Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 05:41 AM JST

PDB ID	:	6KAF / pdb_00006kaf
EMDB ID	:	EMD-9957
Title	:	C2S2M2N2-type PSII-LHCII
Authors	:	Chang, S.H.; Shen, L.L.; Huang, Z.H.; Wang, W.D.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on	:	2019-06-22
Resolution	:	3.73 Å(reported)

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:

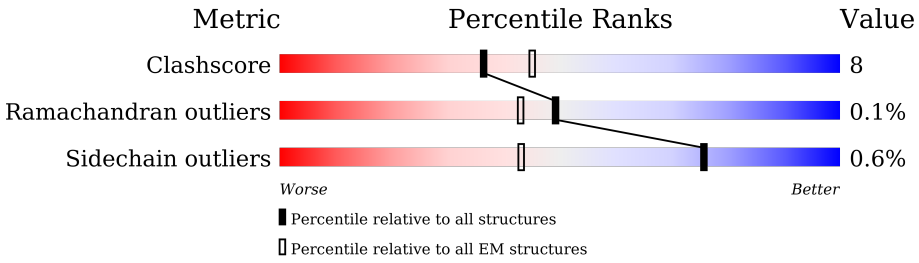
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

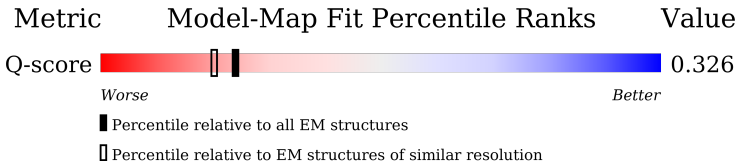
1 Overall quality at a glance

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

The reported resolution of this entry is 3.73 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.





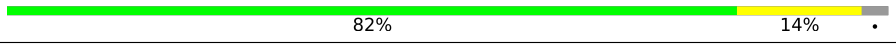
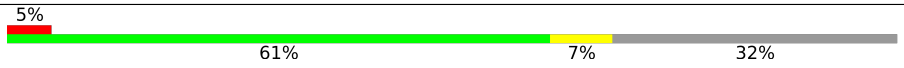
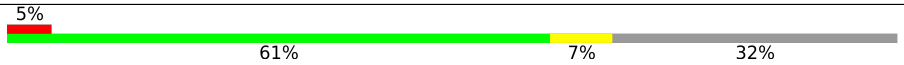
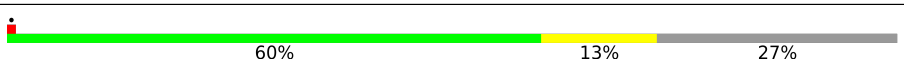
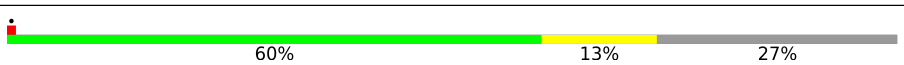
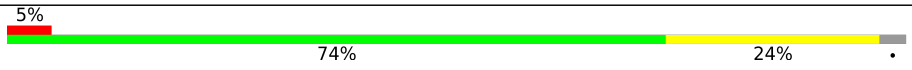
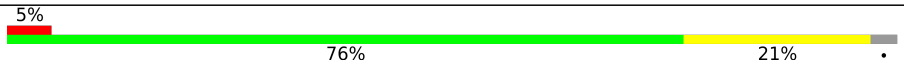
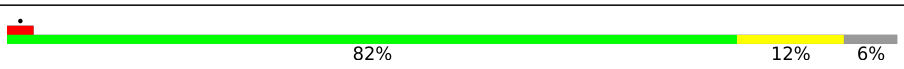
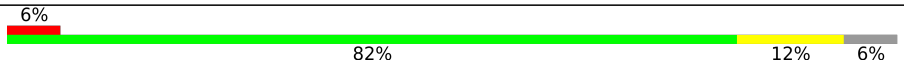
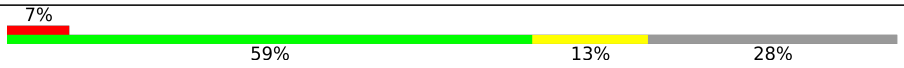
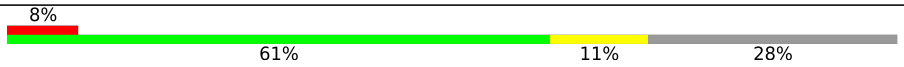
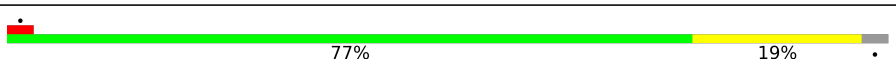
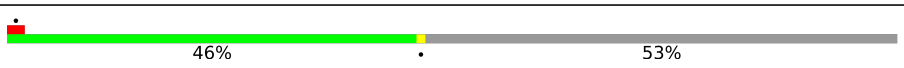
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10415 (3.23 - 4.23)

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	R	280	16% 64% 16% 20%
1	r	280	15% 64% 15% 20%
2	A	352	80% 14% 5%
2	a	352	82% 13% 5%

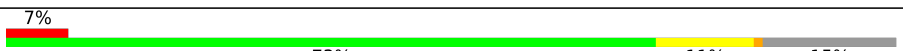
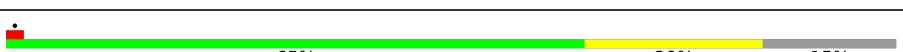
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Mol	Chain	Length	Quality of chain
3	D	352	
3	d	352	
4	F	44	
4	f	44	
5	H	88	
5	h	88	
6	I	37	
6	i	37	
7	J	50	
7	j	50	
8	K	46	
8	k	46	
9	L	38	
9	l	38	
10	M	34	
10	m	34	
11	O	291	
11	o	291	
12	T	31	
12	t	31	
13	W	115	
13	w	115	
14	X	101	
14	x	101	
15	Z	62	

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Mol	Chain	Length	Quality of chain
15	z	62	
16	Y	33	
16	y	33	
17	E	82	
17	e	82	
18	1	257	
18	2	257	
18	3	257	
18	4	257	
18	5	257	
18	6	257	
18	G	257	
18	N	257	
18	P	257	
18	Q	257	
18	U	257	
18	V	257	
18	g	257	
18	n	257	
18	p	257	
18	q	257	
18	u	257	
18	v	257	
19	S	289	
19	s	289	

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Mol	Chain	Length	Quality of chain
20	C	461	84% 14%
20	c	461	85% 13%
21	B	508	85% 14%
21	b	508	5% 84% 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
29	CL	A	402	-	-	X	-
29	CL	a	402	-	-	X	-
29	CL	a	403	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 104363 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 Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	r	223	Total	C	N	O	S	0	0
			1701	1081	286	329	5		
1	R	223	Total	C	N	O	S	0	0
			1698	1080	285	328	5		

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	333	Total	C	N	O	S	0	0
			2614	1707	430	462	15		
2	A	333	Total	C	N	O	S	0	0
			2614	1707	430	462	15		

- Molecule 3 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	341	Total	C	N	O	S	0	0
			2714	1791	447	464	12		
3	D	341	Total	C	N	O	S	0	0
			2714	1791	447	464	12		

- Molecule 4 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	30	Total	C	N	O	S	0	0
			243	165	41	36	1		
4	F	30	Total	C	N	O	S	0	0
			243	165	41	36	1		

- Molecule 5 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	64	Total	C	N	O	S	0	0
			488	327	72	87	2		
5	H	64	Total	C	N	O	S	0	0
			488	327	72	87	2		

- Molecule 6 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	34	Total	C	N	O	S	0	0
			275	189	41	43	2		
6	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

- Molecule 7 is a protein called Photosystem II reaction center protein J, PsbJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	31	Total	C	N	O	S	0	0
			245	168	36	39	2		
7	J	31	Total	C	N	O	S	0	0
			245	168	36	39	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	k	36	Total	C	N	O	0	0
			288	203	41	44		
8	K	36	Total	C	N	O	0	0
			288	203	41	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	l	37	Total	C	N	O	0	0
			306	205	50	51		
9	L	37	Total	C	N	O	0	0
			306	205	50	51		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	m	32	Total	C	N	O	0	0
			248	168	35	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	32	Total 248	C 168	N 35	O 45	0	0

- Molecule 11 is a protein called Oxygen-evolving enhancer protein 1 of photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	o	210	Total 1592	C 1016	N 254	O 318	S 4	0	0
11	O	210	Total 1592	C 1016	N 254	O 318	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total 247	C 171	N 36	O 38	S 2	0	0
12	T	30	Total 247	C 171	N 36	O 38	S 2	0	0

- Molecule 13 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	w	54	Total 417	C 269	N 67	O 79	S 2	0	0
13	W	54	Total 417	C 269	N 67	O 79	S 2	0	0

- Molecule 14 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	x	35	Total 242	C 159	N 39	O 44	0	0
14	X	35	Total 242	C 159	N 39	O 44	0	0

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	z	62	Total 465	C 319	N 69	O 76	S 1	0	0
15	Z	62	Total 465	C 319	N 69	O 76	S 1	0	0

- Molecule 16 is a protein called Photosystem II reaction center protein 30, Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	30	Total 208	C 137	N 34	O 37	0	0
16	y	30	Total 208	C 137	N 34	O 37	0	0

- Molecule 17 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	E	68	Total 555	C 366	N 90	O 99	0	0
17	e	68	Total 555	C 366	N 90	O 99	0	0

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	2	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	3	219	Total 1675	C 1084	N 272	O 314	S 5	0	0
18	4	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	5	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	6	219	Total 1675	C 1084	N 272	O 314	S 5	0	0
18	v	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	p	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	q	219	Total 1675	C 1084	N 272	O 314	S 5	0	0
18	V	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	P	218	Total 1669	C 1081	N 271	O 312	S 5	0	0
18	Q	219	Total 1675	C 1084	N 272	O 314	S 5	0	0
18	U	218	Total 1669	C 1081	N 271	O 312	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
18	G	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
18	u	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	n	218	Total	C	N	O	S	0	0
			1669	1081	271	312	5		
18	g	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	236	Total	C	N	O	S	0	0
			1797	1166	290	337	4		
19	s	236	Total	C	N	O	S	0	0
			1797	1166	290	337	4		

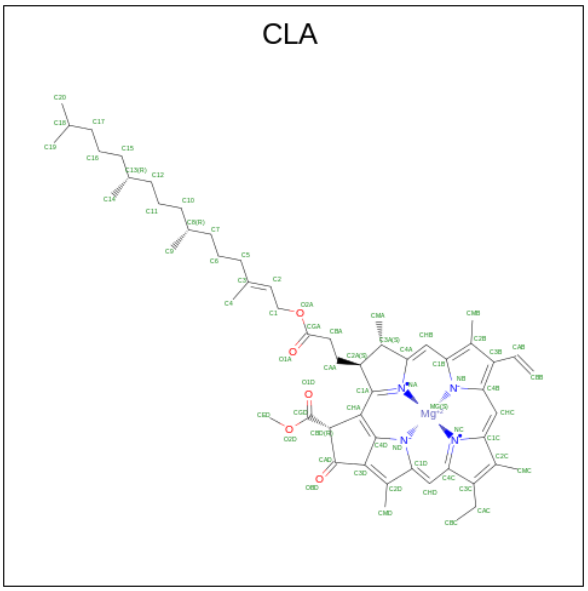
- Molecule 20 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	450	Total	C	N	O	S	0	0
			3502	2290	585	610	17		
20	c	450	Total	C	N	O	S	0	0
			3502	2290	585	610	17		

- Molecule 21 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	503	Total	C	N	O	S	0	0
			3937	2575	658	692	12		
21	b	503	Total	C	N	O	S	0	0
			3937	2575	658	692	12		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	x	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	v	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	p	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			48	38	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	u	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	u	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	u	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	u	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	n	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	g	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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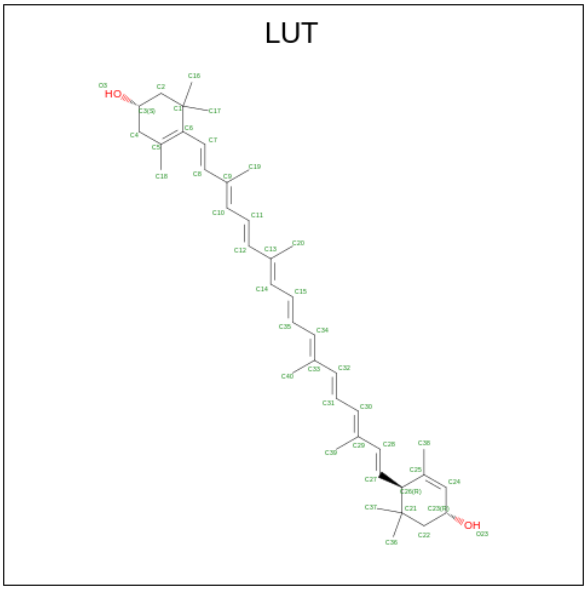
Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	s	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

- Molecule 23 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
23	r	1	Total	C	O	0
			42	40	2	
23	1	1	Total	C	O	0
			42	40	2	
23	1	1	Total	C	O	0
			42	40	2	
23	2	1	Total	C	O	0
			42	40	2	

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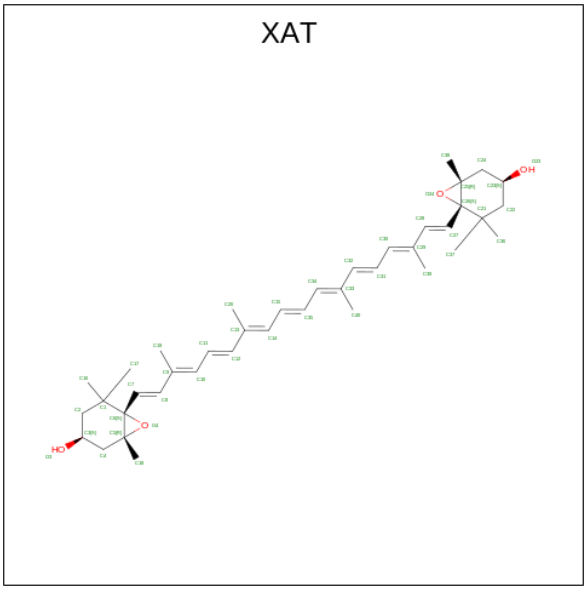
Mol	Chain	Residues	Atoms			AltConf
23	2	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	
23	4	1	Total	C	O	0
			42	40	2	
23	5	1	Total	C	O	0
			42	40	2	
23	5	1	Total	C	O	0
			42	40	2	
23	v	1	Total	C	O	0
			42	40	2	
23	v	1	Total	C	O	0
			42	40	2	
23	p	1	Total	C	O	0
			42	40	2	
23	p	1	Total	C	O	0
			42	40	2	
23	V	1	Total	C	O	0
			42	40	2	
23	V	1	Total	C	O	0
			42	40	2	
23	P	1	Total	C	O	0
			42	40	2	
23	P	1	Total	C	O	0
			42	40	2	
23	U	1	Total	C	O	0
			42	40	2	
23	U	1	Total	C	O	0
			42	40	2	
23	N	1	Total	C	O	0
			42	40	2	
23	N	1	Total	C	O	0
			42	40	2	
23	u	1	Total	C	O	0
			42	40	2	
23	u	1	Total	C	O	0
			42	40	2	
23	n	1	Total	C	O	0
			42	40	2	
23	n	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
23	R	1	Total C O 42 40 2	0
23	S	1	Total C O 42 40 2	0
23	S	1	Total C O 42 40 2	0
23	s	1	Total C O 42 40 2	0
23	s	1	Total C O 42 40 2	0

- Molecule 24 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: $C_{40}H_{56}O_4$).



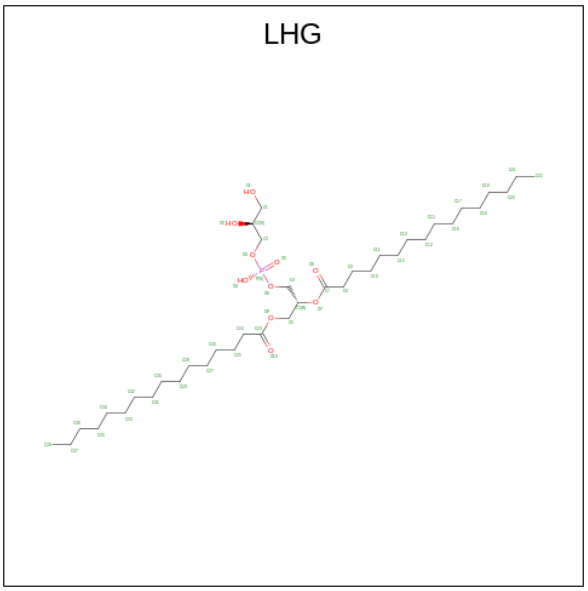
Mol	Chain	Residues	Atoms	AltConf
24	r	1	Total C O 44 40 4	0
24	1	1	Total C O 44 40 4	0
24	2	1	Total C O 44 40 4	0
24	3	1	Total C O 44 40 4	0
24	4	1	Total C O 44 40 4	0
24	5	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms			AltConf
24	6	1	Total	C	O	0
			44	40	4	
24	v	1	Total	C	O	0
			44	40	4	
24	p	1	Total	C	O	0
			44	40	4	
24	q	1	Total	C	O	0
			44	40	4	
24	V	1	Total	C	O	0
			44	40	4	
24	P	1	Total	C	O	0
			44	40	4	
24	Q	1	Total	C	O	0
			44	40	4	
24	U	1	Total	C	O	0
			44	40	4	
24	N	1	Total	C	O	0
			44	40	4	
24	G	1	Total	C	O	0
			44	40	4	
24	u	1	Total	C	O	0
			44	40	4	
24	n	1	Total	C	O	0
			44	40	4	
24	g	1	Total	C	O	0
			44	40	4	
24	R	1	Total	C	O	0
			44	40	4	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
25	r	1	Total	C	O	P	0
			42	31	10	1	
25	a	1	Total	C	O	P	0
			43	32	10	1	
25	d	1	Total	C	O	P	0
			46	35	10	1	
25	d	1	Total	C	O	P	0
			49	38	10	1	
25	l	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			43	32	10	1	
25	L	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	2	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	6	1	Total	C	O	P	0
			49	38	10	1	
25	v	1	Total	C	O	P	0
			49	38	10	1	

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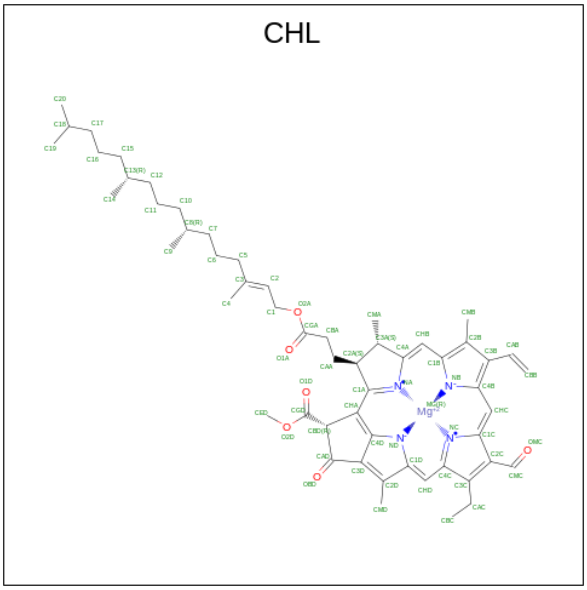
Mol	Chain	Residues	Atoms				AltConf
25	p	1	Total	C	O	P	0
			49	38	10	1	
25	q	1	Total	C	O	P	0
			49	38	10	1	
25	V	1	Total	C	O	P	0
			49	38	10	1	
25	P	1	Total	C	O	P	0
			49	38	10	1	
25	Q	1	Total	C	O	P	0
			49	38	10	1	
25	U	1	Total	C	O	P	0
			49	38	10	1	
25	N	1	Total	C	O	P	0
			49	38	10	1	
25	G	1	Total	C	O	P	0
			49	38	10	1	
25	u	1	Total	C	O	P	0
			49	38	10	1	
25	n	1	Total	C	O	P	0
			49	38	10	1	
25	g	1	Total	C	O	P	0
			49	38	10	1	
25	R	1	Total	C	O	P	0
			42	31	10	1	
25	S	1	Total	C	O	P	0
			49	38	10	1	
25	C	1	Total	C	O	P	0
			49	38	10	1	
25	C	1	Total	C	O	P	0
			49	38	10	1	
25	C	1	Total	C	O	P	0
			49	38	10	1	
25	B	1	Total	C	O	P	0
			47	36	10	1	
25	B	1	Total	C	O	P	0
			49	38	10	1	
25	D	1	Total	C	O	P	0
			46	35	10	1	
25	D	1	Total	C	O	P	0
			49	38	10	1	
25	b	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
25	b	1	Total	C	O	P	0
			49	38	10	1	
25	c	1	Total	C	O	P	0
			49	38	10	1	
25	c	1	Total	C	O	P	0
			49	38	10	1	
25	c	1	Total	C	O	P	0
			49	38	10	1	
25	s	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 26 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	r	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	r	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	v	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	v	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	v	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	v	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	v	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	v	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	p	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
26	p	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	p	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	q	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	q	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	V	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	V	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	P	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	P	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
26	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	Q	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	Q	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	Q	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	U	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	

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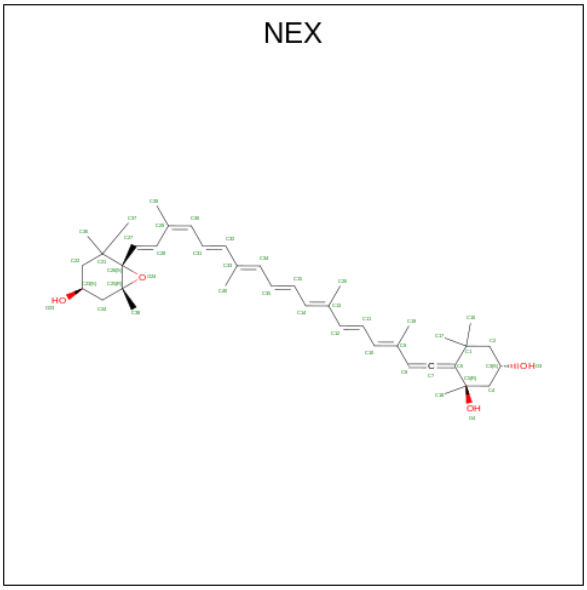
Mol	Chain	Residues	Atoms					AltConf
26	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	G	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	u	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	u	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	u	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
26	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
26	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
26	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
26	R	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
26	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
26	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	S	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
26	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
26	s	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
26	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 27 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
27	r	1	Total	C	O	0
			44	40	4	
27	r	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	v	1	Total	C	O	0
			44	40	4	
27	p	1	Total	C	O	0
			44	40	4	
27	V	1	Total	C	O	0
			44	40	4	
27	P	1	Total	C	O	0
			44	40	4	
27	U	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	u	1	Total	C	O	0
			44	40	4	
27	u	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	S	1	Total	C	O	0
			44	40	4	
27	s	1	Total	C	O	0
			44	40	4	

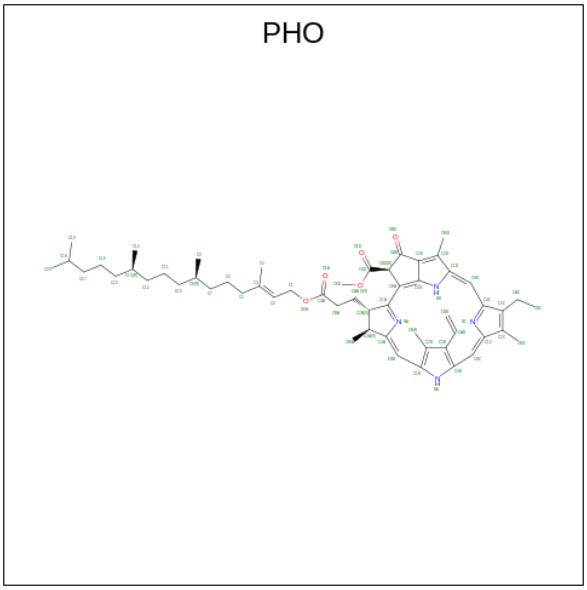
- Molecule 28 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 29 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

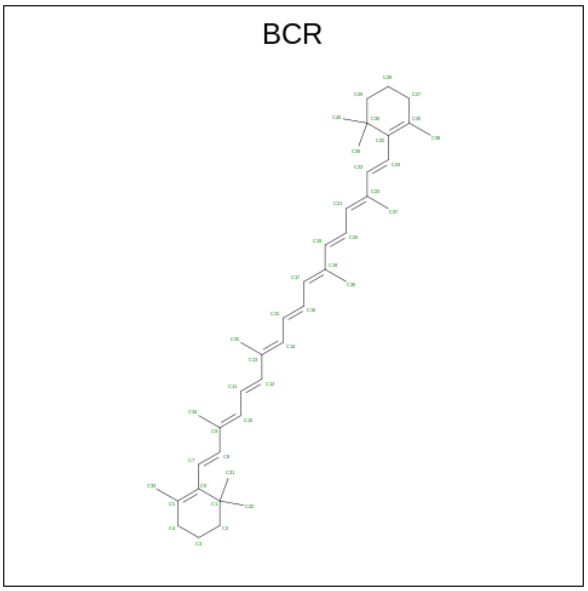
Mol	Chain	Residues	Atoms	AltConf
29	a	2	Total Cl 2 2	0
29	A	2	Total Cl 2 2	0

- Molecule 30 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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



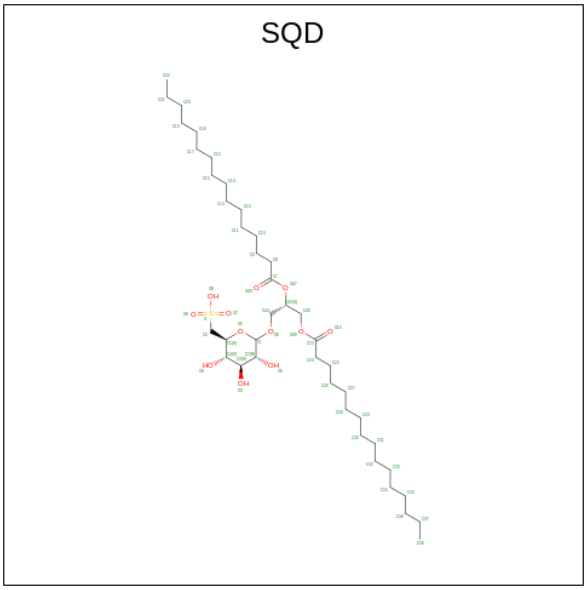
Mol	Chain	Residues	Atoms	AltConf
31	a	1	Total C 40 40	0
31	d	1	Total C 40 40	0
31	k	1	Total C 40 40	0
31	t	1	Total C 40 40	0
31	x	1	Total C 40 40	0
31	z	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	K	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	C	1	Total C 40 40	0
31	B	1	Total C 40 40	0
31	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
31	B	1	Total C 40 40	0
31	D	1	Total C 40 40	0
31	X	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	b	1	Total C 40 40	0
31	c	1	Total C 40 40	0
31	c	1	Total C 40 40	0

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



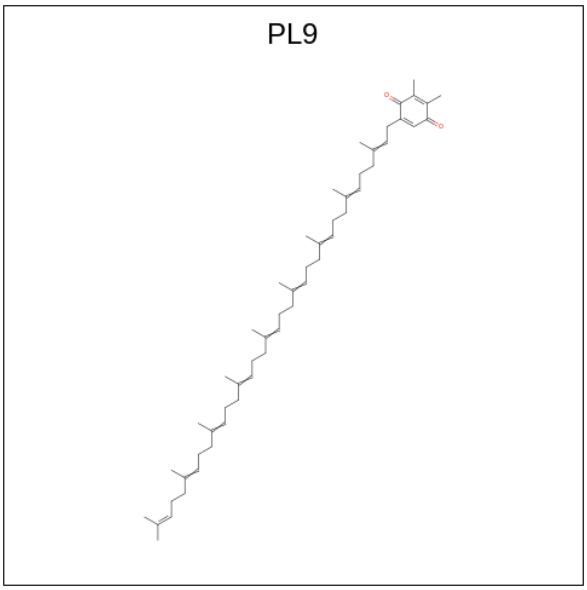
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C O S 50 37 12 1	0
32	a	1	Total C O S 54 41 12 1	0
32	l	1	Total C O S 54 41 12 1	0

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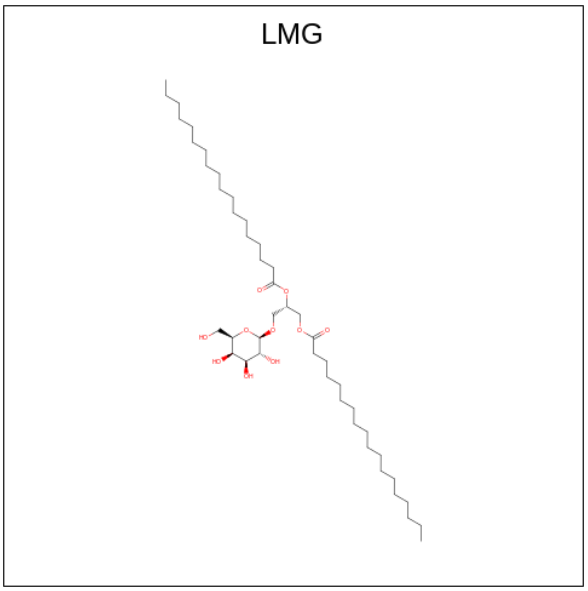
Mol	Chain	Residues	Atoms				AltConf
32	m	1	Total	C	O	S	0
			42	29	12	1	
32	A	1	Total	C	O	S	0
			54	41	12	1	
32	L	1	Total	C	O	S	0
			54	41	12	1	
32	M	1	Total	C	O	S	0
			42	29	12	1	
32	C	1	Total	C	O	S	0
			50	37	12	1	

- Molecule 33 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: $C_{53}H_{80}O_2$).



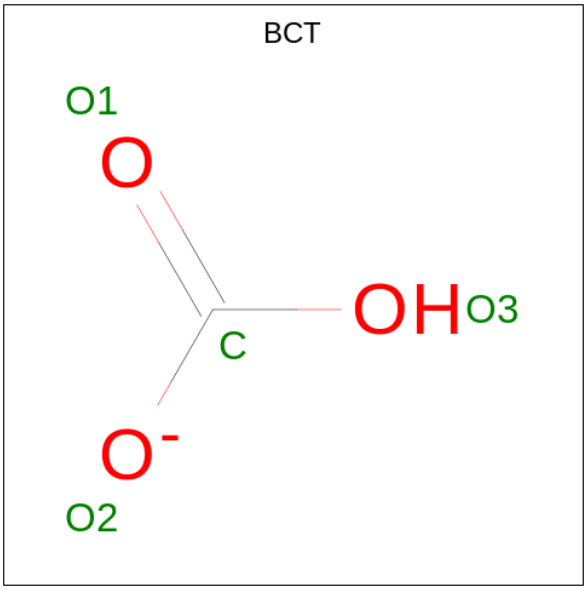
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	C	O	0
			13	11	2	
33	d	1	Total	C	O	0
			55	53	2	
33	A	1	Total	C	O	0
			13	11	2	
33	D	1	Total	C	O	0
			55	53	2	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



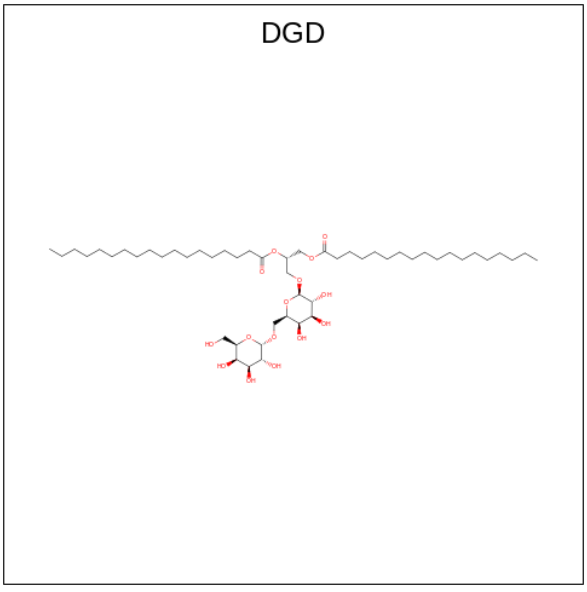
Mol	Chain	Residues	Atoms			AltConf
34	a	1	Total	C	O	0
			40	30	10	
34	d	1	Total	C	O	0
			46	36	10	
34	w	1	Total	C	O	0
			48	38	10	
34	A	1	Total	C	O	0
			40	30	10	
34	W	1	Total	C	O	0
			48	38	10	
34	C	1	Total	C	O	0
			51	41	10	
34	C	1	Total	C	O	0
			51	41	10	
34	B	1	Total	C	O	0
			51	41	10	
34	B	1	Total	C	O	0
			55	45	10	
34	D	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			51	41	10	
34	b	1	Total	C	O	0
			55	45	10	
34	c	1	Total	C	O	0
			51	41	10	
34	c	1	Total	C	O	0
			51	41	10	

- Molecule 35 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



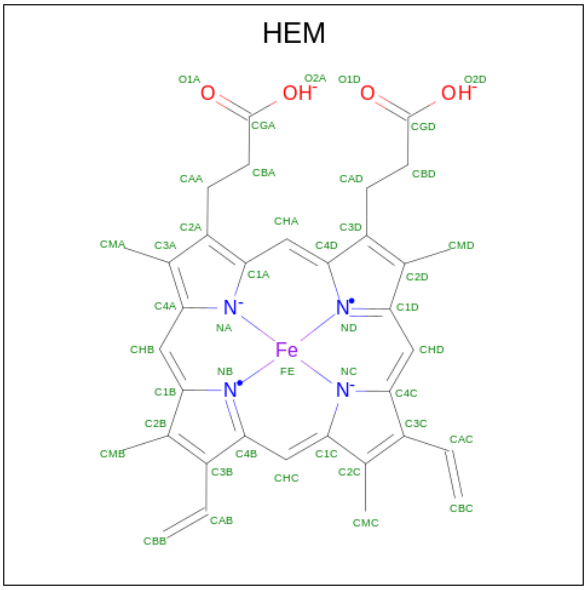
Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			4	1	3	
35	D	1	Total	C	O	0
			4	1	3	

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	AltConf
36	a	1	Total C O 59 44 15	0
36	A	1	Total C O 59 44 15	0
36	J	1	Total C O 60 45 15	0
36	C	1	Total C O 55 40 15	0
36	C	1	Total C O 62 47 15	0
36	B	1	Total C O 62 47 15	0
36	b	1	Total C O 62 47 15	0
36	c	1	Total C O 55 40 15	0
36	c	1	Total C O 62 47 15	0
36	c	1	Total C O 60 45 15	0

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	AltConf
37	E	1	Total C Fe N O 43 34 1 4 4	0

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Mol	Chain	Residues	Atoms					AltConf
37	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

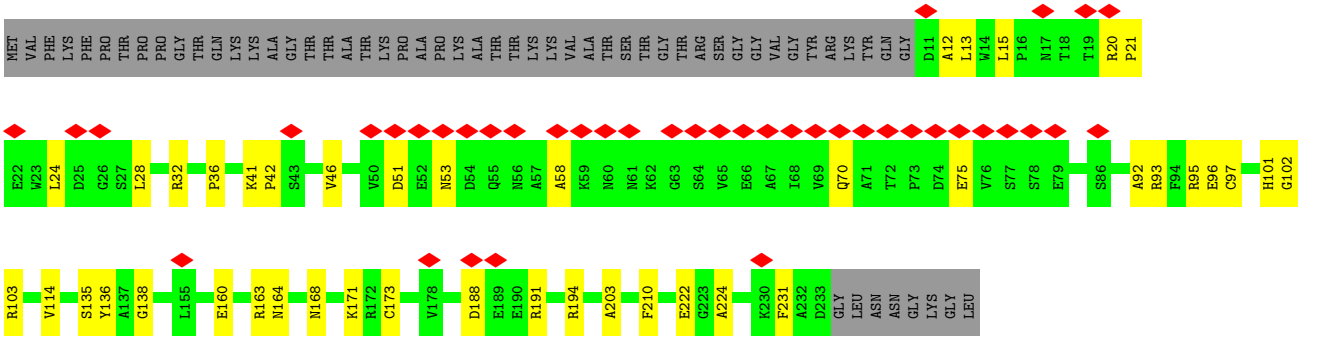
3 Residue-property plots (i)

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: Chlorophyll a-b binding protein CP29

Chain r:

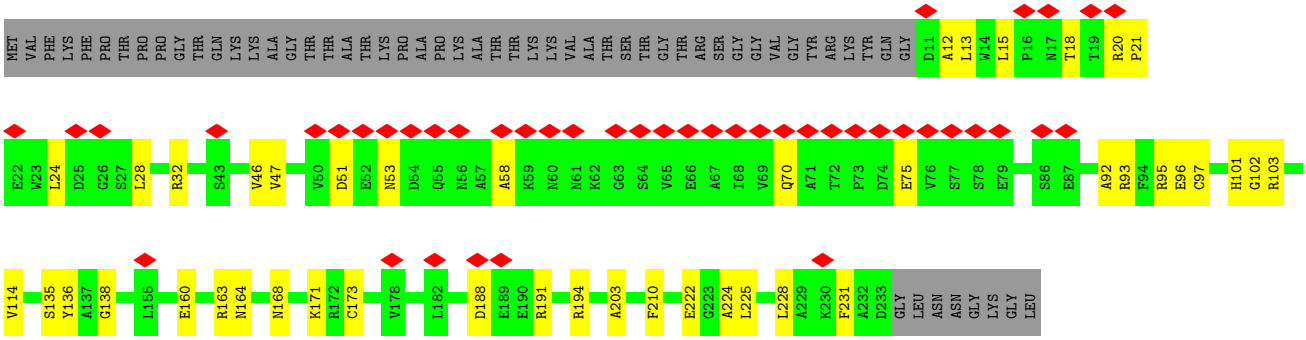




• Molecule 1: Chlorophyll a-b binding protein CP29

Chain R:

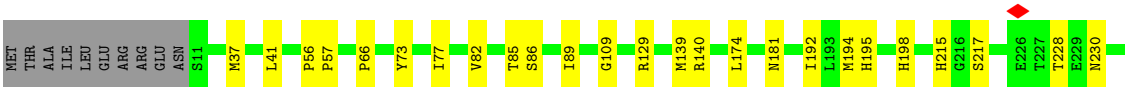




• Molecule 2: Photosystem II protein D1

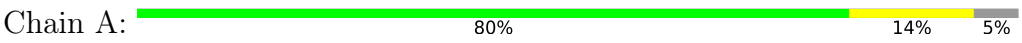
Chain a:

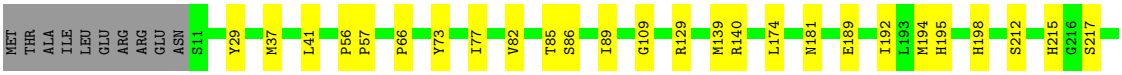






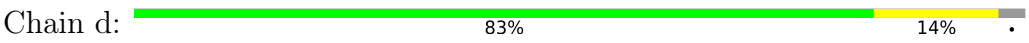
• Molecule 2: Photosystem II protein D1







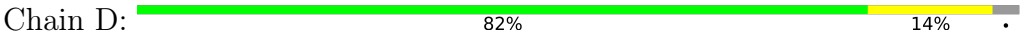
• Molecule 3: Photosystem II D2 protein



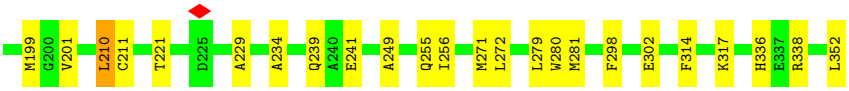




• Molecule 3: Photosystem II D2 protein

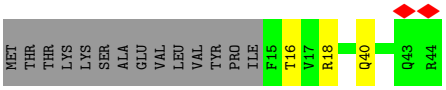






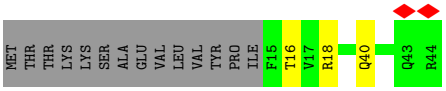
• Molecule 4: Cytochrome b559 subunit beta





• Molecule 4: Cytochrome b559 subunit beta

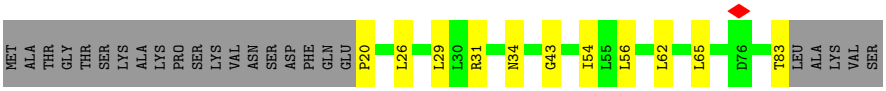




• Molecule 5: Photosystem II reaction center protein H

Chain h:

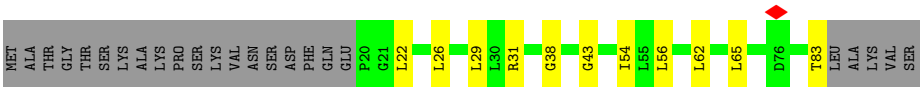




• Molecule 5: Photosystem II reaction center protein H

Chain H:

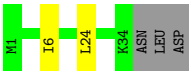




• Molecule 6: Photosystem II reaction center protein I

Chain i:

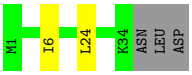




• Molecule 6: Photosystem II reaction center protein I

Chain I:

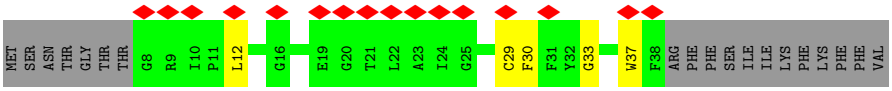




• Molecule 7: Photosystem II reaction center protein J, PsbJ

Chain j:

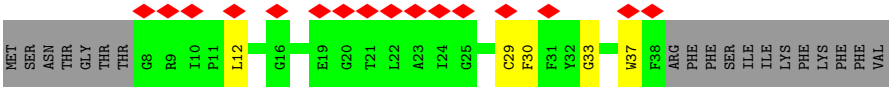




• Molecule 7: Photosystem II reaction center protein J, PsbJ

Chain J:





• Molecule 8: Photosystem II reaction center protein K

Chain k:

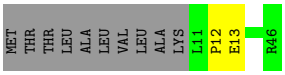




• Molecule 8: Photosystem II reaction center protein K

Chain K:

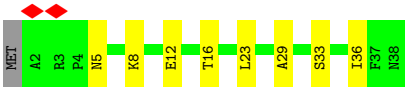




• Molecule 9: Photosystem II reaction center protein L

Chain l:

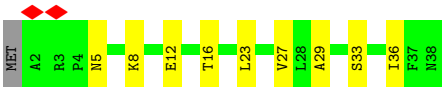




• Molecule 9: Photosystem II reaction center protein L

Chain L:

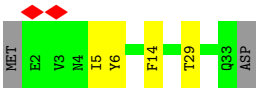




• Molecule 10: Photosystem II reaction center protein M

Chain m:

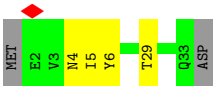




• Molecule 10: Photosystem II reaction center protein M

Chain M:

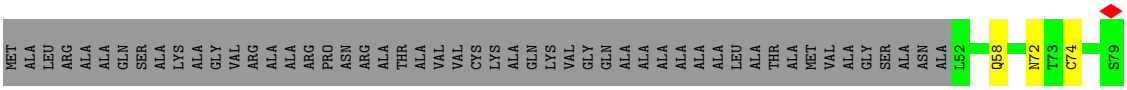


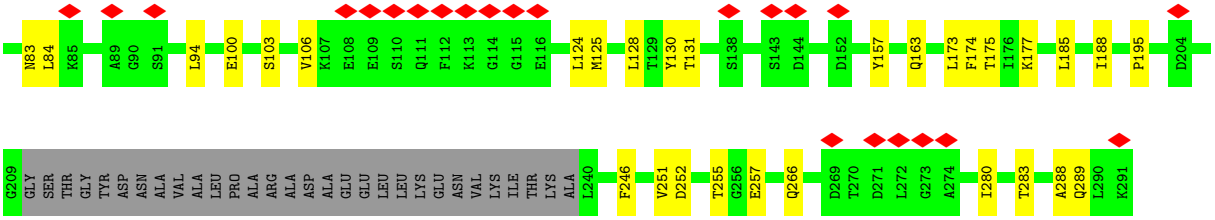


• Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II

Chain o:

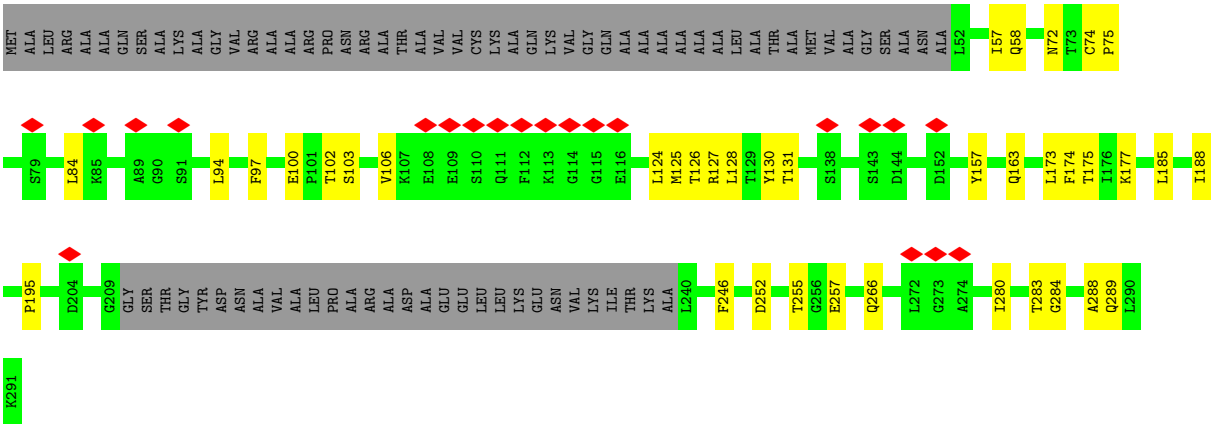




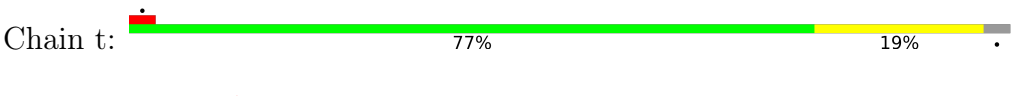


• Molecule 11: Oxygen-evolving enhancer protein 1 of photosystem II

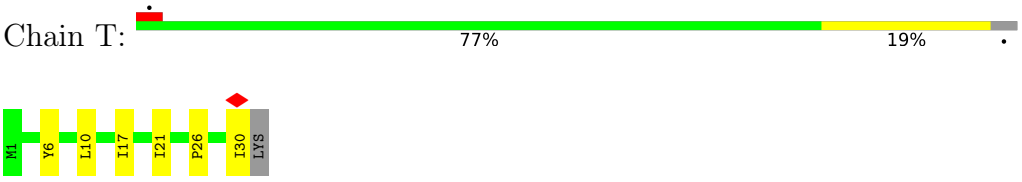




• Molecule 12: Photosystem II reaction center protein T

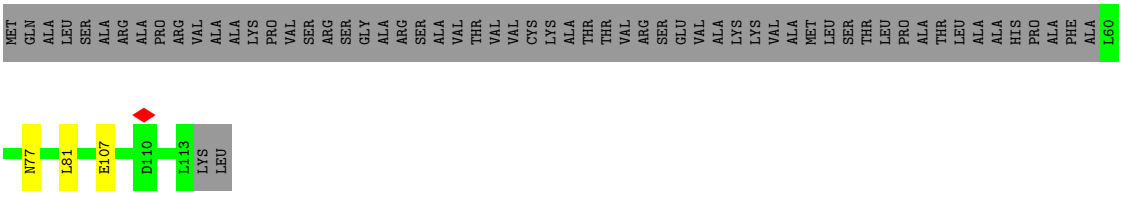


• Molecule 12: Photosystem II reaction center protein T



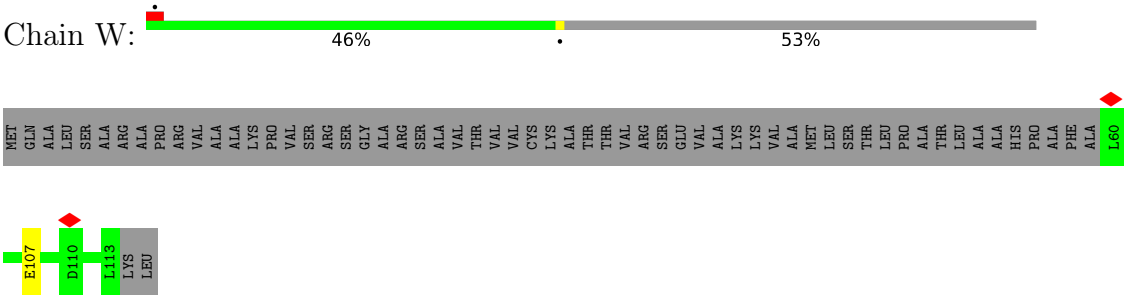
• Molecule 13: Photosystem II reaction center W protein, chloroplastic





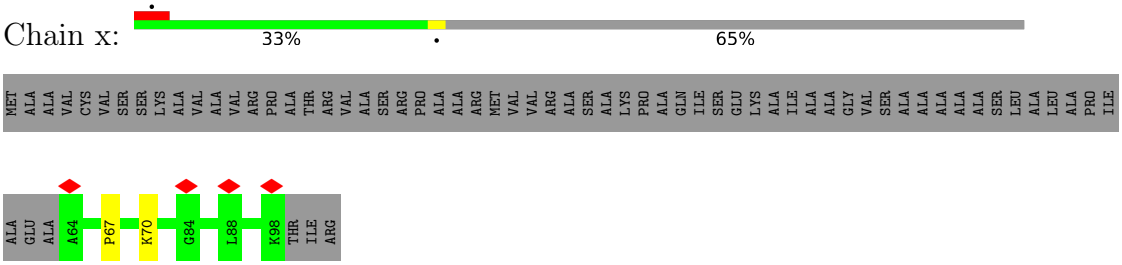
• Molecule 13: Photosystem II reaction center W protein, chloroplastic

Chain W:



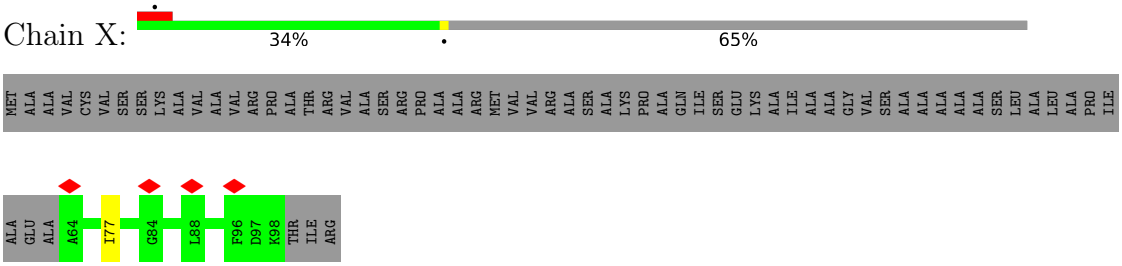
• Molecule 14: 4.1 kDa photosystem II subunit

Chain x:



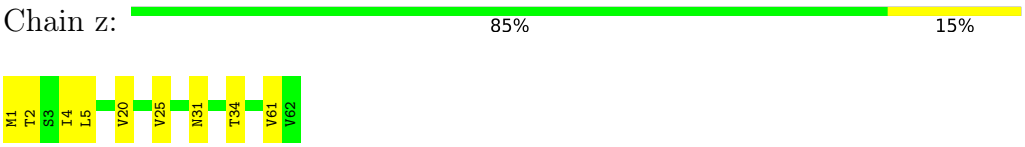
• Molecule 14: 4.1 kDa photosystem II subunit

Chain X:



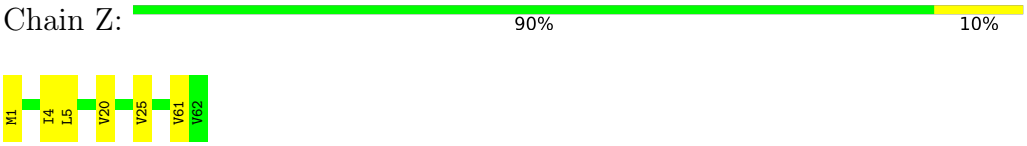
• Molecule 15: Photosystem II reaction center protein Z

Chain z:



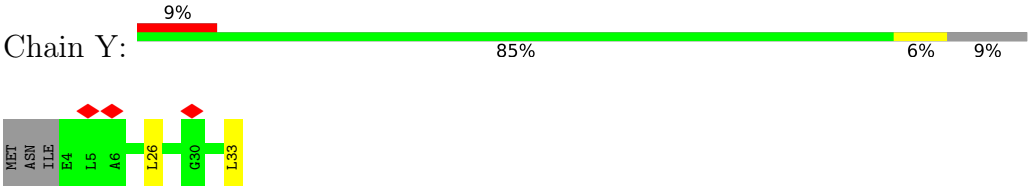
• Molecule 15: Photosystem II reaction center protein Z

Chain Z:



• Molecule 16: Photosystem II reaction center protein 30, Psb30

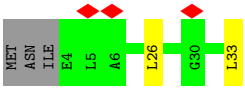
Chain Y:



• Molecule 16: Photosystem II reaction center protein 30, Psb30

Chain y:

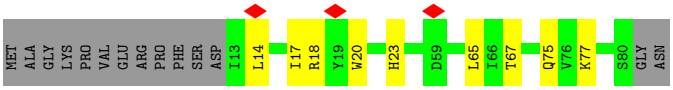




• Molecule 17: Cytochrome b559 subunit alpha

Chain E:

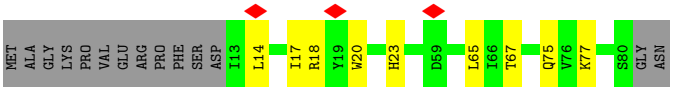




• Molecule 17: Cytochrome b559 subunit alpha

Chain e:

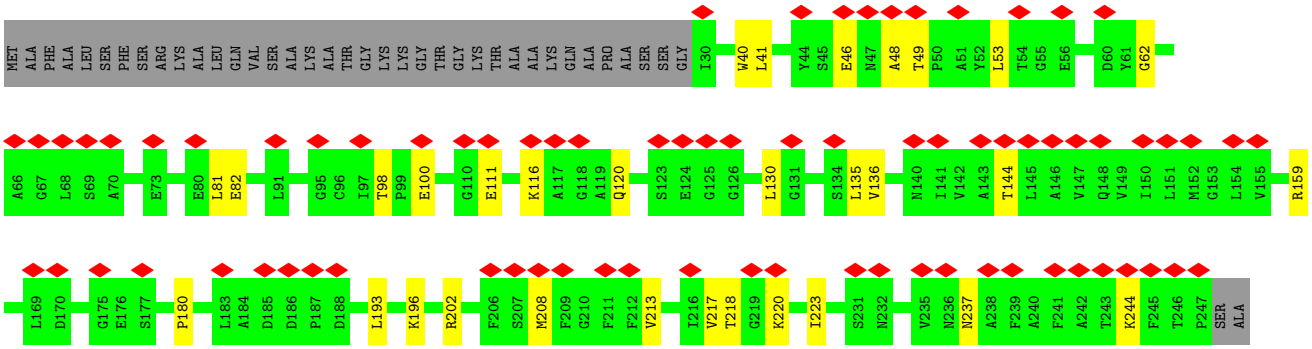




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

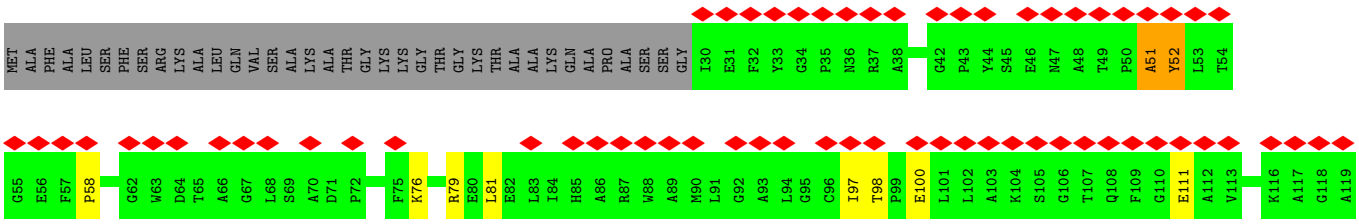




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



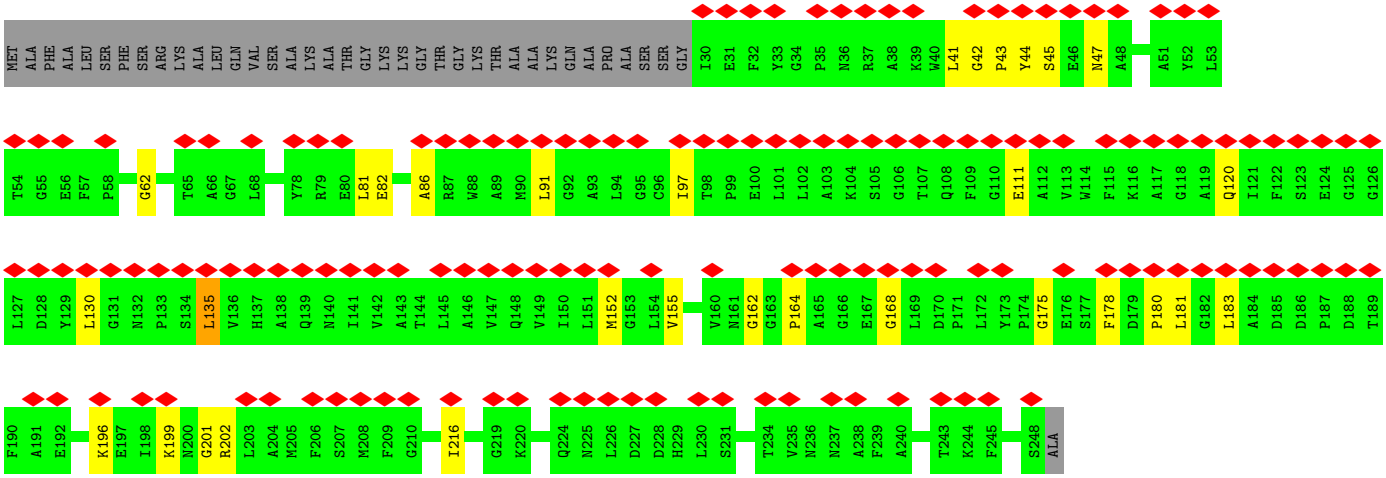




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

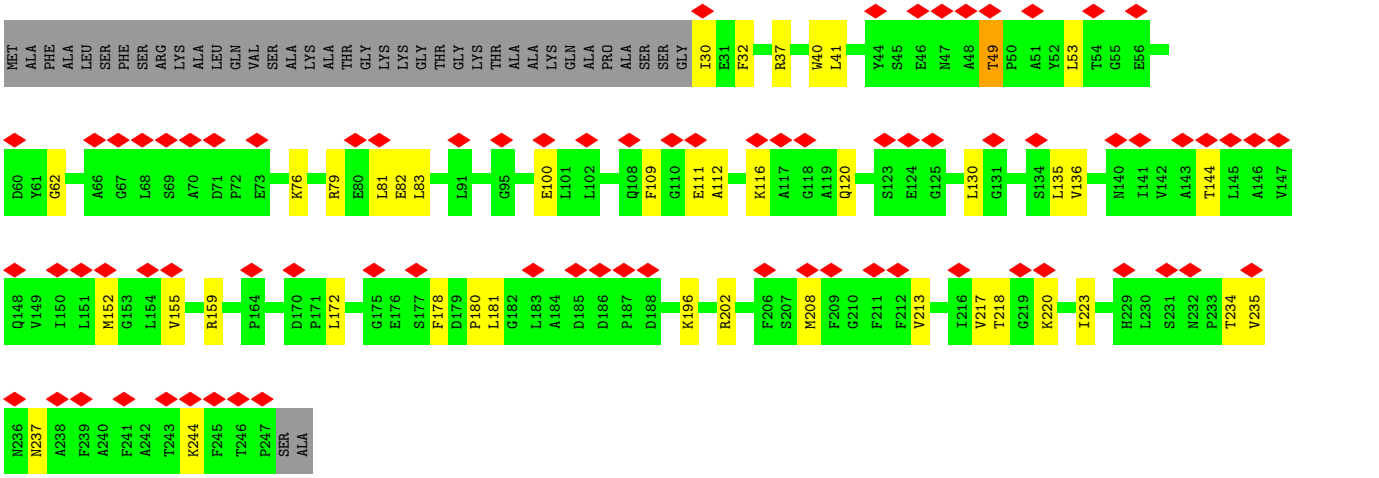




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

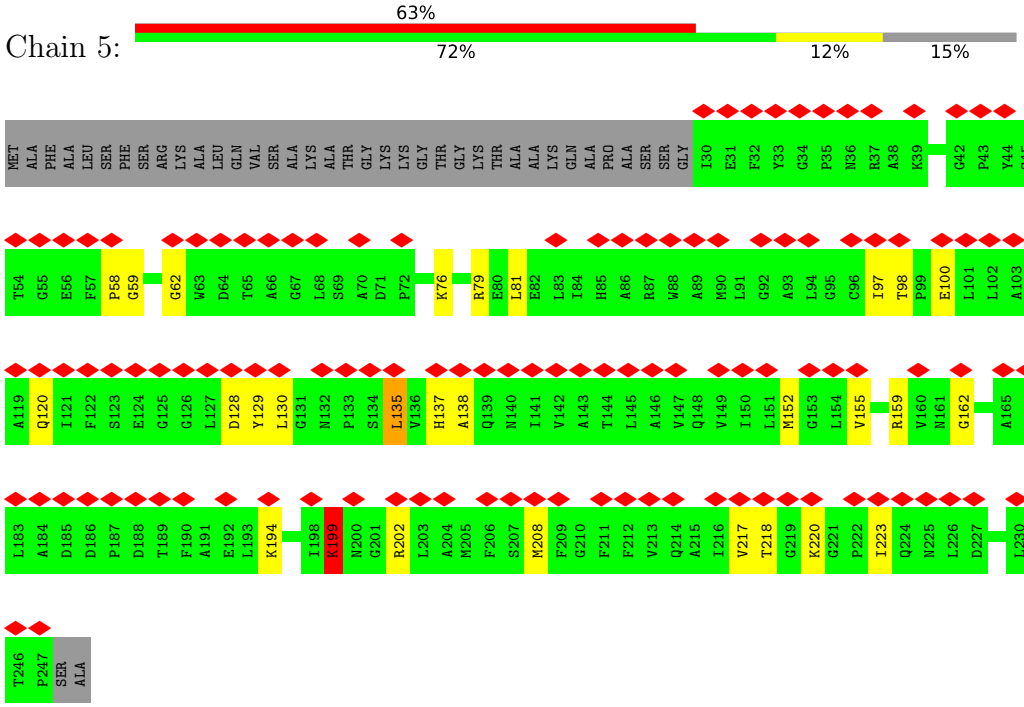
Chain 4:





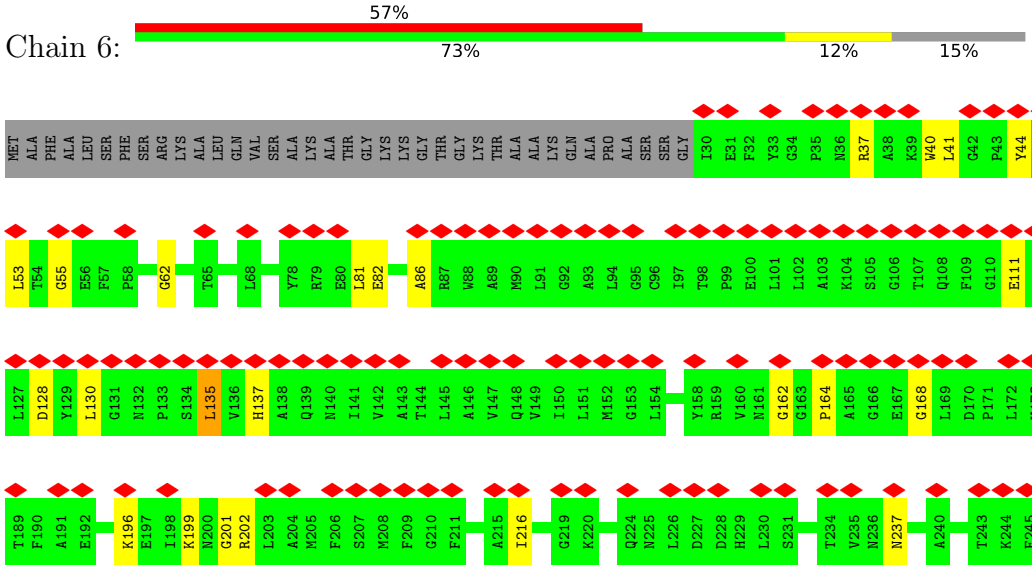
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5:



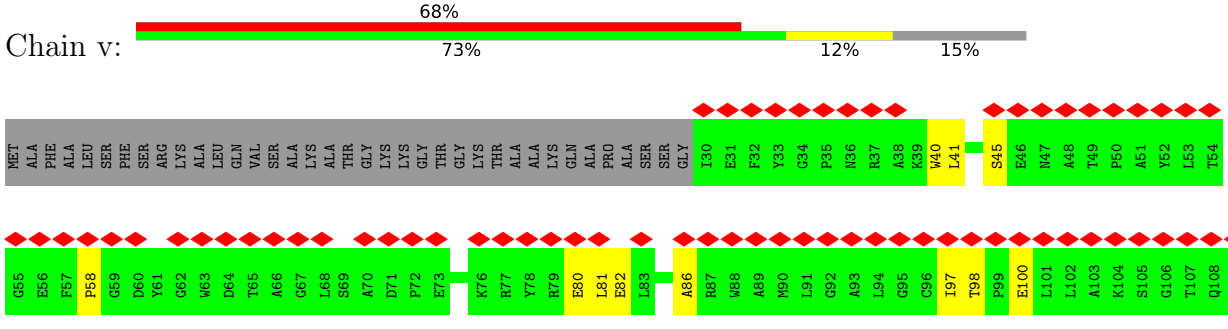
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

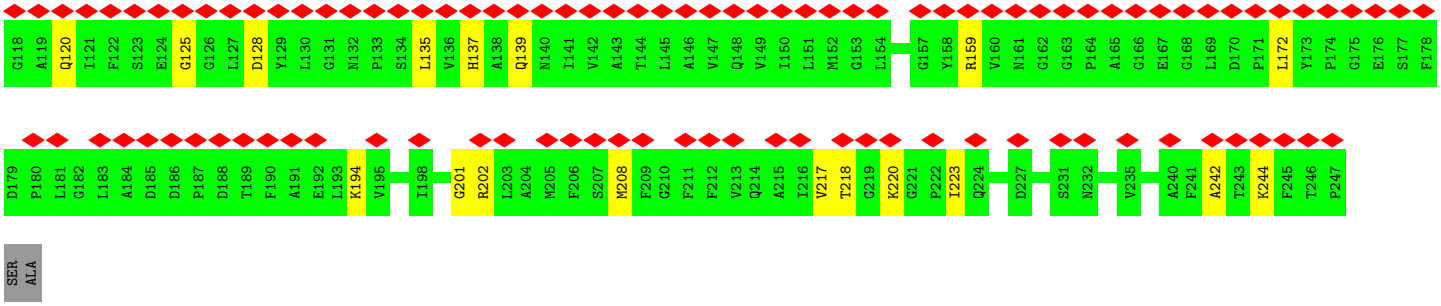
Chain 6:



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain v:

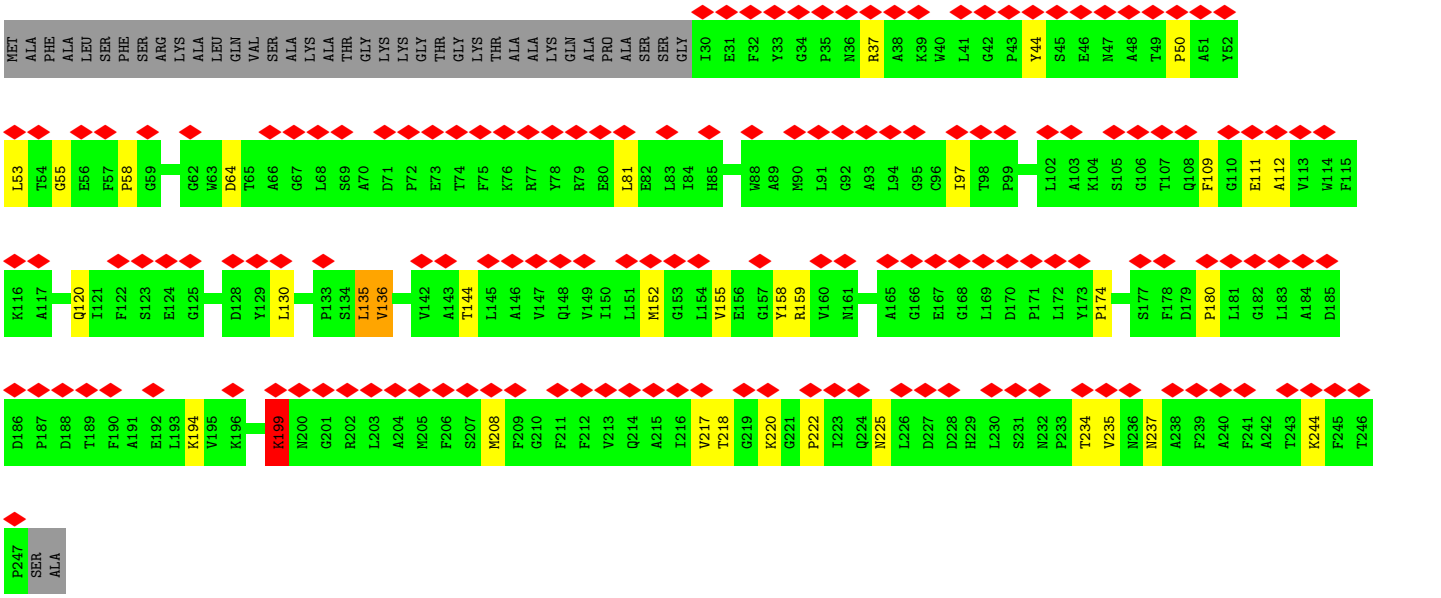




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain p:

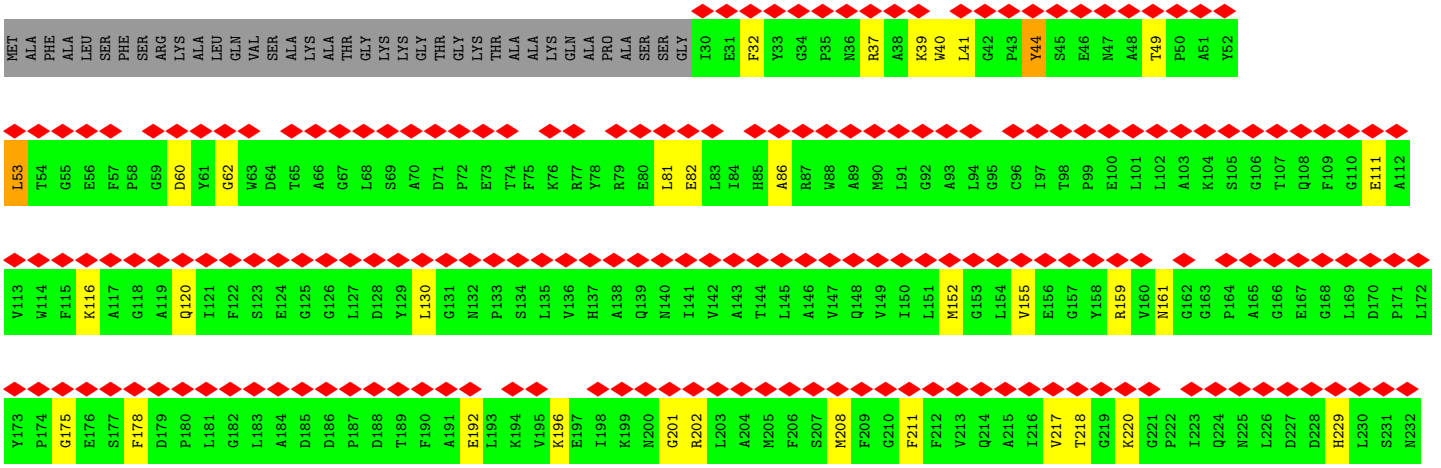


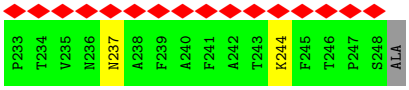


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain q:



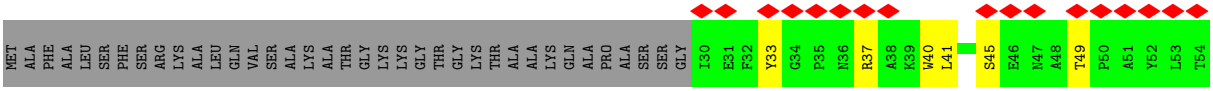


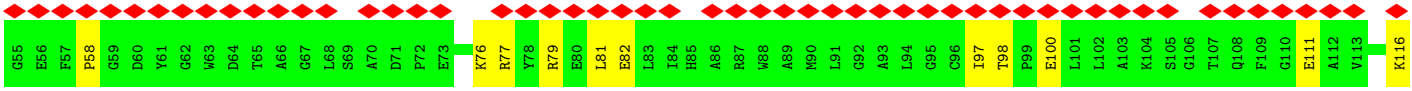


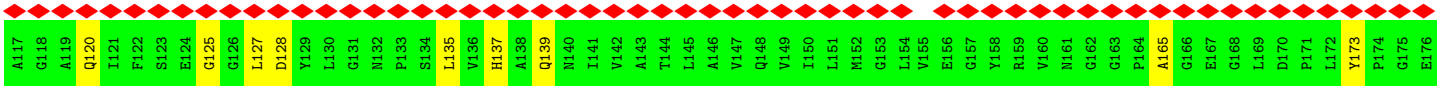
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

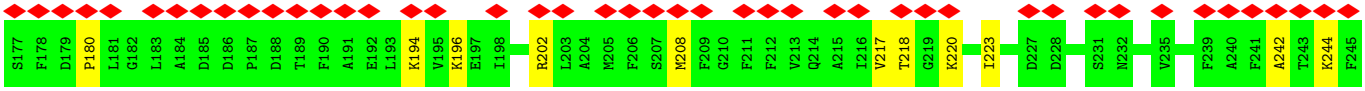
Chain V:









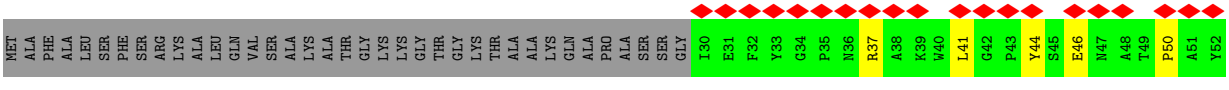


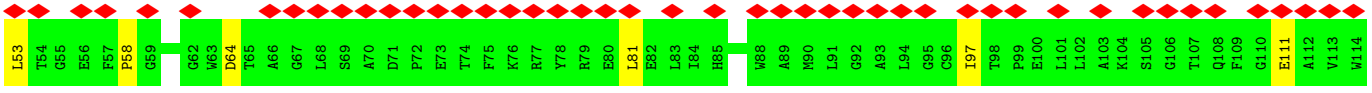


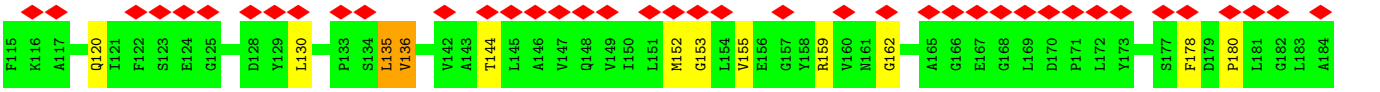
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain P:







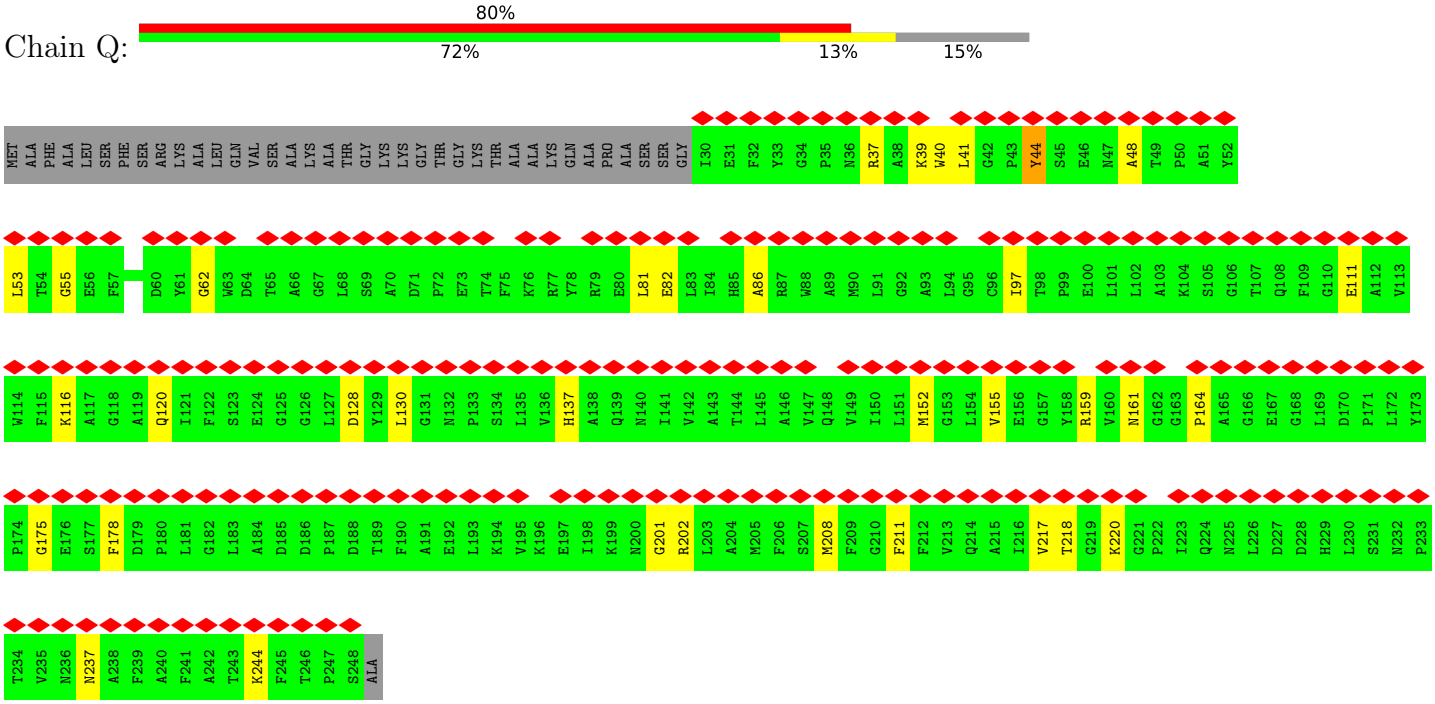






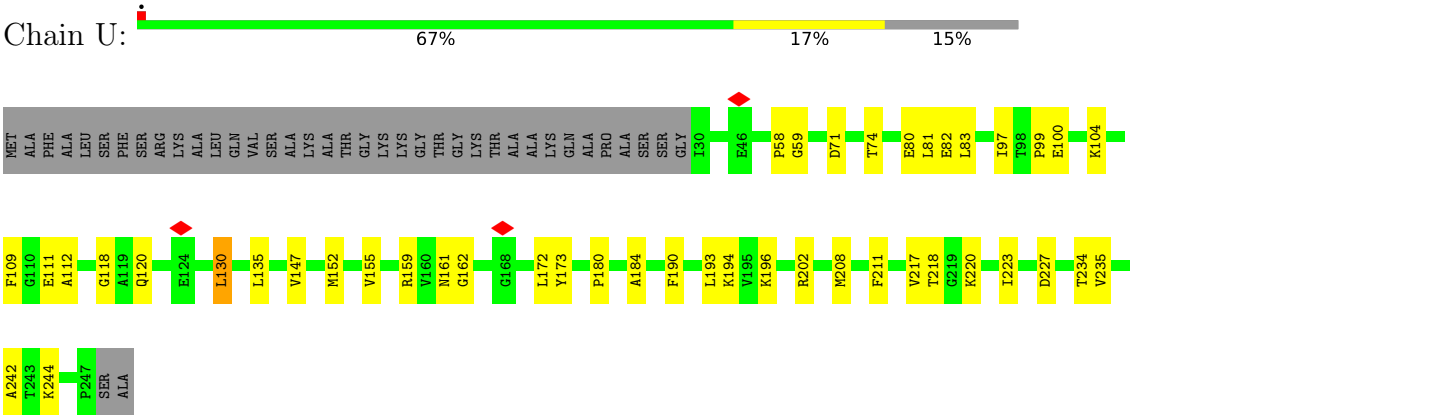
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain Q:



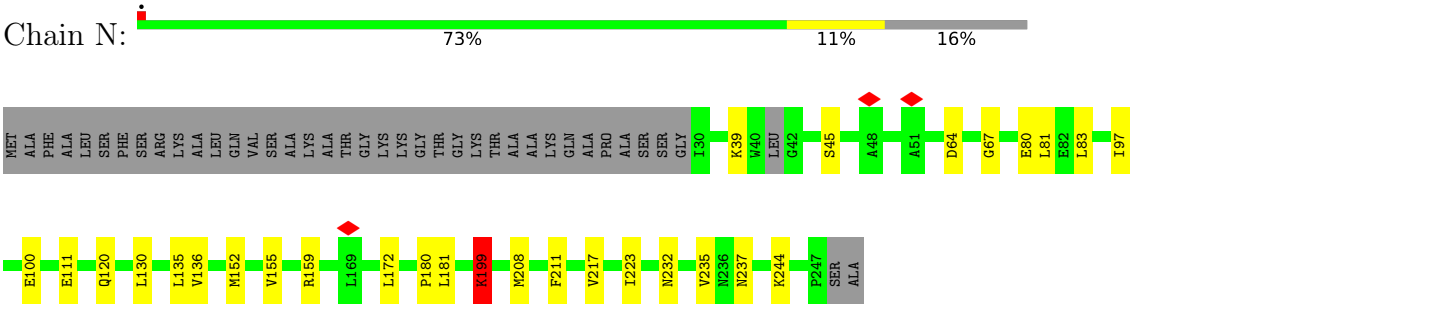
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain U:



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

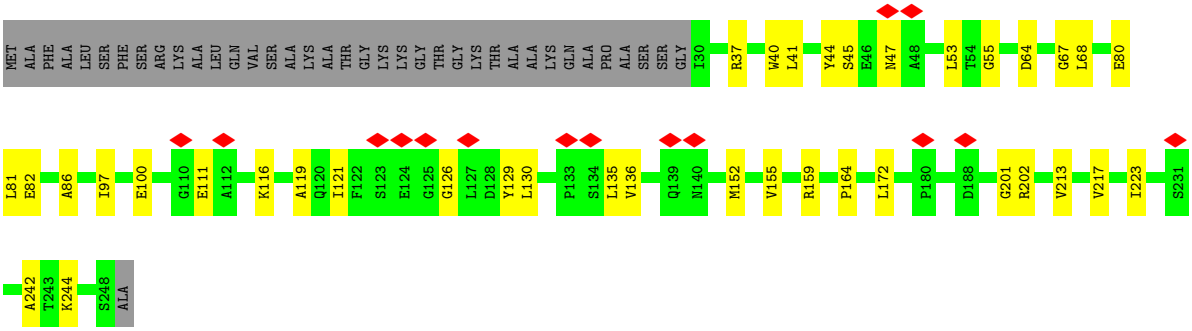
Chain N:



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain G:

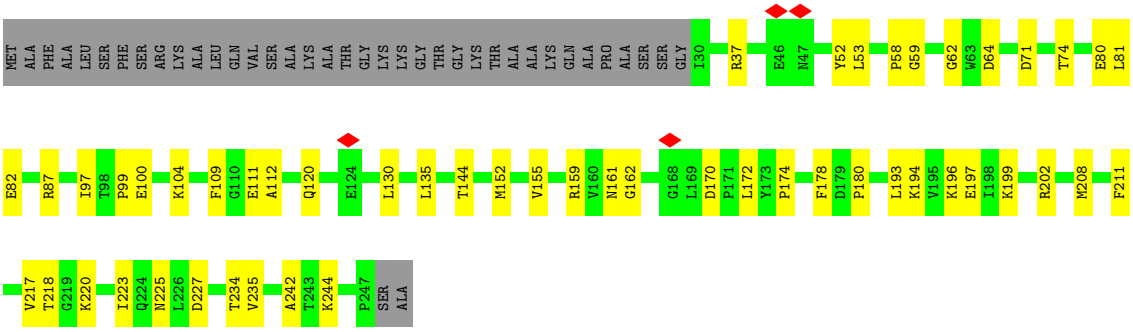




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain u:

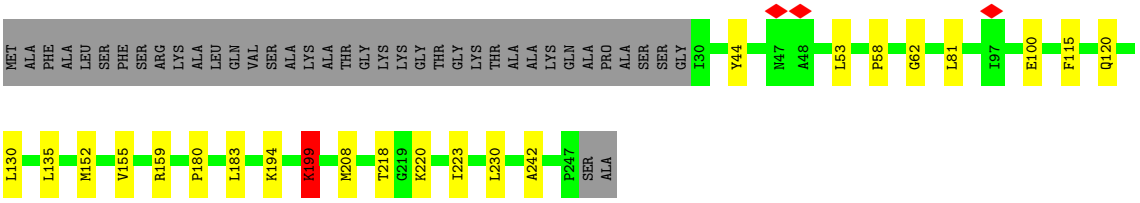




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain n:

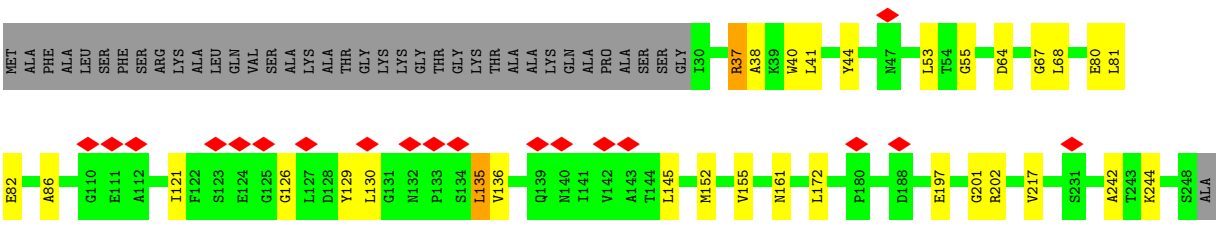




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain g:

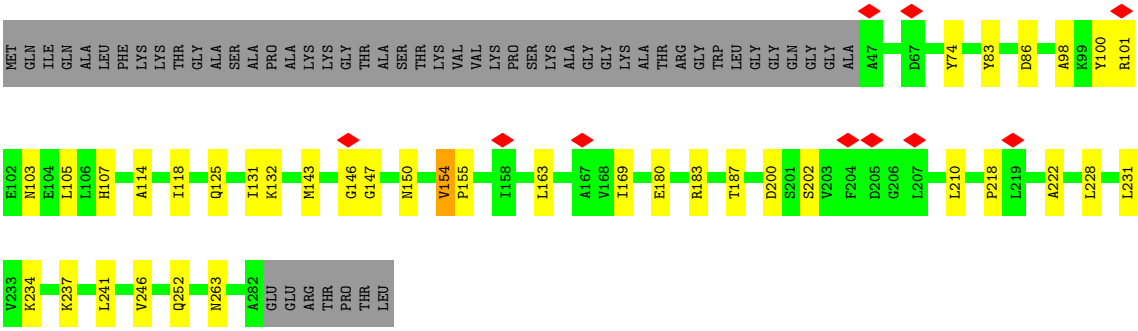




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

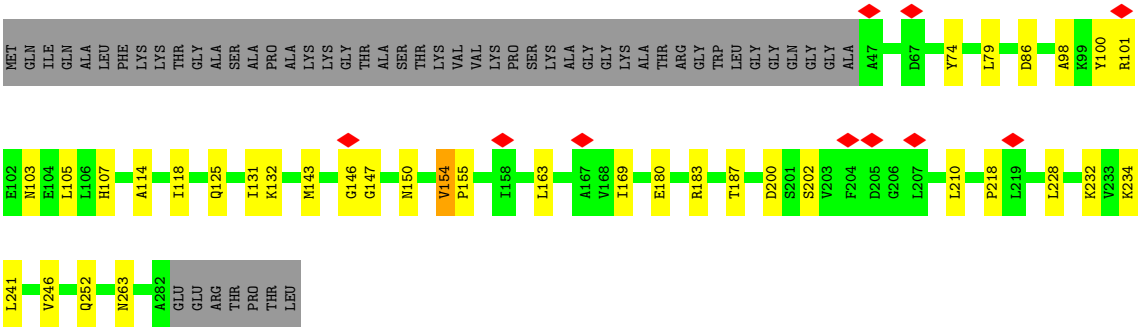
Chain S:



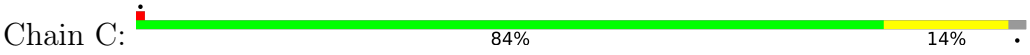


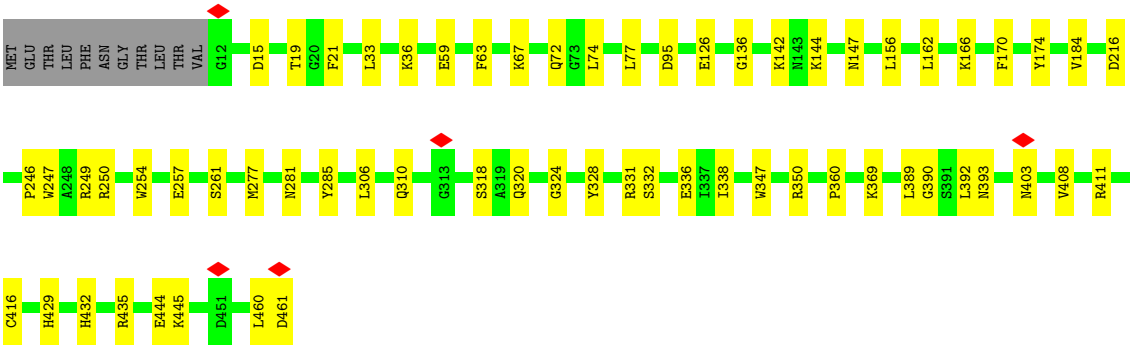
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic



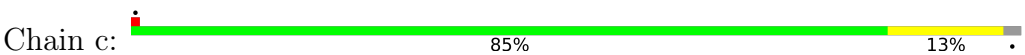


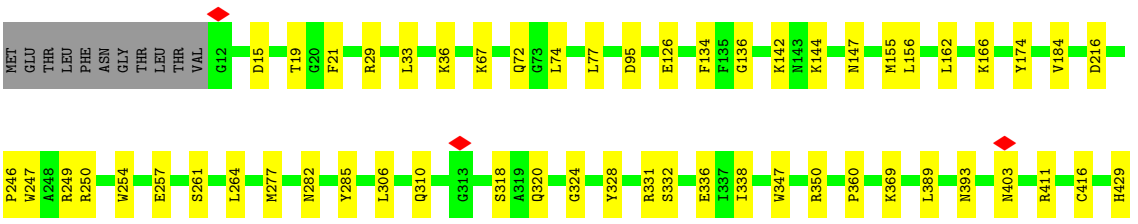
• Molecule 20: Photosystem II CP43 reaction center protein

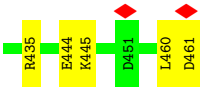




• Molecule 20: Photosystem II CP43 reaction center protein



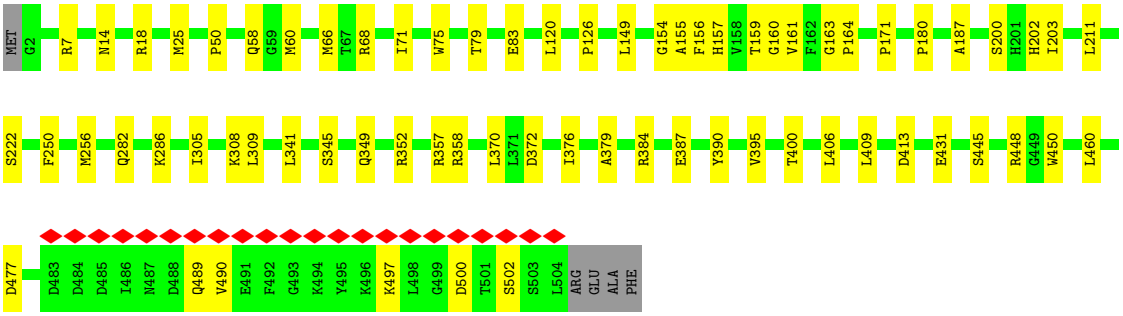




• Molecule 21: Photosystem II CP47 reaction center protein

Chain B:

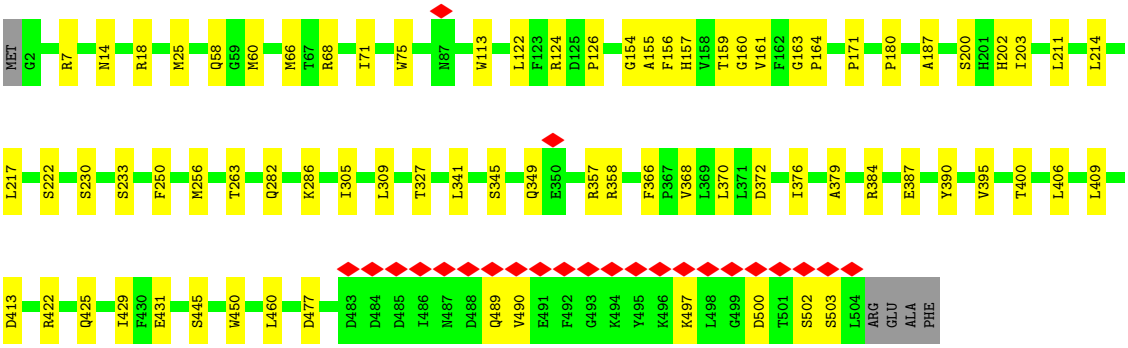




• Molecule 21: Photosystem II CP47 reaction center protein

Chain b:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.181	Depositor
Minimum map value	-1.592	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	392.1, 392.1, 392.1	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, XAT, BCR, CHL, PL9, CLA, BCT, LUT, FE2, LHG, NEX, LMG, PHO, HEM, CL, DGD

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	R	0.21	0/1736	0.56	0/2357
1	r	0.21	0/1739	0.57	0/2361
2	A	0.28	0/2696	0.51	0/3676
2	a	0.29	0/2696	0.53	0/3676
3	D	0.29	0/2808	0.61	0/3830
3	d	0.29	0/2808	0.61	0/3830
4	F	0.25	0/250	0.56	0/338
4	f	0.26	0/250	0.56	0/338
5	H	0.25	0/499	0.51	0/683
5	h	0.25	0/499	0.52	0/683
6	I	0.31	0/283	0.57	0/383
6	i	0.31	0/283	0.57	0/383
7	J	0.18	0/254	0.47	0/345
7	j	0.17	0/254	0.47	0/345
8	K	0.33	0/300	0.74	0/414
8	k	0.35	0/300	0.73	0/414
9	L	0.26	0/314	0.52	0/427
9	l	0.26	0/314	0.55	0/427
10	M	0.24	0/252	0.48	0/345
10	m	0.24	0/252	0.48	0/345
11	O	0.21	0/1620	0.53	0/2184
11	o	0.21	0/1620	0.53	0/2184
12	T	0.22	0/254	0.54	0/343
12	t	0.21	0/254	0.54	0/343
13	W	0.24	0/428	0.48	0/581
13	w	0.24	0/428	0.48	0/581
14	X	0.21	0/244	0.40	0/330
14	x	0.21	0/244	0.40	0/330
15	Z	0.19	0/476	0.41	0/654
15	z	0.19	0/476	0.41	0/654
16	Y	0.19	0/208	0.48	0/285
16	y	0.19	0/208	0.48	0/285

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	E	0.22	0/571	0.54	0/780
17	e	0.22	0/571	0.51	0/780
18	1	0.22	0/1717	0.55	0/2337
18	2	0.25	0/1717	0.63	3/2337 (0.1%)
18	3	0.20	0/1723	0.52	0/2345
18	4	0.22	0/1717	0.56	0/2337
18	5	0.24	0/1717	0.56	1/2337 (0.0%)
18	6	0.21	0/1723	0.54	0/2345
18	G	0.23	0/1723	0.56	0/2345
18	N	0.24	0/1708	0.55	1/2323 (0.0%)
18	P	0.22	0/1717	0.55	1/2337 (0.0%)
18	Q	0.20	0/1723	0.57	0/2345
18	U	0.25	0/1717	0.56	0/2337
18	V	0.21	0/1717	0.53	0/2337
18	g	0.23	0/1723	0.61	0/2345
18	n	0.23	0/1717	0.59	1/2337 (0.0%)
18	p	0.23	0/1717	0.57	1/2337 (0.0%)
18	q	0.21	0/1723	0.57	0/2345
18	u	0.26	0/1717	0.59	0/2337
18	v	0.22	0/1717	0.55	0/2337
19	S	0.25	0/1849	0.65	2/2521 (0.1%)
19	s	0.25	0/1849	0.66	2/2521 (0.1%)
20	C	0.26	0/3623	0.47	0/4936
20	c	0.26	0/3623	0.47	0/4936
21	B	0.23	0/4067	0.45	0/5533
21	b	0.23	0/4067	0.46	0/5533
All	All	0.24	0/76400	0.54	12/103994 (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
1	r	0	1
18	1	0	1
18	2	0	2
18	3	0	1
18	4	0	2
18	5	0	1
18	6	0	2
18	N	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
18	P	0	1
18	Q	0	1
18	U	0	1
18	V	0	1
18	g	0	1
18	n	0	1
18	p	0	1
18	q	0	1
18	u	0	1
18	v	0	1
All	All	0	21

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	199	LYS	CD-CE-NZ	-6.37	91.50	111.90
18	5	199	LYS	CD-CE-NZ	-6.22	91.99	111.90
18	n	199	LYS	CD-CE-NZ	-5.93	92.92	111.90
18	p	199	LYS	CD-CE-NZ	-5.74	93.54	111.90
18	2	51	ALA	CA-C-N	5.30	131.65	121.54
18	2	51	ALA	C-N-CA	5.30	131.65	121.54
18	N	199	LYS	CD-CE-NZ	-5.29	94.98	111.90
19	S	200	ASP	CA-C-N	-5.21	115.33	121.90
19	S	200	ASP	C-N-CA	-5.21	115.33	121.90
19	s	200	ASP	CA-C-N	-5.16	115.40	121.90
19	s	200	ASP	C-N-CA	-5.16	115.40	121.90
18	P	199	LYS	CD-CE-NZ	-5.10	95.59	111.90

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	1	135	LEU	Peptide
18	2	51	ALA	Peptide
18	2	52	TYR	Peptide
18	3	135	LEU	Peptide
18	4	135	LEU	Peptide
18	4	49	THR	Peptide
18	5	135	LEU	Peptide
18	6	135	LEU	Peptide

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Mol	Chain	Res	Type	Group
18	6	44	TYR	Peptide
18	N	135	LEU	Peptide
18	P	135	LEU	Peptide
18	Q	44	TYR	Peptide
18	U	135	LEU	Peptide
18	V	135	LEU	Peptide
18	g	135	LEU	Peptide
18	n	135	LEU	Peptide
18	p	135	LEU	Peptide
18	q	44	TYR	Peptide
1	r	15	LEU	Peptide
18	u	135	LEU	Peptide
18	v	135	LEU	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	R	1698	0	1653	34	0
1	r	1701	0	1656	31	0
2	A	2614	0	2516	41	0
2	a	2614	0	2516	38	0
3	D	2714	0	2596	40	0
3	d	2714	0	2596	38	0
4	F	243	0	252	4	0
4	f	243	0	252	4	0
5	H	488	0	515	9	0
5	h	488	0	515	9	0
6	I	275	0	287	1	0
6	i	275	0	287	1	0
7	J	245	0	236	5	0
7	j	245	0	236	5	0
8	K	288	0	295	1	0
8	k	288	0	295	2	0
9	L	306	0	313	7	0
9	l	306	0	313	6	0
10	M	248	0	266	4	0
10	m	248	0	266	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	O	1592	0	1592	25	0
11	o	1592	0	1592	22	0
12	T	247	0	260	6	0
12	t	247	0	260	7	0
13	W	417	0	387	1	0
13	w	417	0	387	2	0
14	X	242	0	266	1	0
14	x	242	0	266	1	0
15	Z	465	0	499	4	0
15	z	465	0	499	6	0
16	Y	208	0	239	2	0
16	y	208	0	239	2	0
17	E	555	0	550	6	0
17	e	555	0	550	7	0
18	1	1669	0	1612	21	0
18	2	1669	0	1612	16	0
18	3	1675	0	1616	22	0
18	4	1669	0	1612	28	0
18	5	1669	0	1612	22	0
18	6	1675	0	1616	23	0
18	G	1675	0	1617	23	0
18	N	1661	0	1600	19	0
18	P	1669	0	1612	26	0
18	Q	1675	0	1617	24	0
18	U	1669	0	1612	27	0
18	V	1669	0	1612	24	0
18	g	1675	0	1617	21	0
18	n	1669	0	1612	16	0
18	p	1669	0	1612	23	0
18	q	1675	0	1617	24	0
18	u	1669	0	1612	32	0
18	v	1669	0	1612	18	0
19	S	1797	0	1744	25	0
19	s	1797	0	1743	24	0
20	C	3502	0	3373	46	0
20	c	3502	0	3373	44	0
21	B	3937	0	3814	50	0
21	b	3937	0	3814	55	0
22	1	473	0	468	16	0
22	2	473	0	466	22	0
22	3	477	0	475	15	0
22	4	473	0	468	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	5	473	0	466	19	0
22	6	477	0	474	12	0
22	A	240	0	242	8	0
22	B	1040	0	1150	29	0
22	C	845	0	933	25	0
22	D	65	0	71	3	0
22	G	477	0	475	9	0
22	N	473	0	466	15	0
22	P	473	0	466	17	0
22	Q	477	0	475	14	0
22	R	543	0	489	14	0
22	S	465	0	391	10	0
22	U	473	0	468	11	0
22	V	473	0	468	16	0
22	X	65	0	70	1	0
22	a	240	0	242	6	0
22	b	1040	0	1149	33	0
22	c	845	0	933	23	0
22	d	65	0	71	2	0
22	g	477	0	474	5	0
22	n	473	0	466	16	0
22	p	473	0	466	14	0
22	q	477	0	474	10	0
22	r	543	0	487	19	0
22	s	465	0	391	13	0
22	u	473	0	468	14	0
22	v	473	0	468	14	0
22	x	65	0	70	0	0
23	1	84	0	112	5	0
23	2	84	0	112	8	0
23	4	84	0	112	9	0
23	5	84	0	112	14	0
23	N	84	0	112	9	0
23	P	84	0	112	7	0
23	R	42	0	56	2	0
23	S	84	0	112	9	0
23	U	84	0	112	4	0
23	V	84	0	112	11	0
23	n	84	0	112	7	0
23	p	84	0	112	5	0
23	r	42	0	55	4	0
23	s	84	0	111	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	u	84	0	112	6	0
23	v	84	0	112	7	0
24	1	44	0	56	2	0
24	2	44	0	56	5	0
24	3	44	0	56	2	0
24	4	44	0	56	1	0
24	5	44	0	56	3	0
24	6	44	0	56	4	0
24	G	44	0	56	3	0
24	N	44	0	56	2	0
24	P	44	0	56	4	0
24	Q	44	0	56	0	0
24	R	44	0	56	3	0
24	U	44	0	56	5	0
24	V	44	0	56	4	0
24	g	44	0	56	5	0
24	n	44	0	56	1	0
24	p	44	0	56	3	0
24	q	44	0	56	1	0
24	r	44	0	56	4	0
24	u	44	0	56	3	0
24	v	44	0	56	3	0
25	1	49	0	74	0	0
25	2	49	0	74	3	0
25	3	49	0	74	3	0
25	4	49	0	74	1	0
25	5	49	0	74	1	0
25	6	49	0	74	3	0
25	A	43	0	56	3	0
25	B	96	0	139	0	0
25	C	147	0	222	5	0
25	D	95	0	138	11	0
25	G	49	0	74	0	0
25	L	49	0	74	2	0
25	N	49	0	74	4	0
25	P	49	0	74	1	0
25	Q	49	0	74	4	0
25	R	42	0	57	0	0
25	S	49	0	71	5	0
25	U	49	0	74	4	0
25	V	49	0	74	6	0
25	a	43	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	b	96	0	139	0	0
25	c	147	0	222	7	0
25	d	95	0	138	12	0
25	g	49	0	74	2	0
25	l	49	0	74	1	0
25	n	49	0	74	1	0
25	p	49	0	74	2	0
25	q	49	0	74	2	0
25	r	42	0	57	1	0
25	s	49	0	71	3	0
25	u	49	0	74	2	0
25	v	49	0	74	4	0
26	1	362	0	347	10	0
26	2	362	0	349	12	0
26	3	357	0	335	16	0
26	4	296	0	277	11	0
26	5	362	0	349	12	0
26	6	423	0	405	20	0
26	G	357	0	335	13	0
26	N	296	0	280	12	0
26	P	362	0	349	17	0
26	Q	357	0	335	9	0
26	R	183	0	174	5	0
26	S	196	0	141	4	0
26	U	380	0	384	17	0
26	V	362	0	347	15	0
26	g	357	0	335	12	0
26	n	362	0	349	13	0
26	p	428	0	419	12	0
26	q	291	0	265	13	0
26	r	231	0	207	7	0
26	s	196	0	141	2	0
26	u	362	0	347	11	0
26	v	362	0	347	14	0
27	2	44	0	56	1	0
27	5	44	0	56	2	0
27	N	44	0	56	2	0
27	P	44	0	54	1	0
27	R	44	0	54	3	0
27	S	44	0	55	3	0
27	U	44	0	56	0	0
27	V	44	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	n	44	0	56	2	0
27	p	44	0	54	4	0
27	r	88	0	110	7	0
27	s	44	0	55	4	0
27	u	88	0	112	3	0
27	v	44	0	56	2	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	2	0	0	2	0
29	a	2	0	0	4	0
30	A	64	0	74	4	0
30	D	64	0	74	1	0
30	a	64	0	74	2	0
30	d	64	0	74	1	0
31	A	40	0	56	4	0
31	B	120	0	168	11	0
31	C	120	0	168	4	0
31	D	40	0	55	1	0
31	K	40	0	56	2	0
31	T	40	0	56	5	0
31	X	40	0	56	4	0
31	a	40	0	56	3	0
31	b	120	0	168	12	0
31	c	80	0	112	1	0
31	d	40	0	55	0	0
31	k	40	0	56	2	0
31	t	40	0	56	6	0
31	x	40	0	56	3	0
31	z	40	0	56	2	0
32	A	54	0	77	3	0
32	C	50	0	66	2	0
32	L	54	0	76	2	0
32	M	42	0	48	1	0
32	a	104	0	143	6	0
32	l	54	0	76	3	0
32	m	42	0	48	1	0
33	A	13	0	7	0	0
33	D	55	0	80	3	0
33	a	13	0	7	0	0
33	d	55	0	80	3	0
34	A	40	0	50	1	0
34	B	106	0	157	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	102	0	144	4	0
34	D	46	0	61	0	0
34	W	48	0	66	2	0
34	a	40	0	50	1	0
34	b	106	0	157	5	0
34	c	102	0	144	3	0
34	d	46	0	61	0	0
34	w	48	0	66	2	0
35	D	4	0	1	1	0
35	a	4	0	1	1	0
36	A	59	0	76	2	0
36	B	62	0	80	6	0
36	C	117	0	150	7	0
36	J	60	0	78	2	0
36	a	59	0	76	2	0
36	b	62	0	80	7	0
36	c	177	0	228	8	0
37	E	43	0	30	1	0
37	e	43	0	30	1	0
All	All	104363	0	104847	1605	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 8.

All (1605) 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)
18:v:208:MET:HE2	23:v:310:LUT:H10	1.67	0.74
11:o:125:MET:SD	11:o:163:GLN:NE2	2.61	0.73
11:O:125:MET:SD	11:O:163:GLN:NE2	2.62	0.73
18:V:208:MET:HE2	23:V:310:LUT:H10	1.72	0.72
22:2:304:CLA:H52	23:2:309:LUT:H30	1.71	0.71
18:G:111:GLU:HG2	18:G:116:LYS:HB2	1.73	0.71
22:b:616:CLA:H2	22:b:617:CLA:HBB2	1.71	0.71
22:N:301:CLA:HAB	23:N:310:LUT:H32	1.71	0.70
22:2:301:CLA:H52	23:2:310:LUT:H28	1.71	0.70
18:1:208:MET:HE2	23:1:310:LUT:H10	1.73	0.69
18:P:208:MET:HE2	23:P:311:LUT:H10	1.74	0.69
18:4:208:MET:HE2	23:4:310:LUT:H10	1.74	0.69
18:2:199:LYS:NZ	22:2:305:CLA:OBD	2.25	0.68
20:C:320:GLN:HE21	20:C:324:GLY:HA2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:5:301:CLA:H52	23:5:310:LUT:H28	1.76	0.68
18:G:164:PRO:HG2	26:G:315:CHL:HBB2	1.76	0.67
11:O:257:GLU:HG2	11:O:289:GLN:HG2	1.76	0.67
22:S:305:CLA:HAB	23:S:310:LUT:H32	1.75	0.67
22:C:515:CLA:HBB1	31:C:516:BCR:H403	1.74	0.67
20:c:320:GLN:HE21	20:c:324:GLY:HA2	1.59	0.67
18:5:199:LYS:NZ	22:5:305:CLA:OBD	2.26	0.67
18:q:111:GLU:HB3	18:q:120:GLN:HE21	1.60	0.67
18:N:80:GLU:HG2	18:N:172:LEU:HD11	1.77	0.67
22:u:305:CLA:HBB2	25:c:523:LHG:H201	1.77	0.67
31:z:101:BCR:H403	22:c:514:CLA:HBB1	1.77	0.67
27:r:618:NEX:H362	22:p:304:CLA:HAB	1.77	0.66
22:A:406:CLA:HAB	22:D:403:CLA:H72	1.77	0.66
18:p:208:MET:HE2	23:p:311:LUT:H10	1.78	0.66
18:N:199:LYS:NZ	22:N:305:CLA:OBD	2.27	0.66
18:u:208:MET:HE2	23:u:310:LUT:H10	1.78	0.66
22:n:301:CLA:HAB	23:n:310:LUT:H32	1.76	0.66
22:P:304:CLA:HAB	27:R:301:NEX:H362	1.78	0.66
26:v:318:CHL:HBB1	26:q:311:CHL:H51	1.77	0.66
18:P:199:LYS:NZ	22:P:306:CLA:OBD	2.27	0.65
18:Q:111:GLU:HB3	18:Q:120:GLN:HE21	1.62	0.65
22:a:406:CLA:HAB	22:d:402:CLA:H72	1.78	0.65
18:p:199:LYS:NZ	22:p:306:CLA:OBD	2.25	0.65
18:U:208:MET:HE2	23:U:310:LUT:H10	1.77	0.65
18:n:199:LYS:NZ	22:n:305:CLA:OBD	2.25	0.64
18:q:82:GLU:OE2	18:q:202:ARG:NH2	2.30	0.64
18:5:208:MET:HE2	23:5:310:LUT:H10	1.79	0.64
18:Q:82:GLU:OE2	18:Q:202:ARG:NH2	2.31	0.64
22:u:301:CLA:HAB	23:u:310:LUT:H32	1.79	0.64
18:3:180:PRO:HD2	22:3:304:CLA:H2	1.80	0.63
22:U:301:CLA:HAB	23:U:310:LUT:H32	1.80	0.63
2:a:339:PHE:N	29:a:403:CL:CL	2.69	0.63
25:d:406:LHG:H272	25:d:406:LHG:H122	1.81	0.63
18:G:41:LEU:HB3	18:G:44:TYR:HB2	1.80	0.63
24:g:309:XAT:H10	26:g:311:CHL:H142	1.81	0.63
2:a:82:VAL:HB	2:a:174:LEU:HB2	1.81	0.62
22:P:303:CLA:HBB1	26:P:319:CHL:H152	1.82	0.62
31:t:101:BCR:H15C	31:B:619:BCR:H20C	1.82	0.62
22:B:608:CLA:H2	34:B:621:LMG:H151	1.79	0.62
25:c:521:LHG:H171	25:s:312:LHG:H141	1.82	0.62
18:4:81:LEU:HD11	22:4:302:CLA:HBD	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:6:82:GLU:OE2	18:6:202:ARG:NH2	2.32	0.62
22:r:602:CLA:HAB	24:r:612:XAT:H32	1.81	0.62
32:A:412:SQD:H222	31:T:101:BCR:HC21	1.80	0.62
24:G:309:XAT:H10	26:G:311:CHL:H142	1.80	0.62
3:D:24:GLN:O	3:D:26:ARG:NH1	2.33	0.61
18:3:82:GLU:OE2	18:3:202:ARG:NH2	2.32	0.61
22:b:608:CLA:H2	34:b:621:LMG:H151	1.81	0.61
18:1:81:LEU:HD11	22:1:302:CLA:HBD	1.81	0.61
18:4:82:GLU:OE2	18:4:202:ARG:NH2	2.34	0.61
20:C:331:ARG:NH2	11:O:131:THR:O	2.34	0.61
3:d:24:GLN:O	3:d:26:ARG:NH1	2.34	0.61
25:d:405:LHG:HC41	25:d:405:LHG:HC11	1.83	0.61
18:v:111:GLU:O	18:v:120:GLN:NE2	2.34	0.61
22:S:304:CLA:H2A	22:S:304:CLA:HED3	1.83	0.61
21:B:497:LYS:NZ	21:B:502:SER:OG	2.34	0.61
22:b:604:CLA:HAB	22:b:606:CLA:H151	1.83	0.61
22:5:304:CLA:H52	23:5:309:LUT:H30	1.83	0.61
26:5:313:CHL:H51	26:6:317:CHL:HBB1	1.81	0.61
22:s:304:CLA:HED3	22:s:304:CLA:H2A	1.82	0.61
2:A:140:ARG:NH2	25:A:413:LHG:O5	2.34	0.61
19:s:241:LEU:HD11	22:s:306:CLA:HHD	1.83	0.60
31:T:101:BCR:H15C	31:b:619:BCR:H20C	1.82	0.60
3:D:279:LEU:HD22	30:D:401:PHO:HBC3	1.83	0.60
19:S:241:LEU:HD11	22:S:306:CLA:HHD	1.84	0.60
25:D:407:LHG:H122	25:D:407:LHG:H272	1.83	0.60
18:g:129:TYR:H	18:g:135:LEU:HD11	1.66	0.60
25:S:312:LHG:H141	25:C:522:LHG:H171	1.82	0.60
22:A:404:CLA:H52	22:A:405:CLA:HBB1	1.83	0.60
18:1:82:GLU:OE2	18:1:202:ARG:NH2	2.34	0.60
19:s:131:ILE:HG12	19:s:150:ASN:HB2	1.83	0.60
11:o:257:GLU:HG2	11:o:289:GLN:HG2	1.82	0.60
11:o:103:SER:HG	11:o:283:THR:HG1	1.47	0.60
3:d:279:LEU:HD22	30:d:401:PHO:HBC3	1.83	0.60
18:V:111:GLU:O	18:V:120:GLN:NE2	2.34	0.60
1:r:58:ALA:HB2	2:a:228:THR:HA	1.82	0.60
2:A:228:THR:HA	1:R:58:ALA:HB2	1.84	0.60
24:U:311:XAT:H41	26:U:319:CHL:HAA2	1.84	0.60
22:c:507:CLA:H152	31:c:515:BCR:H16C	1.83	0.60
11:O:100:GLU:HA	11:O:131:THR:HG22	1.83	0.60
18:U:82:GLU:OE2	18:U:202:ARG:NH2	2.35	0.59
22:b:608:CLA:H52	34:b:621:LMG:H332	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:o:131:THR:O	20:c:331:ARG:NH2	2.34	0.59
24:g:309:XAT:H28	25:g:310:LHG:H371	1.83	0.59
11:O:103:SER:HG	11:O:283:THR:HG1	1.48	0.59
2:A:254:TYR:HE2	3:D:142:ASN:HD22	1.50	0.59
2:a:140:ARG:NH2	25:a:415:LHG:O5	2.33	0.59
2:A:82:VAL:HB	2:A:174:LEU:HB2	1.83	0.59
18:n:180:PRO:HD2	23:n:309:LUT:H23	1.84	0.59
36:B:601:DGD:HAH2	3:D:123:ILE:HD11	1.83	0.59
21:b:497:LYS:NZ	21:b:502:SER:OG	2.34	0.59
2:a:254:TYR:HE2	3:d:142:ASN:HD22	1.50	0.59
21:B:445:SER:OG	21:B:450:TRP:NE1	2.36	0.59
22:B:614:CLA:H172	31:B:619:BCR:H311	1.85	0.59
32:a:413:SQD:H222	31:t:101:BCR:HC21	1.84	0.59
18:N:81:LEU:HD11	22:N:302:CLA:HBD	1.85	0.59
18:v:81:LEU:HD11	22:v:302:CLA:HBD	1.85	0.59
19:s:187:THR:HB	19:s:202:SER:HB3	1.85	0.59
2:A:139:MET:HE3	3:D:221:THR:HB	1.85	0.59
22:2:304:CLA:H2	23:2:309:LUT:H28	1.85	0.59
18:V:82:GLU:OE2	18:V:202:ARG:NH2	2.35	0.59
25:D:406:LHG:HC11	25:D:406:LHG:HC41	1.84	0.59
3:d:103:ARG:HH21	17:e:77:LYS:HG2	1.68	0.58
18:5:237:ASN:ND2	22:5:308:CLA:O1D	2.35	0.58
26:v:316:CHL:H203	26:v:318:CHL:H51	1.85	0.58
18:u:82:GLU:OE2	18:u:202:ARG:NH2	2.36	0.58
18:n:208:MET:HE2	23:n:310:LUT:H10	1.85	0.58
19:s:218:PRO:HD2	23:s:310:LUT:H23	1.85	0.58
18:v:82:GLU:OE2	18:v:202:ARG:NH2	2.36	0.58
22:a:404:CLA:H52	22:a:405:CLA:HBB1	1.86	0.58
11:o:72:ASN:HD22	11:o:128:LEU:HB3	1.68	0.58
3:D:221:THR:HG21	3:D:249:ALA:HB2	1.86	0.58
18:2:218:THR:HG23	18:2:220:LYS:H	1.67	0.58
18:4:111:GLU:O	18:4:120:GLN:NE2	2.36	0.58
18:v:80:GLU:HA	18:v:172:LEU:HD21	1.85	0.58
1:R:228:LEU:HD21	22:R:310:CLA:HMA1	1.84	0.58
11:O:72:ASN:HD22	11:O:128:LEU:HB3	1.68	0.58
21:b:445:SER:OG	21:b:450:TRP:NE1	2.37	0.58
22:1:301:CLA:HAB	23:1:310:LUT:H32	1.86	0.57
18:p:237:ASN:ND2	22:p:309:CLA:O1D	2.38	0.57
19:S:187:THR:HB	19:S:202:SER:HB3	1.86	0.57
20:c:310:GLN:HE22	20:c:369:LYS:HA	1.69	0.57
11:o:100:GLU:HA	11:o:131:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:THR:HA	2:A:109:GLY:HA3	1.85	0.57
18:1:111:GLU:O	18:1:120:GLN:NE2	2.37	0.57
22:V:301:CLA:H191	26:V:313:CHL:HED1	1.85	0.57
18:g:37:ARG:HH12	18:g:55:GLY:H	1.52	0.57
21:B:155:ALA:O	21:B:159:THR:OG1	2.22	0.57
18:P:237:ASN:ND2	22:P:309:CLA:O1D	2.37	0.57
17:E:77:LYS:HG2	3:D:103:ARG:HH21	1.69	0.57
18:Q:111:GLU:HG2	18:Q:116:LYS:HB2	1.87	0.57
1:R:21:PRO:HG2	1:R:24:LEU:HB2	1.87	0.57
19:s:125:GLN:NE2	19:s:132:LYS:O	2.37	0.57
11:o:106:VAL:HG22	11:o:280:ILE:HG12	1.86	0.57
22:v:301:CLA:HAB	23:v:310:LUT:H32	1.86	0.57
18:q:40:TRP:HD1	18:q:41:LEU:HG	1.70	0.57
20:C:74:LEU:HD13	20:C:77:LEU:HD12	1.87	0.57
2:a:139:MET:HE3	3:d:221:THR:HB	1.85	0.57
22:2:302:CLA:HMA2	22:2:302:CLA:H2	1.86	0.57
22:Q:302:CLA:HMA2	22:Q:302:CLA:H2	1.86	0.57
19:S:131:ILE:HG12	19:S:150:ASN:HB2	1.87	0.57
3:d:221:THR:HG21	3:d:249:ALA:HB2	1.87	0.57
2:A:181:ASN:HD22	3:D:314:PHE:HD1	1.52	0.57
18:2:58:PRO:HG3	18:2:194:LYS:HD3	1.87	0.57
1:r:28:LEU:HD13	1:r:95:ARG:HD3	1.87	0.57
18:4:37:ARG:HH21	18:4:49:THR:HG21	1.69	0.57
20:c:74:LEU:HD13	20:c:77:LEU:HD12	1.87	0.57
18:V:217:VAL:O	18:V:244:LYS:NZ	2.38	0.56
11:O:106:VAL:HG22	11:O:280:ILE:HG12	1.86	0.56
2:a:181:ASN:HD22	3:d:314:PHE:HD1	1.53	0.56
4:F:40:GLN:NE2	7:J:29:CYS:O	2.38	0.56
18:5:128:ASP:OD1	18:5:137:HIS:ND1	2.37	0.56
22:V:302:CLA:HAC2	26:V:316:CHL:H193	1.87	0.56
19:S:105:LEU:HD22	19:S:210:LEU:HD22	1.87	0.56
21:B:68:ARG:NH2	22:B:604:CLA:OBD	2.38	0.56
21:b:155:ALA:O	21:b:159:THR:OG1	2.23	0.56
22:a:405:CLA:H52	33:d:404:PL9:H162	1.86	0.56
3:d:255:GLN:HE21	20:c:460:LEU:HD11	1.70	0.56
4:f:40:GLN:NE2	7:j:29:CYS:O	2.38	0.56
5:h:56:LEU:HB3	31:x:202:BCR:H14C	1.87	0.56
2:A:215:HIS:NE2	35:D:402:BCT:O1	2.35	0.56
18:2:81:LEU:HD11	22:2:302:CLA:HBD	1.87	0.56
18:5:58:PRO:HG3	18:5:194:LYS:HD3	1.87	0.56
18:p:144:THR:HG22	26:p:315:CHL:HAC1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:100:GLU:HB2	18:u:223:ILE:HD12	1.86	0.56
19:S:114:ALA:O	19:S:118:ILE:HB	2.05	0.56
22:b:614:CLA:H172	31:b:619:BCR:H311	1.87	0.56
19:s:105:LEU:HD22	19:s:210:LEU:HD22	1.88	0.56
26:1:316:CHL:H193	26:1:318:CHL:H51	1.87	0.56
18:2:237:ASN:ND2	22:2:308:CLA:O1D	2.38	0.56
18:6:246:THR:HG22	26:6:301:CHL:HBA1	1.87	0.56
18:V:58:PRO:HG3	18:V:194:LYS:HD3	1.87	0.56
18:u:218:THR:HG23	18:u:220:LYS:H	1.70	0.56
1:R:53:ASN:O	21:B:14:ASN:ND2	2.38	0.56
21:b:68:ARG:NH2	22:b:604:CLA:OBD	2.39	0.56
21:b:157:HIS:HA	21:b:163:GLY:HA3	1.88	0.56
1:r:96:GLU:HG3	1:r:173:CYS:HB3	1.85	0.56
17:E:14:LEU:HD13	7:J:12:LEU:HD13	1.87	0.56
22:S:305:CLA:H2	23:S:310:LUT:H28	1.87	0.56
20:C:310:GLN:HE22	20:C:369:LYS:HA	1.71	0.56
21:B:7:ARG:NH2	25:D:406:LHG:O5	2.39	0.56
2:a:234:ASN:ND2	25:l:101:LHG:O5	2.39	0.56
18:v:58:PRO:HG3	18:v:194:LYS:HD3	1.88	0.56
18:2:208:MET:HE2	23:2:310:LUT:H10	1.88	0.56
18:6:175:GLY:HA2	18:6:178:PHE:HB2	1.88	0.56
18:Q:40:TRP:HD1	18:Q:41:LEU:HG	1.70	0.56
18:u:193:LEU:HD23	18:u:196:LYS:HD2	1.88	0.56
19:S:218:PRO:HD2	23:S:310:LUT:H23	1.86	0.56
1:r:231:PHE:HB2	22:r:609:CLA:HED1	1.87	0.56
18:v:217:VAL:O	18:v:244:LYS:NZ	2.39	0.56
1:r:168:ASN:HB3	1:r:171:LYS:HB2	1.88	0.56
18:g:136:VAL:HA	26:g:312:CHL:HMA3	1.88	0.56
21:B:497:LYS:NZ	3:D:20:ASP:OD1	2.36	0.56
2:a:292:THR:HG22	20:c:416:CYS:HB3	1.88	0.55
18:5:217:VAL:O	18:5:244:LYS:NZ	2.39	0.55
18:q:81:LEU:HD11	22:q:302:CLA:HBD	1.88	0.55
18:U:193:LEU:HD23	18:U:196:LYS:HD2	1.88	0.55
18:U:218:THR:HG23	18:U:220:LYS:H	1.71	0.55
18:g:80:GLU:HA	18:g:172:LEU:HD21	1.87	0.55
1:R:96:GLU:HG3	1:R:173:CYS:HB3	1.87	0.55
1:R:168:ASN:HB3	1:R:171:LYS:HB2	1.88	0.55
1:R:191:ARG:HG2	1:R:194:ARG:HH12	1.71	0.55
2:A:292:THR:HG22	20:C:416:CYS:HB3	1.87	0.55
22:A:405:CLA:H52	33:D:405:PL9:H162	1.86	0.55
2:a:56:PRO:HA	2:a:73:TYR:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:x:202:BCR:H351	22:b:602:CLA:HBB2	1.89	0.55
18:P:81:LEU:HD11	22:P:303:CLA:HBD	1.89	0.55
18:N:80:GLU:HA	18:N:172:LEU:HD21	1.88	0.55
18:u:234:THR:HG23	18:u:235:VAL:HG13	1.89	0.55
26:u:316:CHL:HAA2	24:g:309:XAT:H41	1.86	0.55
18:g:82:GLU:OE2	18:g:202:ARG:NH2	2.38	0.55
10:m:5:ILE:HG23	10:M:5:ILE:HD12	1.89	0.55
18:q:217:VAL:O	18:q:244:LYS:NZ	2.40	0.55
18:g:68:LEU:HB2	22:g:301:CLA:H11	1.87	0.55
1:R:28:LEU:HD13	1:R:95:ARG:HD3	1.88	0.55
1:r:53:ASN:O	21:b:14:ASN:ND2	2.39	0.55
2:a:303:ASN:O	20:c:403:ASN:ND2	2.39	0.55
3:d:239:GLN:HE21	3:d:241:GLU:HB2	1.72	0.55
2:A:234:ASN:ND2	25:L:101:LHG:O5	2.40	0.55
2:A:303:ASN:O	20:C:403:ASN:ND2	2.39	0.55
22:N:302:CLA:H152	26:N:317:CHL:H101	1.86	0.55
18:u:58:PRO:HG3	18:u:194:LYS:HD3	1.89	0.55
18:g:41:LEU:HB3	18:g:44:TYR:HB2	1.88	0.55
18:G:82:GLU:OE2	18:G:202:ARG:NH2	2.39	0.55
19:s:114:ALA:O	19:s:118:ILE:HB	2.07	0.55
1:r:93:ARG:NH1	22:r:603:CLA:O1A	2.40	0.55
8:k:12:PRO:HG2	8:k:13:GLU:HG2	1.89	0.55
2:A:56:PRO:HA	2:A:73:TYR:HE2	1.71	0.55
18:2:159:ARG:NH2	26:2:318:CHL:O1D	2.40	0.55
18:5:81:LEU:HD11	22:5:302:CLA:HBD	1.89	0.55
22:v:302:CLA:HAC2	26:v:316:CHL:H193	1.89	0.55
25:c:521:LHG:H152	25:s:312:LHG:H111	1.89	0.55
18:q:159:ARG:NH2	26:q:315:CHL:O1D	2.36	0.55
18:P:144:THR:HG22	26:P:315:CHL:HAC1	1.87	0.55
18:G:68:LEU:HB2	22:G:301:CLA:H11	1.88	0.55
20:C:257:GLU:OE1	20:C:435:ARG:NH1	2.40	0.55
32:L:102:SQD:H131	32:L:102:SQD:H282	1.89	0.55
18:P:180:PRO:HB2	27:P:301:NEX:H163	1.89	0.55
1:R:13:LEU:HD11	1:R:20:ARG:HE	1.72	0.55
20:C:460:LEU:HD11	3:D:255:GLN:HE21	1.72	0.55
3:D:239:GLN:HE21	3:D:241:GLU:HB2	1.72	0.55
2:a:338:ASN:N	29:a:403:CL:CL	2.74	0.54
3:d:129:GLN:NE2	3:d:142:ASN:O	2.40	0.54
25:d:405:LHG:O5	21:b:7:ARG:NH2	2.40	0.54
18:P:180:PRO:HD2	23:P:310:LUT:H23	1.89	0.54
22:B:604:CLA:HAB	22:B:606:CLA:H151	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1:237:ASN:HD21	22:1:308:CLA:H2A	1.71	0.54
20:C:156:LEU:HD13	22:C:509:CLA:H43	1.88	0.54
26:G:315:CHL:HHC	26:G:315:CHL:HBB1	1.89	0.54
20:c:277:MET:HG3	22:c:502:CLA:H12	1.90	0.54
2:a:215:HIS:NE2	35:a:414:BCT:O1	2.35	0.54
22:2:307:CLA:H91	25:2:312:LHG:H311	1.88	0.54
18:6:216:ILE:HG12	26:6:315:CHL:H41	1.89	0.54
18:U:234:THR:HG23	18:U:235:VAL:HG13	1.89	0.54
22:U:307:CLA:HED3	22:U:307:CLA:H2A	1.88	0.54
26:U:315:CHL:H171	26:U:317:CHL:H72	1.89	0.54
26:g:315:CHL:HHC	26:g:315:CHL:HBB1	1.90	0.54
20:C:277:MET:HG3	22:C:503:CLA:H12	1.90	0.54
22:B:602:CLA:HBB2	31:X:201:BCR:H351	1.90	0.54
18:q:111:GLU:HG2	18:q:116:LYS:HB2	1.90	0.54
25:c:521:LHG:H112	22:s:306:CLA:HAB	1.89	0.54
36:A:414:DGD:HD5	21:b:75:TRP:HB3	1.89	0.54
18:3:41:LEU:HB3	18:3:44:TYR:HB2	1.90	0.54
18:P:44:TYR:HB3	18:Q:161:ASN:HD21	1.72	0.54
1:r:21:PRO:HG2	1:r:24:LEU:HB2	1.90	0.54
18:2:181:LEU:HD12	23:2:309:LUT:H222	1.88	0.54
18:4:237:ASN:HD21	22:4:308:CLA:H2A	1.73	0.54
20:C:246:PRO:HA	20:C:249:ARG:HB2	1.88	0.54
1:r:191:ARG:HG2	1:r:194:ARG:HH12	1.73	0.54
18:P:111:GLU:O	18:P:120:GLN:NE2	2.40	0.54
18:g:197:GLU:HA	22:g:304:CLA:HBB1	1.90	0.54
22:g:307:CLA:H121	24:g:309:XAT:H34	1.88	0.54
2:a:37:MET:SD	2:a:129:ARG:NH1	2.81	0.54
36:a:416:DGD:HD5	21:B:75:TRP:HB3	1.89	0.54
18:2:98:THR:HG21	22:2:303:CLA:HAC2	1.90	0.54
18:p:111:GLU:O	18:p:120:GLN:NE2	2.39	0.54
20:C:261:SER:O	20:C:429:HIS:ND1	2.38	0.54
20:c:156:LEU:HD13	22:c:508:CLA:H43	1.89	0.53
18:1:218:THR:HG23	18:1:220:LYS:H	1.73	0.53
7:j:12:LEU:HD13	17:e:14:LEU:HD13	1.90	0.53
22:S:301:CLA:HAB	23:S:311:LUT:H32	1.90	0.53
5:H:56:LEU:HB3	31:X:201:BCR:H14C	1.90	0.53
22:4:301:CLA:HAB	23:4:310:LUT:H32	1.88	0.53
20:c:257:GLU:OE1	20:c:435:ARG:NH1	2.40	0.53
26:4:316:CHL:H171	26:4:316:CHL:H43	1.91	0.53
18:G:81:LEU:HD11	22:G:302:CLA:HBD	1.89	0.53
3:D:129:GLN:NE2	3:D:142:ASN:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:606:CLA:HAB	23:r:611:LUT:H32	1.91	0.53
32:l:102:SQD:H282	32:l:102:SQD:H131	1.89	0.53
18:g:81:LEU:HD11	22:g:302:CLA:HBD	1.91	0.53
21:B:160:GLY:HA3	21:B:180:PRO:HB3	1.91	0.53
26:r:614:CHL:H193	26:r:616:CHL:HBB2	1.91	0.53
3:d:113:PHE:O	3:d:117:HIS:HB2	2.08	0.53
26:4:317:CHL:H43	26:6:312:CHL:H12	1.91	0.53
8:K:12:PRO:HG2	8:K:13:GLU:HG2	1.91	0.53
24:p:312:XAT:H1	25:p:313:LHG:HO1	1.53	0.53
18:U:104:LYS:NZ	18:U:227:ASP:OD2	2.38	0.53
22:R:307:CLA:HAB	23:R:312:LUT:H32	1.90	0.53
22:C:510:CLA:HBC3	22:C:512:CLA:H92	1.91	0.53
31:a:409:BCR:H363	34:a:412:LMG:H342	1.89	0.53
32:A:412:SQD:H241	31:b:620:BCR:H24C	1.90	0.53
22:5:307:CLA:H121	24:5:311:XAT:H34	1.91	0.53
25:u:312:LHG:O3	25:u:312:LHG:O1	2.27	0.53
5:h:34:ASN:ND2	21:b:122:LEU:O	2.42	0.53
2:A:257:ARG:NH2	21:B:489:GLN:O	2.41	0.53
31:A:409:BCR:H363	34:A:411:LMG:H342	1.91	0.53
26:2:316:CHL:H193	26:2:318:CHL:H51	1.90	0.53
26:U:315:CHL:H142	26:U:317:CHL:H122	1.89	0.53
1:R:93:ARG:NH1	22:R:304:CLA:O1A	2.41	0.53
19:S:143:MET:HA	19:S:147:GLY:HA3	1.90	0.53
2:A:333:GLU:OE1	2:A:337:HIS:NE2	2.41	0.52
22:u:307:CLA:HED3	22:u:307:CLA:H2A	1.90	0.52
20:c:136:GLY:O	20:c:144:LYS:NZ	2.42	0.52
22:2:307:CLA:H122	24:2:311:XAT:H34	1.91	0.52
22:4:307:CLA:H111	25:4:312:LHG:H321	1.91	0.52
18:5:111:GLU:HB2	18:5:120:GLN:HG2	1.91	0.52
21:B:305:ILE:HG23	21:B:309:LEU:HD23	1.91	0.52
36:B:601:DGD:HB52	22:B:603:CLA:H61	1.90	0.52
1:r:163:ARG:NH1	26:r:616:CHL:O1D	2.42	0.52
18:p:180:PRO:HB2	27:p:301:NEX:H163	1.90	0.52
18:U:111:GLU:O	18:U:120:GLN:NE2	2.42	0.52
18:u:104:LYS:NZ	18:u:227:ASP:OD2	2.41	0.52
18:g:86:ALA:HB1	18:g:201:GLY:HA3	1.92	0.52
1:R:163:ARG:NH1	26:R:317:CHL:O1D	2.42	0.52
18:q:175:GLY:HA2	18:q:178:PHE:HB2	1.90	0.52
26:u:318:CHL:HHC	26:u:318:CHL:HBB1	1.91	0.52
26:v:317:CHL:HHC	26:v:317:CHL:HBB1	1.90	0.52
22:s:305:CLA:HAB	23:s:310:LUT:H32	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:r:617:NEX:H22	18:U:180:PRO:HB2	1.91	0.52
18:2:217:VAL:O	18:2:244:LYS:NZ	2.42	0.52
18:V:81:LEU:HD11	22:V:302:CLA:HBD	1.91	0.52
19:S:125:GLN:NE2	19:S:132:LYS:O	2.40	0.52
36:b:601:DGD:HB52	22:b:603:CLA:H61	1.91	0.52
20:c:246:PRO:HA	20:c:249:ARG:HB2	1.90	0.52
5:H:43:GLY:O	21:B:222:SER:OG	2.26	0.52
18:N:111:GLU:O	18:N:120:GLN:NE2	2.43	0.52
18:n:242:ALA:HB1	24:n:311:XAT:H42	1.92	0.52
21:B:349:GLN:NE2	21:B:395:VAL:O	2.43	0.52
18:5:159:ARG:NH2	26:5:318:CHL:O1D	2.42	0.52
18:6:135:LEU:HA	26:6:313:CHL:H2A	1.92	0.52
20:C:162:LEU:HD11	22:C:514:CLA:H93	1.90	0.52
18:Q:217:VAL:O	18:Q:244:LYS:NZ	2.41	0.52
21:b:160:GLY:HA3	21:b:180:PRO:HB3	1.91	0.52
18:4:218:THR:HG23	18:4:220:LYS:H	1.75	0.52
18:6:81:LEU:HD11	22:6:303:CLA:HBD	1.92	0.52
18:u:37:ARG:HH22	18:u:53:LEU:HD12	1.74	0.52
19:S:105:LEU:HD13	19:S:210:LEU:HD13	1.91	0.52
3:d:20:ASP:OD1	21:b:497:LYS:NZ	2.36	0.51
18:v:98:THR:HG21	22:v:303:CLA:HAC2	1.92	0.51
21:b:349:GLN:NE2	21:b:395:VAL:O	2.42	0.51
22:c:509:CLA:HBC3	22:c:511:CLA:H92	1.92	0.51
1:r:103:ARG:NH2	26:r:616:CHL:OBD	2.37	0.51
6:i:24:LEU:O	20:c:250:ARG:NH1	2.43	0.51
18:U:58:PRO:HG3	18:U:194:LYS:HD3	1.92	0.51
22:1:302:CLA:H41	22:3:301:CLA:H8	1.90	0.51
18:u:81:LEU:HD11	22:u:302:CLA:HBD	1.92	0.51
18:g:37:ARG:NH2	18:g:53:LEU:O	2.42	0.51
1:R:51:ASP:OD1	1:R:53:ASN:ND2	2.44	0.51
11:O:173:LEU:HB3	11:O:175:THR:HG23	1.92	0.51
21:b:341:LEU:HD13	21:b:429:ILE:HG22	1.93	0.51
19:s:74:TYR:OH	19:s:86:ASP:OD2	2.28	0.51
18:3:62:GLY:N	22:3:301:CLA:OBD	2.43	0.51
18:q:37:ARG:HE	18:q:39:LYS:HE3	1.75	0.51
24:U:311:XAT:H393	25:U:312:LHG:HC92	1.92	0.51
18:u:242:ALA:HA	24:u:311:XAT:H22	1.93	0.51
21:b:305:ILE:HG23	21:b:309:LEU:HD23	1.92	0.51
4:f:40:GLN:HE21	7:j:33:GLY:HA3	1.75	0.51
26:6:314:CHL:HMB1	26:6:317:CHL:HMC	1.93	0.51
18:V:77:ARG:NH2	18:Q:48:ALA:O	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:16:THR:HG22	4:F:18:ARG:H	1.75	0.51
18:1:144:THR:HG22	26:1:314:CHL:HAC1	1.92	0.51
20:c:261:SER:O	20:c:429:HIS:ND1	2.37	0.51
2:A:37:MET:SD	2:A:129:ARG:NH1	2.84	0.51
18:1:217:VAL:O	18:1:244:LYS:NZ	2.44	0.51
18:2:128:ASP:OD1	18:2:137:HIS:ND1	2.39	0.51
22:2:301:CLA:HAB	23:2:310:LUT:H32	1.92	0.51
18:U:80:GLU:HA	18:U:172:LEU:HD21	1.93	0.51
18:3:199:LYS:NZ	25:3:310:LHG:O4	2.43	0.51
18:v:128:ASP:OD1	18:v:137:HIS:ND1	2.43	0.51
22:G:307:CLA:H121	24:G:309:XAT:H34	1.92	0.51
18:3:135:LEU:HA	26:3:312:CHL:H2A	1.93	0.51
26:v:316:CHL:H171	26:v:318:CHL:H72	1.91	0.51
26:n:316:CHL:H192	26:n:318:CHL:H52	1.93	0.51
18:g:40:TRP:HD1	18:g:41:LEU:HG	1.76	0.51
1:R:15:LEU:HD21	22:R:302:CLA:HAA1	1.93	0.51
22:S:302:CLA:HHC	22:S:302:CLA:HBB1	1.93	0.51
20:C:136:GLY:O	20:C:144:LYS:NZ	2.43	0.51
2:a:296:ASN:HD21	20:c:389:LEU:HG	1.76	0.51
4:F:40:GLN:HE21	7:J:33:GLY:HA3	1.74	0.51
18:v:242:ALA:HA	24:v:311:XAT:H22	1.93	0.51
22:v:302:CLA:H142	26:q:315:CHL:H141	1.93	0.51
18:G:86:ALA:HB1	18:G:201:GLY:HA3	1.93	0.51
18:n:115:PHE:HB3	26:n:316:CHL:HED3	1.93	0.51
22:C:508:CLA:H152	31:C:517:BCR:H16C	1.93	0.51
3:D:113:PHE:O	3:D:117:HIS:HB2	2.10	0.51
19:s:252:GLN:OE1	19:s:263:ASN:ND2	2.44	0.51
1:r:51:ASP:OD1	1:r:53:ASN:ND2	2.45	0.50
5:h:83:THR:H	21:b:171:PRO:HG2	1.76	0.50
18:3:175:GLY:HA2	18:3:178:PHE:HB2	1.93	0.50
26:5:316:CHL:H193	26:5:318:CHL:H51	1.93	0.50
18:P:159:ARG:NH2	26:P:319:CHL:O1D	2.39	0.50
25:g:310:LHG:H121	26:g:311:CHL:HED3	1.93	0.50
25:S:312:LHG:H111	25:C:522:LHG:H152	1.93	0.50
19:s:105:LEU:HD13	19:s:210:LEU:HD13	1.92	0.50
22:s:302:CLA:HHC	22:s:302:CLA:HBB1	1.93	0.50
11:o:174:PHE:HA	11:o:266:GLN:HE22	1.76	0.50
6:I:24:LEU:O	20:C:250:ARG:NH1	2.43	0.50
18:2:111:GLU:HB2	18:2:120:GLN:HG2	1.92	0.50
22:4:302:CLA:H41	22:6:302:CLA:H8	1.93	0.50
18:p:180:PRO:HD2	23:p:310:LUT:H23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:311:XAT:H14	26:V:313:CHL:H91	1.93	0.50
18:u:99:PRO:HB2	18:u:112:ALA:HB1	1.93	0.50
11:O:177:LYS:HD2	11:O:195:PRO:HG3	1.92	0.50
1:r:102:GLY:HA3	1:r:203:ALA:HB1	1.94	0.50
18:p:218:THR:HG23	18:p:220:LYS:H	1.76	0.50
22:P:305:CLA:HBB1	22:P:305:CLA:H51	1.94	0.50
18:G:80:GLU:HA	18:G:172:LEU:HD21	1.94	0.50
22:C:510:CLA:HBB1	22:C:512:CLA:HMA1	1.93	0.50
18:v:100:GLU:HB2	18:v:223:ILE:HD12	1.92	0.50
18:p:37:ARG:HH22	18:p:53:LEU:HD12	1.77	0.50
26:V:313:CHL:H152	26:P:317:CHL:HBB1	1.93	0.50
18:Q:175:GLY:HA2	18:Q:178:PHE:HB2	1.94	0.50
22:Q:301:CLA:H191	25:Q:310:LHG:H181	1.94	0.50
18:n:183:LEU:HD22	22:n:304:CLA:H12	1.94	0.50
19:S:246:VAL:HG11	23:S:311:LUT:H14	1.93	0.50
34:c:520:LMG:H292	34:c:520:LMG:H141	1.94	0.50
4:f:16:THR:HG22	4:f:18:ARG:H	1.76	0.50
18:p:159:ARG:NH2	26:p:319:CHL:O1D	2.41	0.50
22:u:305:CLA:HBA1	25:c:523:LHG:HC62	1.94	0.50
25:A:413:LHG:H132	32:C:501:SQD:H251	1.94	0.50
5:H:83:THR:H	21:B:171:PRO:HG2	1.76	0.50
18:q:218:THR:HG23	18:q:220:LYS:H	1.76	0.50
19:S:103:ASN:O	19:S:107:HIS:ND1	2.34	0.50
20:c:162:LEU:HD11	22:c:513:CLA:H93	1.94	0.50
19:s:180:GLU:OE1	19:s:183:ARG:NH2	2.44	0.50
2:a:194:MET:HB3	2:a:300:PHE:HB2	1.94	0.50
16:Y:26:LEU:HD21	15:Z:25:VAL:HA	1.93	0.50
18:5:218:THR:HG23	18:5:220:LYS:H	1.76	0.50
18:6:181:LEU:HB2	22:6:305:CLA:H11	1.93	0.50
18:Q:218:THR:HG23	18:Q:220:LYS:H	1.77	0.50
1:R:103:ARG:NH2	26:R:317:CHL:OBD	2.39	0.50
11:O:173:LEU:O	11:O:266:GLN:NE2	2.45	0.50
2:A:195:HIS:HD2	2:A:299:GLY:HA2	1.77	0.50
12:T:21:ILE:HD11	25:D:407:LHG:H322	1.94	0.50
18:U:100:GLU:HB2	18:U:223:ILE:HD12	1.94	0.50
18:6:62:GLY:N	22:6:302:CLA:OBD	2.44	0.50
26:v:316:CHL:HBB1	26:q:311:CHL:H152	1.93	0.49
18:q:237:ASN:HD21	22:q:308:CLA:H2A	1.77	0.49
18:V:98:THR:HG21	22:V:303:CLA:HAC2	1.94	0.49
22:s:301:CLA:HAB	23:s:311:LUT:H32	1.94	0.49
11:o:177:LYS:HD2	11:o:195:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:412:SQD:H161	31:T:101:BCR:HC31	1.94	0.49
12:T:26:PRO:HB3	20:C:461:ASP:HA	1.94	0.49
13:W:107:GLU:O	20:C:249:ARG:NH1	2.45	0.49
18:3:181:LEU:HB2	22:3:304:CLA:H11	1.94	0.49
18:5:152:MET:HA	18:5:155:VAL:HG22	1.95	0.49
26:p:317:CHL:H203	26:p:319:CHL:H51	1.93	0.49
18:N:180:PRO:HD2	23:N:309:LUT:H23	1.94	0.49
3:D:239:GLN:HG2	3:D:241:GLU:H	1.77	0.49
22:2:306:CLA:H2A	22:2:306:CLA:HED2	1.95	0.49
24:2:311:XAT:H41	26:3:314:CHL:HAA1	1.94	0.49
31:T:101:BCR:H382	31:b:619:BCR:H14C	1.95	0.49
18:6:40:TRP:HD1	18:6:41:LEU:HG	1.78	0.49
22:V:301:CLA:H61	23:V:310:LUT:H28	1.94	0.49
26:V:313:CHL:HBA1	26:P:319:CHL:HMB1	1.95	0.49
19:S:180:GLU:OE1	19:S:183:ARG:NH2	2.45	0.49
18:1:111:GLU:HG2	18:1:116:LYS:HB2	1.94	0.49
18:q:86:ALA:HB1	18:q:201:GLY:HA3	1.93	0.49
18:u:71:ASP:O	18:u:74:THR:OG1	2.29	0.49
1:R:97:CYS:O	1:R:101:HIS:ND1	2.34	0.49
2:a:86:SER:HB3	2:a:89:ILE:HG12	1.95	0.49
32:a:413:SQD:H241	31:B:620:BCR:H24C	1.94	0.49
26:P:319:CHL:H192	22:Q:302:CLA:H13	1.94	0.49
21:B:406:LEU:HB3	21:B:409:LEU:HD12	1.94	0.49
2:a:316:THR:H	2:a:319:ASP:HB2	1.77	0.49
2:A:257:ARG:HH12	21:B:490:VAL:HA	1.77	0.49
2:A:268:SER:O	2:A:272:HIS:ND1	2.41	0.49
18:2:76:LYS:HA	18:2:79:ARG:HE	1.78	0.49
18:6:183:LEU:N	22:6:305:CLA:O1A	2.46	0.49
18:p:58:PRO:HG3	18:p:194:LYS:HD3	1.95	0.49
18:V:128:ASP:OD1	18:V:137:HIS:ND1	2.45	0.49
18:U:242:ALA:HA	24:U:311:XAT:H22	1.94	0.49
1:R:102:GLY:HA3	1:R:203:ALA:HB1	1.93	0.49
19:S:228:LEU:HG	19:S:232:LYS:HE3	1.95	0.49
20:C:360:PRO:HG2	11:O:58:GLN:HG2	1.95	0.49
21:B:250:PHE:HB3	36:B:601:DGD:HB72	1.93	0.49
22:c:509:CLA:HBB1	22:c:511:CLA:HMA1	1.93	0.49
2:a:85:THR:HA	2:a:109:GLY:HA3	1.94	0.49
24:v:311:XAT:H28	25:v:312:LHG:H361	1.94	0.49
26:V:316:CHL:H171	26:V:318:CHL:H72	1.94	0.49
18:u:180:PRO:HD2	23:u:309:LUT:H23	1.95	0.49
1:R:135:SER:HB2	1:R:138:GLY:HA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:C:521:LMG:H141	34:C:521:LMG:H292	1.95	0.49
2:A:316:THR:H	2:A:319:ASP:HB2	1.78	0.49
18:P:50:PRO:HG2	18:P:64:ASP:HB2	1.95	0.49
19:S:252:GLN:OE1	19:S:263:ASN:ND2	2.45	0.49
1:r:36:PRO:HB3	27:r:618:NEX:H3	1.94	0.49
1:r:194:ARG:HH11	18:1:180:PRO:HA	1.78	0.49
11:o:173:LEU:HB3	11:o:175:THR:HG23	1.93	0.49
22:5:306:CLA:HED2	22:5:306:CLA:H2A	1.94	0.49
24:u:311:XAT:H10	26:u:313:CHL:H13	1.95	0.49
21:B:156:PHE:HA	21:B:161:VAL:HB	1.95	0.49
22:B:613:CLA:H111	22:B:614:CLA:HAB	1.95	0.49
11:o:173:LEU:O	11:o:266:GLN:NE2	2.46	0.48
17:E:65:LEU:HD22	3:D:338:ARG:HH21	1.78	0.48
5:H:31:ARG:HE	21:B:126:PRO:HB3	1.78	0.48
18:4:144:THR:HG22	26:4:314:CHL:HAC1	1.94	0.48
26:q:314:CHL:HHC	26:q:314:CHL:HBB1	1.95	0.48
18:N:237:ASN:ND2	22:N:308:CLA:O1D	2.46	0.48
21:b:282:GLN:HE21	21:b:286:LYS:HE3	1.78	0.48
36:c:517:DGD:HA52	36:c:517:DGD:HB71	1.94	0.48
11:o:252:ASP:OD2	11:o:255:THR:OG1	2.30	0.48
22:4:306:CLA:H2A	22:4:306:CLA:HED2	1.95	0.48
18:6:162:GLY:HA3	18:6:168:GLY:H	1.78	0.48
18:U:81:LEU:HD11	22:U:302:CLA:HBD	1.95	0.48
22:U:302:CLA:HMA2	22:U:302:CLA:H2	1.96	0.48
22:G:303:CLA:H3A	22:G:303:CLA:HBA2	1.54	0.48
18:g:217:VAL:O	18:g:244:LYS:NZ	2.41	0.48
2:a:257:ARG:NH2	21:b:489:GLN:O	2.44	0.48
18:4:217:VAL:O	18:4:244:LYS:NZ	2.45	0.48
26:U:319:CHL:H192	26:N:317:CHL:H52	1.95	0.48
18:u:152:MET:HA	18:u:155:VAL:HG22	1.96	0.48
19:S:74:TYR:OH	19:S:86:ASP:OD2	2.30	0.48
21:b:156:PHE:HA	21:b:161:VAL:HB	1.94	0.48
19:s:228:LEU:HG	19:s:232:LYS:HE3	1.94	0.48
13:w:107:GLU:O	20:c:249:ARG:NH1	2.47	0.48
9:L:36:ILE:O	10:M:4:ASN:ND2	2.47	0.48
18:1:46:GLU:HG3	18:1:48:ALA:HB3	1.94	0.48
18:4:100:GLU:HB2	18:4:223:ILE:HD12	1.95	0.48
18:6:181:LEU:HD12	22:6:305:CLA:H42	1.95	0.48
18:N:159:ARG:NH2	26:N:317:CHL:O1D	2.45	0.48
20:C:444:GLU:OE2	20:C:445:LYS:NZ	2.46	0.48
21:B:357:ARG:NH1	21:B:358:ARG:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:126:THR:OG1	11:O:127:ARG:N	2.45	0.48
17:e:20:TRP:HB3	17:e:23:HIS:HB3	1.95	0.48
22:V:303:CLA:HBB1	23:V:310:LUT:H181	1.96	0.48
18:U:159:ARG:NH2	26:U:317:CHL:O1D	2.41	0.48
18:U:173:TYR:HB3	22:U:304:CLA:HED2	1.96	0.48
22:R:304:CLA:H112	21:B:211:LEU:HD22	1.95	0.48
26:R:316:CHL:HBB1	34:B:624:LMG:H172	1.95	0.48
5:h:43:GLY:O	21:b:222:SER:OG	2.24	0.48
31:t:101:BCR:H382	31:B:619:BCR:H14C	1.94	0.48
15:z:25:VAL:HA	16:y:26:LEU:HD21	1.94	0.48
22:1:308:CLA:HBA2	22:1:308:CLA:H3A	1.65	0.48
18:P:214:GLN:HA	18:P:217:VAL:HB	1.96	0.48
18:G:45:SER:OG	18:G:47:ASN:ND2	2.46	0.48
18:G:136:VAL:HA	26:G:312:CHL:HMA3	1.95	0.48
11:o:58:GLN:HG2	20:c:360:PRO:HG2	1.94	0.48
2:A:225:ARG:NH2	21:B:477:ASP:O	2.47	0.48
22:A:406:CLA:HED3	22:A:406:CLA:H2A	1.93	0.48
17:E:20:TRP:HB3	17:E:23:HIS:HB3	1.95	0.48
26:n:316:CHL:HBB2	26:n:318:CHL:HBC1	1.95	0.48
21:b:357:ARG:NH1	21:b:358:ARG:O	2.47	0.48
1:r:135:SER:HB2	1:r:138:GLY:HA2	1.95	0.48
22:r:601:CLA:H12	18:p:158:TYR:HE2	1.79	0.48
18:4:111:GLU:HG2	18:4:116:LYS:HD2	1.96	0.48
18:G:40:TRP:HD1	18:G:41:LEU:HG	1.79	0.48
21:b:406:LEU:HB3	21:b:409:LEU:HD12	1.94	0.48
20:c:216:ASP:OD2	20:c:350:ARG:NH1	2.38	0.48
2:A:86:SER:HB3	2:A:89:ILE:HG12	1.96	0.48
22:3:303:CLA:H3A	22:3:303:CLA:HBA2	1.63	0.48
22:4:302:CLA:H93	26:4:317:CHL:H142	1.95	0.48
22:4:306:CLA:HHC	22:4:306:CLA:HBB1	1.95	0.48
18:5:98:THR:HG21	22:5:303:CLA:HAC2	1.94	0.48
18:Q:37:ARG:NH2	18:Q:53:LEU:O	2.47	0.48
22:Q:307:CLA:H91	25:Q:310:LHG:H322	1.96	0.48
18:n:100:GLU:HB2	18:n:223:ILE:HD12	1.96	0.48
19:S:237:LYS:NZ	22:S:306:CLA:O1D	2.46	0.48
22:C:507:CLA:H18	36:C:519:DGD:HA62	1.95	0.48
21:B:379:ALA:HA	21:B:390:TYR:HB3	1.95	0.48
21:B:413:ASP:N	21:B:413:ASP:OD1	2.46	0.48
18:p:44:TYR:HB3	18:q:161:ASN:HD21	1.79	0.48
22:p:305:CLA:HBB1	22:p:305:CLA:H51	1.95	0.48
24:q:309:XAT:H35	25:q:310:LHG:H171	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:u:59:GLY:O	18:u:202:ARG:NH1	2.47	0.48
20:C:216:ASP:OD2	20:C:350:ARG:NH1	2.38	0.48
21:B:18:ARG:HH22	31:B:618:BCR:H401	1.79	0.48
29:a:402:CL:CL	3:d:317:LYS:HE3	2.51	0.47
25:d:405:LHG:H361	22:b:612:CLA:HBC2	1.95	0.47
18:3:91:LEU:HB3	22:3:303:CLA:HBB2	1.96	0.47
18:G:152:MET:HA	18:G:155:VAL:HG22	1.96	0.47
11:O:252:ASP:OD2	11:O:255:THR:OG1	2.32	0.47
19:s:143:MET:HA	19:s:147:GLY:HA3	1.96	0.47
1:r:210:PHE:CD2	24:r:612:XAT:H12	2.49	0.47
22:q:303:CLA:HMB2	26:q:313:CHL:HBB1	1.96	0.47
18:V:41:LEU:HB2	18:V:45:SER:HA	1.96	0.47
18:u:62:GLY:N	22:u:301:CLA:OBD	2.48	0.47
22:c:506:CLA:H18	36:c:517:DGD:HA62	1.96	0.47
3:d:51:GLY:HA2	3:d:55:VAL:HB	1.96	0.47
3:d:229:ALA:HB3	20:c:21:PHE:HE1	1.79	0.47
24:6:310:XAT:H12	25:6:311:LHG:H191	1.96	0.47
26:p:320:CHL:H193	26:q:315:CHL:H51	1.97	0.47
18:Q:86:ALA:HB1	18:Q:201:GLY:HA3	1.94	0.47
20:c:21:PHE:O	20:c:29:ARG:NH2	2.38	0.47
26:1:313:CHL:HHC	26:1:313:CHL:HBB1	1.95	0.47
22:v:307:CLA:H71	25:v:312:LHG:H171	1.96	0.47
18:U:71:ASP:O	18:U:74:THR:OG1	2.30	0.47
23:U:310:LUT:H35	23:U:310:LUT:H401	1.77	0.47
1:R:136:TYR:HD1	22:R:305:CLA:HBA1	1.79	0.47
22:C:508:CLA:H41	22:C:508:CLA:H62	1.71	0.47
36:C:519:DGD:HB71	36:C:519:DGD:HA52	1.96	0.47
21:b:413:ASP:N	21:b:413:ASP:OD1	2.47	0.47
19:s:154:VAL:HG23	19:s:155:PRO:HD3	1.95	0.47
18:v:159:ARG:NH2	26:v:318:CHL:O1D	2.43	0.47
18:q:32:PHE:HE2	18:q:192:GLU:HG2	1.78	0.47
26:Q:314:CHL:H62	26:Q:314:CHL:H101	1.74	0.47
26:S:314:CHL:HBA2	27:S:317:NEX:H403	1.96	0.47
20:c:36:LYS:HE2	20:c:126:GLU:HG2	1.96	0.47
19:s:169:ILE:HG12	26:s:315:CHL:HBC1	1.97	0.47
2:A:296:ASN:HD21	20:C:389:LEU:HG	1.80	0.47
25:v:312:LHG:H311	25:v:312:LHG:HC91	1.97	0.47
18:V:180:PRO:HD2	23:V:309:LUT:H23	1.97	0.47
26:G:311:CHL:H61	26:G:311:CHL:H41	1.74	0.47
21:B:157:HIS:HA	21:B:163:GLY:HA3	1.96	0.47
22:s:304:CLA:HBA2	22:s:304:CLA:H3A	1.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:609:CLA:H3A	22:r:609:CLA:HBA2	1.56	0.47
34:w:201:LMG:H361	36:c:517:DGD:HB51	1.97	0.47
18:5:76:LYS:HA	18:5:79:ARG:HE	1.80	0.47
22:Q:307:CLA:H93	25:Q:310:LHG:H142	1.97	0.47
18:N:181:LEU:HD12	23:N:309:LUT:H222	1.95	0.47
25:N:312:LHG:H312	25:N:312:LHG:HC91	1.96	0.47
18:g:38:ALA:HB1	26:g:311:CHL:HBC1	1.97	0.47
1:R:160:GLU:HA	1:R:163:ARG:HG2	1.97	0.47
22:R:308:CLA:H3A	22:R:308:CLA:HBA2	1.54	0.47
22:R:311:CLA:H3A	22:R:311:CLA:HBA2	1.54	0.47
20:C:174:TYR:HA	20:C:184:VAL:HA	1.97	0.47
2:a:268:SER:O	2:a:272:HIS:ND1	2.41	0.47
18:2:138:ALA:HA	26:2:314:CHL:HHC	1.97	0.47
22:2:302:CLA:HHC	22:2:302:CLA:HBB1	1.96	0.47
26:3:313:CHL:HBA1	26:3:313:CHL:H3A	1.60	0.47
18:4:53:LEU:HD11	18:4:62:GLY:HA2	1.96	0.47
18:p:50:PRO:HG2	18:p:64:ASP:HB2	1.95	0.47
26:p:317:CHL:H62	26:p:317:CHL:H2	1.60	0.47
18:q:196:LYS:HD3	22:q:306:CLA:HAA2	1.97	0.47
18:Q:159:ARG:NH2	26:Q:316:CHL:O1D	2.38	0.47
18:g:242:ALA:HA	24:g:309:XAT:H22	1.96	0.47
21:b:18:ARG:HH22	31:b:618:BCR:H401	1.79	0.47
21:b:250:PHE:HB3	36:b:601:DGD:HB72	1.97	0.47
26:2:316:CHL:H162	26:2:318:CHL:H93	1.97	0.47
18:3:164:PRO:HG2	26:3:315:CHL:HBB2	1.96	0.47
18:4:116:LYS:HA	26:6:301:CHL:HED3	1.97	0.47
18:4:178:PHE:HB2	26:4:316:CHL:H72	1.97	0.47
22:n:302:CLA:H152	26:n:318:CHL:H101	1.97	0.47
26:n:316:CHL:H172	26:n:318:CHL:H72	1.97	0.47
22:B:609:CLA:H43	22:B:610:CLA:H101	1.95	0.47
22:s:305:CLA:H52	23:s:310:LUT:H30	1.97	0.47
2:a:301:ASN:O	20:c:393:ASN:ND2	2.47	0.47
2:A:77:ILE:HD11	12:T:6:TYR:HB3	1.96	0.47
2:A:194:MET:HB3	2:A:300:PHE:HB2	1.96	0.47
18:6:199:LYS:NZ	25:6:311:LHG:O4	2.47	0.47
22:v:302:CLA:H191	26:q:311:CHL:H202	1.97	0.47
22:P:307:CLA:H2	22:P:307:CLA:H62	1.66	0.47
18:N:100:GLU:HB2	18:N:223:ILE:HD12	1.97	0.47
21:b:113:TRP:HD1	31:b:620:BCR:H403	1.80	0.47
3:d:51:GLY:HA3	3:d:78:VAL:HG22	1.97	0.46
26:5:317:CHL:H122	26:5:317:CHL:H61	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:46:GLU:H	18:Q:161:ASN:HD22	1.62	0.46
24:P:312:XAT:H12	25:P:313:LHG:H211	1.97	0.46
26:U:319:CHL:H172	26:N:317:CHL:H72	1.97	0.46
19:S:234:LYS:HD3	22:S:307:CLA:HAA2	1.97	0.46
20:C:36:LYS:HE2	20:C:126:GLU:HG2	1.97	0.46
2:a:257:ARG:HH12	21:b:490:VAL:HA	1.79	0.46
29:A:402:CL:CL	3:D:317:LYS:HE3	2.51	0.46
18:6:128:ASP:OD1	18:6:137:HIS:ND1	2.40	0.46
26:v:318:CHL:H3A	26:q:311:CHL:HBA2	1.96	0.46
18:V:242:ALA:HA	24:V:311:XAT:H22	1.97	0.46
18:P:153:GLY:HA2	26:P:319:CHL:HAB	1.96	0.46
18:P:178:PHE:HA	26:P:318:CHL:H61	1.97	0.46
18:N:152:MET:HA	18:N:155:VAL:HG22	1.96	0.46
21:b:327:THR:HG22	22:b:608:CLA:H42	1.97	0.46
2:A:301:ASN:O	20:C:393:ASN:ND2	2.48	0.46
18:3:216:ILE:HG12	26:3:314:CHL:H41	1.96	0.46
26:v:313:CHL:H152	26:p:317:CHL:HBB1	1.98	0.46
25:Q:310:LHG:H101	25:Q:310:LHG:H301	1.97	0.46
20:C:21:PHE:HE1	3:D:229:ALA:HB3	1.80	0.46
20:C:33:LEU:HD22	20:C:126:GLU:HB3	1.98	0.46
17:e:17:ILE:HG13	17:e:18:ARG:H	1.81	0.46
20:c:33:LEU:HD22	20:c:126:GLU:HB3	1.98	0.46
19:s:246:VAL:HG11	23:s:311:LUT:H14	1.96	0.46
18:2:152:MET:HA	18:2:155:VAL:HG22	1.97	0.46
18:6:40:TRP:CD1	18:6:41:LEU:HG	2.51	0.46
18:n:53:LEU:HD11	18:n:62:GLY:HA2	1.98	0.46
21:B:18:ARG:HH12	31:B:618:BCR:H401	1.80	0.46
3:D:51:GLY:HA3	3:D:78:VAL:HG22	1.98	0.46
19:s:146:GLY:HA2	19:s:163:LEU:HD22	1.96	0.46
19:s:246:VAL:HG11	23:s:311:LUT:H12	1.98	0.46
2:a:192:ILE:HG13	2:a:293:MET:HE1	1.97	0.46
13:w:77:ASN:H	13:w:81:LEU:HD23	1.80	0.46
18:1:40:TRP:HZ3	18:1:49:THR:HG22	1.80	0.46
26:1:316:CHL:H13	26:1:318:CHL:H102	1.98	0.46
24:V:311:XAT:H28	25:V:312:LHG:H361	1.96	0.46
18:P:162:GLY:HA2	26:P:318:CHL:HAC1	1.97	0.46
18:N:120:GLN:HE22	22:N:303:CLA:HED3	1.81	0.46
1:R:225:LEU:HD23	1:R:228:LEU:HD12	1.97	0.46
3:D:51:GLY:HA2	3:D:55:VAL:HB	1.97	0.46
18:1:100:GLU:HB2	18:1:223:ILE:HD12	1.97	0.46
18:1:196:LYS:HD3	22:1:306:CLA:HAA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:2:310:LUT:H35	23:2:310:LUT:H401	1.79	0.46
26:2:316:CHL:H62	26:2:316:CHL:H2	1.68	0.46
18:4:62:GLY:N	22:4:301:CLA:OBD	2.47	0.46
22:N:307:CLA:H2	22:N:307:CLA:H61	1.66	0.46
18:n:152:MET:HA	18:n:155:VAL:HG22	1.97	0.46
21:B:200:SER:HA	21:B:203:ILE:HD12	1.98	0.46
11:o:83:ASN:HB2	11:o:251:VAL:HB	1.97	0.46
12:t:26:PRO:HB3	20:c:461:ASP:HA	1.97	0.46
2:A:189:GLU:OE2	2:A:332:HIS:NE2	2.48	0.46
27:v:319:NEX:H35	27:v:319:NEX:H401	1.80	0.46
11:O:102:THR:HG22	11:O:284:GLY:HA2	1.97	0.46
21:b:25:MET:HE3	31:b:618:BCR:H23C	1.97	0.46
22:b:613:CLA:H122	22:b:613:CLA:H8	1.77	0.46
1:r:13:LEU:HD11	1:r:20:ARG:HE	1.80	0.46
1:r:136:TYR:HD1	22:r:604:CLA:HBA1	1.80	0.46
2:A:228:THR:OG1	2:A:230:ASN:OD1	2.30	0.46
18:V:100:GLU:HB2	18:V:223:ILE:HD12	1.97	0.46
26:U:317:CHL:H92	26:U:317:CHL:H61	1.85	0.46
23:u:310:LUT:H35	23:u:310:LUT:H401	1.78	0.46
21:B:25:MET:HE3	31:B:618:BCR:H23C	1.97	0.46
21:b:187:ALA:HB2	22:b:602:CLA:HMD3	1.98	0.46
5:H:22:LEU:HB3	21:B:120:LEU:HA	1.97	0.46
9:L:16:THR:HG23	25:D:407:LHG:HC62	1.97	0.46
26:3:314:CHL:H193	26:3:314:CHL:H161	1.79	0.46
18:V:37:ARG:HH21	18:V:49:THR:HG21	1.81	0.46
18:Q:41:LEU:HB3	18:Q:44:TYR:HB2	1.98	0.46
18:Q:128:ASP:OD1	18:Q:137:HIS:ND1	2.47	0.46
22:Q:303:CLA:H3A	22:Q:303:CLA:HBA2	1.58	0.46
18:N:39:LYS:HB2	18:N:45:SER:HB2	1.98	0.46
19:S:154:VAL:HG23	19:S:155:PRO:HD3	1.97	0.46
20:c:174:TYR:HA	20:c:184:VAL:HA	1.97	0.46
22:c:510:CLA:HBA1	22:c:510:CLA:H3A	1.74	0.46
2:a:217:SER:HB2	3:d:142:ASN:HA	1.99	0.46
22:a:406:CLA:HED3	22:a:406:CLA:H2A	1.96	0.46
5:h:65:LEU:HD13	22:b:603:CLA:H62	1.98	0.46
9:L:5:ASN:HB3	9:L:8:LYS:HG3	1.98	0.46
18:4:234:THR:HG23	18:4:235:VAL:HG13	1.97	0.46
18:5:100:GLU:HB2	18:5:223:ILE:HD12	1.98	0.46
25:5:312:LHG:HC82	25:5:312:LHG:H251	1.97	0.46
18:6:86:ALA:HB1	18:6:201:GLY:HA3	1.98	0.46
18:v:125:GLY:O	18:v:139:GLN:NE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:q:37:ARG:HH12	18:q:60:ASP:HB2	1.81	0.46
26:q:311:CHL:H61	26:q:311:CHL:H41	1.72	0.46
25:U:312:LHG:O3	25:U:312:LHG:O1	2.29	0.46
22:B:613:CLA:H3A	22:B:613:CLA:HBA2	1.36	0.46
27:s:317:NEX:H15	27:s:317:NEX:H201	1.82	0.46
2:a:77:ILE:HD11	12:t:6:TYR:HB3	1.96	0.45
31:T:101:BCR:H11C	31:T:101:BCR:H341	1.86	0.45
18:P:37:ARG:HH22	18:P:53:LEU:HD12	1.81	0.45
22:P:307:CLA:H2A	22:P:307:CLA:HED2	1.96	0.45
26:Q:315:CHL:H171	26:Q:315:CHL:H13	1.55	0.45
18:U:83:LEU:HD23	18:U:172:LEU:HD22	1.99	0.45
18:u:109:PHE:O	18:u:120:GLN:NE2	2.49	0.45
19:S:100:TYR:HB3	22:S:301:CLA:H3A	1.98	0.45
20:C:15:ASP:O	20:C:19:THR:OG1	2.30	0.45
20:c:67:LYS:HB3	20:c:72:GLN:HE21	1.81	0.45
25:d:406:LHG:H181	12:t:17:ILE:HD11	1.98	0.45
25:d:406:LHG:H322	12:t:21:ILE:HD11	1.98	0.45
5:h:31:ARG:HE	21:b:126:PRO:HB3	1.79	0.45
2:A:217:SER:HA	3:D:272:LEU:HD12	1.99	0.45
18:N:208:MET:HA	18:N:211:PHE:HD2	1.81	0.45
26:N:313:CHL:H91	26:N:313:CHL:H112	1.82	0.45
33:D:405:PL9:H401	25:D:407:LHG:H211	1.98	0.45
21:b:66:MET:HB3	21:b:71:ILE:HB	1.98	0.45
21:b:345:SER:OG	21:b:400:THR:OG1	2.34	0.45
27:s:317:NEX:H11	27:s:317:NEX:H191	1.78	0.45
22:r:610:CLA:HBA2	22:r:610:CLA:H3A	1.51	0.45
32:m:101:SQD:H142	32:L:102:SQD:H291	1.98	0.45
11:o:94:LEU:HD22	11:o:288:ALA:HB1	1.97	0.45
34:W:201:LMG:H361	36:C:519:DGD:HB51	1.97	0.45
26:3:314:CHL:H91	26:3:314:CHL:H111	1.77	0.45
18:4:30:ILE:HG22	18:4:32:PHE:H	1.82	0.45
24:p:312:XAT:H12	26:p:314:CHL:H112	1.97	0.45
26:U:319:CHL:H151	26:U:319:CHL:H18	1.78	0.45
22:u:302:CLA:H2A	22:u:302:CLA:HED2	1.98	0.45
18:g:121:ILE:HG23	18:g:126:GLY:HA2	1.98	0.45
20:C:338:ILE:HG21	20:C:347:TRP:HB2	1.98	0.45
21:B:187:ALA:HB2	22:B:602:CLA:HMD3	1.98	0.45
22:B:614:CLA:HMA2	22:B:614:CLA:H2	1.98	0.45
22:b:613:CLA:H111	22:b:614:CLA:HAB	1.99	0.45
1:r:188:ASP:HB3	1:r:191:ARG:HB2	1.98	0.45
26:r:615:CHL:HBB1	34:b:624:LMG:H172	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:410:SQD:O49	32:a:410:SQD:O2	2.31	0.45
3:d:239:GLN:HG2	3:d:241:GLU:H	1.81	0.45
18:q:62:GLY:N	22:q:301:CLA:OBD	2.50	0.45
18:q:152:MET:HA	18:q:155:VAL:HG22	1.98	0.45
27:V:319:NEX:H15	27:V:319:NEX:H201	1.80	0.45
18:Q:164:PRO:HG2	26:Q:315:CHL:HBB2	1.98	0.45
22:n:308:CLA:HBA1	22:n:308:CLA:H3A	1.42	0.45
1:r:114:VAL:HG11	22:r:604:CLA:HAC2	1.99	0.45
27:r:618:NEX:H15	27:r:618:NEX:H201	1.75	0.45
2:a:57:PRO:HB2	2:a:66:PRO:HB2	1.98	0.45
22:2:302:CLA:CAD	26:2:318:CHL:H2	2.46	0.45
18:4:213:VAL:HG11	22:4:307:CLA:HAC2	1.99	0.45
27:p:301:NEX:H15	27:p:301:NEX:H201	1.81	0.45
26:U:315:CHL:H91	26:U:317:CHL:H151	1.99	0.45
1:R:188:ASP:HB3	1:R:191:ARG:HB2	1.98	0.45
20:C:247:TRP:NE1	25:C:524:LHG:O9	2.44	0.45
21:B:384:ARG:HH12	21:B:387:GLU:HG2	1.81	0.45
20:c:444:GLU:OE2	20:c:445:LYS:NZ	2.49	0.45
22:c:510:CLA:H91	22:c:510:CLA:H111	1.75	0.45
1:r:12:ALA:O	1:r:32:ARG:NH2	2.48	0.45
1:r:222:GLU:OE1	1:r:224:ALA:N	2.50	0.45
3:d:298:PHE:N	3:d:302:GLU:OE2	2.50	0.45
9:l:36:ILE:HG23	34:b:621:LMG:H301	1.98	0.45
32:l:102:SQD:H291	32:M:101:SQD:H142	1.99	0.45
26:3:313:CHL:HMB1	26:3:316:CHL:HMC	1.98	0.45
26:4:313:CHL:H91	26:4:313:CHL:H112	1.84	0.45
1:R:210:PHE:CD2	24:R:313:XAT:H12	2.51	0.45
22:R:303:CLA:H51	22:R:304:CLA:HBA1	1.98	0.45
22:X:202:CLA:H93	22:X:202:CLA:H112	1.85	0.45
21:b:200:SER:HA	21:b:203:ILE:HD12	1.98	0.45
31:a:409:BCR:H15C	31:a:409:BCR:H351	1.88	0.45
9:l:5:ASN:HB3	9:l:8:LYS:HG3	1.97	0.45
22:A:405:CLA:H152	22:A:405:CLA:H111	1.69	0.45
26:v:316:CHL:H91	26:v:316:CHL:H111	1.84	0.45
18:p:81:LEU:HD11	22:p:303:CLA:HBD	1.97	0.45
26:P:319:CHL:H143	26:P:319:CHL:H162	1.87	0.45
23:R:312:LUT:H35	23:R:312:LUT:H401	1.86	0.45
36:C:520:DGD:HA52	36:C:520:DGD:HA22	1.77	0.45
21:b:379:ALA:HA	21:b:390:TYR:HB3	1.98	0.45
1:r:160:GLU:HA	1:r:163:ARG:HG2	1.98	0.45
2:a:228:THR:OG1	2:a:230:ASN:OD1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:67:THR:H	17:E:75:GLN:HE22	1.65	0.45
31:K:101:BCR:HC7	15:Z:20:VAL:HG21	1.98	0.45
10:M:6:TYR:HB3	31:B:618:BCR:HC31	1.99	0.45
18:1:159:ARG:NH2	26:1:318:CHL:O1D	2.43	0.45
22:2:304:CLA:H43	22:2:306:CLA:HBA1	1.98	0.45
18:5:129:TYR:HB3	18:5:135:LEU:HD11	1.99	0.45
18:6:50:PRO:HD2	18:6:53:LEU:HD11	1.98	0.45
26:V:316:CHL:HBB1	26:Q:311:CHL:H122	1.99	0.45
18:P:58:PRO:HG3	18:P:194:LYS:HD3	1.98	0.45
23:N:310:LUT:H35	23:N:310:LUT:H401	1.77	0.45
26:S:313:CHL:HHC	26:S:313:CHL:HBB1	1.98	0.45
21:B:50:PRO:O	21:B:308:LYS:NZ	2.46	0.45
11:O:174:PHE:HA	11:O:266:GLN:HE22	1.81	0.45
25:D:406:LHG:HC82	25:D:406:LHG:H251	1.99	0.45
21:b:18:ARG:HH12	31:b:618:BCR:H401	1.80	0.45
21:b:154:GLY:HA3	21:b:202:HIS:HB2	1.99	0.45
21:b:372:ASP:OD1	21:b:376:ILE:N	2.47	0.45
27:s:317:NEX:H35	27:s:317:NEX:H401	1.76	0.45
25:d:406:LHG:HC62	9:l:16:THR:HG23	1.98	0.45
36:J:101:DGD:HBE1	36:C:520:DGD:HAE1	1.98	0.45
18:v:40:TRP:CD1	18:v:41:LEU:HG	2.52	0.45
26:V:318:CHL:H203	26:V:318:CHL:H161	1.85	0.45
27:V:319:NEX:H191	27:V:319:NEX:H11	1.72	0.45
18:G:242:ALA:HA	24:G:309:XAT:H22	1.98	0.45
22:G:301:CLA:H41	22:G:301:CLA:H62	1.74	0.45
1:R:75:GLU:HB2	1:R:92:ALA:HB3	1.99	0.45
21:B:154:GLY:HA3	21:B:202:HIS:HB2	1.99	0.45
21:B:157:HIS:CE1	21:B:164:PRO:HD2	2.52	0.45
21:B:460:LEU:HG	3:D:280:TRP:HZ3	1.81	0.45
22:b:602:CLA:H61	22:b:602:CLA:H92	1.81	0.45
22:c:504:CLA:H62	22:c:504:CLA:H41	1.67	0.45
1:r:75:GLU:HB2	1:r:92:ALA:HB3	1.99	0.45
17:E:17:ILE:HG13	17:E:18:ARG:H	1.81	0.45
18:3:86:ALA:HB1	18:3:201:GLY:HA3	1.99	0.45
18:4:109:PHE:HB2	18:4:112:ALA:HB2	1.99	0.45
18:4:196:LYS:HD3	22:4:306:CLA:HAA2	1.99	0.45
22:4:306:CLA:H102	22:4:306:CLA:H61	1.66	0.45
26:6:301:CHL:H62	26:6:301:CHL:H101	1.89	0.45
18:P:152:MET:HA	18:P:155:VAL:HG22	1.99	0.45
22:u:305:CLA:H43	22:u:306:CLA:HMD2	1.99	0.45
27:u:320:NEX:H35	27:u:320:NEX:H401	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:67:LYS:HB3	20:C:72:GLN:HE21	1.81	0.45
21:B:352:ARG:HH21	21:B:372:ASP:HB2	1.80	0.45
22:D:403:CLA:H41	22:D:403:CLA:H62	1.79	0.45
19:s:86:ASP:OD1	23:s:311:LUT:O23	2.34	0.45
19:s:234:LYS:HD3	22:s:307:CLA:HAA2	1.97	0.45
24:3:309:XAT:H15	24:3:309:XAT:H201	1.87	0.44
18:6:111:GLU:O	18:6:120:GLN:NE2	2.50	0.44
24:6:310:XAT:H15	24:6:310:XAT:H201	1.86	0.44
22:N:306:CLA:H2A	22:N:306:CLA:HED2	1.98	0.44
22:N:307:CLA:H52	24:N:311:XAT:H203	1.98	0.44
19:S:169:ILE:HG12	26:S:315:CHL:HBC1	1.98	0.44
22:S:304:CLA:HBA2	22:S:304:CLA:H3A	1.47	0.44
22:b:604:CLA:H41	22:b:604:CLA:H62	1.68	0.44
22:b:610:CLA:H161	22:b:610:CLA:H141	1.78	0.44
33:d:404:PL9:H401	25:d:406:LHG:H211	1.98	0.44
26:p:320:CHL:H101	26:p:320:CHL:H62	1.68	0.44
18:Q:37:ARG:NH1	18:Q:55:GLY:H	2.15	0.44
1:R:114:VAL:HG11	22:R:305:CLA:HAC2	1.99	0.44
21:B:66:MET:HB3	21:B:71:ILE:HB	1.97	0.44
36:b:601:DGD:HB91	36:b:601:DGD:HBW2	1.75	0.44
34:c:520:LMG:H131	34:c:520:LMG:H161	1.85	0.44
5:H:65:LEU:HD13	22:B:603:CLA:H62	1.99	0.44
26:4:313:CHL:HBA1	26:4:313:CHL:H3A	1.84	0.44
26:6:315:CHL:H91	26:6:315:CHL:H111	1.79	0.44
18:v:218:THR:HG23	18:v:220:LYS:H	1.81	0.44
22:q:307:CLA:H152	22:q:308:CLA:HBD	1.99	0.44
18:Q:152:MET:HA	18:Q:155:VAL:HG22	2.00	0.44
18:U:208:MET:HA	18:U:211:PHE:HD2	1.82	0.44
18:U:217:VAL:O	18:U:244:LYS:NZ	2.38	0.44
18:u:87:ARG:NE	18:u:197:GLU:OE2	2.45	0.44
18:n:81:LEU:HD11	22:n:302:CLA:HBD	1.99	0.44
22:n:302:CLA:HHC	22:n:302:CLA:HBB1	1.98	0.44
36:c:519:DGD:HB22	36:c:519:DGD:HB51	1.83	0.44
3:d:280:TRP:HZ3	21:b:460:LEU:HG	1.82	0.44
5:h:54:ILE:HG12	31:x:202:BCR:H312	1.98	0.44
15:z:1:MET:HA	15:z:4:ILE:HD12	1.99	0.44
2:A:57:PRO:HB2	2:A:66:PRO:HB2	1.99	0.44
18:3:111:GLU:O	18:3:120:GLN:NE2	2.50	0.44
23:4:310:LUT:H401	23:4:310:LUT:H35	1.82	0.44
18:U:152:MET:HA	18:U:155:VAL:HG22	2.00	0.44
18:G:100:GLU:HB2	18:G:223:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:g:152:MET:HA	18:g:155:VAL:HG22	1.99	0.44
20:C:332:SER:OG	20:C:336:GLU:N	2.49	0.44
20:c:15:ASP:O	20:c:19:THR:OG1	2.30	0.44
2:A:269:ARG:HH22	3:D:234:ALA:HB3	1.83	0.44
26:2:317:CHL:H13	26:2:317:CHL:H101	1.64	0.44
18:p:135:LEU:HD12	18:p:136:VAL:H	1.82	0.44
22:U:301:CLA:H152	22:N:302:CLA:H143	1.99	0.44
26:U:319:CHL:H91	26:U:319:CHL:H111	1.81	0.44
25:N:312:LHG:H171	26:N:313:CHL:H42	2.00	0.44
27:N:318:NEX:H15	27:N:318:NEX:H201	1.75	0.44
18:n:120:GLN:HE22	22:n:303:CLA:HED2	1.83	0.44
21:b:384:ARG:HH12	21:b:387:GLU:HG2	1.83	0.44
22:r:606:CLA:H143	23:r:611:LUT:H403	2.00	0.44
2:A:174:LEU:HD22	30:A:407:PHO:H141	2.00	0.44
31:A:409:BCR:H401	36:A:414:DGD:HD61	2.00	0.44
27:2:319:NEX:H191	27:2:319:NEX:H11	1.73	0.44
22:5:301:CLA:HBA1	23:5:310:LUT:H382	1.99	0.44
26:v:318:CHL:H143	26:v:318:CHL:H162	1.93	0.44
26:v:318:CHL:H202	26:v:318:CHL:H161	1.90	0.44
23:p:311:LUT:H35	23:p:311:LUT:H401	1.88	0.44
22:G:302:CLA:H92	22:G:302:CLA:H61	1.85	0.44
18:g:64:ASP:HB3	18:g:67:GLY:HA2	2.00	0.44
3:D:192:THR:HG22	3:D:193:LEU:HD22	1.99	0.44
22:c:513:CLA:H8	25:c:521:LHG:H331	2.00	0.44
2:a:217:SER:HA	3:d:272:LEU:HD12	1.99	0.44
3:d:158:LEU:HD11	22:b:603:CLA:H203	1.99	0.44
25:d:405:LHG:H251	25:d:405:LHG:HC82	1.99	0.44
26:1:318:CHL:H43	26:3:311:CHL:H12	1.99	0.44
22:4:306:CLA:H62	22:4:306:CLA:H2	1.80	0.44
26:5:313:CHL:H152	26:6:315:CHL:HBB1	1.99	0.44
22:6:307:CLA:H2	22:6:307:CLA:H61	1.75	0.44
22:v:307:CLA:H2	22:v:307:CLA:H61	1.71	0.44
18:N:217:VAL:O	18:N:244:LYS:NZ	2.35	0.44
22:N:302:CLA:HHC	22:N:302:CLA:HBB1	2.00	0.44
26:u:318:CHL:C4B	26:g:311:CHL:H2	2.48	0.44
26:g:311:CHL:H3A	26:g:311:CHL:HBA1	1.64	0.44
11:O:74:CYS:N	11:O:100:GLU:OE2	2.50	0.44
3:d:210:LEU:HD22	3:d:271:MET:HG2	2.00	0.44
22:3:307:CLA:H2	22:3:307:CLA:H61	1.71	0.44
24:5:311:XAT:H41	26:6:315:CHL:HAA1	2.00	0.44
27:v:319:NEX:H191	27:v:319:NEX:H11	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:p:301:NEX:H35	27:p:301:NEX:H401	1.80	0.44
18:V:125:GLY:O	18:V:139:GLN:NE2	2.51	0.44
18:G:64:ASP:HB3	18:G:67:GLY:HA2	1.99	0.44
26:R:317:CHL:HHC	26:R:317:CHL:H122	2.00	0.44
22:B:605:CLA:HBD	22:B:605:CLA:HBA1	2.00	0.44
22:B:613:CLA:H122	22:B:613:CLA:H8	1.77	0.44
20:c:338:ILE:HG21	20:c:347:TRP:HB2	1.98	0.44
11:o:84:LEU:HD22	11:o:185:LEU:HD22	1.99	0.44
31:t:101:BCR:H11C	31:t:101:BCR:H341	1.87	0.44
2:A:273:PHE:HZ	25:A:413:LHG:HC82	1.56	0.44
7:J:33:GLY:HA2	7:J:37:TRP:CD1	2.53	0.44
26:1:317:CHL:H93	26:1:317:CHL:H112	1.93	0.44
18:3:162:GLY:HA3	18:3:168:GLY:H	1.83	0.44
23:4:309:LUT:H31	23:4:309:LUT:H391	1.87	0.44
22:p:309:CLA:HBA1	22:p:309:CLA:H3A	1.63	0.44
23:V:310:LUT:H35	23:V:310:LUT:H401	1.87	0.44
26:U:319:CHL:H62	26:U:319:CHL:H2	1.69	0.44
26:u:318:CHL:H141	26:u:318:CHL:H162	1.89	0.44
22:C:505:CLA:H162	22:C:505:CLA:H122	1.85	0.44
3:D:48:TRP:HA	3:D:78:VAL:HG21	2.00	0.44
3:D:83:ASN:HD22	3:D:336:HIS:CD2	2.36	0.44
17:e:67:THR:H	17:e:75:GLN:HE22	1.65	0.44
2:a:174:LEU:HD22	30:a:407:PHO:H141	1.99	0.43
3:d:192:THR:HG22	3:d:193:LEU:HD22	1.99	0.43
2:A:238:ARG:HD3	12:T:30:ILE:HA	1.99	0.43
22:4:301:CLA:HBA1	23:4:310:LUT:H382	1.99	0.43
18:v:41:LEU:HB2	18:v:45:SER:HA	1.99	0.43
22:q:308:CLA:H3A	22:q:308:CLA:HBA1	1.56	0.43
18:G:159:ARG:NH2	26:G:316:CHL:O1D	2.38	0.43
18:u:208:MET:HA	18:u:211:PHE:HD2	1.82	0.43
18:n:218:THR:HG23	18:n:220:LYS:H	1.82	0.43
22:n:306:CLA:H2A	22:n:306:CLA:HED2	1.99	0.43
26:n:316:CHL:H91	26:n:316:CHL:H111	1.81	0.43
19:S:146:GLY:HA2	19:S:163:LEU:HD22	2.00	0.43
21:B:345:SER:OG	21:B:400:THR:OG1	2.35	0.43
22:r:602:CLA:H51	22:r:603:CLA:HBA1	2.00	0.43
32:a:413:SQD:H161	31:t:101:BCR:HC31	2.00	0.43
7:j:33:GLY:HA2	7:j:37:TRP:CD1	2.53	0.43
22:2:305:CLA:HMC3	24:2:311:XAT:H372	2.00	0.43
26:3:314:CHL:H2	26:3:314:CHL:H62	1.71	0.43
18:V:196:LYS:HD3	22:V:306:CLA:HBD	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:118:GLY:HA2	26:U:314:CHL:HAC2	1.99	0.43
23:N:309:LUT:H15	23:N:309:LUT:H201	1.90	0.43
27:u:319:NEX:H35	27:u:319:NEX:H401	1.84	0.43
1:R:222:GLU:OE1	1:R:224:ALA:N	2.50	0.43
27:R:301:NEX:H192	27:R:301:NEX:H161	2.00	0.43
4:F:40:GLN:HE22	7:J:30:PHE:HA	1.84	0.43
18:5:162:GLY:HA2	26:5:317:CHL:HMC	1.99	0.43
25:6:311:LHG:H121	26:6:312:CHL:HMA3	1.99	0.43
22:P:302:CLA:HAB	23:P:311:LUT:H32	1.99	0.43
26:P:317:CHL:H193	26:P:319:CHL:H51	2.00	0.43
18:Q:62:GLY:N	22:Q:301:CLA:OBD	2.51	0.43
22:U:305:CLA:HBA1	25:C:524:LHG:HC62	1.99	0.43
22:U:305:CLA:H43	22:U:306:CLA:HMD2	2.00	0.43
18:G:217:VAL:O	18:G:244:LYS:NZ	2.42	0.43
22:n:301:CLA:H192	22:n:301:CLA:H161	1.85	0.43
19:S:222:ALA:HB2	19:S:231:LEU:HD12	1.99	0.43
22:C:506:CLA:O1D	34:C:521:LMG:O3	2.34	0.43
22:B:606:CLA:H143	22:B:606:CLA:H161	1.94	0.43
3:D:298:PHE:N	3:D:302:GLU:OE2	2.50	0.43
20:c:134:PHE:O	20:c:144:LYS:NZ	2.39	0.43
19:s:79:LEU:HD21	19:s:101:ARG:HE	1.83	0.43
31:k:101:BCR:HC7	15:z:20:VAL:HG21	2.00	0.43
5:H:54:ILE:HG12	31:X:201:BCR:H312	1.99	0.43
31:K:101:BCR:H15C	31:K:101:BCR:H351	1.87	0.43
22:1:301:CLA:HBA1	23:1:310:LUT:H382	2.00	0.43
18:3:152:MET:HA	18:3:155:VAL:HG22	2.00	0.43
24:V:311:XAT:H10	26:V:313:CHL:H13	2.01	0.43
18:N:208:MET:HE2	23:N:310:LUT:H10	2.00	0.43
18:u:180:PRO:HB2	27:u:320:NEX:H22	2.01	0.43
23:n:309:LUT:H383	26:n:317:CHL:H11	2.01	0.43
31:B:619:BCR:HC31	34:B:621:LMG:H142	1.99	0.43
2:a:37:MET:HE2	2:a:41:LEU:HD12	2.00	0.43
4:f:40:GLN:HE22	7:j:30:PHE:HA	1.83	0.43
26:4:317:CHL:H203	26:4:317:CHL:H161	1.81	0.43
26:5:316:CHL:H91	26:5:316:CHL:H111	1.87	0.43
22:v:305:CLA:H43	22:v:306:CLA:HMD2	2.01	0.43
23:v:309:LUT:H11	23:v:309:LUT:H191	1.91	0.43
22:p:303:CLA:H141	22:p:303:CLA:H162	1.88	0.43
22:p:307:CLA:H2A	22:p:307:CLA:HED2	1.98	0.43
22:V:308:CLA:HBB1	14:X:77:ILE:HD12	2.00	0.43
27:V:319:NEX:H35	27:V:319:NEX:H401	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:309:CLA:HBA1	22:P:309:CLA:H3A	1.54	0.43
31:B:618:BCR:HC22	34:B:621:LMG:H111	2.00	0.43
22:b:604:CLA:H193	22:b:604:CLA:H162	1.87	0.43
22:b:610:CLA:H2A	22:b:610:CLA:HED2	2.00	0.43
19:s:103:ASN:O	19:s:107:HIS:ND1	2.34	0.43
1:r:41:LYS:HA	1:r:42:PRO:HD3	1.90	0.43
11:o:74:CYS:N	11:o:100:GLU:OE2	2.49	0.43
12:T:17:ILE:HD11	25:D:407:LHG:H181	2.00	0.43
18:5:53:LEU:HD11	18:5:62:GLY:HA2	1.99	0.43
22:Q:305:CLA:H92	22:Q:305:CLA:H61	1.88	0.43
26:G:314:CHL:H62	26:G:314:CHL:H2	1.71	0.43
25:u:312:LHG:H182	25:u:312:LHG:H211	1.84	0.43
20:C:166:LYS:HB2	22:C:504:CLA:H203	1.98	0.43
36:C:520:DGD:HA51	36:C:520:DGD:HA82	1.81	0.43
11:O:188:ILE:HB	11:O:246:PHE:HB2	1.99	0.43
22:b:617:CLA:HHB	31:b:620:BCR:H17C	2.01	0.43
22:r:609:CLA:H91	22:r:609:CLA:H112	1.86	0.43
15:z:5:LEU:HD11	15:z:61:VAL:HG21	1.99	0.43
2:A:217:SER:HB2	3:D:142:ASN:HA	1.99	0.43
22:2:305:CLA:H13	22:2:305:CLA:H102	1.75	0.43
22:5:302:CLA:CAD	26:5:318:CHL:H2	2.49	0.43
22:v:304:CLA:H2	23:v:309:LUT:H28	2.01	0.43
18:V:111:GLU:HG2	18:V:116:LYS:HB2	2.00	0.43
18:Q:237:ASN:HD21	22:Q:308:CLA:H2A	1.84	0.43
18:u:159:ARG:NH2	26:u:318:CHL:O1D	2.41	0.43
23:n:310:LUT:H15	23:n:310:LUT:H201	1.82	0.43
11:O:94:LEU:HD22	11:O:288:ALA:HB1	2.00	0.43
5:h:20:PRO:HD2	21:b:124:ARG:HH22	1.83	0.43
10:m:14:PHE:HD1	34:b:621:LMG:H412	1.84	0.43
18:3:45:SER:OG	18:3:47:ASN:ND2	2.52	0.43
22:3:302:CLA:HBA1	22:3:302:CLA:H11	1.78	0.43
25:3:310:LHG:H121	26:3:311:CHL:HMA3	1.99	0.43
18:6:37:ARG:NH1	18:6:55:GLY:H	2.17	0.43
22:6:304:CLA:HBA2	22:6:304:CLA:H3A	1.43	0.43
26:v:316:CHL:H62	26:v:316:CHL:H101	1.70	0.43
26:V:316:CHL:H203	26:V:318:CHL:H51	1.99	0.43
23:N:309:LUT:H383	26:N:316:CHL:H11	2.01	0.43
26:g:315:CHL:H102	26:g:315:CHL:H61	1.73	0.43
1:R:228:LEU:HA	1:R:231:PHE:HB3	2.00	0.43
22:C:506:CLA:H162	22:C:510:CLA:H121	2.01	0.43
21:B:370:LEU:HD22	21:B:379:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:606:CLA:H92	22:B:606:CLA:H62	1.87	0.43
21:b:230:SER:O	21:b:233:SER:OG	2.36	0.43
19:s:100:TYR:HB3	22:s:301:CLA:H3A	1.99	0.43
2:a:238:ARG:HD3	12:t:30:ILE:HA	2.01	0.43
14:x:67:PRO:HA	14:x:70:LYS:HE2	2.01	0.43
22:v:304:CLA:H111	22:v:304:CLA:H91	1.81	0.43
18:q:202:ARG:HB2	25:q:310:LHG:H241	2.01	0.43
24:P:312:XAT:H15	24:P:312:XAT:H201	1.88	0.43
22:u:301:CLA:H143	22:n:302:CLA:HED1	2.01	0.43
29:a:402:CL:CL	3:d:317:LYS:HB3	2.56	0.43
11:o:130:TYR:HD2	11:o:131:THR:HG23	1.84	0.43
15:Z:1:MET:HA	15:Z:4:ILE:HD12	2.00	0.43
23:5:310:LUT:H11	23:5:310:LUT:H191	1.87	0.43
26:5:316:CHL:H8	26:5:318:CHL:H172	2.01	0.43
26:6:316:CHL:H162	26:6:316:CHL:H122	1.58	0.43
18:V:33:TYR:HA	18:V:37:ARG:HB3	2.01	0.43
18:P:135:LEU:HD12	18:P:136:VAL:H	1.84	0.43
22:U:306:CLA:HBB1	23:U:309:LUT:H14	1.99	0.43
18:u:178:PHE:HA	26:u:317:CHL:H72	2.00	0.43
26:u:316:CHL:H141	26:u:318:CHL:H102	2.00	0.43
27:n:319:NEX:H35	27:n:319:NEX:H401	1.83	0.43
36:B:601:DGD:HB72	36:B:601:DGD:HBT2	1.81	0.43
21:b:71:ILE:HD11	22:b:607:CLA:H2A	2.00	0.43
22:b:602:CLA:H193	22:b:602:CLA:H141	2.01	0.43
22:c:514:CLA:H93	22:c:514:CLA:H61	1.87	0.43
26:s:314:CHL:HBA2	27:s:317:NEX:H403	1.99	0.43
22:r:606:CLA:H52	23:r:611:LUT:H30	2.01	0.42
27:r:617:NEX:H171	27:r:617:NEX:H192	2.01	0.42
3:d:83:ASN:HD22	3:d:336:HIS:CD2	2.37	0.42
2:A:198:HIS:HA	2:A:286:THR:HG22	2.01	0.42
29:A:402:CL:CL	3:D:317:LYS:HB3	2.56	0.42
36:J:101:DGD:HB51	36:J:101:DGD:HB22	1.85	0.42
22:1:307:CLA:H3A	22:1:307:CLA:HBA2	1.72	0.42
26:6:301:CHL:H143	26:6:301:CHL:H111	1.90	0.42
25:V:312:LHG:H311	25:V:312:LHG:HC91	2.01	0.42
18:G:121:ILE:HG23	18:G:126:GLY:HA2	2.00	0.42
1:R:12:ALA:O	1:R:32:ARG:NH2	2.52	0.42
34:C:521:LMG:H191	34:C:521:LMG:H222	1.83	0.42
22:B:602:CLA:H193	22:B:602:CLA:H141	2.00	0.42
3:D:171:PRO:HB3	3:D:181:PHE:CG	2.54	0.42
23:s:310:LUT:H35	23:s:310:LUT:H401	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:603:CLA:H112	21:b:211:LEU:HD22	2.01	0.42
3:d:171:PRO:HB3	3:d:181:PHE:CG	2.54	0.42
11:o:188:ILE:HB	11:o:246:PHE:HB2	2.01	0.42
2:A:37:MET:HE2	2:A:41:LEU:HD12	2.00	0.42
2:A:192:ILE:HG13	2:A:293:MET:HE1	2.00	0.42
15:Z:5:LEU:HD11	15:Z:61:VAL:HG21	2.00	0.42
22:1:302:CLA:H93	26:1:318:CHL:H142	2.00	0.42
26:2:318:CHL:H92	26:2:318:CHL:H62	1.83	0.42
18:4:76:LYS:HA	18:4:79:ARG:HE	1.84	0.42
22:5:302:CLA:HAB	26:5:318:CHL:H152	2.01	0.42
26:6:315:CHL:H161	26:6:315:CHL:H193	1.80	0.42
18:p:180:PRO:HB2	27:p:301:NEX:H172	2.00	0.42
23:V:309:LUT:H31	23:V:309:LUT:H391	1.91	0.42
23:V:309:LUT:H35	23:V:309:LUT:H401	1.87	0.42
23:P:311:LUT:H201	23:P:311:LUT:H15	1.81	0.42
18:U:59:GLY:O	18:U:202:ARG:NH1	2.52	0.42
18:U:99:PRO:HB2	18:U:112:ALA:HB1	2.00	0.42
18:u:111:GLU:O	18:u:120:GLN:NE2	2.52	0.42
22:n:307:CLA:H61	22:n:307:CLA:H2	1.71	0.42
22:R:310:CLA:H3A	22:R:310:CLA:HBA2	1.50	0.42
32:C:501:SQD:H1	32:C:501:SQD:H45	1.87	0.42
21:b:477:ASP:OD1	21:b:477:ASP:N	2.52	0.42
20:c:166:LYS:HB2	22:c:503:CLA:H203	2.01	0.42
22:c:504:CLA:H162	22:c:504:CLA:H122	1.83	0.42
25:d:406:LHG:H171	9:l:23:LEU:HD21	2.00	0.42
22:1:305:CLA:H61	22:1:305:CLA:H41	1.92	0.42
26:2:313:CHL:H91	26:2:313:CHL:H112	1.82	0.42
18:3:111:GLU:HB3	18:3:120:GLN:HE21	1.84	0.42
18:3:196:LYS:HD3	22:3:306:CLA:HBD	2.01	0.42
24:3:309:XAT:H35	24:3:309:XAT:H401	1.87	0.42
18:5:111:GLU:O	18:5:120:GLN:NE2	2.48	0.42
27:5:319:NEX:H191	27:5:319:NEX:H11	1.73	0.42
22:p:305:CLA:H141	22:p:305:CLA:H161	1.87	0.42
22:V:307:CLA:H2	22:V:307:CLA:H61	1.70	0.42
18:P:234:THR:HG23	18:P:235:VAL:HG13	2.01	0.42
22:P:302:CLA:H62	22:P:303:CLA:H3A	2.01	0.42
22:U:306:CLA:H102	22:U:306:CLA:H61	1.83	0.42
26:g:314:CHL:H111	26:g:314:CHL:H91	1.76	0.42
22:R:303:CLA:HAB	24:R:313:XAT:H32	2.02	0.42
23:S:310:LUT:H11	23:S:310:LUT:H191	1.92	0.42
36:b:601:DGD:HB62	36:b:601:DGD:HB32	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:247:TRP:NE1	25:c:523:LHG:O9	2.49	0.42
3:d:48:TRP:HA	3:d:78:VAL:HG21	2.00	0.42
18:1:193:LEU:HD23	18:1:196:LYS:HD2	2.02	0.42
22:1:302:CLA:H3A	22:1:302:CLA:HBA1	1.73	0.42
26:1:316:CHL:H143	26:1:316:CHL:H111	1.87	0.42
26:2:316:CHL:H91	26:2:316:CHL:H111	1.86	0.42
18:4:159:ARG:NH2	26:4:317:CHL:O1D	2.45	0.42
18:4:181:LEU:HD12	23:4:309:LUT:H222	2.00	0.42
26:6:315:CHL:H62	26:6:315:CHL:H101	1.90	0.42
18:p:152:MET:HA	18:p:155:VAL:HG22	2.02	0.42
18:p:217:VAL:O	18:p:244:LYS:NZ	2.36	0.42
23:P:311:LUT:H35	23:P:311:LUT:H401	1.83	0.42
18:Q:40:TRP:CD1	18:Q:41:LEU:HG	2.52	0.42
22:N:301:CLA:H91	22:G:302:CLA:H51	2.00	0.42
23:n:309:LUT:H11	23:n:309:LUT:H191	1.91	0.42
21:B:282:GLN:HE21	21:B:286:LYS:HE3	1.83	0.42
22:B:610:CLA:H2A	22:B:610:CLA:HED2	2.00	0.42
36:b:601:DGD:HB51	36:b:601:DGD:HB22	1.93	0.42
22:b:603:CLA:H61	22:b:603:CLA:H93	1.79	0.42
26:r:614:CHL:H61	26:r:614:CHL:H41	1.77	0.42
30:A:407:PHO:H11	25:D:407:LHG:H361	2.00	0.42
22:2:307:CLA:H2	22:2:307:CLA:H61	1.65	0.42
18:4:180:PRO:HA	1:R:194:ARG:HH11	1.84	0.42
22:4:302:CLA:H91	22:4:302:CLA:H112	1.86	0.42
22:v:304:CLA:H52	23:v:309:LUT:H30	2.02	0.42
22:V:301:CLA:H193	22:V:301:CLA:H161	1.92	0.42
22:V:302:CLA:H143	22:V:302:CLA:H111	1.86	0.42
23:V:309:LUT:H11	23:V:309:LUT:H191	1.92	0.42
23:V:310:LUT:H15	23:V:310:LUT:H201	1.91	0.42
22:P:305:CLA:H52	23:P:310:LUT:H30	2.01	0.42
18:N:83:LEU:HD23	18:N:172:LEU:HD23	2.02	0.42
26:n:313:CHL:H18	26:g:314:CHL:H161	2.00	0.42
26:n:316:CHL:H151	26:n:316:CHL:H18	1.74	0.42
18:g:121:ILE:O	18:g:126:GLY:N	2.53	0.42
22:C:511:CLA:H91	22:C:511:CLA:H111	1.75	0.42
3:D:210:LEU:HD22	3:D:271:MET:HG2	2.00	0.42
36:b:601:DGD:HB51	36:b:601:DGD:HB81	1.70	0.42
26:r:616:CHL:HHC	26:r:616:CHL:H122	2.02	0.42
31:z:101:BCR:H24C	31:z:101:BCR:H371	1.94	0.42
16:y:33:LEU:HD23	22:c:512:CLA:H41	2.02	0.42
22:2:307:CLA:H122	24:2:311:XAT:H32	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:312:LHG:H242	25:2:312:LHG:HC62	1.91	0.42
26:3:315:CHL:H112	26:3:315:CHL:H202	2.02	0.42
26:4:313:CHL:H202	26:4:313:CHL:H161	1.84	0.42
26:5:317:CHL:H61	26:5:317:CHL:H101	1.79	0.42
18:q:208:MET:HA	18:q:211:PHE:HD2	1.85	0.42
18:V:40:TRP:CD1	18:V:41:LEU:HG	2.54	0.42
26:V:317:CHL:H91	26:V:317:CHL:H112	1.84	0.42
18:u:225:ASN:HB3	22:u:307:CLA:HED2	2.00	0.42
18:n:230:LEU:HA	22:n:308:CLA:HAB	2.02	0.42
22:g:303:CLA:HBA2	22:g:303:CLA:H3A	1.38	0.42
21:B:497:LYS:HD3	21:B:500:ASP:HB3	2.02	0.42
11:O:97:PHE:HD1	11:O:288:ALA:HB2	1.84	0.42
21:b:341:LEU:HD11	21:b:431:GLU:HB2	2.02	0.42
22:s:306:CLA:H91	22:s:307:CLA:HMD2	2.01	0.42
1:r:164:ASN:HD22	22:r:610:CLA:HBC3	1.85	0.42
31:a:409:BCR:H401	36:a:416:DGD:HD61	2.01	0.42
3:d:87:HIS:NE2	3:d:162:LEU:O	2.52	0.42
2:A:212:SER:HB2	3:D:211:CYS:HB2	2.02	0.42
23:1:309:LUT:H35	23:1:309:LUT:H401	1.90	0.42
22:q:303:CLA:HBA2	22:q:303:CLA:H3A	1.41	0.42
18:Q:37:ARG:HE	18:Q:39:LYS:HE3	1.85	0.42
18:N:64:ASP:HB3	18:N:67:GLY:HA2	2.01	0.42
26:R:315:CHL:H61	26:R:315:CHL:H41	1.84	0.42
31:C:518:BCR:H15C	31:C:518:BCR:H351	1.92	0.42
22:B:602:CLA:H92	22:B:602:CLA:H61	1.83	0.42
11:O:57:ILE:HD12	11:O:75:PRO:HB3	2.01	0.42
22:b:614:CLA:HMA2	22:b:614:CLA:H2	2.00	0.42
20:c:144:LYS:HA	20:c:147:ASN:HD22	1.84	0.42
20:c:332:SER:OG	20:c:336:GLU:N	2.50	0.42
22:c:514:CLA:H143	22:c:514:CLA:H162	1.90	0.42
36:c:518:DGD:HA82	36:c:518:DGD:HA51	1.85	0.42
25:s:312:LHG:H172	25:s:312:LHG:H201	1.82	0.42
26:p:317:CHL:H13	26:p:319:CHL:H102	2.01	0.42
18:V:127:LEU:O	18:V:137:HIS:ND1	2.51	0.42
18:N:232:ASN:HB3	18:N:235:VAL:HG22	2.01	0.42
26:G:314:CHL:H62	26:G:314:CHL:H101	1.95	0.42
23:u:309:LUT:H15	23:u:309:LUT:H201	1.87	0.42
26:n:318:CHL:H143	26:n:318:CHL:H161	1.88	0.42
20:C:142:LYS:HE3	20:C:254:TRP:CD2	2.55	0.42
22:b:606:CLA:H92	22:b:606:CLA:H62	1.87	0.42
20:c:95:ASP:OD2	34:c:501:LMG:O2	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:282:ASN:OD1	36:c:517:DGD:O5E	2.37	0.42
2:a:269:ARG:HH22	3:d:234:ALA:HB3	1.84	0.42
18:1:53:LEU:HD11	18:1:62:GLY:HA2	2.02	0.42
22:4:302:CLA:H62	22:5:302:CLA:H52	2.02	0.42
26:p:314:CHL:H112	26:p:314:CHL:H91	1.84	0.42
18:q:40:TRP:CD1	18:q:41:LEU:HG	2.52	0.42
22:V:304:CLA:H2	23:V:309:LUT:H28	2.02	0.42
22:N:302:CLA:H92	22:N:302:CLA:H62	1.90	0.42
22:C:511:CLA:HBA1	22:C:511:CLA:H3A	1.73	0.42
31:C:516:BCR:H24C	31:C:516:BCR:H371	1.94	0.42
3:D:78:VAL:O	3:D:172:SER:OG	2.33	0.42
31:b:619:BCR:H11C	31:b:619:BCR:H341	1.93	0.42
20:c:142:LYS:HE3	20:c:254:TRP:CD2	2.55	0.42
22:r:607:CLA:H3A	22:r:607:CLA:HBA2	1.51	0.42
9:L:29:ALA:O	9:L:33:SER:HB3	2.20	0.42
22:2:301:CLA:H203	22:2:301:CLA:H161	1.88	0.42
18:4:152:MET:HA	18:4:155:VAL:HG22	2.02	0.42
22:5:302:CLA:HBB1	23:5:310:LUT:C35	2.50	0.42
27:5:319:NEX:H35	27:5:319:NEX:H401	1.76	0.42
25:V:312:LHG:H311	25:V:312:LHG:H111	2.01	0.42
26:V:318:CHL:H143	26:V:318:CHL:H162	1.88	0.42
18:U:147:VAL:HG11	26:U:314:CHL:HED3	2.01	0.42
18:u:80:GLU:HA	18:u:172:LEU:HD21	2.01	0.42
27:R:301:NEX:H35	27:R:301:NEX:H401	1.83	0.42
19:S:83:TYR:OH	25:S:312:LHG:O5	2.32	0.42
25:S:312:LHG:H162	25:S:312:LHG:H132	1.90	0.42
25:S:312:LHG:H262	25:S:312:LHG:H292	1.78	0.42
20:C:95:ASP:OD2	34:C:502:LMG:O2	2.37	0.42
3:D:161:PRO:HB3	3:D:170:ALA:HB2	2.02	0.42
22:b:613:CLA:HBA2	22:b:613:CLA:H3A	1.36	0.42
20:c:306:LEU:HD12	20:c:328:TYR:HB3	2.01	0.42
22:r:602:CLA:H102	22:r:602:CLA:H13	1.78	0.41
9:l:12:GLU:HG2	10:m:29:THR:HG23	2.01	0.41
24:1:311:XAT:H373	24:1:311:XAT:H23	1.89	0.41
23:4:310:LUT:H31	23:4:310:LUT:H391	1.90	0.41
18:6:111:GLU:HB3	18:6:120:GLN:HE21	1.84	0.41
18:P:208:MET:HA	18:P:211:PHE:HD2	1.85	0.41
18:P:217:VAL:O	18:P:244:LYS:NZ	2.41	0.41
26:P:317:CHL:H101	26:P:317:CHL:H62	1.86	0.41
25:U:312:LHG:H282	25:U:312:LHG:H102	2.02	0.41
22:N:301:CLA:H192	22:N:301:CLA:H161	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:307:CLA:H91	25:N:312:LHG:H341	2.01	0.41
20:C:306:LEU:HD12	20:C:328:TYR:HB3	2.01	0.41
21:b:256:MET:HA	21:b:263:THR:HG21	2.00	0.41
1:r:210:PHE:CZ	24:r:612:XAT:H10	2.55	0.41
3:d:199:MET:HE2	3:d:281:MET:HE2	2.03	0.41
11:o:124:LEU:HD23	11:o:124:LEU:HA	1.91	0.41
22:1:306:CLA:H2	22:1:306:CLA:H62	1.78	0.41
22:4:307:CLA:H2	22:4:307:CLA:H61	1.71	0.41
18:5:138:ALA:HA	26:5:314:CHL:HHC	2.02	0.41
18:v:86:ALA:HB1	18:v:201:GLY:HA3	2.01	0.41
23:v:310:LUT:H15	23:v:310:LUT:H201	1.86	0.41
25:v:312:LHG:H192	25:v:312:LHG:H161	1.87	0.41
18:q:229:HIS:CG	22:q:307:CLA:HAA2	2.55	0.41
18:P:217:VAL:HG11	22:P:308:CLA:HMD1	2.01	0.41
26:G:314:CHL:H91	26:G:314:CHL:H111	1.76	0.41
1:r:97:CYS:O	1:r:101:HIS:ND1	2.34	0.41
3:d:191:TRP:HA	3:d:194:ASN:HD22	1.85	0.41
10:m:6:TYR:HB3	31:b:618:BCR:HC31	2.03	0.41
11:o:74:CYS:SG	11:o:100:GLU:HG3	2.60	0.41
22:A:405:CLA:H2A	22:A:405:CLA:HED3	2.02	0.41
18:1:62:GLY:N	22:1:301:CLA:OBD	2.51	0.41
18:3:183:LEU:N	22:3:304:CLA:O1A	2.41	0.41
18:4:40:TRP:CD1	18:4:41:LEU:HG	2.55	0.41
18:5:180:PRO:HD2	23:5:309:LUT:H23	2.01	0.41
22:5:305:CLA:HMD1	22:5:305:CLA:HHD	1.78	0.41
22:6:308:CLA:H61	22:6:308:CLA:H2	1.72	0.41
22:p:302:CLA:HAB	23:p:311:LUT:H32	2.01	0.41
26:V:313:CHL:H91	26:V:313:CHL:H112	1.84	0.41
18:Q:81:LEU:HD11	22:Q:302:CLA:HBD	2.02	0.41
22:Q:307:CLA:H61	22:Q:307:CLA:H2	1.80	0.41
26:Q:311:CHL:H61	26:Q:311:CHL:H41	1.78	0.41
18:U:184:ALA:HA	18:U:190:PHE:HB2	2.03	0.41
26:N:313:CHL:H11	26:G:316:CHL:H43	2.01	0.41
18:G:37:ARG:HH22	18:G:53:LEU:HD12	1.85	0.41
18:u:52:TYR:OH	18:u:64:ASP:OD2	2.37	0.41
18:u:217:VAL:O	18:u:244:LYS:NZ	2.38	0.41
18:n:44:TYR:HB3	18:g:161:ASN:HD21	1.84	0.41
22:R:304:CLA:H112	22:R:304:CLA:H91	1.86	0.41
23:S:311:LUT:H15	23:S:311:LUT:H201	1.91	0.41
21:b:157:HIS:CE1	21:b:164:PRO:HD2	2.55	0.41
21:b:497:LYS:HZ2	21:b:503:SER:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:603:CLA:H143	22:b:603:CLA:H111	1.85	0.41
20:c:155:MET:HE3	22:c:513:CLA:H51	2.02	0.41
22:r:603:CLA:H112	22:r:603:CLA:H91	1.84	0.41
24:r:612:XAT:H173	24:r:612:XAT:H3	1.89	0.41
16:Y:33:LEU:HD23	22:C:513:CLA:H41	2.02	0.41
18:4:83:LEU:HD23	18:4:172:LEU:HD22	2.01	0.41
26:4:317:CHL:H101	26:6:301:CHL:H13	2.03	0.41
18:6:196:LYS:NZ	22:6:307:CLA:O1A	2.47	0.41
18:p:222:PRO:HA	18:p:225:ASN:HD22	1.85	0.41
22:p:303:CLA:CAD	26:p:319:CHL:H2	2.50	0.41
22:Q:308:CLA:H3A	22:Q:308:CLA:HBA1	1.55	0.41
26:Q:315:CHL:H152	26:Q:315:CHL:H111	1.77	0.41
26:Q:315:CHL:H2	26:Q:315:CHL:H62	1.81	0.41
24:U:311:XAT:H10	26:U:313:CHL:H13	2.01	0.41
22:u:301:CLA:H172	22:u:301:CLA:H13	1.79	0.41
23:S:311:LUT:H31	23:S:311:LUT:H391	1.91	0.41
22:C:511:CLA:H112	22:C:511:CLA:H142	1.83	0.41
3:D:87:HIS:NE2	3:D:162:LEU:O	2.53	0.41
21:b:370:LEU:HD22	21:b:379:ALA:HB3	2.03	0.41
22:b:603:CLA:H141	22:b:603:CLA:H162	1.81	0.41
3:d:201:VAL:HG12	22:d:402:CLA:C1B	2.50	0.41
33:d:404:PL9:H513	12:t:10:LEU:HD22	2.02	0.41
11:o:157:TYR:HE1	20:c:318:SER:HA	1.86	0.41
12:t:30:ILE:H	12:t:30:ILE:HG13	1.70	0.41
31:t:101:BCR:H403	31:B:618:BCR:H342	2.02	0.41
22:A:405:CLA:HMB2	30:A:407:PHO:H172	2.02	0.41
22:4:307:CLA:HBA2	22:4:307:CLA:H3A	1.75	0.41
22:5:301:CLA:H101	23:5:310:LUT:H371	2.01	0.41
23:5:309:LUT:H31	23:5:309:LUT:H391	1.96	0.41
22:6:302:CLA:H72	22:6:302:CLA:H111	1.60	0.41
26:6:315:CHL:H111	26:6:315:CHL:H143	1.86	0.41
18:P:159:ARG:HG3	26:P:318:CHL:C1D	2.51	0.41
23:N:310:LUT:H11	23:N:310:LUT:H191	1.93	0.41
22:u:306:CLA:H8	22:u:306:CLA:H122	1.82	0.41
26:u:318:CHL:H92	26:u:318:CHL:H61	1.86	0.41
25:n:312:LHG:H141	26:n:313:CHL:HED3	2.01	0.41
26:g:315:CHL:H62	26:g:315:CHL:H2	1.76	0.41
20:C:144:LYS:HA	20:C:144:LYS:HD2	1.88	0.41
20:C:144:LYS:HA	20:C:147:ASN:HD22	1.84	0.41
20:C:392:LEU:HD23	20:C:392:LEU:HA	1.91	0.41
20:C:444:GLU:HG2	20:C:445:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:505:CLA:H62	22:C:505:CLA:H41	1.67	0.41
21:B:79:THR:OG1	21:B:83:GLU:O	2.29	0.41
3:D:191:TRP:HA	3:D:194:ASN:HD22	1.86	0.41
21:b:214:LEU:HD23	21:b:217:LEU:HD12	2.02	0.41
2:a:198:HIS:HA	2:a:286:THR:HG22	2.01	0.41
22:a:405:CLA:H111	22:a:405:CLA:H152	1.73	0.41
5:H:38:GLY:O	1:R:47:VAL:HA	2.20	0.41
26:2:316:CHL:H111	26:2:316:CHL:H143	1.88	0.41
26:3:314:CHL:H111	26:3:314:CHL:H143	1.87	0.41
24:5:311:XAT:H15	24:5:311:XAT:H201	1.89	0.41
26:v:316:CHL:HBB1	26:q:311:CHL:H122	2.02	0.41
18:P:41:LEU:HD12	18:P:46:GLU:HB2	2.01	0.41
22:Q:301:CLA:H141	22:Q:301:CLA:H161	1.89	0.41
18:U:109:PHE:HE1	18:U:130:LEU:HA	1.86	0.41
18:u:199:LYS:NZ	22:u:305:CLA:O1D	2.44	0.41
24:u:311:XAT:H373	24:u:311:XAT:H23	1.93	0.41
27:n:319:NEX:H15	27:n:319:NEX:H201	1.70	0.41
1:R:15:LEU:HB2	1:R:18:THR:HG23	2.01	0.41
1:R:46:VAL:HG22	1:R:70:GLN:HG2	2.02	0.41
1:R:210:PHE:CZ	24:R:313:XAT:H10	2.56	0.41
27:S:317:NEX:H191	27:S:317:NEX:H11	1.78	0.41
20:C:285:TYR:O	20:C:411:ARG:NH2	2.50	0.41
22:B:615:CLA:H141	22:B:615:CLA:H161	1.89	0.41
3:D:201:VAL:HG12	22:D:403:CLA:C1B	2.50	0.41
21:b:497:LYS:HD3	21:b:500:ASP:HB3	2.02	0.41
17:e:20:TRP:HD1	17:e:23:HIS:H	1.68	0.41
22:s:305:CLA:H52	23:s:310:LUT:H28	2.03	0.41
27:r:617:NEX:H11	27:r:617:NEX:H191	1.74	0.41
32:a:410:SQD:O9	3:d:230:ASN:ND2	2.50	0.41
5:h:26:LEU:HD23	5:h:29:LEU:HD12	2.03	0.41
22:A:408:CLA:H92	22:A:408:CLA:H62	1.85	0.41
24:1:311:XAT:H35	24:1:311:XAT:H401	1.87	0.41
26:3:315:CHL:H13	26:3:315:CHL:H171	1.68	0.41
25:V:312:LHG:O3	25:V:312:LHG:O1	2.37	0.41
22:P:308:CLA:H121	24:P:312:XAT:H34	2.02	0.41
22:U:306:CLA:H2	22:U:306:CLA:H62	1.81	0.41
24:U:311:XAT:H173	24:U:311:XAT:H3	1.91	0.41
25:U:312:LHG:H182	25:U:312:LHG:H211	1.81	0.41
26:N:313:CHL:H193	26:G:314:CHL:HHB	2.03	0.41
19:S:98:ALA:HA	19:S:101:ARG:HH11	1.86	0.41
22:C:506:CLA:H62	22:C:506:CLA:H41	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:603:CLA:H143	22:B:603:CLA:H111	1.86	0.41
22:B:614:CLA:H142	22:B:614:CLA:H112	1.94	0.41
11:O:130:TYR:HD2	11:O:131:THR:HG23	1.85	0.41
3:d:338:ARG:HH21	17:e:65:LEU:HD22	1.85	0.41
18:1:213:VAL:HG11	22:1:307:CLA:HAC2	2.02	0.41
22:2:301:CLA:H91	22:3:302:CLA:H71	2.02	0.41
26:2:316:CHL:H13	26:2:318:CHL:H101	2.03	0.41
26:6:314:CHL:H3A	26:6:314:CHL:HBA1	1.64	0.41
18:p:109:PHE:HB2	18:p:112:ALA:HB2	2.02	0.41
26:P:319:CHL:H203	26:P:319:CHL:H161	1.83	0.41
23:N:309:LUT:H35	23:N:309:LUT:H401	1.91	0.41
26:N:317:CHL:H91	26:N:317:CHL:H111	1.84	0.41
18:u:144:THR:HG22	26:u:314:CHL:HAC1	2.01	0.41
1:R:164:ASN:HD22	22:R:311:CLA:HBC3	1.85	0.41
22:C:505:CLA:H61	22:C:505:CLA:H102	1.77	0.41
22:C:515:CLA:H93	22:C:515:CLA:H61	1.87	0.41
11:O:84:LEU:HD22	11:O:185:LEU:HD22	2.02	0.41
21:b:366:PHE:HD2	21:b:425:GLN:HE21	1.68	0.41
22:b:615:CLA:H161	22:b:615:CLA:H141	1.88	0.41
19:s:98:ALA:HA	19:s:101:ARG:HH11	1.86	0.41
1:r:46:VAL:HG22	1:r:70:GLN:HG2	2.03	0.41
22:r:606:CLA:H2	23:r:611:LUT:H28	2.03	0.41
30:a:407:PHO:H11	25:d:406:LHG:H361	2.01	0.41
22:a:408:CLA:H13	34:w:201:LMG:H321	2.02	0.41
3:d:160:TYR:HH	3:d:189:HIS:HE2	1.68	0.41
8:k:14:ALA:HB1	15:z:2:THR:HG23	2.02	0.41
31:A:409:BCR:H15C	31:A:409:BCR:H351	1.88	0.41
37:E:101:HEM:HHD	37:E:101:HEM:HBC2	2.03	0.41
5:H:26:LEU:HD23	5:H:29:LEU:HD12	2.02	0.41
18:1:40:TRP:CD1	18:1:41:LEU:HG	2.56	0.41
26:1:317:CHL:H143	26:1:317:CHL:H162	1.88	0.41
24:2:311:XAT:H173	24:2:311:XAT:H3	1.90	0.41
25:2:312:LHG:H132	25:2:312:LHG:H161	1.90	0.41
22:3:301:CLA:H111	22:3:301:CLA:H72	1.58	0.41
22:5:302:CLA:H62	22:5:302:CLA:H2	1.85	0.41
23:5:309:LUT:H15	23:5:309:LUT:H201	1.83	0.41
23:5:310:LUT:H35	23:5:310:LUT:H401	1.76	0.41
24:6:310:XAT:H31	24:6:310:XAT:H391	1.99	0.41
18:p:37:ARG:NH1	18:p:55:GLY:H	2.19	0.41
22:p:302:CLA:HBA1	23:p:311:LUT:H382	2.03	0.41
22:p:307:CLA:H62	22:p:307:CLA:H2	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:p:308:CLA:H142	24:p:312:XAT:H34	2.03	0.41
18:q:41:LEU:HB3	18:q:44:TYR:HB2	2.02	0.41
18:q:49:THR:HB	18:q:53:LEU:HD11	2.02	0.41
18:V:76:LYS:HA	18:V:79:ARG:HE	1.85	0.41
22:V:306:CLA:H2A	22:V:306:CLA:HED2	2.02	0.41
26:V:313:CHL:H52	26:P:319:CHL:HBB1	2.03	0.41
26:Q:316:CHL:H91	26:Q:316:CHL:H112	1.83	0.41
26:U:315:CHL:H152	26:G:311:CHL:H161	2.03	0.41
22:G:307:CLA:H2	22:G:307:CLA:H61	1.75	0.41
22:u:301:CLA:H152	22:n:302:CLA:H143	2.03	0.41
23:u:310:LUT:H372	22:n:302:CLA:HED3	2.01	0.41
19:S:86:ASP:OD1	23:S:311:LUT:O23	2.39	0.41
27:S:317:NEX:H35	27:S:317:NEX:H401	1.76	0.41
20:C:257:GLU:OE2	20:C:432:HIS:ND1	2.47	0.41
21:B:256:MET:O	21:B:448:ARG:NH1	2.54	0.41
21:B:372:ASP:OD1	21:B:376:ILE:N	2.47	0.41
21:B:477:ASP:OD1	21:B:477:ASP:N	2.53	0.41
22:B:604:CLA:H142	22:B:604:CLA:H112	1.89	0.41
22:B:606:CLA:HBB1	22:B:607:CLA:H52	2.02	0.41
22:B:610:CLA:H93	22:B:610:CLA:H61	1.90	0.41
11:O:124:LEU:HD23	11:O:124:LEU:HA	1.91	0.41
22:b:604:CLA:HBB2	22:b:606:CLA:H18	2.02	0.41
22:b:605:CLA:H202	22:b:605:CLA:H162	1.95	0.41
20:c:285:TYR:O	20:c:411:ARG:NH2	2.51	0.41
22:c:504:CLA:H102	22:c:504:CLA:H61	1.77	0.41
15:z:31:ASN:O	15:z:34:THR:OG1	2.35	0.41
2:A:337:HIS:HB2	3:D:352:LEU:HD22	2.02	0.41
31:A:409:BCR:H11C	31:A:409:BCR:H341	1.91	0.41
9:L:12:GLU:HG2	10:M:29:THR:HG23	2.03	0.41
26:3:311:CHL:H91	26:3:311:CHL:H112	1.84	0.41
18:p:234:THR:HG23	18:p:235:VAL:HG13	2.03	0.41
22:q:302:CLA:H92	22:q:302:CLA:H61	1.90	0.41
25:V:312:LHG:H192	25:V:312:LHG:H161	1.85	0.41
22:P:308:CLA:H2	22:P:308:CLA:H61	1.67	0.41
18:Q:208:MET:HA	18:Q:211:PHE:HD2	1.86	0.41
25:N:312:LHG:H251	26:N:313:CHL:HMD1	2.02	0.41
18:G:129:TYR:HB3	18:G:135:LEU:HD21	2.03	0.41
18:n:58:PRO:HG3	18:n:194:LYS:HD3	2.03	0.41
20:C:281:ASN:OD1	36:C:519:DGD:O5E	2.38	0.41
22:B:610:CLA:H141	22:B:610:CLA:H161	1.78	0.41
3:D:199:MET:HE2	3:D:281:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:444:GLU:HG2	20:c:445:LYS:HG3	2.03	0.41
30:A:407:PHO:H141	30:A:407:PHO:H162	1.83	0.40
9:L:23:LEU:HD21	25:D:407:LHG:H171	2.02	0.40
23:1:309:LUT:H15	23:1:309:LUT:H201	1.77	0.40
23:2:309:LUT:H11	23:2:309:LUT:H191	1.95	0.40
18:3:196:LYS:HD3	22:3:306:CLA:HAA2	2.02	0.40
22:3:307:CLA:H71	25:3:310:LHG:H151	2.01	0.40
18:4:40:TRP:HZ3	18:4:49:THR:HG22	1.86	0.40
18:5:59:GLY:HA3	18:5:202:ARG:HH22	1.85	0.40
18:6:164:PRO:HG2	26:6:316:CHL:HBB2	2.03	0.40
22:v:302:CLA:H111	22:v:302:CLA:H152	1.68	0.40
25:p:313:LHG:H251	26:p:314:CHL:HMD1	2.02	0.40
23:P:310:LUT:H15	23:P:310:LUT:H201	1.85	0.40
18:g:40:TRP:CD1	18:g:41:LEU:HG	2.54	0.40
26:g:311:CHL:H91	26:g:311:CHL:H111	1.85	0.40
20:C:166:LYS:HA	20:C:170:PHE:HB2	2.03	0.40
22:C:505:CLA:H192	22:C:512:CLA:HBB2	2.02	0.40
21:B:71:ILE:HD11	22:B:607:CLA:H2A	2.02	0.40
21:B:149:LEU:HG	22:B:605:CLA:H162	1.88	0.40
36:B:601:DGD:HBW2	36:B:601:DGD:HB91	1.79	0.40
21:b:368:VAL:HG21	21:b:422:ARG:HG2	2.03	0.40
22:s:305:CLA:H2	23:s:310:LUT:H28	2.03	0.40
1:r:32:ARG:HH22	25:r:613:LHG:HC31	1.85	0.40
22:2:302:CLA:HED2	22:2:302:CLA:H2A	2.03	0.40
18:3:42:GLY:HA3	18:3:43:PRO:HD3	1.97	0.40
22:4:301:CLA:H13	22:4:301:CLA:H172	1.81	0.40
18:5:181:LEU:HD12	23:5:309:LUT:H222	2.04	0.40
18:V:173:TYR:HB3	22:V:304:CLA:HED2	2.03	0.40
18:V:218:THR:HG23	18:V:220:LYS:H	1.85	0.40
22:V:305:CLA:H8	22:V:305:CLA:H122	1.91	0.40
26:P:317:CHL:H143	26:P:317:CHL:H111	1.88	0.40
26:U:317:CHL:C4B	26:G:311:CHL:H2	2.51	0.40
26:N:316:CHL:H93	26:N:316:CHL:H112	1.88	0.40
18:G:37:ARG:NH1	18:G:55:GLY:H	2.19	0.40
26:n:313:CHL:H91	26:n:313:CHL:H112	1.92	0.40
26:S:315:CHL:H3A	26:S:315:CHL:HBA1	1.83	0.40
20:C:59:GLU:O	20:C:63:PHE:HB2	2.22	0.40
20:C:318:SER:HA	11:O:157:TYR:HE1	1.86	0.40
31:X:201:BCR:H11C	31:X:201:BCR:H341	1.98	0.40
20:c:264:LEU:HD23	20:c:264:LEU:HA	1.87	0.40
22:c:504:CLA:H192	22:c:511:CLA:HBB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:r:615:CHL:H2	26:r:615:CHL:H61	1.79	0.40
2:a:257:ARG:HH22	21:b:490:VAL:HA	1.86	0.40
9:l:29:ALA:O	9:l:33:SER:HB3	2.21	0.40
32:l:102:SQD:H321	32:l:102:SQD:H351	1.85	0.40
2:A:301:ASN:OD1	2:A:303:ASN:ND2	2.54	0.40
12:T:10:LEU:HD22	33:D:405:PL9:H513	2.02	0.40
34:W:201:LMG:H402	34:W:201:LMG:H371	1.91	0.40
18:2:100:GLU:HB2	18:2:223:ILE:HD12	2.02	0.40
24:v:311:XAT:H35	24:v:311:XAT:H401	1.89	0.40
26:q:311:CHL:H91	26:q:311:CHL:H112	1.85	0.40
26:q:314:CHL:H2	26:q:314:CHL:H62	1.69	0.40
22:V:307:CLA:H71	25:V:312:LHG:H171	2.04	0.40
23:V:310:LUT:H372	22:P:303:CLA:HED2	2.03	0.40
22:P:302:CLA:H91	22:Q:302:CLA:H61	2.03	0.40
24:N:311:XAT:H373	24:N:311:XAT:H23	1.89	0.40
18:u:161:ASN:OD1	18:u:162:GLY:N	2.54	0.40
18:u:170:ASP:HB2	18:u:174:PRO:HA	2.04	0.40
26:u:316:CHL:H91	26:u:316:CHL:H111	1.89	0.40
1:R:228:LEU:HA	1:R:228:LEU:HD23	1.85	0.40
20:C:390:GLY:HA3	20:C:408:VAL:HG13	2.02	0.40
21:B:341:LEU:HD11	21:B:431:GLU:HB2	2.03	0.40
22:B:604:CLA:H41	22:B:604:CLA:H62	1.68	0.40
11:O:74:CYS:SG	11:O:100:GLU:HG3	2.61	0.40
3:D:49:LEU:HD21	31:D:404:BCR:H362	2.04	0.40
25:D:406:LHG:H141	25:D:406:LHG:H351	2.02	0.40
36:b:601:DGD:HB72	36:b:601:DGD:HBT2	1.75	0.40
36:c:518:DGD:HBW1	36:c:518:DGD:HBN1	1.91	0.40
2:a:274:PHE:HD1	32:a:410:SQD:H112	1.86	0.40
2:a:337:HIS:HB2	3:d:352:LEU:HD22	2.01	0.40
25:d:405:LHG:H362	22:b:614:CLA:H41	2.02	0.40
31:k:101:BCR:H15C	31:k:101:BCR:H351	1.89	0.40
2:A:29:TYR:O	2:A:129:ARG:NH2	2.54	0.40
9:L:27:VAL:HG11	25:L:101:LHG:H201	2.03	0.40
22:1:307:CLA:H2	22:1:307:CLA:H61	1.67	0.40
18:3:81:LEU:HD11	22:3:302:CLA:HBD	2.02	0.40
26:3:311:CHL:H61	26:3:311:CHL:H41	1.80	0.40
22:5:304:CLA:H51	22:5:306:CLA:HMA2	2.04	0.40
22:5:307:CLA:H61	22:5:307:CLA:H2	1.72	0.40
18:6:237:ASN:ND2	22:6:309:CLA:O1D	2.47	0.40
24:6:310:XAT:H35	24:6:310:XAT:H401	1.90	0.40
18:v:111:GLU:HG2	18:v:116:LYS:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:v:310:LUT:H31	23:v:310:LUT:H391	1.93	0.40
18:V:165:ALA:HB3	26:V:317:CHL:HBB1	2.03	0.40
24:P:312:XAT:H373	24:P:312:XAT:H23	1.89	0.40
26:P:317:CHL:H203	26:P:317:CHL:H161	1.88	0.40
27:N:318:NEX:H11	27:N:318:NEX:H191	1.79	0.40
18:G:116:LYS:HB3	18:G:119:ALA:HB3	2.03	0.40
18:G:213:VAL:HG11	22:G:307:CLA:HAC2	2.04	0.40
22:n:301:CLA:H61	23:n:310:LUT:H28	2.04	0.40
22:C:504:CLA:H92	22:C:514:CLA:H42	2.04	0.40
3:D:160:TYR:HH	3:D:189:HIS:HE2	1.69	0.40
21:b:58:GLN:HB2	21:b:60:MET:HG2	2.03	0.40
31:b:618:BCR:H24C	31:b:618:BCR:H371	1.93	0.40
22:c:505:CLA:H162	22:c:509:CLA:H121	2.04	0.40
22:c:505:CLA:H11	36:c:518:DGD:HB32	2.04	0.40
22:c:507:CLA:H62	22:c:507:CLA:H41	1.69	0.40
27:r:617:NEX:H401	27:r:617:NEX:H35	1.85	0.40
2:a:195:HIS:HD2	2:a:299:GLY:HA2	1.85	0.40
3:d:78:VAL:O	3:d:172:SER:OG	2.34	0.40
18:1:98:THR:HG21	22:1:303:CLA:HAC2	2.03	0.40
23:4:309:LUT:H11	23:4:309:LUT:H191	1.96	0.40
23:4:309:LUT:H201	23:4:309:LUT:H15	1.77	0.40
24:4:311:XAT:H173	24:4:311:XAT:H3	1.89	0.40
22:5:301:CLA:HAB	23:5:310:LUT:H32	2.02	0.40
23:5:309:LUT:H35	23:5:309:LUT:H401	1.88	0.40
22:v:302:CLA:H61	22:v:302:CLA:H2	1.78	0.40
18:U:161:ASN:OD1	18:U:162:GLY:N	2.54	0.40
26:U:315:CHL:H143	26:U:315:CHL:H111	1.82	0.40
18:n:159:ARG:NH2	26:n:318:CHL:O1D	2.54	0.40
22:C:510:CLA:H62	22:C:510:CLA:H41	1.95	0.40
22:C:515:CLA:H52	25:C:522:LHG:H102	2.04	0.40
21:B:58:GLN:HB2	21:B:60:MET:HG2	2.04	0.40
36:B:601:DGD:HB32	36:B:601:DGD:HB62	1.87	0.40
37:e:101:HEM:HHD	37:e:101:HEM:HBC2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	221/280 (79%)	201 (91%)	20 (9%)	0	100	100
1	r	221/280 (79%)	197 (89%)	24 (11%)	0	100	100
2	A	331/352 (94%)	314 (95%)	17 (5%)	0	100	100
2	a	331/352 (94%)	316 (96%)	15 (4%)	0	100	100
3	D	339/352 (96%)	304 (90%)	35 (10%)	0	100	100
3	d	339/352 (96%)	307 (91%)	32 (9%)	0	100	100
4	F	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
4	f	28/44 (64%)	27 (96%)	1 (4%)	0	100	100
5	H	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
5	h	62/88 (70%)	61 (98%)	1 (2%)	0	100	100
6	I	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
6	i	32/37 (86%)	29 (91%)	3 (9%)	0	100	100
7	J	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
7	j	29/50 (58%)	27 (93%)	2 (7%)	0	100	100
8	K	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
8	k	34/46 (74%)	30 (88%)	4 (12%)	0	100	100
9	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
10	M	30/34 (88%)	30 (100%)	0	0	100	100
10	m	30/34 (88%)	30 (100%)	0	0	100	100
11	O	206/291 (71%)	176 (85%)	30 (15%)	0	100	100
11	o	206/291 (71%)	175 (85%)	31 (15%)	0	100	100
12	T	28/31 (90%)	25 (89%)	3 (11%)	0	100	100
12	t	28/31 (90%)	26 (93%)	2 (7%)	0	100	100
13	W	52/115 (45%)	49 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	w	52/115 (45%)	49 (94%)	3 (6%)	0	100	100
14	X	33/101 (33%)	33 (100%)	0	0	100	100
14	x	33/101 (33%)	33 (100%)	0	0	100	100
15	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
15	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
16	Y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
16	y	28/33 (85%)	26 (93%)	2 (7%)	0	100	100
17	E	66/82 (80%)	58 (88%)	8 (12%)	0	100	100
17	e	66/82 (80%)	57 (86%)	9 (14%)	0	100	100
18	1	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	24	56
18	2	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	24	56
18	3	217/257 (84%)	191 (88%)	26 (12%)	0	100	100
18	4	216/257 (84%)	189 (88%)	26 (12%)	1 (0%)	24	56
18	5	216/257 (84%)	190 (88%)	26 (12%)	0	100	100
18	6	217/257 (84%)	190 (88%)	27 (12%)	0	100	100
18	G	217/257 (84%)	185 (85%)	32 (15%)	0	100	100
18	N	213/257 (83%)	188 (88%)	24 (11%)	1 (0%)	24	56
18	P	216/257 (84%)	188 (87%)	27 (12%)	1 (0%)	24	56
18	Q	217/257 (84%)	184 (85%)	33 (15%)	0	100	100
18	U	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	V	216/257 (84%)	187 (87%)	29 (13%)	0	100	100
18	g	217/257 (84%)	183 (84%)	34 (16%)	0	100	100
18	n	216/257 (84%)	184 (85%)	32 (15%)	0	100	100
18	p	216/257 (84%)	186 (86%)	28 (13%)	2 (1%)	14	45
18	q	217/257 (84%)	186 (86%)	31 (14%)	0	100	100
18	u	216/257 (84%)	183 (85%)	33 (15%)	0	100	100
18	v	216/257 (84%)	186 (86%)	30 (14%)	0	100	100
19	S	234/289 (81%)	201 (86%)	33 (14%)	0	100	100
19	s	234/289 (81%)	202 (86%)	32 (14%)	0	100	100
20	C	448/461 (97%)	429 (96%)	19 (4%)	0	100	100
20	c	448/461 (97%)	430 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	B	501/508 (99%)	472 (94%)	29 (6%)	0	100	100
21	b	501/508 (99%)	470 (94%)	31 (6%)	0	100	100
All	All	9485/11214 (85%)	8533 (90%)	945 (10%)	7 (0%)	49	78

