47
11:K:45:PHE:HE2	45:K:101:4RF:H5	1.78	0.47
14:O:151:ASN:OD1	14:O:152:ASP:N	2.47	0.47
22:S:58:LYS:HE3	38:S:624:LHG:HC11	1.97	0.47
1:a:269:ARG:HG3	5:d:235:PHE:HB2	1.95	0.47
3:v:13:PHE:HA	3:v:16:VAL:HG12	1.97	0.47
28:c:502:CLA:H43	28:c:503:CLA:H52	1.97	0.47
35:c:520:DGD:HA41	32:d:411:LMG:H121	1.96	0.47
2:B:256:MET:HG3	2:B:448:ARG:HG3	1.96	0.47
30:B:619:BCR:HC42	32:B:622:LMG:H341	1.96	0.47
17:W:81:LEU:O	17:W:85:ILE:HG12	2.15	0.47
38:Y:624:LHG:H332	38:Y:624:LHG:H361	1.62	0.47
1:a:156:ALA:HA	1:a:160:ILE:HB	1.97	0.47
1:a:306:VAL:HA	10:j:39:GLY:HA2	1.96	0.47
5:d:274:VAL:HG12	41:d:405:PL9:H253	1.97	0.47
1:A:102:LEU:HG	33:A:414:SPH:H5	1.97	0.47
2:B:456:LEU:HD21	32:H:102:LMG:H201	1.96	0.47
28:B:603:CLA:H202	32:H:102:LMG:H371	1.96	0.47
3:V:16:VAL:HG22	30:C:516:BCR:H363	1.97	0.47
4:C:203:LYS:HB3	4:C:211:TRP:HA	1.96	0.47
6:E:82:GLN:O	15:P:58:ALA:N	2.48	0.47
1:a:173:PRO:HB2	1:a:178:GLY:HA3	1.94	0.47
28:a:405:CLA:H112	28:a:406:CLA:HBB1	1.96	0.47
2:b:149:LEU:HD22	28:b:605:CLA:H171	1.95	0.47
4:c:139:TRP:O	4:c:259:TYR:OH	2.21	0.47
6:e:65:LEU:HB3	6:e:67:THR:HG23	1.96	0.47
11:k:22:VAL:HA	11:k:25:LEU:HG	1.95	0.47
14:o:251:SER:HB3	14:o:273:ILE:HB	1.97	0.47
5:D:51:GLY:HA3	5:D:78:VAL:HG22	1.96	0.47
1:a:142:TRP:CZ2	4:c:435:ARG:HD2	2.50	0.47
28:b:608:CLA:H41	28:b:608:CLA:H62	1.53	0.47
7:f:44:ARG:HH21	10:j:40:SER:H	1.61	0.47
14:o:84:CYS:SG	14:o:110:GLU:HB2	2.55	0.47
28:C:507:CLA:H41	28:C:507:CLA:H61	1.55	0.47
18:X:64:SER:OG	18:X:65:VAL:N	2.43	0.47
20:N:138:TYR:OH	49:N:623:NEX:O23	2.27	0.47
1:a:195:HIS:ND1	1:a:293:MET:SD	2.88	0.47
1:a:254:TYR:HE2	5:d:138:LEU:HB2	1.79	0.47
2:b:283:GLU:HG3	2:b:309:LEU:HD21	1.96	0.47
2:b:364:GLU:H	5:d:326:ARG:NH1	2.13	0.47
28:B:603:CLA:HAA1	8:H:64:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:126:MET:HB2	5:D:146:PHE:HD2	1.79	0.47
6:E:62:ASP:OD1	6:E:62:ASP:N	2.48	0.47
14:o:62:LEU:HD21	14:o:80:ILE:HG23	1.97	0.47
1:A:14:TRP:NE1	9:I:25:SER:OG	2.39	0.46
2:B:201:HIS:HB2	28:B:603:CLA:C1B	2.46	0.46
2:b:273:TYR:OH	5:d:164:GLN:O	2.28	0.46
2:b:470:GLY:HA2	28:b:609:CLA:HED1	1.97	0.46
4:c:42:VAL:HG22	28:c:512:CLA:HED1	1.97	0.46
28:c:505:CLA:H203	35:c:518:DGD:HA71	1.96	0.46
5:d:141:TYR:HA	5:d:144:ILE:HD12	1.97	0.46
5:d:188:PHE:O	5:d:294:ARG:NH1	2.49	0.46
2:B:181:VAL:HG13	2:B:199:PRO:HG3	1.96	0.46
28:C:503:CLA:H61	28:C:503:CLA:H41	1.56	0.46
5:D:182:ILE:HG23	28:D:402:CLA:HAC1	1.97	0.46
15:P:132:GLY:O	15:P:185:TYR:OH	2.31	0.46
4:c:205:PRO:HG2	35:c:518:DGD:HA42	1.97	0.46
28:c:501:CLA:HMB1	30:c:515:BCR:H23C	1.97	0.46
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.97	0.46
1:A:269:ARG:NH1	5:D:234:ALA:O	2.48	0.46
5:D:141:TYR:OH	38:D:408:LHG:O4	2.28	0.46
1:a:127:MET:HB3	1:a:147:TYR:CD2	2.50	0.46
2:b:91:TRP:CD2	28:b:607:CLA:HBA2	2.49	0.46
28:b:615:CLA:H91	28:b:615:CLA:H112	1.75	0.46
38:d:410:LHG:H322	38:d:410:LHG:H291	1.63	0.46
1:A:25:GLU:O	4:C:458:ARG:NH2	2.47	0.46
1:A:103:ASP:OD1	31:b:626:SQD:O2	2.33	0.46
29:A:409:PHO:OBD	5:D:129:GLN:NE2	2.35	0.46
15:P:120:ALA:HB1	15:P:213:LYS:HD2	1.97	0.46
22:S:233:VAL:HA	22:S:236:ILE:HG22	1.97	0.46
1:a:42:LEU:HD11	36:t:101:3PH:H2B1	1.98	0.46
1:a:301:ASN:OD1	1:a:303:ASN:ND2	2.48	0.46
28:a:405:CLA:H141	28:a:405:CLA:H162	1.73	0.46
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.97	0.46
28:b:602:CLA:HAC1	43:h:101:RRX:H55	1.96	0.46
28:c:511:CLA:H101	30:c:517:BCR:H402	1.98	0.46
5:d:162:LEU:HD11	32:h:102:LMG:H292	1.98	0.46
1:A:323:ARG:NH1	15:P:110:PHE:O	2.49	0.46
4:C:216:ASP:OD2	4:C:216:ASP:N	2.47	0.46
6:E:66:ILE:O	6:E:75:GLN:NE2	2.48	0.46
1:a:304:GLN:N	1:a:319:ASP:OD1	2.48	0.46
5:d:172:SER:HB3	5:d:177:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:VAL:HG11	2:B:422:ARG:HH12	1.81	0.46
28:B:608:CLA:HMC1	30:B:619:BCR:H10C	1.97	0.46
20:N:247:ALA:HB3	48:G:622:XAT:H193	1.98	0.46
46:N:606:CHL:HHC	46:N:606:CHL:HBB1	1.96	0.46
22:S:217:ASP:OD1	47:S:620:LUT:O23	2.28	0.46
23:Y:168:PHE:CD2	28:Y:608:CLA:HAB	2.51	0.46
1:a:43:THR:HG23	30:a:411:BCR:H16C	1.98	0.46
1:a:52:PHE:CE2	41:d:405:PL9:H462	2.51	0.46
28:B:609:CLA:H3A	28:B:609:CLA:HBA2	1.68	0.46
31:B:626:SQD:O2	1:a:103:ASP:OD1	2.34	0.46
5:D:312:GLU:HB2	14:O:213:PRO:HG3	1.98	0.46
46:N:606:CHL:H72	46:N:606:CHL:HED1	1.97	0.46
1:a:164:GLY:O	4:c:279:TRP:NE1	2.49	0.46
1:a:304:GLN:HG2	1:a:313:VAL:HG21	1.98	0.46
2:b:36:ALA:HB2	30:b:619:BCR:H362	1.96	0.46
28:b:609:CLA:H3A	28:b:609:CLA:HBA2	1.68	0.46
37:c:524:DGA:HAW1	37:c:524:DGA:HAN2	1.68	0.46
10:j:12:LEU:HD13	45:k:101:4RF:H69	1.98	0.46
1:A:267:ASN:HD21	5:D:235:PHE:HB3	1.81	0.46
28:A:406:CLA:H43	38:L:101:LHG:H211	1.97	0.46
29:A:408:PHO:HAB	5:D:205:LEU:HD13	1.98	0.46
2:B:220:ARG:NE	8:H:39:LYS:O	2.45	0.46
4:C:14:ARG:O	11:K:46:ARG:NH1	2.49	0.46
23:Y:119:GLU:OE2	23:Y:133:LYS:NZ	2.39	0.46
28:b:610:CLA:H193	28:b:610:CLA:H162	1.82	0.46
4:c:282:ASN:N	35:c:518:DGD:O5E	2.41	0.46
28:c:507:CLA:H142	30:c:515:BCR:H16C	1.98	0.46
14:o:228:LEU:HD13	14:o:231:LYS:HG3	1.97	0.46
4:C:270:MET:HE1	28:C:503:CLA:H91	1.97	0.46
4:C:315:ASN:HD21	14:O:161:GLU:HB2	1.80	0.46
38:D:410:LHG:H322	38:D:410:LHG:H291	1.74	0.46
20:N:226:VAL:HG23	20:N:227:THR:HG23	1.97	0.46
46:N:609:CHL:HAA2	23:Y:73:THR:HG21	1.98	0.46
46:S:607:CHL:HHC	46:S:607:CHL:HBB1	1.97	0.46
28:Y:602:CLA:CAB	47:Y:621:LUT:H32	2.46	0.46
4:c:309:ASP:OD2	4:c:328:TYR:OH	2.29	0.46
14:o:148:LYS:NZ	14:o:156:GLU:OE2	2.44	0.46
1:A:296:ASN:HB3	4:C:389:LEU:HD13	1.98	0.46
2:B:183:PRO:HG3	2:B:199:PRO:HB2	1.98	0.46
4:C:272:PHE:HB3	35:C:518:DGD:HB62	1.97	0.46
21:G:188:ASP:OD1	21:G:188:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:G:620:LUT:H15	47:G:620:LUT:H201	1.78	0.46
23:Y:102:LEU:HD21	28:Y:612:CLA:H202	1.98	0.46
1:a:225:ARG:NH2	2:b:481:GLY:O	2.49	0.46
28:b:606:CLA:H141	28:b:606:CLA:H162	1.77	0.46
28:c:503:CLA:H41	28:c:503:CLA:H62	1.54	0.46
5:d:225:ASP:HB2	5:d:234:ALA:HB1	1.98	0.46
28:d:403:CLA:H41	28:d:403:CLA:H61	1.55	0.46
6:e:13:ILE:O	6:e:16:SER:OG	2.34	0.46
2:B:175:THR:OG1	2:B:176:GLY:N	2.49	0.45
2:B:191:ASP:HB3	2:B:194:ASN:HB2	1.97	0.45
2:B:242:ILE:HG23	2:B:462:PHE:HD2	1.80	0.45
32:C:523:LMG:H411	33:Y:625:SPH:H122	1.98	0.45
48:G:622:XAT:H201	48:G:622:XAT:H15	1.69	0.45
24:U:107:LYS:HA	24:U:110:ARG:HG2	1.99	0.45
30:a:411:BCR:H351	30:a:411:BCR:H15C	1.77	0.45
2:b:172:TYR:CE1	2:b:283:GLU:HB2	2.50	0.45
2:b:315:ILE:HG22	2:b:426:LEU:HB3	1.97	0.45
28:b:605:CLA:HBB2	30:b:619:BCR:H343	1.97	0.45
38:c:525:LHG:H331	38:c:525:LHG:H361	1.76	0.45
2:B:281:GLN:HE22	24:U:101:ALA:HB3	1.82	0.45
28:B:611:CLA:HHC	28:B:611:CLA:HBB1	1.98	0.45
21:G:41:LEU:O	21:G:44:PHE:HB2	2.15	0.45
28:a:406:CLA:H12	38:l:101:LHG:H211	1.97	0.45
5:d:85:LEU:HA	6:e:69:ARG:HG3	1.98	0.45
1:A:45:ILE:O	1:A:49:ILE:HG12	2.16	0.45
28:A:410:CLA:H2	9:I:12:VAL:HG11	1.99	0.45
28:A:410:CLA:HBC1	33:A:414:SPH:H152	1.98	0.45
30:C:517:BCR:H351	30:C:517:BCR:H15C	1.75	0.45
15:P:99:VAL:HB	15:P:102:ILE:HG13	1.99	0.45
47:N:621:LUT:H11	47:N:621:LUT:H191	1.86	0.45
22:S:244:ILE:HG21	38:S:624:LHG:H282	1.98	0.45
1:a:334:ARG:HH11	5:d:320:LEU:HD22	1.81	0.45
31:b:626:SQD:H223	31:b:626:SQD:H321	1.99	0.45
28:c:510:CLA:H193	28:c:510:CLA:H162	1.79	0.45
2:B:426:LEU:HD13	2:B:443:PHE:HZ	1.81	0.45
38:D:409:LHG:H322	16:T:21:ILE:HD11	1.99	0.45
28:N:613:CLA:H111	28:N:613:CLA:H152	1.75	0.45
21:G:150:VAL:HG23	46:G:609:CHL:HBB2	1.97	0.45
32:a:413:LMG:H322	4:c:205:PRO:HD3	1.99	0.45
2:b:171:PRO:HA	8:h:84:LEU:HD12	1.97	0.45
2:b:325:PHE:CZ	5:d:195:PRO:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:465:GLY:O	2:b:469:HIS:ND1	2.33	0.45
28:b:605:CLA:H2	28:b:613:CLA:H152	1.97	0.45
28:b:609:CLA:H172	8:h:62:LEU:HD11	1.98	0.45
4:c:176:THR:HG23	4:c:177:TRP:HD1	1.79	0.45
4:c:344:MET:O	4:c:347:TRP:HB3	2.16	0.45
15:p:99:VAL:HB	15:p:102:ILE:HD11	1.98	0.45
1:A:321:ILE:O	1:A:325:ASN:ND2	2.49	0.45
30:C:516:BCR:H351	30:C:516:BCR:H15C	1.72	0.45
32:W:201:LMG:H131	32:W:201:LMG:H301	1.99	0.45
23:Y:137:LEU:HD21	28:Y:604:CLA:HAA2	1.99	0.45
24:U:95:LEU:HD12	24:U:108:GLU:HG2	1.98	0.45
1:a:248:ILE:HG23	1:a:252:HIS:CE1	2.52	0.45
5:d:12:ARG:NH2	5:d:20:ASP:OD2	2.39	0.45
14:o:253:VAL:O	14:o:271:GLU:N	2.47	0.45
2:B:327:THR:HG22	28:B:608:CLA:H11	1.98	0.45
28:N:604:CLA:H121	49:N:623:NEX:H402	1.99	0.45
1:a:202:VAL:HG23	28:a:405:CLA:HMB2	1.97	0.45
28:b:615:CLA:H51	31:m:101:SQD:H272	1.99	0.45
31:b:621:SQD:H151	31:b:621:SQD:H272	1.99	0.45
4:c:132:TYR:O	4:c:136:GLY:N	2.50	0.45
28:S:602:CLA:H93	28:S:603:CLA:HMD3	1.98	0.45
4:c:16:GLN:HG2	4:c:22:ALA:HA	1.98	0.45
4:c:303:PHE:HE2	4:c:377:GLU:HA	1.80	0.45
15:p:165:VAL:O	15:p:194:ALA:N	2.50	0.45
15:p:171:LEU:HB2	15:p:188:GLU:HG2	1.98	0.45
1:A:216:GLY:HA2	5:D:268:HIS:HB3	1.99	0.45
2:B:327:THR:O	2:B:444:ARG:NE	2.48	0.45
28:B:604:CLA:CAD	28:B:606:CLA:H12	2.47	0.45
4:C:44:HIS:HD2	28:C:509:CLA:HMB3	1.82	0.45
14:O:258:LYS:HD2	14:O:258:LYS:HA	1.88	0.45
48:N:622:XAT:H391	48:N:622:XAT:H31	1.66	0.45
21:G:190:PRO:HA	21:G:193:PHE:HB3	1.99	0.45
28:Y:613:CLA:H143	38:Y:624:LHG:H361	1.97	0.45
2:b:414:PRO:HA	2:b:417:VAL:HG22	1.99	0.45
6:e:8:ARG:HE	6:e:12:ASP:HB3	1.82	0.45
16:t:11:ILE:HA	16:t:14:LEU:HG	1.98	0.45
17:w:62:ASP:OD1	17:w:64:ARG:NH1	2.50	0.45
4:C:64:VAL:O	4:C:72:GLN:NE2	2.44	0.45
4:C:449:ARG:NH2	5:D:225:ASP:OD2	2.49	0.45
14:O:228:LEU:HA	14:O:229:PRO:HD3	1.80	0.45
20:N:45:ARG:NE	20:N:67:ASP:O	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:287:PRO:HB2	22:S:289:LEU:HD22	1.99	0.45
2:b:10:THR:HA	2:b:13:ILE:HG23	1.98	0.45
28:b:608:CLA:H152	28:b:608:CLA:H112	1.65	0.45
4:c:106:HIS:CE1	28:c:503:CLA:HED2	2.51	0.45
4:c:395:VAL:HG13	4:c:403:ASN:HA	1.99	0.45
5:d:201:VAL:HG23	28:d:402:CLA:HMB2	1.99	0.45
1:A:50:ILE:HG21	30:A:411:BCR:H23C	1.99	0.45
28:B:608:CLA:H62	28:B:608:CLA:H41	1.59	0.45
6:E:8:ARG:NH1	6:E:12:ASP:OD2	2.50	0.45
22:S:61:LEU:HD22	22:S:65:LEU:HG	1.98	0.45
28:Y:614:CLA:HMB2	51:Y:626:PTY:H161	1.98	0.45
30:c:517:BCR:H341	19:z:16:SER:OG	2.17	0.45
5:d:57:SER:O	5:d:57:SER:OG	2.35	0.45
5:d:100:ASP:OD2	5:d:103:ARG:NH1	2.50	0.45
2:B:382:PRO:HG2	2:B:385:LYS:HG3	2.00	0.44
45:I:102:4RF:H54	45:I:102:4RF:H60	1.61	0.44
21:G:220:VAL:HG21	28:G:613:CLA:HMD2	1.98	0.44
46:S:606:CHL:HHC	46:S:606:CHL:HBB1	1.98	0.44
23:Y:237:LEU:HB2	47:Y:620:LUT:H22	1.99	0.44
28:Y:612:CLA:H192	28:Y:612:CLA:H162	1.80	0.44
4:c:177:TRP:HA	4:c:352:PRO:HB3	1.99	0.44
28:c:504:CLA:H62	35:c:519:DGD:HB62	1.98	0.44
5:d:221:THR:HG23	5:d:244:TYR:HB2	1.99	0.44
7:f:32:PHE:O	7:f:36:ILE:HG12	2.17	0.44
32:B:622:LMG:H171	32:B:622:LMG:H142	1.79	0.44
20:N:204:VAL:HG12	20:N:208:LYS:HE2	1.98	0.44
38:N:624:LHG:H131	48:G:622:XAT:H403	2.00	0.44
21:G:41:LEU:HB3	21:G:44:PHE:HB2	1.99	0.44
1:a:52:PHE:HZ	1:a:77:ILE:HG22	1.81	0.44
29:a:408:PHO:H3A	29:a:408:PHO:HBA2	1.53	0.44
2:b:462:PHE:HA	28:b:612:CLA:HMC2	1.99	0.44
28:b:604:CLA:H192	28:b:610:CLA:H91	1.99	0.44
6:e:51:ARG:HB2	6:e:54:GLU:HG2	1.99	0.44
1:A:9:GLU:OE1	1:A:11:THR:OG1	2.28	0.44
29:A:409:PHO:H62	28:D:402:CLA:H111	1.98	0.44
2:B:142:HIS:ND1	28:B:611:CLA:OBD	2.38	0.44
28:B:612:CLA:H162	28:B:612:CLA:H193	1.76	0.44
45:I:102:4RF:H1	28:b:607:CLA:H192	2.00	0.44
28:G:610:CLA:H52	47:G:620:LUT:H30	1.99	0.44
30:c:515:BCR:H351	30:c:515:BCR:H15C	1.66	0.44
35:c:519:DGD:HA72	35:c:520:DGD:HB91	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:88:SER:O	5:d:167:TRP:NE1	2.44	0.44
5:d:231:THR:O	5:d:234:ALA:HB3	2.17	0.44
31:A:412:SQD:H341	35:C:519:DGD:HAF2	2.00	0.44
1:a:32:TRP:HA	1:a:35:VAL:HG12	2.00	0.44
28:b:614:CLA:HBD	28:b:615:CLA:HAB	1.98	0.44
28:c:509:CLA:H112	28:c:509:CLA:H142	1.86	0.44
1:A:334:ARG:HB2	14:O:211:LEU:HD12	2.00	0.44
28:B:614:CLA:H162	28:B:614:CLA:H141	1.75	0.44
28:S:613:CLA:H11	28:S:613:CLA:H52	1.68	0.44
47:S:620:LUT:H35	47:S:620:LUT:H401	1.82	0.44
1:a:120:PHE:HD2	28:c:505:CLA:H202	1.82	0.44
1:a:157:VAL:HG22	1:a:290:ILE:HG21	2.00	0.44
28:b:605:CLA:H71	28:b:611:CLA:H62	1.99	0.44
16:t:13:THR:O	16:t:17:ILE:HG12	2.17	0.44
28:B:602:CLA:H3A	28:B:602:CLA:HBA2	1.45	0.44
28:C:501:CLA:H61	28:C:501:CLA:H41	1.67	0.44
28:C:501:CLA:H203	28:C:507:CLA:H162	2.00	0.44
28:D:403:CLA:H161	28:D:403:CLA:H141	1.75	0.44
28:G:602:CLA:CAB	47:G:621:LUT:H32	2.47	0.44
28:S:602:CLA:H41	28:S:602:CLA:H62	1.70	0.44
28:S:611:CLA:H91	28:S:611:CLA:H142	1.99	0.44
47:Y:620:LUT:H35	47:Y:620:LUT:H401	1.85	0.44
28:a:406:CLA:HED1	41:d:405:PL9:H351	1.98	0.44
29:a:409:PHO:OBD	5:d:129:GLN:NE2	2.50	0.44
28:a:410:CLA:H2	9:i:12:VAL:HG11	1.99	0.44
2:b:75:TRP:HZ2	2:b:90:ILE:HA	1.83	0.44
36:b:624:3PH:H3D2	36:b:624:3PH:H3G2	1.79	0.44
5:d:189:HIS:HA	5:d:294:ARG:HG2	1.99	0.44
28:A:405:CLA:H42	28:A:406:CLA:HMC1	2.00	0.44
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.00	0.44
2:B:387:GLU:HA	15:P:146:GLY:HA3	2.00	0.44
46:N:605:CHL:HAA1	36:S:626:3PH:H3C2	1.99	0.44
46:G:606:CHL:HHC	46:G:606:CHL:HBB1	1.98	0.44
22:S:218:PRO:HD2	47:S:620:LUT:H23	2.00	0.44
22:S:271:PRO:HG2	28:S:614:CLA:HMB2	1.99	0.44
22:S:275:ASN:H	22:S:278:THR:HB	1.82	0.44
1:a:320:ILE:HG21	5:d:180:ARG:HG3	1.99	0.44
30:b:618:BCR:HC32	32:b:622:LMG:H311	1.98	0.44
4:c:443:PHE:HZ	4:c:447:ILE:HG22	1.82	0.44
28:c:503:CLA:H93	28:c:503:CLA:H111	1.87	0.44
28:c:510:CLA:H122	28:c:510:CLA:H8	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:54:PHE:HB3	6:e:47:PHE:CZ	2.53	0.44
12:l:25:ILE:HG13	13:m:18:PRO:HB2	1.99	0.44
14:o:171:LYS:HE3	14:o:175:GLY:HA2	2.00	0.44
28:B:615:CLA:H91	28:B:615:CLA:H112	1.76	0.44
4:C:218:LEU:HA	4:C:221:ILE:HB	2.00	0.44
4:C:221:ILE:O	4:C:225:HIS:ND1	2.46	0.44
4:C:298:SER:HB3	4:C:343:THR:HG22	2.00	0.44
4:C:413:TRP:CE2	28:C:504:CLA:HBA1	2.52	0.44
28:G:604:CLA:HBB1	49:G:623:NEX:H27	2.00	0.44
47:Y:621:LUT:H11	47:Y:621:LUT:H191	1.91	0.44
28:b:609:CLA:H161	28:d:403:CLA:HMA3	1.99	0.44
35:c:519:DGD:HA22	35:c:520:DGD:HB22	2.00	0.44
35:c:520:DGD:HAW2	32:d:411:LMG:H191	1.99	0.44
5:d:338:LYS:HE3	5:d:338:LYS:HB3	1.88	0.44
5:d:343:GLU:OE2	5:d:348:ARG:NH2	2.46	0.44
14:O:208:SER:O	14:O:219:ALA:N	2.43	0.44
28:a:405:CLA:H161	28:a:406:CLA:H72	1.99	0.44
2:b:260:SER:N	2:b:263:THR:OG1	2.39	0.44
28:c:511:CLA:H93	28:c:511:CLA:H61	1.79	0.44
28:d:403:CLA:HBA1	28:d:403:CLA:H12	1.78	0.44
14:o:286:LYS:HD3	14:o:286:LYS:HA	1.81	0.44
1:A:331:MET:HA	1:A:331:MET:HE2	2.00	0.43
4:C:200:TYR:HA	4:C:203:LYS:HE3	2.00	0.43
35:C:519:DGD:HA21	37:J:101:DGA:HA72	1.99	0.43
1:a:274:PHE:HA	1:a:277:VAL:HG12	2.00	0.43
2:b:75:TRP:HD1	2:b:88:PRO:HG2	1.82	0.43
2:b:175:THR:OG1	2:b:176:GLY:N	2.49	0.43
28:b:605:CLA:H93	28:b:605:CLA:H61	1.85	0.43
28:b:613:CLA:H61	28:b:613:CLA:H102	1.60	0.43
28:c:511:CLA:H91	28:c:511:CLA:H111	1.71	0.43
38:d:409:LHG:H252	12:l:19:TYR:HB3	1.99	0.43
14:o:246:THR:HA	15:p:153:GLN:HE22	1.82	0.43
28:B:603:CLA:H193	32:H:102:LMG:H171	2.00	0.43
4:C:246:PRO:HG3	4:C:249:ARG:HH21	1.83	0.43
5:D:343:GLU:OE1	15:P:201:ARG:NH2	2.51	0.43
38:D:409:LHG:H292	16:T:17:ILE:HG23	2.00	0.43
13:M:12:ALA:O	13:M:16:ILE:HG12	2.18	0.43
14:O:119:VAL:HG12	14:O:121:ASP:H	1.83	0.43
14:O:233:ASP:OD1	14:O:233:ASP:N	2.51	0.43
20:N:158:VAL:HG22	46:Y:601:CHL:H93	2.00	0.43
46:N:606:CHL:HBB2	46:N:607:CHL:HAB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N:607:CHL:H162	46:N:609:CHL:H101	2.00	0.43
21:G:91:LEU:HB3	28:G:604:CLA:HAB	2.00	0.43
48:G:622:XAT:H31	48:G:622:XAT:H391	1.76	0.43
28:S:602:CLA:H51	47:S:621:LUT:H28	2.00	0.43
28:Y:611:CLA:H61	28:Y:611:CLA:H41	1.69	0.43
47:Y:621:LUT:H35	47:Y:621:LUT:H401	1.81	0.43
51:Y:626:PTY:H342	51:Y:626:PTY:H371	1.80	0.43
24:U:94:VAL:HG13	24:U:107:LYS:HE3	2.00	0.43
5:d:188:PHE:HE1	5:d:329:MET:HG3	1.83	0.43
8:h:19:GLU:HA	8:h:20:PRO:HD3	1.89	0.43
45:i:101:4RF:H36	45:i:101:4RF:H31	1.67	0.43
12:l:14:ASN:OD1	12:l:14:ASN:N	2.51	0.43
2:B:349:GLN:HG2	2:B:396:GLY:HA3	2.00	0.43
5:D:123:ILE:HD11	32:H:102:LMG:H392	2.01	0.43
15:P:78:TYR:HB3	15:P:87:LEU:HD13	1.99	0.43
28:Y:614:CLA:H152	28:Y:614:CLA:H18	1.75	0.43
1:a:43:THR:HG23	30:a:411:BCR:H362	2.00	0.43
1:a:86:SER:HB3	1:a:89:ILE:HG12	2.00	0.43
28:b:613:CLA:H111	28:b:614:CLA:CAB	2.47	0.43
31:b:626:SQD:H91	31:b:626:SQD:H121	1.76	0.43
28:c:510:CLA:H112	28:c:510:CLA:H152	1.70	0.43
29:A:409:PHO:HBA1	29:A:409:PHO:H3A	1.45	0.43
2:B:185:TRP:HB2	28:B:602:CLA:HED2	2.01	0.43
28:B:605:CLA:H61	28:B:605:CLA:H41	1.76	0.43
28:B:612:CLA:H92	38:D:408:LHG:H351	2.00	0.43
28:B:615:CLA:H3A	28:B:615:CLA:HBA2	1.83	0.43
5:D:201:VAL:HG13	28:D:402:CLA:HMB1	1.99	0.43
28:G:603:CLA:H93	28:Y:603:CLA:H101	2.00	0.43
23:Y:162:MET:CE	49:Y:623:NEX:H30	2.48	0.43
1:a:65:GLU:HA	1:a:66:PRO:HD3	1.83	0.43
2:b:34:ALA:O	2:b:38:THR:HG22	2.19	0.43
2:b:257:TRP:NE1	5:d:163:GLY:O	2.49	0.43
2:b:378:ARG:CZ	15:p:97:LYS:HE3	2.48	0.43
2:b:385:LYS:HB3	15:p:149:ALA:HB3	2.00	0.43
4:c:175:ASP:O	4:c:182:GLY:CA	2.61	0.43
2:B:109:LEU:HD11	30:B:619:BCR:H282	2.00	0.43
28:C:504:CLA:H142	35:C:520:DGD:HBT2	2.01	0.43
5:D:48:TRP:HA	5:D:78:VAL:HG21	2.00	0.43
47:S:621:LUT:H35	47:S:621:LUT:H401	1.81	0.43
28:Y:602:CLA:H91	28:Y:602:CLA:H111	1.69	0.43
46:Y:606:CHL:HBB2	46:Y:607:CHL:HAB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:405:CLA:H201	38:d:409:LHG:H161	2.00	0.43
2:b:170:ASP:CG	2:b:174:LEU:H	2.26	0.43
4:c:330:MET:HE3	4:c:340:GLY:HA2	2.00	0.43
30:d:404:BCR:H15C	7:f:29:THR:HG22	2.00	0.43
6:e:51:ARG:NH1	6:e:54:GLU:OE2	2.50	0.43
14:o:214:LYS:HA	14:o:214:LYS:HD2	1.71	0.43
28:A:405:CLA:H142	28:A:405:CLA:H112	1.83	0.43
28:B:617:CLA:H51	28:B:617:CLA:H11	1.77	0.43
5:D:36:LEU:HA	28:D:403:CLA:HBB2	2.01	0.43
5:D:219:GLU:HG2	38:D:410:LHG:HC62	2.00	0.43
22:S:94:GLU:HA	22:S:97:VAL:HG12	2.01	0.43
2:b:18:ARG:HH12	12:l:5:ASN:ND2	2.16	0.43
28:b:614:CLA:H71	28:b:614:CLA:H112	1.81	0.43
28:c:505:CLA:H91	28:c:505:CLA:H111	1.78	0.43
28:c:509:CLA:HBB1	28:c:509:CLA:HMB3	2.01	0.43
1:A:106:LEU:HD11	30:A:411:BCR:H292	2.00	0.43
28:C:513:CLA:H91	28:C:513:CLA:H112	1.78	0.43
46:G:607:CHL:H13	46:G:607:CHL:H102	1.89	0.43
31:a:412:SQD:H461	4:c:24:TRP:CH2	2.54	0.43
2:b:272:ARG:NH2	2:b:276:ASP:OD2	2.50	0.43
2:b:326:ARG:HH21	5:d:297:ASP:HB2	1.83	0.43
28:b:612:CLA:H71	28:b:612:CLA:H112	1.94	0.43
30:b:618:BCR:H15C	30:b:618:BCR:H351	1.80	0.43
4:c:133:PRO:O	4:c:144:LYS:NZ	2.39	0.43
17:w:65:MET:HG2	17:w:67:GLY:H	1.83	0.43
2:B:9:HIS:CG	28:B:613:CLA:HAB	2.54	0.43
28:B:609:CLA:HMA1	5:D:130:PHE:HE1	1.83	0.43
1:a:219:VAL:HG11	5:d:268:HIS:HD1	1.82	0.43
1:a:269:ARG:NH1	5:d:231:THR:OG1	2.49	0.43
2:b:184:SER:N	2:b:196:GLY:O	2.51	0.43
4:c:166:LYS:NZ	4:c:172:GLY:O	2.51	0.43
4:c:244:PRO:HA	28:c:506:CLA:HED3	1.99	0.43
5:d:61:HIS:HE2	5:d:80:THR:HG1	1.60	0.43
15:p:190:LEU:HD13	15:p:202:HIS:CE1	2.53	0.43
2:B:331:ASN:O	2:B:439:SER:OG	2.36	0.43
28:B:609:CLA:H143	28:B:609:CLA:H161	1.82	0.43
4:C:447:ILE:O	5:D:224:GLU:N	2.43	0.43
28:C:508:CLA:HED2	38:D:410:LHG:HC2	2.01	0.43
5:D:321:LEU:O	5:D:325:ILE:HG12	2.19	0.43
2:b:329:ALA:O	2:b:332:SER:OG	2.30	0.43
2:b:363:PHE:CE2	5:d:326:ARG:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:428:GLY:N	28:c:508:CLA:HBC2	2.34	0.43
14:o:72:TYR:HA	14:o:75:VAL:HG22	2.00	0.43
5:D:129:GLN:HB2	5:D:143:ALA:HB2	2.00	0.43
12:L:5:ASN:HD21	12:L:8:LYS:HE2	1.84	0.43
22:S:85:TYR:HE2	46:S:601:CHL:HAA2	1.84	0.43
28:S:611:CLA:H162	28:S:611:CLA:H192	1.78	0.43
36:S:626:3PH:H262	36:S:626:3PH:H292	1.82	0.43
38:Y:624:LHG:H331	38:Y:624:LHG:H301	1.77	0.43
29:a:409:PHO:HBA1	29:a:409:PHO:H3A	1.47	0.43
29:a:409:PHO:H11	5:d:125:PHE:HB2	2.00	0.43
28:c:513:CLA:H91	28:c:513:CLA:H112	1.80	0.43
19:z:56:VAL:O	19:z:59:SER:OG	2.36	0.43
1:A:131:TRP:CZ3	28:C:505:CLA:HAA2	2.53	0.42
2:B:471:SER:HB2	5:D:140:PRO:HG2	2.00	0.42
28:B:609:CLA:HMB2	5:D:126:MET:HE2	2.00	0.42
3:V:13:PHE:HA	3:V:16:VAL:HG12	2.01	0.42
4:C:281:ASN:O	4:C:411:ARG:NH1	2.51	0.42
5:D:325:ILE:O	5:D:329:MET:CB	2.67	0.42
16:T:19:PHE:CD1	31:b:621:SQD:H152	2.54	0.42
19:Z:26:VAL:HG11	19:Z:40:VAL:HG21	2.01	0.42
28:N:613:CLA:H162	28:N:613:CLA:H203	1.82	0.42
49:N:623:NEX:H15	49:N:623:NEX:H201	1.92	0.42
28:G:602:CLA:H3A	28:G:602:CLA:HBA2	1.58	0.42
28:G:603:CLA:HAC1	46:G:607:CHL:HBB2	2.00	0.42
47:S:621:LUT:H15	47:S:621:LUT:H201	1.90	0.42
23:Y:217:PHE:CD2	28:Y:613:CLA:HAB	2.54	0.42
2:b:16:PRO:HG2	2:b:123:PHE:HB3	2.00	0.42
2:b:44:VAL:HG12	36:b:624:3PH:H351	2.00	0.42
28:b:610:CLA:HMA2	28:b:611:CLA:C2C	2.49	0.42
4:c:27:ASN:HD22	28:c:509:CLA:CAB	2.32	0.42
5:d:54:PHE:HB3	6:e:47:PHE:CE1	2.54	0.42
1:A:51:ALA:O	1:A:55:ALA:CB	2.66	0.42
1:A:260:PHE:O	1:A:264:SER:OG	2.28	0.42
2:B:12:VAL:HG23	28:B:613:CLA:HMC2	2.01	0.42
2:B:26:HIS:CE1	28:B:613:CLA:HMA3	2.54	0.42
4:C:228:ILE:HD13	30:C:515:BCR:H372	2.00	0.42
32:C:523:LMG:H171	32:C:523:LMG:H202	1.88	0.42
5:D:146:PHE:O	5:D:149:PRO:HD2	2.19	0.42
14:O:147:MET:HE2	14:O:298:LEU:HD21	2.01	0.42
28:N:613:CLA:H91	28:N:613:CLA:H112	1.83	0.42
29:a:408:PHO:NB	5:d:209:LEU:HD21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:417:SER:HB2	35:c:519:DGD:HBT2	2.00	0.42
28:c:512:CLA:H91	28:c:512:CLA:H112	1.83	0.42
32:h:102:LMG:H152	32:h:102:LMG:H181	1.66	0.42
15:p:134:PRO:HB3	15:p:187:PHE:CE1	2.54	0.42
18:x:65:VAL:HG13	18:x:69:LEU:HD22	2.01	0.42
2:B:474:ILE:HG23	37:B:625:DGA:HG2	2.01	0.42
30:C:515:BCR:HC31	9:I:24:LEU:HD22	2.01	0.42
5:D:56:THR:HG21	6:E:50:PRO:HD3	2.01	0.42
5:D:262:SER:OG	38:D:409:LHG:O4	2.32	0.42
9:I:14:PHE:O	9:I:18:LEU:HG	2.19	0.42
12:L:18:LEU:HD22	13:M:26:TYR:CG	2.54	0.42
46:N:605:CHL:H62	22:S:120:ILE:HD11	2.01	0.42
46:Y:607:CHL:HAA1	48:Y:622:XAT:H41	2.01	0.42
2:b:5:TRP:NE1	38:l:101:LHG:O10	2.52	0.42
2:b:156:PHE:HB3	2:b:162:PHE:HB3	1.99	0.42
3:v:15:VAL:HG12	30:c:516:BCR:H323	2.00	0.42
4:c:177:TRP:CD1	4:c:352:PRO:HG3	2.54	0.42
28:c:506:CLA:HMC1	28:c:507:CLA:H101	2.00	0.42
5:d:312:GLU:HG2	14:o:213:PRO:HG3	2.01	0.42
30:d:404:BCR:H15C	30:d:404:BCR:H351	1.74	0.42
15:p:127:SER:HA	15:p:209:VAL:HG21	2.00	0.42
28:A:405:CLA:NB	28:D:402:CLA:HBB1	2.35	0.42
31:A:412:SQD:H381	11:K:30:VAL:HG13	2.01	0.42
5:D:79:SER:HA	5:D:172:SER:HB3	2.01	0.42
49:S:623:NEX:H11	49:S:623:NEX:H191	1.88	0.42
28:b:617:CLA:H141	28:b:617:CLA:H162	1.81	0.42
29:A:409:PHO:H112	29:A:409:PHO:H72	1.85	0.42
6:E:78:LYS:HB2	6:E:78:LYS:HE2	1.88	0.42
14:O:211:LEU:HD21	14:O:220:THR:HG23	2.01	0.42
20:N:36:THR:OG1	20:N:37:ILE:N	2.51	0.42
20:N:41:TYR:CE2	20:N:200:ALA:HB1	2.55	0.42
46:N:601:CHL:H41	46:N:601:CHL:H61	1.78	0.42
36:S:626:3PH:H342	36:S:626:3PH:H371	1.82	0.42
48:Y:622:XAT:H391	48:Y:622:XAT:H31	1.71	0.42
1:a:49:ILE:HG12	41:d:405:PL9:H503	2.01	0.42
4:c:63:PHE:HZ	4:c:93:VAL:HG21	1.85	0.42
4:c:120:HIS:HA	4:c:124:GLY:HA3	2.01	0.42
4:c:421:LEU:HB3	28:c:502:CLA:HMC2	2.00	0.42
15:p:104:LEU:HD11	15:p:106:TYR:HE1	1.84	0.42
2:B:24:LEU:HD21	28:B:617:CLA:CAB	2.50	0.42
28:B:603:CLA:H203	5:D:154:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:ASN:HD22	32:H:102:LMG:HC8	1.85	0.42
15:P:206:LYS:HD3	15:P:241:PHE:HB3	2.02	0.42
20:N:158:VAL:HG13	46:N:609:CHL:HBB2	2.01	0.42
28:G:613:CLA:H143	28:G:613:CLA:H111	1.91	0.42
28:S:610:CLA:H3A	28:S:610:CLA:HBA2	1.49	0.42
28:b:607:CLA:H152	28:b:607:CLA:H111	1.85	0.42
28:b:617:CLA:H51	28:b:617:CLA:H11	1.75	0.42
5:d:156:VAL:HG23	5:d:157:PHE:CD2	2.54	0.42
12:l:36:ILE:HG22	13:m:7:GLY:HA2	2.00	0.42
1:A:131:TRP:HE1	4:C:434:GLY:HA2	1.85	0.42
1:A:300:PHE:HD1	4:C:393:ASN:HD21	1.68	0.42
28:B:607:CLA:OBD	35:B:623:DGD:O3D	2.32	0.42
3:V:8:GLN:NE2	11:K:23:ASP:OD1	2.52	0.42
4:C:141:ASP:O	4:C:145:MET:HG2	2.20	0.42
28:C:512:CLA:NB	30:C:514:BCR:H401	2.34	0.42
6:E:57:THR:OG1	6:E:59:ASP:OD1	2.30	0.42
1:a:314:LEU:HG	6:e:55:TYR:CZ	2.55	0.42
28:b:613:CLA:H192	28:b:613:CLA:H162	1.84	0.42
28:B:608:CLA:H201	13:M:11:THR:HA	2.01	0.42
28:C:506:CLA:H8	28:C:506:CLA:H122	1.87	0.42
7:F:44:ARG:HB3	15:P:69:VAL:HG23	2.01	0.42
11:K:12:PRO:HB2	11:K:15:TYR:HD2	1.84	0.42
47:N:621:LUT:H15	47:N:621:LUT:H201	1.85	0.42
22:S:264:ILE:HD13	47:S:620:LUT:H163	2.02	0.42
4:c:166:LYS:HB2	28:c:502:CLA:H203	2.02	0.42
28:c:512:CLA:HMB1	38:c:525:LHG:H121	2.02	0.42
38:d:408:LHG:H152	12:l:24:LEU:HD11	2.02	0.42
4:C:295:PRO:HB3	4:C:346:PHE:HB3	2.02	0.42
4:C:338:ILE:HG21	4:C:347:TRP:HB2	2.01	0.42
7:F:20:LEU:HD23	7:F:20:LEU:HA	1.90	0.42
1:a:218:LEU:HB3	1:a:251:ALA:HB1	2.00	0.42
2:b:321:LYS:HD2	2:b:321:LYS:HA	1.76	0.42
2:b:376:VAL:O	2:b:378:ARG:NH1	2.53	0.42
28:b:609:CLA:H61	28:b:609:CLA:H41	1.81	0.42
28:b:609:CLA:H91	37:b:625:DGA:HBF1	2.02	0.42
28:b:610:CLA:H92	28:b:610:CLA:H61	1.77	0.42
38:c:525:LHG:H161	38:c:525:LHG:H192	1.88	0.42
19:z:12:LEU:HA	19:z:15:VAL:HG12	2.02	0.42
1:A:184:ILE:HG23	1:A:328:MET:HG2	2.02	0.42
1:A:228:THR:OG1	1:A:230:ASN:OD1	2.28	0.42
28:B:612:CLA:H52	28:B:614:CLA:HED3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:60:VAL:HG12	4:C:77:LEU:HD21	2.02	0.42
28:C:501:CLA:H161	28:C:506:CLA:HBB1	2.01	0.42
14:O:212:ASP:OD2	14:O:216:ARG:NE	2.52	0.42
47:N:621:LUT:H35	47:N:621:LUT:H401	1.80	0.42
28:G:604:CLA:C2B	47:G:621:LUT:H183	2.50	0.42
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.02	0.42
2:b:106:LEU:HD11	28:b:607:CLA:H143	2.00	0.42
2:b:340:TRP:CD1	2:b:342:GLY:H	2.38	0.42
37:b:625:DGA:HBH1	37:b:625:DGA:HBS1	1.86	0.42
14:o:236:GLU:HB2	14:o:239:ARG:HB2	2.02	0.42
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.02	0.41
2:B:192:PRO:HG3	8:H:68:TYR:HD1	1.85	0.41
28:B:610:CLA:HMA2	28:B:611:CLA:C2C	2.49	0.41
28:B:613:CLA:HBB1	28:B:615:CLA:HMB2	2.01	0.41
37:B:625:DGA:HAH1	37:B:625:DGA:HAS2	1.78	0.41
28:C:502:CLA:HBB1	32:C:521:LMG:H422	2.02	0.41
5:D:343:GLU:HG3	5:D:348:ARG:HH22	1.84	0.41
15:P:99:VAL:HG12	15:P:101:SER:H	1.84	0.41
2:b:85:SER:O	2:b:85:SER:OG	2.38	0.41
3:v:7:LEU:HD22	11:k:20:PRO:HG2	2.00	0.41
28:c:507:CLA:H112	30:c:515:BCR:H362	2.01	0.41
7:f:19:TRP:HE3	7:f:20:LEU:HD22	1.85	0.41
2:B:170:ASP:OD1	2:B:170:ASP:N	2.53	0.41
4:C:213:VAL:HG13	4:C:277:PHE:HA	2.01	0.41
4:C:274:ALA:HA	4:C:277:PHE:HD2	1.84	0.41
28:C:506:CLA:H2	28:C:507:CLA:H202	2.02	0.41
21:G:160:ARG:HH22	46:G:609:CHL:CGD	2.32	0.41
21:G:173:ASP:OD1	21:G:173:ASP:N	2.52	0.41
23:Y:194:LEU:HD22	28:Y:610:CLA:H11	2.02	0.41
1:a:27:ARG:NH2	16:t:21:ILE:O	2.52	0.41
32:b:622:LMG:H142	32:b:622:LMG:H171	1.91	0.41
5:d:193:LEU:HA	5:d:198:MET:HE2	2.02	0.41
10:j:32:TYR:HD1	37:j:101:DGA:HA31	1.85	0.41
15:p:185:TYR:HB3	15:p:187:PHE:CZ	2.54	0.41
4:C:392:LEU:HD13	35:C:520:DGD:HB51	2.02	0.41
5:D:180:ARG:NH2	5:D:333:ASP:OD1	2.50	0.41
14:O:235:ASP:OD1	14:O:235:ASP:N	2.51	0.41
28:G:603:CLA:H91	28:G:603:CLA:H111	1.77	0.41
22:S:183:ARG:NH2	28:S:609:CLA:O1D	2.53	0.41
1:a:33:PHE:CE2	1:a:128:GLY:HA3	2.56	0.41
1:a:225:ARG:HA	2:b:481:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:308:ASP:HB2	6:e:52:PRO:HB3	2.01	0.41
29:a:409:PHO:H8	29:a:409:PHO:H121	1.80	0.41
2:b:91:TRP:HE1	35:b:623:DGD:HD2	1.84	0.41
2:b:251:VAL:HG22	28:b:603:CLA:H72	2.02	0.41
4:c:205:PRO:HB2	35:c:518:DGD:HA21	2.03	0.41
1:A:290:ILE:HG13	28:A:405:CLA:HED3	2.02	0.41
1:A:341:LEU:HD23	1:A:341:LEU:HA	1.92	0.41
28:B:616:CLA:H202	28:B:616:CLA:H162	1.85	0.41
28:C:506:CLA:H93	28:C:506:CLA:H61	1.86	0.41
28:G:613:CLA:H8	28:G:613:CLA:H122	1.88	0.41
28:S:603:CLA:H41	28:S:603:CLA:H62	1.77	0.41
28:Y:613:CLA:H12	28:Y:614:CLA:HED2	2.02	0.41
29:a:408:PHO:H141	29:a:408:PHO:H162	1.83	0.41
31:a:412:SQD:H131	31:a:412:SQD:H162	1.91	0.41
31:a:412:SQD:H4	45:k:101:4RF:H34	2.02	0.41
28:b:602:CLA:HMC1	8:h:63:ILE:HG21	2.01	0.41
28:b:609:CLA:HMB1	28:b:609:CLA:HBB1	2.02	0.41
30:b:619:BCR:H15C	30:b:619:BCR:H351	1.69	0.41
15:p:164:LYS:HB3	15:p:164:LYS:HE3	1.92	0.41
2:B:347:LYS:O	2:B:397:VAL:HA	2.21	0.41
47:N:620:LUT:H11	47:N:620:LUT:H191	1.92	0.41
28:G:602:CLA:H93	28:G:602:CLA:H111	1.84	0.41
28:Y:613:CLA:H101	38:Y:624:LHG:H331	2.02	0.41
28:Y:614:CLA:H143	28:Y:614:CLA:H161	1.80	0.41
1:a:300:PHE:CE1	4:c:392:LEU:HD11	2.55	0.41
2:b:13:ILE:HA	28:b:613:CLA:HAC2	2.01	0.41
35:c:519:DGD:HA61	35:c:519:DGD:HA92	1.65	0.41
12:l:29:ALA:O	12:l:33:SER:HB3	2.20	0.41
32:A:413:LMG:H322	32:A:413:LMG:H291	1.93	0.41
2:B:460:LEU:HB3	5:D:280:TRP:HZ3	1.85	0.41
2:B:462:PHE:CE2	28:B:612:CLA:HAB	2.55	0.41
12:L:19:TYR:HE1	16:T:19:PHE:CE2	2.39	0.41
13:M:23:LEU:HD23	13:M:23:LEU:HA	1.91	0.41
47:N:620:LUT:H31	47:N:620:LUT:H391	1.95	0.41
21:G:177:PRO:HB3	46:G:608:CHL:HBC2	2.03	0.41
2:b:183:PRO:HA	2:b:199:PRO:HG2	2.02	0.41
28:c:506:CLA:H93	28:c:506:CLA:H61	1.76	0.41
5:d:250:ASN:ND2	5:d:261:PHE:O	2.43	0.41
38:d:409:LHG:H331	16:t:21:ILE:HD11	2.02	0.41
15:p:83:PHE:HB2	15:p:243:VAL:HG22	2.01	0.41
1:A:85:THR:OG1	1:A:113:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:CE1	35:C:520:DGD:HAT2	2.55	0.41
28:A:405:CLA:HBA2	28:A:405:CLA:H3A	1.89	0.41
2:B:225:LEU:HB3	2:B:231:MET:HE3	2.01	0.41
4:C:75:ILE:O	4:C:79:HIS:ND1	2.43	0.41
4:C:150:GLY:O	4:C:154:ILE:HG12	2.20	0.41
14:O:252:ALA:HA	14:O:272:SER:HA	2.03	0.41
20:N:154:LEU:HD13	46:N:607:CHL:HAC2	2.03	0.41
38:N:624:LHG:H201	38:N:624:LHG:H172	1.91	0.41
21:G:214:PHE:CZ	47:G:620:LUT:H8	2.56	0.41
28:b:603:CLA:H172	32:h:102:LMG:H162	2.03	0.41
28:b:615:CLA:HBA1	31:b:621:SQD:H241	2.03	0.41
35:c:519:DGD:HB52	35:c:519:DGD:HB81	1.81	0.41
5:d:87:HIS:CD2	5:d:166:GLY:HA2	2.55	0.41
1:A:29:TYR:O	1:A:129:ARG:NE	2.37	0.41
28:A:406:CLA:H71	29:A:408:PHO:HMB2	2.03	0.41
28:B:609:CLA:H202	28:B:609:CLA:H162	1.95	0.41
4:C:163:LEU:HD22	28:C:501:CLA:C2D	2.51	0.41
4:C:225:HIS:HA	4:C:228:ILE:HG22	2.01	0.41
5:D:130:PHE:CE2	5:D:143:ALA:HB3	2.55	0.41
21:G:152:LEU:HD21	49:G:623:NEX:C34	2.50	0.41
28:S:614:CLA:H41	28:S:614:CLA:H62	1.89	0.41
28:a:406:CLA:H162	28:a:406:CLA:H122	1.88	0.41
2:b:25:MET:HE2	2:b:111:SER:HB2	2.02	0.41
2:b:128:THR:HG23	2:b:130:LYS:H	1.84	0.41
28:c:502:CLA:H141	28:c:502:CLA:H161	1.88	0.41
5:d:152:VAL:HG11	28:d:402:CLA:HBA1	2.02	0.41
28:d:402:CLA:H62	28:d:402:CLA:H41	1.51	0.41
9:i:8:VAL:HA	9:i:11:VAL:HG12	2.03	0.41
1:A:89:ILE:HD11	1:A:108:ASN:HB3	2.02	0.41
2:B:326:ARG:HB3	2:B:444:ARG:HD3	2.02	0.41
28:B:602:CLA:H143	28:B:602:CLA:H111	1.78	0.41
28:B:607:CLA:H13	28:B:607:CLA:H172	1.84	0.41
28:B:610:CLA:H91	28:B:610:CLA:H112	1.89	0.41
4:C:265:ALA:HB2	4:C:429:HIS:CG	2.56	0.41
5:D:148:ALA:HB2	5:D:276:VAL:HG13	2.02	0.41
12:L:27:VAL:HG11	38:L:101:LHG:H192	2.02	0.41
14:O:169:THR:HA	14:O:179:PRO:HA	2.02	0.41
47:N:620:LUT:H35	47:N:620:LUT:H401	1.86	0.41
28:Y:613:CLA:H91	38:Y:624:LHG:H311	2.03	0.41
48:Y:622:XAT:H11	48:Y:622:XAT:H191	1.95	0.41
1:a:281:VAL:O	1:a:285:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:307:VAL:HG12	1:a:313:VAL:HA	2.03	0.41
28:a:406:CLA:H152	41:d:405:PL9:H472	2.01	0.41
28:b:610:CLA:H3A	28:b:610:CLA:HBA1	1.70	0.41
28:b:611:CLA:H151	28:b:613:CLA:HBD	2.03	0.41
31:b:621:SQD:H131	31:b:621:SQD:H102	1.85	0.41
4:c:265:ALA:HB2	4:c:429:HIS:CG	2.55	0.41
5:d:174:GLY:O	5:d:178:ILE:HG12	2.21	0.41
7:f:44:ARG:NH2	10:j:40:SER:H	2.19	0.41
14:o:132:LEU:HD12	14:o:170:VAL:HG12	2.02	0.41
24:u:90:ARG:HG3	24:u:92:ARG:H	1.85	0.41
31:B:626:SQD:H132	33:a:414:SPH:H61	2.03	0.41
5:D:167:TRP:O	5:D:170:ALA:HB3	2.21	0.41
15:P:225:ARG:HA	15:P:228:LYS:HG3	2.03	0.41
46:N:605:CHL:H41	28:S:611:CLA:H171	2.02	0.41
23:Y:42:TYR:CE1	23:Y:202:ALA:HB1	2.56	0.41
28:a:406:CLA:H41	41:d:405:PL9:H162	2.03	0.41
32:a:413:LMG:H362	35:c:518:DGD:HA81	2.03	0.41
28:b:612:CLA:H122	28:b:614:CLA:H121	2.03	0.41
1:A:340:PRO:HB2	15:P:224:LYS:HD3	2.03	0.40
2:B:383:PHE:CD2	5:D:347:PRO:HA	2.56	0.40
3:V:15:VAL:O	30:C:516:BCR:H14C	2.21	0.40
28:C:511:CLA:HBC2	11:K:40:GLN:HG3	2.02	0.40
6:E:69:ARG:NH2	8:H:69:ASN:O	2.39	0.40
21:G:53:LEU:HD11	21:G:64:ASP:HB2	2.03	0.40
38:G:624:LHG:H201	38:G:624:LHG:H172	1.83	0.40
1:a:297:LEU:HD22	4:c:416:THR:HG21	2.02	0.40
2:b:258:TYR:HB2	8:h:68:TYR:OH	2.21	0.40
2:b:474:ILE:HG22	5:d:134:ARG:HH21	1.87	0.40
28:b:614:CLA:H43	38:d:408:LHG:H371	2.03	0.40
5:d:61:HIS:NE2	5:d:80:THR:OG1	2.31	0.40
5:d:246:MET:SD	5:d:264:LYS:HG3	2.61	0.40
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.03	0.40
1:A:206:PHE:CE1	28:D:402:CLA:HBA2	2.56	0.40
28:B:606:CLA:H61	28:B:606:CLA:H41	1.98	0.40
28:B:614:CLA:H71	28:B:614:CLA:H112	1.93	0.40
28:C:510:CLA:H102	28:C:510:CLA:H61	1.81	0.40
23:Y:213:ARG:HA	23:Y:216:MET:HE3	2.04	0.40
2:b:312:TYR:HA	2:b:317:ASN:ND2	2.35	0.40
2:b:445:SER:HB3	2:b:450:TRP:NE1	2.36	0.40
28:b:607:CLA:H91	28:b:607:CLA:H112	1.86	0.40
28:b:616:CLA:H2	28:b:617:CLA:CBB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:145:MET:HE1	4:c:259:TYR:OH	2.21	0.40
4:c:435:ARG:NE	4:c:435:ARG:HA	2.36	0.40
5:d:320:LEU:HA	5:d:323:GLU:CD	2.47	0.40
32:D:411:LMG:H181	32:D:411:LMG:H152	1.83	0.40
45:I:102:4RF:H50	45:I:102:4RF:H55	1.65	0.40
38:L:101:LHG:HC61	38:L:101:LHG:H111	2.04	0.40
15:P:138:ILE:HD12	15:P:138:ILE:HA	1.95	0.40
20:N:223:GLN:O	20:N:227:THR:OG1	2.25	0.40
20:N:248:PHE:HB3	21:G:123:PHE:HZ	1.85	0.40
21:G:199:LYS:HD3	28:G:612:CLA:HBD	2.04	0.40
21:G:202:LYS:NZ	38:G:624:LHG:O4	2.54	0.40
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.56	0.40
1:a:222:SER:HA	5:d:138:LEU:HD13	2.03	0.40
29:a:409:PHO:H92	29:a:409:PHO:H62	1.79	0.40
2:b:115:TRP:CZ3	30:b:618:BCR:H391	2.56	0.40
2:b:141:ILE:O	2:b:145:LEU:HG	2.21	0.40
2:b:376:VAL:HG12	2:b:378:ARG:HH22	1.86	0.40
38:d:408:LHG:H311	38:d:408:LHG:H161	2.03	0.40
14:o:95:ARG:HH12	14:o:193:LEU:HD23	1.86	0.40
28:C:505:CLA:H193	28:C:505:CLA:H161	1.92	0.40
38:D:408:LHG:H112	38:L:101:LHG:HC92	2.04	0.40
20:N:135:GLY:HA3	20:N:148:GLN:HG3	2.03	0.40
28:N:602:CLA:H112	28:N:602:CLA:H152	1.62	0.40
21:G:150:VAL:HA	46:G:609:CHL:HBB2	2.02	0.40
22:S:92:LYS:HB2	22:S:96:GLN:HG2	2.04	0.40
22:S:244:ILE:HG13	38:S:624:LHG:H272	2.03	0.40
2:b:23:HIS:ND1	28:b:616:CLA:OBD	2.30	0.40
2:b:25:MET:HE2	2:b:25:MET:HB3	1.89	0.40
2:b:75:TRP:O	31:b:626:SQD:O3	2.38	0.40
2:b:265:ILE:HG13	2:b:274:GLN:HE22	1.87	0.40
2:b:454:GLY:HA2	32:b:622:LMG:H191	2.03	0.40
28:c:509:CLA:H91	28:c:509:CLA:H111	1.84	0.40
28:c:513:CLA:H102	28:c:513:CLA:H61	1.96	0.40
32:c:523:LMG:HC91	37:c:524:DGA:HB21	2.03	0.40
5:d:162:LEU:HD13	32:h:102:LMG:H182	2.04	0.40
8:h:66:GLU:OE2	8:h:72:LEU:HD22	2.22	0.40
1:A:200:PHE:HZ	35:C:520:DGD:HBN2	1.87	0.40
2:B:248:ALA:HB2	28:B:604:CLA:H61	2.02	0.40
4:C:221:ILE:HG12	30:C:515:BCR:H282	2.03	0.40
37:C:524:DGA:HB91	28:Y:611:CLA:H102	2.03	0.40
45:K:101:4RF:H55	45:K:101:4RF:H50	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:G:601:CHL:HHB	46:Y:609:CHL:HMB2	2.04	0.40
22:S:120:ILE:HD12	28:S:605:CLA:HED2	2.03	0.40
2:b:148:LEU:HD23	2:b:148:LEU:HA	1.94	0.40
28:b:614:CLA:H141	28:b:614:CLA:H162	1.79	0.40
4:c:51:TRP:HB2	28:c:510:CLA:HAC2	2.02	0.40
30:c:514:BCR:HC7	19:z:55:GLY:HA3	2.03	0.40
5:d:18:ALA:O	5:d:22:LEU:HB2	2.22	0.40
5:d:137:ASN:O	5:d:138:LEU:HD23	2.22	0.40
5:d:210:LEU:HD12	5:d:274:VAL:HG21	2.04	0.40
32:h:102:LMG:H111	32:h:102:LMG:H291	2.02	0.40
15:p:228:LYS:HD2	15:p:228:LYS:HA	1.83	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%)	323 (96%)	12 (4%)	0	100	100
1	a	335/336 (100%)	317 (95%)	18 (5%)	0	100	100
2	B	481/484 (99%)	463 (96%)	18 (4%)	0	100	100
2	b	481/484 (99%)	465 (97%)	16 (3%)	0	100	100
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	428 (96%)	19 (4%)	0	100	100
4	c	447/449 (100%)	420 (94%)	27 (6%)	0	100	100
5	D	346/348 (99%)	334 (96%)	12 (4%)	0	100	100
5	d	346/348 (99%)	329 (95%)	17 (5%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	e	74/76 (97%)	72 (97%)	2 (3%)	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%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
9	i	33/35 (94%)	30 (91%)	3 (9%)	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%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	32 (91%)	3 (9%)	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	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m	29/31 (94%)	29 (100%)	0	0	100	100
14	O	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	30	59
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	30	59
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	p	185/187 (99%)	168 (91%)	17 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	2	20
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
18	X	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	14	44
21	G	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
22	S	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	10	39
23	Y	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	24	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	U	25/27 (93%)	25 (100%)	0	0	100	100
24	u	25/27 (93%)	25 (100%)	0	0	100	100
All	All	6054/6142 (99%)	5755 (95%)	290 (5%)	9 (0%)	49	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
22	S	284	ASP
23	Y	146	ILE
20	N	145	ILE
22	S	158	VAL
22	S	92	LYS
16	T	29	ILE

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%)	276 (100%)	0	100	100
2	B	387/387 (100%)	387 (100%)	0	100	100
2	b	387/387 (100%)	387 (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%)	349 (100%)	1 (0%)	86	81
5	D	279/279 (100%)	278 (100%)	1 (0%)	84	79
5	d	279/279 (100%)	278 (100%)	1 (0%)	84	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
14	O	197/197 (100%)	197 (100%)	0	100	100
14	o	197/197 (100%)	197 (100%)	0	100	100
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
21	G	168/168 (100%)	167 (99%)	1 (1%)	78	77
22	S	190/190 (100%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	Y	167/167 (100%)	167 (100%)	0	100 100
24	U	26/26 (100%)	26 (100%)	0	100 100
24	u	26/26 (100%)	26 (100%)	0	100 100
All	All	4942/4940 (100%)	4938 (100%)	4 (0%)	87 87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	332	GLN
21	G	73	GLN
4	c	403	ASN
5	d	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	325	ASN
2	B	282	GLN
2	B	290	GLN
4	C	120	HIS
4	C	406	ASN
5	D	186	GLN
5	D	250	ASN
5	D	322	ASN
5	D	332	GLN
5	D	350	ASN
8	H	69	ASN
8	H	79	ASN
14	O	68	GLN
14	O	274	GLN
14	O	297	GLN
15	P	203	GLN
20	N	234	ASN
21	G	129	ASN
21	G	133	ASN
21	G	217	GLN
22	S	160	GLN
23	Y	225	GLN
23	Y	236	ASN

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Mol	Chain	Res	Type
23	Y	247	ASN
24	U	115	ASN
1	a	247	ASN
1	a	303	ASN
1	a	315	ASN
1	a	335	ASN
2	b	282	GLN
2	b	290	GLN
2	b	317	ASN
2	b	331	ASN
4	c	44	HIS
4	c	189	ASN
4	c	320	GLN
4	c	373	GLN
4	c	403	ASN
5	d	194	ASN
5	d	230	ASN
6	e	53	ASN
6	e	82	GLN
14	o	283	HIS
15	p	140	GLN
15	p	202	HIS
17	w	66	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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	$\#\|Z\| > 2$
2	CSD	b	218	2	3,7,8	0.93	0	1,8,10	0.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CSD	B	218	2	3,7,8	0.85	0	1,8,10	0.20	0

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
2	CSD	b	218	2	-	1/2/6/8	-
2	CSD	B	218	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	N-CA-CB-SG
2	b	218	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 250 ligands modelled in this entry, 6 are monoatomic - leaving 244 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	$\#\|Z\|>2$
36	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
28	CLA	B	604	-	69,73,73	1.38	8 (11%)	83,113,113	1.88	18 (21%)
37	DGA	B	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.49	3 (6%)
49	NEX	N	623	-	38,46,46	3.34	10 (26%)	50,70,70	1.49	9 (18%)
33	SPH	A	414	-	19,20,20	0.65	0	18,21,21	1.06	1 (5%)
40	BCT	d	401	26	2,3,3	1.16	0	2,3,3	4.43	2 (100%)
42	HEM	F	101	6,7	50,50,50	1.48	7 (14%)	66,82,82	1.18	6 (9%)
46	CHL	N	601	-	70,74,74	0.77	2 (2%)	80,114,114	1.25	13 (16%)
32	LMG	w	201	-	39,39,55	0.86	2 (5%)	47,47,63	1.05	2 (4%)
35	DGD	C	519	-	63,63,67	1.13	6 (9%)	77,77,81	0.97	3 (3%)
28	CLA	c	505	-	69,73,73	1.37	7 (10%)	83,113,113	2.05	19 (22%)
31	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.91	2 (3%)
51	PTY	Y	626	-	49,49,49	0.88	4 (8%)	52,54,54	1.06	2 (3%)
30	BCR	C	517	-	41,41,41	1.83	4 (9%)	56,56,56	4.29	15 (26%)
30	BCR	a	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.31	16 (28%)
28	CLA	b	614	-	69,73,73	1.37	7 (10%)	83,113,113	1.90	17 (20%)
31	SQD	C	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
41	PL9	D	405	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
32	LMG	b	622	-	44,44,55	0.87	2 (4%)	52,52,63	1.11	2 (3%)
32	LMG	B	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.09	2 (3%)
28	CLA	S	605	-	54,58,73	1.58	9 (16%)	65,95,113	2.17	18 (27%)
47	LUT	S	621	-	42,43,43	2.34	1 (2%)	51,60,60	1.99	15 (29%)
28	CLA	c	510	4	69,73,73	1.33	7 (10%)	83,113,113	1.99	18 (21%)
28	CLA	c	506	-	69,73,73	1.36	6 (8%)	83,113,113	1.88	18 (21%)
33	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.05	1 (5%)
31	SQD	M	101	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
28	CLA	c	503	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	19 (22%)
30	BCR	d	404	-	41,41,41	1.87	4 (9%)	56,56,56	4.39	17 (30%)
44	GOL	I	101	-	5,5,5	0.55	0	5,5,5	0.29	0
28	CLA	B	616	-	69,73,73	1.36	7 (10%)	83,113,113	1.87	17 (20%)
45	4RF	I	102	-	56,56,56	1.05	3 (5%)	59,59,59	0.88	3 (5%)
38	LHG	S	624	28	44,44,48	0.41	0	47,50,54	1.12	3 (6%)
28	CLA	b	615	-	69,73,73	1.36	7 (10%)	83,113,113	1.91	17 (20%)
36	3PH	S	626	-	47,47,47	0.86	4 (8%)	51,52,52	4.42	4 (7%)
28	CLA	B	612	-	69,73,73	1.36	6 (8%)	83,113,113	1.87	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	BCR	c	517	-	41,41,41	1.88	4 (9%)	56,56,56	4.48	15 (26%)
48	XAT	G	622	-	39,47,47	0.69	1 (2%)	54,74,74	1.90	13 (24%)
46	CHL	S	608	-	65,69,74	0.80	2 (3%)	74,108,114	1.26	12 (16%)
28	CLA	c	507	-	69,73,73	1.38	7 (10%)	83,113,113	1.96	19 (22%)
29	PHO	a	409	-	58,69,69	2.03	8 (13%)	56,99,99	1.76	8 (14%)
39	LMK	C	527	-	38,39,53	1.51	2 (5%)	41,46,60	1.47	2 (4%)
28	CLA	C	505	-	69,73,73	1.38	8 (11%)	83,113,113	1.87	17 (20%)
28	CLA	c	501	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
47	LUT	Y	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.02	14 (27%)
37	DGA	c	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.48	3 (6%)
28	CLA	b	609	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	17 (20%)
36	3PH	T	101	-	47,47,47	0.86	4 (8%)	51,52,52	1.11	2 (3%)
28	CLA	S	603	-	69,73,73	1.37	8 (11%)	83,113,113	2.02	19 (22%)
28	CLA	b	603	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	20 (24%)
38	LHG	C	525	-	46,46,48	0.40	0	49,52,54	1.02	2 (4%)
49	NEX	Y	623	-	38,46,46	3.29	9 (23%)	50,70,70	1.80	14 (28%)
28	CLA	A	405	-	69,73,73	1.36	7 (10%)	83,113,113	1.86	16 (19%)
28	CLA	D	402	-	69,73,73	1.38	8 (11%)	83,113,113	1.89	19 (22%)
28	CLA	C	504	-	69,73,73	1.34	6 (8%)	83,113,113	1.97	19 (22%)
46	CHL	G	609	-	70,74,74	0.81	2 (2%)	80,114,114	1.23	10 (12%)
28	CLA	Y	614	-	69,73,73	1.35	7 (10%)	83,113,113	1.89	19 (22%)
28	CLA	C	503	-	69,73,73	1.37	8 (11%)	83,113,113	1.93	19 (22%)
38	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.45	5 (9%)
28	CLA	S	604	-	59,63,73	1.47	7 (11%)	71,101,113	2.13	19 (26%)
28	CLA	a	410	-	64,68,73	1.42	7 (10%)	77,107,113	1.97	18 (23%)
28	CLA	A	407	-	54,58,73	1.54	7 (12%)	65,95,113	2.17	20 (30%)
45	4RF	i	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.89	3 (5%)
38	LHG	d	408	-	43,43,48	0.40	0	46,49,54	0.99	2 (4%)
36	3PH	t	101	-	47,47,47	0.87	4 (8%)	51,52,52	1.15	2 (3%)
28	CLA	S	613	-	59,63,73	1.47	7 (11%)	71,101,113	2.09	20 (28%)
32	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.17	4 (7%)
25	OEX	A	401	4,1	0,14,14	-	-	-		
38	LHG	G	624	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
28	CLA	Y	612	-	69,73,73	1.36	8 (11%)	83,113,113	1.94	18 (21%)
28	CLA	B	603	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
46	CHL	G	601	21	70,74,74	0.78	2 (2%)	80,114,114	1.24	12 (15%)
28	CLA	B	610	-	69,73,73	1.37	6 (8%)	83,113,113	1.80	16 (19%)
31	SQD	B	626	-	53,54,54	0.80	0	62,65,65	0.91	2 (3%)
28	CLA	S	610	-	69,73,73	1.37	7 (10%)	83,113,113	1.86	21 (25%)
46	CHL	S	607	-	47,51,74	0.94	2 (4%)	52,86,114	1.43	9 (17%)
28	CLA	C	501	-	69,73,73	1.36	7 (10%)	83,113,113	1.96	20 (24%)
28	CLA	b	617	-	69,73,73	1.36	6 (8%)	83,113,113	1.89	18 (21%)
38	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
46	CHL	N	606	-	70,74,74	0.79	1 (1%)	80,114,114	1.22	12 (15%)
28	CLA	N	612	-	49,53,73	1.62	8 (16%)	59,89,113	2.02	15 (25%)
28	CLA	B	602	-	69,73,73	1.36	8 (11%)	83,113,113	1.93	19 (22%)
46	CHL	Y	601	23	70,74,74	0.81	2 (2%)	80,114,114	1.14	8 (10%)
46	CHL	Y	606	-	70,74,74	0.78	1 (1%)	80,114,114	1.23	11 (13%)
28	CLA	A	406	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	16 (19%)
28	CLA	S	617	-	54,58,73	1.54	7 (12%)	65,95,113	2.18	19 (29%)
28	CLA	N	610	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	20 (24%)
30	BCR	C	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.41	15 (26%)
35	DGD	C	518	-	56,56,67	1.00	4 (7%)	70,70,81	0.91	2 (2%)
46	CHL	Y	609	-	70,74,74	0.77	2 (2%)	80,114,114	1.26	12 (15%)
35	DGD	C	520	-	60,60,67	1.07	6 (10%)	74,74,81	0.92	2 (2%)
28	CLA	C	511	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	19 (22%)
28	CLA	c	513	-	69,73,73	1.36	7 (10%)	83,113,113	2.01	22 (26%)
32	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.03	2 (3%)
32	LMG	D	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.05	2 (3%)
35	DGD	b	623	-	44,44,67	0.87	1 (2%)	58,58,81	1.23	5 (8%)
41	PL9	d	405	-	55,55,55	1.16	5 (9%)	68,69,69	1.59	13 (19%)
43	RRX	h	101	-	42,42,42	4.91	24 (57%)	57,58,58	2.40	20 (35%)
28	CLA	c	508	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	18 (21%)
28	CLA	B	615	-	69,73,73	1.37	8 (11%)	83,113,113	1.93	16 (19%)
28	CLA	G	612	-	47,51,73	1.64	7 (14%)	56,86,113	2.09	15 (26%)
39	LMK	c	527	-	38,39,53	1.49	2 (5%)	41,46,60	1.26	2 (4%)
28	CLA	B	608	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	17 (20%)
31	SQD	m	101	-	41,42,54	0.88	0	50,53,65	0.97	2 (4%)
38	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.02	3 (6%)
46	CHL	S	606	-	48,52,74	0.93	2 (4%)	53,87,114	1.43	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	b	611	-	69,73,73	1.37	8 (11%)	83,113,113	1.97	19 (22%)
28	CLA	N	604	-	69,73,73	1.36	8 (11%)	83,113,113	1.98	21 (25%)
28	CLA	D	403	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	18 (21%)
28	CLA	N	602	-	69,73,73	1.35	6 (8%)	83,113,113	1.94	19 (22%)
28	CLA	B	605	-	69,73,73	1.38	6 (8%)	83,113,113	2.06	19 (22%)
28	CLA	G	613	-	69,73,73	1.36	7 (10%)	83,113,113	1.95	18 (21%)
38	LHG	D	409	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
32	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.06	3 (4%)
28	CLA	c	502	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	17 (20%)
34	C7Z	B	620	-	43,43,43	5.35	26 (60%)	58,60,60	2.27	22 (37%)
37	DGA	j	101	-	28,28,43	1.30	3 (10%)	30,30,45	1.20	2 (6%)
38	LHG	d	410	-	38,38,48	0.42	0	41,44,54	1.13	3 (7%)
30	BCR	c	514	-	41,41,41	1.83	4 (9%)	56,56,56	4.45	15 (26%)
28	CLA	C	512	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	18 (21%)
28	CLA	Y	603	-	69,73,73	1.34	7 (10%)	83,113,113	1.96	20 (24%)
28	CLA	G	602	-	69,73,73	1.39	7 (10%)	83,113,113	1.93	19 (22%)
47	LUT	N	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.92	12 (23%)
47	LUT	Y	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.96	12 (23%)
28	CLA	a	406	-	69,73,73	1.37	7 (10%)	83,113,113	1.84	17 (20%)
28	CLA	C	502	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	17 (20%)
28	CLA	C	513	-	69,73,73	1.39	7 (10%)	83,113,113	1.94	17 (20%)
30	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.50	16 (28%)
38	LHG	D	408	-	43,43,48	0.40	0	46,49,54	1.00	2 (4%)
30	BCR	C	515	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	12 (21%)
28	CLA	C	510	4	69,73,73	1.34	6 (8%)	83,113,113	1.99	17 (20%)
28	CLA	B	606	-	69,73,73	1.34	6 (8%)	83,113,113	2.04	19 (22%)
28	CLA	Y	602	-	69,73,73	1.36	7 (10%)	83,113,113	1.91	20 (24%)
28	CLA	b	606	-	69,73,73	1.34	6 (8%)	83,113,113	2.02	19 (22%)
28	CLA	B	609	-	69,73,73	1.36	7 (10%)	83,113,113	1.95	18 (21%)
28	CLA	A	410	-	64,68,73	1.41	7 (10%)	77,107,113	2.03	18 (23%)
28	CLA	C	508	-	69,73,73	1.37	6 (8%)	83,113,113	1.85	18 (21%)
30	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.51	16 (28%)
28	CLA	d	403	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	18 (21%)
46	CHL	N	605	20	70,74,74	0.78	1 (1%)	80,114,114	1.22	10 (12%)
47	LUT	G	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.96	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	B	611	-	69,73,73	1.38	8 (11%)	83,113,113	1.92	18 (21%)
31	SQD	B	621	-	41,42,54	0.88	0	50,53,65	0.94	2 (4%)
43	RRX	H	101	-	42,42,42	4.83	24 (57%)	57,58,58	2.76	22 (38%)
46	CHL	Y	605	23	50,54,74	0.90	2 (4%)	56,90,114	1.34	9 (16%)
28	CLA	Y	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.90	20 (24%)
29	PHO	A	408	-	58,69,69	2.07	10 (17%)	56,99,99	1.53	8 (14%)
28	CLA	b	612	-	69,73,73	1.35	6 (8%)	83,113,113	1.91	15 (18%)
48	XAT	Y	622	-	39,47,47	0.68	1 (2%)	54,74,74	3.70	19 (35%)
28	CLA	G	614	-	53,57,73	1.53	7 (13%)	62,93,113	2.22	18 (29%)
28	CLA	G	611	-	69,73,73	1.38	8 (11%)	83,113,113	1.91	18 (21%)
28	CLA	C	506	-	69,73,73	1.36	6 (8%)	83,113,113	1.89	17 (20%)
32	LMG	c	521	-	51,51,55	1.07	4 (7%)	59,59,63	1.01	2 (3%)
28	CLA	B	617	-	69,73,73	1.36	6 (8%)	83,113,113	1.92	19 (22%)
28	CLA	c	512	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	17 (20%)
28	CLA	b	608	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	17 (20%)
28	CLA	d	402	-	69,73,73	1.38	8 (11%)	83,113,113	1.86	19 (22%)
46	CHL	G	606	-	54,58,74	0.90	2 (3%)	59,94,114	1.40	10 (16%)
28	CLA	a	405	-	69,73,73	1.33	7 (10%)	83,113,113	1.95	19 (22%)
37	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.52	3 (6%)
28	CLA	S	614	-	59,63,73	1.46	7 (11%)	71,101,113	2.01	16 (22%)
28	CLA	B	613	-	69,73,73	1.37	8 (11%)	83,113,113	1.87	15 (18%)
28	CLA	b	613	-	69,73,73	1.36	7 (10%)	83,113,113	1.84	18 (21%)
49	NEX	G	623	-	38,46,46	3.25	10 (26%)	50,70,70	1.87	9 (18%)
30	BCR	D	404	-	41,41,41	1.82	4 (9%)	56,56,56	4.24	16 (28%)
33	SPH	a	414	-	19,20,20	0.67	0	18,21,21	1.03	0
38	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.18	3 (7%)
28	CLA	c	511	-	69,73,73	1.37	7 (10%)	83,113,113	1.97	17 (20%)
31	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.93	3 (5%)
28	CLA	b	616	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	19 (22%)
28	CLA	N	614	-	53,57,73	1.55	8 (15%)	62,93,113	2.23	18 (29%)
28	CLA	c	509	-	69,73,73	1.37	6 (8%)	83,113,113	1.87	15 (18%)
30	BCR	C	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.42	14 (25%)
46	CHL	N	608	-	54,58,74	0.89	2 (3%)	59,94,114	1.32	10 (16%)
28	CLA	B	607	-	69,73,73	1.36	8 (11%)	83,113,113	1.92	19 (22%)
29	PHO	A	409	-	58,69,69	2.06	10 (17%)	56,99,99	1.71	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMG	h	102	-	48,48,55	1.01	6 (12%)	56,56,63	1.17	3 (5%)
25	OEX	a	401	4,1	0,14,14	-	-	-		
28	CLA	Y	610	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	21 (25%)
47	LUT	N	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.04	11 (21%)
38	LHG	d	409	-	48,48,48	0.38	0	51,54,54	0.99	2 (3%)
28	CLA	G	604	-	53,57,73	1.55	8 (15%)	62,93,113	2.19	21 (33%)
30	BCR	B	619	-	41,41,41	1.84	4 (9%)	56,56,56	4.31	18 (32%)
29	PHO	a	408	-	58,69,69	2.06	10 (17%)	56,99,99	1.57	7 (12%)
50	LPX	S	625	-	29,29,29	1.00	2 (6%)	31,33,33	0.97	1 (3%)
28	CLA	S	612	-	49,53,73	1.61	7 (14%)	59,89,113	2.03	15 (25%)
28	CLA	N	603	-	69,73,73	1.35	7 (10%)	83,113,113	1.98	18 (21%)
32	LMG	C	521	-	51,51,55	1.06	6 (11%)	59,59,63	1.09	4 (6%)
28	CLA	b	605	-	69,73,73	1.37	8 (11%)	83,113,113	1.96	18 (21%)
28	CLA	c	504	-	69,73,73	1.36	6 (8%)	83,113,113	1.97	16 (19%)
42	HEM	f	101	6,7	50,50,50	1.43	7 (14%)	66,82,82	1.20	6 (9%)
46	CHL	G	608	-	48,52,74	0.96	2 (4%)	53,87,114	1.42	10 (18%)
40	BCT	D	401	-	2,3,3	1.27	0	2,3,3	4.06	2 (100%)
31	SQD	b	621	-	41,42,54	0.89	0	50,53,65	0.93	2 (4%)
46	CHL	N	607	-	70,74,74	0.78	2 (2%)	80,114,114	1.19	9 (11%)
38	LHG	N	624	-	48,48,48	0.38	0	51,54,54	1.07	3 (5%)
46	CHL	G	605	-	52,56,74	0.88	2 (3%)	58,92,114	1.41	10 (17%)
30	BCR	b	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.61	20 (35%)
30	BCR	c	515	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	14 (25%)
28	CLA	G	610	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	22 (26%)
34	C7Z	b	620	-	43,43,43	5.37	26 (60%)	58,60,60	2.26	19 (32%)
35	DGD	B	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.14	3 (5%)
46	CHL	G	607	-	70,74,74	0.79	2 (2%)	80,114,114	1.18	10 (12%)
47	LUT	G	621	-	42,43,43	2.35	1 (2%)	51,60,60	2.02	12 (23%)
47	LUT	S	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.94	14 (27%)
28	CLA	B	614	-	69,73,73	1.35	6 (8%)	83,113,113	1.91	17 (20%)
28	CLA	G	603	-	69,73,73	1.34	6 (8%)	83,113,113	2.01	20 (24%)
46	CHL	S	601	22	50,54,74	0.92	2 (4%)	56,90,114	1.40	10 (17%)
28	CLA	C	507	-	69,73,73	1.38	8 (11%)	83,113,113	1.96	20 (24%)
32	LMG	H	102	-	48,48,55	1.00	5 (10%)	56,56,63	1.11	2 (3%)
36	3PH	b	624	-	47,47,47	0.87	4 (8%)	51,52,52	1.11	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	CLA	b	604	-	69,73,73	1.36	7 (10%)	83,113,113	1.87	18 (21%)
32	LMG	a	413	-	48,48,55	1.00	4 (8%)	56,56,63	1.14	3 (5%)
28	CLA	b	607	-	69,73,73	1.36	8 (11%)	83,113,113	1.91	18 (21%)
28	CLA	S	609	-	64,68,73	1.41	7 (10%)	77,107,113	1.98	18 (23%)
28	CLA	C	509	-	69,73,73	1.37	7 (10%)	83,113,113	1.89	16 (19%)
48	XAT	N	622	-	39,47,47	0.68	1 (2%)	54,74,74	1.96	12 (22%)
28	CLA	S	611	38	69,73,73	1.36	8 (11%)	83,113,113	1.97	19 (22%)
35	DGD	c	519	-	63,63,67	1.13	6 (9%)	77,77,81	0.94	2 (2%)
28	CLA	Y	613	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	18 (21%)
28	CLA	Y	611	-	69,73,73	1.36	8 (11%)	83,113,113	1.88	17 (20%)
30	BCR	b	619	-	41,41,41	1.87	4 (9%)	56,56,56	4.37	13 (23%)
30	BCR	A	411	-	41,41,41	1.85	4 (9%)	56,56,56	4.25	13 (23%)
28	CLA	a	407	-	53,57,73	1.55	7 (13%)	62,93,113	2.33	19 (30%)
28	CLA	S	602	-	64,68,73	1.40	7 (10%)	77,107,113	2.06	21 (27%)
32	LMG	W	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.15	2 (4%)
37	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.24	2 (6%)
31	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
35	DGD	c	520	-	60,60,67	1.09	6 (10%)	74,74,81	0.90	2 (2%)
45	4RF	K	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.86	3 (5%)
35	DGD	c	518	-	56,56,67	0.98	3 (5%)	70,70,81	0.99	2 (2%)
28	CLA	b	610	-	69,73,73	1.36	6 (8%)	83,113,113	1.91	17 (20%)
31	SQD	b	626	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
46	CHL	N	609	-	70,74,74	0.79	2 (2%)	80,114,114	1.20	12 (15%)
51	PTY	Y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.41	2 (9%)
28	CLA	N	611	-	53,57,73	1.55	7 (13%)	62,93,113	2.16	18 (29%)
46	CHL	Y	607	-	70,74,74	0.75	2 (2%)	80,114,114	1.16	9 (11%)
32	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.09	4 (6%)
37	DGA	b	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.52	3 (6%)
49	NEX	S	623	-	38,46,46	3.36	10 (26%)	50,70,70	1.72	12 (24%)
45	4RF	k	101	-	56,56,56	1.05	3 (5%)	59,59,59	0.87	3 (5%)
28	CLA	b	602	-	69,73,73	1.36	8 (11%)	83,113,113	1.92	17 (20%)
38	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
28	CLA	N	613	-	69,73,73	1.37	8 (11%)	83,113,113	1.95	19 (22%)
28	CLA	Y	608	-	54,58,73	1.54	8 (14%)	65,95,113	2.12	18 (27%)

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
36	3PH	B	624	-	-	28/49/49/49	-
28	CLA	B	604	-	-	19/39/115/115	-
37	DGA	B	625	-	-	25/45/45/45	-
49	NEX	N	623	-	-	2/27/83/83	1/3/3/3
33	SPH	A	414	-	-	8/21/21/21	-
46	CHL	N	601	-	1/1/15/21	8/41/117/117	-
42	HEM	F	101	6,7	-	0/14/54/54	-
32	LMG	w	201	-	-	10/34/54/70	0/1/1/1
35	DGD	C	519	-	-	14/51/91/95	0/2/2/2
28	CLA	c	505	-	-	18/39/115/115	-
31	SQD	a	412	-	-	22/46/66/69	0/1/1/1
51	PTY	Y	626	-	-	21/53/53/53	-
30	BCR	C	517	-	-	10/29/63/63	0/2/2/2
30	BCR	a	411	-	-	10/29/63/63	0/2/2/2
28	CLA	b	614	-	-	12/39/115/115	-
31	SQD	C	526	-	-	17/49/69/69	0/1/1/1
41	PL9	D	405	-	-	7/53/73/73	0/1/1/1
32	LMG	b	622	-	-	11/39/59/70	0/1/1/1
32	LMG	B	622	-	-	12/39/59/70	0/1/1/1
28	CLA	S	605	-	-	12/21/97/115	-
47	LUT	S	621	-	-	1/29/67/67	0/2/2/2
28	CLA	c	510	4	-	20/39/115/115	-
28	CLA	c	506	-	-	19/39/115/115	-
33	SPH	Y	625	-	-	11/21/21/21	-
31	SQD	M	101	-	-	18/37/57/69	0/1/1/1
28	CLA	c	503	-	-	20/39/115/115	-
30	BCR	d	404	-	-	13/29/63/63	0/2/2/2
44	GOL	I	101	-	-	2/4/4/4	-
28	CLA	B	616	-	-	17/39/115/115	-
45	4RF	I	102	-	-	28/59/59/59	-
38	LHG	S	624	28	-	31/49/49/53	-
28	CLA	b	615	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	3PH	S	626	-	-	25/49/49/49	-
28	CLA	B	612	-	-	17/39/115/115	-
30	BCR	c	517	-	-	8/29/63/63	0/2/2/2
48	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
46	CHL	S	608	-	1/1/14/21	8/35/111/117	-
28	CLA	c	507	-	-	18/39/115/115	-
29	PHO	a	409	-	-	9/37/103/103	0/5/6/6
39	LMK	C	527	-	2/2/6/6	15/46/46/60	-
28	CLA	C	505	-	-	20/39/115/115	-
28	CLA	c	501	-	-	22/39/115/115	-
47	LUT	Y	621	-	-	3/29/67/67	0/2/2/2
37	DGA	c	524	-	-	25/45/45/45	-
28	CLA	b	609	-	-	20/39/115/115	-
36	3PH	T	101	-	-	22/49/49/49	-
28	CLA	S	603	-	-	20/39/115/115	-
28	CLA	b	603	-	-	18/39/115/115	-
38	LHG	C	525	-	-	32/51/51/53	-
49	NEX	Y	623	-	-	5/27/83/83	0/3/3/3
28	CLA	A	405	-	-	13/39/115/115	-
28	CLA	D	402	-	-	21/39/115/115	-
28	CLA	C	504	-	-	15/39/115/115	-
46	CHL	G	609	-	1/1/15/21	8/41/117/117	-
28	CLA	Y	614	-	-	16/39/115/115	-
28	CLA	C	503	-	-	18/39/115/115	-
38	LHG	L	101	-	-	42/53/53/53	-
28	CLA	S	604	-	-	11/27/103/115	-
28	CLA	a	410	-	-	7/33/109/115	-
28	CLA	A	407	-	-	9/21/97/115	-
45	4RF	i	101	-	-	31/59/59/59	-
38	LHG	d	408	-	-	30/48/48/53	-
36	3PH	t	101	-	-	26/49/49/49	-
28	CLA	S	613	-	-	11/27/103/115	-
32	LMG	A	413	-	-	14/43/63/70	0/1/1/1
38	LHG	G	624	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	Y	612	-	-	15/39/115/115	-
28	CLA	B	603	-	-	17/39/115/115	-
46	CHL	G	601	21	1/1/15/21	11/41/117/117	-
28	CLA	B	610	-	-	16/39/115/115	-
31	SQD	B	626	-	-	22/49/69/69	0/1/1/1
28	CLA	S	610	-	-	23/39/115/115	-
46	CHL	S	607	-	-	0/14/90/117	-
28	CLA	C	501	-	-	18/39/115/115	-
46	CHL	N	606	-	1/1/15/21	11/41/117/117	-
28	CLA	b	617	-	-	14/39/115/115	-
38	LHG	l	101	-	-	38/53/53/53	-
28	CLA	N	612	-	-	5/15/91/115	-
28	CLA	B	602	-	-	24/39/115/115	-
46	CHL	Y	601	23	1/1/15/21	6/41/117/117	-
46	CHL	Y	606	-	1/1/15/21	7/41/117/117	-
28	CLA	A	406	-	-	19/39/115/115	-
28	CLA	S	617	-	-	7/21/97/115	-
28	CLA	N	610	-	-	24/39/115/115	-
30	BCR	C	514	-	-	13/29/63/63	0/2/2/2
46	CHL	Y	609	-	1/1/15/21	11/41/117/117	-
35	DGD	C	518	-	-	15/44/84/95	0/2/2/2
35	DGD	C	520	-	-	8/48/88/95	0/2/2/2
28	CLA	C	511	-	-	13/39/115/115	-
28	CLA	c	513	-	-	12/39/115/115	-
32	LMG	d	411	-	-	8/41/61/70	0/1/1/1
32	LMG	D	411	-	-	10/41/61/70	0/1/1/1
43	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2
35	DGD	b	623	-	-	11/32/72/95	0/2/2/2
41	PL9	d	405	-	-	21/53/73/73	0/1/1/1
28	CLA	c	508	-	-	10/39/115/115	-
39	LMK	c	527	-	2/2/6/6	12/46/46/60	-
28	CLA	G	612	-	-	6/13/89/115	-
28	CLA	B	615	-	-	11/39/115/115	-
28	CLA	B	608	-	-	27/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SQD	m	101	-	-	20/37/57/69	0/1/1/1
38	LHG	c	525	-	-	31/51/51/53	-
46	CHL	S	606	-	-	1/15/91/117	-
28	CLA	b	611	-	-	11/39/115/115	-
28	CLA	N	604	-	-	15/39/115/115	-
28	CLA	D	403	-	-	16/39/115/115	-
28	CLA	N	602	-	-	18/39/115/115	-
28	CLA	B	605	-	-	14/39/115/115	-
28	CLA	G	613	-	-	17/39/115/115	-
38	LHG	D	409	-	-	28/53/53/53	-
32	LMG	c	523	-	-	14/50/70/70	0/1/1/1
28	CLA	c	502	-	-	9/39/115/115	-
34	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
37	DGA	j	101	-	-	14/30/30/45	-
38	LHG	d	410	-	-	23/43/43/53	-
30	BCR	c	514	-	-	12/29/63/63	0/2/2/2
28	CLA	C	512	-	-	23/39/115/115	-
28	CLA	Y	603	-	-	17/39/115/115	-
28	CLA	G	602	-	-	21/39/115/115	-
47	LUT	N	620	-	-	3/29/67/67	0/2/2/2
47	LUT	Y	620	-	-	3/29/67/67	0/2/2/2
28	CLA	a	406	-	-	15/39/115/115	-
28	CLA	C	502	-	-	17/39/115/115	-
28	CLA	C	513	-	-	20/39/115/115	-
30	BCR	B	618	-	-	7/29/63/63	0/2/2/2
38	LHG	D	408	-	-	24/48/48/53	-
30	BCR	C	515	-	-	11/29/63/63	0/2/2/2
28	CLA	C	510	4	-	18/39/115/115	-
28	CLA	B	606	-	-	17/39/115/115	-
28	CLA	Y	602	-	-	19/39/115/115	-
28	CLA	b	606	-	-	16/39/115/115	-
46	CHL	N	605	20	1/1/15/21	3/41/117/117	-
28	CLA	A	410	-	-	11/33/109/115	-
28	CLA	B	609	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	C	508	-	-	13/39/115/115	-
28	CLA	d	403	-	-	23/39/115/115	-
30	BCR	c	516	-	-	14/29/63/63	0/2/2/2
47	LUT	G	620	-	-	4/29/67/67	0/2/2/2
28	CLA	B	611	-	-	11/39/115/115	-
43	RRX	H	101	-	1/1/11/25	6/29/65/65	0/2/2/2
31	SQD	B	621	-	-	13/37/57/69	0/1/1/1
46	CHL	Y	605	23	-	4/17/93/117	-
28	CLA	Y	604	-	-	17/39/115/115	-
29	PHO	A	408	-	-	13/37/103/103	0/5/6/6
28	CLA	b	612	-	-	15/39/115/115	-
48	XAT	Y	622	-	-	1/31/93/93	0/4/4/4
28	CLA	G	614	-	-	12/20/96/115	-
28	CLA	G	611	-	-	16/39/115/115	-
28	CLA	C	506	-	-	16/39/115/115	-
32	LMG	c	521	-	-	13/46/66/70	0/1/1/1
28	CLA	B	617	-	-	19/39/115/115	-
28	CLA	c	512	-	-	21/39/115/115	-
28	CLA	b	608	-	-	26/39/115/115	-
28	CLA	d	402	-	-	21/39/115/115	-
46	CHL	G	606	-	-	5/22/98/117	-
28	CLA	a	405	-	-	13/39/115/115	-
37	DGA	C	524	-	-	22/45/45/45	-
28	CLA	S	614	-	-	9/27/103/115	-
28	CLA	B	613	-	-	17/39/115/115	-
28	CLA	b	613	-	-	19/39/115/115	-
49	NEX	G	623	-	-	6/27/83/83	0/3/3/3
30	BCR	D	404	-	-	12/29/63/63	0/2/2/2
33	SPH	a	414	-	-	13/21/21/21	-
38	LHG	D	410	-	-	30/43/43/53	-
28	CLA	c	511	-	-	16/39/115/115	-
31	SQD	A	412	-	-	16/46/66/69	0/1/1/1
28	CLA	b	616	-	-	12/39/115/115	-
28	CLA	N	614	-	-	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	c	509	-	-	14/39/115/115	-
30	BCR	C	516	-	-	15/29/63/63	0/2/2/2
46	CHL	N	608	-	-	4/22/98/117	-
28	CLA	B	607	-	-	15/39/115/115	-
29	PHO	A	409	-	-	4/37/103/103	0/5/6/6
32	LMG	h	102	-	-	11/43/63/70	0/1/1/1
28	CLA	Y	610	-	-	17/39/115/115	-
47	LUT	N	621	-	-	2/29/67/67	0/2/2/2
38	LHG	d	409	-	-	28/53/53/53	-
28	CLA	G	604	-	-	12/20/96/115	-
30	BCR	B	619	-	-	6/29/63/63	0/2/2/2
29	PHO	a	408	-	-	6/37/103/103	0/5/6/6
50	LPX	S	625	-	-	12/31/31/31	-
28	CLA	S	612	-	-	5/15/91/115	-
28	CLA	N	603	-	-	20/39/115/115	-
32	LMG	C	521	-	-	13/46/66/70	0/1/1/1
28	CLA	b	605	-	-	19/39/115/115	-
28	CLA	c	504	-	-	21/39/115/115	-
42	HEM	f	101	6,7	-	1/14/54/54	-
46	CHL	G	608	-	-	2/15/91/117	-
46	CHL	N	607	-	1/1/15/21	12/41/117/117	-
31	SQD	b	621	-	-	18/37/57/69	0/1/1/1
38	LHG	N	624	-	-	33/53/53/53	-
46	CHL	G	605	-	1/1/11/21	7/20/96/117	-
30	BCR	b	618	-	-	7/29/63/63	0/2/2/2
30	BCR	c	515	-	-	15/29/63/63	0/2/2/2
28	CLA	G	610	-	-	20/39/115/115	-
34	C7Z	b	620	-	1/1/12/26	14/29/67/67	0/2/2/2
35	DGD	B	623	-	-	14/32/72/95	0/2/2/2
46	CHL	G	607	-	1/1/15/21	11/41/117/117	-
47	LUT	G	621	-	-	5/29/67/67	0/2/2/2
47	LUT	S	620	-	-	4/29/67/67	0/2/2/2
28	CLA	B	614	-	-	11/39/115/115	-
28	CLA	G	603	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	CHL	S	601	22	-	3/17/93/117	-
28	CLA	C	507	-	-	20/39/115/115	-
32	LMG	H	102	-	-	9/43/63/70	0/1/1/1
36	3PH	b	624	-	-	21/49/49/49	-
28	CLA	b	604	-	-	21/39/115/115	-
32	LMG	a	413	-	-	13/43/63/70	0/1/1/1
28	CLA	b	607	-	-	11/39/115/115	-
28	CLA	S	609	-	-	12/33/109/115	-
48	XAT	N	622	-	1/1/12/26	0/31/93/93	0/4/4/4
28	CLA	C	509	-	-	18/39/115/115	-
28	CLA	S	611	38	-	17/39/115/115	-
35	DGD	c	519	-	-	19/51/91/95	0/2/2/2
28	CLA	Y	613	-	-	20/39/115/115	-
28	CLA	Y	611	-	-	18/39/115/115	-
30	BCR	b	619	-	-	11/29/63/63	0/2/2/2
30	BCR	A	411	-	-	11/29/63/63	0/2/2/2
28	CLA	a	407	-	-	11/20/96/115	-
28	CLA	S	602	-	-	20/33/109/115	-
46	CHL	N	609	-	1/1/15/21	6/41/117/117	-
32	LMG	W	201	-	-	12/34/54/70	0/1/1/1
31	SQD	c	526	-	-	13/49/69/69	0/1/1/1
35	DGD	c	520	-	-	7/48/88/95	0/2/2/2
37	DGA	J	101	-	-	10/30/30/45	-
35	DGD	c	518	-	-	19/44/84/95	0/2/2/2
28	CLA	b	610	-	-	14/39/115/115	-
31	SQD	b	626	-	-	21/49/69/69	0/1/1/1
45	4RF	K	101	-	-	32/59/59/59	-
51	PTY	Y	627	-	-	13/20/20/53	-
46	CHL	Y	607	-	1/1/15/21	8/41/117/117	-
28	CLA	N	611	-	-	13/20/96/115	-
32	LMG	C	523	-	-	18/50/70/70	0/1/1/1
37	DGA	b	625	-	-	28/45/45/45	-
49	NEX	S	623	-	-	2/27/83/83	0/3/3/3
45	4RF	k	101	-	-	30/59/59/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	b	602	-	-	28/39/115/115	-
38	LHG	Y	624	-	-	31/53/53/53	-
28	CLA	N	613	-	-	19/39/115/115	-
28	CLA	Y	608	-	-	11/21/97/115	-

All (1211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	620	C7Z	C25-C26	15.90	1.62	1.34
34	B	620	C7Z	C25-C26	15.72	1.61	1.34
43	h	101	RRX	C26-C25	15.50	1.61	1.34
43	H	101	RRX	C26-C25	15.18	1.60	1.34
34	b	620	C7Z	C5-C6	15.02	1.60	1.34
43	h	101	RRX	C5-C6	15.01	1.60	1.34
34	B	620	C7Z	C5-C6	14.94	1.60	1.34
43	H	101	RRX	C5-C6	14.75	1.60	1.34
47	N	620	LUT	C24-C25	14.69	1.51	1.33
47	Y	620	LUT	C24-C25	14.53	1.51	1.33
47	N	621	LUT	C24-C25	14.52	1.51	1.33
47	G	620	LUT	C24-C25	14.48	1.51	1.33
47	Y	621	LUT	C24-C25	14.45	1.51	1.33
47	G	621	LUT	C24-C25	14.44	1.51	1.33
47	S	620	LUT	C24-C25	14.42	1.51	1.33
47	S	621	LUT	C24-C25	14.38	1.51	1.33
34	B	620	C7Z	C24-C23	11.77	1.72	1.52
34	b	620	C7Z	C24-C23	11.76	1.72	1.52
43	H	101	RRX	C29-C28	-10.40	1.37	1.52
43	h	101	RRX	C29-C28	-10.39	1.37	1.52
34	B	620	C7Z	C22-C23	-10.25	1.37	1.52
34	b	620	C7Z	C2-C3	-10.24	1.37	1.52
34	b	620	C7Z	C22-C23	-10.23	1.37	1.52
34	B	620	C7Z	C2-C3	-10.21	1.37	1.52
29	a	408	PHO	C1B-C2B	9.45	1.50	1.39
29	A	408	PHO	C1B-C2B	9.38	1.50	1.39
29	A	409	PHO	C1B-C2B	9.33	1.49	1.39
29	a	409	PHO	C1B-C2B	9.07	1.49	1.39
34	B	620	C7Z	C4-C3	8.64	1.67	1.52
34	b	620	C7Z	C4-C3	8.61	1.67	1.52
29	A	408	PHO	C3B-C4B	7.82	1.50	1.41
43	h	101	RRX	C27-C28	7.78	1.65	1.52
29	a	409	PHO	C3B-C4B	7.76	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S	623	NEX	C14-C13	-7.74	1.25	1.35
29	A	409	PHO	C3B-C4B	7.69	1.50	1.41
49	S	623	NEX	C30-C29	-7.63	1.25	1.35
30	c	515	BCR	C10-C9	7.59	1.45	1.35
49	N	623	NEX	C14-C13	-7.57	1.25	1.35
49	G	623	NEX	C34-C33	-7.56	1.25	1.35
30	C	516	BCR	C10-C9	7.56	1.45	1.35
49	S	623	NEX	C34-C33	-7.55	1.25	1.35
49	N	623	NEX	C30-C29	-7.52	1.25	1.35
30	c	517	BCR	C10-C9	7.48	1.45	1.35
49	N	623	NEX	C34-C33	-7.47	1.25	1.35
29	a	408	PHO	C3B-C4B	7.46	1.50	1.41
43	H	101	RRX	C27-C28	7.45	1.65	1.52
30	d	404	BCR	C10-C9	7.44	1.45	1.35
49	G	623	NEX	C30-C29	-7.43	1.25	1.35
30	c	516	BCR	C10-C9	7.42	1.45	1.35
49	Y	623	NEX	C34-C33	-7.36	1.26	1.35
49	S	623	NEX	C10-C9	-7.30	1.26	1.35
49	G	623	NEX	C14-C13	-7.29	1.26	1.35
49	Y	623	NEX	C14-C13	-7.29	1.26	1.35
49	Y	623	NEX	C30-C29	-7.26	1.26	1.35
49	Y	623	NEX	C10-C9	-7.25	1.26	1.35
49	N	623	NEX	C10-C9	-7.23	1.26	1.35
30	b	618	BCR	C10-C9	7.17	1.45	1.35
30	c	514	BCR	C10-C9	7.16	1.45	1.35
30	A	411	BCR	C10-C9	7.15	1.45	1.35
39	C	527	LMK	O3-C4	7.14	1.43	1.22
30	C	517	BCR	C10-C9	7.13	1.45	1.35
30	b	619	BCR	C10-C9	7.13	1.45	1.35
39	c	527	LMK	O3-C4	7.09	1.43	1.22
30	a	411	BCR	C10-C9	7.09	1.45	1.35
30	C	514	BCR	C10-C9	7.04	1.45	1.35
30	B	618	BCR	C10-C9	6.97	1.45	1.35
30	D	404	BCR	C10-C9	6.93	1.45	1.35
30	B	619	BCR	C10-C9	6.85	1.44	1.35
30	C	515	BCR	C10-C9	6.83	1.44	1.35
49	S	623	NEX	C35-C15	-6.78	1.18	1.36
49	N	623	NEX	C35-C15	-6.76	1.18	1.36
49	Y	623	NEX	C35-C15	-6.67	1.18	1.36
49	G	623	NEX	C35-C15	-6.66	1.18	1.36
43	h	101	RRX	C2-C3	-6.56	1.36	1.52
28	S	605	CLA	MG-NA	6.49	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	603	CLA	MG-NA	6.48	2.21	2.06
28	c	511	CLA	MG-NA	6.47	2.21	2.06
28	c	503	CLA	MG-NA	6.47	2.21	2.06
28	G	611	CLA	MG-NA	6.45	2.21	2.06
28	N	613	CLA	MG-NA	6.44	2.21	2.06
28	Y	608	CLA	MG-NA	6.44	2.21	2.06
28	N	612	CLA	MG-NA	6.44	2.21	2.06
28	G	613	CLA	MG-NA	6.43	2.21	2.06
28	C	501	CLA	MG-NA	6.43	2.21	2.06
28	C	503	CLA	MG-NA	6.43	2.21	2.06
28	B	602	CLA	MG-NA	6.42	2.21	2.06
28	B	616	CLA	MG-NA	6.42	2.21	2.06
28	B	611	CLA	MG-NA	6.41	2.21	2.06
43	H	101	RRX	C2-C3	-6.41	1.36	1.52
28	b	616	CLA	MG-NA	6.41	2.21	2.06
28	C	511	CLA	MG-NA	6.41	2.21	2.06
28	a	407	CLA	MG-NA	6.40	2.21	2.06
28	a	406	CLA	MG-NA	6.40	2.21	2.06
28	B	608	CLA	MG-NA	6.39	2.21	2.06
28	C	512	CLA	MG-NA	6.39	2.21	2.06
28	Y	612	CLA	MG-NA	6.39	2.21	2.06
28	C	507	CLA	MG-NA	6.38	2.21	2.06
28	N	611	CLA	MG-NA	6.38	2.21	2.06
28	S	617	CLA	MG-NA	6.38	2.21	2.06
28	a	410	CLA	MG-NA	6.38	2.21	2.06
49	S	623	NEX	C31-C32	-6.38	1.18	1.34
28	B	605	CLA	MG-NA	6.37	2.21	2.06
28	N	614	CLA	MG-NA	6.37	2.21	2.06
28	b	602	CLA	MG-NA	6.37	2.21	2.06
28	S	611	CLA	MG-NA	6.37	2.21	2.06
28	b	614	CLA	MG-NA	6.37	2.21	2.06
28	B	603	CLA	MG-NA	6.36	2.21	2.06
28	A	407	CLA	MG-NA	6.36	2.21	2.06
28	b	605	CLA	MG-NA	6.36	2.21	2.06
28	S	613	CLA	MG-NA	6.36	2.21	2.06
28	G	612	CLA	MG-NA	6.35	2.21	2.06
28	B	615	CLA	MG-NA	6.35	2.21	2.06
28	G	604	CLA	MG-NA	6.34	2.21	2.06
28	c	512	CLA	MG-NA	6.34	2.21	2.06
28	c	501	CLA	MG-NA	6.34	2.21	2.06
28	Y	611	CLA	MG-NA	6.34	2.21	2.06
28	Y	613	CLA	MG-NA	6.34	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	502	CLA	MG-NA	6.34	2.21	2.06
28	B	604	CLA	MG-NA	6.33	2.21	2.06
28	C	513	CLA	MG-NA	6.32	2.21	2.06
28	N	603	CLA	MG-NA	6.32	2.21	2.06
28	S	609	CLA	MG-NA	6.32	2.21	2.06
28	b	608	CLA	MG-NA	6.31	2.21	2.06
28	b	611	CLA	MG-NA	6.31	2.21	2.06
28	N	604	CLA	MG-NA	6.31	2.21	2.06
28	S	612	CLA	MG-NA	6.29	2.21	2.06
49	S	623	NEX	C11-C12	-6.29	1.18	1.34
28	c	506	CLA	MG-NA	6.29	2.21	2.06
28	c	513	CLA	MG-NA	6.29	2.21	2.06
28	Y	602	CLA	MG-NA	6.29	2.21	2.06
49	N	623	NEX	C31-C32	-6.29	1.18	1.34
49	G	623	NEX	C31-C32	-6.29	1.18	1.34
28	Y	604	CLA	MG-NA	6.28	2.21	2.06
28	d	402	CLA	MG-NA	6.28	2.21	2.06
28	b	615	CLA	MG-NA	6.28	2.21	2.06
28	D	402	CLA	MG-NA	6.28	2.21	2.06
28	S	610	CLA	MG-NA	6.27	2.21	2.06
28	b	609	CLA	MG-NA	6.27	2.21	2.06
28	c	509	CLA	MG-NA	6.27	2.21	2.06
28	c	507	CLA	MG-NA	6.27	2.21	2.06
49	N	623	NEX	C11-C12	-6.27	1.18	1.34
28	Y	603	CLA	MG-NA	6.27	2.21	2.06
28	B	617	CLA	MG-NA	6.27	2.21	2.06
28	G	602	CLA	MG-NA	6.26	2.21	2.06
28	G	614	CLA	MG-NA	6.26	2.21	2.06
28	Y	614	CLA	MG-NA	6.26	2.21	2.06
28	N	602	CLA	MG-NA	6.26	2.21	2.06
28	C	502	CLA	MG-NA	6.26	2.21	2.06
28	G	603	CLA	MG-NA	6.26	2.21	2.06
28	D	403	CLA	MG-NA	6.26	2.21	2.06
28	C	506	CLA	MG-NA	6.26	2.21	2.06
28	c	504	CLA	MG-NA	6.25	2.21	2.06
28	b	604	CLA	MG-NA	6.25	2.21	2.06
28	G	610	CLA	MG-NA	6.25	2.21	2.06
28	S	602	CLA	MG-NA	6.25	2.21	2.06
28	B	609	CLA	MG-NA	6.25	2.21	2.06
28	C	505	CLA	MG-NA	6.25	2.21	2.06
28	b	613	CLA	MG-NA	6.24	2.21	2.06
28	b	617	CLA	MG-NA	6.24	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	604	CLA	MG-NA	6.24	2.21	2.06
28	B	614	CLA	MG-NA	6.24	2.21	2.06
28	b	607	CLA	MG-NA	6.23	2.21	2.06
49	Y	623	NEX	C11-C12	-6.22	1.18	1.34
49	G	623	NEX	C10-C9	-6.22	1.27	1.35
28	B	607	CLA	MG-NA	6.22	2.21	2.06
28	Y	610	CLA	MG-NA	6.22	2.21	2.06
28	N	610	CLA	MG-NA	6.22	2.21	2.06
28	b	603	CLA	MG-NA	6.22	2.21	2.06
28	C	504	CLA	MG-NA	6.22	2.21	2.06
28	S	614	CLA	MG-NA	6.22	2.21	2.06
28	B	610	CLA	MG-NA	6.21	2.21	2.06
28	A	410	CLA	MG-NA	6.21	2.21	2.06
28	C	509	CLA	MG-NA	6.20	2.21	2.06
49	G	623	NEX	C11-C12	-6.20	1.18	1.34
49	Y	623	NEX	C31-C32	-6.20	1.18	1.34
28	B	613	CLA	MG-NA	6.20	2.21	2.06
28	C	508	CLA	MG-NA	6.18	2.21	2.06
28	c	505	CLA	MG-NA	6.17	2.20	2.06
28	d	403	CLA	MG-NA	6.17	2.20	2.06
28	A	406	CLA	MG-NA	6.16	2.20	2.06
28	b	606	CLA	MG-NA	6.15	2.20	2.06
28	B	612	CLA	MG-NA	6.14	2.20	2.06
28	A	405	CLA	MG-NA	6.14	2.20	2.06
43	H	101	RRX	C1-C6	-6.13	1.45	1.53
28	c	510	CLA	MG-NA	6.13	2.20	2.06
28	b	610	CLA	MG-NA	6.13	2.20	2.06
28	B	606	CLA	MG-NA	6.12	2.20	2.06
28	C	510	CLA	MG-NA	6.11	2.20	2.06
28	a	405	CLA	MG-NA	6.07	2.20	2.06
28	b	612	CLA	MG-NA	6.05	2.20	2.06
28	c	508	CLA	MG-NA	5.97	2.20	2.06
30	b	619	BCR	C24-C23	5.93	1.51	1.33
30	d	404	BCR	C24-C23	5.84	1.50	1.33
30	C	516	BCR	C24-C23	5.80	1.50	1.33
30	c	516	BCR	C24-C23	5.80	1.50	1.33
30	c	517	BCR	C24-C23	5.78	1.50	1.33
34	b	620	C7Z	C12-C13	5.78	1.58	1.45
30	b	618	BCR	C24-C23	5.77	1.50	1.33
30	B	618	BCR	C24-C23	5.76	1.50	1.33
30	c	515	BCR	C24-C23	5.73	1.50	1.33
30	D	404	BCR	C24-C23	5.72	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	411	BCR	C24-C23	5.70	1.50	1.33
30	A	411	BCR	C24-C23	5.70	1.50	1.33
30	B	619	BCR	C24-C23	5.67	1.50	1.33
30	c	514	BCR	C24-C23	5.65	1.50	1.33
30	C	517	BCR	C24-C23	5.64	1.50	1.33
30	C	514	BCR	C24-C23	5.62	1.50	1.33
34	B	620	C7Z	C12-C13	5.60	1.58	1.45
30	C	515	BCR	C24-C23	5.59	1.50	1.33
43	h	101	RRX	C1-C6	-5.54	1.46	1.53
34	B	620	C7Z	C1-C6	-5.47	1.46	1.53
49	Y	623	NEX	C7-C8	5.46	1.41	1.32
49	N	623	NEX	C7-C8	5.44	1.41	1.32
34	b	620	C7Z	C1-C6	-5.39	1.46	1.53
49	S	623	NEX	C28-C29	-5.32	1.34	1.45
30	C	515	BCR	C11-C12	-5.28	1.21	1.34
30	B	619	BCR	C11-C12	-5.28	1.21	1.34
30	b	618	BCR	C11-C12	-5.27	1.21	1.34
49	N	623	NEX	C28-C29	-5.23	1.34	1.45
30	C	514	BCR	C11-C12	-5.21	1.21	1.34
49	Y	623	NEX	C28-C29	-5.20	1.34	1.45
43	H	101	RRX	C2-C1	5.19	1.66	1.54
49	G	623	NEX	C28-C29	-5.18	1.34	1.45
30	A	411	BCR	C11-C12	-5.18	1.21	1.34
30	C	517	BCR	C11-C12	-5.18	1.21	1.34
30	a	411	BCR	C11-C12	-5.17	1.21	1.34
43	h	101	RRX	C8-C9	5.17	1.57	1.45
30	b	619	BCR	C11-C12	-5.16	1.21	1.34
30	c	514	BCR	C11-C12	-5.15	1.21	1.34
34	B	620	C7Z	C28-C29	5.13	1.57	1.45
30	D	404	BCR	C11-C12	-5.13	1.21	1.34
30	B	618	BCR	C11-C12	-5.12	1.21	1.34
34	b	620	C7Z	C28-C29	5.11	1.56	1.45
43	h	101	RRX	C19-C18	5.10	1.56	1.45
43	h	101	RRX	C2-C1	5.07	1.65	1.54
30	c	517	BCR	C11-C12	-5.02	1.21	1.34
30	d	404	BCR	C11-C12	-5.01	1.21	1.34
30	c	516	BCR	C11-C12	-5.00	1.21	1.34
30	C	516	BCR	C11-C12	-4.97	1.21	1.34
43	H	101	RRX	C19-C18	4.93	1.56	1.45
49	S	623	NEX	C7-C8	4.85	1.40	1.32
34	B	620	C7Z	C24-C25	-4.81	1.43	1.51
34	b	620	C7Z	C32-C33	4.81	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	515	BCR	C11-C12	-4.80	1.22	1.34
34	B	620	C7Z	C32-C33	4.76	1.56	1.45
34	b	620	C7Z	C24-C25	-4.69	1.43	1.51
49	G	623	NEX	C7-C8	4.68	1.39	1.32
43	H	101	RRX	C8-C9	4.66	1.55	1.45
43	H	101	RRX	C27-C26	-4.64	1.43	1.51
43	h	101	RRX	C30-C25	-4.62	1.47	1.53
43	H	101	RRX	C30-C25	-4.60	1.47	1.53
43	h	101	RRX	C27-C26	-4.45	1.44	1.51
43	h	101	RRX	C12-C13	4.44	1.55	1.45
43	h	101	RRX	C23-C22	4.42	1.55	1.45
34	B	620	C7Z	C31-C30	4.41	1.57	1.43
34	b	620	C7Z	C31-C30	4.40	1.57	1.43
30	B	619	BCR	C16-C17	-4.40	1.29	1.43
30	C	515	BCR	C16-C17	-4.39	1.29	1.43
46	N	608	CHL	CBB-CAB	4.38	1.52	1.30
34	b	620	C7Z	C8-C9	4.37	1.55	1.45
35	c	520	DGD	O1G-C1A	4.36	1.46	1.33
35	b	623	DGD	O1G-C1A	4.36	1.46	1.33
46	Y	601	CHL	CBB-CAB	4.36	1.51	1.30
28	c	504	CLA	CBB-CAB	4.36	1.51	1.30
46	G	607	CHL	CBB-CAB	4.35	1.51	1.30
34	B	620	C7Z	C4-C5	-4.34	1.44	1.51
46	G	605	CHL	CBB-CAB	4.34	1.51	1.30
28	b	611	CLA	CBB-CAB	4.34	1.51	1.30
35	B	623	DGD	O1G-C1A	4.33	1.46	1.33
28	c	512	CLA	CBB-CAB	4.33	1.51	1.30
28	d	402	CLA	CBB-CAB	4.32	1.51	1.30
28	c	508	CLA	CBB-CAB	4.32	1.51	1.30
28	S	612	CLA	CBB-CAB	4.32	1.51	1.30
28	B	612	CLA	CBB-CAB	4.32	1.51	1.30
28	S	603	CLA	CBB-CAB	4.32	1.51	1.30
28	G	603	CLA	CBB-CAB	4.32	1.51	1.30
46	Y	605	CHL	CBB-CAB	4.32	1.51	1.30
46	N	601	CHL	CBB-CAB	4.32	1.51	1.30
28	b	612	CLA	CBB-CAB	4.32	1.51	1.30
28	c	509	CLA	CBB-CAB	4.32	1.51	1.30
28	c	513	CLA	CBB-CAB	4.32	1.51	1.30
28	C	508	CLA	CBB-CAB	4.31	1.51	1.30
46	S	608	CHL	CBB-CAB	4.31	1.51	1.30
28	b	608	CLA	CBB-CAB	4.31	1.51	1.30
28	C	509	CLA	CBB-CAB	4.31	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	511	CLA	CBB-CAB	4.31	1.51	1.30
28	b	614	CLA	CBB-CAB	4.31	1.51	1.30
46	G	601	CHL	CBB-CAB	4.31	1.51	1.30
28	A	405	CLA	CBB-CAB	4.31	1.51	1.30
46	G	608	CHL	CBB-CAB	4.31	1.51	1.30
28	c	507	CLA	CBB-CAB	4.31	1.51	1.30
28	G	614	CLA	CBB-CAB	4.31	1.51	1.30
28	b	610	CLA	CBB-CAB	4.31	1.51	1.30
28	c	503	CLA	CBB-CAB	4.30	1.51	1.30
28	C	503	CLA	CBB-CAB	4.30	1.51	1.30
28	N	614	CLA	CBB-CAB	4.30	1.51	1.30
28	Y	610	CLA	CBB-CAB	4.30	1.51	1.30
28	c	505	CLA	CBB-CAB	4.30	1.51	1.30
28	a	405	CLA	CBB-CAB	4.30	1.51	1.30
28	B	610	CLA	CBB-CAB	4.30	1.51	1.30
30	C	514	BCR	C16-C17	-4.30	1.30	1.43
30	B	618	BCR	C16-C17	-4.30	1.30	1.43
46	N	605	CHL	CBB-CAB	4.30	1.51	1.30
30	a	411	BCR	C16-C17	-4.30	1.30	1.43
28	a	407	CLA	CBB-CAB	4.30	1.51	1.30
28	d	403	CLA	CBB-CAB	4.30	1.51	1.30
28	B	609	CLA	CBB-CAB	4.30	1.51	1.30
28	G	610	CLA	CBB-CAB	4.30	1.51	1.30
28	N	613	CLA	CBB-CAB	4.30	1.51	1.30
28	B	614	CLA	CBB-CAB	4.30	1.51	1.30
28	B	611	CLA	CBB-CAB	4.29	1.51	1.30
28	B	608	CLA	CBB-CAB	4.29	1.51	1.30
46	G	609	CHL	CBB-CAB	4.29	1.51	1.30
28	B	604	CLA	CBB-CAB	4.29	1.51	1.30
28	Y	602	CLA	CBB-CAB	4.29	1.51	1.30
30	A	411	BCR	C16-C17	-4.29	1.30	1.43
28	S	605	CLA	CBB-CAB	4.29	1.51	1.30
28	S	614	CLA	CBB-CAB	4.29	1.51	1.30
28	B	602	CLA	CBB-CAB	4.29	1.51	1.30
28	C	512	CLA	CBB-CAB	4.29	1.51	1.30
28	B	605	CLA	CBB-CAB	4.29	1.51	1.30
28	G	604	CLA	CBB-CAB	4.29	1.51	1.30
28	b	604	CLA	CBB-CAB	4.29	1.51	1.30
28	S	602	CLA	CBB-CAB	4.29	1.51	1.30
28	Y	604	CLA	CBB-CAB	4.29	1.51	1.30
28	Y	608	CLA	CBB-CAB	4.29	1.51	1.30
28	c	501	CLA	CBB-CAB	4.29	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	611	CLA	CBB-CAB	4.29	1.51	1.30
28	C	511	CLA	CBB-CAB	4.28	1.51	1.30
28	S	617	CLA	CBB-CAB	4.28	1.51	1.30
28	S	604	CLA	CBB-CAB	4.28	1.51	1.30
28	B	606	CLA	CBB-CAB	4.28	1.51	1.30
28	N	610	CLA	CBB-CAB	4.28	1.51	1.30
28	C	507	CLA	CBB-CAB	4.28	1.51	1.30
28	N	612	CLA	CBB-CAB	4.28	1.51	1.30
28	G	611	CLA	CBB-CAB	4.28	1.51	1.30
28	B	615	CLA	CBB-CAB	4.28	1.51	1.30
28	C	502	CLA	CBB-CAB	4.28	1.51	1.30
43	H	101	RRX	C3-C4	4.28	1.65	1.52
28	S	610	CLA	CBB-CAB	4.28	1.51	1.30
28	N	602	CLA	CBB-CAB	4.28	1.51	1.30
28	B	603	CLA	CBB-CAB	4.28	1.51	1.30
28	c	502	CLA	CBB-CAB	4.28	1.51	1.30
28	b	609	CLA	CBB-CAB	4.28	1.51	1.30
28	c	506	CLA	CBB-CAB	4.28	1.51	1.30
28	B	617	CLA	CBB-CAB	4.27	1.51	1.30
34	B	620	C7Z	C8-C9	4.27	1.55	1.45
28	b	607	CLA	CBB-CAB	4.27	1.51	1.30
28	B	607	CLA	CBB-CAB	4.27	1.51	1.30
28	S	613	CLA	CBB-CAB	4.27	1.51	1.30
28	Y	603	CLA	CBB-CAB	4.27	1.51	1.30
28	Y	613	CLA	CBB-CAB	4.27	1.51	1.30
46	N	607	CHL	CBB-CAB	4.27	1.51	1.30
46	Y	607	CHL	CBB-CAB	4.27	1.51	1.30
28	N	604	CLA	CBB-CAB	4.27	1.51	1.30
28	a	406	CLA	CBB-CAB	4.27	1.51	1.30
46	S	607	CHL	CBB-CAB	4.27	1.51	1.30
28	c	510	CLA	CBB-CAB	4.27	1.51	1.30
28	G	602	CLA	CBB-CAB	4.27	1.51	1.30
35	C	518	DGD	O1G-C1A	4.27	1.45	1.33
46	N	609	CHL	CBB-CAB	4.27	1.51	1.30
28	b	616	CLA	CBB-CAB	4.26	1.51	1.30
28	G	612	CLA	CBB-CAB	4.26	1.51	1.30
28	b	603	CLA	CBB-CAB	4.26	1.51	1.30
30	D	404	BCR	C16-C17	-4.26	1.30	1.43
28	b	615	CLA	CBB-CAB	4.26	1.51	1.30
28	C	501	CLA	CBB-CAB	4.26	1.51	1.30
28	b	617	CLA	CBB-CAB	4.26	1.51	1.30
28	b	602	CLA	CBB-CAB	4.26	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	613	CLA	CBB-CAB	4.26	1.51	1.30
28	N	611	CLA	CBB-CAB	4.26	1.51	1.30
28	b	613	CLA	CBB-CAB	4.26	1.51	1.30
30	C	517	BCR	C16-C17	-4.26	1.30	1.43
28	C	505	CLA	CBB-CAB	4.26	1.51	1.30
28	b	606	CLA	CBB-CAB	4.26	1.51	1.30
28	Y	612	CLA	CBB-CAB	4.26	1.51	1.30
28	A	407	CLA	CBB-CAB	4.26	1.51	1.30
28	D	402	CLA	CBB-CAB	4.25	1.51	1.30
28	S	609	CLA	CBB-CAB	4.25	1.51	1.30
46	Y	609	CHL	CBB-CAB	4.25	1.51	1.30
35	c	519	DGD	O1G-C1A	4.25	1.45	1.33
28	B	616	CLA	CBB-CAB	4.25	1.51	1.30
28	C	506	CLA	CBB-CAB	4.25	1.51	1.30
28	C	504	CLA	CBB-CAB	4.25	1.51	1.30
28	N	603	CLA	CBB-CAB	4.25	1.51	1.30
28	S	611	CLA	CBB-CAB	4.25	1.51	1.30
43	H	101	RRX	C12-C13	4.25	1.55	1.45
35	C	519	DGD	O1G-C1A	4.25	1.45	1.33
28	B	613	CLA	CBB-CAB	4.25	1.51	1.30
35	c	518	DGD	O1G-C1A	4.24	1.45	1.33
28	b	605	CLA	CBB-CAB	4.24	1.51	1.30
28	Y	614	CLA	CBB-CAB	4.24	1.51	1.30
34	b	620	C7Z	C4-C5	-4.24	1.44	1.51
35	C	520	DGD	O1G-C1A	4.23	1.45	1.33
28	C	505	CLA	MG-ND	-4.23	1.97	2.05
28	C	513	CLA	CBB-CAB	4.23	1.51	1.30
28	C	510	CLA	CBB-CAB	4.23	1.51	1.30
30	b	619	BCR	C16-C17	-4.23	1.30	1.43
28	C	513	CLA	MG-ND	-4.22	1.97	2.05
29	A	408	PHO	C1D-C2D	4.22	1.44	1.39
28	A	406	CLA	CBB-CAB	4.21	1.51	1.30
46	S	601	CHL	CBB-CAB	4.20	1.51	1.30
28	D	403	CLA	CBB-CAB	4.20	1.51	1.30
34	b	620	C7Z	C11-C10	4.20	1.56	1.43
46	Y	606	CHL	CBB-CAB	4.20	1.51	1.30
46	G	606	CHL	CBB-CAB	4.18	1.51	1.30
30	c	517	BCR	C16-C17	-4.18	1.30	1.43
30	c	514	BCR	C16-C17	-4.16	1.30	1.43
28	D	402	CLA	MG-ND	-4.16	1.97	2.05
30	b	618	BCR	C16-C17	-4.15	1.30	1.43
43	h	101	RRX	C3-C4	4.15	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	410	CLA	CBB-CAB	4.14	1.50	1.30
30	c	515	BCR	C16-C17	-4.13	1.30	1.43
30	d	404	BCR	C16-C17	-4.13	1.30	1.43
34	B	620	C7Z	C11-C10	4.12	1.56	1.43
46	N	606	CHL	CBB-CAB	4.12	1.50	1.30
30	C	516	BCR	C16-C17	-4.11	1.30	1.43
28	a	410	CLA	CBB-CAB	4.11	1.50	1.30
30	c	516	BCR	C16-C17	-4.10	1.30	1.43
28	C	507	CLA	MG-ND	-4.09	1.97	2.05
46	S	606	CHL	CBB-CAB	4.08	1.50	1.30
43	H	101	RRX	C23-C22	4.08	1.54	1.45
28	c	507	CLA	MG-ND	-4.08	1.97	2.05
42	F	101	HEM	FE-ND	4.05	2.07	1.94
39	C	527	LMK	O2-C4	4.05	1.43	1.30
28	b	613	CLA	MG-ND	-4.05	1.97	2.05
28	C	508	CLA	MG-ND	-4.04	1.97	2.05
28	C	506	CLA	MG-ND	-4.02	1.97	2.05
28	B	613	CLA	MG-ND	-4.00	1.97	2.05
39	c	527	LMK	O2-C4	3.99	1.43	1.30
28	c	505	CLA	MG-ND	-3.98	1.97	2.05
41	d	405	PL9	C7-C3	-3.98	1.47	1.51
28	b	612	CLA	MG-ND	-3.97	1.97	2.05
34	B	620	C7Z	C22-C21	3.97	1.67	1.54
28	B	612	CLA	MG-ND	-3.96	1.97	2.05
28	b	604	CLA	MG-ND	-3.96	1.97	2.05
28	S	611	CLA	MG-ND	-3.95	1.98	2.05
28	b	617	CLA	MG-ND	-3.95	1.98	2.05
28	A	405	CLA	MG-ND	-3.95	1.98	2.05
28	B	617	CLA	MG-ND	-3.94	1.98	2.05
28	B	604	CLA	MG-ND	-3.94	1.98	2.05
42	f	101	HEM	FE-NB	3.94	2.07	1.94
28	d	402	CLA	MG-ND	-3.94	1.98	2.05
29	A	409	PHO	C1D-C2D	3.93	1.43	1.39
43	h	101	RRX	C20-C21	3.93	1.55	1.43
34	b	620	C7Z	C22-C21	3.92	1.67	1.54
28	c	504	CLA	MG-ND	-3.92	1.98	2.05
28	A	410	CLA	MG-ND	-3.92	1.98	2.05
28	b	611	CLA	MG-ND	-3.91	1.98	2.05
28	b	607	CLA	MG-ND	-3.91	1.98	2.05
28	c	506	CLA	MG-ND	-3.91	1.98	2.05
28	b	609	CLA	MG-ND	-3.91	1.98	2.05
28	a	410	CLA	MG-ND	-3.91	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	605	CLA	MG-ND	-3.90	1.98	2.05
28	a	406	CLA	MG-ND	-3.90	1.98	2.05
28	C	509	CLA	MG-ND	-3.90	1.98	2.05
43	h	101	RRX	C15-C14	3.89	1.55	1.43
28	C	512	CLA	MG-ND	-3.89	1.98	2.05
28	b	605	CLA	MG-ND	-3.89	1.98	2.05
28	c	508	CLA	MG-ND	-3.89	1.98	2.05
28	B	609	CLA	MG-ND	-3.88	1.98	2.05
28	B	611	CLA	MG-ND	-3.88	1.98	2.05
28	N	604	CLA	MG-ND	-3.87	1.98	2.05
28	B	608	CLA	MG-ND	-3.87	1.98	2.05
28	Y	608	CLA	MG-ND	-3.87	1.98	2.05
28	G	604	CLA	MG-ND	-3.87	1.98	2.05
28	S	603	CLA	MG-ND	-3.86	1.98	2.05
28	B	605	CLA	MG-ND	-3.86	1.98	2.05
28	a	407	CLA	MG-ND	-3.86	1.98	2.05
28	N	613	CLA	MG-ND	-3.85	1.98	2.05
29	a	408	PHO	C1D-C2D	3.85	1.43	1.39
28	B	610	CLA	MG-ND	-3.85	1.98	2.05
28	G	602	CLA	MG-ND	-3.85	1.98	2.05
28	S	614	CLA	MG-ND	-3.85	1.98	2.05
28	b	608	CLA	MG-ND	-3.85	1.98	2.05
28	B	615	CLA	MG-ND	-3.84	1.98	2.05
28	B	607	CLA	MG-ND	-3.84	1.98	2.05
28	c	502	CLA	MG-ND	-3.83	1.98	2.05
34	B	620	C7Z	C15-C14	3.83	1.55	1.43
28	c	512	CLA	MG-ND	-3.83	1.98	2.05
28	S	617	CLA	MG-ND	-3.83	1.98	2.05
28	A	406	CLA	MG-ND	-3.83	1.98	2.05
28	C	503	CLA	MG-ND	-3.83	1.98	2.05
28	b	603	CLA	MG-ND	-3.83	1.98	2.05
28	C	510	CLA	MG-ND	-3.83	1.98	2.05
28	b	615	CLA	MG-ND	-3.83	1.98	2.05
28	b	614	CLA	MG-ND	-3.82	1.98	2.05
28	A	407	CLA	MG-ND	-3.82	1.98	2.05
28	G	612	CLA	MG-ND	-3.82	1.98	2.05
28	N	614	CLA	MG-ND	-3.82	1.98	2.05
29	A	409	PHO	C4D-CHA	3.81	1.45	1.39
34	b	620	C7Z	C15-C14	3.81	1.55	1.43
28	S	610	CLA	MG-ND	-3.81	1.98	2.05
28	G	613	CLA	MG-ND	-3.81	1.98	2.05
28	b	610	CLA	MG-ND	-3.81	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	509	CLA	MG-ND	-3.80	1.98	2.05
28	N	610	CLA	MG-ND	-3.80	1.98	2.05
43	H	101	RRX	C15-C14	3.80	1.55	1.43
28	N	611	CLA	MG-ND	-3.80	1.98	2.05
28	Y	612	CLA	MG-ND	-3.80	1.98	2.05
43	H	101	RRX	C20-C21	3.80	1.55	1.43
28	S	612	CLA	MG-ND	-3.79	1.98	2.05
28	S	602	CLA	MG-ND	-3.79	1.98	2.05
28	N	612	CLA	MG-ND	-3.79	1.98	2.05
28	Y	604	CLA	MG-ND	-3.79	1.98	2.05
28	B	616	CLA	MG-ND	-3.78	1.98	2.05
28	S	609	CLA	MG-ND	-3.78	1.98	2.05
28	G	611	CLA	MG-ND	-3.78	1.98	2.05
28	b	602	CLA	MG-ND	-3.78	1.98	2.05
28	D	403	CLA	MG-ND	-3.78	1.98	2.05
28	Y	614	CLA	MG-ND	-3.78	1.98	2.05
28	C	502	CLA	MG-ND	-3.78	1.98	2.05
28	C	501	CLA	MG-ND	-3.78	1.98	2.05
29	a	409	PHO	C1D-C2D	3.78	1.43	1.39
28	S	604	CLA	MG-ND	-3.77	1.98	2.05
41	D	405	PL9	C7-C3	-3.77	1.47	1.51
28	B	603	CLA	MG-ND	-3.77	1.98	2.05
28	Y	610	CLA	MG-ND	-3.76	1.98	2.05
28	c	503	CLA	MG-ND	-3.76	1.98	2.05
29	a	409	PHO	C4D-CHA	3.76	1.45	1.39
28	c	501	CLA	MG-ND	-3.76	1.98	2.05
28	c	513	CLA	MG-ND	-3.76	1.98	2.05
28	Y	602	CLA	MG-ND	-3.75	1.98	2.05
28	b	606	CLA	MG-ND	-3.75	1.98	2.05
28	B	606	CLA	MG-ND	-3.75	1.98	2.05
28	B	602	CLA	MG-ND	-3.75	1.98	2.05
28	c	511	CLA	MG-ND	-3.75	1.98	2.05
28	C	511	CLA	MG-ND	-3.74	1.98	2.05
28	Y	611	CLA	MG-ND	-3.73	1.98	2.05
28	S	613	CLA	MG-ND	-3.73	1.98	2.05
28	B	614	CLA	MG-ND	-3.73	1.98	2.05
28	d	403	CLA	MG-ND	-3.72	1.98	2.05
28	N	603	CLA	MG-ND	-3.72	1.98	2.05
28	a	405	CLA	MG-ND	-3.71	1.98	2.05
34	B	620	C7Z	C27-C26	3.70	1.58	1.45
28	Y	613	CLA	MG-ND	-3.69	1.98	2.05
28	b	616	CLA	MG-ND	-3.69	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	610	CLA	MG-ND	-3.68	1.98	2.05
28	Y	603	CLA	MG-ND	-3.68	1.98	2.05
34	b	620	C7Z	C27-C26	3.68	1.58	1.45
29	a	408	PHO	C4D-CHA	3.68	1.45	1.39
28	C	504	CLA	MG-ND	-3.68	1.98	2.05
37	b	625	DGA	OG2-CB1	3.67	1.44	1.34
28	N	602	CLA	MG-ND	-3.66	1.98	2.05
28	B	612	CLA	C1C-NC	-3.65	1.32	1.37
28	G	603	CLA	MG-ND	-3.64	1.98	2.05
37	B	625	DGA	OG2-CB1	3.64	1.44	1.34
28	G	614	CLA	MG-ND	-3.64	1.98	2.05
34	b	620	C7Z	C35-C34	3.64	1.54	1.43
28	c	510	CLA	MG-ND	-3.63	1.98	2.05
34	B	620	C7Z	C35-C34	3.60	1.54	1.43
34	b	620	C7Z	C2-C1	3.60	1.66	1.54
28	B	611	CLA	C1C-NC	-3.59	1.32	1.37
28	A	406	CLA	C1C-NC	-3.59	1.32	1.37
34	B	620	C7Z	C2-C1	3.59	1.66	1.54
28	c	508	CLA	C1C-NC	-3.58	1.32	1.37
28	C	508	CLA	C1C-NC	-3.55	1.32	1.37
42	F	101	HEM	FE-NB	3.55	2.05	1.94
28	B	605	CLA	C1C-NC	-3.54	1.32	1.37
37	J	101	DGA	OG2-CB1	3.53	1.44	1.34
28	c	504	CLA	C1C-NC	-3.53	1.32	1.37
37	j	101	DGA	OG2-CB1	3.51	1.44	1.34
37	c	524	DGA	OG2-CB1	3.51	1.44	1.34
28	b	611	CLA	C1C-NC	-3.50	1.32	1.37
45	k	101	4RF	O18-C16	3.49	1.43	1.33
28	b	617	CLA	C1C-NC	-3.48	1.32	1.37
28	c	507	CLA	C1C-NC	-3.48	1.32	1.37
28	G	602	CLA	C1C-NC	-3.47	1.32	1.37
45	i	101	4RF	O18-C16	3.46	1.43	1.33
34	B	620	C7Z	C38-C25	3.46	1.56	1.50
28	C	509	CLA	C1C-NC	-3.45	1.32	1.37
45	K	101	4RF	O18-C16	3.45	1.43	1.33
28	c	506	CLA	C1C-NC	-3.45	1.32	1.37
45	I	102	4RF	O18-C16	3.44	1.43	1.33
43	h	101	RRX	C11-C10	3.44	1.54	1.43
28	B	617	CLA	C1C-NC	-3.44	1.32	1.37
28	b	605	CLA	C1C-NC	-3.44	1.32	1.37
37	C	524	DGA	OG2-CB1	3.44	1.44	1.34
28	C	502	CLA	C1C-NC	-3.43	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	620	C7Z	C7-C6	3.42	1.57	1.45
28	N	610	CLA	C1C-NC	-3.42	1.32	1.37
28	C	506	CLA	C1C-NC	-3.41	1.32	1.37
34	b	620	C7Z	C38-C25	3.41	1.56	1.50
28	B	610	CLA	C1C-NC	-3.41	1.32	1.37
28	C	513	CLA	C1C-NC	-3.41	1.32	1.37
37	J	101	DGA	OG1-CA1	3.40	1.43	1.33
28	B	606	CLA	C1C-NC	-3.39	1.32	1.37
28	b	610	CLA	C1C-NC	-3.39	1.32	1.37
28	a	407	CLA	C1C-NC	-3.38	1.32	1.37
43	H	101	RRX	C11-C10	3.38	1.53	1.43
34	B	620	C7Z	C7-C6	3.36	1.57	1.45
28	C	504	CLA	C1C-NC	-3.36	1.32	1.37
29	A	408	PHO	C4D-CHA	3.36	1.44	1.39
28	b	612	CLA	C1C-NC	-3.36	1.32	1.37
28	A	405	CLA	C1C-NC	-3.35	1.32	1.37
37	c	524	DGA	OG1-CA1	3.35	1.43	1.33
43	h	101	RRX	C16-C17	3.35	1.53	1.43
37	B	625	DGA	OG1-CA1	3.35	1.43	1.33
37	j	101	DGA	OG1-CA1	3.33	1.43	1.33
28	c	509	CLA	C1C-NC	-3.31	1.32	1.37
28	c	502	CLA	C1C-NC	-3.31	1.32	1.37
28	D	403	CLA	C1C-NC	-3.30	1.32	1.37
28	D	402	CLA	C1C-NC	-3.30	1.32	1.37
28	a	405	CLA	C1C-NC	-3.30	1.32	1.37
37	C	524	DGA	OG1-CA1	3.29	1.43	1.33
28	d	402	CLA	C1C-NC	-3.29	1.32	1.37
28	b	606	CLA	C1C-NC	-3.29	1.32	1.37
28	B	613	CLA	C1C-NC	-3.29	1.32	1.37
28	G	603	CLA	C1C-NC	-3.29	1.32	1.37
32	H	102	LMG	C37-C36	-3.28	1.33	1.51
28	S	610	CLA	C1C-NC	-3.28	1.32	1.37
28	G	612	CLA	C1C-NC	-3.28	1.32	1.37
28	S	604	CLA	C1C-NC	-3.28	1.32	1.37
28	S	605	CLA	C1C-NC	-3.28	1.32	1.37
35	c	519	DGD	CAB-C9B	-3.28	1.33	1.51
28	G	611	CLA	C1C-NC	-3.28	1.32	1.37
37	b	625	DGA	OG1-CA1	3.28	1.42	1.33
28	N	604	CLA	C1C-NC	-3.27	1.32	1.37
32	h	102	LMG	C19-C18	-3.27	1.33	1.51
35	C	519	DGD	CAB-C9B	-3.27	1.33	1.51
28	B	608	CLA	C1C-NC	-3.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	407	CLA	C1C-NC	-3.26	1.32	1.37
43	h	101	RRX	C29-C30	3.26	1.65	1.54
28	C	507	CLA	C1C-NC	-3.26	1.32	1.37
32	b	622	LMG	C22-C21	-3.26	1.33	1.51
32	c	521	LMG	C22-C21	-3.26	1.33	1.51
43	H	101	RRX	C29-C30	3.26	1.65	1.54
28	a	406	CLA	C1C-NC	-3.26	1.32	1.37
32	B	622	LMG	C22-C21	-3.25	1.33	1.51
28	S	603	CLA	C1C-NC	-3.25	1.33	1.37
43	H	101	RRX	C16-C17	3.25	1.53	1.43
35	c	519	DGD	CDA-CCA	-3.25	1.33	1.51
32	H	102	LMG	C19-C18	-3.24	1.33	1.51
28	S	613	CLA	C1C-NC	-3.24	1.33	1.37
35	C	520	DGD	CAB-C9B	-3.24	1.33	1.51
35	c	520	DGD	CAB-C9B	-3.24	1.33	1.51
28	b	616	CLA	C1C-NC	-3.24	1.33	1.37
35	c	518	DGD	CDB-CCB	-3.24	1.33	1.51
43	h	101	RRX	C24-C25	3.24	1.56	1.45
35	C	519	DGD	CDA-CCA	-3.24	1.33	1.51
28	Y	602	CLA	C1C-NC	-3.24	1.33	1.37
28	N	602	CLA	C1C-NC	-3.23	1.33	1.37
32	c	521	LMG	C40-C39	-3.23	1.33	1.51
28	Y	603	CLA	C1C-NC	-3.23	1.33	1.37
32	C	521	LMG	C40-C39	-3.23	1.33	1.51
32	C	521	LMG	C22-C21	-3.23	1.33	1.51
28	S	614	CLA	C1C-NC	-3.23	1.33	1.37
35	c	520	DGD	CAA-C9A	-3.23	1.33	1.51
32	c	523	LMG	C40-C39	-3.23	1.33	1.51
35	C	518	DGD	CDB-CCB	-3.23	1.33	1.51
28	Y	610	CLA	C1C-NC	-3.23	1.33	1.37
32	C	523	LMG	C40-C39	-3.23	1.33	1.51
28	G	610	CLA	C1C-NC	-3.23	1.33	1.37
32	C	523	LMG	C25-C24	-3.23	1.33	1.51
32	c	523	LMG	C25-C24	-3.23	1.33	1.51
32	c	521	LMG	C37-C36	-3.23	1.33	1.51
32	C	523	LMG	C37-C36	-3.23	1.33	1.51
32	c	523	LMG	C37-C36	-3.22	1.33	1.51
28	N	611	CLA	C1C-NC	-3.22	1.33	1.37
28	b	608	CLA	C1C-NC	-3.22	1.33	1.37
28	c	505	CLA	C1C-NC	-3.22	1.33	1.37
32	C	523	LMG	C22-C21	-3.22	1.33	1.51
32	W	201	LMG	C40-C39	-3.22	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	h	102	LMG	C37-C36	-3.22	1.33	1.51
35	c	520	DGD	CDB-CCB	-3.22	1.33	1.51
28	C	503	CLA	C1C-NC	-3.22	1.33	1.37
32	a	413	LMG	C19-C18	-3.22	1.33	1.51
35	C	520	DGD	CAA-C9A	-3.22	1.33	1.51
32	c	523	LMG	C22-C21	-3.22	1.33	1.51
32	A	413	LMG	C40-C39	-3.22	1.33	1.51
28	C	510	CLA	C1C-NC	-3.22	1.33	1.37
28	b	613	CLA	C1C-NC	-3.22	1.33	1.37
32	a	413	LMG	C37-C36	-3.21	1.33	1.51
28	G	604	CLA	C1C-NC	-3.21	1.33	1.37
28	c	510	CLA	C1C-NC	-3.21	1.33	1.37
35	c	519	DGD	CAA-C9A	-3.21	1.33	1.51
35	C	519	DGD	CDB-CCB	-3.21	1.33	1.51
32	D	411	LMG	C22-C21	-3.21	1.33	1.51
28	Y	612	CLA	C1C-NC	-3.21	1.33	1.37
35	C	518	DGD	CAB-C9B	-3.21	1.33	1.51
35	C	519	DGD	CAA-C9A	-3.21	1.33	1.51
32	A	413	LMG	C37-C36	-3.21	1.33	1.51
32	H	102	LMG	C40-C39	-3.21	1.33	1.51
28	c	503	CLA	C1C-NC	-3.21	1.33	1.37
28	C	505	CLA	C1C-NC	-3.20	1.33	1.37
28	G	602	CLA	C4B-NB	-3.20	1.33	1.37
32	b	622	LMG	C19-C18	-3.20	1.33	1.51
28	B	614	CLA	C1C-NC	-3.20	1.33	1.37
28	N	612	CLA	C1C-NC	-3.20	1.33	1.37
28	b	602	CLA	C1C-NC	-3.20	1.33	1.37
35	c	519	DGD	CDB-CCB	-3.20	1.33	1.51
28	b	614	CLA	C1C-NC	-3.20	1.33	1.37
28	B	607	CLA	C1C-NC	-3.20	1.33	1.37
42	F	101	HEM	FE-NA	3.20	2.06	1.95
28	A	410	CLA	C1C-NC	-3.20	1.33	1.37
42	F	101	HEM	CAC-C3C	3.20	1.56	1.47
42	f	101	HEM	FE-ND	3.20	2.04	1.94
28	N	614	CLA	C1C-NC	-3.20	1.33	1.37
32	A	413	LMG	C19-C18	-3.20	1.33	1.51
35	c	518	DGD	CAB-C9B	-3.20	1.33	1.51
28	Y	614	CLA	C1C-NC	-3.20	1.33	1.37
32	C	523	LMG	C43-C42	-3.20	1.33	1.51
32	D	411	LMG	C19-C18	-3.20	1.33	1.51
32	a	413	LMG	C40-C39	-3.19	1.33	1.51
32	C	521	LMG	C19-C18	-3.19	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	411	LMG	C22-C21	-3.19	1.33	1.51
28	S	612	CLA	C1C-NC	-3.19	1.33	1.37
32	w	201	LMG	C37-C36	-3.19	1.33	1.51
28	B	616	CLA	C1C-NC	-3.19	1.33	1.37
32	W	201	LMG	C37-C36	-3.19	1.33	1.51
32	B	622	LMG	C19-C18	-3.19	1.33	1.51
28	N	613	CLA	C1C-NC	-3.19	1.33	1.37
32	C	521	LMG	C37-C36	-3.19	1.33	1.51
32	h	102	LMG	C40-C39	-3.19	1.33	1.51
32	c	523	LMG	C43-C42	-3.19	1.33	1.51
28	S	611	CLA	C1C-NC	-3.19	1.33	1.37
28	b	604	CLA	C1C-NC	-3.19	1.33	1.37
32	c	523	LMG	C19-C18	-3.19	1.33	1.51
28	S	617	CLA	C1C-NC	-3.18	1.33	1.37
32	d	411	LMG	C19-C18	-3.18	1.33	1.51
35	C	520	DGD	CDB-CCB	-3.18	1.33	1.51
28	S	602	CLA	C1C-NC	-3.18	1.33	1.37
28	B	603	CLA	C1C-NC	-3.18	1.33	1.37
42	f	101	HEM	FE-NA	3.18	2.05	1.95
28	B	602	CLA	C1C-NC	-3.18	1.33	1.37
28	b	609	CLA	C1C-NC	-3.18	1.33	1.37
43	H	101	RRX	C24-C25	3.17	1.56	1.45
28	c	513	CLA	C1C-NC	-3.17	1.33	1.37
28	A	410	CLA	C4B-NB	-3.17	1.33	1.37
28	c	507	CLA	C4B-NB	-3.17	1.33	1.37
28	B	604	CLA	C1C-NC	-3.17	1.33	1.37
28	N	603	CLA	C1C-NC	-3.17	1.33	1.37
28	b	603	CLA	C1C-NC	-3.16	1.33	1.37
28	b	615	CLA	C1C-NC	-3.16	1.33	1.37
32	c	521	LMG	C19-C18	-3.16	1.33	1.51
28	G	614	CLA	C1C-NC	-3.16	1.33	1.37
28	C	501	CLA	C1C-NC	-3.16	1.33	1.37
28	a	410	CLA	C1C-NC	-3.16	1.33	1.37
28	Y	604	CLA	C1C-NC	-3.16	1.33	1.37
28	c	512	CLA	C1C-NC	-3.16	1.33	1.37
28	S	609	CLA	C1C-NC	-3.15	1.33	1.37
42	F	101	HEM	CAB-C3B	3.15	1.56	1.47
28	G	613	CLA	C1C-NC	-3.15	1.33	1.37
28	Y	613	CLA	C1C-NC	-3.15	1.33	1.37
32	C	523	LMG	C19-C18	-3.15	1.33	1.51
32	w	201	LMG	C40-C39	-3.14	1.33	1.51
42	f	101	HEM	CAC-C3C	3.14	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	615	CLA	C1C-NC	-3.14	1.33	1.37
28	B	609	CLA	C1C-NC	-3.14	1.33	1.37
28	A	406	CLA	C4B-NB	-3.14	1.33	1.37
28	C	512	CLA	C1C-NC	-3.14	1.33	1.37
28	c	511	CLA	C1C-NC	-3.14	1.33	1.37
42	f	101	HEM	CAB-C3B	3.13	1.56	1.47
28	C	507	CLA	C4B-NB	-3.13	1.33	1.37
28	b	607	CLA	C1C-NC	-3.12	1.33	1.37
28	c	501	CLA	C1C-NC	-3.12	1.33	1.37
28	d	403	CLA	C1C-NC	-3.11	1.33	1.37
28	C	511	CLA	C1C-NC	-3.11	1.33	1.37
28	Y	611	CLA	C1C-NC	-3.10	1.33	1.37
45	K	101	4RF	O40-C41	3.09	1.42	1.33
28	A	405	CLA	C4B-NB	-3.08	1.34	1.37
45	I	102	4RF	O40-C41	3.08	1.42	1.33
28	c	509	CLA	C4B-NB	-3.08	1.34	1.37
43	H	101	RRX	C4-C5	-3.07	1.44	1.51
28	a	406	CLA	C4B-NB	-3.07	1.34	1.37
45	i	101	4RF	O40-C41	3.06	1.42	1.33
28	Y	608	CLA	C1C-NC	-3.05	1.33	1.37
28	a	410	CLA	C4B-NB	-3.05	1.34	1.37
43	h	101	RRX	C7-C6	3.03	1.55	1.45
28	c	502	CLA	C4B-NB	-3.03	1.34	1.37
41	D	405	PL9	C3-C4	-3.02	1.44	1.49
28	b	610	CLA	C4B-NB	-3.02	1.34	1.37
45	k	101	4RF	O40-C41	2.98	1.42	1.33
28	c	508	CLA	C4B-NB	-2.98	1.34	1.37
28	C	509	CLA	C4B-NB	-2.97	1.34	1.37
28	C	502	CLA	C4B-NB	-2.96	1.34	1.37
28	b	609	CLA	C4B-NB	-2.95	1.34	1.37
43	h	101	RRX	C4-C5	-2.95	1.45	1.51
28	b	614	CLA	C4B-NB	-2.95	1.34	1.37
28	B	605	CLA	C4B-NB	-2.95	1.34	1.37
42	F	101	HEM	FE-NC	2.94	2.05	1.95
28	B	615	CLA	C4B-NB	-2.93	1.34	1.37
43	H	101	RRX	C7-C6	2.93	1.55	1.45
28	B	613	CLA	C4B-NB	-2.92	1.34	1.37
28	a	405	CLA	C4B-NB	-2.92	1.34	1.37
28	D	403	CLA	C4B-NB	-2.91	1.34	1.37
28	b	617	CLA	C4B-NB	-2.89	1.34	1.37
28	C	506	CLA	C4B-NB	-2.89	1.34	1.37
28	N	610	CLA	C4B-NB	-2.88	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	c	512	CLA	C4B-NB	-2.88	1.34	1.37
28	G	611	CLA	C4B-NB	-2.87	1.34	1.37
28	c	503	CLA	C4B-NB	-2.87	1.34	1.37
28	C	513	CLA	C4B-NB	-2.87	1.34	1.37
28	S	612	CLA	C4B-NB	-2.87	1.34	1.37
28	B	617	CLA	C4B-NB	-2.86	1.34	1.37
28	C	512	CLA	C4B-NB	-2.86	1.34	1.37
50	S	625	LPX	P1-O1	2.86	1.70	1.59
28	c	506	CLA	C4B-NB	-2.85	1.34	1.37
43	h	101	RRX	C32-C1	2.85	1.59	1.53
28	B	614	CLA	C4B-NB	-2.85	1.34	1.37
28	c	505	CLA	C4B-NB	-2.85	1.34	1.37
28	b	606	CLA	C4B-NB	-2.85	1.34	1.37
28	B	612	CLA	C4B-NB	-2.84	1.34	1.37
28	b	605	CLA	C4B-NB	-2.84	1.34	1.37
45	k	101	4RF	O21-C22	2.84	1.42	1.34
28	Y	610	CLA	C4B-NB	-2.84	1.34	1.37
28	S	604	CLA	C4B-NB	-2.83	1.34	1.37
28	B	609	CLA	C4B-NB	-2.83	1.34	1.37
28	b	612	CLA	C4B-NB	-2.83	1.34	1.37
28	b	615	CLA	C4B-NB	-2.83	1.34	1.37
28	Y	611	CLA	C4B-NB	-2.83	1.34	1.37
28	Y	613	CLA	C4B-NB	-2.81	1.34	1.37
28	C	510	CLA	C4B-NB	-2.80	1.34	1.37
28	b	602	CLA	C4B-NB	-2.80	1.34	1.37
28	B	604	CLA	C4B-NB	-2.80	1.34	1.37
28	A	407	CLA	C4B-NB	-2.79	1.34	1.37
28	d	403	CLA	C4B-NB	-2.79	1.34	1.37
28	C	503	CLA	C4B-NB	-2.79	1.34	1.37
28	C	508	CLA	C4B-NB	-2.79	1.34	1.37
28	S	602	CLA	C4B-NB	-2.79	1.34	1.37
28	b	607	CLA	C4B-NB	-2.78	1.34	1.37
28	Y	604	CLA	C4B-NB	-2.78	1.34	1.37
28	N	602	CLA	C4B-NB	-2.77	1.34	1.37
45	K	101	4RF	O21-C22	2.77	1.42	1.34
28	N	604	CLA	C4B-NB	-2.76	1.34	1.37
28	S	610	CLA	C4B-NB	-2.76	1.34	1.37
28	C	505	CLA	C4B-NB	-2.76	1.34	1.37
28	b	604	CLA	C4B-NB	-2.76	1.34	1.37
28	c	511	CLA	C4B-NB	-2.76	1.34	1.37
43	H	101	RRX	C32-C1	2.76	1.59	1.53
28	G	610	CLA	C4B-NB	-2.76	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	614	CLA	C4B-NB	-2.76	1.34	1.37
28	B	610	CLA	C4B-NB	-2.76	1.34	1.37
28	b	603	CLA	C4B-NB	-2.76	1.34	1.37
28	B	606	CLA	C4B-NB	-2.75	1.34	1.37
28	G	604	CLA	C4B-NB	-2.75	1.34	1.37
28	Y	612	CLA	C4B-NB	-2.75	1.34	1.37
28	c	513	CLA	C4B-NB	-2.75	1.34	1.37
28	G	614	CLA	C4B-NB	-2.74	1.34	1.37
28	S	609	CLA	C4B-NB	-2.74	1.34	1.37
28	S	613	CLA	C4B-NB	-2.74	1.34	1.37
28	B	603	CLA	C4B-NB	-2.74	1.34	1.37
28	B	607	CLA	C4B-NB	-2.74	1.34	1.37
28	c	510	CLA	C4B-NB	-2.74	1.34	1.37
28	b	608	CLA	C4B-NB	-2.74	1.34	1.37
34	b	620	C7Z	C21-C26	-2.73	1.50	1.53
28	b	616	CLA	C4B-NB	-2.73	1.34	1.37
28	S	617	CLA	C4B-NB	-2.73	1.34	1.37
28	B	616	CLA	C4B-NB	-2.73	1.34	1.37
45	I	102	4RF	O21-C22	2.72	1.42	1.34
28	N	613	CLA	C4B-NB	-2.72	1.34	1.37
28	N	603	CLA	C4B-NB	-2.71	1.34	1.37
28	N	614	CLA	C4B-NB	-2.71	1.34	1.37
28	N	612	CLA	C4B-NB	-2.70	1.34	1.37
41	d	405	PL9	C3-C4	-2.70	1.45	1.49
28	G	613	CLA	C4B-NB	-2.70	1.34	1.37
28	N	611	CLA	C4B-NB	-2.70	1.34	1.37
45	i	101	4RF	O21-C22	2.70	1.41	1.34
34	B	620	C7Z	C21-C26	-2.70	1.50	1.53
28	C	501	CLA	C4B-NB	-2.70	1.34	1.37
28	G	612	CLA	C4B-NB	-2.69	1.34	1.37
28	B	608	CLA	C4B-NB	-2.69	1.34	1.37
28	b	613	CLA	C4B-NB	-2.67	1.34	1.37
28	C	511	CLA	C4B-NB	-2.67	1.34	1.37
28	Y	602	CLA	C4B-NB	-2.66	1.34	1.37
28	Y	608	CLA	C4B-NB	-2.66	1.34	1.37
28	S	605	CLA	C4B-NB	-2.66	1.34	1.37
28	S	611	CLA	C4B-NB	-2.66	1.34	1.37
46	N	609	CHL	C1B-NB	-2.65	1.34	1.37
28	a	407	CLA	C4B-NB	-2.65	1.34	1.37
28	C	504	CLA	C4B-NB	-2.63	1.34	1.37
28	Y	614	CLA	C4B-NB	-2.63	1.34	1.37
28	Y	603	CLA	C4B-NB	-2.61	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	411	LMG	C37-C36	-2.57	1.33	1.51
28	c	504	CLA	C4B-NB	-2.57	1.34	1.37
32	D	411	LMG	C37-C36	-2.56	1.33	1.51
28	c	501	CLA	C4B-NB	-2.55	1.34	1.37
46	Y	601	CHL	C1B-NB	-2.55	1.34	1.37
36	b	624	3PH	O21-C2	-2.54	1.40	1.46
28	S	603	CLA	C4B-NB	-2.54	1.34	1.37
29	a	408	PHO	CMC-C2C	-2.54	1.46	1.50
28	B	611	CLA	C4B-NB	-2.54	1.34	1.37
29	A	409	PHO	CMC-C2C	-2.54	1.46	1.50
46	N	607	CHL	C1B-NB	-2.53	1.34	1.37
51	Y	627	PTY	O7-C6	-2.53	1.40	1.46
28	B	602	CLA	C4B-NB	-2.53	1.34	1.37
28	G	603	CLA	C4B-NB	-2.53	1.34	1.37
29	a	409	PHO	CMC-C2C	-2.49	1.46	1.50
28	D	402	CLA	C4B-NB	-2.49	1.34	1.37
29	A	408	PHO	CMC-C2C	-2.48	1.46	1.50
34	b	620	C7Z	C20-C13	2.48	1.56	1.50
46	G	607	CHL	C1B-NB	-2.48	1.34	1.37
36	t	101	3PH	O21-C2	-2.48	1.40	1.46
29	a	409	PHO	CMD-C2D	-2.47	1.46	1.51
36	S	626	3PH	O21-C2	-2.47	1.40	1.46
42	f	101	HEM	FE-NC	2.46	2.03	1.95
36	B	624	3PH	O21-C2	-2.45	1.40	1.46
36	b	624	3PH	O31-C31	2.44	1.40	1.33
36	S	626	3PH	O31-C31	2.43	1.40	1.33
51	Y	626	PTY	O7-C6	-2.43	1.40	1.46
51	Y	626	PTY	O4-C30	2.42	1.40	1.33
48	G	622	XAT	O24-C25	-2.42	1.42	1.46
29	A	408	PHO	CMD-C2D	-2.42	1.46	1.51
29	A	409	PHO	CMD-C2D	-2.42	1.46	1.51
43	H	101	RRX	C35-C13	2.42	1.55	1.50
46	Y	607	CHL	C1B-NB	-2.41	1.34	1.37
43	h	101	RRX	C35-C13	2.41	1.55	1.50
36	B	624	3PH	O31-C31	2.40	1.40	1.33
36	T	101	3PH	O31-C31	2.40	1.40	1.33
29	A	408	PHO	C4D-ND	-2.40	1.35	1.38
34	B	620	C7Z	C18-C5	2.39	1.54	1.50
29	a	408	PHO	CMB-C2B	-2.39	1.46	1.51
29	a	408	PHO	CMD-C2D	-2.39	1.46	1.51
36	T	101	3PH	O21-C21	2.39	1.41	1.34
36	t	101	3PH	O31-C31	2.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	402	CLA	C4B-NB	-2.37	1.34	1.37
28	G	602	CLA	C1C-C2C	2.37	1.49	1.44
28	b	611	CLA	C1C-C2C	2.36	1.49	1.44
34	b	620	C7Z	C18-C5	2.35	1.54	1.50
29	a	408	PHO	CAC-C3C	-2.35	1.47	1.51
29	A	409	PHO	CMB-C2B	-2.35	1.46	1.51
29	A	408	PHO	CMB-C2B	-2.34	1.46	1.51
46	G	606	CHL	C1B-NB	-2.33	1.34	1.37
50	S	625	LPX	P1-O2	2.32	1.68	1.59
28	B	605	CLA	C1A-CHA	2.32	1.52	1.43
28	S	603	CLA	C1A-CHA	2.31	1.52	1.43
51	Y	627	PTY	O7-C8	2.31	1.40	1.35
28	S	611	CLA	C1A-CHA	2.31	1.52	1.43
30	B	618	BCR	C1-C6	-2.31	1.50	1.53
28	B	602	CLA	C1A-CHA	2.31	1.52	1.43
34	B	620	C7Z	C20-C13	2.30	1.55	1.50
29	A	409	PHO	CAC-C3C	-2.30	1.47	1.51
29	a	408	PHO	C4D-ND	-2.30	1.35	1.38
28	b	614	CLA	C1A-CHA	2.29	1.52	1.43
41	D	405	PL9	C6-C1	-2.29	1.44	1.48
28	b	611	CLA	C4B-NB	-2.29	1.35	1.37
29	a	409	PHO	CMB-C2B	-2.29	1.46	1.51
28	C	512	CLA	C1A-CHA	2.27	1.52	1.43
28	c	512	CLA	C1A-CHA	2.27	1.52	1.43
46	G	608	CHL	C1B-NB	-2.27	1.35	1.37
28	N	611	CLA	C1A-CHA	2.26	1.52	1.43
28	a	407	CLA	C1A-CHA	2.25	1.52	1.43
29	a	409	PHO	C3D-C4D	2.25	1.44	1.41
28	G	613	CLA	C1C-C2C	2.25	1.48	1.44
28	b	613	CLA	C1C-C2C	2.25	1.48	1.44
51	Y	626	PTY	O7-C8	2.24	1.40	1.34
28	c	501	CLA	C1C-C2C	2.24	1.48	1.44
28	N	610	CLA	C1A-CHA	2.24	1.52	1.43
28	S	605	CLA	C1A-CHA	2.24	1.52	1.43
28	d	402	CLA	C1C-C2C	2.24	1.48	1.44
46	N	608	CHL	C1B-NB	-2.24	1.35	1.37
28	C	513	CLA	C1C-C2C	2.24	1.48	1.44
28	A	406	CLA	C1A-CHA	2.24	1.52	1.43
28	B	616	CLA	C1A-CHA	2.23	1.52	1.43
48	Y	622	XAT	O24-C25	-2.23	1.43	1.46
28	b	609	CLA	C1A-CHA	2.23	1.52	1.43
36	t	101	3PH	O21-C21	2.23	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	409	PHO	C3D-C4D	2.22	1.44	1.41
28	b	605	CLA	C1A-CHA	2.22	1.52	1.43
28	N	613	CLA	C1A-CHA	2.22	1.52	1.43
28	c	501	CLA	C1A-CHA	2.22	1.52	1.43
28	b	615	CLA	C1C-C2C	2.22	1.48	1.44
28	S	613	CLA	C1A-CHA	2.22	1.52	1.43
28	a	406	CLA	C1A-CHA	2.22	1.52	1.43
28	c	511	CLA	C1A-CHA	2.22	1.52	1.43
28	S	617	CLA	C1A-CHA	2.22	1.52	1.43
28	S	609	CLA	C1A-CHA	2.21	1.52	1.43
41	d	405	PL9	C53-C6	-2.21	1.46	1.50
28	C	512	CLA	C1C-C2C	2.21	1.48	1.44
28	B	608	CLA	C1A-CHA	2.21	1.52	1.43
28	Y	608	CLA	C1A-CHA	2.21	1.52	1.43
28	c	503	CLA	C1C-C2C	2.21	1.48	1.44
28	C	513	CLA	C1A-CHA	2.20	1.52	1.43
28	b	608	CLA	C1A-CHA	2.20	1.52	1.43
28	Y	611	CLA	C1A-CHA	2.20	1.52	1.43
28	c	505	CLA	C1A-CHA	2.20	1.52	1.43
28	b	603	CLA	C1C-C2C	2.20	1.48	1.44
28	c	504	CLA	C1A-CHA	2.20	1.52	1.43
28	N	614	CLA	C1C-C2C	2.20	1.48	1.44
34	b	620	C7Z	C40-C33	2.20	1.55	1.50
28	N	603	CLA	C1A-CHA	2.20	1.52	1.43
28	A	407	CLA	C1A-CHA	2.20	1.52	1.43
48	N	622	XAT	O24-C25	-2.20	1.43	1.46
28	Y	613	CLA	C1A-CHA	2.19	1.52	1.43
28	G	613	CLA	C1A-CHA	2.19	1.52	1.43
28	N	604	CLA	C1A-CHA	2.19	1.52	1.43
28	B	614	CLA	C1A-CHA	2.19	1.52	1.43
28	Y	612	CLA	C1A-CHA	2.19	1.52	1.43
28	c	513	CLA	C1A-CHA	2.19	1.52	1.43
28	N	614	CLA	C1A-CHA	2.19	1.52	1.43
28	b	602	CLA	C1A-CHA	2.19	1.52	1.43
28	C	503	CLA	C1C-C2C	2.18	1.48	1.44
28	S	604	CLA	C1A-CHA	2.18	1.52	1.43
28	b	616	CLA	C1A-CHA	2.18	1.52	1.43
28	S	612	CLA	C1C-C2C	2.18	1.48	1.44
28	C	505	CLA	C1A-CHA	2.18	1.52	1.43
28	N	613	CLA	C1C-C2C	2.18	1.48	1.44
28	B	603	CLA	C1A-CHA	2.18	1.52	1.43
28	C	503	CLA	C1A-CHA	2.18	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	612	CLA	C1A-CHA	2.18	1.52	1.43
28	N	612	CLA	C1A-CHA	2.17	1.52	1.43
28	C	504	CLA	C1A-CHA	2.17	1.52	1.43
28	d	403	CLA	C1A-CHA	2.17	1.52	1.43
28	G	610	CLA	C1C-C2C	2.17	1.48	1.44
28	a	410	CLA	C1C-C2C	2.17	1.48	1.44
49	S	623	NEX	C1-C6	-2.17	1.50	1.54
28	b	606	CLA	C1A-CHA	2.17	1.52	1.43
28	b	609	CLA	C1C-C2C	2.17	1.48	1.44
28	B	611	CLA	C1C-C2C	2.16	1.48	1.44
28	c	513	CLA	C1C-C2C	2.16	1.48	1.44
28	b	607	CLA	C1A-CHA	2.16	1.52	1.43
34	B	620	C7Z	C40-C33	2.16	1.55	1.50
28	b	611	CLA	C3B-C4B	2.16	1.47	1.42
28	C	501	CLA	C1C-C2C	2.16	1.48	1.44
28	G	612	CLA	C1A-CHA	2.16	1.52	1.43
28	Y	608	CLA	C1C-C2C	2.16	1.48	1.44
28	G	614	CLA	C1A-CHA	2.16	1.52	1.43
28	G	611	CLA	C1A-CHA	2.16	1.52	1.43
28	B	617	CLA	C1A-CHA	2.16	1.52	1.43
28	Y	614	CLA	C1A-CHA	2.16	1.52	1.43
28	G	603	CLA	C1A-CHA	2.16	1.52	1.43
28	B	602	CLA	C1C-C2C	2.16	1.48	1.44
29	A	409	PHO	C4D-ND	-2.16	1.35	1.38
36	B	624	3PH	O21-C21	2.16	1.40	1.34
28	Y	613	CLA	C1C-C2C	2.15	1.48	1.44
28	c	502	CLA	C1A-CHA	2.15	1.52	1.43
46	G	601	CHL	C1B-NB	-2.15	1.35	1.37
28	Y	610	CLA	C1A-CHA	2.15	1.52	1.43
28	c	509	CLA	C1A-CHA	2.15	1.52	1.43
28	B	607	CLA	C1A-CHA	2.15	1.52	1.43
28	b	610	CLA	C1A-CHA	2.15	1.52	1.43
29	a	408	PHO	C3D-C4D	2.15	1.44	1.41
41	d	405	PL9	C6-C1	-2.15	1.44	1.48
28	c	506	CLA	C1A-CHA	2.15	1.52	1.43
28	A	410	CLA	C1A-CHA	2.15	1.52	1.43
28	b	615	CLA	C1A-CHA	2.14	1.52	1.43
28	C	506	CLA	C1A-CHA	2.14	1.52	1.43
28	C	509	CLA	C1A-CHA	2.14	1.52	1.43
28	b	604	CLA	C1A-CHA	2.14	1.52	1.43
28	B	603	CLA	C1C-C2C	2.14	1.48	1.44
28	d	403	CLA	C1C-C2C	2.14	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	G	614	CLA	C1C-C2C	2.14	1.48	1.44
36	S	626	3PH	O21-C21	2.14	1.40	1.34
28	S	613	CLA	C1C-C2C	2.14	1.48	1.44
29	A	408	PHO	CAC-C3C	-2.14	1.47	1.51
28	b	603	CLA	C1A-CHA	2.14	1.52	1.43
36	T	101	3PH	O31-C3	-2.14	1.40	1.45
28	c	505	CLA	C1C-C2C	2.14	1.48	1.44
28	c	511	CLA	C1C-C2C	2.14	1.48	1.44
28	b	617	CLA	C1A-CHA	2.14	1.52	1.43
28	Y	602	CLA	C1C-C2C	2.14	1.48	1.44
37	C	524	DGA	OG2-CG2	-2.13	1.41	1.46
36	b	624	3PH	O21-C21	2.13	1.40	1.34
28	C	502	CLA	C1A-CHA	2.13	1.52	1.43
28	C	507	CLA	C1A-CHA	2.13	1.51	1.43
28	B	611	CLA	C1A-CHA	2.13	1.51	1.43
29	A	408	PHO	C3D-C4D	2.13	1.44	1.41
28	A	410	CLA	C1C-C2C	2.13	1.48	1.44
28	S	610	CLA	C1C-C2C	2.13	1.48	1.44
28	S	609	CLA	C1C-C2C	2.13	1.48	1.44
28	C	511	CLA	C1A-CHA	2.13	1.51	1.43
28	G	602	CLA	C1A-CHA	2.13	1.51	1.43
28	a	410	CLA	C1A-CHA	2.12	1.51	1.43
28	N	602	CLA	C1C-C2C	2.12	1.48	1.44
28	B	604	CLA	C1A-CHA	2.12	1.51	1.43
28	G	610	CLA	C1A-CHA	2.12	1.51	1.43
28	S	610	CLA	C1A-CHA	2.12	1.51	1.43
28	Y	604	CLA	C1A-CHA	2.12	1.51	1.43
28	N	612	CLA	C1C-C2C	2.12	1.48	1.44
28	B	610	CLA	C1A-CHA	2.11	1.51	1.43
28	Y	612	CLA	C1C-C2C	2.11	1.48	1.44
28	c	507	CLA	C1A-CHA	2.11	1.51	1.43
28	b	613	CLA	C1A-CHA	2.11	1.51	1.43
28	G	604	CLA	C1C-C2C	2.11	1.48	1.44
28	C	501	CLA	C1A-CHA	2.11	1.51	1.43
28	c	512	CLA	C1C-C2C	2.11	1.48	1.44
36	B	624	3PH	O31-C3	-2.11	1.40	1.45
28	B	615	CLA	C1A-CHA	2.11	1.51	1.43
28	b	614	CLA	C1C-C2C	2.11	1.48	1.44
28	G	604	CLA	C1A-CHA	2.11	1.51	1.43
28	B	604	CLA	C1C-C2C	2.11	1.48	1.44
28	B	606	CLA	C1A-CHA	2.11	1.51	1.43
46	G	609	CHL	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	D	405	PL9	C53-C6	-2.10	1.46	1.50
28	Y	603	CLA	C1A-CHA	2.10	1.51	1.43
28	B	611	CLA	C3B-C4B	2.10	1.47	1.42
28	Y	611	CLA	C1C-C2C	2.10	1.48	1.44
28	S	603	CLA	C1C-C2C	2.10	1.48	1.44
28	C	510	CLA	C3D-C4D	-2.10	1.39	1.44
28	c	510	CLA	C1A-CHA	2.10	1.51	1.43
28	D	403	CLA	C1A-CHA	2.10	1.51	1.43
28	S	605	CLA	C1C-C2C	2.10	1.48	1.44
36	b	624	3PH	O31-C3	-2.10	1.40	1.45
28	S	605	CLA	MG-NC	2.10	2.11	2.06
28	S	614	CLA	C1A-CHA	2.10	1.51	1.43
42	F	101	HEM	CMB-C2B	2.09	1.55	1.50
28	c	503	CLA	C1A-CHA	2.09	1.51	1.43
37	j	101	DGA	OG2-CG2	-2.09	1.41	1.46
28	G	612	CLA	C1C-C2C	2.09	1.48	1.44
28	B	615	CLA	C1C-C2C	2.09	1.48	1.44
28	D	402	CLA	C1C-C2C	2.09	1.48	1.44
28	b	608	CLA	C1C-C2C	2.09	1.48	1.44
28	S	602	CLA	C1C-C2C	2.09	1.48	1.44
28	d	402	CLA	C3B-C4B	2.09	1.47	1.42
28	b	611	CLA	C1A-CHA	2.09	1.51	1.43
28	C	511	CLA	C1C-C2C	2.09	1.48	1.44
28	b	616	CLA	C1C-C2C	2.09	1.48	1.44
28	a	405	CLA	C1A-CHA	2.09	1.51	1.43
36	t	101	3PH	O31-C3	-2.09	1.40	1.45
28	S	602	CLA	C1A-CHA	2.09	1.51	1.43
28	Y	610	CLA	C1C-C2C	2.09	1.48	1.44
28	Y	603	CLA	C1C-C2C	2.08	1.48	1.44
42	f	101	HEM	CMB-C2B	2.08	1.55	1.50
37	c	524	DGA	OG2-CG2	-2.08	1.41	1.46
28	B	613	CLA	C1A-CHA	2.08	1.51	1.43
28	S	617	CLA	C1C-C2C	2.08	1.48	1.44
28	B	616	CLA	C1C-C2C	2.08	1.48	1.44
28	a	407	CLA	C3D-C4D	-2.08	1.39	1.44
28	C	507	CLA	C3D-C4D	-2.08	1.39	1.44
36	S	626	3PH	O31-C3	-2.07	1.40	1.45
28	b	607	CLA	C1C-C2C	2.07	1.48	1.44
36	T	101	3PH	O21-C2	-2.07	1.41	1.46
28	Y	602	CLA	C1A-CHA	2.07	1.51	1.43
28	S	605	CLA	C3D-C4D	-2.07	1.39	1.44
28	b	612	CLA	C1A-CHA	2.07	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y	604	CLA	C1C-C2C	2.07	1.48	1.44
28	S	614	CLA	C1C-C2C	2.06	1.48	1.44
28	Y	614	CLA	C1C-C2C	2.06	1.48	1.44
28	c	508	CLA	C1A-CHA	2.06	1.51	1.43
28	C	505	CLA	C1C-C2C	2.06	1.48	1.44
28	b	602	CLA	C1C-C2C	2.06	1.48	1.44
28	a	406	CLA	C1C-C2C	2.06	1.48	1.44
49	G	623	NEX	C2-C3	2.06	1.55	1.52
28	B	612	CLA	C1A-CHA	2.06	1.51	1.43
28	B	609	CLA	C3D-C4D	-2.06	1.39	1.44
28	N	611	CLA	C1C-C2C	2.06	1.48	1.44
41	d	405	PL9	C26-C24	-2.06	1.47	1.51
28	A	405	CLA	C1A-CHA	2.06	1.51	1.43
28	N	603	CLA	C1C-C2C	2.06	1.48	1.44
28	N	613	CLA	MG-NC	2.05	2.11	2.06
32	h	102	LMG	C22-C21	-2.05	1.33	1.49
28	N	604	CLA	C1C-C2C	2.05	1.48	1.44
37	J	101	DGA	OG2-CG2	-2.05	1.41	1.46
28	C	508	CLA	C1A-CHA	2.05	1.51	1.43
28	c	507	CLA	C3D-C4D	-2.05	1.39	1.44
28	S	603	CLA	MG-NC	2.05	2.11	2.06
28	b	607	CLA	C3D-C4D	-2.04	1.39	1.44
46	Y	609	CHL	C1B-NB	-2.04	1.35	1.37
28	S	611	CLA	MG-NC	2.04	2.11	2.06
28	G	611	CLA	MG-NC	2.04	2.11	2.06
28	A	407	CLA	C1C-C2C	2.04	1.48	1.44
46	G	605	CHL	C1B-NB	-2.04	1.35	1.37
46	S	601	CHL	C1B-NB	-2.04	1.35	1.37
32	A	413	LMG	C43-C42	-2.04	1.33	1.49
28	C	507	CLA	C1C-C2C	2.04	1.48	1.44
28	S	611	CLA	C1C-C2C	2.03	1.48	1.44
32	h	102	LMG	O1-C1	2.03	1.43	1.40
51	Y	627	PTY	O4-C1	-2.03	1.40	1.45
28	b	602	CLA	MG-NC	2.03	2.11	2.06
28	d	402	CLA	C3D-C4D	-2.03	1.39	1.44
46	Y	605	CHL	C1B-NB	-2.03	1.35	1.37
28	B	607	CLA	C3D-C4D	-2.02	1.39	1.44
28	N	612	CLA	MG-NC	2.02	2.11	2.06
28	N	604	CLA	C3D-C4D	-2.02	1.39	1.44
28	B	604	CLA	C3D-C4D	-2.02	1.39	1.44
28	D	402	CLA	C3D-C4D	-2.02	1.39	1.44
35	C	518	DGD	CGB-CFB	-2.02	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	N	623	NEX	C1-C6	-2.02	1.51	1.54
46	S	608	CHL	C1B-NB	-2.02	1.35	1.37
28	D	402	CLA	C3B-C4B	2.02	1.47	1.42
28	B	608	CLA	C3D-C4D	-2.02	1.39	1.44
28	B	609	CLA	C1C-C2C	2.02	1.48	1.44
28	b	605	CLA	C1C-C2C	2.02	1.48	1.44
28	C	505	CLA	C3D-C4D	-2.02	1.39	1.44
28	A	405	CLA	C3D-C4D	-2.02	1.39	1.44
35	C	519	DGD	CGB-CFB	-2.01	1.33	1.49
28	B	602	CLA	MG-NC	2.01	2.11	2.06
28	B	613	CLA	C3D-C4D	-2.01	1.39	1.44
46	N	601	CHL	C1B-NB	-2.01	1.35	1.37
35	c	520	DGD	CDA-CCA	-2.01	1.33	1.49
35	c	519	DGD	CGB-CFB	-2.01	1.33	1.49
28	C	503	CLA	MG-NC	2.01	2.11	2.06
46	S	606	CHL	C1B-NB	-2.01	1.35	1.37
28	G	604	CLA	C3D-C4D	-2.01	1.39	1.44
35	C	520	DGD	CDA-CCA	-2.01	1.33	1.49
28	b	605	CLA	MG-NC	2.01	2.11	2.06
28	b	604	CLA	C1C-C2C	2.01	1.48	1.44
28	S	604	CLA	CHD-C1D	2.01	1.42	1.38
28	C	509	CLA	C3D-C4D	-2.01	1.39	1.44
28	B	613	CLA	C1C-C2C	2.01	1.48	1.44
28	a	405	CLA	C1C-C2C	2.01	1.48	1.44
28	N	614	CLA	MG-NC	2.01	2.11	2.06
28	G	611	CLA	CHD-C1D	2.01	1.42	1.38
35	C	520	DGD	CGB-CFB	-2.01	1.33	1.49
28	Y	608	CLA	MG-NC	2.01	2.11	2.06
28	c	510	CLA	C1C-C2C	2.01	1.48	1.44
32	A	413	LMG	C22-C21	-2.01	1.33	1.49
28	Y	611	CLA	MG-NC	2.01	2.11	2.06
32	H	102	LMG	C43-C42	-2.01	1.33	1.49
46	S	607	CHL	C1B-NB	-2.01	1.35	1.37
32	C	521	LMG	C43-C42	-2.00	1.33	1.49
32	H	102	LMG	C22-C21	-2.00	1.33	1.49
32	a	413	LMG	C22-C21	-2.00	1.33	1.49
32	h	102	LMG	C43-C42	-2.00	1.33	1.49
32	B	622	LMG	C25-C24	-2.00	1.33	1.49
51	Y	626	PTY	O4-C1	-2.00	1.40	1.45
35	c	520	DGD	CGB-CFB	-2.00	1.33	1.49
28	B	615	CLA	C3D-C4D	-2.00	1.39	1.44
28	Y	612	CLA	MG-NC	2.00	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	607	CLA	C1C-C2C	2.00	1.48	1.44
32	C	521	LMG	C25-C24	-2.00	1.33	1.49