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	2	52	TYR
18	p	136	VAL
18	P	136	VAL
18	1	136	VAL
18	N	136	VAL
18	p	174	PRO
18	4	136	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	175/218 (80%)	175 (100%)	0	100	100
1	r	176/218 (81%)	176 (100%)	0	100	100
2	A	272/289 (94%)	272 (100%)	0	100	100
2	a	272/289 (94%)	272 (100%)	0	100	100
3	D	272/281 (97%)	270 (99%)	2 (1%)	76	77
3	d	272/281 (97%)	270 (99%)	2 (1%)	76	77
4	F	24/37 (65%)	24 (100%)	0	100	100
4	f	24/37 (65%)	24 (100%)	0	100	100
5	H	55/75 (73%)	54 (98%)	1 (2%)	51	66
5	h	55/75 (73%)	54 (98%)	1 (2%)	51	66
6	I	31/34 (91%)	30 (97%)	1 (3%)	34	56
6	i	31/34 (91%)	30 (97%)	1 (3%)	34	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	J	24/42 (57%)	24 (100%)	0	100	100
7	j	24/42 (57%)	24 (100%)	0	100	100
8	K	30/38 (79%)	30 (100%)	0	100	100
8	k	30/38 (79%)	30 (100%)	0	100	100
9	L	34/35 (97%)	34 (100%)	0	100	100
9	l	34/35 (97%)	34 (100%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	100	100
10	m	28/30 (93%)	28 (100%)	0	100	100
11	O	174/223 (78%)	174 (100%)	0	100	100
11	o	174/223 (78%)	174 (100%)	0	100	100
12	T	27/28 (96%)	27 (100%)	0	100	100
12	t	27/28 (96%)	27 (100%)	0	100	100
13	W	42/87 (48%)	42 (100%)	0	100	100
13	w	42/87 (48%)	42 (100%)	0	100	100
14	X	25/67 (37%)	25 (100%)	0	100	100
14	x	25/67 (37%)	25 (100%)	0	100	100
15	Z	52/52 (100%)	52 (100%)	0	100	100
15	z	52/52 (100%)	52 (100%)	0	100	100
16	Y	24/27 (89%)	24 (100%)	0	100	100
16	y	24/27 (89%)	24 (100%)	0	100	100
17	E	60/71 (84%)	60 (100%)	0	100	100
17	e	60/71 (84%)	60 (100%)	0	100	100
18	1	169/194 (87%)	168 (99%)	1 (1%)	78	79
18	2	169/194 (87%)	166 (98%)	3 (2%)	51	66
18	3	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	4	169/194 (87%)	168 (99%)	1 (1%)	78	79
18	5	169/194 (87%)	166 (98%)	3 (2%)	51	66
18	6	170/194 (88%)	169 (99%)	1 (1%)	78	79
18	G	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	N	168/194 (87%)	165 (98%)	3 (2%)	51	66
18	P	169/194 (87%)	166 (98%)	3 (2%)	51	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	U	169/194 (87%)	167 (99%)	2 (1%)	63	71
18	V	169/194 (87%)	168 (99%)	1 (1%)	78	79
18	g	170/194 (88%)	167 (98%)	3 (2%)	51	66
18	n	169/194 (87%)	167 (99%)	2 (1%)	63	71
18	p	169/194 (87%)	166 (98%)	3 (2%)	51	66
18	q	170/194 (88%)	168 (99%)	2 (1%)	63	71
18	u	169/194 (87%)	167 (99%)	2 (1%)	63	71
18	v	169/194 (87%)	168 (99%)	1 (1%)	78	79
19	S	181/217 (83%)	180 (99%)	1 (1%)	78	79
19	s	181/217 (83%)	180 (99%)	1 (1%)	78	79
20	C	352/362 (97%)	352 (100%)	0	100	100
20	c	352/362 (97%)	352 (100%)	0	100	100
21	B	403/407 (99%)	403 (100%)	0	100	100
21	b	403/407 (99%)	403 (100%)	0	100	100
All	All	7618/8732 (87%)	7571 (99%)	47 (1%)	76	79

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	d	210	LEU
3	d	256	ILE
5	h	62	LEU
6	i	6	ILE
5	H	62	LEU
6	I	6	ILE
18	1	130	LEU
18	2	97	ILE
18	2	130	LEU
18	2	199	LYS
18	3	97	ILE
18	3	130	LEU
18	4	130	LEU
18	5	97	ILE
18	5	130	LEU
18	5	199	LYS
18	6	130	LEU

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Mol	Chain	Res	Type
18	v	97	ILE
18	p	97	ILE
18	p	130	LEU
18	p	199	LYS
18	q	53	LEU
18	q	130	LEU
18	V	97	ILE
18	P	97	ILE
18	P	130	LEU
18	P	199	LYS
18	Q	97	ILE
18	Q	130	LEU
18	U	97	ILE
18	U	130	LEU
18	N	97	ILE
18	N	130	LEU
18	N	199	LYS
18	G	97	ILE
18	G	130	LEU
18	u	97	ILE
18	u	130	LEU
18	n	130	LEU
18	n	199	LYS
18	g	37	ARG
18	g	130	LEU
18	g	145	LEU
19	S	154	VAL
3	D	210	LEU
3	D	256	ILE
19	s	154	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	r	55	GLN
1	r	56	ASN
1	r	168	ASN
2	a	113	GLN
2	a	181	ASN
2	a	187	GLN
2	a	195	HIS
2	a	266	ASN

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Mol	Chain	Res	Type
2	a	296	ASN
2	a	322	ASN
3	d	83	ASN
3	d	98	GLN
3	d	129	GLN
3	d	142	ASN
3	d	194	ASN
3	d	197	HIS
3	d	236	ASN
3	d	239	GLN
3	d	255	GLN
3	d	263	ASN
3	d	292	ASN
3	d	350	ASN
4	f	40	GLN
5	h	69	ASN
11	o	266	GLN
2	A	113	GLN
2	A	181	ASN
2	A	187	GLN
2	A	195	HIS
2	A	296	ASN
2	A	303	ASN
2	A	322	ASN
17	E	61	GLN
4	F	40	GLN
4	F	43	GLN
5	H	69	ASN
18	1	140	ASN
18	1	237	ASN
18	3	47	ASN
18	3	120	GLN
18	3	140	ASN
18	3	225	ASN
18	3	236	ASN
18	4	225	ASN
18	4	237	ASN
18	5	140	ASN
18	5	236	ASN
18	6	120	GLN
18	6	236	ASN
18	v	140	ASN

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Mol	Chain	Res	Type
18	v	229	HIS
18	v	232	ASN
18	v	237	ASN
18	p	132	ASN
18	p	225	ASN
18	p	236	ASN
18	q	120	GLN
18	q	229	HIS
18	q	237	ASN
18	V	140	ASN
18	V	229	HIS
18	V	232	ASN
18	V	237	ASN
18	P	132	ASN
18	P	139	GLN
18	P	140	ASN
18	P	236	ASN
18	Q	120	GLN
18	Q	140	ASN
18	Q	161	ASN
18	Q	229	HIS
18	Q	237	ASN
18	U	140	ASN
18	N	120	GLN
18	N	140	ASN
18	N	161	ASN
18	N	229	HIS
18	N	237	ASN
18	G	47	ASN
18	G	120	GLN
18	G	140	ASN
18	G	200	ASN
18	G	229	HIS
18	u	140	ASN
18	n	140	ASN
18	n	225	ASN
18	g	120	GLN
18	g	140	ASN
18	g	200	ASN
18	g	229	HIS
1	R	53	ASN
1	R	55	GLN

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Mol	Chain	Res	Type
1	R	56	ASN
1	R	168	ASN
19	S	263	ASN
19	S	275	ASN
20	C	147	ASN
20	C	310	GLN
20	C	320	GLN
20	C	361	ASN
20	C	386	HIS
21	B	9	HIS
21	B	53	ASN
21	B	87	ASN
21	B	157	HIS
21	B	282	GLN
11	O	266	GLN
3	D	83	ASN
3	D	98	GLN
3	D	129	GLN
3	D	137	ASN
3	D	142	ASN
3	D	194	ASN
3	D	197	HIS
3	D	236	ASN
3	D	239	GLN
3	D	255	GLN
3	D	263	ASN
3	D	292	ASN
3	D	350	ASN
21	b	9	HIS
21	b	53	ASN
21	b	87	ASN
21	b	114	HIS
21	b	157	HIS
21	b	282	GLN
21	b	331	ASN
17	e	23	HIS
20	c	147	ASN
20	c	310	GLN
20	c	320	GLN
20	c	361	ASN
20	c	386	HIS
19	s	127	ASN

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Mol	Chain	Res	Type
19	s	263	ASN
19	s	275	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 552 ligands modelled in this entry, 6 are monoatomic - leaving 546 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	$\#\|Z\| > 2$
22	CLA	b	608	-	69,73,73	1.24	9 (13%)	83,113,113	1.40	8 (9%)
22	CLA	v	302	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	7 (8%)
25	LHG	C	522	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	s	308	-	59,63,73	1.33	9 (15%)	71,101,113	1.40	5 (7%)
23	LUT	2	309	-	42,43,43	0.76	0	51,60,60	1.68	14 (27%)
26	CHL	U	319	-	70,74,74	1.93	20 (28%)	80,114,114	2.63	24 (30%)
27	NEX	r	618	22,1	38,46,46	1.04	2 (5%)	50,70,70	2.49	16 (32%)
26	CHL	6	315	-	70,74,74	1.96	20 (28%)	80,114,114	2.61	25 (31%)
22	CLA	R	309	-	53,57,73	1.41	7 (13%)	62,93,113	1.48	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	606	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	6 (7%)
22	CLA	C	503	-	69,73,73	1.25	9 (13%)	83,113,113	1.35	8 (9%)
25	LHG	5	312	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
34	LMG	b	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	7 (11%)
26	CHL	n	317	-	70,74,74	1.94	21 (30%)	80,114,114	2.69	25 (31%)
23	LUT	V	309	-	42,43,43	0.78	0	51,60,60	1.63	13 (25%)
31	BCR	b	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.46	23 (41%)
26	CHL	Q	311	-	70,74,74	1.92	20 (28%)	80,114,114	2.70	27 (33%)
25	LHG	R	314	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
22	CLA	r	601	27	53,57,73	1.44	10 (18%)	62,93,113	1.51	6 (9%)
22	CLA	G	304	18	68,72,73	1.25	9 (13%)	81,111,113	1.39	10 (12%)
32	SQD	a	413	-	53,54,54	0.95	5 (9%)	62,65,65	1.51	9 (14%)
22	CLA	g	302	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
22	CLA	1	304	-	64,68,73	1.28	10 (15%)	77,107,113	1.36	6 (7%)
26	CHL	2	316	-	70,74,74	1.95	20 (28%)	80,114,114	2.61	23 (28%)
22	CLA	p	307	-	64,68,73	1.29	7 (10%)	77,107,113	1.36	6 (7%)
22	CLA	b	603	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	5 (6%)
26	CHL	3	311	-	70,74,74	1.90	18 (25%)	80,114,114	2.71	27 (33%)
27	NEX	2	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	14 (28%)
25	LHG	D	407	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
23	LUT	5	309	-	42,43,43	0.76	0	51,60,60	1.75	13 (25%)
24	XAT	4	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.07	21 (38%)
22	CLA	p	309	-	52,56,73	1.42	9 (17%)	62,92,113	1.45	5 (8%)
24	XAT	1	311	-	39,47,47	2.54	17 (43%)	54,74,74	12.16	18 (33%)
22	CLA	3	307	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	6 (7%)
22	CLA	B	602	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	9 (10%)
22	CLA	g	306	22	64,68,73	1.31	8 (12%)	77,107,113	1.27	4 (5%)
24	XAT	P	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.98	19 (35%)
22	CLA	c	512	-	69,73,73	1.26	11 (15%)	83,113,113	1.40	8 (9%)
22	CLA	N	306	-	64,68,73	1.29	7 (10%)	77,107,113	1.39	8 (10%)
22	CLA	U	303	-	54,58,73	1.40	9 (16%)	65,95,113	1.43	8 (12%)
25	LHG	b	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.04	2 (4%)
22	CLA	B	611	-	69,73,73	1.26	9 (13%)	83,113,113	1.39	7 (8%)
33	PL9	d	404	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
31	BCR	b	620	-	41,41,41	4.77	24 (58%)	56,56,56	2.21	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CHL	2	318	-	70,74,74	1.90	20 (28%)	80,114,114	2.66	25 (31%)
22	CLA	5	301	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
35	BCT	a	414	-	2,3,3	1.35	0	2,3,3	0.20	0
22	CLA	v	304	-	64,68,73	1.28	8 (12%)	77,107,113	1.39	8 (10%)
22	CLA	C	513	-	69,73,73	1.27	11 (15%)	83,113,113	1.41	8 (9%)
25	LHG	s	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.14	3 (5%)
34	LMG	a	412	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
23	LUT	1	310	-	42,43,43	0.80	0	51,60,60	1.74	14 (27%)
25	LHG	b	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
22	CLA	q	303	-	54,58,73	1.40	9 (16%)	65,95,113	1.49	9 (13%)
22	CLA	c	513	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	6 (7%)
22	CLA	b	615	-	69,73,73	1.22	10 (14%)	83,113,113	1.38	7 (8%)
22	CLA	1	308	-	52,56,73	1.41	9 (17%)	62,92,113	1.44	5 (8%)
22	CLA	Q	303	-	54,58,73	1.41	8 (14%)	65,95,113	1.41	5 (7%)
26	CHL	v	314	-	52,56,74	2.20	16 (30%)	58,92,114	3.11	23 (39%)
31	BCR	c	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	21 (37%)
33	PL9	A	410	-	13,13,55	3.64	7 (53%)	17,17,69	1.47	3 (17%)
22	CLA	5	304	18	69,73,73	1.23	10 (14%)	83,113,113	1.40	8 (9%)
34	LMG	b	624	21	55,55,55	1.17	6 (10%)	63,63,63	1.07	2 (3%)
22	CLA	B	606	-	69,73,73	1.25	9 (13%)	83,113,113	1.37	5 (6%)
22	CLA	U	302	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	4 (4%)
22	CLA	2	304	18	69,73,73	1.22	10 (14%)	83,113,113	1.37	7 (8%)
22	CLA	q	301	-	69,73,73	1.28	10 (14%)	83,113,113	1.30	8 (9%)
22	CLA	G	306	22	64,68,73	1.30	8 (12%)	77,107,113	1.28	4 (5%)
26	CHL	u	314	-	52,56,74	2.20	20 (38%)	58,92,114	3.03	24 (41%)
22	CLA	Q	301	-	69,73,73	1.28	10 (14%)	83,113,113	1.31	8 (9%)
26	CHL	6	314	-	54,58,74	2.28	19 (35%)	59,94,114	2.84	25 (42%)
22	CLA	s	301	19	65,69,73	1.26	11 (16%)	78,108,113	1.37	11 (14%)
24	XAT	Q	309	-	39,47,47	2.60	18 (46%)	54,74,74	11.94	19 (35%)
22	CLA	6	307	22	64,68,73	1.30	8 (12%)	77,107,113	1.33	5 (6%)
25	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
22	CLA	v	303	-	54,58,73	1.41	9 (16%)	65,95,113	1.48	5 (7%)
27	NEX	R	301	22,1	38,46,46	1.03	2 (5%)	50,70,70	2.42	13 (26%)
36	DGD	B	601	21	63,63,67	1.22	7 (11%)	77,77,81	1.07	3 (3%)
31	BCR	C	517	-	41,41,41	4.69	24 (58%)	56,56,56	2.67	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	n	304	18	69,73,73	1.22	10 (14%)	83,113,113	1.40	9 (10%)
22	CLA	V	302	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
22	CLA	G	308	-	52,56,73	1.43	9 (17%)	62,92,113	1.47	6 (9%)
22	CLA	C	506	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	6 (7%)
26	CHL	4	315	-	54,58,74	2.25	19 (35%)	59,94,114	2.84	21 (35%)
23	LUT	p	310	-	42,43,43	0.74	0	51,60,60	1.72	14 (27%)
27	NEX	s	317	19	38,46,46	0.87	1 (2%)	50,70,70	2.39	16 (32%)
22	CLA	C	511	-	69,73,73	1.23	10 (14%)	83,113,113	1.39	11 (13%)
26	CHL	U	317	-	70,74,74	1.88	19 (27%)	80,114,114	2.65	22 (27%)
26	CHL	3	314	-	70,74,74	1.97	20 (28%)	80,114,114	2.59	23 (28%)
22	CLA	c	502	-	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
36	DGD	C	520	-	63,63,67	1.22	6 (9%)	77,77,81	1.16	4 (5%)
26	CHL	U	315	-	70,74,74	1.87	18 (25%)	80,114,114	2.75	26 (32%)
22	CLA	C	508	-	69,73,73	1.26	10 (14%)	83,113,113	1.38	7 (8%)
31	BCR	d	403	3	41,41,41	4.76	24 (58%)	56,56,56	2.26	23 (41%)
24	XAT	p	312	-	39,47,47	2.59	18 (46%)	54,74,74	11.83	18 (33%)
24	XAT	r	612	-	39,47,47	2.52	17 (43%)	54,74,74	11.45	25 (46%)
26	CHL	g	311	-	70,74,74	1.90	19 (27%)	80,114,114	2.66	25 (31%)
22	CLA	P	303	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	5 (6%)
26	CHL	n	318	-	70,74,74	1.96	20 (28%)	80,114,114	2.59	26 (32%)
37	HEM	E	101	4,17	50,50,50	1.43	6 (12%)	66,82,82	1.21	4 (6%)
36	DGD	J	101	-	61,61,67	1.26	6 (9%)	75,75,81	1.17	3 (4%)
25	LHG	V	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.10	2 (3%)
25	LHG	d	406	3	48,48,48	0.90	4 (8%)	51,54,54	1.07	3 (5%)
25	LHG	6	311	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
31	BCR	t	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
26	CHL	N	313	-	70,74,74	1.91	19 (27%)	80,114,114	2.63	25 (31%)
30	PHO	D	401	-	58,69,69	1.98	9 (15%)	56,99,99	1.79	9 (16%)
22	CLA	B	603	-	69,73,73	1.24	9 (13%)	83,113,113	1.34	5 (6%)
22	CLA	r	609	26	64,68,73	1.30	7 (10%)	77,107,113	1.46	9 (11%)
22	CLA	b	607	-	69,73,73	1.25	9 (13%)	83,113,113	1.42	7 (8%)
22	CLA	r	610	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	4 (6%)
22	CLA	n	303	-	54,58,73	1.40	9 (16%)	65,95,113	1.43	8 (12%)
31	BCR	T	101	-	41,41,41	4.79	24 (58%)	56,56,56	2.38	22 (39%)
34	LMG	C	502	-	51,51,55	1.15	4 (7%)	59,59,63	1.16	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CHL	R	317	-	65,69,74	2.02	21 (32%)	74,108,114	2.57	23 (31%)
25	LHG	P	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
22	CLA	s	302	-	49,53,73	1.50	8 (16%)	59,89,113	1.49	6 (10%)
26	CHL	S	313	-	50,54,74	2.31	18 (36%)	56,90,114	3.06	23 (41%)
24	XAT	v	311	-	39,47,47	2.56	18 (46%)	54,74,74	12.01	19 (35%)
26	CHL	p	320	-	70,74,74	1.88	19 (27%)	80,114,114	2.69	24 (30%)
22	CLA	4	306	-	64,68,73	1.32	9 (14%)	77,107,113	1.33	7 (9%)
22	CLA	U	305	-	64,68,73	1.29	10 (15%)	77,107,113	1.31	4 (5%)
26	CHL	4	317	-	70,74,74	1.89	20 (28%)	80,114,114	2.67	25 (31%)
36	DGD	b	601	21	63,63,67	1.23	7 (11%)	77,77,81	1.06	3 (3%)
22	CLA	A	406	-	54,58,73	1.41	10 (18%)	65,95,113	1.44	6 (9%)
22	CLA	C	514	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	5 (6%)
23	LUT	u	309	-	42,43,43	0.75	0	51,60,60	1.52	10 (19%)
22	CLA	6	304	-	54,58,73	1.41	10 (18%)	65,95,113	1.43	9 (13%)
22	CLA	5	303	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	6 (9%)
26	CHL	5	317	-	70,74,74	1.87	18 (25%)	80,114,114	2.72	25 (31%)
26	CHL	n	316	-	70,74,74	1.92	20 (28%)	80,114,114	2.63	23 (28%)
22	CLA	4	304	-	64,68,73	1.28	10 (15%)	77,107,113	1.36	5 (6%)
22	CLA	B	617	-	69,73,73	1.25	9 (13%)	83,113,113	1.37	8 (9%)
22	CLA	b	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	8 (9%)
22	CLA	5	302	-	69,73,73	1.26	8 (11%)	83,113,113	1.32	6 (7%)
22	CLA	b	609	-	69,73,73	1.25	11 (15%)	83,113,113	1.32	7 (8%)
22	CLA	q	306	22	64,68,73	1.29	6 (9%)	77,107,113	1.31	4 (5%)
24	XAT	u	311	-	39,47,47	2.54	18 (46%)	54,74,74	11.77	18 (33%)
22	CLA	U	304	-	64,68,73	1.28	9 (14%)	77,107,113	1.39	8 (10%)
26	CHL	u	318	-	70,74,74	1.87	18 (25%)	80,114,114	2.66	26 (32%)
32	SQD	L	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
22	CLA	b	602	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	6 (7%)
31	BCR	B	618	-	41,41,41	4.74	24 (58%)	56,56,56	2.45	22 (39%)
24	XAT	2	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
22	CLA	v	301	-	69,73,73	1.26	10 (14%)	83,113,113	1.26	5 (6%)
22	CLA	b	612	-	69,73,73	1.25	10 (14%)	83,113,113	1.42	7 (8%)
22	CLA	C	515	-	69,73,73	1.24	9 (13%)	83,113,113	1.38	7 (8%)
23	LUT	S	311	-	42,43,43	0.77	0	51,60,60	1.64	17 (33%)
22	CLA	B	607	-	69,73,73	1.25	9 (13%)	83,113,113	1.41	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	615	-	69,73,73	1.21	10 (14%)	83,113,113	1.38	7 (8%)
25	LHG	l	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	3 (5%)
25	LHG	4	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.07	2 (3%)
22	CLA	B	612	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	7 (8%)
22	CLA	R	304	-	64,68,73	1.29	7 (10%)	77,107,113	1.36	4 (5%)
26	CHL	U	316	18	70,74,74	1.88	20 (28%)	80,114,114	2.80	27 (33%)
22	CLA	P	309	-	52,56,73	1.43	9 (17%)	62,92,113	1.45	5 (8%)
26	CHL	1	315	-	54,58,74	2.22	19 (35%)	59,94,114	2.87	21 (35%)
23	LUT	U	310	-	42,43,43	0.79	0	51,60,60	1.61	9 (17%)
22	CLA	c	514	-	69,73,73	1.24	10 (14%)	83,113,113	1.37	8 (9%)
22	CLA	r	605	-	62,66,73	1.30	9 (14%)	74,104,113	1.42	5 (6%)
22	CLA	x	201	14	69,73,73	1.24	9 (13%)	83,113,113	1.38	8 (9%)
22	CLA	S	301	19	65,69,73	1.25	9 (13%)	78,108,113	1.36	10 (12%)
26	CHL	Q	312	-	52,56,74	2.27	18 (34%)	58,92,114	3.01	24 (41%)
23	LUT	4	309	-	42,43,43	0.73	0	51,60,60	1.60	11 (21%)
31	BCR	C	518	-	41,41,41	4.75	24 (58%)	56,56,56	2.29	19 (33%)
26	CHL	P	319	-	70,74,74	1.89	20 (28%)	80,114,114	2.67	23 (28%)
22	CLA	G	305	22	64,68,73	1.27	9 (14%)	77,107,113	1.44	6 (7%)
26	CHL	1	317	18	70,74,74	1.91	20 (28%)	80,114,114	2.78	28 (35%)
22	CLA	X	202	14	69,73,73	1.23	9 (13%)	83,113,113	1.36	8 (9%)
22	CLA	S	308	-	59,63,73	1.34	9 (15%)	71,101,113	1.39	5 (7%)
22	CLA	R	307	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	4 (4%)
22	CLA	1	306	-	64,68,73	1.30	10 (15%)	77,107,113	1.36	8 (10%)
22	CLA	b	613	-	69,73,73	1.27	12 (17%)	83,113,113	1.34	10 (12%)
23	LUT	r	611	1	42,43,43	0.75	0	51,60,60	1.66	10 (19%)
25	LHG	n	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.03	2 (3%)
23	LUT	P	311	-	42,43,43	0.76	0	51,60,60	1.58	12 (23%)
22	CLA	3	302	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
22	CLA	N	308	-	52,56,73	1.44	9 (17%)	62,92,113	1.41	5 (8%)
22	CLA	r	604	-	52,56,73	1.43	8 (15%)	62,92,113	1.51	6 (9%)
23	LUT	n	309	-	42,43,43	0.74	0	51,60,60	1.62	11 (21%)
26	CHL	q	313	-	54,58,74	2.17	18 (33%)	59,94,114	2.96	22 (37%)
22	CLA	u	307	-	69,73,73	1.22	9 (13%)	83,113,113	1.37	7 (8%)
26	CHL	Q	313	-	54,58,74	2.19	19 (35%)	59,94,114	2.94	23 (38%)
26	CHL	S	315	19	62,66,74	2.15	19 (30%)	70,104,114	2.67	23 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	611	-	69,73,73	1.27	9 (13%)	83,113,113	1.39	7 (8%)
34	LMG	d	407	3	46,46,55	1.26	6 (13%)	54,54,63	1.01	2 (3%)
22	CLA	3	306	22	64,68,73	1.29	8 (12%)	77,107,113	1.33	5 (6%)
23	LUT	s	311	-	42,43,43	0.76	0	51,60,60	1.65	16 (31%)
22	CLA	2	307	-	64,68,73	1.28	9 (14%)	77,107,113	1.39	6 (7%)
22	CLA	4	307	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	8 (9%)
22	CLA	4	308	-	52,56,73	1.42	9 (17%)	62,92,113	1.46	5 (8%)
25	LHG	q	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.05	2 (3%)
26	CHL	q	312	-	52,56,74	2.34	20 (38%)	58,92,114	3.08	24 (41%)
26	CHL	u	317	18	70,74,74	1.87	20 (28%)	80,114,114	2.77	27 (33%)
22	CLA	c	505	-	69,73,73	1.23	9 (13%)	83,113,113	1.36	6 (7%)
22	CLA	B	614	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	8 (9%)
25	LHG	Q	310	-	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
26	CHL	5	318	-	70,74,74	1.90	20 (28%)	80,114,114	2.65	25 (31%)
22	CLA	G	302	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
26	CHL	u	315	-	54,58,74	2.13	18 (33%)	59,94,114	2.91	23 (38%)
30	PHO	A	407	-	58,69,69	2.02	10 (17%)	56,99,99	1.63	9 (16%)
22	CLA	6	303	-	69,73,73	1.24	8 (11%)	83,113,113	1.26	5 (6%)
22	CLA	R	306	-	62,66,73	1.30	9 (14%)	74,104,113	1.42	5 (6%)
36	DGD	c	519	-	61,61,67	1.25	6 (9%)	75,75,81	1.17	3 (4%)
22	CLA	B	609	-	69,73,73	1.25	11 (15%)	83,113,113	1.32	7 (8%)
27	NEX	v	319	-	38,46,46	0.89	1 (2%)	50,70,70	2.45	14 (28%)
22	CLA	4	303	-	54,58,73	1.41	9 (16%)	65,95,113	1.43	9 (13%)
26	CHL	n	313	18	70,74,74	1.94	18 (25%)	80,114,114	2.66	27 (33%)
31	BCR	c	515	-	41,41,41	4.70	24 (58%)	56,56,56	2.67	23 (41%)
22	CLA	N	305	18	64,68,73	1.25	9 (14%)	77,107,113	1.80	12 (15%)
26	CHL	q	311	-	70,74,74	1.90	19 (27%)	80,114,114	2.68	26 (32%)
26	CHL	N	314	-	52,56,74	2.31	19 (36%)	58,92,114	3.03	23 (39%)
22	CLA	s	305	-	59,63,73	1.35	9 (15%)	71,101,113	1.37	6 (8%)
27	NEX	U	318	-	38,46,46	0.96	1 (2%)	50,70,70	2.38	12 (24%)
23	LUT	R	312	-	42,43,43	0.73	0	51,60,60	1.52	11 (21%)
22	CLA	c	509	-	69,73,73	1.28	12 (17%)	83,113,113	1.44	9 (10%)
26	CHL	P	317	-	70,74,74	1.95	21 (30%)	80,114,114	2.66	27 (33%)
26	CHL	r	614	-	70,74,74	1.89	17 (24%)	80,114,114	2.68	25 (31%)
22	CLA	5	305	18	64,68,73	1.26	9 (14%)	77,107,113	1.92	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	p	302	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
22	CLA	6	305	18	68,72,73	1.25	9 (13%)	81,111,113	1.36	10 (12%)
26	CHL	v	317	18	70,74,74	1.92	19 (27%)	80,114,114	2.78	30 (37%)
22	CLA	B	605	21	69,73,73	1.25	9 (13%)	83,113,113	1.66	11 (13%)
22	CLA	N	302	-	69,73,73	1.28	9 (13%)	83,113,113	1.30	6 (7%)
32	SQD	l	102	9	53,54,54	0.93	4 (7%)	62,65,65	1.80	12 (19%)
22	CLA	A	404	-	69,73,73	1.26	11 (15%)	83,113,113	1.44	9 (10%)
26	CHL	p	317	-	70,74,74	1.93	19 (27%)	80,114,114	2.65	24 (30%)
22	CLA	P	308	-	64,68,73	1.29	10 (15%)	77,107,113	1.37	5 (6%)
22	CLA	p	306	18	64,68,73	1.25	7 (10%)	77,107,113	1.97	15 (19%)
22	CLA	b	617	21	69,73,73	1.29	10 (14%)	83,113,113	1.49	12 (14%)
22	CLA	g	303	-	54,58,73	1.42	9 (16%)	65,95,113	1.51	7 (10%)
26	CHL	1	313	-	70,74,74	1.96	20 (28%)	80,114,114	2.60	26 (32%)
25	LHG	A	413	2	42,42,48	0.93	3 (7%)	45,48,54	1.11	2 (4%)
32	SQD	m	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.75	11 (22%)
22	CLA	Q	308	-	52,56,73	1.43	8 (15%)	62,92,113	1.42	6 (9%)
22	CLA	A	408	-	64,68,73	1.29	12 (18%)	77,107,113	1.49	9 (11%)
26	CHL	G	313	-	54,58,74	2.18	18 (33%)	59,94,114	2.96	21 (35%)
27	NEX	r	617	-	38,46,46	1.01	3 (7%)	50,70,70	2.42	17 (34%)
22	CLA	P	305	18	69,73,73	1.22	8 (11%)	83,113,113	1.33	6 (7%)
25	LHG	G	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.10	2 (3%)
22	CLA	P	306	18	64,68,73	1.24	7 (10%)	77,107,113	1.88	11 (14%)
22	CLA	n	301	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
26	CHL	v	313	-	70,74,74	1.94	20 (28%)	80,114,114	2.67	26 (32%)
22	CLA	5	308	-	52,56,73	1.42	8 (15%)	62,92,113	1.43	5 (8%)
24	XAT	q	309	-	39,47,47	2.58	18 (46%)	54,74,74	11.94	18 (33%)
22	CLA	a	408	-	64,68,73	1.29	12 (18%)	77,107,113	1.50	9 (11%)
22	CLA	C	510	-	69,73,73	1.28	12 (17%)	83,113,113	1.44	9 (10%)
22	CLA	u	304	-	64,68,73	1.29	11 (17%)	77,107,113	1.39	8 (10%)
22	CLA	g	305	22	64,68,73	1.28	8 (12%)	77,107,113	1.42	9 (11%)
34	LMG	B	621	-	51,51,55	1.18	6 (11%)	59,59,63	1.44	6 (10%)
34	LMG	D	408	3	46,46,55	1.26	6 (13%)	54,54,63	1.02	2 (3%)
25	LHG	C	524	-	48,48,48	0.90	4 (8%)	51,54,54	1.13	2 (3%)
22	CLA	N	307	-	64,68,73	1.28	10 (15%)	77,107,113	1.38	5 (6%)
26	CHL	6	301	-	70,74,74	1.92	20 (28%)	80,114,114	2.67	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	BCR	x	202	-	41,41,41	4.78	24 (58%)	56,56,56	2.27	18 (32%)
22	CLA	p	303	-	69,73,73	1.25	9 (13%)	83,113,113	1.36	6 (7%)
26	CHL	S	316	-	50,54,74	2.35	19 (38%)	56,90,114	2.98	23 (41%)
22	CLA	3	304	18	68,72,73	1.26	10 (14%)	81,111,113	1.37	10 (12%)
26	CHL	s	313	-	50,54,74	2.33	18 (36%)	56,90,114	3.04	23 (41%)
25	LHG	D	406	3	45,45,48	0.92	4 (8%)	48,51,54	1.08	2 (4%)
26	CHL	q	315	-	65,69,74	2.01	20 (30%)	74,108,114	2.74	26 (35%)
30	PHO	d	401	-	58,69,69	1.98	9 (15%)	56,99,99	1.80	9 (16%)
25	LHG	B	622	-	46,46,48	0.91	4 (8%)	49,52,54	1.06	2 (4%)
25	LHG	p	313	-	48,48,48	0.90	4 (8%)	51,54,54	1.04	2 (3%)
26	CHL	Q	315	18	70,74,74	1.88	18 (25%)	80,114,114	2.70	25 (31%)
22	CLA	P	302	-	69,73,73	1.24	10 (14%)	83,113,113	1.34	8 (9%)
26	CHL	Q	314	-	70,74,74	1.94	19 (27%)	80,114,114	2.59	25 (31%)
22	CLA	q	308	-	52,56,73	1.42	8 (15%)	62,92,113	1.46	6 (9%)
22	CLA	S	304	19	49,53,73	1.48	8 (16%)	59,89,113	1.43	4 (6%)
26	CHL	s	315	19	62,66,74	2.14	19 (30%)	70,104,114	2.68	23 (32%)
22	CLA	n	302	-	69,73,73	1.28	9 (13%)	83,113,113	1.30	6 (7%)
22	CLA	2	302	-	69,73,73	1.27	9 (13%)	83,113,113	1.30	6 (7%)
26	CHL	u	316	-	70,74,74	1.91	18 (25%)	80,114,114	2.76	30 (37%)
25	LHG	u	312	-	48,48,48	0.88	4 (8%)	51,54,54	1.13	3 (5%)
26	CHL	U	314	-	54,58,74	2.15	19 (35%)	59,94,114	2.95	23 (38%)
25	LHG	c	521	-	48,48,48	0.90	4 (8%)	51,54,54	1.08	2 (3%)
26	CHL	Q	316	-	65,69,74	2.00	20 (30%)	74,108,114	2.72	25 (33%)
27	NEX	P	301	18	38,46,46	0.94	1 (2%)	50,70,70	2.35	18 (36%)
22	CLA	U	307	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	6 (7%)
22	CLA	q	302	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	5 (6%)
37	HEM	e	101	4,17	50,50,50	1.44	6 (12%)	66,82,82	1.20	4 (6%)
22	CLA	g	301	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	7 (8%)
23	LUT	1	309	-	42,43,43	0.72	0	51,60,60	1.57	10 (19%)
25	LHG	2	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
26	CHL	6	317	-	65,69,74	1.99	19 (29%)	74,108,114	2.80	25 (33%)
22	CLA	G	303	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	7 (10%)
24	XAT	g	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.71	20 (37%)
25	LHG	v	312	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
22	CLA	B	610	-	69,73,73	1.23	10 (14%)	83,113,113	1.35	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	V	307	-	69,73,73	1.24	10 (14%)	83,113,113	1.36	6 (7%)
31	BCR	X	201	-	41,41,41	4.79	24 (58%)	56,56,56	2.26	17 (30%)
25	LHG	3	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.11	2 (3%)
22	CLA	S	305	-	59,63,73	1.35	9 (15%)	71,101,113	1.37	5 (7%)
26	CHL	V	315	-	54,58,74	2.27	19 (35%)	59,94,114	2.87	23 (38%)
27	NEX	V	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.46	16 (32%)
22	CLA	v	308	-	52,56,73	1.42	8 (15%)	62,92,113	1.43	4 (6%)
26	CHL	g	315	18	70,74,74	1.89	18 (25%)	80,114,114	2.69	25 (31%)
22	CLA	3	301	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	8 (9%)
22	CLA	S	309	-	53,57,73	1.42	10 (18%)	62,93,113	1.42	4 (6%)
26	CHL	3	312	-	52,56,74	2.35	20 (38%)	58,92,114	3.02	26 (44%)
22	CLA	G	301	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	7 (8%)
22	CLA	b	616	21	69,73,73	1.24	8 (11%)	83,113,113	1.38	8 (9%)
27	NEX	u	320	-	38,46,46	0.89	2 (5%)	50,70,70	2.32	18 (36%)
22	CLA	S	302	-	49,53,73	1.51	8 (16%)	59,89,113	1.49	6 (10%)
24	XAT	U	311	-	39,47,47	2.51	17 (43%)	54,74,74	11.93	20 (37%)
26	CHL	V	317	18	70,74,74	1.92	19 (27%)	80,114,114	2.78	29 (36%)
22	CLA	U	306	-	64,68,73	1.31	10 (15%)	77,107,113	1.34	6 (7%)
26	CHL	g	312	-	52,56,74	2.25	18 (34%)	58,92,114	3.08	24 (41%)
31	BCR	a	409	-	41,41,41	4.73	24 (58%)	56,56,56	2.22	22 (39%)
27	NEX	5	319	-	38,46,46	0.91	1 (2%)	50,70,70	2.43	16 (32%)
22	CLA	4	305	-	64,68,73	1.29	9 (14%)	77,107,113	1.34	7 (9%)
22	CLA	v	306	-	64,68,73	1.30	9 (14%)	77,107,113	1.35	7 (9%)
22	CLA	s	304	19	49,53,73	1.47	8 (16%)	59,89,113	1.44	4 (6%)
33	PL9	a	411	-	13,13,55	3.63	7 (53%)	17,17,69	1.48	3 (17%)
26	CHL	R	315	-	70,74,74	1.89	16 (22%)	80,114,114	2.67	26 (32%)
31	BCR	C	516	-	41,41,41	4.76	24 (58%)	56,56,56	2.30	20 (35%)
23	LUT	n	310	-	42,43,43	0.79	0	51,60,60	1.75	14 (27%)
24	XAT	6	310	-	39,47,47	2.56	18 (46%)	54,74,74	11.74	17 (31%)
32	SQD	M	101	-	41,42,54	1.06	5 (12%)	50,53,65	1.74	11 (22%)
31	BCR	k	101	-	41,41,41	4.73	25 (60%)	56,56,56	2.52	19 (33%)
22	CLA	1	303	-	54,58,73	1.40	10 (18%)	65,95,113	1.46	9 (13%)
26	CHL	v	316	-	70,74,74	1.89	19 (27%)	80,114,114	2.68	26 (32%)
22	CLA	C	505	-	69,73,73	1.25	11 (15%)	83,113,113	1.34	6 (7%)
22	CLA	V	301	-	69,73,73	1.27	10 (14%)	83,113,113	1.24	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	405	-	69,73,73	1.27	10 (14%)	83,113,113	1.39	9 (10%)
36	DGD	C	519	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
22	CLA	U	308	-	52,56,73	1.42	8 (15%)	62,92,113	1.46	5 (8%)
22	CLA	3	303	-	54,58,73	1.41	8 (14%)	65,95,113	1.47	8 (12%)
24	XAT	R	313	-	39,47,47	2.54	17 (43%)	54,74,74	11.48	22 (40%)
22	CLA	u	303	-	54,58,73	1.41	9 (16%)	65,95,113	1.47	8 (12%)
22	CLA	V	306	-	64,68,73	1.32	9 (14%)	77,107,113	1.34	7 (9%)
26	CHL	5	314	-	52,56,74	2.33	20 (38%)	58,92,114	3.05	23 (39%)
22	CLA	a	405	-	69,73,73	1.27	10 (14%)	83,113,113	1.39	7 (8%)
22	CLA	C	509	20	69,73,73	1.23	10 (14%)	83,113,113	1.43	10 (12%)
25	LHG	B	623	21	48,48,48	0.90	4 (8%)	51,54,54	1.06	2 (3%)
22	CLA	q	305	22	64,68,73	1.29	9 (14%)	77,107,113	1.34	4 (5%)
34	LMG	w	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)
26	CHL	s	316	-	50,54,74	2.35	19 (38%)	56,90,114	2.99	23 (41%)
34	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.07	2 (3%)
22	CLA	Q	305	22	64,68,73	1.29	9 (14%)	77,107,113	1.30	5 (6%)
22	CLA	S	307	-	53,57,73	1.42	8 (15%)	62,93,113	1.49	8 (12%)
24	XAT	3	309	-	39,47,47	2.56	18 (46%)	54,74,74	11.80	17 (31%)
24	XAT	G	309	-	39,47,47	2.53	17 (43%)	54,74,74	11.82	19 (35%)
22	CLA	1	301	-	69,73,73	1.26	10 (14%)	83,113,113	1.31	7 (8%)
22	CLA	V	304	-	64,68,73	1.28	8 (12%)	77,107,113	1.38	9 (11%)
23	LUT	s	310	19	42,43,43	0.79	0	51,60,60	1.72	13 (25%)
26	CHL	5	316	-	70,74,74	1.95	19 (27%)	80,114,114	2.60	24 (30%)
26	CHL	N	316	-	70,74,74	1.87	19 (27%)	80,114,114	2.71	24 (30%)
32	SQD	C	501	-	49,50,54	1.00	5 (10%)	58,61,65	1.75	11 (18%)
22	CLA	s	307	-	53,57,73	1.42	9 (16%)	62,93,113	1.49	8 (12%)
22	CLA	D	403	3	69,73,73	1.24	10 (14%)	83,113,113	1.28	6 (7%)
22	CLA	S	303	19	54,58,73	1.40	9 (16%)	65,95,113	1.47	8 (12%)
25	LHG	a	415	2	42,42,48	0.93	3 (7%)	45,48,54	1.10	2 (4%)
22	CLA	q	304	18	68,72,73	1.25	9 (13%)	81,111,113	1.47	9 (11%)
22	CLA	s	309	-	53,57,73	1.39	9 (16%)	62,93,113	1.41	4 (6%)
26	CHL	v	315	-	54,58,74	2.22	18 (33%)	59,94,114	2.89	24 (40%)
22	CLA	c	507	-	69,73,73	1.27	10 (14%)	83,113,113	1.39	8 (9%)
22	CLA	2	305	18	64,68,73	1.25	8 (12%)	77,107,113	1.91	13 (16%)
22	CLA	Q	304	18	68,72,73	1.25	9 (13%)	81,111,113	1.40	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	NEX	n	319	-	38,46,46	0.96	2 (5%)	50,70,70	2.64	17 (34%)
26	CHL	P	314	18	70,74,74	1.98	19 (27%)	80,114,114	2.64	25 (31%)
34	LMG	A	411	-	40,40,55	1.30	6 (15%)	48,48,63	1.16	2 (4%)
23	LUT	u	310	-	42,43,43	0.78	0	51,60,60	1.60	10 (19%)
22	CLA	a	404	-	69,73,73	1.26	11 (15%)	83,113,113	1.45	9 (10%)
26	CHL	n	314	-	52,56,74	2.32	20 (38%)	58,92,114	3.02	23 (39%)
23	LUT	P	310	-	42,43,43	0.73	0	51,60,60	1.67	14 (27%)
22	CLA	n	307	-	64,68,73	1.29	10 (15%)	77,107,113	1.37	5 (6%)
26	CHL	G	312	-	52,56,74	2.31	21 (40%)	58,92,114	3.10	23 (39%)
26	CHL	P	316	-	54,58,74	2.23	20 (37%)	59,94,114	2.92	23 (38%)
26	CHL	V	313	-	70,74,74	1.96	19 (27%)	80,114,114	2.64	24 (30%)
22	CLA	R	311	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	4 (6%)
22	CLA	u	301	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
22	CLA	b	604	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	8 (9%)
22	CLA	n	305	18	64,68,73	1.26	7 (10%)	77,107,113	1.96	15 (19%)
22	CLA	a	406	-	54,58,73	1.42	10 (18%)	65,95,113	1.44	7 (10%)
22	CLA	r	603	-	64,68,73	1.29	9 (14%)	77,107,113	1.36	4 (5%)
26	CHL	6	312	-	70,74,74	1.91	19 (27%)	80,114,114	2.72	27 (33%)
26	CHL	g	316	-	65,69,74	1.97	19 (29%)	74,108,114	2.73	27 (36%)
25	LHG	r	613	-	41,41,48	0.96	3 (7%)	44,47,54	1.09	2 (4%)
32	SQD	A	412	-	53,54,54	0.95	5 (9%)	62,65,65	1.50	10 (16%)
26	CHL	P	318	-	70,74,74	1.87	19 (27%)	80,114,114	2.68	24 (30%)
26	CHL	1	314	22	52,56,74	2.24	19 (36%)	58,92,114	3.09	23 (39%)
36	DGD	c	518	-	63,63,67	1.22	6 (9%)	77,77,81	1.15	5 (6%)
26	CHL	r	619	1	52,56,74	2.19	20 (38%)	58,92,114	3.10	23 (39%)
22	CLA	r	607	1	53,57,73	1.40	8 (15%)	62,93,113	1.53	8 (12%)
25	LHG	g	310	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
31	BCR	z	101	-	41,41,41	4.76	24 (58%)	56,56,56	2.32	20 (35%)
27	NEX	N	318	-	38,46,46	0.93	2 (5%)	50,70,70	2.40	17 (34%)
24	XAT	N	311	-	39,47,47	2.53	17 (43%)	54,74,74	11.91	18 (33%)
22	CLA	b	610	-	69,73,73	1.23	10 (14%)	83,113,113	1.33	7 (8%)
26	CHL	p	314	18	70,74,74	1.95	18 (25%)	80,114,114	2.67	26 (32%)
33	PL9	D	405	-	55,55,55	1.54	6 (10%)	68,69,69	1.68	18 (26%)
25	LHG	1	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
34	LMG	W	201	-	48,48,55	1.23	6 (12%)	56,56,63	1.12	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	s	303	19	54,58,73	1.40	9 (16%)	65,95,113	1.47	7 (10%)
35	BCT	D	402	-	2,3,3	1.35	0	2,3,3	0.19	0
31	BCR	K	101	-	41,41,41	4.72	24 (58%)	56,56,56	2.53	19 (33%)
31	BCR	B	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.26	22 (39%)
22	CLA	P	307	-	64,68,73	1.28	7 (10%)	77,107,113	1.36	8 (10%)
22	CLA	R	303	-	64,68,73	1.30	9 (14%)	77,107,113	1.35	7 (9%)
26	CHL	p	316	-	54,58,74	2.22	19 (35%)	59,94,114	2.96	25 (42%)
22	CLA	s	306	-	60,64,73	1.35	10 (16%)	72,102,113	1.40	9 (12%)
26	CHL	g	314	-	70,74,74	1.97	19 (27%)	80,114,114	2.63	26 (32%)
24	XAT	5	311	-	39,47,47	2.58	18 (46%)	54,74,74	11.93	19 (35%)
26	CHL	S	314	-	50,54,74	2.26	19 (38%)	56,90,114	3.12	21 (37%)
31	BCR	D	404	3	41,41,41	4.77	24 (58%)	56,56,56	2.26	23 (41%)
26	CHL	v	318	-	70,74,74	1.93	19 (27%)	80,114,114	2.59	24 (30%)
22	CLA	1	305	-	64,68,73	1.28	8 (12%)	77,107,113	1.37	7 (9%)
23	LUT	U	309	-	42,43,43	0.74	0	51,60,60	1.54	10 (19%)
22	CLA	n	308	-	52,56,73	1.45	8 (15%)	62,92,113	1.52	8 (12%)
26	CHL	G	316	-	65,69,74	1.96	20 (30%)	74,108,114	2.76	25 (33%)
22	CLA	R	308	1	53,57,73	1.39	7 (13%)	62,93,113	1.53	6 (9%)
22	CLA	5	306	-	64,68,73	1.28	8 (12%)	77,107,113	1.39	7 (9%)
26	CHL	2	317	-	70,74,74	1.87	17 (24%)	80,114,114	2.71	26 (32%)
26	CHL	G	314	-	70,74,74	1.95	20 (28%)	80,114,114	2.57	24 (30%)
22	CLA	V	303	-	54,58,73	1.41	10 (18%)	65,95,113	1.51	8 (12%)
22	CLA	G	307	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	5 (6%)
22	CLA	v	305	-	64,68,73	1.29	8 (12%)	77,107,113	1.33	5 (6%)
23	LUT	5	310	-	42,43,43	0.77	0	51,60,60	1.64	12 (23%)
26	CHL	r	616	-	65,69,74	2.03	20 (30%)	74,108,114	2.56	22 (29%)
22	CLA	B	608	-	69,73,73	1.23	8 (11%)	83,113,113	1.39	8 (9%)
25	LHG	c	523	-	48,48,48	0.90	4 (8%)	51,54,54	1.12	2 (3%)
27	NEX	u	319	-	38,46,46	0.93	1 (2%)	50,70,70	2.45	18 (36%)
22	CLA	B	613	-	69,73,73	1.26	12 (17%)	83,113,113	1.34	9 (10%)
22	CLA	U	301	-	69,73,73	1.24	10 (14%)	83,113,113	1.31	8 (9%)
22	CLA	3	305	22	64,68,73	1.28	9 (14%)	77,107,113	1.42	8 (10%)
31	BCR	A	409	-	41,41,41	4.74	24 (58%)	56,56,56	2.25	22 (39%)
22	CLA	c	510	-	69,73,73	1.22	9 (13%)	83,113,113	1.38	9 (10%)
22	CLA	C	507	-	69,73,73	1.23	10 (14%)	83,113,113	1.49	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	P	304	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	6 (9%)
26	CHL	V	314	-	52,56,74	2.27	20 (38%)	58,92,114	3.09	24 (41%)
23	LUT	p	311	-	42,43,43	0.76	0	51,60,60	1.54	12 (23%)
22	CLA	d	402	3	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
26	CHL	q	314	18	70,74,74	1.89	19 (27%)	80,114,114	2.72	24 (30%)
26	CHL	p	318	-	70,74,74	1.86	19 (27%)	80,114,114	2.72	23 (28%)
26	CHL	n	315	-	54,58,74	2.21	19 (35%)	59,94,114	2.95	23 (38%)
23	LUT	N	310	-	42,43,43	0.78	0	51,60,60	1.69	15 (29%)
26	CHL	V	316	-	70,74,74	1.94	19 (27%)	80,114,114	2.60	25 (31%)
22	CLA	6	309	-	52,56,73	1.42	8 (15%)	62,92,113	1.41	5 (8%)
26	CHL	N	315	-	54,58,74	2.16	19 (35%)	59,94,114	2.97	23 (38%)
22	CLA	c	503	-	69,73,73	1.27	11 (15%)	83,113,113	1.47	8 (9%)
26	CHL	6	316	18	70,74,74	1.90	20 (28%)	80,114,114	2.72	23 (28%)
22	CLA	5	307	-	64,68,73	1.28	10 (15%)	77,107,113	1.38	6 (7%)
22	CLA	g	308	-	52,56,73	1.43	9 (17%)	62,92,113	1.45	6 (9%)
22	CLA	2	301	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	9 (10%)
22	CLA	p	305	18	69,73,73	1.22	8 (11%)	83,113,113	1.34	6 (7%)
22	CLA	4	301	-	69,73,73	1.26	10 (14%)	83,113,113	1.33	8 (9%)
23	LUT	N	309	-	42,43,43	0.72	0	51,60,60	1.55	11 (21%)
26	CHL	u	313	-	70,74,74	1.94	20 (28%)	80,114,114	2.59	26 (32%)
22	CLA	q	307	-	69,73,73	1.23	9 (13%)	83,113,113	1.36	6 (7%)
26	CHL	4	314	-	52,56,74	2.19	19 (36%)	58,92,114	3.15	24 (41%)
36	DGD	a	416	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
22	CLA	Q	307	-	69,73,73	1.23	9 (13%)	83,113,113	1.33	6 (7%)
26	CHL	U	313	-	70,74,74	1.96	19 (27%)	80,114,114	2.62	25 (31%)
27	NEX	p	301	18	38,46,46	0.98	2 (5%)	50,70,70	2.43	19 (38%)
26	CHL	3	313	-	54,58,74	2.25	19 (35%)	59,94,114	2.86	24 (40%)
23	LUT	v	310	-	42,43,43	0.77	0	51,60,60	1.63	10 (19%)
22	CLA	c	508	20	69,73,73	1.24	10 (14%)	83,113,113	1.42	10 (12%)
36	DGD	A	414	-	60,60,67	1.27	7 (11%)	74,74,81	1.25	6 (8%)
22	CLA	4	302	-	69,73,73	1.27	9 (13%)	83,113,113	1.26	6 (7%)
32	SQD	a	410	-	49,50,54	1.01	5 (10%)	58,61,65	1.74	11 (18%)
22	CLA	p	308	-	64,68,73	1.29	10 (15%)	77,107,113	1.39	5 (6%)
23	LUT	v	309	-	42,43,43	0.79	0	51,60,60	1.65	12 (23%)
22	CLA	c	504	-	69,73,73	1.25	11 (15%)	83,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	CHL	V	318	-	70,74,74	1.95	20 (28%)	80,114,114	2.58	24 (30%)
26	CHL	6	313	-	52,56,74	2.34	20 (38%)	58,92,114	3.04	26 (44%)
24	XAT	n	311	-	39,47,47	2.53	18 (46%)	54,74,74	11.76	23 (42%)
22	CLA	r	602	-	64,68,73	1.30	9 (14%)	77,107,113	1.34	5 (6%)
23	LUT	S	310	-	42,43,43	0.77	0	51,60,60	1.69	14 (27%)
22	CLA	N	304	18	69,73,73	1.22	10 (14%)	83,113,113	1.39	9 (10%)
34	LMG	c	501	-	51,51,55	1.15	5 (9%)	59,59,63	1.16	3 (5%)
25	LHG	d	405	3	45,45,48	0.92	4 (8%)	48,51,54	1.07	2 (4%)
26	CHL	N	317	-	70,74,74	1.95	20 (28%)	80,114,114	2.59	25 (31%)
22	CLA	B	604	-	69,73,73	1.23	8 (11%)	83,113,113	1.32	8 (9%)
22	CLA	1	302	-	69,73,73	1.28	8 (11%)	83,113,113	1.23	6 (7%)
26	CHL	G	315	18	70,74,74	1.89	20 (28%)	80,114,114	2.69	24 (30%)
22	CLA	2	306	-	64,68,73	1.28	8 (12%)	77,107,113	1.39	7 (9%)
25	LHG	C	523	-	48,48,48	0.89	3 (6%)	51,54,54	1.07	2 (3%)
22	CLA	V	305	-	64,68,73	1.29	9 (14%)	77,107,113	1.38	5 (6%)
26	CHL	p	315	-	52,56,74	2.39	20 (38%)	58,92,114	2.92	22 (37%)
22	CLA	u	308	-	52,56,73	1.42	8 (15%)	62,92,113	1.45	6 (9%)
31	BCR	b	619	-	41,41,41	4.74	24 (58%)	56,56,56	2.27	20 (35%)
22	CLA	S	306	-	60,64,73	1.35	10 (16%)	72,102,113	1.41	7 (9%)
22	CLA	N	301	-	69,73,73	1.26	10 (14%)	83,113,113	1.35	7 (8%)
22	CLA	6	308	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	6 (7%)
26	CHL	G	311	-	70,74,74	1.88	19 (27%)	80,114,114	2.71	27 (33%)
25	LHG	U	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.17	3 (5%)
30	PHO	a	407	-	58,69,69	2.01	11 (18%)	56,99,99	1.62	9 (16%)
22	CLA	Q	302	-	69,73,73	1.24	8 (11%)	83,113,113	1.27	5 (6%)
26	CHL	r	615	-	60,64,74	2.06	20 (33%)	68,102,114	2.92	24 (35%)
22	CLA	2	308	-	52,56,73	1.42	9 (17%)	62,92,113	1.47	5 (8%)
34	LMG	c	520	-	51,51,55	1.20	6 (11%)	59,59,63	1.08	2 (3%)
25	LHG	N	312	-	48,48,48	0.89	4 (8%)	51,54,54	1.09	2 (3%)
22	CLA	3	308	-	52,56,73	1.43	8 (15%)	62,92,113	1.41	5 (8%)
22	CLA	C	504	-	69,73,73	1.28	11 (15%)	83,113,113	1.48	8 (9%)
22	CLA	V	308	-	52,56,73	1.42	8 (15%)	62,92,113	1.45	4 (6%)
26	CHL	R	316	-	60,64,74	2.06	19 (31%)	68,102,114	2.94	24 (35%)
34	LMG	B	624	21	55,55,55	1.16	6 (10%)	63,63,63	1.07	2 (3%)
22	CLA	g	307	-	69,73,73	1.24	9 (13%)	83,113,113	1.35	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	u	305	-	64,68,73	1.29	10 (15%)	77,107,113	1.31	5 (6%)
26	CHL	5	313	18	70,74,74	2.02	20 (28%)	80,114,114	2.65	24 (30%)
22	CLA	u	306	-	64,68,73	1.31	10 (15%)	77,107,113	1.36	5 (6%)
22	CLA	g	304	18	68,72,73	1.26	9 (13%)	81,111,113	1.38	9 (11%)
22	CLA	R	305	-	52,56,73	1.44	8 (15%)	62,92,113	1.51	6 (9%)
22	CLA	2	303	-	54,58,73	1.39	9 (16%)	65,95,113	1.43	5 (7%)
22	CLA	C	512	8,20	69,73,73	1.26	9 (13%)	83,113,113	1.21	5 (6%)
26	CHL	1	316	-	70,74,74	1.92	20 (28%)	80,114,114	2.67	25 (31%)
22	CLA	6	306	22	64,68,73	1.28	9 (14%)	77,107,113	1.41	8 (10%)
25	LHG	S	312	19	48,48,48	0.89	4 (8%)	51,54,54	1.13	3 (5%)
22	CLA	Q	306	22	64,68,73	1.29	7 (10%)	77,107,113	1.28	3 (3%)
25	LHG	c	522	-	48,48,48	0.90	3 (6%)	51,54,54	1.07	2 (3%)
23	LUT	4	310	-	42,43,43	0.83	1 (2%)	51,60,60	1.79	14 (27%)
22	CLA	r	606	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	5 (6%)
22	CLA	N	303	-	54,58,73	1.40	9 (16%)	65,95,113	1.53	7 (10%)
22	CLA	c	506	-	69,73,73	1.23	10 (14%)	83,113,113	1.50	11 (13%)
22	CLA	1	307	-	69,73,73	1.24	11 (15%)	83,113,113	1.37	8 (9%)
22	CLA	r	608	-	53,57,73	1.40	8 (15%)	62,93,113	1.47	8 (12%)
26	CHL	s	314	-	50,54,74	2.26	18 (36%)	56,90,114	3.11	22 (39%)
27	NEX	S	317	19	38,46,46	0.88	1 (2%)	50,70,70	2.45	17 (34%)
22	CLA	R	302	27	53,57,73	1.44	9 (16%)	62,93,113	1.49	6 (9%)
24	XAT	V	311	-	39,47,47	2.58	18 (46%)	54,74,74	12.00	18 (33%)
26	CHL	1	318	-	70,74,74	1.90	20 (28%)	80,114,114	2.64	25 (31%)
26	CHL	3	315	18	70,74,74	1.91	19 (27%)	80,114,114	2.67	23 (28%)
22	CLA	B	616	21	69,73,73	1.23	9 (13%)	83,113,113	1.38	8 (9%)
22	CLA	b	605	21	69,73,73	1.24	9 (13%)	83,113,113	1.66	10 (12%)
26	CHL	3	316	-	65,69,74	2.00	19 (29%)	74,108,114	2.75	25 (33%)
26	CHL	4	316	18	70,74,74	1.92	20 (28%)	80,114,114	2.75	28 (35%)
22	CLA	v	307	-	69,73,73	1.24	10 (14%)	83,113,113	1.35	6 (7%)
26	CHL	5	315	-	54,58,74	2.16	20 (37%)	59,94,114	3.06	23 (38%)
31	BCR	B	620	-	41,41,41	4.75	24 (58%)	56,56,56	2.28	23 (41%)
22	CLA	c	511	8,20	69,73,73	1.26	10 (14%)	83,113,113	1.22	5 (6%)
22	CLA	n	306	-	64,68,73	1.27	7 (10%)	77,107,113	1.39	8 (10%)
26	CHL	2	314	-	52,56,74	2.36	20 (38%)	58,92,114	3.15	24 (41%)
22	CLA	u	302	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	LUT	2	310	-	42,43,43	0.78	0	51,60,60	1.64	12 (23%)
26	CHL	p	319	-	70,74,74	1.91	20 (28%)	80,114,114	2.64	24 (30%)
26	CHL	2	313	18	70,74,74	2.00	20 (28%)	80,114,114	2.65	25 (31%)
22	CLA	6	302	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	8 (9%)
26	CHL	2	315	-	54,58,74	2.17	19 (35%)	59,94,114	3.04	22 (37%)
26	CHL	4	313	-	70,74,74	1.96	20 (28%)	80,114,114	2.57	25 (31%)
36	DGD	c	517	-	56,56,67	1.30	8 (14%)	70,70,81	1.19	5 (7%)
22	CLA	p	304	-	54,58,73	1.41	8 (14%)	65,95,113	1.42	6 (9%)
22	CLA	R	310	-	64,68,73	1.31	7 (10%)	77,107,113	1.43	7 (9%)
26	CHL	g	313	-	54,58,74	2.17	17 (31%)	59,94,114	3.02	20 (33%)
26	CHL	P	315	-	52,56,74	2.43	20 (38%)	58,92,114	2.90	21 (36%)
23	LUT	V	310	-	42,43,43	0.78	0	51,60,60	1.62	12 (23%)

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
22	CLA	b	608	-	-	11/39/115/115	-
22	CLA	v	302	-	-	14/39/115/115	-
25	LHG	C	522	-	-	16/53/53/53	-
22	CLA	s	308	-	-	9/27/103/115	-
23	LUT	2	309	-	-	4/29/67/67	0/2/2/2
26	CHL	U	319	-	-	22/41/117/117	-
27	NEX	r	618	22,1	-	7/27/83/83	0/3/3/3
26	CHL	6	315	-	-	17/41/117/117	-
22	CLA	R	309	-	-	7/20/96/115	-
22	CLA	b	606	-	-	20/39/115/115	-
22	CLA	C	503	-	-	9/39/115/115	-
25	LHG	5	312	-	-	23/53/53/53	-
34	LMG	b	621	-	-	24/46/66/70	0/1/1/1
26	CHL	n	317	-	-	18/41/117/117	-
23	LUT	V	309	-	-	2/29/67/67	0/2/2/2
31	BCR	b	618	-	-	8/29/63/63	0/2/2/2
26	CHL	Q	311	-	-	19/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	R	314	-	-	24/46/46/53	-
22	CLA	r	601	27	-	9/20/96/115	-
22	CLA	G	304	18	-	10/38/114/115	-
32	SQD	a	413	-	-	22/49/69/69	0/1/1/1
22	CLA	g	302	-	-	15/39/115/115	-
22	CLA	1	304	-	-	9/33/109/115	-
26	CHL	2	316	-	-	19/41/117/117	-
22	CLA	p	307	-	-	9/33/109/115	-
22	CLA	b	603	-	-	14/39/115/115	-
26	CHL	3	311	-	-	16/41/117/117	-
27	NEX	2	319	-	-	7/27/83/83	0/3/3/3
25	LHG	D	407	3	-	18/53/53/53	-
23	LUT	5	309	-	-	4/29/67/67	0/2/2/2
24	XAT	4	311	-	-	8/31/93/93	0/4/4/4
22	CLA	p	309	-	-	8/19/95/115	-
24	XAT	1	311	-	-	7/31/93/93	0/4/4/4
22	CLA	3	307	-	-	12/39/115/115	-
22	CLA	B	602	-	-	21/39/115/115	-
22	CLA	g	306	22	-	15/33/109/115	-
24	XAT	P	312	-	-	8/31/93/93	0/4/4/4
22	CLA	c	512	-	-	9/39/115/115	-
22	CLA	N	306	-	-	9/33/109/115	-
22	CLA	U	303	-	-	7/21/97/115	-
25	LHG	b	622	-	-	22/51/51/53	-
22	CLA	B	611	-	-	16/39/115/115	-
33	PL9	d	404	-	-	9/53/73/73	0/1/1/1
31	BCR	b	620	-	-	12/29/63/63	0/2/2/2
26	CHL	2	318	-	-	20/41/117/117	-
22	CLA	5	301	-	-	12/39/115/115	-
22	CLA	v	304	-	-	14/33/109/115	-
22	CLA	C	513	-	-	10/39/115/115	-
25	LHG	s	312	19	-	17/53/53/53	-
34	LMG	a	412	-	-	8/35/55/70	0/1/1/1
23	LUT	1	310	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	b	623	21	-	24/53/53/53	-
22	CLA	q	303	-	-	10/21/97/115	-
22	CLA	c	513	-	-	10/39/115/115	-
22	CLA	b	615	-	-	20/39/115/115	-
22	CLA	1	308	-	-	13/19/95/115	-
22	CLA	Q	303	-	-	12/21/97/115	-
26	CHL	v	314	-	-	14/20/96/117	-
31	BCR	c	516	-	-	11/29/63/63	0/2/2/2
33	PL9	A	410	-	-	0/5/18/73	0/1/1/1
22	CLA	5	304	18	-	14/39/115/115	-
34	LMG	b	624	21	-	22/50/70/70	0/1/1/1
22	CLA	B	606	-	-	20/39/115/115	-
22	CLA	U	302	-	-	14/39/115/115	-
22	CLA	2	304	18	-	11/39/115/115	-
22	CLA	q	301	-	-	17/39/115/115	-
22	CLA	G	306	22	-	11/33/109/115	-
26	CHL	u	314	-	-	13/20/96/117	-
22	CLA	Q	301	-	-	16/39/115/115	-
26	CHL	6	314	-	-	13/22/98/117	-
22	CLA	s	301	19	-	17/35/111/115	-
24	XAT	Q	309	-	-	10/31/93/93	0/4/4/4
22	CLA	6	307	22	-	18/33/109/115	-
25	LHG	L	101	-	-	28/53/53/53	-
22	CLA	v	303	-	-	9/21/97/115	-
27	NEX	R	301	22,1	-	10/27/83/83	0/3/3/3
36	DGD	B	601	21	-	22/51/91/95	0/2/2/2
31	BCR	C	517	-	-	14/29/63/63	0/2/2/2
22	CLA	n	304	18	-	15/39/115/115	-
22	CLA	V	302	-	-	14/39/115/115	-
22	CLA	G	308	-	-	11/19/95/115	-
22	CLA	C	506	-	-	15/39/115/115	-
26	CHL	4	315	-	-	8/22/98/117	-
23	LUT	p	310	-	-	2/29/67/67	0/2/2/2
27	NEX	s	317	19	-	4/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	511	-	-	14/39/115/115	-
26	CHL	U	317	-	-	20/41/117/117	-
26	CHL	3	314	-	-	18/41/117/117	-
22	CLA	c	502	-	-	10/39/115/115	-
36	DGD	C	520	-	-	31/51/91/95	0/2/2/2
26	CHL	U	315	-	-	16/41/117/117	-
22	CLA	C	508	-	-	22/39/115/115	-
31	BCR	d	403	3	-	12/29/63/63	0/2/2/2
24	XAT	p	312	-	-	7/31/93/93	0/4/4/4
24	XAT	r	612	-	-	7/31/93/93	0/4/4/4
26	CHL	g	311	-	-	21/41/117/117	-
22	CLA	P	303	-	-	15/39/115/115	-
26	CHL	n	318	-	-	25/41/117/117	-
37	HEM	E	101	4,17	-	2/14/54/54	-
36	DGD	J	101	-	-	21/49/89/95	0/2/2/2
25	LHG	V	312	-	-	18/53/53/53	-
25	LHG	d	406	3	-	19/53/53/53	-
25	LHG	6	311	-	-	19/53/53/53	-
31	BCR	t	101	-	-	12/29/63/63	0/2/2/2
26	CHL	N	313	-	-	14/41/117/117	-
30	PHO	D	401	-	-	11/37/103/103	0/5/6/6
22	CLA	B	603	-	-	16/39/115/115	-
22	CLA	r	609	26	-	12/33/109/115	-
22	CLA	b	607	-	-	15/39/115/115	-
22	CLA	r	610	-	-	10/15/91/115	-
22	CLA	n	303	-	-	7/21/97/115	-
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
34	LMG	C	502	-	-	26/46/66/70	0/1/1/1
26	CHL	R	317	-	-	16/35/111/117	-
25	LHG	P	313	-	-	24/53/53/53	-
22	CLA	s	302	-	-	6/15/91/115	-
26	CHL	S	313	-	-	7/17/93/117	-
24	XAT	v	311	-	-	11/31/93/93	0/4/4/4
26	CHL	p	320	-	-	20/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	306	-	-	16/33/109/115	-
22	CLA	U	305	-	-	12/33/109/115	-
26	CHL	4	317	-	-	16/41/117/117	-
36	DGD	b	601	21	-	21/51/91/95	0/2/2/2
22	CLA	A	406	-	-	9/21/97/115	-
22	CLA	C	514	-	-	14/39/115/115	-
23	LUT	u	309	-	-	2/29/67/67	0/2/2/2
22	CLA	6	304	-	-	11/21/97/115	-
22	CLA	5	303	-	-	7/21/97/115	-
26	CHL	5	317	-	-	17/41/117/117	-
26	CHL	n	316	-	-	27/41/117/117	-
22	CLA	4	304	-	-	11/33/109/115	-
22	CLA	B	617	-	-	11/39/115/115	-
22	CLA	b	614	-	-	16/39/115/115	-
22	CLA	5	302	-	-	18/39/115/115	-
22	CLA	b	609	-	-	12/39/115/115	-
22	CLA	q	306	22	-	14/33/109/115	-
24	XAT	u	311	-	-	7/31/93/93	0/4/4/4
22	CLA	U	304	-	-	7/33/109/115	-
26	CHL	u	318	-	-	20/41/117/117	-
32	SQD	L	102	9	-	21/49/69/69	0/1/1/1
22	CLA	b	602	-	-	19/39/115/115	-
31	BCR	B	618	-	-	8/29/63/63	0/2/2/2
24	XAT	2	311	-	-	6/31/93/93	0/4/4/4
22	CLA	v	301	-	-	13/39/115/115	-
22	CLA	b	612	-	-	15/39/115/115	-
22	CLA	C	515	-	-	12/39/115/115	-
23	LUT	S	311	-	-	8/29/67/67	0/2/2/2
22	CLA	B	607	-	-	15/39/115/115	-
22	CLA	B	615	-	-	19/39/115/115	-
25	LHG	l	101	-	-	27/53/53/53	-
25	LHG	4	312	-	-	18/53/53/53	-
22	CLA	B	612	-	-	17/39/115/115	-
22	CLA	R	304	-	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	U	316	18	-	13/41/117/117	-
22	CLA	P	309	-	-	12/19/95/115	-
26	CHL	1	315	-	-	8/22/98/117	-
23	LUT	U	310	-	-	3/29/67/67	0/2/2/2
22	CLA	c	514	-	-	11/39/115/115	-
22	CLA	r	605	-	-	9/31/107/115	-
22	CLA	x	201	14	-	10/39/115/115	-
22	CLA	S	301	19	-	17/35/111/115	-
26	CHL	Q	312	-	-	16/20/96/117	-
23	LUT	4	309	-	-	2/29/67/67	0/2/2/2
31	BCR	C	518	-	-	11/29/63/63	0/2/2/2
26	CHL	P	319	-	-	22/41/117/117	-
22	CLA	G	305	22	-	12/33/109/115	-
26	CHL	1	317	18	-	21/41/117/117	-
22	CLA	X	202	14	-	9/39/115/115	-
22	CLA	S	308	-	-	9/27/103/115	-
22	CLA	R	307	-	-	18/39/115/115	-
22	CLA	1	306	-	-	16/33/109/115	-
22	CLA	b	613	-	-	16/39/115/115	-
23	LUT	r	611	1	-	2/29/67/67	0/2/2/2
25	LHG	n	312	-	-	19/53/53/53	-
23	LUT	P	311	-	-	3/29/67/67	0/2/2/2
22	CLA	3	302	-	-	15/39/115/115	-
22	CLA	N	308	-	-	16/19/95/115	-
22	CLA	r	604	-	-	9/19/95/115	-
23	LUT	n	309	-	-	0/29/67/67	0/2/2/2
26	CHL	q	313	-	-	11/22/98/117	-
22	CLA	u	307	-	-	16/39/115/115	-
26	CHL	Q	313	-	-	11/22/98/117	-
26	CHL	S	315	19	-	17/32/108/117	-
22	CLA	b	611	-	-	16/39/115/115	-
34	LMG	d	407	3	-	17/41/61/70	0/1/1/1
22	CLA	3	306	22	-	18/33/109/115	-
23	LUT	s	311	-	-	7/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	307	-	-	10/33/109/115	-
22	CLA	4	307	-	-	9/39/115/115	-
22	CLA	4	308	-	-	13/19/95/115	-
25	LHG	q	310	-	-	22/53/53/53	-
26	CHL	q	312	-	-	14/20/96/117	-
26	CHL	u	317	18	-	13/41/117/117	-
22	CLA	c	505	-	-	11/39/115/115	-
22	CLA	B	614	-	-	14/39/115/115	-
25	LHG	Q	310	-	-	19/53/53/53	-
26	CHL	5	318	-	-	18/41/117/117	-
22	CLA	G	302	-	-	19/39/115/115	-
26	CHL	u	315	-	-	10/22/98/117	-
30	PHO	A	407	-	-	10/37/103/103	0/5/6/6
22	CLA	6	303	-	-	14/39/115/115	-
22	CLA	R	306	-	-	9/31/107/115	-
36	DGD	c	519	-	-	21/49/89/95	0/2/2/2
22	CLA	B	609	-	-	12/39/115/115	-
27	NEX	v	319	-	-	4/27/83/83	0/3/3/3
22	CLA	4	303	-	-	11/21/97/115	-
26	CHL	n	313	18	-	21/41/117/117	-
31	BCR	c	515	-	-	14/29/63/63	0/2/2/2
22	CLA	N	305	18	-	14/33/109/115	-
26	CHL	q	311	-	-	18/41/117/117	-
26	CHL	N	314	-	-	12/20/96/117	-
22	CLA	s	305	-	-	7/27/103/115	-
27	NEX	U	318	-	-	3/27/83/83	0/3/3/3
23	LUT	R	312	-	-	4/29/67/67	0/2/2/2
22	CLA	c	509	-	-	10/39/115/115	-
26	CHL	P	317	-	-	17/41/117/117	-
26	CHL	r	614	-	-	20/41/117/117	-
22	CLA	5	305	18	-	13/33/109/115	-
22	CLA	p	302	-	-	17/39/115/115	-
22	CLA	6	305	18	-	19/38/114/115	-
26	CHL	v	317	18	-	12/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	21	-	20/39/115/115	-
22	CLA	N	302	-	-	20/39/115/115	-
32	SQD	l	102	9	-	21/49/69/69	0/1/1/1
22	CLA	A	404	-	-	15/39/115/115	-
26	CHL	p	317	-	-	16/41/117/117	-
22	CLA	P	308	-	-	15/33/109/115	-
22	CLA	p	306	18	-	13/33/109/115	-
22	CLA	b	617	21	-	14/39/115/115	-
22	CLA	g	303	-	-	13/21/97/115	-
26	CHL	1	313	-	-	12/41/117/117	-
25	LHG	A	413	2	-	27/47/47/53	-
32	SQD	m	101	-	-	21/37/57/69	0/1/1/1
22	CLA	Q	308	-	-	11/19/95/115	-
22	CLA	A	408	-	-	12/33/109/115	-
26	CHL	G	313	-	-	9/22/98/117	-
27	NEX	r	617	-	-	2/27/83/83	0/3/3/3
22	CLA	P	305	18	-	12/39/115/115	-
25	LHG	G	310	-	-	19/53/53/53	-
22	CLA	P	306	18	-	12/33/109/115	-
22	CLA	n	301	-	-	14/39/115/115	-
26	CHL	v	313	-	-	17/41/117/117	-
22	CLA	5	308	-	-	5/19/95/115	-
24	XAT	q	309	-	-	12/31/93/93	0/4/4/4
22	CLA	a	408	-	-	11/33/109/115	-
22	CLA	C	510	-	-	9/39/115/115	-
22	CLA	u	304	-	-	5/33/109/115	-
22	CLA	g	305	22	-	12/33/109/115	-
34	LMG	B	621	-	-	20/46/66/70	0/1/1/1
34	LMG	D	408	3	-	17/41/61/70	0/1/1/1
25	LHG	C	524	-	-	13/53/53/53	-
22	CLA	N	307	-	-	15/33/109/115	-
26	CHL	6	301	-	-	22/41/117/117	-
31	BCR	x	202	-	-	9/29/63/63	0/2/2/2
22	CLA	p	303	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	S	316	-	-	13/17/93/117	-
22	CLA	3	304	18	-	15/38/114/115	-
26	CHL	s	313	-	-	7/17/93/117	-
25	LHG	D	406	3	-	28/50/50/53	-
26	CHL	q	315	-	-	13/35/111/117	-
30	PHO	d	401	-	-	11/37/103/103	0/5/6/6
25	LHG	B	622	-	-	21/51/51/53	-
25	LHG	p	313	-	-	22/53/53/53	-
26	CHL	Q	315	18	-	20/41/117/117	-
22	CLA	P	302	-	-	18/39/115/115	-
26	CHL	Q	314	-	-	22/41/117/117	-
22	CLA	q	308	-	-	13/19/95/115	-
22	CLA	S	304	19	-	11/15/91/115	-
26	CHL	s	315	19	-	17/32/108/117	-
22	CLA	n	302	-	-	16/39/115/115	-
22	CLA	2	302	-	-	14/39/115/115	-
26	CHL	u	316	-	-	24/41/117/117	-
25	LHG	u	312	-	-	25/53/53/53	-
26	CHL	U	314	-	-	12/22/98/117	-
25	LHG	c	521	-	-	14/53/53/53	-
26	CHL	Q	316	-	-	14/35/111/117	-
27	NEX	P	301	18	-	3/27/83/83	0/3/3/3
22	CLA	U	307	-	-	17/39/115/115	-
22	CLA	q	302	-	-	13/39/115/115	-
37	HEM	e	101	4,17	-	3/14/54/54	-
22	CLA	g	301	-	-	14/39/115/115	-
23	LUT	1	309	-	-	2/29/67/67	0/2/2/2
25	LHG	2	312	-	-	24/53/53/53	-
26	CHL	6	317	-	-	18/35/111/117	-
22	CLA	G	303	-	-	12/21/97/115	-
24	XAT	g	309	-	-	10/31/93/93	0/4/4/4
25	LHG	v	312	-	-	19/53/53/53	-
22	CLA	B	610	-	-	18/39/115/115	-
22	CLA	V	307	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	X	201	-	-	9/29/63/63	0/2/2/2
25	LHG	3	310	-	-	18/53/53/53	-
22	CLA	S	305	-	-	8/27/103/115	-
26	CHL	V	315	-	-	8/22/98/117	-
27	NEX	V	319	-	-	6/27/83/83	0/3/3/3
22	CLA	v	308	-	-	11/19/95/115	-
26	CHL	g	315	18	-	23/41/117/117	-
22	CLA	3	301	-	-	14/39/115/115	-
22	CLA	S	309	-	-	4/20/96/115	-
26	CHL	3	312	-	-	10/20/96/117	-
22	CLA	G	301	-	-	19/39/115/115	-
22	CLA	b	616	21	-	11/39/115/115	-
27	NEX	u	320	-	-	2/27/83/83	0/3/3/3
22	CLA	S	302	-	-	6/15/91/115	-
24	XAT	U	311	-	-	7/31/93/93	0/4/4/4
26	CHL	V	317	18	-	14/41/117/117	-
22	CLA	U	306	-	-	12/33/109/115	-
26	CHL	g	312	-	-	12/20/96/117	-
31	BCR	a	409	-	-	2/29/63/63	0/2/2/2
27	NEX	5	319	-	-	8/27/83/83	0/3/3/3
22	CLA	4	305	-	-	8/33/109/115	-
22	CLA	v	306	-	-	15/33/109/115	-
22	CLA	s	304	19	-	11/15/91/115	-
33	PL9	a	411	-	-	0/5/18/73	0/1/1/1
26	CHL	R	315	-	-	20/41/117/117	-
31	BCR	C	516	-	-	8/29/63/63	0/2/2/2
23	LUT	n	310	-	-	3/29/67/67	0/2/2/2
24	XAT	6	310	-	-	8/31/93/93	0/4/4/4
32	SQD	M	101	-	-	22/37/57/69	0/1/1/1
31	BCR	k	101	-	-	13/29/63/63	0/2/2/2
22	CLA	1	303	-	-	10/21/97/115	-
26	CHL	v	316	-	-	17/41/117/117	-
22	CLA	C	505	-	-	19/39/115/115	-
22	CLA	V	301	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	405	-	-	12/39/115/115	-
36	DGD	C	519	-	-	23/44/84/95	0/2/2/2
22	CLA	U	308	-	-	12/19/95/115	-
22	CLA	3	303	-	-	12/21/97/115	-
24	XAT	R	313	-	-	8/31/93/93	0/4/4/4
22	CLA	u	303	-	-	8/21/97/115	-
22	CLA	V	306	-	-	7/33/109/115	-
26	CHL	5	314	-	-	13/20/96/117	-
22	CLA	a	405	-	-	12/39/115/115	-
22	CLA	C	509	20	-	16/39/115/115	-
25	LHG	B	623	21	-	21/53/53/53	-
22	CLA	q	305	22	-	14/33/109/115	-
34	LMG	w	201	-	-	22/43/63/70	0/1/1/1
26	CHL	s	316	-	-	13/17/93/117	-
34	LMG	C	521	-	-	19/46/66/70	0/1/1/1
22	CLA	Q	305	22	-	18/33/109/115	-
22	CLA	S	307	-	-	6/20/96/115	-
24	XAT	3	309	-	-	8/31/93/93	0/4/4/4
24	XAT	G	309	-	-	10/31/93/93	0/4/4/4
22	CLA	1	301	-	-	9/39/115/115	-
22	CLA	V	304	-	-	12/33/109/115	-
23	LUT	s	310	19	-	2/29/67/67	0/2/2/2
26	CHL	5	316	-	-	20/41/117/117	-
26	CHL	N	316	-	-	19/41/117/117	-
32	SQD	C	501	-	-	27/45/65/69	0/1/1/1
22	CLA	s	307	-	-	6/20/96/115	-
22	CLA	D	403	3	-	17/39/115/115	-
22	CLA	S	303	19	-	6/21/97/115	-
25	LHG	a	415	2	-	26/47/47/53	-
22	CLA	q	304	18	-	15/38/114/115	-
22	CLA	s	309	-	-	4/20/96/115	-
26	CHL	v	315	-	-	8/22/98/117	-
22	CLA	c	507	-	-	22/39/115/115	-
22	CLA	2	305	18	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Q	304	18	-	14/38/114/115	-
27	NEX	n	319	-	-	7/27/83/83	0/3/3/3
26	CHL	P	314	18	-	16/41/117/117	-
34	LMG	A	411	-	-	11/35/55/70	0/1/1/1
23	LUT	u	310	-	-	2/29/67/67	0/2/2/2
22	CLA	a	404	-	-	15/39/115/115	-
26	CHL	n	314	-	-	11/20/96/117	-
23	LUT	P	310	-	-	2/29/67/67	0/2/2/2
22	CLA	n	307	-	-	13/33/109/115	-
26	CHL	G	312	-	-	8/20/96/117	-
26	CHL	P	316	-	-	9/22/98/117	-
26	CHL	V	313	-	-	20/41/117/117	-
22	CLA	R	311	-	-	10/15/91/115	-
22	CLA	u	301	-	-	9/39/115/115	-
22	CLA	b	604	-	-	18/39/115/115	-
22	CLA	n	305	18	-	13/33/109/115	-
22	CLA	a	406	-	-	10/21/97/115	-
22	CLA	r	603	-	-	13/33/109/115	-
26	CHL	6	312	-	-	17/41/117/117	-
26	CHL	g	316	-	-	17/35/111/117	-
25	LHG	r	613	-	-	19/46/46/53	-
32	SQD	A	412	-	-	21/49/69/69	0/1/1/1
26	CHL	P	318	-	-	19/41/117/117	-
26	CHL	1	314	22	-	16/20/96/117	-
36	DGD	c	518	-	-	31/51/91/95	0/2/2/2
26	CHL	r	619	1	-	10/20/96/117	-
22	CLA	r	607	1	-	11/20/96/115	-
25	LHG	g	310	-	-	20/53/53/53	-
31	BCR	z	101	-	-	8/29/63/63	0/2/2/2
27	NEX	N	318	-	-	9/27/83/83	0/3/3/3
24	XAT	N	311	-	-	8/31/93/93	0/4/4/4
22	CLA	b	610	-	-	18/39/115/115	-
26	CHL	p	314	18	-	13/41/117/117	-
33	PL9	D	405	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	1	312	-	-	14/53/53/53	-
34	LMG	W	201	-	-	21/43/63/70	0/1/1/1
22	CLA	s	303	19	-	6/21/97/115	-
31	BCR	K	101	-	-	13/29/63/63	0/2/2/2
31	BCR	B	619	-	-	14/29/63/63	0/2/2/2
22	CLA	P	307	-	-	12/33/109/115	-
22	CLA	R	303	-	-	9/33/109/115	-
26	CHL	p	316	-	-	9/22/98/117	-
22	CLA	s	306	-	-	7/29/105/115	-
26	CHL	g	314	-	-	22/41/117/117	-
24	XAT	5	311	-	-	6/31/93/93	0/4/4/4
26	CHL	S	314	-	-	9/17/93/117	-
31	BCR	D	404	3	-	13/29/63/63	0/2/2/2
26	CHL	v	318	-	-	22/41/117/117	-
22	CLA	1	305	-	-	10/33/109/115	-
23	LUT	U	309	-	-	4/29/67/67	0/2/2/2
22	CLA	n	308	-	-	13/19/95/115	-
26	CHL	G	316	-	-	15/35/111/117	-
22	CLA	R	308	1	-	12/20/96/115	-
22	CLA	5	306	-	-	13/33/109/115	-
26	CHL	2	317	-	-	13/41/117/117	-
26	CHL	G	314	-	-	17/41/117/117	-
22	CLA	V	303	-	-	8/21/97/115	-
22	CLA	G	307	-	-	14/39/115/115	-
22	CLA	v	305	-	-	9/33/109/115	-
23	LUT	5	310	-	-	1/29/67/67	0/2/2/2
26	CHL	r	616	-	-	16/35/111/117	-
22	CLA	B	608	-	-	14/39/115/115	-
25	LHG	c	523	-	-	17/53/53/53	-
27	NEX	u	319	-	-	7/27/83/83	0/3/3/3
22	CLA	B	613	-	-	16/39/115/115	-
22	CLA	U	301	-	-	10/39/115/115	-
22	CLA	3	305	22	-	11/33/109/115	-
31	BCR	A	409	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	510	-	-	15/39/115/115	-
22	CLA	C	507	-	-	19/39/115/115	-
22	CLA	P	304	-	-	12/21/97/115	-
26	CHL	V	314	-	-	13/20/96/117	-
23	LUT	p	311	-	-	3/29/67/67	0/2/2/2
22	CLA	d	402	3	-	15/39/115/115	-
26	CHL	q	314	18	-	23/41/117/117	-
26	CHL	p	318	-	-	19/41/117/117	-
26	CHL	n	315	-	-	12/22/98/117	-
23	LUT	N	310	-	-	1/29/67/67	0/2/2/2
26	CHL	V	316	-	-	19/41/117/117	-
22	CLA	6	309	-	-	12/19/95/115	-
26	CHL	N	315	-	-	9/22/98/117	-
22	CLA	c	503	-	-	22/39/115/115	-
26	CHL	6	316	18	-	23/41/117/117	-
22	CLA	5	307	-	-	12/33/109/115	-
22	CLA	g	308	-	-	10/19/95/115	-
22	CLA	2	301	-	-	13/39/115/115	-
22	CLA	p	305	18	-	13/39/115/115	-
22	CLA	4	301	-	-	9/39/115/115	-
23	LUT	N	309	-	-	2/29/67/67	0/2/2/2
26	CHL	u	313	-	-	16/41/117/117	-
22	CLA	q	307	-	-	17/39/115/115	-
26	CHL	4	314	-	-	12/20/96/117	-
36	DGD	a	416	-	-	24/48/88/95	0/2/2/2
22	CLA	Q	307	-	-	12/39/115/115	-
26	CHL	U	313	-	-	17/41/117/117	-
27	NEX	p	301	18	-	3/27/83/83	0/3/3/3
26	CHL	3	313	-	-	16/22/98/117	-
23	LUT	v	310	-	-	0/29/67/67	0/2/2/2
22	CLA	c	508	20	-	16/39/115/115	-
36	DGD	A	414	-	-	22/48/88/95	0/2/2/2
22	CLA	4	302	-	-	15/39/115/115	-
32	SQD	a	410	-	-	25/45/65/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	p	308	-	-	13/33/109/115	-
23	LUT	v	309	-	-	2/29/67/67	0/2/2/2
22	CLA	c	504	-	-	19/39/115/115	-
26	CHL	V	318	-	-	19/41/117/117	-
26	CHL	6	313	-	-	10/20/96/117	-
24	XAT	n	311	-	-	9/31/93/93	0/4/4/4
22	CLA	r	602	-	-	9/33/109/115	-
23	LUT	S	310	-	-	2/29/67/67	0/2/2/2
22	CLA	N	304	18	-	19/39/115/115	-
34	LMG	c	501	-	-	25/46/66/70	0/1/1/1
25	LHG	d	405	3	-	26/50/50/53	-
26	CHL	N	317	-	-	22/41/117/117	-
22	CLA	B	604	-	-	17/39/115/115	-
22	CLA	1	302	-	-	14/39/115/115	-
26	CHL	G	315	18	-	19/41/117/117	-
22	CLA	2	306	-	-	11/33/109/115	-
25	LHG	C	523	-	-	24/53/53/53	-
22	CLA	V	305	-	-	10/33/109/115	-
26	CHL	p	315	-	-	8/20/96/117	-
22	CLA	u	308	-	-	12/19/95/115	-
31	BCR	b	619	-	-	14/29/63/63	0/2/2/2
22	CLA	S	306	-	-	8/29/105/115	-
22	CLA	N	301	-	-	14/39/115/115	-
22	CLA	6	308	-	-	12/39/115/115	-
26	CHL	G	311	-	-	18/41/117/117	-
25	LHG	U	312	-	-	29/53/53/53	-
30	PHO	a	407	-	-	10/37/103/103	0/5/6/6
22	CLA	Q	302	-	-	13/39/115/115	-
26	CHL	r	615	-	-	12/29/105/117	-
22	CLA	2	308	-	-	8/19/95/115	-
34	LMG	c	520	-	-	21/46/66/70	0/1/1/1
25	LHG	N	312	-	-	16/53/53/53	-
22	CLA	3	308	-	-	12/19/95/115	-
22	CLA	C	504	-	-	23/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	V	308	-	-	11/19/95/115	-
26	CHL	R	316	-	-	13/29/105/117	-
34	LMG	B	624	21	-	21/50/70/70	0/1/1/1
22	CLA	g	307	-	-	14/39/115/115	-
22	CLA	u	305	-	-	14/33/109/115	-
26	CHL	5	313	18	-	21/41/117/117	-
22	CLA	u	306	-	-	12/33/109/115	-
22	CLA	g	304	18	-	9/38/114/115	-
22	CLA	R	305	-	-	9/19/95/115	-
22	CLA	2	303	-	-	8/21/97/115	-
22	CLA	C	512	8,20	-	22/39/115/115	-
26	CHL	1	316	-	-	23/41/117/117	-
22	CLA	6	306	22	-	15/33/109/115	-
25	LHG	S	312	19	-	17/53/53/53	-
22	CLA	Q	306	22	-	13/33/109/115	-
25	LHG	c	522	-	-	24/53/53/53	-
23	LUT	4	310	-	-	0/29/67/67	0/2/2/2
22	CLA	r	606	-	-	18/39/115/115	-
22	CLA	N	303	-	-	7/21/97/115	-
22	CLA	c	506	-	-	19/39/115/115	-
22	CLA	1	307	-	-	13/39/115/115	-
22	CLA	r	608	-	-	7/20/96/115	-
26	CHL	s	314	-	-	8/17/93/117	-
27	NEX	S	317	19	-	4/27/83/83	0/3/3/3
22	CLA	R	302	27	-	10/20/96/115	-
24	XAT	V	311	-	-	11/31/93/93	0/4/4/4
26	CHL	1	318	-	-	16/41/117/117	-
26	CHL	3	315	18	-	23/41/117/117	-
22	CLA	B	616	21	-	8/39/115/115	-
22	CLA	b	605	21	-	18/39/115/115	-
26	CHL	3	316	-	-	18/35/111/117	-
26	CHL	4	316	18	-	16/41/117/117	-
22	CLA	v	307	-	-	12/39/115/115	-
26	CHL	5	315	-	-	8/22/98/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	BCR	B	620	-	-	12/29/63/63	0/2/2/2
22	CLA	c	511	8,20	-	20/39/115/115	-
22	CLA	n	306	-	-	9/33/109/115	-
26	CHL	2	314	-	-	9/20/96/117	-
22	CLA	u	302	-	-	16/39/115/115	-
23	LUT	2	310	-	-	1/29/67/67	0/2/2/2
26	CHL	p	319	-	-	17/41/117/117	-
26	CHL	2	313	18	-	20/41/117/117	-
22	CLA	6	302	-	-	17/39/115/115	-
26	CHL	2	315	-	-	7/22/98/117	-
26	CHL	4	313	-	-	18/41/117/117	-
36	DGD	c	517	-	-	22/44/84/95	0/2/2/2
22	CLA	p	304	-	-	12/21/97/115	-
22	CLA	R	310	-	-	12/33/109/115	-
26	CHL	g	313	-	-	10/22/98/117	-
26	CHL	P	315	-	-	11/20/96/117	-
23	LUT	V	310	-	-	0/29/67/67	0/2/2/2