All (2908) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	l	101	LHG	O7-C7-C8	23.08	161.24	111.50
38	L	101	LHG	O7-C7-C8	22.88	160.81	111.50
36	S	626	3PH	O21-C21-C22	22.37	159.71	111.50
30	b	618	BCR	C10-C11-C12	18.18	179.96	123.22
36	S	626	3PH	O21-C21-O22	-18.16	79.82	123.70
38	L	101	LHG	O7-C7-O9	-18.13	79.88	123.70
38	l	101	LHG	O7-C7-O9	-17.93	80.36	123.70
30	B	618	BCR	C10-C11-C12	17.88	179.02	123.22
30	C	515	BCR	C10-C11-C12	17.76	178.66	123.22
30	c	514	BCR	C10-C11-C12	17.70	178.47	123.22
30	C	517	BCR	C10-C11-C12	17.58	178.09	123.22
30	c	516	BCR	C10-C11-C12	17.53	177.91	123.22
30	C	516	BCR	C10-C11-C12	17.52	177.88	123.22
30	A	411	BCR	C10-C11-C12	17.52	177.88	123.22
30	C	514	BCR	C10-C11-C12	17.47	177.74	123.22
30	d	404	BCR	C10-C11-C12	17.41	177.54	123.22
30	b	619	BCR	C10-C11-C12	17.40	177.52	123.22
30	c	517	BCR	C10-C11-C12	17.38	177.45	123.22
30	a	411	BCR	C10-C11-C12	17.31	177.22	123.22
30	B	619	BCR	C10-C11-C12	17.27	177.11	123.22
30	c	515	BCR	C10-C11-C12	17.25	177.05	123.22
30	D	404	BCR	C10-C11-C12	17.24	177.01	123.22
48	Y	622	XAT	C37-C21-C36	-16.67	82.78	107.37
30	c	514	BCR	C16-C15-C14	15.35	154.92	123.47
30	c	516	BCR	C16-C15-C14	15.25	154.72	123.47
30	C	514	BCR	C16-C15-C14	15.00	154.20	123.47
30	c	517	BCR	C16-C15-C14	14.40	152.97	123.47
30	b	619	BCR	C16-C15-C14	14.39	152.94	123.47
30	b	618	BCR	C16-C15-C14	14.29	152.75	123.47
30	B	618	BCR	C16-C15-C14	14.23	152.63	123.47
30	C	516	BCR	C11-C10-C9	14.07	147.40	127.31
30	c	515	BCR	C16-C15-C14	14.02	152.19	123.47
30	d	404	BCR	C16-C15-C14	13.92	151.98	123.47
30	C	515	BCR	C16-C15-C14	13.60	151.34	123.47
30	C	517	BCR	C21-C20-C19	13.39	164.99	123.22
30	c	516	BCR	C11-C10-C9	13.21	146.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	618	BCR	C11-C10-C9	13.13	146.04	127.31
30	B	618	BCR	C11-C10-C9	13.11	146.03	127.31
30	C	516	BCR	C16-C15-C14	13.03	150.17	123.47
30	c	517	BCR	C21-C20-C19	12.84	163.28	123.22
30	c	517	BCR	C11-C10-C9	12.81	145.60	127.31
30	C	514	BCR	C11-C10-C9	12.80	145.57	127.31
48	Y	622	XAT	C37-C21-C22	-12.76	86.80	108.98
30	D	404	BCR	C21-C20-C19	12.75	163.01	123.22
30	b	619	BCR	C11-C10-C9	12.68	145.40	127.31
30	c	516	BCR	C21-C20-C19	12.59	162.51	123.22
30	B	619	BCR	C16-C15-C14	12.57	149.22	123.47
30	A	411	BCR	C11-C10-C9	12.54	145.21	127.31
30	a	411	BCR	C21-C20-C19	12.52	162.28	123.22
30	a	411	BCR	C11-C10-C9	12.43	145.05	127.31
30	C	516	BCR	C21-C20-C19	12.43	162.01	123.22
30	d	404	BCR	C11-C10-C9	12.39	144.99	127.31
30	D	404	BCR	C16-C15-C14	12.38	148.84	123.47
30	c	514	BCR	C21-C20-C19	12.36	161.78	123.22
30	A	411	BCR	C21-C20-C19	12.35	161.77	123.22
30	a	411	BCR	C16-C15-C14	12.30	148.66	123.47
30	C	517	BCR	C11-C10-C9	12.26	144.81	127.31
30	B	619	BCR	C21-C20-C19	12.18	161.23	123.22
30	c	514	BCR	C11-C10-C9	12.08	144.55	127.31
30	A	411	BCR	C16-C15-C14	12.05	148.16	123.47
30	d	404	BCR	C21-C20-C19	12.04	160.80	123.22
30	B	619	BCR	C11-C10-C9	12.03	144.48	127.31
30	C	517	BCR	C16-C15-C14	11.99	148.03	123.47
30	b	618	BCR	C21-C20-C19	11.91	160.38	123.22
30	b	619	BCR	C21-C20-C19	11.69	159.70	123.22
30	c	515	BCR	C21-C20-C19	11.50	159.11	123.22
30	B	618	BCR	C21-C20-C19	11.26	158.35	123.22
36	S	626	3PH	O22-C21-C22	-11.24	79.90	123.73
30	C	514	BCR	C21-C20-C19	11.20	158.17	123.22
30	D	404	BCR	C11-C10-C9	11.18	143.27	127.31
30	C	515	BCR	C11-C10-C9	11.14	143.20	127.31
30	B	619	BCR	C11-C12-C13	11.03	157.40	126.42
38	L	101	LHG	O9-C7-C8	-10.97	80.95	123.73
38	l	101	LHG	O9-C7-C8	-10.95	81.03	123.73
30	D	404	BCR	C11-C12-C13	10.66	156.36	126.42
30	b	618	BCR	C11-C12-C13	10.65	156.34	126.42
30	a	411	BCR	C11-C12-C13	10.63	156.29	126.42
30	c	515	BCR	C11-C10-C9	10.52	142.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	515	BCR	C11-C12-C13	10.50	155.92	126.42
30	C	517	BCR	C11-C12-C13	10.47	155.83	126.42
30	A	411	BCR	C11-C12-C13	10.44	155.75	126.42
30	d	404	BCR	C11-C12-C13	10.38	155.57	126.42
30	c	517	BCR	C11-C12-C13	10.36	155.52	126.42
30	C	516	BCR	C11-C12-C13	10.18	155.02	126.42
30	c	515	BCR	C11-C12-C13	10.14	154.91	126.42
28	a	407	CLA	C4A-NA-C1A	10.07	111.23	106.71
30	C	515	BCR	C21-C20-C19	10.06	154.62	123.22
30	B	618	BCR	C11-C12-C13	10.04	154.62	126.42
30	b	619	BCR	C11-C12-C13	9.94	154.35	126.42
28	b	606	CLA	C4A-NA-C1A	9.93	111.17	106.71
30	c	514	BCR	C11-C12-C13	9.93	154.31	126.42
28	B	605	CLA	C4A-NA-C1A	9.79	111.11	106.71
30	C	514	BCR	C11-C12-C13	9.76	153.82	126.42
28	c	505	CLA	C4A-NA-C1A	9.69	111.06	106.71
28	c	512	CLA	C4A-NA-C1A	9.65	111.05	106.71
28	c	513	CLA	C4A-NA-C1A	9.61	111.03	106.71
28	A	406	CLA	C4A-NA-C1A	9.58	111.02	106.71
28	C	513	CLA	C4A-NA-C1A	9.57	111.01	106.71
28	b	610	CLA	C4A-NA-C1A	9.56	111.01	106.71
28	N	610	CLA	C4A-NA-C1A	9.56	111.00	106.71
28	a	405	CLA	C4A-NA-C1A	9.53	110.99	106.71
28	C	504	CLA	C4A-NA-C1A	9.52	110.99	106.71
28	S	603	CLA	C4A-NA-C1A	9.47	110.97	106.71
28	G	603	CLA	C4A-NA-C1A	9.39	110.93	106.71
28	B	606	CLA	C4A-NA-C1A	9.39	110.93	106.71
28	b	609	CLA	C4A-NA-C1A	9.37	110.92	106.71
28	C	512	CLA	C4A-NA-C1A	9.34	110.90	106.71
28	c	504	CLA	C4A-NA-C1A	9.32	110.89	106.71
28	c	510	CLA	C4A-NA-C1A	9.32	110.89	106.71
28	S	611	CLA	C4A-NA-C1A	9.31	110.89	106.71
28	Y	612	CLA	C4A-NA-C1A	9.30	110.89	106.71
28	Y	603	CLA	C4A-NA-C1A	9.29	110.88	106.71
28	N	613	CLA	C4A-NA-C1A	9.28	110.88	106.71
28	C	509	CLA	C4A-NA-C1A	9.27	110.88	106.71
30	c	516	BCR	C11-C12-C13	9.27	152.45	126.42
28	S	617	CLA	C4A-NA-C1A	9.26	110.87	106.71
28	C	502	CLA	C4A-NA-C1A	9.24	110.86	106.71
28	B	602	CLA	C4A-NA-C1A	9.24	110.86	106.71
30	C	515	BCR	C20-C19-C18	9.23	152.35	126.42
28	N	614	CLA	C4A-NA-C1A	9.23	110.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	608	CLA	C4A-NA-C1A	9.23	110.86	106.71
28	B	608	CLA	C4A-NA-C1A	9.22	110.85	106.71
28	C	510	CLA	C4A-NA-C1A	9.22	110.85	106.71
28	N	603	CLA	C4A-NA-C1A	9.22	110.85	106.71
28	B	613	CLA	C4A-NA-C1A	9.21	110.84	106.71
28	B	614	CLA	C4A-NA-C1A	9.19	110.84	106.71
28	B	617	CLA	C4A-NA-C1A	9.19	110.84	106.71
28	c	509	CLA	C4A-NA-C1A	9.17	110.83	106.71
28	b	614	CLA	C4A-NA-C1A	9.17	110.83	106.71
28	S	613	CLA	C4A-NA-C1A	9.17	110.83	106.71
28	c	511	CLA	C4A-NA-C1A	9.12	110.81	106.71
28	C	511	CLA	C4A-NA-C1A	9.09	110.79	106.71
28	S	604	CLA	C4A-NA-C1A	9.08	110.79	106.71
28	b	605	CLA	C4A-NA-C1A	9.07	110.78	106.71
28	Y	613	CLA	C4A-NA-C1A	9.06	110.78	106.71
28	N	604	CLA	C4A-NA-C1A	9.05	110.78	106.71
28	c	506	CLA	C4A-NA-C1A	9.04	110.77	106.71
28	A	407	CLA	C4A-NA-C1A	9.04	110.77	106.71
28	S	609	CLA	C4A-NA-C1A	9.03	110.76	106.71
28	B	615	CLA	C4A-NA-C1A	9.02	110.76	106.71
28	b	617	CLA	C4A-NA-C1A	9.01	110.76	106.71
28	c	502	CLA	C4A-NA-C1A	9.00	110.75	106.71
28	B	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
28	b	612	CLA	C4A-NA-C1A	8.97	110.74	106.71
28	B	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
28	G	613	CLA	C4A-NA-C1A	8.91	110.71	106.71
28	G	614	CLA	C4A-NA-C1A	8.90	110.71	106.71
28	B	610	CLA	C4A-NA-C1A	8.89	110.70	106.71
28	N	611	CLA	C4A-NA-C1A	8.88	110.70	106.71
28	b	602	CLA	C4A-NA-C1A	8.87	110.69	106.71
28	b	615	CLA	C4A-NA-C1A	8.83	110.68	106.71
28	A	410	CLA	C4A-NA-C1A	8.83	110.67	106.71
28	b	603	CLA	C4A-NA-C1A	8.83	110.67	106.71
28	Y	610	CLA	C4A-NA-C1A	8.82	110.67	106.71
28	C	506	CLA	C4A-NA-C1A	8.82	110.67	106.71
28	G	604	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	S	612	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	b	616	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	Y	608	CLA	C4A-NA-C1A	8.81	110.67	106.71
28	d	403	CLA	C4A-NA-C1A	8.79	110.66	106.71
28	Y	611	CLA	C4A-NA-C1A	8.78	110.65	106.71
28	c	508	CLA	C4A-NA-C1A	8.78	110.65	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	610	CLA	C4A-NA-C1A	8.76	110.65	106.71
28	B	607	CLA	C4A-NA-C1A	8.74	110.64	106.71
28	S	605	CLA	C4A-NA-C1A	8.74	110.64	106.71
28	C	505	CLA	C4A-NA-C1A	8.73	110.63	106.71
28	Y	614	CLA	C4A-NA-C1A	8.73	110.63	106.71
28	Y	604	CLA	C4A-NA-C1A	8.71	110.62	106.71
28	c	507	CLA	C4A-NA-C1A	8.70	110.62	106.71
28	D	403	CLA	C4A-NA-C1A	8.68	110.61	106.71
28	C	507	CLA	C4A-NA-C1A	8.67	110.60	106.71
28	C	501	CLA	C4A-NA-C1A	8.66	110.60	106.71
28	b	613	CLA	C4A-NA-C1A	8.65	110.59	106.71
28	G	602	CLA	C4A-NA-C1A	8.63	110.59	106.71
28	A	405	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	C	503	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	G	612	CLA	C4A-NA-C1A	8.62	110.58	106.71
28	b	607	CLA	C4A-NA-C1A	8.61	110.58	106.71
28	Y	602	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	G	611	CLA	C4A-NA-C1A	8.60	110.57	106.71
28	c	501	CLA	C4A-NA-C1A	8.59	110.57	106.71
30	B	618	BCR	C20-C19-C18	8.57	150.50	126.42
28	B	616	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	B	609	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	b	611	CLA	C4A-NA-C1A	8.55	110.55	106.71
30	C	514	BCR	C20-C19-C18	8.55	150.44	126.42
28	N	602	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	a	410	CLA	C4A-NA-C1A	8.55	110.55	106.71
28	S	602	CLA	C4A-NA-C1A	8.54	110.55	106.71
28	b	604	CLA	C4A-NA-C1A	8.53	110.54	106.71
28	N	612	CLA	C4A-NA-C1A	8.49	110.53	106.71
29	A	409	PHO	C4D-CHA-CBD	-8.49	104.67	108.52
28	S	610	CLA	C4A-NA-C1A	8.48	110.52	106.71
28	D	402	CLA	C4A-NA-C1A	8.47	110.52	106.71
28	c	503	CLA	C4A-NA-C1A	8.47	110.51	106.71
28	B	604	CLA	C4A-NA-C1A	8.35	110.46	106.71
30	b	618	BCR	C20-C19-C18	8.35	149.88	126.42
28	a	406	CLA	C4A-NA-C1A	8.34	110.45	106.71
28	B	611	CLA	C4A-NA-C1A	8.33	110.45	106.71
30	c	515	BCR	C20-C19-C18	8.32	149.79	126.42
30	b	619	BCR	C20-C19-C18	8.32	149.78	126.42
28	S	614	CLA	C4A-NA-C1A	8.31	110.44	106.71
43	H	101	RRX	C38-C26-C25	-8.19	115.33	124.53
30	d	404	BCR	C20-C19-C18	8.05	149.02	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	508	CLA	C4A-NA-C1A	8.03	110.31	106.71
29	a	409	PHO	C4D-CHA-CBD	-8.02	104.89	108.52
39	C	527	LMK	O2-C4-O3	-7.94	106.06	124.09
30	c	514	BCR	C20-C19-C18	7.78	148.27	126.42
28	d	402	CLA	C4A-NA-C1A	7.77	110.20	106.71
29	a	408	PHO	C4D-CHA-CBD	-7.73	105.02	108.52
30	C	516	BCR	C20-C19-C18	7.66	147.93	126.42
30	B	619	BCR	C20-C19-C18	7.61	147.78	126.42
43	h	101	RRX	C38-C26-C25	-7.36	116.27	124.53
30	c	517	BCR	C20-C19-C18	7.34	147.04	126.42
48	Y	622	XAT	C36-C21-C22	7.22	121.53	108.98
30	a	411	BCR	C20-C19-C18	7.21	146.68	126.42
30	c	516	BCR	C20-C19-C18	7.20	146.63	126.42
30	A	411	BCR	C20-C19-C18	7.14	146.46	126.42
48	Y	622	XAT	C37-C21-C26	-7.09	90.91	110.05
30	D	404	BCR	C20-C19-C18	6.95	145.93	126.42
37	C	524	DGA	CDB-CCB-CBB	-6.83	79.75	114.42
37	b	625	DGA	CDB-CCB-CBB	-6.82	79.81	114.42
37	B	625	DGA	CDB-CCB-CBB	-6.61	80.85	114.42
29	A	408	PHO	C4D-CHA-CBD	-6.61	105.53	108.52
30	C	517	BCR	C20-C19-C18	6.60	144.94	126.42
43	H	101	RRX	C15-C14-C13	-6.54	117.97	127.31
28	S	603	CLA	O2D-CGD-CBD	6.52	122.86	111.27
28	S	602	CLA	O2D-CGD-CBD	6.50	122.82	111.27
37	c	524	DGA	CDB-CCB-CBB	-6.49	81.48	114.42
28	B	606	CLA	O2A-C1-C2	6.39	125.43	108.64
39	c	527	LMK	O2-C4-O3	-6.35	109.67	124.09
28	a	407	CLA	CMD-C2D-C1D	6.29	135.80	124.71
28	B	609	CLA	O2D-CGD-CBD	6.21	122.31	111.27
28	b	606	CLA	CMD-C2D-C1D	6.15	135.56	124.71
28	b	612	CLA	O2A-C1-C2	6.08	124.62	108.64
28	S	604	CLA	O2A-C1-C2	6.04	124.52	108.64
28	B	606	CLA	CMD-C2D-C1D	6.04	135.35	124.71
28	b	615	CLA	CMD-C2D-C1D	5.99	135.27	124.71
28	d	402	CLA	O2A-C1-C2	5.99	124.37	108.64
28	c	505	CLA	O2A-C1-C2	5.95	124.28	108.64
28	B	608	CLA	CMD-C2D-C1D	5.91	135.12	124.71
28	B	615	CLA	CMD-C2D-C1D	5.87	135.06	124.71
43	H	101	RRX	C11-C10-C9	-5.86	118.94	127.31
28	c	505	CLA	O2D-CGD-CBD	5.86	121.69	111.27
28	C	507	CLA	O2A-C1-C2	5.85	124.02	108.64
28	C	510	CLA	CMD-C2D-C1D	5.84	135.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	605	CLA	O2D-CGD-CBD	5.84	121.64	111.27
43	H	101	RRX	C24-C25-C26	-5.77	107.48	121.46
28	a	406	CLA	CMD-C2D-C1D	5.77	134.88	124.71
28	A	405	CLA	CMD-C2D-C1D	5.76	134.86	124.71
28	G	614	CLA	CMD-C2D-C1D	5.75	134.85	124.71
28	C	511	CLA	CMD-C2D-C1D	5.75	134.84	124.71
28	S	602	CLA	O2A-C1-C2	5.74	123.72	108.64
28	G	604	CLA	O2D-CGD-CBD	5.72	121.43	111.27
48	N	622	XAT	C31-C30-C29	-5.71	119.16	127.31
28	G	614	CLA	O2A-C1-C2	5.68	122.25	108.97
28	a	405	CLA	CMD-C2D-C1D	5.68	134.72	124.71
28	S	614	CLA	CMD-C2D-C1D	5.68	134.72	124.71
28	a	407	CLA	O2D-CGD-CBD	5.67	121.35	111.27
28	C	501	CLA	CMD-C2D-C1D	5.66	134.69	124.71
49	G	623	NEX	C2-C1-C6	5.66	114.71	109.21
28	N	604	CLA	O2D-CGD-CBD	5.65	121.31	111.27
28	C	509	CLA	CMD-C2D-C1D	5.65	134.67	124.71
47	G	621	LUT	C21-C26-C25	5.65	121.54	111.42
28	S	613	CLA	CMD-C2D-C1D	5.64	134.66	124.71
28	N	614	CLA	O2A-C1-C2	5.64	122.15	108.97
34	b	620	C7Z	C38-C25-C26	-5.64	118.20	124.53
28	c	509	CLA	CMD-C2D-C1D	5.63	134.64	124.71
28	N	610	CLA	CMD-C2D-C1D	5.63	134.63	124.71
28	B	614	CLA	CMD-C2D-C1D	5.63	134.63	124.71
28	c	510	CLA	CMD-C2D-C1D	5.61	134.59	124.71
28	Y	613	CLA	CMD-C2D-C1D	5.60	134.58	124.71
28	N	604	CLA	CMD-C2D-C1D	5.58	134.55	124.71
28	c	513	CLA	CMD-C2D-C1D	5.58	134.55	124.71
28	G	604	CLA	CMD-C2D-C1D	5.57	134.53	124.71
28	c	502	CLA	CMD-C2D-C1D	5.57	134.53	124.71
28	C	504	CLA	O2A-C1-C2	5.57	123.27	108.64
28	c	501	CLA	CMD-C2D-C1D	5.56	134.51	124.71
28	B	617	CLA	O2D-CGD-CBD	5.56	121.14	111.27
28	S	611	CLA	O2D-CGD-CBD	5.56	121.14	111.27
28	b	616	CLA	CMD-C2D-C1D	5.56	134.50	124.71
28	N	611	CLA	CMD-C2D-C1D	5.55	134.50	124.71
28	b	609	CLA	O2D-CGD-CBD	5.55	121.12	111.27
28	N	602	CLA	O2D-CGD-CBD	5.54	121.12	111.27
47	N	621	LUT	C21-C26-C25	5.54	121.34	111.42
28	B	603	CLA	O2A-C1-C2	5.54	123.19	108.64
47	Y	621	LUT	C21-C26-C25	5.53	121.33	111.42
28	C	503	CLA	CMD-C2D-C1D	5.53	134.46	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	603	CLA	CMD-C2D-C1D	5.52	134.44	124.71
28	D	403	CLA	CMD-C2D-C1D	5.52	134.44	124.71
28	B	605	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	B	607	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	G	613	CLA	O2A-C1-C2	5.51	123.11	108.64
28	d	403	CLA	CMD-C2D-C1D	5.51	134.42	124.71
28	Y	602	CLA	O2D-CGD-CBD	5.51	121.06	111.27
28	c	503	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	b	607	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	b	602	CLA	CMD-C2D-C1D	5.50	134.41	124.71
28	Y	604	CLA	CMD-C2D-C1D	5.50	134.40	124.71
28	S	605	CLA	CMD-C2D-C1D	5.49	134.38	124.71
28	C	501	CLA	O2D-CGD-CBD	5.48	121.01	111.27
28	b	614	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	N	602	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	b	603	CLA	CMD-C2D-C1D	5.48	134.37	124.71
28	b	610	CLA	O2A-C1-C2	5.48	123.03	108.64
28	C	502	CLA	O2A-C1-C2	5.48	123.03	108.64
34	b	620	C7Z	C15-C14-C13	-5.48	119.50	127.31
28	c	504	CLA	CMD-C2D-C1D	5.47	134.36	124.71
28	D	403	CLA	O2D-CGD-CBD	5.47	120.99	111.27
28	N	604	CLA	O2A-C1-C2	5.47	123.02	108.64
28	G	612	CLA	CMD-C2D-C1D	5.47	134.35	124.71
28	N	603	CLA	CMD-C2D-C1D	5.47	134.34	124.71
28	c	511	CLA	CMD-C2D-C1D	5.46	134.34	124.71
28	S	604	CLA	CMD-C2D-C1D	5.46	134.34	124.71
28	b	605	CLA	CMD-C2D-C1D	5.46	134.34	124.71
28	b	603	CLA	O2A-C1-C2	5.46	122.99	108.64
47	S	621	LUT	C21-C26-C25	5.46	121.20	111.42
28	b	608	CLA	O2A-C1-C2	5.45	122.97	108.64
28	B	607	CLA	O2D-CGD-CBD	5.45	120.96	111.27
28	C	507	CLA	CMD-C2D-C1D	5.45	134.32	124.71
28	Y	608	CLA	CMD-C2D-C1D	5.45	134.32	124.71
28	b	610	CLA	CMD-C2D-C1D	5.45	134.31	124.71
28	G	603	CLA	CMD-C2D-C1D	5.45	134.31	124.71
28	S	605	CLA	O2A-C1-C2	5.44	122.94	108.64
28	a	407	CLA	O2A-C1-C2	5.44	121.69	108.97
28	B	602	CLA	CMD-C2D-C1D	5.43	134.28	124.71
28	N	614	CLA	CMD-C2D-C1D	5.42	134.27	124.71
48	N	622	XAT	C15-C14-C13	-5.42	119.57	127.31
47	G	620	LUT	C21-C26-C25	5.42	121.12	111.42
28	S	610	CLA	CMD-C2D-C1D	5.41	134.26	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	604	CLA	O2D-CGD-CBD	5.41	120.89	111.27
28	B	609	CLA	CMD-C2D-C1D	5.41	134.25	124.71
28	C	513	CLA	O2A-C1-C2	5.41	122.85	108.64
28	b	604	CLA	CMD-C2D-C1D	5.41	134.24	124.71
28	Y	610	CLA	CMD-C2D-C1D	5.41	134.24	124.71
28	b	608	CLA	CMD-C2D-C1D	5.40	134.23	124.71
28	C	504	CLA	CMD-C2D-C1D	5.40	134.22	124.71
28	B	604	CLA	CMD-C2D-C1D	5.40	134.22	124.71
28	b	611	CLA	CMD-C2D-C1D	5.40	134.22	124.71
28	c	504	CLA	O2A-C1-C2	5.40	122.81	108.64
28	N	612	CLA	CMD-C2D-C1D	5.39	134.22	124.71
28	A	406	CLA	CMD-C2D-C1D	5.39	134.21	124.71
28	G	603	CLA	O2A-C1-C2	5.39	122.79	108.64
47	Y	620	LUT	C21-C26-C25	5.39	121.07	111.42
28	G	612	CLA	O2D-CGD-CBD	5.38	120.83	111.27
28	C	506	CLA	CMD-C2D-C1D	5.38	134.19	124.71
48	G	622	XAT	C15-C14-C13	-5.37	119.65	127.31
28	S	602	CLA	CMD-C2D-C1D	5.37	134.17	124.71
28	b	613	CLA	O2D-CGD-CBD	5.37	120.80	111.27
28	Y	603	CLA	CMD-C2D-C1D	5.37	134.17	124.71
28	N	613	CLA	O2A-C1-C2	5.36	122.73	108.64
40	d	401	BCT	O2-C-O1	5.36	133.45	119.55
28	G	610	CLA	CMD-C2D-C1D	5.36	134.15	124.71
28	C	509	CLA	O2D-CGD-CBD	5.35	120.78	111.27
28	b	617	CLA	O2D-CGD-CBD	5.35	120.78	111.27
28	A	410	CLA	O2D-CGD-CBD	5.34	120.76	111.27
28	G	610	CLA	O2A-C1-C2	5.34	122.66	108.64
28	B	613	CLA	O2D-CGD-CBD	5.33	120.75	111.27
28	B	612	CLA	O2D-CGD-CBD	5.33	120.74	111.27
28	d	403	CLA	O2D-CGD-CBD	5.33	120.74	111.27
28	Y	603	CLA	O2D-CGD-CBD	5.33	120.73	111.27
28	A	407	CLA	O2D-CGD-CBD	5.32	120.73	111.27
34	B	620	C7Z	C15-C14-C13	-5.32	119.72	127.31
28	c	511	CLA	O2A-C1-C2	5.32	122.62	108.64
28	B	613	CLA	CMD-C2D-C1D	5.32	134.09	124.71
28	G	611	CLA	O2D-CGD-CBD	5.32	120.72	111.27
28	c	507	CLA	CMD-C2D-C1D	5.32	134.08	124.71
40	D	401	BCT	O2-C-O1	5.31	133.32	119.55
28	B	611	CLA	CMD-C2D-C1D	5.31	134.07	124.71
28	c	507	CLA	O2A-C1-C2	5.31	122.58	108.64
28	Y	614	CLA	CMD-C2D-C1D	5.30	134.06	124.71
28	C	502	CLA	CMD-C2D-C1D	5.30	134.06	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	402	CLA	O2A-C1-C2	5.30	122.56	108.64
28	G	602	CLA	O2D-CGD-CBD	5.29	120.67	111.27
28	c	506	CLA	CMD-C2D-C1D	5.29	134.03	124.71
28	Y	611	CLA	CMD-C2D-C1D	5.27	134.01	124.71
28	A	410	CLA	CMD-C2D-C1D	5.27	134.00	124.71
28	b	606	CLA	O2A-C1-C2	5.27	122.48	108.64
28	N	613	CLA	CMD-C2D-C1D	5.27	134.00	124.71
48	Y	622	XAT	C31-C30-C29	-5.27	119.79	127.31
28	G	611	CLA	CMD-C2D-C1D	5.26	133.99	124.71
28	B	605	CLA	O2A-C1-C2	5.26	122.47	108.64
28	Y	610	CLA	O2A-C1-C2	5.26	122.45	108.64
34	B	620	C7Z	C11-C10-C9	-5.26	119.81	127.31
28	Y	602	CLA	CMD-C2D-C1D	5.26	133.98	124.71
35	B	623	DGD	O2G-C1B-C2B	5.26	122.83	111.50
28	C	505	CLA	O2A-C1-C2	5.25	122.44	108.64
28	C	513	CLA	O2D-CGD-CBD	5.25	120.59	111.27
28	B	607	CLA	O2A-C1-C2	5.25	122.42	108.64
28	G	614	CLA	O2D-CGD-CBD	5.24	120.57	111.27
28	A	407	CLA	CMD-C2D-C1D	5.24	133.94	124.71
28	c	508	CLA	CMD-C2D-C1D	5.24	133.94	124.71
28	B	611	CLA	O2D-CGD-CBD	5.23	120.56	111.27
41	d	405	PL9	C7-C3-C4	5.23	121.13	116.88
28	B	616	CLA	CMD-C2D-C1D	5.23	133.93	124.71
28	C	503	CLA	O2D-CGD-CBD	5.22	120.55	111.27
28	C	506	CLA	O2D-CGD-CBD	5.22	120.54	111.27
28	S	609	CLA	CMD-C2D-C1D	5.22	133.91	124.71
28	a	410	CLA	CMD-C2D-C1D	5.22	133.91	124.71
28	S	605	CLA	O2D-CGD-CBD	5.22	120.54	111.27
28	N	603	CLA	O2D-CGD-CBD	5.21	120.53	111.27
28	C	512	CLA	O2D-CGD-CBD	5.21	120.52	111.27
47	G	621	LUT	C21-C26-C27	5.20	119.28	112.70
28	G	602	CLA	O2A-C1-C2	5.20	122.31	108.64
28	S	609	CLA	O2D-CGD-CBD	5.20	120.51	111.27
28	B	617	CLA	O2A-C1-C2	5.20	122.30	108.64
28	Y	604	CLA	O2D-CGD-CBD	5.20	120.50	111.27
28	S	617	CLA	CMD-C2D-C1D	5.20	133.87	124.71
28	c	512	CLA	O2D-CGD-CBD	5.19	120.49	111.27
28	B	602	CLA	O2D-CGD-CBD	5.19	120.48	111.27
28	S	612	CLA	CMD-C2D-C1D	5.18	133.84	124.71
28	B	608	CLA	O2A-C1-C2	5.18	122.24	108.64
28	G	613	CLA	CMD-C2D-C1D	5.18	133.83	124.71
43	H	101	RRX	C24-C23-C22	5.17	134.05	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	617	CLA	O2A-C1-C2	5.17	122.22	108.64
47	N	620	LUT	C21-C26-C25	5.17	120.68	111.42
28	b	616	CLA	O2D-CGD-CBD	5.17	120.45	111.27
28	S	614	CLA	O2D-CGD-CBD	5.17	120.45	111.27
28	S	603	CLA	CMD-C2D-C1D	5.17	133.82	124.71
28	Y	612	CLA	O2D-CGD-CBD	5.16	120.44	111.27
28	B	604	CLA	O2A-C1-C2	5.15	122.17	108.64
28	d	403	CLA	O2A-C1-C2	5.15	122.16	108.64
28	Y	612	CLA	CMD-C2D-C1D	5.15	133.78	124.71
41	D	405	PL9	C7-C3-C4	5.14	121.06	116.88
28	A	407	CLA	O2A-C1-C2	5.14	122.15	108.64
28	B	616	CLA	O2D-CGD-CBD	5.14	120.40	111.27
28	N	611	CLA	O2A-C1-C2	5.13	120.97	108.97
28	N	614	CLA	O2D-CGD-CBD	5.13	120.39	111.27
28	c	512	CLA	O2A-C1-C2	5.13	122.12	108.64
28	b	607	CLA	O2D-CGD-CBD	5.13	120.39	111.27
28	B	612	CLA	O2A-C1-C2	5.13	122.11	108.64
28	a	410	CLA	O2D-CGD-CBD	5.13	120.38	111.27
28	c	502	CLA	O2A-C1-C2	5.13	122.11	108.64
28	d	402	CLA	O2D-CGD-CBD	5.13	120.38	111.27
28	B	604	CLA	O2D-CGD-CBD	5.12	120.37	111.27
28	C	511	CLA	O2D-CGD-CBD	5.12	120.37	111.27
28	c	505	CLA	CMD-C2D-C1D	5.12	133.73	124.71
30	c	516	BCR	C15-C14-C13	-5.11	120.02	127.31
47	S	620	LUT	C21-C26-C25	5.11	120.56	111.42
28	C	508	CLA	CMD-C2D-C1D	5.10	133.71	124.71
28	B	606	CLA	O2D-CGD-CBD	5.10	120.34	111.27
28	C	508	CLA	O2A-C1-C2	5.10	122.04	108.64
28	B	603	CLA	O2D-CGD-CBD	5.10	120.33	111.27
28	b	616	CLA	O2A-C1-C2	5.10	122.03	108.64
28	S	617	CLA	O2A-C1-C2	5.10	122.03	108.64
28	G	604	CLA	O2A-C1-C2	5.09	120.88	108.97
28	N	603	CLA	O2A-C1-C2	5.09	122.02	108.64
28	C	504	CLA	O2D-CGD-CBD	5.09	120.32	111.27
28	G	603	CLA	O2D-CGD-CBD	5.09	120.32	111.27
28	c	506	CLA	O2D-CGD-CBD	5.09	120.32	111.27
28	c	501	CLA	O2D-CGD-CBD	5.09	120.30	111.27
28	b	609	CLA	CMD-C2D-C1D	5.08	133.66	124.71
28	Y	611	CLA	O2D-CGD-CBD	5.08	120.29	111.27
28	C	510	CLA	O2A-C1-C2	5.08	121.98	108.64
28	c	510	CLA	O2D-CGD-CBD	5.07	120.29	111.27
28	S	612	CLA	O2D-CGD-CBD	5.07	120.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	502	CLA	O2D-CGD-CBD	5.06	120.27	111.27
43	H	101	RRX	C23-C22-C21	-5.06	111.18	118.94
28	Y	614	CLA	O2D-CGD-CBD	5.06	120.26	111.27
28	S	611	CLA	CMD-C2D-C1D	5.06	133.62	124.71
28	b	607	CLA	O2A-C1-C2	5.06	121.92	108.64
28	b	609	CLA	O2A-C1-C2	5.05	121.92	108.64
28	S	603	CLA	O2A-C1-C2	5.05	121.91	108.64
28	B	611	CLA	O2A-C1-C2	5.05	121.90	108.64
28	b	612	CLA	O2D-CGD-CBD	5.04	120.22	111.27
28	b	603	CLA	O2D-CGD-CBD	5.03	120.21	111.27
28	C	505	CLA	O2D-CGD-CBD	5.03	120.21	111.27
28	c	513	CLA	O2D-CGD-CBD	5.03	120.21	111.27
28	N	610	CLA	O2D-CGD-CBD	5.02	120.19	111.27
28	C	510	CLA	O2D-CGD-CBD	5.02	120.18	111.27
28	b	611	CLA	O2A-C1-C2	5.01	121.79	108.64
28	c	509	CLA	O2D-CGD-CBD	5.00	120.16	111.27
28	c	502	CLA	O2D-CGD-CBD	5.00	120.16	111.27
28	S	610	CLA	O2D-CGD-CBD	5.00	120.15	111.27
28	c	508	CLA	O2A-C1-C2	4.99	121.75	108.64
28	Y	604	CLA	O2A-C1-C2	4.99	121.75	108.64
28	b	606	CLA	O2D-CGD-CBD	4.99	120.13	111.27
28	c	503	CLA	O2D-CGD-CBD	4.99	120.13	111.27
28	C	512	CLA	O2A-C1-C2	4.98	121.73	108.64
28	d	402	CLA	CMD-C2D-C1D	4.98	133.49	124.71
28	b	602	CLA	O2A-C1-C2	4.98	121.72	108.64
28	S	611	CLA	O2A-C1-C2	4.98	121.71	108.64
28	c	503	CLA	O2A-C1-C2	4.96	121.68	108.64
28	c	512	CLA	CMD-C2D-C1D	4.96	133.46	124.71
34	b	620	C7Z	C35-C34-C33	-4.96	120.23	127.31
28	S	613	CLA	O2A-C1-C2	4.96	121.66	108.64
28	Y	611	CLA	O2A-C1-C2	4.96	121.66	108.64
28	Y	602	CLA	O2A-C1-C2	4.95	121.66	108.64
28	D	402	CLA	CMD-C2D-C1D	4.95	133.44	124.71
28	C	507	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	b	604	CLA	O2D-CGD-CBD	4.94	120.05	111.27
28	b	605	CLA	O2D-CGD-CBD	4.94	120.04	111.27
47	N	621	LUT	C21-C26-C27	4.93	118.94	112.70
28	A	410	CLA	O2A-C1-C2	4.93	121.58	108.64
28	D	402	CLA	O2D-CGD-CBD	4.92	120.02	111.27
28	b	615	CLA	O2A-C1-C2	4.92	121.56	108.64
34	b	620	C7Z	C31-C30-C29	-4.92	120.30	127.31
28	N	602	CLA	O2A-C1-C2	4.91	121.54	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	602	CLA	CMD-C2D-C1D	4.90	133.35	124.71
28	B	612	CLA	CMD-C2D-C1D	4.89	133.34	124.71
28	c	511	CLA	O2D-CGD-CBD	4.89	119.96	111.27
28	C	501	CLA	O2A-C1-C2	4.89	121.49	108.64
43	H	101	RRX	C37-C22-C23	4.89	125.78	118.08
28	G	611	CLA	O2A-C1-C2	4.89	121.48	108.64
28	S	614	CLA	O2A-C1-C2	4.88	121.47	108.64
28	c	510	CLA	O2A-C1-C2	4.88	121.47	108.64
28	B	616	CLA	O2A-C1-C2	4.88	121.47	108.64
49	Y	623	NEX	C2-C1-C6	4.88	113.95	109.21
28	N	611	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	c	504	CLA	O2D-CGD-CBD	4.88	119.94	111.27
28	B	614	CLA	O2A-C1-C2	4.87	121.43	108.64
28	b	605	CLA	O2A-C1-C2	4.86	121.41	108.64
28	N	612	CLA	O2D-CGD-CBD	4.85	119.89	111.27
28	C	505	CLA	CMD-C2D-C1D	4.85	133.26	124.71
28	D	403	CLA	O2A-C1-C2	4.84	121.36	108.64
28	C	503	CLA	O2A-C1-C2	4.84	121.36	108.64
28	G	610	CLA	O2D-CGD-CBD	4.84	119.87	111.27
28	c	507	CLA	O2D-CGD-CBD	4.84	119.87	111.27
48	G	622	XAT	C31-C30-C29	-4.84	120.41	127.31
28	S	617	CLA	O2D-CGD-CBD	4.83	119.86	111.27
28	Y	610	CLA	O2D-CGD-CBD	4.83	119.86	111.27
28	b	602	CLA	O2D-CGD-CBD	4.83	119.85	111.27
28	Y	603	CLA	O2A-C1-C2	4.83	121.33	108.64
28	b	613	CLA	CMD-C2D-C1D	4.83	133.22	124.71
35	b	623	DGD	O2G-C1B-C2B	4.83	121.90	111.50
51	Y	627	PTY	O7-C8-C11	4.82	119.97	111.09
43	h	101	RRX	C24-C23-C22	4.82	133.53	126.23
28	Y	613	CLA	O2A-C1-C2	4.82	121.30	108.64
49	Y	623	NEX	C38-C25-C24	4.82	119.70	114.28
28	b	611	CLA	O2D-CGD-CBD	4.81	119.82	111.27
47	Y	621	LUT	C21-C26-C27	4.81	118.78	112.70
28	Y	608	CLA	O2D-CGD-CBD	4.81	119.81	111.27
28	B	608	CLA	O2D-CGD-CBD	4.80	119.80	111.27
28	b	614	CLA	O2A-C1-C2	4.80	121.24	108.64
28	c	513	CLA	O2A-C1-C2	4.80	121.24	108.64
28	C	511	CLA	O2A-C1-C2	4.79	121.23	108.64
28	Y	612	CLA	O2A-C1-C2	4.79	121.22	108.64
28	c	501	CLA	O2A-C1-C2	4.78	121.21	108.64
28	B	609	CLA	O2A-C1-C2	4.78	121.21	108.64
28	S	609	CLA	O2A-C1-C2	4.78	121.19	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	N	610	CLA	O2A-C1-C2	4.77	121.18	108.64
28	B	613	CLA	O2A-C1-C2	4.77	121.18	108.64
28	B	615	CLA	O2D-CGD-CBD	4.76	119.73	111.27
28	b	615	CLA	O2D-CGD-CBD	4.75	119.71	111.27
28	A	406	CLA	O2A-C1-C2	4.75	121.12	108.64
28	b	608	CLA	O2D-CGD-CBD	4.75	119.70	111.27
28	S	610	CLA	O2A-C1-C2	4.74	121.10	108.64
28	G	613	CLA	O2D-CGD-CBD	4.74	119.68	111.27
28	b	612	CLA	CMD-C2D-C1D	4.73	133.04	124.71
28	b	604	CLA	O2A-C1-C2	4.71	121.02	108.64
48	Y	622	XAT	C15-C14-C13	-4.71	120.59	127.31
49	S	623	NEX	C38-C25-C24	4.70	119.57	114.28
43	H	101	RRX	C21-C20-C19	-4.70	108.55	123.22
28	Y	614	CLA	O2A-C1-C2	4.69	120.96	108.64
28	B	615	CLA	O2A-C1-C2	4.69	120.96	108.64
28	b	617	CLA	CMD-C2D-C1D	4.68	132.96	124.71
28	b	614	CLA	O2D-CGD-CBD	4.66	119.56	111.27
28	B	610	CLA	CMD-C2D-C1D	4.65	132.90	124.71
28	C	508	CLA	O2D-CGD-CBD	4.64	119.52	111.27
43	h	101	RRX	C37-C22-C23	4.64	125.39	118.08
28	B	610	CLA	O2A-C1-C2	4.64	120.82	108.64
28	B	602	CLA	O2A-C1-C2	4.64	120.82	108.64
28	B	614	CLA	O2D-CGD-CBD	4.63	119.50	111.27
28	Y	613	CLA	O2D-CGD-CBD	4.63	119.50	111.27
28	c	506	CLA	O2A-C1-C2	4.63	120.80	108.64
28	a	405	CLA	O2A-C1-C2	4.63	120.79	108.64
28	N	613	CLA	O2D-CGD-CBD	4.63	119.49	111.27
28	C	512	CLA	CMD-C2D-C1D	4.62	132.86	124.71
30	c	514	BCR	C15-C14-C13	-4.62	120.71	127.31
28	B	617	CLA	CMD-C2D-C1D	4.62	132.86	124.71
28	B	610	CLA	O2D-CGD-CBD	4.61	119.46	111.27
49	G	623	NEX	C38-C25-C24	4.61	119.46	114.28
34	B	620	C7Z	C7-C8-C9	-4.60	119.29	126.23
43	h	101	RRX	C24-C25-C26	-4.59	110.35	121.46
28	Y	608	CLA	O2A-C1-C2	4.58	120.68	108.64
28	b	613	CLA	O2A-C1-C2	4.58	120.67	108.64
29	a	408	PHO	C2B-C1B-NB	-4.57	106.37	109.53
38	S	624	LHG	O7-C7-C8	4.56	121.33	111.50
32	W	201	LMG	O7-C10-C11	4.56	121.33	111.50
30	C	516	BCR	C33-C5-C6	-4.55	119.42	124.53
28	S	613	CLA	O2D-CGD-CBD	4.55	119.35	111.27
34	B	620	C7Z	C35-C34-C33	-4.53	120.84	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	G	622	XAT	C18-C5-C4	4.51	119.35	114.28
32	B	622	LMG	O7-C10-C11	4.50	121.20	111.50
48	N	622	XAT	C18-C5-C4	4.49	119.33	114.28
48	Y	622	XAT	C18-C5-C4	4.49	119.33	114.28
28	A	405	CLA	O2D-CGD-CBD	4.48	119.24	111.27
28	a	410	CLA	O2A-C1-C2	4.46	120.37	108.64
28	c	508	CLA	O2D-CGD-CBD	4.46	119.20	111.27
32	b	622	LMG	O7-C10-C11	4.46	121.11	111.50
43	h	101	RRX	C33-C5-C6	-4.45	119.53	124.53
28	A	405	CLA	O2A-C1-C2	4.44	120.31	108.64
29	A	408	PHO	C2B-C1B-NB	-4.44	106.46	109.53
47	S	620	LUT	C35-C34-C33	-4.43	120.99	127.31
30	c	516	BCR	C33-C5-C6	-4.41	119.57	124.53
34	b	620	C7Z	C7-C8-C9	-4.39	119.59	126.23
28	b	610	CLA	O2D-CGD-CBD	4.38	119.06	111.27
47	G	621	LUT	C35-C34-C33	-4.38	121.06	127.31
47	Y	620	LUT	C21-C26-C27	4.36	118.22	112.70
34	B	620	C7Z	C18-C5-C6	-4.36	119.63	124.53
32	A	413	LMG	O7-C10-C11	4.36	120.90	111.50
28	C	506	CLA	O2A-C1-C2	4.36	120.09	108.64
49	S	623	NEX	C2-C1-C6	4.35	113.43	109.21
48	G	622	XAT	C38-C25-C24	4.32	119.14	114.28
28	a	406	CLA	O2D-CGD-CBD	4.32	118.95	111.27
28	a	405	CLA	O2D-CGD-CBD	4.31	118.93	111.27
34	b	620	C7Z	C11-C10-C9	-4.31	121.17	127.31
38	N	624	LHG	O7-C7-C8	4.30	120.78	111.50
47	N	620	LUT	C21-C26-C27	4.30	118.14	112.70
34	B	620	C7Z	C1-C6-C5	-4.29	116.56	122.61
36	t	101	3PH	O21-C21-C22	4.29	120.75	111.50
43	H	101	RRX	C7-C8-C9	-4.29	119.75	126.23
29	A	409	PHO	C2B-C1B-NB	-4.28	106.57	109.53
43	h	101	RRX	C23-C22-C21	-4.28	112.38	118.94
43	h	101	RRX	C7-C8-C9	4.26	132.68	126.23
47	S	620	LUT	C21-C26-C27	4.26	118.09	112.70
48	N	622	XAT	O24-C25-C24	4.24	116.57	113.38
48	N	622	XAT	C38-C25-C24	4.23	119.04	114.28
47	G	620	LUT	C15-C14-C13	-4.22	121.28	127.31
32	C	521	LMG	O7-C10-C11	4.22	120.60	111.50
47	N	621	LUT	C22-C23-C24	-4.22	106.94	111.74
38	d	410	LHG	O7-C7-C8	4.21	120.58	111.50
43	h	101	RRX	C21-C20-C19	-4.21	110.07	123.22
47	G	620	LUT	C21-C26-C27	4.19	118.00	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	N	621	LUT	C35-C34-C33	-4.18	121.34	127.31
34	B	620	C7Z	C38-C25-C26	-4.18	119.83	124.53
34	b	620	C7Z	C1-C6-C5	-4.18	116.73	122.61
48	Y	622	XAT	C38-C25-C24	4.17	118.97	114.28
49	N	623	NEX	C38-C25-C24	4.16	118.97	114.28
28	A	406	CLA	O2D-CGD-CBD	4.16	118.66	111.27
47	S	621	LUT	C21-C26-C27	4.15	117.95	112.70
47	N	621	LUT	C7-C8-C9	-4.15	119.96	126.23
32	H	102	LMG	O7-C10-C11	4.13	120.41	111.50
43	h	101	RRX	C34-C9-C8	4.13	124.58	118.08
32	h	102	LMG	O7-C10-C11	4.11	120.37	111.50
47	Y	621	LUT	C22-C23-C24	-4.11	107.06	111.74
43	h	101	RRX	C15-C14-C13	-4.08	121.49	127.31
38	C	525	LHG	O7-C7-C8	4.07	120.28	111.50
48	Y	622	XAT	C7-C8-C9	-4.07	119.22	125.53
38	D	410	LHG	O7-C7-C8	4.06	120.26	111.50
38	c	525	LHG	O7-C7-C8	4.05	120.24	111.50
32	C	523	LMG	O7-C10-C11	4.05	120.23	111.50
30	B	618	BCR	C15-C14-C13	-4.05	121.53	127.31
32	c	523	LMG	O7-C10-C11	4.04	120.20	111.50
30	b	618	BCR	C27-C26-C25	-4.04	116.87	122.73
47	N	620	LUT	C15-C14-C13	-4.02	121.57	127.31
37	b	625	DGA	OG2-CB1-CB2	4.02	120.16	111.50
34	b	620	C7Z	C27-C28-C29	-4.02	120.17	126.23
38	G	624	LHG	O7-C7-C8	4.01	120.14	111.50
46	Y	609	CHL	CHD-C1D-ND	-4.00	120.78	124.45
36	B	624	3PH	O21-C21-C22	3.99	120.10	111.50
46	G	609	CHL	CHD-C1D-ND	-3.99	120.79	124.45
38	Y	624	LHG	O7-C7-C8	3.99	120.09	111.50
32	a	413	LMG	O7-C10-C11	3.99	120.09	111.50
48	Y	622	XAT	C36-C21-C26	3.98	120.79	110.05
38	D	409	LHG	O7-C7-C8	3.97	120.05	111.50
30	A	411	BCR	C33-C5-C6	-3.96	120.08	124.53
47	G	620	LUT	C22-C23-C24	-3.96	107.23	111.74
47	Y	621	LUT	C35-C34-C33	-3.95	121.67	127.31
47	G	621	LUT	C22-C23-C24	-3.94	107.26	111.74
37	B	625	DGA	OG2-CB1-CB2	3.94	119.98	111.50
36	b	624	3PH	O21-C21-C22	3.93	119.98	111.50
28	C	509	CLA	O2A-C1-C2	3.91	118.91	108.64
37	c	524	DGA	OG2-CB1-CB2	3.91	119.93	111.50
51	Y	626	PTY	O7-C8-C11	3.91	119.92	111.50
28	c	507	CLA	C2C-C1C-NC	3.91	113.63	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S	621	LUT	C22-C23-C24	-3.91	107.30	111.74
37	J	101	DGA	OG2-CB1-CB2	3.90	119.90	111.50
37	C	524	DGA	OG2-CB1-CB2	3.88	119.87	111.50
28	b	612	CLA	C1-C2-C3	-3.88	119.34	126.04
30	b	618	BCR	C15-C14-C13	-3.87	121.79	127.31
35	C	519	DGD	O2G-C1B-C2B	3.86	119.83	111.50
38	d	409	LHG	O7-C7-C8	3.86	119.81	111.50
47	G	621	LUT	C7-C8-C9	-3.85	120.42	126.23
47	S	621	LUT	C35-C34-C33	-3.85	121.82	127.31
46	G	601	CHL	CHD-C1D-ND	-3.85	120.92	124.45
46	Y	601	CHL	CHD-C1D-ND	-3.84	120.92	124.45
49	G	623	NEX	C17-C1-C6	-3.83	107.05	110.47
28	b	611	CLA	C2D-C1D-ND	3.82	112.92	110.10
32	w	201	LMG	O7-C10-C11	3.80	119.70	111.50
28	A	406	CLA	C2C-C1C-NC	3.79	113.52	109.97
32	D	411	LMG	O7-C10-C11	3.78	119.66	111.50
47	Y	620	LUT	C22-C23-C24	-3.78	107.44	111.74
48	G	622	XAT	O24-C25-C24	3.78	116.22	113.38
36	T	101	3PH	O21-C21-C22	3.78	119.64	111.50
38	D	408	LHG	O7-C7-C8	3.78	119.64	111.50
45	i	101	4RF	O21-C22-C24	3.77	119.62	111.50
45	I	102	4RF	O21-C22-C24	3.77	119.62	111.50
47	S	620	LUT	C7-C8-C9	-3.76	120.55	126.23
45	k	101	4RF	O21-C22-C24	3.76	119.60	111.50
28	B	605	CLA	C2C-C1C-NC	3.75	113.49	109.97
47	N	621	LUT	C15-C14-C13	-3.75	121.96	127.31
47	Y	621	LUT	C7-C8-C9	-3.75	120.57	126.23
43	H	101	RRX	C33-C5-C6	-3.74	120.33	124.53
28	B	606	CLA	CHD-C1D-ND	-3.74	121.02	124.45
37	j	101	DGA	OG2-CB1-CB2	3.73	119.53	111.50
29	a	409	PHO	C2B-C1B-NB	-3.73	106.95	109.53
28	c	509	CLA	O2A-C1-C2	3.72	118.42	108.64
30	B	618	BCR	C1-C6-C5	-3.70	117.40	122.61
47	G	620	LUT	C35-C34-C33	-3.70	122.03	127.31
28	B	605	CLA	C1-C2-C3	-3.69	119.65	126.04
28	N	613	CLA	CMA-C3A-C4A	3.69	121.69	111.77
47	N	620	LUT	C35-C34-C33	-3.69	122.04	127.31
46	G	605	CHL	C2C-C3C-C4C	3.68	109.11	106.49
46	N	601	CHL	CHD-C1D-ND	-3.67	121.08	124.45
35	c	518	DGD	O2G-C1B-C2B	3.67	119.42	111.50
30	b	618	BCR	C33-C5-C6	-3.67	120.40	124.53
28	c	502	CLA	C2C-C1C-NC	3.67	113.41	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	c	527	LMK	O3-C4-C3	-3.67	110.40	122.98
28	b	605	CLA	CMA-C3A-C4A	3.67	121.63	111.77
49	S	623	NEX	C27-C28-C29	-3.67	119.84	125.53
49	S	623	NEX	C16-C1-C6	-3.66	107.19	110.47
35	C	518	DGD	O2G-C1B-C2B	3.66	119.39	111.50
30	c	515	BCR	C33-C5-C6	-3.66	120.42	124.53
28	b	609	CLA	C1-C2-C3	-3.66	119.71	126.04
28	G	603	CLA	C1-C2-C3	-3.66	119.72	126.04
28	c	504	CLA	C2C-C1C-NC	3.66	113.40	109.97
28	a	405	CLA	C2D-C1D-ND	3.66	112.80	110.10
49	G	623	NEX	C27-C28-C29	-3.65	119.86	125.53
31	m	101	SQD	O7-S-C6	-3.65	102.61	106.94
46	N	608	CHL	CHD-C1D-ND	-3.65	121.10	124.45
35	C	520	DGD	O2G-C1B-C2B	3.64	119.34	111.50
41	d	405	PL9	C7-C3-C2	-3.64	118.52	123.30
47	G	621	LUT	C15-C14-C13	-3.64	122.12	127.31
32	d	411	LMG	O7-C10-C11	3.63	119.33	111.50
43	H	101	RRX	C15-C16-C17	-3.63	116.04	123.47
43	H	101	RRX	C1-C6-C5	-3.63	117.50	122.61
31	a	412	SQD	O7-S-C6	-3.63	102.63	106.94
29	a	409	PHO	CMB-C2B-C3B	3.62	131.45	124.68
28	S	617	CLA	C1-C2-C3	-3.61	120.90	126.75
28	G	613	CLA	C1-C2-C3	-3.60	119.81	126.04
28	C	508	CLA	C1-C2-C3	-3.60	119.82	126.04
47	S	621	LUT	C7-C8-C9	-3.60	120.80	126.23
28	c	505	CLA	C1-C2-C3	-3.59	119.83	126.04
28	G	611	CLA	C2C-C1C-NC	3.59	113.34	109.97
28	C	513	CLA	C2D-C1D-ND	3.59	112.75	110.10
45	K	101	4RF	O21-C22-C24	3.59	119.24	111.50
30	a	411	BCR	C33-C5-C6	-3.59	120.50	124.53
31	B	626	SQD	O7-S-C6	-3.59	102.68	106.94
30	B	618	BCR	C33-C5-C4	3.59	120.50	113.62
30	c	517	BCR	C33-C5-C4	3.59	120.50	113.62
47	N	620	LUT	C22-C23-C24	-3.58	107.66	111.74
32	c	521	LMG	O7-C10-C11	3.58	119.22	111.50
28	b	606	CLA	CHD-C1D-ND	-3.58	121.16	124.45
28	c	509	CLA	C2C-C1C-NC	3.58	113.32	109.97
46	S	606	CHL	CHD-C1D-ND	-3.58	121.17	124.45
31	C	526	SQD	O7-S-C6	-3.57	102.69	106.94
28	b	605	CLA	C2C-C1C-NC	3.57	113.32	109.97
28	S	605	CLA	C2C-C1C-NC	3.57	113.32	109.97
31	M	101	SQD	O7-S-C6	-3.57	102.70	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	621	SQD	O7-S-C6	-3.56	102.70	106.94
46	Y	606	CHL	CHD-C1D-ND	-3.56	121.18	124.45
47	Y	621	LUT	C11-C10-C9	-3.55	122.25	127.31
28	Y	608	CLA	C1-C2-C3	-3.55	121.01	126.75
47	N	621	LUT	C18-C5-C6	-3.55	120.55	124.53
28	C	509	CLA	C2C-C1C-NC	3.54	113.29	109.97
28	B	611	CLA	C2C-C1C-NC	3.54	113.29	109.97
47	S	621	LUT	C18-C5-C6	-3.54	120.55	124.53
28	G	603	CLA	C2C-C1C-NC	3.54	113.29	109.97
31	b	626	SQD	O7-S-C6	-3.54	102.73	106.94
30	B	618	BCR	C33-C5-C6	-3.54	120.56	124.53
28	a	406	CLA	O2A-C1-C2	3.54	117.93	108.64
47	Y	620	LUT	C35-C34-C33	-3.54	122.26	127.31
46	S	607	CHL	CHD-C1D-ND	-3.54	121.20	124.45
47	Y	621	LUT	C15-C14-C13	-3.53	122.27	127.31
35	c	520	DGD	O2G-C1B-C2B	3.53	119.12	111.50
28	c	503	CLA	C1-C2-C3	-3.53	119.93	126.04
47	Y	620	LUT	C15-C14-C13	-3.53	122.28	127.31
31	A	412	SQD	O7-S-C6	-3.52	102.75	106.94
47	Y	620	LUT	C7-C8-C9	-3.52	120.91	126.23
47	N	621	LUT	C11-C10-C9	-3.51	122.30	127.31
48	G	622	XAT	C7-C8-C9	-3.50	120.09	125.53
28	G	610	CLA	C1-C2-C3	-3.50	119.98	126.04
38	d	408	LHG	O7-C7-C8	3.50	119.05	111.50
28	b	603	CLA	C1-C2-C3	-3.50	119.99	126.04
28	G	614	CLA	CHD-C1D-ND	-3.49	121.25	124.45
31	B	621	SQD	O7-S-C6	-3.49	102.79	106.94
31	c	526	SQD	O7-S-C6	-3.49	102.79	106.94
28	S	605	CLA	C1-C2-C3	-3.48	121.11	126.75
49	N	623	NEX	C5-C4-C3	3.48	115.87	111.75
28	d	403	CLA	C1-C2-C3	-3.48	120.02	126.04
28	S	611	CLA	C2C-C1C-NC	3.48	113.23	109.97
28	D	402	CLA	C1-C2-C3	-3.48	120.03	126.04
41	D	405	PL9	C7-C3-C2	-3.48	118.73	123.30
28	C	510	CLA	C1C-C2C-C3C	-3.47	103.30	106.96
49	N	623	NEX	C27-C28-C29	-3.47	120.15	125.53
28	S	613	CLA	C1-C2-C3	-3.46	120.05	126.04
28	S	603	CLA	C2C-C1C-NC	3.46	113.21	109.97
28	N	604	CLA	C1-C2-C3	-3.45	120.07	126.04
28	b	611	CLA	C2C-C1C-NC	3.45	113.21	109.97
28	b	615	CLA	CHD-C1D-ND	-3.45	121.28	124.45
30	b	618	BCR	C33-C5-C4	3.45	120.24	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	N	605	CHL	CHD-C1D-ND	-3.45	121.28	124.45
46	G	605	CHL	CHD-C1D-ND	-3.45	121.29	124.45
43	H	101	RRX	C4-C5-C6	-3.44	117.74	122.73
28	A	406	CLA	C1-C2-C3	-3.43	120.10	126.04
43	h	101	RRX	C1-C6-C5	-3.43	117.78	122.61
30	c	517	BCR	C37-C22-C21	-3.43	118.12	122.92
28	C	506	CLA	C2C-C1C-NC	3.43	113.18	109.97
34	b	620	C7Z	C18-C5-C4	3.42	120.69	114.36
46	S	601	CHL	CHD-C1D-ND	-3.42	121.31	124.45
47	G	621	LUT	C11-C10-C9	-3.41	122.44	127.31
28	C	501	CLA	CHD-C1D-ND	-3.41	121.32	124.45
28	b	614	CLA	C2C-C1C-NC	3.41	113.17	109.97
46	G	606	CHL	CHD-C1D-ND	-3.41	121.32	124.45
28	a	405	CLA	CHD-C1D-ND	-3.41	121.32	124.45
28	c	512	CLA	C2C-C1C-NC	3.40	113.16	109.97
49	Y	623	NEX	C31-C30-C29	3.40	132.17	127.31
28	S	614	CLA	CHD-C1D-ND	-3.40	121.33	124.45
46	Y	605	CHL	CHD-C1D-ND	-3.40	121.33	124.45
28	C	507	CLA	C2C-C1C-NC	3.40	113.16	109.97
28	c	508	CLA	CHD-C1D-ND	-3.39	121.34	124.45
28	a	406	CLA	C2C-C1C-NC	3.39	113.15	109.97
28	c	511	CLA	C1-C2-C3	-3.39	120.19	126.04
28	c	504	CLA	C1-C2-C3	-3.38	120.19	126.04
28	A	405	CLA	C1-C2-C3	-3.38	120.19	126.04
35	c	519	DGD	O2G-C1B-C2B	3.38	118.78	111.50
46	G	609	CHL	C4B-CHC-C1C	3.38	134.34	126.34
28	C	510	CLA	C1-C2-C3	-3.37	120.21	126.04
46	G	601	CHL	C2C-C3C-C4C	3.37	108.89	106.49
28	c	513	CLA	CHD-C1D-ND	-3.37	121.36	124.45
28	S	604	CLA	C2C-C1C-NC	3.37	113.12	109.97
34	B	620	C7Z	C31-C30-C29	-3.36	122.52	127.31
34	b	620	C7Z	C18-C5-C6	-3.35	120.76	124.53
46	G	605	CHL	C3C-C4C-NC	-3.35	106.81	110.57
28	C	511	CLA	CHD-C1D-ND	-3.35	121.38	124.45
28	N	602	CLA	CHD-C1D-ND	-3.35	121.38	124.45
28	Y	612	CLA	C2C-C1C-NC	3.34	113.11	109.97
28	c	506	CLA	C2C-C1C-NC	3.34	113.10	109.97
49	Y	623	NEX	C27-C28-C29	-3.34	120.34	125.53
28	d	403	CLA	CHD-C1D-ND	-3.34	121.39	124.45
47	S	620	LUT	C35-C15-C14	-3.34	116.64	123.47
28	b	603	CLA	CHD-C1D-ND	-3.34	121.39	124.45
28	c	510	CLA	C1C-C2C-C3C	-3.33	103.45	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	620	C7Z	C27-C28-C29	-3.33	121.20	126.23
46	S	608	CHL	CHD-C1D-ND	-3.33	121.39	124.45
28	c	510	CLA	CHD-C1D-ND	-3.33	121.39	124.45
28	B	606	CLA	C1-C2-C3	-3.33	120.28	126.04
46	G	607	CHL	CHD-C1D-ND	-3.33	121.39	124.45
30	c	515	BCR	C15-C14-C13	-3.33	122.56	127.31
28	c	510	CLA	C2D-C1D-ND	3.33	112.56	110.10
28	D	403	CLA	C2C-C1C-NC	3.33	113.09	109.97
48	G	622	XAT	C38-C25-C26	-3.32	116.69	122.26
28	C	510	CLA	CHD-C1D-ND	-3.32	121.40	124.45
28	C	501	CLA	CMA-C3A-C4A	3.32	120.70	111.77
46	N	607	CHL	CHD-C1D-ND	-3.32	121.40	124.45
47	S	620	LUT	C15-C14-C13	-3.32	122.57	127.31
28	A	407	CLA	C1-C2-C3	-3.32	121.39	126.75
28	A	407	CLA	C2C-C1C-NC	3.31	113.08	109.97
46	N	606	CHL	C3B-C4B-NB	-3.31	107.45	110.52
28	B	606	CLA	C2C-C1C-NC	3.31	113.07	109.97
46	N	609	CHL	CHD-C1D-ND	-3.30	121.42	124.45
28	c	503	CLA	CHD-C1D-ND	-3.30	121.42	124.45
28	B	615	CLA	C1-C2-C3	-3.30	120.33	126.04
46	G	601	CHL	C3C-C4C-NC	-3.30	106.87	110.57
46	N	601	CHL	C2C-C3C-C4C	3.30	108.84	106.49
47	G	620	LUT	C7-C8-C9	-3.30	121.25	126.23
30	c	517	BCR	C4-C5-C6	-3.30	117.94	122.73
28	c	508	CLA	C1-C2-C3	-3.29	120.34	126.04
28	G	610	CLA	CHD-C1D-ND	-3.29	121.43	124.45
28	S	602	CLA	C1-C2-C3	-3.29	120.35	126.04
28	C	501	CLA	C1-C2-C3	-3.29	120.36	126.04
28	N	612	CLA	C2C-C1C-NC	3.28	113.05	109.97
28	N	614	CLA	CHD-C1D-ND	-3.28	121.44	124.45
28	Y	610	CLA	C1-C2-C3	-3.28	120.37	126.04
28	b	602	CLA	C2C-C1C-NC	3.28	113.04	109.97
48	N	622	XAT	C6-C7-C8	-3.27	119.07	125.99
28	G	603	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
30	B	619	BCR	C33-C5-C6	-3.27	120.86	124.53
28	c	507	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
28	S	613	CLA	CMA-C3A-C4A	3.27	120.56	111.77
28	N	602	CLA	C1-C2-C3	-3.27	120.39	126.04
46	S	606	CHL	C2C-C3C-C4C	3.27	108.82	106.49
28	G	612	CLA	C2C-C1C-NC	3.27	113.03	109.97
28	Y	610	CLA	CHD-C1D-ND	-3.26	121.45	124.45
30	B	619	BCR	C33-C5-C4	3.26	119.89	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	602	CLA	C2C-C1C-NC	3.26	113.03	109.97
28	B	607	CLA	CHD-C1D-ND	-3.26	121.46	124.45
28	Y	613	CLA	CHD-C1D-ND	-3.26	121.46	124.45
28	B	609	CLA	C1-C2-C3	-3.26	120.41	126.04
28	A	410	CLA	CHD-C1D-ND	-3.26	121.46	124.45
28	B	614	CLA	C2C-C1C-NC	3.26	113.02	109.97
28	c	511	CLA	CMA-C3A-C4A	3.25	120.52	111.77
28	S	617	CLA	C2C-C1C-NC	3.25	113.02	109.97
28	c	501	CLA	C1-C2-C3	-3.25	120.42	126.04
46	G	608	CHL	CHD-C1D-ND	-3.25	121.47	124.45
28	B	603	CLA	CHD-C1D-ND	-3.25	121.47	124.45
28	B	602	CLA	C2C-C1C-NC	3.25	113.02	109.97
28	C	502	CLA	C2C-C1C-NC	3.25	113.02	109.97
46	Y	606	CHL	C2C-C3C-C4C	3.25	108.81	106.49
28	b	616	CLA	C1-C2-C3	-3.25	120.42	126.04
46	S	607	CHL	C2C-C3C-C4C	3.25	108.80	106.49
49	G	623	NEX	C20-C13-C14	-3.25	118.38	122.92
40	d	401	BCT	O3-C-O1	-3.24	111.14	119.55
28	S	604	CLA	CHD-C1D-ND	-3.24	121.48	124.45
43	H	101	RRX	C33-C5-C4	3.24	119.84	113.62
28	D	403	CLA	CHD-C1D-ND	-3.24	121.48	124.45
30	c	514	BCR	C33-C5-C6	-3.24	120.89	124.53
47	S	620	LUT	C18-C5-C6	-3.24	120.89	124.53
46	N	605	CHL	C2C-C3C-C4C	3.23	108.80	106.49
28	B	614	CLA	CHD-C1D-ND	-3.23	121.48	124.45
28	a	407	CLA	C2D-C1D-ND	3.23	112.48	110.10
28	B	608	CLA	C2C-C1C-NC	3.22	112.99	109.97
30	a	411	BCR	C33-C5-C4	3.22	119.80	113.62
28	C	502	CLA	C1-C2-C3	-3.22	120.48	126.04
28	N	611	CLA	C2C-C1C-NC	3.22	112.98	109.97
28	N	603	CLA	C1-C2-C3	-3.21	120.49	126.04
46	Y	609	CHL	CMA-C3A-C4A	3.21	120.40	111.77
28	C	510	CLA	C2C-C1C-NC	3.20	112.97	109.97
30	C	514	BCR	C33-C5-C6	-3.20	120.93	124.53
49	G	623	NEX	C39-C29-C30	-3.20	118.44	122.92
28	C	503	CLA	CMA-C3A-C4A	3.20	120.38	111.77
28	S	611	CLA	C1-C2-C3	-3.20	120.51	126.04
28	B	617	CLA	C2C-C1C-NC	3.20	112.97	109.97
28	B	609	CLA	C2C-C1C-NC	3.20	112.97	109.97
28	N	610	CLA	CHD-C1D-ND	-3.19	121.52	124.45
28	c	501	CLA	CHD-C1D-ND	-3.19	121.52	124.45
46	N	607	CHL	CHB-C4A-NA	3.19	128.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	508	CLA	CHD-C1D-ND	-3.19	121.52	124.45
28	b	607	CLA	CHD-C1D-ND	-3.19	121.52	124.45
46	Y	609	CHL	C3C-C4C-NC	-3.19	107.00	110.57
28	Y	614	CLA	C2C-C1C-NC	3.19	112.96	109.97
30	b	619	BCR	C15-C14-C13	-3.19	122.76	127.31
28	B	603	CLA	C2C-C1C-NC	3.19	112.96	109.97
28	N	614	CLA	C2C-C1C-NC	3.19	112.96	109.97
30	b	619	BCR	C33-C5-C4	3.19	119.74	113.62
28	Y	603	CLA	CHD-C1D-ND	-3.18	121.53	124.45
46	G	609	CHL	CMA-C3A-C4A	3.18	120.33	111.77
28	D	402	CLA	C2D-C1D-ND	3.18	112.45	110.10
28	Y	608	CLA	C2C-C1C-NC	3.18	112.95	109.97
28	C	512	CLA	C2C-C1C-NC	3.18	112.95	109.97
28	B	604	CLA	C2C-C1C-NC	3.17	112.94	109.97
30	C	517	BCR	C36-C18-C17	-3.17	118.48	122.92
46	Y	606	CHL	C3B-C4B-NB	-3.17	107.57	110.52
28	S	610	CLA	CHD-C1D-ND	-3.17	121.54	124.45
28	S	603	CLA	CMA-C3A-C4A	3.17	120.29	111.77
28	b	610	CLA	CHD-C1D-ND	-3.17	121.54	124.45
28	B	615	CLA	CHD-C1D-ND	-3.16	121.55	124.45
28	B	605	CLA	CMA-C3A-C4A	3.16	120.27	111.77
28	N	603	CLA	C2C-C1C-NC	3.16	112.93	109.97
28	C	512	CLA	C2D-C1D-ND	3.16	112.43	110.10
46	N	606	CHL	C2C-C3C-C4C	3.16	108.74	106.49
28	b	604	CLA	C2C-C1C-NC	3.16	112.93	109.97
46	N	601	CHL	C3C-C4C-NC	-3.16	107.03	110.57
30	c	515	BCR	C33-C5-C4	3.15	119.68	113.62
28	B	611	CLA	C1-C2-C3	-3.15	120.59	126.04
48	N	622	XAT	C38-C25-C26	-3.15	116.98	122.26
30	B	619	BCR	C23-C24-C25	-3.15	118.35	127.20
28	B	613	CLA	C2C-C1C-NC	3.15	112.92	109.97
28	B	609	CLA	CHD-C1D-ND	-3.15	121.56	124.45
28	b	616	CLA	C2C-C1C-NC	3.15	112.92	109.97
46	N	607	CHL	C2C-C3C-C4C	3.15	108.73	106.49
28	A	405	CLA	CHD-C1D-ND	-3.15	121.56	124.45
28	c	503	CLA	C2D-C1D-ND	3.15	112.42	110.10
28	b	611	CLA	C1-C2-C3	-3.14	120.60	126.04
46	N	607	CHL	C3C-C4C-NC	-3.14	107.05	110.57
28	A	410	CLA	C2C-C1C-NC	3.14	112.91	109.97
28	C	505	CLA	C2C-C1C-NC	3.14	112.91	109.97
46	G	608	CHL	CMA-C3A-C4A	3.14	120.21	111.77
30	a	411	BCR	C38-C26-C25	-3.14	121.00	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	N	604	CLA	C2C-C1C-NC	3.14	112.91	109.97
28	b	606	CLA	C2C-C1C-NC	3.14	112.91	109.97
29	A	409	PHO	CMB-C2B-C3B	3.14	130.54	124.68
34	B	620	C7Z	C2-C3-C4	3.14	114.60	110.30
28	D	402	CLA	C3B-C4B-NB	-3.13	107.61	110.52
28	c	513	CLA	C1-C2-C3	-3.13	120.63	126.04
28	b	608	CLA	C2C-C1C-NC	3.13	112.90	109.97
28	S	613	CLA	C2C-C1C-NC	3.13	112.90	109.97
28	B	615	CLA	C2C-C1C-NC	3.13	112.90	109.97
46	S	606	CHL	C3C-C4C-NC	-3.12	107.07	110.57
28	c	503	CLA	CMA-C3A-C4A	3.12	120.16	111.77
28	C	506	CLA	CHD-C1D-ND	-3.12	121.59	124.45
46	S	606	CHL	C3B-C4B-NB	-3.12	107.62	110.52
28	Y	603	CLA	C2C-C1C-NC	3.12	112.89	109.97
46	S	608	CHL	CMA-C3A-C4A	3.11	120.14	111.77
46	S	601	CHL	C3C-C4C-NC	-3.11	107.09	110.57
28	S	603	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
29	a	409	PHO	CBC-CAC-C3C	3.11	117.43	112.88
46	Y	607	CHL	CHD-C1D-ND	-3.10	121.60	124.45
49	Y	623	NEX	C39-C29-C30	-3.10	118.58	122.92
46	N	605	CHL	C3C-C4C-NC	-3.10	107.09	110.57
28	G	602	CLA	C4B-CHC-C1C	3.10	133.69	126.34
46	N	609	CHL	CMA-C3A-C4A	3.10	120.10	111.77
46	S	601	CHL	C2C-C3C-C4C	3.10	108.70	106.49
28	b	603	CLA	C2C-C1C-NC	3.10	112.87	109.97
47	N	620	LUT	C11-C10-C9	-3.10	122.89	127.31
28	c	505	CLA	C2C-C1C-NC	3.09	112.87	109.97
46	S	607	CHL	CMA-C3A-C4A	3.09	120.07	111.77
28	N	613	CLA	C2C-C1C-NC	3.09	112.86	109.97
28	D	403	CLA	C1-C2-C3	-3.09	120.70	126.04
28	C	504	CLA	C1-C2-C3	-3.09	120.70	126.04
47	S	621	LUT	C38-C25-C24	-3.09	116.96	123.56
46	S	607	CHL	C3C-C4C-NC	-3.09	107.11	110.57
28	G	613	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	c	502	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	c	501	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	b	614	CLA	C1-C2-C3	-3.08	120.71	126.04
28	c	511	CLA	C2C-C1C-NC	3.08	112.86	109.97
28	b	611	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
28	a	407	CLA	CMA-C3A-C4A	3.08	120.06	111.77
28	C	513	CLA	CMD-C2D-C1D	3.08	130.14	124.71
28	S	612	CLA	C2D-C1D-ND	3.08	112.37	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	602	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	S	613	CLA	CHD-C1D-ND	-3.08	121.62	124.45
28	C	504	CLA	C2D-C1D-ND	3.08	112.37	110.10
28	Y	604	CLA	CHD-C1D-ND	-3.08	121.63	124.45
46	Y	606	CHL	C3C-C4C-NC	-3.08	107.12	110.57
28	Y	611	CLA	C2C-C1C-NC	3.08	112.85	109.97
28	c	508	CLA	C2D-C1D-ND	3.07	112.37	110.10
46	G	605	CHL	CMA-C3A-C4A	3.07	120.04	111.77
46	Y	609	CHL	C2C-C3C-C4C	3.07	108.68	106.49
28	b	602	CLA	CHD-C1D-ND	-3.07	121.63	124.45
28	a	405	CLA	C1-C2-C3	-3.07	120.73	126.04
28	a	410	CLA	C2C-C1C-NC	3.07	112.85	109.97
28	G	603	CLA	CHD-C1D-ND	-3.07	121.63	124.45
28	G	604	CLA	C2C-C1C-NC	3.07	112.84	109.97
28	c	502	CLA	CHD-C1D-ND	-3.07	121.64	124.45
28	Y	608	CLA	CHD-C1D-ND	-3.06	121.64	124.45
28	b	616	CLA	CHD-C1D-ND	-3.06	121.64	124.45
28	B	610	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	B	616	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	b	606	CLA	C2D-C1D-ND	3.06	112.36	110.10
28	N	613	CLA	O2A-CGA-CBA	3.06	121.51	111.91
30	d	404	BCR	C1-C6-C5	-3.06	118.31	122.61
28	c	504	CLA	CMA-C3A-C4A	3.06	119.99	111.77
30	D	404	BCR	C34-C9-C10	-3.06	118.64	122.92
49	Y	623	NEX	C17-C1-C6	-3.06	107.74	110.47
46	G	607	CHL	CMA-C3A-C4A	3.06	119.99	111.77
28	S	609	CLA	CHD-C1D-ND	-3.06	121.65	124.45
28	c	509	CLA	CHD-C1D-ND	-3.06	121.65	124.45
28	c	511	CLA	CHD-C1D-ND	-3.06	121.65	124.45
28	C	511	CLA	C2C-C1C-NC	3.06	112.83	109.97
46	S	606	CHL	CMA-C3A-C4A	3.05	119.98	111.77
28	c	510	CLA	C1-C2-C3	-3.05	120.76	126.04
46	Y	601	CHL	CMA-C3A-C4A	3.05	119.98	111.77
28	S	609	CLA	CMA-C3A-C4A	3.05	119.97	111.77
46	G	606	CHL	C2C-C3C-C4C	3.05	108.66	106.49
28	Y	614	CLA	CHD-C1D-ND	-3.05	121.65	124.45
46	N	601	CHL	CMA-C3A-C4A	3.05	119.96	111.77
46	Y	606	CHL	CMA-C3A-C4A	3.05	119.96	111.77
46	G	607	CHL	C4A-NA-C1A	3.05	108.08	106.71
28	G	602	CLA	CMA-C3A-C4A	3.04	119.96	111.77
28	b	617	CLA	C1-C2-C3	-3.04	120.78	126.04
28	b	607	CLA	C2C-C1C-NC	3.04	112.82	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	S	601	CHL	C3B-C4B-NB	-3.04	107.69	110.52
28	C	509	CLA	CHD-C1D-ND	-3.04	121.66	124.45
28	a	410	CLA	CMA-C3A-C4A	3.04	119.94	111.77
49	G	623	NEX	C31-C30-C29	3.03	131.64	127.31
46	Y	605	CHL	C3C-C4C-NC	-3.03	107.17	110.57
30	C	515	BCR	C33-C5-C6	-3.03	121.12	124.53
30	d	404	BCR	C4-C5-C6	-3.03	118.33	122.73
30	C	517	BCR	C37-C22-C21	-3.03	118.68	122.92
28	C	503	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	b	609	CLA	C2C-C1C-NC	3.03	112.81	109.97
46	G	606	CHL	C3C-C4C-NC	-3.03	107.17	110.57
28	c	510	CLA	C2C-C1C-NC	3.03	112.81	109.97
28	Y	612	CLA	C2D-C1D-ND	3.03	112.33	110.10
28	B	602	CLA	C2D-C1D-ND	3.02	112.33	110.10
30	d	404	BCR	C33-C5-C4	3.02	119.42	113.62
28	C	513	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
28	B	614	CLA	C1-C2-C3	-3.02	120.82	126.04
28	A	406	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
30	C	514	BCR	C15-C14-C13	-3.02	123.00	127.31
28	S	612	CLA	C2C-C1C-NC	3.02	112.80	109.97
28	A	407	CLA	CMA-C3A-C4A	3.02	119.89	111.77
28	G	611	CLA	CMA-C3A-C4A	3.02	119.88	111.77
28	B	603	CLA	C1-C2-C3	-3.02	120.83	126.04
28	S	609	CLA	C2C-C1C-NC	3.02	112.80	109.97
49	N	623	NEX	C39-C29-C30	-3.01	118.70	122.92
28	Y	604	CLA	C2C-C1C-NC	3.01	112.80	109.97
28	b	602	CLA	CMA-C3A-C4A	3.01	119.87	111.77
47	S	621	LUT	C15-C14-C13	-3.01	123.01	127.31
28	c	513	CLA	C2C-C1C-NC	3.01	112.79	109.97
28	c	513	CLA	C2D-C1D-ND	3.01	112.32	110.10
46	Y	605	CHL	CMA-C3A-C4A	3.01	119.86	111.77
28	b	611	CLA	CHD-C1D-ND	-3.01	121.69	124.45
28	C	507	CLA	CHD-C1D-ND	-3.01	121.69	124.45
28	B	614	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
28	S	614	CLA	C2C-C1C-NC	3.01	112.79	109.97
28	d	402	CLA	CHD-C1D-ND	-3.01	121.69	124.45
28	G	613	CLA	C2C-C1C-NC	3.00	112.79	109.97
28	C	504	CLA	CHD-C1D-ND	-3.00	121.70	124.45
28	N	610	CLA	C2D-C1D-ND	3.00	112.31	110.10
46	S	601	CHL	CMA-C3A-C4A	3.00	119.83	111.77
28	G	611	CLA	CHD-C1D-ND	-2.99	121.70	124.45
28	N	614	CLA	CMA-C3A-C4A	2.99	119.82	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	S	608	CHL	C2C-C3C-C4C	2.99	108.62	106.49
46	N	608	CHL	CMA-C3A-C4A	2.99	119.82	111.77
28	Y	610	CLA	C2D-C1D-ND	2.99	112.31	110.10
46	G	601	CHL	CMA-C3A-C4A	2.99	119.81	111.77
28	S	614	CLA	C1-C2-C3	-2.99	120.87	126.04
28	Y	602	CLA	CHD-C1D-ND	-2.99	121.71	124.45
28	a	406	CLA	CMA-C3A-C4A	2.99	119.81	111.77
28	b	610	CLA	C2D-C1D-ND	2.99	112.31	110.10
28	A	406	CLA	CHD-C1D-ND	-2.99	121.71	124.45
28	B	611	CLA	CHD-C1D-ND	-2.99	121.71	124.45
28	B	614	CLA	C2D-C1D-ND	2.99	112.30	110.10
28	b	609	CLA	C2D-C1D-ND	2.99	112.30	110.10
28	b	617	CLA	C2C-C1C-NC	2.98	112.77	109.97
30	C	517	BCR	C19-C18-C17	2.98	123.52	118.94
28	N	603	CLA	CHD-C1D-ND	-2.98	121.71	124.45
28	C	501	CLA	C2C-C1C-NC	2.98	112.77	109.97
28	G	604	CLA	CHD-C1D-ND	-2.98	121.71	124.45
28	C	513	CLA	C2C-C1C-NC	2.98	112.76	109.97
28	c	502	CLA	C1-C2-C3	-2.98	120.89	126.04
28	S	617	CLA	CMA-C3A-C4A	2.98	119.78	111.77
46	G	606	CHL	CMA-C3A-C4A	2.98	119.78	111.77
28	N	611	CLA	C2D-C1D-ND	2.98	112.30	110.10
28	c	504	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
28	Y	608	CLA	CMA-C3A-C4A	2.98	119.77	111.77
28	c	503	CLA	C2C-C1C-NC	2.98	112.76	109.97
34	B	620	C7Z	C21-C26-C25	-2.98	118.42	122.61
28	B	611	CLA	C4B-CHC-C1C	2.97	133.39	126.34
46	Y	607	CHL	C2C-C3C-C4C	2.97	108.61	106.49
28	B	608	CLA	CHD-C1D-ND	-2.97	121.72	124.45
29	A	408	PHO	O1D-CGD-CBD	2.97	129.69	124.74
28	B	609	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
46	N	609	CHL	C4B-CHC-C1C	2.97	133.38	126.34
28	b	606	CLA	C1-C2-C3	-2.97	120.91	126.04
28	d	402	CLA	C2C-C1C-NC	2.97	112.75	109.97
41	d	405	PL9	C27-C28-C29	-2.96	120.53	127.66
28	B	611	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
46	G	609	CHL	C3B-C4B-NB	-2.96	107.77	110.52
46	Y	609	CHL	C4B-CHC-C1C	2.96	133.36	126.34
28	B	606	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
28	C	511	CLA	CMA-C3A-C4A	2.96	119.72	111.77
28	G	614	CLA	C2C-C1C-NC	2.96	112.74	109.97
28	S	617	CLA	CHD-C1D-ND	-2.96	121.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	618	BCR	C34-C9-C10	-2.95	118.79	122.92
28	S	602	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
28	S	605	CLA	CMA-C3A-C4A	2.95	119.71	111.77
28	a	407	CLA	CHD-C1D-ND	-2.95	121.74	124.45
28	B	612	CLA	C1-C2-C3	-2.95	120.94	126.04
28	Y	603	CLA	C2D-C1D-ND	2.95	112.28	110.10
28	C	507	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
28	B	607	CLA	C2C-C1C-NC	2.95	112.73	109.97
46	Y	607	CHL	CMA-C3A-C4A	2.95	119.70	111.77
28	N	614	CLA	C2D-C1D-ND	2.95	112.28	110.10
46	N	608	CHL	C4B-CHC-C1C	2.95	133.32	126.34
28	a	407	CLA	OBD-CAD-C3D	-2.95	121.43	128.52
28	Y	613	CLA	C2C-C1C-NC	2.95	112.73	109.97
28	b	614	CLA	CHD-C1D-ND	-2.94	121.75	124.45
28	Y	613	CLA	CMA-C3A-C4A	2.94	119.68	111.77
28	b	605	CLA	O2A-CGA-CBA	2.94	121.14	111.91
34	B	620	C7Z	C38-C25-C24	2.94	119.80	114.36
28	C	503	CLA	CHD-C1D-ND	-2.94	121.75	124.45
28	B	603	CLA	C2D-C1D-ND	2.94	112.27	110.10
28	S	610	CLA	C2D-C1D-ND	2.93	112.27	110.10
47	S	621	LUT	C35-C15-C14	-2.93	117.47	123.47
28	b	611	CLA	C4B-CHC-C1C	2.93	133.29	126.34
28	S	602	CLA	C2D-C1D-ND	2.93	112.26	110.10
28	S	612	CLA	CHD-C1D-ND	-2.93	121.76	124.45
30	b	619	BCR	C33-C5-C6	-2.93	121.24	124.53
28	N	602	CLA	C2D-C1D-ND	2.93	112.26	110.10
48	N	622	XAT	C7-C8-C9	-2.93	120.99	125.53
28	b	614	CLA	C2D-C1D-ND	2.93	112.26	110.10
28	b	603	CLA	C2D-C1D-ND	2.93	112.26	110.10
28	b	608	CLA	CMA-C3A-C4A	2.92	119.63	111.77
28	b	608	CLA	CHD-C1D-ND	-2.92	121.77	124.45
28	c	501	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
28	C	505	CLA	C1-C2-C3	-2.92	120.99	126.04
28	A	406	CLA	CMA-C3A-C4A	2.92	119.62	111.77
28	a	406	CLA	CHD-C1D-ND	-2.92	121.77	124.45
46	N	606	CHL	CMA-C3A-C4A	2.92	119.62	111.77
30	D	404	BCR	C36-C18-C17	-2.92	118.83	122.92
46	N	608	CHL	C3C-C4C-NC	-2.92	107.30	110.57
28	c	502	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
28	b	615	CLA	C2C-C1C-NC	2.91	112.70	109.97
46	N	606	CHL	CHD-C1D-ND	-2.91	121.78	124.45
28	b	605	CLA	O2D-CGD-O1D	-2.91	118.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	N	622	XAT	O4-C5-C4	-2.91	111.19	113.38
28	b	607	CLA	C1-C2-C3	-2.91	121.01	126.04
28	N	610	CLA	C2C-C1C-NC	2.91	112.70	109.97
28	S	602	CLA	O2A-CGA-CBA	2.91	121.04	111.91
28	C	503	CLA	C1-C2-C3	-2.91	121.01	126.04
28	b	610	CLA	C1-C2-C3	-2.91	121.02	126.04
28	b	613	CLA	C2D-C1D-ND	2.91	112.25	110.10
28	Y	611	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	b	604	CLA	CHD-C1D-ND	-2.91	121.78	124.45
28	c	505	CLA	C1-O2A-CGA	2.90	124.06	116.44
42	f	101	HEM	C4D-ND-C1D	2.90	108.07	105.07
46	Y	605	CHL	C2C-C3C-C4C	2.90	108.56	106.49
28	N	603	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
28	b	611	CLA	C3B-C4B-NB	-2.90	107.83	110.52
28	C	512	CLA	CMA-C3A-C4A	2.90	119.56	111.77
28	S	617	CLA	C2D-C1D-ND	2.90	112.24	110.10
28	B	604	CLA	C1-C2-C3	-2.90	121.03	126.04
28	G	610	CLA	C2D-C1D-ND	2.89	112.24	110.10
46	G	608	CHL	C2C-C3C-C4C	2.89	108.55	106.49
28	S	609	CLA	C2D-C1D-ND	2.89	112.23	110.10
28	A	407	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
28	S	603	CLA	C1-C2-C3	-2.89	121.05	126.04
28	B	610	CLA	O2A-CGA-CBA	2.89	120.97	111.91
47	G	620	LUT	C31-C30-C29	-2.89	123.19	127.31
34	B	620	C7Z	C11-C12-C13	-2.89	118.31	126.42
46	S	607	CHL	C3B-C4B-NB	-2.89	107.84	110.52
28	b	614	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
28	G	603	CLA	CMA-C3A-C4A	2.88	119.52	111.77
28	B	616	CLA	C2D-C1D-ND	2.88	112.23	110.10
28	a	410	CLA	CHD-C1D-ND	-2.88	121.81	124.45
30	C	516	BCR	C34-C9-C10	-2.88	118.89	122.92
28	c	508	CLA	CMA-C3A-C4A	2.88	119.51	111.77
28	A	407	CLA	CHD-C1D-ND	-2.88	121.81	124.45
46	Y	607	CHL	C3C-C4C-NC	-2.88	107.34	110.57
28	B	609	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
28	c	504	CLA	CHD-C1D-ND	-2.88	121.81	124.45
47	G	620	LUT	C11-C10-C9	-2.87	123.21	127.31
30	C	514	BCR	C38-C26-C25	-2.87	121.30	124.53
28	S	611	CLA	CMA-C3A-C4A	2.87	119.50	111.77
28	c	512	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
28	G	613	CLA	C2D-C1D-ND	2.87	112.22	110.10
28	b	613	CLA	C3B-C4B-NB	-2.87	107.85	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	G	608	CHL	C3B-C4B-NB	-2.87	107.85	110.52
46	S	608	CHL	C3C-C4C-NC	-2.87	107.35	110.57
30	c	517	BCR	C36-C18-C17	-2.87	118.90	122.92
32	d	411	LMG	O8-C28-C29	2.87	120.91	111.91
46	G	601	CHL	C4B-CHC-C1C	2.87	133.14	126.34
28	C	501	CLA	C2D-C1D-ND	2.87	112.22	110.10
28	B	603	CLA	CMA-C3A-C4A	2.87	119.48	111.77
28	Y	610	CLA	C2C-C1C-NC	2.87	112.66	109.97
28	Y	603	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
28	G	602	CLA	C2D-C1D-ND	2.87	112.22	110.10
34	B	620	C7Z	C22-C23-C24	2.87	114.23	110.30
28	N	604	CLA	CHD-C1D-ND	-2.87	121.82	124.45
28	c	501	CLA	C2C-C1C-NC	2.87	112.66	109.97
28	Y	612	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
38	l	101	LHG	O8-C23-C24	2.86	120.89	111.91
28	a	405	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	A	410	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
28	b	611	CLA	C1D-ND-C4D	-2.86	104.30	106.33
28	S	613	CLA	C2D-C1D-ND	2.86	112.21	110.10
28	a	406	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
28	c	506	CLA	CHD-C1D-ND	-2.86	121.83	124.45
38	d	410	LHG	O8-C23-C24	2.86	120.87	111.91
28	b	608	CLA	C1-C2-C3	-2.86	121.10	126.04
28	B	602	CLA	CHD-C1D-ND	-2.86	121.83	124.45
38	D	410	LHG	O8-C23-C24	2.85	120.87	111.91
28	B	610	CLA	C2D-C1D-ND	2.85	112.21	110.10
46	G	607	CHL	C4B-CHC-C1C	2.85	133.10	126.34
28	c	507	CLA	CMA-C3A-C4A	2.85	119.44	111.77
28	B	616	CLA	CHD-C1D-ND	-2.85	121.83	124.45
46	Y	607	CHL	CHB-C4A-NA	2.85	128.46	124.51
28	B	606	CLA	C2D-C1D-ND	2.85	112.20	110.10
29	a	409	PHO	C2D-C1D-ND	-2.85	107.56	109.53
46	N	609	CHL	C3C-C4C-NC	-2.85	107.38	110.57
47	Y	620	LUT	C18-C5-C6	-2.85	121.33	124.53
28	A	407	CLA	C2D-C1D-ND	2.85	112.20	110.10
28	b	616	CLA	C2D-C1D-ND	2.85	112.20	110.10
28	C	511	CLA	C1-C2-C3	-2.85	121.12	126.04
28	G	612	CLA	CHD-C1D-ND	-2.85	121.84	124.45
28	G	613	CLA	CHD-C1D-ND	-2.85	121.84	124.45
30	A	411	BCR	C33-C5-C4	2.85	119.08	113.62
28	N	611	CLA	CHD-C1D-ND	-2.84	121.84	124.45
28	c	512	CLA	C2D-C1D-ND	2.84	112.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	410	CLA	CMA-C3A-C4A	2.84	119.41	111.77
28	S	603	CLA	C2D-C1D-ND	2.84	112.20	110.10
46	N	605	CHL	CMA-C3A-C4A	2.84	119.41	111.77
28	C	513	CLA	C1-C2-C3	-2.84	121.13	126.04
28	N	604	CLA	C2D-C1D-ND	2.84	112.20	110.10
46	G	609	CHL	C1-O2A-CGA	2.84	123.89	116.44
28	B	616	CLA	C1-C2-C3	-2.84	121.14	126.04
47	Y	620	LUT	C38-C25-C24	-2.84	117.49	123.56
28	c	505	CLA	CMA-C3A-C4A	2.84	119.39	111.77
28	a	407	CLA	C2C-C1C-NC	2.83	112.63	109.97
48	G	622	XAT	C26-C27-C28	-2.83	120.00	125.99
28	d	403	CLA	C2C-C1C-NC	2.83	112.63	109.97
49	G	623	NEX	C38-C25-C26	-2.83	117.51	122.26
29	A	408	PHO	CMB-C2B-C3B	2.83	129.98	124.68
28	C	502	CLA	CHD-C1D-ND	-2.83	121.85	124.45
29	a	408	PHO	O1D-CGD-CBD	2.83	129.46	124.74
30	c	515	BCR	C23-C24-C25	-2.83	119.25	127.20
46	Y	607	CHL	C4A-NA-C1A	2.83	107.98	106.71
28	G	604	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
46	N	601	CHL	C4B-CHC-C1C	2.83	133.05	126.34
43	h	101	RRX	C33-C5-C4	2.83	119.05	113.62
32	C	523	LMG	O8-C28-C29	2.83	120.78	111.91
28	c	502	CLA	C2D-C1D-ND	2.83	112.19	110.10
28	N	613	CLA	C2D-C1D-ND	2.82	112.19	110.10
28	B	612	CLA	CHD-C1D-ND	-2.82	121.86	124.45
28	G	610	CLA	C2C-C1C-NC	2.82	112.62	109.97
28	S	605	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	S	611	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
29	a	409	PHO	O1D-CGD-CBD	2.82	129.44	124.74
28	c	507	CLA	CHD-C1D-ND	-2.82	121.86	124.45
46	N	605	CHL	C1-C2-C3	-2.82	121.17	126.04
28	S	604	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
28	G	603	CLA	C2D-C1D-ND	2.81	112.18	110.10
46	G	606	CHL	CHB-C4A-NA	2.81	128.40	124.51
28	b	610	CLA	C2C-C1C-NC	2.81	112.61	109.97
28	Y	602	CLA	C1-C2-C3	-2.81	121.19	126.04
28	B	617	CLA	C1-C2-C3	-2.81	121.19	126.04
28	b	613	CLA	C2C-C1C-NC	2.81	112.60	109.97
46	G	607	CHL	C1-O2A-CGA	2.81	123.81	116.44
28	B	610	CLA	CHD-C1D-ND	-2.81	121.88	124.45
32	W	201	LMG	O8-C28-C29	2.81	120.71	111.91
28	B	608	CLA	CMA-C3A-C4A	2.80	119.31	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	513	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
28	B	611	CLA	C3B-C4B-NB	-2.80	107.91	110.52
46	N	606	CHL	C3C-C4C-NC	-2.80	107.43	110.57
28	Y	614	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
28	B	604	CLA	CHD-C1D-ND	-2.80	121.88	124.45
28	Y	612	CLA	CHD-C1D-ND	-2.80	121.88	124.45
49	N	623	NEX	C19-C9-C10	-2.80	119.00	122.92
41	d	405	PL9	C40-C39-C41	2.80	119.98	115.27
32	c	521	LMG	O8-C28-C29	2.80	120.69	111.91
28	N	612	CLA	CHD-C1D-ND	-2.80	121.88	124.45
29	a	408	PHO	CMB-C2B-C3B	2.80	129.91	124.68
47	Y	620	LUT	C11-C10-C9	-2.80	123.32	127.31
28	N	614	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
28	N	612	CLA	C2D-C1D-ND	2.80	112.17	110.10
28	a	407	CLA	CHA-C4D-ND	2.79	138.34	132.50
35	C	519	DGD	O1G-C1A-C2A	2.79	120.68	111.91
30	C	515	BCR	C34-C9-C10	-2.79	119.01	122.92
46	G	608	CHL	C4B-CHC-C1C	2.79	132.96	126.34
28	b	612	CLA	CHD-C1D-ND	-2.79	121.89	124.45
47	S	620	LUT	C22-C23-C24	-2.79	108.56	111.74
28	Y	613	CLA	C2D-C1D-ND	2.79	112.16	110.10
28	S	613	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
28	c	505	CLA	CHD-C1D-ND	-2.79	121.89	124.45
47	N	620	LUT	C18-C5-C6	-2.78	121.40	124.53
47	N	620	LUT	C38-C25-C24	-2.78	117.60	123.56
28	N	603	CLA	C2D-C1D-ND	2.78	112.16	110.10
28	G	602	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
28	B	612	CLA	C2D-C1D-ND	2.78	112.16	110.10
28	Y	602	CLA	CMA-C3A-C4A	2.78	119.25	111.77
28	A	410	CLA	C1-C2-C3	-2.78	121.23	126.04
28	S	614	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
28	B	611	CLA	C2D-C1D-ND	2.78	112.15	110.10
28	C	512	CLA	O2A-CGA-CBA	2.78	120.63	111.91
28	S	611	CLA	C2D-C1D-ND	2.78	112.15	110.10
28	c	509	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
28	c	512	CLA	CMA-C3A-C4A	2.78	119.23	111.77
46	G	607	CHL	CHB-C4A-NA	2.78	128.35	124.51
30	c	516	BCR	C33-C5-C4	2.78	118.95	113.62
28	G	614	CLA	CMA-C3A-C4A	2.77	119.23	111.77
28	B	605	CLA	O2A-CGA-CBA	2.77	120.61	111.91
46	G	609	CHL	C4D-CHA-C1A	2.77	124.62	121.25
28	c	502	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	d	405	PL9	C7-C8-C9	-2.77	122.18	126.79
28	b	604	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
46	S	601	CHL	C4B-CHC-C1C	2.77	132.90	126.34
28	d	402	CLA	C3B-C4B-NB	-2.77	107.95	110.52
28	Y	610	CLA	O2A-CGA-CBA	2.77	120.59	111.91
38	D	409	LHG	O8-C23-C24	2.77	120.58	111.91
28	B	603	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
29	a	409	PHO	O2D-CGD-O1D	-2.76	118.44	123.84
28	D	402	CLA	C1D-ND-C4D	-2.76	104.37	106.33
30	B	618	BCR	C23-C24-C25	-2.76	119.45	127.20
28	C	513	CLA	CMA-C3A-C4A	2.76	119.19	111.77
46	G	608	CHL	C2B-C1B-NB	-2.76	108.38	110.23
28	Y	602	CLA	C2D-C1D-ND	2.76	112.14	110.10
28	b	612	CLA	C2D-C1D-ND	2.76	112.14	110.10
28	b	603	CLA	CMA-C3A-C4A	2.75	119.18	111.77
46	N	608	CHL	C2C-C3C-C4C	2.75	108.45	106.49
46	N	605	CHL	C3B-C4B-NB	-2.75	107.96	110.52
28	C	504	CLA	C2C-C1C-NC	2.75	112.55	109.97
35	c	520	DGD	O1G-C1A-C2A	2.75	120.55	111.91
28	Y	604	CLA	C1-C2-C3	-2.75	121.28	126.04
28	D	403	CLA	O2A-CGA-CBA	2.75	120.54	111.91
46	N	609	CHL	C1-O2A-CGA	2.75	123.66	116.44
35	C	518	DGD	O1G-C1A-C2A	2.75	120.54	111.91
28	c	509	CLA	CMA-C3A-C4A	2.75	119.16	111.77
28	b	609	CLA	CHD-C1D-ND	-2.75	121.93	124.45
30	C	514	BCR	C23-C24-C25	-2.75	119.48	127.20
28	N	602	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
46	Y	609	CHL	C3B-C4B-NB	-2.75	107.97	110.52
28	A	410	CLA	CAA-C2A-C3A	-2.75	105.26	112.78
28	G	614	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
28	N	613	CLA	CHD-C1D-ND	-2.74	121.93	124.45
50	S	625	LPX	O3-P1-O4	2.74	125.80	112.24
49	Y	623	NEX	C16-C1-C6	-2.74	108.02	110.47
28	b	603	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
28	C	502	CLA	C2D-C1D-ND	2.74	112.12	110.10
28	b	612	CLA	CMA-C3A-C4A	2.74	119.14	111.77
28	C	505	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
28	b	617	CLA	C2D-C1D-ND	2.74	112.12	110.10
28	G	610	CLA	O2A-CGA-CBA	2.74	120.50	111.91
28	D	403	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
51	Y	626	PTY	O4-C30-C31	2.74	120.50	111.91
28	b	605	CLA	C1C-C2C-C3C	-2.74	104.08	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	603	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
28	G	604	CLA	CMA-C3A-C4A	2.73	119.12	111.77
28	C	512	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
28	c	512	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
48	Y	622	XAT	C38-C25-C26	-2.73	117.69	122.26
49	S	623	NEX	C38-C25-C26	-2.73	117.69	122.26
28	Y	613	CLA	O2A-CGA-CBA	2.73	120.47	111.91
28	Y	608	CLA	C2D-C1D-ND	2.73	112.11	110.10
28	d	402	CLA	C2D-C1D-ND	2.73	112.11	110.10
36	t	101	3PH	O31-C31-C32	2.72	120.46	111.91
28	c	501	CLA	C2D-C1D-ND	2.72	112.11	110.10
38	C	525	LHG	O8-C23-C24	2.72	120.46	111.91
34	B	620	C7Z	C28-C27-C26	-2.72	119.56	127.20
46	Y	601	CHL	CHB-C4A-NA	2.72	128.28	124.51
28	B	602	CLA	CMA-C3A-C4A	2.72	119.09	111.77
46	N	607	CHL	CMA-C3A-C4A	2.72	119.09	111.77
43	h	101	RRX	C2-C1-C6	2.72	114.67	110.48
38	d	409	LHG	O8-C23-C24	2.72	120.44	111.91
28	S	617	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
28	B	605	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
38	L	101	LHG	O8-C23-C24	2.72	120.43	111.91
28	N	613	CLA	C1-C2-C3	-2.72	121.34	126.04
28	G	611	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
28	Y	614	CLA	C2D-C1D-ND	2.72	112.11	110.10
28	S	611	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
28	N	602	CLA	CMA-C3A-C4A	2.71	119.07	111.77
28	G	614	CLA	C2D-C1D-ND	2.71	112.10	110.10
46	G	608	CHL	C3C-C4C-NC	-2.71	107.53	110.57
46	S	607	CHL	C4B-CHC-C1C	2.71	132.76	126.34
43	h	101	RRX	C30-C25-C26	-2.71	118.80	122.61
28	a	410	CLA	O2A-CGA-CBA	2.71	120.40	111.91
28	N	604	CLA	OBD-CAD-C3D	-2.71	122.01	128.52
34	B	620	C7Z	C18-C5-C4	2.70	119.36	114.36
28	S	602	CLA	C2C-C1C-NC	2.70	112.50	109.97
46	S	608	CHL	C3B-C4B-NB	-2.70	108.01	110.52
30	A	411	BCR	C36-C18-C17	-2.70	119.14	122.92
46	G	606	CHL	C3B-C4B-NB	-2.70	108.01	110.52
30	C	515	BCR	C23-C24-C25	-2.70	119.62	127.20
49	Y	623	NEX	C38-C25-C26	-2.70	117.74	122.26
46	N	606	CHL	C2B-C1B-NB	-2.70	108.42	110.23
28	D	403	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
30	C	516	BCR	C27-C26-C25	-2.70	118.82	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	520	DGD	O1G-C1A-C2A	2.69	120.36	111.91
28	B	602	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
28	D	402	CLA	CHA-C4D-ND	2.69	138.13	132.50
28	C	512	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
28	S	611	CLA	CHD-C1D-ND	-2.69	121.98	124.45
42	F	101	HEM	C4D-ND-C1D	2.69	107.85	105.07
46	Y	601	CHL	C1-C2-C3	-2.69	121.40	126.04
28	B	617	CLA	C2D-C1D-ND	2.69	112.08	110.10
28	b	604	CLA	CMA-C3A-C4A	2.69	118.99	111.77
32	C	521	LMG	O8-C28-C29	2.69	120.34	111.91
28	c	511	CLA	C2D-C1D-ND	2.69	112.08	110.10
28	C	510	CLA	CMD-C2D-C3D	-2.68	121.44	127.61
28	b	609	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
28	c	508	CLA	C4B-CHC-C1C	2.68	132.70	126.34
28	b	613	CLA	C1-C2-C3	-2.68	121.40	126.04
28	c	512	CLA	C1-C2-C3	-2.68	121.40	126.04
45	K	101	4RF	O18-C16-C15	2.68	120.32	111.91
28	A	410	CLA	C2D-C1D-ND	2.68	112.08	110.10
47	N	620	LUT	C7-C8-C9	-2.68	122.19	126.23
28	b	602	CLA	C1-C2-C3	-2.68	121.41	126.04
28	S	610	CLA	C3B-C4B-NB	-2.68	108.03	110.52
35	c	519	DGD	O1G-C1A-C2A	2.68	120.31	111.91
28	B	615	CLA	CMD-C2D-C3D	-2.68	121.45	127.61
28	c	501	CLA	C3B-C4B-NB	-2.68	108.03	110.52
28	B	607	CLA	O2A-CGA-CBA	2.68	120.31	111.91
28	B	608	CLA	CMD-C2D-C3D	-2.68	121.45	127.61
30	d	404	BCR	C38-C26-C25	-2.68	121.52	124.53
28	b	609	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
30	D	404	BCR	C38-C26-C25	-2.68	121.52	124.53
28	B	605	CLA	CHD-C1D-ND	-2.68	122.00	124.45
28	B	607	CLA	C1-C2-C3	-2.68	121.42	126.04
28	c	513	CLA	CMA-C3A-C4A	2.68	118.96	111.77
28	B	613	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
28	G	604	CLA	C2D-C1D-ND	2.67	112.08	110.10
28	Y	604	CLA	C2D-C1D-ND	2.67	112.08	110.10
46	G	601	CHL	C3B-C4B-NB	-2.67	108.03	110.52
28	C	509	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
45	I	102	4RF	O40-C41-C43	2.67	120.30	111.91
28	B	608	CLA	C1-C2-C3	-2.67	121.42	126.04
28	d	403	CLA	C2D-C1D-ND	2.67	112.07	110.10
46	S	608	CHL	C1-O2A-CGA	2.67	123.45	116.44
28	C	505	CLA	C3B-C4B-NB	-2.67	108.04	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	413	LMG	C8-O7-C10	-2.67	111.21	117.79
28	b	605	CLA	CHD-C1D-ND	-2.67	122.00	124.45
28	N	612	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	b	606	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
28	c	512	CLA	O2A-CGA-CBA	2.67	120.28	111.91
46	Y	601	CHL	C3C-C4C-NC	-2.67	107.58	110.57
47	G	620	LUT	C38-C25-C24	-2.66	117.86	123.56
28	C	508	CLA	CMA-C3A-C4A	2.66	118.93	111.77
46	N	601	CHL	C1-C2-C3	-2.66	121.44	126.04
28	d	402	CLA	C4B-CHC-C1C	2.66	132.65	126.34
30	a	411	BCR	C38-C26-C27	2.66	118.73	113.62
46	S	606	CHL	C4B-CHC-C1C	2.66	132.65	126.34
28	C	513	CLA	C3B-C4B-NB	-2.66	108.05	110.52
28	C	505	CLA	CHA-C4D-ND	2.66	138.06	132.50
46	Y	605	CHL	C3B-C4B-NB	-2.66	108.05	110.52
28	C	502	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
46	N	607	CHL	C4B-CHC-C1C	2.66	132.64	126.34
46	Y	606	CHL	C4B-CHC-C1C	2.66	132.64	126.34
37	J	101	DGA	OG1-CA1-CA2	2.66	120.24	111.91
28	B	615	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
28	C	503	CLA	C2D-C1D-ND	2.66	112.06	110.10
28	C	504	CLA	CMA-C3A-C4A	2.66	118.91	111.77
28	N	611	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
30	c	516	BCR	C34-C9-C10	-2.65	119.20	122.92
46	Y	605	CHL	C4B-CHC-C1C	2.65	132.63	126.34
28	Y	608	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
28	b	608	CLA	C2D-C1D-ND	2.65	112.06	110.10
28	N	602	CLA	O2A-CGA-CBA	2.65	120.23	111.91
37	C	524	DGA	OG1-CA1-CA2	2.65	120.23	111.91
28	b	606	CLA	CMD-C2D-C3D	-2.65	121.52	127.61
30	c	517	BCR	C33-C5-C6	-2.65	121.55	124.53
28	B	605	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
38	D	410	LHG	C5-O7-C7	-2.65	111.27	117.79
30	b	618	BCR	C38-C26-C27	2.65	118.70	113.62
28	Y	602	CLA	O2A-CGA-CBA	2.65	120.22	111.91
46	Y	606	CHL	C1-C2-C3	-2.65	121.46	126.04
36	T	101	3PH	O31-C31-C32	2.65	120.22	111.91
28	c	505	CLA	O2A-CGA-CBA	2.65	120.21	111.91
29	A	409	PHO	O2D-CGD-O1D	-2.64	118.67	123.84
30	C	517	BCR	C23-C24-C25	-2.64	119.78	127.20
46	Y	609	CHL	C1-O2A-CGA	2.64	123.38	116.44
28	Y	613	CLA	C1C-C2C-C3C	-2.64	104.18	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	403	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
28	b	602	CLA	C2D-C1D-ND	2.64	112.05	110.10
28	B	612	CLA	C2C-C1C-NC	2.64	112.45	109.97
38	S	624	LHG	O8-C23-C24	2.64	120.20	111.91
28	Y	603	CLA	CMA-C3A-C4A	2.64	118.87	111.77
28	G	612	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
28	G	612	CLA	C2D-C1D-ND	2.64	112.05	110.10
28	Y	611	CLA	C2D-C1D-ND	2.64	112.05	110.10
47	Y	620	LUT	C10-C11-C12	-2.64	114.98	123.22
28	C	513	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
46	G	606	CHL	C1-O2A-CGA	2.64	123.36	116.44
34	b	620	C7Z	C28-C27-C26	-2.64	119.80	127.20
28	B	615	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	C	506	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
46	G	605	CHL	CHB-C4A-NA	2.63	128.15	124.51
47	G	620	LUT	C18-C5-C6	-2.63	121.57	124.53
28	Y	602	CLA	C2C-C1C-NC	2.63	112.44	109.97
28	S	605	CLA	O2A-CGA-CBA	2.63	120.17	111.91
28	C	511	CLA	C2D-C1D-ND	2.63	112.04	110.10
28	c	507	CLA	O2A-CGA-CBA	2.63	120.16	111.91
28	A	410	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
35	b	623	DGD	O1G-C1A-C2A	2.63	120.16	111.91
46	N	605	CHL	C4B-CHC-C1C	2.63	132.57	126.34
28	S	604	CLA	O2A-CGA-CBA	2.63	120.16	111.91
30	C	514	BCR	C40-C30-C25	-2.63	106.04	110.30
28	S	605	CLA	CHA-C4D-ND	2.63	137.99	132.50
28	c	510	CLA	C1D-ND-C4D	-2.63	104.47	106.33
28	b	602	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
28	b	616	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
47	Y	620	LUT	C31-C30-C29	-2.63	123.56	127.31
28	S	605	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	c	505	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	S	602	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
28	b	615	CLA	CMD-C2D-C3D	-2.62	121.58	127.61
28	c	506	CLA	CMA-C3A-C4A	2.62	118.82	111.77
30	C	514	BCR	C38-C26-C27	2.62	118.66	113.62
28	C	507	CLA	C1-O2A-CGA	2.62	123.33	116.44
28	B	613	CLA	CHA-C4D-ND	2.62	137.99	132.50
32	a	413	LMG	O8-C28-C29	2.62	120.14	111.91
46	S	608	CHL	C4B-CHC-C1C	2.62	132.56	126.34
30	B	618	BCR	C4-C5-C6	-2.62	118.93	122.73
28	A	405	CLA	C2C-C1C-NC	2.62	112.43	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	N	602	CLA	C2C-C1C-NC	2.62	112.43	109.97
28	b	615	CLA	C2D-C1D-ND	2.62	112.03	110.10
32	c	523	LMG	O8-C28-C29	2.62	120.13	111.91
43	H	101	RRX	C30-C25-C26	-2.62	118.92	122.61
28	B	606	CLA	C1-O2A-CGA	2.62	123.31	116.44
28	Y	612	CLA	O2A-CGA-CBA	2.62	120.12	111.91
28	c	507	CLA	C4B-CHC-C1C	2.62	132.55	126.34
28	C	511	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	a	410	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
28	G	602	CLA	C1-C2-C3	-2.62	121.52	126.04
28	B	606	CLA	CMD-C2D-C3D	-2.62	121.59	127.61
41	d	405	PL9	C22-C23-C24	-2.62	121.36	127.66
47	N	621	LUT	C38-C25-C24	-2.62	117.96	123.56
30	B	618	BCR	C34-C9-C10	-2.62	119.26	122.92
28	B	608	CLA	CHA-C4D-ND	2.61	137.97	132.50
28	c	505	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
28	B	609	CLA	CMA-C3A-C4A	2.61	118.79	111.77
28	c	501	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
47	Y	621	LUT	C38-C25-C24	-2.61	117.97	123.56
28	B	604	CLA	O2A-CGA-CBA	2.61	120.10	111.91
43	h	101	RRX	C7-C6-C5	-2.61	115.14	121.46
38	D	408	LHG	O8-C23-C24	2.61	120.10	111.91
28	b	610	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
46	N	609	CHL	C4A-NA-C1A	2.61	107.88	106.71
29	A	409	PHO	C2D-C1D-ND	-2.61	107.72	109.53
46	Y	605	CHL	CHB-C4A-NA	2.61	128.12	124.51
28	B	604	CLA	CHA-C4D-ND	2.61	137.95	132.50
28	S	603	CLA	CHA-C4D-ND	2.61	137.95	132.50
30	C	516	BCR	C28-C27-C26	-2.61	109.42	114.08
28	B	604	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
28	N	611	CLA	CMA-C3A-C4A	2.60	118.77	111.77
28	b	611	CLA	CMA-C3A-C4A	2.60	118.77	111.77
49	S	623	NEX	C39-C29-C30	-2.60	119.28	122.92
30	B	618	BCR	C1-C6-C7	2.60	123.14	115.78
36	b	624	3PH	O31-C31-C32	2.60	120.08	111.91
28	B	615	CLA	CHA-C4D-ND	2.60	137.94	132.50
28	S	617	CLA	O2A-CGA-CBA	2.60	120.08	111.91
43	H	101	RRX	C36-C18-C19	2.60	122.18	118.08
47	G	621	LUT	C35-C15-C14	-2.60	118.14	123.47
28	B	613	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
28	C	513	CLA	CBA-CAA-C2A	2.60	121.54	113.86
46	G	605	CHL	C4A-NA-C1A	2.60	107.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	G	605	CHL	C3B-C4B-NB	-2.60	108.10	110.52
47	Y	621	LUT	C31-C30-C29	-2.60	123.60	127.31
28	C	511	CLA	O2A-CGA-CBA	2.60	120.06	111.91
28	S	612	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
28	C	509	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
35	c	518	DGD	O1G-C1A-C2A	2.60	120.06	111.91
28	C	510	CLA	C2D-C1D-ND	2.60	112.02	110.10
28	C	506	CLA	C1-C2-C3	-2.59	121.56	126.04
28	S	602	CLA	CMA-C3A-C4A	2.59	118.74	111.77
28	C	501	CLA	C3B-C4B-NB	-2.59	108.11	110.52
28	B	613	CLA	C1-C2-C3	-2.59	121.56	126.04
28	N	604	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
28	G	602	CLA	CHD-C1D-ND	-2.59	122.07	124.45
46	S	608	CHL	CHB-C4A-NA	2.59	128.09	124.51
37	j	101	DGA	OG1-CA1-CA2	2.59	120.04	111.91
28	C	501	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
28	B	609	CLA	C2D-C1D-ND	2.59	112.01	110.10
36	S	626	3PH	O31-C31-C32	2.59	120.03	111.91
28	B	611	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
38	Y	624	LHG	C6-C5-C4	-2.59	105.67	111.79
28	G	604	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
28	N	604	CLA	CHA-C4D-ND	2.59	137.91	132.50
30	C	516	BCR	C33-C5-C4	2.58	118.58	113.62
28	S	605	CLA	CHD-C1D-ND	-2.58	122.08	124.45
28	b	605	CLA	CHA-C4D-ND	2.58	137.90	132.50
28	N	610	CLA	C1-C2-C3	-2.58	121.58	126.04
28	D	403	CLA	CMA-C3A-C4A	2.58	118.72	111.77
28	A	405	CLA	CHA-C4D-ND	2.58	137.90	132.50
46	G	605	CHL	C4B-CHC-C1C	2.58	132.46	126.34
28	S	604	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	B	617	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
28	C	501	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
28	c	501	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
28	d	402	CLA	C1-C2-C3	-2.58	121.58	126.04
28	Y	611	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
28	C	508	CLA	C2D-C1D-ND	2.58	112.00	110.10
29	A	409	PHO	O1D-CGD-CBD	2.58	129.03	124.74
28	c	511	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
28	c	508	CLA	C1D-ND-C4D	-2.57	104.51	106.33
28	S	611	CLA	CHA-C4D-ND	2.57	137.88	132.50
28	b	608	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
30	b	618	BCR	C28-C27-C26	-2.57	109.49	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	604	CLA	CHA-C4D-ND	2.57	137.88	132.50
45	i	101	4RF	O40-C41-C43	2.57	119.97	111.91
30	b	618	BCR	C1-C6-C5	-2.57	119.00	122.61
42	F	101	HEM	C4A-NA-C1A	2.57	107.86	105.35
39	C	527	LMK	O3-C4-C3	-2.57	114.18	122.98
28	B	602	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
28	B	609	CLA	CHA-C4D-ND	2.57	137.87	132.50
46	N	601	CHL	C3B-C4B-NB	-2.56	108.14	110.52
28	a	407	CLA	CMD-C2D-C3D	-2.56	121.72	127.61
28	a	406	CLA	CHA-C4D-ND	2.56	137.85	132.50
28	b	607	CLA	C2D-C1D-ND	2.56	111.99	110.10
28	G	611	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
41	D	405	PL9	C7-C8-C9	-2.56	122.53	126.79
28	C	506	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
28	C	508	CLA	C2C-C1C-NC	2.56	112.37	109.97
28	Y	611	CLA	C1-C2-C3	-2.56	121.62	126.04
47	N	621	LUT	C35-C15-C14	-2.56	118.24	123.47
28	N	603	CLA	CMA-C3A-C4A	2.56	118.64	111.77
36	B	624	3PH	O31-C31-C32	2.56	119.93	111.91
28	N	604	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
30	b	619	BCR	C4-C5-C6	-2.55	119.02	122.73
28	c	513	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
28	C	510	CLA	CHA-C4D-ND	2.55	137.83	132.50
28	N	611	CLA	CHA-C4D-ND	2.55	137.83	132.50
28	S	603	CLA	CHD-C1D-ND	-2.55	122.11	124.45
28	b	615	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
48	G	622	XAT	C6-C7-C8	-2.55	120.60	125.99
46	Y	606	CHL	C2B-C1B-NB	-2.55	108.52	110.23
49	Y	623	NEX	C1-C2-C3	2.55	119.39	113.64
28	C	507	CLA	C2D-C1D-ND	2.54	111.98	110.10
28	S	604	CLA	C1-O2A-CGA	2.54	123.12	116.44
28	c	504	CLA	C2D-C1D-ND	2.54	111.98	110.10
28	b	613	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
46	S	601	CHL	CHB-C4A-NA	2.54	128.03	124.51
32	w	201	LMG	O8-C28-C29	2.54	119.88	111.91
28	c	505	CLA	C2D-C1D-ND	2.54	111.98	110.10
28	G	611	CLA	C1-C2-C3	-2.54	121.65	126.04
47	S	620	LUT	C38-C25-C24	-2.54	118.13	123.56
28	c	508	CLA	C2C-C1C-NC	2.54	112.35	109.97
28	B	608	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
28	Y	604	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
30	d	404	BCR	C15-C14-C13	-2.54	123.69	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	603	CLA	C1-O2A-CGA	2.54	123.10	116.44
28	b	613	CLA	CHD-C1D-ND	-2.54	122.12	124.45
28	C	510	CLA	C1D-ND-C4D	-2.54	104.53	106.33
28	a	410	CLA	C2D-C1D-ND	2.53	111.97	110.10
28	B	602	CLA	C4B-CHC-C1C	2.53	132.35	126.34
28	C	503	CLA	CHA-C4D-ND	2.53	137.80	132.50
28	S	602	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
28	N	603	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
28	B	603	CLA	O2A-CGA-CBA	2.53	119.86	111.91
32	D	411	LMG	O8-C28-C29	2.53	119.86	111.91
28	B	604	CLA	CMA-C3A-C4A	2.53	118.58	111.77
28	b	604	CLA	O2A-CGA-CBA	2.53	119.85	111.91
28	b	615	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	D	404	BCR	C19-C18-C17	2.53	122.83	118.94
28	G	613	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
28	Y	611	CLA	CHA-C4D-ND	2.53	137.79	132.50
28	c	512	CLA	CHA-C4D-ND	2.53	137.79	132.50
28	c	504	CLA	C4B-CHC-C1C	2.53	132.34	126.34
28	C	507	CLA	CHA-C4D-ND	2.53	137.79	132.50
28	C	505	CLA	O2A-CGA-CBA	2.53	119.84	111.91
28	c	506	CLA	C2D-C1D-ND	2.53	111.97	110.10
28	B	607	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
46	N	608	CHL	C1-O2A-CGA	2.53	123.07	116.44
38	N	624	LHG	O8-C23-C24	2.53	119.83	111.91
28	Y	611	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
28	G	610	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
43	H	101	RRX	C11-C12-C13	-2.52	119.33	126.42
28	B	616	CLA	C3B-C4B-NB	-2.52	108.18	110.52
46	N	606	CHL	CHB-C4A-NA	2.52	128.00	124.51
28	B	607	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
38	c	525	LHG	O8-C23-C24	2.52	119.82	111.91
28	D	402	CLA	C2C-C1C-NC	2.52	112.33	109.97
28	C	511	CLA	CHA-C4D-ND	2.52	137.77	132.50
28	N	612	CLA	CHA-C4D-ND	2.52	137.77	132.50
46	N	609	CHL	C4D-CHA-C1A	2.52	124.31	121.25
30	A	411	BCR	C38-C26-C25	-2.52	121.70	124.53
47	S	620	LUT	C11-C10-C9	-2.52	123.72	127.31
32	B	622	LMG	O8-C28-C29	2.52	119.81	111.91
45	i	101	4RF	O18-C16-C15	2.52	119.81	111.91
28	b	606	CLA	C1D-ND-C4D	-2.52	104.55	106.33
28	S	610	CLA	C1-C2-C3	-2.52	121.69	126.04
28	b	607	CLA	CHA-C4D-ND	2.52	137.76	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	616	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
28	N	613	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
28	B	607	CLA	CHA-C4D-ND	2.51	137.76	132.50
28	N	603	CLA	CHA-C4D-ND	2.51	137.76	132.50
28	C	507	CLA	O2A-CGA-CBA	2.51	119.80	111.91
28	c	512	CLA	CHD-C1D-ND	-2.51	122.14	124.45
28	B	605	CLA	CHA-C4D-ND	2.51	137.76	132.50
28	G	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
32	b	622	LMG	O8-C28-C29	2.51	119.79	111.91
28	C	506	CLA	CMA-C3A-C4A	2.51	118.52	111.77
28	d	403	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
28	d	402	CLA	O2A-CGA-CBA	2.51	119.79	111.91
28	c	507	CLA	CHA-C4D-ND	2.51	137.75	132.50
28	C	504	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
28	C	505	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
46	N	601	CHL	CHB-C4A-NA	2.51	127.98	124.51
28	Y	610	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
28	B	615	CLA	OBD-CAD-C3D	-2.51	122.48	128.52
46	N	605	CHL	CHB-C4A-NA	2.51	127.98	124.51
28	Y	608	CLA	CHA-C4D-ND	2.51	137.74	132.50
28	B	608	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
45	K	101	4RF	O40-C41-C43	2.51	119.77	111.91
28	N	611	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
28	c	510	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
28	Y	614	CLA	C3B-C4B-NB	-2.51	108.19	110.52
28	a	410	CLA	CHA-C4D-ND	2.50	137.74	132.50
28	b	604	CLA	CHA-C4D-ND	2.50	137.74	132.50
38	G	624	LHG	O8-C23-C24	2.50	119.76	111.91
45	I	102	4RF	O18-C16-C15	2.50	119.76	111.91
30	b	618	BCR	C36-C18-C17	-2.50	119.42	122.92
28	b	610	CLA	CHA-C4D-ND	2.50	137.73	132.50
28	b	617	CLA	CMA-C3A-C4A	2.50	118.50	111.77
28	b	615	CLA	CHA-C4D-ND	2.50	137.73	132.50
28	d	402	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
43	H	101	RRX	C8-C7-C6	-2.50	120.18	127.20
28	S	609	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
28	c	513	CLA	CBA-CAA-C2A	2.50	121.24	113.86
42	f	101	HEM	C4A-NA-C1A	2.50	107.80	105.35
28	b	616	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
28	S	603	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
28	S	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
37	c	524	DGA	OG1-CA1-CA2	2.50	119.74	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	602	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
47	Y	621	LUT	C3-C4-C5	-2.50	106.88	111.85
28	c	501	CLA	C4B-CHC-C1C	2.50	132.26	126.34
46	Y	607	CHL	C1-O2A-CGA	2.50	122.99	116.44
30	a	411	BCR	C23-C24-C25	-2.50	120.19	127.20
28	B	611	CLA	CMA-C3A-C4A	2.49	118.48	111.77
30	c	517	BCR	C8-C9-C10	2.49	122.77	118.94
28	b	609	CLA	CHA-C4D-ND	2.49	137.72	132.50
28	G	614	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
28	c	507	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
30	c	514	BCR	C36-C18-C17	-2.49	119.43	122.92
28	b	614	CLA	CHA-C4D-ND	2.49	137.71	132.50
30	c	517	BCR	C15-C14-C13	-2.49	123.75	127.31
30	c	516	BCR	C37-C22-C23	2.49	122.00	118.08
28	a	407	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
28	S	610	CLA	C2C-C1C-NC	2.49	112.31	109.97
28	C	506	CLA	CHA-C4D-ND	2.49	137.71	132.50
46	G	609	CHL	CHC-C1C-NC	2.49	127.98	124.20
49	S	623	NEX	C19-C9-C10	-2.49	119.44	122.92
28	a	410	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	A	409	PHO	C1C-C2C-C3C	-2.49	106.54	108.61
28	d	403	CLA	O2A-CGA-CBA	2.49	119.71	111.91
45	k	101	4RF	O18-C16-C15	2.49	119.71	111.91
28	C	502	CLA	CHA-C4D-ND	2.49	137.70	132.50
28	S	614	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
45	k	101	4RF	O40-C41-C43	2.49	119.71	111.91
28	S	610	CLA	CHA-C4D-ND	2.48	137.70	132.50
46	N	608	CHL	CHB-C4A-NA	2.48	127.95	124.51
28	c	506	CLA	C1-C2-C3	-2.48	121.75	126.04
28	G	612	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
28	b	606	CLA	CHA-C4D-ND	2.48	137.69	132.50
28	b	613	CLA	CHA-C4D-ND	2.48	137.69	132.50
28	S	609	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
28	N	610	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
43	h	101	RRX	C8-C9-C10	-2.48	115.14	118.94
28	C	511	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
30	c	515	BCR	C38-C26-C25	-2.48	121.75	124.53
28	B	607	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
28	B	602	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	C	509	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	b	616	CLA	CHA-C4D-ND	2.48	137.68	132.50
28	G	613	CLA	O2A-CGA-CBA	2.48	119.68	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	503	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
28	Y	612	CLA	CMA-C3A-C4A	2.47	118.42	111.77
32	h	102	LMG	O8-C28-C29	2.47	119.67	111.91
46	Y	607	CHL	C4B-CHC-C1C	2.47	132.21	126.34
29	a	408	PHO	C1C-C2C-C3C	-2.47	106.55	108.61
28	C	507	CLA	CMA-C3A-C4A	2.47	118.42	111.77
47	S	621	LUT	C11-C10-C9	-2.47	123.78	127.31
28	Y	612	CLA	CHA-C4D-ND	2.47	137.67	132.50
28	A	407	CLA	CHA-C4D-ND	2.47	137.67	132.50
28	B	606	CLA	CHA-C4D-ND	2.47	137.67	132.50
30	A	411	BCR	C23-C24-C25	-2.47	120.26	127.20
28	G	602	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
28	b	608	CLA	CHA-C4D-ND	2.47	137.66	132.50
28	c	505	CLA	CHA-C4D-ND	2.47	137.66	132.50
46	G	608	CHL	C4A-NA-C1A	2.47	107.82	106.71
28	D	403	CLA	C3B-C4B-NB	-2.47	108.22	110.52
28	b	610	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
47	N	620	LUT	C31-C30-C29	-2.47	123.79	127.31
28	A	405	CLA	CMD-C2D-C3D	-2.47	121.94	127.61
35	B	623	DGD	O1G-C1A-C2A	2.47	119.64	111.91
28	Y	614	CLA	CMA-C3A-C4A	2.46	118.40	111.77
47	G	621	LUT	C38-C25-C24	-2.46	118.28	123.56
30	C	515	BCR	C33-C5-C4	2.46	118.35	113.62
28	b	617	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
28	A	410	CLA	O2A-CGA-CBA	2.46	119.64	111.91
28	c	502	CLA	CHA-C4D-ND	2.46	137.65	132.50
28	C	512	CLA	CHA-C4D-ND	2.46	137.65	132.50
28	Y	603	CLA	C3B-C4B-NB	-2.46	108.23	110.52
30	a	411	BCR	C36-C18-C17	-2.46	119.48	122.92
28	C	510	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
46	S	606	CHL	CHB-C4A-NA	2.46	127.91	124.51
28	b	612	CLA	O2A-CGA-CBA	2.46	119.63	111.91
28	D	402	CLA	C4B-CHC-C1C	2.46	132.17	126.34
28	a	407	CLA	C3D-C2D-C1D	-2.46	102.47	105.83
28	B	616	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	S	613	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	b	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
28	c	501	CLA	CHA-C4D-ND	2.46	137.64	132.50
37	B	625	DGA	OG1-CA1-CA2	2.46	119.62	111.91
28	N	612	CLA	C3B-C4B-NB	-2.46	108.23	110.52
28	A	406	CLA	C2D-C1D-ND	2.46	111.92	110.10
47	S	620	LUT	C10-C11-C12	-2.46	115.55	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	C	517	BCR	C23-C22-C21	2.46	122.71	118.94
28	B	616	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
28	C	507	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
28	S	604	CLA	C2D-C1D-ND	2.45	111.91	110.10
28	B	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
38	Y	624	LHG	O8-C23-C24	2.45	119.61	111.91
28	b	612	CLA	C2C-C1C-NC	2.45	112.27	109.97
28	Y	603	CLA	C1-C2-C3	-2.45	121.80	126.04
28	S	609	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
41	D	405	PL9	C22-C23-C24	-2.45	121.76	127.66
28	G	603	CLA	CHA-C4D-ND	2.45	137.62	132.50
28	Y	614	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
28	G	611	CLA	CHA-C4D-ND	2.45	137.62	132.50
28	Y	612	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
28	N	612	CLA	C4B-CHC-C1C	2.45	132.15	126.34
28	a	406	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
30	B	619	BCR	C35-C13-C12	2.45	121.93	118.08
49	N	623	NEX	C38-C25-C26	-2.45	118.16	122.26
28	b	607	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
28	B	612	CLA	CMA-C3A-C4A	2.45	118.35	111.77
28	D	402	CLA	CAC-C3C-C4C	2.45	127.98	124.81
28	C	503	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
28	c	506	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
28	D	403	CLA	C2D-C1D-ND	2.45	111.91	110.10
28	c	509	CLA	CHA-C4D-ND	2.45	137.62	132.50
46	N	606	CHL	C1-C2-C3	-2.45	121.81	126.04
30	C	516	BCR	C31-C1-C6	-2.45	106.33	110.30
28	B	609	CLA	O1D-CGD-CBD	-2.45	119.48	124.48
32	A	413	LMG	O8-C28-C29	2.44	119.58	111.91
28	G	614	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
30	B	619	BCR	C28-C27-C26	-2.44	109.71	114.08
28	B	617	CLA	CMA-C3A-C4A	2.44	118.34	111.77
28	Y	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	B	602	CLA	C1-C2-C3	-2.44	121.82	126.04
28	S	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
28	G	603	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
28	b	604	CLA	C1-C2-C3	-2.44	121.82	126.04
46	G	609	CHL	CHD-C4C-C3C	2.44	128.43	124.84
28	B	613	CLA	CHD-C1D-ND	-2.44	122.21	124.45
28	d	403	CLA	CHA-C4D-ND	2.44	137.60	132.50
28	b	611	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
46	Y	601	CHL	C4A-NA-C1A	2.44	107.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	613	CLA	CHA-C4D-ND	2.44	137.60	132.50
28	N	603	CLA	C3B-C4B-NB	-2.44	108.25	110.52
28	b	607	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
28	b	611	CLA	CHA-C4D-ND	2.44	137.60	132.50
46	N	608	CHL	C4D-CHA-C1A	2.44	124.22	121.25
28	C	503	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
28	Y	610	CLA	C4B-CHC-C1C	2.44	132.12	126.34
46	G	601	CHL	C1-O2A-CGA	2.44	122.84	116.44
28	B	613	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
28	B	614	CLA	CHA-C4D-ND	2.44	137.59	132.50
28	N	613	CLA	CHA-C4D-ND	2.44	137.59	132.50
28	b	607	CLA	O2A-CGA-CBA	2.44	119.55	111.91
30	d	404	BCR	C36-C18-C17	-2.44	119.51	122.92
28	S	605	CLA	C1-O2A-CGA	2.44	122.83	116.44
28	Y	602	CLA	CHA-C4D-ND	2.44	137.59	132.50
28	b	607	CLA	C3B-C4B-NB	-2.44	108.26	110.52
28	d	402	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
28	S	610	CLA	C4B-CHC-C1C	2.43	132.11	126.34
28	b	610	CLA	O2A-CGA-CBA	2.43	119.54	111.91
28	Y	612	CLA	C1-C2-C3	-2.43	121.83	126.04
28	c	507	CLA	C2D-C1D-ND	2.43	111.90	110.10
28	b	616	CLA	C3B-C4B-NB	-2.43	108.26	110.52
28	c	504	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	B	611	CLA	CHA-C4D-ND	2.43	137.59	132.50
32	C	521	LMG	C8-O7-C10	-2.43	111.80	117.79
28	C	504	CLA	C3B-C4B-NB	-2.43	108.26	110.52
28	C	501	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	S	617	CLA	CHA-C4D-ND	2.43	137.59	132.50
28	S	605	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
28	b	617	CLA	CHD-C1D-ND	-2.43	122.22	124.45
46	N	607	CHL	C1-O2A-CGA	2.43	122.82	116.44
28	c	513	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	B	603	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
28	B	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
28	c	510	CLA	CHA-C4D-ND	2.43	137.58	132.50
28	B	610	CLA	C1-O2A-CGA	2.43	122.82	116.44
30	C	517	BCR	C33-C5-C6	-2.43	121.80	124.53
28	Y	613	CLA	CHA-C4D-ND	2.43	137.58	132.50
30	D	404	BCR	C33-C5-C4	2.43	118.28	113.62
28	S	612	CLA	CHA-C4D-ND	2.43	137.57	132.50
28	Y	614	CLA	CHA-C4D-ND	2.43	137.57	132.50
28	B	617	CLA	CHA-C4D-ND	2.43	137.57	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	c	515	BCR	C34-C9-C10	-2.43	119.53	122.92
29	A	408	PHO	O2D-CGD-O1D	-2.42	119.10	123.84
28	S	614	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
28	N	602	CLA	C1D-ND-C4D	-2.42	104.61	106.33
28	C	509	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
28	B	612	CLA	O2A-CGA-CBA	2.42	119.51	111.91
28	G	612	CLA	C4B-CHC-C1C	2.42	132.08	126.34
46	Y	609	CHL	C1-C2-C3	-2.42	121.85	126.04
28	C	513	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
28	Y	604	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
46	G	607	CHL	C1-C2-C3	-2.42	121.86	126.04
28	a	405	CLA	CHA-C4D-ND	2.42	137.56	132.50
28	D	403	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
29	a	408	PHO	O2D-CGD-O1D	-2.42	119.11	123.84
28	c	511	CLA	CHA-C4D-ND	2.42	137.56	132.50
30	c	514	BCR	C38-C26-C25	-2.42	121.81	124.53
37	b	625	DGA	OG1-CA1-CA2	2.42	119.50	111.91
46	N	605	CHL	C2B-C1B-NB	-2.42	108.61	110.23
33	Y	625	SPH	C3-C4-C5	-2.42	119.40	124.79
28	C	511	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
47	Y	621	LUT	C18-C5-C6	-2.42	121.81	124.53
28	Y	608	CLA	C3B-C4B-NB	-2.42	108.27	110.52
28	b	617	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	b	604	CLA	C2D-C1D-ND	2.41	111.88	110.10
28	S	602	CLA	CHA-C4D-ND	2.41	137.55	132.50
28	Y	611	CLA	CMA-C3A-C4A	2.41	118.26	111.77
30	d	404	BCR	C37-C22-C21	-2.41	119.55	122.92
28	G	613	CLA	C3B-C4B-NB	-2.41	108.28	110.52
38	d	408	LHG	O8-C23-C24	2.41	119.47	111.91
46	S	607	CHL	CHB-C4A-NA	2.41	127.84	124.51
28	Y	603	CLA	CHA-C4D-ND	2.41	137.54	132.50
28	A	405	CLA	C2D-C1D-ND	2.41	111.88	110.10
28	B	614	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
28	N	602	CLA	C4B-CHC-C1C	2.41	132.05	126.34
28	b	608	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
28	Y	610	CLA	CMA-C3A-C4A	2.41	118.24	111.77
46	G	601	CHL	CHB-C4A-NA	2.40	127.84	124.51
28	C	503	CLA	C4B-CHC-C1C	2.40	132.04	126.34
28	c	506	CLA	CHA-C4D-ND	2.40	137.53	132.50
28	N	610	CLA	CMA-C3A-C4A	2.40	118.23	111.77
28	c	503	CLA	C4B-CHC-C1C	2.40	132.04	126.34
28	b	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	620	C7Z	C8-C7-C6	-2.40	120.45	127.20
49	S	623	NEX	C1-C2-C3	2.40	119.07	113.64
28	G	602	CLA	CMC-C2C-C1C	2.40	128.70	125.04
28	N	610	CLA	CHA-C4D-ND	2.40	137.53	132.50
46	Y	601	CHL	C1-O2A-CGA	2.40	122.75	116.44
28	N	614	CLA	CHA-C4D-ND	2.40	137.52	132.50
28	c	509	CLA	C2D-C1D-ND	2.40	111.87	110.10
28	G	603	CLA	C4B-CHC-C1C	2.40	132.03	126.34
28	C	502	CLA	CMA-C3A-C4A	2.40	118.22	111.77
28	b	606	CLA	O2A-CGA-CBA	2.40	119.44	111.91
28	d	402	CLA	CHA-C4D-ND	2.40	137.52	132.50
46	N	609	CHL	C2C-C3C-C4C	2.40	108.20	106.49
28	b	607	CLA	CAA-C2A-C3A	-2.40	106.22	112.78
28	b	603	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
28	S	609	CLA	CHA-C4D-ND	2.40	137.51	132.50
28	G	614	CLA	CHA-C4D-ND	2.39	137.51	132.50
28	C	503	CLA	O2A-CGA-CBA	2.39	119.42	111.91
28	c	511	CLA	O2A-CGA-CBA	2.39	119.42	111.91
30	B	619	BCR	C4-C5-C6	-2.39	119.26	122.73
28	N	614	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
28	S	603	CLA	C4B-CHC-C1C	2.39	132.01	126.34
28	B	606	CLA	C1D-ND-C4D	-2.39	104.64	106.33
28	c	509	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
28	G	612	CLA	C3B-C4B-NB	-2.39	108.30	110.52
28	Y	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
28	a	406	CLA	CHA-C1A-NA	-2.39	120.93	126.40
28	c	511	CLA	CHA-C1A-NA	-2.39	120.93	126.40
28	C	501	CLA	C4B-CHC-C1C	2.39	132.00	126.34
28	S	611	CLA	C3B-C4B-NB	-2.39	108.30	110.52
28	Y	612	CLA	C3B-C4B-NB	-2.39	108.30	110.52
46	G	607	CHL	C4D-CHA-C1A	2.39	124.15	121.25
28	c	505	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
28	Y	603	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
47	G	621	LUT	C10-C11-C12	-2.38	115.78	123.22
28	B	604	CLA	C3B-C4B-NB	-2.38	108.30	110.52
28	c	513	CLA	CHA-C1A-NA	-2.38	120.94	126.40
28	c	509	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
28	c	507	CLA	C3B-C4B-NB	-2.38	108.30	110.52
28	B	604	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
28	A	410	CLA	CHA-C4D-ND	2.38	137.48	132.50
28	C	505	CLA	CHD-C1D-ND	-2.38	122.27	124.45
28	B	617	CLA	C1-O2A-CGA	2.38	122.69	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	503	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
28	A	406	CLA	CHA-C4D-ND	2.38	137.47	132.50
28	D	403	CLA	CHA-C4D-ND	2.38	137.47	132.50
28	b	603	CLA	CHA-C4D-ND	2.38	137.47	132.50
28	C	507	CLA	CHA-C1A-NA	-2.38	120.95	126.40
28	S	613	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
28	N	604	CLA	CMA-C3A-C4A	2.38	118.16	111.77
30	C	517	BCR	C38-C26-C25	-2.38	121.86	124.53
28	D	402	CLA	CAA-CBA-CGA	-2.38	106.31	113.25
46	S	606	CHL	C2B-C1B-NB	-2.38	108.64	110.23
28	S	603	CLA	C3B-C4B-NB	-2.38	108.31	110.52
28	C	508	CLA	CHA-C4D-ND	2.37	137.47	132.50
42	F	101	HEM	C1B-NB-C4B	2.37	107.53	105.07
30	b	618	BCR	C30-C25-C26	-2.37	119.27	122.61
28	Y	613	CLA	C1-C2-C3	-2.37	121.94	126.04
28	B	605	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
46	N	606	CHL	C1-O2A-CGA	2.37	122.67	116.44
28	N	610	CLA	C4B-CHC-C1C	2.37	131.97	126.34
28	S	612	CLA	C4B-CHC-C1C	2.37	131.97	126.34
46	G	601	CHL	C1-C2-C3	-2.37	121.94	126.04
28	C	504	CLA	CHA-C4D-ND	2.37	137.46	132.50
28	G	610	CLA	CHA-C4D-ND	2.37	137.46	132.50
34	b	620	C7Z	C22-C23-C24	2.37	113.55	110.30
28	Y	604	CLA	CMA-C3A-C4A	2.37	118.15	111.77
28	N	611	CLA	C4B-CHC-C1C	2.37	131.96	126.34
28	B	602	CLA	C3B-C4B-NB	-2.37	108.32	110.52
30	c	516	BCR	C37-C22-C21	-2.37	119.60	122.92
28	B	610	CLA	CHA-C4D-ND	2.37	137.46	132.50
28	d	402	CLA	C1D-ND-C4D	-2.37	104.65	106.33
34	b	620	C7Z	C31-C32-C33	-2.37	119.76	126.42
28	B	612	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
28	G	610	CLA	C4B-CHC-C1C	2.37	131.95	126.34
28	Y	614	CLA	C4B-CHC-C1C	2.37	131.95	126.34
46	N	605	CHL	C1-O2A-CGA	2.37	122.66	116.44
28	A	405	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
28	N	611	CLA	C3B-C4B-NB	-2.37	108.32	110.52
28	C	509	CLA	CMA-C3A-C4A	2.37	118.14	111.77
28	G	614	CLA	O2A-CGA-CBA	2.37	119.33	111.91
28	Y	613	CLA	C1-O2A-CGA	2.36	122.64	116.44
28	G	602	CLA	CHA-C4D-ND	2.36	137.44	132.50
28	A	407	CLA	C4B-CHC-C1C	2.36	131.94	126.34
47	G	621	LUT	C31-C30-C29	-2.36	123.94	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	509	CLA	C2D-C1D-ND	2.36	111.84	110.10
31	B	626	SQD	O3-C3-C2	-2.36	104.89	110.35
28	N	602	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
28	c	503	CLA	CHA-C1A-NA	-2.36	120.99	126.40
28	b	605	CLA	C1-C2-C3	-2.36	121.96	126.04
28	A	407	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
28	Y	602	CLA	C4B-CHC-C1C	2.36	131.94	126.34
47	G	620	LUT	C10-C11-C12	-2.36	115.85	123.22
46	Y	601	CHL	C4B-CHC-C1C	2.36	131.93	126.34
28	C	512	CLA	CHD-C1D-ND	-2.36	122.29	124.45
28	S	609	CLA	C3B-C4B-NB	-2.36	108.33	110.52
28	B	606	CLA	O2A-CGA-CBA	2.36	119.30	111.91
48	Y	622	XAT	C6-C7-C8	-2.36	121.01	125.99
28	C	507	CLA	OBD-CAD-C3D	-2.35	122.85	128.52
28	a	407	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
46	G	609	CHL	C3C-C4C-NC	-2.35	107.93	110.57
42	F	101	HEM	C4C-NC-C1C	2.35	107.65	105.35
29	a	408	PHO	C2D-C1D-ND	-2.35	107.90	109.53
28	B	607	CLA	C2D-C1D-ND	2.35	111.84	110.10
42	f	101	HEM	C4C-NC-C1C	2.35	107.65	105.35
28	b	610	CLA	C4B-CHC-C1C	2.35	131.92	126.34
28	b	605	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
28	a	407	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
28	S	614	CLA	C2D-C1D-ND	2.35	111.84	110.10
28	c	503	CLA	CHA-C4D-ND	2.35	137.42	132.50
28	a	410	CLA	C3B-C4B-NB	-2.35	108.33	110.52
28	b	614	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
30	C	514	BCR	C36-C18-C17	-2.35	119.63	122.92
28	S	610	CLA	O2A-CGA-CBA	2.35	119.28	111.91
46	N	609	CHL	CHB-C4A-NA	2.35	127.76	124.51
30	C	514	BCR	C34-C9-C10	-2.35	119.63	122.92
28	S	617	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
28	c	506	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
28	N	602	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	B	612	CLA	CHA-C4D-ND	2.35	137.41	132.50
28	C	506	CLA	O2A-CGA-CBA	2.35	119.27	111.91
30	B	618	BCR	C36-C18-C17	-2.35	119.64	122.92
48	Y	622	XAT	C19-C9-C10	-2.35	119.64	122.92
28	S	602	CLA	C4B-CHC-C1C	2.35	131.90	126.34
28	b	611	CLA	C3D-C2D-C1D	-2.34	102.63	105.83
28	G	603	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
28	B	610	CLA	C1C-C2C-C3C	-2.34	104.49	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	602	CLA	C3B-C4B-NB	-2.34	108.34	110.52
28	b	604	CLA	C3B-C4B-NB	-2.34	108.34	110.52
46	S	601	CHL	C4A-NA-C1A	2.34	107.76	106.71
28	B	607	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
28	b	613	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
46	G	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
49	S	623	NEX	C26-C27-C28	-2.34	121.05	125.99
28	c	507	CLA	CHA-C1A-NA	-2.34	121.04	126.40
30	A	411	BCR	C19-C18-C17	2.34	122.53	118.94
28	B	614	CLA	O2A-CGA-CBA	2.34	119.25	111.91
28	C	504	CLA	C4B-CHC-C1C	2.34	131.88	126.34
28	B	605	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
28	a	405	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
32	h	102	LMG	O1-C1-C2	2.34	111.95	108.30
28	c	510	CLA	O2A-CGA-CBA	2.34	119.24	111.91
28	b	604	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
28	G	611	CLA	C4B-CHC-C1C	2.33	131.88	126.34
28	S	611	CLA	C4B-CHC-C1C	2.33	131.88	126.34
28	S	613	CLA	CMD-C2D-C3D	-2.33	122.24	127.61
30	c	515	BCR	C1-C6-C7	2.33	122.38	115.78
28	b	603	CLA	C3B-C4B-NB	-2.33	108.35	110.52
30	C	515	BCR	C15-C14-C13	-2.33	123.98	127.31
28	b	609	CLA	CMA-C3A-C4A	2.33	118.04	111.77
46	N	607	CHL	C1-C2-C3	-2.33	122.01	126.04
28	A	407	CLA	O2A-CGA-CBA	2.33	119.22	111.91
43	h	101	RRX	C36-C18-C19	2.33	121.75	118.08
28	d	403	CLA	C4B-CHC-C1C	2.33	131.86	126.34
28	C	501	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
46	Y	609	CHL	CHB-C4A-NA	2.33	127.73	124.51
28	a	405	CLA	C4B-CHC-C1C	2.33	131.86	126.34
28	Y	610	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
47	S	620	LUT	C39-C29-C28	2.33	121.74	118.08
30	b	618	BCR	C4-C5-C6	-2.33	119.36	122.73
28	N	614	CLA	C3B-C4B-NB	-2.32	108.36	110.52
49	S	623	NEX	C4-C3-C2	2.32	115.26	110.77
28	b	613	CLA	C4B-CHC-C1C	2.32	131.84	126.34
47	G	621	LUT	C18-C5-C6	-2.32	121.92	124.53
47	S	620	LUT	C30-C31-C32	-2.32	115.98	123.22
34	b	620	C7Z	C2-C3-C4	2.32	113.48	110.30
46	N	606	CHL	C4B-CHC-C1C	2.32	131.84	126.34
31	c	526	SQD	O3-C3-C2	-2.32	104.99	110.35
28	S	602	CLA	C1C-C2C-C3C	-2.32	104.52	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	S	608	CHL	C4A-NA-C1A	2.32	107.75	106.71
28	c	511	CLA	C4B-CHC-C1C	2.32	131.83	126.34
28	C	501	CLA	C1D-ND-C4D	-2.32	104.69	106.33
47	S	621	LUT	C39-C29-C28	2.32	121.73	118.08
42	F	101	HEM	CAD-CBD-CGD	-2.32	108.62	113.60
46	N	606	CHL	C4A-NA-C1A	2.32	107.75	106.71
48	Y	622	XAT	O24-C25-C38	-2.32	112.28	115.06
28	c	513	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
28	d	403	CLA	CHA-C1A-NA	-2.31	121.10	126.40
46	G	606	CHL	C4B-CHC-C1C	2.31	131.83	126.34
32	H	102	LMG	O8-C28-C29	2.31	119.17	111.91
28	Y	614	CLA	C1-C2-C3	-2.31	122.04	126.04
28	S	613	CLA	C3B-C4B-NB	-2.31	108.37	110.52
28	G	604	CLA	C3B-C4B-NB	-2.31	108.37	110.52
28	G	610	CLA	CMA-C3A-C4A	2.31	117.98	111.77
28	c	509	CLA	C4B-CHC-C1C	2.31	131.82	126.34
28	Y	604	CLA	C4B-CHC-C1C	2.31	131.82	126.34
28	B	606	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
28	Y	614	CLA	O2A-CGA-CBA	2.31	119.16	111.91
28	S	612	CLA	C1D-ND-C4D	-2.31	104.69	106.33
31	b	626	SQD	O3-C3-C2	-2.31	105.01	110.35
28	B	615	CLA	C4B-CHC-C1C	2.31	131.81	126.34
28	Y	613	CLA	C4B-CHC-C1C	2.31	131.81	126.34
30	c	516	BCR	C35-C13-C14	-2.31	119.69	122.92
28	C	502	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
28	c	507	CLA	OBD-CAD-C3D	-2.30	122.97	128.52
28	S	614	CLA	O2A-CGA-CBA	2.30	119.14	111.91
28	Y	613	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
28	C	504	CLA	C1D-ND-C4D	-2.30	104.70	106.33
28	a	407	CLA	C1D-ND-C4D	-2.30	104.70	106.33
28	C	507	CLA	C4B-CHC-C1C	2.30	131.80	126.34
28	S	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
28	S	602	CLA	C1D-ND-C4D	-2.30	104.70	106.33
28	D	403	CLA	C4B-CHC-C1C	2.30	131.80	126.34
28	N	604	CLA	C4B-CHC-C1C	2.30	131.80	126.34
28	N	610	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
49	Y	623	NEX	C19-C9-C10	-2.30	119.70	122.92
28	b	602	CLA	C3B-C4B-NB	-2.30	108.38	110.52
28	G	613	CLA	C4B-CHC-C1C	2.30	131.79	126.34
46	G	607	CHL	C3C-C4C-NC	-2.30	107.99	110.57
28	c	501	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
28	B	611	CLA	CHA-C1A-NA	-2.30	121.13	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	G	606	CHL	C2B-C1B-NB	-2.30	108.69	110.23
28	B	615	CLA	CMA-C3A-C4A	2.30	117.95	111.77
30	B	619	BCR	C36-C18-C17	-2.30	119.70	122.92
28	b	616	CLA	C4B-CHC-C1C	2.30	131.79	126.34
49	G	623	NEX	C4-C3-C2	2.30	115.21	110.77
28	G	614	CLA	C4B-CHC-C1C	2.30	131.79	126.34
28	A	410	CLA	C3B-C4B-NB	-2.30	108.39	110.52
35	b	623	DGD	O6D-C5D-C6D	2.30	111.30	106.67
49	S	623	NEX	C20-C13-C14	-2.30	119.71	122.92
41	d	405	PL9	C32-C33-C34	-2.29	122.14	127.66
30	c	517	BCR	C19-C18-C17	2.29	122.46	118.94
28	N	602	CLA	C3B-C4B-NB	-2.29	108.39	110.52
31	M	101	SQD	O3-C3-C2	-2.29	105.05	110.35
28	a	406	CLA	C4B-CHC-C1C	2.29	131.78	126.34
31	C	526	SQD	O3-C3-C2	-2.29	105.05	110.35
28	N	613	CLA	C4B-CHC-C1C	2.29	131.78	126.34
28	d	403	CLA	C3B-C4B-NB	-2.29	108.39	110.52
28	C	504	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
28	B	616	CLA	CHA-C1A-NA	-2.29	121.15	126.40
28	S	609	CLA	C4B-CHC-C1C	2.29	131.77	126.34
28	S	605	CLA	C4B-CHC-C1C	2.29	131.77	126.34
28	b	605	CLA	C4B-CHC-C1C	2.29	131.77	126.34
28	b	607	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
28	Y	603	CLA	C1D-ND-C4D	-2.29	104.71	106.33
28	Y	608	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
28	Y	602	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
31	m	101	SQD	O3-C3-C2	-2.29	105.06	110.35
28	b	612	CLA	CHA-C4D-ND	2.29	137.29	132.50
31	b	621	SQD	O3-C3-C2	-2.29	105.06	110.35
28	Y	611	CLA	C4B-CHC-C1C	2.29	131.76	126.34
28	C	513	CLA	CHA-C4D-ND	2.29	137.28	132.50
28	B	616	CLA	C4B-CHC-C1C	2.29	131.76	126.34
28	a	406	CLA	C2A-C1A-CHA	2.29	127.86	123.86
28	b	616	CLA	C1-O2A-CGA	2.29	122.44	116.44
28	b	615	CLA	C4B-CHC-C1C	2.29	131.76	126.34
28	a	405	CLA	C2C-C1C-NC	2.29	112.11	109.97
31	a	412	SQD	O3-C3-C2	-2.28	105.07	110.35
28	c	513	CLA	C4B-CHC-C1C	2.28	131.76	126.34
28	B	603	CLA	C4B-CHC-C1C	2.28	131.75	126.34
29	A	408	PHO	C2D-C1D-ND	-2.28	107.95	109.53
28	N	603	CLA	C4B-CHC-C1C	2.28	131.75	126.34
28	b	603	CLA	CAA-C2A-C3A	-2.28	106.53	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	610	CLA	C1D-ND-C4D	-2.28	104.71	106.33
28	Y	608	CLA	CHA-C1A-NA	-2.28	121.17	126.40
48	N	622	XAT	C18-C5-C6	-2.28	118.44	122.26
28	N	614	CLA	CHA-C1A-NA	-2.28	121.17	126.40
28	b	614	CLA	C4B-CHC-C1C	2.28	131.75	126.34
28	D	403	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
28	S	614	CLA	CHA-C1A-NA	-2.28	121.18	126.40
46	N	601	CHL	C2B-C1B-NB	-2.28	108.70	110.23
28	A	406	CLA	O2A-CGA-CBA	2.28	119.06	111.91
28	B	612	CLA	C4B-CHC-C1C	2.28	131.74	126.34
28	N	612	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
28	b	602	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
28	b	603	CLA	C4B-CHC-C1C	2.28	131.74	126.34
28	S	614	CLA	C3B-C4B-NB	-2.28	108.40	110.52
28	c	503	CLA	C1D-ND-C4D	-2.28	104.72	106.33
28	S	602	CLA	C3B-C4B-NB	-2.28	108.40	110.52
43	h	101	RRX	C20-C21-C22	2.27	130.56	127.31
46	Y	606	CHL	C4D-CHA-C1A	2.27	124.02	121.25
47	Y	621	LUT	C10-C11-C12	-2.27	116.12	123.22
49	Y	623	NEX	C26-C27-C28	-2.27	121.19	125.99
28	C	502	CLA	C4B-CHC-C1C	2.27	131.73	126.34
41	D	405	PL9	C20-C19-C21	2.27	119.09	115.27
28	B	609	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
28	C	504	CLA	C1-O2A-CGA	2.27	122.40	116.44
28	S	604	CLA	C1-C2-C3	-2.27	122.11	126.04
48	G	622	XAT	O4-C5-C18	-2.27	112.33	115.06
28	Y	603	CLA	C4B-CHC-C1C	2.27	131.72	126.34
28	C	511	CLA	CHA-C1A-NA	-2.27	121.20	126.40
30	c	514	BCR	C34-C9-C10	-2.27	119.74	122.92
43	H	101	RRX	C35-C13-C14	-2.27	119.74	122.92
28	N	604	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
28	Y	613	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
28	N	612	CLA	CHA-C1A-NA	-2.27	121.20	126.40
28	c	503	CLA	C3B-C4B-NB	-2.27	108.41	110.52
28	c	506	CLA	O2A-CGA-CBA	2.27	119.03	111.91
28	b	603	CLA	O2A-CGA-CBA	2.27	119.03	111.91
46	Y	609	CHL	C2B-C1B-NB	-2.27	108.71	110.23
28	b	602	CLA	C4B-CHC-C1C	2.27	131.72	126.34
28	G	612	CLA	CMA-C3A-C4A	2.27	117.87	111.77
28	b	611	CLA	O2A-CGA-CBA	2.27	119.02	111.91
28	b	608	CLA	C4B-CHC-C1C	2.27	131.71	126.34
28	S	605	CLA	C3B-C4B-NB	-2.27	108.41	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	N	601	CHL	C1-O2A-CGA	2.27	122.39	116.44
28	A	410	CLA	C4B-CHC-C1C	2.26	131.71	126.34
28	N	610	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
38	c	525	LHG	C5-O7-C7	-2.26	112.22	117.79
28	G	614	CLA	CAA-C2A-C3A	-2.26	106.58	112.78
30	B	619	BCR	C34-C9-C10	-2.26	119.75	122.92
28	b	604	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
46	G	607	CHL	CHC-C1C-NC	2.26	127.64	124.20
28	G	610	CLA	C1D-ND-C4D	-2.26	104.73	106.33
30	D	404	BCR	C37-C22-C21	-2.26	119.75	122.92
28	C	509	CLA	C4B-CHC-C1C	2.26	131.70	126.34
28	C	512	CLA	C4B-CHC-C1C	2.26	131.70	126.34
28	B	608	CLA	O2A-CGA-CBA	2.26	119.00	111.91
28	b	605	CLA	C2D-C1D-ND	2.26	111.77	110.10
28	a	406	CLA	O2A-CGA-CBA	2.26	119.00	111.91
30	b	618	BCR	C23-C24-C25	-2.26	120.86	127.20
28	b	617	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
32	c	523	LMG	C8-O7-C10	-2.26	112.23	117.79
28	S	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
28	Y	612	CLA	CHA-C1A-NA	-2.26	121.23	126.40
28	C	501	CLA	O2A-CGA-CBA	2.26	118.99	111.91
28	B	603	CLA	C3B-C4B-NB	-2.26	108.42	110.52
31	B	621	SQD	O3-C3-C2	-2.26	105.13	110.35
28	b	606	CLA	CMA-C3A-C4A	2.26	117.84	111.77
28	C	511	CLA	C4B-CHC-C1C	2.26	131.69	126.34
30	B	618	BCR	C8-C7-C6	-2.26	120.87	127.20
28	b	611	CLA	CHA-C1A-NA	-2.26	121.23	126.40
31	A	412	SQD	O3-C3-C2	-2.26	105.13	110.35
28	Y	604	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
46	S	608	CHL	C2B-C1B-NB	-2.25	108.72	110.23
49	S	623	NEX	C17-C1-C6	-2.25	108.45	110.47
28	c	506	CLA	C4B-CHC-C1C	2.25	131.68	126.34
28	a	406	CLA	C2D-C1D-ND	2.25	111.76	110.10
28	G	613	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
28	c	513	CLA	C1D-ND-C4D	-2.25	104.73	106.33
28	C	503	CLA	CHA-C1A-NA	-2.25	121.24	126.40
28	G	604	CLA	C4B-CHC-C1C	2.25	131.68	126.34
28	Y	612	CLA	C4B-CHC-C1C	2.25	131.68	126.34
28	B	604	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
28	B	617	CLA	CHD-C1D-ND	-2.25	122.39	124.45
28	c	512	CLA	C4B-CHC-C1C	2.25	131.68	126.34
30	C	514	BCR	C33-C5-C4	2.25	117.94	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	604	CLA	C4B-CHC-C1C	2.25	131.68	126.34
28	S	613	CLA	C4B-CHC-C1C	2.25	131.67	126.34
28	c	502	CLA	C4B-CHC-C1C	2.25	131.67	126.34
28	c	504	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
41	D	405	PL9	C27-C28-C29	-2.25	122.24	127.66
42	f	101	HEM	C1B-NB-C4B	2.25	107.40	105.07
28	b	608	CLA	O2A-CGA-CBA	2.25	118.97	111.91
28	c	504	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
28	a	410	CLA	C4B-CHC-C1C	2.25	131.67	126.34
28	C	511	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
28	G	604	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
28	C	503	CLA	C3B-C4B-NB	-2.25	108.43	110.52
28	d	403	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
28	A	405	CLA	C4B-CHC-C1C	2.25	131.67	126.34
28	G	610	CLA	C3B-C4B-NB	-2.25	108.43	110.52
28	S	617	CLA	C3B-C4B-NB	-2.25	108.43	110.52
28	G	611	CLA	C2D-C1D-ND	2.25	111.76	110.10
28	G	614	CLA	C1D-ND-C4D	-2.25	104.74	106.33
28	C	508	CLA	C4B-CHC-C1C	2.25	131.66	126.34
43	H	101	RRX	C2-C1-C6	2.24	113.94	110.48
28	S	614	CLA	C4B-CHC-C1C	2.24	131.66	126.34
28	N	613	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
28	b	609	CLA	C4B-CHC-C1C	2.24	131.66	126.34
46	Y	609	CHL	C4D-CHA-C1A	2.24	123.98	121.25
28	d	403	CLA	CMA-C3A-C2A	2.24	122.87	113.83
28	N	614	CLA	C4B-CHC-C1C	2.24	131.65	126.34
28	c	508	CLA	CAC-C3C-C4C	2.24	127.72	124.81
28	N	613	CLA	C3B-C4B-NB	-2.24	108.44	110.52
47	S	621	LUT	C31-C32-C33	-2.24	120.13	126.42
48	Y	622	XAT	C40-C33-C34	-2.24	119.79	122.92
43	h	101	RRX	C19-C18-C17	-2.24	115.51	118.94
28	B	614	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
28	b	617	CLA	C4B-CHC-C1C	2.24	131.64	126.34
28	N	614	CLA	C1D-ND-C4D	-2.24	104.75	106.33
28	c	510	CLA	C3B-C4B-NB	-2.23	108.44	110.52
28	b	603	CLA	C1D-ND-C4D	-2.23	104.75	106.33
28	c	513	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
28	B	605	CLA	C2D-C1D-ND	2.23	111.75	110.10
29	A	408	PHO	C1C-C2C-C3C	-2.23	106.75	108.61
28	b	616	CLA	CHA-C1A-NA	-2.23	121.28	126.40
28	c	505	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
28	b	602	CLA	CMD-C2D-C3D	-2.23	122.48	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	502	CLA	CHA-C1A-NA	-2.23	121.29	126.40
28	C	503	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
28	B	611	CLA	O2A-CGA-CBA	2.23	118.90	111.91
28	b	616	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
28	Y	604	CLA	C3B-C4B-NB	-2.23	108.45	110.52
28	C	513	CLA	CHA-C1A-NA	-2.23	121.30	126.40
28	c	503	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
28	c	511	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
28	D	402	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
30	c	514	BCR	C37-C22-C21	-2.23	119.81	122.92
28	b	616	CLA	CMA-C3A-C4A	2.23	117.75	111.77
28	a	410	CLA	CHA-C1A-NA	-2.23	121.30	126.40
47	N	620	LUT	C10-C11-C12	-2.23	116.27	123.22
28	C	509	CLA	C1-C2-C3	-2.22	122.19	126.04
30	b	619	BCR	C34-C9-C10	-2.22	119.81	122.92
28	N	604	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
28	C	506	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
28	S	617	CLA	C4B-CHC-C1C	2.22	131.61	126.34
28	B	608	CLA	C4B-CHC-C1C	2.22	131.61	126.34
28	b	602	CLA	CHA-C1A-NA	-2.22	121.31	126.40
28	G	612	CLA	CHA-C1A-NA	-2.22	121.31	126.40
28	b	614	CLA	CHA-C1A-NA	-2.22	121.31	126.40
28	S	605	CLA	CHA-C1A-NA	-2.22	121.31	126.40
28	B	604	CLA	C2D-C1D-ND	2.22	111.74	110.10
46	N	607	CHL	C4A-NA-C1A	2.22	107.70	106.71
41	D	405	PL9	C40-C39-C41	2.22	119.00	115.27
28	c	508	CLA	CHA-C4D-ND	2.22	137.14	132.50
30	A	411	BCR	C34-C9-C10	-2.22	119.81	122.92
28	S	604	CLA	C4B-CHC-C1C	2.22	131.60	126.34
28	B	610	CLA	C4B-CHC-C1C	2.22	131.60	126.34
28	c	501	CLA	O2A-CGA-CBA	2.22	118.86	111.91
28	B	605	CLA	CHA-C1A-NA	-2.22	121.32	126.40
28	B	610	CLA	CHA-C1A-NA	-2.22	121.32	126.40
28	N	603	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
28	N	610	CLA	C1D-ND-C4D	-2.21	104.76	106.33
28	B	602	CLA	O2A-CGA-CBA	2.21	118.86	111.91
28	c	510	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
28	S	603	CLA	CHA-C1A-NA	-2.21	121.33	126.40
28	G	603	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
28	B	615	CLA	C2D-C1D-ND	2.21	111.73	110.10
28	c	501	CLA	C1D-ND-C4D	-2.21	104.76	106.33
28	C	510	CLA	O2A-CGA-CBA	2.21	118.85	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y	610	CLA	C3B-C4B-NB	-2.21	108.47	110.52
28	a	407	CLA	CHA-C1A-NA	-2.21	121.34	126.40
28	D	402	CLA	CHD-C1D-ND	-2.21	122.42	124.45
28	b	611	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
28	c	511	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
28	S	611	CLA	CHA-C1A-NA	-2.21	121.34	126.40
28	Y	604	CLA	O2A-CGA-CBA	2.21	118.83	111.91
41	d	405	PL9	C26-C24-C23	-2.21	116.65	121.12
28	N	604	CLA	C3B-C4B-NB	-2.21	108.47	110.52
46	G	609	CHL	CHB-C4A-NA	2.20	127.56	124.51
46	G	605	CHL	C2B-C1B-NB	-2.20	108.75	110.23
28	A	407	CLA	C3B-C4B-NB	-2.20	108.47	110.52
35	B	623	DGD	O2G-C1B-O1B	-2.20	118.38	123.70
28	G	612	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
28	B	617	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
42	f	101	HEM	CMC-C2C-C1C	-2.20	120.84	124.71
34	b	620	C7Z	C20-C13-C14	-2.20	119.84	122.92
28	c	502	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
28	B	607	CLA	C4B-CHC-C1C	2.20	131.55	126.34
30	c	516	BCR	C38-C26-C25	-2.20	122.06	124.53
28	G	611	CLA	O2A-CGA-CBA	2.20	118.80	111.91
28	Y	602	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
28	b	613	CLA	CHA-C1A-NA	-2.20	121.37	126.40
28	A	405	CLA	CHA-C1A-NA	-2.20	121.37	126.40
28	b	607	CLA	C4B-CHC-C1C	2.20	131.55	126.34
28	B	617	CLA	C4B-CHC-C1C	2.20	131.55	126.34
28	B	605	CLA	C4B-CHC-C1C	2.20	131.54	126.34
28	b	608	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
28	G	603	CLA	C1D-ND-C4D	-2.19	104.78	106.33
28	B	608	CLA	C2D-C1D-ND	2.19	111.72	110.10
28	c	508	CLA	C3B-C4B-NB	-2.19	108.48	110.52
28	b	606	CLA	C4B-CHC-C1C	2.19	131.54	126.34
28	N	602	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
51	Y	627	PTY	C6-O7-C8	-2.19	113.81	117.90
28	C	507	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
28	C	512	CLA	C1-O2A-CGA	2.19	122.19	116.44
28	G	611	CLA	CHA-C1A-NA	-2.19	121.38	126.40
28	G	604	CLA	OBD-CAD-C3D	-2.19	123.25	128.52
28	b	605	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
28	Y	603	CLA	O2A-CGA-CBA	2.19	118.78	111.91
28	B	614	CLA	C1D-ND-C4D	-2.19	104.78	106.33
28	b	612	CLA	C4B-CHC-C1C	2.19	131.53	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	606	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
47	S	621	LUT	C10-C11-C12	-2.19	116.39	123.22
28	D	402	CLA	CMC-C2C-C1C	2.19	128.37	125.04
28	Y	608	CLA	C4B-CHC-C1C	2.19	131.53	126.34
30	C	516	BCR	C8-C9-C10	2.19	122.30	118.94
46	G	601	CHL	C4D-CHA-C1A	2.19	123.91	121.25
28	B	614	CLA	C4B-CHC-C1C	2.19	131.52	126.34
28	N	611	CLA	CHA-C1A-NA	-2.19	121.39	126.40
49	N	623	NEX	C31-C30-C29	2.19	130.43	127.31
40	D	401	BCT	O3-C-O1	-2.18	113.88	119.55
28	A	406	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
28	Y	608	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
49	N	623	NEX	C20-C13-C14	-2.18	119.86	122.92
28	b	605	CLA	C3B-C4B-NB	-2.18	108.49	110.52
46	Y	609	CHL	CHD-C4C-C3C	2.18	128.05	124.84
28	b	610	CLA	C1D-ND-C4D	-2.18	104.78	106.33
28	c	510	CLA	C4B-CHC-C1C	2.18	131.51	126.34
30	c	514	BCR	C33-C5-C4	2.18	117.81	113.62
28	b	617	CLA	C1-O2A-CGA	2.18	122.17	116.44
28	b	604	CLA	C4B-CHC-C1C	2.18	131.51	126.34
30	D	404	BCR	C33-C5-C6	-2.18	122.08	124.53
28	S	613	CLA	C1D-ND-C4D	-2.18	104.79	106.33
28	N	611	CLA	O2A-CGA-CBA	2.18	118.74	111.91
28	B	607	CLA	CMA-C3A-C4A	2.18	117.63	111.77
28	N	611	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
28	B	614	CLA	CHA-C1A-NA	-2.18	121.42	126.40
28	G	614	CLA	C3B-C4B-NB	-2.18	108.50	110.52
28	b	615	CLA	C3B-C4B-NB	-2.18	108.50	110.52
28	A	406	CLA	C4B-CHC-C1C	2.17	131.49	126.34
28	G	611	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
28	G	602	CLA	O2A-CGA-CBA	2.17	118.72	111.91
28	N	613	CLA	C1D-ND-C4D	-2.17	104.79	106.33
28	S	613	CLA	C1-O2A-CGA	2.17	122.14	116.44
34	b	620	C7Z	C1-C6-C7	2.17	121.92	115.78
30	C	515	BCR	C38-C26-C25	-2.17	122.09	124.53
30	d	404	BCR	C30-C25-C24	2.17	121.92	115.78
28	B	609	CLA	C1D-ND-C4D	-2.17	104.79	106.33
28	B	603	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
28	B	607	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
28	c	505	CLA	C3B-C4B-NB	-2.17	108.50	110.52
46	Y	606	CHL	CHB-C4A-NA	2.17	127.51	124.51
28	S	617	CLA	CHA-C1A-NA	-2.17	121.43	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	612	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
28	B	607	CLA	C3B-C4B-NB	-2.17	108.50	110.52
28	B	602	CLA	CHA-C1A-NA	-2.17	121.44	126.40
28	b	603	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
28	S	604	CLA	CMA-C3A-C4A	2.17	117.59	111.77
28	C	502	CLA	CHA-C1A-NA	-2.17	121.44	126.40
28	c	504	CLA	CHA-C1A-NA	-2.17	121.44	126.40
28	C	505	CLA	C1-O2A-CGA	2.17	122.12	116.44
30	d	404	BCR	C34-C9-C10	-2.17	119.89	122.92
28	G	604	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
28	C	506	CLA	C2D-C1D-ND	2.16	111.70	110.10
28	b	609	CLA	CHA-C1A-NA	-2.16	121.44	126.40
28	Y	614	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
28	S	612	CLA	CHA-C1A-NA	-2.16	121.44	126.40
34	B	620	C7Z	C4-C5-C6	-2.16	116.03	120.85
30	C	517	BCR	C31-C1-C6	-2.16	106.79	110.30
28	S	610	CLA	CHA-C1A-NA	-2.16	121.44	126.40
28	a	405	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
28	G	603	CLA	C3B-C4B-NB	-2.16	108.51	110.52
28	c	504	CLA	C3B-C4B-NB	-2.16	108.51	110.52
28	B	617	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
28	c	502	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
28	c	505	CLA	C4B-CHC-C1C	2.16	131.47	126.34
28	Y	613	CLA	C1D-ND-C4D	-2.16	104.80	106.33
28	c	503	CLA	O2A-CGA-CBA	2.16	118.69	111.91
30	c	517	BCR	C38-C26-C27	2.16	117.77	113.62
28	c	510	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
48	N	622	XAT	C39-C29-C30	-2.16	119.90	122.92
43	H	101	RRX	C19-C18-C17	-2.16	115.63	118.94
28	A	407	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
35	b	623	DGD	C4D-C3D-C2D	2.16	114.59	110.82
28	C	501	CLA	CHA-C1A-NA	-2.16	121.45	126.40
28	b	607	CLA	CHA-C1A-NA	-2.16	121.45	126.40
41	D	405	PL9	O1-C4-C3	-2.16	118.34	120.72
28	B	609	CLA	C4B-CHC-C1C	2.16	131.46	126.34
38	d	410	LHG	C5-O7-C7	-2.16	112.48	117.79
28	b	614	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
28	Y	611	CLA	C3B-C4B-NB	-2.16	108.51	110.52
28	S	610	CLA	C1D-ND-C4D	-2.16	104.80	106.33
28	B	606	CLA	C4B-CHC-C1C	2.16	131.45	126.34
28	B	603	CLA	CHA-C1A-NA	-2.16	121.46	126.40
28	c	513	CLA	C2A-C1A-CHA	2.16	127.63	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Y	622	XAT	C26-C27-C28	-2.16	121.44	125.99
28	B	602	CLA	C1D-ND-C4D	-2.16	104.80	106.33
28	N	603	CLA	CHA-C1A-NA	-2.15	121.46	126.40
28	c	509	CLA	CHA-C1A-NA	-2.15	121.46	126.40
28	C	506	CLA	CHA-C1A-NA	-2.15	121.47	126.40
28	N	604	CLA	CHA-C1A-NA	-2.15	121.47	126.40
38	S	624	LHG	C5-O7-C7	-2.15	112.49	117.79
41	D	405	PL9	C31-C32-C33	-2.15	104.81	111.88
34	b	620	C7Z	C8-C7-C6	-2.15	121.16	127.20
28	b	616	CLA	C1D-ND-C4D	-2.15	104.81	106.33
28	c	506	CLA	CHA-C1A-NA	-2.15	121.47	126.40
28	c	512	CLA	CHA-C1A-NA	-2.15	121.47	126.40
49	N	623	NEX	C40-C33-C34	-2.15	119.91	122.92
48	G	622	XAT	C19-C9-C10	-2.15	119.91	122.92
28	S	610	CLA	C1C-C2C-C3C	-2.15	104.69	106.96
28	S	610	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
28	C	508	CLA	CAC-C3C-C4C	2.15	127.60	124.81
28	N	611	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
28	b	617	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
28	c	505	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
28	B	614	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
28	c	508	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
28	C	513	CLA	C4B-CHC-C1C	2.15	131.43	126.34
28	Y	603	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
38	N	624	LHG	C5-O7-C7	-2.15	112.51	117.79
28	S	609	CLA	C1D-ND-C4D	-2.15	104.81	106.33
28	d	402	CLA	CMA-C3A-C4A	2.14	117.54	111.77
28	B	602	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
28	Y	611	CLA	CHA-C1A-NA	-2.14	121.49	126.40
46	S	607	CHL	C4D-CHA-C1A	2.14	123.86	121.25
30	c	514	BCR	C23-C24-C25	-2.14	121.18	127.20
28	Y	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
28	G	614	CLA	CHA-C1A-NA	-2.14	121.49	126.40
28	c	510	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
28	a	405	CLA	CMC-C2C-C1C	2.14	128.30	125.04
28	C	508	CLA	C3B-C4B-NB	-2.14	108.53	110.52
46	G	605	CHL	C1-O2A-CGA	2.14	122.95	116.73
28	c	501	CLA	CHA-C1A-NA	-2.14	121.50	126.40
28	B	604	CLA	CHA-C1A-NA	-2.14	121.50	126.40
46	N	608	CHL	C4A-NA-C1A	2.14	107.67	106.71
30	B	619	BCR	C27-C26-C25	-2.14	119.63	122.73
28	b	610	CLA	CMD-C2D-C3D	-2.14	122.70	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Y	622	XAT	O4-C5-C4	-2.14	111.78	113.38
28	Y	610	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
28	b	612	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
41	d	405	PL9	C36-C34-C33	-2.13	116.80	121.12
38	L	101	LHG	C5-O7-C7	-2.13	112.54	117.79
28	B	617	CLA	CHA-C1A-NA	-2.13	121.51	126.40
28	b	615	CLA	CMA-C3A-C4A	2.13	117.51	111.77
28	C	512	CLA	CHA-C1A-NA	-2.13	121.51	126.40
28	Y	608	CLA	O2A-CGA-CBA	2.13	118.60	111.91
46	N	609	CHL	C1-C2-C3	-2.13	122.36	126.04
28	b	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	S	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	C	506	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
28	Y	614	CLA	C1D-ND-C4D	-2.13	104.82	106.33
28	S	609	CLA	CHA-C1A-NA	-2.13	121.52	126.40
28	N	614	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
28	A	405	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
46	N	608	CHL	C3B-C4B-NB	-2.13	108.54	110.52
28	C	508	CLA	O2A-CGA-CBA	2.13	118.59	111.91
30	D	404	BCR	C4-C5-C6	-2.13	119.64	122.73
28	C	512	CLA	C1-C2-C3	-2.13	122.36	126.04
28	N	612	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
46	N	601	CHL	C4D-CHA-C1A	2.13	123.84	121.25
28	b	606	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
28	C	513	CLA	C1D-ND-C4D	-2.13	104.82	106.33
28	c	509	CLA	O2A-CGA-CBA	2.13	118.59	111.91
28	G	613	CLA	CHA-C1A-NA	-2.13	121.53	126.40
28	Y	611	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
28	C	510	CLA	C4B-CHC-C1C	2.13	131.38	126.34
28	G	603	CLA	O2A-CGA-CBA	2.13	118.58	111.91
46	S	601	CHL	C4D-CHA-C1A	2.13	123.84	121.25
33	A	414	SPH	C3-C4-C5	-2.13	120.05	124.79
28	S	609	CLA	C1-C2-C3	-2.13	122.37	126.04
28	B	613	CLA	C4B-CHC-C1C	2.12	131.37	126.34
28	B	603	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
28	B	617	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
29	A	408	PHO	C1-C2-C3	-2.12	122.37	126.04
28	B	603	CLA	C1D-ND-C4D	-2.12	104.83	106.33
28	Y	604	CLA	C1D-ND-C4D	-2.12	104.83	106.33
28	c	511	CLA	C1D-ND-C4D	-2.12	104.83	106.33
34	b	620	C7Z	C38-C25-C24	2.12	118.28	114.36
34	b	620	C7Z	C11-C12-C13	-2.12	120.46	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	614	CLA	CMA-C3A-C4A	2.12	117.47	111.77
28	N	613	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
28	C	507	CLA	C1-C2-C3	-2.12	122.38	126.04
48	Y	622	XAT	O4-C5-C18	-2.12	112.52	115.06
28	S	610	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
28	N	612	CLA	CMA-C3A-C4A	2.12	117.47	111.77
28	c	512	CLA	C1-O2A-CGA	2.12	122.01	116.44
28	a	405	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
41	D	405	PL9	O2-C1-C6	2.12	124.26	120.59
28	Y	603	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
28	b	614	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
41	d	405	PL9	O2-C1-C6	2.12	124.26	120.59
28	A	405	CLA	CAC-C3C-C4C	2.12	127.56	124.81
28	S	602	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
28	C	508	CLA	CHA-C1A-NA	-2.12	121.55	126.40
28	C	505	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
28	C	506	CLA	C4B-CHC-C1C	2.12	131.36	126.34
28	c	512	CLA	C2A-C1A-CHA	2.12	127.56	123.86
28	Y	602	CLA	C1D-ND-C4D	-2.12	104.83	106.33
28	b	614	CLA	O2A-CGA-CBA	2.12	118.55	111.91
30	b	618	BCR	C29-C28-C27	2.11	116.10	111.38
28	N	610	CLA	CHA-C1A-NA	-2.11	121.56	126.40
28	a	407	CLA	C4B-CHC-C1C	2.11	131.34	126.34
28	G	610	CLA	C6-C5-C3	-2.11	107.92	113.45
28	N	604	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
46	G	601	CHL	CHD-C4C-C3C	2.11	127.94	124.84
28	C	504	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
28	G	603	CLA	CHA-C1A-NA	-2.11	121.57	126.40
28	B	612	CLA	C1D-ND-C4D	-2.11	104.84	106.33
28	Y	614	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
43	h	101	RRX	C16-C15-C14	-2.11	119.16	123.47
28	G	610	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
28	C	511	CLA	C3B-C4B-NB	-2.11	108.56	110.52
46	G	608	CHL	C4D-CHA-C1A	2.11	123.81	121.25
28	S	602	CLA	CHA-C1A-NA	-2.11	121.58	126.40
28	D	402	CLA	CHA-C1A-NA	-2.10	121.58	126.40
28	B	615	CLA	CHA-C1A-NA	-2.10	121.58	126.40
28	G	602	CLA	C3B-C4B-NB	-2.10	108.56	110.52
28	S	604	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
28	N	610	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
28	Y	614	CLA	CHA-C1A-NA	-2.10	121.58	126.40
28	B	604	CLA	O1D-CGD-CBD	-2.10	120.18	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	612	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
28	a	410	CLA	C3B-C2B-C1B	-2.10	104.62	107.16
28	c	508	CLA	O2A-CGA-CBA	2.10	118.50	111.91
28	b	613	CLA	C1D-ND-C4D	-2.10	104.84	106.33
28	C	505	CLA	CHA-C1A-NA	-2.10	121.59	126.40
28	N	610	CLA	O2A-CGA-CBA	2.10	118.49	111.91
30	b	619	BCR	C1-C6-C5	-2.10	119.66	122.61
46	S	601	CHL	C2B-C1B-NB	-2.10	108.83	110.23
28	S	611	CLA	O2A-CGA-CBA	2.10	118.49	111.91
28	A	407	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
28	c	503	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
28	b	610	CLA	CHA-C1A-NA	-2.10	121.60	126.40
28	a	405	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
28	b	617	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
28	b	608	CLA	CHA-C1A-NA	-2.09	121.60	126.40
28	c	513	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
30	D	404	BCR	C30-C25-C24	2.09	121.70	115.78
30	b	618	BCR	C37-C22-C21	-2.09	119.99	122.92
46	S	606	CHL	C4D-CHA-C1A	2.09	123.80	121.25
30	C	517	BCR	C34-C9-C10	-2.09	119.99	122.92
28	N	604	CLA	O2A-CGA-CBA	2.09	118.47	111.91
30	a	411	BCR	C40-C30-C25	-2.09	106.91	110.30
28	G	610	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
28	S	610	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
28	B	613	CLA	C2D-C1D-ND	2.09	111.64	110.10
28	S	610	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
28	C	511	CLA	C1D-ND-C4D	-2.09	104.85	106.33
28	C	501	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
28	a	405	CLA	OBD-CAD-C3D	-2.09	123.50	128.52
28	N	602	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
28	Y	610	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
28	B	608	CLA	CHA-C1A-NA	-2.09	121.62	126.40
30	a	411	BCR	C4-C5-C6	-2.09	119.70	122.73
47	S	620	LUT	C20-C13-C12	2.09	121.36	118.08
38	D	409	LHG	C5-O7-C7	-2.09	112.66	117.79
28	b	608	CLA	C1-O2A-CGA	2.09	121.92	116.44
46	Y	606	CHL	C1-O2A-CGA	2.09	121.92	116.44
28	S	613	CLA	CHA-C1A-NA	-2.08	121.62	126.40
28	B	605	CLA	CAA-CBA-CGA	-2.08	107.16	113.25
28	b	615	CLA	C1-O2A-CGA	2.08	121.91	116.44
30	B	619	BCR	C8-C7-C6	-2.08	121.35	127.20
28	b	610	CLA	C3D-C2D-C1D	-2.08	102.99	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	609	CLA	O2A-CGA-CBA	2.08	118.45	111.91
28	c	507	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
28	D	403	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	c	515	BCR	C36-C18-C17	-2.08	120.00	122.92
28	G	610	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
28	G	602	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	a	409	PHO	C1-C2-C3	-2.08	122.44	126.04
46	N	609	CHL	CHD-C4C-C3C	2.08	127.90	124.84
46	G	601	CHL	C2B-C1B-NB	-2.08	108.84	110.23
28	b	617	CLA	CHA-C1A-NA	-2.08	121.63	126.40
28	C	505	CLA	C4B-CHC-C1C	2.08	131.27	126.34
30	a	411	BCR	C35-C13-C12	2.08	121.35	118.08
28	G	613	CLA	C1D-ND-C4D	-2.08	104.86	106.33
41	d	405	PL9	C37-C38-C39	-2.08	122.66	127.66
28	C	507	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
46	Y	607	CHL	C1-C2-C3	-2.08	122.45	126.04
32	a	413	LMG	C8-O7-C10	-2.08	112.68	117.79
28	A	410	CLA	CHA-C1A-NA	-2.08	121.64	126.40
28	Y	602	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
28	A	407	CLA	CHA-C1A-NA	-2.08	121.64	126.40
28	C	510	CLA	C3B-C4B-NB	-2.08	108.59	110.52
28	b	604	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
28	c	513	CLA	C3B-C4B-NB	-2.07	108.59	110.52
28	b	603	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
28	b	613	CLA	O2A-CGA-CBA	2.07	118.41	111.91
28	B	613	CLA	CHA-C1A-NA	-2.07	121.65	126.40
28	A	406	CLA	CHA-C1A-NA	-2.07	121.65	126.40
46	N	601	CHL	C4A-NA-C1A	2.07	107.64	106.71
28	b	616	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
28	A	407	CLA	C1D-ND-C4D	-2.07	104.86	106.33
48	G	622	XAT	C20-C13-C14	-2.07	120.02	122.92
46	N	609	CHL	CHC-C1C-NC	2.07	127.34	124.20
28	C	507	CLA	C3B-C4B-NB	-2.07	108.59	110.52
28	C	508	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
28	Y	612	CLA	C1D-ND-C4D	-2.07	104.86	106.33
46	S	607	CHL	C2B-C1B-NB	-2.07	108.85	110.23
28	C	504	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
30	B	619	BCR	C38-C26-C27	2.07	117.59	113.62
28	d	402	CLA	CHA-C1A-NA	-2.07	121.66	126.40
41	d	405	PL9	O2-C1-C2	-2.07	117.05	121.78
28	Y	611	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
29	A	409	PHO	C1-C2-C3	-2.07	122.47	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	d	405	PL9	O1-C4-C3	-2.07	118.44	120.72
28	N	613	CLA	CHA-C1A-NA	-2.07	121.67	126.40
28	Y	612	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
28	A	410	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
30	C	516	BCR	C19-C18-C17	2.06	122.11	118.94
28	N	614	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
28	B	617	CLA	O2A-CGA-CBA	2.06	118.38	111.91
28	G	604	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
28	B	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
28	b	615	CLA	C1D-ND-C4D	-2.06	104.87	106.33
28	C	509	CLA	O2A-CGA-CBA	2.06	118.38	111.91
28	B	610	CLA	C3B-C4B-NB	-2.06	108.60	110.52
47	Y	621	LUT	C16-C1-C6	-2.06	106.95	110.30
28	a	407	CLA	O2A-CGA-CBA	2.06	118.38	111.91
28	B	608	CLA	C3B-C4B-NB	-2.06	108.60	110.52
32	A	413	LMG	O7-C10-O9	-2.06	118.72	123.70
46	S	608	CHL	C1-C2-C3	-2.06	122.48	126.04
28	B	612	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
28	G	611	CLA	C3B-C4B-NB	-2.06	108.61	110.52
28	Y	604	CLA	CHA-C1A-NA	-2.06	121.69	126.40
28	C	504	CLA	O2A-CGA-CBA	2.06	118.36	111.91
46	Y	605	CHL	C2B-C1B-NB	-2.06	108.85	110.23
28	G	604	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
28	a	406	CLA	C1-C2-C3	-2.06	122.49	126.04
28	Y	602	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
47	G	620	LUT	C31-C32-C33	-2.06	120.64	126.42
28	b	603	CLA	CHA-C1A-NA	-2.06	121.69	126.40
41	D	405	PL9	O2-C1-C2	-2.06	117.07	121.78
28	D	402	CLA	O2A-CGA-CBA	2.06	118.36	111.91
35	b	623	DGD	O5D-C1E-C2E	2.06	111.51	108.30
48	G	622	XAT	C18-C5-C6	-2.06	118.82	122.26
28	C	512	CLA	C1D-ND-C4D	-2.06	104.88	106.33
28	G	604	CLA	CHA-C1A-NA	-2.05	121.69	126.40
30	c	516	BCR	C31-C1-C6	-2.05	106.97	110.30
28	b	606	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
28	G	611	CLA	CAC-C3C-C4C	2.05	127.47	124.81
28	C	502	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
28	a	410	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
28	b	609	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
28	c	506	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
47	N	621	LUT	C16-C1-C6	-2.05	106.97	110.30
30	c	516	BCR	C19-C18-C17	2.05	122.09	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	508	CLA	C1-O2A-CGA	2.05	121.82	116.44
28	N	610	CLA	C2A-C1A-CHA	2.05	127.44	123.86
28	B	602	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	c	514	BCR	C38-C26-C27	2.05	117.55	113.62
38	G	624	LHG	C6-C5-C4	-2.05	106.94	111.79
28	c	506	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
28	Y	613	CLA	C3B-C4B-NB	-2.05	108.61	110.52
28	C	510	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
28	b	615	CLA	CHA-C1A-NA	-2.05	121.71	126.40
28	B	610	CLA	C1D-ND-C4D	-2.05	104.88	106.33
43	H	101	RRX	C16-C17-C18	-2.05	124.39	127.31
28	A	405	CLA	C1C-C2C-C3C	-2.05	104.81	106.96
28	G	603	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
48	Y	622	XAT	C39-C29-C30	-2.04	120.06	122.92
30	d	404	BCR	C38-C26-C27	2.04	117.54	113.62
28	N	614	CLA	C1-O2A-CGA	2.04	121.81	116.44
47	Y	620	LUT	C15-C35-C34	-2.04	119.29	123.47
28	N	603	CLA	C1D-ND-C4D	-2.04	104.88	106.33
28	C	509	CLA	CHA-C1A-NA	-2.04	121.72	126.40
28	B	611	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
28	G	604	CLA	O2A-CGA-CBA	2.04	118.32	111.91
34	B	620	C7Z	C21-C26-C27	2.04	121.56	115.78
28	N	611	CLA	C1D-ND-C4D	-2.04	104.88	106.33
28	S	610	CLA	C1-O2A-CGA	2.04	121.80	116.44
35	C	519	DGD	O1G-C1A-O1A	-2.04	118.44	123.59
28	B	607	CLA	CHA-C1A-NA	-2.04	121.72	126.40
28	c	513	CLA	C1-O2A-CGA	2.04	121.80	116.44
49	Y	623	NEX	C31-C32-C33	2.04	132.15	126.42
28	C	501	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	S	617	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
47	N	620	LUT	C15-C35-C34	-2.04	119.29	123.47
28	C	512	CLA	C3B-C4B-NB	-2.04	108.62	110.52
28	C	502	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
47	S	621	LUT	C20-C13-C12	2.04	121.29	118.08
28	B	616	CLA	C1D-ND-C4D	-2.04	104.89	106.33
46	Y	605	CHL	C4A-NA-C1A	2.04	107.62	106.71
28	S	603	CLA	C1-O2A-CGA	2.04	121.80	116.44
28	S	603	CLA	C2A-C1A-CHA	2.04	127.42	123.86
28	b	606	CLA	C3B-C4B-NB	-2.04	108.62	110.52
28	c	508	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
28	B	606	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	G	602	CLA	O1D-CGD-CBD	-2.04	120.31	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	N	622	XAT	C20-C13-C14	-2.04	120.07	122.92
28	S	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	S	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
28	B	613	CLA	O2A-CGA-CBA	2.04	118.30	111.91
28	N	610	CLA	C3B-C4B-NB	-2.04	108.63	110.52
28	c	507	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
28	S	604	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
28	G	604	CLA	C1D-ND-C4D	-2.04	104.89	106.33
28	S	611	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
28	c	507	CLA	C1-C2-C3	-2.03	122.53	126.04
30	d	404	BCR	C33-C5-C6	-2.03	122.25	124.53
28	S	605	CLA	C2D-C1D-ND	2.03	111.60	110.10
30	B	619	BCR	C15-C14-C13	-2.03	124.41	127.31
28	C	503	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
28	S	611	CLA	C2A-C1A-CHA	2.03	127.41	123.86
28	b	613	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
28	N	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
28	C	505	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
28	Y	610	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
28	B	617	CLA	C3B-C4B-NB	-2.03	108.63	110.52
47	G	620	LUT	C20-C13-C12	2.03	121.28	118.08
28	d	403	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
28	Y	604	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
28	B	605	CLA	C2A-C1A-CHA	2.03	127.41	123.86
32	C	521	LMG	O7-C10-O9	-2.03	118.80	123.70
49	Y	623	NEX	C20-C13-C14	-2.03	120.08	122.92
28	b	612	CLA	C1D-ND-C4D	-2.03	104.89	106.33
47	S	621	LUT	C18-C5-C4	2.03	118.11	114.36
46	N	601	CHL	CHD-C4C-C3C	2.03	127.82	124.84
28	S	617	CLA	C1D-ND-C4D	-2.03	104.90	106.33
41	D	405	PL9	C36-C34-C33	-2.03	117.02	121.12
28	b	609	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
28	B	606	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
34	B	620	C7Z	C24-C25-C26	-2.02	116.33	120.85
28	N	612	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	G	610	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
28	S	603	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	c	506	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
28	b	605	CLA	CHA-C1A-NA	-2.02	121.76	126.40
34	B	620	C7Z	C1-C6-C7	2.02	121.50	115.78
28	b	609	CLA	C2A-C1A-CHA	2.02	127.40	123.86
28	N	603	CLA	CAA-C2A-C3A	-2.02	107.24	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	617	CLA	C3B-C4B-NB	-2.02	108.64	110.52
28	D	402	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
42	F	101	HEM	CMB-C2B-C1B	-2.02	121.96	125.04
28	B	616	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
28	S	613	CLA	O2A-CGA-CBA	2.02	118.25	111.91
42	f	101	HEM	C3D-C4D-ND	-2.02	107.92	110.17
28	C	508	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
28	d	402	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
28	G	602	CLA	CHA-C1A-NA	-2.02	121.78	126.40
32	C	523	LMG	O7-C10-O9	-2.02	118.83	123.70
28	c	502	CLA	O2A-CGA-CBA	2.02	118.24	111.91
49	Y	623	NEX	C4-C3-C2	2.02	114.67	110.77
28	G	610	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	A	412	SQD	O8-S-C6	-2.02	102.53	105.74
28	N	613	CLA	CMC-C2C-C1C	2.02	128.11	125.04
28	B	612	CLA	CHA-C1A-NA	-2.02	121.78	126.40
46	G	606	CHL	CHA-C1A-NA	-2.02	121.78	126.40
28	S	602	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
28	Y	610	CLA	CHA-C1A-NA	-2.01	121.78	126.40
28	S	612	CLA	CMA-C3A-C4A	2.01	117.19	111.77
32	C	523	LMG	C8-O7-C10	-2.01	112.83	117.79
46	S	608	CHL	C4D-CHA-C1A	2.01	123.70	121.25
28	Y	610	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
46	N	606	CHL	C4D-CHA-C1A	2.01	123.70	121.25
28	S	609	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
28	a	405	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
28	S	617	CLA	C1-O2A-CGA	2.01	121.72	116.44
41	D	405	PL9	C37-C38-C39	-2.01	122.82	127.66
28	B	616	CLA	CMA-C3A-C4A	2.01	117.18	111.77
28	Y	602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
28	A	407	CLA	C1-O2A-CGA	2.01	121.72	116.44
30	a	411	BCR	C34-C9-C10	-2.01	120.11	122.92
47	Y	621	LUT	C35-C15-C14	-2.01	119.36	123.47
28	a	406	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
28	Y	608	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	Y	603	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
28	C	503	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
28	B	606	CLA	CHA-C1A-NA	-2.01	121.80	126.40
28	d	402	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
28	A	406	CLA	C2A-C1A-CHA	2.01	127.37	123.86
28	a	410	CLA	C1-C2-C3	-2.01	122.58	126.04
28	B	609	CLA	CBC-CAC-C3C	-2.00	106.91	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	610	CLA	CHA-C1A-NA	-2.00	121.81	126.40
30	D	404	BCR	C38-C26-C27	2.00	117.47	113.62
28	b	602	CLA	O2A-CGA-CBA	2.00	118.19	111.91
28	S	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
28	C	502	CLA	C1-O2A-CGA	2.00	121.70	116.44
28	b	613	CLA	CMA-C3A-C4A	2.00	117.16	111.77
28	G	613	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
28	a	405	CLA	CHA-C1A-NA	-2.00	121.81	126.40
28	N	604	CLA	C1D-ND-C4D	-2.00	104.91	106.33
28	S	610	CLA	CMA-C3A-C4A	2.00	117.15	111.77
34	B	620	C7Z	C15-C35-C34	-2.00	119.37	123.47
28	C	508	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
28	b	607	CLA	CMA-C3A-C4A	2.00	117.15	111.77
30	b	619	BCR	C36-C18-C17	-2.00	120.12	122.92
28	S	612	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	Y	604	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

All (25) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	B	620	C7Z	C3
34	b	620	C7Z	C3
39	C	527	LMK	C8
39	C	527	LMK	C3
39	c	527	LMK	C8
39	c	527	LMK	C3
43	H	101	RRX	C28
43	h	101	RRX	C28
46	N	601	CHL	C8
46	N	605	CHL	C8
46	N	606	CHL	C8
46	N	607	CHL	C8
46	N	609	CHL	C8
46	G	601	CHL	C8
46	G	605	CHL	C3A
46	G	607	CHL	C8
46	G	609	CHL	C8
46	S	608	CHL	C8
46	Y	601	CHL	C8
46	Y	606	CHL	C8
46	Y	607	CHL	C8
46	Y	609	CHL	C8

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Mol	Chain	Res	Type	Atom
48	N	622	XAT	C6
48	G	622	XAT	C6
48	G	622	XAT	C26

All (3517) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	405	CLA	C1A-C2A-CAA-CBA
28	A	405	CLA	C3A-C2A-CAA-CBA
28	A	405	CLA	CBD-CGD-O2D-CED
28	A	406	CLA	C1A-C2A-CAA-CBA
28	A	406	CLA	C3A-C2A-CAA-CBA
28	A	406	CLA	CHA-CBD-CGD-O1D
28	A	406	CLA	CHA-CBD-CGD-O2D
28	A	407	CLA	C2-C1-O2A-CGA
28	A	407	CLA	CHA-CBD-CGD-O1D
28	A	407	CLA	CHA-CBD-CGD-O2D
28	B	602	CLA	C3A-C2A-CAA-CBA
28	B	602	CLA	CHA-CBD-CGD-O1D
28	B	602	CLA	CHA-CBD-CGD-O2D
28	B	602	CLA	CAD-CBD-CGD-O1D
28	B	603	CLA	CHA-CBD-CGD-O1D
28	B	603	CLA	CHA-CBD-CGD-O2D
28	B	603	CLA	CBD-CGD-O2D-CED
28	B	603	CLA	C2-C3-C5-C6
28	B	603	CLA	C4-C3-C5-C6
28	B	604	CLA	C2-C3-C5-C6
28	B	604	CLA	C4-C3-C5-C6
28	B	604	CLA	C14-C13-C15-C16
28	B	605	CLA	C2-C3-C5-C6
28	B	605	CLA	C4-C3-C5-C6
28	B	607	CLA	CBD-CGD-O2D-CED
28	B	608	CLA	C1A-C2A-CAA-CBA
28	B	608	CLA	C3A-C2A-CAA-CBA
28	B	608	CLA	CHA-CBD-CGD-O1D
28	B	608	CLA	CHA-CBD-CGD-O2D
28	B	608	CLA	CAD-CBD-CGD-O1D
28	B	608	CLA	C2-C3-C5-C6
28	B	608	CLA	C4-C3-C5-C6
28	B	609	CLA	C1A-C2A-CAA-CBA
28	B	610	CLA	C1A-C2A-CAA-CBA
28	B	610	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	B	610	CLA	CHA-CBD-CGD-O1D
28	B	610	CLA	CHA-CBD-CGD-O2D
28	B	610	CLA	CAD-CBD-CGD-O1D
28	B	610	CLA	CAD-CBD-CGD-O2D
28	B	612	CLA	CHA-CBD-CGD-O1D
28	B	612	CLA	CHA-CBD-CGD-O2D
28	B	612	CLA	CBD-CGD-O2D-CED
28	B	613	CLA	C1A-C2A-CAA-CBA
28	B	613	CLA	C2-C1-O2A-CGA
28	B	615	CLA	CBD-CGD-O2D-CED
28	B	616	CLA	CHA-CBD-CGD-O1D
28	B	616	CLA	CHA-CBD-CGD-O2D
28	B	617	CLA	CHA-CBD-CGD-O1D
28	B	617	CLA	CHA-CBD-CGD-O2D
28	C	502	CLA	CHA-CBD-CGD-O1D
28	C	502	CLA	CHA-CBD-CGD-O2D
28	C	502	CLA	CAD-CBD-CGD-O1D
28	C	502	CLA	CBD-CGD-O2D-CED
28	C	503	CLA	CBD-CGD-O2D-CED
28	C	503	CLA	C2-C3-C5-C6
28	C	503	CLA	C4-C3-C5-C6
28	C	504	CLA	CBD-CGD-O2D-CED
28	C	504	CLA	C2-C3-C5-C6
28	C	504	CLA	C4-C3-C5-C6
28	C	505	CLA	CHA-CBD-CGD-O1D
28	C	505	CLA	CHA-CBD-CGD-O2D
28	C	505	CLA	CAD-CBD-CGD-O1D
28	C	505	CLA	CAD-CBD-CGD-O2D
28	C	506	CLA	C2-C1-O2A-CGA
28	C	506	CLA	CBD-CGD-O2D-CED
28	C	508	CLA	CHA-CBD-CGD-O1D
28	C	508	CLA	CHA-CBD-CGD-O2D
28	C	509	CLA	C6-C7-C8-C9
28	C	511	CLA	CBD-CGD-O2D-CED
28	C	512	CLA	CBA-CGA-O2A-C1
28	C	512	CLA	CHA-CBD-CGD-O1D
28	C	512	CLA	CHA-CBD-CGD-O2D
28	C	512	CLA	CAD-CBD-CGD-O1D
28	C	513	CLA	C1A-C2A-CAA-CBA
28	C	513	CLA	CBD-CGD-O2D-CED
28	D	402	CLA	C3A-C2A-CAA-CBA
28	D	402	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	D	402	CLA	C4-C3-C5-C6
28	D	403	CLA	O1A-CGA-O2A-C1
28	D	403	CLA	C2B-C3B-CAB-CBB
28	D	403	CLA	C4B-C3B-CAB-CBB
28	D	403	CLA	CBD-CGD-O2D-CED
28	N	604	CLA	C1A-C2A-CAA-CBA
28	N	604	CLA	C3A-C2A-CAA-CBA
28	N	610	CLA	C1A-C2A-CAA-CBA
28	N	610	CLA	C3A-C2A-CAA-CBA
28	N	610	CLA	C2-C3-C5-C6
28	N	610	CLA	C4-C3-C5-C6
28	N	611	CLA	CHA-CBD-CGD-O1D
28	N	611	CLA	CHA-CBD-CGD-O2D
28	N	612	CLA	CBD-CGD-O2D-CED
28	N	613	CLA	C1A-C2A-CAA-CBA
28	N	613	CLA	CHA-CBD-CGD-O1D
28	N	613	CLA	CHA-CBD-CGD-O2D
28	N	614	CLA	C1A-C2A-CAA-CBA
28	G	602	CLA	C1A-C2A-CAA-CBA
28	G	602	CLA	C3A-C2A-CAA-CBA
28	G	603	CLA	CBD-CGD-O2D-CED
28	G	610	CLA	CBD-CGD-O2D-CED
28	G	614	CLA	CBD-CGD-O2D-CED
28	S	602	CLA	C2-C1-O2A-CGA
28	S	602	CLA	CHA-CBD-CGD-O1D
28	S	602	CLA	CHA-CBD-CGD-O2D
28	S	603	CLA	C1A-C2A-CAA-CBA
28	S	603	CLA	C3A-C2A-CAA-CBA
28	S	603	CLA	CHA-CBD-CGD-O1D
28	S	603	CLA	CHA-CBD-CGD-O2D
28	S	604	CLA	CBA-CGA-O2A-C1
28	S	604	CLA	O1A-CGA-O2A-C1
28	S	604	CLA	CBD-CGD-O2D-CED
28	S	605	CLA	C1A-C2A-CAA-CBA
28	S	605	CLA	CHA-CBD-CGD-O1D
28	S	605	CLA	CHA-CBD-CGD-O2D
28	S	609	CLA	C2B-C3B-CAB-CBB
28	S	609	CLA	C4B-C3B-CAB-CBB
28	S	609	CLA	CBD-CGD-O2D-CED
28	S	610	CLA	C1A-C2A-CAA-CBA
28	S	610	CLA	C3A-C2A-CAA-CBA
28	S	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	S	611	CLA	C1A-C2A-CAA-CBA
28	S	611	CLA	C3A-C2A-CAA-CBA
28	S	611	CLA	CAD-CBD-CGD-O2D
28	S	611	CLA	CBD-CGD-O2D-CED
28	S	612	CLA	CBD-CGD-O2D-CED
28	S	613	CLA	CHA-CBD-CGD-O1D
28	S	613	CLA	CHA-CBD-CGD-O2D
28	S	614	CLA	CBD-CGD-O2D-CED
28	Y	604	CLA	CBD-CGD-O2D-CED
28	Y	608	CLA	C2-C1-O2A-CGA
28	Y	610	CLA	CBD-CGD-O2D-CED
28	Y	611	CLA	CHA-CBD-CGD-O1D
28	Y	611	CLA	CHA-CBD-CGD-O2D
28	Y	612	CLA	C2B-C3B-CAB-CBB
28	Y	612	CLA	C4B-C3B-CAB-CBB
28	Y	614	CLA	CBD-CGD-O2D-CED
28	a	405	CLA	C1A-C2A-CAA-CBA
28	a	405	CLA	C3A-C2A-CAA-CBA
28	a	405	CLA	CBD-CGD-O2D-CED
28	a	406	CLA	C3A-C2A-CAA-CBA
28	a	406	CLA	C2-C1-O2A-CGA
28	a	406	CLA	CHA-CBD-CGD-O1D
28	a	406	CLA	CHA-CBD-CGD-O2D
28	b	602	CLA	CHA-CBD-CGD-O1D
28	b	602	CLA	CHA-CBD-CGD-O2D
28	b	603	CLA	CHA-CBD-CGD-O1D
28	b	603	CLA	CHA-CBD-CGD-O2D
28	b	603	CLA	CBD-CGD-O2D-CED
28	b	604	CLA	CBD-CGD-O2D-CED
28	b	606	CLA	CBD-CGD-O2D-CED
28	b	606	CLA	C4-C3-C5-C6
28	b	607	CLA	C1A-C2A-CAA-CBA
28	b	607	CLA	CHA-CBD-CGD-O1D
28	b	607	CLA	CHA-CBD-CGD-O2D
28	b	607	CLA	CBD-CGD-O2D-CED
28	b	608	CLA	C1A-C2A-CAA-CBA
28	b	608	CLA	C3A-C2A-CAA-CBA
28	b	608	CLA	CHA-CBD-CGD-O1D
28	b	608	CLA	CHA-CBD-CGD-O2D
28	b	608	CLA	CAD-CBD-CGD-O1D
28	b	608	CLA	C2-C3-C5-C6
28	b	608	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	b	609	CLA	C1A-C2A-CAA-CBA
28	b	609	CLA	C3A-C2A-CAA-CBA
28	b	609	CLA	CHA-CBD-CGD-O1D
28	b	609	CLA	CHA-CBD-CGD-O2D
28	b	610	CLA	C1A-C2A-CAA-CBA
28	b	610	CLA	C3A-C2A-CAA-CBA
28	b	610	CLA	CAD-CBD-CGD-O1D
28	b	610	CLA	CAD-CBD-CGD-O2D
28	b	611	CLA	CBD-CGD-O2D-CED
28	b	613	CLA	C2-C1-O2A-CGA
28	b	614	CLA	CHA-CBD-CGD-O1D
28	b	614	CLA	CHA-CBD-CGD-O2D
28	b	616	CLA	C4B-C3B-CAB-CBB
28	b	616	CLA	CHA-CBD-CGD-O1D
28	b	616	CLA	CHA-CBD-CGD-O2D
28	c	501	CLA	CHA-CBD-CGD-O1D
28	c	501	CLA	CHA-CBD-CGD-O2D
28	c	501	CLA	CAD-CBD-CGD-O1D
28	c	501	CLA	CBD-CGD-O2D-CED
28	c	502	CLA	CAD-CBD-CGD-O1D
28	c	502	CLA	CAD-CBD-CGD-O2D
28	c	502	CLA	CBD-CGD-O2D-CED
28	c	503	CLA	C2-C3-C5-C6
28	c	503	CLA	C4-C3-C5-C6
28	c	504	CLA	C1A-C2A-CAA-CBA
28	c	504	CLA	C3A-C2A-CAA-CBA
28	c	504	CLA	C6-C7-C8-C9
28	c	506	CLA	C2-C1-O2A-CGA
28	c	506	CLA	CBD-CGD-O2D-CED
28	c	507	CLA	C4B-C3B-CAB-CBB
28	c	508	CLA	CHA-CBD-CGD-O1D
28	c	508	CLA	CHA-CBD-CGD-O2D
28	c	509	CLA	C2-C1-O2A-CGA
28	c	509	CLA	CBD-CGD-O2D-CED
28	c	510	CLA	CHA-CBD-CGD-O1D
28	c	510	CLA	CHA-CBD-CGD-O2D
28	c	510	CLA	CBD-CGD-O2D-CED
28	c	511	CLA	C1A-C2A-CAA-CBA
28	c	511	CLA	CHA-CBD-CGD-O1D
28	c	511	CLA	CHA-CBD-CGD-O2D
28	c	512	CLA	CBA-CGA-O2A-C1
28	c	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	c	512	CLA	CHA-CBD-CGD-O1D
28	c	512	CLA	CHA-CBD-CGD-O2D
28	c	512	CLA	CAD-CBD-CGD-O1D
28	c	513	CLA	C1A-C2A-CAA-CBA
28	d	402	CLA	C2-C1-O2A-CGA
28	d	402	CLA	CHA-CBD-CGD-O1D
28	d	402	CLA	CHA-CBD-CGD-O2D
28	d	402	CLA	CBD-CGD-O2D-CED
28	d	403	CLA	CBA-CGA-O2A-C1
28	d	403	CLA	O1A-CGA-O2A-C1
28	d	403	CLA	C2-C3-C5-C6
28	d	403	CLA	C4-C3-C5-C6
29	A	409	PHO	C3A-C2A-CAA-CBA
29	a	409	PHO	C3A-C2A-CAA-CBA
30	A	411	BCR	C7-C8-C9-C10
30	A	411	BCR	C7-C8-C9-C34
30	A	411	BCR	C11-C10-C9-C8
30	A	411	BCR	C11-C10-C9-C34
30	A	411	BCR	C10-C11-C12-C13
30	A	411	BCR	C17-C18-C19-C20
30	A	411	BCR	C36-C18-C19-C20
30	B	618	BCR	C11-C10-C9-C8
30	B	618	BCR	C11-C10-C9-C34
30	B	618	BCR	C10-C11-C12-C13
30	B	618	BCR	C17-C18-C19-C20
30	B	618	BCR	C36-C18-C19-C20
30	B	619	BCR	C11-C10-C9-C8
30	B	619	BCR	C11-C10-C9-C34
30	C	514	BCR	C11-C10-C9-C8
30	C	514	BCR	C11-C10-C9-C34
30	C	514	BCR	C9-C10-C11-C12
30	C	514	BCR	C10-C11-C12-C13
30	C	514	BCR	C13-C14-C15-C16
30	C	514	BCR	C36-C18-C19-C20
30	C	514	BCR	C37-C22-C23-C24
30	C	515	BCR	C11-C10-C9-C8
30	C	515	BCR	C11-C10-C9-C34
30	C	515	BCR	C10-C11-C12-C13
30	C	515	BCR	C17-C18-C19-C20
30	C	515	BCR	C36-C18-C19-C20
30	C	515	BCR	C19-C20-C21-C22
30	C	516	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	C	516	BCR	C5-C6-C7-C8
30	C	516	BCR	C7-C8-C9-C10
30	C	516	BCR	C7-C8-C9-C34
30	C	516	BCR	C11-C10-C9-C8
30	C	516	BCR	C11-C10-C9-C34
30	C	516	BCR	C10-C11-C12-C13
30	C	516	BCR	C23-C24-C25-C30
30	C	517	BCR	C11-C10-C9-C8
30	C	517	BCR	C11-C10-C9-C34
30	C	517	BCR	C10-C11-C12-C13
30	C	517	BCR	C17-C18-C19-C20
30	C	517	BCR	C36-C18-C19-C20
30	D	404	BCR	C11-C10-C9-C8
30	D	404	BCR	C11-C10-C9-C34
30	D	404	BCR	C10-C11-C12-C13
30	D	404	BCR	C17-C18-C19-C20
30	D	404	BCR	C36-C18-C19-C20
30	D	404	BCR	C21-C22-C23-C24
30	D	404	BCR	C37-C22-C23-C24
30	D	404	BCR	C23-C24-C25-C26
30	D	404	BCR	C23-C24-C25-C30
30	a	411	BCR	C11-C10-C9-C8
30	a	411	BCR	C11-C10-C9-C34
30	a	411	BCR	C17-C18-C19-C20
30	a	411	BCR	C36-C18-C19-C20
30	b	618	BCR	C11-C10-C9-C8
30	b	618	BCR	C11-C10-C9-C34
30	b	618	BCR	C10-C11-C12-C13
30	b	619	BCR	C7-C8-C9-C10
30	b	619	BCR	C7-C8-C9-C34
30	b	619	BCR	C11-C10-C9-C8
30	b	619	BCR	C11-C10-C9-C34
30	b	619	BCR	C10-C11-C12-C13
30	b	619	BCR	C36-C18-C19-C20
30	b	619	BCR	C23-C24-C25-C30
30	c	514	BCR	C11-C10-C9-C8
30	c	514	BCR	C11-C10-C9-C34
30	c	514	BCR	C9-C10-C11-C12
30	c	514	BCR	C10-C11-C12-C13
30	c	514	BCR	C17-C18-C19-C20
30	c	514	BCR	C36-C18-C19-C20
30	c	515	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
30	c	515	BCR	C11-C10-C9-C8
30	c	515	BCR	C11-C10-C9-C34
30	c	516	BCR	C7-C8-C9-C10
30	c	516	BCR	C7-C8-C9-C34
30	c	516	BCR	C9-C10-C11-C12
30	c	516	BCR	C10-C11-C12-C13
30	c	516	BCR	C21-C22-C23-C24
30	c	516	BCR	C37-C22-C23-C24
30	c	517	BCR	C11-C10-C9-C8
30	c	517	BCR	C11-C10-C9-C34
30	c	517	BCR	C10-C11-C12-C13
30	d	404	BCR	C11-C10-C9-C8
30	d	404	BCR	C11-C10-C9-C34
30	d	404	BCR	C10-C11-C12-C13
30	d	404	BCR	C36-C18-C19-C20
30	d	404	BCR	C23-C24-C25-C26
30	d	404	BCR	C23-C24-C25-C30
31	B	621	SQD	C2-C1-O6-C44
31	B	621	SQD	O5-C1-O6-C44
31	B	621	SQD	O5-C5-C6-S
31	B	626	SQD	O47-C45-C46-O48
31	B	626	SQD	C5-C6-S-O7
31	B	626	SQD	C5-C6-S-O8
31	B	626	SQD	C5-C6-S-O9
31	C	526	SQD	O5-C5-C6-S
31	C	526	SQD	C5-C6-S-O7
31	C	526	SQD	C5-C6-S-O8
31	C	526	SQD	C5-C6-S-O9
31	M	101	SQD	O5-C5-C6-S
31	a	412	SQD	O47-C45-C46-O48
31	a	412	SQD	O5-C5-C6-S
31	b	621	SQD	C2-C1-O6-C44
31	b	621	SQD	O5-C1-O6-C44
31	b	621	SQD	O5-C5-C6-S
31	b	626	SQD	C2-C1-O6-C44
31	b	626	SQD	O5-C1-O6-C44
31	b	626	SQD	C5-C6-S-O7
31	b	626	SQD	C5-C6-S-O8
31	b	626	SQD	C5-C6-S-O9
31	c	526	SQD	O5-C5-C6-S
31	m	101	SQD	C2-C1-O6-C44
31	m	101	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
31	m	101	SQD	O5-C5-C6-S
31	m	101	SQD	C5-C6-S-O7
31	m	101	SQD	C5-C6-S-O8
31	m	101	SQD	C5-C6-S-O9
32	A	413	LMG	C2-C1-O1-C7
32	A	413	LMG	O6-C1-O1-C7
32	B	622	LMG	O6-C1-O1-C7
32	B	622	LMG	O9-C10-O7-C8
32	B	622	LMG	C11-C10-O7-C8
32	C	523	LMG	C2-C1-O1-C7
32	C	523	LMG	O6-C1-O1-C7
32	W	201	LMG	O6-C1-O1-C7
32	W	201	LMG	C7-C8-O7-C10
32	W	201	LMG	C11-C10-O7-C8
32	W	201	LMG	O10-C28-O8-C9
32	b	622	LMG	O9-C10-O7-C8
32	b	622	LMG	C11-C10-O7-C8
32	c	523	LMG	C11-C10-O7-C8
33	A	414	SPH	C1-C2-C3-O3
33	Y	625	SPH	O1-C1-C2-N2
33	Y	625	SPH	O1-C1-C2-C3
33	Y	625	SPH	C2-C3-C4-C5
33	Y	625	SPH	O3-C3-C4-C5
33	a	414	SPH	O1-C1-C2-N2
33	a	414	SPH	O1-C1-C2-C3
33	a	414	SPH	C1-C2-C3-O3
33	a	414	SPH	C1-C2-C3-C4
33	a	414	SPH	N2-C2-C3-O3
33	a	414	SPH	N2-C2-C3-C4
34	B	620	C7Z	C11-C12-C13-C20
34	B	620	C7Z	C11-C12-C13-C14
34	B	620	C7Z	C27-C28-C29-C30
34	B	620	C7Z	C27-C28-C29-C39
34	b	620	C7Z	C21-C26-C27-C28
34	b	620	C7Z	C11-C12-C13-C20
34	b	620	C7Z	C11-C12-C13-C14
34	b	620	C7Z	C31-C32-C33-C40
34	b	620	C7Z	C27-C28-C29-C30
34	b	620	C7Z	C27-C28-C29-C39
35	B	623	DGD	O1B-C1B-O2G-C2G
35	B	623	DGD	O6D-C1D-O3G-C3G
35	B	623	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
35	B	623	DGD	O6E-C1E-O5D-C6D
35	b	623	DGD	O1B-C1B-O2G-C2G
35	b	623	DGD	O6D-C1D-O3G-C3G
35	c	518	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	O6E-C1E-O5D-C6D
36	B	624	3PH	C1-O11-P-O13
36	B	624	3PH	C1-O11-P-O14
36	B	624	3PH	C1-O11-P-O12
36	T	101	3PH	C1-O11-P-O13
36	T	101	3PH	C1-O11-P-O14
36	S	626	3PH	O22-C21-O21-C2
36	b	624	3PH	O21-C2-C3-O31
36	t	101	3PH	O22-C21-O21-C2
36	t	101	3PH	C22-C21-O21-C2
37	B	625	DGA	CB2-CB1-OG2-CG2
37	B	625	DGA	OB1-CB1-OG2-CG2
37	B	625	DGA	CG1-CG2-CG3-OXT
37	B	625	DGA	OG2-CG2-CG3-OXT
37	J	101	DGA	CG1-CG2-CG3-OXT
37	J	101	DGA	OG2-CG2-CG3-OXT
37	b	625	DGA	CB2-CB1-OG2-CG2
37	b	625	DGA	OB1-CB1-OG2-CG2
37	b	625	DGA	CG1-CG2-CG3-OXT
37	b	625	DGA	OG2-CG2-CG3-OXT
38	C	525	LHG	O1-C1-C2-O2
38	C	525	LHG	C3-O3-P-O6
38	C	525	LHG	C4-O6-P-O4
38	D	408	LHG	O1-C1-C2-C3
38	D	408	LHG	C3-O3-P-O5
38	D	408	LHG	C4-O6-P-O3
38	D	408	LHG	C4-O6-P-O4
38	D	408	LHG	C4-O6-P-O5
38	D	409	LHG	C4-O6-P-O4
38	D	410	LHG	C3-O3-P-O4
38	D	410	LHG	C3-O3-P-O5
38	D	410	LHG	C4-O6-P-O5
38	D	410	LHG	O7-C5-C6-O8
38	L	101	LHG	O1-C1-C2-O2
38	L	101	LHG	C3-O3-P-O4
38	L	101	LHG	C3-O3-P-O5
38	L	101	LHG	C3-O3-P-O6
38	L	101	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
38	L	101	LHG	C8-C7-O7-C5
38	N	624	LHG	O1-C1-C2-C3
38	N	624	LHG	C4-O6-P-O4
38	N	624	LHG	O7-C5-C6-O8
38	G	624	LHG	C4-O6-P-O4
38	G	624	LHG	O7-C5-C6-O8
38	S	624	LHG	O1-C1-C2-C3
38	S	624	LHG	O2-C2-C3-O3
38	S	624	LHG	C3-O3-P-O5
38	S	624	LHG	C4-O6-P-O3
38	S	624	LHG	C4-O6-P-O4
38	S	624	LHG	C4-O6-P-O5
38	S	624	LHG	C8-C7-O7-C5
38	Y	624	LHG	C1-C2-C3-O3
38	Y	624	LHG	C4-O6-P-O4
38	Y	624	LHG	C4-O6-P-O5
38	c	525	LHG	C1-C2-C3-O3
38	c	525	LHG	C3-O3-P-O5
38	c	525	LHG	C3-O3-P-O6
38	c	525	LHG	C4-O6-P-O4
38	d	408	LHG	O1-C1-C2-C3
38	d	408	LHG	C3-O3-P-O4
38	d	408	LHG	C4-O6-P-O3
38	d	408	LHG	C4-O6-P-O4
38	d	408	LHG	C4-O6-P-O5
38	d	409	LHG	C3-O3-P-O5
38	d	410	LHG	O1-C1-C2-C3
38	d	410	LHG	C3-O3-P-O5
38	d	410	LHG	C4-O6-P-O3
38	d	410	LHG	C4-O6-P-O4
38	d	410	LHG	C4-O6-P-O5
38	l	101	LHG	O1-C1-C2-C3
38	l	101	LHG	C3-O3-P-O4
38	l	101	LHG	C3-O3-P-O5
38	l	101	LHG	C3-O3-P-O6
38	l	101	LHG	O9-C7-O7-C5
38	l	101	LHG	C8-C7-O7-C5
39	C	527	LMK	O9-C10-O7-C8
39	C	527	LMK	C1-C2-C3-C4
39	C	527	LMK	C1-C2-C3-N4
39	C	527	LMK	C2-C3-N4-C5
39	C	527	LMK	C2-C3-N4-C6

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Mol	Chain	Res	Type	Atoms
39	C	527	LMK	C2-C3-N4-C46
39	c	527	LMK	O1-C7-C8-O7
39	c	527	LMK	O9-C10-C11-C12
39	c	527	LMK	O10-C28-O8-C9
41	d	405	PL9	C12-C13-C14-C16
41	d	405	PL9	C22-C23-C24-C25
41	d	405	PL9	C24-C26-C27-C28
41	d	405	PL9	C27-C28-C29-C31
41	d	405	PL9	C32-C33-C34-C36
41	d	405	PL9	C37-C38-C39-C40
43	H	101	RRX	C23-C24-C25-C26
43	h	101	RRX	C23-C24-C25-C26
43	h	101	RRX	C36-C18-C19-C20
43	h	101	RRX	C17-C18-C19-C20
43	h	101	RRX	C5-C6-C7-C8
44	I	101	GOL	C1-C2-C3-O3
45	I	102	4RF	O18-C19-C20-O21
45	I	102	4RF	C24-C22-O21-C20
45	K	101	4RF	O21-C20-C39-O40
45	i	101	4RF	C24-C22-O21-C20
46	N	606	CHL	C2-C3-C5-C6
46	G	601	CHL	CHA-CBD-CGD-O1D
46	G	601	CHL	CHA-CBD-CGD-O2D
46	G	605	CHL	C1A-C2A-CAA-CBA
46	G	605	CHL	C3A-C2A-CAA-CBA
46	G	605	CHL	CHA-CBD-CGD-O1D
46	G	605	CHL	CHA-CBD-CGD-O2D
46	G	607	CHL	C1A-C2A-CAA-CBA
46	G	609	CHL	CHA-CBD-CGD-O1D
46	G	609	CHL	CHA-CBD-CGD-O2D
46	G	609	CHL	C2-C3-C5-C6
46	G	609	CHL	C4-C3-C5-C6
46	Y	601	CHL	CHA-CBD-CGD-O1D
46	Y	601	CHL	CHA-CBD-CGD-O2D
47	N	620	LUT	C1-C6-C7-C8
47	N	621	LUT	C21-C26-C27-C28
47	G	620	LUT	C27-C28-C29-C30
47	G	620	LUT	C27-C28-C29-C39
47	G	621	LUT	C21-C26-C27-C28
47	S	620	LUT	C25-C26-C27-C28
47	Y	621	LUT	C21-C26-C27-C28
50	S	625	LPX	C3-C4-C5-O6

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Mol	Chain	Res	Type	Atoms
50	S	625	LPX	O1-C3-C4-C5
50	S	625	LPX	C1-O2-P1-O3
50	S	625	LPX	C1-O2-P1-O4
51	Y	626	PTY	N1-C2-C3-O11
51	Y	627	PTY	C11-C8-O7-C6
28	G	613	CLA	O1D-CGD-O2D-CED
28	S	613	CLA	O1D-CGD-O2D-CED
28	b	614	CLA	O1D-CGD-O2D-CED
28	N	613	CLA	O1D-CGD-O2D-CED
28	Y	608	CLA	O1D-CGD-O2D-CED
28	Y	613	CLA	O1D-CGD-O2D-CED
28	a	405	CLA	O1D-CGD-O2D-CED
28	b	608	CLA	O1D-CGD-O2D-CED
28	A	410	CLA	CBD-CGD-O2D-CED
28	B	604	CLA	CBD-CGD-O2D-CED
28	B	606	CLA	CBD-CGD-O2D-CED
28	B	608	CLA	CBD-CGD-O2D-CED
28	B	610	CLA	CBD-CGD-O2D-CED
28	B	611	CLA	CBD-CGD-O2D-CED
28	B	613	CLA	CBD-CGD-O2D-CED
28	B	614	CLA	CBD-CGD-O2D-CED
28	B	616	CLA	CBD-CGD-O2D-CED
28	C	501	CLA	CBD-CGD-O2D-CED
28	C	507	CLA	CBD-CGD-O2D-CED
28	C	509	CLA	CBD-CGD-O2D-CED
28	C	510	CLA	CBD-CGD-O2D-CED
28	C	512	CLA	CBD-CGD-O2D-CED
28	N	602	CLA	CBD-CGD-O2D-CED
28	N	610	CLA	CBD-CGD-O2D-CED
28	N	613	CLA	CBD-CGD-O2D-CED
28	N	614	CLA	CBD-CGD-O2D-CED
28	G	602	CLA	CBD-CGD-O2D-CED
28	G	604	CLA	CBD-CGD-O2D-CED
28	G	612	CLA	CBD-CGD-O2D-CED
28	G	613	CLA	CBD-CGD-O2D-CED
28	S	603	CLA	CBD-CGD-O2D-CED
28	S	605	CLA	CBD-CGD-O2D-CED
28	S	613	CLA	CBD-CGD-O2D-CED
28	S	617	CLA	CBD-CGD-O2D-CED
28	Y	603	CLA	CBD-CGD-O2D-CED
28	Y	608	CLA	CBD-CGD-O2D-CED
28	Y	611	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	Y	612	CLA	CBD-CGD-O2D-CED
28	Y	613	CLA	CBD-CGD-O2D-CED
28	b	602	CLA	CBD-CGD-O2D-CED
28	b	605	CLA	CBD-CGD-O2D-CED
28	b	608	CLA	CBD-CGD-O2D-CED
28	b	609	CLA	CBD-CGD-O2D-CED
28	b	610	CLA	CBD-CGD-O2D-CED
28	b	612	CLA	CBD-CGD-O2D-CED
28	b	613	CLA	CBD-CGD-O2D-CED
28	b	614	CLA	CBD-CGD-O2D-CED
28	b	615	CLA	CBD-CGD-O2D-CED
28	b	616	CLA	CBD-CGD-O2D-CED
28	b	617	CLA	CBD-CGD-O2D-CED
28	c	504	CLA	CBD-CGD-O2D-CED
28	c	507	CLA	CBD-CGD-O2D-CED
28	c	511	CLA	CBD-CGD-O2D-CED
28	c	513	CLA	CBD-CGD-O2D-CED
28	d	403	CLA	CBD-CGD-O2D-CED
29	a	409	PHO	CBD-CGD-O2D-CED
28	C	512	CLA	O1A-CGA-O2A-C1
28	N	603	CLA	O1A-CGA-O2A-C1
28	G	611	CLA	O1A-CGA-O2A-C1
28	S	605	CLA	O1A-CGA-O2A-C1
28	S	613	CLA	O1A-CGA-O2A-C1
28	b	603	CLA	O1A-CGA-O2A-C1
31	c	526	SQD	O10-C23-O48-C46
45	I	102	4RF	O17-C16-O18-C19
28	A	405	CLA	O1D-CGD-O2D-CED
28	B	608	CLA	O1D-CGD-O2D-CED
28	B	614	CLA	O1D-CGD-O2D-CED
28	C	504	CLA	O1D-CGD-O2D-CED
28	N	612	CLA	O1D-CGD-O2D-CED
28	S	604	CLA	O1D-CGD-O2D-CED
28	S	609	CLA	O1D-CGD-O2D-CED
28	S	617	CLA	O1D-CGD-O2D-CED
28	Y	610	CLA	O1D-CGD-O2D-CED
28	b	602	CLA	O1D-CGD-O2D-CED
28	b	610	CLA	O1D-CGD-O2D-CED
28	b	612	CLA	O1D-CGD-O2D-CED
28	b	615	CLA	O1D-CGD-O2D-CED
28	c	501	CLA	O1D-CGD-O2D-CED
28	c	504	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	c	513	CLA	O1D-CGD-O2D-CED
28	d	402	CLA	O1D-CGD-O2D-CED
35	c	518	DGD	C2G-C1G-O1G-C1A
28	B	604	CLA	O1D-CGD-O2D-CED
28	B	606	CLA	O1D-CGD-O2D-CED
28	B	607	CLA	O1D-CGD-O2D-CED
28	B	612	CLA	O1D-CGD-O2D-CED
28	B	615	CLA	O1D-CGD-O2D-CED
28	C	503	CLA	O1D-CGD-O2D-CED
28	C	506	CLA	O1D-CGD-O2D-CED
28	C	511	CLA	O1D-CGD-O2D-CED
28	C	513	CLA	O1D-CGD-O2D-CED
28	N	614	CLA	O1D-CGD-O2D-CED
28	G	603	CLA	O1D-CGD-O2D-CED
28	G	610	CLA	O1D-CGD-O2D-CED
28	S	610	CLA	O1D-CGD-O2D-CED
28	Y	604	CLA	O1D-CGD-O2D-CED
28	b	603	CLA	O1D-CGD-O2D-CED
28	b	604	CLA	O1D-CGD-O2D-CED
28	b	606	CLA	O1D-CGD-O2D-CED
28	c	502	CLA	O1D-CGD-O2D-CED
28	c	506	CLA	O1D-CGD-O2D-CED
28	c	511	CLA	O1D-CGD-O2D-CED
28	N	611	CLA	CBA-CGA-O2A-C1
28	G	604	CLA	CBA-CGA-O2A-C1
28	S	605	CLA	CBA-CGA-O2A-C1
32	W	201	LMG	C29-C28-O8-C9
36	t	101	3PH	C32-C31-O31-C3
45	I	102	4RF	C15-C16-O18-C19
51	Y	627	PTY	O30-C30-O4-C1
28	B	609	CLA	CBD-CGD-O2D-CED
28	B	617	CLA	CBD-CGD-O2D-CED
28	D	402	CLA	CBD-CGD-O2D-CED
28	N	603	CLA	CBD-CGD-O2D-CED
28	N	604	CLA	CBD-CGD-O2D-CED
28	N	611	CLA	CBD-CGD-O2D-CED
28	G	611	CLA	CBD-CGD-O2D-CED
28	S	602	CLA	CBD-CGD-O2D-CED
28	Y	602	CLA	CBD-CGD-O2D-CED
28	a	407	CLA	CBD-CGD-O2D-CED
28	a	410	CLA	CBD-CGD-O2D-CED
28	c	503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	A	406	CLA	O1A-CGA-O2A-C1
28	B	603	CLA	O1A-CGA-O2A-C1
28	C	505	CLA	O1A-CGA-O2A-C1
28	N	611	CLA	O1A-CGA-O2A-C1
28	G	604	CLA	O1A-CGA-O2A-C1
28	G	614	CLA	O1A-CGA-O2A-C1
28	S	609	CLA	O1A-CGA-O2A-C1
28	S	617	CLA	O1A-CGA-O2A-C1
28	Y	602	CLA	O1A-CGA-O2A-C1
28	Y	604	CLA	O1A-CGA-O2A-C1
28	Y	608	CLA	O1A-CGA-O2A-C1
28	Y	611	CLA	O1A-CGA-O2A-C1
28	c	505	CLA	O1A-CGA-O2A-C1
28	c	506	CLA	O1A-CGA-O2A-C1
32	C	521	LMG	O10-C28-O8-C9
32	c	521	LMG	O10-C28-O8-C9
32	c	523	LMG	O10-C28-O8-C9
36	T	101	3PH	O32-C31-O31-C3
36	b	624	3PH	O32-C31-O31-C3
36	t	101	3PH	O32-C31-O31-C3
45	i	101	4RF	O17-C16-O18-C19
28	D	403	CLA	O1D-CGD-O2D-CED
28	S	611	CLA	O1D-CGD-O2D-CED
28	Y	614	CLA	O1D-CGD-O2D-CED
28	b	607	CLA	O1D-CGD-O2D-CED
28	b	611	CLA	O1D-CGD-O2D-CED
32	d	411	LMG	C4-C5-C6-O5
28	B	603	CLA	O1D-CGD-O2D-CED
28	C	502	CLA	O1D-CGD-O2D-CED
28	S	612	CLA	O1D-CGD-O2D-CED
28	S	614	CLA	O1D-CGD-O2D-CED
28	c	509	CLA	O1D-CGD-O2D-CED
28	c	510	CLA	O1D-CGD-O2D-CED
51	Y	627	PTY	C31-C30-O4-C1
28	c	512	CLA	CBD-CGD-O2D-CED
28	N	610	CLA	O1D-CGD-O2D-CED
28	G	614	CLA	O1D-CGD-O2D-CED
28	Y	603	CLA	O1D-CGD-O2D-CED
32	W	201	LMG	O9-C10-O7-C8
32	a	413	LMG	O9-C10-O7-C8
32	c	523	LMG	O9-C10-O7-C8
36	T	101	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
38	S	624	LHG	O9-C7-O7-C5
45	i	101	4RF	O23-C22-O21-C20
51	Y	627	PTY	O10-C8-O7-C6
28	d	403	CLA	O1D-CGD-O2D-CED
28	B	605	CLA	C3-C5-C6-C7
28	B	608	CLA	C3-C5-C6-C7
28	B	610	CLA	C3-C5-C6-C7
28	S	613	CLA	C3-C5-C6-C7
28	b	617	CLA	C3-C5-C6-C7
28	c	504	CLA	C3-C5-C6-C7
28	c	508	CLA	C3-C5-C6-C7
28	d	403	CLA	C3-C5-C6-C7
29	A	409	PHO	C3-C5-C6-C7
28	A	406	CLA	CBA-CGA-O2A-C1
28	B	603	CLA	CBA-CGA-O2A-C1
28	B	608	CLA	CBA-CGA-O2A-C1
28	C	505	CLA	CBA-CGA-O2A-C1
28	C	509	CLA	CBA-CGA-O2A-C1
28	D	403	CLA	CBA-CGA-O2A-C1
28	N	603	CLA	CBA-CGA-O2A-C1
28	G	611	CLA	CBA-CGA-O2A-C1
28	S	610	CLA	CBA-CGA-O2A-C1
28	S	613	CLA	CBA-CGA-O2A-C1
28	S	617	CLA	CBA-CGA-O2A-C1
28	Y	603	CLA	CBA-CGA-O2A-C1
28	Y	604	CLA	CBA-CGA-O2A-C1
28	Y	611	CLA	CBA-CGA-O2A-C1
28	b	603	CLA	CBA-CGA-O2A-C1
28	c	505	CLA	CBA-CGA-O2A-C1
28	c	511	CLA	CBA-CGA-O2A-C1
31	c	526	SQD	C24-C23-O48-C46
32	C	521	LMG	C29-C28-O8-C9
32	c	521	LMG	C29-C28-O8-C9
36	T	101	3PH	C32-C31-O31-C3
45	i	101	4RF	C15-C16-O18-C19
32	a	413	LMG	C11-C10-O7-C8
35	B	623	DGD	C2B-C1B-O2G-C2G
35	b	623	DGD	C2B-C1B-O2G-C2G
36	T	101	3PH	C22-C21-O21-C2
28	N	602	CLA	O1D-CGD-O2D-CED
28	a	406	CLA	CBD-CGD-O2D-CED
31	b	626	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
28	B	606	CLA	C4-C3-C5-C6
28	c	504	CLA	C4-C3-C5-C6
46	N	606	CHL	C4-C3-C5-C6
28	G	613	CLA	C2A-CAA-CBA-CGA
28	G	614	CLA	C2A-CAA-CBA-CGA
28	S	602	CLA	C2A-CAA-CBA-CGA
28	S	614	CLA	C2A-CAA-CBA-CGA
28	c	507	CLA	C2A-CAA-CBA-CGA
28	C	506	CLA	O1A-CGA-O2A-C1
32	A	413	LMG	C17-C18-C19-C20
32	A	413	LMG	C35-C36-C37-C38
32	A	413	LMG	C38-C39-C40-C41
32	B	622	LMG	C17-C18-C19-C20
32	C	521	LMG	C17-C18-C19-C20
32	C	521	LMG	C35-C36-C37-C38
32	C	523	LMG	C17-C18-C19-C20
32	C	523	LMG	C41-C42-C43-C44
32	D	411	LMG	C17-C18-C19-C20
32	D	411	LMG	C20-C21-C22-C23
32	H	102	LMG	C38-C39-C40-C41
32	W	201	LMG	C35-C36-C37-C38
32	W	201	LMG	C38-C39-C40-C41
32	a	413	LMG	C17-C18-C19-C20
32	a	413	LMG	C35-C36-C37-C38
32	a	413	LMG	C38-C39-C40-C41
32	b	622	LMG	C17-C18-C19-C20
32	c	521	LMG	C17-C18-C19-C20
32	c	521	LMG	C35-C36-C37-C38
32	c	523	LMG	C17-C18-C19-C20
32	c	523	LMG	C41-C42-C43-C44
32	d	411	LMG	C17-C18-C19-C20
32	d	411	LMG	C20-C21-C22-C23
32	h	102	LMG	C38-C39-C40-C41
32	w	201	LMG	C35-C36-C37-C38
32	w	201	LMG	C38-C39-C40-C41
35	C	518	DGD	C8B-C9B-CAB-CBB
35	C	519	DGD	C8A-C9A-CAA-CBA
35	C	519	DGD	CBB-CCB-CDB-CEB
35	C	520	DGD	CBB-CCB-CDB-CEB
35	c	518	DGD	C8B-C9B-CAB-CBB
35	c	519	DGD	C8A-C9A-CAA-CBA
35	c	519	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
35	c	520	DGD	CBB-CCB-CDB-CEB
28	N	610	CLA	C3-C5-C6-C7
28	G	611	CLA	C3-C5-C6-C7
28	G	613	CLA	C3-C5-C6-C7
28	S	610	CLA	C3-C5-C6-C7
28	Y	604	CLA	C3-C5-C6-C7
28	b	604	CLA	C3-C5-C6-C7
28	b	605	CLA	C3-C5-C6-C7
28	N	602	CLA	CBA-CGA-O2A-C1
28	G	614	CLA	CBA-CGA-O2A-C1
28	S	609	CLA	CBA-CGA-O2A-C1
28	Y	602	CLA	CBA-CGA-O2A-C1
28	Y	608	CLA	CBA-CGA-O2A-C1
28	a	407	CLA	CBA-CGA-O2A-C1
28	b	606	CLA	CBA-CGA-O2A-C1
28	b	608	CLA	CBA-CGA-O2A-C1
28	b	611	CLA	CBA-CGA-O2A-C1
28	c	506	CLA	CBA-CGA-O2A-C1
32	c	523	LMG	C29-C28-O8-C9
35	B	623	DGD	C2A-C1A-O1G-C1G
36	b	624	3PH	C32-C31-O31-C3
32	d	411	LMG	O6-C5-C6-O5
28	C	510	CLA	O1D-CGD-O2D-CED
28	G	602	CLA	O1D-CGD-O2D-CED
28	S	605	CLA	O1D-CGD-O2D-CED
28	Y	611	CLA	O1D-CGD-O2D-CED
28	B	610	CLA	O1D-CGD-O2D-CED
28	B	613	CLA	O1D-CGD-O2D-CED
28	B	616	CLA	O1D-CGD-O2D-CED
28	C	509	CLA	O1D-CGD-O2D-CED
28	Y	612	CLA	O1D-CGD-O2D-CED
28	b	609	CLA	O1D-CGD-O2D-CED
36	b	624	3PH	O22-C21-O21-C2
45	I	102	4RF	O23-C22-O21-C20
41	d	405	PL9	C22-C23-C24-C26
41	d	405	PL9	C37-C38-C39-C41
28	G	602	CLA	O1A-CGA-O2A-C1
28	G	613	CLA	O1A-CGA-O2A-C1
28	S	602	CLA	O1A-CGA-O2A-C1
28	Y	603	CLA	O1A-CGA-O2A-C1
28	a	406	CLA	O1A-CGA-O2A-C1
28	b	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	c	509	CLA	O1A-CGA-O2A-C1
32	C	523	LMG	O10-C28-O8-C9
28	A	410	CLA	O1D-CGD-O2D-CED
28	B	611	CLA	O1D-CGD-O2D-CED
28	C	512	CLA	O1D-CGD-O2D-CED
28	c	507	CLA	O1D-CGD-O2D-CED
30	B	618	BCR	C9-C10-C11-C12
30	b	619	BCR	C9-C10-C11-C12
43	h	101	RRX	C15-C16-C17-C18
28	C	507	CLA	O1D-CGD-O2D-CED
38	D	409	LHG	O2-C2-C3-O3
38	G	624	LHG	O2-C2-C3-O3
38	Y	624	LHG	O2-C2-C3-O3
38	c	525	LHG	O2-C2-C3-O3
38	l	101	LHG	O2-C2-C3-O3
50	S	625	LPX	O1-C3-C4-O5
28	C	506	CLA	C3-C5-C6-C7
28	b	608	CLA	C3-C5-C6-C7
28	A	407	CLA	CBA-CGA-O2A-C1
28	B	613	CLA	CBA-CGA-O2A-C1
28	G	602	CLA	CBA-CGA-O2A-C1
28	G	613	CLA	CBA-CGA-O2A-C1
28	S	602	CLA	CBA-CGA-O2A-C1
28	Y	612	CLA	CBA-CGA-O2A-C1
28	Y	613	CLA	CBA-CGA-O2A-C1
28	a	410	CLA	CBA-CGA-O2A-C1
28	c	501	CLA	CBA-CGA-O2A-C1
28	c	509	CLA	CBA-CGA-O2A-C1
31	b	626	SQD	C24-C23-O48-C46
38	l	101	LHG	C24-C23-O8-C6
28	B	608	CLA	O1A-CGA-O2A-C1
28	C	509	CLA	O1A-CGA-O2A-C1
28	S	610	CLA	O1A-CGA-O2A-C1
28	Y	612	CLA	O1A-CGA-O2A-C1
28	c	511	CLA	O1A-CGA-O2A-C1
38	l	101	LHG	O10-C23-O8-C6
28	S	603	CLA	O1D-CGD-O2D-CED
28	b	616	CLA	O1D-CGD-O2D-CED
28	b	617	CLA	O1D-CGD-O2D-CED
50	S	625	LPX	O5-C4-C5-O6
31	m	101	SQD	C8-C7-O47-C45
32	C	523	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
36	b	624	3PH	C22-C21-O21-C2
38	N	624	LHG	C8-C7-O7-C5
28	G	604	CLA	O1D-CGD-O2D-CED
28	b	605	CLA	O1D-CGD-O2D-CED
38	C	525	LHG	C11-C12-C13-C14
28	Y	613	CLA	O1A-CGA-O2A-C1
38	c	525	LHG	C11-C12-C13-C14
28	C	501	CLA	O1D-CGD-O2D-CED
28	G	612	CLA	O1D-CGD-O2D-CED
28	S	609	CLA	C3-C5-C6-C7
28	c	509	CLA	C3-C5-C6-C7
28	c	511	CLA	C3-C5-C6-C7
28	c	512	CLA	C3-C5-C6-C7
28	d	402	CLA	C3-C5-C6-C7
28	C	506	CLA	CBA-CGA-O2A-C1
28	N	610	CLA	CBA-CGA-O2A-C1
28	a	406	CLA	CBA-CGA-O2A-C1
32	C	523	LMG	C29-C28-O8-C9
28	A	407	CLA	O1A-CGA-O2A-C1
28	B	613	CLA	O1A-CGA-O2A-C1
28	c	501	CLA	O1A-CGA-O2A-C1
42	f	101	HEM	C3D-CAD-CBD-CGD
28	C	507	CLA	C4-C3-C5-C6
28	c	501	CLA	C4-C3-C5-C6
28	d	402	CLA	C4-C3-C5-C6
28	C	507	CLA	C2-C3-C5-C6
28	b	606	CLA	C2-C3-C5-C6
28	c	501	CLA	C2-C3-C5-C6
28	d	402	CLA	C2-C3-C5-C6
28	N	602	CLA	C2A-CAA-CBA-CGA
28	c	502	CLA	C2A-CAA-CBA-CGA
28	b	613	CLA	O1D-CGD-O2D-CED
29	a	409	PHO	O1D-CGD-O2D-CED
28	B	610	CLA	O1A-CGA-O2A-C1
28	N	602	CLA	O1A-CGA-O2A-C1
28	a	407	CLA	O1A-CGA-O2A-C1
28	b	606	CLA	O1A-CGA-O2A-C1
28	b	608	CLA	O1A-CGA-O2A-C1
35	B	623	DGD	O1A-C1A-O1G-C1G
31	a	412	SQD	O5-C1-O6-C44
32	b	622	LMG	O6-C1-O1-C7
41	d	405	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
41	d	405	PL9	C19-C21-C22-C23
41	d	405	PL9	C39-C41-C42-C43
28	B	606	CLA	CBA-CGA-O2A-C1
28	B	610	CLA	CBA-CGA-O2A-C1
28	C	511	CLA	CBA-CGA-O2A-C1
36	S	626	3PH	C32-C31-O31-C3
45	K	101	4RF	C43-C41-O40-C39
38	l	101	LHG	C7-C8-C9-C10
45	I	102	4RF	C33-C34-C35-C36
28	B	617	CLA	O1D-CGD-O2D-CED
28	Y	602	CLA	O1D-CGD-O2D-CED
28	a	407	CLA	O1D-CGD-O2D-CED
28	a	410	CLA	O1D-CGD-O2D-CED
28	a	410	CLA	O1A-CGA-O2A-C1
31	B	621	SQD	C8-C7-O47-C45
28	N	603	CLA	O1D-CGD-O2D-CED
28	N	604	CLA	O1D-CGD-O2D-CED
28	B	602	CLA	CBD-CGD-O2D-CED
38	L	101	LHG	C1-C2-C3-O3
38	G	624	LHG	C1-C2-C3-O3
38	S	624	LHG	C1-C2-C3-O3
38	l	101	LHG	C1-C2-C3-O3
31	B	621	SQD	O49-C7-O47-C45
31	m	101	SQD	O49-C7-O47-C45
38	N	624	LHG	O9-C7-O7-C5
28	C	511	CLA	O1A-CGA-O2A-C1
28	D	403	CLA	C3-C5-C6-C7
28	S	603	CLA	C3-C5-C6-C7
28	c	506	CLA	C3-C5-C6-C7
28	N	611	CLA	O1D-CGD-O2D-CED
28	A	405	CLA	CBA-CGA-O2A-C1
28	B	604	CLA	CBA-CGA-O2A-C1
28	B	611	CLA	CBA-CGA-O2A-C1
28	C	503	CLA	CBA-CGA-O2A-C1
28	b	610	CLA	CBA-CGA-O2A-C1
28	b	613	CLA	CBA-CGA-O2A-C1
28	b	614	CLA	CBA-CGA-O2A-C1
28	c	503	CLA	CBA-CGA-O2A-C1
28	c	508	CLA	CBA-CGA-O2A-C1
28	c	510	CLA	CBA-CGA-O2A-C1
28	d	402	CLA	CBA-CGA-O2A-C1
31	C	526	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
31	M	101	SQD	C24-C23-O48-C46
31	m	101	SQD	C24-C23-O48-C46
35	C	520	DGD	C2A-C1A-O1G-C1G
35	c	518	DGD	C2A-C1A-O1G-C1G
36	B	624	3PH	C32-C31-O31-C3
38	L	101	LHG	C24-C23-O8-C6
43	H	101	RRX	C9-C10-C11-C12
28	G	610	CLA	C13-C15-C16-C17
28	S	611	CLA	C5-C6-C7-C8
28	N	610	CLA	O1A-CGA-O2A-C1
41	d	405	PL9	C47-C48-C49-C51
45	I	102	4RF	C31-C32-C33-C34
28	S	602	CLA	O1D-CGD-O2D-CED
36	t	101	3PH	O11-C1-C2-O21
31	b	621	SQD	C10-C11-C12-C13
28	B	602	CLA	C15-C16-C17-C18
28	B	604	CLA	C10-C11-C12-C13
28	B	607	CLA	C10-C11-C12-C13
28	B	608	CLA	C8-C10-C11-C12
28	B	610	CLA	C5-C6-C7-C8
28	B	611	CLA	C15-C16-C17-C18
28	N	613	CLA	C15-C16-C17-C18
28	G	603	CLA	C5-C6-C7-C8
28	S	603	CLA	C5-C6-C7-C8
28	S	613	CLA	C5-C6-C7-C8
28	b	604	CLA	C15-C16-C17-C18
28	b	611	CLA	C15-C16-C17-C18
28	b	613	CLA	C10-C11-C12-C13
28	c	503	CLA	C13-C15-C16-C17
38	D	410	LHG	C7-C8-C9-C10
45	I	102	4RF	C13-C14-C15-C16
31	a	412	SQD	C2-C1-O6-C44
31	c	526	SQD	C2-C1-O6-C44
35	B	623	DGD	C2D-C1D-O3G-C3G
35	b	623	DGD	C2D-C1D-O3G-C3G
28	B	611	CLA	O1A-CGA-O2A-C1
28	C	503	CLA	O1A-CGA-O2A-C1
31	C	526	SQD	O10-C23-O48-C46
31	M	101	SQD	O10-C23-O48-C46
31	m	101	SQD	O10-C23-O48-C46
28	C	501	CLA	C4-C3-C5-C6
28	B	606	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	A	405	CLA	C11-C12-C13-C14
28	B	603	CLA	C14-C13-C15-C16
28	B	605	CLA	C6-C7-C8-C9
28	C	505	CLA	C11-C10-C8-C9
28	C	513	CLA	C11-C10-C8-C9
28	D	402	CLA	C6-C7-C8-C9
28	b	602	CLA	C11-C12-C13-C14
28	b	604	CLA	C14-C13-C15-C16
28	b	605	CLA	C6-C7-C8-C9
28	b	606	CLA	C6-C7-C8-C9
28	b	608	CLA	C11-C10-C8-C9
28	b	612	CLA	C11-C12-C13-C14
28	b	616	CLA	C11-C10-C8-C9
28	d	402	CLA	C6-C7-C8-C9
28	d	403	CLA	C14-C13-C15-C16
46	N	606	CHL	C14-C13-C15-C16
46	G	609	CHL	C11-C10-C8-C9
46	Y	609	CHL	C11-C12-C13-C14
28	D	402	CLA	O1D-CGD-O2D-CED
28	B	615	CLA	C10-C11-C12-C13
28	D	403	CLA	C5-C6-C7-C8
28	Y	602	CLA	C2A-CAA-CBA-CGA
28	a	407	CLA	C2A-CAA-CBA-CGA
30	B	619	BCR	C36-C18-C19-C20
30	C	516	BCR	C36-C18-C19-C20
30	C	517	BCR	C37-C22-C23-C24
30	b	618	BCR	C36-C18-C19-C20
30	c	515	BCR	C11-C12-C13-C35
30	c	515	BCR	C36-C18-C19-C20
34	b	620	C7Z	C7-C8-C9-C19
43	H	101	RRX	C7-C8-C9-C34
47	Y	620	LUT	C31-C32-C33-C40
49	Y	623	NEX	C11-C12-C13-C20
30	C	517	BCR	C21-C22-C23-C24
30	c	515	BCR	C7-C8-C9-C10
34	b	620	C7Z	C7-C8-C9-C10
43	H	101	RRX	C7-C8-C9-C10
32	C	523	LMG	O9-C10-O7-C8
45	K	101	4RF	C31-C32-C33-C34
31	a	412	SQD	C7-C8-C9-C10
38	d	409	LHG	C7-C8-C9-C10
28	A	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	B	604	CLA	O1A-CGA-O2A-C1
28	B	613	CLA	C10-C11-C12-C13
28	S	609	CLA	C10-C11-C12-C13
28	Y	612	CLA	C8-C10-C11-C12
28	b	602	CLA	C15-C16-C17-C18
28	b	609	CLA	C5-C6-C7-C8
28	c	505	CLA	C10-C11-C12-C13
28	c	506	CLA	C13-C15-C16-C17
28	c	508	CLA	C15-C16-C17-C18
45	k	101	4RF	C12-C13-C14-C15
28	S	604	CLA	C3-C5-C6-C7
28	B	614	CLA	CBA-CGA-O2A-C1
28	b	604	CLA	CBA-CGA-O2A-C1
37	C	524	DGA	CA2-CA1-OG1-CG1
45	i	101	4RF	C43-C41-O40-C39
28	B	604	CLA	C13-C15-C16-C17
28	B	608	CLA	C13-C15-C16-C17
28	C	502	CLA	C13-C15-C16-C17
28	C	504	CLA	C10-C11-C12-C13
28	C	512	CLA	C13-C15-C16-C17
28	C	513	CLA	C10-C11-C12-C13
28	N	602	CLA	C8-C10-C11-C12
28	G	613	CLA	C13-C15-C16-C17
28	S	611	CLA	C8-C10-C11-C12
28	Y	603	CLA	C13-C15-C16-C17
28	Y	604	CLA	C8-C10-C11-C12
28	Y	610	CLA	C13-C15-C16-C17
28	Y	613	CLA	C5-C6-C7-C8
28	Y	613	CLA	C15-C16-C17-C18
28	Y	614	CLA	C8-C10-C11-C12
28	b	603	CLA	C5-C6-C7-C8
28	b	605	CLA	C8-C10-C11-C12
28	b	606	CLA	C15-C16-C17-C18
28	d	403	CLA	C8-C10-C11-C12
37	j	101	DGA	CB1-CB2-CB3-CB4
38	G	624	LHG	C7-C8-C9-C10
38	d	409	LHG	C23-C24-C25-C26
38	l	101	LHG	C23-C24-C25-C26
51	Y	626	PTY	C8-C11-C12-C13
28	B	605	CLA	C15-C16-C17-C18
28	B	614	CLA	C5-C6-C7-C8
28	C	510	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	C	512	CLA	C5-C6-C7-C8
28	N	602	CLA	C15-C16-C17-C18
28	N	613	CLA	C13-C15-C16-C17
28	G	603	CLA	C15-C16-C17-C18
28	S	603	CLA	C13-C15-C16-C17
28	Y	602	CLA	C8-C10-C11-C12
28	Y	602	CLA	C13-C15-C16-C17
28	b	602	CLA	C10-C11-C12-C13
28	b	612	CLA	C5-C6-C7-C8
28	b	617	CLA	C13-C15-C16-C17
28	c	501	CLA	C13-C15-C16-C17
28	c	503	CLA	C15-C16-C17-C18
28	c	510	CLA	C15-C16-C17-C18
28	c	511	CLA	C8-C10-C11-C12
28	c	512	CLA	C5-C6-C7-C8
28	B	609	CLA	O1D-CGD-O2D-CED
28	c	503	CLA	O1D-CGD-O2D-CED
38	D	410	LHG	O1-C1-C2-O2
38	l	101	LHG	O1-C1-C2-O2
36	B	624	3PH	O32-C31-O31-C3
31	B	621	SQD	C23-C24-C25-C26
32	A	413	LMG	C10-C11-C12-C13
32	H	102	LMG	C28-C29-C30-C31
32	b	622	LMG	C10-C11-C12-C13
32	b	622	LMG	C28-C29-C30-C31
32	h	102	LMG	C28-C29-C30-C31
35	C	518	DGD	C1B-C2B-C3B-C4B
36	S	626	3PH	C31-C32-C33-C34
37	C	524	DGA	CB1-CB2-CB3-CB4
37	J	101	DGA	CB1-CB2-CB3-CB4
37	c	524	DGA	CB1-CB2-CB3-CB4
38	C	525	LHG	C23-C24-C25-C26
38	D	408	LHG	C7-C8-C9-C10
38	D	409	LHG	C7-C8-C9-C10
38	D	410	LHG	C23-C24-C25-C26
38	N	624	LHG	C7-C8-C9-C10
38	c	525	LHG	C23-C24-C25-C26
38	d	408	LHG	C23-C24-C25-C26
38	d	410	LHG	C7-C8-C9-C10
38	d	410	LHG	C23-C24-C25-C26
45	I	102	4RF	C22-C24-C25-C26
45	i	101	4RF	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
45	k	101	4RF	C22-C24-C25-C26
28	B	614	CLA	C13-C15-C16-C17
28	C	508	CLA	C15-C16-C17-C18
28	N	613	CLA	C5-C6-C7-C8
28	G	602	CLA	C8-C10-C11-C12
28	G	610	CLA	C8-C10-C11-C12
28	Y	610	CLA	C8-C10-C11-C12
28	Y	611	CLA	C10-C11-C12-C13
28	b	606	CLA	C8-C10-C11-C12
28	c	508	CLA	C5-C6-C7-C8
28	c	512	CLA	C15-C16-C17-C18
28	B	603	CLA	C3-C5-C6-C7
28	Y	614	CLA	CBA-CGA-O2A-C1
28	c	504	CLA	CBA-CGA-O2A-C1
28	G	611	CLA	O1D-CGD-O2D-CED
28	A	406	CLA	C2-C1-O2A-CGA
28	B	602	CLA	C2-C1-O2A-CGA
28	B	608	CLA	C2-C1-O2A-CGA
28	B	614	CLA	C2-C1-O2A-CGA
28	C	509	CLA	C2-C1-O2A-CGA
28	N	611	CLA	C2-C1-O2A-CGA
28	G	604	CLA	C2-C1-O2A-CGA
28	G	611	CLA	C2-C1-O2A-CGA
28	G	614	CLA	C2-C1-O2A-CGA
28	Y	603	CLA	C2-C1-O2A-CGA
28	Y	604	CLA	C2-C1-O2A-CGA
28	Y	614	CLA	C2-C1-O2A-CGA
28	a	407	CLA	C2-C1-O2A-CGA
28	b	602	CLA	C2-C1-O2A-CGA
28	b	605	CLA	C2-C1-O2A-CGA
28	b	608	CLA	C2-C1-O2A-CGA
28	b	614	CLA	C2-C1-O2A-CGA
28	B	608	CLA	C5-C6-C7-C8
28	B	609	CLA	C5-C6-C7-C8
28	N	603	CLA	C13-C15-C16-C17
28	N	604	CLA	C10-C11-C12-C13
28	N	613	CLA	C8-C10-C11-C12
28	G	603	CLA	C8-C10-C11-C12
28	Y	604	CLA	C13-C15-C16-C17
28	b	615	CLA	C10-C11-C12-C13
28	b	617	CLA	C10-C11-C12-C13
31	c	526	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
45	k	101	4RF	C41-C43-C44-C45
28	A	406	CLA	CBD-CGD-O2D-CED
46	G	608	CHL	C2A-CAA-CBA-CGA
31	c	526	SQD	C8-C7-O47-C45
28	C	503	CLA	C15-C16-C17-C18
28	C	506	CLA	C5-C6-C7-C8
28	G	611	CLA	C10-C11-C12-C13
28	A	406	CLA	C11-C12-C13-C15
28	b	604	CLA	C11-C12-C13-C15
46	G	601	CHL	C12-C13-C15-C16
28	a	406	CLA	C3-C5-C6-C7
28	B	606	CLA	O1A-CGA-O2A-C1
28	b	610	CLA	O1A-CGA-O2A-C1
28	b	614	CLA	O1A-CGA-O2A-C1
28	c	508	CLA	O1A-CGA-O2A-C1
28	c	510	CLA	O1A-CGA-O2A-C1
28	d	402	CLA	O1A-CGA-O2A-C1
38	L	101	LHG	O10-C23-O8-C6
30	B	619	BCR	C19-C20-C21-C22
30	b	618	BCR	C9-C10-C11-C12
30	c	514	BCR	C15-C16-C17-C18
30	c	516	BCR	C19-C20-C21-C22
30	c	517	BCR	C9-C10-C11-C12
30	d	404	BCR	C9-C10-C11-C12
47	G	621	LUT	C29-C30-C31-C32
47	S	621	LUT	C29-C30-C31-C32
28	A	407	CLA	C2A-CAA-CBA-CGA
28	B	602	CLA	C2A-CAA-CBA-CGA
29	A	408	PHO	C2A-CAA-CBA-CGA
46	N	606	CHL	C2A-CAA-CBA-CGA
46	S	608	CHL	C2A-CAA-CBA-CGA
46	Y	607	CHL	C2A-CAA-CBA-CGA
28	c	512	CLA	O1D-CGD-O2D-CED
28	C	510	CLA	C5-C6-C7-C8
28	C	510	CLA	C8-C10-C11-C12
28	C	513	CLA	C8-C10-C11-C12
28	N	602	CLA	C13-C15-C16-C17
28	S	602	CLA	C10-C11-C12-C13
28	b	604	CLA	C8-C10-C11-C12
28	b	607	CLA	C10-C11-C12-C13
28	b	612	CLA	C8-C10-C11-C12
28	b	615	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	c	504	CLA	C13-C15-C16-C17
28	c	504	CLA	C15-C16-C17-C18
38	c	525	LHG	C33-C34-C35-C36
28	b	613	CLA	O1A-CGA-O2A-C1
28	c	503	CLA	O1A-CGA-O2A-C1
35	C	520	DGD	O1A-C1A-O1G-C1G
35	c	518	DGD	O1A-C1A-O1G-C1G
31	B	626	SQD	O5-C1-O6-C44
35	C	519	DGD	O6E-C1E-O5D-C6D
28	G	602	CLA	C13-C15-C16-C17
28	c	506	CLA	C8-C10-C11-C12
38	S	624	LHG	C9-C10-C11-C12
35	c	518	DGD	C1B-C2B-C3B-C4B
30	c	515	BCR	C10-C11-C12-C13
48	Y	622	XAT	C10-C11-C12-C13
49	Y	623	NEX	C30-C31-C32-C33
38	C	525	LHG	O2-C2-C3-O3
38	L	101	LHG	O2-C2-C3-O3
38	d	408	LHG	O2-C2-C3-O3
31	M	101	SQD	O49-C7-O47-C45
31	b	621	SQD	O49-C7-O47-C45
28	B	608	CLA	C15-C16-C17-C18
28	B	610	CLA	C8-C10-C11-C12
28	B	617	CLA	C15-C16-C17-C18
28	C	508	CLA	C13-C15-C16-C17
28	N	603	CLA	C8-C10-C11-C12
28	G	611	CLA	C15-C16-C17-C18
28	Y	611	CLA	C15-C16-C17-C18
28	Y	614	CLA	C5-C6-C7-C8
28	b	608	CLA	C10-C11-C12-C13
28	c	501	CLA	C15-C16-C17-C18
28	c	512	CLA	C10-C11-C12-C13
36	S	626	3PH	O32-C31-O31-C3
38	C	525	LHG	C33-C34-C35-C36
38	D	409	LHG	C9-C10-C11-C12
28	A	410	CLA	C8-C10-C11-C12
28	A	410	CLA	C10-C11-C12-C13
28	B	612	CLA	C15-C16-C17-C18
28	C	502	CLA	C5-C6-C7-C8
28	C	508	CLA	C5-C6-C7-C8
28	b	609	CLA	C8-C10-C11-C12
28	b	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	a	406	CLA	O1D-CGD-O2D-CED
28	B	614	CLA	O1A-CGA-O2A-C1
28	c	504	CLA	O1A-CGA-O2A-C1
37	C	524	DGA	OA1-CA1-OG1-CG1
45	K	101	4RF	O42-C41-O40-C39
45	i	101	4RF	O42-C41-O40-C39
31	M	101	SQD	C8-C7-O47-C45
31	b	621	SQD	C8-C7-O47-C45
31	b	626	SQD	C8-C7-O47-C45
32	A	413	LMG	C11-C10-O7-C8
38	G	624	LHG	C8-C7-O7-C5
28	B	602	CLA	C13-C15-C16-C17
28	B	612	CLA	C5-C6-C7-C8
28	B	612	CLA	C13-C15-C16-C17
28	C	507	CLA	C15-C16-C17-C18
28	C	508	CLA	C8-C10-C11-C12
28	G	613	CLA	C5-C6-C7-C8
28	S	610	CLA	C10-C11-C12-C13
28	b	610	CLA	C5-C6-C7-C8
28	b	616	CLA	C13-C15-C16-C17
28	c	506	CLA	C5-C6-C7-C8
28	d	403	CLA	C13-C15-C16-C17
46	N	606	CHL	C5-C6-C7-C8
38	C	525	LHG	C4-O6-P-O3
38	D	409	LHG	C4-O6-P-O3
38	D	410	LHG	C3-O3-P-O6
38	D	410	LHG	C4-O6-P-O3
38	N	624	LHG	C4-O6-P-O3
38	G	624	LHG	C4-O6-P-O3
38	Y	624	LHG	C4-O6-P-O3
38	c	525	LHG	C4-O6-P-O3
38	d	408	LHG	C3-O3-P-O6
38	d	410	LHG	C3-O3-P-O6
50	S	625	LPX	C1-O2-P1-O1
51	Y	627	PTY	C5-O14-P1-O11
38	L	101	LHG	C7-C8-C9-C10
28	C	510	CLA	CBA-CGA-O2A-C1
28	a	405	CLA	CBA-CGA-O2A-C1
28	B	608	CLA	C10-C11-C12-C13
28	C	510	CLA	C13-C15-C16-C17
28	d	403	CLA	C10-C11-C12-C13
31	m	101	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
38	C	525	LHG	C1-C2-C3-O3
38	D	409	LHG	C1-C2-C3-O3
38	d	408	LHG	C1-C2-C3-O3
31	b	626	SQD	O49-C7-O47-C45
31	c	526	SQD	O49-C7-O47-C45
32	A	413	LMG	O9-C10-O7-C8
38	G	624	LHG	O9-C7-O7-C5
28	Y	611	CLA	C4-C3-C5-C6
46	N	601	CHL	C4-C3-C5-C6
28	S	609	CLA	C5-C6-C7-C8
28	S	611	CLA	C13-C15-C16-C17
28	Y	602	CLA	C15-C16-C17-C18
28	b	604	CLA	C13-C15-C16-C17
28	c	512	CLA	C13-C15-C16-C17
38	S	624	LHG	C30-C31-C32-C33
28	B	604	CLA	C2A-CAA-CBA-CGA
28	C	505	CLA	C2A-CAA-CBA-CGA
28	C	507	CLA	C2A-CAA-CBA-CGA
28	S	603	CLA	C2A-CAA-CBA-CGA
28	S	613	CLA	C2A-CAA-CBA-CGA
28	Y	613	CLA	C2A-CAA-CBA-CGA
28	c	505	CLA	C2A-CAA-CBA-CGA
28	C	507	CLA	C16-C17-C18-C20
28	D	402	CLA	C16-C17-C18-C19
28	G	613	CLA	C16-C17-C18-C20
28	c	511	CLA	C16-C17-C18-C19
28	B	602	CLA	CBA-CGA-O2A-C1
28	G	603	CLA	CBA-CGA-O2A-C1
38	d	408	LHG	C24-C23-O8-C6
28	D	402	CLA	C15-C16-C17-C18
28	b	608	CLA	C13-C15-C16-C17
47	N	621	LUT	C29-C30-C31-C32
33	a	414	SPH	C5-C6-C7-C8
38	D	409	LHG	C23-C24-C25-C26
37	c	524	DGA	CA4-CA5-CA6-CA7
45	k	101	4RF	C29-C30-C31-C32
32	h	102	LMG	C11-C10-O7-C8
28	C	505	CLA	C8-C10-C11-C12
28	b	604	CLA	C10-C11-C12-C13
49	G	623	NEX	C39-C29-C30-C31
49	G	623	NEX	C40-C33-C34-C35
49	Y	623	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
31	A	412	SQD	C13-C14-C15-C16
35	c	519	DGD	C4B-C5B-C6B-C7B
36	B	624	3PH	C29-C2A-C2B-C2C
36	t	101	3PH	C2A-C2B-C2C-C2D
37	C	524	DGA	CB7-CB8-CB9-CAB
37	J	101	DGA	CB7-CB8-CB9-CAB
38	D	408	LHG	C30-C31-C32-C33
28	C	509	CLA	C16-C17-C18-C19
28	C	513	CLA	C16-C17-C18-C19
28	b	602	CLA	C16-C17-C18-C20
28	b	609	CLA	C16-C17-C18-C20
28	d	402	CLA	C16-C17-C18-C20
36	B	624	3PH	C3C-C3D-C3E-C3F
36	T	101	3PH	C29-C2A-C2B-C2C
37	B	625	DGA	CB9-CAB-CBB-CCB
37	c	524	DGA	CA2-CA3-CA4-CA5
37	c	524	DGA	CB7-CB8-CB9-CAB
38	C	525	LHG	C29-C30-C31-C32
38	D	408	LHG	C25-C26-C27-C28
38	N	624	LHG	C33-C34-C35-C36
38	S	624	LHG	C12-C13-C14-C15
38	Y	624	LHG	C13-C14-C15-C16
45	I	102	4RF	C46-C47-C48-C49
45	i	101	4RF	C07-C08-C09-C10
45	k	101	4RF	C26-C27-C28-C29
32	h	102	LMG	O9-C10-O7-C8
31	M	101	SQD	C7-C8-C9-C10
31	a	412	SQD	C30-C31-C32-C33
36	b	624	3PH	C37-C38-C39-C3A
37	c	524	DGA	CA5-CA6-CA7-CA8
37	c	524	DGA	CAA-CBA-CCA-CDA
37	c	524	DGA	CEA-CFA-CGA-CHA
37	c	524	DGA	CBB-CAB-CB9-CB8
38	L	101	LHG	C26-C27-C28-C29
38	G	624	LHG	C13-C14-C15-C16
38	d	408	LHG	C28-C29-C30-C31
38	d	408	LHG	C30-C31-C32-C33
38	l	101	LHG	C11-C12-C13-C14
45	i	101	4RF	C05-C06-C07-C08
28	Y	614	CLA	O1A-CGA-O2A-C1
36	S	626	3PH	C2B-C2C-C2D-C2E
37	b	625	DGA	CB7-CB8-CB9-CAB