All (5975) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	409	BCR	C26-C25	15.51	1.61	1.34
31	a	409	BCR	C26-C25	15.51	1.61	1.34
31	b	619	BCR	C5-C6	15.49	1.61	1.34
31	B	619	BCR	C5-C6	15.47	1.61	1.34
31	x	202	BCR	C5-C6	15.45	1.61	1.34
31	z	101	BCR	C5-C6	15.44	1.61	1.34
31	X	201	BCR	C5-C6	15.44	1.61	1.34
31	c	516	BCR	C26-C25	15.40	1.61	1.34
31	C	516	BCR	C5-C6	15.39	1.61	1.34
31	d	403	BCR	C26-C25	15.35	1.61	1.34
31	D	404	BCR	C26-C25	15.35	1.61	1.34
31	T	101	BCR	C5-C6	15.34	1.61	1.34
31	t	101	BCR	C5-C6	15.34	1.61	1.34
31	C	518	BCR	C26-C25	15.33	1.61	1.34
31	b	619	BCR	C26-C25	15.31	1.61	1.34
31	b	618	BCR	C5-C6	15.30	1.60	1.34
31	k	101	BCR	C5-C6	15.29	1.60	1.34
31	x	202	BCR	C26-C25	15.28	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	201	BCR	C26-C25	15.27	1.60	1.34
31	B	619	BCR	C26-C25	15.27	1.60	1.34
31	K	101	BCR	C5-C6	15.25	1.60	1.34
31	K	101	BCR	C26-C25	15.25	1.60	1.34
31	k	101	BCR	C26-C25	15.25	1.60	1.34
31	C	518	BCR	C5-C6	15.23	1.60	1.34
31	b	620	BCR	C5-C6	15.22	1.60	1.34
31	c	516	BCR	C5-C6	15.22	1.60	1.34
31	B	618	BCR	C5-C6	15.20	1.60	1.34
31	t	101	BCR	C26-C25	15.19	1.60	1.34
31	C	516	BCR	C26-C25	15.19	1.60	1.34
31	B	620	BCR	C5-C6	15.18	1.60	1.34
31	B	618	BCR	C26-C25	15.15	1.60	1.34
31	T	101	BCR	C26-C25	15.14	1.60	1.34
31	z	101	BCR	C26-C25	15.13	1.60	1.34
31	d	403	BCR	C5-C6	15.12	1.60	1.34
31	D	404	BCR	C5-C6	15.11	1.60	1.34
31	b	618	BCR	C26-C25	15.08	1.60	1.34
31	A	409	BCR	C5-C6	15.05	1.60	1.34
31	a	409	BCR	C5-C6	14.98	1.60	1.34
31	B	620	BCR	C26-C25	14.97	1.60	1.34
31	b	620	BCR	C26-C25	14.97	1.60	1.34
31	c	515	BCR	C5-C6	14.92	1.60	1.34
31	c	515	BCR	C26-C25	14.88	1.60	1.34
31	C	517	BCR	C5-C6	14.88	1.60	1.34
31	C	517	BCR	C26-C25	14.85	1.60	1.34
30	A	407	PHO	C1B-C2B	8.82	1.49	1.39
30	a	407	PHO	C1B-C2B	8.71	1.49	1.39
30	d	401	PHO	C1B-C2B	8.71	1.49	1.39
30	D	401	PHO	C1B-C2B	8.71	1.49	1.39
33	a	411	PL9	C6-C5	8.00	1.53	1.35
33	A	410	PL9	C6-C5	7.98	1.53	1.35
31	B	618	BCR	C30-C25	-7.96	1.42	1.53
31	b	618	BCR	C30-C25	-7.92	1.42	1.53
30	A	407	PHO	C3B-C4B	7.63	1.50	1.41
30	a	407	PHO	C3B-C4B	7.56	1.50	1.41
30	d	401	PHO	C3B-C4B	7.37	1.49	1.41
30	D	401	PHO	C3B-C4B	7.36	1.49	1.41
33	A	410	PL9	C2-C3	7.26	1.53	1.34
33	a	411	PL9	C2-C3	7.23	1.53	1.34
31	c	515	BCR	C30-C25	-7.18	1.43	1.53
31	C	517	BCR	C30-C25	-7.11	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	620	BCR	C30-C25	-7.01	1.44	1.53
31	B	620	BCR	C30-C25	-7.00	1.44	1.53
31	z	101	BCR	C30-C25	-6.93	1.44	1.53
33	d	404	PL9	C2-C3	6.88	1.52	1.34
33	D	405	PL9	C2-C3	6.86	1.52	1.34
31	c	516	BCR	C30-C25	-6.86	1.44	1.53
31	C	516	BCR	C30-C25	-6.86	1.44	1.53
31	C	518	BCR	C30-C25	-6.83	1.44	1.53
31	b	619	BCR	C30-C25	-6.79	1.44	1.53
31	x	202	BCR	C30-C25	-6.77	1.44	1.53
31	B	619	BCR	C30-C25	-6.76	1.44	1.53
31	A	409	BCR	C30-C25	-6.71	1.44	1.53
31	X	201	BCR	C30-C25	-6.70	1.44	1.53
31	a	409	BCR	C30-C25	-6.69	1.44	1.53
31	C	517	BCR	C29-C28	-6.62	1.36	1.52
31	c	515	BCR	C29-C28	-6.62	1.36	1.52
31	C	516	BCR	C29-C28	-6.56	1.36	1.52
31	z	101	BCR	C29-C28	-6.54	1.36	1.52
31	A	409	BCR	C29-C28	-6.52	1.36	1.52
31	k	101	BCR	C30-C25	-6.52	1.44	1.53
31	K	101	BCR	C30-C25	-6.52	1.44	1.53
31	a	409	BCR	C29-C28	-6.51	1.36	1.52
31	B	618	BCR	C29-C28	-6.50	1.36	1.52
31	b	618	BCR	C29-C28	-6.47	1.36	1.52
31	C	518	BCR	C29-C28	-6.44	1.36	1.52
31	c	516	BCR	C29-C28	-6.43	1.36	1.52
31	X	201	BCR	C29-C28	-6.42	1.36	1.52
31	B	619	BCR	C29-C28	-6.41	1.36	1.52
31	D	404	BCR	C30-C25	-6.40	1.45	1.53
31	b	619	BCR	C29-C28	-6.40	1.36	1.52
31	b	620	BCR	C29-C28	-6.39	1.36	1.52
31	B	620	BCR	C29-C28	-6.38	1.36	1.52
31	t	101	BCR	C29-C28	-6.38	1.36	1.52
31	t	101	BCR	C30-C25	-6.37	1.45	1.53
31	d	403	BCR	C30-C25	-6.36	1.45	1.53
31	b	618	BCR	C2-C3	-6.36	1.36	1.52
31	x	202	BCR	C29-C28	-6.35	1.36	1.52
31	T	101	BCR	C29-C28	-6.35	1.36	1.52
31	T	101	BCR	C30-C25	-6.31	1.45	1.53
31	k	101	BCR	C29-C28	-6.31	1.37	1.52
31	K	101	BCR	C29-C28	-6.30	1.37	1.52
31	c	516	BCR	C2-C3	-6.27	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	516	BCR	C2-C3	-6.27	1.37	1.52
31	B	618	BCR	C2-C3	-6.26	1.37	1.52
31	x	202	BCR	C2-C3	-6.26	1.37	1.52
31	B	619	BCR	C2-C3	-6.25	1.37	1.52
31	a	409	BCR	C2-C3	-6.25	1.37	1.52
31	z	101	BCR	C2-C3	-6.25	1.37	1.52
31	C	518	BCR	C2-C3	-6.24	1.37	1.52
31	B	620	BCR	C2-C3	-6.24	1.37	1.52
31	A	409	BCR	C2-C3	-6.24	1.37	1.52
31	t	101	BCR	C2-C3	-6.23	1.37	1.52
31	X	201	BCR	C2-C3	-6.23	1.37	1.52
31	T	101	BCR	C2-C3	-6.23	1.37	1.52
31	b	619	BCR	C2-C3	-6.23	1.37	1.52
31	D	404	BCR	C2-C3	-6.22	1.37	1.52
31	d	403	BCR	C2-C3	-6.21	1.37	1.52
31	b	620	BCR	C2-C3	-6.21	1.37	1.52
31	d	403	BCR	C29-C28	-6.20	1.37	1.52
31	D	404	BCR	C29-C28	-6.17	1.37	1.52
31	A	409	BCR	C1-C6	-6.15	1.45	1.53
31	k	101	BCR	C2-C3	-6.15	1.37	1.52
31	a	409	BCR	C1-C6	-6.14	1.45	1.53
31	C	517	BCR	C2-C3	-6.13	1.37	1.52
31	K	101	BCR	C2-C3	-6.12	1.37	1.52
31	c	515	BCR	C2-C3	-6.09	1.37	1.52
31	T	101	BCR	C8-C9	6.02	1.58	1.45
31	t	101	BCR	C8-C9	6.00	1.58	1.45
31	c	515	BCR	C1-C6	-5.98	1.45	1.53
31	C	517	BCR	C1-C6	-5.95	1.45	1.53
31	D	404	BCR	C8-C9	5.83	1.58	1.45
31	B	620	BCR	C1-C6	-5.81	1.45	1.53
31	X	201	BCR	C1-C6	-5.81	1.45	1.53
31	b	618	BCR	C1-C6	-5.80	1.45	1.53
31	b	620	BCR	C1-C6	-5.80	1.45	1.53
31	d	403	BCR	C8-C9	5.80	1.58	1.45
31	b	620	BCR	C8-C9	5.80	1.58	1.45
31	C	516	BCR	C1-C6	-5.79	1.45	1.53
31	x	202	BCR	C1-C6	-5.78	1.45	1.53
31	X	201	BCR	C8-C9	5.76	1.58	1.45
31	B	620	BCR	C8-C9	5.75	1.58	1.45
31	x	202	BCR	C8-C9	5.73	1.58	1.45
31	z	101	BCR	C1-C6	-5.70	1.45	1.53
31	D	404	BCR	C1-C6	-5.65	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	K	101	BCR	C8-C9	5.65	1.58	1.45
31	B	618	BCR	C1-C6	-5.63	1.46	1.53
31	d	403	BCR	C1-C6	-5.63	1.46	1.53
31	k	101	BCR	C8-C9	5.63	1.58	1.45
31	c	516	BCR	C8-C9	5.60	1.58	1.45
31	C	518	BCR	C8-C9	5.58	1.57	1.45
31	z	101	BCR	C8-C9	5.56	1.57	1.45
31	B	619	BCR	C8-C9	5.53	1.57	1.45
31	t	101	BCR	C19-C18	5.53	1.57	1.45
31	C	516	BCR	C8-C9	5.53	1.57	1.45
31	b	619	BCR	C8-C9	5.52	1.57	1.45
31	T	101	BCR	C19-C18	5.51	1.57	1.45
31	B	618	BCR	C8-C9	5.48	1.57	1.45
26	1	317	CHL	O2D-CGD	5.46	1.46	1.33
26	4	316	CHL	O2D-CGD	5.44	1.46	1.33
31	b	618	BCR	C8-C9	5.44	1.57	1.45
31	A	409	BCR	C8-C9	5.42	1.57	1.45
31	c	515	BCR	C8-C9	5.38	1.57	1.45
31	C	517	BCR	C8-C9	5.37	1.57	1.45
31	a	409	BCR	C8-C9	5.36	1.57	1.45
26	v	317	CHL	O2D-CGD	5.36	1.46	1.33
31	k	101	BCR	C1-C6	-5.35	1.46	1.53
31	D	404	BCR	C29-C30	5.35	1.66	1.54
31	C	518	BCR	C1-C6	-5.33	1.46	1.53
31	X	201	BCR	C19-C18	5.32	1.57	1.45
31	T	101	BCR	C29-C30	5.32	1.66	1.54
31	t	101	BCR	C29-C30	5.32	1.66	1.54
31	x	202	BCR	C19-C18	5.31	1.57	1.45
31	d	403	BCR	C29-C30	5.31	1.66	1.54
31	c	516	BCR	C1-C6	-5.30	1.46	1.53
31	K	101	BCR	C1-C6	-5.29	1.46	1.53
26	V	317	CHL	O2D-CGD	5.29	1.46	1.33
31	K	101	BCR	C29-C30	5.25	1.66	1.54
31	b	619	BCR	C1-C6	-5.25	1.46	1.53
26	U	316	CHL	O2D-CGD	5.24	1.46	1.33
26	g	313	CHL	O2D-CGD	5.24	1.46	1.33
31	b	620	BCR	C19-C18	5.23	1.57	1.45
26	n	316	CHL	O2D-CGD	5.23	1.46	1.33
26	u	317	CHL	O2D-CGD	5.23	1.46	1.33
31	c	516	BCR	C19-C18	5.22	1.57	1.45
31	D	404	BCR	C19-C18	5.22	1.57	1.45
31	k	101	BCR	C29-C30	5.22	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	518	BCR	C19-C18	5.21	1.57	1.45
26	Q	312	CHL	O2D-CGD	5.21	1.45	1.33
26	q	312	CHL	O2D-CGD	5.20	1.45	1.33
31	d	403	BCR	C19-C18	5.19	1.57	1.45
26	P	315	CHL	CHC-C1C	5.19	1.49	1.38
31	B	620	BCR	C19-C18	5.18	1.57	1.45
26	s	313	CHL	O2D-CGD	5.17	1.45	1.33
26	g	316	CHL	O2D-CGD	5.17	1.45	1.33
26	s	314	CHL	O2D-CGD	5.16	1.45	1.33
31	z	101	BCR	C19-C18	5.16	1.57	1.45
26	V	316	CHL	O2D-CGD	5.16	1.45	1.33
26	n	315	CHL	O2D-CGD	5.16	1.45	1.33
31	B	619	BCR	C1-C6	-5.16	1.46	1.53
31	b	620	BCR	C29-C30	5.15	1.66	1.54
26	p	320	CHL	O2D-CGD	5.15	1.45	1.33
26	S	314	CHL	O2D-CGD	5.15	1.45	1.33
26	3	312	CHL	O2D-CGD	5.15	1.45	1.33
26	G	316	CHL	O2D-CGD	5.15	1.45	1.33
31	C	516	BCR	C19-C18	5.14	1.57	1.45
31	x	202	BCR	C29-C30	5.14	1.66	1.54
26	g	314	CHL	O2D-CGD	5.14	1.45	1.33
26	3	314	CHL	O2D-CGD	5.14	1.45	1.33
26	r	615	CHL	O2D-CGD	5.13	1.45	1.33
26	2	316	CHL	O2D-CGD	5.13	1.45	1.33
26	S	313	CHL	O2D-CGD	5.13	1.45	1.33
31	B	620	BCR	C29-C30	5.13	1.66	1.54
26	v	315	CHL	O2D-CGD	5.13	1.45	1.33
31	T	101	BCR	C1-C6	-5.13	1.46	1.53
26	p	315	CHL	O2D-CGD	5.12	1.45	1.33
26	G	312	CHL	O2D-CGD	5.12	1.45	1.33
26	R	315	CHL	O2D-CGD	5.12	1.45	1.33
26	6	315	CHL	O2D-CGD	5.12	1.45	1.33
26	G	313	CHL	O2D-CGD	5.12	1.45	1.33
31	X	201	BCR	C29-C30	5.12	1.65	1.54
26	Q	313	CHL	O2D-CGD	5.12	1.45	1.33
26	P	317	CHL	O2D-CGD	5.12	1.45	1.33
26	Q	314	CHL	O2D-CGD	5.12	1.45	1.33
26	G	314	CHL	O2D-CGD	5.12	1.45	1.33
31	z	101	BCR	C29-C30	5.12	1.65	1.54
26	4	314	CHL	O2D-CGD	5.11	1.45	1.33
26	6	313	CHL	O2D-CGD	5.11	1.45	1.33
26	P	319	CHL	O2D-CGD	5.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v	316	CHL	O2D-CGD	5.11	1.45	1.33
26	u	314	CHL	O2D-CGD	5.11	1.45	1.33
26	p	317	CHL	O2D-CGD	5.10	1.45	1.33
26	5	313	CHL	O2D-CGD	5.10	1.45	1.33
26	g	312	CHL	O2D-CGD	5.10	1.45	1.33
26	p	318	CHL	O2D-CGD	5.10	1.45	1.33
26	1	314	CHL	O2D-CGD	5.10	1.45	1.33
26	U	314	CHL	O2D-CGD	5.10	1.45	1.33
26	u	315	CHL	O2D-CGD	5.10	1.45	1.33
26	5	316	CHL	O2D-CGD	5.10	1.45	1.33
26	v	318	CHL	O2D-CGD	5.10	1.45	1.33
26	N	315	CHL	O2D-CGD	5.09	1.45	1.33
26	r	614	CHL	O2D-CGD	5.09	1.45	1.33
26	3	316	CHL	O2D-CGD	5.09	1.45	1.33
26	v	314	CHL	O2D-CGD	5.09	1.45	1.33
26	2	314	CHL	O2D-CGD	5.09	1.45	1.33
26	5	314	CHL	O2D-CGD	5.09	1.45	1.33
26	Q	316	CHL	O2D-CGD	5.09	1.45	1.33
26	R	316	CHL	O2D-CGD	5.09	1.45	1.33
26	P	314	CHL	O2D-CGD	5.09	1.45	1.33
26	U	315	CHL	O2D-CGD	5.09	1.45	1.33
26	V	315	CHL	O2D-CGD	5.09	1.45	1.33
26	P	316	CHL	O2D-CGD	5.09	1.45	1.33
26	1	318	CHL	O2D-CGD	5.08	1.45	1.33
26	u	316	CHL	O2D-CGD	5.08	1.45	1.33
26	r	616	CHL	O2D-CGD	5.08	1.45	1.33
26	G	315	CHL	O2D-CGD	5.08	1.45	1.33
31	C	516	BCR	C29-C30	5.08	1.65	1.54
26	q	313	CHL	O2D-CGD	5.08	1.45	1.33
26	V	314	CHL	O2D-CGD	5.08	1.45	1.33
26	q	311	CHL	O2D-CGD	5.08	1.45	1.33
26	N	313	CHL	O2D-CGD	5.08	1.45	1.33
26	p	314	CHL	O2D-CGD	5.07	1.45	1.33
26	6	317	CHL	O2D-CGD	5.07	1.45	1.33
26	5	318	CHL	O2D-CGD	5.07	1.45	1.33
26	q	314	CHL	O2D-CGD	5.07	1.45	1.33
26	P	318	CHL	O2D-CGD	5.07	1.45	1.33
26	N	314	CHL	O2D-CGD	5.07	1.45	1.33
26	6	314	CHL	O2D-CGD	5.07	1.45	1.33
26	S	315	CHL	O2D-CGD	5.07	1.45	1.33
26	4	315	CHL	O2D-CGD	5.07	1.45	1.33
26	V	318	CHL	O2D-CGD	5.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	314	CHL	O2D-CGD	5.07	1.45	1.33
26	R	317	CHL	O2D-CGD	5.07	1.45	1.33
26	Q	315	CHL	O2D-CGD	5.06	1.45	1.33
26	2	315	CHL	O2D-CGD	5.06	1.45	1.33
26	s	315	CHL	O2D-CGD	5.06	1.45	1.33
26	U	319	CHL	O2D-CGD	5.06	1.45	1.33
26	n	313	CHL	O2D-CGD	5.06	1.45	1.33
26	p	319	CHL	O2D-CGD	5.06	1.45	1.33
26	n	317	CHL	O2D-CGD	5.06	1.45	1.33
26	5	315	CHL	O2D-CGD	5.06	1.45	1.33
26	n	318	CHL	O2D-CGD	5.06	1.45	1.33
31	b	619	BCR	C19-C18	5.06	1.56	1.45
31	K	101	BCR	C19-C18	5.05	1.56	1.45
31	t	101	BCR	C1-C6	-5.05	1.46	1.53
26	p	316	CHL	O2D-CGD	5.05	1.45	1.33
26	r	619	CHL	O2D-CGD	5.04	1.45	1.33
26	u	313	CHL	O2D-CGD	5.04	1.45	1.33
26	2	318	CHL	O2D-CGD	5.04	1.45	1.33
26	4	317	CHL	O2D-CGD	5.04	1.45	1.33
26	Q	311	CHL	O2D-CGD	5.04	1.45	1.33
26	2	313	CHL	O2D-CGD	5.03	1.45	1.33
26	1	313	CHL	C3D-C4D	-5.03	1.32	1.44
31	b	619	BCR	C29-C30	5.03	1.65	1.54
26	3	315	CHL	O2D-CGD	5.03	1.45	1.33
26	g	311	CHL	O2D-CGD	5.03	1.45	1.33
26	N	317	CHL	O2D-CGD	5.03	1.45	1.33
26	3	313	CHL	O2D-CGD	5.02	1.45	1.33
26	U	313	CHL	O2D-CGD	5.02	1.45	1.33
31	B	619	BCR	C29-C30	5.02	1.65	1.54
26	s	316	CHL	O2D-CGD	5.02	1.45	1.33
26	q	315	CHL	O2D-CGD	5.01	1.45	1.33
26	5	317	CHL	O2D-CGD	5.01	1.45	1.33
26	4	313	CHL	O2D-CGD	5.01	1.45	1.33
26	2	317	CHL	O2D-CGD	5.01	1.45	1.33
26	1	315	CHL	O2D-CGD	5.01	1.45	1.33
31	k	101	BCR	C19-C18	5.01	1.56	1.45
31	a	409	BCR	C29-C30	5.01	1.65	1.54
31	B	619	BCR	C19-C18	5.01	1.56	1.45
26	g	315	CHL	O2D-CGD	5.01	1.45	1.33
26	6	312	CHL	O2D-CGD	5.00	1.45	1.33
31	c	516	BCR	C29-C30	5.00	1.65	1.54
26	v	313	CHL	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	315	CHL	C2C-C3C	5.00	1.47	1.36
26	p	315	CHL	CHC-C1C	5.00	1.48	1.38
26	V	313	CHL	O2D-CGD	5.00	1.45	1.33
31	A	409	BCR	C29-C30	4.99	1.65	1.54
26	u	318	CHL	O2D-CGD	4.99	1.45	1.33
31	C	517	BCR	C19-C18	4.99	1.56	1.45
26	1	313	CHL	O2D-CGD	4.99	1.45	1.33
26	n	317	CHL	C3D-C4D	-4.99	1.32	1.44
31	c	515	BCR	C19-C18	4.99	1.56	1.45
26	P	314	CHL	CHC-C1C	4.98	1.48	1.38
31	B	618	BCR	C29-C30	4.98	1.65	1.54
31	b	618	BCR	C29-C30	4.98	1.65	1.54
26	N	316	CHL	O2D-CGD	4.98	1.45	1.33
26	G	311	CHL	O2D-CGD	4.98	1.45	1.33
26	1	316	CHL	O2D-CGD	4.98	1.45	1.33
26	S	316	CHL	O2D-CGD	4.98	1.45	1.33
26	R	317	CHL	C3D-C4D	-4.98	1.32	1.44
26	U	313	CHL	C3D-C4D	-4.97	1.32	1.44
26	2	314	CHL	C2C-C3C	4.97	1.47	1.36
31	C	518	BCR	C29-C30	4.96	1.65	1.54
26	4	313	CHL	C3D-C4D	-4.95	1.33	1.44
31	c	515	BCR	C29-C30	4.95	1.65	1.54
31	C	517	BCR	C29-C30	4.95	1.65	1.54
26	U	317	CHL	O2D-CGD	4.95	1.45	1.33
26	6	301	CHL	C3D-C4D	-4.94	1.33	1.44
26	3	311	CHL	O2D-CGD	4.94	1.45	1.33
26	S	313	CHL	C3D-C4D	-4.94	1.33	1.44
26	r	616	CHL	C3D-C4D	-4.94	1.33	1.44
26	6	316	CHL	O2D-CGD	4.94	1.45	1.33
26	1	315	CHL	C3D-C4D	-4.93	1.33	1.44
26	p	315	CHL	C2C-C3C	4.93	1.47	1.36
26	P	315	CHL	C3D-C4D	-4.93	1.33	1.44
26	5	316	CHL	C3D-C4D	-4.92	1.33	1.44
24	r	612	XAT	C2-C3	-4.91	1.45	1.52
26	1	316	CHL	C3D-C4D	-4.91	1.33	1.44
26	6	301	CHL	O2D-CGD	4.91	1.45	1.33
26	V	313	CHL	C3D-C4D	-4.91	1.33	1.44
26	s	313	CHL	C3D-C4D	-4.91	1.33	1.44
26	P	315	CHL	O2D-CGD	4.91	1.45	1.33
26	n	318	CHL	C3D-C4D	-4.90	1.33	1.44
26	4	315	CHL	C3D-C4D	-4.90	1.33	1.44
26	v	313	CHL	C3D-C4D	-4.89	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p	315	CHL	C3D-C4D	-4.89	1.33	1.44
26	u	316	CHL	C3D-C4D	-4.89	1.33	1.44
26	N	316	CHL	C3D-C4D	-4.88	1.33	1.44
24	R	313	XAT	C8-C9	4.87	1.56	1.45
24	R	313	XAT	C2-C3	-4.87	1.45	1.52
26	5	314	CHL	C2C-C3C	4.87	1.47	1.36
26	2	316	CHL	C3D-C4D	-4.87	1.33	1.44
26	3	312	CHL	C2C-C3C	4.87	1.47	1.36
24	U	311	XAT	C22-C23	-4.87	1.45	1.52
26	v	316	CHL	C3D-C4D	-4.86	1.33	1.44
26	N	315	CHL	C3D-C4D	-4.86	1.33	1.44
26	P	317	CHL	C3D-C4D	-4.85	1.33	1.44
26	v	315	CHL	C3D-C4D	-4.85	1.33	1.44
31	a	409	BCR	C19-C18	4.85	1.56	1.45
26	p	317	CHL	C3D-C4D	-4.85	1.33	1.44
26	6	313	CHL	CHD-C1D	4.85	1.47	1.38
26	4	316	CHL	C3D-C4D	-4.85	1.33	1.44
26	6	314	CHL	C3D-C4D	-4.85	1.33	1.44
26	3	313	CHL	C3D-C4D	-4.84	1.33	1.44
26	G	311	CHL	C3D-C4D	-4.84	1.33	1.44
26	N	317	CHL	C3D-C4D	-4.84	1.33	1.44
26	s	315	CHL	C2C-C3C	4.84	1.47	1.36
26	6	313	CHL	C2C-C3C	4.83	1.47	1.36
26	v	317	CHL	C3D-C4D	-4.83	1.33	1.44
26	u	313	CHL	C3D-C4D	-4.83	1.33	1.44
26	q	312	CHL	CHD-C1D	4.83	1.47	1.38
31	B	618	BCR	C19-C18	4.83	1.56	1.45
24	q	309	XAT	C8-C9	4.83	1.56	1.45
26	g	316	CHL	C3D-C4D	-4.83	1.33	1.44
24	Q	309	XAT	C8-C9	4.82	1.56	1.45
26	V	315	CHL	C3D-C4D	-4.82	1.33	1.44
24	u	311	XAT	C22-C23	-4.82	1.45	1.52
26	n	314	CHL	CHC-C1C	4.82	1.48	1.38
24	r	612	XAT	C8-C9	4.82	1.56	1.45
26	2	313	CHL	C3D-C4D	-4.81	1.33	1.44
26	p	314	CHL	CHC-C1C	4.81	1.48	1.38
26	p	314	CHL	C3D-C4D	-4.81	1.33	1.44
26	U	314	CHL	C3D-C4D	-4.81	1.33	1.44
31	A	409	BCR	C19-C18	4.81	1.56	1.45
24	G	309	XAT	C28-C29	4.81	1.56	1.45
26	6	317	CHL	C3D-C4D	-4.81	1.33	1.44
26	5	318	CHL	C3D-C4D	-4.81	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	312	CHL	C2C-C3C	4.81	1.47	1.36
26	P	316	CHL	C3D-C4D	-4.81	1.33	1.44
26	S	315	CHL	C3D-C4D	-4.81	1.33	1.44
26	3	312	CHL	CHD-C1D	4.80	1.47	1.38
26	s	315	CHL	C3D-C4D	-4.80	1.33	1.44
26	2	314	CHL	CHC-C1C	4.80	1.48	1.38
26	V	317	CHL	C3D-C4D	-4.80	1.33	1.44
26	S	315	CHL	C2C-C3C	4.80	1.47	1.36
26	6	312	CHL	C3D-C4D	-4.80	1.33	1.44
26	3	311	CHL	C3D-C4D	-4.80	1.33	1.44
26	p	316	CHL	C3D-C4D	-4.80	1.33	1.44
26	U	315	CHL	C3D-C4D	-4.80	1.33	1.44
26	u	314	CHL	C3D-C4D	-4.80	1.33	1.44
26	n	315	CHL	C3D-C4D	-4.80	1.33	1.44
31	b	618	BCR	C19-C18	4.79	1.56	1.45
26	5	313	CHL	C3D-C4D	-4.79	1.33	1.44
26	3	312	CHL	CHC-C1C	4.79	1.48	1.38
26	1	317	CHL	C3D-C4D	-4.79	1.33	1.44
26	s	316	CHL	C3D-C4D	-4.79	1.33	1.44
26	u	317	CHL	C3D-C4D	-4.79	1.33	1.44
26	q	313	CHL	C3D-C4D	-4.79	1.33	1.44
26	V	316	CHL	C3D-C4D	-4.79	1.33	1.44
26	3	314	CHL	C3D-C4D	-4.79	1.33	1.44
26	P	314	CHL	C3D-C4D	-4.78	1.33	1.44
26	6	315	CHL	C3D-C4D	-4.78	1.33	1.44
26	S	316	CHL	C3D-C4D	-4.78	1.33	1.44
26	Q	313	CHL	C3D-C4D	-4.78	1.33	1.44
24	V	311	XAT	C8-C9	4.78	1.56	1.45
24	3	309	XAT	C28-C29	4.78	1.56	1.45
26	Q	311	CHL	C3D-C4D	-4.78	1.33	1.44
26	3	316	CHL	C3D-C4D	-4.77	1.33	1.44
24	R	313	XAT	C22-C23	-4.77	1.45	1.52
26	2	318	CHL	C3D-C4D	-4.77	1.33	1.44
26	Q	316	CHL	C3D-C4D	-4.77	1.33	1.44
26	3	315	CHL	C2C-C3C	4.77	1.47	1.36
24	g	309	XAT	C22-C23	-4.77	1.45	1.52
26	N	314	CHL	C3D-C4D	-4.77	1.33	1.44
26	1	318	CHL	C3D-C4D	-4.77	1.33	1.44
26	U	316	CHL	C3D-C4D	-4.76	1.33	1.44
24	6	310	XAT	C28-C29	4.76	1.56	1.45
24	g	309	XAT	C8-C9	4.76	1.56	1.45
24	Q	309	XAT	C28-C29	4.76	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	312	CHL	C2C-C3C	4.76	1.46	1.36
26	G	316	CHL	C3D-C4D	-4.76	1.33	1.44
24	5	311	XAT	C8-C9	4.76	1.56	1.45
26	S	314	CHL	C2C-C3C	4.76	1.46	1.36
26	p	319	CHL	C3D-C4D	-4.75	1.33	1.44
26	5	317	CHL	C3D-C4D	-4.75	1.33	1.44
24	v	311	XAT	C8-C9	4.75	1.56	1.45
26	3	313	CHL	C2C-C3C	4.75	1.46	1.36
24	g	309	XAT	C2-C3	-4.75	1.45	1.52
26	P	318	CHL	C3D-C4D	-4.75	1.33	1.44
26	N	313	CHL	C3D-C4D	-4.75	1.33	1.44
26	4	317	CHL	C3D-C4D	-4.75	1.33	1.44
26	q	315	CHL	C3D-C4D	-4.75	1.33	1.44
26	s	314	CHL	C2C-C3C	4.75	1.46	1.36
24	r	612	XAT	C22-C23	-4.75	1.45	1.52
26	q	312	CHL	CHC-C1C	4.74	1.48	1.38
24	p	312	XAT	C28-C29	4.74	1.56	1.45
26	s	315	CHL	CHC-C1C	4.74	1.48	1.38
26	6	313	CHL	CHC-C1C	4.74	1.48	1.38
26	P	315	CHL	CHD-C1D	4.74	1.47	1.38
26	6	316	CHL	C2C-C3C	4.74	1.46	1.36
26	p	318	CHL	C3D-C4D	-4.74	1.33	1.44
26	u	315	CHL	C3D-C4D	-4.74	1.33	1.44
26	V	315	CHL	C2C-C3C	4.74	1.46	1.36
26	s	314	CHL	C3D-C4D	-4.74	1.33	1.44
26	G	313	CHL	C3D-C4D	-4.74	1.33	1.44
24	P	312	XAT	C8-C9	4.74	1.56	1.45
24	2	311	XAT	C8-C9	4.73	1.56	1.45
24	V	311	XAT	C28-C29	4.73	1.56	1.45
26	3	315	CHL	C3D-C4D	-4.73	1.33	1.44
24	G	309	XAT	C2-C3	-4.73	1.45	1.52
26	2	317	CHL	C3D-C4D	-4.73	1.33	1.44
26	U	319	CHL	C3D-C4D	-4.73	1.33	1.44
24	5	311	XAT	C28-C29	4.73	1.56	1.45
24	G	309	XAT	C8-C9	4.73	1.56	1.45
26	S	316	CHL	C2C-C3C	4.72	1.46	1.36
26	s	316	CHL	C2C-C3C	4.72	1.46	1.36
26	G	312	CHL	CHC-C1C	4.72	1.48	1.38
24	p	312	XAT	C8-C9	4.72	1.56	1.45
26	4	314	CHL	C3D-C4D	-4.72	1.33	1.44
26	5	313	CHL	CHC-C1C	4.72	1.48	1.38
26	g	315	CHL	C3D-C4D	-4.72	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	313	CHL	C3D-C4D	-4.72	1.33	1.44
26	S	315	CHL	CHC-C1C	4.72	1.48	1.38
26	6	314	CHL	C2C-C3C	4.72	1.46	1.36
26	5	315	CHL	C3D-C4D	-4.72	1.33	1.44
24	P	312	XAT	C28-C29	4.71	1.56	1.45
24	P	312	XAT	C32-C33	4.71	1.56	1.45
26	2	314	CHL	CHD-C1D	4.71	1.47	1.38
24	q	309	XAT	C22-C23	-4.71	1.45	1.52
24	n	311	XAT	C8-C9	4.71	1.56	1.45
24	3	309	XAT	C22-C23	-4.71	1.45	1.52
26	6	316	CHL	C3D-C4D	-4.71	1.33	1.44
26	5	314	CHL	CHC-C1C	4.71	1.48	1.38
24	4	311	XAT	C22-C23	-4.71	1.45	1.52
26	Q	315	CHL	C3D-C4D	-4.71	1.33	1.44
24	p	312	XAT	C2-C3	-4.71	1.45	1.52
26	q	311	CHL	C3D-C4D	-4.70	1.33	1.44
26	g	312	CHL	C2C-C3C	4.70	1.46	1.36
26	r	619	CHL	C3D-C4D	-4.70	1.33	1.44
31	t	101	BCR	C23-C22	4.70	1.56	1.45
24	1	311	XAT	C2-C3	-4.70	1.45	1.52
31	T	101	BCR	C23-C22	4.70	1.56	1.45
26	2	315	CHL	C3D-C4D	-4.70	1.33	1.44
24	v	311	XAT	C22-C23	-4.70	1.45	1.52
26	g	311	CHL	C3D-C4D	-4.69	1.33	1.44
24	G	309	XAT	C22-C23	-4.69	1.45	1.52
24	N	311	XAT	C28-C29	4.69	1.56	1.45
24	g	309	XAT	C28-C29	4.69	1.56	1.45
24	N	311	XAT	C22-C23	-4.69	1.45	1.52
26	v	315	CHL	C2C-C3C	4.69	1.46	1.36
24	q	309	XAT	C28-C29	4.69	1.56	1.45
24	n	311	XAT	C28-C29	4.69	1.56	1.45
26	v	318	CHL	C3D-C4D	-4.68	1.33	1.44
26	V	314	CHL	C2C-C3C	4.68	1.46	1.36
26	G	315	CHL	C3D-C4D	-4.68	1.33	1.44
26	V	315	CHL	CHC-C1C	4.68	1.48	1.38
24	1	311	XAT	C28-C29	4.68	1.56	1.45
26	3	314	CHL	CHC-C1C	4.68	1.48	1.38
26	S	314	CHL	C3D-C4D	-4.68	1.33	1.44
26	n	313	CHL	CHC-C1C	4.68	1.48	1.38
24	1	311	XAT	C22-C23	-4.68	1.45	1.52
26	q	314	CHL	C2C-C3C	4.68	1.46	1.36
26	n	316	CHL	C3D-C4D	-4.68	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	313	XAT	C28-C29	4.67	1.56	1.45
26	4	315	CHL	C2C-C3C	4.67	1.46	1.36
26	6	314	CHL	CHC-C1C	4.67	1.48	1.38
26	V	314	CHL	CHD-C1D	4.67	1.47	1.38
26	S	316	CHL	CHC-C1C	4.67	1.48	1.38
26	U	317	CHL	C3D-C4D	-4.67	1.33	1.44
24	r	612	XAT	C28-C29	4.67	1.56	1.45
26	1	315	CHL	C2C-C3C	4.67	1.46	1.36
24	n	311	XAT	C22-C23	-4.67	1.45	1.52
24	6	310	XAT	C8-C9	4.67	1.56	1.45
24	V	311	XAT	C32-C33	4.67	1.56	1.45
26	R	315	CHL	C3D-C4D	-4.67	1.33	1.44
24	6	310	XAT	C2-C3	-4.66	1.45	1.52
24	v	311	XAT	C28-C29	4.66	1.56	1.45
24	u	311	XAT	C28-C29	4.66	1.56	1.45
24	5	311	XAT	C32-C33	4.66	1.56	1.45
26	5	313	CHL	C2C-C3C	4.66	1.46	1.36
26	g	314	CHL	C2C-C3C	4.66	1.46	1.36
24	p	312	XAT	C32-C33	4.66	1.55	1.45
26	V	318	CHL	C2C-C3C	4.66	1.46	1.36
24	u	311	XAT	C8-C9	4.66	1.55	1.45
26	Q	312	CHL	C2C-C3C	4.65	1.46	1.36
26	6	314	CHL	CHD-C1D	4.65	1.47	1.38
24	p	312	XAT	C22-C23	-4.65	1.45	1.52
24	2	311	XAT	C28-C29	4.65	1.55	1.45
24	R	313	XAT	C32-C33	4.65	1.55	1.45
26	s	315	CHL	CHD-C1D	4.65	1.47	1.38
24	Q	309	XAT	C32-C33	4.65	1.55	1.45
26	g	314	CHL	CHC-C1C	4.65	1.48	1.38
26	G	314	CHL	C3D-C4D	-4.64	1.33	1.44
24	q	309	XAT	C2-C3	-4.64	1.45	1.52
26	N	314	CHL	CHD-C1D	4.64	1.47	1.38
26	6	315	CHL	CHC-C1C	4.64	1.47	1.38
26	r	614	CHL	C3D-C4D	-4.64	1.33	1.44
26	q	314	CHL	C3D-C4D	-4.64	1.33	1.44
24	3	309	XAT	C8-C9	4.64	1.55	1.45
26	5	314	CHL	CHD-C1D	4.64	1.47	1.38
26	V	318	CHL	C3D-C4D	-4.64	1.33	1.44
26	Q	316	CHL	C2C-C3C	4.64	1.46	1.36
24	4	311	XAT	C28-C29	4.64	1.55	1.45
24	2	311	XAT	C2-C3	-4.64	1.45	1.52
26	n	314	CHL	CHD-C1D	4.63	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	312	CHL	CHD-C1D	4.63	1.47	1.38
26	p	320	CHL	C3D-C4D	-4.63	1.33	1.44
26	n	314	CHL	C3D-C4D	-4.63	1.33	1.44
24	2	311	XAT	C22-C23	-4.63	1.45	1.52
24	4	311	XAT	C2-C3	-4.63	1.45	1.52
26	Q	314	CHL	C3D-C4D	-4.63	1.33	1.44
24	N	311	XAT	C8-C9	4.63	1.55	1.45
26	V	314	CHL	CHC-C1C	4.63	1.47	1.38
24	2	311	XAT	C32-C33	4.62	1.55	1.45
26	q	315	CHL	C2C-C3C	4.62	1.46	1.36
24	P	312	XAT	C22-C23	-4.62	1.45	1.52
26	2	313	CHL	CHC-C1C	4.62	1.47	1.38
26	u	318	CHL	C3D-C4D	-4.62	1.33	1.44
26	P	319	CHL	C3D-C4D	-4.62	1.33	1.44
26	2	313	CHL	C2C-C3C	4.62	1.46	1.36
24	U	311	XAT	C28-C29	4.62	1.55	1.45
24	5	311	XAT	C2-C3	-4.62	1.45	1.52
26	n	315	CHL	C2C-C3C	4.62	1.46	1.36
31	b	620	BCR	C23-C22	4.62	1.55	1.45
26	S	315	CHL	CHD-C1D	4.61	1.47	1.38
26	G	314	CHL	C2C-C3C	4.61	1.46	1.36
26	2	315	CHL	C2C-C3C	4.61	1.46	1.36
26	3	316	CHL	C2C-C3C	4.61	1.46	1.36
26	3	313	CHL	CHD-C1D	4.61	1.47	1.38
24	V	311	XAT	C22-C23	-4.61	1.45	1.52
26	R	316	CHL	C3D-C4D	-4.61	1.33	1.44
24	P	312	XAT	C12-C13	4.61	1.55	1.45
26	6	317	CHL	C2C-C3C	4.61	1.46	1.36
24	r	612	XAT	C32-C33	4.61	1.55	1.45
24	U	311	XAT	C8-C9	4.60	1.55	1.45
26	p	319	CHL	C2C-C3C	4.60	1.46	1.36
26	s	316	CHL	CHC-C1C	4.60	1.47	1.38
24	1	311	XAT	C8-C9	4.60	1.55	1.45
26	P	316	CHL	C2C-C3C	4.60	1.46	1.36
26	6	315	CHL	C2C-C3C	4.60	1.46	1.36
24	q	309	XAT	C32-C33	4.59	1.55	1.45
26	v	318	CHL	C2C-C3C	4.59	1.46	1.36
26	Q	312	CHL	C3D-C4D	-4.59	1.33	1.44
26	5	315	CHL	C2C-C3C	4.59	1.46	1.36
24	4	311	XAT	C8-C9	4.59	1.55	1.45
24	v	311	XAT	C32-C33	4.59	1.55	1.45
26	N	314	CHL	CHC-C1C	4.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	309	XAT	C2-C3	-4.59	1.45	1.52
26	s	316	CHL	CHD-C1D	4.59	1.47	1.38
24	6	310	XAT	C22-C23	-4.59	1.45	1.52
26	N	317	CHL	C2C-C3C	4.58	1.46	1.36
26	p	315	CHL	CHD-C1D	4.58	1.47	1.38
26	3	314	CHL	C2C-C3C	4.58	1.46	1.36
26	r	615	CHL	C3D-C4D	-4.58	1.33	1.44
26	S	316	CHL	CHD-C1D	4.58	1.47	1.38
24	U	311	XAT	C2-C3	-4.58	1.45	1.52
26	1	314	CHL	C3D-C4D	-4.58	1.33	1.44
24	3	309	XAT	C32-C33	4.58	1.55	1.45
26	Q	315	CHL	C2C-C3C	4.58	1.46	1.36
24	u	311	XAT	C32-C33	4.57	1.55	1.45
24	Q	309	XAT	C22-C23	-4.57	1.45	1.52
26	g	312	CHL	CHD-C1D	4.57	1.47	1.38
26	3	316	CHL	CHD-C1D	4.57	1.47	1.38
26	q	312	CHL	C3D-C4D	-4.57	1.33	1.44
24	6	310	XAT	C12-C13	4.57	1.55	1.45
26	P	314	CHL	C2C-C3C	4.56	1.46	1.36
24	V	311	XAT	C2-C3	-4.56	1.45	1.52
26	R	316	CHL	C2C-C3C	4.56	1.46	1.36
24	P	312	XAT	C2-C3	-4.56	1.45	1.52
24	6	310	XAT	C32-C33	4.56	1.55	1.45
26	n	314	CHL	C2C-C3C	4.56	1.46	1.36
26	p	316	CHL	C2C-C3C	4.56	1.46	1.36
26	V	316	CHL	C2C-C3C	4.55	1.46	1.36
26	V	313	CHL	C2C-C3C	4.55	1.46	1.36
24	1	311	XAT	C32-C33	4.55	1.55	1.45
26	n	318	CHL	CHD-C1D	4.55	1.47	1.38
26	N	314	CHL	C2C-C3C	4.54	1.46	1.36
26	V	316	CHL	CHC-C1C	4.54	1.47	1.38
26	V	313	CHL	CHC-C1C	4.54	1.47	1.38
24	5	311	XAT	C22-C23	-4.54	1.45	1.52
26	5	314	CHL	C3D-C4D	-4.54	1.33	1.44
26	G	314	CHL	CHC-C1C	4.54	1.47	1.38
24	Q	309	XAT	C2-C3	-4.54	1.45	1.52
31	B	620	BCR	C23-C22	4.54	1.55	1.45
24	Q	309	XAT	C12-C13	4.54	1.55	1.45
26	U	313	CHL	C2C-C3C	4.54	1.46	1.36
26	1	314	CHL	CHC-C1C	4.54	1.47	1.38
31	C	517	BCR	C3-C4	4.54	1.66	1.52
26	v	313	CHL	CHC-C1C	4.54	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	312	CHL	CHC-C1C	4.53	1.47	1.38
26	V	315	CHL	CHD-C1D	4.53	1.47	1.38
26	g	314	CHL	C3D-C4D	-4.53	1.33	1.44
26	6	317	CHL	CHD-C1D	4.53	1.47	1.38
24	4	311	XAT	C32-C33	4.53	1.55	1.45
24	g	309	XAT	C32-C33	4.53	1.55	1.45
26	U	319	CHL	CHC-C1C	4.53	1.47	1.38
31	t	101	BCR	C11-C10	4.53	1.57	1.43
24	3	309	XAT	C12-C13	4.53	1.55	1.45
24	N	311	XAT	C32-C33	4.53	1.55	1.45
24	V	311	XAT	C12-C13	4.53	1.55	1.45
26	5	313	CHL	CHD-C1D	4.53	1.47	1.38
24	5	311	XAT	C12-C13	4.52	1.55	1.45
31	X	201	BCR	C11-C10	4.52	1.57	1.43
26	P	319	CHL	C2C-C3C	4.52	1.46	1.36
26	p	316	CHL	CHD-C1D	4.52	1.47	1.38
26	Q	313	CHL	C2C-C3C	4.52	1.46	1.36
31	c	515	BCR	C3-C4	4.52	1.66	1.52
24	N	311	XAT	C2-C3	-4.52	1.45	1.52
24	v	311	XAT	C12-C13	4.52	1.55	1.45
26	n	318	CHL	C2C-C3C	4.51	1.46	1.36
24	v	311	XAT	C2-C3	-4.51	1.45	1.52
26	3	313	CHL	CHC-C1C	4.51	1.47	1.38
26	g	313	CHL	C3D-C4D	-4.51	1.34	1.44
26	1	313	CHL	C2C-C3C	4.51	1.46	1.36
31	T	101	BCR	C11-C10	4.51	1.57	1.43
26	r	615	CHL	C2C-C3C	4.51	1.46	1.36
26	4	313	CHL	CHC-C1C	4.51	1.47	1.38
26	s	313	CHL	O2A-CGA	4.51	1.45	1.30
26	1	318	CHL	C2C-C3C	4.50	1.46	1.36
26	Q	314	CHL	CHC-C1C	4.50	1.47	1.38
26	1	317	CHL	O2A-CGA	4.50	1.46	1.33
24	p	312	XAT	C12-C13	4.50	1.55	1.45
26	v	316	CHL	C2C-C3C	4.50	1.46	1.36
26	U	313	CHL	CHC-C1C	4.50	1.47	1.38
26	2	316	CHL	C2C-C3C	4.50	1.46	1.36
26	S	314	CHL	O2A-CGA	4.50	1.45	1.30
24	n	311	XAT	C12-C13	4.49	1.55	1.45
26	u	313	CHL	C2C-C3C	4.49	1.46	1.36
26	P	317	CHL	CHD-C1D	4.49	1.47	1.38
26	s	314	CHL	O2A-CGA	4.49	1.45	1.30
26	4	315	CHL	CHD-C1D	4.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	317	CHL	CHD-C1D	4.49	1.47	1.38
26	4	316	CHL	C2C-C3C	4.49	1.46	1.36
24	u	311	XAT	C2-C3	-4.49	1.45	1.52
24	2	311	XAT	C12-C13	4.49	1.55	1.45
24	U	311	XAT	C32-C33	4.49	1.55	1.45
26	Q	312	CHL	CHD-C1D	4.49	1.47	1.38
26	g	312	CHL	CHC-C1C	4.49	1.47	1.38
26	v	314	CHL	C2C-C3C	4.49	1.46	1.36
26	2	313	CHL	CHD-C1D	4.49	1.47	1.38
26	2	318	CHL	C2C-C3C	4.49	1.46	1.36
24	R	313	XAT	C12-C13	4.49	1.55	1.45
26	2	314	CHL	C3D-C4D	-4.49	1.34	1.44
24	G	309	XAT	C32-C33	4.49	1.55	1.45
26	s	313	CHL	CHC-C1C	4.49	1.47	1.38
31	x	202	BCR	C11-C10	4.49	1.57	1.43
26	r	616	CHL	CHC-C1C	4.48	1.47	1.38
31	d	403	BCR	C11-C10	4.48	1.57	1.43
26	S	313	CHL	O2A-CGA	4.48	1.45	1.30
24	g	309	XAT	C12-C13	4.48	1.55	1.45
26	G	315	CHL	C2C-C3C	4.48	1.46	1.36
26	5	316	CHL	C2C-C3C	4.48	1.46	1.36
26	N	315	CHL	C2C-C3C	4.48	1.46	1.36
26	R	317	CHL	C2C-C3C	4.48	1.46	1.36
24	n	311	XAT	C2-C3	-4.48	1.45	1.52
26	r	616	CHL	CHD-C1D	4.48	1.47	1.38
26	5	317	CHL	O2A-CGA	4.48	1.46	1.33
26	G	313	CHL	C2C-C3C	4.48	1.46	1.36
26	S	313	CHL	CHC-C1C	4.48	1.47	1.38
26	S	316	CHL	O2A-CGA	4.48	1.45	1.30
26	R	317	CHL	CHC-C1C	4.48	1.47	1.38
31	B	620	BCR	C3-C4	4.48	1.66	1.52
26	2	317	CHL	O2A-CGA	4.48	1.46	1.33
26	r	616	CHL	C2C-C3C	4.48	1.46	1.36
31	D	404	BCR	C11-C10	4.47	1.57	1.43
26	R	317	CHL	CHD-C1D	4.47	1.47	1.38
24	u	311	XAT	C12-C13	4.47	1.55	1.45
26	v	313	CHL	C2C-C3C	4.47	1.46	1.36
26	P	317	CHL	C2C-C3C	4.47	1.46	1.36
26	P	316	CHL	CHD-C1D	4.47	1.47	1.38
26	s	313	CHL	CHD-C1D	4.47	1.47	1.38
31	b	620	BCR	C3-C4	4.47	1.66	1.52
26	n	317	CHL	CHC-C1C	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	516	BCR	C11-C10	4.46	1.57	1.43
31	X	201	BCR	C23-C22	4.46	1.55	1.45
26	4	317	CHL	C2C-C3C	4.46	1.46	1.36
26	U	314	CHL	C2C-C3C	4.46	1.46	1.36
26	v	314	CHL	C3D-C4D	-4.46	1.34	1.44
26	s	316	CHL	O2A-CGA	4.46	1.45	1.30
26	3	315	CHL	CHC-C1C	4.46	1.47	1.38
24	n	311	XAT	C32-C33	4.46	1.55	1.45
26	3	311	CHL	C2C-C3C	4.46	1.46	1.36
26	s	313	CHL	C2C-C3C	4.46	1.46	1.36
26	1	313	CHL	CHC-C1C	4.45	1.47	1.38
26	4	313	CHL	C2C-C3C	4.45	1.46	1.36
26	V	318	CHL	CHC-C1C	4.45	1.47	1.38
26	U	313	CHL	CHD-C1D	4.45	1.47	1.38
24	q	309	XAT	C12-C13	4.45	1.55	1.45
26	n	315	CHL	CHD-C1D	4.45	1.47	1.38
26	p	317	CHL	CHC-C1C	4.45	1.47	1.38
26	g	311	CHL	CHC-C1C	4.45	1.47	1.38
26	Q	314	CHL	C2C-C3C	4.45	1.46	1.36
26	g	312	CHL	C3D-C4D	-4.45	1.34	1.44
24	G	309	XAT	C12-C13	4.45	1.55	1.45
31	K	101	BCR	C3-C4	4.44	1.66	1.52
31	C	518	BCR	C11-C10	4.44	1.57	1.43
26	r	619	CHL	CHC-C1C	4.44	1.47	1.38
26	3	312	CHL	C3D-C4D	-4.44	1.34	1.44
26	n	315	CHL	CHC-C1C	4.44	1.47	1.38
31	t	101	BCR	C3-C4	4.44	1.66	1.52
26	5	316	CHL	CHC-C1C	4.44	1.47	1.38
26	G	313	CHL	O2A-CGA	4.44	1.46	1.33
26	6	313	CHL	C3D-C4D	-4.44	1.34	1.44
31	k	101	BCR	C2-C1	4.44	1.64	1.54
26	V	313	CHL	CHD-C1D	4.44	1.47	1.38
26	u	313	CHL	CHD-C1D	4.44	1.47	1.38
26	u	315	CHL	C2C-C3C	4.44	1.46	1.36
26	n	316	CHL	CHC-C1C	4.44	1.47	1.38
26	g	315	CHL	O2A-CGA	4.44	1.46	1.33
26	g	315	CHL	C2C-C3C	4.44	1.46	1.36
31	k	101	BCR	C3-C4	4.44	1.66	1.52
26	G	315	CHL	CHC-C1C	4.44	1.47	1.38
26	q	313	CHL	C2C-C3C	4.44	1.46	1.36
26	r	619	CHL	O2A-CGA	4.44	1.46	1.33
26	5	313	CHL	O2A-CGA	4.43	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	313	CHL	O2A-CGA	4.43	1.46	1.33
24	r	612	XAT	C12-C13	4.43	1.55	1.45
26	G	312	CHL	C3D-C4D	-4.43	1.34	1.44
26	4	315	CHL	CHC-C1C	4.43	1.47	1.38
26	6	316	CHL	O2A-CGA	4.43	1.46	1.33
26	N	315	CHL	CHC-C1C	4.43	1.47	1.38
31	D	404	BCR	C23-C22	4.43	1.55	1.45
31	z	101	BCR	C3-C4	4.43	1.66	1.52
31	C	516	BCR	C3-C4	4.43	1.66	1.52
26	u	315	CHL	O2A-CGA	4.43	1.46	1.33
26	U	319	CHL	C2C-C3C	4.43	1.46	1.36
26	2	313	CHL	O2A-CGA	4.43	1.46	1.33
26	6	312	CHL	C2C-C3C	4.43	1.46	1.36
24	4	311	XAT	C12-C13	4.42	1.55	1.45
31	K	101	BCR	C2-C1	4.42	1.64	1.54
26	P	317	CHL	CHC-C1C	4.42	1.47	1.38
26	Q	311	CHL	C2C-C3C	4.42	1.46	1.36
26	1	317	CHL	C2C-C3C	4.42	1.46	1.36
31	T	101	BCR	C3-C4	4.42	1.66	1.52
26	p	317	CHL	C2C-C3C	4.42	1.46	1.36
26	U	317	CHL	C2C-C3C	4.42	1.46	1.36
26	u	316	CHL	CHC-C1C	4.41	1.47	1.38
24	1	311	XAT	C12-C13	4.41	1.55	1.45
26	3	315	CHL	O2A-CGA	4.41	1.46	1.33
31	x	202	BCR	C23-C22	4.41	1.55	1.45
26	S	313	CHL	C2C-C3C	4.41	1.46	1.36
31	d	403	BCR	C23-C22	4.41	1.55	1.45
26	g	313	CHL	CHD-C1D	4.41	1.47	1.38
26	g	313	CHL	C2C-C3C	4.41	1.46	1.36
26	5	318	CHL	C2C-C3C	4.41	1.46	1.36
26	U	314	CHL	O2A-CGA	4.41	1.46	1.33
26	S	313	CHL	CHD-C1D	4.40	1.46	1.38
26	4	314	CHL	CHC-C1C	4.40	1.47	1.38
26	g	311	CHL	C2C-C3C	4.40	1.46	1.36
26	P	319	CHL	O2A-CGA	4.40	1.46	1.33
26	1	315	CHL	CHC-C1C	4.40	1.47	1.38
31	B	618	BCR	C3-C4	4.40	1.66	1.52
31	b	619	BCR	C3-C4	4.40	1.66	1.52
26	g	315	CHL	CHC-C1C	4.40	1.47	1.38
26	v	317	CHL	C2C-C3C	4.40	1.46	1.36
24	U	311	XAT	C12-C13	4.40	1.55	1.45
26	1	314	CHL	C2C-C3C	4.40	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	316	CHL	C2C-C3C	4.40	1.46	1.36
26	6	301	CHL	C2C-C3C	4.40	1.46	1.36
26	n	316	CHL	C2C-C3C	4.40	1.46	1.36
31	d	403	BCR	C3-C4	4.40	1.66	1.52
26	2	316	CHL	CHC-C1C	4.40	1.47	1.38
26	R	316	CHL	CHC-C1C	4.40	1.47	1.38
26	3	314	CHL	CHD-C1D	4.39	1.46	1.38
26	G	313	CHL	CHD-C1D	4.39	1.46	1.38
26	u	314	CHL	CHC-C1C	4.39	1.47	1.38
31	D	404	BCR	C3-C4	4.39	1.66	1.52
26	N	313	CHL	C2C-C3C	4.39	1.46	1.36
26	g	314	CHL	CHD-C1D	4.39	1.46	1.38
26	N	315	CHL	O2A-CGA	4.39	1.46	1.33
26	V	318	CHL	CHD-C1D	4.39	1.46	1.38
26	P	316	CHL	CHC-C1C	4.39	1.47	1.38
26	G	316	CHL	C2C-C3C	4.39	1.46	1.36
26	u	313	CHL	CHC-C1C	4.39	1.47	1.38
26	p	316	CHL	CHC-C1C	4.39	1.47	1.38
26	Q	313	CHL	CHD-C1D	4.38	1.46	1.38
26	V	317	CHL	C2C-C3C	4.38	1.46	1.36
26	5	316	CHL	CHD-C1D	4.38	1.46	1.38
26	n	315	CHL	O2A-CGA	4.38	1.46	1.33
26	g	313	CHL	CHC-C1C	4.38	1.47	1.38
26	Q	316	CHL	CHD-C1D	4.38	1.46	1.38
26	1	315	CHL	CHD-C1D	4.38	1.46	1.38
26	6	315	CHL	CHD-C1D	4.38	1.46	1.38
26	2	318	CHL	CHD-C1D	4.38	1.46	1.38
26	r	615	CHL	CHC-C1C	4.38	1.47	1.38
26	4	316	CHL	O2A-CGA	4.37	1.46	1.33
26	Q	313	CHL	O2A-CGA	4.37	1.46	1.33
31	c	516	BCR	C3-C4	4.37	1.66	1.52
26	g	316	CHL	C2C-C3C	4.37	1.46	1.36
31	C	518	BCR	C3-C4	4.37	1.66	1.52
31	B	619	BCR	C3-C4	4.37	1.66	1.52
26	v	314	CHL	CHC-C1C	4.37	1.47	1.38
31	B	620	BCR	C11-C10	4.37	1.57	1.43
26	P	315	CHL	O2A-CGA	4.37	1.46	1.33
26	n	317	CHL	CHD-C1D	4.37	1.46	1.38
31	a	409	BCR	C3-C4	4.37	1.66	1.52
31	A	409	BCR	C3-C4	4.36	1.66	1.52
26	V	314	CHL	C3D-C4D	-4.36	1.34	1.44
26	2	316	CHL	CHD-C1D	4.36	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	313	CHL	CHD-C1D	4.36	1.46	1.38
26	v	317	CHL	O2A-CGA	4.36	1.46	1.33
31	b	618	BCR	C3-C4	4.36	1.66	1.52
31	b	620	BCR	C11-C10	4.36	1.57	1.43
24	N	311	XAT	C12-C13	4.36	1.55	1.45
26	u	315	CHL	CHC-C1C	4.36	1.47	1.38
26	G	314	CHL	CHD-C1D	4.36	1.46	1.38
26	G	315	CHL	O2A-CGA	4.36	1.46	1.33
26	P	314	CHL	CHD-C1D	4.36	1.46	1.38
26	n	317	CHL	C2C-C3C	4.36	1.46	1.36
26	v	315	CHL	CHC-C1C	4.35	1.47	1.38
26	g	316	CHL	O2A-CGA	4.35	1.46	1.33
26	V	317	CHL	O2A-CGA	4.35	1.46	1.33
26	q	315	CHL	CHC-C1C	4.35	1.47	1.38
26	V	314	CHL	O2A-CGA	4.35	1.46	1.33
26	q	315	CHL	CHD-C1D	4.34	1.46	1.38
26	v	318	CHL	CHD-C1D	4.34	1.46	1.38
31	C	518	BCR	C4-C5	-4.34	1.42	1.51
31	B	620	BCR	C2-C1	4.34	1.64	1.54
26	G	311	CHL	C2C-C3C	4.34	1.46	1.36
31	B	618	BCR	C4-C5	-4.34	1.42	1.51
26	q	311	CHL	C2C-C3C	4.34	1.46	1.36
26	v	316	CHL	CHC-C1C	4.34	1.47	1.38
31	X	201	BCR	C3-C4	4.34	1.66	1.52
26	6	312	CHL	CHC-C1C	4.34	1.47	1.38
26	6	301	CHL	CHD-C1D	4.34	1.46	1.38
26	R	315	CHL	O2A-CGA	4.34	1.46	1.33
31	z	101	BCR	C11-C10	4.33	1.56	1.43
26	v	313	CHL	CHD-C1D	4.33	1.46	1.38
26	4	313	CHL	CHD-C1D	4.33	1.46	1.38
26	g	316	CHL	CHD-C1D	4.33	1.46	1.38
31	x	202	BCR	C3-C4	4.33	1.66	1.52
26	p	320	CHL	C2C-C3C	4.33	1.46	1.36
26	4	315	CHL	O2A-CGA	4.33	1.46	1.33
31	C	516	BCR	C11-C10	4.33	1.56	1.43
26	Q	315	CHL	O2A-CGA	4.33	1.46	1.33
26	5	315	CHL	O2A-CGA	4.33	1.46	1.33
26	q	312	CHL	O2A-CGA	4.33	1.46	1.33
26	G	313	CHL	CHC-C1C	4.33	1.47	1.38
31	c	515	BCR	C23-C22	4.33	1.55	1.45
26	U	316	CHL	C2C-C3C	4.33	1.46	1.36
26	3	311	CHL	CHC-C1C	4.33	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	316	CHL	C2C-C3C	4.32	1.46	1.36
26	U	314	CHL	CHC-C1C	4.32	1.47	1.38
31	K	101	BCR	C11-C10	4.32	1.56	1.43
26	v	314	CHL	CHD-C1D	4.32	1.46	1.38
26	V	315	CHL	O2A-CGA	4.32	1.46	1.33
26	1	315	CHL	O2A-CGA	4.32	1.46	1.33
26	q	314	CHL	O2A-CGA	4.32	1.46	1.33
26	2	314	CHL	O2A-CGA	4.32	1.46	1.33
26	5	318	CHL	CHD-C1D	4.32	1.46	1.38
31	k	101	BCR	C11-C10	4.32	1.56	1.43
26	G	316	CHL	CHD-C1D	4.32	1.46	1.38
31	c	515	BCR	C11-C10	4.32	1.56	1.43
26	5	314	CHL	O2A-CGA	4.32	1.46	1.33
26	s	314	CHL	CHC-C1C	4.31	1.47	1.38
31	b	618	BCR	C4-C5	-4.31	1.42	1.51
26	N	317	CHL	O2A-CGA	4.31	1.45	1.33
26	R	316	CHL	O2A-CGA	4.31	1.45	1.33
26	1	314	CHL	CHD-C1D	4.31	1.46	1.38
31	b	620	BCR	C2-C1	4.31	1.64	1.54
26	1	314	CHL	O2A-CGA	4.31	1.45	1.33
26	v	315	CHL	CHD-C1D	4.31	1.46	1.38
26	4	314	CHL	C2C-C3C	4.31	1.46	1.36
31	b	619	BCR	C2-C1	4.31	1.64	1.54
26	2	315	CHL	CHC-C1C	4.31	1.47	1.38
26	r	614	CHL	C2C-C3C	4.31	1.46	1.36
31	C	516	BCR	C23-C22	4.31	1.55	1.45
26	v	315	CHL	O2A-CGA	4.31	1.45	1.33
26	n	313	CHL	C2C-C3C	4.31	1.46	1.36
26	P	318	CHL	O2A-CGA	4.31	1.45	1.33
26	Q	311	CHL	O2A-CGA	4.31	1.45	1.33
26	N	316	CHL	O2A-CGA	4.31	1.45	1.33
26	4	317	CHL	O2A-CGA	4.30	1.45	1.33
26	6	314	CHL	O2A-CGA	4.30	1.45	1.33
26	p	320	CHL	CHC-C1C	4.30	1.47	1.38
26	Q	311	CHL	CHC-C1C	4.30	1.47	1.38
26	v	314	CHL	O2A-CGA	4.30	1.45	1.33
26	q	311	CHL	O2A-CGA	4.30	1.45	1.33
26	r	614	CHL	O2A-CGA	4.30	1.45	1.33
26	n	316	CHL	CHD-C1D	4.30	1.46	1.38
26	p	317	CHL	CHD-C1D	4.30	1.46	1.38
26	G	311	CHL	O2A-CGA	4.30	1.45	1.33
26	q	314	CHL	CHC-C1C	4.30	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	316	CHL	O2A-CGA	4.30	1.45	1.33
26	p	319	CHL	O2A-CGA	4.30	1.45	1.33
26	n	313	CHL	CHD-C1D	4.29	1.46	1.38
31	c	516	BCR	C4-C5	-4.29	1.42	1.51
26	r	615	CHL	O2A-CGA	4.29	1.45	1.33
31	C	517	BCR	C11-C10	4.29	1.56	1.43
26	P	316	CHL	O2A-CGA	4.29	1.45	1.33
26	S	315	CHL	O2A-CGA	4.29	1.45	1.33
26	s	315	CHL	O2A-CGA	4.29	1.45	1.33
31	z	101	BCR	C23-C22	4.29	1.55	1.45
26	G	312	CHL	O2A-CGA	4.29	1.45	1.33
26	Q	316	CHL	CHC-C1C	4.29	1.47	1.38
31	B	619	BCR	C11-C10	4.29	1.56	1.43
26	2	315	CHL	O2A-CGA	4.29	1.45	1.33
26	5	315	CHL	CHC-C1C	4.28	1.47	1.38
26	Q	314	CHL	CHD-C1D	4.28	1.46	1.38
31	C	517	BCR	C23-C22	4.28	1.55	1.45
26	R	315	CHL	C2C-C3C	4.28	1.45	1.36
26	p	319	CHL	CHD-C1D	4.28	1.46	1.38
26	u	318	CHL	C2C-C3C	4.28	1.45	1.36
26	v	317	CHL	CHD-C1D	4.28	1.46	1.38
26	5	318	CHL	O2A-CGA	4.28	1.45	1.33
26	u	316	CHL	O2A-CGA	4.28	1.45	1.33
26	n	318	CHL	O2A-CGA	4.28	1.45	1.33
31	a	409	BCR	C4-C5	-4.28	1.42	1.51
31	b	619	BCR	C11-C10	4.28	1.56	1.43
26	4	314	CHL	O2A-CGA	4.27	1.45	1.33
26	v	318	CHL	O2A-CGA	4.27	1.45	1.33
26	S	314	CHL	CHC-C1C	4.27	1.47	1.38
26	6	316	CHL	CHC-C1C	4.27	1.47	1.38
26	g	311	CHL	CHD-C1D	4.27	1.46	1.38
31	B	619	BCR	C2-C1	4.27	1.64	1.54
26	g	313	CHL	O2A-CGA	4.27	1.45	1.33
26	u	317	CHL	C2C-C3C	4.27	1.45	1.36
26	N	316	CHL	CHC-C1C	4.27	1.47	1.38
26	p	316	CHL	O2A-CGA	4.27	1.45	1.33
26	6	312	CHL	O2A-CGA	4.27	1.45	1.33
26	Q	312	CHL	O2A-CGA	4.27	1.45	1.33
31	d	403	BCR	C2-C1	4.26	1.64	1.54
26	6	301	CHL	CHC-C1C	4.26	1.47	1.38
26	V	318	CHL	O2A-CGA	4.26	1.45	1.33
26	r	616	CHL	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	316	CHL	CHD-C1D	4.26	1.46	1.38
31	B	618	BCR	C2-C1	4.26	1.63	1.54
31	c	516	BCR	C2-C1	4.26	1.63	1.54
31	C	517	BCR	C2-C1	4.26	1.63	1.54
31	c	516	BCR	C23-C22	4.26	1.55	1.45
26	u	316	CHL	CHD-C1D	4.26	1.46	1.38
26	V	317	CHL	CHC-C1C	4.26	1.47	1.38
26	6	313	CHL	O2A-CGA	4.26	1.45	1.33
26	q	313	CHL	CHC-C1C	4.26	1.47	1.38
26	V	316	CHL	CHD-C1D	4.26	1.46	1.38
26	p	318	CHL	O2A-CGA	4.25	1.45	1.33
31	C	518	BCR	C23-C22	4.25	1.55	1.45
26	u	314	CHL	O2A-CGA	4.25	1.45	1.33
26	R	315	CHL	CHD-C1D	4.25	1.46	1.38
26	g	312	CHL	O2A-CGA	4.25	1.45	1.33
26	q	315	CHL	O2A-CGA	4.25	1.45	1.33
26	5	317	CHL	C2C-C3C	4.25	1.45	1.36
26	P	315	CHL	CHD-C4C	4.25	1.48	1.39
26	3	311	CHL	O2A-CGA	4.25	1.45	1.33
26	3	312	CHL	O2A-CGA	4.25	1.45	1.33
26	2	318	CHL	O2A-CGA	4.25	1.45	1.33
26	n	318	CHL	CHC-C1C	4.25	1.47	1.38
26	P	317	CHL	O2A-CGA	4.25	1.45	1.33
31	D	404	BCR	C4-C5	-4.25	1.42	1.51
26	v	318	CHL	CHC-C1C	4.25	1.47	1.38
26	1	317	CHL	CHD-C1D	4.25	1.46	1.38
26	Q	315	CHL	CHC-C1C	4.25	1.47	1.38
31	d	403	BCR	C4-C5	-4.25	1.42	1.51
26	r	615	CHL	CHD-C1D	4.24	1.46	1.38
26	6	301	CHL	O2A-CGA	4.24	1.45	1.33
31	C	518	BCR	C2-C1	4.24	1.63	1.54
26	p	314	CHL	C2C-C3C	4.24	1.45	1.36
26	p	314	CHL	O2A-CGA	4.24	1.45	1.33
26	U	319	CHL	CHD-C1D	4.24	1.46	1.38
26	6	317	CHL	O2A-CGA	4.24	1.45	1.33
26	R	317	CHL	O2A-CGA	4.24	1.45	1.33
26	r	614	CHL	CHD-C1D	4.24	1.46	1.38
31	c	515	BCR	C2-C1	4.24	1.63	1.54
31	d	403	BCR	C28-C27	4.24	1.65	1.52
31	D	404	BCR	C2-C1	4.24	1.63	1.54
26	U	319	CHL	O2A-CGA	4.24	1.45	1.33
31	A	409	BCR	C4-C5	-4.23	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	t	101	BCR	C2-C1	4.23	1.63	1.54
31	T	101	BCR	C2-C1	4.23	1.63	1.54
26	N	313	CHL	CHC-C1C	4.23	1.47	1.38
37	e	101	HEM	FE-NB	4.23	2.08	1.94
26	3	312	CHL	CHD-C4C	4.23	1.48	1.39
26	u	318	CHL	CHC-C1C	4.23	1.47	1.38
26	g	311	CHL	O2A-CGA	4.23	1.45	1.33
26	g	314	CHL	O2A-CGA	4.23	1.45	1.33
26	P	318	CHL	C2C-C3C	4.23	1.45	1.36
31	x	202	BCR	C2-C1	4.23	1.63	1.54
26	G	314	CHL	O2A-CGA	4.23	1.45	1.33
26	4	317	CHL	CHD-C1D	4.23	1.46	1.38
26	q	312	CHL	CHD-C4C	4.23	1.48	1.39
26	1	313	CHL	CHD-C1D	4.23	1.46	1.38
26	p	315	CHL	O2A-CGA	4.23	1.45	1.33
26	4	316	CHL	CHD-C1D	4.23	1.46	1.38
31	a	409	BCR	C11-C10	4.23	1.56	1.43
26	P	319	CHL	CHD-C1D	4.22	1.46	1.38
26	V	317	CHL	CHD-C1D	4.22	1.46	1.38
26	1	316	CHL	O2A-CGA	4.22	1.45	1.33
26	5	316	CHL	O2A-CGA	4.22	1.45	1.33
26	3	313	CHL	O2A-CGA	4.22	1.45	1.33
26	u	318	CHL	O2A-CGA	4.22	1.45	1.33
26	2	317	CHL	C2C-C3C	4.22	1.45	1.36
26	2	315	CHL	CHD-C1D	4.22	1.46	1.38
26	p	317	CHL	O2A-CGA	4.22	1.45	1.33
26	n	316	CHL	O2A-CGA	4.22	1.45	1.33
26	p	318	CHL	C2C-C3C	4.22	1.45	1.36
26	n	314	CHL	CHD-C4C	4.22	1.48	1.39
26	U	315	CHL	C2C-C3C	4.22	1.45	1.36
26	p	320	CHL	O2A-CGA	4.22	1.45	1.33
26	Q	316	CHL	O2A-CGA	4.22	1.45	1.33
31	B	618	BCR	C11-C10	4.22	1.56	1.43
31	A	409	BCR	C11-C10	4.22	1.56	1.43
31	A	409	BCR	C2-C1	4.21	1.63	1.54
26	4	316	CHL	CHC-C1C	4.21	1.47	1.38
26	1	316	CHL	CHC-C1C	4.21	1.47	1.38
26	V	316	CHL	O2A-CGA	4.21	1.45	1.33
26	Q	311	CHL	CHD-C1D	4.21	1.46	1.38
26	1	318	CHL	O2A-CGA	4.21	1.45	1.33
26	N	313	CHL	CHD-C1D	4.21	1.46	1.38
26	r	614	CHL	CHC-C1C	4.21	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	316	CHL	O2A-CGA	4.21	1.45	1.33
26	6	313	CHL	CHD-C4C	4.21	1.48	1.39
26	v	313	CHL	O2A-CGA	4.21	1.45	1.33
26	N	317	CHL	CHC-C1C	4.21	1.47	1.38
31	D	404	BCR	C28-C27	4.21	1.65	1.52
26	U	317	CHL	O2A-CGA	4.21	1.45	1.33
26	U	316	CHL	CHD-C1D	4.21	1.46	1.38
26	3	314	CHL	O2A-CGA	4.20	1.45	1.33
26	P	314	CHL	O2A-CGA	4.20	1.45	1.33
31	B	619	BCR	C23-C22	4.20	1.55	1.45
26	R	315	CHL	CHC-C1C	4.20	1.47	1.38
26	N	316	CHL	C2C-C3C	4.20	1.45	1.36
26	q	311	CHL	CHC-C1C	4.20	1.47	1.38
26	N	315	CHL	CHD-C1D	4.20	1.46	1.38
26	N	313	CHL	O2A-CGA	4.20	1.45	1.33
26	3	311	CHL	CHD-C1D	4.20	1.46	1.38
31	k	101	BCR	C28-C27	4.19	1.65	1.52
31	b	619	BCR	C23-C22	4.19	1.55	1.45
31	b	618	BCR	C11-C10	4.19	1.56	1.43
31	X	201	BCR	C2-C1	4.19	1.63	1.54
26	2	317	CHL	CHC-C1C	4.19	1.47	1.38
26	P	318	CHL	CHC-C1C	4.19	1.47	1.38
31	K	101	BCR	C28-C27	4.19	1.65	1.52
26	q	311	CHL	CHD-C1D	4.19	1.46	1.38
26	s	314	CHL	CHD-C1D	4.19	1.46	1.38
26	U	317	CHL	CHC-C1C	4.19	1.47	1.38
31	a	409	BCR	C2-C1	4.19	1.63	1.54
31	K	101	BCR	C23-C22	4.19	1.54	1.45
26	N	314	CHL	O2A-CGA	4.19	1.45	1.33
37	E	101	HEM	FE-NB	4.18	2.07	1.94
26	R	316	CHL	CHD-C1D	4.18	1.46	1.38
26	U	315	CHL	CHC-C1C	4.18	1.47	1.38
26	1	318	CHL	CHD-C1D	4.18	1.46	1.38
26	V	313	CHL	O2A-CGA	4.18	1.45	1.33
26	n	314	CHL	O2A-CGA	4.18	1.45	1.33
26	N	314	CHL	CHD-C4C	4.18	1.48	1.39
31	A	409	BCR	C23-C22	4.18	1.54	1.45
26	1	318	CHL	CHC-C1C	4.18	1.47	1.38
26	U	317	CHL	CHD-C1D	4.18	1.46	1.38
26	2	316	CHL	O2A-CGA	4.18	1.45	1.33
31	a	409	BCR	C23-C22	4.18	1.54	1.45
26	v	316	CHL	O2A-CGA	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	314	CHL	O2A-CGA	4.17	1.45	1.33
26	1	313	CHL	O2A-CGA	4.17	1.45	1.33
26	u	313	CHL	O2A-CGA	4.17	1.45	1.33
26	n	317	CHL	O2A-CGA	4.17	1.45	1.33
26	u	314	CHL	C2C-C3C	4.17	1.45	1.36
26	r	619	CHL	C2C-C3C	4.17	1.45	1.36
31	z	101	BCR	C2-C1	4.17	1.63	1.54
26	u	314	CHL	CHD-C1D	4.17	1.46	1.38
26	U	313	CHL	O2A-CGA	4.17	1.45	1.33
26	1	317	CHL	CHC-C1C	4.17	1.47	1.38
26	6	315	CHL	O2A-CGA	4.16	1.45	1.33
26	n	313	CHL	O2A-CGA	4.16	1.45	1.33
31	b	618	BCR	C2-C1	4.16	1.63	1.54
31	K	101	BCR	C4-C5	-4.16	1.42	1.51
26	p	314	CHL	CHC-C4B	4.16	1.48	1.39
26	5	318	CHL	CHC-C1C	4.16	1.47	1.38
31	C	516	BCR	C2-C1	4.15	1.63	1.54
31	k	101	BCR	C4-C5	-4.15	1.42	1.51
26	4	313	CHL	O2A-CGA	4.15	1.45	1.33
26	U	316	CHL	CHC-C1C	4.15	1.46	1.38
26	S	314	CHL	CHD-C1D	4.14	1.46	1.38
26	4	317	CHL	CHC-C1C	4.14	1.46	1.38
31	b	618	BCR	C28-C27	4.14	1.65	1.52
26	U	315	CHL	CHD-C1D	4.14	1.46	1.38
26	5	317	CHL	CHC-C1C	4.13	1.46	1.38
26	U	316	CHL	O2A-CGA	4.13	1.45	1.33
26	p	315	CHL	CHD-C4C	4.13	1.48	1.39
26	S	315	CHL	CHD-C4C	4.13	1.48	1.39
26	6	312	CHL	CHD-C1D	4.13	1.46	1.38
26	u	317	CHL	O2A-CGA	4.13	1.45	1.33
31	k	101	BCR	C23-C22	4.13	1.54	1.45
26	n	318	CHL	CHD-C4C	4.13	1.48	1.39
26	G	311	CHL	CHC-C1C	4.13	1.46	1.38
26	G	311	CHL	CHD-C1D	4.13	1.46	1.38
31	b	620	BCR	C4-C5	-4.13	1.42	1.51
26	v	317	CHL	CHC-C1C	4.13	1.46	1.38
31	z	101	BCR	C4-C5	-4.13	1.42	1.51
26	u	317	CHL	CHC-C1C	4.13	1.46	1.38
26	u	317	CHL	CHD-C1D	4.12	1.46	1.38
31	x	202	BCR	C28-C27	4.12	1.65	1.52
26	U	315	CHL	O2A-CGA	4.12	1.45	1.33
26	3	316	CHL	CHC-C1C	4.12	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	314	CHL	CHD-C4C	4.12	1.48	1.39
26	6	314	CHL	CHD-C4C	4.12	1.48	1.39
31	B	618	BCR	C28-C27	4.11	1.65	1.52
31	b	620	BCR	C28-C27	4.11	1.65	1.52
26	p	314	CHL	CHD-C1D	4.11	1.46	1.38
26	3	316	CHL	CHD-C4C	4.10	1.48	1.39
26	s	315	CHL	CHD-C4C	4.10	1.48	1.39
31	B	620	BCR	C4-C5	-4.10	1.42	1.51
26	p	319	CHL	CHC-C1C	4.10	1.46	1.38
31	B	620	BCR	C28-C27	4.10	1.65	1.52
31	t	101	BCR	C28-C27	4.10	1.65	1.52
31	b	619	BCR	C4-C5	-4.10	1.42	1.51
26	P	314	CHL	CHD-C4C	4.09	1.48	1.39
26	5	313	CHL	CHD-C4C	4.09	1.48	1.39
26	2	314	CHL	CHD-C4C	4.09	1.48	1.39
26	V	315	CHL	CHD-C4C	4.09	1.48	1.39
31	b	619	BCR	C28-C27	4.09	1.65	1.52
26	g	312	CHL	CHD-C4C	4.09	1.48	1.39
26	Q	313	CHL	CHC-C1C	4.08	1.46	1.38
26	r	619	CHL	CHD-C1D	4.08	1.46	1.38
31	B	619	BCR	C28-C27	4.08	1.65	1.52
26	g	316	CHL	CHC-C1C	4.08	1.46	1.38
26	5	315	CHL	CHD-C1D	4.08	1.46	1.38
31	C	516	BCR	C4-C5	-4.08	1.43	1.51
26	P	317	CHL	CHD-C4C	4.08	1.48	1.39
26	u	318	CHL	CHD-C1D	4.08	1.46	1.38
31	X	201	BCR	C28-C27	4.08	1.65	1.52
31	T	101	BCR	C28-C27	4.08	1.65	1.52
26	6	317	CHL	CHD-C4C	4.07	1.48	1.39
26	5	317	CHL	CHD-C1D	4.07	1.46	1.38
26	P	314	CHL	CHC-C4B	4.07	1.48	1.39
26	Q	312	CHL	CHD-C4C	4.07	1.48	1.39
26	G	312	CHL	CHD-C4C	4.07	1.48	1.39
26	N	317	CHL	CHD-C4C	4.07	1.48	1.39
26	2	313	CHL	CHD-C4C	4.07	1.48	1.39
31	c	516	BCR	C28-C27	4.06	1.65	1.52
31	t	101	BCR	C4-C5	-4.06	1.43	1.51
31	X	201	BCR	C4-C5	-4.06	1.43	1.51
26	3	313	CHL	CHD-C4C	4.06	1.48	1.39
31	C	518	BCR	C28-C27	4.06	1.65	1.52
26	g	314	CHL	CHD-C4C	4.06	1.48	1.39
26	G	316	CHL	CHC-C1C	4.06	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	318	CHL	CHD-C1D	4.06	1.46	1.38
31	B	619	BCR	C4-C5	-4.06	1.43	1.51
31	x	202	BCR	C4-C5	-4.05	1.43	1.51
26	p	318	CHL	CHD-C1D	4.04	1.46	1.38
31	C	517	BCR	C4-C5	-4.04	1.43	1.51
31	c	515	BCR	C4-C5	-4.04	1.43	1.51
31	A	409	BCR	C28-C27	4.04	1.65	1.52
26	p	318	CHL	CHC-C1C	4.04	1.46	1.38
26	3	314	CHL	CHD-C4C	4.03	1.48	1.39
26	S	316	CHL	CHD-C4C	4.03	1.48	1.39
26	r	616	CHL	CHD-C4C	4.03	1.48	1.39
26	P	315	CHL	CHC-C4B	4.03	1.48	1.39
26	s	316	CHL	CHD-C4C	4.03	1.48	1.39
31	T	101	BCR	C4-C5	-4.03	1.43	1.51
26	4	314	CHL	CHD-C1D	4.02	1.46	1.38
26	u	313	CHL	CHD-C4C	4.02	1.48	1.39
26	U	313	CHL	CHD-C4C	4.02	1.48	1.39
26	6	315	CHL	CHD-C4C	4.02	1.48	1.39
26	N	316	CHL	CHD-C1D	4.02	1.46	1.38
26	R	317	CHL	CHD-C4C	4.02	1.48	1.39
26	2	317	CHL	CHD-C1D	4.01	1.46	1.38
22	q	301	CLA	C1D-ND	4.01	1.42	1.37
26	V	316	CHL	CHD-C4C	4.01	1.48	1.39
26	2	318	CHL	CHC-C1C	4.01	1.46	1.38
31	a	409	BCR	C28-C27	4.01	1.65	1.52
26	n	313	CHL	CHD-C4C	4.00	1.48	1.39
26	V	314	CHL	CHD-C4C	3.99	1.48	1.39
31	C	517	BCR	C28-C27	3.99	1.65	1.52
26	n	315	CHL	CHD-C4C	3.99	1.48	1.39
26	6	317	CHL	CHC-C1C	3.99	1.46	1.38
26	q	315	CHL	CHD-C4C	3.98	1.48	1.39
26	N	313	CHL	CHD-C4C	3.98	1.48	1.39
26	p	320	CHL	CHD-C1D	3.98	1.46	1.38
31	c	515	BCR	C28-C27	3.97	1.64	1.52
26	2	318	CHL	CHD-C4C	3.97	1.48	1.39
26	p	316	CHL	CHD-C4C	3.97	1.48	1.39
26	V	313	CHL	CHD-C4C	3.97	1.48	1.39
26	P	316	CHL	CHD-C4C	3.96	1.48	1.39
31	B	618	BCR	C23-C22	3.96	1.54	1.45
26	5	318	CHL	CHD-C4C	3.95	1.48	1.39
26	s	313	CHL	CHD-C4C	3.95	1.48	1.39
26	Q	313	CHL	CHD-C4C	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	316	CHL	CHD-C4C	3.95	1.48	1.39
22	R	310	CLA	C1D-ND	3.95	1.42	1.37
26	q	311	CHL	CHD-C4C	3.95	1.48	1.39
26	P	319	CHL	CHC-C1C	3.95	1.46	1.38
26	2	316	CHL	CHD-C4C	3.95	1.48	1.39
26	v	316	CHL	CHD-C1D	3.95	1.46	1.38
26	Q	314	CHL	CHD-C4C	3.95	1.48	1.39
26	Q	316	CHL	CHD-C4C	3.95	1.48	1.39
26	G	314	CHL	CHD-C4C	3.94	1.48	1.39
26	5	316	CHL	CHD-C4C	3.94	1.48	1.39
31	t	101	BCR	C12-C13	3.94	1.54	1.45
26	n	316	CHL	CHD-C4C	3.94	1.48	1.39
26	p	315	CHL	CHC-C4B	3.94	1.48	1.39
26	U	314	CHL	CHD-C1D	3.94	1.46	1.38
26	u	316	CHL	CHD-C4C	3.94	1.48	1.39
31	T	101	BCR	C12-C13	3.93	1.54	1.45
22	Q	301	CLA	C1D-ND	3.93	1.42	1.37
26	p	317	CHL	CHD-C4C	3.93	1.48	1.39
22	R	302	CLA	C1D-ND	3.93	1.42	1.37
26	4	313	CHL	CHD-C4C	3.93	1.48	1.39
31	X	201	BCR	C12-C13	3.93	1.54	1.45
26	S	313	CHL	CHD-C4C	3.92	1.48	1.39
26	q	313	CHL	CHD-C4C	3.92	1.48	1.39
24	u	311	XAT	C31-C30	3.92	1.55	1.43
26	4	315	CHL	CHD-C4C	3.92	1.48	1.39
26	6	301	CHL	CHD-C4C	3.92	1.48	1.39
31	d	403	BCR	C12-C13	3.92	1.54	1.45
26	G	316	CHL	CHD-C4C	3.91	1.48	1.39
26	2	313	CHL	CHC-C4B	3.91	1.48	1.39
26	p	314	CHL	CHD-C4C	3.90	1.48	1.39
26	Q	311	CHL	CHD-C4C	3.90	1.48	1.39
26	U	319	CHL	CHD-C4C	3.90	1.48	1.39
22	V	301	CLA	C1D-ND	3.90	1.42	1.37
26	V	317	CHL	CHD-C4C	3.90	1.48	1.39
22	r	609	CLA	C1D-ND	3.90	1.42	1.37
26	G	313	CHL	CHD-C4C	3.90	1.48	1.39
31	x	202	BCR	C12-C13	3.90	1.54	1.45
26	V	318	CHL	CHD-C4C	3.90	1.48	1.39
31	D	404	BCR	C12-C13	3.89	1.54	1.45
26	5	313	CHL	CHC-C4B	3.89	1.48	1.39
26	1	316	CHL	CHD-C4C	3.89	1.48	1.39
26	4	316	CHL	CHD-C4C	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	313	CHL	CHD-C4C	3.89	1.48	1.39
24	V	311	XAT	C31-C30	3.88	1.55	1.43
22	n	308	CLA	C1D-ND	3.88	1.42	1.37
22	r	601	CLA	C1D-ND	3.88	1.42	1.37
26	1	313	CHL	CHD-C4C	3.88	1.48	1.39
26	v	315	CHL	CHD-C4C	3.88	1.48	1.39
26	U	316	CHL	CHD-C4C	3.88	1.48	1.39
26	p	319	CHL	CHD-C4C	3.87	1.48	1.39
31	C	516	BCR	C28-C27	3.87	1.64	1.52
26	1	315	CHL	CHD-C4C	3.87	1.48	1.39
36	a	416	DGD	O6E-C1E	3.87	1.51	1.41
24	P	312	XAT	C35-C34	3.87	1.55	1.43
31	b	618	BCR	C23-C22	3.87	1.54	1.45
26	u	314	CHL	CHD-C4C	3.87	1.48	1.39
26	v	314	CHL	CHD-C4C	3.87	1.48	1.39
31	T	101	BCR	C15-C14	3.87	1.55	1.43
26	r	614	CHL	CHD-C4C	3.87	1.48	1.39
26	6	312	CHL	CHD-C4C	3.86	1.48	1.39
36	A	414	DGD	O6E-C1E	3.86	1.51	1.41
31	z	101	BCR	C28-C27	3.86	1.64	1.52
24	p	312	XAT	C35-C34	3.86	1.55	1.43
22	g	306	CLA	C1D-ND	3.86	1.42	1.37
24	p	312	XAT	C31-C30	3.86	1.55	1.43
24	P	312	XAT	C31-C30	3.86	1.55	1.43
26	v	317	CHL	CHD-C4C	3.85	1.48	1.39
26	v	313	CHL	CHD-C4C	3.85	1.48	1.39
26	1	317	CHL	CHD-C4C	3.85	1.48	1.39
24	R	313	XAT	C31-C30	3.85	1.55	1.43
26	n	313	CHL	CHC-C4B	3.84	1.48	1.39
26	v	318	CHL	CHD-C4C	3.84	1.48	1.39
24	Q	309	XAT	C35-C34	3.84	1.55	1.43
31	t	101	BCR	C15-C14	3.84	1.55	1.43
24	6	310	XAT	C35-C34	3.84	1.55	1.43
22	v	301	CLA	C1D-ND	3.84	1.42	1.37
24	R	313	XAT	C35-C34	3.84	1.55	1.43
26	n	317	CHL	CHD-C4C	3.83	1.48	1.39
26	3	311	CHL	CHD-C4C	3.83	1.48	1.39
26	R	315	CHL	CHD-C4C	3.83	1.48	1.39
24	3	309	XAT	C35-C34	3.83	1.55	1.43
24	v	311	XAT	C31-C30	3.83	1.55	1.43
24	U	311	XAT	C31-C30	3.83	1.55	1.43
22	3	301	CLA	C1D-ND	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	309	XAT	C31-C30	3.82	1.55	1.43
31	c	516	BCR	C12-C13	3.82	1.54	1.45
24	3	309	XAT	C15-C14	3.82	1.55	1.43
22	R	304	CLA	C1D-ND	3.82	1.42	1.37
24	Q	309	XAT	C15-C14	3.82	1.55	1.43
24	5	311	XAT	C31-C30	3.82	1.55	1.43
24	3	309	XAT	C31-C30	3.82	1.55	1.43
26	g	315	CHL	CHD-C1D	3.81	1.45	1.38
24	2	311	XAT	C31-C30	3.81	1.55	1.43
26	v	316	CHL	CHD-C4C	3.81	1.47	1.39
24	6	310	XAT	C15-C14	3.81	1.55	1.43
24	P	312	XAT	C15-C14	3.81	1.55	1.43
26	g	312	CHL	OBD-CAD	3.81	1.29	1.22
26	G	311	CHL	CHD-C4C	3.81	1.47	1.39
24	r	612	XAT	C31-C30	3.81	1.55	1.43
26	g	311	CHL	CHD-C4C	3.81	1.47	1.39
26	P	319	CHL	CHD-C4C	3.81	1.47	1.39
24	5	311	XAT	C35-C34	3.81	1.55	1.43
26	u	315	CHL	CHD-C1D	3.80	1.45	1.38
26	4	317	CHL	CHD-C4C	3.80	1.47	1.39
22	6	302	CLA	C1D-ND	3.80	1.42	1.37
26	U	315	CHL	CHD-C4C	3.80	1.47	1.39
24	Q	309	XAT	C31-C30	3.80	1.55	1.43
26	g	315	CHL	CHC-C4B	3.80	1.47	1.39
26	u	317	CHL	CHD-C4C	3.80	1.47	1.39
26	G	312	CHL	OBD-CAD	3.80	1.29	1.22
24	V	311	XAT	C35-C34	3.80	1.55	1.43
26	V	314	CHL	OBD-CAD	3.80	1.29	1.22
24	p	312	XAT	C15-C14	3.80	1.55	1.43
24	2	311	XAT	C15-C14	3.80	1.55	1.43
26	s	314	CHL	CHD-C4C	3.80	1.47	1.39
24	2	311	XAT	C35-C34	3.80	1.55	1.43
26	r	615	CHL	CHD-C4C	3.80	1.47	1.39
24	6	310	XAT	C31-C30	3.80	1.55	1.43
22	R	309	CLA	C1D-ND	3.79	1.42	1.37
26	R	316	CHL	CHD-C4C	3.79	1.47	1.39
26	S	314	CHL	CHD-C4C	3.79	1.47	1.39
26	P	315	CHL	CHB-C1B	3.79	1.47	1.39
26	1	318	CHL	CHD-C4C	3.79	1.47	1.39
26	n	314	CHL	CHC-C4B	3.79	1.47	1.39
26	1	314	CHL	CHD-C4C	3.78	1.47	1.39
24	4	311	XAT	C35-C34	3.78	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	315	CHL	CHC-C4B	3.78	1.47	1.39
26	G	315	CHL	CHD-C1D	3.78	1.45	1.38
22	r	603	CLA	C1D-ND	3.78	1.42	1.37
24	q	309	XAT	C11-C10	3.78	1.55	1.43
24	Q	309	XAT	C11-C10	3.78	1.55	1.43
24	q	309	XAT	C31-C30	3.78	1.55	1.43
24	4	311	XAT	C31-C30	3.78	1.55	1.43
26	v	314	CHL	OBD-CAD	3.78	1.29	1.22
24	5	311	XAT	C15-C14	3.78	1.55	1.43
24	1	311	XAT	C31-C30	3.78	1.55	1.43
24	P	312	XAT	C11-C10	3.78	1.55	1.43
24	G	309	XAT	C31-C30	3.77	1.55	1.43
24	1	311	XAT	C35-C34	3.77	1.55	1.43
24	q	309	XAT	C35-C34	3.77	1.55	1.43
24	V	311	XAT	C15-C14	3.77	1.55	1.43
22	p	304	CLA	C1D-ND	3.77	1.42	1.37
24	q	309	XAT	C15-C14	3.77	1.55	1.43
22	b	611	CLA	C1D-ND	3.77	1.42	1.37
24	r	612	XAT	C35-C34	3.77	1.55	1.43
24	1	311	XAT	C15-C14	3.76	1.55	1.43
24	u	311	XAT	C15-C14	3.76	1.55	1.43
26	3	312	CHL	OBD-CAD	3.76	1.29	1.22
24	N	311	XAT	C31-C30	3.76	1.55	1.43
31	C	518	BCR	C12-C13	3.76	1.54	1.45
22	3	308	CLA	C1D-ND	3.76	1.42	1.37
34	C	521	LMG	O6-C1	3.76	1.51	1.41
24	u	311	XAT	C35-C34	3.76	1.55	1.43
31	k	101	BCR	C12-C13	3.76	1.54	1.45
22	4	301	CLA	C1D-ND	3.75	1.42	1.37
26	p	320	CHL	CHD-C4C	3.75	1.47	1.39
22	n	301	CLA	C1D-ND	3.75	1.42	1.37
24	V	311	XAT	C11-C10	3.75	1.55	1.43
26	r	619	CHL	CHD-C4C	3.75	1.47	1.39
22	G	301	CLA	C1D-ND	3.75	1.42	1.37
26	U	317	CHL	CHD-C4C	3.75	1.47	1.39
31	K	101	BCR	C12-C13	3.75	1.54	1.45
26	6	313	CHL	OBD-CAD	3.75	1.28	1.22
34	b	621	LMG	O6-C1	3.75	1.51	1.41
24	v	311	XAT	C35-C34	3.75	1.55	1.43
26	2	314	CHL	CHC-C4B	3.75	1.47	1.39
26	Q	312	CHL	OBD-CAD	3.75	1.28	1.22
22	r	610	CLA	C1D-ND	3.75	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	308	CLA	C1D-ND	3.75	1.42	1.37
26	2	315	CHL	CHD-C4C	3.74	1.47	1.39
24	4	311	XAT	C15-C14	3.74	1.55	1.43
30	D	401	PHO	C1D-C2D	3.74	1.43	1.39
34	b	624	LMG	O6-C1	3.74	1.51	1.41
24	R	313	XAT	C15-C14	3.74	1.55	1.43
22	S	302	CLA	C4B-NB	3.74	1.42	1.37
22	B	611	CLA	C1D-ND	3.74	1.42	1.37
26	g	314	CHL	OBD-CAD	3.74	1.28	1.22
24	6	310	XAT	C11-C10	3.73	1.55	1.43
24	r	612	XAT	C11-C10	3.73	1.55	1.43
24	n	311	XAT	C31-C30	3.73	1.55	1.43
26	G	315	CHL	CHC-C4B	3.73	1.47	1.39
24	R	313	XAT	C11-C10	3.73	1.55	1.43
22	R	311	CLA	C1D-ND	3.73	1.42	1.37
31	b	620	BCR	C12-C13	3.73	1.54	1.45
22	R	306	CLA	C1D-ND	3.73	1.42	1.37
31	z	101	BCR	C12-C13	3.73	1.53	1.45
24	N	311	XAT	C35-C34	3.73	1.55	1.43
24	v	311	XAT	C11-C10	3.72	1.55	1.43
24	g	309	XAT	C35-C34	3.72	1.55	1.43
26	s	315	CHL	CHC-C4B	3.72	1.47	1.39
22	P	304	CLA	C1D-ND	3.72	1.42	1.37
22	Q	302	CLA	C1D-ND	3.72	1.42	1.37
22	G	306	CLA	C1D-ND	3.72	1.42	1.37
34	B	624	LMG	O6-C1	3.72	1.51	1.41
22	G	308	CLA	C1D-ND	3.72	1.42	1.37
24	n	311	XAT	C35-C34	3.72	1.55	1.43
24	r	612	XAT	C15-C14	3.72	1.55	1.43
24	p	312	XAT	C11-C10	3.72	1.55	1.43
22	v	302	CLA	C1D-ND	3.72	1.42	1.37
26	2	314	CHL	OBD-CAD	3.72	1.28	1.22
31	d	403	BCR	C15-C14	3.72	1.55	1.43
31	D	404	BCR	C15-C14	3.72	1.55	1.43
26	q	312	CHL	OBD-CAD	3.72	1.28	1.22
34	D	408	LMG	O6-C1	3.72	1.51	1.41
22	r	605	CLA	C1D-ND	3.71	1.42	1.37
22	r	608	CLA	C1D-ND	3.71	1.42	1.37
22	B	605	CLA	C1D-ND	3.71	1.42	1.37
34	d	407	LMG	O6-C1	3.71	1.51	1.41
24	G	309	XAT	C15-C14	3.71	1.55	1.43
24	5	311	XAT	C11-C10	3.71	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	309	XAT	C15-C14	3.71	1.55	1.43
22	N	301	CLA	C1D-ND	3.71	1.42	1.37
26	4	314	CHL	CHD-C4C	3.71	1.47	1.39
26	V	313	CHL	CHC-C4B	3.71	1.47	1.39
24	v	311	XAT	C15-C14	3.71	1.54	1.43
22	1	301	CLA	C1D-ND	3.71	1.42	1.37
22	6	307	CLA	C1D-ND	3.71	1.42	1.37
24	3	309	XAT	C11-C10	3.71	1.54	1.43
34	C	502	LMG	O6-C1	3.71	1.51	1.41
24	2	311	XAT	C11-C10	3.71	1.54	1.43
26	N	316	CHL	CHD-C4C	3.71	1.47	1.39
30	d	401	PHO	C1D-C2D	3.71	1.43	1.39
34	c	501	LMG	O6-C1	3.71	1.51	1.41
26	g	313	CHL	OBD-CAD	3.71	1.28	1.22
22	G	305	CLA	C1D-ND	3.70	1.42	1.37
22	g	301	CLA	C1D-ND	3.70	1.42	1.37
22	g	308	CLA	C1D-ND	3.70	1.42	1.37
22	4	302	CLA	C1D-ND	3.70	1.42	1.37
34	B	621	LMG	O6-C1	3.70	1.51	1.41
26	s	313	CHL	CHC-C4B	3.70	1.47	1.39
34	c	520	LMG	O6-C1	3.70	1.51	1.41
24	g	309	XAT	C11-C10	3.70	1.54	1.43
26	4	315	CHL	OBD-CAD	3.70	1.28	1.22
22	N	306	CLA	C1D-ND	3.70	1.42	1.37
22	s	302	CLA	C4B-NB	3.70	1.42	1.37
26	Q	315	CHL	CHC-C4B	3.70	1.47	1.39
26	u	314	CHL	OBD-CAD	3.70	1.28	1.22
26	n	315	CHL	OBD-CAD	3.70	1.28	1.22
26	3	315	CHL	CHD-C1D	3.69	1.45	1.38
26	6	313	CHL	CHC-C4B	3.69	1.47	1.39
26	3	314	CHL	CHC-C4B	3.69	1.47	1.39
26	S	314	CHL	OBD-CAD	3.69	1.28	1.22
26	5	314	CHL	OBD-CAD	3.69	1.28	1.22
26	3	312	CHL	CHC-C4B	3.69	1.47	1.39
22	q	302	CLA	C1D-ND	3.69	1.42	1.37
22	n	302	CLA	C4B-NB	3.69	1.42	1.37
22	g	305	CLA	C1D-ND	3.69	1.42	1.37
22	G	307	CLA	C1D-ND	3.69	1.42	1.37
26	N	314	CHL	OBD-CAD	3.69	1.28	1.22
26	p	315	CHL	CHB-C1B	3.69	1.47	1.39
26	2	317	CHL	CHD-C4C	3.68	1.47	1.39
22	6	309	CLA	C1D-ND	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	309	XAT	C35-C34	3.68	1.54	1.43
31	C	516	BCR	C12-C13	3.68	1.53	1.45
22	S	305	CLA	C1D-ND	3.68	1.42	1.37
26	s	314	CHL	OBD-CAD	3.68	1.28	1.22
24	u	311	XAT	C11-C10	3.68	1.54	1.43
26	3	315	CHL	CHD-C4C	3.68	1.47	1.39
36	J	101	DGD	O6D-C1D	3.68	1.51	1.41
31	X	201	BCR	C15-C14	3.68	1.54	1.43
22	n	303	CLA	C1D-ND	3.68	1.42	1.37
26	1	314	CHL	OBD-CAD	3.68	1.28	1.22
22	U	305	CLA	C1D-ND	3.68	1.42	1.37
22	3	303	CLA	C1D-ND	3.68	1.42	1.37
26	5	315	CHL	CHD-C4C	3.68	1.47	1.39
22	V	306	CLA	C1D-ND	3.68	1.42	1.37
24	U	311	XAT	C15-C14	3.68	1.54	1.43
26	u	318	CHL	CHD-C4C	3.68	1.47	1.39
31	B	620	BCR	C12-C13	3.68	1.53	1.45
26	S	313	CHL	CHC-C4B	3.68	1.47	1.39
24	U	311	XAT	C35-C34	3.67	1.54	1.43
22	s	303	CLA	C1D-ND	3.67	1.42	1.37
26	5	317	CHL	CHD-C4C	3.67	1.47	1.39
31	A	409	BCR	C12-C13	3.67	1.53	1.45
24	4	311	XAT	C11-C10	3.67	1.54	1.43
26	6	314	CHL	CHC-C4B	3.67	1.47	1.39
22	u	305	CLA	C1D-ND	3.67	1.42	1.37
26	V	315	CHL	CHC-C4B	3.67	1.47	1.39
26	r	619	CHL	OBD-CAD	3.67	1.28	1.22
22	B	607	CLA	C1D-ND	3.67	1.42	1.37
31	c	516	BCR	C15-C14	3.66	1.54	1.43
22	s	304	CLA	C1D-ND	3.66	1.42	1.37
22	N	302	CLA	C4B-NB	3.66	1.42	1.37
22	N	307	CLA	C1D-ND	3.66	1.42	1.37
34	A	411	LMG	O6-C1	3.66	1.51	1.41
24	G	309	XAT	C11-C10	3.66	1.54	1.43
22	g	307	CLA	C1D-ND	3.66	1.42	1.37
26	1	315	CHL	OBD-CAD	3.66	1.28	1.22
31	b	620	BCR	C15-C14	3.66	1.54	1.43
22	5	304	CLA	C1D-ND	3.66	1.42	1.37
26	6	316	CHL	CHC-C4B	3.66	1.47	1.39
22	s	302	CLA	C1D-ND	3.66	1.42	1.37
26	4	314	CHL	OBD-CAD	3.66	1.28	1.22
22	Q	308	CLA	C1D-ND	3.66	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	318	CHL	OBD-CAD	3.66	1.28	1.22
22	S	304	CLA	C1D-ND	3.66	1.42	1.37
24	N	311	XAT	C15-C14	3.65	1.54	1.43
31	x	202	BCR	C15-C14	3.65	1.54	1.43
26	G	313	CHL	OBD-CAD	3.65	1.28	1.22
26	1	313	CHL	CHC-C4B	3.65	1.47	1.39
31	a	409	BCR	C12-C13	3.65	1.53	1.45
24	U	311	XAT	C11-C10	3.65	1.54	1.43
36	c	518	DGD	O6E-C1E	3.65	1.51	1.41
26	U	315	CHL	OBD-CAD	3.65	1.28	1.22
26	n	314	CHL	OBD-CAD	3.65	1.28	1.22
22	G	303	CLA	C1D-ND	3.65	1.42	1.37
22	s	305	CLA	C1D-ND	3.65	1.42	1.37
22	b	607	CLA	C1D-ND	3.64	1.42	1.37
34	a	412	LMG	O6-C1	3.64	1.51	1.41
26	q	312	CHL	CHC-C4B	3.64	1.47	1.39
22	q	303	CLA	C1D-ND	3.64	1.42	1.37
22	n	307	CLA	C1D-ND	3.64	1.42	1.37
22	b	617	CLA	C1D-ND	3.64	1.42	1.37
24	n	311	XAT	C15-C14	3.64	1.54	1.43
22	P	307	CLA	C1D-ND	3.64	1.42	1.37
26	3	315	CHL	CHC-C4B	3.64	1.47	1.39
26	v	313	CHL	CHC-C4B	3.64	1.47	1.39
26	5	316	CHL	OBD-CAD	3.64	1.28	1.22
24	n	311	XAT	C11-C10	3.64	1.54	1.43
26	V	316	CHL	OBD-CAD	3.64	1.28	1.22
36	c	519	DGD	O6D-C1D	3.64	1.51	1.41
22	a	404	CLA	C4D-ND	-3.64	1.32	1.37
22	p	307	CLA	C1D-ND	3.64	1.42	1.37
26	5	313	CHL	OBD-CAD	3.64	1.28	1.22
26	q	313	CHL	OBD-CAD	3.64	1.28	1.22
22	q	308	CLA	C1D-ND	3.64	1.42	1.37
26	G	315	CHL	CHD-C4C	3.64	1.47	1.39
26	u	316	CHL	OBD-CAD	3.63	1.28	1.22
26	Q	312	CHL	CHC-C4B	3.63	1.47	1.39
26	Q	314	CHL	OBD-CAD	3.63	1.28	1.22
22	5	301	CLA	C1D-ND	3.63	1.42	1.37
22	S	302	CLA	C1D-ND	3.63	1.42	1.37
26	3	313	CHL	CHC-C4B	3.63	1.47	1.39
26	q	314	CHL	CHC-C4B	3.63	1.47	1.39
22	a	406	CLA	C1D-ND	3.63	1.42	1.37
26	2	316	CHL	OBD-CAD	3.63	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	315	CHL	CHC-C4B	3.63	1.47	1.39
26	N	314	CHL	CHC-C4B	3.63	1.47	1.39
22	A	406	CLA	C1D-ND	3.63	1.42	1.37
22	1	302	CLA	C1D-ND	3.63	1.42	1.37
22	P	309	CLA	C1D-ND	3.63	1.42	1.37
26	P	316	CHL	OBD-CAD	3.63	1.28	1.22
26	Q	311	CHL	OBD-CAD	3.63	1.28	1.22
26	Q	313	CHL	OBD-CAD	3.63	1.28	1.22
22	2	308	CLA	C1D-ND	3.63	1.42	1.37
36	C	520	DGD	O6E-C1E	3.63	1.51	1.41
24	1	311	XAT	C11-C10	3.63	1.54	1.43
26	r	614	CHL	OBD-CAD	3.63	1.28	1.22
26	G	312	CHL	CHC-C4B	3.63	1.47	1.39
31	C	518	BCR	C15-C14	3.63	1.54	1.43
26	6	314	CHL	OBD-CAD	3.63	1.28	1.22
22	P	305	CLA	C1D-ND	3.63	1.42	1.37
22	N	303	CLA	C1D-ND	3.63	1.42	1.37
26	v	315	CHL	CHC-C4B	3.62	1.47	1.39
26	r	615	CHL	OBD-CAD	3.62	1.28	1.22
22	r	602	CLA	C1D-ND	3.62	1.42	1.37
26	5	315	CHL	OBD-CAD	3.62	1.28	1.22
26	P	316	CHL	CHC-C4B	3.62	1.47	1.39
22	V	308	CLA	C1D-ND	3.62	1.42	1.37
26	N	315	CHL	OBD-CAD	3.62	1.28	1.22
26	5	314	CHL	CHC-C4B	3.62	1.47	1.39
22	6	304	CLA	C1D-ND	3.62	1.42	1.37
22	s	307	CLA	C1D-ND	3.62	1.42	1.37
22	5	308	CLA	C1D-ND	3.62	1.42	1.37
22	Q	303	CLA	C1D-ND	3.62	1.42	1.37
26	P	319	CHL	OBD-CAD	3.62	1.28	1.22
22	6	306	CLA	C1D-ND	3.62	1.42	1.37
26	s	316	CHL	CHC-C4B	3.62	1.47	1.39
22	2	304	CLA	C1D-ND	3.62	1.42	1.37
26	v	317	CHL	CHC-C4B	3.62	1.47	1.39
26	Q	315	CHL	CHD-C1D	3.62	1.45	1.38
26	R	316	CHL	OBD-CAD	3.62	1.28	1.22
26	g	314	CHL	CHC-C4B	3.61	1.47	1.39
26	N	315	CHL	CHD-C4C	3.61	1.47	1.39
22	q	305	CLA	C1D-ND	3.61	1.42	1.37
22	b	608	CLA	C1D-ND	3.61	1.42	1.37
22	V	303	CLA	C1D-ND	3.61	1.42	1.37
26	r	616	CHL	CHC-C4B	3.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	315	CHL	OBD-CAD	3.61	1.28	1.22
26	p	316	CHL	OBD-CAD	3.61	1.28	1.22
26	S	316	CHL	CHC-C4B	3.61	1.47	1.39
22	u	302	CLA	C1D-ND	3.61	1.42	1.37
22	S	303	CLA	C1D-ND	3.61	1.42	1.37
36	a	416	DGD	O6D-C1D	3.61	1.51	1.41
26	3	313	CHL	OBD-CAD	3.61	1.28	1.22
36	A	414	DGD	O6D-C1D	3.61	1.51	1.41
26	N	317	CHL	OBD-CAD	3.61	1.28	1.22
22	R	303	CLA	C1D-ND	3.60	1.42	1.37
26	U	319	CHL	OBD-CAD	3.60	1.28	1.22
31	C	517	BCR	C12-C13	3.60	1.53	1.45
26	P	318	CHL	CHD-C4C	3.60	1.47	1.39
26	g	315	CHL	CHD-C4C	3.60	1.47	1.39
22	A	404	CLA	C4D-ND	-3.60	1.32	1.37
22	4	308	CLA	C1D-ND	3.60	1.42	1.37
22	R	305	CLA	C1D-ND	3.60	1.42	1.37
26	P	314	CHL	OBD-CAD	3.60	1.28	1.22
26	6	301	CHL	OBD-CAD	3.60	1.28	1.22
26	s	316	CHL	OBD-CAD	3.60	1.28	1.22
26	V	315	CHL	CHB-C1B	3.60	1.47	1.39
22	3	306	CLA	C1D-ND	3.60	1.42	1.37
22	u	301	CLA	C1D-ND	3.60	1.42	1.37
26	p	320	CHL	OBD-CAD	3.60	1.28	1.22
26	N	313	CHL	OBD-CAD	3.60	1.28	1.22
36	b	601	DGD	O6E-C1E	3.60	1.51	1.41
26	p	318	CHL	CHD-C4C	3.60	1.47	1.39
31	K	101	BCR	C15-C14	3.60	1.54	1.43
22	b	605	CLA	C1D-ND	3.60	1.42	1.37
26	G	314	CHL	OBD-CAD	3.60	1.28	1.22
31	c	515	BCR	C12-C13	3.60	1.53	1.45
26	G	311	CHL	OBD-CAD	3.60	1.28	1.22
22	v	308	CLA	C1D-ND	3.59	1.42	1.37
26	q	314	CHL	CHD-C4C	3.59	1.47	1.39
22	A	405	CLA	C1D-ND	3.59	1.42	1.37
31	k	101	BCR	C15-C14	3.59	1.54	1.43
26	R	317	CHL	CHC-C4B	3.59	1.47	1.39
22	B	608	CLA	C1D-ND	3.59	1.42	1.37
22	q	307	CLA	C1D-ND	3.59	1.42	1.37
26	n	313	CHL	OBD-CAD	3.59	1.28	1.22
26	2	313	CHL	OBD-CAD	3.59	1.28	1.22
26	V	315	CHL	OBD-CAD	3.59	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	308	CLA	C1D-ND	3.59	1.42	1.37
26	1	316	CHL	OBD-CAD	3.59	1.28	1.22
31	B	620	BCR	C15-C14	3.59	1.54	1.43
22	q	306	CLA	C1D-ND	3.59	1.42	1.37
26	6	316	CHL	CHD-C4C	3.59	1.47	1.39
26	S	316	CHL	OBD-CAD	3.59	1.28	1.22
26	Q	314	CHL	CHC-C4B	3.59	1.47	1.39
26	p	319	CHL	OBD-CAD	3.59	1.28	1.22
26	R	315	CHL	OBD-CAD	3.59	1.28	1.22
22	s	306	CLA	C1D-ND	3.59	1.42	1.37
26	3	316	CHL	OBD-CAD	3.59	1.28	1.22
26	n	316	CHL	OBD-CAD	3.59	1.28	1.22
22	S	306	CLA	C1D-ND	3.59	1.42	1.37
26	6	312	CHL	OBD-CAD	3.59	1.28	1.22
22	v	303	CLA	C1D-ND	3.58	1.42	1.37
22	Q	304	CLA	C1D-ND	3.58	1.42	1.37
22	Q	306	CLA	C1D-ND	3.58	1.42	1.37
26	U	319	CHL	CHC-C4B	3.58	1.47	1.39
22	Q	307	CLA	C1D-ND	3.58	1.42	1.37
22	g	304	CLA	C1D-ND	3.58	1.42	1.37
26	6	317	CHL	OBD-CAD	3.58	1.28	1.22
22	6	308	CLA	C1D-ND	3.58	1.42	1.37
26	Q	315	CHL	CHD-C4C	3.58	1.47	1.39
22	g	302	CLA	C1D-ND	3.58	1.42	1.37
26	s	315	CHL	OBD-CAD	3.58	1.28	1.22
26	V	314	CHL	CHC-C4B	3.58	1.47	1.39
26	3	311	CHL	OBD-CAD	3.58	1.28	1.22
22	2	306	CLA	C1D-ND	3.58	1.42	1.37
26	S	314	CHL	CHC-C4B	3.57	1.47	1.39
26	V	316	CHL	CHC-C4B	3.57	1.47	1.39
26	V	313	CHL	OBD-CAD	3.57	1.28	1.22
22	n	302	CLA	C1D-ND	3.57	1.42	1.37
26	P	317	CHL	OBD-CAD	3.57	1.28	1.22
30	a	407	PHO	C1D-C2D	3.57	1.43	1.39
22	A	408	CLA	C1D-ND	3.57	1.42	1.37
22	V	302	CLA	C1D-ND	3.57	1.42	1.37
22	R	307	CLA	C1D-ND	3.57	1.42	1.37
22	3	307	CLA	C1D-ND	3.57	1.42	1.37
26	6	316	CHL	CHD-C1D	3.57	1.45	1.38
26	3	314	CHL	OBD-CAD	3.57	1.28	1.22
22	v	306	CLA	C1D-ND	3.56	1.42	1.37
22	p	305	CLA	C1D-ND	3.56	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	303	CLA	C1D-ND	3.56	1.42	1.37
26	u	313	CHL	OBD-CAD	3.56	1.28	1.22
26	s	314	CHL	CHC-C4B	3.56	1.47	1.39
26	1	318	CHL	OBD-CAD	3.56	1.28	1.22
26	U	314	CHL	OBD-CAD	3.56	1.28	1.22
26	p	315	CHL	OBD-CAD	3.56	1.28	1.22
22	4	306	CLA	C1D-ND	3.56	1.42	1.37
22	V	304	CLA	C1D-ND	3.56	1.42	1.37
31	B	619	BCR	C12-C13	3.56	1.53	1.45
22	r	604	CLA	C1D-ND	3.56	1.42	1.37
36	B	601	DGD	O6E-C1E	3.56	1.50	1.41
22	q	304	CLA	C1D-ND	3.56	1.42	1.37
26	P	317	CHL	CHC-C4B	3.56	1.47	1.39
26	5	318	CHL	OBD-CAD	3.56	1.28	1.22
26	U	313	CHL	CHC-C4B	3.56	1.47	1.39
26	u	315	CHL	OBD-CAD	3.56	1.28	1.22
26	2	315	CHL	OBD-CAD	3.56	1.28	1.22
26	p	316	CHL	CHC-C4B	3.56	1.47	1.39
26	4	317	CHL	OBD-CAD	3.56	1.28	1.22
22	1	308	CLA	C1D-ND	3.56	1.42	1.37
22	3	305	CLA	C1D-ND	3.56	1.42	1.37
26	V	318	CHL	OBD-CAD	3.55	1.28	1.22
26	r	614	CHL	CHC-C4B	3.55	1.47	1.39
26	S	315	CHL	OBD-CAD	3.55	1.28	1.22
22	U	308	CLA	C1D-ND	3.55	1.42	1.37
37	E	101	HEM	FE-ND	3.55	2.05	1.94
22	u	308	CLA	C1D-ND	3.55	1.42	1.37
22	S	307	CLA	C1D-ND	3.55	1.42	1.37
22	g	303	CLA	C1D-ND	3.55	1.42	1.37
22	p	309	CLA	C1D-ND	3.55	1.42	1.37
22	a	405	CLA	C4D-ND	-3.55	1.32	1.37
22	n	304	CLA	C1D-ND	3.55	1.42	1.37
26	g	311	CHL	OBD-CAD	3.55	1.28	1.22
22	a	405	CLA	C1D-ND	3.54	1.42	1.37
24	N	311	XAT	C11-C10	3.54	1.54	1.43
31	b	619	BCR	C12-C13	3.54	1.53	1.45
22	G	302	CLA	C1D-ND	3.54	1.42	1.37
22	4	305	CLA	C1D-ND	3.54	1.42	1.37
22	N	302	CLA	C1D-ND	3.54	1.42	1.37
22	5	306	CLA	C1D-ND	3.54	1.42	1.37
26	g	316	CHL	OBD-CAD	3.54	1.28	1.22
31	b	619	BCR	C15-C14	3.54	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	316	CHL	CHC-C4B	3.54	1.47	1.39
26	2	318	CHL	OBD-CAD	3.54	1.28	1.22
26	v	313	CHL	OBD-CAD	3.54	1.28	1.22
22	U	302	CLA	C1D-ND	3.54	1.42	1.37
31	B	619	BCR	C15-C14	3.54	1.54	1.43
22	G	304	CLA	C1D-ND	3.54	1.42	1.37
31	C	516	BCR	C15-C14	3.54	1.54	1.43
26	q	311	CHL	OBD-CAD	3.54	1.28	1.22
31	c	515	BCR	C27-C26	-3.54	1.44	1.51
31	C	517	BCR	C27-C26	-3.54	1.44	1.51
26	P	315	CHL	OBD-CAD	3.54	1.28	1.22
26	3	311	CHL	CHC-C4B	3.54	1.47	1.39
26	p	317	CHL	CHC-C4B	3.54	1.47	1.39
26	G	314	CHL	CHC-C4B	3.53	1.47	1.39
26	U	314	CHL	CHD-C4C	3.53	1.47	1.39
26	v	317	CHL	OBD-CAD	3.53	1.28	1.22
26	6	312	CHL	CHC-C4B	3.53	1.47	1.39
26	6	313	CHL	CHB-C1B	3.53	1.47	1.39
22	1	302	CLA	C4B-NB	3.53	1.42	1.37
22	p	303	CLA	C1D-ND	3.53	1.42	1.37
26	v	314	CHL	CHC-C4B	3.53	1.47	1.39
22	4	306	CLA	C4B-NB	3.53	1.42	1.37
22	C	510	CLA	C4D-ND	-3.53	1.32	1.37
30	A	407	PHO	C1D-C2D	3.53	1.43	1.39
26	V	317	CHL	CHC-C4B	3.53	1.47	1.39
26	S	316	CHL	CHB-C1B	3.53	1.47	1.39
22	U	306	CLA	C1D-ND	3.53	1.42	1.37
26	V	317	CHL	OBD-CAD	3.53	1.28	1.22
37	e	101	HEM	FE-ND	3.53	2.05	1.94
22	n	306	CLA	C1D-ND	3.53	1.42	1.37
31	z	101	BCR	C15-C14	3.52	1.54	1.43
31	C	516	BCR	C27-C26	-3.52	1.44	1.51
22	1	305	CLA	C1D-ND	3.52	1.42	1.37
26	n	314	CHL	CHB-C1B	3.52	1.47	1.39
26	n	316	CHL	CHC-C4B	3.52	1.47	1.39
26	3	312	CHL	CHB-C1B	3.52	1.47	1.39
26	s	316	CHL	CHB-C1B	3.52	1.47	1.39
22	v	307	CLA	C1D-ND	3.52	1.42	1.37
26	2	315	CHL	CHC-C4B	3.52	1.47	1.39
26	v	316	CHL	OBD-CAD	3.52	1.28	1.22
22	5	307	CLA	C1D-ND	3.52	1.42	1.37
22	6	303	CLA	C1D-ND	3.52	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	301	CLA	C1D-ND	3.52	1.42	1.37
22	V	306	CLA	C4B-NB	3.52	1.42	1.37
22	P	308	CLA	C1D-ND	3.52	1.42	1.37
26	v	315	CHL	OBD-CAD	3.52	1.28	1.22
26	v	318	CHL	OBD-CAD	3.52	1.28	1.22
22	b	604	CLA	C1D-ND	3.52	1.42	1.37
26	5	315	CHL	CHC-C4B	3.52	1.47	1.39
22	c	510	CLA	C4D-ND	-3.51	1.32	1.37
26	u	315	CHL	CHC-C4B	3.51	1.47	1.39
26	1	317	CHL	OBD-CAD	3.51	1.28	1.22
26	p	314	CHL	OBD-CAD	3.51	1.28	1.22
22	v	305	CLA	C1D-ND	3.51	1.42	1.37
22	V	307	CLA	C1D-ND	3.51	1.42	1.37
26	2	317	CHL	OBD-CAD	3.51	1.28	1.22
26	r	619	CHL	CHC-C4B	3.51	1.47	1.39
26	S	315	CHL	CHB-C1B	3.51	1.47	1.39
31	z	101	BCR	C27-C26	-3.50	1.44	1.51
26	u	313	CHL	CHC-C4B	3.50	1.47	1.39
22	3	302	CLA	C1D-ND	3.50	1.42	1.37
22	v	304	CLA	C1D-ND	3.50	1.42	1.37
22	c	512	CLA	C1D-ND	3.50	1.42	1.37
31	C	517	BCR	C15-C14	3.50	1.54	1.43
26	5	317	CHL	OBD-CAD	3.50	1.28	1.22
26	U	313	CHL	OBD-CAD	3.50	1.28	1.22
31	A	409	BCR	C15-C14	3.50	1.54	1.43
31	b	619	BCR	C27-C26	-3.50	1.44	1.51
22	c	503	CLA	C4D-ND	-3.50	1.32	1.37
26	4	316	CHL	OBD-CAD	3.50	1.28	1.22
26	1	315	CHL	CHC-C4B	3.50	1.47	1.39
34	W	201	LMG	O6-C1	3.50	1.50	1.41
22	a	408	CLA	C1D-ND	3.50	1.42	1.37
22	p	308	CLA	C1D-ND	3.50	1.42	1.37
36	J	101	DGD	O6E-C1E	3.49	1.50	1.41
22	U	301	CLA	C1D-ND	3.49	1.42	1.37
26	p	317	CHL	OBD-CAD	3.49	1.28	1.22
31	t	101	BCR	C24-C25	3.49	1.57	1.45
31	c	515	BCR	C15-C14	3.49	1.54	1.43
26	5	316	CHL	CHC-C4B	3.49	1.47	1.39
26	4	313	CHL	OBD-CAD	3.49	1.28	1.22
26	n	315	CHL	CHC-C4B	3.49	1.47	1.39
22	1	307	CLA	C1D-ND	3.49	1.42	1.37
22	r	606	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	316	CHL	OBD-CAD	3.48	1.28	1.22
22	Q	305	CLA	C1D-ND	3.48	1.42	1.37
31	D	404	BCR	C24-C25	3.48	1.57	1.45
31	a	409	BCR	C15-C14	3.48	1.54	1.43
22	u	306	CLA	C1D-ND	3.48	1.42	1.37
26	u	314	CHL	CHC-C4B	3.48	1.47	1.39
26	4	315	CHL	CHC-C4B	3.48	1.47	1.39
26	6	314	CHL	CHB-C1B	3.48	1.47	1.39
26	1	313	CHL	OBD-CAD	3.48	1.28	1.22
26	s	313	CHL	OBD-CAD	3.48	1.28	1.22
31	T	101	BCR	C24-C25	3.48	1.57	1.45
26	U	314	CHL	CHC-C4B	3.48	1.47	1.39
26	u	318	CHL	CHC-C4B	3.48	1.47	1.39
22	C	504	CLA	C4D-ND	-3.48	1.32	1.37
22	2	302	CLA	C1D-ND	3.48	1.42	1.37
26	v	315	CHL	CHB-C1B	3.48	1.47	1.39
26	R	315	CHL	CHC-C4B	3.48	1.47	1.39
26	g	311	CHL	CHC-C4B	3.48	1.47	1.39
22	u	303	CLA	C1D-ND	3.48	1.42	1.37
22	B	610	CLA	C1D-ND	3.48	1.42	1.37
22	C	505	CLA	C1D-ND	3.48	1.42	1.37
31	B	618	BCR	C12-C13	3.48	1.53	1.45
26	q	315	CHL	CHC-C4B	3.47	1.47	1.39
22	3	304	CLA	C1D-ND	3.47	1.42	1.37
22	4	306	CLA	C3B-C4B	3.47	1.50	1.42
26	S	313	CHL	OBD-CAD	3.47	1.28	1.22
22	B	604	CLA	C1D-ND	3.47	1.42	1.37
22	b	610	CLA	C1D-ND	3.47	1.42	1.37
22	C	511	CLA	C4D-ND	-3.47	1.32	1.37
26	v	316	CHL	CHC-C4B	3.47	1.47	1.39
31	d	403	BCR	C24-C25	3.47	1.57	1.45
31	c	516	BCR	C27-C26	-3.47	1.44	1.51
31	B	619	BCR	C27-C26	-3.46	1.44	1.51
26	q	314	CHL	CHD-C1D	3.46	1.45	1.38
22	b	613	CLA	C4D-ND	-3.46	1.32	1.37
26	2	316	CHL	CHC-C4B	3.46	1.47	1.39
22	r	607	CLA	C1D-ND	3.46	1.42	1.37
26	G	316	CHL	OBD-CAD	3.46	1.28	1.22
22	1	303	CLA	C1D-ND	3.46	1.42	1.37
26	3	313	CHL	CHB-C1B	3.46	1.47	1.39
26	g	312	CHL	CHC-C4B	3.46	1.47	1.39
22	u	307	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	305	CLA	C1D-ND	3.46	1.42	1.37
26	q	312	CHL	CHB-C1B	3.45	1.47	1.39
31	B	618	BCR	C15-C14	3.45	1.54	1.43
22	S	302	CLA	C3B-C4B	3.45	1.50	1.42
26	4	313	CHL	CHC-C4B	3.45	1.47	1.39
26	G	311	CHL	CHC-C4B	3.45	1.47	1.39
22	1	302	CLA	C3B-C4B	3.45	1.50	1.42
22	4	307	CLA	C1D-ND	3.45	1.42	1.37
34	w	201	LMG	O6-C1	3.45	1.50	1.41
26	U	317	CHL	OBD-CAD	3.45	1.28	1.22
22	5	302	CLA	C1D-ND	3.45	1.42	1.37
22	4	302	CLA	C4B-NB	3.45	1.42	1.37
22	x	201	CLA	C1D-ND	3.45	1.42	1.37
22	n	302	CLA	C3B-C4B	3.45	1.50	1.42
26	V	318	CHL	CHC-C4B	3.45	1.47	1.39
26	s	315	CHL	CHB-C1B	3.45	1.47	1.39
26	r	616	CHL	OBD-CAD	3.45	1.28	1.22
22	b	609	CLA	C4D-ND	-3.45	1.33	1.37
26	1	314	CHL	CHC-C4B	3.44	1.47	1.39
22	U	307	CLA	C1D-ND	3.44	1.42	1.37
26	N	313	CHL	CHC-C4B	3.44	1.47	1.39
26	P	318	CHL	OBD-CAD	3.44	1.28	1.22
22	b	616	CLA	C1D-ND	3.44	1.42	1.37
22	5	302	CLA	C4D-ND	-3.44	1.33	1.37
26	u	315	CHL	CHD-C4C	3.44	1.47	1.39
22	n	308	CLA	C4B-NB	3.44	1.42	1.37
26	V	313	CHL	CHB-C1B	3.44	1.47	1.39
22	c	509	CLA	C4D-ND	-3.44	1.33	1.37
22	2	302	CLA	C3B-C4B	3.44	1.50	1.42
26	Q	311	CHL	CHC-C4B	3.44	1.47	1.39
22	S	309	CLA	C1D-ND	3.43	1.42	1.37
31	a	409	BCR	C24-C25	3.43	1.57	1.45
22	4	303	CLA	C1D-ND	3.43	1.42	1.37
26	u	318	CHL	OBD-CAD	3.43	1.28	1.22
22	N	304	CLA	C1D-ND	3.43	1.42	1.37
22	C	513	CLA	C1D-ND	3.43	1.42	1.37
36	c	519	DGD	O6E-C1E	3.43	1.50	1.41
22	c	504	CLA	C1D-ND	3.43	1.42	1.37
22	c	506	CLA	C1D-ND	3.43	1.42	1.37
26	2	314	CHL	CHB-C1B	3.42	1.47	1.39
22	6	305	CLA	C1D-ND	3.42	1.42	1.37
22	2	307	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	301	CHL	CHC-C4B	3.42	1.47	1.39
22	B	602	CLA	C1D-ND	3.42	1.42	1.37
26	N	314	CHL	CHB-C1B	3.42	1.47	1.39
22	1	306	CLA	C1D-ND	3.42	1.42	1.37
26	N	316	CHL	CHC-C4B	3.42	1.47	1.39
22	C	507	CLA	C1D-ND	3.42	1.42	1.37
22	Q	301	CLA	C4D-ND	-3.42	1.33	1.37
22	s	309	CLA	C1D-ND	3.42	1.42	1.37
22	5	303	CLA	C1D-ND	3.42	1.42	1.37
31	b	618	BCR	C15-C14	3.42	1.54	1.43
22	B	613	CLA	C4D-ND	-3.42	1.33	1.37
22	B	617	CLA	C1D-ND	3.41	1.42	1.37
22	v	302	CLA	C4D-ND	-3.41	1.33	1.37
22	s	308	CLA	C1D-ND	3.41	1.42	1.37
22	s	302	CLA	C3B-C4B	3.41	1.50	1.42
26	N	315	CHL	CHC-C4B	3.41	1.47	1.39
26	n	317	CHL	CHC-C4B	3.41	1.47	1.39
31	C	518	BCR	C27-C26	-3.41	1.44	1.51
26	U	316	CHL	OBD-CAD	3.41	1.28	1.22
22	5	305	CLA	C4B-NB	3.41	1.42	1.37
31	A	409	BCR	C24-C25	3.41	1.57	1.45
26	p	318	CHL	OBD-CAD	3.41	1.28	1.22
22	p	302	CLA	C1D-ND	3.41	1.42	1.37
22	X	202	CLA	C1D-ND	3.41	1.42	1.37
22	N	302	CLA	C3B-C4B	3.41	1.50	1.42
26	n	317	CHL	CHB-C1B	3.41	1.47	1.39
26	q	315	CHL	OBD-CAD	3.41	1.28	1.22
22	A	405	CLA	C4D-ND	-3.40	1.33	1.37
22	R	305	CLA	C4B-NB	3.40	1.42	1.37
26	1	316	CHL	CHC-C4B	3.40	1.47	1.39
22	R	302	CLA	C4B-NB	3.40	1.42	1.37
22	c	507	CLA	C4D-ND	-3.40	1.33	1.37
26	U	315	CHL	CHC-C4B	3.40	1.47	1.39
26	s	313	CHL	CHB-C1B	3.40	1.47	1.39
22	b	603	CLA	C1D-ND	3.40	1.42	1.37
26	3	315	CHL	OBD-CAD	3.40	1.28	1.22
26	n	315	CHL	CHB-C1B	3.40	1.47	1.39
26	g	313	CHL	CHC-C4B	3.40	1.47	1.39
22	2	303	CLA	C1D-ND	3.40	1.42	1.37
22	U	303	CLA	C1D-ND	3.39	1.42	1.37
22	C	508	CLA	C4D-ND	-3.39	1.33	1.37
26	Q	312	CHL	CHB-C1B	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C4D-ND	-3.39	1.33	1.37
22	c	504	CLA	C4D-ND	-3.39	1.33	1.37
22	S	308	CLA	C1D-ND	3.39	1.42	1.37
22	V	306	CLA	C3B-C4B	3.39	1.50	1.42
26	Q	316	CHL	OBD-CAD	3.39	1.28	1.22
22	c	509	CLA	C4B-NB	3.39	1.42	1.37
26	Q	316	CHL	CHC-C4B	3.39	1.47	1.39
22	2	301	CLA	C4D-ND	-3.39	1.33	1.37
22	B	606	CLA	C1D-ND	3.39	1.41	1.37
26	G	313	CHL	CHC-C4B	3.39	1.47	1.39
22	b	614	CLA	C1D-ND	3.38	1.41	1.37
26	4	314	CHL	CHC-C4B	3.38	1.47	1.39
26	4	315	CHL	CHB-C1B	3.38	1.47	1.39
22	r	601	CLA	C4B-NB	3.38	1.41	1.37
22	B	614	CLA	C1D-ND	3.38	1.41	1.37
26	V	316	CHL	CHB-C1B	3.38	1.47	1.39
26	n	313	CHL	CHB-C1B	3.38	1.47	1.39
22	b	615	CLA	C1D-ND	3.38	1.41	1.37
31	b	618	BCR	C12-C13	3.38	1.53	1.45
22	3	301	CLA	C4D-ND	-3.38	1.33	1.37
26	g	314	CHL	CHB-C1B	3.37	1.47	1.39
22	v	306	CLA	C4B-NB	3.37	1.41	1.37
22	u	304	CLA	C1D-ND	3.37	1.41	1.37
22	Q	303	CLA	C4B-NB	3.37	1.41	1.37
26	p	320	CHL	CHC-C4B	3.37	1.47	1.39
22	C	505	CLA	C4D-ND	-3.37	1.33	1.37
22	N	308	CLA	C4B-NB	3.37	1.41	1.37
26	6	315	CHL	CHB-C1B	3.37	1.47	1.39
22	C	506	CLA	C4D-ND	-3.37	1.33	1.37
26	2	313	CHL	CHB-C1B	3.37	1.47	1.39
22	q	301	CLA	C4D-ND	-3.37	1.33	1.37
26	q	311	CHL	CHC-C4B	3.36	1.47	1.39
22	P	302	CLA	C1D-ND	3.36	1.41	1.37
26	P	315	CHL	MG-NA	-3.36	1.98	2.06
22	b	612	CLA	C1D-ND	3.36	1.41	1.37
22	B	606	CLA	C4D-ND	-3.36	1.33	1.37
22	r	610	CLA	C4B-NB	3.36	1.41	1.37
22	b	606	CLA	C1D-ND	3.36	1.41	1.37
22	B	616	CLA	C1D-ND	3.36	1.41	1.37
22	C	510	CLA	C4B-NB	3.36	1.41	1.37
22	c	514	CLA	C4D-ND	-3.36	1.33	1.37
26	r	615	CHL	CHC-C4B	3.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	317	CHL	OBD-CAD	3.36	1.28	1.22
26	3	315	CHL	CHB-C1B	3.36	1.46	1.39
26	n	317	CHL	OBD-CAD	3.36	1.28	1.22
26	5	314	CHL	CHB-C1B	3.36	1.46	1.39
22	2	302	CLA	C4B-NB	3.36	1.41	1.37
22	5	305	CLA	C3D-C4D	3.35	1.51	1.44
26	R	316	CHL	CHC-C4B	3.35	1.46	1.39
26	R	317	CHL	OBD-CAD	3.35	1.28	1.22
22	V	302	CLA	C4D-ND	-3.35	1.33	1.37
22	C	507	CLA	C4D-ND	-3.35	1.33	1.37
36	C	520	DGD	O6D-C1D	3.35	1.50	1.41
31	X	201	BCR	C24-C25	3.35	1.57	1.45
36	c	518	DGD	O6D-C1D	3.35	1.50	1.41
22	c	505	CLA	C4D-ND	-3.35	1.33	1.37
31	b	620	BCR	C24-C25	3.35	1.57	1.45
26	2	317	CHL	CHC-C4B	3.35	1.46	1.39
22	B	603	CLA	C1D-ND	3.35	1.41	1.37
26	S	313	CHL	CHB-C1B	3.35	1.46	1.39
22	B	614	CLA	C4D-ND	-3.35	1.33	1.37
22	b	602	CLA	C1D-ND	3.35	1.41	1.37
22	p	306	CLA	C3D-C4D	3.35	1.51	1.44
31	b	618	BCR	C27-C26	-3.35	1.44	1.51
31	x	202	BCR	C24-C25	3.35	1.57	1.45
22	g	306	CLA	C4B-NB	3.34	1.41	1.37
22	d	402	CLA	C4D-ND	-3.34	1.33	1.37
31	b	619	BCR	C24-C25	3.34	1.57	1.45
22	B	615	CLA	C1D-ND	3.34	1.41	1.37
22	c	506	CLA	C4D-ND	-3.34	1.33	1.37
26	5	313	CHL	CHB-C1B	3.34	1.46	1.39
26	u	317	CHL	CHC-C4B	3.34	1.46	1.39
22	4	304	CLA	C1D-ND	3.34	1.41	1.37
22	c	507	CLA	C4B-NB	3.34	1.41	1.37
31	b	620	BCR	C27-C26	-3.34	1.44	1.51
22	c	503	CLA	C1D-ND	3.34	1.41	1.37
22	c	511	CLA	C1D-ND	3.34	1.41	1.37
31	A	409	BCR	C27-C26	-3.34	1.44	1.51
22	R	309	CLA	C4B-NB	3.33	1.41	1.37
31	B	619	BCR	C24-C25	3.33	1.56	1.45
22	A	406	CLA	C4D-ND	-3.33	1.33	1.37
22	b	606	CLA	C4D-ND	-3.33	1.33	1.37
26	1	317	CHL	CHC-C4B	3.33	1.46	1.39
26	G	312	CHL	CHB-C1B	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	CLA	C4D-ND	-3.33	1.33	1.37
26	U	317	CHL	CHC-C4B	3.33	1.46	1.39
31	C	518	BCR	C24-C25	3.33	1.56	1.45
31	B	620	BCR	C24-C25	3.33	1.56	1.45
22	1	301	CLA	C4D-ND	-3.33	1.33	1.37
22	B	612	CLA	C1D-ND	3.33	1.41	1.37
22	c	513	CLA	C4D-ND	-3.33	1.33	1.37
22	C	514	CLA	C4D-ND	-3.33	1.33	1.37
22	u	305	CLA	C4D-ND	-3.33	1.33	1.37
31	c	516	BCR	C24-C25	3.33	1.56	1.45
22	p	302	CLA	C4D-ND	-3.33	1.33	1.37
31	B	618	BCR	C27-C26	-3.32	1.44	1.51
31	T	101	BCR	C37-C22	3.32	1.57	1.50
22	4	301	CLA	C4D-ND	-3.32	1.33	1.37
22	b	614	CLA	C4D-ND	-3.32	1.33	1.37
22	D	403	CLA	C4D-ND	-3.32	1.33	1.37
22	n	305	CLA	C4B-NB	3.32	1.41	1.37
22	R	311	CLA	C4B-NB	3.32	1.41	1.37
22	b	602	CLA	C4D-ND	-3.32	1.33	1.37
26	v	313	CHL	CHB-C1B	3.32	1.46	1.39
26	3	314	CHL	CHB-C1B	3.32	1.46	1.39
22	C	504	CLA	C1D-ND	3.31	1.41	1.37
26	u	313	CHL	CHB-C1B	3.31	1.46	1.39
22	C	515	CLA	C4D-ND	-3.31	1.33	1.37
26	P	316	CHL	CHB-C1B	3.31	1.46	1.39
26	p	314	CHL	CHB-C1B	3.31	1.46	1.39
26	P	314	CHL	CHB-C1B	3.31	1.46	1.39
22	A	408	CLA	C4D-ND	-3.31	1.33	1.37
36	J	101	DGD	O2G-C1B	3.31	1.43	1.34
26	G	313	CHL	CHB-C1B	3.31	1.46	1.39
26	5	316	CHL	CHB-C1B	3.31	1.46	1.39
26	4	316	CHL	CHC-C4B	3.31	1.46	1.39
26	q	313	CHL	CHC-C4B	3.31	1.46	1.39
26	U	316	CHL	CHC-C4B	3.31	1.46	1.39
22	a	406	CLA	C4D-ND	-3.31	1.33	1.37
26	U	313	CHL	CHB-C1B	3.31	1.46	1.39
22	a	408	CLA	C4D-ND	-3.31	1.33	1.37
26	v	318	CHL	CHC-C4B	3.31	1.46	1.39
26	n	318	CHL	CHB-C1B	3.31	1.46	1.39
22	C	512	CLA	C1D-ND	3.31	1.41	1.37
22	6	302	CLA	C4D-ND	-3.31	1.33	1.37
22	A	404	CLA	C1D-ND	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	C4B-NB	3.30	1.41	1.37
26	Q	314	CHL	CHB-C1B	3.30	1.46	1.39
31	B	620	BCR	C27-C26	-3.30	1.44	1.51
26	Q	313	CHL	CHB-C1B	3.30	1.46	1.39
22	5	301	CLA	C4D-ND	-3.30	1.33	1.37
22	G	301	CLA	C4D-ND	-3.30	1.33	1.37
22	u	304	CLA	C4D-ND	-3.30	1.33	1.37
26	q	314	CHL	OBD-CAD	3.30	1.28	1.22
31	a	409	BCR	C27-C26	-3.30	1.44	1.51
22	4	302	CLA	C3B-C4B	3.30	1.50	1.42
22	2	305	CLA	C4B-NB	3.30	1.41	1.37
26	p	316	CHL	CHB-C1B	3.29	1.46	1.39
26	q	315	CHL	CHB-C1B	3.29	1.46	1.39
22	4	304	CLA	C4D-ND	-3.29	1.33	1.37
31	C	516	BCR	C24-C25	3.29	1.56	1.45
22	b	613	CLA	C1D-ND	3.29	1.41	1.37
22	n	305	CLA	C3D-C4D	3.29	1.51	1.44
26	1	315	CHL	CHB-C1B	3.29	1.46	1.39
26	N	316	CHL	CHB-C1B	3.28	1.46	1.39
26	N	315	CHL	CHB-C1B	3.28	1.46	1.39
26	1	316	CHL	CHB-C1B	3.28	1.46	1.39
22	r	608	CLA	C4B-NB	3.28	1.41	1.37
22	q	303	CLA	C4B-NB	3.28	1.41	1.37
22	c	514	CLA	C1D-ND	3.28	1.41	1.37
22	4	303	CLA	C4D-ND	-3.28	1.33	1.37
22	v	301	CLA	C4D-ND	-3.28	1.33	1.37
22	B	602	CLA	C4D-ND	-3.28	1.33	1.37
31	k	101	BCR	C27-C26	-3.28	1.44	1.51
22	Q	306	CLA	C4B-NB	3.28	1.41	1.37
22	r	604	CLA	C4B-NB	3.28	1.41	1.37
26	Q	315	CHL	CHB-C1B	3.28	1.46	1.39
22	V	301	CLA	C4D-ND	-3.27	1.33	1.37
22	v	307	CLA	C4D-ND	-3.27	1.33	1.37
22	u	306	CLA	C4D-ND	-3.27	1.33	1.37
31	t	101	BCR	C27-C26	-3.27	1.44	1.51
22	C	503	CLA	C1D-ND	3.27	1.41	1.37
22	C	514	CLA	C1D-ND	3.27	1.41	1.37
22	r	609	CLA	C4B-NB	3.27	1.41	1.37
22	B	603	CLA	C4D-ND	-3.27	1.33	1.37
22	C	515	CLA	C1D-ND	3.27	1.41	1.37
31	z	101	BCR	C24-C25	3.27	1.56	1.45
26	P	318	CHL	CHC-C4B	3.27	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	307	CLA	C4D-ND	-3.27	1.33	1.37
22	g	304	CLA	C4B-NB	3.27	1.41	1.37
26	r	616	CHL	CHB-C1B	3.27	1.46	1.39
31	t	101	BCR	C37-C22	3.26	1.57	1.50
22	1	304	CLA	C4D-ND	-3.26	1.33	1.37
22	u	301	CLA	C4D-ND	-3.26	1.33	1.37
26	Q	316	CHL	CHB-C1B	3.26	1.46	1.39
26	Q	315	CHL	OBD-CAD	3.26	1.28	1.22
22	U	301	CLA	C4D-ND	-3.26	1.33	1.37
26	p	317	CHL	CHB-C1B	3.26	1.46	1.39
22	b	612	CLA	C4D-ND	-3.26	1.33	1.37
22	3	302	CLA	C4D-ND	-3.26	1.33	1.37
36	c	519	DGD	O2G-C1B	3.26	1.43	1.34
26	1	318	CHL	CHC-C4B	3.26	1.46	1.39
26	g	316	CHL	CHC-C4B	3.26	1.46	1.39
26	Q	313	CHL	CHC-C4B	3.26	1.46	1.39
26	P	317	CHL	CHB-C1B	3.26	1.46	1.39
22	2	307	CLA	C4D-ND	-3.26	1.33	1.37
22	b	603	CLA	C4D-ND	-3.25	1.33	1.37
22	G	304	CLA	C4B-NB	3.25	1.41	1.37
22	2	302	CLA	C4D-ND	-3.25	1.33	1.37
26	2	316	CHL	CHB-C1B	3.25	1.46	1.39
22	g	301	CLA	C4D-ND	-3.25	1.33	1.37
22	n	303	CLA	C4B-NB	3.25	1.41	1.37
22	x	201	CLA	C4D-ND	-3.25	1.33	1.37
26	q	313	CHL	CHB-C1B	3.25	1.46	1.39
26	G	314	CHL	CHB-C1B	3.25	1.46	1.39
26	V	314	CHL	CHB-C1B	3.25	1.46	1.39
22	5	307	CLA	C4D-ND	-3.25	1.33	1.37
22	U	302	CLA	C4D-ND	-3.25	1.33	1.37
26	N	317	CHL	CHB-C1B	3.25	1.46	1.39
22	G	303	CLA	C4B-NB	3.25	1.41	1.37
22	C	508	CLA	C4B-NB	3.24	1.41	1.37
22	2	305	CLA	C3D-C4D	3.24	1.51	1.44
26	G	315	CHL	OBD-CAD	3.24	1.28	1.22
22	X	202	CLA	C4D-ND	-3.24	1.33	1.37
22	c	502	CLA	C1D-ND	3.24	1.41	1.37
22	V	307	CLA	C4D-ND	-3.24	1.33	1.37
22	P	302	CLA	C4D-ND	-3.24	1.33	1.37
22	U	306	CLA	C4B-NB	3.24	1.41	1.37
22	R	306	CLA	C4B-NB	3.24	1.41	1.37
26	N	316	CHL	OBD-CAD	3.24	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	C4D-ND	-3.24	1.33	1.37
26	6	301	CHL	CHB-C1B	3.24	1.46	1.39
22	b	604	CLA	C4D-ND	-3.24	1.33	1.37
22	1	304	CLA	C1D-ND	3.24	1.41	1.37
26	4	313	CHL	CHB-C1B	3.23	1.46	1.39
26	p	318	CHL	CHC-C4B	3.23	1.46	1.39
26	N	313	CHL	CHB-C1B	3.23	1.46	1.39
22	C	513	CLA	C4D-ND	-3.23	1.33	1.37
31	x	202	BCR	C27-C26	-3.23	1.44	1.51
31	K	101	BCR	C27-C26	-3.23	1.44	1.51
22	S	308	CLA	C4D-ND	-3.23	1.33	1.37
26	q	314	CHL	CHB-C1B	3.23	1.46	1.39
26	g	313	CHL	CHB-C1B	3.23	1.46	1.39
26	R	317	CHL	CHB-C1B	3.23	1.46	1.39
22	b	607	CLA	C4D-ND	-3.23	1.33	1.37
22	q	306	CLA	C4B-NB	3.23	1.41	1.37
22	C	511	CLA	C1D-ND	3.23	1.41	1.37
31	X	201	BCR	C27-C26	-3.23	1.44	1.51
31	T	101	BCR	C20-C21	3.23	1.53	1.43
36	c	517	DGD	O6E-C1E	3.23	1.50	1.41
22	r	607	CLA	C4B-NB	3.23	1.41	1.37
26	v	316	CHL	CHB-C1B	3.22	1.46	1.39
26	V	318	CHL	CHB-C1B	3.22	1.46	1.39
22	1	307	CLA	C4D-ND	-3.22	1.33	1.37
22	U	305	CLA	C4D-ND	-3.22	1.33	1.37
31	T	101	BCR	C27-C26	-3.22	1.44	1.51
22	B	608	CLA	C4D-ND	-3.22	1.33	1.37
22	b	617	CLA	C4D-ND	-3.22	1.33	1.37
22	B	604	CLA	C4D-ND	-3.22	1.33	1.37
26	N	317	CHL	CHC-C4B	3.22	1.46	1.39
22	1	303	CLA	C4D-ND	-3.22	1.33	1.37
36	b	601	DGD	O6D-C1D	3.22	1.50	1.41
26	G	316	CHL	CHC-C4B	3.22	1.46	1.39
22	B	610	CLA	C4B-NB	3.22	1.41	1.37
22	S	305	CLA	C4D-ND	-3.21	1.33	1.37
36	B	601	DGD	O6D-C1D	3.21	1.50	1.41
22	r	605	CLA	C4B-NB	3.21	1.41	1.37
26	p	319	CHL	CHC-C4B	3.21	1.46	1.39
22	c	513	CLA	C1D-ND	3.21	1.41	1.37
31	D	404	BCR	C27-C26	-3.21	1.44	1.51
26	v	318	CHL	CHB-C1B	3.21	1.46	1.39
22	s	305	CLA	C4D-ND	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	C4B-NB	3.21	1.41	1.37
36	C	520	DGD	O2G-C1B	3.21	1.43	1.34
22	V	305	CLA	C4B-NB	3.21	1.41	1.37
22	p	309	CLA	C4B-NB	3.20	1.41	1.37
22	S	303	CLA	C4B-NB	3.20	1.41	1.37
26	S	314	CHL	CHB-C1B	3.20	1.46	1.39
22	a	404	CLA	C1D-ND	3.20	1.41	1.37
26	s	314	CHL	CHB-C1B	3.20	1.46	1.39
31	C	517	BCR	C24-C25	3.20	1.56	1.45
36	C	519	DGD	O6E-C1E	3.20	1.50	1.41
22	R	310	CLA	C4B-NB	3.20	1.41	1.37
26	u	314	CHL	CHB-C1B	3.20	1.46	1.39
26	4	317	CHL	CHC-C4B	3.20	1.46	1.39
22	s	303	CLA	C4B-NB	3.20	1.41	1.37
31	t	101	BCR	C20-C21	3.20	1.53	1.43
31	c	515	BCR	C24-C25	3.20	1.56	1.45
22	5	308	CLA	C4B-NB	3.20	1.41	1.37
22	c	508	CLA	C4D-ND	-3.20	1.33	1.37
22	b	611	CLA	C4D-ND	-3.20	1.33	1.37
26	g	315	CHL	OBD-CAD	3.20	1.28	1.22
26	n	318	CHL	CHC-C4B	3.20	1.46	1.39
22	1	306	CLA	C4D-ND	-3.20	1.33	1.37
22	Q	304	CLA	C4B-NB	3.20	1.41	1.37
26	v	314	CHL	CHB-C1B	3.19	1.46	1.39
22	b	610	CLA	C4D-ND	-3.19	1.33	1.37
26	3	316	CHL	CHC-C4B	3.19	1.46	1.39
31	k	101	BCR	C24-C25	3.19	1.56	1.45
22	u	301	CLA	C4B-NB	3.19	1.41	1.37
22	B	613	CLA	C1D-ND	3.19	1.41	1.37
22	1	302	CLA	C4D-ND	-3.19	1.33	1.37
22	b	612	CLA	C4B-NB	3.19	1.41	1.37
22	B	607	CLA	C4D-ND	-3.19	1.33	1.37
22	v	304	CLA	C4D-ND	-3.19	1.33	1.37
22	V	305	CLA	C4D-ND	-3.19	1.33	1.37
22	B	610	CLA	C4D-ND	-3.19	1.33	1.37
26	g	316	CHL	CHB-C1B	3.19	1.46	1.39
22	V	301	CLA	C4B-NB	3.19	1.41	1.37
22	P	308	CLA	C4B-NB	3.19	1.41	1.37
22	g	303	CLA	C4B-NB	3.19	1.41	1.37
31	K	101	BCR	C24-C25	3.19	1.56	1.45
22	4	307	CLA	C4D-ND	-3.19	1.33	1.37
22	p	308	CLA	C4D-ND	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	304	CLA	C4B-NB	3.19	1.41	1.37
22	R	308	CLA	C4B-NB	3.19	1.41	1.37
26	2	314	CHL	C3D-C2D	3.19	1.47	1.39
22	S	309	CLA	C4B-NB	3.19	1.41	1.37
26	6	316	CHL	CHB-C1B	3.19	1.46	1.39
26	P	315	CHL	C3D-C2D	3.19	1.47	1.39
26	5	318	CHL	CHC-C4B	3.18	1.46	1.39
31	B	618	BCR	C24-C25	3.18	1.56	1.45
22	P	303	CLA	C4D-ND	-3.18	1.33	1.37
22	g	307	CLA	C4B-NB	3.18	1.41	1.37
22	C	508	CLA	C1D-ND	3.18	1.41	1.37
22	c	507	CLA	C1D-ND	3.18	1.41	1.37
33	d	404	PL9	C6-C5	3.18	1.51	1.35
22	U	308	CLA	C4D-ND	-3.18	1.33	1.37
22	S	307	CLA	C4D-ND	-3.18	1.33	1.37
22	U	306	CLA	C4D-ND	-3.18	1.33	1.37
36	c	518	DGD	O2G-C1B	3.18	1.43	1.34
22	s	301	CLA	C1D-ND	3.18	1.41	1.37
22	c	510	CLA	C1D-ND	3.18	1.41	1.37
26	1	313	CHL	CHB-C1B	3.18	1.46	1.39
22	P	308	CLA	C4D-ND	-3.18	1.33	1.37
22	b	608	CLA	C4D-ND	-3.18	1.33	1.37
22	r	606	CLA	C4D-ND	-3.18	1.33	1.37
22	p	303	CLA	C4D-ND	-3.18	1.33	1.37
26	5	317	CHL	CHC-C4B	3.18	1.46	1.39
22	c	512	CLA	C4D-ND	-3.17	1.33	1.37
30	D	401	PHO	C4D-CHA	3.17	1.44	1.39
31	d	403	BCR	C27-C26	-3.17	1.44	1.51
33	D	405	PL9	C6-C5	3.17	1.51	1.35
22	U	304	CLA	C1D-ND	3.17	1.41	1.37
22	s	306	CLA	C4D-ND	-3.17	1.33	1.37
22	3	304	CLA	C4B-NB	3.17	1.41	1.37
22	c	511	CLA	C4D-ND	-3.17	1.33	1.37
26	p	315	CHL	MG-NA	-3.17	1.98	2.06
22	3	308	CLA	C4B-NB	3.17	1.41	1.37
22	6	309	CLA	C4B-NB	3.17	1.41	1.37
22	6	303	CLA	C4D-ND	-3.17	1.33	1.37
22	g	303	CLA	C4D-ND	-3.17	1.33	1.37
31	D	404	BCR	C37-C22	3.17	1.57	1.50
22	6	307	CLA	C4B-NB	3.17	1.41	1.37
22	Q	308	CLA	C4D-ND	-3.17	1.33	1.37
22	G	307	CLA	C4B-NB	3.17	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	C4D-ND	-3.17	1.33	1.37
22	g	302	CLA	C4B-NB	3.17	1.41	1.37
22	b	609	CLA	C1D-ND	3.16	1.41	1.37
32	M	101	SQD	O48-C23	3.16	1.42	1.33
22	s	301	CLA	C4D-ND	-3.16	1.33	1.37
22	p	308	CLA	C4B-NB	3.16	1.41	1.37
22	5	306	CLA	C4D-ND	-3.16	1.33	1.37
22	R	307	CLA	C4D-ND	-3.16	1.33	1.37
33	a	411	PL9	C6-C1	3.16	1.53	1.45
22	u	303	CLA	C4B-NB	3.16	1.41	1.37
22	q	301	CLA	C4B-NB	3.16	1.41	1.37
33	A	410	PL9	C6-C1	3.16	1.53	1.45
22	v	305	CLA	C4B-NB	3.16	1.41	1.37
26	6	312	CHL	CHB-C1B	3.16	1.46	1.39
22	r	602	CLA	C4D-ND	-3.16	1.33	1.37
26	R	315	CHL	CHB-C1B	3.16	1.46	1.39
34	d	407	LMG	O7-C10	3.16	1.43	1.34
22	R	303	CLA	C4D-ND	-3.16	1.33	1.37
22	4	302	CLA	C4D-ND	-3.16	1.33	1.37
22	q	304	CLA	C4B-NB	3.16	1.41	1.37
22	S	301	CLA	C1D-ND	3.16	1.41	1.37
22	Q	307	CLA	C4D-ND	-3.15	1.33	1.37
22	U	307	CLA	C4D-ND	-3.15	1.33	1.37
22	p	303	CLA	C4B-NB	3.15	1.41	1.37
22	G	306	CLA	C4B-NB	3.15	1.41	1.37
31	B	619	BCR	C37-C22	3.15	1.57	1.50
22	3	306	CLA	C4B-NB	3.15	1.41	1.37
36	c	517	DGD	O6D-C1D	3.15	1.49	1.41
26	Q	311	CHL	CHB-C1B	3.15	1.46	1.39
22	6	308	CLA	C4D-ND	-3.15	1.33	1.37
22	p	306	CLA	C4B-NB	3.15	1.41	1.37
37	e	101	HEM	CAB-C3B	3.15	1.56	1.47
22	1	305	CLA	C4D-ND	-3.15	1.33	1.37
22	v	303	CLA	C4D-ND	-3.15	1.33	1.37
22	6	304	CLA	C4B-NB	3.15	1.41	1.37
31	b	618	BCR	C24-C25	3.15	1.56	1.45
26	g	315	CHL	C3B-C4B	3.15	1.50	1.42
22	B	611	CLA	C4D-ND	-3.15	1.33	1.37
32	m	101	SQD	O48-C23	3.14	1.42	1.33
26	3	311	CHL	CHB-C1B	3.14	1.46	1.39
22	3	308	CLA	C4D-ND	-3.14	1.33	1.37
26	6	317	CHL	C1D-C2D	3.14	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	304	CLA	C4D-ND	-3.14	1.33	1.37
31	c	516	BCR	C20-C21	3.14	1.53	1.43
22	Q	305	CLA	C4D-ND	-3.14	1.33	1.37
22	u	302	CLA	C4B-NB	3.14	1.41	1.37
22	c	502	CLA	C4D-ND	-3.14	1.33	1.37
22	4	305	CLA	C4D-ND	-3.14	1.33	1.37
22	v	308	CLA	C4D-ND	-3.14	1.33	1.37
22	C	503	CLA	C4D-ND	-3.14	1.33	1.37
22	p	307	CLA	C4B-NB	3.14	1.41	1.37
22	N	305	CLA	C4B-NB	3.14	1.41	1.37
22	C	509	CLA	C4D-ND	-3.14	1.33	1.37
22	4	306	CLA	C4D-ND	-3.14	1.33	1.37
22	B	609	CLA	C1D-ND	3.14	1.41	1.37
37	E	101	HEM	CAB-C3B	3.14	1.56	1.47
22	u	308	CLA	C4D-ND	-3.14	1.33	1.37
26	1	318	CHL	CHB-C1B	3.14	1.46	1.39
30	d	401	PHO	C4D-CHA	3.14	1.44	1.39
22	v	305	CLA	C4D-ND	-3.13	1.33	1.37
34	D	408	LMG	O7-C10	3.13	1.43	1.34
22	r	603	CLA	C4B-NB	3.13	1.41	1.37
36	C	519	DGD	O6D-C1D	3.13	1.49	1.41
36	a	416	DGD	O2G-C1B	3.13	1.43	1.34
31	d	403	BCR	C37-C22	3.13	1.57	1.50
26	u	316	CHL	CHB-C1B	3.13	1.46	1.39
22	S	306	CLA	C4D-ND	-3.13	1.33	1.37
26	G	315	CHL	C3B-C4B	3.13	1.50	1.42
22	q	307	CLA	C4D-ND	-3.13	1.33	1.37
22	N	301	CLA	C4D-ND	-3.13	1.33	1.37
22	S	301	CLA	C4D-ND	-3.13	1.33	1.37
32	a	410	SQD	O48-C23	3.13	1.42	1.33
26	u	317	CHL	CHB-C1B	3.13	1.46	1.39
22	q	303	CLA	C4D-ND	-3.13	1.33	1.37
26	r	614	CHL	CHB-C1B	3.13	1.46	1.39
36	A	414	DGD	O2G-C1B	3.13	1.43	1.34
30	A	407	PHO	C4D-CHA	3.13	1.44	1.39
22	Q	303	CLA	C4D-ND	-3.13	1.33	1.37
26	v	317	CHL	CHB-C1B	3.13	1.46	1.39
22	s	308	CLA	C4D-ND	-3.13	1.33	1.37
31	C	518	BCR	C20-C21	3.13	1.53	1.43
26	n	316	CHL	CHB-C1B	3.13	1.46	1.39
22	P	309	CLA	C4B-NB	3.13	1.41	1.37
26	U	319	CHL	CHB-C1B	3.12	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	501	SQD	O48-C23	3.12	1.42	1.33
22	V	304	CLA	C4B-NB	3.12	1.41	1.37
22	U	301	CLA	C4B-NB	3.12	1.41	1.37
22	u	302	CLA	C4D-ND	-3.12	1.33	1.37
26	g	312	CHL	CHB-C1B	3.12	1.46	1.39
31	b	619	BCR	C37-C22	3.12	1.57	1.50
26	5	317	CHL	CHB-C1B	3.12	1.46	1.39
22	b	615	CLA	C4D-ND	-3.12	1.33	1.37
22	c	508	CLA	C4B-NB	3.12	1.41	1.37
26	3	316	CHL	C1D-C2D	3.12	1.51	1.45
26	p	319	CHL	CHB-C1B	3.12	1.46	1.39
22	6	304	CLA	C4D-ND	-3.12	1.33	1.37
22	6	305	CLA	C4B-NB	3.12	1.41	1.37
26	6	313	CHL	C3D-C2D	3.12	1.47	1.39
22	4	303	CLA	C4B-NB	3.12	1.41	1.37
26	3	312	CHL	C3D-C2D	3.12	1.47	1.39
22	V	308	CLA	C4D-ND	-3.12	1.33	1.37
30	a	407	PHO	C4D-CHA	3.12	1.44	1.39
22	G	302	CLA	C4D-ND	-3.12	1.33	1.37
22	3	307	CLA	C4D-ND	-3.11	1.33	1.37
22	3	306	CLA	C4D-ND	-3.11	1.33	1.37
26	S	315	CHL	C3D-C2D	3.11	1.47	1.39
22	B	615	CLA	C4D-ND	-3.11	1.33	1.37
22	p	304	CLA	C4D-ND	-3.11	1.33	1.37
22	S	308	CLA	C4B-NB	3.11	1.41	1.37
33	a	411	PL9	C5-C4	3.11	1.53	1.45
26	2	318	CHL	CHC-C4B	3.11	1.46	1.39
22	V	302	CLA	C4B-NB	3.11	1.41	1.37
22	G	308	CLA	C4D-ND	-3.11	1.33	1.37
22	g	306	CLA	C3B-C4B	3.11	1.50	1.42
26	2	317	CHL	CHB-C1B	3.11	1.46	1.39
26	q	311	CHL	CHB-C1B	3.11	1.46	1.39
22	6	308	CLA	C4B-NB	3.10	1.41	1.37
26	6	317	CHL	CHC-C4B	3.10	1.46	1.39
22	3	303	CLA	C4D-ND	-3.10	1.33	1.37
22	Q	305	CLA	C4B-NB	3.10	1.41	1.37
26	g	315	CHL	CHB-C1B	3.10	1.46	1.39
31	b	620	BCR	C37-C22	3.10	1.57	1.50
22	3	305	CLA	C4B-NB	3.10	1.41	1.37
22	n	303	CLA	C4D-ND	-3.10	1.33	1.37
31	K	101	BCR	C37-C22	3.10	1.57	1.50
26	4	316	CHL	CHB-C1B	3.10	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	g	308	CLA	C4D-ND	-3.10	1.33	1.37
22	P	306	CLA	C4B-NB	3.10	1.41	1.37
22	U	302	CLA	C4B-NB	3.10	1.41	1.37
26	p	320	CHL	CHB-C1B	3.10	1.46	1.39
22	P	306	CLA	C3D-C4D	3.10	1.51	1.44
33	A	410	PL9	C5-C4	3.10	1.53	1.45
22	G	308	CLA	C4B-NB	3.10	1.41	1.37
22	S	301	CLA	C4B-NB	3.10	1.41	1.37
22	U	304	CLA	C4D-ND	-3.10	1.33	1.37
22	c	502	CLA	C4B-NB	3.10	1.41	1.37
22	U	303	CLA	C4D-ND	-3.10	1.33	1.37
26	P	319	CHL	CHC-C4B	3.10	1.46	1.39
27	R	301	NEX	C7-C8	-3.10	1.26	1.32
26	u	315	CHL	CHB-C1B	3.10	1.46	1.39
26	v	317	CHL	C3B-C4B	3.10	1.50	1.42
22	3	303	CLA	C4B-NB	3.10	1.41	1.37
22	q	308	CLA	C4D-ND	-3.10	1.33	1.37
22	u	307	CLA	C4D-ND	-3.09	1.33	1.37
22	5	303	CLA	C4B-NB	3.09	1.41	1.37
26	U	314	CHL	CHB-C1B	3.09	1.46	1.39
22	4	308	CLA	C4B-NB	3.09	1.41	1.37
22	6	307	CLA	C4D-ND	-3.09	1.33	1.37
22	U	303	CLA	C4B-NB	3.09	1.41	1.37
26	4	317	CHL	CHB-C1B	3.09	1.46	1.39
26	3	312	CHL	C1D-C2D	3.09	1.51	1.45
22	N	307	CLA	C4B-NB	3.09	1.41	1.37
22	s	309	CLA	C4D-ND	-3.09	1.33	1.37
22	n	302	CLA	C4D-ND	-3.09	1.33	1.37
31	b	620	BCR	C20-C21	3.09	1.53	1.43
26	P	315	CHL	C1D-C2D	3.09	1.51	1.45
22	Q	307	CLA	C4B-NB	3.09	1.41	1.37
26	s	316	CHL	C1D-C2D	3.09	1.51	1.45
26	p	315	CHL	C3D-C2D	3.08	1.47	1.39
22	G	306	CLA	C4D-ND	-3.08	1.33	1.37
22	q	305	CLA	C4D-ND	-3.08	1.33	1.37
31	X	201	BCR	C37-C22	3.08	1.57	1.50
22	S	309	CLA	C4D-ND	-3.08	1.33	1.37
33	a	411	PL9	C2-C1	3.08	1.53	1.45
22	r	604	CLA	C4D-ND	-3.08	1.33	1.37
22	2	303	CLA	C4D-ND	-3.08	1.33	1.37
27	2	319	NEX	C7-C8	-3.08	1.26	1.32
22	5	302	CLA	C4B-NB	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	306	CLA	C4D-ND	-3.08	1.33	1.37
22	2	308	CLA	C4D-ND	-3.08	1.33	1.37
26	1	314	CHL	CHB-C1B	3.08	1.46	1.39
22	5	307	CLA	C4B-NB	3.08	1.41	1.37
22	S	304	CLA	C4B-NB	3.08	1.41	1.37
31	B	620	BCR	C37-C22	3.08	1.57	1.50
26	s	315	CHL	C3D-C2D	3.08	1.47	1.39
22	5	303	CLA	C4D-ND	-3.08	1.33	1.37
22	q	307	CLA	C4B-NB	3.08	1.41	1.37
22	G	303	CLA	C4D-ND	-3.08	1.33	1.37
31	a	409	BCR	C37-C22	3.08	1.57	1.50
22	s	309	CLA	C4B-NB	3.08	1.41	1.37
22	Q	301	CLA	C4B-NB	3.07	1.41	1.37
22	2	307	CLA	C4B-NB	3.07	1.41	1.37
31	k	101	BCR	C37-C22	3.07	1.57	1.50
31	x	202	BCR	C37-C22	3.07	1.57	1.50
22	C	503	CLA	C4B-NB	3.07	1.41	1.37
31	X	201	BCR	C20-C21	3.07	1.53	1.43
22	N	302	CLA	C4D-ND	-3.07	1.33	1.37
26	3	316	CHL	CHB-C1B	3.07	1.46	1.39
22	s	301	CLA	C4B-NB	3.07	1.41	1.37
26	r	619	CHL	CHB-C1B	3.07	1.46	1.39
26	G	316	CHL	CHB-C1B	3.07	1.46	1.39
26	2	315	CHL	CHB-C1B	3.07	1.46	1.39
26	U	316	CHL	CHB-C1B	3.07	1.46	1.39
27	r	618	NEX	C7-C8	-3.07	1.26	1.32
22	P	309	CLA	C4D-ND	-3.07	1.33	1.37
22	6	303	CLA	C4B-NB	3.07	1.41	1.37
22	V	303	CLA	C4D-ND	-3.06	1.33	1.37
33	A	410	PL9	C2-C1	3.06	1.53	1.45
22	U	308	CLA	C4B-NB	3.06	1.41	1.37
22	p	304	CLA	C4B-NB	3.06	1.41	1.37
26	5	314	CHL	C3D-C2D	3.06	1.47	1.39
31	D	404	BCR	C20-C21	3.06	1.52	1.43
22	R	305	CLA	C4D-ND	-3.06	1.33	1.37
22	C	506	CLA	C4B-NB	3.06	1.41	1.37
22	S	307	CLA	C4B-NB	3.06	1.41	1.37
31	A	409	BCR	C37-C22	3.06	1.57	1.50
22	g	308	CLA	C4B-NB	3.06	1.41	1.37
27	U	318	NEX	C7-C8	-3.06	1.26	1.32
36	C	519	DGD	O2G-C1B	3.06	1.42	1.34
22	g	302	CLA	C4D-ND	-3.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	n	301	CLA	C4D-ND	-3.06	1.33	1.37
22	5	308	CLA	C4D-ND	-3.06	1.33	1.37
22	v	302	CLA	C4B-NB	3.06	1.41	1.37
22	V	306	CLA	C4D-ND	-3.06	1.33	1.37
22	2	308	CLA	C4B-NB	3.06	1.41	1.37
22	C	506	CLA	C1D-ND	3.06	1.41	1.37
22	C	509	CLA	C4B-NB	3.06	1.41	1.37
22	b	604	CLA	C4B-NB	3.06	1.41	1.37
26	g	311	CHL	CHB-C1B	3.05	1.46	1.39
22	6	309	CLA	C4D-ND	-3.05	1.33	1.37
22	v	306	CLA	C4D-ND	-3.05	1.33	1.37
22	q	302	CLA	C4D-ND	-3.05	1.33	1.37
26	5	313	CHL	C3B-C4B	3.05	1.49	1.42
22	p	309	CLA	C4D-ND	-3.05	1.33	1.37
22	S	306	CLA	C4B-NB	3.05	1.41	1.37
22	4	308	CLA	C4D-ND	-3.05	1.33	1.37
22	3	307	CLA	C4B-NB	3.05	1.41	1.37
26	q	312	CHL	C3D-C2D	3.05	1.47	1.39
22	p	307	CLA	C4D-ND	-3.05	1.33	1.37
22	s	306	CLA	C4B-NB	3.04	1.41	1.37
31	x	202	BCR	C20-C21	3.04	1.52	1.43
22	u	303	CLA	C4D-ND	-3.04	1.33	1.37
26	N	314	CHL	C3D-C2D	3.04	1.47	1.39
22	v	303	CLA	C4B-NB	3.04	1.41	1.37
22	V	307	CLA	C4B-NB	3.04	1.41	1.37
22	s	308	CLA	C4B-NB	3.04	1.41	1.37
22	1	308	CLA	C4B-NB	3.04	1.41	1.37
26	q	314	CHL	C3B-C4B	3.04	1.49	1.42
31	B	620	BCR	C20-C21	3.04	1.52	1.43
22	q	306	CLA	C4D-ND	-3.04	1.33	1.37
22	N	303	CLA	C4D-ND	-3.04	1.33	1.37
31	z	101	BCR	C37-C22	3.04	1.57	1.50
31	d	403	BCR	C20-C21	3.04	1.52	1.43
26	5	315	CHL	CHB-C1B	3.04	1.46	1.39
26	S	316	CHL	C1D-C2D	3.04	1.51	1.45
22	v	304	CLA	C4B-NB	3.04	1.41	1.37
22	g	305	CLA	C4B-NB	3.04	1.41	1.37
22	V	303	CLA	C4B-NB	3.03	1.41	1.37
22	n	307	CLA	C4B-NB	3.03	1.41	1.37
22	B	604	CLA	C4B-NB	3.03	1.41	1.37
31	c	515	BCR	C37-C22	3.03	1.57	1.50
22	P	304	CLA	C4B-NB	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	309	XAT	C4-C3	3.03	1.56	1.52
22	S	303	CLA	C4D-ND	-3.03	1.33	1.37
26	6	317	CHL	CHB-C1B	3.03	1.46	1.39
31	C	517	BCR	C37-C22	3.03	1.57	1.50
26	G	311	CHL	CHB-C1B	3.03	1.46	1.39
22	v	301	CLA	C4B-NB	3.03	1.41	1.37
22	R	307	CLA	C4B-NB	3.03	1.41	1.37
31	C	516	BCR	C37-C22	3.03	1.57	1.50
26	6	313	CHL	C1D-C2D	3.03	1.51	1.45
22	G	301	CLA	C4B-NB	3.03	1.41	1.37
26	U	317	CHL	CHB-C1B	3.03	1.46	1.39
22	n	306	CLA	C4B-NB	3.03	1.41	1.37
22	S	304	CLA	C4D-ND	-3.03	1.33	1.37
22	P	305	CLA	C4D-ND	-3.03	1.33	1.37
22	r	602	CLA	C4B-NB	3.03	1.41	1.37
36	B	601	DGD	O2G-C1B	3.03	1.42	1.34
22	s	301	CLA	C3B-C4B	3.03	1.49	1.42
27	r	617	NEX	C7-C8	-3.02	1.26	1.32
36	c	517	DGD	O2G-C1B	3.02	1.42	1.34
22	1	308	CLA	C4D-ND	-3.02	1.33	1.37
22	2	304	CLA	C4D-ND	-3.02	1.33	1.37
26	1	317	CHL	CHB-C1B	3.02	1.46	1.39
24	N	311	XAT	C38-C25	3.02	1.56	1.51
26	V	314	CHL	C3D-C2D	3.02	1.47	1.39
26	n	314	CHL	C3D-C2D	3.02	1.47	1.39
22	q	305	CLA	C4B-NB	3.02	1.41	1.37
22	s	307	CLA	C4B-NB	3.02	1.41	1.37
31	C	516	BCR	C20-C21	3.02	1.52	1.43
26	G	315	CHL	CHB-C1B	3.02	1.46	1.39
26	V	318	CHL	C3D-C2D	3.02	1.47	1.39
22	V	308	CLA	C4B-NB	3.02	1.41	1.37
22	u	305	CLA	C4B-NB	3.02	1.41	1.37
31	z	101	BCR	C20-C21	3.02	1.52	1.43
22	P	307	CLA	C4D-ND	-3.01	1.33	1.37
26	n	314	CHL	MG-NA	-3.01	1.99	2.06
22	6	306	CLA	C4B-NB	3.01	1.41	1.37
22	n	307	CLA	C4D-ND	-3.01	1.33	1.37
22	Q	306	CLA	C4D-ND	-3.01	1.33	1.37
22	g	306	CLA	C4D-ND	-3.01	1.33	1.37
22	P	304	CLA	C4D-ND	-3.01	1.33	1.37
26	u	318	CHL	C3B-C4B	3.01	1.49	1.42
22	6	302	CLA	C4B-NB	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	315	CHL	C3D-C2D	3.01	1.47	1.39
34	w	201	LMG	O7-C10	3.01	1.42	1.34
26	G	312	CHL	C3D-C2D	3.01	1.47	1.39
22	3	301	CLA	C4B-NB	3.01	1.41	1.37
31	B	619	BCR	C20-C21	3.01	1.52	1.43
24	2	311	XAT	C24-C23	3.01	1.56	1.52
22	s	304	CLA	C4B-NB	3.01	1.41	1.37
26	g	312	CHL	C3D-C2D	3.01	1.47	1.39
26	P	318	CHL	CHB-C1B	3.01	1.46	1.39
22	r	606	CLA	C4B-NB	3.01	1.41	1.37
22	c	505	CLA	C1D-ND	3.00	1.41	1.37
26	v	318	CHL	C3D-C2D	3.00	1.47	1.39
22	C	510	CLA	C1D-ND	3.00	1.41	1.37
22	S	301	CLA	C3B-C4B	3.00	1.49	1.42
24	5	311	XAT	C24-C23	3.00	1.56	1.52
22	N	306	CLA	C4B-NB	3.00	1.41	1.37
22	N	304	CLA	C4D-ND	-3.00	1.33	1.37
22	G	302	CLA	C4B-NB	3.00	1.41	1.37
26	1	314	CHL	C3D-C2D	3.00	1.47	1.39
22	4	305	CLA	C4B-NB	3.00	1.41	1.37
22	v	307	CLA	C4B-NB	3.00	1.41	1.37
22	C	512	CLA	C4B-NB	3.00	1.41	1.37
31	b	619	BCR	C20-C21	3.00	1.52	1.43
27	5	319	NEX	C7-C8	-3.00	1.27	1.32
22	2	303	CLA	C4B-NB	3.00	1.41	1.37
26	p	314	CHL	C3B-C4B	3.00	1.49	1.42
26	4	314	CHL	CHB-C1B	3.00	1.46	1.39
22	g	304	CLA	C3B-C4B	3.00	1.49	1.42
22	b	617	CLA	C4B-NB	3.00	1.41	1.37
22	3	305	CLA	C4D-ND	-3.00	1.33	1.37
27	n	319	NEX	C7-C8	-3.00	1.27	1.32
22	N	304	CLA	C3B-C4B	3.00	1.49	1.42
31	B	618	BCR	C37-C22	3.00	1.57	1.50
24	v	311	XAT	C4-C3	3.00	1.56	1.52
22	6	305	CLA	C4D-ND	-3.00	1.33	1.37
22	B	607	CLA	C4B-NB	3.00	1.41	1.37
26	Q	312	CHL	C3D-C2D	2.99	1.47	1.39
24	Q	309	XAT	C38-C25	2.99	1.56	1.51
26	V	317	CHL	CHB-C1B	2.99	1.46	1.39
36	b	601	DGD	O2G-C1B	2.99	1.42	1.34
22	1	306	CLA	C4B-NB	2.99	1.41	1.37
22	c	508	CLA	C1D-ND	2.99	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	C1D-ND	2.99	1.41	1.37
32	L	102	SQD	O48-C23	2.99	1.42	1.33
22	v	308	CLA	C4B-NB	2.99	1.41	1.37
22	1	303	CLA	C4B-NB	2.99	1.41	1.37
26	S	315	CHL	C1D-C2D	2.99	1.51	1.45
22	u	308	CLA	C4B-NB	2.99	1.41	1.37
26	2	314	CHL	C1B-NB	-2.99	1.34	1.37
22	b	607	CLA	C4B-NB	2.99	1.41	1.37
26	6	314	CHL	C3D-C2D	2.99	1.47	1.39
22	b	611	CLA	C4B-NB	2.98	1.41	1.37
22	p	305	CLA	C4D-ND	-2.98	1.33	1.37
22	g	307	CLA	C4D-ND	-2.98	1.33	1.37
31	b	618	BCR	C37-C22	2.98	1.57	1.50
22	n	301	CLA	C4B-NB	2.98	1.41	1.37
32	l	102	SQD	O48-C23	2.98	1.42	1.33
22	G	305	CLA	C4B-NB	2.98	1.41	1.37
26	V	313	CHL	C1D-C2D	2.98	1.51	1.45
22	s	303	CLA	C4D-ND	-2.98	1.33	1.37
34	b	624	LMG	O7-C10	2.98	1.42	1.34
26	2	318	CHL	CHB-C1B	2.98	1.46	1.39
26	n	318	CHL	C3D-C2D	2.98	1.47	1.39
31	t	101	BCR	C7-C6	2.98	1.55	1.45
22	c	511	CLA	C4B-NB	2.98	1.41	1.37
22	U	305	CLA	C4B-NB	2.98	1.41	1.37
22	N	303	CLA	C4B-NB	2.98	1.41	1.37
26	U	315	CHL	CHB-C1B	2.97	1.46	1.39
22	4	307	CLA	C4B-NB	2.97	1.41	1.37
26	3	313	CHL	C3D-C2D	2.97	1.47	1.39
22	Q	302	CLA	C4D-ND	-2.97	1.33	1.37
26	S	313	CHL	C3B-C4B	2.97	1.49	1.42
22	R	303	CLA	C4B-NB	2.97	1.41	1.37
22	3	304	CLA	C4D-ND	-2.97	1.33	1.37
26	p	315	CHL	C1D-C2D	2.97	1.51	1.45
22	s	304	CLA	C4D-ND	-2.97	1.33	1.37
26	6	316	CHL	C3B-C4B	2.97	1.49	1.42
22	N	308	CLA	C4D-ND	-2.97	1.33	1.37
22	g	301	CLA	C4B-NB	2.97	1.41	1.37
32	A	412	SQD	O48-C23	2.97	1.42	1.33
24	q	309	XAT	C38-C25	2.97	1.56	1.51
34	B	624	LMG	O7-C10	2.96	1.42	1.34
22	G	307	CLA	C4D-ND	-2.96	1.33	1.37
22	V	304	CLA	C3B-C4B	2.96	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	313	CHL	C3B-C4B	2.96	1.49	1.42
22	C	504	CLA	C4B-NB	2.96	1.41	1.37
22	b	606	CLA	C4B-NB	2.96	1.41	1.37
26	S	316	CHL	C3D-C2D	2.96	1.47	1.39
33	A	410	PL9	C3-C4	2.96	1.53	1.49
26	u	316	CHL	C1D-C2D	2.96	1.51	1.45
22	n	304	CLA	C3B-C4B	2.96	1.49	1.42
26	N	317	CHL	C3D-C2D	2.96	1.47	1.39
22	Q	302	CLA	C4B-NB	2.96	1.41	1.37
26	5	318	CHL	CHB-C1B	2.96	1.46	1.39
22	c	505	CLA	C4B-NB	2.96	1.41	1.37
22	r	608	CLA	C4D-ND	-2.96	1.33	1.37
22	5	304	CLA	C4D-ND	-2.96	1.33	1.37
22	G	304	CLA	C3B-C4B	2.96	1.49	1.42
22	N	301	CLA	C3B-C4B	2.96	1.49	1.42
22	r	603	CLA	C4D-ND	-2.96	1.33	1.37
22	C	513	CLA	C4B-NB	2.96	1.41	1.37
22	Q	301	CLA	C3B-C4B	2.95	1.49	1.42
26	5	313	CHL	C3D-C2D	2.95	1.47	1.39
31	T	101	BCR	C7-C6	2.95	1.55	1.45
26	s	316	CHL	C3D-C2D	2.95	1.47	1.39
22	N	304	CLA	C4B-NB	2.95	1.41	1.37
26	P	317	CHL	C1D-C2D	2.95	1.51	1.45
22	U	304	CLA	C4B-NB	2.95	1.41	1.37
22	2	306	CLA	C4B-NB	2.95	1.41	1.37
22	n	306	CLA	C4D-ND	-2.95	1.33	1.37
22	S	302	CLA	C4D-ND	-2.95	1.33	1.37
22	v	304	CLA	C3B-C4B	2.95	1.49	1.42
22	6	306	CLA	C4D-ND	-2.95	1.33	1.37
22	P	303	CLA	C4B-NB	2.95	1.41	1.37
22	B	611	CLA	C4B-NB	2.95	1.41	1.37
22	P	302	CLA	C3B-C4B	2.95	1.49	1.42
22	c	503	CLA	C4B-NB	2.95	1.41	1.37
22	C	509	CLA	C1D-ND	2.95	1.41	1.37
26	P	319	CHL	CHB-C1B	2.94	1.46	1.39
24	p	312	XAT	C24-C23	2.94	1.56	1.52
22	c	512	CLA	C4B-NB	2.94	1.41	1.37
22	n	304	CLA	C4D-ND	-2.94	1.33	1.37
32	l	102	SQD	O47-C7	2.94	1.42	1.34
24	V	311	XAT	C4-C3	2.94	1.56	1.52
24	q	309	XAT	C4-C3	2.94	1.56	1.52
32	L	102	SQD	O47-C7	2.94	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	302	CLA	C4D-ND	-2.94	1.33	1.37
24	Q	309	XAT	C24-C23	2.94	1.56	1.52
26	U	313	CHL	C1D-C2D	2.94	1.51	1.45
22	B	605	CLA	C4D-ND	-2.94	1.33	1.37
22	s	302	CLA	C4D-ND	-2.94	1.33	1.37
26	Q	312	CHL	C1D-C2D	2.94	1.51	1.45
22	u	306	CLA	C4B-NB	2.94	1.41	1.37
24	6	310	XAT	C4-C3	2.94	1.56	1.52
22	N	307	CLA	C4D-ND	-2.94	1.33	1.37
24	1	311	XAT	C38-C25	2.94	1.56	1.51
37	E	101	HEM	CAC-C3C	2.94	1.55	1.47
22	1	301	CLA	C4B-NB	2.94	1.41	1.37
22	N	301	CLA	C4B-NB	2.94	1.41	1.37
26	u	318	CHL	CHB-C1B	2.94	1.46	1.39
26	G	312	CHL	C1D-C2D	2.93	1.51	1.45
34	W	201	LMG	O7-C10	2.93	1.42	1.34
22	q	308	CLA	C4B-NB	2.93	1.41	1.37
24	6	310	XAT	C38-C25	2.93	1.56	1.51
24	v	311	XAT	C38-C25	2.93	1.56	1.51
26	q	315	CHL	C1D-C2D	2.93	1.51	1.45
32	a	413	SQD	O48-C23	2.93	1.41	1.33
24	V	311	XAT	C38-C25	2.93	1.56	1.51
26	s	313	CHL	C3B-C4B	2.93	1.49	1.42
22	b	612	CLA	C3B-C4B	2.93	1.49	1.42
24	4	311	XAT	C38-C25	2.93	1.56	1.51
26	g	313	CHL	C3D-C2D	2.92	1.47	1.39
26	5	313	CHL	C1D-C2D	2.92	1.51	1.45
26	4	315	CHL	C3D-C2D	2.92	1.47	1.39
27	p	301	NEX	C7-C8	-2.92	1.27	1.32
22	3	302	CLA	C4B-NB	2.92	1.41	1.37
22	5	301	CLA	C4B-NB	2.92	1.41	1.37
26	p	316	CHL	C3D-C2D	2.92	1.47	1.39
26	P	316	CHL	C3D-C2D	2.92	1.47	1.39
37	e	101	HEM	CAC-C3C	2.92	1.55	1.47
26	P	314	CHL	C3D-C2D	2.92	1.47	1.39
22	5	304	CLA	C4B-NB	2.92	1.41	1.37
22	N	306	CLA	C4D-ND	-2.92	1.33	1.37
24	P	312	XAT	C4-C3	2.92	1.56	1.52
24	q	309	XAT	C18-C5	2.92	1.56	1.51
24	P	312	XAT	C38-C25	2.92	1.56	1.51
22	2	304	CLA	C3B-C4B	2.92	1.49	1.42
22	p	305	CLA	C4B-NB	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	C3B-C4B	2.92	1.49	1.42
22	R	304	CLA	C4D-ND	-2.92	1.33	1.37
24	g	309	XAT	C38-C25	2.92	1.56	1.51
26	s	315	CHL	C1D-C2D	2.92	1.51	1.45
24	G	309	XAT	C38-C25	2.92	1.56	1.51
26	V	314	CHL	C1D-C2D	2.92	1.51	1.45
31	C	517	BCR	C20-C21	2.92	1.52	1.43
32	a	410	SQD	O47-C7	2.91	1.42	1.34
26	s	313	CHL	C1D-C2D	2.91	1.51	1.45
22	r	605	CLA	C4D-ND	-2.91	1.33	1.37
22	U	307	CLA	C4B-NB	2.91	1.41	1.37
26	N	314	CHL	MG-NA	-2.91	1.99	2.06
22	s	305	CLA	C4B-NB	2.91	1.41	1.37
26	G	313	CHL	C3D-C2D	2.91	1.47	1.39
22	r	601	CLA	C4D-ND	-2.91	1.33	1.37
22	b	605	CLA	C4D-ND	-2.91	1.33	1.37
22	Q	308	CLA	C4B-NB	2.91	1.41	1.37
26	p	318	CHL	CHB-C1B	2.91	1.45	1.39
26	2	313	CHL	C1B-NB	-2.91	1.34	1.37
24	2	311	XAT	C4-C3	2.91	1.56	1.52
24	2	311	XAT	C38-C25	2.91	1.56	1.51
26	q	312	CHL	C1D-C2D	2.91	1.51	1.45
22	6	305	CLA	C3B-C4B	2.91	1.49	1.42
31	k	101	BCR	C20-C21	2.91	1.52	1.43
31	c	516	BCR	C37-C22	2.91	1.56	1.50
22	2	301	CLA	C4B-NB	2.91	1.41	1.37
22	P	307	CLA	C4B-NB	2.91	1.41	1.37
26	G	314	CHL	C3D-C2D	2.91	1.47	1.39
22	4	301	CLA	C4B-NB	2.91	1.41	1.37
31	K	101	BCR	C20-C21	2.90	1.52	1.43
26	Q	316	CHL	C1D-C2D	2.90	1.51	1.45
22	c	509	CLA	C3B-C4B	2.90	1.49	1.42
26	v	315	CHL	C3D-C2D	2.90	1.47	1.39
32	a	413	SQD	O47-C7	2.90	1.42	1.34
31	c	515	BCR	C20-C21	2.90	1.52	1.43
22	B	609	CLA	C4B-NB	2.90	1.41	1.37
22	5	304	CLA	C3B-C4B	2.90	1.49	1.42
24	4	311	XAT	C4-C3	2.90	1.56	1.52
26	2	313	CHL	C3D-C2D	2.90	1.47	1.39
26	g	314	CHL	C3D-C2D	2.90	1.47	1.39
22	R	306	CLA	C4D-ND	-2.90	1.33	1.37
26	q	311	CHL	C1D-C2D	2.90	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	313	CHL	C3D-C2D	2.90	1.47	1.39
26	V	317	CHL	C1D-C2D	2.90	1.51	1.45
24	5	311	XAT	C4-C3	2.90	1.56	1.52
22	R	311	CLA	C4D-ND	-2.89	1.33	1.37
22	v	306	CLA	C3B-C4B	2.89	1.49	1.42
22	C	503	CLA	C3B-C4B	2.89	1.49	1.42
22	B	612	CLA	C3B-C4B	2.89	1.49	1.42
26	n	317	CHL	C3D-C2D	2.89	1.47	1.39
22	P	302	CLA	C4B-NB	2.89	1.41	1.37
32	A	412	SQD	O47-C7	2.89	1.42	1.34
26	4	313	CHL	C3D-C2D	2.89	1.47	1.39
26	2	313	CHL	C3B-C4B	2.89	1.49	1.42
22	q	302	CLA	C4B-NB	2.89	1.41	1.37
26	2	313	CHL	C1D-C2D	2.89	1.51	1.45
22	c	509	CLA	CMC-C2C	-2.89	1.44	1.50
26	n	313	CHL	C3D-C2D	2.89	1.47	1.39
31	C	518	BCR	C37-C22	2.89	1.56	1.50
24	3	309	XAT	C38-C25	2.89	1.56	1.51
32	C	501	SQD	O47-C7	2.89	1.42	1.34
26	g	313	CHL	C1D-C2D	2.89	1.51	1.45
22	Q	304	CLA	C3B-C4B	2.89	1.49	1.42
22	B	606	CLA	C4B-NB	2.89	1.41	1.37
22	R	309	CLA	C4D-ND	-2.88	1.33	1.37
22	4	304	CLA	C4B-NB	2.88	1.41	1.37
22	n	304	CLA	C4B-NB	2.88	1.41	1.37
22	S	305	CLA	C4B-NB	2.88	1.41	1.37
26	S	313	CHL	C1D-C2D	2.88	1.51	1.45
22	2	304	CLA	C4B-NB	2.88	1.41	1.37
31	A	409	BCR	C20-C21	2.88	1.52	1.43
22	b	609	CLA	C4B-NB	2.88	1.41	1.37
33	a	411	PL9	C3-C4	2.88	1.53	1.49
22	3	304	CLA	C3B-C4B	2.88	1.49	1.42
22	5	301	CLA	C3B-C4B	2.88	1.49	1.42
24	p	312	XAT	C38-C25	2.88	1.56	1.51
26	g	312	CHL	C1D-C2D	2.88	1.51	1.45
24	u	311	XAT	C38-C25	2.88	1.56	1.51
26	2	314	CHL	C1D-C2D	2.88	1.51	1.45
26	p	317	CHL	C1D-C2D	2.88	1.51	1.45
22	C	510	CLA	C3B-C4B	2.88	1.49	1.42
22	2	301	CLA	C3B-C4B	2.87	1.49	1.42
26	5	314	CHL	MG-NA	-2.87	1.99	2.06
26	1	315	CHL	C3D-C2D	2.87	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	311	CHL	C3B-C4B	2.87	1.49	1.42
26	5	316	CHL	C1D-C2D	2.87	1.51	1.45
26	r	615	CHL	CHB-C1B	2.87	1.45	1.39
22	N	305	CLA	C3D-C4D	2.87	1.50	1.44
22	p	302	CLA	C3B-C4B	2.87	1.49	1.42
26	g	316	CHL	C3D-C2D	2.87	1.47	1.39
27	u	319	NEX	C7-C8	-2.87	1.27	1.32
22	d	402	CLA	C1D-ND	2.87	1.41	1.37
26	2	313	CHL	MG-NA	-2.87	1.99	2.06
22	r	607	CLA	C4D-ND	-2.87	1.33	1.37
26	V	313	CHL	C3D-C2D	2.87	1.46	1.39
22	G	303	CLA	C3B-C4B	2.87	1.49	1.42
31	a	409	BCR	C20-C21	2.87	1.52	1.43
22	q	304	CLA	C3B-C4B	2.87	1.49	1.42
27	v	319	NEX	C7-C8	-2.87	1.27	1.32
22	r	610	CLA	C4D-ND	-2.87	1.33	1.37
22	G	304	CLA	C4D-ND	-2.87	1.33	1.37
22	1	305	CLA	C4B-NB	2.87	1.41	1.37
26	6	312	CHL	C1D-C2D	2.87	1.51	1.45
24	3	309	XAT	C18-C5	2.86	1.56	1.51
24	Q	309	XAT	C18-C5	2.86	1.56	1.51
22	g	301	CLA	C3B-C4B	2.86	1.49	1.42
26	Q	314	CHL	C3D-C2D	2.86	1.46	1.39
26	Q	311	CHL	C1D-C2D	2.86	1.51	1.45
22	b	605	CLA	C4B-NB	2.86	1.41	1.37
22	R	308	CLA	C4D-ND	-2.86	1.33	1.37
22	P	305	CLA	C4B-NB	2.86	1.41	1.37
30	d	401	PHO	C4D-ND	-2.86	1.34	1.38
26	q	313	CHL	C1D-C2D	2.86	1.51	1.45
26	V	315	CHL	C1D-C2D	2.86	1.51	1.45
26	Q	313	CHL	C1D-C2D	2.86	1.51	1.45
26	R	316	CHL	CHB-C1B	2.86	1.45	1.39
26	q	315	CHL	C3D-C2D	2.86	1.46	1.39
22	q	301	CLA	C3B-C4B	2.86	1.49	1.42
22	u	307	CLA	C4B-NB	2.86	1.41	1.37
26	S	315	CHL	MG-NA	-2.86	1.99	2.06
26	4	317	CHL	C3D-C2D	2.86	1.46	1.39
34	C	502	LMG	O7-C10	2.86	1.42	1.34
33	D	405	PL9	C2-C1	2.86	1.52	1.44
26	v	317	CHL	C3D-C2D	2.86	1.46	1.39
26	Q	315	CHL	C3B-C4B	2.85	1.49	1.42
26	v	314	CHL	C1D-C2D	2.85	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	316	CHL	C3D-C2D	2.85	1.46	1.39
26	2	316	CHL	C1D-C2D	2.85	1.51	1.45
26	g	316	CHL	C1D-C2D	2.85	1.51	1.45
26	s	315	CHL	MG-NA	-2.85	1.99	2.06
26	5	313	CHL	MG-NA	-2.85	1.99	2.06
26	n	317	CHL	C1D-C2D	2.85	1.50	1.45
26	3	316	CHL	C3D-C2D	2.85	1.46	1.39
31	b	620	BCR	C7-C6	2.85	1.55	1.45
26	Q	311	CHL	C3D-C2D	2.85	1.46	1.39
26	5	318	CHL	C3D-C2D	2.85	1.46	1.39
24	3	309	XAT	C4-C3	2.85	1.56	1.52
22	D	403	CLA	C1D-ND	2.85	1.41	1.37
26	s	313	CHL	C3D-C2D	2.85	1.46	1.39
22	U	302	CLA	C3B-C4B	2.85	1.49	1.42
26	G	311	CHL	C3B-C4B	2.84	1.49	1.42
26	5	314	CHL	C1D-C2D	2.84	1.50	1.45
22	r	601	CLA	C3B-C4B	2.84	1.49	1.42
26	Q	316	CHL	C3D-C2D	2.84	1.46	1.39
22	5	308	CLA	C3B-C4B	2.84	1.49	1.42
22	G	306	CLA	C3B-C4B	2.84	1.49	1.42
22	B	615	CLA	C4B-NB	2.84	1.41	1.37
31	k	101	BCR	C7-C6	2.84	1.55	1.45
22	n	301	CLA	C3B-C4B	2.84	1.49	1.42
31	B	620	BCR	C7-C6	2.84	1.55	1.45
22	1	304	CLA	C4B-NB	2.84	1.41	1.37
30	D	401	PHO	C4D-ND	-2.84	1.34	1.38
26	v	313	CHL	C1D-C2D	2.84	1.50	1.45
24	v	311	XAT	C18-C5	2.84	1.56	1.51
26	r	614	CHL	C3D-C2D	2.84	1.46	1.39
22	1	307	CLA	C4B-NB	2.84	1.41	1.37
26	5	313	CHL	C1B-NB	-2.84	1.34	1.37
31	A	409	BCR	C39-C30	-2.84	1.48	1.53
30	a	407	PHO	CMC-C2C	-2.84	1.46	1.50
30	d	401	PHO	CMC-C2C	-2.84	1.46	1.50
22	5	306	CLA	C4B-NB	2.84	1.41	1.37
33	d	404	PL9	C2-C1	2.84	1.52	1.44
26	v	314	CHL	C3D-C2D	2.84	1.46	1.39
26	2	314	CHL	MG-NA	-2.84	1.99	2.06
24	V	311	XAT	C18-C5	2.83	1.56	1.51
22	5	305	CLA	C3B-C4B	2.83	1.49	1.42
31	x	202	BCR	C7-C6	2.83	1.55	1.45
26	4	316	CHL	C3D-C2D	2.83	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	407	PHO	CMC-C2C	-2.83	1.46	1.50
22	G	301	CLA	C3B-C4B	2.83	1.49	1.42
22	N	308	CLA	C3B-C4B	2.83	1.49	1.42
26	1	317	CHL	C3D-C2D	2.83	1.46	1.39
22	C	510	CLA	CMC-C2C	-2.83	1.44	1.50
26	q	313	CHL	C3D-C2D	2.83	1.46	1.39
22	G	305	CLA	C4D-ND	-2.83	1.33	1.37
22	C	505	CLA	C4B-NB	2.83	1.41	1.37
22	b	615	CLA	C4B-NB	2.83	1.41	1.37
26	p	319	CHL	C3D-C2D	2.83	1.46	1.39
26	5	316	CHL	C3D-C2D	2.83	1.46	1.39
26	V	317	CHL	C3D-C2D	2.83	1.46	1.39
26	6	317	CHL	C3D-C2D	2.83	1.46	1.39
26	r	616	CHL	C3D-C2D	2.83	1.46	1.39
31	X	201	BCR	C7-C6	2.83	1.55	1.45
26	u	314	CHL	C3D-C2D	2.83	1.46	1.39
26	n	315	CHL	C1D-C2D	2.83	1.50	1.45
22	C	510	CLA	CMB-C2B	-2.83	1.44	1.50
27	N	318	NEX	C7-C8	-2.83	1.27	1.32
31	b	619	BCR	C7-C6	2.83	1.55	1.45
22	c	509	CLA	CMB-C2B	-2.83	1.44	1.50
22	b	608	CLA	C4B-NB	2.83	1.41	1.37
22	2	308	CLA	C3B-C4B	2.82	1.49	1.42
26	V	317	CHL	C3B-C4B	2.82	1.49	1.42
22	C	514	CLA	C4B-NB	2.82	1.41	1.37
22	b	610	CLA	C3B-C4B	2.82	1.49	1.42
31	K	101	BCR	C7-C6	2.82	1.55	1.45
34	c	501	LMG	O7-C10	2.82	1.42	1.34
31	C	518	BCR	C7-C6	2.82	1.55	1.45
26	v	317	CHL	C1D-C2D	2.82	1.50	1.45
22	P	305	CLA	C3B-C4B	2.82	1.49	1.42
31	C	516	BCR	C7-C6	2.82	1.55	1.45
26	4	314	CHL	C3D-C2D	2.82	1.46	1.39
26	u	313	CHL	C1D-C2D	2.82	1.50	1.45
26	P	314	CHL	C1D-C2D	2.82	1.50	1.45
26	1	314	CHL	MG-NA	-2.82	1.99	2.06
26	G	316	CHL	C1D-C2D	2.82	1.50	1.45
31	B	618	BCR	C20-C21	2.82	1.52	1.43
26	4	316	CHL	C1D-C2D	2.82	1.50	1.45
22	v	307	CLA	C3B-C4B	2.82	1.49	1.42
24	4	311	XAT	C18-C5	2.82	1.56	1.51
32	m	101	SQD	O47-C7	2.82	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	q	303	CLA	C3B-C4B	2.82	1.49	1.42
22	B	612	CLA	CMC-C2C	-2.81	1.44	1.50
26	1	318	CHL	C3D-C2D	2.81	1.46	1.39
22	B	608	CLA	C4B-NB	2.81	1.41	1.37
31	B	619	BCR	C7-C6	2.81	1.55	1.45
26	R	315	CHL	C3D-C2D	2.81	1.46	1.39
26	S	313	CHL	C3D-C2D	2.81	1.46	1.39
26	r	615	CHL	C3D-C2D	2.81	1.46	1.39
26	2	318	CHL	C3D-C2D	2.81	1.46	1.39
26	V	316	CHL	C1D-C2D	2.81	1.50	1.45
22	u	304	CLA	C4B-NB	2.81	1.41	1.37
22	Q	305	CLA	C3B-C4B	2.81	1.49	1.42
26	q	311	CHL	C3D-C2D	2.81	1.46	1.39
26	g	314	CHL	C1D-C2D	2.81	1.50	1.45
24	N	311	XAT	C24-C23	2.81	1.56	1.52
22	5	302	CLA	C3B-C4B	2.81	1.49	1.42
24	p	312	XAT	C18-C5	2.81	1.56	1.51
22	c	507	CLA	CMB-C2B	-2.81	1.44	1.50
26	R	316	CHL	C3D-C2D	2.81	1.46	1.39
24	P	312	XAT	C24-C23	2.81	1.56	1.52
31	z	101	BCR	C7-C6	2.81	1.55	1.45
24	P	312	XAT	C18-C5	2.81	1.56	1.51
26	p	316	CHL	C1D-C2D	2.81	1.50	1.45
22	q	307	CLA	C3B-C4B	2.81	1.49	1.42
24	5	311	XAT	C38-C25	2.81	1.56	1.51
34	B	621	LMG	O7-C8	-2.81	1.39	1.46
30	D	401	PHO	CMC-C2C	-2.81	1.46	1.50
22	r	609	CLA	C4D-ND	-2.81	1.33	1.37
26	P	316	CHL	C1D-C2D	2.81	1.50	1.45
22	g	305	CLA	C4D-ND	-2.80	1.33	1.37
22	B	605	CLA	C4B-NB	2.80	1.41	1.37
22	V	307	CLA	C3B-C4B	2.80	1.49	1.42
24	1	311	XAT	C18-C5	2.80	1.56	1.51
24	U	311	XAT	C38-C25	2.80	1.56	1.51
26	n	314	CHL	C3B-C4B	2.80	1.49	1.42
22	C	515	CLA	C4B-NB	2.80	1.41	1.37
26	2	316	CHL	C3D-C2D	2.80	1.46	1.39
26	N	313	CHL	C1D-C2D	2.80	1.50	1.45
26	P	319	CHL	C3D-C2D	2.80	1.46	1.39
26	3	311	CHL	C1D-C2D	2.80	1.50	1.45
24	1	311	XAT	C4-C3	2.80	1.56	1.52
26	R	317	CHL	C3D-C2D	2.80	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	309	XAT	C18-C5	2.80	1.56	1.51
34	C	521	LMG	O7-C10	2.80	1.42	1.34
22	g	304	CLA	C4D-ND	-2.80	1.33	1.37
26	G	316	CHL	C3D-C2D	2.80	1.46	1.39
26	u	317	CHL	C3D-C2D	2.80	1.46	1.39
26	Q	311	CHL	C3B-C4B	2.80	1.49	1.42
26	6	314	CHL	C1D-C2D	2.80	1.50	1.45
31	c	515	BCR	C39-C30	-2.80	1.48	1.53
34	b	624	LMG	O8-C28	2.80	1.41	1.33
26	1	316	CHL	C1D-C2D	2.80	1.50	1.45
26	6	301	CHL	C1D-C2D	2.80	1.50	1.45
22	p	302	CLA	C4B-NB	2.79	1.41	1.37
32	M	101	SQD	O47-C7	2.79	1.42	1.34
26	N	317	CHL	C1D-C2D	2.79	1.50	1.45
26	n	318	CHL	C1D-C2D	2.79	1.50	1.45
22	C	508	CLA	CMB-C2B	-2.79	1.44	1.50
22	R	302	CLA	C1B-C2B	2.79	1.49	1.43
22	2	305	CLA	C3B-C4B	2.79	1.49	1.42
22	R	306	CLA	C3B-C4B	2.79	1.49	1.42
26	n	316	CHL	C3D-C2D	2.79	1.46	1.39
31	D	404	BCR	C7-C6	2.79	1.55	1.45
27	V	319	NEX	C7-C8	-2.79	1.27	1.32
26	R	317	CHL	C1D-C2D	2.79	1.50	1.45
31	t	101	BCR	C16-C17	2.79	1.52	1.43
24	u	311	XAT	C18-C5	2.79	1.56	1.51
22	6	309	CLA	C3B-C4B	2.79	1.49	1.42
22	B	610	CLA	C3B-C4B	2.79	1.49	1.42
24	n	311	XAT	C24-C23	2.79	1.56	1.52
26	2	318	CHL	C1D-C2D	2.79	1.50	1.45
31	c	516	BCR	C7-C6	2.79	1.55	1.45
34	a	412	LMG	O7-C10	2.79	1.42	1.34
34	C	521	LMG	O8-C28	2.79	1.41	1.33
26	N	317	CHL	C4B-NB	-2.79	1.34	1.37
34	B	624	LMG	O8-C28	2.79	1.41	1.33
24	6	310	XAT	C18-C5	2.79	1.56	1.51
26	v	313	CHL	C3D-C2D	2.79	1.46	1.39
24	G	309	XAT	C18-C5	2.79	1.56	1.51
22	d	402	CLA	MG-NB	-2.79	2.00	2.05
31	a	409	BCR	C39-C30	-2.78	1.48	1.53
31	T	101	BCR	C16-C17	2.78	1.52	1.43
22	6	308	CLA	C3B-C4B	2.78	1.49	1.42
24	N	311	XAT	C4-C3	2.78	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	p	309	CLA	C3B-C4B	2.78	1.49	1.42
22	Q	307	CLA	C3B-C4B	2.78	1.49	1.42
22	b	611	CLA	C3B-C4B	2.78	1.49	1.42
22	q	304	CLA	C4D-ND	-2.78	1.33	1.37
24	p	312	XAT	C4-C3	2.78	1.56	1.52
34	c	520	LMG	O7-C10	2.78	1.42	1.34
22	n	303	CLA	C3B-C4B	2.78	1.49	1.42
26	3	311	CHL	C3D-C2D	2.78	1.46	1.39
26	p	314	CHL	C3D-C2D	2.78	1.46	1.39
34	A	411	LMG	O7-C10	2.78	1.42	1.34
26	U	316	CHL	C1D-C2D	2.78	1.50	1.45
22	r	607	CLA	C3B-C4B	2.78	1.49	1.42
22	r	610	CLA	C3B-C4B	2.78	1.49	1.42
22	3	305	CLA	C3B-C4B	2.78	1.49	1.42
24	u	311	XAT	C4-C3	2.78	1.56	1.52
22	a	404	CLA	CMC-C2C	-2.78	1.44	1.50
26	N	313	CHL	C3D-C2D	2.78	1.46	1.39
34	a	412	LMG	O8-C28	2.78	1.41	1.33
26	1	313	CHL	C1D-C2D	2.78	1.50	1.45
31	b	618	BCR	C20-C21	2.78	1.52	1.43
26	4	313	CHL	C1D-C2D	2.78	1.50	1.45
22	5	306	CLA	C3B-C4B	2.78	1.49	1.42
24	V	311	XAT	C24-C23	2.78	1.56	1.52
22	P	309	CLA	C3B-C4B	2.78	1.49	1.42
22	r	608	CLA	C3B-C4B	2.78	1.49	1.42
22	q	308	CLA	C3B-C4B	2.77	1.49	1.42
26	u	313	CHL	C3D-C2D	2.77	1.46	1.39
22	2	307	CLA	C3B-C4B	2.77	1.49	1.42
22	R	308	CLA	C3B-C4B	2.77	1.49	1.42
22	b	612	CLA	CMC-C2C	-2.77	1.44	1.50
22	4	308	CLA	C3B-C4B	2.77	1.49	1.42
26	G	313	CHL	C1D-C2D	2.77	1.50	1.45
26	V	315	CHL	MG-NA	-2.77	1.99	2.06
22	n	308	CLA	C4D-ND	-2.77	1.33	1.37
26	2	315	CHL	C3D-C2D	2.77	1.46	1.39
22	5	307	CLA	C3B-C4B	2.77	1.49	1.42
26	r	614	CHL	C3B-C4B	2.77	1.49	1.42
26	N	316	CHL	C1D-C2D	2.77	1.50	1.45
22	3	308	CLA	C3B-C4B	2.77	1.49	1.42
26	r	619	CHL	C3D-C2D	2.77	1.46	1.39
26	r	616	CHL	C1B-NB	-2.77	1.34	1.37
25	l	101	LHG	O7-C5	-2.77	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	311	CLA	C3B-C4B	2.77	1.49	1.42
22	X	202	CLA	C3B-C4B	2.77	1.49	1.42
26	3	313	CHL	C1D-C2D	2.77	1.50	1.45
26	5	318	CHL	C1D-C2D	2.77	1.50	1.45
31	B	620	BCR	C39-C30	-2.77	1.48	1.53
22	q	306	CLA	C3B-C4B	2.77	1.49	1.42
24	5	311	XAT	C18-C5	2.77	1.56	1.51
26	g	311	CHL	C3D-C2D	2.77	1.46	1.39
25	c	522	LHG	O7-C5	-2.77	1.39	1.46
22	r	605	CLA	C3B-C4B	2.77	1.49	1.42
24	q	309	XAT	C24-C23	2.76	1.56	1.52
31	b	620	BCR	C39-C30	-2.76	1.48	1.53
26	5	315	CHL	C1D-C2D	2.76	1.50	1.45
22	A	404	CLA	CMC-C2C	-2.76	1.44	1.50
22	c	514	CLA	C4B-NB	2.76	1.41	1.37
22	r	603	CLA	C3B-C4B	2.76	1.49	1.42
24	2	311	XAT	C18-C5	2.76	1.56	1.51
22	6	306	CLA	C3B-C4B	2.76	1.49	1.42
26	p	320	CHL	C3D-C2D	2.76	1.46	1.39
26	r	615	CHL	C1D-C2D	2.76	1.50	1.45
26	6	315	CHL	C1D-C2D	2.76	1.50	1.45
22	B	611	CLA	C3B-C4B	2.76	1.49	1.42
22	C	512	CLA	C1B-C2B	2.76	1.49	1.43
24	1	311	XAT	C24-C23	2.76	1.56	1.52
26	r	616	CHL	C1D-C2D	2.76	1.50	1.45
22	b	613	CLA	C4B-NB	2.76	1.41	1.37
26	R	315	CHL	C3B-C4B	2.76	1.49	1.42
22	c	513	CLA	C4B-NB	2.76	1.41	1.37
22	R	310	CLA	C4D-ND	-2.76	1.33	1.37
31	d	403	BCR	C16-C17	2.76	1.52	1.43
22	Q	304	CLA	C4D-ND	-2.76	1.33	1.37
22	p	305	CLA	C3B-C4B	2.76	1.49	1.42
22	b	603	CLA	C4B-NB	2.76	1.41	1.37
31	C	517	BCR	C39-C30	-2.76	1.48	1.53
22	2	306	CLA	C3B-C4B	2.76	1.49	1.42
26	3	311	CHL	C3B-C4B	2.75	1.49	1.42
24	6	310	XAT	C24-C23	2.75	1.56	1.52
22	V	301	CLA	C3B-C4B	2.75	1.49	1.42
31	d	403	BCR	C7-C6	2.75	1.54	1.45
22	Q	308	CLA	C3B-C4B	2.75	1.49	1.42
22	n	307	CLA	C3B-C4B	2.75	1.49	1.42
22	S	309	CLA	C3B-C4B	2.75	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	317	CHL	C1D-C2D	2.75	1.50	1.45
34	c	520	LMG	O8-C28	2.75	1.41	1.33
22	R	304	CLA	C3B-C4B	2.75	1.49	1.42
22	3	307	CLA	C3B-C4B	2.75	1.49	1.42
22	u	302	CLA	C3B-C4B	2.75	1.49	1.42
25	C	523	LHG	O7-C5	-2.75	1.39	1.46
26	q	312	CHL	MG-NA	-2.75	1.99	2.06
26	P	315	CHL	C4B-NB	-2.75	1.34	1.37
22	r	604	CLA	C1B-C2B	2.75	1.49	1.43
30	a	407	PHO	C4D-ND	-2.75	1.34	1.38
22	r	606	CLA	C3B-C4B	2.75	1.49	1.42
26	v	313	CHL	C3B-C4B	2.75	1.49	1.42
26	1	313	CHL	C3D-C2D	2.75	1.46	1.39
26	3	314	CHL	C1D-C2D	2.75	1.50	1.45
22	3	301	CLA	C3B-C4B	2.75	1.49	1.42
22	g	303	CLA	C3B-C4B	2.75	1.49	1.42
34	A	411	LMG	O8-C28	2.75	1.41	1.33
26	n	316	CHL	C1D-C2D	2.75	1.50	1.45
22	x	201	CLA	C3B-C4B	2.75	1.49	1.42
26	r	616	CHL	C3B-C4B	2.75	1.49	1.42
26	n	318	CHL	C4B-NB	-2.75	1.34	1.37
22	p	307	CLA	C3B-C4B	2.75	1.49	1.42
26	3	315	CHL	C3D-C2D	2.75	1.46	1.39
26	G	314	CHL	C1D-C2D	2.75	1.50	1.45
31	C	517	BCR	C7-C6	2.75	1.54	1.45
24	U	311	XAT	C4-C3	2.75	1.56	1.52
24	U	311	XAT	C18-C5	2.75	1.56	1.51
22	x	201	CLA	C4B-NB	2.75	1.41	1.37
22	n	305	CLA	C3B-C4B	2.75	1.49	1.42
24	R	313	XAT	C38-C25	2.74	1.56	1.51
22	q	305	CLA	C3B-C4B	2.74	1.49	1.42
22	V	302	CLA	C3B-C4B	2.74	1.49	1.42
26	4	313	CHL	C1B-NB	-2.74	1.34	1.37
22	1	308	CLA	C3B-C4B	2.74	1.49	1.42
26	5	314	CHL	C1B-NB	-2.74	1.34	1.37
26	U	313	CHL	C3D-C2D	2.74	1.46	1.39
25	L	101	LHG	O7-C5	-2.74	1.39	1.46
26	1	318	CHL	C1D-C2D	2.74	1.50	1.45
26	V	318	CHL	C1D-C2D	2.74	1.50	1.45
26	g	311	CHL	C1D-C2D	2.74	1.50	1.45
22	5	303	CLA	C3B-C4B	2.74	1.49	1.42
26	R	317	CHL	C3B-C4B	2.74	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v	315	CHL	C1D-C2D	2.74	1.50	1.45
26	G	311	CHL	C1D-C2D	2.74	1.50	1.45
22	N	303	CLA	C3B-C4B	2.74	1.49	1.42
22	D	403	CLA	MG-NB	-2.74	2.00	2.05
26	4	313	CHL	MG-NA	-2.74	1.99	2.06
30	A	407	PHO	C4D-ND	-2.74	1.34	1.38
26	5	315	CHL	C3D-C2D	2.74	1.46	1.39
22	G	307	CLA	C3B-C4B	2.74	1.49	1.42
26	p	315	CHL	C3B-C4B	2.74	1.49	1.42
26	6	312	CHL	C3D-C2D	2.74	1.46	1.39
22	R	307	CLA	C3B-C4B	2.73	1.49	1.42
31	D	404	BCR	C16-C17	2.73	1.51	1.43
22	c	504	CLA	C4B-NB	2.73	1.41	1.37
22	1	307	CLA	C3B-C4B	2.73	1.49	1.42
26	s	316	CHL	MG-NA	-2.73	1.99	2.06
22	X	202	CLA	C4B-NB	2.73	1.41	1.37
22	6	302	CLA	C3B-C4B	2.73	1.49	1.42
22	6	307	CLA	C3B-C4B	2.73	1.49	1.42
26	G	315	CHL	C3D-C2D	2.73	1.46	1.39
22	u	301	CLA	C3B-C4B	2.73	1.49	1.42
31	c	515	BCR	C7-C6	2.73	1.54	1.45
24	n	311	XAT	C4-C3	2.73	1.56	1.52
26	2	314	CHL	C3B-C4B	2.73	1.49	1.42
26	1	317	CHL	C1D-C2D	2.73	1.50	1.45
26	U	319	CHL	C3D-C2D	2.73	1.46	1.39
26	N	316	CHL	C3D-C2D	2.73	1.46	1.39
31	C	516	BCR	C39-C30	-2.73	1.48	1.53
26	u	318	CHL	C3D-C2D	2.73	1.46	1.39
26	Q	314	CHL	C1D-C2D	2.73	1.50	1.45
22	V	303	CLA	C3B-C4B	2.73	1.49	1.42
22	g	302	CLA	C3B-C4B	2.73	1.49	1.42
24	r	612	XAT	C38-C25	2.73	1.56	1.51
22	g	308	CLA	C3B-C4B	2.73	1.49	1.42
31	z	101	BCR	C39-C30	-2.73	1.48	1.53
22	N	307	CLA	C3B-C4B	2.73	1.49	1.42
22	n	308	CLA	C3B-C4B	2.73	1.49	1.42
26	5	317	CHL	C3D-C2D	2.73	1.46	1.39
26	P	314	CHL	MG-NA	-2.72	1.99	2.06
25	U	312	LHG	O7-C5	-2.72	1.39	1.46
22	c	511	CLA	C1B-C2B	2.72	1.49	1.43
22	g	307	CLA	C3B-C4B	2.72	1.49	1.42
22	S	303	CLA	C3B-C4B	2.72	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	317	CHL	C3D-C2D	2.72	1.46	1.39
26	1	314	CHL	C1D-C2D	2.72	1.50	1.45
22	R	305	CLA	C1B-C2B	2.72	1.49	1.43
22	v	308	CLA	C3B-C4B	2.72	1.49	1.42
26	s	313	CHL	MG-NA	-2.72	1.99	2.06
22	4	301	CLA	C3B-C4B	2.72	1.49	1.42
26	2	315	CHL	C1D-C2D	2.72	1.50	1.45
26	n	315	CHL	C3D-C2D	2.72	1.46	1.39
26	6	312	CHL	C3B-C4B	2.72	1.49	1.42
26	N	315	CHL	C3D-C2D	2.72	1.46	1.39
26	P	315	CHL	C3B-C4B	2.72	1.49	1.42
24	3	309	XAT	C24-C23	2.72	1.56	1.52
24	4	311	XAT	C24-C23	2.72	1.56	1.52
31	c	516	BCR	C39-C30	-2.72	1.48	1.53
24	g	309	XAT	C24-C23	2.72	1.56	1.52
26	p	314	CHL	C1D-C2D	2.72	1.50	1.45
31	C	518	BCR	C39-C30	-2.72	1.48	1.53
22	r	603	CLA	C1B-C2B	2.72	1.49	1.43
25	d	405	LHG	O7-C5	-2.72	1.39	1.46
22	2	303	CLA	C3B-C4B	2.72	1.49	1.42
26	S	314	CHL	C3D-C2D	2.72	1.46	1.39
22	v	301	CLA	C3B-C4B	2.71	1.49	1.42
26	P	318	CHL	C3D-C2D	2.71	1.46	1.39
22	B	606	CLA	C1B-C2B	2.71	1.49	1.43
26	3	314	CHL	C3D-C2D	2.71	1.46	1.39
26	U	317	CHL	C3D-C2D	2.71	1.46	1.39
26	s	314	CHL	C3D-C2D	2.71	1.46	1.39
26	6	314	CHL	MG-NA	-2.71	1.99	2.06
24	n	311	XAT	C18-C5	2.71	1.56	1.51
25	5	312	LHG	O7-C5	-2.71	1.39	1.46
26	u	317	CHL	C1D-C2D	2.71	1.50	1.45
22	p	303	CLA	C3B-C4B	2.71	1.49	1.42
25	D	407	LHG	O7-C5	-2.71	1.39	1.46
26	S	316	CHL	MG-NA	-2.71	1.99	2.06
22	4	305	CLA	C3B-C4B	2.71	1.49	1.42
24	N	311	XAT	C18-C5	2.71	1.56	1.51
22	v	305	CLA	C3B-C4B	2.71	1.49	1.42
26	u	318	CHL	C1B-NB	-2.71	1.34	1.37
26	n	313	CHL	C1D-C2D	2.71	1.50	1.45
22	3	306	CLA	C3B-C4B	2.71	1.49	1.42
22	Q	306	CLA	C3B-C4B	2.71	1.49	1.42
25	D	406	LHG	O7-C5	-2.71	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	408	CLA	C3B-C4B	2.71	1.49	1.42
26	4	315	CHL	C1B-NB	-2.71	1.34	1.37
26	6	315	CHL	C3D-C2D	2.71	1.46	1.39
22	B	603	CLA	C4B-NB	2.71	1.41	1.37
22	R	302	CLA	C3B-C4B	2.71	1.49	1.42
26	V	314	CHL	C3B-C4B	2.71	1.49	1.42
26	U	319	CHL	C1D-C2D	2.71	1.50	1.45
22	v	302	CLA	C3B-C4B	2.71	1.49	1.42
34	b	621	LMG	O7-C8	-2.71	1.39	1.46
26	4	315	CHL	C1D-C2D	2.71	1.50	1.45
22	b	609	CLA	C3B-C4B	2.70	1.49	1.42
22	U	306	CLA	C3B-C4B	2.70	1.49	1.42
26	1	313	CHL	C1B-NB	-2.70	1.34	1.37
25	d	406	LHG	O7-C5	-2.70	1.39	1.46
26	Q	312	CHL	C3B-C4B	2.70	1.49	1.42
25	u	312	LHG	O7-C5	-2.70	1.39	1.46
24	v	311	XAT	C24-C23	2.70	1.56	1.52
27	P	301	NEX	C7-C8	-2.70	1.27	1.32
22	B	613	CLA	C4B-NB	2.70	1.41	1.37
22	4	307	CLA	C3B-C4B	2.70	1.49	1.42
22	P	308	CLA	C3B-C4B	2.70	1.49	1.42
22	1	305	CLA	C3B-C4B	2.70	1.49	1.42
22	r	602	CLA	C3B-C4B	2.70	1.49	1.42
22	R	310	CLA	C3B-C4B	2.70	1.49	1.42
22	C	513	CLA	C3B-C4B	2.70	1.49	1.42
26	p	320	CHL	C1D-C2D	2.70	1.50	1.45
26	v	315	CHL	C3B-C4B	2.70	1.49	1.42
22	p	308	CLA	C3B-C4B	2.70	1.49	1.42
22	V	305	CLA	C3B-C4B	2.70	1.49	1.42
26	R	316	CHL	C1D-C2D	2.70	1.50	1.45
26	5	314	CHL	C4B-NB	-2.70	1.34	1.37
22	s	304	CLA	C3B-C4B	2.70	1.49	1.42
22	c	512	CLA	C3B-C4B	2.70	1.49	1.42
26	4	317	CHL	C1D-C2D	2.70	1.50	1.45
22	R	309	CLA	C3B-C4B	2.70	1.49	1.42
26	6	313	CHL	C3B-C4B	2.70	1.49	1.42
26	u	316	CHL	C3B-C4B	2.70	1.49	1.42
26	N	314	CHL	C1D-C2D	2.69	1.50	1.45
26	u	314	CHL	C1D-C2D	2.69	1.50	1.45
22	N	305	CLA	C3B-C4B	2.69	1.49	1.42
26	1	313	CHL	MG-NA	-2.69	1.99	2.06
22	U	301	CLA	C3B-C4B	2.69	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	C3B-C4B	2.69	1.49	1.42
22	R	303	CLA	C3B-C4B	2.69	1.49	1.42
22	6	304	CLA	C3B-C4B	2.69	1.49	1.42
22	V	308	CLA	C3B-C4B	2.69	1.49	1.42
22	A	405	CLA	C4B-NB	2.69	1.41	1.37
26	U	315	CHL	C1D-C2D	2.69	1.50	1.45
22	a	408	CLA	C3B-C4B	2.69	1.49	1.42
26	P	319	CHL	C1D-C2D	2.69	1.50	1.45
22	s	303	CLA	C3B-C4B	2.69	1.49	1.42
22	a	406	CLA	C4B-NB	2.69	1.41	1.37
26	2	317	CHL	C1D-C2D	2.69	1.50	1.45
26	p	318	CHL	C3D-C2D	2.69	1.46	1.39
31	B	619	BCR	C39-C30	-2.69	1.48	1.53
31	b	618	BCR	C39-C30	-2.69	1.48	1.53
22	b	606	CLA	C1B-C2B	2.69	1.49	1.43
26	r	614	CHL	C1D-C2D	2.69	1.50	1.45
26	Q	315	CHL	C3D-C2D	2.69	1.46	1.39
22	B	608	CLA	C3B-C4B	2.68	1.49	1.42
24	G	309	XAT	C24-C23	2.68	1.56	1.52
22	B	617	CLA	C4B-NB	2.68	1.41	1.37
26	R	317	CHL	C1B-NB	-2.68	1.34	1.37
22	B	609	CLA	C3B-C4B	2.68	1.49	1.42
26	V	316	CHL	C3D-C2D	2.68	1.46	1.39
22	n	308	CLA	C1B-C2B	2.68	1.49	1.43
31	A	409	BCR	C7-C6	2.68	1.54	1.45
26	P	317	CHL	C3D-C2D	2.68	1.46	1.39
22	a	406	CLA	C3B-C4B	2.68	1.49	1.42
22	a	404	CLA	MG-NB	-2.68	2.00	2.05
26	g	315	CHL	C3D-C2D	2.68	1.46	1.39
22	A	404	CLA	MG-NB	-2.68	2.00	2.05
26	3	314	CHL	MG-NA	-2.68	1.99	2.06
25	C	522	LHG	O7-C5	-2.68	1.39	1.46
26	R	315	CHL	C1D-C2D	2.68	1.50	1.45
22	r	609	CLA	C3B-C4B	2.68	1.49	1.42
22	P	303	CLA	C3B-C4B	2.68	1.49	1.42
22	q	306	CLA	C1B-C2B	2.68	1.49	1.43
22	G	308	CLA	C3B-C4B	2.68	1.49	1.42
22	a	405	CLA	C4B-NB	2.67	1.41	1.37
22	d	402	CLA	C4B-NB	2.67	1.41	1.37
26	v	316	CHL	C1D-C2D	2.67	1.50	1.45
22	C	511	CLA	C3B-C4B	2.67	1.49	1.42
22	c	510	CLA	C3B-C4B	2.67	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	315	CHL	C3D-C2D	2.67	1.46	1.39
26	q	314	CHL	C3D-C2D	2.67	1.46	1.39
22	b	608	CLA	C3B-C4B	2.67	1.49	1.42
31	a	409	BCR	C7-C6	2.67	1.54	1.45
26	q	311	CHL	C3B-C4B	2.67	1.49	1.42
26	U	319	CHL	MG-NA	-2.67	1.99	2.06
22	P	306	CLA	C3B-C4B	2.67	1.49	1.42
22	Q	306	CLA	C1B-C2B	2.67	1.49	1.43
22	A	406	CLA	C4B-NB	2.67	1.41	1.37
31	x	202	BCR	C16-C17	2.67	1.51	1.43
22	B	613	CLA	C3B-C4B	2.67	1.49	1.42
22	b	613	CLA	C3B-C4B	2.67	1.49	1.42
22	S	306	CLA	C3B-C4B	2.66	1.49	1.42
22	n	305	CLA	C1B-C2B	2.66	1.49	1.43
31	b	619	BCR	C39-C30	-2.66	1.48	1.53
22	P	307	CLA	C3B-C4B	2.66	1.49	1.42
22	b	616	CLA	C4D-ND	-2.66	1.34	1.37
22	s	305	CLA	C3B-C4B	2.66	1.49	1.42
22	r	601	CLA	C1B-C2B	2.66	1.49	1.43
22	S	305	CLA	C3B-C4B	2.66	1.49	1.42
25	c	521	LHG	O7-C5	-2.66	1.39	1.46
22	n	306	CLA	C3B-C4B	2.66	1.49	1.42
26	2	315	CHL	C3B-C4B	2.66	1.49	1.42
25	3	310	LHG	O7-C5	-2.66	1.39	1.46
26	q	312	CHL	C3B-C4B	2.66	1.49	1.42
22	U	303	CLA	C3B-C4B	2.66	1.49	1.42
26	n	317	CHL	MG-NA	-2.66	2.00	2.06
26	v	318	CHL	C1D-C2D	2.66	1.50	1.45
31	B	618	BCR	C7-C6	2.66	1.54	1.45
22	Q	302	CLA	C3B-C4B	2.66	1.49	1.42
22	S	304	CLA	C3B-C4B	2.66	1.49	1.42
22	p	306	CLA	C3B-C4B	2.66	1.49	1.42
26	S	314	CHL	C1D-C2D	2.66	1.50	1.45
26	V	313	CHL	C3B-C4B	2.66	1.49	1.42
25	c	523	LHG	O7-C5	-2.66	1.39	1.46
26	P	318	CHL	C1D-C2D	2.66	1.50	1.45
26	n	313	CHL	MG-NA	-2.66	2.00	2.06
26	p	315	CHL	C4B-NB	-2.66	1.34	1.37
31	B	618	BCR	C39-C30	-2.66	1.48	1.53
22	b	617	CLA	MG-NB	-2.66	2.00	2.05
22	B	616	CLA	C4D-ND	-2.65	1.34	1.37
22	r	604	CLA	C3B-C4B	2.65	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	C3B-C4B	2.65	1.49	1.42
26	N	313	CHL	C3B-C4B	2.65	1.49	1.42
26	u	315	CHL	C1D-ND	-2.65	1.34	1.37
26	4	314	CHL	C1D-C2D	2.65	1.50	1.45
26	S	313	CHL	MG-NA	-2.65	2.00	2.06
22	R	305	CLA	C3B-C4B	2.65	1.49	1.42
26	3	312	CHL	C3B-C4B	2.65	1.49	1.42
22	u	305	CLA	C3B-C4B	2.65	1.49	1.42
26	v	314	CHL	C3B-C4B	2.65	1.49	1.42
31	X	201	BCR	C16-C17	2.65	1.51	1.43
26	p	317	CHL	C3D-C2D	2.65	1.46	1.39
26	G	312	CHL	C3B-C4B	2.65	1.49	1.42
22	S	304	CLA	C1B-C2B	2.65	1.49	1.43
30	D	401	PHO	CMD-C2D	-2.65	1.46	1.51
22	b	614	CLA	C4B-NB	2.65	1.41	1.37
22	C	504	CLA	C1B-C2B	2.65	1.49	1.43
31	x	202	BCR	C39-C30	-2.65	1.48	1.53
22	G	302	CLA	C3B-C4B	2.65	1.49	1.42
22	A	406	CLA	C3B-C4B	2.65	1.49	1.42
26	2	314	CHL	C4B-NB	-2.65	1.34	1.37
34	b	621	LMG	O7-C10	2.65	1.41	1.34
26	4	315	CHL	MG-NA	-2.65	2.00	2.06
24	u	311	XAT	C24-C23	2.64	1.56	1.52
22	N	306	CLA	C3B-C4B	2.64	1.49	1.42
22	S	308	CLA	C3B-C4B	2.64	1.49	1.42
22	B	614	CLA	C4B-NB	2.64	1.41	1.37
25	C	524	LHG	O7-C5	-2.64	1.40	1.46
22	D	403	CLA	CMD-C2D	-2.64	1.45	1.50
22	b	617	CLA	C3B-C4B	2.64	1.48	1.42
26	n	314	CHL	C1D-C2D	2.64	1.50	1.45
22	c	503	CLA	CMB-C2B	-2.64	1.45	1.50
22	g	306	CLA	C1B-C2B	2.64	1.49	1.43
22	d	402	CLA	CMD-C2D	-2.64	1.45	1.50
34	W	201	LMG	O8-C28	2.64	1.41	1.33
26	u	315	CHL	C1B-NB	-2.64	1.34	1.37
31	X	201	BCR	C39-C30	-2.64	1.48	1.53
26	r	619	CHL	C1D-C2D	2.64	1.50	1.45
26	3	313	CHL	MG-NA	-2.64	2.00	2.06
22	6	303	CLA	C3B-C4B	2.64	1.48	1.42
22	c	503	CLA	C1B-C2B	2.64	1.49	1.43
26	6	313	CHL	MG-NA	-2.64	2.00	2.06
36	C	520	DGD	O1G-C1A	2.64	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	315	CHL	C3B-C4B	2.63	1.48	1.42
26	N	314	CHL	C3B-C4B	2.63	1.48	1.42
22	u	304	CLA	C3B-C4B	2.63	1.48	1.42
26	v	316	CHL	C3D-C2D	2.63	1.46	1.39
22	Q	303	CLA	C1B-C2B	2.63	1.49	1.43
26	U	314	CHL	C3D-C2D	2.63	1.46	1.39
36	J	101	DGD	O1G-C1A	2.63	1.41	1.33
22	s	308	CLA	C3B-C4B	2.63	1.48	1.42
31	b	618	BCR	C7-C6	2.63	1.54	1.45
26	3	312	CHL	MG-NA	-2.63	2.00	2.06
22	u	303	CLA	CMB-C2B	-2.63	1.45	1.50
22	C	506	CLA	C3B-C4B	2.63	1.48	1.42
22	u	303	CLA	C3B-C4B	2.63	1.48	1.42
26	g	312	CHL	C3B-C4B	2.63	1.48	1.42
26	S	315	CHL	C3B-C4B	2.63	1.48	1.42
22	S	307	CLA	C3B-C4B	2.63	1.48	1.42
22	D	403	CLA	C4B-NB	2.63	1.41	1.37
22	P	307	CLA	C1B-C2B	2.63	1.49	1.43
22	R	304	CLA	C1B-C2B	2.63	1.49	1.43
34	A	411	LMG	O7-C8	-2.63	1.40	1.46
26	6	314	CHL	C1B-NB	-2.63	1.34	1.37
31	b	620	BCR	C16-C17	2.63	1.51	1.43
26	N	313	CHL	MG-NA	-2.63	2.00	2.06
22	R	311	CLA	C1B-C2B	2.63	1.49	1.43
22	s	306	CLA	C3B-C4B	2.62	1.48	1.42
26	g	315	CHL	C1D-C2D	2.62	1.50	1.45
30	d	401	PHO	CMD-C2D	-2.62	1.46	1.51
22	3	302	CLA	C3B-C4B	2.62	1.48	1.42
22	b	616	CLA	C4B-NB	2.62	1.41	1.37
26	1	315	CHL	C1D-C2D	2.62	1.50	1.45
34	w	201	LMG	O8-C28	2.62	1.41	1.33
22	r	609	CLA	C1B-C2B	2.62	1.49	1.43
22	R	310	CLA	C1B-C2B	2.62	1.49	1.43
22	B	602	CLA	C4B-NB	2.62	1.41	1.37
22	a	405	CLA	C3B-C4B	2.62	1.48	1.42
26	6	316	CHL	C3D-C2D	2.62	1.46	1.39
26	3	315	CHL	C1B-C2B	2.62	1.49	1.43
22	s	307	CLA	C3B-C4B	2.62	1.48	1.42
26	5	314	CHL	C3B-C4B	2.62	1.48	1.42
22	5	308	CLA	C1B-C2B	2.62	1.49	1.43
34	a	412	LMG	O7-C8	-2.62	1.40	1.46
26	5	315	CHL	C3B-C4B	2.62	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q	315	CHL	C3B-C4B	2.62	1.48	1.42
25	s	312	LHG	O7-C5	-2.62	1.40	1.46
22	2	305	CLA	C4D-ND	-2.62	1.34	1.37
22	c	505	CLA	C3B-C4B	2.62	1.48	1.42
26	1	315	CHL	C1B-NB	-2.62	1.34	1.37
22	V	305	CLA	C1B-C2B	2.61	1.49	1.43
26	N	317	CHL	C1B-NB	-2.61	1.34	1.37
31	t	101	BCR	C39-C30	-2.61	1.48	1.53
26	G	312	CHL	C1B-NB	-2.61	1.34	1.37
22	b	607	CLA	C3B-C4B	2.61	1.48	1.42
22	C	505	CLA	MG-NB	-2.61	2.00	2.05
36	c	519	DGD	O1G-C1A	2.61	1.41	1.33
26	n	316	CHL	MG-NA	-2.61	2.00	2.06
34	d	407	LMG	O8-C28	2.61	1.41	1.33
25	q	310	LHG	O7-C5	-2.61	1.40	1.46
22	P	304	CLA	C3B-C4B	2.61	1.48	1.42
27	u	320	NEX	C7-C8	-2.61	1.27	1.32
25	b	623	LHG	O7-C5	-2.61	1.40	1.46
22	N	306	CLA	C1B-C2B	2.61	1.49	1.43
26	q	312	CHL	C1B-NB	-2.61	1.34	1.37
22	2	308	CLA	C1B-C2B	2.61	1.49	1.43
22	U	305	CLA	C3B-C4B	2.61	1.48	1.42
24	n	311	XAT	C38-C25	2.61	1.55	1.51
25	6	311	LHG	O7-C5	-2.61	1.40	1.46
22	b	609	CLA	MG-NB	-2.61	2.00	2.05
31	T	101	BCR	C39-C30	-2.61	1.48	1.53
22	U	308	CLA	C3B-C4B	2.61	1.48	1.42
26	r	619	CHL	C3B-C4B	2.61	1.48	1.42
22	q	302	CLA	C3B-C4B	2.61	1.48	1.42
26	U	314	CHL	C1B-NB	-2.61	1.34	1.37
26	U	315	CHL	C3B-C4B	2.61	1.48	1.42
22	B	617	CLA	C1B-C2B	2.61	1.49	1.43
26	6	315	CHL	MG-NA	-2.61	2.00	2.06
22	G	305	CLA	C3B-C4B	2.61	1.48	1.42
26	g	314	CHL	MG-NA	-2.61	2.00	2.06
26	p	319	CHL	C1D-C2D	2.61	1.50	1.45
34	B	621	LMG	O7-C10	2.61	1.41	1.34
22	B	616	CLA	C4B-NB	2.60	1.41	1.37
26	1	314	CHL	C3B-C4B	2.60	1.48	1.42
22	C	504	CLA	CMB-C2B	-2.60	1.45	1.50
22	1	306	CLA	C1B-C2B	2.60	1.49	1.43
25	B	623	LHG	O7-C5	-2.60	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	308	CLA	C1B-C2B	2.60	1.49	1.43
26	3	314	CHL	C3B-C4B	2.60	1.48	1.42
22	4	303	CLA	C3B-C4B	2.60	1.48	1.42
22	p	307	CLA	C1B-C2B	2.60	1.49	1.43
22	1	304	CLA	C3B-C4B	2.60	1.48	1.42
26	R	316	CHL	C3B-C4B	2.60	1.48	1.42
26	p	318	CHL	C1D-C2D	2.60	1.50	1.45
25	V	312	LHG	O7-C5	-2.60	1.40	1.46
26	Q	316	CHL	C3B-C4B	2.60	1.48	1.42
31	C	518	BCR	C16-C17	2.60	1.51	1.43
22	s	304	CLA	C1B-C2B	2.60	1.49	1.43
22	4	304	CLA	C3B-C4B	2.60	1.48	1.42
26	r	615	CHL	C3B-C4B	2.60	1.48	1.42
22	n	306	CLA	C1B-C2B	2.59	1.49	1.43
26	G	314	CHL	MG-NA	-2.59	2.00	2.06
26	Q	314	CHL	MG-NA	-2.59	2.00	2.06
26	P	314	CHL	C3B-C4B	2.59	1.48	1.42
22	Q	303	CLA	C3B-C4B	2.59	1.48	1.42
26	S	314	CHL	C3B-C4B	2.59	1.48	1.42
26	N	314	CHL	C4B-NB	-2.59	1.34	1.37
36	c	518	DGD	O1G-C1A	2.59	1.40	1.33
26	s	314	CHL	C1D-C2D	2.59	1.50	1.45
34	b	621	LMG	O8-C28	2.59	1.40	1.33
26	q	312	CHL	C4B-NB	-2.59	1.34	1.37
31	c	516	BCR	C16-C17	2.59	1.51	1.43
22	v	303	CLA	C3B-C4B	2.59	1.48	1.42
22	c	504	CLA	MG-NB	-2.59	2.00	2.05
25	S	312	LHG	O7-C5	-2.59	1.40	1.46
22	1	301	CLA	C3B-C4B	2.59	1.48	1.42
25	p	313	LHG	O7-C5	-2.59	1.40	1.46
26	1	314	CHL	C1B-NB	-2.59	1.34	1.37
26	4	314	CHL	C3B-C4B	2.59	1.48	1.42
34	D	408	LMG	O8-C28	2.59	1.40	1.33
25	P	313	LHG	O7-C5	-2.59	1.40	1.46
22	b	617	CLA	CMD-C2D	-2.59	1.45	1.50
22	c	513	CLA	C3B-C4B	2.59	1.48	1.42
22	Q	305	CLA	C1B-C2B	2.59	1.49	1.43
26	n	313	CHL	C3B-C4B	2.58	1.48	1.42
22	B	607	CLA	C3B-C4B	2.58	1.48	1.42
22	B	617	CLA	CMD-C2D	-2.58	1.45	1.50
22	b	602	CLA	C4B-NB	2.58	1.41	1.37
26	P	315	CHL	C1D-ND	-2.58	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	515	CLA	C3B-C4B	2.58	1.48	1.42
22	b	616	CLA	C1B-C2B	2.58	1.49	1.43
22	P	309	CLA	C1B-C2B	2.58	1.49	1.43
22	p	304	CLA	C3B-C4B	2.58	1.48	1.42
22	3	302	CLA	C1B-C2B	2.58	1.49	1.43
22	D	403	CLA	C3B-C4B	2.58	1.48	1.42
26	s	315	CHL	C1B-NB	-2.58	1.34	1.37
22	1	303	CLA	MG-NB	-2.58	2.00	2.05
22	3	303	CLA	C3B-C4B	2.58	1.48	1.42
22	P	308	CLA	C1B-C2B	2.58	1.49	1.43
27	S	317	NEX	C7-C8	-2.58	1.27	1.32
22	N	307	CLA	C1B-C2B	2.58	1.49	1.43
22	C	514	CLA	C3B-C4B	2.58	1.48	1.42
22	u	308	CLA	C3B-C4B	2.58	1.48	1.42
26	1	315	CHL	MG-NA	-2.58	2.00	2.06
26	V	316	CHL	MG-NA	-2.57	2.00	2.06
26	s	314	CHL	C3B-C4B	2.57	1.48	1.42
22	r	610	CLA	C1B-C2B	2.57	1.49	1.43
22	A	404	CLA	C3B-C4B	2.57	1.48	1.42
26	6	315	CHL	C3B-C4B	2.57	1.48	1.42
22	q	305	CLA	C1B-C2B	2.57	1.49	1.43
22	g	305	CLA	C1B-C2B	2.57	1.49	1.43
22	u	302	CLA	C1B-C2B	2.57	1.49	1.43
26	v	318	CHL	C1B-NB	-2.57	1.34	1.37
22	d	402	CLA	C3B-C4B	2.57	1.48	1.42
22	c	514	CLA	C3B-C4B	2.57	1.48	1.42
22	B	616	CLA	C1B-C2B	2.57	1.49	1.43
22	c	510	CLA	MG-NB	-2.57	2.00	2.05
26	P	316	CHL	C1B-NB	-2.57	1.34	1.37
22	b	613	CLA	CMC-C2C	-2.57	1.45	1.50
22	v	305	CLA	C1B-C2B	2.57	1.49	1.43
26	S	315	CHL	C1B-NB	-2.57	1.34	1.37
36	C	519	DGD	O1G-C1G	-2.57	1.39	1.45
22	g	302	CLA	C1B-C2B	2.57	1.49	1.43
31	K	101	BCR	C16-C17	2.57	1.51	1.43
34	C	502	LMG	O7-C8	-2.57	1.40	1.46
22	g	305	CLA	C3B-C4B	2.57	1.48	1.42
26	1	316	CHL	C3D-C2D	2.57	1.46	1.39
22	S	305	CLA	C1B-C2B	2.57	1.49	1.43
22	s	307	CLA	C1B-C2B	2.57	1.49	1.43
26	n	317	CHL	C3B-C4B	2.56	1.48	1.42
26	U	313	CHL	MG-NA	-2.56	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	p	309	CLA	C1B-C2B	2.56	1.49	1.43
26	U	319	CHL	C3B-C4B	2.56	1.48	1.42
26	V	313	CHL	MG-NA	-2.56	2.00	2.06
26	n	314	CHL	C4B-NB	-2.56	1.34	1.37
26	q	315	CHL	MG-NA	-2.56	2.00	2.06
26	V	318	CHL	C1B-NB	-2.56	1.34	1.37
22	c	506	CLA	MG-NB	-2.56	2.00	2.05
22	2	305	CLA	C1B-C2B	2.56	1.49	1.43
26	6	313	CHL	C1B-C2B	2.56	1.49	1.43
30	A	407	PHO	CAC-C3C	-2.56	1.47	1.51
25	b	622	LHG	O7-C5	-2.56	1.40	1.46
22	a	404	CLA	C3B-C4B	2.56	1.48	1.42
22	p	305	CLA	C1B-C2B	2.56	1.49	1.43
22	q	302	CLA	C1B-C2B	2.56	1.49	1.43
36	c	517	DGD	O1G-C1A	2.56	1.40	1.33
22	r	608	CLA	C1B-C2B	2.56	1.49	1.43
22	1	306	CLA	C3B-C4B	2.56	1.48	1.42
22	u	306	CLA	C3B-C4B	2.56	1.48	1.42
26	G	315	CHL	C1D-C2D	2.56	1.50	1.45
22	3	305	CLA	C1B-C2B	2.56	1.49	1.43
26	P	315	CHL	C1B-NB	-2.56	1.34	1.37
22	s	305	CLA	C1B-C2B	2.56	1.49	1.43
34	B	621	LMG	O1-C1	-2.56	1.35	1.40
22	N	305	CLA	C4D-ND	-2.56	1.34	1.37
31	D	404	BCR	C39-C30	-2.56	1.48	1.53
26	U	317	CHL	C1D-C2D	2.56	1.50	1.45
22	C	507	CLA	MG-NB	-2.55	2.00	2.05
22	r	607	CLA	C1B-C2B	2.55	1.49	1.43
26	Q	314	CHL	C3B-C4B	2.55	1.48	1.42
22	c	502	CLA	CMD-C2D	-2.55	1.45	1.50
22	B	617	CLA	C3B-C4B	2.55	1.48	1.42
26	P	317	CHL	C3B-C4B	2.55	1.48	1.42
22	P	306	CLA	C1B-C2B	2.55	1.49	1.43
22	n	307	CLA	C1B-C2B	2.55	1.49	1.43
25	r	613	LHG	O8-C23	2.55	1.40	1.33
34	B	621	LMG	O8-C28	2.55	1.40	1.33
31	k	101	BCR	C16-C17	2.55	1.51	1.43
22	B	609	CLA	MG-NB	-2.55	2.00	2.05
22	6	309	CLA	C1B-C2B	2.55	1.49	1.43
26	5	316	CHL	MG-NA	-2.55	2.00	2.06
22	C	512	CLA	C3B-C4B	2.55	1.48	1.42
26	n	313	CHL	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	303	CLA	C1B-C2B	2.55	1.49	1.43
22	4	303	CLA	MG-NB	-2.55	2.00	2.05
22	6	303	CLA	C1B-C2B	2.55	1.49	1.43
34	c	501	LMG	O7-C8	-2.55	1.40	1.46
26	4	313	CHL	C4B-NB	-2.55	1.34	1.37
22	U	302	CLA	C1B-C2B	2.54	1.49	1.43
26	U	317	CHL	C1B-NB	-2.54	1.34	1.37
31	C	516	BCR	C16-C17	2.54	1.51	1.43
22	G	302	CLA	C1B-C2B	2.54	1.49	1.43
26	6	301	CHL	C3D-C2D	2.54	1.46	1.39
22	A	405	CLA	C3B-C4B	2.54	1.48	1.42
22	p	306	CLA	C1B-C2B	2.54	1.49	1.43
31	B	620	BCR	C16-C17	2.54	1.51	1.43
26	Q	315	CHL	C1D-C2D	2.54	1.50	1.45
22	6	306	CLA	C1B-C2B	2.54	1.49	1.43
36	c	517	DGD	O1G-C1G	-2.54	1.39	1.45
25	Q	310	LHG	O7-C5	-2.54	1.40	1.46
25	R	314	LHG	O8-C23	2.54	1.40	1.33
25	1	312	LHG	O7-C5	-2.54	1.40	1.46
22	Q	302	CLA	C1B-C2B	2.54	1.49	1.43
22	G	306	CLA	C1B-C2B	2.54	1.49	1.43
22	G	308	CLA	C1B-C2B	2.54	1.49	1.43
22	3	308	CLA	C1B-C2B	2.54	1.49	1.43
22	P	305	CLA	C1B-C2B	2.54	1.49	1.43
22	S	307	CLA	C1B-C2B	2.54	1.49	1.43
26	p	315	CHL	C1B-NB	-2.54	1.34	1.37
26	3	312	CHL	C1B-C2B	2.54	1.49	1.43
26	p	316	CHL	C1B-NB	-2.54	1.34	1.37
26	V	314	CHL	C1B-C2B	2.54	1.49	1.43
36	C	519	DGD	O1G-C1A	2.54	1.40	1.33
26	P	316	CHL	C3B-C4B	2.53	1.48	1.42
25	B	622	LHG	O7-C5	-2.53	1.40	1.46
26	2	317	CHL	C3B-C4B	2.53	1.48	1.42
26	3	313	CHL	C1B-NB	-2.53	1.34	1.37
22	b	602	CLA	C3B-C4B	2.53	1.48	1.42
22	B	606	CLA	C3B-C4B	2.53	1.48	1.42
25	v	312	LHG	O7-C5	-2.53	1.40	1.46
22	R	309	CLA	C1B-C2B	2.53	1.49	1.43
22	C	503	CLA	CMD-C2D	-2.53	1.45	1.50
26	u	314	CHL	C3B-C4B	2.53	1.48	1.42
22	G	307	CLA	C1B-C2B	2.53	1.49	1.43
31	b	619	BCR	C16-C17	2.53	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	308	CLA	C1B-C2B	2.53	1.49	1.43
22	U	303	CLA	CMB-C2B	-2.53	1.45	1.50
22	B	613	CLA	CMC-C2C	-2.53	1.45	1.50
22	c	511	CLA	C3B-C4B	2.53	1.48	1.42
22	G	305	CLA	C1B-C2B	2.53	1.49	1.43
24	U	311	XAT	C24-C23	2.53	1.56	1.52
22	2	303	CLA	C1B-C2B	2.53	1.49	1.43
22	g	308	CLA	C1B-C2B	2.53	1.49	1.43
22	3	306	CLA	C1B-C2B	2.53	1.49	1.43
22	b	614	CLA	MG-NB	-2.53	2.00	2.05
22	v	308	CLA	C1B-C2B	2.53	1.49	1.43
26	R	316	CHL	C1B-NB	-2.53	1.34	1.37
22	C	511	CLA	MG-NB	-2.53	2.00	2.05
26	n	318	CHL	MG-NA	-2.53	2.00	2.06
31	z	101	BCR	C16-C17	2.53	1.51	1.43
31	B	619	BCR	C16-C17	2.53	1.51	1.43
30	a	407	PHO	CMD-C2D	-2.53	1.46	1.51
26	P	317	CHL	MG-NA	-2.53	2.00	2.06
22	B	602	CLA	C3B-C4B	2.53	1.48	1.42
22	P	303	CLA	C1B-C2B	2.53	1.49	1.43
22	u	306	CLA	C1B-C2B	2.53	1.49	1.43
31	K	101	BCR	C39-C30	-2.53	1.48	1.53
22	q	308	CLA	C1B-C2B	2.52	1.49	1.43
22	S	309	CLA	C1B-C2B	2.52	1.49	1.43
22	a	406	CLA	MG-NB	-2.52	2.00	2.05
22	s	309	CLA	C1B-C2B	2.52	1.49	1.43
34	W	201	LMG	O7-C8	-2.52	1.40	1.46
26	3	315	CHL	C3B-C4B	2.52	1.48	1.42
22	2	307	CLA	C1B-C2B	2.52	1.49	1.43
22	b	606	CLA	C3B-C4B	2.52	1.48	1.42
22	5	305	CLA	C1B-C2B	2.52	1.49	1.43
22	C	508	CLA	MG-NB	-2.52	2.00	2.05
22	C	514	CLA	MG-NB	-2.52	2.00	2.05
22	p	308	CLA	C1B-C2B	2.52	1.49	1.43
26	U	313	CHL	C3B-C4B	2.52	1.48	1.42
22	V	302	CLA	C1B-C2B	2.52	1.49	1.43
27	r	618	NEX	C1-C6	-2.52	1.50	1.54
26	u	313	CHL	C3B-C4B	2.52	1.48	1.42
22	v	306	CLA	C1B-C2B	2.52	1.49	1.43
22	Q	308	CLA	C1B-C2B	2.52	1.49	1.43
26	p	318	CHL	C4B-NB	-2.52	1.34	1.37
26	u	318	CHL	C1D-C2D	2.52	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	304	CLA	C1B-C2B	2.52	1.49	1.43
26	5	317	CHL	C3B-C4B	2.52	1.48	1.42
25	b	623	LHG	O8-C23	2.52	1.40	1.33
22	g	307	CLA	C1B-C2B	2.52	1.49	1.43
22	R	307	CLA	C1B-C2B	2.51	1.49	1.43
30	a	407	PHO	CAC-C3C	-2.51	1.47	1.51
22	A	408	CLA	MG-NB	-2.51	2.00	2.05
22	c	514	CLA	C1B-C2B	2.51	1.49	1.43
22	b	604	CLA	C3B-C4B	2.51	1.48	1.42
22	r	605	CLA	C1B-C2B	2.51	1.49	1.43
22	c	513	CLA	MG-NB	-2.51	2.00	2.05
26	U	314	CHL	C1D-ND	-2.51	1.34	1.37
30	A	407	PHO	CMB-C2B	-2.51	1.46	1.51
22	b	602	CLA	MG-NB	-2.51	2.00	2.05
25	B	623	LHG	O8-C23	2.51	1.40	1.33
26	6	314	CHL	C3B-C4B	2.51	1.48	1.42
26	6	313	CHL	C1B-NB	-2.51	1.34	1.37
22	A	406	CLA	MG-NB	-2.51	2.00	2.05
22	r	606	CLA	C1B-C2B	2.51	1.49	1.43
26	N	314	CHL	C1B-NB	-2.51	1.34	1.37
26	6	301	CHL	MG-NA	-2.51	2.00	2.06
30	A	407	PHO	CMD-C2D	-2.51	1.46	1.51
25	c	523	LHG	O8-C23	2.51	1.40	1.33
22	U	304	CLA	C3B-C4B	2.51	1.48	1.42
26	1	316	CHL	MG-NA	-2.51	2.00	2.06
26	v	315	CHL	MG-NA	-2.51	2.00	2.06
25	C	524	LHG	O8-C23	2.51	1.40	1.33
22	s	308	CLA	C1B-C2B	2.51	1.49	1.43
22	N	308	CLA	C1B-C2B	2.50	1.49	1.43
22	p	304	CLA	C1B-C2B	2.50	1.49	1.43
22	S	308	CLA	C1B-C2B	2.50	1.49	1.43
22	B	602	CLA	C1B-C2B	2.50	1.49	1.43
22	1	303	CLA	C3B-C4B	2.50	1.48	1.42
26	6	317	CHL	MG-NA	-2.50	2.00	2.06
22	c	507	CLA	C3B-C4B	2.50	1.48	1.42
22	B	605	CLA	CMB-C2B	-2.50	1.45	1.50
25	4	312	LHG	O8-C23	2.50	1.40	1.33
34	C	502	LMG	O8-C28	2.50	1.40	1.33
26	p	316	CHL	MG-NA	-2.50	2.00	2.06
31	k	101	BCR	C39-C30	-2.50	1.48	1.53
22	4	308	CLA	C1B-C2B	2.50	1.49	1.43
22	B	607	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	C1B-C2B	2.50	1.49	1.43
24	g	309	XAT	C4-C3	2.50	1.55	1.52
22	6	307	CLA	C1B-C2B	2.50	1.49	1.43
22	x	201	CLA	C1B-C2B	2.50	1.49	1.43
22	B	604	CLA	C3B-C4B	2.50	1.48	1.42
26	6	317	CHL	C4C-C3C	2.50	1.49	1.45
36	a	416	DGD	O1G-C1A	2.50	1.40	1.33
26	2	316	CHL	MG-NA	-2.50	2.00	2.06
26	G	311	CHL	C3D-C2D	2.50	1.45	1.39
22	b	605	CLA	CMB-C2B	-2.50	1.45	1.50
25	4	312	LHG	O7-C5	-2.50	1.40	1.46
22	u	304	CLA	MG-NB	-2.50	2.00	2.05
22	6	308	CLA	C1B-C2B	2.50	1.49	1.43
25	1	312	LHG	O8-C23	2.50	1.40	1.33
26	3	316	CHL	MG-NA	-2.50	2.00	2.06
26	N	315	CHL	C1B-NB	-2.50	1.34	1.37
26	s	316	CHL	C4B-NB	-2.50	1.34	1.37
26	4	316	CHL	C3B-C4B	2.50	1.48	1.42
36	A	414	DGD	O1G-C1A	2.49	1.40	1.33
22	v	301	CLA	MG-NB	-2.49	2.00	2.05
26	p	315	CHL	C1D-ND	-2.49	1.34	1.37
26	P	319	CHL	C1B-NB	-2.49	1.34	1.37
34	c	520	LMG	O7-C8	-2.49	1.40	1.46
26	S	316	CHL	C3B-C4B	2.49	1.48	1.42
33	D	405	PL9	O1-C4	-2.49	1.17	1.23
26	G	314	CHL	C3B-C4B	2.49	1.48	1.42
26	5	317	CHL	C1B-C2B	2.49	1.49	1.43
22	5	305	CLA	C4D-ND	-2.49	1.34	1.37
22	B	602	CLA	MG-NB	-2.49	2.00	2.05
31	d	403	BCR	C39-C30	-2.49	1.48	1.53
22	B	603	CLA	C1B-C2B	2.49	1.49	1.43
34	b	624	LMG	O7-C8	-2.49	1.40	1.46
22	c	508	CLA	C3B-C4B	2.49	1.48	1.42
26	p	316	CHL	C3B-C4B	2.49	1.48	1.42
26	p	314	CHL	MG-NA	-2.49	2.00	2.06
26	4	314	CHL	MG-NA	-2.49	2.00	2.06
22	C	513	CLA	MG-NB	-2.49	2.00	2.05
26	V	318	CHL	C3B-C4B	2.49	1.48	1.42
26	G	312	CHL	C1B-C2B	2.49	1.49	1.43
26	Q	313	CHL	C1B-C2B	2.49	1.49	1.43
26	S	316	CHL	C1B-NB	-2.49	1.34	1.37
26	3	312	CHL	C1B-NB	-2.49	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	314	CHL	C1D-ND	-2.49	1.34	1.37
26	g	313	CHL	C3B-C4B	2.49	1.48	1.42
22	u	307	CLA	C1B-C2B	2.49	1.49	1.43
25	2	312	LHG	O7-C5	-2.49	1.40	1.46
22	a	408	CLA	C4B-NB	2.49	1.40	1.37
22	P	306	CLA	C4D-ND	-2.49	1.34	1.37
27	s	317	NEX	C7-C8	-2.49	1.27	1.32
22	b	615	CLA	C3B-C4B	2.49	1.48	1.42
22	5	306	CLA	C1B-C2B	2.49	1.49	1.43
26	4	315	CHL	C4B-NB	-2.49	1.34	1.37
26	V	315	CHL	C1B-NB	-2.49	1.34	1.37
26	P	314	CHL	C1B-NB	-2.49	1.34	1.37
22	s	303	CLA	C1B-C2B	2.49	1.49	1.43
26	q	315	CHL	C1B-NB	-2.49	1.34	1.37
22	2	306	CLA	C1B-C2B	2.49	1.49	1.43
26	v	314	CHL	C1B-C2B	2.48	1.49	1.43
26	p	317	CHL	C3B-C4B	2.48	1.48	1.42
26	g	314	CHL	C3B-C4B	2.48	1.48	1.42
25	A	413	LHG	O7-C7	2.48	1.41	1.34
26	q	311	CHL	MG-NA	-2.48	2.00	2.06
22	s	309	CLA	C3B-C4B	2.48	1.48	1.42
22	R	303	CLA	C1B-C2B	2.48	1.49	1.43
36	b	601	DGD	O1G-C1A	2.48	1.40	1.33
26	s	313	CHL	C1B-NB	-2.48	1.34	1.37
26	Q	316	CHL	MG-NA	-2.48	2.00	2.06
22	c	512	CLA	MG-NB	-2.48	2.00	2.05
34	w	201	LMG	O7-C8	-2.48	1.40	1.46
22	b	613	CLA	MG-NB	-2.48	2.00	2.05
22	p	303	CLA	C1B-C2B	2.48	1.49	1.43
26	n	314	CHL	C1B-C2B	2.48	1.49	1.43
26	n	318	CHL	C4C-C3C	2.48	1.49	1.45
22	C	509	CLA	C3B-C4B	2.48	1.48	1.42
22	s	306	CLA	CMD-C2D	-2.48	1.45	1.50
22	3	304	CLA	C1B-C2B	2.48	1.49	1.43
26	3	313	CHL	C1B-C2B	2.48	1.49	1.43
22	C	515	CLA	C1B-C2B	2.48	1.49	1.43
22	5	307	CLA	C1B-C2B	2.48	1.49	1.43
26	v	316	CHL	C3B-C4B	2.48	1.48	1.42
25	n	312	LHG	O8-C23	2.48	1.40	1.33
22	G	301	CLA	MG-NB	-2.48	2.00	2.05
22	V	307	CLA	C1B-C2B	2.48	1.49	1.43
22	U	304	CLA	MG-NB	-2.48	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	415	LHG	O7-C7	2.48	1.41	1.34
30	a	407	PHO	CMB-C2B	-2.48	1.46	1.51
22	S	303	CLA	C1B-C2B	2.48	1.49	1.43
33	d	404	PL9	O1-C4	-2.48	1.18	1.23
25	n	312	LHG	O7-C5	-2.48	1.40	1.46
26	p	320	CHL	C3B-C4B	2.47	1.48	1.42
26	3	315	CHL	C1D-ND	-2.47	1.34	1.37
26	V	318	CHL	C4B-NB	-2.47	1.34	1.37
22	4	305	CLA	MG-NB	-2.47	2.00	2.05
22	B	614	CLA	MG-NB	-2.47	2.00	2.05
26	S	316	CHL	C4B-NB	-2.47	1.34	1.37
34	C	521	LMG	O7-C8	-2.47	1.40	1.46
22	c	507	CLA	MG-NB	-2.47	2.00	2.05
26	g	314	CHL	C1B-C2B	2.47	1.49	1.43
34	c	501	LMG	O8-C28	2.47	1.40	1.33
26	v	315	CHL	C1B-NB	-2.47	1.34	1.37
22	P	304	CLA	C1B-C2B	2.47	1.49	1.43
22	c	506	CLA	C4B-NB	2.47	1.40	1.37
24	G	309	XAT	C4-C3	2.47	1.55	1.52
26	V	316	CHL	C3B-C4B	2.47	1.48	1.42
22	X	202	CLA	C1B-C2B	2.47	1.49	1.43
22	b	602	CLA	C1B-C2B	2.47	1.49	1.43
26	r	615	CHL	C1B-NB	-2.47	1.34	1.37
22	4	301	CLA	MG-NB	-2.47	2.00	2.05
22	b	603	CLA	C1B-C2B	2.47	1.49	1.43
22	N	305	CLA	C1B-C2B	2.47	1.49	1.43
26	2	318	CHL	C1B-NB	-2.47	1.34	1.37
26	U	313	CHL	C4B-NB	-2.47	1.34	1.37
22	b	614	CLA	C1B-C2B	2.47	1.49	1.43
26	p	319	CHL	C1B-NB	-2.47	1.34	1.37
26	P	316	CHL	MG-NA	-2.47	2.00	2.06
22	b	617	CLA	CMC-C2C	-2.47	1.45	1.50
25	r	613	LHG	O7-C5	-2.47	1.40	1.46
36	B	601	DGD	O1G-C1A	2.47	1.40	1.33
26	3	315	CHL	C1D-C2D	2.47	1.50	1.45
26	p	317	CHL	MG-NA	-2.47	2.00	2.06
26	2	318	CHL	C4B-NB	-2.47	1.34	1.37
26	4	315	CHL	C1D-ND	-2.47	1.34	1.37
26	6	316	CHL	C1D-ND	-2.47	1.34	1.37
26	n	318	CHL	C1B-NB	-2.47	1.34	1.37
26	Q	314	CHL	C1B-C2B	2.47	1.49	1.43
22	C	515	CLA	MG-NB	-2.47	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p	314	CHL	C1B-NB	-2.46	1.34	1.37
24	r	612	XAT	C4-C3	2.46	1.55	1.52
26	n	317	CHL	C1B-C2B	2.46	1.49	1.43
22	4	304	CLA	MG-NB	-2.46	2.00	2.05
26	3	314	CHL	C4B-NB	-2.46	1.34	1.37
26	P	315	CHL	C1B-C2B	2.46	1.49	1.43
22	4	304	CLA	C1B-C2B	2.46	1.49	1.43
22	C	508	CLA	C3B-C4B	2.46	1.48	1.42
26	n	315	CHL	C1B-NB	-2.46	1.34	1.37
26	s	316	CHL	C3B-C4B	2.46	1.48	1.42
26	n	314	CHL	C1B-NB	-2.46	1.34	1.37
22	3	307	CLA	C1B-C2B	2.46	1.49	1.43
22	R	306	CLA	C1B-C2B	2.46	1.49	1.43
22	b	605	CLA	C1B-C2B	2.46	1.49	1.43
22	1	301	CLA	MG-NB	-2.46	2.00	2.05
22	A	405	CLA	MG-NB	-2.46	2.00	2.05
26	N	314	CHL	C1B-C2B	2.46	1.49	1.43
22	a	408	CLA	C1B-NB	-2.46	1.34	1.37
26	S	313	CHL	C1B-NB	-2.46	1.34	1.37
22	1	305	CLA	MG-NB	-2.46	2.00	2.05
26	6	313	CHL	C4C-C3C	2.46	1.49	1.45
25	v	312	LHG	O8-C23	2.46	1.40	1.33
22	A	408	CLA	C4B-NB	2.46	1.40	1.37
26	q	313	CHL	C1B-C2B	2.46	1.49	1.43
22	U	307	CLA	C1B-C2B	2.46	1.49	1.43
22	B	615	CLA	C3B-C4B	2.46	1.48	1.42
22	Q	304	CLA	C1B-C2B	2.46	1.49	1.43
26	v	313	CHL	MG-NA	-2.46	2.00	2.06
26	n	316	CHL	C3B-C4B	2.45	1.48	1.42
22	r	602	CLA	C1B-C2B	2.45	1.49	1.43
22	c	514	CLA	MG-NB	-2.45	2.00	2.05
26	p	319	CHL	C4B-NB	-2.45	1.34	1.37
26	U	315	CHL	C3D-C2D	2.45	1.45	1.39
22	b	614	CLA	C3B-C4B	2.45	1.48	1.42
22	U	307	CLA	C3B-C4B	2.45	1.48	1.42
22	S	306	CLA	CMD-C2D	-2.45	1.45	1.50
22	1	308	CLA	C1B-C2B	2.45	1.49	1.43
26	6	313	CHL	C4B-NB	-2.45	1.34	1.37
26	p	317	CHL	C1B-NB	-2.45	1.34	1.37
36	B	601	DGD	O1G-C1G	-2.45	1.39	1.45
26	6	316	CHL	C1D-C2D	2.45	1.50	1.45
22	5	302	CLA	C1B-C2B	2.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	317	CHL	C1B-C2B	2.45	1.49	1.43
26	2	316	CHL	C3B-C4B	2.45	1.48	1.42
22	Q	307	CLA	C1B-C2B	2.45	1.49	1.43
22	u	306	CLA	CMD-C2D	-2.45	1.45	1.50
33	D	405	PL9	O2-C1	-2.45	1.18	1.24
22	b	613	CLA	C1B-C2B	2.45	1.49	1.43
22	p	302	CLA	MG-NB	-2.45	2.00	2.05
26	N	317	CHL	C1B-C2B	2.45	1.49	1.43
26	6	317	CHL	C4B-NB	-2.45	1.34	1.37
25	q	310	LHG	O8-C23	2.45	1.40	1.33
22	B	613	CLA	MG-NB	-2.45	2.00	2.05
22	B	614	CLA	C3B-C4B	2.45	1.48	1.42
26	V	315	CHL	C1D-ND	-2.45	1.34	1.37
26	V	315	CHL	C3B-C4B	2.45	1.48	1.42
22	v	302	CLA	C1B-C2B	2.45	1.49	1.43
26	q	312	CHL	C1B-C2B	2.44	1.49	1.43
26	N	316	CHL	C3B-C4B	2.44	1.48	1.42
22	b	603	CLA	MG-NB	-2.44	2.00	2.05
26	u	316	CHL	MG-NA	-2.44	2.00	2.06
22	6	305	CLA	C1B-C2B	2.44	1.49	1.43
26	g	312	CHL	C1B-C2B	2.44	1.49	1.43
36	J	101	DGD	O1G-C1G	-2.44	1.39	1.45
22	4	305	CLA	C1B-C2B	2.44	1.49	1.43
27	R	301	NEX	C1-C6	-2.44	1.50	1.54
26	1	318	CHL	C1B-C2B	2.44	1.49	1.43
22	C	506	CLA	MG-NB	-2.44	2.00	2.05
22	B	605	CLA	C1B-C2B	2.44	1.49	1.43
26	6	315	CHL	C1B-NB	-2.44	1.34	1.37
26	S	315	CHL	C1B-C2B	2.44	1.49	1.43
26	P	318	CHL	C4B-NB	-2.44	1.34	1.37
26	u	313	CHL	MG-NA	-2.44	2.00	2.06
26	q	314	CHL	C1D-C2D	2.44	1.50	1.45
22	B	614	CLA	C1B-C2B	2.44	1.49	1.43
22	n	305	CLA	C1D-ND	2.44	1.40	1.37
22	b	611	CLA	MG-NB	-2.44	2.01	2.05
22	B	603	CLA	MG-NB	-2.44	2.01	2.05
22	X	202	CLA	MG-NB	-2.44	2.01	2.05
34	A	411	LMG	O1-C1	-2.44	1.36	1.40
26	2	316	CHL	C4B-NB	-2.44	1.34	1.37
26	2	317	CHL	C1B-C2B	2.44	1.49	1.43
24	R	313	XAT	C4-C3	2.44	1.55	1.52
26	s	315	CHL	C1B-C2B	2.44	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	408	CLA	MG-NB	-2.44	2.01	2.05
22	P	306	CLA	C1D-ND	2.43	1.40	1.37
22	S	306	CLA	C1B-C2B	2.43	1.49	1.43
26	G	313	CHL	C1B-C2B	2.43	1.49	1.43
26	P	318	CHL	C1B-NB	-2.43	1.34	1.37
26	3	313	CHL	C3B-C4B	2.43	1.48	1.42
22	V	306	CLA	C1B-C2B	2.43	1.49	1.43
24	r	612	XAT	C18-C5	2.43	1.55	1.51
22	A	408	CLA	C1B-NB	-2.43	1.34	1.37
22	B	603	CLA	C3B-C4B	2.43	1.48	1.42
36	b	601	DGD	O1G-C1G	-2.43	1.39	1.45
26	g	313	CHL	C1B-C2B	2.43	1.49	1.43
25	5	312	LHG	O8-C23	2.43	1.40	1.33
22	b	603	CLA	C3B-C4B	2.43	1.48	1.42
22	U	303	CLA	MG-NB	-2.43	2.01	2.05
26	N	316	CHL	C1B-C2B	2.43	1.49	1.43
25	c	522	LHG	O8-C23	2.43	1.40	1.33
22	C	512	CLA	CMD-C2D	-2.43	1.45	1.50
26	v	314	CHL	C4C-C3C	2.43	1.49	1.45
26	s	316	CHL	C1B-C2B	2.43	1.49	1.43
26	4	313	CHL	C3B-C4B	2.43	1.48	1.42
26	u	313	CHL	C4B-NB	-2.43	1.34	1.37
22	1	306	CLA	MG-NB	-2.43	2.01	2.05
30	d	401	PHO	CAC-C3C	-2.43	1.47	1.51
22	B	610	CLA	C1B-C2B	2.43	1.49	1.43
26	N	316	CHL	MG-NA	-2.43	2.00	2.06
22	1	304	CLA	MG-NB	-2.43	2.01	2.05
26	V	314	CHL	C1B-NB	-2.43	1.34	1.37
22	1	307	CLA	C1B-C2B	2.43	1.49	1.43
22	4	307	CLA	C1B-C2B	2.43	1.49	1.43
26	g	312	CHL	MG-NA	-2.43	2.00	2.06
22	U	305	CLA	C1B-C2B	2.43	1.49	1.43
26	u	316	CHL	C3D-C2D	2.43	1.45	1.39
22	b	604	CLA	MG-NB	-2.43	2.01	2.05
22	c	511	CLA	CMD-C2D	-2.43	1.45	1.50
26	2	314	CHL	C1B-C2B	2.43	1.49	1.43
22	p	306	CLA	C4D-ND	-2.43	1.34	1.37
26	q	314	CHL	C1D-ND	-2.42	1.34	1.37
27	r	617	NEX	C1-C6	-2.42	1.50	1.54
26	N	317	CHL	MG-NA	-2.42	2.00	2.06
26	V	314	CHL	C4C-C3C	2.42	1.49	1.45
26	5	316	CHL	C4B-NB	-2.42	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	315	CHL	MG-NA	-2.42	2.00	2.06
26	1	314	CHL	C1B-C2B	2.42	1.49	1.43
26	n	318	CHL	C1B-C2B	2.42	1.49	1.43
22	N	305	CLA	C1D-ND	2.42	1.40	1.37
22	V	303	CLA	MG-NB	-2.42	2.01	2.05
25	g	310	LHG	O7-C5	-2.42	1.40	1.46
25	s	312	LHG	O8-C23	2.42	1.40	1.33
22	b	612	CLA	C1B-C2B	2.42	1.49	1.43
22	A	404	CLA	CMD-C2D	-2.42	1.45	1.50
22	2	301	CLA	MG-NB	-2.42	2.01	2.05
26	3	316	CHL	C4B-NB	-2.42	1.34	1.37
22	a	404	CLA	CMD-C2D	-2.42	1.45	1.50
25	V	312	LHG	O8-C23	2.42	1.40	1.33
22	S	306	CLA	MG-NB	-2.42	2.01	2.05
26	N	317	CHL	C4C-C3C	2.42	1.49	1.45
34	a	412	LMG	O1-C1	-2.42	1.36	1.40
26	s	316	CHL	C1B-NB	-2.42	1.34	1.37
22	B	613	CLA	C1B-C2B	2.42	1.48	1.43
26	5	314	CHL	C1B-C2B	2.42	1.48	1.43
22	u	305	CLA	C1B-C2B	2.42	1.48	1.43
26	5	316	CHL	C3B-C4B	2.42	1.48	1.42
25	R	314	LHG	O7-C5	-2.42	1.40	1.46
34	B	624	LMG	O7-C8	-2.42	1.40	1.46
22	c	503	CLA	MG-NB	-2.42	2.01	2.05
22	v	307	CLA	C1B-C2B	2.42	1.48	1.43
26	1	313	CHL	C1D-ND	-2.42	1.34	1.37
22	1	305	CLA	C1B-C2B	2.42	1.48	1.43
30	d	401	PHO	CMB-C2B	-2.42	1.46	1.51
22	g	301	CLA	MG-NB	-2.42	2.01	2.05
26	S	315	CHL	C4B-NB	-2.41	1.34	1.37
24	R	313	XAT	C18-C5	2.41	1.55	1.51
22	U	306	CLA	CMD-C2D	-2.41	1.45	1.50
22	s	301	CLA	CHC-C1C	2.41	1.43	1.38
22	B	604	CLA	MG-NB	-2.41	2.01	2.05
26	3	312	CHL	C4C-C3C	2.41	1.49	1.45
22	B	611	CLA	MG-NB	-2.41	2.01	2.05
25	S	312	LHG	O8-C23	2.41	1.40	1.33
25	C	523	LHG	O8-C23	2.41	1.40	1.33
26	P	317	CHL	C1B-NB	-2.41	1.34	1.37
26	1	317	CHL	C3B-C4B	2.41	1.48	1.42
26	G	313	CHL	C3B-C4B	2.41	1.48	1.42
30	D	401	PHO	CAC-C3C	-2.41	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	616	CLA	C3B-C4B	2.41	1.48	1.42
33	d	404	PL9	O2-C1	-2.41	1.18	1.24
22	b	610	CLA	C1B-C2B	2.41	1.48	1.43
26	Q	315	CHL	C1B-C2B	2.41	1.48	1.43
26	Q	316	CHL	C1B-C2B	2.41	1.48	1.43
22	x	201	CLA	MG-NB	-2.41	2.01	2.05
22	B	617	CLA	CMC-C2C	-2.41	1.45	1.50
26	U	317	CHL	C3B-C4B	2.41	1.48	1.42
25	Q	310	LHG	O8-C23	2.41	1.40	1.33
25	g	310	LHG	O8-C23	2.41	1.40	1.33
22	4	302	CLA	C1B-C2B	2.41	1.48	1.43
26	4	314	CHL	C1B-NB	-2.41	1.34	1.37
26	Q	316	CHL	C1B-NB	-2.41	1.34	1.37
22	q	304	CLA	C1B-C2B	2.41	1.48	1.43
26	S	316	CHL	C1B-C2B	2.41	1.48	1.43
22	B	608	CLA	MG-NB	-2.41	2.01	2.05
26	q	312	CHL	C4C-C3C	2.41	1.49	1.45
26	V	316	CHL	C1B-C2B	2.41	1.48	1.43
26	Q	312	CHL	C1B-C2B	2.41	1.48	1.43
26	G	311	CHL	C1B-NB	-2.41	1.34	1.37
22	B	615	CLA	C1B-C2B	2.41	1.48	1.43
25	2	312	LHG	O8-C23	2.41	1.40	1.33
26	V	318	CHL	MG-NA	-2.40	2.00	2.06
36	A	414	DGD	O1G-C1G	-2.40	1.39	1.45
26	p	315	CHL	C1B-C2B	2.40	1.48	1.43
22	B	609	CLA	CMB-C2B	-2.40	1.45	1.50
22	c	504	CLA	C1B-C2B	2.40	1.48	1.43
26	3	313	CHL	C1D-ND	-2.40	1.34	1.37
26	N	314	CHL	C4C-C3C	2.40	1.49	1.45
22	V	304	CLA	C1B-C2B	2.40	1.48	1.43
22	s	306	CLA	MG-NB	-2.40	2.01	2.05
22	g	304	CLA	C1B-C2B	2.40	1.48	1.43
26	3	314	CHL	C1B-C2B	2.40	1.48	1.43
26	2	316	CHL	C1B-NB	-2.40	1.34	1.37
26	6	301	CHL	C4B-NB	-2.40	1.34	1.37
22	C	506	CLA	C1B-C2B	2.40	1.48	1.43
26	p	316	CHL	C1B-C2B	2.40	1.48	1.43
22	a	405	CLA	MG-NB	-2.40	2.01	2.05
26	1	314	CHL	C4B-NB	-2.40	1.34	1.37
26	1	316	CHL	C1B-NB	-2.40	1.34	1.37
26	p	319	CHL	C1B-C2B	2.40	1.48	1.43
31	a	409	BCR	C16-C17	2.40	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	W	201	LMG	O1-C1	-2.40	1.36	1.40
22	P	302	CLA	MG-NB	-2.40	2.01	2.05
26	1	315	CHL	C1D-ND	-2.40	1.34	1.37
31	A	409	BCR	C16-C17	2.40	1.50	1.43
22	u	306	CLA	MG-NB	-2.40	2.01	2.05
26	v	318	CHL	C1B-C2B	2.39	1.48	1.43
26	q	311	CHL	C1B-C2B	2.39	1.48	1.43
36	C	519	DGD	O5D-C1E	-2.39	1.36	1.40
22	b	615	CLA	C1B-C2B	2.39	1.48	1.43
22	c	513	CLA	C1B-C2B	2.39	1.48	1.43
36	c	517	DGD	O5D-C1E	-2.39	1.36	1.40
26	g	312	CHL	C1B-NB	-2.39	1.34	1.37
22	c	505	CLA	MG-NB	-2.39	2.01	2.05
26	u	313	CHL	C1B-C2B	2.39	1.48	1.43
26	3	316	CHL	C3B-C4B	2.39	1.48	1.42
26	P	317	CHL	C1B-C2B	2.39	1.48	1.43
31	B	618	BCR	C16-C17	2.39	1.50	1.43
26	s	315	CHL	C4B-NB	-2.39	1.34	1.37
30	D	401	PHO	CMB-C2B	-2.39	1.46	1.51
22	G	304	CLA	C1B-C2B	2.39	1.48	1.43
26	4	314	CHL	C1B-C2B	2.39	1.48	1.43
26	U	316	CHL	C3B-C4B	2.39	1.48	1.42
26	V	315	CHL	C4B-NB	-2.39	1.34	1.37
26	n	315	CHL	C1B-C2B	2.39	1.48	1.43
22	s	305	CLA	MG-NB	-2.39	2.01	2.05
26	n	316	CHL	C1B-C2B	2.39	1.48	1.43
26	V	313	CHL	C1B-C2B	2.39	1.48	1.43
22	u	308	CLA	C1B-C2B	2.39	1.48	1.43
36	c	519	DGD	O1G-C1G	-2.39	1.39	1.45
22	v	303	CLA	MG-NB	-2.39	2.01	2.05
26	1	316	CHL	C1B-C2B	2.39	1.48	1.43
26	3	316	CHL	C4C-C3C	2.39	1.49	1.45
22	c	508	CLA	MG-NB	-2.39	2.01	2.05
22	s	306	CLA	C1B-C2B	2.39	1.48	1.43
26	G	316	CHL	C1B-C2B	2.39	1.48	1.43
26	3	312	CHL	C4B-NB	-2.38	1.34	1.37
26	p	317	CHL	C1B-C2B	2.38	1.48	1.43
26	1	315	CHL	C4B-NB	-2.38	1.34	1.37
26	n	317	CHL	C4B-NB	-2.38	1.34	1.37
26	Q	311	CHL	MG-NA	-2.38	2.00	2.06
22	u	303	CLA	MG-NB	-2.38	2.01	2.05
26	4	317	CHL	C3B-C4B	2.38	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	315	CHL	C1D-C2D	2.38	1.50	1.45
34	d	407	LMG	O7-C8	-2.38	1.40	1.46
26	6	301	CHL	C1B-C2B	2.38	1.48	1.43
22	C	507	CLA	C3B-C4B	2.38	1.48	1.42
26	5	318	CHL	C3B-C4B	2.38	1.48	1.42
26	Q	313	CHL	C4C-C3C	2.38	1.49	1.45
34	D	408	LMG	O7-C8	-2.38	1.40	1.46
26	v	315	CHL	C1D-ND	-2.38	1.34	1.37
22	b	616	CLA	C3B-C4B	2.38	1.48	1.42
22	C	505	CLA	C1B-C2B	2.38	1.48	1.43
26	3	314	CHL	C1B-NB	-2.38	1.34	1.37
22	p	306	CLA	C1D-ND	2.38	1.40	1.37
26	p	318	CHL	C3B-C4B	2.38	1.48	1.42
22	4	306	CLA	C1B-C2B	2.38	1.48	1.43
22	S	301	CLA	CHC-C1C	2.38	1.43	1.38
32	a	410	SQD	O2-C2	-2.38	1.37	1.43
22	q	307	CLA	C1B-C2B	2.38	1.48	1.43
26	2	315	CHL	C1B-NB	-2.38	1.34	1.37
26	V	315	CHL	C1B-C2B	2.38	1.48	1.43
22	u	307	CLA	C3B-C4B	2.38	1.48	1.42
22	N	303	CLA	MG-NB	-2.38	2.01	2.05
26	p	320	CHL	C1B-C2B	2.38	1.48	1.43
25	G	310	LHG	O8-C23	2.38	1.40	1.33
22	B	612	CLA	C1B-C2B	2.38	1.48	1.43
25	N	312	LHG	O8-C23	2.38	1.40	1.33
26	v	318	CHL	C3B-C4B	2.38	1.48	1.42
22	S	305	CLA	MG-NB	-2.38	2.01	2.05
22	B	607	CLA	CMD-C2D	-2.38	1.45	1.50
26	1	317	CHL	C1B-NB	-2.38	1.34	1.37
22	C	509	CLA	MG-NB	-2.37	2.01	2.05
22	B	617	CLA	MG-NB	-2.37	2.01	2.05
26	3	316	CHL	C1B-NB	-2.37	1.34	1.37
26	6	317	CHL	C1B-C2B	2.37	1.48	1.43
26	U	319	CHL	C1B-C2B	2.37	1.48	1.43
22	C	507	CLA	C4B-NB	2.37	1.40	1.37
26	U	313	CHL	C1B-NB	-2.37	1.34	1.37
22	c	505	CLA	C1B-C2B	2.37	1.48	1.43
26	s	314	CHL	C1B-C2B	2.37	1.48	1.43
22	c	506	CLA	C3B-C4B	2.37	1.48	1.42
26	r	619	CHL	C1B-NB	-2.37	1.34	1.37
26	U	315	CHL	C1B-NB	-2.37	1.34	1.37
26	S	314	CHL	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	315	CHL	MG-NA	-2.37	2.00	2.06
26	5	318	CHL	C4B-NB	-2.37	1.34	1.37
22	u	301	CLA	MG-NB	-2.37	2.01	2.05
26	6	314	CHL	C4C-C3C	2.37	1.49	1.45
26	6	315	CHL	C4B-NB	-2.37	1.34	1.37
26	P	314	CHL	C1B-C2B	2.37	1.48	1.43
26	G	314	CHL	C1B-C2B	2.37	1.48	1.43
31	c	515	BCR	C16-C17	2.37	1.50	1.43
22	q	305	CLA	MG-NB	-2.37	2.01	2.05
26	g	312	CHL	C4C-C3C	2.37	1.49	1.45
22	1	303	CLA	CMB-C2B	-2.37	1.45	1.50
26	u	317	CHL	C3B-C4B	2.37	1.48	1.42
26	1	318	CHL	C3B-C4B	2.37	1.48	1.42
26	g	316	CHL	C1B-C2B	2.37	1.48	1.43
26	G	312	CHL	MG-NA	-2.37	2.00	2.06
26	s	314	CHL	C4C-C3C	2.37	1.49	1.45
26	1	316	CHL	C3B-C4B	2.37	1.48	1.42
26	q	313	CHL	C3B-C4B	2.37	1.48	1.42
25	p	313	LHG	O8-C23	2.37	1.40	1.33
22	A	404	CLA	C4B-NB	2.37	1.40	1.37
26	4	316	CHL	C1B-NB	-2.37	1.34	1.37
22	C	504	CLA	C3B-C4B	2.37	1.48	1.42
26	5	316	CHL	C1B-C2B	2.37	1.48	1.43
26	G	314	CHL	C1B-NB	-2.36	1.34	1.37
31	C	517	BCR	C16-C17	2.36	1.50	1.43
22	C	514	CLA	C1B-C2B	2.36	1.48	1.43
25	G	310	LHG	O7-C5	-2.36	1.40	1.46
34	w	201	LMG	O1-C1	-2.36	1.36	1.40
22	b	607	CLA	CMD-C2D	-2.36	1.45	1.50
22	C	504	CLA	MG-NB	-2.36	2.01	2.05
26	1	316	CHL	C4B-NB	-2.36	1.34	1.37
34	c	520	LMG	O1-C1	-2.36	1.36	1.40
22	b	607	CLA	MG-NB	-2.36	2.01	2.05
22	b	608	CLA	MG-NB	-2.36	2.01	2.05
26	5	318	CHL	C1B-NB	-2.36	1.34	1.37
26	v	318	CHL	C4C-C3C	2.36	1.49	1.45
26	v	315	CHL	C1B-C2B	2.36	1.48	1.43
26	5	316	CHL	C1B-NB	-2.36	1.34	1.37
25	D	407	LHG	O8-C23	2.36	1.40	1.33
25	N	312	LHG	O7-C5	-2.36	1.40	1.46
26	4	316	CHL	C1B-C2B	2.36	1.48	1.43
26	N	315	CHL	C1B-C2B	2.36	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	303	CLA	C1B-C2B	2.36	1.48	1.43
31	b	618	BCR	C16-C17	2.36	1.50	1.43
26	G	312	CHL	C4B-NB	-2.36	1.34	1.37
26	S	314	CHL	C4C-C3C	2.36	1.49	1.45
22	V	301	CLA	MG-NB	-2.36	2.01	2.05
25	l	101	LHG	O8-C23	2.36	1.40	1.33
26	2	318	CHL	MG-NA	-2.36	2.00	2.06
26	V	318	CHL	C1B-C2B	2.36	1.48	1.43
22	D	403	CLA	MG-ND	-2.36	2.01	2.05
22	b	609	CLA	CMB-C2B	-2.36	1.45	1.50
22	5	301	CLA	MG-NB	-2.36	2.01	2.05
26	v	316	CHL	C1B-C2B	2.36	1.48	1.43
22	U	301	CLA	MG-NB	-2.36	2.01	2.05
25	A	413	LHG	O8-C6	-2.36	1.39	1.45
22	C	503	CLA	C1B-C2B	2.36	1.48	1.43
22	3	303	CLA	CMB-C2B	-2.36	1.45	1.50
22	U	308	CLA	C1B-C2B	2.36	1.48	1.43
26	P	317	CHL	C4B-NB	-2.36	1.34	1.37
22	U	304	CLA	CMB-C2B	-2.36	1.45	1.50
22	C	510	CLA	MG-NB	-2.35	2.01	2.05
22	b	616	CLA	MG-NB	-2.35	2.01	2.05
36	a	416	DGD	O1G-C1G	-2.35	1.39	1.45
26	p	318	CHL	C1B-C2B	2.35	1.48	1.43
22	B	608	CLA	C1B-C2B	2.35	1.48	1.43
26	G	314	CHL	C4B-NB	-2.35	1.34	1.37
22	U	306	CLA	C1B-C2B	2.35	1.48	1.43
22	B	605	CLA	MG-NB	-2.35	2.01	2.05
26	5	318	CHL	MG-NA	-2.35	2.00	2.06
22	n	302	CLA	C1B-C2B	2.35	1.48	1.43
26	P	319	CHL	C1B-C2B	2.35	1.48	1.43
25	P	313	LHG	O8-C23	2.35	1.40	1.33
26	g	314	CHL	C4B-NB	-2.35	1.34	1.37
22	b	613	CLA	CMD-C2D	-2.35	1.45	1.50
26	2	314	CHL	C4C-C3C	2.35	1.49	1.45
26	G	316	CHL	C3B-C4B	2.35	1.48	1.42
26	v	318	CHL	C4B-NB	-2.35	1.34	1.37
26	p	319	CHL	MG-NA	-2.35	2.00	2.06
22	A	405	CLA	CMD-C2D	-2.35	1.45	1.50
25	C	522	LHG	O8-C23	2.35	1.40	1.33
26	v	313	CHL	C1B-C2B	2.35	1.48	1.43
22	c	513	CLA	CMD-C2D	-2.35	1.45	1.50
26	6	317	CHL	C3B-C4B	2.35	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	315	CHL	C3B-C4B	2.35	1.48	1.42
26	R	315	CHL	C1B-NB	-2.35	1.34	1.37
22	b	617	CLA	C1B-C2B	2.35	1.48	1.43
26	2	316	CHL	C1B-C2B	2.35	1.48	1.43
22	B	609	CLA	CMD-C2D	-2.35	1.45	1.50
22	b	611	CLA	C1B-C2B	2.35	1.48	1.43
22	B	605	CLA	C3B-C4B	2.35	1.48	1.42
22	B	616	CLA	MG-NB	-2.35	2.01	2.05
22	2	304	CLA	C1B-C2B	2.35	1.48	1.43
26	N	315	CHL	C1D-ND	-2.35	1.34	1.37
33	A	410	PL9	O1-C4	-2.35	1.18	1.24
22	U	306	CLA	CMB-C2B	-2.35	1.45	1.50
25	L	101	LHG	O8-C23	2.35	1.40	1.33
26	6	301	CHL	C3B-C4B	2.35	1.48	1.42
26	Q	311	CHL	C1B-C2B	2.35	1.48	1.43
22	Q	301	CLA	MG-NB	-2.35	2.01	2.05
26	1	318	CHL	C1B-NB	-2.35	1.34	1.37
22	S	302	CLA	C1B-C2B	2.34	1.48	1.43
22	4	303	CLA	CMB-C2B	-2.34	1.45	1.50
34	C	521	LMG	O1-C1	-2.34	1.36	1.40
22	d	402	CLA	MG-ND	-2.34	2.01	2.05
22	n	303	CLA	C1B-C2B	2.34	1.48	1.43
26	2	318	CHL	C1B-C2B	2.34	1.48	1.43
22	P	307	CLA	MG-NB	-2.34	2.01	2.05
22	G	303	CLA	CMB-C2B	-2.34	1.45	1.50
22	g	303	CLA	CMB-C2B	-2.34	1.45	1.50
26	Q	312	CHL	C1B-NB	-2.34	1.34	1.37
22	c	509	CLA	MG-NB	-2.34	2.01	2.05
22	a	405	CLA	CMD-C2D	-2.34	1.45	1.50
26	u	316	CHL	C1B-C2B	2.34	1.48	1.43
26	Q	314	CHL	C4B-NB	-2.34	1.34	1.37
22	B	607	CLA	MG-NB	-2.34	2.01	2.05
32	C	501	SQD	O2-C2	-2.34	1.37	1.43
26	R	316	CHL	C4C-C3C	2.34	1.49	1.45
22	P	304	CLA	MG-NB	-2.34	2.01	2.05
22	S	308	CLA	MG-NB	-2.34	2.01	2.05
22	D	403	CLA	CMC-C2C	-2.34	1.45	1.50
26	3	313	CHL	C4C-C3C	2.34	1.49	1.45
26	2	315	CHL	C1B-C2B	2.34	1.48	1.43
26	6	315	CHL	C1B-C2B	2.34	1.48	1.43
26	q	314	CHL	C1B-C2B	2.34	1.48	1.43
26	u	317	CHL	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	C1B-C2B	2.33	1.48	1.43
22	C	511	CLA	C4B-NB	2.33	1.40	1.37
25	a	415	LHG	O8-C6	-2.33	1.39	1.45
22	3	303	CLA	MG-NB	-2.33	2.01	2.05
26	5	317	CHL	MG-NA	-2.33	2.00	2.06
36	c	518	DGD	O1G-C1G	-2.33	1.39	1.45
26	Q	312	CHL	C4C-C3C	2.33	1.49	1.45
26	G	312	CHL	C4C-C3C	2.33	1.49	1.45
26	4	317	CHL	C1B-NB	-2.33	1.34	1.37
26	S	315	CHL	C1D-ND	-2.33	1.34	1.37
26	U	314	CHL	C3B-C4B	2.33	1.48	1.42
22	Q	305	CLA	MG-NB	-2.33	2.01	2.05
26	4	313	CHL	C1B-C2B	2.33	1.48	1.43
26	q	315	CHL	C1B-C2B	2.33	1.48	1.43
26	5	316	CHL	C1D-ND	-2.33	1.34	1.37
22	c	509	CLA	CMD-C2D	-2.33	1.45	1.50
22	B	613	CLA	CMD-C2D	-2.33	1.45	1.50
26	4	316	CHL	MG-NA	-2.33	2.00	2.06
26	U	313	CHL	C1B-C2B	2.33	1.48	1.43
22	5	302	CLA	MG-NB	-2.33	2.01	2.05
26	g	314	CHL	C4C-C3C	2.33	1.49	1.45
26	Q	313	CHL	C3B-C4B	2.33	1.48	1.42
22	a	405	CLA	CMB-C2B	-2.33	1.45	1.50
26	g	314	CHL	C1B-NB	-2.33	1.34	1.37
26	g	316	CHL	C3B-C4B	2.33	1.48	1.42
25	d	406	LHG	O8-C23	2.33	1.40	1.33
26	6	314	CHL	C1B-C2B	2.32	1.48	1.43
26	g	311	CHL	C1B-C2B	2.32	1.48	1.43
22	Q	308	CLA	MG-NB	-2.32	2.01	2.05
26	g	313	CHL	C4C-C3C	2.32	1.49	1.45
26	6	316	CHL	C1B-C2B	2.32	1.48	1.43
26	R	315	CHL	C1B-C2B	2.32	1.48	1.43
22	v	307	CLA	MG-NB	-2.32	2.01	2.05
22	g	303	CLA	MG-NB	-2.32	2.01	2.05
26	6	301	CHL	C1B-NB	-2.32	1.34	1.37
26	p	316	CHL	C4B-NB	-2.32	1.34	1.37
22	b	608	CLA	C1B-C2B	2.32	1.48	1.43
22	v	304	CLA	C1B-C2B	2.32	1.48	1.43
22	C	513	CLA	C1B-C2B	2.32	1.48	1.43
22	6	307	CLA	MG-NB	-2.32	2.01	2.05
26	r	614	CHL	C1B-NB	-2.32	1.34	1.37
26	4	315	CHL	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	615	CHL	C4C-C3C	2.32	1.49	1.45
22	U	301	CLA	CMC-C2C	-2.32	1.45	1.50
22	q	301	CLA	MG-NB	-2.32	2.01	2.05
22	A	405	CLA	C1B-C2B	2.32	1.48	1.43
26	P	319	CHL	C3B-C4B	2.32	1.48	1.42
26	p	317	CHL	C4B-NB	-2.32	1.34	1.37
22	B	611	CLA	C1B-C2B	2.32	1.48	1.43
22	d	402	CLA	CMC-C2C	-2.32	1.45	1.50
22	a	404	CLA	C4B-NB	2.32	1.40	1.37
22	C	511	CLA	C1B-C2B	2.32	1.48	1.43
22	v	303	CLA	CMB-C2B	-2.32	1.45	1.50
22	d	402	CLA	C1B-C2B	2.32	1.48	1.43
22	1	307	CLA	MG-NB	-2.32	2.01	2.05
22	a	408	CLA	CMD-C2D	-2.32	1.45	1.50
22	s	301	CLA	C1B-C2B	2.32	1.48	1.43
26	g	316	CHL	MG-NA	-2.32	2.00	2.06
25	3	310	LHG	O8-C6	-2.32	1.39	1.45
22	6	302	CLA	MG-NB	-2.32	2.01	2.05
22	A	405	CLA	CMB-C2B	-2.32	1.45	1.50
22	B	604	CLA	CMB-C2B	-2.32	1.45	1.50
26	r	615	CHL	C1B-C2B	2.31	1.48	1.43
25	6	311	LHG	O8-C23	2.31	1.40	1.33
26	6	314	CHL	C4B-NB	-2.31	1.34	1.37
22	C	510	CLA	CMD-C2D	-2.31	1.45	1.50
26	U	316	CHL	C1B-C2B	2.31	1.48	1.43
22	S	309	CLA	CMD-C2D	-2.31	1.45	1.50
22	A	408	CLA	CMD-C2D	-2.31	1.45	1.50
22	N	301	CLA	MG-NB	-2.31	2.01	2.05
34	B	621	LMG	O1-C7	-2.31	1.39	1.43
26	2	313	CHL	C1B-C2B	2.31	1.48	1.43
22	u	301	CLA	CHC-C1C	2.31	1.43	1.38
22	1	302	CLA	C1B-C2B	2.31	1.48	1.43
26	4	313	CHL	C1D-ND	-2.31	1.34	1.37
22	b	605	CLA	C3B-C4B	2.31	1.48	1.42
22	c	503	CLA	C3B-C4B	2.31	1.48	1.42
22	A	406	CLA	C1B-C2B	2.31	1.48	1.43
22	s	302	CLA	C1B-C2B	2.31	1.48	1.43
26	G	311	CHL	C1B-C2B	2.31	1.48	1.43
26	2	318	CHL	C4C-C3C	2.31	1.49	1.45
26	v	316	CHL	MG-NA	-2.31	2.00	2.06
22	C	513	CLA	CMB-C2B	-2.31	1.45	1.50
22	c	508	CLA	CMD-C2D	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	312	CHL	C1B-C2B	2.31	1.48	1.43
22	R	303	CLA	CMD-C2D	-2.31	1.45	1.50
22	B	614	CLA	CMC-C2C	-2.31	1.45	1.50
24	N	311	XAT	C20-C13	2.31	1.55	1.50
25	d	406	LHG	O8-C6	-2.31	1.39	1.45
22	u	304	CLA	CMC-C2C	-2.31	1.45	1.50
25	D	406	LHG	O8-C6	-2.31	1.39	1.45
36	C	520	DGD	O1G-C1G	-2.31	1.39	1.45
22	a	405	CLA	C1B-C2B	2.31	1.48	1.43
26	1	318	CHL	MG-NA	-2.31	2.00	2.06
22	p	304	CLA	MG-NB	-2.31	2.01	2.05
22	N	303	CLA	CMB-C2B	-2.31	1.45	1.50
22	c	508	CLA	C1B-C2B	2.31	1.48	1.43
22	b	607	CLA	CMC-C2C	-2.31	1.45	1.50
26	6	316	CHL	MG-NA	-2.31	2.00	2.06
25	c	521	LHG	O8-C23	2.31	1.40	1.33
22	C	509	CLA	CMD-C2D	-2.31	1.45	1.50
26	u	314	CHL	C1B-C2B	2.31	1.48	1.43
22	B	607	CLA	CMC-C2C	-2.31	1.45	1.50
22	5	307	CLA	MG-NB	-2.31	2.01	2.05
26	V	317	CHL	C1B-C2B	2.31	1.48	1.43
22	b	609	CLA	CMD-C2D	-2.31	1.45	1.50
26	3	316	CHL	C1B-C2B	2.31	1.48	1.43
25	c	521	LHG	O8-C6	-2.31	1.39	1.45
22	v	305	CLA	MG-NB	-2.30	2.01	2.05
22	q	308	CLA	MG-NB	-2.30	2.01	2.05
26	P	316	CHL	C1B-C2B	2.30	1.48	1.43
22	U	301	CLA	CHC-C1C	2.30	1.43	1.38
25	N	312	LHG	O7-C7	2.30	1.40	1.34
26	R	315	CHL	C4C-C3C	2.30	1.49	1.45
26	2	316	CHL	C1D-ND	-2.30	1.35	1.37
26	g	311	CHL	C1B-NB	-2.30	1.35	1.37
33	a	411	PL9	O1-C4	-2.30	1.18	1.24
26	R	316	CHL	C1B-C2B	2.30	1.48	1.43
26	V	316	CHL	C4B-NB	-2.30	1.35	1.37
26	5	313	CHL	C1B-C2B	2.30	1.48	1.43
22	b	604	CLA	CMB-C2B	-2.30	1.45	1.50
26	N	313	CHL	C1B-C2B	2.30	1.48	1.43
26	1	317	CHL	C1B-C2B	2.30	1.48	1.43
26	1	315	CHL	C3B-C4B	2.30	1.48	1.42
26	G	316	CHL	MG-NA	-2.30	2.00	2.06
22	b	605	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	315	CHL	C1B-C2B	2.30	1.48	1.43
26	U	319	CHL	C1B-NB	-2.30	1.35	1.37
22	S	307	CLA	MG-NB	-2.30	2.01	2.05
26	r	616	CHL	MG-NA	-2.30	2.00	2.06
22	u	301	CLA	CMC-C2C	-2.30	1.45	1.50
22	4	307	CLA	MG-NB	-2.30	2.01	2.05
22	C	511	CLA	CMD-C2D	-2.30	1.45	1.50
22	2	306	CLA	MG-NB	-2.30	2.01	2.05
22	S	301	CLA	C1B-C2B	2.30	1.48	1.43
26	U	315	CHL	C1B-C2B	2.30	1.48	1.43
22	1	308	CLA	MG-NB	-2.30	2.01	2.05
22	V	303	CLA	C1B-C2B	2.30	1.48	1.43
26	r	614	CHL	C1B-C2B	2.30	1.48	1.43
22	Q	307	CLA	MG-NB	-2.30	2.01	2.05
26	q	315	CHL	C4B-NB	-2.30	1.35	1.37
34	d	407	LMG	O1-C1	-2.30	1.36	1.40
22	u	307	CLA	MG-NB	-2.30	2.01	2.05
22	V	301	CLA	CMB-C2B	-2.30	1.45	1.50
22	v	301	CLA	C1B-C2B	2.30	1.48	1.43
22	6	304	CLA	MG-NB	-2.30	2.01	2.05
22	V	305	CLA	MG-NB	-2.30	2.01	2.05
26	P	316	CHL	C4B-NB	-2.29	1.35	1.37
22	N	302	CLA	C1B-C2B	2.29	1.48	1.43
22	c	512	CLA	C1B-C2B	2.29	1.48	1.43
26	3	311	CHL	C1B-C2B	2.29	1.48	1.43
26	p	319	CHL	C3B-C4B	2.29	1.48	1.42
25	6	311	LHG	O8-C6	-2.29	1.39	1.45
22	B	603	CLA	CMD-C2D	-2.29	1.45	1.50
22	c	502	CLA	C1B-C2B	2.29	1.48	1.43
34	D	408	LMG	O1-C1	-2.29	1.36	1.40
22	Q	301	CLA	CHC-C1C	2.29	1.43	1.38
26	q	311	CHL	C1B-NB	-2.29	1.35	1.37
22	a	406	CLA	C1B-C2B	2.29	1.48	1.43
22	5	304	CLA	C1B-C2B	2.29	1.48	1.43
22	U	304	CLA	C1B-C2B	2.29	1.48	1.43
22	c	510	CLA	CMD-C2D	-2.29	1.45	1.50
26	Q	312	CHL	MG-NA	-2.29	2.00	2.06
26	5	314	CHL	C4C-C3C	2.29	1.49	1.45
22	N	304	CLA	CHC-C1C	2.29	1.43	1.38
26	p	318	CHL	C1B-NB	-2.29	1.35	1.37
22	v	304	CLA	MG-NB	-2.29	2.01	2.05
22	S	304	CLA	MG-NB	-2.29	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	MG-NB	-2.29	2.01	2.05
22	C	507	CLA	CMD-C2D	-2.29	1.45	1.50
22	P	308	CLA	MG-NB	-2.29	2.01	2.05
25	U	312	LHG	O8-C23	2.29	1.40	1.33
22	S	303	CLA	CMB-C2B	-2.29	1.45	1.50
22	g	303	CLA	C1B-C2B	2.29	1.48	1.43
26	P	318	CHL	C3B-C4B	2.29	1.48	1.42
22	v	301	CLA	CMB-C2B	-2.29	1.46	1.50
26	Q	315	CHL	C1D-ND	-2.29	1.35	1.37
22	b	617	CLA	CMB-C2B	-2.29	1.46	1.50
24	q	309	XAT	C20-C13	2.29	1.55	1.50
22	V	307	CLA	MG-NB	-2.29	2.01	2.05
26	5	315	CHL	C1B-C2B	2.29	1.48	1.43
22	P	303	CLA	MG-NB	-2.29	2.01	2.05
26	P	314	CHL	C1D-ND	-2.29	1.35	1.37
26	N	314	CHL	C1D-ND	-2.29	1.35	1.37
22	B	615	CLA	MG-NB	-2.29	2.01	2.05
25	D	407	LHG	O8-C6	-2.28	1.39	1.45
26	4	316	CHL	C4C-C3C	2.28	1.49	1.45
22	C	508	CLA	CMD-C2D	-2.28	1.46	1.50
22	s	303	CLA	CMB-C2B	-2.28	1.46	1.50
22	v	302	CLA	MG-NB	-2.28	2.01	2.05
25	d	405	LHG	O8-C6	-2.28	1.39	1.45
22	S	306	CLA	CMB-C2B	-2.28	1.46	1.50
22	R	303	CLA	MG-NB	-2.28	2.01	2.05
22	6	308	CLA	MG-NB	-2.28	2.01	2.05
26	Q	313	CHL	MG-NA	-2.28	2.00	2.06
22	6	304	CLA	CMB-C2B	-2.28	1.46	1.50
26	1	318	CHL	C4B-NB	-2.28	1.35	1.37
26	q	313	CHL	C1B-NB	-2.28	1.35	1.37
22	U	305	CLA	MG-NB	-2.28	2.01	2.05
26	Q	313	CHL	C4B-NB	-2.28	1.35	1.37
22	U	308	CLA	MG-NB	-2.28	2.01	2.05
25	B	622	LHG	O8-C6	-2.28	1.40	1.45
22	p	308	CLA	MG-NB	-2.28	2.01	2.05
22	5	306	CLA	MG-NB	-2.28	2.01	2.05
26	6	316	CHL	C4C-C3C	2.28	1.49	1.45
22	2	307	CLA	MG-NB	-2.28	2.01	2.05
25	4	312	LHG	O7-C7	2.28	1.40	1.34
22	n	304	CLA	C1B-C2B	2.28	1.48	1.43
26	S	316	CHL	C1D-ND	-2.28	1.35	1.37
22	3	301	CLA	MG-NB	-2.28	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	306	CLA	CMB-C2B	-2.28	1.46	1.50
26	V	313	CHL	C1B-NB	-2.28	1.35	1.37
26	6	312	CHL	MG-NA	-2.28	2.00	2.06
22	b	603	CLA	CMD-C2D	-2.28	1.46	1.50
24	5	311	XAT	C20-C13	2.28	1.55	1.50
22	C	514	CLA	CMD-C2D	-2.28	1.46	1.50
24	Q	309	XAT	C20-C13	2.28	1.55	1.50
22	V	304	CLA	CHC-C1C	2.28	1.43	1.38
25	3	310	LHG	O8-C23	2.27	1.40	1.33
25	b	622	LHG	O8-C6	-2.27	1.40	1.45
22	b	614	CLA	CMC-C2C	-2.27	1.46	1.50
22	C	504	CLA	CMC-C2C	-2.27	1.46	1.50
22	1	301	CLA	CMB-C2B	-2.27	1.46	1.50
26	Q	316	CHL	C4B-NB	-2.27	1.35	1.37
22	3	301	CLA	C1B-C2B	2.27	1.48	1.43
26	5	318	CHL	C1B-C2B	2.27	1.48	1.43
26	2	315	CHL	MG-NA	-2.27	2.00	2.06
22	4	308	CLA	MG-NB	-2.27	2.01	2.05
22	c	506	CLA	CMD-C2D	-2.27	1.46	1.50
26	P	319	CHL	C4B-NB	-2.27	1.35	1.37
26	3	311	CHL	MG-NA	-2.27	2.00	2.06
26	4	315	CHL	C3B-C4B	2.27	1.48	1.42
22	p	307	CLA	MG-NB	-2.27	2.01	2.05
22	U	306	CLA	MG-NB	-2.27	2.01	2.05
22	V	308	CLA	MG-NB	-2.27	2.01	2.05
22	6	304	CLA	C1B-C2B	2.27	1.48	1.43
22	q	303	CLA	C1B-C2B	2.27	1.48	1.43
22	n	301	CLA	MG-NB	-2.27	2.01	2.05
22	c	510	CLA	C1B-C2B	2.27	1.48	1.43
22	U	304	CLA	CMC-C2C	-2.27	1.46	1.50
22	B	606	CLA	MG-NB	-2.27	2.01	2.05
26	6	317	CHL	C1B-NB	-2.27	1.35	1.37
26	v	317	CHL	C4C-C3C	2.27	1.48	1.45
26	U	317	CHL	C4C-C3C	2.27	1.48	1.45
22	b	617	CLA	MG-ND	-2.27	2.01	2.05
22	u	303	CLA	C1B-C2B	2.27	1.48	1.43
22	R	302	CLA	CMC-C2C	-2.27	1.46	1.50
22	r	602	CLA	MG-NB	-2.27	2.01	2.05
26	q	313	CHL	C4C-C3C	2.27	1.48	1.45
22	s	307	CLA	MG-NB	-2.27	2.01	2.05
26	p	319	CHL	C4C-C3C	2.27	1.48	1.45
26	p	318	CHL	MG-NA	-2.27	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	303	CLA	CMB-C2B	-2.27	1.46	1.50
22	U	303	CLA	C1B-C2B	2.27	1.48	1.43
24	p	312	XAT	C20-C13	2.27	1.55	1.50
22	3	306	CLA	MG-NB	-2.27	2.01	2.05
22	3	307	CLA	MG-NB	-2.27	2.01	2.05
26	G	313	CHL	C1B-NB	-2.27	1.35	1.37
22	c	510	CLA	C4B-NB	2.27	1.40	1.37
26	5	313	CHL	C1D-ND	-2.27	1.35	1.37
22	U	302	CLA	CMD-C2D	-2.27	1.46	1.50
22	P	302	CLA	CHC-C1C	2.27	1.43	1.38
22	D	403	CLA	C1B-C2B	2.26	1.48	1.43
24	V	311	XAT	C20-C13	2.26	1.55	1.50
26	5	318	CHL	C4C-C3C	2.26	1.48	1.45
26	V	318	CHL	C4C-C3C	2.26	1.48	1.45
22	r	602	CLA	CMD-C2D	-2.26	1.46	1.50
36	b	601	DGD	O2G-C2G	-2.26	1.40	1.46
32	l	102	SQD	O2-C2	-2.26	1.37	1.43
26	P	319	CHL	MG-NA	-2.26	2.00	2.06
26	n	313	CHL	C1B-NB	-2.26	1.35	1.37
26	2	318	CHL	C3B-C4B	2.26	1.48	1.42
22	n	303	CLA	CMD-C2D	-2.26	1.46	1.50
26	4	317	CHL	MG-NA	-2.26	2.00	2.06
22	U	308	CLA	CMD-C2D	-2.26	1.46	1.50
24	R	313	XAT	C24-C23	2.26	1.55	1.52
22	u	306	CLA	CMB-C2B	-2.26	1.46	1.50
22	u	308	CLA	CMD-C2D	-2.26	1.46	1.50
26	S	314	CHL	C1B-NB	-2.26	1.35	1.37
22	c	507	CLA	CMD-C2D	-2.26	1.46	1.50
36	C	519	DGD	O2G-C2G	-2.26	1.40	1.46
26	n	315	CHL	C4C-C3C	2.26	1.48	1.45
26	r	614	CHL	C4C-C3C	2.26	1.48	1.45
26	U	317	CHL	C1B-C2B	2.26	1.48	1.43
22	5	303	CLA	CMD-C2D	-2.26	1.46	1.50
22	c	512	CLA	CMB-C2B	-2.26	1.46	1.50
22	G	308	CLA	MG-NB	-2.26	2.01	2.05
26	s	313	CHL	C1B-C2B	2.26	1.48	1.43
26	R	317	CHL	MG-NA	-2.26	2.00	2.06
22	g	307	CLA	CMD-C2D	-2.26	1.46	1.50
22	u	305	CLA	MG-NB	-2.26	2.01	2.05
26	n	314	CHL	C1D-ND	-2.26	1.35	1.37
24	2	311	XAT	C40-C33	2.26	1.55	1.50
26	G	313	CHL	C4C-C3C	2.26	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C1B-C2B	2.26	1.48	1.43
22	C	513	CLA	C1B-NB	-2.26	1.35	1.37
26	1	314	CHL	C1D-ND	-2.26	1.35	1.37
25	P	313	LHG	O8-C6	-2.26	1.40	1.45
22	B	606	CLA	CMB-C2B	-2.26	1.46	1.50
26	Q	314	CHL	C1B-NB	-2.26	1.35	1.37
26	s	315	CHL	C1D-ND	-2.26	1.35	1.37
22	V	302	CLA	MG-NB	-2.26	2.01	2.05
25	u	312	LHG	O8-C23	2.26	1.39	1.33
22	N	301	CLA	CHC-C1C	2.26	1.43	1.38
26	g	313	CHL	C1B-NB	-2.26	1.35	1.37
26	R	316	CHL	CHB-C4A	-2.26	1.32	1.37
22	C	503	CLA	CMB-C2B	-2.26	1.46	1.50
26	2	317	CHL	MG-NA	-2.26	2.00	2.06
22	q	302	CLA	MG-NB	-2.25	2.01	2.05
22	u	304	CLA	C1B-C2B	2.25	1.48	1.43
26	V	317	CHL	MG-NA	-2.25	2.00	2.06
26	4	315	CHL	C4C-C3C	2.25	1.48	1.45
22	b	606	CLA	MG-NB	-2.25	2.01	2.05
22	s	308	CLA	MG-NB	-2.25	2.01	2.05
26	n	315	CHL	C3B-C4B	2.25	1.48	1.42
22	4	301	CLA	CMB-C2B	-2.25	1.46	1.50
26	3	311	CHL	C1B-NB	-2.25	1.35	1.37
26	s	316	CHL	C1D-ND	-2.25	1.35	1.37
22	s	309	CLA	CMD-C2D	-2.25	1.46	1.50
22	U	302	CLA	MG-NB	-2.25	2.01	2.05
22	g	304	CLA	CHC-C1C	2.25	1.43	1.38
25	B	622	LHG	O8-C23	2.25	1.39	1.33
22	A	404	CLA	C1B-C2B	2.25	1.48	1.43
22	c	511	CLA	CMB-C2B	-2.25	1.46	1.50
24	r	612	XAT	C24-C23	2.25	1.55	1.52
22	2	308	CLA	MG-NB	-2.25	2.01	2.05
22	5	304	CLA	MG-NB	-2.25	2.01	2.05
36	c	517	DGD	O2G-C2G	-2.25	1.41	1.46
32	A	412	SQD	O2-C2	-2.25	1.37	1.43
26	P	319	CHL	C4C-C3C	2.25	1.48	1.45
26	n	317	CHL	C4C-C3C	2.25	1.48	1.45
25	d	406	LHG	O7-C7	2.25	1.40	1.34
22	c	507	CLA	C1B-C2B	2.25	1.48	1.43
24	P	312	XAT	C20-C13	2.25	1.55	1.50
26	p	314	CHL	C1D-ND	-2.25	1.35	1.37
25	G	310	LHG	O7-C7	2.25	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	C1B-C2B	2.25	1.48	1.43
22	b	612	CLA	CMB-C2B	-2.25	1.46	1.50
22	1	303	CLA	C1B-C2B	2.25	1.48	1.43
24	N	311	XAT	C40-C33	2.25	1.55	1.50
22	G	303	CLA	MG-NB	-2.25	2.01	2.05
26	v	317	CHL	C1B-NB	-2.25	1.35	1.37
22	n	301	CLA	CHC-C1C	2.25	1.43	1.38
22	6	306	CLA	MG-NB	-2.25	2.01	2.05
22	G	307	CLA	CMD-C2D	-2.25	1.46	1.50
22	u	301	CLA	CMB-C2B	-2.25	1.46	1.50
22	6	303	CLA	MG-NB	-2.25	2.01	2.05
22	s	301	CLA	CMC-C2C	-2.25	1.46	1.50
26	1	317	CHL	MG-NA	-2.25	2.00	2.06
26	V	317	CHL	C1B-NB	-2.25	1.35	1.37
22	B	612	CLA	CMB-C2B	-2.25	1.46	1.50
22	c	513	CLA	MG-ND	-2.25	2.01	2.05
22	c	506	CLA	C1B-C2B	2.25	1.48	1.43
22	g	308	CLA	MG-NB	-2.25	2.01	2.05
22	A	406	CLA	CMD-C2D	-2.25	1.46	1.50
22	c	512	CLA	CMD-C2D	-2.24	1.46	1.50
25	n	312	LHG	O7-C7	2.24	1.40	1.34
25	D	406	LHG	O8-C23	2.24	1.39	1.33
24	r	612	XAT	C20-C13	2.24	1.55	1.50
22	B	602	CLA	CMD-C2D	-2.24	1.46	1.50
22	N	303	CLA	C1B-C2B	2.24	1.48	1.43
22	b	602	CLA	CMD-C2D	-2.24	1.46	1.50
26	u	318	CHL	CHB-C4A	-2.24	1.32	1.37
26	2	317	CHL	C1B-NB	-2.24	1.35	1.37
26	G	316	CHL	C1B-NB	-2.24	1.35	1.37
22	n	303	CLA	CMB-C2B	-2.24	1.46	1.50
26	q	314	CHL	C4C-C3C	2.24	1.48	1.45
26	V	317	CHL	C4C-C3C	2.24	1.48	1.45
24	n	311	XAT	C20-C13	2.24	1.55	1.50
22	2	302	CLA	CMD-C2D	-2.24	1.46	1.50
22	P	304	CLA	CMB-C2B	-2.24	1.46	1.50
22	Q	303	CLA	CMB-C2B	-2.24	1.46	1.50
22	u	302	CLA	MG-NB	-2.24	2.01	2.05
26	P	316	CHL	C4C-C3C	2.24	1.48	1.45
32	L	102	SQD	O2-C2	-2.24	1.37	1.43
22	V	304	CLA	MG-NB	-2.24	2.01	2.05
22	G	303	CLA	C1B-C2B	2.24	1.48	1.43
26	g	316	CHL	C4C-C3C	2.24	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	302	CLA	MG-NB	-2.24	2.01	2.05
26	n	316	CHL	C4B-NB	-2.24	1.35	1.37
26	n	318	CHL	C1D-ND	-2.24	1.35	1.37
22	6	302	CLA	C1B-C2B	2.24	1.48	1.43
25	d	405	LHG	O8-C23	2.24	1.39	1.33
25	D	407	LHG	O7-C7	2.24	1.40	1.34
22	S	301	CLA	CMC-C2C	-2.24	1.46	1.50
22	u	308	CLA	MG-NB	-2.24	2.01	2.05
26	U	316	CHL	MG-NA	-2.24	2.01	2.06
22	B	612	CLA	CMD-C2D	-2.24	1.46	1.50
26	U	313	CHL	C1D-ND	-2.24	1.35	1.37
26	G	314	CHL	C4C-C3C	2.24	1.48	1.45
22	6	309	CLA	MG-NB	-2.24	2.01	2.05
22	n	304	CLA	CHC-C1C	2.24	1.43	1.38
22	b	612	CLA	CMD-C2D	-2.24	1.46	1.50
26	u	317	CHL	MG-NA	-2.24	2.01	2.06
26	r	616	CHL	C1D-ND	-2.24	1.35	1.37
26	u	317	CHL	C1D-ND	-2.24	1.35	1.37
22	C	505	CLA	MG-ND	-2.24	2.01	2.05
26	P	318	CHL	MG-NA	-2.23	2.01	2.06
26	P	318	CHL	C1B-C2B	2.23	1.48	1.43
22	r	606	CLA	MG-NB	-2.23	2.01	2.05
26	r	619	CHL	C1B-C2B	2.23	1.48	1.43
22	c	505	CLA	CMB-C2B	-2.23	1.46	1.50
26	S	313	CHL	C1B-C2B	2.23	1.48	1.43
22	4	306	CLA	CMD-C2D	-2.23	1.46	1.50
26	v	318	CHL	MG-NA	-2.23	2.01	2.06
26	s	316	CHL	C4C-C3C	2.23	1.48	1.45
22	c	503	CLA	CMC-C2C	-2.23	1.46	1.50
22	C	514	CLA	MG-ND	-2.23	2.01	2.05
22	c	502	CLA	MG-NB	-2.23	2.01	2.05
26	V	315	CHL	C4C-C3C	2.23	1.48	1.45
26	G	316	CHL	C4B-NB	-2.23	1.35	1.37
22	G	302	CLA	MG-NB	-2.23	2.01	2.05
25	v	312	LHG	O7-C7	2.23	1.40	1.34
26	v	313	CHL	C1B-NB	-2.23	1.35	1.37
25	U	312	LHG	O8-C6	-2.23	1.40	1.45
22	n	307	CLA	CMD-C2D	-2.23	1.46	1.50
26	r	616	CHL	CHB-C4A	-2.23	1.32	1.37
22	q	307	CLA	MG-NB	-2.23	2.01	2.05
25	b	622	LHG	O8-C23	2.23	1.39	1.33
22	N	305	CLA	MG-NB	-2.23	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q	311	CHL	C1B-NB	-2.23	1.35	1.37
26	U	314	CHL	C4B-NB	-2.23	1.35	1.37
22	B	611	CLA	CMB-C2B	-2.23	1.46	1.50
26	g	315	CHL	C1B-C2B	2.23	1.48	1.43
24	2	311	XAT	C20-C13	2.23	1.55	1.50
22	R	307	CLA	MG-NB	-2.23	2.01	2.05
22	U	307	CLA	CMC-C2C	-2.23	1.46	1.50
32	a	413	SQD	O2-C2	-2.23	1.37	1.43
22	2	302	CLA	C1B-C2B	2.23	1.48	1.43
22	N	302	CLA	CMB-C2B	-2.23	1.46	1.50
26	3	313	CHL	C4B-NB	-2.23	1.35	1.37
22	1	306	CLA	CMD-C2D	-2.23	1.46	1.50
22	U	301	CLA	CMB-C2B	-2.23	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.23	1.46	1.50
25	B	622	LHG	O7-C7	2.23	1.40	1.34
26	s	313	CHL	C4C-C3C	2.23	1.48	1.45
25	C	522	LHG	O8-C6	-2.23	1.40	1.45
26	P	318	CHL	CHB-C4A	-2.23	1.32	1.37
22	2	303	CLA	CMD-C2D	-2.23	1.46	1.50
22	n	304	CLA	CMD-C2D	-2.23	1.46	1.50
24	v	311	XAT	C20-C13	2.23	1.55	1.50
22	p	303	CLA	MG-NB	-2.23	2.01	2.05
22	v	304	CLA	CHC-C1C	2.23	1.43	1.38
22	p	302	CLA	CHC-C1C	2.23	1.43	1.38
22	2	303	CLA	MG-NB	-2.23	2.01	2.05
25	u	312	LHG	O8-C6	-2.22	1.40	1.45
26	n	317	CHL	C1B-NB	-2.22	1.35	1.37
26	R	317	CHL	C1D-ND	-2.22	1.35	1.37
22	a	404	CLA	C1B-C2B	2.22	1.48	1.43
22	n	305	CLA	C4D-ND	-2.22	1.34	1.37
26	6	315	CHL	C1D-ND	-2.22	1.35	1.37
26	u	314	CHL	C1B-NB	-2.22	1.35	1.37
26	S	316	CHL	C4C-C3C	2.22	1.48	1.45
36	B	601	DGD	O2G-C2G	-2.22	1.41	1.46
22	s	304	CLA	MG-NB	-2.22	2.01	2.05
26	s	314	CHL	C1B-NB	-2.22	1.35	1.37
34	c	520	LMG	O1-C7	-2.22	1.39	1.43
25	1	312	LHG	O7-C7	2.22	1.40	1.34
22	V	301	CLA	C1B-C2B	2.22	1.48	1.43
24	3	309	XAT	C20-C13	2.22	1.55	1.50
26	U	314	CHL	C1D-C2D	2.22	1.49	1.45
22	U	307	CLA	MG-NB	-2.22	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	317	CHL	CHB-C4A	-2.22	1.32	1.37
22	C	506	CLA	CMB-C2B	-2.22	1.46	1.50
24	6	310	XAT	C20-C13	2.22	1.55	1.50
25	g	310	LHG	O7-C7	2.22	1.40	1.34
26	g	316	CHL	C1B-NB	-2.22	1.35	1.37
26	S	313	CHL	C4C-C3C	2.22	1.48	1.45
22	5	303	CLA	MG-NB	-2.22	2.01	2.05
26	v	317	CHL	MG-NA	-2.22	2.01	2.06
25	L	101	LHG	O8-C6	-2.22	1.40	1.45
26	V	313	CHL	C4C-C3C	2.22	1.48	1.45
26	R	317	CHL	C4C-C3C	2.22	1.48	1.45
34	b	621	LMG	O1-C1	-2.22	1.36	1.40
24	5	311	XAT	C40-C33	2.22	1.55	1.50
22	g	302	CLA	MG-NB	-2.22	2.01	2.05
26	g	315	CHL	C1B-NB	-2.22	1.35	1.37
22	n	301	CLA	C1B-C2B	2.22	1.48	1.43
22	n	302	CLA	CMB-C2B	-2.22	1.46	1.50
24	4	311	XAT	C20-C13	2.22	1.55	1.50
24	V	311	XAT	C40-C33	2.22	1.55	1.50
22	c	504	CLA	MG-ND	-2.22	2.01	2.05
26	1	317	CHL	C4B-NB	-2.22	1.35	1.37
22	c	512	CLA	C1B-NB	-2.21	1.35	1.37
22	3	303	CLA	C1B-C2B	2.21	1.48	1.43
26	r	615	CHL	CHB-C4A	-2.21	1.32	1.37
26	v	317	CHL	C1B-C2B	2.21	1.48	1.43
22	b	611	CLA	CMB-C2B	-2.21	1.46	1.50
22	c	508	CLA	CMB-C2B	-2.21	1.46	1.50
22	C	504	CLA	CMD-C2D	-2.21	1.46	1.50
22	C	505	CLA	CMD-C2D	-2.21	1.46	1.50
26	N	315	CHL	C3B-C4B	2.21	1.48	1.42
26	3	314	CHL	C1D-ND	-2.21	1.35	1.37
26	G	316	CHL	C4C-C3C	2.21	1.48	1.45
22	a	406	CLA	CMB-C2B	-2.21	1.46	1.50
23	4	310	LUT	C1-C6	-2.21	1.50	1.53
22	P	309	CLA	MG-NB	-2.21	2.01	2.05
22	c	503	CLA	CMD-C2D	-2.21	1.46	1.50
22	c	514	CLA	CMB-C2B	-2.21	1.46	1.50
24	p	312	XAT	C40-C33	2.21	1.55	1.50
25	p	313	LHG	O7-C7	2.21	1.40	1.34
22	1	304	CLA	MG-ND	-2.21	2.01	2.05
22	q	301	CLA	C1B-C2B	2.21	1.48	1.43
22	B	615	CLA	CMB-C2B	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	q	301	CLA	CHC-C1C	2.21	1.43	1.38
22	4	303	CLA	C1B-C2B	2.21	1.48	1.43
24	P	312	XAT	C40-C33	2.21	1.55	1.50
26	V	316	CHL	C4C-C3C	2.21	1.48	1.45
25	N	312	LHG	O8-C6	-2.21	1.40	1.45
22	P	305	CLA	MG-NB	-2.21	2.01	2.05
34	b	624	LMG	O1-C1	-2.21	1.36	1.40
22	N	306	CLA	MG-NB	-2.21	2.01	2.05
26	N	313	CHL	C1B-NB	-2.21	1.35	1.37
22	S	303	CLA	MG-NB	-2.21	2.01	2.05
25	l	101	LHG	O8-C6	-2.21	1.40	1.45
26	G	314	CHL	C1D-ND	-2.21	1.35	1.37
22	S	307	CLA	CMD-C2D	-2.21	1.46	1.50
22	G	302	CLA	CMB-C2B	-2.21	1.46	1.50
22	g	303	CLA	CMD-C2D	-2.21	1.46	1.50
26	P	319	CHL	CHB-C4A	-2.21	1.32	1.37
22	a	406	CLA	CMD-C2D	-2.20	1.46	1.50
22	c	504	CLA	CMD-C2D	-2.20	1.46	1.50
26	3	312	CHL	C2C-C1C	2.20	1.49	1.44
22	b	606	CLA	CMB-C2B	-2.20	1.46	1.50
26	U	319	CHL	C1D-ND	-2.20	1.35	1.37
25	Q	310	LHG	O8-C6	-2.20	1.40	1.45
26	p	316	CHL	C4C-C3C	2.20	1.48	1.45
22	B	611	CLA	CMD-C2D	-2.20	1.46	1.50
22	b	615	CLA	CMB-C2B	-2.20	1.46	1.50
22	n	306	CLA	MG-NB	-2.20	2.01	2.05
22	p	305	CLA	MG-NB	-2.20	2.01	2.05
26	n	315	CHL	C4B-NB	-2.20	1.35	1.37
26	p	318	CHL	CHB-C4A	-2.20	1.32	1.37
22	b	604	CLA	C1B-C2B	2.20	1.48	1.43
22	C	512	CLA	CMB-C2B	-2.20	1.46	1.50
25	p	313	LHG	O8-C6	-2.20	1.40	1.45
22	c	507	CLA	CMC-C2C	-2.20	1.46	1.50
22	n	303	CLA	MG-NB	-2.20	2.01	2.05
22	N	304	CLA	C1B-C2B	2.20	1.48	1.43
22	S	301	CLA	MG-NB	-2.20	2.01	2.05
26	p	314	CHL	C1B-C2B	2.20	1.48	1.43
22	C	503	CLA	CMC-C2C	-2.20	1.46	1.50
22	C	513	CLA	CMD-C2D	-2.20	1.46	1.50
26	Q	315	CHL	C4C-C3C	2.20	1.48	1.45
22	u	302	CLA	CMD-C2D	-2.20	1.46	1.50
25	V	312	LHG	O7-C7	2.20	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u	313	CHL	C1B-NB	-2.20	1.35	1.37
22	P	303	CLA	CMD-C2D	-2.20	1.46	1.50
22	3	305	CLA	MG-NB	-2.20	2.01	2.05
24	4	311	XAT	C40-C33	2.20	1.55	1.50
25	b	622	LHG	O7-C7	2.20	1.40	1.34
26	4	316	CHL	C4B-NB	-2.20	1.35	1.37
30	a	407	PHO	CBD-CGD	-2.20	1.49	1.52
22	u	304	CLA	CMB-C2B	-2.20	1.46	1.50
22	C	509	CLA	CMB-C2B	-2.20	1.46	1.50
22	6	305	CLA	MG-NB	-2.20	2.01	2.05
26	G	311	CHL	C4C-C3C	2.20	1.48	1.45
24	Q	309	XAT	C40-C33	2.20	1.55	1.50
26	Q	313	CHL	C1B-NB	-2.20	1.35	1.37
26	U	316	CHL	C1D-ND	-2.20	1.35	1.37
22	b	613	CLA	CMB-C2B	-2.20	1.46	1.50
22	2	305	CLA	C1D-ND	2.20	1.40	1.37
22	5	305	CLA	C1D-ND	2.20	1.40	1.37
22	q	303	CLA	MG-NB	-2.20	2.01	2.05
26	U	314	CHL	C1B-C2B	2.20	1.48	1.43
22	C	515	CLA	CMB-C2B	-2.19	1.46	1.50
30	A	407	PHO	CBD-CGD	-2.19	1.49	1.52
24	R	313	XAT	C20-C13	2.19	1.55	1.50
22	N	308	CLA	CHC-C1C	2.19	1.43	1.38
26	2	316	CHL	C4C-C3C	2.19	1.48	1.45
24	q	309	XAT	C40-C33	2.19	1.55	1.50
22	3	302	CLA	MG-NB	-2.19	2.01	2.05
22	C	503	CLA	MG-NB	-2.19	2.01	2.05
26	5	315	CHL	C1B-NB	-2.19	1.35	1.37
26	5	317	CHL	C1B-NB	-2.19	1.35	1.37
26	U	316	CHL	C1B-NB	-2.19	1.35	1.37
26	N	315	CHL	MG-NA	-2.19	2.01	2.06
24	n	311	XAT	C40-C33	2.19	1.55	1.50
26	G	312	CHL	C4D-CHA	2.19	1.46	1.38
22	S	305	CLA	CHC-C1C	2.19	1.43	1.38
26	1	317	CHL	C4C-C3C	2.19	1.48	1.45
26	g	312	CHL	C4B-NB	-2.19	1.35	1.37
22	S	309	CLA	MG-NB	-2.19	2.01	2.05
26	U	315	CHL	MG-NA	-2.19	2.01	2.06
22	C	512	CLA	MG-NB	-2.19	2.01	2.05
22	x	201	CLA	CMD-C2D	-2.19	1.46	1.50
22	2	303	CLA	CMB-C2B	-2.19	1.46	1.50
22	U	307	CLA	CMB-C2B	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	304	CLA	MG-NB	-2.19	2.01	2.05
22	v	308	CLA	MG-NB	-2.19	2.01	2.05
26	G	315	CHL	C2C-C1C	2.19	1.49	1.44
26	V	316	CHL	C1B-NB	-2.19	1.35	1.37
22	c	502	CLA	CMC-C2C	-2.19	1.46	1.50
25	v	312	LHG	O8-C6	-2.19	1.40	1.45
25	c	521	LHG	O7-C7	2.19	1.40	1.34
22	b	607	CLA	CMB-C2B	-2.19	1.46	1.50
22	b	612	CLA	CHC-C1C	2.19	1.43	1.38
22	6	303	CLA	CMB-C2B	-2.19	1.46	1.50
22	B	607	CLA	CMB-C2B	-2.19	1.46	1.50
22	N	301	CLA	C1B-C2B	2.19	1.48	1.43
22	B	615	CLA	CMD-C2D	-2.19	1.46	1.50
26	1	315	CHL	C4C-C3C	2.19	1.48	1.45
26	u	314	CHL	C4C-C3C	2.19	1.48	1.45
26	G	312	CHL	C2C-C1C	2.19	1.49	1.44
26	5	317	CHL	C4B-NB	-2.19	1.35	1.37
26	s	313	CHL	C1D-ND	-2.19	1.35	1.37
22	B	609	CLA	C1B-C2B	2.19	1.48	1.43
22	p	309	CLA	MG-NB	-2.19	2.01	2.05
26	r	616	CHL	C4C-C3C	2.18	1.48	1.45
26	N	316	CHL	C4B-NB	-2.18	1.35	1.37
26	6	313	CHL	C4D-CHA	2.18	1.46	1.38
22	G	301	CLA	CMC-C2C	-2.18	1.46	1.50
22	5	308	CLA	MG-NB	-2.18	2.01	2.05
22	2	301	CLA	CMC-C2C	-2.18	1.46	1.50
22	b	611	CLA	CMC-C2C	-2.18	1.46	1.50
26	R	317	CHL	CHB-C4A	-2.18	1.32	1.37
22	q	302	CLA	CMB-C2B	-2.18	1.46	1.50
26	v	317	CHL	CHB-C4A	-2.18	1.32	1.37
24	6	310	XAT	C40-C33	2.18	1.55	1.50
22	3	308	CLA	MG-NB	-2.18	2.01	2.05
22	P	308	CLA	CMD-C2D	-2.18	1.46	1.50
22	c	511	CLA	MG-NB	-2.18	2.01	2.05
22	u	307	CLA	CMC-C2C	-2.18	1.46	1.50
22	b	610	CLA	CMB-C2B	-2.18	1.46	1.50
22	b	615	CLA	CMD-C2D	-2.18	1.46	1.50
24	P	312	XAT	C28-C27	2.18	1.37	1.32
22	d	402	CLA	CMB-C2B	-2.18	1.46	1.50
22	q	307	CLA	CMD-C2D	-2.18	1.46	1.50
22	C	515	CLA	CMD-C2D	-2.18	1.46	1.50
22	g	305	CLA	CMB-C2B	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	6	312	CHL	C1B-NB	-2.18	1.35	1.37
22	A	406	CLA	CMB-C2B	-2.18	1.46	1.50
22	P	302	CLA	CMB-C2B	-2.18	1.46	1.50
22	X	202	CLA	CMD-C2D	-2.18	1.46	1.50
22	Q	304	CLA	MG-NB	-2.18	2.01	2.05
22	B	604	CLA	C1B-C2B	2.18	1.48	1.43
22	B	612	CLA	CHC-C1C	2.18	1.42	1.38
22	a	408	CLA	CMC-C2C	-2.18	1.46	1.50
22	B	610	CLA	CMB-C2B	-2.18	1.46	1.50
22	a	404	CLA	MG-ND	-2.18	2.01	2.05
22	N	302	CLA	CMD-C2D	-2.18	1.46	1.50
22	g	302	CLA	CMB-C2B	-2.18	1.46	1.50
22	b	609	CLA	C1B-C2B	2.18	1.48	1.43
26	p	320	CHL	MG-NA	-2.18	2.01	2.06
25	2	312	LHG	O8-C6	-2.18	1.40	1.45
32	C	501	SQD	O3-C3	-2.18	1.37	1.43
22	g	301	CLA	CMB-C2B	-2.18	1.46	1.50
26	n	318	CHL	C3B-C4B	2.18	1.47	1.42
22	G	303	CLA	CHC-C1C	2.18	1.42	1.38
22	A	404	CLA	MG-ND	-2.18	2.01	2.05
22	5	303	CLA	CMB-C2B	-2.18	1.46	1.50
22	Q	305	CLA	CMD-C2D	-2.18	1.46	1.50
26	N	317	CHL	C1D-ND	-2.18	1.35	1.37
22	5	302	CLA	CMD-C2D	-2.18	1.46	1.50
22	u	302	CLA	CMB-C2B	-2.18	1.46	1.50
22	g	301	CLA	C1B-C2B	2.18	1.48	1.43
22	3	302	CLA	CMB-C2B	-2.18	1.46	1.50
22	U	302	CLA	CMB-C2B	-2.18	1.46	1.50
22	b	611	CLA	CMD-C2D	-2.18	1.46	1.50
26	2	313	CHL	C1D-ND	-2.18	1.35	1.37
26	G	315	CHL	CHB-C4A	-2.17	1.32	1.37
26	2	314	CHL	C1D-ND	-2.17	1.35	1.37
22	B	609	CLA	MG-ND	-2.17	2.01	2.05
26	v	316	CHL	C1B-NB	-2.17	1.35	1.37
26	p	317	CHL	C1D-ND	-2.17	1.35	1.37
22	B	613	CLA	CMB-C2B	-2.17	1.46	1.50
36	b	601	DGD	O3G-C1D	-2.17	1.36	1.40
22	g	305	CLA	MG-NB	-2.17	2.01	2.05
22	s	303	CLA	MG-NB	-2.17	2.01	2.05
22	u	305	CLA	CMD-C2D	-2.17	1.46	1.50
34	b	621	LMG	O1-C7	-2.17	1.39	1.43
26	r	616	CHL	C4B-NB	-2.17	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	304	CLA	CHC-C1C	2.17	1.42	1.38
26	v	318	CHL	C1D-ND	-2.17	1.35	1.37
22	q	307	CLA	CHC-C1C	2.17	1.42	1.38
26	V	318	CHL	C1D-ND	-2.17	1.35	1.37
22	n	307	CLA	MG-NB	-2.17	2.01	2.05
24	U	311	XAT	C28-C27	2.17	1.37	1.32
26	p	314	CHL	C2C-C1C	2.17	1.49	1.44
22	G	301	CLA	CMB-C2B	-2.17	1.46	1.50
22	C	506	CLA	CMD-C2D	-2.17	1.46	1.50
26	4	317	CHL	C4C-C3C	2.17	1.48	1.45
26	2	314	CHL	C4D-CHA	2.17	1.46	1.38
22	c	513	CLA	CMB-C2B	-2.17	1.46	1.50
22	2	304	CLA	CHC-C1C	2.17	1.42	1.38
26	n	317	CHL	C1D-ND	-2.17	1.35	1.37
22	Q	301	CLA	CMD-C2D	-2.17	1.46	1.50
24	Q	309	XAT	C8-C7	2.17	1.37	1.32
24	1	311	XAT	C20-C13	2.17	1.55	1.50
24	3	309	XAT	C40-C33	2.17	1.55	1.50
22	G	305	CLA	MG-NB	-2.17	2.01	2.05
22	u	308	CLA	CMB-C2B	-2.17	1.46	1.50
26	U	314	CHL	MG-NA	-2.17	2.01	2.06
25	V	312	LHG	O8-C6	-2.17	1.40	1.45
26	4	317	CHL	C4B-NB	-2.17	1.35	1.37
26	5	315	CHL	MG-NA	-2.17	2.01	2.06
24	v	311	XAT	C40-C33	2.17	1.55	1.50
22	N	304	CLA	MG-NB	-2.17	2.01	2.05
26	U	319	CHL	C4B-NB	-2.17	1.35	1.37
22	b	608	CLA	CMD-C2D	-2.17	1.46	1.50
22	v	306	CLA	MG-NB	-2.17	2.01	2.05
22	N	307	CLA	MG-NB	-2.17	2.01	2.05
24	3	309	XAT	C28-C27	2.17	1.37	1.32
26	U	313	CHL	C4C-C3C	2.17	1.48	1.45
22	N	307	CLA	CMD-C2D	-2.17	1.46	1.50
26	G	315	CHL	C1B-NB	-2.17	1.35	1.37
24	U	311	XAT	C40-C33	2.17	1.55	1.50
22	v	306	CLA	CMD-C2D	-2.16	1.46	1.50
26	6	316	CHL	C1B-NB	-2.16	1.35	1.37
26	U	317	CHL	CHB-C4A	-2.16	1.32	1.37
22	P	306	CLA	MG-NB	-2.16	2.01	2.05
26	u	317	CHL	C4C-C3C	2.16	1.48	1.45
22	1	302	CLA	MG-NB	-2.16	2.01	2.05
22	s	309	CLA	MG-NB	-2.16	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	310	LHG	O8-C6	-2.16	1.40	1.45
26	p	316	CHL	C1D-ND	-2.16	1.35	1.37
22	r	606	CLA	CMD-C2D	-2.16	1.46	1.50
26	n	314	CHL	C4C-C3C	2.16	1.48	1.45
26	r	619	CHL	MG-NA	-2.16	2.01	2.06
26	q	314	CHL	C1B-NB	-2.16	1.35	1.37
26	3	312	CHL	C4D-CHA	2.16	1.46	1.38
22	R	305	CLA	CMD-C2D	-2.16	1.46	1.50
24	u	311	XAT	C28-C27	2.16	1.37	1.32
26	v	315	CHL	C4C-C3C	2.16	1.48	1.45
22	U	308	CLA	CMB-C2B	-2.16	1.46	1.50
25	2	312	LHG	O7-C7	2.16	1.40	1.34
26	V	316	CHL	C1D-ND	-2.16	1.35	1.37
26	P	316	CHL	C1D-ND	-2.16	1.35	1.37
26	4	314	CHL	CHB-C4A	-2.16	1.32	1.37
26	U	315	CHL	CHB-C4A	-2.16	1.32	1.37
22	C	509	CLA	CMC-C2C	-2.16	1.46	1.50
26	3	315	CHL	C4C-C3C	2.16	1.48	1.45
22	C	504	CLA	CAC-C3C	-2.16	1.45	1.51
22	p	308	CLA	CMD-C2D	-2.16	1.46	1.50
22	C	508	CLA	CMC-C2C	-2.16	1.46	1.50
26	5	315	CHL	C4C-C3C	2.16	1.48	1.45
24	p	312	XAT	C28-C27	2.16	1.37	1.32
26	v	316	CHL	C1D-ND	-2.16	1.35	1.37
26	g	316	CHL	C4B-NB	-2.16	1.35	1.37
25	C	522	LHG	O7-C7	2.16	1.40	1.34
22	Q	301	CLA	CMB-C2B	-2.16	1.46	1.50
22	U	305	CLA	CMD-C2D	-2.16	1.46	1.50
25	B	623	LHG	O7-C7	2.16	1.40	1.34
22	V	307	CLA	CMD-C2D	-2.16	1.46	1.50
22	b	605	CLA	C1B-NB	-2.16	1.35	1.37
22	1	306	CLA	CMB-C2B	-2.16	1.46	1.50
22	6	306	CLA	CMD-C2D	-2.16	1.46	1.50
24	R	313	XAT	C40-C33	2.16	1.55	1.50
25	R	314	LHG	O7-C7	2.16	1.40	1.34
24	G	309	XAT	C28-C27	2.16	1.37	1.32
26	P	314	CHL	C2C-C1C	2.16	1.49	1.44
22	R	309	CLA	MG-NB	-2.16	2.01	2.05
22	S	308	CLA	CMB-C2B	-2.16	1.46	1.50
22	c	514	CLA	CMD-C2D	-2.16	1.46	1.50
26	u	314	CHL	MG-NA	-2.16	2.01	2.06
22	5	307	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	604	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	611	CLA	CMC-C2C	-2.16	1.46	1.50
26	u	315	CHL	C1B-C2B	2.15	1.48	1.43
26	u	313	CHL	C4C-C3C	2.15	1.48	1.45
25	b	623	LHG	O7-C7	2.15	1.40	1.34
26	S	314	CHL	MG-NA	-2.15	2.01	2.06
22	v	305	CLA	CMD-C2D	-2.15	1.46	1.50
22	p	304	CLA	CMB-C2B	-2.15	1.46	1.50
22	Q	307	CLA	CHC-C1C	2.15	1.42	1.38
24	1	311	XAT	C40-C33	2.15	1.55	1.50
26	S	315	CHL	C4C-C3C	2.15	1.48	1.45
24	V	311	XAT	C28-C27	2.15	1.37	1.32
26	g	314	CHL	C1D-ND	-2.15	1.35	1.37
22	B	606	CLA	CMD-C2D	-2.15	1.46	1.50
22	2	304	CLA	MG-NB	-2.15	2.01	2.05
24	G	309	XAT	C20-C13	2.15	1.55	1.50
26	v	313	CHL	C4C-C3C	2.15	1.48	1.45
22	4	304	CLA	MG-ND	-2.15	2.01	2.05
22	s	301	CLA	MG-NB	-2.15	2.01	2.05
25	6	311	LHG	O7-C7	2.15	1.40	1.34
25	q	310	LHG	O8-C6	-2.15	1.40	1.45
26	q	313	CHL	MG-NA	-2.15	2.01	2.06
22	s	305	CLA	CHC-C1C	2.15	1.42	1.38
26	1	313	CHL	C4B-NB	-2.15	1.35	1.37
25	a	415	LHG	O8-C23	2.15	1.39	1.33
22	S	303	CLA	CMC-C2C	-2.15	1.46	1.50
22	5	301	CLA	CMC-C2C	-2.15	1.46	1.50
26	G	315	CHL	C1B-C2B	2.15	1.48	1.43
34	C	521	LMG	O1-C7	-2.15	1.39	1.43
24	2	311	XAT	C28-C27	2.15	1.37	1.32
22	B	614	CLA	MG-ND	-2.15	2.01	2.05
22	v	303	CLA	CMD-C2D	-2.15	1.46	1.50
27	p	301	NEX	C1-C6	-2.15	1.50	1.54
22	1	301	CLA	C1B-C2B	2.15	1.48	1.43
26	p	320	CHL	C1B-NB	-2.15	1.35	1.37
22	r	610	CLA	MG-NB	-2.15	2.01	2.05
22	p	303	CLA	CMD-C2D	-2.15	1.46	1.50
22	N	301	CLA	CMB-C2B	-2.15	1.46	1.50
22	g	301	CLA	CMC-C2C	-2.15	1.46	1.50
22	a	408	CLA	C1B-C2B	2.15	1.48	1.43
22	b	616	CLA	CMD-C2D	-2.15	1.46	1.50
24	Q	309	XAT	C28-C27	2.15	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	316	CHL	C1D-ND	-2.15	1.35	1.37
26	6	301	CHL	C4C-C3C	2.15	1.48	1.45
32	C	501	SQD	O4-C4	-2.15	1.37	1.43
25	Q	310	LHG	O7-C7	2.15	1.40	1.34
22	S	302	CLA	MG-NB	-2.15	2.01	2.05
22	b	606	CLA	CMC-C2C	-2.15	1.46	1.50
22	B	614	CLA	CMD-C2D	-2.15	1.46	1.50
22	s	301	CLA	CMD-C2D	-2.15	1.46	1.50
26	p	320	CHL	C4B-NB	-2.15	1.35	1.37
26	Q	314	CHL	C1D-ND	-2.15	1.35	1.37
22	A	405	CLA	MG-ND	-2.14	2.01	2.05
22	c	505	CLA	CMC-C2C	-2.14	1.46	1.50
22	3	305	CLA	CMD-C2D	-2.14	1.46	1.50
22	s	307	CLA	CMD-C2D	-2.14	1.46	1.50
32	a	410	SQD	O3-C3	-2.14	1.37	1.43
26	N	317	CHL	C3B-C4B	2.14	1.47	1.42
22	V	307	CLA	CHC-C1C	2.14	1.42	1.38
25	5	312	LHG	O8-C6	-2.14	1.40	1.45
26	5	316	CHL	C4C-C3C	2.14	1.48	1.45
22	R	302	CLA	CMD-C2D	-2.14	1.46	1.50
25	n	312	LHG	O8-C6	-2.14	1.40	1.45
26	n	316	CHL	C1B-NB	-2.14	1.35	1.37
22	u	307	CLA	CMB-C2B	-2.14	1.46	1.50
22	b	606	CLA	CMD-C2D	-2.14	1.46	1.50
22	4	303	CLA	CMD-C2D	-2.14	1.46	1.50
22	5	304	CLA	CMB-C2B	-2.14	1.46	1.50
26	u	315	CHL	C4B-NB	-2.14	1.35	1.37
22	r	605	CLA	CMB-C2B	-2.14	1.46	1.50
22	U	305	CLA	CMB-C2B	-2.14	1.46	1.50
26	v	314	CHL	C2C-C1C	2.14	1.49	1.44
26	1	318	CHL	C4C-C3C	2.14	1.48	1.45
22	B	614	CLA	CMB-C2B	-2.14	1.46	1.50
26	N	313	CHL	C1D-ND	-2.14	1.35	1.37
22	Q	303	CLA	MG-NB	-2.14	2.01	2.05
26	6	315	CHL	C4C-C3C	2.14	1.48	1.45
22	s	308	CLA	CMB-C2B	-2.14	1.46	1.50
22	A	408	CLA	C1B-C2B	2.14	1.48	1.43
22	R	311	CLA	CMB-C2B	-2.14	1.46	1.50
25	C	524	LHG	O7-C7	2.14	1.40	1.34
26	6	317	CHL	CHB-C4A	-2.14	1.32	1.37
26	u	317	CHL	C1B-NB	-2.14	1.35	1.37
22	u	307	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	302	CLA	CMD-C2D	-2.14	1.46	1.50
22	4	302	CLA	CMD-C2D	-2.14	1.46	1.50
22	6	308	CLA	CMD-C2D	-2.14	1.46	1.50
22	S	301	CLA	CMD-C2D	-2.14	1.46	1.50
22	B	610	CLA	CMD-C2D	-2.14	1.46	1.50
22	3	307	CLA	CMD-C2D	-2.14	1.46	1.50
26	u	313	CHL	C1D-ND	-2.14	1.35	1.37
24	u	311	XAT	C40-C33	2.14	1.55	1.50
22	s	302	CLA	CMD-C2D	-2.14	1.46	1.50
26	q	312	CHL	C4D-CHA	2.14	1.46	1.38
22	S	302	CLA	CMD-C2D	-2.14	1.46	1.50
22	C	513	CLA	CMC-C2C	-2.14	1.46	1.50
32	m	101	SQD	O2-C2	-2.14	1.37	1.43
26	Q	315	CHL	MG-NA	-2.14	2.01	2.06
26	u	314	CHL	C4B-NB	-2.14	1.35	1.37
22	B	608	CLA	CMC-C2C	-2.13	1.46	1.50
26	1	317	CHL	CHB-C4A	-2.13	1.32	1.37
26	3	316	CHL	CHB-C4A	-2.13	1.32	1.37
22	C	514	CLA	CMB-C2B	-2.13	1.46	1.50
22	B	613	CLA	MG-ND	-2.13	2.01	2.05
33	D	405	PL9	C6-C1	2.13	1.52	1.48
22	V	306	CLA	CMD-C2D	-2.13	1.46	1.50
22	q	304	CLA	MG-NB	-2.13	2.01	2.05
22	r	601	CLA	CMC-C2C	-2.13	1.46	1.50
22	c	505	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	512	CLA	CMC-C2C	-2.13	1.46	1.50
26	G	315	CHL	MG-NA	-2.13	2.01	2.06
22	b	614	CLA	MG-ND	-2.13	2.01	2.05
22	v	307	CLA	CHC-C1C	2.13	1.42	1.38
22	B	606	CLA	CMC-C2C	-2.13	1.46	1.50
36	B	601	DGD	O3G-C1D	-2.13	1.36	1.40
22	4	302	CLA	MG-NB	-2.13	2.01	2.05
22	R	307	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	503	CLA	CAC-C3C	-2.13	1.45	1.51
25	3	310	LHG	O7-C7	2.13	1.40	1.34
22	C	510	CLA	C1B-NB	-2.13	1.35	1.37
26	p	319	CHL	C1D-ND	-2.13	1.35	1.37
22	S	303	CLA	CMD-C2D	-2.13	1.46	1.50
22	B	616	CLA	CMB-C2B	-2.13	1.46	1.50
22	c	514	CLA	CMC-C2C	-2.13	1.46	1.50
22	5	305	CLA	MG-NB	-2.13	2.01	2.05
34	A	411	LMG	O1-C7	-2.13	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	316	CHL	C1D-ND	-2.13	1.35	1.37
22	Q	307	CLA	CMD-C2D	-2.13	1.46	1.50
22	b	614	CLA	CMB-C2B	-2.13	1.46	1.50
26	g	311	CHL	CHB-C4A	-2.13	1.32	1.37
22	n	304	CLA	MG-NB	-2.13	2.01	2.05
22	R	311	CLA	MG-NB	-2.13	2.01	2.05
22	u	306	CLA	CMC-C2C	-2.13	1.46	1.50
22	s	308	CLA	CMD-C2D	-2.13	1.46	1.50
26	G	313	CHL	MG-NA	-2.13	2.01	2.06
34	B	624	LMG	O1-C1	-2.13	1.36	1.40
26	2	315	CHL	C4C-C3C	2.13	1.48	1.45
22	3	302	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	506	CLA	CMC-C2C	-2.13	1.46	1.50
22	A	408	CLA	CMC-C2C	-2.13	1.46	1.50
25	P	313	LHG	O7-C7	2.13	1.40	1.34
22	Q	304	CLA	CHC-C1C	2.13	1.42	1.38
22	N	308	CLA	MG-NB	-2.13	2.01	2.05
22	6	309	CLA	CHC-C1C	2.13	1.42	1.38
22	4	305	CLA	CMB-C2B	-2.13	1.46	1.50
22	U	307	CLA	CMD-C2D	-2.13	1.46	1.50
22	4	301	CLA	C1B-C2B	2.13	1.48	1.43
22	b	613	CLA	C1B-NB	-2.13	1.35	1.37
25	A	413	LHG	O8-C23	2.13	1.39	1.33
22	c	508	CLA	CMC-C2C	-2.13	1.46	1.50
24	1	311	XAT	C28-C27	2.13	1.37	1.32
26	2	318	CHL	CHB-C4A	-2.13	1.32	1.37
22	u	303	CLA	CMC-C2C	-2.13	1.46	1.50
24	q	309	XAT	C8-C7	2.12	1.37	1.32
22	6	305	CLA	CHC-C1C	2.12	1.42	1.38
26	s	314	CHL	MG-NA	-2.12	2.01	2.06
22	U	306	CLA	CMC-C2C	-2.12	1.46	1.50
26	N	316	CHL	C1D-ND	-2.12	1.35	1.37
22	b	608	CLA	CMC-C2C	-2.12	1.46	1.50
26	u	316	CHL	CHB-C4A	-2.12	1.32	1.37
22	Q	306	CLA	MG-NB	-2.12	2.01	2.05
22	q	301	CLA	CMC-C2C	-2.12	1.46	1.50
26	u	317	CHL	C4B-NB	-2.12	1.35	1.37
22	4	307	CLA	CMD-C2D	-2.12	1.46	1.50
22	C	507	CLA	CMC-C2C	-2.12	1.46	1.50
22	s	303	CLA	CMD-C2D	-2.12	1.46	1.50
22	U	304	CLA	CMD-C2D	-2.12	1.46	1.50
22	b	610	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	CMB-C2B	-2.12	1.46	1.50
32	a	410	SQD	O4-C4	-2.12	1.38	1.43
22	1	301	CLA	CMC-C2C	-2.12	1.46	1.50
37	e	101	HEM	C2A-C3A	-2.12	1.33	1.38
22	r	607	CLA	CMB-C2B	-2.12	1.46	1.50
22	n	302	CLA	CMD-C2D	-2.12	1.46	1.50
26	r	619	CHL	CHB-C4A	-2.12	1.32	1.37
22	Q	301	CLA	C1B-C2B	2.12	1.48	1.43
22	B	603	CLA	CMB-C2B	-2.12	1.46	1.50
22	G	304	CLA	MG-NB	-2.12	2.01	2.05
26	V	314	CHL	MG-NA	-2.12	2.01	2.06
22	C	515	CLA	CMC-C2C	-2.12	1.46	1.50
25	r	613	LHG	O7-C7	2.12	1.40	1.34
26	6	312	CHL	C1D-ND	-2.12	1.35	1.37
32	M	101	SQD	O2-C2	-2.12	1.38	1.43
22	2	301	CLA	C1B-C2B	2.12	1.48	1.43
26	g	311	CHL	MG-NA	-2.12	2.01	2.06
22	4	306	CLA	CMB-C2B	-2.12	1.46	1.50
22	g	304	CLA	CMD-C2D	-2.12	1.46	1.50
22	s	304	CLA	CMD-C2D	-2.12	1.46	1.50
22	s	307	CLA	CMC-C2C	-2.12	1.46	1.50
22	c	509	CLA	C1B-NB	-2.12	1.35	1.37
26	R	317	CHL	C4B-NB	-2.12	1.35	1.37
26	r	619	CHL	C4C-C3C	2.12	1.48	1.45
22	G	308	CLA	CHC-C1C	2.12	1.42	1.38
22	q	307	CLA	CMC-C2C	-2.12	1.46	1.50
26	5	318	CHL	CHB-C4A	-2.12	1.32	1.37
24	g	309	XAT	C20-C13	2.12	1.55	1.50
22	g	308	CLA	CHC-C1C	2.12	1.42	1.38
26	q	314	CHL	MG-NA	-2.12	2.01	2.06
22	2	302	CLA	MG-NB	-2.12	2.01	2.05
26	P	315	CHL	C2C-C1C	2.12	1.49	1.44
22	v	308	CLA	CMD-C2D	-2.12	1.46	1.50
22	N	304	CLA	CMB-C2B	-2.12	1.46	1.50
26	P	318	CHL	C1D-ND	-2.12	1.35	1.37
22	g	304	CLA	MG-NB	-2.12	2.01	2.05
22	C	514	CLA	CMC-C2C	-2.12	1.46	1.50
22	g	301	CLA	CHC-C1C	2.12	1.42	1.38
25	q	310	LHG	O7-C7	2.12	1.40	1.34
22	r	610	CLA	CMB-C2B	-2.12	1.46	1.50
22	G	305	CLA	CMB-C2B	-2.12	1.46	1.50
22	s	303	CLA	CMC-C2C	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	301	CLA	CHC-C1C	2.12	1.42	1.38
26	q	315	CHL	C4C-C3C	2.12	1.48	1.45
22	p	303	CLA	CMB-C2B	-2.12	1.46	1.50
22	Q	308	CLA	CMD-C2D	-2.12	1.46	1.50
22	b	603	CLA	CMB-C2B	-2.12	1.46	1.50
26	Q	316	CHL	C4C-C3C	2.12	1.48	1.45
22	a	406	CLA	MG-ND	-2.12	2.01	2.05
22	a	404	CLA	CMB-C2B	-2.12	1.46	1.50
22	C	504	CLA	C1B-NB	-2.11	1.35	1.37
26	V	314	CHL	C4D-CHA	2.11	1.45	1.38
22	V	302	CLA	CMD-C2D	-2.11	1.46	1.50
26	1	316	CHL	C4C-C3C	2.11	1.48	1.45
22	q	301	CLA	CMB-C2B	-2.11	1.46	1.50
22	C	506	CLA	CMC-C2C	-2.11	1.46	1.50
22	G	301	CLA	C1B-C2B	2.11	1.48	1.43
26	s	315	CHL	C4C-C3C	2.11	1.48	1.45
22	6	302	CLA	CHC-C1C	2.11	1.42	1.38
22	p	306	CLA	MG-NB	-2.11	2.01	2.05
26	2	315	CHL	CHB-C4A	-2.11	1.32	1.37
25	1	312	LHG	O8-C6	-2.11	1.40	1.45
24	5	311	XAT	C28-C27	2.11	1.37	1.32
25	g	310	LHG	O8-C6	-2.11	1.40	1.45
25	c	522	LHG	O8-C6	-2.11	1.40	1.45
26	6	315	CHL	C2C-C1C	2.11	1.49	1.44
22	a	404	CLA	C1B-NB	-2.11	1.35	1.37
22	x	201	CLA	C1B-NB	-2.11	1.35	1.37
22	S	305	CLA	CMC-C2C	-2.11	1.46	1.50
22	R	308	CLA	MG-NB	-2.11	2.01	2.05
32	A	412	SQD	O4-C4	-2.11	1.38	1.43
22	V	305	CLA	CMD-C2D	-2.11	1.46	1.50
22	N	303	CLA	CMD-C2D	-2.11	1.46	1.50
24	r	612	XAT	C40-C33	2.11	1.55	1.50
22	3	304	CLA	CHC-C1C	2.11	1.42	1.38
22	4	301	CLA	CMC-C2C	-2.11	1.46	1.50
22	n	308	CLA	CMB-C2B	-2.11	1.46	1.50
22	2	301	CLA	CMB-C2B	-2.11	1.46	1.50
22	b	614	CLA	CMD-C2D	-2.11	1.46	1.50
26	U	316	CHL	C4C-C3C	2.11	1.48	1.45
22	2	305	CLA	MG-NB	-2.11	2.01	2.05
22	S	304	CLA	CMD-C2D	-2.11	1.46	1.50
24	6	310	XAT	C28-C27	2.11	1.37	1.32
22	5	304	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	p	305	CLA	CMC-C2C	-2.11	1.46	1.50
22	U	303	CLA	CMD-C2D	-2.11	1.46	1.50
22	u	304	CLA	CMD-C2D	-2.11	1.46	1.50
36	c	519	DGD	O5D-C1E	-2.11	1.36	1.40
26	p	319	CHL	CHB-C4A	-2.11	1.32	1.37
26	G	311	CHL	CHB-C4A	-2.11	1.32	1.37
22	r	608	CLA	MG-NB	-2.11	2.01	2.05
26	p	315	CHL	C2C-C1C	2.11	1.49	1.44
26	g	315	CHL	CHB-C4A	-2.11	1.32	1.37
24	U	311	XAT	C20-C13	2.11	1.55	1.50
26	u	318	CHL	C4C-C3C	2.11	1.48	1.45
22	R	305	CLA	MG-NB	-2.11	2.01	2.05
22	v	302	CLA	CMC-C2C	-2.11	1.46	1.50
22	q	301	CLA	CMD-C2D	-2.11	1.46	1.50
22	3	308	CLA	CHC-C1C	2.11	1.42	1.38
22	s	304	CLA	CHC-C1C	2.11	1.42	1.38
37	E	101	HEM	C2A-C3A	-2.11	1.33	1.38
26	V	313	CHL	C4B-NB	-2.11	1.35	1.37
26	u	314	CHL	C1D-ND	-2.11	1.35	1.37
22	r	604	CLA	CMB-C2B	-2.11	1.46	1.50
22	5	301	CLA	CHC-C1C	2.11	1.42	1.38
26	n	316	CHL	C1D-ND	-2.11	1.35	1.37
22	R	303	CLA	CMB-C2B	-2.11	1.46	1.50
26	4	316	CHL	CHB-C4A	-2.11	1.32	1.37
22	B	602	CLA	MG-ND	-2.11	2.01	2.05
26	n	313	CHL	C2C-C1C	2.11	1.49	1.44
22	2	304	CLA	CMC-C2C	-2.11	1.46	1.50
22	2	307	CLA	CMD-C2D	-2.11	1.46	1.50
22	4	304	CLA	CMB-C2B	-2.11	1.46	1.50
22	b	605	CLA	CMD-C2D	-2.11	1.46	1.50
22	v	302	CLA	CMB-C2B	-2.11	1.46	1.50
22	u	303	CLA	CMD-C2D	-2.11	1.46	1.50
26	1	313	CHL	C1B-C2B	2.11	1.48	1.43
22	N	306	CLA	CMD-C2D	-2.11	1.46	1.50
22	1	306	CLA	MG-ND	-2.11	2.01	2.05
22	b	613	CLA	MG-ND	-2.11	2.01	2.05
22	b	602	CLA	CMC-C2C	-2.10	1.46	1.50
34	a	412	LMG	O1-C7	-2.10	1.39	1.43
22	V	303	CLA	CMD-C2D	-2.10	1.46	1.50
26	v	313	CHL	C1D-ND	-2.10	1.35	1.37
22	b	609	CLA	MG-ND	-2.10	2.01	2.05
22	B	605	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	311	CHL	C1D-ND	-2.10	1.35	1.37
26	Q	313	CHL	C1D-ND	-2.10	1.35	1.37
22	b	610	CLA	MG-NB	-2.10	2.01	2.05
22	U	306	CLA	MG-ND	-2.10	2.01	2.05
22	1	305	CLA	CMB-C2B	-2.10	1.46	1.50
26	g	315	CHL	MG-NA	-2.10	2.01	2.06
26	r	619	CHL	C1D-ND	-2.10	1.35	1.37
26	R	316	CHL	C4B-NB	-2.10	1.35	1.37
26	5	313	CHL	C2C-C1C	2.10	1.49	1.44
26	5	314	CHL	C1D-ND	-2.10	1.35	1.37
22	b	602	CLA	MG-ND	-2.10	2.01	2.05
22	A	404	CLA	CMB-C2B	-2.10	1.46	1.50
22	G	307	CLA	CMB-C2B	-2.10	1.46	1.50
25	4	312	LHG	O8-C6	-2.10	1.40	1.45
22	p	302	CLA	CMB-C2B	-2.10	1.46	1.50
22	S	308	CLA	CMD-C2D	-2.10	1.46	1.50
22	c	511	CLA	CMC-C2C	-2.10	1.46	1.50
24	q	309	XAT	C28-C27	2.10	1.37	1.32
22	4	307	CLA	CMC-C2C	-2.10	1.46	1.50
22	b	612	CLA	MG-NB	-2.10	2.01	2.05
36	A	414	DGD	O6E-C5E	2.10	1.49	1.44
22	6	303	CLA	CMD-C2D	-2.10	1.46	1.50
22	g	307	CLA	CMB-C2B	-2.10	1.46	1.50
22	n	308	CLA	MG-NB	-2.10	2.01	2.05
22	1	308	CLA	CMD-C2D	-2.10	1.46	1.50
22	u	305	CLA	CMB-C2B	-2.10	1.46	1.50
22	R	306	CLA	CMD-C2D	-2.10	1.46	1.50
24	u	311	XAT	C20-C13	2.10	1.55	1.50
22	Q	305	CLA	CHC-C1C	2.10	1.42	1.38
22	Q	303	CLA	CMD-C2D	-2.10	1.46	1.50
22	G	305	CLA	CMD-C2D	-2.10	1.46	1.50
36	C	520	DGD	O2G-C2G	-2.10	1.41	1.46
22	v	307	CLA	CMD-C2D	-2.10	1.46	1.50
22	D	403	CLA	CMB-C2B	-2.10	1.46	1.50
32	A	412	SQD	O3-C3	-2.10	1.38	1.43
26	4	314	CHL	C4B-NB	-2.10	1.35	1.37
26	N	316	CHL	C1B-NB	-2.10	1.35	1.37
22	2	307	CLA	CHC-C1C	2.10	1.42	1.38
22	N	304	CLA	CMD-C2D	-2.10	1.46	1.50
26	u	318	CHL	C1B-C2B	2.10	1.48	1.43
26	4	317	CHL	C1D-ND	-2.10	1.35	1.37
22	R	306	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	414	DGD	O2G-C2G	-2.10	1.41	1.46
22	q	308	CLA	CMD-C2D	-2.10	1.46	1.50
22	A	408	CLA	CHC-C1C	2.10	1.42	1.38
26	v	317	CHL	C1D-ND	-2.10	1.35	1.37
22	G	307	CLA	MG-NB	-2.10	2.01	2.05
26	r	615	CHL	C4B-NB	-2.10	1.35	1.37
26	3	315	CHL	C4B-NB	-2.10	1.35	1.37
26	Q	312	CHL	C4B-NB	-2.10	1.35	1.37
26	N	315	CHL	C4B-NB	-2.10	1.35	1.37
22	r	604	CLA	MG-NB	-2.09	2.01	2.05
22	6	307	CLA	CMD-C2D	-2.09	1.46	1.50
22	c	506	CLA	C1B-NB	-2.09	1.35	1.37
22	v	307	CLA	CMC-C2C	-2.09	1.46	1.50
22	Q	302	CLA	CMB-C2B	-2.09	1.46	1.50
26	3	314	CHL	C4C-C3C	2.09	1.48	1.45
26	q	314	CHL	C2C-C1C	2.09	1.49	1.44
26	v	316	CHL	C4C-C3C	2.09	1.48	1.45
26	P	317	CHL	C1D-ND	-2.09	1.35	1.37
36	J	101	DGD	O5D-C1E	-2.09	1.36	1.40
22	c	513	CLA	CMC-C2C	-2.09	1.46	1.50
24	4	311	XAT	C28-C27	2.09	1.37	1.32
22	r	607	CLA	MG-NB	-2.09	2.01	2.05
22	n	301	CLA	CMB-C2B	-2.09	1.46	1.50
22	S	307	CLA	CMC-C2C	-2.09	1.46	1.50
26	q	312	CHL	C1D-ND	-2.09	1.35	1.37
26	P	314	CHL	C4B-NB	-2.09	1.35	1.37
22	B	612	CLA	MG-NB	-2.09	2.01	2.05
22	B	609	CLA	C1B-NB	-2.09	1.35	1.37
26	S	313	CHL	C1D-ND	-2.09	1.35	1.37
22	1	307	CLA	CMD-C2D	-2.09	1.46	1.50
22	n	303	CLA	CHC-C1C	2.09	1.42	1.38
36	c	518	DGD	O2G-C2G	-2.09	1.41	1.46
22	1	305	CLA	CMD-C2D	-2.09	1.46	1.50
22	p	304	CLA	CMD-C2D	-2.09	1.46	1.50
26	u	316	CHL	C1B-NB	-2.09	1.35	1.37
32	a	413	SQD	O4-C4	-2.09	1.38	1.43
22	g	302	CLA	CMD-C2D	-2.09	1.46	1.50
22	R	302	CLA	CMB-C2B	-2.09	1.46	1.50
22	A	406	CLA	MG-ND	-2.09	2.01	2.05
26	n	316	CHL	C4C-C3C	2.09	1.48	1.45
26	R	317	CHL	C2C-C1C	2.09	1.49	1.44
22	n	307	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	313	CHL	CHB-C4A	-2.09	1.32	1.37
22	1	304	CLA	CMB-C2B	-2.09	1.46	1.50
26	n	314	CHL	C4D-CHA	2.09	1.45	1.38
22	r	605	CLA	CMD-C2D	-2.09	1.46	1.50
26	V	314	CHL	C2C-C1C	2.09	1.49	1.44
22	S	309	CLA	CHC-C1C	2.09	1.42	1.38
22	v	301	CLA	CMC-C2C	-2.09	1.46	1.50
22	v	302	CLA	CMD-C2D	-2.09	1.46	1.50
22	S	309	CLA	CMB-C2B	-2.09	1.46	1.50
22	G	302	CLA	CMD-C2D	-2.09	1.46	1.50
26	4	314	CHL	C1D-ND	-2.09	1.35	1.37
26	V	313	CHL	C1D-ND	-2.09	1.35	1.37
22	5	304	CLA	CHC-C1C	2.09	1.42	1.38
22	1	307	CLA	CMC-C2C	-2.09	1.46	1.50
22	C	511	CLA	CMB-C2B	-2.09	1.46	1.50
26	2	313	CHL	C2C-C1C	2.09	1.49	1.44
26	5	314	CHL	C4D-CHA	2.09	1.45	1.38
37	E	101	HEM	CMB-C2B	2.09	1.55	1.50
26	Q	311	CHL	C4C-C3C	2.09	1.48	1.45
22	q	305	CLA	CMD-C2D	-2.09	1.46	1.50
24	g	309	XAT	C28-C27	2.08	1.37	1.32
22	r	602	CLA	CMB-C2B	-2.08	1.46	1.50
33	d	404	PL9	C6-C1	2.08	1.52	1.48
26	2	313	CHL	C4C-C3C	2.08	1.48	1.45
22	V	308	CLA	CMD-C2D	-2.08	1.46	1.50
22	g	305	CLA	CMD-C2D	-2.08	1.46	1.50
26	6	312	CHL	C2C-C1C	2.08	1.49	1.44
22	g	307	CLA	MG-NB	-2.08	2.01	2.05
32	a	413	SQD	O3-C3	-2.08	1.38	1.43
24	v	311	XAT	C28-C27	2.08	1.37	1.32
26	5	315	CHL	CHB-C4A	-2.08	1.32	1.37
24	N	311	XAT	C28-C27	2.08	1.37	1.32
22	5	301	CLA	CMB-C2B	-2.08	1.46	1.50
22	v	301	CLA	CMD-C2D	-2.08	1.46	1.50
22	V	301	CLA	CMC-C2C	-2.08	1.46	1.50
22	N	307	CLA	CMC-C2C	-2.08	1.46	1.50
26	U	317	CHL	C4B-NB	-2.08	1.35	1.37
22	q	306	CLA	MG-NB	-2.08	2.01	2.05
22	p	308	CLA	CMC-C2C	-2.08	1.46	1.50
26	2	315	CHL	C1D-ND	-2.08	1.35	1.37
34	D	408	LMG	O1-C7	-2.08	1.39	1.43
22	q	305	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	u	305	CLA	CHC-C1C	2.08	1.42	1.38
26	G	316	CHL	CHB-C4A	-2.08	1.32	1.37
26	6	313	CHL	C2C-C1C	2.08	1.49	1.44
22	r	601	CLA	CMD-C2D	-2.08	1.46	1.50
22	p	302	CLA	CMD-C2D	-2.08	1.46	1.50
22	X	202	CLA	CMC-C2C	-2.08	1.46	1.50
22	r	605	CLA	CHC-C1C	2.08	1.42	1.38
22	n	302	CLA	MG-NB	-2.08	2.01	2.05
22	R	306	CLA	MG-NB	-2.08	2.01	2.05
22	q	303	CLA	CMB-C2B	-2.08	1.46	1.50
22	P	308	CLA	CMC-C2C	-2.08	1.46	1.50
25	S	312	LHG	O7-C7	2.08	1.40	1.34
25	s	312	LHG	O7-C7	2.08	1.40	1.34
22	N	302	CLA	MG-NB	-2.08	2.01	2.05
22	3	308	CLA	CMD-C2D	-2.08	1.46	1.50
22	v	308	CLA	CHC-C1C	2.08	1.42	1.38
22	B	608	CLA	CMD-C2D	-2.08	1.46	1.50
26	3	315	CHL	C1B-NB	-2.08	1.35	1.37
26	U	319	CHL	CHB-C4A	-2.08	1.32	1.37
26	3	314	CHL	C2C-C1C	2.08	1.49	1.44
36	a	416	DGD	O2G-C2G	-2.08	1.41	1.46
26	4	317	CHL	CHB-C4A	-2.08	1.32	1.37
22	4	306	CLA	MG-NB	-2.08	2.01	2.05
22	B	617	CLA	MG-ND	-2.08	2.01	2.05
22	2	301	CLA	CHC-C1C	2.08	1.42	1.38
22	u	304	CLA	CHC-C1C	2.08	1.42	1.38
22	p	309	CLA	CMD-C2D	-2.08	1.46	1.50
22	V	307	CLA	CMC-C2C	-2.08	1.46	1.50
22	N	301	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	602	CLA	CMB-C2B	-2.08	1.46	1.50
22	r	609	CLA	MG-NB	-2.08	2.01	2.05
27	N	318	NEX	O24-C25	-2.08	1.43	1.46
22	C	512	CLA	CMC-C2C	-2.08	1.46	1.50
26	3	311	CHL	CHB-C4A	-2.08	1.32	1.37
26	n	316	CHL	CHB-C4A	-2.08	1.32	1.37
22	3	307	CLA	CMC-C2C	-2.08	1.46	1.50
22	P	302	CLA	CMD-C2D	-2.08	1.46	1.50
22	n	301	CLA	CMD-C2D	-2.08	1.46	1.50
26	V	317	CHL	C1D-ND	-2.08	1.35	1.37
22	r	601	CLA	CMB-C2B	-2.08	1.46	1.50
22	R	308	CLA	CMD-C2D	-2.08	1.46	1.50
22	c	504	CLA	CMB-C2B	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	313	CHL	C4C-C3C	2.08	1.48	1.45
22	r	605	CLA	MG-NB	-2.07	2.01	2.05
22	u	306	CLA	MG-ND	-2.07	2.01	2.05
26	v	313	CHL	C4B-NB	-2.07	1.35	1.37
22	1	302	CLA	CMB-C2B	-2.07	1.46	1.50
22	Q	308	CLA	CHC-C1C	2.07	1.42	1.38
22	2	304	CLA	CMB-C2B	-2.07	1.46	1.50
22	3	304	CLA	CMD-C2D	-2.07	1.46	1.50
22	U	303	CLA	CMC-C2C	-2.07	1.46	1.50
22	R	305	CLA	CMB-C2B	-2.07	1.46	1.50
22	b	604	CLA	CMC-C2C	-2.07	1.46	1.50
26	1	313	CHL	CHB-C4A	-2.07	1.32	1.37
26	6	312	CHL	CHB-C4A	-2.07	1.32	1.37
26	U	314	CHL	CHB-C4A	-2.07	1.32	1.37
22	V	301	CLA	CMD-C2D	-2.07	1.46	1.50
22	N	308	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	615	CLA	CMC-C2C	-2.07	1.46	1.50
22	r	601	CLA	MG-NB	-2.07	2.01	2.05
22	r	601	CLA	CHC-C1C	2.07	1.42	1.38
25	B	623	LHG	O8-C6	-2.07	1.40	1.45
22	s	306	CLA	MG-ND	-2.07	2.01	2.05
26	q	315	CHL	CHB-C4A	-2.07	1.32	1.37
22	b	603	CLA	CMC-C2C	-2.07	1.46	1.50
22	1	303	CLA	CMD-C2D	-2.07	1.46	1.50
22	1	306	CLA	CMC-C2C	-2.07	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.07	1.46	1.50
22	c	508	CLA	C1B-NB	-2.07	1.35	1.37
22	a	408	CLA	MG-ND	-2.07	2.01	2.05
22	B	610	CLA	CMC-C2C	-2.07	1.46	1.50
22	P	305	CLA	CHC-C1C	2.07	1.42	1.38
26	n	313	CHL	C4C-C3C	2.07	1.48	1.45
22	u	304	CLA	C1B-NB	-2.07	1.35	1.37
22	p	302	CLA	C1B-C2B	2.07	1.48	1.43
26	4	313	CHL	C4C-C3C	2.07	1.48	1.45
22	6	309	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	305	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	309	CLA	CMC-C2C	-2.07	1.46	1.50
26	Q	316	CHL	CHB-C4A	-2.07	1.32	1.37
22	2	303	CLA	CMC-C2C	-2.07	1.46	1.50
22	3	306	CLA	CMD-C2D	-2.07	1.46	1.50
22	G	308	CLA	CMD-C2D	-2.07	1.46	1.50
22	r	607	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	619	CHL	C4B-NB	-2.07	1.35	1.37
22	V	307	CLA	CMB-C2B	-2.07	1.46	1.50
22	B	610	CLA	MG-NB	-2.07	2.01	2.05
22	c	512	CLA	MG-ND	-2.07	2.01	2.05
26	g	311	CHL	C4C-C3C	2.07	1.48	1.45
22	r	603	CLA	CHC-C1C	2.07	1.42	1.38
24	n	311	XAT	C28-C27	2.07	1.37	1.32
22	A	405	CLA	CMC-C2C	-2.07	1.46	1.50
22	4	302	CLA	CMB-C2B	-2.07	1.46	1.50
22	n	307	CLA	CMC-C2C	-2.07	1.46	1.50
22	V	301	CLA	CHC-C1C	2.07	1.42	1.38
26	g	311	CHL	C2C-C1C	2.07	1.49	1.44
26	g	315	CHL	C4C-C3C	2.07	1.48	1.45
22	P	304	CLA	CMD-C2D	-2.07	1.46	1.50
36	a	416	DGD	O6E-C5E	2.07	1.49	1.44
22	3	301	CLA	CMD-C2D	-2.07	1.46	1.50
22	S	302	CLA	CMB-C2B	-2.07	1.46	1.50
26	q	311	CHL	C1D-ND	-2.07	1.35	1.37
22	s	302	CLA	CMB-C2B	-2.07	1.46	1.50
26	r	615	CHL	C2C-C1C	2.07	1.49	1.44
22	C	511	CLA	CMC-C2C	-2.07	1.46	1.50
22	s	305	CLA	CMC-C2C	-2.07	1.46	1.50
22	S	306	CLA	MG-ND	-2.07	2.01	2.05
22	4	301	CLA	CHC-C1C	2.07	1.42	1.38
22	R	306	CLA	CHC-C1C	2.07	1.42	1.38
22	v	306	CLA	CMB-C2B	-2.07	1.46	1.50
22	s	302	CLA	MG-NB	-2.06	2.01	2.05
22	3	304	CLA	CMC-C2C	-2.06	1.46	1.50
22	u	301	CLA	CMD-C2D	-2.06	1.46	1.50
22	6	302	CLA	CMB-C2B	-2.06	1.46	1.50
22	b	610	CLA	CMC-C2C	-2.06	1.46	1.50
22	B	613	CLA	C1B-NB	-2.06	1.35	1.37
26	N	317	CHL	CHB-C4A	-2.06	1.32	1.37
22	4	305	CLA	CMD-C2D	-2.06	1.46	1.50
22	4	308	CLA	CMD-C2D	-2.06	1.46	1.50
22	6	304	CLA	CMC-C2C	-2.06	1.46	1.50
26	n	315	CHL	C1D-ND	-2.06	1.35	1.37
22	1	308	CLA	CMB-C2B	-2.06	1.46	1.50
25	b	623	LHG	O8-C6	-2.06	1.40	1.45
26	p	320	CHL	CHB-C4A	-2.06	1.32	1.37
32	M	101	SQD	O4-C4	-2.06	1.38	1.43
26	n	317	CHL	C1C-NC	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	507	CLA	CMB-C2B	-2.06	1.46	1.50
34	w	201	LMG	O1-C7	-2.06	1.40	1.43
22	B	616	CLA	CMD-C2D	-2.06	1.46	1.50
36	c	517	DGD	O3G-C1D	-2.06	1.36	1.40
22	u	302	CLA	CMC-C2C	-2.06	1.46	1.50
22	C	505	CLA	CMC-C2C	-2.06	1.46	1.50
26	G	315	CHL	C4C-C3C	2.06	1.48	1.45
26	1	317	CHL	C1D-ND	-2.06	1.35	1.37
22	2	301	CLA	CMD-C2D	-2.06	1.46	1.50
22	4	308	CLA	CMB-C2B	-2.06	1.46	1.50
22	s	306	CLA	CMC-C2C	-2.06	1.46	1.50
22	P	302	CLA	C1B-C2B	2.06	1.48	1.43
24	2	311	XAT	C8-C7	2.06	1.37	1.32
22	b	609	CLA	C1B-NB	-2.06	1.35	1.37
22	r	606	CLA	CHC-C1C	2.06	1.42	1.38
22	g	303	CLA	CHC-C1C	2.06	1.42	1.38
27	u	320	NEX	O24-C25	-2.06	1.43	1.46
22	G	306	CLA	MG-NB	-2.06	2.01	2.05
22	v	307	CLA	CMB-C2B	-2.06	1.46	1.50
22	G	304	CLA	CMD-C2D	-2.06	1.46	1.50
22	C	505	CLA	CMB-C2B	-2.06	1.46	1.50
26	N	316	CHL	CHB-C4A	-2.06	1.32	1.37
22	P	303	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	604	CLA	CMC-C2C	-2.06	1.46	1.50
22	c	510	CLA	CMC-C2C	-2.06	1.46	1.50
37	e	101	HEM	CMB-C2B	2.06	1.55	1.50
22	x	201	CLA	CMC-C2C	-2.06	1.46	1.50
22	g	302	CLA	CMC-C2C	-2.06	1.46	1.50
22	c	509	CLA	MG-ND	-2.06	2.01	2.05
22	r	606	CLA	CMB-C2B	-2.06	1.46	1.50
22	G	303	CLA	CMD-C2D	-2.06	1.46	1.50
22	6	308	CLA	CHC-C1C	2.06	1.42	1.38
26	G	313	CHL	C4B-NB	-2.06	1.35	1.37
32	m	101	SQD	O4-C4	-2.06	1.38	1.43
22	V	302	CLA	CMB-C2B	-2.06	1.46	1.50
26	1	314	CHL	CHB-C4A	-2.06	1.32	1.37
26	U	316	CHL	CHB-C4A	-2.06	1.32	1.37
26	r	615	CHL	MG-NA	-2.06	2.01	2.06
22	B	610	CLA	CHC-C1C	2.06	1.42	1.38
22	P	307	CLA	CMD-C2D	-2.06	1.46	1.50
22	n	304	CLA	CMB-C2B	-2.06	1.46	1.50
22	G	304	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	CLA	C1B-NB	-2.05	1.35	1.37
26	6	301	CHL	C1D-ND	-2.05	1.35	1.37
32	l	102	SQD	O3-C3	-2.05	1.38	1.43
22	6	302	CLA	CMD-C2D	-2.05	1.46	1.50
22	p	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	R	302	CLA	MG-NB	-2.05	2.01	2.05
22	R	303	CLA	CHC-C1C	2.05	1.42	1.38
22	a	405	CLA	MG-ND	-2.05	2.01	2.05
22	6	304	CLA	CMD-C2D	-2.05	1.46	1.50
22	V	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	N	307	CLA	CMB-C2B	-2.05	1.46	1.50
22	5	301	CLA	C1B-C2B	2.05	1.48	1.43
26	1	316	CHL	CHB-C4A	-2.05	1.32	1.37
22	B	605	CLA	C1B-NB	-2.05	1.35	1.37
22	1	303	CLA	MG-ND	-2.05	2.01	2.05
26	N	313	CHL	CHB-C4A	-2.05	1.32	1.37
22	5	307	CLA	CMD-C2D	-2.05	1.46	1.50
22	c	510	CLA	CMB-C2B	-2.05	1.46	1.50
22	b	610	CLA	CHC-C1C	2.05	1.42	1.38
22	n	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	g	301	CLA	CMD-C2D	-2.05	1.46	1.50
22	P	309	CLA	CHC-C1C	2.05	1.42	1.38
34	W	201	LMG	O1-C7	-2.05	1.40	1.43
22	4	304	CLA	CMD-C2D	-2.05	1.46	1.50
22	S	308	CLA	CMC-C2C	-2.05	1.46	1.50
22	v	302	CLA	CHC-C1C	2.05	1.42	1.38
26	1	318	CHL	C1D-ND	-2.05	1.35	1.37
34	B	624	LMG	O1-C7	-2.05	1.40	1.43
22	v	303	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	602	CLA	CMC-C2C	-2.05	1.46	1.50
22	q	308	CLA	CHC-C1C	2.05	1.42	1.38
26	6	316	CHL	CHB-C4A	-2.05	1.32	1.37
26	2	318	CHL	C1D-ND	-2.05	1.35	1.37
24	P	312	XAT	C8-C7	2.05	1.37	1.32
22	4	301	CLA	CMD-C2D	-2.05	1.46	1.50
22	g	308	CLA	CMD-C2D	-2.05	1.46	1.50
26	5	315	CHL	C1D-ND	-2.05	1.35	1.37
22	S	304	CLA	CHC-C1C	2.05	1.42	1.38
22	C	510	CLA	MG-ND	-2.05	2.01	2.05
22	3	307	CLA	CMB-C2B	-2.05	1.46	1.50
22	G	306	CLA	CMD-C2D	-2.05	1.46	1.50
22	g	304	CLA	CMC-C2C	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	CMC-C2C	-2.05	1.46	1.50
22	U	305	CLA	CHC-C1C	2.05	1.42	1.38
27	n	319	NEX	O24-C25	-2.05	1.43	1.46
22	3	307	CLA	CHC-C1C	2.05	1.42	1.38
26	P	317	CHL	C4C-C3C	2.05	1.48	1.45
26	2	317	CHL	CHB-C4A	-2.05	1.32	1.37
26	G	314	CHL	CHB-C4A	-2.05	1.32	1.37
22	3	305	CLA	CMB-C2B	-2.05	1.46	1.50
22	C	510	CLA	C1B-C2B	2.05	1.48	1.43
22	1	307	CLA	CHC-C1C	2.05	1.42	1.38
26	U	319	CHL	C4C-C3C	2.05	1.48	1.45
25	c	523	LHG	O7-C7	2.05	1.40	1.34
22	c	504	CLA	CMC-C2C	-2.05	1.46	1.50
22	r	602	CLA	CHC-C1C	2.05	1.42	1.38
22	B	613	CLA	CHC-C1C	2.05	1.42	1.38
24	G	309	XAT	C40-C33	2.05	1.55	1.50
26	U	317	CHL	MG-NA	-2.05	2.01	2.06
22	1	301	CLA	CMD-C2D	-2.05	1.46	1.50
22	5	307	CLA	CMC-C2C	-2.05	1.46	1.50
22	P	309	CLA	CMD-C2D	-2.05	1.46	1.50
26	Q	311	CHL	C1D-ND	-2.05	1.35	1.37
26	5	317	CHL	CHB-C4A	-2.05	1.32	1.37
22	c	514	CLA	CHC-C1C	2.05	1.42	1.38
22	V	308	CLA	CMB-C2B	-2.05	1.46	1.50
22	P	305	CLA	CMC-C2C	-2.05	1.46	1.50
22	U	302	CLA	CMC-C2C	-2.05	1.46	1.50
22	N	301	CLA	CMC-C2C	-2.05	1.46	1.50
26	u	318	CHL	MG-NA	-2.04	2.01	2.06
24	g	309	XAT	C40-C33	2.04	1.55	1.50
22	n	308	CLA	CMD-C2D	-2.04	1.46	1.50
22	q	304	CLA	CHC-C1C	2.04	1.42	1.38
22	a	405	CLA	CMC-C2C	-2.04	1.46	1.50
22	Q	307	CLA	CMC-C2C	-2.04	1.46	1.50
25	C	523	LHG	O8-C6	-2.04	1.40	1.45
22	G	307	CLA	CHC-C1C	2.04	1.42	1.38
22	g	308	CLA	CMB-C2B	-2.04	1.46	1.50
26	p	317	CHL	C4C-C3C	2.04	1.48	1.45
26	Q	311	CHL	CHB-C4A	-2.04	1.32	1.37
22	3	306	CLA	CMB-C2B	-2.04	1.46	1.50
22	q	303	CLA	CMD-C2D	-2.04	1.46	1.50
22	X	202	CLA	C1B-NB	-2.04	1.35	1.37
22	6	306	CLA	CMB-C2B	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	308	CLA	CMB-C2B	-2.04	1.46	1.50
27	r	617	NEX	O24-C25	-2.04	1.43	1.46
22	3	301	CLA	CHC-C1C	2.04	1.42	1.38
22	V	305	CLA	CHC-C1C	2.04	1.42	1.38
22	q	302	CLA	CMD-C2D	-2.04	1.46	1.50
22	3	301	CLA	CMB-C2B	-2.04	1.46	1.50
22	3	303	CLA	CMD-C2D	-2.04	1.46	1.50
22	5	304	CLA	CMD-C2D	-2.04	1.46	1.50
22	R	310	CLA	CMB-C2B	-2.04	1.46	1.50
22	6	305	CLA	CMC-C2C	-2.04	1.46	1.50
22	R	307	CLA	CMB-C2B	-2.04	1.46	1.50
24	V	311	XAT	C8-C7	2.04	1.37	1.32
22	c	509	CLA	C1B-C2B	2.04	1.48	1.43
22	G	308	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	602	CLA	CMB-C2B	-2.04	1.46	1.50
25	s	312	LHG	O8-C6	-2.04	1.40	1.45
22	1	304	CLA	CMC-C2C	-2.04	1.46	1.50
22	n	305	CLA	C3D-C2D	2.04	1.44	1.39
26	Q	314	CHL	C4C-C3C	2.04	1.48	1.45
22	n	306	CLA	CMD-C2D	-2.04	1.46	1.50
36	C	519	DGD	O3G-C1D	-2.04	1.36	1.40
26	S	314	CHL	C1D-ND	-2.04	1.35	1.37
32	L	102	SQD	O3-C3	-2.04	1.38	1.43
22	5	308	CLA	CMB-C2B	-2.04	1.46	1.50
22	P	303	CLA	CMC-C2C	-2.04	1.46	1.50
24	5	311	XAT	C8-C7	2.04	1.37	1.32
26	u	316	CHL	C4C-C3C	2.04	1.48	1.45
22	2	305	CLA	CMC-C2C	-2.04	1.46	1.50
22	p	308	CLA	CHC-C1C	2.04	1.42	1.38
26	2	313	CHL	C4B-NB	-2.04	1.35	1.37
22	2	306	CLA	CMD-C2D	-2.04	1.46	1.50
22	Q	304	CLA	CMC-C2C	-2.04	1.46	1.50
22	S	306	CLA	CMC-C2C	-2.04	1.46	1.50
26	v	316	CHL	CHB-C4A	-2.04	1.32	1.37
22	N	304	CLA	CMC-C2C	-2.04	1.46	1.50
22	s	309	CLA	CMC-C2C	-2.04	1.46	1.50
22	b	615	CLA	CHC-C1C	2.04	1.42	1.38
22	a	408	CLA	CHC-C1C	2.04	1.42	1.38
22	P	308	CLA	CHC-C1C	2.04	1.42	1.38
25	S	312	LHG	O8-C6	-2.04	1.40	1.45
22	C	513	CLA	MG-ND	-2.04	2.01	2.05
22	a	406	CLA	CMC-C2C	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	303	CLA	CMC-C2C	-2.03	1.46	1.50
26	V	314	CHL	C4B-NB	-2.03	1.35	1.37
22	1	308	CLA	CHC-C1C	2.03	1.42	1.38
22	U	301	CLA	CMD-C2D	-2.03	1.46	1.50
24	v	311	XAT	C8-C7	2.03	1.37	1.32
22	V	302	CLA	CHC-C1C	2.03	1.42	1.38
26	n	317	CHL	CHB-C4A	-2.03	1.32	1.37
22	p	309	CLA	CHC-C1C	2.03	1.42	1.38
22	N	307	CLA	CHC-C1C	2.03	1.42	1.38
22	6	307	CLA	CMB-C2B	-2.03	1.46	1.50
22	n	307	CLA	CMB-C2B	-2.03	1.46	1.50
22	s	305	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	408	CLA	MG-ND	-2.03	2.01	2.05
22	2	308	CLA	CHC-C1C	2.03	1.42	1.38
22	P	309	CLA	CMB-C2B	-2.03	1.46	1.50
22	s	301	CLA	CMB-C2B	-2.03	1.46	1.50
22	4	304	CLA	CMC-C2C	-2.03	1.46	1.50
22	Q	301	CLA	CMC-C2C	-2.03	1.46	1.50
22	c	506	CLA	CMB-C2B	-2.03	1.46	1.50
22	4	307	CLA	CHC-C1C	2.03	1.42	1.38
22	v	301	CLA	CHC-C1C	2.03	1.42	1.38
24	3	309	XAT	C8-C7	2.03	1.37	1.32
22	P	302	CLA	CMC-C2C	-2.03	1.46	1.50
22	Q	306	CLA	CMB-C2B	-2.03	1.46	1.50
22	u	305	CLA	CMC-C2C	-2.03	1.46	1.50
22	3	305	CLA	CHC-C1C	2.03	1.42	1.38
22	q	303	CLA	CHC-C1C	2.03	1.42	1.38
22	C	510	CLA	CHC-C1C	2.03	1.42	1.38
22	v	305	CLA	CMB-C2B	-2.03	1.46	1.50
22	V	305	CLA	CMB-C2B	-2.03	1.46	1.50
22	g	306	CLA	CMD-C2D	-2.03	1.46	1.50
26	r	616	CHL	C2C-C1C	2.03	1.48	1.44
22	5	302	CLA	CMB-C2B	-2.03	1.46	1.50
22	Q	304	CLA	CMD-C2D	-2.03	1.46	1.50
26	R	317	CHL	C1B-C2B	2.03	1.48	1.43
22	V	303	CLA	CMC-C2C	-2.03	1.46	1.50
22	s	309	CLA	CMB-C2B	-2.03	1.46	1.50
25	D	406	LHG	O7-C7	2.03	1.40	1.34
25	C	524	LHG	O8-C6	-2.03	1.40	1.45
30	a	407	PHO	C3D-C4D	2.03	1.44	1.41
26	G	316	CHL	C1D-ND	-2.03	1.35	1.37
26	u	315	CHL	CHB-C4A	-2.03	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	608	CLA	CMD-C2D	-2.03	1.46	1.50
32	M	101	SQD	O3-C3	-2.03	1.38	1.43
22	P	308	CLA	CMB-C2B	-2.03	1.46	1.50
22	a	408	CLA	CMB-C2B	-2.03	1.46	1.50
22	2	308	CLA	CMD-C2D	-2.03	1.46	1.50
26	1	318	CHL	CHB-C4A	-2.03	1.32	1.37
22	A	406	CLA	CMC-C2C	-2.03	1.46	1.50
22	p	303	CLA	CMC-C2C	-2.03	1.46	1.50
22	N	302	CLA	CMC-C2C	-2.02	1.46	1.50
26	q	313	CHL	C1D-ND	-2.02	1.35	1.37
26	Q	316	CHL	C1D-ND	-2.02	1.35	1.37
22	5	306	CLA	CMD-C2D	-2.02	1.46	1.50
22	6	304	CLA	CHC-C1C	2.02	1.42	1.38
22	6	306	CLA	CHC-C1C	2.02	1.42	1.38
26	4	313	CHL	CHB-C4A	-2.02	1.32	1.37
22	2	307	CLA	CMB-C2B	-2.02	1.46	1.50
22	2	308	CLA	CMB-C2B	-2.02	1.46	1.50
22	V	306	CLA	CMC-C2C	-2.02	1.46	1.50
24	u	311	XAT	C8-C7	2.02	1.37	1.32
26	2	316	CHL	CHB-C4A	-2.02	1.32	1.37
22	R	304	CLA	MG-NB	-2.02	2.01	2.05
34	d	407	LMG	O1-C7	-2.02	1.40	1.43
22	2	302	CLA	CMB-C2B	-2.02	1.46	1.50
22	c	507	CLA	C1B-NB	-2.02	1.35	1.37
25	U	312	LHG	O7-C7	2.02	1.40	1.34
26	q	311	CHL	CHB-C4A	-2.02	1.32	1.37
24	R	313	XAT	C8-C7	2.02	1.37	1.32
26	Q	315	CHL	C1B-NB	-2.02	1.35	1.37
34	b	624	LMG	O1-C7	-2.02	1.40	1.43
32	m	101	SQD	O3-C3	-2.02	1.38	1.43
22	r	610	CLA	CMD-C2D	-2.02	1.46	1.50
22	G	305	CLA	CHC-C1C	2.02	1.42	1.38
22	g	306	CLA	CHC-C1C	2.02	1.42	1.38
22	c	503	CLA	C1B-NB	-2.02	1.35	1.37
22	2	302	CLA	CMC-C2C	-2.02	1.46	1.50
22	3	301	CLA	CMC-C2C	-2.02	1.46	1.50
22	U	301	CLA	C1B-C2B	2.02	1.48	1.43
22	b	613	CLA	CHC-C1C	2.02	1.42	1.38
25	u	312	LHG	O7-C7	2.02	1.40	1.34
22	p	307	CLA	CMB-C2B	-2.02	1.46	1.50
22	4	302	CLA	CMC-C2C	-2.02	1.46	1.50
22	1	301	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	614	CHL	CHB-C4A	-2.02	1.32	1.37
22	6	308	CLA	CMB-C2B	-2.02	1.46	1.50
26	6	301	CHL	CHB-C4A	-2.02	1.32	1.37
26	V	318	CHL	CHB-C4A	-2.02	1.32	1.37
22	s	301	CLA	MG-ND	-2.02	2.01	2.05
22	U	305	CLA	CMC-C2C	-2.02	1.46	1.50
26	p	318	CHL	C1D-ND	-2.02	1.35	1.37
22	G	301	CLA	CMD-C2D	-2.02	1.46	1.50
24	6	310	XAT	C8-C7	2.02	1.37	1.32
22	2	304	CLA	CMD-C2D	-2.02	1.46	1.50
22	b	608	CLA	CMB-C2B	-2.02	1.46	1.50
26	1	313	CHL	C4C-C3C	2.02	1.48	1.45
22	C	511	CLA	C1B-NB	-2.02	1.35	1.37
26	5	318	CHL	C1D-ND	-2.02	1.35	1.37
22	q	305	CLA	CMC-C2C	-2.02	1.46	1.50
22	G	306	CLA	CMB-C2B	-2.02	1.46	1.50
22	4	303	CLA	MG-ND	-2.02	2.01	2.05
25	d	405	LHG	O7-C7	2.02	1.40	1.34
22	A	408	CLA	CMB-C2B	-2.02	1.46	1.50
22	v	306	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	523	LHG	O8-C6	-2.02	1.40	1.45
26	N	315	CHL	C4C-C3C	2.02	1.48	1.45
22	5	301	CLA	CMD-C2D	-2.02	1.46	1.50
22	p	309	CLA	CMB-C2B	-2.02	1.46	1.50
26	q	311	CHL	C4C-C3C	2.02	1.48	1.45
26	v	313	CHL	CHB-C4A	-2.02	1.32	1.37
22	R	310	CLA	MG-NB	-2.02	2.01	2.05
26	p	320	CHL	C1D-ND	-2.02	1.35	1.37
22	r	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	R	311	CLA	CMD-C2D	-2.02	1.46	1.50
26	p	315	CHL	C4C-C3C	2.02	1.48	1.45
22	6	308	CLA	CMC-C2C	-2.01	1.46	1.50
22	b	609	CLA	CMC-C2C	-2.01	1.46	1.50
26	s	314	CHL	C1D-ND	-2.01	1.35	1.37
22	1	304	CLA	CMD-C2D	-2.01	1.46	1.50
26	P	315	CHL	C3B-C2B	2.01	1.48	1.41
26	Q	311	CHL	C2C-C1C	2.01	1.48	1.44
22	s	307	CLA	CMB-C2B	-2.01	1.46	1.50
26	U	316	CHL	C4B-NB	-2.01	1.35	1.37
22	4	308	CLA	CHC-C1C	2.01	1.42	1.38
26	n	318	CHL	CHB-C4A	-2.01	1.32	1.37
22	r	603	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	302	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	609	CLA	CMC-C2C	-2.01	1.46	1.50
22	B	616	CLA	CMC-C2C	-2.01	1.46	1.50
26	G	315	CHL	C1D-ND	-2.01	1.35	1.37
22	s	308	CLA	CMC-C2C	-2.01	1.46	1.50
26	u	315	CHL	MG-NA	-2.01	2.01	2.06
22	R	307	CLA	CHC-C1C	2.01	1.42	1.38
24	n	311	XAT	C8-C7	2.01	1.37	1.32
22	q	304	CLA	CMC-C2C	-2.01	1.46	1.50
26	6	316	CHL	C2C-C1C	2.01	1.48	1.44
22	C	509	CLA	C1B-NB	-2.01	1.35	1.37
22	Q	305	CLA	CMC-C2C	-2.01	1.46	1.50
22	R	304	CLA	CHC-C1C	2.01	1.42	1.38
26	u	317	CHL	CHB-C4A	-2.01	1.32	1.37
22	6	305	CLA	C3D-C4D	2.01	1.48	1.44
22	4	307	CLA	CMB-C2B	-2.01	1.46	1.50
26	5	315	CHL	C4B-NB	-2.01	1.35	1.37
22	r	603	CLA	MG-NB	-2.01	2.01	2.05
22	V	306	CLA	MG-NB	-2.01	2.01	2.05
22	r	608	CLA	CHC-C1C	2.01	1.42	1.38
22	C	508	CLA	C1B-NB	-2.01	1.35	1.37
26	G	311	CHL	C1D-ND	-2.01	1.35	1.37
22	5	303	CLA	CMC-C2C	-2.01	1.46	1.50
24	r	612	XAT	C8-C7	2.01	1.37	1.32
22	V	306	CLA	CMB-C2B	-2.01	1.46	1.50
22	N	303	CLA	CMC-C2C	-2.01	1.46	1.50
22	n	304	CLA	CMC-C2C	-2.01	1.46	1.50
22	1	307	CLA	CMB-C2B	-2.01	1.46	1.50
22	p	308	CLA	CMB-C2B	-2.01	1.46	1.50
22	1	307	CLA	MG-ND	-2.01	2.01	2.05
22	c	504	CLA	CHC-C1C	2.01	1.42	1.38
31	k	101	BCR	C32-C1	2.01	1.57	1.53
26	P	316	CHL	CHB-C4A	-2.01	1.32	1.37
26	P	317	CHL	CHB-C4A	-2.01	1.32	1.37
22	p	305	CLA	CHC-C1C	2.01	1.42	1.38
22	g	307	CLA	CHC-C1C	2.01	1.42	1.38
22	C	507	CLA	C1B-NB	-2.01	1.35	1.37
22	N	305	CLA	CMB-C2B	-2.01	1.46	1.50
22	r	609	CLA	CMC-C2C	-2.01	1.46	1.50
22	q	304	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	615	CLA	MG-ND	-2.01	2.01	2.05
26	g	316	CHL	C1D-ND	-2.01	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	315	CHL	C4C-C3C	2.01	1.48	1.45
22	c	511	CLA	CHC-C1C	2.01	1.42	1.38
22	g	306	CLA	CMC-C2C	-2.01	1.46	1.50
22	R	309	CLA	CMD-C2D	-2.01	1.46	1.50
22	n	301	CLA	CMC-C2C	-2.01	1.46	1.50
34	c	501	LMG	O1-C1	-2.01	1.36	1.40
26	S	314	CHL	CHB-C4A	-2.01	1.32	1.37
22	c	509	CLA	CHC-C1C	2.01	1.42	1.38
22	5	305	CLA	CMB-C2B	-2.01	1.46	1.50
22	P	304	CLA	CMC-C2C	-2.01	1.46	1.50
26	u	314	CHL	CHB-C4A	-2.00	1.32	1.37
26	5	313	CHL	C4B-NB	-2.00	1.35	1.37
22	N	305	CLA	CHC-C1C	2.00	1.42	1.38
22	C	505	CLA	CHC-C1C	2.00	1.42	1.38
26	u	313	CHL	CMC-C2C	2.00	1.49	1.45
26	G	311	CHL	MG-NA	-2.00	2.01	2.06
22	4	305	CLA	MG-ND	-2.00	2.01	2.05
26	R	316	CHL	C2C-C1C	2.00	1.48	1.44
26	q	315	CHL	C1D-ND	-2.00	1.35	1.37
22	5	306	CLA	CMC-C2C	-2.00	1.46	1.50
22	v	304	CLA	CMD-C2D	-2.00	1.46	1.50
22	V	303	CLA	MG-ND	-2.00	2.01	2.05
26	N	313	CHL	C4B-NB	-2.00	1.35	1.37
26	G	312	CHL	CMC-C2C	2.00	1.49	1.45
22	3	304	CLA	C3D-C4D	2.00	1.48	1.44
26	P	319	CHL	C1D-ND	-2.00	1.35	1.37
26	P	317	CHL	C2C-C1C	2.00	1.48	1.44
22	4	306	CLA	CMC-C2C	-2.00	1.46	1.50
22	5	308	CLA	CMD-C2D	-2.00	1.46	1.50
22	V	304	CLA	CMC-C2C	-2.00	1.46	1.50
22	2	306	CLA	CMC-C2C	-2.00	1.46	1.50
22	5	307	CLA	CMB-C2B	-2.00	1.46	1.50
22	5	305	CLA	CMC-C2C	-2.00	1.46	1.50
22	b	604	CLA	CMD-C2D	-2.00	1.46	1.50
24	p	312	XAT	C8-C7	2.00	1.37	1.32

All (6551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	311	XAT	O4-C5-C4	60.27	158.66	113.38
24	2	311	XAT	O4-C5-C4	60.01	158.46	113.38
24	n	311	XAT	O24-C25-C24	59.81	158.31	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	311	XAT	O24-C25-C24	59.80	158.31	113.38
24	4	311	XAT	O4-C5-C4	59.80	158.31	113.38
24	Q	309	XAT	O4-C5-C4	59.77	158.28	113.38
24	q	309	XAT	O4-C5-C4	59.61	158.16	113.38
24	5	311	XAT	O4-C5-C4	59.57	158.13	113.38
24	V	311	XAT	O24-C25-C24	59.37	157.98	113.38
24	P	312	XAT	O24-C25-C24	59.35	157.97	113.38
24	1	311	XAT	O24-C25-C24	59.31	157.94	113.38
24	v	311	XAT	O24-C25-C24	59.18	157.84	113.38
24	G	309	XAT	O24-C25-C24	59.03	157.72	113.38
24	v	311	XAT	O4-C5-C4	58.85	157.59	113.38
24	4	311	XAT	O24-C25-C24	58.84	157.58	113.38
24	U	311	XAT	O24-C25-C24	58.82	157.57	113.38
24	V	311	XAT	O4-C5-C4	58.57	157.38	113.38
24	P	312	XAT	O4-C5-C4	58.52	157.35	113.38
24	U	311	XAT	O4-C5-C4	58.49	157.32	113.38
24	p	312	XAT	O4-C5-C4	58.42	157.27	113.38
24	u	311	XAT	O24-C25-C24	58.38	157.23	113.38
24	p	312	XAT	O24-C25-C24	58.11	157.03	113.38
24	3	309	XAT	O4-C5-C4	58.05	156.99	113.38
24	g	309	XAT	O24-C25-C24	57.98	156.94	113.38
24	3	309	XAT	O24-C25-C24	57.85	156.84	113.38
24	6	310	XAT	O4-C5-C4	57.76	156.77	113.38
24	5	311	XAT	O24-C25-C24	57.57	156.63	113.38
24	6	310	XAT	O24-C25-C24	57.53	156.60	113.38
24	q	309	XAT	O24-C25-C24	57.46	156.55	113.38
24	u	311	XAT	O4-C5-C4	57.28	156.41	113.38
24	Q	309	XAT	O24-C25-C24	57.27	156.40	113.38
24	2	311	XAT	O24-C25-C24	57.15	156.32	113.38
24	G	309	XAT	O4-C5-C4	57.05	156.24	113.38
24	g	309	XAT	O4-C5-C4	57.01	156.21	113.38
24	N	311	XAT	O4-C5-C4	56.93	156.15	113.38
24	R	313	XAT	O24-C25-C24	56.54	155.86	113.38
24	r	612	XAT	O4-C5-C4	56.22	155.62	113.38
24	r	612	XAT	O24-C25-C24	55.98	155.43	113.38
24	R	313	XAT	O4-C5-C4	55.96	155.42	113.38
24	n	311	XAT	O4-C5-C4	55.65	155.19	113.38
24	Q	309	XAT	C18-C5-C4	-13.45	99.14	114.28
24	u	311	XAT	C38-C25-C24	-13.32	99.30	114.28
24	1	311	XAT	C18-C5-C4	-13.13	99.51	114.28
24	4	311	XAT	C18-C5-C4	-13.09	99.55	114.28
24	p	312	XAT	C38-C25-C24	-13.09	99.55	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	311	XAT	O24-C25-C38	-12.99	99.49	115.06
24	P	312	XAT	C18-C5-C4	-12.99	99.67	114.28
24	U	311	XAT	C18-C5-C4	-12.98	99.68	114.28
24	5	311	XAT	C38-C25-C24	-12.98	99.68	114.28
24	v	311	XAT	C18-C5-C4	-12.93	99.73	114.28
24	N	311	XAT	C18-C5-C4	-12.93	99.74	114.28
24	q	309	XAT	C18-C5-C4	-12.92	99.74	114.28
24	2	311	XAT	C38-C25-C24	-12.92	99.75	114.28
24	5	311	XAT	C18-C5-C4	-12.92	99.75	114.28
24	1	311	XAT	C38-C25-C24	-12.91	99.75	114.28
24	u	311	XAT	C18-C5-C4	-12.91	99.76	114.28
24	2	311	XAT	C18-C5-C4	-12.89	99.78	114.28
24	4	311	XAT	C38-C25-C24	-12.83	99.85	114.28
24	N	311	XAT	C38-C25-C24	-12.83	99.85	114.28
24	V	311	XAT	C38-C25-C24	-12.82	99.85	114.28
24	V	311	XAT	C18-C5-C4	-12.81	99.87	114.28
24	U	311	XAT	C38-C25-C24	-12.81	99.87	114.28
24	p	312	XAT	C18-C5-C4	-12.70	99.99	114.28
24	R	313	XAT	C18-C5-C4	-12.70	99.99	114.28
24	3	309	XAT	C18-C5-C4	-12.67	100.03	114.28
24	N	311	XAT	O24-C25-C38	-12.60	99.96	115.06
24	P	312	XAT	C38-C25-C24	-12.60	100.11	114.28
24	6	310	XAT	C18-C5-C4	-12.60	100.11	114.28
24	q	309	XAT	O4-C5-C18	-12.59	99.97	115.06
24	P	312	XAT	O24-C25-C38	-12.58	99.98	115.06
24	2	311	XAT	O4-C5-C18	-12.57	99.99	115.06
24	r	612	XAT	C18-C5-C4	-12.57	100.14	114.28
24	v	311	XAT	C38-C25-C24	-12.57	100.14	114.28
24	G	309	XAT	C38-C25-C24	-12.56	100.15	114.28
24	Q	309	XAT	O4-C5-C18	-12.53	100.04	115.06
24	n	311	XAT	C18-C5-C4	-12.48	100.24	114.28
24	1	311	XAT	O4-C5-C18	-12.48	100.10	115.06
24	5	311	XAT	O4-C5-C18	-12.43	100.16	115.06
24	1	311	XAT	O24-C25-C38	-12.43	100.17	115.06
24	4	311	XAT	O4-C5-C18	-12.41	100.19	115.06
24	v	311	XAT	O24-C25-C38	-12.39	100.21	115.06
24	G	309	XAT	O24-C25-C38	-12.39	100.21	115.06
24	Q	309	XAT	C38-C25-C24	-12.39	100.34	114.28
24	V	311	XAT	O24-C25-C38	-12.38	100.22	115.06
24	G	309	XAT	C18-C5-C4	-12.37	100.37	114.28
24	g	309	XAT	C18-C5-C4	-12.32	100.42	114.28
24	v	311	XAT	O4-C5-C18	-12.32	100.30	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	309	XAT	C38-C25-C24	-12.30	100.44	114.28
24	n	311	XAT	C38-C25-C24	-12.30	100.44	114.28
24	6	310	XAT	C38-C25-C24	-12.30	100.44	114.28
24	3	309	XAT	C38-C25-C24	-12.28	100.46	114.28
24	U	311	XAT	O24-C25-C38	-12.27	100.35	115.06
24	g	309	XAT	C38-C25-C24	-12.27	100.48	114.28
24	4	311	XAT	O24-C25-C38	-12.20	100.44	115.06
24	V	311	XAT	O4-C5-C18	-12.16	100.49	115.06
24	r	612	XAT	C38-C25-C24	-12.11	100.66	114.28
24	3	309	XAT	O24-C25-C38	-12.03	100.64	115.06
24	g	309	XAT	O24-C25-C38	-12.00	100.68	115.06
24	R	313	XAT	C38-C25-C24	-11.98	100.80	114.28
24	P	312	XAT	O4-C5-C18	-11.95	100.74	115.06
24	6	310	XAT	O24-C25-C38	-11.93	100.76	115.06
24	p	312	XAT	O4-C5-C18	-11.91	100.79	115.06
24	5	311	XAT	O24-C25-C38	-11.87	100.83	115.06
24	3	309	XAT	O4-C5-C18	-11.86	100.85	115.06
24	U	311	XAT	O4-C5-C18	-11.85	100.86	115.06
24	u	311	XAT	O24-C25-C38	-11.81	100.91	115.06
24	6	310	XAT	O4-C5-C18	-11.80	100.91	115.06
24	p	312	XAT	O24-C25-C38	-11.79	100.94	115.06
24	Q	309	XAT	O24-C25-C38	-11.77	100.95	115.06
24	q	309	XAT	O24-C25-C38	-11.67	101.08	115.06
24	2	311	XAT	O24-C25-C38	-11.65	101.09	115.06
24	u	311	XAT	O4-C5-C18	-11.43	101.36	115.06
24	g	309	XAT	O4-C5-C18	-11.28	101.54	115.06
24	R	313	XAT	O24-C25-C38	-11.27	101.55	115.06
24	G	309	XAT	O4-C5-C18	-11.23	101.60	115.06
24	N	311	XAT	O4-C5-C18	-11.19	101.65	115.06
24	r	612	XAT	O24-C25-C38	-10.95	101.94	115.06
24	n	311	XAT	O4-C5-C18	-10.92	101.97	115.06
27	r	618	NEX	O24-C25-C24	10.78	121.48	113.38
26	R	316	CHL	C2B-C1B-NB	10.68	117.39	110.23
26	r	615	CHL	C2B-C1B-NB	10.66	117.38	110.23
26	V	317	CHL	C2B-C1B-NB	10.61	117.35	110.23
26	1	317	CHL	C2B-C1B-NB	10.38	117.19	110.23
26	u	318	CHL	C2B-C1B-NB	10.38	117.19	110.23
26	p	318	CHL	C2B-C1B-NB	10.36	117.18	110.23
26	U	315	CHL	C2B-C1B-NB	10.36	117.18	110.23
26	v	317	CHL	C2B-C1B-NB	10.31	117.14	110.23
26	4	316	CHL	C2B-C1B-NB	10.30	117.14	110.23
26	5	318	CHL	C2B-C1B-NB	10.27	117.12	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	314	CHL	C2B-C1B-NB	10.25	117.10	110.23
26	r	619	CHL	C2B-C1B-NB	10.24	117.10	110.23
24	r	612	XAT	O4-C5-C18	-10.24	102.79	115.06
26	5	315	CHL	C2B-C1B-NB	10.23	117.09	110.23
26	G	315	CHL	C2B-C1B-NB	10.22	117.08	110.23
26	v	314	CHL	C2B-C1B-NB	10.21	117.08	110.23
26	2	318	CHL	C2B-C1B-NB	10.19	117.06	110.23
27	R	301	NEX	O24-C25-C24	10.18	121.03	113.38
26	5	317	CHL	C2B-C1B-NB	10.16	117.04	110.23
26	g	312	CHL	C2B-C1B-NB	10.16	117.04	110.23
26	P	319	CHL	C2B-C1B-NB	10.15	117.03	110.23
26	g	315	CHL	C2B-C1B-NB	10.13	117.02	110.23
26	p	320	CHL	C2B-C1B-NB	10.12	117.02	110.23
26	U	317	CHL	C2B-C1B-NB	10.10	117.01	110.23
26	2	317	CHL	C2B-C1B-NB	10.09	117.00	110.23
26	Q	311	CHL	C2B-C1B-NB	10.08	116.99	110.23
26	6	317	CHL	C2B-C1B-NB	10.07	116.98	110.23
26	U	316	CHL	C2B-C1B-NB	10.07	116.98	110.23
26	6	316	CHL	C2B-C1B-NB	10.04	116.96	110.23
26	2	315	CHL	C2B-C1B-NB	10.03	116.95	110.23
26	G	311	CHL	C2B-C1B-NB	10.02	116.95	110.23
26	3	311	CHL	C2B-C1B-NB	10.02	116.95	110.23
24	R	313	XAT	O4-C5-C18	-10.01	103.06	115.06
26	G	316	CHL	C2B-C1B-NB	10.00	116.93	110.23
26	u	317	CHL	C2B-C1B-NB	10.00	116.93	110.23
26	g	313	CHL	C2B-C1B-NB	10.00	116.93	110.23
26	g	311	CHL	C2B-C1B-NB	9.97	116.92	110.23
26	r	614	CHL	C2B-C1B-NB	9.95	116.90	110.23
26	P	318	CHL	C2B-C1B-NB	9.95	116.90	110.23
27	n	319	NEX	O24-C25-C24	9.95	120.85	113.38
26	6	312	CHL	C2B-C1B-NB	9.94	116.89	110.23
26	n	316	CHL	C2B-C1B-NB	9.94	116.89	110.23
26	q	311	CHL	C2B-C1B-NB	9.92	116.88	110.23
26	S	314	CHL	C2B-C1B-NB	9.92	116.88	110.23
26	u	316	CHL	C2B-C1B-NB	9.91	116.88	110.23
26	1	314	CHL	C2B-C1B-NB	9.87	116.85	110.23
26	3	316	CHL	C2B-C1B-NB	9.86	116.84	110.23
26	4	317	CHL	C2B-C1B-NB	9.85	116.84	110.23
26	q	314	CHL	C2B-C1B-NB	9.85	116.83	110.23
26	R	315	CHL	C2B-C1B-NB	9.85	116.83	110.23
26	V	314	CHL	C2B-C1B-NB	9.85	116.83	110.23
26	s	314	CHL	C2B-C1B-NB	9.83	116.82	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	319	CHL	C2B-C1B-NB	9.74	116.76	110.23
26	u	314	CHL	C2B-C1B-NB	9.72	116.75	110.23
26	g	316	CHL	C2B-C1B-NB	9.72	116.75	110.23
27	U	318	NEX	O24-C25-C24	9.72	120.68	113.38
26	u	316	CHL	CMD-C2D-C1D	9.72	141.84	124.71
26	N	313	CHL	C2B-C1B-NB	9.67	116.72	110.23
26	Q	315	CHL	C2B-C1B-NB	9.65	116.70	110.23
26	U	319	CHL	C2B-C1B-NB	9.62	116.68	110.23
26	v	316	CHL	C2B-C1B-NB	9.60	116.67	110.23
26	1	318	CHL	C2B-C1B-NB	9.60	116.67	110.23
26	v	318	CHL	C2B-C1B-NB	9.60	116.67	110.23
26	u	315	CHL	C2B-C1B-NB	9.59	116.66	110.23
26	G	312	CHL	C2B-C1B-NB	9.58	116.66	110.23
26	U	314	CHL	C2B-C1B-NB	9.57	116.65	110.23
26	N	316	CHL	C2B-C1B-NB	9.56	116.64	110.23
27	v	319	NEX	O24-C25-C24	9.55	120.56	113.38
26	p	314	CHL	C2B-C1B-NB	9.54	116.62	110.23
26	q	315	CHL	C2B-C1B-NB	9.51	116.61	110.23
26	Q	312	CHL	C2B-C1B-NB	9.51	116.61	110.23
26	G	314	CHL	C2B-C1B-NB	9.51	116.61	110.23
26	V	318	CHL	C2B-C1B-NB	9.48	116.59	110.23
26	p	317	CHL	C2B-C1B-NB	9.47	116.58	110.23
26	P	317	CHL	C2B-C1B-NB	9.45	116.57	110.23
26	Q	316	CHL	C2B-C1B-NB	9.45	116.56	110.23
26	n	313	CHL	C2B-C1B-NB	9.43	116.55	110.23
26	1	316	CHL	C2B-C1B-NB	9.35	116.50	110.23
26	6	301	CHL	C2B-C1B-NB	9.32	116.48	110.23
26	N	317	CHL	C2B-C1B-NB	9.26	116.44	110.23
26	N	315	CHL	C2B-C1B-NB	9.25	116.44	110.23
26	Q	314	CHL	C2B-C1B-NB	9.24	116.43	110.23
26	2	316	CHL	C2B-C1B-NB	9.24	116.43	110.23
26	v	313	CHL	C2B-C1B-NB	9.22	116.42	110.23
26	U	315	CHL	CMD-C2D-C1D	9.22	140.96	124.71
26	1	313	CHL	C2B-C1B-NB	9.20	116.40	110.23
26	P	314	CHL	C2B-C1B-NB	9.18	116.39	110.23
26	6	301	CHL	CMD-C2D-C1D	9.17	140.87	124.71
26	q	312	CHL	C2B-C1B-NB	9.14	116.36	110.23
26	V	316	CHL	C2B-C1B-NB	9.13	116.35	110.23
26	5	316	CHL	C2B-C1B-NB	9.12	116.34	110.23
26	p	316	CHL	C2B-C1B-NB	9.12	116.34	110.23
26	6	315	CHL	C2B-C1B-NB	9.11	116.34	110.23
26	5	313	CHL	C2B-C1B-NB	9.10	116.33	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	313	CHL	C2B-C1B-NB	9.08	116.32	110.23
26	2	313	CHL	C2B-C1B-NB	9.06	116.31	110.23
26	S	313	CHL	C2B-C1B-NB	9.06	116.31	110.23
26	G	313	CHL	C2B-C1B-NB	9.06	116.31	110.23
26	P	317	CHL	CMD-C2D-C1D	9.05	140.67	124.71
26	n	318	CHL	C2B-C1B-NB	9.05	116.30	110.23
26	G	311	CHL	CMD-C2D-C1D	9.04	140.64	124.71
26	3	314	CHL	C2B-C1B-NB	9.04	116.29	110.23
26	1	316	CHL	CMD-C2D-C1D	9.03	140.63	124.71
26	P	316	CHL	C2B-C1B-NB	9.02	116.28	110.23
26	u	313	CHL	C2B-C1B-NB	8.99	116.26	110.23
26	g	314	CHL	C2B-C1B-NB	8.98	116.25	110.23
26	V	313	CHL	C2B-C1B-NB	8.98	116.25	110.23
26	n	317	CHL	C2B-C1B-NB	8.97	116.25	110.23
26	3	315	CHL	C2B-C1B-NB	8.95	116.23	110.23
26	5	314	CHL	C2B-C1B-NB	8.94	116.22	110.23
26	N	314	CHL	C2B-C1B-NB	8.94	116.22	110.23
27	s	317	NEX	O24-C25-C24	8.93	120.09	113.38
26	s	313	CHL	C2B-C1B-NB	8.93	116.22	110.23
26	q	313	CHL	C2B-C1B-NB	8.92	116.21	110.23
22	B	605	CLA	C4A-NA-C1A	8.88	110.70	106.71
26	6	315	CHL	CMD-C2D-C1D	8.88	140.36	124.71
26	U	313	CHL	C2B-C1B-NB	8.86	116.17	110.23
27	5	319	NEX	O24-C25-C24	8.86	120.04	113.38
22	b	605	CLA	C4A-NA-C1A	8.85	110.69	106.71
27	V	319	NEX	O24-C25-C24	8.84	120.02	113.38
26	n	315	CHL	C2B-C1B-NB	8.83	116.15	110.23
26	V	316	CHL	CMD-C2D-C1D	8.81	140.24	124.71
26	3	314	CHL	CMD-C2D-C1D	8.80	140.22	124.71
26	U	313	CHL	CMD-C2D-C1D	8.79	140.21	124.71
26	p	317	CHL	CMD-C2D-C1D	8.79	140.20	124.71
26	n	317	CHL	C2C-C3C-C4C	-8.78	100.23	106.49
27	r	617	NEX	O24-C25-C24	8.78	119.98	113.38
26	r	616	CHL	C2B-C1B-NB	8.78	116.11	110.23
27	S	317	NEX	O24-C25-C24	8.77	119.97	113.38
26	n	315	CHL	CMD-C2D-C1D	8.77	140.16	124.71
26	2	314	CHL	C2B-C1B-NB	8.75	116.10	110.23
26	R	317	CHL	C2B-C1B-NB	8.75	116.10	110.23
22	p	306	CLA	C4A-NA-C1A	8.73	110.63	106.71
26	v	316	CHL	CMD-C2D-C1D	8.73	140.10	124.71
26	Q	313	CHL	C2B-C1B-NB	8.73	116.08	110.23
26	S	313	CHL	CMD-C2D-C1D	8.69	140.02	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	p	301	NEX	O24-C25-C24	8.68	119.90	113.38
26	6	317	CHL	CMD-C2D-C1D	8.67	140.00	124.71
22	C	504	CLA	C4A-NA-C1A	8.67	110.60	106.71
27	u	320	NEX	O24-C25-C24	8.65	119.88	113.38
26	3	312	CHL	C2B-C1B-NB	8.65	116.03	110.23
26	s	313	CHL	CMD-C2D-C1D	8.63	139.93	124.71
26	V	313	CHL	CMD-C2D-C1D	8.63	139.93	124.71
26	6	313	CHL	C2B-C1B-NB	8.63	116.02	110.23
27	2	319	NEX	O24-C25-C24	8.61	119.85	113.38
26	3	316	CHL	CMD-C2D-C1D	8.59	139.86	124.71
26	s	315	CHL	C2B-C1B-NB	8.59	115.99	110.23
26	1	313	CHL	CMD-C2D-C1D	8.59	139.84	124.71
26	n	314	CHL	C2B-C1B-NB	8.58	115.98	110.23
26	v	313	CHL	CMD-C2D-C1D	8.57	139.82	124.71
26	S	315	CHL	C2B-C1B-NB	8.55	115.97	110.23
22	c	503	CLA	C4A-NA-C1A	8.54	110.55	106.71
26	1	315	CHL	C2B-C1B-NB	8.52	115.94	110.23
26	Q	316	CHL	CMD-C2D-C1D	8.51	139.72	124.71
26	6	312	CHL	CMD-C2D-C1D	8.51	139.71	124.71
26	2	316	CHL	CMD-C2D-C1D	8.51	139.71	124.71
26	N	313	CHL	CMD-C2D-C1D	8.49	139.68	124.71
26	q	315	CHL	CMD-C2D-C1D	8.49	139.67	124.71
26	5	316	CHL	CMD-C2D-C1D	8.48	139.67	124.71
26	q	314	CHL	C2C-C3C-C4C	-8.47	100.45	106.49
26	6	314	CHL	C2B-C1B-NB	8.47	115.91	110.23
26	3	313	CHL	C2B-C1B-NB	8.46	115.90	110.23
26	6	316	CHL	C2C-C3C-C4C	-8.45	100.47	106.49
26	U	319	CHL	CMD-C2D-C1D	8.44	139.59	124.71
26	g	314	CHL	CMD-C2D-C1D	8.42	139.56	124.71
26	s	316	CHL	CMD-C2D-C1D	8.41	139.53	124.71
26	S	316	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	G	312	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	q	311	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	g	315	CHL	CMD-C2D-C1D	8.40	139.52	124.71
26	S	314	CHL	CMD-C2D-C1D	8.40	139.51	124.71
26	g	311	CHL	CMD-C2D-C1D	8.39	139.49	124.71
22	P	306	CLA	C4A-NA-C1A	8.39	110.48	106.71
26	n	316	CHL	CMD-C2D-C1D	8.38	139.49	124.71
26	5	317	CHL	CMD-C2D-C1D	8.38	139.49	124.71
26	u	315	CHL	C2C-C3C-C4C	-8.38	100.52	106.49
26	2	317	CHL	CMD-C2D-C1D	8.38	139.48	124.71
26	N	316	CHL	CMD-C2D-C1D	8.38	139.48	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	311	CHL	CMD-C2D-C1D	8.38	139.47	124.71
26	s	314	CHL	CMD-C2D-C1D	8.37	139.47	124.71
26	v	315	CHL	C2B-C1B-NB	8.37	115.84	110.23
26	P	318	CHL	CMD-C2D-C1D	8.36	139.45	124.71
26	R	317	CHL	CMD-C2D-C1D	8.36	139.44	124.71
26	Q	315	CHL	C2C-C3C-C4C	-8.36	100.53	106.49
26	r	615	CHL	CMD-C2D-C1D	8.35	139.44	124.71
26	p	318	CHL	CMD-C2D-C1D	8.35	139.43	124.71
26	p	320	CHL	CMD-C2D-C1D	8.33	139.40	124.71
26	u	313	CHL	CMD-C2D-C1D	8.33	139.40	124.71
26	2	315	CHL	CMD-C2D-C1D	8.32	139.38	124.71
26	v	314	CHL	CMD-C2D-C1D	8.32	139.38	124.71
26	q	313	CHL	CMD-C2D-C1D	8.31	139.36	124.71
22	5	305	CLA	C4A-NA-C1A	8.31	110.44	106.71
26	P	314	CHL	CMD-C2D-C1D	8.31	139.35	124.71
26	q	312	CHL	CMD-C2D-C1D	8.30	139.35	124.71
26	Q	314	CHL	CMD-C2D-C1D	8.30	139.34	124.71
22	n	305	CLA	C4A-NA-C1A	8.30	110.44	106.71
26	R	316	CHL	CMD-C2D-C1D	8.29	139.33	124.71
26	r	616	CHL	CMD-C2D-C1D	8.29	139.32	124.71
26	g	313	CHL	CMD-C2D-C1D	8.29	139.32	124.71
27	N	318	NEX	O24-C25-C24	8.28	119.60	113.38
26	2	313	CHL	CMD-C2D-C1D	8.28	139.31	124.71
26	3	315	CHL	C2C-C3C-C4C	-8.27	100.59	106.49
26	r	614	CHL	CMD-C2D-C1D	8.27	139.29	124.71
26	V	317	CHL	CMD-C2D-C1D	8.27	139.28	124.71
26	5	315	CHL	CMD-C2D-C1D	8.27	139.28	124.71
26	R	315	CHL	CMD-C2D-C1D	8.27	139.28	124.71
26	4	314	CHL	CMD-C2D-C1D	8.26	139.28	124.71
26	Q	311	CHL	CMD-C2D-C1D	8.25	139.26	124.71
26	p	314	CHL	CMD-C2D-C1D	8.24	139.24	124.71
26	4	313	CHL	CMD-C2D-C1D	8.24	139.23	124.71
26	V	314	CHL	CMD-C2D-C1D	8.23	139.22	124.71
26	6	313	CHL	CMD-C2D-C1D	8.23	139.22	124.71
26	5	314	CHL	CMD-C2D-C1D	8.23	139.22	124.71
22	2	305	CLA	C4A-NA-C1A	8.23	110.41	106.71
26	U	317	CHL	CMD-C2D-C1D	8.23	139.22	124.71
26	n	317	CHL	CMD-C2D-C1D	8.22	139.21	124.71
26	G	313	CHL	CMD-C2D-C1D	8.22	139.21	124.71
26	3	312	CHL	CMD-C2D-C1D	8.22	139.20	124.71
26	P	315	CHL	CHD-C1D-ND	-8.21	116.91	124.45
26	s	316	CHL	C2B-C1B-NB	8.21	115.74	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	317	CHL	CMD-C2D-C1D	8.21	139.18	124.71
27	P	301	NEX	O24-C25-C24	8.21	119.55	113.38
26	r	619	CHL	CMD-C2D-C1D	8.21	139.18	124.71
26	5	313	CHL	CMD-C2D-C1D	8.21	139.18	124.71
26	p	315	CHL	CMD-C2D-C1D	8.20	139.17	124.71
26	p	316	CHL	CMD-C2D-C1D	8.20	139.17	124.71
26	Q	315	CHL	CMD-C2D-C1D	8.20	139.17	124.71
26	s	314	CHL	C2C-C3C-C4C	-8.19	100.65	106.49
26	G	315	CHL	CMD-C2D-C1D	8.19	139.14	124.71
26	g	315	CHL	C2C-C3C-C4C	-8.18	100.66	106.49
26	v	317	CHL	CMD-C2D-C1D	8.18	139.13	124.71
26	1	314	CHL	CMD-C2D-C1D	8.18	139.12	124.71
26	4	315	CHL	C2B-C1B-NB	8.17	115.71	110.23
26	1	318	CHL	CMD-C2D-C1D	8.17	139.10	124.71
26	2	318	CHL	CMD-C2D-C1D	8.17	139.10	124.71
26	S	316	CHL	C2B-C1B-NB	8.17	115.71	110.23
26	g	312	CHL	CMD-C2D-C1D	8.16	139.09	124.71
26	2	314	CHL	CMD-C2D-C1D	8.16	139.09	124.71
26	P	315	CHL	CMD-C2D-C1D	8.16	139.09	124.71
26	4	316	CHL	CMD-C2D-C1D	8.15	139.08	124.71
26	u	314	CHL	CMD-C2D-C1D	8.14	139.06	124.71
26	G	316	CHL	CMD-C2D-C1D	8.13	139.05	124.71
26	u	318	CHL	CMD-C2D-C1D	8.13	139.04	124.71
26	N	315	CHL	C2C-C3C-C4C	-8.13	100.70	106.49
26	Q	313	CHL	CMD-C2D-C1D	8.11	139.01	124.71
26	q	314	CHL	CMD-C2D-C1D	8.11	139.00	124.71
26	P	316	CHL	CMD-C2D-C1D	8.11	139.00	124.71
26	4	317	CHL	CMD-C2D-C1D	8.11	139.00	124.71
26	V	315	CHL	C2B-C1B-NB	8.09	115.66	110.23
26	S	314	CHL	C2C-C3C-C4C	-8.09	100.72	106.49
26	N	314	CHL	CMD-C2D-C1D	8.09	138.97	124.71
26	n	314	CHL	CMD-C2D-C1D	8.08	138.96	124.71
26	G	314	CHL	CMD-C2D-C1D	8.08	138.96	124.71
26	s	315	CHL	CMD-C2D-C1D	8.06	138.92	124.71
26	g	316	CHL	CMD-C2D-C1D	8.06	138.92	124.71
26	Q	312	CHL	CMD-C2D-C1D	8.05	138.90	124.71
26	n	318	CHL	CMD-C2D-C1D	8.04	138.89	124.71
26	P	319	CHL	CMD-C2D-C1D	8.02	138.85	124.71
26	5	318	CHL	CMD-C2D-C1D	8.02	138.84	124.71
22	c	509	CLA	C4A-NA-C1A	8.01	110.31	106.71
26	N	317	CHL	CMD-C2D-C1D	8.01	138.82	124.71
26	S	315	CHL	CMD-C2D-C1D	8.00	138.82	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	314	CHL	C2C-C3C-C4C	-8.00	100.79	106.49
26	p	315	CHL	C2B-C1B-NB	7.98	115.58	110.23
22	C	510	CLA	C4A-NA-C1A	7.98	110.30	106.71
26	6	316	CHL	CMD-C2D-C1D	7.98	138.78	124.71
26	1	315	CHL	CMD-C2D-C1D	7.98	138.78	124.71
22	r	609	CLA	C4A-NA-C1A	7.98	110.29	106.71
26	U	316	CHL	CMD-C2D-C1D	7.98	138.77	124.71
22	R	308	CLA	C4A-NA-C1A	7.96	110.28	106.71
26	p	319	CHL	CMD-C2D-C1D	7.96	138.74	124.71
22	B	612	CLA	C4A-NA-C1A	7.96	110.28	106.71
26	2	315	CHL	C2C-C3C-C4C	-7.95	100.82	106.49
26	3	315	CHL	CMD-C2D-C1D	7.94	138.71	124.71
26	n	313	CHL	CMD-C2D-C1D	7.94	138.71	124.71
22	b	617	CLA	C4A-NA-C1A	7.93	110.27	106.71
26	V	315	CHL	CMD-C2D-C1D	7.93	138.69	124.71
22	b	612	CLA	C4A-NA-C1A	7.92	110.27	106.71
26	u	317	CHL	CMD-C2D-C1D	7.92	138.67	124.71
26	4	315	CHL	CMD-C2D-C1D	7.92	138.66	124.71
26	N	316	CHL	C2C-C3C-C4C	-7.91	100.85	106.49
26	v	315	CHL	CMD-C2D-C1D	7.91	138.65	124.71
30	d	401	PHO	C4D-CHA-CBD	-7.91	104.94	108.52
26	5	315	CHL	C2C-C3C-C4C	-7.90	100.86	106.49
26	3	313	CHL	CMD-C2D-C1D	7.88	138.60	124.71
26	G	315	CHL	C2C-C3C-C4C	-7.86	100.89	106.49
26	6	314	CHL	CMD-C2D-C1D	7.86	138.56	124.71
22	c	506	CLA	C4A-NA-C1A	7.85	110.23	106.71
26	N	315	CHL	CMD-C2D-C1D	7.84	138.54	124.71
22	q	304	CLA	C4A-NA-C1A	7.83	110.23	106.71
30	D	401	PHO	C4D-CHA-CBD	-7.79	104.99	108.52
26	p	315	CHL	CHD-C1D-ND	-7.78	117.30	124.45
26	r	614	CHL	C2C-C3C-C4C	-7.78	100.94	106.49
26	U	314	CHL	CMD-C2D-C1D	7.77	138.41	124.71
26	R	316	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
26	R	315	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
22	C	507	CLA	C4A-NA-C1A	7.75	110.19	106.71
22	n	305	CLA	CMD-C2D-C1D	-7.73	111.08	124.71
26	5	313	CHL	C2C-C3C-C4C	-7.73	100.98	106.49
22	b	607	CLA	C4A-NA-C1A	7.72	110.17	106.71
26	1	314	CHL	C2C-C3C-C4C	-7.72	100.99	106.49
26	4	314	CHL	C2C-C3C-C4C	-7.71	100.99	106.49
26	V	318	CHL	CMD-C2D-C1D	7.71	138.30	124.71
22	C	509	CLA	C4A-NA-C1A	7.70	110.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	305	CLA	C4A-NA-C1A	7.68	110.16	106.71
22	r	607	CLA	C4A-NA-C1A	7.67	110.16	106.71
22	p	303	CLA	C4A-NA-C1A	7.66	110.15	106.71
26	p	318	CHL	C2C-C3C-C4C	-7.65	101.04	106.49
26	r	615	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
26	P	318	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
22	B	607	CLA	C4A-NA-C1A	7.62	110.13	106.71
22	G	305	CLA	C4A-NA-C1A	7.62	110.13	106.71
22	2	305	CLA	CMD-C2D-C1D	-7.61	111.30	124.71
22	b	608	CLA	C4A-NA-C1A	7.60	110.12	106.71
26	v	318	CHL	CMD-C2D-C1D	7.60	138.10	124.71
22	n	308	CLA	C4A-NA-C1A	7.59	110.12	106.71
26	v	315	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
22	2	307	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	N	305	CLA	C4A-NA-C1A	7.58	110.11	106.71
22	g	305	CLA	C4A-NA-C1A	7.57	110.11	106.71
26	u	317	CHL	C2C-C3C-C4C	-7.57	101.09	106.49
26	U	319	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
22	R	310	CLA	C4A-NA-C1A	7.56	110.10	106.71
26	r	619	CHL	C2C-C3C-C4C	-7.56	101.10	106.49
26	v	318	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
22	p	306	CLA	CMD-C2D-C1D	-7.55	111.41	124.71
22	c	505	CLA	C4A-NA-C1A	7.55	110.10	106.71
26	v	316	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
26	2	314	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
22	r	605	CLA	C4A-NA-C1A	7.50	110.08	106.71
22	g	307	CLA	C4A-NA-C1A	7.50	110.08	106.71
26	1	315	CHL	C2C-C3C-C4C	-7.50	101.14	106.49
22	B	606	CLA	C4A-NA-C1A	7.50	110.08	106.71
22	c	508	CLA	C4A-NA-C1A	7.49	110.08	106.71
22	5	305	CLA	CMD-C2D-C1D	-7.49	111.51	124.71
26	U	316	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
26	P	316	CHL	C2C-C3C-C4C	-7.48	101.15	106.49
31	k	101	BCR	C24-C23-C22	-7.48	114.93	126.23
22	5	307	CLA	C4A-NA-C1A	7.48	110.07	106.71
26	v	313	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
22	G	307	CLA	C4A-NA-C1A	7.47	110.06	106.71
22	R	306	CLA	C4A-NA-C1A	7.47	110.06	106.71
26	P	315	CHL	C2B-C1B-NB	7.47	115.24	110.23
22	C	506	CLA	C4A-NA-C1A	7.46	110.06	106.71
26	p	314	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
22	6	306	CLA	C4A-NA-C1A	7.45	110.06	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	305	CLA	C4A-NA-C1A	7.45	110.06	106.71
26	4	315	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
22	s	308	CLA	C4A-NA-C1A	7.43	110.05	106.71
26	5	317	CHL	C2C-C3C-C4C	-7.43	101.19	106.49
22	r	604	CLA	C4A-NA-C1A	7.42	110.04	106.71
22	p	308	CLA	C4A-NA-C1A	7.41	110.04	106.71
22	b	606	CLA	C4A-NA-C1A	7.41	110.04	106.71
31	K	101	BCR	C24-C23-C22	-7.41	115.03	126.23
22	R	305	CLA	C4A-NA-C1A	7.41	110.04	106.71
26	2	313	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
22	B	608	CLA	C4A-NA-C1A	7.40	110.03	106.71
22	P	308	CLA	C4A-NA-C1A	7.40	110.03	106.71
26	S	313	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
31	C	517	BCR	C15-C14-C13	-7.39	116.76	127.31
26	s	316	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
26	6	317	CHL	C2C-C3C-C4C	-7.37	101.23	106.49
26	p	319	CHL	C2C-C3C-C4C	-7.37	101.24	106.49
22	U	307	CLA	C4A-NA-C1A	7.37	110.02	106.71
26	s	313	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
26	n	315	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
26	N	314	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
26	U	315	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
22	C	515	CLA	C4A-NA-C1A	7.36	110.01	106.71
22	b	615	CLA	C4A-NA-C1A	7.36	110.01	106.71
26	g	312	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
22	B	603	CLA	C4A-NA-C1A	7.34	110.01	106.71
26	n	313	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
22	N	303	CLA	C4A-NA-C1A	7.34	110.01	106.71
26	u	318	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
22	r	603	CLA	C4A-NA-C1A	7.34	110.00	106.71
26	g	316	CHL	C2C-C3C-C4C	-7.34	101.26	106.49
26	2	314	CHL	CHD-C1D-ND	-7.33	117.72	124.45
31	c	515	BCR	C15-C14-C13	-7.33	116.85	127.31
26	P	319	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
26	G	316	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
26	v	317	CHL	C2C-C3C-C4C	-7.32	101.27	106.49
22	1	306	CLA	C4A-NA-C1A	7.31	109.99	106.71
26	3	313	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
22	N	307	CLA	C4A-NA-C1A	7.31	109.99	106.71
26	4	316	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
26	P	314	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
26	4	317	CHL	C2C-C3C-C4C	-7.30	101.28	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	315	CHL	C2C-C3C-C4C	-7.30	101.29	106.49
22	v	306	CLA	C4A-NA-C1A	7.29	109.98	106.71
26	5	314	CHL	C2C-C3C-C4C	-7.29	101.29	106.49
22	n	307	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	P	303	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	S	308	CLA	C4A-NA-C1A	7.28	109.98	106.71
22	B	615	CLA	C4A-NA-C1A	7.27	109.98	106.71
26	V	318	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
22	c	514	CLA	C4A-NA-C1A	7.27	109.97	106.71
26	p	316	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
26	6	314	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
22	u	307	CLA	C4A-NA-C1A	7.27	109.97	106.71
26	S	316	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
22	b	603	CLA	C4A-NA-C1A	7.26	109.97	106.71
26	V	313	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
22	c	507	CLA	C4A-NA-C1A	7.25	109.97	106.71
26	1	317	CHL	C2C-C3C-C4C	-7.24	101.33	106.49
22	2	308	CLA	C4A-NA-C1A	7.24	109.96	106.71
26	U	317	CHL	C2C-C3C-C4C	-7.23	101.33	106.49
26	n	314	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
26	Q	312	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
26	u	314	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
22	V	307	CLA	C4A-NA-C1A	7.20	109.94	106.71
26	S	315	CHL	CHD-C1D-ND	-7.20	117.84	124.45
26	v	314	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
22	P	306	CLA	CMD-C2D-C1D	-7.19	112.03	124.71
26	n	316	CHL	C2C-C3C-C4C	-7.19	101.36	106.49
22	Q	304	CLA	C4A-NA-C1A	7.19	109.94	106.71
22	v	303	CLA	C4A-NA-C1A	7.19	109.94	106.71
26	V	314	CHL	C2C-C3C-C4C	-7.18	101.37	106.49
26	s	315	CHL	CHD-C1D-ND	-7.18	117.86	124.45
22	5	306	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	Q	303	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	n	306	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	R	304	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	5	303	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	C	513	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	R	311	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	G	304	CLA	C4A-NA-C1A	7.16	109.93	106.71
26	V	316	CHL	C2C-C3C-C4C	-7.16	101.38	106.49
26	G	314	CHL	C2C-C3C-C4C	-7.16	101.38	106.49
26	u	315	CHL	CMD-C2D-C1D	7.16	137.33	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	304	CLA	C4A-NA-C1A	7.15	109.92	106.71
26	1	318	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
22	r	610	CLA	C4A-NA-C1A	7.14	109.92	106.71
22	b	616	CLA	C4A-NA-C1A	7.13	109.91	106.71
26	U	316	CHL	O2D-CGD-CBD	7.12	123.93	111.27
22	p	305	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	3	307	CLA	C4A-NA-C1A	7.12	109.91	106.71
26	6	312	CHL	C2C-C3C-C4C	-7.12	101.42	106.49
26	v	317	CHL	O2D-CGD-CBD	7.12	123.92	111.27
26	S	316	CHL	CHD-C1D-ND	-7.12	117.91	124.45
22	2	306	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	U	308	CLA	C4A-NA-C1A	7.11	109.90	106.71
26	s	316	CHL	CHD-C1D-ND	-7.10	117.93	124.45
26	g	313	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
26	3	316	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
22	5	304	CLA	C4A-NA-C1A	7.10	109.90	106.71
22	R	302	CLA	C4A-NA-C1A	7.10	109.90	106.71
26	2	314	CHL	CHB-C1B-NB	-7.10	116.74	124.26
22	r	601	CLA	C4A-NA-C1A	7.09	109.89	106.71
22	v	305	CLA	C4A-NA-C1A	7.09	109.89	106.71
26	V	313	CHL	CHD-C1D-ND	-7.08	117.94	124.45
22	5	308	CLA	C4A-NA-C1A	7.08	109.89	106.71
22	p	307	CLA	C4A-NA-C1A	7.08	109.89	106.71
26	2	317	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
26	2	318	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
22	u	306	CLA	C4A-NA-C1A	7.07	109.89	106.71
26	5	316	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
22	N	306	CLA	C4A-NA-C1A	7.07	109.88	106.71
26	1	317	CHL	O2D-CGD-CBD	7.06	123.82	111.27
22	g	304	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	B	613	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	C	514	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	4	308	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	4	307	CLA	C4A-NA-C1A	7.05	109.87	106.71
22	u	302	CLA	C4A-NA-C1A	7.04	109.87	106.71
26	G	313	CHL	C2C-C3C-C4C	-7.04	101.47	106.49
22	b	611	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	C	503	CLA	C4A-NA-C1A	7.03	109.87	106.71
26	g	314	CHL	C2C-C3C-C4C	-7.03	101.48	106.49
22	s	307	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	C	508	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	v	307	CLA	C4A-NA-C1A	7.03	109.86	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	q	307	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	B	610	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	c	512	CLA	C4A-NA-C1A	7.02	109.86	106.71
26	Q	316	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
22	c	513	CLA	C4A-NA-C1A	7.02	109.86	106.71
26	3	311	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
26	u	316	CHL	C2C-C3C-C4C	-7.02	101.48	106.49
26	p	320	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
22	2	304	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	V	306	CLA	C4A-NA-C1A	7.01	109.86	106.71
26	2	316	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
26	n	318	CHL	C2C-C3C-C4C	-7.01	101.49	106.49
22	q	306	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	g	306	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	2	303	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	u	308	CLA	C4A-NA-C1A	7.00	109.86	106.71
22	n	304	CLA	C4A-NA-C1A	7.00	109.86	106.71
26	Q	314	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
22	U	302	CLA	C4A-NA-C1A	7.00	109.85	106.71
26	G	311	CHL	C2C-C3C-C4C	-7.00	101.50	106.49
26	2	314	CHL	C4A-NA-C1A	6.99	109.85	106.71
26	s	313	CHL	CHD-C1D-ND	-6.99	118.03	124.45
26	N	317	CHL	C2C-C3C-C4C	-6.99	101.51	106.49
22	B	611	CLA	C4A-NA-C1A	6.98	109.84	106.71
26	5	314	CHL	CHD-C1D-ND	-6.98	118.04	124.45
22	a	405	CLA	C4A-NA-C1A	6.98	109.84	106.71
26	6	313	CHL	CHD-C1D-ND	-6.98	118.04	124.45
26	V	317	CHL	C2C-C3C-C4C	-6.98	101.52	106.49
22	P	304	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	A	405	CLA	C4A-NA-C1A	6.97	109.84	106.71
22	N	305	CLA	CMD-C2D-C1D	-6.97	112.43	124.71
22	3	304	CLA	C4A-NA-C1A	6.97	109.84	106.71
26	Q	311	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
22	4	306	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	6	308	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	Q	307	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	x	201	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	V	308	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	b	613	CLA	C4A-NA-C1A	6.95	109.83	106.71
26	g	311	CHL	C2C-C3C-C4C	-6.95	101.53	106.49
22	s	309	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	q	308	CLA	C4A-NA-C1A	6.94	109.83	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	616	CLA	C4A-NA-C1A	6.94	109.82	106.71
22	c	502	CLA	C4A-NA-C1A	6.94	109.82	106.71
22	S	307	CLA	C4A-NA-C1A	6.93	109.82	106.71
26	R	317	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
26	q	315	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
22	u	305	CLA	C4A-NA-C1A	6.93	109.82	106.71
26	4	313	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
26	6	301	CHL	C2C-C3C-C4C	-6.93	101.55	106.49
26	p	317	CHL	C2C-C3C-C4C	-6.92	101.55	106.49
26	6	315	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
22	5	302	CLA	C4A-NA-C1A	6.92	109.82	106.71
22	V	303	CLA	C4A-NA-C1A	6.92	109.82	106.71
26	3	314	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
26	q	312	CHL	C2C-C3C-C4C	-6.91	101.56	106.49
22	b	610	CLA	C4A-NA-C1A	6.91	109.81	106.71
26	5	318	CHL	C2C-C3C-C4C	-6.91	101.56	106.49
26	3	312	CHL	CHD-C1D-ND	-6.90	118.11	124.45
22	X	202	CLA	C4A-NA-C1A	6.90	109.81	106.71
26	5	313	CHL	CHD-C1D-ND	-6.90	118.11	124.45
22	G	303	CLA	C4A-NA-C1A	6.90	109.81	106.71
22	u	303	CLA	C4A-NA-C1A	6.90	109.81	106.71
26	U	313	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
26	1	313	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
22	v	308	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	1	308	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	U	306	CLA	C4A-NA-C1A	6.88	109.80	106.71
22	3	308	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	P	305	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	q	303	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	P	307	CLA	C4A-NA-C1A	6.87	109.80	106.71
24	r	612	XAT	C26-C27-C28	-6.87	111.47	125.99
31	C	518	BCR	C11-C10-C9	-6.87	117.51	127.31
22	U	305	CLA	C4A-NA-C1A	6.87	109.79	106.71
26	5	316	CHL	CHD-C1D-ND	-6.86	118.15	124.45
26	1	316	CHL	C2C-C3C-C4C	-6.86	101.60	106.49
26	1	313	CHL	CHD-C1D-ND	-6.86	118.15	124.45
22	3	306	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	S	309	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	1	307	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	a	408	CLA	C4A-NA-C1A	6.85	109.79	106.71
22	c	510	CLA	C4A-NA-C1A	6.85	109.78	106.71
26	r	616	CHL	C2C-C3C-C4C	-6.84	101.61	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	516	BCR	C11-C10-C9	-6.83	117.56	127.31
26	S	313	CHL	CHD-C1D-ND	-6.83	118.17	124.45
22	Q	306	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	v	302	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	C	511	CLA	C4A-NA-C1A	6.82	109.77	106.71
26	2	316	CHL	CHD-C1D-ND	-6.82	118.19	124.45
22	N	308	CLA	C4A-NA-C1A	6.81	109.77	106.71
30	A	407	PHO	C4D-CHA-CBD	-6.81	105.44	108.52
22	A	408	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	b	609	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	r	608	CLA	C4A-NA-C1A	6.80	109.77	106.71
22	N	304	CLA	C4A-NA-C1A	6.80	109.77	106.71
22	4	304	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	6	307	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	p	304	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	R	309	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	1	304	CLA	C4A-NA-C1A	6.80	109.76	106.71
26	V	315	CHL	CHD-C1D-ND	-6.79	118.21	124.45
22	6	309	CLA	C4A-NA-C1A	6.79	109.76	106.71
26	V	317	CHL	O2D-CGD-CBD	6.78	123.31	111.27
24	N	311	XAT	C15-C14-C13	-6.78	117.64	127.31
26	q	315	CHL	CHD-C1D-ND	-6.78	118.23	124.45
26	s	315	CHL	C2C-C3C-C4C	-6.78	101.66	106.49
22	s	304	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	s	302	CLA	C4A-NA-C1A	6.77	109.75	106.71
26	3	316	CHL	CHD-C1D-ND	-6.77	118.23	124.45
22	a	404	CLA	C4A-NA-C1A	6.76	109.75	106.71
22	V	302	CLA	C4A-NA-C1A	6.76	109.74	106.71
26	q	313	CHL	C2C-C3C-C4C	-6.75	101.68	106.49
26	2	313	CHL	CHD-C1D-ND	-6.75	118.25	124.45
22	B	609	CLA	C4A-NA-C1A	6.75	109.74	106.71
26	3	314	CHL	CHD-C1D-ND	-6.74	118.26	124.45
22	Q	308	CLA	C4A-NA-C1A	6.74	109.74	106.71
26	n	318	CHL	CHD-C1D-ND	-6.74	118.26	124.45
22	S	302	CLA	C4A-NA-C1A	6.74	109.73	106.71
26	6	314	CHL	CHD-C1D-ND	-6.73	118.27	124.45
26	P	314	CHL	CHD-C1D-ND	-6.73	118.27	124.45
26	Q	313	CHL	C2C-C3C-C4C	-6.73	101.69	106.49
22	R	307	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	617	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	6	305	CLA	C4A-NA-C1A	6.73	109.73	106.71
26	p	315	CHL	C2C-C3C-C4C	-6.73	101.69	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	C4A-NA-C1A	6.72	109.73	106.71
30	a	407	PHO	C4D-CHA-CBD	-6.72	105.48	108.52
26	4	313	CHL	CHD-C1D-ND	-6.72	118.28	124.45
26	v	313	CHL	CHD-C1D-ND	-6.72	118.28	124.45
26	P	317	CHL	CHD-C1D-ND	-6.72	118.28	124.45
22	b	602	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	g	303	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	B	614	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	r	606	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	S	304	CLA	C4A-NA-C1A	6.70	109.72	106.71
26	G	312	CHL	C2C-C3C-C4C	-6.70	101.72	106.49
22	p	309	CLA	C4A-NA-C1A	6.69	109.71	106.71
26	N	317	CHL	CHD-C1D-ND	-6.68	118.31	124.45
22	A	404	CLA	C4A-NA-C1A	6.68	109.71	106.71
26	6	313	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
26	u	313	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
26	q	312	CHL	CHD-C1D-ND	-6.67	118.32	124.45
26	U	313	CHL	CHD-C1D-ND	-6.67	118.32	124.45
26	S	315	CHL	C2C-C3C-C4C	-6.67	101.73	106.49
26	P	317	CHL	C2C-C3C-C4C	-6.66	101.74	106.49
22	S	303	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	G	306	CLA	C4A-NA-C1A	6.66	109.70	106.71
26	g	314	CHL	CHD-C1D-ND	-6.65	118.34	124.45
26	6	317	CHL	CHD-C1D-ND	-6.65	118.34	124.45
26	q	311	CHL	CHD-C1D-ND	-6.64	118.35	124.45
22	P	309	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	G	308	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	1	305	CLA	C4A-NA-C1A	6.63	109.69	106.71
26	3	315	CHL	CHD-C1D-ND	-6.63	118.36	124.45
26	6	315	CHL	CHD-C1D-ND	-6.63	118.36	124.45
22	s	303	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	q	302	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	3	302	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	s	305	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	6	303	CLA	C4A-NA-C1A	6.60	109.67	106.71
26	N	313	CHL	CHD-C1D-ND	-6.60	118.39	124.45
26	q	311	CHL	C2C-C3C-C4C	-6.59	101.79	106.49
26	5	314	CHL	CHB-C1B-NB	-6.59	117.28	124.26
26	n	317	CHL	CHD-C1D-ND	-6.59	118.40	124.45
22	A	406	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	c	504	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	N	302	CLA	C4A-NA-C1A	6.58	109.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	303	CLA	C4A-NA-C1A	6.58	109.66	106.71
26	3	312	CHL	C2C-C3C-C4C	-6.58	101.80	106.49
22	C	505	CLA	C4A-NA-C1A	6.58	109.66	106.71
26	G	312	CHL	CHD-C1D-ND	-6.57	118.42	124.45
26	4	316	CHL	O2D-CGD-CBD	6.57	122.94	111.27
26	P	315	CHL	C2C-C3C-C4C	-6.57	101.81	106.49
22	2	302	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	q	305	CLA	C4A-NA-C1A	6.56	109.66	106.71
26	Q	316	CHL	CHD-C1D-ND	-6.56	118.43	124.45
22	3	303	CLA	C4A-NA-C1A	6.55	109.65	106.71
22	n	302	CLA	C4A-NA-C1A	6.55	109.65	106.71
26	3	313	CHL	CHD-C1D-ND	-6.55	118.44	124.45
26	p	317	CHL	CHD-C1D-ND	-6.55	118.44	124.45
26	u	316	CHL	CHD-C1D-ND	-6.54	118.44	124.45
22	Q	305	CLA	C4A-NA-C1A	6.53	109.64	106.71
26	u	313	CHL	CHD-C1D-ND	-6.53	118.45	124.45
22	R	303	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	S	305	CLA	C4A-NA-C1A	6.52	109.64	106.71
26	N	316	CHL	CHD-C1D-ND	-6.52	118.46	124.45
22	g	308	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	a	406	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	u	304	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	b	614	CLA	C4A-NA-C1A	6.51	109.63	106.71
26	6	313	CHL	CHB-C1B-NB	-6.51	117.37	124.26
26	n	314	CHL	CHD-C1D-ND	-6.50	118.48	124.45
26	r	616	CHL	CHD-C1D-ND	-6.49	118.49	124.45
26	p	316	CHL	CHD-C1D-ND	-6.49	118.49	124.45
27	u	319	NEX	O24-C25-C24	6.48	118.25	113.38
22	n	303	CLA	C4A-NA-C1A	6.48	109.62	106.71
26	3	311	CHL	CHD-C1D-ND	-6.48	118.50	124.45
26	3	312	CHL	CHB-C1B-NB	-6.48	117.40	124.26
22	g	302	CLA	C4A-NA-C1A	6.47	109.62	106.71
26	1	314	CHL	CHD-C1D-ND	-6.47	118.51	124.45
26	q	312	CHL	CHB-C1B-NB	-6.46	117.41	124.26
22	4	305	CLA	C4A-NA-C1A	6.45	109.61	106.71
26	v	315	CHL	CHD-C1D-ND	-6.44	118.53	124.45
26	N	314	CHL	CHD-C1D-ND	-6.44	118.54	124.45
22	V	304	CLA	C4A-NA-C1A	6.43	109.60	106.71
26	g	313	CHL	CHD-C1D-ND	-6.42	118.55	124.45
22	G	302	CLA	C4A-NA-C1A	6.42	109.59	106.71
26	R	317	CHL	CHD-C1D-ND	-6.42	118.56	124.45
26	6	312	CHL	CHD-C1D-ND	-6.41	118.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V	316	CHL	CHD-C1D-ND	-6.41	118.56	124.45
26	n	315	CHL	CHD-C1D-ND	-6.40	118.57	124.45
26	G	314	CHL	CHD-C1D-ND	-6.40	118.58	124.45
22	v	304	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	r	602	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	4	302	CLA	C4A-NA-C1A	6.39	109.58	106.71
26	G	313	CHL	CHD-C1D-ND	-6.39	118.59	124.45
26	Q	312	CHL	CHD-C1D-ND	-6.38	118.59	124.45
26	Q	311	CHL	CHD-C1D-ND	-6.38	118.59	124.45
26	4	315	CHL	CHD-C1D-ND	-6.37	118.60	124.45
26	N	313	CHL	C2C-C3C-C4C	-6.37	101.95	106.49
26	V	314	CHL	CHD-C1D-ND	-6.36	118.61	124.45
26	u	317	CHL	O2D-CGD-CBD	6.36	122.57	111.27
22	b	604	CLA	C4A-NA-C1A	6.36	109.57	106.71
22	B	604	CLA	C4A-NA-C1A	6.36	109.56	106.71
26	P	316	CHL	CHD-C1D-ND	-6.35	118.62	124.45
26	1	316	CHL	CHD-C1D-ND	-6.35	118.62	124.45
26	g	312	CHL	CHD-C1D-ND	-6.35	118.62	124.45
26	Q	314	CHL	CHD-C1D-ND	-6.34	118.63	124.45
22	1	303	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	Q	302	CLA	C4A-NA-C1A	6.34	109.56	106.71
26	1	315	CHL	CHD-C1D-ND	-6.32	118.64	124.45
26	U	316	CHL	CHD-C1D-ND	-6.32	118.65	124.45
26	6	301	CHL	CHD-C1D-ND	-6.32	118.65	124.45
26	u	314	CHL	CHD-C1D-ND	-6.30	118.66	124.45
26	Q	315	CHL	CHD-C1D-ND	-6.30	118.67	124.45
24	R	313	XAT	C26-C27-C28	-6.29	112.69	125.99
26	p	314	CHL	CHD-C1D-ND	-6.29	118.68	124.45
31	C	516	BCR	C15-C14-C13	-6.28	118.34	127.31
26	v	316	CHL	CHD-C1D-ND	-6.28	118.68	124.45
26	N	314	CHL	CHB-C1B-NB	-6.27	117.62	124.26
26	n	313	CHL	CHD-C1D-ND	-6.27	118.69	124.45
26	V	317	CHL	CHD-C1D-ND	-6.26	118.70	124.45
31	z	101	BCR	C15-C14-C13	-6.25	118.39	127.31
26	q	313	CHL	CHD-C1D-ND	-6.24	118.72	124.45
26	Q	313	CHL	CHD-C1D-ND	-6.24	118.72	124.45
26	n	314	CHL	CHB-C1B-NB	-6.23	117.66	124.26
22	6	304	CLA	C4A-NA-C1A	6.23	109.51	106.71
26	U	319	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	R	313	XAT	C6-C7-C8	-6.21	112.86	125.99
26	n	316	CHL	CHD-C1D-ND	-6.21	118.75	124.45
26	u	317	CHL	CHD-C1D-ND	-6.20	118.75	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	316	CHL	CHD-C1D-ND	-6.20	118.76	124.45
26	4	316	CHL	CHD-C1D-ND	-6.19	118.76	124.45
26	p	320	CHL	CHD-C1D-ND	-6.18	118.78	124.45
26	q	314	CHL	CHD-C1D-ND	-6.17	118.78	124.45
26	V	318	CHL	CHD-C1D-ND	-6.17	118.79	124.45
26	1	317	CHL	CHD-C1D-ND	-6.15	118.80	124.45
26	g	315	CHL	CHD-C1D-ND	-6.14	118.81	124.45
22	c	511	CLA	C4A-NA-C1A	6.14	109.47	106.71
26	g	316	CHL	CHD-C1D-ND	-6.14	118.82	124.45
22	S	306	CLA	C4A-NA-C1A	6.13	109.46	106.71
22	U	301	CLA	C4A-NA-C1A	6.12	109.46	106.71
26	1	318	CHL	CHD-C1D-ND	-6.12	118.83	124.45
22	4	301	CLA	C4A-NA-C1A	6.12	109.46	106.71
26	v	317	CHL	CHD-C1D-ND	-6.12	118.83	124.45
22	v	301	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	d	402	CLA	C4A-NA-C1A	6.09	109.45	106.71
26	2	317	CHL	CHD-C1D-ND	-6.09	118.86	124.45
22	p	302	CLA	C4A-NA-C1A	6.09	109.44	106.71
24	r	612	XAT	C6-C7-C8	-6.08	113.13	125.99
26	g	311	CHL	CHD-C1D-ND	-6.07	118.87	124.45
26	2	318	CHL	CHD-C1D-ND	-6.06	118.88	124.45
22	n	305	CLA	CMD-C2D-C3D	6.06	141.55	127.61
22	2	305	CLA	CMD-C2D-C3D	6.05	141.53	127.61
26	5	317	CHL	CHD-C1D-ND	-6.05	118.90	124.45
26	p	319	CHL	CHD-C1D-ND	-6.05	118.90	124.45
31	B	620	BCR	C16-C17-C18	-6.03	118.70	127.31
22	1	302	CLA	C4A-NA-C1A	6.03	109.42	106.71
22	s	301	CLA	C4A-NA-C1A	6.03	109.42	106.71
26	5	318	CHL	CHD-C1D-ND	-6.03	118.92	124.45
26	6	316	CHL	CHD-C1D-ND	-6.03	118.92	124.45
22	P	306	CLA	CMD-C2D-C3D	6.02	141.47	127.61
26	G	315	CHL	CHD-C1D-ND	-6.02	118.92	124.45
22	p	306	CLA	CMD-C2D-C3D	6.02	141.45	127.61
26	G	312	CHL	CHB-C1B-NB	-6.02	117.89	124.26
22	D	403	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	V	301	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	s	306	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	n	301	CLA	C4A-NA-C1A	6.01	109.41	106.71
26	r	615	CHL	CHD-C1D-ND	-6.00	118.94	124.45
22	4	303	CLA	C4A-NA-C1A	6.00	109.40	106.71
22	u	301	CLA	C4A-NA-C1A	6.00	109.40	106.71
22	C	512	CLA	C4A-NA-C1A	5.99	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	301	CLA	C4A-NA-C1A	5.99	109.40	106.71
26	r	614	CHL	CHD-C1D-ND	-5.98	118.96	124.45
26	2	315	CHL	CHD-C1D-ND	-5.98	118.96	124.45
26	P	315	CHL	CHB-C1B-NB	-5.98	117.93	124.26
22	5	305	CLA	CMD-C2D-C3D	5.97	141.36	127.61
26	4	314	CHL	CHD-C1D-ND	-5.97	118.97	124.45
26	4	317	CHL	CHD-C1D-ND	-5.97	118.97	124.45
26	P	318	CHL	CHD-C1D-ND	-5.97	118.97	124.45
26	R	316	CHL	CHD-C1D-ND	-5.95	118.99	124.45
26	r	619	CHL	CHD-C1D-ND	-5.94	119.00	124.45
31	b	620	BCR	C16-C17-C18	-5.93	118.85	127.31
26	q	314	CHL	C3C-C4C-NC	5.91	117.20	110.57
22	S	301	CLA	C4A-NA-C1A	5.91	109.36	106.71
26	5	315	CHL	CHD-C1D-ND	-5.90	119.04	124.45
22	1	301	CLA	C4A-NA-C1A	5.89	109.35	106.71
22	P	302	CLA	C4A-NA-C1A	5.89	109.35	106.71
22	3	301	CLA	C4A-NA-C1A	5.88	109.35	106.71
26	u	315	CHL	C3C-C4C-NC	5.88	117.17	110.57
26	P	319	CHL	CHD-C1D-ND	-5.88	119.05	124.45
31	C	517	BCR	C1-C6-C5	-5.87	114.34	122.61
26	R	315	CHL	CHD-C1D-ND	-5.87	119.06	124.45
26	U	317	CHL	CHD-C1D-ND	-5.85	119.08	124.45
26	v	318	CHL	CHD-C1D-ND	-5.84	119.08	124.45
31	c	515	BCR	C1-C6-C5	-5.83	114.40	122.61
26	U	315	CHL	CHD-C1D-ND	-5.83	119.10	124.45
26	G	311	CHL	CHD-C1D-ND	-5.82	119.11	124.45
26	p	315	CHL	CHB-C1B-NB	-5.82	118.10	124.26
22	q	301	CLA	C4A-NA-C1A	5.80	109.31	106.71
26	u	318	CHL	CHD-C1D-ND	-5.78	119.14	124.45
26	Q	315	CHL	C3C-C4C-NC	5.76	117.04	110.57
22	N	301	CLA	C4A-NA-C1A	5.76	109.30	106.71
26	6	316	CHL	C3C-C4C-NC	5.76	117.03	110.57
26	p	318	CHL	C3B-C2B-C1B	-5.75	100.22	107.16
26	n	318	CHL	O2D-CGD-CBD	5.73	121.44	111.27
22	N	305	CLA	CMD-C2D-C3D	5.72	140.76	127.61
22	g	301	CLA	C4A-NA-C1A	5.71	109.27	106.71
26	v	314	CHL	CHD-C1D-ND	-5.71	119.21	124.45
26	p	318	CHL	CHD-C1D-ND	-5.71	119.21	124.45
24	V	311	XAT	C15-C14-C13	-5.70	119.18	127.31
22	5	301	CLA	C4A-NA-C1A	5.69	109.27	106.71
27	V	319	NEX	C11-C10-C9	-5.68	119.21	127.31
26	n	316	CHL	C3B-C2B-C1B	-5.68	100.31	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	302	CLA	C4A-NA-C1A	5.67	109.26	106.71
26	g	314	CHL	CHB-C1B-NB	-5.67	118.26	124.26
31	x	202	BCR	C11-C10-C9	-5.66	119.23	127.31
26	s	314	CHL	CHD-C1D-ND	-5.66	119.26	124.45
26	g	312	CHL	C3B-C2B-C1B	-5.65	100.34	107.16
26	S	314	CHL	CHD-C1D-ND	-5.64	119.27	124.45
24	n	311	XAT	C6-C7-C8	-5.64	114.07	125.99
26	G	315	CHL	C3C-C4C-NC	5.64	116.89	110.57
31	x	202	BCR	C7-C8-C9	-5.63	117.72	126.23
26	q	312	CHL	C3B-C2B-C1B	-5.61	100.39	107.16
26	G	312	CHL	C3B-C2B-C1B	-5.60	100.40	107.16
26	P	318	CHL	C3B-C2B-C1B	-5.60	100.41	107.16
26	4	316	CHL	C3B-C2B-C1B	-5.60	100.41	107.16
26	R	316	CHL	C3B-C2B-C1B	-5.59	100.41	107.16
26	g	315	CHL	C3C-C4C-NC	5.59	116.84	110.57
26	1	317	CHL	C3B-C2B-C1B	-5.59	100.41	107.16
26	r	615	CHL	C3B-C2B-C1B	-5.58	100.42	107.16
31	X	201	BCR	C7-C8-C9	-5.58	117.80	126.23
22	Q	301	CLA	C4A-NA-C1A	5.58	109.21	106.71
31	X	201	BCR	C11-C10-C9	-5.58	119.35	127.31
26	2	318	CHL	C3B-C2B-C1B	-5.56	100.44	107.16
31	C	516	BCR	C16-C17-C18	-5.56	119.38	127.31
26	5	318	CHL	C3B-C2B-C1B	-5.56	100.45	107.16
26	1	314	CHL	C3B-C2B-C1B	-5.55	100.46	107.16
26	p	320	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
26	g	313	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
26	u	317	CHL	C3B-C2B-C1B	-5.54	100.47	107.16
31	z	101	BCR	C16-C17-C18	-5.54	119.41	127.31
26	U	314	CHL	C3C-C4C-NC	5.53	116.77	110.57
26	3	315	CHL	C3C-C4C-NC	5.52	116.76	110.57
26	G	314	CHL	C3B-C2B-C1B	-5.52	100.50	107.16
26	v	313	CHL	O2D-CGD-CBD	5.52	121.07	111.27
26	N	317	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
26	5	314	CHL	C3B-C2B-C1B	-5.51	100.51	107.16
27	u	319	NEX	C38-C25-C26	-5.51	113.03	122.26
26	g	312	CHL	O2D-CGD-CBD	5.50	121.04	111.27
22	G	301	CLA	C4A-NA-C1A	5.49	109.18	106.71
26	p	319	CHL	C3B-C2B-C1B	-5.49	100.54	107.16
26	N	315	CHL	CHD-C1D-ND	-5.48	119.41	124.45
26	4	314	CHL	C3B-C2B-C1B	-5.48	100.54	107.16
26	Q	314	CHL	C3B-C2B-C1B	-5.48	100.55	107.16
26	5	318	CHL	O2D-CGD-CBD	5.47	121.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	314	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
26	3	314	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
26	2	314	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
26	U	319	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
26	g	314	CHL	C3B-C2B-C1B	-5.47	100.56	107.16
26	V	318	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
26	U	316	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
26	G	316	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
26	V	314	CHL	C3B-C2B-C1B	-5.46	100.57	107.16
26	6	315	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
26	V	317	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
26	R	316	CHL	C3C-C4C-NC	5.45	116.69	110.57
26	N	314	CHL	C3B-C2B-C1B	-5.45	100.58	107.16
26	s	314	CHL	C3C-C4C-NC	5.44	116.68	110.57
26	n	318	CHL	C3B-C2B-C1B	-5.44	100.59	107.16
26	p	317	CHL	C3B-C2B-C1B	-5.44	100.60	107.16
26	V	316	CHL	C3B-C2B-C1B	-5.44	100.60	107.16
26	N	315	CHL	C3C-C4C-NC	5.44	116.67	110.57
26	6	301	CHL	C3B-C2B-C1B	-5.43	100.60	107.16
26	5	315	CHL	C3B-C2B-C1B	-5.43	100.60	107.16
24	Q	309	XAT	C15-C14-C13	-5.43	119.56	127.31
26	S	314	CHL	C3C-C4C-NC	5.43	116.66	110.57
26	Q	313	CHL	O2D-CGD-CBD	5.43	120.92	111.27
26	P	317	CHL	C3B-C2B-C1B	-5.43	100.61	107.16
26	1	314	CHL	CHB-C1B-NB	-5.43	118.51	124.26
26	4	313	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
26	p	316	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
26	N	316	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
26	3	314	CHL	CHB-C1B-NB	-5.42	118.52	124.26
31	t	101	BCR	C24-C23-C22	-5.42	118.05	126.23
26	6	317	CHL	C3B-C2B-C1B	-5.42	100.62	107.16
26	2	316	CHL	C3B-C2B-C1B	-5.41	100.62	107.16
26	5	315	CHL	C3C-C4C-NC	5.41	116.64	110.57
26	V	313	CHL	O2D-CGD-CBD	5.41	120.88	111.27
26	V	314	CHL	CHB-C1B-NB	-5.41	118.53	124.26
26	v	318	CHL	C3B-C2B-C1B	-5.41	100.64	107.16
26	p	318	CHL	C3C-C4C-NC	5.41	116.63	110.57
26	5	316	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
26	N	315	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
26	3	312	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
26	3	316	CHL	C3B-C2B-C1B	-5.40	100.64	107.16
26	r	619	CHL	C3B-C2B-C1B	-5.40	100.65	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	314	CHL	C3B-C2B-C1B	-5.39	100.65	107.16
24	G	309	XAT	C6-C7-C8	-5.39	114.60	125.99
26	3	315	CHL	C3B-C2B-C1B	-5.38	100.66	107.16
26	q	314	CHL	C2D-C1D-ND	5.38	114.07	110.10
24	6	310	XAT	C6-C7-C8	-5.38	114.63	125.99
26	P	319	CHL	C3B-C2B-C1B	-5.37	100.67	107.16
26	s	314	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
26	6	313	CHL	C3B-C2B-C1B	-5.37	100.68	107.16
26	P	314	CHL	C3B-C2B-C1B	-5.36	100.69	107.16
26	v	314	CHL	C3B-C2B-C1B	-5.36	100.70	107.16
26	3	311	CHL	O2D-CGD-CBD	5.35	120.78	111.27
26	q	312	CHL	C4A-NA-C1A	5.35	109.11	106.71
26	1	316	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
26	5	317	CHL	C3B-C2B-C1B	-5.35	100.70	107.16
26	P	318	CHL	C3C-C4C-NC	5.35	116.57	110.57
26	q	315	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
26	U	315	CHL	C3B-C2B-C1B	-5.35	100.71	107.16
26	U	314	CHL	C3B-C2B-C1B	-5.34	100.72	107.16
26	v	316	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
26	2	315	CHL	C3B-C2B-C1B	-5.33	100.73	107.16
26	4	317	CHL	C3B-C2B-C1B	-5.32	100.73	107.16
26	u	314	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
26	Q	316	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
26	Q	312	CHL	C3B-C2B-C1B	-5.32	100.74	107.16
26	r	615	CHL	C3C-C4C-NC	5.32	116.53	110.57
24	q	309	XAT	C15-C14-C13	-5.31	119.72	127.31
26	6	315	CHL	CHB-C1B-NB	-5.31	118.63	124.26
26	u	315	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
27	n	319	NEX	C15-C14-C13	-5.31	119.73	127.31
26	n	317	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
26	s	315	CHL	C3B-C2B-C1B	-5.31	100.75	107.16
26	q	313	CHL	O2D-CGD-CBD	5.31	120.70	111.27
26	2	317	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
26	g	316	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
26	1	318	CHL	C3B-C2B-C1B	-5.30	100.76	107.16
31	K	101	BCR	C16-C17-C18	-5.30	119.74	127.31
31	T	101	BCR	C24-C23-C22	-5.30	118.23	126.23
26	S	316	CHL	O2D-CGD-CBD	5.29	120.67	111.27
26	u	316	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
26	S	315	CHL	C3B-C2B-C1B	-5.29	100.77	107.16
24	g	309	XAT	C6-C7-C8	-5.29	114.80	125.99
26	P	315	CHL	C4A-NA-C1A	5.29	109.08	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	316	CHL	O2D-CGD-CBD	5.29	120.67	111.27
26	u	313	CHL	C3B-C2B-C1B	-5.29	100.78	107.16
26	v	314	CHL	C3C-C4C-NC	5.29	116.50	110.57
31	B	618	BCR	C15-C14-C13	-5.29	119.77	127.31
26	2	313	CHL	CHC-C4B-NB	-5.28	118.66	124.26
26	U	313	CHL	C3B-C2B-C1B	-5.28	100.79	107.16
26	2	315	CHL	C3C-C4C-NC	5.27	116.49	110.57
26	n	315	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
26	q	312	CHL	O2D-CGD-CBD	5.27	120.64	111.27
27	n	319	NEX	C11-C10-C9	-5.27	119.79	127.31
26	2	318	CHL	O2D-CGD-CBD	5.27	120.63	111.27
26	G	311	CHL	O2D-CGD-CBD	5.27	120.63	111.27
26	U	317	CHL	C3B-C2B-C1B	-5.27	100.80	107.16
26	p	315	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
26	6	312	CHL	O2D-CGD-CBD	5.26	120.62	111.27
26	n	314	CHL	C4A-NA-C1A	5.26	109.07	106.71
26	U	314	CHL	CHD-C1D-ND	-5.26	119.62	124.45
26	3	313	CHL	C3B-C2B-C1B	-5.26	100.81	107.16
26	G	312	CHL	O2D-CGD-CBD	5.25	120.60	111.27
26	Q	311	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
26	P	316	CHL	C3B-C2B-C1B	-5.25	100.82	107.16
31	C	518	BCR	C16-C17-C18	-5.25	119.82	127.31
31	B	619	BCR	C16-C17-C18	-5.25	119.82	127.31
26	6	314	CHL	C3B-C2B-C1B	-5.25	100.83	107.16
26	6	312	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
26	P	315	CHL	C3B-C2B-C1B	-5.24	100.83	107.16
31	b	618	BCR	C15-C14-C13	-5.24	119.83	127.31
26	3	311	CHL	C3B-C2B-C1B	-5.24	100.84	107.16
26	u	317	CHL	C3C-C4C-NC	5.24	116.44	110.57
26	q	311	CHL	C3B-C2B-C1B	-5.23	100.85	107.16
31	K	101	BCR	C1-C6-C5	-5.23	115.25	122.61
26	p	316	CHL	O2D-CGD-CBD	5.22	120.54	111.27
31	k	101	BCR	C1-C6-C5	-5.21	115.27	122.61
26	N	313	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
26	V	313	CHL	C3B-C2B-C1B	-5.21	100.87	107.16
26	p	314	CHL	O2D-CGD-CBD	5.21	120.52	111.27
26	6	316	CHL	C2D-C1D-ND	5.21	113.94	110.10
26	2	317	CHL	C3C-C4C-NC	5.20	116.41	110.57
26	U	316	CHL	C3C-C4C-NC	5.20	116.41	110.57
26	R	315	CHL	O2D-CGD-CBD	5.20	120.52	111.27
26	u	318	CHL	C3C-C4C-NC	5.20	116.41	110.57
26	N	317	CHL	O2D-CGD-CBD	5.20	120.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	r	614	CHL	O2D-CGD-CBD	5.20	120.51	111.27
26	p	320	CHL	C3C-C4C-NC	5.20	116.40	110.57
26	g	316	CHL	O2D-CGD-CBD	5.20	120.50	111.27
26	Q	315	CHL	C2D-C1D-ND	5.20	113.93	110.10
31	c	516	BCR	C16-C17-C18	-5.19	119.90	127.31
26	n	313	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
26	v	313	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
26	r	614	CHL	C3B-C2B-C1B	-5.19	100.89	107.16
26	r	619	CHL	C3C-C4C-NC	5.19	116.39	110.57
31	b	618	BCR	C11-C10-C9	-5.19	119.90	127.31
26	4	314	CHL	O2D-CGD-CBD	5.19	120.48	111.27
26	4	314	CHL	C3C-C4C-NC	5.18	116.38	110.57
26	g	312	CHL	CHB-C1B-NB	-5.18	118.77	124.26
31	k	101	BCR	C16-C17-C18	-5.18	119.92	127.31
27	u	319	NEX	C15-C14-C13	-5.18	119.92	127.31
26	P	314	CHL	O2D-CGD-CBD	5.18	120.47	111.27
26	6	314	CHL	O2D-CGD-CBD	5.18	120.47	111.27
26	U	317	CHL	C3C-C4C-NC	5.17	116.37	110.57
31	b	619	BCR	C16-C17-C18	-5.17	119.93	127.31
26	q	315	CHL	O2D-CGD-CBD	5.16	120.44	111.27
26	s	314	CHL	O2D-CGD-CBD	5.16	120.44	111.27
26	v	316	CHL	C3C-C4C-NC	5.16	116.36	110.57
26	n	317	CHL	O2D-CGD-CBD	5.16	120.44	111.27
26	S	314	CHL	O2D-CGD-CBD	5.16	120.43	111.27
27	2	319	NEX	C11-C10-C9	-5.15	119.96	127.31
26	s	316	CHL	C3B-C2B-C1B	-5.15	100.94	107.16
26	6	316	CHL	C3B-C2B-C1B	-5.15	100.95	107.16
26	3	313	CHL	O2D-CGD-CBD	5.15	120.41	111.27
26	G	311	CHL	C3C-C4C-NC	5.14	116.34	110.57
31	x	202	BCR	C16-C17-C18	-5.14	119.97	127.31
26	3	311	CHL	C3C-C4C-NC	5.14	116.33	110.57
26	6	312	CHL	C3C-C4C-NC	5.13	116.33	110.57
26	V	315	CHL	O2D-CGD-CBD	5.13	120.39	111.27
26	Q	315	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
26	g	315	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
31	c	515	BCR	C4-C5-C6	-5.13	115.28	122.73
26	P	319	CHL	C3C-C4C-NC	5.12	116.32	110.57
26	N	316	CHL	C3C-C4C-NC	5.12	116.31	110.57
31	B	618	BCR	C11-C10-C9	-5.12	120.00	127.31
26	R	315	CHL	C3B-C2B-C1B	-5.12	100.98	107.16
26	V	315	CHL	C3B-C2B-C1B	-5.12	100.98	107.16
26	Q	315	CHL	C3B-C2B-C1B	-5.12	100.98	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	201	BCR	C16-C17-C18	-5.11	120.01	127.31
26	p	319	CHL	O2D-CGD-CBD	5.11	120.36	111.27
31	c	515	BCR	C33-C5-C6	-5.11	118.79	124.53
26	6	313	CHL	C4A-NA-C1A	5.11	109.00	106.71
26	q	314	CHL	C3D-C2D-C1D	-5.11	98.86	105.83
26	1	315	CHL	C3B-C2B-C1B	-5.11	100.99	107.16
26	Q	311	CHL	O2D-CGD-CBD	5.11	120.34	111.27
26	5	317	CHL	C3C-C4C-NC	5.10	116.30	110.57
24	4	311	XAT	C35-C34-C33	-5.10	120.03	127.31
26	g	311	CHL	C3C-C4C-NC	5.10	116.29	110.57
27	N	318	NEX	C38-C25-C26	-5.10	113.71	122.26
26	4	315	CHL	O2D-CGD-CBD	5.10	120.33	111.27
26	V	315	CHL	CHB-C1B-NB	-5.10	118.86	124.26
26	v	318	CHL	C3C-C4C-NC	5.10	116.28	110.57
26	5	313	CHL	CHC-C4B-NB	-5.09	118.87	124.26
26	4	317	CHL	C3C-C4C-NC	5.09	116.28	110.57
26	G	313	CHL	C3B-C2B-C1B	-5.09	101.02	107.16
26	4	317	CHL	O2D-CGD-CBD	5.09	120.31	111.27
26	G	315	CHL	C3B-C2B-C1B	-5.09	101.02	107.16
31	C	517	BCR	C33-C5-C6	-5.08	118.82	124.53
26	5	314	CHL	C4A-NA-C1A	5.08	108.99	106.71
26	P	316	CHL	O2D-CGD-CBD	5.08	120.30	111.27
26	r	614	CHL	C3C-C4C-NC	5.08	116.27	110.57
22	B	605	CLA	CAA-C2A-C3A	-5.08	98.87	112.78
26	v	315	CHL	O2D-CGD-CBD	5.08	120.29	111.27
31	C	517	BCR	C4-C5-C6	-5.08	115.36	122.73
26	g	311	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
26	S	316	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
26	g	315	CHL	C3B-C2B-C1B	-5.07	101.04	107.16
24	Q	309	XAT	C11-C10-C9	-5.07	120.07	127.31
26	R	315	CHL	C3C-C4C-NC	5.07	116.25	110.57
22	b	605	CLA	CAA-C2A-C3A	-5.07	98.90	112.78
30	D	401	PHO	C2B-C1B-NB	-5.07	106.03	109.53
26	6	316	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
26	G	315	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
26	1	317	CHL	C3C-C4C-NC	5.06	116.24	110.57
26	g	313	CHL	C3C-C4C-NC	5.06	116.24	110.57
26	V	318	CHL	O2D-CGD-CBD	5.05	120.25	111.27
24	3	309	XAT	C6-C7-C8	-5.05	115.32	125.99
24	q	309	XAT	C11-C10-C9	-5.04	120.11	127.31
31	B	618	BCR	C16-C17-C18	-5.04	120.11	127.31
26	g	311	CHL	O2D-CGD-CBD	5.04	120.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	315	CHL	O2D-CGD-CBD	5.04	120.22	111.27
26	1	316	CHL	O2D-CGD-CBD	5.04	120.22	111.27
31	b	618	BCR	C38-C26-C25	-5.04	118.87	124.53
27	S	317	NEX	C11-C10-C9	-5.03	120.12	127.31
26	n	313	CHL	C3C-C4C-NC	5.03	116.22	110.57
31	K	101	BCR	C20-C21-C22	-5.03	120.13	127.31
31	b	618	BCR	C16-C17-C18	-5.03	120.13	127.31
26	p	319	CHL	C3C-C4C-NC	5.03	116.21	110.57
31	k	101	BCR	C20-C21-C22	-5.03	120.14	127.31
26	N	313	CHL	O2D-CGD-CBD	5.03	120.20	111.27
27	2	319	NEX	C38-C25-C26	-5.02	113.84	122.26
27	V	319	NEX	C27-C28-C29	-5.02	117.74	125.53
27	2	319	NEX	C27-C28-C29	-5.02	117.74	125.53
26	q	313	CHL	C3B-C2B-C1B	-5.02	101.10	107.16
30	d	401	PHO	C2B-C1B-NB	-5.02	106.06	109.53
26	p	317	CHL	O2D-CGD-CBD	5.01	120.18	111.27
26	4	316	CHL	C3C-C4C-NC	5.01	116.19	110.57
26	4	315	CHL	C3B-C2B-C1B	-5.01	101.11	107.16
27	U	318	NEX	C15-C14-C13	-5.01	120.16	127.31
27	u	319	NEX	C11-C10-C9	-5.01	120.16	127.31
26	Q	313	CHL	C3B-C2B-C1B	-5.01	101.11	107.16
26	v	317	CHL	C3B-C2B-C1B	-5.01	101.12	107.16
26	1	315	CHL	O2D-CGD-CBD	5.00	120.15	111.27
31	T	101	BCR	C11-C10-C9	-4.99	120.18	127.31
26	N	315	CHL	O2D-CGD-CBD	4.99	120.14	111.27
26	1	318	CHL	C3C-C4C-NC	4.99	116.17	110.57
27	5	319	NEX	C11-C10-C9	-4.99	120.19	127.31
26	Q	312	CHL	O2D-CGD-CBD	4.98	120.12	111.27
24	R	313	XAT	C18-C5-C6	-4.98	113.91	122.26
27	P	301	NEX	C38-C25-C26	-4.98	113.92	122.26
26	q	314	CHL	C3B-C2B-C1B	-4.97	101.16	107.16
27	S	317	NEX	C38-C25-C26	-4.97	113.92	122.26
26	U	315	CHL	C3C-C4C-NC	4.97	116.15	110.57
26	n	317	CHL	C3C-C4C-NC	4.97	116.15	110.57
32	L	102	SQD	O9-S-C6	4.97	112.85	106.94
26	v	314	CHL	O2D-CGD-CBD	4.97	120.11	111.27
31	t	101	BCR	C11-C10-C9	-4.97	120.21	127.31
26	Q	311	CHL	C3C-C4C-NC	4.97	116.15	110.57
26	v	318	CHL	O2D-CGD-CBD	4.97	120.09	111.27
26	P	319	CHL	O2D-CGD-CBD	4.97	120.09	111.27
26	2	316	CHL	O2D-CGD-CBD	4.96	120.08	111.27
27	5	319	NEX	C27-C28-C29	-4.96	117.84	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	315	CHL	C3D-C2D-C1D	-4.96	99.07	105.83
26	V	314	CHL	O2D-CGD-CBD	4.95	120.07	111.27
26	s	315	CHL	O2D-CGD-CBD	4.95	120.07	111.27
26	1	314	CHL	O2D-CGD-CBD	4.95	120.06	111.27
26	N	316	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
26	5	316	CHL	O2D-CGD-CBD	4.94	120.05	111.27
26	1	313	CHL	O2D-CGD-CBD	4.94	120.05	111.27
24	N	311	XAT	C6-C7-C8	-4.94	115.55	125.99
26	S	313	CHL	O2D-CGD-CBD	4.94	120.05	111.27
26	p	318	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
26	p	314	CHL	C3C-C4C-NC	4.94	116.11	110.57
31	t	101	BCR	C33-C5-C6	-4.94	118.98	124.53
26	p	314	CHL	C3B-C2B-C1B	-4.93	101.21	107.16
26	5	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
26	n	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
26	2	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
27	v	319	NEX	C27-C28-C29	-4.93	117.88	125.53
26	U	313	CHL	O2D-CGD-CBD	4.93	120.03	111.27
26	s	316	CHL	CHB-C1B-NB	-4.93	119.04	124.26
26	u	314	CHL	C3C-C4C-NC	4.93	116.10	110.57
26	V	317	CHL	C3C-C4C-NC	4.93	116.10	110.57
26	G	316	CHL	C3C-C4C-NC	4.92	116.09	110.57
27	s	317	NEX	C38-C25-C26	-4.92	114.01	122.26
26	v	317	CHL	C3C-C4C-NC	4.92	116.09	110.57
26	G	311	CHL	C3B-C2B-C1B	-4.92	101.22	107.16
27	u	320	NEX	C38-C25-C26	-4.92	114.02	122.26
32	l	102	SQD	O9-S-C6	4.91	112.78	106.94
27	v	319	NEX	C11-C10-C9	-4.91	120.30	127.31
26	S	316	CHL	CHB-C1B-NB	-4.91	119.06	124.26
26	v	313	CHL	C3C-C4C-NC	4.91	116.08	110.57
26	G	313	CHL	C3C-C4C-NC	4.91	116.08	110.57
27	r	617	NEX	C38-C25-C26	-4.91	114.03	122.26
26	Q	316	CHL	O2D-CGD-CBD	4.91	119.99	111.27
26	g	313	CHL	O2D-CGD-CBD	4.90	119.98	111.27
26	G	312	CHL	C4A-NA-C1A	4.90	108.91	106.71
26	1	313	CHL	C3B-C2B-C1B	-4.90	101.24	107.16
26	4	313	CHL	O2D-CGD-CBD	4.90	119.98	111.27
31	b	619	BCR	C1-C6-C5	-4.90	115.71	122.61
24	U	311	XAT	C6-C7-C8	-4.90	115.64	125.99
26	V	318	CHL	C3C-C4C-NC	4.89	116.05	110.57
26	P	318	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
26	1	318	CHL	O2D-CGD-CBD	4.88	119.94	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	316	CHL	C3C-C4C-NC	4.88	116.04	110.57
27	N	318	NEX	C15-C14-C13	-4.88	120.35	127.31
31	T	101	BCR	C33-C5-C6	-4.88	119.05	124.53
26	s	313	CHL	O2D-CGD-CBD	4.88	119.93	111.27
27	u	319	NEX	O24-C25-C38	4.88	120.90	115.06
31	b	619	BCR	C15-C14-C13	-4.88	120.35	127.31
31	D	404	BCR	C24-C23-C22	-4.87	118.87	126.23
26	6	317	CHL	O2D-CGD-CBD	4.87	119.93	111.27
26	R	316	CHL	O2D-CGD-CBD	4.87	119.93	111.27
26	Q	314	CHL	CHB-C1B-NB	-4.87	119.10	124.26
26	G	315	CHL	C2D-C1D-ND	4.87	113.69	110.10
31	B	619	BCR	C1-C6-C5	-4.86	115.76	122.61
26	p	317	CHL	C3C-C4C-NC	4.86	116.03	110.57
27	U	318	NEX	C38-C25-C26	-4.86	114.11	122.26
27	V	319	NEX	C38-C25-C26	-4.86	114.11	122.26
36	C	519	DGD	O2G-C1B-C2B	4.86	121.97	111.50
26	3	312	CHL	C4A-NA-C1A	4.86	108.89	106.71
26	5	313	CHL	C3B-C2B-C1B	-4.85	101.30	107.16
26	s	313	CHL	C3B-C2B-C1B	-4.85	101.30	107.16
31	B	619	BCR	C15-C14-C13	-4.85	120.39	127.31
26	s	315	CHL	CHB-C1B-NB	-4.85	119.12	124.26
26	G	314	CHL	CHB-C1B-NB	-4.85	119.12	124.26
26	V	314	CHL	C3C-C4C-NC	4.85	116.01	110.57
36	c	517	DGD	O2G-C1B-C2B	4.85	121.95	111.50
31	B	618	BCR	C38-C26-C25	-4.85	119.09	124.53
31	d	403	BCR	C24-C23-C22	-4.85	118.91	126.23
26	2	317	CHL	O2D-CGD-CBD	4.84	119.87	111.27
26	6	301	CHL	O2D-CGD-CBD	4.84	119.87	111.27
26	6	313	CHL	O2D-CGD-CBD	4.84	119.87	111.27
26	U	319	CHL	C3C-C4C-NC	4.84	116.00	110.57
26	2	317	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
27	5	319	NEX	C38-C25-C26	-4.84	114.15	122.26
26	2	318	CHL	C3C-C4C-NC	4.84	116.00	110.57
24	u	311	XAT	C6-C7-C8	-4.83	115.79	125.99
27	n	319	NEX	C17-C1-C6	-4.82	106.16	110.47
26	U	317	CHL	O2D-CGD-CBD	4.82	119.84	111.27
26	2	313	CHL	C3B-C2B-C1B	-4.82	101.34	107.16
31	d	403	BCR	C30-C25-C26	-4.82	115.82	122.61
26	v	315	CHL	C3C-C4C-NC	4.82	115.98	110.57
26	5	317	CHL	C3D-C2D-C1D	-4.82	99.25	105.83
31	A	409	BCR	C11-C10-C9	-4.82	120.43	127.31
26	5	318	CHL	C3C-C4C-NC	4.82	115.97	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	320	CHL	C3D-C2D-C1D	-4.81	99.27	105.83
26	g	315	CHL	C2D-C1D-ND	4.81	113.65	110.10
27	p	301	NEX	C38-C25-C26	-4.81	114.21	122.26
26	q	313	CHL	C3C-C4C-NC	4.80	115.96	110.57
26	3	311	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
26	Q	312	CHL	C3C-C4C-NC	4.80	115.95	110.57
26	v	316	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
26	5	317	CHL	O2D-CGD-CBD	4.79	119.78	111.27
26	S	315	CHL	CHB-C1B-NB	-4.79	119.18	124.26
31	a	409	BCR	C1-C6-C5	-4.79	115.87	122.61
26	v	315	CHL	C3B-C2B-C1B	-4.79	101.38	107.16
26	3	316	CHL	O2D-CGD-CBD	4.79	119.77	111.27
26	R	316	CHL	C3D-C2D-C1D	-4.79	99.30	105.83
31	t	101	BCR	C20-C21-C22	-4.78	120.48	127.31
26	G	316	CHL	O2D-CGD-CBD	4.78	119.77	111.27
24	v	311	XAT	C15-C14-C13	-4.78	120.49	127.31
27	u	319	NEX	C31-C30-C29	-4.78	120.49	127.31
31	T	101	BCR	C7-C8-C9	-4.78	119.02	126.23
26	S	313	CHL	C3B-C2B-C1B	-4.78	101.40	107.16
26	P	317	CHL	O2D-CGD-CBD	4.77	119.75	111.27
27	R	301	NEX	C17-C1-C6	-4.77	106.20	110.47
31	D	404	BCR	C30-C25-C26	-4.77	115.90	122.61
24	r	612	XAT	C18-C5-C6	-4.77	114.27	122.26
26	2	313	CHL	CHB-C1B-NB	-4.77	119.21	124.26
26	5	315	CHL	O2D-CGD-CBD	4.76	119.73	111.27
26	G	315	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
26	3	312	CHL	O2D-CGD-CBD	4.76	119.73	111.27
26	u	317	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
27	2	319	NEX	C35-C34-C33	-4.76	120.52	127.31
26	u	318	CHL	O2D-CGD-CBD	4.75	119.72	111.27
24	p	312	XAT	C6-C7-C8	-4.75	115.94	125.99
26	R	317	CHL	C3C-C4C-NC	4.75	115.90	110.57
31	A	409	BCR	C1-C6-C5	-4.75	115.92	122.61
26	G	313	CHL	O2D-CGD-CBD	4.75	119.70	111.27
24	q	309	XAT	C26-C27-C28	-4.75	115.96	125.99
26	g	311	CHL	C3D-C2D-C1D	-4.74	99.36	105.83
27	n	319	NEX	C38-C25-C26	-4.74	114.31	122.26
31	c	515	BCR	C11-C10-C9	-4.74	120.54	127.31
26	P	318	CHL	CHD-C4C-C3C	-4.74	117.87	124.84
26	r	619	CHL	C3D-C2D-C1D	-4.74	99.37	105.83
26	n	318	CHL	CHB-C1B-NB	-4.74	119.24	124.26
26	r	615	CHL	C3D-C2D-C1D	-4.73	99.37	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	t	101	BCR	C7-C8-C9	-4.73	119.08	126.23
27	r	617	NEX	C15-C14-C13	-4.73	120.56	127.31
24	6	310	XAT	C15-C14-C13	-4.73	120.56	127.31
26	1	315	CHL	C3C-C4C-NC	4.72	115.87	110.57
26	p	318	CHL	CHD-C4C-C3C	-4.72	117.90	124.84
26	2	313	CHL	C3C-C4C-NC	4.72	115.87	110.57
26	1	316	CHL	C3C-C4C-NC	4.72	115.86	110.57
26	n	317	CHL	C3D-C2D-C1D	-4.72	99.39	105.83
26	p	316	CHL	CHB-C1B-NB	-4.72	119.26	124.26
26	3	315	CHL	C2D-C1D-ND	4.72	113.58	110.10
26	r	616	CHL	C3B-C2B-C1B	-4.72	101.47	107.16
26	u	318	CHL	C3B-C2B-C1B	-4.72	101.47	107.16
32	l	102	SQD	O5-C5-C4	4.72	118.26	109.69
26	q	311	CHL	C3C-C4C-NC	4.71	115.86	110.57
27	p	301	NEX	C27-C28-C29	-4.71	118.22	125.53
26	1	314	CHL	C3C-C4C-NC	4.71	115.86	110.57
31	C	517	BCR	C27-C26-C25	-4.71	115.89	122.73
24	6	310	XAT	C26-C27-C28	-4.71	116.03	125.99
26	r	615	CHL	O2D-CGD-CBD	4.71	119.64	111.27
27	P	301	NEX	C27-C28-C29	-4.71	118.22	125.53
26	g	312	CHL	C3C-C4C-NC	4.70	115.85	110.57
26	P	317	CHL	CHB-C1B-NB	-4.70	119.28	124.26
26	R	317	CHL	C3B-C2B-C1B	-4.70	101.49	107.16
26	2	317	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
27	5	319	NEX	C35-C34-C33	-4.70	120.60	127.31
31	a	409	BCR	C11-C10-C9	-4.70	120.60	127.31
31	b	618	BCR	C24-C23-C22	-4.70	119.14	126.23
26	6	312	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
26	2	315	CHL	O2D-CGD-CBD	4.69	119.60	111.27
26	U	316	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
31	T	101	BCR	C20-C21-C22	-4.69	120.62	127.31
32	C	501	SQD	C1-O5-C5	4.69	122.89	113.69
26	5	313	CHL	C3C-C4C-NC	4.68	115.82	110.57
26	n	314	CHL	O2D-CGD-CBD	4.68	119.59	111.27
24	3	309	XAT	C15-C14-C13	-4.68	120.63	127.31
31	x	202	BCR	C15-C14-C13	-4.68	120.63	127.31
32	a	410	SQD	C1-O5-C5	4.68	122.88	113.69
27	v	319	NEX	C38-C25-C26	-4.68	114.42	122.26
26	P	314	CHL	C3C-C4C-NC	4.68	115.82	110.57
26	P	319	CHL	C3D-C2D-C1D	-4.68	99.45	105.83
26	r	619	CHL	O2D-CGD-CBD	4.68	119.58	111.27
26	4	314	CHL	C3D-C2D-C1D	-4.68	99.45	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q	313	CHL	C3C-C4C-NC	4.68	115.81	110.57
26	3	313	CHL	CHB-C1B-NB	-4.67	119.31	124.26
26	g	315	CHL	CHD-C4C-C3C	-4.67	117.97	124.84
26	v	314	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
26	U	319	CHL	C3D-C2D-C1D	-4.67	99.46	105.83
31	c	515	BCR	C27-C26-C25	-4.67	115.95	122.73
26	P	316	CHL	C3C-C4C-NC	4.66	115.80	110.57
26	u	315	CHL	CHD-C4C-C3C	-4.66	117.99	124.84
26	r	616	CHL	C3C-C4C-NC	4.66	115.80	110.57
32	L	102	SQD	O5-C5-C4	4.66	118.16	109.69
26	g	314	CHL	C3D-C2D-C1D	-4.66	99.47	105.83
31	X	201	BCR	C15-C14-C13	-4.65	120.67	127.31
27	u	320	NEX	C15-C14-C13	-4.65	120.67	127.31
26	1	318	CHL	C3D-C2D-C1D	-4.65	99.48	105.83
26	6	314	CHL	CHB-C1B-NB	-4.65	119.34	124.26
26	V	316	CHL	CHB-C1B-NB	-4.65	119.34	124.26
26	V	313	CHL	C3C-C4C-NC	4.64	115.78	110.57
26	u	314	CHL	C3D-C2D-C1D	-4.64	99.49	105.83
26	2	314	CHL	O2D-CGD-CBD	4.64	119.52	111.27
26	5	313	CHL	CHB-C1B-NB	-4.64	119.34	124.26
26	5	316	CHL	C3C-C4C-NC	4.64	115.77	110.57
26	u	313	CHL	C3C-C4C-NC	4.64	115.77	110.57
24	P	312	XAT	C15-C14-C13	-4.64	120.69	127.31
26	U	319	CHL	O2D-CGD-CBD	4.63	119.50	111.27
26	Q	314	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
26	Q	316	CHL	C3D-C2D-C1D	-4.63	99.51	105.83
26	V	316	CHL	C3C-C4C-NC	4.63	115.76	110.57
26	u	316	CHL	C3C-C4C-NC	4.63	115.76	110.57
26	P	317	CHL	C3C-C4C-NC	4.63	115.76	110.57
26	r	616	CHL	O2D-CGD-CBD	4.63	119.49	111.27
26	N	314	CHL	O2D-CGD-CBD	4.63	119.49	111.27
26	R	315	CHL	C3D-C2D-C1D	-4.63	99.52	105.83
26	P	318	CHL	O2D-CGD-CBD	4.63	119.49	111.27
26	2	315	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
31	K	101	BCR	C15-C14-C13	-4.62	120.71	127.31
26	n	313	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
26	G	313	CHL	C3D-C2D-C1D	-4.62	99.52	105.83
26	S	313	CHL	C3C-C4C-NC	4.62	115.75	110.57
26	G	311	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	2	316	CHL	C3C-C4C-NC	4.62	115.75	110.57
27	V	319	NEX	C15-C14-C13	-4.62	120.72	127.31
31	A	409	BCR	C15-C14-C13	-4.62	120.72	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	314	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	q	315	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	u	318	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
26	p	317	CHL	C3D-C2D-C1D	-4.61	99.53	105.83
26	G	314	CHL	C3C-C4C-NC	4.61	115.75	110.57
26	6	301	CHL	C3C-C4C-NC	4.61	115.74	110.57
26	g	313	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
26	4	317	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
26	5	314	CHL	O2D-CGD-CBD	4.61	119.46	111.27
26	p	314	CHL	CHD-C4C-C3C	-4.61	118.06	124.84
27	u	320	NEX	C11-C10-C9	-4.61	120.73	127.31
26	5	315	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
26	Q	314	CHL	C3C-C4C-NC	4.61	115.74	110.57
26	Q	316	CHL	C3C-C4C-NC	4.61	115.74	110.57
23	r	611	LUT	C35-C34-C33	-4.61	120.73	127.31
26	6	312	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
26	n	316	CHL	C3C-C4C-NC	4.60	115.73	110.57
26	q	311	CHL	O2D-CGD-CBD	4.60	119.44	111.27
26	q	314	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
26	4	315	CHL	C3C-C4C-NC	4.60	115.73	110.57
26	Q	315	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
26	r	614	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
26	n	316	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
26	n	315	CHL	C3C-C4C-NC	4.59	115.72	110.57
26	U	317	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
26	N	313	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
31	C	517	BCR	C11-C10-C9	-4.58	120.77	127.31
26	p	319	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
26	4	316	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
26	1	317	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
26	U	313	CHL	C3C-C4C-NC	4.57	115.70	110.57
26	V	318	CHL	CHB-C1B-NB	-4.57	119.42	124.26
26	G	312	CHL	C3C-C4C-NC	4.57	115.69	110.57
26	u	315	CHL	CHD-C1D-ND	-4.57	120.26	124.45
26	1	314	CHL	C3D-C2D-C1D	-4.57	99.60	105.83
26	p	318	CHL	O2D-CGD-CBD	4.56	119.38	111.27
26	V	316	CHL	C3D-C2D-C1D	-4.56	99.60	105.83
26	p	314	CHL	C3D-C2D-C1D	-4.56	99.60	105.83
26	R	317	CHL	O2D-CGD-CBD	4.56	119.37	111.27
26	R	317	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
26	6	315	CHL	C3C-C4C-NC	4.56	115.68	110.57
26	V	314	CHL	C3D-C2D-C1D	-4.56	99.61	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s	313	CHL	C3C-C4C-NC	4.56	115.68	110.57
26	Q	312	CHL	CHB-C1B-NB	-4.56	119.43	124.26
26	3	311	CHL	CHD-C4C-C3C	-4.55	118.14	124.84
26	V	317	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
26	1	316	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
26	1	313	CHL	C3C-C4C-NC	4.55	115.67	110.57
26	n	315	CHL	CHB-C1B-NB	-4.55	119.44	124.26
24	q	309	XAT	C31-C30-C29	-4.55	120.82	127.31
26	q	313	CHL	C3D-C2D-C1D	-4.55	99.63	105.83
26	Q	311	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
26	v	315	CHL	C3D-C2D-C1D	-4.54	99.63	105.83
26	u	314	CHL	O2D-CGD-CBD	4.54	119.33	111.27
26	6	317	CHL	C3C-C4C-NC	4.54	115.66	110.57
31	B	618	BCR	C24-C23-C22	-4.54	119.38	126.23
26	p	315	CHL	C4A-NA-C1A	4.54	108.75	106.71
26	N	316	CHL	O2D-CGD-CBD	4.54	119.33	111.27
26	p	320	CHL	CHD-C4C-C3C	-4.54	118.17	124.84
26	S	314	CHL	C3D-C2D-C1D	-4.53	99.64	105.83
26	q	311	CHL	C3D-C2D-C1D	-4.53	99.64	105.83
31	K	101	BCR	C4-C5-C6	-4.53	116.15	122.73
31	c	516	BCR	C1-C6-C5	-4.53	116.23	122.61
26	N	317	CHL	CHB-C1B-NB	-4.53	119.46	124.26
32	m	101	SQD	O9-S-C6	4.53	112.32	106.94
26	v	313	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
26	G	312	CHL	C3D-C2D-C1D	-4.53	99.65	105.83
26	p	316	CHL	C3C-C4C-NC	4.52	115.64	110.57
26	4	314	CHL	CHD-C4C-C3C	-4.52	118.19	124.84
31	a	409	BCR	C15-C14-C13	-4.52	120.86	127.31
26	P	314	CHL	C3D-C2D-C1D	-4.52	99.67	105.83
27	N	318	NEX	C27-C28-C29	-4.52	118.52	125.53
26	2	314	CHL	C3D-C2D-C1D	-4.52	99.67	105.83
26	V	313	CHL	C3D-C2D-C1D	-4.51	99.67	105.83
26	1	313	CHL	C3D-C2D-C1D	-4.51	99.67	105.83
26	4	313	CHL	C3C-C4C-NC	4.51	115.63	110.57
30	a	407	PHO	C2B-C1B-NB	-4.51	106.41	109.53
26	3	316	CHL	C3C-C4C-NC	4.51	115.63	110.57
31	k	101	BCR	C15-C14-C13	-4.51	120.87	127.31
31	C	517	BCR	C24-C23-C22	-4.51	119.42	126.23
26	g	314	CHL	C3C-C4C-NC	4.51	115.63	110.57
26	S	313	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
26	v	318	CHL	C3D-C2D-C1D	-4.51	99.68	105.83
26	3	314	CHL	C3C-C4C-NC	4.50	115.62	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q	315	CHL	C3C-C4C-NC	4.50	115.62	110.57
26	5	317	CHL	CHD-C4C-C3C	-4.50	118.22	124.84
26	6	316	CHL	CHD-C4C-C3C	-4.50	118.22	124.84
26	v	317	CHL	C3D-C2D-C1D	-4.50	99.70	105.83
26	s	313	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
26	s	316	CHL	C3C-C4C-NC	4.49	115.61	110.57
26	r	619	CHL	CHD-C4C-C3C	-4.49	118.24	124.84
26	u	313	CHL	O2D-CGD-CBD	4.49	119.25	111.27
26	r	616	CHL	C3D-C2D-C1D	-4.49	99.70	105.83
26	q	314	CHL	C1D-ND-C4D	-4.49	103.15	106.33
26	2	316	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
26	g	314	CHL	O2D-CGD-CBD	4.49	119.24	111.27
26	s	314	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
26	4	313	CHL	C3D-C2D-C1D	-4.49	99.71	105.83
32	M	101	SQD	O9-S-C6	4.49	112.27	106.94
26	S	316	CHL	C3C-C4C-NC	4.48	115.60	110.57
27	s	317	NEX	C11-C10-C9	-4.48	120.91	127.31
26	P	317	CHL	C3D-C2D-C1D	-4.48	99.71	105.83
30	A	407	PHO	C2B-C1B-NB	-4.48	106.43	109.53
23	U	310	LUT	C35-C34-C33	-4.48	120.92	127.31
24	n	311	XAT	C18-C5-C6	-4.47	114.76	122.26
24	Q	309	XAT	C26-C27-C28	-4.47	116.54	125.99
24	1	311	XAT	C35-C34-C33	-4.47	120.94	127.31
26	G	316	CHL	C3D-C2D-C1D	-4.47	99.74	105.83
26	V	318	CHL	C3D-C2D-C1D	-4.47	99.74	105.83
26	2	313	CHL	C3D-C2D-C1D	-4.46	99.74	105.83
26	u	316	CHL	O2D-CGD-CBD	4.46	119.20	111.27
26	P	314	CHL	CHB-C1B-NB	-4.46	119.53	124.26
31	c	515	BCR	C16-C17-C18	-4.46	120.94	127.31
26	N	314	CHL	C4A-NA-C1A	4.46	108.71	106.71
26	n	313	CHL	CHD-C4C-C3C	-4.46	118.29	124.84
31	c	515	BCR	C24-C23-C22	-4.46	119.50	126.23
26	u	313	CHL	C3D-C2D-C1D	-4.46	99.75	105.83
26	Q	312	CHL	C3D-C2D-C1D	-4.46	99.75	105.83
27	r	618	NEX	C2-C1-C6	4.45	113.54	109.21
26	5	317	CHL	C3B-C4B-NB	4.45	114.65	110.52
26	N	313	CHL	C3C-C4C-NC	4.45	115.56	110.57
26	N	314	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
31	k	101	BCR	C4-C5-C6	-4.45	116.27	122.73
26	6	301	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
26	p	316	CHL	C3D-C2D-C1D	-4.45	99.76	105.83
26	n	314	CHL	C3D-C2D-C1D	-4.45	99.76	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	316	CHL	O2D-CGD-CBD	4.45	119.17	111.27
26	u	316	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	5	314	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	5	313	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	3	313	CHL	C3C-C4C-NC	4.44	115.56	110.57
26	U	313	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	5	316	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
32	m	101	SQD	O7-S-C6	4.44	112.22	106.94
26	p	315	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
27	v	319	NEX	C15-C14-C13	-4.44	120.97	127.31
26	6	317	CHL	C3D-C2D-C1D	-4.44	99.77	105.83
26	N	316	CHL	CHD-C4C-C3C	-4.44	118.32	124.84
32	M	101	SQD	O7-S-C6	4.43	112.21	106.94
26	Q	315	CHL	C1D-ND-C4D	-4.43	103.19	106.33
27	r	617	NEX	C11-C10-C9	-4.43	120.99	127.31
26	U	314	CHL	CHD-C4C-C3C	-4.43	118.33	124.84
26	2	318	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
26	n	315	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
26	P	316	CHL	CHB-C1B-NB	-4.43	119.57	124.26
26	p	320	CHL	C2D-C1D-ND	4.43	113.37	110.10
27	p	301	NEX	C15-C14-C13	-4.43	120.99	127.31
27	s	317	NEX	C35-C34-C33	-4.43	120.99	127.31
26	s	316	CHL	C3D-C2D-C1D	-4.43	99.79	105.83
26	q	312	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
27	N	318	NEX	C11-C10-C9	-4.42	121.00	127.31
26	v	318	CHL	CHB-C1B-NB	-4.42	119.58	124.26
26	5	318	CHL	C3D-C2D-C1D	-4.42	99.80	105.83
26	P	315	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
26	g	316	CHL	C3D-C2D-C1D	-4.41	99.81	105.83
27	n	319	NEX	C27-C28-C29	-4.41	118.69	125.53
27	r	617	NEX	C27-C28-C29	-4.41	118.69	125.53
27	P	301	NEX	O24-C25-C38	4.41	120.34	115.06
26	6	316	CHL	C1D-ND-C4D	-4.41	103.20	106.33
26	N	317	CHL	C3D-C2D-C1D	-4.41	99.82	105.83
26	n	318	CHL	C3D-C2D-C1D	-4.40	99.82	105.83
26	N	315	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
26	3	312	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
26	3	316	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
26	S	316	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
31	C	518	BCR	C1-C6-C5	-4.40	116.42	122.61
33	d	404	PL9	C7-C8-C9	-4.39	119.48	126.79
26	s	315	CHL	C3D-C2D-C1D	-4.39	99.84	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q	313	CHL	C3D-C2D-C1D	-4.39	99.84	105.83
26	v	316	CHL	CHD-C4C-C3C	-4.39	118.39	124.84
27	p	301	NEX	C2-C1-C6	4.39	113.47	109.21
26	S	315	CHL	C3D-C2D-C1D	-4.39	99.85	105.83
26	4	315	CHL	CHB-C1B-NB	-4.38	119.62	124.26
26	V	315	CHL	C3D-C2D-C1D	-4.38	99.85	105.83
27	S	317	NEX	C35-C34-C33	-4.38	121.06	127.31
26	u	317	CHL	C2D-C1D-ND	4.38	113.33	110.10
26	5	315	CHL	CHD-C4C-C3C	-4.38	118.41	124.84
25	G	310	LHG	O7-C7-C8	4.37	120.92	111.50
23	N	310	LUT	C35-C34-C33	-4.37	121.07	127.31
26	3	314	CHL	C3D-C2D-C1D	-4.37	99.87	105.83
26	6	313	CHL	C3D-C2D-C1D	-4.37	99.87	105.83
26	U	315	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
26	g	312	CHL	C3D-C2D-C1D	-4.36	99.88	105.83
26	p	317	CHL	CHB-C1B-NB	-4.36	119.64	124.26
33	D	405	PL9	C7-C8-C9	-4.36	119.53	126.79
24	3	309	XAT	C26-C27-C28	-4.36	116.78	125.99
26	N	317	CHL	C3C-C4C-NC	4.36	115.46	110.57
26	n	315	CHL	O2D-CGD-CBD	4.35	119.00	111.27
26	2	317	CHL	C2D-C1D-ND	4.35	113.31	110.10
26	U	319	CHL	CHB-C1B-NB	-4.35	119.65	124.26
24	V	311	XAT	C6-C7-C8	-4.35	116.80	125.99
26	P	319	CHL	C3B-C4B-NB	4.35	114.55	110.52
26	6	315	CHL	C3D-C2D-C1D	-4.35	99.90	105.83
31	C	517	BCR	C16-C17-C18	-4.34	121.11	127.31
26	N	316	CHL	C2D-C1D-ND	4.34	113.30	110.10
31	c	515	BCR	C38-C26-C25	-4.34	119.65	124.53
26	6	317	CHL	C3B-C4B-NB	4.34	114.54	110.52
26	V	315	CHL	C3C-C4C-NC	4.34	115.44	110.57
36	c	519	DGD	O2G-C1B-C2B	4.34	120.85	111.50
24	g	309	XAT	C26-C27-C28	-4.34	116.83	125.99
26	P	316	CHL	C3D-C2D-C1D	-4.33	99.92	105.83
27	R	301	NEX	C2-C1-C6	4.33	113.42	109.21
27	R	301	NEX	C38-C25-C26	-4.33	115.00	122.26
36	J	101	DGD	O2G-C1B-C2B	4.33	120.83	111.50
24	v	311	XAT	C6-C7-C8	-4.33	116.84	125.99
26	6	301	CHL	CHB-C1B-NB	-4.31	119.69	124.26
32	L	102	SQD	O7-S-C6	4.31	112.06	106.94
26	U	314	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
26	p	318	CHL	C2D-C1D-ND	4.31	113.28	110.10
26	1	315	CHL	C3D-C2D-C1D	-4.30	99.96	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	r	618	NEX	C38-C25-C26	-4.30	115.06	122.26
25	g	310	LHG	O7-C7-C8	4.30	120.76	111.50
23	u	310	LUT	C35-C34-C33	-4.30	121.18	127.31
22	n	305	CLA	C4D-C3D-CAD	-4.29	103.03	108.10
27	R	301	NEX	C27-C28-C29	-4.29	118.87	125.53
26	Q	311	CHL	CHD-C4C-C3C	-4.29	118.54	124.84
23	5	310	LUT	C35-C34-C33	-4.29	121.19	127.31
26	U	315	CHL	O2D-CGD-CBD	4.28	118.88	111.27
26	Q	314	CHL	O2D-CGD-CBD	4.28	118.87	111.27
26	U	315	CHL	CHD-C4C-C3C	-4.28	118.55	124.84
25	C	524	LHG	O7-C7-C8	4.27	120.71	111.50
24	r	612	XAT	C38-C25-C26	-4.27	115.10	122.26
26	3	314	CHL	O2D-CGD-CBD	4.27	118.85	111.27
24	N	311	XAT	C18-C5-C6	-4.27	115.11	122.26
26	v	314	CHL	CHD-C4C-C3C	-4.27	118.57	124.84
26	p	319	CHL	CHB-C1B-NB	-4.26	119.74	124.26
23	P	310	LUT	C35-C34-C33	-4.26	121.23	127.31
26	q	315	CHL	CHB-C1B-NB	-4.26	119.74	124.26
26	4	315	CHL	C3D-C2D-C1D	-4.26	100.02	105.83
25	N	312	LHG	O7-C7-C8	4.25	120.67	111.50
31	C	517	BCR	C38-C26-C25	-4.25	119.75	124.53
31	b	619	BCR	C4-C5-C6	-4.25	116.56	122.73
31	c	515	BCR	C7-C8-C9	-4.25	119.81	126.23
26	U	316	CHL	C2D-C1D-ND	4.25	113.24	110.10
31	t	101	BCR	C30-C25-C26	-4.25	116.63	122.61
31	b	620	BCR	C38-C26-C25	-4.24	119.76	124.53
23	1	309	LUT	C15-C14-C13	-4.24	121.26	127.31
22	p	306	CLA	C4D-C3D-CAD	-4.24	103.10	108.10
26	v	316	CHL	C2D-C1D-ND	4.24	113.23	110.10
26	S	314	CHL	CHD-C4C-C3C	-4.23	118.62	124.84
26	3	312	CHL	C3C-C4C-NC	4.23	115.32	110.57
32	l	102	SQD	O7-S-C6	4.23	111.97	106.94
27	S	317	NEX	C15-C14-C13	-4.23	121.27	127.31
24	R	313	XAT	C15-C14-C13	-4.23	121.27	127.31
31	A	409	BCR	C16-C17-C18	-4.23	121.28	127.31
26	6	314	CHL	C3C-C4C-NC	4.23	115.31	110.57
31	T	101	BCR	C30-C25-C26	-4.23	116.66	122.61
26	u	317	CHL	CHD-C4C-C3C	-4.23	118.63	124.84
23	4	309	LUT	C15-C14-C13	-4.22	121.28	127.31
26	3	311	CHL	C2D-C1D-ND	4.22	113.22	110.10
26	U	316	CHL	CHD-C4C-C3C	-4.22	118.63	124.84
31	a	409	BCR	C16-C17-C18	-4.22	121.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	5	311	XAT	C31-C30-C29	-4.22	121.29	127.31
27	r	618	NEX	C27-C28-C29	-4.22	118.99	125.53
26	4	314	CHL	CHB-C1B-NB	-4.22	119.79	124.26
31	B	620	BCR	C38-C26-C25	-4.22	119.79	124.53
23	4	310	LUT	C7-C8-C9	-4.21	119.87	126.23
26	g	311	CHL	CHD-C4C-C3C	-4.21	118.66	124.84
26	s	314	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
26	N	315	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
26	4	317	CHL	C3B-C4B-NB	4.20	114.41	110.52
24	G	309	XAT	C15-C14-C13	-4.20	121.31	127.31
32	l	102	SQD	O47-C7-C8	4.20	120.56	111.50
32	L	102	SQD	O47-C7-C8	4.20	120.56	111.50
26	u	314	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
27	u	320	NEX	C27-C28-C29	-4.20	119.02	125.53
26	2	314	CHL	C3C-C4C-NC	4.20	115.28	110.57
26	G	311	CHL	CHD-C4C-C3C	-4.20	118.67	124.84
26	2	315	CHL	CHD-C4C-C3C	-4.19	118.67	124.84
24	g	309	XAT	C15-C14-C13	-4.19	121.32	127.31
26	v	315	CHL	CHB-C1B-NB	-4.19	119.82	124.26
31	B	619	BCR	C4-C5-C6	-4.19	116.64	122.73
26	s	315	CHL	C3C-C4C-NC	4.19	115.27	110.57
31	C	517	BCR	C7-C8-C9	-4.19	119.91	126.23
26	G	314	CHL	O2D-CGD-CBD	4.19	118.71	111.27
27	V	319	NEX	C35-C34-C33	-4.18	121.34	127.31
26	1	317	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
26	6	313	CHL	C3C-C4C-NC	4.18	115.26	110.57
26	6	315	CHL	O2D-CGD-CBD	4.18	118.70	111.27
26	5	317	CHL	C2D-C1D-ND	4.18	113.18	110.10
23	n	309	LUT	C7-C8-C9	-4.18	119.92	126.23
27	5	319	NEX	C15-C14-C13	-4.18	121.35	127.31
27	s	317	NEX	C15-C14-C13	-4.18	121.35	127.31
26	5	314	CHL	C3C-C4C-NC	4.18	115.26	110.57
26	u	318	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
26	r	619	CHL	C2D-C1D-ND	4.18	113.18	110.10
26	u	318	CHL	C2D-C1D-ND	4.18	113.18	110.10
26	R	315	CHL	CAC-C3C-C4C	4.17	130.23	124.81
26	P	314	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
26	v	316	CHL	O2D-CGD-CBD	4.17	118.68	111.27
27	r	618	NEX	C15-C14-C13	-4.17	121.36	127.31
25	c	523	LHG	O7-C7-C8	4.17	120.48	111.50
26	2	317	CHL	C3B-C4B-NB	4.17	114.38	110.52
24	2	311	XAT	C15-C14-C13	-4.17	121.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	v	312	LHG	O7-C7-C8	4.16	120.47	111.50
26	u	315	CHL	C3D-C2D-C1D	-4.16	100.15	105.83
26	r	615	CHL	CHD-C4C-C3C	-4.16	118.72	124.84
31	z	101	BCR	C24-C23-C22	-4.16	119.95	126.23
26	p	314	CHL	CHC-C4B-NB	-4.16	119.85	124.26
26	n	317	CHL	CHB-C1B-NB	-4.16	119.85	124.26
26	4	317	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
23	n	310	LUT	C35-C34-C33	-4.16	121.38	127.31
26	n	318	CHL	C3C-C4C-NC	4.16	115.23	110.57
26	2	318	CHL	C3B-C4B-NB	4.16	114.37	110.52
34	B	624	LMG	O7-C10-C11	4.16	120.46	111.50
24	5	311	XAT	C26-C27-C28	-4.15	117.21	125.99
26	3	315	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
31	B	618	BCR	C4-C5-C6	-4.15	116.70	122.73
26	P	318	CHL	C2D-C1D-ND	4.15	113.16	110.10
31	B	620	BCR	C1-C6-C5	-4.15	116.77	122.61
26	q	312	CHL	C3C-C4C-NC	4.15	115.22	110.57
31	D	404	BCR	C4-C5-C6	-4.15	116.71	122.73
26	n	313	CHL	CHB-C1B-NB	-4.14	119.87	124.26
26	3	313	CHL	C3D-C2D-C1D	-4.14	100.18	105.83
31	d	403	BCR	C33-C5-C6	-4.14	119.88	124.53
26	u	316	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
31	d	403	BCR	C4-C5-C6	-4.14	116.73	122.73
26	P	319	CHL	CHD-C4C-C3C	-4.14	118.76	124.84
26	R	316	CHL	CHD-C4C-C3C	-4.13	118.76	124.84
27	N	318	NEX	O24-C25-C38	4.13	120.01	115.06
34	b	624	LMG	O7-C10-C11	4.13	120.40	111.50
26	3	315	CHL	CHB-C1B-NB	-4.13	119.89	124.26
22	5	305	CLA	C4D-C3D-CAD	-4.12	103.23	108.10
32	C	501	SQD	C44-O6-C1	4.12	121.79	113.74
25	S	312	LHG	O7-C7-C8	4.12	120.38	111.50
27	2	319	NEX	O24-C25-C38	4.12	119.99	115.06
31	t	101	BCR	C38-C26-C25	-4.12	119.90	124.53
26	S	315	CHL	C3C-C4C-NC	4.12	115.19	110.57
26	v	314	CHL	C2D-C1D-ND	4.12	113.14	110.10
25	s	312	LHG	O7-C7-C8	4.11	120.36	111.50
24	R	313	XAT	C38-C25-C26	-4.11	115.37	122.26
25	2	312	LHG	O7-C7-C8	4.11	120.36	111.50
31	T	101	BCR	C38-C26-C25	-4.11	119.91	124.53
24	u	311	XAT	C18-C5-C6	-4.11	115.37	122.26
31	b	618	BCR	C4-C5-C6	-4.11	116.76	122.73
23	p	310	LUT	C15-C14-C13	-4.11	121.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	t	101	BCR	C16-C17-C18	-4.11	121.45	127.31
31	B	620	BCR	C15-C14-C13	-4.11	121.45	127.31
31	B	619	BCR	C11-C10-C9	-4.11	121.45	127.31
24	r	612	XAT	C15-C14-C13	-4.10	121.45	127.31
24	Q	309	XAT	C31-C30-C29	-4.10	121.45	127.31
26	p	320	CHL	O2D-CGD-CBD	4.10	118.56	111.27
26	V	317	CHL	CHD-C4C-C3C	-4.10	118.81	124.84
34	c	501	LMG	O7-C10-C11	4.10	120.34	111.50
27	r	617	NEX	C2-C1-C6	4.10	113.19	109.21
26	1	316	CHL	CHB-C1B-NB	-4.10	119.92	124.26
23	R	312	LUT	C35-C34-C33	-4.10	121.46	127.31
24	2	311	XAT	C38-C25-C26	-4.09	115.40	122.26
24	P	312	XAT	C6-C7-C8	-4.09	117.34	125.99
26	6	312	CHL	C2D-C1D-ND	4.09	113.12	110.10
34	C	502	LMG	O7-C10-C11	4.09	120.31	111.50
24	P	312	XAT	C31-C30-C29	-4.09	121.48	127.31
24	G	309	XAT	C31-C30-C29	-4.09	121.48	127.31
26	q	311	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
31	D	404	BCR	C33-C5-C6	-4.08	119.94	124.53
26	6	316	CHL	O2D-CGD-CBD	4.08	118.52	111.27
24	V	311	XAT	C31-C30-C29	-4.08	121.48	127.31
27	2	319	NEX	C15-C14-C13	-4.08	121.48	127.31
24	v	311	XAT	C31-C30-C29	-4.08	121.49	127.31
26	4	313	CHL	CHB-C1B-NB	-4.08	119.94	124.26
31	b	620	BCR	C1-C6-C5	-4.08	116.87	122.61
26	g	316	CHL	C3B-C4B-NB	4.08	114.30	110.52
24	N	311	XAT	C26-C27-C28	-4.07	117.38	125.99
26	4	316	CHL	CHD-C4C-C3C	-4.07	118.85	124.84
26	U	317	CHL	C3B-C4B-NB	4.07	114.29	110.52
27	u	319	NEX	C35-C34-C33	-4.07	121.50	127.31
26	P	319	CHL	C2D-C1D-ND	4.07	113.10	110.10
27	P	301	NEX	C15-C14-C13	-4.07	121.51	127.31
24	3	309	XAT	C11-C10-C9	-4.07	121.51	127.31
23	5	309	LUT	C35-C34-C33	-4.06	121.51	127.31
26	1	318	CHL	C3B-C4B-NB	4.06	114.28	110.52
26	p	317	CHL	CHD-C4C-C3C	-4.06	118.87	124.84
26	n	314	CHL	C3C-C4C-NC	4.06	115.12	110.57
26	R	316	CHL	C2D-C1D-ND	4.06	113.09	110.10
26	G	315	CHL	C1D-ND-C4D	-4.06	103.45	106.33
27	p	301	NEX	O24-C25-C38	4.06	119.92	115.06
26	r	614	CHL	CAC-C3C-C4C	4.06	130.07	124.81
26	1	315	CHL	CHB-C1B-NB	-4.06	119.96	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	619	BCR	C33-C5-C6	-4.05	119.98	124.53
27	N	318	NEX	C35-C34-C33	-4.05	121.53	127.31
26	G	316	CHL	C3B-C4B-NB	4.04	114.27	110.52
26	n	317	CHL	CAC-C3C-C4C	4.04	130.05	124.81
31	X	201	BCR	C38-C26-C25	-4.04	119.99	124.53
25	R	314	LHG	O7-C7-C8	4.04	120.21	111.50
26	N	314	CHL	C3C-C4C-NC	4.04	115.10	110.57
25	V	312	LHG	O7-C7-C8	4.04	120.20	111.50
31	A	409	BCR	C33-C5-C6	-4.04	120.00	124.53
26	4	314	CHL	C2D-C1D-ND	4.04	113.08	110.10
24	3	309	XAT	C35-C34-C33	-4.03	121.56	127.31
26	u	314	CHL	C2D-C1D-ND	4.03	113.07	110.10
26	N	313	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
24	G	309	XAT	C26-C27-C28	-4.02	117.49	125.99
26	g	315	CHL	C1D-ND-C4D	-4.02	103.48	106.33
26	r	614	CHL	CHD-C4C-C3C	-4.02	118.93	124.84
24	5	311	XAT	C38-C25-C26	-4.02	115.52	122.26
31	C	516	BCR	C24-C23-C22	-4.02	120.16	126.23
26	u	317	CHL	C1D-ND-C4D	-4.02	103.48	106.33
26	R	315	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
31	c	516	BCR	C15-C14-C13	-4.01	121.59	127.31
26	v	314	CHL	C3B-C4B-NB	4.01	114.23	110.52
23	v	309	LUT	C7-C8-C9	-4.01	120.18	126.23
24	g	309	XAT	C18-C5-C6	-4.01	115.55	122.26
26	u	316	CHL	CMD-C2D-C3D	-4.01	118.40	127.61
26	v	313	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
26	V	316	CHL	O2D-CGD-CBD	4.00	118.38	111.27
23	V	309	LUT	C7-C8-C9	-4.00	120.19	126.23
22	C	507	CLA	O2D-CGD-O1D	-4.00	116.01	123.84
27	v	319	NEX	C35-C34-C33	-4.00	121.60	127.31
22	2	305	CLA	C4D-C3D-CAD	-4.00	103.38	108.10
26	6	314	CHL	C3D-C2D-C1D	-4.00	100.38	105.83
23	5	309	LUT	C15-C14-C13	-4.00	121.61	127.31
34	w	201	LMG	O7-C10-C11	4.00	120.11	111.50
22	c	506	CLA	O2D-CGD-O1D	-3.99	116.03	123.84
26	1	318	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
26	G	316	CHL	CHD-C4C-C3C	-3.99	118.97	124.84
31	B	618	BCR	C1-C6-C5	-3.99	117.00	122.61
26	v	317	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
31	z	101	BCR	C38-C26-C25	-3.98	120.06	124.53
32	a	410	SQD	C44-O6-C1	3.98	121.52	113.74
22	P	306	CLA	C4D-C3D-CAD	-3.98	103.40	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	310	XAT	C38-C25-C26	-3.98	115.59	122.26
26	Q	313	CHL	CAC-C3C-C4C	3.98	129.97	124.81
24	R	313	XAT	C35-C15-C14	-3.98	115.33	123.47
31	a	409	BCR	C33-C5-C6	-3.98	120.06	124.53
26	3	315	CHL	CMB-C2B-C1B	3.98	131.42	125.37
26	N	315	CHL	CHB-C1B-NB	-3.97	120.05	124.26
31	T	101	BCR	C16-C17-C18	-3.97	121.64	127.31
26	p	315	CHL	C3C-C4C-NC	3.97	115.02	110.57
27	S	317	NEX	C31-C30-C29	-3.97	121.64	127.31
26	U	319	CHL	CHD-C4C-C3C	-3.97	119.00	124.84
26	n	316	CHL	CHB-C1B-NB	-3.97	120.06	124.26
24	Q	309	XAT	C38-C25-C26	-3.97	115.61	122.26
27	p	301	NEX	C35-C34-C33	-3.96	121.65	127.31
26	r	615	CHL	C2D-C1D-ND	3.96	113.02	110.10
26	2	316	CHL	CHB-C1B-NB	-3.96	120.06	124.26
26	s	313	CHL	CHB-C1B-NB	-3.96	120.06	124.26
24	n	311	XAT	C26-C27-C28	-3.96	117.62	125.99
26	G	313	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
23	s	310	LUT	C35-C34-C33	-3.96	121.66	127.31
26	p	319	CHL	C3B-C4B-NB	3.96	114.19	110.52
31	A	409	BCR	C7-C8-C9	-3.96	120.25	126.23
24	2	311	XAT	C31-C30-C29	-3.96	121.66	127.31
26	N	314	CHL	CAC-C3C-C4C	3.96	129.94	124.81
26	G	311	CHL	C3B-C4B-NB	3.95	114.18	110.52
25	U	312	LHG	O7-C7-C8	3.95	120.02	111.50
23	p	310	LUT	C35-C34-C33	-3.95	121.67	127.31
26	U	316	CHL	C1D-ND-C4D	-3.95	103.53	106.33
26	3	315	CHL	O2D-CGD-CBD	3.95	118.28	111.27
26	n	316	CHL	CHD-C4C-C3C	-3.95	119.04	124.84
31	b	619	BCR	C11-C10-C9	-3.95	121.68	127.31
24	1	311	XAT	C31-C30-C29	-3.94	121.68	127.31
26	4	317	CHL	C2D-C1D-ND	3.94	113.01	110.10
31	K	101	BCR	C30-C25-C26	-3.94	117.06	122.61
24	1	311	XAT	C6-C7-C8	-3.94	117.66	125.99
26	3	316	CHL	C3B-C4B-NB	3.94	114.17	110.52
26	5	316	CHL	CHB-C1B-NB	-3.94	120.09	124.26
25	n	312	LHG	O7-C7-C8	3.94	119.99	111.50
32	C	501	SQD	O47-C7-C8	3.94	119.99	111.50
24	p	312	XAT	C26-C27-C28	-3.94	117.67	125.99
26	g	313	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
26	n	314	CHL	CHC-C4B-NB	-3.94	120.09	124.26
26	1	316	CHL	CHD-C4C-C3C	-3.93	119.06	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q	316	CHL	CHB-C1B-NB	-3.93	120.09	124.26
26	q	311	CHL	C2D-C1D-ND	3.93	113.00	110.10
32	A	412	SQD	O7-S-C6	3.93	111.61	106.94
26	g	316	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
26	U	317	CHL	CHD-C4C-C3C	-3.93	119.07	124.84
24	5	311	XAT	C6-C7-C8	-3.93	117.69	125.99
36	A	414	DGD	O2G-C1B-C2B	3.93	119.97	111.50
26	Q	311	CHL	C2D-C1D-ND	3.93	113.00	110.10
36	a	416	DGD	O2G-C1B-C2B	3.92	119.96	111.50
27	V	319	NEX	O24-C25-C38	3.92	119.76	115.06
34	b	621	LMG	O7-C10-C11	3.92	119.96	111.50
26	Q	313	CHL	C3B-C4B-NB	3.92	114.15	110.52
26	5	318	CHL	C3B-C4B-NB	3.92	114.15	110.52
26	6	312	CHL	C1D-ND-C4D	-3.92	103.55	106.33
24	5	311	XAT	C15-C14-C13	-3.92	121.72	127.31
24	q	309	XAT	C38-C25-C26	-3.92	115.69	122.26
31	k	101	BCR	C30-C25-C26	-3.92	117.09	122.61
24	v	311	XAT	C26-C27-C28	-3.92	117.71	125.99
26	U	314	CHL	O2D-CGD-CBD	3.92	118.22	111.27
32	a	413	SQD	O7-S-C6	3.92	111.59	106.94
26	U	317	CHL	C2D-C1D-ND	3.91	112.99	110.10
26	V	313	CHL	CHB-C1B-NB	-3.91	120.11	124.26
25	r	613	LHG	O7-C7-C8	3.91	119.94	111.50
23	1	310	LUT	C7-C8-C9	-3.91	120.32	126.23
31	B	619	BCR	C23-C24-C25	-3.91	116.22	127.20
26	1	313	CHL	CHB-C1B-NB	-3.91	120.12	124.26
24	g	309	XAT	C31-C30-C29	-3.91	121.73	127.31
24	3	309	XAT	C38-C25-C26	-3.91	115.71	122.26
24	2	311	XAT	C35-C34-C33	-3.91	121.73	127.31
25	6	311	LHG	O7-C7-C8	3.91	119.92	111.50
26	5	318	CHL	CHD-C4C-C3C	-3.91	119.10	124.84
27	u	319	NEX	C26-C27-C28	-3.91	117.73	125.99
31	b	619	BCR	C23-C24-C25	-3.90	116.24	127.20
26	v	316	CHL	C1D-ND-C4D	-3.90	103.56	106.33
24	U	311	XAT	C15-C14-C13	-3.90	121.74	127.31
31	K	101	BCR	C33-C5-C6	-3.90	120.15	124.53
26	N	316	CHL	C1D-ND-C4D	-3.90	103.56	106.33
34	B	621	LMG	O7-C10-C11	3.90	119.91	111.50
25	u	312	LHG	O7-C7-C8	3.90	119.91	111.50
31	x	202	BCR	C38-C26-C25	-3.90	120.15	124.53
24	G	309	XAT	C18-C5-C6	-3.90	115.73	122.26
31	C	518	BCR	C15-C14-C13	-3.89	121.75	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	311	XAT	C6-C7-C8	-3.89	117.76	125.99
23	2	310	LUT	C35-C34-C33	-3.89	121.75	127.31
26	u	318	CHL	C3B-C4B-NB	3.89	114.12	110.52
25	Q	310	LHG	O7-C7-C8	3.88	119.87	111.50
26	g	313	CHL	CAC-C3C-C4C	3.88	129.85	124.81
34	B	621	LMG	C1-C2-C3	3.88	118.08	110.00
25	P	313	LHG	O7-C7-C8	3.88	119.86	111.50
24	N	311	XAT	C11-C10-C9	-3.88	121.77	127.31
26	g	311	CHL	C2D-C1D-ND	3.88	112.96	110.10
26	p	318	CHL	C3B-C4B-NB	3.88	114.11	110.52
23	U	309	LUT	C35-C34-C33	-3.88	121.78	127.31
34	W	201	LMG	O7-C10-C11	3.87	119.85	111.50
26	p	320	CHL	C1D-ND-C4D	-3.87	103.58	106.33
23	v	310	LUT	C7-C8-C9	-3.87	120.39	126.23
24	1	311	XAT	C26-C27-C28	-3.87	117.81	125.99
31	k	101	BCR	C33-C5-C6	-3.87	120.18	124.53
23	N	309	LUT	C7-C8-C9	-3.87	120.39	126.23
26	2	317	CHL	C1D-ND-C4D	-3.86	103.59	106.33
26	Q	311	CHL	C1D-ND-C4D	-3.86	103.59	106.33
31	b	618	BCR	C8-C7-C6	-3.86	116.35	127.20
26	1	317	CHL	C2D-C1D-ND	3.86	112.95	110.10
26	1	317	CHL	C3B-C4B-NB	3.86	114.10	110.52
27	s	317	NEX	C31-C30-C29	-3.86	121.80	127.31
26	r	619	CHL	CAC-C3C-C4C	3.86	129.82	124.81
25	C	523	LHG	O7-C7-C8	3.86	119.82	111.50
26	n	318	CHL	CAC-C3C-C4C	3.86	129.81	124.81
26	R	315	CHL	C2D-C1D-ND	3.86	112.94	110.10
34	A	411	LMG	O7-C10-C11	3.85	119.81	111.50
34	a	412	LMG	O7-C10-C11	3.85	119.80	111.50
26	u	314	CHL	CAC-C3C-C4C	3.85	129.81	124.81
26	3	311	CHL	C1D-ND-C4D	-3.85	103.60	106.33
26	V	317	CHL	C2D-C1D-ND	3.85	112.94	110.10
26	q	313	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
32	C	501	SQD	O9-S-C6	3.85	111.51	106.94
27	5	319	NEX	O24-C25-C38	3.85	119.67	115.06
31	B	618	BCR	C7-C8-C9	-3.85	120.42	126.23
27	2	319	NEX	C39-C29-C30	-3.85	117.54	122.92
25	4	312	LHG	O7-C7-C8	3.84	119.78	111.50
27	S	317	NEX	O24-C25-C38	3.84	119.66	115.06
24	u	311	XAT	C15-C14-C13	-3.84	121.83	127.31
25	c	522	LHG	O7-C7-C8	3.84	119.78	111.50
26	U	319	CHL	C2D-C1D-ND	3.84	112.93	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	620	BCR	C38-C26-C27	3.84	120.99	113.62
26	N	313	CHL	C2D-C1D-ND	3.84	112.93	110.10
24	p	312	XAT	C38-C25-C26	-3.83	115.83	122.26
26	2	314	CHL	CHC-C4B-NB	-3.83	120.20	124.26
26	N	317	CHL	C3B-C4B-NB	3.83	114.07	110.52
26	5	315	CHL	C2D-C1D-ND	3.83	112.93	110.10
25	D	406	LHG	O7-C7-C8	3.83	119.75	111.50
32	a	410	SQD	O47-C7-C8	3.83	119.75	111.50
26	q	311	CHL	C1D-ND-C4D	-3.82	103.62	106.33
26	q	313	CHL	CAC-C3C-C4C	3.82	129.77	124.81
26	N	313	CHL	CHB-C1B-NB	-3.82	120.21	124.26
26	2	313	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
26	Q	316	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
26	5	313	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
34	b	621	LMG	C4-C3-C2	3.82	117.49	110.82
24	4	311	XAT	C26-C27-C28	-3.81	117.93	125.99
26	4	314	CHL	C3B-C4B-NB	3.81	114.05	110.52
27	S	317	NEX	C27-C28-C29	-3.81	119.61	125.53
26	r	615	CHL	C3B-C4B-NB	3.81	114.05	110.52
24	n	311	XAT	C15-C14-C13	-3.81	121.87	127.31
26	1	314	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
27	U	318	NEX	C27-C28-C29	-3.81	119.62	125.53
25	d	405	LHG	O7-C7-C8	3.81	119.71	111.50
26	6	301	CHL	CHD-C4C-C3C	-3.81	119.24	124.84
31	d	403	BCR	C7-C8-C9	-3.81	120.48	126.23
25	l	101	LHG	O7-C7-C8	3.81	119.70	111.50
26	2	318	CHL	CHD-C4C-C3C	-3.81	119.25	124.84
26	Q	314	CHL	CHD-C4C-C3C	-3.81	119.25	124.84
26	1	318	CHL	C2D-C1D-ND	3.80	112.91	110.10
27	s	317	NEX	O24-C25-C38	3.80	119.61	115.06
26	U	315	CHL	C3B-C4B-NB	3.80	114.04	110.52
26	3	315	CHL	C1D-ND-C4D	-3.80	103.64	106.33
34	B	621	LMG	C4-C3-C2	3.80	117.45	110.82
26	p	319	CHL	CHD-C4C-C3C	-3.80	119.26	124.84
31	B	619	BCR	C33-C5-C6	-3.80	120.27	124.53
31	D	404	BCR	C27-C26-C25	-3.79	117.22	122.73
36	a	416	DGD	O6E-C5E-C4E	3.79	116.58	109.69
26	u	315	CHL	O2D-CGD-CBD	3.79	118.00	111.27
26	n	313	CHL	CAC-C3C-C4C	3.79	129.73	124.81
24	v	311	XAT	C35-C34-C33	-3.79	121.90	127.31
26	u	317	CHL	CAC-C3C-C4C	3.79	129.72	124.81
26	5	317	CHL	C1D-ND-C4D	-3.78	103.65	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	316	CHL	C2D-C1D-ND	3.78	112.89	110.10
31	d	403	BCR	C27-C26-C25	-3.78	117.24	122.73
24	u	311	XAT	C27-C28-C29	-3.78	119.67	125.53
26	p	320	CHL	C3B-C4B-NB	3.78	114.02	110.52
26	q	315	CHL	CHD-C4C-C3C	-3.78	119.29	124.84
26	r	614	CHL	C2D-C1D-ND	3.78	112.89	110.10
31	z	101	BCR	C30-C25-C26	-3.78	117.29	122.61
26	n	316	CHL	C2D-C1D-ND	3.78	112.89	110.10
26	P	317	CHL	CHD-C4C-C3C	-3.78	119.29	124.84
31	D	404	BCR	C7-C8-C9	-3.78	120.53	126.23
32	a	410	SQD	O9-S-C6	3.78	111.43	106.94
26	R	316	CHL	C3B-C4B-NB	3.77	114.02	110.52
25	L	101	LHG	O7-C7-C8	3.77	119.63	111.50
31	z	101	BCR	C1-C6-C5	-3.77	117.30	122.61
26	U	317	CHL	CAC-C3C-C4C	3.77	129.70	124.81
25	q	310	LHG	O7-C7-C8	3.77	119.63	111.50
26	S	313	CHL	CHC-C4B-NB	-3.77	120.27	124.26
36	C	520	DGD	O2G-C1B-C2B	3.77	119.62	111.50
26	V	318	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
26	q	314	CHL	O2D-CGD-CBD	3.77	117.97	111.27
26	q	311	CHL	C3B-C4B-NB	3.77	114.01	110.52
26	v	318	CHL	CHD-C4C-C3C	-3.77	119.30	124.84
31	c	516	BCR	C23-C24-C25	-3.77	116.63	127.20
26	g	311	CHL	C3B-C4B-NB	3.76	114.01	110.52
26	V	316	CHL	CHD-C4C-C3C	-3.76	119.31	124.84
26	r	615	CHL	CHB-C1B-NB	-3.76	120.27	124.26
31	C	518	BCR	C23-C24-C25	-3.76	116.64	127.20
25	3	310	LHG	O7-C7-C8	3.76	119.61	111.50
27	P	301	NEX	C35-C34-C33	-3.76	121.94	127.31
26	2	315	CHL	C2D-C1D-ND	3.76	112.87	110.10
25	1	312	LHG	O7-C7-C8	3.76	119.60	111.50
26	g	313	CHL	C2D-C1D-ND	3.76	112.87	110.10
26	V	317	CHL	C1D-ND-C4D	-3.76	103.67	106.33
31	a	409	BCR	C7-C8-C9	-3.76	120.56	126.23
26	n	313	CHL	C3B-C4B-NB	3.76	114.00	110.52
26	v	317	CHL	C2D-C1D-ND	3.75	112.87	110.10
26	4	316	CHL	C3B-C4B-NB	3.75	114.00	110.52
26	Q	313	CHL	CHB-C1B-NB	-3.75	120.28	124.26
26	U	313	CHL	CHB-C1B-NB	-3.75	120.28	124.26
31	C	516	BCR	C1-C6-C5	-3.75	117.33	122.61
22	A	408	CLA	CMB-C2B-C1B	-3.75	119.66	125.37
23	V	309	LUT	C35-C34-C33	-3.75	121.96	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	315	CHL	O2D-CGD-CBD	3.75	117.93	111.27
24	4	311	XAT	C31-C30-C29	-3.75	121.96	127.31
24	6	310	XAT	C35-C34-C33	-3.75	121.96	127.31
27	U	318	NEX	C31-C30-C29	-3.75	121.96	127.31
24	V	311	XAT	C35-C34-C33	-3.74	121.97	127.31
27	v	319	NEX	C39-C29-C30	-3.74	117.68	122.92
24	2	311	XAT	C6-C7-C8	-3.74	118.08	125.99
26	U	316	CHL	C3B-C4B-NB	3.74	113.99	110.52
32	L	102	SQD	C1-O5-C5	3.74	121.03	113.69
26	g	313	CHL	CHB-C1B-NB	-3.74	120.30	124.26
36	A	414	DGD	O6E-C5E-C4E	3.74	116.49	109.69
31	D	404	BCR	C38-C26-C25	-3.74	120.33	124.53
26	G	311	CHL	C2D-C1D-ND	3.74	112.86	110.10
26	1	318	CHL	CHB-C1B-NB	-3.74	120.30	124.26
22	N	305	CLA	C4D-C3D-CAD	-3.74	103.69	108.10
31	D	404	BCR	C1-C6-C5	-3.74	117.35	122.61
23	4	310	LUT	C35-C34-C33	-3.74	121.98	127.31
24	g	309	XAT	C38-C25-C26	-3.74	116.00	122.26
22	b	605	CLA	CHB-C4A-NA	3.74	129.68	124.51
23	2	309	LUT	C35-C34-C33	-3.73	121.98	127.31
26	R	316	CHL	CHB-C1B-NB	-3.73	120.31	124.26
31	T	101	BCR	C1-C6-C5	-3.73	117.36	122.61
26	u	316	CHL	C1D-ND-C4D	-3.73	103.69	106.33
26	G	316	CHL	C2D-C1D-ND	3.73	112.85	110.10
36	c	518	DGD	O2G-C1B-C2B	3.73	119.54	111.50
26	n	318	CHL	C3B-C4B-NB	3.73	113.97	110.52
22	b	607	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
31	b	620	BCR	C38-C26-C27	3.73	120.77	113.62
26	v	318	CHL	C3B-C4B-NB	3.73	113.97	110.52
31	C	516	BCR	C38-C26-C25	-3.72	120.35	124.53
26	Q	312	CHL	CHD-C4C-C3C	-3.72	119.37	124.84
24	U	311	XAT	C18-C5-C6	-3.72	116.02	122.26
27	s	317	NEX	C27-C28-C29	-3.72	119.76	125.53
31	C	516	BCR	C8-C7-C6	-3.72	116.76	127.20
26	u	318	CHL	CAC-C3C-C4C	3.72	129.63	124.81
31	z	101	BCR	C4-C5-C6	-3.72	117.33	122.73
31	z	101	BCR	C8-C7-C6	-3.71	116.77	127.20
25	p	313	LHG	O7-C7-C8	3.71	119.50	111.50
31	d	403	BCR	C1-C6-C5	-3.71	117.38	122.61
32	C	501	SQD	O7-S-C6	3.71	111.35	106.94
32	M	101	SQD	O47-C7-C8	3.71	119.50	111.50
24	6	310	XAT	C11-C10-C9	-3.71	122.01	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	r	611	LUT	C7-C8-C9	-3.71	120.63	126.23
26	p	314	CHL	C2D-C1D-ND	3.71	112.84	110.10
31	c	515	BCR	C30-C25-C26	-3.71	117.39	122.61
32	A	412	SQD	O9-S-O7	-3.71	101.11	113.95
26	v	314	CHL	CAC-C3C-C4C	3.71	129.62	124.81
32	m	101	SQD	O47-C7-C8	3.70	119.48	111.50
22	G	305	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
26	G	311	CHL	CAC-C3C-C4C	3.70	129.62	124.81
23	S	310	LUT	C35-C34-C33	-3.70	122.03	127.31
26	p	314	CHL	CHB-C1B-NB	-3.70	120.34	124.26
26	P	315	CHL	CHC-C4B-NB	-3.70	120.34	124.26
26	n	317	CHL	OMC-CMC-C2C	-3.70	117.32	125.69
31	X	201	BCR	C1-C6-C5	-3.70	117.40	122.61
22	B	605	CLA	CHB-C4A-NA	3.70	129.63	124.51
26	S	314	CHL	C2D-C1D-ND	3.70	112.83	110.10
22	a	408	CLA	CMB-C2B-C1B	-3.70	119.74	125.37
26	s	313	CHL	CHC-C4B-NB	-3.69	120.35	124.26
24	6	310	XAT	C18-C5-C6	-3.69	116.07	122.26
31	K	101	BCR	C38-C26-C27	3.69	120.71	113.62
27	u	320	NEX	O24-C25-C38	3.69	119.48	115.06
23	P	311	LUT	C15-C14-C13	-3.69	122.04	127.31
31	k	101	BCR	C38-C26-C27	3.69	120.70	113.62
24	P	312	XAT	C18-C5-C6	-3.69	116.08	122.26
31	C	516	BCR	C4-C5-C6	-3.69	117.38	122.73
24	P	312	XAT	C26-C27-C28	-3.69	118.20	125.99
32	a	410	SQD	O9-S-O7	-3.69	101.19	113.95
26	g	311	CHL	CAC-C3C-C4C	3.68	129.59	124.81
31	C	518	BCR	C4-C5-C6	-3.68	117.38	122.73
26	S	313	CHL	CHB-C1B-NB	-3.68	120.36	124.26
26	G	313	CHL	C2D-C1D-ND	3.68	112.81	110.10
32	a	413	SQD	O47-C7-C8	3.68	119.43	111.50
26	s	314	CHL	C2D-C1D-ND	3.68	112.81	110.10
31	d	403	BCR	C38-C26-C25	-3.68	120.40	124.53
26	v	317	CHL	CAC-C3C-C4C	3.67	129.58	124.81
26	U	315	CHL	CMD-C2D-C3D	-3.67	119.16	127.61
31	x	202	BCR	C1-C6-C5	-3.67	117.44	122.61
32	l	102	SQD	C1-O5-C5	3.67	120.90	113.69
26	q	313	CHL	C3B-C4B-NB	3.67	113.92	110.52
31	C	517	BCR	C30-C25-C26	-3.67	117.44	122.61
26	P	315	CHL	C3C-C4C-NC	3.67	114.69	110.57
25	A	413	LHG	O7-C7-C8	3.67	119.41	111.50
26	u	317	CHL	C3B-C4B-NB	3.67	113.92	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v	317	CHL	C1D-ND-C4D	-3.67	103.73	106.33
31	a	409	BCR	C33-C5-C4	3.67	120.66	113.62
26	1	316	CHL	C3B-C4B-NB	3.66	113.91	110.52
26	u	313	CHL	CHB-C1B-NB	-3.66	120.38	124.26
27	U	318	NEX	O24-C25-C38	3.66	119.44	115.06
32	a	410	SQD	O7-S-C6	3.66	111.29	106.94
26	u	313	CHL	CHD-C4C-C3C	-3.66	119.46	124.84
27	r	618	NEX	C5-C6-C1	3.66	123.33	119.70
25	5	312	LHG	O7-C7-C8	3.66	119.39	111.50
24	3	309	XAT	C18-C5-C6	-3.66	116.13	122.26
26	5	315	CHL	C3B-C4B-NB	3.66	113.91	110.52
26	n	313	CHL	C2D-C1D-ND	3.66	112.80	110.10
26	6	317	CHL	C3D-C4D-ND	3.66	116.15	110.24
32	A	412	SQD	O47-C7-C8	3.66	119.38	111.50
31	A	409	BCR	C33-C5-C4	3.66	120.64	113.62
31	t	101	BCR	C38-C26-C27	3.65	120.64	113.62
32	C	501	SQD	O9-S-O7	-3.65	101.31	113.95
32	m	101	SQD	O9-S-O7	-3.65	101.31	113.95
26	g	315	CHL	O2D-CGD-CBD	3.65	117.75	111.27
26	u	318	CHL	C1D-ND-C4D	-3.65	103.74	106.33
22	g	301	CLA	CMB-C2B-C1B	-3.65	119.81	125.37
26	p	319	CHL	C2D-C1D-ND	3.65	112.79	110.10
25	a	415	LHG	O7-C7-C8	3.65	119.36	111.50
26	g	314	CHL	C4A-NA-C1A	3.65	108.35	106.71
26	V	317	CHL	C3B-C4B-NB	3.65	113.90	110.52
26	6	315	CHL	CHD-C4C-C3C	-3.65	119.48	124.84
26	u	314	CHL	C1D-ND-C4D	-3.65	103.75	106.33
26	g	311	CHL	CHB-C1B-NB	-3.65	120.40	124.26
31	D	404	BCR	C11-C10-C9	-3.64	122.11	127.31
26	q	313	CHL	CMB-C2B-C1B	3.64	130.91	125.37
31	B	620	BCR	C33-C5-C4	3.64	120.61	113.62
22	B	615	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
26	N	316	CHL	CAC-C3C-C4C	3.64	129.53	124.81
26	Q	311	CHL	C3B-C4B-NB	3.64	113.89	110.52
32	l	102	SQD	C4-C3-C2	3.64	117.17	110.82
26	G	313	CHL	C3B-C4B-NB	3.64	113.89	110.52
24	q	309	XAT	C35-C34-C33	-3.64	122.12	127.31
32	L	102	SQD	O9-S-O7	-3.64	101.37	113.95
26	R	317	CHL	CHD-C4C-C3C	-3.63	119.50	124.84
26	1	313	CHL	CHC-C4B-NB	-3.63	120.41	124.26
27	R	301	NEX	C39-C29-C30	-3.63	117.83	122.92
26	u	314	CHL	C3B-C4B-NB	3.63	113.89	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	314	CHL	CHC-C4B-NB	-3.63	120.41	124.26
22	b	617	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
26	V	313	CHL	CHD-C4C-C3C	-3.63	119.50	124.84
22	B	607	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
26	q	313	CHL	CHB-C1B-NB	-3.63	120.42	124.26
26	2	315	CHL	C3B-C4B-NB	3.63	113.88	110.52
23	v	309	LUT	C35-C34-C33	-3.63	122.13	127.31
31	A	409	BCR	C4-C5-C6	-3.63	117.47	122.73
32	M	101	SQD	O9-S-O7	-3.63	101.40	113.95
24	5	311	XAT	C11-C10-C9	-3.62	122.14	127.31
25	c	521	LHG	O7-C7-C8	3.62	119.31	111.50
32	a	413	SQD	O9-S-O7	-3.62	101.43	113.95
27	r	617	NEX	C35-C34-C33	-3.62	122.15	127.31
26	p	315	CHL	CHC-C4B-NB	-3.62	120.43	124.26
26	r	619	CHL	C3B-C4B-NB	3.62	113.87	110.52
27	U	318	NEX	C35-C34-C33	-3.62	122.15	127.31
27	r	617	NEX	O24-C25-C38	3.61	119.39	115.06
26	R	317	CHL	CHB-C1B-NB	-3.61	120.43	124.26
31	b	620	BCR	C33-C5-C4	3.61	120.56	113.62
23	N	309	LUT	C35-C34-C33	-3.61	122.16	127.31
24	R	313	XAT	C35-C34-C33	-3.61	122.16	127.31
26	2	315	CHL	CHB-C1B-NB	-3.61	120.44	124.26
31	t	101	BCR	C1-C6-C5	-3.61	117.53	122.61
26	N	316	CHL	C3B-C4B-NB	3.60	113.86	110.52
26	G	313	CHL	CAC-C3C-C4C	3.60	129.48	124.81
26	U	314	CHL	C2D-C1D-ND	3.60	112.76	110.10
24	u	311	XAT	C38-C25-C26	-3.60	116.23	122.26
26	N	313	CHL	C3B-C4B-NB	3.60	113.85	110.52
26	n	317	CHL	CHD-C4C-C3C	-3.60	119.55	124.84
26	G	316	CHL	C1D-ND-C4D	-3.60	103.78	106.33
31	c	516	BCR	C4-C5-C6	-3.59	117.51	122.73
27	n	319	NEX	C35-C34-C33	-3.59	122.18	127.31
25	C	522	LHG	O7-C7-C8	3.59	119.24	111.50
31	d	403	BCR	C11-C10-C9	-3.59	122.19	127.31
26	6	312	CHL	C3B-C4B-NB	3.59	113.85	110.52
23	4	309	LUT	C7-C8-C9	-3.59	120.81	126.23
23	n	310	LUT	C15-C14-C13	-3.59	122.19	127.31
34	B	621	LMG	O6-C1-C2	3.59	117.94	110.35
26	6	301	CHL	CMD-C2D-C3D	-3.59	119.36	127.61
26	u	315	CHL	C2D-C1D-ND	3.59	112.75	110.10
31	B	620	BCR	C4-C5-C6	-3.59	117.53	122.73
26	U	316	CHL	CAC-C3C-C4C	3.58	129.46	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	u	309	LUT	C35-C34-C33	-3.58	122.19	127.31
34	c	520	LMG	O7-C10-C11	3.58	119.22	111.50
32	l	102	SQD	O9-S-O7	-3.58	101.55	113.95
26	1	317	CHL	C1D-ND-C4D	-3.58	103.79	106.33
26	Q	311	CHL	C3D-C4D-ND	3.58	116.03	110.24
24	p	312	XAT	C18-C5-C6	-3.58	116.26	122.26
26	6	317	CHL	C1D-ND-C4D	-3.58	103.79	106.33
26	N	317	CHL	CAC-C3C-C4C	3.58	129.45	124.81
25	B	622	LHG	O7-C7-C8	3.58	119.21	111.50
26	v	314	CHL	C1D-ND-C4D	-3.57	103.80	106.33
23	n	309	LUT	C35-C34-C33	-3.57	122.21	127.31
24	U	311	XAT	C38-C25-C26	-3.57	116.28	122.26
26	U	313	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
26	v	313	CHL	CHB-C1B-NB	-3.57	120.48	124.26
24	V	311	XAT	C11-C10-C9	-3.57	122.22	127.31
31	a	409	BCR	C4-C5-C6	-3.57	117.56	122.73
26	4	316	CHL	CHB-C1B-NB	-3.56	120.48	124.26
31	b	620	BCR	C30-C25-C26	-3.56	117.59	122.61
26	p	314	CHL	CAC-C3C-C4C	3.56	129.43	124.81
22	b	615	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
34	C	521	LMG	O7-C10-C11	3.56	119.18	111.50
31	b	620	BCR	C8-C7-C6	-3.56	117.20	127.20
26	1	314	CHL	CAC-C3C-C4C	3.56	129.43	124.81
27	v	319	NEX	O24-C25-C38	3.56	119.32	115.06
26	G	313	CHL	CHB-C1B-NB	-3.56	120.49	124.26
26	Q	315	CHL	O2D-CGD-CBD	3.56	117.59	111.27
23	s	310	LUT	C35-C15-C14	-3.56	116.19	123.47
26	4	316	CHL	C1D-ND-C4D	-3.56	103.81	106.33
26	p	318	CHL	C1D-ND-C4D	-3.56	103.81	106.33
26	G	314	CHL	CHD-C4C-C3C	-3.56	119.61	124.84
22	g	303	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
26	Q	314	CHL	C2D-C1D-ND	3.55	112.72	110.10
26	r	615	CHL	CAC-C3C-C4C	3.55	129.42	124.81
26	S	313	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
31	B	618	BCR	C20-C21-C22	-3.55	122.24	127.31
27	V	319	NEX	C39-C29-C30	-3.55	117.95	122.92
26	6	317	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
26	Q	313	CHL	CHD-C4C-C3C	-3.55	119.62	124.84
26	p	318	CHL	CAC-C3C-C4C	3.55	129.41	124.81
26	g	316	CHL	CAC-C3C-C4C	3.55	129.41	124.81
31	b	618	BCR	C20-C21-C22	-3.55	122.25	127.31
26	4	313	CHL	CAC-C3C-C4C	3.55	129.41	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	n	311	XAT	C38-C25-C26	-3.55	116.31	122.26
26	V	314	CHL	C3B-C4B-NB	3.55	113.81	110.52
26	U	316	CHL	C3D-C4D-ND	3.55	115.98	110.24
23	1	310	LUT	C35-C34-C33	-3.55	122.25	127.31
23	4	310	LUT	C2-C3-C4	3.55	115.16	110.30
31	b	618	BCR	C27-C26-C25	-3.54	117.58	122.73
24	G	309	XAT	C35-C34-C33	-3.54	122.25	127.31
26	3	311	CHL	C3B-C4B-NB	3.54	113.80	110.52
26	g	316	CHL	C2D-C1D-ND	3.54	112.71	110.10
26	r	616	CHL	CHB-C1B-NB	-3.54	120.51	124.26
24	Q	309	XAT	C35-C34-C33	-3.54	122.26	127.31
23	5	309	LUT	C11-C10-C9	-3.54	122.26	127.31
26	3	314	CHL	CHD-C4C-C3C	-3.54	119.64	124.84
26	5	314	CHL	CHC-C4B-NB	-3.54	120.51	124.26
26	v	313	CHL	CAC-C3C-C4C	3.54	129.40	124.81
31	T	101	BCR	C38-C26-C27	3.54	120.42	113.62
31	D	404	BCR	C38-C26-C27	3.54	120.42	113.62
23	v	310	LUT	C35-C34-C33	-3.54	122.26	127.31
24	1	311	XAT	C15-C14-C13	-3.54	122.26	127.31
31	b	620	BCR	C4-C5-C6	-3.54	117.60	122.73
26	q	311	CHL	C3D-C4D-ND	3.54	115.96	110.24
26	V	317	CHL	CAC-C3C-C4C	3.54	129.40	124.81
23	N	310	LUT	C15-C14-C13	-3.54	122.26	127.31
24	g	309	XAT	C11-C10-C9	-3.53	122.27	127.31
26	G	311	CHL	C1D-ND-C4D	-3.53	103.82	106.33
26	1	313	CHL	CHD-C4C-C3C	-3.53	119.64	124.84
26	4	317	CHL	CAC-C3C-C4C	3.53	129.40	124.81
26	V	313	CHL	CAC-C3C-C4C	3.53	129.39	124.81
31	B	618	BCR	C33-C5-C4	3.53	120.40	113.62
26	q	313	CHL	C2D-C1D-ND	3.53	112.71	110.10
26	r	619	CHL	C1D-ND-C4D	-3.53	103.83	106.33
24	2	311	XAT	C26-C27-C28	-3.53	118.53	125.99
26	P	314	CHL	CHC-C4B-NB	-3.53	120.52	124.26
31	X	201	BCR	C20-C21-C22	-3.53	122.27	127.31
26	v	317	CHL	C3D-C4D-ND	3.53	115.95	110.24
26	n	314	CHL	CAC-C3C-C4C	3.53	129.39	124.81
26	Q	316	CHL	C2D-C1D-ND	3.53	112.70	110.10
26	V	314	CHL	C4A-NA-C1A	3.53	108.29	106.71
27	R	301	NEX	C5-C6-C1	3.53	123.20	119.70
26	V	314	CHL	CAC-C3C-C4C	3.53	129.39	124.81
26	U	315	CHL	C1D-ND-C4D	-3.53	103.83	106.33
24	V	311	XAT	C18-C5-C6	-3.53	116.35	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	U	310	LUT	C15-C14-C13	-3.53	122.28	127.31
31	C	517	BCR	C20-C21-C22	-3.52	122.28	127.31
26	6	301	CHL	C3B-C4B-NB	3.52	113.78	110.52
26	P	318	CHL	C3B-C4B-NB	3.52	113.78	110.52
24	G	309	XAT	C11-C10-C9	-3.52	122.28	127.31
32	L	102	SQD	C4-C3-C2	3.52	116.97	110.82
23	v	310	LUT	C15-C14-C13	-3.52	122.29	127.31
23	5	309	LUT	C7-C8-C9	-3.52	120.92	126.23
24	2	311	XAT	C11-C10-C9	-3.52	122.29	127.31
22	g	305	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
26	2	318	CHL	CAC-C3C-C4C	3.52	129.37	124.81
26	3	316	CHL	C3D-C4D-ND	3.52	115.92	110.24
26	r	616	CHL	CHD-C4C-C3C	-3.52	119.67	124.84
27	5	319	NEX	C39-C29-C30	-3.52	118.00	122.92
26	V	317	CHL	C3D-C4D-ND	3.52	115.92	110.24
26	G	316	CHL	CAC-C3C-C4C	3.51	129.37	124.81
26	G	313	CHL	CMB-C2B-C1B	3.51	130.72	125.37
31	d	403	BCR	C38-C26-C27	3.51	120.36	113.62
26	5	318	CHL	C2D-C1D-ND	3.51	112.69	110.10
26	V	316	CHL	CAC-C3C-C4C	3.51	129.37	124.81
26	v	315	CHL	CHD-C4C-C3C	-3.51	119.68	124.84
26	v	317	CHL	C3B-C4B-NB	3.51	113.77	110.52
31	C	516	BCR	C30-C25-C26	-3.51	117.67	122.61
31	k	101	BCR	C27-C26-C25	-3.51	117.64	122.73
31	B	620	BCR	C8-C7-C6	-3.51	117.36	127.20
26	P	319	CHL	CHB-C1B-NB	-3.51	120.55	124.26
26	u	317	CHL	C3D-C4D-ND	3.51	115.91	110.24
26	4	317	CHL	C1D-ND-C4D	-3.51	103.84	106.33
26	R	315	CHL	C3B-C4B-NB	3.50	113.77	110.52
31	B	618	BCR	C27-C26-C25	-3.50	117.64	122.73
26	S	314	CHL	C3B-C4B-NB	3.50	113.77	110.52
26	6	312	CHL	C3D-C4D-ND	3.50	115.90	110.24
26	4	313	CHL	CHD-C4C-C3C	-3.50	119.69	124.84
26	u	316	CHL	C3B-C4B-NB	3.50	113.76	110.52
31	K	101	BCR	C11-C10-C9	-3.50	122.31	127.31
26	1	314	CHL	C3B-C4B-NB	3.50	113.76	110.52
26	5	317	CHL	CAC-C3C-C4C	3.50	129.35	124.81
24	G	309	XAT	C38-C25-C26	-3.50	116.39	122.26
31	B	618	BCR	C8-C7-C6	-3.50	117.37	127.20
26	G	314	CHL	C2D-C1D-ND	3.50	112.68	110.10
26	v	316	CHL	C3B-C4B-NB	3.50	113.76	110.52
26	V	314	CHL	CHD-C4C-C3C	-3.50	119.70	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q	316	CHL	C3B-C4B-NB	3.50	113.76	110.52
31	K	101	BCR	C7-C8-C9	-3.50	120.95	126.23
34	b	621	LMG	O6-C5-C4	3.49	116.04	109.69
32	a	410	SQD	O6-C1-C2	3.49	113.76	108.30
27	p	301	NEX	C39-C29-C30	-3.49	118.03	122.92
26	3	316	CHL	CHD-C4C-C3C	-3.49	119.71	124.84
26	p	317	CHL	C2D-C1D-ND	3.49	112.67	110.10
31	T	101	BCR	C33-C5-C4	3.49	120.31	113.62
31	x	202	BCR	C20-C21-C22	-3.49	122.34	127.31
23	P	310	LUT	C15-C14-C13	-3.48	122.34	127.31
26	g	313	CHL	C3B-C4B-NB	3.48	113.75	110.52
26	g	312	CHL	C3B-C4B-NB	3.48	113.74	110.52
26	g	316	CHL	C1D-ND-C4D	-3.48	103.86	106.33
26	q	315	CHL	C2D-C1D-ND	3.48	112.67	110.10
26	3	312	CHL	CHC-C4B-NB	-3.48	120.57	124.26
26	6	313	CHL	CHC-C4B-NB	-3.48	120.57	124.26
26	s	314	CHL	C3B-C4B-NB	3.48	113.74	110.52
31	B	620	BCR	C24-C23-C22	-3.48	120.98	126.23
24	q	309	XAT	C35-C15-C14	-3.48	116.35	123.47
24	5	311	XAT	C35-C34-C33	-3.48	122.35	127.31
26	P	317	CHL	CMD-C2D-C3D	-3.48	119.62	127.61
27	N	318	NEX	C39-C29-C30	-3.48	118.05	122.92
23	r	611	LUT	C15-C14-C13	-3.47	122.35	127.31
26	1	314	CHL	C2D-C1D-ND	3.47	112.66	110.10
26	g	312	CHL	CHD-C4C-C3C	-3.47	119.73	124.84
26	r	615	CHL	CHB-C4A-NA	3.47	129.31	124.51
24	4	311	XAT	C15-C14-C13	-3.47	122.35	127.31
31	K	101	BCR	C27-C26-C25	-3.47	117.69	122.73
23	u	310	LUT	C15-C14-C13	-3.47	122.36	127.31
26	2	317	CHL	O2A-CGA-CBA	3.47	122.80	111.91
31	x	202	BCR	C23-C24-C25	-3.47	117.46	127.20
26	n	315	CHL	CHD-C4C-C3C	-3.47	119.74	124.84
26	g	315	CHL	CAC-C3C-C4C	3.47	129.31	124.81
24	q	309	XAT	C6-C7-C8	-3.46	118.67	125.99
22	n	304	CLA	CHB-C4A-NA	3.46	129.30	124.51
31	B	619	BCR	C8-C7-C6	-3.46	117.48	127.20
26	6	314	CHL	CAC-C3C-C4C	3.46	129.30	124.81
24	p	312	XAT	C35-C34-C33	-3.46	122.37	127.31
26	1	316	CHL	CAC-C3C-C4C	3.46	129.30	124.81
30	A	407	PHO	CMB-C2B-C3B	3.46	131.15	124.68
26	P	318	CHL	CAC-C3C-C4C	3.46	129.30	124.81
31	B	620	BCR	C30-C25-C26	-3.46	117.74	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	318	CHL	CAC-C3C-C4C	3.46	129.30	124.81
23	p	311	LUT	C15-C14-C13	-3.46	122.38	127.31
26	v	318	CHL	C2D-C1D-ND	3.46	112.65	110.10
26	U	315	CHL	CAC-C3C-C4C	3.46	129.29	124.81
31	C	518	BCR	C27-C26-C25	-3.45	117.72	122.73
26	1	315	CHL	CHD-C4C-C3C	-3.45	119.76	124.84
24	4	311	XAT	C38-C25-C26	-3.45	116.47	122.26
31	C	516	BCR	C16-C15-C14	-3.45	116.40	123.47
26	r	614	CHL	C3B-C4B-NB	3.45	113.72	110.52
31	b	619	BCR	C38-C26-C25	-3.45	120.66	124.53
22	n	308	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
31	b	618	BCR	C7-C8-C9	-3.44	121.03	126.23
26	Q	313	CHL	CMB-C2B-C1B	3.44	130.61	125.37
26	1	317	CHL	CHB-C1B-NB	-3.44	120.61	124.26
26	4	316	CHL	C3D-C4D-ND	3.44	115.81	110.24
26	5	318	CHL	CAC-C3C-C4C	3.44	129.28	124.81
26	4	314	CHL	CAC-C3C-C4C	3.44	129.27	124.81
26	P	319	CHL	C1D-ND-C4D	-3.44	103.89	106.33
31	k	101	BCR	C11-C10-C9	-3.44	122.40	127.31
26	5	315	CHL	C1D-ND-C4D	-3.44	103.89	106.33
26	q	314	CHL	C3B-C4B-NB	3.44	113.70	110.52
26	g	316	CHL	C3D-C4D-ND	3.44	115.80	110.24
26	2	316	CHL	CHD-C4C-C3C	-3.43	119.79	124.84
26	N	313	CHL	C1D-ND-C4D	-3.43	103.89	106.33
22	a	408	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
30	a	407	PHO	CMB-C2B-C3B	3.43	131.10	124.68
31	c	516	BCR	C27-C26-C25	-3.43	117.75	122.73
31	c	516	BCR	C7-C8-C9	-3.43	121.05	126.23
26	r	616	CHL	CAC-C3C-C4C	3.43	129.26	124.81
26	2	318	CHL	C2D-C1D-ND	3.43	112.63	110.10
26	R	316	CHL	CAC-C3C-C4C	3.43	129.26	124.81
36	A	414	DGD	C1E-O6E-C5E	3.43	120.42	113.69
26	r	614	CHL	CHB-C1B-NB	-3.43	120.63	124.26
26	U	319	CHL	CAC-C3C-C4C	3.43	129.26	124.81
23	2	310	LUT	C7-C8-C9	-3.43	121.06	126.23
26	4	317	CHL	CHB-C1B-NB	-3.43	120.63	124.26
22	u	304	CLA	CMB-C2B-C1B	-3.43	120.15	125.37
26	U	315	CHL	C2D-C1D-ND	3.43	112.63	110.10
26	s	313	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
31	B	619	BCR	C15-C16-C17	-3.42	116.46	123.47
26	6	315	CHL	CMD-C2D-C3D	-3.42	119.74	127.61
31	X	201	BCR	C23-C24-C25	-3.42	117.59	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	311	CHL	C3D-C4D-ND	3.42	115.77	110.24
26	1	316	CHL	CMD-C2D-C3D	-3.42	119.75	127.61
26	R	317	CHL	CAC-C3C-C4C	3.42	129.25	124.81
24	5	311	XAT	C18-C5-C6	-3.42	116.53	122.26
26	5	316	CHL	CHD-C4C-C3C	-3.42	119.82	124.84
32	m	101	SQD	C44-O6-C1	3.42	120.41	113.74
31	b	619	BCR	C8-C7-C6	-3.42	117.61	127.20
26	U	313	CHL	CAC-C3C-C4C	3.42	129.24	124.81
23	4	309	LUT	C35-C34-C33	-3.41	122.44	127.31
31	k	101	BCR	C38-C26-C25	-3.41	120.69	124.53
36	a	416	DGD	C1E-O6E-C5E	3.41	120.39	113.69
26	2	317	CHL	CAC-C3C-C4C	3.41	129.24	124.81
31	D	404	BCR	C33-C5-C4	3.41	120.17	113.62
31	C	518	BCR	C20-C21-C22	-3.41	122.44	127.31
26	U	317	CHL	CHB-C1B-NB	-3.41	120.65	124.26
24	U	311	XAT	C26-C27-C28	-3.40	118.79	125.99
26	6	317	CHL	CAC-C3C-C4C	3.40	129.23	124.81
26	3	316	CHL	CHB-C1B-NB	-3.40	120.65	124.26
26	n	317	CHL	C2D-C1D-ND	3.40	112.61	110.10
26	5	318	CHL	C3D-C4D-ND	3.40	115.74	110.24
31	C	518	BCR	C7-C8-C9	-3.40	121.10	126.23
26	G	316	CHL	C3D-C4D-ND	3.40	115.73	110.24
31	C	518	BCR	C21-C20-C19	-3.40	112.61	123.22
26	6	301	CHL	CAC-C3C-C4C	3.40	129.22	124.81
26	g	312	CHL	CAC-C3C-C4C	3.40	129.22	124.81
25	b	623	LHG	O7-C7-C8	3.39	118.82	111.50
26	1	317	CHL	C3D-C4D-ND	3.39	115.73	110.24
24	N	311	XAT	C35-C15-C14	-3.39	116.52	123.47
26	N	316	CHL	CHB-C1B-NB	-3.39	120.67	124.26
26	Q	312	CHL	CAC-C3C-C4C	3.39	129.21	124.81
26	6	316	CHL	C3B-C4B-NB	3.39	113.66	110.52
31	b	620	BCR	C15-C14-C13	-3.39	122.47	127.31
31	c	515	BCR	C20-C21-C22	-3.39	122.47	127.31
26	n	313	CHL	CHC-C4B-NB	-3.39	120.67	124.26
26	1	317	CHL	CAC-C3C-C4C	3.39	129.21	124.81
26	G	311	CHL	CMD-C2D-C3D	-3.39	119.83	127.61
26	u	313	CHL	CAC-C3C-C4C	3.39	129.20	124.81
27	r	617	NEX	C39-C29-C30	-3.38	118.18	122.92
26	G	314	CHL	CAC-C3C-C4C	3.38	129.20	124.81
23	2	309	LUT	C15-C14-C13	-3.38	122.48	127.31
22	G	301	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
26	P	318	CHL	C1D-ND-C4D	-3.38	103.93	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v	318	CHL	CAC-C3C-C4C	3.38	129.20	124.81
27	U	318	NEX	C11-C10-C9	-3.38	122.49	127.31
31	t	101	BCR	C33-C5-C4	3.38	120.11	113.62
26	u	316	CHL	CAC-C3C-C4C	3.38	129.19	124.81
31	c	516	BCR	C33-C5-C4	3.38	120.11	113.62
23	P	311	LUT	C35-C34-C33	-3.38	122.49	127.31
32	M	101	SQD	C44-O6-C1	3.38	120.34	113.74
26	Q	313	CHL	C3D-C4D-ND	3.38	115.70	110.24
26	5	317	CHL	CHB-C1B-NB	-3.38	120.68	124.26
26	Q	315	CHL	C3B-C4B-NB	3.38	113.65	110.52
26	u	313	CHL	C2D-C1D-ND	3.38	112.59	110.10
25	B	623	LHG	O7-C7-C8	3.38	118.78	111.50
26	N	316	CHL	C3D-C4D-ND	3.38	115.70	110.24
30	d	401	PHO	CMB-C2B-C3B	3.38	130.99	124.68
30	D	401	PHO	CMB-C2B-C3B	3.38	130.99	124.68
31	k	101	BCR	C7-C8-C9	-3.37	121.14	126.23
25	b	622	LHG	O7-C7-C8	3.37	118.77	111.50
26	U	314	CHL	C3B-C4B-NB	3.37	113.64	110.52
24	P	312	XAT	C38-C25-C26	-3.37	116.61	122.26
26	Q	311	CHL	CAC-C3C-C4C	3.37	129.19	124.81
31	a	409	BCR	C8-C7-C6	-3.37	117.73	127.20
26	V	316	CHL	C2D-C1D-ND	3.37	112.59	110.10
26	R	316	CHL	CHB-C4A-NA	3.37	129.17	124.51
27	n	319	NEX	C2-C1-C6	3.37	112.48	109.21
26	Q	315	CHL	C3D-C4D-ND	3.37	115.69	110.24
26	q	312	CHL	CHC-C4B-NB	-3.37	120.69	124.26
26	S	313	CHL	CAC-C3C-C4C	3.37	129.18	124.81
31	B	619	BCR	C38-C26-C25	-3.37	120.75	124.53
27	P	301	NEX	C39-C29-C30	-3.37	118.21	122.92
26	5	318	CHL	C1D-ND-C4D	-3.36	103.94	106.33
26	u	316	CHL	C2D-C1D-ND	3.36	112.58	110.10
26	u	314	CHL	C3D-C4D-ND	3.36	115.68	110.24
31	d	403	BCR	C33-C5-C4	3.36	120.08	113.62
22	B	605	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
22	B	617	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
26	5	316	CHL	CAC-C3C-C4C	3.36	129.17	124.81
26	u	316	CHL	C3D-C4D-ND	3.36	115.67	110.24
26	v	316	CHL	C3D-C4D-ND	3.36	115.67	110.24
22	b	605	CLA	O2D-CGD-O1D	-3.36	117.28	123.84
27	u	319	NEX	C24-C23-C22	-3.35	104.29	110.77
26	U	315	CHL	CHB-C1B-NB	-3.35	120.71	124.26
26	n	316	CHL	C3B-C4B-NB	3.35	113.62	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	620	BCR	C27-C26-C25	-3.35	117.86	122.73
26	3	314	CHL	CMD-C2D-C3D	-3.35	119.91	127.61
22	B	604	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
27	p	301	NEX	C11-C10-C9	-3.35	122.53	127.31
26	q	314	CHL	C3D-C4D-ND	3.35	115.66	110.24
26	N	315	CHL	C2D-C1D-ND	3.35	112.57	110.10
26	U	313	CHL	C3D-C4D-ND	3.35	115.66	110.24
22	q	304	CLA	CHB-C4A-NA	3.35	129.14	124.51
26	4	314	CHL	C1D-ND-C4D	-3.35	103.96	106.33
26	2	316	CHL	CAC-C3C-C4C	3.35	129.15	124.81
31	c	516	BCR	C21-C20-C19	-3.35	112.77	123.22
26	s	316	CHL	CAC-C3C-C4C	3.35	129.15	124.81
26	4	316	CHL	CAC-C3C-C4C	3.34	129.15	124.81
31	b	619	BCR	C15-C16-C17	-3.34	116.62	123.47
26	p	316	CHL	CHD-C4C-C3C	-3.34	119.93	124.84
26	v	315	CHL	C2D-C1D-ND	3.34	112.57	110.10
24	1	311	XAT	C38-C25-C26	-3.34	116.66	122.26
26	4	317	CHL	C3D-C4D-ND	3.34	115.64	110.24
26	6	317	CHL	C2D-C1D-ND	3.34	112.57	110.10
23	n	310	LUT	C7-C8-C9	-3.34	121.19	126.23
32	C	501	SQD	O6-C1-C2	3.34	113.52	108.30
22	b	604	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
31	A	409	BCR	C38-C26-C25	-3.34	120.78	124.53
23	5	310	LUT	C7-C8-C9	-3.34	121.19	126.23
24	v	311	XAT	C38-C25-C26	-3.34	116.67	122.26
26	V	318	CHL	C3B-C4B-NB	3.34	113.61	110.52
23	s	310	LUT	C7-C8-C9	-3.34	121.19	126.23
26	u	313	CHL	C3D-C4D-ND	3.34	115.63	110.24
26	Q	312	CHL	C2D-C1D-ND	3.33	112.56	110.10
26	P	316	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	6	316	CHL	C3D-C4D-ND	3.33	115.63	110.24
26	S	316	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	P	316	CHL	CHD-C4C-C3C	-3.33	119.94	124.84
24	V	311	XAT	C38-C25-C26	-3.33	116.68	122.26
26	q	315	CHL	C3B-C4B-NB	3.33	113.61	110.52
26	s	313	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	n	316	CHL	CAC-C3C-C4C	3.33	129.13	124.81
26	P	314	CHL	C2D-C1D-ND	3.33	112.56	110.10
26	p	319	CHL	CAC-C3C-C4C	3.33	129.13	124.81
22	6	306	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
31	K	101	BCR	C38-C26-C25	-3.33	120.79	124.53
26	P	319	CHL	CHB-C4A-NA	3.33	129.11	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	q	309	XAT	C30-C31-C32	-3.33	112.84	123.22
26	V	318	CHL	C2D-C1D-ND	3.33	112.56	110.10
31	z	101	BCR	C16-C15-C14	-3.33	116.66	123.47
26	p	318	CHL	CHB-C4A-NA	3.33	129.11	124.51
26	U	317	CHL	C1D-ND-C4D	-3.32	103.97	106.33
31	x	202	BCR	C4-C5-C6	-3.32	117.90	122.73
26	V	313	CHL	C3D-C4D-ND	3.32	115.61	110.24
22	S	305	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
27	R	301	NEX	C35-C34-C33	-3.32	122.57	127.31
26	G	315	CHL	CAC-C3C-C4C	3.32	129.12	124.81
26	5	317	CHL	C3D-C4D-ND	3.32	115.61	110.24
24	v	311	XAT	C18-C5-C6	-3.32	116.70	122.26
23	n	310	LUT	C18-C5-C4	3.32	120.51	114.36
22	3	305	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
26	1	316	CHL	C2D-C1D-ND	3.32	112.55	110.10
26	v	313	CHL	C2D-C1D-ND	3.32	112.55	110.10
26	3	316	CHL	CAC-C3C-C4C	3.32	129.11	124.81
26	2	318	CHL	C3D-C4D-ND	3.32	115.60	110.24
26	5	317	CHL	O2A-CGA-CBA	3.32	122.32	111.91
31	X	201	BCR	C4-C5-C6	-3.32	117.92	122.73
26	4	317	CHL	CHB-C4A-NA	3.31	129.10	124.51
26	Q	312	CHL	C3B-C4B-NB	3.31	113.59	110.52
31	a	409	BCR	C24-C23-C22	-3.31	121.23	126.23
27	u	320	NEX	C39-C29-C30	-3.31	118.28	122.92
26	1	318	CHL	C1D-ND-C4D	-3.31	103.98	106.33
22	5	304	CLA	CHB-C4A-NA	3.31	129.09	124.51
26	3	314	CHL	CAC-C3C-C4C	3.31	129.11	124.81
31	b	618	BCR	C1-C6-C5	-3.31	117.95	122.61
36	B	601	DGD	O2G-C1B-C2B	3.31	118.63	111.50
26	g	314	CHL	C2D-C1D-ND	3.31	112.54	110.10
26	R	315	CHL	CHB-C1B-NB	-3.31	120.75	124.26
31	A	409	BCR	C24-C23-C22	-3.31	121.24	126.23
31	b	620	BCR	C24-C23-C22	-3.31	121.24	126.23
31	B	620	BCR	C27-C26-C25	-3.30	117.94	122.73
26	6	315	CHL	CAC-C3C-C4C	3.30	129.09	124.81
26	u	315	CHL	C3B-C4B-NB	3.30	113.58	110.52
26	s	314	CHL	CHB-C1B-NB	-3.30	120.76	124.26
26	U	313	CHL	CMD-C2D-C3D	-3.30	120.02	127.61
26	p	320	CHL	C3D-C4D-ND	3.30	115.58	110.24
26	p	315	CHL	CED-O2D-CGD	3.30	123.40	115.94
26	S	314	CHL	CHB-C1B-NB	-3.30	120.77	124.26
26	p	317	CHL	C3B-C4B-NB	3.30	113.57	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	S	310	LUT	C7-C8-C9	-3.30	121.25	126.23
24	v	311	XAT	C11-C10-C9	-3.30	122.61	127.31
26	s	314	CHL	C1D-ND-C4D	-3.29	104.00	106.33
26	1	313	CHL	CAC-C3C-C4C	3.29	129.08	124.81
22	R	310	CLA	CHB-C4A-NA	3.29	129.06	124.51
31	A	409	BCR	C8-C7-C6	-3.29	117.96	127.20
26	2	317	CHL	CHB-C1B-NB	-3.29	120.77	124.26
26	v	316	CHL	CAC-C3C-C4C	3.29	129.08	124.81
26	g	314	CHL	CAC-C3C-C4C	3.29	129.08	124.81
26	u	313	CHL	C3B-C4B-NB	3.29	113.56	110.52
26	n	315	CHL	CMD-C2D-C3D	-3.29	120.05	127.61
26	s	316	CHL	CHD-C4C-C3C	-3.29	120.01	124.84
26	2	314	CHL	CAC-C3C-C4C	3.29	129.07	124.81
26	V	318	CHL	CAC-C3C-C4C	3.28	129.07	124.81
22	s	305	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	1	310	LUT	C3-C4-C5	-3.28	105.32	111.85
26	n	315	CHL	CAC-C3C-C4C	3.28	129.07	124.81
31	C	518	BCR	C33-C5-C4	3.28	119.92	113.62
31	c	516	BCR	C20-C21-C22	-3.28	122.63	127.31
26	G	312	CHL	CAC-C3C-C4C	3.28	129.07	124.81
26	Q	313	CHL	C2D-C1D-ND	3.28	112.52	110.10
22	2	304	CLA	CHB-C4A-NA	3.28	129.05	124.51
26	N	315	CHL	C3B-C4B-NB	3.28	113.56	110.52
24	4	311	XAT	C18-C5-C6	-3.28	116.77	122.26
24	U	311	XAT	C31-C30-C29	-3.28	122.64	127.31
26	p	316	CHL	CAC-C3C-C4C	3.28	129.06	124.81
23	v	309	LUT	C15-C14-C13	-3.28	122.64	127.31
24	V	311	XAT	C26-C27-C28	-3.27	119.07	125.99
26	6	317	CHL	CHB-C1B-NB	-3.27	120.79	124.26
26	N	317	CHL	CMB-C2B-C1B	3.27	130.35	125.37
34	b	621	LMG	C1-C2-C3	3.27	116.81	110.00
26	u	316	CHL	CHB-C1B-NB	-3.27	120.79	124.26
26	q	311	CHL	CAC-C3C-C4C	3.27	129.05	124.81
26	p	314	CHL	C1D-ND-C4D	-3.27	104.01	106.33
26	v	317	CHL	O2A-CGA-CBA	3.27	122.17	111.91
26	S	313	CHL	C3D-C4D-ND	3.27	115.53	110.24
26	u	315	CHL	CHB-C1B-NB	-3.27	120.80	124.26
31	b	618	BCR	C33-C5-C4	3.27	119.89	113.62
26	U	314	CHL	CHB-C1B-NB	-3.27	120.80	124.26
26	2	317	CHL	C3D-C4D-ND	3.27	115.52	110.24
26	5	316	CHL	C3D-C4D-ND	3.27	115.52	110.24
26	P	317	CHL	C3B-C4B-NB	3.27	113.54	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q	315	CHL	CMB-C2B-C1B	3.26	130.34	125.37
26	S	316	CHL	CHD-C4C-C3C	-3.26	120.04	124.84
27	P	301	NEX	C17-C1-C6	-3.26	107.55	110.47
26	g	311	CHL	C1D-ND-C4D	-3.26	104.02	106.33
26	V	314	CHL	C2D-C1D-ND	3.26	112.51	110.10
30	d	401	PHO	C2D-C1D-ND	-3.26	107.28	109.53
30	D	401	PHO	C2D-C1D-ND	-3.26	107.28	109.53
26	p	314	CHL	C3D-C4D-ND	3.26	115.51	110.24
26	v	313	CHL	C3D-C4D-ND	3.26	115.50	110.24
26	R	315	CHL	C1D-ND-C4D	-3.26	104.02	106.33
26	P	315	CHL	O2D-CGD-CBD	3.25	117.05	111.27
22	C	507	CLA	CMB-C2B-C1B	-3.25	120.41	125.37
26	V	317	CHL	O2A-CGA-CBA	3.25	122.11	111.91
26	P	319	CHL	CAC-C3C-C4C	3.25	129.03	124.81
22	p	309	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
26	3	315	CHL	C3D-C4D-ND	3.25	115.49	110.24
23	V	310	LUT	C35-C34-C33	-3.25	122.67	127.31
26	q	312	CHL	O2D-CGD-O1D	-3.25	117.49	123.84
26	q	313	CHL	C3D-C4D-ND	3.25	115.49	110.24
31	C	517	BCR	C8-C7-C6	-3.25	118.08	127.20
32	C	501	SQD	O5-C5-C4	3.25	115.59	109.69
26	5	315	CHL	C3D-C4D-ND	3.25	115.49	110.24
26	5	313	CHL	CAC-C3C-C4C	3.25	129.02	124.81
26	2	316	CHL	C3D-C4D-ND	3.24	115.49	110.24
26	2	316	CHL	C2D-C1D-ND	3.24	112.49	110.10
24	P	312	XAT	C35-C34-C33	-3.24	122.68	127.31
31	c	515	BCR	C8-C7-C6	-3.24	118.10	127.20
26	V	316	CHL	CMD-C2D-C3D	-3.24	120.16	127.61
26	2	313	CHL	C3B-C4B-NB	3.24	113.52	110.52
26	g	312	CHL	C2D-C1D-ND	3.23	112.49	110.10
26	N	313	CHL	C3D-C4D-ND	3.23	115.47	110.24
24	2	311	XAT	C27-C28-C29	-3.23	120.51	125.53
22	U	304	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
26	G	314	CHL	C3B-C4B-NB	3.23	113.51	110.52
24	2	311	XAT	C18-C5-C6	-3.23	116.84	122.26
22	u	304	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
26	1	318	CHL	C3D-C4D-ND	3.23	115.46	110.24
31	b	619	BCR	C38-C26-C27	3.23	119.82	113.62
32	l	102	SQD	C44-O6-C1	3.23	120.05	113.74
27	n	319	NEX	C39-C29-C30	-3.23	118.40	122.92
32	A	412	SQD	O9-S-C6	3.23	110.77	106.94
26	S	314	CHL	C1D-ND-C4D	-3.23	104.04	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	317	NEX	C17-C1-C6	-3.23	107.58	110.47
22	4	304	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
36	b	601	DGD	O2G-C1B-C2B	3.22	118.45	111.50
26	N	317	CHL	C3D-C4D-ND	3.22	115.45	110.24
22	P	309	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
26	5	316	CHL	C3B-C4B-NB	3.22	113.50	110.52
26	1	314	CHL	C4A-NA-C1A	3.22	108.15	106.71
26	U	319	CHL	C3B-C4B-NB	3.22	113.50	110.52
27	u	319	NEX	C2-C1-C6	3.22	112.34	109.21
26	G	313	CHL	C3D-C4D-ND	3.22	115.44	110.24
26	p	315	CHL	O2D-CGD-CBD	3.22	116.99	111.27
26	2	316	CHL	C3B-C4B-NB	3.22	113.50	110.52
22	A	408	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
32	a	410	SQD	O5-C5-C4	3.22	115.54	109.69
22	c	506	CLA	CMB-C2B-C1B	-3.22	120.47	125.37
26	Q	314	CHL	CAC-C3C-C4C	3.22	128.98	124.81
26	G	312	CHL	CHD-C4C-C3C	-3.22	120.11	124.84
26	p	317	CHL	CAC-C3C-C4C	3.22	128.98	124.81
34	D	408	LMG	O7-C10-C11	3.22	118.43	111.50
26	5	314	CHL	CAC-C3C-C4C	3.21	128.98	124.81
26	v	314	CHL	CHB-C1B-NB	-3.21	120.85	124.26
22	1	304	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
26	g	316	CHL	CHB-C1B-NB	-3.21	120.86	124.26
31	z	101	BCR	C33-C5-C4	3.21	119.79	113.62
26	6	313	CHL	CAC-C3C-C4C	3.21	128.98	124.81
26	n	315	CHL	C3B-C4B-NB	3.21	113.50	110.52
27	S	317	NEX	C2-C1-C6	3.21	112.33	109.21
26	6	317	CHL	CMD-C2D-C3D	-3.21	120.23	127.61
22	N	304	CLA	CHB-C4A-NA	3.21	128.95	124.51
26	g	314	CHL	CHD-C4C-C3C	-3.21	120.13	124.84
26	n	315	CHL	CMB-C2B-C1B	3.20	130.25	125.37
31	B	619	BCR	C38-C26-C27	3.20	119.77	113.62
26	P	317	CHL	CAC-C3C-C4C	3.20	128.97	124.81
26	N	315	CHL	CMB-C2B-C1B	3.20	130.25	125.37
26	U	315	CHL	C3D-C4D-ND	3.20	115.42	110.24
26	4	315	CHL	CHD-C4C-C3C	-3.20	120.14	124.84
31	C	516	BCR	C33-C5-C4	3.20	119.76	113.62
24	N	311	XAT	C38-C25-C26	-3.20	116.90	122.26
23	p	310	LUT	C11-C10-C9	-3.20	122.75	127.31
31	C	516	BCR	C21-C20-C19	-3.20	113.24	123.22
26	n	317	CHL	C3B-C4B-NB	3.20	113.48	110.52
22	p	306	CLA	CHB-C4A-NA	3.20	128.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	309	XAT	C18-C5-C6	-3.20	116.91	122.26
26	p	317	CHL	CMD-C2D-C3D	-3.20	120.26	127.61
26	3	316	CHL	C1D-ND-C4D	-3.19	104.07	106.33
26	2	318	CHL	CHB-C1B-NB	-3.19	120.88	124.26
26	U	319	CHL	C1D-ND-C4D	-3.19	104.07	106.33
31	b	618	BCR	C23-C24-C25	-3.19	118.24	127.20
26	s	313	CHL	C3D-C4D-ND	3.19	115.40	110.24
26	r	615	CHL	C1D-ND-C4D	-3.19	104.07	106.33
26	n	318	CHL	CMB-C2B-C1B	3.19	130.22	125.37
27	n	319	NEX	O24-C25-C38	3.19	118.87	115.06
23	1	310	LUT	C15-C14-C13	-3.19	122.76	127.31
22	u	303	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
26	n	317	CHL	C3D-C4D-ND	3.18	115.39	110.24
26	2	318	CHL	C1D-ND-C4D	-3.18	104.07	106.33
26	q	313	CHL	C1D-ND-C4D	-3.18	104.07	106.33
26	R	316	CHL	C1D-ND-C4D	-3.18	104.07	106.33
26	u	318	CHL	CHC-C4B-NB	-3.18	120.89	124.26
31	B	620	BCR	C20-C21-C22	-3.18	122.77	127.31
26	Q	316	CHL	C3D-C4D-ND	3.18	115.39	110.24
26	n	316	CHL	C1D-ND-C4D	-3.18	104.07	106.33
26	S	313	CHL	CMD-C2D-C3D	-3.18	120.29	127.61
26	r	614	CHL	C1D-ND-C4D	-3.18	104.08	106.33
26	Q	314	CHL	C3B-C4B-NB	3.18	113.47	110.52
26	Q	313	CHL	C1C-C2C-C3C	-3.18	104.59	107.11
26	V	315	CHL	C4A-NA-C1A	3.18	108.14	106.71
34	d	407	LMG	O7-C10-C11	3.18	118.35	111.50
31	B	618	BCR	C23-C24-C25	-3.18	118.28	127.20
26	G	315	CHL	C3D-C4D-ND	3.18	115.38	110.24
31	z	101	BCR	C21-C20-C19	-3.18	113.30	123.22
26	s	314	CHL	C3D-C4D-ND	3.18	115.38	110.24
26	5	318	CHL	CHB-C1B-NB	-3.18	120.89	124.26
32	L	102	SQD	C44-O6-C1	3.17	119.94	113.74
26	n	318	CHL	C3D-C4D-ND	3.17	115.37	110.24
26	3	316	CHL	CMD-C2D-C3D	-3.17	120.32	127.61
26	q	312	CHL	CAC-C3C-C4C	3.17	128.93	124.81
24	n	311	XAT	C35-C34-C33	-3.17	122.78	127.31
22	b	609	CLA	CMB-C2B-C1B	-3.17	120.54	125.37
26	Q	315	CHL	CAC-C3C-C4C	3.17	128.92	124.81
23	s	310	LUT	C30-C31-C32	-3.17	113.33	123.22
22	A	404	CLA	CMB-C2B-C1B	-3.17	120.55	125.37
31	C	517	BCR	C33-C5-C4	3.17	119.70	113.62
22	a	404	CLA	CMB-C2B-C1B	-3.16	120.55	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q	315	CHL	C3D-C4D-ND	3.16	115.36	110.24
26	3	316	CHL	C2D-C1D-ND	3.16	112.43	110.10
26	4	315	CHL	CAC-C3C-C4C	3.16	128.91	124.81
26	G	311	CHL	CHB-C4A-NA	3.16	128.88	124.51
26	r	619	CHL	C3D-C4D-ND	3.16	115.35	110.24
26	u	317	CHL	CHB-C1B-NB	-3.16	120.91	124.26
26	u	313	CHL	C1D-ND-C4D	-3.16	104.09	106.33
31	x	202	BCR	C38-C26-C27	3.16	119.68	113.62
26	1	313	CHL	C3D-C4D-ND	3.15	115.34	110.24
26	S	314	CHL	C3D-C4D-ND	3.15	115.34	110.24
24	1	311	XAT	C18-C5-C6	-3.15	116.97	122.26
24	q	309	XAT	C18-C5-C6	-3.15	116.97	122.26
26	U	317	CHL	CHB-C4A-NA	3.15	128.87	124.51
22	3	305	CLA	CHB-C4A-NA	3.15	128.87	124.51
26	S	316	CHL	C3D-C4D-ND	3.15	115.34	110.24
26	q	314	CHL	CAC-C3C-C4C	3.15	128.90	124.81
24	r	612	XAT	C10-C11-C12	-3.15	113.38	123.22
26	2	313	CHL	CAC-C3C-C4C	3.15	128.90	124.81
26	s	316	CHL	C3D-C4D-ND	3.15	115.33	110.24
26	3	313	CHL	CMB-C2B-C1B	3.15	130.17	125.37
26	s	313	CHL	CMD-C2D-C3D	-3.15	120.37	127.61
23	2	309	LUT	C11-C10-C9	-3.15	122.82	127.31
31	z	101	BCR	C29-C30-C25	3.15	115.33	110.48
26	u	318	CHL	CHB-C4A-NA	3.15	128.86	124.51
31	b	619	BCR	C27-C26-C25	-3.15	118.16	122.73
31	z	101	BCR	C27-C26-C25	-3.15	118.16	122.73
26	v	315	CHL	C3D-C4D-ND	3.14	115.32	110.24
26	P	314	CHL	C3D-C4D-ND	3.14	115.32	110.24
26	p	320	CHL	CAC-C3C-C4C	3.14	128.89	124.81
26	Q	316	CHL	CAC-C3C-C4C	3.14	128.89	124.81
22	b	608	CLA	CHB-C4A-NA	3.14	128.86	124.51
26	6	301	CHL	C3D-C4D-ND	3.14	115.32	110.24
26	P	319	CHL	C3D-C4D-ND	3.14	115.32	110.24
26	p	317	CHL	C3D-C4D-ND	3.14	115.32	110.24
27	r	618	NEX	C39-C29-C30	-3.14	118.52	122.92
26	n	316	CHL	CMB-C2B-C1B	3.14	130.15	125.37
31	c	515	BCR	C33-C5-C4	3.14	119.64	113.62
26	V	313	CHL	C2D-C1D-ND	3.14	112.42	110.10
24	g	309	XAT	C35-C34-C33	-3.14	122.83	127.31
22	N	308	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
26	V	313	CHL	CMD-C2D-C3D	-3.14	120.40	127.61
26	G	313	CHL	C1D-ND-C4D	-3.14	104.11	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	313	CHL	C3D-C4D-ND	3.14	115.31	110.24
26	U	316	CHL	O2A-CGA-CBA	3.13	121.75	111.91
31	x	202	BCR	C30-C25-C26	-3.13	118.20	122.61
26	v	317	CHL	CHC-C4B-NB	-3.13	120.94	124.26
23	u	309	LUT	C15-C14-C13	-3.13	122.84	127.31
22	x	201	CLA	CMB-C2B-C1B	-3.13	120.60	125.37
26	S	315	CHL	CHC-C4B-NB	-3.13	120.94	124.26
24	u	311	XAT	C26-C27-C28	-3.13	119.37	125.99
26	2	315	CHL	C1D-ND-C4D	-3.13	104.11	106.33
26	G	311	CHL	C1C-C2C-C3C	-3.13	104.63	107.11
25	d	406	LHG	O7-C7-C8	3.13	118.25	111.50
26	g	315	CHL	C3D-C4D-ND	3.13	115.30	110.24
31	b	619	BCR	C20-C21-C22	-3.13	122.85	127.31
26	g	314	CHL	CMB-C2B-C1B	3.13	130.13	125.37
26	G	311	CHL	C3D-C4D-ND	3.13	115.29	110.24
31	B	619	BCR	C27-C26-C25	-3.12	118.19	122.73
26	V	316	CHL	C3B-C4B-NB	3.12	113.41	110.52
22	q	307	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
26	N	317	CHL	C2D-C1D-ND	3.12	112.41	110.10
26	1	315	CHL	C3D-C4D-ND	3.12	115.29	110.24
26	V	315	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
26	1	316	CHL	C3D-C4D-ND	3.12	115.28	110.24
26	1	317	CHL	O1D-CGD-CBD	-3.12	118.10	124.48
31	c	516	BCR	C38-C26-C25	-3.12	121.03	124.53
26	1	315	CHL	C3B-C4B-NB	3.12	113.41	110.52
26	p	317	CHL	C1D-ND-C4D	-3.12	104.12	106.33
26	v	317	CHL	O2D-CGD-O1D	-3.12	117.75	123.84
26	p	320	CHL	CHB-C4A-NA	3.11	128.82	124.51
26	G	315	CHL	C3B-C4B-NB	3.11	113.40	110.52
26	n	316	CHL	C3D-C4D-ND	3.11	115.27	110.24
22	v	304	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
31	C	516	BCR	C23-C24-C25	-3.11	118.47	127.20
26	3	313	CHL	CHD-C4C-C3C	-3.11	120.27	124.84
26	6	301	CHL	C2D-C1D-ND	3.11	112.40	110.10
26	2	318	CHL	C1C-C2C-C3C	-3.11	104.65	107.11
22	p	306	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
26	P	318	CHL	CHB-C1B-NB	-3.11	120.97	124.26
22	5	304	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
26	3	315	CHL	C3B-C4B-NB	3.11	113.40	110.52
26	R	315	CHL	C3D-C4D-ND	3.11	115.26	110.24
23	V	310	LUT	C7-C8-C9	-3.11	121.54	126.23
31	C	518	BCR	C38-C26-C25	-3.10	121.04	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	U	311	XAT	C27-C28-C29	-3.10	120.72	125.53
26	G	312	CHL	C3B-C4B-NB	3.10	113.39	110.52
26	u	318	CHL	C3D-C4D-ND	3.10	115.25	110.24
26	p	318	CHL	C3D-C4D-ND	3.10	115.25	110.24
26	q	311	CHL	CMB-C2B-C1B	3.10	130.09	125.37
26	1	313	CHL	CMD-C2D-C3D	-3.10	120.48	127.61
27	u	319	NEX	C27-C28-C29	-3.10	120.72	125.53
31	C	516	BCR	C20-C21-C22	-3.10	122.89	127.31
22	6	302	CLA	CMB-C2B-C1B	-3.10	120.65	125.37
24	G	309	XAT	C30-C31-C32	-3.10	113.55	123.22
22	b	616	CLA	CHB-C4A-NA	3.10	128.80	124.51
26	g	313	CHL	C1D-ND-C4D	-3.10	104.13	106.33
26	Q	312	CHL	C3D-C4D-ND	3.10	115.25	110.24
26	6	317	CHL	CMB-C2B-C1B	3.10	130.08	125.37
26	6	312	CHL	CAC-C3C-C4C	3.10	128.83	124.81
22	X	202	CLA	CMB-C2B-C1B	-3.10	120.66	125.37
26	5	317	CHL	CHB-C4A-NA	3.10	128.79	124.51
25	D	407	LHG	O7-C7-C8	3.09	118.17	111.50
23	P	311	LUT	C31-C30-C29	-3.09	122.89	127.31
26	U	319	CHL	C3D-C4D-ND	3.09	115.24	110.24
22	C	514	CLA	C3B-C4B-NB	-3.09	107.65	110.52
26	p	317	CHL	CMB-C2B-C1B	3.09	130.07	125.37
31	z	101	BCR	C23-C24-C25	-3.09	118.53	127.20
26	P	318	CHL	C3D-C4D-ND	3.09	115.23	110.24
26	5	317	CHL	CMB-C2B-C1B	3.09	130.07	125.37
26	v	315	CHL	CMB-C2B-C1B	3.09	130.07	125.37
31	c	516	BCR	C30-C25-C26	-3.09	118.26	122.61
23	S	311	LUT	C35-C34-C33	-3.09	122.90	127.31
31	X	201	BCR	C38-C26-C27	3.09	119.55	113.62
26	5	318	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
31	K	101	BCR	C8-C7-C6	-3.09	118.54	127.20
23	1	309	LUT	C7-C8-C9	-3.09	121.57	126.23
22	p	308	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
26	q	311	CHL	CHB-C1B-NB	-3.09	120.99	124.26
26	r	614	CHL	C3D-C4D-ND	3.08	115.23	110.24
26	p	319	CHL	C3D-C4D-ND	3.08	115.23	110.24
31	b	618	BCR	C21-C20-C19	-3.08	113.59	123.22
26	s	315	CHL	CHD-C4C-C3C	-3.08	120.31	124.84
31	k	101	BCR	C8-C7-C6	-3.08	118.54	127.20
26	u	314	CHL	CHB-C1B-NB	-3.08	120.99	124.26
27	2	319	NEX	C11-C12-C13	-3.08	117.76	126.42
26	P	317	CHL	C2D-C1D-ND	3.08	112.38	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	315	CHL	CAC-C3C-C4C	3.08	128.81	124.81
22	B	616	CLA	CHB-C4A-NA	3.08	128.77	124.51
22	4	308	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
26	p	318	CHL	CHB-C1B-NB	-3.08	121.00	124.26
26	n	313	CHL	C3D-C4D-ND	3.08	115.22	110.24
26	U	316	CHL	CHB-C1B-NB	-3.08	121.00	124.26
26	v	313	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
31	B	620	BCR	C10-C11-C12	-3.08	113.62	123.22
26	V	315	CHL	CAC-C3C-C4C	3.08	128.80	124.81
26	S	313	CHL	C3B-C4B-NB	3.08	113.37	110.52
32	M	101	SQD	C4-C3-C2	3.07	116.19	110.82
26	S	313	CHL	C2D-C1D-ND	3.07	112.37	110.10
22	q	308	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	C	505	CLA	C3B-C4B-NB	-3.07	107.67	110.52
26	v	314	CHL	C3D-C4D-ND	3.07	115.21	110.24
22	V	304	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
27	r	618	NEX	C5-C4-C3	3.07	115.38	111.75
26	g	313	CHL	C3D-C4D-ND	3.07	115.20	110.24
26	2	315	CHL	C3D-C4D-ND	3.07	115.20	110.24
22	p	305	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	C	506	CLA	CHB-C4A-NA	3.07	128.76	124.51
22	B	608	CLA	CHB-C4A-NA	3.07	128.75	124.51
22	c	505	CLA	CHB-C4A-NA	3.07	128.75	124.51
23	2	310	LUT	C11-C10-C9	-3.07	122.93	127.31
26	U	316	CHL	O1D-CGD-CBD	-3.07	118.21	124.48
22	P	302	CLA	CMB-C2B-C1B	-3.07	120.70	125.37
22	1	308	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
26	5	316	CHL	C2D-C1D-ND	3.07	112.36	110.10
31	b	618	BCR	C38-C26-C27	3.07	119.51	113.62
26	5	316	CHL	CMD-C2D-C3D	-3.07	120.56	127.61
31	t	101	BCR	C4-C5-C6	-3.07	118.28	122.73
22	P	302	CLA	C3B-C4B-NB	-3.06	107.67	110.52
26	1	316	CHL	C1D-ND-C4D	-3.06	104.16	106.33
31	C	518	BCR	C30-C25-C26	-3.06	118.30	122.61
22	N	301	CLA	C3B-C4B-NB	-3.06	107.67	110.52
26	5	318	CHL	C4-C3-C5	3.06	120.42	115.27
26	U	313	CHL	C2D-C1D-ND	3.06	112.36	110.10
22	n	304	CLA	CMA-C3A-C4A	-3.06	103.54	111.77
23	n	309	LUT	C15-C14-C13	-3.06	122.94	127.31
31	B	620	BCR	C23-C24-C25	-3.06	118.60	127.20
31	B	618	BCR	C38-C26-C27	3.06	119.50	113.62
22	c	513	CLA	C3B-C4B-NB	-3.06	107.67	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	317	CHL	C3D-C4D-ND	3.06	115.19	110.24
26	S	315	CHL	CHD-C4C-C3C	-3.06	120.34	124.84
23	V	309	LUT	C15-C14-C13	-3.06	122.94	127.31
33	D	405	PL9	C17-C18-C19	-3.06	120.30	127.66
32	m	101	SQD	C4-C3-C2	3.06	116.16	110.82
26	3	312	CHL	CAC-C3C-C4C	3.06	128.78	124.81
26	V	318	CHL	C3D-C4D-ND	3.06	115.18	110.24
26	2	316	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
31	T	101	BCR	C4-C5-C6	-3.06	118.29	122.73
26	2	313	CHL	C3D-C4D-ND	3.06	115.18	110.24
26	U	316	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
26	4	315	CHL	C3B-C4B-NB	3.05	113.35	110.52
22	r	609	CLA	CHB-C4A-NA	3.05	128.74	124.51
26	v	314	CHL	CHB-C4A-NA	3.05	128.74	124.51
22	N	303	CLA	CHB-C4A-NA	3.05	128.73	124.51
31	X	201	BCR	C30-C25-C26	-3.05	118.31	122.61
31	z	101	BCR	C20-C21-C22	-3.05	122.95	127.31
31	T	101	BCR	C27-C26-C25	-3.05	118.30	122.73
22	5	305	CLA	CHB-C4A-NA	3.05	128.73	124.51
26	v	316	CHL	CHB-C1B-NB	-3.05	121.03	124.26
26	4	315	CHL	C3D-C4D-ND	3.05	115.17	110.24
26	6	314	CHL	C3D-C4D-ND	3.05	115.17	110.24
26	V	315	CHL	C3D-C4D-ND	3.05	115.17	110.24
23	5	310	LUT	C11-C10-C9	-3.05	122.96	127.31
22	c	504	CLA	C3B-C4B-NB	-3.05	107.69	110.52
26	4	314	CHL	C3D-C4D-ND	3.05	115.17	110.24
26	5	313	CHL	C4-C3-C5	3.05	120.40	115.27
26	q	311	CHL	C4-C3-C5	3.05	120.40	115.27
23	V	310	LUT	C15-C35-C34	-3.05	117.23	123.47
26	P	316	CHL	C3D-C4D-ND	3.05	115.17	110.24
22	Q	301	CLA	C3B-C4B-NB	-3.05	107.69	110.52
26	U	315	CHL	CMB-C2B-C1B	3.05	130.01	125.37
26	g	311	CHL	CMB-C2B-C1B	3.05	130.01	125.37
26	N	313	CHL	C1C-C2C-C3C	-3.04	104.70	107.11
26	n	315	CHL	C3D-C4D-ND	3.04	115.16	110.24
22	B	609	CLA	CMB-C2B-C1B	-3.04	120.73	125.37
26	P	318	CHL	CHB-C4A-NA	3.04	128.72	124.51
26	n	315	CHL	C2D-C1D-ND	3.04	112.35	110.10
23	1	310	LUT	C16-C1-C6	-3.04	105.36	110.30
22	c	510	CLA	CHB-C4A-NA	3.04	128.72	124.51
26	u	317	CHL	O2A-CGA-CBA	3.04	121.46	111.91
32	l	102	SQD	C3-C4-C5	3.04	115.67	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	R	312	LUT	C15-C14-C13	-3.04	122.97	127.31
26	v	316	CHL	CMD-C2D-C3D	-3.04	120.62	127.61
26	q	311	CHL	CHB-C4A-NA	3.04	128.72	124.51
26	Q	316	CHL	C1D-ND-C4D	-3.04	104.17	106.33
26	g	311	CHL	C3D-C4D-ND	3.04	115.16	110.24
26	2	318	CHL	C4-C3-C5	3.04	120.38	115.27
26	U	317	CHL	C3D-C4D-ND	3.04	115.15	110.24
22	P	306	CLA	CHB-C4A-NA	3.04	128.71	124.51
22	N	304	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
26	1	313	CHL	C2D-C1D-ND	3.04	112.34	110.10
26	r	619	CHL	CHB-C4A-NA	3.04	128.71	124.51
22	x	201	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	n	304	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	C	511	CLA	CHB-C4A-NA	3.04	128.71	124.51
26	Q	313	CHL	C1D-ND-C4D	-3.04	104.18	106.33
26	q	312	CHL	CMB-C2B-C1B	3.04	129.99	125.37
22	p	305	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
31	c	515	BCR	C21-C20-C19	-3.03	113.75	123.22
26	P	317	CHL	CMB-C2B-C1B	3.03	129.99	125.37
26	u	313	CHL	C1C-C2C-C3C	-3.03	104.71	107.11
31	b	618	BCR	C40-C30-C25	-3.03	105.38	110.30
26	s	315	CHL	CAC-C3C-C4C	3.03	128.75	124.81
26	u	313	CHL	CMB-C2B-C1B	3.03	129.99	125.37
24	g	309	XAT	C30-C31-C32	-3.03	113.75	123.22
26	2	318	CHL	CMB-C2B-C1B	3.03	129.99	125.37
22	2	304	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	U	314	CHL	C3D-C4D-ND	3.03	115.14	110.24
22	c	509	CLA	C3B-C4B-NB	-3.03	107.70	110.52
26	U	313	CHL	C3B-C4B-NB	3.03	113.33	110.52
26	4	313	CHL	C3D-C4D-ND	3.03	115.14	110.24
26	1	314	CHL	CHC-C4B-NB	-3.03	121.05	124.26
22	6	309	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	4	310	LUT	C15-C14-C13	-3.03	122.99	127.31
31	b	620	BCR	C23-C24-C25	-3.03	118.69	127.20
22	6	306	CLA	CHB-C4A-NA	3.03	128.70	124.51
26	S	316	CHL	CMD-C2D-C3D	-3.03	120.65	127.61
31	b	618	BCR	C15-C16-C17	-3.03	117.27	123.47
26	3	311	CHL	CHB-C4A-NA	3.03	128.70	124.51
22	Q	301	CLA	CMB-C2B-C1B	-3.03	120.76	125.37
26	v	313	CHL	C1D-ND-C4D	-3.03	104.19	106.33
23	S	310	LUT	C30-C31-C32	-3.02	113.78	123.22
26	p	316	CHL	C3B-C4B-NB	3.02	113.32	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	316	CHL	CHB-C4A-NA	3.02	128.69	124.51
23	V	310	LUT	C15-C14-C13	-3.02	122.99	127.31
27	u	320	NEX	C35-C34-C33	-3.02	122.99	127.31
22	P	305	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	5	313	CHL	C3D-C4D-ND	3.02	115.13	110.24
26	4	313	CHL	C3B-C4B-NB	3.02	113.32	110.52
27	n	319	NEX	C16-C1-C6	3.02	113.18	110.47
26	p	315	CHL	C3D-C4D-ND	3.02	115.13	110.24
26	g	315	CHL	O2A-CGA-CBA	3.02	121.39	111.91
26	g	316	CHL	CMB-C2B-C1B	3.02	129.97	125.37
26	6	317	CHL	CHB-C4A-NA	3.02	128.69	124.51
23	s	311	LUT	C15-C14-C13	-3.02	123.00	127.31
24	3	309	XAT	C31-C30-C29	-3.02	123.00	127.31
26	P	319	CHL	C1C-C2C-C3C	-3.02	104.72	107.11
22	C	513	CLA	CHB-C4A-NA	3.02	128.69	124.51
26	1	318	CHL	CMB-C2B-C1B	3.02	129.97	125.37
26	n	313	CHL	C1D-ND-C4D	-3.02	104.19	106.33
22	R	308	CLA	CHB-C4A-NA	3.02	128.69	124.51
22	2	306	CLA	CMB-C2B-C1B	-3.02	120.77	125.37
26	u	316	CHL	CMB-C2B-C1B	3.02	129.97	125.37
31	D	404	BCR	C8-C7-C6	-3.02	118.73	127.20
26	6	316	CHL	CMB-C2B-C1B	3.02	129.96	125.37
26	6	301	CHL	C1D-ND-C4D	-3.02	104.19	106.33
26	1	318	CHL	CHB-C4A-NA	3.02	128.68	124.51
26	G	316	CHL	CHB-C1B-NB	-3.02	121.06	124.26
33	d	404	PL9	C17-C18-C19	-3.01	120.40	127.66
26	n	317	CHL	CMB-C2B-C1B	3.01	129.96	125.37
26	6	316	CHL	CAC-C3C-C4C	3.01	128.72	124.81
26	v	317	CHL	O1D-CGD-CBD	-3.01	118.32	124.48
26	s	316	CHL	CMD-C2D-C3D	-3.01	120.68	127.61
24	G	309	XAT	C10-C11-C12	-3.01	113.82	123.22
26	v	318	CHL	C3D-C4D-ND	3.01	115.11	110.24
22	3	301	CLA	CMB-C2B-C1B	-3.01	120.78	125.37
26	v	313	CHL	C3B-C4B-NB	3.01	113.31	110.52
23	n	309	LUT	C18-C5-C6	-3.01	121.15	124.53
26	p	314	CHL	C3B-C4B-NB	3.01	113.31	110.52
26	P	316	CHL	C3B-C4B-NB	3.01	113.31	110.52
26	U	319	CHL	CMB-C2B-C1B	3.01	129.95	125.37
26	g	315	CHL	C3B-C4B-NB	3.01	113.31	110.52
22	X	202	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	2	308	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	Q	304	CLA	CHB-C4A-NA	3.00	128.67	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	309	LUT	C11-C10-C9	-3.00	123.02	127.31
26	R	317	CHL	C2D-C1D-ND	3.00	112.32	110.10
26	G	315	CHL	CHC-C4B-NB	-3.00	121.08	124.26
36	J	101	DGD	O1G-C1A-C2A	3.00	121.33	111.91
31	a	409	BCR	C38-C26-C25	-3.00	121.16	124.53
27	P	301	NEX	C11-C10-C9	-3.00	123.03	127.31
31	T	101	BCR	C20-C19-C18	-3.00	117.98	126.42
26	2	313	CHL	C4A-NA-C1A	3.00	108.06	106.71
26	r	615	CHL	C3D-C4D-ND	3.00	115.09	110.24
33	D	405	PL9	C22-C23-C24	-3.00	120.44	127.66
25	c	523	LHG	O8-C23-C24	3.00	121.32	111.91
26	V	316	CHL	C3D-C4D-ND	3.00	115.09	110.24
22	3	308	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
26	G	312	CHL	CHC-C4B-NB	-3.00	121.08	124.26
26	Q	311	CHL	CMB-C2B-C1B	3.00	129.94	125.37
31	d	403	BCR	C8-C7-C6	-3.00	118.78	127.20
33	d	404	PL9	C22-C23-C24	-3.00	120.44	127.66
26	v	313	CHL	C1-C2-C3	-3.00	120.86	126.04
26	3	313	CHL	CAC-C3C-C4C	3.00	128.70	124.81
26	Q	312	CHL	O2D-CGD-O1D	-3.00	117.98	123.84
26	N	315	CHL	C3D-C4D-ND	3.00	115.08	110.24
22	c	507	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
26	U	314	CHL	C1D-ND-C4D	-2.99	104.21	106.33
31	C	516	BCR	C29-C30-C25	2.99	115.09	110.48
26	N	317	CHL	CHD-C4C-C3C	-2.99	120.44	124.84
26	s	315	CHL	CHC-C4B-NB	-2.99	121.09	124.26
26	G	311	CHL	C4-C3-C5	2.99	120.30	115.27
26	g	314	CHL	C3B-C4B-NB	2.99	113.29	110.52
33	D	405	PL9	C12-C13-C14	-2.99	120.46	127.66
26	q	311	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
33	d	404	PL9	C12-C13-C14	-2.99	120.46	127.66
26	4	316	CHL	CMB-C2B-C1B	2.99	129.92	125.37
26	U	317	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
23	4	309	LUT	C31-C30-C29	-2.99	123.05	127.31
22	b	610	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
32	L	102	SQD	C3-C4-C5	2.99	115.57	110.24
26	V	317	CHL	CHB-C1B-NB	-2.99	121.10	124.26
26	s	315	CHL	C3D-C4D-ND	2.99	115.07	110.24
26	3	315	CHL	O2A-CGA-CBA	2.98	121.28	111.91
26	1	314	CHL	CMB-C2B-C1B	2.98	129.91	125.37
26	1	315	CHL	CAC-C3C-C4C	2.98	128.68	124.81
26	q	314	CHL	CMB-C2B-C1B	2.98	129.91	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	313	CHL	CMD-C2D-C3D	-2.98	120.75	127.61
26	p	316	CHL	C3D-C4D-ND	2.98	115.06	110.24
22	C	510	CLA	CHB-C1B-NB	2.98	127.41	124.26
22	U	308	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	c	512	CLA	CHB-C4A-NA	2.98	128.63	124.51
24	Q	309	XAT	C7-C8-C9	-2.98	120.90	125.53
22	B	610	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
36	c	519	DGD	O1G-C1A-C2A	2.98	121.26	111.91
22	B	611	CLA	CHB-C4A-NA	2.98	128.63	124.51
22	P	306	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	4	314	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
22	4	307	CLA	CHB-C4A-NA	2.98	128.63	124.51
27	5	319	NEX	C11-C12-C13	-2.98	118.05	126.42
26	u	317	CHL	CMB-C2B-C1B	2.98	129.90	125.37
24	r	612	XAT	C35-C15-C14	-2.98	117.38	123.47
26	q	315	CHL	C1D-ND-C4D	-2.98	104.22	106.33
22	q	304	CLA	CMB-C2B-C1B	-2.98	120.84	125.37
26	2	317	CHL	CHB-C4A-NA	2.98	128.63	124.51
36	A	414	DGD	C3E-C4E-C5E	2.97	115.55	110.24
26	p	319	CHL	C1D-ND-C4D	-2.97	104.22	106.33
26	V	316	CHL	CMB-C2B-C1B	2.97	129.90	125.37
22	C	509	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	C	503	CLA	C3B-C4B-NB	-2.97	107.76	110.52
26	Q	316	CHL	CMD-C2D-C3D	-2.97	120.77	127.61
26	S	315	CHL	C3D-C4D-ND	2.97	115.05	110.24
26	6	316	CHL	O2A-CGA-CBA	2.97	121.24	111.91
31	C	517	BCR	C21-C20-C19	-2.97	113.94	123.22
22	u	301	CLA	CHB-C1B-NB	2.97	127.40	124.26
26	P	314	CHL	CAC-C3C-C4C	2.97	128.67	124.81
26	V	314	CHL	CMB-C2B-C1B	2.97	129.90	125.37
22	2	305	CLA	CHB-C4A-NA	2.97	128.62	124.51
26	G	311	CHL	CMB-C2B-C1B	2.97	129.89	125.37
22	p	302	CLA	C3B-C4B-NB	-2.97	107.76	110.52
22	A	408	CLA	CMB-C2B-C3B	2.97	133.78	126.59
25	Q	310	LHG	O8-C23-C24	2.97	121.22	111.91
31	A	409	BCR	C20-C21-C22	-2.97	123.07	127.31
26	V	317	CHL	O1D-CGD-CBD	-2.97	118.41	124.48
26	q	313	CHL	C1C-C2C-C3C	-2.97	104.76	107.11
26	2	317	CHL	CMB-C2B-C1B	2.97	129.89	125.37
22	n	305	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
27	r	618	NEX	C35-C34-C33	-2.97	123.08	127.31
22	b	611	CLA	CHB-C4A-NA	2.97	128.61	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	304	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
26	q	315	CHL	CMD-C2D-C3D	-2.96	120.79	127.61
26	N	314	CHL	C3B-C4B-NB	2.96	113.27	110.52
24	N	311	XAT	C10-C11-C12	-2.96	113.97	123.22
22	5	303	CLA	CHB-C4A-NA	2.96	128.61	124.51
22	V	303	CLA	CHB-C4A-NA	2.96	128.61	124.51
26	r	614	CHL	C4-C3-C5	2.96	120.25	115.27
26	5	315	CHL	CHB-C1B-NB	-2.96	121.12	124.26
26	p	320	CHL	CHB-C1B-NB	-2.96	121.12	124.26
22	C	508	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	P	310	LUT	C11-C10-C9	-2.96	123.09	127.31
22	Q	308	CLA	CHB-C4A-NA	2.96	128.60	124.51
23	S	311	LUT	C15-C14-C13	-2.96	123.09	127.31
26	R	317	CHL	C3D-C4D-ND	2.96	115.02	110.24
26	S	315	CHL	CAC-C3C-C4C	2.96	128.65	124.81
22	C	510	CLA	C3B-C4B-NB	-2.96	107.77	110.52
26	V	313	CHL	C3B-C4B-NB	2.96	113.26	110.52
26	P	315	CHL	C3D-C4D-ND	2.96	115.02	110.24
24	u	311	XAT	C11-C10-C9	-2.96	123.09	127.31
22	5	308	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	5	301	CLA	CMB-C2B-C1B	-2.96	120.87	125.37
26	4	317	CHL	CMB-C2B-C1B	2.95	129.87	125.37
31	k	101	BCR	C33-C5-C4	2.95	119.29	113.62
26	n	318	CHL	C2D-C1D-ND	2.95	112.28	110.10
26	s	314	CHL	CMD-C2D-C3D	-2.95	120.82	127.61
26	6	315	CHL	CMB-C2B-C1B	2.95	129.87	125.37
26	g	312	CHL	CMB-C2B-C1B	2.95	129.87	125.37
26	G	312	CHL	CMD-C2D-C3D	-2.95	120.82	127.61
22	a	408	CLA	CMB-C2B-C3B	2.95	133.74	126.59
26	S	316	CHL	C4A-NA-C1A	2.95	108.03	106.71
22	P	305	CLA	CHB-C4A-NA	2.95	128.59	124.51
26	U	313	CHL	C1D-ND-C4D	-2.95	104.24	106.33
22	c	506	CLA	CHB-C4A-NA	2.95	128.59	124.51
24	g	309	XAT	C10-C11-C12	-2.95	114.01	123.22
26	s	313	CHL	C2D-C1D-ND	2.95	112.28	110.10
26	g	315	CHL	CHC-C4B-NB	-2.95	121.13	124.26
26	P	319	CHL	CMB-C2B-C1B	2.95	129.86	125.37
22	c	502	CLA	C3B-C4B-NB	-2.95	107.78	110.52
26	u	315	CHL	C3D-C4D-ND	2.95	115.01	110.24
24	P	312	XAT	C11-C10-C9	-2.95	123.10	127.31
31	B	619	BCR	C20-C21-C22	-2.95	123.10	127.31
22	c	508	CLA	CHB-C4A-NA	2.95	128.59	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	312	CHL	O2D-CGD-O1D	-2.95	118.07	123.84
26	v	318	CHL	CMB-C2B-C1B	2.95	129.86	125.37
26	U	315	CHL	O2A-CGA-CBA	2.95	121.16	111.91
26	1	317	CHL	O2D-CGD-O1D	-2.95	118.08	123.84
31	t	101	BCR	C20-C19-C18	-2.95	118.14	126.42
26	q	311	CHL	CMD-C2D-C3D	-2.95	120.84	127.61
32	a	413	SQD	O9-S-C6	2.95	110.44	106.94
22	1	302	CLA	C3B-C4B-NB	-2.94	107.78	110.52
26	u	313	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
26	S	314	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
26	1	313	CHL	C1-C2-C3	-2.94	120.95	126.04
22	D	403	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
26	G	316	CHL	CMB-C2B-C1B	2.94	129.85	125.37
26	s	315	CHL	C4A-NA-C1A	2.94	108.03	106.71
22	2	302	CLA	C3B-C4B-NB	-2.94	107.78	110.52
22	C	507	CLA	CHB-C4A-NA	2.94	128.58	124.51
26	3	314	CHL	CMB-C2B-C1B	2.94	129.85	125.37
31	d	403	BCR	C30-C25-C24	2.94	124.10	115.78
22	3	302	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	1	309	LUT	C31-C30-C29	-2.94	123.11	127.31
22	u	308	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
26	Q	315	CHL	CHB-C1B-NB	-2.94	121.14	124.26
22	U	301	CLA	CHB-C1B-NB	2.94	127.37	124.26
22	n	305	CLA	CHB-C4A-NA	2.94	128.58	124.51
26	u	315	CHL	CAC-C3C-C4C	2.94	128.62	124.81
26	2	313	CHL	C2D-C1D-ND	2.94	112.27	110.10
26	q	312	CHL	CMD-C2D-C3D	-2.94	120.86	127.61
23	2	309	LUT	C30-C31-C32	-2.94	114.05	123.22
31	K	101	BCR	C33-C5-C4	2.94	119.26	113.62
26	6	312	CHL	CMD-C2D-C3D	-2.94	120.86	127.61
31	b	620	BCR	C15-C16-C17	-2.94	117.46	123.47
22	a	408	CLA	CHB-C4A-NA	2.94	128.57	124.51
26	v	315	CHL	CAC-C3C-C4C	2.94	128.62	124.81
22	p	302	CLA	CMB-C2B-C1B	-2.94	120.90	125.37
22	N	301	CLA	CMB-C2B-C1B	-2.94	120.90	125.37
22	g	308	CLA	C3B-C4B-NB	-2.94	107.79	110.52
26	p	319	CHL	C1C-C2C-C3C	-2.93	104.78	107.11
26	p	319	CHL	CMB-C2B-C1B	2.93	129.84	125.37
31	c	515	BCR	C23-C24-C25	-2.93	118.96	127.20
23	S	310	LUT	C35-C15-C14	-2.93	117.46	123.47
26	G	312	CHL	C2D-C1D-ND	2.93	112.27	110.10
26	4	315	CHL	CMB-C2B-C1B	2.93	129.84	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	311	XAT	C35-C34-C33	-2.93	123.12	127.31
26	R	317	CHL	CHC-C4B-NB	-2.93	121.15	124.26
22	2	307	CLA	CHB-C4A-NA	2.93	128.57	124.51
23	U	310	LUT	C38-C25-C24	-2.93	117.29	123.56
31	B	618	BCR	C21-C20-C19	-2.93	114.07	123.22
26	3	315	CHL	CAC-C3C-C4C	2.93	128.61	124.81
22	g	305	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	1	316	CHL	CMB-C2B-C1B	2.93	129.83	125.37
26	q	315	CHL	CAC-C3C-C4C	2.93	128.61	124.81
26	U	314	CHL	CAC-C3C-C4C	2.93	128.61	124.81
26	6	312	CHL	CHB-C4A-NA	2.93	128.56	124.51
22	N	307	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	r	616	CHL	CHC-C4B-NB	-2.93	121.16	124.26
24	R	313	XAT	C10-C11-C12	-2.93	114.08	123.22
26	p	315	CHL	CHD-C4C-C3C	-2.93	120.54	124.84
22	g	303	CLA	C3B-C4B-NB	-2.93	107.80	110.52
26	v	315	CHL	C3B-C4B-NB	2.93	113.23	110.52
26	p	316	CHL	C2D-C1D-ND	2.93	112.26	110.10
33	d	404	PL9	C42-C43-C44	-2.93	120.61	127.66
31	C	517	BCR	C23-C24-C25	-2.93	118.98	127.20
22	b	606	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
31	a	409	BCR	C20-C21-C22	-2.93	123.14	127.31
22	B	602	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	u	313	CHL	C1-C2-C3	-2.93	120.98	126.04
26	V	315	CHL	CMB-C2B-C1B	2.92	129.82	125.37
22	P	308	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
31	D	404	BCR	C30-C25-C24	2.92	124.05	115.78
26	u	317	CHL	CHB-C4A-NA	2.92	128.55	124.51
26	Q	316	CHL	O2A-CGA-CBA	2.92	121.08	111.91
26	3	311	CHL	CHB-C1B-NB	-2.92	121.16	124.26
26	R	316	CHL	C3D-C4D-ND	2.92	114.97	110.24
22	4	308	CLA	CHB-C4A-NA	2.92	128.55	124.51
36	a	416	DGD	C3E-C4E-C5E	2.92	115.45	110.24
26	s	315	CHL	CMB-C2B-C1B	2.92	129.82	125.37
26	s	316	CHL	C4A-NA-C1A	2.92	108.02	106.71
22	R	306	CLA	CHB-C4A-NA	2.92	128.55	124.51
26	p	318	CHL	CMB-C2B-C1B	2.92	129.82	125.37
26	r	615	CHL	CMB-C2B-C1B	2.92	129.81	125.37
26	g	311	CHL	C1C-C2C-C3C	-2.92	104.80	107.11
26	P	314	CHL	O2A-CGA-CBA	2.92	121.06	111.91
36	c	518	DGD	O1G-C1A-C2A	2.92	121.06	111.91
26	r	616	CHL	C3D-C4D-ND	2.92	114.96	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	313	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
26	U	313	CHL	CMB-C2B-C1B	2.92	129.81	125.37
22	b	615	CLA	CHB-C4A-NA	2.92	128.54	124.51
26	N	316	CHL	CMB-C2B-C1B	2.92	129.81	125.37
26	g	313	CHL	CMB-C2B-C1B	2.92	129.81	125.37
33	d	404	PL9	C37-C38-C39	-2.92	120.64	127.66
22	r	605	CLA	CHB-C4A-NA	2.92	128.54	124.51
27	s	317	NEX	C17-C1-C6	-2.91	107.86	110.47
26	S	315	CHL	C4A-NA-C1A	2.91	108.02	106.71
26	5	313	CHL	C3B-C4B-NB	2.91	113.22	110.52
22	G	303	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	2	316	CHL	CMB-C2B-C1B	2.91	129.81	125.37
26	G	312	CHL	CMB-C2B-C1B	2.91	129.81	125.37
30	a	407	PHO	C2D-C1D-ND	-2.91	107.52	109.53
22	c	509	CLA	CHB-C1B-NB	2.91	127.34	124.26
26	r	616	CHL	C2D-C1D-ND	2.91	112.25	110.10
33	D	405	PL9	C37-C38-C39	-2.91	120.65	127.66
31	t	101	BCR	C27-C26-C25	-2.91	118.50	122.73
22	r	607	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	g	312	CHL	C3D-C4D-ND	2.91	114.95	110.24
26	Q	313	CHL	O2A-CGA-CBA	2.91	121.04	111.91
24	U	311	XAT	C10-C11-C12	-2.91	114.14	123.22
22	G	305	CLA	CHB-C4A-NA	2.91	128.54	124.51
22	b	602	CLA	CHB-C4A-NA	2.91	128.54	124.51
31	c	516	BCR	C8-C7-C6	-2.91	119.03	127.20
30	D	401	PHO	O2D-CGD-O1D	-2.91	118.15	123.84
26	P	314	CHL	C3B-C4B-NB	2.91	113.21	110.52
26	S	315	CHL	CMB-C2B-C1B	2.91	129.80	125.37
22	d	402	CLA	C3B-C4B-NB	-2.91	107.82	110.52
26	s	313	CHL	C3B-C4B-NB	2.91	113.21	110.52
22	1	307	CLA	CHB-C4A-NA	2.91	128.53	124.51
26	Q	311	CHL	CHB-C4A-NA	2.91	128.53	124.51
26	V	313	CHL	CMB-C2B-C1B	2.91	129.80	125.37
26	1	317	CHL	CMB-C2B-C1B	2.91	129.79	125.37
25	C	524	LHG	O8-C23-C24	2.91	121.03	111.91
33	D	405	PL9	C42-C43-C44	-2.90	120.67	127.66
22	b	617	CLA	CHB-C4A-NA	2.90	128.53	124.51
22	2	304	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
26	Q	311	CHL	CHB-C1B-NB	-2.90	121.18	124.26
22	n	306	CLA	CMB-C2B-C1B	-2.90	120.95	125.37
22	d	402	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
26	q	315	CHL	O2A-CGA-CBA	2.90	121.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	617	CLA	C3B-C4B-NB	-2.90	107.83	110.52
26	n	316	CHL	CMD-C2D-C3D	-2.90	120.94	127.61
26	V	317	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
26	V	313	CHL	C1D-ND-C4D	-2.90	104.28	106.33
26	U	319	CHL	CMD-C2D-C3D	-2.90	120.95	127.61
26	Q	314	CHL	C3D-C4D-ND	2.90	114.92	110.24
26	R	317	CHL	CMD-C2D-C3D	-2.90	120.95	127.61
22	b	617	CLA	C2A-C1A-CHA	2.90	128.93	123.86
22	B	610	CLA	CHB-C4A-NA	2.90	128.52	124.51
31	b	620	BCR	C10-C11-C12	-2.90	114.18	123.22
22	G	308	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
26	G	311	CHL	CHB-C1B-NB	-2.90	121.19	124.26
26	2	313	CHL	CMD-C2D-C3D	-2.89	120.95	127.61
22	N	301	CLA	CHB-C1B-NB	2.89	127.32	124.26
22	D	403	CLA	C3B-C4B-NB	-2.89	107.83	110.52
22	q	305	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	2	304	CLA	C3B-C4B-NB	-2.89	107.83	110.52
22	U	307	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
26	g	311	CHL	C4-C3-C5	2.89	120.14	115.27
26	N	315	CHL	O2A-CGA-CBA	2.89	120.98	111.91
26	U	314	CHL	O2A-CGA-CBA	2.89	120.98	111.91
26	N	313	CHL	CAC-C3C-C4C	2.89	128.56	124.81
26	1	318	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
22	b	610	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	g	314	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
26	g	312	CHL	O2A-CGA-CBA	2.89	120.98	111.91
26	N	314	CHL	O2A-CGA-CBA	2.89	120.98	111.91
27	v	319	NEX	C11-C12-C13	-2.89	118.30	126.42
22	r	603	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	B	613	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	b	613	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	3	312	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
23	2	309	LUT	C10-C11-C12	-2.89	114.21	123.22
26	r	616	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
26	U	313	CHL	C1-C2-C3	-2.89	121.05	126.04
22	V	308	CLA	CHB-C4A-NA	2.89	128.50	124.51
22	B	611	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
26	5	313	CHL	C2D-C1D-ND	2.88	112.23	110.10
22	2	303	CLA	CHB-C4A-NA	2.88	128.50	124.51
26	6	316	CHL	CHB-C1B-NB	-2.88	121.20	124.26
22	g	308	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