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Mol	Chain	Res	Type	Atoms
38	D	408	LHG	C33-C34-C35-C36
51	Y	626	PTY	C19-C20-C21-C22
31	b	621	SQD	C11-C10-C9-C8
36	T	101	3PH	C2B-C2C-C2D-C2E
37	c	524	DGA	CA6-CA7-CA8-CA9
37	j	101	DGA	CB7-CB8-CB9-CAB
38	S	624	LHG	C13-C14-C15-C16
45	K	101	4RF	C24-C25-C26-C27
28	A	410	CLA	C3-C5-C6-C7
28	b	602	CLA	C3-C5-C6-C7
31	b	626	SQD	C7-C8-C9-C10
32	w	201	LMG	C28-C29-C30-C31
31	B	626	SQD	C2-C1-O6-C44
32	B	622	LMG	C2-C1-O1-C7
35	C	519	DGD	C2E-C1E-O5D-C6D
49	G	623	NEX	C28-C29-C30-C31
49	G	623	NEX	C32-C33-C34-C35
49	Y	623	NEX	C28-C29-C30-C31
39	c	527	LMK	O7-C8-C9-O8
28	C	508	CLA	CBA-CGA-O2A-C1
28	b	612	CLA	CBA-CGA-O2A-C1
35	C	518	DGD	C3A-C4A-C5A-C6A
36	B	624	3PH	C2B-C2C-C2D-C2E
38	N	624	LHG	C13-C14-C15-C16
38	G	624	LHG	C11-C10-C9-C8
45	K	101	4RF	C26-C27-C28-C29
45	K	101	4RF	C46-C47-C48-C49
28	C	507	CLA	C13-C15-C16-C17
28	Y	613	CLA	C10-C11-C12-C13
28	a	405	CLA	C5-C6-C7-C8
28	G	603	CLA	O1A-CGA-O2A-C1
28	b	604	CLA	O1A-CGA-O2A-C1
28	Y	610	CLA	C16-C17-C18-C20
36	b	624	3PH	C28-C29-C2A-C2B
38	L	101	LHG	C11-C10-C9-C8
38	c	525	LHG	C24-C25-C26-C27
45	I	102	4RF	C07-C08-C09-C10
45	K	101	4RF	C44-C45-C46-C47
28	c	504	CLA	C2-C3-C5-C6
28	B	602	CLA	C11-C12-C13-C14
28	B	605	CLA	C11-C10-C8-C9
28	C	503	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	C	513	CLA	C11-C12-C13-C14
28	a	406	CLA	C11-C12-C13-C14
28	d	403	CLA	C11-C12-C13-C14
46	G	601	CHL	C11-C12-C13-C14
46	G	601	CHL	C14-C13-C15-C16
46	G	607	CHL	C14-C13-C15-C16
38	D	408	LHG	C23-C24-C25-C26
38	L	101	LHG	C23-C24-C25-C26
38	N	624	LHG	C23-C24-C25-C26
38	c	525	LHG	C7-C8-C9-C10
31	c	526	SQD	C17-C18-C19-C20
32	C	523	LMG	C18-C19-C20-C21
36	B	624	3PH	C24-C25-C26-C27
36	B	624	3PH	C3D-C3E-C3F-C3G
37	J	101	DGA	CB5-CB6-CB7-CB8
37	b	625	DGA	CA9-CAA-CBA-CCA
38	S	624	LHG	C11-C12-C13-C14
38	l	101	LHG	C28-C29-C30-C31
45	I	102	4RF	C32-C33-C34-C35
28	G	602	CLA	C10-C11-C12-C13
28	b	614	CLA	C15-C16-C17-C18
28	c	506	CLA	C10-C11-C12-C13
28	Y	608	CLA	C2A-CAA-CBA-CGA
28	a	406	CLA	C2A-CAA-CBA-CGA
28	c	501	CLA	C2A-CAA-CBA-CGA
46	N	608	CHL	C2A-CAA-CBA-CGA
30	a	411	BCR	C11-C12-C13-C35
30	d	404	BCR	C37-C22-C23-C24
34	B	620	C7Z	C7-C8-C9-C19
32	H	102	LMG	C13-C14-C15-C16
35	c	520	DGD	C5A-C6A-C7A-C8A
36	B	624	3PH	C25-C26-C27-C28
37	c	524	DGA	CAB-CBB-CCB-CDB
38	N	624	LHG	C14-C15-C16-C17
38	l	101	LHG	C26-C27-C28-C29
45	K	101	4RF	C45-C46-C47-C48
45	i	101	4RF	C09-C10-C11-C12
51	Y	626	PTY	C39-C40-C41-C42
38	C	525	LHG	O1-C1-C2-C3
38	D	409	LHG	O1-C1-C2-C3
38	D	410	LHG	O1-C1-C2-C3
38	L	101	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	G	624	LHG	O1-C1-C2-C3
38	Y	624	LHG	O1-C1-C2-C3
38	c	525	LHG	O1-C1-C2-C3
38	d	409	LHG	O1-C1-C2-C3
30	b	619	BCR	C17-C18-C19-C20
30	d	404	BCR	C21-C22-C23-C24
34	B	620	C7Z	C7-C8-C9-C10
28	B	617	CLA	C3-C5-C6-C7
28	Y	611	CLA	C3-C5-C6-C7
32	C	521	LMG	O9-C10-O7-C8
38	C	525	LHG	O9-C7-O7-C5
28	C	503	CLA	C8-C10-C11-C12
28	d	402	CLA	C15-C16-C17-C18
31	B	626	SQD	C8-C7-O47-C45
32	C	521	LMG	C11-C10-O7-C8
38	C	525	LHG	C8-C7-O7-C5
31	B	626	SQD	C16-C17-C18-C19
32	c	521	LMG	C11-C12-C13-C14
33	Y	625	SPH	C14-C15-C16-C17
38	D	409	LHG	C11-C12-C13-C14
38	S	624	LHG	C23-C24-C25-C26
31	A	412	SQD	C11-C12-C13-C14
31	b	621	SQD	C9-C10-C11-C12
32	w	201	LMG	C36-C37-C38-C39
36	t	101	3PH	C2B-C2C-C2D-C2E
37	B	625	DGA	CA4-CA5-CA6-CA7
37	J	101	DGA	CA4-CA5-CA6-CA7
37	c	524	DGA	CB3-CB4-CB5-CB6
38	C	525	LHG	C28-C29-C30-C31
38	D	408	LHG	C11-C12-C13-C14
38	Y	624	LHG	C16-C17-C18-C19
38	c	525	LHG	C13-C14-C15-C16
38	c	525	LHG	C26-C27-C28-C29
45	i	101	4RF	C43-C44-C45-C46
32	H	102	LMG	O6-C5-C6-O5
28	B	603	CLA	C4B-C3B-CAB-CBB
28	B	616	CLA	C4B-C3B-CAB-CBB
28	C	501	CLA	C4B-C3B-CAB-CBB
28	C	504	CLA	C4B-C3B-CAB-CBB
28	C	510	CLA	C4B-C3B-CAB-CBB
28	C	513	CLA	C4B-C3B-CAB-CBB
28	N	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	N	611	CLA	C4B-C3B-CAB-CBB
28	N	612	CLA	C4B-C3B-CAB-CBB
28	N	614	CLA	C4B-C3B-CAB-CBB
28	G	604	CLA	C4B-C3B-CAB-CBB
28	G	612	CLA	C4B-C3B-CAB-CBB
28	G	613	CLA	C4B-C3B-CAB-CBB
28	S	605	CLA	C4B-C3B-CAB-CBB
28	S	610	CLA	C4B-C3B-CAB-CBB
28	S	611	CLA	C4B-C3B-CAB-CBB
28	S	613	CLA	C4B-C3B-CAB-CBB
28	S	617	CLA	C4B-C3B-CAB-CBB
28	Y	603	CLA	C4B-C3B-CAB-CBB
28	Y	608	CLA	C4B-C3B-CAB-CBB
28	Y	614	CLA	C4B-C3B-CAB-CBB
28	b	602	CLA	C4B-C3B-CAB-CBB
28	b	603	CLA	C4B-C3B-CAB-CBB
28	b	605	CLA	C4B-C3B-CAB-CBB
28	b	606	CLA	C4B-C3B-CAB-CBB
28	b	607	CLA	C4B-C3B-CAB-CBB
28	c	510	CLA	C4B-C3B-CAB-CBB
28	C	509	CLA	C16-C17-C18-C20
28	D	402	CLA	C16-C17-C18-C20
28	G	602	CLA	C16-C17-C18-C19
28	G	602	CLA	C16-C17-C18-C20
28	G	611	CLA	C16-C17-C18-C19
28	G	611	CLA	C16-C17-C18-C20
28	G	613	CLA	C16-C17-C18-C19
28	Y	613	CLA	C16-C17-C18-C19
28	c	501	CLA	C16-C17-C18-C19
28	c	501	CLA	C16-C17-C18-C20
28	c	507	CLA	C16-C17-C18-C19
28	c	507	CLA	C16-C17-C18-C20
31	M	101	SQD	O5-C1-O6-C44
31	c	526	SQD	O5-C1-O6-C44
28	c	505	CLA	C5-C6-C7-C8
28	c	506	CLA	C15-C16-C17-C18
31	B	626	SQD	C28-C29-C30-C31
36	S	626	3PH	C24-C25-C26-C27
36	t	101	3PH	C27-C28-C29-C2A
37	J	101	DGA	CA2-CA3-CA4-CA5
37	j	101	DGA	CB6-CB7-CB8-CB9
38	Y	624	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
38	Y	624	LHG	C31-C32-C33-C34
38	c	525	LHG	C29-C30-C31-C32
45	K	101	4RF	C10-C11-C12-C13
45	k	101	4RF	C27-C28-C29-C30
33	Y	625	SPH	C11-C10-C9-C8
33	a	414	SPH	C7-C8-C9-C10
36	b	624	3PH	C3E-C3F-C3G-C3H
37	B	625	DGA	CA5-CA6-CA7-CA8
38	Y	624	LHG	C29-C30-C31-C32
38	d	409	LHG	C28-C29-C30-C31
45	K	101	4RF	C27-C28-C29-C30
45	i	101	4RF	C22-C24-C25-C26
28	B	602	CLA	C10-C11-C12-C13
28	c	508	CLA	C10-C11-C12-C13
28	C	510	CLA	O1A-CGA-O2A-C1
28	a	405	CLA	O1A-CGA-O2A-C1
33	A	414	SPH	C12-C13-C14-C15
38	l	101	LHG	C13-C14-C15-C16
28	C	504	CLA	CBA-CGA-O2A-C1
28	S	603	CLA	CBA-CGA-O2A-C1
28	Y	610	CLA	CBA-CGA-O2A-C1
31	A	412	SQD	C24-C23-O48-C46
32	d	411	LMG	C19-C20-C21-C22
36	S	626	3PH	C29-C2A-C2B-C2C
37	c	524	DGA	CA8-CA9-CAA-CBA
51	Y	626	PTY	C36-C37-C38-C39
28	B	609	CLA	C3A-C2A-CAA-CBA
28	B	613	CLA	C3A-C2A-CAA-CBA
28	C	507	CLA	C3A-C2A-CAA-CBA
28	C	512	CLA	C3A-C2A-CAA-CBA
28	C	513	CLA	C3A-C2A-CAA-CBA
28	N	603	CLA	C3A-C2A-CAA-CBA
28	N	614	CLA	C3A-C2A-CAA-CBA
28	G	603	CLA	C3A-C2A-CAA-CBA
28	S	605	CLA	C3A-C2A-CAA-CBA
28	Y	603	CLA	C3A-C2A-CAA-CBA
28	c	507	CLA	C3A-C2A-CAA-CBA
28	c	513	CLA	C3A-C2A-CAA-CBA
29	A	408	PHO	C3A-C2A-CAA-CBA
46	G	606	CHL	C3A-C2A-CAA-CBA
46	G	607	CHL	C3A-C2A-CAA-CBA
30	C	515	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	b	625	DGA	CA4-CA5-CA6-CA7
37	b	625	DGA	CDB-CEB-CFB-CGB
37	c	524	DGA	CB9-CAB-CBB-CCB
38	D	409	LHG	C10-C11-C12-C13
28	C	501	CLA	C16-C17-C18-C20
28	C	513	CLA	C16-C17-C18-C20
32	h	102	LMG	C12-C13-C14-C15
33	Y	625	SPH	C6-C7-C8-C9
37	b	625	DGA	CA6-CA7-CA8-CA9
38	D	409	LHG	C25-C26-C27-C28
38	D	409	LHG	C28-C29-C30-C31
38	Y	624	LHG	C11-C10-C9-C8
38	l	101	LHG	C11-C10-C9-C8
45	I	102	4RF	C44-C45-C46-C47
32	b	622	LMG	C7-C8-C9-O8
38	Y	624	LHG	C4-C5-C6-O8
31	B	626	SQD	O49-C7-O47-C45
38	d	408	LHG	C11-C12-C13-C14
28	C	511	CLA	C3-C5-C6-C7
38	L	101	LHG	C9-C10-C11-C12
38	G	624	LHG	C28-C29-C30-C31
45	k	101	4RF	C34-C35-C36-C37
51	Y	626	PTY	C22-C23-C24-C25
29	A	408	PHO	C4-C3-C5-C6
29	a	408	PHO	C4-C3-C5-C6
46	Y	607	CHL	C4-C3-C5-C6
29	A	408	PHO	C2-C3-C5-C6
29	a	408	PHO	C2-C3-C5-C6
46	Y	607	CHL	C2-C3-C5-C6
36	B	624	3PH	C22-C21-O21-C2
35	C	519	DGD	C4B-C5B-C6B-C7B
37	c	524	DGA	CB5-CB6-CB7-CB8
38	D	408	LHG	O1-C1-C2-O2
38	D	409	LHG	O1-C1-C2-O2
38	G	624	LHG	O1-C1-C2-O2
38	S	624	LHG	O1-C1-C2-O2
38	c	525	LHG	O1-C1-C2-O2
38	d	408	LHG	O1-C1-C2-O2
38	d	409	LHG	O1-C1-C2-O2
38	d	410	LHG	O1-C1-C2-O2
39	C	527	LMK	O9-C10-C11-C12
44	I	101	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	Y	610	CLA	C5-C6-C7-C8
32	D	411	LMG	C19-C20-C21-C22
36	T	101	3PH	C24-C25-C26-C27
36	T	101	3PH	C25-C26-C27-C28
38	N	624	LHG	C28-C29-C30-C31
38	c	525	LHG	C25-C26-C27-C28
38	d	409	LHG	C13-C14-C15-C16
28	B	602	CLA	O1A-CGA-O2A-C1
38	d	408	LHG	O10-C23-O8-C6
28	b	602	CLA	C16-C17-C18-C19
28	c	513	CLA	C16-C17-C18-C19
28	d	402	CLA	C16-C17-C18-C19
28	A	407	CLA	C2B-C3B-CAB-CBB
28	B	603	CLA	C2B-C3B-CAB-CBB
28	B	616	CLA	C2B-C3B-CAB-CBB
28	C	501	CLA	C2B-C3B-CAB-CBB
28	C	504	CLA	C2B-C3B-CAB-CBB
28	C	513	CLA	C2B-C3B-CAB-CBB
28	N	603	CLA	C2B-C3B-CAB-CBB
28	N	611	CLA	C2B-C3B-CAB-CBB
28	N	612	CLA	C2B-C3B-CAB-CBB
28	N	614	CLA	C2B-C3B-CAB-CBB
28	G	612	CLA	C2B-C3B-CAB-CBB
28	G	613	CLA	C2B-C3B-CAB-CBB
28	S	605	CLA	C2B-C3B-CAB-CBB
28	S	610	CLA	C2B-C3B-CAB-CBB
28	S	611	CLA	C2B-C3B-CAB-CBB
28	S	613	CLA	C2B-C3B-CAB-CBB
28	S	617	CLA	C2B-C3B-CAB-CBB
28	Y	603	CLA	C2B-C3B-CAB-CBB
28	Y	608	CLA	C2B-C3B-CAB-CBB
28	a	407	CLA	C2B-C3B-CAB-CBB
28	b	602	CLA	C2B-C3B-CAB-CBB
28	b	603	CLA	C2B-C3B-CAB-CBB
28	b	605	CLA	C2B-C3B-CAB-CBB
28	b	606	CLA	C2B-C3B-CAB-CBB
28	b	607	CLA	C2B-C3B-CAB-CBB
28	b	613	CLA	C2B-C3B-CAB-CBB
28	b	616	CLA	C2B-C3B-CAB-CBB
28	c	507	CLA	C2B-C3B-CAB-CBB
28	c	510	CLA	C2B-C3B-CAB-CBB
28	Y	612	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	b	603	CLA	C8-C10-C11-C12
37	B	625	DGA	CA3-CA4-CA5-CA6
37	B	625	DGA	CB3-CB4-CB5-CB6
51	Y	626	PTY	C40-C41-C42-C43
28	C	508	CLA	C3-C5-C6-C7
35	c	518	DGD	O6E-C5E-C6E-O5E
31	b	621	SQD	C24-C23-O48-C46
37	C	524	DGA	CA9-CAA-CBA-CCA
38	d	408	LHG	C13-C14-C15-C16
38	d	408	LHG	C25-C26-C27-C28
28	Y	611	CLA	C13-C15-C16-C17
38	D	410	LHG	C1-C2-C3-O3
31	B	621	SQD	C13-C14-C15-C16
31	m	101	SQD	C27-C28-C29-C30
35	C	519	DGD	C3A-C4A-C5A-C6A
38	c	525	LHG	C28-C29-C30-C31
45	k	101	4RF	C28-C29-C30-C31
36	B	624	3PH	O22-C21-O21-C2
28	B	606	CLA	C2-C1-O2A-CGA
28	B	616	CLA	C2-C1-O2A-CGA
28	B	617	CLA	C2-C1-O2A-CGA
28	C	502	CLA	C2-C1-O2A-CGA
28	C	503	CLA	C2-C1-O2A-CGA
28	C	507	CLA	C2-C1-O2A-CGA
28	C	510	CLA	C2-C1-O2A-CGA
28	N	613	CLA	C2-C1-O2A-CGA
28	S	614	CLA	C2-C1-O2A-CGA
28	b	611	CLA	C2-C1-O2A-CGA
28	b	617	CLA	C2-C1-O2A-CGA
28	c	502	CLA	C2-C1-O2A-CGA
28	c	503	CLA	C2-C1-O2A-CGA
28	c	504	CLA	C2-C1-O2A-CGA
28	c	510	CLA	C2-C1-O2A-CGA
37	C	524	DGA	CA6-CA7-CA8-CA9
38	D	408	LHG	C26-C27-C28-C29
38	d	409	LHG	C34-C35-C36-C37
45	K	101	4RF	C11-C12-C13-C14
28	D	403	CLA	C8-C10-C11-C12
31	A	412	SQD	O10-C23-O48-C46
38	L	101	LHG	C16-C17-C18-C19
38	N	624	LHG	C25-C26-C27-C28
38	l	101	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	S	604	CLA	C6-C7-C8-C9
28	b	605	CLA	C16-C17-C18-C19
37	c	524	DGA	CA1-CA2-CA3-CA4
45	k	101	4RF	C13-C14-C15-C16
30	A	411	BCR	C23-C24-C25-C26
30	A	411	BCR	C23-C24-C25-C30
30	C	514	BCR	C1-C6-C7-C8
30	C	514	BCR	C5-C6-C7-C8
30	C	515	BCR	C1-C6-C7-C8
30	C	515	BCR	C5-C6-C7-C8
30	C	516	BCR	C23-C24-C25-C26
30	C	517	BCR	C23-C24-C25-C30
30	D	404	BCR	C1-C6-C7-C8
30	D	404	BCR	C5-C6-C7-C8
30	a	411	BCR	C23-C24-C25-C26
30	a	411	BCR	C23-C24-C25-C30
30	b	619	BCR	C23-C24-C25-C26
30	c	514	BCR	C1-C6-C7-C8
30	c	514	BCR	C5-C6-C7-C8
30	c	515	BCR	C23-C24-C25-C26
30	c	515	BCR	C23-C24-C25-C30
30	c	516	BCR	C1-C6-C7-C8
30	c	516	BCR	C5-C6-C7-C8
30	c	516	BCR	C23-C24-C25-C26
30	c	516	BCR	C23-C24-C25-C30
30	d	404	BCR	C1-C6-C7-C8
30	d	404	BCR	C5-C6-C7-C8
34	B	620	C7Z	C1-C6-C7-C8
34	B	620	C7Z	C5-C6-C7-C8
34	B	620	C7Z	C21-C26-C27-C28
34	B	620	C7Z	C25-C26-C27-C28
34	b	620	C7Z	C1-C6-C7-C8
34	b	620	C7Z	C5-C6-C7-C8
34	b	620	C7Z	C25-C26-C27-C28
43	H	101	RRX	C5-C6-C7-C8
47	N	620	LUT	C5-C6-C7-C8
38	D	410	LHG	C24-C23-O8-C6
38	c	525	LHG	C24-C23-O8-C6
45	k	101	4RF	C43-C41-O40-C39
28	C	501	CLA	C5-C6-C7-C8
28	C	511	CLA	C8-C10-C11-C12
28	C	513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	N	604	CLA	C13-C15-C16-C17
28	S	611	CLA	C15-C16-C17-C18
28	Y	602	CLA	C5-C6-C7-C8
37	b	625	DGA	CB9-CAB-CBB-CCB
38	d	410	LHG	C33-C34-C35-C36
45	k	101	4RF	C24-C25-C26-C27
28	C	508	CLA	O1A-CGA-O2A-C1
28	S	603	CLA	O1A-CGA-O2A-C1
36	t	101	3PH	C22-C23-C24-C25
38	C	525	LHG	C26-C27-C28-C29
41	d	405	PL9	C47-C48-C49-C50
28	B	614	CLA	C8-C10-C11-C12
28	B	616	CLA	C10-C11-C12-C13
37	C	524	DGA	CB9-CAB-CBB-CCB
28	N	603	CLA	C4-C3-C5-C6
28	c	510	CLA	C4-C3-C5-C6
41	D	405	PL9	C40-C39-C41-C42
28	B	603	CLA	C12-C13-C15-C16
28	B	605	CLA	C6-C7-C8-C10
28	B	605	CLA	C11-C10-C8-C7
28	B	613	CLA	C12-C13-C15-C16
28	B	615	CLA	C6-C7-C8-C10
28	C	501	CLA	C2-C3-C5-C6
28	C	503	CLA	C6-C7-C8-C10
28	C	505	CLA	C6-C7-C8-C10
28	C	513	CLA	C11-C12-C13-C15
28	N	613	CLA	C2-C3-C5-C6
28	S	603	CLA	C11-C10-C8-C7
28	a	406	CLA	C11-C12-C13-C15
28	b	605	CLA	C6-C7-C8-C10
28	b	608	CLA	C11-C12-C13-C15
28	b	610	CLA	C11-C12-C13-C15
28	c	509	CLA	C12-C13-C15-C16
28	c	510	CLA	C2-C3-C5-C6
28	c	511	CLA	C11-C12-C13-C15
28	d	402	CLA	C6-C7-C8-C10
28	d	402	CLA	C11-C12-C13-C15
28	d	403	CLA	C11-C10-C8-C7
41	D	405	PL9	C38-C39-C41-C42
41	d	405	PL9	C13-C14-C16-C17
28	C	504	CLA	O1A-CGA-O2A-C1
28	Y	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	b	612	CLA	O1A-CGA-O2A-C1
36	T	101	3PH	C37-C38-C39-C3A
38	N	624	LHG	C11-C12-C13-C14
28	B	617	CLA	C10-C11-C12-C13
28	C	507	CLA	C5-C6-C7-C8
28	S	611	CLA	C10-C11-C12-C13
28	b	616	CLA	C8-C10-C11-C12
28	c	503	CLA	C8-C10-C11-C12
38	l	101	LHG	C5-C6-O8-C23
30	B	618	BCR	C13-C14-C15-C16
30	C	514	BCR	C15-C16-C17-C18
30	C	516	BCR	C9-C10-C11-C12
30	C	517	BCR	C9-C10-C11-C12
28	N	610	CLA	C16-C17-C18-C20
38	D	410	LHG	O9-C7-O7-C5
38	Y	624	LHG	O9-C7-O7-C5
36	b	624	3PH	C21-C22-C23-C24
28	A	410	CLA	CBA-CGA-O2A-C1
28	G	610	CLA	CBA-CGA-O2A-C1
38	C	525	LHG	C30-C31-C32-C33
28	b	604	CLA	C2A-CAA-CBA-CGA
28	A	406	CLA	C13-C15-C16-C17
28	b	607	CLA	C5-C6-C7-C8
36	t	101	3PH	C3C-C3D-C3E-C3F
37	B	625	DGA	CB5-CB6-CB7-CB8
38	C	525	LHG	C25-C26-C27-C28
38	D	409	LHG	C34-C35-C36-C37
38	c	525	LHG	C30-C31-C32-C33
35	c	519	DGD	C1B-C2B-C3B-C4B
28	B	602	CLA	O1D-CGD-O2D-CED
28	C	509	CLA	C10-C11-C12-C13
28	Y	604	CLA	C10-C11-C12-C13
28	b	614	CLA	C8-C10-C11-C12
32	D	411	LMG	C12-C13-C14-C15
35	c	519	DGD	C6B-C7B-C8B-C9B
36	B	624	3PH	C22-C23-C24-C25
37	b	625	DGA	CB5-CB6-CB7-CB8
38	L	101	LHG	C28-C29-C30-C31
28	b	610	CLA	C3-C5-C6-C7
38	d	409	LHG	C10-C11-C12-C13
32	D	411	LMG	O6-C5-C6-O5
35	C	518	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
28	C	510	CLA	C16-C17-C18-C20
35	c	519	DGD	O6E-C1E-O5D-C6D
28	B	609	CLA	C13-C15-C16-C17
28	b	611	CLA	C13-C15-C16-C17
28	b	617	CLA	C5-C6-C7-C8
32	C	521	LMG	C14-C15-C16-C17
35	C	519	DGD	CCB-CDB-CEB-CFB
37	B	625	DGA	CA8-CA9-CAA-CBA
38	D	410	LHG	C33-C34-C35-C36
45	k	101	4RF	C08-C09-C10-C11
51	Y	626	PTY	C23-C24-C25-C26
35	C	519	DGD	C1B-C2B-C3B-C4B
36	B	624	3PH	C21-C22-C23-C24
37	B	625	DGA	CB1-CB2-CB3-CB4
37	b	625	DGA	CB1-CB2-CB3-CB4
38	G	624	LHG	C23-C24-C25-C26
32	D	411	LMG	C11-C10-O7-C8
32	c	521	LMG	C11-C10-O7-C8
38	D	410	LHG	C8-C7-O7-C5
38	Y	624	LHG	C8-C7-O7-C5
37	B	625	DGA	CB7-CB8-CB9-CAB
38	l	101	LHG	C25-C26-C27-C28
45	k	101	4RF	C43-C44-C45-C46
28	B	606	CLA	C8-C10-C11-C12
28	G	610	CLA	C10-C11-C12-C13
28	b	617	CLA	C15-C16-C17-C18
28	c	501	CLA	C8-C10-C11-C12
31	C	526	SQD	C9-C10-C11-C12
35	c	518	DGD	C3A-C4A-C5A-C6A
38	Y	624	LHG	C30-C31-C32-C33
39	c	527	LMK	C2-C3-C4-O2
28	B	607	CLA	C3-C5-C6-C7
28	B	609	CLA	C3-C5-C6-C7
38	G	624	LHG	C9-C10-C11-C12
38	d	408	LHG	C29-C30-C31-C32
38	l	101	LHG	C31-C32-C33-C34
39	C	527	LMK	C12-C13-C14-C15
38	Y	624	LHG	O7-C5-C6-O8
38	d	410	LHG	O7-C5-C6-O8
45	I	102	4RF	O21-C20-C39-O40
38	d	408	LHG	C24-C25-C26-C27
45	K	101	4RF	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
45	k	101	4RF	C48-C49-C50-C51
28	Y	610	CLA	C16-C17-C18-C19
46	S	608	CHL	C11-C12-C13-C14
38	L	101	LHG	C10-C11-C12-C13
32	c	521	LMG	O6-C5-C6-O5
35	C	519	DGD	O6E-C5E-C6E-O5E
28	B	604	CLA	C5-C6-C7-C8
28	B	612	CLA	C8-C10-C11-C12
28	S	602	CLA	C4-C3-C5-C6
41	D	405	PL9	C15-C14-C16-C17
36	T	101	3PH	C31-C32-C33-C34
38	Y	624	LHG	C23-C24-C25-C26
28	N	603	CLA	C2-C3-C5-C6
28	Y	611	CLA	C2-C3-C5-C6
46	N	601	CHL	C2-C3-C5-C6
28	A	406	CLA	C11-C12-C13-C14
28	B	613	CLA	C14-C13-C15-C16
28	B	615	CLA	C6-C7-C8-C9
28	B	616	CLA	C14-C13-C15-C16
28	C	505	CLA	C6-C7-C8-C9
28	C	512	CLA	C14-C13-C15-C16
28	N	604	CLA	C6-C7-C8-C9
28	N	610	CLA	C6-C7-C8-C9
28	G	603	CLA	C6-C7-C8-C9
28	G	611	CLA	C6-C7-C8-C9
28	S	603	CLA	C11-C10-C8-C9
28	b	602	CLA	C6-C7-C8-C9
28	b	602	CLA	C11-C10-C8-C9
28	b	604	CLA	C11-C12-C13-C14
28	b	606	CLA	C11-C10-C8-C9
28	b	613	CLA	C14-C13-C15-C16
28	c	509	CLA	C14-C13-C15-C16
28	c	510	CLA	C14-C13-C15-C16
28	c	511	CLA	C11-C12-C13-C14
28	d	402	CLA	C11-C12-C13-C14
28	d	403	CLA	C11-C10-C8-C9
46	N	605	CHL	C11-C10-C8-C9
35	c	519	DGD	O6E-C5E-C6E-O5E
28	A	410	CLA	O1A-CGA-O2A-C1
31	c	526	SQD	C9-C10-C11-C12
36	t	101	3PH	C37-C38-C39-C3A
37	j	101	DGA	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
45	K	101	4RF	C08-C09-C10-C11
36	B	624	3PH	C3B-C3C-C3D-C3E
37	c	524	DGA	CDB-CEB-CFB-CGB
38	D	408	LHG	C29-C30-C31-C32
38	L	101	LHG	C25-C26-C27-C28
45	K	101	4RF	C09-C10-C11-C12
32	h	102	LMG	O6-C5-C6-O5
35	b	623	DGD	O6E-C5E-C6E-O5E
28	S	614	CLA	CBA-CGA-O2A-C1
28	c	502	CLA	C13-C15-C16-C17
37	b	625	DGA	CA8-CA9-CAA-CBA
45	i	101	4RF	C10-C11-C12-C13
30	C	514	BCR	C17-C18-C19-C20
30	C	514	BCR	C21-C22-C23-C24
30	C	516	BCR	C17-C18-C19-C20
34	b	620	C7Z	C31-C32-C33-C34
45	k	101	4RF	O42-C41-O40-C39
28	A	407	CLA	C1A-C2A-CAA-CBA
28	B	602	CLA	C1A-C2A-CAA-CBA
28	B	605	CLA	C1A-C2A-CAA-CBA
28	B	607	CLA	C1A-C2A-CAA-CBA
28	C	501	CLA	C1A-C2A-CAA-CBA
28	C	503	CLA	C1A-C2A-CAA-CBA
28	C	507	CLA	C1A-C2A-CAA-CBA
28	C	511	CLA	C1A-C2A-CAA-CBA
28	D	402	CLA	C1A-C2A-CAA-CBA
28	N	603	CLA	C1A-C2A-CAA-CBA
28	G	603	CLA	C1A-C2A-CAA-CBA
28	G	604	CLA	C1A-C2A-CAA-CBA
28	G	610	CLA	C1A-C2A-CAA-CBA
28	G	614	CLA	C1A-C2A-CAA-CBA
28	S	602	CLA	C1A-C2A-CAA-CBA
28	S	604	CLA	C1A-C2A-CAA-CBA
28	S	609	CLA	C1A-C2A-CAA-CBA
28	S	617	CLA	C1A-C2A-CAA-CBA
28	Y	603	CLA	C1A-C2A-CAA-CBA
28	Y	608	CLA	C1A-C2A-CAA-CBA
28	Y	610	CLA	C1A-C2A-CAA-CBA
28	Y	611	CLA	C1A-C2A-CAA-CBA
28	Y	614	CLA	C1A-C2A-CAA-CBA
28	a	406	CLA	C1A-C2A-CAA-CBA
28	a	407	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	b	604	CLA	C1A-C2A-CAA-CBA
28	c	501	CLA	C1A-C2A-CAA-CBA
28	c	503	CLA	C1A-C2A-CAA-CBA
28	c	507	CLA	C1A-C2A-CAA-CBA
28	c	512	CLA	C1A-C2A-CAA-CBA
46	N	607	CHL	C1A-C2A-CAA-CBA
46	G	606	CHL	C1A-C2A-CAA-CBA
28	G	610	CLA	C16-C17-C18-C19
28	Y	613	CLA	C16-C17-C18-C20
28	b	605	CLA	C16-C17-C18-C20
28	b	609	CLA	C16-C17-C18-C19
28	c	513	CLA	C16-C17-C18-C20
32	D	411	LMG	O9-C10-O7-C8
32	c	521	LMG	O9-C10-O7-C8
37	C	524	DGA	OB1-CB1-OG2-CG2
37	C	524	DGA	CB2-CB1-OG2-CG2
38	c	525	LHG	C8-C7-O7-C5
32	H	102	LMG	C37-C38-C39-C40
36	S	626	3PH	C22-C23-C24-C25
37	b	625	DGA	CA5-CA6-CA7-CA8
38	d	408	LHG	C33-C34-C35-C36
43	h	101	RRX	C9-C10-C11-C12
28	b	602	CLA	C13-C15-C16-C17
28	b	607	CLA	C8-C10-C11-C12
38	L	101	LHG	C13-C14-C15-C16
28	C	507	CLA	C3-C5-C6-C7
28	S	602	CLA	C3-C5-C6-C7
45	k	101	4RF	C45-C46-C47-C48
38	c	525	LHG	O10-C23-O8-C6
28	D	403	CLA	C13-C15-C16-C17
28	Y	613	CLA	C8-C10-C11-C12
28	B	612	CLA	CBA-CGA-O2A-C1
36	B	624	3PH	O11-C1-C2-C3
36	t	101	3PH	O11-C1-C2-C3
38	N	624	LHG	O6-C4-C5-C6
38	G	624	LHG	O6-C4-C5-C6
38	d	408	LHG	O6-C4-C5-C6
38	d	409	LHG	O6-C4-C5-C6
51	Y	627	PTY	O14-C5-C6-C1
38	d	408	LHG	C7-C8-C9-C10
32	C	523	LMG	C16-C17-C18-C19
28	C	501	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	C	507	CLA	C16-C17-C18-C19
28	S	604	CLA	C6-C7-C8-C10
28	c	511	CLA	C16-C17-C18-C20
38	D	410	LHG	C25-C26-C27-C28
38	Y	624	LHG	C11-C12-C13-C14
38	l	101	LHG	C30-C31-C32-C33
28	b	608	CLA	C15-C16-C17-C18
31	a	412	SQD	C26-C27-C28-C29
38	D	409	LHG	C15-C16-C17-C18
45	I	102	4RF	C51-C52-C53-C54
28	N	613	CLA	C4-C3-C5-C6
31	b	621	SQD	C24-C25-C26-C27
37	C	524	DGA	CCA-CDA-CEA-CFA
28	B	603	CLA	C5-C6-C7-C8
28	B	616	CLA	C13-C15-C16-C17
28	Y	612	CLA	C13-C15-C16-C17
38	d	409	LHG	C11-C12-C13-C14
38	d	410	LHG	C28-C29-C30-C31
45	i	101	4RF	C33-C34-C35-C36
31	b	621	SQD	O10-C23-O48-C46
38	D	410	LHG	O10-C23-O8-C6
36	b	624	3PH	C2E-C2F-C2G-C2H
36	t	101	3PH	C25-C26-C27-C28
37	b	625	DGA	CA2-CA3-CA4-CA5
31	A	412	SQD	O6-C44-C45-C46
31	B	626	SQD	C44-C45-C46-O48
31	C	526	SQD	C44-C45-C46-O48
31	M	101	SQD	C44-C45-C46-O48
31	a	412	SQD	O6-C44-C45-C46
32	a	413	LMG	C7-C8-C9-O8
32	w	201	LMG	O1-C7-C8-C9
35	C	520	DGD	CCB-CDB-CEB-CFB
35	b	623	DGD	O1G-C1G-C2G-C3G
36	S	626	3PH	C1-C2-C3-O31
37	j	101	DGA	OG1-CG1-CG2-CG3
38	L	101	LHG	C4-C5-C6-O8
38	N	624	LHG	C15-C16-C17-C18
38	S	624	LHG	C4-C5-C6-O8
38	d	410	LHG	C4-C5-C6-O8
38	l	101	LHG	C4-C5-C6-O8
39	C	527	LMK	O1-C7-C8-C9
35	c	520	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
28	B	617	CLA	C8-C10-C11-C12
32	c	521	LMG	C19-C20-C21-C22
37	b	625	DGA	CBB-CAB-CB9-CB8
38	d	409	LHG	C25-C26-C27-C28
45	I	102	4RF	C09-C10-C11-C12
32	W	201	LMG	C8-C7-O1-C1
35	C	519	DGD	C2G-C3G-O3G-C1D
35	c	519	DGD	C2G-C3G-O3G-C1D
31	a	412	SQD	C31-C32-C33-C34
37	C	524	DGA	CA8-CA9-CAA-CBA
38	d	410	LHG	C29-C30-C31-C32
28	A	405	CLA	C5-C6-C7-C8
28	C	512	CLA	C15-C16-C17-C18
28	Y	611	CLA	C5-C6-C7-C8
28	b	603	CLA	C13-C15-C16-C17
38	L	101	LHG	C31-C32-C33-C34
38	N	624	LHG	O8-C23-C24-C25
35	C	518	DGD	O1A-C1A-O1G-C1G
35	c	519	DGD	CAB-CBB-CCB-CDB
35	c	519	DGD	CCB-CDB-CEB-CFB
38	N	624	LHG	O1-C1-C2-O2
38	Y	624	LHG	O1-C1-C2-O2
28	D	403	CLA	C10-C11-C12-C13
28	G	610	CLA	O1A-CGA-O2A-C1
38	D	409	LHG	C29-C30-C31-C32
38	D	409	LHG	C30-C31-C32-C33
38	S	624	LHG	C28-C29-C30-C31
50	S	625	LPX	C10-C11-C12-C13
37	C	524	DGA	CB4-CB5-CB6-CB7
28	B	615	CLA	C5-C6-C7-C8
30	c	516	BCR	C11-C10-C9-C34
32	C	521	LMG	O6-C5-C6-O5
35	B	623	DGD	O6E-C5E-C6E-O5E
35	C	518	DGD	O6E-C5E-C6E-O5E
28	b	602	CLA	C4-C3-C5-C6
45	i	101	4RF	C06-C07-C08-C09
38	S	624	LHG	C7-C8-C9-C10
45	K	101	4RF	C41-C43-C44-C45
28	B	617	CLA	CBA-CGA-O2A-C1
35	c	519	DGD	C2A-C1A-O1G-C1G
39	C	527	LMK	C11-C12-C13-C14
28	N	610	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	c	505	CLA	C8-C10-C11-C12
31	B	621	SQD	C46-C45-O47-C7
33	a	414	SPH	O3-C3-C4-C5
36	T	101	3PH	C3-C2-O21-C21
37	B	625	DGA	CG1-CG2-OG2-CB1
37	b	625	DGA	CG1-CG2-OG2-CB1
28	C	502	CLA	C2A-CAA-CBA-CGA
28	b	606	CLA	C2A-CAA-CBA-CGA
28	S	614	CLA	O1A-CGA-O2A-C1
28	c	507	CLA	C2-C1-O2A-CGA
29	a	409	PHO	C2-C1-O2A-CGA
36	b	624	3PH	C27-C28-C29-C2A
33	a	414	SPH	C12-C13-C14-C15
38	S	624	LHG	C31-C32-C33-C34
51	Y	626	PTY	C41-C42-C43-C44
36	T	101	3PH	C1-O11-P-O12
36	t	101	3PH	C36-C37-C38-C39
37	b	625	DGA	CCB-CDB-CEB-CFB
38	L	101	LHG	C11-C12-C13-C14
28	b	602	CLA	CBA-CGA-O2A-C1
28	B	617	CLA	C16-C17-C18-C20
28	N	610	CLA	C16-C17-C18-C19
28	B	604	CLA	C15-C16-C17-C18
31	a	412	SQD	C25-C26-C27-C28
33	a	414	SPH	C14-C15-C16-C17
28	B	612	CLA	O1A-CGA-O2A-C1
28	A	406	CLA	C5-C6-C7-C8
28	b	610	CLA	C13-C15-C16-C17
28	b	615	CLA	C13-C15-C16-C17
31	M	101	SQD	C2-C1-O6-C44
35	c	519	DGD	C2E-C1E-O5D-C6D
31	A	412	SQD	O6-C44-C45-O47
36	S	626	3PH	O21-C2-C3-O31
37	j	101	DGA	OG1-CG1-CG2-OG2
51	Y	627	PTY	O4-C1-C6-O7
38	c	525	LHG	O9-C7-O7-C5
28	S	602	CLA	C5-C6-C7-C8
28	b	608	CLA	C8-C10-C11-C12
35	c	520	DGD	O1A-C1A-O1G-C1G
28	C	510	CLA	C16-C17-C18-C19
28	A	406	CLA	O1D-CGD-O2D-CED
31	b	626	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
38	Y	624	LHG	C34-C35-C36-C37
41	d	405	PL9	C15-C14-C16-C17
37	b	625	DGA	CB3-CB4-CB5-CB6
28	A	405	CLA	C12-C13-C15-C16
28	A	406	CLA	C11-C10-C8-C7
28	B	602	CLA	C11-C12-C13-C15
28	B	616	CLA	C12-C13-C15-C16
28	C	502	CLA	C11-C12-C13-C15
28	C	512	CLA	C12-C13-C15-C16
28	D	402	CLA	C11-C12-C13-C15
28	N	604	CLA	C6-C7-C8-C10
28	N	610	CLA	C6-C7-C8-C10
28	G	603	CLA	C6-C7-C8-C10
28	G	610	CLA	C12-C13-C15-C16
28	G	611	CLA	C6-C7-C8-C10
28	S	602	CLA	C6-C7-C8-C10
28	Y	611	CLA	C6-C7-C8-C10
28	b	602	CLA	C2-C3-C5-C6
28	b	602	CLA	C6-C7-C8-C10
28	b	602	CLA	C11-C10-C8-C7
28	b	602	CLA	C11-C12-C13-C15
28	b	609	CLA	C12-C13-C15-C16
28	b	612	CLA	C11-C10-C8-C7
28	b	613	CLA	C12-C13-C15-C16
28	b	616	CLA	C11-C10-C8-C7
28	b	616	CLA	C11-C12-C13-C15
28	b	617	CLA	C6-C7-C8-C10
28	c	505	CLA	C12-C13-C15-C16
28	c	507	CLA	C12-C13-C15-C16
28	c	510	CLA	C11-C12-C13-C15
28	c	510	CLA	C12-C13-C15-C16
46	N	605	CHL	C11-C10-C8-C7
46	N	606	CHL	C11-C12-C13-C15
46	N	607	CHL	C11-C10-C8-C7
46	G	609	CHL	C11-C12-C13-C15
46	S	608	CHL	C11-C10-C8-C7
46	Y	606	CHL	C11-C12-C13-C15
46	Y	609	CHL	C12-C13-C15-C16
32	A	413	LMG	O7-C10-C11-C12
28	A	405	CLA	C14-C13-C15-C16
28	B	604	CLA	C11-C12-C13-C14
28	B	607	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	B	609	CLA	C11-C10-C8-C9
28	B	617	CLA	C6-C7-C8-C9
28	C	501	CLA	C14-C13-C15-C16
28	C	502	CLA	C11-C12-C13-C14
28	C	505	CLA	C14-C13-C15-C16
28	C	509	CLA	C14-C13-C15-C16
28	C	513	CLA	C6-C7-C8-C9
28	D	402	CLA	C11-C12-C13-C14
28	N	603	CLA	C14-C13-C15-C16
28	G	610	CLA	C14-C13-C15-C16
28	Y	612	CLA	C11-C10-C8-C9
28	b	602	CLA	C14-C13-C15-C16
28	b	617	CLA	C6-C7-C8-C9
28	c	504	CLA	C11-C10-C8-C9
28	c	505	CLA	C14-C13-C15-C16
28	c	507	CLA	C14-C13-C15-C16
28	c	513	CLA	C11-C12-C13-C14
46	N	606	CHL	C11-C10-C8-C9
46	N	607	CHL	C11-C10-C8-C9
46	N	607	CHL	C11-C12-C13-C14
46	G	609	CHL	C11-C12-C13-C14
46	S	608	CHL	C11-C10-C8-C9
46	Y	606	CHL	C6-C7-C8-C9
46	Y	607	CHL	C6-C7-C8-C9
46	Y	609	CHL	C14-C13-C15-C16
31	A	412	SQD	C33-C34-C35-C36
31	a	412	SQD	C10-C11-C12-C13
33	Y	625	SPH	C12-C13-C14-C15
37	c	524	DGA	CEB-CFB-CGB-CHB
38	C	525	LHG	C34-C35-C36-C37
38	L	101	LHG	C33-C34-C35-C36
38	Y	624	LHG	C33-C34-C35-C36
28	S	610	CLA	C2A-CAA-CBA-CGA
28	Y	610	CLA	C2A-CAA-CBA-CGA
32	C	523	LMG	C42-C43-C44-C45
38	L	101	LHG	C34-C35-C36-C37
45	i	101	4RF	C11-C12-C13-C14
30	C	516	BCR	C37-C22-C23-C24
30	c	517	BCR	C37-C22-C23-C24
32	c	521	LMG	C29-C30-C31-C32
33	A	414	SPH	C6-C7-C8-C9
30	B	619	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	c	515	BCR	C17-C18-C19-C20
30	d	404	BCR	C17-C18-C19-C20
28	C	512	CLA	C3-C5-C6-C7
28	B	615	CLA	C15-C16-C17-C18
28	a	410	CLA	C8-C10-C11-C12
28	b	610	CLA	C15-C16-C17-C18
28	c	510	CLA	C5-C6-C7-C8
36	b	624	3PH	C3F-C3G-C3H-C3I
36	t	101	3PH	C3D-C3E-C3F-C3G
38	N	624	LHG	C16-C17-C18-C19
38	d	409	LHG	C29-C30-C31-C32
35	c	519	DGD	O1A-C1A-O1G-C1G
28	c	513	CLA	CBA-CGA-O2A-C1
36	b	624	3PH	C2F-C2G-C2H-C2I
38	G	624	LHG	C11-C12-C13-C14
28	N	613	CLA	CAA-CBA-CGA-O2A
38	D	410	LHG	C24-C25-C26-C27
28	A	407	CLA	C4B-C3B-CAB-CBB
28	B	604	CLA	C4B-C3B-CAB-CBB
28	B	606	CLA	C4B-C3B-CAB-CBB
28	B	608	CLA	C4B-C3B-CAB-CBB
28	B	610	CLA	C4B-C3B-CAB-CBB
28	B	617	CLA	C4B-C3B-CAB-CBB
28	C	502	CLA	C4B-C3B-CAB-CBB
28	C	505	CLA	C4B-C3B-CAB-CBB
28	N	602	CLA	C4B-C3B-CAB-CBB
28	N	610	CLA	C4B-C3B-CAB-CBB
28	N	613	CLA	C4B-C3B-CAB-CBB
28	G	602	CLA	C4B-C3B-CAB-CBB
28	G	610	CLA	C4B-C3B-CAB-CBB
28	G	611	CLA	C4B-C3B-CAB-CBB
28	S	604	CLA	C4B-C3B-CAB-CBB
28	S	614	CLA	C4B-C3B-CAB-CBB
28	Y	604	CLA	C4B-C3B-CAB-CBB
28	a	407	CLA	C4B-C3B-CAB-CBB
28	b	604	CLA	C4B-C3B-CAB-CBB
28	b	613	CLA	C4B-C3B-CAB-CBB
28	c	506	CLA	C4B-C3B-CAB-CBB
28	d	403	CLA	C4B-C3B-CAB-CBB
28	G	610	CLA	C16-C17-C18-C20
28	Y	603	CLA	C8-C10-C11-C12
36	b	624	3PH	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
38	C	525	LHG	O6-C4-C5-C6
38	D	410	LHG	O6-C4-C5-C6
35	C	520	DGD	C7A-C8A-C9A-CAA
35	C	519	DGD	C1A-C2A-C3A-C4A
35	c	519	DGD	C1A-C2A-C3A-C4A
38	D	408	LHG	C24-C25-C26-C27
38	d	408	LHG	C11-C10-C9-C8
28	B	615	CLA	C8-C10-C11-C12
28	G	602	CLA	C5-C6-C7-C8
45	K	101	4RF	C22-C24-C25-C26
45	K	101	4RF	C02-C03-C04-C05
28	N	603	CLA	C5-C6-C7-C8
28	c	507	CLA	C13-C15-C16-C17
45	k	101	4RF	C30-C31-C32-C33
36	B	624	3PH	C27-C28-C29-C2A
36	T	101	3PH	C2D-C2E-C2F-C2G
36	S	626	3PH	C36-C37-C38-C39
38	Y	624	LHG	C9-C10-C11-C12
38	d	408	LHG	C26-C27-C28-C29
31	b	621	SQD	O47-C7-C8-C9
37	b	625	DGA	CA1-CA2-CA3-CA4
31	B	626	SQD	C33-C34-C35-C36
36	T	101	3PH	C2-C1-O11-P
38	C	525	LHG	C2-C3-O3-P
38	D	410	LHG	C2-C3-O3-P
38	d	410	LHG	C2-C3-O3-P
28	N	613	CLA	C3A-C2A-CAA-CBA
29	a	408	PHO	C3A-C2A-CAA-CBA
38	c	525	LHG	C35-C36-C37-C38
45	k	101	4RF	C47-C48-C49-C50
30	c	517	BCR	C13-C14-C15-C16
34	B	620	C7Z	C29-C30-C31-C32
34	b	620	C7Z	C9-C10-C11-C12
43	h	101	RRX	C19-C20-C21-C22
47	Y	621	LUT	C29-C30-C31-C32
31	b	621	SQD	C14-C15-C16-C17
32	c	523	LMG	C18-C19-C20-C21
36	T	101	3PH	C36-C37-C38-C39
36	S	626	3PH	C2A-C2B-C2C-C2D
37	j	101	DGA	CA7-CA8-CA9-CAA
38	C	525	LHG	C13-C14-C15-C16
28	Y	614	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	B	622	LMG	C32-C33-C34-C35
36	t	101	3PH	C3A-C3B-C3C-C3D
37	J	101	DGA	CB3-CB4-CB5-CB6
37	b	625	DGA	CFB-CGB-CHB-CIB
28	A	410	CLA	C11-C12-C13-C15
28	G	603	CLA	C16-C17-C18-C20
45	K	101	4RF	C15-C16-O18-C19
38	d	408	LHG	C31-C32-C33-C34
28	d	403	CLA	C5-C6-C7-C8
31	a	412	SQD	C44-C45-C46-O48
35	B	623	DGD	O1G-C1G-C2G-C3G
36	t	101	3PH	C1-C2-C3-O31
39	c	527	LMK	O1-C7-C8-C9
39	c	527	LMK	C7-C8-C9-O8
45	I	102	4RF	C19-C20-C39-O40
45	k	101	4RF	O18-C19-C20-C39
31	b	621	SQD	C12-C13-C14-C15
38	C	525	LHG	C9-C10-C11-C12
38	C	525	LHG	C35-C36-C37-C38
38	G	624	LHG	C33-C34-C35-C36
38	G	624	LHG	C35-C36-C37-C38
38	L	101	LHG	C19-C20-C21-C22
38	d	410	LHG	C24-C25-C26-C27
51	Y	626	PTY	C35-C36-C37-C38
28	C	504	CLA	C8-C10-C11-C12
45	I	102	4RF	C25-C26-C27-C28
38	D	409	LHG	C13-C14-C15-C16
28	b	602	CLA	O1A-CGA-O2A-C1
28	b	615	CLA	C8-C10-C11-C12
37	b	625	DGA	CCA-CDA-CEA-CFA
32	A	413	LMG	C34-C35-C36-C37
35	c	518	DGD	C9B-CAB-CBB-CCB
45	k	101	4RF	C32-C33-C34-C35
39	C	527	LMK	C7-C8-O7-C10
39	C	527	LMK	C9-C8-O7-C10
28	B	617	CLA	O1A-CGA-O2A-C1
38	G	624	LHG	C26-C27-C28-C29
45	k	101	4RF	C46-C47-C48-C49
32	d	411	LMG	C30-C31-C32-C33
33	Y	625	SPH	C11-C12-C13-C14
37	C	524	DGA	CBB-CAB-CB9-CB8
38	c	525	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	N	624	LHG	O6-C4-C5-O7
38	d	409	LHG	O6-C4-C5-O7
32	a	413	LMG	C29-C28-O8-C9
28	b	612	CLA	C16-C17-C18-C19
28	N	610	CLA	C5-C6-C7-C8
32	C	521	LMG	O7-C10-C11-C12
28	B	604	CLA	C2B-C3B-CAB-CBB
28	B	617	CLA	C2B-C3B-CAB-CBB
28	C	505	CLA	C2B-C3B-CAB-CBB
28	C	510	CLA	C2B-C3B-CAB-CBB
28	N	610	CLA	C2B-C3B-CAB-CBB
28	N	613	CLA	C2B-C3B-CAB-CBB
28	G	604	CLA	C2B-C3B-CAB-CBB
28	G	611	CLA	C2B-C3B-CAB-CBB
28	Y	614	CLA	C2B-C3B-CAB-CBB
28	b	604	CLA	C2B-C3B-CAB-CBB
28	c	506	CLA	C2B-C3B-CAB-CBB
28	d	403	CLA	C2B-C3B-CAB-CBB
38	D	410	LHG	O2-C2-C3-O3
32	A	413	LMG	C40-C41-C42-C43
38	D	408	LHG	C28-C29-C30-C31
38	S	624	LHG	C26-C27-C28-C29
38	d	409	LHG	C35-C36-C37-C38
28	Y	613	CLA	C13-C15-C16-C17
38	N	624	LHG	C31-C32-C33-C34
45	K	101	4RF	C12-C13-C14-C15
35	c	518	DGD	O6D-C5D-C6D-O5D
31	B	626	SQD	O6-C44-C45-O47
35	B	623	DGD	O1G-C1G-C2G-O2G
38	L	101	LHG	O7-C5-C6-O8
45	i	101	4RF	O18-C19-C20-O21
37	b	625	DGA	CAA-CBA-CCA-CDA
38	d	409	LHG	C30-C31-C32-C33
46	S	608	CHL	C11-C12-C13-C15
31	a	412	SQD	C15-C16-C17-C18
45	K	101	4RF	C29-C30-C31-C32
45	k	101	4RF	C49-C50-C51-C52
32	a	413	LMG	O6-C1-O1-C7
38	d	409	LHG	C1-C2-C3-O3
31	B	621	SQD	C14-C15-C16-C17
31	b	626	SQD	C19-C20-C21-C22
33	a	414	SPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
35	c	519	DGD	C2A-C3A-C4A-C5A
37	b	625	DGA	CB6-CB7-CB8-CB9
38	D	409	LHG	C35-C36-C37-C38
38	N	624	LHG	C35-C36-C37-C38
41	d	405	PL9	C40-C39-C41-C42
28	N	602	CLA	C2-C1-O2A-CGA
28	G	610	CLA	C2-C1-O2A-CGA
28	Y	602	CLA	C2-C1-O2A-CGA
28	Y	610	CLA	C2-C1-O2A-CGA
28	c	511	CLA	C15-C16-C17-C18
28	B	602	CLA	C14-C13-C15-C16
28	B	609	CLA	C11-C12-C13-C14
28	B	616	CLA	C11-C12-C13-C14
28	S	609	CLA	C6-C7-C8-C9
28	Y	602	CLA	C6-C7-C8-C9
28	Y	602	CLA	C11-C10-C8-C9
28	b	616	CLA	C11-C12-C13-C14
28	c	505	CLA	C11-C10-C8-C9
46	N	601	CHL	C14-C13-C15-C16
46	G	601	CHL	C6-C7-C8-C9
35	C	518	DGD	C2B-C3B-C4B-C5B
36	S	626	3PH	C2C-C2D-C2E-C2F
36	T	101	3PH	C2C-C2D-C2E-C2F
45	k	101	4RF	C35-C36-C37-C38
50	S	625	LPX	C13-C14-C15-C16
29	A	408	PHO	C1A-C2A-CAA-CBA
38	D	409	LHG	C2-C3-O3-P
38	l	101	LHG	C2-C3-O3-P
38	D	408	LHG	C11-C10-C9-C8
45	i	101	4RF	C51-C52-C53-C54
28	C	501	CLA	C2A-CAA-CBA-CGA
28	S	611	CLA	C2A-CAA-CBA-CGA
28	b	617	CLA	C2A-CAA-CBA-CGA
30	C	515	BCR	C23-C24-C25-C26
30	C	515	BCR	C23-C24-C25-C30
30	c	514	BCR	C23-C24-C25-C26
30	c	514	BCR	C23-C24-C25-C30
47	G	621	LUT	C1-C6-C7-C8
28	C	508	CLA	C10-C11-C12-C13
28	C	509	CLA	C15-C16-C17-C18
28	S	602	CLA	C8-C10-C11-C12
28	b	605	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	c	513	CLA	C8-C10-C11-C12
32	h	102	LMG	C15-C16-C17-C18
28	b	602	CLA	CAA-CBA-CGA-O2A
41	D	405	PL9	C47-C48-C49-C50
36	t	101	3PH	C38-C39-C3A-C3B
38	S	624	LHG	C14-C15-C16-C17
38	c	525	LHG	C34-C35-C36-C37
45	I	102	4RF	C52-C53-C54-C55
45	K	101	4RF	C03-C04-C05-C06
30	b	618	BCR	C17-C18-C19-C20
47	Y	620	LUT	C31-C32-C33-C34
49	Y	623	NEX	C11-C12-C13-C14
28	A	405	CLA	C10-C11-C12-C13
28	B	611	CLA	C13-C15-C16-C17
51	Y	626	PTY	C11-C8-O7-C6
37	B	625	DGA	CBB-CAB-CB9-CB8
32	w	201	LMG	C37-C38-C39-C40
28	A	406	CLA	C3-C5-C6-C7
28	a	405	CLA	C13-C15-C16-C17
31	A	412	SQD	C10-C11-C12-C13
38	G	624	LHG	C24-C25-C26-C27
28	c	513	CLA	O1A-CGA-O2A-C1
39	c	527	LMK	O7-C10-C11-C12
38	L	101	LHG	O6-C4-C5-C6
38	c	525	LHG	O6-C4-C5-C6
38	l	101	LHG	O6-C4-C5-C6
36	b	624	3PH	C22-C23-C24-C25
28	B	602	CLA	C12-C13-C15-C16
28	B	604	CLA	C11-C12-C13-C15
28	B	604	CLA	C12-C13-C15-C16
28	B	607	CLA	C11-C10-C8-C7
28	B	609	CLA	C11-C10-C8-C7
28	B	616	CLA	C6-C7-C8-C10
28	B	617	CLA	C6-C7-C8-C10
28	C	501	CLA	C12-C13-C15-C16
28	C	505	CLA	C12-C13-C15-C16
28	C	507	CLA	C12-C13-C15-C16
28	C	509	CLA	C6-C7-C8-C10
28	C	509	CLA	C12-C13-C15-C16
28	C	510	CLA	C12-C13-C15-C16
28	C	512	CLA	C11-C10-C8-C7
28	C	513	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
28	N	603	CLA	C12-C13-C15-C16
28	G	602	CLA	C6-C7-C8-C10
28	G	602	CLA	C12-C13-C15-C16
28	G	610	CLA	C11-C10-C8-C7
28	S	609	CLA	C6-C7-C8-C10
28	S	610	CLA	C11-C10-C8-C7
28	Y	602	CLA	C6-C7-C8-C10
28	Y	612	CLA	C11-C10-C8-C7
28	Y	613	CLA	C11-C12-C13-C15
28	Y	613	CLA	C12-C13-C15-C16
28	b	602	CLA	C12-C13-C15-C16
28	b	604	CLA	C6-C7-C8-C10
28	b	613	CLA	C11-C10-C8-C7
28	c	501	CLA	C11-C10-C8-C7
28	c	504	CLA	C6-C7-C8-C10
28	c	504	CLA	C11-C10-C8-C7
28	c	513	CLA	C11-C12-C13-C15
28	d	402	CLA	C11-C10-C8-C7
28	d	403	CLA	C11-C12-C13-C15
28	d	403	CLA	C12-C13-C15-C16
46	N	601	CHL	C12-C13-C15-C16
46	N	606	CHL	C11-C10-C8-C7
46	N	607	CHL	C11-C12-C13-C15
46	G	601	CHL	C6-C7-C8-C10
46	Y	606	CHL	C6-C7-C8-C10
31	m	101	SQD	C26-C27-C28-C29
30	A	411	BCR	C9-C10-C11-C12
30	b	618	BCR	C13-C14-C15-C16
30	b	619	BCR	C19-C20-C21-C22
30	c	515	BCR	C19-C20-C21-C22
30	d	404	BCR	C19-C20-C21-C22
28	A	410	CLA	C11-C12-C13-C14
28	B	617	CLA	C16-C17-C18-C19
38	d	410	LHG	C24-C23-O8-C6
28	a	405	CLA	C8-C10-C11-C12
37	C	524	DGA	CA4-CA5-CA6-CA7
38	D	408	LHG	C13-C14-C15-C16
38	S	624	LHG	C34-C35-C36-C37
29	a	409	PHO	C3-C5-C6-C7
28	C	513	CLA	CBA-CGA-O2A-C1
28	D	402	CLA	CAA-CBA-CGA-O2A
37	B	625	DGA	CA9-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
37	B	625	DGA	CFA-CGA-CHA-CIA
45	k	101	4RF	C11-C12-C13-C14
35	C	518	DGD	O6D-C5D-C6D-O5D
28	B	602	CLA	CAD-CBD-CGD-O2D
28	B	608	CLA	CAD-CBD-CGD-O2D
28	C	502	CLA	CAD-CBD-CGD-O2D
28	G	602	CLA	CAD-CBD-CGD-O2D
28	G	603	CLA	CAD-CBD-CGD-O2D
28	Y	604	CLA	CAD-CBD-CGD-O2D
28	c	501	CLA	CAD-CBD-CGD-O2D
28	c	512	CLA	CAD-CBD-CGD-O2D
29	A	408	PHO	CAD-CBD-CGD-O2D
31	m	101	SQD	C46-C45-O47-C7
36	S	626	3PH	C1-C2-O21-C21
46	N	607	CHL	CAD-CBD-CGD-O2D
51	Y	626	PTY	O10-C8-O7-C6
28	c	505	CLA	C4-C3-C5-C6
31	b	626	SQD	O6-C44-C45-C46
36	T	101	3PH	C1-C2-C3-O31
38	C	525	LHG	C4-C5-C6-O8
38	N	624	LHG	C4-C5-C6-O8
38	G	624	LHG	C4-C5-C6-O8
38	d	408	LHG	C2-C3-O3-P
45	I	102	4RF	O18-C19-C20-C39
36	b	624	3PH	O11-C1-C2-O21
38	D	410	LHG	O6-C4-C5-O7
38	c	525	LHG	O6-C4-C5-O7
28	N	613	CLA	C10-C11-C12-C13
28	b	603	CLA	C10-C11-C12-C13
28	B	612	CLA	C10-C11-C12-C13
28	a	406	CLA	C5-C6-C7-C8
31	b	626	SQD	C10-C11-C12-C13
28	B	605	CLA	CHA-CBD-CGD-O1D
28	B	605	CLA	CHA-CBD-CGD-O2D
28	B	607	CLA	CHA-CBD-CGD-O1D
28	B	607	CLA	CHA-CBD-CGD-O2D
28	B	609	CLA	CHA-CBD-CGD-O1D
28	B	609	CLA	CHA-CBD-CGD-O2D
28	B	613	CLA	CHA-CBD-CGD-O1D
28	B	613	CLA	CHA-CBD-CGD-O2D
28	C	504	CLA	CHA-CBD-CGD-O1D
28	C	504	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	C	506	CLA	CHA-CBD-CGD-O1D
28	C	506	CLA	CHA-CBD-CGD-O2D
28	C	507	CLA	CHA-CBD-CGD-O1D
28	C	507	CLA	CHA-CBD-CGD-O2D
28	N	604	CLA	CHA-CBD-CGD-O1D
28	N	604	CLA	CHA-CBD-CGD-O2D
28	G	604	CLA	CHA-CBD-CGD-O1D
28	G	604	CLA	CHA-CBD-CGD-O2D
28	G	612	CLA	CHA-CBD-CGD-O1D
28	G	612	CLA	CHA-CBD-CGD-O2D
28	Y	602	CLA	CHA-CBD-CGD-O1D
28	Y	602	CLA	CHA-CBD-CGD-O2D
28	Y	612	CLA	CHA-CBD-CGD-O1D
28	Y	612	CLA	CHA-CBD-CGD-O2D
28	b	613	CLA	CHA-CBD-CGD-O1D
28	b	613	CLA	CHA-CBD-CGD-O2D
28	b	617	CLA	CHA-CBD-CGD-O1D
28	b	617	CLA	CHA-CBD-CGD-O2D
28	c	503	CLA	CHA-CBD-CGD-O1D
28	c	503	CLA	CHA-CBD-CGD-O2D
28	c	504	CLA	CHA-CBD-CGD-O1D
28	c	504	CLA	CHA-CBD-CGD-O2D
28	c	505	CLA	CHA-CBD-CGD-O1D
28	c	505	CLA	CHA-CBD-CGD-O2D
28	c	506	CLA	CHA-CBD-CGD-O1D
46	N	601	CHL	CHA-CBD-CGD-O1D
46	N	601	CHL	CHA-CBD-CGD-O2D
46	N	609	CHL	CHA-CBD-CGD-O1D
46	N	609	CHL	CHA-CBD-CGD-O2D
45	K	101	4RF	O17-C16-O18-C19
30	c	516	BCR	C11-C10-C9-C8
32	a	413	LMG	C11-C12-C13-C14
37	C	524	DGA	CCB-CDB-CEB-CFB
31	C	526	SQD	O6-C44-C45-O47
31	b	626	SQD	O6-C44-C45-O47
32	H	102	LMG	O7-C8-C9-O8
32	a	413	LMG	O7-C8-C9-O8
32	c	521	LMG	O7-C8-C9-O8
35	b	623	DGD	O1G-C1G-C2G-O2G
36	t	101	3PH	O21-C2-C3-O31
38	C	525	LHG	O7-C5-C6-O8
38	S	624	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
31	B	621	SQD	C12-C13-C14-C15
38	l	101	LHG	C12-C13-C14-C15
38	Y	624	LHG	C26-C27-C28-C29
31	M	101	SQD	C11-C10-C9-C8
37	B	625	DGA	CEA-CFA-CGA-CHA
38	L	101	LHG	C30-C31-C32-C33
46	Y	609	CHL	C4-C3-C5-C6
32	a	413	LMG	O10-C28-O8-C9
41	D	405	PL9	C4-C3-C7-C8
31	m	101	SQD	C10-C11-C12-C13
38	C	525	LHG	C24-C25-C26-C27
32	w	201	LMG	O7-C10-C11-C12
28	C	512	CLA	C11-C10-C8-C9
28	D	403	CLA	C11-C12-C13-C14
28	N	602	CLA	C6-C7-C8-C9
28	N	610	CLA	C11-C12-C13-C14
28	S	610	CLA	C11-C10-C8-C9
28	Y	613	CLA	C11-C12-C13-C14
28	Y	613	CLA	C14-C13-C15-C16
28	c	503	CLA	C14-C13-C15-C16
46	N	606	CHL	C11-C12-C13-C14
35	C	518	DGD	C4A-C5A-C6A-C7A
36	t	101	3PH	C35-C36-C37-C38
38	d	408	LHG	C34-C35-C36-C37
28	C	513	CLA	O1A-CGA-O2A-C1
31	a	412	SQD	C4-C5-C6-S
31	b	621	SQD	C4-C5-C6-S
31	c	526	SQD	C4-C5-C6-S
31	m	101	SQD	C4-C5-C6-S
31	B	626	SQD	C12-C13-C14-C15
38	G	624	LHG	C31-C32-C33-C34
28	B	607	CLA	C2A-CAA-CBA-CGA
28	G	610	CLA	C2A-CAA-CBA-CGA
46	Y	605	CHL	C2A-CAA-CBA-CGA
29	a	409	PHO	C2C-C3C-CAC-CBC
31	M	101	SQD	O47-C7-C8-C9
31	B	626	SQD	C32-C33-C34-C35
30	c	515	BCR	C37-C22-C23-C24
30	C	516	BCR	C21-C22-C23-C24
30	c	517	BCR	C21-C22-C23-C24
36	B	624	3PH	C35-C36-C37-C38
28	A	410	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	C	512	CLA	C1A-C2A-CAA-CBA
28	D	403	CLA	C1A-C2A-CAA-CBA
28	G	611	CLA	C1A-C2A-CAA-CBA
28	b	602	CLA	C1A-C2A-CAA-CBA
28	c	508	CLA	C1A-C2A-CAA-CBA
28	d	403	CLA	C1A-C2A-CAA-CBA
28	G	603	CLA	C16-C17-C18-C19
36	T	101	3PH	C38-C39-C3A-C3B
28	B	611	CLA	C2-C1-O2A-CGA
28	N	603	CLA	C2-C1-O2A-CGA
28	N	614	CLA	C2-C1-O2A-CGA
28	b	603	CLA	C2-C1-O2A-CGA
29	A	408	PHO	CBA-CGA-O2A-C1
29	a	408	PHO	CBA-CGA-O2A-C1
38	C	525	LHG	C24-C23-O8-C6
45	i	101	4RF	C32-C33-C34-C35
43	H	101	RRX	C19-C20-C21-C22
38	S	624	LHG	C3-O3-P-O6
31	B	621	SQD	C25-C26-C27-C28
37	c	524	DGA	CCA-CDA-CEA-CFA
45	i	101	4RF	C29-C30-C31-C32
45	i	101	4RF	C47-C48-C49-C50
36	b	624	3PH	C2-C1-O11-P
38	S	624	LHG	C2-C3-O3-P
28	S	602	CLA	C2-C3-C5-C6
31	b	621	SQD	C25-C26-C27-C28
45	k	101	4RF	C25-C26-C27-C28
28	B	602	CLA	C4B-C3B-CAB-CBB
28	G	603	CLA	C4B-C3B-CAB-CBB
28	S	603	CLA	C4B-C3B-CAB-CBB
28	c	501	CLA	C4B-C3B-CAB-CBB
38	C	525	LHG	C3-O3-P-O4
38	D	410	LHG	C4-O6-P-O4
38	d	408	LHG	C3-O3-P-O5
38	d	410	LHG	C3-O3-P-O4
50	S	625	LPX	C3-O1-P1-O4
51	Y	627	PTY	C5-O14-P1-O13
28	B	608	CLA	C16-C17-C18-C20
28	Y	604	CLA	C16-C17-C18-C19
28	b	612	CLA	C16-C17-C18-C20
31	C	526	SQD	O5-C1-O6-C44
28	c	510	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	C	505	CLA	C15-C16-C17-C18
28	Y	610	CLA	C15-C16-C17-C18
28	B	611	CLA	C2A-CAA-CBA-CGA
28	C	505	CLA	C3-C5-C6-C7
46	N	607	CHL	C3-C5-C6-C7
46	S	608	CHL	C3-C5-C6-C7
36	S	626	3PH	C2F-C2G-C2H-C2I
28	B	605	CLA	CAD-CBD-CGD-O1D
28	B	613	CLA	CAD-CBD-CGD-O1D
28	C	504	CLA	CAD-CBD-CGD-O1D
28	C	506	CLA	CAD-CBD-CGD-O1D
28	G	604	CLA	CAD-CBD-CGD-O1D
28	S	611	CLA	CAD-CBD-CGD-O1D
28	c	503	CLA	CAD-CBD-CGD-O1D
28	c	504	CLA	CAD-CBD-CGD-O1D
28	c	506	CLA	CAD-CBD-CGD-O1D
28	c	510	CLA	CAD-CBD-CGD-O1D
31	B	626	SQD	O5-C5-C6-S
39	C	527	LMK	C29-C28-O8-C9
46	N	601	CHL	CAD-CBD-CGD-O1D
46	N	609	CHL	CAD-CBD-CGD-O1D
35	B	623	DGD	C1B-C2B-C3B-C4B
32	b	622	LMG	C18-C19-C20-C21
36	b	624	3PH	C32-C33-C34-C35
32	a	413	LMG	C30-C31-C32-C33
38	Y	624	LHG	C35-C36-C37-C38
28	D	402	CLA	C3-C5-C6-C7
32	C	523	LMG	C11-C12-C13-C14
38	S	624	LHG	C33-C34-C35-C36
38	c	525	LHG	C15-C16-C17-C18
45	i	101	4RF	C49-C50-C51-C52
28	B	608	CLA	C11-C12-C13-C15
28	B	613	CLA	C11-C10-C8-C7
28	B	616	CLA	C11-C12-C13-C15
28	C	506	CLA	C11-C10-C8-C7
28	C	507	CLA	C11-C12-C13-C15
28	C	509	CLA	C11-C10-C8-C7
28	C	512	CLA	C11-C12-C13-C15
28	C	513	CLA	C11-C10-C8-C7
28	D	403	CLA	C11-C12-C13-C15
28	N	602	CLA	C6-C7-C8-C10
28	N	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
28	N	610	CLA	C12-C13-C15-C16
28	S	610	CLA	C11-C12-C13-C15
28	S	611	CLA	C11-C12-C13-C15
28	b	603	CLA	C6-C7-C8-C10
28	b	604	CLA	C12-C13-C15-C16
28	b	606	CLA	C6-C7-C8-C10
28	b	608	CLA	C11-C10-C8-C7
28	b	609	CLA	C11-C12-C13-C15
28	c	503	CLA	C12-C13-C15-C16
28	c	505	CLA	C6-C7-C8-C10
38	C	525	LHG	O6-C4-C5-O7
38	D	408	LHG	O6-C4-C5-O7
38	L	101	LHG	O6-C4-C5-O7
38	d	408	LHG	O6-C4-C5-O7
38	l	101	LHG	O6-C4-C5-O7
41	D	405	PL9	C13-C14-C16-C17
46	N	606	CHL	C12-C13-C15-C16
46	G	607	CHL	C6-C7-C8-C10
46	Y	609	CHL	C11-C12-C13-C15
51	Y	627	PTY	O14-C5-C6-O7
38	D	409	LHG	C27-C28-C29-C30
29	a	408	PHO	O1A-CGA-O2A-C1
31	a	412	SQD	C24-C25-C26-C27
30	C	514	BCR	C19-C20-C21-C22
35	c	518	DGD	C4D-C5D-C6D-O5D
32	H	102	LMG	O7-C10-C11-C12
38	L	101	LHG	C14-C15-C16-C17
38	Y	624	LHG	C32-C33-C34-C35
28	N	604	CLA	C2A-CAA-CBA-CGA
28	b	608	CLA	C16-C17-C18-C20
36	T	101	3PH	C3D-C3E-C3F-C3G
37	C	524	DGA	CA2-CA3-CA4-CA5
35	C	518	DGD	C4D-C5D-C6D-O5D
46	S	608	CHL	CAA-CBA-CGA-O2A
31	B	626	SQD	O6-C44-C45-C46
31	C	526	SQD	O6-C44-C45-C46
33	A	414	SPH	C1-C2-C3-C4
36	b	624	3PH	C1-C2-C3-O31
37	j	101	DGA	CB5-CB6-CB7-CB8
38	D	409	LHG	C16-C17-C18-C19
38	D	410	LHG	C4-C5-C6-O8
45	K	101	4RF	C19-C20-C39-O40

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Mol	Chain	Res	Type	Atoms
31	C	526	SQD	O47-C45-C46-O48
31	M	101	SQD	O47-C45-C46-O48
31	a	412	SQD	O6-C44-C45-O47
32	b	622	LMG	O7-C8-C9-O8
32	w	201	LMG	O1-C7-C8-O7
31	A	412	SQD	C14-C15-C16-C17
32	c	523	LMG	C33-C34-C35-C36
29	A	408	PHO	O1A-CGA-O2A-C1
38	D	410	LHG	C11-C10-C9-C8
31	A	412	SQD	C45-C44-O6-C1
32	w	201	LMG	C8-C7-O1-C1
35	C	519	DGD	C5D-C6D-O5D-C1E
35	c	519	DGD	C5D-C6D-O5D-C1E
28	B	611	CLA	C8-C10-C11-C12
28	B	616	CLA	O1A-CGA-O2A-C1
28	S	610	CLA	C4-C3-C5-C6
28	B	616	CLA	CBA-CGA-O2A-C1
31	B	626	SQD	C24-C23-O48-C46
45	K	101	4RF	C50-C51-C52-C53
28	N	602	CLA	C10-C11-C12-C13
28	A	406	CLA	C11-C10-C8-C9
28	C	502	CLA	C11-C10-C8-C9
28	C	507	CLA	C14-C13-C15-C16
28	C	510	CLA	C14-C13-C15-C16
28	G	602	CLA	C6-C7-C8-C9
28	G	602	CLA	C14-C13-C15-C16
28	G	610	CLA	C11-C10-C8-C9
28	b	604	CLA	C6-C7-C8-C9
28	b	609	CLA	C11-C12-C13-C14
28	b	611	CLA	C11-C12-C13-C14
28	c	501	CLA	C11-C10-C8-C9
31	b	626	SQD	C30-C31-C32-C33
32	H	102	LMG	C12-C13-C14-C15
28	d	402	CLA	CAA-CBA-CGA-O2A
32	C	523	LMG	C14-C15-C16-C17
38	S	624	LHG	C29-C30-C31-C32
38	d	409	LHG	C33-C34-C35-C36
38	l	101	LHG	C35-C36-C37-C38
28	c	507	CLA	C15-C16-C17-C18
38	d	410	LHG	O10-C23-O8-C6
37	c	524	DGA	CFA-CGA-CHA-CIA
38	N	624	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	C	526	SQD	C29-C30-C31-C32
35	c	520	DGD	C4A-C5A-C6A-C7A
38	d	408	LHG	C35-C36-C37-C38
38	l	101	LHG	C29-C30-C31-C32
45	k	101	4RF	C33-C34-C35-C36
30	a	411	BCR	C11-C12-C13-C14
28	B	606	CLA	C2B-C3B-CAB-CBB
28	B	607	CLA	C2B-C3B-CAB-CBB
28	B	608	CLA	C2B-C3B-CAB-CBB
28	B	610	CLA	C2B-C3B-CAB-CBB
28	C	502	CLA	C2B-C3B-CAB-CBB
28	C	506	CLA	C2B-C3B-CAB-CBB
28	N	602	CLA	C2B-C3B-CAB-CBB
28	N	604	CLA	C2B-C3B-CAB-CBB
28	G	602	CLA	C2B-C3B-CAB-CBB
28	G	610	CLA	C2B-C3B-CAB-CBB
28	G	614	CLA	C2B-C3B-CAB-CBB
28	S	603	CLA	C2B-C3B-CAB-CBB
28	S	604	CLA	C2B-C3B-CAB-CBB
28	S	614	CLA	C2B-C3B-CAB-CBB
28	Y	604	CLA	C2B-C3B-CAB-CBB
28	c	501	CLA	C2B-C3B-CAB-CBB
33	A	414	SPH	C10-C11-C12-C13
35	c	520	DGD	O6D-C5D-C6D-O5D
36	B	624	3PH	C39-C3A-C3B-C3C
38	D	409	LHG	C33-C34-C35-C36
28	N	611	CLA	C1-C2-C3-C4
28	G	604	CLA	C1-C2-C3-C4
28	G	614	CLA	C1-C2-C3-C4
33	a	414	SPH	C2-C3-C4-C5
46	N	608	CHL	C1-C2-C3-C4
46	G	606	CHL	C1-C2-C3-C4
28	B	605	CLA	O1A-CGA-O2A-C1
28	B	602	CLA	C3-C5-C6-C7
28	a	405	CLA	CAA-CBA-CGA-O2A
31	M	101	SQD	C46-C45-O47-C7
31	b	621	SQD	C46-C45-O47-C7
32	B	622	LMG	C9-C8-O7-C10
32	b	622	LMG	C9-C8-O7-C10
38	l	101	LHG	C6-C5-O7-C7
32	B	622	LMG	C11-C12-C13-C14
28	A	410	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
28	B	604	CLA	C2-C1-O2A-CGA
28	C	513	CLA	C2-C1-O2A-CGA
28	D	402	CLA	C2-C1-O2A-CGA
28	N	610	CLA	C2-C1-O2A-CGA
28	b	612	CLA	C2-C1-O2A-CGA
46	N	601	CHL	C2-C1-O2A-CGA
46	Y	609	CHL	C2-C1-O2A-CGA
32	C	521	LMG	C29-C30-C31-C32
45	k	101	4RF	C44-C45-C46-C47
28	A	405	CLA	CAA-CBA-CGA-O2A
28	C	511	CLA	C13-C15-C16-C17
31	B	626	SQD	O10-C23-O48-C46
38	G	624	LHG	C16-C17-C18-C19
38	D	410	LHG	C30-C31-C32-C33
37	C	524	DGA	CB3-CB4-CB5-CB6
50	S	625	LPX	C15-C16-C17-C18
47	G	620	LUT	C29-C30-C31-C32
38	C	525	LHG	O10-C23-O8-C6
36	B	624	3PH	O11-C1-C2-O21
38	G	624	LHG	O6-C4-C5-O7
38	N	624	LHG	C9-C10-C11-C12
38	d	410	LHG	C26-C27-C28-C29
28	C	510	CLA	C4-C3-C5-C6
30	C	517	BCR	C23-C24-C25-C26
46	G	601	CHL	C3-C5-C6-C7
47	G	621	LUT	C5-C6-C7-C8
28	c	505	CLA	C2-C3-C5-C6
46	Y	609	CHL	C2-C3-C5-C6
45	i	101	4RF	C26-C27-C28-C29
35	c	519	DGD	C3B-C4B-C5B-C6B
28	B	602	CLA	C16-C17-C18-C20
36	S	626	3PH	C22-C21-O21-C2
32	c	523	LMG	O6-C1-O1-C7
32	h	102	LMG	O6-C1-O1-C7
35	C	518	DGD	O6E-C1E-O5D-C6D
35	b	623	DGD	O6E-C1E-O5D-C6D
51	Y	626	PTY	C37-C38-C39-C40
35	b	623	DGD	C2E-C1E-O5D-C6D
49	N	623	NEX	C28-C29-C30-C31
35	c	518	DGD	C2B-C3B-C4B-C5B
38	D	410	LHG	C34-C35-C36-C37
38	l	101	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
39	C	527	LMK	O1-C7-C8-O7
38	D	408	LHG	C3-O3-P-O6
38	D	409	LHG	C3-O3-P-O6
38	L	101	LHG	C4-O6-P-O3
38	N	624	LHG	C3-O3-P-O6
38	G	624	LHG	C3-O3-P-O6
38	Y	624	LHG	C3-O3-P-O6
38	d	409	LHG	C3-O3-P-O6
38	d	409	LHG	C4-O6-P-O3
38	l	101	LHG	C4-O6-P-O3
50	S	625	LPX	C3-O1-P1-O2
51	Y	626	PTY	C3-O11-P1-O14
51	Y	626	PTY	C5-O14-P1-O11
51	Y	627	PTY	C3-O11-P1-O14
35	c	518	DGD	C4A-C5A-C6A-C7A
37	C	524	DGA	CB5-CB6-CB7-CB8
38	l	101	LHG	C17-C18-C19-C20
45	K	101	4RF	C07-C08-C09-C10
29	A	409	PHO	CHA-CBD-CGD-O1D
29	A	409	PHO	CHA-CBD-CGD-O2D
29	a	409	PHO	CHA-CBD-CGD-O1D
29	a	409	PHO	CHA-CBD-CGD-O2D
32	D	411	LMG	C28-C29-C30-C31
28	B	605	CLA	CBA-CGA-O2A-C1
31	B	621	SQD	C44-C45-C46-O48
32	B	622	LMG	C7-C8-C9-O8
32	H	102	LMG	C7-C8-C9-O8
35	c	518	DGD	O1G-C1G-C2G-C3G
51	Y	627	PTY	O4-C1-C6-C5
37	B	625	DGA	CA2-CA3-CA4-CA5
45	i	101	4RF	C01-C02-C03-C04
28	B	617	CLA	C5-C6-C7-C8
28	B	609	CLA	C11-C12-C13-C15
28	N	603	CLA	C11-C10-C8-C7
46	N	607	CHL	C12-C13-C15-C16
46	G	607	CHL	C11-C12-C13-C15
46	Y	606	CHL	C12-C13-C15-C16
46	Y	607	CHL	C6-C7-C8-C10
28	B	608	CLA	C11-C12-C13-C14
28	B	613	CLA	C11-C10-C8-C9
28	B	616	CLA	C6-C7-C8-C9
28	C	512	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	S	602	CLA	C6-C7-C8-C9
28	Y	611	CLA	C6-C7-C8-C9
28	b	613	CLA	C11-C10-C8-C9
28	c	505	CLA	C6-C7-C8-C9
28	c	511	CLA	C11-C10-C8-C9
28	d	402	CLA	C11-C10-C8-C9
46	G	607	CHL	C6-C7-C8-C9
28	B	608	CLA	C16-C17-C18-C19
38	N	624	LHG	C34-C35-C36-C37
36	b	624	3PH	C38-C39-C3A-C3B
28	C	504	CLA	C2A-CAA-CBA-CGA
28	b	613	CLA	C3-C5-C6-C7
37	b	625	DGA	CA3-CA4-CA5-CA6
37	B	625	DGA	CA6-CA7-CA8-CA9
38	S	624	LHG	C5-C4-O6-P
28	Y	612	CLA	C15-C16-C17-C18
28	S	605	CLA	C2C-C3C-CAC-CBC
32	C	521	LMG	C13-C14-C15-C16
28	Y	604	CLA	C4-C3-C5-C6
33	Y	625	SPH	C10-C11-C12-C13
28	d	403	CLA	C16-C17-C18-C20
29	A	408	PHO	C16-C17-C18-C19
28	b	605	CLA	CBA-CGA-O2A-C1
38	N	624	LHG	O10-C23-C24-C25
32	b	622	LMG	O6-C5-C6-O5
28	S	605	CLA	C4C-C3C-CAC-CBC
46	S	601	CHL	CAA-CBA-CGA-O2A
36	B	624	3PH	C2C-C2D-C2E-C2F
45	I	102	4RF	C03-C04-C05-C06
32	D	411	LMG	C18-C19-C20-C21
28	B	607	CLA	C4B-C3B-CAB-CBB
28	C	503	CLA	C4B-C3B-CAB-CBB
28	C	506	CLA	C4B-C3B-CAB-CBB
28	C	511	CLA	C4B-C3B-CAB-CBB
28	N	604	CLA	C4B-C3B-CAB-CBB
28	G	614	CLA	C4B-C3B-CAB-CBB
28	S	602	CLA	C4B-C3B-CAB-CBB
28	Y	611	CLA	C4B-C3B-CAB-CBB
28	b	617	CLA	C4B-C3B-CAB-CBB
30	C	516	BCR	C19-C20-C21-C22
47	Y	620	LUT	C29-C30-C31-C32
28	G	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	G	603	CLA	C3-C5-C6-C7
51	Y	627	PTY	N1-C2-C3-O11
32	W	201	LMG	C29-C30-C31-C32
45	I	102	4RF	C05-C06-C07-C08
45	I	102	4RF	C49-C50-C51-C52
30	B	619	BCR	C10-C11-C12-C13
32	c	523	LMG	C30-C31-C32-C33
28	N	602	CLA	C3-C5-C6-C7
32	C	523	LMG	C36-C37-C38-C39
28	S	603	CLA	C4-C3-C5-C6
28	b	609	CLA	C4-C3-C5-C6
46	Y	605	CHL	CAA-CBA-CGA-O1A
32	B	622	LMG	C19-C20-C21-C22
45	I	102	4RF	C43-C44-C45-C46
28	B	610	CLA	C2-C1-O2A-CGA
28	D	403	CLA	C2-C1-O2A-CGA
46	Y	606	CHL	C2-C1-O2A-CGA
32	c	523	LMG	C2-C1-O1-C7
35	C	518	DGD	C2E-C1E-O5D-C6D
45	k	101	4RF	O18-C19-C20-O21
45	I	102	4RF	C47-C48-C49-C50
28	b	605	CLA	CAA-CBA-CGA-O2A
38	L	101	LHG	C2-C3-O3-P
28	c	511	CLA	C3A-C2A-CAA-CBA
28	c	512	CLA	C3A-C2A-CAA-CBA
46	N	607	CHL	C3A-C2A-CAA-CBA
46	Y	601	CHL	C3A-C2A-CAA-CBA
31	m	101	SQD	O47-C7-C8-C9
38	G	624	LHG	O8-C23-C24-C25
30	A	411	BCR	C19-C20-C21-C22
28	C	501	CLA	C13-C15-C16-C17
36	B	624	3PH	C2F-C2G-C2H-C2I
36	S	626	3PH	C3C-C3D-C3E-C3F
28	b	604	CLA	C4-C3-C5-C6
28	c	509	CLA	C4-C3-C5-C6
31	C	526	SQD	C11-C10-C9-C8
38	D	408	LHG	C34-C35-C36-C37
28	S	610	CLA	C2-C3-C5-C6
32	c	521	LMG	O7-C10-C11-C12
28	B	606	CLA	C6-C7-C8-C9
28	B	614	CLA	C14-C13-C15-C16
28	C	503	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	C	507	CLA	C11-C12-C13-C14
28	N	610	CLA	C14-C13-C15-C16
28	S	610	CLA	C11-C12-C13-C14
28	Y	603	CLA	C6-C7-C8-C9
28	a	405	CLA	C14-C13-C15-C16
28	c	501	CLA	C11-C12-C13-C14
28	c	506	CLA	C6-C7-C8-C9
46	N	607	CHL	C14-C13-C15-C16
46	G	607	CHL	C11-C10-C8-C9
46	Y	609	CHL	C11-C10-C8-C9
28	Y	604	CLA	C16-C17-C18-C20
35	c	518	DGD	CAB-CBB-CCB-CDB
38	L	101	LHG	C29-C30-C31-C32
51	Y	626	PTY	C11-C12-C13-C14
38	c	525	LHG	C10-C11-C12-C13
37	C	524	DGA	OG1-CG1-CG2-CG3
38	d	409	LHG	C4-C5-C6-O8
49	N	623	NEX	C39-C29-C30-C31
49	S	623	NEX	C39-C29-C30-C31
41	d	405	PL9	C17-C18-C19-C21
28	N	611	CLA	C2A-CAA-CBA-CGA
28	C	511	CLA	C5-C6-C7-C8
38	l	101	LHG	C34-C35-C36-C37
28	b	608	CLA	C16-C17-C18-C19
31	B	626	SQD	C13-C14-C15-C16
38	d	410	LHG	C9-C10-C11-C12
45	i	101	4RF	C25-C26-C27-C28
35	C	519	DGD	C2A-C3A-C4A-C5A
28	b	609	CLA	C15-C16-C17-C18
31	b	626	SQD	C31-C32-C33-C34
38	D	410	LHG	C9-C10-C11-C12
31	c	526	SQD	C25-C26-C27-C28
35	B	623	DGD	C1G-C2G-O2G-C1B
35	b	623	DGD	C1G-C2G-O2G-C1B
38	L	101	LHG	C6-C5-O7-C7
28	Y	603	CLA	C4-C3-C5-C6
28	B	604	CLA	C1A-C2A-CAA-CBA
28	N	602	CLA	C1A-C2A-CAA-CBA
28	b	605	CLA	C1A-C2A-CAA-CBA
45	K	101	4RF	C43-C44-C45-C46
28	C	502	CLA	C6-C7-C8-C10
28	Y	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
28	Y	614	CLA	C11-C10-C8-C7
28	b	613	CLA	C6-C7-C8-C10
28	c	512	CLA	C6-C7-C8-C10
46	Y	605	CHL	CAA-CBA-CGA-O2A
37	c	524	DGA	CDA-CEA-CFA-CGA
32	h	102	LMG	O7-C10-C11-C12
31	a	412	SQD	C14-C15-C16-C17
38	N	624	LHG	C19-C20-C21-C22
28	C	509	CLA	C8-C10-C11-C12
28	C	503	CLA	C3-C5-C6-C7
28	c	503	CLA	C3-C5-C6-C7
28	N	613	CLA	C2A-CAA-CBA-CGA
28	B	606	CLA	C10-C11-C12-C13
28	B	606	CLA	C15-C16-C17-C18
36	S	626	3PH	C25-C26-C27-C28
45	i	101	4RF	C53-C54-C55-C56
51	Y	626	PTY	C24-C25-C26-C27
36	S	626	3PH	O11-C1-C2-O21
45	k	101	4RF	C09-C10-C11-C12
37	j	101	DGA	CA2-CA3-CA4-CA5
28	Y	614	CLA	C16-C17-C18-C19
28	b	615	CLA	C16-C17-C18-C20
46	S	601	CHL	CAA-CBA-CGA-O1A
41	d	405	PL9	C30-C29-C31-C32
31	B	626	SQD	C11-C10-C9-C8
35	c	518	DGD	C6B-C7B-C8B-C9B
28	c	508	CLA	C13-C15-C16-C17
28	C	510	CLA	C2-C3-C5-C6
28	Y	604	CLA	C2-C3-C5-C6
28	c	509	CLA	C2-C3-C5-C6
28	C	511	CLA	C2B-C3B-CAB-CBB
28	G	603	CLA	C2B-C3B-CAB-CBB
28	S	602	CLA	C2B-C3B-CAB-CBB
28	Y	602	CLA	C2B-C3B-CAB-CBB
28	Y	610	CLA	C2B-C3B-CAB-CBB
28	Y	611	CLA	C2B-C3B-CAB-CBB
45	k	101	4RF	C05-C06-C07-C08
38	G	624	LHG	C29-C30-C31-C32
28	b	611	CLA	C8-C10-C11-C12
31	a	412	SQD	O49-C7-O47-C45
49	S	623	NEX	C28-C29-C30-C31
35	C	520	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
37	c	524	DGA	CB2-CB3-CB4-CB5
28	c	504	CLA	C2A-CAA-CBA-CGA
38	L	101	LHG	C35-C36-C37-C38
30	D	404	BCR	C19-C20-C21-C22
30	c	514	BCR	C13-C14-C15-C16
31	a	412	SQD	C8-C7-O47-C45
28	S	603	CLA	C16-C17-C18-C19
35	C	520	DGD	C4A-C5A-C6A-C7A
35	c	519	DGD	C2B-C3B-C4B-C5B
28	b	614	CLA	C13-C15-C16-C17
41	D	405	PL9	C39-C41-C42-C43
28	B	612	CLA	C4-C3-C5-C6
28	C	512	CLA	C4-C3-C5-C6
46	N	609	CHL	C4-C3-C5-C6
28	B	612	CLA	C2-C1-O2A-CGA
28	C	501	CLA	C2-C1-O2A-CGA
28	b	605	CLA	O1A-CGA-O2A-C1
37	j	101	DGA	CA5-CA6-CA7-CA8
28	C	508	CLA	C11-C12-C13-C14
32	A	413	LMG	O9-C10-C11-C12
38	D	409	LHG	C24-C25-C26-C27
31	A	412	SQD	C15-C16-C17-C18
32	d	411	LMG	C12-C13-C14-C15
28	B	606	CLA	C2A-CAA-CBA-CGA
28	B	613	CLA	C2A-CAA-CBA-CGA
28	c	510	CLA	C2A-CAA-CBA-CGA
46	S	601	CHL	C2A-CAA-CBA-CGA
38	N	624	LHG	C18-C19-C20-C21
30	c	515	BCR	C1-C6-C7-C8
30	c	517	BCR	C23-C24-C25-C30
47	G	620	LUT	C1-C6-C7-C8
47	S	620	LUT	C1-C6-C7-C8
47	Y	621	LUT	C1-C6-C7-C8
46	G	607	CHL	C5-C6-C7-C8
32	d	411	LMG	C18-C19-C20-C21
38	D	408	LHG	C32-C33-C34-C35
38	l	101	LHG	C33-C34-C35-C36
28	N	613	CLA	CAA-CBA-CGA-O1A
30	a	411	BCR	C19-C20-C21-C22
34	b	620	C7Z	C13-C14-C15-C35
47	S	620	LUT	C29-C30-C31-C32
31	m	101	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	C2A-C3A-C4A-C5A
36	t	101	3PH	C29-C2A-C2B-C2C
28	C	506	CLA	C4-C3-C5-C6
46	G	607	CHL	C4-C3-C5-C6
29	A	408	PHO	C16-C17-C18-C20
28	D	402	CLA	C10-C11-C12-C13
28	N	603	CLA	C15-C16-C17-C18
46	S	608	CHL	C10-C11-C12-C13
28	Y	603	CLA	C2-C3-C5-C6
46	N	606	CHL	C3-C5-C6-C7
28	N	602	CLA	C5-C6-C7-C8
31	c	526	SQD	C27-C28-C29-C30
36	B	624	3PH	C26-C27-C28-C29
36	t	101	3PH	C24-C25-C26-C27
32	h	102	LMG	C11-C12-C13-C14
28	S	610	CLA	C13-C15-C16-C17
36	B	624	3PH	C2D-C2E-C2F-C2G
36	S	626	3PH	C34-C35-C36-C37
35	C	520	DGD	O6D-C5D-C6D-O5D
28	C	501	CLA	O1A-CGA-O2A-C1
28	Y	602	CLA	C4B-C3B-CAB-CBB
28	Y	610	CLA	C4B-C3B-CAB-CBB
38	D	408	LHG	O6-C4-C5-C6
38	Y	624	LHG	O6-C4-C5-C6
28	C	505	CLA	C11-C10-C8-C7
41	d	405	PL9	C18-C19-C21-C22
29	A	408	PHO	CBD-CGD-O2D-CED
36	T	101	3PH	C3A-C3B-C3C-C3D
45	I	102	4RF	C27-C28-C29-C30
37	j	101	DGA	OG2-CG2-CG3-OXT
49	G	623	NEX	C33-C34-C35-C15
31	A	412	SQD	O47-C7-C8-C9
45	K	101	4RF	C01-C02-C03-C04
32	B	622	LMG	O7-C8-C9-O8
29	A	408	PHO	O1D-CGD-O2D-CED
46	N	608	CHL	O2A-C1-C2-C3
46	G	606	CHL	O2A-C1-C2-C3
36	t	101	3PH	O31-C31-C32-C33
28	C	512	CLA	C2A-CAA-CBA-CGA
28	B	602	CLA	C16-C17-C18-C19
37	J	101	DGA	CA5-CA6-CA7-CA8
45	I	102	4RF	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
36	B	624	3PH	C2A-C2B-C2C-C2D
37	B	625	DGA	OG2-CB1-CB2-CB3
32	C	521	LMG	O9-C10-C11-C12
31	M	101	SQD	C26-C27-C28-C29
28	S	611	CLA	C4-C3-C5-C6
28	a	405	CLA	C4-C3-C5-C6
46	N	607	CHL	C4-C3-C5-C6
46	G	601	CHL	C4-C3-C5-C6
28	B	615	CLA	C13-C15-C16-C17
46	N	609	CHL	C2-C3-C5-C6
32	c	523	LMG	O7-C10-C11-C12
28	B	612	CLA	C11-C12-C13-C14
28	C	506	CLA	C11-C10-C8-C9
28	C	509	CLA	C11-C10-C8-C9
28	G	613	CLA	C14-C13-C15-C16
28	S	611	CLA	C11-C12-C13-C14
28	a	405	CLA	C11-C12-C13-C14
28	b	603	CLA	C6-C7-C8-C9
28	b	609	CLA	C6-C7-C8-C9
28	b	610	CLA	C11-C12-C13-C14
28	b	612	CLA	C11-C10-C8-C9
28	c	507	CLA	C11-C12-C13-C14
28	c	510	CLA	C11-C12-C13-C14
28	d	403	CLA	C6-C7-C8-C9
29	a	409	PHO	C6-C7-C8-C9
46	G	609	CHL	C14-C13-C15-C16
46	Y	606	CHL	C11-C12-C13-C14
33	A	414	SPH	C2-C3-C4-C5
36	S	626	3PH	C3B-C3C-C3D-C3E
28	b	614	CLA	C3A-C2A-CAA-CBA
31	b	626	SQD	C15-C16-C17-C18
38	N	624	LHG	O2-C2-C3-O3
28	Y	613	CLA	CAA-CBA-CGA-O2A
28	C	510	CLA	CAD-CBD-CGD-O2D
28	C	512	CLA	CAD-CBD-CGD-O2D
28	N	602	CLA	CAD-CBD-CGD-O2D
28	N	603	CLA	CAD-CBD-CGD-O2D
28	N	612	CLA	CAD-CBD-CGD-O2D
28	S	612	CLA	CAD-CBD-CGD-O2D
28	Y	603	CLA	CAD-CBD-CGD-O2D
28	Y	614	CLA	CAD-CBD-CGD-O2D
28	b	606	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
28	b	608	CLA	CAD-CBD-CGD-O2D
38	L	101	LHG	C4-C5-O7-C7
46	S	606	CHL	CAD-CBD-CGD-O2D
46	Y	605	CHL	CAD-CBD-CGD-O2D
41	d	405	PL9	C12-C13-C14-C15
32	a	413	LMG	C29-C30-C31-C32
28	N	604	CLA	CAA-CBA-CGA-O2A
28	S	614	CLA	CAA-CBA-CGA-O2A
28	c	503	CLA	CAA-CBA-CGA-O2A
37	j	101	DGA	OG2-CB1-CB2-CB3
38	L	101	LHG	O9-C7-C8-C9
45	i	101	4RF	C24-C25-C26-C27
32	A	413	LMG	C33-C34-C35-C36
28	G	613	CLA	C4-C3-C5-C6
28	a	406	CLA	C4-C3-C5-C6
36	t	101	3PH	C2E-C2F-C2G-C2H
28	B	612	CLA	C2-C3-C5-C6
41	d	405	PL9	C38-C39-C41-C42
46	G	607	CHL	C2-C3-C5-C6
28	B	615	CLA	CAA-CBA-CGA-O2A
45	i	101	4RF	O40-C41-C43-C44
30	c	515	BCR	C11-C12-C13-C14
30	c	515	BCR	C21-C22-C23-C24
45	K	101	4RF	C48-C49-C50-C51
45	K	101	4RF	C51-C52-C53-C54
38	d	409	LHG	C2-C3-O3-P
39	c	527	LMK	C11-C10-O7-C8
51	Y	626	PTY	O4-C1-C6-C5
38	c	525	LHG	C14-C15-C16-C17
38	D	409	LHG	O6-C4-C5-O7
38	Y	624	LHG	O6-C4-C5-O7
32	C	523	LMG	O7-C10-C11-C12
36	S	626	3PH	O21-C21-C22-C23
46	G	605	CHL	CAA-CBA-CGA-O2A
28	d	403	CLA	C16-C17-C18-C19
30	a	411	BCR	C10-C11-C12-C13
28	S	610	CLA	C8-C10-C11-C12
29	a	408	PHO	O2A-C1-C2-C3
46	Y	607	CHL	O2A-C1-C2-C3
31	a	412	SQD	C35-C36-C37-C38
28	b	603	CLA	CAA-CBA-CGA-O2A
28	S	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	S	603	CLA	C16-C17-C18-C20
37	B	625	DGA	CA1-CA2-CA3-CA4
38	d	409	LHG	O2-C2-C3-O3
31	M	101	SQD	O49-C7-C8-C9
28	B	611	CLA	CHA-CBD-CGD-O1D
28	B	611	CLA	CHA-CBD-CGD-O2D
28	B	614	CLA	CHA-CBD-CGD-O1D
28	B	614	CLA	CHA-CBD-CGD-O2D
28	C	509	CLA	CHA-CBD-CGD-O1D
28	C	509	CLA	CHA-CBD-CGD-O2D
28	C	511	CLA	CHA-CBD-CGD-O1D
28	C	511	CLA	CHA-CBD-CGD-O2D
28	D	402	CLA	CHA-CBD-CGD-O1D
28	D	402	CLA	CHA-CBD-CGD-O2D
28	N	610	CLA	CHA-CBD-CGD-O1D
28	N	610	CLA	CHA-CBD-CGD-O2D
28	G	610	CLA	CHA-CBD-CGD-O1D
28	G	610	CLA	CHA-CBD-CGD-O2D
28	G	613	CLA	CHA-CBD-CGD-O2D
28	S	610	CLA	CHA-CBD-CGD-O2D
28	Y	608	CLA	CHA-CBD-CGD-O1D
28	Y	608	CLA	CHA-CBD-CGD-O2D
28	Y	610	CLA	CHA-CBD-CGD-O1D
28	Y	610	CLA	CHA-CBD-CGD-O2D
28	Y	613	CLA	CHA-CBD-CGD-O1D
28	Y	613	CLA	CHA-CBD-CGD-O2D
28	a	407	CLA	CHA-CBD-CGD-O1D
28	a	407	CLA	CHA-CBD-CGD-O2D
28	a	410	CLA	CHA-CBD-CGD-O1D
28	a	410	CLA	CHA-CBD-CGD-O2D
28	b	611	CLA	CHA-CBD-CGD-O1D
28	b	611	CLA	CHA-CBD-CGD-O2D
28	c	502	CLA	CHA-CBD-CGD-O1D
28	c	502	CLA	CHA-CBD-CGD-O2D
28	c	506	CLA	CHA-CBD-CGD-O2D
28	c	507	CLA	CHA-CBD-CGD-O1D
28	c	507	CLA	CHA-CBD-CGD-O2D
28	c	509	CLA	CHA-CBD-CGD-O1D
28	c	509	CLA	CHA-CBD-CGD-O2D
39	C	527	LMK	C2-C3-C4-O3
46	Y	609	CHL	CHA-CBD-CGD-O1D
46	Y	609	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
49	G	623	NEX	C13-C14-C15-C35
28	S	612	CLA	CAA-CBA-CGA-O1A
28	G	613	CLA	CAA-CBA-CGA-O2A
31	C	526	SQD	C32-C33-C34-C35
28	C	506	CLA	C2-C3-C5-C6
31	b	626	SQD	C25-C26-C27-C28
36	S	626	3PH	C32-C33-C34-C35
36	B	624	3PH	C33-C34-C35-C36
38	D	410	LHG	C10-C11-C12-C13
36	S	626	3PH	O11-C1-C2-C3
38	D	409	LHG	O6-C4-C5-C6
28	B	603	CLA	CAA-CBA-CGA-O2A
28	G	603	CLA	CAA-CBA-CGA-O2A
45	K	101	4RF	O21-C22-C24-C25
32	h	102	LMG	O7-C8-C9-O8
32	C	521	LMG	C28-C29-C30-C31
28	B	608	CLA	CAA-CBA-CGA-O2A
28	B	609	CLA	CAA-CBA-CGA-O2A
28	b	615	CLA	CAA-CBA-CGA-O2A
37	c	524	DGA	OG2-CB1-CB2-CB3
38	d	409	LHG	O7-C7-C8-C9
29	A	408	PHO	CHA-CBD-CGD-O1D
33	A	414	SPH	N2-C2-C3-O3
28	b	608	CLA	C5-C6-C7-C8
28	C	501	CLA	CBA-CGA-O2A-C1
31	B	626	SQD	C10-C11-C12-C13
31	C	526	SQD	C33-C34-C35-C36
28	A	405	CLA	C11-C12-C13-C15
28	B	617	CLA	C11-C12-C13-C15
28	C	508	CLA	C11-C12-C13-C15
28	Y	603	CLA	C11-C10-C8-C7
28	b	605	CLA	C12-C13-C15-C16
28	b	609	CLA	C2-C3-C5-C6
28	b	612	CLA	C2-C3-C5-C6
28	c	507	CLA	C11-C12-C13-C15
46	Y	607	CHL	C11-C12-C13-C15
31	b	626	SQD	C35-C36-C37-C38
33	Y	625	SPH	C4-C5-C6-C7
28	B	607	CLA	CAA-CBA-CGA-O2A
31	M	101	SQD	O48-C23-C24-C25
32	W	201	LMG	O7-C10-C11-C12
28	C	504	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
28	N	603	CLA	C11-C10-C8-C9
28	Y	602	CLA	C11-C12-C13-C14
28	Y	603	CLA	C11-C10-C8-C9
28	Y	614	CLA	C11-C10-C8-C9
28	b	605	CLA	C14-C13-C15-C16
28	b	609	CLA	C14-C13-C15-C16
28	c	512	CLA	C6-C7-C8-C9
28	c	512	CLA	C14-C13-C15-C16
28	C	501	CLA	C15-C16-C17-C18
28	B	602	CLA	C2B-C3B-CAB-CBB
46	N	607	CHL	C2B-C3B-CAB-CBB
46	N	608	CHL	C2B-C3B-CAB-CBB
46	G	607	CHL	C2B-C3B-CAB-CBB
46	Y	601	CHL	C2B-C3B-CAB-CBB
46	Y	607	CHL	C2B-C3B-CAB-CBB
31	B	621	SQD	C4-C5-C6-S
38	d	409	LHG	C15-C16-C17-C18
45	i	101	4RF	C31-C32-C33-C34
28	b	607	CLA	C13-C15-C16-C17
28	b	603	CLA	C2A-CAA-CBA-CGA
46	G	606	CHL	C2A-CAA-CBA-CGA
46	Y	606	CHL	C2A-CAA-CBA-CGA
28	B	615	CLA	CAA-CBA-CGA-O1A
28	S	610	CLA	CAA-CBA-CGA-O2A
37	B	625	DGA	CBB-CCB-CDB-CEB
38	l	101	LHG	C19-C20-C21-C22
28	G	614	CLA	CAA-CBA-CGA-O2A
32	C	523	LMG	C12-C13-C14-C15
28	b	602	CLA	CAA-CBA-CGA-O1A
47	N	620	LUT	C27-C28-C29-C30
28	b	612	CLA	C13-C15-C16-C17
38	C	525	LHG	C16-C17-C18-C19
28	B	606	CLA	C1A-C2A-CAA-CBA
28	Y	604	CLA	C1A-C2A-CAA-CBA
28	b	614	CLA	C1A-C2A-CAA-CBA
28	c	506	CLA	C1A-C2A-CAA-CBA
38	d	410	LHG	C1-C2-C3-O3
46	Y	601	CHL	C1A-C2A-CAA-CBA
32	A	413	LMG	C36-C37-C38-C39
28	N	604	CLA	CAA-CBA-CGA-O1A
28	Y	613	CLA	CAA-CBA-CGA-O1A
28	c	503	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
36	t	101	3PH	O32-C31-C32-C33
37	B	625	DGA	OB1-CB1-CB2-CB3
39	c	527	LMK	C12-C13-C14-C15
28	c	509	CLA	C8-C10-C11-C12
45	i	101	4RF	O42-C41-C43-C44
45	i	101	4RF	O18-C19-C20-C39
28	N	614	CLA	CAA-CBA-CGA-O2A
37	b	625	DGA	OG1-CA1-CA2-CA3
28	A	406	CLA	C2A-CAA-CBA-CGA
28	b	608	CLA	C2A-CAA-CBA-CGA
35	c	520	DGD	CCB-CDB-CEB-CFB
31	A	412	SQD	O49-C7-C8-C9
32	c	523	LMG	O9-C10-C11-C12
31	m	101	SQD	C11-C10-C9-C8
28	c	513	CLA	C10-C11-C12-C13
31	M	101	SQD	C10-C11-C12-C13
37	C	524	DGA	CA1-CA2-CA3-CA4
28	B	603	CLA	CAA-CBA-CGA-O1A
28	B	609	CLA	CAA-CBA-CGA-O1A
28	S	603	CLA	C2-C3-C5-C6
31	C	526	SQD	C2-C1-O6-C44
28	B	613	CLA	C4B-C3B-CAB-CBB
28	D	402	CLA	C4B-C3B-CAB-CBB
28	c	505	CLA	C4B-C3B-CAB-CBB
38	L	101	LHG	C4-O6-P-O5
38	N	624	LHG	C4-O6-P-O5
38	d	409	LHG	C4-O6-P-O5
38	l	101	LHG	C4-O6-P-O5
46	N	605	CHL	C4B-C3B-CAB-CBB
46	G	605	CHL	C4B-C3B-CAB-CBB
46	G	608	CHL	C4B-C3B-CAB-CBB
51	Y	626	PTY	C3-O11-P1-O13
32	c	521	LMG	C10-C11-C12-C13
31	m	101	SQD	C28-C29-C30-C31
28	B	607	CLA	CAA-CBA-CGA-O1A
28	G	613	CLA	CAA-CBA-CGA-O1A
31	M	101	SQD	O10-C23-C24-C25
37	c	524	DGA	OB1-CB1-CB2-CB3
31	A	412	SQD	C35-C36-C37-C38
47	S	620	LUT	C5-C6-C7-C8
28	C	505	CLA	C5-C6-C7-C8
28	c	503	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	G	603	CLA	CAA-CBA-CGA-O1A
28	b	603	CLA	CAA-CBA-CGA-O1A
36	S	626	3PH	O22-C21-C22-C23
31	A	412	SQD	C12-C13-C14-C15
36	t	101	3PH	C2C-C2D-C2E-C2F
28	D	402	CLA	CAA-CBA-CGA-O1A
37	j	101	DGA	OB1-CB1-CB2-CB3
28	B	606	CLA	C5-C6-C7-C8
35	c	519	DGD	C5B-C6B-C7B-C8B
45	K	101	4RF	O23-C22-C24-C25
28	c	506	CLA	C4-C3-C5-C6
46	G	601	CHL	C2-C3-C5-C6
28	B	612	CLA	C16-C17-C18-C19
28	C	503	CLA	CAD-CBD-CGD-O1D
28	G	611	CLA	CAD-CBD-CGD-O1D
28	S	604	CLA	CAD-CBD-CGD-O1D
28	b	605	CLA	CAD-CBD-CGD-O1D
28	b	615	CLA	CAD-CBD-CGD-O1D
31	A	412	SQD	O5-C5-C6-S
31	b	626	SQD	O5-C5-C6-S
35	B	623	DGD	C3G-C2G-O2G-C1B
35	b	623	DGD	C3G-C2G-O2G-C1B
39	c	527	LMK	C29-C28-O8-C9
46	Y	609	CHL	CAD-CBD-CGD-O1D
51	Y	626	PTY	C2-C3-O11-P1
51	Y	627	PTY	C2-C3-O11-P1
32	C	523	LMG	O9-C10-C11-C12
46	G	605	CHL	CAA-CBA-CGA-O1A
35	C	519	DGD	C3B-C4B-C5B-C6B
36	b	624	3PH	C26-C27-C28-C29
38	L	101	LHG	C17-C18-C19-C20
32	c	523	LMG	O8-C28-C29-C30
37	C	524	DGA	OG2-CB1-CB2-CB3
28	S	610	CLA	C5-C6-C7-C8
28	c	509	CLA	C13-C15-C16-C17
28	C	502	CLA	C6-C7-C8-C9
46	Y	601	CHL	C11-C12-C13-C14
38	C	525	LHG	C31-C32-C33-C34
32	C	523	LMG	C34-C35-C36-C37
32	w	201	LMG	O9-C10-C11-C12
28	B	606	CLA	CAA-CBA-CGA-O2A
28	N	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
28	b	609	CLA	CAA-CBA-CGA-O2A
35	C	518	DGD	O2G-C1B-C2B-C3B
38	S	624	LHG	O8-C23-C24-C25
38	d	409	LHG	C11-C10-C9-C8
28	b	615	CLA	CAA-CBA-CGA-O1A
36	B	624	3PH	C2E-C2F-C2G-C2H
28	G	602	CLA	C15-C16-C17-C18
28	c	505	CLA	CAA-CBA-CGA-O2A
28	c	512	CLA	CAA-CBA-CGA-O2A
32	B	622	LMG	O7-C10-C11-C12
37	J	101	DGA	OG2-CB1-CB2-CB3
37	c	524	DGA	OG1-CA1-CA2-CA3
28	b	613	CLA	C8-C10-C11-C12
38	D	408	LHG	C35-C36-C37-C38
32	W	201	LMG	O9-C10-C11-C12
38	d	409	LHG	O9-C7-C8-C9
38	G	624	LHG	C34-C35-C36-C37
28	b	606	CLA	C13-C15-C16-C17
28	B	612	CLA	C6-C7-C8-C10
28	D	403	CLA	C6-C7-C8-C10
28	S	602	CLA	C11-C10-C8-C7
28	Y	602	CLA	C11-C12-C13-C15
28	b	604	CLA	C2-C3-C5-C6
28	b	615	CLA	C11-C12-C13-C15
28	c	512	CLA	C12-C13-C15-C16
45	I	102	4RF	C41-C43-C44-C45
46	N	609	CHL	C12-C13-C15-C16
46	G	601	CHL	C11-C12-C13-C15
28	B	608	CLA	CAA-CBA-CGA-O1A
31	b	621	SQD	O49-C7-C8-C9
35	c	518	DGD	O1B-C1B-C2B-C3B
37	C	524	DGA	OB1-CB1-CB2-CB3
37	B	625	DGA	CBA-CCA-CDA-CEA
28	C	503	CLA	CAA-CBA-CGA-O2A
28	C	505	CLA	CAA-CBA-CGA-O2A
28	b	608	CLA	CAA-CBA-CGA-O2A
28	b	613	CLA	CAA-CBA-CGA-O2A
31	a	412	SQD	O47-C7-C8-C9
35	c	518	DGD	O2G-C1B-C2B-C3B
38	D	409	LHG	O7-C7-C8-C9
38	Y	624	LHG	O8-C23-C24-C25
37	j	101	DGA	CBB-CAB-CB9-CB8

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Mol	Chain	Res	Type	Atoms
38	D	410	LHG	C29-C30-C31-C32
38	L	101	LHG	C12-C13-C14-C15
32	D	411	LMG	C10-C11-C12-C13
30	c	516	BCR	C17-C18-C19-C20
28	A	406	CLA	CAA-CBA-CGA-O1A
28	N	614	CLA	CAA-CBA-CGA-O1A
28	b	613	CLA	CAA-CBA-CGA-O1A
28	c	505	CLA	CAA-CBA-CGA-O1A
35	C	518	DGD	O1B-C1B-C2B-C3B
37	b	625	DGA	OA1-CA1-CA2-CA3
47	G	621	LUT	C9-C10-C11-C12
33	A	414	SPH	C14-C15-C16-C17
28	Y	614	CLA	C16-C17-C18-C20
28	b	615	CLA	C16-C17-C18-C19
28	A	406	CLA	CAA-CBA-CGA-O2A
31	a	412	SQD	C32-C33-C34-C35
28	B	603	CLA	C8-C10-C11-C12
28	B	607	CLA	C5-C6-C7-C8
28	c	504	CLA	C8-C10-C11-C12
28	d	402	CLA	C5-C6-C7-C8
38	d	410	LHG	C34-C35-C36-C37
51	Y	626	PTY	C13-C14-C15-C16
28	C	503	CLA	CAA-CBA-CGA-O1A
28	G	614	CLA	CAA-CBA-CGA-O1A
28	b	609	CLA	CAA-CBA-CGA-O1A
28	c	512	CLA	CAA-CBA-CGA-O1A
38	S	624	LHG	O10-C23-C24-C25
38	Y	624	LHG	O10-C23-C24-C25
37	c	524	DGA	CA2-CA1-OG1-CG1
38	N	624	LHG	O7-C7-C8-C9
28	N	611	CLA	CAA-CBA-CGA-O1A
28	S	610	CLA	CAA-CBA-CGA-O1A
28	D	402	CLA	C8-C10-C11-C12
28	b	612	CLA	C15-C16-C17-C18
39	c	527	LMK	C29-C30-C31-C32
28	C	508	CLA	CAA-CBA-CGA-O2A
28	C	512	CLA	CAA-CBA-CGA-O2A
37	b	625	DGA	OG2-CB1-CB2-CB3

All (1) ring outliers are listed below:

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Mol	Chain	Res	Type	Atoms

Mol	Chain	Res	Type	Atoms
49	N	623	NEX	C1-C2-C3-C4-C5-C6

228 monomers are involved in 667 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	624	3PH	1	0
28	B	604	CLA	3	0
37	B	625	DGA	4	0
49	N	623	NEX	3	0
33	A	414	SPH	2	0
42	F	101	HEM	2	0
46	N	601	CHL	7	0
35	C	519	DGD	3	0
28	c	505	CLA	4	0
31	a	412	SQD	4	0
51	Y	626	PTY	7	0
30	C	517	BCR	2	0
30	a	411	BCR	6	0
28	b	614	CLA	9	0
31	C	526	SQD	2	0
41	D	405	PL9	3	0
32	b	622	LMG	3	0
32	B	622	LMG	6	0
28	S	605	CLA	1	0
47	S	621	LUT	4	0
28	c	510	CLA	7	0
28	c	506	CLA	5	0
33	Y	625	SPH	2	0
31	M	101	SQD	1	0
28	c	503	CLA	6	0
30	d	404	BCR	3	0
28	B	616	CLA	4	0
45	I	102	4RF	4	0
38	S	624	LHG	4	0
28	b	615	CLA	4	0
36	S	626	3PH	4	0
28	B	612	CLA	5	0
30	c	517	BCR	6	0
48	G	622	XAT	7	0
46	S	608	CHL	2	0
28	c	507	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	409	PHO	7	0
28	C	505	CLA	6	0
28	c	501	CLA	1	0
47	Y	621	LUT	4	0
37	c	524	DGA	2	0
28	b	609	CLA	10	0
36	T	101	3PH	1	0
28	S	603	CLA	2	0
28	b	603	CLA	2	0
38	C	525	LHG	5	0
49	Y	623	NEX	2	0
28	A	405	CLA	9	0
28	D	402	CLA	8	0
28	C	504	CLA	3	0
46	G	609	CHL	7	0
28	Y	614	CLA	8	0
28	C	503	CLA	2	0
38	L	101	LHG	5	0
28	S	604	CLA	1	0
28	a	410	CLA	3	0
45	i	101	4RF	3	0
38	d	408	LHG	3	0
36	t	101	3PH	2	0
28	S	613	CLA	1	0
32	A	413	LMG	6	0
25	A	401	OEX	1	0
38	G	624	LHG	4	0
28	Y	612	CLA	3	0
28	B	603	CLA	6	0
46	G	601	CHL	4	0
28	B	610	CLA	3	0
31	B	626	SQD	3	0
28	S	610	CLA	2	0
46	S	607	CHL	1	0
28	C	501	CLA	5	0
28	b	617	CLA	3	0
38	l	101	LHG	3	0
46	N	606	CHL	4	0
28	B	602	CLA	3	0
46	Y	601	CHL	3	0
46	Y	606	CHL	2	0
28	A	406	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	N	610	CLA	4	0
30	C	514	BCR	5	0
35	C	518	DGD	6	0
46	Y	609	CHL	5	0
35	C	520	DGD	5	0
28	C	511	CLA	1	0
28	c	513	CLA	8	0
32	d	411	LMG	5	0
32	D	411	LMG	1	0
35	b	623	DGD	2	0
41	d	405	PL9	9	0
43	h	101	RRX	4	0
28	c	508	CLA	5	0
28	B	615	CLA	6	0
28	G	612	CLA	1	0
28	B	608	CLA	7	0
31	m	101	SQD	1	0
38	c	525	LHG	4	0
46	S	606	CHL	2	0
28	b	611	CLA	5	0
28	N	604	CLA	2	0
28	D	403	CLA	4	0
28	N	602	CLA	2	0
28	B	605	CLA	5	0
28	G	613	CLA	4	0
38	D	409	LHG	5	0
32	c	523	LMG	1	0
28	c	502	CLA	5	0
37	j	101	DGA	3	0
38	d	410	LHG	3	0
30	c	514	BCR	6	0
28	C	512	CLA	2	0
28	Y	603	CLA	5	0
28	G	602	CLA	3	0
47	N	620	LUT	5	0
47	Y	620	LUT	3	0
28	a	406	CLA	7	0
28	C	502	CLA	3	0
28	C	513	CLA	6	0
30	B	618	BCR	1	0
38	D	408	LHG	4	0
30	C	515	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	C	510	CLA	2	0
28	B	606	CLA	5	0
28	Y	602	CLA	4	0
28	b	606	CLA	2	0
28	B	609	CLA	6	0
28	A	410	CLA	3	0
28	C	508	CLA	3	0
30	c	516	BCR	3	0
28	d	403	CLA	5	0
46	N	605	CHL	5	0
47	G	620	LUT	3	0
28	B	611	CLA	3	0
31	B	621	SQD	3	0
43	H	101	RRX	3	0
46	Y	605	CHL	1	0
28	Y	604	CLA	1	0
29	A	408	PHO	4	0
28	b	612	CLA	5	0
48	Y	622	XAT	3	0
28	G	614	CLA	1	0
28	C	506	CLA	7	0
32	c	521	LMG	1	0
28	B	617	CLA	4	0
28	c	512	CLA	4	0
28	b	608	CLA	3	0
28	d	402	CLA	5	0
46	G	606	CHL	1	0
28	a	405	CLA	9	0
37	C	524	DGA	3	0
28	S	614	CLA	2	0
28	B	613	CLA	5	0
28	b	613	CLA	11	0
49	G	623	NEX	2	0
30	D	404	BCR	1	0
33	a	414	SPH	2	0
38	D	410	LHG	5	0
28	c	511	CLA	7	0
31	A	412	SQD	3	0
28	b	616	CLA	2	0
28	N	614	CLA	1	0
28	c	509	CLA	4	0
30	C	516	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	607	CLA	5	0
29	A	409	PHO	4	0
32	h	102	LMG	7	0
28	Y	610	CLA	3	0
47	N	621	LUT	4	0
38	d	409	LHG	7	0
28	G	604	CLA	4	0
30	B	619	BCR	4	0
29	a	408	PHO	7	0
50	S	625	LPX	1	0
28	N	603	CLA	2	0
32	C	521	LMG	2	0
28	b	605	CLA	6	0
28	c	504	CLA	3	0
42	f	101	HEM	1	0
46	G	608	CHL	3	0
31	b	621	SQD	6	0
46	N	607	CHL	4	0
38	N	624	LHG	4	0
46	G	605	CHL	1	0
30	b	618	BCR	4	0
30	c	515	BCR	4	0
28	G	610	CLA	2	0
35	B	623	DGD	1	0
46	G	607	CHL	7	0
47	G	621	LUT	2	0
47	S	620	LUT	4	0
28	B	614	CLA	6	0
28	G	603	CLA	5	0
46	S	601	CHL	2	0
28	C	507	CLA	6	0
32	H	102	LMG	8	0
36	b	624	3PH	2	0
28	b	604	CLA	1	0
32	a	413	LMG	4	0
28	b	607	CLA	7	0
28	S	609	CLA	1	0
28	C	509	CLA	2	0
48	N	622	XAT	1	0
28	S	611	CLA	6	0
35	c	519	DGD	10	0
28	Y	613	CLA	7	0

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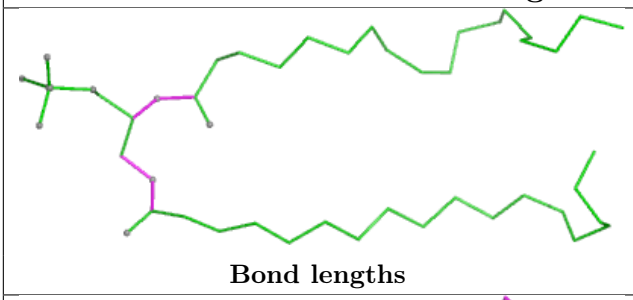
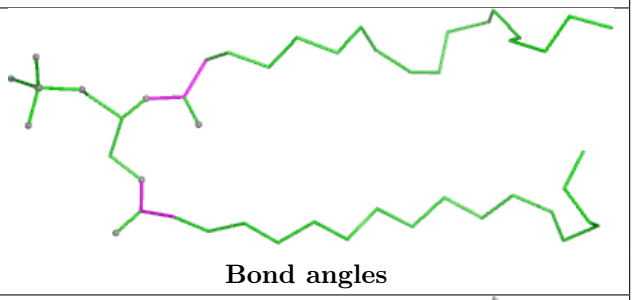
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	Y	611	CLA	3	0
30	b	619	BCR	4	0
30	A	411	BCR	3	0
28	a	407	CLA	1	0
28	S	602	CLA	3	0
32	W	201	LMG	2	0
37	J	101	DGA	1	0
31	c	526	SQD	2	0
35	c	520	DGD	6	0
45	K	101	4RF	3	0
35	c	518	DGD	6	0
28	b	610	CLA	6	0
31	b	626	SQD	4	0
46	N	609	CHL	5	0
28	N	611	CLA	1	0
46	Y	607	CHL	4	0
32	C	523	LMG	4	0
37	b	625	DGA	4	0
49	S	623	NEX	1	0
45	k	101	4RF	2	0
28	b	602	CLA	4	0
38	Y	624	LHG	6	0
28	N	613	CLA	3	0
28	Y	608	CLA	2	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.

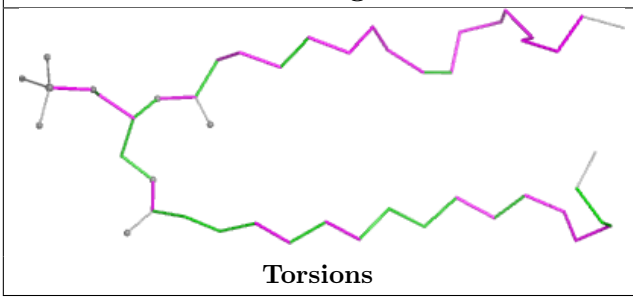
Ligand 3PH B 624



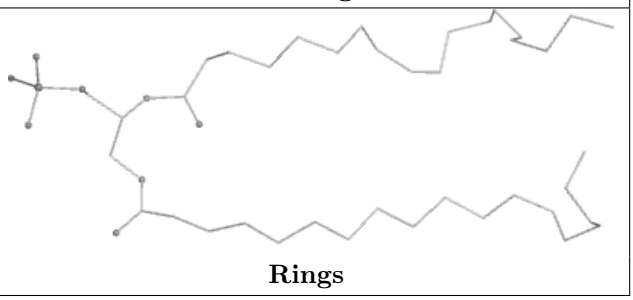
Bond lengths



Bond angles

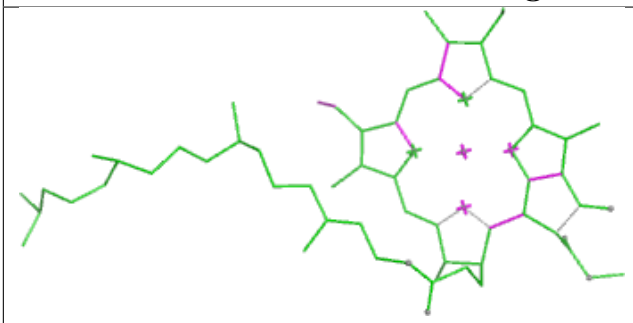


Torsions

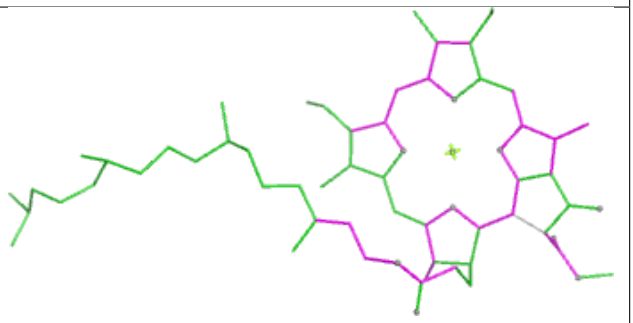


Rings

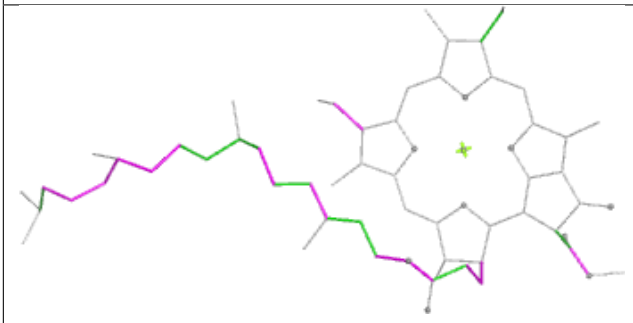
Ligand CLA B 604



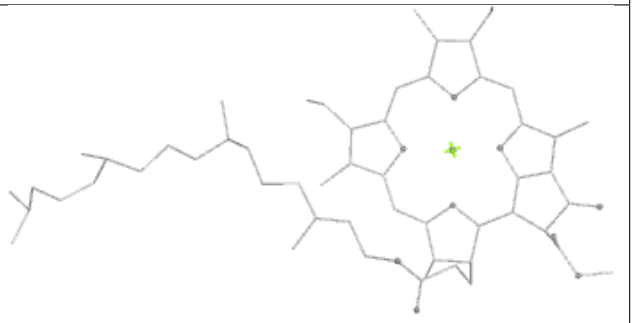
Bond lengths



Bond angles

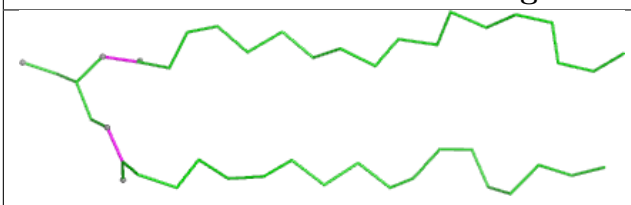


Torsions

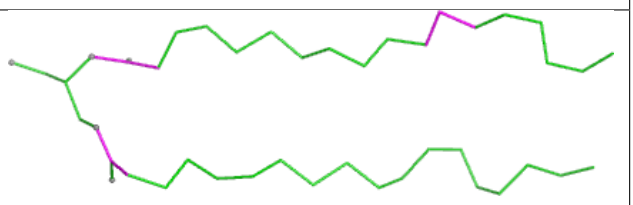


Rings

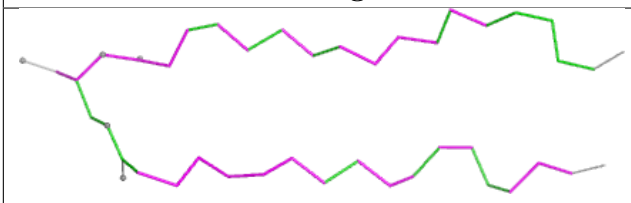
Ligand DGA B 625



Bond lengths



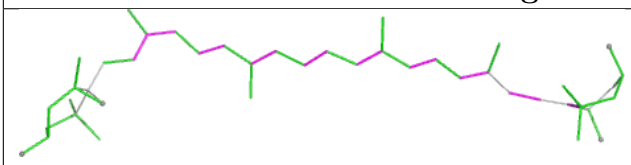
Bond angles



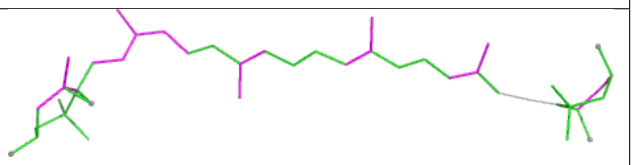
Torsions

Rings

Ligand NEX N 623

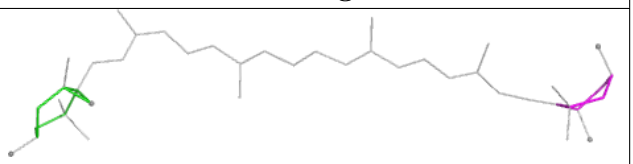


Bond lengths



Bond angles

Torsions

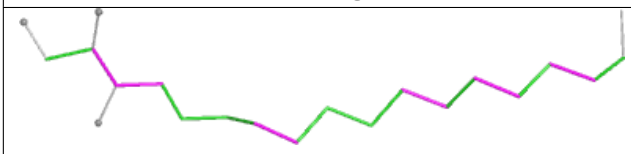


Rings

Ligand SPH A 414

Bond lengths

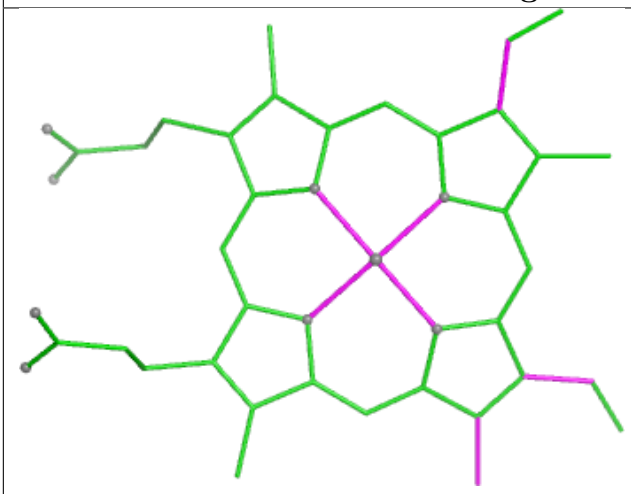
Bond angles



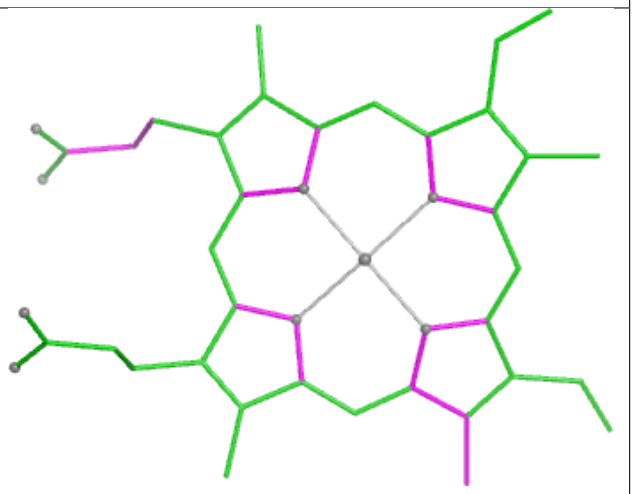
Torsions

Rings

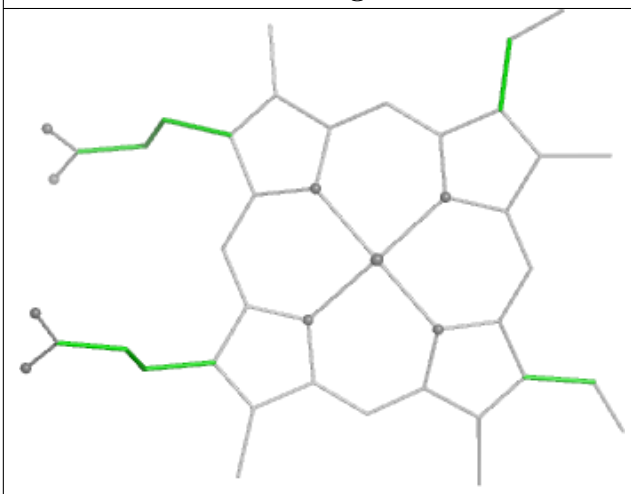
Ligand HEM F 101



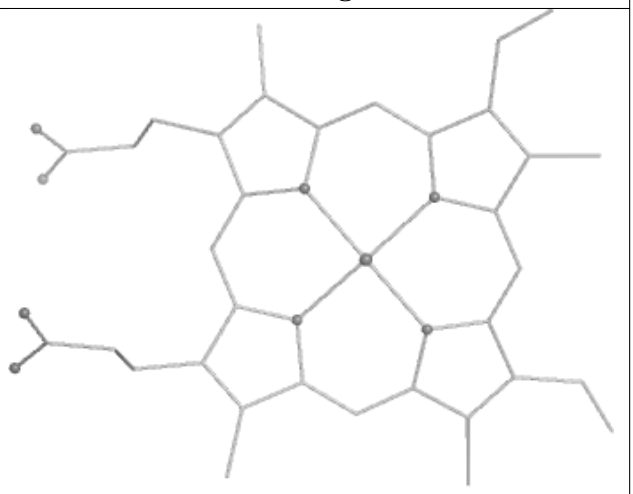
Bond lengths



Bond angles

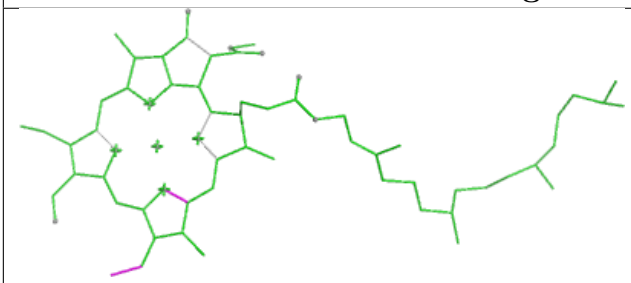


Torsions

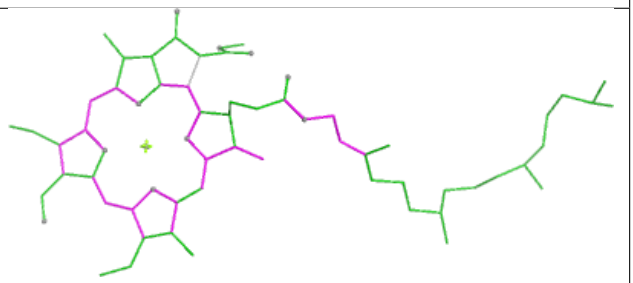


Rings

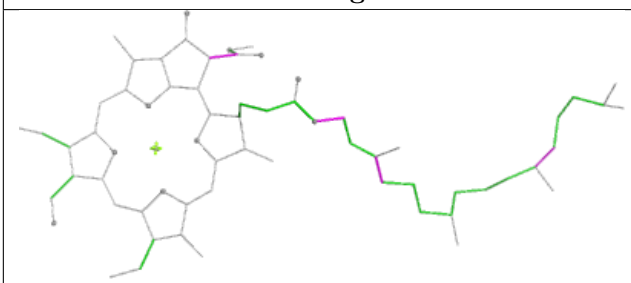
Ligand CHL N 601



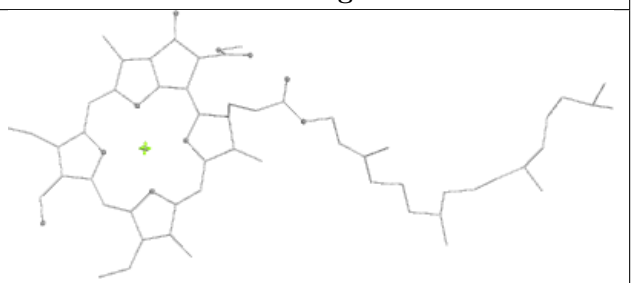
Bond lengths



Bond angles

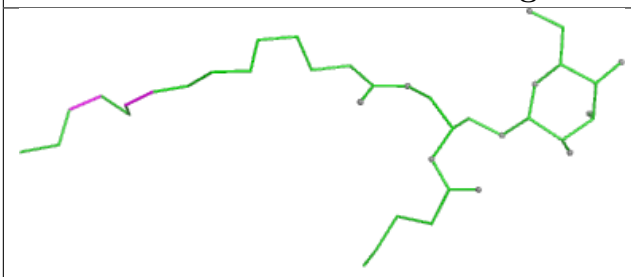


Torsions

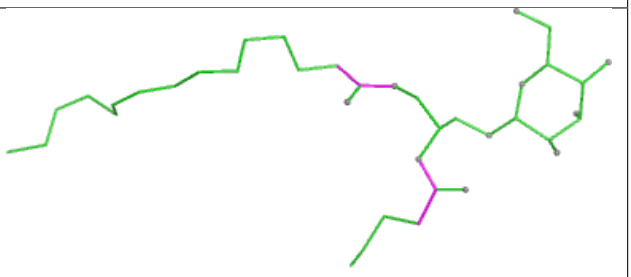


Rings

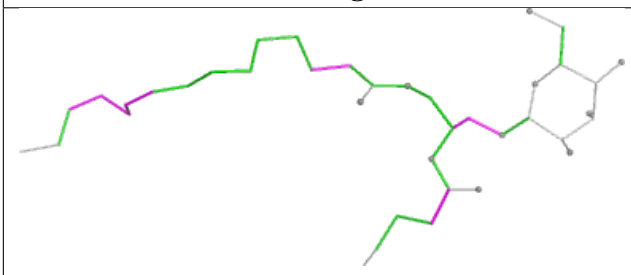
Ligand LMG w 201



Bond lengths



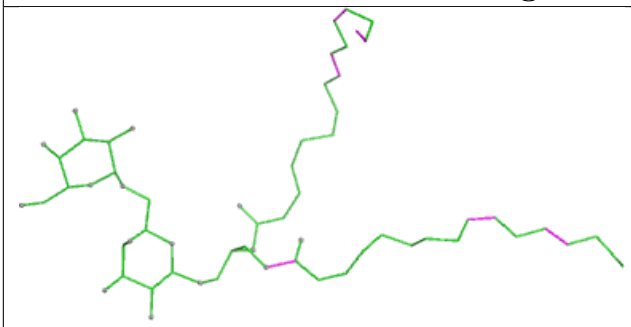
Bond angles



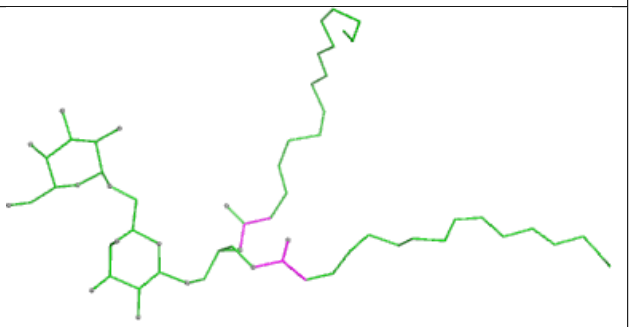
Torsions

Rings

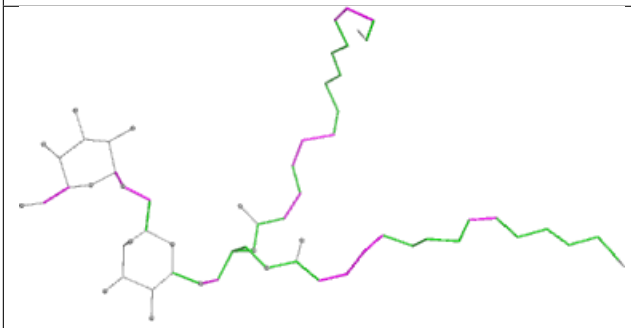
Ligand DGD C 519



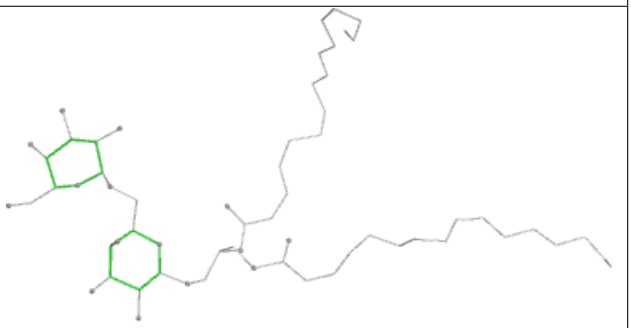
Bond lengths



Bond angles

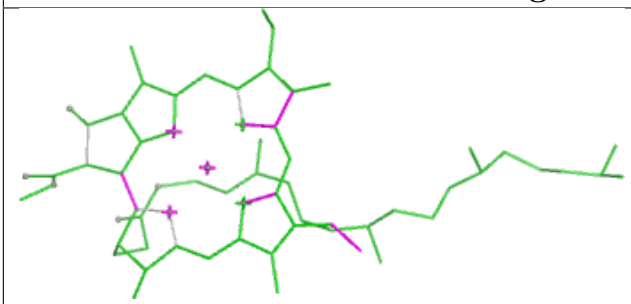


Torsions



Rings

Ligand CLA c 505



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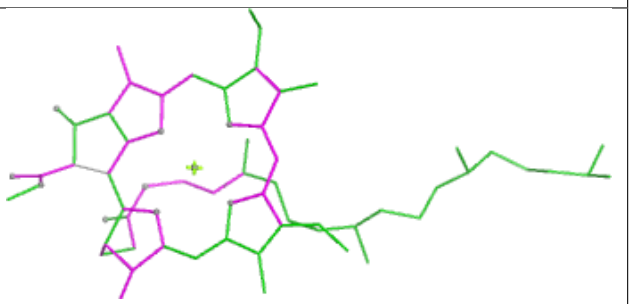
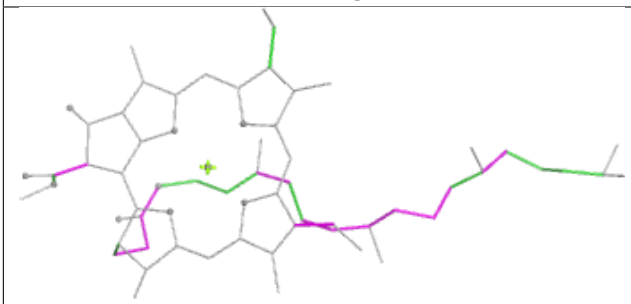
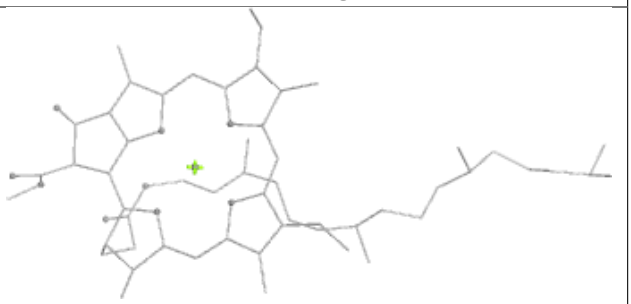


Bond angles

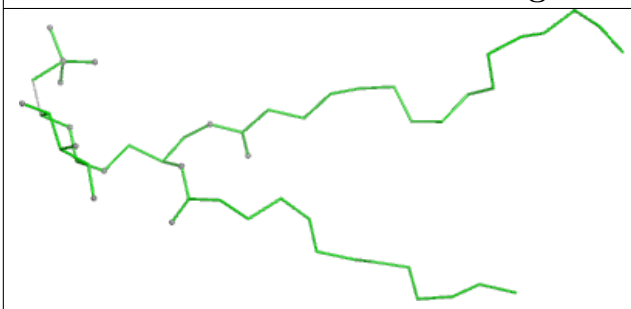


Torsions

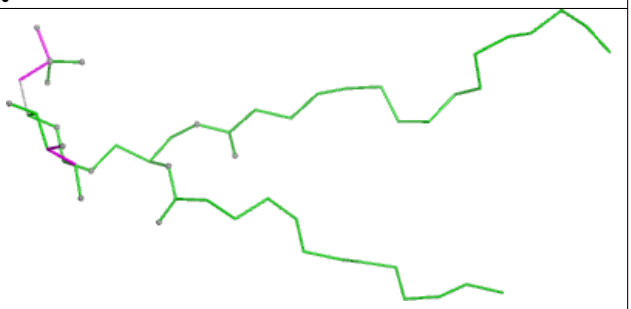


Rings

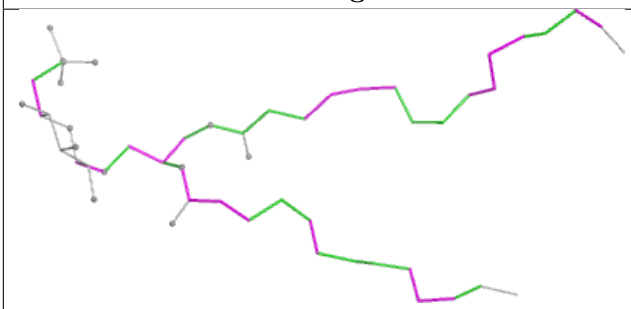
Ligand SQD a 412



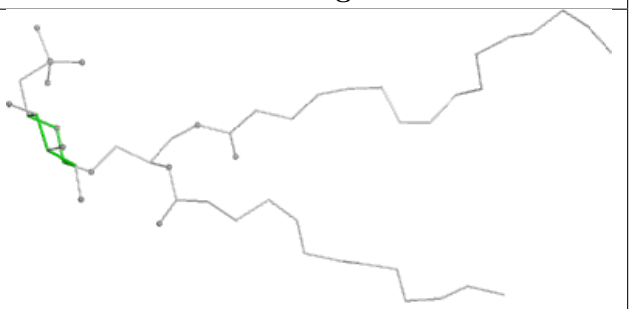
Bond lengths



Bond angles

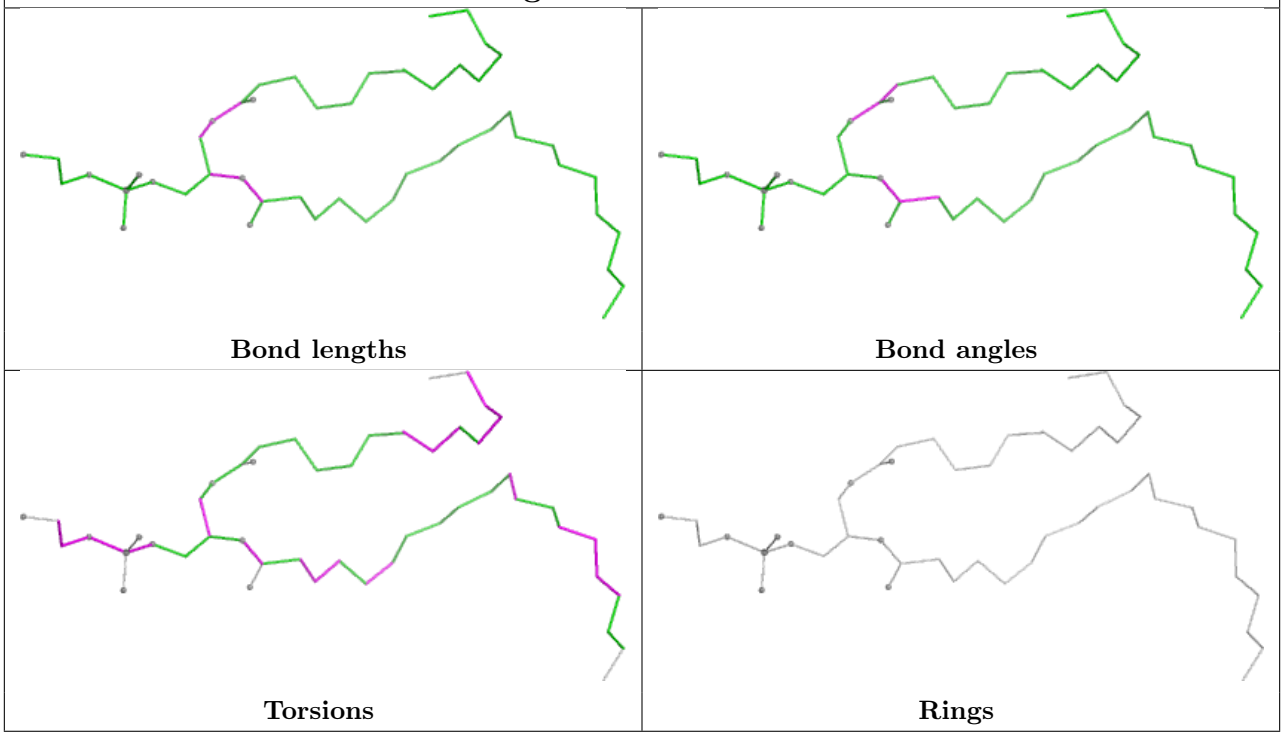


Torsions

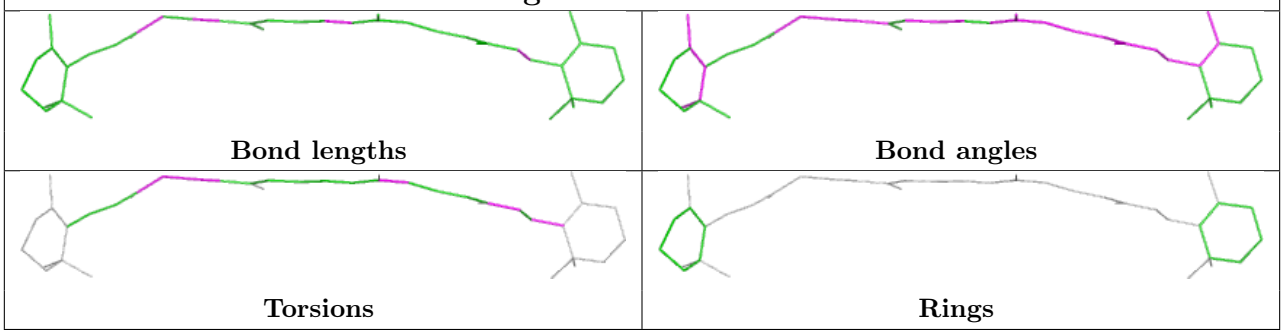


Rings

Ligand PTY Y 626



Ligand BCR C 517



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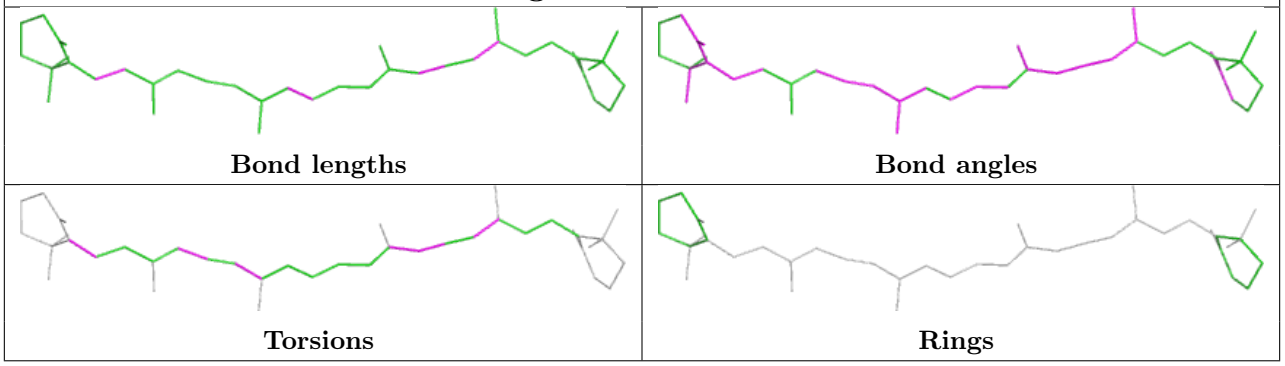
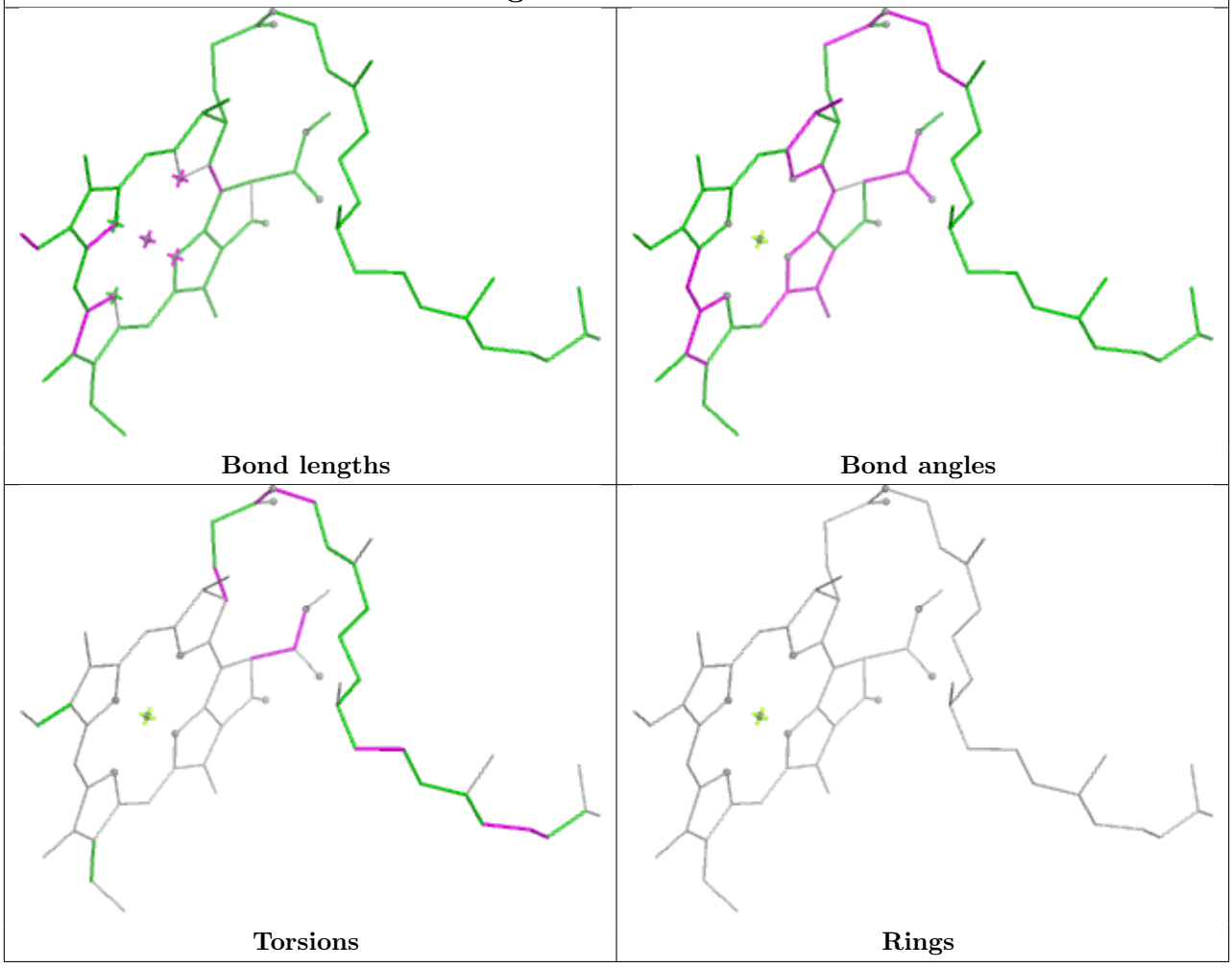
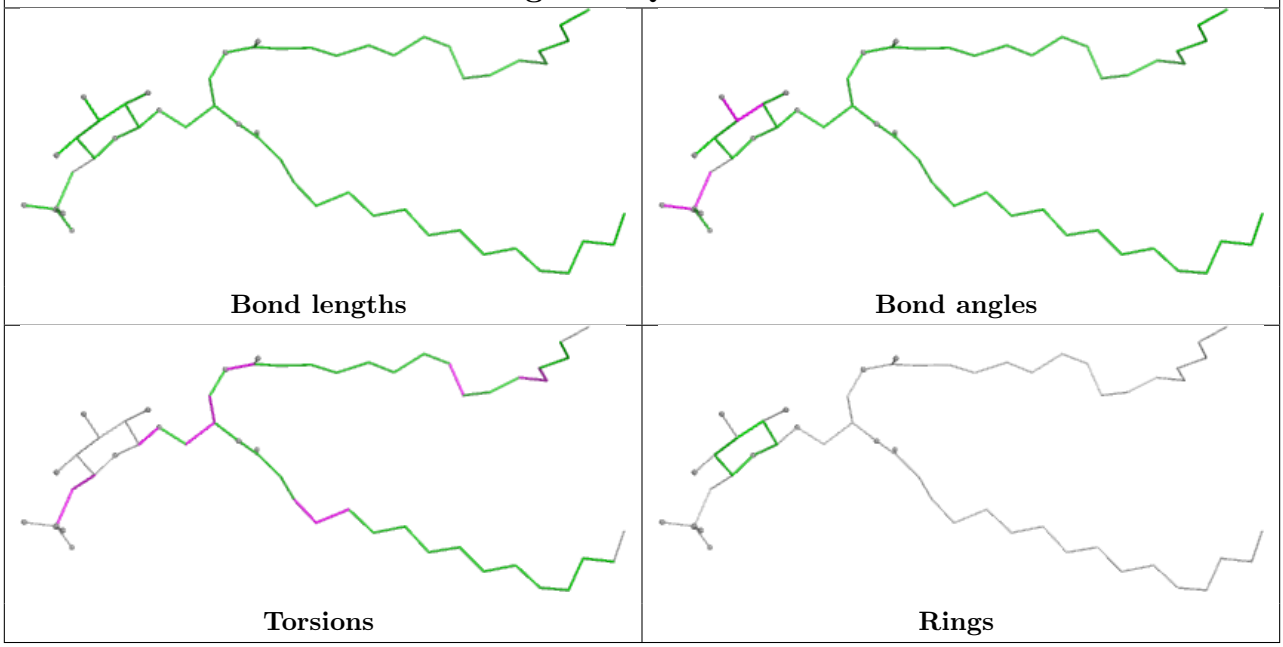


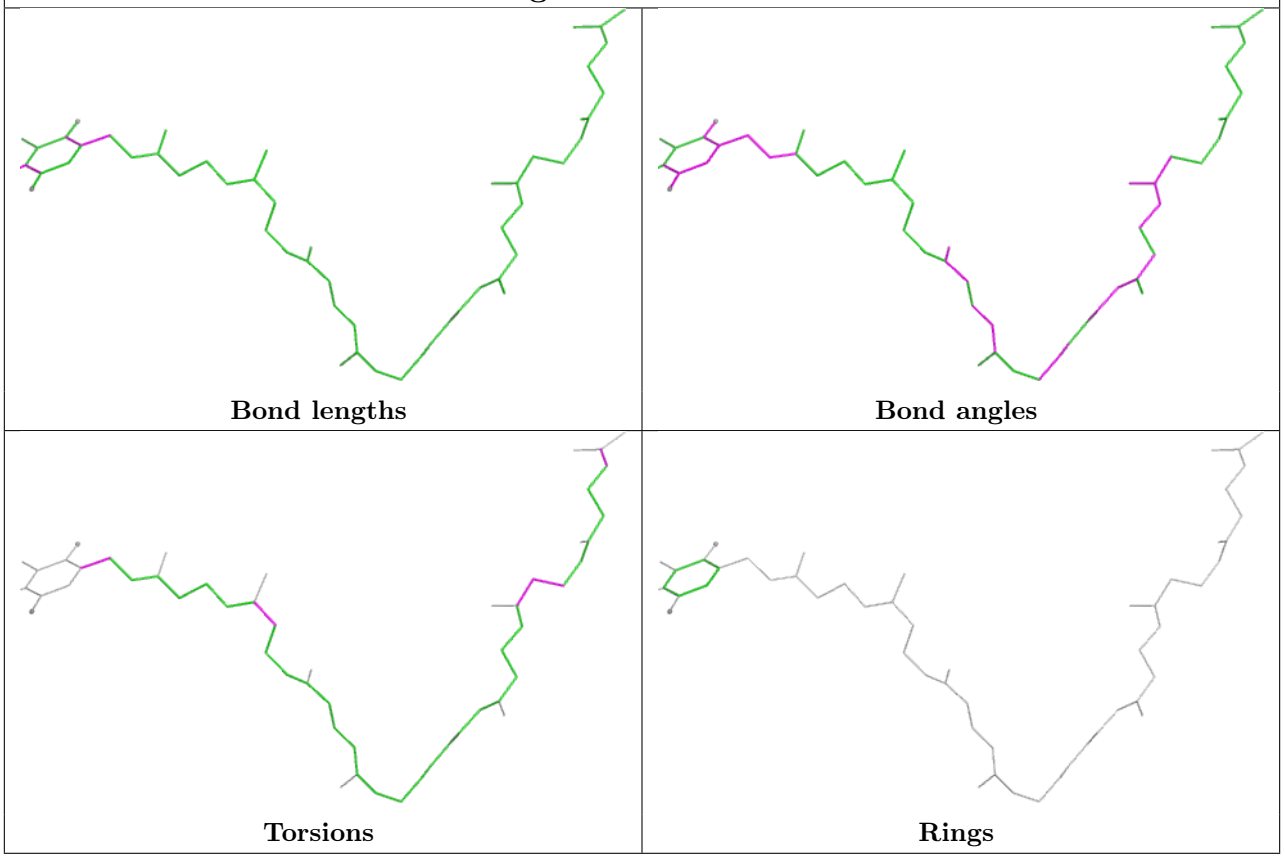
Ligand CLA b 614



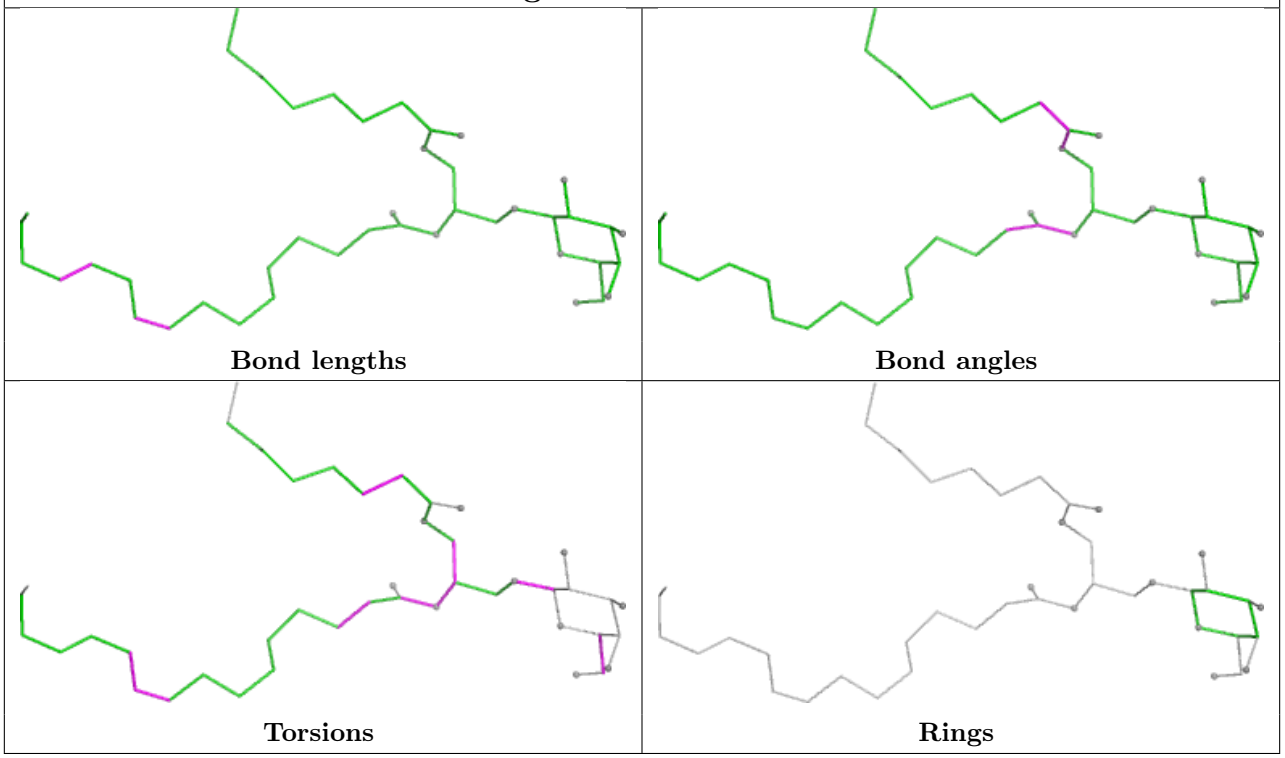
Ligand SQD C 526



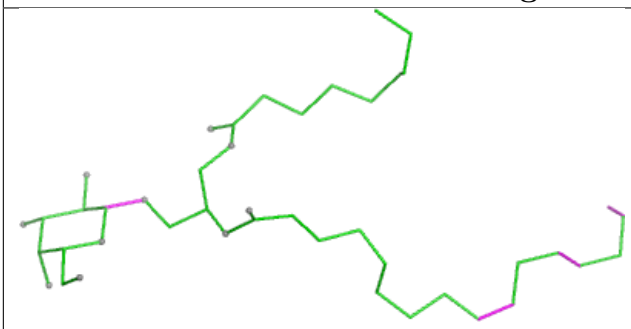
Ligand PL9 D 405



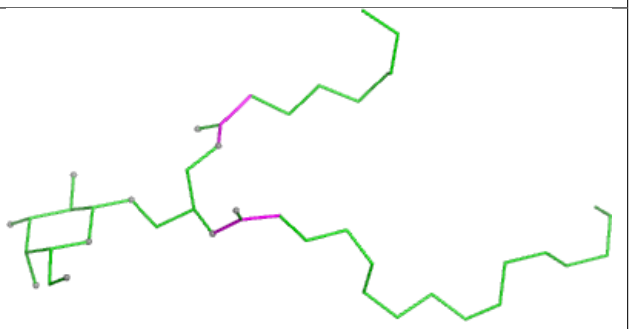
Ligand LMG b 622



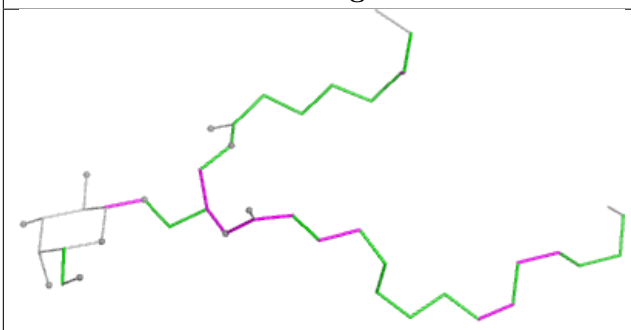
Ligand LMG B 622



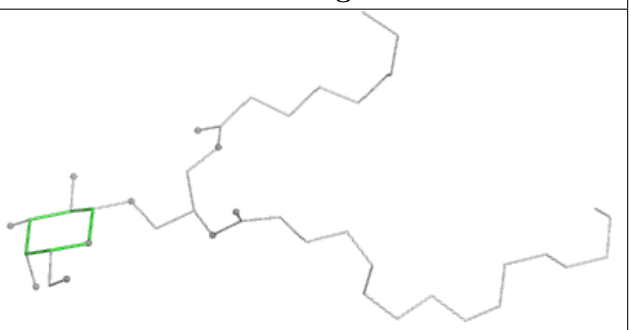
Bond lengths



Bond angles

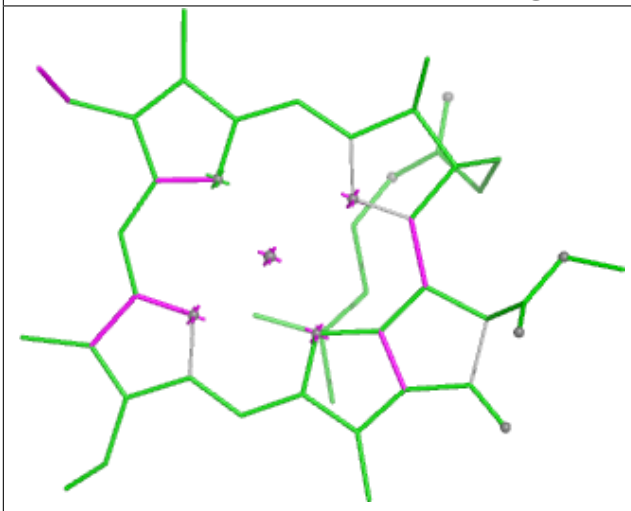


Torsions



Rings

Ligand CLA S 605



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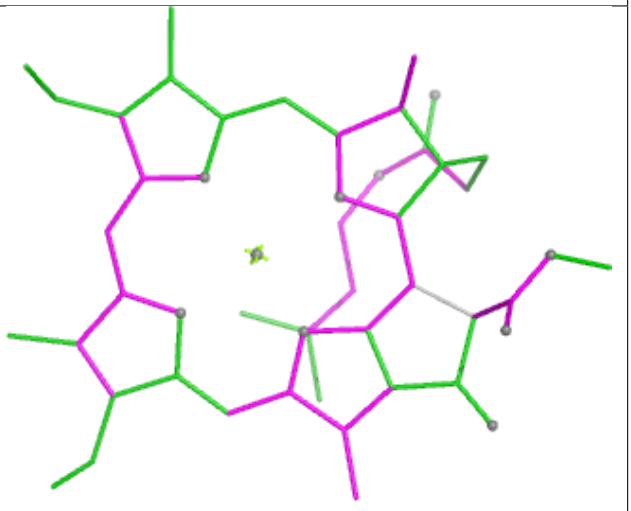
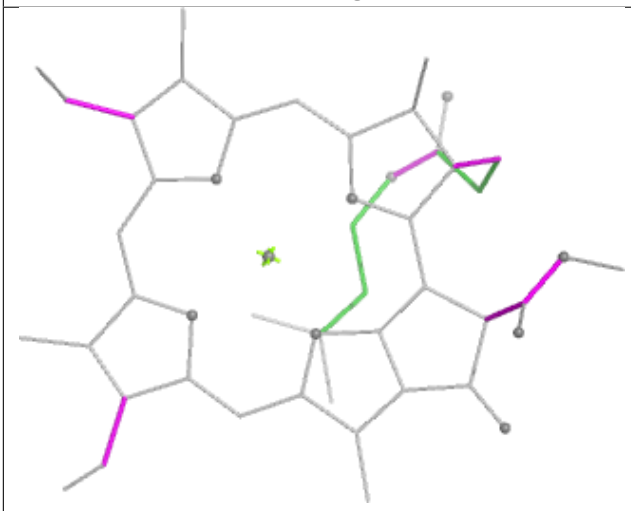


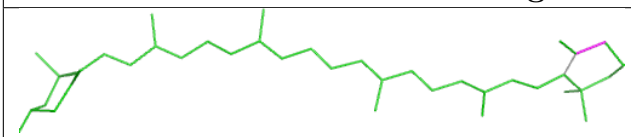
Bond angles



Torsions

Rings

Ligand LUT S 621



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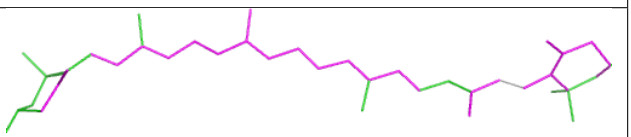
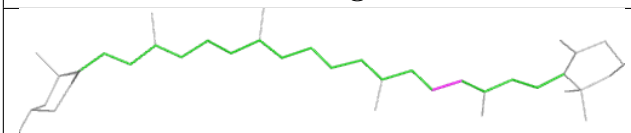


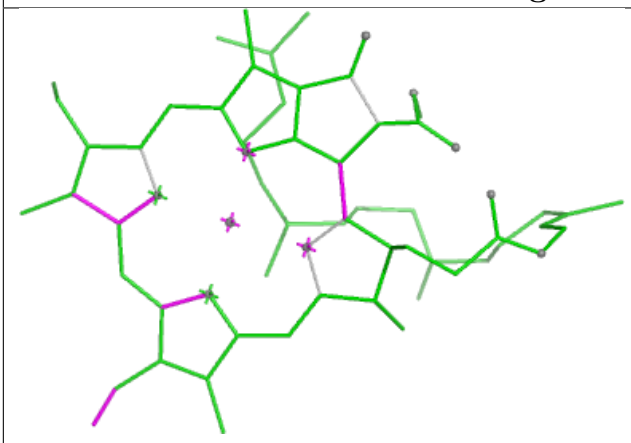
Bond angles



Torsions

Rings

Ligand CLA c 510



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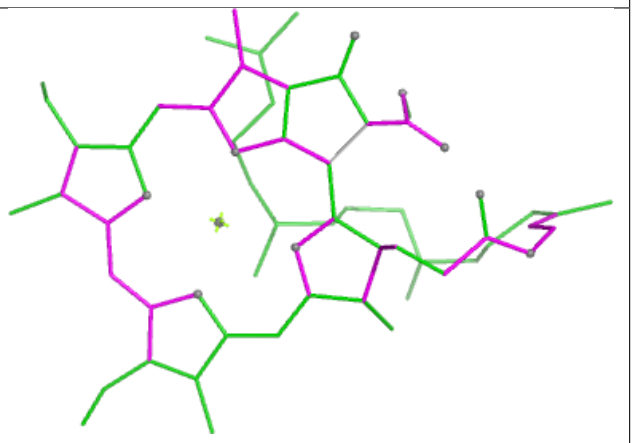
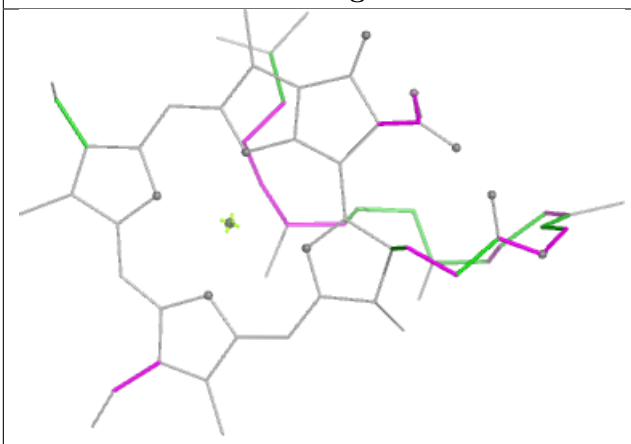
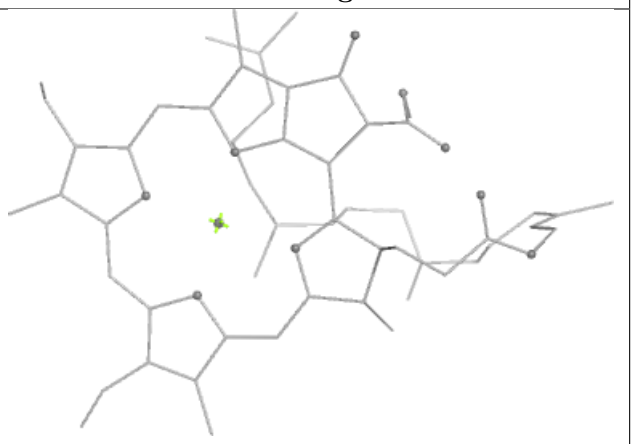


Bond angles

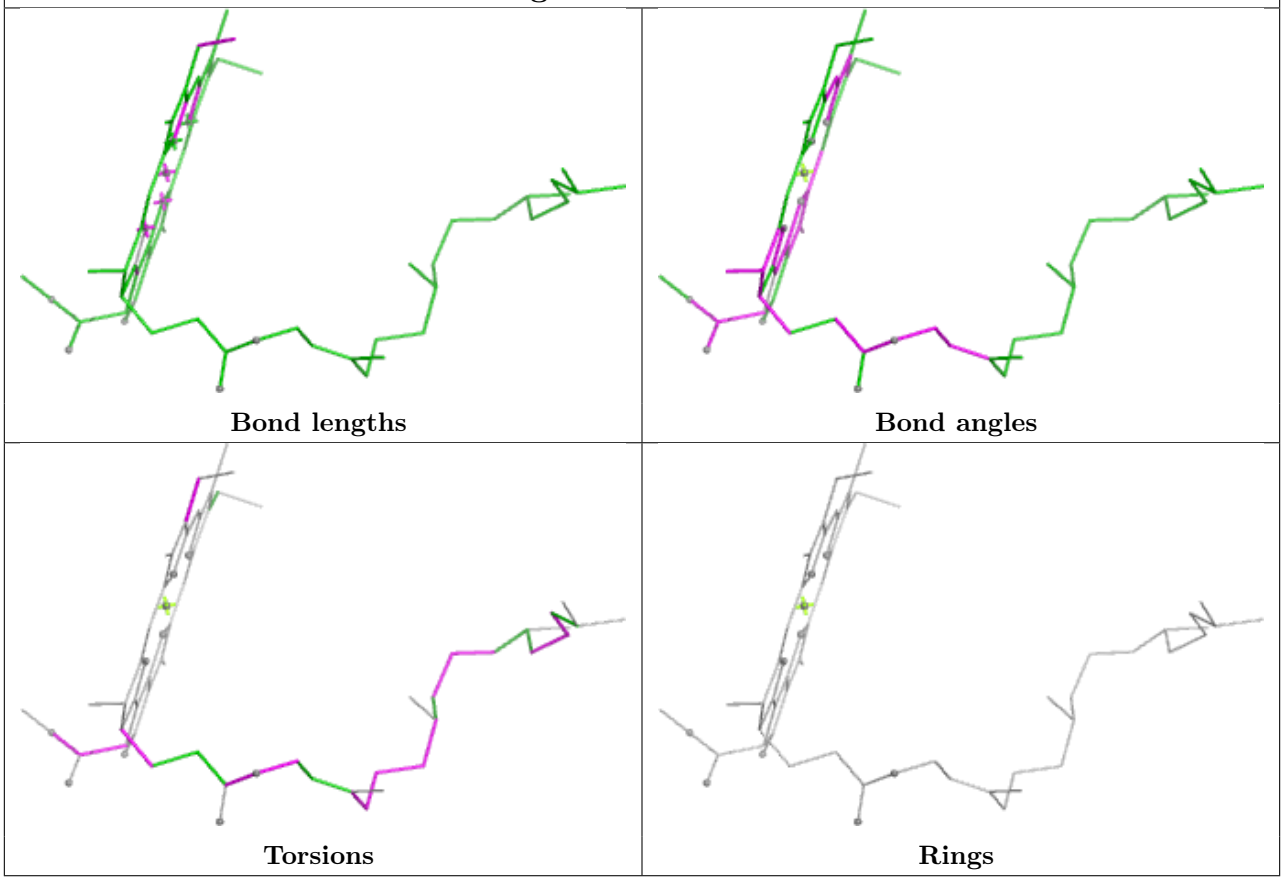


Torsions

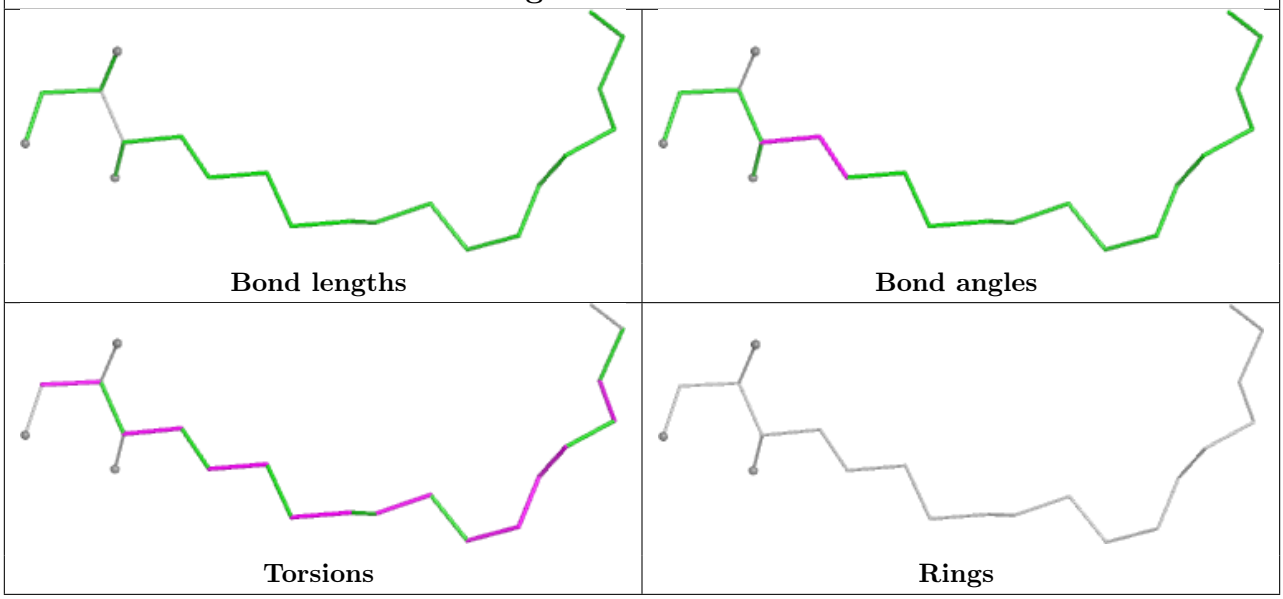


Rings

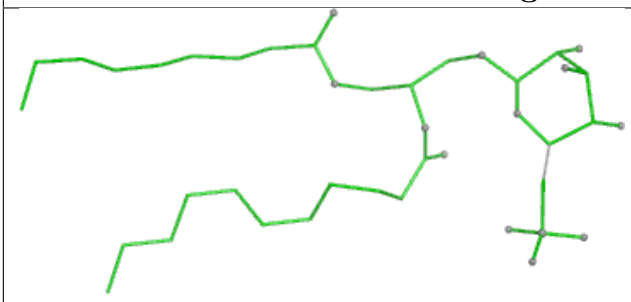
Ligand CLA c 506



Ligand SPH Y 625



Ligand SQD M 101



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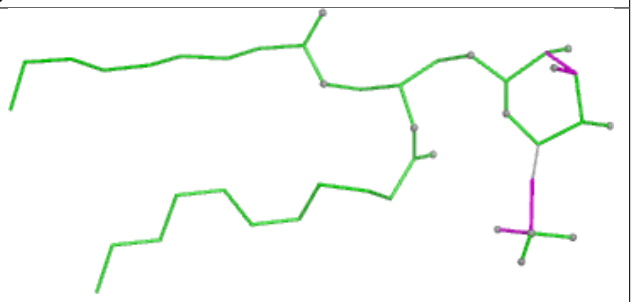
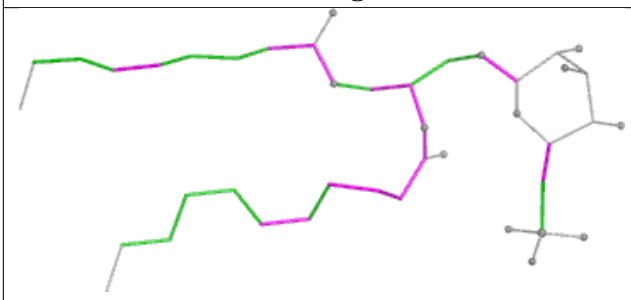


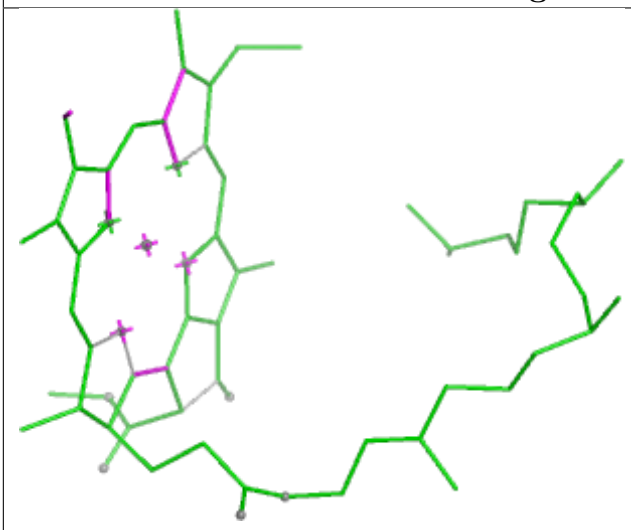
Bond angles



Torsions

Rings

Ligand CLA c 503



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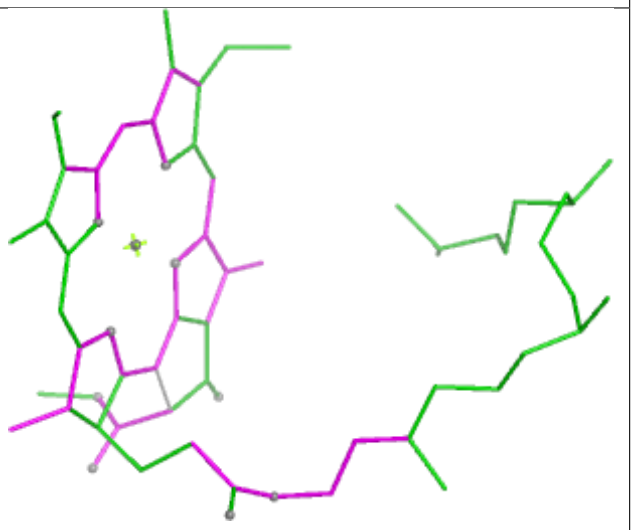
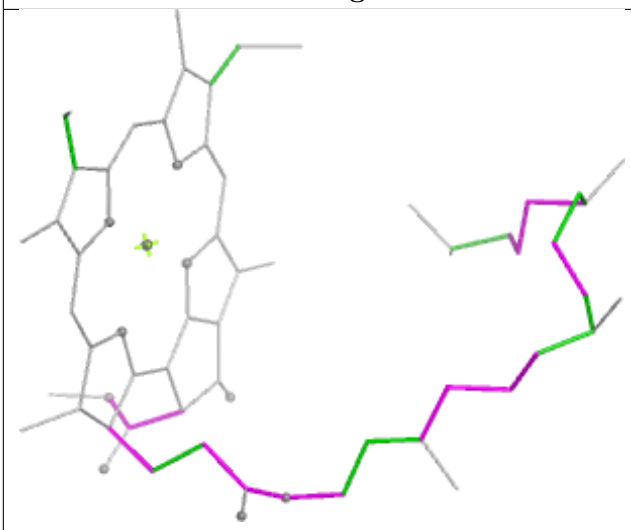


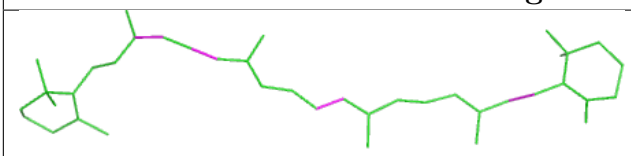
Bond angles



Torsions

Rings

Ligand BCR d 404



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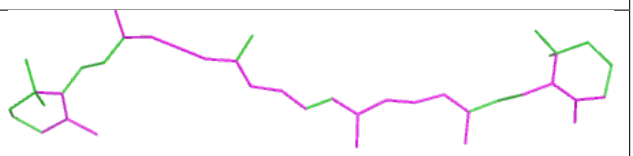
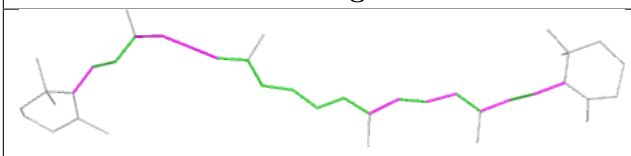
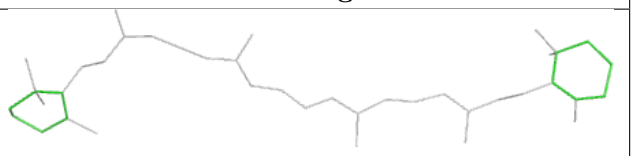


Bond angles

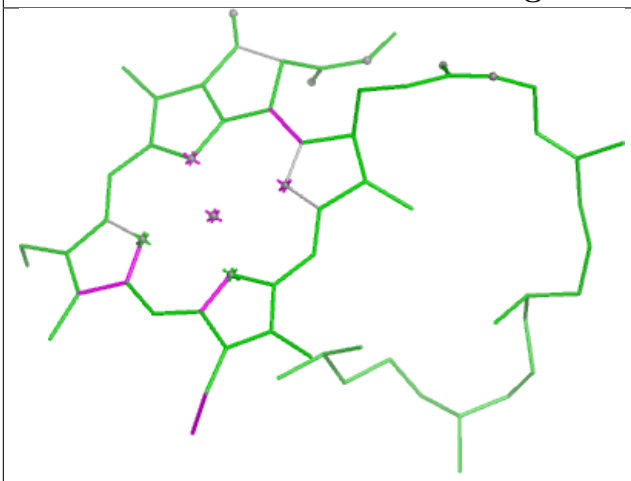


Torsions



Rings

Ligand CLA B 616



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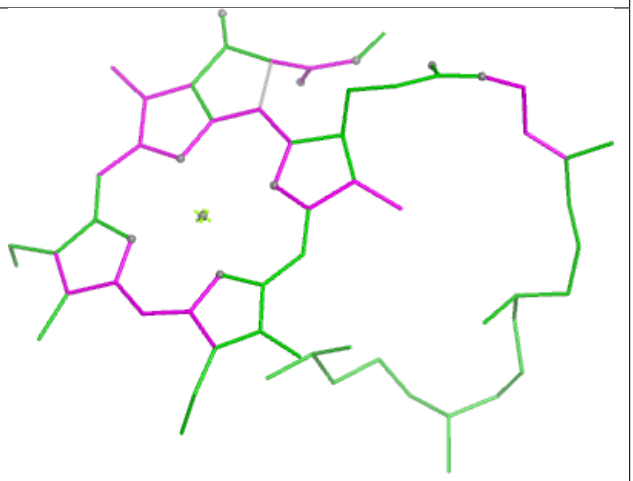
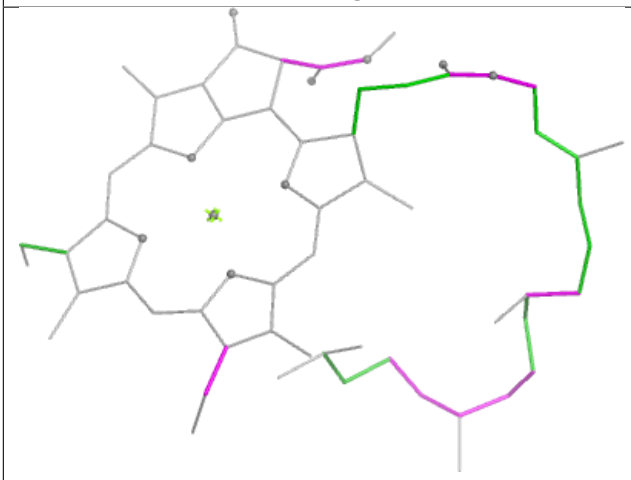


Bond angles



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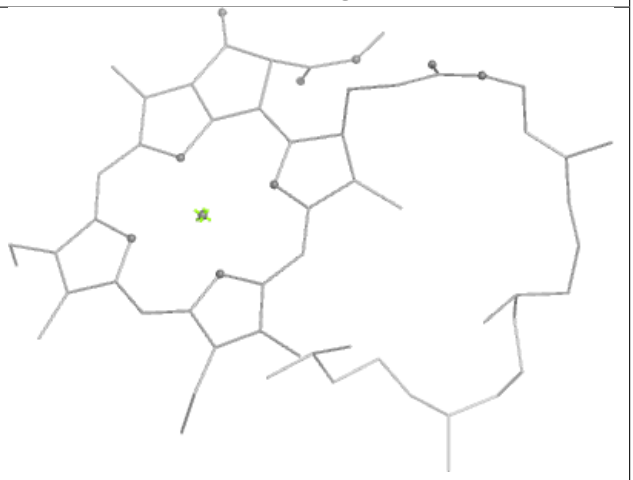
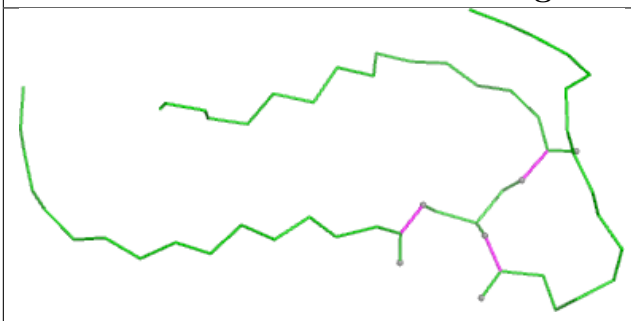


Rings

Ligand 4RF I 102



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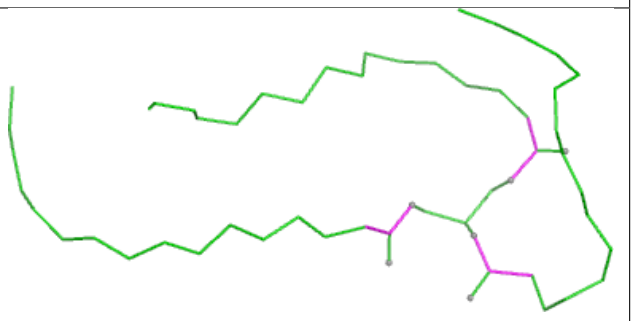
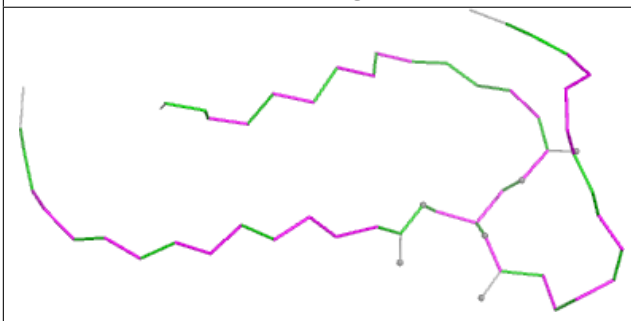
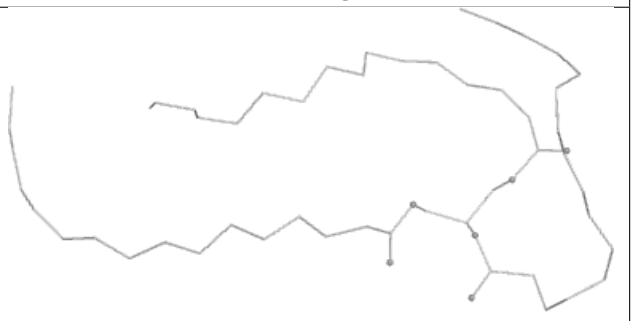


Bond angles

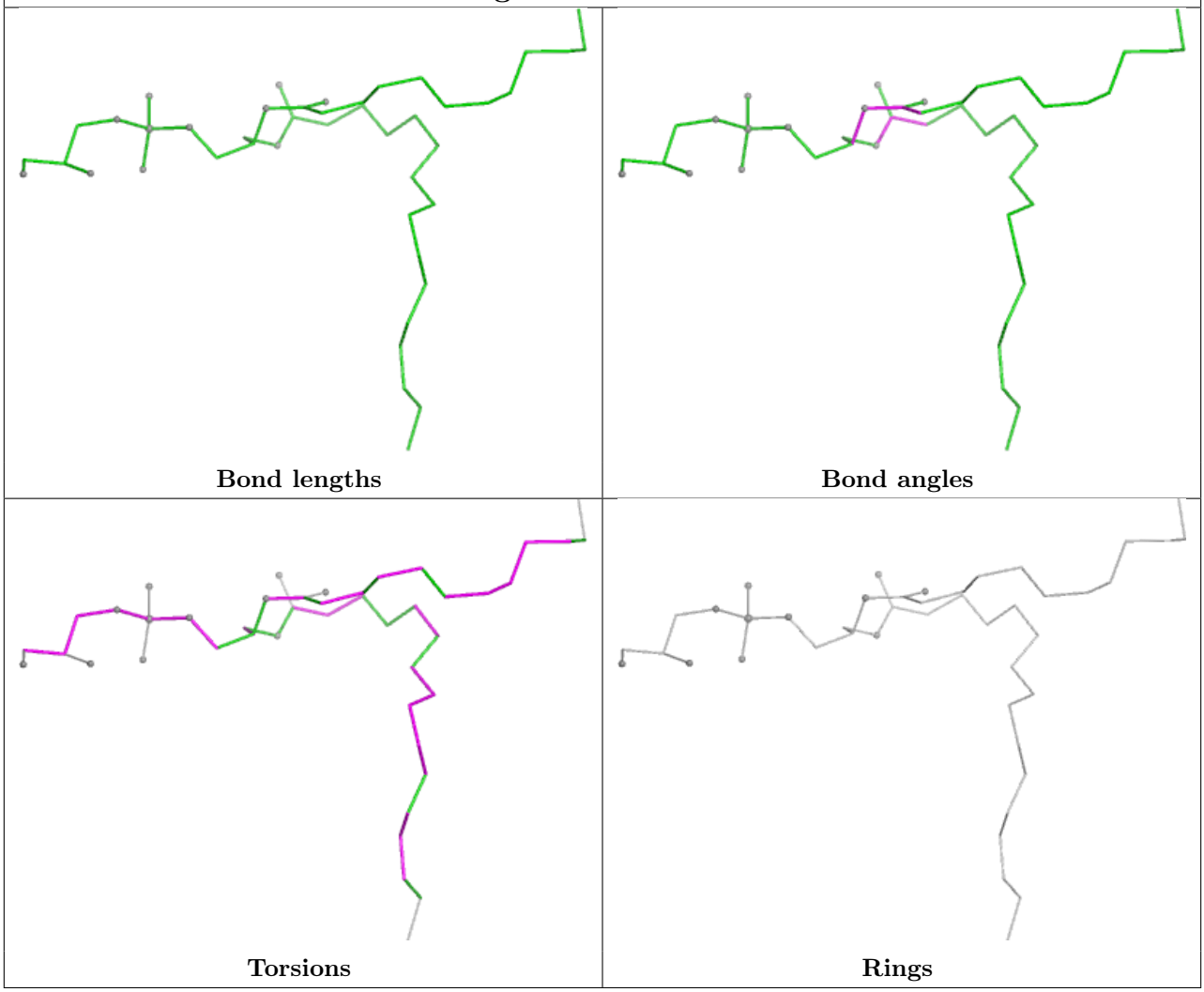


Torsions

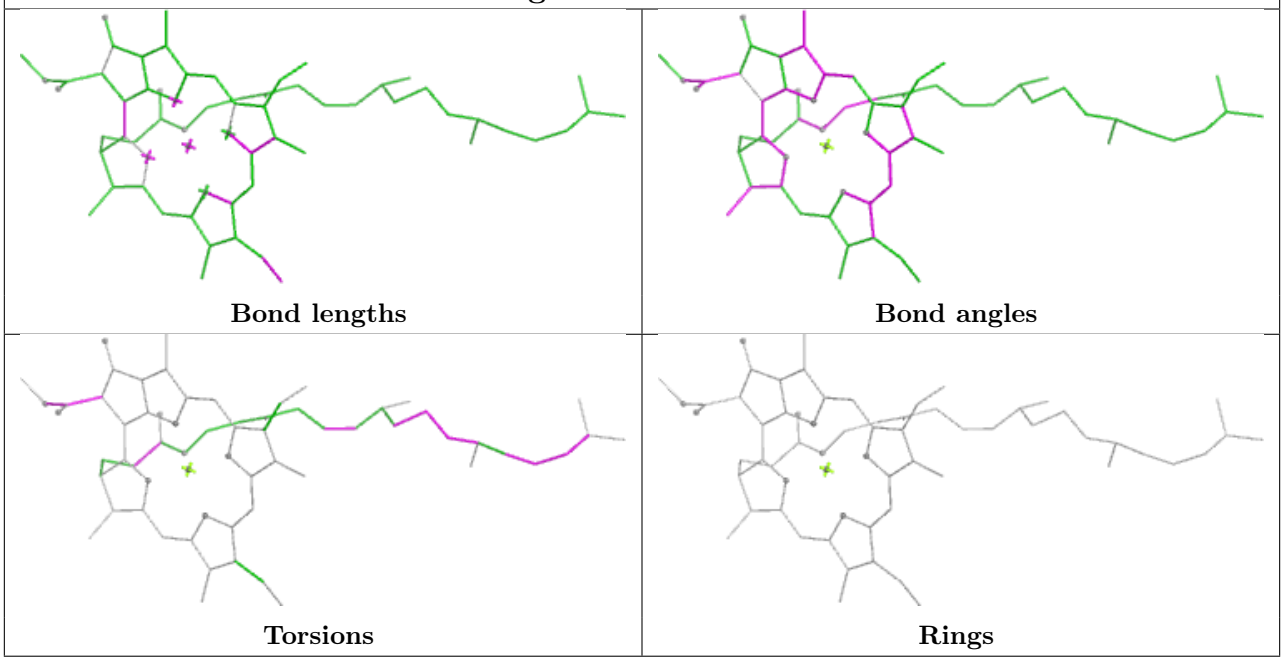


Rings

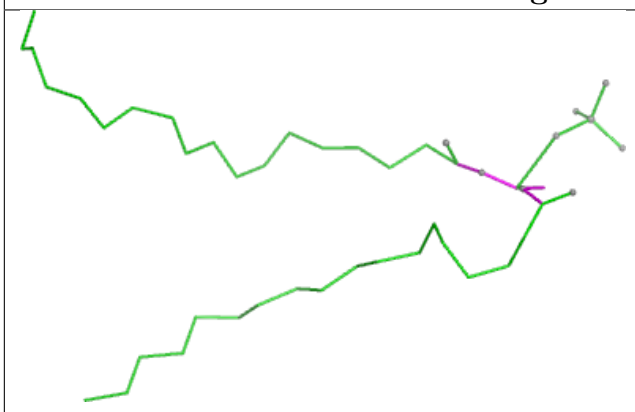
Ligand LHG S 624



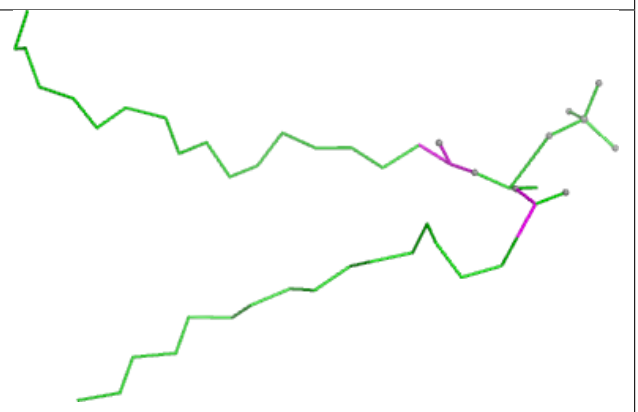
Ligand CLA b 615



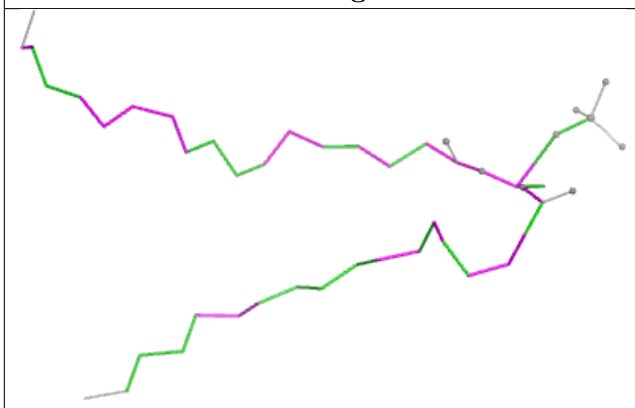
Ligand 3PH S 626



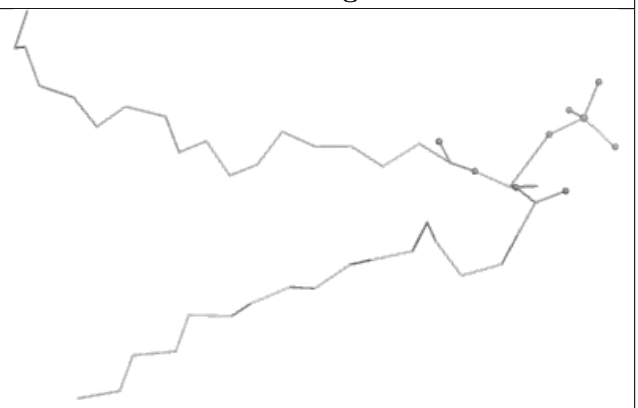
Bond lengths



Bond angles

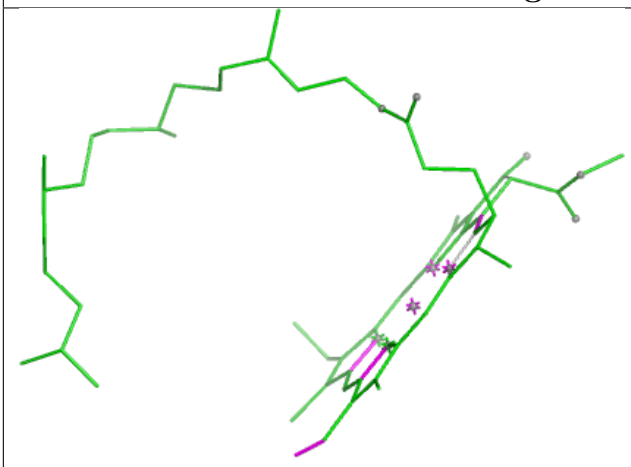


Torsions



Rings

Ligand CLA B 612



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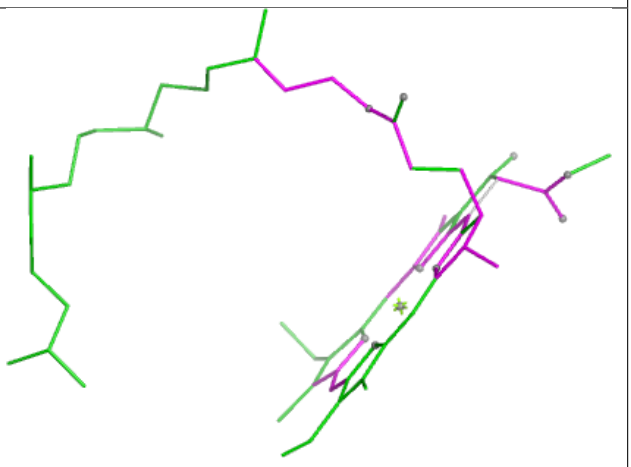
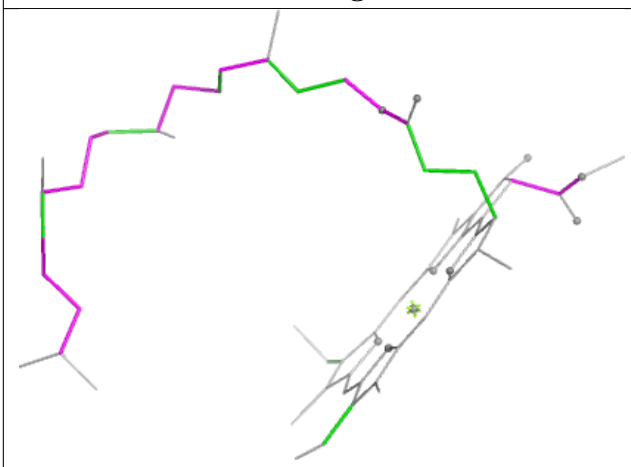


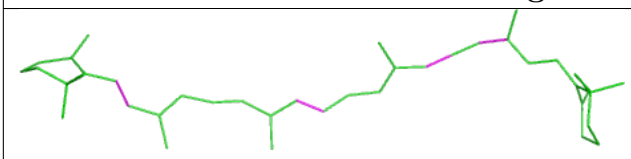
Bond angles



Torsions

Rings

Ligand BCR c 517



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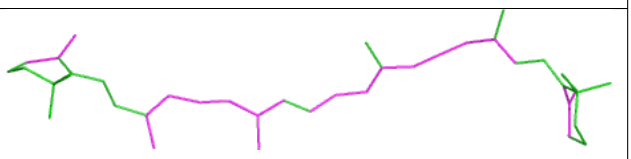
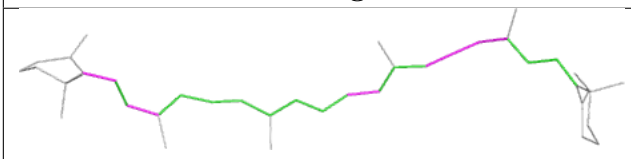
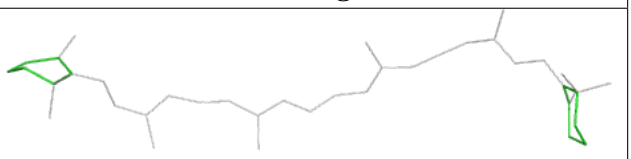


Bond angles

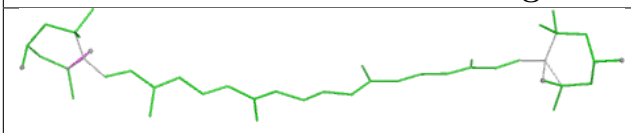


Torsions



Rings

Ligand XAT G 622



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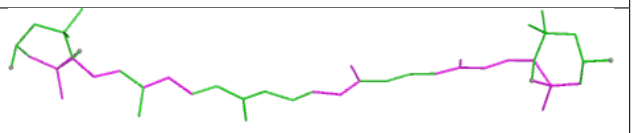
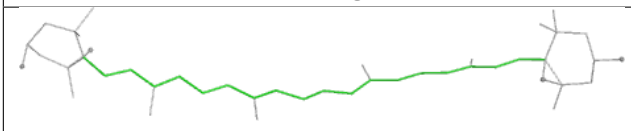
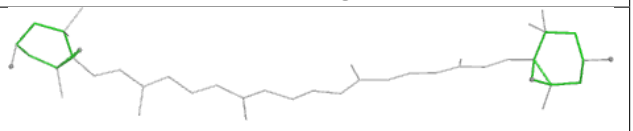


Bond angles



Torsions



Rings

Ligand CHL S 608

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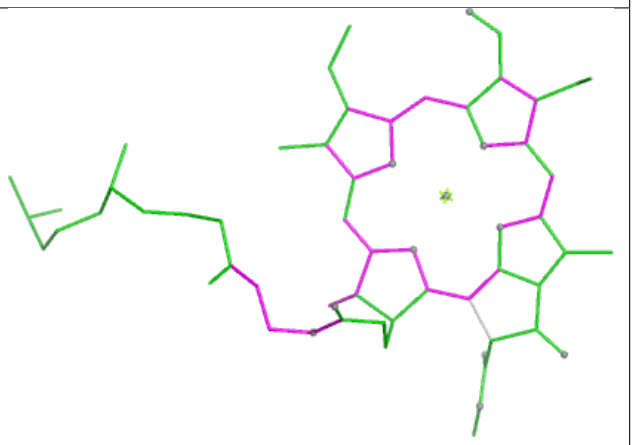
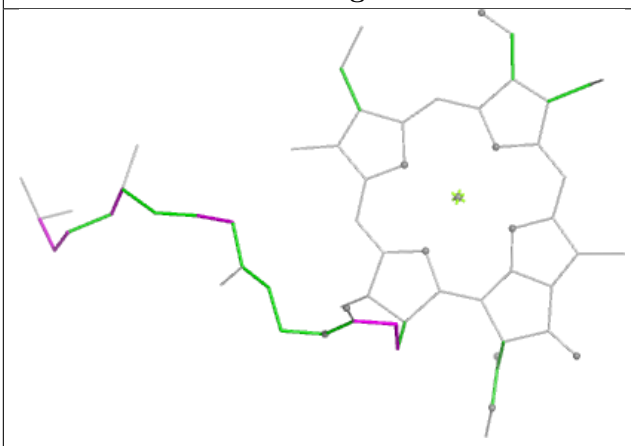


Bond angles



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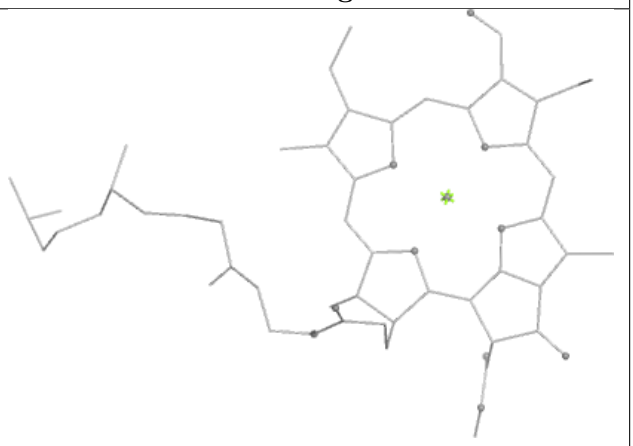
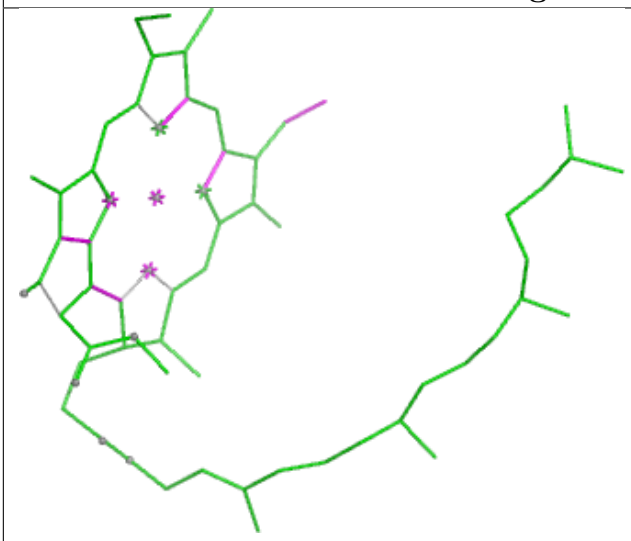


Rings

Ligand CLA c 507



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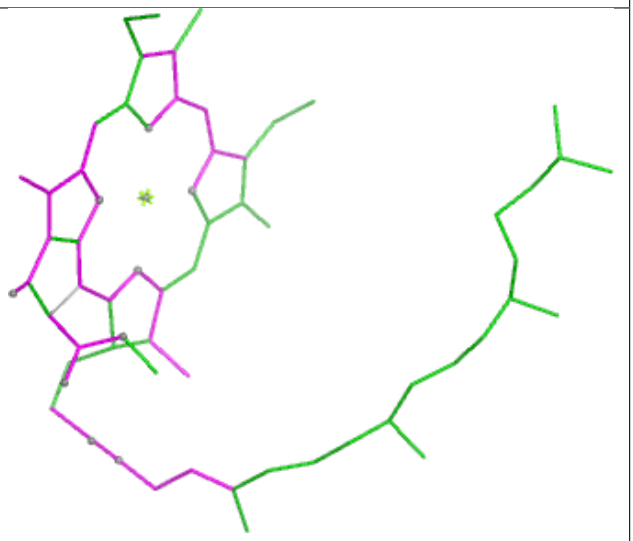
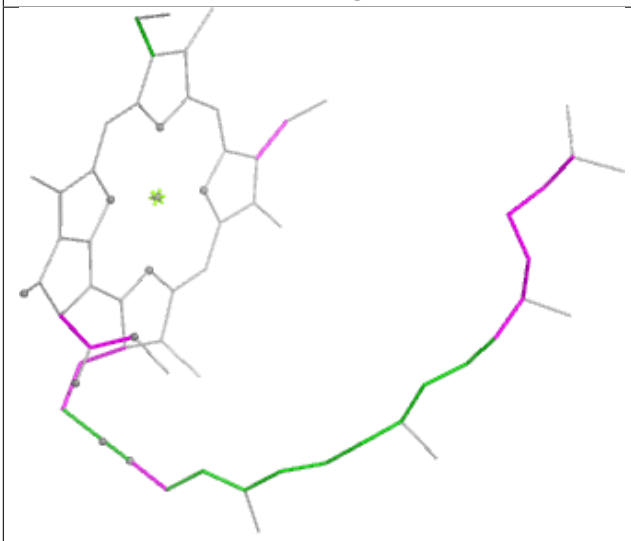


Bond angles



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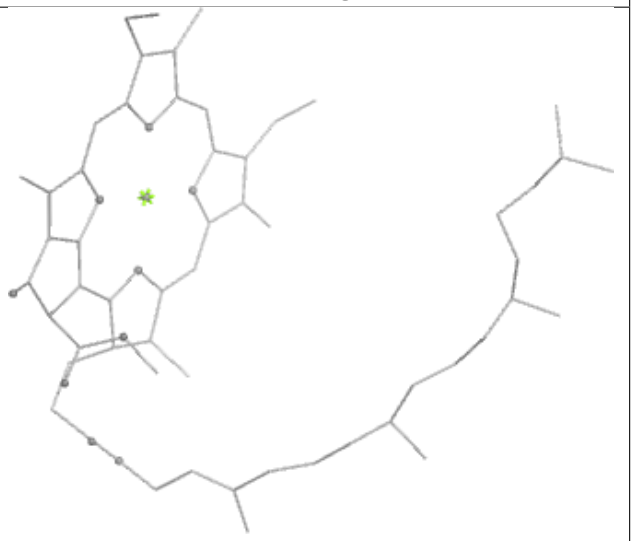
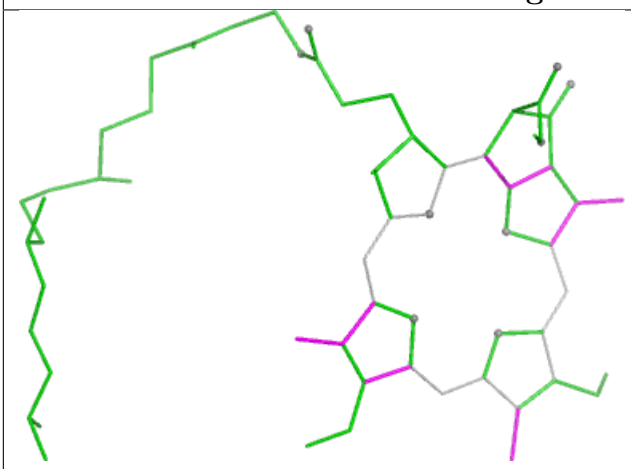
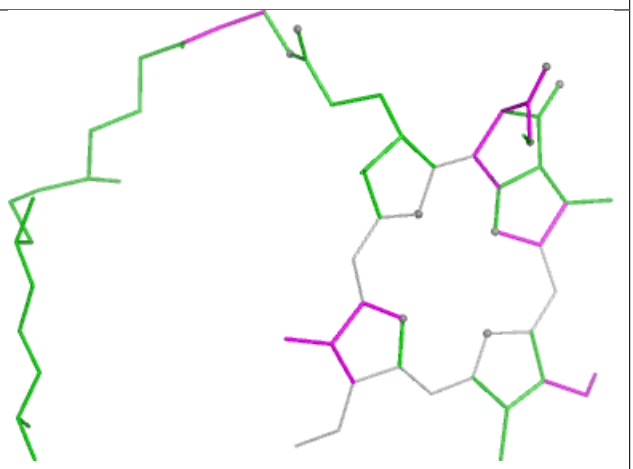


Rings

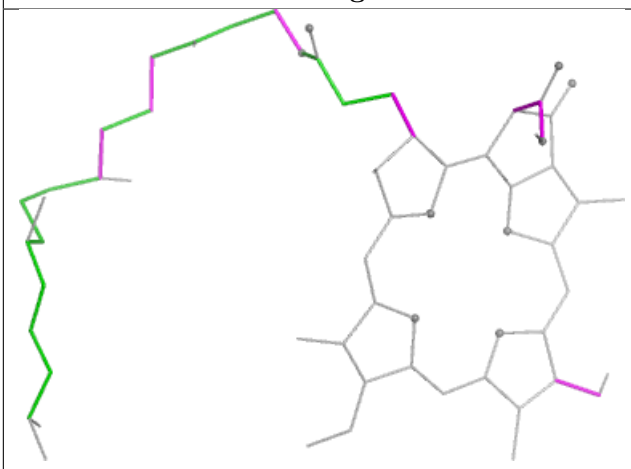
Ligand PHO a 409



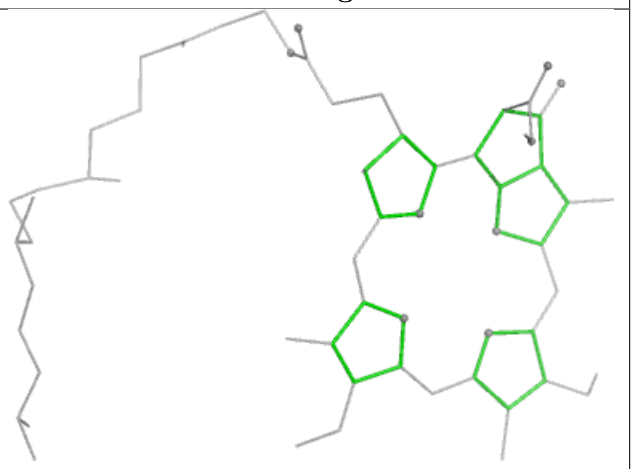
Bond lengths



Bond angles

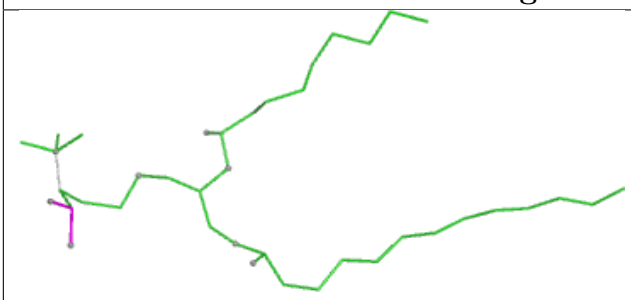


Torsions



Rings

Ligand LMK C 527



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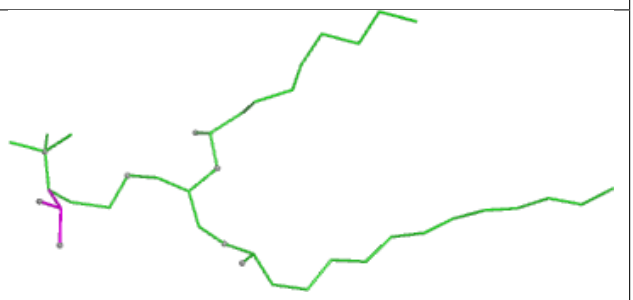
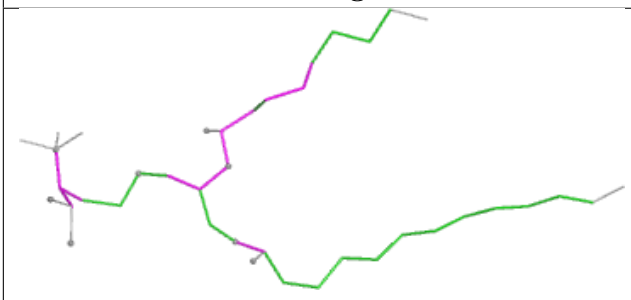
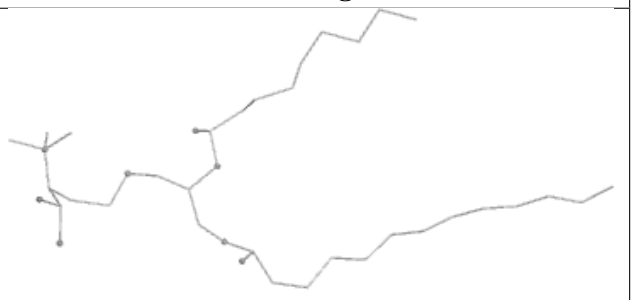


Bond angles

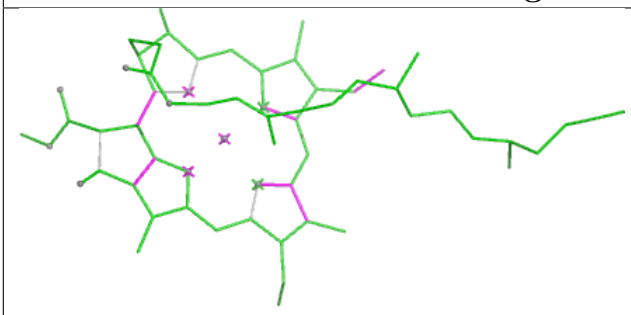


Torsions



Rings

Ligand CLA C 505



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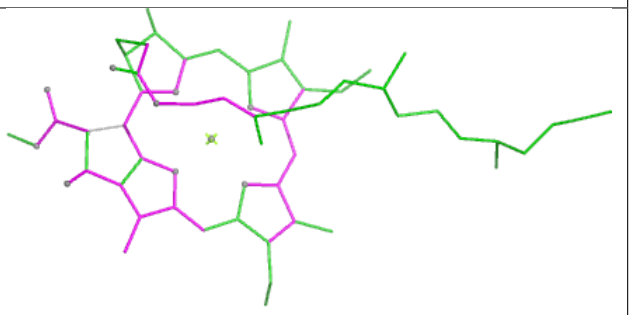
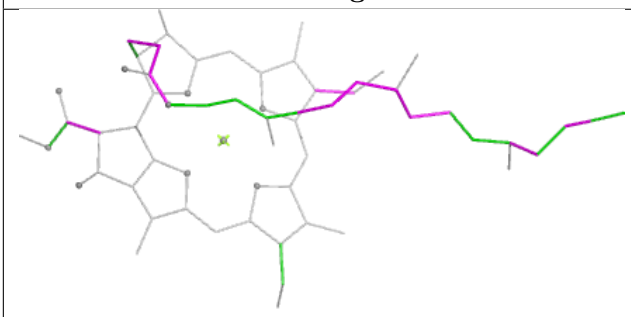


Bond angles



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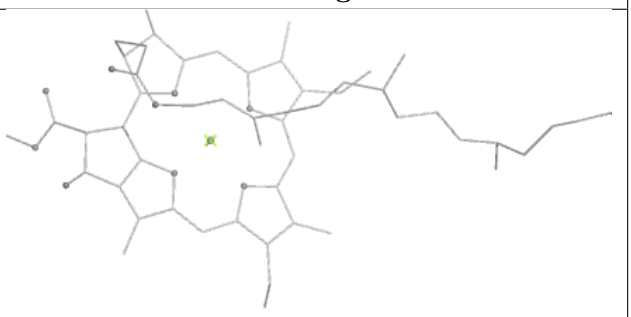

Rings

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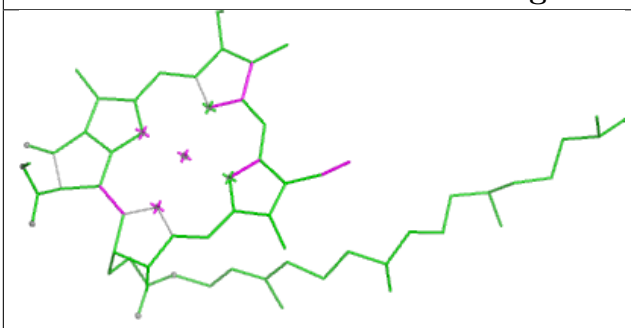

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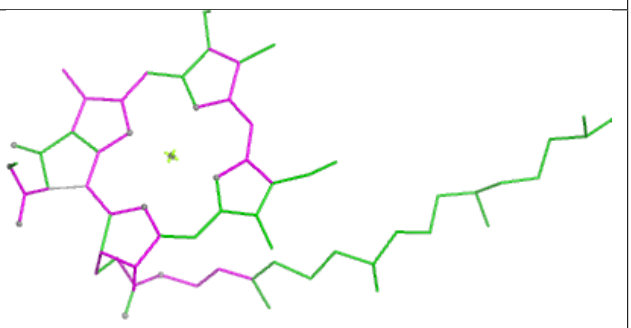
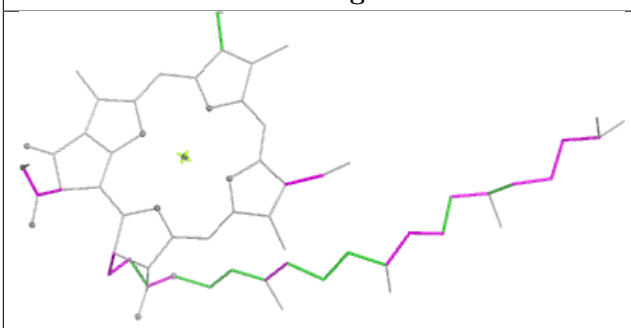
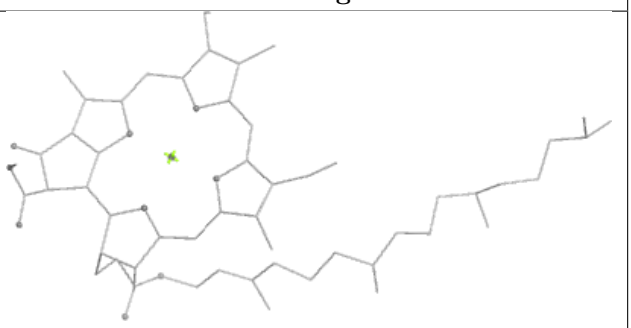


Bond angles

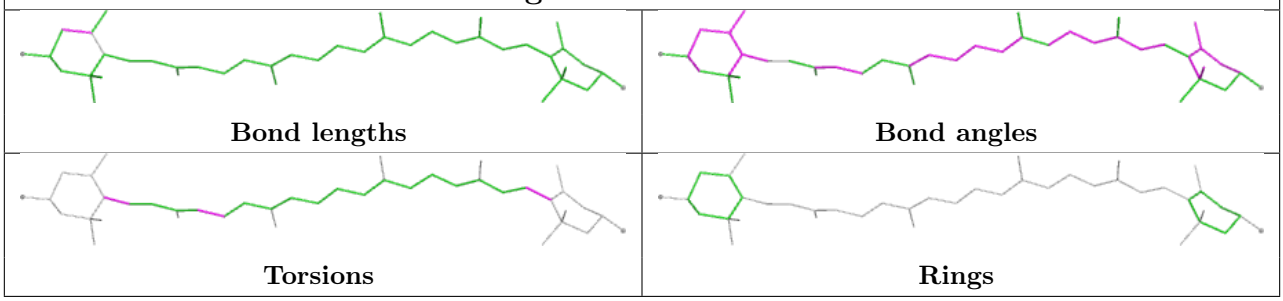


Torsions



Rings

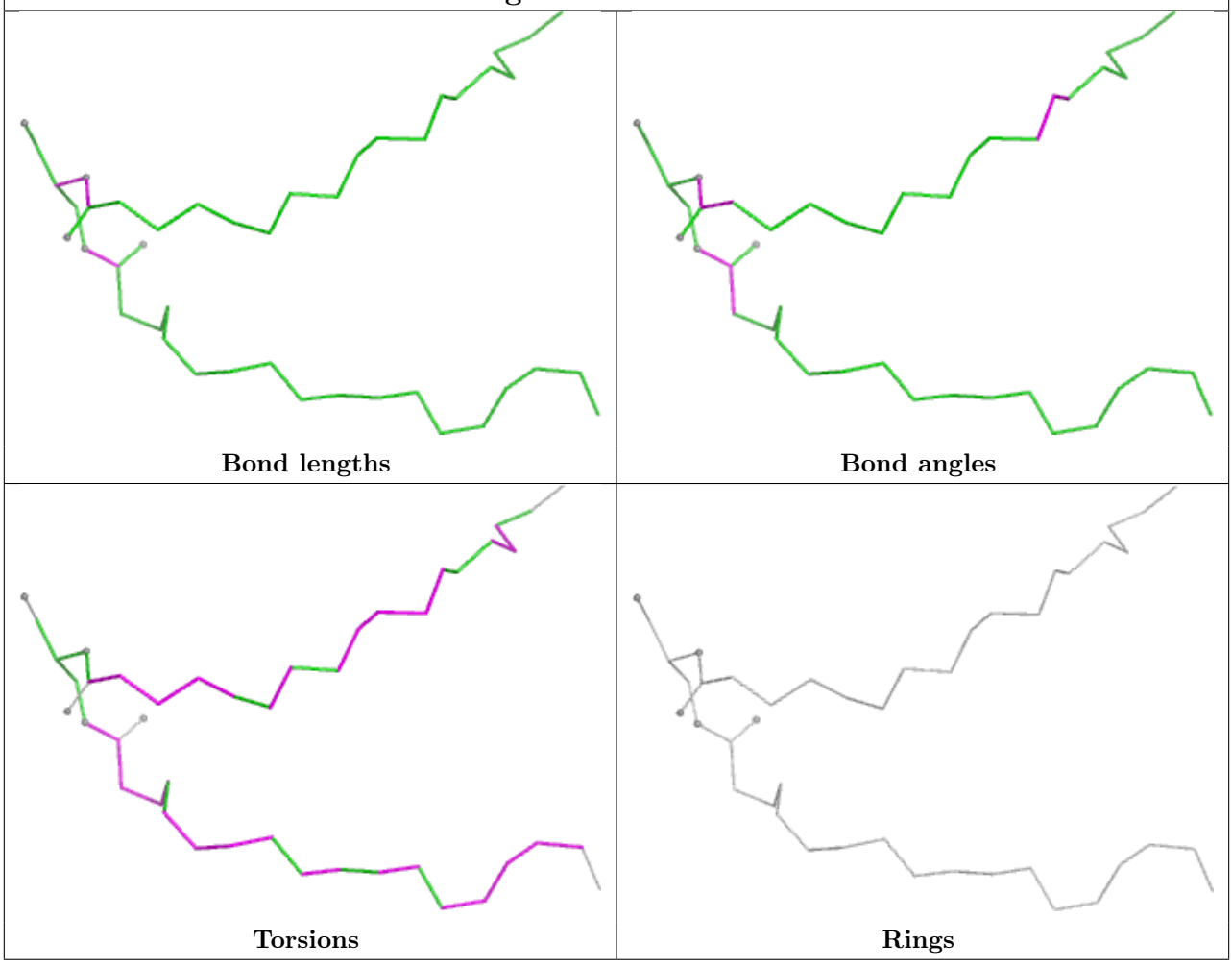
Ligand LUT Y 621



Bond lengths | Bond angles

Torsions | Rings

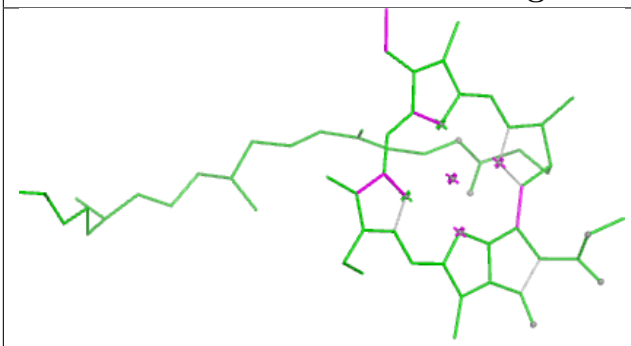
Ligand DGA c 524



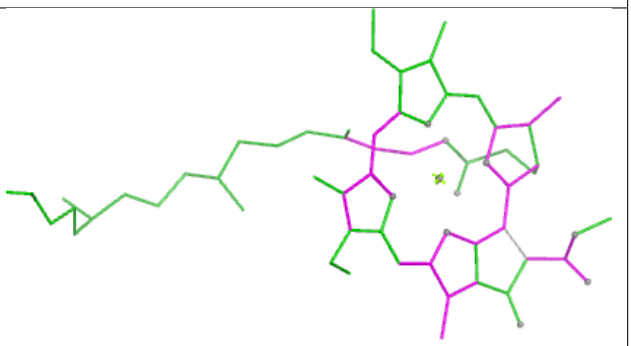
Bond lengths | Bond angles

Torsions | Rings

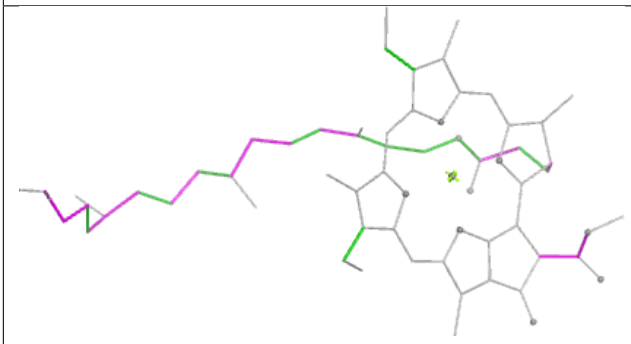
Ligand CLA b 609



Bond lengths



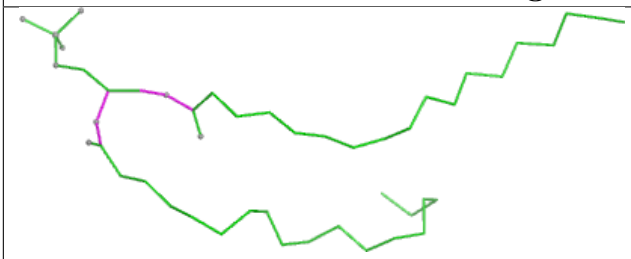
Bond angles



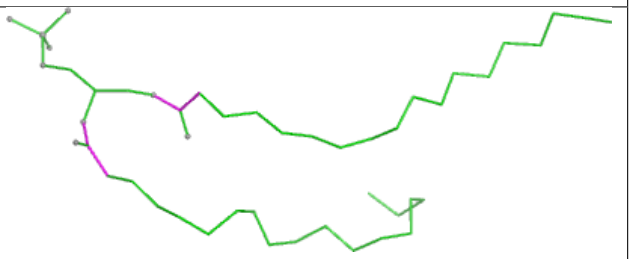
Torsions

Rings

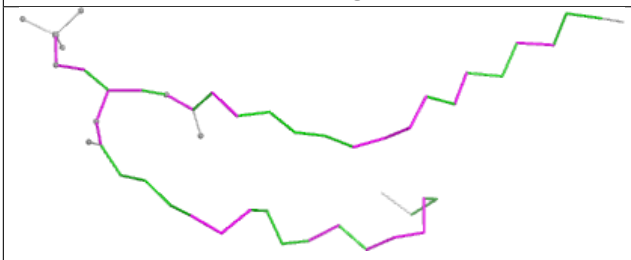
Ligand 3PH T 101



Bond lengths



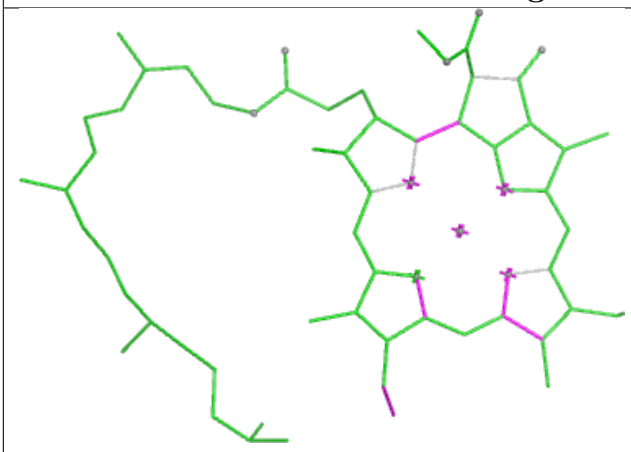
Bond angles



Torsions

Rings

Ligand CLA S 603



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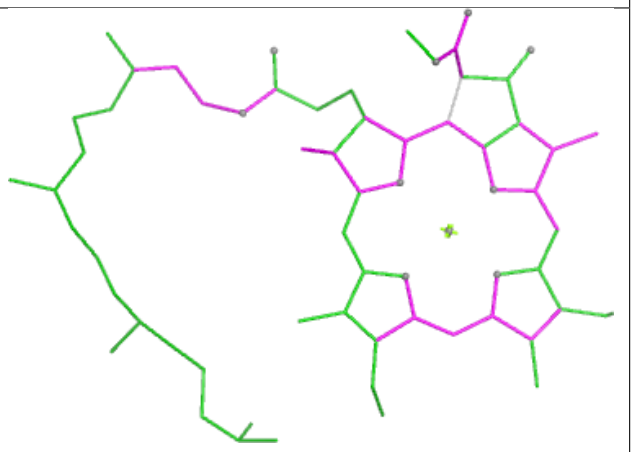
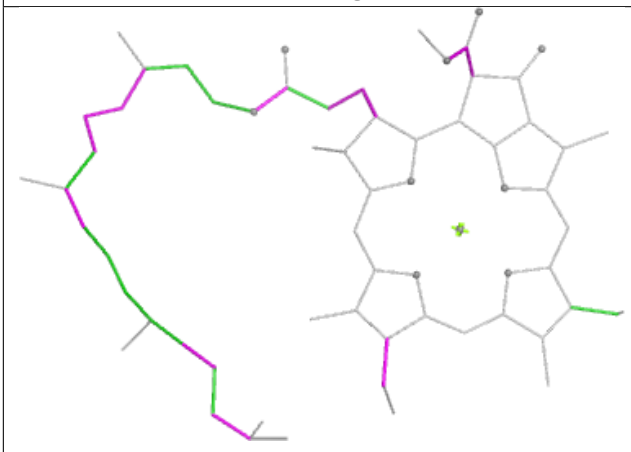
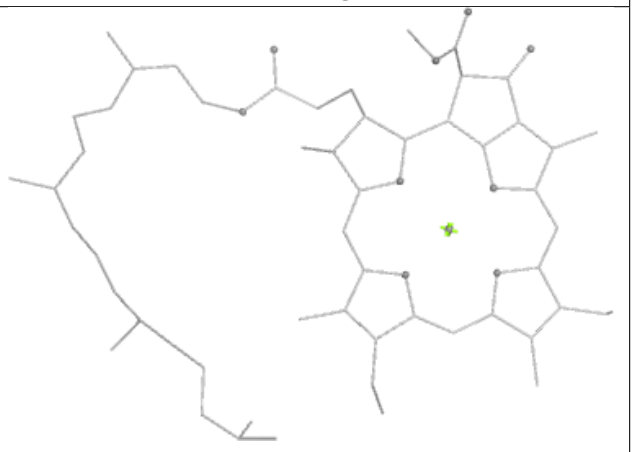


Bond angles

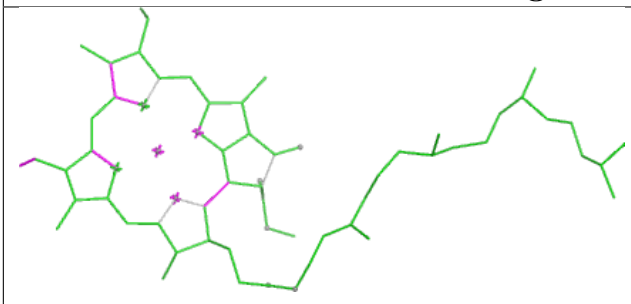


Torsions



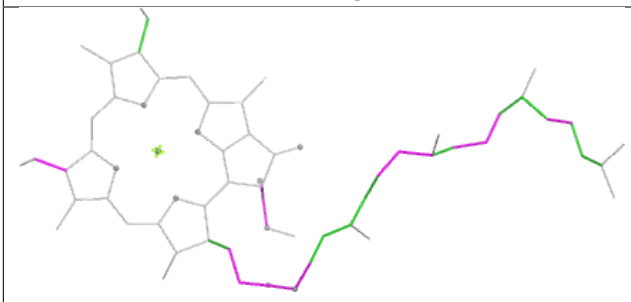
Rings

Ligand CLA b 603

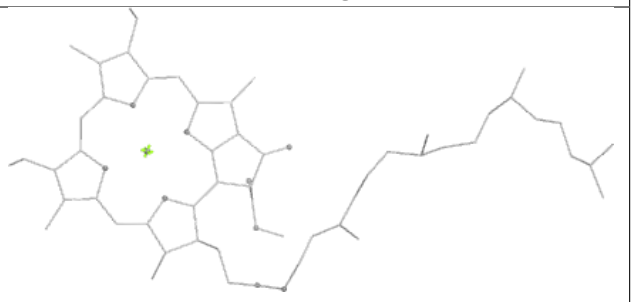


Bond lengths

Bond angles

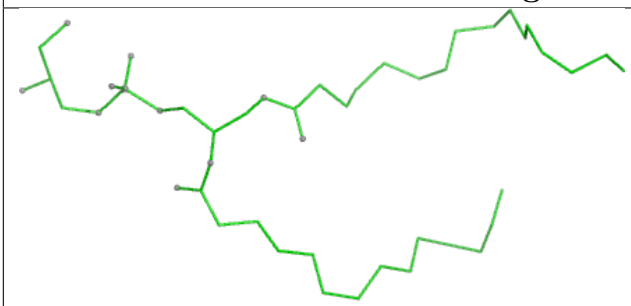


Torsions

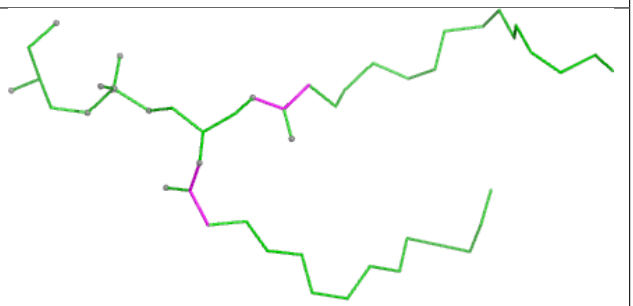


Rings

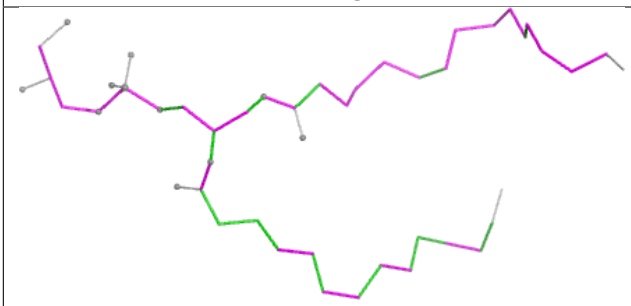
Ligand LHG C 525



Bond lengths



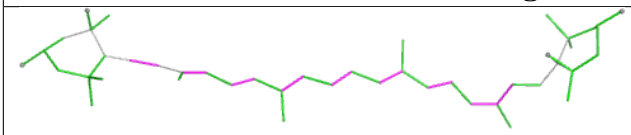
Bond angles



Torsions

Rings

Ligand NEX Y 623



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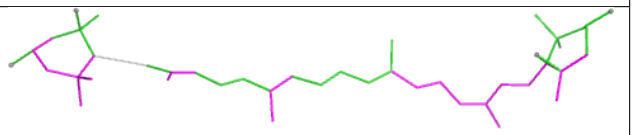

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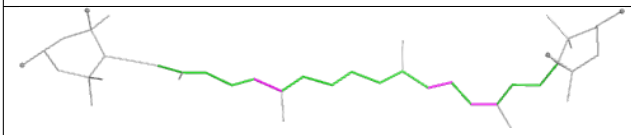
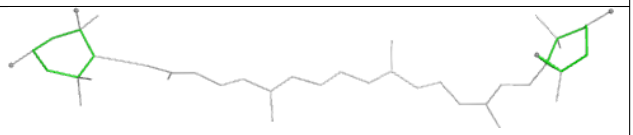
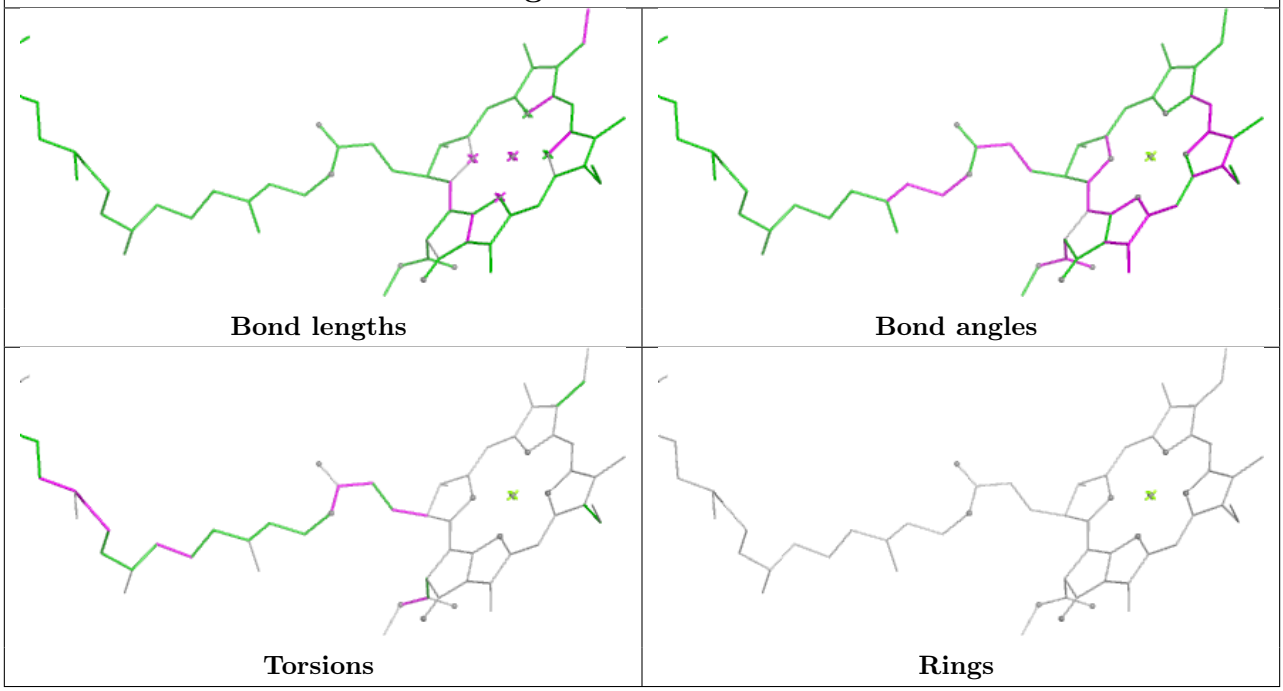


Torsions

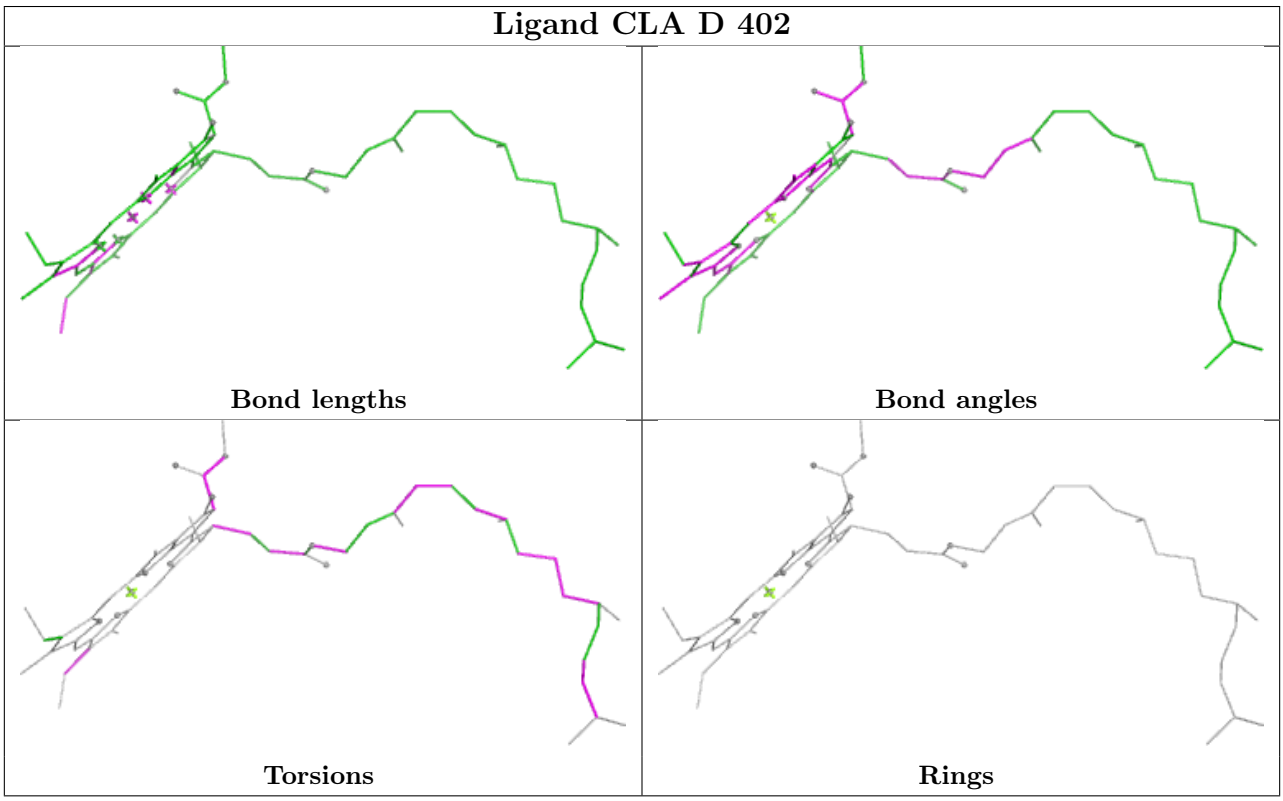


Rings

Ligand CLA A 405



Ligand CLA D 402



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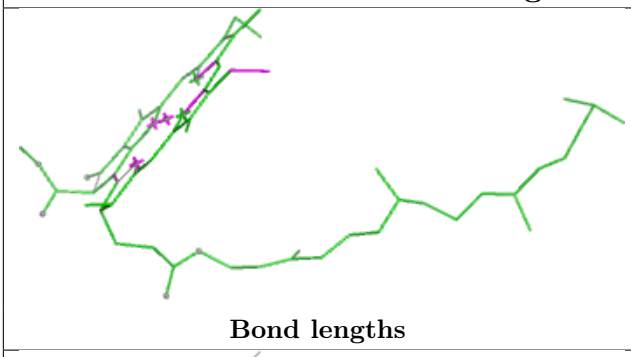

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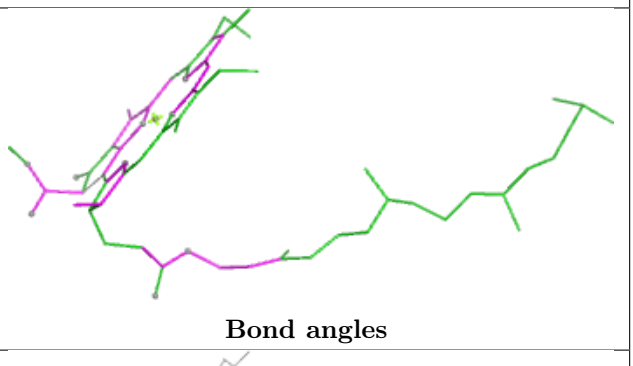

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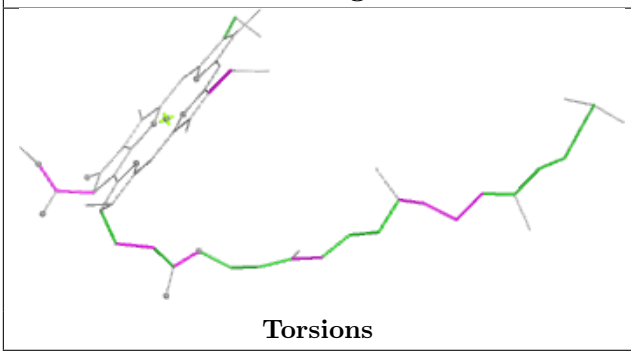

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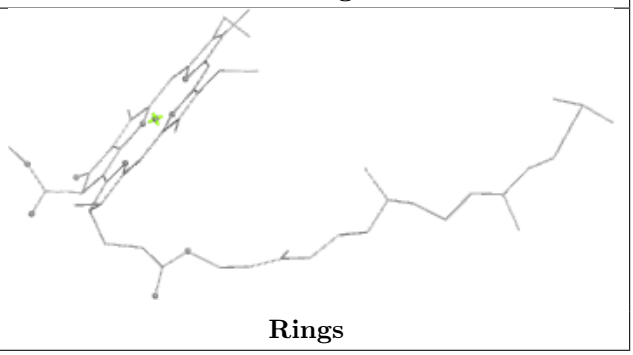
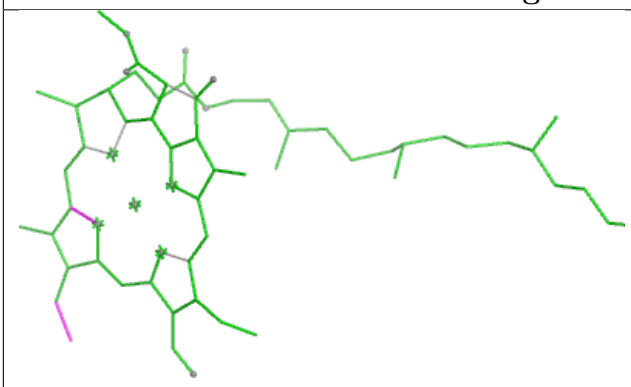


Rings

Ligand CHL G 609



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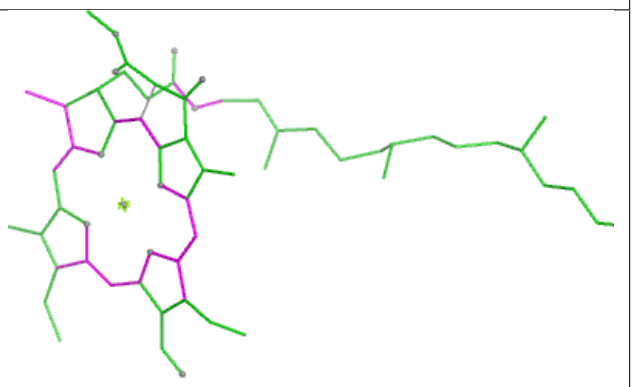
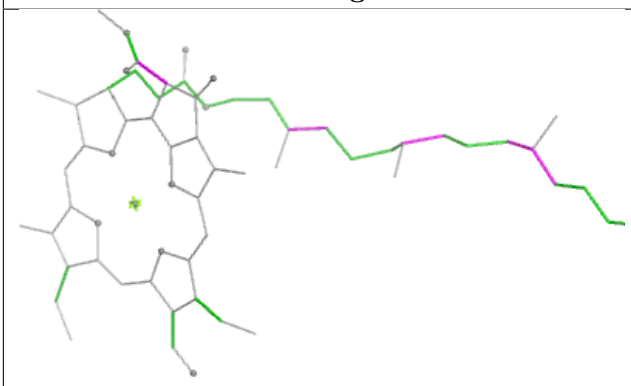


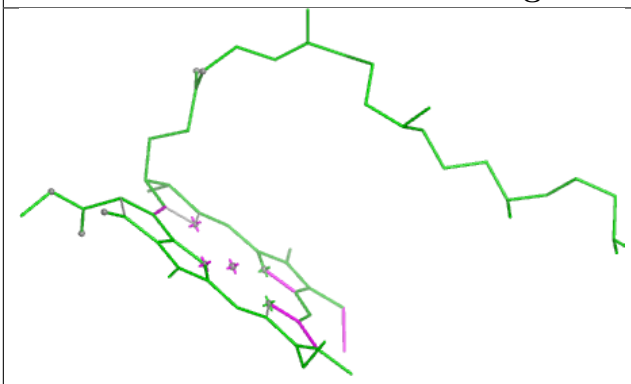
Bond angles



Torsions

Rings

Ligand CLA Y 614



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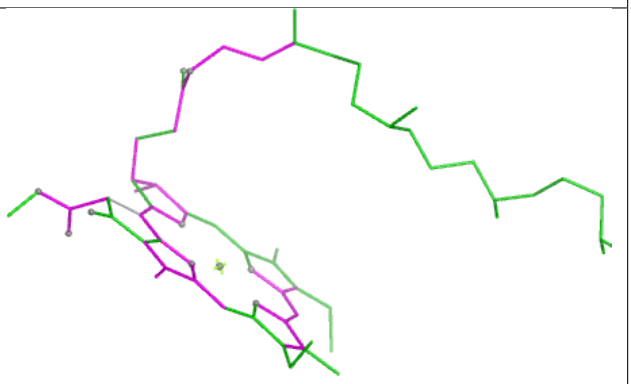

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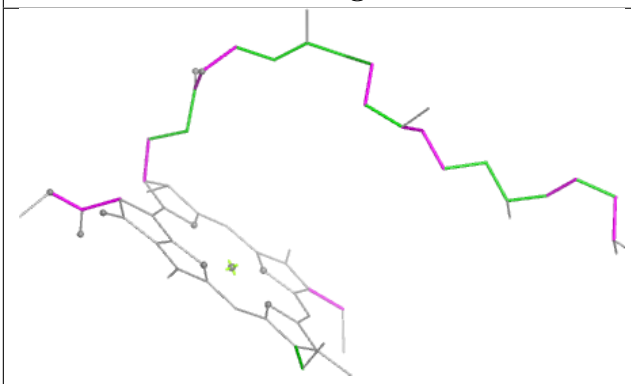

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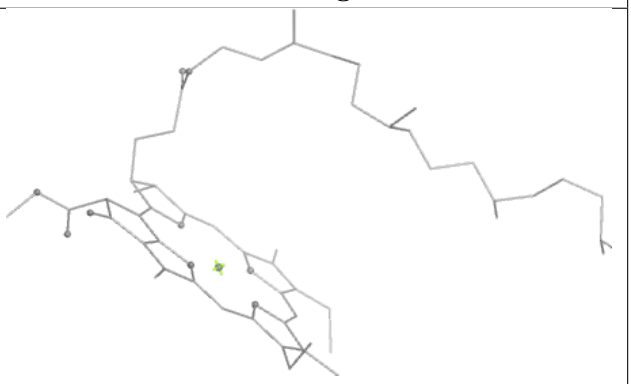
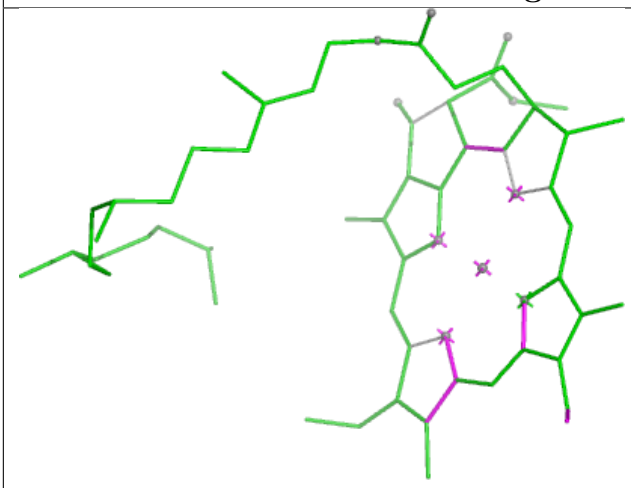


Rings

Ligand CLA C 503



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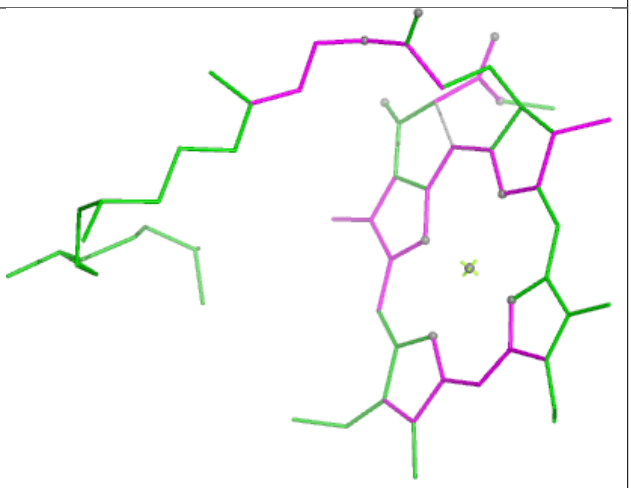
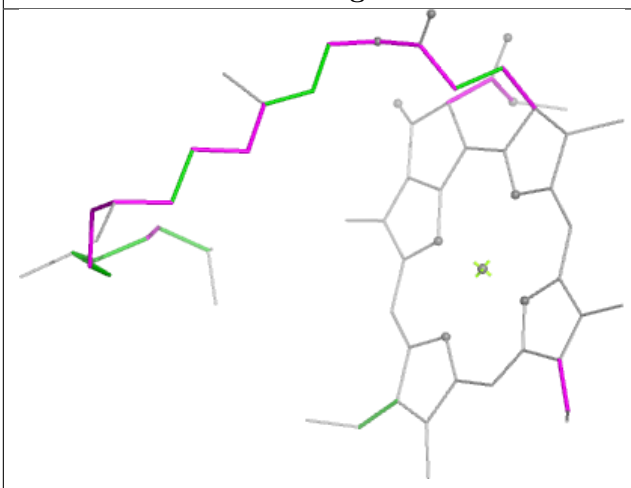


Bond angles



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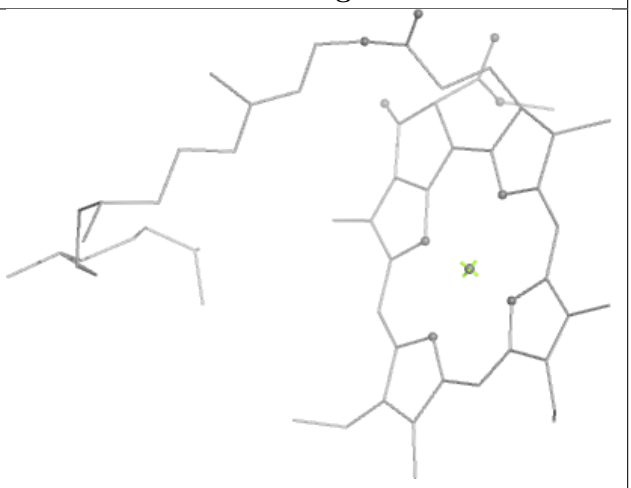


Rings

Ligand LHG L 101

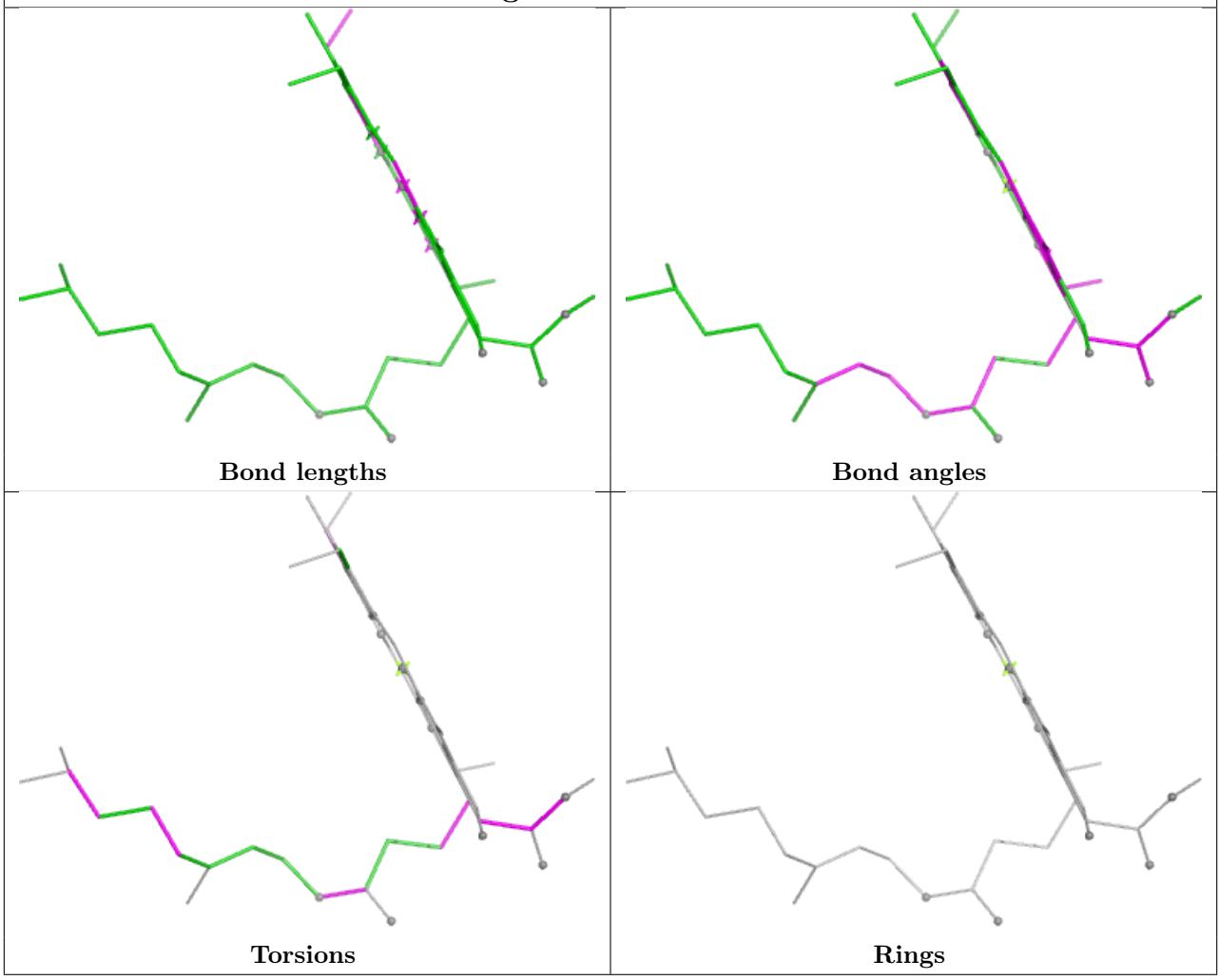
Bond lengths

Bond angles

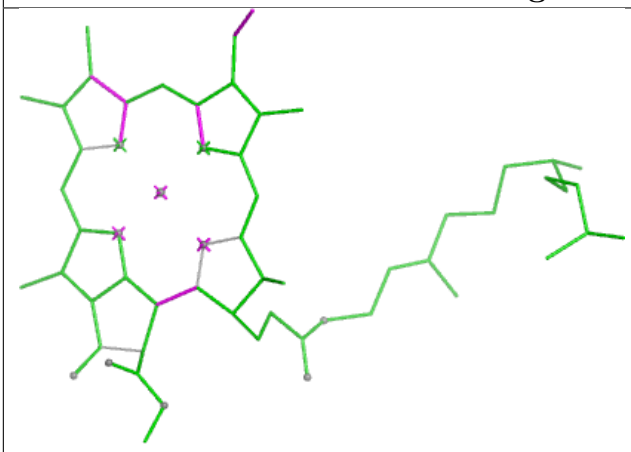
Torsions

Rings

Ligand CLA S 604



Ligand CLA a 410



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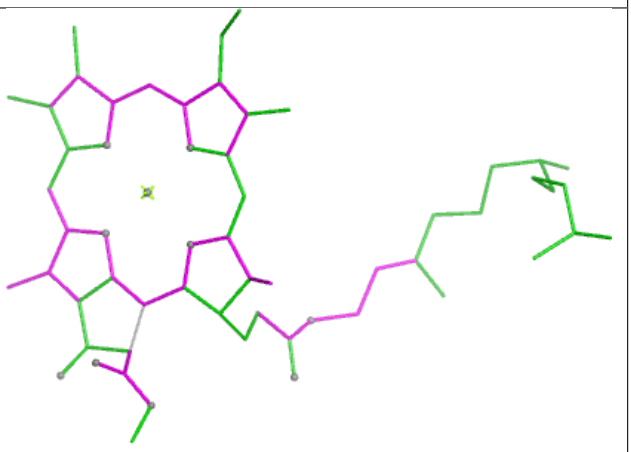
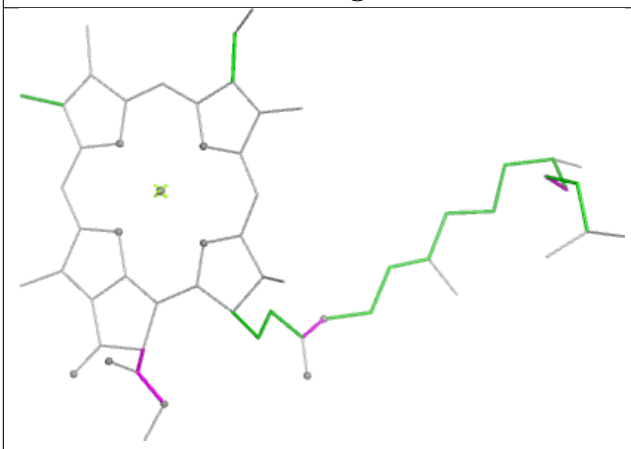


Bond angles



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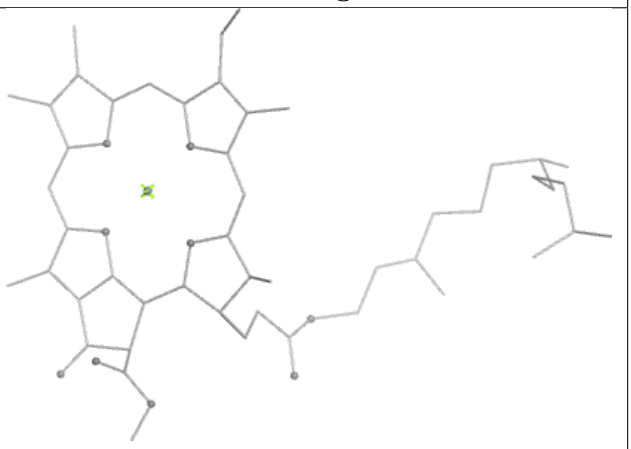
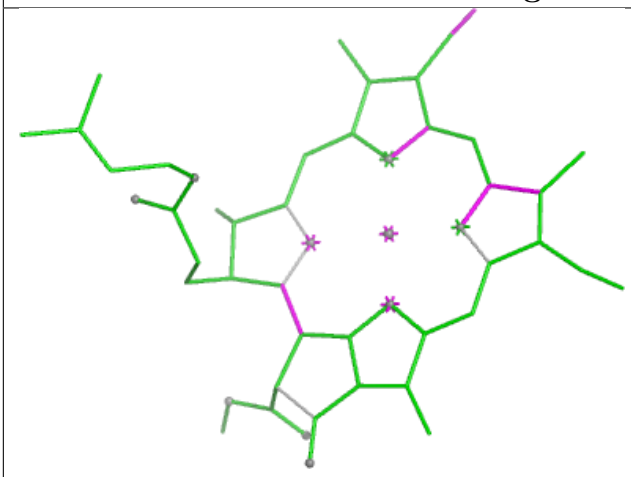


Rings

Ligand CLA A 407



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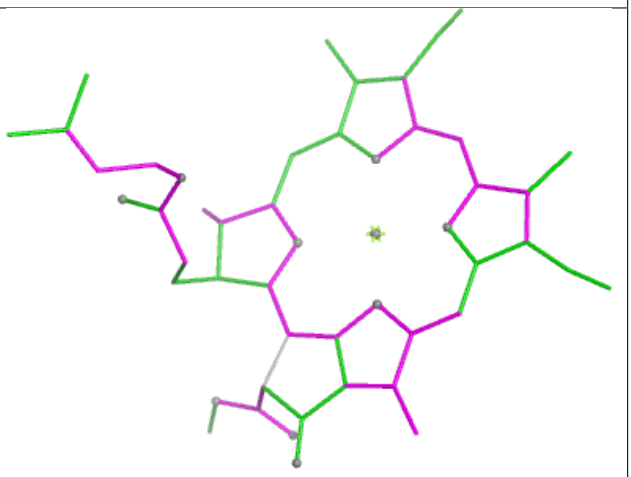
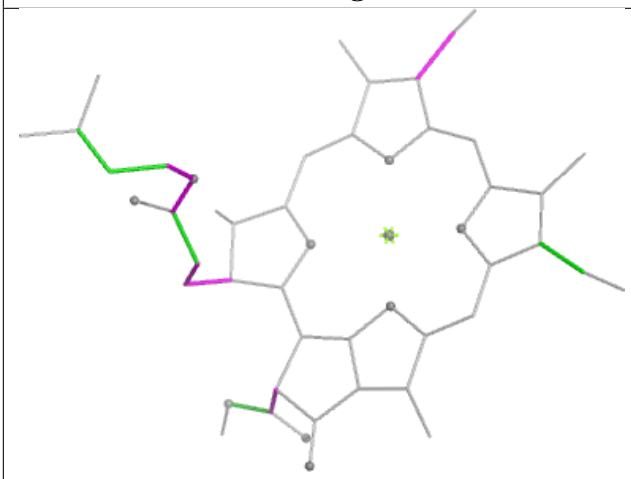


Bond angles



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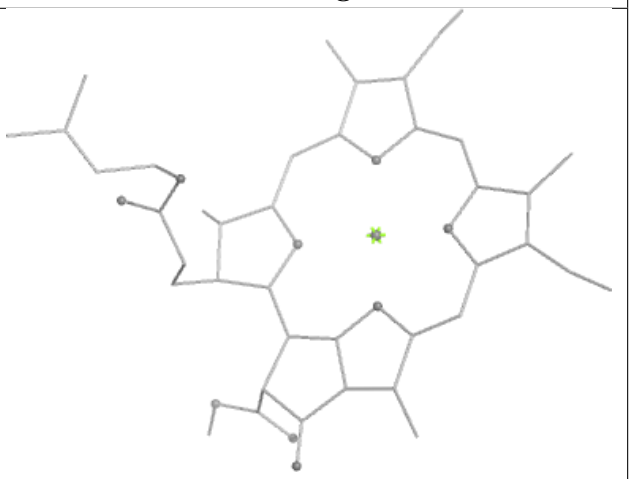
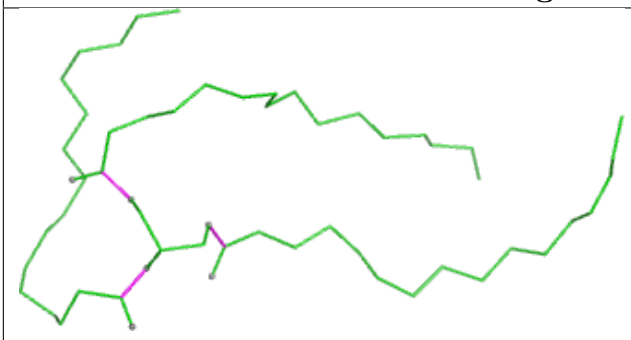


Rings

Ligand 4RF i 101



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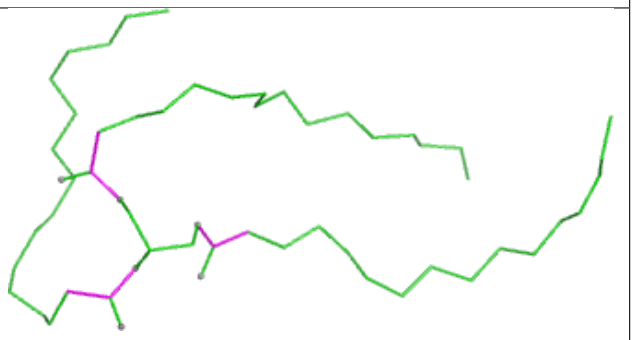

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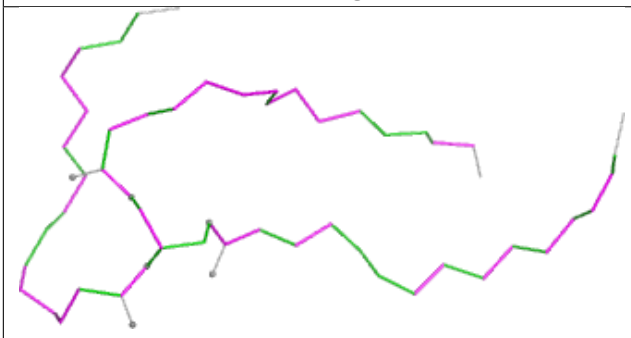
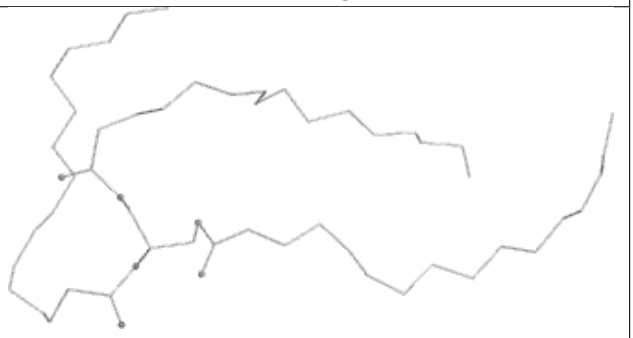
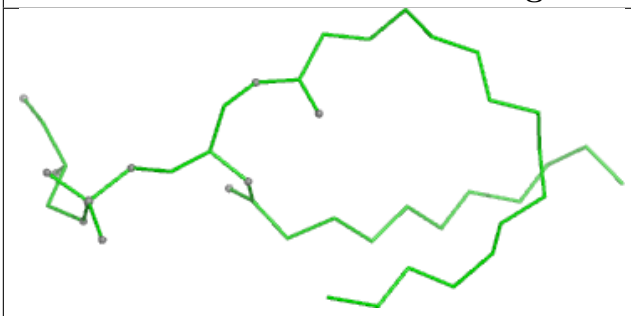


Torsions



Rings

Ligand LHG d 408



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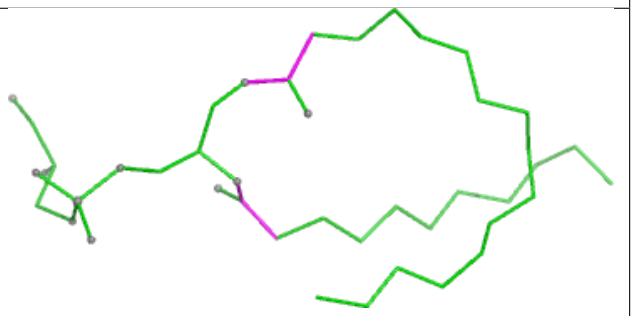
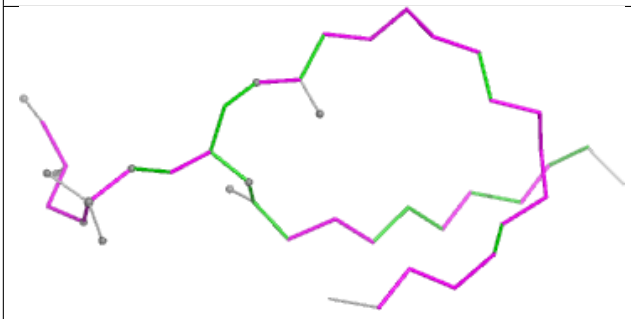


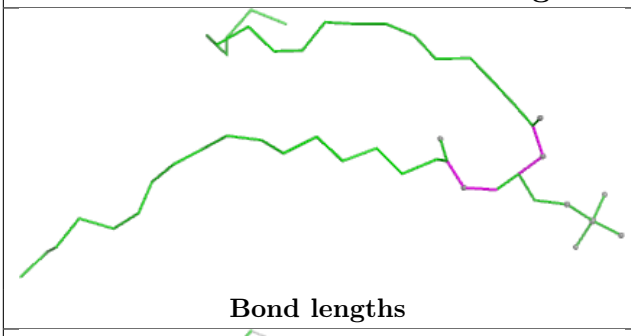
Bond angles



Torsions

Rings

Ligand 3PH t 101



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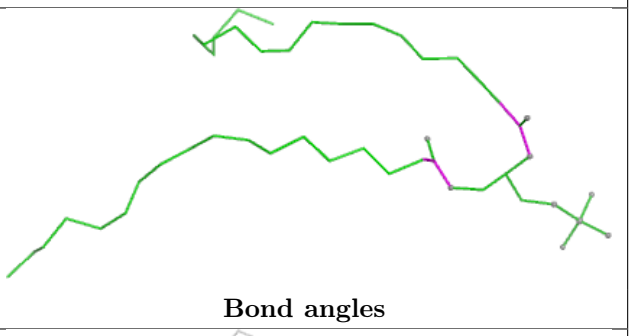
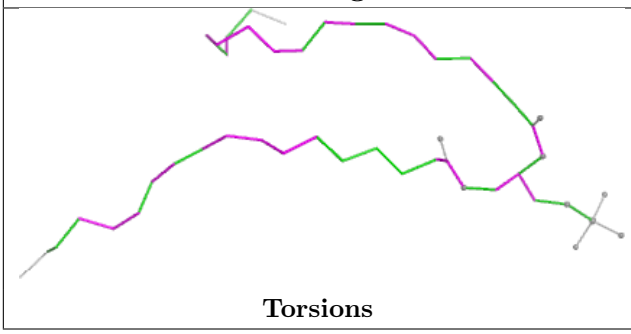
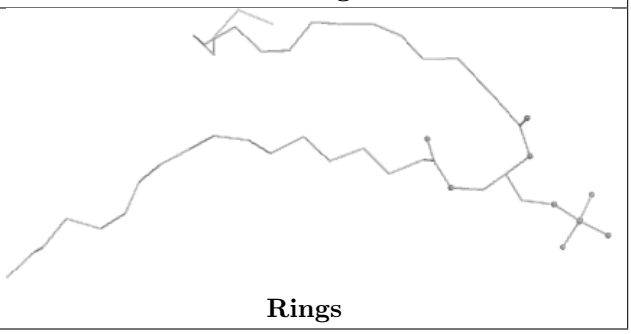


Bond angles

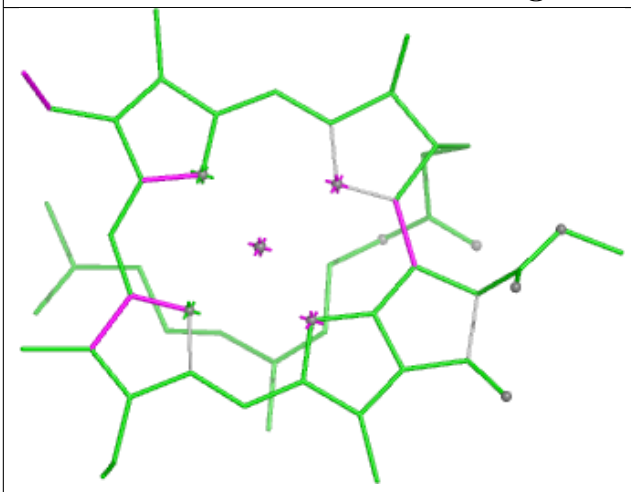


Torsions



Rings

Ligand CLA S 613



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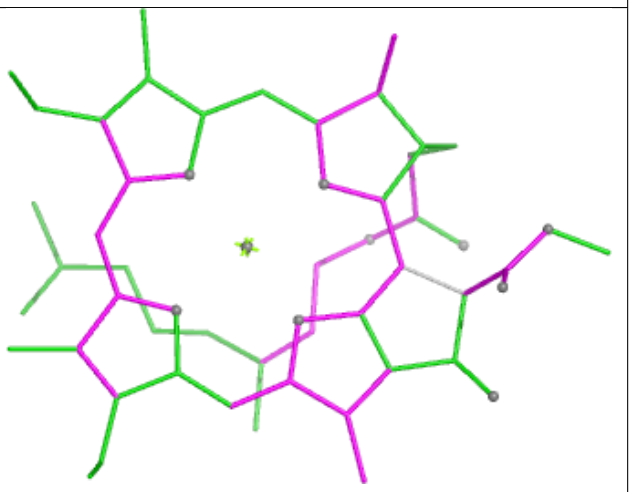
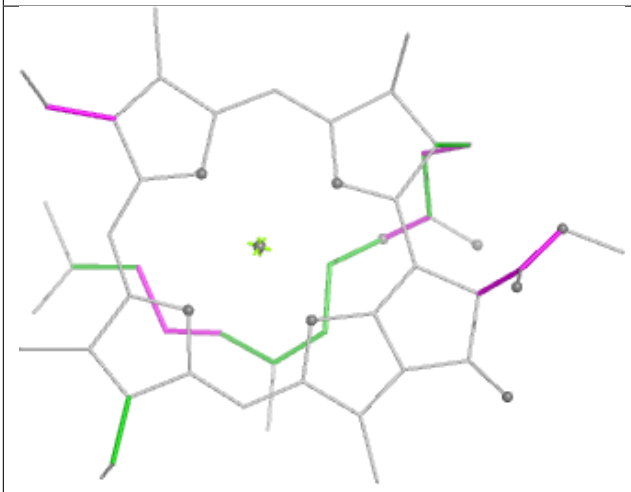


Bond angles



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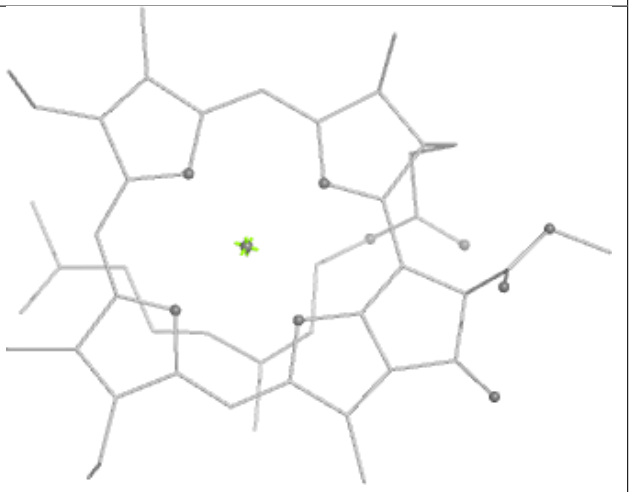
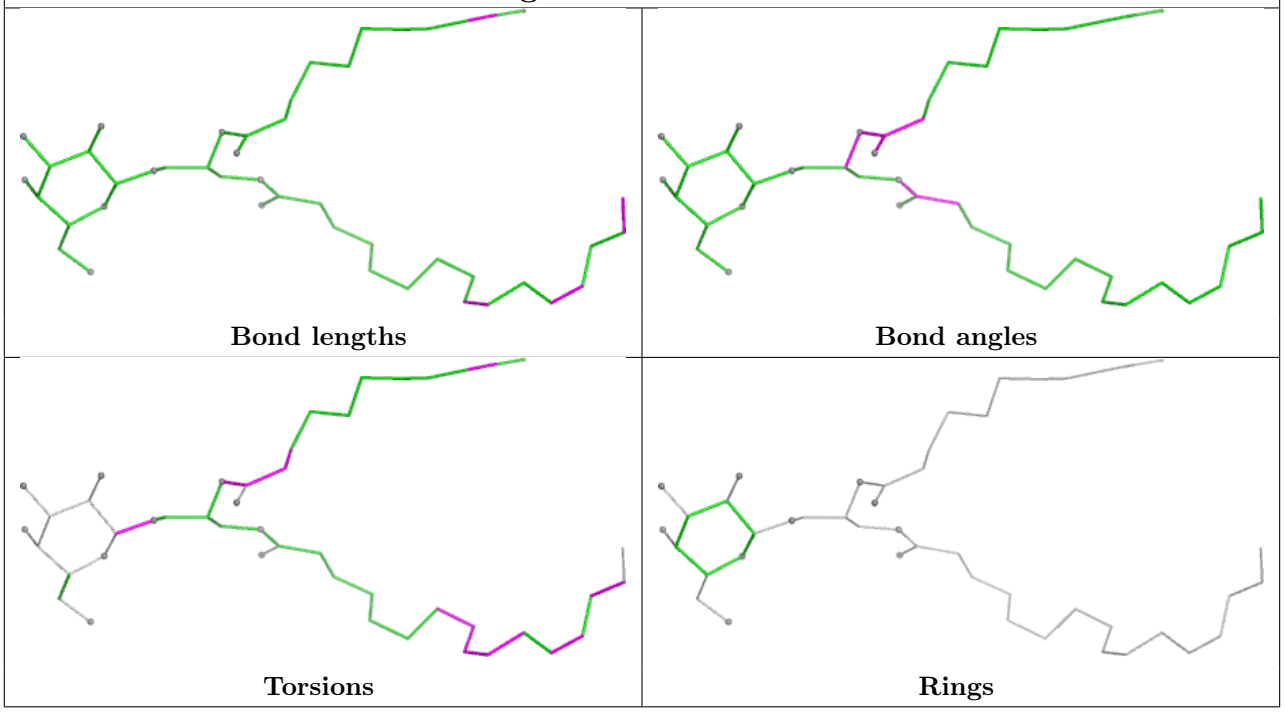
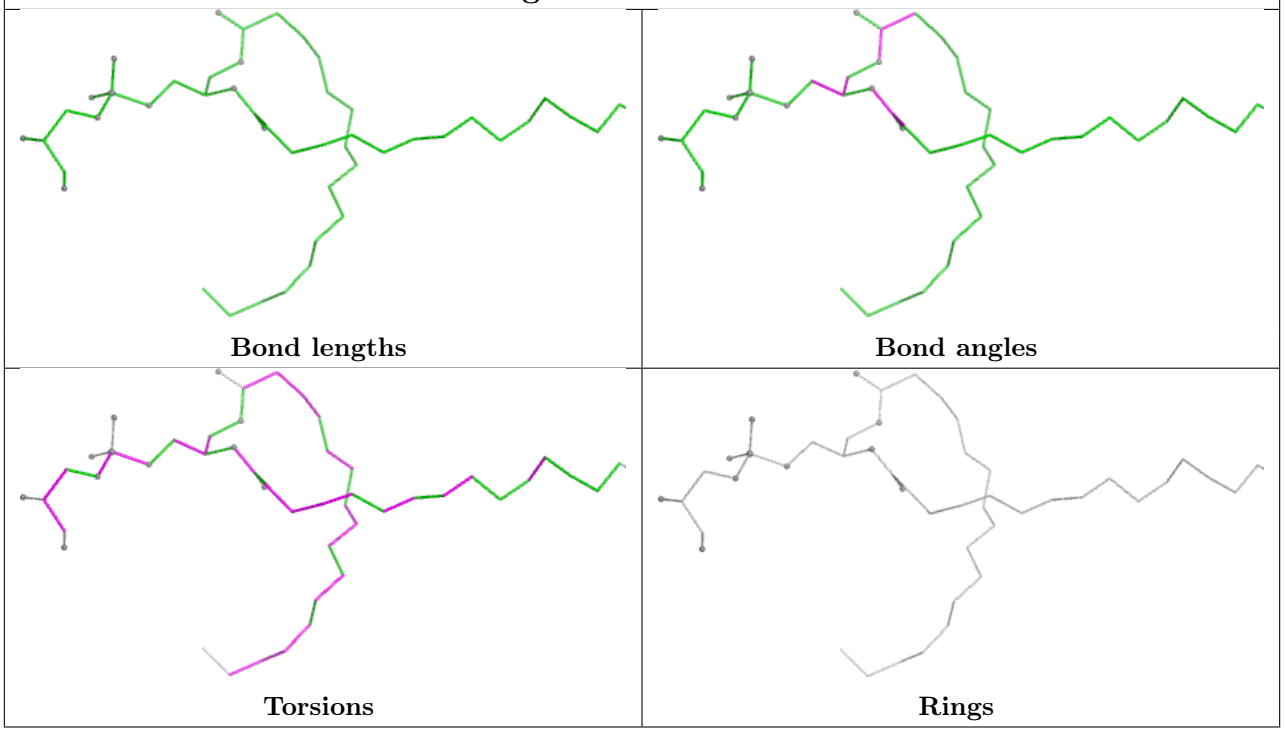


Rings

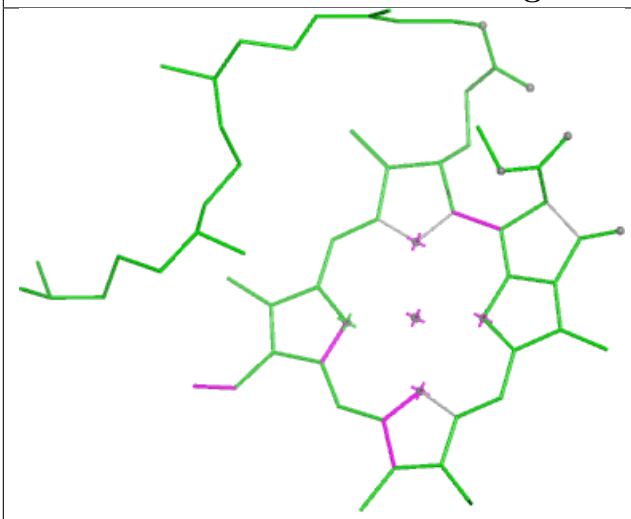
Ligand LMG A 413



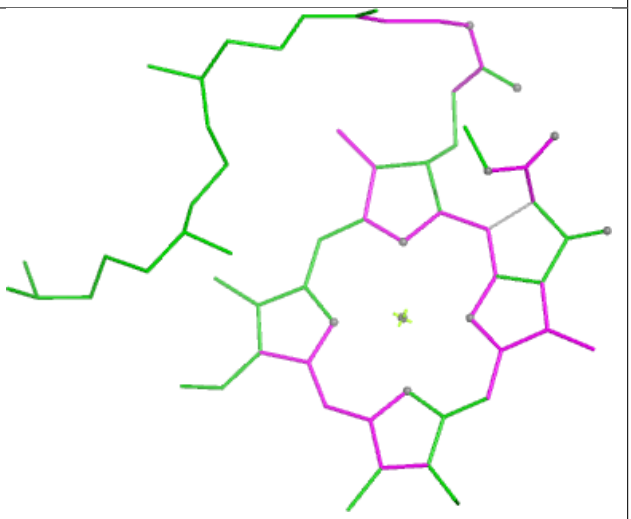
Ligand LHG G 624



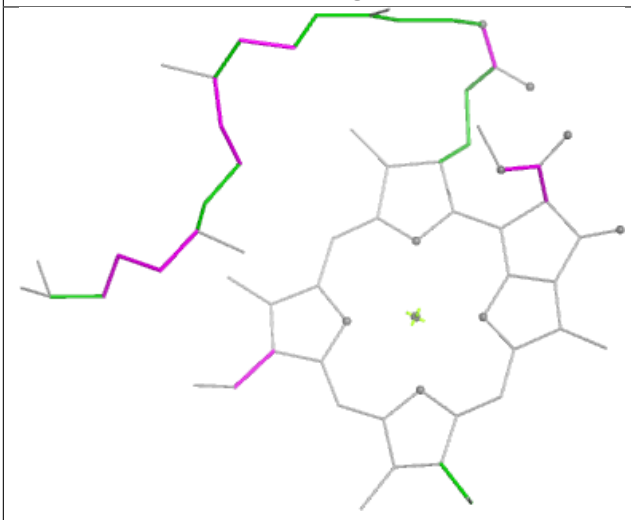
Ligand CLA Y 612



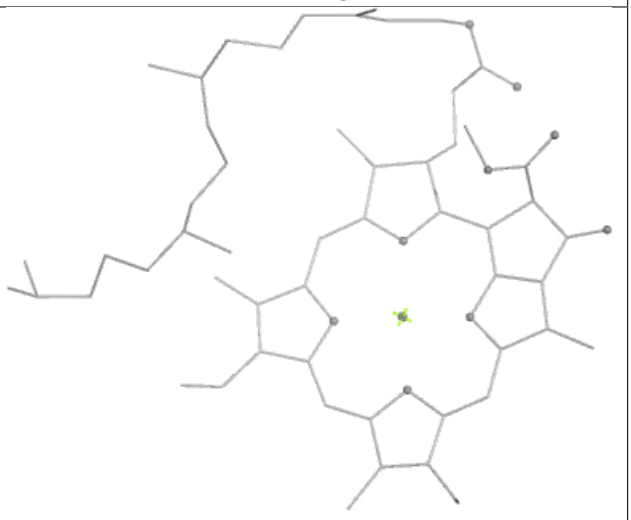
Bond lengths



Bond angles

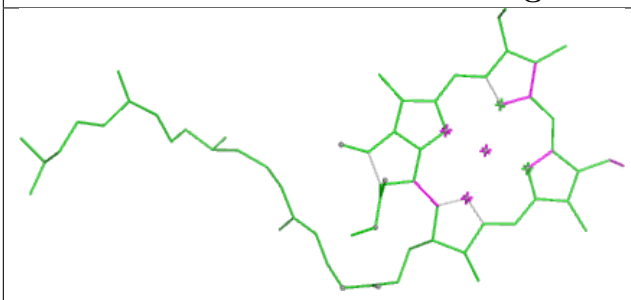


Torsions

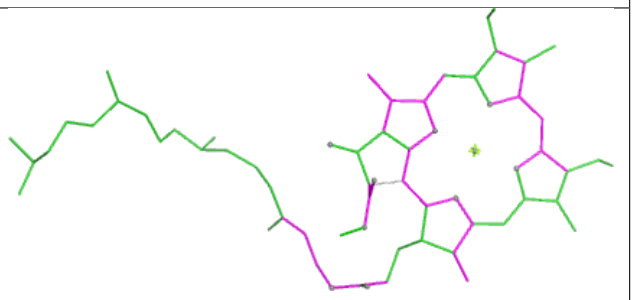


Rings

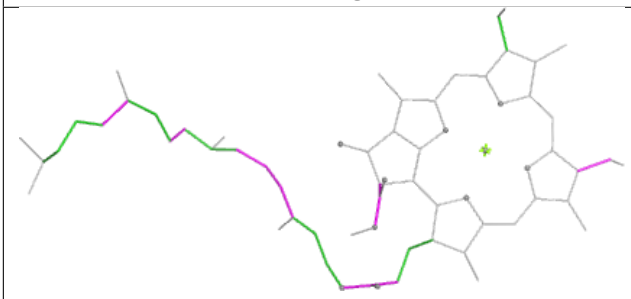
Ligand CLA B 603



Bond lengths



Bond angles



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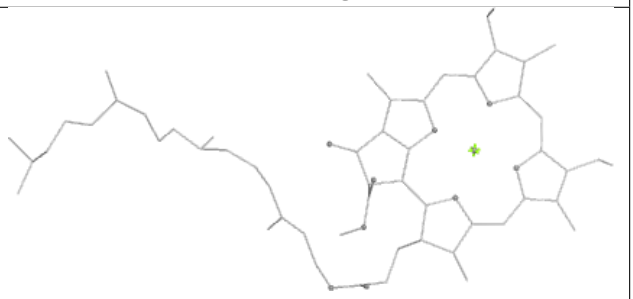
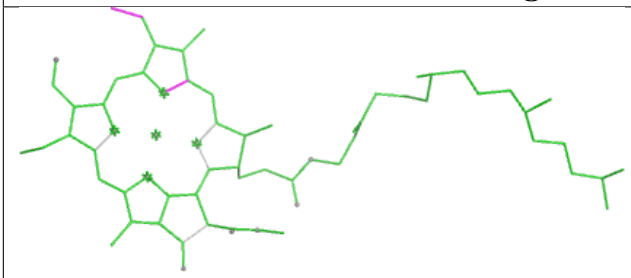


Rings

Ligand CHL G 601



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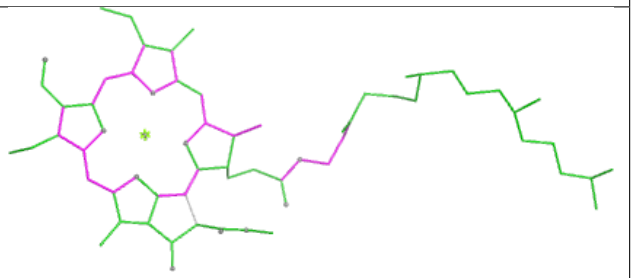
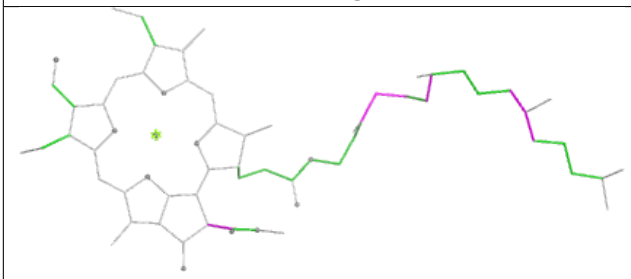


Bond angles



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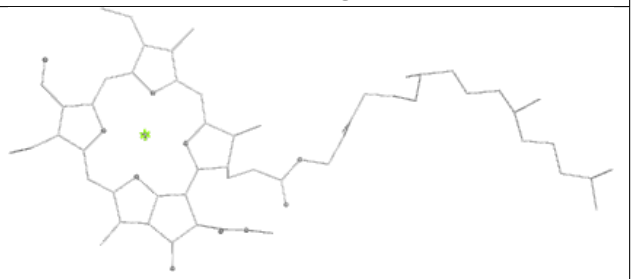
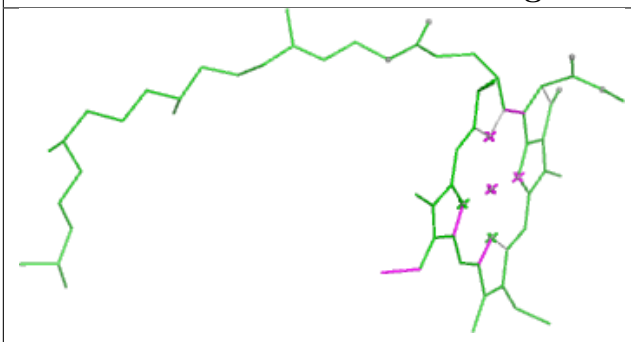


Rings

Ligand CLA B 610



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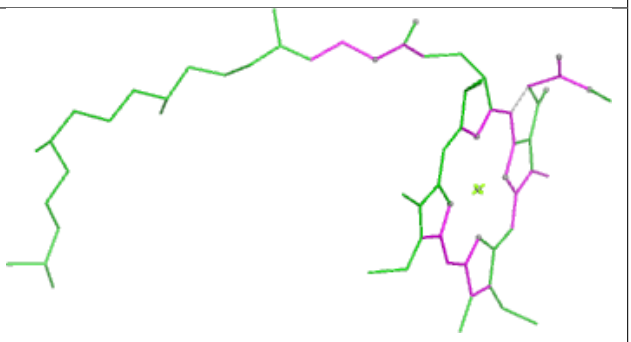

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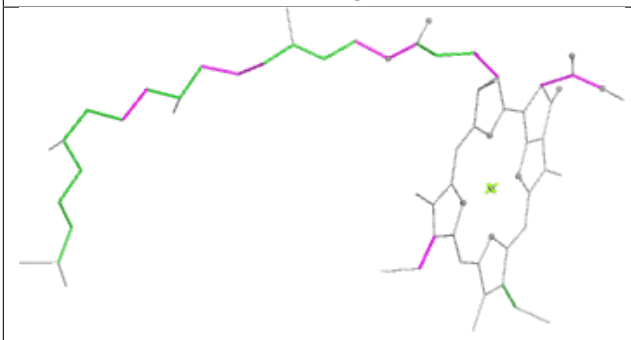

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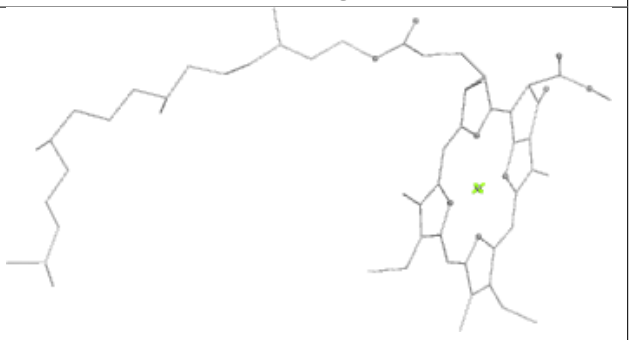
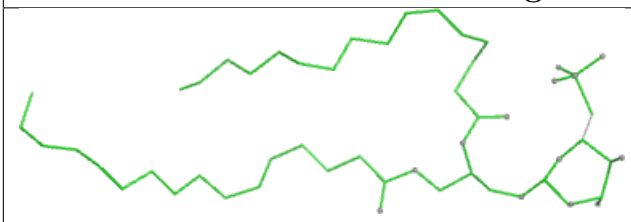


Rings

Ligand SQD B 626



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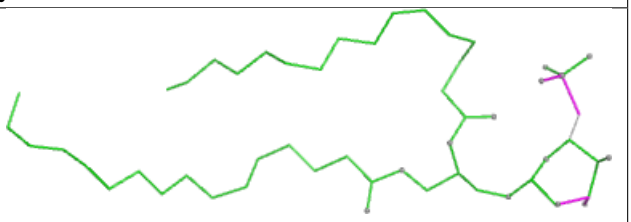
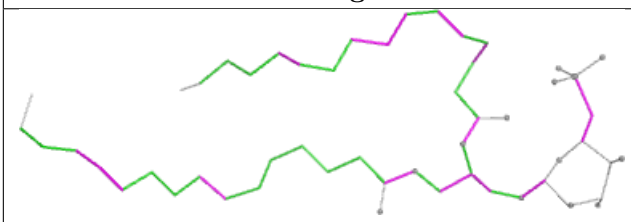


Bond angles



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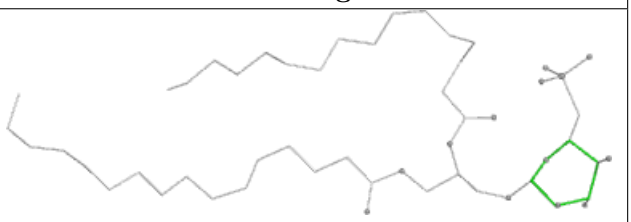
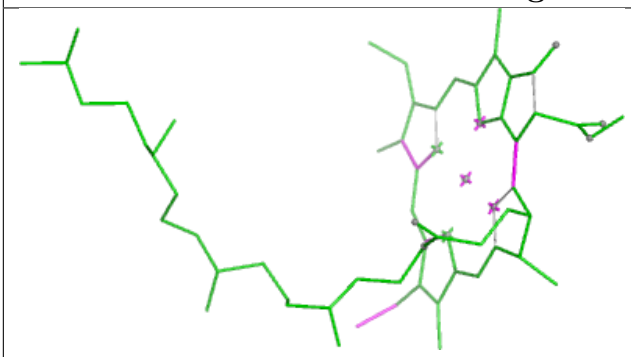


Rings

Ligand CLA S 610



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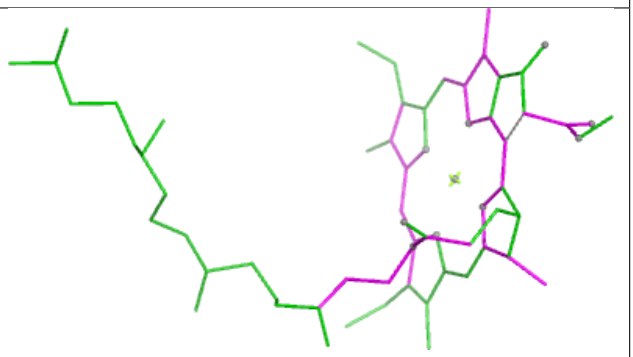
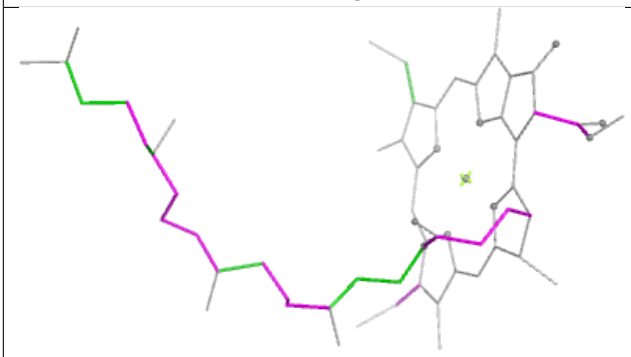


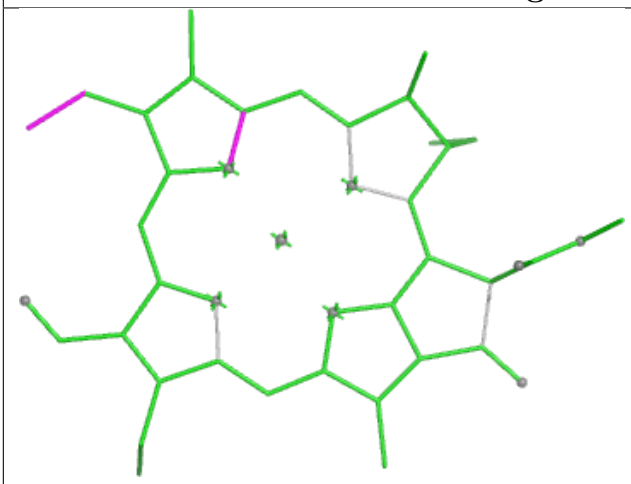
Bond angles



Torsions

Rings

Ligand CHL S 607



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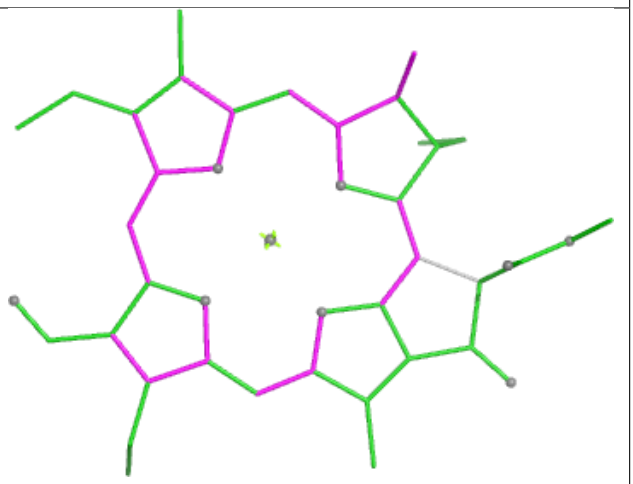
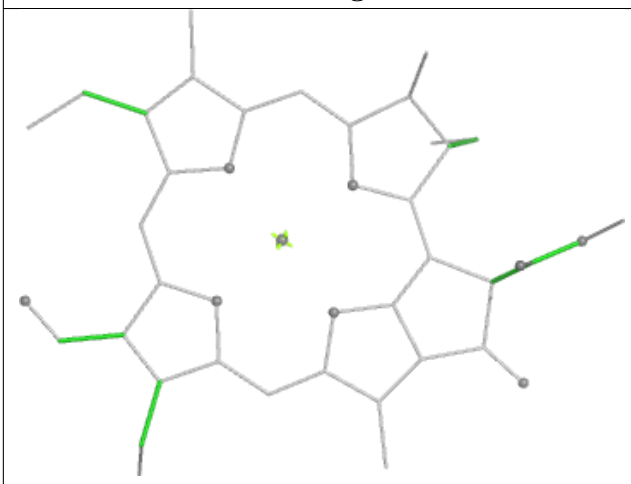
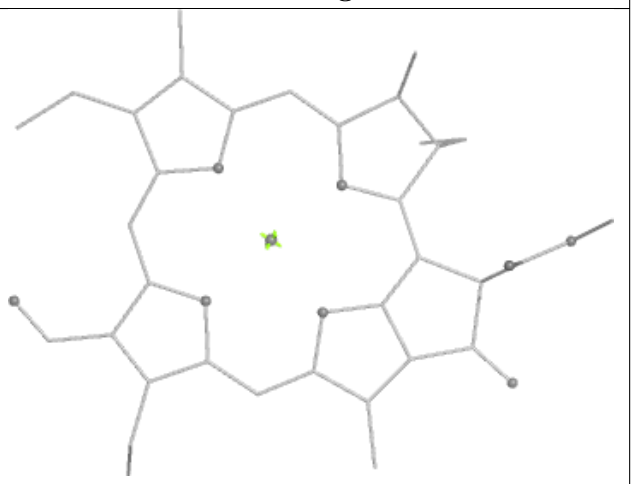


Bond angles

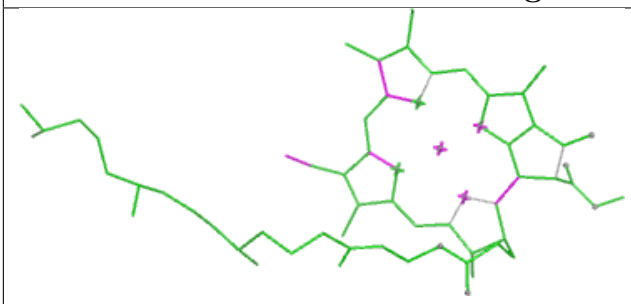


Torsions



Rings

Ligand CLA C 501



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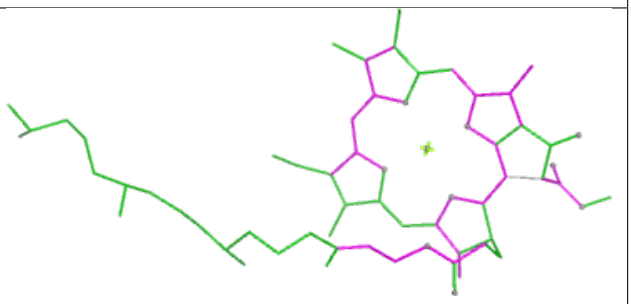

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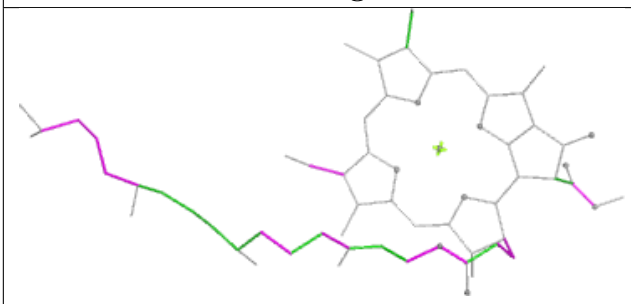

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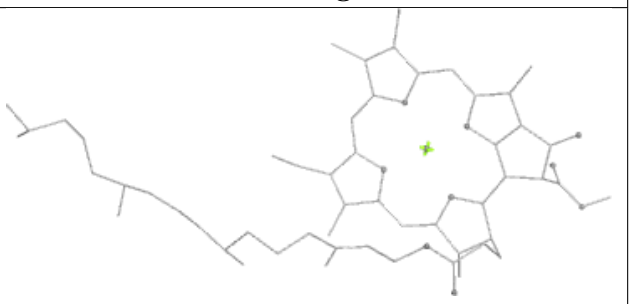
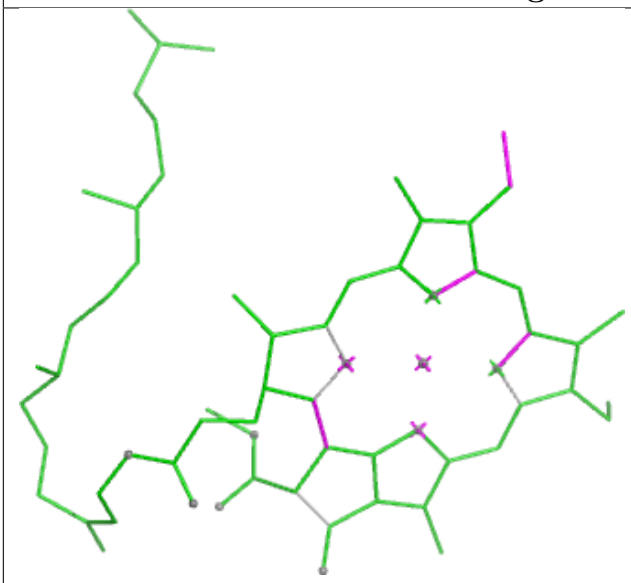


Rings

Ligand CLA b 617



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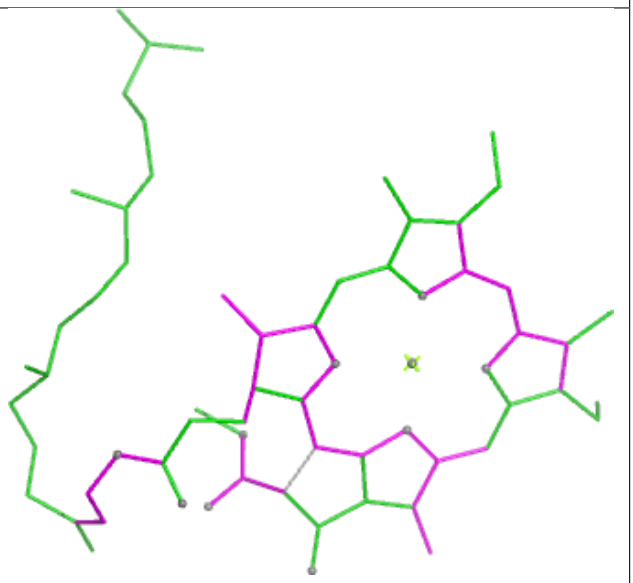
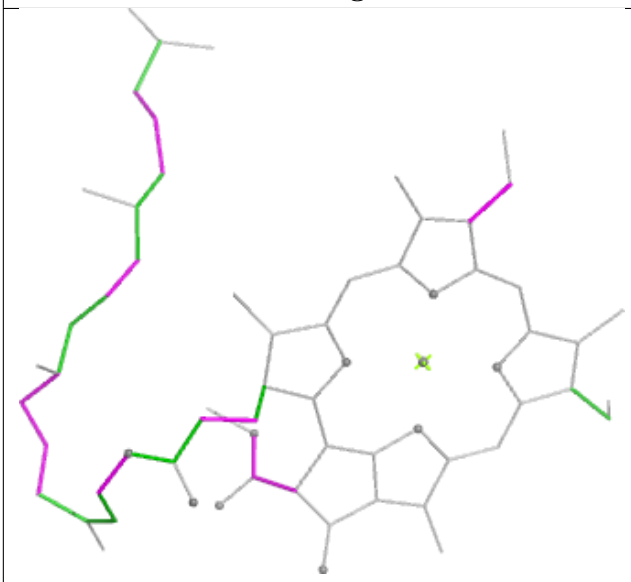


Bond angles



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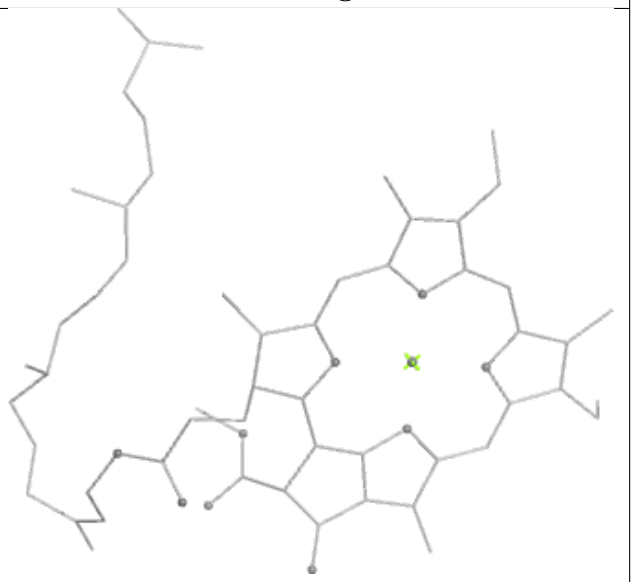
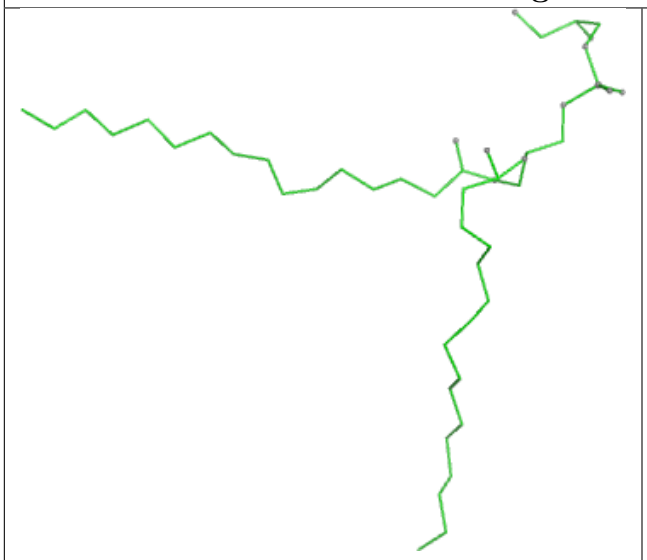


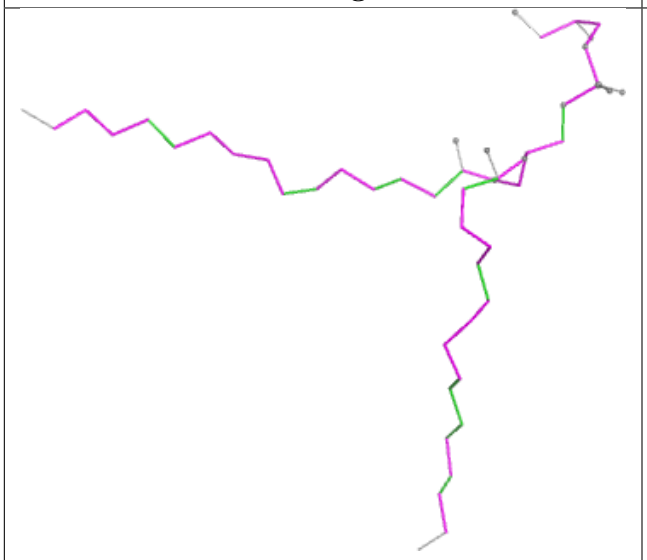
Rings

Ligand LHG l 101



Bond lengths

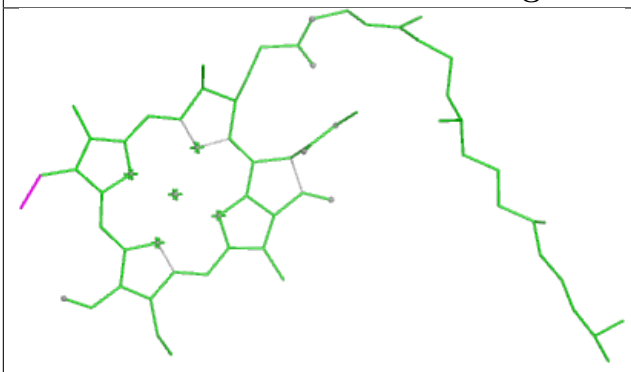
Bond angles



Torsions

Rings

Ligand CHL N 606



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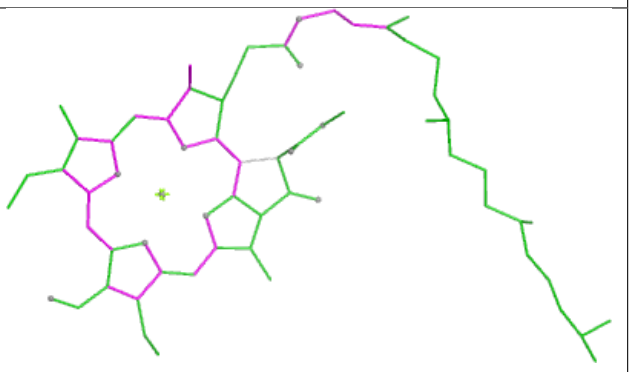
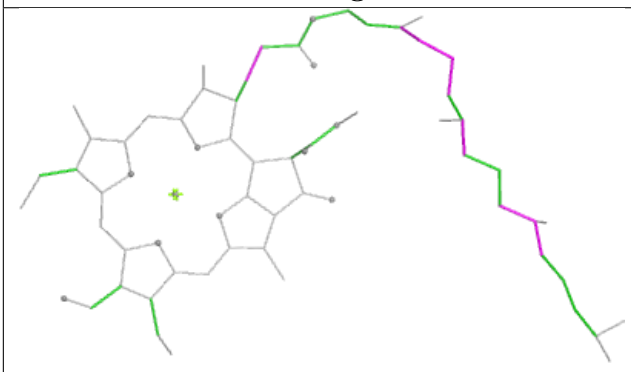
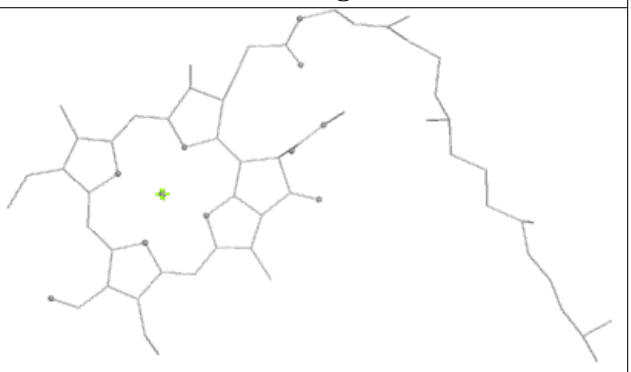


Bond angles

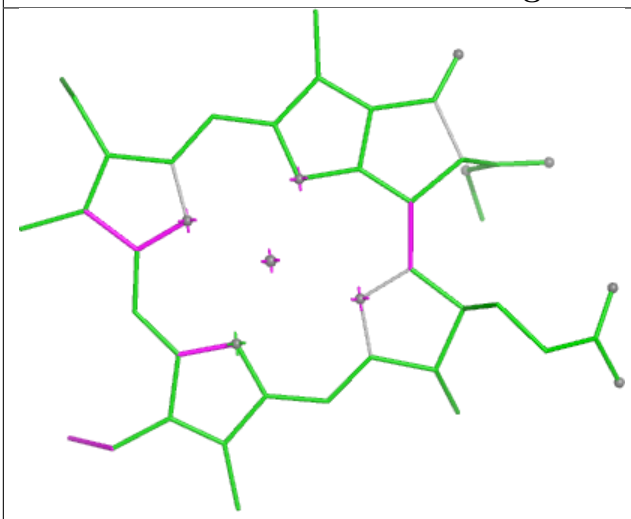


Torsions



Rings

Ligand CLA N 612



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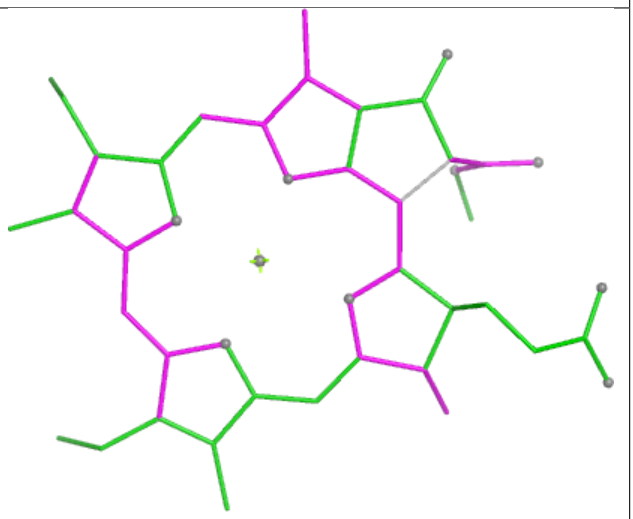
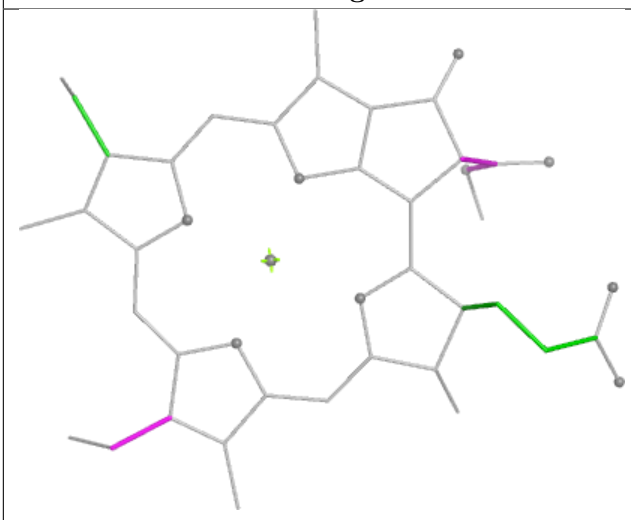


Bond angles



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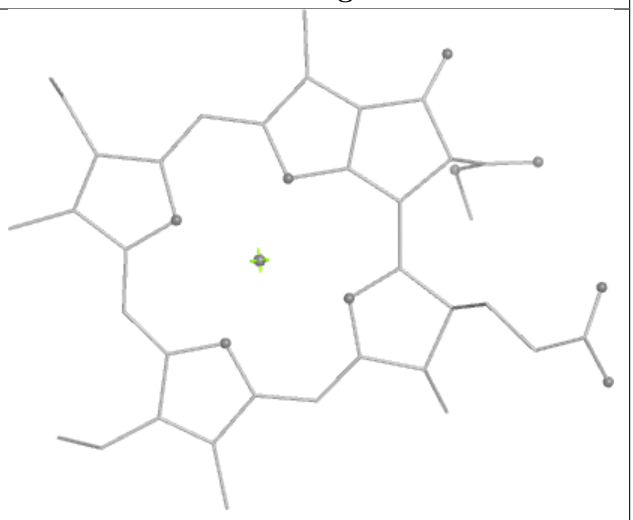
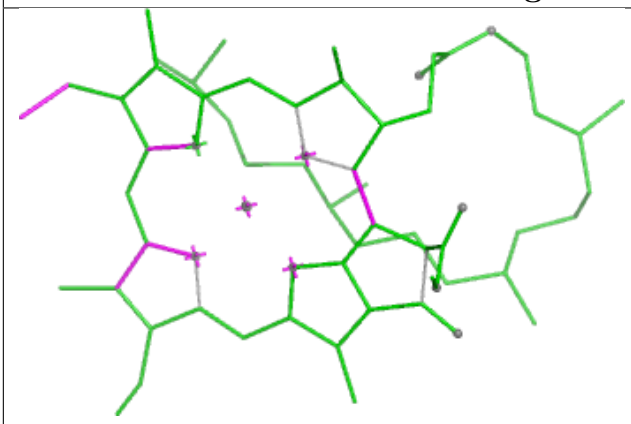


Rings

Ligand CLA B 602



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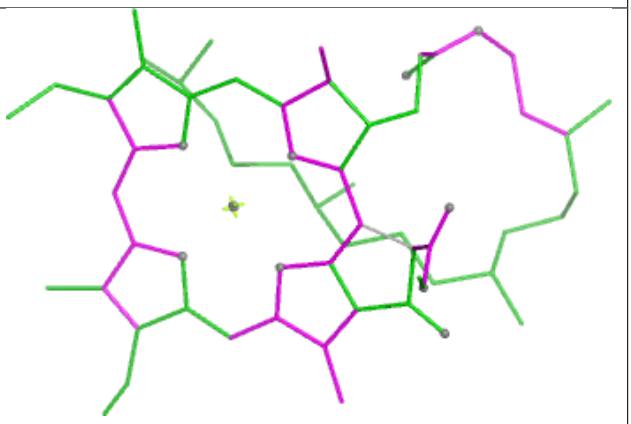
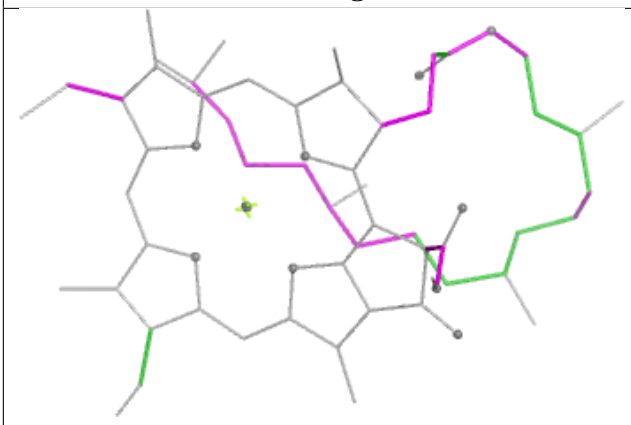
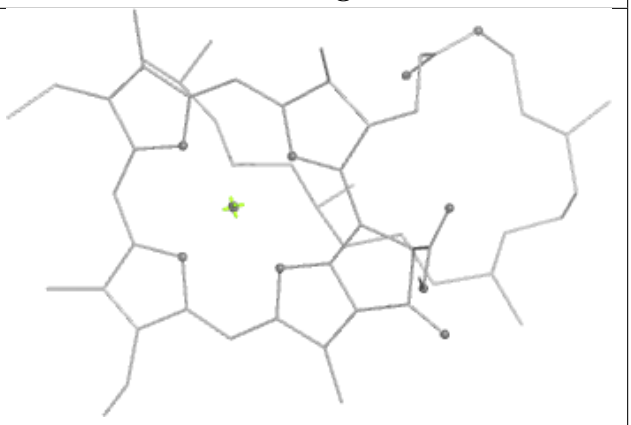


Bond angles

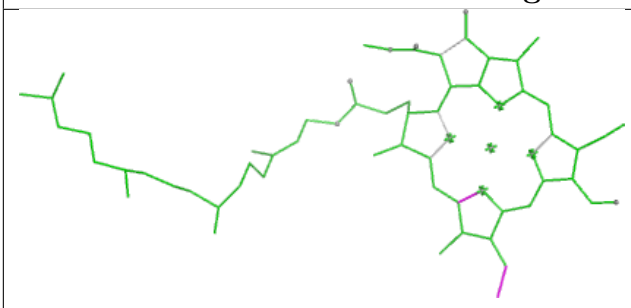


Torsions



Rings

Ligand CHL Y 601



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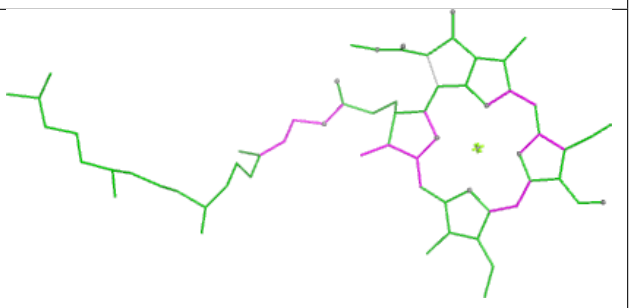
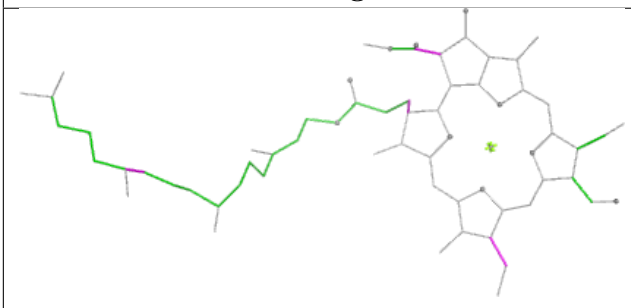
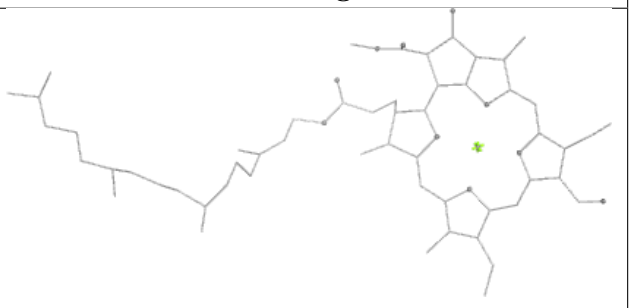


Bond angles

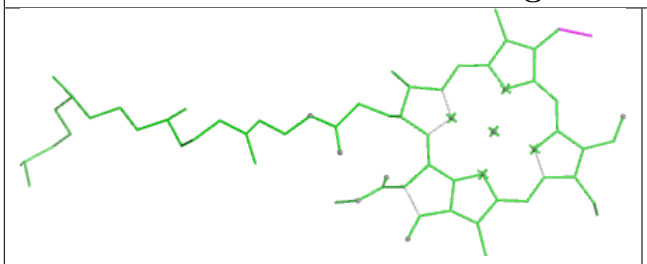


Torsions



Rings

Ligand CHL Y 606



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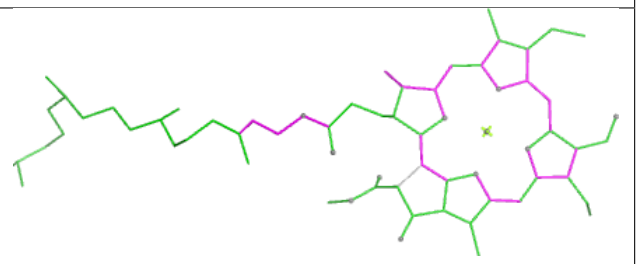
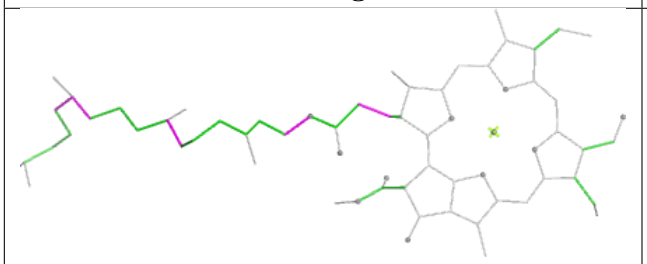
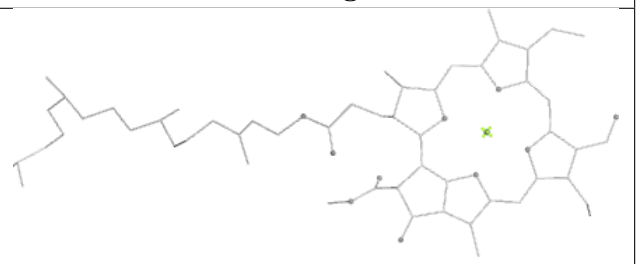


Bond angles

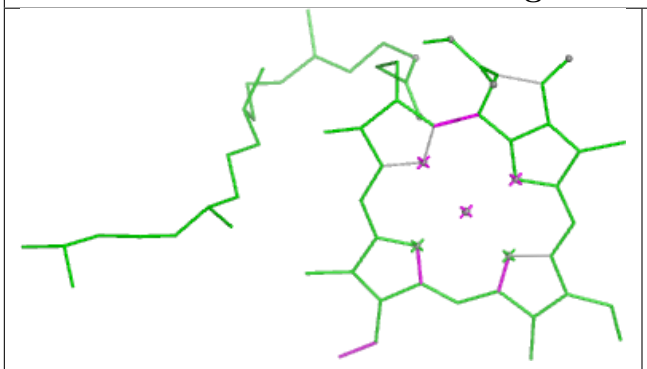


Torsions



Rings

Ligand CLA A 406



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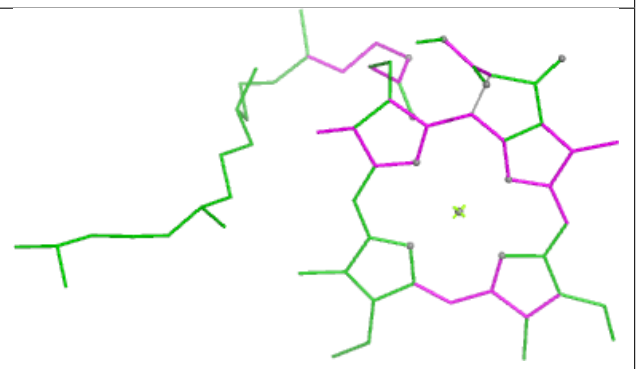
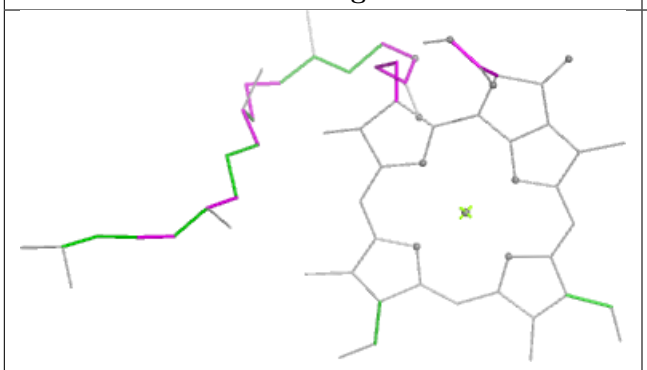