30	d	401	PHO	O2D-CGD-O1D	-2.88	118.20	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	314	CHL	CMD-C2D-C3D	-2.88	120.98	127.61
26	R	316	CHL	CMB-C2B-C1B	2.88	129.76	125.37
24	4	311	XAT	C27-C28-C29	-2.88	121.06	125.53
27	R	301	NEX	O24-C25-C38	2.88	118.51	115.06
31	B	618	BCR	C40-C30-C25	-2.88	105.63	110.30
22	B	606	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	4	313	CHL	C1-C2-C3	-2.88	121.06	126.04
26	Q	314	CHL	CMB-C2B-C1B	2.88	129.75	125.37
22	3	304	CLA	CMB-C2B-C1B	-2.88	120.98	125.37
26	U	316	CHL	CMB-C2B-C1B	2.88	129.75	125.37
22	A	408	CLA	CHB-C4A-NA	2.88	128.49	124.51
31	A	409	BCR	C30-C25-C26	-2.88	118.56	122.61
22	c	505	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	1	317	CHL	C1-O2A-CGA	2.88	123.99	116.44
26	G	316	CHL	CHB-C4A-NA	2.88	128.49	124.51
26	s	316	CHL	C3B-C4B-NB	2.88	113.18	110.52
22	Q	301	CLA	CHB-C1B-NB	2.88	127.30	124.26
22	C	504	CLA	CHB-C4A-NA	2.88	128.49	124.51
26	U	315	CHL	CHB-C4A-NA	2.88	128.49	124.51
31	b	619	BCR	C33-C5-C4	2.88	119.14	113.62
22	3	307	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	u	310	LUT	C38-C25-C24	-2.87	117.41	123.56
26	4	314	CHL	CMB-C2B-C1B	2.87	129.75	125.37
36	C	520	DGD	O1G-C1A-C2A	2.87	120.93	111.91
26	5	316	CHL	CMB-C2B-C1B	2.87	129.75	125.37
22	v	303	CLA	CHB-C4A-NA	2.87	128.49	124.51
27	S	317	NEX	C39-C29-C30	-2.87	118.90	122.92
31	C	518	BCR	C8-C7-C6	-2.87	119.14	127.20
31	b	620	BCR	C30-C25-C24	2.87	123.90	115.78
31	c	516	BCR	C15-C16-C17	-2.87	117.59	123.47
26	6	313	CHL	O2A-CGA-CBA	2.87	120.92	111.91
26	1	317	CHL	CHB-C4A-NA	2.87	128.48	124.51
26	5	318	CHL	CMB-C2B-C1B	2.87	129.74	125.37
26	v	313	CHL	CMB-C2B-C1B	2.87	129.74	125.37
26	q	313	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
22	n	307	CLA	CHB-C4A-NA	2.87	128.48	124.51
26	5	314	CHL	CMD-C2D-C3D	-2.87	121.01	127.61
22	4	305	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	a	413	SQD	O8-S-C6	2.87	110.31	105.74
22	n	308	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	B	615	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	V	302	CLA	C3B-C4B-NB	-2.87	107.86	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	507	CLA	C3B-C4B-NB	-2.87	107.86	110.52
22	b	611	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
31	C	518	BCR	C15-C16-C17	-2.87	117.60	123.47
26	V	318	CHL	CMB-C2B-C1B	2.87	129.73	125.37
22	C	508	CLA	C3B-C4B-NB	-2.87	107.86	110.52
23	V	310	LUT	C38-C25-C24	-2.87	117.43	123.56
26	5	313	CHL	C4A-NA-C1A	2.86	107.99	106.71
22	u	307	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	s	301	CLA	CHB-C4A-NA	2.86	128.47	124.51
26	u	314	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
34	A	411	LMG	O8-C28-C29	2.86	120.90	111.91
22	b	617	CLA	O1D-CGD-CBD	2.86	130.34	124.48
26	G	312	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
26	3	311	CHL	CMB-C2B-C1B	2.86	129.73	125.37
27	R	301	NEX	C28-C29-C30	2.86	123.33	118.94
26	q	314	CHL	CHB-C1B-NB	-2.86	121.23	124.26
23	S	310	LUT	C18-C5-C6	-2.86	121.31	124.53
26	g	312	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
26	R	317	CHL	C3B-C4B-NB	2.86	113.17	110.52
26	P	318	CHL	CMB-C2B-C1B	2.86	129.73	125.37
22	g	304	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	P	310	LUT	C7-C8-C9	-2.86	121.92	126.23
22	5	307	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	B	612	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	2	301	CLA	CMB-C2B-C1B	-2.86	121.02	125.37
26	1	315	CHL	CMB-C2B-C1B	2.86	129.72	125.37
26	4	313	CHL	C2D-C1D-ND	2.86	112.21	110.10
31	C	516	BCR	C27-C26-C25	-2.86	118.58	122.73
22	1	305	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	p	303	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	B	606	CLA	CHB-C4A-NA	2.86	128.46	124.51
26	n	314	CHL	O2A-CGA-CBA	2.86	120.87	111.91
25	L	101	LHG	O8-C23-C24	2.85	120.87	111.91
23	U	309	LUT	C15-C14-C13	-2.85	123.24	127.31
22	X	202	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	p	310	LUT	C3-C4-C5	-2.85	106.17	111.85
22	U	303	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	5	313	CHL	CMD-C2D-C3D	-2.85	121.05	127.61
23	N	309	LUT	C15-C14-C13	-2.85	123.24	127.31
23	R	312	LUT	C7-C8-C9	-2.85	121.93	126.23
22	g	307	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	2	316	CHL	C1D-ND-C4D	-2.85	104.31	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	317	CHL	C1D-ND-C4D	-2.85	104.31	106.33
23	p	310	LUT	C31-C30-C29	-2.85	123.24	127.31
23	s	311	LUT	C35-C34-C33	-2.85	123.24	127.31
26	q	315	CHL	C1C-C2C-C3C	-2.85	104.85	107.11
26	4	313	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
26	p	315	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
26	4	313	CHL	CMB-C2B-C1B	2.85	129.71	125.37
26	6	314	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
26	q	313	CHL	O2A-CGA-CBA	2.85	120.85	111.91
22	R	311	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	V	317	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
22	v	306	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	p	315	CHL	O2A-CGA-CBA	2.85	120.84	111.91
23	u	309	LUT	C16-C1-C6	-2.85	105.68	110.30
26	4	317	CHL	C1C-C2C-C3C	-2.85	104.86	107.11
26	Q	311	CHL	C1C-C2C-C3C	-2.85	104.86	107.11
26	p	316	CHL	CMD-C2D-C3D	-2.85	121.07	127.61
22	5	306	CLA	CMB-C2B-C1B	-2.85	121.03	125.37
22	x	201	CLA	CHB-C4A-NA	2.85	128.45	124.51
22	n	307	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
22	b	612	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
26	6	315	CHL	C3D-C4D-ND	2.85	114.84	110.24
26	P	319	CHL	O2A-CGA-CBA	2.84	120.83	111.91
26	G	314	CHL	C3D-C4D-ND	2.84	114.84	110.24
31	X	201	BCR	C33-C5-C4	2.84	119.08	113.62
26	1	315	CHL	C2D-C1D-ND	2.84	112.20	110.10
26	S	316	CHL	C3B-C4B-NB	2.84	113.15	110.52
22	V	307	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	4	310	LUT	C18-C5-C6	-2.84	121.33	124.53
26	3	312	CHL	C1C-C2C-C3C	-2.84	104.86	107.11
22	B	617	CLA	CMB-C2B-C1B	-2.84	121.04	125.37
26	P	316	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
31	C	516	BCR	C10-C11-C12	-2.84	114.35	123.22
22	b	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	C	513	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	1	308	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	5	306	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	6	312	CHL	CHB-C1B-NB	-2.84	121.25	124.26
22	N	304	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	B	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	u	317	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
24	V	311	XAT	C27-C28-C29	-2.84	121.12	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	620	BCR	C15-C16-C17	-2.84	117.66	123.47
22	C	503	CLA	CHB-C4A-NA	2.84	128.44	124.51
26	3	316	CHL	C1C-C2C-C3C	-2.84	104.86	107.11
23	P	310	LUT	C3-C4-C5	-2.84	106.20	111.85
26	V	317	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
22	n	301	CLA	CMB-C2B-C1B	-2.84	121.05	125.37
26	n	315	CHL	O2A-CGA-CBA	2.84	120.81	111.91
22	g	301	CLA	CMB-C2B-C3B	2.84	133.46	126.59
26	p	320	CHL	CMB-C2B-C1B	2.84	129.69	125.37
22	c	512	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	v	314	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
31	D	404	BCR	C16-C17-C18	-2.84	123.26	127.31
27	u	319	NEX	C17-C1-C6	-2.84	107.93	110.47
26	n	318	CHL	CHD-C4C-C3C	-2.84	120.67	124.84
22	R	311	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	b	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	4	315	CHL	O2A-CGA-CBA	2.84	120.81	111.91
31	c	515	BCR	C11-C12-C13	-2.83	118.45	126.42
31	z	101	BCR	C33-C5-C6	-2.83	121.34	124.53
26	P	315	CHL	CHD-C1D-C2D	2.83	131.43	125.48
26	Q	311	CHL	C4-C3-C5	2.83	120.04	115.27
22	P	304	CLA	CHB-C4A-NA	2.83	128.43	124.51
31	b	618	BCR	C30-C25-C26	-2.83	118.62	122.61
23	v	310	LUT	C3-C4-C5	-2.83	106.21	111.85
26	1	315	CHL	O2A-CGA-CBA	2.83	120.80	111.91
26	2	315	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
34	a	412	LMG	O8-C28-C29	2.83	120.80	111.91
26	P	315	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
22	N	302	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	p	312	XAT	C15-C14-C13	-2.83	123.27	127.31
26	v	315	CHL	CHC-C4B-NB	-2.83	121.26	124.26
22	S	305	CLA	C3B-C4B-NB	-2.83	107.89	110.52
25	C	522	LHG	O8-C23-C24	2.83	120.79	111.91
26	p	320	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
22	B	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	p	316	CHL	O2A-CGA-CBA	2.83	120.79	111.91
22	2	306	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	4	316	CHL	O1D-CGD-CBD	-2.83	118.70	124.48
22	v	304	CLA	C3B-C4B-NB	-2.83	107.89	110.52
26	2	318	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
26	Q	311	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
26	V	316	CHL	C1D-ND-C4D	-2.83	104.33	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	r	612	XAT	C4-C3-C2	-2.83	105.31	110.77
26	3	311	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
22	R	303	CLA	CHB-C4A-NA	2.83	128.42	124.51
22	4	301	CLA	C3B-C4B-NB	-2.83	107.89	110.52
22	q	308	CLA	C3B-C4B-NB	-2.83	107.89	110.52
22	n	301	CLA	C3B-C4B-NB	-2.83	107.89	110.52
22	b	606	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	S	311	LUT	C31-C30-C29	-2.83	123.28	127.31
22	C	515	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
22	5	305	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
32	A	412	SQD	C4-C3-C2	2.83	115.76	110.82
22	c	514	CLA	C3B-C4B-NB	-2.82	107.89	110.52
22	G	302	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	6	313	CHL	C3B-C4B-NB	2.82	113.13	110.52
22	r	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	3	311	CHL	C1-C2-C3	-2.82	121.16	126.04
23	2	309	LUT	C7-C8-C9	-2.82	121.97	126.23
26	2	314	CHL	CMB-C2B-C1B	2.82	129.67	125.37
24	q	309	XAT	C10-C11-C12	-2.82	114.41	123.22
22	G	308	CLA	C3B-C4B-NB	-2.82	107.90	110.52
26	6	312	CHL	CMB-C2B-C1B	2.82	129.66	125.37
26	5	315	CHL	CHB-C4A-NA	2.82	128.41	124.51
31	B	618	BCR	C15-C16-C17	-2.82	117.70	123.47
26	3	314	CHL	C3D-C4D-ND	2.82	114.80	110.24
22	r	610	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	G	307	CLA	CHB-C4A-NA	2.82	128.41	124.51
22	N	302	CLA	C3B-C4B-NB	-2.82	107.90	110.52
26	n	314	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
31	a	409	BCR	C30-C25-C26	-2.82	118.64	122.61
26	2	313	CHL	C4-C3-C5	2.82	120.01	115.27
26	6	301	CHL	CMB-C2B-C1B	2.82	129.66	125.37
25	l	101	LHG	O8-C23-C24	2.82	120.75	111.91
30	A	407	PHO	C2D-C1D-ND	-2.82	107.58	109.53
26	v	317	CHL	CHB-C4A-NA	2.82	128.41	124.51
26	3	314	CHL	C3B-C4B-NB	2.82	113.13	110.52
26	6	314	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
26	q	312	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
23	4	310	LUT	C18-C5-C4	2.82	119.57	114.36
26	r	614	CHL	CMD-C2D-C3D	-2.82	121.14	127.61
22	c	514	CLA	CAA-C2A-C3A	-2.82	105.07	112.78
22	u	302	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
26	g	313	CHL	CMD-C2D-C3D	-2.82	121.14	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	310	LUT	C38-C25-C24	-2.82	117.53	123.56
31	z	101	BCR	C10-C11-C12	-2.82	114.43	123.22
26	n	317	CHL	CHC-C4B-NB	-2.81	121.28	124.26
31	X	201	BCR	C33-C5-C6	-2.81	121.37	124.53
26	V	317	CHL	CHB-C4A-NA	2.81	128.40	124.51
22	Q	304	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	g	311	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
31	B	618	BCR	C30-C25-C26	-2.81	118.65	122.61
22	P	302	CLA	CHB-C1B-NB	2.81	127.23	124.26
22	R	305	CLA	CHB-C4A-NA	2.81	128.40	124.51
22	r	601	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	Q	313	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
26	Q	316	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
22	2	301	CLA	CHB-C1B-NB	2.81	127.23	124.26
22	5	301	CLA	CHB-C1B-NB	2.81	127.23	124.26
24	Q	309	XAT	C30-C31-C32	-2.81	114.45	123.22
31	x	202	BCR	C33-C5-C4	2.81	119.01	113.62
26	q	314	CHL	CHC-C4B-NB	-2.81	121.28	124.26
26	p	314	CHL	CMD-C2D-C3D	-2.81	121.15	127.61
31	B	619	BCR	C33-C5-C4	2.81	119.01	113.62
26	6	312	CHL	C1-C2-C3	-2.81	121.19	126.04
22	5	302	CLA	C3B-C4B-NB	-2.81	107.91	110.52
26	Q	314	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
26	3	311	CHL	CAC-C3C-C4C	2.81	128.45	124.81
23	1	310	LUT	C31-C30-C29	-2.81	123.31	127.31
31	C	517	BCR	C11-C12-C13	-2.81	118.53	126.42
26	S	313	CHL	C1D-ND-C4D	-2.81	104.34	106.33
22	C	509	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	6	315	CHL	O2A-CGA-CBA	2.81	120.71	111.91
26	v	314	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
26	V	314	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
22	v	308	CLA	CHB-C4A-NA	2.81	128.39	124.51
23	1	309	LUT	C38-C25-C24	-2.80	117.56	123.56
22	u	302	CLA	C3B-C4B-NB	-2.80	107.91	110.52
26	s	316	CHL	CHC-C4B-NB	-2.80	121.29	124.26
22	c	508	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	v	302	CLA	C3B-C4B-NB	-2.80	107.92	110.52
26	6	313	CHL	CMB-C2B-C1B	2.80	129.64	125.37
26	v	314	CHL	O2A-CGA-CBA	2.80	120.70	111.91
31	B	620	BCR	C30-C25-C24	2.80	123.71	115.78
26	G	314	CHL	CMB-C2B-C1B	2.80	129.64	125.37
22	p	303	CLA	C3B-C4B-NB	-2.80	107.92	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	306	CLA	CHB-C4A-NA	2.80	128.39	124.51
24	5	311	XAT	C10-C11-C12	-2.80	114.47	123.22
26	5	315	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
25	c	522	LHG	O8-C23-C24	2.80	120.70	111.91
33	d	404	PL9	C40-C39-C41	2.80	119.98	115.27
22	4	305	CLA	C3B-C4B-NB	-2.80	107.92	110.52
26	4	316	CHL	O2D-CGD-O1D	-2.80	118.36	123.84
26	v	317	CHL	CMD-C2D-C3D	-2.80	121.17	127.61
22	c	510	CLA	CMB-C2B-C1B	-2.80	121.11	125.37
26	S	314	CHL	CMB-C2B-C1B	2.80	129.63	125.37
26	v	314	CHL	C1C-C2C-C3C	-2.80	104.89	107.11
26	5	314	CHL	CHD-C4C-C3C	-2.80	120.73	124.84
22	N	306	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	B	607	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	S	301	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	c	503	CLA	CHB-C4A-NA	2.80	128.38	124.51
26	u	315	CHL	C1D-ND-C4D	-2.80	104.35	106.33
26	g	311	CHL	CHC-C4B-NB	-2.80	121.30	124.26
26	u	318	CHL	CHB-C1B-NB	-2.80	121.30	124.26
31	d	403	BCR	C16-C17-C18	-2.80	123.32	127.31
26	4	314	CHL	C4D-CHA-C1A	-2.80	117.85	121.25
26	n	313	CHL	CMB-C2B-C1B	2.80	129.63	125.37
26	3	312	CHL	O2A-CGA-CBA	2.79	120.68	111.91
22	R	304	CLA	CHB-C4A-NA	2.79	128.38	124.51
26	1	313	CHL	C3B-C4B-NB	2.79	113.11	110.52
26	S	314	CHL	CHB-C4A-NA	2.79	128.38	124.51
22	U	302	CLA	C3B-C4B-NB	-2.79	107.92	110.52
22	C	515	CLA	C3B-C4B-NB	-2.79	107.92	110.52
22	c	512	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
26	6	315	CHL	C2D-C1D-ND	2.79	112.16	110.10
26	P	316	CHL	C2D-C1D-ND	2.79	112.16	110.10
25	C	523	LHG	O8-C23-C24	2.79	120.67	111.91
26	1	317	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
22	n	302	CLA	C3B-C4B-NB	-2.79	107.92	110.52
26	3	313	CHL	C3B-C4B-NB	2.79	113.11	110.52
22	B	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	S	316	CHL	CHC-C4B-NB	-2.79	121.30	124.26
22	6	307	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	R	315	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
26	1	314	CHL	C3D-C4D-ND	2.79	114.75	110.24
22	6	308	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
26	r	615	CHL	CMD-C2D-C3D	-2.79	121.19	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	v	307	CLA	C3B-C4B-NB	-2.79	107.93	110.52
22	G	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	2	308	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	c	502	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	r	619	CHL	CHB-C1B-NB	-2.79	121.31	124.26
23	s	311	LUT	C31-C30-C29	-2.79	123.33	127.31
26	V	314	CHL	O2A-CGA-CBA	2.79	120.65	111.91
22	r	601	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	r	604	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	3	303	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	r	602	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	p	314	CHL	O2A-CGA-CBA	2.79	120.65	111.91
26	N	317	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
22	G	304	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	U	311	XAT	C11-C10-C9	-2.79	123.33	127.31
22	N	304	CLA	CMA-C3A-C4A	-2.78	104.29	111.77
22	V	307	CLA	C3B-C4B-NB	-2.78	107.93	110.52
26	U	317	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
22	5	304	CLA	C3B-C4B-NB	-2.78	107.93	110.52
22	s	305	CLA	C3B-C4B-NB	-2.78	107.93	110.52
26	G	316	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
22	p	307	CLA	CHB-C4A-NA	2.78	128.36	124.51
22	B	614	CLA	CHB-C4A-NA	2.78	128.36	124.51
24	u	311	XAT	C31-C30-C29	-2.78	123.34	127.31
26	1	317	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
36	C	520	DGD	C4E-C3E-C2E	2.78	115.68	110.82
22	C	511	CLA	CMB-C2B-C1B	-2.78	121.13	125.37
26	v	315	CHL	O2A-CGA-CBA	2.78	120.64	111.91
26	G	313	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
26	1	313	CHL	O2A-CGA-CBA	2.78	120.63	111.91
26	S	316	CHL	CMB-C2B-C1B	2.78	129.60	125.37
26	1	316	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
26	G	315	CHL	C4-C3-C5	2.78	119.94	115.27
24	1	311	XAT	C11-C10-C9	-2.78	123.35	127.31
26	P	316	CHL	O2A-CGA-CBA	2.78	120.62	111.91
22	v	304	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
26	3	313	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
22	v	307	CLA	CHB-C4A-NA	2.78	128.35	124.51
22	q	308	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
26	r	616	CHL	C3B-C4B-NB	2.78	113.09	110.52
26	g	314	CHL	CHC-C4B-NB	-2.78	121.32	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	314	CHL	C3B-C4B-NB	2.78	113.09	110.52
22	N	306	CLA	CMB-C2B-C1B	-2.78	121.14	125.37
27	U	318	NEX	C39-C29-C30	-2.77	119.04	122.92
26	s	315	CHL	CMD-C2D-C3D	-2.77	121.23	127.61
23	p	311	LUT	C31-C30-C29	-2.77	123.35	127.31
22	1	305	CLA	C3B-C4B-NB	-2.77	107.94	110.52
23	4	310	LUT	C31-C30-C29	-2.77	123.36	127.31
26	3	314	CHL	C2D-C1D-ND	2.77	112.15	110.10
26	2	314	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
26	V	315	CHL	O2A-CGA-CBA	2.77	120.60	111.91
26	G	314	CHL	O2A-CGA-CBA	2.77	120.60	111.91
22	3	304	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	3	312	CHL	CHD-C4C-C3C	-2.77	120.77	124.84
23	s	310	LUT	C18-C5-C6	-2.77	121.42	124.53
26	3	311	CHL	CMD-C2D-C3D	-2.77	121.24	127.61
37	E	101	HEM	C4C-NC-C1C	2.77	108.06	105.35
22	b	607	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	5	314	CHL	CMB-C2B-C1B	2.77	129.59	125.37
26	p	316	CHL	CMB-C2B-C1B	2.77	129.59	125.37
22	G	304	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	3	312	CHL	CMB-C2B-C1B	2.77	129.58	125.37
26	s	316	CHL	CMB-C2B-C1B	2.77	129.58	125.37
22	S	306	CLA	C3B-C4B-NB	-2.77	107.95	110.52
24	R	313	XAT	C4-C3-C2	-2.77	105.43	110.77
37	e	101	HEM	C4C-NC-C1C	2.77	108.06	105.35
22	g	302	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
32	C	501	SQD	O8-S-C6	2.76	110.14	105.74
31	C	516	BCR	C33-C5-C6	-2.76	121.42	124.53
22	Q	308	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	V	303	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	P	317	CHL	C1D-ND-C4D	-2.76	104.37	106.33
22	a	405	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	g	303	CLA	CHB-C4A-NA	2.76	128.33	124.51
26	v	316	CHL	CMB-C2B-C1B	2.76	129.58	125.37
24	N	311	XAT	C31-C30-C29	-2.76	123.37	127.31
22	4	302	CLA	C3B-C4B-NB	-2.76	107.95	110.52
23	2	310	LUT	C38-C25-C24	-2.76	117.65	123.56
36	B	601	DGD	O1G-C1A-C2A	2.76	120.58	111.91
22	Q	307	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	1	312	LHG	O8-C23-C24	2.76	120.58	111.91
26	5	315	CHL	O2A-CGA-CBA	2.76	120.58	111.91
26	g	316	CHL	CMD-C2D-C3D	-2.76	121.26	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	308	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	5	317	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
26	N	314	CHL	CMB-C2B-C1B	2.76	129.57	125.37
26	1	315	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
26	6	315	CHL	C3B-C4B-NB	2.76	113.08	110.52
24	Q	309	XAT	C10-C11-C12	-2.76	114.60	123.22
22	C	513	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
26	R	315	CHL	CMB-C2B-C1B	2.76	129.57	125.37
26	s	314	CHL	CMB-C2B-C1B	2.76	129.57	125.37
26	3	312	CHL	C3B-C4B-NB	2.76	113.08	110.52
24	4	311	XAT	C11-C12-C13	-2.76	118.66	126.42
26	g	312	CHL	O2D-CGD-O1D	-2.76	118.44	123.84
26	2	314	CHL	O2A-CGA-CBA	2.76	120.57	111.91
27	s	317	NEX	C39-C29-C30	-2.76	119.06	122.92
26	N	314	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
26	Q	312	CHL	CMB-C2B-C1B	2.76	129.57	125.37
33	D	405	PL9	C40-C39-C41	2.76	119.91	115.27
22	R	303	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	p	309	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	q	305	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	S	306	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	p	304	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	p	308	CLA	CHB-C4A-NA	2.76	128.33	124.51
27	2	319	NEX	C28-C29-C30	2.76	123.17	118.94
26	4	314	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
26	V	315	CHL	C2D-C1D-ND	2.76	112.14	110.10
26	G	313	CHL	CMD-C2D-C3D	-2.76	121.27	127.61
31	x	202	BCR	C33-C5-C6	-2.76	121.43	124.53
22	S	302	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	s	308	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
26	V	314	CHL	O2D-CGD-O1D	-2.76	118.45	123.84
22	g	307	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	C	506	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
31	A	409	BCR	C23-C24-C25	-2.76	119.46	127.20
22	S	309	CLA	CHB-C4A-NA	2.76	128.32	124.51
36	b	601	DGD	O1G-C1A-C2A	2.76	120.56	111.91
26	v	318	CHL	C1C-C2C-C3C	-2.76	104.93	107.11
26	1	314	CHL	CMD-C2D-C3D	-2.76	121.28	127.61
24	u	311	XAT	C10-C11-C12	-2.76	114.62	123.22
22	B	608	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
31	k	101	BCR	C10-C11-C12	-2.76	114.62	123.22
26	P	317	CHL	C1C-C2C-C3C	-2.75	104.93	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	405	CLA	CHB-C4A-NA	2.75	128.32	124.51
26	n	314	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
22	3	303	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	V	305	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	N	305	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
22	V	304	CLA	CMB-C2B-C1B	-2.75	121.18	125.37
22	C	507	CLA	CMB-C2B-C3B	2.75	133.25	126.59
26	n	318	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
22	P	308	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	C	515	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	s	303	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	s	306	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	u	306	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	c	509	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	C	505	CLA	CHB-C4A-NA	2.75	128.31	124.51
26	2	313	CHL	O2A-CGA-CBA	2.75	120.53	111.91
26	S	316	CHL	C2D-C1D-ND	2.75	112.13	110.10
26	2	317	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
22	v	301	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	n	304	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	v	303	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	u	316	CHL	C4-C3-C5	2.75	119.89	115.27
26	V	317	CHL	CMB-C2B-C1B	2.75	129.55	125.37
22	3	306	CLA	CHB-C4A-NA	2.75	128.31	124.51
26	u	318	CHL	C1C-C2C-C3C	-2.75	104.94	107.11
23	5	309	LUT	C30-C31-C32	-2.75	114.65	123.22
22	N	307	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	r	613	LHG	O8-C23-C24	2.74	120.52	111.91
25	6	311	LHG	O8-C23-C24	2.74	120.52	111.91
26	G	315	CHL	CMB-C2B-C1B	2.74	129.55	125.37
22	a	406	CLA	C3B-C4B-NB	-2.74	107.97	110.52
22	P	303	CLA	CHB-C4A-NA	2.74	128.31	124.51
26	V	314	CHL	CAA-C2A-C3A	-2.74	105.27	112.78
31	a	409	BCR	C21-C20-C19	-2.74	114.66	123.22
22	u	301	CLA	C3B-C4B-NB	-2.74	107.97	110.52
26	r	614	CHL	OMC-CMC-C2C	-2.74	119.49	125.69
26	R	315	CHL	OMC-CMC-C2C	-2.74	119.49	125.69
22	s	306	CLA	C3B-C4B-NB	-2.74	107.97	110.52
27	n	319	NEX	C11-C12-C13	-2.74	118.72	126.42
22	C	510	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	c	506	CLA	CMB-C2B-C3B	2.74	133.22	126.59
22	4	304	CLA	CHB-C4A-NA	2.74	128.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	304	CLA	C3B-C4B-NB	-2.74	107.97	110.52
26	5	314	CHL	O2A-CGA-CBA	2.74	120.50	111.91
22	6	304	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	p	307	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	V	301	CLA	CHB-C1B-NB	2.74	127.16	124.26
23	S	310	LUT	C16-C1-C6	-2.74	105.86	110.30
22	6	308	CLA	C3B-C4B-NB	-2.74	107.97	110.52
23	v	310	LUT	C15-C35-C34	-2.74	117.87	123.47
22	V	304	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	5	310	LUT	C38-C25-C24	-2.74	117.70	123.56
26	4	315	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
26	5	315	CHL	CMB-C2B-C1B	2.74	129.53	125.37
22	u	302	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	g	315	CHL	CMB-C2B-C1B	2.73	129.53	125.37
22	1	301	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	U	304	CLA	C3B-C4B-NB	-2.73	107.98	110.52
26	U	313	CHL	C4-C3-C5	2.73	119.87	115.27
26	4	316	CHL	C1C-C2C-C3C	-2.73	104.94	107.11
22	6	305	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	4	316	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
26	S	315	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
26	N	316	CHL	O2A-CGA-CBA	2.73	120.48	111.91
22	v	306	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	s	316	CHL	C2D-C1D-ND	2.73	112.12	110.10
22	c	504	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	v	310	LUT	C31-C30-C29	-2.73	123.41	127.31
26	V	313	CHL	C1-C2-C3	-2.73	121.32	126.04
23	1	310	LUT	C38-C25-C24	-2.73	117.72	123.56
26	Q	315	CHL	CHB-C4A-NA	2.73	128.29	124.51
22	G	307	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	p	320	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
26	R	317	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
26	2	315	CHL	O2A-CGA-CBA	2.73	120.47	111.91
22	G	303	CLA	C3B-C4B-NB	-2.73	107.98	110.52
26	3	316	CHL	CMB-C2B-C1B	2.73	129.52	125.37
26	r	616	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
22	6	307	CLA	CHB-C4A-NA	2.73	128.28	124.51
26	U	314	CHL	CHB-C4A-NA	2.73	128.28	124.51
26	s	313	CHL	CMB-C2B-C1B	2.73	129.52	125.37
22	U	306	CLA	CHB-C4A-NA	2.73	128.28	124.51
22	6	305	CLA	CMB-C2B-C1B	-2.73	121.22	125.37
27	u	319	NEX	C11-C12-C13	-2.72	118.76	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	301	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	s	302	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	3	306	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	R	302	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
27	n	319	NEX	C15-C35-C34	-2.72	117.89	123.47
22	A	406	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	c	507	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	v	317	CHL	C1C-C2C-C3C	-2.72	104.95	107.11
24	Q	309	XAT	C35-C15-C14	-2.72	117.90	123.47
22	P	309	CLA	CHB-C4A-NA	2.72	128.28	124.51
26	3	316	CHL	CHB-C4A-NA	2.72	128.28	124.51
25	v	312	LHG	O8-C23-C24	2.72	120.45	111.91
26	u	315	CHL	O2A-CGA-CBA	2.72	120.45	111.91
22	s	309	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	S	313	CHL	CMB-C2B-C1B	2.72	129.51	125.37
26	5	318	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
27	V	319	NEX	C24-C23-C22	-2.72	105.52	110.77
22	1	305	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	c	514	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	Q	312	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
22	C	508	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	N	317	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
27	V	319	NEX	C11-C12-C13	-2.72	118.78	126.42
22	6	308	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	u	317	CHL	C1-C2-C3	-2.72	121.34	126.04
26	Q	312	CHL	O2A-CGA-CBA	2.72	120.44	111.91
24	4	311	XAT	C15-C35-C34	-2.72	117.91	123.47
22	v	304	CLA	CHB-C4A-NA	2.72	128.27	124.51
27	r	618	NEX	C17-C1-C6	-2.72	108.04	110.47
26	5	313	CHL	CMB-C2B-C1B	2.72	129.51	125.37
26	2	316	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
24	u	311	XAT	C15-C35-C34	-2.72	117.91	123.47
27	R	301	NEX	C24-C23-C22	-2.72	105.53	110.77
22	1	304	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	u	314	CHL	CHB-C4A-NA	2.72	128.27	124.51
34	d	407	LMG	O8-C28-C29	2.72	120.43	111.91
26	v	314	CHL	CMB-C2B-C1B	2.72	129.50	125.37
22	V	305	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	6	304	CLA	CHB-C4A-NA	2.71	128.27	124.51
22	R	306	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
22	P	303	CLA	C3B-C4B-NB	-2.71	108.00	110.52
22	3	302	CLA	O2A-CGA-O1A	-2.71	116.74	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p	320	CHL	O2A-CGA-CBA	2.71	120.42	111.91
22	3	307	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	4	301	CLA	CHB-C4A-NA	2.71	128.26	124.51
31	K	101	BCR	C10-C11-C12	-2.71	114.75	123.22
26	5	313	CHL	O2A-CGA-CBA	2.71	120.42	111.91
26	R	316	CHL	CMD-C2D-C3D	-2.71	121.38	127.61
22	2	307	CLA	C3B-C4B-NB	-2.71	108.00	110.52
22	V	304	CLA	C3B-C4B-NB	-2.71	108.00	110.52
22	G	301	CLA	CHB-C1B-NB	2.71	127.13	124.26
26	q	315	CHL	CHC-C4B-NB	-2.71	121.39	124.26
26	Q	311	CHL	O2A-CGA-CBA	2.71	120.42	111.91
26	G	315	CHL	O2A-CGA-CBA	2.71	120.42	111.91
26	V	318	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
22	A	404	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
33	d	404	PL9	C53-C6-C1	2.71	120.53	114.99
26	6	316	CHL	CHC-C4B-NB	-2.71	121.39	124.26
22	U	301	CLA	C3B-C4B-NB	-2.71	108.00	110.52
26	5	316	CHL	C1D-ND-C4D	-2.71	104.41	106.33
26	p	315	CHL	CMB-C2B-C1B	2.71	129.50	125.37
32	A	412	SQD	O8-S-C6	2.71	110.06	105.74
22	2	305	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
32	m	101	SQD	O5-C5-C4	2.71	114.61	109.69
25	R	314	LHG	O8-C23-C24	2.71	120.41	111.91
26	U	313	CHL	C1C-C2C-C3C	-2.71	104.97	107.11
22	v	305	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	5	304	CLA	CMA-C3A-C4A	-2.71	104.50	111.77
23	1	309	LUT	C35-C34-C33	-2.71	123.45	127.31
22	2	307	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	4	303	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	n	306	CLA	CHB-C4A-NA	2.71	128.25	124.51
26	P	318	CHL	CMD-C2D-C3D	-2.71	121.39	127.61
22	q	301	CLA	CMB-C2B-C1B	-2.71	121.25	125.37
26	G	316	CHL	C1C-C2C-C3C	-2.71	104.97	107.11
22	S	303	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
31	b	619	BCR	C30-C25-C26	-2.70	118.80	122.61
26	n	313	CHL	CHB-C4A-NA	2.70	128.25	124.51
26	P	314	CHL	CMB-C2B-C1B	2.70	129.49	125.37
26	U	317	CHL	CMB-C2B-C1B	2.70	129.49	125.37
26	2	317	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
26	6	317	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
22	B	617	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	R	313	XAT	C30-C31-C32	-2.70	114.78	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	312	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
26	N	315	CHL	C1D-ND-C4D	-2.70	104.42	106.33
26	2	315	CHL	CMB-C2B-C1B	2.70	129.48	125.37
23	p	311	LUT	C38-C25-C24	-2.70	117.78	123.56
22	1	306	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	r	605	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
26	Q	312	CHL	C1D-ND-C4D	-2.70	104.42	106.33
26	q	312	CHL	C3B-C4B-NB	2.70	113.02	110.52
22	V	302	CLA	CHB-C4A-NA	2.70	128.25	124.51
33	D	405	PL9	C53-C6-C1	2.70	120.51	114.99
26	n	317	CHL	CMD-C2D-C3D	-2.70	121.40	127.61
26	g	314	CHL	O2A-CGA-CBA	2.70	120.38	111.91
22	G	305	CLA	O2D-CGD-CBD	2.70	116.06	111.27
34	D	408	LMG	O8-C28-C29	2.70	120.38	111.91
24	U	311	XAT	C15-C35-C34	-2.70	117.94	123.47
22	n	301	CLA	CHB-C1B-NB	2.70	127.11	124.26
26	p	319	CHL	C4-C3-C5	2.70	119.81	115.27
25	c	521	LHG	O8-C23-C24	2.70	120.37	111.91
26	v	317	CHL	CMB-C2B-C1B	2.70	129.48	125.37
26	P	317	CHL	O2A-CGA-CBA	2.70	120.37	111.91
22	U	307	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	C	514	CLA	CHB-C4A-NA	2.70	128.24	124.51
22	c	513	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	1	318	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
22	4	306	CLA	CHB-C4A-NA	2.69	128.24	124.51
26	g	315	CHL	CHB-C4A-NA	2.69	128.24	124.51
26	s	314	CHL	CHB-C4A-NA	2.69	128.24	124.51
22	5	304	CLA	C1-C2-C3	-2.69	121.39	126.04
24	r	612	XAT	C39-C29-C28	2.69	122.32	118.08
27	p	301	NEX	C17-C1-C6	-2.69	108.06	110.47
26	Q	314	CHL	O2A-CGA-CBA	2.69	120.36	111.91
31	t	101	BCR	C11-C12-C13	-2.69	118.85	126.42
24	v	311	XAT	C10-C11-C12	-2.69	114.82	123.22
23	v	310	LUT	C38-C25-C24	-2.69	117.80	123.56
26	P	315	CHL	O2A-CGA-CBA	2.69	120.35	111.91
32	M	101	SQD	O5-C5-C4	2.69	114.58	109.69
22	Q	307	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	S	312	LHG	O8-C23-C24	2.69	120.35	111.91
25	s	312	LHG	O8-C23-C24	2.69	120.35	111.91
26	V	318	CHL	O2A-CGA-CBA	2.69	120.35	111.91
26	s	315	CHL	O2A-CGA-CBA	2.69	120.35	111.91
31	T	101	BCR	C30-C25-C24	2.69	123.39	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	406	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	q	307	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	b	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
24	1	311	XAT	C11-C12-C13	-2.69	118.86	126.42
22	p	304	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	p	316	CHL	C4A-NA-C1A	2.69	107.92	106.71
26	5	315	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
26	S	315	CHL	O2A-CGA-CBA	2.69	120.34	111.91
22	V	306	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	n	316	CHL	C2A-C3A-C4A	-2.69	97.53	101.87
22	u	303	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	s	307	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	u	318	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
26	V	313	CHL	O2A-CGA-CBA	2.69	120.34	111.91
31	A	409	BCR	C21-C20-C19	-2.69	114.83	123.22
22	a	404	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	Q	305	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	1	307	CLA	C3B-C4B-NB	-2.68	108.03	110.52
26	u	316	CHL	C4D-CHA-C1A	-2.68	117.98	121.25
22	a	406	CLA	CHB-C4A-NA	2.68	128.22	124.51
22	g	301	CLA	CHB-C1B-NB	2.68	127.10	124.26
26	P	316	CHL	CMB-C2B-C1B	2.68	129.46	125.37
26	u	313	CHL	O2A-CGA-CBA	2.68	120.33	111.91
23	s	311	LUT	C18-C5-C6	-2.68	121.52	124.53
26	P	314	CHL	C1D-ND-C4D	-2.68	104.43	106.33
26	N	316	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
26	p	317	CHL	C1C-C2C-C3C	-2.68	104.98	107.11
26	6	313	CHL	CHD-C4C-C3C	-2.68	120.90	124.84
26	5	316	CHL	O2A-CGA-CBA	2.68	120.32	111.91
22	G	301	CLA	CMB-C2B-C3B	2.68	133.08	126.59
22	S	309	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	2	308	CLA	C3B-C4B-NB	-2.68	108.03	110.52
22	U	307	CLA	C3B-C4B-NB	-2.68	108.03	110.52
22	B	603	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	6	313	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
26	u	314	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
26	6	317	CHL	C4-C3-C5	2.68	119.78	115.27
26	2	313	CHL	CMB-C2B-C1B	2.68	129.45	125.37
26	p	317	CHL	O2A-CGA-CBA	2.68	120.31	111.91
26	r	619	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
31	x	202	BCR	C27-C26-C25	-2.68	118.84	122.73
31	X	201	BCR	C27-C26-C25	-2.68	118.84	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	304	CLA	C3B-C4B-NB	-2.68	108.03	110.52
26	2	316	CHL	O2A-CGA-CBA	2.68	120.31	111.91
26	V	315	CHL	CMD-C2D-C3D	-2.68	121.46	127.61
22	q	303	CLA	CHB-C4A-NA	2.68	128.21	124.51
26	3	316	CHL	C4-C3-C5	2.68	119.77	115.27
31	T	101	BCR	C11-C12-C13	-2.67	118.90	126.42
22	3	305	CLA	C3B-C4B-NB	-2.67	108.03	110.52
26	4	317	CHL	CMD-C2D-C3D	-2.67	121.46	127.61
26	v	317	CHL	CHB-C1B-NB	-2.67	121.43	124.26
26	N	314	CHL	OMC-CMC-C2C	-2.67	119.64	125.69
22	P	303	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
27	R	301	NEX	C11-C12-C13	-2.67	118.91	126.42
22	N	308	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	G	308	CLA	CHB-C4A-NA	2.67	128.21	124.51
33	d	404	PL9	C20-C19-C21	2.67	119.77	115.27
22	v	305	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	q	306	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	P	311	LUT	C11-C10-C9	-2.67	123.50	127.31
26	v	316	CHL	O2A-CGA-CBA	2.67	120.29	111.91
22	S	307	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
26	G	312	CHL	O2A-CGA-CBA	2.67	120.29	111.91
23	4	310	LUT	C38-C25-C24	-2.67	117.84	123.56
22	R	310	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
22	G	303	CLA	CHB-C1B-NB	2.67	127.08	124.26
23	V	310	LUT	C31-C30-C29	-2.67	123.50	127.31
26	R	315	CHL	C4-C3-C5	2.67	119.76	115.27
23	5	309	LUT	C3-C4-C5	-2.67	106.53	111.85
26	r	614	CHL	CMB-C2B-C1B	2.67	129.44	125.37
22	n	301	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
26	V	316	CHL	O2A-CGA-CBA	2.67	120.28	111.91
23	r	611	LUT	C18-C5-C6	-2.67	121.53	124.53
37	e	101	HEM	CAA-CBA-CGA	-2.67	107.86	113.60
26	p	318	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
22	G	304	CLA	CMB-C2B-C1B	-2.67	121.31	125.37
22	c	513	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
26	6	316	CHL	CHB-C4A-NA	2.67	128.20	124.51
31	t	101	BCR	C30-C25-C24	2.67	123.32	115.78
31	a	409	BCR	C16-C15-C14	-2.67	118.01	123.47
22	r	602	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
31	a	409	BCR	C23-C24-C25	-2.67	119.72	127.20
22	P	304	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	v	313	CHL	O2A-CGA-CBA	2.66	120.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	409	BCR	C16-C15-C14	-2.66	118.02	123.47
24	6	310	XAT	C31-C30-C29	-2.66	123.51	127.31
33	a	411	PL9	C6-C1-C2	2.66	119.85	117.13
24	Q	309	XAT	C6-C7-C8	-2.66	120.36	125.99
26	U	313	CHL	O2A-CGA-CBA	2.66	120.27	111.91
23	U	309	LUT	C16-C1-C6	-2.66	105.98	110.30
23	2	310	LUT	C15-C14-C13	-2.66	123.51	127.31
22	4	304	CLA	C3B-C4B-NB	-2.66	108.05	110.52
22	r	606	CLA	CHB-C4A-NA	2.66	128.19	124.51
26	u	315	CHL	CHB-C4A-NA	2.66	128.19	124.51
26	4	313	CHL	O2A-CGA-CBA	2.66	120.26	111.91
27	v	319	NEX	C28-C29-C30	2.66	123.03	118.94
26	u	313	CHL	C4-C3-C5	2.66	119.75	115.27
23	2	309	LUT	C35-C15-C14	-2.66	118.02	123.47
26	Q	312	CHL	CHC-C4B-NB	-2.66	121.44	124.26
33	A	410	PL9	C6-C1-C2	2.66	119.84	117.13
23	S	311	LUT	C18-C5-C6	-2.66	121.54	124.53
23	N	310	LUT	C38-C25-C24	-2.66	117.87	123.56
22	v	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	S	307	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	r	604	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	5	301	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	q	304	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	g	311	CHL	O2A-CGA-CBA	2.66	120.25	111.91
22	g	301	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	R	307	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	U	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	s	306	CLA	CHB-C4A-NA	2.66	128.19	124.51
32	a	413	SQD	C4-C3-C2	2.66	115.46	110.82
26	R	316	CHL	C4-C3-C5	2.66	119.74	115.27
26	V	314	CHL	CHC-C4B-NB	-2.66	121.44	124.26
32	a	410	SQD	O8-S-C6	2.66	109.97	105.74
22	b	615	CLA	C3B-C4B-NB	-2.66	108.05	110.52
22	R	302	CLA	O2A-CGA-O1A	-2.66	116.89	123.59
26	U	315	CHL	C4-C3-C5	2.65	119.74	115.27
22	1	301	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	v	301	CLA	CHB-C1B-NB	2.65	127.07	124.26
26	N	317	CHL	C1D-ND-C4D	-2.65	104.45	106.33
26	2	314	CHL	CAA-C2A-C3A	-2.65	105.51	112.78
27	P	301	NEX	C24-C23-C22	-2.65	105.65	110.77
31	B	619	BCR	C30-C25-C26	-2.65	118.88	122.61
26	G	314	CHL	CMD-C2D-C3D	-2.65	121.51	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	313	CHL	O2A-CGA-CBA	2.65	120.23	111.91
22	g	308	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	6	306	CLA	C3B-C4B-NB	-2.65	108.06	110.52
26	G	311	CHL	O2A-CGA-CBA	2.65	120.23	111.91
26	v	315	CHL	C1D-ND-C4D	-2.65	104.45	106.33
26	3	314	CHL	CHC-C4B-NB	-2.65	121.45	124.26
27	r	617	NEX	C4-C3-C2	-2.65	105.66	110.77
22	n	303	CLA	CMB-C2B-C1B	-2.65	121.33	125.37
27	r	617	NEX	C17-C1-C6	-2.65	108.10	110.47
22	r	606	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	q	301	CLA	C3B-C4B-NB	-2.65	108.06	110.52
22	p	302	CLA	CHB-C4A-NA	2.65	128.17	124.51
30	a	407	PHO	O1D-CGD-CBD	2.65	129.15	124.74
22	b	603	CLA	CHB-C4A-NA	2.65	128.17	124.51
27	p	301	NEX	C24-C23-C22	-2.65	105.67	110.77
23	u	309	LUT	C38-C25-C24	-2.64	117.90	123.56
22	2	301	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
27	U	318	NEX	C26-C27-C28	-2.64	120.40	125.99
27	v	319	NEX	C24-C23-C22	-2.64	105.67	110.77
22	2	305	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
22	u	301	CLA	CMB-C2B-C1B	-2.64	121.34	125.37
26	V	315	CHL	C3B-C4B-NB	2.64	112.97	110.52
25	U	312	LHG	O8-C23-C24	2.64	120.20	111.91
22	4	307	CLA	C3B-C4B-NB	-2.64	108.06	110.52
22	1	303	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	6	314	CHL	CMB-C2B-C1B	2.64	129.39	125.37
22	Q	307	CLA	C3B-C4B-NB	-2.64	108.07	110.52
22	S	308	CLA	C3B-C4B-NB	-2.64	108.07	110.52
22	1	306	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
27	5	319	NEX	C24-C23-C22	-2.64	105.68	110.77
27	N	318	NEX	C24-C23-C22	-2.64	105.68	110.77
26	g	316	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
36	c	518	DGD	C4E-C3E-C2E	2.64	115.43	110.82
22	P	307	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
32	a	413	SQD	C44-O6-C1	2.64	118.89	113.74
31	d	403	BCR	C1-C6-C7	2.64	123.24	115.78
26	q	315	CHL	C4-C3-C5	2.64	119.71	115.27
25	2	312	LHG	O8-C23-C24	2.64	120.18	111.91
25	3	310	LHG	O8-C23-C24	2.64	120.18	111.91
22	s	307	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
26	1	314	CHL	O2D-CGD-O1D	-2.64	118.69	123.84
22	s	301	CLA	C3B-C4B-NB	-2.64	108.07	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	302	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	n	315	CHL	C1D-ND-C4D	-2.64	104.46	106.33
22	r	609	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
22	P	304	CLA	C1-C2-C3	-2.63	122.49	126.75
22	S	302	CLA	C3B-C4B-NB	-2.63	108.07	110.52
26	4	314	CHL	O2A-CGA-CBA	2.63	120.17	111.91
26	U	313	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
26	4	316	CHL	CHB-C4A-NA	2.63	128.15	124.51
22	P	309	CLA	C3B-C4B-NB	-2.63	108.07	110.52
22	S	306	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	R	307	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	5	309	LUT	C10-C11-C12	-2.63	115.01	123.22
23	s	311	LUT	C10-C11-C12	-2.63	115.01	123.22
22	s	303	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
26	r	619	CHL	CMB-C2B-C1B	2.63	129.38	125.37
22	U	308	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	4	315	CHL	C2D-C1D-ND	2.63	112.04	110.10
22	s	304	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	n	303	CLA	C1-C2-C3	-2.63	122.50	126.75
22	v	301	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	q	302	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	s	315	CHL	C2D-C1D-ND	2.63	112.04	110.10
26	n	317	CHL	O2A-CGA-CBA	2.63	120.15	111.91
22	1	303	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
22	Q	308	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
25	5	312	LHG	O8-C23-C24	2.63	120.15	111.91
26	n	314	CHL	CMB-C2B-C1B	2.62	129.37	125.37
22	5	305	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
26	P	315	CHL	CMB-C2B-C1B	2.62	129.37	125.37
26	Q	316	CHL	CMB-C2B-C1B	2.62	129.37	125.37
22	6	309	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	b	623	LHG	O8-C23-C24	2.62	120.14	111.91
26	g	314	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
23	s	311	LUT	C3-C4-C5	-2.62	106.63	111.85
22	U	302	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
22	s	302	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	S	302	CLA	CHB-C1B-NB	2.62	127.03	124.26
26	N	314	CHL	CHD-C4C-C3C	-2.62	120.99	124.84
22	S	301	CLA	C3B-C4B-NB	-2.62	108.08	110.52
22	c	511	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
23	P	311	LUT	C38-C25-C24	-2.62	117.95	123.56
22	S	304	CLA	CHB-C4A-NA	2.62	128.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q	315	CHL	CMB-C2B-C1B	2.62	129.36	125.37
27	5	319	NEX	C35-C15-C14	-2.62	118.11	123.47
22	s	308	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	S	306	CLA	C2D-C1D-ND	-2.62	108.17	110.10
22	b	608	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	B	623	LHG	O8-C23-C24	2.62	120.12	111.91
26	S	315	CHL	C3B-C4B-NB	2.62	112.94	110.52
22	S	302	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	C	512	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
26	V	314	CHL	C3D-C4D-ND	2.62	114.47	110.24
23	4	310	LUT	C11-C10-C9	-2.62	123.58	127.31
22	s	306	CLA	C2D-C1D-ND	-2.62	108.18	110.10
22	V	306	CLA	C3B-C4B-NB	-2.62	108.09	110.52
22	6	302	CLA	CHB-C1B-NB	2.62	127.03	124.26
22	U	303	CLA	CHB-C4A-NA	2.61	128.13	124.51
24	6	310	XAT	C10-C11-C12	-2.61	115.06	123.22
22	4	305	CLA	CHB-C4A-NA	2.61	128.13	124.51
26	2	315	CHL	CAC-C3C-C4C	2.61	128.20	124.81
22	C	514	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	4	308	CLA	C3B-C4B-NB	-2.61	108.09	110.52
23	5	310	LUT	C15-C14-C13	-2.61	123.58	127.31
22	N	305	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	u	317	CHL	O1D-CGD-CBD	-2.61	119.14	124.48
22	P	302	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	R	302	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	N	316	CHL	CHB-C4A-NA	2.61	128.12	124.51
22	R	308	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
26	n	318	CHL	O2A-CGA-CBA	2.61	120.09	111.91
22	3	301	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
26	u	316	CHL	CAA-CBA-CGA	-2.61	105.63	113.25
37	E	101	HEM	CAA-CBA-CGA	-2.61	107.99	113.60
22	C	506	CLA	C3B-C4B-NB	-2.61	108.10	110.52
26	N	313	CHL	O2A-CGA-CBA	2.61	120.09	111.91
26	G	311	CHL	C1-C2-C3	-2.61	121.53	126.04
26	U	316	CHL	C1-C2-C3	-2.61	121.54	126.04
22	B	615	CLA	C3B-C4B-NB	-2.61	108.10	110.52
26	V	315	CHL	CHC-C4B-NB	-2.61	121.50	124.26
25	u	312	LHG	O8-C23-C24	2.61	120.08	111.91
22	n	306	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	N	310	LUT	C18-C5-C4	2.60	119.18	114.36
22	P	302	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	5	306	CLA	O2D-CGD-O1D	-2.60	118.75	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	308	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	g	314	CHL	C3D-C4D-ND	2.60	114.44	110.24
26	6	301	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	S	314	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	N	315	CHL	CMD-C2D-C3D	-2.60	121.63	127.61
23	p	311	LUT	C35-C34-C33	-2.60	123.60	127.31
26	Q	314	CHL	C1D-ND-C4D	-2.60	104.49	106.33
22	q	305	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	N	301	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	D	404	BCR	C1-C6-C7	2.60	123.13	115.78
26	U	314	CHL	CMD-C2D-C3D	-2.60	121.64	127.61
26	G	316	CHL	O2A-CGA-CBA	2.60	120.06	111.91
23	v	309	LUT	C38-C25-C24	-2.60	118.00	123.56
22	N	307	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	5	307	CLA	C3B-C4B-NB	-2.60	108.11	110.52
22	5	307	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	V	312	LHG	O8-C23-C24	2.60	120.06	111.91
26	1	316	CHL	O1D-CGD-CBD	-2.60	119.17	124.48
36	B	601	DGD	O6E-C5E-C4E	2.60	114.41	109.69
22	2	306	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	1	313	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	s	315	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
22	q	301	CLA	CHB-C1B-NB	2.60	127.00	124.26
22	c	505	CLA	C3B-C4B-NB	-2.60	108.11	110.52
26	s	315	CHL	C3B-C4B-NB	2.60	112.92	110.52
26	V	313	CHL	CHC-C4B-NB	-2.59	121.51	124.26
22	v	307	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	Q	305	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	U	305	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	1	313	CHL	C1D-ND-C4D	-2.59	104.49	106.33
24	r	612	XAT	C35-C34-C33	-2.59	123.61	127.31
26	3	314	CHL	O2A-CGA-CBA	2.59	120.05	111.91
26	Q	315	CHL	O2A-CGA-CBA	2.59	120.05	111.91
27	r	617	NEX	C11-C12-C13	-2.59	119.13	126.42
26	r	616	CHL	C4-C3-C5	2.59	119.63	115.27
22	p	307	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	B	612	CLA	C3B-C4B-NB	-2.59	108.11	110.52
26	g	313	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
26	G	311	CHL	CHC-C4B-NB	-2.59	121.51	124.26
22	C	515	CLA	CBA-CAA-C2A	2.59	121.51	113.86
26	g	315	CHL	CMD-C2D-C3D	-2.59	121.65	127.61
32	a	413	SQD	C1-O5-C5	2.59	118.78	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	307	CLA	C3B-C4B-NB	-2.59	108.11	110.52
23	S	311	LUT	C3-C4-C5	-2.59	106.69	111.85
22	s	302	CLA	C3B-C4B-NB	-2.59	108.11	110.52
33	D	405	PL9	C20-C19-C21	2.59	119.63	115.27
26	6	314	CHL	CHC-C4B-NB	-2.59	121.52	124.26
22	5	308	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	G	306	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	S	310	LUT	C15-C14-C13	-2.59	123.62	127.31
32	m	101	SQD	O48-C23-C24	2.59	120.03	111.91
22	4	302	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	V	308	CLA	C3B-C4B-NB	-2.59	108.11	110.52
22	A	408	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
36	C	519	DGD	O1G-C1A-C2A	2.59	120.03	111.91
25	4	312	LHG	O8-C23-C24	2.59	120.02	111.91
26	v	318	CHL	O2A-CGA-CBA	2.59	120.02	111.91
32	l	102	SQD	O6-C1-C2	2.59	112.34	108.30
27	P	301	NEX	C2-C1-C6	2.58	111.72	109.21
26	5	316	CHL	C1C-C2C-C3C	-2.58	105.06	107.11
22	6	303	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
22	P	308	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	Q	304	CLA	CMB-C2B-C1B	-2.58	121.43	125.37
30	A	407	PHO	O1D-CGD-CBD	2.58	129.04	124.74
31	c	516	BCR	C33-C5-C6	-2.58	121.63	124.53
36	c	517	DGD	O1G-C1A-C2A	2.58	120.01	111.91
22	d	402	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	3	313	CHL	C2D-C1D-ND	2.58	112.01	110.10
22	6	303	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	p	319	CHL	CMD-C2D-C3D	-2.58	121.68	127.61
26	v	318	CHL	C1D-ND-C4D	-2.58	104.50	106.33
22	v	308	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
27	S	317	NEX	C24-C23-C22	-2.58	105.79	110.77
22	G	307	CLA	C3B-C4B-NB	-2.58	108.12	110.52
32	M	101	SQD	O48-C23-C24	2.58	120.00	111.91
22	c	510	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	n	310	LUT	C18-C5-C6	-2.58	121.63	124.53
26	u	314	CHL	O2A-CGA-CBA	2.58	120.00	111.91
22	4	303	CLA	CHB-C1B-NB	2.58	126.99	124.26
22	V	301	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
26	v	313	CHL	C4-C3-C5	2.58	119.61	115.27
26	G	312	CHL	CAA-C2A-C3A	-2.58	105.72	112.78
22	n	302	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
22	P	307	CLA	CHB-C4A-NA	2.58	128.07	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	312	CHL	C4-C3-C5	2.58	119.61	115.27
26	R	315	CHL	O2A-CGA-CBA	2.58	119.99	111.91
27	2	319	NEX	C24-C23-C22	-2.58	105.80	110.77
23	P	311	LUT	C3-C4-C5	-2.58	106.72	111.85
26	5	315	CHL	CAC-C3C-C4C	2.57	128.15	124.81
23	p	311	LUT	C3-C4-C5	-2.57	106.73	111.85
23	v	309	LUT	C18-C5-C6	-2.57	121.64	124.53
34	w	201	LMG	C6-C5-C4	-2.57	106.98	113.00
26	n	318	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
22	6	302	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	u	307	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	s	309	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	S	315	CHL	C1C-C2C-C3C	-2.57	105.07	107.11
26	P	319	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
22	A	404	CLA	CMB-C2B-C3B	2.57	132.82	126.59
25	P	313	LHG	O8-C23-C24	2.57	119.98	111.91
22	p	309	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	q	307	CLA	C3B-C4B-NB	-2.57	108.13	110.52
26	n	318	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
22	1	302	CLA	CHB-C1B-NB	2.57	126.98	124.26
22	a	404	CLA	CMB-C2B-C3B	2.57	132.81	126.59
33	D	405	PL9	C27-C28-C29	-2.57	121.47	127.66
22	s	303	CLA	C1-C2-C3	-2.57	122.59	126.75
22	s	304	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	R	305	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
23	U	310	LUT	C16-C1-C6	-2.57	106.13	110.30
22	u	308	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	p	313	LHG	O8-C23-C24	2.57	119.97	111.91
23	N	310	LUT	C7-C8-C9	-2.57	122.35	126.23
22	3	304	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	2	302	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	2	318	CHL	CHB-C4A-NA	2.57	128.06	124.51
22	b	609	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	C	511	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
22	A	404	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	s	314	CHL	CAC-C3C-C4C	2.57	128.14	124.81
26	1	316	CHL	C4-C3-C5	2.57	119.59	115.27
22	B	609	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
26	6	312	CHL	O2A-CGA-CBA	2.56	119.96	111.91
22	b	605	CLA	C2A-C1A-CHA	2.56	128.34	123.86
23	S	311	LUT	C10-C11-C12	-2.56	115.21	123.22
26	S	315	CHL	C2D-C1D-ND	2.56	111.99	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	301	CHL	O2A-CGA-CBA	2.56	119.96	111.91
22	s	302	CLA	CHB-C1B-NB	2.56	126.97	124.26
26	g	316	CHL	CHB-C4A-NA	2.56	128.06	124.51
27	u	319	NEX	C15-C35-C34	-2.56	118.22	123.47
31	d	403	BCR	C20-C21-C22	-2.56	123.65	127.31
26	6	314	CHL	O2A-CGA-CBA	2.56	119.95	111.91
22	3	308	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	4	303	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	R	311	CLA	C3B-C4B-NB	-2.56	108.14	110.52
26	v	315	CHL	CMD-C2D-C3D	-2.56	121.72	127.61
22	N	306	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	S	310	LUT	C1-C2-C3	2.56	119.43	113.64
22	6	307	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	r	605	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	a	404	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	5	314	CHL	C2D-C1D-ND	2.56	111.99	110.10
22	R	306	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	C	510	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	6	315	CHL	C4-C3-C5	2.56	119.58	115.27
22	V	305	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	r	607	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
22	6	302	CLA	CMB-C2B-C3B	2.56	132.78	126.59
23	r	611	LUT	C35-C15-C14	-2.56	118.23	123.47
27	U	318	NEX	C15-C35-C34	-2.56	118.23	123.47
22	4	306	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	1	309	LUT	C3-C4-C5	-2.56	106.76	111.85
26	U	314	CHL	CMB-C2B-C1B	2.56	129.26	125.37
22	1	307	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
22	B	602	CLA	C3B-C4B-NB	-2.56	108.14	110.52
26	N	314	CHL	O2D-CGD-O1D	-2.56	118.84	123.84
26	1	313	CHL	CMB-C2B-C1B	2.56	129.26	125.37
25	N	312	LHG	O8-C23-C24	2.56	119.93	111.91
27	r	618	NEX	C24-C23-C22	-2.56	105.84	110.77
26	R	317	CHL	C4-C3-C5	2.56	119.57	115.27
22	V	301	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	g	306	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
24	r	612	XAT	C28-C29-C30	-2.56	115.02	118.94
22	3	301	CLA	CHB-C1B-NB	2.56	126.96	124.26
31	C	518	BCR	C33-C5-C6	-2.55	121.66	124.53
30	D	401	PHO	O1D-CGD-CBD	2.55	128.99	124.74
22	b	606	CLA	C3B-C4B-NB	-2.55	108.14	110.52
26	V	314	CHL	C1C-C2C-C3C	-2.55	105.09	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	301	CLA	CHB-C1B-NB	2.55	126.96	124.26
26	S	314	CHL	CAC-C3C-C4C	2.55	128.12	124.81
23	N	309	LUT	C11-C10-C9	-2.55	123.67	127.31
26	q	311	CHL	C1-C2-C3	-2.55	121.63	126.04
22	p	302	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
33	D	405	PL9	C32-C33-C34	-2.55	121.51	127.66
23	V	309	LUT	C18-C5-C6	-2.55	121.66	124.53
23	u	310	LUT	C16-C1-C6	-2.55	106.16	110.30
26	R	315	CHL	CHB-C4A-NA	2.55	128.04	124.51
26	G	315	CHL	CHB-C4A-NA	2.55	128.04	124.51
22	2	303	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
22	u	308	CLA	C3B-C4B-NB	-2.55	108.15	110.52
26	4	317	CHL	O2A-CGA-CBA	2.55	119.91	111.91
26	U	313	CHL	CHC-C4B-NB	-2.55	121.56	124.26
26	U	316	CHL	C2A-C1A-CHA	-2.55	119.40	123.86
33	d	404	PL9	C32-C33-C34	-2.55	121.52	127.66
31	D	404	BCR	C20-C21-C22	-2.55	123.67	127.31
22	4	301	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
23	U	310	LUT	C39-C29-C28	2.55	122.09	118.08
22	1	302	CLA	CHB-C4A-NA	2.55	128.04	124.51
27	V	319	NEX	C28-C29-C30	2.55	122.85	118.94
26	2	313	CHL	C1-C2-C3	-2.55	121.64	126.04
26	q	311	CHL	O2A-CGA-CBA	2.55	119.91	111.91
22	N	303	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
22	V	307	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	3	302	CLA	CHB-C4A-NA	2.55	128.03	124.51
27	r	618	NEX	O24-C25-C38	2.55	118.11	115.06
22	6	305	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	G	302	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	R	304	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	2	306	CLA	C2A-C1A-CHA	2.55	128.31	123.86
22	u	304	CLA	CMB-C2B-C3B	2.55	132.75	126.59
22	2	306	CLA	CMB-C2B-C3B	2.54	132.75	126.59
23	V	309	LUT	C38-C25-C24	-2.54	118.11	123.56
26	n	314	CHL	O2D-CGD-O1D	-2.54	118.86	123.84
22	r	608	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	6	315	CHL	CHC-C4B-NB	-2.54	121.56	124.26
23	s	310	LUT	C11-C10-C9	-2.54	123.68	127.31
26	N	317	CHL	O2A-CGA-CBA	2.54	119.89	111.91
22	g	302	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	c	509	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	R	308	CLA	C3B-C4B-NB	-2.54	108.16	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	313	CHL	CMD-C2D-C3D	-2.54	121.77	127.61
26	3	311	CHL	C4-C3-C5	2.54	119.55	115.27
34	B	621	LMG	O8-C28-C29	2.54	119.88	111.91
22	b	602	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	s	308	CLA	C3B-C4B-NB	-2.54	108.16	110.52
26	r	614	CHL	O2A-CGA-CBA	2.54	119.87	111.91
23	S	310	LUT	C11-C10-C9	-2.54	123.69	127.31
25	g	310	LHG	O8-C23-C24	2.54	119.87	111.91
22	G	306	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	g	302	CLA	C3B-C4B-NB	-2.54	108.16	110.52
23	s	310	LUT	C16-C1-C6	-2.54	106.18	110.30
27	s	317	NEX	C24-C23-C22	-2.54	105.87	110.77
22	r	609	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
26	G	311	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
22	Q	305	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	1	303	CLA	CHB-C1B-NB	2.54	126.94	124.26
22	S	303	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	V	309	LUT	C11-C10-C9	-2.54	123.69	127.31
23	2	310	LUT	C18-C5-C6	-2.54	121.68	124.53
22	U	303	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	r	608	CLA	CMB-C2B-C1B	-2.54	121.51	125.37
26	U	316	CHL	CMD-C2D-C3D	-2.53	121.78	127.61
26	P	315	CHL	CHD-C4C-C3C	-2.53	121.11	124.84
22	B	613	CLA	C3B-C4B-NB	-2.53	108.16	110.52
26	s	313	CHL	C1D-ND-C4D	-2.53	104.53	106.33
22	U	303	CLA	CHB-C1B-NB	2.53	126.94	124.26
22	u	305	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	D	403	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	s	310	LUT	C21-C26-C27	-2.53	109.50	112.70
22	c	514	CLA	CBA-CAA-C2A	2.53	121.33	113.86
22	g	305	CLA	C3B-C4B-NB	-2.53	108.17	110.52
23	r	611	LUT	C11-C10-C9	-2.53	123.70	127.31
22	5	303	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
24	P	312	XAT	C10-C11-C12	-2.53	115.32	123.22
23	1	309	LUT	C15-C35-C34	-2.53	118.29	123.47
22	4	307	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	6	304	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
22	R	309	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
22	U	308	CLA	C3B-C4B-NB	-2.53	108.17	110.52
23	N	309	LUT	C16-C1-C6	-2.53	106.20	110.30
22	Q	303	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	4	303	CLA	CHB-C4A-NA	2.53	128.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	622	LHG	O8-C23-C24	2.53	119.84	111.91
31	B	619	BCR	C7-C8-C9	-2.53	122.42	126.23
34	C	521	LMG	O8-C28-C29	2.53	119.84	111.91
26	G	313	CHL	CHB-C4A-NA	2.53	128.01	124.51
22	r	601	CLA	C3B-C4B-NB	-2.53	108.17	110.52
26	Q	312	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
31	X	201	BCR	C24-C23-C22	-2.53	122.42	126.23
26	P	317	CHL	C4-C3-C5	2.53	119.52	115.27
26	3	313	CHL	O2A-CGA-CBA	2.53	119.83	111.91
31	c	516	BCR	C38-C26-C27	2.53	118.47	113.62
26	R	316	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
26	Q	313	CHL	O2D-CGD-O1D	-2.53	118.90	123.84
27	u	319	NEX	C4-C3-C2	-2.52	105.90	110.77
22	b	612	CLA	C3B-C4B-NB	-2.52	108.17	110.52
22	S	304	CLA	C3B-C4B-NB	-2.52	108.17	110.52
26	6	314	CHL	C3B-C4B-NB	2.52	112.86	110.52
33	a	411	PL9	C7-C3-C2	-2.52	119.98	123.30
22	x	201	CLA	CMB-C2B-C3B	2.52	132.70	126.59
22	u	303	CLA	CHB-C1B-NB	2.52	126.93	124.26
33	d	404	PL9	C15-C14-C16	2.52	119.52	115.27
26	q	311	CHL	C4D-CHA-C1A	-2.52	118.18	121.25
22	R	309	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	S	309	CLA	C3B-C4B-NB	-2.52	108.17	110.52
22	n	305	CLA	CAD-C3D-C2D	2.52	152.97	140.80
27	n	319	NEX	C24-C23-C22	-2.52	105.90	110.77
26	p	315	CHL	CHD-C1D-C2D	2.52	130.77	125.48
23	n	310	LUT	C22-C23-C24	-2.52	108.87	111.74
26	U	316	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
22	V	302	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
33	D	405	PL9	C25-C24-C26	2.52	119.51	115.27
26	Q	316	CHL	CHC-C4B-NB	-2.52	121.59	124.26
22	B	608	CLA	C3B-C4B-NB	-2.52	108.18	110.52
26	Q	316	CHL	O2D-CGD-O1D	-2.52	118.91	123.84
26	p	314	CHL	CMB-C2B-C1B	2.52	129.21	125.37
22	B	608	CLA	CMB-C2B-C1B	-2.52	121.53	125.37
23	s	310	LUT	C1-C2-C3	2.52	119.33	113.64
26	v	317	CHL	C4-C3-C5	2.52	119.51	115.27
22	c	514	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
26	4	316	CHL	C1-O2A-CGA	2.52	123.05	116.44
22	1	308	CLA	C3B-C4B-NB	-2.52	108.18	110.52
26	N	313	CHL	CMB-C2B-C1B	2.52	129.20	125.37
22	V	308	CLA	O2D-CGD-O1D	-2.52	118.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	g	303	CLA	CHB-C1B-NB	2.52	126.92	124.26
22	n	307	CLA	C3B-C4B-NB	-2.52	108.18	110.52
22	C	511	CLA	CMB-C2B-C3B	2.52	132.68	126.59
33	A	410	PL9	C7-C3-C2	-2.51	119.99	123.30
27	r	617	NEX	C24-C23-C22	-2.51	105.92	110.77
23	p	310	LUT	C38-C25-C24	-2.51	118.18	123.56
23	U	310	LUT	C7-C8-C9	-2.51	122.44	126.23
33	d	404	PL9	C27-C28-C29	-2.51	121.61	127.66
26	N	316	CHL	C4-C3-C5	2.51	119.50	115.27
22	Q	301	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
30	d	401	PHO	O1D-CGD-CBD	2.51	128.92	124.74
23	5	310	LUT	C18-C5-C6	-2.51	121.71	124.53
34	W	201	LMG	C6-C5-C4	-2.51	107.12	113.00
22	s	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	r	615	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
26	v	315	CHL	C1C-C2C-C3C	-2.51	105.12	107.11
30	a	407	PHO	O2D-CGD-O1D	-2.51	118.93	123.84
22	b	613	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	Q	306	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	2	311	XAT	C10-C11-C12	-2.51	115.39	123.22
26	q	314	CHL	CHB-C4A-NA	2.51	127.98	124.51
26	2	314	CHL	CHD-C4C-C3C	-2.51	121.15	124.84
26	S	316	CHL	O2D-CGD-O1D	-2.51	118.94	123.84
33	d	404	PL9	C25-C24-C26	2.51	119.49	115.27
22	c	503	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
23	S	310	LUT	C10-C11-C12	-2.51	115.39	123.22
23	u	310	LUT	C39-C29-C28	2.51	122.03	118.08
31	d	403	BCR	C35-C13-C12	2.51	122.03	118.08
26	q	312	CHL	C2D-C1D-ND	2.51	111.95	110.10
27	2	319	NEX	C35-C15-C14	-2.51	118.34	123.47
22	G	307	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
22	p	302	CLA	CHB-C1B-NB	2.51	126.91	124.26
26	u	316	CHL	O2A-CGA-CBA	2.51	119.77	111.91
22	X	202	CLA	CMB-C2B-C3B	2.50	132.66	126.59
25	B	622	LHG	O8-C23-C24	2.50	119.77	111.91
23	n	309	LUT	C31-C30-C29	-2.50	123.74	127.31
23	s	310	LUT	C15-C14-C13	-2.50	123.74	127.31
31	b	619	BCR	C7-C8-C9	-2.50	122.45	126.23
26	2	315	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
31	c	515	BCR	C16-C15-C14	-2.50	118.35	123.47
26	u	314	CHL	CMB-C2B-C1B	2.50	129.18	125.37
25	G	310	LHG	O8-C23-C24	2.50	119.76	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	501	LMG	O8-C28-C29	2.50	119.76	111.91
22	g	306	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	N	309	LUT	C30-C31-C32	-2.50	115.42	123.22
26	G	314	CHL	CHC-C4B-NB	-2.50	121.61	124.26
26	s	316	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
22	N	308	CLA	C3B-C4B-NB	-2.50	108.20	110.52
26	6	301	CHL	C4-C3-C5	2.50	119.47	115.27
22	1	303	CLA	C3B-C4B-NB	-2.50	108.20	110.52
32	L	102	SQD	O6-C1-C2	2.50	112.20	108.30
30	A	407	PHO	O2D-CGD-O1D	-2.50	118.96	123.84
26	3	313	CHL	C4A-NA-C1A	2.50	107.83	106.71
22	C	504	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
22	A	404	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	n	305	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
22	2	301	CLA	C3B-C4B-NB	-2.49	108.20	110.52
22	b	608	CLA	C3B-C4B-NB	-2.49	108.20	110.52
34	c	520	LMG	O8-C28-C29	2.49	119.73	111.91
26	P	319	CHL	C4-C3-C5	2.49	119.47	115.27
23	p	310	LUT	C8-C7-C6	-2.49	120.20	127.20
22	G	302	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	n	306	CLA	CMB-C2B-C3B	2.49	132.62	126.59
22	C	505	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	p	304	CLA	C1-C2-C3	-2.49	122.72	126.75
30	d	401	PHO	C4A-C3A-C2A	-2.49	100.47	102.84
22	Q	301	CLA	CHB-C4A-NA	2.49	127.96	124.51
26	r	619	CHL	O2D-CGD-O1D	-2.49	118.97	123.84
22	5	305	CLA	CAD-C3D-C2D	2.49	152.82	140.80
22	g	307	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
26	q	314	CHL	O2A-CGA-CBA	2.49	119.72	111.91
33	d	404	PL9	C35-C34-C36	2.49	119.46	115.27
27	N	318	NEX	C16-C1-C6	2.49	112.70	110.47
26	p	319	CHL	CHB-C4A-NA	2.49	127.95	124.51
22	4	302	CLA	CHB-C1B-NB	2.49	126.89	124.26
26	n	318	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
22	4	302	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	V	318	CHL	C1D-ND-C4D	-2.49	104.57	106.33
22	u	303	CLA	C3B-C4B-NB	-2.49	108.21	110.52
26	V	318	CHL	C4-C3-C5	2.49	119.45	115.27
22	G	306	CLA	C3B-C4B-NB	-2.49	108.21	110.52
22	P	302	CLA	CMB-C2B-C3B	2.49	132.61	126.59
26	n	316	CHL	CED-O2D-CGD	2.48	121.56	115.94
26	1	318	CHL	O2A-CGA-CBA	2.48	119.70	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	304	CLA	C1-C2-C3	-2.48	121.75	126.04
26	3	311	CHL	O2A-CGA-CBA	2.48	119.70	111.91
22	r	608	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
26	P	318	CHL	O2A-CGA-CBA	2.48	119.70	111.91
33	D	405	PL9	C15-C14-C16	2.48	119.45	115.27
22	B	606	CLA	C3B-C4B-NB	-2.48	108.21	110.52
26	G	315	CHL	C1C-C2C-C3C	-2.48	105.14	107.11
27	u	320	NEX	C28-C29-C30	2.48	122.75	118.94
27	u	320	NEX	C24-C23-C22	-2.48	105.98	110.77
22	r	607	CLA	C3B-C4B-NB	-2.48	108.21	110.52
23	r	611	LUT	C38-C25-C24	-2.48	118.25	123.56
26	1	316	CHL	O2A-CGA-CBA	2.48	119.69	111.91
23	v	309	LUT	C11-C10-C9	-2.48	123.77	127.31
22	n	303	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
22	B	616	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
23	1	310	LUT	C10-C11-C12	-2.48	115.48	123.22
26	G	315	CHL	CHB-C1B-NB	-2.48	121.63	124.26
31	D	404	BCR	C35-C13-C12	2.48	121.98	118.08
26	6	313	CHL	O2D-CGD-O1D	-2.48	118.99	123.84
22	1	301	CLA	CHB-C1B-NB	2.48	126.88	124.26
23	4	309	LUT	C38-C25-C24	-2.48	118.25	123.56
24	N	311	XAT	C30-C31-C32	-2.48	115.48	123.22
26	G	314	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
22	b	609	CLA	CHB-C1B-NB	2.48	126.88	124.26
23	s	311	LUT	C20-C13-C12	2.48	121.98	118.08
26	p	318	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
26	G	312	CHL	C3D-C4D-ND	2.48	114.25	110.24
23	p	310	LUT	C7-C8-C9	-2.48	122.49	126.23
22	p	308	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	S	301	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
22	P	307	CLA	CMB-C2B-C1B	-2.48	121.60	125.37
22	c	504	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
22	q	304	CLA	CMB-C2B-C3B	2.48	132.59	126.59
26	r	616	CHL	O2A-CGA-CBA	2.48	119.68	111.91
22	U	305	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
22	c	510	CLA	CMB-C2B-C3B	2.48	132.58	126.59
26	n	314	CHL	C2D-C1D-ND	2.48	111.93	110.10
22	5	301	CLA	CMB-C2B-C3B	2.47	132.58	126.59
23	R	312	LUT	C18-C5-C6	-2.47	121.75	124.53
31	b	620	BCR	C34-C9-C8	2.47	121.98	118.08
26	3	315	CHL	C4-C3-C5	2.47	119.43	115.27
22	5	302	CLA	O2D-CGD-O1D	-2.47	119.00	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	306	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
22	2	303	CLA	C3B-C4B-NB	-2.47	108.22	110.52
26	s	314	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
34	C	502	LMG	O8-C28-C29	2.47	119.67	111.91
26	Q	311	CHL	C1-C2-C3	-2.47	121.77	126.04
26	Q	311	CHL	C2A-C1A-CHA	-2.47	119.53	123.86
23	u	310	LUT	C3-C4-C5	-2.47	106.93	111.85
26	q	313	CHL	CHB-C4A-NA	2.47	127.93	124.51
22	2	302	CLA	CHB-C1B-NB	2.47	126.87	124.26
22	r	610	CLA	C3B-C4B-NB	-2.47	108.22	110.52
22	B	603	CLA	C3B-C4B-NB	-2.47	108.22	110.52
23	r	611	LUT	C30-C31-C32	-2.47	115.50	123.22
22	Q	302	CLA	C3B-C4B-NB	-2.47	108.22	110.52
26	G	314	CHL	C1D-ND-C4D	-2.47	104.58	106.33
22	R	309	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
26	G	315	CHL	CMD-C2D-C3D	-2.47	121.93	127.61
22	b	608	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
22	C	515	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
23	2	310	LUT	C3-C4-C5	-2.47	106.94	111.85
26	Q	316	CHL	C4-C3-C5	2.47	119.42	115.27
24	3	309	XAT	C10-C11-C12	-2.47	115.51	123.22
27	n	319	NEX	C31-C30-C29	-2.47	123.79	127.31
22	5	306	CLA	CMB-C2B-C3B	2.47	132.57	126.59
26	R	317	CHL	O2A-CGA-CBA	2.47	119.65	111.91
22	U	301	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
26	P	315	CHL	CED-O2D-CGD	2.47	121.52	115.94
22	a	408	CLA	CHB-C1B-NB	2.47	126.87	124.26
26	u	318	CHL	CMB-C2B-C1B	2.47	129.12	125.37
23	2	309	LUT	C38-C25-C24	-2.47	118.28	123.56
22	N	303	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	a	404	CLA	CAA-C2A-C3A	-2.47	106.03	112.78
26	r	614	CHL	CHB-C4A-NA	2.47	127.92	124.51
22	G	305	CLA	C3B-C4B-NB	-2.47	108.23	110.52
26	p	320	CHL	C4-C3-C5	2.47	119.42	115.27
22	S	303	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
26	4	314	CHL	CHB-C4A-NA	2.46	127.92	124.51
22	s	301	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
33	D	405	PL9	C35-C34-C36	2.46	119.41	115.27
26	3	313	CHL	CHC-C4B-NB	-2.46	121.65	124.26
26	N	313	CHL	C2A-C3A-C4A	-2.46	97.89	101.87
23	V	310	LUT	C3-C4-C5	-2.46	106.95	111.85
26	V	317	CHL	C1-C2-C3	-2.46	121.79	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	302	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	6	305	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
26	Q	314	CHL	C1C-C2C-C3C	-2.46	105.16	107.11
31	b	618	BCR	C33-C5-C6	-2.46	121.77	124.53
22	r	603	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
22	u	305	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
26	V	318	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
26	4	313	CHL	CHC-C4B-NB	-2.46	121.66	124.26
26	P	314	CHL	C1-C2-C3	-2.46	121.79	126.04
32	A	412	SQD	C44-O6-C1	2.46	118.54	113.74
23	P	310	LUT	C30-C31-C32	-2.46	115.55	123.22
26	p	318	CHL	O2A-CGA-CBA	2.46	119.61	111.91
26	g	314	CHL	C4-C3-C5	2.46	119.40	115.27
22	V	307	CLA	O2A-CGA-O1A	-2.46	117.40	123.59
26	U	319	CHL	CHC-C4B-NB	-2.46	121.66	124.26
26	4	317	CHL	C4-C3-C5	2.45	119.40	115.27
22	N	302	CLA	CHB-C4A-NA	2.45	127.91	124.51
26	u	317	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
22	3	301	CLA	CMB-C2B-C3B	2.45	132.53	126.59
26	g	312	CHL	CHC-C4B-NB	-2.45	121.66	124.26
25	d	405	LHG	O8-C23-C24	2.45	119.61	111.91
31	d	403	BCR	C37-C22-C23	2.45	121.94	118.08
23	R	312	LUT	C38-C25-C24	-2.45	118.31	123.56
22	P	305	CLA	C3B-C4B-NB	-2.45	108.24	110.52
22	N	307	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
26	3	312	CHL	C2D-C1D-ND	2.45	111.91	110.10
26	u	317	CHL	CMD-C2D-C3D	-2.45	121.97	127.61
22	S	307	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
22	Q	302	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	s	304	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	C	518	BCR	C38-C26-C27	2.45	118.33	113.62
26	4	315	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
26	n	313	CHL	OMC-CMC-C2C	-2.45	120.15	125.69
26	g	316	CHL	C4-C3-C5	2.45	119.39	115.27
22	N	303	CLA	CHB-C1B-NB	2.45	126.85	124.26
26	P	314	CHL	O2A-CGA-O1A	-2.45	117.41	123.59
22	5	306	CLA	C2A-C1A-CHA	2.45	128.14	123.86
22	b	616	CLA	C2A-C1A-CHA	2.45	128.14	123.86
31	B	620	BCR	C34-C9-C8	2.45	121.94	118.08
26	g	311	CHL	C1-C2-C3	-2.45	121.81	126.04
26	1	315	CHL	C1C-C2C-C3C	-2.45	105.17	107.11
31	k	101	BCR	C16-C15-C14	-2.45	118.46	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	p	302	CLA	CMB-C2B-C3B	2.45	132.52	126.59
22	B	609	CLA	CHB-C1B-NB	2.45	126.85	124.26
26	G	316	CHL	C4-C3-C5	2.45	119.39	115.27
22	4	306	CLA	C3B-C4B-NB	-2.45	108.24	110.52
22	q	302	CLA	C3B-C4B-NB	-2.45	108.24	110.52
24	4	311	XAT	C11-C10-C9	-2.45	123.81	127.31
22	B	605	CLA	C2A-C1A-CHA	2.45	128.14	123.86
26	2	317	CHL	C1-C2-C3	-2.45	121.81	126.04
22	A	404	CLA	CAA-CBA-CGA	-2.45	106.10	113.25
22	u	306	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
22	b	609	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	q	312	CHL	C4D-CHA-C1A	-2.45	118.27	121.25
26	6	312	CHL	C2A-C1A-CHA	-2.45	119.58	123.86
25	D	406	LHG	O8-C23-C24	2.45	119.58	111.91
22	U	304	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	S	305	CLA	CHB-C4A-NA	2.45	127.89	124.51
26	p	315	CHL	C2D-C1D-ND	2.45	111.91	110.10
36	A	414	DGD	O1G-C1A-C2A	2.44	119.58	111.91
31	B	620	BCR	C33-C5-C6	-2.44	121.78	124.53
27	r	617	NEX	C28-C29-C30	2.44	122.69	118.94
32	m	101	SQD	O6-C1-C2	2.44	112.12	108.30
24	n	311	XAT	C39-C29-C28	2.44	121.93	118.08
22	A	408	CLA	CHB-C1B-NB	2.44	126.84	124.26
22	b	611	CLA	C3B-C4B-NB	-2.44	108.25	110.52
26	5	313	CHL	C1-C2-C3	-2.44	121.82	126.04
26	P	315	CHL	CAC-C3C-C4C	2.44	127.98	124.81
22	p	306	CLA	CAD-C3D-C2D	2.44	152.59	140.80
22	B	609	CLA	C3B-C4B-NB	-2.44	108.25	110.52
26	6	313	CHL	C2D-C1D-ND	2.44	111.90	110.10
26	u	315	CHL	CMB-C2B-C1B	2.44	129.09	125.37
23	V	309	LUT	C3-C4-C5	-2.44	106.99	111.85
22	n	301	CLA	CHB-C4A-NA	2.44	127.89	124.51
26	3	316	CHL	O2A-CGA-CBA	2.44	119.57	111.91
22	q	303	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	S	301	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
26	N	314	CHL	C2D-C1D-ND	2.44	111.90	110.10
27	u	320	NEX	C15-C35-C34	-2.44	118.47	123.47
23	p	311	LUT	C11-C10-C9	-2.44	123.83	127.31
36	a	416	DGD	O1G-C1A-C2A	2.44	119.57	111.91
26	p	315	CHL	CAC-C3C-C4C	2.44	127.98	124.81
34	W	201	LMG	O8-C28-C29	2.44	119.56	111.91
22	1	302	CLA	O2D-CGD-O1D	-2.44	119.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	408	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
22	U	306	CLA	C2A-C1A-CHA	2.44	128.12	123.86
24	v	311	XAT	C30-C31-C32	-2.44	115.61	123.22
34	w	201	LMG	O6-C5-C4	2.44	114.12	109.69
26	u	317	CHL	C2A-C1A-CHA	-2.44	119.59	123.86
23	4	310	LUT	C16-C1-C6	-2.44	106.34	110.30
26	P	316	CHL	CHC-C4B-NB	-2.44	121.68	124.26
26	g	312	CHL	C4A-NA-C1A	2.44	107.80	106.71
26	Q	315	CHL	CMD-C2D-C3D	-2.44	122.01	127.61
23	S	311	LUT	C20-C13-C12	2.44	121.92	118.08
22	b	616	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
34	b	624	LMG	O8-C28-C29	2.44	119.56	111.91
23	s	311	LUT	C7-C8-C9	-2.44	122.55	126.23
23	s	310	LUT	C10-C11-C12	-2.44	115.61	123.22
22	s	305	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	B	611	CLA	C3B-C4B-NB	-2.44	108.25	110.52
36	b	601	DGD	O6E-C5E-C4E	2.44	114.12	109.69
23	1	310	LUT	C18-C5-C4	2.43	118.87	114.36
26	N	313	CHL	C4D-CHA-C1A	-2.43	118.29	121.25
26	V	318	CHL	CHC-C4B-NB	-2.43	121.68	124.26
37	E	101	HEM	CMB-C2B-C1B	-2.43	121.33	125.04
23	4	310	LUT	C22-C23-C24	-2.43	108.97	111.74
26	r	615	CHL	C4-C3-C5	2.43	119.36	115.27
26	g	312	CHL	C1D-ND-C4D	-2.43	104.61	106.33
24	4	311	XAT	C30-C31-C32	-2.43	115.63	123.22
24	n	311	XAT	C11-C12-C13	-2.43	119.59	126.42
22	C	507	CLA	O1D-CGD-CBD	2.43	129.46	124.48
23	5	310	LUT	C22-C23-C24	-2.43	108.98	111.74
31	D	404	BCR	C37-C22-C23	2.43	121.90	118.08
23	U	309	LUT	C22-C23-C24	2.43	114.50	111.74
26	v	317	CHL	C2A-C1A-CHA	-2.43	119.61	123.86
26	n	318	CHL	C1D-ND-C4D	-2.43	104.61	106.33
26	U	316	CHL	C4-C3-C5	2.43	119.36	115.27
26	Q	314	CHL	C4-C3-C5	2.43	119.35	115.27
26	4	313	CHL	C1C-C2C-C3C	-2.43	105.19	107.11
23	5	309	LUT	C35-C15-C14	-2.43	118.50	123.47
22	c	506	CLA	O1D-CGD-CBD	2.43	129.45	124.48
31	B	620	BCR	C11-C10-C9	-2.43	123.85	127.31
22	N	305	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	B	617	CLA	CMB-C2B-C3B	2.43	132.46	126.59
22	S	304	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
22	p	303	CLA	O2D-CGD-O1D	-2.43	119.10	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	303	CLA	C3B-C4B-NB	-2.43	108.27	110.52
26	V	313	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
25	D	407	LHG	O8-C23-C24	2.42	119.52	111.91
22	q	301	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
26	q	313	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
22	a	404	CLA	CAA-CBA-CGA	-2.42	106.17	113.25
26	3	312	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
22	3	304	CLA	CMB-C2B-C3B	2.42	132.46	126.59
26	g	315	CHL	OMC-CMC-C2C	-2.42	120.21	125.69
26	N	313	CHL	C1-C2-C3	-2.42	121.85	126.04
26	3	312	CHL	C3D-C4D-ND	2.42	114.16	110.24
26	6	313	CHL	C3D-C4D-ND	2.42	114.16	110.24
23	1	310	LUT	C22-C23-C24	-2.42	108.98	111.74
26	q	311	CHL	C2A-C1A-CHA	-2.42	119.62	123.86
22	b	603	CLA	C3B-C4B-NB	-2.42	108.27	110.52
26	p	316	CHL	CHC-C4B-NB	-2.42	121.69	124.26
22	q	306	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	P	306	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	a	405	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	C	513	CLA	C3B-C4B-NB	-2.42	108.27	110.52
26	3	311	CHL	O2D-CGD-O1D	-2.42	119.11	123.84
26	q	312	CHL	O2A-CGA-CBA	2.42	119.50	111.91
26	U	319	CHL	O2A-CGA-CBA	2.42	119.50	111.91
26	3	313	CHL	C1C-C2C-C3C	-2.42	105.19	107.11
26	v	313	CHL	CHC-C4B-NB	-2.42	121.70	124.26
22	B	614	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	c	512	CLA	C3B-C4B-NB	-2.42	108.27	110.52
31	b	618	BCR	C16-C15-C14	-2.42	118.52	123.47
22	r	609	CLA	C2A-C1A-CHA	2.42	128.09	123.86
34	B	624	LMG	O8-C28-C29	2.42	119.49	111.91
26	1	316	CHL	CGD-CBD-CAD	-2.42	102.91	110.73
23	P	310	LUT	C35-C15-C14	-2.42	118.52	123.47
31	t	101	BCR	C15-C16-C17	-2.42	118.52	123.47
22	6	303	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	v	308	CLA	C3B-C4B-NB	-2.42	108.27	110.52
22	c	511	CLA	CHB-C4A-NA	2.42	127.85	124.51
34	b	621	LMG	O8-C28-C29	2.42	119.49	111.91
22	5	307	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
22	g	304	CLA	CMB-C2B-C1B	-2.41	121.69	125.37
23	u	310	LUT	C7-C8-C9	-2.41	122.59	126.23
22	A	405	CLA	O2D-CGD-O1D	-2.41	119.12	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	406	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
22	q	302	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	u	304	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	N	309	LUT	C18-C5-C6	-2.41	121.82	124.53
22	b	609	CLA	C3B-C4B-NB	-2.41	108.28	110.52
26	6	314	CHL	C4A-NA-C1A	2.41	107.79	106.71
26	U	315	CHL	C4D-CHA-C1A	-2.41	118.31	121.25
34	w	201	LMG	O8-C28-C29	2.41	119.48	111.91
22	q	307	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
25	n	312	LHG	O8-C23-C24	2.41	119.48	111.91
22	r	603	CLA	C3B-C4B-NB	-2.41	108.28	110.52
22	U	301	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	r	609	CLA	C1-C2-C3	-2.41	121.87	126.04
22	B	610	CLA	C4-C3-C5	2.41	119.33	115.27
26	3	315	CHL	CHB-C4A-NA	2.41	127.84	124.51
26	6	315	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
26	q	314	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
27	2	319	NEX	C30-C31-C32	-2.41	115.70	123.22
26	v	318	CHL	C4-C3-C5	2.41	119.32	115.27
22	S	303	CLA	C1-C2-C3	-2.41	122.85	126.75
26	2	314	CHL	OMC-CMC-C2C	-2.41	120.24	125.69
22	c	502	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
31	T	101	BCR	C15-C16-C17	-2.41	118.54	123.47
22	X	202	CLA	O2D-CGD-CBD	2.41	115.55	111.27
26	p	315	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
26	p	316	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
34	b	621	LMG	C1-O6-C5	2.41	118.41	113.69
23	U	309	LUT	C30-C31-C32	-2.41	115.71	123.22
22	5	308	CLA	C3B-C4B-NB	-2.41	108.28	110.52
22	V	303	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
23	P	310	LUT	C38-C25-C24	-2.40	118.41	123.56
22	x	201	CLA	O2D-CGD-CBD	2.40	115.54	111.27
26	n	313	CHL	C4-C3-C5	2.40	119.32	115.27
22	s	301	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
26	q	312	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
22	N	306	CLA	CMB-C2B-C3B	2.40	132.41	126.59
22	v	307	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
33	D	405	PL9	C30-C29-C31	2.40	119.31	115.27
22	C	503	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
34	W	201	LMG	O6-C5-C4	2.40	114.06	109.69
26	v	313	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
25	A	413	LHG	O8-C23-C24	2.40	119.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	303	CLA	CHB-C1B-NB	2.40	126.80	124.26
23	N	310	LUT	C1-C2-C3	2.40	119.07	113.64
26	p	314	CHL	C4-C3-C5	2.40	119.31	115.27
26	P	317	CHL	C4D-CHA-C1A	-2.40	118.33	121.25
22	4	307	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
26	6	312	CHL	O2D-CGD-O1D	-2.40	119.14	123.84
23	V	310	LUT	C10-C11-C12	-2.40	115.73	123.22
25	q	310	LHG	O8-C23-C24	2.40	119.44	111.91
22	p	305	CLA	C3B-C4B-NB	-2.40	108.29	110.52
26	2	314	CHL	C3B-C4B-NB	2.40	112.74	110.52
22	4	306	CLA	CHB-C1B-NB	2.40	126.80	124.26
26	6	301	CHL	CGD-CBD-CAD	-2.40	102.97	110.73
26	N	317	CHL	C4-C3-C5	2.40	119.30	115.27
26	g	315	CHL	CHB-C1B-NB	-2.40	121.72	124.26
22	G	304	CLA	C3B-C4B-NB	-2.40	108.29	110.52
33	d	404	PL9	C30-C29-C31	2.40	119.30	115.27
27	u	320	NEX	C16-C1-C6	2.40	112.62	110.47
27	5	319	NEX	C17-C1-C6	-2.40	108.33	110.47
26	Q	314	CHL	CHC-C4B-NB	-2.40	121.72	124.26
26	5	314	CHL	C3D-C4D-ND	2.39	114.11	110.24
26	G	311	CHL	C4D-CHA-C1A	-2.39	118.33	121.25
31	b	620	BCR	C20-C21-C22	-2.39	123.89	127.31
26	s	314	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
25	d	406	LHG	O8-C23-C24	2.39	119.42	111.91
24	g	309	XAT	C15-C35-C34	-2.39	118.57	123.47
26	3	314	CHL	C4-C3-C5	2.39	119.30	115.27
31	A	409	BCR	C38-C26-C27	2.39	118.21	113.62
27	5	319	NEX	C28-C29-C30	2.39	122.61	118.94
22	Q	306	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	1	317	CHL	C4-C3-C5	2.39	119.30	115.27
23	r	611	LUT	C10-C11-C12	-2.39	115.75	123.22
26	u	317	CHL	C4-C3-C5	2.39	119.30	115.27
23	4	309	LUT	C3-C4-C5	-2.39	107.09	111.85
22	2	301	CLA	CMB-C2B-C3B	2.39	132.38	126.59
26	N	313	CHL	CHC-C4B-NB	-2.39	121.72	124.26
22	u	307	CLA	CHC-C4B-NB	2.39	126.79	124.26
27	r	617	NEX	C19-C9-C10	-2.39	119.57	122.92
26	Q	313	CHL	CHB-C4A-NA	2.39	127.82	124.51
24	R	313	XAT	C19-C9-C8	2.39	121.84	118.08
22	C	509	CLA	C2A-C1A-CHA	2.39	128.04	123.86
22	N	301	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	S	314	CHL	O2D-CGD-O1D	-2.39	119.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	s	311	LUT	C38-C25-C24	-2.39	118.44	123.56
25	a	415	LHG	O8-C23-C24	2.39	119.41	111.91
26	1	317	CHL	O2A-CGA-CBA	2.39	119.41	111.91
26	R	317	CHL	C1D-ND-C4D	-2.39	104.64	106.33
31	C	518	BCR	C10-C11-C12	-2.39	115.76	123.22
22	g	307	CLA	C3B-C4B-NB	-2.39	108.30	110.52
37	e	101	HEM	CMB-C2B-C1B	-2.39	121.40	125.04
22	A	405	CLA	C2A-C1A-CHA	2.39	128.04	123.86
26	P	314	CHL	C4-C3-C5	2.39	119.29	115.27
26	5	318	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
26	P	317	CHL	CHC-C4B-NB	-2.39	121.73	124.26
22	n	302	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	c	508	CLA	C2A-C1A-CHA	2.39	128.03	123.86
31	b	620	BCR	C33-C5-C6	-2.39	121.85	124.53
26	1	314	CHL	C4D-CHA-C1A	-2.39	118.34	121.25
23	u	309	LUT	C3-C4-C5	-2.39	107.10	111.85
22	g	301	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	2	303	CLA	C1-C2-C3	-2.39	122.89	126.75
23	P	311	LUT	C7-C8-C9	-2.39	122.63	126.23
30	A	407	PHO	C1C-C2C-C3C	-2.38	106.63	108.61
22	2	305	CLA	C3B-C4B-NB	-2.38	108.30	110.52
26	S	315	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
31	t	101	BCR	C1-C6-C7	2.38	122.52	115.78
36	J	101	DGD	O6D-C5D-C4D	2.38	114.02	109.69
26	V	317	CHL	C2A-C1A-CHA	-2.38	119.69	123.86
23	4	309	LUT	C18-C5-C6	-2.38	121.85	124.53
26	N	314	CHL	C3D-C4D-ND	2.38	114.09	110.24
22	2	305	CLA	CAD-C3D-C2D	2.38	152.29	140.80
26	r	619	CHL	CAA-C2A-C3A	-2.38	106.26	112.78
31	B	620	BCR	C21-C20-C19	-2.38	115.79	123.22
26	q	314	CHL	CMD-C2D-C3D	-2.38	122.14	127.61
26	p	318	CHL	C1-C2-C3	-2.38	121.93	126.04
22	3	306	CLA	C3B-C4B-NB	-2.38	108.31	110.52
32	M	101	SQD	O6-C1-C2	2.38	112.02	108.30
23	s	310	LUT	C39-C29-C28	2.38	121.83	118.08
22	Q	303	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	6	316	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
22	R	310	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
22	n	303	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	s	313	CHL	C4A-NA-C1A	2.38	107.78	106.71
30	a	407	PHO	C1C-C2C-C3C	-2.38	106.63	108.61
31	c	515	BCR	C36-C18-C19	2.38	121.82	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	316	CHL	O2A-CGA-CBA	2.38	119.37	111.91
23	S	310	LUT	C39-C29-C28	2.38	121.82	118.08
22	a	406	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
27	N	318	NEX	C17-C1-C6	-2.38	108.34	110.47
26	P	316	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
22	3	304	CLA	C3B-C4B-NB	-2.38	108.31	110.52
31	x	202	BCR	C24-C23-C22	-2.38	122.65	126.23
22	N	301	CLA	CMB-C2B-C3B	2.37	132.34	126.59
22	u	301	CLA	CHB-C4A-NA	2.37	127.80	124.51
22	s	305	CLA	C1-C2-C3	-2.37	121.94	126.04
26	U	315	CHL	C1-C2-C3	-2.37	121.94	126.04
26	n	315	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
22	V	303	CLA	CHB-C1B-NB	2.37	126.77	124.26
26	u	313	CHL	CHB-C4A-NA	2.37	127.79	124.51
26	g	314	CHL	CED-O2D-CGD	2.37	121.30	115.94
22	q	303	CLA	CHB-C1B-NB	2.37	126.77	124.26
26	p	317	CHL	C4D-CHA-C1A	-2.37	118.36	121.25
31	K	101	BCR	C16-C15-C14	-2.37	118.62	123.47
26	3	314	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
26	n	317	CHL	C4-C3-C5	2.37	119.26	115.27
22	q	304	CLA	O1D-CGD-CBD	2.37	129.33	124.48
22	S	301	CLA	C1-C2-C3	-2.37	121.94	126.04
22	v	301	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	Q	304	CLA	O1D-CGD-CBD	2.37	129.33	124.48
24	U	311	XAT	C35-C34-C33	-2.37	123.93	127.31
22	6	308	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
22	a	405	CLA	C3B-C4B-NB	-2.37	108.32	110.52
23	5	309	LUT	C15-C35-C34	-2.37	118.62	123.47
26	5	317	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
26	n	314	CHL	C4D-CHA-C1A	-2.37	118.37	121.25
26	5	318	CHL	CHB-C4A-NA	2.37	127.78	124.51
22	b	614	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
26	v	317	CHL	OMC-CMC-C2C	-2.37	120.34	125.69
26	p	317	CHL	O1D-CGD-CBD	-2.37	119.64	124.48
22	a	405	CLA	C2A-C1A-CHA	2.37	128.00	123.86
22	q	301	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	2	314	CHL	CHD-C1D-C2D	2.36	130.44	125.48
22	B	605	CLA	CAA-CBA-CGA	-2.36	106.35	113.25
22	u	301	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
26	5	313	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
30	D	401	PHO	C4A-C3A-C2A	-2.36	100.59	102.84
22	r	607	CLA	C2A-C1A-CHA	2.36	127.99	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n	318	CHL	C4-C3-C5	2.36	119.24	115.27
22	s	301	CLA	C1-C2-C3	-2.36	121.96	126.04
24	p	312	XAT	C11-C10-C9	-2.36	123.94	127.31
22	Q	301	CLA	CMB-C2B-C3B	2.36	132.30	126.59
22	b	610	CLA	C3B-C4B-NB	-2.36	108.33	110.52
26	4	316	CHL	C4-C3-C5	2.36	119.24	115.27
23	s	311	LUT	C18-C5-C4	2.36	118.72	114.36
26	p	316	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
22	C	512	CLA	C3B-C4B-NB	-2.36	108.33	110.52
26	g	314	CHL	C1-C2-C3	-2.36	121.97	126.04
26	4	315	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
24	5	311	XAT	C30-C31-C32	-2.36	115.86	123.22
23	S	311	LUT	C7-C8-C9	-2.36	122.67	126.23
22	N	302	CLA	CHB-C1B-NB	2.36	126.75	124.26
22	B	614	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
26	r	614	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
22	B	610	CLA	C3B-C4B-NB	-2.36	108.33	110.52
26	6	317	CHL	C2A-C1A-CHA	-2.36	119.74	123.86
27	p	301	NEX	C11-C12-C13	-2.35	119.80	126.42
26	g	313	CHL	O2A-CGA-CBA	2.35	119.29	111.91
22	b	614	CLA	C3B-C4B-NB	-2.35	108.33	110.52
24	r	612	XAT	C27-C28-C29	2.35	129.18	125.53
31	C	517	BCR	C16-C15-C14	-2.35	118.65	123.47
26	v	317	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
22	V	301	CLA	CHB-C4A-NA	2.35	127.77	124.51
31	K	101	BCR	C21-C20-C19	-2.35	115.88	123.22
26	p	320	CHL	CED-O2D-CGD	2.35	121.26	115.94
22	A	405	CLA	C3B-C4B-NB	-2.35	108.33	110.52
22	n	308	CLA	C2A-C1A-CHA	2.35	127.97	123.86
26	s	315	CHL	O2D-CGD-O1D	-2.35	119.24	123.84
22	C	508	CLA	CHB-C1B-NB	2.35	126.75	124.26
31	C	517	BCR	C36-C18-C19	2.35	121.78	118.08
26	u	318	CHL	C4-C3-C5	2.35	119.22	115.27
22	v	306	CLA	C2A-C1A-CHA	2.35	127.97	123.86
27	N	318	NEX	C11-C12-C13	-2.35	119.81	126.42
22	C	512	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	u	315	CHL	OMC-CMC-C2C	-2.35	120.37	125.69
26	V	316	CHL	C4-C3-C5	2.35	119.22	115.27
26	v	316	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
22	g	305	CLA	O2D-CGD-CBD	2.35	115.44	111.27
23	p	310	LUT	C30-C31-C32	-2.35	115.89	123.22
22	6	304	CLA	CHB-C1B-NB	2.35	126.74	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v	318	CHL	CMD-C2D-C3D	-2.35	122.22	127.61
26	q	312	CHL	C3D-C4D-ND	2.35	114.03	110.24
23	2	310	LUT	C18-C5-C4	2.35	118.70	114.36
22	r	602	CLA	C3B-C4B-NB	-2.35	108.34	110.52
26	p	316	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
26	u	316	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
26	4	316	CHL	O2A-CGA-CBA	2.35	119.27	111.91
22	b	602	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
36	C	520	DGD	C1E-C2E-C3E	2.35	114.88	110.00
22	6	305	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
26	g	316	CHL	O2A-CGA-CBA	2.34	119.27	111.91
31	k	101	BCR	C21-C20-C19	-2.34	115.90	123.22
22	c	503	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
26	5	317	CHL	C1-C2-C3	-2.34	121.99	126.04
26	6	301	CHL	O1D-CGD-CBD	-2.34	119.69	124.48
26	3	311	CHL	C2A-C1A-CHA	-2.34	119.76	123.86
22	v	305	CLA	C3B-C4B-NB	-2.34	108.34	110.52
22	Q	303	CLA	C1-C2-C3	-2.34	122.96	126.75
22	r	606	CLA	C3B-C4B-NB	-2.34	108.34	110.52
26	6	317	CHL	O2A-CGA-CBA	2.34	119.26	111.91
26	3	315	CHL	CMD-C2D-C3D	-2.34	122.23	127.61
26	N	315	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
22	R	308	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
24	P	312	XAT	C30-C31-C32	-2.34	115.92	123.22
24	p	312	XAT	C30-C31-C32	-2.34	115.92	123.22
31	b	620	BCR	C11-C10-C9	-2.34	123.97	127.31
26	p	319	CHL	O2A-CGA-CBA	2.34	119.25	111.91
26	2	314	CHL	C2D-C1D-ND	2.34	111.83	110.10
22	n	308	CLA	O2D-CGD-CBD	2.34	115.42	111.27
26	V	318	CHL	C1-C2-C3	-2.34	122.00	126.04
26	N	316	CHL	OMC-CMC-C2C	-2.34	120.41	125.69
22	P	302	CLA	CHD-C1D-ND	-2.33	122.31	124.45
22	N	304	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
22	S	301	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
22	b	613	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
26	P	316	CHL	O2D-CGD-O1D	-2.33	119.28	123.84
26	v	316	CHL	C4-C3-C5	2.33	119.19	115.27
23	U	309	LUT	C35-C15-C14	-2.33	118.70	123.47
26	2	313	CHL	C1D-ND-C4D	-2.33	104.68	106.33
26	Q	311	CHL	C4D-CHA-C1A	-2.33	118.42	121.25
26	1	318	CHL	C4-C3-C5	2.33	119.19	115.27
26	u	316	CHL	C1-C2-C3	-2.33	122.02	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	513	CLA	C2A-C1A-CHA	2.33	127.93	123.86
26	Q	315	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
22	R	309	CLA	CHB-C1B-NB	2.33	126.72	124.26
26	U	316	CHL	O2A-CGA-O1A	-2.33	117.72	123.59
26	N	313	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
22	n	302	CLA	CHB-C1B-NB	2.33	126.72	124.26
26	S	316	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
31	B	618	BCR	C16-C15-C14	-2.33	118.71	123.47
26	p	314	CHL	O1D-CGD-CBD	-2.33	119.73	124.48
26	q	315	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
22	B	616	CLA	C3B-C4B-NB	-2.33	108.36	110.52
26	u	314	CHL	C1C-C2C-C3C	-2.33	105.27	107.11
26	p	314	CHL	C1-C2-C3	-2.32	122.02	126.04
26	G	316	CHL	C1-C2-C3	-2.32	122.02	126.04
24	n	311	XAT	C19-C9-C8	2.32	121.74	118.08
22	b	617	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
23	5	309	LUT	C38-C25-C24	-2.32	118.59	123.56
27	V	319	NEX	C16-C1-C6	2.32	112.55	110.47
31	x	202	BCR	C34-C9-C10	-2.32	119.67	122.92
22	c	511	CLA	C3B-C4B-NB	-2.32	108.36	110.52
22	b	611	CLA	C2A-C1A-CHA	2.32	127.92	123.86
23	v	310	LUT	C10-C11-C12	-2.32	115.97	123.22
22	A	405	CLA	CHB-C1B-NB	2.32	126.72	124.26
26	r	614	CHL	CHC-C4B-NB	-2.32	121.80	124.26
22	r	607	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
22	B	611	CLA	C2A-C1A-CHA	2.32	127.92	123.86
23	u	310	LUT	C22-C23-C24	-2.32	109.10	111.74
26	U	314	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
26	n	318	CHL	O1D-CGD-CBD	-2.32	119.73	124.48
22	u	306	CLA	C3B-C4B-NB	-2.32	108.36	110.52
22	R	307	CLA	C3B-C4B-NB	-2.32	108.36	110.52
23	N	309	LUT	C10-C11-C12	-2.32	115.97	123.22
23	v	309	LUT	C16-C1-C6	-2.32	106.54	110.30
26	V	317	CHL	C4D-CHA-C1A	-2.32	118.43	121.25
22	G	301	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	P	318	CHL	C1C-C2C-C3C	-2.32	105.27	107.11
31	b	618	BCR	C10-C11-C12	-2.32	115.98	123.22
26	n	313	CHL	O2A-CGA-CBA	2.32	119.18	111.91
27	v	319	NEX	C17-C1-C6	-2.32	108.40	110.47
26	R	315	CHL	O2D-CGD-O1D	-2.32	119.31	123.84
31	C	516	BCR	C34-C9-C8	2.32	121.73	118.08
22	b	613	CLA	CAA-CBA-CGA	-2.32	106.48	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	410	SQD	O48-C23-C24	2.32	119.18	111.91
26	Q	315	CHL	C4-C3-C5	2.32	119.17	115.27
22	B	613	CLA	CAA-CBA-CGA	-2.32	106.48	113.25
26	v	313	CHL	CHB-C4A-NA	2.32	127.72	124.51
24	G	309	XAT	C15-C35-C34	-2.32	118.73	123.47
22	V	303	CLA	C3B-C4B-NB	-2.32	108.37	110.52
22	R	305	CLA	C3B-C4B-NB	-2.32	108.37	110.52
27	2	319	NEX	C17-C1-C6	-2.32	108.40	110.47
23	S	311	LUT	C38-C25-C24	-2.32	118.60	123.56
22	5	303	CLA	C3B-C4B-NB	-2.32	108.37	110.52
26	n	314	CHL	C3B-C4B-NB	2.32	112.66	110.52
27	u	319	NEX	C39-C29-C30	-2.32	119.68	122.92
26	6	316	CHL	C4-C3-C5	2.31	119.17	115.27
33	D	405	PL9	C45-C44-C46	2.31	119.17	115.27
22	a	404	CLA	C3B-C4B-NB	-2.31	108.37	110.52
26	V	316	CHL	C4D-CHA-C1A	-2.31	118.43	121.25
24	r	612	XAT	C19-C9-C8	2.31	121.72	118.08
26	P	316	CHL	C4A-NA-C1A	2.31	107.75	106.71
26	n	316	CHL	C4D-CHA-C1A	-2.31	118.43	121.25
23	2	310	LUT	C31-C30-C29	-2.31	124.01	127.31
22	b	609	CLA	CMB-C2B-C3B	2.31	132.19	126.59
23	p	311	LUT	C10-C11-C12	-2.31	116.00	123.22
31	A	409	BCR	C10-C11-C12	-2.31	116.00	123.22
22	q	303	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
22	1	307	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
26	6	316	CHL	CMD-C2D-C3D	-2.31	122.30	127.61
26	1	315	CHL	C1D-ND-C4D	-2.31	104.69	106.33
22	B	612	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
26	g	312	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
26	R	317	CHL	CMB-C2B-C1B	2.31	128.89	125.37
34	B	621	LMG	C8-O7-C10	-2.31	112.11	117.79
23	1	310	LUT	C18-C5-C6	-2.31	121.94	124.53
23	v	309	LUT	C1-C2-C3	2.31	118.86	113.64
27	N	318	NEX	C31-C30-C29	-2.31	124.02	127.31
26	v	316	CHL	C1-C2-C3	-2.31	122.05	126.04
22	b	605	CLA	CBA-CAA-C2A	2.31	120.67	113.86
22	s	301	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
22	v	304	CLA	CHB-C1B-NB	2.31	126.70	124.26
22	U	304	CLA	CHB-C1B-NB	2.31	126.70	124.26
23	5	309	LUT	C39-C29-C28	2.30	121.71	118.08
23	S	311	LUT	C18-C5-C4	2.30	118.62	114.36
31	D	404	BCR	C23-C24-C25	-2.30	120.73	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	501	SQD	O48-C23-C24	2.30	119.14	111.91
22	V	304	CLA	CMB-C2B-C3B	2.30	132.17	126.59
24	P	312	XAT	C27-C28-C29	-2.30	121.96	125.53
22	3	301	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	5	303	CLA	C1-C2-C3	-2.30	123.03	126.75
26	2	317	CHL	O2A-CGA-O1A	-2.30	117.78	123.59
23	N	310	LUT	C2-C3-C4	2.30	113.45	110.30
23	U	309	LUT	C10-C11-C12	-2.30	116.04	123.22
24	n	311	XAT	C20-C13-C12	2.30	121.70	118.08
26	V	315	CHL	OMC-CMC-C2C	-2.30	120.49	125.69
26	v	313	CHL	O1D-CGD-CBD	-2.30	119.78	124.48
24	g	309	XAT	C36-C21-C26	2.30	116.25	110.05
22	r	609	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
31	a	409	BCR	C38-C26-C27	2.30	118.03	113.62
22	b	604	CLA	CHB-C1B-NB	2.30	126.69	124.26
26	6	314	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
23	1	309	LUT	C10-C11-C12	-2.30	116.04	123.22
22	A	406	CLA	C2D-C1D-ND	-2.30	108.41	110.10
22	b	614	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
22	c	512	CLA	C2A-C1A-CHA	2.30	127.88	123.86
23	n	310	LUT	C1-C6-C5	-2.30	119.38	122.61
31	C	517	BCR	C29-C30-C25	2.30	114.02	110.48
22	u	304	CLA	C3B-C4B-NB	-2.30	108.38	110.52
26	Q	311	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
26	N	315	CHL	O2D-CGD-O1D	-2.30	119.35	123.84
26	p	314	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
26	V	317	CHL	O2A-CGA-O1A	-2.29	117.80	123.59
22	A	404	CLA	C3B-C4B-NB	-2.29	108.39	110.52
26	P	318	CHL	C4-C3-C5	2.29	119.13	115.27
26	1	314	CHL	C1D-ND-C4D	-2.29	104.70	106.33
22	3	307	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
24	p	312	XAT	C31-C30-C29	-2.29	124.04	127.31
27	u	320	NEX	C11-C12-C13	-2.29	119.97	126.42
36	c	519	DGD	O6D-C5D-C4D	2.29	113.86	109.69
23	s	311	LUT	C15-C35-C34	-2.29	118.78	123.47
26	U	316	CHL	C4D-CHA-C1A	-2.29	118.46	121.25
23	N	310	LUT	C11-C10-C9	-2.29	124.04	127.31
26	U	315	CHL	C4D-C3D-CAD	2.29	110.80	108.10
23	s	311	LUT	C30-C31-C32	-2.29	116.06	123.22
32	L	102	SQD	O48-C23-C24	2.29	119.10	111.91
22	v	304	CLA	CMB-C2B-C3B	2.29	132.14	126.59
26	Q	315	CHL	C1C-C2C-C3C	-2.29	105.30	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	317	CHL	C1-C2-C3	-2.29	122.08	126.04
22	b	616	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	3	305	CLA	O2D-CGD-CBD	2.29	115.34	111.27
22	n	301	CLA	CMB-C2B-C3B	2.29	132.13	126.59
27	N	318	NEX	C30-C31-C32	-2.29	116.07	123.22
26	U	317	CHL	O2A-CGA-CBA	2.29	119.09	111.91
24	R	313	XAT	C39-C29-C28	2.29	121.68	118.08
22	B	607	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	b	607	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	C	509	CLA	CHD-C1D-ND	-2.29	122.35	124.45
31	T	101	BCR	C1-C6-C7	2.29	122.25	115.78
31	c	515	BCR	C29-C30-C25	2.29	114.00	110.48
26	U	315	CHL	OMC-CMC-C2C	-2.29	120.52	125.69
26	U	315	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
24	r	612	XAT	C31-C32-C33	-2.29	119.99	126.42
22	2	301	CLA	CHB-C4A-NA	2.29	127.67	124.51
32	C	501	SQD	O5-C1-C2	2.29	115.19	110.35
22	a	406	CLA	C2D-C1D-ND	-2.29	108.42	110.10
22	R	308	CLA	C2A-C1A-CHA	2.29	127.86	123.86
22	r	609	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	R	303	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	u	304	CLA	CHB-C1B-NB	2.28	126.68	124.26
23	V	309	LUT	C31-C30-C29	-2.28	124.05	127.31
23	n	310	LUT	C11-C10-C9	-2.28	124.05	127.31
32	m	101	SQD	O8-S-C6	2.28	109.38	105.74
22	5	301	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	4	315	CHL	C4A-NA-C1A	2.28	107.73	106.71
26	N	316	CHL	C2A-C1A-CHA	-2.28	119.86	123.86
22	a	405	CLA	CHB-C1B-NB	2.28	126.67	124.26
22	1	301	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
22	6	305	CLA	CMB-C2B-C3B	2.28	132.12	126.59
22	q	303	CLA	C1-C2-C3	-2.28	123.06	126.75
26	p	318	CHL	C4-C3-C5	2.28	119.11	115.27
33	d	404	PL9	C45-C44-C46	2.28	119.11	115.27
23	N	310	LUT	C18-C5-C6	-2.28	121.96	124.53
26	1	315	CHL	O2D-CGD-O1D	-2.28	119.37	123.84
32	M	101	SQD	O8-S-C6	2.28	109.38	105.74
26	s	313	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
34	C	502	LMG	C8-O7-C10	-2.28	112.17	117.79
22	Q	302	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	b	604	CLA	C3B-C4B-NB	-2.28	108.40	110.52
32	L	102	SQD	O48-C23-O10	-2.28	117.83	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	6	313	CHL	CAA-C2A-C3A	-2.28	106.53	112.78
26	2	313	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
22	u	303	CLA	O2D-CGD-CBD	2.28	115.32	111.27
26	4	317	CHL	C2A-C1A-CHA	-2.28	119.87	123.86
26	Q	316	CHL	C1-C2-C3	-2.28	122.10	126.04
22	6	306	CLA	O2D-CGD-CBD	2.28	115.32	111.27
26	4	314	CHL	CHC-C4B-NB	-2.28	121.84	124.26
31	B	618	BCR	C10-C11-C12	-2.28	116.10	123.22
22	1	305	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
22	2	307	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
23	S	311	LUT	C30-C31-C32	-2.28	116.11	123.22
36	c	517	DGD	C6D-C5D-C4D	-2.28	107.33	112.09
23	P	310	LUT	C31-C30-C29	-2.28	124.06	127.31
26	3	313	CHL	O2D-CGD-O1D	-2.28	119.38	123.84
22	4	306	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
23	P	311	LUT	C22-C23-C24	-2.28	109.15	111.74
22	P	306	CLA	CAD-C3D-C2D	2.28	151.79	140.80
26	V	316	CHL	CED-O2D-CGD	2.28	121.09	115.94
22	u	307	CLA	C3B-C4B-NB	-2.28	108.40	110.52
22	v	302	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
26	R	317	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
31	d	403	BCR	C10-C11-C12	-2.28	116.11	123.22
31	a	409	BCR	C37-C22-C23	2.28	121.67	118.08
31	A	409	BCR	C37-C22-C23	2.28	121.67	118.08
26	U	314	CHL	OMC-CMC-C2C	-2.28	120.54	125.69
31	A	409	BCR	C15-C16-C17	-2.28	118.81	123.47
31	z	101	BCR	C34-C9-C8	2.28	121.66	118.08
26	G	316	CHL	C2A-C1A-CHA	-2.28	119.88	123.86
31	d	403	BCR	C23-C24-C25	-2.28	120.81	127.20
27	N	318	NEX	C15-C35-C34	-2.28	118.81	123.47
22	5	305	CLA	C3B-C4B-NB	-2.28	108.40	110.52
27	p	301	NEX	C30-C31-C32	-2.28	116.12	123.22
32	l	102	SQD	O48-C23-O10	-2.27	117.85	123.59
22	C	507	CLA	CHC-C4B-NB	2.27	126.66	124.26
26	V	315	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
22	3	301	CLA	C3B-C4B-NB	-2.27	108.41	110.52
22	B	604	CLA	C3B-C4B-NB	-2.27	108.41	110.52
26	5	318	CHL	O1D-CGD-CBD	-2.27	119.83	124.48
24	R	313	XAT	C16-C1-C6	2.27	116.18	110.05
27	p	301	NEX	C28-C29-C30	2.27	122.43	118.94
22	1	306	CLA	C3B-C4B-NB	-2.27	108.41	110.52
26	P	315	CHL	C1C-C2C-C3C	-2.27	105.31	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	313	CHL	O2D-CGD-O1D	-2.27	119.40	123.84
22	p	305	CLA	CMA-C3A-C4A	-2.27	105.67	111.77
22	V	306	CLA	CHB-C1B-NB	2.27	126.66	124.26
26	U	317	CHL	C4-C3-C5	2.27	119.09	115.27
24	q	309	XAT	C36-C21-C26	2.27	116.17	110.05
26	P	316	CHL	C1C-C2C-C3C	-2.27	105.31	107.11
22	q	303	CLA	C2A-C1A-CHA	2.27	127.83	123.86
23	5	310	LUT	C35-C15-C14	-2.27	118.83	123.47
27	S	317	NEX	C26-C27-C28	-2.27	121.20	125.99
23	2	310	LUT	C22-C23-C24	-2.27	109.16	111.74
22	G	304	CLA	CMB-C2B-C3B	2.27	132.08	126.59
22	4	305	CLA	CHB-C1B-NB	2.27	126.66	124.26
22	c	507	CLA	CHB-C1B-NB	2.27	126.66	124.26
22	a	406	CLA	C1-C2-C3	-2.27	123.08	126.75
22	q	308	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	6	302	CLA	CHB-C4A-NA	2.27	127.64	124.51
26	p	319	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
26	n	317	CHL	O2D-CGD-O1D	-2.27	119.41	123.84
26	u	318	CHL	O2A-CGA-CBA	2.27	119.02	111.91
26	2	314	CHL	C1D-CHD-C4C	-2.26	121.17	126.06
22	C	507	CLA	C3A-C2A-C1A	2.26	104.73	101.34
22	G	303	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
31	c	516	BCR	C10-C11-C12	-2.26	116.15	123.22
22	B	616	CLA	CHC-C4B-NB	2.26	126.65	124.26
22	B	604	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	u	307	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
26	v	317	CHL	C1-C2-C3	-2.26	122.13	126.04
22	c	506	CLA	C3A-C2A-C1A	2.26	104.73	101.34
24	1	311	XAT	C30-C31-C32	-2.26	116.16	123.22
26	p	320	CHL	C1-C2-C3	-2.26	122.13	126.04
22	B	613	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
26	U	317	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
23	p	311	LUT	C15-C35-C34	-2.26	118.84	123.47
24	n	311	XAT	C35-C15-C14	-2.26	118.84	123.47
26	U	319	CHL	C2A-C3A-C4A	-2.26	98.22	101.87
26	Q	315	CHL	C2A-C1A-CHA	-2.26	119.91	123.86
23	p	311	LUT	C7-C8-C9	-2.26	122.82	126.23
23	p	311	LUT	C22-C23-C24	-2.26	109.17	111.74
24	3	309	XAT	C36-C21-C26	2.26	116.15	110.05
22	S	303	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
26	3	312	CHL	CAA-C2A-C3A	-2.26	106.59	112.78
26	6	314	CHL	OMC-CMC-C2C	-2.26	120.58	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	502	CLA	C2D-C1D-ND	-2.26	108.44	110.10
22	5	301	CLA	C3B-C4B-NB	-2.26	108.42	110.52
22	B	602	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
26	v	314	CHL	CAA-C2A-C3A	-2.26	106.59	112.78
22	B	607	CLA	O2D-CGD-CBD	2.26	115.28	111.27
27	s	317	NEX	C26-C27-C28	-2.26	121.22	125.99
31	b	620	BCR	C37-C22-C23	2.26	121.64	118.08
26	Q	315	CHL	CHC-C4B-NB	-2.26	121.87	124.26
26	V	316	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
32	l	102	SQD	O48-C23-C24	2.26	118.99	111.91
22	Q	307	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
22	4	305	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
22	b	607	CLA	O2D-CGD-CBD	2.25	115.28	111.27
22	b	612	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
22	3	303	CLA	C1-C2-C3	-2.25	123.10	126.75
22	c	503	CLA	C2A-C1A-CHA	2.25	127.80	123.86
22	r	602	CLA	CHD-C1D-ND	-2.25	122.38	124.45
22	B	609	CLA	CMB-C2B-C3B	2.25	132.04	126.59
22	r	604	CLA	C3B-C4B-NB	-2.25	108.42	110.52
22	s	307	CLA	C3B-C4B-NB	-2.25	108.42	110.52
23	2	310	LUT	C1-C2-C3	2.25	118.73	113.64
22	B	615	CLA	O2D-CGD-CBD	2.25	115.27	111.27
27	5	319	NEX	C30-C31-C32	-2.25	116.19	123.22
32	a	413	SQD	O48-C23-O10	-2.25	117.91	123.59
26	4	317	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	n	313	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
26	2	318	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
22	q	307	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
31	a	409	BCR	C10-C11-C12	-2.25	116.19	123.22
22	6	304	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
22	r	608	CLA	CHB-C1B-NB	2.25	126.64	124.26
26	5	314	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
22	V	305	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
24	r	612	XAT	C16-C1-C6	2.25	116.12	110.05
27	r	618	NEX	C15-C35-C34	-2.25	118.87	123.47
22	a	408	CLA	O2D-CGD-CBD	2.25	115.27	111.27
26	N	317	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
36	c	517	DGD	O2G-C1B-O1B	-2.25	118.27	123.70
26	g	313	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
22	c	512	CLA	CMB-C2B-C1B	-2.25	121.94	125.37
32	a	410	SQD	O5-C1-C2	2.25	115.11	110.35
26	V	317	CHL	C4-C3-C5	2.25	119.05	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g	311	CHL	CHB-C4A-NA	2.25	127.62	124.51
22	b	616	CLA	CHC-C4B-NB	2.25	126.64	124.26
26	u	318	CHL	O2D-CGD-O1D	-2.25	119.45	123.84
22	c	508	CLA	C3B-C4B-NB	-2.25	108.43	110.52
26	r	616	CHL	C1D-ND-C4D	-2.25	104.74	106.33
22	c	506	CLA	C3B-C4B-NB	-2.24	108.43	110.52
22	n	307	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
22	c	513	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
26	S	313	CHL	OMC-CMC-C2C	-2.24	120.61	125.69
26	q	315	CHL	C1-C2-C3	-2.24	122.16	126.04
22	R	309	CLA	CMB-C2B-C3B	2.24	132.02	126.59
22	C	503	CLA	C2D-C1D-ND	-2.24	108.45	110.10
22	1	301	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
33	D	405	PL9	C51-C49-C50	2.24	119.56	114.60
36	C	519	DGD	C6D-C5D-C4D	-2.24	107.41	112.09
22	n	305	CLA	C3D-C4D-ND	2.24	113.86	110.24
22	n	303	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	S	310	LUT	C18-C5-C4	2.24	118.51	114.36
31	C	516	BCR	C11-C10-C9	-2.24	124.11	127.31
22	R	302	CLA	C3B-C4B-NB	-2.24	108.44	110.52
22	C	507	CLA	C3B-C4B-NB	-2.24	108.44	110.52
26	6	315	CHL	C1-C2-C3	-2.24	122.17	126.04
23	p	311	LUT	C18-C5-C6	-2.24	122.01	124.53
26	2	315	CHL	CHC-C4B-NB	-2.24	121.89	124.26
26	V	313	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
26	V	317	CHL	CHC-C4B-NB	-2.24	121.89	124.26
22	B	608	CLA	CHB-C1B-NB	2.24	126.63	124.26
22	C	504	CLA	C2A-C1A-CHA	2.24	127.77	123.86
22	n	305	CLA	C4D-CHA-C1A	2.24	123.97	121.25
26	U	319	CHL	C4D-CHA-C1A	-2.24	118.53	121.25
36	C	519	DGD	O2G-C1B-O1B	-2.24	118.29	123.70
22	P	307	CLA	CMB-C2B-C3B	2.24	132.01	126.59
23	S	311	LUT	C35-C15-C14	-2.24	118.89	123.47
31	d	403	BCR	C16-C15-C14	-2.24	118.89	123.47
22	B	614	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
23	u	309	LUT	C10-C11-C12	-2.24	116.24	123.22
27	S	317	NEX	C16-C1-C6	2.24	112.47	110.47
34	c	501	LMG	C8-O7-C10	-2.24	112.28	117.79
22	S	307	CLA	C3B-C4B-NB	-2.24	108.44	110.52
22	s	303	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
22	c	508	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	6	313	CHL	CAA-C2A-C1A	2.24	119.30	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	5	310	LUT	C18-C5-C4	2.24	118.50	114.36
22	c	506	CLA	CHC-C4B-NB	2.23	126.62	124.26
31	B	619	BCR	C24-C23-C22	-2.23	122.86	126.23
22	6	309	CLA	C3B-C4B-NB	-2.23	108.44	110.52
22	p	306	CLA	C2A-C1A-CHA	2.23	127.77	123.86
23	v	309	LUT	C3-C4-C5	-2.23	107.40	111.85
22	b	604	CLA	CHB-C4A-NA	2.23	127.60	124.51
27	P	301	NEX	C28-C29-C30	2.23	122.37	118.94
22	B	602	CLA	CHC-C4B-NB	2.23	126.62	124.26
22	b	612	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
26	u	315	CHL	CED-O2D-CGD	2.23	120.98	115.94
23	N	310	LUT	C16-C1-C6	-2.23	106.68	110.30
22	U	306	CLA	CHB-C1B-NB	2.23	126.62	124.26
22	b	611	CLA	CHB-C1B-NB	2.23	126.62	124.26
23	p	310	LUT	C15-C35-C34	-2.23	118.91	123.47
31	a	409	BCR	C15-C16-C17	-2.23	118.91	123.47
22	q	303	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
22	B	611	CLA	CHB-C1B-NB	2.23	126.62	124.26
26	S	315	CHL	CHD-C1D-C2D	2.23	130.16	125.48
26	P	317	CHL	O1D-CGD-CBD	-2.23	119.92	124.48
26	u	317	CHL	C4D-CHA-C1A	-2.23	118.54	121.25
26	g	316	CHL	O1D-CGD-CBD	-2.23	119.93	124.48
22	p	302	CLA	CHD-C1D-ND	-2.23	122.41	124.45
26	r	616	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
26	5	315	CHL	O2D-CGD-O1D	-2.23	119.48	123.84
22	2	301	CLA	C1-C2-C3	-2.23	122.19	126.04
22	N	305	CLA	C2A-C1A-CHA	2.23	127.75	123.86
36	c	518	DGD	C1E-C2E-C3E	2.23	114.63	110.00
22	Q	304	CLA	C3B-C4B-NB	-2.23	108.45	110.52
26	g	316	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
22	b	617	CLA	CHA-C4D-ND	2.23	137.15	132.50
26	P	314	CHL	O1D-CGD-CBD	-2.23	119.93	124.48
23	R	312	LUT	C35-C15-C14	-2.23	118.92	123.47
30	a	407	PHO	OBD-CAD-CBD	-2.22	122.56	125.82
22	C	509	CLA	C3B-C4B-NB	-2.22	108.45	110.52
26	U	313	CHL	C4D-CHA-C1A	-2.22	118.54	121.25
26	2	318	CHL	O1D-CGD-CBD	-2.22	119.93	124.48
26	P	316	CHL	C1D-ND-C4D	-2.22	104.75	106.33
31	D	404	BCR	C10-C11-C12	-2.22	116.28	123.22
23	R	312	LUT	C30-C31-C32	-2.22	116.28	123.22
26	s	316	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
36	C	519	DGD	C6E-C5E-C4E	-2.22	107.80	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	p	311	LUT	C16-C1-C6	-2.22	106.69	110.30
26	v	316	CHL	C2A-C1A-CHA	-2.22	119.97	123.86
22	b	615	CLA	O2D-CGD-CBD	2.22	115.22	111.27
23	1	310	LUT	C15-C35-C34	-2.22	118.92	123.47
23	R	312	LUT	C10-C11-C12	-2.22	116.29	123.22
31	X	201	BCR	C34-C9-C10	-2.22	119.81	122.92
26	5	314	CHL	OMC-CMC-C2C	-2.22	120.67	125.69
22	4	303	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
22	u	303	CLA	C1-C2-C3	-2.22	123.16	126.75
26	u	316	CHL	CHC-C4B-NB	-2.22	121.91	124.26
24	6	310	XAT	C36-C21-C26	2.22	116.03	110.05
23	S	310	LUT	C21-C26-C27	-2.22	109.90	112.70
22	B	612	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
26	p	316	CHL	C1D-ND-C4D	-2.22	104.76	106.33
22	2	305	CLA	C3D-C4D-ND	2.22	113.82	110.24
27	N	318	NEX	C28-C29-C30	2.22	122.34	118.94
22	4	301	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
22	b	608	CLA	CHB-C1B-NB	2.22	126.60	124.26
22	B	605	CLA	CBA-CAA-C2A	2.22	120.40	113.86
36	c	517	DGD	C6E-C5E-C4E	-2.22	107.81	113.00
26	u	315	CHL	CMD-C2D-C3D	-2.22	122.52	127.61
26	4	313	CHL	CHB-C4A-NA	2.22	127.58	124.51
26	P	319	CHL	O2D-CGD-O1D	-2.21	119.51	123.84
26	4	316	CHL	C1-C2-C3	-2.21	122.22	126.04
26	P	314	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
23	v	309	LUT	C31-C30-C29	-2.21	124.15	127.31
26	Q	314	CHL	C1-C2-C3	-2.21	122.22	126.04
22	1	305	CLA	CHB-C1B-NB	2.21	126.60	124.26
22	v	303	CLA	CHB-C1B-NB	2.21	126.60	124.26
22	3	305	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	r	608	CLA	CMB-C2B-C3B	2.21	131.94	126.59
26	N	313	CHL	C4-C3-C5	2.21	118.99	115.27
22	A	406	CLA	CHB-C1B-NB	2.21	126.60	124.26
23	S	311	LUT	C19-C9-C8	2.21	121.56	118.08
22	S	301	CLA	CMB-C2B-C3B	2.21	131.94	126.59
22	r	604	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
23	n	310	LUT	C8-C7-C6	-2.21	120.99	127.20
26	g	315	CHL	C2A-C1A-CHA	-2.21	119.99	123.86
22	N	303	CLA	C1-C2-C3	-2.21	123.18	126.75
24	v	311	XAT	C27-C28-C29	-2.21	122.10	125.53
23	V	310	LUT	C18-C5-C4	2.21	118.45	114.36
22	Q	305	CLA	O2A-CGA-O1A	-2.21	118.02	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	412	SQD	O6-C1-C2	2.21	111.75	108.30
27	R	301	NEX	C4-C3-C2	-2.21	106.51	110.77
23	n	309	LUT	C30-C31-C32	-2.21	116.32	123.22
22	3	303	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
26	4	316	CHL	CED-O2D-CGD	2.21	120.93	115.94
22	g	304	CLA	O1D-CGD-CBD	2.21	129.00	124.48
22	N	304	CLA	C1-C2-C3	-2.21	122.22	126.04
26	N	314	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
26	2	315	CHL	CHB-C4A-NA	2.21	127.56	124.51
22	u	301	CLA	CMB-C2B-C3B	2.21	131.93	126.59
22	s	309	CLA	CHC-C4B-NB	2.21	126.59	124.26
26	s	313	CHL	OMC-CMC-C2C	-2.21	120.70	125.69
22	C	513	CLA	CMB-C2B-C1B	-2.21	122.01	125.37
26	u	316	CHL	C4D-C3D-CAD	2.21	110.70	108.10
22	S	305	CLA	C1-C2-C3	-2.21	122.23	126.04
22	N	304	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
33	d	404	PL9	C51-C49-C50	2.21	119.47	114.60
27	S	317	NEX	C11-C12-C13	-2.21	120.22	126.42
22	6	306	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
22	U	307	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
26	G	313	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
22	C	511	CLA	C3B-C4B-NB	-2.20	108.47	110.52
23	v	309	LUT	C18-C5-C4	2.20	118.44	114.36
26	v	318	CHL	CHB-C4A-NA	2.20	127.56	124.51
26	5	317	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
22	Q	303	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
26	u	313	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
23	n	310	LUT	C3-C4-C5	-2.20	107.47	111.85
26	n	318	CHL	C1-C2-C3	-2.20	122.23	126.04
22	S	301	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
22	n	304	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
26	V	318	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
26	p	320	CHL	C2A-C1A-CHA	-2.20	120.01	123.86
26	n	313	CHL	C4D-CHA-C1A	-2.20	118.57	121.25
23	P	310	LUT	C10-C11-C12	-2.20	116.35	123.22
22	C	504	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	V	309	LUT	C18-C5-C4	2.20	118.43	114.36
26	s	315	CHL	CHD-C1D-C2D	2.20	130.09	125.48
22	3	303	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
26	u	316	CHL	CHB-C4A-NA	2.20	127.55	124.51
31	K	101	BCR	C23-C24-C25	-2.20	121.03	127.20
26	2	313	CHL	C1C-C2C-C3C	-2.20	105.37	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	4	310	LUT	C1-C6-C5	-2.20	119.52	122.61
26	V	315	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
23	u	309	LUT	C7-C8-C9	-2.20	122.92	126.23
22	C	514	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
31	k	101	BCR	C23-C24-C25	-2.20	121.03	127.20
26	1	316	CHL	C4D-CHA-C1A	-2.20	118.58	121.25
22	6	305	CLA	O1D-CGD-CBD	2.20	128.98	124.48
24	u	311	XAT	C35-C34-C33	-2.20	124.18	127.31
22	R	310	CLA	C3B-C4B-NB	-2.20	108.48	110.52
22	c	510	CLA	C3B-C4B-NB	-2.20	108.48	110.52
23	5	310	LUT	C1-C2-C3	2.20	118.60	113.64
31	C	516	BCR	C38-C26-C27	2.20	117.83	113.62
24	n	311	XAT	C36-C21-C26	2.20	115.97	110.05
22	C	510	CLA	C4-C3-C5	2.19	118.96	115.27
22	Q	308	CLA	C2A-C1A-CHA	2.19	127.70	123.86
26	V	316	CHL	C2A-C3A-C4A	-2.19	98.33	101.87
26	q	311	CHL	CHC-C4B-NB	-2.19	121.94	124.26
22	q	308	CLA	C2A-C1A-CHA	2.19	127.69	123.86
22	Q	304	CLA	CMB-C2B-C3B	2.19	131.90	126.59
23	V	309	LUT	C16-C1-C6	-2.19	106.74	110.30
23	V	309	LUT	C1-C2-C3	2.19	118.59	113.64
24	n	311	XAT	C27-C28-C29	-2.19	122.13	125.53
31	z	101	BCR	C11-C10-C9	-2.19	124.18	127.31
23	P	311	LUT	C18-C5-C6	-2.19	122.07	124.53
22	2	305	CLA	C4D-CHA-C1A	2.19	123.92	121.25
26	Q	311	CHL	CHC-C4B-NB	-2.19	121.94	124.26
23	u	309	LUT	C30-C31-C32	-2.19	116.38	123.22
26	n	313	CHL	C4A-NA-C1A	2.19	107.69	106.71
33	a	411	PL9	C11-C9-C10	2.19	119.44	114.60
22	5	305	CLA	C3D-C4D-ND	2.19	113.78	110.24
26	4	313	CHL	C1D-ND-C4D	-2.19	104.78	106.33
32	A	412	SQD	O48-C23-O10	-2.19	118.06	123.59
31	b	619	BCR	C24-C23-C22	-2.19	122.93	126.23
26	v	316	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
26	g	312	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
26	v	315	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
22	Q	307	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
31	B	619	BCR	C30-C25-C24	2.19	121.97	115.78
22	C	508	CLA	O1D-CGD-CBD	2.19	128.96	124.48
31	C	517	BCR	C37-C22-C23	2.19	121.53	118.08
26	5	313	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
22	B	604	CLA	CHB-C1B-NB	2.19	126.57	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u	316	CHL	C2A-C1A-CHA	-2.19	120.03	123.86
23	S	311	LUT	C16-C1-C6	-2.19	106.75	110.30
22	C	510	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
22	s	301	CLA	CMB-C2B-C3B	2.19	131.88	126.59
22	u	305	CLA	O2A-CGA-O1A	-2.19	118.08	123.59
24	1	311	XAT	C27-C28-C29	-2.19	122.14	125.53
24	2	311	XAT	C30-C31-C32	-2.19	116.40	123.22
30	A	407	PHO	OBD-CAD-CBD	-2.19	122.62	125.82
27	r	618	NEX	C28-C29-C30	2.19	122.29	118.94
22	P	307	CLA	C2A-C1A-CHA	2.18	127.68	123.86
31	T	101	BCR	C2-C1-C6	2.18	113.84	110.48
22	U	301	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
26	g	316	CHL	C1-C2-C3	-2.18	122.27	126.04
22	R	305	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
26	p	314	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
26	u	317	CHL	O2A-CGA-O1A	-2.18	118.08	123.59
26	G	314	CHL	C2A-C3A-C4A	-2.18	98.34	101.87
26	n	316	CHL	C1C-C2C-C3C	-2.18	105.38	107.11
24	Q	309	XAT	C36-C21-C26	2.18	115.94	110.05
26	g	316	CHL	O2D-CGD-O1D	-2.18	119.57	123.84
22	q	301	CLA	CMB-C2B-C3B	2.18	131.88	126.59
22	N	305	CLA	C4D-CHA-C1A	2.18	123.91	121.25
26	n	314	CHL	C3D-C4D-ND	2.18	113.77	110.24
22	B	617	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
22	C	507	CLA	CHB-C1B-NB	2.18	126.57	124.26
24	v	311	XAT	C36-C21-C26	2.18	115.94	110.05
27	r	618	NEX	C20-C13-C14	-2.18	119.87	122.92
26	u	315	CHL	C1C-C2C-C3C	-2.18	105.38	107.11
26	Q	314	CHL	C2A-C3A-C4A	-2.18	98.35	101.87
31	B	620	BCR	C7-C8-C9	-2.18	122.94	126.23
27	v	319	NEX	C30-C31-C32	-2.18	116.41	123.22
22	n	304	CLA	C2D-C1D-ND	-2.18	108.50	110.10
22	c	506	CLA	C2A-C1A-CHA	2.18	127.67	123.86
26	5	313	CHL	C1D-ND-C4D	-2.18	104.79	106.33
22	b	613	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
37	e	101	HEM	CAC-C3C-C4C	2.18	130.16	124.90
26	3	314	CHL	C4A-NA-C1A	2.18	107.69	106.71
22	c	507	CLA	O1D-CGD-CBD	2.18	128.94	124.48
26	V	313	CHL	O1D-CGD-CBD	-2.18	120.03	124.48
26	6	314	CHL	CHD-C1D-C2D	2.18	130.05	125.48
36	a	416	DGD	O6E-C1E-C2E	2.18	114.96	110.35
30	A	407	PHO	CMD-C2D-C3D	2.18	128.75	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	n	305	CLA	C3B-C4B-NB	-2.18	108.49	110.52
23	4	309	LUT	C11-C10-C9	-2.18	124.20	127.31
26	6	313	CHL	CHD-C1D-C2D	2.18	130.05	125.48
22	V	306	CLA	C2A-C1A-CHA	2.18	127.67	123.86
24	g	309	XAT	C40-C33-C32	2.18	121.51	118.08
26	N	315	CHL	CHB-C4A-NA	2.18	127.52	124.51
23	s	310	LUT	C18-C5-C4	2.18	118.39	114.36
26	3	311	CHL	CHC-C4B-NB	-2.18	121.95	124.26
22	P	304	CLA	CHC-C4B-NB	2.18	126.56	124.26
22	b	604	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
27	P	301	NEX	C30-C31-C32	-2.18	116.42	123.22
26	6	301	CHL	C1-C2-C3	-2.18	122.28	126.04
22	q	306	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	n	310	LUT	C10-C11-C12	-2.18	116.42	123.22
27	s	317	NEX	C2-C1-C6	2.18	111.33	109.21
22	r	608	CLA	C2A-C1A-CHA	2.18	127.66	123.86
22	4	306	CLA	C2A-C1A-CHA	2.18	127.66	123.86
26	v	317	CHL	O2A-CGA-O1A	-2.18	118.10	123.59
26	5	317	CHL	C2A-C1A-CHA	-2.18	120.06	123.86
26	g	311	CHL	O1D-CGD-CBD	-2.18	120.03	124.48
23	2	309	LUT	C3-C4-C5	-2.18	107.52	111.85
32	A	412	SQD	C1-O5-C5	2.17	117.96	113.69
26	S	316	CHL	C1D-ND-C4D	-2.17	104.79	106.33
26	s	316	CHL	C1D-ND-C4D	-2.17	104.79	106.33
22	r	609	CLA	C3A-C2A-C1A	2.17	104.60	101.34
31	t	101	BCR	C36-C18-C17	-2.17	119.88	122.92
22	q	304	CLA	CHB-C1B-NB	2.17	126.56	124.26
24	1	311	XAT	C16-C1-C6	2.17	115.92	110.05
22	P	307	CLA	CHC-C4B-NB	2.17	126.56	124.26
22	p	305	CLA	C1-C2-C3	-2.17	122.28	126.04
22	C	510	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
25	u	312	LHG	C5-O7-C7	-2.17	112.44	117.79
26	3	315	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
37	E	101	HEM	CAC-C3C-C4C	2.17	130.14	124.90
24	R	313	XAT	C24-C23-C22	-2.17	106.58	110.77
22	q	302	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	6	315	CHL	C1D-ND-C4D	-2.17	104.79	106.33
23	p	310	LUT	C16-C1-C6	-2.17	106.78	110.30
23	V	309	LUT	C30-C31-C32	-2.17	116.44	123.22
23	n	309	LUT	C16-C1-C6	-2.17	106.78	110.30
26	P	314	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
22	b	616	CLA	O2A-CGA-O1A	-2.17	118.11	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	313	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
26	5	316	CHL	O1D-CGD-CBD	-2.17	120.04	124.48
22	c	508	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	2	314	CHL	C3D-C4D-ND	2.17	113.75	110.24
26	Q	316	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
22	6	302	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	u	306	CLA	C2A-C1A-CHA	2.17	127.65	123.86
22	U	303	CLA	C1-C2-C3	-2.17	123.24	126.75
22	n	305	CLA	C2A-C1A-CHA	2.17	127.65	123.86
26	s	313	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
26	2	315	CHL	O2D-CGD-O1D	-2.17	119.60	123.84
22	6	306	CLA	C2A-C1A-CHA	2.17	127.65	123.86
26	4	313	CHL	O2A-CGA-O1A	-2.17	118.12	123.59
26	r	616	CHL	CMB-C2B-C1B	2.17	128.67	125.37
30	a	407	PHO	CMD-C2D-C3D	2.17	128.73	124.68
22	G	308	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	U	309	LUT	C8-C7-C6	-2.17	121.11	127.20
26	N	317	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
22	S	301	CLA	C2A-C1A-CHA	2.17	127.65	123.86
31	D	404	BCR	C16-C15-C14	-2.17	119.03	123.47
31	c	515	BCR	C37-C22-C23	2.17	121.49	118.08
31	a	409	BCR	C27-C26-C25	-2.17	119.59	122.73
27	N	318	NEX	C26-C27-C28	-2.17	121.41	125.99
33	A	410	PL9	C11-C9-C10	2.17	119.39	114.60
27	P	301	NEX	C31-C30-C29	-2.17	124.22	127.31
22	4	307	CLA	CAC-C3C-C4C	2.17	127.62	124.81
27	u	320	NEX	C19-C9-C10	-2.17	119.89	122.92
26	2	317	CHL	C2A-C1A-CHA	-2.17	120.07	123.86
23	P	310	LUT	C8-C7-C6	-2.17	121.12	127.20
36	A	414	DGD	O6E-C1E-C2E	2.16	114.93	110.35
23	N	310	LUT	C8-C7-C6	-2.16	121.12	127.20
23	s	311	LUT	C39-C29-C28	2.16	121.49	118.08
22	n	305	CLA	C3A-C2A-C1A	2.16	104.58	101.34
26	6	312	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
22	C	515	CLA	C2A-C1A-CHA	2.16	127.64	123.86
24	G	309	XAT	C36-C21-C26	2.16	115.89	110.05
23	u	309	LUT	C18-C5-C6	-2.16	122.10	124.53
26	Q	314	CHL	CED-O2D-CGD	2.16	120.83	115.94
22	b	602	CLA	CHC-C4B-NB	2.16	126.55	124.26
23	v	310	LUT	C16-C1-C6	-2.16	106.79	110.30
24	4	311	XAT	C16-C1-C6	2.16	115.88	110.05
26	6	317	CHL	C1-C2-C3	-2.16	122.30	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	s	301	CLA	C2A-C1A-CHA	2.16	127.64	123.86
22	A	408	CLA	C3B-C4B-NB	-2.16	108.51	110.52
22	C	504	CLA	C3B-C4B-NB	-2.16	108.51	110.52
22	q	301	CLA	CHD-C1D-ND	-2.16	122.47	124.45
22	C	509	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	V	310	LUT	C1-C2-C3	2.16	118.52	113.64
26	V	315	CHL	O1D-CGD-CBD	-2.16	120.06	124.48
22	3	308	CLA	C3B-C4B-NB	-2.16	108.51	110.52
26	q	311	CHL	O2D-CGD-O1D	-2.16	119.61	123.84
22	r	601	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	1	313	CHL	O1D-CGD-CBD	-2.16	120.06	124.48
26	2	318	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
22	G	302	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
31	b	619	BCR	C30-C25-C24	2.16	121.89	115.78
22	p	303	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
26	5	314	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
23	U	310	LUT	C18-C5-C6	-2.16	122.10	124.53
22	P	306	CLA	CHC-C4B-NB	2.16	126.54	124.26
22	s	306	CLA	CHB-C1B-NB	2.16	126.54	124.26
26	R	315	CHL	CHC-C4B-NB	-2.16	121.97	124.26
22	3	302	CLA	C1-O2A-CGA	2.16	122.10	116.44
26	u	318	CHL	C1-C2-C3	-2.16	122.31	126.04
23	U	309	LUT	C38-C25-C24	-2.16	118.94	123.56
26	u	313	CHL	C2A-C1A-CHA	-2.16	120.09	123.86
31	A	409	BCR	C27-C26-C25	-2.16	119.60	122.73
26	G	315	CHL	C2A-C1A-CHA	-2.16	120.09	123.86
26	6	301	CHL	CHC-C4B-NB	-2.15	121.98	124.26
22	p	304	CLA	CHC-C4B-NB	2.15	126.54	124.26
22	s	301	CLA	CMA-C3A-C4A	-2.15	105.98	111.77
22	B	614	CLA	CHC-C4B-NB	2.15	126.54	124.26
23	n	309	LUT	C10-C11-C12	-2.15	116.50	123.22
26	G	311	CHL	C2A-C1A-CHA	-2.15	120.09	123.86
26	n	315	CHL	OMC-CMC-C2C	-2.15	120.82	125.69
27	r	618	NEX	C26-C27-C28	-2.15	121.44	125.99
22	b	614	CLA	CMB-C2B-C3B	2.15	131.80	126.59
22	C	503	CLA	CHB-C1B-NB	2.15	126.54	124.26
22	b	614	CLA	CHC-C4B-NB	2.15	126.54	124.26
26	1	317	CHL	C2A-C1A-CHA	-2.15	120.09	123.86
26	6	314	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
26	q	314	CHL	C4-C3-C5	2.15	118.89	115.27
23	S	310	LUT	C38-C25-C24	-2.15	118.95	123.56
22	p	306	CLA	CAA-C2A-C3A	-2.15	106.89	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	2	317	CHL	CBC-CAC-C3C	-2.15	106.50	112.43
24	p	312	XAT	C20-C13-C12	2.15	121.47	118.08
22	c	514	CLA	C2A-C1A-CHA	2.15	127.62	123.86
22	C	509	CLA	CHC-C4B-NB	2.15	126.53	124.26
23	u	310	LUT	C18-C5-C6	-2.15	122.11	124.53
26	1	317	CHL	C4D-CHA-C1A	-2.15	118.63	121.25
22	B	616	CLA	C2A-C1A-CHA	2.15	127.62	123.86
27	u	320	NEX	C17-C1-C6	-2.15	108.55	110.47
23	1	309	LUT	C18-C5-C6	-2.15	122.11	124.53
27	P	301	NEX	C19-C9-C10	-2.15	119.91	122.92
22	b	610	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	c	506	CLA	CHB-C1B-NB	2.15	126.53	124.26
22	b	611	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
24	n	311	XAT	C28-C29-C30	-2.15	115.64	118.94
26	G	312	CHL	C4D-CHA-C1A	-2.15	118.64	121.25
22	a	408	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	R	309	CLA	C2A-C1A-CHA	2.15	127.61	123.86
22	B	611	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
22	c	509	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
26	R	315	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
22	S	308	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
22	P	309	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
31	C	517	BCR	C15-C16-C17	-2.15	119.08	123.47
22	a	406	CLA	CHB-C1B-NB	2.14	126.53	124.26
22	G	301	CLA	C3B-C4B-NB	-2.14	108.53	110.52
22	s	307	CLA	CMB-C2B-C1B	-2.14	122.10	125.37
22	s	308	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
26	P	317	CHL	CED-O2D-CGD	2.14	120.78	115.94
22	B	608	CLA	CMB-C2B-C3B	2.14	131.78	126.59
22	n	308	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
24	v	311	XAT	C35-C15-C14	-2.14	119.08	123.47
26	u	313	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
26	Q	315	CHL	CED-O2D-CGD	2.14	120.78	115.94
22	U	305	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
22	1	306	CLA	CHC-C4B-NB	2.14	126.53	124.26
22	b	615	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
26	3	316	CHL	C2A-C1A-CHA	-2.14	120.11	123.86
22	P	307	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
26	3	312	CHL	CHD-C1D-C2D	2.14	129.97	125.48
26	S	313	CHL	C1C-C2C-C3C	-2.14	105.42	107.11
22	B	614	CLA	CMB-C2B-C3B	2.14	131.77	126.59
26	3	312	CHL	CAA-C2A-C1A	2.14	118.99	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G	316	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
22	1	303	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
23	n	310	LUT	C1-C2-C3	2.14	118.47	113.64
26	1	318	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
26	4	316	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
23	s	311	LUT	C19-C9-C8	2.14	121.45	118.08
22	R	302	CLA	CAC-C3C-C4C	2.14	127.58	124.81
22	S	303	CLA	C3B-C4B-NB	-2.14	108.53	110.52
22	B	604	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
22	P	303	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
31	c	515	BCR	C7-C6-C5	-2.14	116.28	121.46
26	g	316	CHL	C2A-C1A-CHA	-2.14	120.12	123.86
26	n	315	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
22	C	507	CLA	C2A-C1A-CHA	2.14	127.60	123.86
22	b	613	CLA	C2A-C1A-CHA	2.14	127.60	123.86
26	1	318	CHL	C2A-C1A-CHA	-2.14	120.12	123.86
31	c	516	BCR	C34-C9-C10	-2.14	119.93	122.92
22	C	511	CLA	C11-C12-C13	-2.14	109.01	115.92
26	v	318	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
22	V	304	CLA	CHB-C1B-NB	2.14	126.52	124.26
26	5	314	CHL	CHD-C1D-C2D	2.14	129.96	125.48
26	G	316	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
26	S	313	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
26	3	311	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
31	T	101	BCR	C29-C30-C25	2.14	113.77	110.48
26	6	317	CHL	O2D-CGD-O1D	-2.13	119.66	123.84
22	g	304	CLA	CHB-C1B-NB	2.13	126.52	124.26
26	6	314	CHL	C2D-C1D-ND	2.13	111.68	110.10
22	3	304	CLA	O1D-CGD-CBD	2.13	128.85	124.48
23	U	310	LUT	C10-C11-C12	-2.13	116.56	123.22
22	1	304	CLA	CHB-C1B-NB	2.13	126.52	124.26
26	R	316	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
26	q	314	CHL	C2A-C1A-CHA	-2.13	120.13	123.86
22	c	504	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	R	312	LUT	C11-C10-C9	-2.13	124.27	127.31
26	S	313	CHL	CHB-C4A-NA	2.13	127.46	124.51
26	1	314	CHL	O2A-CGA-CBA	2.13	118.60	111.91
22	b	617	CLA	CHB-C1B-NB	2.13	126.52	124.26
26	S	316	CHL	CHD-C1D-C2D	2.13	129.95	125.48
26	v	315	CHL	OMC-CMC-C2C	-2.13	120.86	125.69
23	u	309	LUT	C8-C7-C6	-2.13	121.21	127.20
22	x	201	CLA	CAA-C2A-C3A	-2.13	106.94	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	303	CLA	C3B-C4B-NB	-2.13	108.54	110.52
22	p	306	CLA	CHC-C4B-NB	2.13	126.51	124.26
26	P	317	CHL	C1-C2-C3	-2.13	122.36	126.04
23	V	310	LUT	C16-C1-C6	-2.13	106.84	110.30
22	1	307	CLA	CHB-C1B-NB	2.13	126.51	124.26
22	V	307	CLA	CHB-C1B-NB	2.13	126.51	124.26
22	S	307	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
27	r	617	NEX	C31-C30-C29	-2.13	124.27	127.31
22	g	303	CLA	CMB-C2B-C1B	-2.13	122.12	125.37
22	B	616	CLA	C2D-C1D-ND	-2.13	108.53	110.10
22	v	305	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
22	2	307	CLA	CHB-C1B-NB	2.13	126.51	124.26
22	5	301	CLA	C1-C2-C3	-2.13	122.36	126.04
22	c	510	CLA	C11-C12-C13	-2.13	109.03	115.92
26	s	316	CHL	CHD-C1D-C2D	2.13	129.95	125.48
24	N	311	XAT	C40-C33-C32	2.13	121.43	118.08
22	B	613	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
24	5	311	XAT	C16-C1-C6	2.13	115.79	110.05
26	6	313	CHL	O2A-CGA-O1A	-2.13	118.22	123.59
26	1	314	CHL	CED-O2D-CGD	2.13	120.75	115.94
26	3	316	CHL	C1-C2-C3	-2.13	122.36	126.04
22	b	615	CLA	CHC-C4B-NB	2.13	126.51	124.26
26	u	313	CHL	CHC-C4B-NB	-2.13	122.00	124.26
26	n	318	CHL	CHC-C4B-NB	-2.13	122.00	124.26
22	b	610	CLA	C4-C3-C5	2.13	118.85	115.27
22	C	505	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	p	312	XAT	C35-C15-C14	-2.13	119.11	123.47
22	B	617	CLA	C2D-C1D-ND	-2.13	108.54	110.10
24	V	311	XAT	C10-C11-C12	-2.13	116.58	123.22
32	m	101	SQD	O48-C23-O10	-2.13	118.22	123.59
27	u	320	NEX	C4-C3-C2	-2.13	106.67	110.77
22	U	301	CLA	CMB-C2B-C3B	2.13	131.74	126.59
26	p	315	CHL	C3B-C4B-NB	2.13	112.49	110.52
22	4	301	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	P	304	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	2	309	LUT	C8-C7-C6	-2.12	121.23	127.20
26	g	316	CHL	C4D-CHA-C1A	-2.12	118.66	121.25
24	U	311	XAT	C36-C21-C26	2.12	115.78	110.05
31	B	618	BCR	C33-C5-C6	-2.12	122.14	124.53
22	Q	304	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	2	316	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
26	v	316	CHL	CHB-C4A-NA	2.12	127.45	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	305	CLA	CAD-C3D-C2D	2.12	151.05	140.80
26	n	313	CHL	C1-C2-C3	-2.12	122.37	126.04
26	3	315	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
23	1	310	LUT	C11-C10-C9	-2.12	124.28	127.31
22	n	303	CLA	CMB-C2B-C3B	2.12	131.73	126.59
36	c	518	DGD	O5D-C1E-C2E	2.12	111.62	108.30
23	N	309	LUT	C38-C25-C24	-2.12	119.02	123.56
22	6	307	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
22	r	607	CLA	CHB-C1B-NB	2.12	126.50	124.26
22	B	615	CLA	CHC-C4B-NB	2.12	126.50	124.26
22	3	304	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
31	C	518	BCR	C34-C9-C10	-2.12	119.95	122.92
22	4	305	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
26	v	315	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
22	n	305	CLA	OBD-CAD-C3D	2.12	133.62	128.52
22	R	310	CLA	C1-C2-C3	-2.12	122.38	126.04
26	V	316	CHL	CHC-C4B-NB	-2.12	122.01	124.26
23	N	309	LUT	C35-C15-C14	-2.12	119.13	123.47
26	4	316	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
22	v	302	CLA	CHD-C1D-ND	-2.12	122.51	124.45
26	V	313	CHL	C4-C3-C5	2.12	118.83	115.27
26	4	313	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
26	U	319	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
26	n	317	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
22	d	402	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
32	M	101	SQD	O48-C23-O10	-2.12	118.25	123.59
26	g	315	CHL	CHB-C1B-C2B	-2.12	121.26	127.24
26	n	317	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
22	c	509	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
22	4	307	CLA	C1-C2-C3	-2.12	122.38	126.04
26	u	314	CHL	C4D-CHA-C1A	-2.12	118.67	121.25
24	U	311	XAT	C30-C31-C32	-2.12	116.61	123.22
22	1	305	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
22	c	510	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
24	2	311	XAT	C16-C1-C6	2.12	115.76	110.05
22	n	306	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	S	306	CLA	CHB-C1B-NB	2.11	126.50	124.26
26	6	316	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
26	N	317	CHL	C1-C2-C3	-2.11	122.39	126.04
22	g	304	CLA	CMB-C2B-C3B	2.11	131.71	126.59
22	V	304	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
26	g	314	CHL	C4D-CHA-C1A	-2.11	118.68	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	617	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	4	311	XAT	C36-C21-C26	2.11	115.75	110.05
23	r	611	LUT	C31-C30-C29	-2.11	124.30	127.31
22	s	301	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
31	C	517	BCR	C7-C6-C5	-2.11	116.34	121.46
22	N	306	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	s	317	NEX	C11-C12-C13	-2.11	120.49	126.42
23	R	312	LUT	C16-C1-C6	-2.11	106.88	110.30
22	U	306	CLA	CHA-C1A-NA	-2.11	121.56	126.40
22	3	304	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	4	310	LUT	C1-C2-C3	2.11	118.41	113.64
27	V	319	NEX	C30-C31-C32	-2.11	116.63	123.22
22	B	605	CLA	O2D-CGD-CBD	2.11	115.02	111.27
23	N	310	LUT	C10-C11-C12	-2.11	116.64	123.22
31	t	101	BCR	C34-C9-C10	-2.11	119.97	122.92
26	v	318	CHL	CHC-C4B-NB	-2.11	122.03	124.26
22	6	306	CLA	C3A-C2A-C1A	2.11	104.50	101.34
26	3	311	CHL	C4D-CHA-C1A	-2.11	118.68	121.25
26	V	316	CHL	C1-C2-C3	-2.11	122.40	126.04
22	b	617	CLA	CHC-C4B-NB	2.11	126.49	124.26
26	G	315	CHL	CHB-C1B-C2B	-2.11	121.28	127.24
26	Q	313	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
22	p	306	CLA	C4D-CHA-C1A	2.11	123.81	121.25
27	5	319	NEX	C26-C27-C28	-2.11	121.54	125.99
22	6	302	CLA	C3B-C4B-NB	-2.11	108.56	110.52
26	S	314	CHL	C4D-CHA-C1A	-2.11	118.69	121.25
25	D	407	LHG	C6-C5-C4	-2.11	106.81	111.79
24	g	309	XAT	C16-C1-C6	2.11	115.73	110.05
22	v	307	CLA	CHB-C1B-NB	2.11	126.49	124.26
23	n	309	LUT	C18-C5-C4	2.11	118.25	114.36
22	c	509	CLA	C4-C3-C5	2.10	118.81	115.27
22	c	507	CLA	CHC-C4B-NB	2.10	126.48	124.26
22	b	608	CLA	CMB-C2B-C3B	2.10	131.69	126.59
26	3	314	CHL	C1D-ND-C4D	-2.10	104.84	106.33
26	R	315	CHL	O1D-CGD-CBD	-2.10	120.18	124.48
22	1	303	CLA	C1-C2-C3	-2.10	123.35	126.75
31	b	620	BCR	C21-C20-C19	-2.10	116.65	123.22
26	5	318	CHL	O2A-CGA-CBA	2.10	118.51	111.91
22	B	615	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
22	R	309	CLA	CHC-C4B-NB	2.10	126.48	124.26
22	X	202	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
22	1	306	CLA	O2A-CGA-O1A	-2.10	118.28	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	T	101	BCR	C34-C9-C10	-2.10	119.98	122.92
23	5	309	LUT	C16-C1-C6	-2.10	106.89	110.30
26	5	318	CHL	C2A-C1A-CHA	-2.10	120.18	123.86
31	x	202	BCR	C30-C25-C24	2.10	121.72	115.78
23	v	309	LUT	C30-C31-C32	-2.10	116.66	123.22
23	s	311	LUT	C16-C1-C6	-2.10	106.89	110.30
26	p	318	CHL	C1-O2A-CGA	2.10	121.96	116.44
26	4	314	CHL	CED-O2D-CGD	2.10	120.69	115.94
22	V	303	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
22	A	408	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	s	307	CLA	C2A-C1A-CHA	2.10	127.53	123.86
26	6	314	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
26	u	315	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
26	g	311	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
22	B	616	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	2	309	LUT	C39-C29-C28	2.10	121.38	118.08
26	p	317	CHL	CAA-CBA-CGA	-2.10	107.12	113.25
31	D	404	BCR	C15-C14-C13	-2.10	124.32	127.31
26	2	318	CHL	O2A-CGA-CBA	2.10	118.49	111.91
22	B	617	CLA	C3B-C4B-NB	-2.10	108.57	110.52
23	N	310	LUT	C22-C23-C24	-2.10	109.35	111.74
22	4	304	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	5	307	CLA	CHB-C1B-NB	2.10	126.48	124.26
26	6	301	CHL	C4D-CHA-C1A	-2.10	118.70	121.25
22	v	306	CLA	C3B-C4B-NB	-2.10	108.57	110.52
27	V	319	NEX	C31-C30-C29	-2.10	124.32	127.31
31	d	403	BCR	C21-C20-C19	-2.10	116.67	123.22
22	C	511	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
23	4	309	LUT	C15-C35-C34	-2.10	119.18	123.47
22	6	303	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	R	304	CLA	C3B-C4B-NB	-2.10	108.57	110.52
22	n	306	CLA	C2A-C1A-CHA	2.10	127.52	123.86
26	q	313	CHL	O1D-CGD-CBD	-2.10	120.20	124.48
22	B	612	CLA	CHB-C1B-NB	2.10	126.47	124.26
24	u	311	XAT	C30-C31-C32	-2.10	116.68	123.22
26	6	315	CHL	CED-O2D-CGD	2.09	120.67	115.94
27	p	301	NEX	C35-C15-C14	-2.09	119.18	123.47
26	6	315	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
22	v	304	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	g	306	CLA	C3B-C4B-NB	-2.09	108.57	110.52
31	z	101	BCR	C38-C26-C27	2.09	117.64	113.62
22	5	302	CLA	CHB-C1B-NB	2.09	126.47	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	r	615	CHL	CHC-C4B-NB	-2.09	122.04	124.26
22	v	302	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	B	608	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	x	201	CLA	C3B-C4B-NB	-2.09	108.57	110.52
22	g	302	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	b	604	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	c	509	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
24	n	311	XAT	C40-C33-C32	2.09	121.38	118.08
26	p	319	CHL	C1-C2-C3	-2.09	122.42	126.04
22	S	307	CLA	CMB-C2B-C3B	2.09	131.66	126.59
22	D	403	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
26	U	314	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
22	B	613	CLA	C2A-C1A-CHA	2.09	127.52	123.86
26	p	314	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
22	C	508	CLA	CHC-C4B-NB	2.09	126.47	124.26
22	b	612	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	p	312	XAT	C16-C1-C6	2.09	115.69	110.05
26	1	318	CHL	C1-C2-C3	-2.09	122.42	126.04
26	V	314	CHL	C1D-ND-C4D	-2.09	104.85	106.33
31	B	618	BCR	C29-C30-C25	2.09	113.70	110.48
31	T	101	BCR	C36-C18-C17	-2.09	119.99	122.92
22	B	603	CLA	CHC-C4B-NB	2.09	126.47	124.26
26	3	313	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
26	p	316	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
22	U	304	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	a	404	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	C	505	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	C	509	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	p	307	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	r	601	CLA	C2A-C1A-CHA	2.09	127.51	123.86
22	C	510	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	3	305	CLA	C2A-C1A-CHA	2.09	127.51	123.86
26	Q	312	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
26	2	314	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
31	D	404	BCR	C21-C20-C19	-2.09	116.70	123.22
26	u	314	CHL	C2A-C1A-CHA	-2.09	120.21	123.86
22	4	307	CLA	CHB-C1B-NB	2.09	126.47	124.26
26	2	313	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
22	N	302	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	5	316	CHL	CHC-C4B-NB	-2.09	122.05	124.26
22	n	306	CLA	CHC-C4B-NB	2.09	126.47	124.26
26	5	316	CHL	C4D-CHA-C1A	-2.09	118.71	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v	313	CHL	C1C-C2C-C3C	-2.09	105.46	107.11
22	Q	302	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
31	t	101	BCR	C2-C1-C6	2.09	113.69	110.48
26	v	315	CHL	C4A-NA-C1A	2.09	107.64	106.71
26	U	314	CHL	CED-O2D-CGD	2.09	120.66	115.94
31	a	409	BCR	C1-C6-C7	2.09	121.68	115.78
26	R	316	CHL	O2A-CGA-CBA	2.09	118.45	111.91
22	g	305	CLA	C3A-C2A-C1A	2.09	104.46	101.34
24	G	309	XAT	C16-C1-C6	2.09	115.68	110.05
26	2	318	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
26	S	315	CHL	C4D-CHA-C1A	-2.09	118.71	121.25
26	2	316	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
23	U	309	LUT	C20-C13-C12	2.08	121.36	118.08
26	n	315	CHL	O2D-CGD-O1D	-2.08	119.76	123.84
22	n	303	CLA	CHB-C1B-NB	2.08	126.46	124.26
31	B	620	BCR	C37-C22-C23	2.08	121.36	118.08
27	P	301	NEX	O4-C5-C18	-2.08	105.68	109.39
26	u	316	CHL	OMC-CMC-C2C	-2.08	120.97	125.69
22	b	603	CLA	CHC-C4B-NB	2.08	126.46	124.26
22	q	303	CLA	CMB-C2B-C3B	2.08	131.63	126.59
22	1	302	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	b	605	CLA	O2D-CGD-CBD	2.08	114.97	111.27
23	P	310	LUT	C39-C29-C28	2.08	121.36	118.08
22	4	303	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	u	316	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
22	p	303	CLA	C2A-C1A-CHA	2.08	127.50	123.86
22	U	308	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	3	313	CHL	C1D-ND-C4D	-2.08	104.86	106.33
24	R	313	XAT	C36-C21-C26	2.08	115.67	110.05
23	P	311	LUT	C10-C11-C12	-2.08	116.72	123.22
22	s	307	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	n	311	XAT	C15-C35-C34	-2.08	119.21	123.47
31	A	409	BCR	C1-C6-C7	2.08	121.66	115.78
26	V	318	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
26	p	317	CHL	CHC-C4B-NB	-2.08	122.06	124.26
27	U	318	NEX	C11-C12-C13	-2.08	120.57	126.42
23	4	309	LUT	C16-C1-C6	-2.08	106.93	110.30
22	1	306	CLA	C2A-C1A-CHA	2.08	127.50	123.86
26	p	314	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
26	4	315	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
26	6	312	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
22	R	310	CLA	C2A-C1A-CHA	2.08	127.49	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	508	CLA	CHB-C1B-NB	2.08	126.46	124.26
26	N	316	CHL	O2D-CGD-O1D	-2.08	119.78	123.84
23	u	310	LUT	C10-C11-C12	-2.08	116.73	123.22
27	p	301	NEX	O24-C25-C26	-2.08	57.24	58.96
26	1	315	CHL	OMC-CMC-C2C	-2.08	120.99	125.69
22	b	613	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	c	515	BCR	C30-C25-C24	2.08	121.66	115.78
22	4	303	CLA	C1-C2-C3	-2.08	123.39	126.75
27	n	319	NEX	C28-C29-C30	2.08	122.13	118.94
23	R	312	LUT	C31-C30-C29	-2.08	124.35	127.31
26	p	319	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
26	N	316	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
22	g	304	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	1	303	CLA	CHC-C4B-NB	2.08	126.45	124.26
22	g	305	CLA	CHC-C4B-NB	2.08	126.45	124.26
22	V	303	CLA	C1-C2-C3	-2.08	123.39	126.75
26	P	317	CHL	C2A-C3A-C4A	-2.08	98.52	101.87
22	p	309	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	5	304	CLA	C2A-C1A-CHA	2.08	127.49	123.86
26	q	314	CHL	CED-O2D-CGD	2.08	120.63	115.94
22	C	506	CLA	CHB-C1B-NB	2.08	126.45	124.26
22	d	402	CLA	C2D-C1D-ND	-2.07	108.58	110.10
23	P	311	LUT	C16-C1-C6	-2.07	106.93	110.30
22	c	504	CLA	CHB-C1B-NB	2.07	126.45	124.26
23	U	310	LUT	C3-C4-C5	-2.07	107.72	111.85
26	Q	313	CHL	C2A-C1A-CHA	-2.07	120.23	123.86
27	p	301	NEX	C31-C30-C29	-2.07	124.35	127.31
26	v	314	CHL	C4D-CHA-C1A	-2.07	118.72	121.25
26	s	313	CHL	C4D-CHA-C1A	-2.07	118.72	121.25
31	b	619	BCR	C10-C11-C12	-2.07	116.75	123.22
27	s	317	NEX	C4-C3-C2	-2.07	106.77	110.77
22	2	305	CLA	C2A-C1A-CHA	2.07	127.48	123.86
26	R	316	CHL	CHC-C4B-NB	-2.07	122.06	124.26
33	D	405	PL9	C12-C11-C9	-2.07	106.16	112.98
26	g	312	CHL	O2A-CGA-O1A	-2.07	118.36	123.59
23	p	310	LUT	C10-C11-C12	-2.07	116.75	123.22
26	P	315	CHL	C2D-C1D-ND	2.07	111.63	110.10
22	G	305	CLA	C3A-C2A-C1A	2.07	104.44	101.34
24	P	312	XAT	C36-C21-C26	2.07	115.64	110.05
22	1	306	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
22	6	305	CLA	CHB-C1B-NB	2.07	126.45	124.26
22	U	304	CLA	CHC-C4B-NB	2.07	126.45	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	616	CLA	C2D-C1D-ND	-2.07	108.58	110.10
22	B	614	CLA	C2A-C1A-CHA	2.07	127.48	123.86
26	4	317	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
26	v	318	CHL	O2D-CGD-O1D	-2.07	119.79	123.84
22	B	613	CLA	O1D-CGD-CBD	2.07	128.72	124.48
23	N	310	LUT	C30-C31-C32	-2.07	116.76	123.22
33	d	404	PL9	C12-C11-C9	-2.07	106.17	112.98
23	5	310	LUT	C16-C1-C6	-2.07	106.94	110.30
22	s	305	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
22	N	305	CLA	CHC-C4B-NB	2.07	126.45	124.26
22	r	607	CLA	C3A-C2A-C1A	2.07	104.44	101.34
22	P	306	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
26	g	315	CHL	C1C-C2C-C3C	-2.07	105.47	107.11
23	p	310	LUT	C1-C2-C3	2.07	118.31	113.64
31	d	403	BCR	C15-C14-C13	-2.07	124.36	127.31
26	u	314	CHL	CHC-C4B-NB	-2.07	122.07	124.26
22	u	304	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
22	B	604	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	P	311	LUT	C15-C35-C34	-2.07	119.24	123.47
26	s	315	CHL	C4D-CHA-C1A	-2.07	118.73	121.25
22	5	308	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
26	r	615	CHL	C1-O2A-CGA	2.07	121.87	116.44
26	2	317	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
22	N	306	CLA	C2A-C1A-CHA	2.07	127.47	123.86
22	N	306	CLA	CHC-C4B-NB	2.07	126.44	124.26
22	1	303	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	5	302	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
31	B	619	BCR	C10-C11-C12	-2.07	116.77	123.22
31	b	619	BCR	C34-C9-C8	2.07	121.33	118.08
24	2	311	XAT	C35-C15-C14	-2.07	119.24	123.47
26	r	614	CHL	O1D-CGD-CBD	-2.07	120.26	124.48
22	p	306	CLA	C3B-C4B-NB	-2.07	108.60	110.52
22	c	503	CLA	C3B-C4B-NB	-2.07	108.60	110.52
22	c	508	CLA	CHC-C4B-NB	2.06	126.44	124.26
22	c	510	CLA	O1D-CGD-CBD	2.06	128.71	124.48
26	U	315	CHL	C2A-C1A-CHA	-2.06	120.25	123.86
27	s	317	NEX	O24-C25-C26	-2.06	57.25	58.96
26	v	316	CHL	CED-O2D-CGD	2.06	120.61	115.94
27	V	319	NEX	O24-C25-C26	-2.06	57.25	58.96
22	B	605	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	p	306	CLA	C3A-C2A-C1A	2.06	104.43	101.34
22	p	304	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	312	CHL	O2A-CGA-O1A	-2.06	118.39	123.59
24	n	311	XAT	C16-C1-C6	2.06	115.61	110.05
24	R	313	XAT	C17-C1-C6	-2.06	104.48	110.05
22	s	302	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
22	2	306	CLA	CHA-C1A-NA	-2.06	121.68	126.40
26	r	614	CHL	C1C-C2C-C3C	-2.06	105.48	107.11
22	4	302	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
26	q	315	CHL	O1D-CGD-CBD	-2.06	120.27	124.48
22	p	306	CLA	C3D-C4D-ND	2.06	113.57	110.24
22	Q	304	CLA	CHB-C1B-NB	2.06	126.44	124.26
26	R	316	CHL	C1-O2A-CGA	2.06	121.85	116.44
22	6	308	CLA	CHB-C1B-NB	2.06	126.44	124.26
22	g	305	CLA	C2A-C1A-CHA	2.06	127.46	123.86
31	x	202	BCR	C15-C16-C17	-2.06	119.25	123.47
26	P	318	CHL	C1-O2A-CGA	2.06	121.85	116.44
23	2	309	LUT	C31-C30-C29	-2.06	124.37	127.31
23	5	310	LUT	C3-C4-C5	-2.06	107.75	111.85
22	n	304	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	V	309	LUT	C35-C15-C14	-2.06	119.26	123.47
27	p	301	NEX	C5-C4-C3	-2.06	109.31	111.75
26	1	316	CHL	CHC-C4B-NB	-2.06	122.08	124.26
22	R	305	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
22	U	303	CLA	CMB-C2B-C1B	-2.06	122.24	125.37
22	G	304	CLA	CHB-C1B-NB	2.06	126.43	124.26
31	b	618	BCR	C11-C12-C13	-2.06	120.64	126.42
26	1	316	CHL	C1-C2-C3	-2.06	122.49	126.04
22	1	308	CLA	C2A-C1A-CHA	2.06	127.45	123.86
26	v	317	CHL	CHB-C1B-C2B	-2.06	121.43	127.24
22	c	502	CLA	CHB-C1B-NB	2.06	126.43	124.26
26	N	314	CHL	O2A-CGA-O1A	-2.06	118.41	123.59
26	g	314	CHL	O2D-CGD-O1D	-2.06	119.82	123.84
22	c	513	CLA	C1-C2-C3	-2.05	122.49	126.04
22	p	307	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	s	314	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
31	C	517	BCR	C30-C25-C24	2.05	121.59	115.78
26	3	315	CHL	OMC-CMC-C2C	-2.05	121.04	125.69
24	V	311	XAT	C36-C21-C26	2.05	115.59	110.05
26	1	318	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
26	n	316	CHL	O1D-CGD-CBD	-2.05	120.28	124.48
27	u	320	NEX	C26-C27-C28	-2.05	121.65	125.99
22	c	508	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
22	6	304	CLA	C3B-C4B-NB	-2.05	108.61	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	S	312	LHG	C5-O7-C7	-2.05	112.74	117.79
22	B	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
26	q	315	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
26	R	315	CHL	C1-C2-C3	-2.05	122.50	126.04
22	4	308	CLA	C2A-C1A-CHA	2.05	127.44	123.86
22	n	308	CLA	C3B-C4B-NB	-2.05	108.61	110.52
26	N	315	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
23	S	311	LUT	C39-C29-C28	2.05	121.31	118.08
22	4	301	CLA	CMB-C2B-C3B	2.05	131.55	126.59
22	3	304	CLA	CHB-C1B-NB	2.05	126.43	124.26
23	5	309	LUT	C31-C30-C29	-2.05	124.39	127.31
22	Q	304	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	g	308	CLA	CHB-C1B-NB	2.05	126.43	124.26
22	s	307	CLA	CHC-C4B-NB	2.05	126.43	124.26
27	5	319	NEX	C16-C1-C6	2.05	112.31	110.47
22	B	607	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
26	u	316	CHL	CED-O2D-CGD	2.05	120.57	115.94
26	v	313	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
24	P	312	XAT	C16-C1-C6	2.05	115.57	110.05
26	3	314	CHL	C4D-CHA-C1A	-2.05	118.76	121.25
26	6	312	CHL	CHC-C4B-NB	-2.05	122.09	124.26
22	1	304	CLA	CHC-C4B-NB	2.05	126.42	124.26
23	p	310	LUT	C35-C15-C14	-2.05	119.28	123.47
22	3	302	CLA	C3B-C4B-NB	-2.05	108.62	110.52
22	Q	308	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
26	5	315	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
26	v	316	CHL	OMC-CMC-C2C	-2.04	121.06	125.69
22	2	308	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
22	B	607	CLA	O2A-C1-C2	-2.04	103.26	108.64
23	2	309	LUT	C16-C1-C6	-2.04	106.98	110.30
31	t	101	BCR	C29-C30-C25	2.04	113.63	110.48
22	S	307	CLA	C2A-C1A-CHA	2.04	127.43	123.86
22	c	505	CLA	C3C-C4C-NC	-2.04	108.28	110.57
27	v	319	NEX	C16-C1-C6	2.04	112.30	110.47
22	G	304	CLA	O1D-CGD-CBD	2.04	128.66	124.48
27	u	319	NEX	O24-C25-C26	-2.04	57.27	58.96
22	C	506	CLA	C3C-C4C-NC	-2.04	108.28	110.57
22	b	613	CLA	O1D-CGD-CBD	2.04	128.66	124.48
22	5	304	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	n	314	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
26	Q	312	CHL	C4A-NA-C1A	2.04	107.62	106.71
30	D	401	PHO	C4B-NB-C1B	2.04	111.99	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	p	306	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	r	619	CHL	C4D-CHA-C1A	-2.04	118.77	121.25
27	V	319	NEX	C15-C35-C34	-2.04	119.29	123.47
22	B	602	CLA	C2D-C1D-ND	-2.04	108.60	110.10
22	v	306	CLA	C1-C2-C3	-2.04	122.51	126.04
26	Q	311	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
25	d	406	LHG	C6-C5-C4	-2.04	106.96	111.79
22	R	303	CLA	CHD-C1D-ND	-2.04	122.58	124.45
30	d	401	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
22	N	304	CLA	CMB-C2B-C3B	2.04	131.53	126.59
22	U	304	CLA	O2D-CGD-CBD	2.04	114.89	111.27
23	P	310	LUT	C1-C2-C3	2.04	118.25	113.64
22	G	308	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	B	604	CLA	CHC-C4B-NB	2.04	126.42	124.26
23	S	311	LUT	C8-C7-C6	-2.04	121.47	127.20
25	s	312	LHG	C5-O7-C7	-2.04	112.77	117.79
22	b	604	CLA	CHC-C4B-NB	2.04	126.42	124.26
26	3	316	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
26	P	318	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
22	R	309	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
23	N	310	LUT	C39-C29-C28	2.04	121.29	118.08
26	r	619	CHL	C1C-C2C-C3C	-2.04	105.50	107.11
23	S	311	LUT	C11-C10-C9	-2.04	124.40	127.31
22	S	303	CLA	CHB-C1B-NB	2.04	126.41	124.26
22	6	309	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
26	1	317	CHL	CED-O2D-CGD	2.04	120.55	115.94
22	X	202	CLA	C3B-C4B-NB	-2.04	108.62	110.52
22	q	304	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	g	305	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
30	D	401	PHO	O2A-CGA-O1A	-2.04	118.45	123.59
31	B	619	BCR	C34-C9-C8	2.04	121.29	118.08
26	n	313	CHL	C1C-C2C-C3C	-2.04	105.50	107.11
22	1	307	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
26	q	315	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
26	4	317	CHL	C4D-CHA-C1A	-2.04	118.77	121.25
22	V	304	CLA	CHD-C1D-ND	-2.03	122.58	124.45
26	5	317	CHL	O1D-CGD-CBD	-2.03	120.32	124.48
26	6	314	CHL	C4D-CHA-C1A	-2.03	118.77	121.25
27	n	319	NEX	C4-C3-C2	-2.03	106.84	110.77
22	2	301	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
26	V	314	CHL	CHB-C4A-NA	2.03	127.33	124.51
26	U	319	CHL	C1-O2A-CGA	2.03	121.78	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	V	311	XAT	C16-C1-C6	2.03	115.54	110.05
22	v	303	CLA	C3B-C4B-NB	-2.03	108.63	110.52
22	r	608	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	V	306	CLA	O1D-CGD-CBD	2.03	128.65	124.48
22	b	613	CLA	CMB-C2B-C3B	2.03	131.51	126.59
23	n	309	LUT	C8-C7-C6	-2.03	121.49	127.20
23	s	311	LUT	C11-C10-C9	-2.03	124.41	127.31
22	u	307	CLA	CAC-C3C-C4C	2.03	127.45	124.81
22	P	306	CLA	O1D-CGD-CBD	2.03	128.64	124.48
26	n	318	CHL	C4A-NA-C1A	2.03	107.62	106.71
26	u	318	CHL	CHB-C1B-C2B	-2.03	121.50	127.24
22	r	604	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
23	2	309	LUT	C15-C35-C34	-2.03	119.31	123.47
22	b	605	CLA	CMC-C2C-C3C	2.03	131.63	126.12
26	4	313	CHL	O2D-CGD-O1D	-2.03	119.86	123.84
26	P	317	CHL	CAA-CBA-CGA	-2.03	107.31	113.25
22	b	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	6	304	CLA	CMB-C2B-C3B	2.03	131.51	126.59
22	c	502	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
24	6	310	XAT	C16-C1-C6	2.03	115.53	110.05
22	B	602	CLA	C2A-C1A-CHA	2.03	127.41	123.86
22	3	301	CLA	CHD-C1D-ND	-2.03	122.59	124.45
27	P	301	NEX	C11-C12-C13	-2.03	120.71	126.42
23	N	309	LUT	C31-C30-C29	-2.03	124.41	127.31
26	G	311	CHL	C4D-C3D-CAD	2.03	110.49	108.10
22	c	511	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	U	311	XAT	C40-C33-C32	2.03	121.28	118.08
22	3	307	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
22	u	308	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	B	610	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	P	318	CHL	C1-C2-C3	-2.03	122.53	126.04
22	N	305	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
22	3	305	CLA	C3A-C2A-C1A	2.03	104.38	101.34
24	3	309	XAT	C16-C1-C6	2.03	115.52	110.05
22	B	613	CLA	CHA-C1A-NA	-2.03	121.75	126.40
26	2	317	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
22	c	503	CLA	CHC-C4B-NB	2.03	126.41	124.26
26	2	316	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
22	C	512	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	b	607	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	5	306	CLA	C3B-C4B-NB	-2.03	108.63	110.52
22	q	304	CLA	C3B-C4B-NB	-2.03	108.63	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	619	BCR	C20-C19-C18	-2.03	120.72	126.42
22	C	511	CLA	O1D-CGD-CBD	2.03	128.63	124.48
22	c	505	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	G	304	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	405	CLA	C1-C2-C3	-2.03	122.54	126.04
22	b	605	CLA	C3B-C4B-NB	-2.03	108.63	110.52
22	4	303	CLA	CHC-C4B-NB	2.03	126.40	124.26
22	v	306	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
26	1	313	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
30	d	401	PHO	C4B-NB-C1B	2.03	111.97	108.83
22	b	617	CLA	CAA-C2A-C1A	2.03	118.62	111.97
26	Q	314	CHL	O1D-CGD-CBD	-2.03	120.34	124.48
26	1	313	CHL	C6-C5-C3	-2.03	108.14	113.45
22	C	509	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
22	R	309	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	u	302	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
22	c	507	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	D	403	CLA	C2D-C1D-ND	-2.02	108.61	110.10
26	U	313	CHL	C2A-C1A-CHA	-2.02	120.32	123.86
26	q	312	CHL	CHD-C1D-C2D	2.02	129.73	125.48
22	S	306	CLA	CHA-C1A-NA	-2.02	121.76	126.40
22	U	307	CLA	CHC-C4B-NB	2.02	126.40	124.26
23	P	310	LUT	C16-C1-C6	-2.02	107.02	110.30
22	b	614	CLA	C2A-C1A-CHA	2.02	127.40	123.86
22	R	303	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
22	3	306	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
22	1	307	CLA	CAC-C3C-C4C	2.02	127.44	124.81
26	G	314	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
23	V	310	LUT	C22-C23-C24	-2.02	109.44	111.74
22	b	605	CLA	CHC-C4B-NB	2.02	126.40	124.26
22	u	305	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
22	s	306	CLA	CHA-C1A-NA	-2.02	121.77	126.40
26	p	316	CHL	O2A-CGA-O1A	-2.02	118.49	123.59
26	6	313	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
25	L	101	LHG	C5-O7-C7	-2.02	112.81	117.79
22	6	304	CLA	C1-C2-C3	-2.02	123.48	126.75
31	B	619	BCR	C11-C12-C13	-2.02	120.74	126.42
26	1	313	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
22	n	301	CLA	C2D-C1D-ND	-2.02	108.61	110.10
26	2	316	CHL	CHC-C4B-NB	-2.02	122.12	124.26
22	u	303	CLA	CHC-C4B-NB	2.02	126.40	124.26
22	C	503	CLA	O2A-CGA-O1A	-2.02	118.49	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	5	316	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
26	5	315	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
22	G	303	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	G	304	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	s	303	CLA	CHB-C1B-NB	2.02	126.39	124.26
27	S	317	NEX	O24-C25-C26	-2.02	57.29	58.96
24	r	612	XAT	C17-C1-C6	-2.02	104.59	110.05
22	A	404	CLA	CHB-C1B-NB	2.02	126.39	124.26
22	u	308	CLA	CHB-C1B-NB	2.02	126.39	124.26
27	p	301	NEX	C26-C27-C28	-2.02	121.72	125.99
22	P	305	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
26	3	316	CHL	O1D-CGD-CBD	-2.02	120.36	124.48
23	n	310	LUT	C30-C31-C32	-2.02	116.92	123.22
22	R	303	CLA	C2D-C1D-ND	-2.02	108.62	110.10
26	5	317	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
22	C	503	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
26	P	319	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
22	c	512	CLA	CHA-C1A-NA	-2.02	121.78	126.40
26	G	314	CHL	C1-C2-C3	-2.02	122.56	126.04
22	n	304	CLA	CMB-C2B-C3B	2.02	131.47	126.59
31	b	618	BCR	C29-C30-C25	2.02	113.58	110.48
22	2	302	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	3	313	CHL	C4D-CHA-C1A	-2.02	118.80	121.25
22	1	301	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	U	301	CLA	CHD-C1D-ND	-2.02	122.60	124.45
26	5	318	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
26	s	314	CHL	O2A-CGA-CBA	2.01	120.50	114.03
31	B	620	BCR	C1-C6-C7	2.01	121.48	115.78
31	c	516	BCR	C30-C25-C24	2.01	121.48	115.78
22	C	511	CLA	CHD-C1D-ND	-2.01	122.60	124.45
22	U	303	CLA	CHC-C4B-NB	2.01	126.39	124.26
22	g	308	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
27	u	320	NEX	O24-C25-C26	-2.01	57.29	58.96
26	Q	312	CHL	CAA-C2A-C1A	2.01	118.57	111.97
23	1	310	LUT	C30-C31-C32	-2.01	116.93	123.22
26	p	317	CHL	C2A-C3A-C4A	-2.01	98.62	101.87
24	4	311	XAT	C7-C8-C9	-2.01	122.41	125.53
26	u	318	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
26	N	317	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
24	r	612	XAT	C36-C21-C26	2.01	115.48	110.05
26	6	315	CHL	C4A-NA-C1A	2.01	107.61	106.71
22	n	308	CLA	CHC-C4B-NB	2.01	126.39	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	605	CLA	CHC-C4B-NB	2.01	126.39	124.26
26	n	314	CHL	CAA-C2A-C3A	-2.01	107.27	112.78
26	N	315	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
22	B	602	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
26	r	619	CHL	CHC-C4B-NB	-2.01	122.13	124.26
22	b	607	CLA	CHC-C4B-NB	2.01	126.39	124.26
26	V	317	CHL	CHB-C1B-C2B	-2.01	121.56	127.24
26	G	314	CHL	CED-O2D-CGD	2.01	120.49	115.94
22	C	513	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	5	311	XAT	C40-C33-C32	2.01	121.25	118.08
22	g	303	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	c	514	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
26	n	317	CHL	CHB-C4A-NA	2.01	127.29	124.51
22	n	305	CLA	CHC-C4B-NB	2.01	126.39	124.26
26	Q	316	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
24	r	612	XAT	C20-C13-C12	2.01	121.25	118.08
27	S	317	NEX	C31-C32-C33	-2.01	120.77	126.42
23	1	309	LUT	C16-C1-C6	-2.01	107.04	110.30
22	B	605	CLA	CMC-C2C-C3C	2.01	131.57	126.12
26	s	316	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
22	S	302	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
22	C	504	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
34	b	621	LMG	C8-O7-C10	-2.01	112.84	117.79
22	r	605	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	v	302	CLA	CHB-C1B-NB	2.01	126.38	124.26
27	r	617	NEX	C26-C27-C28	-2.01	121.75	125.99
22	2	304	CLA	C2A-C1A-CHA	2.01	127.37	123.86
26	U	319	CHL	C1C-C2C-C3C	-2.01	105.52	107.11
27	u	319	NEX	C31-C32-C33	-2.01	120.77	126.42
22	b	606	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
26	q	312	CHL	CAA-C2A-C3A	-2.01	107.28	112.78
24	r	612	XAT	C24-C23-C22	-2.01	106.89	110.77
22	3	308	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	2	310	LUT	C16-C1-C6	-2.01	107.04	110.30
23	4	309	LUT	C10-C11-C12	-2.01	116.95	123.22
22	a	405	CLA	C1-C2-C3	-2.01	122.57	126.04
31	X	201	BCR	C15-C16-C17	-2.01	119.36	123.47
22	b	606	CLA	CHC-C4B-NB	2.01	126.38	124.26
24	5	311	XAT	C36-C21-C26	2.01	115.46	110.05
22	c	503	CLA	C1-C2-C3	-2.01	122.57	126.04
22	C	511	CLA	C2A-C1A-CHA	2.01	127.37	123.86
22	s	306	CLA	O2A-CGA-O1A	-2.01	118.53	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	N	317	CHL	CHC-C4B-NB	-2.01	122.13	124.26
26	r	615	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
22	A	405	CLA	CHA-C1A-NA	-2.01	121.80	126.40
22	V	302	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
22	s	306	CLA	CAC-C3C-C4C	2.00	127.41	124.81
26	g	314	CHL	C1D-ND-C4D	-2.00	104.91	106.33
26	g	315	CHL	O2A-CGA-O1A	-2.00	118.53	123.59
22	b	608	CLA	C2A-C1A-CHA	2.00	127.36	123.86
22	P	308	CLA	CHB-C1B-NB	2.00	126.38	124.26
22	6	305	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	S	316	CHL	O1D-CGD-CBD	-2.00	120.38	124.48
23	4	310	LUT	C30-C31-C32	-2.00	116.96	123.22
27	P	301	NEX	O24-C25-C26	-2.00	57.30	58.96
22	2	305	CLA	C3A-C2A-C1A	2.00	104.34	101.34
22	p	308	CLA	CHB-C1B-NB	2.00	126.38	124.26
26	5	316	CHL	C2A-C1A-CHA	-2.00	120.36	123.86
26	3	312	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
26	n	315	CHL	CED-O2D-CGD	2.00	120.47	115.94
22	N	308	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	g	301	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
31	c	516	BCR	C24-C23-C22	-2.00	123.21	126.23
26	4	314	CHL	C1C-C2C-C3C	-2.00	105.53	107.11
22	R	306	CLA	CHB-C1B-NB	2.00	126.38	124.26
23	v	310	LUT	C18-C5-C4	2.00	118.06	114.36
26	r	615	CHL	O2A-CGA-CBA	2.00	118.19	111.91
22	Q	301	CLA	CHD-C1D-ND	-2.00	122.61	124.45
22	A	405	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
22	P	305	CLA	C1-C2-C3	-2.00	122.58	126.04
22	B	606	CLA	CHC-C4B-NB	2.00	126.38	124.26
22	n	302	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	U	312	LHG	C5-O7-C7	-2.00	112.86	117.79
22	r	606	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	5	305	CLA	C4D-CHA-C1A	2.00	123.68	121.25
22	C	504	CLA	CHC-C4B-NB	2.00	126.38	124.26
22	5	303	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	l	101	LHG	C5-O7-C7	-2.00	112.87	117.79
26	6	317	CHL	O1D-CGD-CBD	-2.00	120.39	124.48
26	R	317	CHL	C4D-CHA-C1A	-2.00	118.81	121.25