Bond angles



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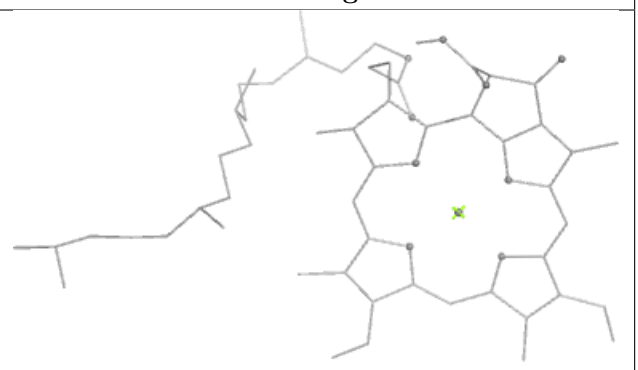

Rings

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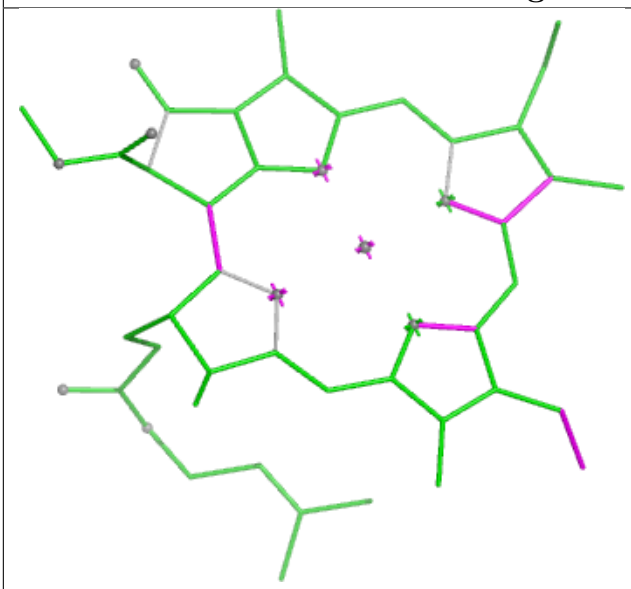

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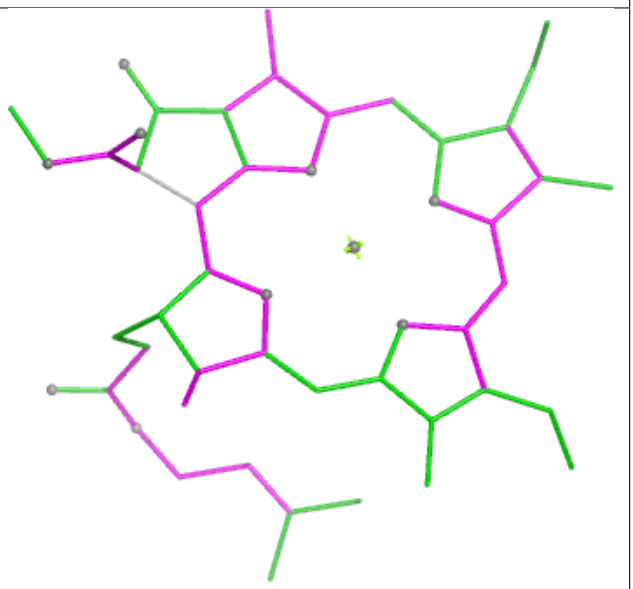
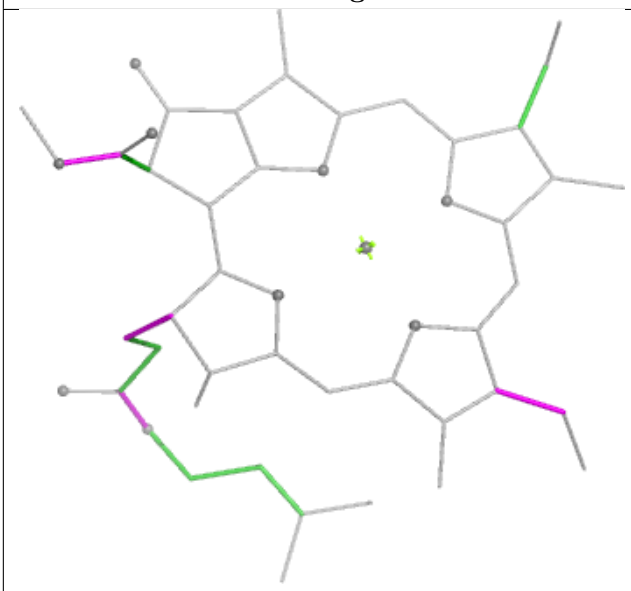


Bond angles



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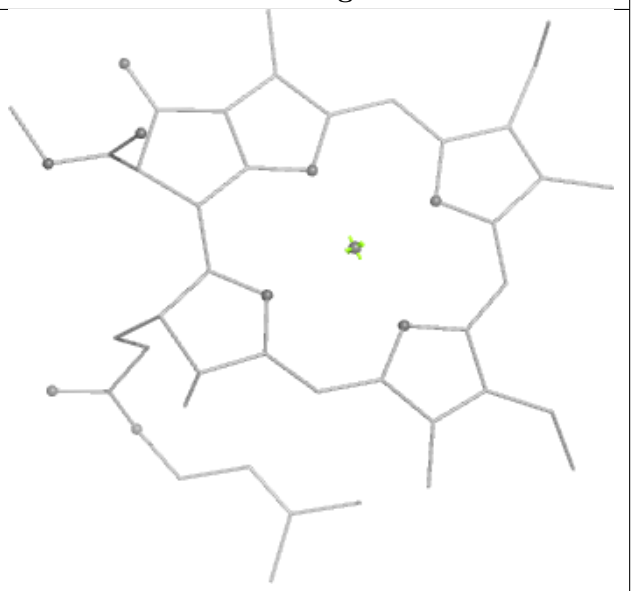
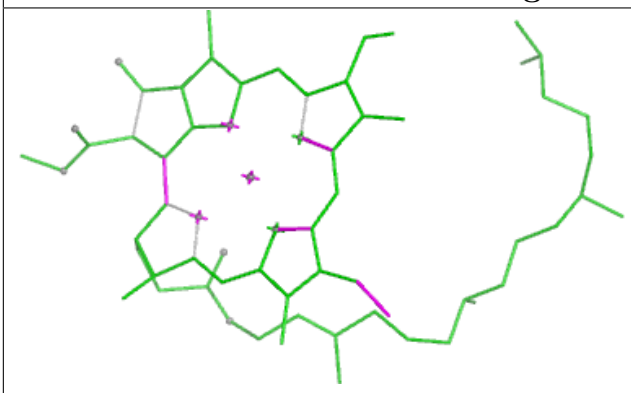


Rings

Ligand CLA N 610



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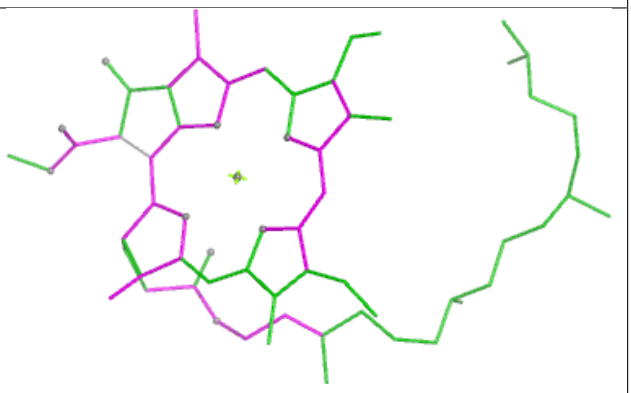
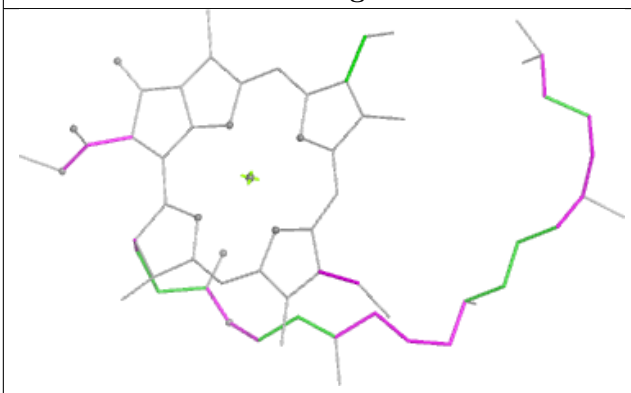


Bond angles



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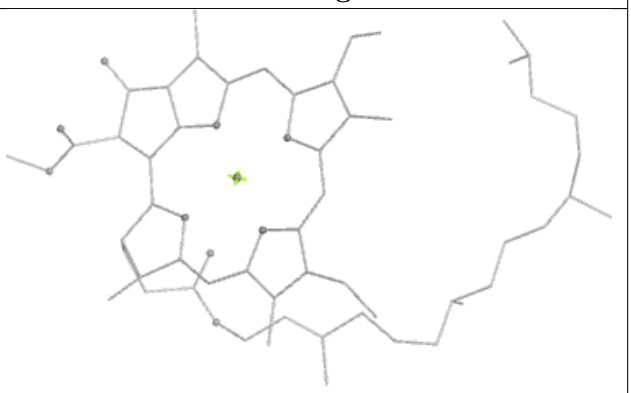
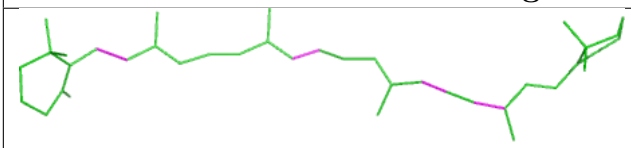


Rings

Ligand BCR C 514



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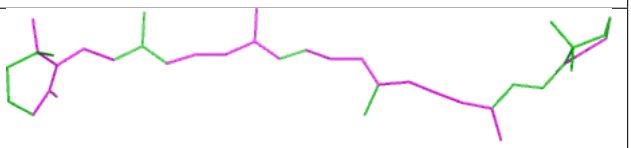

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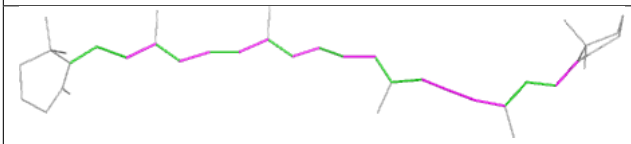

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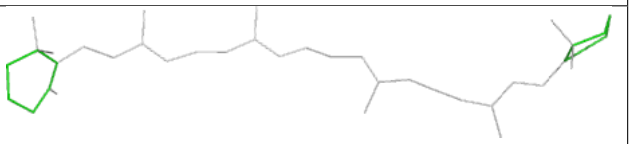
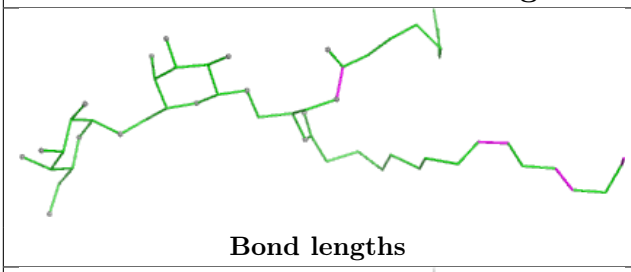


Rings

Ligand DGD C 518



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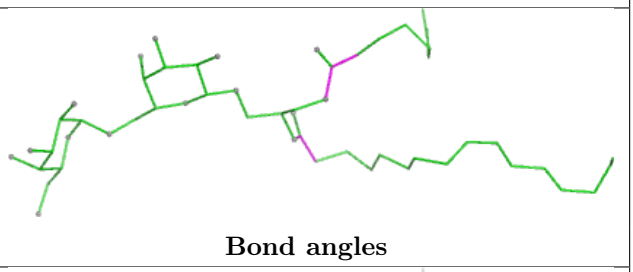
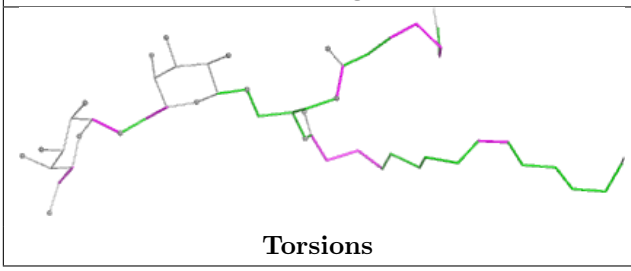


Bond angles



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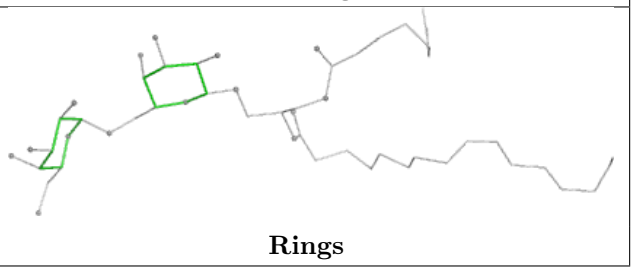
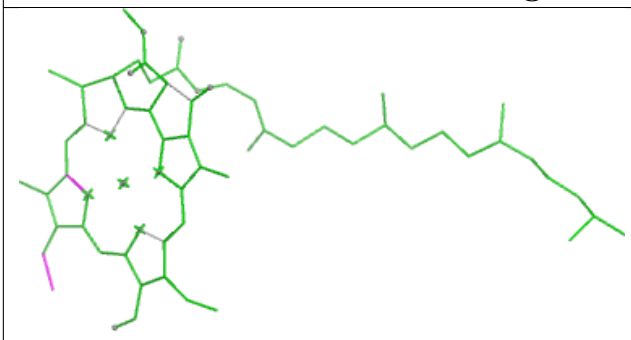


Rings

Ligand CHL Y 609



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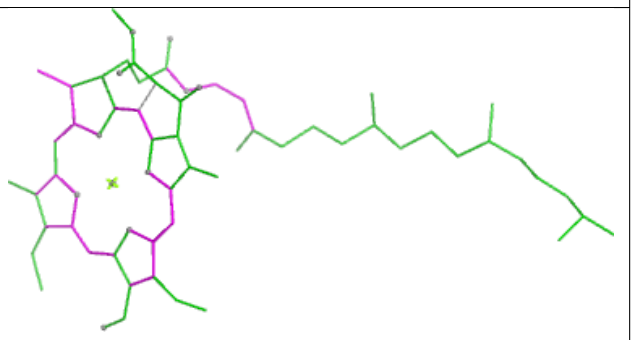
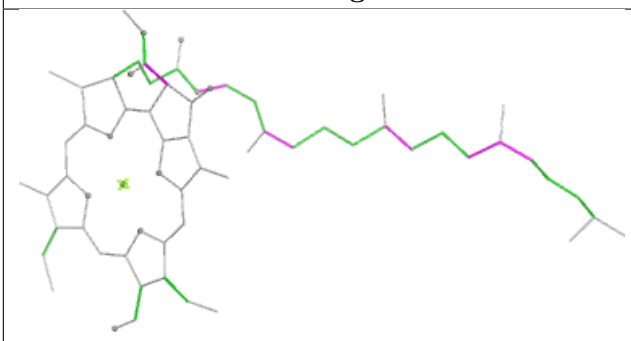
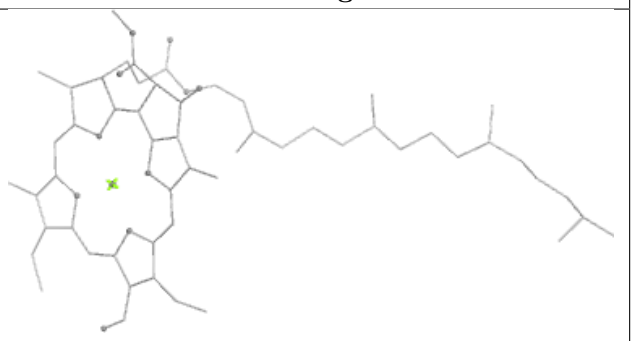


Bond angles

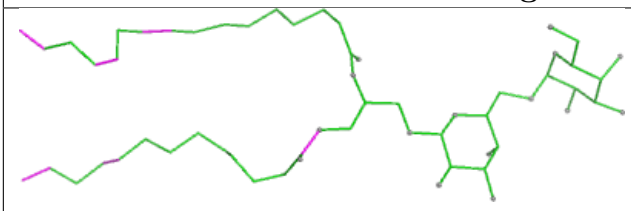


Torsions



Rings

Ligand DGD C 520



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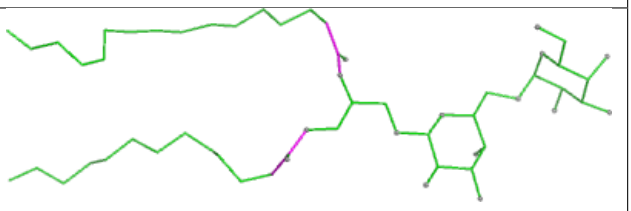

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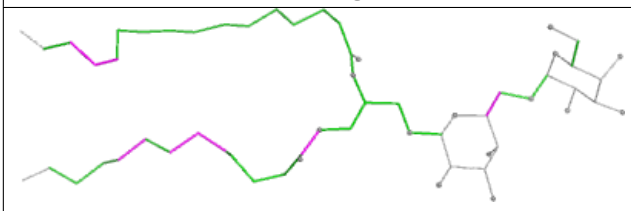

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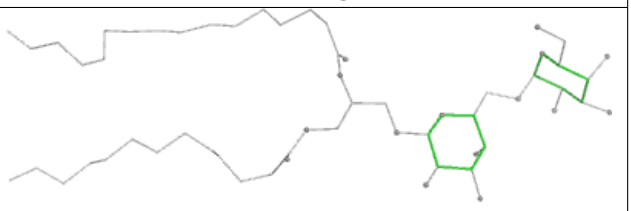
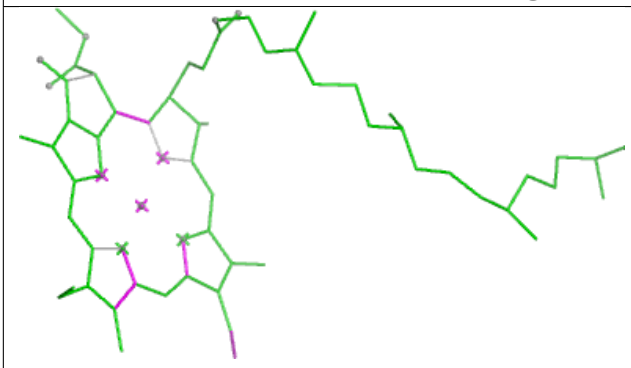


Rings

Ligand CLA C 511



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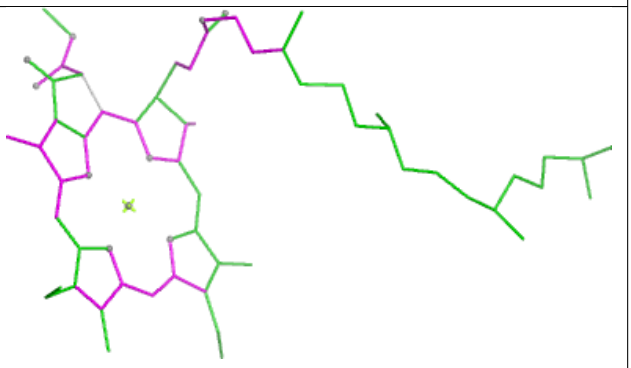
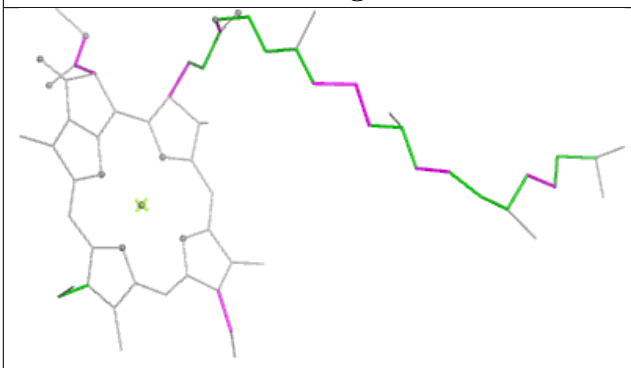


Bond angles



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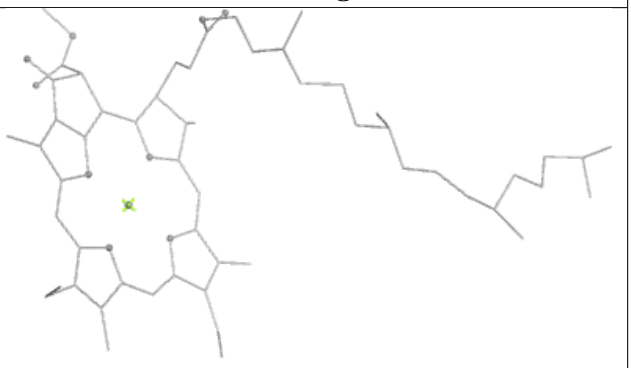

Rings

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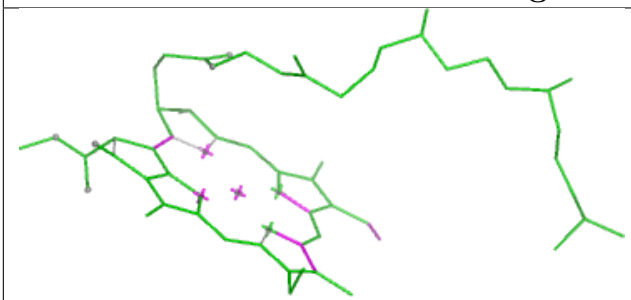

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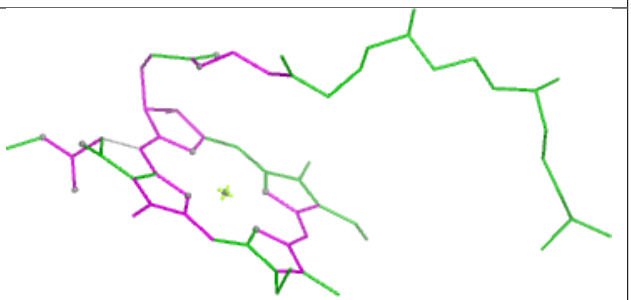
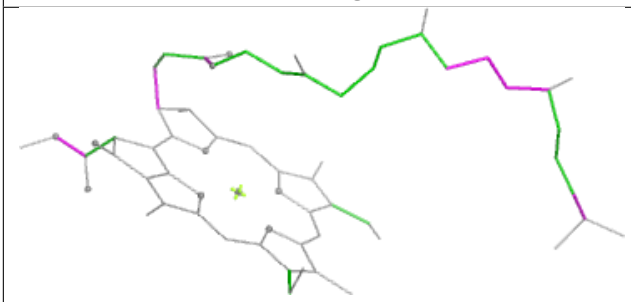


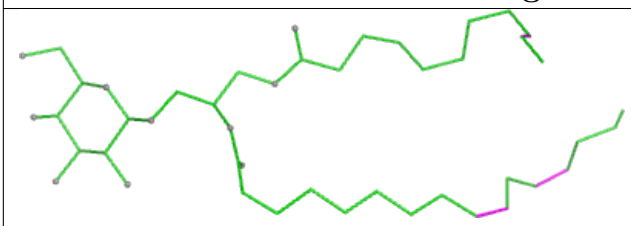
Bond angles



Torsions

Rings

Ligand LMG d 411



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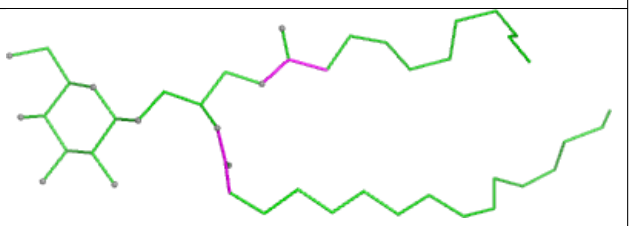

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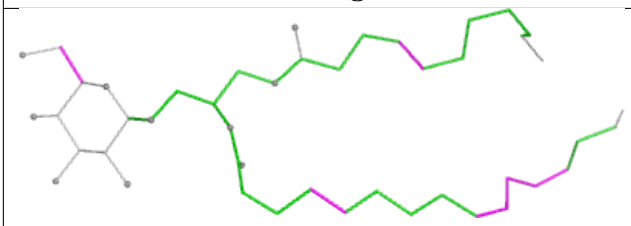

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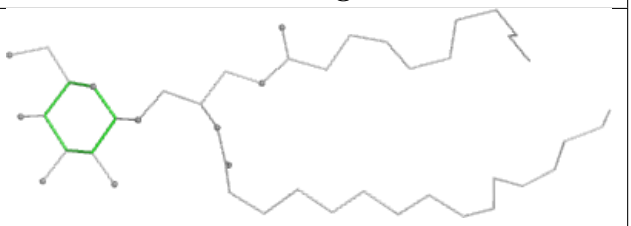

Rings

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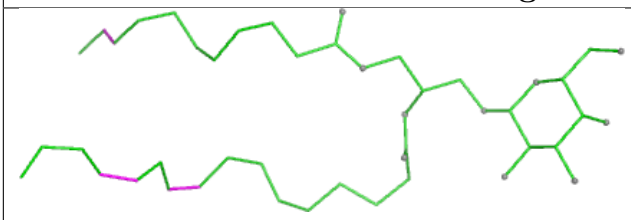

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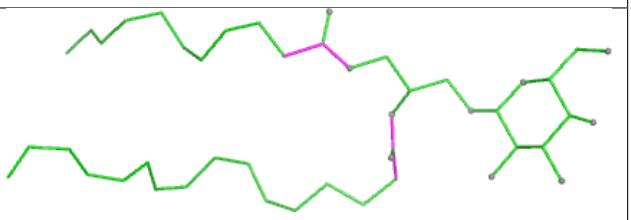

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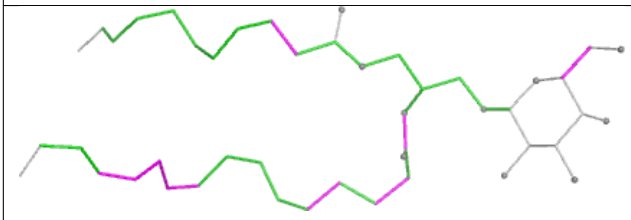

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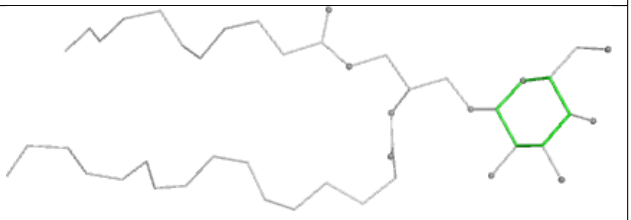
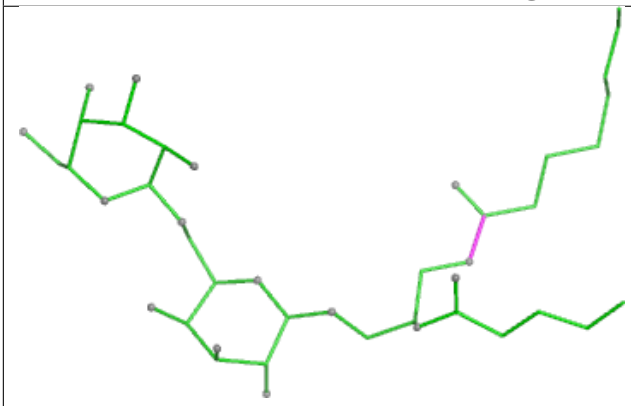


Rings

Ligand DGD b 623



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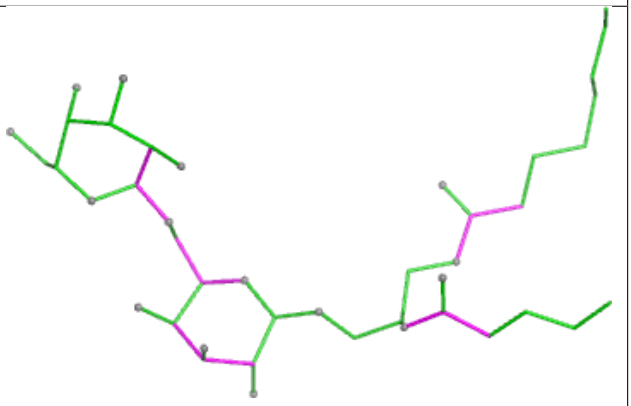
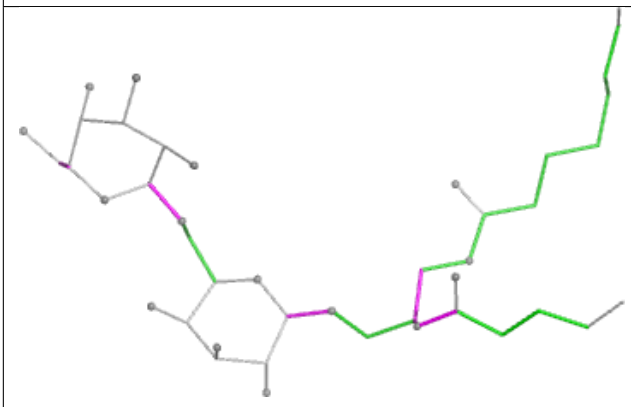


Bond angles



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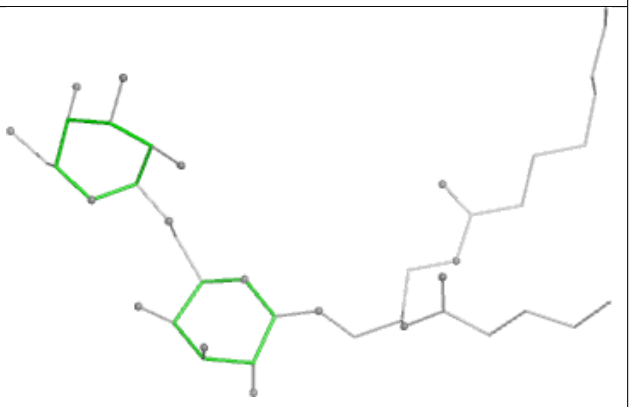
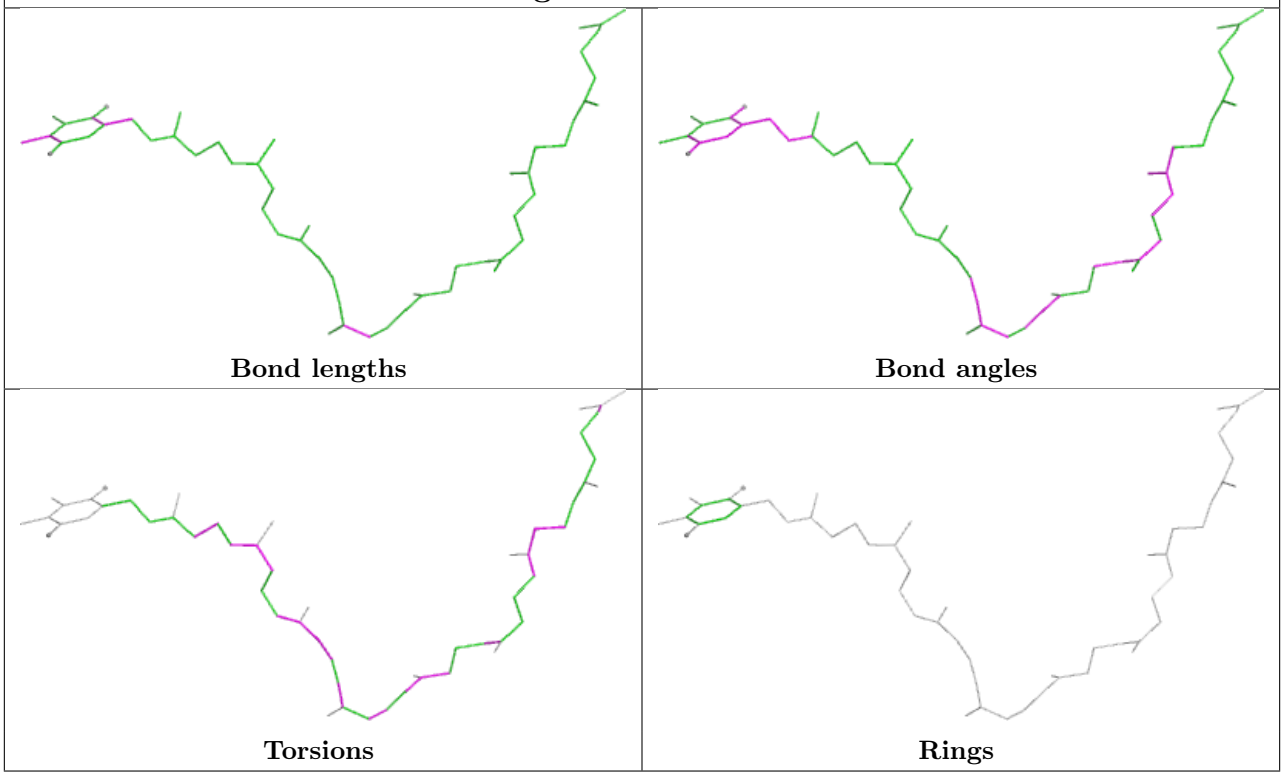


Rings

Ligand PL9 d 405



Ligand RRX h 101

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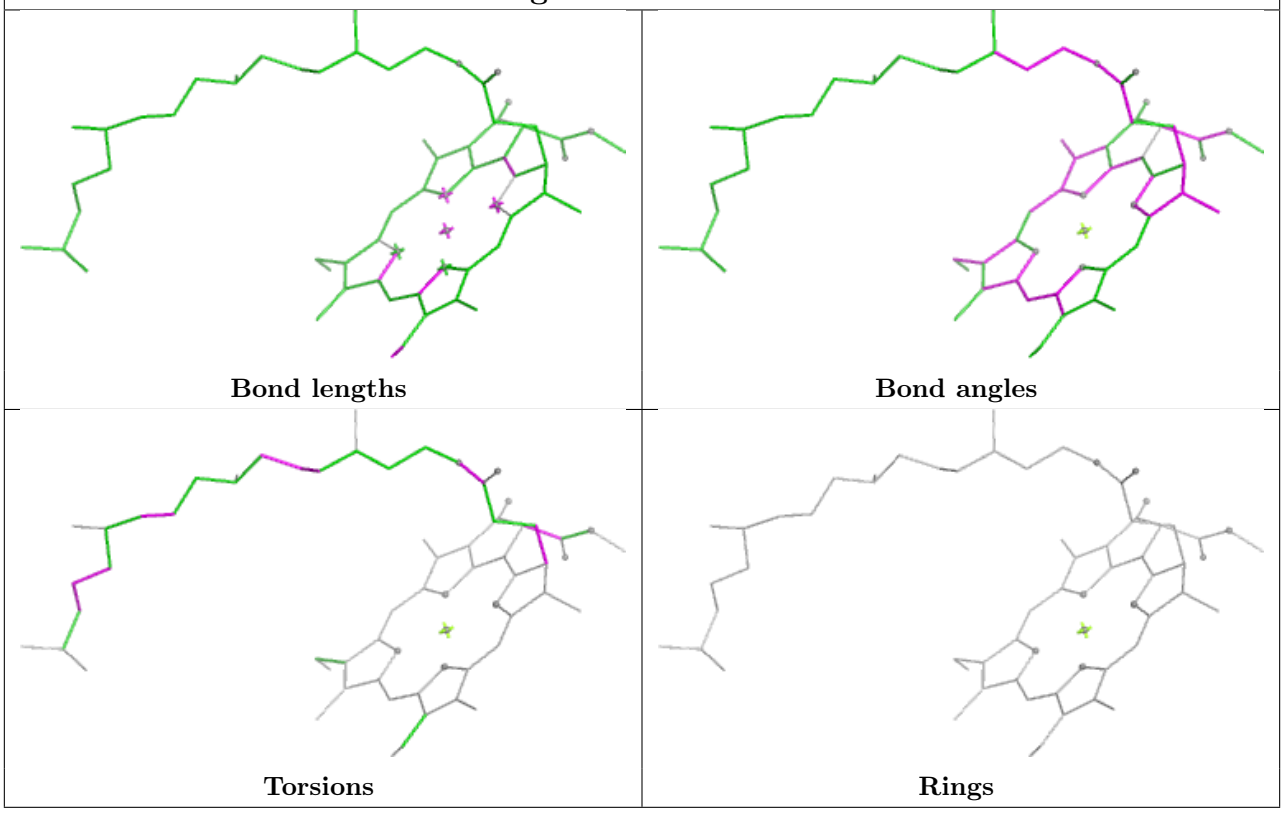
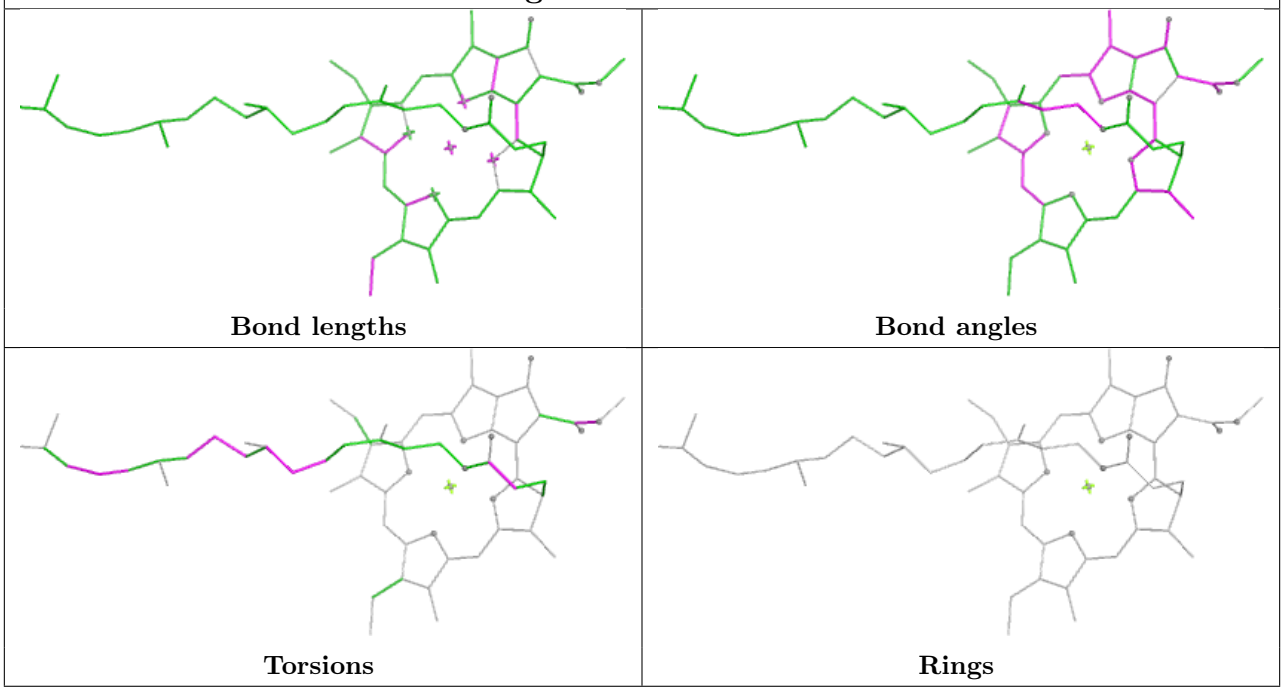


Ligand CLA B 615



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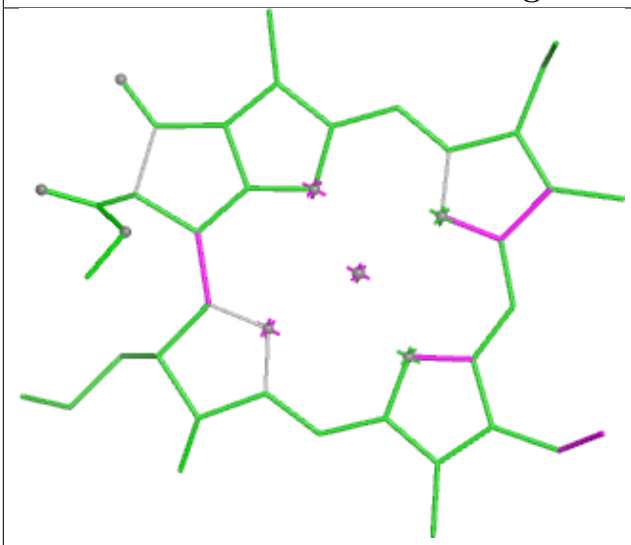
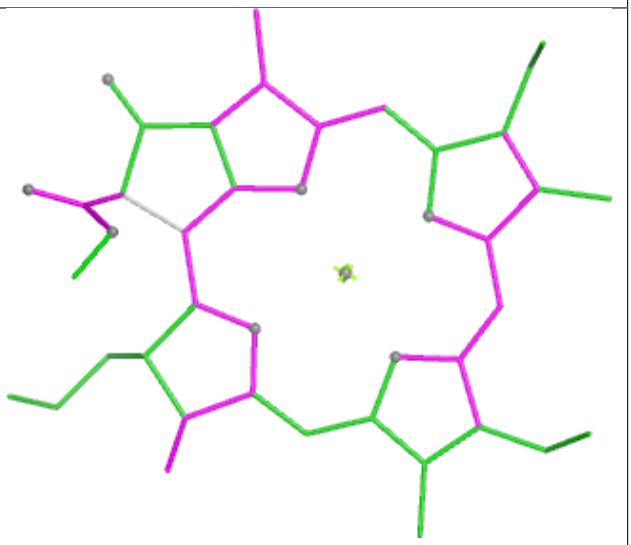
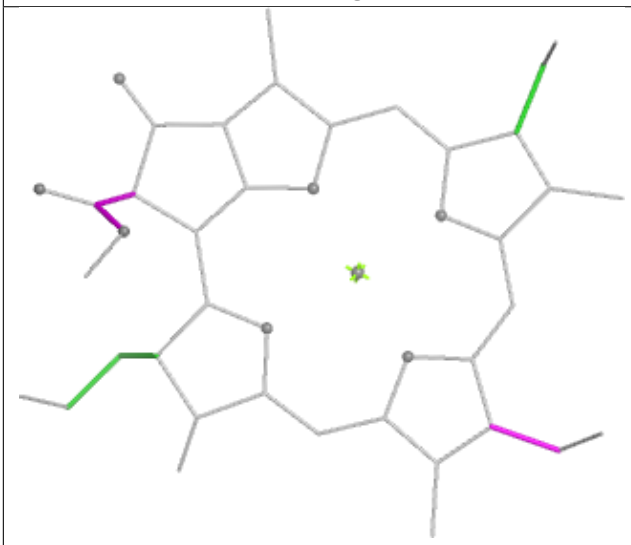


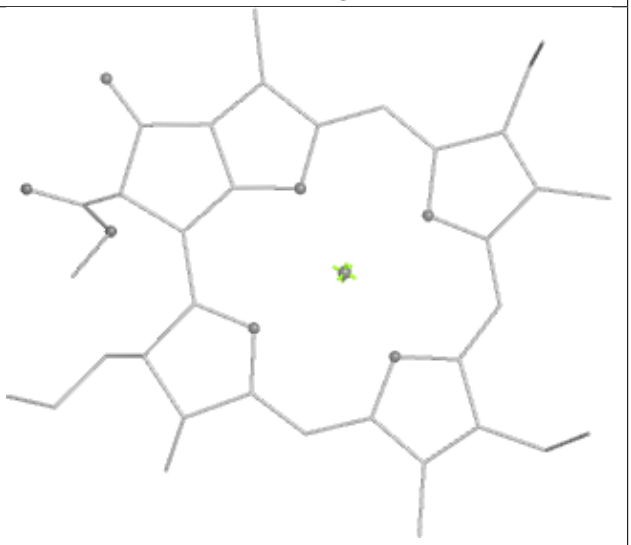
Bond lengths



Bond angles

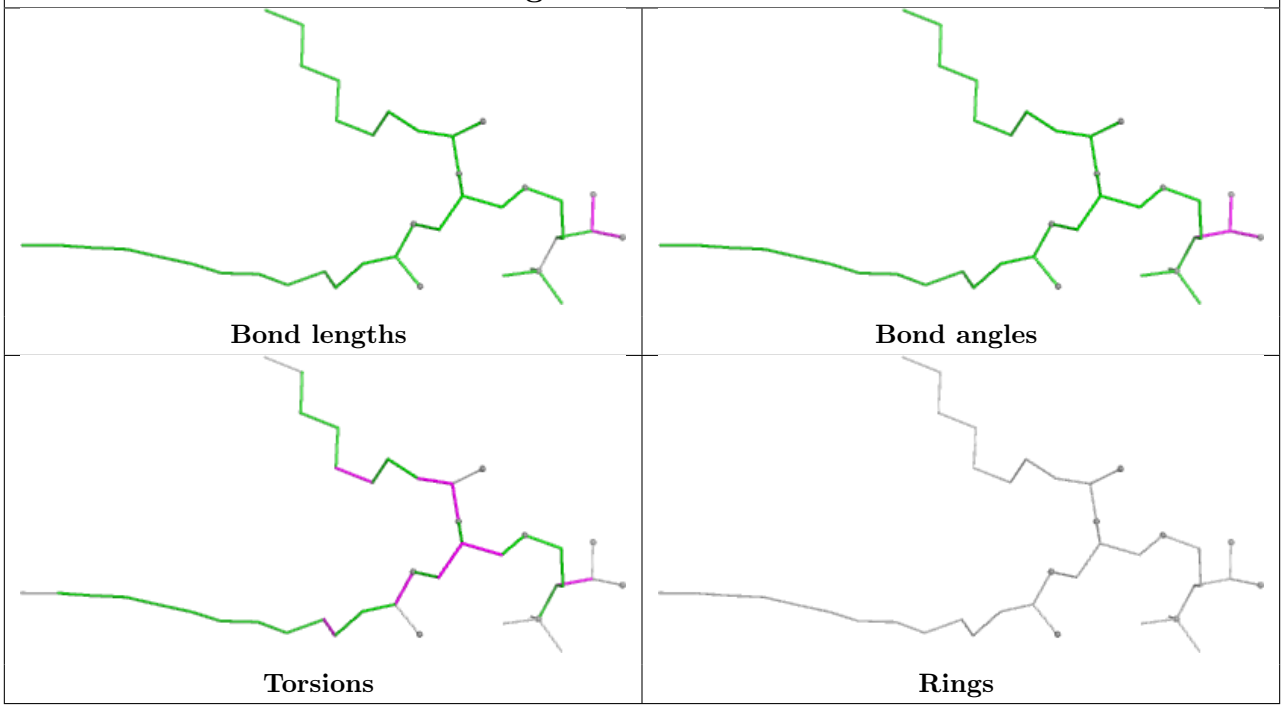


Torsions

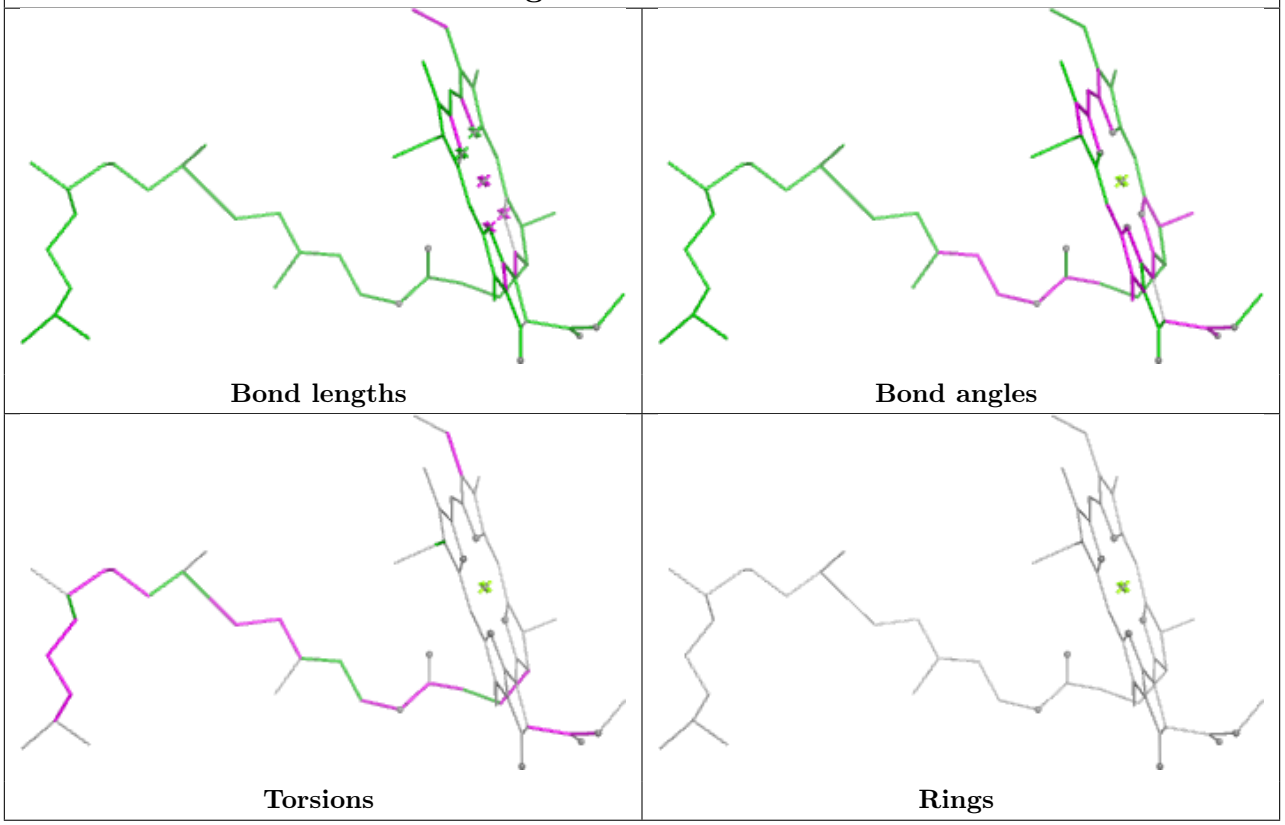


Rings

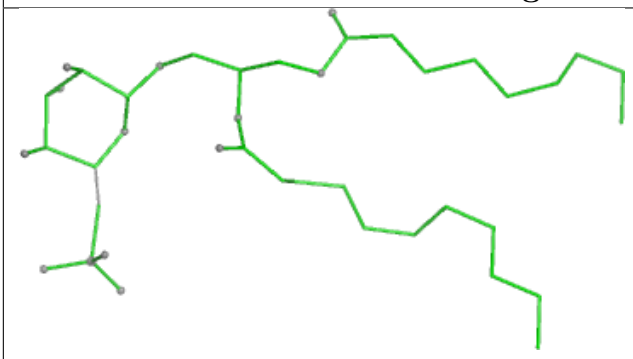
Ligand LMK c 527



Ligand CLA B 608



Ligand SQD m 101



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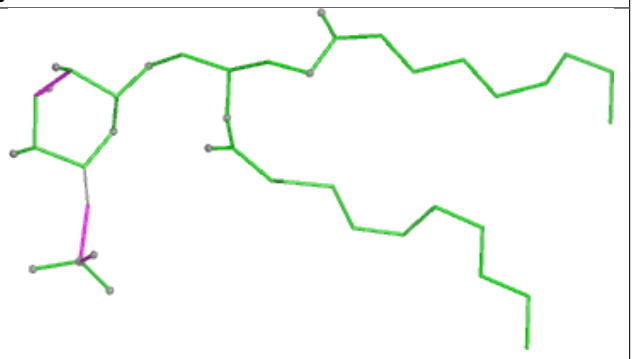
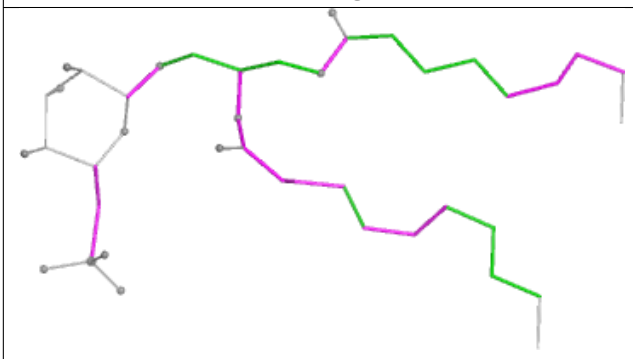
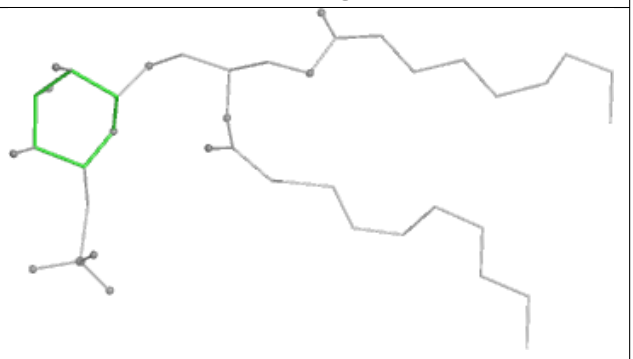


Bond angles

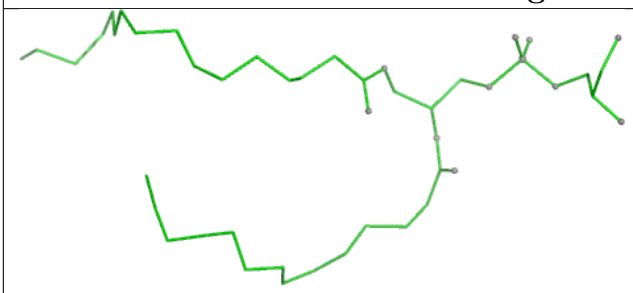


Torsions



Rings

Ligand LHG c 525



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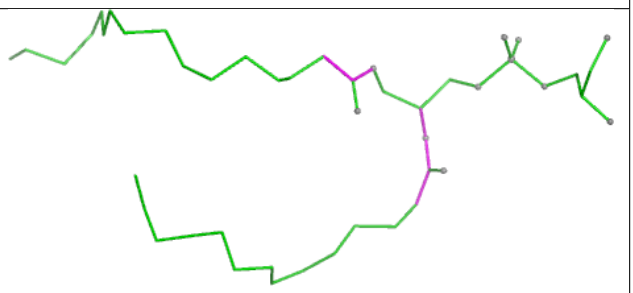
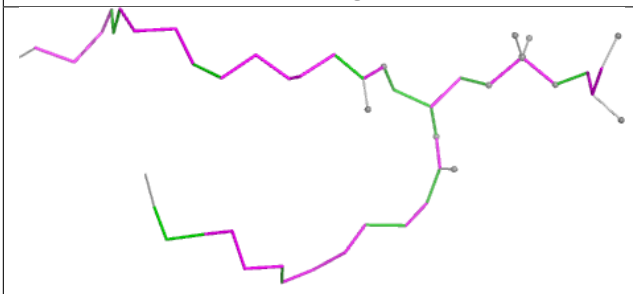


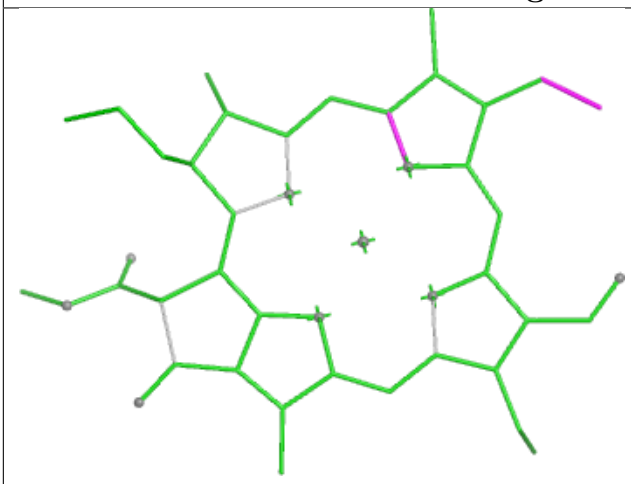
Bond angles



Torsions

Rings

Ligand CHL S 606



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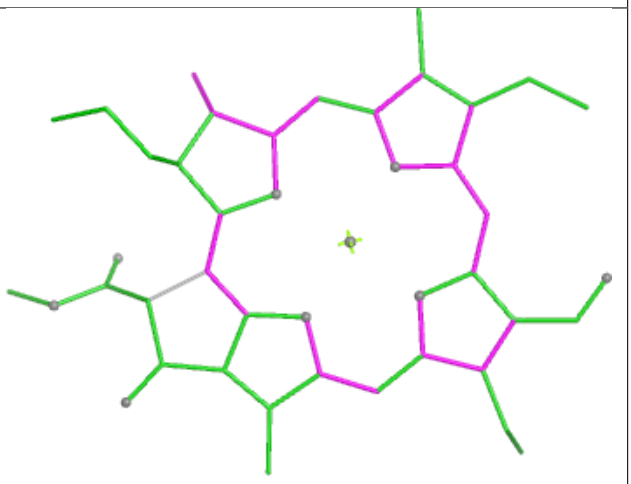
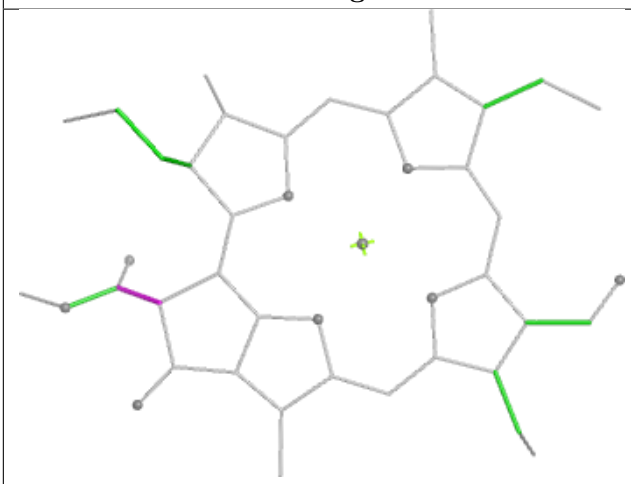
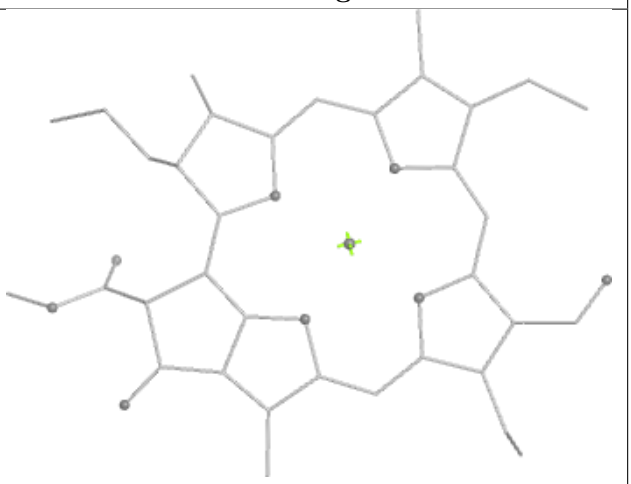


Bond angles

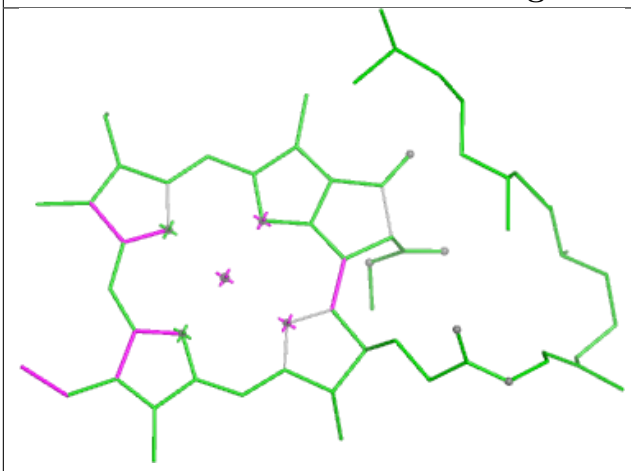


Torsions



Rings

Ligand CLA b 611



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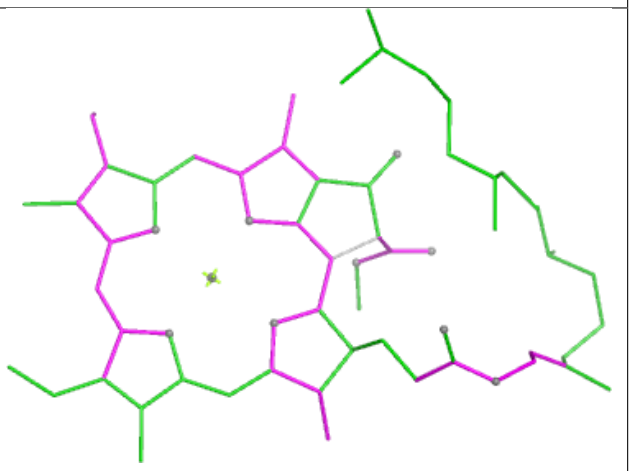
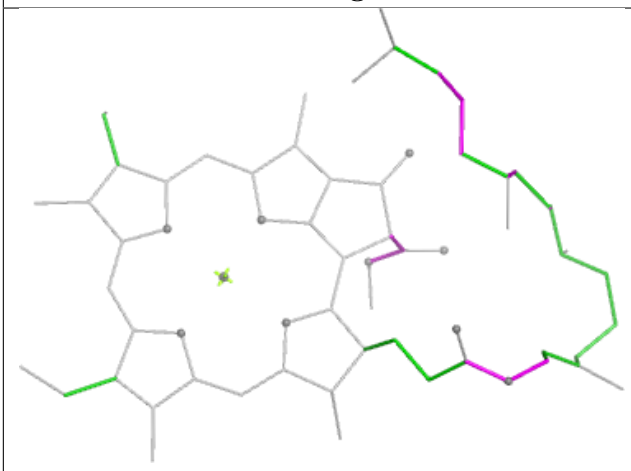


Bond angles



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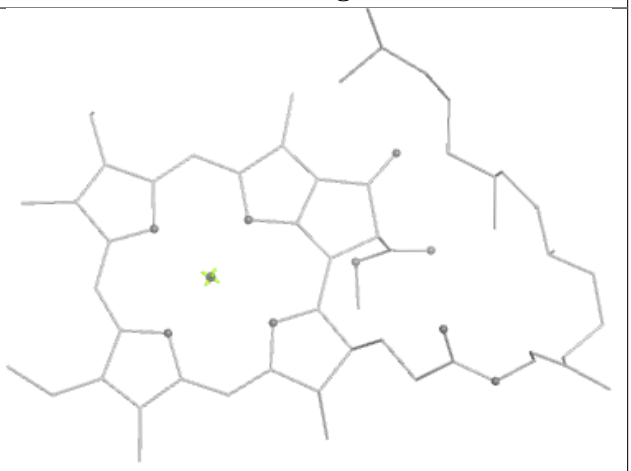
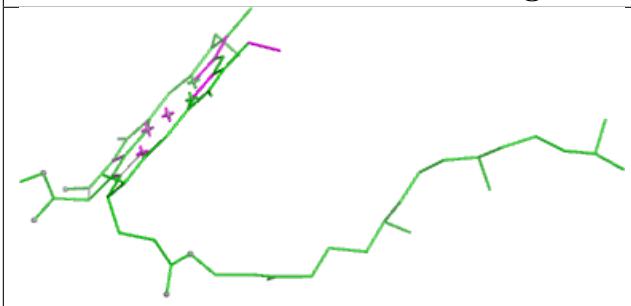


Rings

Ligand CLA N 604



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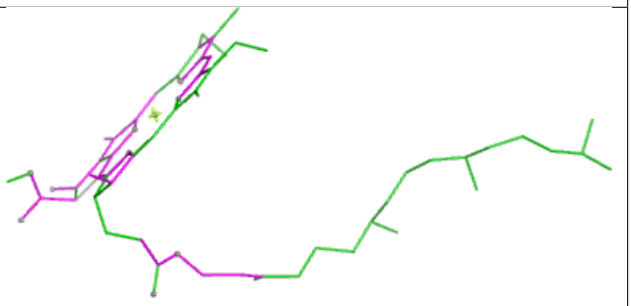
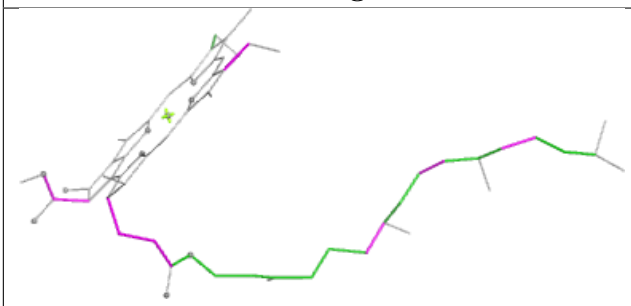


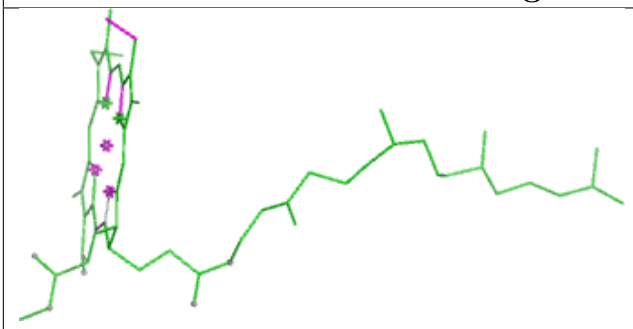
Bond angles



Torsions

Rings

Ligand CLA D 403



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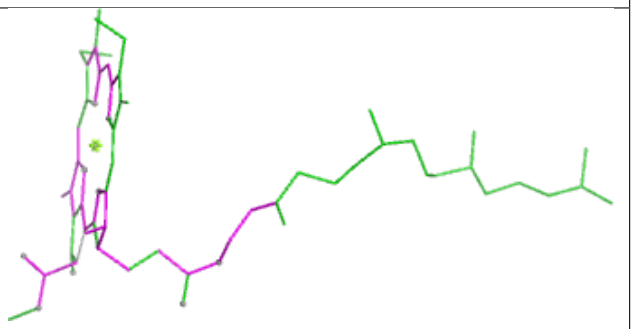
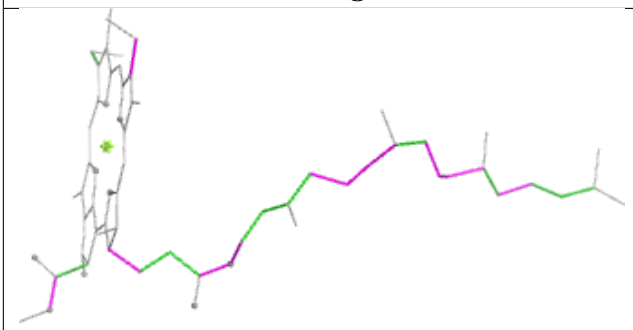


Bond angles



Torsions

Rings

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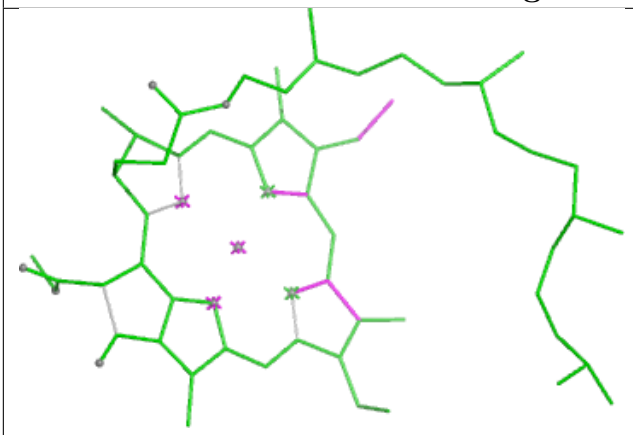

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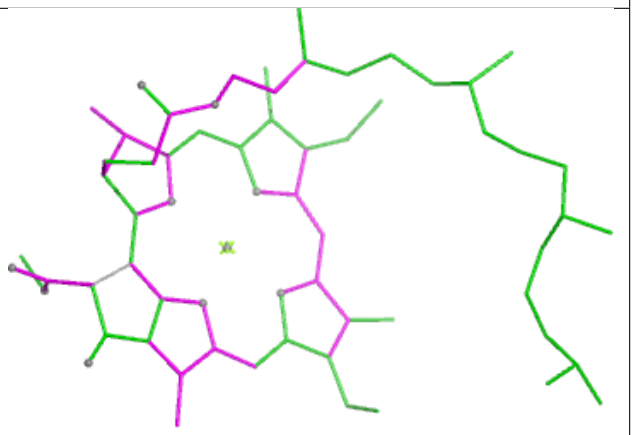
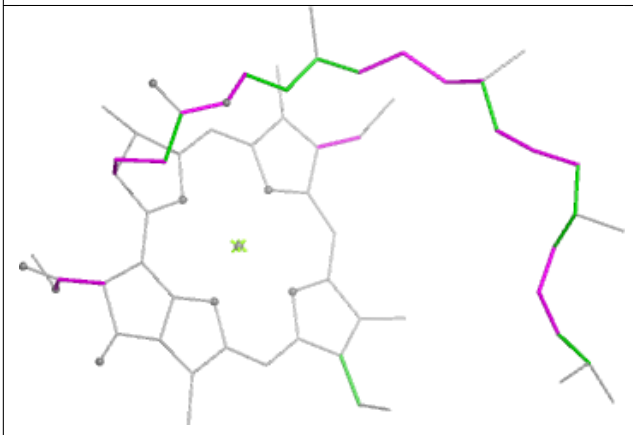


Bond angles



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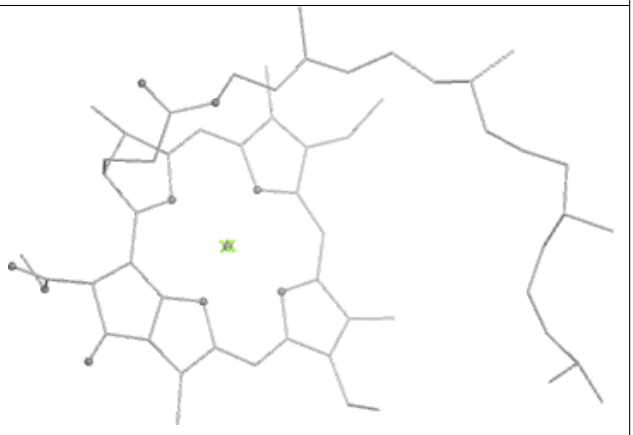

Rings

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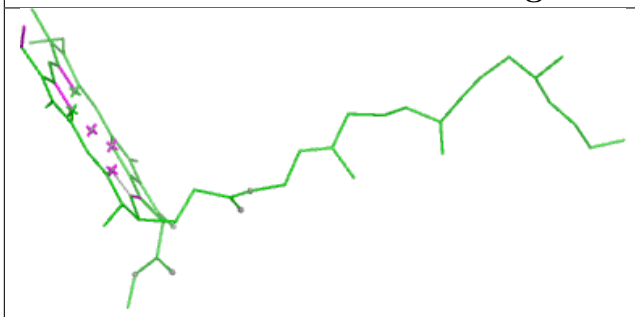

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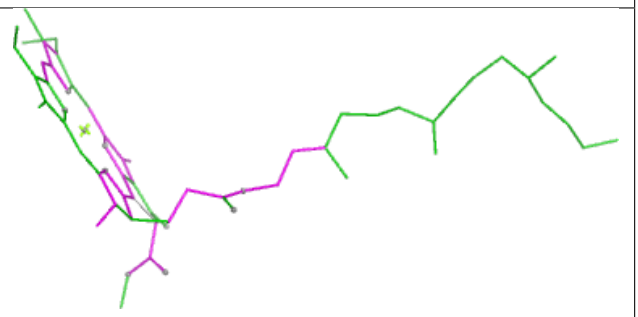

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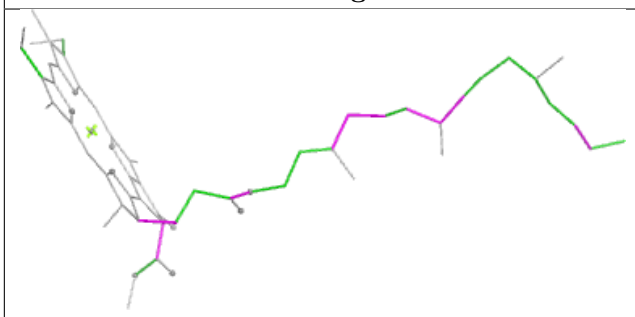

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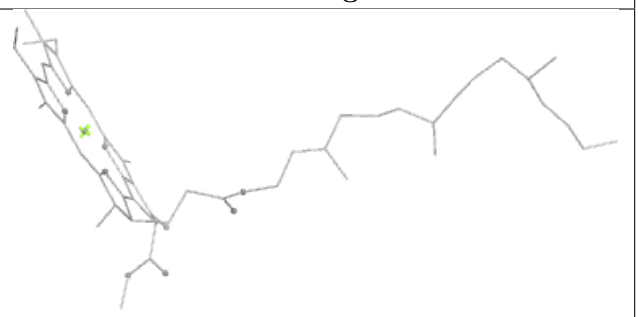

Rings

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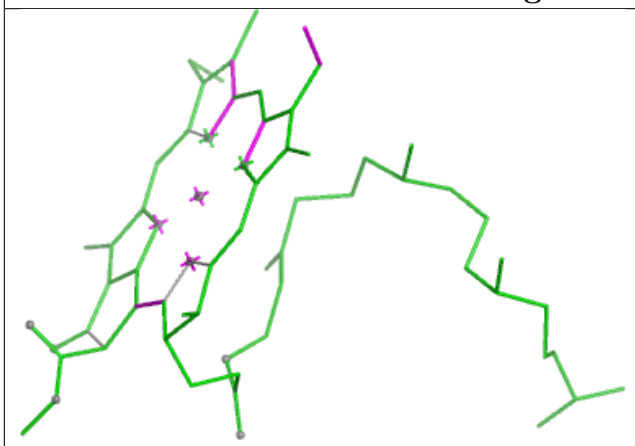

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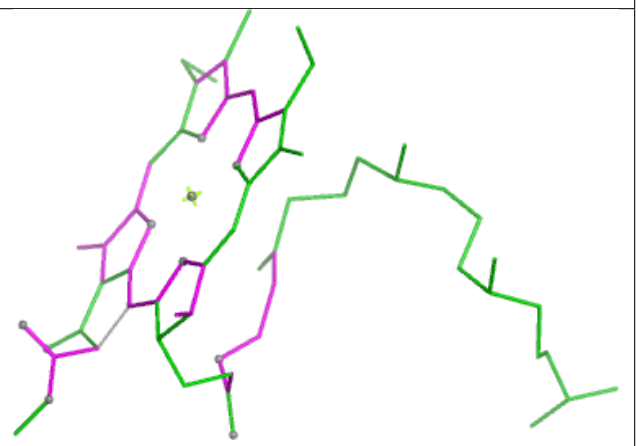
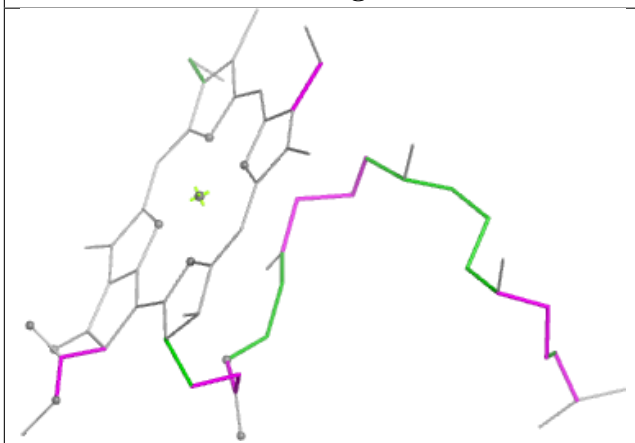


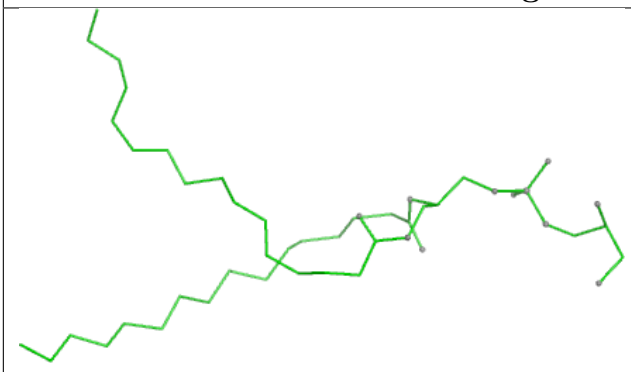
Bond angles



Torsions

Rings

Ligand LHG D 409



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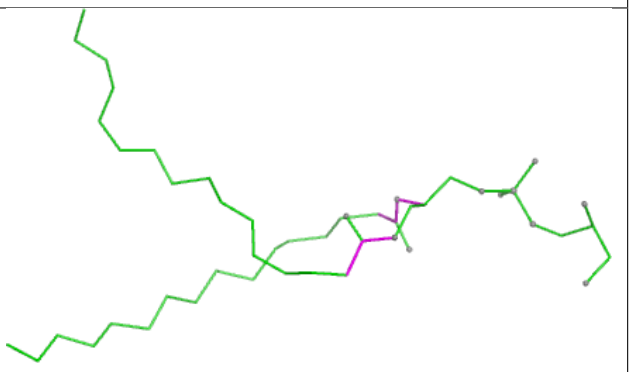
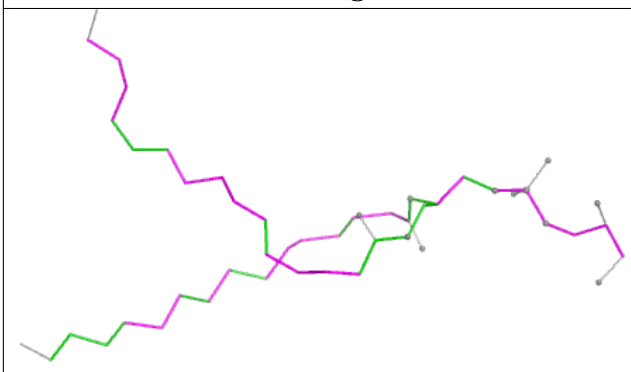


Bond angles



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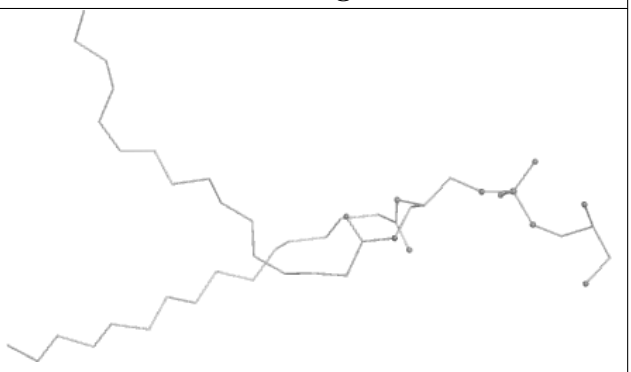
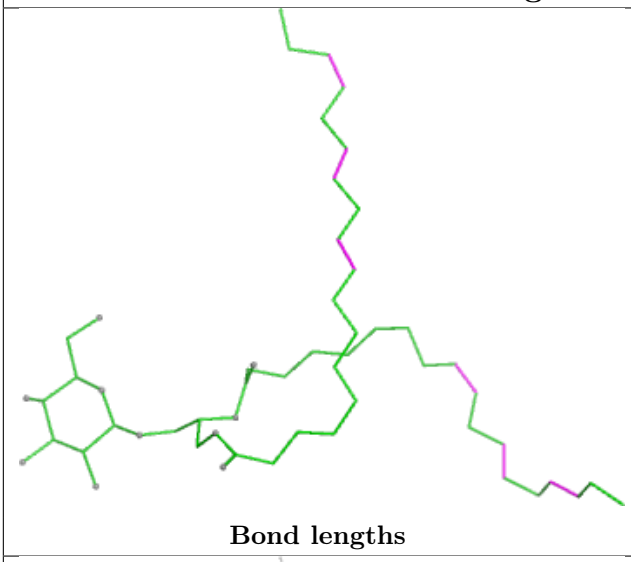


Rings

Ligand LMG c 523



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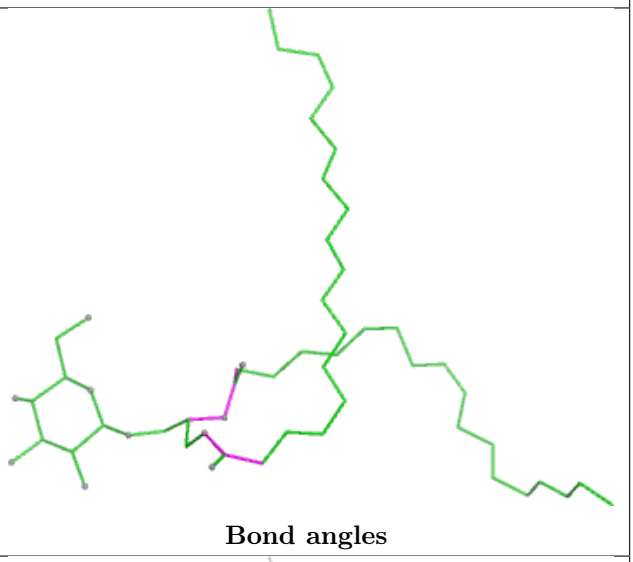

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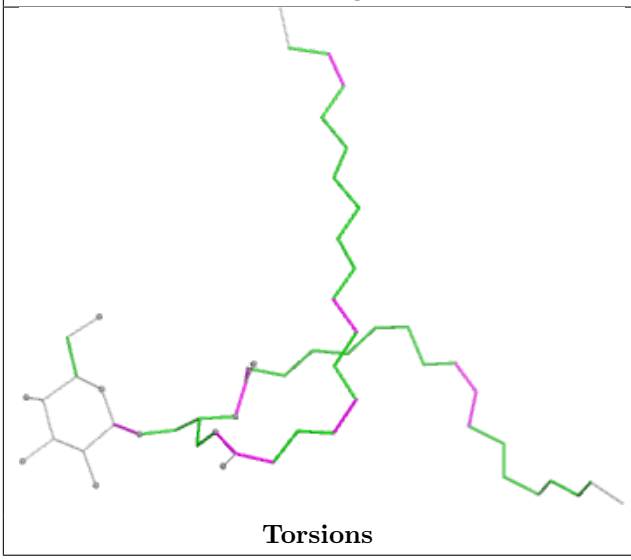
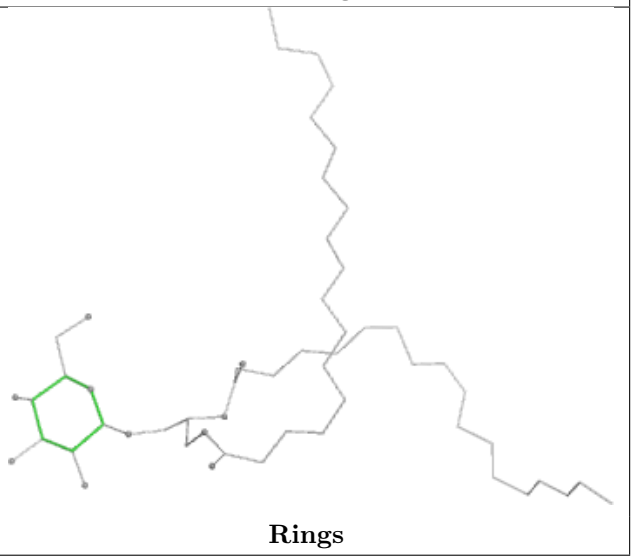
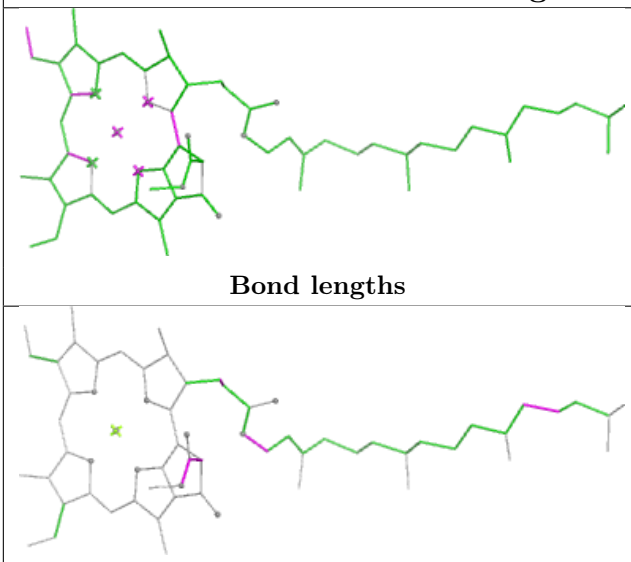


Torsions

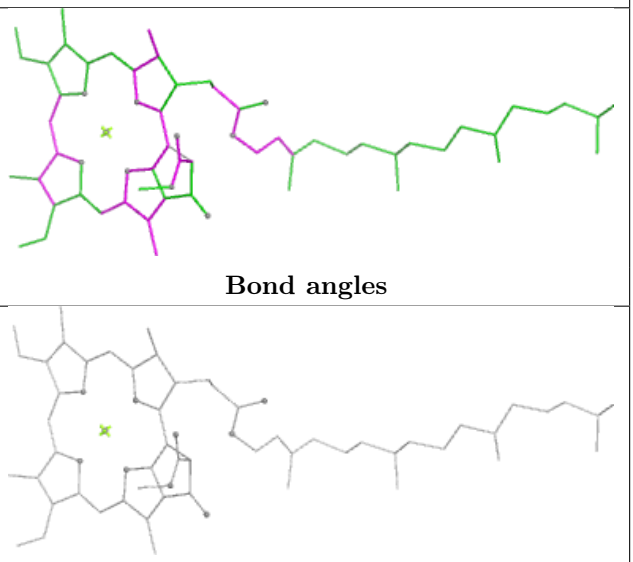


Rings

Ligand CLA c 502



Bond lengths

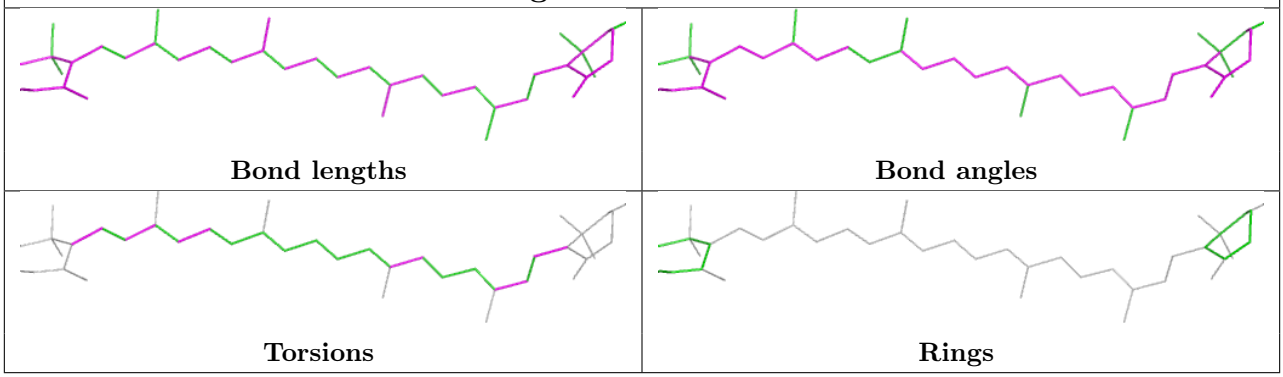


Bond angles

Torsions

Rings

Ligand C7Z B 620



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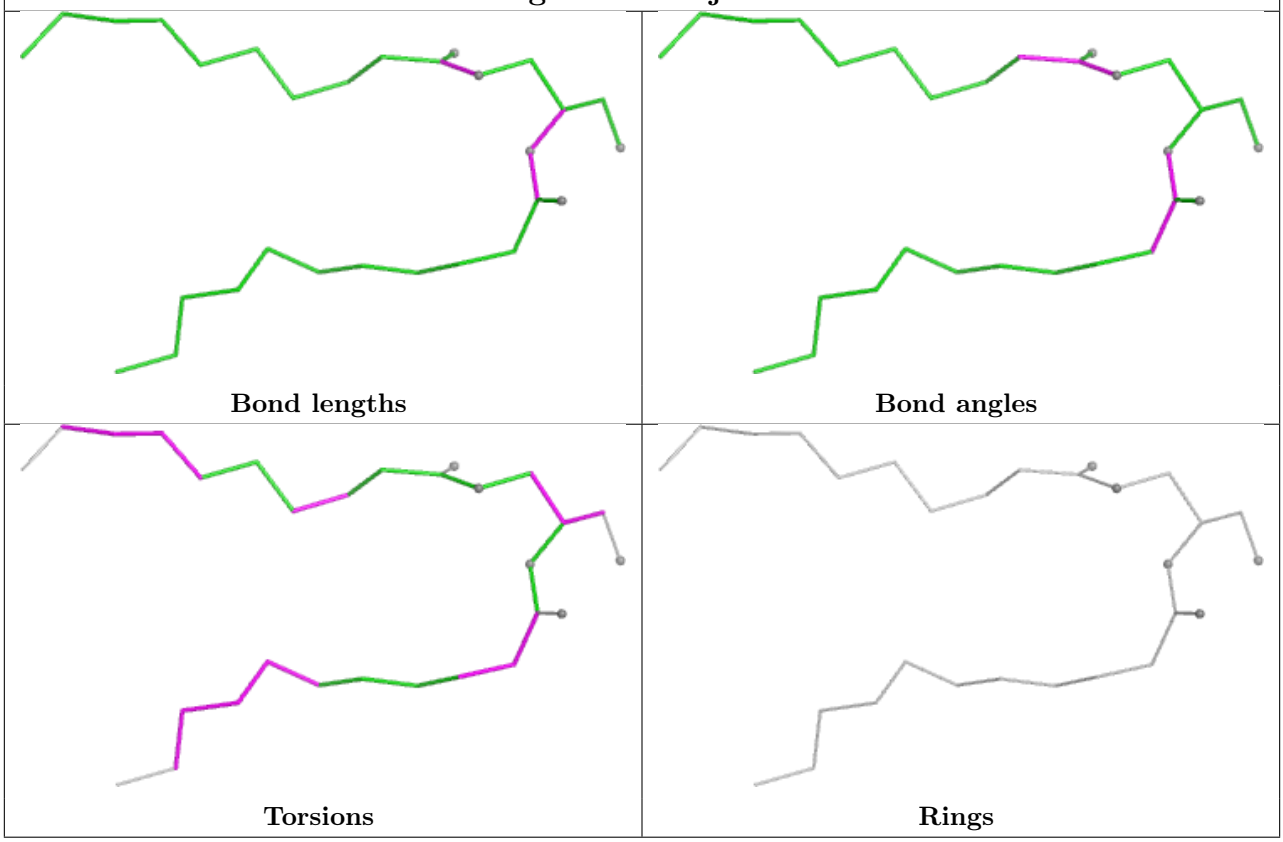
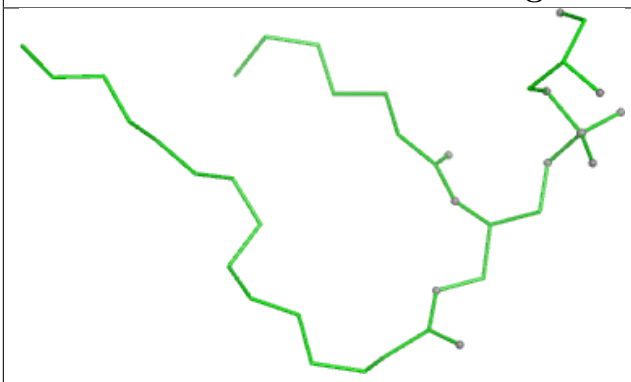


Ligand LHG d 410



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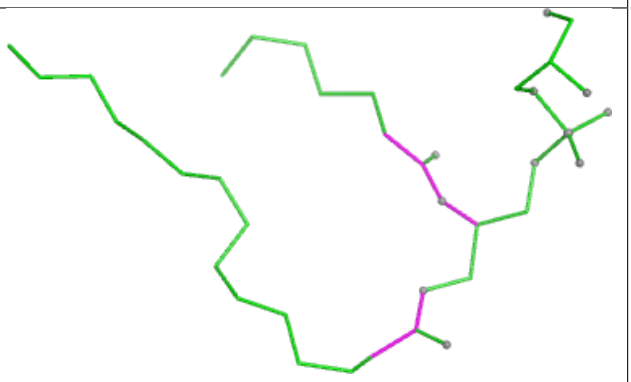
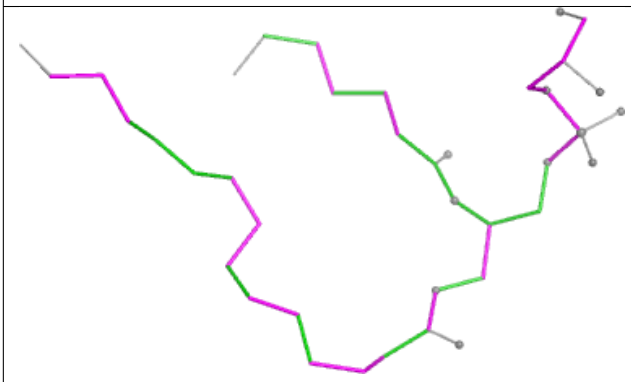
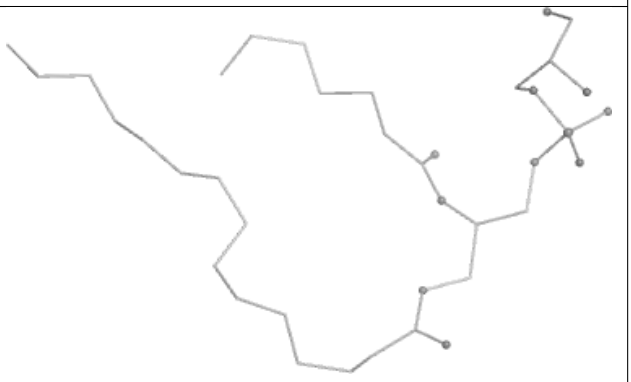


Bond angles



Torsions



Rings

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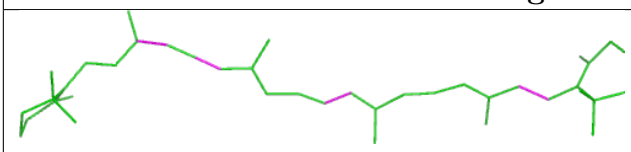
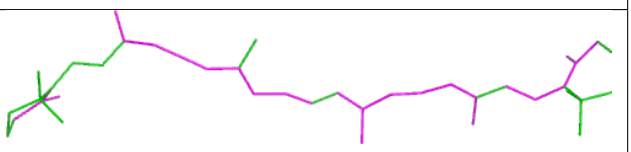
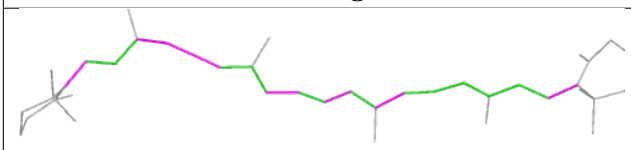


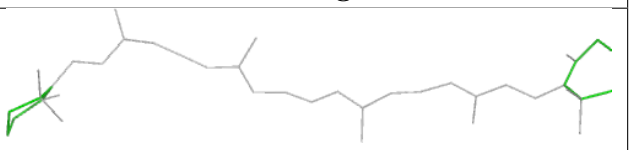
Bond lengths



Bond angles

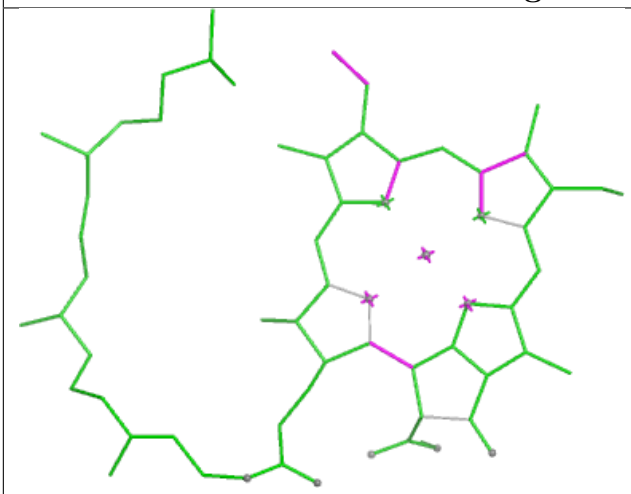


Torsions



Rings

Ligand CLA C 512



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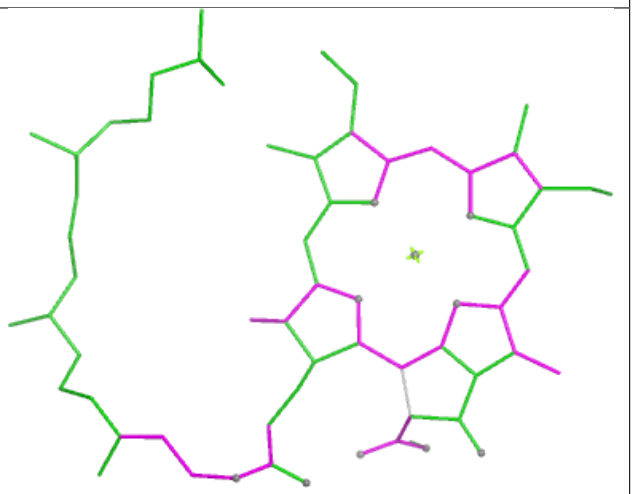

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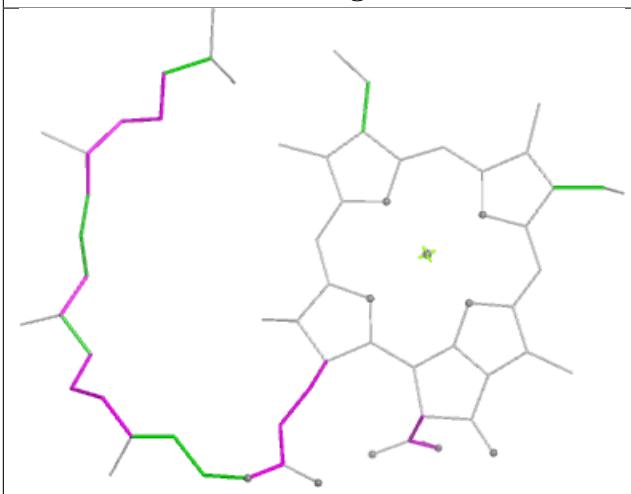

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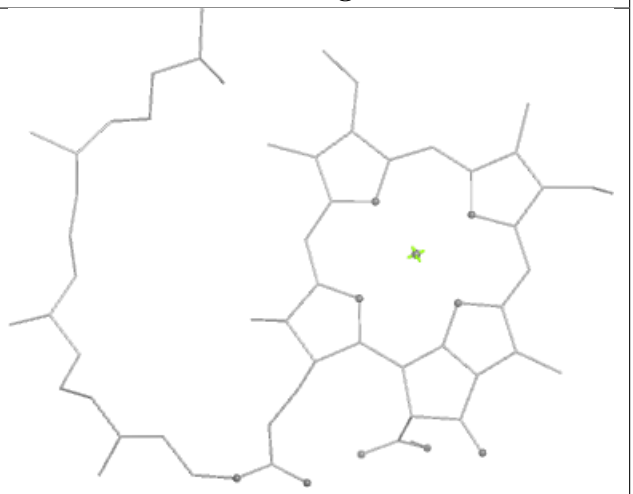
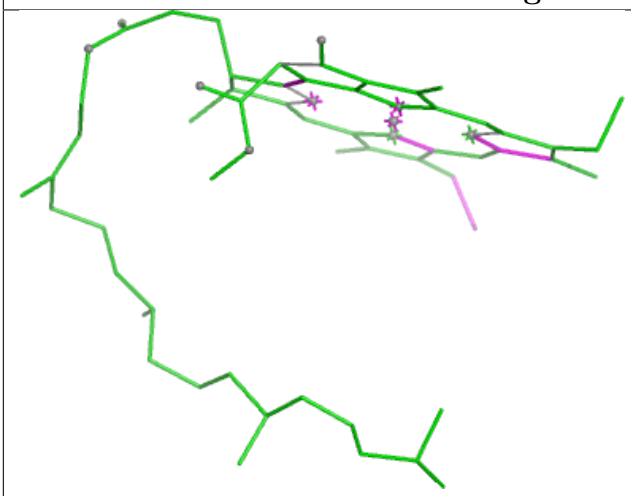


Rings

Ligand CLA Y 603



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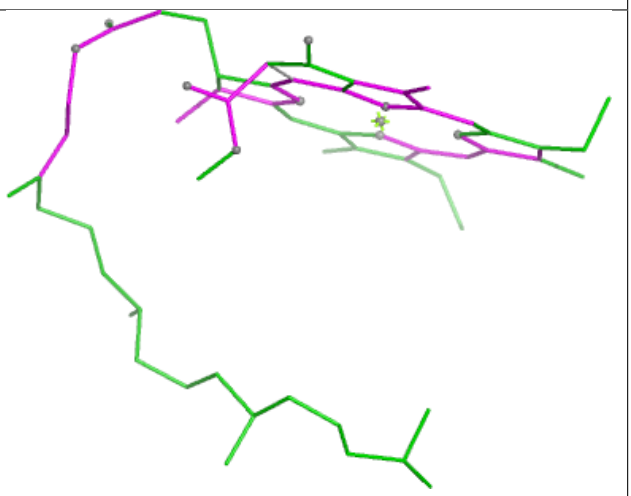

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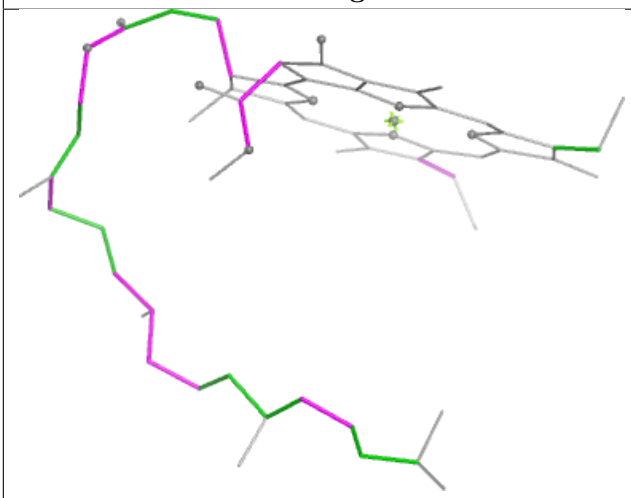

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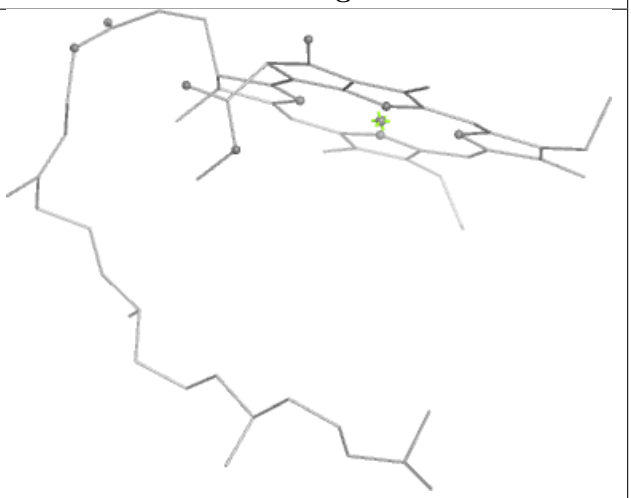
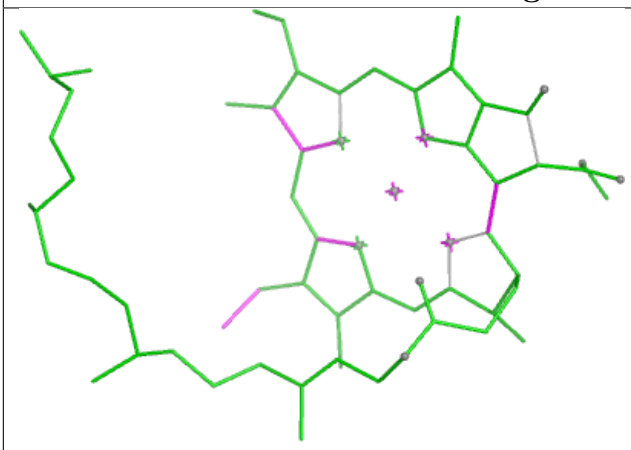


Rings

Ligand CLA G 602



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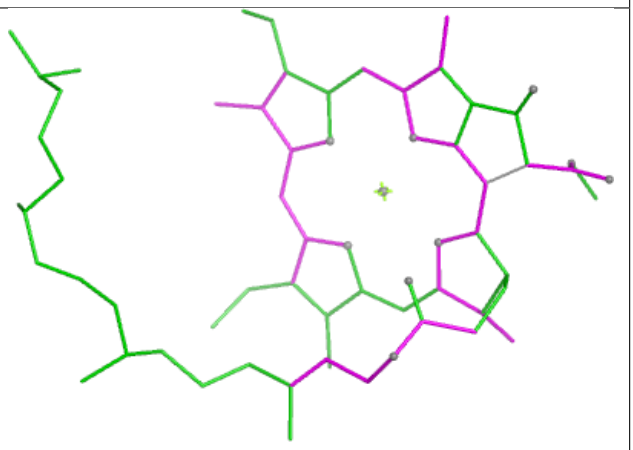
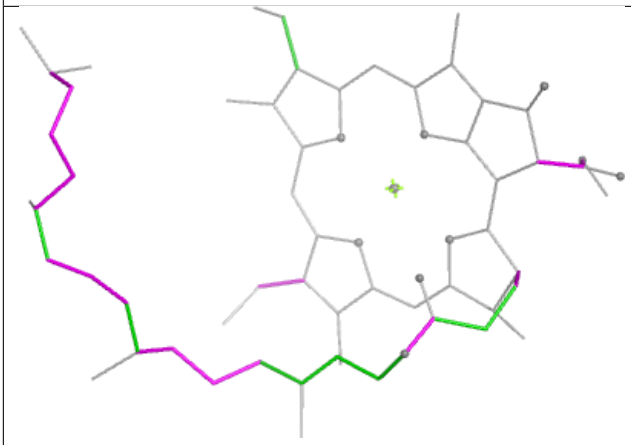


Bond angles



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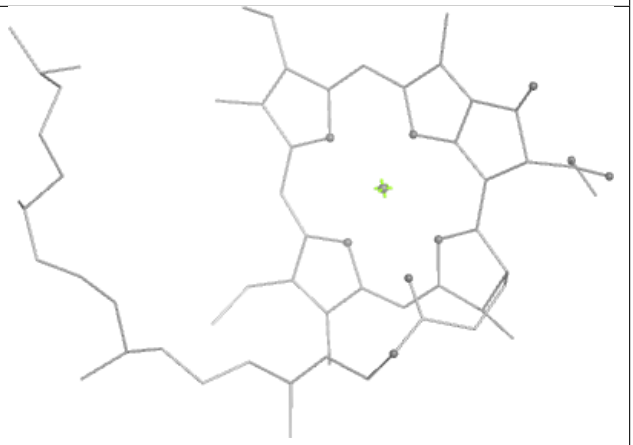
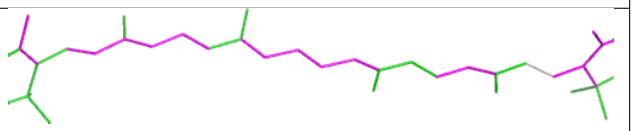


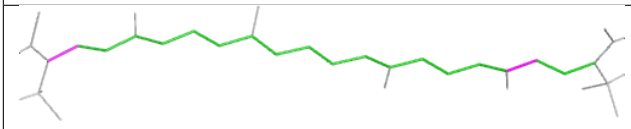
Rings

Ligand LUT N 620

Bond lengths



Bond angles



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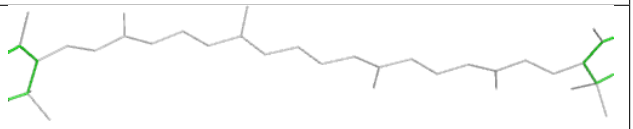
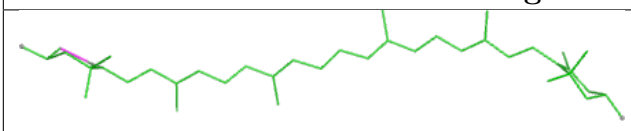


Rings

Ligand LUT Y 620



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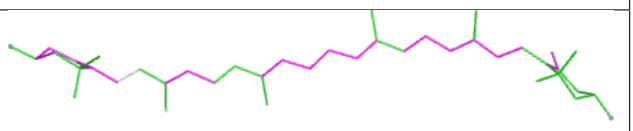
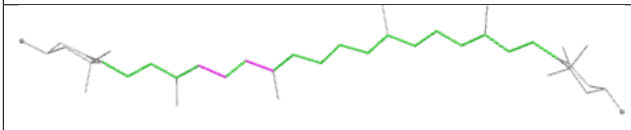


Bond angles



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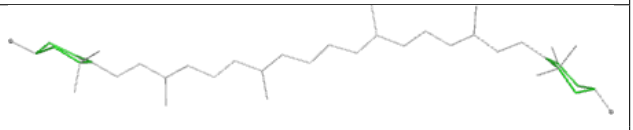
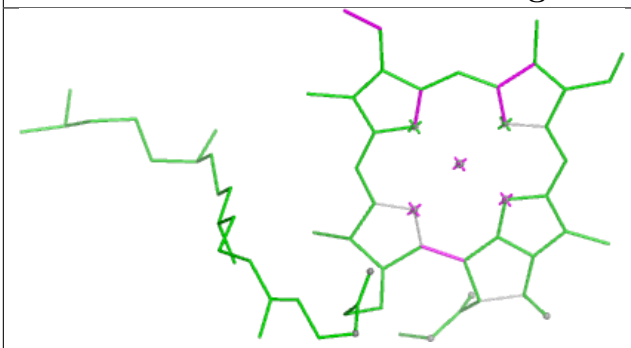


Rings

Ligand CLA a 406



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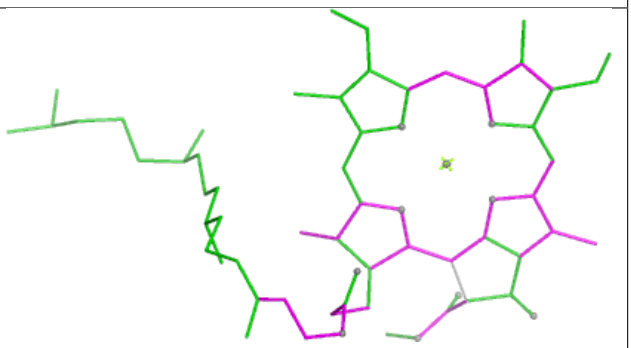
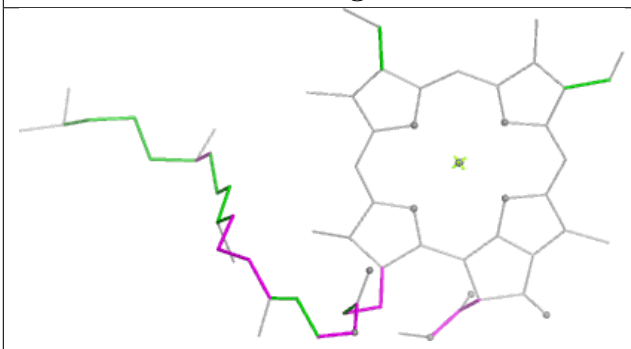
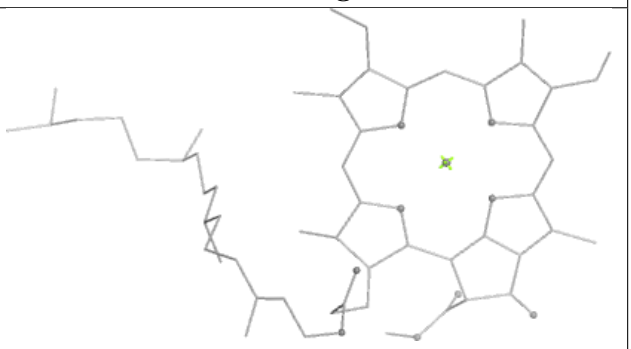


Bond angles

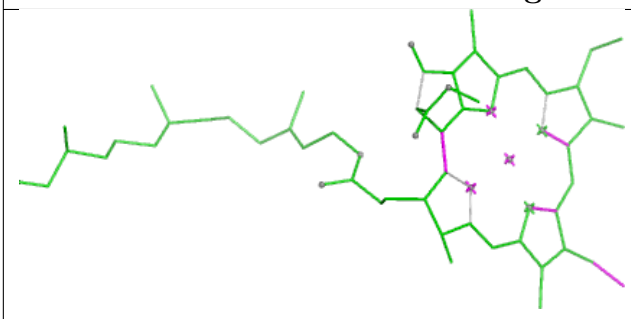


Torsions



Rings

Ligand CLA C 502



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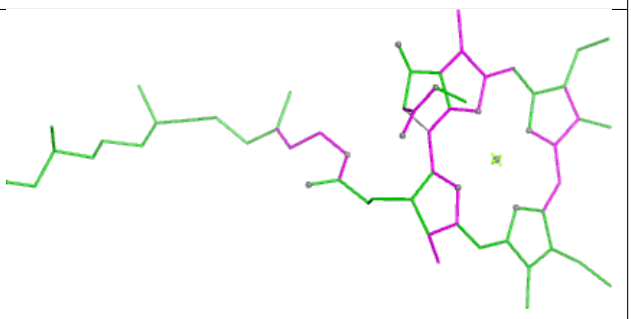
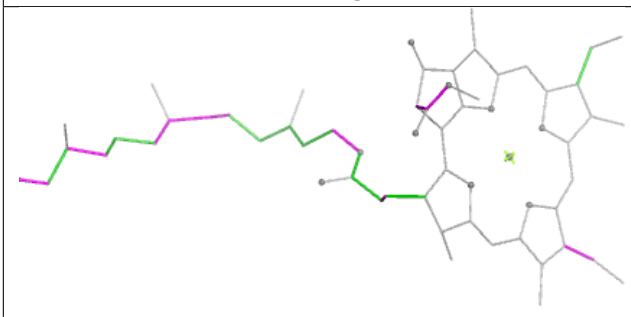


Bond angles



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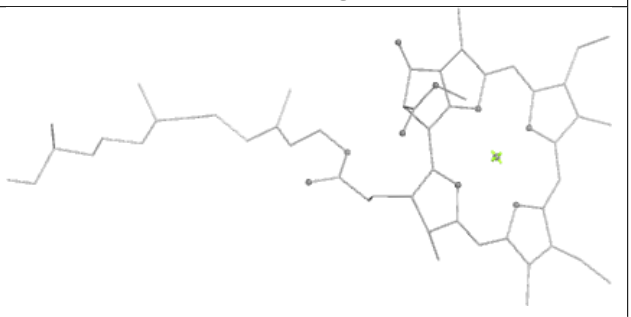
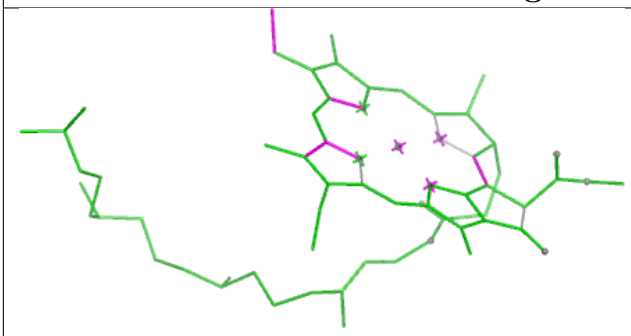


Rings

Ligand CLA C 513



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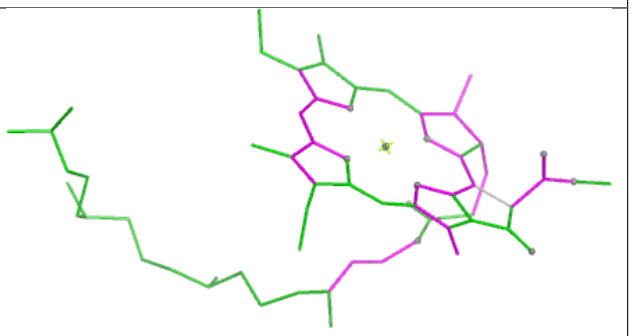
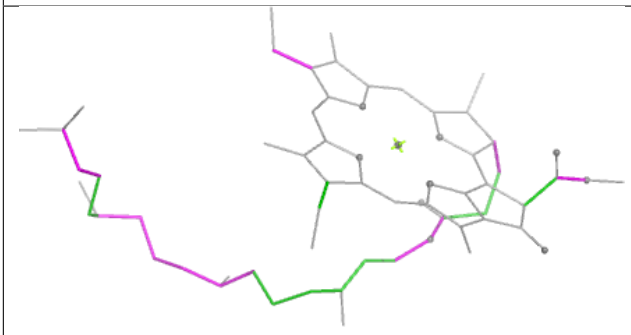
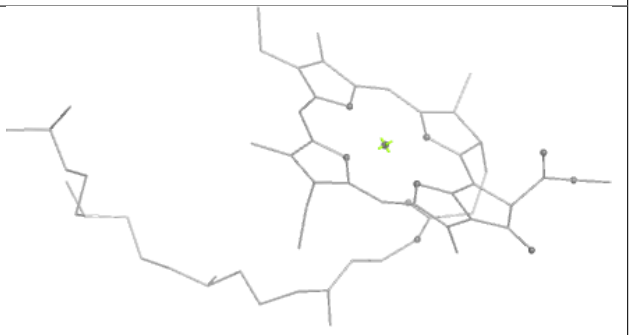


Bond angles

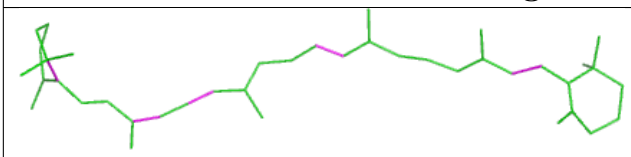


Torsions



Rings

Ligand BCR B 618



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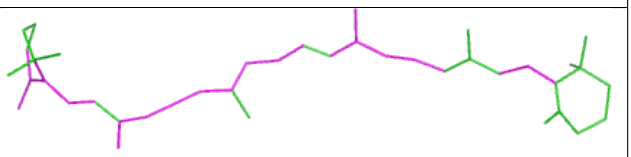
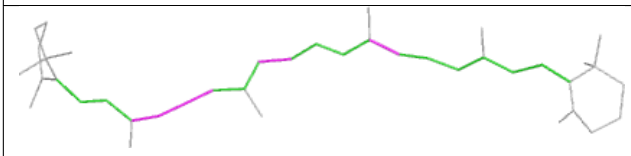


Bond angles



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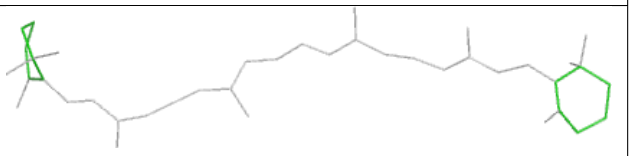
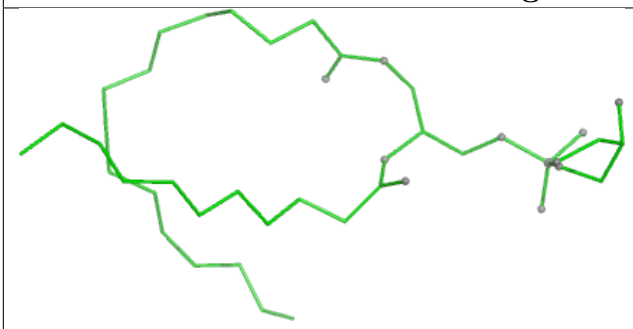


Rings

Ligand LHG D 408



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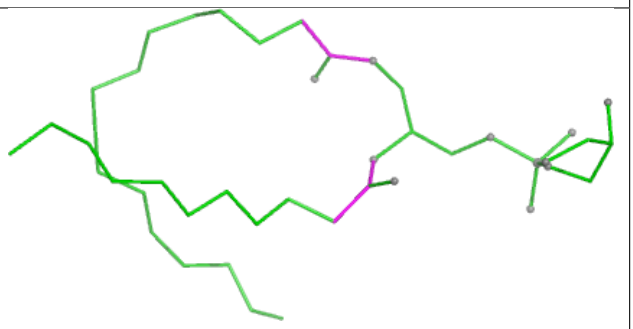
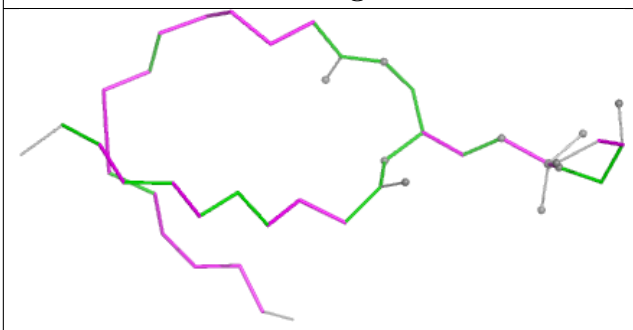


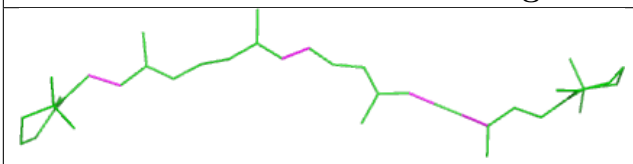
Bond angles



Torsions

Rings

Ligand BCR C 515



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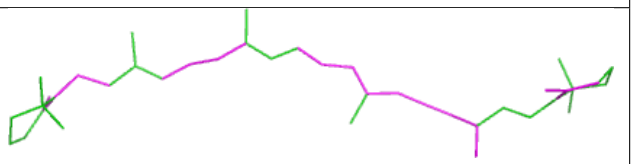
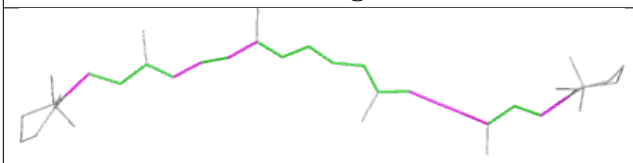
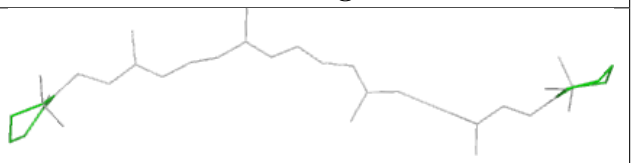


Bond angles

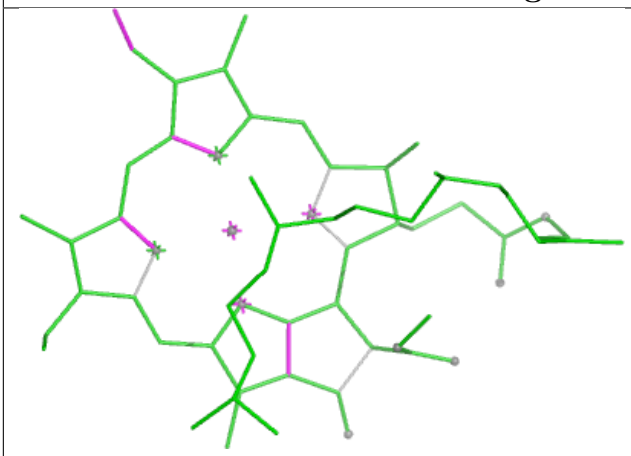


Torsions



Rings

Ligand CLA C 510



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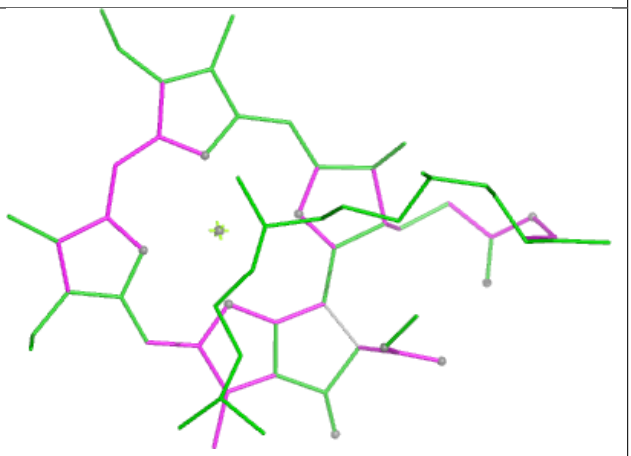
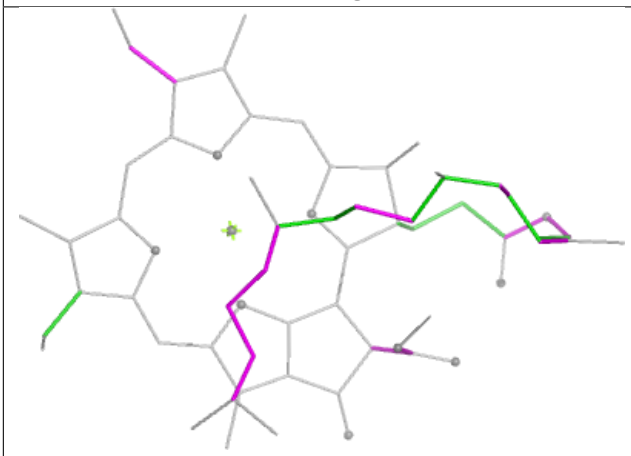


Bond angles



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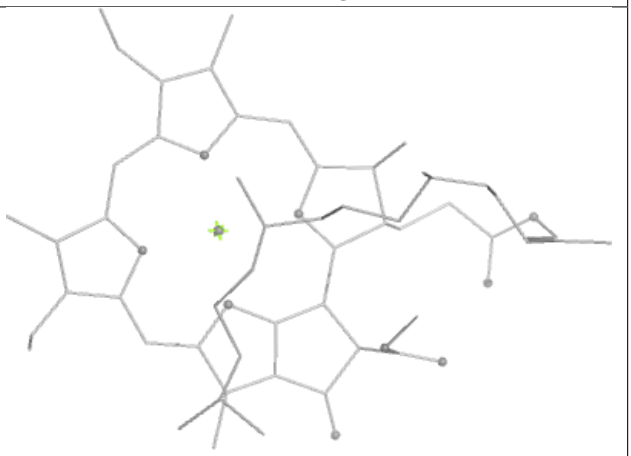
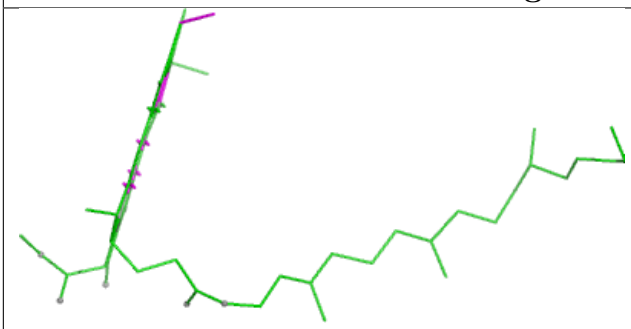


Rings

Ligand CLA B 606



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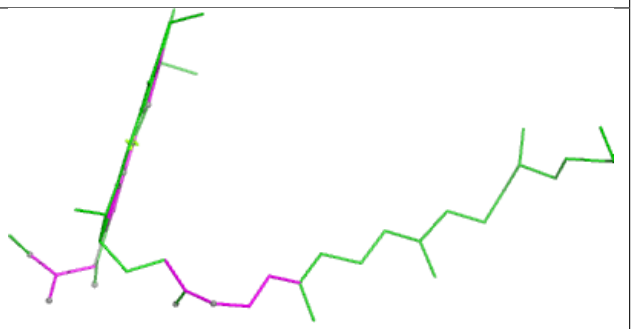
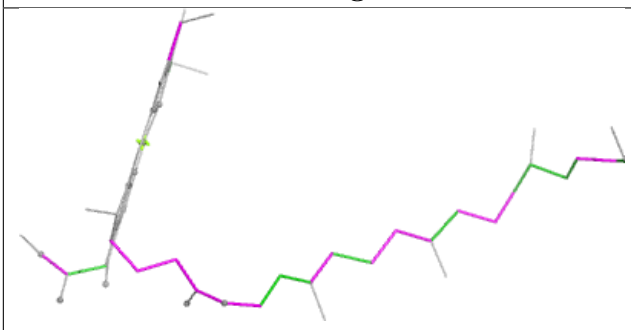


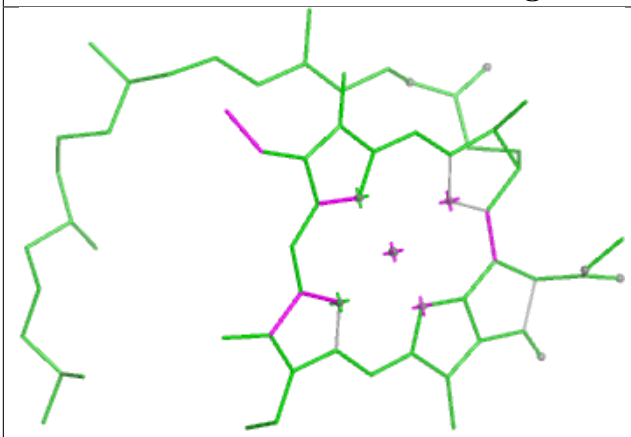
Bond angles



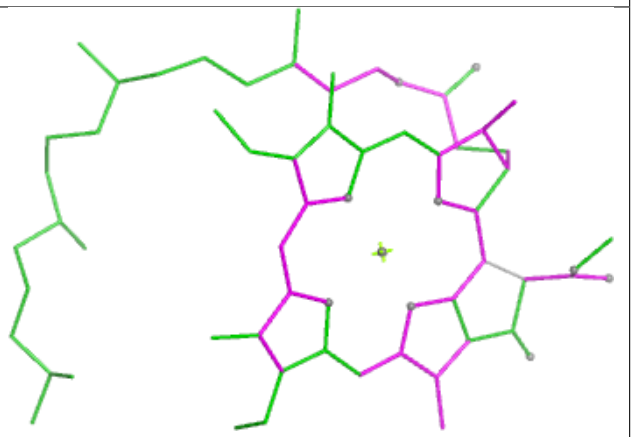
Torsions

Rings

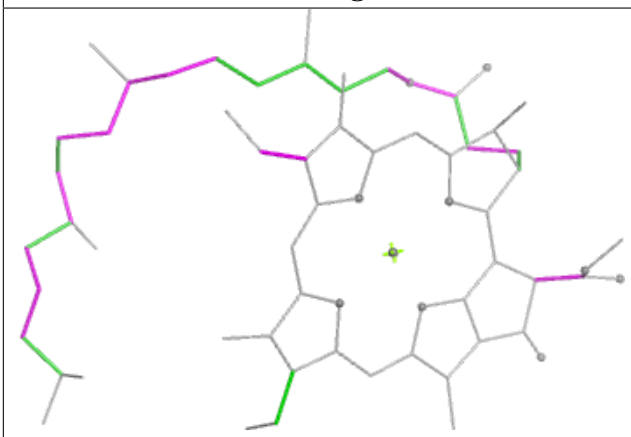
Ligand CLA Y 602



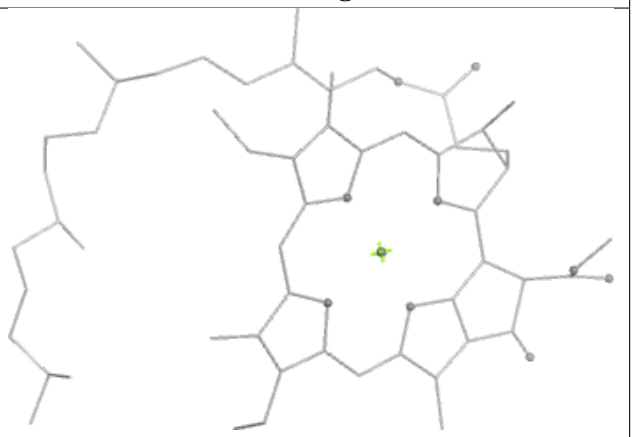
Bond lengths



Bond angles

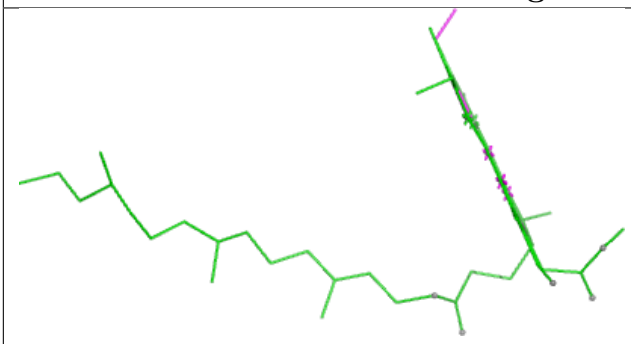


Torsions



Rings

Ligand CLA b 606



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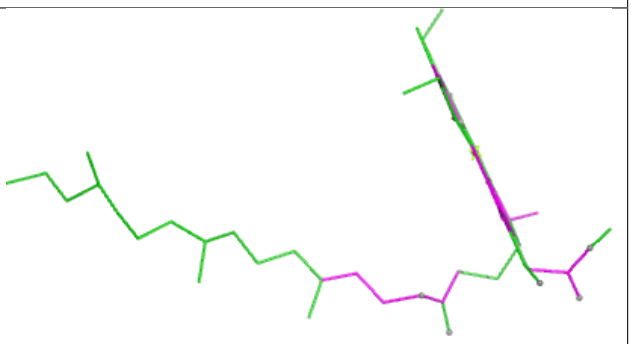
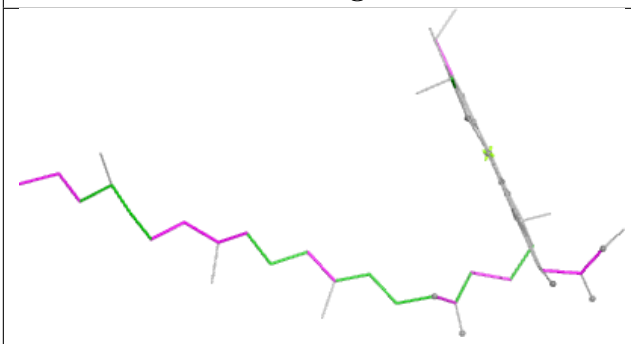


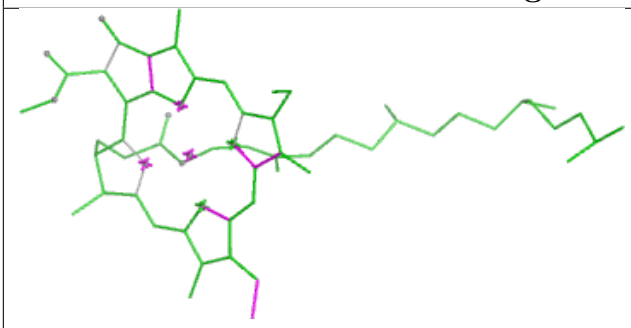
Bond angles



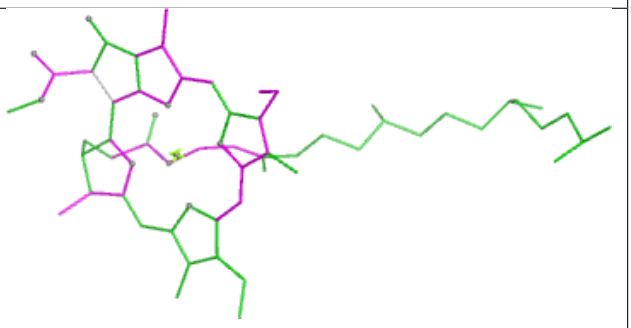
Torsions

Rings

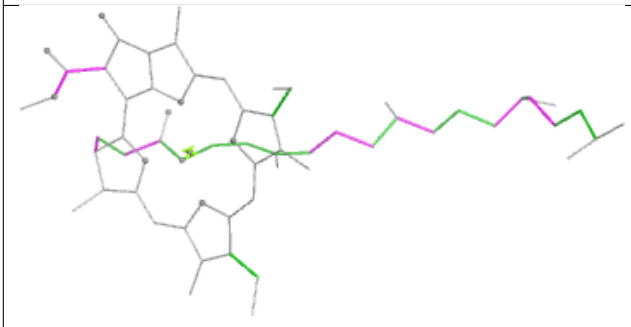
Ligand CLA B 609



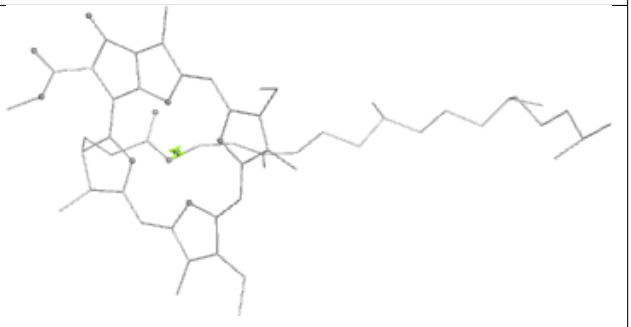
Bond lengths



Bond angles

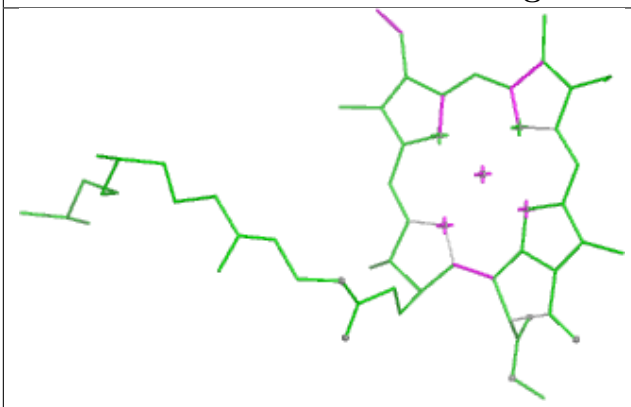


Torsions



Rings

Ligand CLA A 410



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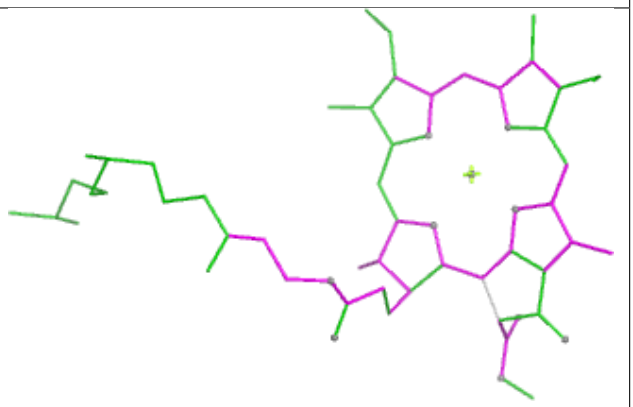
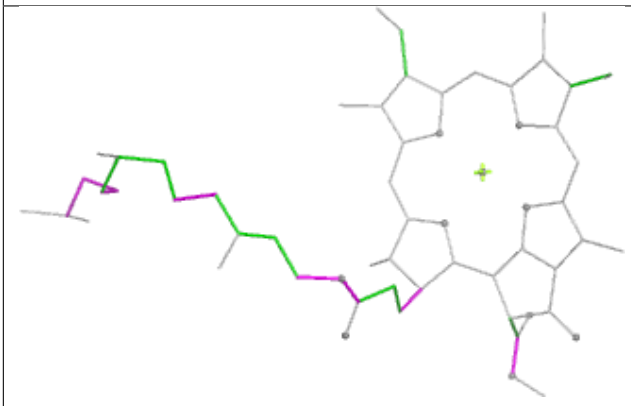


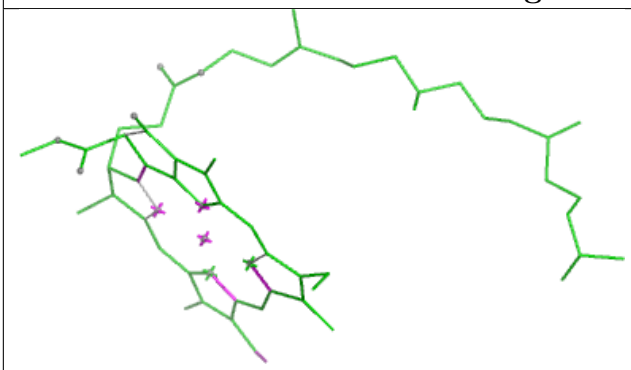
Bond angles



Torsions

Rings

Ligand CLA C 508



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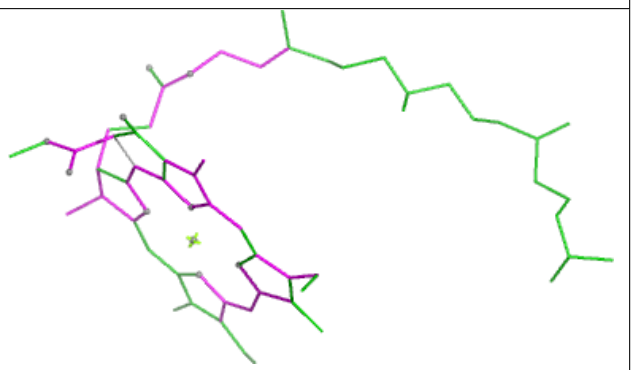
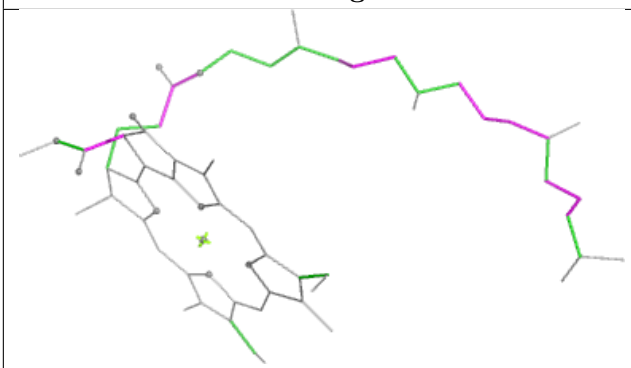
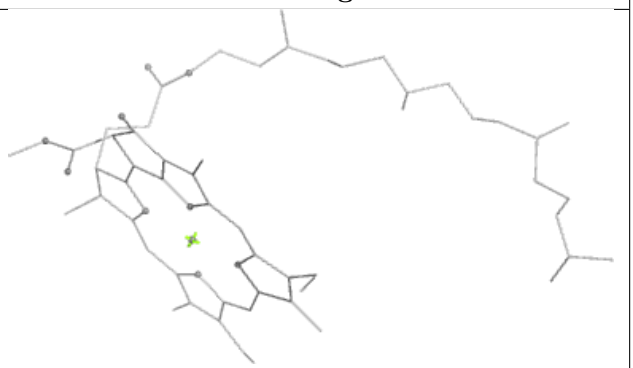


Bond angles

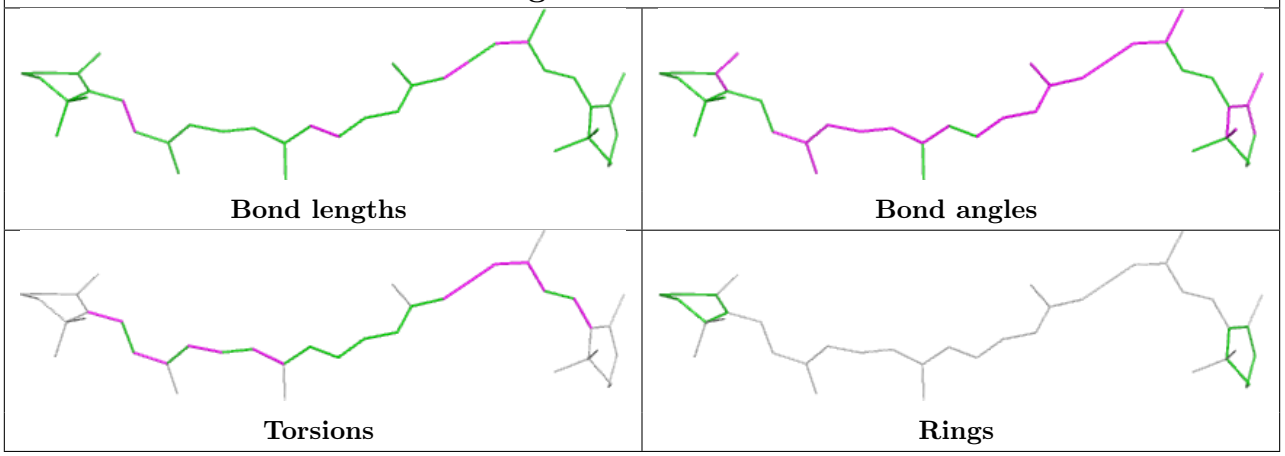


Torsions

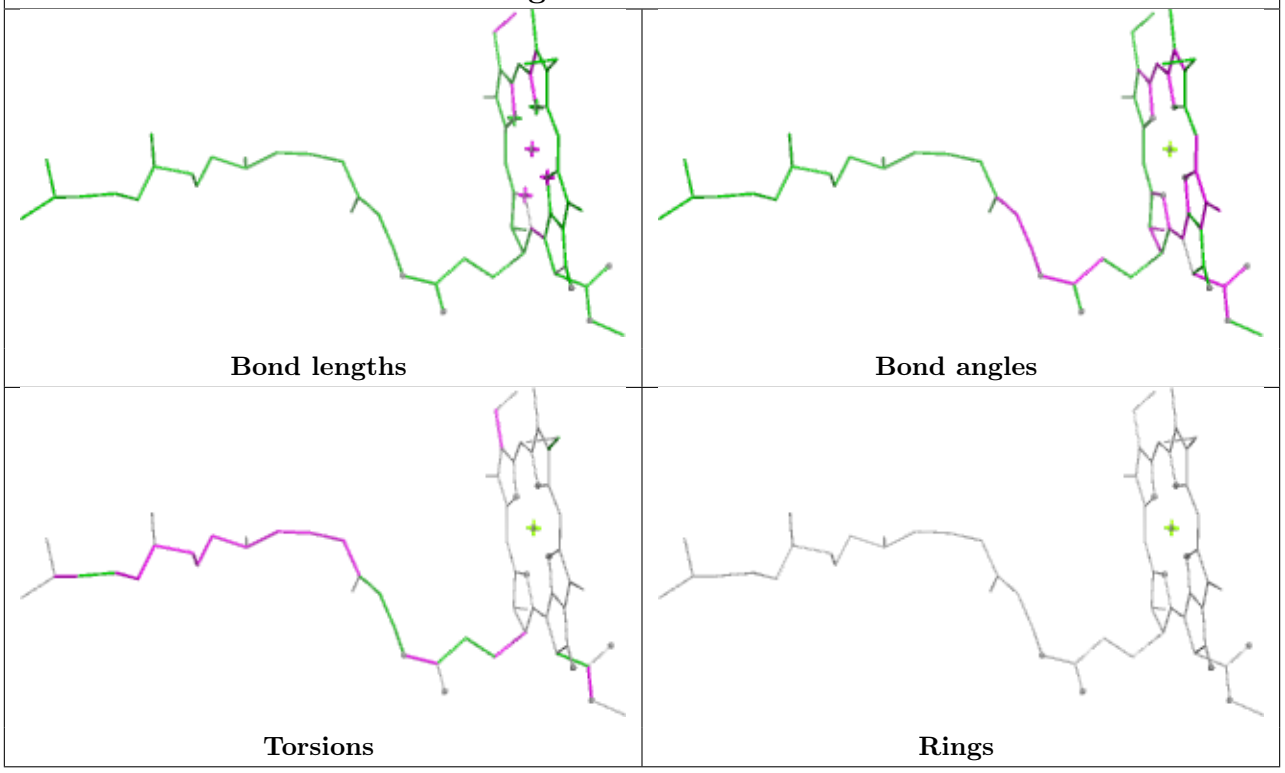


Rings

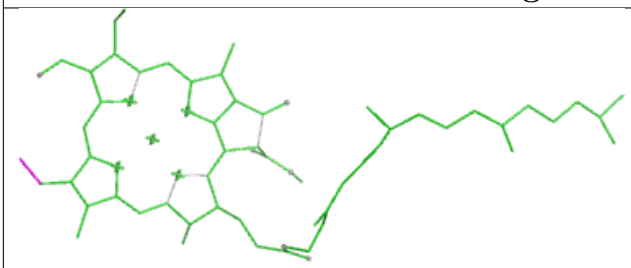
Ligand BCR c 516



Ligand CLA d 403



Ligand CHL N 605



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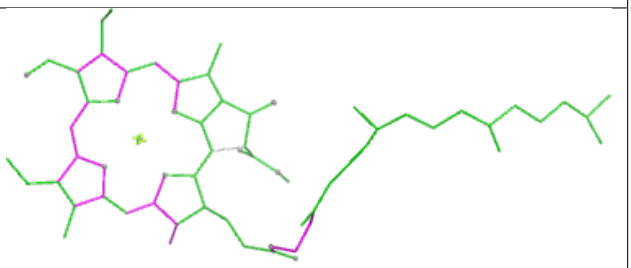
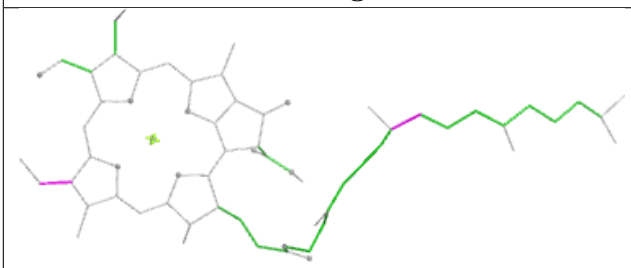
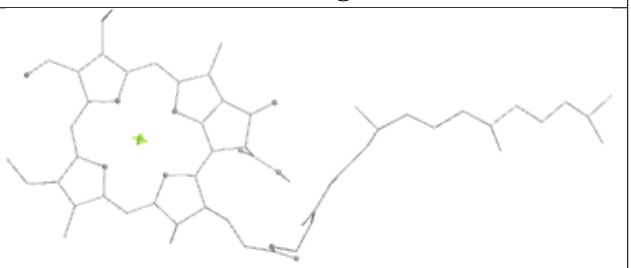


Bond angles

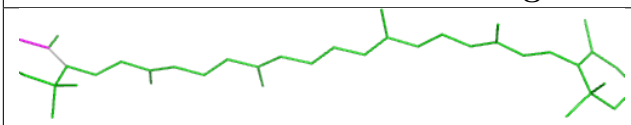


Torsions



Rings

Ligand LUT G 620



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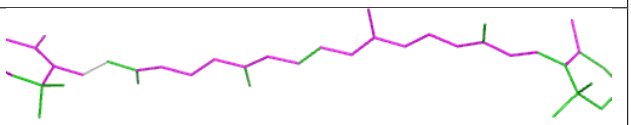
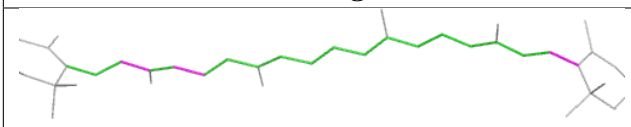


Bond angles



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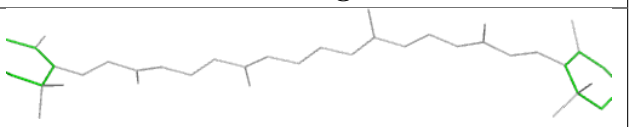
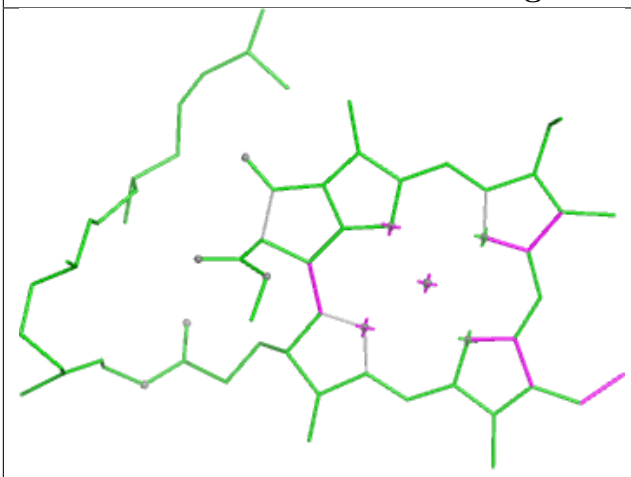


Rings

Ligand CLA B 611



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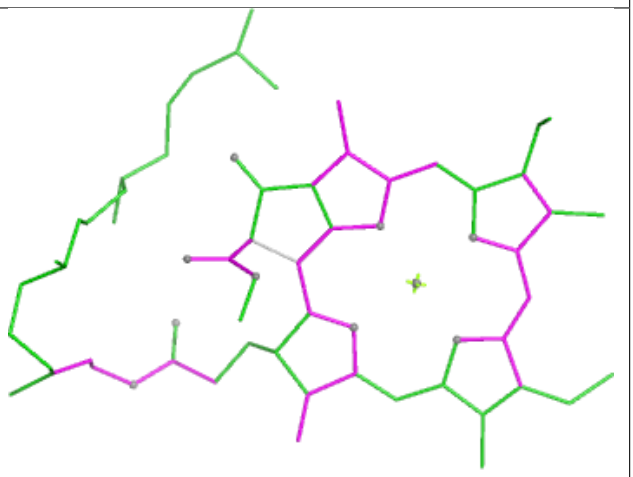
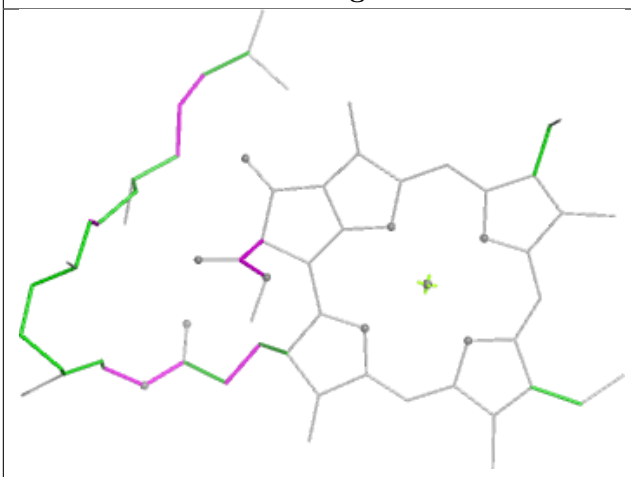
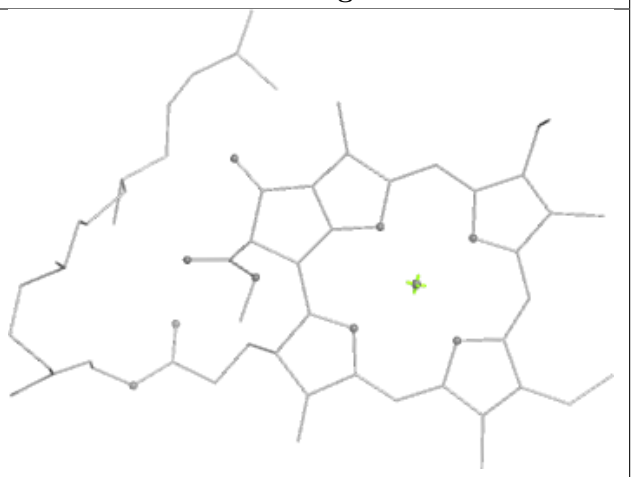


Bond angles

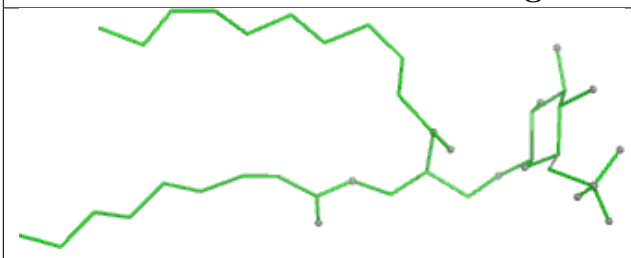


Torsions

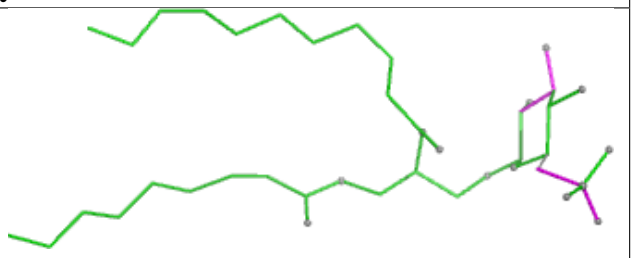


Rings

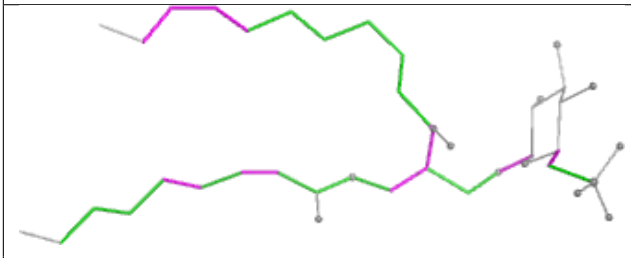
Ligand SQD B 621



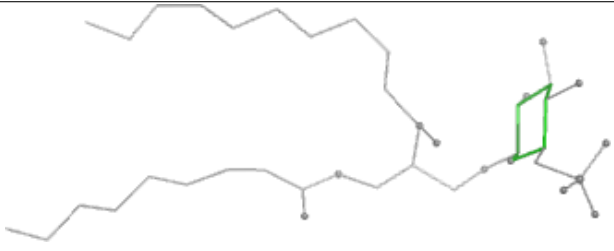
Bond lengths



Bond angles

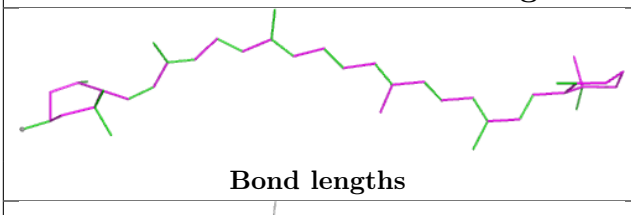


Torsions



Rings

Ligand RRX H 101



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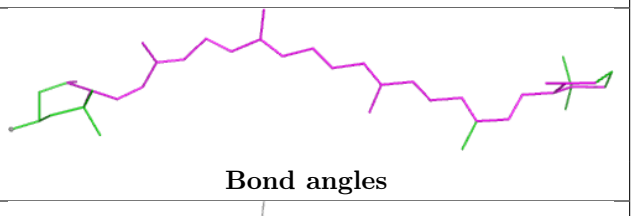
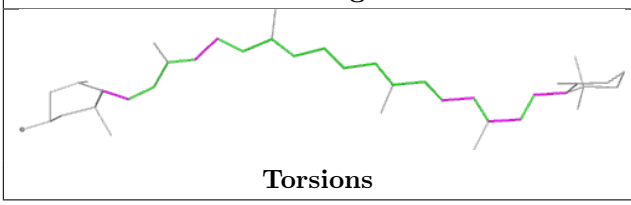
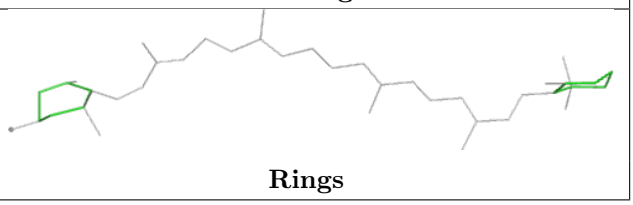


Bond angles

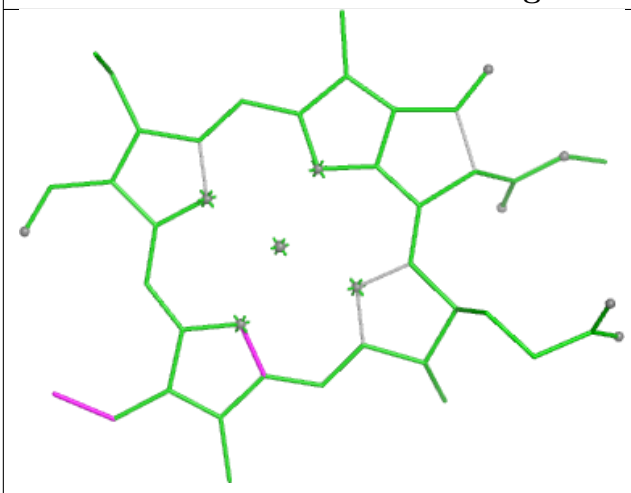


Torsions



Rings

Ligand CHL Y 605



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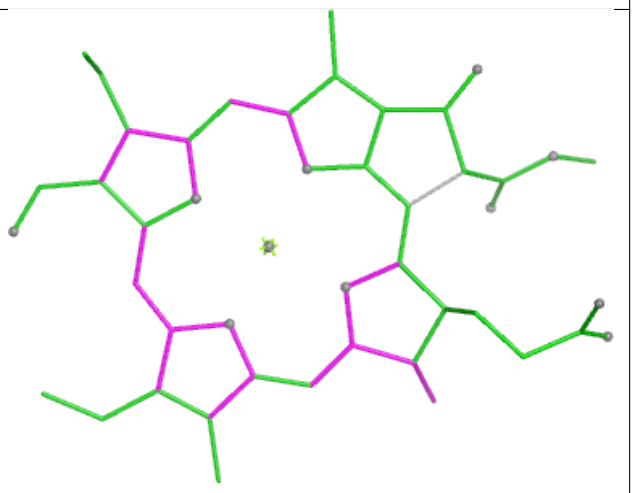
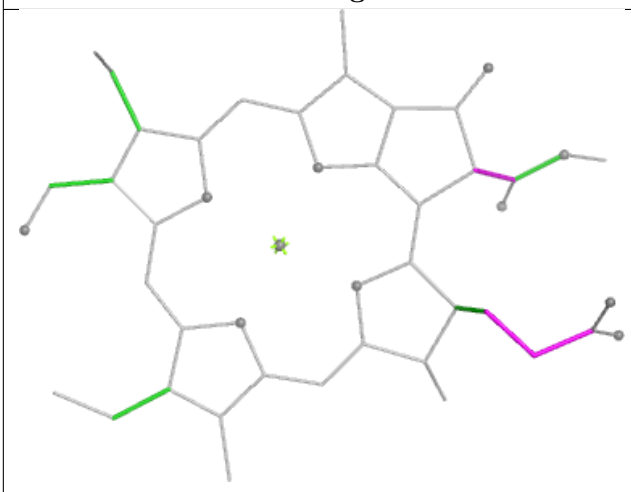
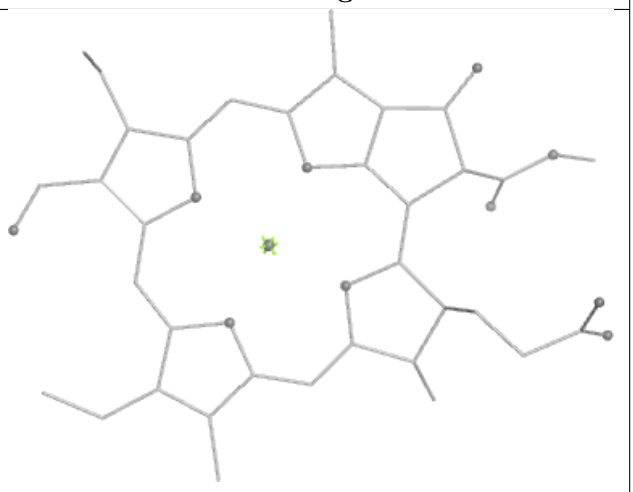