There are no chirality outliers.

All (7284) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	r	601	CLA	C2B-C3B-CAB-CBB
22	r	601	CLA	C4B-C3B-CAB-CBB
22	r	604	CLA	C1A-C2A-CAA-CBA
22	r	605	CLA	C4B-C3B-CAB-CBB
22	r	606	CLA	CBD-CGD-O2D-CED
22	r	606	CLA	C2-C3-C5-C6
22	r	606	CLA	C4-C3-C5-C6
22	r	607	CLA	C1A-C2A-CAA-CBA
22	r	607	CLA	C3A-C2A-CAA-CBA
22	r	607	CLA	C4B-C3B-CAB-CBB
22	r	608	CLA	CBD-CGD-O2D-CED
22	r	609	CLA	CBD-CGD-O2D-CED
22	r	610	CLA	C1A-C2A-CAA-CBA
22	r	610	CLA	C3A-C2A-CAA-CBA
22	r	610	CLA	C4B-C3B-CAB-CBB
22	a	404	CLA	CHA-CBD-CGD-O1D
22	a	404	CLA	CHA-CBD-CGD-O2D
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
22	a	406	CLA	C2B-C3B-CAB-CBB
22	a	406	CLA	C4B-C3B-CAB-CBB
22	a	406	CLA	CHA-CBD-CGD-O1D
22	a	406	CLA	CHA-CBD-CGD-O2D
22	A	404	CLA	CHA-CBD-CGD-O1D
22	A	404	CLA	CHA-CBD-CGD-O2D
22	A	405	CLA	CHA-CBD-CGD-O1D
22	A	405	CLA	CHA-CBD-CGD-O2D
22	A	406	CLA	C2B-C3B-CAB-CBB
22	A	406	CLA	C4B-C3B-CAB-CBB
22	A	406	CLA	CHA-CBD-CGD-O1D
22	A	406	CLA	CHA-CBD-CGD-O2D
22	1	302	CLA	CHA-CBD-CGD-O1D
22	1	302	CLA	CHA-CBD-CGD-O2D
22	1	302	CLA	CBD-CGD-O2D-CED
22	1	303	CLA	CHA-CBD-CGD-O1D
22	1	303	CLA	CHA-CBD-CGD-O2D
22	1	303	CLA	CAD-CBD-CGD-O1D
22	1	303	CLA	CBD-CGD-O2D-CED
22	1	304	CLA	CBD-CGD-O2D-CED
22	1	305	CLA	C2B-C3B-CAB-CBB
22	1	305	CLA	C4B-C3B-CAB-CBB
22	1	305	CLA	CBD-CGD-O2D-CED
22	1	306	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	1	306	CLA	C4B-C3B-CAB-CBB
22	1	307	CLA	CBD-CGD-O2D-CED
22	1	308	CLA	C1A-C2A-CAA-CBA
22	1	308	CLA	C3A-C2A-CAA-CBA
22	1	308	CLA	C2B-C3B-CAB-CBB
22	1	308	CLA	C4B-C3B-CAB-CBB
22	1	308	CLA	CHA-CBD-CGD-O1D
22	1	308	CLA	CHA-CBD-CGD-O2D
22	1	308	CLA	CAD-CBD-CGD-O1D
22	2	301	CLA	CBD-CGD-O2D-CED
22	2	303	CLA	CBD-CGD-O2D-CED
22	2	304	CLA	C2B-C3B-CAB-CBB
22	2	304	CLA	C4B-C3B-CAB-CBB
22	2	304	CLA	CBD-CGD-O2D-CED
22	2	305	CLA	C4B-C3B-CAB-CBB
22	2	305	CLA	CHA-CBD-CGD-O1D
22	2	305	CLA	CHA-CBD-CGD-O2D
22	2	308	CLA	C2B-C3B-CAB-CBB
22	2	308	CLA	C4B-C3B-CAB-CBB
22	2	308	CLA	CBD-CGD-O2D-CED
22	3	301	CLA	CBD-CGD-O2D-CED
22	3	302	CLA	CBA-CGA-O2A-C1
22	3	302	CLA	O1A-CGA-O2A-C1
22	3	302	CLA	CHA-CBD-CGD-O1D
22	3	302	CLA	CHA-CBD-CGD-O2D
22	3	302	CLA	CAD-CBD-CGD-O1D
22	3	302	CLA	C6-C7-C8-C9
22	3	303	CLA	C1A-C2A-CAA-CBA
22	3	303	CLA	C3A-C2A-CAA-CBA
22	3	304	CLA	CBD-CGD-O2D-CED
22	3	305	CLA	C4B-C3B-CAB-CBB
22	3	305	CLA	CBD-CGD-O2D-CED
22	3	306	CLA	C4B-C3B-CAB-CBB
22	3	307	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CHA-CBD-CGD-O1D
22	3	308	CLA	CHA-CBD-CGD-O2D
22	3	308	CLA	CAD-CBD-CGD-O1D
22	3	308	CLA	CAD-CBD-CGD-O2D
22	4	302	CLA	CHA-CBD-CGD-O1D
22	4	302	CLA	CHA-CBD-CGD-O2D
22	4	303	CLA	CHA-CBD-CGD-O1D
22	4	303	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	4	303	CLA	CAD-CBD-CGD-O1D
22	4	303	CLA	CAD-CBD-CGD-O2D
22	4	303	CLA	CBD-CGD-O2D-CED
22	4	305	CLA	C2B-C3B-CAB-CBB
22	4	305	CLA	C4B-C3B-CAB-CBB
22	4	305	CLA	CBD-CGD-O2D-CED
22	4	307	CLA	CBD-CGD-O2D-CED
22	4	308	CLA	C1A-C2A-CAA-CBA
22	4	308	CLA	C3A-C2A-CAA-CBA
22	4	308	CLA	C2B-C3B-CAB-CBB
22	4	308	CLA	C4B-C3B-CAB-CBB
22	4	308	CLA	CHA-CBD-CGD-O1D
22	4	308	CLA	CHA-CBD-CGD-O2D
22	4	308	CLA	CAD-CBD-CGD-O1D
22	5	301	CLA	CBD-CGD-O2D-CED
22	5	304	CLA	C2B-C3B-CAB-CBB
22	5	304	CLA	C4B-C3B-CAB-CBB
22	5	304	CLA	CBD-CGD-O2D-CED
22	5	305	CLA	C4B-C3B-CAB-CBB
22	5	305	CLA	CHA-CBD-CGD-O1D
22	5	305	CLA	CHA-CBD-CGD-O2D
22	5	307	CLA	CBD-CGD-O2D-CED
22	5	308	CLA	C4B-C3B-CAB-CBB
22	5	308	CLA	CBD-CGD-O2D-CED
22	6	302	CLA	CBD-CGD-O2D-CED
22	6	303	CLA	CHA-CBD-CGD-O1D
22	6	303	CLA	CHA-CBD-CGD-O2D
22	6	304	CLA	C1A-C2A-CAA-CBA
22	6	304	CLA	C3A-C2A-CAA-CBA
22	6	304	CLA	CBD-CGD-O2D-CED
22	6	305	CLA	CBD-CGD-O2D-CED
22	6	306	CLA	C2B-C3B-CAB-CBB
22	6	306	CLA	C4B-C3B-CAB-CBB
22	6	306	CLA	CBD-CGD-O2D-CED
22	6	307	CLA	C4B-C3B-CAB-CBB
22	6	308	CLA	CBD-CGD-O2D-CED
22	6	309	CLA	CHA-CBD-CGD-O1D
22	6	309	CLA	CHA-CBD-CGD-O2D
22	6	309	CLA	CAD-CBD-CGD-O1D
22	6	309	CLA	CAD-CBD-CGD-O2D
22	v	301	CLA	C2B-C3B-CAB-CBB
22	v	302	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	v	302	CLA	C4B-C3B-CAB-CBB
22	v	303	CLA	C1A-C2A-CAA-CBA
22	v	304	CLA	C1A-C2A-CAA-CBA
22	v	304	CLA	CBD-CGD-O2D-CED
22	v	305	CLA	C2B-C3B-CAB-CBB
22	v	305	CLA	C4B-C3B-CAB-CBB
22	v	305	CLA	CBD-CGD-O2D-CED
22	v	307	CLA	CBD-CGD-O2D-CED
22	v	308	CLA	C1A-C2A-CAA-CBA
22	v	308	CLA	C3A-C2A-CAA-CBA
22	p	302	CLA	CBD-CGD-O2D-CED
22	p	303	CLA	C2B-C3B-CAB-CBB
22	p	303	CLA	C4B-C3B-CAB-CBB
22	p	304	CLA	C1A-C2A-CAA-CBA
22	p	304	CLA	C3A-C2A-CAA-CBA
22	p	304	CLA	CHA-CBD-CGD-O1D
22	p	304	CLA	CBD-CGD-O2D-CED
22	p	306	CLA	CHA-CBD-CGD-O1D
22	p	306	CLA	CHA-CBD-CGD-O2D
22	p	308	CLA	CBD-CGD-O2D-CED
22	p	309	CLA	C1A-C2A-CAA-CBA
22	p	309	CLA	C3A-C2A-CAA-CBA
22	p	309	CLA	C2B-C3B-CAB-CBB
22	p	309	CLA	C4B-C3B-CAB-CBB
22	p	309	CLA	CBD-CGD-O2D-CED
22	q	302	CLA	C2B-C3B-CAB-CBB
22	q	302	CLA	C4B-C3B-CAB-CBB
22	q	302	CLA	CHA-CBD-CGD-O1D
22	q	302	CLA	CHA-CBD-CGD-O2D
22	q	303	CLA	C1A-C2A-CAA-CBA
22	q	303	CLA	C3A-C2A-CAA-CBA
22	q	304	CLA	CBD-CGD-O2D-CED
22	q	305	CLA	CBD-CGD-O2D-CED
22	q	306	CLA	C2B-C3B-CAB-CBB
22	q	306	CLA	C4B-C3B-CAB-CBB
22	q	307	CLA	CBD-CGD-O2D-CED
22	q	308	CLA	C3A-C2A-CAA-CBA
22	q	308	CLA	CHA-CBD-CGD-O1D
22	q	308	CLA	CHA-CBD-CGD-O2D
22	q	308	CLA	CBD-CGD-O2D-CED
22	V	301	CLA	C2B-C3B-CAB-CBB
22	V	301	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	V	302	CLA	C2B-C3B-CAB-CBB
22	V	302	CLA	C4B-C3B-CAB-CBB
22	V	303	CLA	C1A-C2A-CAA-CBA
22	V	303	CLA	C3A-C2A-CAA-CBA
22	V	304	CLA	C1A-C2A-CAA-CBA
22	V	304	CLA	CBD-CGD-O2D-CED
22	V	305	CLA	CBD-CGD-O2D-CED
22	V	306	CLA	CBD-CGD-O2D-CED
22	V	308	CLA	C2A-CAA-CBA-CGA
22	P	302	CLA	CBD-CGD-O2D-CED
22	P	304	CLA	C1A-C2A-CAA-CBA
22	P	304	CLA	C3A-C2A-CAA-CBA
22	P	304	CLA	CHA-CBD-CGD-O1D
22	P	304	CLA	CHA-CBD-CGD-O2D
22	P	304	CLA	CAD-CBD-CGD-O1D
22	P	306	CLA	CHA-CBD-CGD-O1D
22	P	306	CLA	CHA-CBD-CGD-O2D
22	P	308	CLA	CBD-CGD-O2D-CED
22	P	309	CLA	C1A-C2A-CAA-CBA
22	P	309	CLA	C3A-C2A-CAA-CBA
22	P	309	CLA	C2B-C3B-CAB-CBB
22	P	309	CLA	C4B-C3B-CAB-CBB
22	P	309	CLA	CBD-CGD-O2D-CED
22	Q	301	CLA	CBD-CGD-O2D-CED
22	Q	302	CLA	C2B-C3B-CAB-CBB
22	Q	302	CLA	C4B-C3B-CAB-CBB
22	Q	303	CLA	C1A-C2A-CAA-CBA
22	Q	303	CLA	C3A-C2A-CAA-CBA
22	Q	303	CLA	CHA-CBD-CGD-O1D
22	Q	303	CLA	CHA-CBD-CGD-O2D
22	Q	304	CLA	CBD-CGD-O2D-CED
22	Q	304	CLA	O1D-CGD-O2D-CED
22	Q	305	CLA	CHA-CBD-CGD-O1D
22	Q	305	CLA	CHA-CBD-CGD-O2D
22	Q	305	CLA	CBD-CGD-O2D-CED
22	Q	305	CLA	O1D-CGD-O2D-CED
22	Q	306	CLA	C2B-C3B-CAB-CBB
22	Q	306	CLA	C4B-C3B-CAB-CBB
22	Q	308	CLA	C3A-C2A-CAA-CBA
22	Q	308	CLA	CHA-CBD-CGD-O1D
22	Q	308	CLA	CHA-CBD-CGD-O2D
22	U	301	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	U	304	CLA	C2B-C3B-CAB-CBB
22	U	305	CLA	CBD-CGD-O2D-CED
22	U	305	CLA	O1D-CGD-O2D-CED
22	U	306	CLA	C4B-C3B-CAB-CBB
22	U	307	CLA	C2B-C3B-CAB-CBB
22	U	307	CLA	C4B-C3B-CAB-CBB
22	U	307	CLA	CBD-CGD-O2D-CED
22	U	308	CLA	C2B-C3B-CAB-CBB
22	U	308	CLA	C4B-C3B-CAB-CBB
22	U	308	CLA	CHA-CBD-CGD-O1D
22	U	308	CLA	CAD-CBD-CGD-O1D
22	U	308	CLA	CAD-CBD-CGD-O2D
22	N	302	CLA	CHA-CBD-CGD-O1D
22	N	302	CLA	CHA-CBD-CGD-O2D
22	N	302	CLA	CAD-CBD-CGD-O1D
22	N	302	CLA	CBD-CGD-O2D-CED
22	N	303	CLA	CHA-CBD-CGD-O1D
22	N	303	CLA	CHA-CBD-CGD-O2D
22	N	303	CLA	CAD-CBD-CGD-O1D
22	N	304	CLA	CBD-CGD-O2D-CED
22	N	305	CLA	C2B-C3B-CAB-CBB
22	N	305	CLA	C4B-C3B-CAB-CBB
22	N	305	CLA	CHA-CBD-CGD-O1D
22	N	305	CLA	CHA-CBD-CGD-O2D
22	N	306	CLA	CBD-CGD-O2D-CED
22	N	308	CLA	C1A-C2A-CAA-CBA
22	N	308	CLA	C4B-C3B-CAB-CBB
22	N	308	CLA	CAD-CBD-CGD-O1D
22	N	308	CLA	CAD-CBD-CGD-O2D
22	G	301	CLA	C2-C3-C5-C6
22	G	301	CLA	C4-C3-C5-C6
22	G	302	CLA	CHA-CBD-CGD-O1D
22	G	302	CLA	CHA-CBD-CGD-O2D
22	G	302	CLA	CAD-CBD-CGD-O1D
22	G	302	CLA	CBD-CGD-O2D-CED
22	G	303	CLA	C1A-C2A-CAA-CBA
22	G	303	CLA	C3A-C2A-CAA-CBA
22	G	303	CLA	CHA-CBD-CGD-O1D
22	G	303	CLA	CHA-CBD-CGD-O2D
22	G	304	CLA	CBD-CGD-O2D-CED
22	G	304	CLA	O1D-CGD-O2D-CED
22	G	305	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	G	307	CLA	C4B-C3B-CAB-CBB
22	G	307	CLA	CBD-CGD-O2D-CED
22	G	307	CLA	O1D-CGD-O2D-CED
22	G	308	CLA	CHA-CBD-CGD-O1D
22	G	308	CLA	CHA-CBD-CGD-O2D
22	G	308	CLA	CAD-CBD-CGD-O1D
22	u	301	CLA	CBD-CGD-O2D-CED
22	u	305	CLA	CBD-CGD-O2D-CED
22	u	305	CLA	O1D-CGD-O2D-CED
22	u	307	CLA	CBD-CGD-O2D-CED
22	u	308	CLA	C2B-C3B-CAB-CBB
22	u	308	CLA	C4B-C3B-CAB-CBB
22	u	308	CLA	CHA-CBD-CGD-O1D
22	u	308	CLA	CHA-CBD-CGD-O2D
22	u	308	CLA	CAD-CBD-CGD-O1D
22	u	308	CLA	CAD-CBD-CGD-O2D
22	n	303	CLA	CHA-CBD-CGD-O1D
22	n	303	CLA	CHA-CBD-CGD-O2D
22	n	305	CLA	C2B-C3B-CAB-CBB
22	n	305	CLA	C4B-C3B-CAB-CBB
22	n	305	CLA	CHA-CBD-CGD-O1D
22	n	305	CLA	CHA-CBD-CGD-O2D
22	n	306	CLA	CBD-CGD-O2D-CED
22	n	308	CLA	C1A-C2A-CAA-CBA
22	n	308	CLA	C3A-C2A-CAA-CBA
22	n	308	CLA	C2B-C3B-CAB-CBB
22	n	308	CLA	C4B-C3B-CAB-CBB
22	n	308	CLA	CBD-CGD-O2D-CED
22	g	301	CLA	C2-C3-C5-C6
22	g	301	CLA	C4-C3-C5-C6
22	g	302	CLA	CHA-CBD-CGD-O1D
22	g	302	CLA	CHA-CBD-CGD-O2D
22	g	302	CLA	CAD-CBD-CGD-O1D
22	g	302	CLA	CBD-CGD-O2D-CED
22	g	303	CLA	C3A-C2A-CAA-CBA
22	g	303	CLA	CAD-CBD-CGD-O1D
22	g	303	CLA	CAD-CBD-CGD-O2D
22	g	304	CLA	CBD-CGD-O2D-CED
22	g	304	CLA	O1D-CGD-O2D-CED
22	g	305	CLA	C1A-C2A-CAA-CBA
22	g	305	CLA	C3A-C2A-CAA-CBA
22	g	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	g	305	CLA	C4B-C3B-CAB-CBB
22	g	305	CLA	CBD-CGD-O2D-CED
22	g	307	CLA	C4B-C3B-CAB-CBB
22	g	307	CLA	CBD-CGD-O2D-CED
22	g	307	CLA	O1D-CGD-O2D-CED
22	g	308	CLA	CHA-CBD-CGD-O1D
22	g	308	CLA	CHA-CBD-CGD-O2D
22	g	308	CLA	CAD-CBD-CGD-O1D
22	g	308	CLA	CAD-CBD-CGD-O2D
22	R	302	CLA	C2B-C3B-CAB-CBB
22	R	302	CLA	C4B-C3B-CAB-CBB
22	R	304	CLA	CBD-CGD-O2D-CED
22	R	305	CLA	C1A-C2A-CAA-CBA
22	R	306	CLA	C4B-C3B-CAB-CBB
22	R	307	CLA	CBD-CGD-O2D-CED
22	R	308	CLA	C1A-C2A-CAA-CBA
22	R	308	CLA	C3A-C2A-CAA-CBA
22	R	308	CLA	C4B-C3B-CAB-CBB
22	R	309	CLA	CBD-CGD-O2D-CED
22	R	310	CLA	C1A-C2A-CAA-CBA
22	R	310	CLA	C3A-C2A-CAA-CBA
22	R	310	CLA	CHA-CBD-CGD-O1D
22	R	310	CLA	CHA-CBD-CGD-O2D
22	R	310	CLA	CBD-CGD-O2D-CED
22	R	311	CLA	C1A-C2A-CAA-CBA
22	R	311	CLA	C3A-C2A-CAA-CBA
22	R	311	CLA	C4B-C3B-CAB-CBB
22	S	301	CLA	C1A-C2A-CAA-CBA
22	S	302	CLA	CBD-CGD-O2D-CED
22	S	303	CLA	CBD-CGD-O2D-CED
22	S	304	CLA	C1A-C2A-CAA-CBA
22	S	304	CLA	C3A-C2A-CAA-CBA
22	S	304	CLA	C2B-C3B-CAB-CBB
22	S	304	CLA	C4B-C3B-CAB-CBB
22	S	304	CLA	CBD-CGD-O2D-CED
22	S	305	CLA	CBD-CGD-O2D-CED
22	S	306	CLA	C4B-C3B-CAB-CBB
22	S	309	CLA	C2B-C3B-CAB-CBB
22	S	309	CLA	C4B-C3B-CAB-CBB
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	C	506	CLA	C2B-C3B-CAB-CBB
22	C	506	CLA	C4B-C3B-CAB-CBB
22	C	507	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O2D
22	C	508	CLA	C2B-C3B-CAB-CBB
22	C	508	CLA	C4B-C3B-CAB-CBB
22	C	510	CLA	C2-C3-C5-C6
22	C	510	CLA	C4-C3-C5-C6
22	C	513	CLA	CHA-CBD-CGD-O1D
22	C	513	CLA	CHA-CBD-CGD-O2D
22	C	513	CLA	CBD-CGD-O2D-CED
22	C	514	CLA	C4B-C3B-CAB-CBB
22	C	514	CLA	CBD-CGD-O2D-CED
22	C	515	CLA	C1A-C2A-CAA-CBA
22	B	603	CLA	C2B-C3B-CAB-CBB
22	B	603	CLA	C4B-C3B-CAB-CBB
22	B	604	CLA	CAD-CBD-CGD-O1D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	C2-C3-C5-C6
22	B	604	CLA	C4-C3-C5-C6
22	B	605	CLA	C2B-C3B-CAB-CBB
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	605	CLA	CAD-CBD-CGD-O1D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	B	606	CLA	C2B-C3B-CAB-CBB
22	B	606	CLA	C4B-C3B-CAB-CBB
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O2D
22	B	607	CLA	C2B-C3B-CAB-CBB
22	B	607	CLA	C4B-C3B-CAB-CBB
22	B	608	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	CBD-CGD-O2D-CED
22	B	615	CLA	C2-C3-C5-C6
22	B	615	CLA	C4-C3-C5-C6
22	B	615	CLA	C6-C7-C8-C9
22	B	616	CLA	CHA-CBD-CGD-O1D
22	B	616	CLA	CHA-CBD-CGD-O2D
22	B	617	CLA	CAD-CBD-CGD-O1D
22	B	617	CLA	CAD-CBD-CGD-O2D
22	X	202	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	CAD-CBD-CGD-O1D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	C2-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
22	b	605	CLA	C2B-C3B-CAB-CBB
22	b	605	CLA	C4B-C3B-CAB-CBB
22	b	605	CLA	CAD-CBD-CGD-O1D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	b	606	CLA	C2B-C3B-CAB-CBB
22	b	606	CLA	C4B-C3B-CAB-CBB
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	C2B-C3B-CAB-CBB
22	b	607	CLA	C4B-C3B-CAB-CBB
22	b	609	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	C2-C3-C5-C6
22	b	610	CLA	C4-C3-C5-C6
22	b	610	CLA	C6-C7-C8-C9
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	613	CLA	C1A-C2A-CAA-CBA
22	b	613	CLA	C3A-C2A-CAA-CBA
22	b	615	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CHA-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	b	617	CLA	C2B-C3B-CAB-CBB
22	b	617	CLA	C4B-C3B-CAB-CBB
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	C2-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
22	c	505	CLA	C2B-C3B-CAB-CBB
22	c	505	CLA	C4B-C3B-CAB-CBB
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	C2B-C3B-CAB-CBB
22	c	507	CLA	C4B-C3B-CAB-CBB
22	c	507	CLA	C2-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C4-C3-C5-C6
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CHA-CBD-CGD-O1D
22	c	512	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	C4B-C3B-CAB-CBB
22	c	513	CLA	CBD-CGD-O2D-CED
22	c	514	CLA	C1A-C2A-CAA-CBA
22	s	301	CLA	C1A-C2A-CAA-CBA
22	s	301	CLA	C3A-C2A-CAA-CBA
22	s	302	CLA	CBD-CGD-O2D-CED
22	s	303	CLA	CBD-CGD-O2D-CED
22	s	304	CLA	C1A-C2A-CAA-CBA
22	s	304	CLA	C3A-C2A-CAA-CBA
22	s	304	CLA	C2B-C3B-CAB-CBB
22	s	304	CLA	C4B-C3B-CAB-CBB
22	s	304	CLA	CBD-CGD-O2D-CED
22	s	305	CLA	CBD-CGD-O2D-CED
22	s	306	CLA	C4B-C3B-CAB-CBB
23	1	309	LUT	C1-C6-C7-C8
23	2	309	LUT	C27-C28-C29-C30
23	2	309	LUT	C27-C28-C29-C39
23	4	309	LUT	C1-C6-C7-C8
23	5	309	LUT	C27-C28-C29-C30
23	5	309	LUT	C27-C28-C29-C39
23	U	309	LUT	C1-C6-C7-C8
23	S	311	LUT	C11-C12-C13-C20
23	S	311	LUT	C27-C28-C29-C30
23	S	311	LUT	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
23	s	311	LUT	C27-C28-C29-C30
23	s	311	LUT	C27-C28-C29-C39
24	r	612	XAT	C27-C28-C29-C30
24	r	612	XAT	C27-C28-C29-C39
24	r	612	XAT	C31-C32-C33-C34
24	r	612	XAT	C31-C32-C33-C40
24	1	311	XAT	C9-C10-C11-C12
24	1	311	XAT	C31-C32-C33-C34
24	1	311	XAT	C31-C32-C33-C40
24	2	311	XAT	C7-C8-C9-C10
24	2	311	XAT	C7-C8-C9-C19
24	3	309	XAT	C7-C8-C9-C10
24	3	309	XAT	C7-C8-C9-C19
24	3	309	XAT	C31-C32-C33-C40
24	4	311	XAT	C9-C10-C11-C12
24	4	311	XAT	C31-C32-C33-C34
24	4	311	XAT	C31-C32-C33-C40
24	5	311	XAT	C7-C8-C9-C10
24	5	311	XAT	C7-C8-C9-C19
24	5	311	XAT	C11-C12-C13-C14
24	5	311	XAT	C11-C12-C13-C20
24	6	310	XAT	C7-C8-C9-C10
24	6	310	XAT	C7-C8-C9-C19
24	6	310	XAT	C31-C32-C33-C34
24	6	310	XAT	C31-C32-C33-C40
24	v	311	XAT	C7-C8-C9-C10
24	v	311	XAT	C7-C8-C9-C19
24	v	311	XAT	C27-C28-C29-C30
24	v	311	XAT	C27-C28-C29-C39
24	v	311	XAT	C31-C32-C33-C40
24	p	312	XAT	C27-C28-C29-C30
24	p	312	XAT	C27-C28-C29-C39
24	p	312	XAT	C31-C32-C33-C40
24	q	309	XAT	C7-C8-C9-C19
24	q	309	XAT	C13-C14-C15-C35
24	q	309	XAT	C31-C32-C33-C34
24	q	309	XAT	C31-C32-C33-C40
24	V	311	XAT	C7-C8-C9-C10
24	V	311	XAT	C7-C8-C9-C19
24	V	311	XAT	C11-C12-C13-C14
24	V	311	XAT	C11-C12-C13-C20
24	V	311	XAT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	V	311	XAT	C27-C28-C29-C39
24	P	312	XAT	C11-C12-C13-C14
24	P	312	XAT	C11-C12-C13-C20
24	P	312	XAT	C31-C32-C33-C34
24	P	312	XAT	C31-C32-C33-C40
24	Q	309	XAT	C7-C8-C9-C10
24	Q	309	XAT	C7-C8-C9-C19
24	Q	309	XAT	C31-C32-C33-C34
24	Q	309	XAT	C31-C32-C33-C40
24	U	311	XAT	C7-C8-C9-C10
24	U	311	XAT	C7-C8-C9-C19
24	U	311	XAT	C11-C12-C13-C14
24	U	311	XAT	C11-C12-C13-C20
24	U	311	XAT	C31-C32-C33-C34
24	U	311	XAT	C31-C32-C33-C40
24	N	311	XAT	C7-C8-C9-C19
24	N	311	XAT	C9-C10-C11-C12
24	G	309	XAT	C7-C8-C9-C10
24	G	309	XAT	C7-C8-C9-C19
24	G	309	XAT	C11-C12-C13-C14
24	G	309	XAT	C11-C12-C13-C20
24	G	309	XAT	C27-C28-C29-C39
24	G	309	XAT	C31-C32-C33-C34
24	G	309	XAT	C31-C32-C33-C40
24	u	311	XAT	C7-C8-C9-C10
24	u	311	XAT	C7-C8-C9-C19
24	u	311	XAT	C11-C12-C13-C14
24	u	311	XAT	C11-C12-C13-C20
24	n	311	XAT	C27-C28-C29-C30
24	n	311	XAT	C27-C28-C29-C39
24	g	309	XAT	C7-C8-C9-C10
24	g	309	XAT	C7-C8-C9-C19
24	g	309	XAT	C11-C12-C13-C14
24	g	309	XAT	C11-C12-C13-C20
24	g	309	XAT	C27-C28-C29-C39
24	g	309	XAT	C31-C32-C33-C34
24	g	309	XAT	C31-C32-C33-C40
24	R	313	XAT	C27-C28-C29-C30
24	R	313	XAT	C27-C28-C29-C39
25	r	613	LHG	C4-O6-P-O5
25	a	415	LHG	C2-C3-O3-P
25	a	415	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
25	a	415	LHG	C4-O6-P-O4
25	a	415	LHG	C4-O6-P-O5
25	a	415	LHG	C8-C7-O7-C5
25	d	405	LHG	O1-C1-C2-C3
25	d	405	LHG	C3-O3-P-O4
25	d	405	LHG	C3-O3-P-O5
25	d	406	LHG	C4-O6-P-O4
25	l	101	LHG	C3-O3-P-O4
25	l	101	LHG	C3-O3-P-O5
25	l	101	LHG	C4-O6-P-O4
25	A	413	LHG	C2-C3-O3-P
25	A	413	LHG	C4-O6-P-O3
25	A	413	LHG	C4-O6-P-O4
25	A	413	LHG	C4-O6-P-O5
25	A	413	LHG	C8-C7-O7-C5
25	L	101	LHG	O1-C1-C2-O2
25	L	101	LHG	C3-O3-P-O4
25	L	101	LHG	C3-O3-P-O5
25	L	101	LHG	C4-O6-P-O4
25	1	312	LHG	O1-C1-C2-C3
25	1	312	LHG	O2-C2-C3-O3
25	1	312	LHG	C4-O6-P-O5
25	2	312	LHG	O1-C1-C2-C3
25	2	312	LHG	C4-O6-P-O5
25	3	310	LHG	C4-O6-P-O5
25	4	312	LHG	C4-O6-P-O5
25	5	312	LHG	C4-O6-P-O5
25	6	311	LHG	O1-C1-C2-C3
25	6	311	LHG	C4-O6-P-O5
25	v	312	LHG	C3-O3-P-O4
25	v	312	LHG	C4-O6-P-O5
25	p	313	LHG	O1-C1-C2-O2
25	p	313	LHG	O1-C1-C2-C3
25	p	313	LHG	C1-C2-C3-O3
25	p	313	LHG	C4-O6-P-O5
25	q	310	LHG	C1-C2-C3-O3
25	q	310	LHG	C4-O6-P-O5
25	V	312	LHG	O1-C1-C2-O2
25	V	312	LHG	O1-C1-C2-C3
25	V	312	LHG	C3-O3-P-O4
25	V	312	LHG	C3-O3-P-O5
25	V	312	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
25	Q	310	LHG	O1-C1-C2-C3
25	Q	310	LHG	C4-O6-P-O5
25	U	312	LHG	C3-O3-P-O5
25	G	310	LHG	O1-C1-C2-C3
25	G	310	LHG	C4-O6-P-O5
25	u	312	LHG	C3-O3-P-O5
25	n	312	LHG	C1-C2-C3-O3
25	n	312	LHG	C4-O6-P-O5
25	g	310	LHG	O1-C1-C2-C3
25	g	310	LHG	C4-O6-P-O5
25	R	314	LHG	O1-C1-C2-C3
25	R	314	LHG	O2-C2-C3-O3
25	R	314	LHG	C3-O3-P-O4
25	R	314	LHG	C3-O3-P-O5
25	R	314	LHG	C3-O3-P-O6
25	R	314	LHG	C4-O6-P-O5
25	S	312	LHG	C4-O6-P-O5
25	C	522	LHG	C24-C23-O8-C6
25	C	524	LHG	O1-C1-C2-C3
25	C	524	LHG	C1-C2-C3-O3
25	C	524	LHG	O9-C7-O7-C5
25	C	524	LHG	C8-C7-O7-C5
25	B	622	LHG	C4-O6-P-O4
25	B	623	LHG	O1-C1-C2-C3
25	B	623	LHG	O2-C2-C3-O3
25	B	623	LHG	C3-O3-P-O4
25	B	623	LHG	C4-O6-P-O4
25	B	623	LHG	C4-O6-P-O5
25	B	623	LHG	O7-C5-C6-O8
25	D	406	LHG	C3-O3-P-O4
25	D	407	LHG	C4-O6-P-O4
25	b	622	LHG	C3-O3-P-O6
25	b	622	LHG	C4-O6-P-O4
25	b	622	LHG	C4-O6-P-O5
25	b	623	LHG	O1-C1-C2-O2
25	b	623	LHG	O1-C1-C2-C3
25	b	623	LHG	O2-C2-C3-O3
25	b	623	LHG	C3-O3-P-O4
25	b	623	LHG	C4-O6-P-O4
25	b	623	LHG	C4-O6-P-O5
25	b	623	LHG	O7-C5-C6-O8
25	c	521	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	c	521	LHG	C4-O6-P-O5
25	c	523	LHG	O1-C1-C2-C3
25	c	523	LHG	C1-C2-C3-O3
25	c	523	LHG	O9-C7-O7-C5
25	s	312	LHG	C4-O6-P-O5
26	r	614	CHL	C1C-C2C-CMC-OMC
26	r	614	CHL	C3C-C2C-CMC-OMC
26	1	314	CHL	C3C-C2C-CMC-OMC
26	1	314	CHL	CHA-CBD-CGD-O1D
26	1	314	CHL	CHA-CBD-CGD-O2D
26	1	314	CHL	CAD-CBD-CGD-O1D
26	1	314	CHL	CAD-CBD-CGD-O2D
26	1	314	CHL	CBD-CGD-O2D-CED
26	1	315	CHL	C2B-C3B-CAB-CBB
26	1	315	CHL	C4B-C3B-CAB-CBB
26	1	315	CHL	C1C-C2C-CMC-OMC
26	1	317	CHL	C1C-C2C-CMC-OMC
26	1	317	CHL	C3C-C2C-CMC-OMC
26	2	313	CHL	C2-C3-C5-C6
26	2	313	CHL	C4-C3-C5-C6
26	2	314	CHL	C1C-C2C-CMC-OMC
26	2	314	CHL	C3C-C2C-CMC-OMC
26	2	314	CHL	CHA-CBD-CGD-O1D
26	2	314	CHL	CHA-CBD-CGD-O2D
26	2	314	CHL	CBD-CGD-O2D-CED
26	2	315	CHL	CBD-CGD-O2D-CED
26	2	316	CHL	C1C-C2C-CMC-OMC
26	2	316	CHL	C3C-C2C-CMC-OMC
26	2	316	CHL	CHA-CBD-CGD-O1D
26	2	316	CHL	CHA-CBD-CGD-O2D
26	2	318	CHL	C3C-C2C-CMC-OMC
26	3	312	CHL	CHA-CBD-CGD-O1D
26	3	312	CHL	CHA-CBD-CGD-O2D
26	3	312	CHL	CAD-CBD-CGD-O1D
26	3	313	CHL	C3A-C2A-CAA-CBA
26	3	313	CHL	C2B-C3B-CAB-CBB
26	3	313	CHL	C4B-C3B-CAB-CBB
26	3	313	CHL	C1C-C2C-CMC-OMC
26	3	314	CHL	CBD-CGD-O2D-CED
26	3	315	CHL	C1C-C2C-CMC-OMC
26	3	315	CHL	C3C-C2C-CMC-OMC
26	3	316	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	3	316	CHL	C1C-C2C-CMC-OMC
26	3	316	CHL	C3C-C2C-CMC-OMC
26	3	316	CHL	CHA-CBD-CGD-O1D
26	3	316	CHL	CHA-CBD-CGD-O2D
26	4	314	CHL	CHA-CBD-CGD-O1D
26	4	314	CHL	CHA-CBD-CGD-O2D
26	4	314	CHL	CAD-CBD-CGD-O1D
26	4	314	CHL	CAD-CBD-CGD-O2D
26	4	314	CHL	CBD-CGD-O2D-CED
26	4	315	CHL	C2B-C3B-CAB-CBB
26	4	315	CHL	C4B-C3B-CAB-CBB
26	4	315	CHL	C1C-C2C-CMC-OMC
26	4	316	CHL	C1A-C2A-CAA-CBA
26	4	316	CHL	C1C-C2C-CMC-OMC
26	4	316	CHL	C3C-C2C-CMC-OMC
26	4	317	CHL	C3C-C2C-CMC-OMC
26	5	313	CHL	C2-C3-C5-C6
26	5	313	CHL	C4-C3-C5-C6
26	5	314	CHL	C1C-C2C-CMC-OMC
26	5	314	CHL	C3C-C2C-CMC-OMC
26	5	314	CHL	CHA-CBD-CGD-O1D
26	5	314	CHL	CHA-CBD-CGD-O2D
26	5	314	CHL	CAD-CBD-CGD-O1D
26	5	314	CHL	CBD-CGD-O2D-CED
26	5	316	CHL	C1C-C2C-CMC-OMC
26	5	316	CHL	C3C-C2C-CMC-OMC
26	5	316	CHL	CHA-CBD-CGD-O1D
26	5	316	CHL	CHA-CBD-CGD-O2D
26	5	318	CHL	C3C-C2C-CMC-OMC
26	5	318	CHL	C14-C13-C15-C16
26	6	301	CHL	C3C-C2C-CMC-OMC
26	6	301	CHL	C11-C10-C8-C9
26	6	313	CHL	CHA-CBD-CGD-O1D
26	6	313	CHL	CHA-CBD-CGD-O2D
26	6	313	CHL	CAD-CBD-CGD-O1D
26	6	314	CHL	C2B-C3B-CAB-CBB
26	6	314	CHL	C4B-C3B-CAB-CBB
26	6	314	CHL	C1C-C2C-CMC-OMC
26	6	315	CHL	C2A-CAA-CBA-CGA
26	6	315	CHL	CBD-CGD-O2D-CED
26	6	316	CHL	C1A-C2A-CAA-CBA
26	6	316	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	6	316	CHL	C3C-C2C-CMC-OMC
26	6	317	CHL	C1A-C2A-CAA-CBA
26	6	317	CHL	C1C-C2C-CMC-OMC
26	6	317	CHL	C3C-C2C-CMC-OMC
26	v	313	CHL	C3C-C2C-CMC-OMC
26	v	314	CHL	C3C-C2C-CMC-OMC
26	v	314	CHL	CHA-CBD-CGD-O1D
26	v	314	CHL	CHA-CBD-CGD-O2D
26	v	314	CHL	CAD-CBD-CGD-O1D
26	v	314	CHL	CAD-CBD-CGD-O2D
26	v	315	CHL	C1C-C2C-CMC-OMC
26	v	316	CHL	C1C-C2C-CMC-OMC
26	v	316	CHL	C3C-C2C-CMC-OMC
26	v	317	CHL	C1C-C2C-CMC-OMC
26	v	317	CHL	C3C-C2C-CMC-OMC
26	v	317	CHL	C11-C10-C8-C9
26	v	318	CHL	C1C-C2C-CMC-OMC
26	v	318	CHL	C3C-C2C-CMC-OMC
26	v	318	CHL	C6-C7-C8-C9
26	p	315	CHL	CHA-CBD-CGD-O1D
26	p	315	CHL	CHA-CBD-CGD-O2D
26	p	315	CHL	CAD-CBD-CGD-O1D
26	p	315	CHL	CBD-CGD-O2D-CED
26	p	316	CHL	C1C-C2C-CMC-OMC
26	p	317	CHL	CHA-CBD-CGD-O1D
26	p	318	CHL	CBD-CGD-O2D-CED
26	p	319	CHL	C1C-C2C-CMC-OMC
26	p	319	CHL	C3C-C2C-CMC-OMC
26	p	320	CHL	C11-C10-C8-C9
26	q	311	CHL	C2-C3-C5-C6
26	q	311	CHL	C4-C3-C5-C6
26	q	312	CHL	C2A-CAA-CBA-CGA
26	q	312	CHL	C3C-C2C-CMC-OMC
26	q	312	CHL	CHA-CBD-CGD-O1D
26	q	312	CHL	CHA-CBD-CGD-O2D
26	q	312	CHL	CAD-CBD-CGD-O1D
26	q	312	CHL	CAD-CBD-CGD-O2D
26	q	313	CHL	CHA-CBD-CGD-O1D
26	q	313	CHL	CHA-CBD-CGD-O2D
26	q	314	CHL	C1A-C2A-CAA-CBA
26	q	314	CHL	C3C-C2C-CMC-OMC
26	q	315	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	q	315	CHL	C3C-C2C-CMC-OMC
26	V	313	CHL	C3C-C2C-CMC-OMC
26	V	314	CHL	C3C-C2C-CMC-OMC
26	V	314	CHL	CHA-CBD-CGD-O1D
26	V	314	CHL	CHA-CBD-CGD-O2D
26	V	314	CHL	CAD-CBD-CGD-O1D
26	V	315	CHL	C1C-C2C-CMC-OMC
26	V	316	CHL	C3C-C2C-CMC-OMC
26	V	317	CHL	C3C-C2C-CMC-OMC
26	V	318	CHL	C3C-C2C-CMC-OMC
26	V	318	CHL	C6-C7-C8-C9
26	P	315	CHL	CHA-CBD-CGD-O1D
26	P	315	CHL	CHA-CBD-CGD-O2D
26	P	315	CHL	CAD-CBD-CGD-O1D
26	P	316	CHL	C1C-C2C-CMC-OMC
26	P	317	CHL	C2A-CAA-CBA-CGA
26	P	317	CHL	CHA-CBD-CGD-O1D
26	P	317	CHL	CHA-CBD-CGD-O2D
26	P	317	CHL	C11-C10-C8-C9
26	P	318	CHL	C3C-C2C-CMC-OMC
26	P	319	CHL	C1A-C2A-CAA-CBA
26	P	319	CHL	C3C-C2C-CMC-OMC
26	Q	312	CHL	C1A-C2A-CAA-CBA
26	Q	312	CHL	C3C-C2C-CMC-OMC
26	Q	312	CHL	CHA-CBD-CGD-O1D
26	Q	312	CHL	CHA-CBD-CGD-O2D
26	Q	312	CHL	CAD-CBD-CGD-O1D
26	Q	312	CHL	CAD-CBD-CGD-O2D
26	Q	313	CHL	CHA-CBD-CGD-O1D
26	Q	313	CHL	CHA-CBD-CGD-O2D
26	Q	314	CHL	C3C-C2C-CMC-OMC
26	Q	314	CHL	C11-C10-C8-C9
26	Q	315	CHL	C1A-C2A-CAA-CBA
26	Q	315	CHL	C1C-C2C-CMC-OMC
26	Q	315	CHL	C3C-C2C-CMC-OMC
26	Q	315	CHL	C11-C10-C8-C9
26	Q	316	CHL	C1C-C2C-CMC-OMC
26	Q	316	CHL	C3C-C2C-CMC-OMC
26	U	314	CHL	C2B-C3B-CAB-CBB
26	U	314	CHL	C4B-C3B-CAB-CBB
26	U	314	CHL	C1C-C2C-CMC-OMC
26	U	314	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	U	314	CHL	CHA-CBD-CGD-O2D
26	U	315	CHL	C1C-C2C-CMC-OMC
26	U	315	CHL	C3C-C2C-CMC-OMC
26	U	315	CHL	CHA-CBD-CGD-O1D
26	U	315	CHL	CHA-CBD-CGD-O2D
26	U	316	CHL	C1C-C2C-CMC-OMC
26	U	316	CHL	C3C-C2C-CMC-OMC
26	U	316	CHL	C6-C7-C8-C9
26	U	317	CHL	C1C-C2C-CMC-OMC
26	U	317	CHL	C3C-C2C-CMC-OMC
26	U	317	CHL	C14-C13-C15-C16
26	U	319	CHL	C1A-C2A-CAA-CBA
26	U	319	CHL	C2A-CAA-CBA-CGA
26	U	319	CHL	C1C-C2C-CMC-OMC
26	U	319	CHL	C3C-C2C-CMC-OMC
26	U	319	CHL	CHA-CBD-CGD-O1D
26	U	319	CHL	CHA-CBD-CGD-O2D
26	U	319	CHL	C11-C10-C8-C9
26	N	313	CHL	C3C-C2C-CMC-OMC
26	N	314	CHL	C1C-C2C-CMC-OMC
26	N	314	CHL	C3C-C2C-CMC-OMC
26	N	314	CHL	CHA-CBD-CGD-O1D
26	N	314	CHL	CHA-CBD-CGD-O2D
26	N	314	CHL	CAD-CBD-CGD-O1D
26	N	314	CHL	CAD-CBD-CGD-O2D
26	N	314	CHL	CBD-CGD-O2D-CED
26	N	315	CHL	C2B-C3B-CAB-CBB
26	N	315	CHL	C4B-C3B-CAB-CBB
26	N	315	CHL	C1C-C2C-CMC-OMC
26	N	316	CHL	C1C-C2C-CMC-OMC
26	N	316	CHL	C3C-C2C-CMC-OMC
26	N	316	CHL	CHA-CBD-CGD-O1D
26	N	316	CHL	CHA-CBD-CGD-O2D
26	N	317	CHL	C1C-C2C-CMC-OMC
26	N	317	CHL	C3C-C2C-CMC-OMC
26	G	311	CHL	C2-C3-C5-C6
26	G	311	CHL	C4-C3-C5-C6
26	G	312	CHL	CHA-CBD-CGD-O1D
26	G	312	CHL	CHA-CBD-CGD-O2D
26	G	312	CHL	CAD-CBD-CGD-O1D
26	G	312	CHL	CAD-CBD-CGD-O2D
26	G	313	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	G	313	CHL	C4B-C3B-CAB-CBB
26	G	313	CHL	C3C-C2C-CMC-OMC
26	G	314	CHL	C1C-C2C-CMC-OMC
26	G	314	CHL	C3C-C2C-CMC-OMC
26	G	314	CHL	CBD-CGD-O2D-CED
26	G	315	CHL	C1A-C2A-CAA-CBA
26	G	316	CHL	C1A-C2A-CAA-CBA
26	G	316	CHL	C1C-C2C-CMC-OMC
26	G	316	CHL	C3C-C2C-CMC-OMC
26	u	314	CHL	CHA-CBD-CGD-O1D
26	u	314	CHL	CHA-CBD-CGD-O2D
26	u	314	CHL	CAD-CBD-CGD-O1D
26	u	314	CHL	CAD-CBD-CGD-O2D
26	u	315	CHL	C2B-C3B-CAB-CBB
26	u	315	CHL	C4B-C3B-CAB-CBB
26	u	315	CHL	C1C-C2C-CMC-OMC
26	u	315	CHL	CHA-CBD-CGD-O1D
26	u	315	CHL	CHA-CBD-CGD-O2D
26	u	316	CHL	C1C-C2C-CMC-OMC
26	u	316	CHL	C3C-C2C-CMC-OMC
26	u	316	CHL	CHA-CBD-CGD-O1D
26	u	317	CHL	C1C-C2C-CMC-OMC
26	u	317	CHL	C3C-C2C-CMC-OMC
26	u	317	CHL	C6-C7-C8-C9
26	u	318	CHL	C1C-C2C-CMC-OMC
26	u	318	CHL	C3C-C2C-CMC-OMC
26	n	313	CHL	C1C-C2C-CMC-OMC
26	n	313	CHL	C3C-C2C-CMC-OMC
26	n	314	CHL	C3C-C2C-CMC-OMC
26	n	314	CHL	CHA-CBD-CGD-O1D
26	n	314	CHL	CHA-CBD-CGD-O2D
26	n	314	CHL	CAD-CBD-CGD-O1D
26	n	314	CHL	CAD-CBD-CGD-O2D
26	n	314	CHL	CBD-CGD-O2D-CED
26	n	315	CHL	C2B-C3B-CAB-CBB
26	n	315	CHL	C4B-C3B-CAB-CBB
26	n	315	CHL	C1C-C2C-CMC-OMC
26	n	316	CHL	C1A-C2A-CAA-CBA
26	n	316	CHL	C2B-C3B-CAB-CBB
26	n	316	CHL	C4B-C3B-CAB-CBB
26	n	316	CHL	C1C-C2C-CMC-OMC
26	n	316	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	n	316	CHL	CHA-CBD-CGD-O2D
26	n	317	CHL	C1C-C2C-CMC-OMC
26	n	317	CHL	C3C-C2C-CMC-OMC
26	n	317	CHL	CHA-CBD-CGD-O1D
26	n	317	CHL	CHA-CBD-CGD-O2D
26	n	318	CHL	C1C-C2C-CMC-OMC
26	n	318	CHL	C3C-C2C-CMC-OMC
26	g	312	CHL	C1C-C2C-CMC-OMC
26	g	312	CHL	C3C-C2C-CMC-OMC
26	g	312	CHL	CHA-CBD-CGD-O1D
26	g	312	CHL	CHA-CBD-CGD-O2D
26	g	313	CHL	C2B-C3B-CAB-CBB
26	g	313	CHL	C4B-C3B-CAB-CBB
26	g	313	CHL	C3C-C2C-CMC-OMC
26	g	314	CHL	C3C-C2C-CMC-OMC
26	g	315	CHL	C1C-C2C-CMC-OMC
26	g	315	CHL	C3C-C2C-CMC-OMC
26	g	316	CHL	C1A-C2A-CAA-CBA
26	g	316	CHL	C1C-C2C-CMC-OMC
26	g	316	CHL	C3C-C2C-CMC-OMC
26	R	315	CHL	C1C-C2C-CMC-OMC
26	R	315	CHL	C3C-C2C-CMC-OMC
26	R	316	CHL	C3C-C2C-CMC-OMC
26	R	316	CHL	CHA-CBD-CGD-O1D
26	S	313	CHL	C1C-C2C-CMC-OMC
26	S	313	CHL	C3C-C2C-CMC-OMC
26	S	316	CHL	C1A-C2A-CAA-CBA
26	S	316	CHL	CHA-CBD-CGD-O1D
26	S	316	CHL	CHA-CBD-CGD-O2D
26	s	313	CHL	C1C-C2C-CMC-OMC
26	s	313	CHL	C3C-C2C-CMC-OMC
26	s	316	CHL	C1A-C2A-CAA-CBA
26	s	316	CHL	C3C-C2C-CMC-OMC
26	s	316	CHL	CHA-CBD-CGD-O1D
26	s	316	CHL	CHA-CBD-CGD-O2D
27	r	618	NEX	C7-C8-C9-C10
27	r	618	NEX	C7-C8-C9-C19
27	r	618	NEX	O24-C26-C27-C28
27	2	319	NEX	C7-C8-C9-C19
27	2	319	NEX	C11-C12-C13-C14
27	2	319	NEX	C11-C12-C13-C20
27	5	319	NEX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
27	5	319	NEX	C7-C8-C9-C19
27	5	319	NEX	C11-C12-C13-C14
27	5	319	NEX	C11-C12-C13-C20
27	v	319	NEX	C11-C12-C13-C14
27	v	319	NEX	C11-C12-C13-C20
27	V	319	NEX	C7-C8-C9-C19
27	V	319	NEX	C11-C12-C13-C14
27	V	319	NEX	C11-C12-C13-C20
27	N	318	NEX	C7-C8-C9-C10
27	N	318	NEX	C7-C8-C9-C19
27	n	319	NEX	C7-C8-C9-C10
27	n	319	NEX	C7-C8-C9-C19
27	n	319	NEX	C11-C12-C13-C20
27	R	301	NEX	C7-C8-C9-C10
27	R	301	NEX	C7-C8-C9-C19
27	R	301	NEX	C11-C12-C13-C14
27	R	301	NEX	C11-C12-C13-C20
27	R	301	NEX	O24-C26-C27-C28
27	S	317	NEX	C7-C8-C9-C10
27	S	317	NEX	C7-C8-C9-C19
27	s	317	NEX	C7-C8-C9-C10
27	s	317	NEX	C7-C8-C9-C19
31	a	409	BCR	C7-C8-C9-C10
31	a	409	BCR	C7-C8-C9-C34
31	d	403	BCR	C1-C6-C7-C8
31	d	403	BCR	C11-C12-C13-C14
31	d	403	BCR	C11-C12-C13-C35
31	d	403	BCR	C15-C16-C17-C18
31	d	403	BCR	C17-C18-C19-C20
31	d	403	BCR	C36-C18-C19-C20
31	d	403	BCR	C21-C22-C23-C24
31	d	403	BCR	C37-C22-C23-C24
31	d	403	BCR	C23-C24-C25-C30
31	k	101	BCR	C11-C12-C13-C14
31	k	101	BCR	C11-C12-C13-C35
31	k	101	BCR	C17-C18-C19-C20
31	k	101	BCR	C36-C18-C19-C20
31	k	101	BCR	C21-C22-C23-C24
31	k	101	BCR	C37-C22-C23-C24
31	t	101	BCR	C7-C8-C9-C10
31	t	101	BCR	C17-C18-C19-C20
31	t	101	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	t	101	BCR	C21-C22-C23-C24
31	t	101	BCR	C37-C22-C23-C24
31	t	101	BCR	C23-C24-C25-C26
31	x	202	BCR	C7-C8-C9-C10
31	x	202	BCR	C7-C8-C9-C34
31	x	202	BCR	C11-C12-C13-C14
31	x	202	BCR	C11-C12-C13-C35
31	z	101	BCR	C11-C12-C13-C35
31	A	409	BCR	C7-C8-C9-C10
31	A	409	BCR	C7-C8-C9-C34
31	K	101	BCR	C11-C12-C13-C14
31	K	101	BCR	C11-C12-C13-C35
31	K	101	BCR	C17-C18-C19-C20
31	K	101	BCR	C36-C18-C19-C20
31	K	101	BCR	C21-C22-C23-C24
31	K	101	BCR	C37-C22-C23-C24
31	T	101	BCR	C17-C18-C19-C20
31	T	101	BCR	C36-C18-C19-C20
31	T	101	BCR	C21-C22-C23-C24
31	T	101	BCR	C37-C22-C23-C24
31	T	101	BCR	C23-C24-C25-C26
31	C	516	BCR	C11-C12-C13-C35
31	C	516	BCR	C13-C14-C15-C16
31	C	517	BCR	C17-C18-C19-C20
31	C	517	BCR	C36-C18-C19-C20
31	C	517	BCR	C21-C22-C23-C24
31	C	517	BCR	C37-C22-C23-C24
31	C	518	BCR	C7-C8-C9-C10
31	C	518	BCR	C7-C8-C9-C34
31	C	518	BCR	C17-C18-C19-C20
31	C	518	BCR	C36-C18-C19-C20
31	C	518	BCR	C21-C22-C23-C24
31	C	518	BCR	C37-C22-C23-C24
31	C	518	BCR	C23-C24-C25-C30
31	B	618	BCR	C11-C12-C13-C14
31	B	618	BCR	C11-C12-C13-C35
31	B	619	BCR	C1-C6-C7-C8
31	B	619	BCR	C7-C8-C9-C10
31	B	619	BCR	C7-C8-C9-C34
31	B	619	BCR	C17-C18-C19-C20
31	B	619	BCR	C36-C18-C19-C20
31	B	619	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
31	B	619	BCR	C37-C22-C23-C24
31	B	620	BCR	C11-C12-C13-C14
31	B	620	BCR	C11-C12-C13-C35
31	B	620	BCR	C17-C18-C19-C20
31	B	620	BCR	C36-C18-C19-C20
31	B	620	BCR	C37-C22-C23-C24
31	D	404	BCR	C1-C6-C7-C8
31	D	404	BCR	C11-C12-C13-C14
31	D	404	BCR	C11-C12-C13-C35
31	D	404	BCR	C15-C16-C17-C18
31	D	404	BCR	C17-C18-C19-C20
31	D	404	BCR	C36-C18-C19-C20
31	D	404	BCR	C21-C22-C23-C24
31	D	404	BCR	C37-C22-C23-C24
31	D	404	BCR	C23-C24-C25-C30
31	X	201	BCR	C7-C8-C9-C10
31	X	201	BCR	C7-C8-C9-C34
31	X	201	BCR	C11-C12-C13-C14
31	X	201	BCR	C11-C12-C13-C35
31	b	619	BCR	C1-C6-C7-C8
31	b	619	BCR	C7-C8-C9-C10
31	b	619	BCR	C7-C8-C9-C34
31	b	619	BCR	C13-C14-C15-C16
31	b	619	BCR	C17-C18-C19-C20
31	b	619	BCR	C36-C18-C19-C20
31	b	619	BCR	C21-C22-C23-C24
31	b	619	BCR	C37-C22-C23-C24
31	b	620	BCR	C11-C12-C13-C14
31	b	620	BCR	C11-C12-C13-C35
31	b	620	BCR	C36-C18-C19-C20
31	b	620	BCR	C21-C22-C23-C24
31	b	620	BCR	C37-C22-C23-C24
31	c	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C36-C18-C19-C20
31	c	515	BCR	C21-C22-C23-C24
31	c	515	BCR	C37-C22-C23-C24
31	c	516	BCR	C7-C8-C9-C10
31	c	516	BCR	C7-C8-C9-C34
31	c	516	BCR	C17-C18-C19-C20
31	c	516	BCR	C36-C18-C19-C20
31	c	516	BCR	C21-C22-C23-C24
31	c	516	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
31	c	516	BCR	C23-C24-C25-C30
32	a	410	SQD	C45-C44-O6-C1
32	a	410	SQD	O5-C1-O6-C44
32	a	410	SQD	C5-C6-S-O7
32	a	410	SQD	C5-C6-S-O8
32	a	410	SQD	C5-C6-S-O9
32	a	413	SQD	C5-C6-S-O9
32	l	102	SQD	C2-C1-O6-C44
32	l	102	SQD	O5-C1-O6-C44
32	l	102	SQD	O49-C7-O47-C45
32	l	102	SQD	C8-C7-O47-C45
32	m	101	SQD	O49-C7-O47-C45
32	m	101	SQD	O5-C5-C6-S
32	A	412	SQD	C5-C6-S-O7
32	A	412	SQD	C5-C6-S-O8
32	A	412	SQD	C5-C6-S-O9
32	L	102	SQD	C2-C1-O6-C44
32	L	102	SQD	O5-C1-O6-C44
32	L	102	SQD	O49-C7-O47-C45
32	L	102	SQD	C8-C7-O47-C45
32	M	101	SQD	O49-C7-O47-C45
32	M	101	SQD	O5-C5-C6-S
32	C	501	SQD	C45-C44-O6-C1
32	C	501	SQD	O5-C1-O6-C44
32	C	501	SQD	C5-C6-S-O7
32	C	501	SQD	C5-C6-S-O8
34	C	521	LMG	C2-C1-O1-C7
34	C	521	LMG	O6-C1-O1-C7
34	B	624	LMG	O6-C1-O1-C7
34	B	624	LMG	C11-C10-O7-C8
34	b	624	LMG	O6-C1-O1-C7
34	b	624	LMG	C11-C10-O7-C8
34	c	520	LMG	C2-C1-O1-C7
34	c	520	LMG	O6-C1-O1-C7
36	a	416	DGD	C2D-C1D-O3G-C3G
36	a	416	DGD	O6D-C1D-O3G-C3G
36	A	414	DGD	C2D-C1D-O3G-C3G
36	A	414	DGD	O6D-C1D-O3G-C3G
36	A	414	DGD	C2E-C1E-O5D-C6D
36	J	101	DGD	C2B-C1B-O2G-C2G
36	C	519	DGD	C2B-C1B-O2G-C2G
36	C	520	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
36	C	520	DGD	O6E-C1E-O5D-C6D
36	c	517	DGD	C2B-C1B-O2G-C2G
36	c	518	DGD	C2E-C1E-O5D-C6D
36	c	518	DGD	O6E-C1E-O5D-C6D
36	c	519	DGD	C2B-C1B-O2G-C2G
22	r	602	CLA	O1D-CGD-O2D-CED
22	r	608	CLA	O1D-CGD-O2D-CED
22	1	305	CLA	O1D-CGD-O2D-CED
22	1	307	CLA	O1D-CGD-O2D-CED
22	3	303	CLA	O1D-CGD-O2D-CED
22	3	304	CLA	O1D-CGD-O2D-CED
22	3	307	CLA	O1D-CGD-O2D-CED
22	4	305	CLA	O1D-CGD-O2D-CED
22	6	304	CLA	O1D-CGD-O2D-CED
22	6	305	CLA	O1D-CGD-O2D-CED
22	6	306	CLA	O1D-CGD-O2D-CED
22	6	308	CLA	O1D-CGD-O2D-CED
22	v	303	CLA	O1D-CGD-O2D-CED
22	v	305	CLA	O1D-CGD-O2D-CED
22	p	308	CLA	O1D-CGD-O2D-CED
22	q	305	CLA	O1D-CGD-O2D-CED
22	q	307	CLA	O1D-CGD-O2D-CED
22	V	303	CLA	O1D-CGD-O2D-CED
22	V	305	CLA	O1D-CGD-O2D-CED
22	V	307	CLA	O1D-CGD-O2D-CED
22	P	308	CLA	O1D-CGD-O2D-CED
22	Q	307	CLA	O1D-CGD-O2D-CED
22	g	305	CLA	O1D-CGD-O2D-CED
22	R	303	CLA	O1D-CGD-O2D-CED
22	R	309	CLA	O1D-CGD-O2D-CED
22	S	302	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
22	B	614	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
22	b	614	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	s	302	CLA	O1D-CGD-O2D-CED
22	r	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	r	609	CLA	O1D-CGD-O2D-CED
22	3	305	CLA	O1D-CGD-O2D-CED
22	4	302	CLA	O1D-CGD-O2D-CED
22	4	307	CLA	O1D-CGD-O2D-CED
22	5	307	CLA	O1D-CGD-O2D-CED
22	6	303	CLA	O1D-CGD-O2D-CED
22	v	306	CLA	O1D-CGD-O2D-CED
22	q	304	CLA	O1D-CGD-O2D-CED
22	G	305	CLA	O1D-CGD-O2D-CED
22	G	306	CLA	O1D-CGD-O2D-CED
22	n	301	CLA	O1D-CGD-O2D-CED
22	n	307	CLA	O1D-CGD-O2D-CED
22	R	307	CLA	O1D-CGD-O2D-CED
22	R	310	CLA	O1D-CGD-O2D-CED
22	S	308	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	602	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	s	308	CLA	O1D-CGD-O2D-CED
22	r	602	CLA	CBD-CGD-O2D-CED
22	r	603	CLA	CBD-CGD-O2D-CED
22	x	201	CLA	CBD-CGD-O2D-CED
22	1	301	CLA	CBD-CGD-O2D-CED
22	2	302	CLA	CBD-CGD-O2D-CED
22	2	306	CLA	CBD-CGD-O2D-CED
22	2	307	CLA	CBD-CGD-O2D-CED
22	3	302	CLA	CBD-CGD-O2D-CED
22	3	303	CLA	CBD-CGD-O2D-CED
22	3	308	CLA	CBD-CGD-O2D-CED
22	4	301	CLA	CBD-CGD-O2D-CED
22	4	302	CLA	CBD-CGD-O2D-CED
22	4	304	CLA	CBD-CGD-O2D-CED
22	4	306	CLA	CBD-CGD-O2D-CED
22	5	302	CLA	CBD-CGD-O2D-CED
22	5	306	CLA	CBD-CGD-O2D-CED
22	6	303	CLA	CBD-CGD-O2D-CED
22	6	309	CLA	CBD-CGD-O2D-CED
22	v	301	CLA	CBD-CGD-O2D-CED
22	v	303	CLA	CBD-CGD-O2D-CED
22	v	306	CLA	CBD-CGD-O2D-CED
22	v	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	p	305	CLA	CBD-CGD-O2D-CED
22	p	307	CLA	CBD-CGD-O2D-CED
22	q	301	CLA	CBD-CGD-O2D-CED
22	q	302	CLA	CBD-CGD-O2D-CED
22	V	301	CLA	CBD-CGD-O2D-CED
22	V	303	CLA	CBD-CGD-O2D-CED
22	V	307	CLA	CBD-CGD-O2D-CED
22	V	308	CLA	CBD-CGD-O2D-CED
22	P	303	CLA	CBD-CGD-O2D-CED
22	P	304	CLA	CBD-CGD-O2D-CED
22	P	305	CLA	CBD-CGD-O2D-CED
22	P	307	CLA	CBD-CGD-O2D-CED
22	Q	307	CLA	CBD-CGD-O2D-CED
22	Q	308	CLA	CBD-CGD-O2D-CED
22	U	308	CLA	CBD-CGD-O2D-CED
22	N	301	CLA	CBD-CGD-O2D-CED
22	N	308	CLA	CBD-CGD-O2D-CED
22	G	303	CLA	CBD-CGD-O2D-CED
22	G	306	CLA	CBD-CGD-O2D-CED
22	G	308	CLA	CBD-CGD-O2D-CED
22	u	303	CLA	CBD-CGD-O2D-CED
22	u	304	CLA	CBD-CGD-O2D-CED
22	u	308	CLA	CBD-CGD-O2D-CED
22	n	301	CLA	CBD-CGD-O2D-CED
22	n	302	CLA	CBD-CGD-O2D-CED
22	n	303	CLA	CBD-CGD-O2D-CED
22	n	304	CLA	CBD-CGD-O2D-CED
22	n	307	CLA	CBD-CGD-O2D-CED
22	g	303	CLA	CBD-CGD-O2D-CED
22	g	306	CLA	CBD-CGD-O2D-CED
22	g	308	CLA	CBD-CGD-O2D-CED
22	R	303	CLA	CBD-CGD-O2D-CED
22	S	308	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	CBD-CGD-O2D-CED
22	B	617	CLA	CBD-CGD-O2D-CED
22	b	602	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	s	308	CLA	CBD-CGD-O2D-CED
26	r	616	CHL	CBD-CGD-O2D-CED
26	r	619	CHL	CBD-CGD-O2D-CED
26	3	312	CHL	CBD-CGD-O2D-CED
26	3	315	CHL	CBD-CGD-O2D-CED
26	3	316	CHL	CBD-CGD-O2D-CED
26	5	315	CHL	CBD-CGD-O2D-CED
26	6	313	CHL	CBD-CGD-O2D-CED
26	6	316	CHL	CBD-CGD-O2D-CED
26	6	317	CHL	CBD-CGD-O2D-CED
26	P	315	CHL	CBD-CGD-O2D-CED
26	P	318	CHL	CBD-CGD-O2D-CED
26	Q	314	CHL	CBD-CGD-O2D-CED
26	Q	315	CHL	CBD-CGD-O2D-CED
26	G	313	CHL	CBD-CGD-O2D-CED
26	G	315	CHL	CBD-CGD-O2D-CED
26	u	314	CHL	CBD-CGD-O2D-CED
26	g	313	CHL	CBD-CGD-O2D-CED
26	g	314	CHL	CBD-CGD-O2D-CED
26	g	315	CHL	CBD-CGD-O2D-CED
26	R	317	CHL	CBD-CGD-O2D-CED
22	2	302	CLA	O1A-CGA-O2A-C1
22	P	306	CLA	O1A-CGA-O2A-C1
22	n	308	CLA	O1A-CGA-O2A-C1
25	2	312	LHG	O10-C23-O8-C6
25	5	312	LHG	O10-C23-O8-C6
25	C	522	LHG	O10-C23-O8-C6
25	c	521	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
26	G	315	CHL	O1A-CGA-O2A-C1
34	C	502	LMG	O10-C28-O8-C9
34	B	621	LMG	O10-C28-O8-C9
34	c	501	LMG	O10-C28-O8-C9
36	J	101	DGD	O1A-C1A-O1G-C1G
36	c	519	DGD	O1A-C1A-O1G-C1G
22	r	603	CLA	O1D-CGD-O2D-CED
22	2	304	CLA	O1D-CGD-O2D-CED
22	2	307	CLA	O1D-CGD-O2D-CED
22	P	303	CLA	O1D-CGD-O2D-CED
22	P	305	CLA	O1D-CGD-O2D-CED
22	Q	301	CLA	O1D-CGD-O2D-CED
22	U	307	CLA	O1D-CGD-O2D-CED
22	N	301	CLA	O1D-CGD-O2D-CED
22	n	306	CLA	O1D-CGD-O2D-CED
22	g	306	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	B	617	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
26	3	315	CHL	O1D-CGD-O2D-CED
26	6	316	CHL	O1D-CGD-O2D-CED
26	Q	314	CHL	O1D-CGD-O2D-CED
22	2	303	CLA	O1D-CGD-O2D-CED
22	3	301	CLA	O1D-CGD-O2D-CED
22	5	301	CLA	O1D-CGD-O2D-CED
22	5	308	CLA	O1D-CGD-O2D-CED
22	6	302	CLA	O1D-CGD-O2D-CED
22	v	307	CLA	O1D-CGD-O2D-CED
22	p	302	CLA	O1D-CGD-O2D-CED
22	p	305	CLA	O1D-CGD-O2D-CED
22	p	309	CLA	O1D-CGD-O2D-CED
22	P	302	CLA	O1D-CGD-O2D-CED
22	N	302	CLA	O1D-CGD-O2D-CED
22	N	304	CLA	O1D-CGD-O2D-CED
22	N	306	CLA	O1D-CGD-O2D-CED
22	G	302	CLA	O1D-CGD-O2D-CED
22	n	308	CLA	O1D-CGD-O2D-CED
22	g	302	CLA	O1D-CGD-O2D-CED
22	S	303	CLA	O1D-CGD-O2D-CED
22	S	305	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
22	s	303	CLA	O1D-CGD-O2D-CED
22	s	304	CLA	O1D-CGD-O2D-CED
22	s	305	CLA	O1D-CGD-O2D-CED
26	1	314	CHL	O1D-CGD-O2D-CED
26	2	314	CHL	O1D-CGD-O2D-CED
26	3	314	CHL	O1D-CGD-O2D-CED
26	6	315	CHL	O1D-CGD-O2D-CED
26	p	315	CHL	O1D-CGD-O2D-CED
26	n	314	CHL	O1D-CGD-O2D-CED
22	P	303	CLA	CBA-CGA-O2A-C1
22	P	306	CLA	CBA-CGA-O2A-C1
22	n	308	CLA	CBA-CGA-O2A-C1
25	2	312	LHG	C24-C23-O8-C6
25	5	312	LHG	C24-C23-O8-C6
25	c	521	LHG	C24-C23-O8-C6
36	J	101	DGD	C2A-C1A-O1G-C1G
36	c	519	DGD	C2A-C1A-O1G-C1G
22	r	601	CLA	CBD-CGD-O2D-CED
22	a	404	CLA	CBD-CGD-O2D-CED
22	a	406	CLA	CBD-CGD-O2D-CED
22	A	404	CLA	CBD-CGD-O2D-CED
22	A	406	CLA	CBD-CGD-O2D-CED
22	1	306	CLA	CBD-CGD-O2D-CED
22	3	306	CLA	CBD-CGD-O2D-CED
22	5	303	CLA	CBD-CGD-O2D-CED
22	6	307	CLA	CBD-CGD-O2D-CED
22	q	306	CLA	CBD-CGD-O2D-CED
22	V	302	CLA	CBD-CGD-O2D-CED
22	U	302	CLA	CBD-CGD-O2D-CED
22	U	304	CLA	CBD-CGD-O2D-CED
22	N	307	CLA	CBD-CGD-O2D-CED
22	u	302	CLA	CBD-CGD-O2D-CED
22	S	307	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	2	317	CHL	CBD-CGD-O2D-CED
26	5	317	CHL	CBD-CGD-O2D-CED
26	6	301	CHL	CBD-CGD-O2D-CED
26	q	311	CHL	CBD-CGD-O2D-CED
26	q	314	CHL	CBD-CGD-O2D-CED
26	N	316	CHL	CBD-CGD-O2D-CED
26	n	315	CHL	CBD-CGD-O2D-CED
26	g	316	CHL	CBD-CGD-O2D-CED
30	a	407	PHO	CBD-CGD-O2D-CED
30	d	401	PHO	CBD-CGD-O2D-CED
30	A	407	PHO	CBD-CGD-O2D-CED
30	D	401	PHO	CBD-CGD-O2D-CED
22	r	601	CLA	O1A-CGA-O2A-C1
22	r	607	CLA	O1A-CGA-O2A-C1
22	1	305	CLA	O1A-CGA-O2A-C1
22	2	305	CLA	O1A-CGA-O2A-C1
22	4	305	CLA	O1A-CGA-O2A-C1
22	5	302	CLA	O1A-CGA-O2A-C1
22	6	305	CLA	O1A-CGA-O2A-C1
22	v	305	CLA	O1A-CGA-O2A-C1
22	p	306	CLA	O1A-CGA-O2A-C1
22	q	304	CLA	O1A-CGA-O2A-C1
22	V	305	CLA	O1A-CGA-O2A-C1
22	V	308	CLA	O1A-CGA-O2A-C1
22	P	303	CLA	O1A-CGA-O2A-C1
22	U	305	CLA	O1A-CGA-O2A-C1
22	N	302	CLA	O1A-CGA-O2A-C1
22	N	306	CLA	O1A-CGA-O2A-C1
22	G	302	CLA	O1A-CGA-O2A-C1
22	u	305	CLA	O1A-CGA-O2A-C1
22	g	302	CLA	O1A-CGA-O2A-C1
22	R	302	CLA	O1A-CGA-O2A-C1
22	R	308	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	O1A-CGA-O2A-C1
22	C	512	CLA	O1A-CGA-O2A-C1
22	c	507	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	O1A-CGA-O2A-C1
25	B	622	LHG	O10-C23-O8-C6
25	b	622	LHG	O10-C23-O8-C6
30	a	407	PHO	O1A-CGA-O2A-C1
30	A	407	PHO	O1A-CGA-O2A-C1
32	m	101	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
32	M	101	SQD	O10-C23-O48-C46
36	a	416	DGD	O1A-C1A-O1G-C1G
36	A	414	DGD	O1A-C1A-O1G-C1G
22	1	303	CLA	O1D-CGD-O2D-CED
22	5	304	CLA	O1D-CGD-O2D-CED
22	p	304	CLA	O1D-CGD-O2D-CED
22	V	304	CLA	O1D-CGD-O2D-CED
22	P	309	CLA	O1D-CGD-O2D-CED
22	u	307	CLA	O1D-CGD-O2D-CED
22	R	304	CLA	O1D-CGD-O2D-CED
22	C	513	CLA	O1D-CGD-O2D-CED
22	C	514	CLA	O1D-CGD-O2D-CED
26	4	314	CHL	O1D-CGD-O2D-CED
26	N	314	CHL	O1D-CGD-O2D-CED
34	A	411	LMG	O6-C5-C6-O5
22	1	304	CLA	O1D-CGD-O2D-CED
22	2	301	CLA	O1D-CGD-O2D-CED
22	2	308	CLA	O1D-CGD-O2D-CED
22	4	303	CLA	O1D-CGD-O2D-CED
22	5	306	CLA	O1D-CGD-O2D-CED
22	v	304	CLA	O1D-CGD-O2D-CED
22	q	308	CLA	O1D-CGD-O2D-CED
22	V	306	CLA	O1D-CGD-O2D-CED
22	U	301	CLA	O1D-CGD-O2D-CED
22	S	304	CLA	O1D-CGD-O2D-CED
26	2	315	CHL	O1D-CGD-O2D-CED
26	5	314	CHL	O1D-CGD-O2D-CED
26	p	318	CHL	O1D-CGD-O2D-CED
26	G	314	CHL	O1D-CGD-O2D-CED
36	A	414	DGD	O6D-C5D-C6D-O5D
22	R	308	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	CBD-CGD-O2D-CED
22	s	307	CLA	CBD-CGD-O2D-CED
26	p	320	CHL	CBD-CGD-O2D-CED
26	s	316	CHL	CBD-CGD-O2D-CED
26	Q	315	CHL	C13-C15-C16-C17
22	x	201	CLA	O1D-CGD-O2D-CED
22	1	302	CLA	O1D-CGD-O2D-CED
22	v	301	CLA	O1D-CGD-O2D-CED
22	u	301	CLA	O1D-CGD-O2D-CED
22	u	308	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	X	202	CLA	O1D-CGD-O2D-CED
25	D	406	LHG	O9-C7-O7-C5
34	B	624	LMG	O9-C10-O7-C8
34	b	624	LMG	O9-C10-O7-C8
36	J	101	DGD	O1B-C1B-O2G-C2G
36	C	519	DGD	O1B-C1B-O2G-C2G
36	c	517	DGD	O1B-C1B-O2G-C2G
36	c	519	DGD	O1B-C1B-O2G-C2G
22	5	302	CLA	O1D-CGD-O2D-CED
22	x	201	CLA	C3-C5-C6-C7
22	1	307	CLA	C3-C5-C6-C7
22	p	302	CLA	C3-C5-C6-C7
22	P	307	CLA	C3-C5-C6-C7
22	P	308	CLA	C3-C5-C6-C7
22	Q	304	CLA	C3-C5-C6-C7
22	U	307	CLA	C3-C5-C6-C7
22	G	307	CLA	C3-C5-C6-C7
22	u	307	CLA	C3-C5-C6-C7
22	g	307	CLA	C3-C5-C6-C7
22	R	304	CLA	C3-C5-C6-C7
22	R	310	CLA	C3-C5-C6-C7
22	C	505	CLA	C3-C5-C6-C7
22	B	602	CLA	C3-C5-C6-C7
22	B	605	CLA	C3-C5-C6-C7
22	B	615	CLA	C3-C5-C6-C7
22	X	202	CLA	C3-C5-C6-C7
22	b	615	CLA	C3-C5-C6-C7
22	c	504	CLA	C3-C5-C6-C7
26	r	616	CHL	C3-C5-C6-C7
26	5	313	CHL	C3-C5-C6-C7
26	p	314	CHL	C3-C5-C6-C7
26	p	317	CHL	C3-C5-C6-C7
26	q	314	CHL	C3-C5-C6-C7
26	q	315	CHL	C3-C5-C6-C7
26	V	317	CHL	C3-C5-C6-C7
26	P	314	CHL	C3-C5-C6-C7
26	N	313	CHL	C3-C5-C6-C7
26	n	313	CHL	C3-C5-C6-C7
26	n	316	CHL	C3-C5-C6-C7
26	R	317	CHL	C3-C5-C6-C7
26	S	315	CHL	C3-C5-C6-C7
26	s	315	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	d	401	PHO	C3-C5-C6-C7
30	D	401	PHO	C3-C5-C6-C7
22	r	607	CLA	CBA-CGA-O2A-C1
22	1	305	CLA	CBA-CGA-O2A-C1
22	2	302	CLA	CBA-CGA-O2A-C1
22	4	302	CLA	CBA-CGA-O2A-C1
22	4	305	CLA	CBA-CGA-O2A-C1
22	5	302	CLA	CBA-CGA-O2A-C1
22	6	303	CLA	CBA-CGA-O2A-C1
22	v	305	CLA	CBA-CGA-O2A-C1
22	p	306	CLA	CBA-CGA-O2A-C1
22	q	304	CLA	CBA-CGA-O2A-C1
22	V	305	CLA	CBA-CGA-O2A-C1
22	V	308	CLA	CBA-CGA-O2A-C1
22	Q	302	CLA	CBA-CGA-O2A-C1
22	U	305	CLA	CBA-CGA-O2A-C1
22	N	302	CLA	CBA-CGA-O2A-C1
22	N	306	CLA	CBA-CGA-O2A-C1
22	G	302	CLA	CBA-CGA-O2A-C1
22	u	302	CLA	CBA-CGA-O2A-C1
22	n	306	CLA	CBA-CGA-O2A-C1
22	g	302	CLA	CBA-CGA-O2A-C1
22	R	302	CLA	CBA-CGA-O2A-C1
22	R	308	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
22	c	511	CLA	CBA-CGA-O2A-C1
25	B	622	LHG	C24-C23-O8-C6
25	b	622	LHG	C24-C23-O8-C6
26	G	311	CHL	CBA-CGA-O2A-C1
26	G	315	CHL	CBA-CGA-O2A-C1
30	a	407	PHO	CBA-CGA-O2A-C1
30	A	407	PHO	CBA-CGA-O2A-C1
34	C	502	LMG	C29-C28-O8-C9
34	B	621	LMG	C29-C28-O8-C9
34	c	501	LMG	C29-C28-O8-C9
36	a	416	DGD	C2A-C1A-O1G-C1G
36	A	414	DGD	C2A-C1A-O1G-C1G
36	C	520	DGD	O6E-C5E-C6E-O5E
36	c	518	DGD	O6E-C5E-C6E-O5E
25	d	405	LHG	C8-C7-O7-C5
25	D	406	LHG	C8-C7-O7-C5
25	c	523	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
32	m	101	SQD	C8-C7-O47-C45
32	M	101	SQD	C8-C7-O47-C45
22	2	306	CLA	O1D-CGD-O2D-CED
22	3	308	CLA	O1D-CGD-O2D-CED
22	4	304	CLA	O1D-CGD-O2D-CED
22	q	301	CLA	O1D-CGD-O2D-CED
22	V	301	CLA	O1D-CGD-O2D-CED
22	U	308	CLA	O1D-CGD-O2D-CED
22	N	308	CLA	O1D-CGD-O2D-CED
22	u	304	CLA	O1D-CGD-O2D-CED
22	n	303	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
26	r	616	CHL	O1D-CGD-O2D-CED
26	P	315	CHL	O1D-CGD-O2D-CED
26	P	318	CHL	O1D-CGD-O2D-CED
26	R	317	CHL	O1D-CGD-O2D-CED
22	r	607	CLA	CBD-CGD-O2D-CED
26	S	316	CHL	CBD-CGD-O2D-CED
22	U	302	CLA	O1A-CGA-O2A-C1
36	a	416	DGD	O6D-C5D-C6D-O5D
36	a	416	DGD	C4D-C5D-C6D-O5D
36	A	414	DGD	C4D-C5D-C6D-O5D
22	P	302	CLA	C4-C3-C5-C6
22	C	508	CLA	C4-C3-C5-C6
22	b	615	CLA	C4-C3-C5-C6
22	c	505	CLA	C4-C3-C5-C6
26	r	614	CHL	C4-C3-C5-C6
26	Q	311	CHL	C4-C3-C5-C6
26	g	311	CHL	C4-C3-C5-C6
22	C	508	CLA	C2-C3-C5-C6
22	b	615	CLA	C2-C3-C5-C6
26	r	614	CHL	C2-C3-C5-C6
26	g	311	CHL	C2-C3-C5-C6
22	C	509	CLA	CBD-CGD-O2D-CED
26	5	318	CHL	CBD-CGD-O2D-CED
26	G	316	CHL	CBD-CGD-O2D-CED
22	P	306	CLA	C2A-CAA-CBA-CGA
22	N	308	CLA	C2A-CAA-CBA-CGA
22	G	301	CLA	C2A-CAA-CBA-CGA
22	g	301	CLA	C2A-CAA-CBA-CGA
22	C	514	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	b	602	CLA	C2A-CAA-CBA-CGA
22	b	608	CLA	C2A-CAA-CBA-CGA
26	r	616	CHL	C2A-CAA-CBA-CGA
26	1	314	CHL	C2A-CAA-CBA-CGA
26	2	314	CHL	C2A-CAA-CBA-CGA
26	2	315	CHL	C2A-CAA-CBA-CGA
26	2	316	CHL	C2A-CAA-CBA-CGA
26	3	314	CHL	C2A-CAA-CBA-CGA
26	3	315	CHL	C2A-CAA-CBA-CGA
26	5	314	CHL	C2A-CAA-CBA-CGA
26	5	316	CHL	C2A-CAA-CBA-CGA
26	6	316	CHL	C2A-CAA-CBA-CGA
26	v	314	CHL	C2A-CAA-CBA-CGA
26	V	314	CHL	C2A-CAA-CBA-CGA
26	V	315	CHL	C2A-CAA-CBA-CGA
26	V	316	CHL	C2A-CAA-CBA-CGA
26	Q	312	CHL	C2A-CAA-CBA-CGA
26	U	314	CHL	C2A-CAA-CBA-CGA
26	U	315	CHL	C2A-CAA-CBA-CGA
26	G	314	CHL	C2A-CAA-CBA-CGA
26	n	316	CHL	C2A-CAA-CBA-CGA
26	g	312	CHL	C2A-CAA-CBA-CGA
26	R	317	CHL	C2A-CAA-CBA-CGA
25	Q	310	LHG	O10-C23-O8-C6
34	b	621	LMG	O10-C28-O8-C9
22	4	301	CLA	O1D-CGD-O2D-CED
26	5	315	CHL	O1D-CGD-O2D-CED
22	r	603	CLA	C3-C5-C6-C7
22	p	307	CLA	C3-C5-C6-C7
22	V	301	CLA	C3-C5-C6-C7
22	V	306	CLA	C3-C5-C6-C7
22	P	302	CLA	C3-C5-C6-C7
22	B	607	CLA	C3-C5-C6-C7
22	b	605	CLA	C3-C5-C6-C7
22	b	607	CLA	C3-C5-C6-C7
22	r	601	CLA	CBA-CGA-O2A-C1
22	A	405	CLA	CBA-CGA-O2A-C1
22	2	305	CLA	CBA-CGA-O2A-C1
22	6	305	CLA	CBA-CGA-O2A-C1
22	6	306	CLA	CBA-CGA-O2A-C1
22	p	303	CLA	CBA-CGA-O2A-C1
22	U	302	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	u	305	CLA	CBA-CGA-O2A-C1
22	R	309	CLA	CBA-CGA-O2A-C1
22	C	507	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	CBA-CGA-O2A-C1
22	c	507	CLA	CBA-CGA-O2A-C1
25	Q	310	LHG	C24-C23-O8-C6
32	l	102	SQD	C24-C23-O48-C46
32	m	101	SQD	C24-C23-O48-C46
32	L	102	SQD	C24-C23-O48-C46
32	M	101	SQD	C24-C23-O48-C46
34	d	407	LMG	C29-C28-O8-C9
34	D	408	LMG	C29-C28-O8-C9
22	1	301	CLA	O1D-CGD-O2D-CED
22	Q	308	CLA	O1D-CGD-O2D-CED
26	3	312	CHL	O1D-CGD-O2D-CED
26	G	315	CHL	O1D-CGD-O2D-CED
22	P	306	CLA	CBD-CGD-O2D-CED
22	U	303	CLA	CBD-CGD-O2D-CED
26	V	314	CHL	CBD-CGD-O2D-CED
26	Q	312	CHL	CBD-CGD-O2D-CED
22	2	302	CLA	O1D-CGD-O2D-CED
22	3	302	CLA	O1D-CGD-O2D-CED
22	q	302	CLA	O1D-CGD-O2D-CED
22	P	307	CLA	O1D-CGD-O2D-CED
22	G	308	CLA	O1D-CGD-O2D-CED
22	g	308	CLA	O1D-CGD-O2D-CED
26	6	313	CHL	O1D-CGD-O2D-CED
26	u	314	CHL	O1D-CGD-O2D-CED
25	d	405	LHG	O9-C7-O7-C5
22	3	305	CLA	O1A-CGA-O2A-C1
22	4	302	CLA	O1A-CGA-O2A-C1
22	6	303	CLA	O1A-CGA-O2A-C1
22	6	306	CLA	O1A-CGA-O2A-C1
22	p	303	CLA	O1A-CGA-O2A-C1
22	u	302	CLA	O1A-CGA-O2A-C1
22	g	304	CLA	O1A-CGA-O2A-C1
26	q	311	CHL	O1A-CGA-O2A-C1
26	G	311	CHL	O1A-CGA-O2A-C1
34	d	407	LMG	O10-C28-O8-C9
34	D	408	LMG	O10-C28-O8-C9
22	6	309	CLA	O1D-CGD-O2D-CED
26	g	314	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	V	311	XAT	C13-C14-C15-C35
24	N	311	XAT	C33-C34-C35-C15
31	t	101	BCR	C13-C14-C15-C16
31	z	101	BCR	C13-C14-C15-C16
31	T	101	BCR	C13-C14-C15-C16
31	C	517	BCR	C13-C14-C15-C16
31	B	619	BCR	C13-C14-C15-C16
31	B	620	BCR	C15-C16-C17-C18
31	b	618	BCR	C9-C10-C11-C12
31	c	516	BCR	C9-C10-C11-C12
34	a	412	LMG	O6-C5-C6-O5
36	B	601	DGD	O6E-C5E-C6E-O5E
22	a	405	CLA	CBD-CGD-O2D-CED
22	a	408	CLA	CBD-CGD-O2D-CED
22	A	405	CLA	CBD-CGD-O2D-CED
22	N	305	CLA	CBD-CGD-O2D-CED
22	n	305	CLA	CBD-CGD-O2D-CED
22	R	302	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	611	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
26	1	316	CHL	CBD-CGD-O2D-CED
26	2	313	CHL	CBD-CGD-O2D-CED
26	2	318	CHL	CBD-CGD-O2D-CED
26	5	313	CHL	CBD-CGD-O2D-CED
26	q	312	CHL	CBD-CGD-O2D-CED
26	q	313	CHL	CBD-CGD-O2D-CED
26	P	316	CHL	CBD-CGD-O2D-CED
26	Q	311	CHL	CBD-CGD-O2D-CED
26	Q	313	CHL	CBD-CGD-O2D-CED
26	N	315	CHL	CBD-CGD-O2D-CED
22	P	304	CLA	O1D-CGD-O2D-CED
22	g	303	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
26	r	619	CHL	O1D-CGD-O2D-CED
25	C	523	LHG	O2-C2-C3-O3
25	C	524	LHG	O2-C2-C3-O3
25	c	521	LHG	O2-C2-C3-O3
25	c	522	LHG	O2-C2-C3-O3
25	c	523	LHG	O2-C2-C3-O3
22	2	307	CLA	C3-C5-C6-C7
22	4	307	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	q	301	CLA	C3-C5-C6-C7
22	N	307	CLA	C3-C5-C6-C7
26	5	316	CHL	C3-C5-C6-C7
26	G	315	CHL	C3-C5-C6-C7
22	a	405	CLA	CBA-CGA-O2A-C1
22	3	304	CLA	CBA-CGA-O2A-C1
22	q	302	CLA	CBA-CGA-O2A-C1
22	Q	304	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	CBA-CGA-O2A-C1
26	6	312	CHL	CBA-CGA-O2A-C1
26	g	311	CHL	CBA-CGA-O2A-C1
32	a	413	SQD	C24-C23-O48-C46
34	b	621	LMG	C29-C28-O8-C9
22	Q	302	CLA	O1A-CGA-O2A-C1
22	n	306	CLA	O1A-CGA-O2A-C1
36	b	601	DGD	O6E-C5E-C6E-O5E
34	C	502	LMG	C4-C5-C6-O5
22	v	308	CLA	O1D-CGD-O2D-CED
22	p	307	CLA	O1D-CGD-O2D-CED
22	V	308	CLA	O1D-CGD-O2D-CED
22	n	302	CLA	O1D-CGD-O2D-CED
22	n	304	CLA	O1D-CGD-O2D-CED
26	Q	315	CHL	O1D-CGD-O2D-CED
25	r	613	LHG	C8-C7-O7-C5
32	C	501	SQD	C8-C7-O47-C45
22	2	305	CLA	CBD-CGD-O2D-CED
22	p	306	CLA	CBD-CGD-O2D-CED
22	S	301	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
26	v	314	CHL	CBD-CGD-O2D-CED
26	p	316	CHL	CBD-CGD-O2D-CED
26	U	314	CHL	CBD-CGD-O2D-CED
26	n	317	CHL	CBD-CGD-O2D-CED
34	A	411	LMG	C4-C5-C6-O5
36	c	518	DGD	C4E-C5E-C6E-O5E
26	g	315	CHL	O1D-CGD-O2D-CED
22	a	405	CLA	O1A-CGA-O2A-C1
34	c	501	LMG	C4-C5-C6-O5
36	C	520	DGD	C4E-C5E-C6E-O5E
22	c	503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	5	305	CLA	CBD-CGD-O2D-CED
22	p	303	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
26	2	317	CHL	C10-C11-C12-C13
22	C	513	CLA	C3-C5-C6-C7
22	c	512	CLA	C3-C5-C6-C7
26	6	315	CHL	C3-C5-C6-C7
26	U	319	CHL	C3-C5-C6-C7
22	3	305	CLA	CBA-CGA-O2A-C1
22	g	304	CLA	CBA-CGA-O2A-C1
26	q	311	CHL	CBA-CGA-O2A-C1
32	A	412	SQD	C24-C23-O48-C46
22	C	504	CLA	O1D-CGD-O2D-CED
25	a	415	LHG	O9-C7-O7-C5
25	A	413	LHG	O9-C7-O7-C5
36	B	601	DGD	C4E-C5E-C6E-O5E
22	R	309	CLA	O1A-CGA-O2A-C1
22	C	507	CLA	O1A-CGA-O2A-C1
26	6	312	CHL	O1A-CGA-O2A-C1
26	g	311	CHL	O1A-CGA-O2A-C1
37	E	101	HEM	C2A-CAA-CBA-CGA
34	c	501	LMG	O6-C5-C6-O5
22	R	307	CLA	C4-C3-C5-C6
22	B	610	CLA	C4-C3-C5-C6
22	R	307	CLA	C2-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
22	V	302	CLA	C2A-CAA-CBA-CGA
22	Q	305	CLA	C2A-CAA-CBA-CGA
22	g	303	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	C2A-CAA-CBA-CGA
22	b	613	CLA	C2A-CAA-CBA-CGA
22	c	505	CLA	C2A-CAA-CBA-CGA
26	5	315	CHL	C2A-CAA-CBA-CGA
26	Q	314	CHL	C2A-CAA-CBA-CGA
26	Q	315	CHL	C2A-CAA-CBA-CGA
26	G	312	CHL	C2A-CAA-CBA-CGA
26	u	314	CHL	C2A-CAA-CBA-CGA
26	s	314	CHL	C2A-CAA-CBA-CGA
22	3	306	CLA	O1D-CGD-O2D-CED
22	4	306	CLA	O1D-CGD-O2D-CED
22	G	303	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	6	317	CHL	O1D-CGD-O2D-CED
34	w	201	LMG	O6-C5-C6-O5
34	W	201	LMG	O6-C5-C6-O5
34	C	521	LMG	O6-C5-C6-O5
22	A	405	CLA	O1A-CGA-O2A-C1
22	q	302	CLA	O1A-CGA-O2A-C1
22	Q	304	CLA	O1A-CGA-O2A-C1
22	B	602	CLA	O1A-CGA-O2A-C1
22	b	608	CLA	O1A-CGA-O2A-C1
22	c	506	CLA	O1A-CGA-O2A-C1
36	c	519	DGD	C4E-C5E-C6E-O5E
26	g	313	CHL	O1D-CGD-O2D-CED
22	r	608	CLA	CBA-CGA-O2A-C1
22	x	201	CLA	CBA-CGA-O2A-C1
22	u	306	CLA	CBA-CGA-O2A-C1
22	C	515	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	CBA-CGA-O2A-C1
22	b	613	CLA	CBA-CGA-O2A-C1
26	6	301	CHL	CBA-CGA-O2A-C1
26	V	313	CHL	CBA-CGA-O2A-C1
26	Q	311	CHL	CBA-CGA-O2A-C1
26	U	313	CHL	CBA-CGA-O2A-C1
26	u	313	CHL	CBA-CGA-O2A-C1
26	g	314	CHL	CBA-CGA-O2A-C1
36	c	517	DGD	C2A-C1A-O1G-C1G
34	C	502	LMG	O6-C5-C6-O5
36	J	101	DGD	C4E-C5E-C6E-O5E
36	b	601	DGD	C4E-C5E-C6E-O5E
22	u	303	CLA	O1D-CGD-O2D-CED
26	3	316	CHL	O1D-CGD-O2D-CED
26	G	313	CHL	O1D-CGD-O2D-CED
22	3	304	CLA	O1A-CGA-O2A-C1
32	a	410	SQD	C8-C7-O47-C45
22	a	404	CLA	O1D-CGD-O2D-CED
22	A	404	CLA	O1D-CGD-O2D-CED
22	6	307	CLA	O1D-CGD-O2D-CED
22	u	302	CLA	O1D-CGD-O2D-CED
26	n	315	CHL	O1D-CGD-O2D-CED
26	r	614	CHL	CBD-CGD-O2D-CED
26	R	315	CHL	CBD-CGD-O2D-CED
26	5	317	CHL	O1D-CGD-O2D-CED
26	q	314	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	d	406	LHG	C1-C2-C3-O3
25	1	312	LHG	C1-C2-C3-O3
25	P	313	LHG	C1-C2-C3-O3
25	R	314	LHG	C1-C2-C3-O3
25	B	623	LHG	C1-C2-C3-O3
25	D	407	LHG	C1-C2-C3-O3
25	b	623	LHG	C1-C2-C3-O3
25	r	613	LHG	O9-C7-O7-C5
22	a	408	CLA	O1A-CGA-O2A-C1
22	u	306	CLA	O1A-CGA-O2A-C1
22	S	308	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	O1A-CGA-O2A-C1
22	b	613	CLA	O1A-CGA-O2A-C1
26	6	301	CHL	O1A-CGA-O2A-C1
26	v	313	CHL	O1A-CGA-O2A-C1
26	U	313	CHL	O1A-CGA-O2A-C1
26	u	313	CHL	O1A-CGA-O2A-C1
26	g	314	CHL	O1A-CGA-O2A-C1
36	c	517	DGD	O1A-C1A-O1G-C1G
22	r	609	CLA	C3-C5-C6-C7
22	a	408	CLA	CBA-CGA-O2A-C1
22	A	408	CLA	CBA-CGA-O2A-C1
22	1	302	CLA	CBA-CGA-O2A-C1
22	p	304	CLA	CBA-CGA-O2A-C1
22	q	303	CLA	CBA-CGA-O2A-C1
22	q	306	CLA	CBA-CGA-O2A-C1
22	U	306	CLA	CBA-CGA-O2A-C1
22	G	303	CLA	CBA-CGA-O2A-C1
22	u	308	CLA	CBA-CGA-O2A-C1
22	S	303	CLA	CBA-CGA-O2A-C1
22	S	306	CLA	CBA-CGA-O2A-C1
22	S	308	CLA	CBA-CGA-O2A-C1
22	B	607	CLA	CBA-CGA-O2A-C1
22	B	611	CLA	CBA-CGA-O2A-C1
22	X	202	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	CBA-CGA-O2A-C1
22	b	607	CLA	CBA-CGA-O2A-C1
22	b	611	CLA	CBA-CGA-O2A-C1
22	b	617	CLA	CBA-CGA-O2A-C1
22	c	514	CLA	CBA-CGA-O2A-C1
22	s	301	CLA	CBA-CGA-O2A-C1
22	s	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	s	306	CLA	CBA-CGA-O2A-C1
22	s	308	CLA	CBA-CGA-O2A-C1
25	3	310	LHG	C24-C23-O8-C6
25	6	311	LHG	C24-C23-O8-C6
26	1	313	CHL	CBA-CGA-O2A-C1
26	1	316	CHL	CBA-CGA-O2A-C1
26	3	311	CHL	CBA-CGA-O2A-C1
26	v	313	CHL	CBA-CGA-O2A-C1
26	p	319	CHL	CBA-CGA-O2A-C1
26	g	315	CHL	CBA-CGA-O2A-C1
26	S	315	CHL	CBA-CGA-O2A-C1
36	C	519	DGD	C2A-C1A-O1G-C1G
34	w	201	LMG	C4-C5-C6-O5
22	r	601	CLA	O1D-CGD-O2D-CED
24	4	311	XAT	C33-C34-C35-C15
24	v	311	XAT	C9-C10-C11-C12
24	Q	309	XAT	C29-C30-C31-C32
24	N	311	XAT	C13-C14-C15-C35
24	u	311	XAT	C9-C10-C11-C12
31	k	101	BCR	C9-C10-C11-C12
31	K	101	BCR	C9-C10-C11-C12
31	C	518	BCR	C9-C10-C11-C12
31	c	515	BCR	C13-C14-C15-C16
34	c	520	LMG	C28-C29-C30-C31
22	U	306	CLA	C5-C6-C7-C8
22	C	503	CLA	C15-C16-C17-C18
22	B	606	CLA	C13-C15-C16-C17
26	4	316	CHL	C8-C10-C11-C12
26	6	301	CHL	C13-C15-C16-C17
36	C	519	DGD	O1A-C1A-O1G-C1G
34	a	412	LMG	C4-C5-C6-O5
34	W	201	LMG	C4-C5-C6-O5
22	C	504	CLA	C8-C10-C11-C12
22	C	507	CLA	C5-C6-C7-C8
22	b	613	CLA	C15-C16-C17-C18
26	4	317	CHL	C13-C15-C16-C17
26	v	317	CHL	C13-C15-C16-C17
26	v	318	CHL	C13-C15-C16-C17
26	V	317	CHL	C8-C10-C11-C12
26	P	318	CHL	C13-C15-C16-C17
26	n	317	CHL	C13-C15-C16-C17
25	a	415	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	A	413	LHG	O2-C2-C3-O3
25	p	313	LHG	O2-C2-C3-O3
25	q	310	LHG	O2-C2-C3-O3
25	n	312	LHG	O2-C2-C3-O3
34	C	521	LMG	C28-C29-C30-C31
22	6	309	CLA	O2A-C1-C2-C3
22	q	308	CLA	O2A-C1-C2-C3
22	g	308	CLA	O2A-C1-C2-C3
32	m	101	SQD	C2-C1-O6-C44
32	M	101	SQD	C2-C1-O6-C44
36	a	416	DGD	C2E-C1E-O5D-C6D
32	a	413	SQD	O6-C44-C45-O47
22	p	304	CLA	O1A-CGA-O2A-C1
22	q	306	CLA	O1A-CGA-O2A-C1
22	U	306	CLA	O1A-CGA-O2A-C1
22	S	306	CLA	O1A-CGA-O2A-C1
22	b	611	CLA	O1A-CGA-O2A-C1
22	s	306	CLA	O1A-CGA-O2A-C1
22	s	308	CLA	O1A-CGA-O2A-C1
26	Q	311	CHL	C2-C3-C5-C6
22	v	305	CLA	C6-C7-C8-C9
22	V	305	CLA	C6-C7-C8-C9
22	P	303	CLA	C6-C7-C8-C9
22	U	302	CLA	C6-C7-C8-C9
22	U	305	CLA	C6-C7-C8-C9
22	u	305	CLA	C6-C7-C8-C9
22	n	304	CLA	C14-C13-C15-C16
22	C	508	CLA	C14-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C9
22	B	602	CLA	C14-C13-C15-C16
22	B	603	CLA	C11-C12-C13-C14
22	B	603	CLA	C14-C13-C15-C16
22	B	605	CLA	C6-C7-C8-C9
22	B	606	CLA	C14-C13-C15-C16
22	B	610	CLA	C6-C7-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	b	602	CLA	C14-C13-C15-C16
22	b	603	CLA	C14-C13-C15-C16
22	b	605	CLA	C6-C7-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	b	615	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C14-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C9
26	1	316	CHL	C11-C10-C8-C9
26	1	317	CHL	C6-C7-C8-C9
26	1	317	CHL	C14-C13-C15-C16
26	1	318	CHL	C14-C13-C15-C16
26	2	316	CHL	C11-C10-C8-C9
26	2	318	CHL	C14-C13-C15-C16
26	4	316	CHL	C6-C7-C8-C9
26	4	317	CHL	C14-C13-C15-C16
26	5	316	CHL	C11-C10-C8-C9
26	5	317	CHL	C11-C10-C8-C9
26	6	316	CHL	C6-C7-C8-C9
26	v	316	CHL	C11-C10-C8-C9
26	v	317	CHL	C11-C12-C13-C14
26	v	318	CHL	C14-C13-C15-C16
26	p	318	CHL	C6-C7-C8-C9
26	V	317	CHL	C11-C10-C8-C9
26	P	318	CHL	C6-C7-C8-C9
26	P	319	CHL	C14-C13-C15-C16
26	U	316	CHL	C14-C13-C15-C16
26	U	317	CHL	C6-C7-C8-C9
26	U	317	CHL	C11-C10-C8-C9
26	N	316	CHL	C6-C7-C8-C9
26	N	317	CHL	C6-C7-C8-C9
26	G	311	CHL	C11-C12-C13-C14
26	G	314	CHL	C11-C10-C8-C9
26	u	316	CHL	C11-C12-C13-C14
26	u	318	CHL	C6-C7-C8-C9
26	u	318	CHL	C14-C13-C15-C16
26	n	318	CHL	C6-C7-C8-C9
26	g	311	CHL	C11-C12-C13-C14
22	A	406	CLA	O1D-CGD-O2D-CED
22	1	306	CLA	O1D-CGD-O2D-CED
22	5	303	CLA	O1D-CGD-O2D-CED
22	N	307	CLA	O1D-CGD-O2D-CED
26	q	311	CHL	O1D-CGD-O2D-CED
30	D	401	PHO	O1D-CGD-O2D-CED
26	s	313	CHL	CBD-CGD-O2D-CED
22	c	507	CLA	C13-C15-C16-C17
26	2	318	CHL	C8-C10-C11-C12
26	q	311	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	g	314	CHL	C13-C15-C16-C17
22	G	302	CLA	C2A-CAA-CBA-CGA
22	g	302	CLA	C2A-CAA-CBA-CGA
22	g	308	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	C2A-CAA-CBA-CGA
26	4	314	CHL	C2A-CAA-CBA-CGA
26	P	315	CHL	C2A-CAA-CBA-CGA
26	S	314	CHL	C2A-CAA-CBA-CGA
23	N	309	LUT	C31-C32-C33-C40
23	n	310	LUT	C7-C8-C9-C19
23	s	311	LUT	C11-C12-C13-C20
24	2	311	XAT	C11-C12-C13-C20
24	3	309	XAT	C11-C12-C13-C20
24	6	310	XAT	C11-C12-C13-C20
24	v	311	XAT	C11-C12-C13-C20
24	q	309	XAT	C11-C12-C13-C20
24	V	311	XAT	C31-C32-C33-C40
24	n	311	XAT	C11-C12-C13-C20
24	n	311	XAT	C31-C32-C33-C40
27	N	318	NEX	C11-C12-C13-C20
27	u	319	NEX	C11-C12-C13-C20
31	d	403	BCR	C7-C8-C9-C34
31	k	101	BCR	C7-C8-C9-C34
31	t	101	BCR	C7-C8-C9-C34
31	K	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C7-C8-C9-C34
31	C	517	BCR	C7-C8-C9-C34
31	B	619	BCR	C11-C12-C13-C35
31	D	404	BCR	C7-C8-C9-C34
31	b	618	BCR	C11-C12-C13-C35
24	2	311	XAT	C11-C12-C13-C14
24	6	310	XAT	C11-C12-C13-C14
24	v	311	XAT	C11-C12-C13-C14
24	v	311	XAT	C31-C32-C33-C34
24	q	309	XAT	C7-C8-C9-C10
24	q	309	XAT	C11-C12-C13-C14
24	V	311	XAT	C31-C32-C33-C34
24	n	311	XAT	C11-C12-C13-C14
24	n	311	XAT	C31-C32-C33-C34
31	d	403	BCR	C7-C8-C9-C10
31	k	101	BCR	C7-C8-C9-C10
31	K	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	T	101	BCR	C7-C8-C9-C10
31	C	517	BCR	C7-C8-C9-C10
31	D	404	BCR	C7-C8-C9-C10
31	b	618	BCR	C11-C12-C13-C14
31	c	515	BCR	C7-C8-C9-C10
25	5	312	LHG	C8-C7-O7-C5
34	C	521	LMG	C4-C5-C6-O5
25	d	406	LHG	C7-C8-C9-C10
25	D	407	LHG	C7-C8-C9-C10
22	A	408	CLA	O1A-CGA-O2A-C1
22	G	303	CLA	O1A-CGA-O2A-C1
22	B	611	CLA	O1A-CGA-O2A-C1
26	3	311	CHL	O1A-CGA-O2A-C1
32	A	412	SQD	O10-C23-O48-C46
22	p	305	CLA	C15-C16-C17-C18
22	P	307	CLA	C8-C10-C11-C12
22	N	301	CLA	C15-C16-C17-C18
22	n	301	CLA	C15-C16-C17-C18
22	n	304	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
22	B	612	CLA	C5-C6-C7-C8
22	X	202	CLA	C8-C10-C11-C12
26	5	313	CHL	C10-C11-C12-C13
26	5	317	CHL	C10-C11-C12-C13
26	6	312	CHL	C13-C15-C16-C17
26	P	318	CHL	C5-C6-C7-C8
26	P	318	CHL	C8-C10-C11-C12
26	R	315	CHL	C13-C15-C16-C17
26	R	317	CHL	C8-C10-C11-C12
22	U	304	CLA	O1D-CGD-O2D-CED
22	S	307	CLA	O1D-CGD-O2D-CED
26	6	301	CHL	O1D-CGD-O2D-CED
26	g	316	CHL	O1D-CGD-O2D-CED
30	d	401	PHO	O1D-CGD-O2D-CED
30	a	407	PHO	O1D-CGD-O2D-CED
22	p	306	CLA	C3-C5-C6-C7
22	B	609	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
26	2	316	CHL	C3-C5-C6-C7
22	1	303	CLA	CBA-CGA-O2A-C1
22	6	304	CLA	CBA-CGA-O2A-C1
22	U	308	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	G	304	CLA	CBA-CGA-O2A-C1
22	S	301	CLA	CBA-CGA-O2A-C1
22	c	503	CLA	CBA-CGA-O2A-C1
26	q	314	CHL	CBA-CGA-O2A-C1
26	g	316	CHL	CBA-CGA-O2A-C1
26	s	315	CHL	CBA-CGA-O2A-C1
22	r	609	CLA	C5-C6-C7-C8
22	1	307	CLA	C10-C11-C12-C13
22	2	305	CLA	C8-C10-C11-C12
22	5	301	CLA	C10-C11-C12-C13
22	q	301	CLA	C8-C10-C11-C12
22	Q	302	CLA	C15-C16-C17-C18
22	U	302	CLA	C13-C15-C16-C17
22	N	306	CLA	C10-C11-C12-C13
22	G	301	CLA	C13-C15-C16-C17
22	C	509	CLA	C5-C6-C7-C8
22	B	603	CLA	C13-C15-C16-C17
22	B	610	CLA	C5-C6-C7-C8
22	B	613	CLA	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
22	c	502	CLA	C15-C16-C17-C18
22	c	504	CLA	C5-C6-C7-C8
22	c	507	CLA	C10-C11-C12-C13
26	1	313	CHL	C13-C15-C16-C17
26	4	313	CHL	C10-C11-C12-C13
26	5	313	CHL	C8-C10-C11-C12
26	5	318	CHL	C8-C10-C11-C12
26	v	317	CHL	C5-C6-C7-C8
26	v	317	CHL	C8-C10-C11-C12
26	p	318	CHL	C13-C15-C16-C17
26	p	319	CHL	C13-C15-C16-C17
26	V	313	CHL	C13-C15-C16-C17
26	V	316	CHL	C8-C10-C11-C12
26	V	317	CHL	C5-C6-C7-C8
26	P	317	CHL	C13-C15-C16-C17
26	Q	315	CHL	C8-C10-C11-C12
26	U	319	CHL	C5-C6-C7-C8
26	N	313	CHL	C13-C15-C16-C17
26	N	316	CHL	C8-C10-C11-C12
26	G	311	CHL	C8-C10-C11-C12
26	u	318	CHL	C13-C15-C16-C17
26	g	311	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	O6E-C5E-C6E-O5E
25	P	313	LHG	C23-C24-C25-C26
25	U	312	LHG	C23-C24-C25-C26
25	G	310	LHG	C23-C24-C25-C26
25	u	312	LHG	C23-C24-C25-C26
25	g	310	LHG	C23-C24-C25-C26
32	A	412	SQD	C7-C8-C9-C10
30	A	407	PHO	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
22	x	201	CLA	C8-C10-C11-C12
22	1	306	CLA	C5-C6-C7-C8
22	2	301	CLA	C10-C11-C12-C13
22	2	302	CLA	C8-C10-C11-C12
22	3	304	CLA	C13-C15-C16-C17
22	5	306	CLA	C8-C10-C11-C12
22	6	303	CLA	C8-C10-C11-C12
22	v	302	CLA	C10-C11-C12-C13
22	v	305	CLA	C5-C6-C7-C8
22	q	305	CLA	C5-C6-C7-C8
22	V	302	CLA	C13-C15-C16-C17
22	V	306	CLA	C10-C11-C12-C13
22	Q	301	CLA	C8-C10-C11-C12
22	Q	304	CLA	C8-C10-C11-C12
22	u	306	CLA	C5-C6-C7-C8
22	C	508	CLA	C10-C11-C12-C13
22	C	512	CLA	C10-C11-C12-C13
22	C	515	CLA	C13-C15-C16-C17
22	B	602	CLA	C13-C15-C16-C17
22	B	612	CLA	C15-C16-C17-C18
22	b	606	CLA	C13-C15-C16-C17
22	b	608	CLA	C8-C10-C11-C12
22	b	608	CLA	C10-C11-C12-C13
22	c	506	CLA	C5-C6-C7-C8
22	c	508	CLA	C5-C6-C7-C8
22	c	509	CLA	C5-C6-C7-C8
22	c	511	CLA	C10-C11-C12-C13
22	c	514	CLA	C13-C15-C16-C17
26	2	317	CHL	C5-C6-C7-C8
26	2	318	CHL	C5-C6-C7-C8
26	3	314	CHL	C13-C15-C16-C17
26	5	313	CHL	C15-C16-C17-C18
26	5	316	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	5	317	CHL	C13-C15-C16-C17
26	5	318	CHL	C13-C15-C16-C17
26	6	315	CHL	C13-C15-C16-C17
26	p	314	CHL	C13-C15-C16-C17
26	p	318	CHL	C5-C6-C7-C8
26	V	317	CHL	C13-C15-C16-C17
26	V	318	CHL	C13-C15-C16-C17
26	P	314	CHL	C10-C11-C12-C13
26	P	314	CHL	C15-C16-C17-C18
26	P	319	CHL	C8-C10-C11-C12
26	P	319	CHL	C13-C15-C16-C17
26	Q	311	CHL	C15-C16-C17-C18
26	Q	315	CHL	C15-C16-C17-C18
26	U	316	CHL	C8-C10-C11-C12
26	G	314	CHL	C13-C15-C16-C17
26	u	316	CHL	C13-C15-C16-C17
26	u	317	CHL	C8-C10-C11-C12
26	u	318	CHL	C5-C6-C7-C8
26	n	316	CHL	C8-C10-C11-C12
26	g	311	CHL	C13-C15-C16-C17
26	g	314	CHL	C8-C10-C11-C12
26	2	317	CHL	O1D-CGD-O2D-CED
26	N	316	CHL	O1D-CGD-O2D-CED
25	l	101	LHG	O1-C1-C2-O2
25	1	312	LHG	O1-C1-C2-O2
25	2	312	LHG	O1-C1-C2-O2
25	g	310	LHG	O1-C1-C2-O2
25	R	314	LHG	O1-C1-C2-O2
25	B	623	LHG	O1-C1-C2-O2
22	1	302	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	O10-C23-O48-C46
25	r	613	LHG	C23-C24-C25-C26
25	l	101	LHG	C7-C8-C9-C10
25	L	101	LHG	C7-C8-C9-C10
25	1	312	LHG	C23-C24-C25-C26
25	6	311	LHG	C23-C24-C25-C26
25	N	312	LHG	C23-C24-C25-C26
25	n	312	LHG	C23-C24-C25-C26
25	R	314	LHG	C23-C24-C25-C26
32	a	413	SQD	C7-C8-C9-C10
32	C	501	SQD	C23-C24-C25-C26
34	w	201	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
34	W	201	LMG	C10-C11-C12-C13
34	C	502	LMG	C10-C11-C12-C13
34	c	501	LMG	C10-C11-C12-C13
22	s	301	CLA	CBD-CGD-O2D-CED
22	a	404	CLA	C8-C10-C11-C12
22	x	201	CLA	C15-C16-C17-C18
22	2	304	CLA	C10-C11-C12-C13
22	3	304	CLA	C10-C11-C12-C13
22	4	307	CLA	C10-C11-C12-C13
22	G	302	CLA	C15-C16-C17-C18
22	C	512	CLA	C15-C16-C17-C18
22	B	605	CLA	C5-C6-C7-C8
22	B	612	CLA	C13-C15-C16-C17
22	b	612	CLA	C5-C6-C7-C8
26	1	313	CHL	C8-C10-C11-C12
26	2	317	CHL	C13-C15-C16-C17
26	3	311	CHL	C8-C10-C11-C12
26	4	313	CHL	C13-C15-C16-C17
26	4	313	CHL	C15-C16-C17-C18
26	6	312	CHL	C8-C10-C11-C12
26	v	313	CHL	C8-C10-C11-C12
26	v	318	CHL	C5-C6-C7-C8
26	v	318	CHL	C15-C16-C17-C18
26	p	319	CHL	C15-C16-C17-C18
26	V	318	CHL	C15-C16-C17-C18
26	Q	314	CHL	C13-C15-C16-C17
26	U	313	CHL	C13-C15-C16-C17
26	n	317	CHL	C8-C10-C11-C12
26	g	315	CHL	C15-C16-C17-C18
22	4	303	CLA	CBA-CGA-O2A-C1
22	Q	303	CLA	CBA-CGA-O2A-C1
22	N	305	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	CBA-CGA-O2A-C1
22	B	614	CLA	CBA-CGA-O2A-C1
22	a	406	CLA	O1D-CGD-O2D-CED
22	q	306	CLA	O1D-CGD-O2D-CED
22	U	302	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	C5-C6-C7-C8
22	A	404	CLA	C5-C6-C7-C8
22	5	305	CLA	C8-C10-C11-C12
22	q	302	CLA	C15-C16-C17-C18
22	P	306	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	U	307	CLA	C8-C10-C11-C12
22	G	301	CLA	C8-C10-C11-C12
22	u	307	CLA	C8-C10-C11-C12
22	g	301	CLA	C15-C16-C17-C18
22	B	603	CLA	C5-C6-C7-C8
22	D	403	CLA	C13-C15-C16-C17
22	b	603	CLA	C5-C6-C7-C8
22	b	612	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
26	r	616	CHL	C8-C10-C11-C12
26	1	313	CHL	C15-C16-C17-C18
26	1	316	CHL	C15-C16-C17-C18
26	2	313	CHL	C15-C16-C17-C18
26	v	317	CHL	C15-C16-C17-C18
26	P	317	CHL	C15-C16-C17-C18
26	U	313	CHL	C8-C10-C11-C12
26	U	319	CHL	C8-C10-C11-C12
26	u	317	CHL	C15-C16-C17-C18
26	n	316	CHL	C5-C6-C7-C8
26	g	314	CHL	C15-C16-C17-C18
26	R	315	CHL	C8-C10-C11-C12
25	3	310	LHG	C23-C24-C25-C26
25	4	312	LHG	C23-C24-C25-C26
25	B	622	LHG	C7-C8-C9-C10
22	G	301	CLA	CBD-CGD-O2D-CED
26	S	315	CHL	C8-C10-C11-C12
26	s	315	CHL	C8-C10-C11-C12
37	e	101	HEM	C2A-CAA-CBA-CGA
22	u	302	CLA	C13-C15-C16-C17
22	g	307	CLA	C8-C10-C11-C12
22	S	301	CLA	C8-C10-C11-C12
22	B	614	CLA	C13-C15-C16-C17
22	b	609	CLA	C8-C10-C11-C12
26	1	317	CHL	C8-C10-C11-C12
26	1	317	CHL	C13-C15-C16-C17
26	1	317	CHL	C15-C16-C17-C18
26	2	318	CHL	C13-C15-C16-C17
26	4	313	CHL	C8-C10-C11-C12
26	4	316	CHL	C13-C15-C16-C17
26	p	320	CHL	C15-C16-C17-C18
26	P	319	CHL	C15-C16-C17-C18
26	n	317	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	3	304	CLA	C6-C7-C8-C10
22	v	307	CLA	C12-C13-C15-C16
22	q	307	CLA	C11-C12-C13-C15
22	q	307	CLA	C12-C13-C15-C16
22	Q	304	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	B	603	CLA	C11-C12-C13-C15
26	1	317	CHL	C6-C7-C8-C10
26	2	313	CHL	C6-C7-C8-C10
26	5	317	CHL	C6-C7-C8-C10
26	U	315	CHL	C6-C7-C8-C10
26	U	319	CHL	C12-C13-C15-C16
26	n	316	CHL	C12-C13-C15-C16
26	g	315	CHL	C6-C7-C8-C10
26	S	315	CHL	C6-C7-C8-C10
26	s	315	CHL	C6-C7-C8-C10
22	b	609	CLA	C3-C5-C6-C7
26	1	316	CHL	C3-C5-C6-C7
22	q	303	CLA	O1A-CGA-O2A-C1
22	u	308	CLA	O1A-CGA-O2A-C1
22	B	607	CLA	O1A-CGA-O2A-C1
22	X	202	CLA	O1A-CGA-O2A-C1
22	b	602	CLA	O1A-CGA-O2A-C1
22	c	514	CLA	O1A-CGA-O2A-C1
22	s	303	CLA	O1A-CGA-O2A-C1
25	3	310	LHG	O10-C23-O8-C6
25	6	311	LHG	O10-C23-O8-C6
26	p	319	CHL	O1A-CGA-O2A-C1
26	S	315	CHL	O1A-CGA-O2A-C1
24	1	311	XAT	C29-C30-C31-C32
24	3	309	XAT	C9-C10-C11-C12
24	6	310	XAT	C9-C10-C11-C12
24	v	311	XAT	C29-C30-C31-C32
24	q	309	XAT	C9-C10-C11-C12
24	q	309	XAT	C29-C30-C31-C32
24	V	311	XAT	C29-C30-C31-C32
24	P	312	XAT	C9-C10-C11-C12
24	P	312	XAT	C29-C30-C31-C32
24	Q	309	XAT	C9-C10-C11-C12
24	U	311	XAT	C9-C10-C11-C12
24	G	309	XAT	C9-C10-C11-C12
24	n	311	XAT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
24	g	309	XAT	C9-C10-C11-C12
31	k	101	BCR	C19-C20-C21-C22
31	K	101	BCR	C15-C16-C17-C18
31	K	101	BCR	C19-C20-C21-C22
31	B	618	BCR	C9-C10-C11-C12
31	B	619	BCR	C19-C20-C21-C22
31	b	619	BCR	C19-C20-C21-C22
31	c	515	BCR	C9-C10-C11-C12
22	1	308	CLA	CBA-CGA-O2A-C1
22	5	305	CLA	CBA-CGA-O2A-C1
22	G	308	CLA	CBA-CGA-O2A-C1
26	R	315	CHL	CBA-CGA-O2A-C1
22	a	406	CLA	C2A-CAA-CBA-CGA
22	6	304	CLA	C2A-CAA-CBA-CGA
22	6	306	CLA	C2A-CAA-CBA-CGA
22	p	306	CLA	C2A-CAA-CBA-CGA
22	N	301	CLA	C2A-CAA-CBA-CGA
22	N	303	CLA	C2A-CAA-CBA-CGA
22	C	504	CLA	C2A-CAA-CBA-CGA
22	c	503	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
22	s	308	CLA	C2A-CAA-CBA-CGA
26	3	312	CHL	C2A-CAA-CBA-CGA
26	6	313	CHL	C2A-CAA-CBA-CGA
26	v	315	CHL	C2A-CAA-CBA-CGA
26	v	316	CHL	C2A-CAA-CBA-CGA
26	p	317	CHL	C2A-CAA-CBA-CGA
26	q	314	CHL	C2A-CAA-CBA-CGA
26	G	313	CHL	C2A-CAA-CBA-CGA
26	n	314	CHL	C2A-CAA-CBA-CGA
22	V	302	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	O1D-CGD-O2D-CED
22	b	604	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
26	p	320	CHL	O1D-CGD-O2D-CED
22	r	605	CLA	C8-C10-C11-C12
22	a	408	CLA	C10-C11-C12-C13
22	x	201	CLA	C13-C15-C16-C17
22	A	404	CLA	C8-C10-C11-C12
22	2	301	CLA	C8-C10-C11-C12
22	4	306	CLA	C8-C10-C11-C12
22	5	301	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	5	302	CLA	C15-C16-C17-C18
22	U	301	CLA	C8-C10-C11-C12
22	G	307	CLA	C8-C10-C11-C12
22	u	301	CLA	C8-C10-C11-C12
22	g	301	CLA	C8-C10-C11-C12
22	R	306	CLA	C8-C10-C11-C12
22	C	509	CLA	C13-C15-C16-C17
22	C	515	CLA	C15-C16-C17-C18
22	B	605	CLA	C8-C10-C11-C12
22	B	609	CLA	C8-C10-C11-C12
22	B	613	CLA	C10-C11-C12-C13
22	B	614	CLA	C15-C16-C17-C18
22	X	202	CLA	C13-C15-C16-C17
22	b	613	CLA	C10-C11-C12-C13
22	b	614	CLA	C13-C15-C16-C17
22	c	514	CLA	C15-C16-C17-C18
22	s	301	CLA	C8-C10-C11-C12
26	1	318	CHL	C15-C16-C17-C18
26	2	316	CHL	C15-C16-C17-C18
26	p	318	CHL	C8-C10-C11-C12
26	U	317	CHL	C5-C6-C7-C8
26	N	313	CHL	C8-C10-C11-C12
26	N	313	CHL	C10-C11-C12-C13
26	u	313	CHL	C8-C10-C11-C12
26	u	313	CHL	C13-C15-C16-C17
22	b	617	CLA	O1A-CGA-O2A-C1
26	1	316	CHL	O1A-CGA-O2A-C1
26	6	312	CHL	CBD-CGD-O2D-CED
26	n	318	CHL	CBD-CGD-O2D-CED
36	c	519	DGD	O6E-C1E-O5D-C6D
22	d	402	CLA	C13-C15-C16-C17
22	5	301	CLA	C13-C15-C16-C17
22	5	301	CLA	C15-C16-C17-C18
22	b	603	CLA	C13-C15-C16-C17
26	5	318	CHL	C15-C16-C17-C18
26	G	315	CHL	C15-C16-C17-C18
26	u	316	CHL	C8-C10-C11-C12
26	u	318	CHL	C15-C16-C17-C18
36	J	101	DGD	O6E-C5E-C6E-O5E
25	d	406	LHG	O2-C2-C3-O3
25	C	522	LHG	O2-C2-C3-O3
25	B	622	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	D	407	LHG	O2-C2-C3-O3
25	b	622	LHG	O2-C2-C3-O3
32	C	501	SQD	O49-C7-O47-C45
22	A	408	CLA	C10-C11-C12-C13
22	4	306	CLA	C5-C6-C7-C8
22	5	305	CLA	C5-C6-C7-C8
22	6	306	CLA	C5-C6-C7-C8
22	p	302	CLA	C8-C10-C11-C12
22	V	304	CLA	C5-C6-C7-C8
22	P	302	CLA	C8-C10-C11-C12
22	g	306	CLA	C10-C11-C12-C13
22	C	515	CLA	C5-C6-C7-C8
22	b	614	CLA	C15-C16-C17-C18
22	c	507	CLA	C5-C6-C7-C8
22	c	508	CLA	C13-C15-C16-C17
26	2	318	CHL	C15-C16-C17-C18
26	3	315	CHL	C8-C10-C11-C12
26	6	316	CHL	C15-C16-C17-C18
26	p	314	CHL	C10-C11-C12-C13
26	p	317	CHL	C8-C10-C11-C12
26	P	317	CHL	C8-C10-C11-C12
26	P	318	CHL	C15-C16-C17-C18
26	U	316	CHL	C13-C15-C16-C17
26	G	314	CHL	C8-C10-C11-C12
26	G	316	CHL	C8-C10-C11-C12
26	n	318	CHL	C15-C16-C17-C18
30	a	407	PHO	C5-C6-C7-C8
22	b	614	CLA	CBA-CGA-O2A-C1
26	v	318	CHL	CBD-CGD-O2D-CED
22	R	308	CLA	O1D-CGD-O2D-CED
22	r	608	CLA	O1A-CGA-O2A-C1
22	x	201	CLA	O1A-CGA-O2A-C1
22	G	304	CLA	O1A-CGA-O2A-C1
22	S	303	CLA	O1A-CGA-O2A-C1
22	C	515	CLA	O1A-CGA-O2A-C1
22	b	607	CLA	O1A-CGA-O2A-C1
22	s	301	CLA	O1A-CGA-O2A-C1
26	1	313	CHL	O1A-CGA-O2A-C1
26	V	313	CHL	O1A-CGA-O2A-C1
26	Q	311	CHL	O1A-CGA-O2A-C1
26	g	315	CHL	O1A-CGA-O2A-C1
26	g	316	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	l	102	SQD	O10-C23-O48-C46
25	b	622	LHG	C7-C8-C9-C10
22	q	304	CLA	C8-C10-C11-C12
22	N	301	CLA	C8-C10-C11-C12
22	S	308	CLA	C5-C6-C7-C8
22	C	508	CLA	C8-C10-C11-C12
22	C	510	CLA	C5-C6-C7-C8
22	b	602	CLA	C13-C15-C16-C17
22	b	605	CLA	C8-C10-C11-C12
22	b	614	CLA	C8-C10-C11-C12
26	1	313	CHL	C10-C11-C12-C13
26	1	316	CHL	C13-C15-C16-C17
26	3	314	CHL	C8-C10-C11-C12
26	3	315	CHL	C15-C16-C17-C18
26	5	316	CHL	C13-C15-C16-C17
26	p	317	CHL	C13-C15-C16-C17
26	p	320	CHL	C8-C10-C11-C12
26	q	314	CHL	C15-C16-C17-C18
26	Q	314	CHL	C8-C10-C11-C12
22	U	308	CLA	O1A-CGA-O2A-C1
22	S	301	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	O1A-CGA-O2A-C1
26	s	315	CHL	O1A-CGA-O2A-C1
32	L	102	SQD	O10-C23-O48-C46
34	C	521	LMG	C11-C10-O7-C8
22	r	602	CLA	C8-C10-C11-C12
22	2	305	CLA	C5-C6-C7-C8
22	v	304	CLA	C8-C10-C11-C12
22	p	302	CLA	C10-C11-C12-C13
22	P	305	CLA	C13-C15-C16-C17
22	Q	305	CLA	C5-C6-C7-C8
22	n	301	CLA	C8-C10-C11-C12
22	C	508	CLA	C13-C15-C16-C17
22	C	511	CLA	C13-C15-C16-C17
22	B	608	CLA	C10-C11-C12-C13
22	B	609	CLA	C13-C15-C16-C17
22	B	614	CLA	C8-C10-C11-C12
22	b	609	CLA	C13-C15-C16-C17
22	c	510	CLA	C13-C15-C16-C17
22	c	514	CLA	C5-C6-C7-C8
22	s	308	CLA	C5-C6-C7-C8
26	r	614	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	1	318	CHL	C13-C15-C16-C17
26	2	316	CHL	C8-C10-C11-C12
26	2	317	CHL	C8-C10-C11-C12
26	3	311	CHL	C13-C15-C16-C17
26	4	313	CHL	C5-C6-C7-C8
26	6	301	CHL	C15-C16-C17-C18
26	v	313	CHL	C13-C15-C16-C17
26	q	311	CHL	C13-C15-C16-C17
26	q	315	CHL	C8-C10-C11-C12
26	N	316	CHL	C13-C15-C16-C17
26	N	317	CHL	C8-C10-C11-C12
26	G	311	CHL	C13-C15-C16-C17
26	n	318	CHL	C8-C10-C11-C12
26	R	316	CHL	C5-C6-C7-C8
30	A	407	PHO	C5-C6-C7-C8
25	r	613	LHG	C3-O3-P-O6
25	r	613	LHG	C4-O6-P-O3
25	a	415	LHG	C3-O3-P-O6
25	d	405	LHG	C4-O6-P-O3
25	l	101	LHG	C3-O3-P-O6
25	A	413	LHG	C3-O3-P-O6
25	L	101	LHG	C3-O3-P-O6
25	V	312	LHG	C3-O3-P-O6
25	Q	310	LHG	C4-O6-P-O3
25	U	312	LHG	C3-O3-P-O6
25	U	312	LHG	C4-O6-P-O3
25	G	310	LHG	C4-O6-P-O3
25	u	312	LHG	C3-O3-P-O6
25	u	312	LHG	C4-O6-P-O3
25	g	310	LHG	C4-O6-P-O3
25	S	312	LHG	C4-O6-P-O3
25	C	523	LHG	C3-O3-P-O6
25	C	523	LHG	C4-O6-P-O3
25	B	622	LHG	C3-O3-P-O6
25	B	622	LHG	C4-O6-P-O3
25	B	623	LHG	C4-O6-P-O3
25	D	406	LHG	C4-O6-P-O3
25	b	622	LHG	C4-O6-P-O3
25	b	623	LHG	C4-O6-P-O3
25	c	522	LHG	C3-O3-P-O6
25	c	522	LHG	C4-O6-P-O3
25	c	523	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
25	s	312	LHG	C4-O6-P-O3
25	d	405	LHG	C23-C24-C25-C26
22	n	307	CLA	C3-C5-C6-C7
22	5	307	CLA	CBA-CGA-O2A-C1
22	v	302	CLA	CBA-CGA-O2A-C1
22	U	303	CLA	CBA-CGA-O2A-C1
22	n	303	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	CBA-CGA-O2A-C1
22	c	504	CLA	CBA-CGA-O2A-C1
26	2	313	CHL	CBA-CGA-O2A-C1
22	b	605	CLA	CBD-CGD-O2D-CED
22	U	302	CLA	C5-C6-C7-C8
22	u	305	CLA	C5-C6-C7-C8
22	c	507	CLA	C8-C10-C11-C12
26	2	313	CHL	C8-C10-C11-C12
26	2	316	CHL	C13-C15-C16-C17
26	3	315	CHL	C10-C11-C12-C13
26	v	316	CHL	C8-C10-C11-C12
26	U	317	CHL	C13-C15-C16-C17
22	3	308	CLA	O2A-C1-C2-C3
22	Q	308	CLA	O2A-C1-C2-C3
22	G	308	CLA	O2A-C1-C2-C3
25	q	310	LHG	C7-C8-C9-C10
34	B	624	LMG	C10-C11-C12-C13
34	b	624	LMG	C10-C11-C12-C13
22	s	307	CLA	O1D-CGD-O2D-CED
26	s	316	CHL	O1D-CGD-O2D-CED
25	C	523	LHG	C1-C2-C3-O3
25	B	622	LHG	C1-C2-C3-O3
25	b	622	LHG	C1-C2-C3-O3
25	c	521	LHG	C1-C2-C3-O3
25	c	522	LHG	C1-C2-C3-O3
25	5	312	LHG	O9-C7-O7-C5
34	C	521	LMG	O9-C10-O7-C8
22	C	506	CLA	C4-C3-C5-C6
26	s	315	CHL	C4-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
22	5	304	CLA	C15-C16-C17-C18
26	6	315	CHL	C8-C10-C11-C12
26	P	314	CHL	C8-C10-C11-C12
26	U	313	CHL	C15-C16-C17-C18
26	S	313	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	Q	303	CLA	O1A-CGA-O2A-C1
22	3	305	CLA	C2A-CAA-CBA-CGA
22	n	301	CLA	C2A-CAA-CBA-CGA
22	n	308	CLA	C2A-CAA-CBA-CGA
22	S	308	CLA	C2A-CAA-CBA-CGA
22	C	509	CLA	C2A-CAA-CBA-CGA
22	b	603	CLA	C2A-CAA-CBA-CGA
26	p	314	CHL	C2A-CAA-CBA-CGA
26	P	314	CHL	C2A-CAA-CBA-CGA
22	u	307	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C19
22	q	305	CLA	C3-C5-C6-C7
22	q	308	CLA	CBA-CGA-O2A-C1
22	P	304	CLA	CBA-CGA-O2A-C1
22	P	307	CLA	CBA-CGA-O2A-C1
26	4	313	CHL	CBA-CGA-O2A-C1
26	5	313	CHL	CBA-CGA-O2A-C1
26	p	317	CHL	CBA-CGA-O2A-C1
26	V	317	CHL	CBA-CGA-O2A-C1
26	G	316	CHL	CBA-CGA-O2A-C1
26	u	316	CHL	CBA-CGA-O2A-C1
26	u	316	CHL	C15-C16-C17-C18
22	C	512	CLA	CBD-CGD-O2D-CED
26	5	317	CHL	C8-C10-C11-C12
26	Q	311	CHL	C13-C15-C16-C17
26	Q	316	CHL	C8-C10-C11-C12
26	N	317	CHL	C15-C16-C17-C18
24	2	311	XAT	C9-C10-C11-C12
24	2	311	XAT	C29-C30-C31-C32
24	5	311	XAT	C9-C10-C11-C12
24	V	311	XAT	C9-C10-C11-C12
24	G	309	XAT	C29-C30-C31-C32
24	g	309	XAT	C29-C30-C31-C32
31	x	202	BCR	C13-C14-C15-C16
31	C	517	BCR	C9-C10-C11-C12
31	C	518	BCR	C19-C20-C21-C22
31	X	201	BCR	C13-C14-C15-C16
31	b	620	BCR	C15-C16-C17-C18
31	c	516	BCR	C19-C20-C21-C22
36	J	101	DGD	C1A-C2A-C3A-C4A
25	P	313	LHG	C17-C18-C19-C20
25	Q	310	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	r	607	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	O1D-CGD-O2D-CED
22	B	605	CLA	CBD-CGD-O2D-CED
34	c	520	LMG	C11-C10-O7-C8
22	5	304	CLA	C10-C11-C12-C13
22	U	305	CLA	C5-C6-C7-C8
22	C	505	CLA	C10-C11-C12-C13
22	B	610	CLA	C13-C15-C16-C17
22	b	615	CLA	C15-C16-C17-C18
22	c	504	CLA	C10-C11-C12-C13
22	v	307	CLA	C3-C5-C6-C7
25	6	311	LHG	C25-C26-C27-C28
25	V	312	LHG	C24-C25-C26-C27
25	u	312	LHG	C16-C17-C18-C19
25	c	522	LHG	C15-C16-C17-C18
32	a	413	SQD	C9-C10-C11-C12
32	A	412	SQD	C9-C10-C11-C12
34	b	621	LMG	C13-C14-C15-C16
34	b	621	LMG	C36-C37-C38-C39
36	C	520	DGD	C4B-C5B-C6B-C7B
36	c	517	DGD	C7B-C8B-C9B-CAB
36	c	518	DGD	C4B-C5B-C6B-C7B
26	S	316	CHL	O1D-CGD-O2D-CED
22	p	308	CLA	C11-C12-C13-C14
22	g	306	CLA	C11-C12-C13-C14
22	B	603	CLA	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C20
22	b	603	CLA	C16-C17-C18-C19
22	b	606	CLA	C16-C17-C18-C19
26	r	616	CHL	C11-C12-C13-C15
26	1	317	CHL	C16-C17-C18-C20
26	6	316	CHL	C16-C17-C18-C20
26	U	319	CHL	C16-C17-C18-C19
26	N	316	CHL	C16-C17-C18-C20
26	n	316	CHL	C16-C17-C18-C19
26	n	317	CHL	C16-C17-C18-C19
26	n	318	CHL	C16-C17-C18-C19
22	3	308	CLA	CBA-CGA-O2A-C1
22	n	305	CLA	CBA-CGA-O2A-C1
22	B	617	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	C2A-C1A-O1G-C1G
25	3	310	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	P	313	LHG	C26-C27-C28-C29
25	Q	310	LHG	C17-C18-C19-C20
25	C	523	LHG	C15-C16-C17-C18
25	C	524	LHG	C16-C17-C18-C19
25	b	623	LHG	C11-C12-C13-C14
32	l	102	SQD	C12-C13-C14-C15
32	C	501	SQD	C29-C30-C31-C32
34	B	621	LMG	C17-C18-C19-C20
34	B	621	LMG	C37-C38-C39-C40
34	B	624	LMG	C11-C12-C13-C14
36	J	101	DGD	C2A-C3A-C4A-C5A
36	C	519	DGD	C7B-C8B-C9B-CAB
26	5	318	CHL	O1D-CGD-O2D-CED
26	G	316	CHL	O1D-CGD-O2D-CED
34	c	520	LMG	O9-C10-O7-C8
26	5	316	CHL	C8-C10-C11-C12
26	3	313	CHL	CBD-CGD-O2D-CED
25	U	312	LHG	C24-C25-C26-C27
32	l	102	SQD	C10-C11-C12-C13
34	w	201	LMG	C29-C30-C31-C32
34	W	201	LMG	C29-C30-C31-C32
34	C	502	LMG	C15-C16-C17-C18
34	B	621	LMG	C29-C30-C31-C32
34	B	621	LMG	C36-C37-C38-C39
34	b	624	LMG	C11-C12-C13-C14
22	5	305	CLA	O1A-CGA-O2A-C1
22	b	614	CLA	O1A-CGA-O2A-C1
26	q	314	CHL	O1A-CGA-O2A-C1
25	d	405	LHG	C24-C25-C26-C27
25	L	101	LHG	C11-C12-C13-C14
25	U	312	LHG	C10-C11-C12-C13
25	N	312	LHG	C26-C27-C28-C29
25	G	310	LHG	C25-C26-C27-C28
25	b	623	LHG	C25-C26-C27-C28
32	a	413	SQD	C14-C15-C16-C17
32	L	102	SQD	C12-C13-C14-C15
34	B	621	LMG	C35-C36-C37-C38
34	b	621	LMG	C38-C39-C40-C41
34	c	501	LMG	C15-C16-C17-C18
36	C	520	DGD	C9B-CAB-CBB-CCB
36	B	601	DGD	CCA-CDA-CEA-CFA
22	P	306	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	O1D-CGD-O2D-CED
22	p	306	CLA	C5-C6-C7-C8
22	B	602	CLA	C8-C10-C11-C12
26	r	614	CHL	C15-C16-C17-C18
25	P	313	LHG	O2-C2-C3-O3
25	p	313	LHG	C24-C25-C26-C27
25	V	312	LHG	C25-C26-C27-C28
25	P	313	LHG	C24-C25-C26-C27
25	R	314	LHG	C16-C17-C18-C19
26	R	316	CHL	C3-C5-C6-C7
22	U	303	CLA	O1D-CGD-O2D-CED
22	B	611	CLA	O1D-CGD-O2D-CED
36	J	101	DGD	C2E-C1E-O5D-C6D
36	c	518	DGD	C2D-C1D-O3G-C3G
36	c	519	DGD	C2E-C1E-O5D-C6D
22	r	609	CLA	CBA-CGA-O2A-C1
22	2	303	CLA	CBA-CGA-O2A-C1
25	d	405	LHG	C12-C13-C14-C15
25	g	310	LHG	C32-C33-C34-C35
25	b	622	LHG	C24-C25-C26-C27
32	L	102	SQD	C10-C11-C12-C13
34	d	407	LMG	C11-C12-C13-C14
34	w	201	LMG	C11-C12-C13-C14
34	C	502	LMG	C37-C38-C39-C40
36	c	517	DGD	CAB-CBB-CCB-CDB
22	d	402	CLA	C15-C16-C17-C18
22	g	306	CLA	C8-C10-C11-C12
22	R	310	CLA	C10-C11-C12-C13
22	D	403	CLA	C15-C16-C17-C18
26	6	301	CHL	C8-C10-C11-C12
26	U	313	CHL	C5-C6-C7-C8
22	4	303	CLA	O1A-CGA-O2A-C1
22	5	307	CLA	O1A-CGA-O2A-C1
22	6	304	CLA	O1A-CGA-O2A-C1
22	P	307	CLA	O1A-CGA-O2A-C1
22	N	305	CLA	O1A-CGA-O2A-C1
22	C	504	CLA	O1A-CGA-O2A-C1
22	c	503	CLA	O1A-CGA-O2A-C1
26	5	313	CHL	O1A-CGA-O2A-C1
22	6	307	CLA	C11-C12-C13-C15
22	v	304	CLA	C11-C12-C13-C14
22	G	301	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	G	305	CLA	C11-C12-C13-C15
22	n	304	CLA	C16-C17-C18-C20
22	n	305	CLA	C11-C12-C13-C14
22	C	504	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C20
26	2	313	CHL	C16-C17-C18-C19
26	3	316	CHL	C11-C12-C13-C15
26	4	316	CHL	C16-C17-C18-C19
26	5	313	CHL	C16-C17-C18-C19
26	6	317	CHL	C11-C12-C13-C14
26	v	317	CHL	C16-C17-C18-C19
26	v	317	CHL	C16-C17-C18-C20
26	q	314	CHL	C16-C17-C18-C19
26	Q	316	CHL	C11-C12-C13-C15
26	N	317	CHL	C16-C17-C18-C20
26	g	311	CHL	C16-C17-C18-C20
26	R	315	CHL	C16-C17-C18-C20
22	N	305	CLA	O1D-CGD-O2D-CED
26	V	314	CHL	O1D-CGD-O2D-CED
26	Q	312	CHL	O1D-CGD-O2D-CED
22	r	605	CLA	C4-C3-C5-C6
22	4	302	CLA	C4-C3-C5-C6
26	3	314	CHL	C4-C3-C5-C6
26	6	315	CHL	C4-C3-C5-C6
26	S	315	CHL	C4-C3-C5-C6
25	5	312	LHG	C28-C29-C30-C31
25	B	623	LHG	C11-C12-C13-C14
25	B	623	LHG	C25-C26-C27-C28
34	B	621	LMG	C13-C14-C15-C16
34	B	621	LMG	C38-C39-C40-C41
36	C	519	DGD	C4A-C5A-C6A-C7A
22	P	302	CLA	C2-C3-C5-C6
26	n	316	CHL	C2-C3-C5-C6
22	2	304	CLA	C11-C12-C13-C14
22	4	306	CLA	C11-C10-C8-C9
22	5	304	CLA	C11-C12-C13-C14
22	U	307	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	b	612	CLA	C11-C10-C8-C9
22	c	508	CLA	C6-C7-C8-C9
26	v	316	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	V	313	CHL	C11-C12-C13-C14
26	V	316	CHL	C14-C13-C15-C16
26	Q	311	CHL	C6-C7-C8-C9
26	N	316	CHL	C14-C13-C15-C16
26	G	311	CHL	C6-C7-C8-C9
26	n	318	CHL	C11-C10-C8-C9
26	g	311	CHL	C6-C7-C8-C9
26	g	314	CHL	C11-C10-C8-C9
26	g	314	CHL	C14-C13-C15-C16
26	g	315	CHL	C11-C10-C8-C9
22	b	611	CLA	O1D-CGD-O2D-CED
25	6	311	LHG	C12-C13-C14-C15
25	p	313	LHG	C26-C27-C28-C29
25	q	310	LHG	C11-C12-C13-C14
25	V	312	LHG	C31-C32-C33-C34
25	G	310	LHG	C10-C11-C12-C13
25	g	310	LHG	C10-C11-C12-C13
25	S	312	LHG	C15-C16-C17-C18
25	C	523	LHG	C14-C15-C16-C17
25	D	406	LHG	C12-C13-C14-C15
25	s	312	LHG	C15-C16-C17-C18
32	a	410	SQD	C24-C25-C26-C27
32	a	413	SQD	C12-C13-C14-C15
32	A	412	SQD	C24-C25-C26-C27
34	d	407	LMG	C33-C34-C35-C36
34	B	624	LMG	C37-C38-C39-C40
34	D	408	LMG	C11-C12-C13-C14
34	c	501	LMG	C37-C38-C39-C40
36	c	517	DGD	C4A-C5A-C6A-C7A
22	C	512	CLA	C13-C15-C16-C17
26	u	313	CHL	C15-C16-C17-C18
26	g	316	CHL	C8-C10-C11-C12
26	R	315	CHL	C15-C16-C17-C18
22	A	406	CLA	C2A-CAA-CBA-CGA
22	2	306	CLA	C2A-CAA-CBA-CGA
22	3	301	CLA	C2A-CAA-CBA-CGA
22	6	302	CLA	C2A-CAA-CBA-CGA
22	P	309	CLA	C2A-CAA-CBA-CGA
26	u	315	CHL	C2A-CAA-CBA-CGA
26	u	316	CHL	C2A-CAA-CBA-CGA
26	n	313	CHL	C2A-CAA-CBA-CGA
26	S	316	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	s	316	CHL	C2A-CAA-CBA-CGA
22	1	303	CLA	O1A-CGA-O2A-C1
22	1	308	CLA	O1A-CGA-O2A-C1
22	G	308	CLA	O1A-CGA-O2A-C1
22	c	504	CLA	O1A-CGA-O2A-C1
26	G	316	CHL	O1A-CGA-O2A-C1
26	R	315	CHL	O1A-CGA-O2A-C1
24	1	311	XAT	C11-C12-C13-C20
24	4	311	XAT	C11-C12-C13-C20
24	p	312	XAT	C11-C12-C13-C20
24	Q	309	XAT	C11-C12-C13-C20
24	N	311	XAT	C11-C12-C13-C20
31	t	101	BCR	C11-C12-C13-C35
31	z	101	BCR	C36-C18-C19-C20
31	T	101	BCR	C11-C12-C13-C35
31	C	516	BCR	C36-C18-C19-C20
31	b	619	BCR	C11-C12-C13-C35
31	c	515	BCR	C7-C8-C9-C34
31	c	515	BCR	C11-C12-C13-C35
25	5	312	LHG	C24-C25-C26-C27
25	p	313	LHG	C31-C32-C33-C34
25	D	406	LHG	C24-C25-C26-C27
32	a	413	SQD	C24-C25-C26-C27
36	a	416	DGD	C5B-C6B-C7B-C8B
36	A	414	DGD	C5B-C6B-C7B-C8B
36	c	518	DGD	C7A-C8A-C9A-CAA
36	c	518	DGD	C8B-C9B-CAB-CBB
25	r	613	LHG	O1-C1-C2-C3
25	a	415	LHG	O1-C1-C2-C3
25	l	101	LHG	O1-C1-C2-C3
25	A	413	LHG	O1-C1-C2-C3
25	L	101	LHG	O1-C1-C2-C3
25	q	310	LHG	O1-C1-C2-C3
25	P	313	LHG	O1-C1-C2-C3
25	u	312	LHG	O1-C1-C2-C3
25	n	312	LHG	O1-C1-C2-C3
25	C	522	LHG	O1-C1-C2-C3
25	B	622	LHG	O1-C1-C2-C3
25	D	406	LHG	O1-C1-C2-C3
25	b	622	LHG	O1-C1-C2-C3
23	S	311	LUT	C11-C12-C13-C14
24	1	311	XAT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	3	309	XAT	C11-C12-C13-C14
24	4	311	XAT	C11-C12-C13-C14
24	p	312	XAT	C11-C12-C13-C14
24	Q	309	XAT	C11-C12-C13-C14
24	N	311	XAT	C11-C12-C13-C14
24	G	309	XAT	C27-C28-C29-C30
31	t	101	BCR	C11-C12-C13-C14
31	z	101	BCR	C11-C12-C13-C14
31	z	101	BCR	C17-C18-C19-C20
31	T	101	BCR	C11-C12-C13-C14
31	C	516	BCR	C11-C12-C13-C14
31	C	516	BCR	C17-C18-C19-C20
31	B	620	BCR	C21-C22-C23-C24
22	N	306	CLA	C3-C5-C6-C7
22	a	408	CLA	O1D-CGD-O2D-CED
25	R	314	LHG	O9-C7-O7-C5
34	W	201	LMG	O9-C10-O7-C8
22	6	302	CLA	C8-C10-C11-C12
22	6	307	CLA	C10-C11-C12-C13
22	P	306	CLA	C5-C6-C7-C8
22	b	610	CLA	C5-C6-C7-C8
26	1	313	CHL	C5-C6-C7-C8
26	2	313	CHL	C10-C11-C12-C13
26	q	311	CHL	C8-C10-C11-C12
26	U	316	CHL	C15-C16-C17-C18
26	G	315	CHL	C13-C15-C16-C17
25	R	314	LHG	C8-C7-O7-C5
34	W	201	LMG	C11-C10-O7-C8
25	p	313	LHG	C9-C10-C11-C12
25	p	313	LHG	C15-C16-C17-C18
32	L	102	SQD	C14-C15-C16-C17
32	M	101	SQD	C27-C28-C29-C30
36	C	519	DGD	CAB-CBB-CCB-CDB
36	C	520	DGD	C7A-C8A-C9A-CAA
22	r	610	CLA	CBD-CGD-O2D-CED
25	r	613	LHG	C7-C8-C9-C10
25	v	312	LHG	C23-C24-C25-C26
25	R	314	LHG	C7-C8-C9-C10
25	D	406	LHG	C23-C24-C25-C26
36	c	519	DGD	C1A-C2A-C3A-C4A
25	a	415	LHG	C30-C31-C32-C33
25	l	101	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	A	413	LHG	C30-C31-C32-C33
25	p	313	LHG	C25-C26-C27-C28
25	P	313	LHG	C11-C10-C9-C8
25	Q	310	LHG	C9-C10-C11-C12
25	Q	310	LHG	C14-C15-C16-C17
25	c	522	LHG	C14-C15-C16-C17
25	c	523	LHG	C16-C17-C18-C19
32	l	102	SQD	C14-C15-C16-C17
32	A	412	SQD	C12-C13-C14-C15
34	C	521	LMG	C35-C36-C37-C38
34	B	624	LMG	C14-C15-C16-C17
34	b	624	LMG	C14-C15-C16-C17
34	b	624	LMG	C37-C38-C39-C40
36	c	519	DGD	C2A-C3A-C4A-C5A
22	r	603	CLA	C4B-C3B-CAB-CBB
22	r	604	CLA	C4B-C3B-CAB-CBB
22	r	609	CLA	C4B-C3B-CAB-CBB
22	a	405	CLA	C4B-C3B-CAB-CBB
22	d	402	CLA	C4B-C3B-CAB-CBB
22	A	405	CLA	C4B-C3B-CAB-CBB
22	1	304	CLA	C4B-C3B-CAB-CBB
22	2	303	CLA	C4B-C3B-CAB-CBB
22	3	302	CLA	C4B-C3B-CAB-CBB
22	3	307	CLA	C4B-C3B-CAB-CBB
22	5	302	CLA	C4B-C3B-CAB-CBB
22	5	303	CLA	C4B-C3B-CAB-CBB
22	6	303	CLA	C4B-C3B-CAB-CBB
22	v	301	CLA	C4B-C3B-CAB-CBB
22	v	307	CLA	C4B-C3B-CAB-CBB
22	p	307	CLA	C4B-C3B-CAB-CBB
22	q	305	CLA	C4B-C3B-CAB-CBB
22	q	308	CLA	C4B-C3B-CAB-CBB
22	V	305	CLA	C4B-C3B-CAB-CBB
22	V	307	CLA	C4B-C3B-CAB-CBB
22	V	308	CLA	C4B-C3B-CAB-CBB
22	P	303	CLA	C4B-C3B-CAB-CBB
22	P	306	CLA	C4B-C3B-CAB-CBB
22	Q	305	CLA	C4B-C3B-CAB-CBB
22	Q	308	CLA	C4B-C3B-CAB-CBB
22	U	304	CLA	C4B-C3B-CAB-CBB
22	G	302	CLA	C4B-C3B-CAB-CBB
22	G	305	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	G	306	CLA	C4B-C3B-CAB-CBB
22	G	308	CLA	C4B-C3B-CAB-CBB
22	u	302	CLA	C4B-C3B-CAB-CBB
22	u	306	CLA	C4B-C3B-CAB-CBB
22	u	307	CLA	C4B-C3B-CAB-CBB
22	g	302	CLA	C4B-C3B-CAB-CBB
22	g	303	CLA	C4B-C3B-CAB-CBB
22	g	308	CLA	C4B-C3B-CAB-CBB
22	R	305	CLA	C4B-C3B-CAB-CBB
22	C	504	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	B	602	CLA	C4B-C3B-CAB-CBB
22	B	616	CLA	C4B-C3B-CAB-CBB
22	b	602	CLA	C4B-C3B-CAB-CBB
22	b	603	CLA	C4B-C3B-CAB-CBB
22	b	616	CLA	C4B-C3B-CAB-CBB
22	c	503	CLA	C4B-C3B-CAB-CBB
22	c	511	CLA	C4B-C3B-CAB-CBB
22	c	514	CLA	C4B-C3B-CAB-CBB
26	V	315	CHL	C4B-C3B-CAB-CBB
26	P	318	CHL	C4B-C3B-CAB-CBB
22	r	603	CLA	C11-C12-C13-C14
22	r	603	CLA	C11-C12-C13-C15
22	6	307	CLA	C11-C12-C13-C14
22	P	308	CLA	C11-C12-C13-C14
22	P	308	CLA	C11-C12-C13-C15
22	Q	305	CLA	C11-C12-C13-C14
22	G	305	CLA	C11-C12-C13-C14
22	R	304	CLA	C11-C12-C13-C14
22	R	304	CLA	C11-C12-C13-C15
22	B	610	CLA	C16-C17-C18-C19
22	b	603	CLA	C16-C17-C18-C20
22	b	606	CLA	C16-C17-C18-C20
22	b	610	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20
26	r	616	CHL	C11-C12-C13-C14
26	6	301	CHL	C16-C17-C18-C19
26	6	301	CHL	C16-C17-C18-C20
26	p	314	CHL	C16-C17-C18-C20
26	q	311	CHL	C16-C17-C18-C19
26	q	311	CHL	C16-C17-C18-C20
26	V	317	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	P	314	CHL	C16-C17-C18-C20
26	P	318	CHL	C16-C17-C18-C19
26	P	318	CHL	C16-C17-C18-C20
26	Q	311	CHL	C16-C17-C18-C19
26	Q	315	CHL	C16-C17-C18-C19
26	Q	315	CHL	C16-C17-C18-C20
26	N	316	CHL	C16-C17-C18-C19
26	N	317	CHL	C16-C17-C18-C19
26	n	316	CHL	C16-C17-C18-C20
26	n	318	CHL	C16-C17-C18-C20
26	g	311	CHL	C16-C17-C18-C19
26	R	317	CHL	C11-C12-C13-C14
26	R	317	CHL	C11-C12-C13-C15
36	a	416	DGD	O6E-C1E-O5D-C6D
36	A	414	DGD	O6E-C1E-O5D-C6D
36	J	101	DGD	O6E-C1E-O5D-C6D
22	3	301	CLA	C8-C10-C11-C12
22	3	302	CLA	C8-C10-C11-C12
22	V	301	CLA	C10-C11-C12-C13
22	c	510	CLA	C8-C10-C11-C12
22	c	511	CLA	C13-C15-C16-C17
26	p	317	CHL	C15-C16-C17-C18
26	V	313	CHL	C8-C10-C11-C12
26	V	313	CHL	C10-C11-C12-C13
26	U	317	CHL	C15-C16-C17-C18
26	P	316	CHL	O1D-CGD-O2D-CED
26	Q	313	CHL	O1D-CGD-O2D-CED
25	1	312	LHG	C25-C26-C27-C28
25	v	312	LHG	C25-C26-C27-C28
25	N	312	LHG	C25-C26-C27-C28
25	u	312	LHG	C25-C26-C27-C28
25	B	622	LHG	C10-C11-C12-C13
36	C	519	DGD	C4B-C5B-C6B-C7B
22	r	605	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
26	4	317	CHL	CBD-CGD-O2D-CED
25	r	613	LHG	C15-C16-C17-C18
25	6	311	LHG	C27-C28-C29-C30
25	B	622	LHG	C9-C10-C11-C12
32	l	102	SQD	C9-C10-C11-C12
32	m	101	SQD	C9-C10-C11-C12
32	m	101	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	A	412	SQD	C17-C18-C19-C20
32	M	101	SQD	C9-C10-C11-C12
34	C	502	LMG	C16-C17-C18-C19
25	V	312	LHG	C23-C24-C25-C26
25	C	522	LHG	C23-C24-C25-C26
22	q	304	CLA	C10-C11-C12-C13
22	n	301	CLA	C5-C6-C7-C8
22	C	511	CLA	C8-C10-C11-C12
26	V	316	CHL	C13-C15-C16-C17
26	2	313	CHL	O1A-CGA-O2A-C1
26	4	313	CHL	O1A-CGA-O2A-C1
25	v	312	LHG	C24-C25-C26-C27
32	a	413	SQD	C28-C29-C30-C31
34	d	407	LMG	C13-C14-C15-C16
34	D	408	LMG	C13-C14-C15-C16
36	A	414	DGD	C7B-C8B-C9B-CAB
26	2	318	CHL	O1D-CGD-O2D-CED
22	5	307	CLA	C3-C5-C6-C7
26	u	316	CHL	C3-C5-C6-C7
22	4	306	CLA	CBA-CGA-O2A-C1
22	Q	305	CLA	CBA-CGA-O2A-C1
22	n	302	CLA	CBA-CGA-O2A-C1
22	B	608	CLA	CBA-CGA-O2A-C1
22	b	612	CLA	CBA-CGA-O2A-C1
25	A	413	LHG	C31-C32-C33-C34
32	A	412	SQD	C14-C15-C16-C17
32	L	102	SQD	C9-C10-C11-C12
34	b	621	LMG	C37-C38-C39-C40
36	c	517	DGD	C4B-C5B-C6B-C7B
22	a	405	CLA	O1D-CGD-O2D-CED
22	R	302	CLA	O1D-CGD-O2D-CED
26	2	313	CHL	O1D-CGD-O2D-CED
26	5	313	CHL	O1D-CGD-O2D-CED
26	q	313	CHL	O1D-CGD-O2D-CED
26	N	315	CHL	O1D-CGD-O2D-CED
22	r	601	CLA	C3A-C2A-CAA-CBA
22	v	303	CLA	C3A-C2A-CAA-CBA
22	S	301	CLA	C3A-C2A-CAA-CBA
22	C	514	CLA	C3A-C2A-CAA-CBA
22	C	515	CLA	C3A-C2A-CAA-CBA
22	B	611	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C3A-C2A-CAA-CBA
22	c	514	CLA	C3A-C2A-CAA-CBA
26	r	614	CHL	C3A-C2A-CAA-CBA
26	1	316	CHL	C3A-C2A-CAA-CBA
26	2	316	CHL	C3A-C2A-CAA-CBA
26	5	316	CHL	C3A-C2A-CAA-CBA
26	Q	312	CHL	C3A-C2A-CAA-CBA
26	U	319	CHL	C3A-C2A-CAA-CBA
26	u	316	CHL	C3A-C2A-CAA-CBA
26	n	316	CHL	C3A-C2A-CAA-CBA
26	g	313	CHL	C3A-C2A-CAA-CBA
26	R	315	CHL	C3A-C2A-CAA-CBA
22	A	405	CLA	C8-C10-C11-C12
22	6	305	CLA	C13-C15-C16-C17
22	U	306	CLA	C10-C11-C12-C13
25	a	415	LHG	C31-C32-C33-C34
25	l	101	LHG	C25-C26-C27-C28
25	A	413	LHG	C25-C26-C27-C28
25	u	312	LHG	C13-C14-C15-C16
25	u	312	LHG	C30-C31-C32-C33
25	C	522	LHG	C24-C25-C26-C27
25	D	406	LHG	C28-C29-C30-C31
32	M	101	SQD	C11-C10-C9-C8
34	c	501	LMG	C16-C17-C18-C19
36	a	416	DGD	C7B-C8B-C9B-CAB
36	c	518	DGD	C9B-CAB-CBB-CCB
22	A	405	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	O1D-CGD-O2D-CED
26	Q	311	CHL	O1D-CGD-O2D-CED
22	v	302	CLA	O1A-CGA-O2A-C1
22	C	505	CLA	O1A-CGA-O2A-C1
22	3	306	CLA	C11-C12-C13-C14
22	6	306	CLA	C11-C12-C13-C14
22	6	306	CLA	C11-C12-C13-C15
22	p	308	CLA	C11-C12-C13-C15
22	Q	305	CLA	C11-C12-C13-C15
22	g	306	CLA	C11-C12-C13-C15
22	C	504	CLA	C16-C17-C18-C19
22	B	603	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C20
26	r	614	CHL	C16-C17-C18-C19
26	r	614	CHL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	1	317	CHL	C16-C17-C18-C19
26	3	315	CHL	C16-C17-C18-C19
26	3	315	CHL	C16-C17-C18-C20
26	3	316	CHL	C11-C12-C13-C14
26	4	316	CHL	C16-C17-C18-C20
26	6	316	CHL	C16-C17-C18-C19
26	6	317	CHL	C11-C12-C13-C15
26	p	318	CHL	C16-C17-C18-C19
26	p	318	CHL	C16-C17-C18-C20
26	q	314	CHL	C16-C17-C18-C20
26	V	317	CHL	C16-C17-C18-C20
26	P	314	CHL	C16-C17-C18-C19
26	Q	316	CHL	C11-C12-C13-C14
26	U	319	CHL	C16-C17-C18-C20
26	G	315	CHL	C16-C17-C18-C20
25	a	415	LHG	C25-C26-C27-C28
25	l	101	LHG	C32-C33-C34-C35
25	P	313	LHG	C25-C26-C27-C28
25	G	310	LHG	C27-C28-C29-C30
25	n	312	LHG	C14-C15-C16-C17
32	A	412	SQD	C28-C29-C30-C31
34	w	201	LMG	C13-C14-C15-C16
34	C	521	LMG	C12-C13-C14-C15
34	B	624	LMG	C22-C23-C24-C25
36	C	520	DGD	C8B-C9B-CAB-CBB
22	r	604	CLA	O2A-C1-C2-C3
22	2	308	CLA	O2A-C1-C2-C3
22	R	305	CLA	O2A-C1-C2-C3
34	c	520	LMG	C7-C8-C9-O8
22	4	308	CLA	CBD-CGD-O2D-CED
22	D	403	CLA	CBD-CGD-O2D-CED
26	U	317	CHL	CBD-CGD-O2D-CED
34	b	621	LMG	C4-C5-C6-O5
25	2	312	LHG	C16-C17-C18-C19
25	B	622	LHG	C24-C25-C26-C27
32	m	101	SQD	C11-C10-C9-C8
34	b	621	LMG	C30-C31-C32-C33
22	1	306	CLA	C3-C5-C6-C7
22	V	307	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
22	s	308	CLA	C3-C5-C6-C7
25	a	415	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	A	413	LHG	C7-C8-C9-C10
34	b	621	LMG	C28-C29-C30-C31
25	S	312	LHG	C11-C12-C13-C14
25	D	407	LHG	C26-C27-C28-C29
34	W	201	LMG	C11-C12-C13-C14
22	Q	301	CLA	C10-C11-C12-C13
22	1	302	CLA	C4-C3-C5-C6
22	2	302	CLA	C4-C3-C5-C6
22	3	306	CLA	C4-C3-C5-C6
22	5	302	CLA	C4-C3-C5-C6
22	6	307	CLA	C4-C3-C5-C6
22	v	302	CLA	C4-C3-C5-C6
22	v	306	CLA	C4-C3-C5-C6
22	q	307	CLA	C4-C3-C5-C6
22	u	302	CLA	C4-C3-C5-C6
26	n	316	CHL	C4-C3-C5-C6
22	g	305	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	CBA-CGA-O2A-C1
22	B	612	CLA	CBA-CGA-O2A-C1
22	b	610	CLA	CBA-CGA-O2A-C1
26	3	314	CHL	CBA-CGA-O2A-C1
22	1	302	CLA	C2-C3-C5-C6
22	2	302	CLA	C2-C3-C5-C6
22	3	306	CLA	C2-C3-C5-C6
22	4	306	CLA	C2-C3-C5-C6
22	5	302	CLA	C2-C3-C5-C6
22	v	302	CLA	C2-C3-C5-C6
22	u	302	CLA	C2-C3-C5-C6
22	u	307	CLA	C2-C3-C5-C6
26	6	315	CHL	C2-C3-C5-C6
26	q	314	CHL	C2-C3-C5-C6
26	S	315	CHL	C2-C3-C5-C6
26	s	315	CHL	C2-C3-C5-C6
25	l	101	LHG	C8-C7-O7-C5
25	L	101	LHG	C8-C7-O7-C5
34	w	201	LMG	C11-C10-O7-C8
22	r	602	CLA	C2A-CAA-CBA-CGA
22	5	303	CLA	C2A-CAA-CBA-CGA
22	p	309	CLA	C2A-CAA-CBA-CGA
22	R	303	CLA	C2A-CAA-CBA-CGA
25	d	405	LHG	O1-C1-C2-O2
25	Q	310	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
25	G	310	LHG	O1-C1-C2-O2
25	n	312	LHG	O1-C1-C2-O2
25	C	522	LHG	O1-C1-C2-O2
25	C	524	LHG	O1-C1-C2-O2
25	c	521	LHG	O1-C1-C2-O2
25	3	310	LHG	C27-C28-C29-C30
25	n	312	LHG	C25-C26-C27-C28
25	s	312	LHG	C11-C12-C13-C14
32	a	410	SQD	C25-C26-C27-C28
34	b	621	LMG	C15-C16-C17-C18
34	b	621	LMG	C17-C18-C19-C20
34	b	621	LMG	C35-C36-C37-C38
36	c	518	DGD	C2B-C3B-C4B-C5B
36	c	519	DGD	C9A-CAA-CBA-CCA
22	U	303	CLA	O1A-CGA-O2A-C1
22	n	303	CLA	O1A-CGA-O2A-C1
22	B	617	CLA	O1A-CGA-O2A-C1
26	p	317	CHL	O1A-CGA-O2A-C1
26	V	317	CHL	O1A-CGA-O2A-C1
22	A	408	CLA	C11-C12-C13-C14
26	Q	311	CHL	C16-C17-C18-C20
26	R	315	CHL	C16-C17-C18-C19
22	r	603	CLA	C2B-C3B-CAB-CBB
22	r	604	CLA	C2B-C3B-CAB-CBB
22	r	605	CLA	C2B-C3B-CAB-CBB
22	r	607	CLA	C2B-C3B-CAB-CBB
22	r	609	CLA	C2B-C3B-CAB-CBB
22	r	610	CLA	C2B-C3B-CAB-CBB
22	A	405	CLA	C2B-C3B-CAB-CBB
22	1	301	CLA	C2B-C3B-CAB-CBB
22	1	304	CLA	C2B-C3B-CAB-CBB
22	2	303	CLA	C2B-C3B-CAB-CBB
22	2	305	CLA	C2B-C3B-CAB-CBB
22	3	302	CLA	C2B-C3B-CAB-CBB
22	3	305	CLA	C2B-C3B-CAB-CBB
22	3	306	CLA	C2B-C3B-CAB-CBB
22	3	307	CLA	C2B-C3B-CAB-CBB
22	4	304	CLA	C2B-C3B-CAB-CBB
22	5	302	CLA	C2B-C3B-CAB-CBB
22	5	303	CLA	C2B-C3B-CAB-CBB
22	5	305	CLA	C2B-C3B-CAB-CBB
22	5	308	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	6	303	CLA	C2B-C3B-CAB-CBB
22	6	307	CLA	C2B-C3B-CAB-CBB
22	6	308	CLA	C2B-C3B-CAB-CBB
22	v	307	CLA	C2B-C3B-CAB-CBB
22	p	307	CLA	C2B-C3B-CAB-CBB
22	q	305	CLA	C2B-C3B-CAB-CBB
22	q	308	CLA	C2B-C3B-CAB-CBB
22	V	305	CLA	C2B-C3B-CAB-CBB
22	V	307	CLA	C2B-C3B-CAB-CBB
22	V	308	CLA	C2B-C3B-CAB-CBB
22	P	303	CLA	C2B-C3B-CAB-CBB
22	P	306	CLA	C2B-C3B-CAB-CBB
22	Q	303	CLA	C2B-C3B-CAB-CBB
22	Q	305	CLA	C2B-C3B-CAB-CBB
22	Q	308	CLA	C2B-C3B-CAB-CBB
22	U	306	CLA	C2B-C3B-CAB-CBB
22	N	307	CLA	C2B-C3B-CAB-CBB
22	N	308	CLA	C2B-C3B-CAB-CBB
22	G	302	CLA	C2B-C3B-CAB-CBB
22	G	305	CLA	C2B-C3B-CAB-CBB
22	G	306	CLA	C2B-C3B-CAB-CBB
22	G	307	CLA	C2B-C3B-CAB-CBB
22	G	308	CLA	C2B-C3B-CAB-CBB
22	u	302	CLA	C2B-C3B-CAB-CBB
22	u	303	CLA	C2B-C3B-CAB-CBB
22	u	306	CLA	C2B-C3B-CAB-CBB
22	u	307	CLA	C2B-C3B-CAB-CBB
22	g	302	CLA	C2B-C3B-CAB-CBB
22	g	303	CLA	C2B-C3B-CAB-CBB
22	g	307	CLA	C2B-C3B-CAB-CBB
22	g	308	CLA	C2B-C3B-CAB-CBB
22	R	305	CLA	C2B-C3B-CAB-CBB
22	R	306	CLA	C2B-C3B-CAB-CBB
22	R	308	CLA	C2B-C3B-CAB-CBB
22	R	311	CLA	C2B-C3B-CAB-CBB
22	S	306	CLA	C2B-C3B-CAB-CBB
22	S	308	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	514	CLA	C2B-C3B-CAB-CBB
22	B	602	CLA	C2B-C3B-CAB-CBB
22	B	616	CLA	C2B-C3B-CAB-CBB
22	b	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	b	603	CLA	C2B-C3B-CAB-CBB
22	b	616	CLA	C2B-C3B-CAB-CBB
22	c	511	CLA	C2B-C3B-CAB-CBB
22	c	513	CLA	C2B-C3B-CAB-CBB
22	s	306	CLA	C2B-C3B-CAB-CBB
22	s	308	CLA	C2B-C3B-CAB-CBB
22	s	309	CLA	C2B-C3B-CAB-CBB
26	p	318	CHL	C2B-C3B-CAB-CBB
26	V	315	CHL	C2B-C3B-CAB-CBB
26	P	318	CHL	C2B-C3B-CAB-CBB
26	N	317	CHL	C2B-C3B-CAB-CBB
26	n	318	CHL	C2B-C3B-CAB-CBB
22	B	608	CLA	C8-C10-C11-C12
22	b	610	CLA	C13-C15-C16-C17
25	5	312	LHG	C11-C10-C9-C8
34	C	502	LMG	C36-C37-C38-C39
36	C	520	DGD	C2B-C3B-C4B-C5B
22	6	308	CLA	C3-C5-C6-C7
22	Q	301	CLA	C3-C5-C6-C7
22	4	308	CLA	CBA-CGA-O2A-C1
25	L	101	LHG	C9-C10-C11-C12
34	C	521	LMG	C21-C22-C23-C24
22	q	308	CLA	O1A-CGA-O2A-C1
22	P	304	CLA	O1A-CGA-O2A-C1
22	n	305	CLA	O1A-CGA-O2A-C1
26	u	316	CHL	O1A-CGA-O2A-C1
32	m	101	SQD	C23-C24-C25-C26
32	M	101	SQD	C23-C24-C25-C26
25	C	522	LHG	C1-C2-C3-O3
25	d	406	LHG	C26-C27-C28-C29
25	V	312	LHG	C32-C33-C34-C35
34	c	520	LMG	C21-C22-C23-C24
36	A	414	DGD	C7A-C8A-C9A-CAA
34	w	201	LMG	O9-C10-O7-C8
26	1	317	CHL	C2-C1-O2A-CGA
25	L	101	LHG	C32-C33-C34-C35
25	1	312	LHG	C26-C27-C28-C29
25	n	312	LHG	C27-C28-C29-C30
25	C	522	LHG	C14-C15-C16-C17
32	m	101	SQD	C25-C26-C27-C28
34	b	621	LMG	C16-C17-C18-C19
22	5	302	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	N	304	CLA	C8-C10-C11-C12
22	C	511	CLA	C10-C11-C12-C13
22	B	615	CLA	C15-C16-C17-C18
26	5	313	CHL	C5-C6-C7-C8
26	p	318	CHL	C15-C16-C17-C18
22	3	308	CLA	O1A-CGA-O2A-C1
22	B	610	CLA	O1A-CGA-O2A-C1
22	b	610	CLA	O1A-CGA-O2A-C1
36	c	518	DGD	O1A-C1A-O1G-C1G
25	d	405	LHG	C33-C34-C35-C36
25	g	310	LHG	C28-C29-C30-C31
25	g	310	LHG	C33-C34-C35-C36
32	M	101	SQD	C25-C26-C27-C28
34	b	624	LMG	C22-C23-C24-C25
22	c	503	CLA	C16-C17-C18-C19
22	c	507	CLA	C16-C17-C18-C20
25	u	312	LHG	C7-C8-C9-C10
22	3	307	CLA	C3-C5-C6-C7
22	S	308	CLA	C3-C5-C6-C7
23	r	611	LUT	C1-C6-C7-C8
23	r	611	LUT	C5-C6-C7-C8
23	1	309	LUT	C5-C6-C7-C8
23	4	309	LUT	C5-C6-C7-C8
23	U	309	LUT	C5-C6-C7-C8
23	R	312	LUT	C5-C6-C7-C8
31	d	403	BCR	C5-C6-C7-C8
31	k	101	BCR	C23-C24-C25-C26
31	t	101	BCR	C5-C6-C7-C8
31	x	202	BCR	C23-C24-C25-C26
31	x	202	BCR	C23-C24-C25-C30
31	z	101	BCR	C1-C6-C7-C8
31	K	101	BCR	C23-C24-C25-C26
31	T	101	BCR	C5-C6-C7-C8
31	C	516	BCR	C1-C6-C7-C8
31	C	517	BCR	C1-C6-C7-C8
31	C	517	BCR	C23-C24-C25-C26
31	C	518	BCR	C23-C24-C25-C26
31	B	618	BCR	C5-C6-C7-C8
31	B	619	BCR	C23-C24-C25-C26
31	B	619	BCR	C23-C24-C25-C30
31	B	620	BCR	C23-C24-C25-C26
31	B	620	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
31	D	404	BCR	C5-C6-C7-C8
31	X	201	BCR	C23-C24-C25-C26
31	X	201	BCR	C23-C24-C25-C30
31	b	618	BCR	C5-C6-C7-C8
31	b	619	BCR	C23-C24-C25-C26
31	b	619	BCR	C23-C24-C25-C30
31	b	620	BCR	C23-C24-C25-C26
31	b	620	BCR	C23-C24-C25-C30
31	c	515	BCR	C1-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C26
31	c	516	BCR	C23-C24-C25-C26
25	D	407	LHG	C33-C34-C35-C36
25	c	521	LHG	C11-C12-C13-C14
34	C	502	LMG	C18-C19-C20-C21
34	c	520	LMG	C12-C13-C14-C15
36	C	520	DGD	CCA-CDA-CEA-CFA
26	p	316	CHL	O1D-CGD-O2D-CED
22	p	307	CLA	CBA-CGA-O2A-C1
25	d	405	LHG	C24-C23-O8-C6
25	D	406	LHG	C24-C23-O8-C6
26	r	614	CHL	CBA-CGA-O2A-C1
26	1	314	CHL	CBA-CGA-O2A-C1
26	V	318	CHL	CBA-CGA-O2A-C1
22	d	402	CLA	C10-C11-C12-C13
22	G	302	CLA	C5-C6-C7-C8
22	G	306	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8
22	c	510	CLA	C10-C11-C12-C13
26	4	317	CHL	C8-C10-C11-C12
26	5	317	CHL	C15-C16-C17-C18
26	v	313	CHL	C10-C11-C12-C13
26	p	320	CHL	C13-C15-C16-C17
26	V	318	CHL	C5-C6-C7-C8
26	Q	311	CHL	C8-C10-C11-C12
26	u	313	CHL	C5-C6-C7-C8
34	d	407	LMG	C11-C10-O7-C8
25	d	405	LHG	C11-C12-C13-C14
25	l	101	LHG	C9-C10-C11-C12
25	3	310	LHG	C31-C32-C33-C34
25	6	311	LHG	C31-C32-C33-C34
25	6	311	LHG	C32-C33-C34-C35
25	Q	310	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	g	310	LHG	C27-C28-C29-C30
25	b	622	LHG	C9-C10-C11-C12
36	J	101	DGD	C7B-C8B-C9B-CAB
22	1	308	CLA	O2A-C1-C2-C3
22	4	308	CLA	O2A-C1-C2-C3
22	v	308	CLA	O2A-C1-C2-C3
22	n	302	CLA	O1A-CGA-O2A-C1
22	s	301	CLA	C14-C13-C15-C16
25	2	312	LHG	C23-C24-C25-C26
25	U	312	LHG	C7-C8-C9-C10
25	c	521	LHG	C23-C24-C25-C26
34	D	408	LMG	C28-C29-C30-C31
25	u	312	LHG	C10-C11-C12-C13
34	c	501	LMG	C18-C19-C20-C21
22	R	303	CLA	C8-C10-C11-C12
22	B	612	CLA	C10-C11-C12-C13
22	D	403	CLA	C10-C11-C12-C13
26	1	316	CHL	C8-C10-C11-C12
26	6	317	CHL	C8-C10-C11-C12
26	G	314	CHL	C15-C16-C17-C18
25	S	312	LHG	C32-C33-C34-C35
22	4	306	CLA	C4-C3-C5-C6
22	u	307	CLA	C4-C3-C5-C6
26	q	314	CHL	C4-C3-C5-C6
26	Q	315	CHL	C4-C3-C5-C6
33	d	404	PL9	C30-C29-C31-C32
26	q	312	CHL	O1D-CGD-O2D-CED
22	r	605	CLA	C2-C3-C5-C6
22	2	304	CLA	C11-C12-C13-C15
22	2	307	CLA	C11-C10-C8-C7
22	3	301	CLA	C11-C10-C8-C7
22	3	302	CLA	C11-C10-C8-C7
22	3	304	CLA	C12-C13-C15-C16
22	4	302	CLA	C2-C3-C5-C6
22	4	306	CLA	C11-C10-C8-C7
22	5	304	CLA	C11-C12-C13-C15
22	5	307	CLA	C2-C3-C5-C6
22	6	302	CLA	C11-C10-C8-C7
22	6	305	CLA	C6-C7-C8-C10
22	6	307	CLA	C2-C3-C5-C6
22	v	302	CLA	C12-C13-C15-C16
22	v	306	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	q	307	CLA	C2-C3-C5-C6
22	Q	307	CLA	C2-C3-C5-C6
22	U	307	CLA	C2-C3-C5-C6
22	U	307	CLA	C11-C10-C8-C7
22	n	307	CLA	C6-C7-C8-C10
22	C	503	CLA	C11-C10-C8-C7
22	C	504	CLA	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	C	514	CLA	C6-C7-C8-C10
22	B	606	CLA	C12-C13-C15-C16
22	B	610	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	B	613	CLA	C6-C7-C8-C10
22	b	605	CLA	C6-C7-C8-C10
22	b	606	CLA	C12-C13-C15-C16
22	b	612	CLA	C11-C10-C8-C7
22	b	613	CLA	C6-C7-C8-C10
22	c	503	CLA	C2-C3-C5-C6
22	c	504	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C12-C13-C15
26	r	615	CHL	C2-C3-C5-C6
26	1	317	CHL	C12-C13-C15-C16
26	2	318	CHL	C11-C10-C8-C7
26	2	318	CHL	C12-C13-C15-C16
26	3	314	CHL	C2-C3-C5-C6
26	6	312	CHL	C6-C7-C8-C10
26	v	318	CHL	C12-C13-C15-C16
26	V	313	CHL	C11-C12-C13-C15
26	V	316	CHL	C12-C13-C15-C16
26	P	319	CHL	C12-C13-C15-C16
26	Q	311	CHL	C6-C7-C8-C10
26	Q	315	CHL	C2-C3-C5-C6
26	N	316	CHL	C12-C13-C15-C16
26	G	311	CHL	C6-C7-C8-C10
26	G	311	CHL	C12-C13-C15-C16
26	g	311	CHL	C6-C7-C8-C10
26	g	315	CHL	C11-C10-C8-C7
33	d	404	PL9	C28-C29-C31-C32
33	D	405	PL9	C28-C29-C31-C32
26	p	319	CHL	C3-C5-C6-C7
22	2	303	CLA	O1A-CGA-O2A-C1
22	4	306	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	4	308	CLA	O1A-CGA-O2A-C1
22	Q	305	CLA	O1A-CGA-O2A-C1
22	g	305	CLA	O1A-CGA-O2A-C1
22	B	608	CLA	O1A-CGA-O2A-C1
22	b	612	CLA	O1A-CGA-O2A-C1
26	3	314	CHL	O1A-CGA-O2A-C1
25	v	312	LHG	C30-C31-C32-C33
25	b	622	LHG	C10-C11-C12-C13
32	a	410	SQD	C30-C31-C32-C33
32	a	413	SQD	C10-C11-C12-C13
32	L	102	SQD	C15-C16-C17-C18
36	C	520	DGD	C7B-C8B-C9B-CAB
22	1	302	CLA	C13-C15-C16-C17
22	5	306	CLA	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
26	1	316	CHL	C5-C6-C7-C8
26	2	317	CHL	C15-C16-C17-C18
26	n	313	CHL	C10-C11-C12-C13
24	5	311	XAT	C29-C30-C31-C32
24	Q	309	XAT	C13-C14-C15-C35
24	n	311	XAT	C9-C10-C11-C12
27	r	618	NEX	C9-C10-C11-C12
31	k	101	BCR	C15-C16-C17-C18
31	B	619	BCR	C15-C16-C17-C18
31	c	515	BCR	C15-C16-C17-C18
22	v	304	CLA	C11-C12-C13-C15
22	N	305	CLA	C11-C12-C13-C14
22	n	304	CLA	C16-C17-C18-C19
22	C	508	CLA	C16-C17-C18-C20
26	2	313	CHL	C16-C17-C18-C20
26	5	313	CHL	C16-C17-C18-C20
26	v	316	CHL	C16-C17-C18-C19
26	G	316	CHL	C11-C12-C13-C15
22	n	305	CLA	O1D-CGD-O2D-CED
25	C	523	LHG	O9-C7-O7-C5
25	c	522	LHG	O9-C7-O7-C5
32	a	410	SQD	O49-C7-O47-C45
34	B	621	LMG	O9-C10-O7-C8
22	1	306	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	CBA-CGA-O2A-C1
22	6	309	CLA	CBA-CGA-O2A-C1
22	G	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	n	304	CLA	CBA-CGA-O2A-C1
22	g	307	CLA	CBA-CGA-O2A-C1
26	3	313	CHL	CBA-CGA-O2A-C1
26	6	315	CHL	CBA-CGA-O2A-C1
26	P	317	CHL	CBA-CGA-O2A-C1
26	Q	315	CHL	CBA-CGA-O2A-C1
26	u	317	CHL	CBA-CGA-O2A-C1
25	d	405	LHG	C26-C27-C28-C29
32	a	410	SQD	C9-C10-C11-C12
36	a	416	DGD	C7A-C8A-C9A-CAA
22	1	304	CLA	C2A-CAA-CBA-CGA
22	v	304	CLA	C2A-CAA-CBA-CGA
22	q	301	CLA	C2A-CAA-CBA-CGA
22	V	304	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	C2A-CAA-CBA-CGA
22	c	502	CLA	C2A-CAA-CBA-CGA
26	p	315	CHL	C2A-CAA-CBA-CGA
26	Q	313	CHL	C2A-CAA-CBA-CGA
22	S	301	CLA	O1D-CGD-O2D-CED
22	a	405	CLA	C8-C10-C11-C12
22	3	301	CLA	C15-C16-C17-C18
22	v	304	CLA	C5-C6-C7-C8
22	n	307	CLA	C5-C6-C7-C8
22	B	607	CLA	C5-C6-C7-C8
22	b	607	CLA	C5-C6-C7-C8
26	r	614	CHL	C13-C15-C16-C17
26	3	314	CHL	C15-C16-C17-C18
26	q	314	CHL	C13-C15-C16-C17
25	L	101	LHG	C25-C26-C27-C28
25	U	312	LHG	C16-C17-C18-C19
25	n	312	LHG	C28-C29-C30-C31
25	c	521	LHG	C24-C25-C26-C27
34	c	501	LMG	C36-C37-C38-C39
22	p	303	CLA	O1D-CGD-O2D-CED
25	4	312	LHG	C25-C26-C27-C28
36	b	601	DGD	C3A-C4A-C5A-C6A
34	d	407	LMG	C28-C29-C30-C31
36	A	414	DGD	C1A-C2A-C3A-C4A
22	2	305	CLA	O1D-CGD-O2D-CED
22	A	404	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	P	302	CLA	C5-C6-C7-C8
22	R	307	CLA	C10-C11-C12-C13
22	c	512	CLA	C8-C10-C11-C12
26	4	317	CHL	C15-C16-C17-C18
25	2	312	LHG	C9-C10-C11-C12
25	S	312	LHG	C16-C17-C18-C19
32	l	102	SQD	C27-C28-C29-C30
22	B	617	CLA	C3-C5-C6-C7
22	b	606	CLA	CBA-CGA-O2A-C1
26	6	317	CHL	CBA-CGA-O2A-C1
22	n	305	CLA	C11-C12-C13-C15
26	V	316	CHL	C16-C17-C18-C19
36	c	518	DGD	O6D-C1D-O3G-C3G
26	V	313	CHL	C5-C6-C7-C8
26	n	317	CHL	O1D-CGD-O2D-CED
25	d	405	LHG	C28-C29-C30-C31
25	U	312	LHG	C25-C26-C27-C28
32	l	102	SQD	C15-C16-C17-C18
32	C	501	SQD	C9-C10-C11-C12
25	3	310	LHG	C8-C7-O7-C5
25	V	312	LHG	C8-C7-O7-C5
25	C	523	LHG	C8-C7-O7-C5
25	B	623	LHG	C8-C7-O7-C5
25	b	623	LHG	C8-C7-O7-C5
25	c	522	LHG	C8-C7-O7-C5
34	C	502	LMG	C11-C10-O7-C8
34	B	621	LMG	C11-C10-O7-C8
34	D	408	LMG	C11-C10-O7-C8
34	c	501	LMG	C11-C10-O7-C8
25	N	312	LHG	O6-C4-C5-O7
25	N	312	LHG	C10-C11-C12-C13
25	u	312	LHG	C9-C10-C11-C12
25	u	312	LHG	C12-C13-C14-C15
25	s	312	LHG	C32-C33-C34-C35
36	b	601	DGD	O6D-C5D-C6D-O5D
22	g	307	CLA	C5-C6-C7-C8
22	c	506	CLA	C15-C16-C17-C18
26	3	316	CHL	C8-C10-C11-C12
26	q	314	CHL	C8-C10-C11-C12
22	R	306	CLA	CBD-CGD-O2D-CED
26	1	315	CHL	CBD-CGD-O2D-CED
26	3	311	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	V	318	CHL	CBD-CGD-O2D-CED
32	C	501	SQD	C25-C26-C27-C28
36	J	101	DGD	C9A-CAA-CBA-CCA
36	c	517	DGD	C8B-C9B-CAB-CBB
25	l	101	LHG	O9-C7-O7-C5
25	L	101	LHG	O9-C7-O7-C5
25	3	310	LHG	O9-C7-O7-C5
25	B	623	LHG	O9-C7-O7-C5
34	d	407	LMG	O9-C10-O7-C8
25	D	407	LHG	C17-C18-C19-C20
25	c	521	LHG	C14-C15-C16-C17
32	L	102	SQD	C27-C28-C29-C30
32	a	410	SQD	C2-C1-O6-C44
32	C	501	SQD	C2-C1-O6-C44
36	C	520	DGD	C2D-C1D-O3G-C3G
26	Q	314	CHL	C15-C16-C17-C18
25	a	415	LHG	O7-C5-C6-O8
25	l	101	LHG	O7-C5-C6-O8
25	A	413	LHG	O7-C5-C6-O8
25	L	101	LHG	O7-C5-C6-O8
25	5	312	LHG	O7-C5-C6-O8
32	m	101	SQD	O47-C45-C46-O48
32	A	412	SQD	O6-C44-C45-O47
32	M	101	SQD	O47-C45-C46-O48
34	B	624	LMG	O1-C7-C8-O7
34	b	624	LMG	O1-C7-C8-O7
26	S	315	CHL	CBD-CGD-O2D-CED
22	p	307	CLA	O1A-CGA-O2A-C1
25	d	405	LHG	O10-C23-O8-C6
22	G	301	CLA	C16-C17-C18-C19
26	v	318	CHL	C16-C17-C18-C19
26	n	317	CHL	C16-C17-C18-C20
25	d	405	LHG	C15-C16-C17-C18
25	G	310	LHG	C32-C33-C34-C35
25	D	406	LHG	C26-C27-C28-C29
36	C	519	DGD	C8B-C9B-CAB-CBB
22	c	511	CLA	C5-C6-C7-C8
26	r	615	CHL	C5-C6-C7-C8
26	3	315	CHL	C13-C15-C16-C17
26	4	316	CHL	C15-C16-C17-C18
26	6	316	CHL	C13-C15-C16-C17
26	G	311	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	5	307	CLA	C4-C3-C5-C6
22	Q	307	CLA	C4-C3-C5-C6
22	U	307	CLA	C4-C3-C5-C6
22	c	503	CLA	C4-C3-C5-C6
26	r	615	CHL	C4-C3-C5-C6
33	D	405	PL9	C30-C29-C31-C32
22	N	302	CLA	C2-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
32	L	102	SQD	C29-C30-C31-C32
36	b	601	DGD	C7B-C8B-C9B-CAB
22	A	404	CLA	C11-C12-C13-C14
22	2	307	CLA	C11-C10-C8-C9
22	3	302	CLA	C11-C10-C8-C9
22	3	304	CLA	C6-C7-C8-C9
22	3	304	CLA	C14-C13-C15-C16
22	6	305	CLA	C6-C7-C8-C9
22	v	302	CLA	C14-C13-C15-C16
22	v	307	CLA	C14-C13-C15-C16
22	q	307	CLA	C11-C12-C13-C14
22	q	307	CLA	C14-C13-C15-C16
22	V	302	CLA	C14-C13-C15-C16
22	Q	304	CLA	C11-C10-C8-C9
22	u	305	CLA	C11-C10-C8-C9
22	n	307	CLA	C6-C7-C8-C9
22	g	301	CLA	C11-C12-C13-C14
22	C	504	CLA	C14-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C12-C13-C14
22	C	507	CLA	C14-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	b	613	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C12-C13-C14
22	c	507	CLA	C6-C7-C8-C9
22	s	301	CLA	C6-C7-C8-C9
26	2	313	CHL	C6-C7-C8-C9
26	2	313	CHL	C14-C13-C15-C16
26	5	313	CHL	C14-C13-C15-C16
26	6	312	CHL	C6-C7-C8-C9
26	v	313	CHL	C6-C7-C8-C9
26	V	313	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	U	315	CHL	C6-C7-C8-C9
26	G	311	CHL	C14-C13-C15-C16
26	n	316	CHL	C14-C13-C15-C16
26	g	311	CHL	C14-C13-C15-C16
26	S	315	CHL	C6-C7-C8-C9
30	a	407	PHO	C11-C10-C8-C9
30	A	407	PHO	C11-C10-C8-C9
26	4	315	CHL	CBD-CGD-O2D-CED
26	u	318	CHL	CBD-CGD-O2D-CED
25	b	622	LHG	C12-C13-C14-C15
22	u	306	CLA	C3-C5-C6-C7
22	C	504	CLA	C3-C5-C6-C7
26	3	314	CHL	C3-C5-C6-C7
22	B	607	CLA	O1D-CGD-O2D-CED
22	A	405	CLA	C2A-CAA-CBA-CGA
22	4	304	CLA	C2A-CAA-CBA-CGA
22	v	301	CLA	C2A-CAA-CBA-CGA
22	V	301	CLA	C2A-CAA-CBA-CGA
22	Q	301	CLA	C2A-CAA-CBA-CGA
22	N	302	CLA	C2A-CAA-CBA-CGA
22	S	301	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	C2A-CAA-CBA-CGA
22	c	504	CLA	C2A-CAA-CBA-CGA
22	c	506	CLA	C2A-CAA-CBA-CGA
22	s	301	CLA	C2A-CAA-CBA-CGA
26	N	314	CHL	C2A-CAA-CBA-CGA
26	g	314	CHL	C2A-CAA-CBA-CGA
25	4	312	LHG	C29-C30-C31-C32
25	4	312	LHG	C31-C32-C33-C34
32	A	412	SQD	C10-C11-C12-C13
36	B	601	DGD	C3A-C4A-C5A-C6A
23	U	309	LUT	C11-C12-C13-C20
23	R	312	LUT	C7-C8-C9-C19
24	P	312	XAT	C7-C8-C9-C19
22	p	306	CLA	O1D-CGD-O2D-CED
26	s	313	CHL	O1D-CGD-O2D-CED
22	G	307	CLA	C5-C6-C7-C8
22	C	511	CLA	C5-C6-C7-C8
26	3	311	CHL	C10-C11-C12-C13
25	d	406	LHG	C17-C18-C19-C20
25	U	312	LHG	C13-C14-C15-C16
25	D	406	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
34	d	407	LMG	C15-C16-C17-C18
34	W	201	LMG	C32-C33-C34-C35
34	C	502	LMG	C19-C20-C21-C22
24	3	309	XAT	C31-C32-C33-C34
24	N	311	XAT	C7-C8-C9-C10
24	g	309	XAT	C27-C28-C29-C30
27	n	319	NEX	C11-C12-C13-C14
31	B	619	BCR	C11-C12-C13-C14
22	n	304	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	O1A-CGA-O2A-C1
25	D	406	LHG	O10-C23-O8-C6
26	r	614	CHL	O1A-CGA-O2A-C1
26	1	314	CHL	O1A-CGA-O2A-C1
26	V	318	CHL	O1A-CGA-O2A-C1
22	r	601	CLA	C1A-C2A-CAA-CBA
22	r	602	CLA	C1A-C2A-CAA-CBA
22	r	606	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C1A-C2A-CAA-CBA
22	A	408	CLA	C1A-C2A-CAA-CBA
22	1	304	CLA	C1A-C2A-CAA-CBA
22	2	301	CLA	C1A-C2A-CAA-CBA
22	2	304	CLA	C1A-C2A-CAA-CBA
22	2	305	CLA	C1A-C2A-CAA-CBA
22	4	304	CLA	C1A-C2A-CAA-CBA
22	5	301	CLA	C1A-C2A-CAA-CBA
22	5	304	CLA	C1A-C2A-CAA-CBA
22	p	305	CLA	C1A-C2A-CAA-CBA
22	q	301	CLA	C1A-C2A-CAA-CBA
22	q	308	CLA	C1A-C2A-CAA-CBA
22	P	305	CLA	C1A-C2A-CAA-CBA
22	Q	301	CLA	C1A-C2A-CAA-CBA
22	Q	305	CLA	C1A-C2A-CAA-CBA
22	Q	308	CLA	C1A-C2A-CAA-CBA
22	N	304	CLA	C1A-C2A-CAA-CBA
22	N	305	CLA	C1A-C2A-CAA-CBA
22	G	301	CLA	C1A-C2A-CAA-CBA
22	G	304	CLA	C1A-C2A-CAA-CBA
22	n	304	CLA	C1A-C2A-CAA-CBA
22	n	305	CLA	C1A-C2A-CAA-CBA
22	g	303	CLA	C1A-C2A-CAA-CBA
22	R	303	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	R	307	CLA	C1A-C2A-CAA-CBA
22	S	305	CLA	C1A-C2A-CAA-CBA
22	C	510	CLA	C1A-C2A-CAA-CBA
22	C	514	CLA	C1A-C2A-CAA-CBA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	b	607	CLA	C1A-C2A-CAA-CBA
22	c	509	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	s	305	CLA	C1A-C2A-CAA-CBA
26	r	614	CHL	C1A-C2A-CAA-CBA
26	1	314	CHL	C1A-C2A-CAA-CBA
26	1	316	CHL	C1A-C2A-CAA-CBA
26	1	317	CHL	C1A-C2A-CAA-CBA
26	1	318	CHL	C1A-C2A-CAA-CBA
26	2	316	CHL	C1A-C2A-CAA-CBA
26	2	318	CHL	C1A-C2A-CAA-CBA
26	3	312	CHL	C1A-C2A-CAA-CBA
26	3	313	CHL	C1A-C2A-CAA-CBA
26	3	315	CHL	C1A-C2A-CAA-CBA
26	4	314	CHL	C1A-C2A-CAA-CBA
26	4	317	CHL	C1A-C2A-CAA-CBA
26	5	316	CHL	C1A-C2A-CAA-CBA
26	5	318	CHL	C1A-C2A-CAA-CBA
26	6	313	CHL	C1A-C2A-CAA-CBA
26	6	314	CHL	C1A-C2A-CAA-CBA
26	v	314	CHL	C1A-C2A-CAA-CBA
26	p	318	CHL	C1A-C2A-CAA-CBA
26	V	317	CHL	C1A-C2A-CAA-CBA
26	U	316	CHL	C1A-C2A-CAA-CBA
26	U	317	CHL	C1A-C2A-CAA-CBA
26	N	314	CHL	C1A-C2A-CAA-CBA
26	u	314	CHL	C1A-C2A-CAA-CBA
26	u	316	CHL	C1A-C2A-CAA-CBA
26	u	317	CHL	C1A-C2A-CAA-CBA
26	u	318	CHL	C1A-C2A-CAA-CBA
26	n	314	CHL	C1A-C2A-CAA-CBA
26	g	311	CHL	C1A-C2A-CAA-CBA
26	g	312	CHL	C1A-C2A-CAA-CBA
26	g	313	CHL	C1A-C2A-CAA-CBA
26	g	315	CHL	C1A-C2A-CAA-CBA
26	R	315	CHL	C1A-C2A-CAA-CBA
22	A	408	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	3	306	CLA	C11-C12-C13-C15
22	N	301	CLA	C16-C17-C18-C20
22	N	302	CLA	C16-C17-C18-C19
22	u	307	CLA	C16-C17-C18-C19
22	n	301	CLA	C16-C17-C18-C20
26	p	314	CHL	C16-C17-C18-C19
26	V	318	CHL	C16-C17-C18-C19
26	P	319	CHL	C16-C17-C18-C19
25	b	623	LHG	O9-C7-O7-C5
34	C	502	LMG	O9-C10-O7-C8
34	c	501	LMG	O9-C10-O7-C8
25	d	406	LHG	C8-C7-O7-C5
25	P	313	LHG	C8-C7-O7-C5
32	a	413	SQD	C17-C18-C19-C20
34	c	501	LMG	C19-C20-C21-C22
36	B	601	DGD	C9A-CAA-CBA-CCA
24	4	311	XAT	C29-C30-C31-C32
31	x	202	BCR	C9-C10-C11-C12
31	C	517	BCR	C15-C16-C17-C18
31	C	517	BCR	C19-C20-C21-C22
31	c	515	BCR	C19-C20-C21-C22
22	V	305	CLA	C5-C6-C7-C8
22	C	513	CLA	C8-C10-C11-C12
25	d	405	LHG	C3-O3-P-O6
25	d	406	LHG	C4-O6-P-O3
25	l	101	LHG	C4-O6-P-O3
25	L	101	LHG	C4-O6-P-O3
25	2	312	LHG	C4-O6-P-O3
25	4	312	LHG	C4-O6-P-O3
25	5	312	LHG	C4-O6-P-O3
25	v	312	LHG	C3-O3-P-O6
25	B	623	LHG	C3-O3-P-O6
25	D	406	LHG	C3-O3-P-O6
25	D	407	LHG	C4-O6-P-O3
25	b	623	LHG	C3-O3-P-O6
25	s	312	LHG	C16-C17-C18-C19
34	C	521	LMG	C10-C11-C12-C13
36	c	518	DGD	C1A-C2A-C3A-C4A
36	c	518	DGD	C1B-C2B-C3B-C4B
22	g	306	CLA	C3-C5-C6-C7
22	B	614	CLA	C3-C5-C6-C7
26	v	314	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	r	609	CLA	O1A-CGA-O2A-C1
22	P	303	CLA	C5-C6-C7-C8
22	B	602	CLA	C15-C16-C17-C18
22	c	510	CLA	C5-C6-C7-C8
26	6	316	CHL	C8-C10-C11-C12
22	u	303	CLA	CBA-CGA-O2A-C1
22	B	606	CLA	CBA-CGA-O2A-C1
25	S	312	LHG	C24-C23-O8-C6
25	D	406	LHG	O6-C4-C5-C6
22	5	305	CLA	O1D-CGD-O2D-CED
25	N	312	LHG	C9-C10-C11-C12
34	w	201	LMG	C30-C31-C32-C33
36	a	416	DGD	C1A-C2A-C3A-C4A
36	C	520	DGD	C1B-C2B-C3B-C4B
25	d	406	LHG	C33-C34-C35-C36
36	c	519	DGD	C7B-C8B-C9B-CAB
36	A	414	DGD	O6E-C5E-C6E-O5E
22	C	512	CLA	C5-C6-C7-C8
34	W	201	LMG	C30-C31-C32-C33
26	r	614	CHL	O1D-CGD-O2D-CED
32	l	102	SQD	C29-C30-C31-C32
26	6	312	CHL	C10-C11-C12-C13
25	3	310	LHG	C24-C25-C26-C27
36	a	416	DGD	C6A-C7A-C8A-C9A
36	b	601	DGD	C4D-C5D-C6D-O5D
25	s	312	LHG	C24-C23-O8-C6
36	a	416	DGD	O6E-C5E-C6E-O5E
25	d	406	LHG	O9-C7-O7-C5
34	D	408	LMG	O9-C10-O7-C8
34	C	502	LMG	C14-C15-C16-C17
34	c	501	LMG	C14-C15-C16-C17
22	3	305	CLA	C5-C6-C7-C8
22	p	305	CLA	C8-C10-C11-C12
26	6	315	CHL	C15-C16-C17-C18
36	B	601	DGD	O6D-C5D-C6D-O5D
34	w	201	LMG	C32-C33-C34-C35
25	D	407	LHG	C8-C7-O7-C5
22	1	306	CLA	O1A-CGA-O2A-C1
22	5	303	CLA	O1A-CGA-O2A-C1
22	6	309	CLA	O1A-CGA-O2A-C1
26	3	313	CHL	O1A-CGA-O2A-C1
26	P	317	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	Q	315	CHL	O1A-CGA-O2A-C1
26	u	317	CHL	O1A-CGA-O2A-C1
25	d	406	LHG	C11-C12-C13-C14
25	G	310	LHG	C24-C25-C26-C27
36	A	414	DGD	C2B-C3B-C4B-C5B
22	6	302	CLA	C15-C16-C17-C18
22	v	303	CLA	C2A-CAA-CBA-CGA
22	V	302	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
26	R	315	CHL	O1D-CGD-O2D-CED
22	N	305	CLA	C3-C5-C6-C7
25	A	413	LHG	C4-C5-C6-O8
25	6	311	LHG	C24-C25-C26-C27
25	v	312	LHG	C4-C5-C6-O8
25	Q	310	LHG	C4-C5-C6-O8
25	R	314	LHG	C4-C5-C6-O8
32	m	101	SQD	C44-C45-C46-O48
32	A	412	SQD	O6-C44-C45-C46
32	A	412	SQD	C11-C12-C13-C14
32	M	101	SQD	C44-C45-C46-O48
34	w	201	LMG	C7-C8-C9-O8
34	C	502	LMG	O1-C7-C8-C9
34	C	521	LMG	O1-C7-C8-C9
34	b	621	LMG	C7-C8-C9-O8
34	c	501	LMG	O1-C7-C8-C9
34	c	501	LMG	C7-C8-C9-O8
34	c	520	LMG	O1-C7-C8-C9
36	C	519	DGD	O1G-C1G-C2G-C3G
36	C	520	DGD	C5B-C6B-C7B-C8B
36	c	517	DGD	O1G-C1G-C2G-C3G
36	c	518	DGD	C7B-C8B-C9B-CAB
22	5	302	CLA	C13-C15-C16-C17
22	b	612	CLA	C10-C11-C12-C13
26	g	315	CHL	C13-C15-C16-C17
25	q	310	LHG	C24-C25-C26-C27
25	R	314	LHG	C28-C29-C30-C31
25	D	406	LHG	C15-C16-C17-C18
26	6	315	CHL	O1A-CGA-O2A-C1
26	6	317	CHL	O1A-CGA-O2A-C1
34	C	502	LMG	C8-C7-O1-C1
34	c	501	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
36	C	520	DGD	C2G-C3G-O3G-C1D
36	c	518	DGD	C2G-C3G-O3G-C1D
25	1	312	LHG	C11-C12-C13-C14
36	C	520	DGD	CDA-CEA-CFA-CGA
36	b	601	DGD	CCA-CDA-CEA-CFA
22	U	306	CLA	CBD-CGD-O2D-CED
22	P	308	CLA	C8-C10-C11-C12
22	c	505	CLA	C5-C6-C7-C8
25	D	406	LHG	C35-C36-C37-C38
34	b	624	LMG	O6-C5-C6-O5
25	c	522	LHG	C23-C24-C25-C26
25	s	312	LHG	C25-C26-C27-C28
25	s	312	LHG	C35-C36-C37-C38
34	D	408	LMG	C15-C16-C17-C18
36	a	416	DGD	C2B-C3B-C4B-C5B
22	v	306	CLA	C3-C5-C6-C7
22	N	305	CLA	C11-C12-C13-C15
22	B	611	CLA	C16-C17-C18-C20
30	D	401	PHO	C10-C11-C12-C13
25	D	407	LHG	C11-C12-C13-C14
34	D	408	LMG	O6-C5-C6-O5
36	C	519	DGD	O6E-C5E-C6E-O5E
36	c	517	DGD	O6E-C5E-C6E-O5E
25	r	613	LHG	O1-C1-C2-O2
25	D	406	LHG	O1-C1-C2-O2
25	c	523	LHG	O1-C1-C2-O2
22	5	308	CLA	O2A-C1-C2-C3
22	U	308	CLA	O2A-C1-C2-C3
22	u	308	CLA	O2A-C1-C2-C3
34	c	520	LMG	C35-C36-C37-C38
36	A	414	DGD	C6A-C7A-C8A-C9A
22	q	305	CLA	C8-C10-C11-C12
25	p	313	LHG	C23-C24-C25-C26
34	A	411	LMG	C28-C29-C30-C31
36	C	519	DGD	C1B-C2B-C3B-C4B
36	b	601	DGD	C1A-C2A-C3A-C4A
36	c	517	DGD	C1B-C2B-C3B-C4B
22	G	304	CLA	C16-C17-C18-C19
25	d	406	LHG	C35-C36-C37-C38
22	Q	306	CLA	C8-C10-C11-C12
30	d	401	PHO	C10-C11-C12-C13
34	d	407	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
34	B	624	LMG	O6-C5-C6-O5
22	Q	302	CLA	C4-C3-C5-C6
22	N	302	CLA	C4-C3-C5-C6
26	2	317	CHL	C4-C3-C5-C6
26	V	316	CHL	C4-C3-C5-C6
26	n	318	CHL	C4-C3-C5-C6
26	R	317	CHL	C4-C3-C5-C6
33	d	404	PL9	C15-C14-C16-C17
33	D	405	PL9	C15-C14-C16-C17
26	V	316	CHL	C2-C3-C5-C6
33	d	404	PL9	C13-C14-C16-C17
25	g	310	LHG	C7-C8-C9-C10
22	a	408	CLA	C11-C12-C13-C14
22	q	301	CLA	C16-C17-C18-C20
22	q	305	CLA	C11-C12-C13-C14
26	G	315	CHL	C16-C17-C18-C19
26	G	316	CHL	C11-C12-C13-C14
22	r	604	CLA	CBA-CGA-O2A-C1
22	5	306	CLA	CBA-CGA-O2A-C1
22	Q	306	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	CBA-CGA-O2A-C1
22	b	605	CLA	CBA-CGA-O2A-C1
25	a	415	LHG	C24-C23-O8-C6
25	A	413	LHG	C24-C23-O8-C6
26	3	316	CHL	CBA-CGA-O2A-C1
26	P	316	CHL	CBA-CGA-O2A-C1
26	n	315	CHL	CBA-CGA-O2A-C1
26	g	312	CHL	CBD-CGD-O2D-CED
22	n	302	CLA	C15-C16-C17-C18
22	C	507	CLA	C13-C15-C16-C17
22	C	507	CLA	C15-C16-C17-C18
22	X	202	CLA	C15-C16-C17-C18
22	b	602	CLA	C5-C6-C7-C8
22	b	604	CLA	C15-C16-C17-C18
26	U	315	CHL	C8-C10-C11-C12
25	S	312	LHG	C25-C26-C27-C28
36	c	519	DGD	CBB-CCB-CDB-CEB
32	l	102	SQD	C46-C45-O47-C7
32	L	102	SQD	C46-C45-O47-C7
22	s	301	CLA	O1D-CGD-O2D-CED
22	a	405	CLA	C2A-CAA-CBA-CGA
22	q	301	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C13-C15-C16-C17
26	Q	311	CHL	C10-C11-C12-C13
26	n	318	CHL	C13-C15-C16-C17
22	4	305	CLA	C2-C1-O2A-CGA
22	p	306	CLA	C2-C1-O2A-CGA
26	r	616	CHL	C2-C1-O2A-CGA
26	R	317	CHL	C2-C1-O2A-CGA
25	d	405	LHG	C10-C11-C12-C13
36	c	518	DGD	C8A-C9A-CAA-CBA
22	G	301	CLA	O1D-CGD-O2D-CED
26	U	314	CHL	O1D-CGD-O2D-CED
26	S	313	CHL	O1D-CGD-O2D-CED
22	C	504	CLA	C10-C11-C12-C13
22	C	506	CLA	C5-C6-C7-C8
25	B	623	LHG	C5-C4-O6-P
25	D	407	LHG	C19-C20-C21-C22
34	C	521	LMG	C11-C12-C13-C14
22	6	307	CLA	CBA-CGA-O2A-C1
22	R	305	CLA	CBA-CGA-O2A-C1
26	v	318	CHL	CBA-CGA-O2A-C1
26	U	316	CHL	CBA-CGA-O2A-C1
26	R	317	CHL	CBA-CGA-O2A-C1
25	4	312	LHG	O6-C4-C5-O7
22	b	611	CLA	C16-C17-C18-C19
26	V	316	CHL	C16-C17-C18-C20
26	g	316	CHL	C11-C12-C13-C15
26	1	318	CHL	CBD-CGD-O2D-CED
25	B	622	LHG	C27-C28-C29-C30
34	c	501	LMG	C32-C33-C34-C35
26	v	316	CHL	C13-C15-C16-C17
26	q	314	CHL	C10-C11-C12-C13
22	r	610	CLA	O1D-CGD-O2D-CED
26	v	318	CHL	O1D-CGD-O2D-CED
22	G	307	CLA	O1A-CGA-O2A-C1
22	g	307	CLA	O1A-CGA-O2A-C1
22	b	606	CLA	O1A-CGA-O2A-C1
25	S	312	LHG	O10-C23-O8-C6
37	E	101	HEM	C3D-CAD-CBD-CGD
32	C	501	SQD	C30-C31-C32-C33
34	B	624	LMG	C28-C29-C30-C31
34	b	624	LMG	C28-C29-C30-C31
22	1	306	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	6	307	CLA	C8-C10-C11-C12
22	N	301	CLA	C5-C6-C7-C8
22	B	606	CLA	C5-C6-C7-C8
22	b	614	CLA	C10-C11-C12-C13
22	b	617	CLA	C10-C11-C12-C13
26	2	313	CHL	C5-C6-C7-C8
25	S	312	LHG	C35-C36-C37-C38
25	R	314	LHG	O7-C5-C6-O8
34	d	407	LMG	O1-C7-C8-O7
34	D	408	LMG	O1-C7-C8-O7
25	d	406	LHG	C19-C20-C21-C22
25	5	312	LHG	C13-C14-C15-C16
25	b	622	LHG	C27-C28-C29-C30
32	C	501	SQD	C24-C25-C26-C27
25	V	312	LHG	O9-C7-O7-C5
25	D	407	LHG	O9-C7-O7-C5
22	A	405	CLA	C13-C15-C16-C17
22	N	302	CLA	C15-C16-C17-C18
22	B	602	CLA	C5-C6-C7-C8
22	c	505	CLA	C15-C16-C17-C18
26	p	319	CHL	C8-C10-C11-C12
22	B	605	CLA	O1A-CGA-O2A-C1
22	B	606	CLA	O1A-CGA-O2A-C1
25	s	312	LHG	O10-C23-O8-C6
26	3	316	CHL	O1A-CGA-O2A-C1
22	n	302	CLA	C16-C17-C18-C19
30	d	401	PHO	CHA-CBD-CGD-O1D
30	d	401	PHO	CHA-CBD-CGD-O2D
30	D	401	PHO	CHA-CBD-CGD-O1D
30	D	401	PHO	CHA-CBD-CGD-O2D
26	4	317	CHL	O1D-CGD-O2D-CED
25	C	524	LHG	C19-C20-C21-C22
34	b	621	LMG	C22-C23-C24-C25
36	c	518	DGD	C3A-C4A-C5A-C6A
26	r	616	CHL	C4-C3-C5-C6
25	U	312	LHG	C12-C13-C14-C15
36	B	601	DGD	C4D-C5D-C6D-O5D
22	r	606	CLA	C11-C10-C8-C7
22	a	404	CLA	C11-C12-C13-C15
22	d	402	CLA	C11-C12-C13-C15
22	A	404	CLA	C11-C12-C13-C15
22	3	301	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	3	306	CLA	C6-C7-C8-C10
22	5	302	CLA	C11-C10-C8-C7
22	5	304	CLA	C6-C7-C8-C10
22	6	302	CLA	C11-C12-C13-C15
22	6	305	CLA	C11-C12-C13-C15
22	v	305	CLA	C6-C7-C8-C10
22	p	302	CLA	C11-C12-C13-C15
22	q	301	CLA	C6-C7-C8-C10
22	q	304	CLA	C11-C12-C13-C15
22	V	301	CLA	C11-C12-C13-C15
22	V	302	CLA	C12-C13-C15-C16
22	Q	304	CLA	C12-C13-C15-C16
22	Q	305	CLA	C11-C10-C8-C7
22	N	304	CLA	C11-C10-C8-C7
22	N	307	CLA	C6-C7-C8-C10
22	n	304	CLA	C12-C13-C15-C16
22	n	306	CLA	C11-C10-C8-C7
22	g	301	CLA	C11-C12-C13-C15
22	g	306	CLA	C11-C10-C8-C7
22	R	307	CLA	C11-C10-C8-C7
22	S	301	CLA	C6-C7-C8-C10
22	S	301	CLA	C11-C12-C13-C15
22	C	505	CLA	C6-C7-C8-C10
22	C	507	CLA	C6-C7-C8-C10
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C12-C13-C15
22	B	602	CLA	C12-C13-C15-C16
22	B	603	CLA	C12-C13-C15-C16
22	B	607	CLA	C6-C7-C8-C10
22	B	612	CLA	C6-C7-C8-C10
22	B	613	CLA	C11-C12-C13-C15
22	B	616	CLA	C11-C12-C13-C15
22	B	617	CLA	C12-C13-C15-C16
22	D	403	CLA	C11-C12-C13-C15
22	b	607	CLA	C6-C7-C8-C10
22	b	612	CLA	C6-C7-C8-C10
22	b	613	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C10-C8-C7
22	b	616	CLA	C6-C7-C8-C10
22	c	503	CLA	C6-C7-C8-C10
22	c	503	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C12-C13-C15-C16
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C12-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C10
22	s	301	CLA	C6-C7-C8-C10
26	1	313	CHL	C11-C12-C13-C15
26	1	318	CHL	C12-C13-C15-C16
26	2	313	CHL	C12-C13-C15-C16
26	2	316	CHL	C12-C13-C15-C16
26	2	317	CHL	C2-C3-C5-C6
26	3	311	CHL	C6-C7-C8-C10
26	4	316	CHL	C6-C7-C8-C10
26	4	317	CHL	C12-C13-C15-C16
26	5	313	CHL	C12-C13-C15-C16
26	5	316	CHL	C12-C13-C15-C16
26	5	317	CHL	C11-C10-C8-C7
26	6	315	CHL	C12-C13-C15-C16
26	v	313	CHL	C6-C7-C8-C10
26	v	313	CHL	C11-C12-C13-C15
26	v	316	CHL	C12-C13-C15-C16
26	v	317	CHL	C11-C10-C8-C7
26	p	320	CHL	C11-C10-C8-C7
26	q	311	CHL	C12-C13-C15-C16
26	q	314	CHL	C12-C13-C15-C16
26	V	313	CHL	C6-C7-C8-C10
26	V	313	CHL	C12-C13-C15-C16
26	P	314	CHL	C12-C13-C15-C16
26	Q	311	CHL	C12-C13-C15-C16
26	Q	314	CHL	C11-C10-C8-C7
26	U	317	CHL	C12-C13-C15-C16
26	N	313	CHL	C11-C12-C13-C15
26	N	316	CHL	C6-C7-C8-C10
26	G	311	CHL	C11-C12-C13-C15
26	G	314	CHL	C12-C13-C15-C16
26	G	315	CHL	C12-C13-C15-C16
26	u	313	CHL	C11-C12-C13-C15
26	u	316	CHL	C12-C13-C15-C16
26	u	318	CHL	C11-C12-C13-C15
26	n	313	CHL	C11-C12-C13-C15
26	n	317	CHL	C6-C7-C8-C10
26	n	318	CHL	C2-C3-C5-C6
26	g	311	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	R	317	CHL	C2-C3-C5-C6
30	a	407	PHO	C11-C10-C8-C7
30	A	407	PHO	C11-C10-C8-C7
33	D	405	PL9	C13-C14-C16-C17
25	b	623	LHG	O7-C7-C8-C9
22	3	306	CLA	C3-C5-C6-C7
34	B	621	LMG	C19-C20-C21-C22
22	r	606	CLA	C14-C13-C15-C16
22	a	404	CLA	C11-C12-C13-C14
22	d	402	CLA	C11-C12-C13-C14
22	3	301	CLA	C6-C7-C8-C9
22	3	301	CLA	C11-C12-C13-C14
22	3	306	CLA	C6-C7-C8-C9
22	5	302	CLA	C11-C10-C8-C9
22	5	307	CLA	C11-C10-C8-C9
22	6	302	CLA	C11-C12-C13-C14
22	6	303	CLA	C11-C10-C8-C9
22	6	305	CLA	C11-C12-C13-C14
22	v	306	CLA	C11-C10-C8-C9
22	q	301	CLA	C11-C12-C13-C14
22	q	304	CLA	C11-C12-C13-C14
22	V	301	CLA	C11-C12-C13-C14
22	P	302	CLA	C11-C12-C13-C14
22	P	305	CLA	C6-C7-C8-C9
22	Q	304	CLA	C11-C12-C13-C14
22	Q	304	CLA	C14-C13-C15-C16
22	Q	306	CLA	C6-C7-C8-C9
22	N	302	CLA	C14-C13-C15-C16
22	N	307	CLA	C6-C7-C8-C9
22	G	301	CLA	C11-C12-C13-C14
22	G	306	CLA	C11-C10-C8-C9
22	G	307	CLA	C14-C13-C15-C16
22	g	306	CLA	C11-C10-C8-C9
22	g	307	CLA	C14-C13-C15-C16
22	R	307	CLA	C14-C13-C15-C16
22	S	301	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C12-C13-C14
22	C	512	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	613	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	b	613	CLA	C11-C12-C13-C14
22	c	503	CLA	C14-C13-C15-C16
22	c	506	CLA	C14-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C14
26	1	313	CHL	C11-C12-C13-C14
26	1	318	CHL	C6-C7-C8-C9
26	2	313	CHL	C11-C12-C13-C14
26	2	317	CHL	C11-C12-C13-C14
26	2	318	CHL	C6-C7-C8-C9
26	2	318	CHL	C11-C10-C8-C9
26	3	311	CHL	C6-C7-C8-C9
26	4	313	CHL	C11-C12-C13-C14
26	v	313	CHL	C11-C12-C13-C14
26	p	314	CHL	C11-C12-C13-C14
26	p	320	CHL	C14-C13-C15-C16
26	q	311	CHL	C14-C13-C15-C16
26	q	314	CHL	C14-C13-C15-C16
26	V	313	CHL	C14-C13-C15-C16
26	P	314	CHL	C14-C13-C15-C16
26	Q	311	CHL	C14-C13-C15-C16
26	U	313	CHL	C11-C12-C13-C14
26	U	315	CHL	C14-C13-C15-C16
26	U	319	CHL	C14-C13-C15-C16
26	u	313	CHL	C11-C12-C13-C14
26	n	313	CHL	C11-C12-C13-C14
26	n	316	CHL	C11-C10-C8-C9
26	s	315	CHL	C6-C7-C8-C9
25	C	523	LHG	C23-C24-C25-C26
25	l	101	LHG	C30-C31-C32-C33
25	6	311	LHG	C11-C12-C13-C14
25	C	523	LHG	C16-C17-C18-C19
22	r	603	CLA	CBA-CGA-O2A-C1
22	3	306	CLA	CBA-CGA-O2A-C1
22	R	306	CLA	CBA-CGA-O2A-C1
26	r	616	CHL	CBA-CGA-O2A-C1
26	3	315	CHL	CBA-CGA-O2A-C1
22	R	307	CLA	C8-C10-C11-C12
26	v	318	CHL	C8-C10-C11-C12
22	a	404	CLA	C2A-CAA-CBA-CGA
22	1	301	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	O1D-CGD-O2D-CED
26	1	316	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	u	303	CLA	O1A-CGA-O2A-C1
22	b	605	CLA	O1A-CGA-O2A-C1
31	C	517	BCR	C11-C12-C13-C35
22	V	302	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
26	v	316	CHL	C16-C17-C18-C20
25	4	312	LHG	O1-C1-C2-C3
31	b	620	BCR	C17-C18-C19-C20
34	C	502	LMG	C32-C33-C34-C35
22	U	306	CLA	C3-C5-C6-C7
22	b	605	CLA	O1D-CGD-O2D-CED
22	n	304	CLA	C15-C16-C17-C18
25	2	312	LHG	C28-C29-C30-C31
36	a	416	DGD	C8B-C9B-CAB-CBB
22	A	406	CLA	CBA-CGA-O2A-C1
22	G	305	CLA	CBA-CGA-O2A-C1
25	c	522	LHG	C24-C23-O8-C6
26	v	316	CHL	CBA-CGA-O2A-C1
26	p	316	CHL	CBA-CGA-O2A-C1
34	C	502	LMG	C22-C23-C24-C25
34	b	624	LMG	C24-C25-C26-C27
22	B	615	CLA	C8-C10-C11-C12
26	U	317	CHL	C8-C10-C11-C12
22	B	605	CLA	O1D-CGD-O2D-CED
36	A	414	DGD	CAB-CBB-CCB-CDB
22	d	402	CLA	CBD-CGD-O2D-CED
34	B	621	LMG	C30-C31-C32-C33
22	r	602	CLA	C4B-C3B-CAB-CBB
22	1	301	CLA	C4B-C3B-CAB-CBB
22	1	303	CLA	C4B-C3B-CAB-CBB
22	1	307	CLA	C4B-C3B-CAB-CBB
22	2	307	CLA	C4B-C3B-CAB-CBB
22	3	308	CLA	C4B-C3B-CAB-CBB
22	4	301	CLA	C4B-C3B-CAB-CBB
22	4	303	CLA	C4B-C3B-CAB-CBB
22	4	304	CLA	C4B-C3B-CAB-CBB
22	4	307	CLA	C4B-C3B-CAB-CBB
22	5	307	CLA	C4B-C3B-CAB-CBB
22	6	308	CLA	C4B-C3B-CAB-CBB
22	6	309	CLA	C4B-C3B-CAB-CBB
22	v	303	CLA	C4B-C3B-CAB-CBB
22	v	306	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	v	308	CLA	C4B-C3B-CAB-CBB
22	p	304	CLA	C4B-C3B-CAB-CBB
22	p	308	CLA	C4B-C3B-CAB-CBB
22	q	301	CLA	C4B-C3B-CAB-CBB
22	q	303	CLA	C4B-C3B-CAB-CBB
22	q	307	CLA	C4B-C3B-CAB-CBB
22	V	303	CLA	C4B-C3B-CAB-CBB
22	P	304	CLA	C4B-C3B-CAB-CBB
22	P	308	CLA	C4B-C3B-CAB-CBB
22	Q	301	CLA	C4B-C3B-CAB-CBB
22	Q	303	CLA	C4B-C3B-CAB-CBB
22	Q	307	CLA	C4B-C3B-CAB-CBB
22	U	301	CLA	C4B-C3B-CAB-CBB
22	U	302	CLA	C4B-C3B-CAB-CBB
22	U	303	CLA	C4B-C3B-CAB-CBB
22	N	307	CLA	C4B-C3B-CAB-CBB
22	G	303	CLA	C4B-C3B-CAB-CBB
22	u	301	CLA	C4B-C3B-CAB-CBB
22	u	303	CLA	C4B-C3B-CAB-CBB
22	R	303	CLA	C4B-C3B-CAB-CBB
22	S	305	CLA	C4B-C3B-CAB-CBB
22	S	308	CLA	C4B-C3B-CAB-CBB
22	C	503	CLA	C4B-C3B-CAB-CBB
22	C	505	CLA	C4B-C3B-CAB-CBB
22	C	509	CLA	C4B-C3B-CAB-CBB
22	C	515	CLA	C4B-C3B-CAB-CBB
22	B	610	CLA	C4B-C3B-CAB-CBB
22	B	611	CLA	C4B-C3B-CAB-CBB
22	D	403	CLA	C4B-C3B-CAB-CBB
22	b	610	CLA	C4B-C3B-CAB-CBB
22	b	611	CLA	C4B-C3B-CAB-CBB
22	c	502	CLA	C4B-C3B-CAB-CBB
22	c	504	CLA	C4B-C3B-CAB-CBB
22	c	508	CLA	C4B-C3B-CAB-CBB
22	s	305	CLA	C4B-C3B-CAB-CBB
22	s	308	CLA	C4B-C3B-CAB-CBB
22	s	309	CLA	C4B-C3B-CAB-CBB
26	p	318	CHL	C4B-C3B-CAB-CBB
26	p	320	CHL	C4B-C3B-CAB-CBB
26	N	317	CHL	C4B-C3B-CAB-CBB
26	n	318	CHL	C4B-C3B-CAB-CBB
22	B	602	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	b	602	CLA	C16-C17-C18-C19
22	a	404	CLA	C13-C15-C16-C17
22	A	408	CLA	C8-C10-C11-C12
22	6	305	CLA	C8-C10-C11-C12
22	B	614	CLA	C10-C11-C12-C13
26	g	315	CHL	C5-C6-C7-C8
25	a	415	LHG	O6-C4-C5-C6
25	d	405	LHG	O6-C4-C5-C6
25	l	101	LHG	O6-C4-C5-C6
25	A	413	LHG	O6-C4-C5-C6
25	L	101	LHG	O6-C4-C5-C6
25	d	405	LHG	C25-C26-C27-C28
34	B	624	LMG	C24-C25-C26-C27
36	B	601	DGD	C7B-C8B-C9B-CAB
34	a	412	LMG	C28-C29-C30-C31
36	C	520	DGD	C1A-C2A-C3A-C4A
34	D	408	LMG	C33-C34-C35-C36
34	c	520	LMG	C11-C12-C13-C14
25	u	312	LHG	C24-C23-O8-C6
26	4	317	CHL	CBA-CGA-O2A-C1
36	C	520	DGD	C2A-C1A-O1G-C1G
22	1	308	CLA	CBD-CGD-O2D-CED
22	3	305	CLA	C10-C11-C12-C13
22	B	611	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
34	c	520	LMG	O6-C5-C6-O5
22	c	511	CLA	O1D-CGD-O2D-CED
26	3	313	CHL	O1D-CGD-O2D-CED
22	C	514	CLA	C4-C3-C5-C6
26	p	320	CHL	C4-C3-C5-C6
26	Q	314	CHL	C4-C3-C5-C6
26	g	314	CHL	C4-C3-C5-C6
22	Q	302	CLA	C2-C3-C5-C6
26	r	616	CHL	C2-C3-C5-C6
26	Q	314	CHL	C2-C3-C5-C6
25	G	310	LHG	C7-C8-C9-C10
22	R	304	CLA	C8-C10-C11-C12
25	P	313	LHG	O9-C7-O7-C5
22	S	301	CLA	C14-C13-C15-C16
26	P	316	CHL	O1A-CGA-O2A-C1
25	C	522	LHG	C25-C26-C27-C28
22	N	304	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	D	401	PHO	C16-C17-C18-C19
34	B	624	LMG	C32-C33-C34-C35
26	n	313	CHL	C8-C10-C11-C12
22	a	404	CLA	CBA-CGA-O2A-C1
22	3	303	CLA	CBA-CGA-O2A-C1
25	N	312	LHG	C24-C23-O8-C6
26	V	316	CHL	CBA-CGA-O2A-C1
26	U	317	CHL	CBA-CGA-O2A-C1
26	u	318	CHL	CBA-CGA-O2A-C1
34	B	624	LMG	C29-C28-O8-C9
36	C	519	DGD	O6D-C5D-C6D-O5D
34	b	621	LMG	C29-C30-C31-C32
25	a	415	LHG	C5-C4-O6-P
25	l	101	LHG	C2-C3-O3-P
25	A	413	LHG	C5-C4-O6-P
25	L	101	LHG	C2-C3-O3-P
25	b	623	LHG	C5-C4-O6-P
25	c	522	LHG	C2-C3-O3-P
22	Q	306	CLA	O1A-CGA-O2A-C1
26	n	315	CHL	O1A-CGA-O2A-C1
22	N	308	CLA	C3A-C2A-CAA-CBA
26	6	314	CHL	C3A-C2A-CAA-CBA
26	P	319	CHL	C3A-C2A-CAA-CBA
26	g	311	CHL	C3A-C2A-CAA-CBA
26	g	316	CHL	C3A-C2A-CAA-CBA
26	S	316	CHL	C3A-C2A-CAA-CBA
26	s	316	CHL	C3A-C2A-CAA-CBA
26	U	315	CHL	C10-C11-C12-C13
25	L	101	LHG	C16-C17-C18-C19
32	m	101	SQD	C12-C13-C14-C15
24	r	612	XAT	C29-C30-C31-C32
24	4	311	XAT	C13-C14-C15-C35
31	X	201	BCR	C9-C10-C11-C12
31	b	619	BCR	C15-C16-C17-C18
25	d	406	LHG	C12-C13-C14-C15
25	U	312	LHG	C11-C12-C13-C14
25	g	310	LHG	C9-C10-C11-C12
25	D	407	LHG	C18-C19-C20-C21
22	P	305	CLA	C15-C16-C17-C18
22	C	514	CLA	C5-C6-C7-C8
22	c	507	CLA	C15-C16-C17-C18
26	6	316	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	v	313	CHL	C5-C6-C7-C8
26	N	316	CHL	C15-C16-C17-C18
26	U	316	CHL	O1A-CGA-O2A-C1
25	G	310	LHG	C33-C34-C35-C36
36	C	520	DGD	C8A-C9A-CAA-CBA
22	q	301	CLA	C16-C17-C18-C19
22	U	307	CLA	C16-C17-C18-C20
30	D	401	PHO	C16-C17-C18-C20
37	e	101	HEM	C3D-CAD-CBD-CGD
22	A	404	CLA	CBA-CGA-O2A-C1
22	Q	307	CLA	CBA-CGA-O2A-C1
25	C	523	LHG	C24-C23-O8-C6
25	N	312	LHG	C29-C30-C31-C32
25	n	312	LHG	C12-C13-C14-C15
25	C	524	LHG	C26-C27-C28-C29
22	b	606	CLA	C5-C6-C7-C8
22	c	510	CLA	C15-C16-C17-C18
22	c	514	CLA	C10-C11-C12-C13
26	p	318	CHL	C10-C11-C12-C13
26	V	318	CHL	C8-C10-C11-C12
25	a	415	LHG	C4-C5-C6-O8
25	l	101	LHG	C4-C5-C6-O8
25	L	101	LHG	C4-C5-C6-O8
25	3	310	LHG	C4-C5-C6-O8
25	V	312	LHG	C4-C5-C6-O8
25	B	623	LHG	C4-C5-C6-O8
25	b	623	LHG	C4-C5-C6-O8
32	a	413	SQD	O6-C44-C45-C46
32	l	102	SQD	C44-C45-C46-O48
32	L	102	SQD	C44-C45-C46-O48
34	d	407	LMG	O1-C7-C8-C9
34	d	407	LMG	C7-C8-C9-O8
34	w	201	LMG	O1-C7-C8-C9
34	W	201	LMG	C7-C8-C9-O8
34	C	502	LMG	C7-C8-C9-O8
34	C	521	LMG	C7-C8-C9-O8
34	B	624	LMG	O1-C7-C8-C9
34	D	408	LMG	O1-C7-C8-C9
34	D	408	LMG	C7-C8-C9-O8
34	b	624	LMG	O1-C7-C8-C9
36	a	416	DGD	O1G-C1G-C2G-C3G
36	A	414	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
36	C	520	DGD	C3A-C4A-C5A-C6A
22	6	307	CLA	O1A-CGA-O2A-C1
25	a	415	LHG	O10-C23-O8-C6
25	A	413	LHG	O10-C23-O8-C6
26	6	312	CHL	O1D-CGD-O2D-CED
34	B	621	LMG	C15-C16-C17-C18
36	c	518	DGD	CDB-CEB-CFB-CGB
36	c	517	DGD	O6D-C5D-C6D-O5D
22	b	602	CLA	C3-C5-C6-C7
22	5	306	CLA	O1A-CGA-O2A-C1
22	C	504	CLA	C5-C6-C7-C8
26	N	317	CHL	C13-C15-C16-C17
22	g	304	CLA	C4-C3-C5-C6
22	D	403	CLA	C4-C3-C5-C6
26	U	313	CHL	C4-C3-C5-C6
22	c	507	CLA	C16-C17-C18-C19
26	U	317	CHL	O1D-CGD-O2D-CED
25	l	101	LHG	C16-C17-C18-C19
34	B	621	LMG	C21-C22-C23-C24
22	g	304	CLA	C16-C17-C18-C19
36	a	416	DGD	C9B-CAB-CBB-CCB
26	1	315	CHL	O1D-CGD-O2D-CED
26	V	318	CHL	O1D-CGD-O2D-CED
26	p	314	CHL	C8-C10-C11-C12
25	3	310	LHG	C4-O6-P-O3
25	R	314	LHG	C4-O6-P-O3
26	r	615	CHL	C3C-C2C-CMC-OMC
26	1	315	CHL	C3C-C2C-CMC-OMC
26	1	316	CHL	C3C-C2C-CMC-OMC
26	1	318	CHL	C3C-C2C-CMC-OMC
26	3	313	CHL	C3C-C2C-CMC-OMC
26	4	314	CHL	C3C-C2C-CMC-OMC
26	4	315	CHL	C3C-C2C-CMC-OMC
26	5	313	CHL	C3C-C2C-CMC-OMC
26	6	314	CHL	C3C-C2C-CMC-OMC
26	v	315	CHL	C3C-C2C-CMC-OMC
26	p	314	CHL	C3C-C2C-CMC-OMC
26	p	316	CHL	C3C-C2C-CMC-OMC
26	p	318	CHL	C3C-C2C-CMC-OMC
26	q	313	CHL	C3C-C2C-CMC-OMC
26	V	315	CHL	C3C-C2C-CMC-OMC
26	P	314	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	P	316	CHL	C3C-C2C-CMC-OMC
26	Q	313	CHL	C3C-C2C-CMC-OMC
26	U	313	CHL	C3C-C2C-CMC-OMC
26	U	314	CHL	C3C-C2C-CMC-OMC
26	N	315	CHL	C3C-C2C-CMC-OMC
26	G	311	CHL	C3C-C2C-CMC-OMC
26	u	315	CHL	C3C-C2C-CMC-OMC
26	n	315	CHL	C3C-C2C-CMC-OMC
26	S	315	CHL	C3C-C2C-CMC-OMC
26	S	316	CHL	C3C-C2C-CMC-OMC
26	s	315	CHL	C3C-C2C-CMC-OMC
25	B	622	LHG	C23-C24-C25-C26
22	r	604	CLA	O1A-CGA-O2A-C1
22	R	305	CLA	O1A-CGA-O2A-C1
22	6	307	CLA	C3-C5-C6-C7
22	4	301	CLA	C2A-CAA-CBA-CGA
26	p	320	CHL	C2A-CAA-CBA-CGA
26	N	315	CHL	C2A-CAA-CBA-CGA
26	G	315	CHL	C2A-CAA-CBA-CGA
25	6	311	LHG	O1-C1-C2-O2
25	b	622	LHG	O1-C1-C2-O2
22	a	408	CLA	C8-C10-C11-C12
22	u	302	CLA	C5-C6-C7-C8
22	g	302	CLA	C5-C6-C7-C8
25	1	312	LHG	C13-C14-C15-C16
25	D	406	LHG	C27-C28-C29-C30
25	D	407	LHG	C12-C13-C14-C15
34	B	621	LMG	C18-C19-C20-C21
25	a	415	LHG	O6-C4-C5-O7
25	A	413	LHG	O6-C4-C5-O7
25	U	312	LHG	O6-C4-C5-O7
25	u	312	LHG	O6-C4-C5-O7
25	n	312	LHG	O6-C4-C5-O7
25	R	314	LHG	O6-C4-C5-O7
25	D	406	LHG	O6-C4-C5-O7
22	g	303	CLA	CBA-CGA-O2A-C1
34	a	412	LMG	C39-C40-C41-C42
22	r	603	CLA	O1A-CGA-O2A-C1
26	v	318	CHL	O1A-CGA-O2A-C1
22	C	508	CLA	C16-C17-C18-C19
26	V	318	CHL	C16-C17-C18-C20
26	g	316	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	C	508	CLA	C15-C16-C17-C18
34	D	408	LMG	C16-C17-C18-C19
36	C	520	DGD	CDB-CEB-CFB-CGB
22	b	602	CLA	CAA-CBA-CGA-O2A
22	a	405	CLA	C2B-C3B-CAB-CBB
22	d	402	CLA	C2B-C3B-CAB-CBB
22	1	303	CLA	C2B-C3B-CAB-CBB
22	1	307	CLA	C2B-C3B-CAB-CBB
22	2	307	CLA	C2B-C3B-CAB-CBB
22	3	308	CLA	C2B-C3B-CAB-CBB
22	4	301	CLA	C2B-C3B-CAB-CBB
22	4	303	CLA	C2B-C3B-CAB-CBB
22	4	307	CLA	C2B-C3B-CAB-CBB
22	5	307	CLA	C2B-C3B-CAB-CBB
22	6	309	CLA	C2B-C3B-CAB-CBB
22	v	303	CLA	C2B-C3B-CAB-CBB
22	v	308	CLA	C2B-C3B-CAB-CBB
22	p	308	CLA	C2B-C3B-CAB-CBB
22	q	307	CLA	C2B-C3B-CAB-CBB
22	P	304	CLA	C2B-C3B-CAB-CBB
22	P	308	CLA	C2B-C3B-CAB-CBB
22	U	301	CLA	C2B-C3B-CAB-CBB
22	U	303	CLA	C2B-C3B-CAB-CBB
22	G	303	CLA	C2B-C3B-CAB-CBB
22	C	505	CLA	C2B-C3B-CAB-CBB
22	C	509	CLA	C2B-C3B-CAB-CBB
22	C	515	CLA	C2B-C3B-CAB-CBB
22	B	610	CLA	C2B-C3B-CAB-CBB
22	D	403	CLA	C2B-C3B-CAB-CBB
22	b	610	CLA	C2B-C3B-CAB-CBB
22	c	502	CLA	C2B-C3B-CAB-CBB
22	c	504	CLA	C2B-C3B-CAB-CBB
22	c	508	CLA	C2B-C3B-CAB-CBB
22	c	514	CLA	C2B-C3B-CAB-CBB
22	s	305	CLA	C2B-C3B-CAB-CBB
26	1	317	CHL	C2B-C3B-CAB-CBB
26	2	318	CHL	C2B-C3B-CAB-CBB
26	p	320	CHL	C2B-C3B-CAB-CBB
26	G	316	CHL	C2B-C3B-CAB-CBB
26	u	317	CHL	C2B-C3B-CAB-CBB
26	g	316	CHL	C2B-C3B-CAB-CBB
25	a	415	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	3	310	LHG	C15-C16-C17-C18
22	3	306	CLA	O1A-CGA-O2A-C1
22	Q	304	CLA	C15-C16-C17-C18
34	c	501	LMG	C22-C23-C24-C25
26	3	311	CHL	C3-C5-C6-C7
25	r	613	LHG	O7-C5-C6-O8
25	2	312	LHG	O7-C5-C6-O8
25	3	310	LHG	O7-C5-C6-O8
25	V	312	LHG	O7-C5-C6-O8
25	N	312	LHG	O7-C5-C6-O8
34	C	502	LMG	O1-C7-C8-O7
34	b	621	LMG	O7-C8-C9-O8
36	C	519	DGD	O1G-C1G-C2G-O2G
36	c	517	DGD	O1G-C1G-C2G-O2G
22	b	602	CLA	C15-C16-C17-C18
22	r	605	CLA	O1D-CGD-O2D-CED
25	u	312	LHG	C8-C7-O7-C5
26	4	315	CHL	O1D-CGD-O2D-CED
26	n	318	CHL	O1D-CGD-O2D-CED
22	q	305	CLA	C11-C12-C13-C15
22	N	301	CLA	C16-C17-C18-C19
22	N	304	CLA	C16-C17-C18-C19
22	B	602	CLA	C16-C17-C18-C19
26	v	318	CHL	C16-C17-C18-C20
26	P	319	CHL	C16-C17-C18-C20
30	d	401	PHO	C16-C17-C18-C19
30	d	401	PHO	C16-C17-C18-C20
22	N	307	CLA	C5-C6-C7-C8
22	B	609	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
25	2	312	LHG	C1-C2-C3-O3
25	d	405	LHG	C27-C28-C29-C30
25	c	522	LHG	C17-C18-C19-C20
34	B	624	LMG	C21-C22-C23-C24
36	c	519	DGD	CCA-CDA-CEA-CFA
26	5	317	CHL	C4-C3-C5-C6
26	q	315	CHL	C4-C3-C5-C6
26	Q	316	CHL	C4-C3-C5-C6
22	n	304	CLA	C2-C1-O2A-CGA
22	S	301	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C2-C1-O2A-CGA
22	b	609	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C2-C1-O2A-CGA
22	c	514	CLA	C2-C1-O2A-CGA
26	N	313	CHL	C2-C1-O2A-CGA
26	N	317	CHL	C2-C1-O2A-CGA
26	n	313	CHL	C2-C1-O2A-CGA
26	n	318	CHL	C2-C1-O2A-CGA
22	U	306	CLA	O1D-CGD-O2D-CED
26	p	320	CHL	C2-C3-C5-C6
25	A	413	LHG	C9-C10-C11-C12
22	q	302	CLA	C5-C6-C7-C8
26	V	317	CHL	C15-C16-C17-C18
36	B	601	DGD	C1A-C2A-C3A-C4A
22	6	305	CLA	C11-C10-C8-C9
22	p	305	CLA	C11-C10-C8-C9
22	q	304	CLA	C14-C13-C15-C16
22	V	307	CLA	C14-C13-C15-C16
22	P	307	CLA	C6-C7-C8-C9
22	U	305	CLA	C11-C10-C8-C9
22	N	304	CLA	C14-C13-C15-C16
22	G	301	CLA	C6-C7-C8-C9
22	u	302	CLA	C6-C7-C8-C9
22	u	307	CLA	C14-C13-C15-C16
22	n	302	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C12-C13-C14
22	B	608	CLA	C11-C10-C8-C9
22	B	617	CLA	C14-C13-C15-C16
22	b	617	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	c	511	CLA	C6-C7-C8-C9
22	s	301	CLA	C11-C12-C13-C14
26	1	317	CHL	C11-C12-C13-C14
26	2	316	CHL	C14-C13-C15-C16
26	3	311	CHL	C11-C12-C13-C14
26	3	311	CHL	C14-C13-C15-C16
26	5	316	CHL	C14-C13-C15-C16
26	5	317	CHL	C6-C7-C8-C9
26	6	312	CHL	C11-C12-C13-C14
26	6	312	CHL	C14-C13-C15-C16
26	v	313	CHL	C14-C13-C15-C16
26	p	317	CHL	C14-C13-C15-C16
26	p	319	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	q	311	CHL	C11-C12-C13-C14
26	q	314	CHL	C11-C12-C13-C14
26	V	318	CHL	C14-C13-C15-C16
26	P	314	CHL	C11-C12-C13-C14
26	Q	311	CHL	C11-C12-C13-C14
26	Q	314	CHL	C11-C12-C13-C14
26	N	313	CHL	C11-C12-C13-C14
26	G	314	CHL	C14-C13-C15-C16
26	u	317	CHL	C14-C13-C15-C16
26	g	315	CHL	C14-C13-C15-C16
26	R	315	CHL	C11-C12-C13-C14
26	R	315	CHL	C14-C13-C15-C16
25	c	523	LHG	C19-C20-C21-C22
34	d	407	LMG	C12-C13-C14-C15
36	A	414	DGD	C8B-C9B-CAB-CBB
36	c	518	DGD	C5B-C6B-C7B-C8B
22	D	403	CLA	O1D-CGD-O2D-CED
22	v	302	CLA	C5-C6-C7-C8
22	b	615	CLA	C8-C10-C11-C12
22	b	617	CLA	C13-C15-C16-C17
26	5	313	CHL	C13-C15-C16-C17
25	4	312	LHG	C2-C3-O3-P
25	5	312	LHG	C2-C3-O3-P
25	Q	310	LHG	C2-C3-O3-P
25	R	314	LHG	C2-C3-O3-P
22	R	306	CLA	O1A-CGA-O2A-C1
26	3	315	CHL	O1A-CGA-O2A-C1
26	R	317	CHL	O1A-CGA-O2A-C1
25	L	101	LHG	C30-C31-C32-C33
22	p	302	CLA	C2A-CAA-CBA-CGA
22	P	302	CLA	C2A-CAA-CBA-CGA
22	U	301	CLA	C2A-CAA-CBA-CGA
22	S	305	CLA	C2A-CAA-CBA-CGA
22	a	408	CLA	C11-C12-C13-C15
26	u	316	CHL	C16-C17-C18-C19
23	2	309	LUT	C1-C6-C7-C8
23	2	309	LUT	C5-C6-C7-C8
23	v	309	LUT	C5-C6-C7-C8
23	V	309	LUT	C5-C6-C7-C8
23	u	309	LUT	C1-C6-C7-C8
23	u	309	LUT	C5-C6-C7-C8
23	R	312	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	k	101	BCR	C1-C6-C7-C8
31	t	101	BCR	C23-C24-C25-C30
31	z	101	BCR	C5-C6-C7-C8
31	K	101	BCR	C1-C6-C7-C8
31	T	101	BCR	C23-C24-C25-C30
31	C	516	BCR	C5-C6-C7-C8
31	B	620	BCR	C5-C6-C7-C8
31	b	618	BCR	C1-C6-C7-C8
31	b	620	BCR	C1-C6-C7-C8
31	b	620	BCR	C5-C6-C7-C8
22	r	606	CLA	C8-C10-C11-C12
22	U	302	CLA	C15-C16-C17-C18
22	b	604	CLA	C5-C6-C7-C8
26	R	315	CHL	C10-C11-C12-C13
34	b	624	LMG	C32-C33-C34-C35
25	d	406	LHG	C18-C19-C20-C21
25	D	406	LHG	C31-C32-C33-C34
25	c	522	LHG	C16-C17-C18-C19
23	s	311	LUT	C11-C12-C13-C14
24	p	312	XAT	C31-C32-C33-C34
27	u	319	NEX	C11-C12-C13-C14
31	b	619	BCR	C11-C12-C13-C14
22	v	307	CLA	C10-C11-C12-C13
22	P	302	CLA	C15-C16-C17-C18
22	P	308	CLA	C5-C6-C7-C8
22	C	511	CLA	C15-C16-C17-C18
22	b	615	CLA	C5-C6-C7-C8
26	5	317	CHL	C5-C6-C7-C8
26	G	315	CHL	C5-C6-C7-C8
25	5	312	LHG	C25-C26-C27-C28
34	C	502	LMG	C35-C36-C37-C38
36	c	517	DGD	C1A-C2A-C3A-C4A
25	U	312	LHG	C8-C7-O7-C5
34	d	407	LMG	C30-C31-C32-C33
36	c	518	DGD	CDA-CEA-CFA-CGA
22	N	308	CLA	O2A-C1-C2-C3
22	B	617	CLA	C13-C15-C16-C17
26	p	316	CHL	O1A-CGA-O2A-C1
22	U	307	CLA	C16-C17-C18-C19
34	A	411	LMG	C10-C11-C12-C13
22	2	301	CLA	C15-C16-C17-C18
26	U	315	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	a	413	SQD	C16-C17-C18-C19
34	b	621	LMG	C11-C12-C13-C14
36	C	520	DGD	CAB-CBB-CCB-CDB
22	4	308	CLA	O1D-CGD-O2D-CED
26	1	318	CHL	O1D-CGD-O2D-CED
26	S	315	CHL	O1D-CGD-O2D-CED
22	B	604	CLA	C5-C6-C7-C8
22	B	617	CLA	C10-C11-C12-C13
25	r	613	LHG	O6-C4-C5-C6
25	G	310	LHG	O6-C4-C5-C6
25	g	310	LHG	O6-C4-C5-C6
25	c	523	LHG	O6-C4-C5-C6
26	u	318	CHL	O1D-CGD-O2D-CED
32	M	101	SQD	C12-C13-C14-C15
22	r	606	CLA	C12-C13-C15-C16
22	1	306	CLA	C11-C10-C8-C7
22	3	302	CLA	C6-C7-C8-C10
22	5	307	CLA	C11-C10-C8-C7
22	6	303	CLA	C11-C10-C8-C7
22	6	305	CLA	C11-C10-C8-C7
22	6	308	CLA	C12-C13-C15-C16
22	v	306	CLA	C11-C10-C8-C7
22	p	305	CLA	C11-C10-C8-C7
22	q	301	CLA	C11-C12-C13-C15
22	q	304	CLA	C12-C13-C15-C16
22	q	306	CLA	C6-C7-C8-C10
22	V	305	CLA	C6-C7-C8-C10
22	V	307	CLA	C12-C13-C15-C16
22	P	302	CLA	C11-C12-C13-C15
22	P	303	CLA	C11-C10-C8-C7
22	P	305	CLA	C6-C7-C8-C10
22	Q	301	CLA	C11-C12-C13-C15
22	Q	304	CLA	C11-C12-C13-C15
22	Q	306	CLA	C6-C7-C8-C10
22	U	305	CLA	C6-C7-C8-C10
22	N	302	CLA	C12-C13-C15-C16
22	G	301	CLA	C6-C7-C8-C10
22	G	301	CLA	C11-C12-C13-C15
22	G	302	CLA	C11-C10-C8-C7
22	G	302	CLA	C12-C13-C15-C16
22	G	306	CLA	C11-C10-C8-C7
22	G	307	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	u	305	CLA	C6-C7-C8-C10
22	u	307	CLA	C12-C13-C15-C16
22	n	302	CLA	C12-C13-C15-C16
22	n	304	CLA	C11-C12-C13-C15
22	g	301	CLA	C6-C7-C8-C10
22	g	301	CLA	C12-C13-C15-C16
22	g	307	CLA	C12-C13-C15-C16
22	R	307	CLA	C12-C13-C15-C16
22	C	508	CLA	C12-C13-C15-C16
22	C	509	CLA	C12-C13-C15-C16
22	C	512	CLA	C6-C7-C8-C10
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C6-C7-C8-C10
22	B	605	CLA	C6-C7-C8-C10
22	B	605	CLA	C11-C10-C8-C7
22	B	608	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7
22	B	615	CLA	C6-C7-C8-C10
22	B	616	CLA	C6-C7-C8-C10
22	b	602	CLA	C12-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	b	610	CLA	C6-C7-C8-C10
22	b	616	CLA	C11-C12-C13-C15
22	b	617	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	c	508	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C15
22	s	301	CLA	C11-C12-C13-C15
26	r	614	CHL	C11-C12-C13-C15
26	r	614	CHL	C12-C13-C15-C16
26	1	316	CHL	C12-C13-C15-C16
26	1	317	CHL	C11-C12-C13-C15
26	2	313	CHL	C11-C12-C13-C15
26	2	316	CHL	C11-C10-C8-C7
26	3	311	CHL	C11-C12-C13-C15
26	3	311	CHL	C12-C13-C15-C16
26	4	313	CHL	C11-C12-C13-C15
26	4	317	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	5	318	CHL	C11-C12-C13-C15
26	5	318	CHL	C12-C13-C15-C16
26	6	312	CHL	C12-C13-C15-C16
26	6	316	CHL	C6-C7-C8-C10
26	6	316	CHL	C11-C12-C13-C15
26	v	313	CHL	C12-C13-C15-C16
26	v	318	CHL	C6-C7-C8-C10
26	p	314	CHL	C11-C12-C13-C15
26	p	320	CHL	C12-C13-C15-C16
26	q	311	CHL	C11-C12-C13-C15
26	q	314	CHL	C11-C12-C13-C15
26	q	315	CHL	C2-C3-C5-C6
26	V	318	CHL	C6-C7-C8-C10
26	P	317	CHL	C11-C10-C8-C7
26	P	317	CHL	C12-C13-C15-C16
26	Q	311	CHL	C11-C12-C13-C15
26	Q	315	CHL	C11-C10-C8-C7
26	Q	315	CHL	C12-C13-C15-C16
26	Q	316	CHL	C2-C3-C5-C6
26	U	313	CHL	C11-C12-C13-C15
26	U	315	CHL	C12-C13-C15-C16
26	U	316	CHL	C6-C7-C8-C10
26	N	313	CHL	C12-C13-C15-C16
26	N	317	CHL	C6-C7-C8-C10
26	N	317	CHL	C11-C12-C13-C15
26	u	316	CHL	C11-C12-C13-C15
26	u	318	CHL	C12-C13-C15-C16
26	n	318	CHL	C11-C12-C13-C15
26	g	311	CHL	C11-C12-C13-C15
26	g	314	CHL	C2-C3-C5-C6
26	g	315	CHL	C12-C13-C15-C16
26	R	315	CHL	C11-C12-C13-C15
26	R	315	CHL	C12-C13-C15-C16
26	4	317	CHL	O1A-CGA-O2A-C1
25	v	312	LHG	C29-C30-C31-C32
22	r	606	CLA	C10-C11-C12-C13
22	P	302	CLA	C10-C11-C12-C13
22	N	304	CLA	C13-C15-C16-C17
22	c	503	CLA	C8-C10-C11-C12
24	R	313	XAT	C13-C14-C15-C35
27	R	301	NEX	C29-C30-C31-C32
31	C	518	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	c	516	BCR	C15-C16-C17-C18
22	N	302	CLA	C16-C17-C18-C20
22	n	301	CLA	C16-C17-C18-C19
26	R	316	CHL	C6-C7-C8-C9
25	p	313	LHG	C16-C17-C18-C19
25	q	310	LHG	C28-C29-C30-C31
32	a	413	SQD	C29-C30-C31-C32
32	m	101	SQD	C26-C27-C28-C29
25	4	312	LHG	C13-C14-C15-C16
25	C	522	LHG	C11-C10-C9-C8
26	Q	316	CHL	C10-C11-C12-C13
26	G	316	CHL	C5-C6-C7-C8
26	v	316	CHL	O1A-CGA-O2A-C1
22	A	404	CLA	C2A-CAA-CBA-CGA
22	u	308	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	C2A-CAA-CBA-CGA
26	P	319	CHL	C2A-CAA-CBA-CGA
25	B	622	LHG	C29-C30-C31-C32
32	M	101	SQD	C26-C27-C28-C29
22	D	403	CLA	C5-C6-C7-C8
34	D	408	LMG	C30-C31-C32-C33
36	b	601	DGD	C2A-C3A-C4A-C5A
26	2	318	CHL	C3-C5-C6-C7
22	r	605	CLA	CBA-CGA-O2A-C1
22	q	307	CLA	CBA-CGA-O2A-C1
32	C	501	SQD	C24-C23-O48-C46
34	b	624	LMG	C29-C28-O8-C9
32	A	412	SQD	C29-C30-C31-C32
25	1	312	LHG	C19-C20-C21-C22
25	n	312	LHG	C29-C30-C31-C32
25	R	314	LHG	C15-C16-C17-C18
25	D	407	LHG	C28-C29-C30-C31
26	3	311	CHL	C5-C6-C7-C8
26	g	315	CHL	C10-C11-C12-C13
25	d	406	LHG	C28-C29-C30-C31
36	C	520	DGD	C9A-CAA-CBA-CCA
22	1	303	CLA	CAD-CBD-CGD-O2D
22	1	308	CLA	CAD-CBD-CGD-O2D
22	2	301	CLA	CAD-CBD-CGD-O2D
22	2	308	CLA	CAD-CBD-CGD-O2D
22	4	308	CLA	CAD-CBD-CGD-O2D
22	6	302	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	v	304	CLA	CAD-CBD-CGD-O2D
22	p	305	CLA	CAD-CBD-CGD-O2D
22	N	307	CLA	CAD-CBD-CGD-O2D
22	G	305	CLA	CAD-CBD-CGD-O2D
22	G	308	CLA	CAD-CBD-CGD-O2D
22	u	304	CLA	CAD-CBD-CGD-O2D
22	g	305	CLA	CAD-CBD-CGD-O2D
22	R	304	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	s	303	CLA	CAD-CBD-CGD-O2D
26	5	313	CHL	CAD-CBD-CGD-O2D
26	5	314	CHL	CAD-CBD-CGD-O2D
26	p	315	CHL	CAD-CBD-CGD-O2D
26	V	314	CHL	CAD-CBD-CGD-O2D
26	P	315	CHL	CAD-CBD-CGD-O2D
26	P	319	CHL	CAD-CBD-CGD-O2D
26	Q	316	CHL	CAD-CBD-CGD-O2D
26	U	313	CHL	CAD-CBD-CGD-O2D
26	u	313	CHL	CAD-CBD-CGD-O2D
22	6	306	CLA	C3-C5-C6-C7
22	1	301	CLA	C15-C16-C17-C18
36	J	101	DGD	CCA-CDA-CEA-CFA
25	c	522	LHG	O10-C23-O8-C6
26	U	317	CHL	O1A-CGA-O2A-C1
22	1	307	CLA	CBA-CGA-O2A-C1
22	2	306	CLA	CBA-CGA-O2A-C1
22	v	307	CLA	CBA-CGA-O2A-C1
26	p	320	CHL	CBA-CGA-O2A-C1
22	R	306	CLA	O1D-CGD-O2D-CED
22	d	402	CLA	C4-C3-C5-C6
22	6	305	CLA	C4-C3-C5-C6
22	p	302	CLA	C4-C3-C5-C6
26	6	301	CHL	C4-C3-C5-C6
33	d	404	PL9	C45-C44-C46-C47
33	D	405	PL9	C45-C44-C46-C47
22	n	302	CLA	C16-C17-C18-C20
26	R	316	CHL	C6-C7-C8-C10
34	W	201	LMG	C17-C18-C19-C20
36	C	520	DGD	O6D-C1D-O3G-C3G
22	b	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	5	317	CHL	C2-C3-C5-C6
26	6	301	CHL	C2-C3-C5-C6
33	D	405	PL9	C43-C44-C46-C47
25	2	312	LHG	C2-C3-O3-P
25	6	311	LHG	C4-C5-C6-O8
25	N	312	LHG	C4-C5-C6-O8
25	g	310	LHG	C4-C5-C6-O8
25	c	523	LHG	C2-C3-O3-P
26	r	616	CHL	O1A-CGA-O2A-C1
25	d	405	LHG	O6-C4-C5-O7
25	P	313	LHG	O6-C4-C5-O7
25	G	310	LHG	O6-C4-C5-O7
25	c	523	LHG	O6-C4-C5-O7
22	6	302	CLA	C5-C6-C7-C8
22	c	503	CLA	C10-C11-C12-C13
22	2	301	CLA	C2A-CAA-CBA-CGA
22	5	301	CLA	C2A-CAA-CBA-CGA
22	u	301	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C2A-CAA-CBA-CGA
34	b	624	LMG	O10-C28-O8-C9
26	u	316	CHL	C16-C17-C18-C20
25	u	312	LHG	O9-C7-O7-C5
22	r	609	CLA	CHA-CBD-CGD-O1D
22	r	609	CLA	CHA-CBD-CGD-O2D
22	r	610	CLA	CHA-CBD-CGD-O1D
22	r	610	CLA	CHA-CBD-CGD-O2D
22	2	301	CLA	CHA-CBD-CGD-O1D
22	5	306	CLA	CHA-CBD-CGD-O1D
22	5	306	CLA	CHA-CBD-CGD-O2D
22	6	307	CLA	CHA-CBD-CGD-O1D
22	v	306	CLA	CHA-CBD-CGD-O1D
22	v	306	CLA	CHA-CBD-CGD-O2D
22	v	308	CLA	CHA-CBD-CGD-O1D
22	v	308	CLA	CHA-CBD-CGD-O2D
22	p	304	CLA	CHA-CBD-CGD-O2D
22	q	303	CLA	CHA-CBD-CGD-O1D
22	q	303	CLA	CHA-CBD-CGD-O2D
22	q	305	CLA	CHA-CBD-CGD-O1D
22	q	305	CLA	CHA-CBD-CGD-O2D
22	V	308	CLA	CHA-CBD-CGD-O1D
22	V	308	CLA	CHA-CBD-CGD-O2D
22	Q	302	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	U	308	CLA	CHA-CBD-CGD-O2D
22	u	303	CLA	CHA-CBD-CGD-O1D
22	u	303	CLA	CHA-CBD-CGD-O2D
22	n	302	CLA	CHA-CBD-CGD-O1D
22	R	311	CLA	CHA-CBD-CGD-O1D
22	R	311	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	511	CLA	CHA-CBD-CGD-O1D
22	C	511	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O1D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	B	610	CLA	CHA-CBD-CGD-O1D
22	B	610	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
26	r	619	CHL	CHA-CBD-CGD-O1D
26	r	619	CHL	CHA-CBD-CGD-O2D
26	p	317	CHL	CHA-CBD-CGD-O2D
26	u	316	CHL	CHA-CBD-CGD-O2D
26	n	316	CHL	CHA-CBD-CGD-O1D
26	R	316	CHL	CHA-CBD-CGD-O2D
22	a	404	CLA	O1A-CGA-O2A-C1
25	u	312	LHG	O10-C23-O8-C6
25	C	523	LHG	O10-C23-O8-C6
26	u	318	CHL	O1A-CGA-O2A-C1
34	B	624	LMG	O10-C28-O8-C9
36	C	520	DGD	O1A-C1A-O1G-C1G
22	V	308	CLA	O2A-C1-C2-C3
22	n	308	CLA	O2A-C1-C2-C3
34	w	201	LMG	C2-C1-O1-C7
26	n	316	CHL	C15-C16-C17-C18
36	B	601	DGD	C2A-C3A-C4A-C5A
25	v	312	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
32	a	410	SQD	O6-C44-C45-O47
32	l	102	SQD	O47-C45-C46-O48
32	L	102	SQD	O47-C45-C46-O48
32	C	501	SQD	O6-C44-C45-O47
34	w	201	LMG	O1-C7-C8-O7
34	w	201	LMG	O7-C8-C9-O8
34	C	521	LMG	O1-C7-C8-O7
34	c	501	LMG	O1-C7-C8-O7
34	c	501	LMG	O7-C8-C9-O8
34	c	520	LMG	O1-C7-C8-O7
36	a	416	DGD	O1G-C1G-C2G-O2G
36	A	414	DGD	O1G-C1G-C2G-O2G
36	b	601	DGD	O2G-C2G-C3G-O3G
22	4	307	CLA	CBA-CGA-O2A-C1
25	2	312	LHG	C26-C27-C28-C29
26	3	311	CHL	O1D-CGD-O2D-CED
22	d	402	CLA	C5-C6-C7-C8
22	G	306	CLA	C10-C11-C12-C13
22	g	306	CLA	C5-C6-C7-C8
26	Q	316	CHL	C5-C6-C7-C8
26	u	313	CHL	C10-C11-C12-C13
22	A	404	CLA	O1A-CGA-O2A-C1
22	A	406	CLA	O1A-CGA-O2A-C1
22	3	303	CLA	O1A-CGA-O2A-C1
22	G	305	CLA	O1A-CGA-O2A-C1
26	V	316	CHL	O1A-CGA-O2A-C1
25	3	310	LHG	O1-C1-C2-O2
25	d	405	LHG	C31-C32-C33-C34
36	A	414	DGD	C9B-CAB-CBB-CCB
22	a	404	CLA	C3-C5-C6-C7
22	Q	305	CLA	C4-C3-C5-C6
26	N	317	CHL	C4-C3-C5-C6
26	n	317	CHL	C4-C3-C5-C6
26	R	316	CHL	C4-C3-C5-C6
25	L	101	LHG	C24-C25-C26-C27
22	g	303	CLA	O1A-CGA-O2A-C1
25	N	312	LHG	O10-C23-O8-C6
26	n	317	CHL	C2-C3-C5-C6
26	R	316	CHL	C2-C3-C5-C6
33	d	404	PL9	C43-C44-C46-C47
33	d	404	PL9	C4-C3-C7-C8
33	D	405	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
25	D	406	LHG	C11-C12-C13-C14
36	c	518	DGD	C9A-CAA-CBA-CCA
25	U	312	LHG	O9-C7-O7-C5
22	2	305	CLA	C10-C11-C12-C13
22	1	306	CLA	C11-C10-C8-C9
22	3	307	CLA	C14-C13-C15-C16
22	q	304	CLA	C6-C7-C8-C9
22	q	304	CLA	C11-C10-C8-C9
22	q	305	CLA	C11-C10-C8-C9
22	q	306	CLA	C6-C7-C8-C9
22	U	307	CLA	C14-C13-C15-C16
22	N	305	CLA	C6-C7-C8-C9
22	g	301	CLA	C6-C7-C8-C9
22	g	301	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
26	3	314	CHL	C11-C10-C8-C9
26	6	301	CHL	C14-C13-C15-C16
26	6	315	CHL	C11-C10-C8-C9
26	n	313	CHL	C6-C7-C8-C9
26	g	315	CHL	C11-C12-C13-C14
32	M	101	SQD	C45-C46-O48-C23
36	C	519	DGD	C4D-C5D-C6D-O5D
25	C	523	LHG	C17-C18-C19-C20
32	a	410	SQD	C27-C28-C29-C30
32	C	501	SQD	C14-C15-C16-C17
32	a	413	SQD	C5-C6-S-O8
32	m	101	SQD	C4-C5-C6-S
32	M	101	SQD	C4-C5-C6-S
25	l	101	LHG	C24-C25-C26-C27
25	V	312	LHG	C9-C10-C11-C12
26	3	313	CHL	C2A-CAA-CBA-CGA
26	P	319	CHL	C10-C11-C12-C13
22	Q	307	CLA	O1A-CGA-O2A-C1
27	N	318	NEX	C31-C32-C33-C40
31	B	618	BCR	C7-C8-C9-C34
32	m	101	SQD	C45-C46-O48-C23
25	v	312	LHG	C31-C32-C33-C34
22	u	305	CLA	C8-C10-C11-C12
22	B	612	CLA	C8-C10-C11-C12
34	c	501	LMG	C35-C36-C37-C38
23	N	309	LUT	C31-C32-C33-C34
23	n	310	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	a	408	CLA	C1A-C2A-CAA-CBA
22	1	301	CLA	C1A-C2A-CAA-CBA
22	3	304	CLA	C1A-C2A-CAA-CBA
22	4	301	CLA	C1A-C2A-CAA-CBA
22	v	301	CLA	C1A-C2A-CAA-CBA
22	P	302	CLA	C1A-C2A-CAA-CBA
22	U	301	CLA	C1A-C2A-CAA-CBA
22	N	301	CLA	C1A-C2A-CAA-CBA
22	u	301	CLA	C1A-C2A-CAA-CBA
22	u	304	CLA	C1A-C2A-CAA-CBA
22	g	301	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
26	v	318	CHL	C1A-C2A-CAA-CBA
26	p	319	CHL	C1A-C2A-CAA-CBA
32	a	413	SQD	C23-C24-C25-C26
22	u	302	CLA	C15-C16-C17-C18
26	1	318	CHL	C5-C6-C7-C8
26	2	313	CHL	C13-C15-C16-C17
22	Q	303	CLA	CBD-CGD-O2D-CED
25	v	312	LHG	C24-C23-O8-C6
26	v	315	CHL	CBA-CGA-O2A-C1
26	q	315	CHL	CBA-CGA-O2A-C1
34	b	624	LMG	C21-C22-C23-C24
36	J	101	DGD	C3A-C4A-C5A-C6A
22	2	306	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	C15-C16-C17-C18
26	G	311	CHL	C5-C6-C7-C8
25	d	406	LHG	C3-O3-P-O6
26	P	319	CHL	CBD-CGD-O2D-CED
22	B	608	CLA	C4-C3-C5-C6
26	v	316	CHL	C4-C3-C5-C6
22	G	305	CLA	C3-C5-C6-C7
22	S	306	CLA	C3-C5-C6-C7
22	C	515	CLA	C3-C5-C6-C7
25	r	613	LHG	C2-C3-O3-P
25	C	523	LHG	C2-C3-O3-P
25	b	623	LHG	C15-C16-C17-C18
25	c	521	LHG	C25-C26-C27-C28
34	w	201	LMG	C12-C13-C14-C15
26	p	320	CHL	O1A-CGA-O2A-C1
22	g	306	CLA	C4B-C3B-CAB-CBB
22	C	510	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C4B-C3B-CAB-CBB
25	r	613	LHG	C3-O3-P-O5
25	a	415	LHG	C3-O3-P-O4
25	a	415	LHG	C3-O3-P-O5
25	d	405	LHG	C4-O6-P-O4
25	d	405	LHG	C4-O6-P-O5
25	d	406	LHG	C4-O6-P-O5
25	l	101	LHG	C4-O6-P-O5
25	A	413	LHG	C3-O3-P-O4
25	A	413	LHG	C3-O3-P-O5
25	L	101	LHG	C4-O6-P-O5
25	v	312	LHG	C3-O3-P-O5
25	U	312	LHG	C4-O6-P-O4
25	U	312	LHG	C4-O6-P-O5
25	u	312	LHG	C4-O6-P-O4
25	u	312	LHG	C4-O6-P-O5
25	C	523	LHG	C3-O3-P-O4
25	C	523	LHG	C3-O3-P-O5
25	C	523	LHG	C4-O6-P-O4
25	C	523	LHG	C4-O6-P-O5
25	B	622	LHG	C3-O3-P-O4
25	B	623	LHG	C3-O3-P-O5
25	D	406	LHG	C3-O3-P-O5
25	D	406	LHG	C4-O6-P-O4
25	D	406	LHG	C4-O6-P-O5
25	D	407	LHG	C4-O6-P-O5
25	b	623	LHG	C3-O3-P-O5
25	c	522	LHG	C3-O3-P-O5
25	c	522	LHG	C4-O6-P-O4
25	c	522	LHG	C4-O6-P-O5
25	c	523	LHG	C4-O6-P-O5
26	r	615	CHL	C4B-C3B-CAB-CBB
26	r	619	CHL	C4B-C3B-CAB-CBB
26	1	314	CHL	C4B-C3B-CAB-CBB
26	1	316	CHL	C4B-C3B-CAB-CBB
26	1	317	CHL	C4B-C3B-CAB-CBB
26	1	318	CHL	C4B-C3B-CAB-CBB
26	2	315	CHL	C4B-C3B-CAB-CBB
26	2	316	CHL	C4B-C3B-CAB-CBB
26	2	317	CHL	C4B-C3B-CAB-CBB
26	2	318	CHL	C4B-C3B-CAB-CBB
26	3	314	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	3	315	CHL	C4B-C3B-CAB-CBB
26	3	316	CHL	C4B-C3B-CAB-CBB
26	4	313	CHL	C4B-C3B-CAB-CBB
26	4	314	CHL	C4B-C3B-CAB-CBB
26	4	316	CHL	C4B-C3B-CAB-CBB
26	4	317	CHL	C4B-C3B-CAB-CBB
26	5	314	CHL	C4B-C3B-CAB-CBB
26	5	315	CHL	C4B-C3B-CAB-CBB
26	5	316	CHL	C4B-C3B-CAB-CBB
26	5	317	CHL	C4B-C3B-CAB-CBB
26	5	318	CHL	C4B-C3B-CAB-CBB
26	6	301	CHL	C4B-C3B-CAB-CBB
26	6	315	CHL	C4B-C3B-CAB-CBB
26	6	317	CHL	C4B-C3B-CAB-CBB
26	v	314	CHL	C4B-C3B-CAB-CBB
26	v	316	CHL	C4B-C3B-CAB-CBB
26	v	318	CHL	C4B-C3B-CAB-CBB
26	p	316	CHL	C4B-C3B-CAB-CBB
26	p	317	CHL	C4B-C3B-CAB-CBB
26	p	319	CHL	C4B-C3B-CAB-CBB
26	q	312	CHL	C4B-C3B-CAB-CBB
26	q	313	CHL	C4B-C3B-CAB-CBB
26	V	314	CHL	C4B-C3B-CAB-CBB
26	V	316	CHL	C4B-C3B-CAB-CBB
26	V	318	CHL	C4B-C3B-CAB-CBB
26	P	314	CHL	C4B-C3B-CAB-CBB
26	P	315	CHL	C4B-C3B-CAB-CBB
26	P	316	CHL	C4B-C3B-CAB-CBB
26	P	317	CHL	C4B-C3B-CAB-CBB
26	P	319	CHL	C4B-C3B-CAB-CBB
26	Q	312	CHL	C4B-C3B-CAB-CBB
26	Q	313	CHL	C4B-C3B-CAB-CBB
26	Q	314	CHL	C4B-C3B-CAB-CBB
26	U	313	CHL	C4B-C3B-CAB-CBB
26	U	315	CHL	C4B-C3B-CAB-CBB
26	U	316	CHL	C4B-C3B-CAB-CBB
26	U	317	CHL	C4B-C3B-CAB-CBB
26	U	319	CHL	C4B-C3B-CAB-CBB
26	N	316	CHL	C4B-C3B-CAB-CBB
26	G	312	CHL	C4B-C3B-CAB-CBB
26	G	314	CHL	C4B-C3B-CAB-CBB
26	G	316	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	u	313	CHL	C4B-C3B-CAB-CBB
26	u	314	CHL	C4B-C3B-CAB-CBB
26	u	317	CHL	C4B-C3B-CAB-CBB
26	n	313	CHL	C4B-C3B-CAB-CBB
26	g	312	CHL	C4B-C3B-CAB-CBB
26	g	314	CHL	C4B-C3B-CAB-CBB
26	g	316	CHL	C4B-C3B-CAB-CBB
26	R	316	CHL	C4B-C3B-CAB-CBB
26	S	314	CHL	C4B-C3B-CAB-CBB
26	S	316	CHL	C4B-C3B-CAB-CBB
26	s	314	CHL	C4B-C3B-CAB-CBB
26	s	316	CHL	C4B-C3B-CAB-CBB
22	5	304	CLA	C16-C17-C18-C20
22	q	307	CLA	C16-C17-C18-C20
22	u	305	CLA	C11-C12-C13-C14
26	q	315	CHL	C11-C12-C13-C15
34	c	520	LMG	C10-C11-C12-C13
32	a	410	SQD	C14-C15-C16-C17
34	w	201	LMG	O6-C1-O1-C7
22	a	406	CLA	CBA-CGA-O2A-C1
22	6	308	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	CBA-CGA-O2A-C1
25	L	101	LHG	C24-C23-O8-C6
25	1	312	LHG	O6-C4-C5-C6
25	4	312	LHG	O6-C4-C5-C6
25	5	312	LHG	O6-C4-C5-C6
25	P	313	LHG	O6-C4-C5-C6
25	U	312	LHG	O6-C4-C5-C6
25	N	312	LHG	O6-C4-C5-C6
25	u	312	LHG	O6-C4-C5-C6
25	n	312	LHG	O6-C4-C5-C6
25	R	314	LHG	O6-C4-C5-C6
22	r	605	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	O47-C7-C8-C9
22	S	309	CLA	C2A-CAA-CBA-CGA
22	A	404	CLA	C3-C5-C6-C7
25	q	310	LHG	C26-C27-C28-C29
25	D	406	LHG	C25-C26-C27-C28
36	J	101	DGD	C3B-C4B-C5B-C6B
25	C	522	LHG	C8-C7-O7-C5
22	b	604	CLA	C16-C17-C18-C19
25	P	313	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
22	1	302	CLA	CAD-CBD-CGD-O1D
22	4	302	CLA	CAD-CBD-CGD-O1D
22	6	303	CLA	CAD-CBD-CGD-O1D
22	v	306	CLA	CAD-CBD-CGD-O1D
22	v	308	CLA	CAD-CBD-CGD-O1D
22	p	304	CLA	CAD-CBD-CGD-O1D
22	q	302	CLA	CAD-CBD-CGD-O1D
22	q	303	CLA	CAD-CBD-CGD-O1D
22	q	308	CLA	CAD-CBD-CGD-O1D
22	V	308	CLA	CAD-CBD-CGD-O1D
22	Q	302	CLA	CAD-CBD-CGD-O1D
22	Q	303	CLA	CAD-CBD-CGD-O1D
22	Q	308	CLA	CAD-CBD-CGD-O1D
22	G	303	CLA	CAD-CBD-CGD-O1D
22	n	302	CLA	CAD-CBD-CGD-O1D
22	n	303	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	511	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	510	CLA	CAD-CBD-CGD-O1D
26	r	619	CHL	CAD-CBD-CGD-O1D
26	2	314	CHL	CAD-CBD-CGD-O1D
26	g	312	CHL	CAD-CBD-CGD-O1D
27	2	319	NEX	C7-C8-C9-C10
27	V	319	NEX	C7-C8-C9-C10
30	a	407	PHO	CAD-CBD-CGD-O1D
30	A	407	PHO	CAD-CBD-CGD-O1D
32	l	102	SQD	C5-C6-S-O7
32	L	102	SQD	C5-C6-S-O7
32	C	501	SQD	C5-C6-S-O9
36	c	517	DGD	C4D-C5D-C6D-O5D
25	B	623	LHG	O7-C7-C8-C9
22	B	610	CLA	C15-C16-C17-C18
25	P	313	LHG	C31-C32-C33-C34
36	a	416	DGD	CAB-CBB-CCB-CDB
25	R	314	LHG	C12-C13-C14-C15
26	G	314	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C15-C16-C17-C18
26	P	319	CHL	O1D-CGD-O2D-CED
25	P	313	LHG	C24-C23-O8-C6
25	U	312	LHG	C24-C23-O8-C6
26	6	316	CHL	CBA-CGA-O2A-C1
26	u	315	CHL	CBA-CGA-O2A-C1
22	c	513	CLA	CAA-CBA-CGA-O2A
22	d	402	CLA	O1D-CGD-O2D-CED
25	C	522	LHG	O9-C7-O7-C5
25	p	313	LHG	C27-C28-C29-C30
22	C	507	CLA	C4-C3-C5-C6
22	c	506	CLA	C4-C3-C5-C6
22	r	609	CLA	C3A-C2A-CAA-CBA
22	1	307	CLA	C6-C7-C8-C10
22	2	302	CLA	C12-C13-C15-C16
22	2	304	CLA	C12-C13-C15-C16
22	3	307	CLA	C11-C10-C8-C7
22	3	307	CLA	C12-C13-C15-C16
22	4	302	CLA	C12-C13-C15-C16
22	4	304	CLA	C11-C10-C8-C7
22	6	308	CLA	C11-C10-C8-C7
22	q	304	CLA	C6-C7-C8-C10
22	q	305	CLA	C11-C10-C8-C7
22	P	303	CLA	C6-C7-C8-C10
22	P	307	CLA	C6-C7-C8-C10
22	U	302	CLA	C6-C7-C8-C10
22	U	307	CLA	C12-C13-C15-C16
22	u	302	CLA	C12-C13-C15-C16
22	g	305	CLA	C6-C7-C8-C10
22	C	509	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C12-C13-C15
22	b	615	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	c	510	CLA	C6-C7-C8-C10
22	c	511	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C10-C8-C7
25	r	613	LHG	O6-C4-C5-O7
25	l	101	LHG	O6-C4-C5-O7
25	L	101	LHG	O6-C4-C5-O7
25	1	312	LHG	O6-C4-C5-O7
25	5	312	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
25	q	310	LHG	O6-C4-C5-O7
25	Q	310	LHG	C7-C8-C9-C10
25	g	310	LHG	O6-C4-C5-O7
26	1	316	CHL	C11-C10-C8-C7
26	1	318	CHL	C11-C12-C13-C15
26	2	317	CHL	C11-C12-C13-C15
26	2	318	CHL	C11-C12-C13-C15
26	3	314	CHL	C12-C13-C15-C16
26	3	315	CHL	C12-C13-C15-C16
26	5	313	CHL	C11-C12-C13-C15
26	5	317	CHL	C11-C12-C13-C15
26	6	301	CHL	C12-C13-C15-C16
26	6	312	CHL	C11-C12-C13-C15
26	v	316	CHL	C11-C10-C8-C7
26	p	317	CHL	C12-C13-C15-C16
26	p	318	CHL	C6-C7-C8-C10
26	p	319	CHL	C11-C12-C13-C15
26	P	314	CHL	C11-C12-C13-C15
26	P	318	CHL	C6-C7-C8-C10
26	Q	314	CHL	C12-C13-C15-C16
26	u	317	CHL	C6-C7-C8-C10
26	u	318	CHL	C6-C7-C8-C10
26	n	313	CHL	C12-C13-C15-C16
26	g	315	CHL	C11-C12-C13-C15
30	d	401	PHO	C11-C12-C13-C15
30	D	401	PHO	C11-C12-C13-C15
25	N	312	LHG	C14-C15-C16-C17
34	A	411	LMG	C32-C33-C34-C35
22	c	507	CLA	C3-C5-C6-C7
23	N	310	LUT	C29-C30-C31-C32
25	2	312	LHG	C27-C28-C29-C30
25	C	524	LHG	C33-C34-C35-C36
25	B	622	LHG	C13-C14-C15-C16
22	C	515	CLA	C10-C11-C12-C13
26	p	317	CHL	C5-C6-C7-C8
36	C	519	DGD	C1A-C2A-C3A-C4A
26	S	314	CHL	O1D-CGD-O2D-CED
26	s	314	CHL	O1D-CGD-O2D-CED
25	2	312	LHG	C8-C7-O7-C5
25	s	312	LHG	C8-C7-O7-C5
25	c	523	LHG	C26-C27-C28-C29
25	U	312	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
26	v	315	CHL	O1A-CGA-O2A-C1
25	2	312	LHG	O2-C2-C3-O3
25	4	312	LHG	C9-C10-C11-C12
25	U	312	LHG	C29-C30-C31-C32
25	D	407	LHG	C35-C36-C37-C38
26	g	311	CHL	C5-C6-C7-C8
22	p	308	CLA	C2A-CAA-CBA-CGA
26	q	313	CHL	C2A-CAA-CBA-CGA
22	u	305	CLA	C11-C12-C13-C15
22	4	306	CLA	C3-C5-C6-C7
26	3	315	CHL	C3-C5-C6-C7
36	C	520	DGD	O6D-C5D-C6D-O5D
22	P	309	CLA	O2A-C1-C2-C3
25	5	312	LHG	C4-C5-C6-O8
25	B	622	LHG	C12-C13-C14-C15
26	r	615	CHL	C1C-C2C-CMC-OMC
26	1	314	CHL	C1C-C2C-CMC-OMC
26	1	316	CHL	C1C-C2C-CMC-OMC
26	1	318	CHL	C1C-C2C-CMC-OMC
26	2	318	CHL	C1C-C2C-CMC-OMC
26	4	314	CHL	C1C-C2C-CMC-OMC
26	4	317	CHL	C1C-C2C-CMC-OMC
26	5	313	CHL	C1C-C2C-CMC-OMC
26	5	318	CHL	C1C-C2C-CMC-OMC
26	6	301	CHL	C1C-C2C-CMC-OMC
26	v	313	CHL	C1C-C2C-CMC-OMC
26	v	314	CHL	C1C-C2C-CMC-OMC
26	p	314	CHL	C1C-C2C-CMC-OMC
26	p	318	CHL	C1C-C2C-CMC-OMC
26	q	312	CHL	C1C-C2C-CMC-OMC
26	q	313	CHL	C1C-C2C-CMC-OMC
26	q	314	CHL	C1C-C2C-CMC-OMC
26	V	313	CHL	C1C-C2C-CMC-OMC
26	V	314	CHL	C1C-C2C-CMC-OMC
26	V	316	CHL	C1C-C2C-CMC-OMC
26	V	317	CHL	C1C-C2C-CMC-OMC
26	V	318	CHL	C1C-C2C-CMC-OMC
26	P	314	CHL	C1C-C2C-CMC-OMC
26	P	318	CHL	C1C-C2C-CMC-OMC
26	P	319	CHL	C1C-C2C-CMC-OMC
26	Q	312	CHL	C1C-C2C-CMC-OMC
26	Q	313	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
26	Q	314	CHL	C1C-C2C-CMC-OMC
26	U	313	CHL	C1C-C2C-CMC-OMC
26	N	313	CHL	C1C-C2C-CMC-OMC
26	G	311	CHL	C1C-C2C-CMC-OMC
26	G	313	CHL	C1C-C2C-CMC-OMC
26	G	315	CHL	C1C-C2C-CMC-OMC
26	n	314	CHL	C1C-C2C-CMC-OMC
26	g	313	CHL	C1C-C2C-CMC-OMC
26	g	314	CHL	C1C-C2C-CMC-OMC
26	R	316	CHL	C1C-C2C-CMC-OMC
26	S	315	CHL	C1C-C2C-CMC-OMC
26	S	316	CHL	C1C-C2C-CMC-OMC
26	s	315	CHL	C1C-C2C-CMC-OMC
26	s	316	CHL	C1C-C2C-CMC-OMC
34	W	201	LMG	O1-C7-C8-C9
36	B	601	DGD	C1G-C2G-C3G-O3G
36	b	601	DGD	C1G-C2G-C3G-O3G
25	6	311	LHG	O7-C5-C6-O8
25	p	313	LHG	O7-C5-C6-O8
25	Q	310	LHG	O7-C5-C6-O8
34	d	407	LMG	O7-C8-C9-O8
34	W	201	LMG	O1-C7-C8-O7
34	W	201	LMG	O7-C8-C9-O8
34	C	502	LMG	O7-C8-C9-O8
34	C	521	LMG	O7-C8-C9-O8
34	D	408	LMG	O7-C8-C9-O8
34	c	520	LMG	O7-C8-C9-O8
36	B	601	DGD	O2G-C2G-C3G-O3G
34	B	621	LMG	C16-C17-C18-C19
25	v	312	LHG	O10-C23-O8-C6
26	q	315	CHL	O1A-CGA-O2A-C1
22	V	304	CLA	C8-C10-C11-C12
22	N	304	CLA	C15-C16-C17-C18
26	3	316	CHL	C10-C11-C12-C13
26	p	319	CHL	C5-C6-C7-C8
36	c	518	DGD	C3B-C4B-C5B-C6B
36	c	519	DGD	C3B-C4B-C5B-C6B
25	S	312	LHG	C2-C3-O3-P
25	s	312	LHG	C2-C3-O3-P
25	b	623	LHG	C12-C13-C14-C15
22	q	307	CLA	O1A-CGA-O2A-C1
26	r	619	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	P	305	CLA	C5-C6-C7-C8
26	g	311	CHL	C15-C16-C17-C18
22	6	303	CLA	C4-C3-C5-C6
26	p	317	CHL	C4-C3-C5-C6
26	G	314	CHL	C4-C3-C5-C6
22	n	307	CLA	CBA-CGA-O2A-C1
22	C	506	CLA	CBA-CGA-O2A-C1
26	r	619	CHL	CBA-CGA-O2A-C1
22	g	304	CLA	C2-C3-C5-C6
26	N	317	CHL	C2-C3-C5-C6
22	1	308	CLA	O1D-CGD-O2D-CED
22	C	514	CLA	CAA-CBA-CGA-O2A
32	A	412	SQD	O47-C7-C8-C9
25	U	312	LHG	C32-C33-C34-C35
36	b	601	DGD	C6B-C7B-C8B-C9B
22	v	301	CLA	C10-C11-C12-C13
22	U	305	CLA	C8-C10-C11-C12
22	r	606	CLA	C11-C10-C8-C9
22	5	304	CLA	C6-C7-C8-C9
22	6	302	CLA	C6-C7-C8-C9
22	6	308	CLA	C14-C13-C15-C16
22	Q	301	CLA	C11-C12-C13-C14
22	Q	305	CLA	C11-C10-C8-C9
22	G	302	CLA	C11-C10-C8-C9
22	G	302	CLA	C14-C13-C15-C16
22	n	302	CLA	C11-C10-C8-C9
22	n	306	CLA	C11-C10-C8-C9
22	R	307	CLA	C11-C10-C8-C9
22	C	507	CLA	C6-C7-C8-C9
22	B	604	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	607	CLA	C6-C7-C8-C9
22	B	610	CLA	C14-C13-C15-C16
22	B	612	CLA	C6-C7-C8-C9
22	B	616	CLA	C6-C7-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C12-C13-C14
22	c	502	CLA	C11-C10-C8-C9
22	c	508	CLA	C14-C13-C15-C16
26	r	614	CHL	C14-C13-C15-C16
26	1	313	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	1	316	CHL	C14-C13-C15-C16
26	Q	314	CHL	C14-C13-C15-C16
26	Q	315	CHL	C14-C13-C15-C16
26	N	313	CHL	C14-C13-C15-C16
26	N	317	CHL	C11-C10-C8-C9
26	G	315	CHL	C14-C13-C15-C16
26	n	317	CHL	C6-C7-C8-C9
26	n	318	CHL	C11-C12-C13-C14
22	a	406	CLA	O1A-CGA-O2A-C1
26	s	314	CHL	CBD-CGD-O2D-CED
34	b	621	LMG	O9-C10-O7-C8
32	a	410	SQD	C18-C19-C20-C21
26	6	316	CHL	O1A-CGA-O2A-C1
22	5	306	CLA	C2A-CAA-CBA-CGA
25	P	313	LHG	O1-C1-C2-O2
25	5	312	LHG	C16-C17-C18-C19
32	C	501	SQD	C18-C19-C20-C21
26	g	312	CHL	O1D-CGD-O2D-CED
25	q	310	LHG	C30-C31-C32-C33
25	b	622	LHG	C29-C30-C31-C32
26	g	315	CHL	C3-C5-C6-C7
22	B	604	CLA	C15-C16-C17-C18
26	R	317	CHL	C10-C11-C12-C13
25	q	310	LHG	C27-C28-C29-C30
36	c	519	DGD	C3A-C4A-C5A-C6A
25	U	312	LHG	C30-C31-C32-C33
22	r	602	CLA	C2B-C3B-CAB-CBB
22	r	606	CLA	C2B-C3B-CAB-CBB
22	3	303	CLA	C2B-C3B-CAB-CBB
22	v	306	CLA	C2B-C3B-CAB-CBB
22	p	304	CLA	C2B-C3B-CAB-CBB
22	p	305	CLA	C2B-C3B-CAB-CBB
22	p	306	CLA	C2B-C3B-CAB-CBB
22	q	301	CLA	C2B-C3B-CAB-CBB
22	q	303	CLA	C2B-C3B-CAB-CBB
22	V	303	CLA	C2B-C3B-CAB-CBB
22	P	302	CLA	C2B-C3B-CAB-CBB
22	P	305	CLA	C2B-C3B-CAB-CBB
22	Q	301	CLA	C2B-C3B-CAB-CBB
22	Q	307	CLA	C2B-C3B-CAB-CBB
22	U	302	CLA	C2B-C3B-CAB-CBB
22	U	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	N	303	CLA	C2B-C3B-CAB-CBB
22	N	304	CLA	C2B-C3B-CAB-CBB
22	u	301	CLA	C2B-C3B-CAB-CBB
22	u	305	CLA	C2B-C3B-CAB-CBB
22	n	307	CLA	C2B-C3B-CAB-CBB
22	g	306	CLA	C2B-C3B-CAB-CBB
22	R	303	CLA	C2B-C3B-CAB-CBB
22	R	304	CLA	C2B-C3B-CAB-CBB
22	R	307	CLA	C2B-C3B-CAB-CBB
22	R	310	CLA	C2B-C3B-CAB-CBB
22	S	305	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C2B-C3B-CAB-CBB
22	C	504	CLA	C2B-C3B-CAB-CBB
22	B	604	CLA	C2B-C3B-CAB-CBB
22	B	611	CLA	C2B-C3B-CAB-CBB
22	B	615	CLA	C2B-C3B-CAB-CBB
22	b	604	CLA	C2B-C3B-CAB-CBB
22	b	611	CLA	C2B-C3B-CAB-CBB
22	b	615	CLA	C2B-C3B-CAB-CBB
22	c	503	CLA	C2B-C3B-CAB-CBB
26	1	318	CHL	C2B-C3B-CAB-CBB
26	2	316	CHL	C2B-C3B-CAB-CBB
26	3	312	CHL	C2B-C3B-CAB-CBB
26	3	316	CHL	C2B-C3B-CAB-CBB
26	4	316	CHL	C2B-C3B-CAB-CBB
26	4	317	CHL	C2B-C3B-CAB-CBB
26	5	316	CHL	C2B-C3B-CAB-CBB
26	5	318	CHL	C2B-C3B-CAB-CBB
26	6	301	CHL	C2B-C3B-CAB-CBB
26	6	317	CHL	C2B-C3B-CAB-CBB
26	v	316	CHL	C2B-C3B-CAB-CBB
26	v	318	CHL	C2B-C3B-CAB-CBB
26	p	317	CHL	C2B-C3B-CAB-CBB
26	p	319	CHL	C2B-C3B-CAB-CBB
26	q	312	CHL	C2B-C3B-CAB-CBB
26	V	316	CHL	C2B-C3B-CAB-CBB
26	P	314	CHL	C2B-C3B-CAB-CBB
26	P	317	CHL	C2B-C3B-CAB-CBB
26	Q	313	CHL	C2B-C3B-CAB-CBB
26	Q	314	CHL	C2B-C3B-CAB-CBB
26	Q	316	CHL	C2B-C3B-CAB-CBB
26	U	316	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	U	317	CHL	C2B-C3B-CAB-CBB
26	G	312	CHL	C2B-C3B-CAB-CBB
26	G	314	CHL	C2B-C3B-CAB-CBB
26	u	314	CHL	C2B-C3B-CAB-CBB
26	g	312	CHL	C2B-C3B-CAB-CBB
26	g	314	CHL	C2B-C3B-CAB-CBB
26	S	314	CHL	C2B-C3B-CAB-CBB
26	S	315	CHL	C2B-C3B-CAB-CBB
26	s	314	CHL	C2B-C3B-CAB-CBB
25	2	312	LHG	O9-C7-O7-C5
34	b	624	LMG	C13-C14-C15-C16
26	u	315	CHL	O1A-CGA-O2A-C1
22	Q	305	CLA	C2-C3-C5-C6
26	n	313	CHL	C16-C17-C18-C20
22	G	306	CLA	C8-C10-C11-C12
22	r	601	CLA	C1-C2-C3-C4
22	r	607	CLA	C1-C2-C3-C4
22	r	608	CLA	C1-C2-C3-C4
22	R	302	CLA	C1-C2-C3-C4
22	R	308	CLA	C1-C2-C3-C4
22	R	309	CLA	C1-C2-C3-C4
22	S	307	CLA	C1-C2-C3-C4
22	s	307	CLA	C1-C2-C3-C4
26	1	315	CHL	C1-C2-C3-C4
26	2	315	CHL	C1-C2-C3-C4
26	3	313	CHL	C1-C2-C3-C4
26	4	315	CHL	C1-C2-C3-C4
26	5	315	CHL	C1-C2-C3-C4
26	6	314	CHL	C1-C2-C3-C4
26	v	315	CHL	C1-C2-C3-C4
26	p	316	CHL	C1-C2-C3-C4
26	q	313	CHL	C1-C2-C3-C4
26	V	315	CHL	C1-C2-C3-C4
26	P	316	CHL	C1-C2-C3-C4
26	Q	313	CHL	C1-C2-C3-C4
26	U	314	CHL	C1-C2-C3-C4
26	N	315	CHL	C1-C2-C3-C4
26	G	313	CHL	C1-C2-C3-C4
26	u	315	CHL	C1-C2-C3-C4
26	n	315	CHL	C1-C2-C3-C4
26	g	313	CHL	C1-C2-C3-C4
25	P	313	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
26	u	314	CHL	O1A-CGA-O2A-C1
25	G	310	LHG	C9-C10-C11-C12
22	B	615	CLA	C5-C6-C7-C8
25	a	415	LHG	C4-C5-O7-C7
25	A	413	LHG	C4-C5-O7-C7
25	2	312	LHG	O6-C4-C5-C6
25	p	313	LHG	O6-C4-C5-C6
25	a	415	LHG	C1-C2-C3-O3
25	A	413	LHG	C1-C2-C3-O3
22	r	606	CLA	C2A-CAA-CBA-CGA
22	Q	308	CLA	C2A-CAA-CBA-CGA
22	U	304	CLA	C2A-CAA-CBA-CGA
22	u	304	CLA	C2A-CAA-CBA-CGA
22	R	307	CLA	C2A-CAA-CBA-CGA
22	S	304	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	C2A-CAA-CBA-CGA
22	b	604	CLA	C2A-CAA-CBA-CGA
22	s	309	CLA	C2A-CAA-CBA-CGA
26	P	318	CHL	C2A-CAA-CBA-CGA
26	g	315	CHL	C2A-CAA-CBA-CGA
25	6	311	LHG	O9-C7-O7-C5
25	q	310	LHG	O9-C7-O7-C5
25	s	312	LHG	O9-C7-O7-C5
22	P	303	CLA	C13-C15-C16-C17
22	d	402	CLA	C2-C1-O2A-CGA
22	6	305	CLA	C2-C1-O2A-CGA
22	p	308	CLA	C2-C1-O2A-CGA
22	P	306	CLA	C2-C1-O2A-CGA
22	g	302	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
22	C	515	CLA	C2-C1-O2A-CGA
22	B	609	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C2-C1-O2A-CGA
22	c	506	CLA	C2-C1-O2A-CGA
22	s	301	CLA	C2-C1-O2A-CGA
26	n	315	CHL	C2-C1-O2A-CGA
25	P	313	LHG	C9-C10-C11-C12
34	A	411	LMG	C39-C40-C41-C42
22	u	306	CLA	C11-C12-C13-C15
22	b	603	CLA	CAA-CBA-CGA-O2A
22	1	307	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	L	101	LHG	O10-C23-O8-C6
22	q	307	CLA	C3-C5-C6-C7
22	Q	307	CLA	C3-C5-C6-C7
25	2	312	LHG	C35-C36-C37-C38
25	C	522	LHG	C9-C10-C11-C12
22	6	305	CLA	C10-C11-C12-C13
32	C	501	SQD	C10-C11-C12-C13
22	Q	303	CLA	O1D-CGD-O2D-CED
26	6	314	CHL	CBA-CGA-O2A-C1
26	u	314	CHL	CBA-CGA-O2A-C1
27	R	301	NEX	C13-C14-C15-C35
22	v	307	CLA	O1A-CGA-O2A-C1
22	V	304	CLA	O1A-CGA-O2A-C1
25	2	312	LHG	O6-C4-C5-O7
25	p	313	LHG	O6-C4-C5-O7
25	S	312	LHG	O8-C23-C24-C25
22	S	309	CLA	O2A-C1-C2-C3
22	s	309	CLA	O2A-C1-C2-C3
26	P	318	CHL	C4-C3-C5-C6
26	R	315	CHL	C4-C3-C5-C6
25	b	623	LHG	C28-C29-C30-C31
26	r	615	CHL	O1D-CGD-O2D-CED
23	v	309	LUT	C1-C6-C7-C8
23	V	309	LUT	C1-C6-C7-C8
23	S	310	LUT	C5-C6-C7-C8
31	B	620	BCR	C1-C6-C7-C8
22	6	305	CLA	C2-C3-C5-C6
22	4	307	CLA	O1A-CGA-O2A-C1
25	4	312	LHG	C7-C8-C9-C10
22	2	308	CLA	CBA-CGA-O2A-C1
22	V	302	CLA	CBA-CGA-O2A-C1
34	W	201	LMG	C29-C28-O8-C9
25	s	312	LHG	O8-C23-C24-C25
26	s	315	CHL	O1D-CGD-O2D-CED
25	6	311	LHG	C8-C7-O7-C5
25	q	310	LHG	C8-C7-O7-C5
34	b	621	LMG	C11-C10-O7-C8
34	W	201	LMG	O6-C1-O1-C7
36	C	519	DGD	O6E-C1E-O5D-C6D
25	b	622	LHG	C13-C14-C15-C16
32	A	412	SQD	C16-C17-C18-C19
22	b	610	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C8-C10-C11-C12
34	W	201	LMG	C2-C1-O1-C7
25	d	406	LHG	C30-C31-C32-C33
25	D	406	LHG	C13-C14-C15-C16
34	B	621	LMG	C22-C23-C24-C25
22	C	511	CLA	CBA-CGA-O2A-C1
22	c	509	CLA	CBA-CGA-O2A-C1
25	6	311	LHG	C4-O6-P-O3
25	q	310	LHG	C4-O6-P-O3
25	n	312	LHG	C4-O6-P-O3
25	C	524	LHG	C3-O3-P-O6
25	C	524	LHG	C4-O6-P-O3
25	D	407	LHG	C3-O3-P-O6
25	c	521	LHG	C4-O6-P-O3
25	c	523	LHG	C3-O3-P-O6
32	A	412	SQD	C23-C24-C25-C26
25	2	312	LHG	C12-C13-C14-C15
25	S	312	LHG	C11-C10-C9-C8
36	C	519	DGD	C2B-C3B-C4B-C5B
25	C	522	LHG	C11-C12-C13-C14
26	p	318	CHL	C4-C3-C5-C6
26	u	316	CHL	C4-C3-C5-C6
22	3	301	CLA	C6-C7-C8-C10
22	V	302	CLA	C11-C10-C8-C7
22	N	305	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C12-C13-C15
22	c	508	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C12-C13-C15
26	V	318	CHL	C12-C13-C15-C16
26	g	314	CHL	C12-C13-C15-C16
22	C	511	CLA	O1A-CGA-O2A-C1
22	4	304	CLA	C11-C10-C8-C9
22	6	308	CLA	C11-C10-C8-C9
22	p	302	CLA	C11-C12-C13-C14
22	q	301	CLA	C6-C7-C8-C9
22	P	303	CLA	C11-C10-C8-C9
22	N	304	CLA	C11-C10-C8-C9
22	n	304	CLA	C11-C12-C13-C14
22	g	305	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	S	301	CLA	C11-C12-C13-C14
22	C	509	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
22	B	616	CLA	C11-C12-C13-C14
22	b	607	CLA	C6-C7-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	b	616	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C10-C8-C9
26	3	314	CHL	C14-C13-C15-C16
26	4	317	CHL	C11-C12-C13-C14
26	5	313	CHL	C11-C12-C13-C14
26	5	318	CHL	C11-C12-C13-C14
26	6	315	CHL	C14-C13-C15-C16
26	6	316	CHL	C11-C12-C13-C14
26	P	317	CHL	C14-C13-C15-C16
26	N	317	CHL	C11-C12-C13-C14
26	u	316	CHL	C14-C13-C15-C16
26	n	313	CHL	C14-C13-C15-C16
26	g	315	CHL	C6-C7-C8-C9
26	3	314	CHL	C10-C11-C12-C13
24	q	309	XAT	C33-C34-C35-C15
24	R	313	XAT	C33-C34-C35-C15
27	r	618	NEX	C29-C30-C31-C32
27	R	301	NEX	C9-C10-C11-C12
31	B	620	BCR	C13-C14-C15-C16
22	Q	307	CLA	C16-C17-C18-C20
32	a	410	SQD	C11-C10-C9-C8
34	B	624	LMG	C12-C13-C14-C15
34	B	624	LMG	C13-C14-C15-C16
36	c	517	DGD	C2B-C3B-C4B-C5B
22	c	510	CLA	CBA-CGA-O2A-C1
25	l	101	LHG	C24-C23-O8-C6
22	G	301	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	O1A-CGA-O2A-C1
34	W	201	LMG	O10-C28-O8-C9
25	n	312	LHG	C11-C12-C13-C14
26	S	314	CHL	CBD-CGD-O2D-CED
22	s	304	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	C8-C10-C11-C12
26	6	317	CHL	C2C-C3C-CAC-CBC
36	A	414	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
32	m	101	SQD	C7-C8-C9-C10
22	2	308	CLA	O1A-CGA-O2A-C1
22	n	307	CLA	O1A-CGA-O2A-C1
22	C	506	CLA	O1A-CGA-O2A-C1
26	6	314	CHL	O1A-CGA-O2A-C1
26	N	317	CHL	O1A-CGA-O2A-C1
24	u	311	XAT	C31-C32-C33-C40
27	2	319	NEX	C31-C32-C33-C40
27	5	319	NEX	C31-C32-C33-C40
31	b	618	BCR	C36-C18-C19-C20
22	5	304	CLA	C16-C17-C18-C19
22	R	310	CLA	CBA-CGA-O2A-C1
26	v	314	CHL	CBA-CGA-O2A-C1
25	U	312	LHG	O1-C1-C2-C3
25	q	310	LHG	C2-C3-O3-P
25	B	623	LHG	C2-C3-O3-P
22	6	308	CLA	O1A-CGA-O2A-C1
27	N	318	NEX	C11-C12-C13-C14
31	c	515	BCR	C11-C12-C13-C14
22	s	301	CLA	C12-C13-C15-C16
22	4	301	CLA	C15-C16-C17-C18
25	S	312	LHG	C8-C7-O7-C5
22	3	304	CLA	C4-C3-C5-C6
26	1	316	CHL	C4-C3-C5-C6
26	g	315	CHL	C4-C3-C5-C6
25	A	413	LHG	O1-C1-C2-O2
22	C	514	CLA	C2-C3-C5-C6
22	D	403	CLA	C2-C3-C5-C6
26	U	313	CHL	C2-C3-C5-C6
26	G	314	CHL	C2-C3-C5-C6
34	b	624	LMG	C12-C13-C14-C15
22	q	306	CLA	C11-C12-C13-C15
22	q	307	CLA	C16-C17-C18-C19
26	q	315	CHL	C11-C12-C13-C14
22	N	304	CLA	CBA-CGA-O2A-C1
22	N	307	CLA	CBA-CGA-O2A-C1
22	G	301	CLA	CBA-CGA-O2A-C1
22	c	505	CLA	CBA-CGA-O2A-C1
26	N	317	CHL	CBA-CGA-O2A-C1
32	a	410	SQD	C24-C23-O48-C46
22	V	302	CLA	O1A-CGA-O2A-C1
26	V	313	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	R	311	CLA	O1D-CGD-O2D-CED
25	C	523	LHG	C11-C12-C13-C14
34	c	501	LMG	C13-C14-C15-C16
26	V	313	CHL	O1D-CGD-O2D-CED
25	n	312	LHG	C11-C10-C9-C8
36	c	518	DGD	O6D-C5D-C6D-O5D
22	V	304	CLA	CBA-CGA-O2A-C1
22	D	403	CLA	CBA-CGA-O2A-C1
36	c	519	DGD	C5A-C6A-C7A-C8A
22	r	606	CLA	C4B-C3B-CAB-CBB
22	2	301	CLA	C4B-C3B-CAB-CBB
22	3	303	CLA	C4B-C3B-CAB-CBB
22	p	302	CLA	C4B-C3B-CAB-CBB
22	p	305	CLA	C4B-C3B-CAB-CBB
22	p	306	CLA	C4B-C3B-CAB-CBB
22	P	302	CLA	C4B-C3B-CAB-CBB
22	P	305	CLA	C4B-C3B-CAB-CBB
22	U	305	CLA	C4B-C3B-CAB-CBB
22	N	303	CLA	C4B-C3B-CAB-CBB
22	u	305	CLA	C4B-C3B-CAB-CBB
22	n	307	CLA	C4B-C3B-CAB-CBB
22	R	307	CLA	C4B-C3B-CAB-CBB
22	R	310	CLA	C4B-C3B-CAB-CBB
22	S	301	CLA	C4B-C3B-CAB-CBB
22	B	604	CLA	C4B-C3B-CAB-CBB
22	B	612	CLA	C4B-C3B-CAB-CBB
22	B	615	CLA	C4B-C3B-CAB-CBB
22	b	604	CLA	C4B-C3B-CAB-CBB
22	b	615	CLA	C4B-C3B-CAB-CBB
26	Q	316	CHL	C4B-C3B-CAB-CBB
26	S	315	CHL	C4B-C3B-CAB-CBB
22	p	305	CLA	C2A-CAA-CBA-CGA
22	q	305	CLA	C2A-CAA-CBA-CGA
22	P	308	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C2A-CAA-CBA-CGA
36	c	517	DGD	O6E-C1E-O5D-C6D
22	R	304	CLA	C5-C6-C7-C8
23	n	310	LUT	C29-C30-C31-C32
23	S	311	LUT	C33-C34-C35-C15
23	s	311	LUT	C33-C34-C35-C15
24	n	311	XAT	C33-C34-C35-C15
31	x	202	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	z	101	BCR	C19-C20-C21-C22
31	C	516	BCR	C19-C20-C21-C22
34	C	502	LMG	C13-C14-C15-C16
25	q	310	LHG	O6-C4-C5-C6
22	N	304	CLA	O1A-CGA-O2A-C1
22	s	301	CLA	CAA-CBA-CGA-O2A
22	B	603	CLA	C10-C11-C12-C13
25	3	310	LHG	C32-C33-C34-C35
25	N	312	LHG	C11-C10-C9-C8
26	3	316	CHL	C2C-C3C-CAC-CBC
26	s	315	CHL	CBD-CGD-O2D-CED
32	a	410	SQD	C7-C8-C9-C10
22	C	508	CLA	C3-C5-C6-C7
25	s	312	LHG	C11-C10-C9-C8
36	C	520	DGD	C3B-C4B-C5B-C6B
22	1	305	CLA	C4-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
26	v	313	CHL	C4-C3-C5-C6
33	d	404	PL9	C35-C34-C36-C37
22	C	506	CLA	C15-C16-C17-C18
32	l	102	SQD	C16-C17-C18-C19
26	p	317	CHL	C2-C3-C5-C6
26	g	315	CHL	C2-C3-C5-C6
22	N	307	CLA	O1A-CGA-O2A-C1
22	R	310	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	C13-C14-C15-C16
26	Q	311	CHL	C5-C6-C7-C8
25	S	312	LHG	O9-C7-O7-C5
25	U	312	LHG	C9-C10-C11-C12
36	c	518	DGD	CAB-CBB-CCB-CDB
22	1	305	CLA	C2-C1-O2A-CGA
22	2	302	CLA	C2-C1-O2A-CGA
22	G	304	CLA	C2-C1-O2A-CGA
22	G	306	CLA	C2-C1-O2A-CGA
22	R	302	CLA	C2-C1-O2A-CGA
22	C	504	CLA	C2-C1-O2A-CGA
22	B	611	CLA	C2-C1-O2A-CGA
26	v	315	CHL	C2-C1-O2A-CGA
26	g	314	CHL	C2-C1-O2A-CGA
25	c	522	LHG	C25-C26-C27-C28
34	d	407	LMG	C16-C17-C18-C19
36	a	416	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	C5-C6-C7-C8
26	g	316	CHL	C5-C6-C7-C8
32	a	410	SQD	C10-C11-C12-C13
22	5	307	CLA	C2A-CAA-CBA-CGA
22	q	308	CLA	C2A-CAA-CBA-CGA
22	N	304	CLA	C2A-CAA-CBA-CGA
22	G	303	CLA	C2A-CAA-CBA-CGA
22	S	303	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
22	B	615	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
22	b	615	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
25	P	313	LHG	O7-C5-C6-O8
22	b	603	CLA	C15-C16-C17-C18
25	b	623	LHG	C2-C3-O3-P
34	w	201	LMG	C16-C17-C18-C19
36	c	518	DGD	C6B-C7B-C8B-C9B
22	r	604	CLA	C3A-C2A-CAA-CBA
22	R	305	CLA	C3A-C2A-CAA-CBA
26	q	314	CHL	C3A-C2A-CAA-CBA
30	d	401	PHO	C3A-C2A-CAA-CBA
30	D	401	PHO	C3A-C2A-CAA-CBA
22	r	606	CLA	C16-C17-C18-C20
25	B	623	LHG	C28-C29-C30-C31
32	a	410	SQD	C26-C27-C28-C29
26	G	313	CHL	O2A-C1-C2-C3
26	n	315	CHL	O2A-C1-C2-C3
22	b	616	CLA	CBD-CGD-O2D-CED
32	C	501	SQD	C28-C29-C30-C31
31	X	201	BCR	C15-C16-C17-C18
25	r	613	LHG	C28-C29-C30-C31
25	q	310	LHG	C9-C10-C11-C12
26	N	317	CHL	C2C-C3C-CAC-CBC
22	a	408	CLA	C4-C3-C5-C6
22	g	307	CLA	C4-C3-C5-C6
26	P	317	CHL	C4-C3-C5-C6
33	D	405	PL9	C35-C34-C36-C37
36	B	601	DGD	C1B-C2B-C3B-C4B
26	v	316	CHL	C2-C3-C5-C6
22	V	301	CLA	C8-C10-C11-C12
22	S	301	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	1	305	CLA	C6-C7-C8-C9
22	6	305	CLA	C14-C13-C15-C16
22	B	605	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C10-C8-C9
26	4	316	CHL	C14-C13-C15-C16
26	p	320	CHL	C11-C12-C13-C14
26	q	311	CHL	C6-C7-C8-C9
26	V	316	CHL	C11-C10-C8-C9
26	V	316	CHL	C11-C12-C13-C14
26	G	311	CHL	C11-C10-C8-C9
26	u	318	CHL	C11-C12-C13-C14
26	g	311	CHL	C11-C10-C8-C9
26	g	314	CHL	C11-C12-C13-C14
22	s	305	CLA	C5-C6-C7-C8
25	l	101	LHG	O10-C23-O8-C6
34	b	624	LMG	C30-C31-C32-C33
26	6	315	CHL	C10-C11-C12-C13
25	r	613	LHG	C4-C5-C6-O8
25	p	313	LHG	C4-C5-C6-O8
27	r	617	NEX	C39-C29-C30-C31
27	r	618	NEX	C39-C29-C30-C31
27	2	319	NEX	C39-C29-C30-C31
27	5	319	NEX	C39-C29-C30-C31
27	v	319	NEX	C39-C29-C30-C31
27	p	301	NEX	C39-C29-C30-C31
27	V	319	NEX	C39-C29-C30-C31
27	P	301	NEX	C39-C29-C30-C31
27	U	318	NEX	C39-C29-C30-C31
27	N	318	NEX	C39-C29-C30-C31
27	u	319	NEX	C39-C29-C30-C31
27	u	320	NEX	C39-C29-C30-C31
27	n	319	NEX	C39-C29-C30-C31
27	R	301	NEX	C39-C29-C30-C31
27	S	317	NEX	C39-C29-C30-C31
27	s	317	NEX	C39-C29-C30-C31
36	c	518	DGD	O1B-C1B-O2G-C2G
25	c	523	LHG	C11-C10-C9-C8
32	L	102	SQD	C16-C17-C18-C19
22	3	306	CLA	C2A-CAA-CBA-CGA
22	B	606	CLA	C2A-CAA-CBA-CGA
34	D	408	LMG	C12-C13-C14-C15
26	v	314	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	623	LHG	C26-C27-C28-C29
34	b	624	LMG	C15-C16-C17-C18
22	u	306	CLA	C11-C12-C13-C14
25	C	523	LHG	C25-C26-C27-C28
24	q	309	XAT	C27-C28-C29-C39
24	R	313	XAT	C7-C8-C9-C19
34	c	520	LMG	C33-C34-C35-C36
22	C	504	CLA	C15-C16-C17-C18
25	v	312	LHG	C9-C10-C11-C12
25	U	312	LHG	C26-C27-C28-C29
23	R	312	LUT	C7-C8-C9-C10
34	C	521	LMG	C9-C8-O7-C10
34	c	520	LMG	C9-C8-O7-C10
22	C	509	CLA	C10-C11-C12-C13
22	B	613	CLA	C8-C10-C11-C12
26	q	315	CHL	C5-C6-C7-C8
22	B	606	CLA	C4-C3-C5-C6
22	r	609	CLA	C1A-C2A-CAA-CBA
22	2	302	CLA	C1A-C2A-CAA-CBA
22	2	306	CLA	C1A-C2A-CAA-CBA
22	3	308	CLA	C1A-C2A-CAA-CBA
22	5	302	CLA	C1A-C2A-CAA-CBA
22	5	305	CLA	C1A-C2A-CAA-CBA
22	5	306	CLA	C1A-C2A-CAA-CBA
22	p	302	CLA	C1A-C2A-CAA-CBA
22	V	301	CLA	C1A-C2A-CAA-CBA
22	U	304	CLA	C1A-C2A-CAA-CBA
22	n	301	CLA	C1A-C2A-CAA-CBA
22	g	304	CLA	C1A-C2A-CAA-CBA
22	R	302	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	C1A-C2A-CAA-CBA
22	B	604	CLA	C1A-C2A-CAA-CBA
22	b	604	CLA	C1A-C2A-CAA-CBA
22	c	504	CLA	C1A-C2A-CAA-CBA
26	P	318	CHL	C1A-C2A-CAA-CBA
22	4	306	CLA	C6-C7-C8-C10
22	6	306	CLA	C6-C7-C8-C10
22	v	301	CLA	C6-C7-C8-C10
22	p	308	CLA	C11-C10-C8-C7
22	q	304	CLA	C11-C10-C8-C7
22	N	304	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	n	302	CLA	C11-C10-C8-C7
22	g	307	CLA	C2-C3-C5-C6
22	b	609	CLA	C11-C12-C13-C15
22	c	502	CLA	C11-C10-C8-C7
26	5	316	CHL	C11-C10-C8-C7
26	6	316	CHL	C12-C13-C15-C16
26	p	320	CHL	C6-C7-C8-C10
26	V	317	CHL	C11-C10-C8-C7
26	P	319	CHL	C11-C12-C13-C15
26	G	314	CHL	C6-C7-C8-C10
26	n	313	CHL	C6-C7-C8-C10
34	a	412	LMG	C10-C11-C12-C13
22	c	509	CLA	O1A-CGA-O2A-C1
32	a	413	SQD	C30-C31-C32-C33
36	b	601	DGD	C9B-CAB-CBB-CCB
26	5	315	CHL	C3C-C2C-CMC-OMC
26	p	320	CHL	C3C-C2C-CMC-OMC
26	G	315	CHL	C3C-C2C-CMC-OMC
25	Q	310	LHG	C25-C26-C27-C28
34	c	520	LMG	C36-C37-C38-C39
22	c	508	CLA	C10-C11-C12-C13
25	L	101	LHG	C31-C32-C33-C34
32	A	412	SQD	C32-C33-C34-C35
34	A	411	LMG	C40-C41-C42-C43
34	B	624	LMG	C15-C16-C17-C18
22	b	616	CLA	O1D-CGD-O2D-CED
22	3	303	CLA	C2A-CAA-CBA-CGA
22	5	304	CLA	C2A-CAA-CBA-CGA
22	q	307	CLA	C2A-CAA-CBA-CGA
22	P	305	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	s	303	CLA	C2A-CAA-CBA-CGA
26	S	313	CHL	C2A-CAA-CBA-CGA
26	s	313	CHL	C2A-CAA-CBA-CGA
22	a	405	CLA	C13-C15-C16-C17
22	4	302	CLA	C13-C15-C16-C17
22	b	613	CLA	C8-C10-C11-C12
36	J	101	DGD	C5A-C6A-C7A-C8A
26	N	315	CHL	O2A-C1-C2-C3
26	n	318	CHL	CBA-CGA-O2A-C1
34	w	201	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	B	624	LMG	C30-C31-C32-C33
25	l	101	LHG	C31-C32-C33-C34
22	Q	307	CLA	C16-C17-C18-C19
22	R	307	CLA	C16-C17-C18-C20
22	g	302	CLA	C15-C16-C17-C18
26	V	316	CHL	C15-C16-C17-C18
26	U	313	CHL	C10-C11-C12-C13
34	a	412	LMG	C32-C33-C34-C35
36	c	518	DGD	C5A-C6A-C7A-C8A
22	A	408	CLA	C4-C3-C5-C6
26	6	316	CHL	C4-C3-C5-C6
26	p	319	CHL	C4-C3-C5-C6
26	U	317	CHL	C4-C3-C5-C6
22	Q	302	CLA	C8-C10-C11-C12
22	B	611	CLA	C15-C16-C17-C18
32	M	101	SQD	C7-C8-C9-C10
22	6	303	CLA	C2-C3-C5-C6
26	1	316	CHL	C2-C3-C5-C6
26	P	318	CHL	C2-C3-C5-C6
22	2	301	CLA	C2B-C3B-CAB-CBB
22	p	302	CLA	C2B-C3B-CAB-CBB
22	n	304	CLA	C2B-C3B-CAB-CBB
22	B	612	CLA	C2B-C3B-CAB-CBB
22	b	612	CLA	C2B-C3B-CAB-CBB
26	r	615	CHL	C2B-C3B-CAB-CBB
26	r	619	CHL	C2B-C3B-CAB-CBB
26	1	314	CHL	C2B-C3B-CAB-CBB
26	1	316	CHL	C2B-C3B-CAB-CBB
26	2	315	CHL	C2B-C3B-CAB-CBB
26	2	317	CHL	C2B-C3B-CAB-CBB
26	3	314	CHL	C2B-C3B-CAB-CBB
26	3	315	CHL	C2B-C3B-CAB-CBB
26	4	313	CHL	C2B-C3B-CAB-CBB
26	4	314	CHL	C2B-C3B-CAB-CBB
26	5	314	CHL	C2B-C3B-CAB-CBB
26	5	315	CHL	C2B-C3B-CAB-CBB
26	5	317	CHL	C2B-C3B-CAB-CBB
26	6	313	CHL	C2B-C3B-CAB-CBB
26	6	315	CHL	C2B-C3B-CAB-CBB
26	v	314	CHL	C2B-C3B-CAB-CBB
26	p	316	CHL	C2B-C3B-CAB-CBB
26	q	313	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
26	V	314	CHL	C2B-C3B-CAB-CBB
26	V	318	CHL	C2B-C3B-CAB-CBB
26	P	315	CHL	C2B-C3B-CAB-CBB
26	P	316	CHL	C2B-C3B-CAB-CBB
26	P	319	CHL	C2B-C3B-CAB-CBB
26	Q	312	CHL	C2B-C3B-CAB-CBB
26	U	313	CHL	C2B-C3B-CAB-CBB
26	U	315	CHL	C2B-C3B-CAB-CBB
26	U	319	CHL	C2B-C3B-CAB-CBB
26	N	314	CHL	C2B-C3B-CAB-CBB
26	N	316	CHL	C2B-C3B-CAB-CBB
26	u	313	CHL	C2B-C3B-CAB-CBB
26	n	313	CHL	C2B-C3B-CAB-CBB
26	R	316	CHL	C2B-C3B-CAB-CBB
26	S	316	CHL	C2B-C3B-CAB-CBB
26	s	315	CHL	C2B-C3B-CAB-CBB
26	s	316	CHL	C2B-C3B-CAB-CBB
34	b	621	LMG	C31-C32-C33-C34
32	m	101	SQD	C29-C30-C31-C32
36	b	601	DGD	CBA-CCA-CDA-CEA
22	C	509	CLA	C8-C10-C11-C12
22	c	505	CLA	O1A-CGA-O2A-C1
26	q	315	CHL	O1D-CGD-O2D-CED
25	V	312	LHG	C13-C14-C15-C16
36	B	601	DGD	C9B-CAB-CBB-CCB
25	v	312	LHG	O9-C7-O7-C5
27	r	617	NEX	C28-C29-C30-C31
27	r	618	NEX	C28-C29-C30-C31
27	2	319	NEX	C28-C29-C30-C31
27	5	319	NEX	C28-C29-C30-C31
27	v	319	NEX	C28-C29-C30-C31
27	p	301	NEX	C28-C29-C30-C31
27	V	319	NEX	C28-C29-C30-C31
27	P	301	NEX	C28-C29-C30-C31
27	U	318	NEX	C28-C29-C30-C31
27	N	318	NEX	C28-C29-C30-C31
27	u	319	NEX	C28-C29-C30-C31
27	u	320	NEX	C28-C29-C30-C31
27	n	319	NEX	C28-C29-C30-C31
27	R	301	NEX	C28-C29-C30-C31
27	S	317	NEX	C28-C29-C30-C31
27	s	317	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	v	306	CLA	C8-C10-C11-C12
22	u	306	CLA	C10-C11-C12-C13
22	c	508	CLA	C8-C10-C11-C12
22	d	402	CLA	CBA-CGA-O2A-C1
26	U	319	CHL	C15-C16-C17-C18
23	p	311	LUT	C9-C10-C11-C12
23	u	310	LUT	C29-C30-C31-C32
24	Q	309	XAT	C33-C34-C35-C15
22	U	302	CLA	C8-C10-C11-C12
22	b	604	CLA	C8-C10-C11-C12
26	4	313	CHL	C16-C17-C18-C20
25	u	312	LHG	C24-C25-C26-C27
25	n	312	LHG	C13-C14-C15-C16
32	a	410	SQD	C31-C32-C33-C34
22	4	302	CLA	C5-C6-C7-C8
22	R	307	CLA	C15-C16-C17-C18
22	D	403	CLA	O1A-CGA-O2A-C1
25	l	101	LHG	C1-C2-C3-O3
25	L	101	LHG	C1-C2-C3-O3
25	S	312	LHG	C1-C2-C3-O3
22	q	303	CLA	C2-C1-O2A-CGA
22	q	304	CLA	C2-C1-O2A-CGA
22	V	305	CLA	C2-C1-O2A-CGA
22	U	305	CLA	C2-C1-O2A-CGA
22	G	302	CLA	C2-C1-O2A-CGA
22	u	305	CLA	C2-C1-O2A-CGA
22	b	611	CLA	C2-C1-O2A-CGA
26	3	313	CHL	C2-C1-O2A-CGA
26	6	314	CHL	C2-C1-O2A-CGA
26	q	314	CHL	C2-C1-O2A-CGA
26	P	319	CHL	C2-C1-O2A-CGA
26	S	315	CHL	C2-C1-O2A-CGA
26	s	315	CHL	C2-C1-O2A-CGA
22	a	408	CLA	C2-C3-C5-C6
22	3	304	CLA	C2-C3-C5-C6
26	p	318	CHL	C2-C3-C5-C6
26	P	317	CHL	C2-C3-C5-C6
26	u	316	CHL	C2-C3-C5-C6
22	C	513	CLA	O1A-CGA-O2A-C1
26	n	318	CHL	O1A-CGA-O2A-C1
34	w	201	LMG	O10-C28-O8-C9
22	1	302	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
36	J	101	DGD	C8A-C9A-CAA-CBA
32	a	410	SQD	C23-C24-C25-C26
22	x	201	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
25	C	523	LHG	C19-C20-C21-C22
26	S	316	CHL	CAA-CBA-CGA-O2A
36	b	601	DGD	C1B-C2B-C3B-C4B
22	P	309	CLA	O1A-CGA-O2A-C1
22	B	604	CLA	C13-C15-C16-C17
22	Q	307	CLA	C2A-CAA-CBA-CGA
22	G	307	CLA	C2A-CAA-CBA-CGA
22	p	302	CLA	C16-C17-C18-C20
26	s	316	CHL	CAA-CBA-CGA-O2A
26	5	315	CHL	O2A-C1-C2-C3
26	2	314	CHL	C2-C1-O2A-CGA
36	C	519	DGD	C2A-C3A-C4A-C5A
36	b	601	DGD	C4B-C5B-C6B-C7B
25	b	623	LHG	O9-C7-C8-C9
22	d	402	CLA	O1A-CGA-O2A-C1
22	V	303	CLA	O1A-CGA-O2A-C1
26	Q	314	CHL	O1A-CGA-O2A-C1
23	2	310	LUT	C1-C6-C7-C8
23	5	309	LUT	C1-C6-C7-C8
23	5	310	LUT	C1-C6-C7-C8
23	p	310	LUT	C1-C6-C7-C8
23	p	311	LUT	C1-C6-C7-C8
23	p	311	LUT	C5-C6-C7-C8
23	P	310	LUT	C1-C6-C7-C8
23	P	310	LUT	C5-C6-C7-C8
23	P	311	LUT	C1-C6-C7-C8
23	U	310	LUT	C1-C6-C7-C8
23	U	310	LUT	C5-C6-C7-C8
23	u	310	LUT	C1-C6-C7-C8
23	S	310	LUT	C1-C6-C7-C8
23	S	311	LUT	C1-C6-C7-C8
23	s	310	LUT	C1-C6-C7-C8
23	s	310	LUT	C5-C6-C7-C8
23	s	311	LUT	C1-C6-C7-C8
31	A	409	BCR	C1-C6-C7-C8
25	2	312	LHG	C24-C25-C26-C27
25	4	312	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	CAA-CBA-CGA-O2A
25	c	522	LHG	C11-C12-C13-C14
36	c	519	DGD	C5B-C6B-C7B-C8B
26	s	316	CHL	CAA-CBA-CGA-O1A
25	3	310	LHG	O1-C1-C2-C3
23	P	311	LUT	C9-C10-C11-C12
24	r	612	XAT	C33-C34-C35-C15
27	u	319	NEX	C29-C30-C31-C32
31	D	404	BCR	C19-C20-C21-C22
31	b	618	BCR	C13-C14-C15-C16
22	V	303	CLA	CBA-CGA-O2A-C1
22	6	302	CLA	C4-C3-C5-C6
22	B	607	CLA	C4-C3-C5-C6
26	P	319	CHL	C4-C3-C5-C6
24	u	311	XAT	C31-C32-C33-C34
31	C	517	BCR	C11-C12-C13-C14
22	r	603	CLA	C5-C6-C7-C8
30	A	407	PHO	C13-C15-C16-C17
22	d	402	CLA	C2-C3-C5-C6
22	R	306	CLA	C2-C3-C5-C6
22	B	602	CLA	CAA-CBA-CGA-O2A
26	6	301	CHL	C3-C5-C6-C7
26	S	313	CHL	CAA-CBA-CGA-O2A
26	p	315	CHL	C2-C1-O2A-CGA
26	N	317	CHL	C4C-C3C-CAC-CBC
26	v	318	CHL	C10-C11-C12-C13
26	Q	314	CHL	CBA-CGA-O2A-C1
26	s	313	CHL	CAA-CBA-CGA-O2A
26	Q	316	CHL	O1A-CGA-O2A-C1
22	3	305	CLA	C11-C12-C13-C15
26	r	614	CHL	C5-C6-C7-C8
26	n	316	CHL	C13-C15-C16-C17
26	S	313	CHL	CAA-CBA-CGA-O1A
26	S	316	CHL	CAA-CBA-CGA-O1A
22	s	306	CLA	C2A-CAA-CBA-CGA
22	P	309	CLA	CBA-CGA-O2A-C1
22	C	513	CLA	CBA-CGA-O2A-C1
25	5	312	LHG	C7-C8-C9-C10
26	S	314	CHL	CAA-CBA-CGA-O2A
26	s	314	CHL	CAA-CBA-CGA-O2A
22	5	301	CLA	C4B-C3B-CAB-CBB
22	N	301	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	N	304	CLA	C4B-C3B-CAB-CBB
22	n	301	CLA	C4B-C3B-CAB-CBB
22	R	304	CLA	C4B-C3B-CAB-CBB
22	b	612	CLA	C4B-C3B-CAB-CBB
22	s	301	CLA	C4B-C3B-CAB-CBB
26	3	312	CHL	C4B-C3B-CAB-CBB
26	s	315	CHL	C4B-C3B-CAB-CBB
26	V	313	CHL	C16-C17-C18-C20
32	a	413	SQD	C11-C12-C13-C14
36	c	519	DGD	C8A-C9A-CAA-CBA
22	1	307	CLA	C8-C10-C11-C12
22	n	301	CLA	C13-C15-C16-C17
22	b	604	CLA	C13-C15-C16-C17
26	G	316	CHL	C4-C3-C5-C6
34	C	521	LMG	C40-C41-C42-C43
22	1	306	CLA	C6-C7-C8-C10
22	v	302	CLA	C11-C12-C13-C15
22	p	302	CLA	C2-C3-C5-C6
22	n	305	CLA	C6-C7-C8-C10
22	C	507	CLA	C2-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
22	B	608	CLA	C2-C3-C5-C6
26	1	313	CHL	C6-C7-C8-C10
26	v	317	CHL	C11-C12-C13-C15
26	q	311	CHL	C6-C7-C8-C10
26	Q	314	CHL	C11-C12-C13-C15
26	U	317	CHL	C2-C3-C5-C6
22	V	307	CLA	CBA-CGA-O2A-C1
26	Q	316	CHL	CBA-CGA-O2A-C1
32	C	501	SQD	C11-C10-C9-C8
25	a	415	LHG	O1-C1-C2-O2
25	u	312	LHG	O1-C1-C2-O2
32	M	101	SQD	C29-C30-C31-C32
23	5	309	LUT	C9-C10-C11-C12
23	U	310	LUT	C29-C30-C31-C32
22	r	608	CLA	CAA-CBA-CGA-O2A
22	C	512	CLA	CAA-CBA-CGA-O2A
26	n	316	CHL	CAA-CBA-CGA-O2A
36	C	519	DGD	C2E-C1E-O5D-C6D
36	c	517	DGD	C2E-C1E-O5D-C6D
22	R	311	CLA	CAA-CBA-CGA-O2A
32	L	102	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	b	622	LHG	O7-C5-C6-O8
34	a	412	LMG	O7-C8-C9-O8
36	c	517	DGD	O2G-C2G-C3G-O3G
36	c	519	DGD	O1G-C1G-C2G-O2G
22	b	602	CLA	CAA-CBA-CGA-O1A
26	5	314	CHL	C2-C1-O2A-CGA
26	1	315	CHL	O2A-C1-C2-C3
26	2	315	CHL	O2A-C1-C2-C3
26	3	313	CHL	O2A-C1-C2-C3
26	4	315	CHL	O2A-C1-C2-C3
26	6	314	CHL	O2A-C1-C2-C3
26	v	315	CHL	O2A-C1-C2-C3
26	V	315	CHL	O2A-C1-C2-C3
26	Q	313	CHL	O2A-C1-C2-C3
26	g	313	CHL	O2A-C1-C2-C3
22	p	303	CLA	CAA-CBA-CGA-O2A
22	u	306	CLA	CAA-CBA-CGA-O2A
26	u	316	CHL	CAA-CBA-CGA-O2A
22	Q	301	CLA	C15-C16-C17-C18
22	C	503	CLA	C13-C15-C16-C17
22	c	502	CLA	C13-C15-C16-C17
26	6	317	CHL	C10-C11-C12-C13
30	a	407	PHO	C13-C15-C16-C17
26	v	318	CHL	C2C-C3C-CAC-CBC
22	r	606	CLA	C16-C17-C18-C19
26	u	313	CHL	C16-C17-C18-C20
26	s	313	CHL	CAA-CBA-CGA-O1A
25	p	313	LHG	C24-C23-O8-C6
22	u	302	CLA	CAA-CBA-CGA-O2A
22	n	308	CLA	CAA-CBA-CGA-O2A
22	R	309	CLA	CAA-CBA-CGA-O2A
22	c	511	CLA	CAA-CBA-CGA-O2A
25	u	312	LHG	O8-C23-C24-C25
26	5	316	CHL	CAA-CBA-CGA-O2A
26	G	315	CHL	CAA-CBA-CGA-O2A
26	q	312	CHL	C2-C1-O2A-CGA
22	B	602	CLA	C4-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	b	608	CLA	C4-C3-C5-C6
26	3	311	CHL	C4-C3-C5-C6
26	u	313	CHL	C4-C3-C5-C6
26	g	316	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	a	407	PHO	C4-C3-C5-C6
22	6	306	CLA	C8-C10-C11-C12
25	1	312	LHG	C4-O6-P-O3
25	p	313	LHG	C4-O6-P-O3
22	A	408	CLA	C2-C3-C5-C6
22	c	506	CLA	C2-C3-C5-C6
26	p	319	CHL	C2-C3-C5-C6
26	R	315	CHL	C2-C3-C5-C6
25	D	406	LHG	C30-C31-C32-C33
36	C	520	DGD	C5A-C6A-C7A-C8A
22	q	306	CLA	CAA-CBA-CGA-O2A
22	P	303	CLA	CAA-CBA-CGA-O2A
25	P	313	LHG	O8-C23-C24-C25
34	w	201	LMG	O7-C10-C11-C12
34	c	501	LMG	O8-C28-C29-C30
34	A	411	LMG	C36-C37-C38-C39
34	c	520	LMG	C40-C41-C42-C43
22	S	301	CLA	C12-C13-C15-C16
22	1	302	CLA	C6-C7-C8-C9
22	1	307	CLA	C6-C7-C8-C9
22	2	301	CLA	C14-C13-C15-C16
22	2	302	CLA	C14-C13-C15-C16
22	2	304	CLA	C14-C13-C15-C16
22	3	301	CLA	C11-C10-C8-C9
22	3	307	CLA	C11-C10-C8-C9
22	4	302	CLA	C14-C13-C15-C16
22	6	302	CLA	C11-C10-C8-C9
22	v	301	CLA	C6-C7-C8-C9
22	u	302	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	C	514	CLA	C6-C7-C8-C9
26	r	614	CHL	C11-C12-C13-C14
26	1	313	CHL	C11-C10-C8-C9
26	2	318	CHL	C11-C12-C13-C14
26	3	315	CHL	C14-C13-C15-C16
26	4	313	CHL	C11-C10-C8-C9
26	p	320	CHL	C6-C7-C8-C9
26	P	317	CHL	C11-C12-C13-C14
25	g	310	LHG	C24-C25-C26-C27
26	S	314	CHL	CAA-CBA-CGA-O1A
22	V	304	CLA	C3A-C2A-CAA-CBA
22	R	302	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C3A-C2A-CAA-CBA
26	6	316	CHL	C3A-C2A-CAA-CBA
26	Q	315	CHL	C3A-C2A-CAA-CBA
22	3	304	CLA	C16-C17-C18-C19
32	l	102	SQD	C11-C10-C9-C8
22	5	302	CLA	CAA-CBA-CGA-O2A
22	v	304	CLA	CAA-CBA-CGA-O2A
22	Q	302	CLA	CAA-CBA-CGA-O2A
22	N	306	CLA	CAA-CBA-CGA-O2A
26	r	615	CHL	CBD-CGD-O2D-CED
26	n	318	CHL	C2C-C3C-CAC-CBC
22	r	603	CLA	CAD-CBD-CGD-O2D
22	A	408	CLA	CAD-CBD-CGD-O2D
22	3	302	CLA	CAD-CBD-CGD-O2D
22	4	304	CLA	CAD-CBD-CGD-O2D
22	5	301	CLA	CAD-CBD-CGD-O2D
22	5	302	CLA	CAD-CBD-CGD-O2D
22	6	306	CLA	CAD-CBD-CGD-O2D
22	v	302	CLA	CAD-CBD-CGD-O2D
22	p	308	CLA	CAD-CBD-CGD-O2D
22	q	306	CLA	CAD-CBD-CGD-O2D
22	q	307	CLA	CAD-CBD-CGD-O2D
22	V	304	CLA	CAD-CBD-CGD-O2D
22	P	302	CLA	CAD-CBD-CGD-O2D
22	P	304	CLA	CAD-CBD-CGD-O2D
22	P	305	CLA	CAD-CBD-CGD-O2D
22	P	308	CLA	CAD-CBD-CGD-O2D
22	P	309	CLA	CAD-CBD-CGD-O2D
22	Q	301	CLA	CAD-CBD-CGD-O2D
22	U	304	CLA	CAD-CBD-CGD-O2D
22	N	301	CLA	CAD-CBD-CGD-O2D
22	N	302	CLA	CAD-CBD-CGD-O2D
22	N	303	CLA	CAD-CBD-CGD-O2D
22	N	304	CLA	CAD-CBD-CGD-O2D
22	N	306	CLA	CAD-CBD-CGD-O2D
22	n	301	CLA	CAD-CBD-CGD-O2D
22	n	306	CLA	CAD-CBD-CGD-O2D
22	g	306	CLA	CAD-CBD-CGD-O2D
22	S	303	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	B	602	CLA	CAD-CBD-CGD-O2D
22	c	511	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	3	312	CHL	CAD-CBD-CGD-O2D
26	6	313	CHL	CAD-CBD-CGD-O2D
26	n	315	CHL	CAD-CBD-CGD-O2D
34	c	520	LMG	C7-C8-O7-C10
22	q	306	CLA	C11-C12-C13-C14
22	R	307	CLA	C16-C17-C18-C19
25	n	312	LHG	C24-C25-C26-C27
25	c	522	LHG	C19-C20-C21-C22
36	c	517	DGD	C2A-C3A-C4A-C5A
26	6	312	CHL	C5-C6-C7-C8
26	N	317	CHL	C5-C6-C7-C8
22	Q	306	CLA	C2A-CAA-CBA-CGA
25	C	524	LHG	C11-C10-C9-C8
22	r	606	CLA	C5-C6-C7-C8
22	S	307	CLA	C2-C1-O2A-CGA
22	C	512	CLA	C2-C1-O2A-CGA
26	4	316	CHL	C2-C1-O2A-CGA
26	s	314	CHL	CAA-CBA-CGA-O1A
25	v	312	LHG	C11-C12-C13-C14
32	a	413	SQD	C32-C33-C34-C35
22	4	302	CLA	CAA-CBA-CGA-O2A
22	6	304	CLA	CAA-CBA-CGA-O2A
22	V	304	CLA	CAA-CBA-CGA-O2A
25	U	312	LHG	O8-C23-C24-C25
25	N	312	LHG	O8-C23-C24-C25
26	r	616	CHL	CAA-CBA-CGA-O2A
26	2	316	CHL	CAA-CBA-CGA-O2A
34	W	201	LMG	O7-C10-C11-C12
36	b	601	DGD	O2G-C1B-C2B-C3B
25	6	311	LHG	C14-C15-C16-C17
25	p	313	LHG	C34-C35-C36-C37
22	R	306	CLA	C4-C3-C5-C6
26	3	315	CHL	C4-C3-C5-C6
26	6	312	CHL	C4-C3-C5-C6
26	u	318	CHL	C4-C3-C5-C6
26	r	615	CHL	C6-C7-C8-C10
22	S	304	CLA	CAA-CBA-CGA-O2A
26	1	314	CHL	C2-C1-O2A-CGA
34	W	201	LMG	C16-C17-C18-C19
26	V	315	CHL	O1D-CGD-O2D-CED
22	C	504	CLA	C2-C3-C5-C6
22	B	607	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C2-C3-C5-C6
26	6	316	CHL	C2-C3-C5-C6
26	v	313	CHL	C2-C3-C5-C6
22	r	603	CLA	CAA-CBA-CGA-O2A
22	v	306	CLA	CAA-CBA-CGA-O2A
22	N	301	CLA	CAA-CBA-CGA-O2A
22	N	307	CLA	CAA-CBA-CGA-O2A
22	G	302	CLA	CAA-CBA-CGA-O2A
22	n	301	CLA	CAA-CBA-CGA-O2A
26	1	316	CHL	CAA-CBA-CGA-O2A
26	3	313	CHL	CAA-CBA-CGA-O2A
26	R	317	CHL	CAA-CBA-CGA-O2A
26	s	315	CHL	CAA-CBA-CGA-O2A
25	c	523	LHG	C18-C19-C20-C21
23	U	309	LUT	C11-C12-C13-C14
24	P	312	XAT	C7-C8-C9-C10
31	B	618	BCR	C7-C8-C9-C10
25	q	310	LHG	C12-C13-C14-C15
24	r	612	XAT	O4-C6-C7-C8
24	3	309	XAT	O24-C26-C27-C28
24	6	310	XAT	O24-C26-C27-C28
24	N	311	XAT	O24-C26-C27-C28
24	R	313	XAT	O4-C6-C7-C8
24	R	313	XAT	O24-C26-C27-C28
25	2	312	LHG	C4-C5-C6-O8
25	G	310	LHG	C2-C3-O3-P
25	B	622	LHG	C4-C5-C6-O8
25	b	622	LHG	C4-C5-C6-O8
27	p	301	NEX	O24-C26-C27-C28
27	P	301	NEX	O24-C26-C27-C28
27	U	318	NEX	O24-C26-C27-C28
27	N	318	NEX	O24-C26-C27-C28
27	u	319	NEX	O24-C26-C27-C28
27	n	319	NEX	O24-C26-C27-C28
32	C	501	SQD	O6-C44-C45-C46
34	b	621	LMG	O1-C7-C8-C9
22	r	610	CLA	CAA-CBA-CGA-O2A
26	V	314	CHL	O1A-CGA-O2A-C1
25	Q	310	LHG	O6-C4-C5-O7
25	c	521	LHG	O6-C4-C5-O7
26	r	616	CHL	C10-C11-C12-C13
22	1	306	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	4	306	CLA	CAA-CBA-CGA-O2A
22	v	302	CLA	CAA-CBA-CGA-O2A
22	P	307	CLA	CAA-CBA-CGA-O2A
22	U	302	CLA	CAA-CBA-CGA-O2A
26	P	315	CHL	CAA-CBA-CGA-O2A
26	g	314	CHL	CAA-CBA-CGA-O2A
22	R	308	CLA	O2A-C1-C2-C3
26	q	313	CHL	O2A-C1-C2-C3
22	s	304	CLA	CAA-CBA-CGA-O2A
22	a	404	CLA	O2A-C1-C2-C3
22	A	404	CLA	O2A-C1-C2-C3
22	c	510	CLA	O2A-C1-C2-C3
26	r	615	CHL	O2A-C1-C2-C3
26	U	319	CHL	O2A-C1-C2-C3
26	n	316	CHL	O2A-C1-C2-C3
26	R	316	CHL	O2A-C1-C2-C3
25	r	613	LHG	C17-C18-C19-C20
22	2	304	CLA	C2A-CAA-CBA-CGA
22	6	307	CLA	C2A-CAA-CBA-CGA
22	p	304	CLA	C2A-CAA-CBA-CGA
22	U	307	CLA	C2A-CAA-CBA-CGA
22	G	304	CLA	C2A-CAA-CBA-CGA
22	g	307	CLA	C2A-CAA-CBA-CGA
22	2	302	CLA	CAA-CBA-CGA-O2A
26	S	315	CHL	CAA-CBA-CGA-O2A
34	C	502	LMG	O8-C28-C29-C30
36	b	601	DGD	O1G-C1A-C2A-C3A
25	p	313	LHG	O10-C23-O8-C6
22	R	311	CLA	CAA-CBA-CGA-O1A
22	S	304	CLA	CAA-CBA-CGA-O1A
36	B	601	DGD	C6B-C7B-C8B-C9B
25	s	312	LHG	C1-C2-C3-O3
22	R	311	CLA	CBD-CGD-O2D-CED
26	n	316	CHL	CBD-CGD-O2D-CED
22	r	604	CLA	CHA-CBD-CGD-O1D
22	r	604	CLA	CHA-CBD-CGD-O2D
22	1	306	CLA	CHA-CBD-CGD-O1D
22	1	306	CLA	CHA-CBD-CGD-O2D
22	2	303	CLA	CHA-CBD-CGD-O2D
22	2	306	CLA	CHA-CBD-CGD-O1D
22	2	306	CLA	CHA-CBD-CGD-O2D
22	3	303	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	3	305	CLA	CHA-CBD-CGD-O1D
22	3	306	CLA	CHA-CBD-CGD-O1D
22	3	306	CLA	CHA-CBD-CGD-O2D
22	4	306	CLA	CHA-CBD-CGD-O1D
22	6	304	CLA	CHA-CBD-CGD-O1D
22	6	304	CLA	CHA-CBD-CGD-O2D
22	6	307	CLA	CHA-CBD-CGD-O2D
22	v	301	CLA	CHA-CBD-CGD-O1D
22	V	301	CLA	CHA-CBD-CGD-O2D
22	V	306	CLA	CHA-CBD-CGD-O1D
22	V	306	CLA	CHA-CBD-CGD-O2D
22	P	307	CLA	CHA-CBD-CGD-O1D
22	Q	302	CLA	CHA-CBD-CGD-O2D
22	Q	306	CLA	CHA-CBD-CGD-O1D
22	Q	306	CLA	CHA-CBD-CGD-O2D
22	U	301	CLA	CHA-CBD-CGD-O1D
22	U	301	CLA	CHA-CBD-CGD-O2D
22	U	303	CLA	CHA-CBD-CGD-O1D
22	N	308	CLA	CHA-CBD-CGD-O1D
22	N	308	CLA	CHA-CBD-CGD-O2D
22	G	301	CLA	CHA-CBD-CGD-O1D
22	G	301	CLA	CHA-CBD-CGD-O2D
22	u	301	CLA	CHA-CBD-CGD-O2D
22	n	302	CLA	CHA-CBD-CGD-O2D
22	g	301	CLA	CHA-CBD-CGD-O1D
22	g	301	CLA	CHA-CBD-CGD-O2D
22	g	303	CLA	CHA-CBD-CGD-O1D
22	g	303	CLA	CHA-CBD-CGD-O2D
22	R	304	CLA	CHA-CBD-CGD-O2D
22	R	305	CLA	CHA-CBD-CGD-O1D
22	R	305	CLA	CHA-CBD-CGD-O2D
22	S	302	CLA	CHA-CBD-CGD-O1D
22	S	302	CLA	CHA-CBD-CGD-O2D
22	S	304	CLA	CHA-CBD-CGD-O1D
22	S	304	CLA	CHA-CBD-CGD-O2D
22	S	307	CLA	CHA-CBD-CGD-O1D
22	S	307	CLA	CHA-CBD-CGD-O2D
22	C	514	CLA	CHA-CBD-CGD-O1D
22	B	604	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	B	611	CLA	CHA-CBD-CGD-O2D
22	B	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	CHA-CBD-CGD-O2D
22	B	613	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CHA-CBD-CGD-O2D
22	b	604	CLA	CHA-CBD-CGD-O2D
22	b	608	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	b	613	CLA	CHA-CBD-CGD-O2D
22	b	614	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	513	CLA	CHA-CBD-CGD-O1D
22	s	302	CLA	CHA-CBD-CGD-O1D
22	s	302	CLA	CHA-CBD-CGD-O2D
22	s	304	CLA	CHA-CBD-CGD-O1D
22	s	304	CLA	CHA-CBD-CGD-O2D
22	s	307	CLA	CHA-CBD-CGD-O1D
22	s	307	CLA	CHA-CBD-CGD-O2D
26	6	312	CHL	CHA-CBD-CGD-O2D
26	6	317	CHL	CHA-CBD-CGD-O1D
26	6	317	CHL	CHA-CBD-CGD-O2D
26	n	313	CHL	CHA-CBD-CGD-O1D
26	n	313	CHL	CHA-CBD-CGD-O2D
26	g	311	CHL	CHA-CBD-CGD-O1D
26	g	311	CHL	CHA-CBD-CGD-O2D
26	g	316	CHL	CHA-CBD-CGD-O1D
26	g	316	CHL	CHA-CBD-CGD-O2D
22	r	610	CLA	CAA-CBA-CGA-O1A
22	q	302	CLA	C4-C3-C5-C6
22	5	306	CLA	CAA-CBA-CGA-O2A
22	p	307	CLA	CAA-CBA-CGA-O2A
22	P	308	CLA	CAA-CBA-CGA-O2A
22	N	302	CLA	CAA-CBA-CGA-O2A
22	R	304	CLA	CAA-CBA-CGA-O2A
34	B	621	LMG	O8-C28-C29-C30
25	g	310	LHG	C29-C30-C31-C32
26	3	315	CHL	C2-C3-C5-C6
22	b	611	CLA	C15-C16-C17-C18
26	p	319	CHL	C2C-C3C-CAC-CBC
22	p	305	CLA	C13-C15-C16-C17
22	2	306	CLA	CAA-CBA-CGA-O2A
22	3	306	CLA	CAA-CBA-CGA-O2A
22	q	301	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	g	302	CLA	CAA-CBA-CGA-O2A
22	C	503	CLA	CAA-CBA-CGA-O2A
26	3	315	CHL	CAA-CBA-CGA-O2A
32	a	410	SQD	O47-C7-C8-C9
36	B	601	DGD	O2G-C1B-C2B-C3B
25	B	622	LHG	O7-C5-C6-O8
25	c	522	LHG	O7-C5-C6-O8
34	A	411	LMG	O7-C8-C9-O8
34	b	621	LMG	O1-C7-C8-O7
36	J	101	DGD	O1G-C1G-C2G-O2G
36	C	519	DGD	O2G-C2G-C3G-O3G
22	v	304	CLA	O1A-CGA-O2A-C1
34	a	412	LMG	C40-C41-C42-C43
22	c	513	CLA	C5-C6-C7-C8
26	n	313	CHL	C13-C15-C16-C17
34	c	520	LMG	C20-C21-C22-C23
36	a	416	DGD	C3B-C4B-C5B-C6B
26	4	313	CHL	O1D-CGD-O2D-CED
22	2	307	CLA	CAA-CBA-CGA-O2A
22	4	301	CLA	CAA-CBA-CGA-O2A
22	5	305	CLA	CAA-CBA-CGA-O2A
22	6	307	CLA	CAA-CBA-CGA-O2A
22	n	302	CLA	CAA-CBA-CGA-O2A
22	g	306	CLA	CAA-CBA-CGA-O2A
22	R	303	CLA	CAA-CBA-CGA-O2A
22	c	502	CLA	CAA-CBA-CGA-O2A
26	6	314	CHL	CAA-CBA-CGA-O2A
32	C	501	SQD	O47-C7-C8-C9
26	n	318	CHL	C4C-C3C-CAC-CBC
26	u	313	CHL	C2A-CAA-CBA-CGA
22	s	304	CLA	CAA-CBA-CGA-O1A
25	4	312	LHG	O1-C1-C2-O2
25	B	622	LHG	O1-C1-C2-O2
22	p	305	CLA	C10-C11-C12-C13
22	r	602	CLA	CAA-CBA-CGA-O2A
22	1	301	CLA	CAA-CBA-CGA-O2A
22	1	302	CLA	CAA-CBA-CGA-O2A
22	Q	306	CLA	CAA-CBA-CGA-O2A
22	N	308	CLA	CAA-CBA-CGA-O2A
22	u	307	CLA	CAA-CBA-CGA-O2A
26	n	317	CHL	CAA-CBA-CGA-O2A
34	b	621	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	4	305	CLA	C8-C10-C11-C12
22	1	304	CLA	C11-C10-C8-C7
22	6	302	CLA	C6-C7-C8-C10
22	6	305	CLA	C12-C13-C15-C16
22	G	307	CLA	C2-C3-C5-C6
26	5	316	CHL	C2-C3-C5-C6
26	6	301	CHL	C11-C10-C8-C7
26	u	318	CHL	C2-C3-C5-C6
22	p	308	CLA	CAA-CBA-CGA-O2A
22	n	306	CLA	CAA-CBA-CGA-O2A
22	S	306	CLA	CAA-CBA-CGA-O2A
25	C	523	LHG	O8-C23-C24-C25
26	u	314	CHL	C2-C1-O2A-CGA
22	6	306	CLA	C6-C7-C8-C9
22	p	308	CLA	C11-C10-C8-C9
22	V	302	CLA	C11-C10-C8-C9
22	n	305	CLA	C6-C7-C8-C9
22	X	202	CLA	C6-C7-C8-C9
22	b	602	CLA	C11-C12-C13-C14
22	b	609	CLA	C11-C12-C13-C14
26	1	318	CHL	C11-C12-C13-C14
26	4	313	CHL	C6-C7-C8-C9
26	5	317	CHL	C11-C12-C13-C14
30	d	401	PHO	C11-C12-C13-C14
30	D	401	PHO	C11-C12-C13-C14
22	R	309	CLA	CAA-CBA-CGA-O1A
22	5	301	CLA	C2B-C3B-CAB-CBB
22	r	607	CLA	O2A-C1-C2-C3
26	V	314	CHL	CBA-CGA-O2A-C1
34	A	411	LMG	C29-C28-O8-C9
22	U	306	CLA	CAA-CBA-CGA-O2A
25	G	310	LHG	O8-C23-C24-C25
36	B	601	DGD	O1G-C1A-C2A-C3A
25	u	312	LHG	O10-C23-C24-C25
22	p	302	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20
36	b	601	DGD	C5B-C6B-C7B-C8B
26	5	318	CHL	C3-C5-C6-C7
25	v	312	LHG	C8-C7-O7-C5
36	c	518	DGD	C2B-C1B-O2G-C2G
22	2	307	CLA	C2A-CAA-CBA-CGA
22	6	308	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	v	307	CLA	C2A-CAA-CBA-CGA
22	V	307	CLA	C2A-CAA-CBA-CGA
22	Q	303	CLA	C2A-CAA-CBA-CGA
32	m	101	SQD	O49-C7-C8-C9
34	c	501	LMG	O10-C28-C29-C30
34	b	624	LMG	C29-C30-C31-C32
22	s	302	CLA	CAA-CBA-CGA-O2A
22	r	603	CLA	CAA-CBA-CGA-O1A
22	v	302	CLA	CAA-CBA-CGA-O1A
22	v	306	CLA	CAA-CBA-CGA-O1A
22	q	306	CLA	CAA-CBA-CGA-O1A
22	N	301	CLA	CAA-CBA-CGA-O1A
22	u	302	CLA	CAA-CBA-CGA-O1A
26	r	616	CHL	CAA-CBA-CGA-O1A
26	3	313	CHL	CAA-CBA-CGA-O1A
34	w	201	LMG	O9-C10-C11-C12
36	B	601	DGD	CDA-CEA-CFA-CGA
22	C	512	CLA	C4-C3-C5-C6
26	Q	312	CHL	O1A-CGA-O2A-C1
33	d	404	PL9	C33-C34-C36-C37
26	n	318	CHL	C5-C6-C7-C8
26	G	312	CHL	CBD-CGD-O2D-CED
36	J	101	DGD	C6A-C7A-C8A-C9A
22	Q	302	CLA	CAA-CBA-CGA-O1A
32	M	101	SQD	O49-C7-C8-C9
23	s	311	LUT	C7-C8-C9-C10
24	R	313	XAT	C7-C8-C9-C10
27	N	318	NEX	C31-C32-C33-C34
31	b	618	BCR	C17-C18-C19-C20
36	c	519	DGD	C6A-C7A-C8A-C9A
22	N	308	CLA	CBA-CGA-O2A-C1
22	a	406	CLA	C1A-C2A-CAA-CBA
22	1	307	CLA	C1A-C2A-CAA-CBA
22	2	303	CLA	C1A-C2A-CAA-CBA
22	3	301	CLA	C1A-C2A-CAA-CBA
22	4	303	CLA	C1A-C2A-CAA-CBA
22	6	302	CLA	C1A-C2A-CAA-CBA
22	6	305	CLA	C1A-C2A-CAA-CBA
22	6	309	CLA	C1A-C2A-CAA-CBA
22	P	303	CLA	C1A-C2A-CAA-CBA
22	P	307	CLA	C1A-C2A-CAA-CBA
22	N	307	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	G	305	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
26	r	616	CHL	C1A-C2A-CAA-CBA
26	4	313	CHL	C1A-C2A-CAA-CBA
26	5	314	CHL	C1A-C2A-CAA-CBA
26	6	301	CHL	C1A-C2A-CAA-CBA
26	q	312	CHL	C1A-C2A-CAA-CBA
26	U	315	CHL	C1A-C2A-CAA-CBA
26	G	311	CHL	C1A-C2A-CAA-CBA
26	g	314	CHL	C1A-C2A-CAA-CBA
26	R	317	CHL	C1A-C2A-CAA-CBA
26	S	314	CHL	C1A-C2A-CAA-CBA
22	1	306	CLA	CAA-CBA-CGA-O1A
22	U	302	CLA	CAA-CBA-CGA-O1A
22	n	301	CLA	CAA-CBA-CGA-O1A
26	2	316	CHL	CAA-CBA-CGA-O1A
26	5	316	CHL	CAA-CBA-CGA-O1A
26	P	315	CHL	CAA-CBA-CGA-O1A
26	R	317	CHL	CAA-CBA-CGA-O1A
36	b	601	DGD	O1A-C1A-C2A-C3A
22	B	615	CLA	CAA-CBA-CGA-O2A
32	M	101	SQD	C13-C14-C15-C16
26	n	316	CHL	O1A-CGA-O2A-C1
22	Q	305	CLA	C2-C1-O2A-CGA
22	Q	306	CLA	C2-C1-O2A-CGA
22	N	302	CLA	C2-C1-O2A-CGA
22	c	511	CLA	C2-C1-O2A-CGA
22	s	307	CLA	C2-C1-O2A-CGA
26	1	318	CHL	C2-C1-O2A-CGA
26	6	317	CHL	C4C-C3C-CAC-CBC
22	N	302	CLA	C10-C11-C12-C13
22	4	306	CLA	CAA-CBA-CGA-O1A
22	5	306	CLA	CAA-CBA-CGA-O1A
22	v	304	CLA	CAA-CBA-CGA-O1A
22	p	303	CLA	CAA-CBA-CGA-O1A
22	G	302	CLA	CAA-CBA-CGA-O1A
22	n	308	CLA	CAA-CBA-CGA-O1A
26	G	315	CHL	CAA-CBA-CGA-O1A
26	u	316	CHL	CAA-CBA-CGA-O1A
26	n	316	CHL	CAA-CBA-CGA-O1A
34	W	201	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	C	502	LMG	O10-C28-C29-C30
36	B	601	DGD	O1A-C1A-C2A-C3A
25	b	623	LHG	C26-C27-C28-C29
32	a	410	SQD	O6-C44-C45-C46
36	C	519	DGD	C1G-C2G-C3G-O3G
36	c	517	DGD	C1G-C2G-C3G-O3G
22	U	307	CLA	CAA-CBA-CGA-O2A
22	s	306	CLA	CAA-CBA-CGA-O2A
25	U	312	LHG	C19-C20-C21-C22
22	3	307	CLA	C2A-CAA-CBA-CGA
22	u	307	CLA	C2A-CAA-CBA-CGA
22	n	307	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	C2A-CAA-CBA-CGA
22	b	614	CLA	C2A-CAA-CBA-CGA
22	s	305	CLA	C2A-CAA-CBA-CGA
36	a	416	DGD	C4B-C5B-C6B-C7B
36	C	519	DGD	CDB-CEB-CFB-CGB
26	3	314	CHL	C16-C17-C18-C19
26	u	318	CHL	C16-C17-C18-C20
22	r	608	CLA	CAA-CBA-CGA-O1A
22	3	306	CLA	CAA-CBA-CGA-O1A
22	6	304	CLA	CAA-CBA-CGA-O1A
22	p	307	CLA	CAA-CBA-CGA-O1A
22	P	308	CLA	CAA-CBA-CGA-O1A
22	N	307	CLA	CAA-CBA-CGA-O1A
22	c	511	CLA	CAA-CBA-CGA-O1A
25	P	313	LHG	O10-C23-C24-C25
22	N	301	CLA	C13-C15-C16-C17
26	q	312	CHL	O1A-CGA-O2A-C1
22	4	304	CLA	CAA-CBA-CGA-O2A
22	4	306	CLA	C10-C11-C12-C13
25	r	613	LHG	C5-C4-O6-P
25	5	312	LHG	C5-C4-O6-P
25	R	314	LHG	C5-C4-O6-P
22	V	304	CLA	CAA-CBA-CGA-O1A
22	u	306	CLA	CAA-CBA-CGA-O1A
22	n	306	CLA	CAA-CBA-CGA-O1A
22	g	302	CLA	CAA-CBA-CGA-O1A
22	C	512	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	CAA-CBA-CGA-O1A
25	U	312	LHG	O10-C23-C24-C25
25	N	312	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	P	308	CLA	C2-C3-C5-C6
22	N	308	CLA	O1A-CGA-O2A-C1
26	5	318	CHL	O1A-CGA-O2A-C1
22	g	304	CLA	C4B-C3B-CAB-CBB
25	3	310	LHG	C3-O3-P-O5
25	4	312	LHG	C3-O3-P-O5
25	5	312	LHG	C3-O3-P-O5
25	5	312	LHG	C4-O6-P-O4
25	P	313	LHG	C4-O6-P-O5
25	G	310	LHG	C3-O3-P-O5
25	g	310	LHG	C3-O3-P-O5
25	g	310	LHG	C4-O6-P-O4
25	S	312	LHG	C3-O3-P-O5
25	C	522	LHG	C4-O6-P-O5
25	b	622	LHG	C3-O3-P-O4
25	s	312	LHG	C3-O3-P-O5
26	6	312	CHL	C4B-C3B-CAB-CBB
26	6	313	CHL	C4B-C3B-CAB-CBB
26	v	313	CHL	C4B-C3B-CAB-CBB
26	q	311	CHL	C4B-C3B-CAB-CBB
26	q	315	CHL	C4B-C3B-CAB-CBB
26	V	313	CHL	C4B-C3B-CAB-CBB
26	N	313	CHL	C4B-C3B-CAB-CBB
26	N	314	CHL	C4B-C3B-CAB-CBB
26	u	316	CHL	C4B-C3B-CAB-CBB
26	n	314	CHL	C4B-C3B-CAB-CBB
26	n	317	CHL	C4B-C3B-CAB-CBB
25	q	310	LHG	C23-C24-C25-C26
26	3	316	CHL	C4C-C3C-CAC-CBC
36	c	518	DGD	CCA-CDA-CEA-CFA
22	2	306	CLA	CAA-CBA-CGA-O1A
22	5	305	CLA	CAA-CBA-CGA-O1A
22	P	303	CLA	CAA-CBA-CGA-O1A
22	N	302	CLA	CAA-CBA-CGA-O1A
22	S	306	CLA	CAA-CBA-CGA-O1A
22	C	503	CLA	CAA-CBA-CGA-O1A
25	G	310	LHG	O10-C23-C24-C25
26	6	314	CHL	CAA-CBA-CGA-O1A
26	s	315	CHL	CAA-CBA-CGA-O1A
36	B	601	DGD	O1B-C1B-C2B-C3B
22	b	609	CLA	CAA-CBA-CGA-O2A
26	6	316	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	O1A-CGA-O2A-C1
34	A	411	LMG	O10-C28-O8-C9
36	A	414	DGD	C3B-C4B-C5B-C6B
36	J	101	DGD	CBB-CCB-CDB-CEB
22	S	302	CLA	CAA-CBA-CGA-O2A
23	p	310	LUT	C5-C6-C7-C8
23	P	311	LUT	C5-C6-C7-C8
23	S	311	LUT	C5-C6-C7-C8
31	B	618	BCR	C1-C6-C7-C8
36	C	520	DGD	C2A-C3A-C4A-C5A
22	q	302	CLA	C13-C15-C16-C17
22	1	302	CLA	CAA-CBA-CGA-O1A
22	p	308	CLA	CAA-CBA-CGA-O1A
22	U	306	CLA	CAA-CBA-CGA-O1A
22	R	304	CLA	CAA-CBA-CGA-O1A
26	1	316	CHL	CAA-CBA-CGA-O1A
26	3	315	CHL	CAA-CBA-CGA-O1A
26	g	314	CHL	CAA-CBA-CGA-O1A
26	S	315	CHL	CAA-CBA-CGA-O1A
34	B	621	LMG	O10-C28-C29-C30
36	b	601	DGD	O1B-C1B-C2B-C3B
25	5	312	LHG	C35-C36-C37-C38
25	P	313	LHG	C27-C28-C29-C30
26	1	317	CHL	O1A-CGA-O2A-C1
26	U	314	CHL	O1A-CGA-O2A-C1
25	4	312	LHG	O8-C23-C24-C25
26	P	314	CHL	CAA-CBA-CGA-O2A
22	G	301	CLA	C5-C6-C7-C8
22	B	613	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C20
22	N	307	CLA	C2A-CAA-CBA-CGA
22	P	307	CLA	CAA-CBA-CGA-O1A
22	N	306	CLA	CAA-CBA-CGA-O1A
22	P	302	CLA	C13-C15-C16-C17
22	Q	304	CLA	C10-C11-C12-C13
22	P	309	CLA	CAA-CBA-CGA-O2A
26	6	301	CHL	CAA-CBA-CGA-O2A
22	G	304	CLA	C13-C15-C16-C17
22	r	602	CLA	CAA-CBA-CGA-O1A
22	2	307	CLA	CAA-CBA-CGA-O1A
30	A	407	PHO	C4-C3-C5-C6
22	1	305	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C2-C3-C5-C6
22	p	306	CLA	C11-C12-C13-C14
22	D	403	CLA	C16-C17-C18-C19
22	s	302	CLA	CAA-CBA-CGA-O1A
22	p	302	CLA	CAD-CBD-CGD-O1D
22	p	309	CLA	CAD-CBD-CGD-O1D
22	U	306	CLA	CAD-CBD-CGD-O1D
22	G	305	CLA	CAD-CBD-CGD-O1D
22	u	306	CLA	CAD-CBD-CGD-O1D
22	n	308	CLA	CAD-CBD-CGD-O1D
22	g	305	CLA	CAD-CBD-CGD-O1D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O1D
26	r	615	CHL	CAD-CBD-CGD-O1D
26	u	317	CHL	CAD-CBD-CGD-O1D
26	n	318	CHL	CAD-CBD-CGD-O1D
26	S	314	CHL	CAD-CBD-CGD-O1D
26	s	314	CHL	CAD-CBD-CGD-O1D
27	u	319	NEX	C7-C8-C9-C10
32	l	102	SQD	O5-C5-C6-S
32	L	102	SQD	O5-C5-C6-S
32	C	501	SQD	O5-C5-C6-S
22	1	301	CLA	CAA-CBA-CGA-O1A
22	2	302	CLA	CAA-CBA-CGA-O1A
22	4	302	CLA	CAA-CBA-CGA-O1A
22	5	302	CLA	CAA-CBA-CGA-O1A
25	C	523	LHG	O10-C23-C24-C25
36	J	101	DGD	C5B-C6B-C7B-C8B
22	3	303	CLA	CAA-CBA-CGA-O2A
22	6	302	CLA	CAA-CBA-CGA-O2A
22	v	301	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
25	c	522	LHG	O8-C23-C24-C25
22	1	304	CLA	C11-C10-C8-C9
22	N	304	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C12-C13-C14
22	b	610	CLA	C14-C13-C15-C16
22	c	508	CLA	C11-C10-C8-C9
26	Q	314	CHL	C6-C7-C8-C9
36	B	601	DGD	C4B-C5B-C6B-C7B
25	q	310	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
22	A	408	CLA	CBD-CGD-O2D-CED
34	C	521	LMG	C20-C21-C22-C23
22	3	304	CLA	C5-C6-C7-C8
26	U	319	CHL	C13-C15-C16-C17
22	4	301	CLA	CAA-CBA-CGA-O1A
22	6	307	CLA	CAA-CBA-CGA-O1A
22	N	308	CLA	CAA-CBA-CGA-O1A
22	g	306	CLA	CAA-CBA-CGA-O1A
26	n	317	CHL	CAA-CBA-CGA-O1A
25	A	413	LHG	C15-C16-C17-C18
25	R	314	LHG	C19-C20-C21-C22
22	v	304	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
26	U	314	CHL	CBA-CGA-O2A-C1
26	n	316	CHL	CBA-CGA-O2A-C1
22	1	307	CLA	CAA-CBA-CGA-O2A
22	3	301	CLA	CAA-CBA-CGA-O2A
22	3	307	CLA	CAA-CBA-CGA-O2A
22	v	303	CLA	CAA-CBA-CGA-O2A
22	V	306	CLA	CAA-CBA-CGA-O2A
22	Q	301	CLA	CAA-CBA-CGA-O2A
22	U	301	CLA	CAA-CBA-CGA-O2A
22	n	307	CLA	CAA-CBA-CGA-O2A
22	R	308	CLA	CAA-CBA-CGA-O2A
22	C	507	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
26	1	314	CHL	CAA-CBA-CGA-O2A
26	1	317	CHL	CAA-CBA-CGA-O2A
26	p	314	CHL	CAA-CBA-CGA-O2A
26	u	313	CHL	CAA-CBA-CGA-O2A
26	n	313	CHL	CAA-CBA-CGA-O2A
22	r	606	CLA	C15-C16-C17-C18
22	C	506	CLA	C8-C10-C11-C12
22	V	307	CLA	O1A-CGA-O2A-C1
36	B	601	DGD	C8A-C9A-CAA-CBA
22	4	307	CLA	CAA-CBA-CGA-O2A
22	5	301	CLA	CAA-CBA-CGA-O2A
22	v	308	CLA	CAA-CBA-CGA-O2A
22	p	302	CLA	CAA-CBA-CGA-O2A
22	P	302	CLA	CAA-CBA-CGA-O2A
22	G	306	CLA	CAA-CBA-CGA-O2A
22	S	305	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	CAA-CBA-CGA-O2A
25	q	310	LHG	O8-C23-C24-C25
26	V	313	CHL	CAA-CBA-CGA-O2A
26	U	313	CHL	CAA-CBA-CGA-O2A
26	N	313	CHL	CAA-CBA-CGA-O2A
32	M	101	SQD	O47-C7-C8-C9
22	R	307	CLA	C5-C6-C7-C8
26	1	317	CHL	C10-C11-C12-C13
25	V	312	LHG	C34-C35-C36-C37
25	Q	310	LHG	C24-C25-C26-C27
26	Q	312	CHL	C2-C1-O2A-CGA
32	C	501	SQD	C7-C8-C9-C10
22	q	301	CLA	CAA-CBA-CGA-O1A
22	Q	306	CLA	CAA-CBA-CGA-O1A
22	R	303	CLA	CAA-CBA-CGA-O1A
25	g	310	LHG	C2-C3-O3-P
22	G	307	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
26	2	318	CHL	C4-C3-C5-C6
26	5	318	CHL	C4-C3-C5-C6
26	V	318	CHL	C4-C3-C5-C6
22	v	301	CLA	C13-C15-C16-C17
25	C	523	LHG	C12-C13-C14-C15
22	x	201	CLA	C6-C7-C8-C10
22	2	302	CLA	C3A-C2A-CAA-CBA
22	2	306	CLA	C3A-C2A-CAA-CBA
22	5	302	CLA	C3A-C2A-CAA-CBA
22	5	306	CLA	C3A-C2A-CAA-CBA
22	v	304	CLA	C3A-C2A-CAA-CBA
22	C	513	CLA	C11-C12-C13-C15
22	B	605	CLA	C3A-C2A-CAA-CBA
22	B	605	CLA	C11-C12-C13-C15
22	B	606	CLA	C2-C3-C5-C6
22	B	609	CLA	C11-C12-C13-C15
22	b	603	CLA	C12-C13-C15-C16
22	b	613	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
26	r	619	CHL	C3A-C2A-CAA-CBA
26	3	316	CHL	C3A-C2A-CAA-CBA
26	4	316	CHL	C12-C13-C15-C16
26	5	318	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	6	317	CHL	C3A-C2A-CAA-CBA
26	V	316	CHL	C6-C7-C8-C10
26	Q	314	CHL	C6-C7-C8-C10
26	U	315	CHL	C3A-C2A-CAA-CBA
26	U	317	CHL	C6-C7-C8-C10
26	U	319	CHL	C11-C10-C8-C7
26	G	315	CHL	C3A-C2A-CAA-CBA
26	G	316	CHL	C3A-C2A-CAA-CBA
26	n	318	CHL	C6-C7-C8-C10
33	D	405	PL9	C33-C34-C36-C37
22	3	301	CLA	CAA-CBA-CGA-O1A
22	6	302	CLA	CAA-CBA-CGA-O1A
22	V	301	CLA	CAA-CBA-CGA-O1A
22	n	302	CLA	CAA-CBA-CGA-O1A
37	e	101	HEM	CAA-CBA-CGA-O1A
32	L	102	SQD	C28-C29-C30-C31
22	r	607	CLA	CAA-CBA-CGA-O2A
22	A	404	CLA	CAA-CBA-CGA-O2A
22	1	304	CLA	CAA-CBA-CGA-O2A
22	2	301	CLA	CAA-CBA-CGA-O2A
22	V	301	CLA	CAA-CBA-CGA-O2A
22	B	611	CLA	CAA-CBA-CGA-O2A
22	c	506	CLA	CAA-CBA-CGA-O2A
25	Q	310	LHG	O8-C23-C24-C25
25	b	622	LHG	O8-C23-C24-C25
26	4	313	CHL	CAA-CBA-CGA-O2A
26	g	312	CHL	CAA-CBA-CGA-O2A
32	l	102	SQD	C28-C29-C30-C31
23	S	311	LUT	C7-C8-C9-C10
24	1	311	XAT	C27-C28-C29-C30
24	q	309	XAT	C27-C28-C29-C30
27	5	319	NEX	C31-C32-C33-C34
31	B	618	BCR	C17-C18-C19-C20
22	C	507	CLA	CAA-CBA-CGA-O1A
22	B	615	CLA	CAA-CBA-CGA-O1A
22	b	611	CLA	CAA-CBA-CGA-O1A
26	n	313	CHL	CAA-CBA-CGA-O1A
32	C	501	SQD	O49-C7-C8-C9
24	v	311	XAT	C13-C14-C15-C35
24	p	312	XAT	C9-C10-C11-C12
31	b	620	BCR	C13-C14-C15-C16
32	C	501	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
34	C	502	LMG	C31-C32-C33-C34
26	u	318	CHL	C16-C17-C18-C19
22	a	404	CLA	CAA-CBA-CGA-O2A
22	2	305	CLA	CAA-CBA-CGA-O2A
25	5	312	LHG	O8-C23-C24-C25
26	4	316	CHL	CAA-CBA-CGA-O2A
26	N	316	CHL	CAA-CBA-CGA-O2A
32	m	101	SQD	O47-C7-C8-C9
22	3	303	CLA	CAA-CBA-CGA-O1A
22	v	301	CLA	CAA-CBA-CGA-O1A
22	v	303	CLA	CAA-CBA-CGA-O1A
22	U	307	CLA	CAA-CBA-CGA-O1A
22	u	307	CLA	CAA-CBA-CGA-O1A
22	n	307	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	CAA-CBA-CGA-O1A
22	b	617	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
22	s	306	CLA	CAA-CBA-CGA-O1A
25	c	522	LHG	O10-C23-C24-C25
26	4	313	CHL	CAA-CBA-CGA-O1A
26	V	313	CHL	CAA-CBA-CGA-O1A
36	a	416	DGD	CDB-CEB-CFB-CGB
22	v	307	CLA	C8-C10-C11-C12
22	Q	301	CLA	C13-C15-C16-C17
25	L	101	LHG	O2-C2-C3-O3
22	u	301	CLA	CAA-CBA-CGA-O2A
26	P	318	CHL	CAA-CBA-CGA-O2A
26	U	319	CHL	CAA-CBA-CGA-O2A
36	C	520	DGD	O1G-C1A-C2A-C3A
25	c	522	LHG	C30-C31-C32-C33
26	P	319	CHL	C2C-C3C-CAC-CBC
22	3	307	CLA	CAA-CBA-CGA-O1A
22	4	304	CLA	CAA-CBA-CGA-O1A
22	R	308	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	CAA-CBA-CGA-O1A
25	4	312	LHG	O10-C23-C24-C25
26	1	317	CHL	CAA-CBA-CGA-O1A
26	p	314	CHL	CAA-CBA-CGA-O1A
26	N	313	CHL	CAA-CBA-CGA-O1A
22	U	308	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C2A-CAA-CBA-CGA
26	p	318	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
26	v	318	CHL	C4C-C3C-CAC-CBC
22	q	306	CLA	C8-C10-C11-C12
22	u	307	CLA	C5-C6-C7-C8
22	S	305	CLA	C5-C6-C7-C8
22	S	306	CLA	C5-C6-C7-C8
22	b	615	CLA	C13-C15-C16-C17
26	Q	312	CHL	CBA-CGA-O2A-C1
36	C	520	DGD	C6B-C7B-C8B-C9B
22	A	408	CLA	C3-C5-C6-C7
22	Q	301	CLA	CAA-CBA-CGA-O1A
26	N	316	CHL	CAA-CBA-CGA-O1A
22	P	308	CLA	C4-C3-C5-C6
25	v	312	LHG	C12-C13-C14-C15
22	G	304	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	CAA-CBA-CGA-O2A
26	2	313	CHL	CAA-CBA-CGA-O2A
22	S	302	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

459 monomers are involved in 949 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	608	CLA	3	0
22	v	302	CLA	6	0
25	C	522	LHG	3	0
23	2	309	LUT	4	0
26	U	319	CHL	6	0
27	r	618	NEX	3	0
26	6	315	CHL	7	0
22	b	606	CLA	3	0
22	C	503	CLA	1	0
25	5	312	LHG	1	0
34	b	621	LMG	4	0
26	n	317	CHL	1	0
23	V	309	LUT	5	0
31	b	618	BCR	5	0
26	Q	311	CHL	2	0
22	r	601	CLA	1	0
32	a	413	SQD	3	0
22	g	302	CLA	1	0
26	2	316	CHL	6	0
22	p	307	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	603	CLA	6	0
26	3	311	CHL	4	0
27	2	319	NEX	1	0
25	D	407	LHG	7	0
23	5	309	LUT	6	0
24	4	311	XAT	1	0
22	p	309	CLA	2	0
24	1	311	XAT	2	0
22	3	307	CLA	2	0
22	B	602	CLA	4	0
24	P	312	XAT	4	0
22	c	512	CLA	1	0
22	N	306	CLA	1	0
33	d	404	PL9	3	0
31	b	620	BCR	3	0
26	2	318	CHL	6	0
22	5	301	CLA	4	0
35	a	414	BCT	1	0
22	v	304	CLA	3	0
22	C	513	CLA	1	0
25	s	312	LHG	3	0
34	a	412	LMG	1	0
23	1	310	LUT	3	0
22	q	303	CLA	2	0
22	c	513	CLA	3	0
22	b	615	CLA	1	0
22	1	308	CLA	2	0
22	Q	303	CLA	1	0
22	5	304	CLA	2	0
34	b	624	LMG	1	0
22	B	606	CLA	4	0
22	U	302	CLA	2	0
22	2	304	CLA	3	0
22	q	301	CLA	1	0
26	u	314	CHL	1	0
22	Q	301	CLA	3	0
26	6	314	CHL	2	0
22	s	301	CLA	2	0
22	6	307	CLA	2	0
25	L	101	LHG	2	0
22	v	303	CLA	1	0
27	R	301	NEX	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	601	DGD	6	0
31	C	517	BCR	1	0
22	n	304	CLA	1	0
22	V	302	CLA	3	0
22	C	506	CLA	3	0
23	p	310	LUT	1	0
27	s	317	NEX	4	0
22	C	511	CLA	3	0
26	U	317	CHL	6	0
26	3	314	CHL	6	0
22	c	502	CLA	1	0
36	C	520	DGD	3	0
26	U	315	CHL	5	0
22	C	508	CLA	2	0
24	p	312	XAT	3	0
24	r	612	XAT	4	0
26	g	311	CHL	6	0
22	P	303	CLA	4	0
26	n	318	CHL	6	0
37	E	101	HEM	1	0
36	J	101	DGD	2	0
25	V	312	LHG	6	0
25	d	406	LHG	7	0
25	6	311	LHG	3	0
31	t	101	BCR	6	0
26	N	313	CHL	5	0
30	D	401	PHO	1	0
22	B	603	CLA	3	0
22	r	609	CLA	3	0
22	b	607	CLA	1	0
22	r	610	CLA	2	0
22	n	303	CLA	1	0
31	T	101	BCR	5	0
34	C	502	LMG	1	0
26	R	317	CHL	3	0
25	P	313	LHG	1	0
22	s	302	CLA	1	0
26	S	313	CHL	1	0
24	v	311	XAT	3	0
26	p	320	CHL	2	0
22	4	306	CLA	5	0
22	U	305	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	317	CHL	5	0
36	b	601	DGD	7	0
22	A	406	CLA	2	0
22	C	514	CLA	2	0
23	u	309	LUT	2	0
22	6	304	CLA	1	0
22	5	303	CLA	1	0
26	5	317	CHL	3	0
26	n	316	CHL	6	0
22	b	614	CLA	4	0
22	5	302	CLA	6	0
22	q	306	CLA	1	0
24	u	311	XAT	3	0
22	U	304	CLA	1	0
26	u	318	CHL	6	0
32	L	102	SQD	2	0
22	b	602	CLA	4	0
31	B	618	BCR	6	0
24	2	311	XAT	5	0
22	v	301	CLA	1	0
22	b	612	CLA	1	0
22	C	515	CLA	3	0
23	S	311	LUT	5	0
22	B	607	CLA	2	0
22	B	615	CLA	1	0
25	l	101	LHG	1	0
25	4	312	LHG	1	0
22	R	304	CLA	4	0
22	P	309	CLA	2	0
23	U	310	LUT	3	0
22	c	514	CLA	3	0
22	S	301	CLA	2	0
23	4	309	LUT	4	0
31	C	518	BCR	1	0
26	P	319	CHL	9	0
26	1	317	CHL	2	0
22	X	202	CLA	1	0
22	R	307	CLA	1	0
22	1	306	CLA	2	0
22	b	613	CLA	3	0
23	r	611	LUT	4	0
25	n	312	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	311	LUT	4	0
22	3	302	CLA	3	0
22	N	308	CLA	1	0
22	r	604	CLA	2	0
23	n	309	LUT	3	0
26	q	313	CHL	1	0
22	u	307	CLA	2	0
26	S	315	CHL	2	0
22	3	306	CLA	2	0
23	s	311	LUT	4	0
22	2	307	CLA	4	0
22	4	307	CLA	4	0
22	4	308	CLA	1	0
25	q	310	LHG	2	0
26	u	317	CHL	1	0
22	c	505	CLA	2	0
22	B	614	CLA	4	0
25	Q	310	LHG	4	0
26	5	318	CHL	5	0
22	G	302	CLA	3	0
30	A	407	PHO	4	0
22	6	303	CLA	1	0
36	c	519	DGD	1	0
22	B	609	CLA	1	0
27	v	319	NEX	2	0
26	n	313	CHL	3	0
31	c	515	BCR	1	0
22	N	305	CLA	1	0
26	q	311	CHL	7	0
22	s	305	CLA	4	0
23	R	312	LUT	2	0
22	c	509	CLA	3	0
26	P	317	CHL	5	0
26	r	614	CHL	2	0
22	5	305	CLA	2	0
22	p	302	CLA	2	0
22	6	305	CLA	3	0
26	v	317	CHL	1	0
22	B	605	CLA	2	0
22	N	302	CLA	5	0
32	l	102	SQD	3	0
22	A	404	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	p	317	CHL	4	0
22	P	308	CLA	3	0
22	p	306	CLA	1	0
22	b	617	CLA	2	0
22	g	303	CLA	1	0
26	1	313	CHL	1	0
25	A	413	LHG	3	0
32	m	101	SQD	1	0
22	Q	308	CLA	2	0
22	A	408	CLA	1	0
27	r	617	NEX	4	0
22	P	305	CLA	2	0
22	P	306	CLA	1	0
22	n	301	CLA	3	0
26	v	313	CHL	1	0
22	5	308	CLA	1	0
24	q	309	XAT	1	0
22	a	408	CLA	1	0
22	C	510	CLA	4	0
34	B	621	LMG	3	0
25	C	524	LHG	2	0
22	N	307	CLA	3	0
26	6	301	CHL	5	0
31	x	202	BCR	3	0
22	p	303	CLA	3	0
22	3	304	CLA	3	0
25	D	406	LHG	4	0
26	q	315	CHL	3	0
30	d	401	PHO	1	0
25	p	313	LHG	2	0
26	Q	315	CHL	4	0
22	P	302	CLA	3	0
26	Q	314	CHL	1	0
22	q	308	CLA	3	0
22	S	304	CLA	2	0
26	s	315	CHL	1	0
22	n	302	CLA	6	0
22	2	302	CLA	5	0
26	u	316	CHL	3	0
25	u	312	LHG	2	0
26	U	314	CHL	2	0
25	c	521	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Q	316	CHL	2	0
27	P	301	NEX	1	0
22	U	307	CLA	1	0
22	q	302	CLA	2	0
37	e	101	HEM	1	0
22	g	301	CLA	1	0
23	1	309	LUT	2	0
25	2	312	LHG	3	0
26	6	317	CHL	2	0
22	G	303	CLA	1	0
24	g	309	XAT	5	0
25	v	312	LHG	4	0
22	B	610	CLA	4	0
22	V	307	CLA	2	0
31	X	201	BCR	4	0
25	3	310	LHG	3	0
22	S	305	CLA	2	0
27	V	319	NEX	3	0
26	g	315	CHL	3	0
22	3	301	CLA	3	0
26	3	312	CHL	1	0
22	G	301	CLA	2	0
22	b	616	CLA	1	0
27	u	320	NEX	2	0
22	S	302	CLA	1	0
24	U	311	XAT	5	0
26	V	317	CHL	2	0
22	U	306	CLA	4	0
26	g	312	CHL	1	0
31	a	409	BCR	3	0
27	5	319	NEX	2	0
22	v	306	CLA	1	0
22	s	304	CLA	2	0
26	R	315	CHL	1	0
31	C	516	BCR	2	0
23	n	310	LUT	4	0
24	6	310	XAT	4	0
32	M	101	SQD	1	0
31	k	101	BCR	2	0
22	1	303	CLA	1	0
26	v	316	CHL	7	0
22	C	505	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	V	301	CLA	3	0
22	A	405	CLA	5	0
36	C	519	DGD	4	0
22	3	303	CLA	2	0
24	R	313	XAT	3	0
22	V	306	CLA	2	0
26	5	314	CHL	1	0
22	a	405	CLA	3	0
22	C	509	CLA	1	0
34	w	201	LMG	2	0
34	C	521	LMG	3	0
22	Q	305	CLA	1	0
22	S	307	CLA	1	0
24	3	309	XAT	2	0
24	G	309	XAT	3	0
22	1	301	CLA	3	0
22	V	304	CLA	2	0
23	s	310	LUT	6	0
26	5	316	CHL	3	0
26	N	316	CHL	2	0
32	C	501	SQD	2	0
22	s	307	CLA	2	0
22	D	403	CLA	3	0
25	a	415	LHG	1	0
22	c	507	CLA	2	0
22	2	305	CLA	3	0
27	n	319	NEX	2	0
34	A	411	LMG	1	0
23	u	310	LUT	4	0
22	a	404	CLA	1	0
23	P	310	LUT	3	0
22	n	307	CLA	1	0
26	G	312	CHL	1	0
26	V	313	CHL	7	0
22	R	311	CLA	2	0
22	u	301	CLA	5	0
22	b	604	CLA	5	0
22	n	305	CLA	1	0
22	a	406	CLA	2	0
22	r	603	CLA	4	0
26	6	312	CHL	2	0
25	r	613	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	412	SQD	3	0
26	P	318	CHL	3	0
26	1	314	CHL	1	0
36	c	518	DGD	3	0
22	r	607	CLA	1	0
25	g	310	LHG	2	0
31	z	101	BCR	2	0
27	N	318	NEX	2	0
24	N	311	XAT	2	0
22	b	610	CLA	2	0
26	p	314	CHL	3	0
33	D	405	PL9	3	0
34	W	201	LMG	2	0
35	D	402	BCT	1	0
31	K	101	BCR	2	0
31	B	619	BCR	4	0
22	P	307	CLA	2	0
22	R	303	CLA	2	0
22	s	306	CLA	3	0
26	g	314	CHL	2	0
24	5	311	XAT	3	0
26	S	314	CHL	1	0
31	D	404	BCR	1	0
26	v	318	CHL	7	0
22	1	305	CLA	1	0
23	U	309	LUT	1	0
22	n	308	CLA	2	0
26	G	316	CHL	2	0
22	R	308	CLA	1	0
22	5	306	CLA	2	0
26	2	317	CHL	1	0
26	G	314	CHL	4	0
22	V	303	CLA	2	0
22	G	307	CLA	3	0
22	v	305	CLA	1	0
23	5	310	LUT	8	0
26	r	616	CHL	4	0
22	B	608	CLA	1	0
25	c	523	LHG	3	0
27	u	319	NEX	1	0
22	B	613	CLA	3	0
22	U	301	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	409	BCR	4	0
22	c	510	CLA	2	0
22	C	507	CLA	1	0
22	P	304	CLA	1	0
23	p	311	LUT	4	0
22	d	402	CLA	2	0
26	q	314	CHL	2	0
23	N	310	LUT	4	0
26	V	316	CHL	4	0
22	6	309	CLA	1	0
22	c	503	CLA	1	0
26	6	316	CHL	2	0
22	5	307	CLA	2	0
22	2	301	CLA	4	0
22	p	305	CLA	2	0
22	4	301	CLA	4	0
23	N	309	LUT	5	0
26	u	313	CHL	1	0
22	q	307	CLA	2	0
26	4	314	CHL	1	0
36	a	416	DGD	2	0
22	Q	307	CLA	3	0
26	U	313	CHL	1	0
27	p	301	NEX	4	0
26	3	313	CHL	2	0
23	v	310	LUT	4	0
22	c	508	CLA	1	0
36	A	414	DGD	2	0
22	4	302	CLA	5	0
32	a	410	SQD	3	0
22	p	308	CLA	1	0
23	v	309	LUT	3	0
22	c	504	CLA	4	0
26	V	318	CHL	4	0
26	6	313	CHL	1	0
24	n	311	XAT	1	0
22	r	602	CLA	3	0
23	S	310	LUT	4	0
34	c	501	LMG	1	0
25	d	405	LHG	5	0
26	N	317	CHL	5	0
22	B	604	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	302	CLA	4	0
26	G	315	CHL	2	0
22	2	306	CLA	2	0
22	V	305	CLA	1	0
26	p	315	CHL	1	0
31	b	619	BCR	4	0
22	S	306	CLA	2	0
22	N	301	CLA	3	0
22	6	308	CLA	1	0
26	G	311	CHL	4	0
25	U	312	LHG	4	0
30	a	407	PHO	2	0
22	Q	302	CLA	4	0
26	r	615	CHL	2	0
22	2	308	CLA	1	0
34	c	520	LMG	2	0
25	N	312	LHG	4	0
22	C	504	CLA	2	0
22	V	308	CLA	1	0
26	R	316	CHL	1	0
34	B	624	LMG	1	0
22	g	307	CLA	1	0
22	u	305	CLA	4	0
26	5	313	CHL	2	0
22	u	306	CLA	2	0
22	g	304	CLA	1	0
22	R	305	CLA	2	0
22	2	303	CLA	1	0
22	C	512	CLA	3	0
26	1	316	CHL	3	0
25	S	312	LHG	5	0
23	4	310	LUT	5	0
22	r	606	CLA	4	0
22	N	303	CLA	1	0
22	c	506	CLA	1	0
22	1	307	CLA	3	0
26	s	314	CHL	1	0
27	S	317	NEX	3	0
22	R	302	CLA	1	0
24	V	311	XAT	4	0
26	1	318	CHL	5	0
26	3	315	CHL	3	0