Bond angles

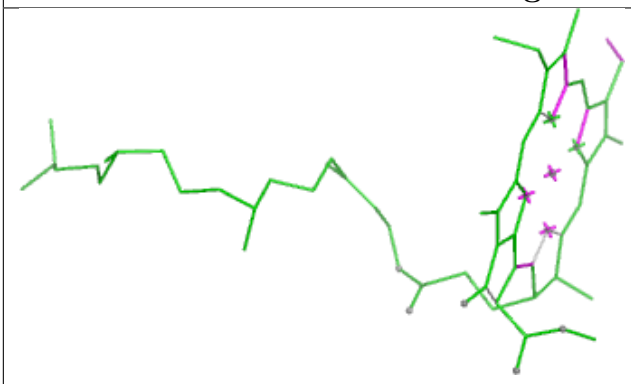


Torsions



Rings

Ligand CLA Y 604



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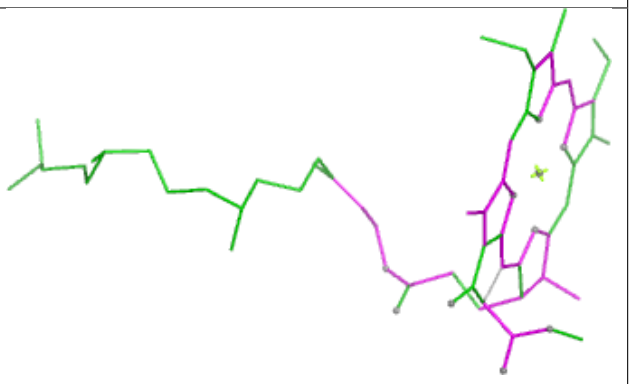
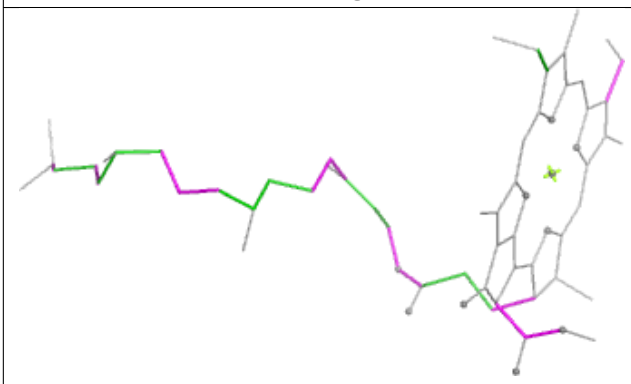


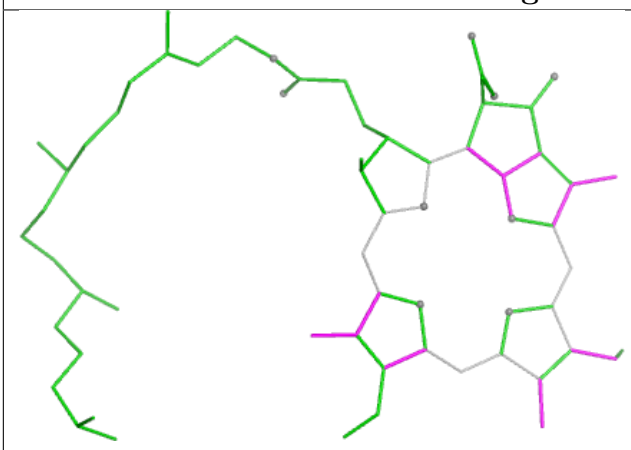
Bond angles



Torsions

Rings

Ligand PHO A 408



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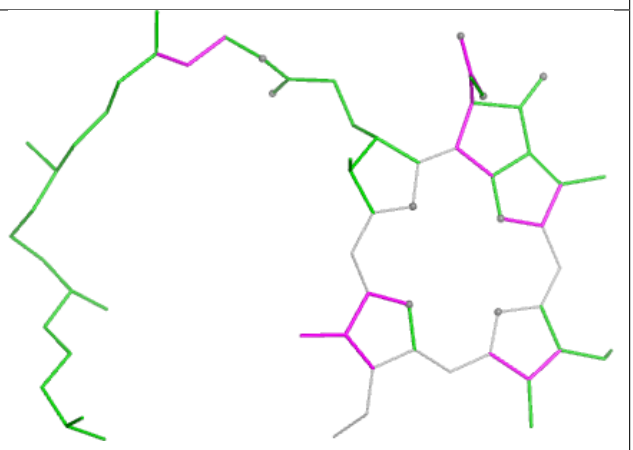
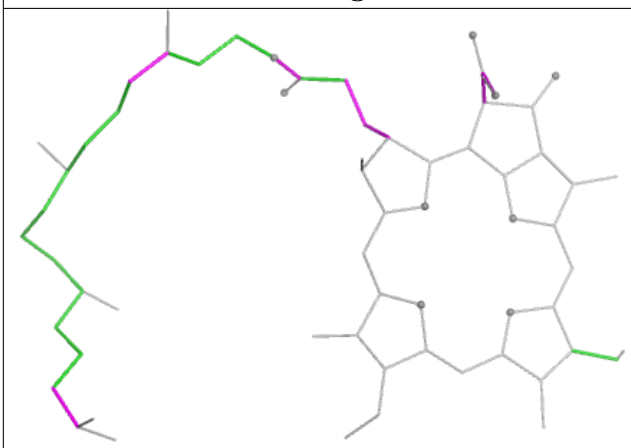
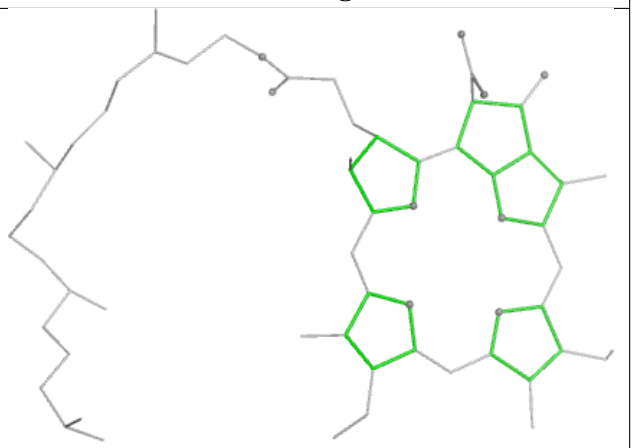


Bond angles

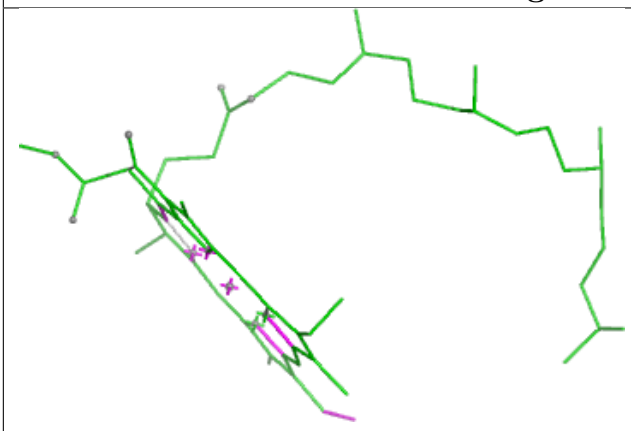


Torsions

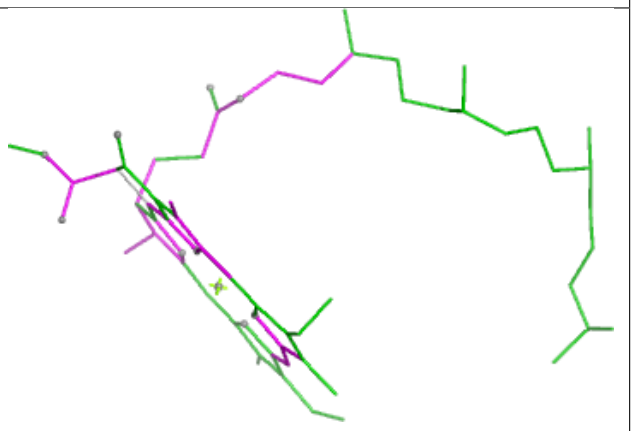


Rings

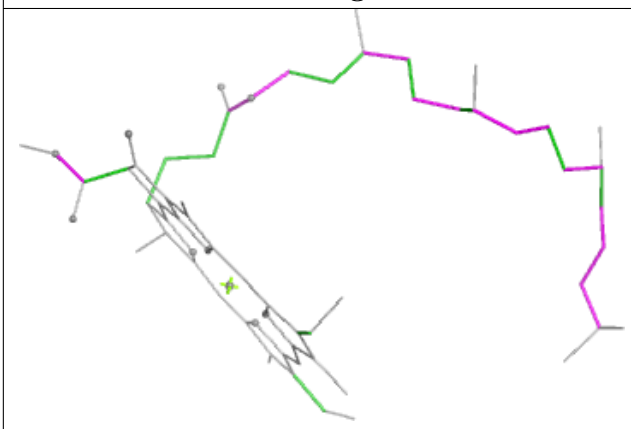
Ligand CLA b 612



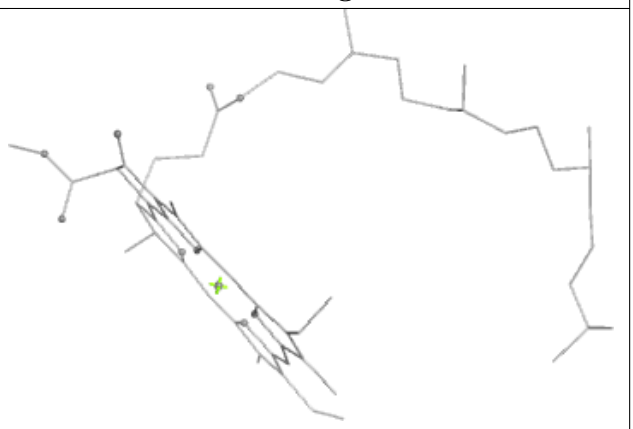
Bond lengths



Bond angles

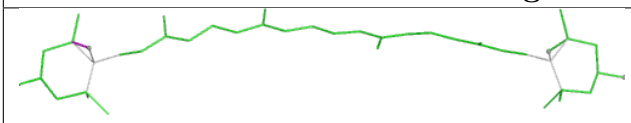


Torsions



Rings

Ligand XAT Y 622



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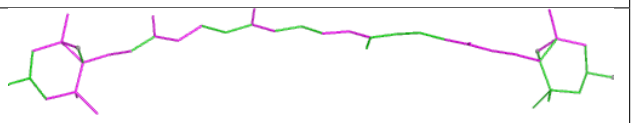
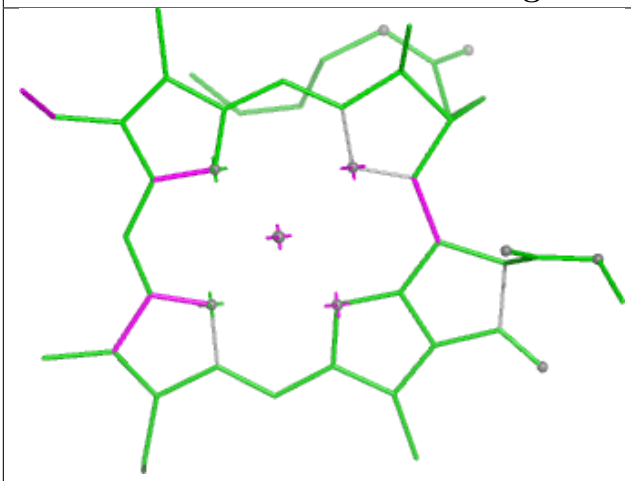


Bond angles

Torsions

Rings

Ligand CLA G 614



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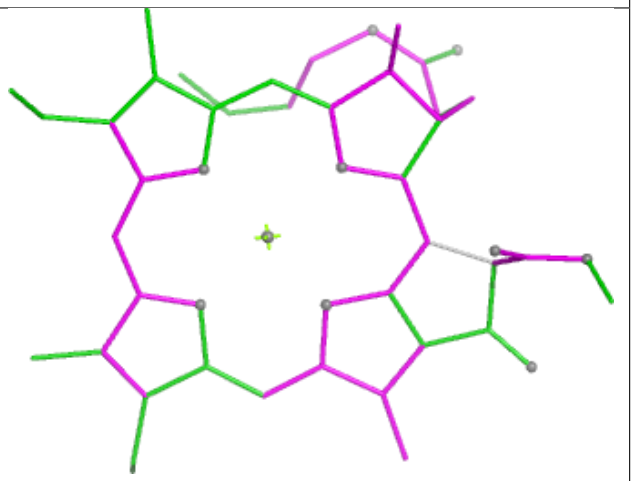
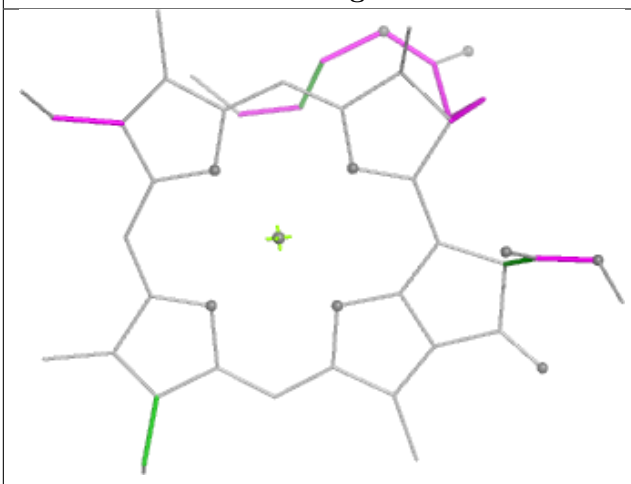


Bond angles



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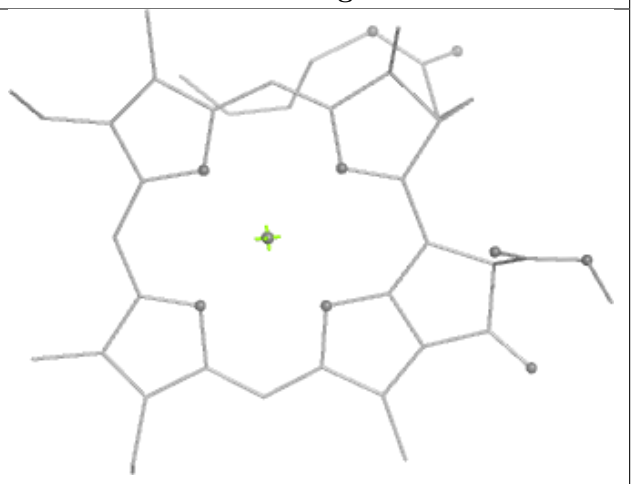

Rings

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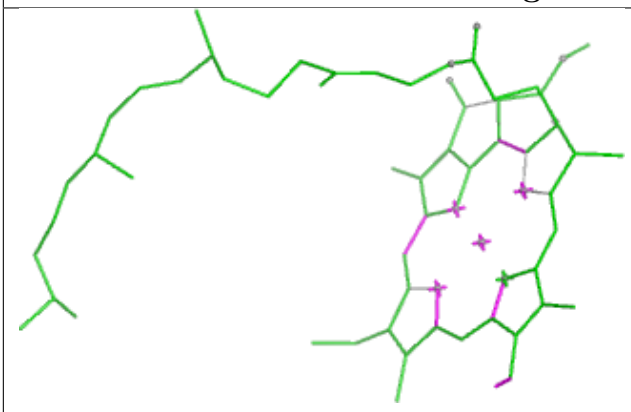

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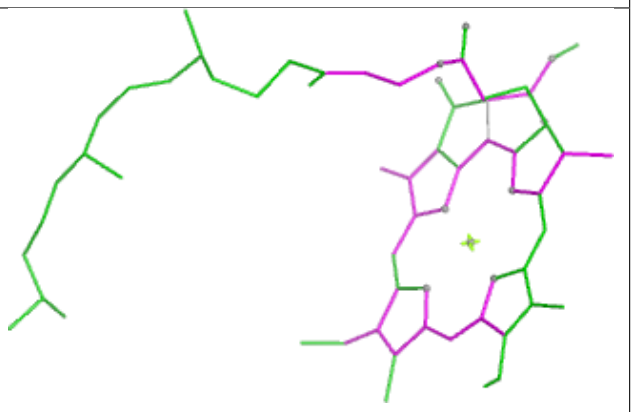
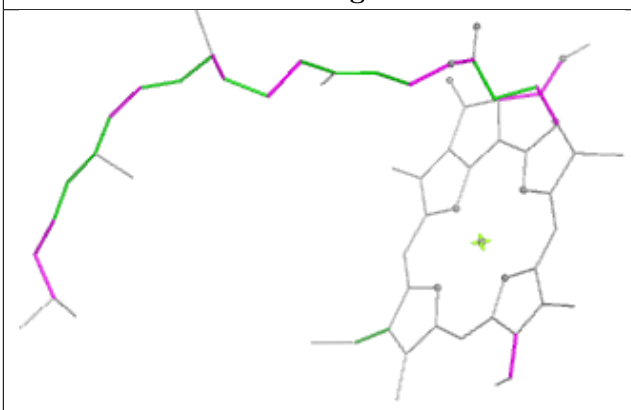


Bond angles



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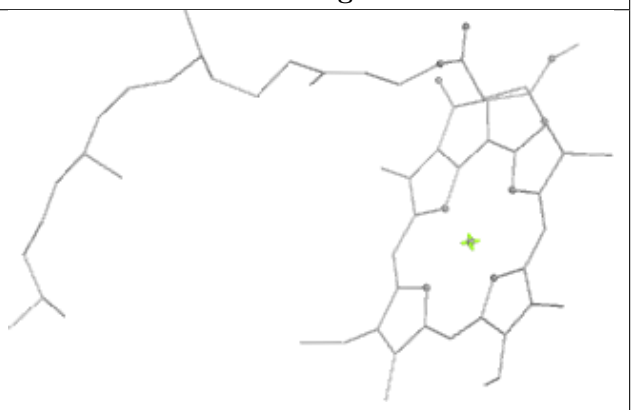
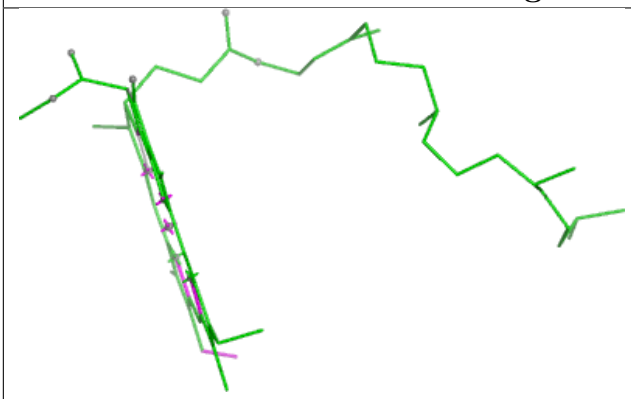


Rings

Ligand CLA C 506



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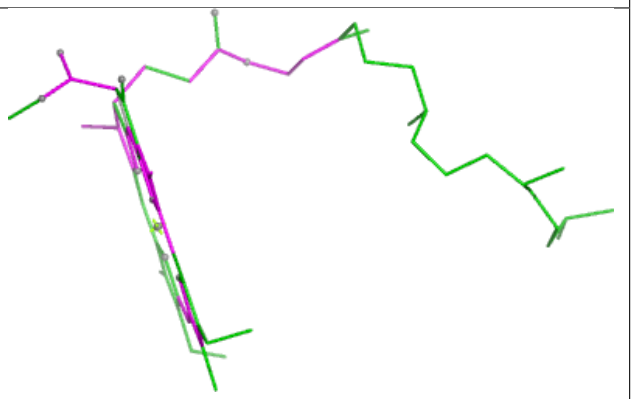

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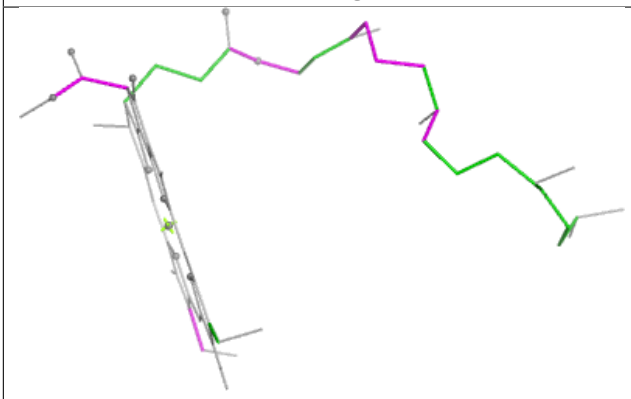

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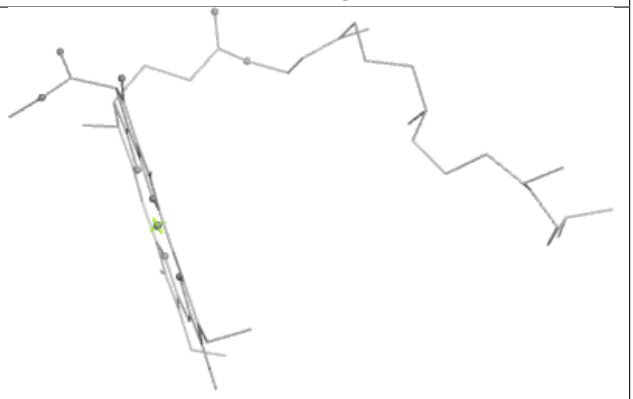
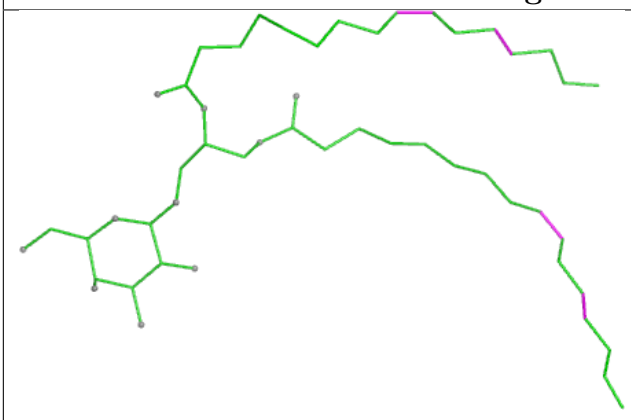


Rings

Ligand LMG c 521



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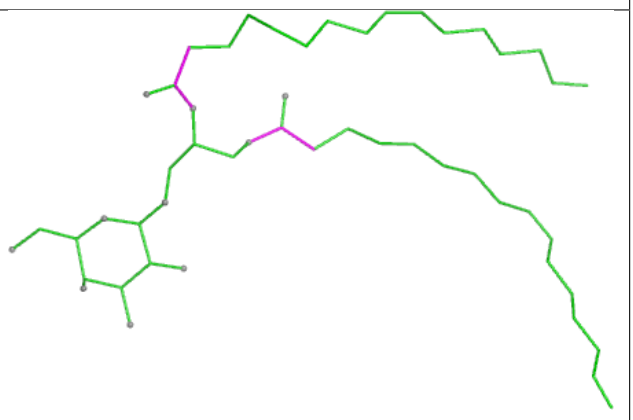

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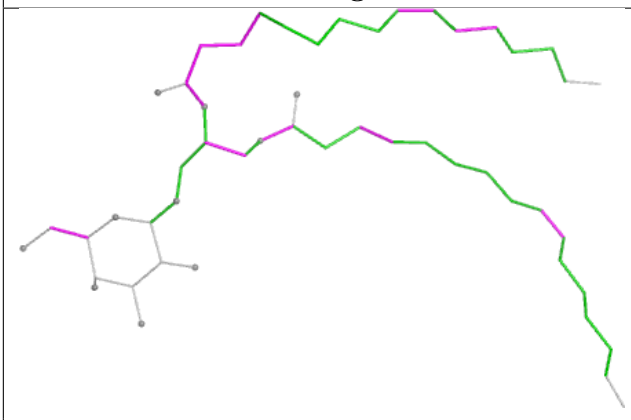

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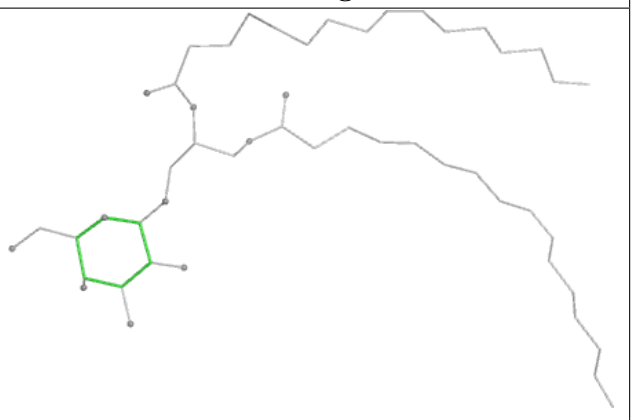
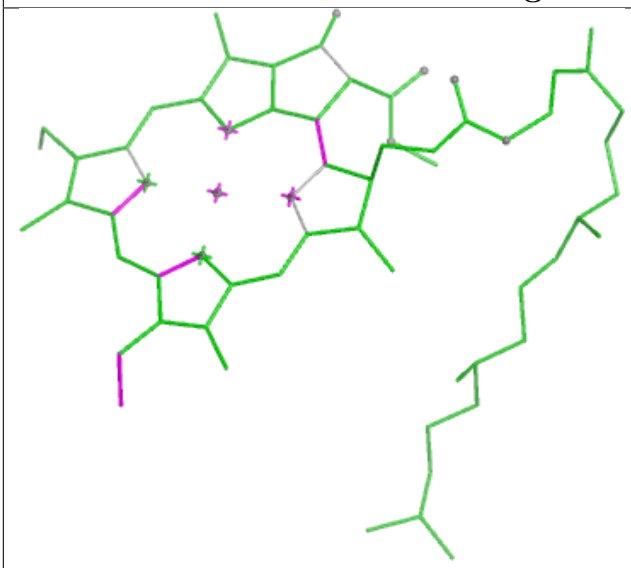


Rings

Ligand CLA B 617



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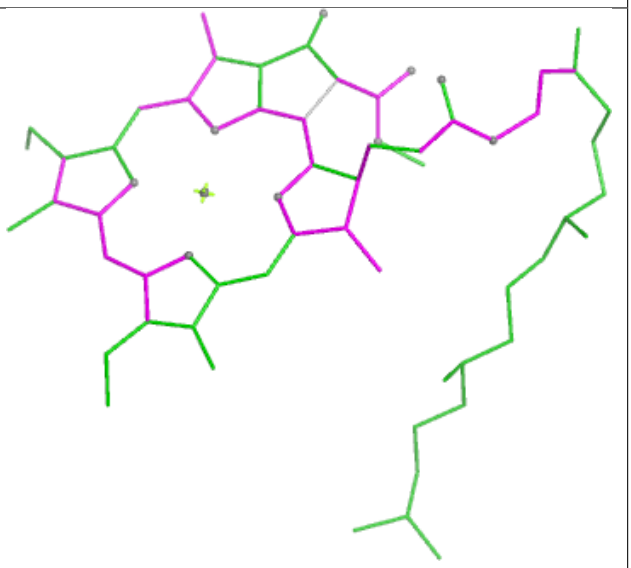
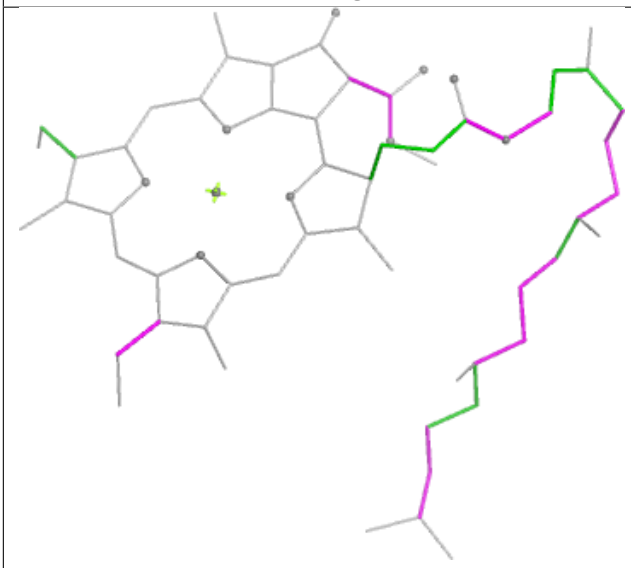


Bond angles



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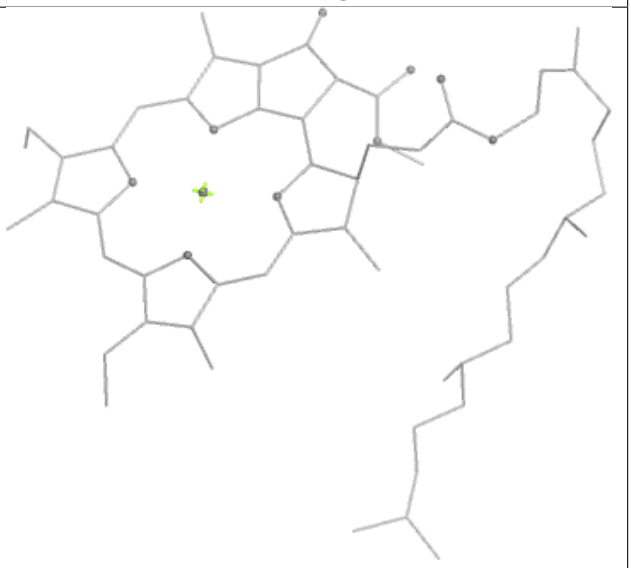
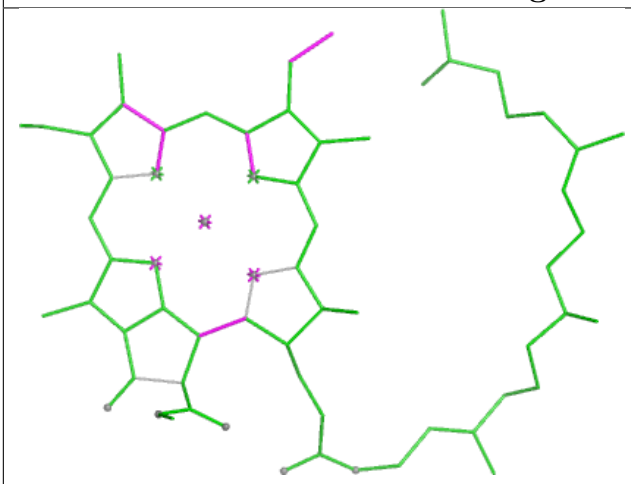


Rings

Ligand CLA c 512



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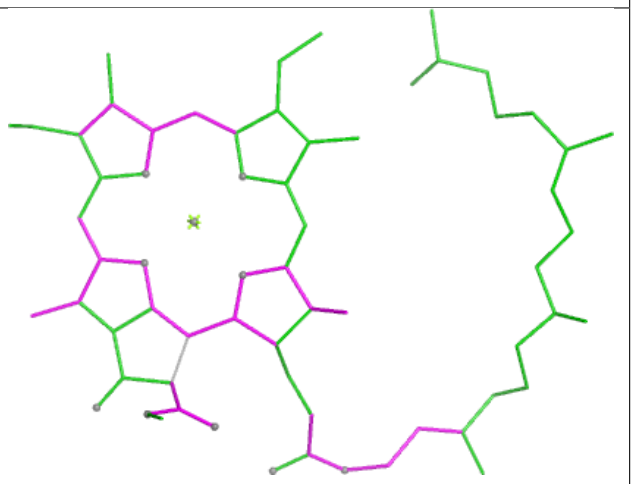
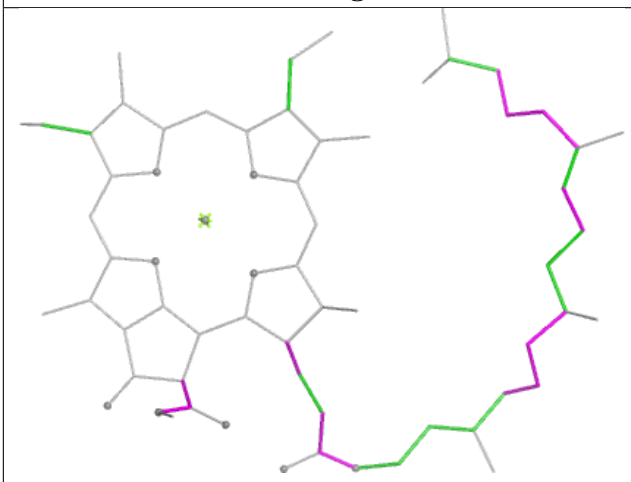


Bond angles



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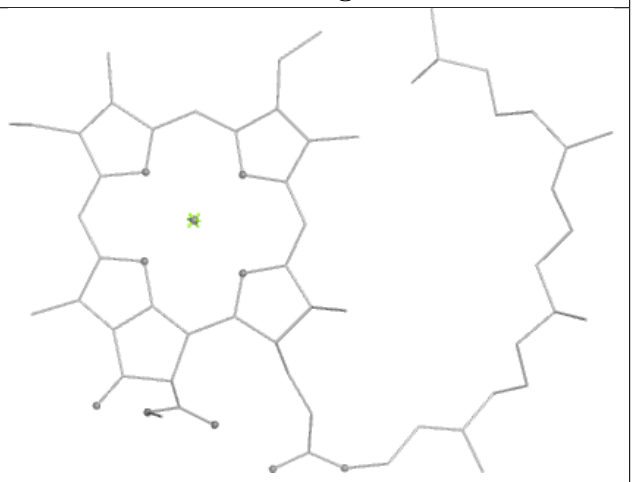
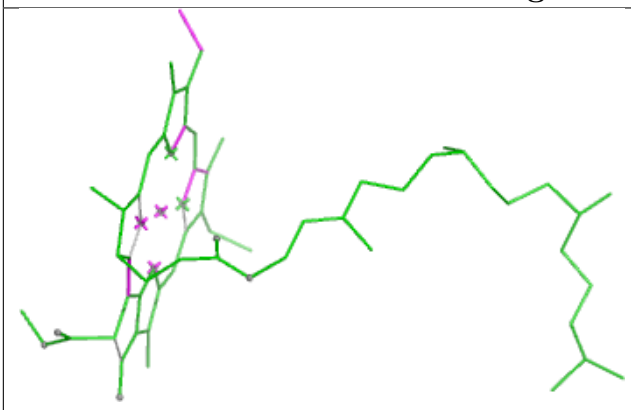


Rings

Ligand CLA b 608



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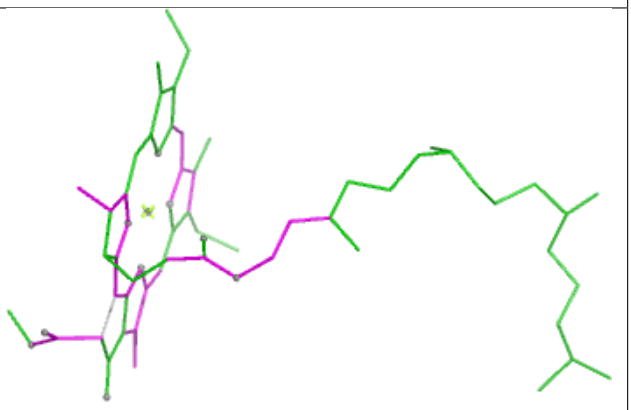

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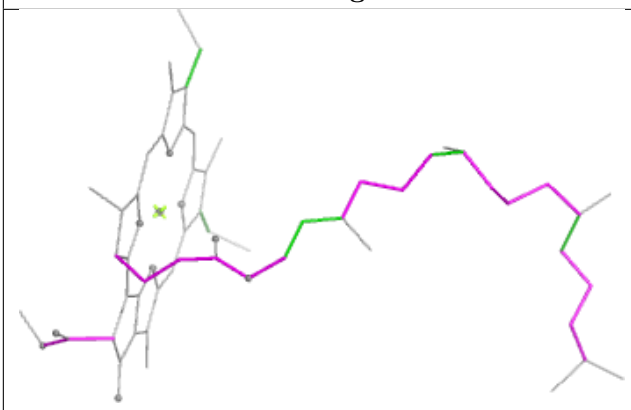
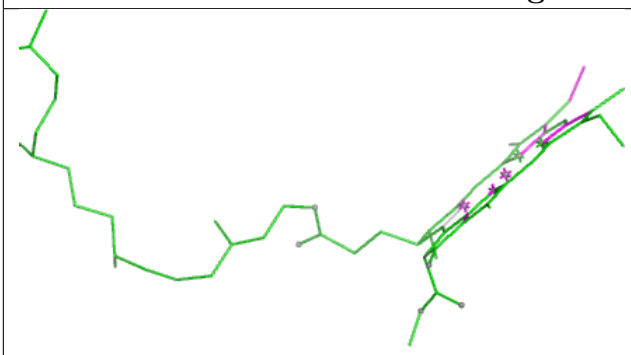


Torsions

Rings

Ligand CLA d 402



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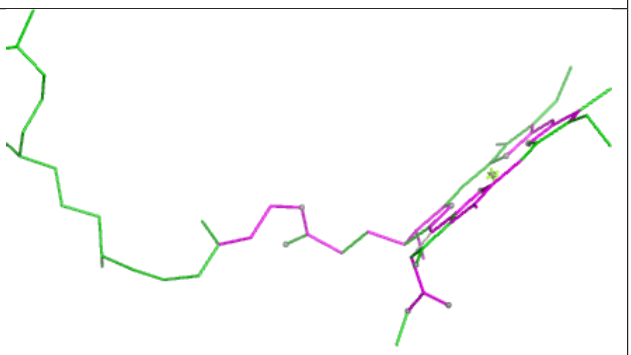

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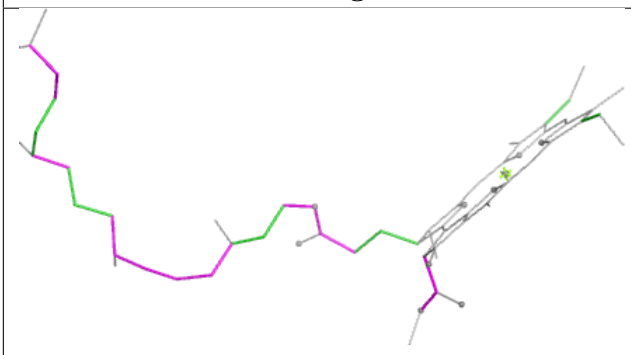

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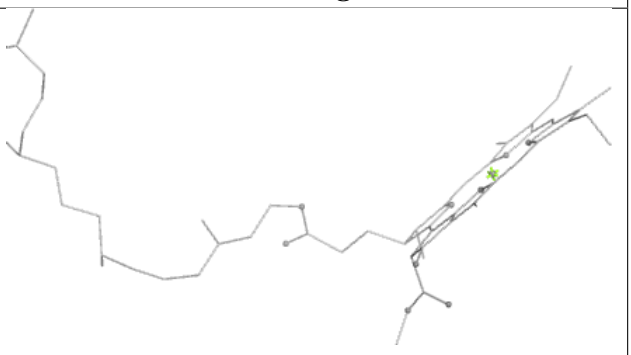
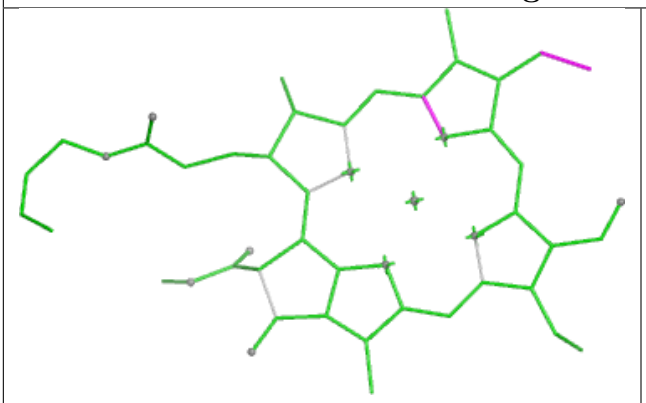


Rings

Ligand CHL G 606



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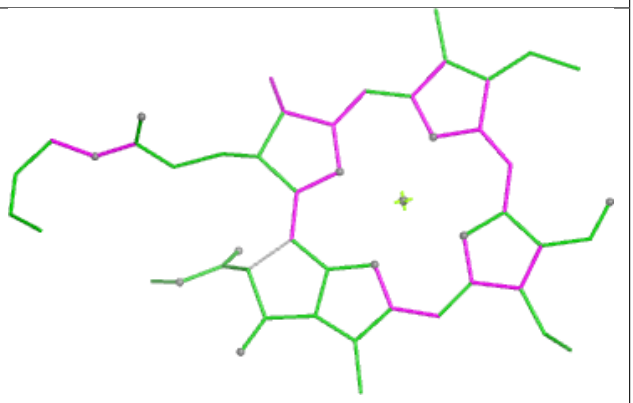
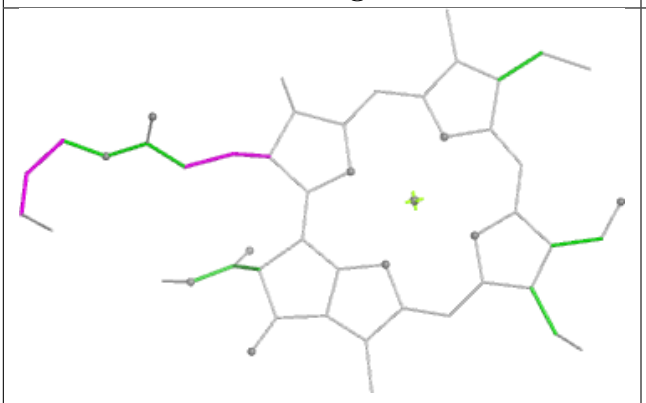


Bond angles



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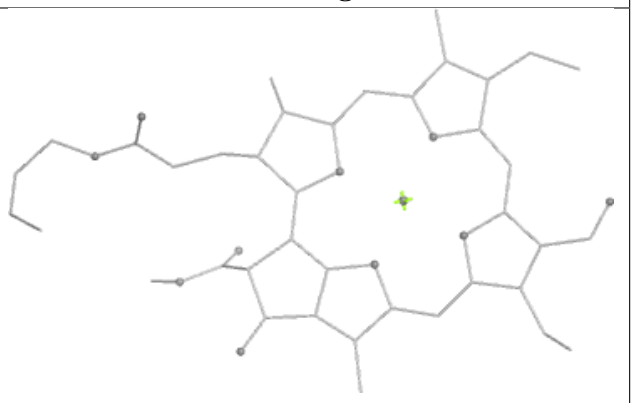
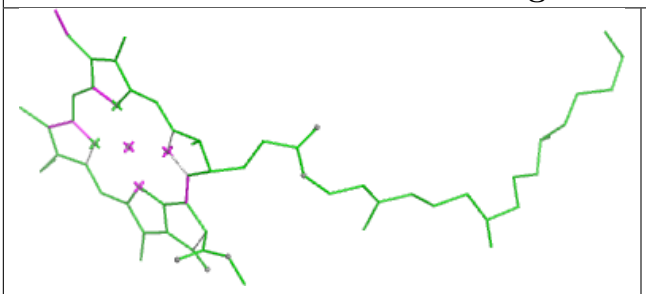


Rings

Ligand CLA a 405



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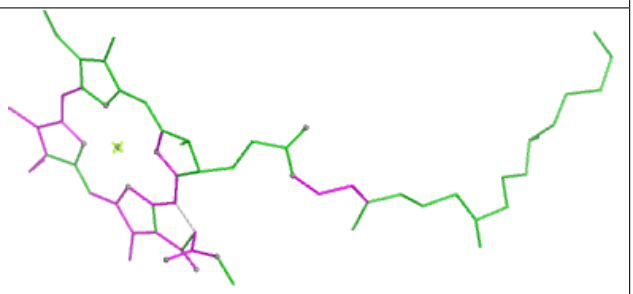
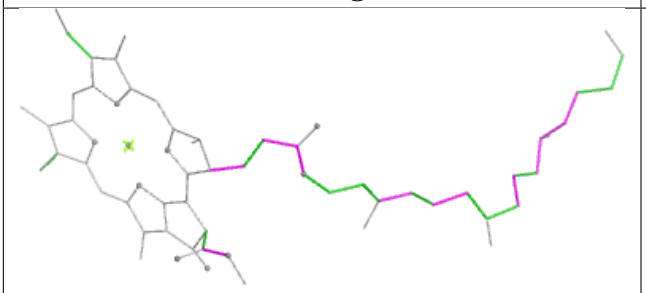


Bond angles



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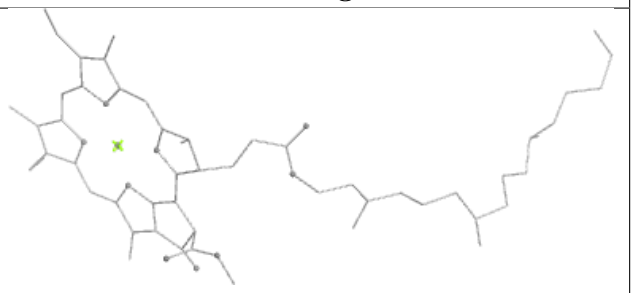
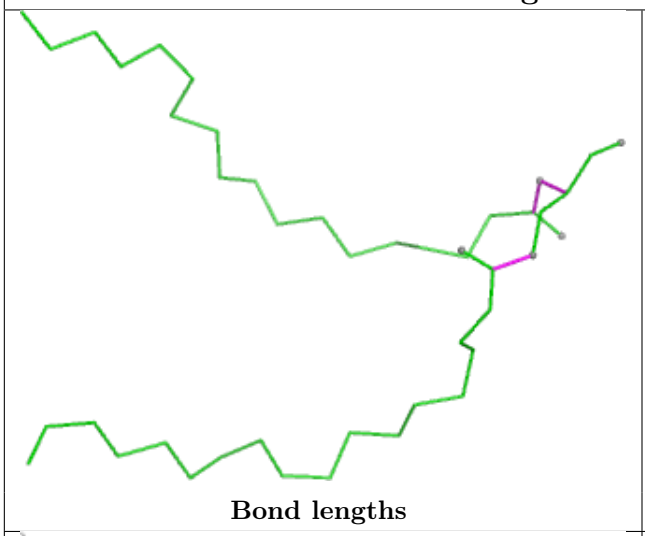


Rings

Ligand DGA C 524



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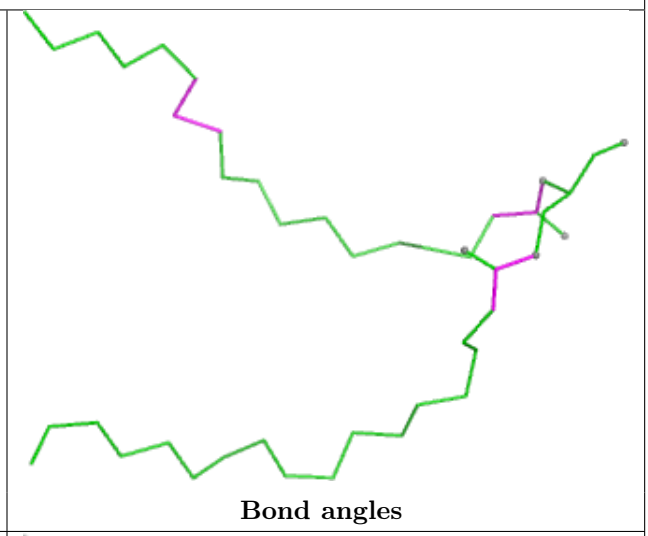
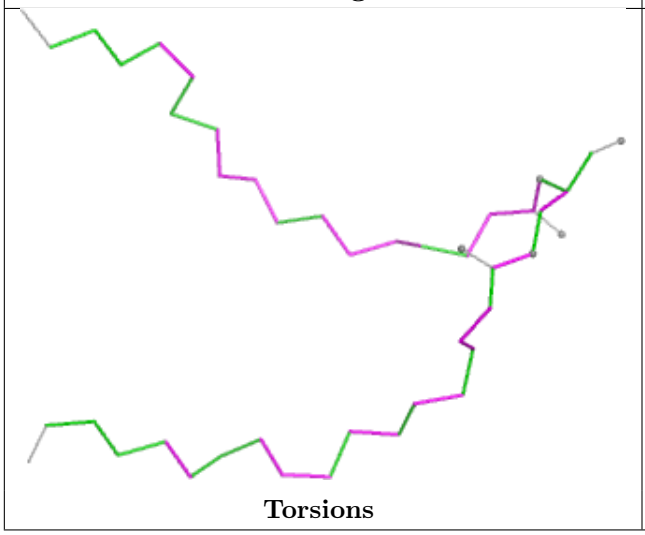


Bond angles



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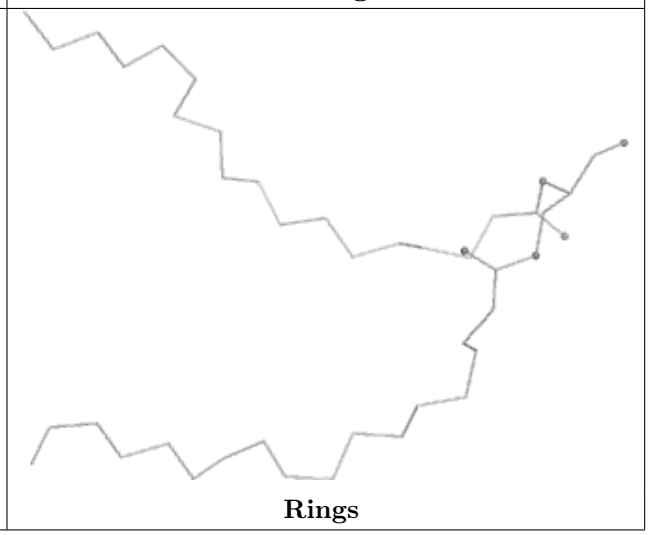
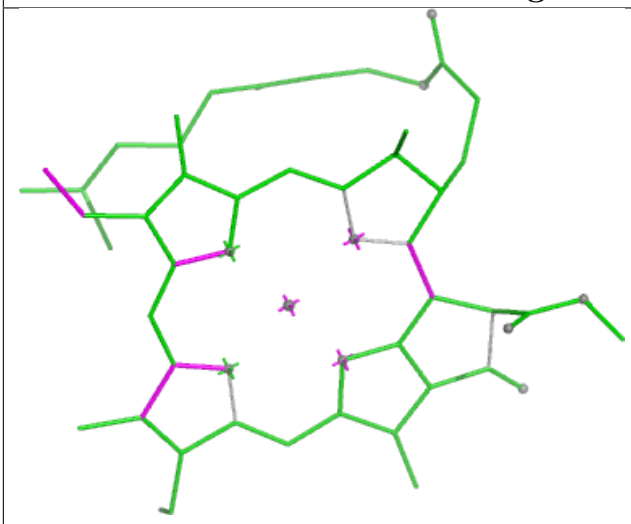


Rings

Ligand CLA S 614



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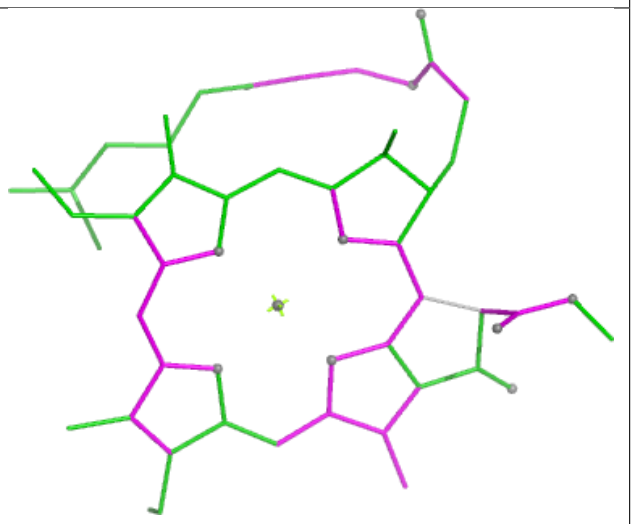
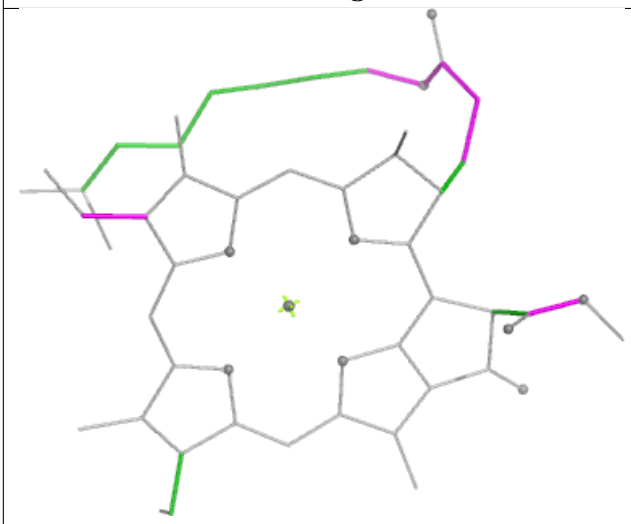


Bond angles



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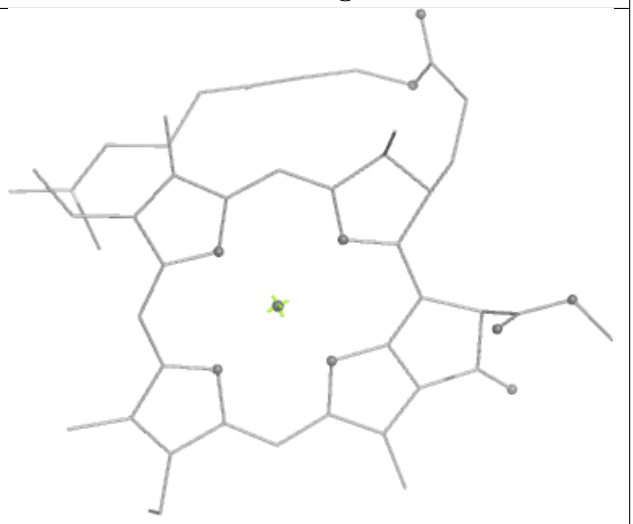
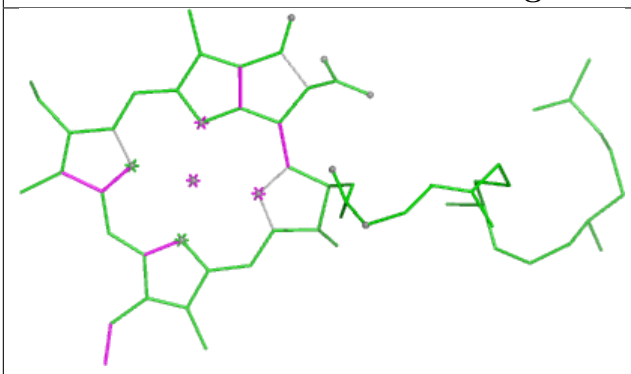


Rings

Ligand CLA B 613



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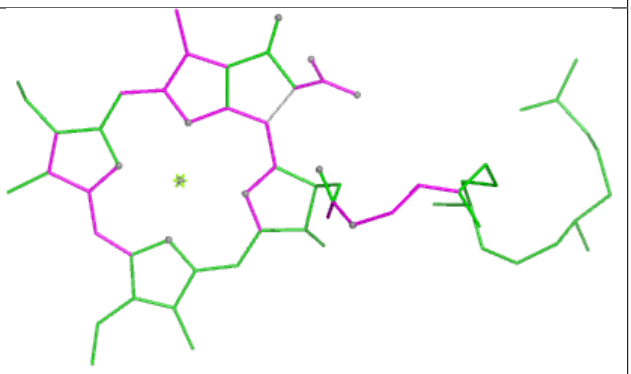
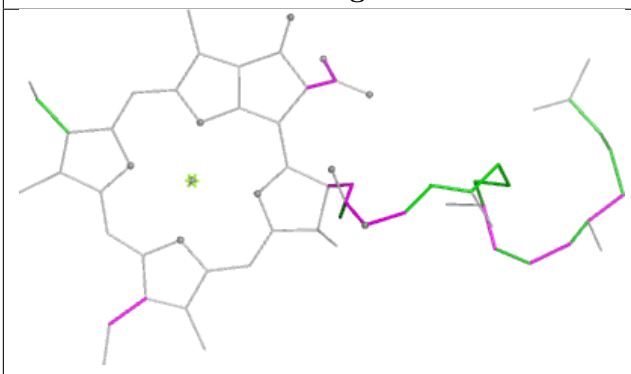
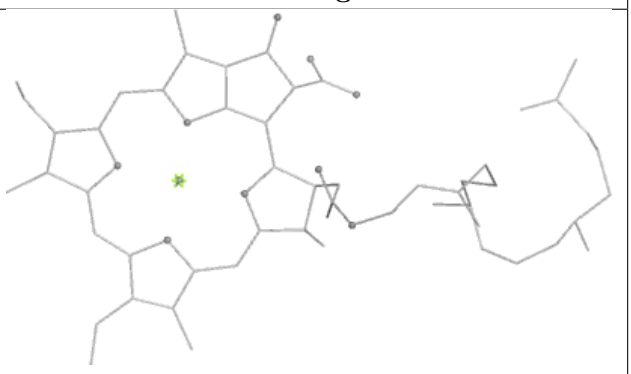


Bond angles

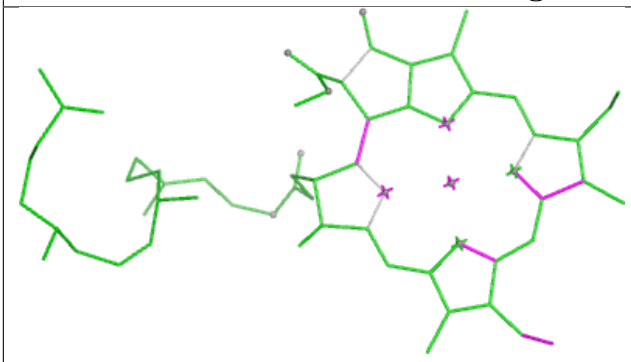


Torsions

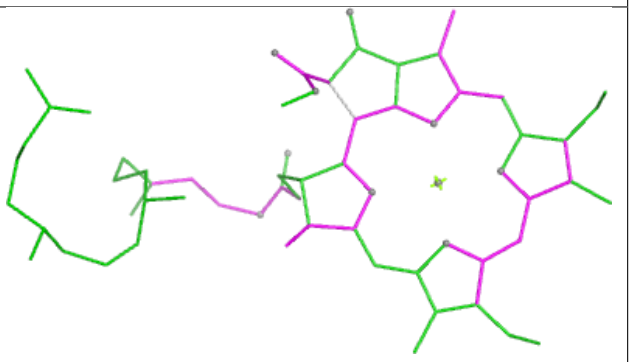


Rings

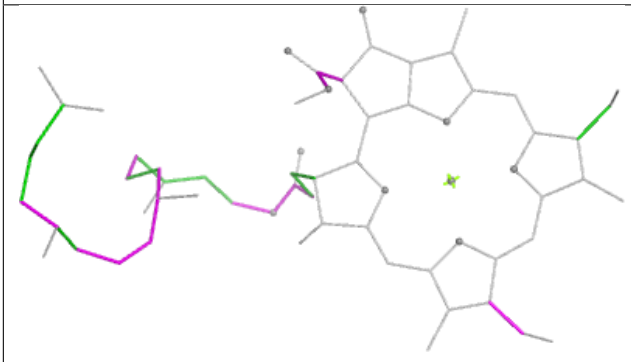
Ligand CLA b 613



Bond lengths



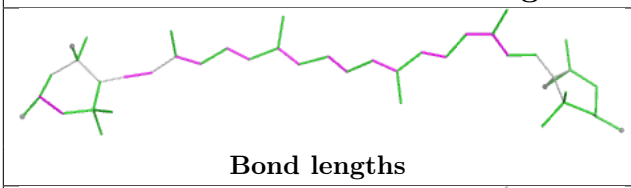
Bond angles



Torsions

Rings

Ligand NEX G 623



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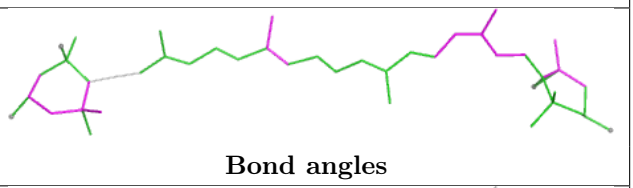
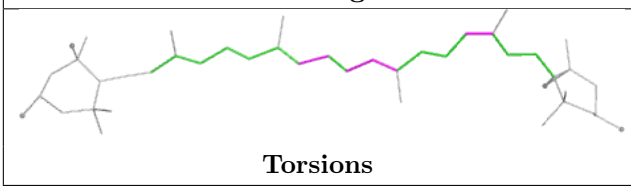
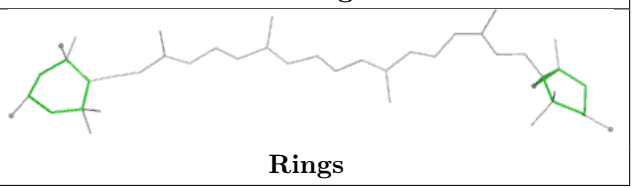


Bond angles

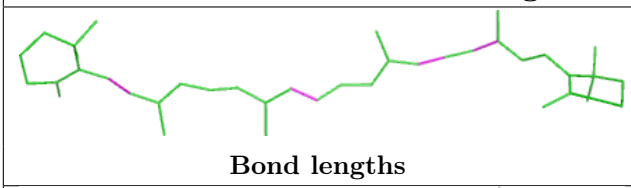


Torsions



Rings

Ligand BCR D 404



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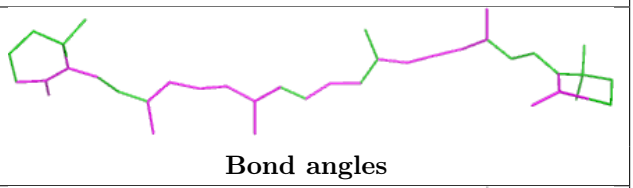
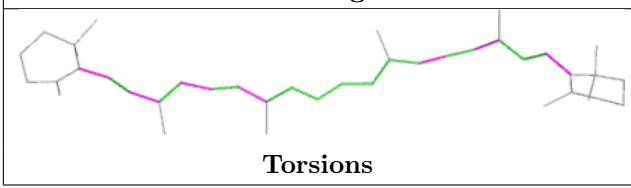
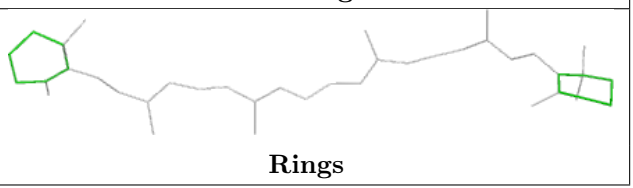


Bond angles

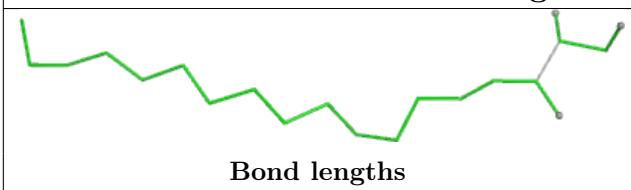


Torsions



Rings

Ligand SPH a 414



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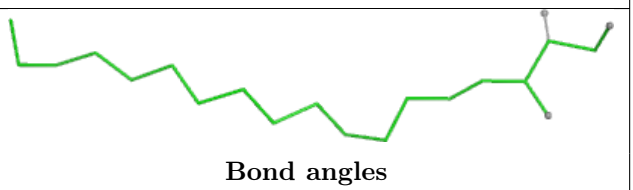
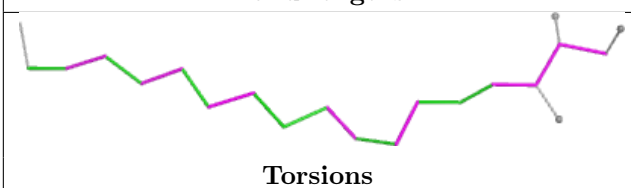


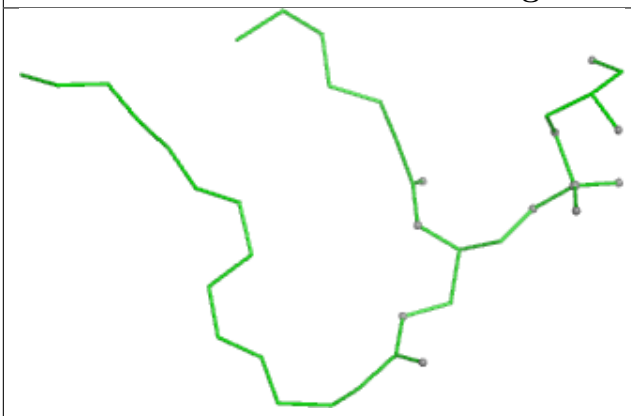
Bond angles



Torsions

Rings

Ligand LHG D 410



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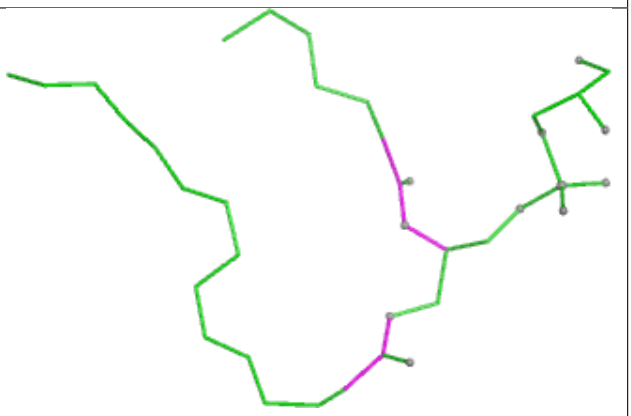
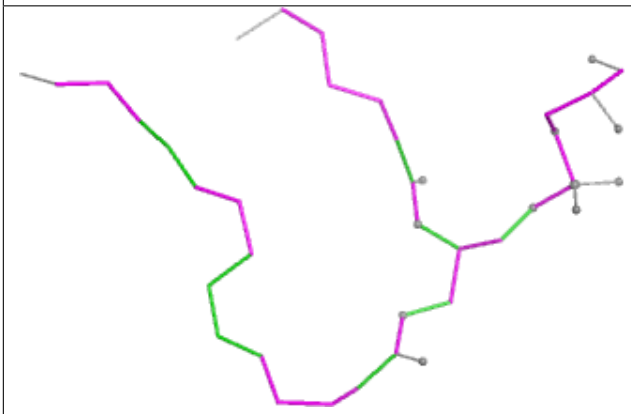
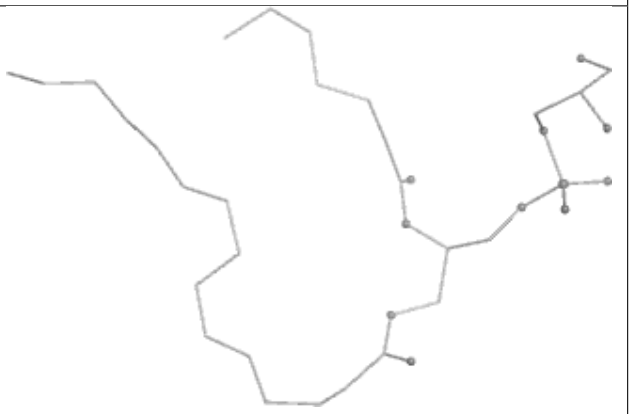


Bond angles

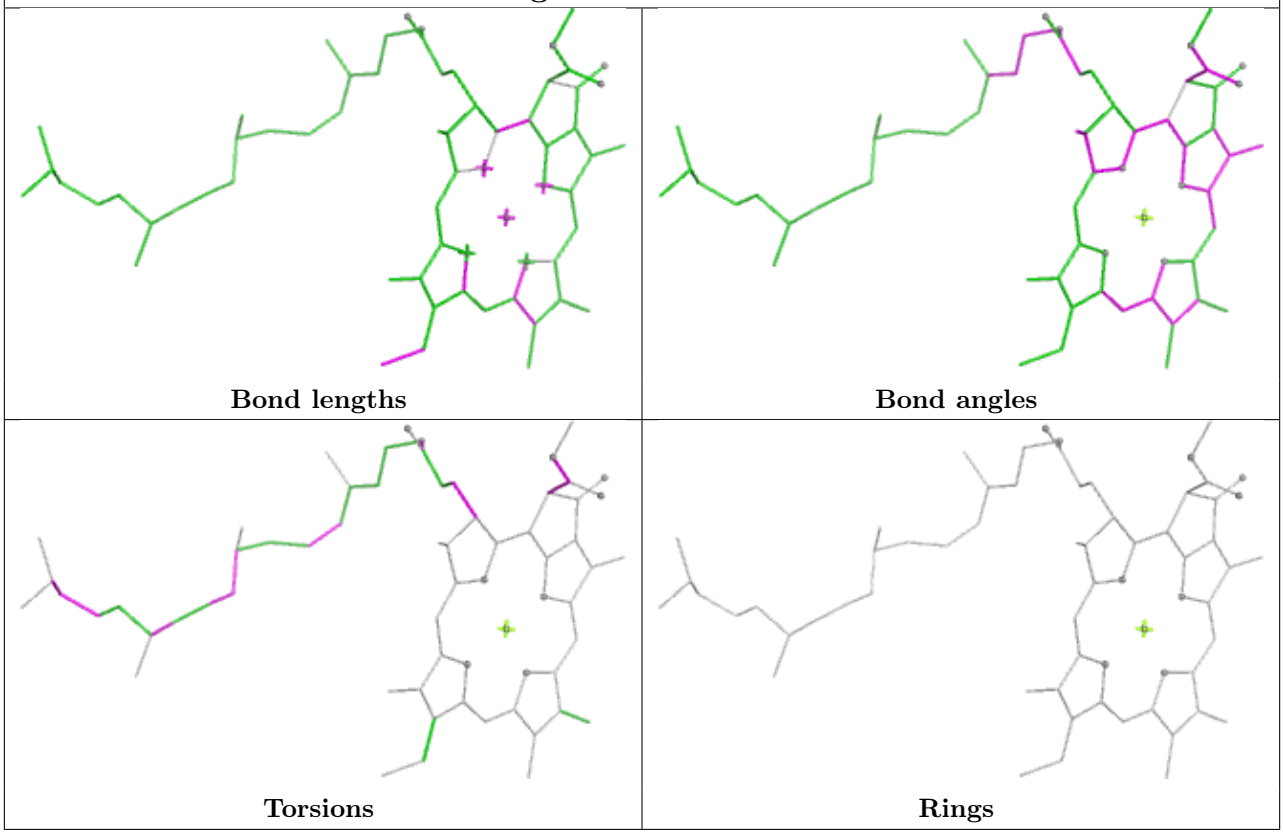


Torsions

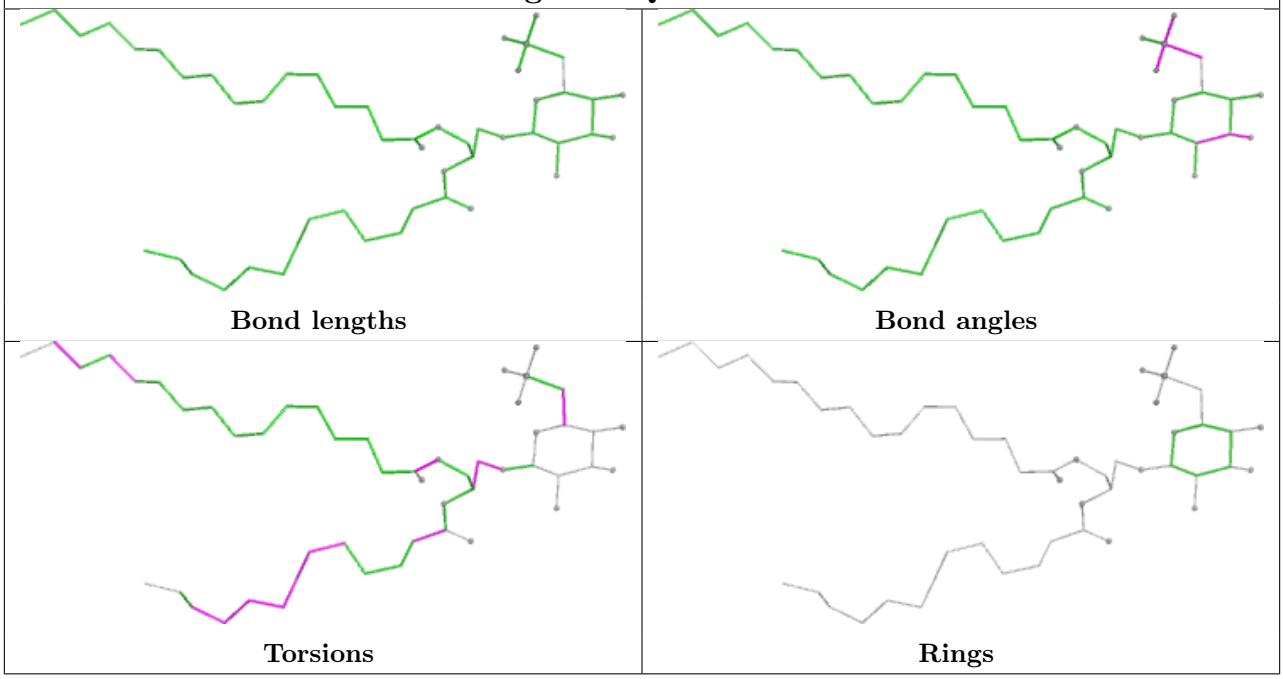


Rings

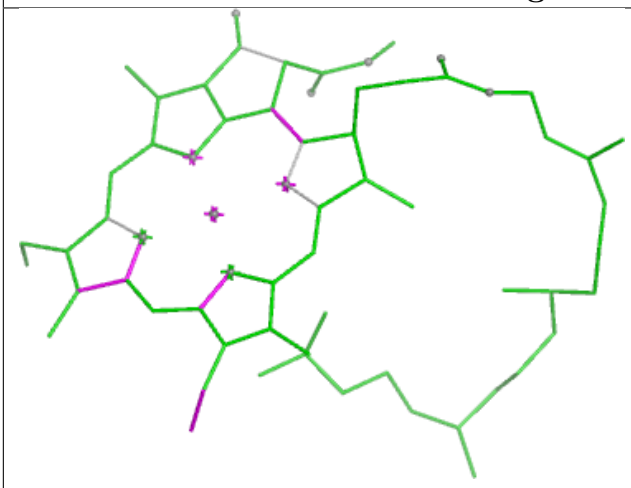
Ligand CLA c 511



Ligand SQD A 412



Ligand CLA b 616



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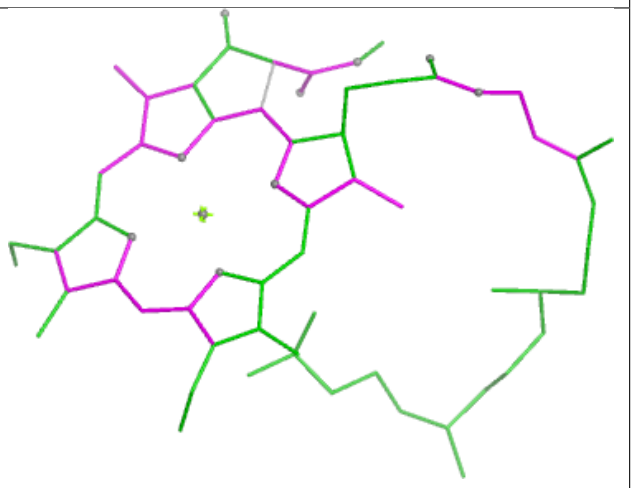
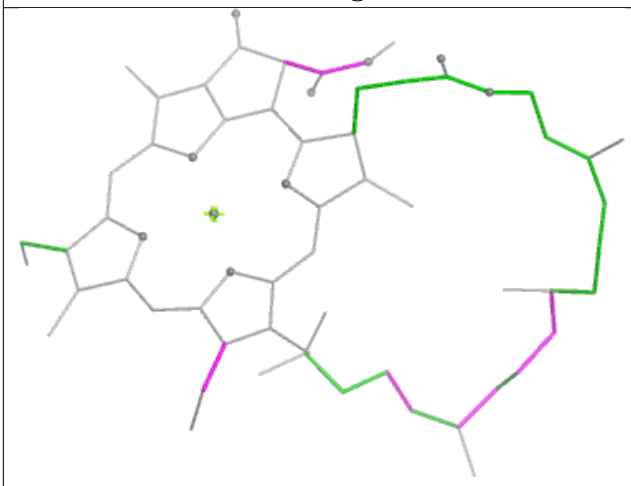


Bond angles



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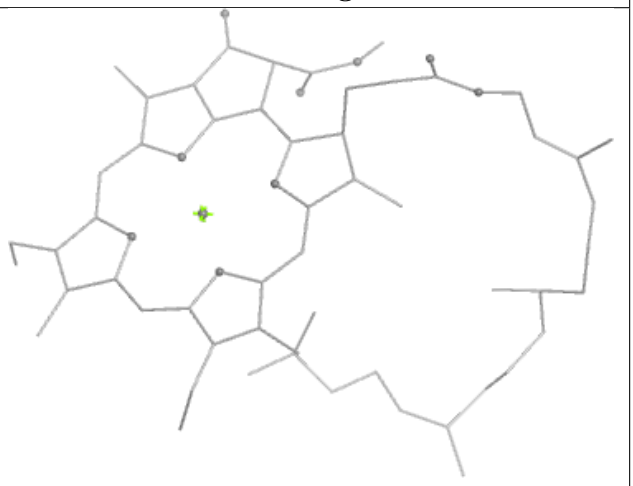
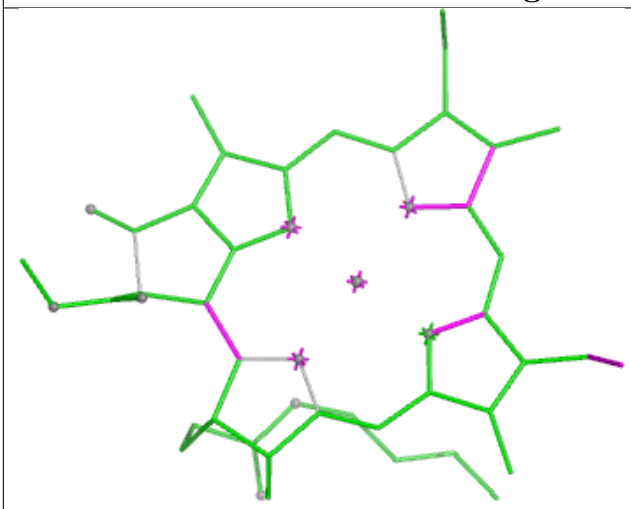


Rings

Ligand CLA N 614



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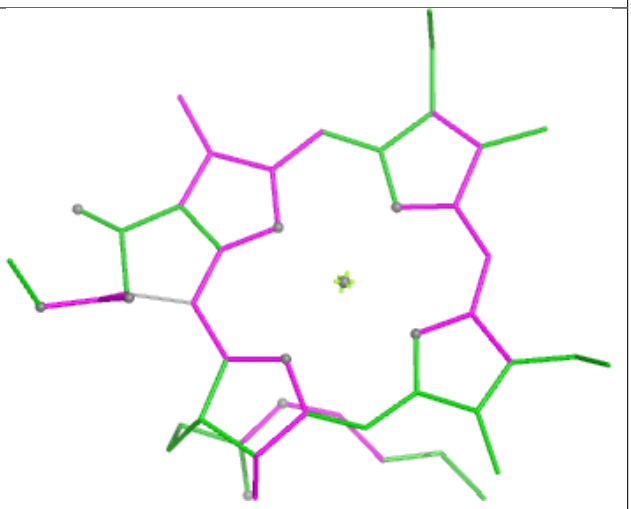
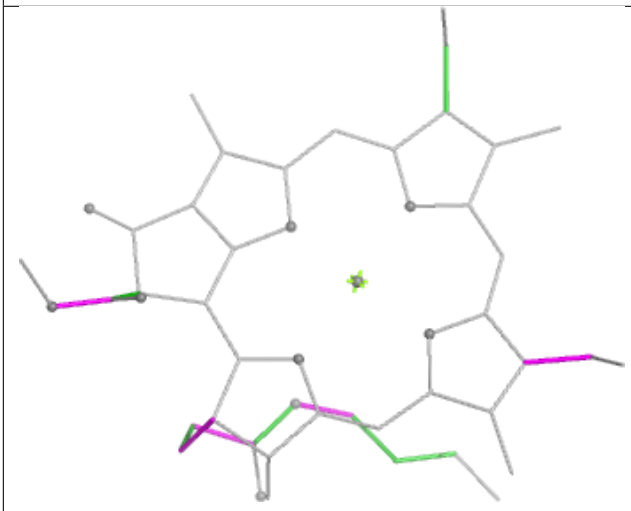


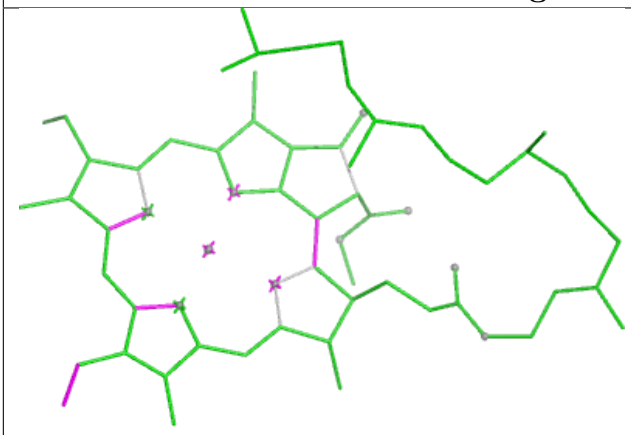
Bond angles



Torsions

Rings

Ligand CLA c 509



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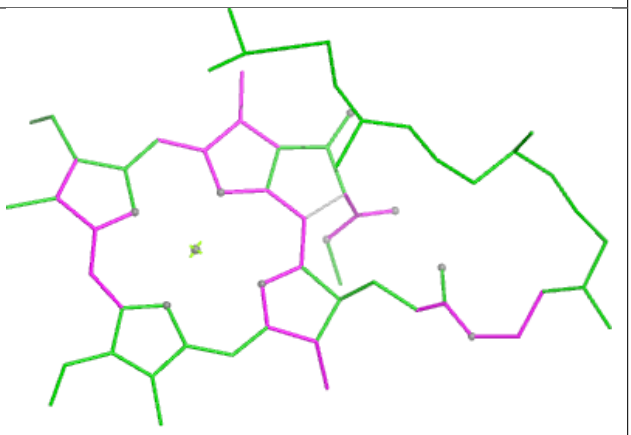
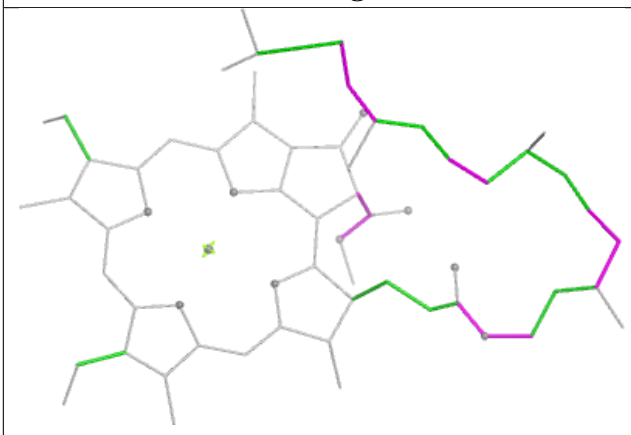
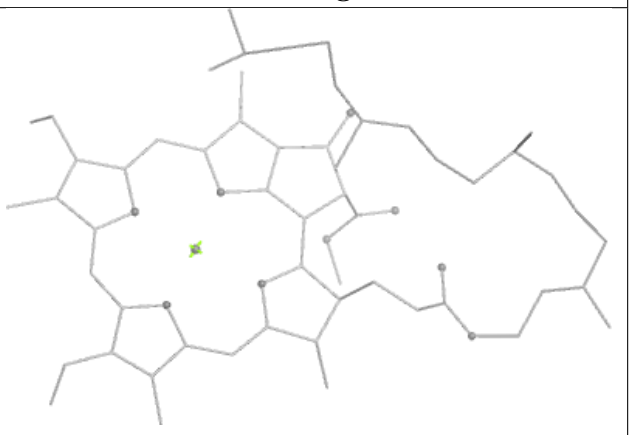


Bond angles

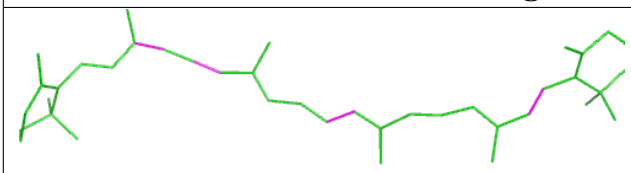


Torsions



Rings

Ligand BCR C 516



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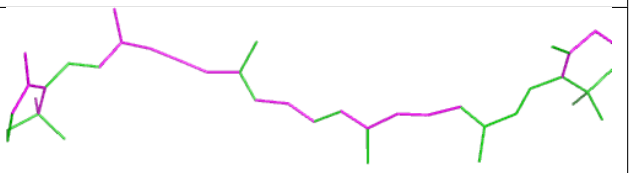
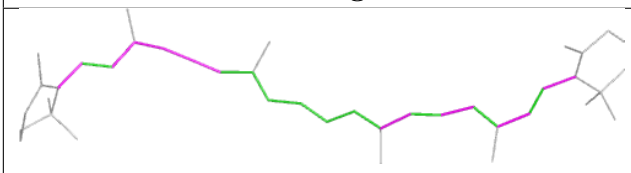


Bond angles



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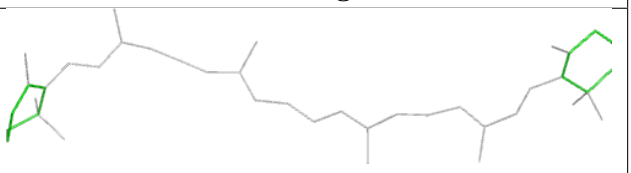
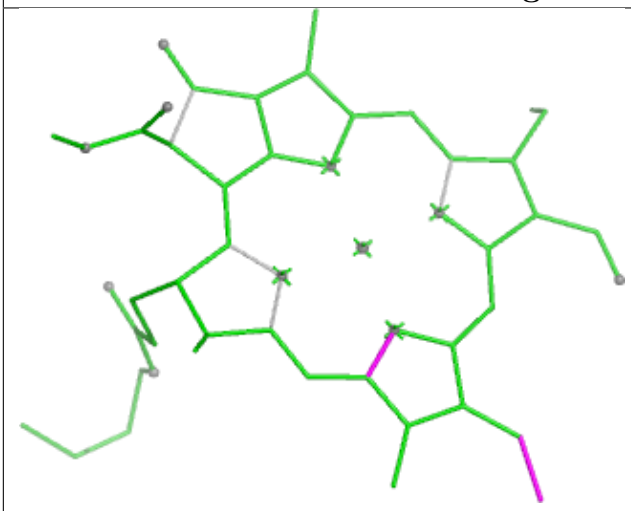


Rings

Ligand CHL N 608



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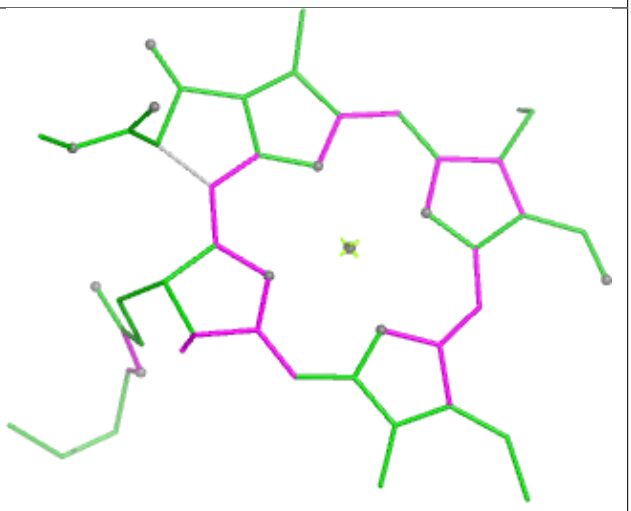
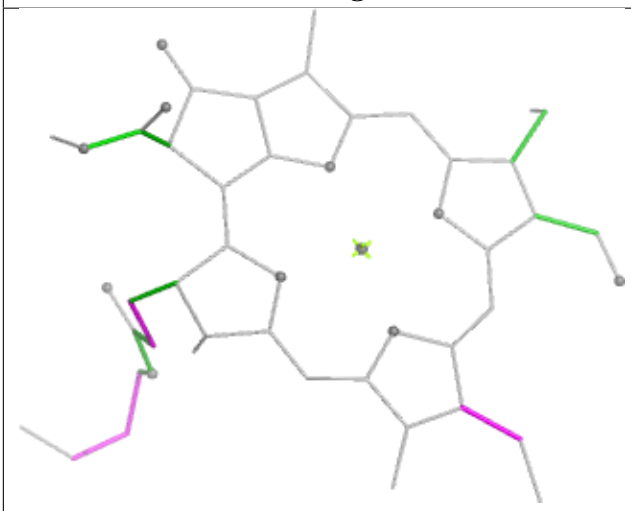


Bond angles



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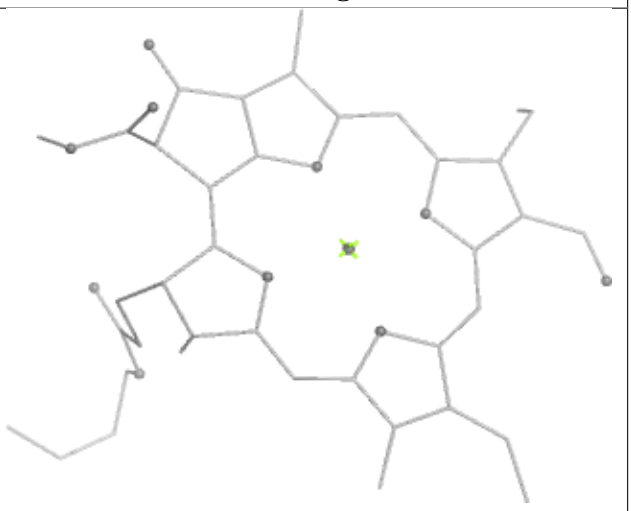
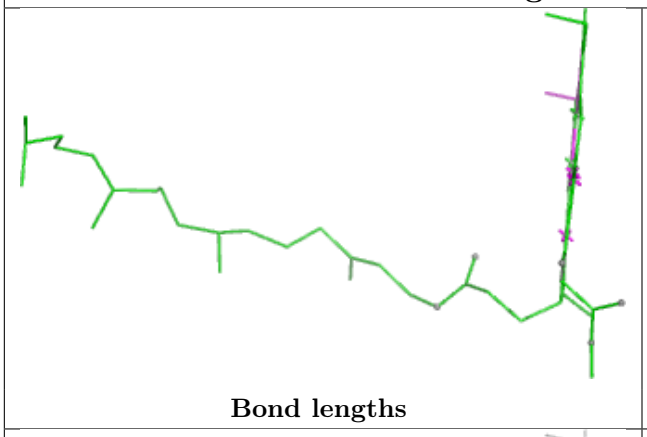


Rings

Ligand CLA B 607



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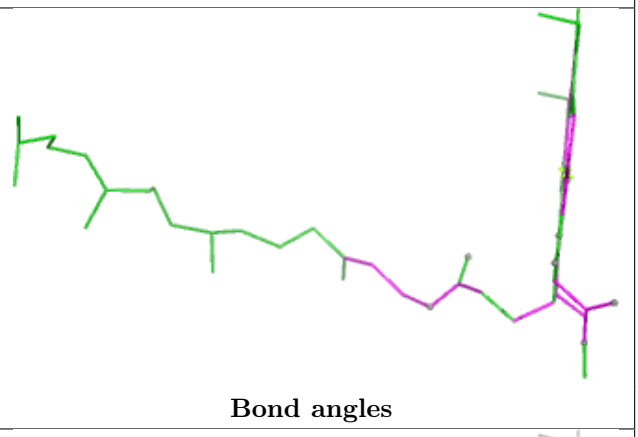
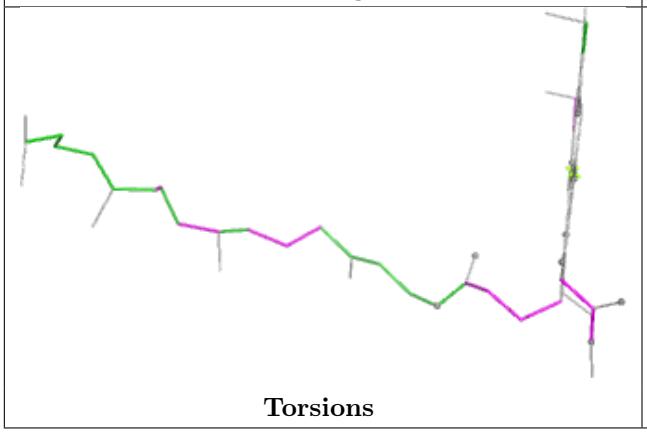


Bond angles



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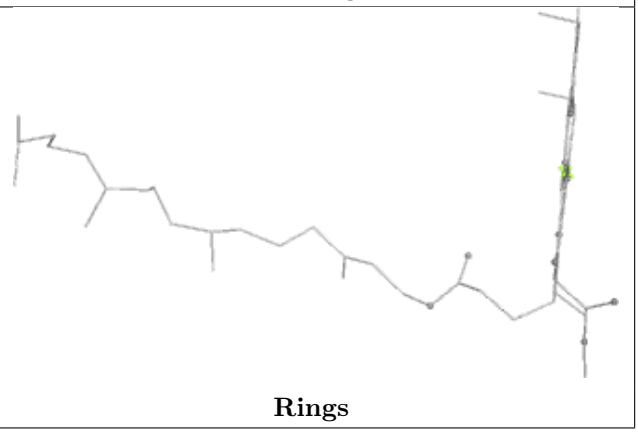
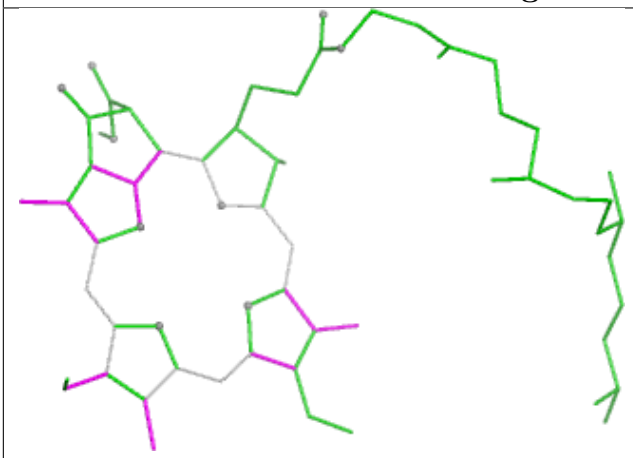


Rings

Ligand PHO A 409



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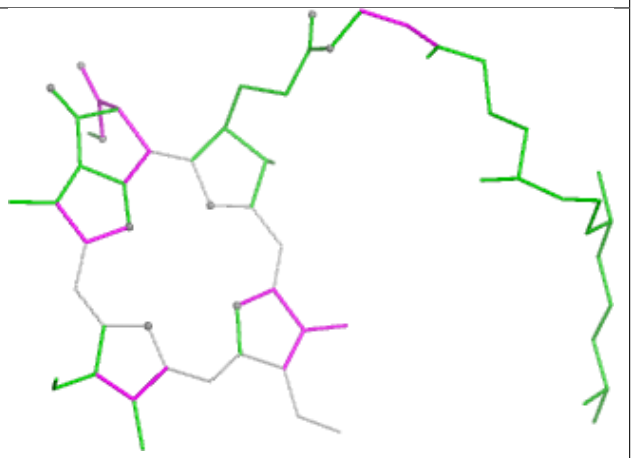
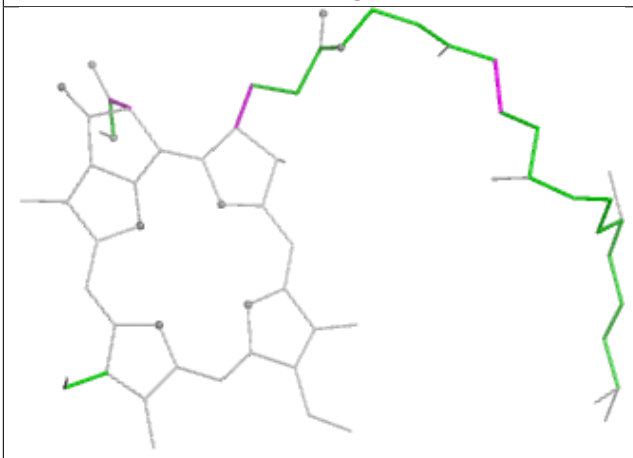


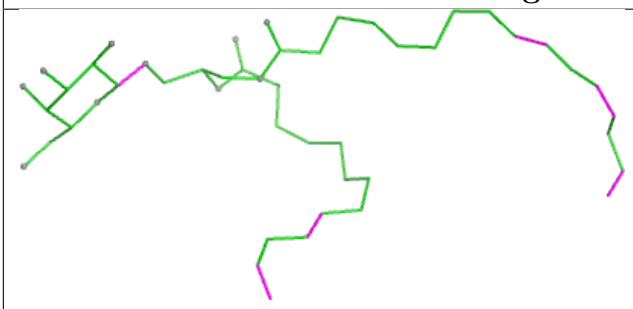
Bond angles



Torsions

Rings

Ligand LMG h 102



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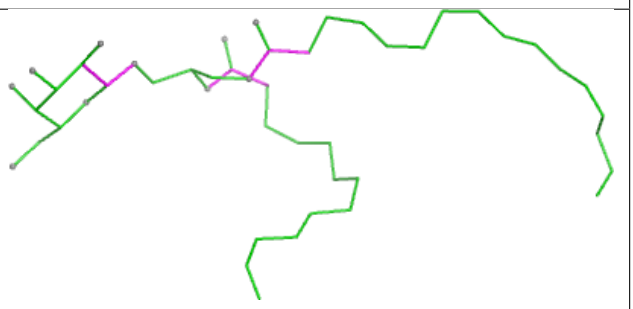
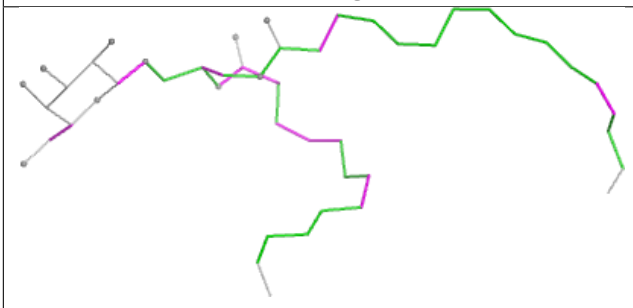
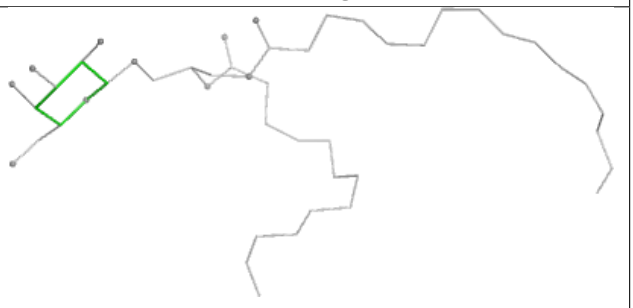


Bond angles

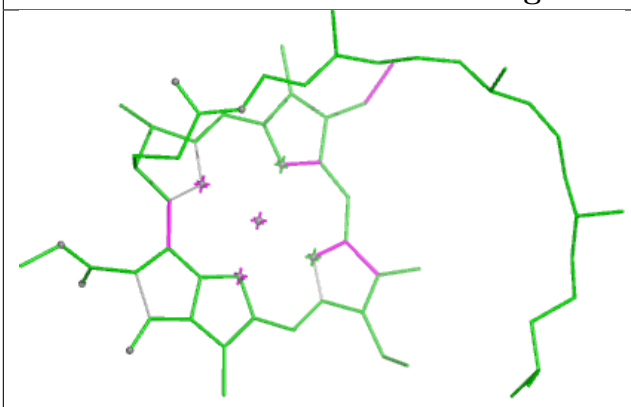


Torsions



Rings

Ligand CLA Y 610



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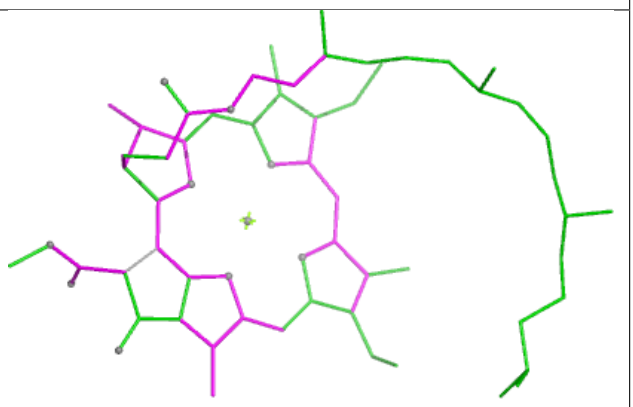
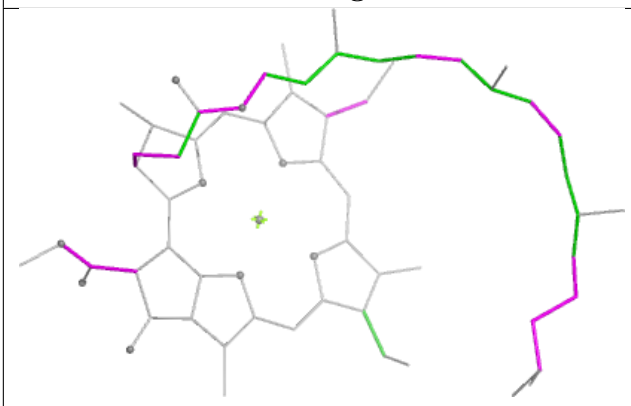
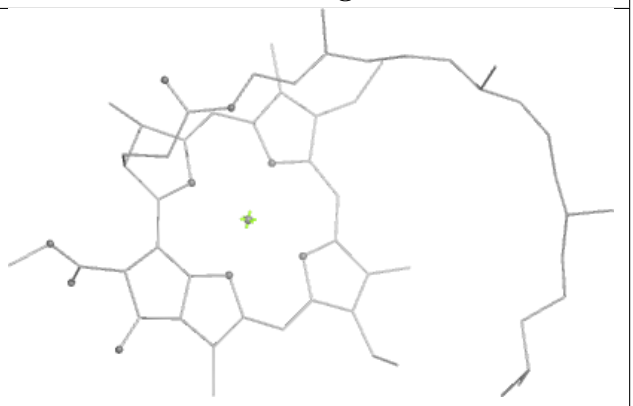


Bond angles



Torsions



Rings

Ligand LUT N 621

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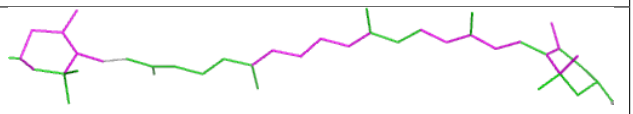
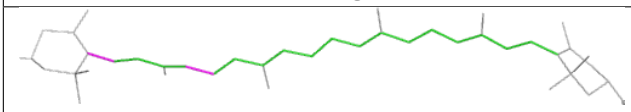


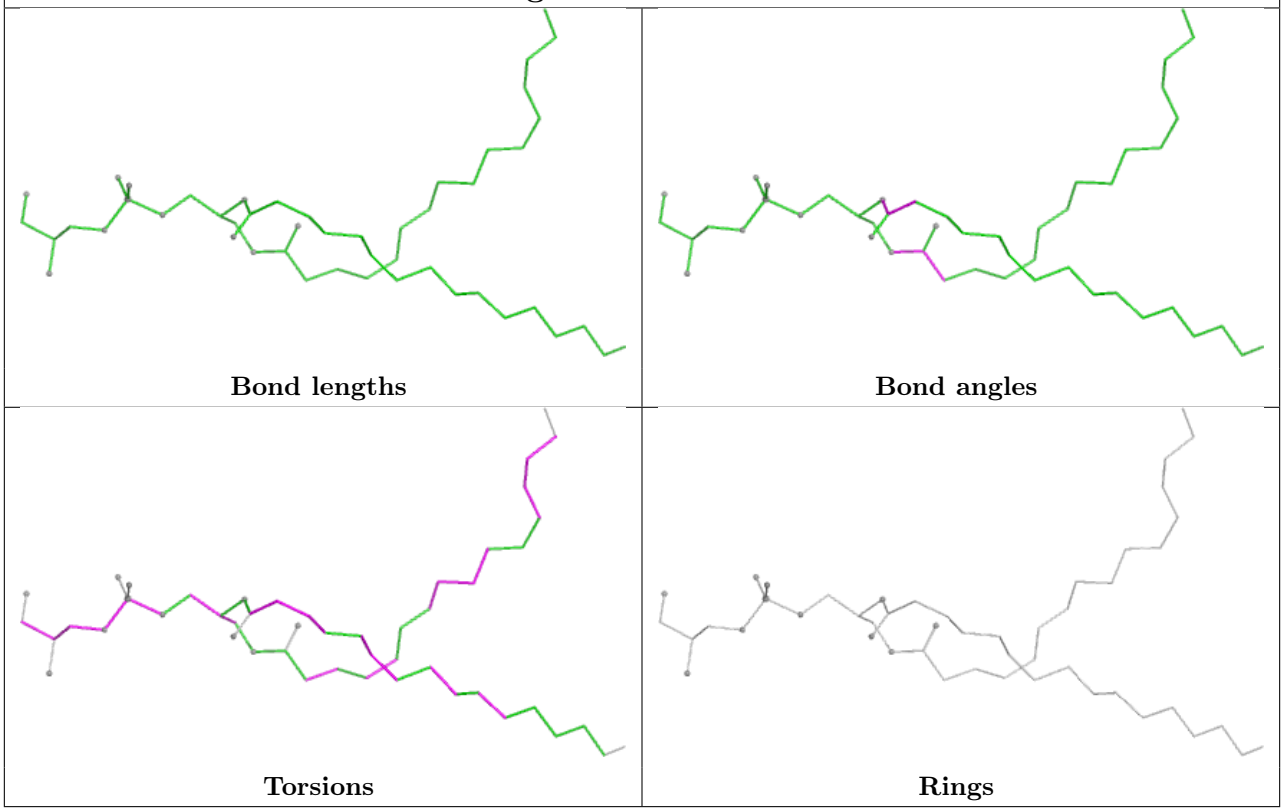
Bond angles



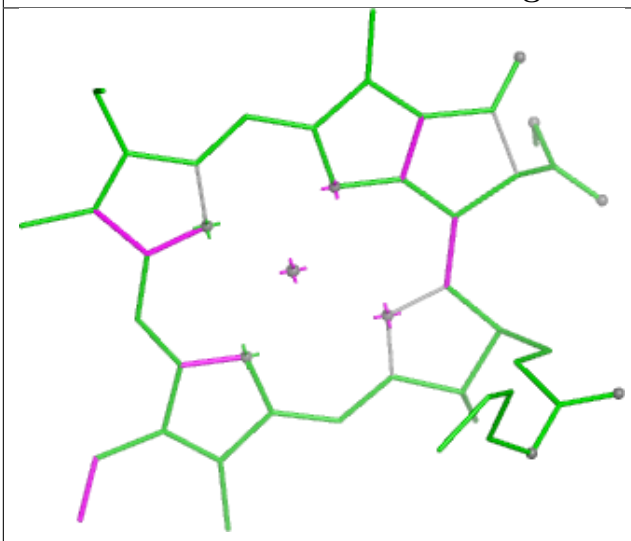
Torsions

Rings

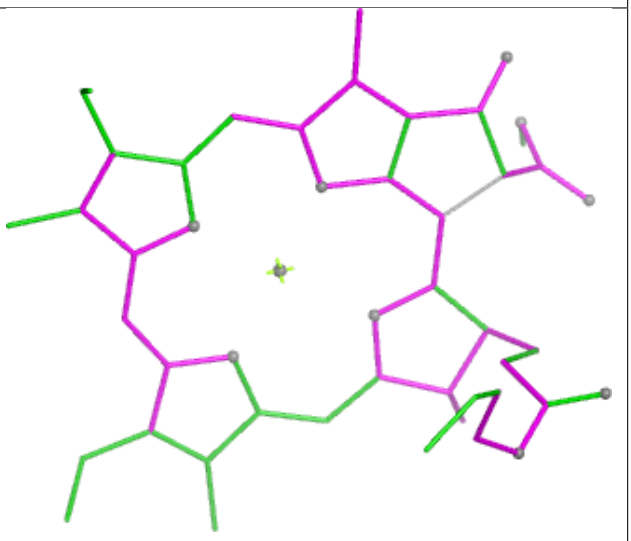
Ligand LHG d 409



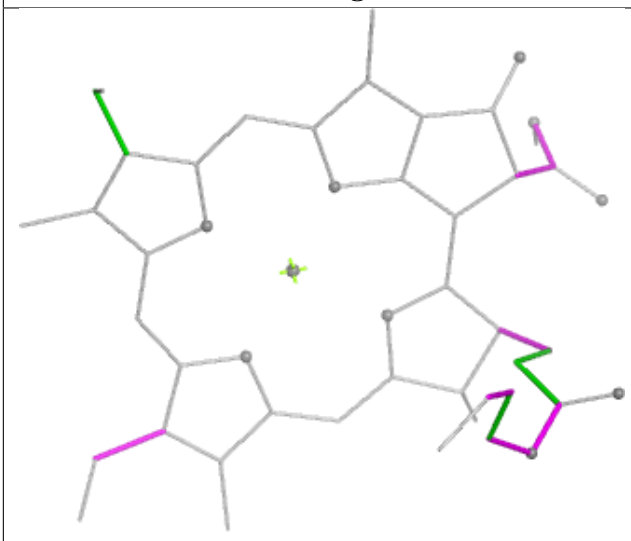
Ligand CLA G 604



Bond lengths



Bond angles



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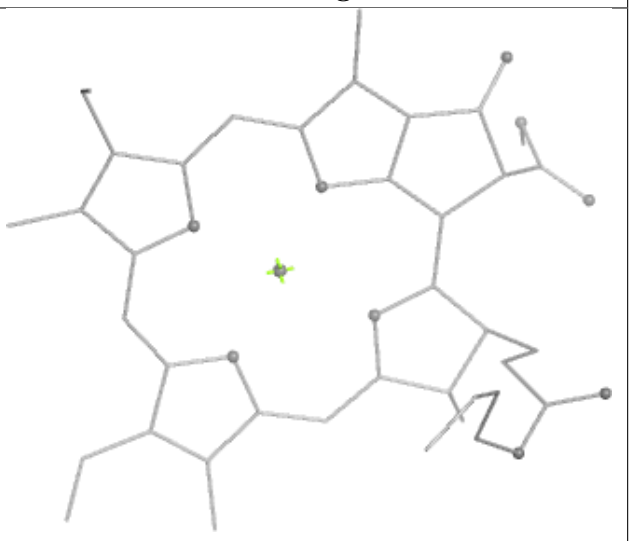
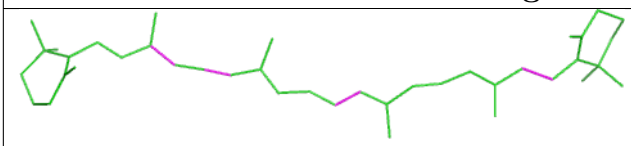


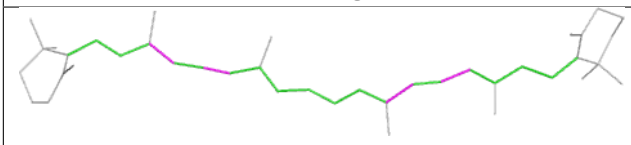
Rings

Ligand BCR B 619

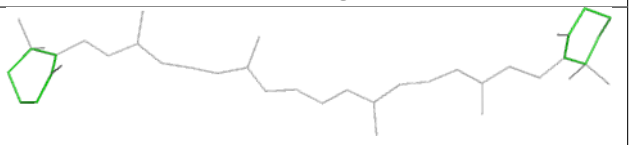


Bond lengths

Bond angles

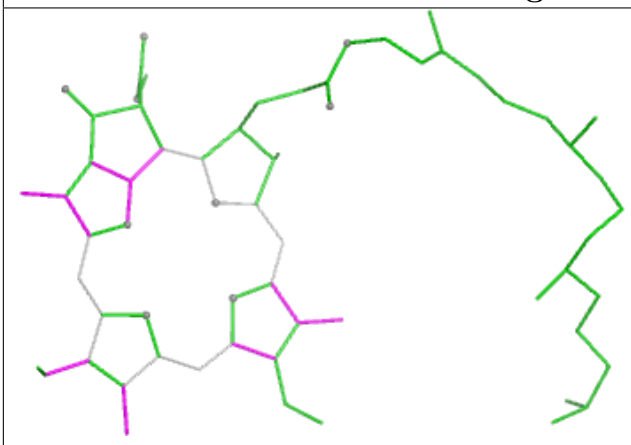


Torsions

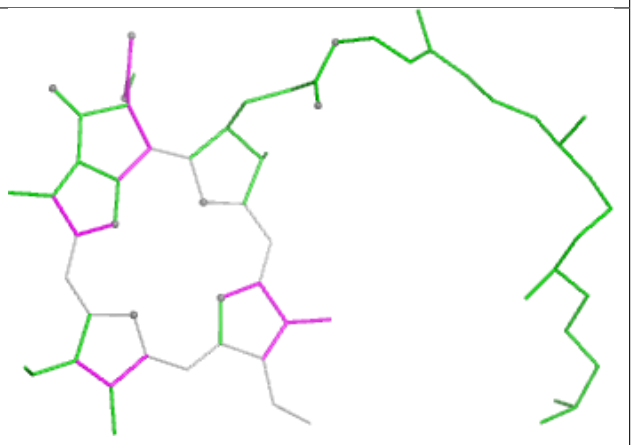


Rings

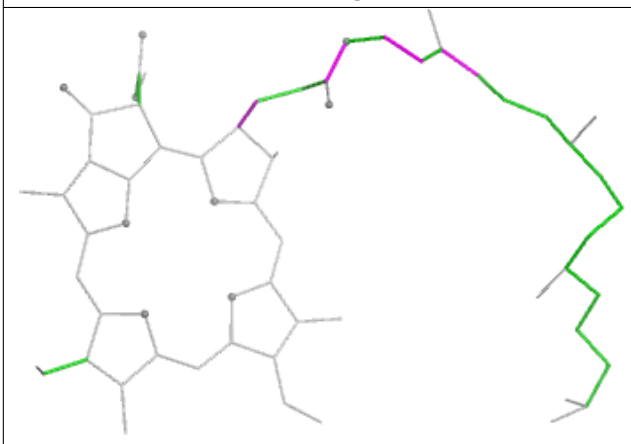
Ligand PHO a 408



Bond lengths



Bond angles



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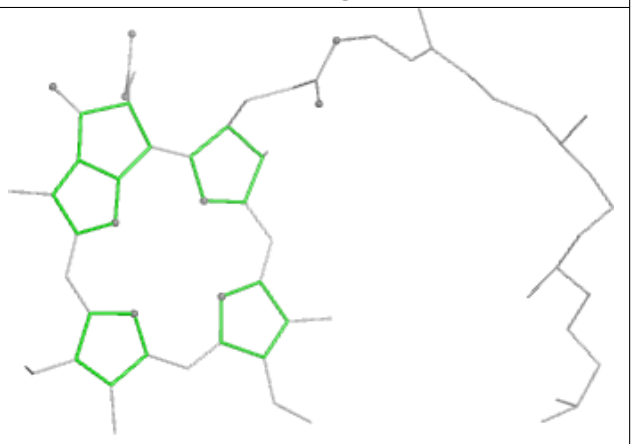
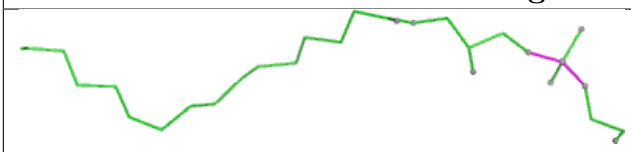


Rings

Ligand LPX S 625



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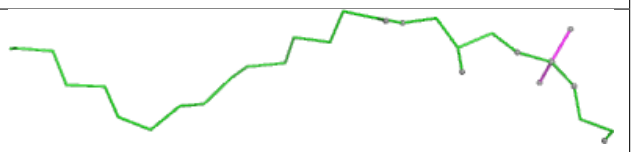
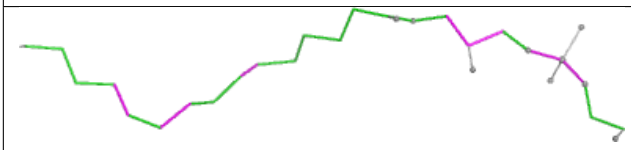


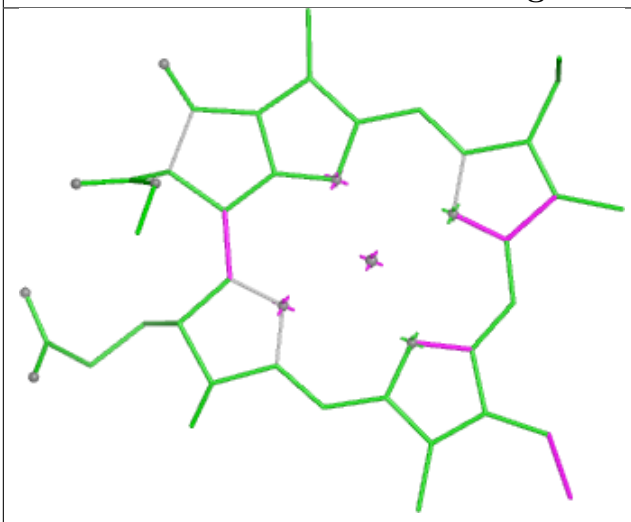
Bond angles



Torsions

Rings

Ligand CLA S 612



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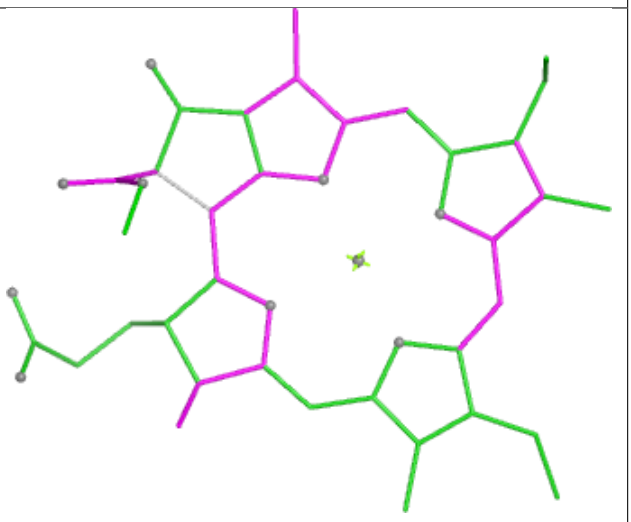
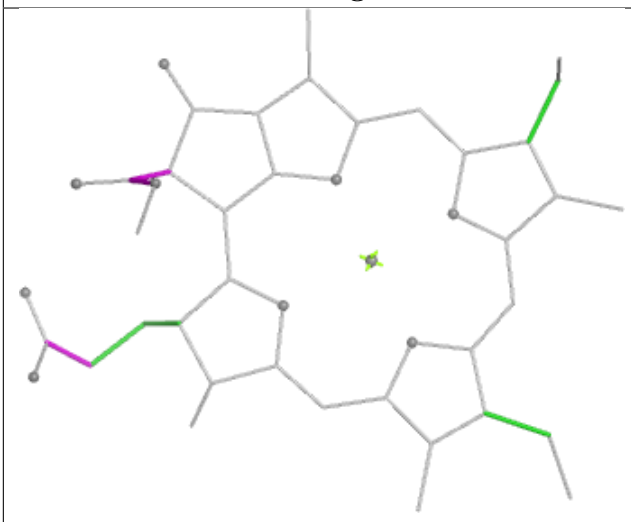
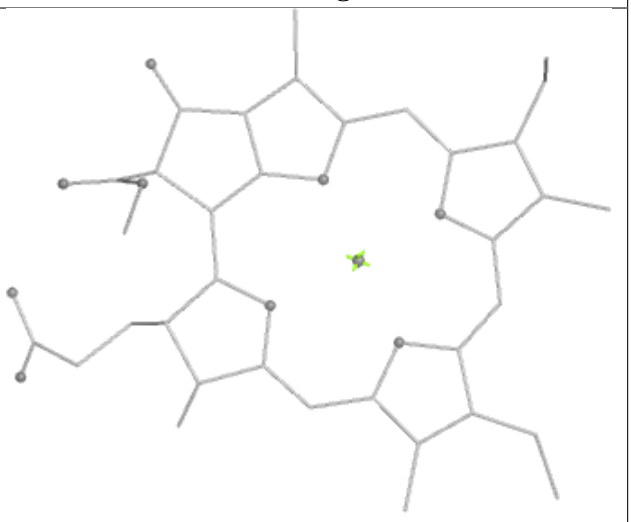


Bond angles



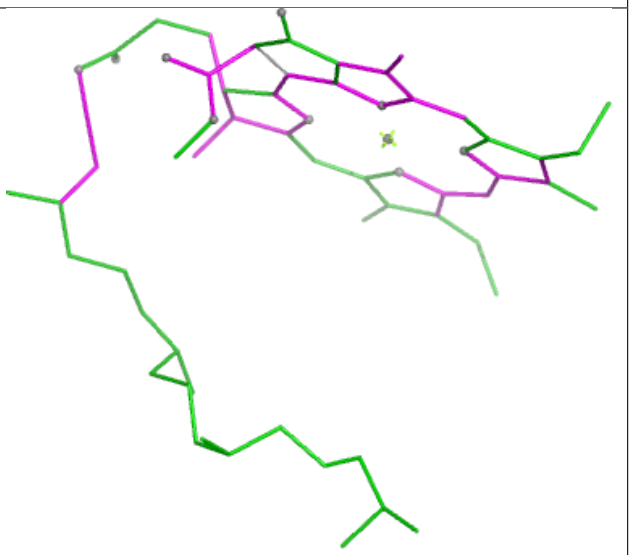
Torsions



Rings

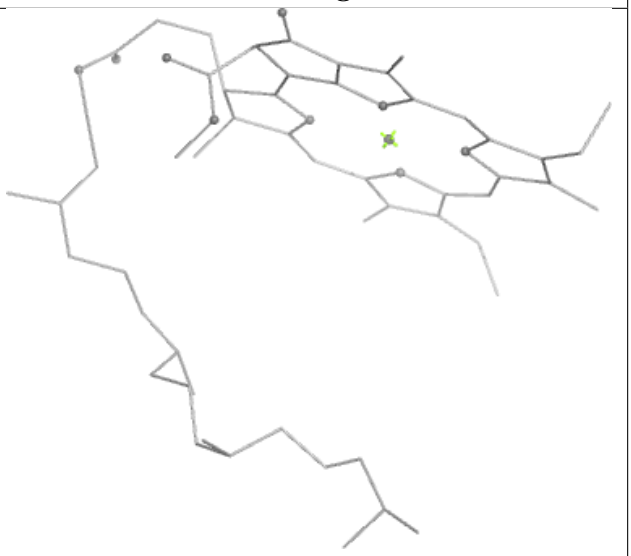
Ligand CLA N 603

Bond lengths



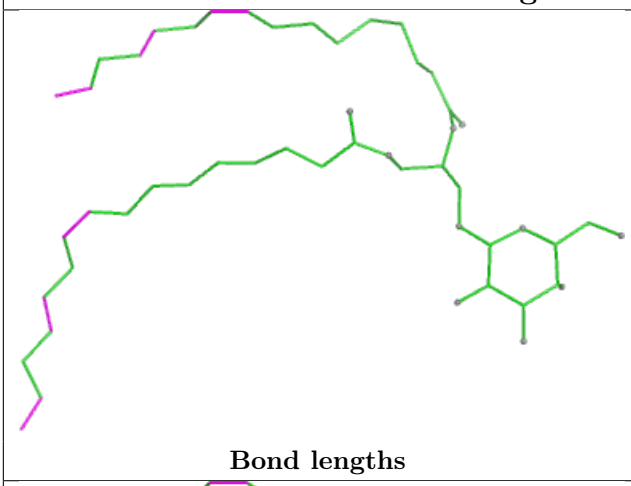
Bond angles

Torsions



Rings

Ligand LMG C 521



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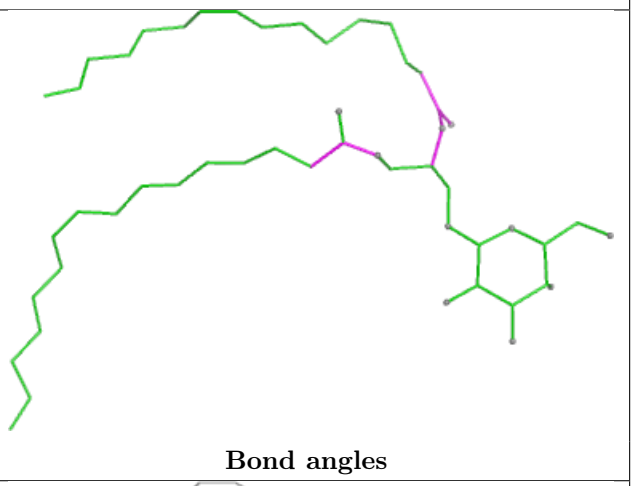
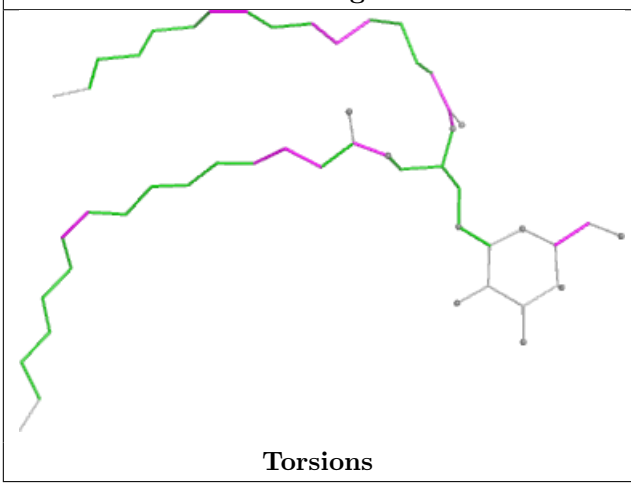


Bond angles



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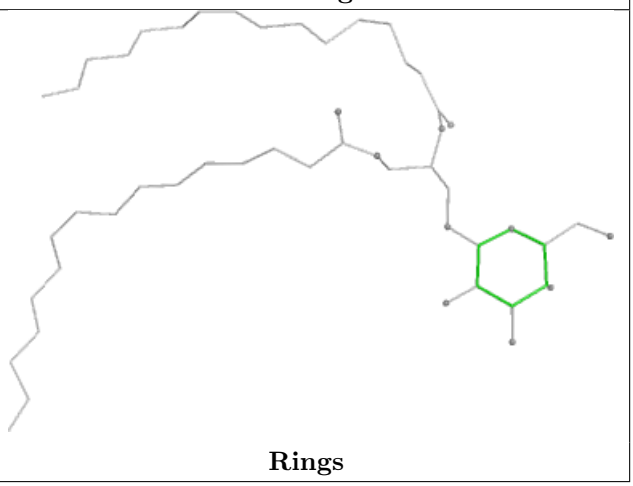
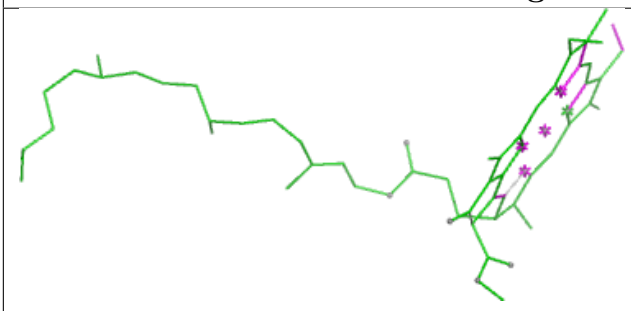
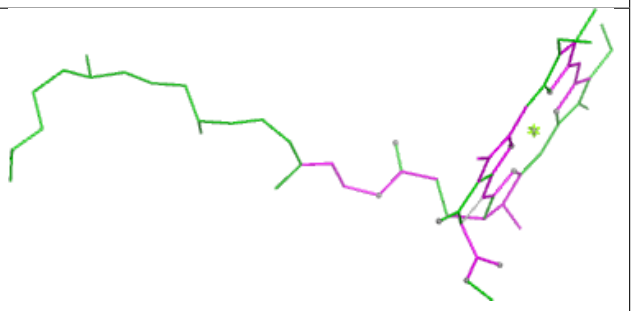


Rings

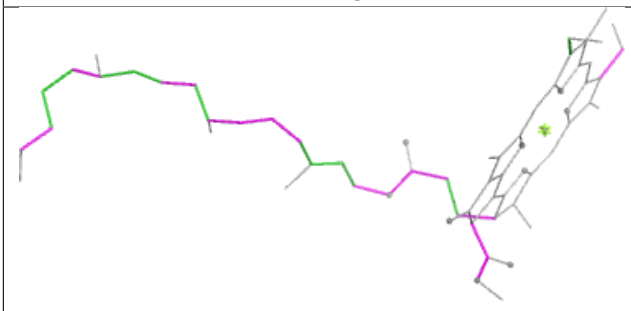
Ligand CLA b 605



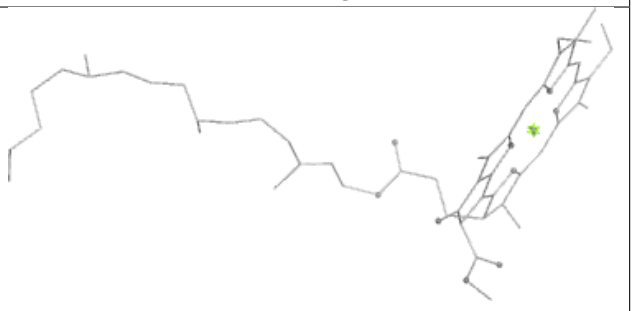
Bond lengths



Bond angles

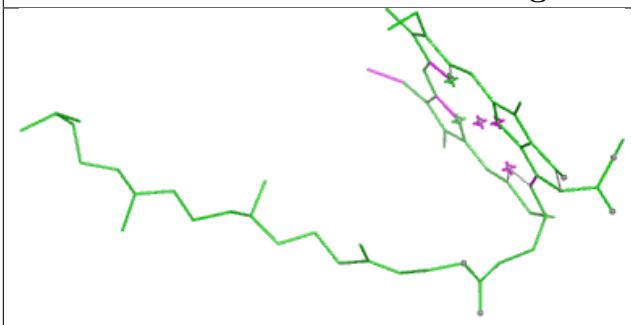


Torsions



Rings

Ligand CLA c 504



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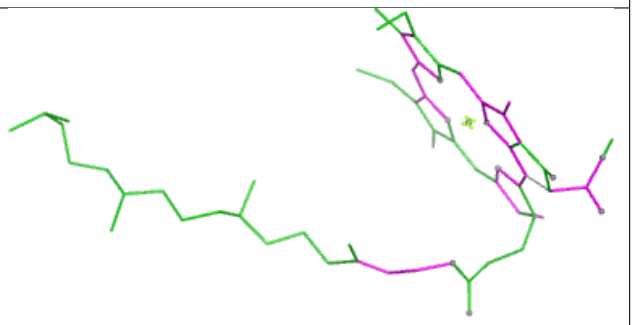
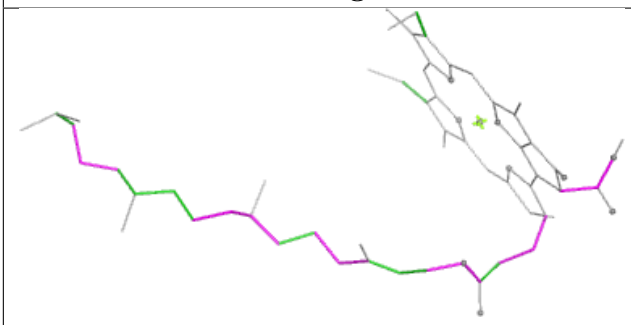


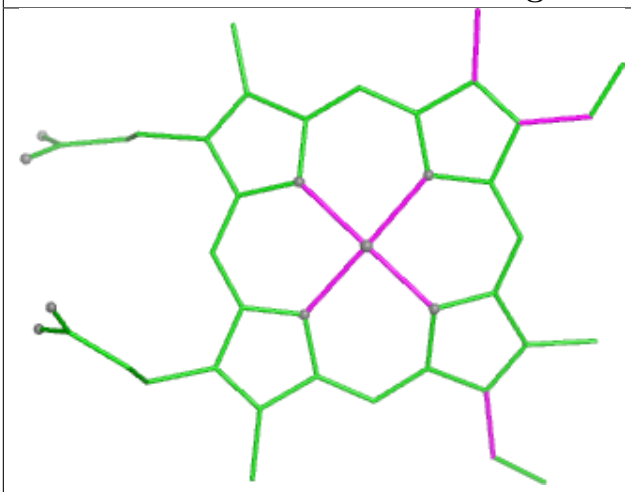
Bond angles



Torsions

Rings

Ligand HEM f 101



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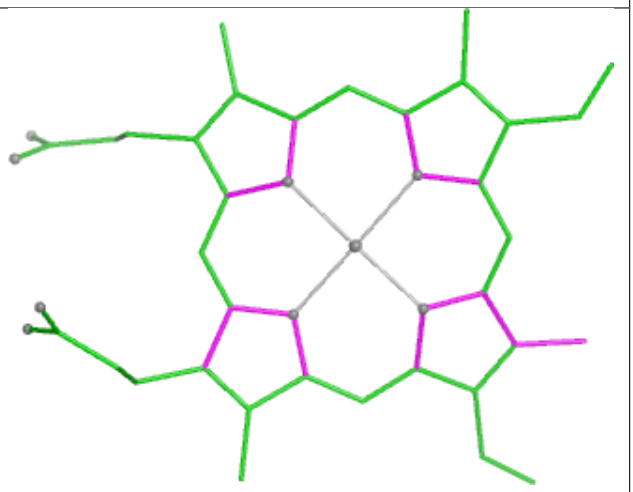
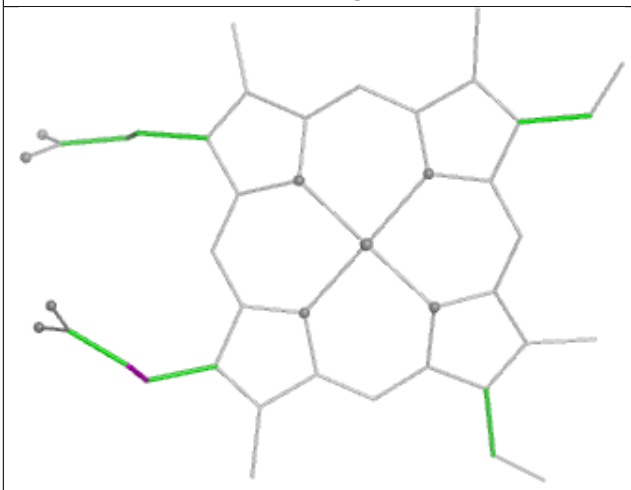


Bond angles



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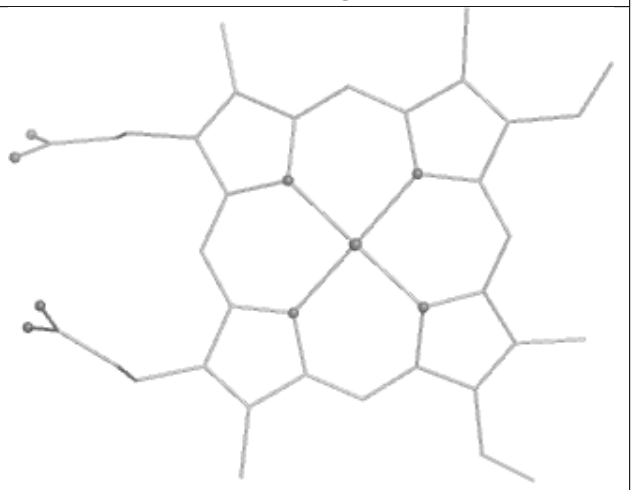
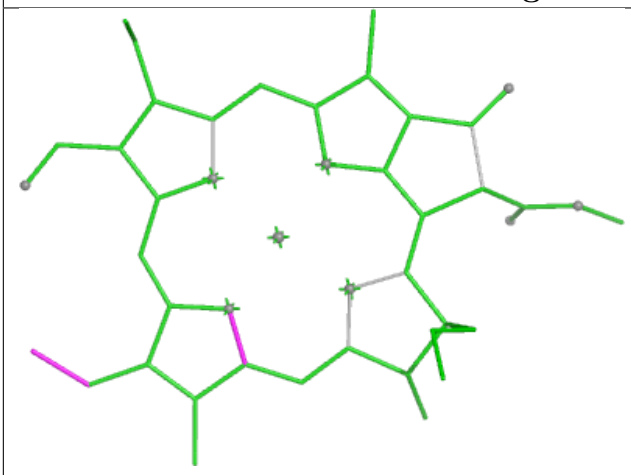


Rings

Ligand CHL G 608



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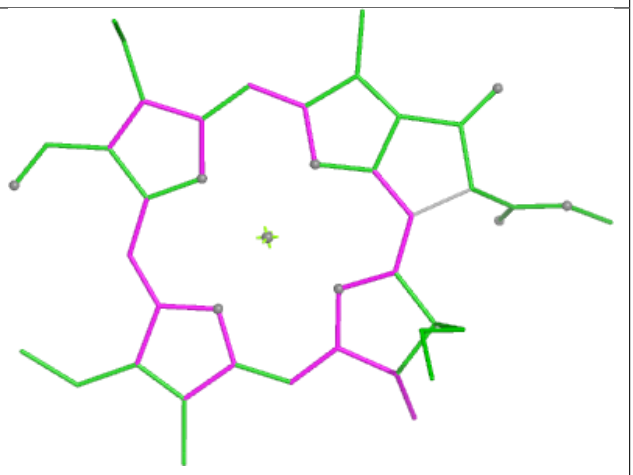
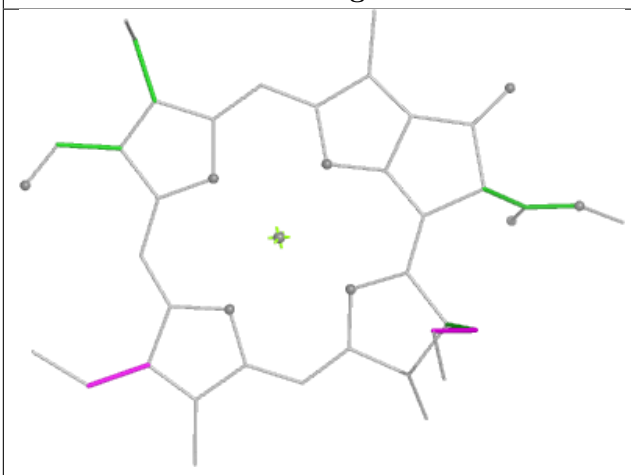


Bond angles



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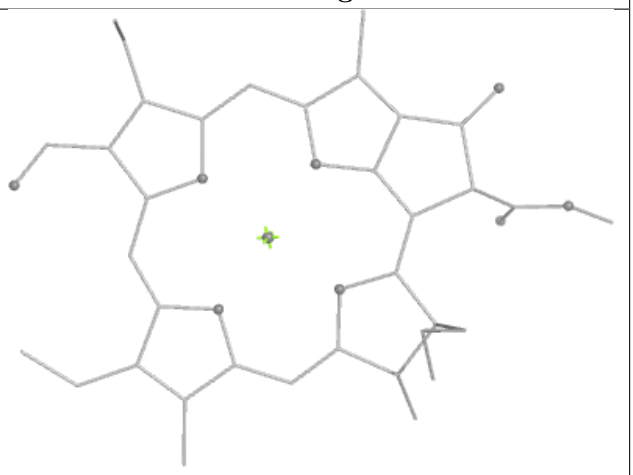
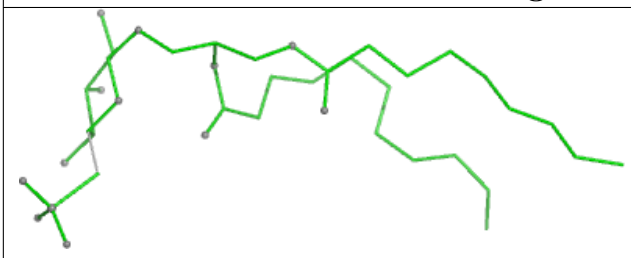


Rings

Ligand SQD b 621



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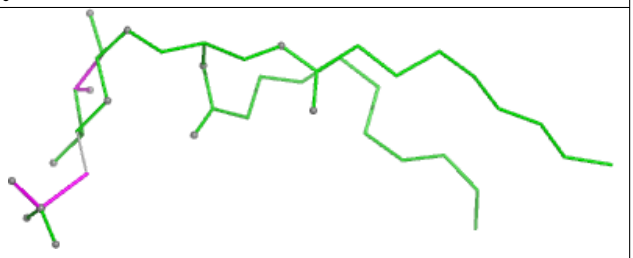
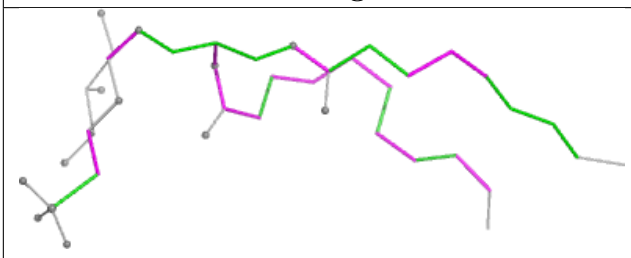
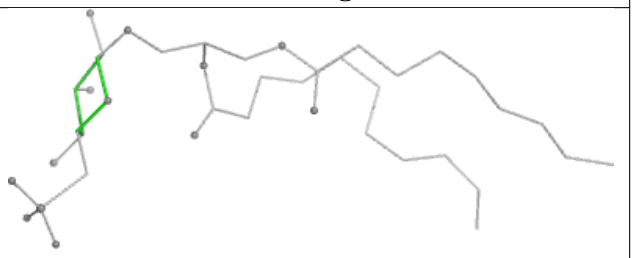


Bond angles

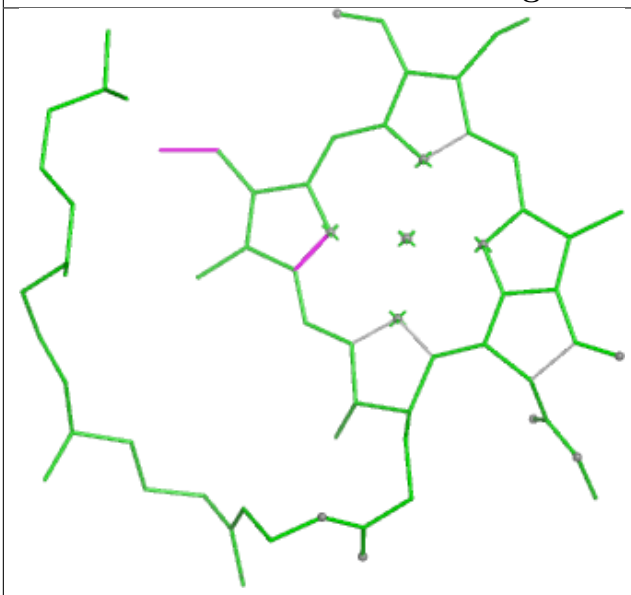


Torsions

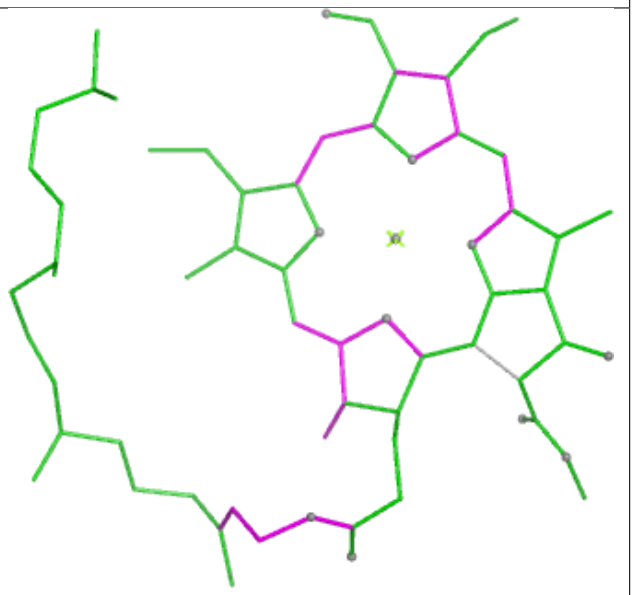


Rings

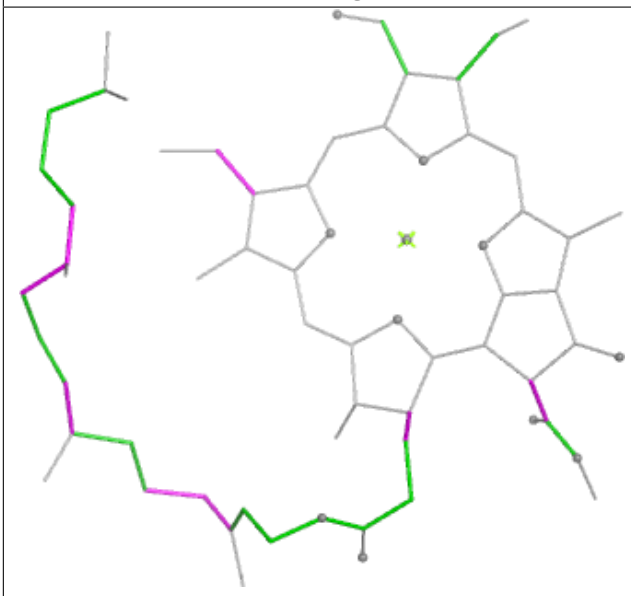
Ligand CHL N 607



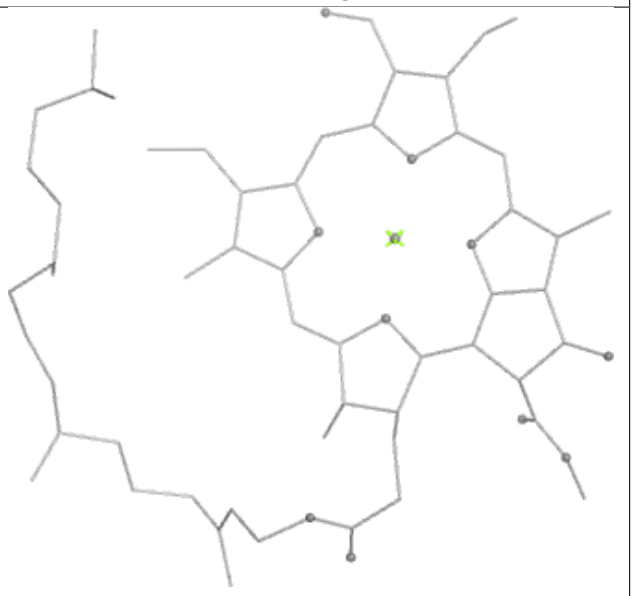
Bond lengths



Bond angles

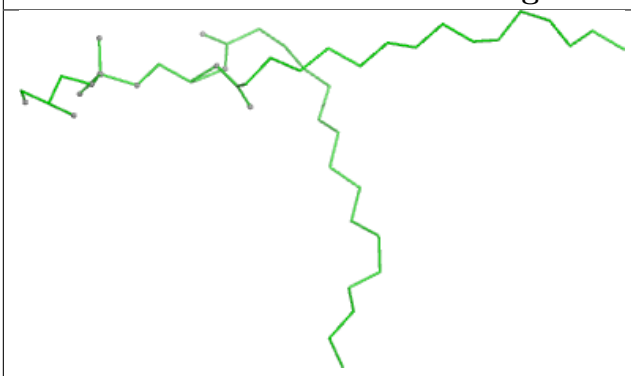


Torsions

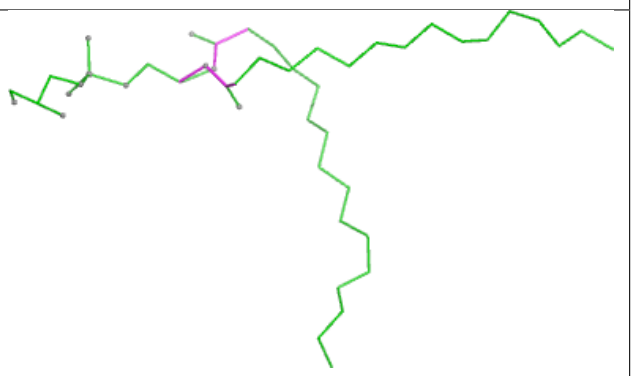


Rings

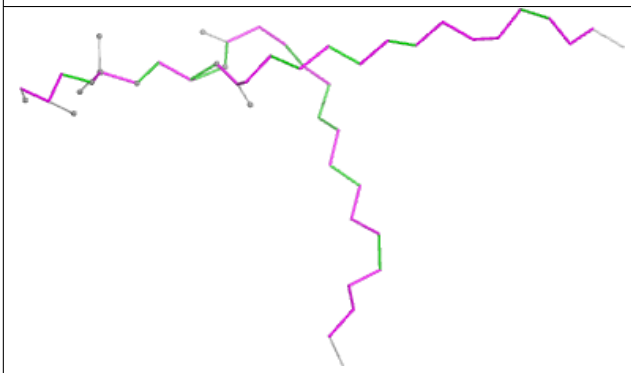
Ligand LHG N 624



Bond lengths



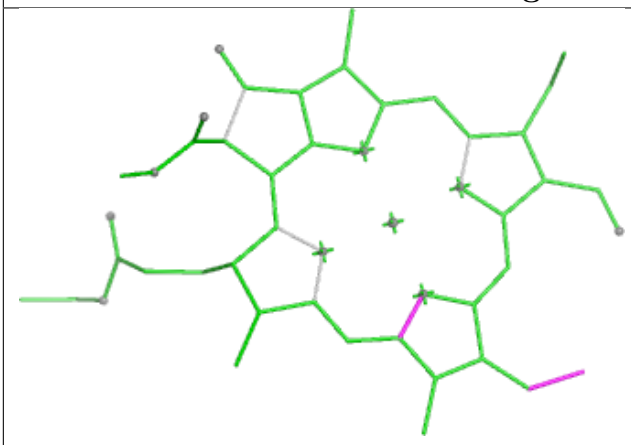
Bond angles



Torsions

Rings

Ligand CHL G 605



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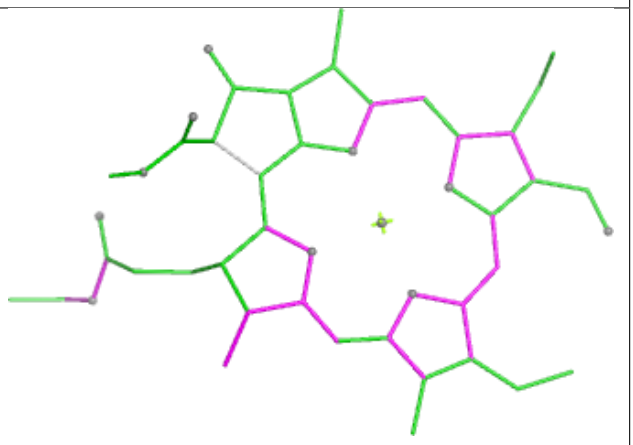
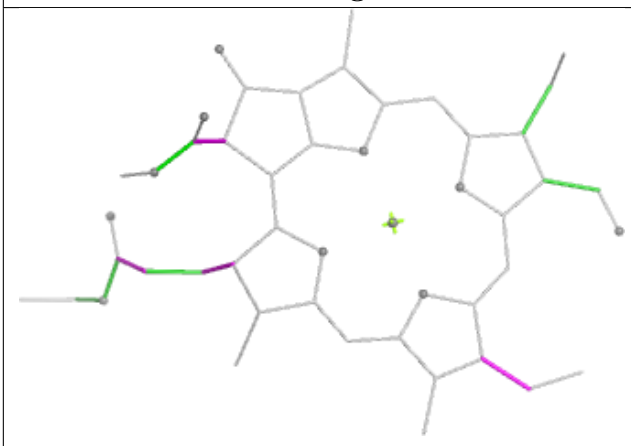
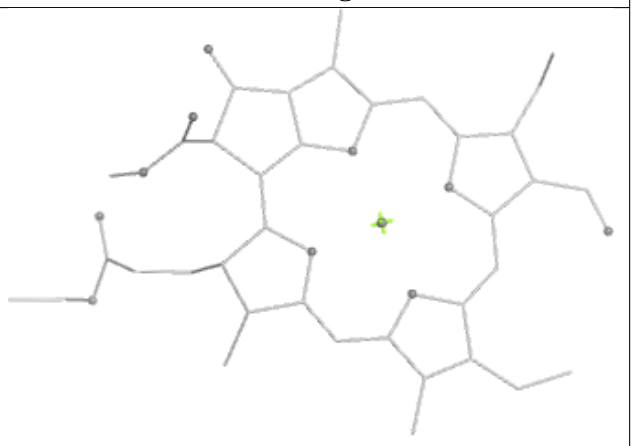


Bond angles

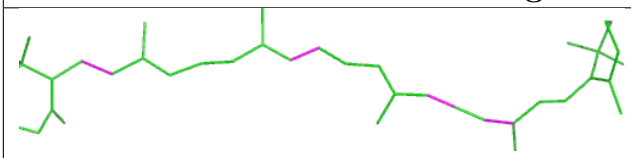


Torsions



Rings

Ligand BCR b 618



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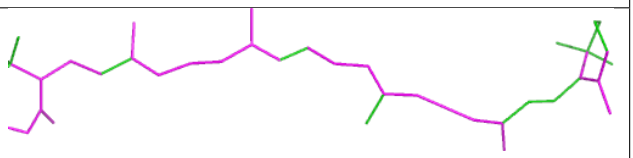
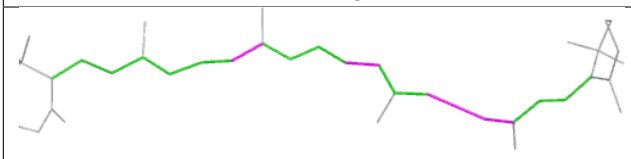
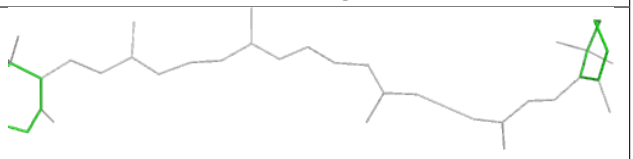


Bond angles

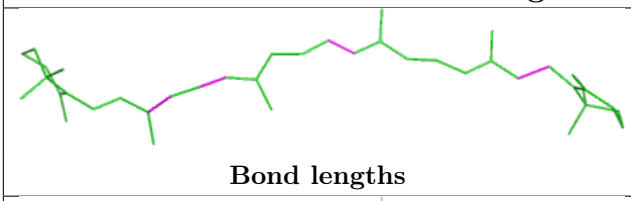


Torsions



Rings

Ligand BCR c 515



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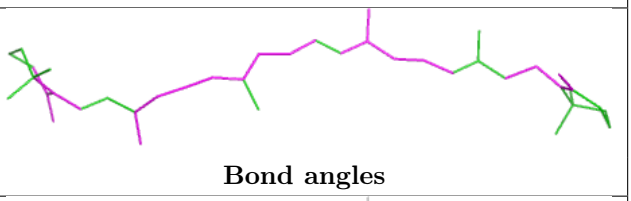
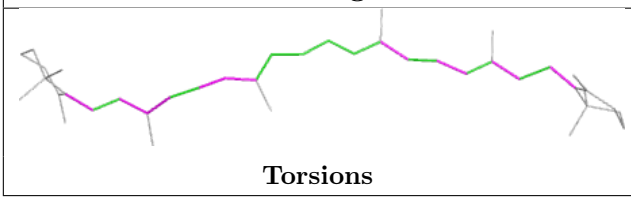


Bond angles



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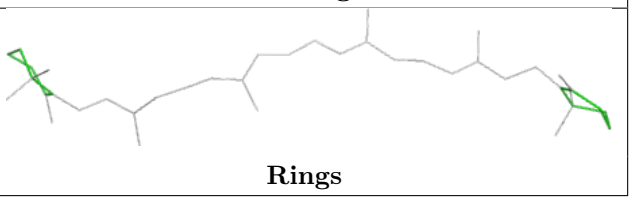
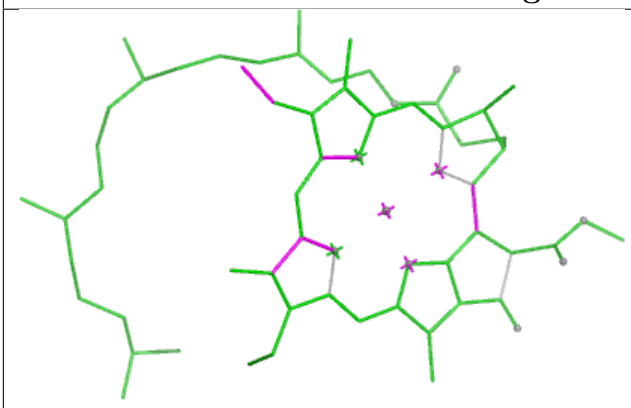


Rings

Ligand CLA G 610



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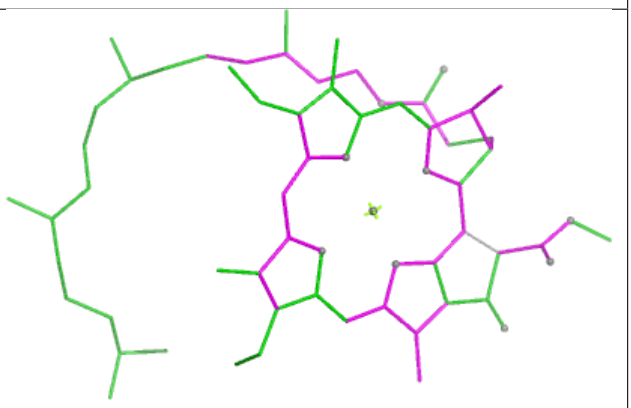
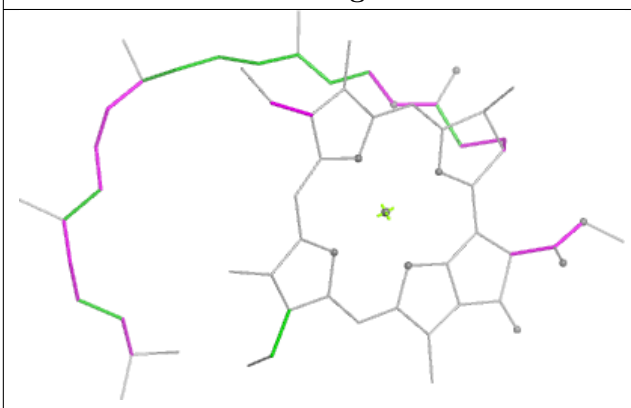
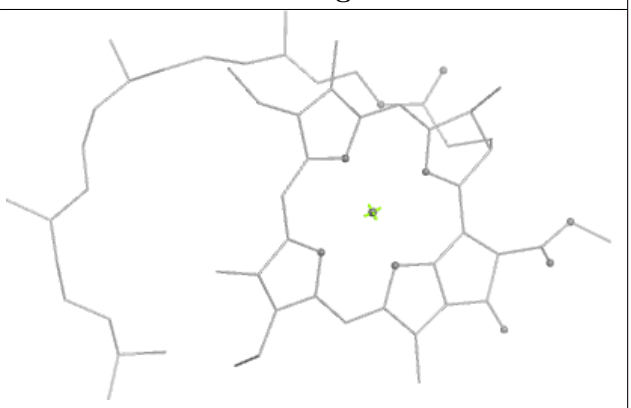


Bond angles

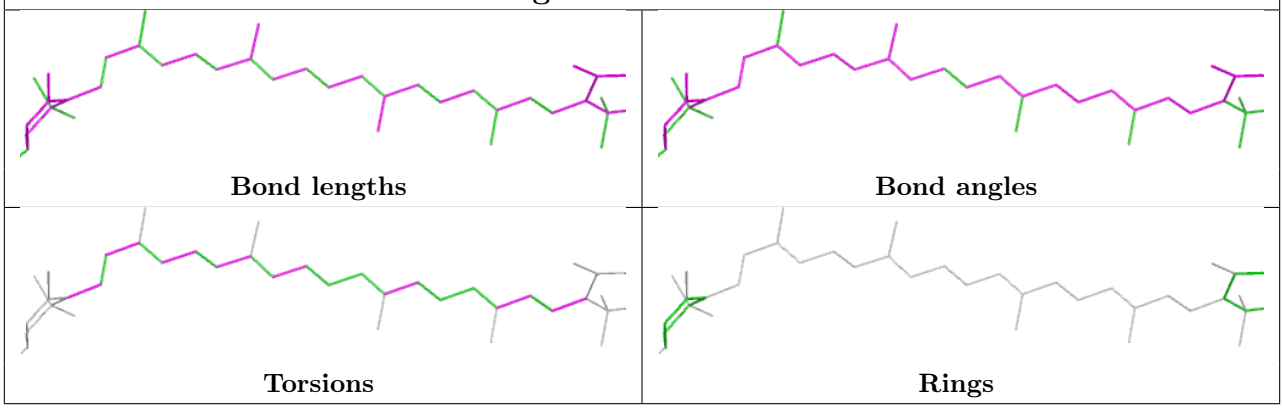


Torsions

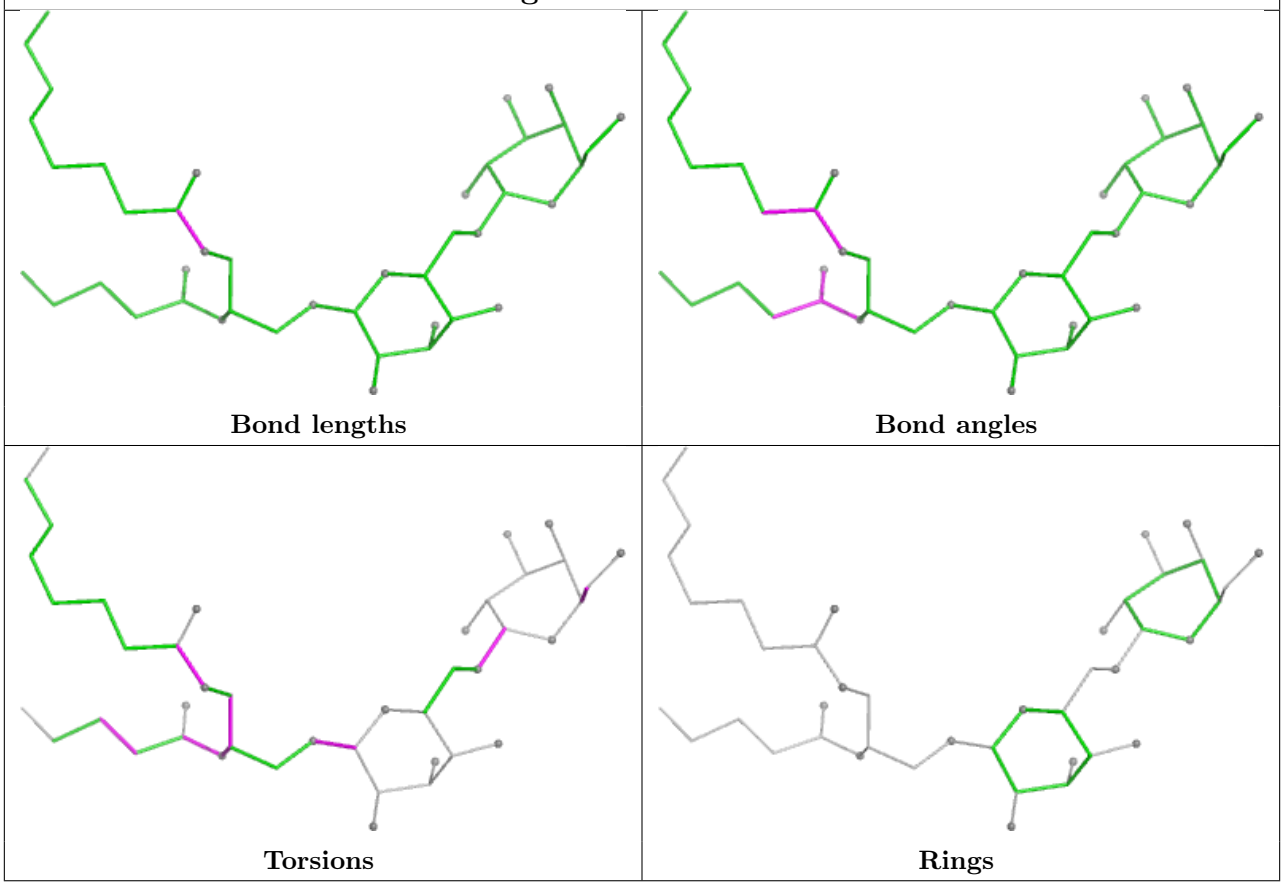


Rings

Ligand C7Z b 620



Ligand DGD B 623



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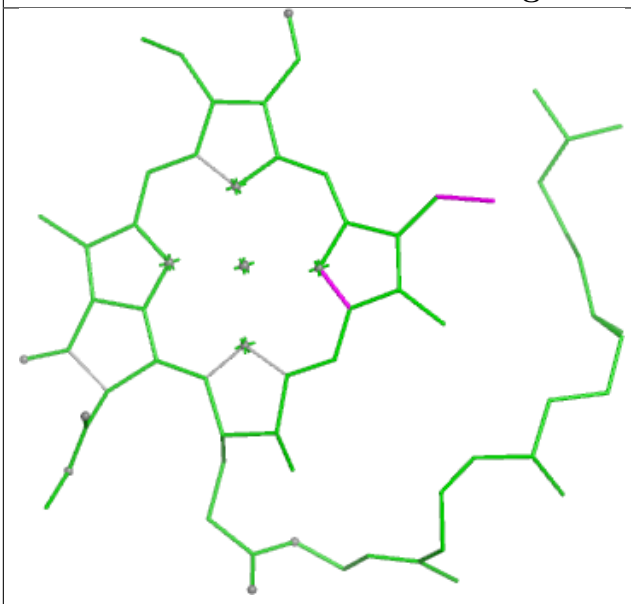
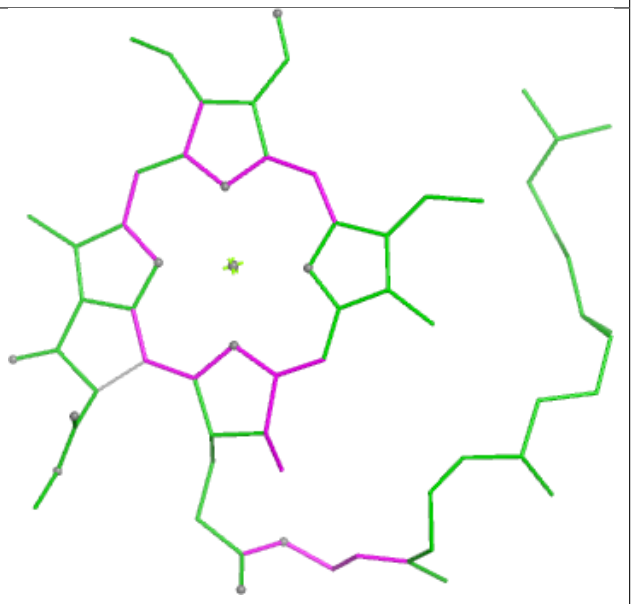
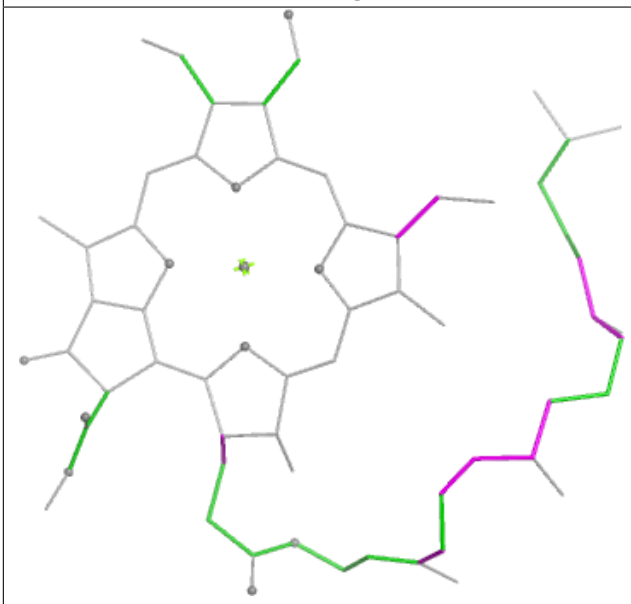


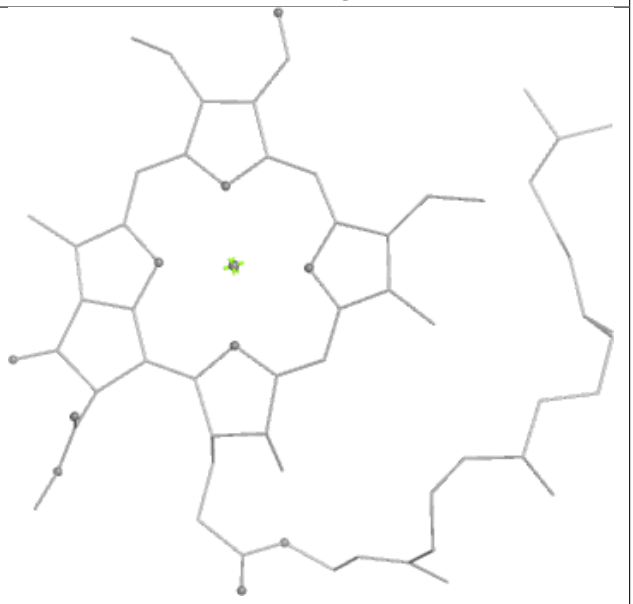
Bond lengths



Bond angles



Torsions



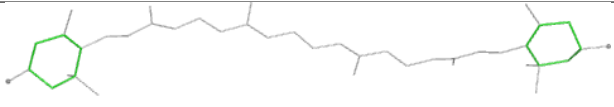
Rings

Ligand LUT G 621

Bond lengths

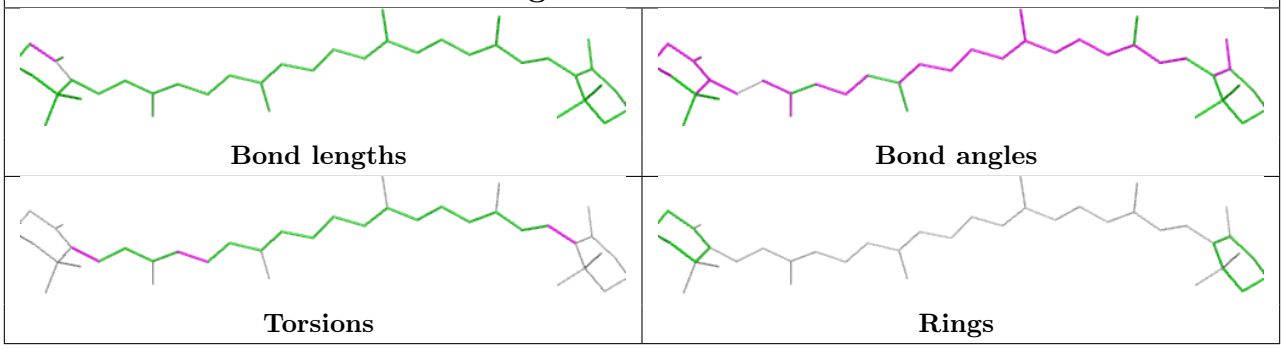
Bond angles

Torsions

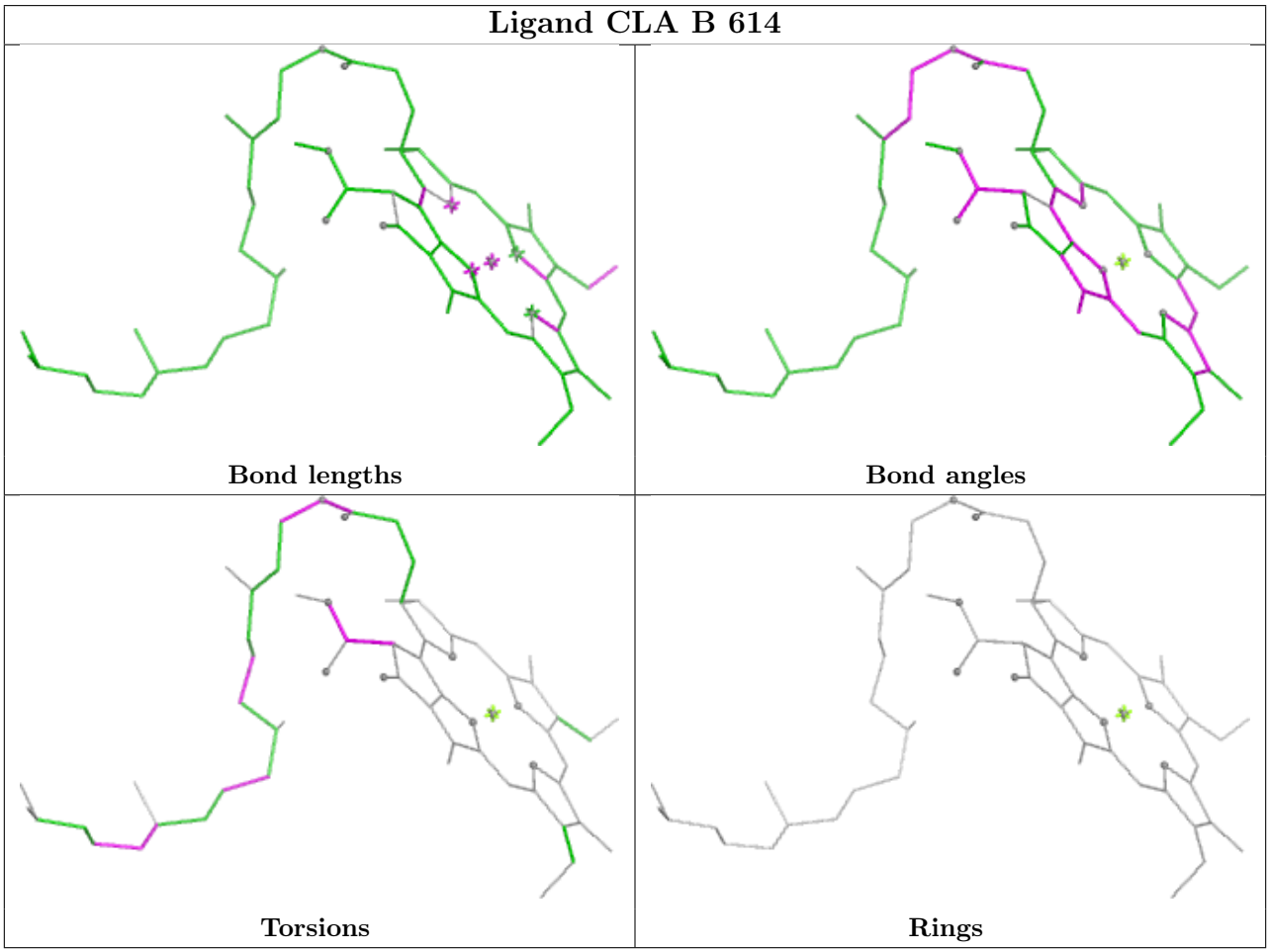


Rings

Ligand LUT S 620



Ligand CLA B 614



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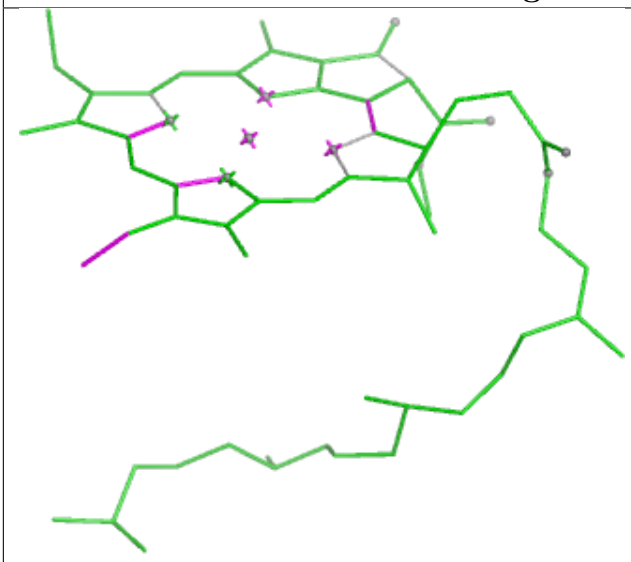
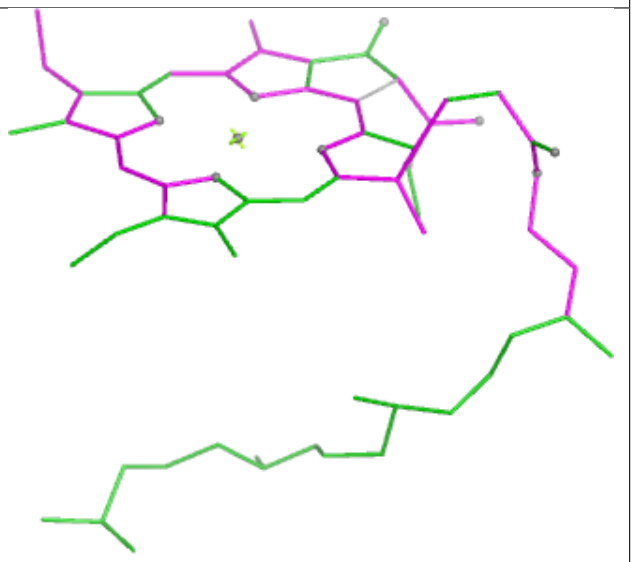
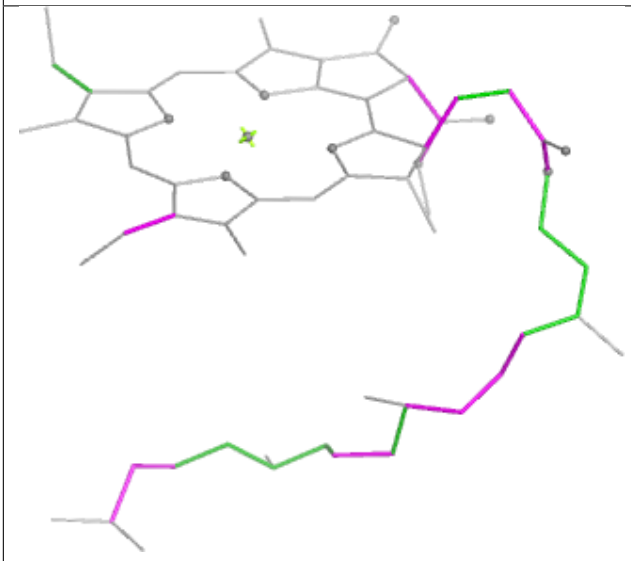


Bond lengths



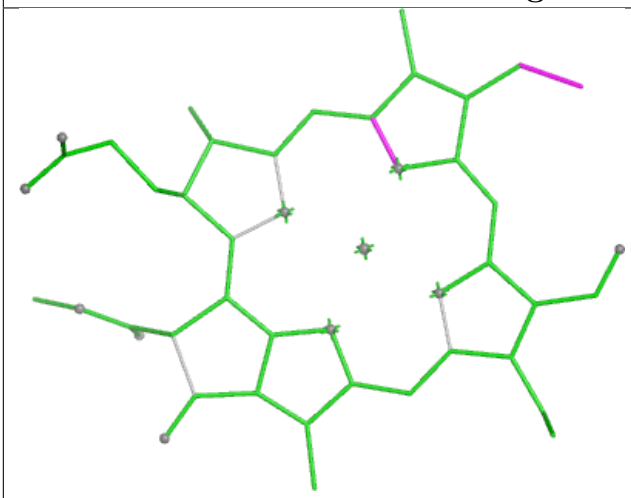
Bond angles



Torsions

Rings

Ligand CHL S 601



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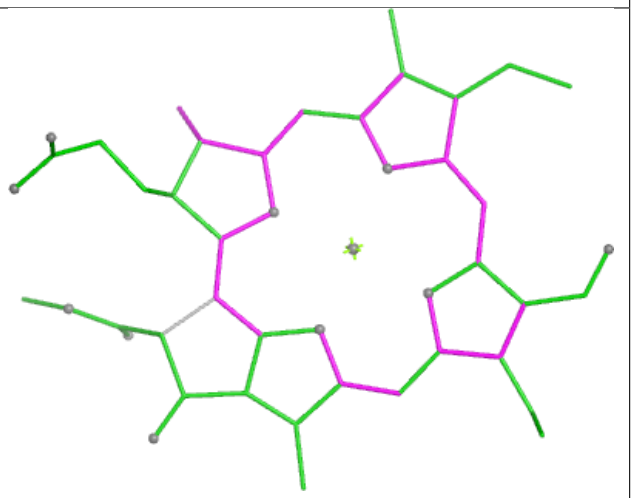
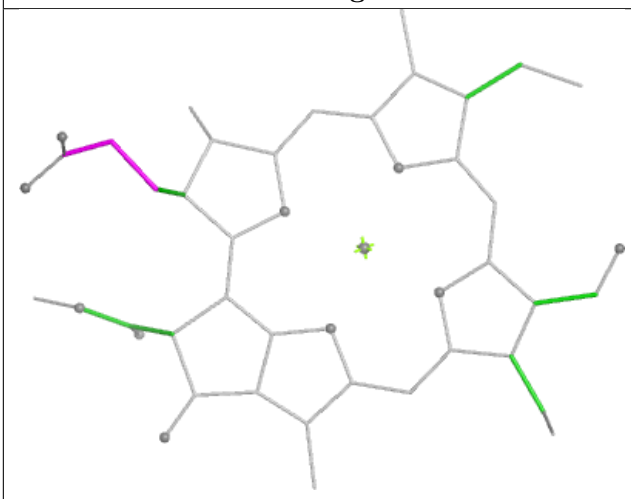
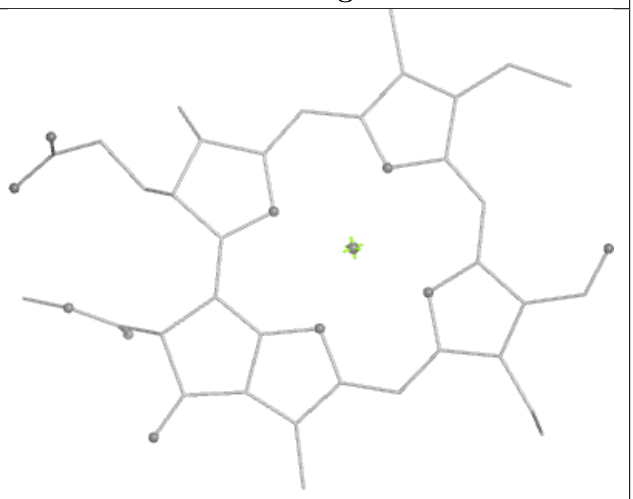


Bond angles

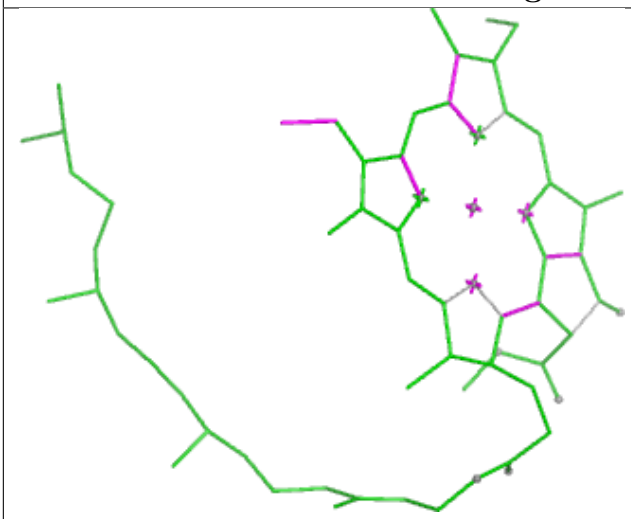


Torsions



Rings

Ligand CLA C 507



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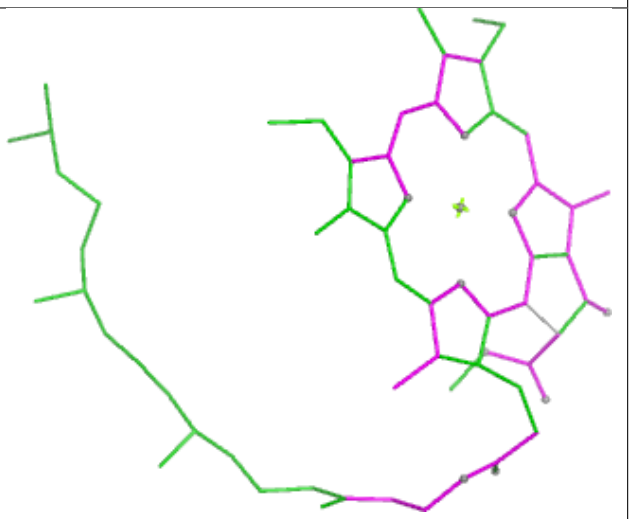
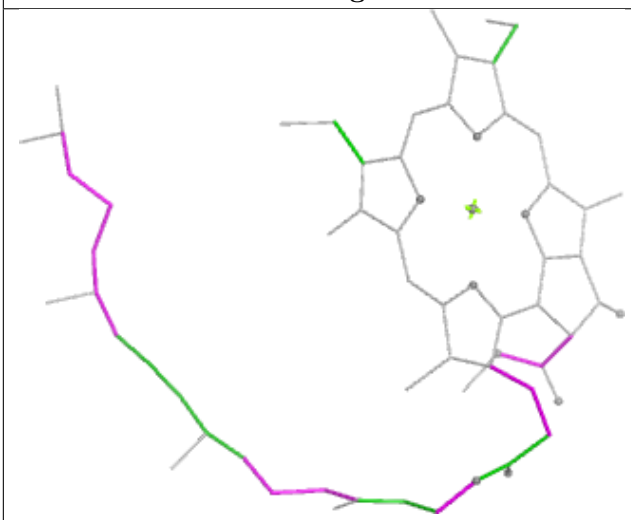
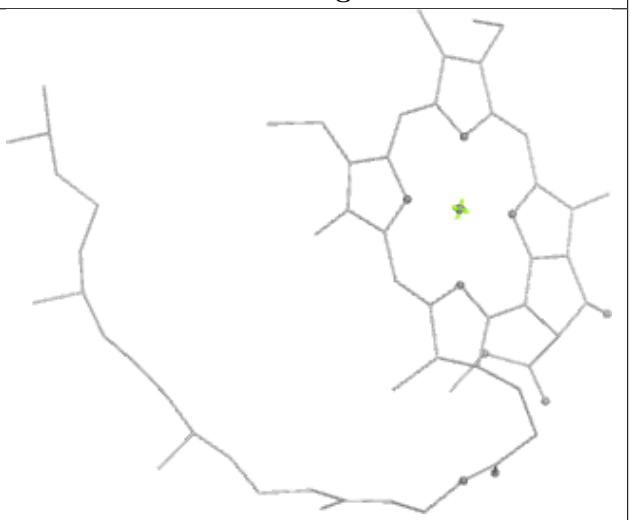


Bond angles

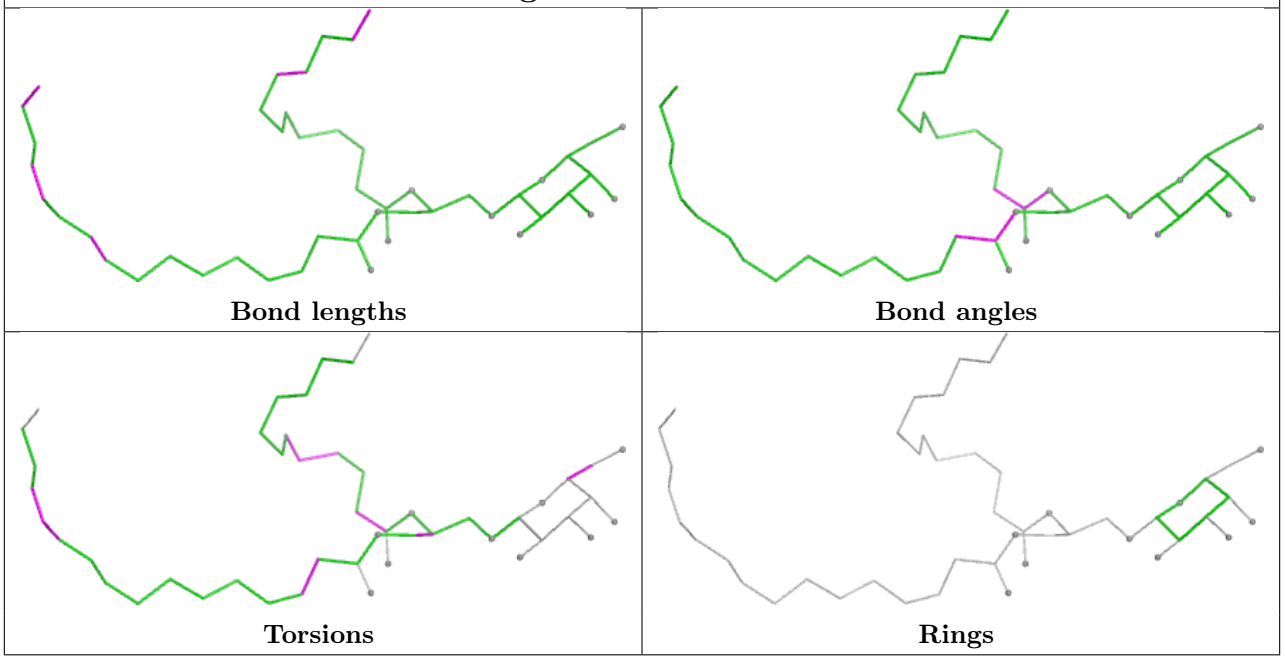


Torsions

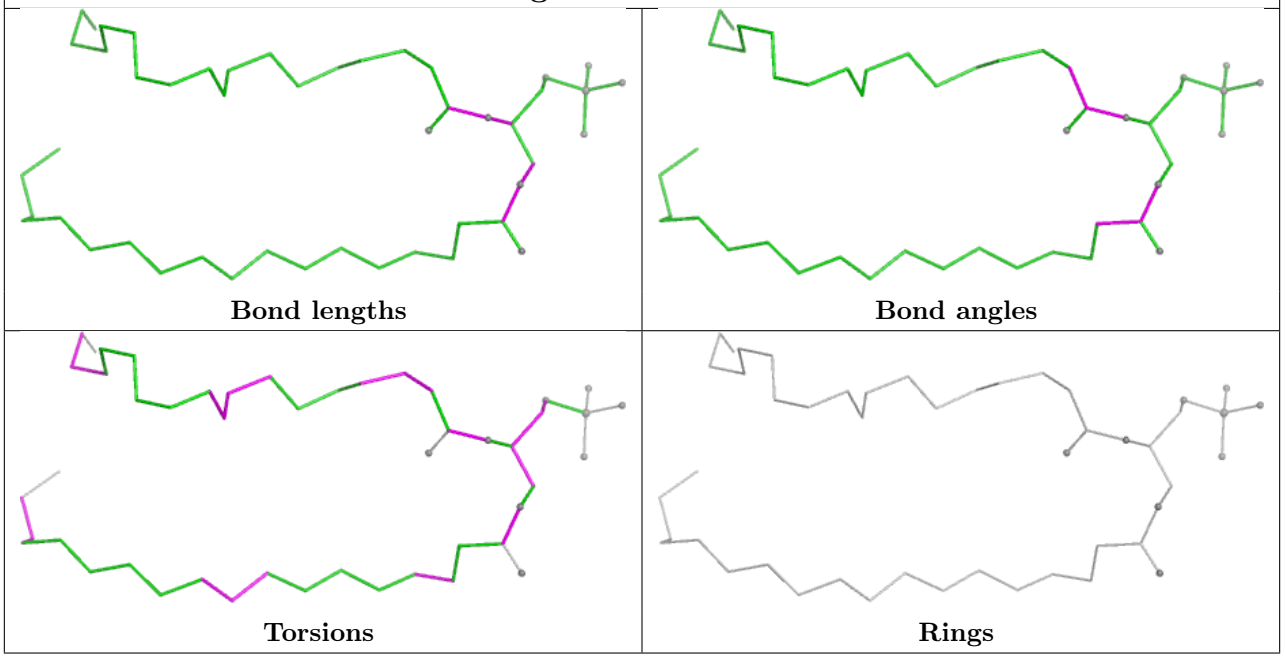


Rings

Ligand LMG H 102



Ligand 3PH b 624



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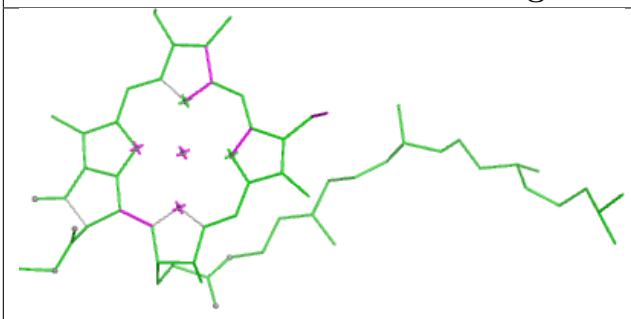
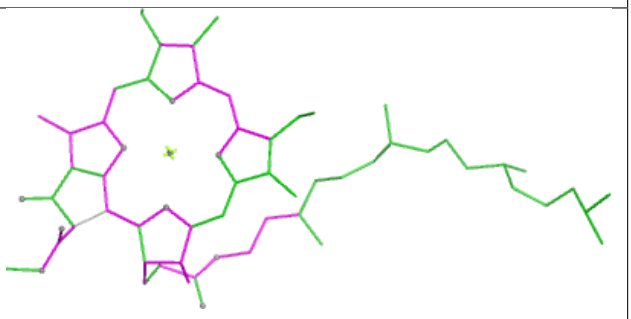
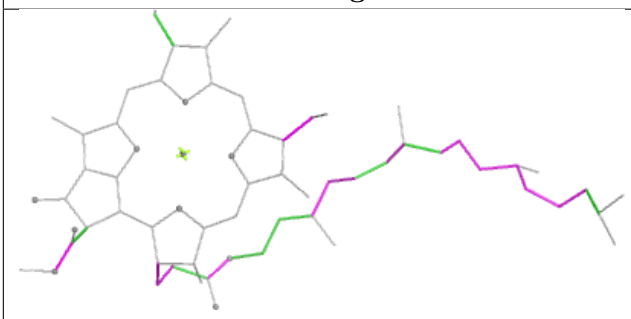


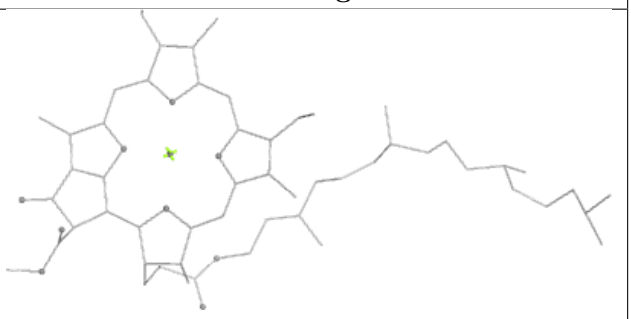
Bond lengths



Bond angles

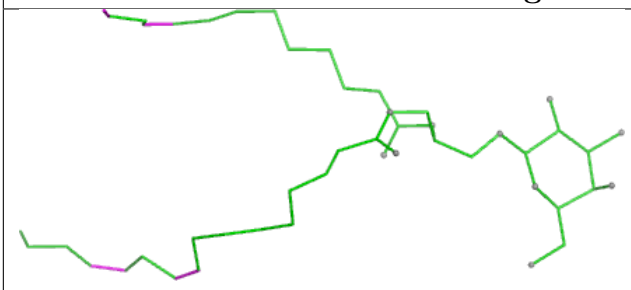


Torsions



Rings

Ligand LMG a 413



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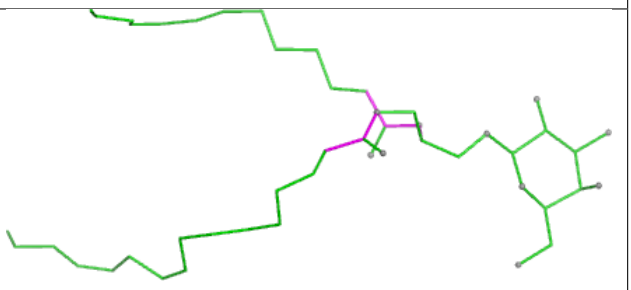
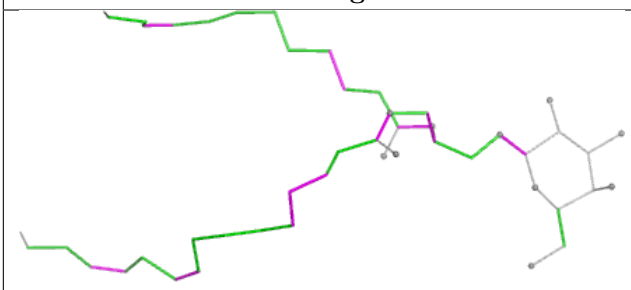
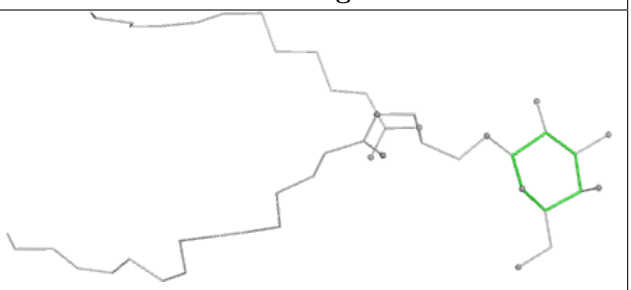


Bond angles

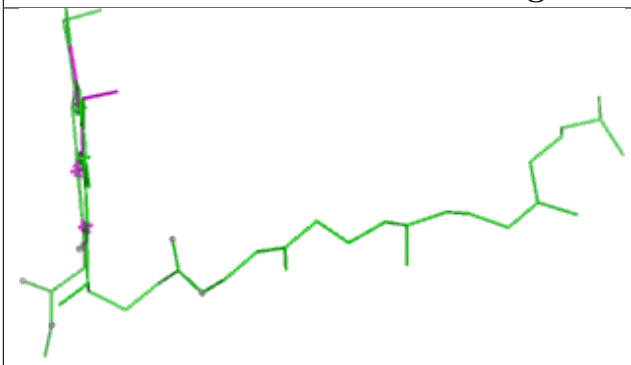


Torsions



Rings

Ligand CLA b 607



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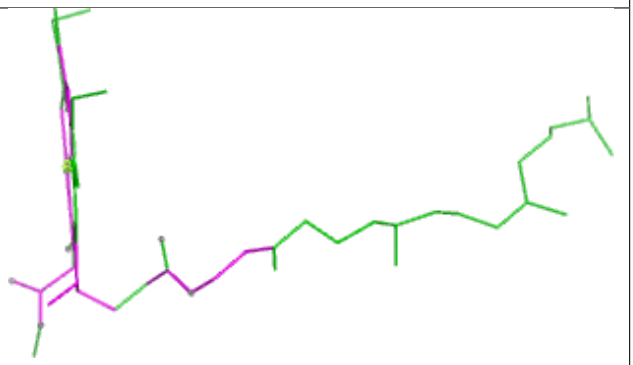
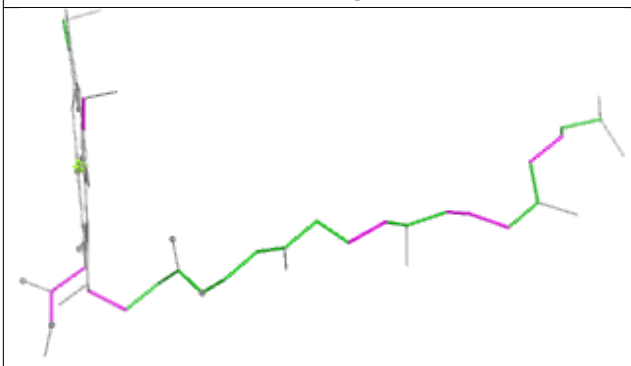
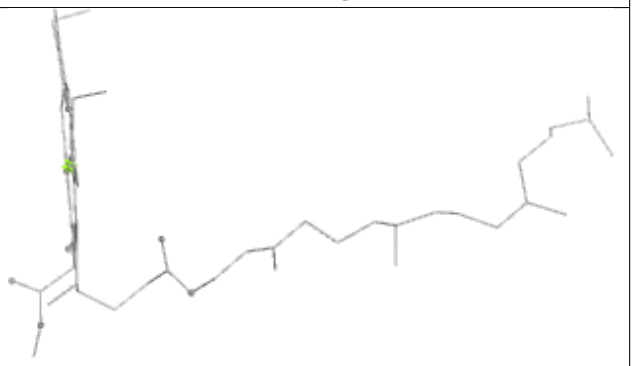


Bond angles

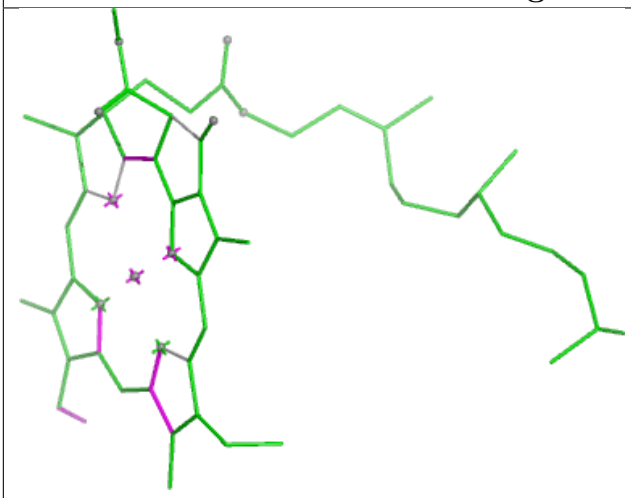


Torsions

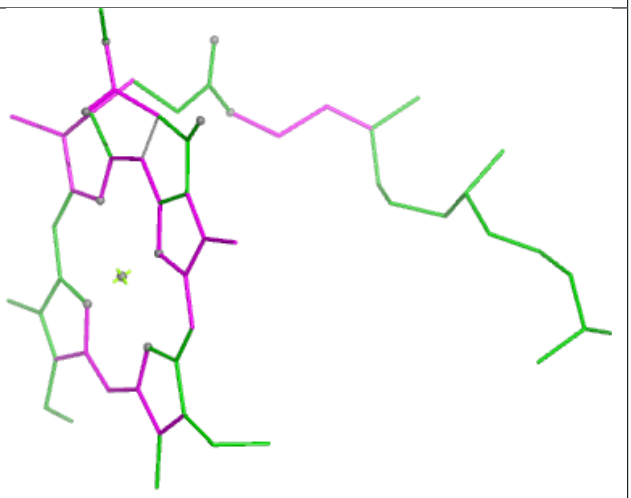


Rings

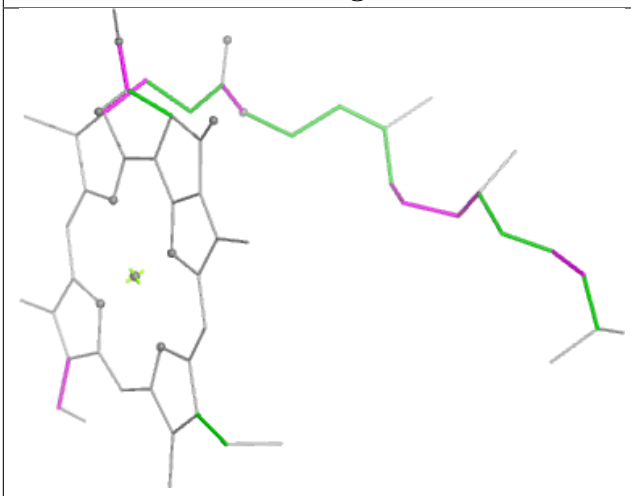
Ligand CLA S 609



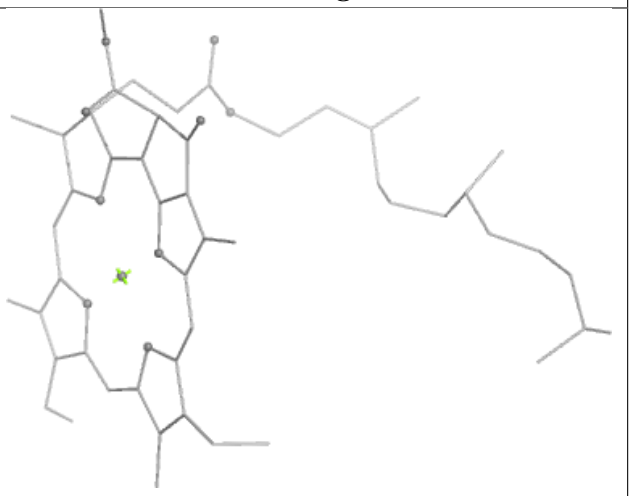
Bond lengths



Bond angles

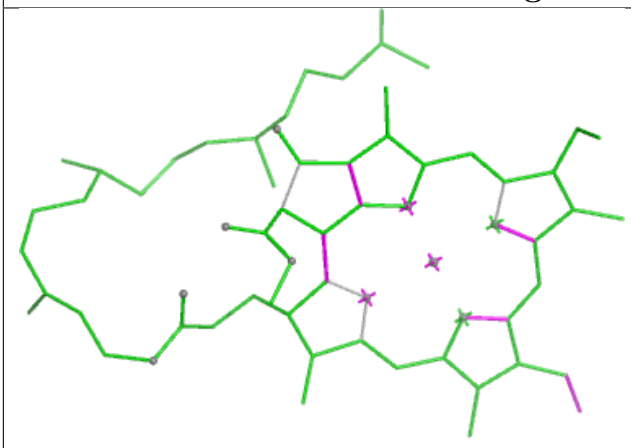


Torsions



Rings

Ligand CLA C 509



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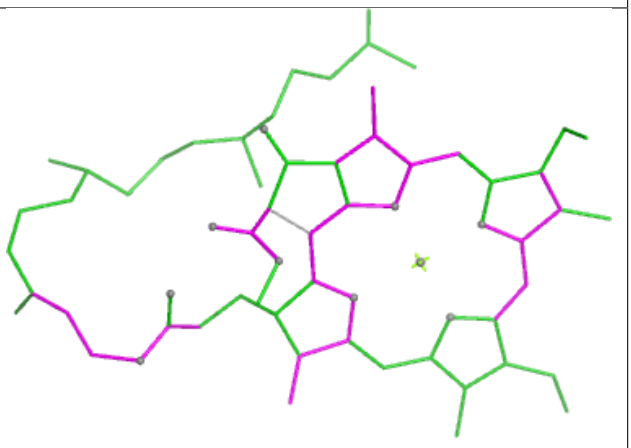

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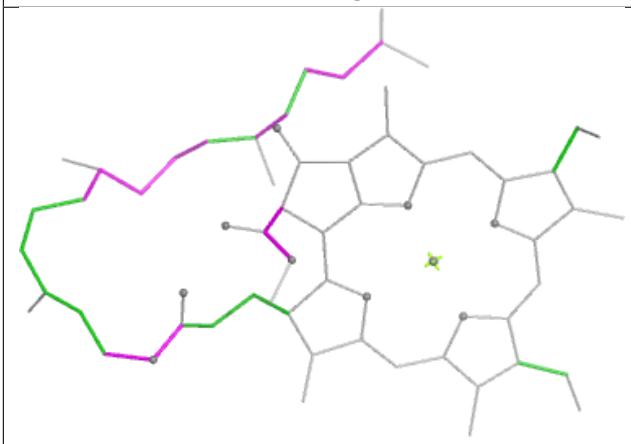

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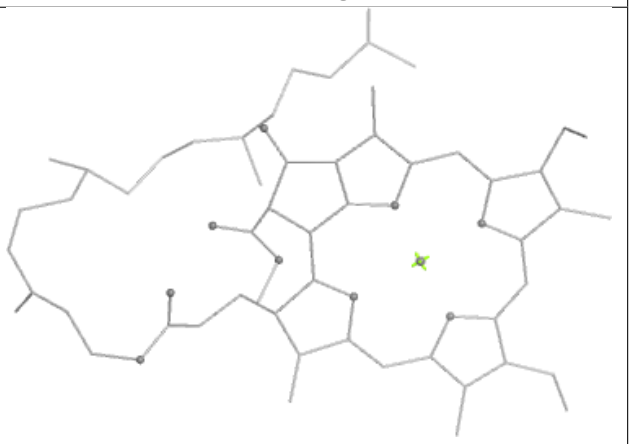
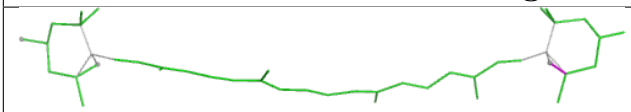


Rings

Ligand XAT N 622



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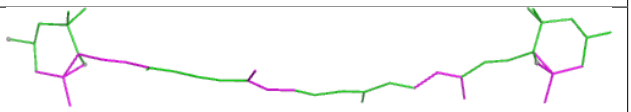

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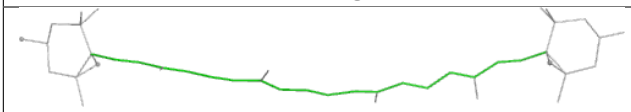
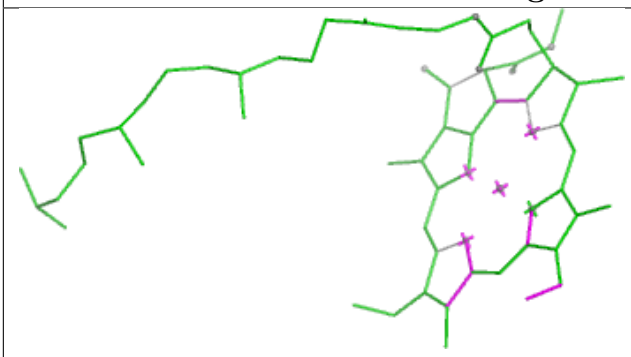


Torsions

Rings

Ligand CLA S 611



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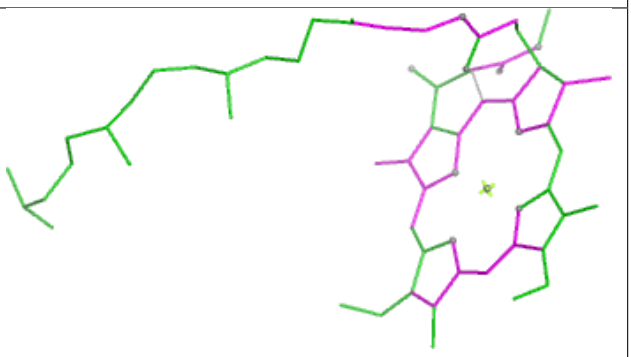

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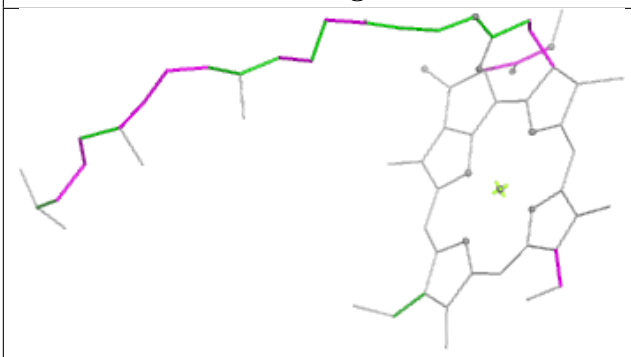
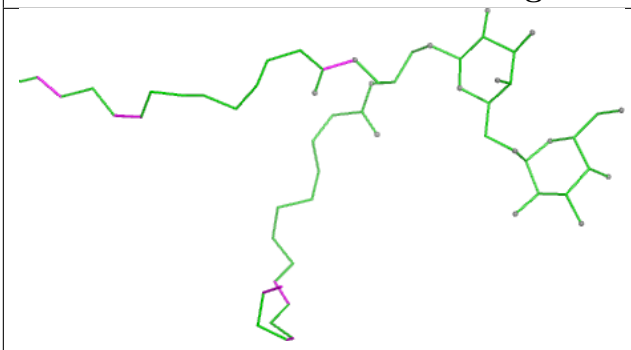


Torsions

Rings

Ligand DGD c 519



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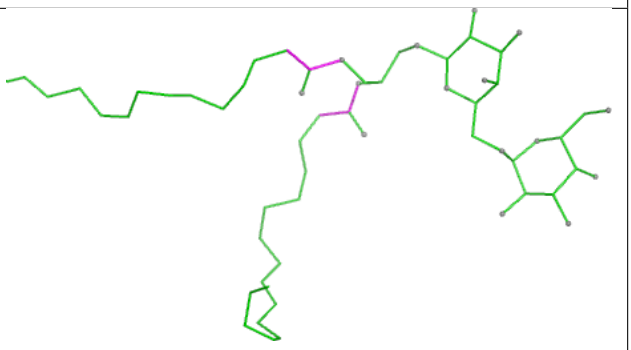
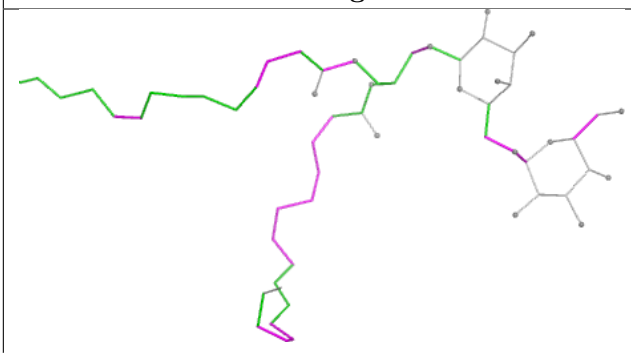


Bond angles



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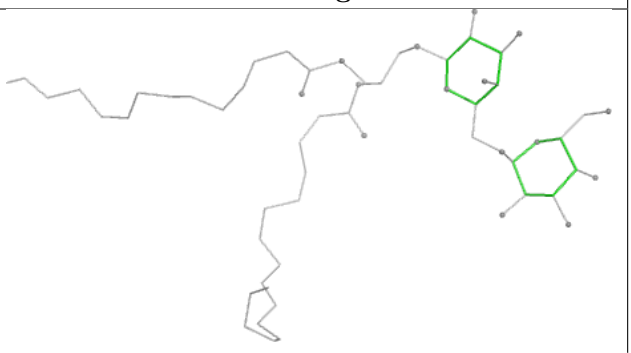
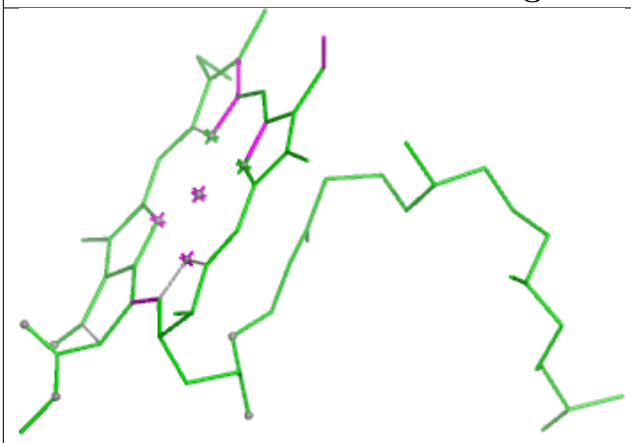


Rings

Ligand CLA Y 613



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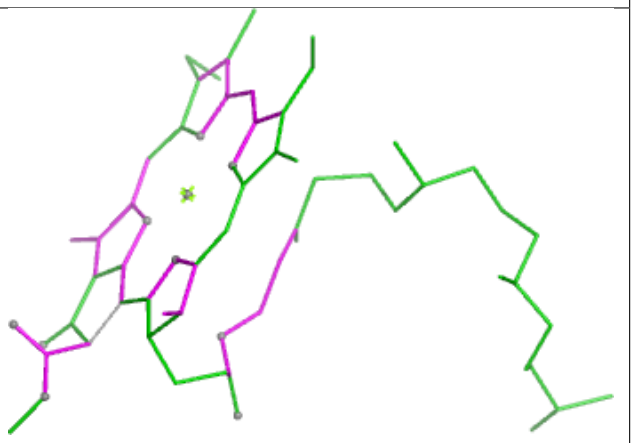

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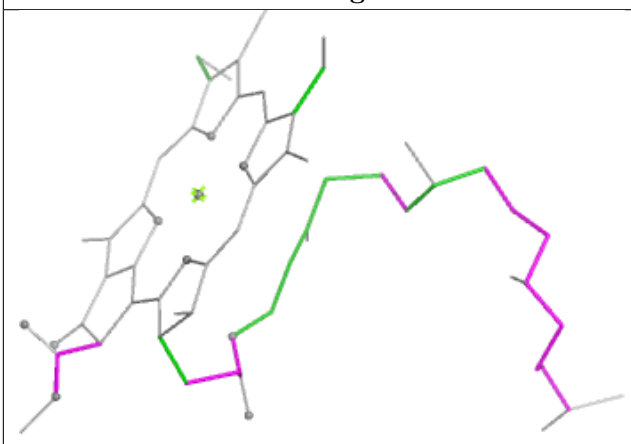

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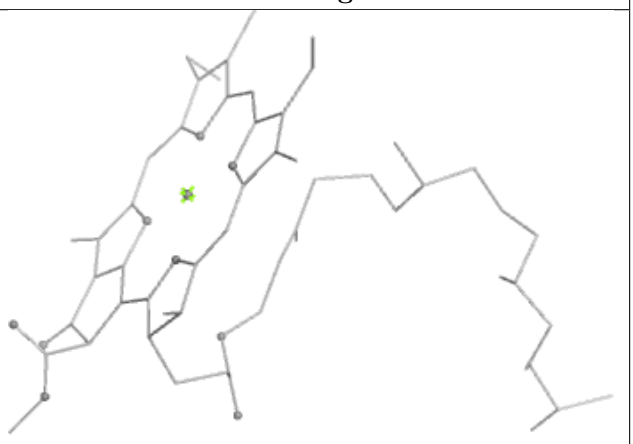
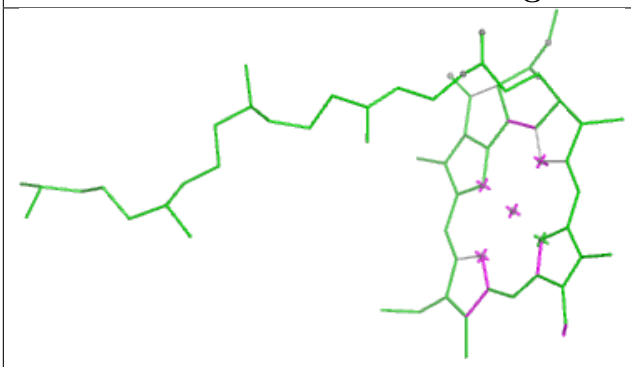


Rings

Ligand CLA Y 611



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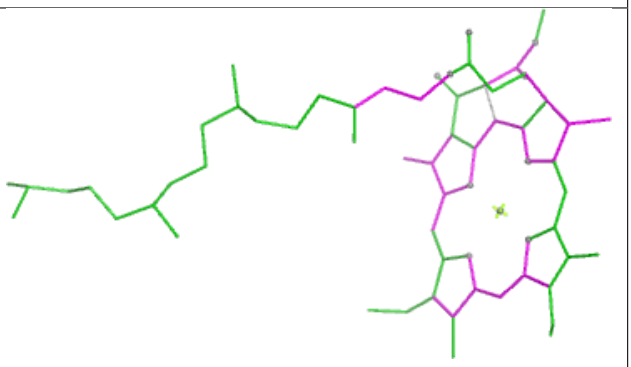

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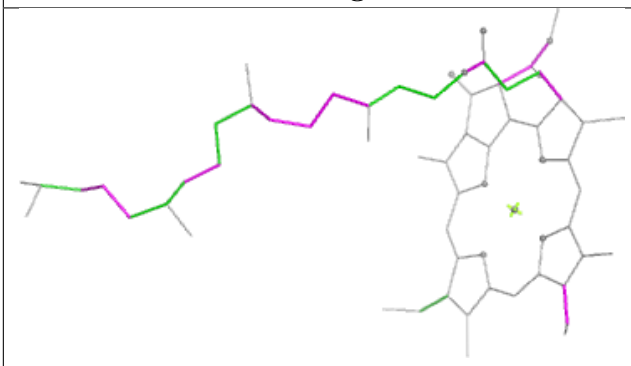

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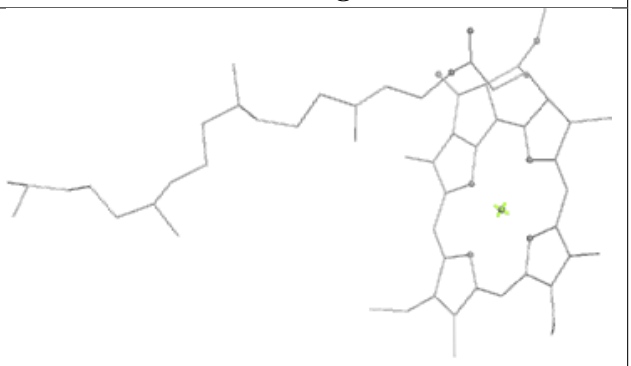
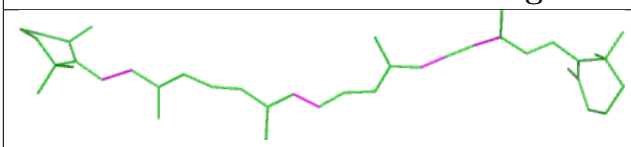


Rings

Ligand BCR b 619



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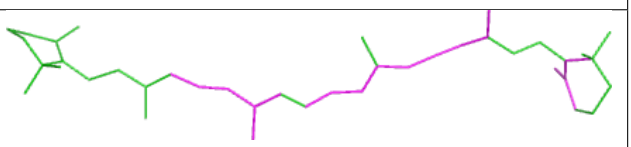

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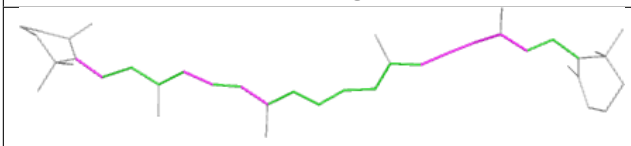

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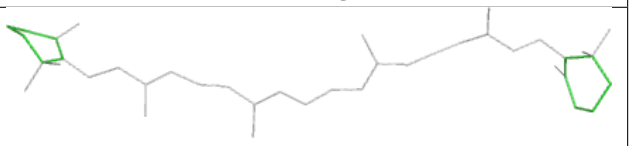
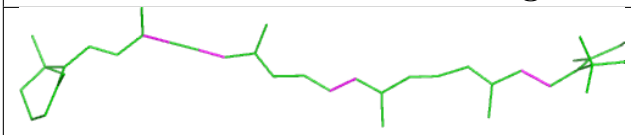


Rings

Ligand BCR A 411



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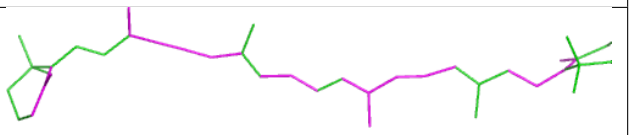

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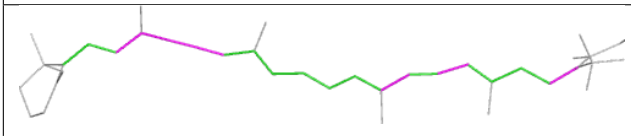

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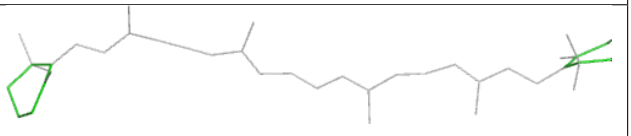
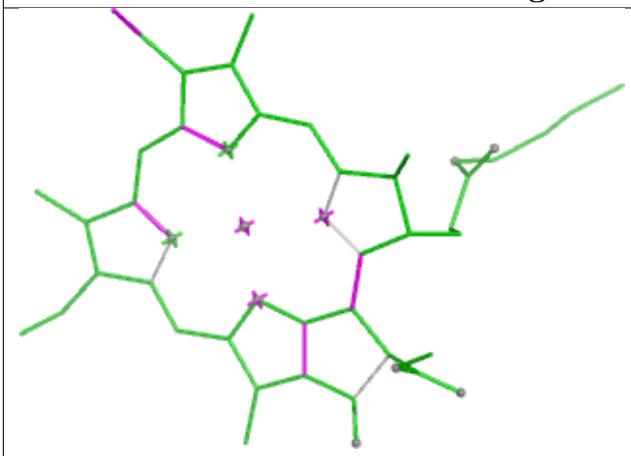


Rings

Ligand CLA a 407



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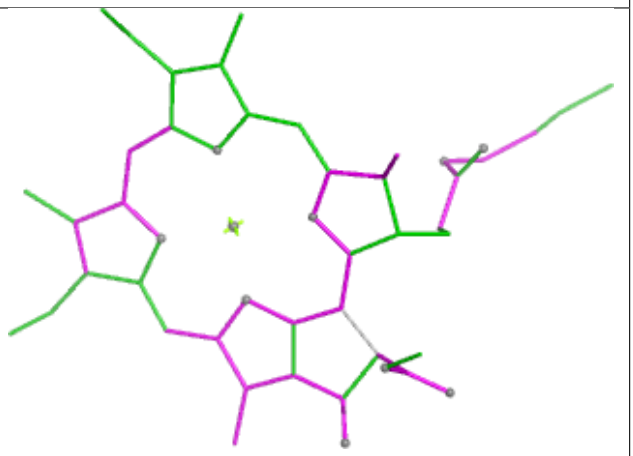

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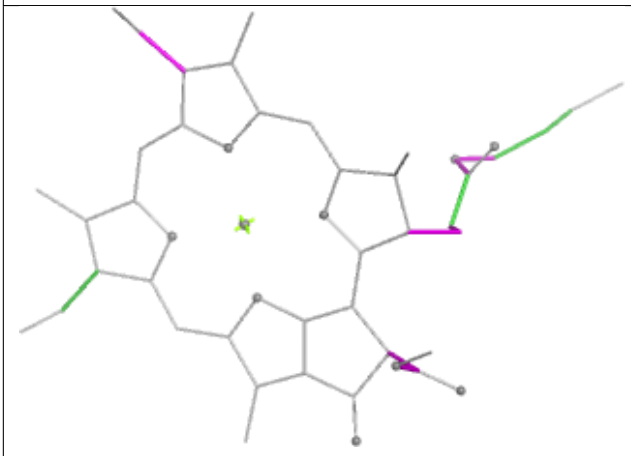

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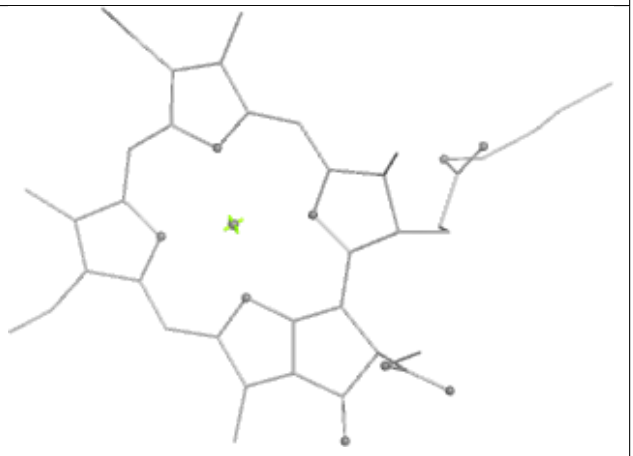
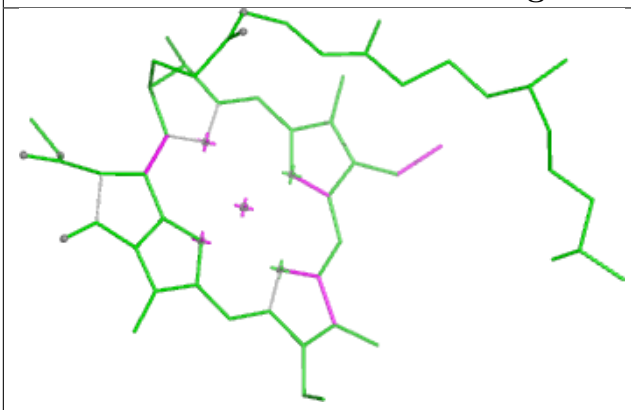


Rings

Ligand CLA S 602



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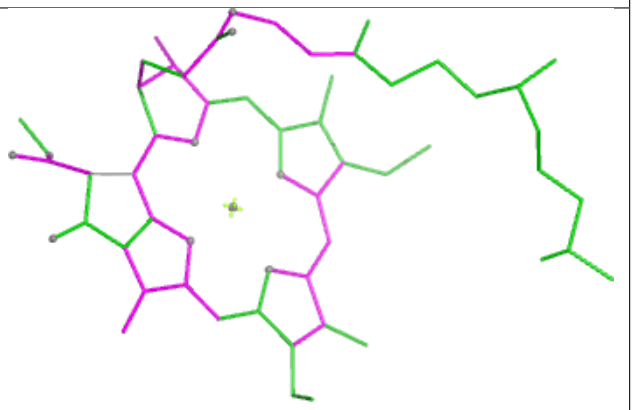
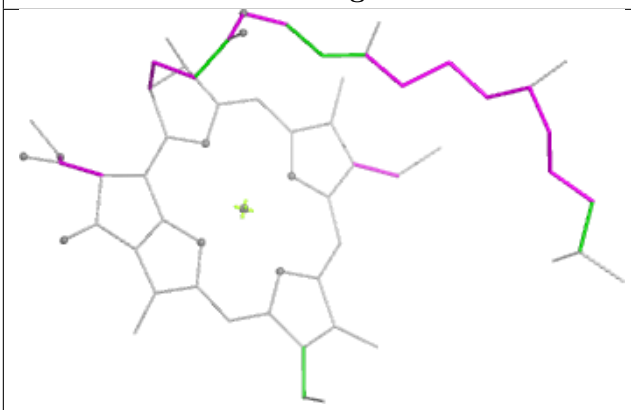


Bond angles



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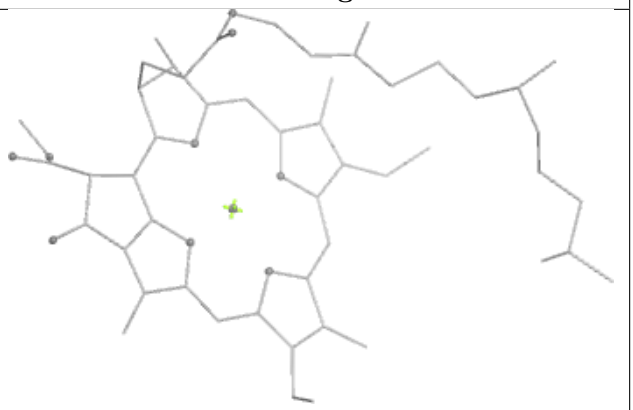
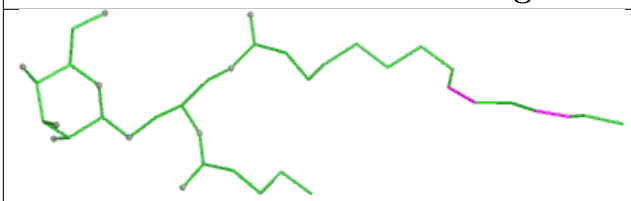


Rings

Ligand LMG W 201



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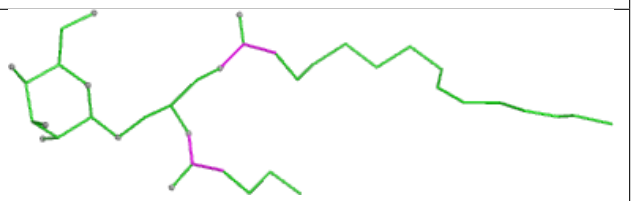
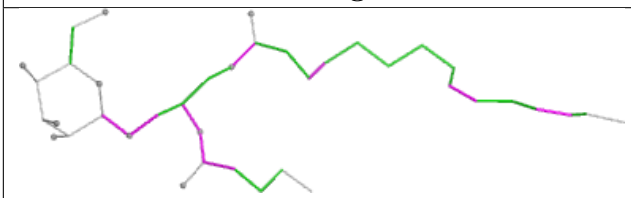


Bond angles



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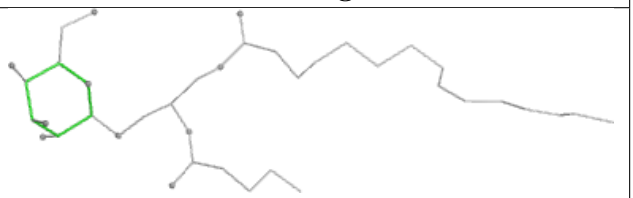
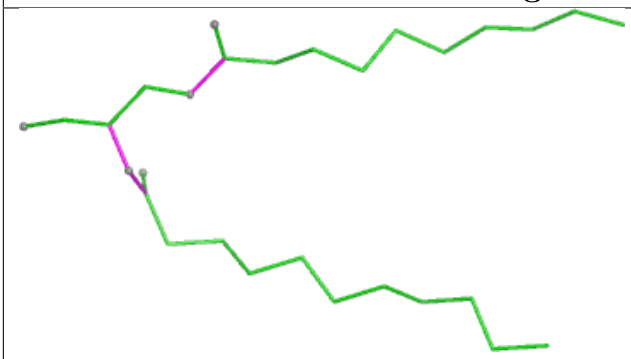


Rings

Ligand DGA J 101



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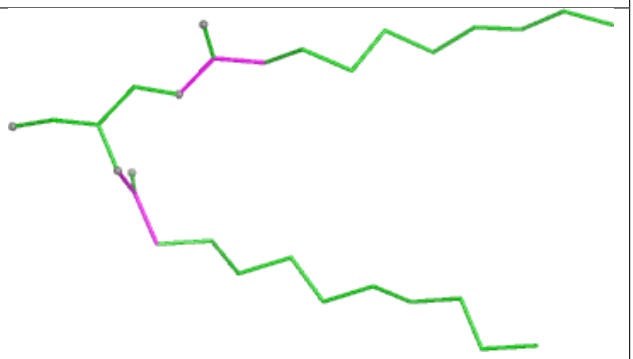
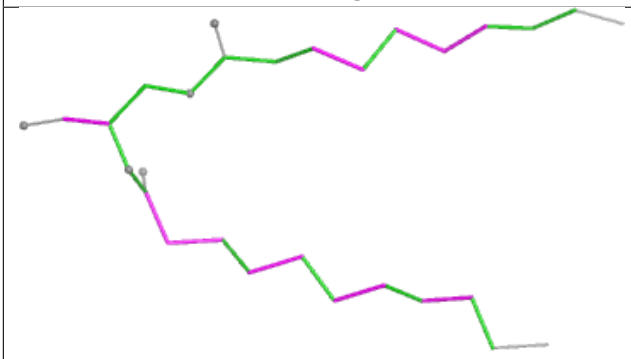


Bond angles



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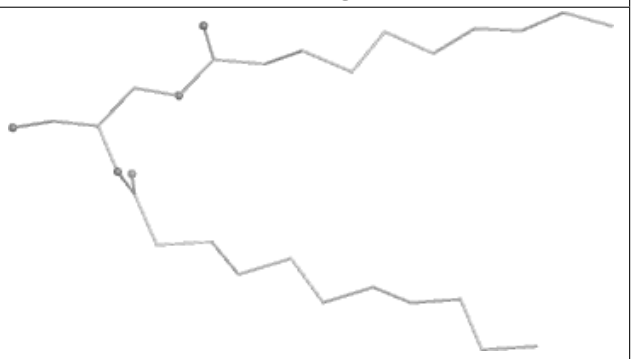
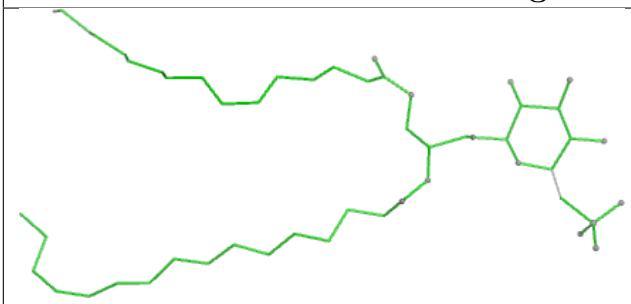


Rings

Ligand SQD c 526



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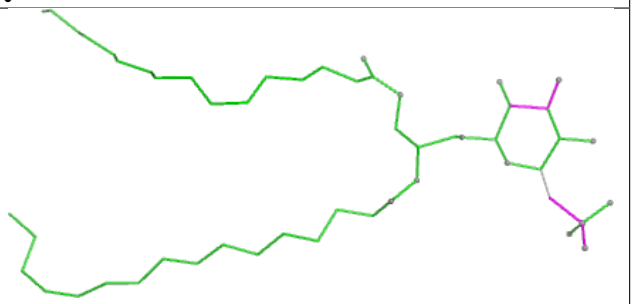
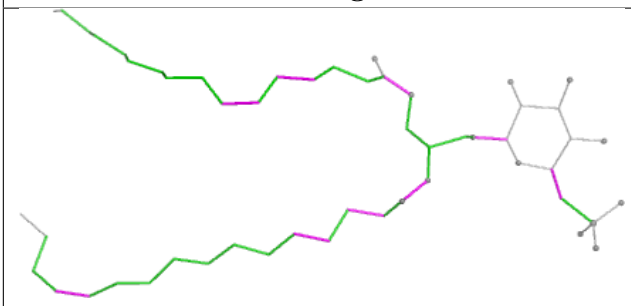
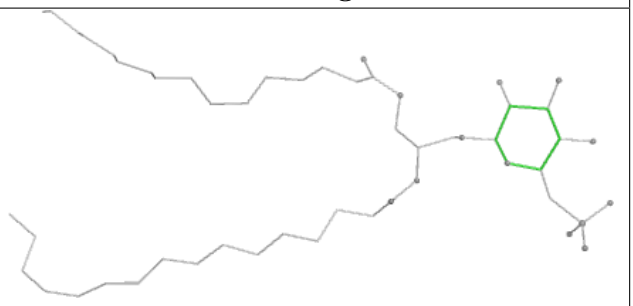


Bond angles

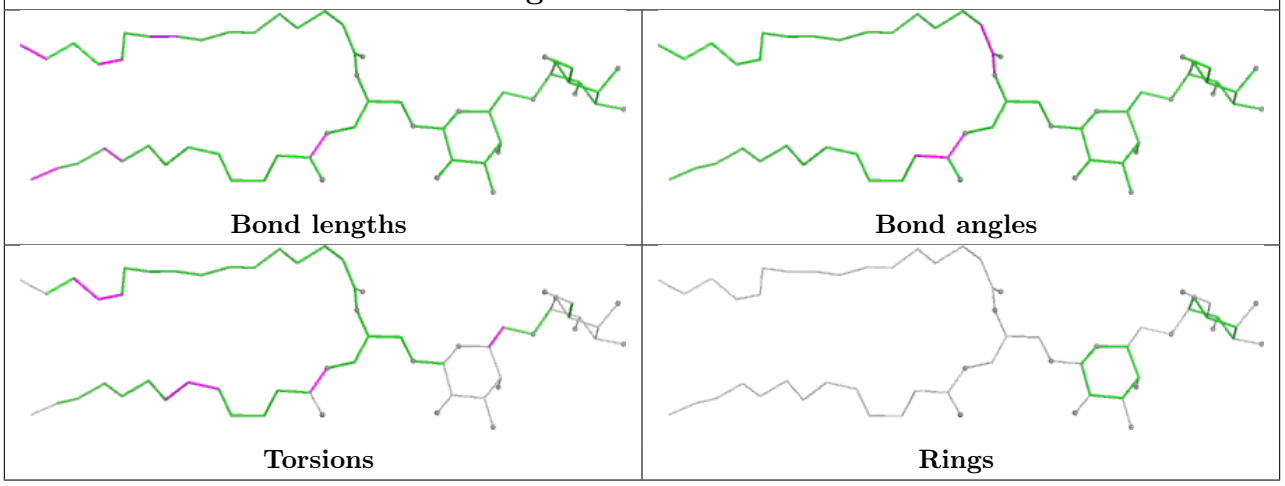


Torsions

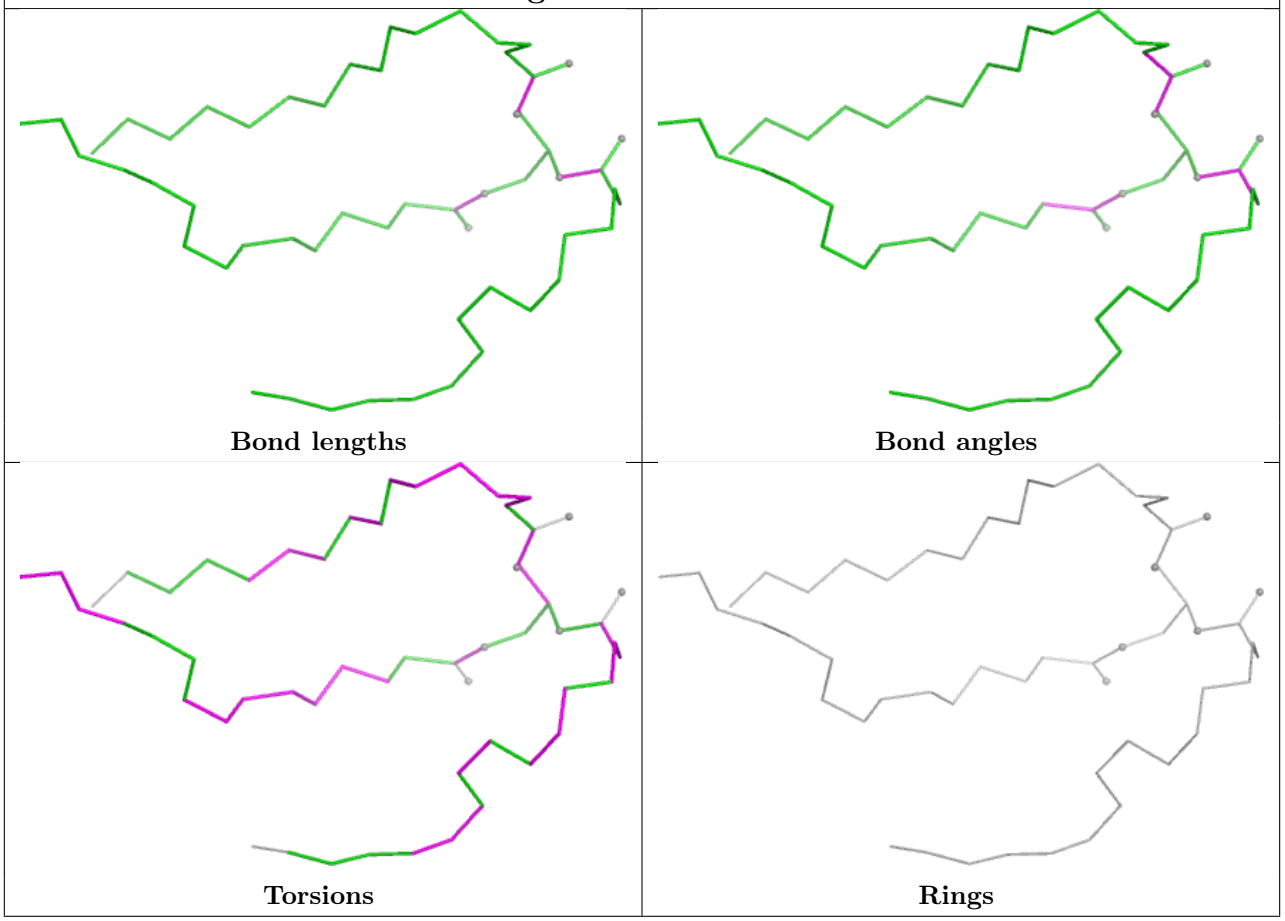


Rings

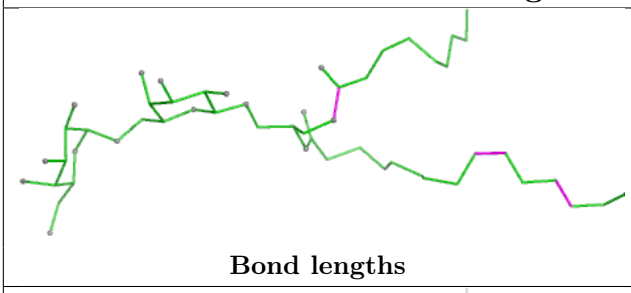
Ligand DGD c 520



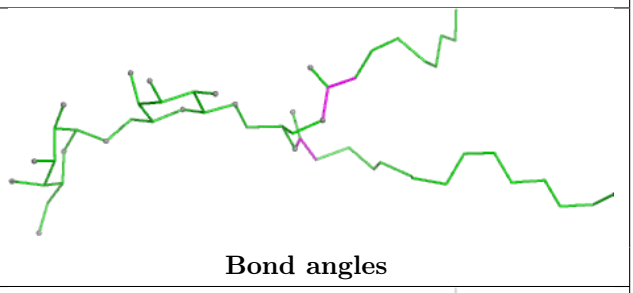
Ligand 4RF K 101



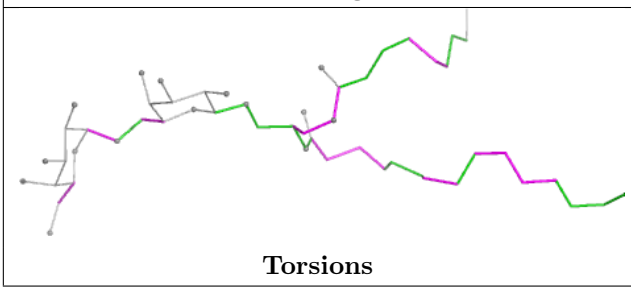
Ligand DGD c 518



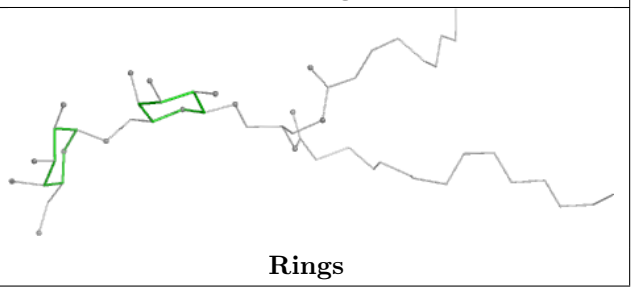
Bond lengths



Bond angles

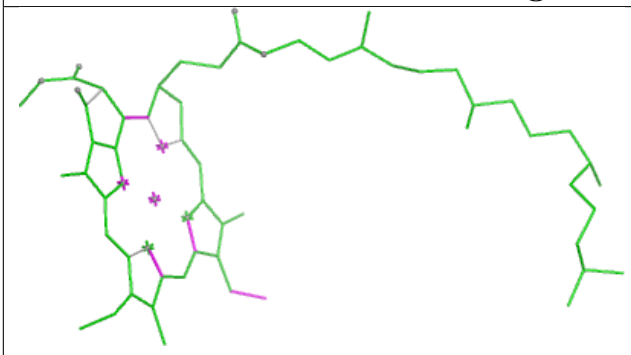


Torsions



Rings

Ligand CLA b 610



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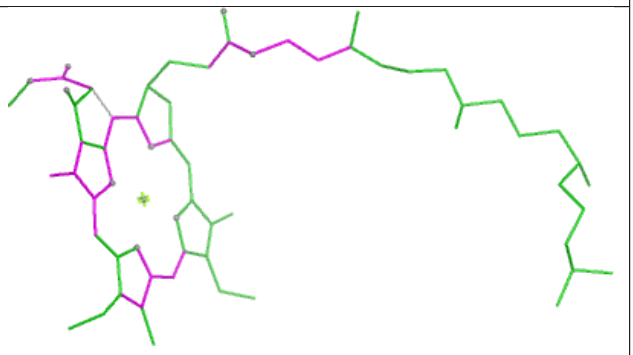
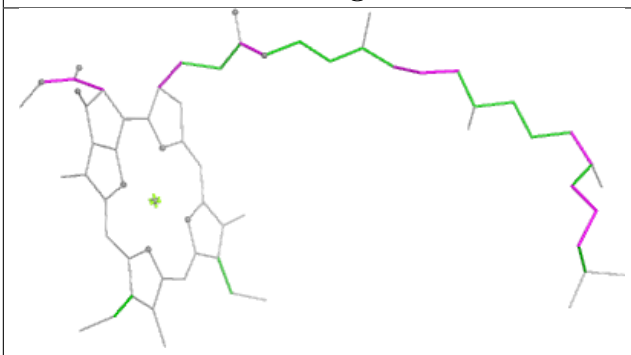
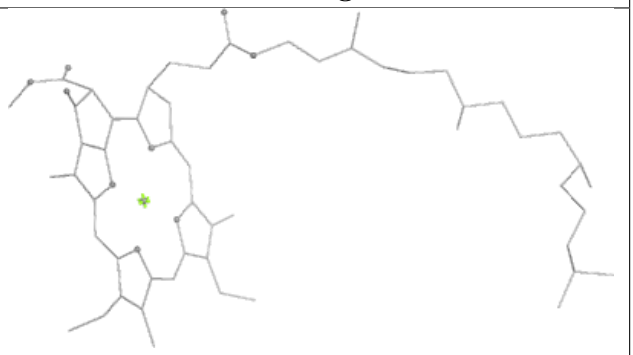


Bond angles

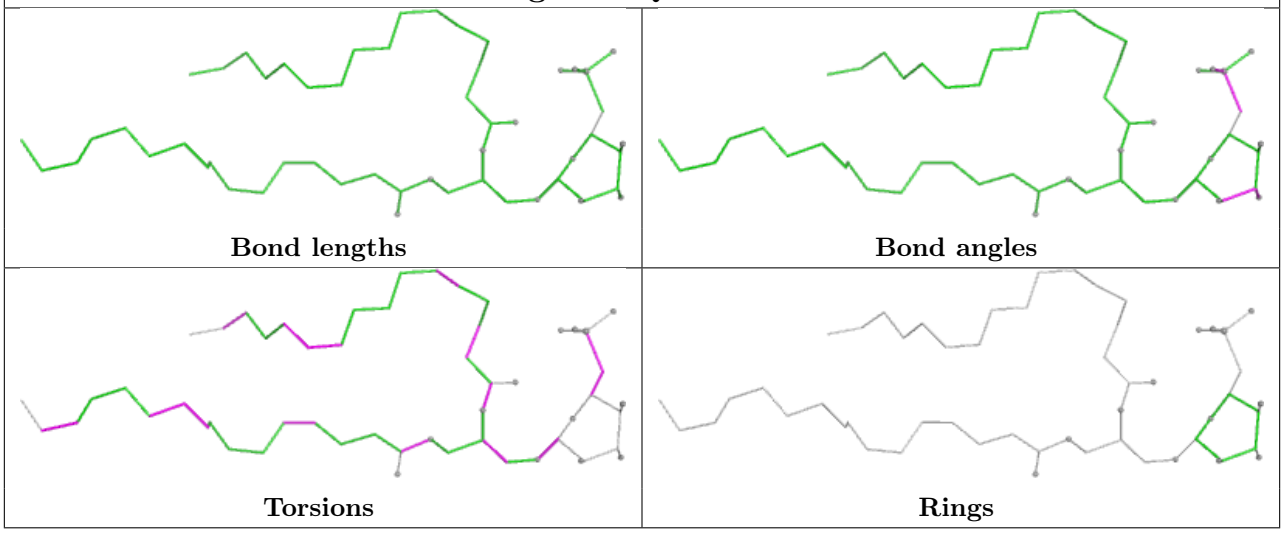


Torsions

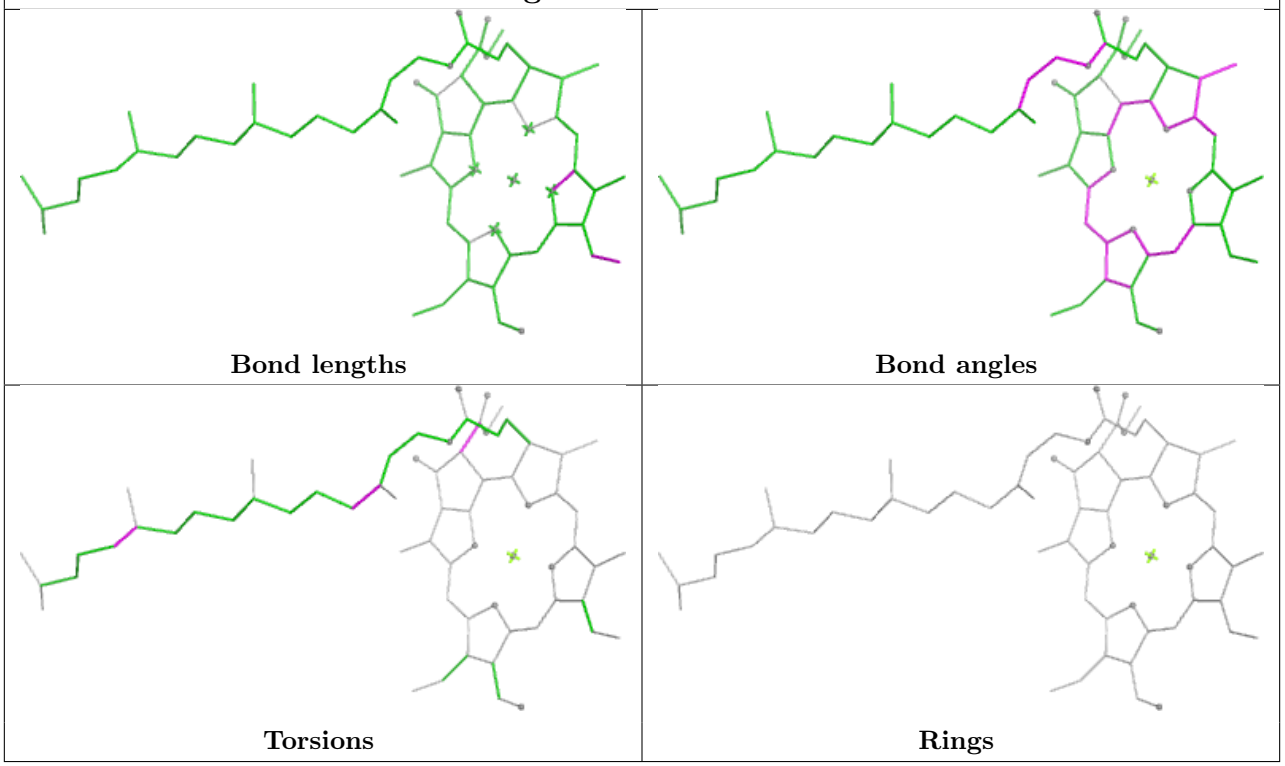


Rings

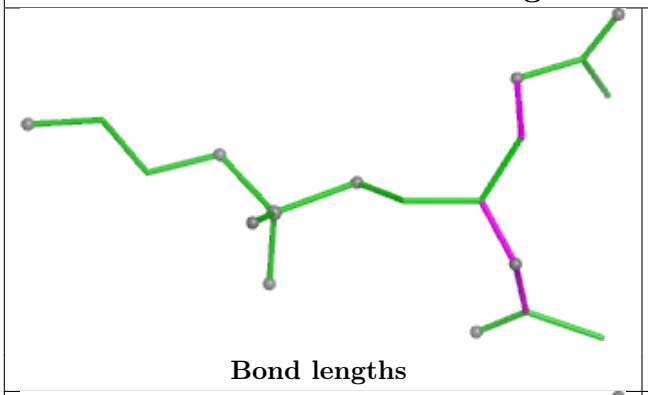
Ligand SQD b 626



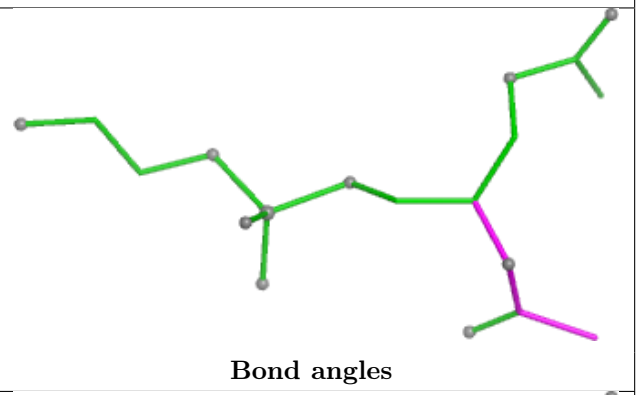
Ligand CHL N 609



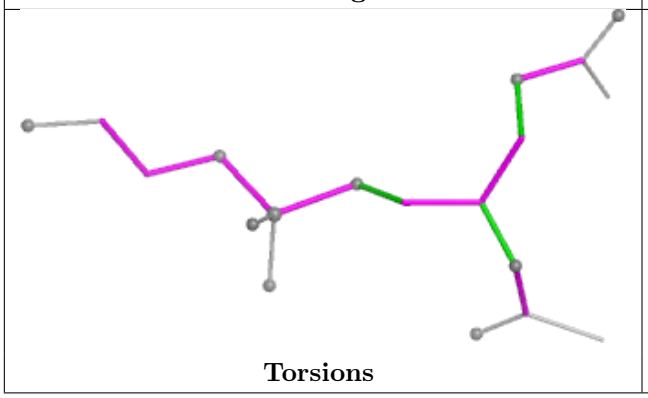
Ligand PTY Y 627



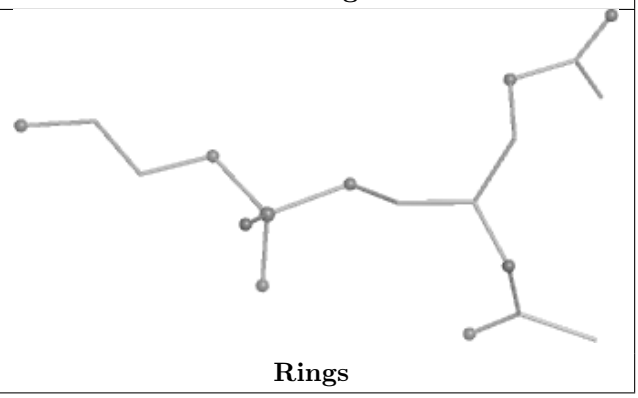
Bond lengths



Bond angles

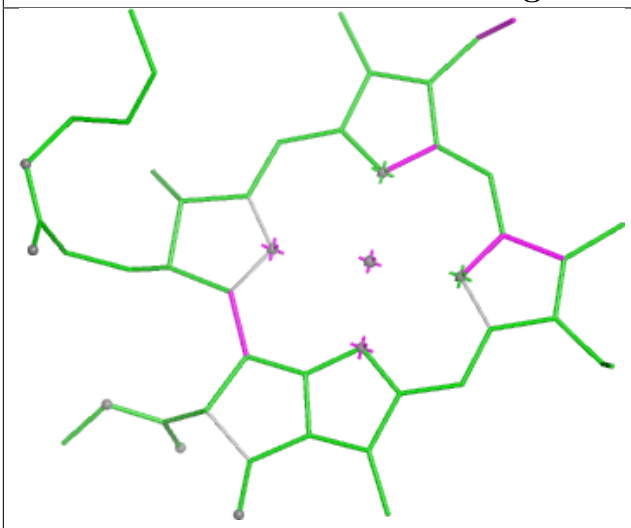


Torsions

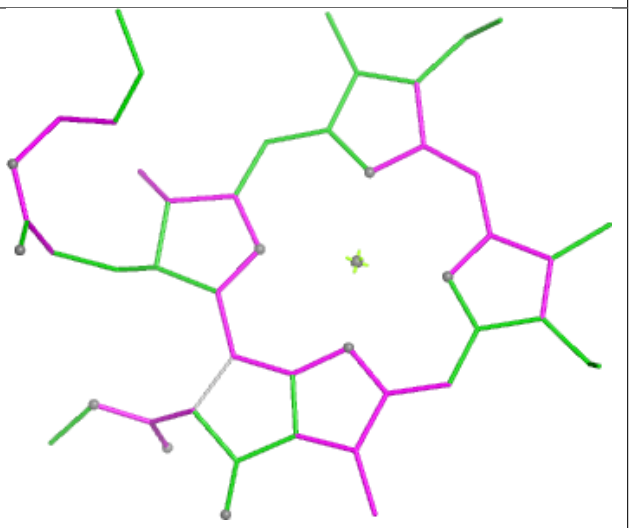


Rings

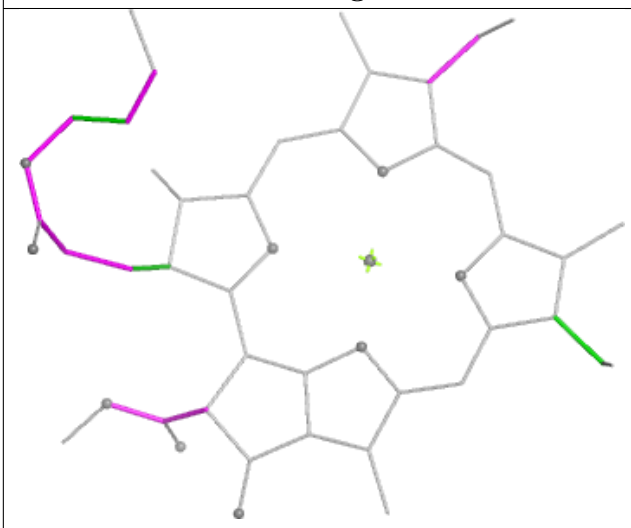
Ligand CLA N 611



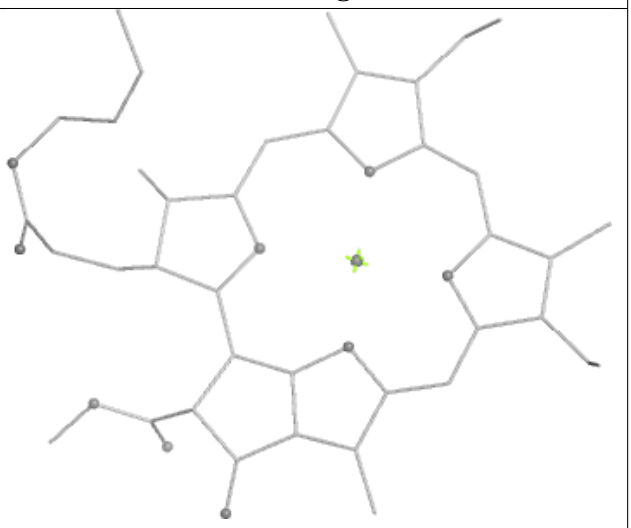
Bond lengths



Bond angles

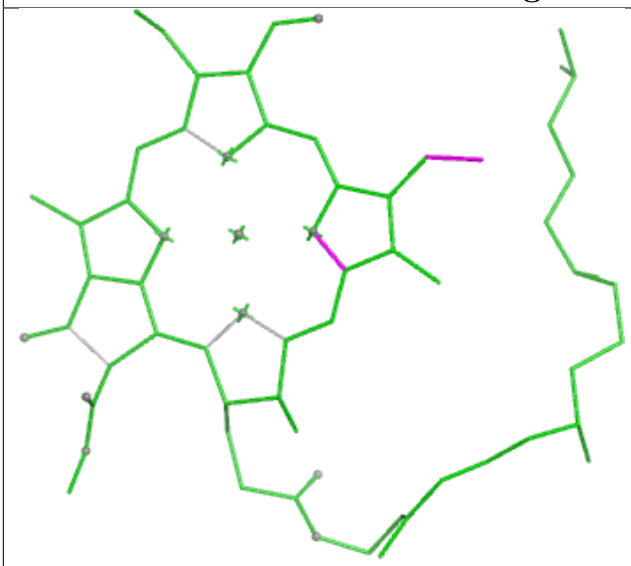


Torsions

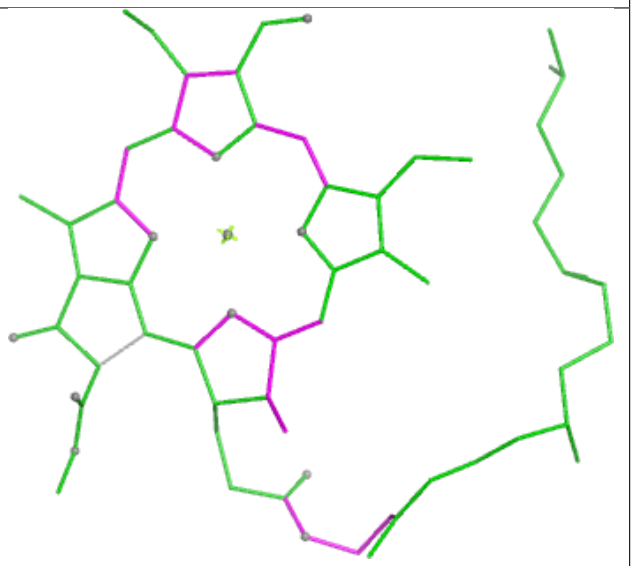


Rings

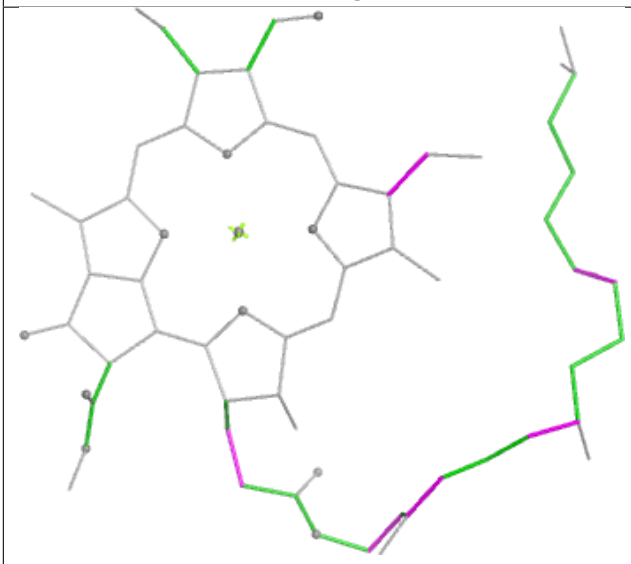
Ligand CHL Y 607



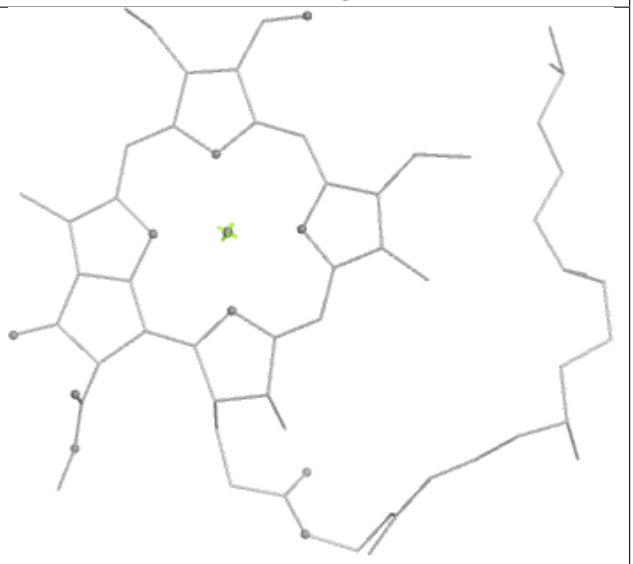
Bond lengths



Bond angles

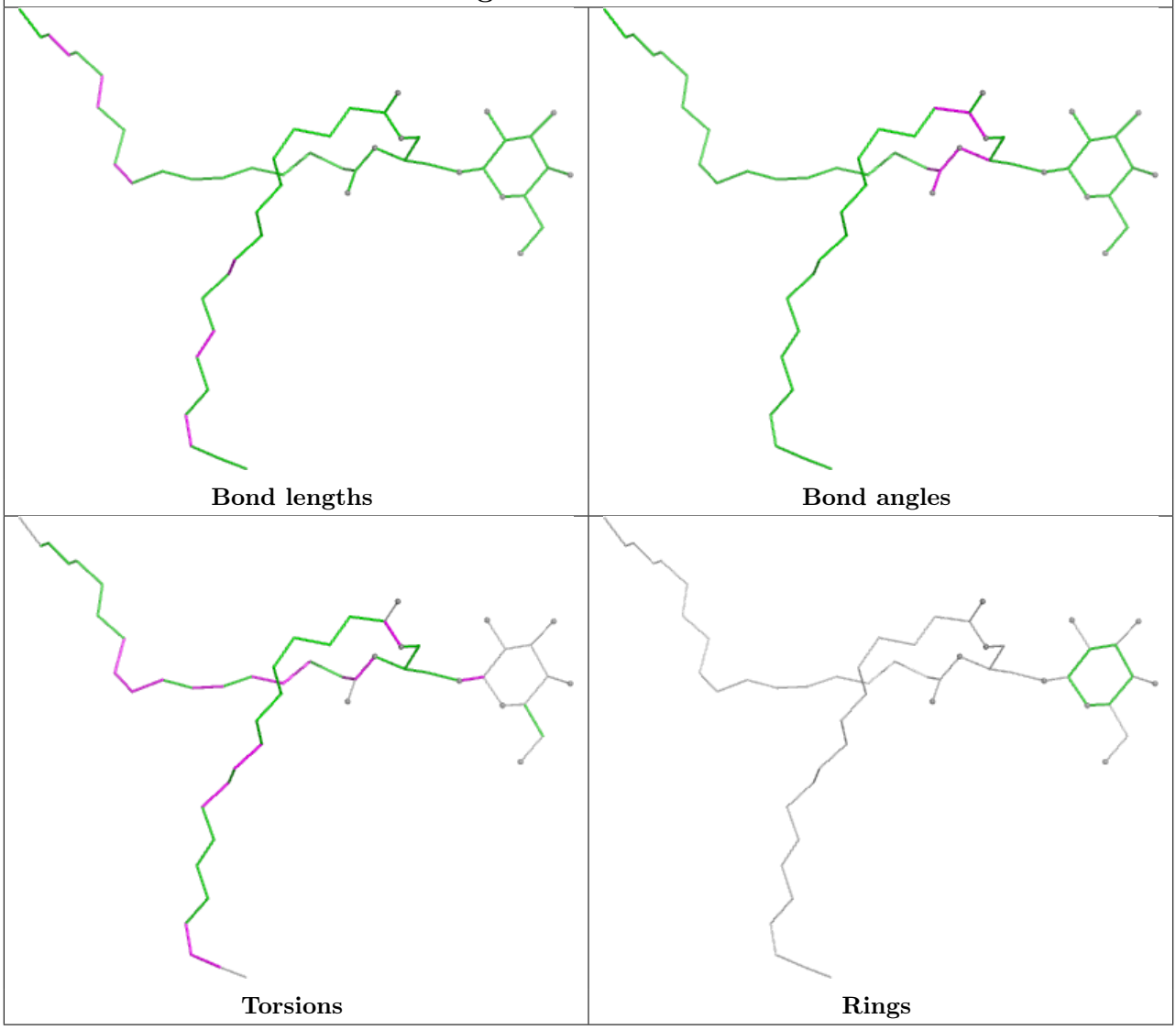


Torsions

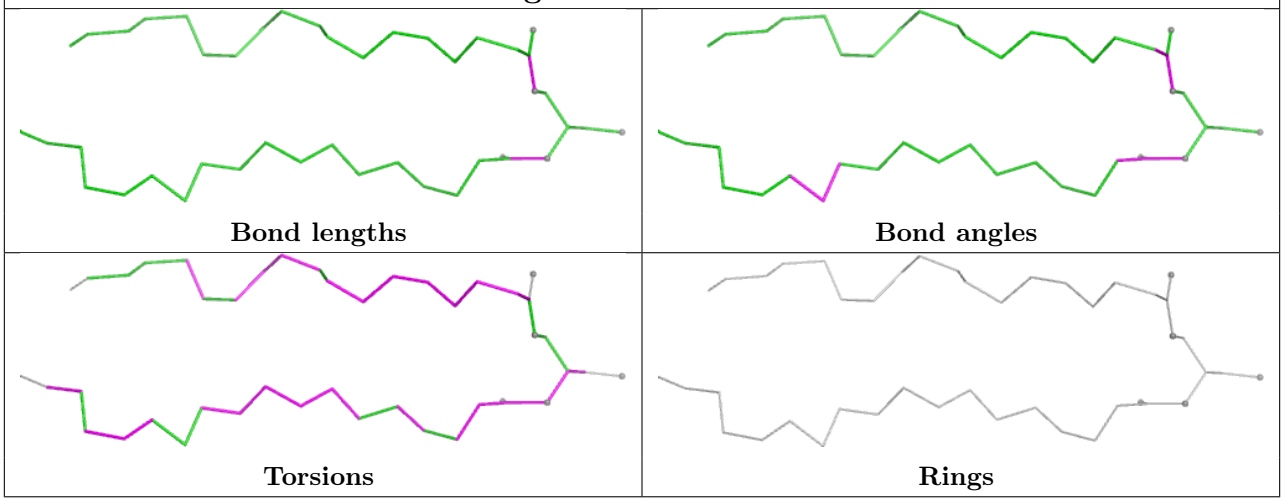


Rings

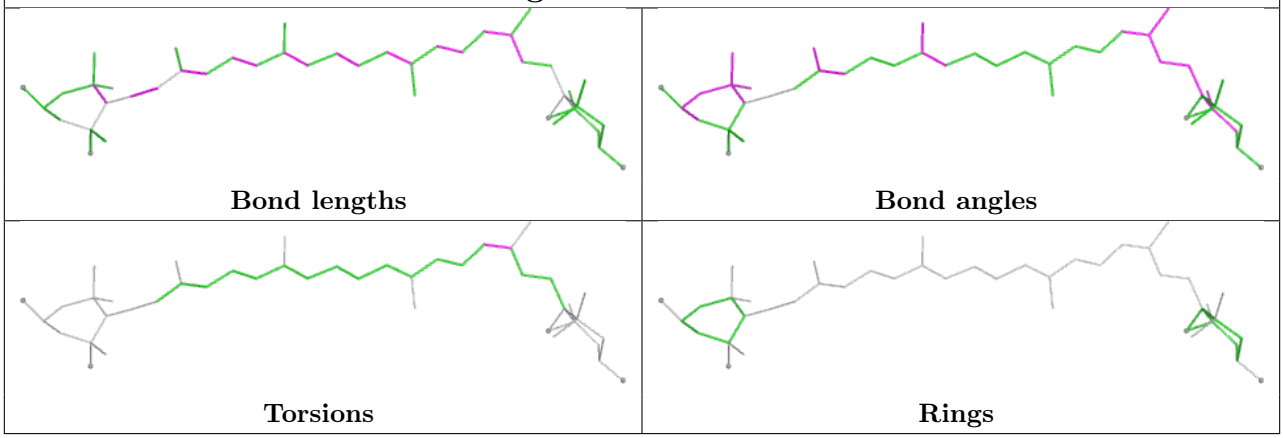
Ligand LMG C 523



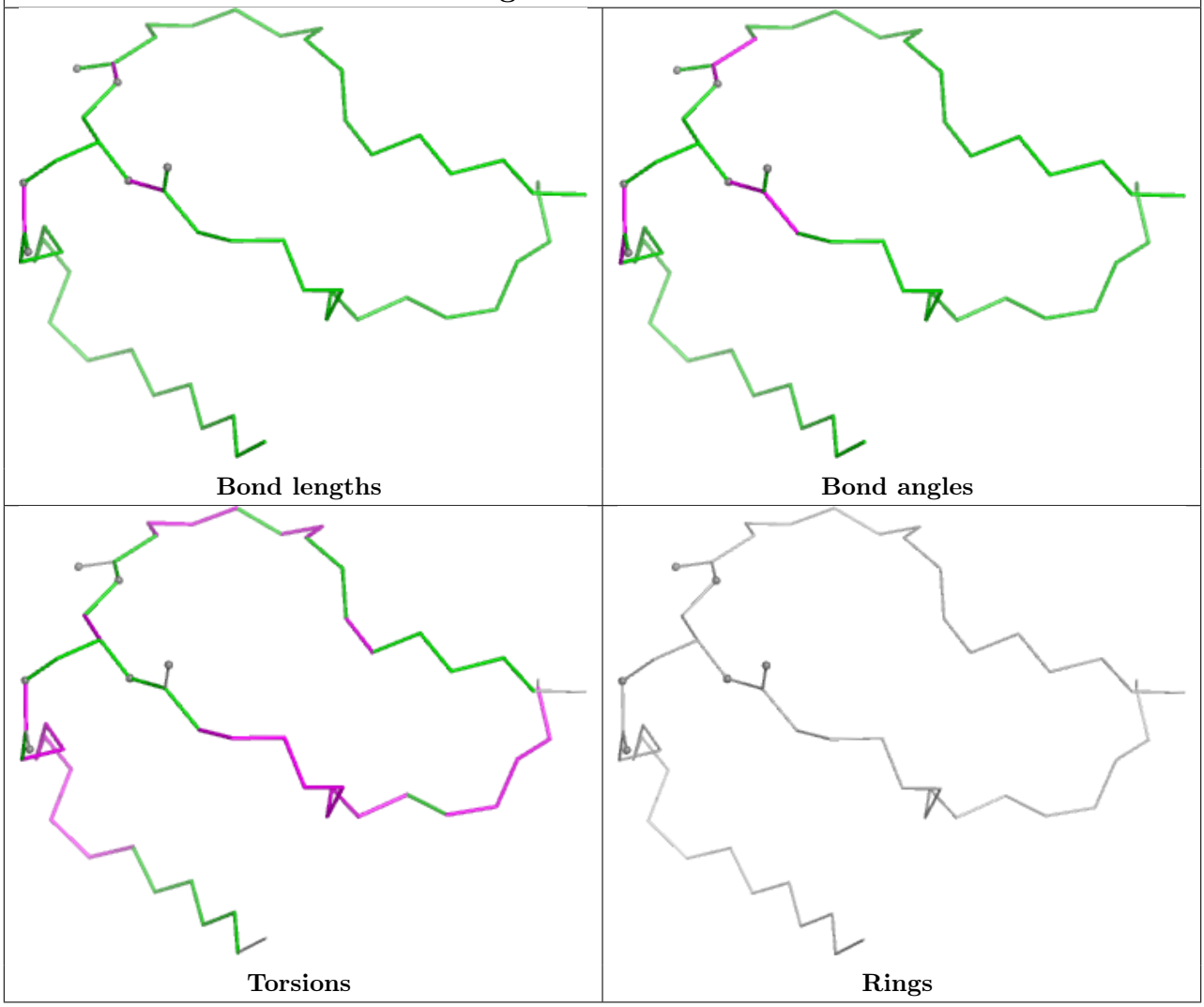
Ligand DGA b 625



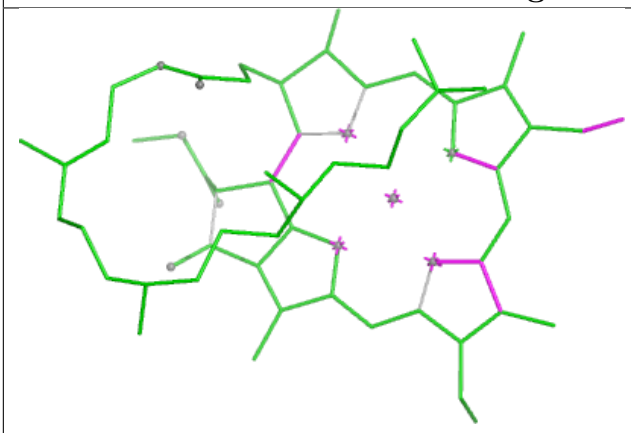
Ligand NEX S 623



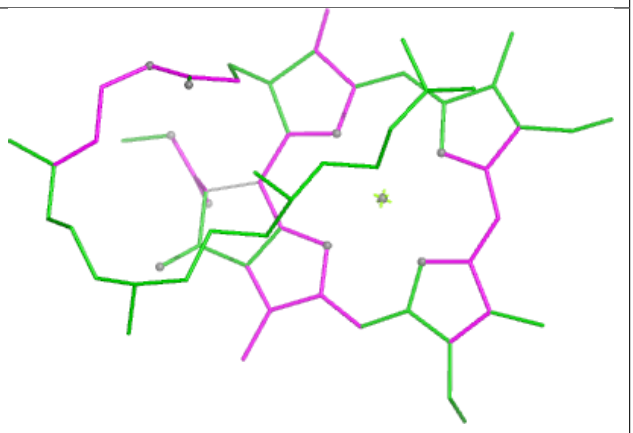
Ligand 4RF k 101



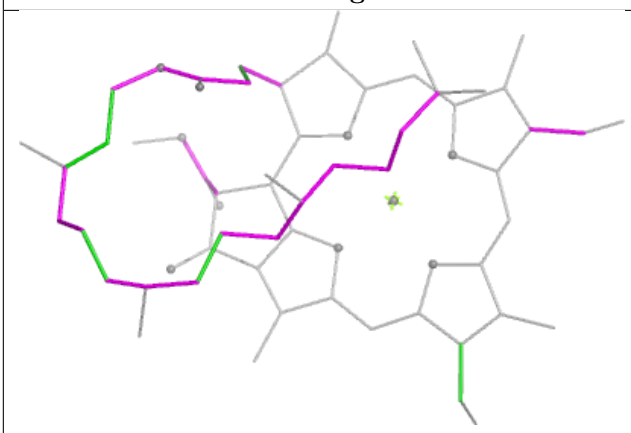
Ligand CLA b 602



Bond lengths



Bond angles

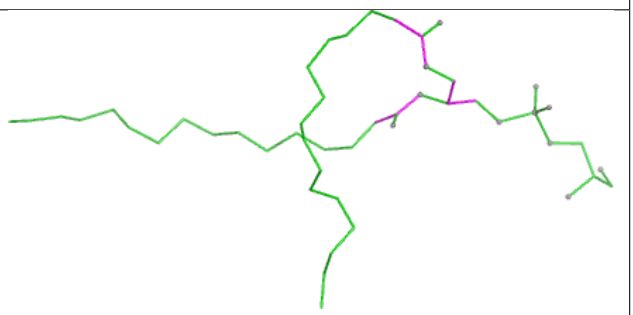


Torsions

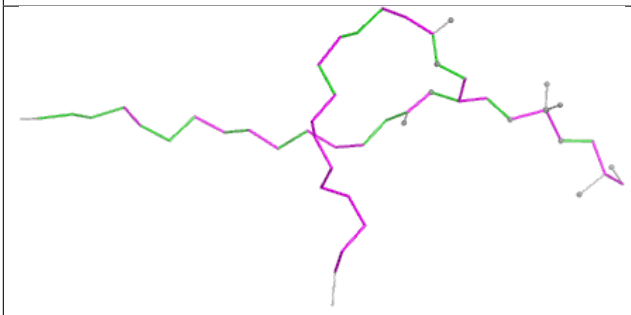
Rings

Ligand LHG Y 624

Bond lengths



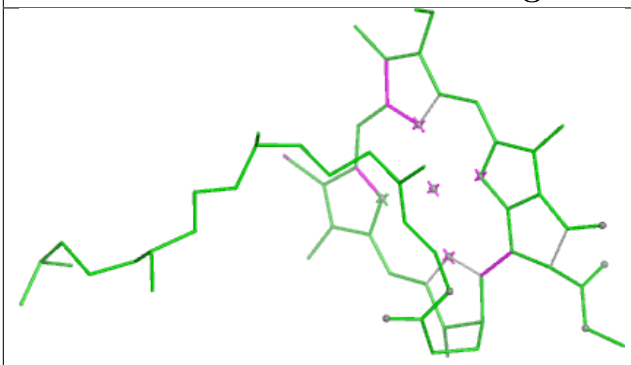
Bond angles



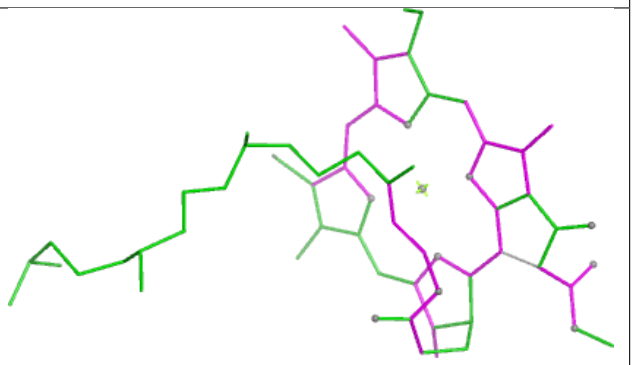
Torsions

Rings

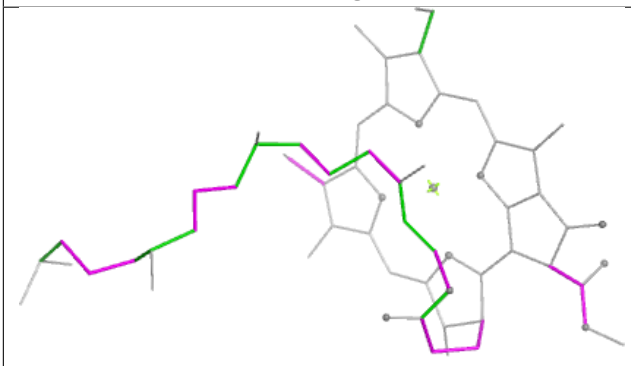
Ligand CLA N 613



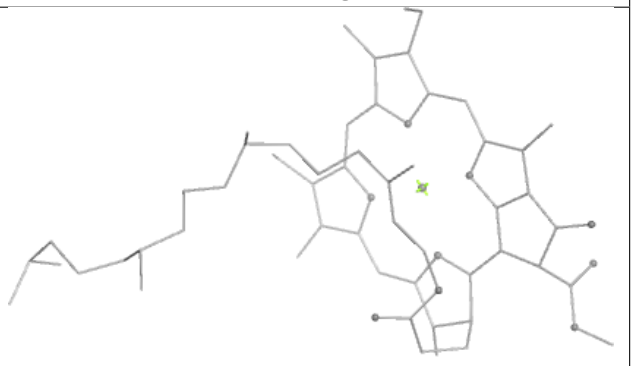
Bond lengths



Bond angles

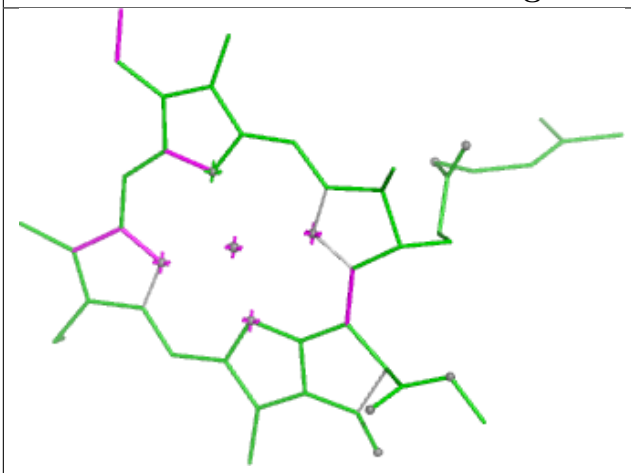


Torsions

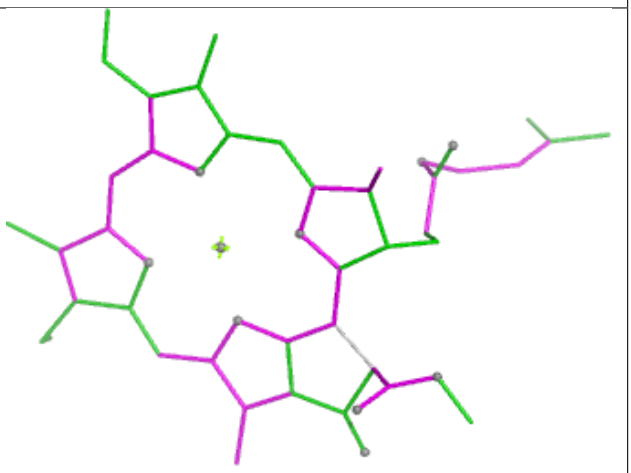


Rings

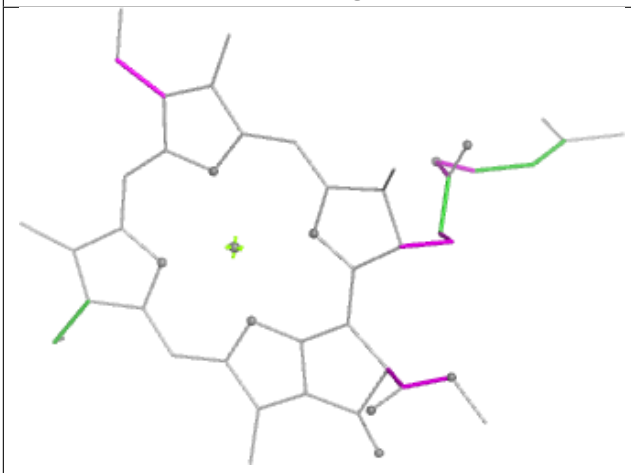
Ligand CLA Y 608



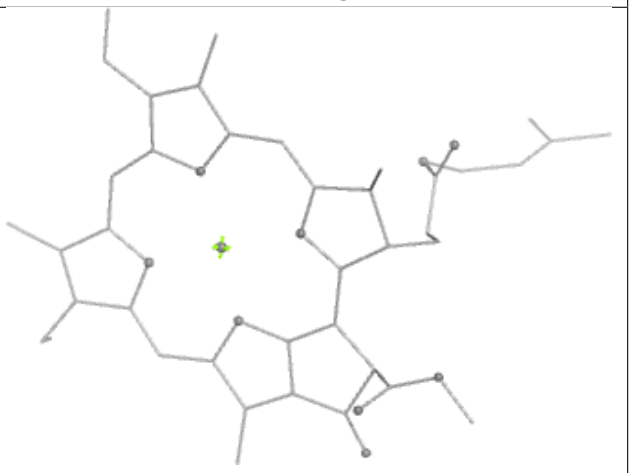
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

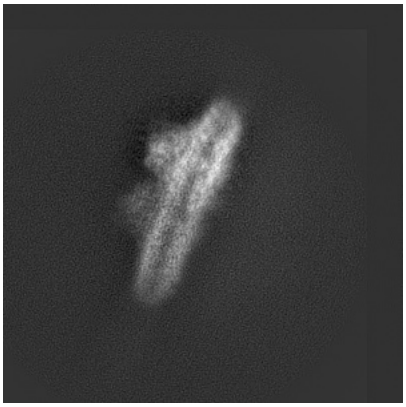
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13548. These allow visual inspection of the internal detail of the map and identification of artifacts.

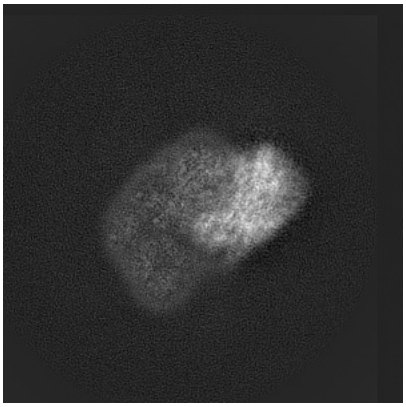
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

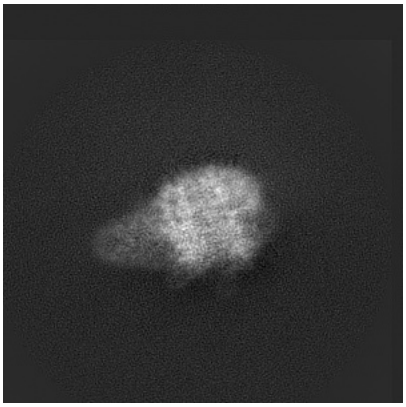
6.1.1 Primary map



X



Y

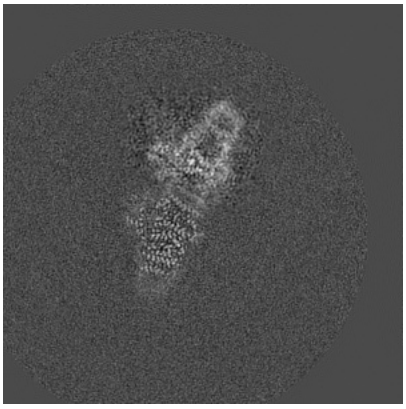


Z

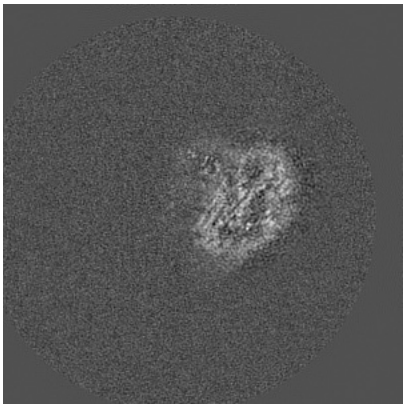
The images above show the map projected in three orthogonal directions.

6.2 Central slices

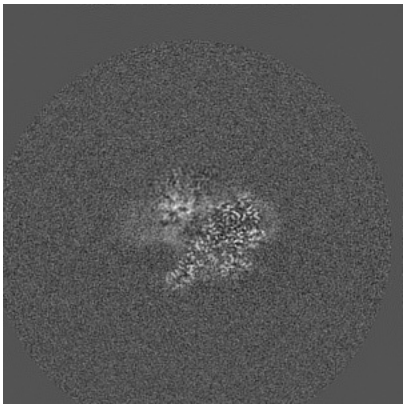
6.2.1 Primary map



X Index: 250



Y Index: 250

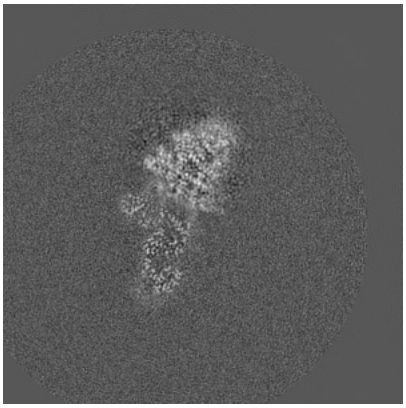


Z Index: 250

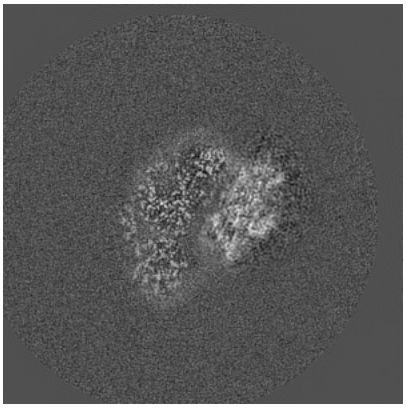
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

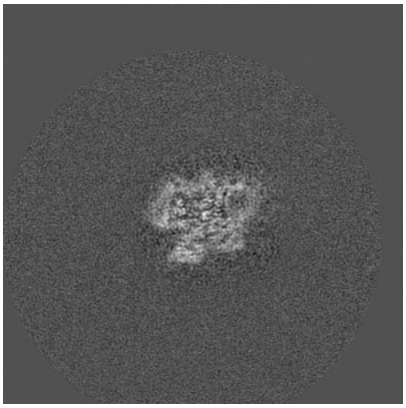
6.3.1 Primary map



X Index: 225



Y Index: 219

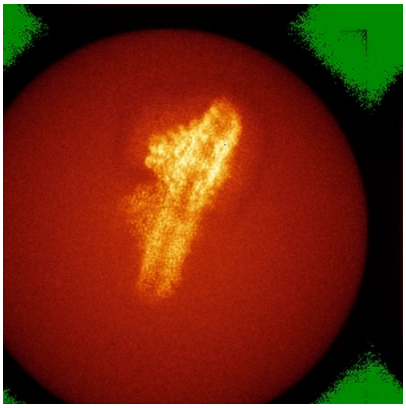


Z Index: 304

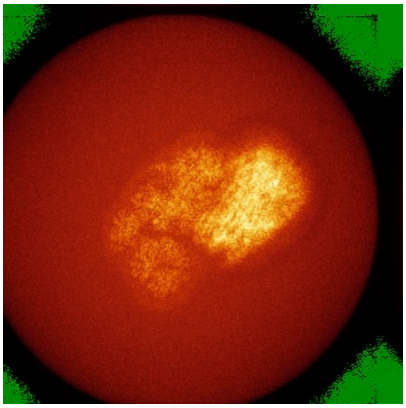
The images above show the largest variance slices of the map in three orthogonal directions.

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

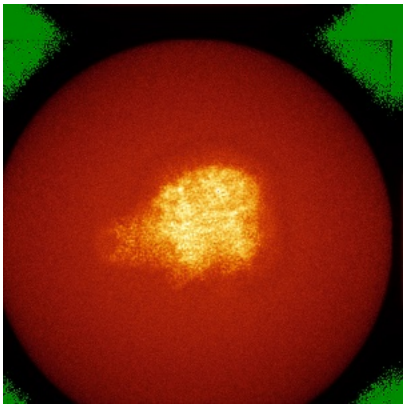
6.4.1 Primary map



X



Y

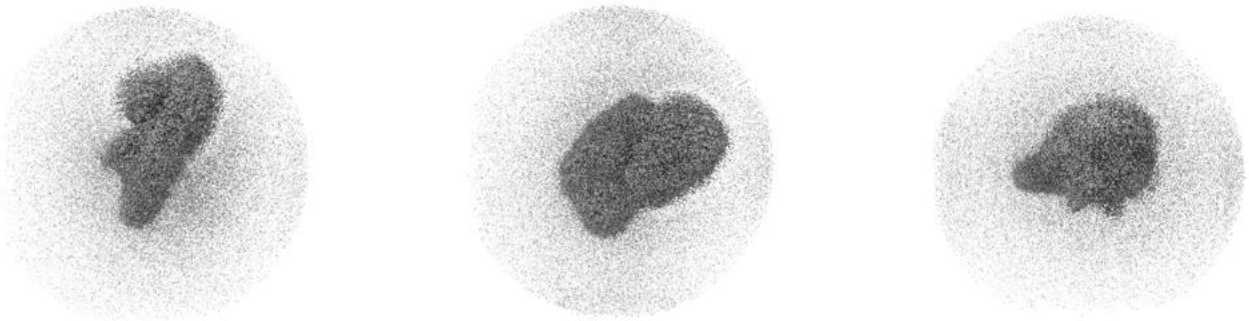


Z

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 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

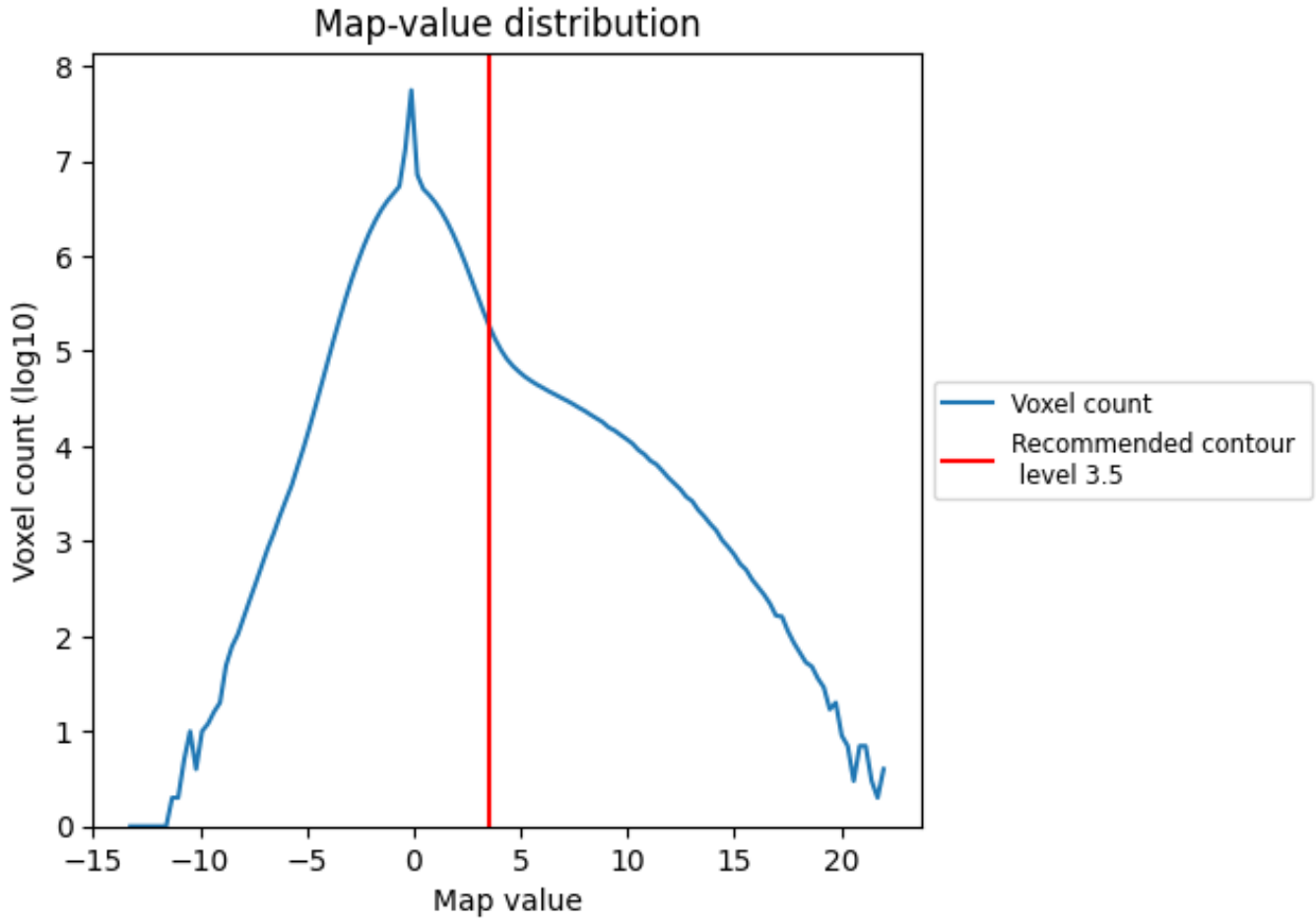
6.6 Mask visualisation (i)

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

7 Map analysis

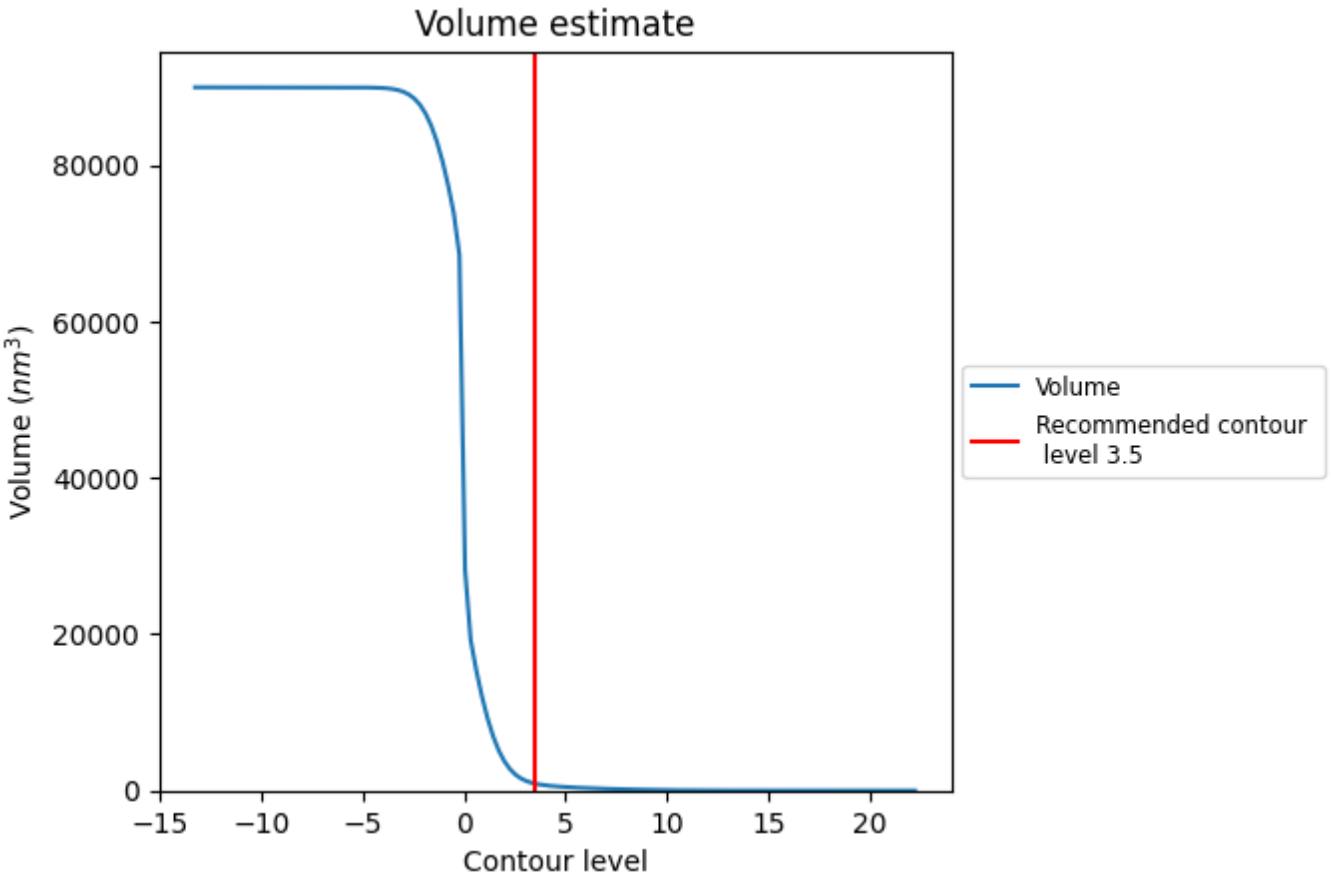
This section contains the results of statistical analysis of the map.

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.

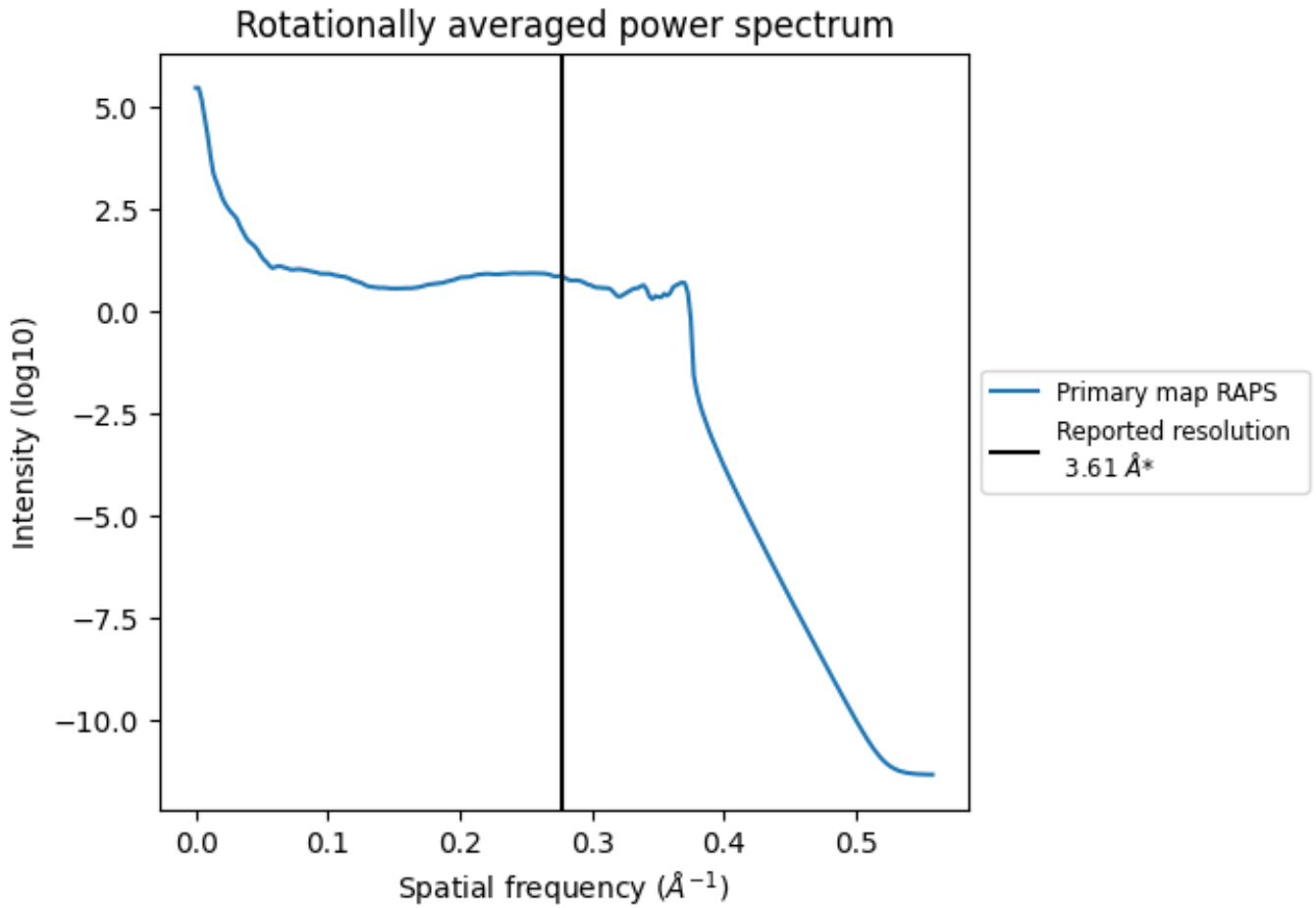
7.2 Volume estimate



The volume at the recommended contour level is 898 nm^3; this corresponds to an approximate mass of 811 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)

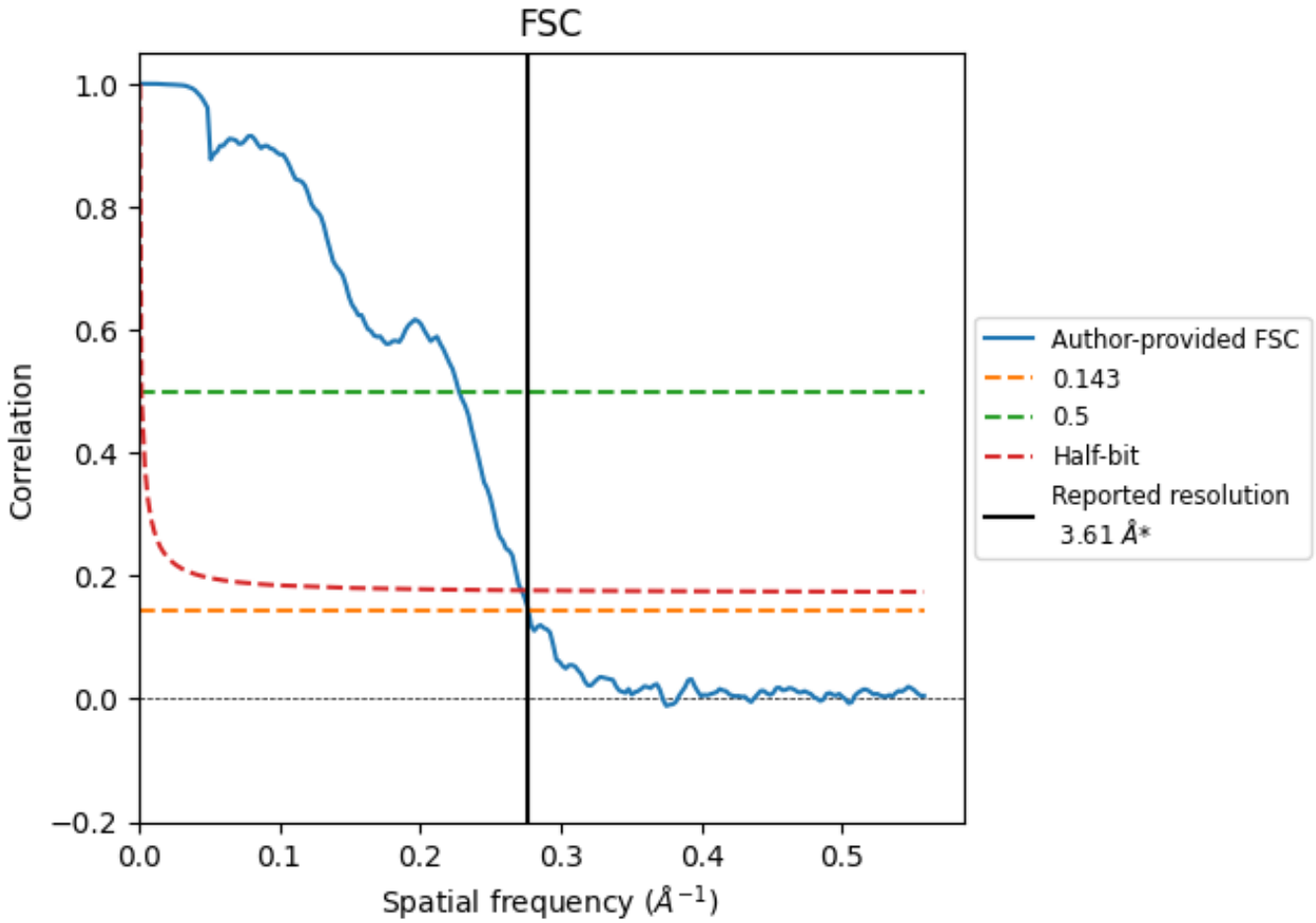


*Reported resolution corresponds to spatial frequency of 0.277 $Å^{-1}$

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 0.277 $Å^{-1}$

8.2 Resolution estimates (i)

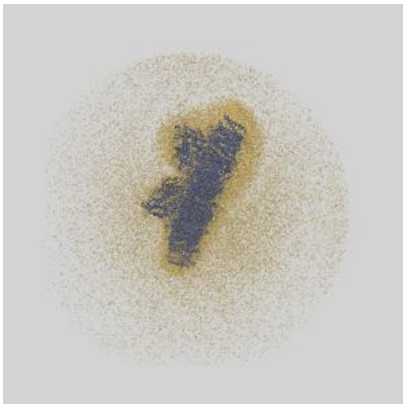
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.61	-	-
Author-provided FSC curve	3.61	4.39	3.67
Unmasked-calculated*	-	-	-

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

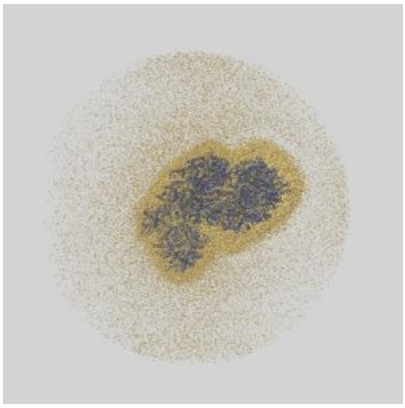
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13548 and PDB model 7PNK. Per-residue inclusion information can be found in section 3 on page 35.

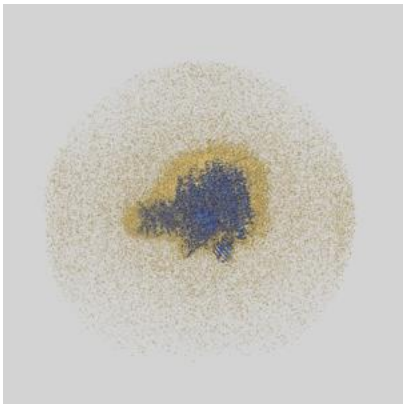
9.1 Map-model overlay



X



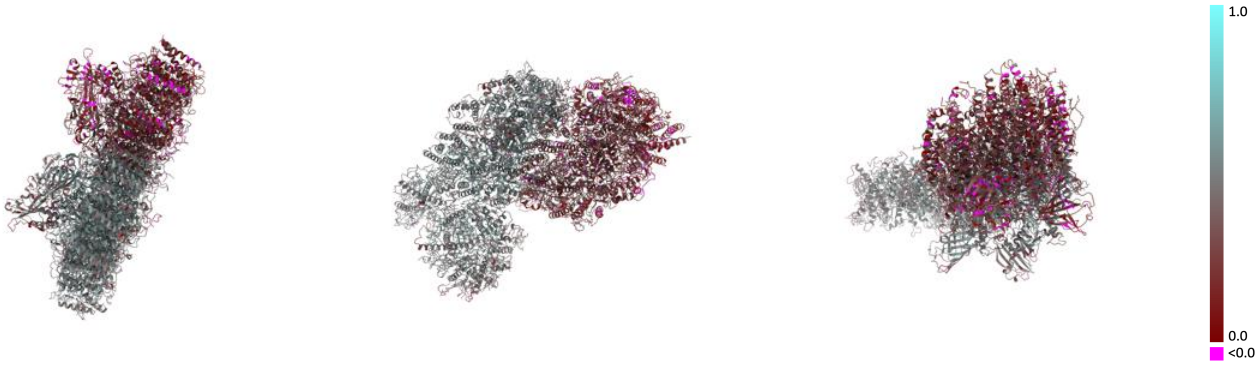
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 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.

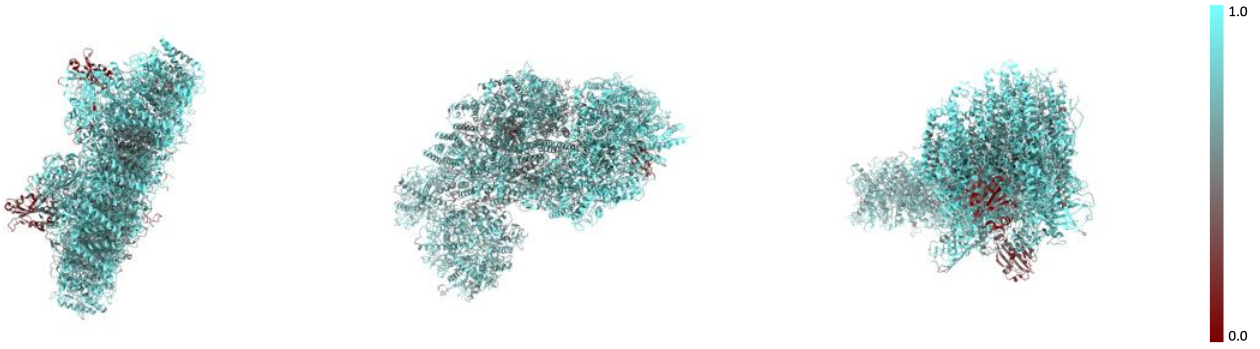
9.2 Q-score mapped to coordinate model



X Y Z

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.

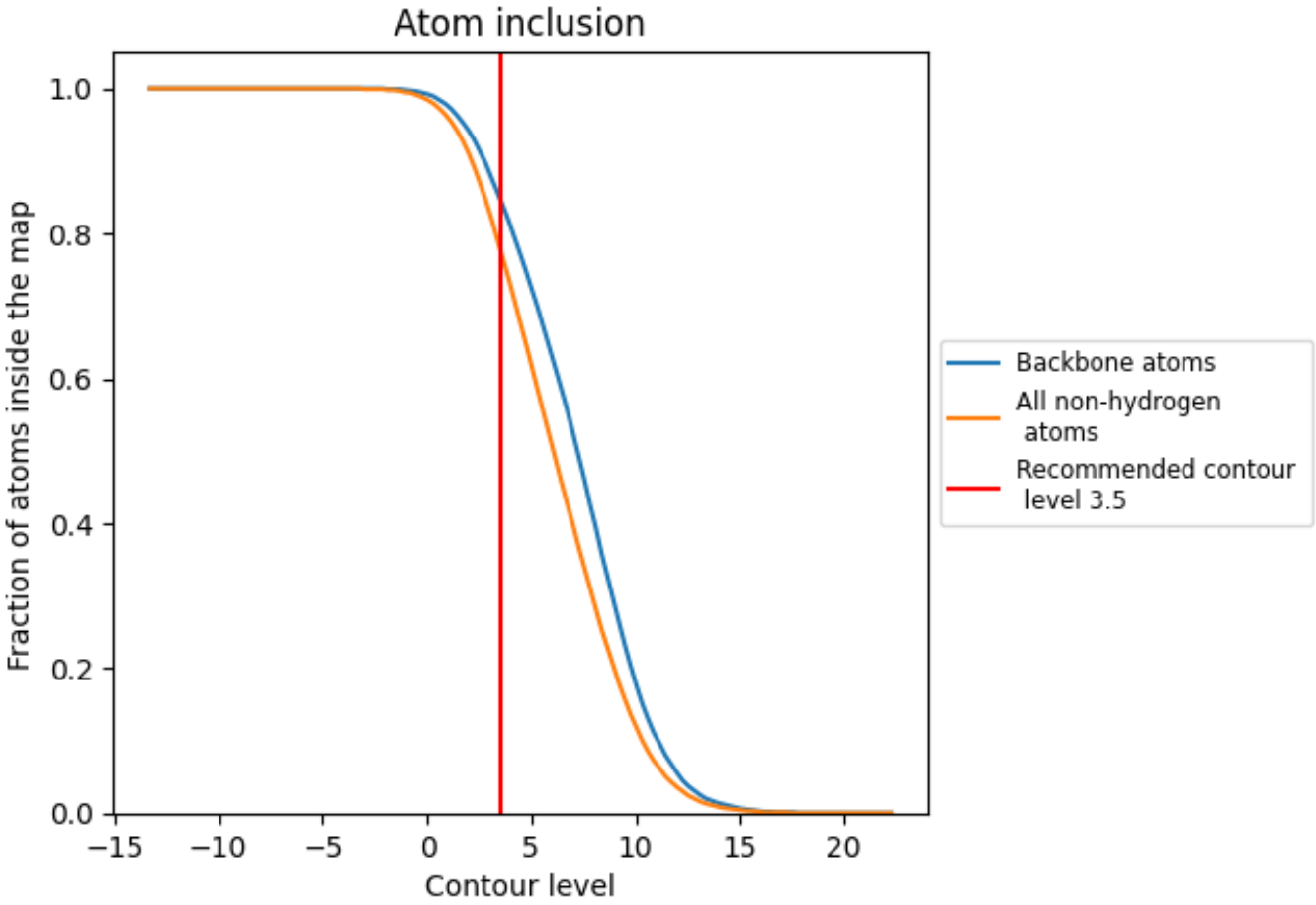
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.3810
A	0.7720	0.5100
B	0.8000	0.4910
C	0.8120	0.5310
D	0.8180	0.5240
E	0.8140	0.4740
F	0.8080	0.4820
G	0.7440	0.4420
H	0.7960	0.4790
I	0.6840	0.4500
J	0.7280	0.4740
K	0.7340	0.4710
L	0.7490	0.4910
M	0.6470	0.3770
N	0.7750	0.4800
O	0.7230	0.4310
P	0.2770	0.3450
S	0.7710	0.4780
T	0.5970	0.4100
U	0.6330	0.3920
V	0.7600	0.4840
W	0.6560	0.4540
X	0.7510	0.4430
Y	0.7500	0.4910
Z	0.7910	0.4930
a	0.8530	0.2340
b	0.8320	0.2570
c	0.8620	0.2170
d	0.8790	0.2770
e	0.9490	0.2380
f	0.8950	0.2490
h	0.8330	0.2430
i	0.7810	0.2010
j	0.8760	0.2850
k	0.8860	0.2450

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	0.6840	0.1810
m	0.6650	0.2260
o	0.8250	0.2010
p	0.3550	0.1570
t	0.6010	0.2440
u	0.9400	0.2420
v	0.8980	0.2180
w	0.7950	0.1740
x	0.8660	0.1970
z	0.8970	0.1980