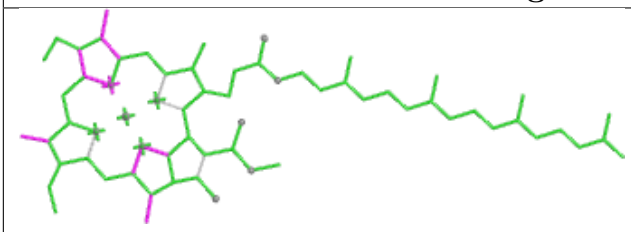
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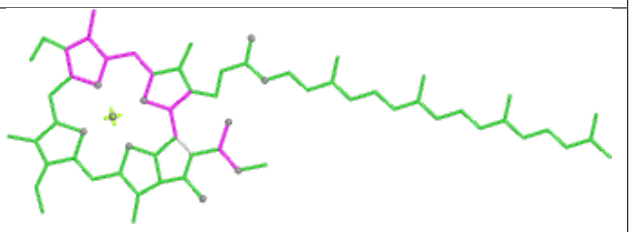
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	605	CLA	1	0
26	3	316	CHL	1	0
26	4	316	CHL	2	0
22	v	307	CLA	2	0
31	B	620	BCR	1	0
22	c	511	CLA	3	0
22	n	306	CLA	1	0
26	2	314	CHL	1	0
22	u	302	CLA	2	0
23	2	310	LUT	4	0
26	p	319	CHL	4	0
26	2	313	CHL	1	0
22	6	302	CLA	3	0
26	4	313	CHL	3	0
36	c	517	DGD	4	0
22	p	304	CLA	1	0
22	R	310	CLA	2	0
26	P	315	CHL	1	0
23	V	310	LUT	6	0

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

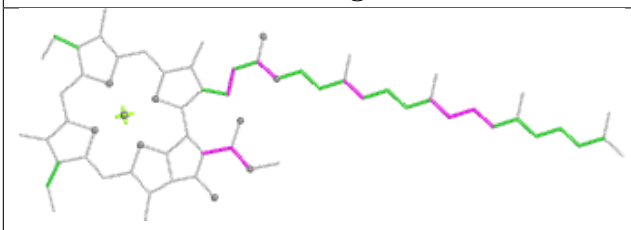
Ligand CLA b 608



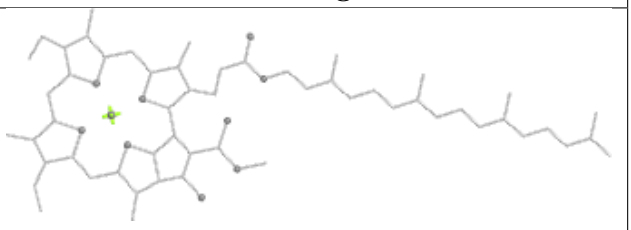
Bond lengths



Bond angles

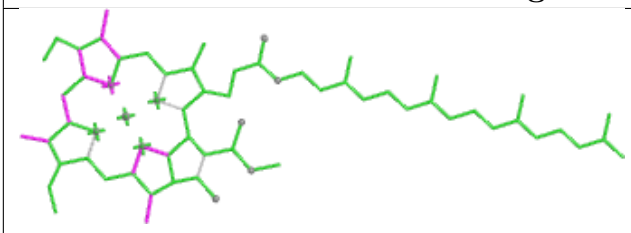


Torsions

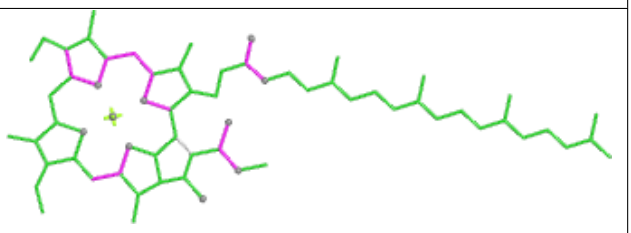


Rings

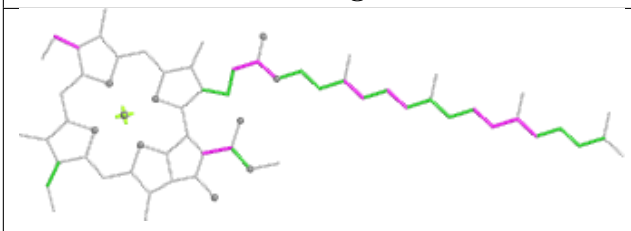
Ligand CLA v 302



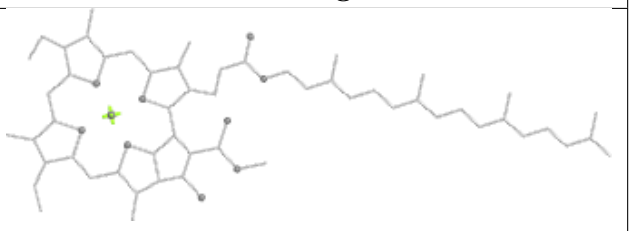
Bond lengths



Bond angles

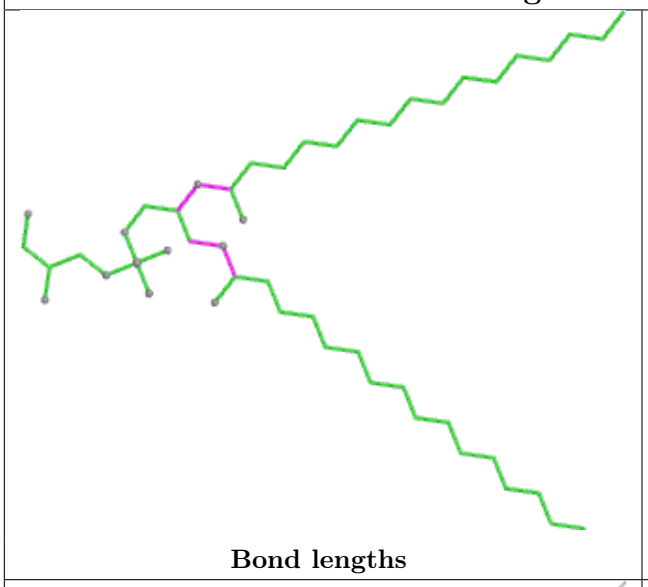


Torsions

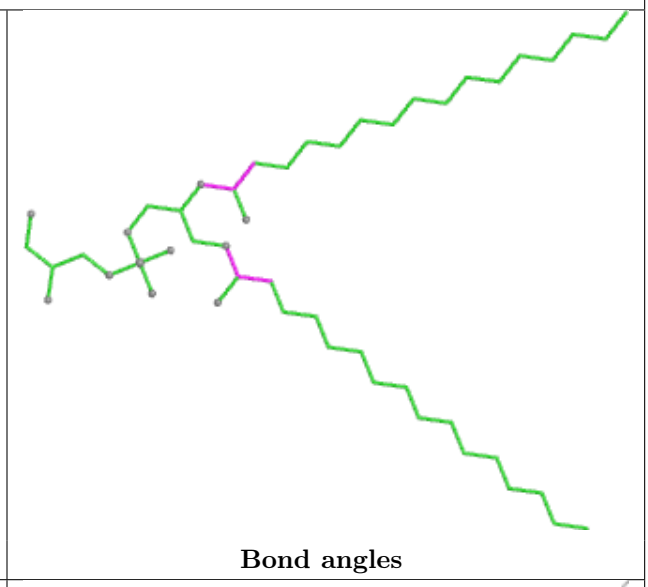


Rings

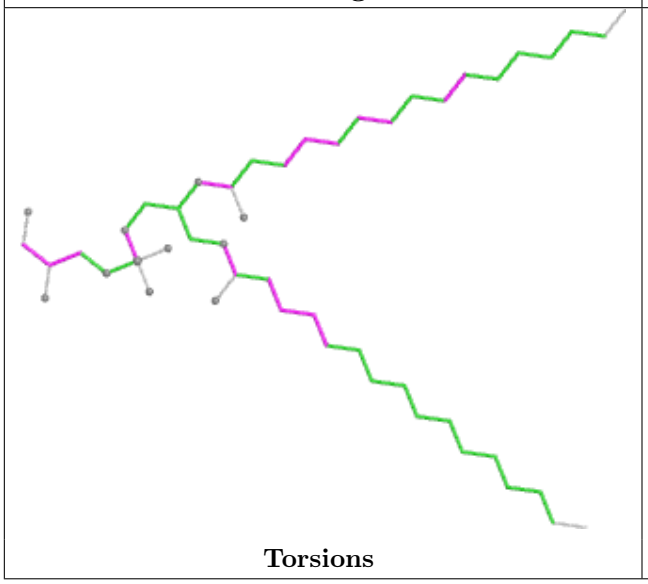
Ligand LHG C 522



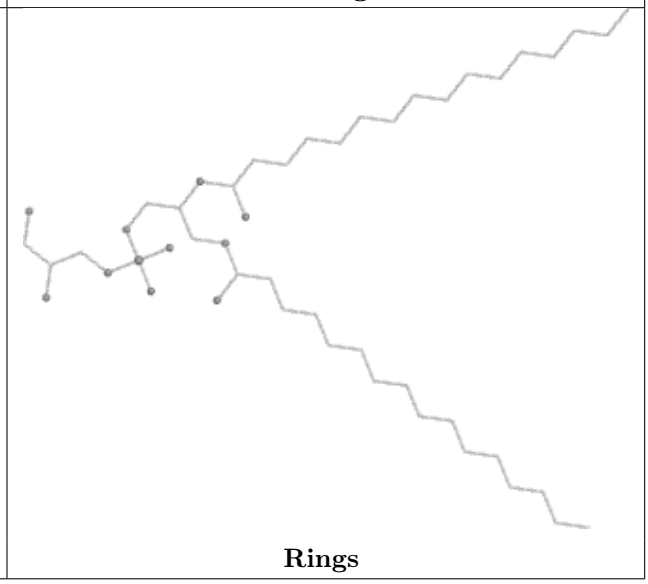
Bond lengths



Bond angles

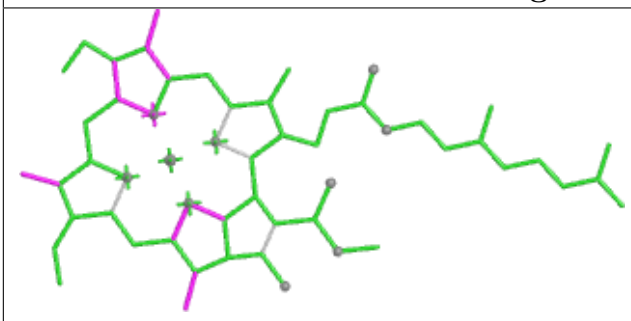


Torsions

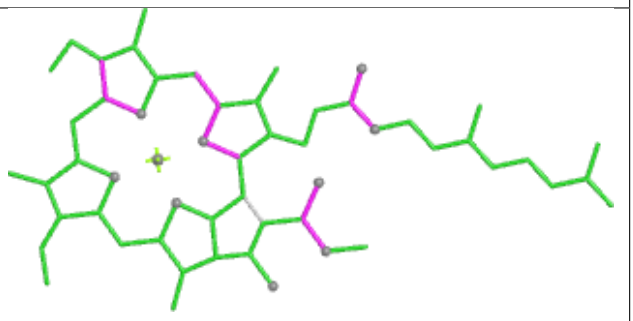


Rings

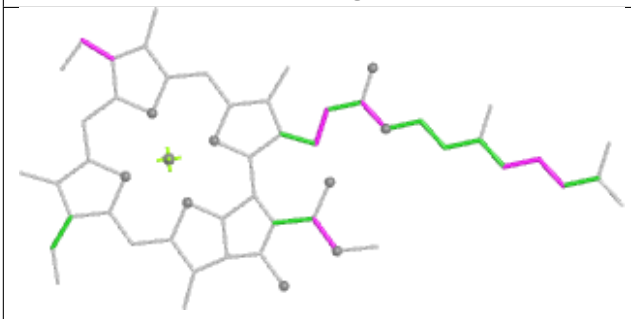
Ligand CLA s 308



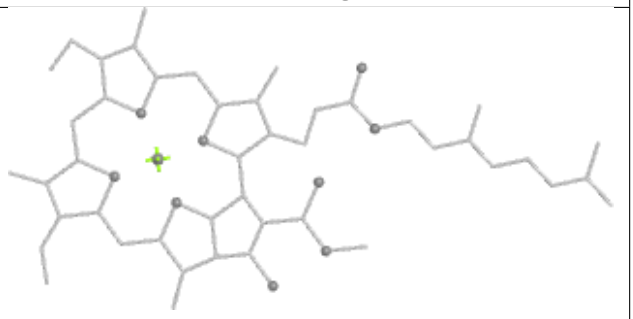
Bond lengths



Bond angles

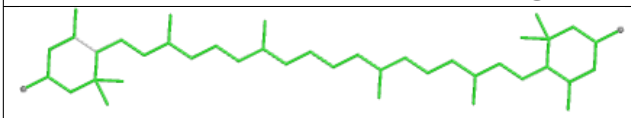


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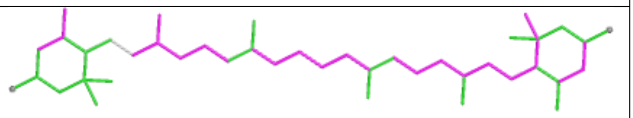


Rings

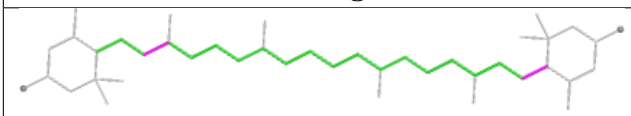
Ligand LUT 2 309



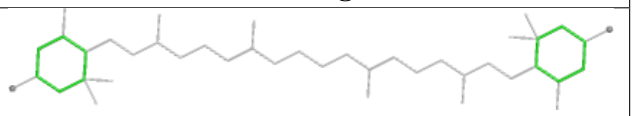
Bond lengths



Bond angles

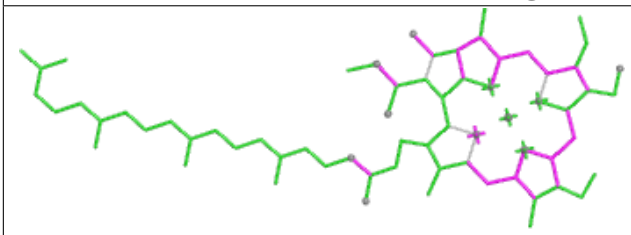


Torsions

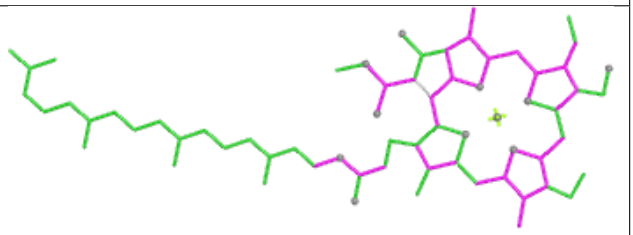


Rings

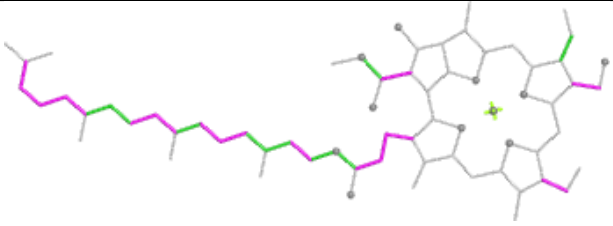
Ligand CHL U 319



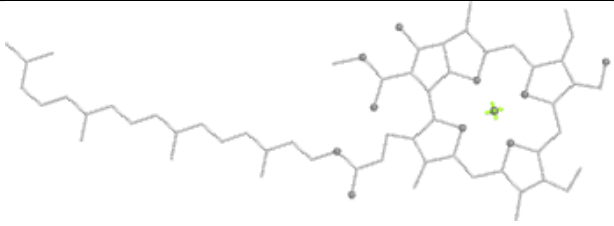
Bond lengths



Bond angles

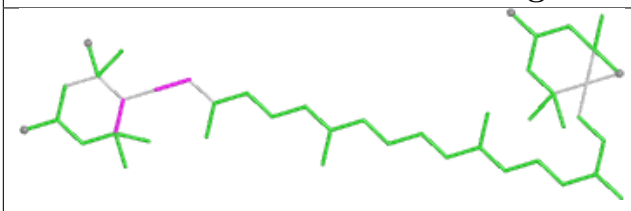


Torsions

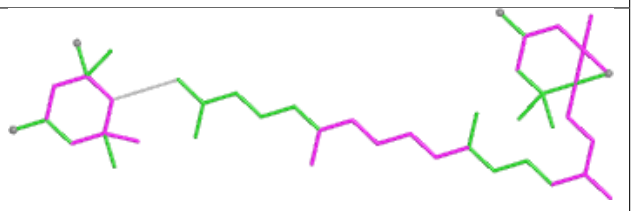


Rings

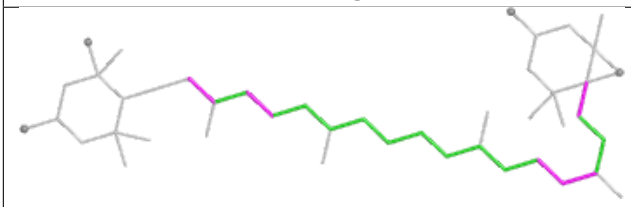
Ligand NEX r 618



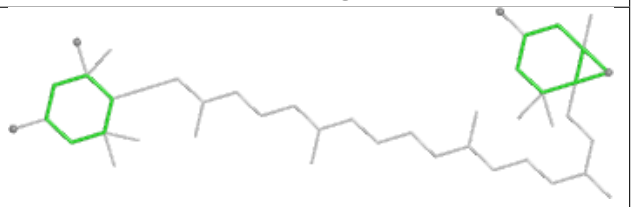
Bond lengths



Bond angles

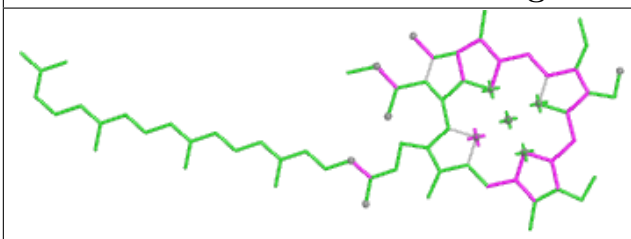


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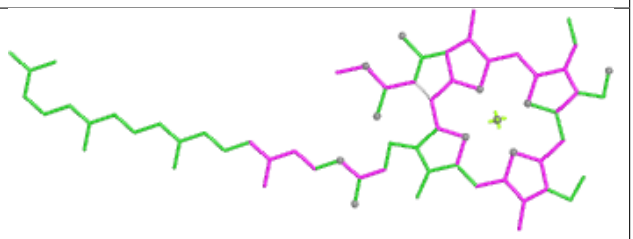


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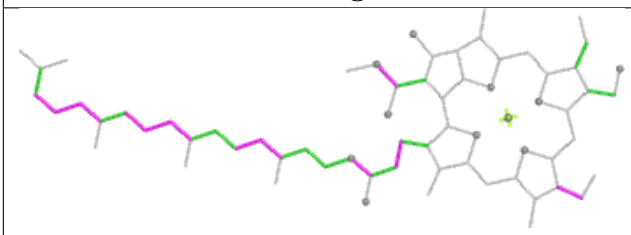
Ligand CHL 6 315



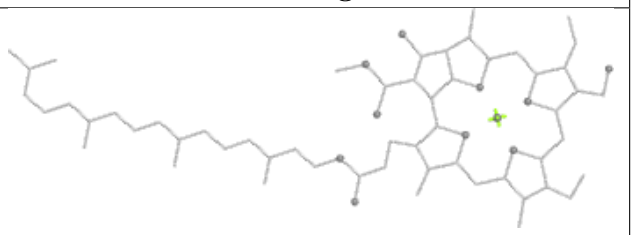
Bond lengths



Bond angles

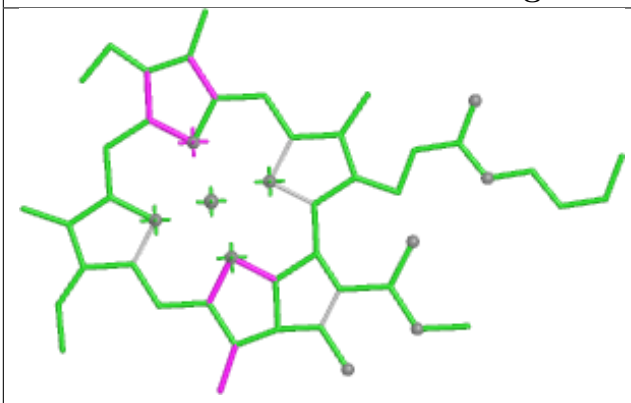


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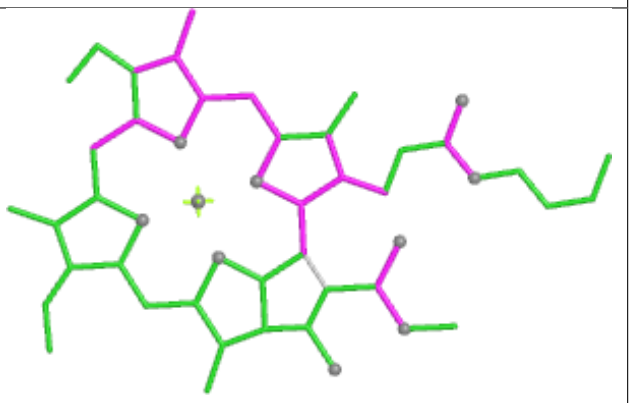


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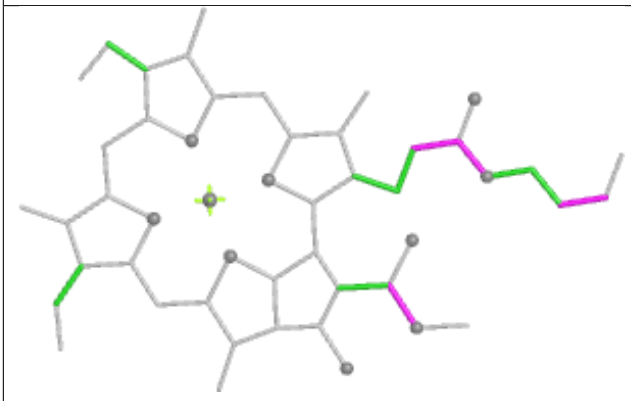
Ligand CLA R 309



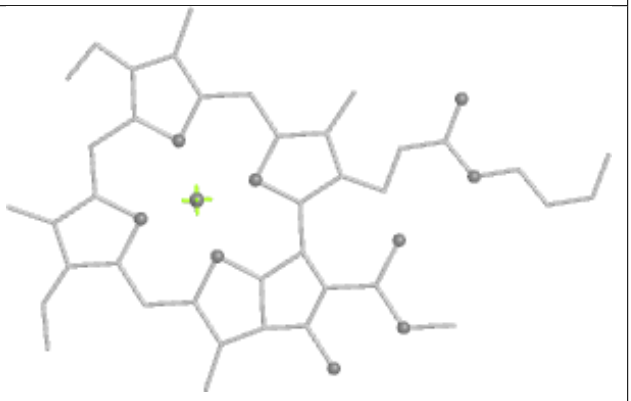
Bond lengths



Bond angles

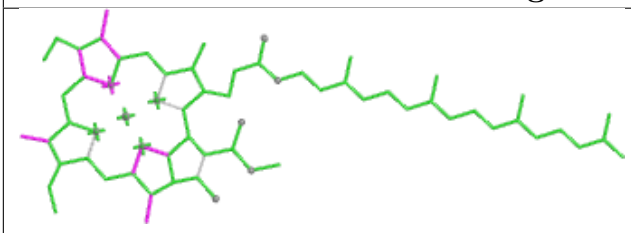


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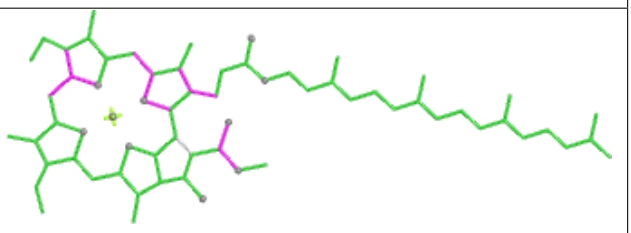


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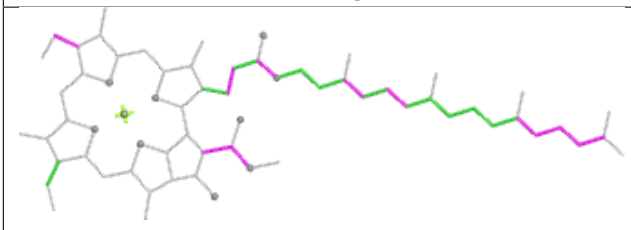
Ligand CLA b 606



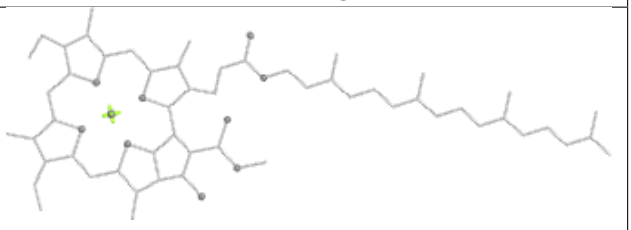
Bond lengths



Bond angles

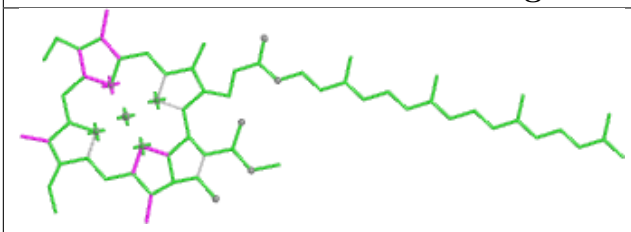


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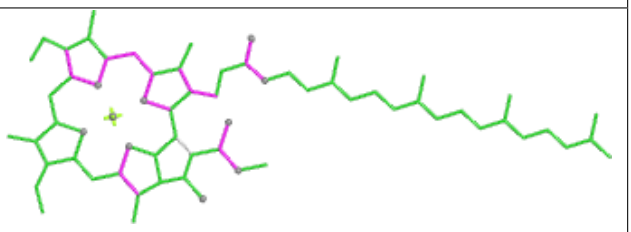


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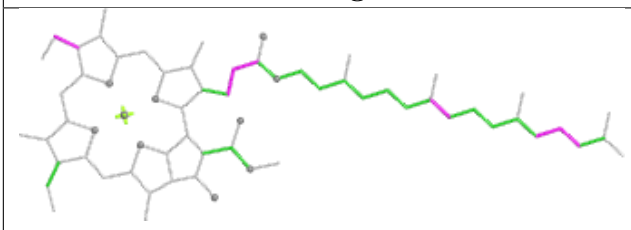
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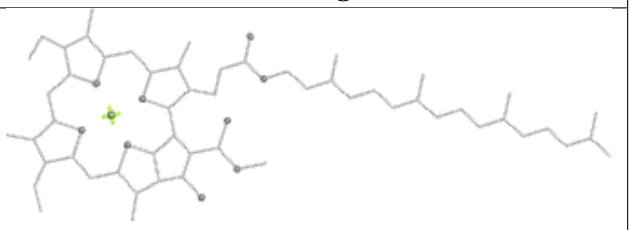
Bond lengths



Bond angles

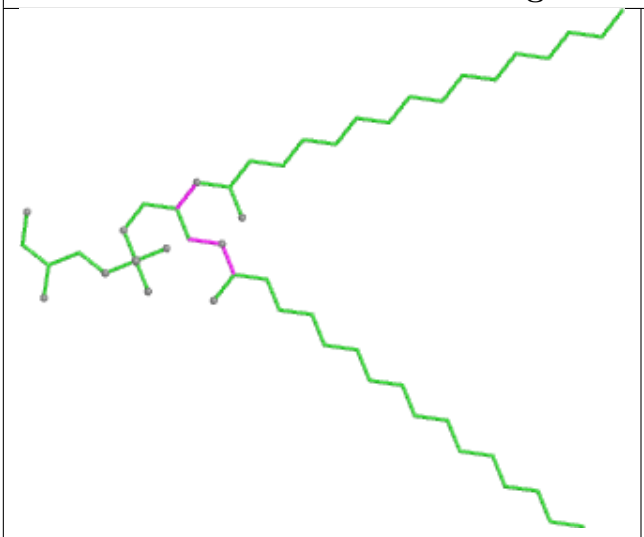


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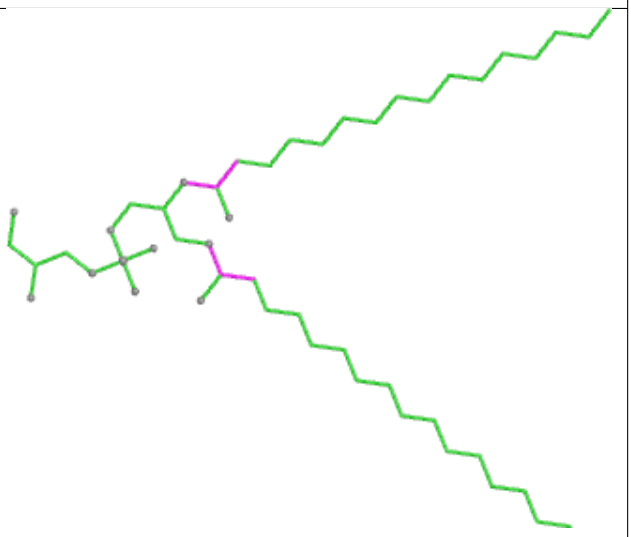


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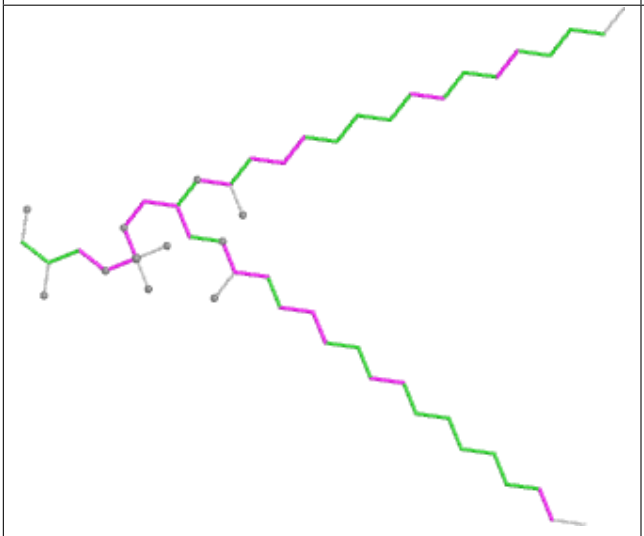
Ligand LHG 5 312



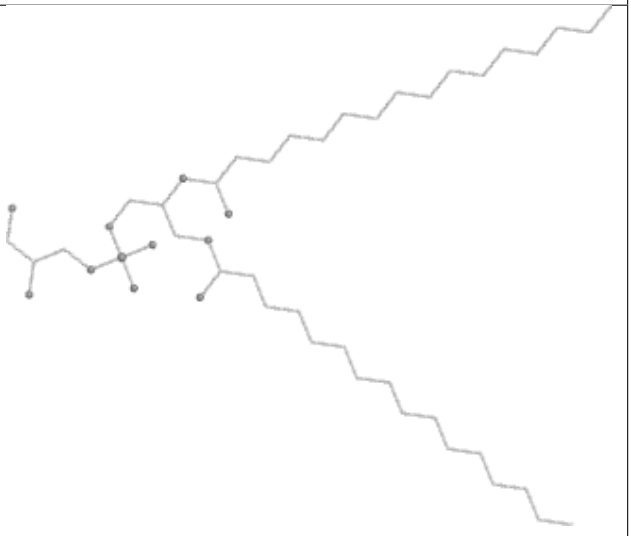
Bond lengths



Bond angles

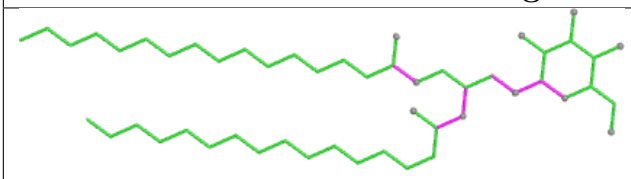


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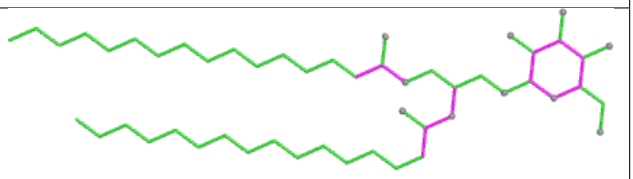


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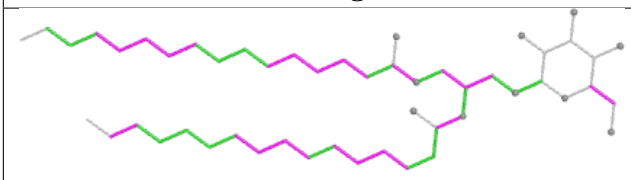
Ligand LMG b 621



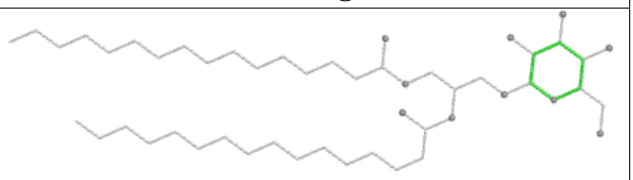
Bond lengths



Bond angles

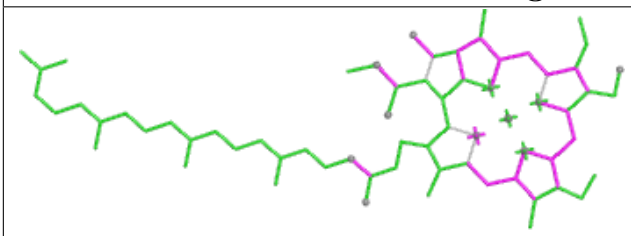


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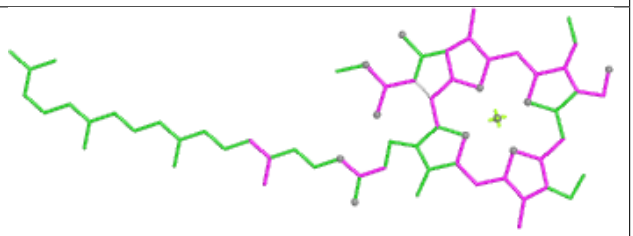


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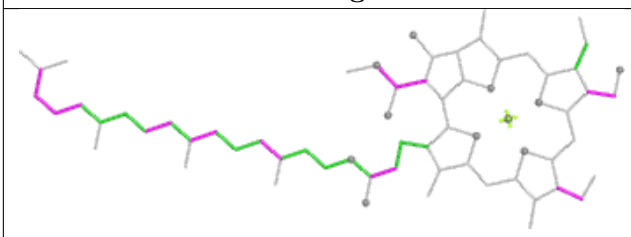
Ligand CHL n 317



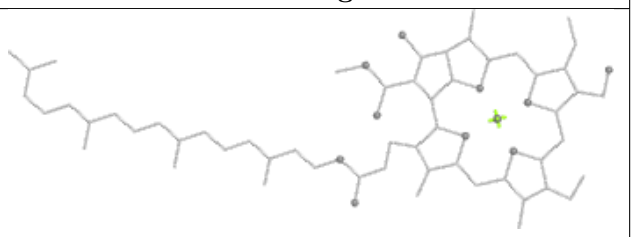
Bond lengths



Bond angles



Torsions

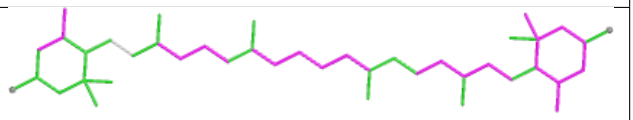


Rings

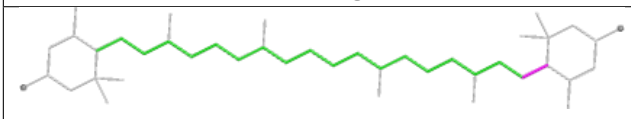
Ligand LUT V 309



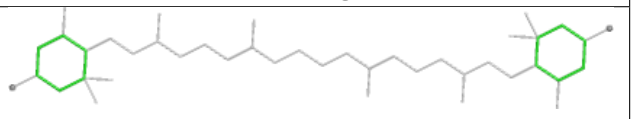
Bond lengths



Bond angles

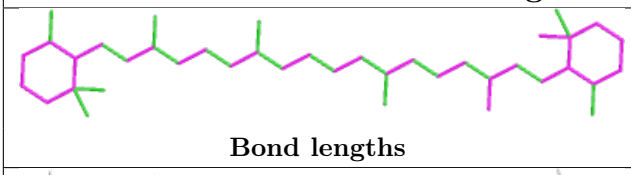


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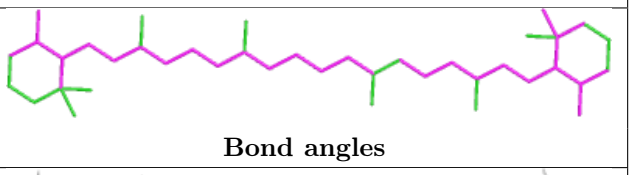


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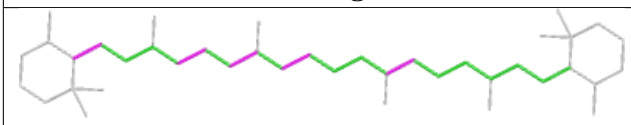
Ligand BCR b 618



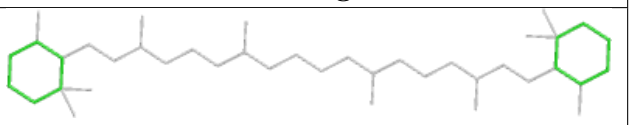
Bond lengths



Bond angles

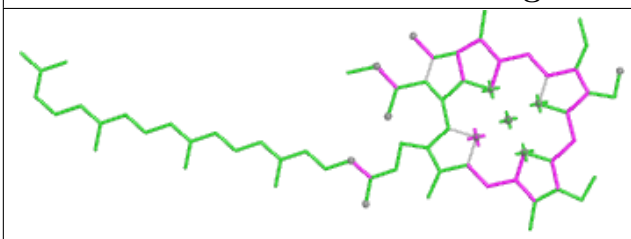


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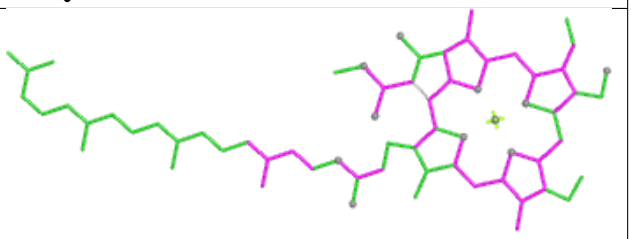


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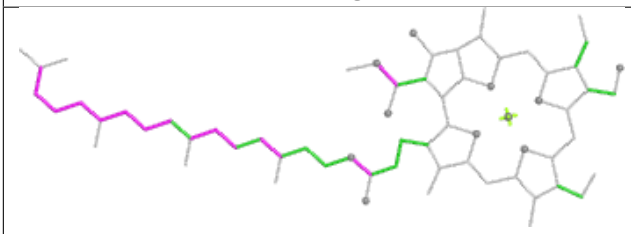
Ligand CHL Q 311



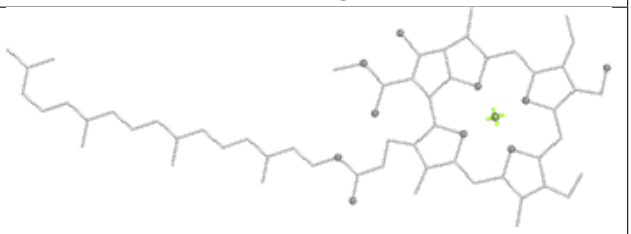
Bond lengths



Bond angles

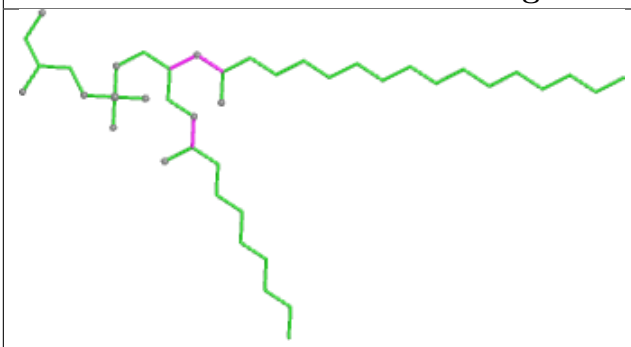


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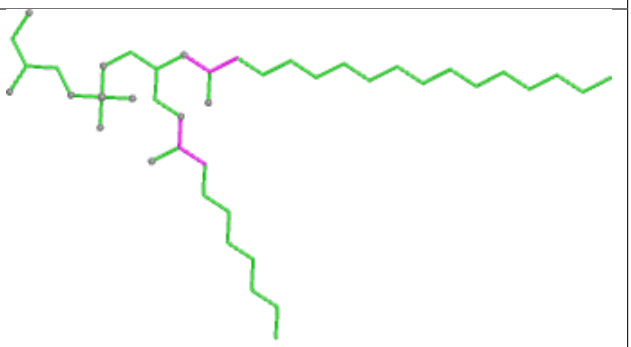


Rings

Ligand LHG R 314



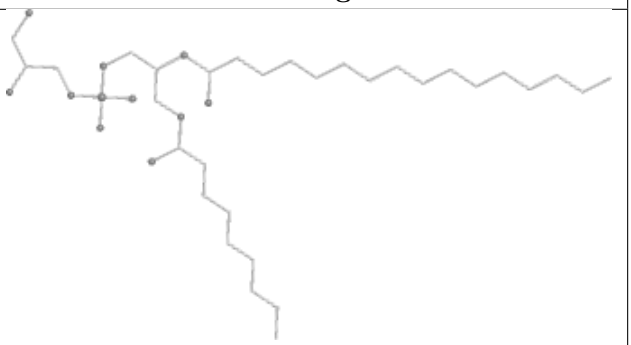
Bond lengths



Bond angles

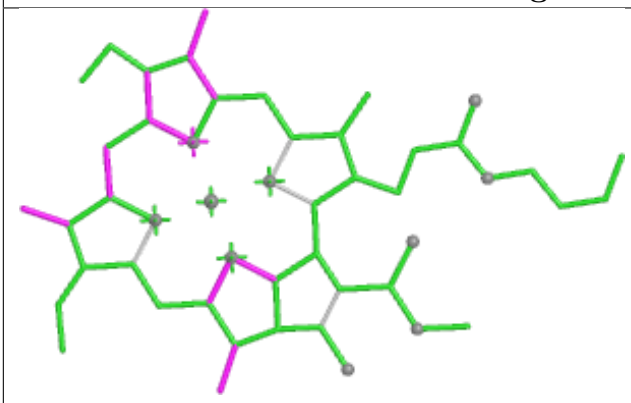


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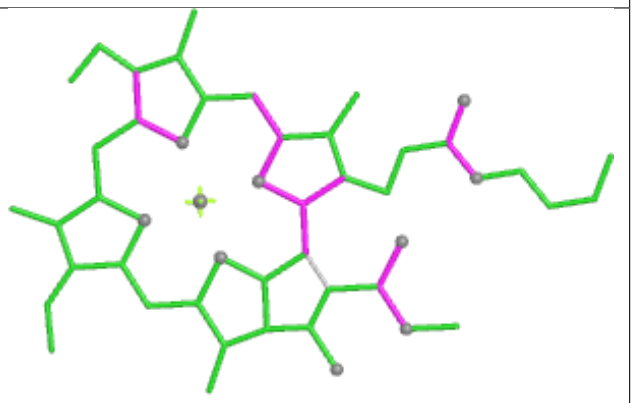


Rings

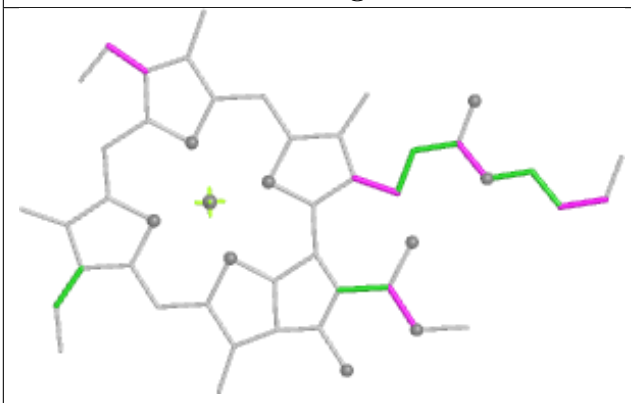
Ligand CLA r 601



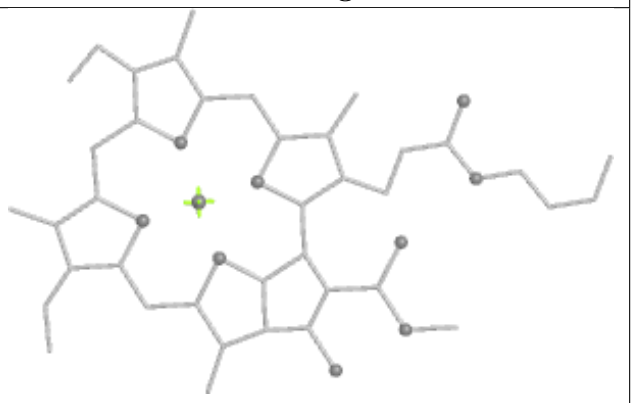
Bond lengths



Bond angles

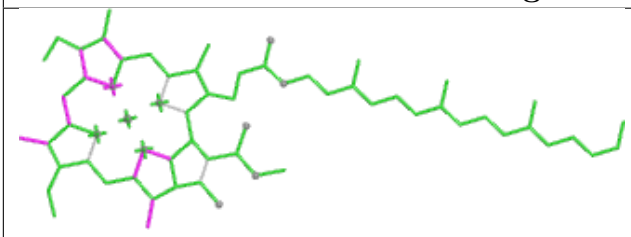


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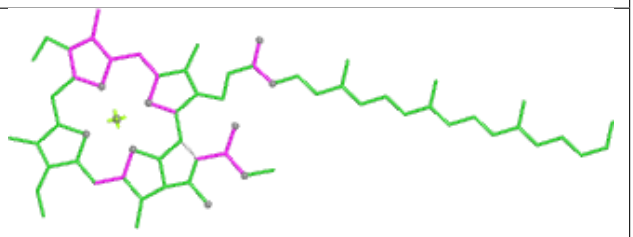


Rings

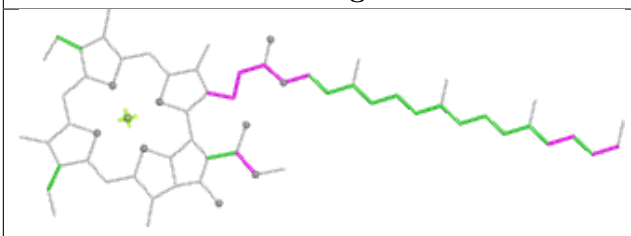
Ligand CLA G 304



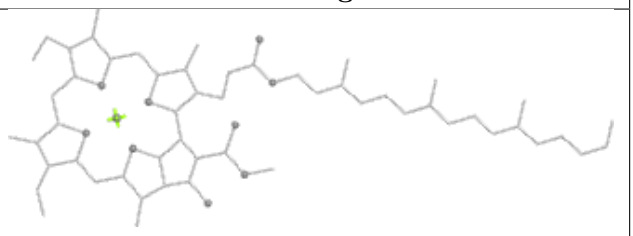
Bond lengths



Bond angles

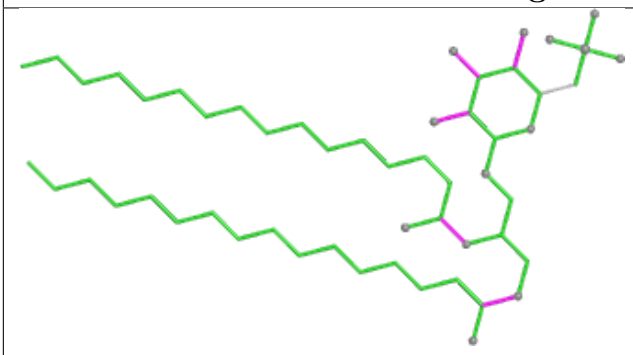


Torsions

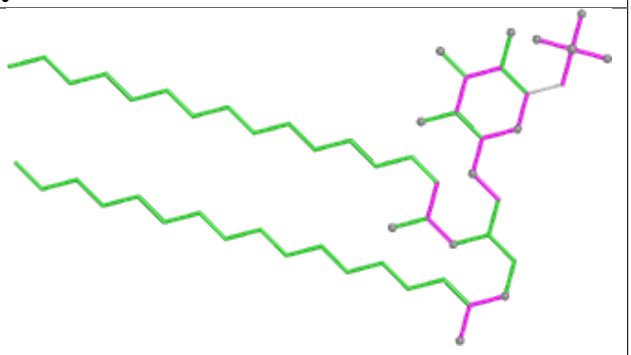


Rings

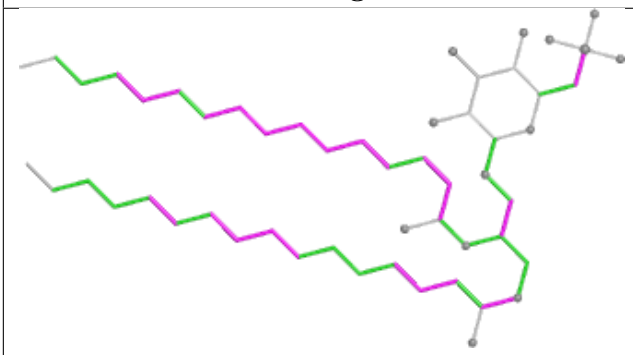
Ligand SQD a 413



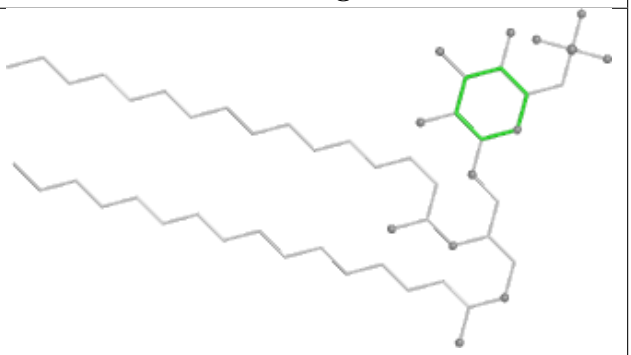
Bond lengths



Bond angles

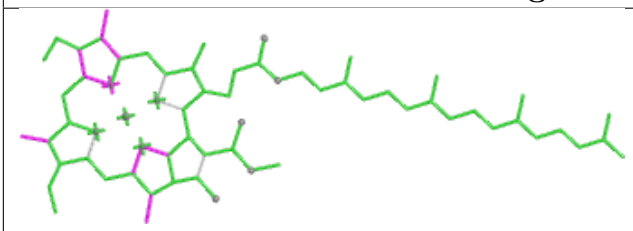


Torsions

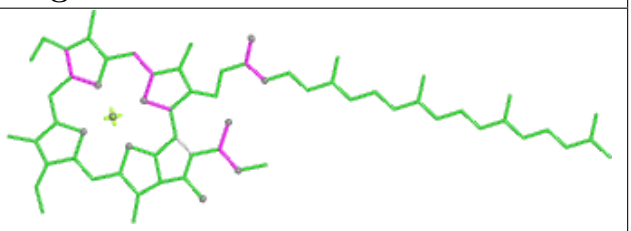


Rings

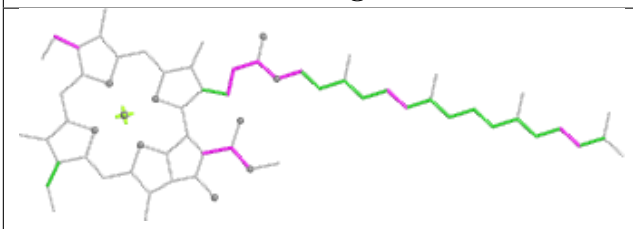
Ligand CLA g 302



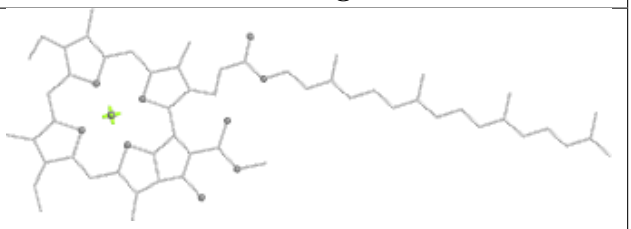
Bond lengths



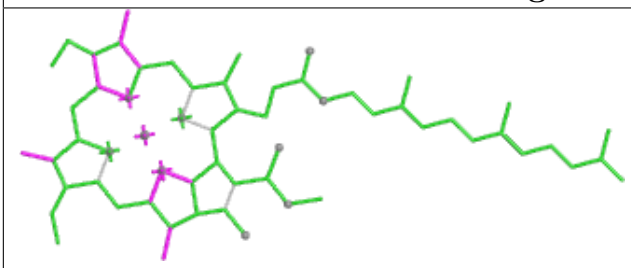
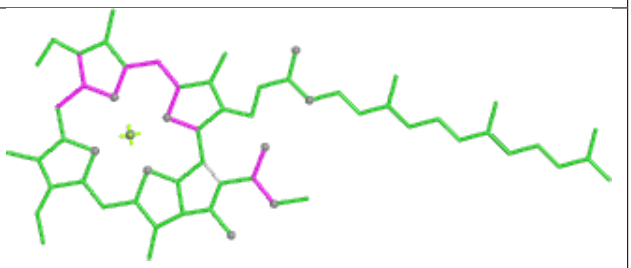
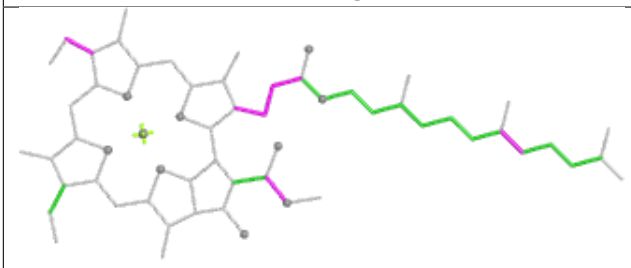
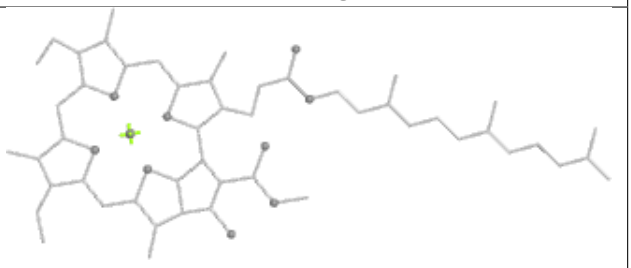
Bond angles

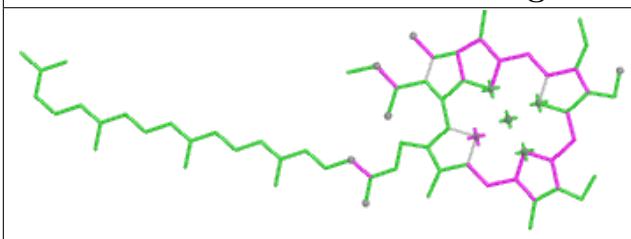
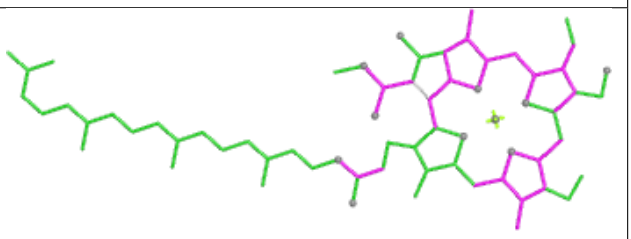
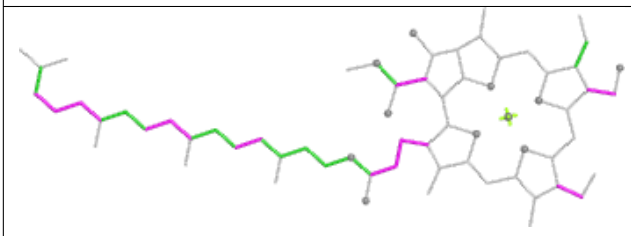
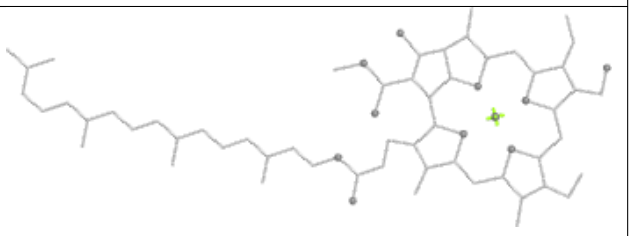


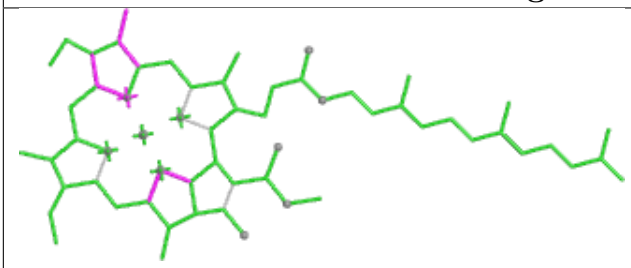
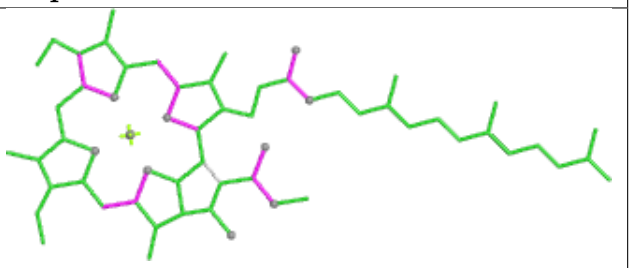
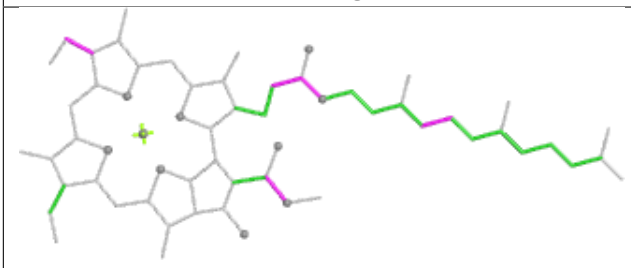
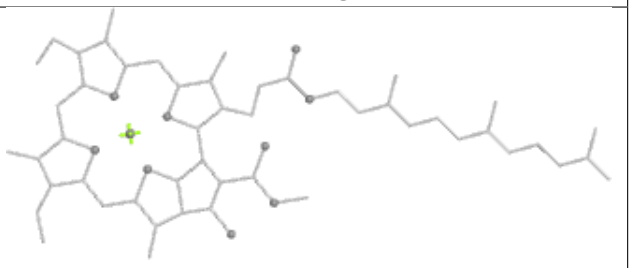
Torsions

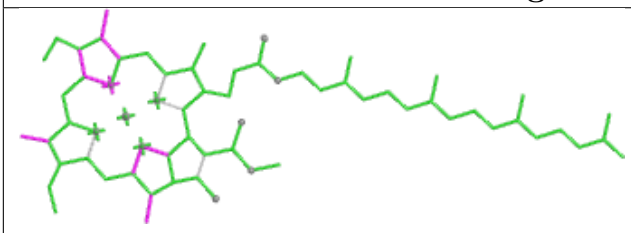
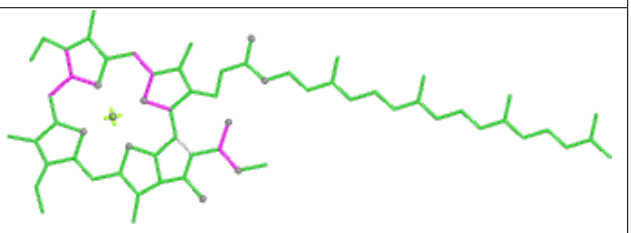
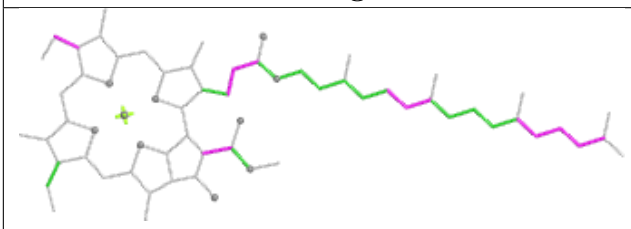
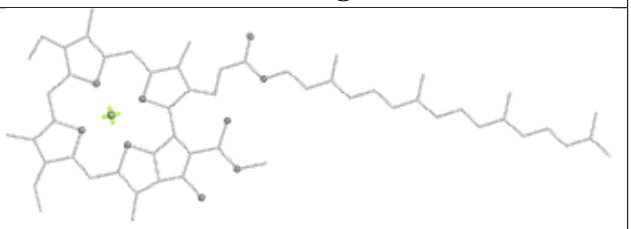


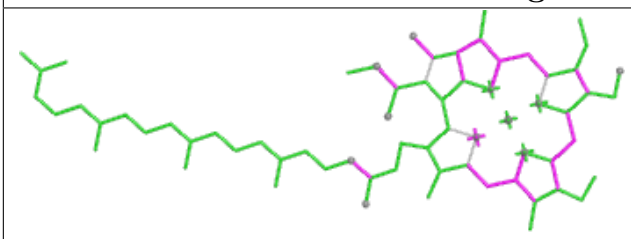
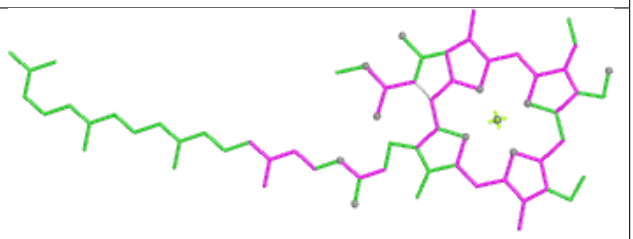
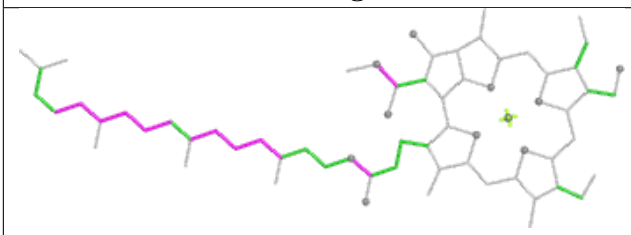
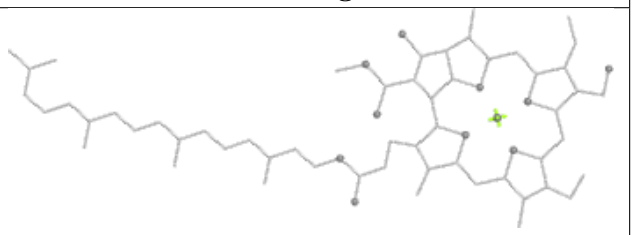
Rings

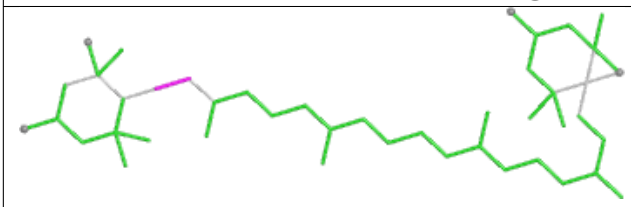
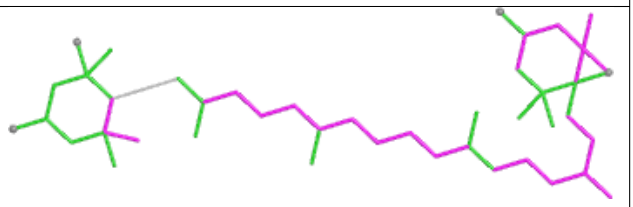
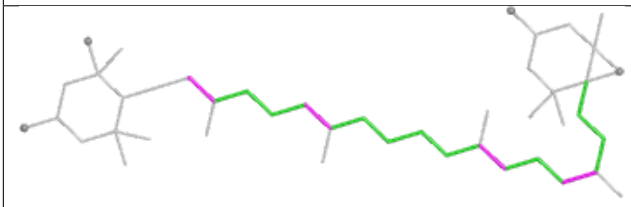
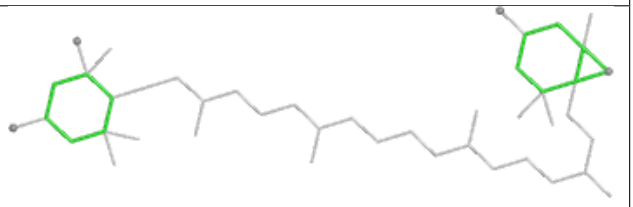
Ligand CLA 1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

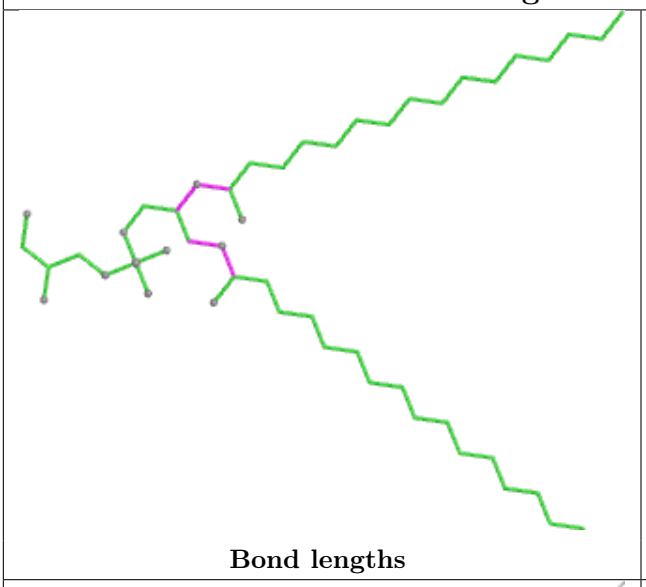
Ligand CLA p 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

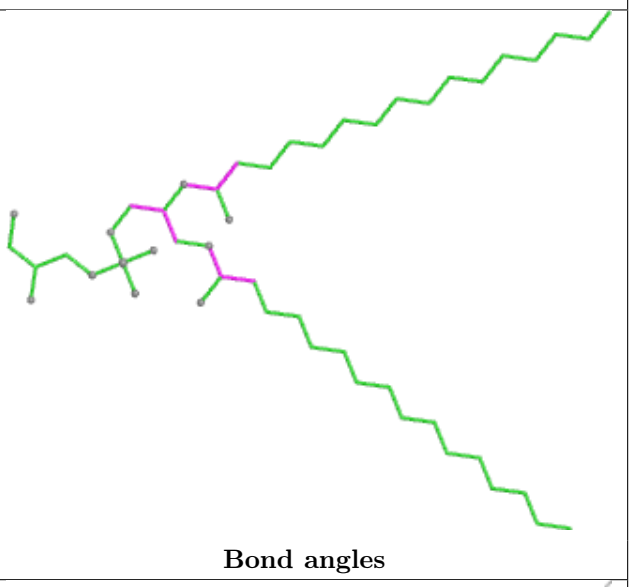
Ligand CHL 3 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX 2 319	
	
Bond lengths	Bond angles
	
Torsions	Rings

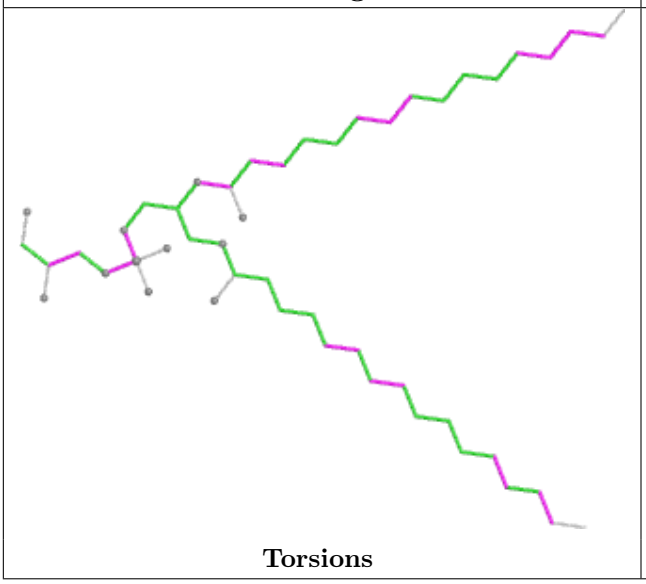
Ligand LHG D 407



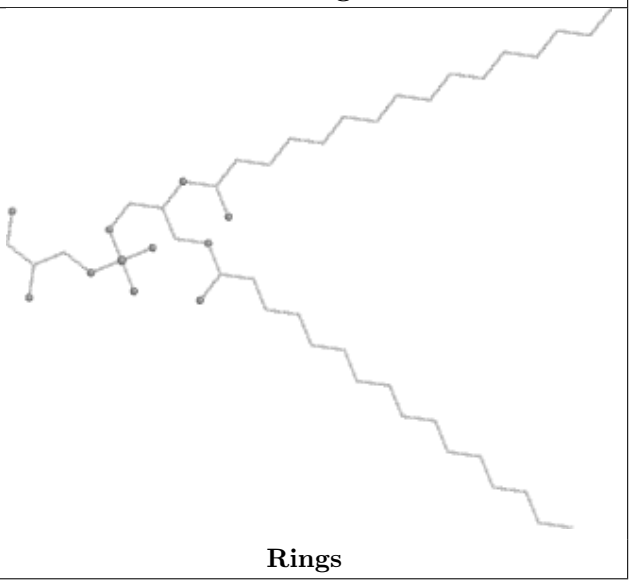
Bond lengths



Bond angles



Torsions

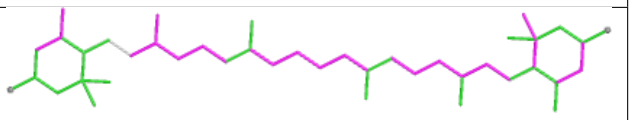


Rings

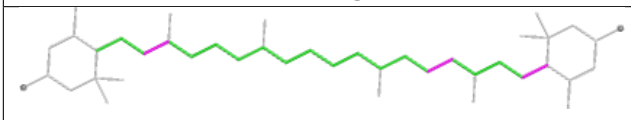
Ligand LUT 5 309



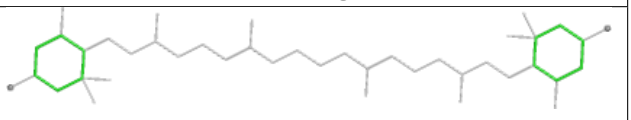
Bond lengths



Bond angles

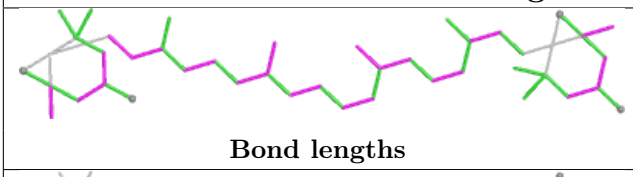


Torsions

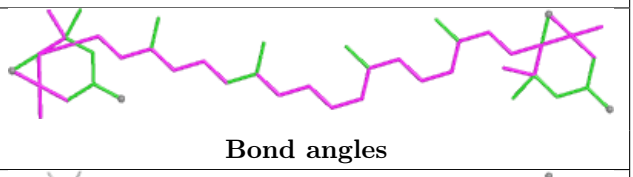


Rings

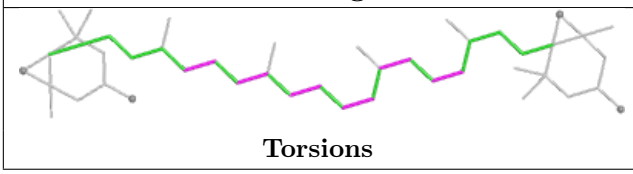
Ligand XAT 4 311



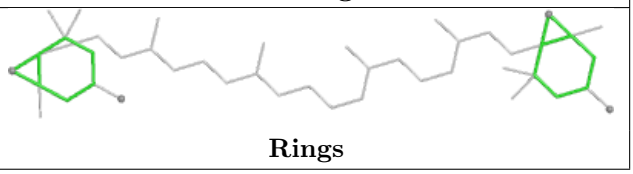
Bond lengths



Bond angles

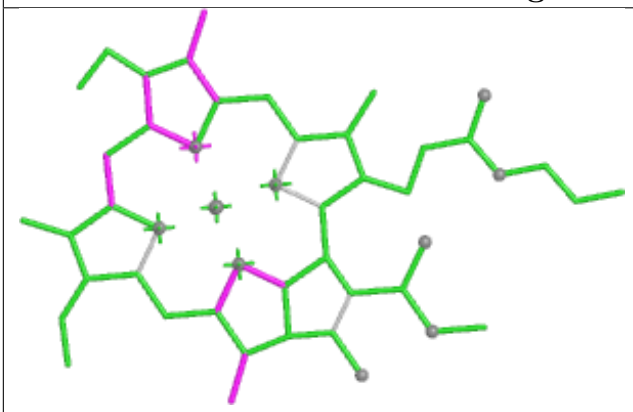


Torsions

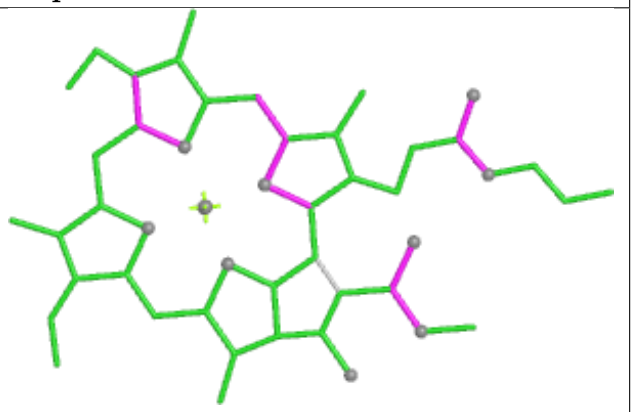


Rings

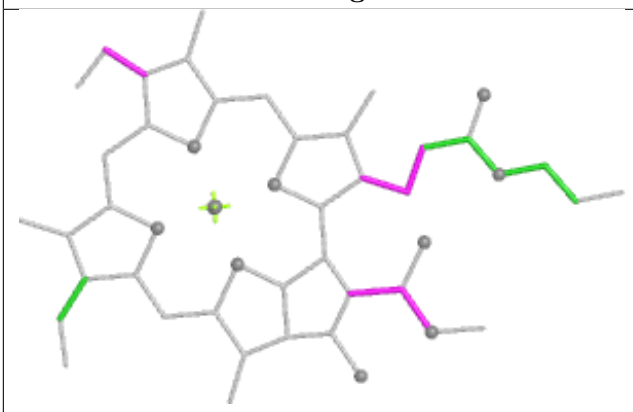
Ligand CLA p 309



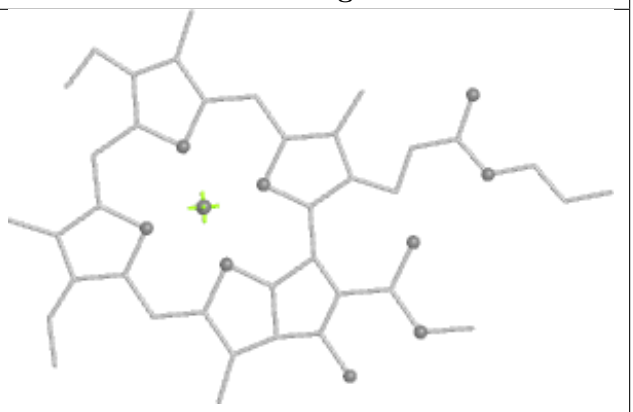
Bond lengths



Bond angles

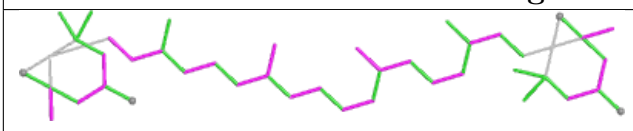


Torsions

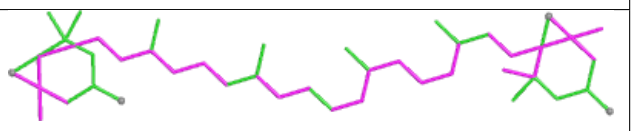


Rings

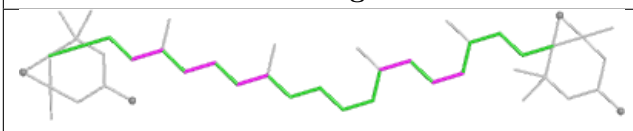
Ligand XAT 1 311



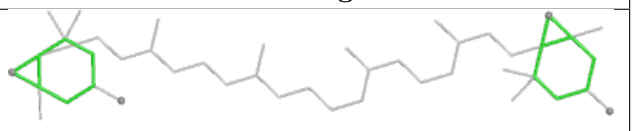
Bond lengths



Bond angles

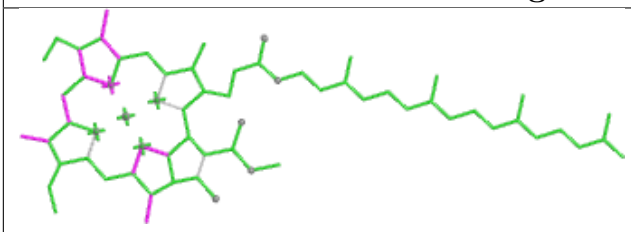


Torsions

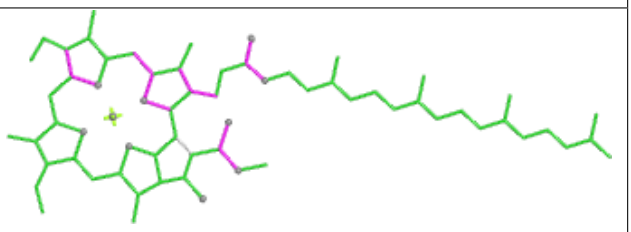


Rings

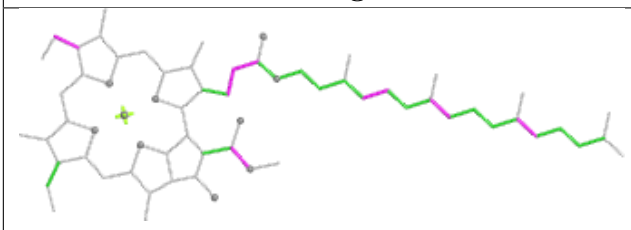
Ligand CLA 3 307



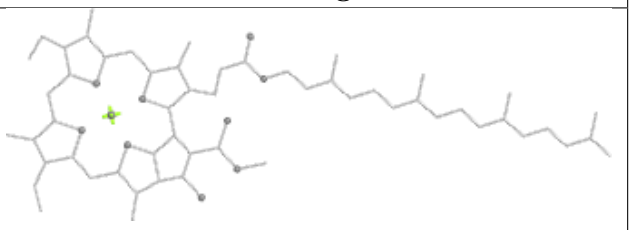
Bond lengths



Bond angles

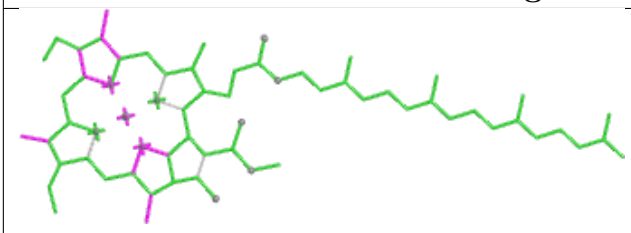


Torsions

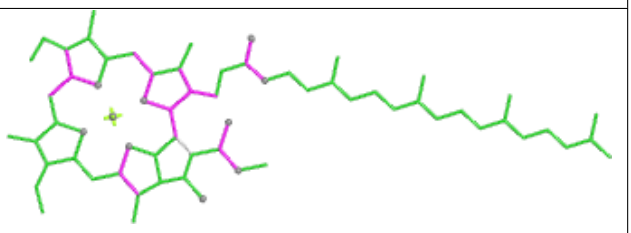


Rings

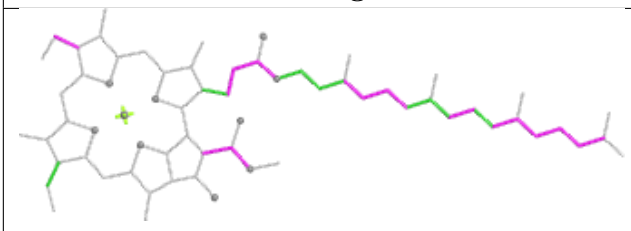
Ligand CLA B 602



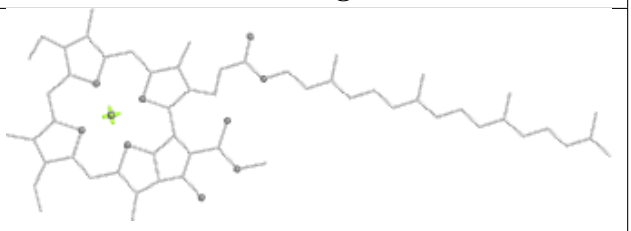
Bond lengths



Bond angles

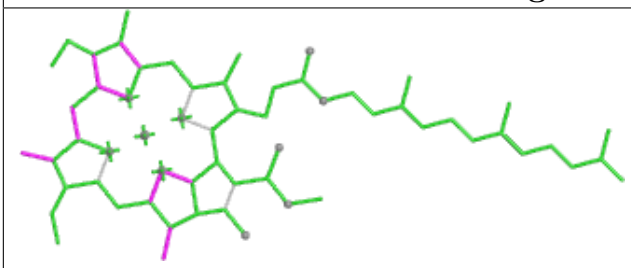


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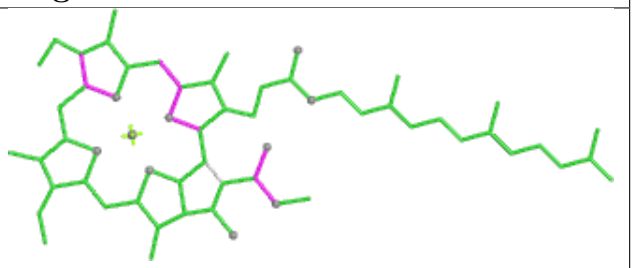


Rings

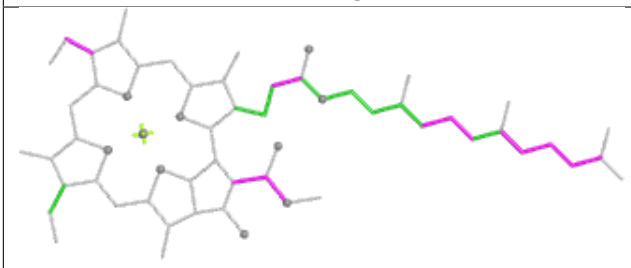
Ligand CLA g 306



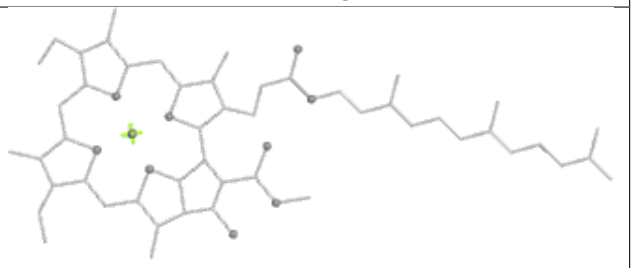
Bond lengths



Bond angles

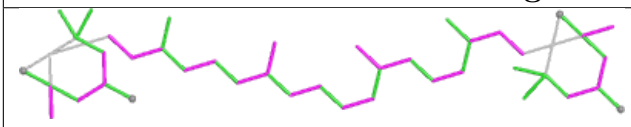


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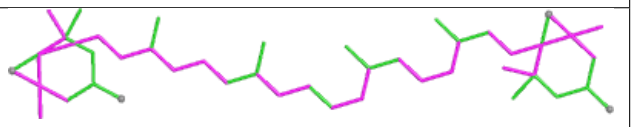


Rings

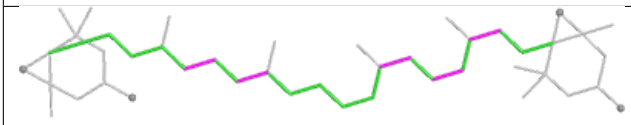
Ligand XAT P 312



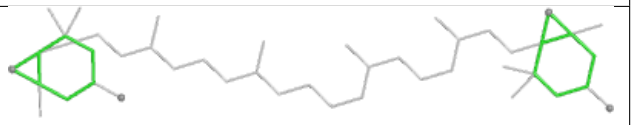
Bond lengths



Bond angles

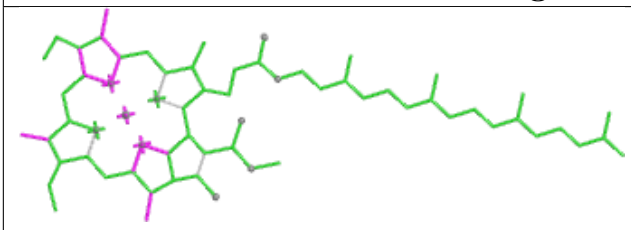


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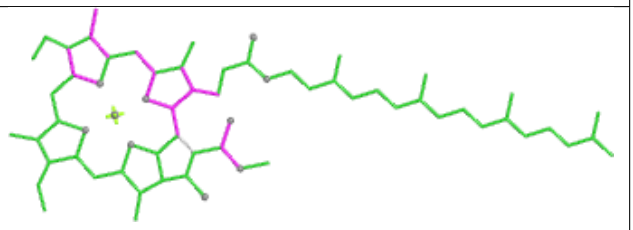


Rings

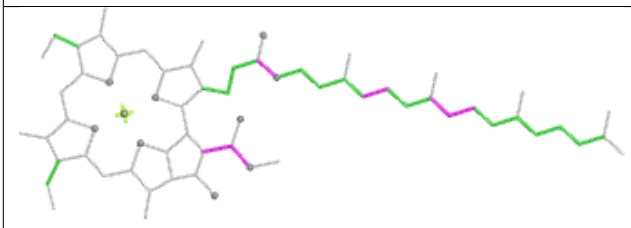
Ligand CLA c 512



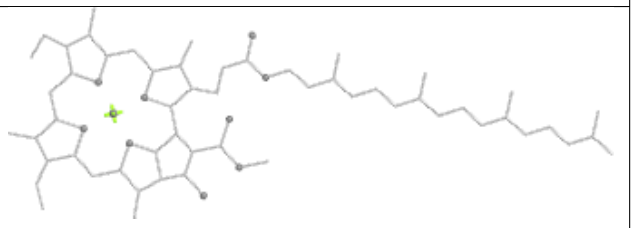
Bond lengths



Bond angles

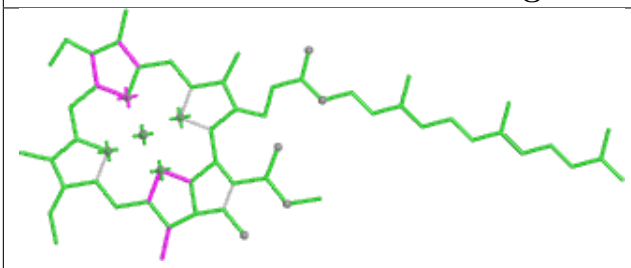


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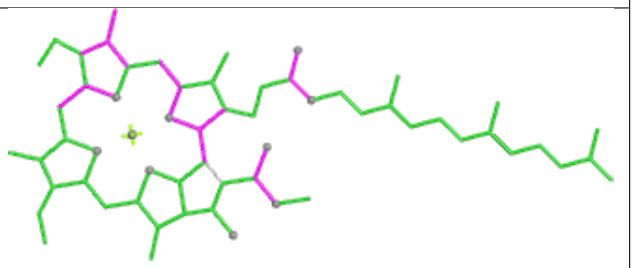


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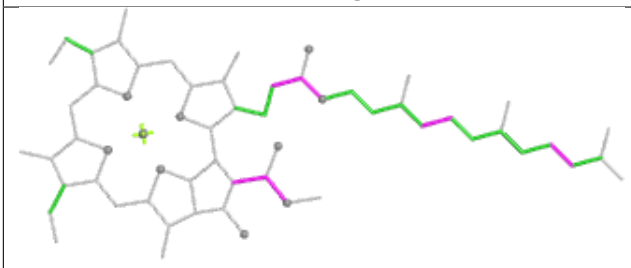
Ligand CLA N 306



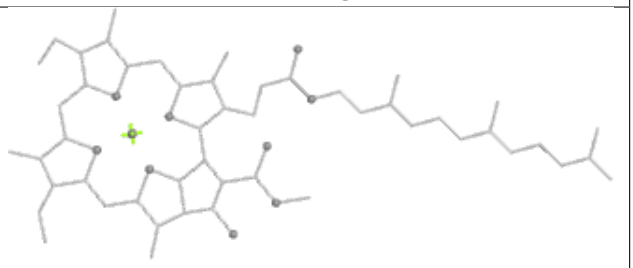
Bond lengths



Bond angles

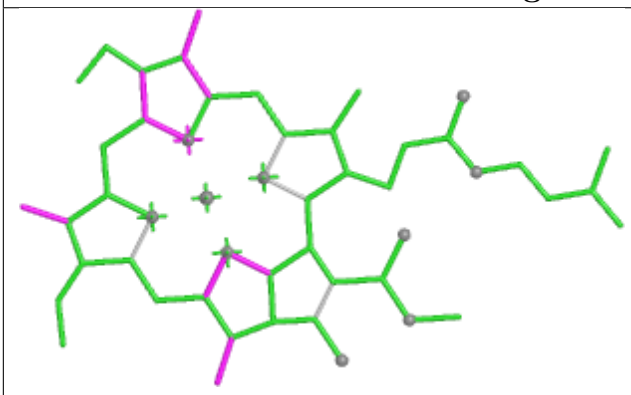


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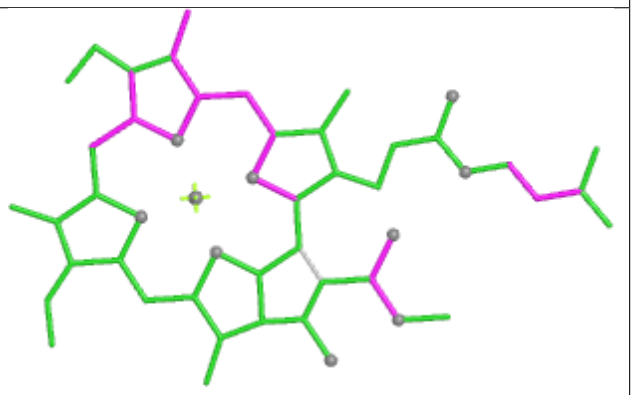


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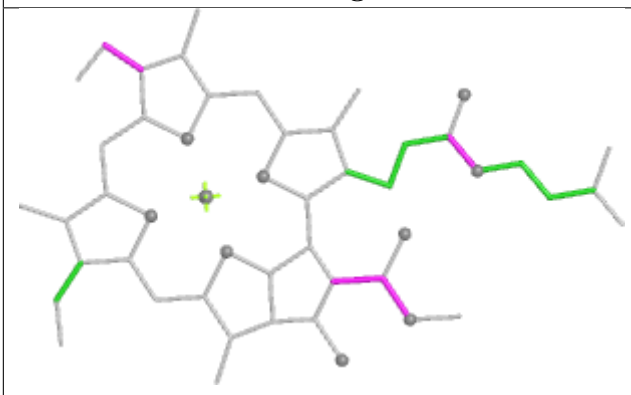
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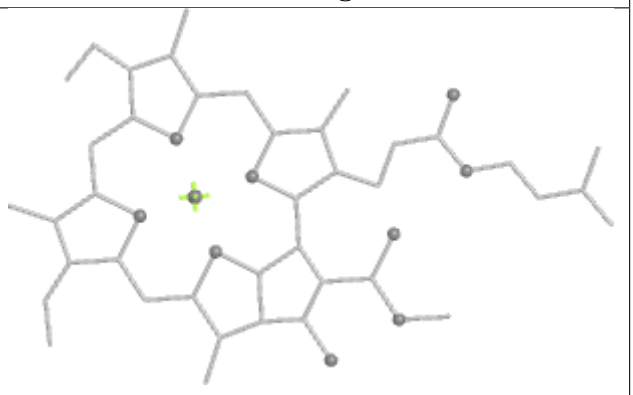
Bond lengths



Bond angles

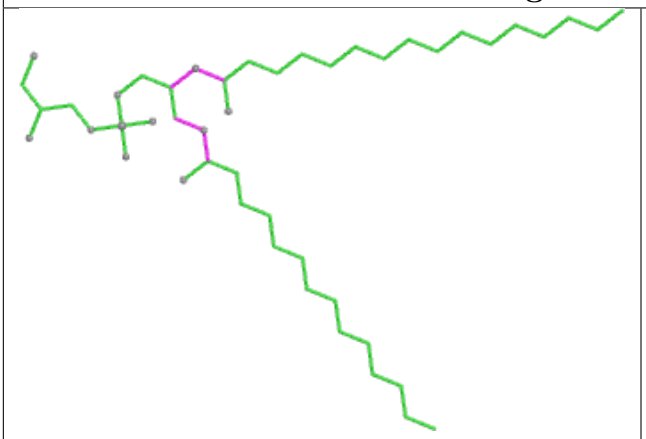


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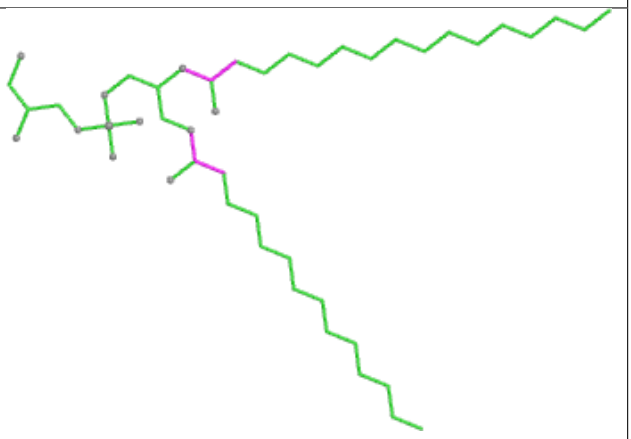


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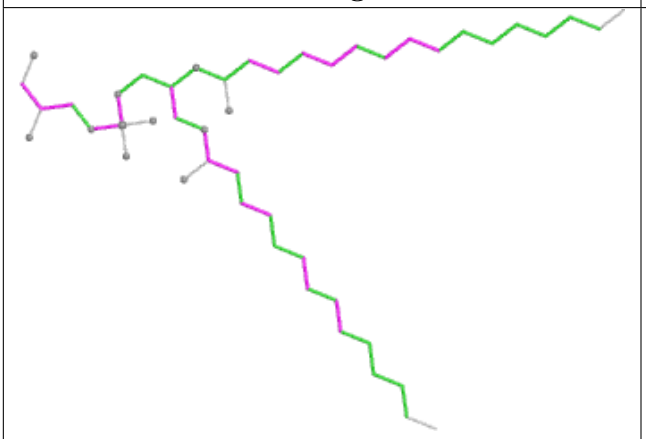
Ligand LHG b 622



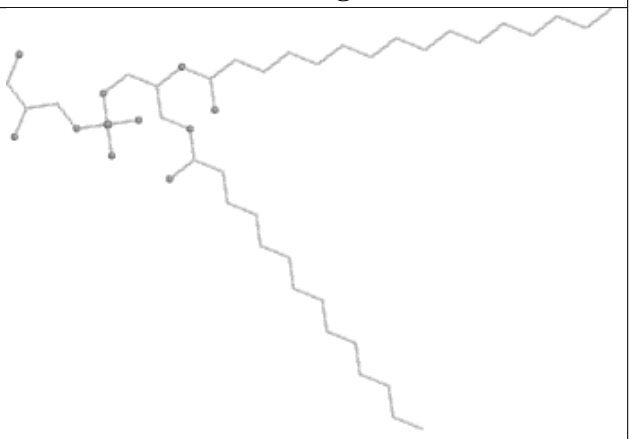
Bond lengths



Bond angles

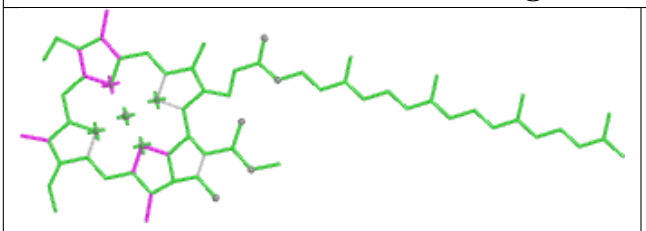


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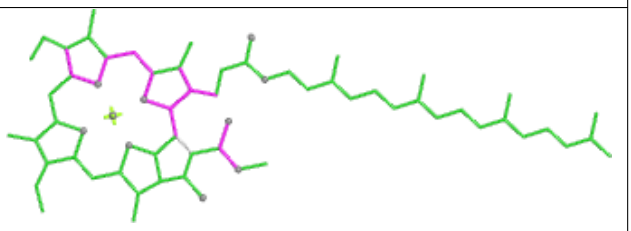


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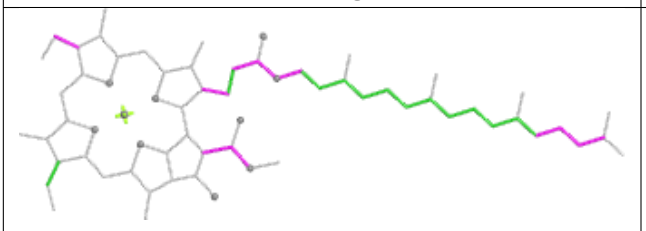
Ligand CLA B 611



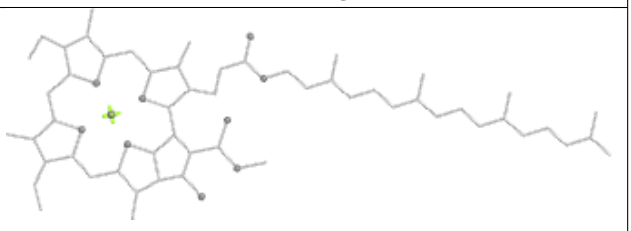
Bond lengths



Bond angles

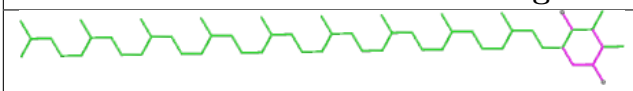


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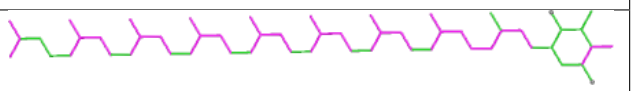


Rings

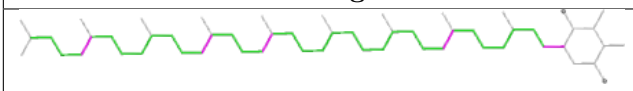
Ligand PL9 d 404



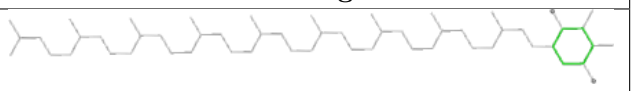
Bond lengths



Bond angles

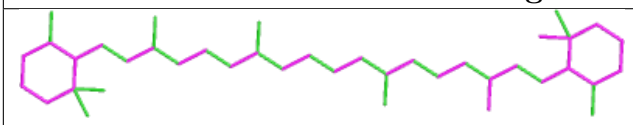


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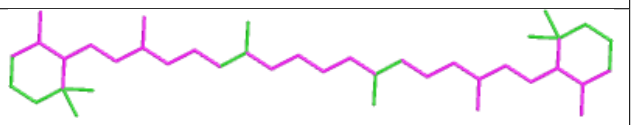


Rings

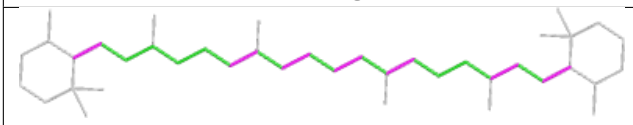
Ligand BCR b 620



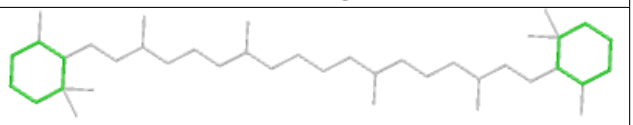
Bond lengths



Bond angles

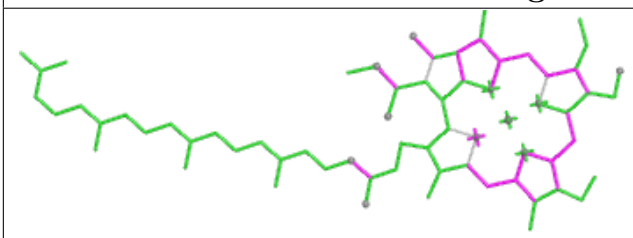


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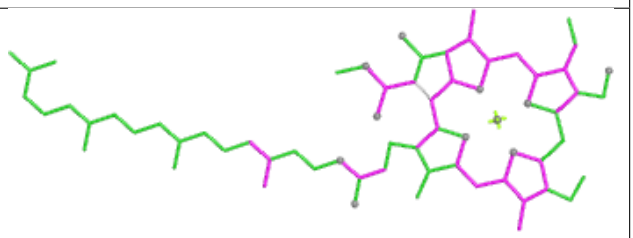


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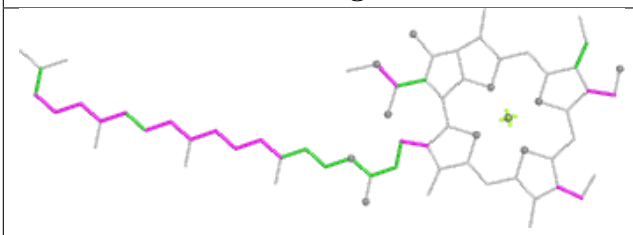
Ligand CHL 2 318



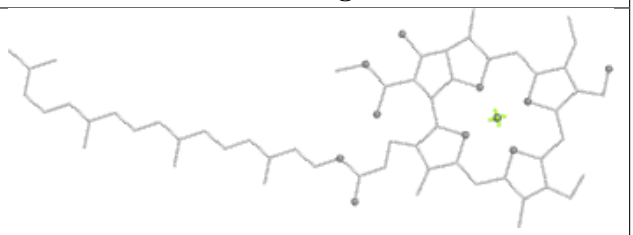
Bond lengths



Bond angles

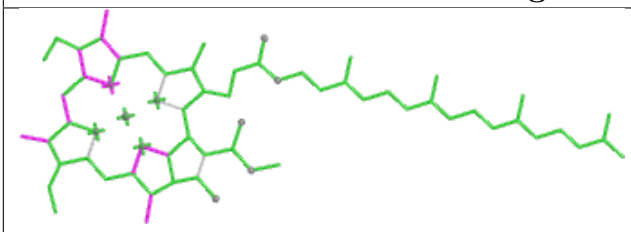


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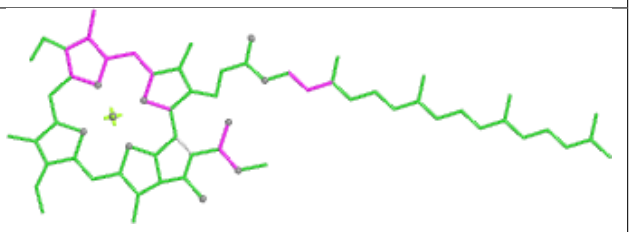


Rings

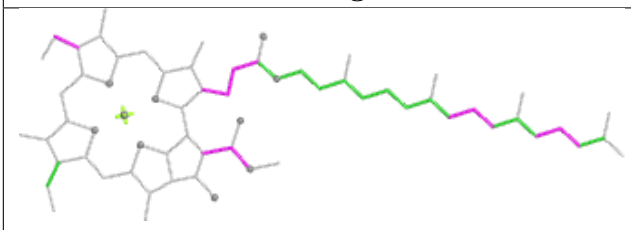
Ligand CLA 5 301



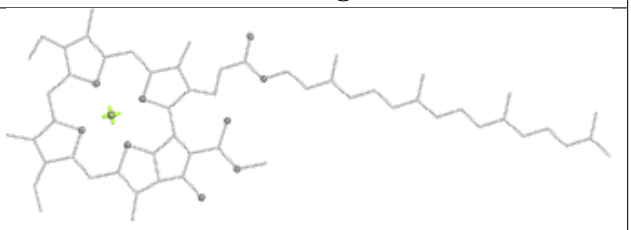
Bond lengths



Bond angles

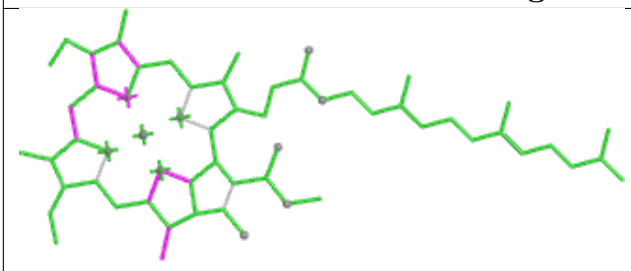


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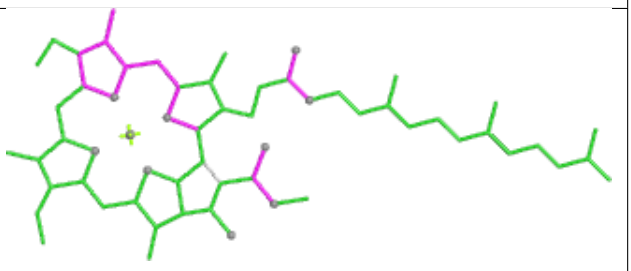


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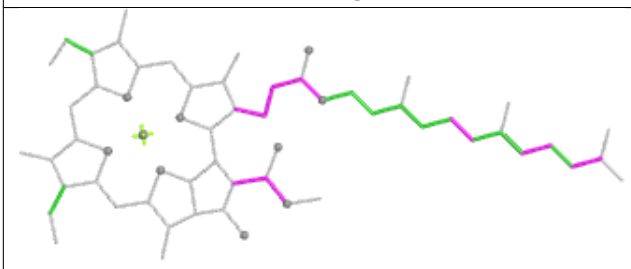
Ligand CLA v 304



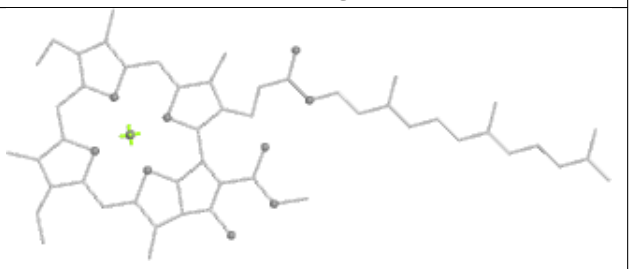
Bond lengths



Bond angles

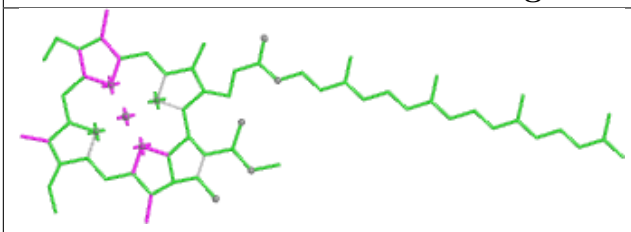


Torsions

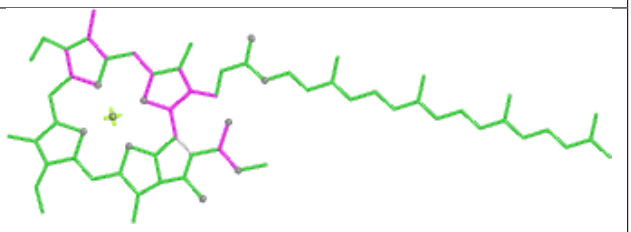


Rings

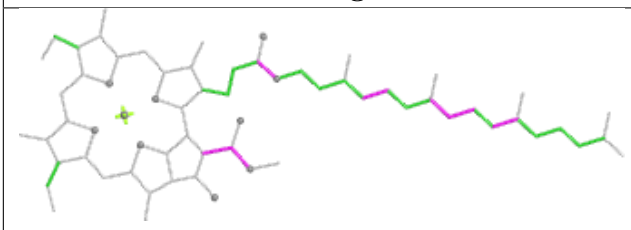
Ligand CLA C 513



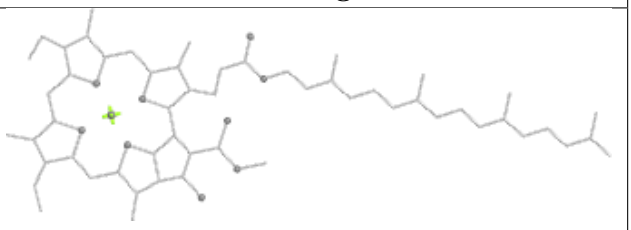
Bond lengths



Bond angles

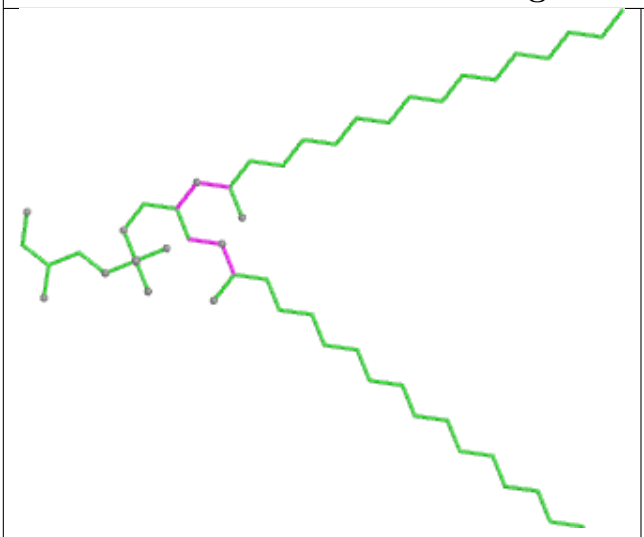


Torsions

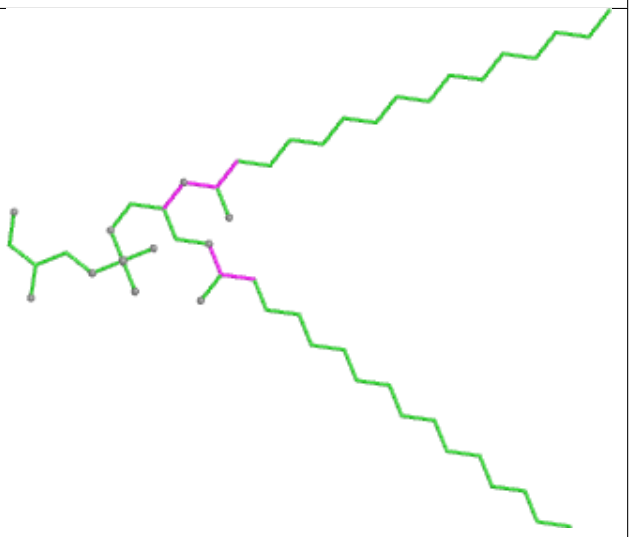


Rings

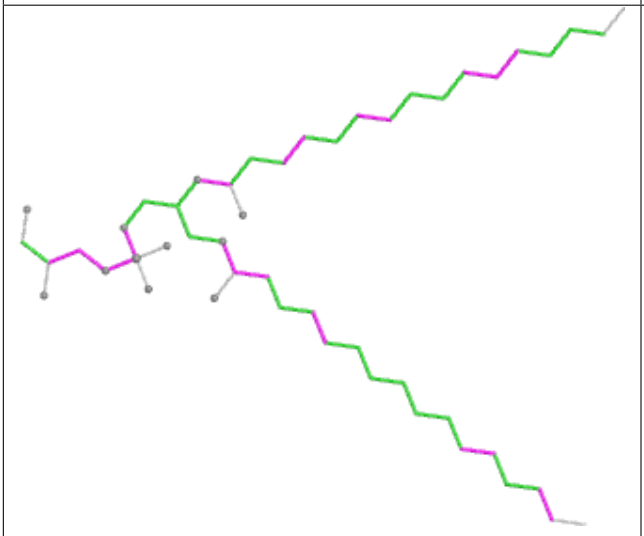
Ligand LHG s 312



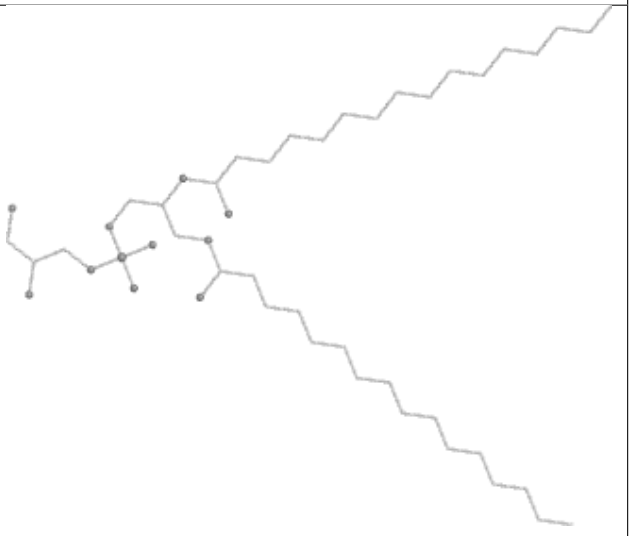
Bond lengths



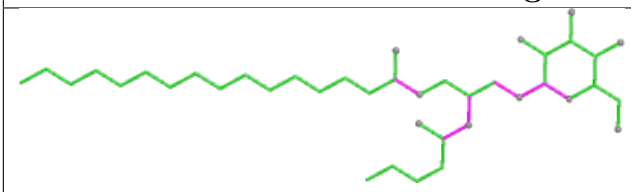
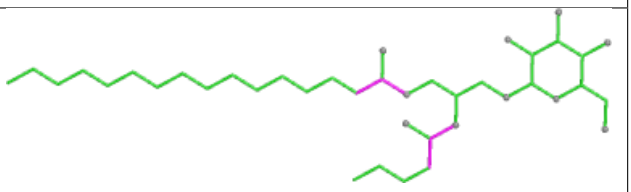
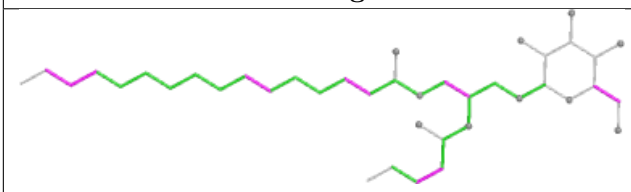
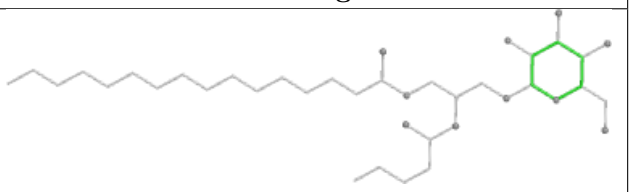
Bond angles

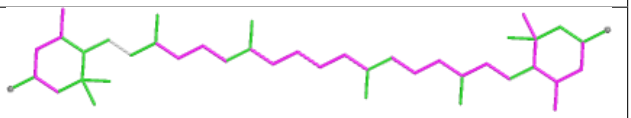
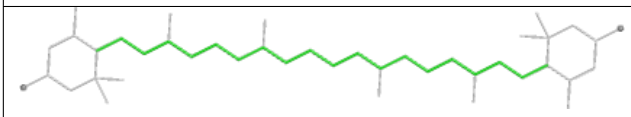
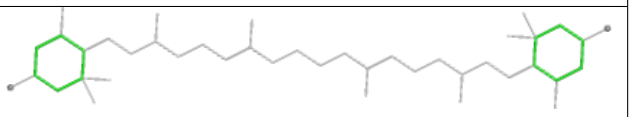


Torsions

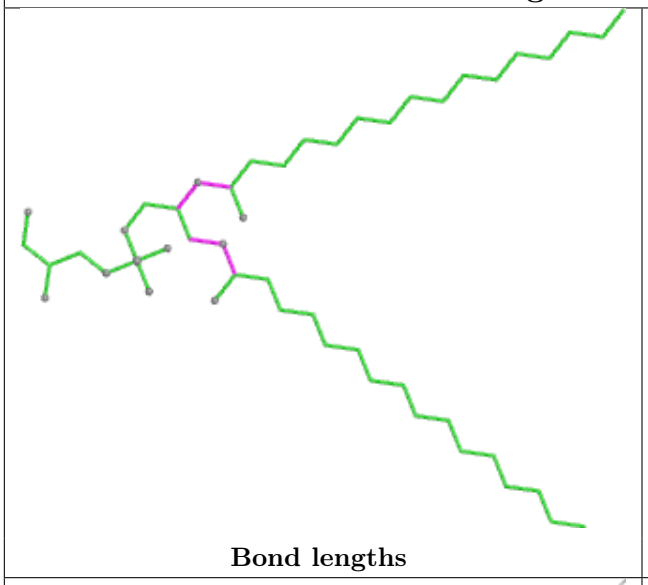


Rings

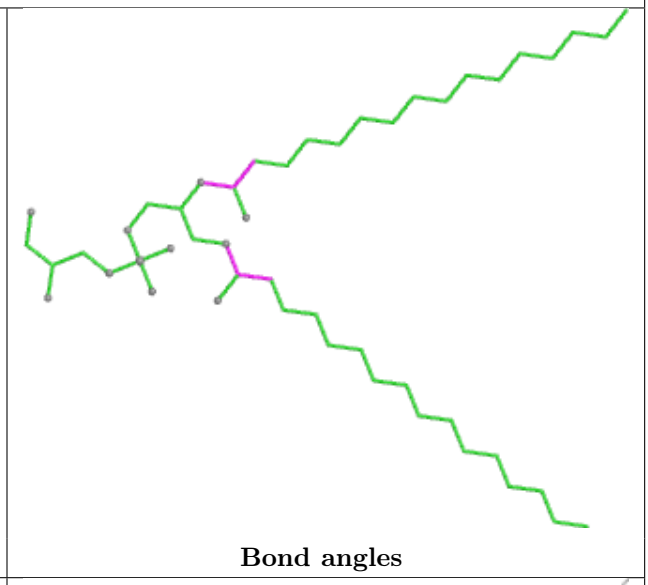
Ligand LMG a 412	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT 1 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

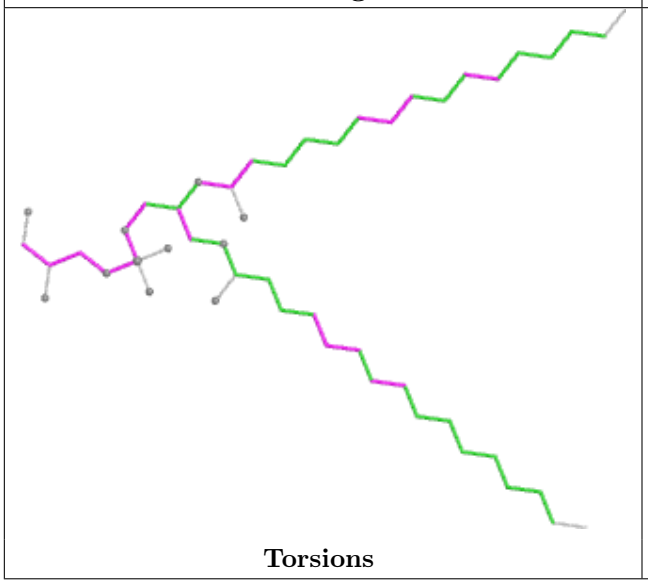
Ligand LHG b 623



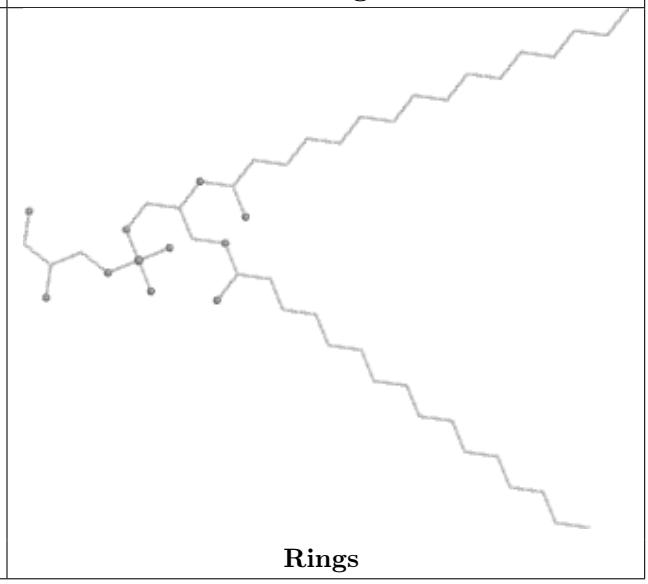
Bond lengths



Bond angles

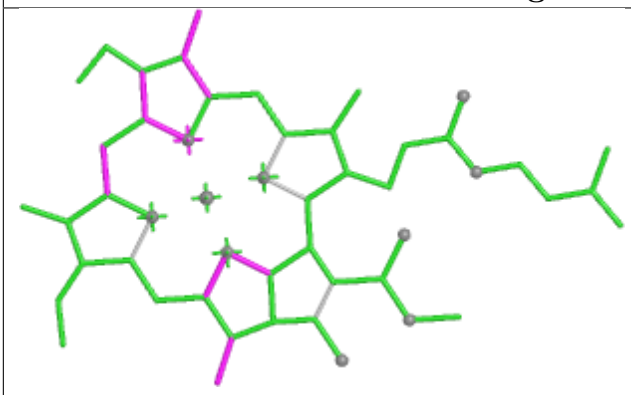


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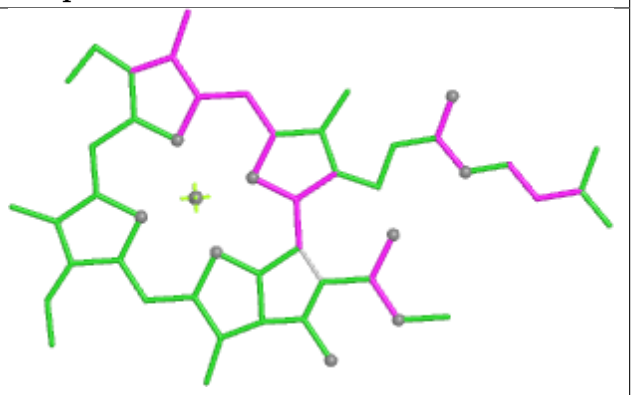


Rings

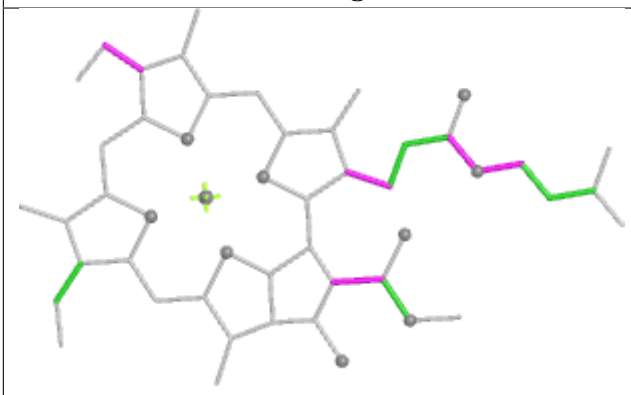
Ligand CLA q 303



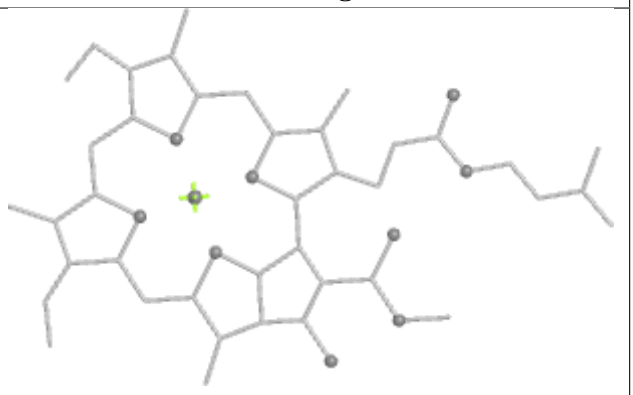
Bond lengths



Bond angles

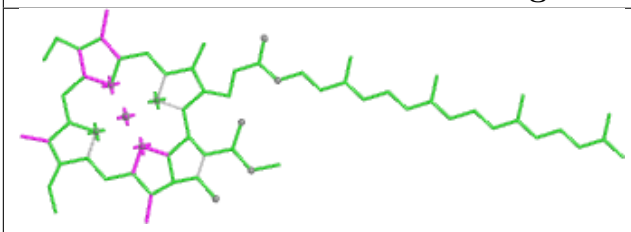


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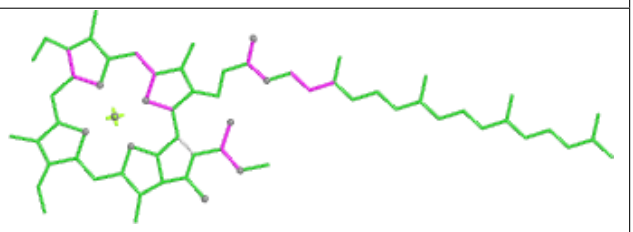


Rings

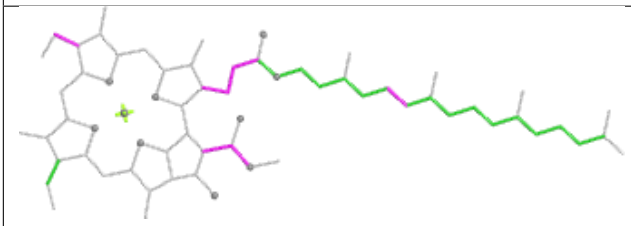
Ligand CLA c 513



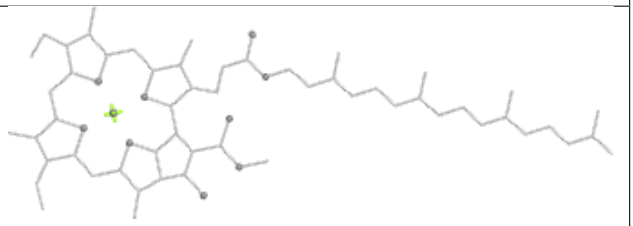
Bond lengths



Bond angles

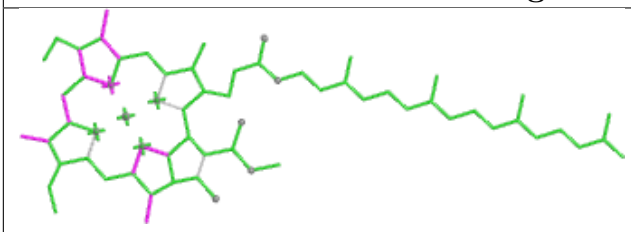


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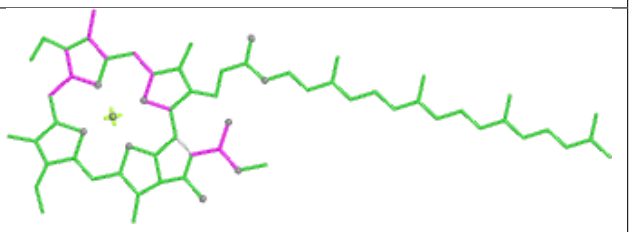


Rings

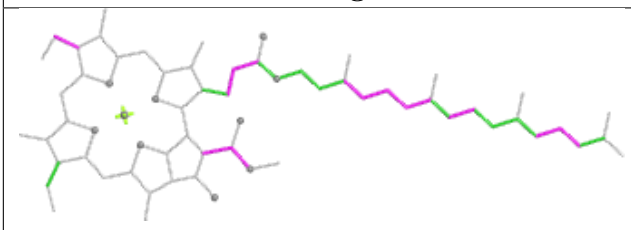
Ligand CLA b 615



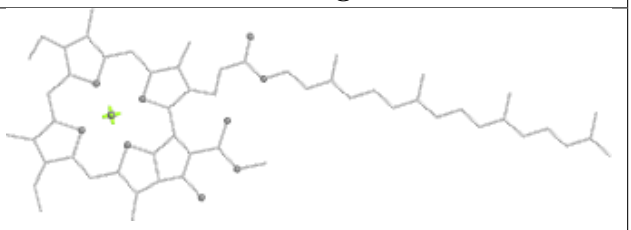
Bond lengths



Bond angles

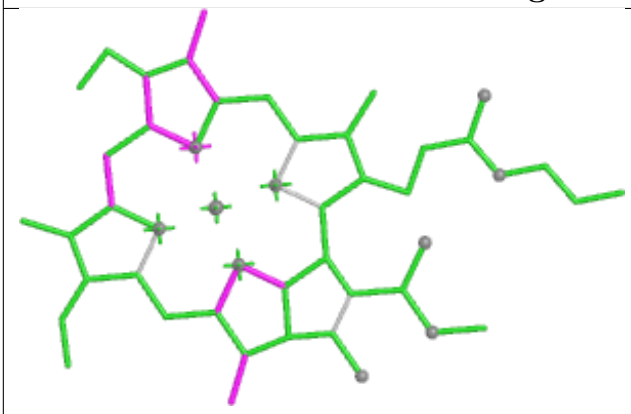


Torsions

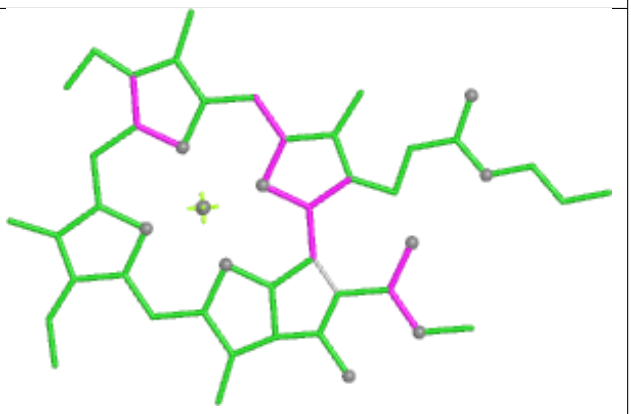


Rings

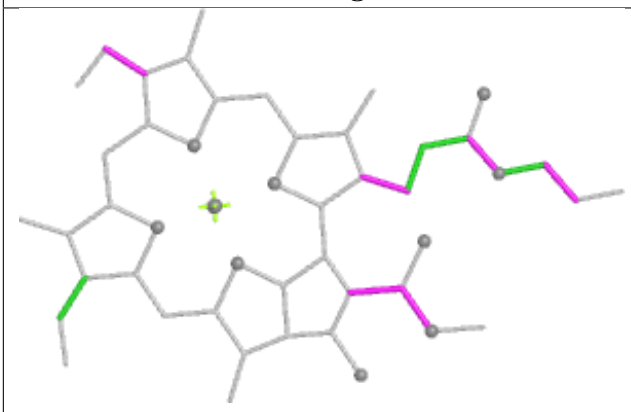
Ligand CLA 1 308



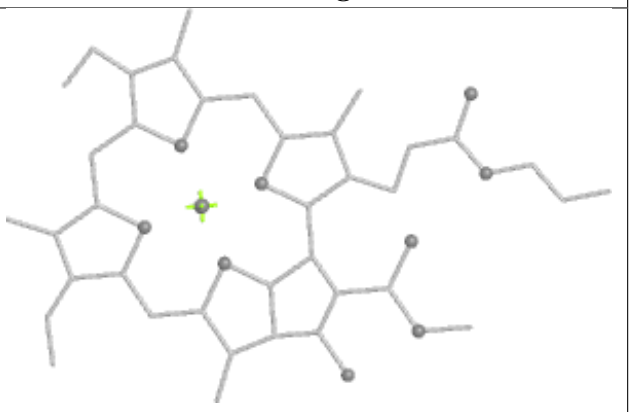
Bond lengths



Bond angles

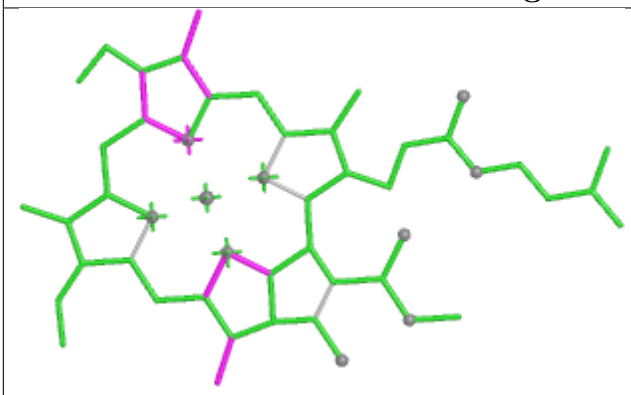


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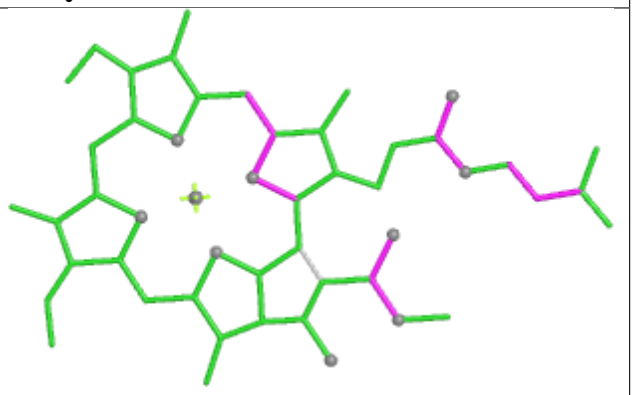


Rings

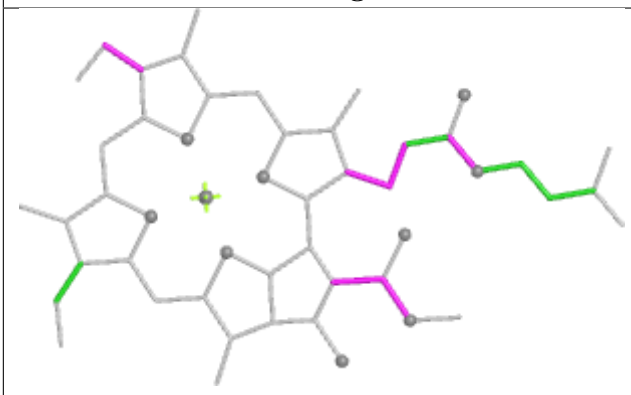
Ligand CLA Q 303



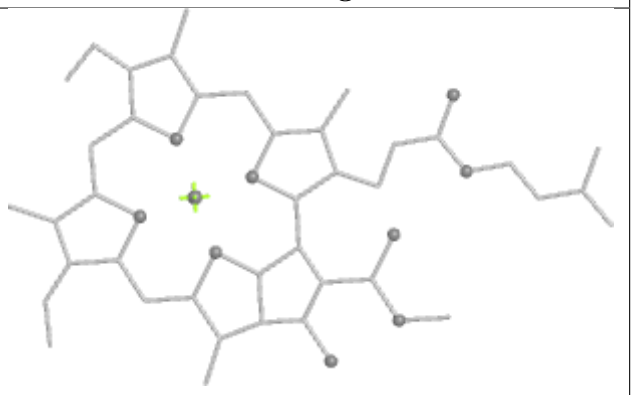
Bond lengths



Bond angles

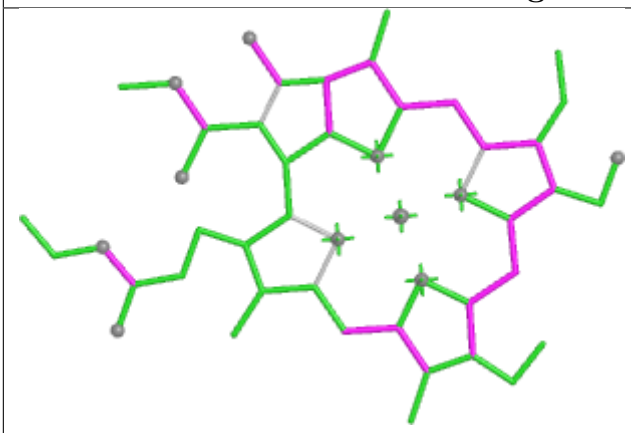


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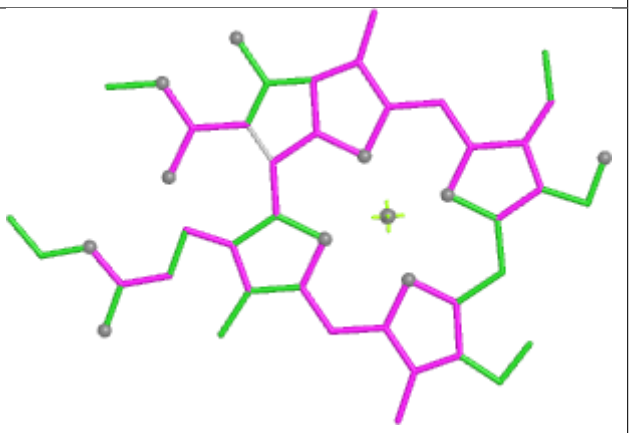


Rings

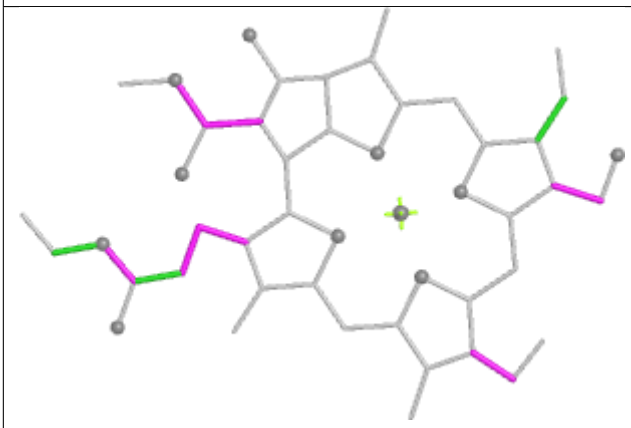
Ligand CHL v 314



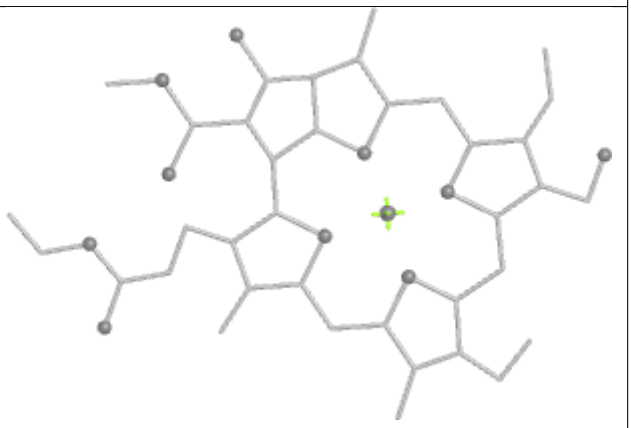
Bond lengths



Bond angles

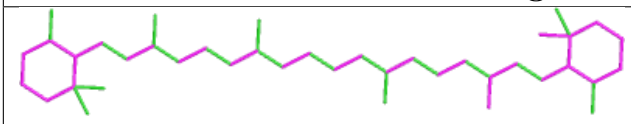


Torsions

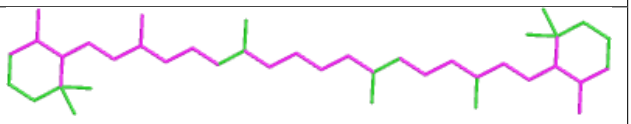


Rings

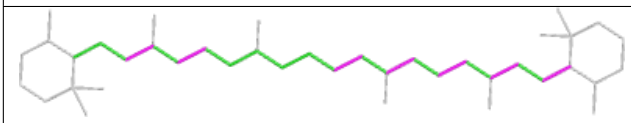
Ligand BCR c 516



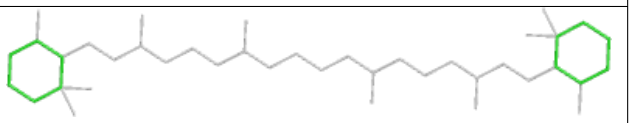
Bond lengths



Bond angles

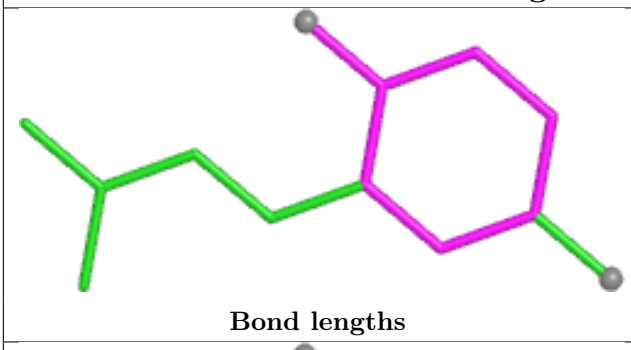


Torsions

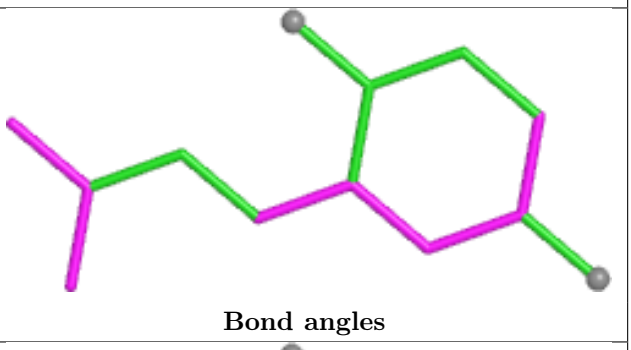


Rings

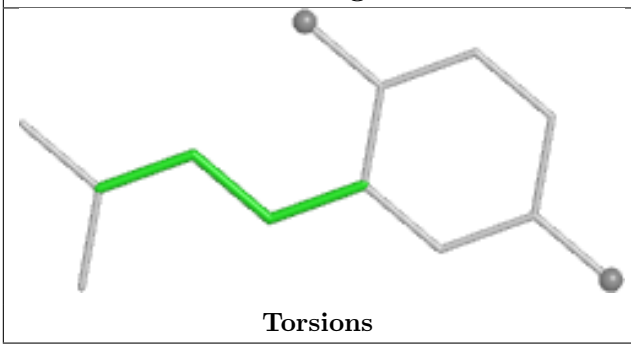
Ligand PL9 A 410



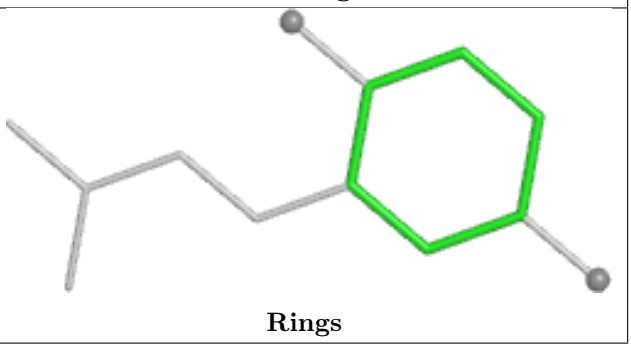
Bond lengths



Bond angles

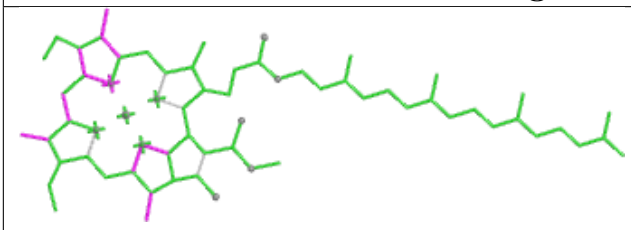


Torsions

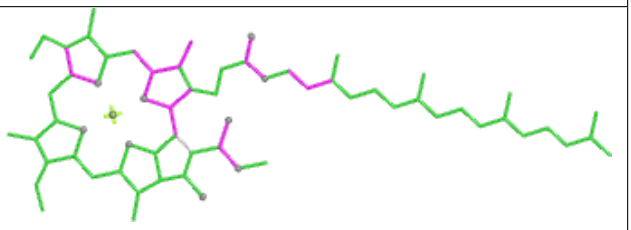


Rings

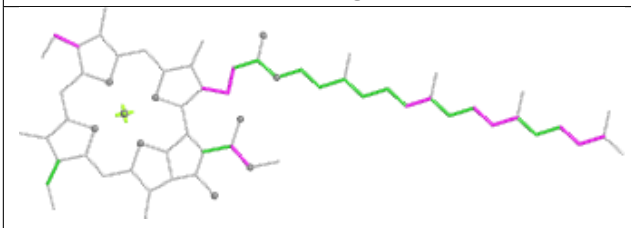
Ligand CLA 5 304



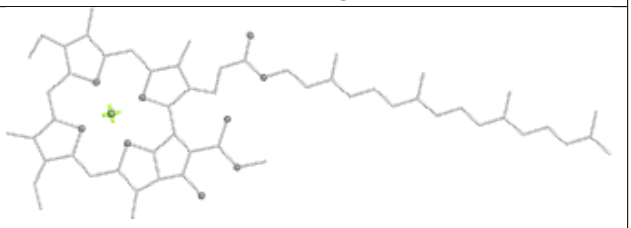
Bond lengths



Bond angles

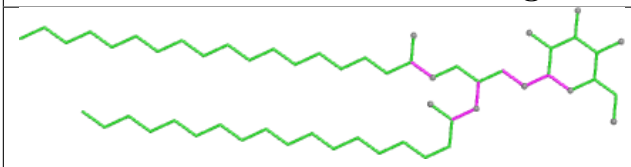


Torsions

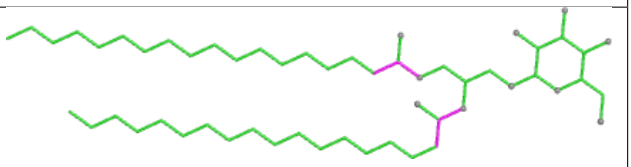


Rings

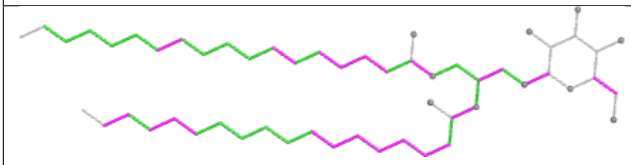
Ligand LMG b 624



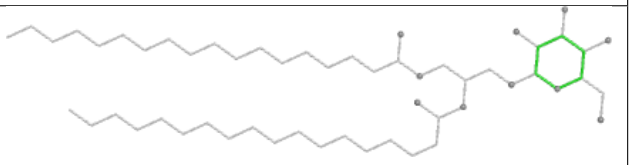
Bond lengths



Bond angles

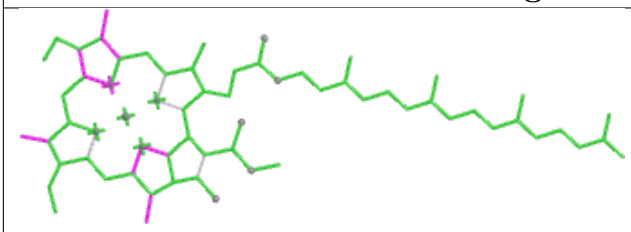


Torsions

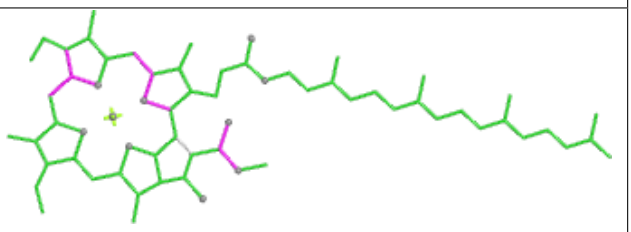


Rings

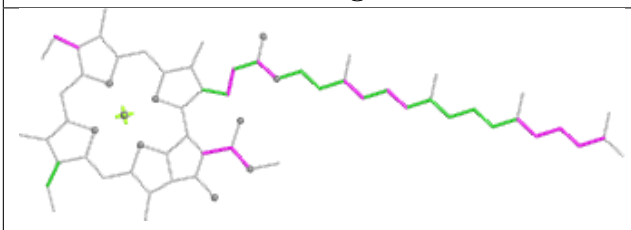
Ligand CLA B 606



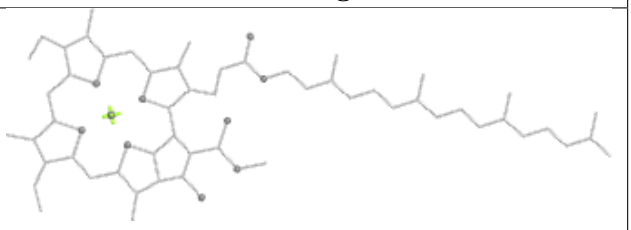
Bond lengths



Bond angles

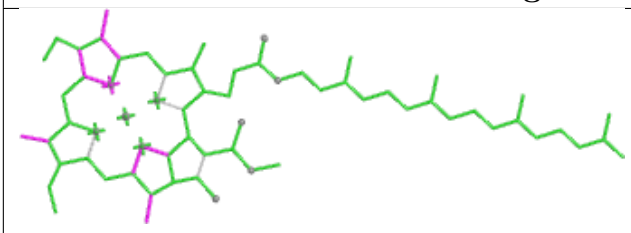


Torsions

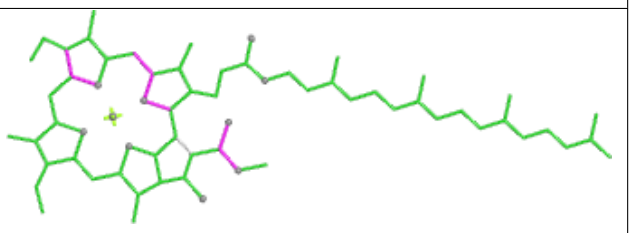


Rings

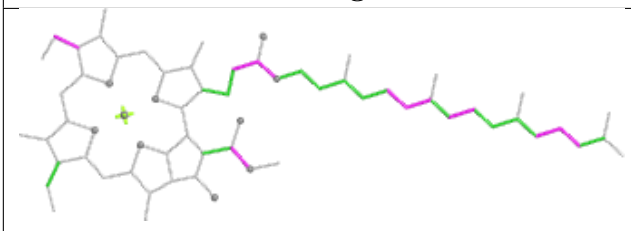
Ligand CLA U 302



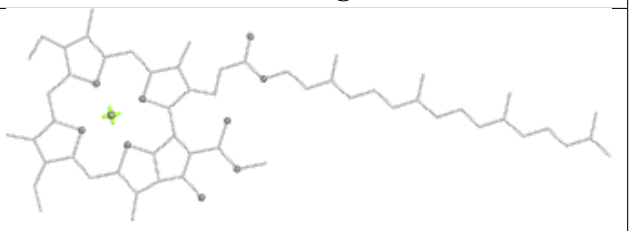
Bond lengths



Bond angles

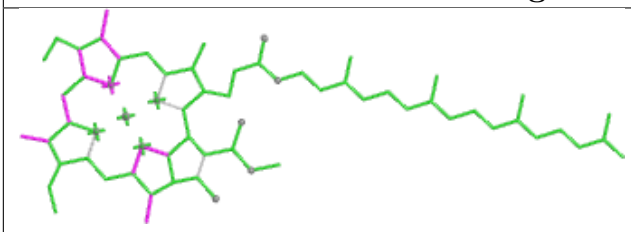


Torsions

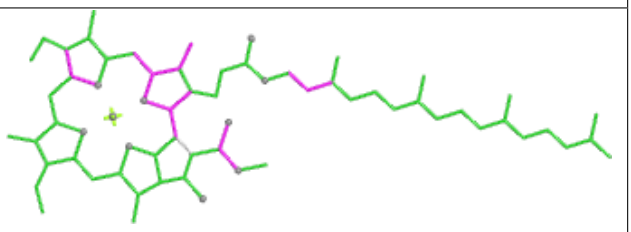


Rings

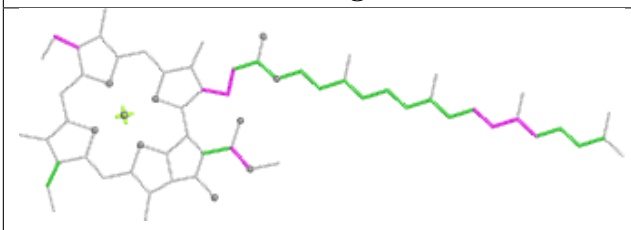
Ligand CLA 2 304



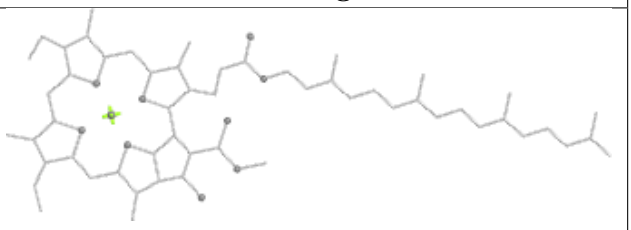
Bond lengths



Bond angles

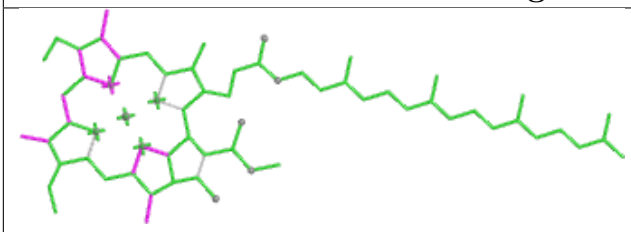


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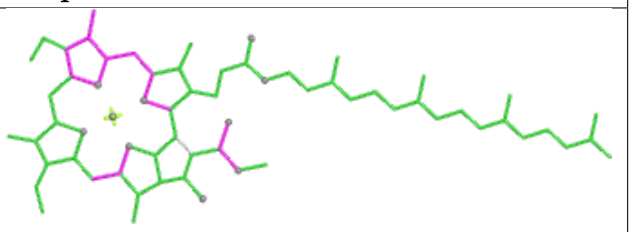


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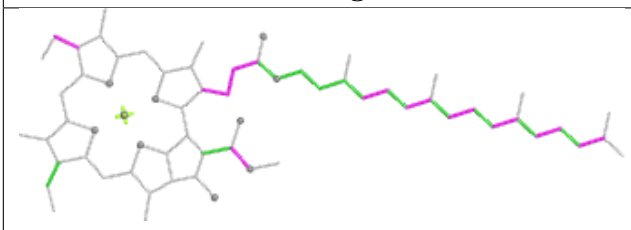
Ligand CLA q 301



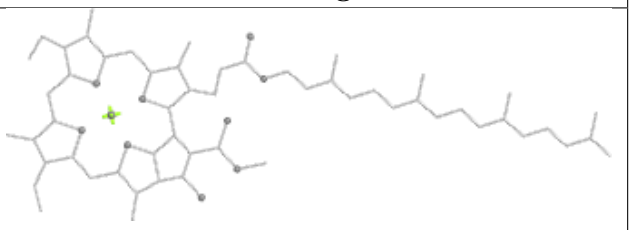
Bond lengths



Bond angles

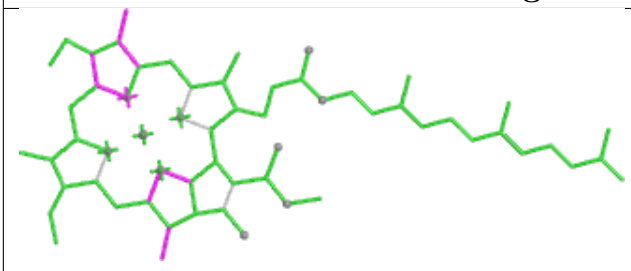


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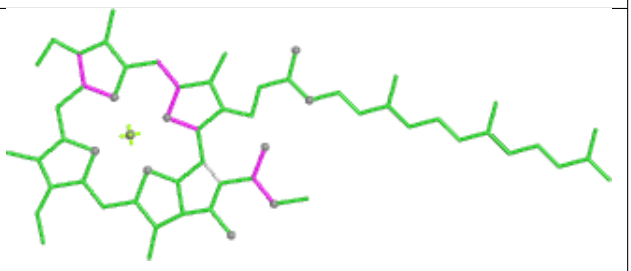


Rings

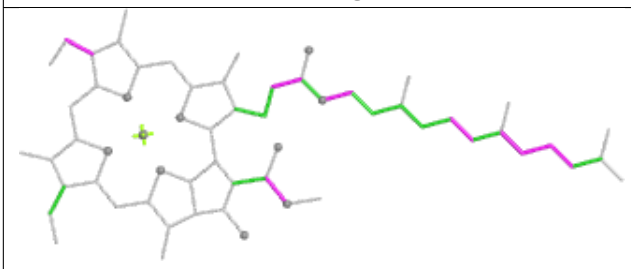
Ligand CLA G 306



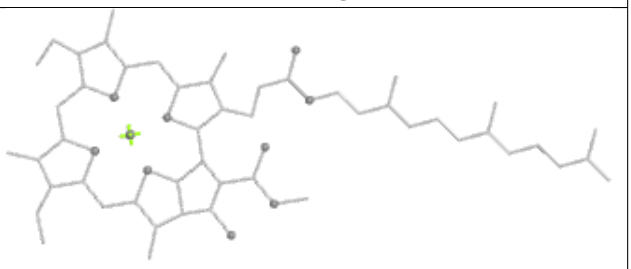
Bond lengths



Bond angles

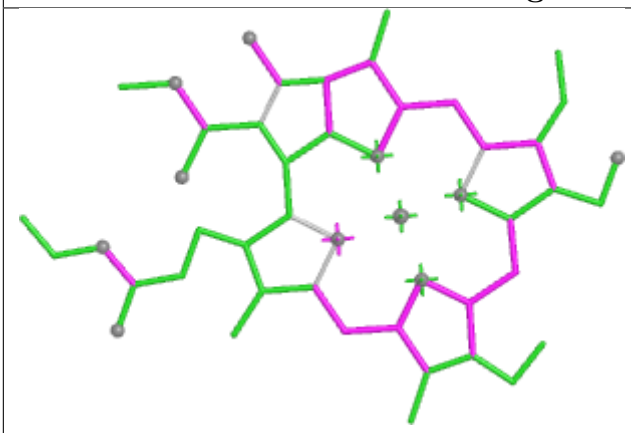


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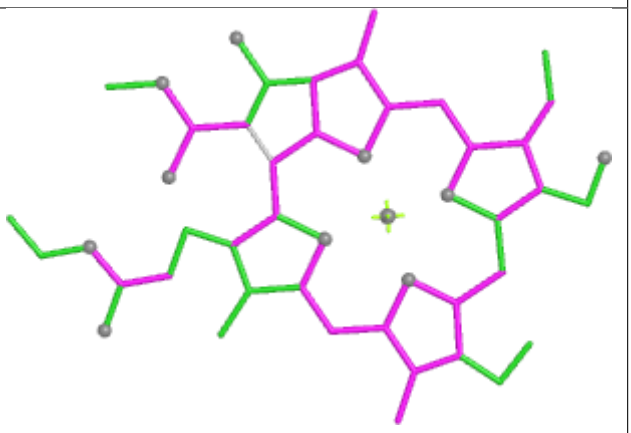


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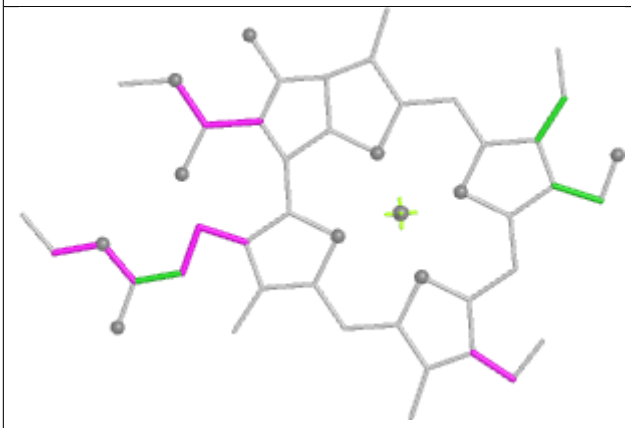
Ligand CHL u 314



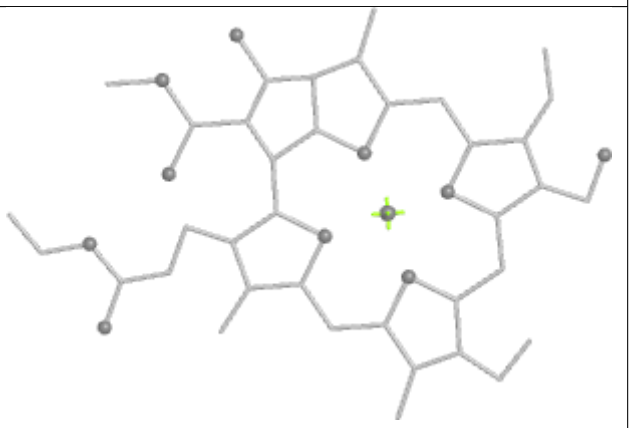
Bond lengths



Bond angles

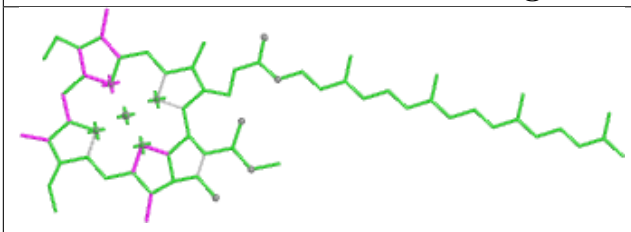


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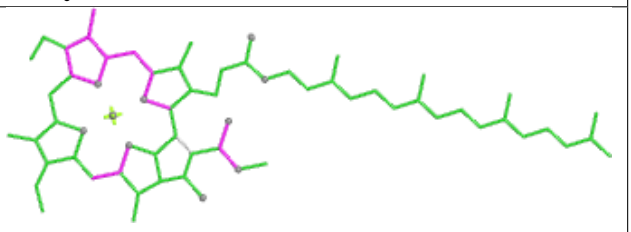


Rings

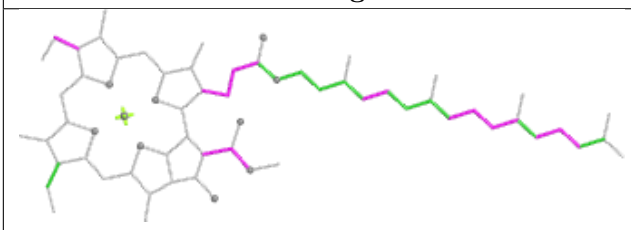
Ligand CLA Q 301



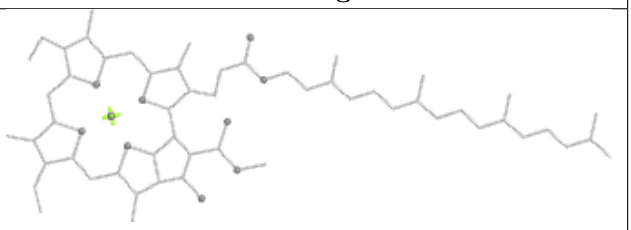
Bond lengths



Bond angles

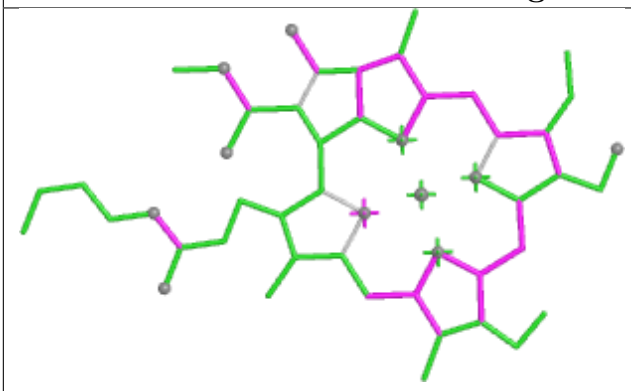


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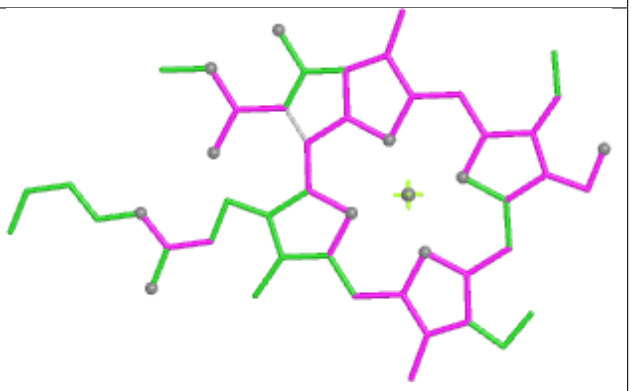


Rings

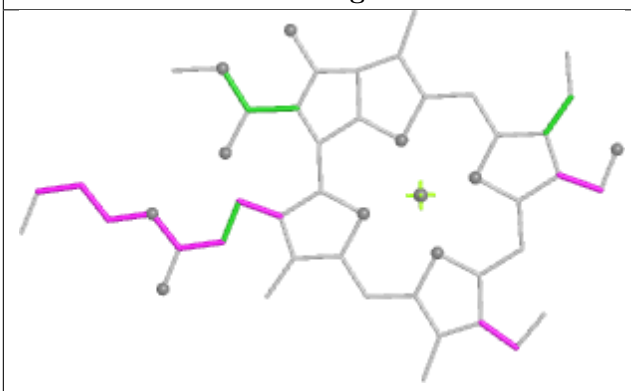
Ligand CHL 6 314



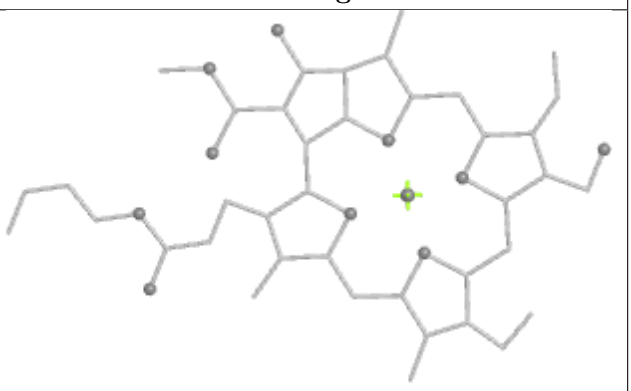
Bond lengths



Bond angles

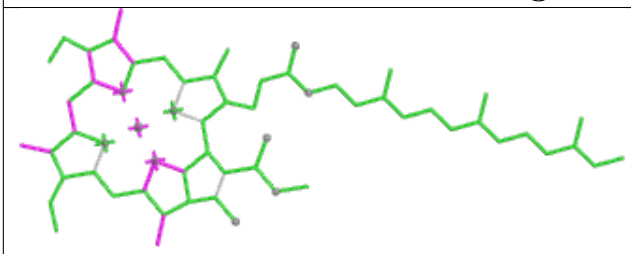


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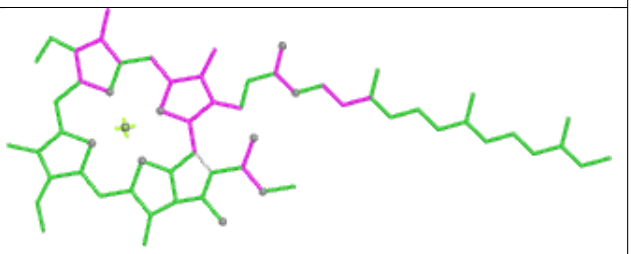


Rings

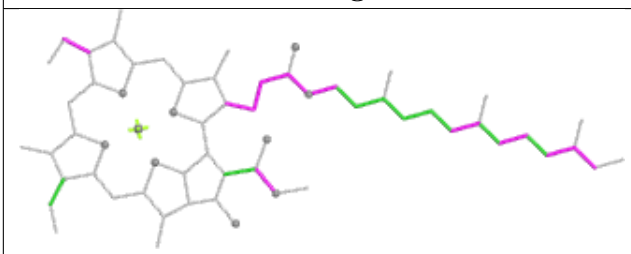
Ligand CLA s 301



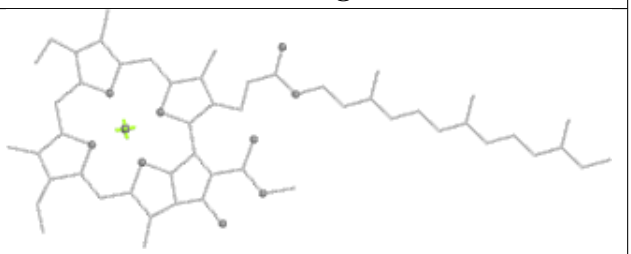
Bond lengths



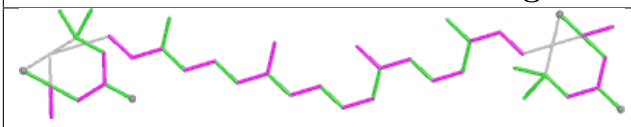
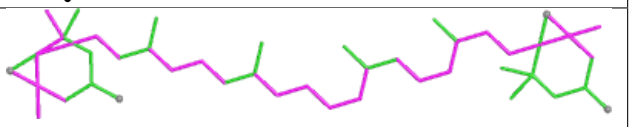
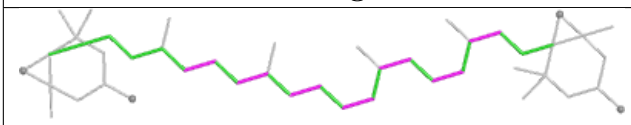
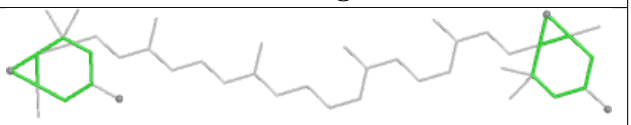
Bond angles

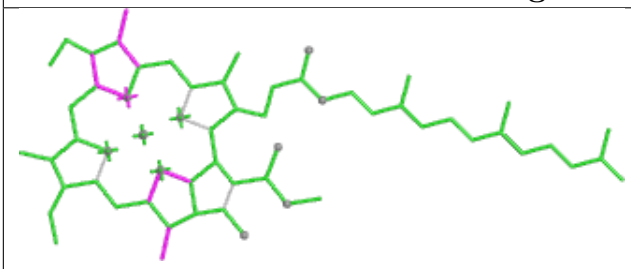
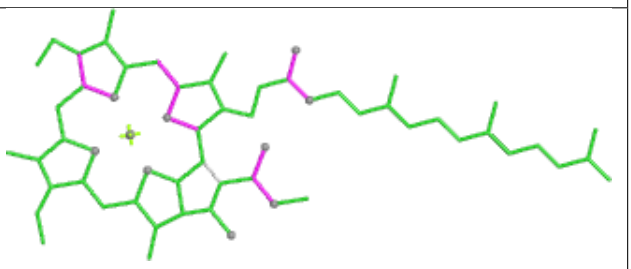
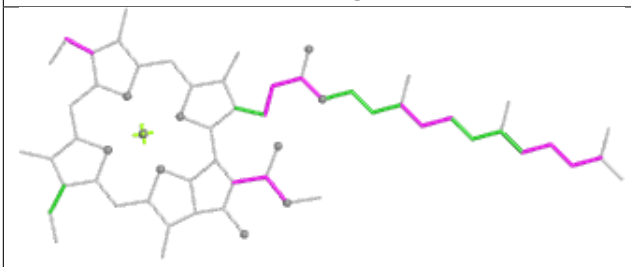
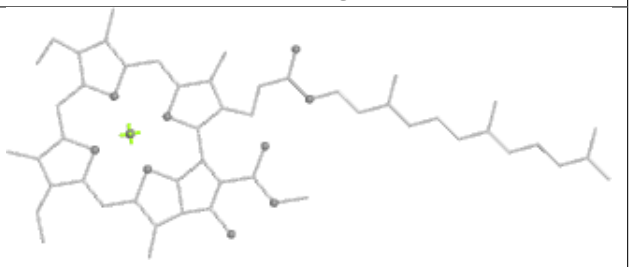


Torsions

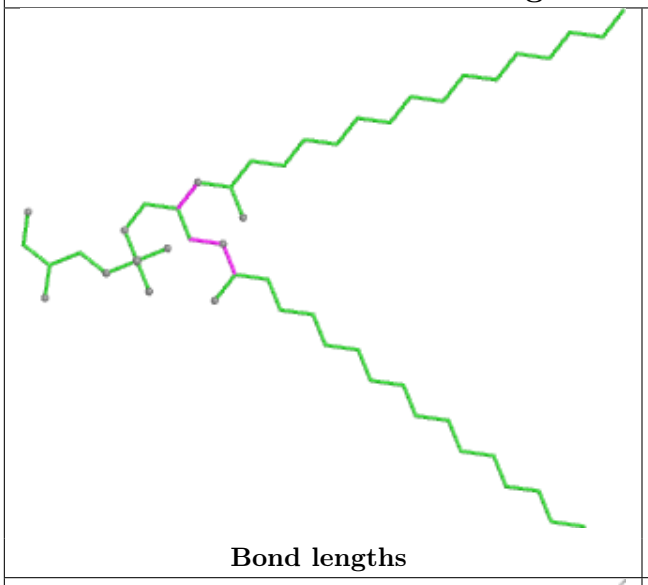


Rings

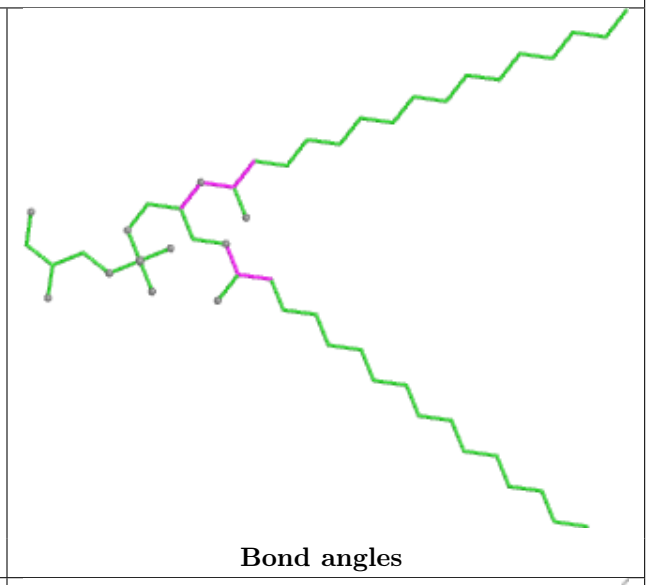
Ligand XAT Q 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

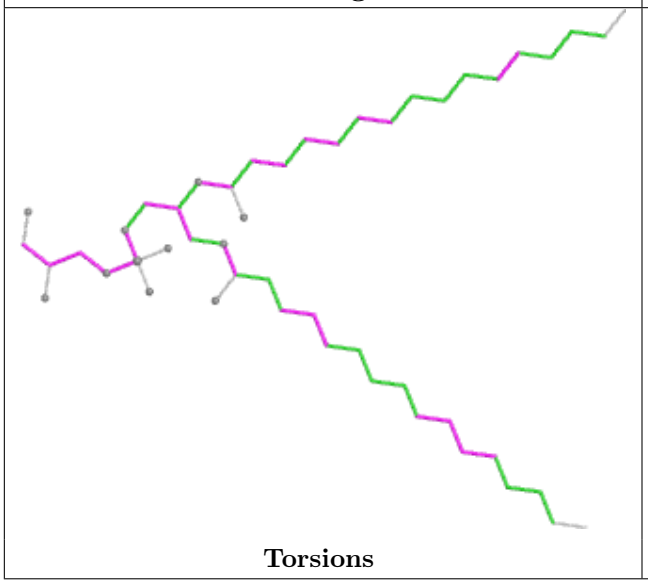
Ligand LHG L 101



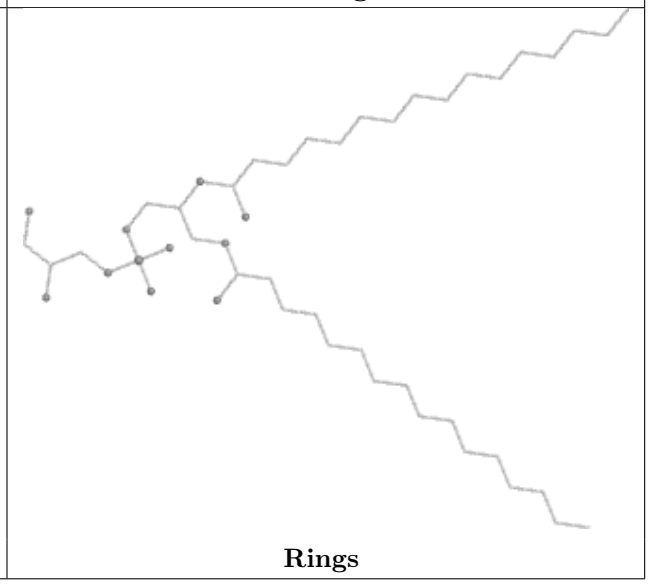
Bond lengths



Bond angles

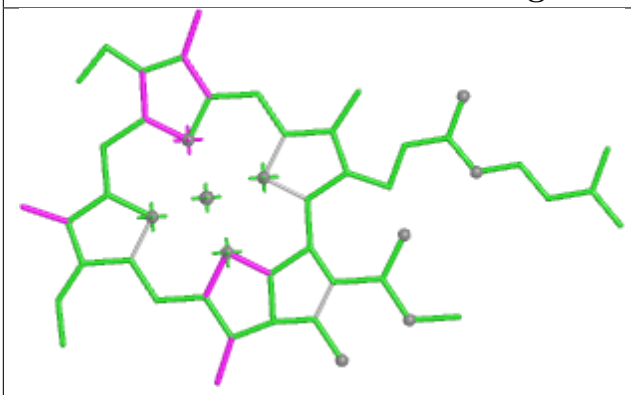


Torsions

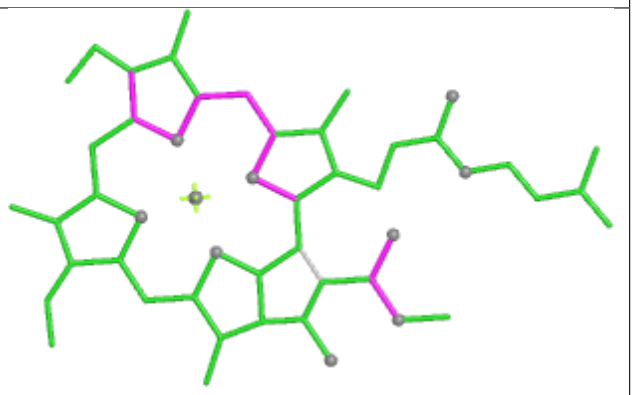


Rings

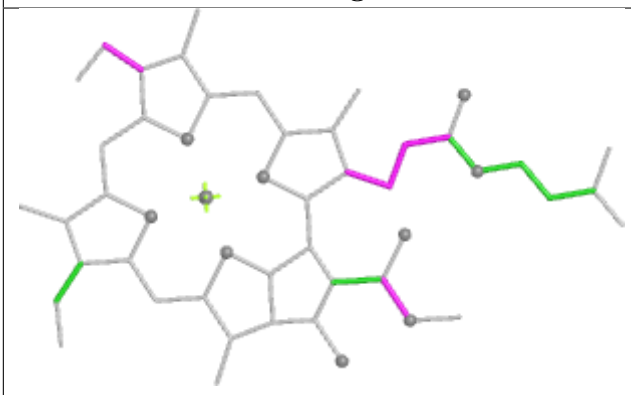
Ligand CLA v 303



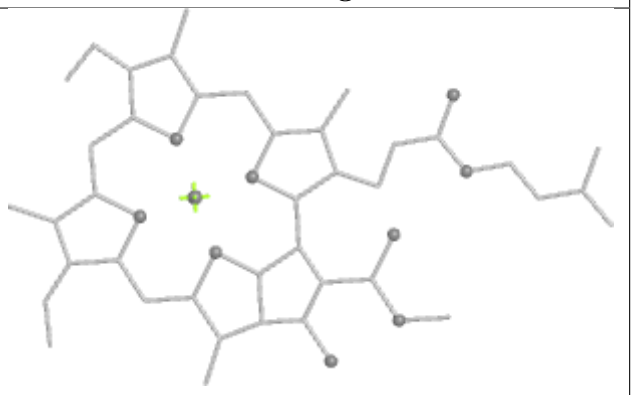
Bond lengths



Bond angles



Torsions

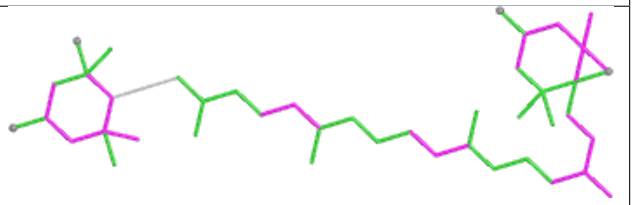


Rings

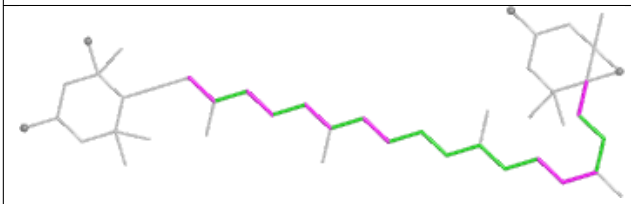
Ligand NEX R 301



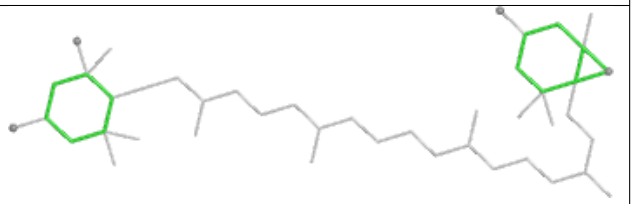
Bond lengths



Bond angles

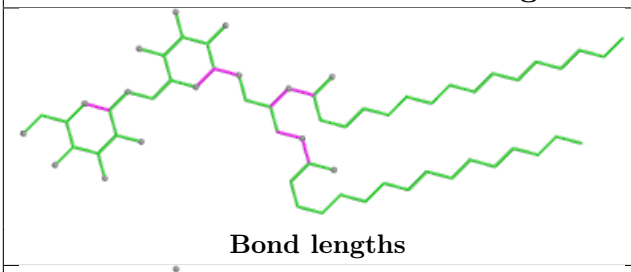


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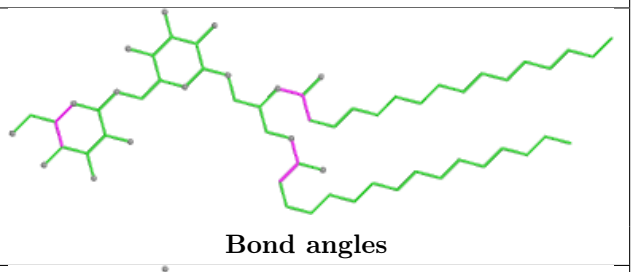


Rings

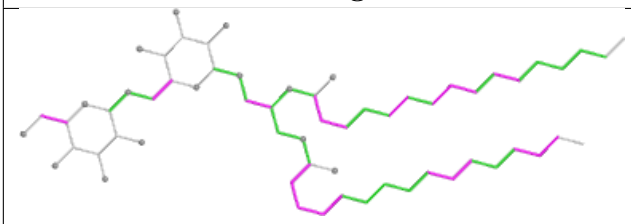
Ligand DGD B 601



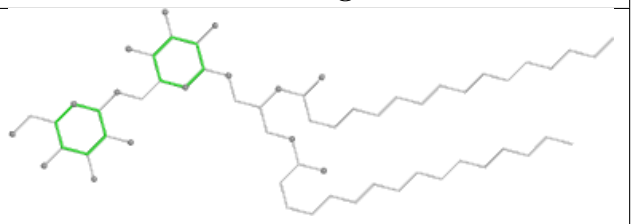
Bond lengths



Bond angles

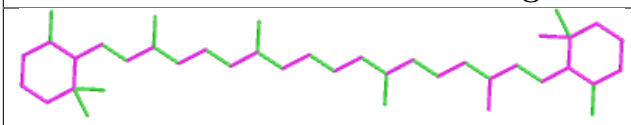


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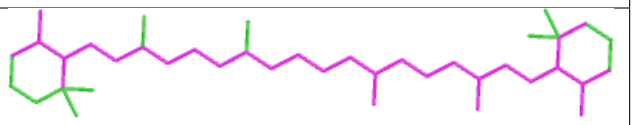


Rings

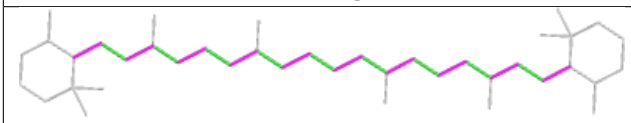
Ligand BCR C 517



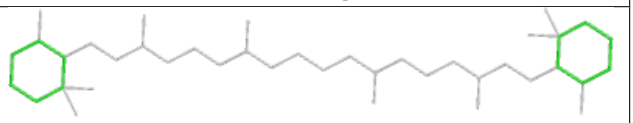
Bond lengths



Bond angles

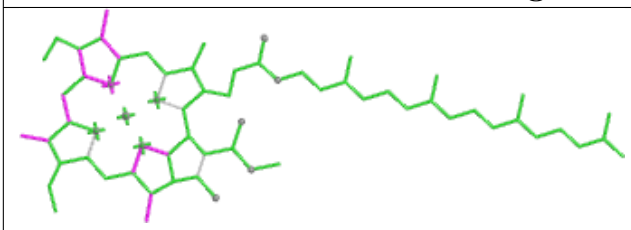


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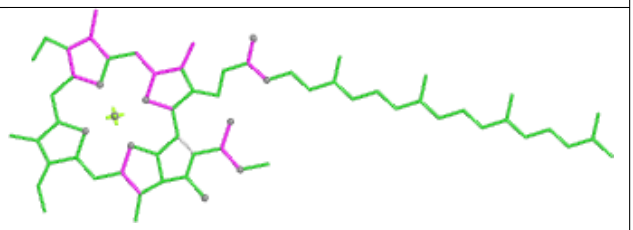


Rings

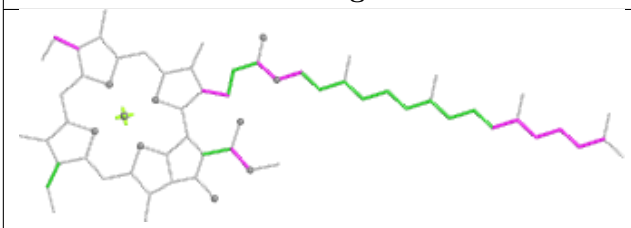
Ligand CLA n 304



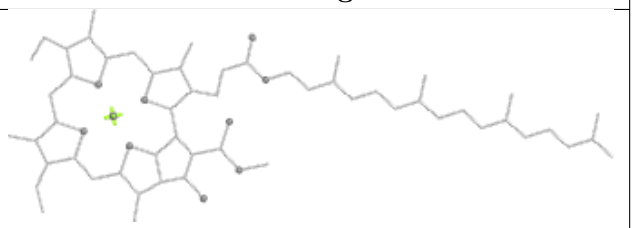
Bond lengths



Bond angles

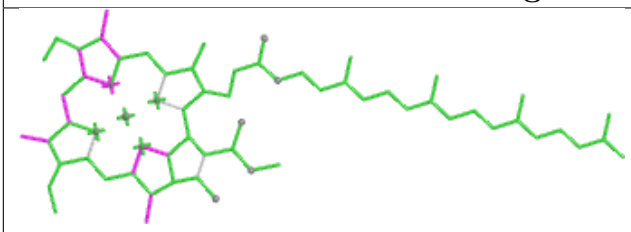


Torsions

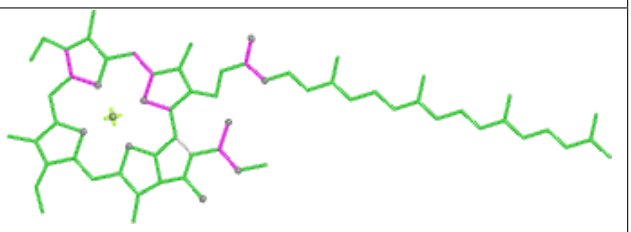


Rings

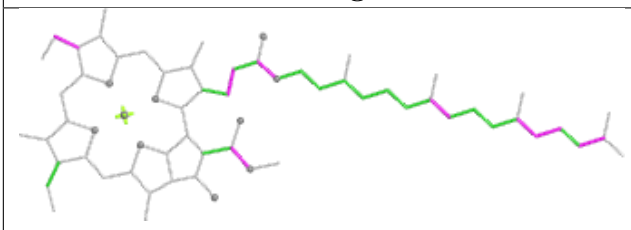
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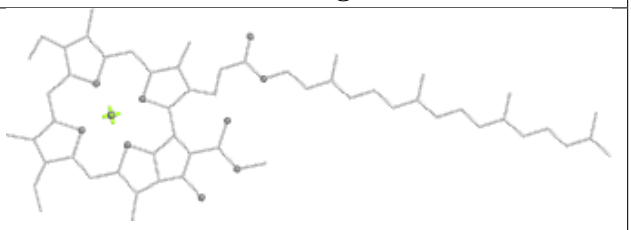
Bond lengths



Bond angles

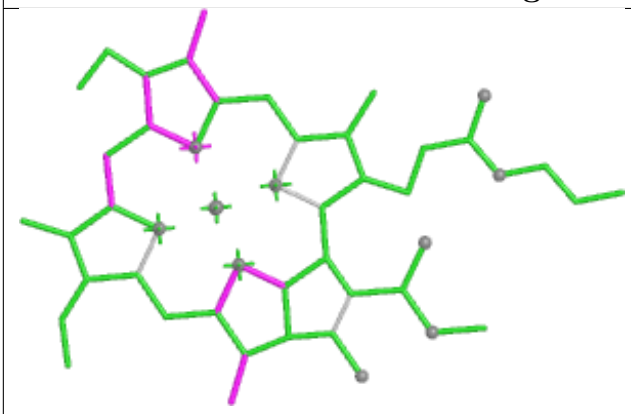


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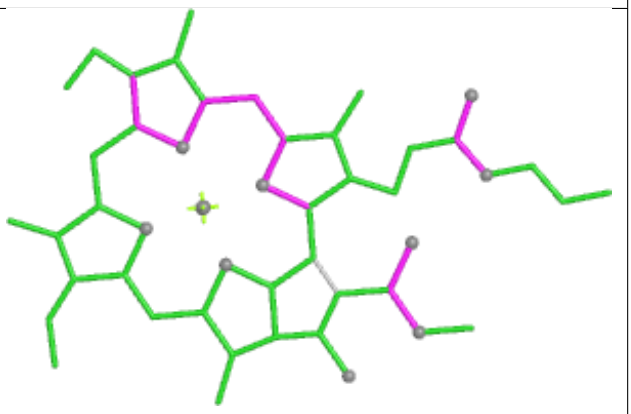


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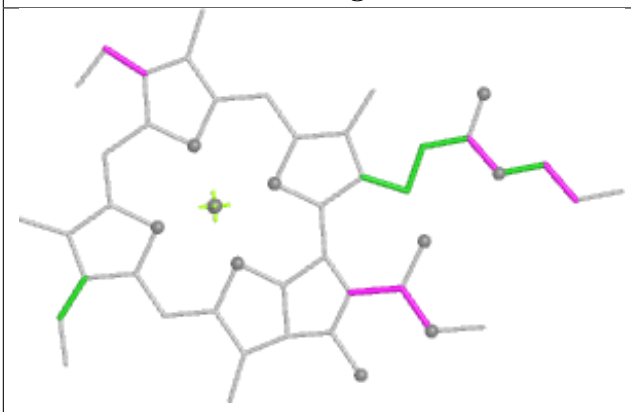
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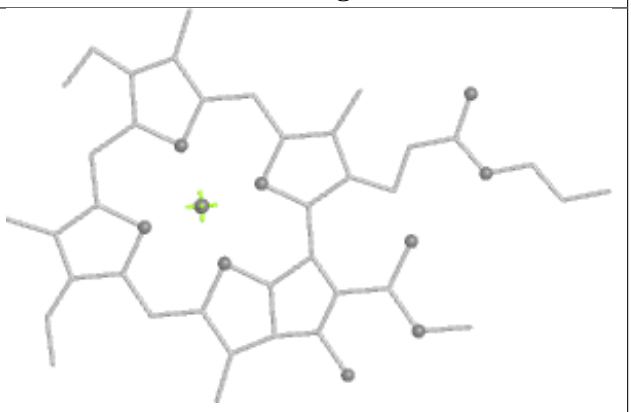
Bond lengths



Bond angles

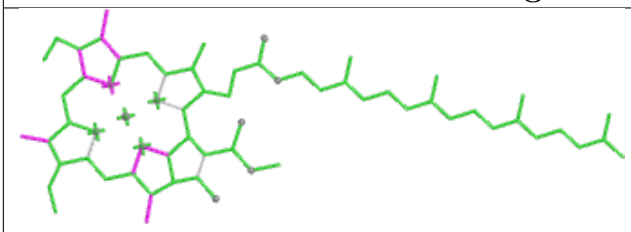


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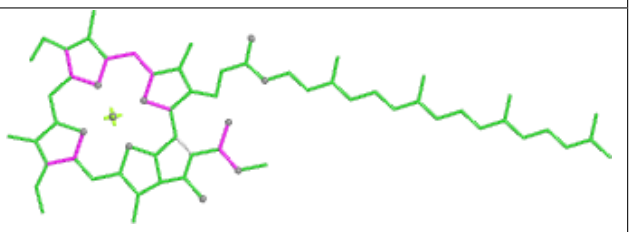


Rings

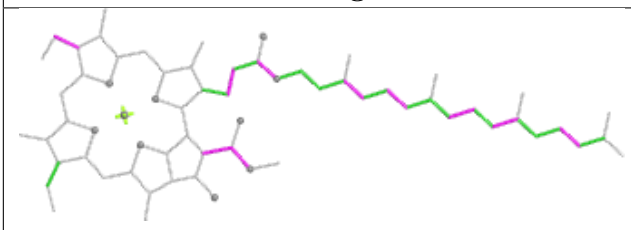
Ligand CLA C 506



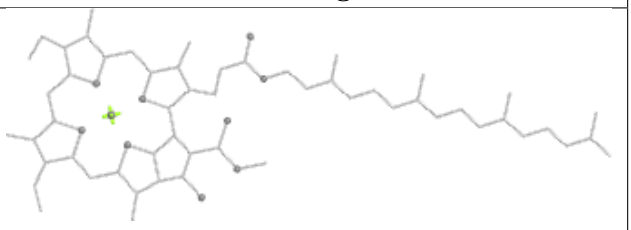
Bond lengths



Bond angles

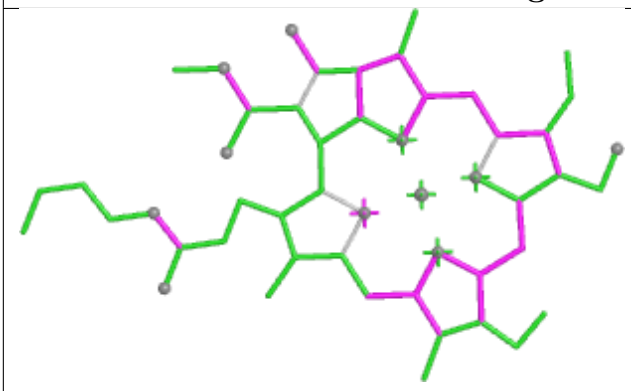


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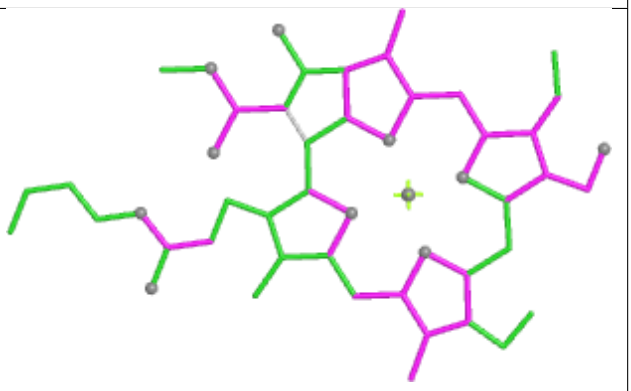


Rings

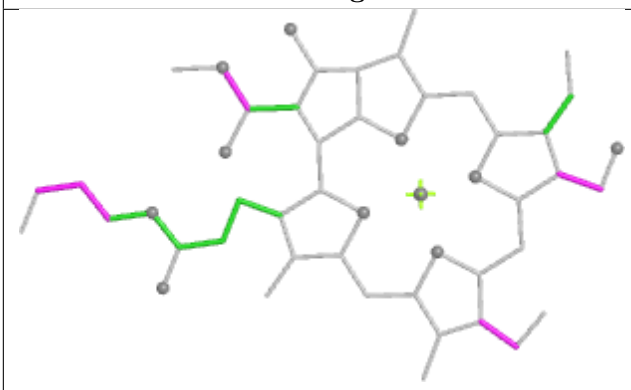
Ligand CHL 4 315



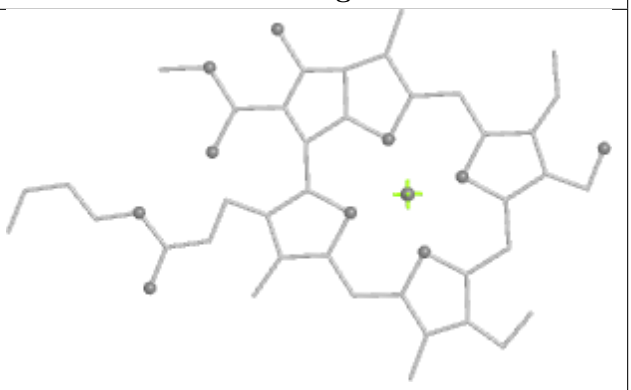
Bond lengths



Bond angles

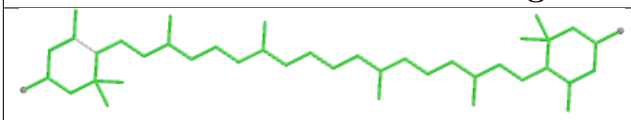


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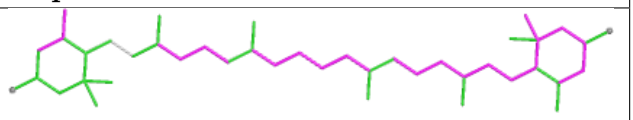


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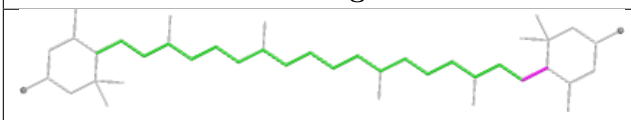
Ligand LUT p 310



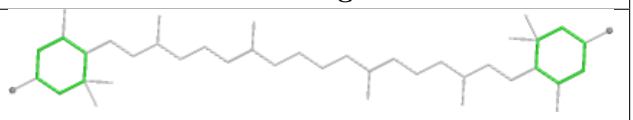
Bond lengths



Bond angles

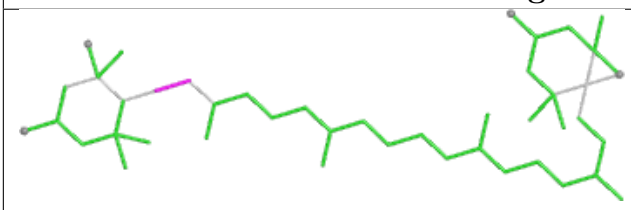


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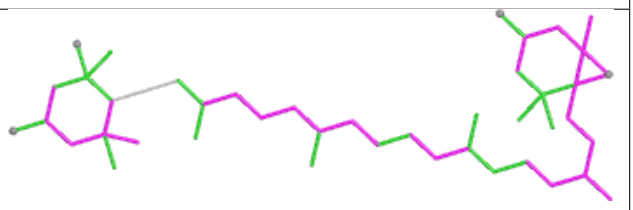


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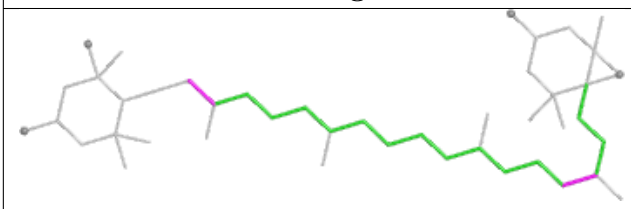
Ligand NEX s 317



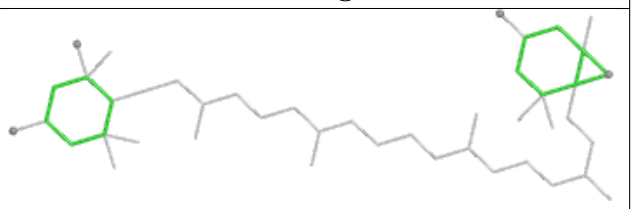
Bond lengths



Bond angles

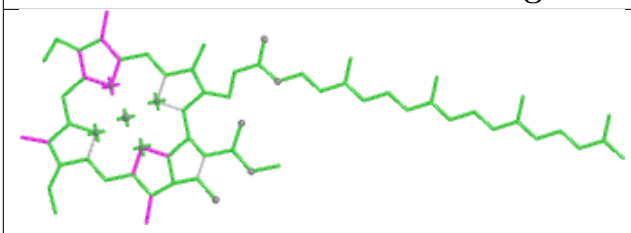


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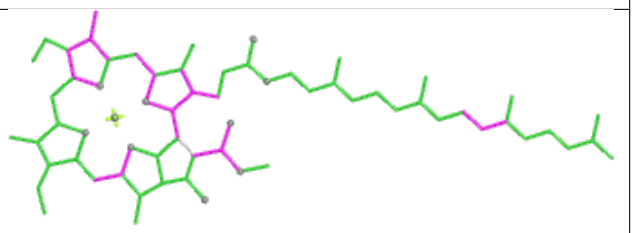


Rings

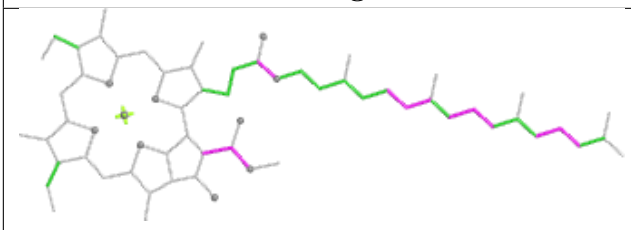
Ligand CLA C 511



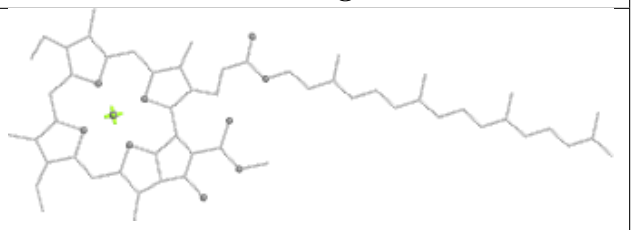
Bond lengths



Bond angles

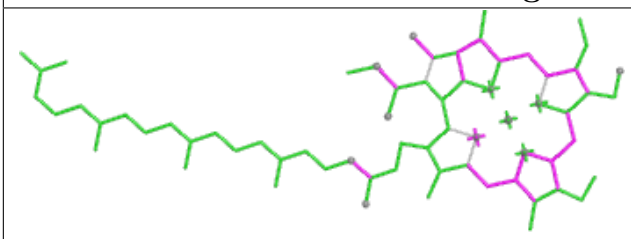


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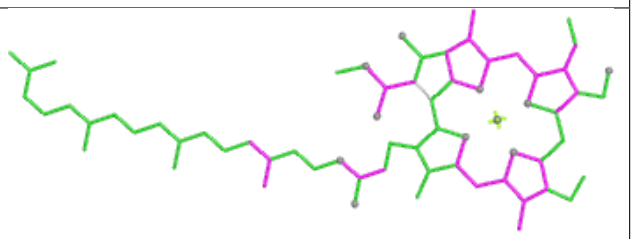


Rings

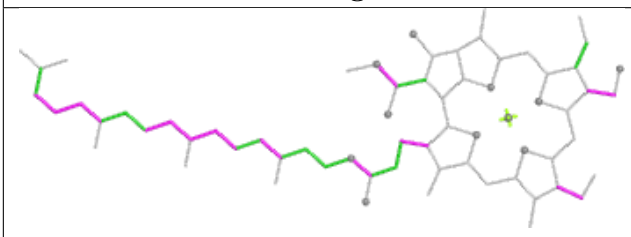
Ligand CHL U 317



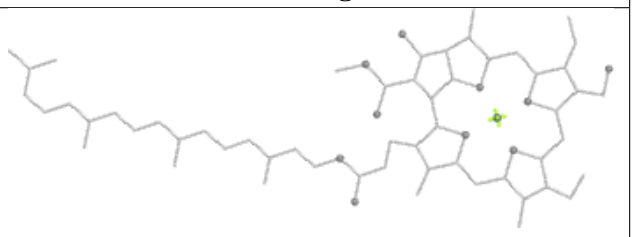
Bond lengths



Bond angles

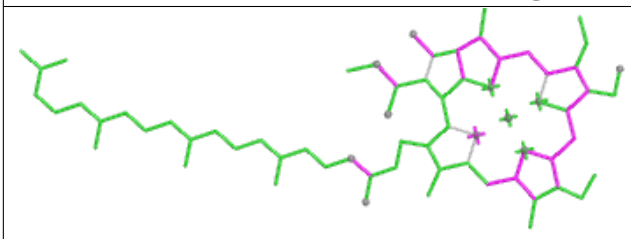


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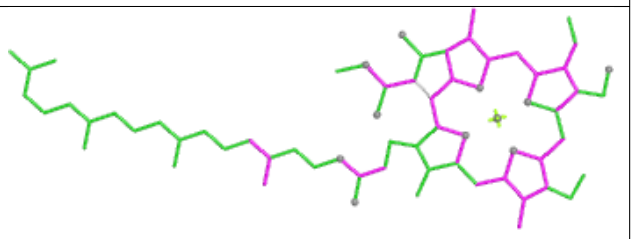


Rings

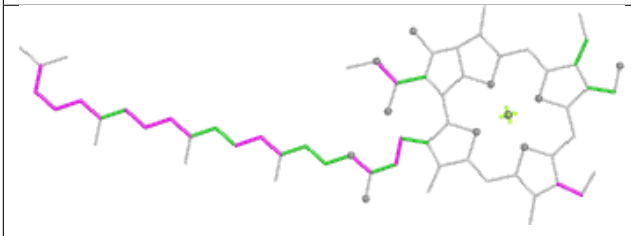
Ligand CHL 3 314



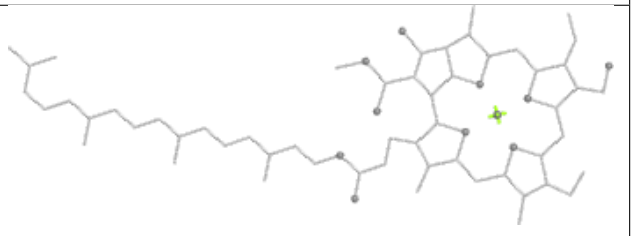
Bond lengths



Bond angles

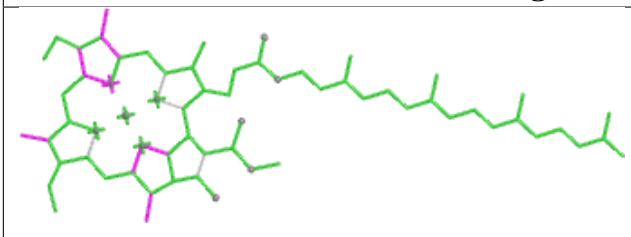


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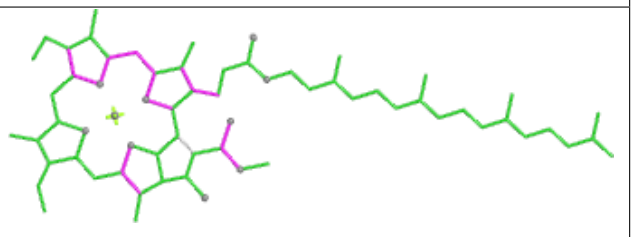


Rings

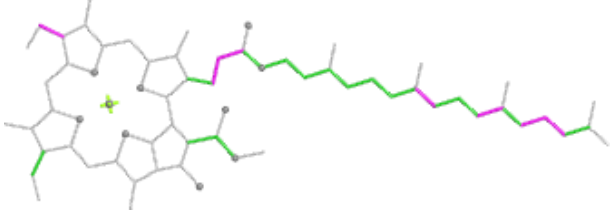
Ligand CLA c 502



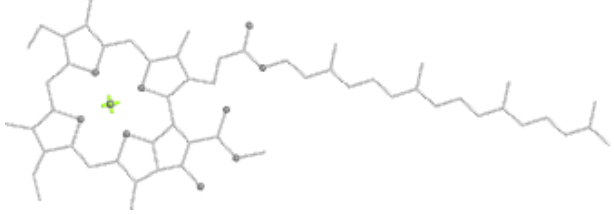
Bond lengths



Bond angles

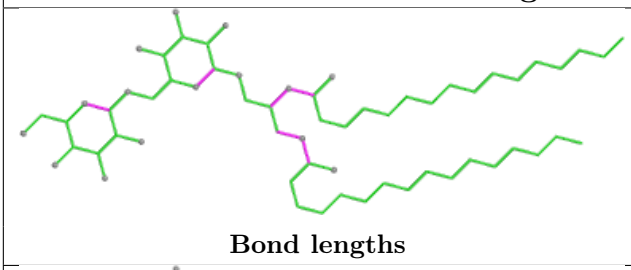


Torsions

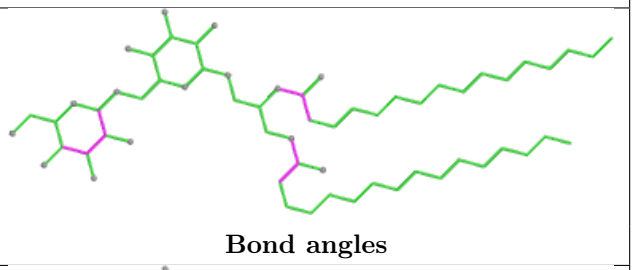


Rings

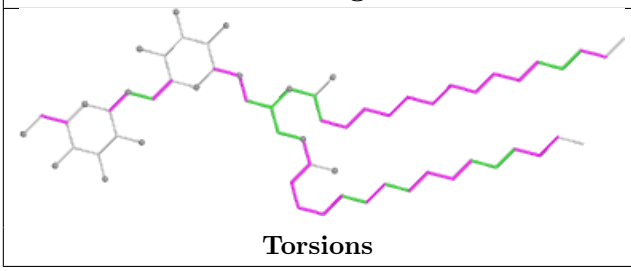
Ligand DGD C 520



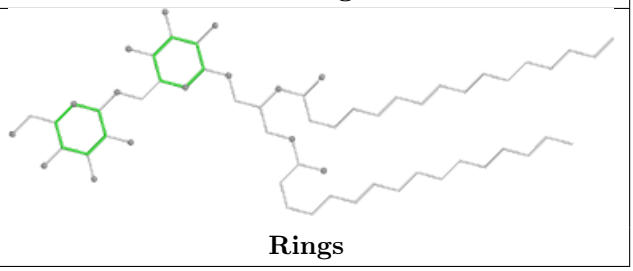
Bond lengths



Bond angles

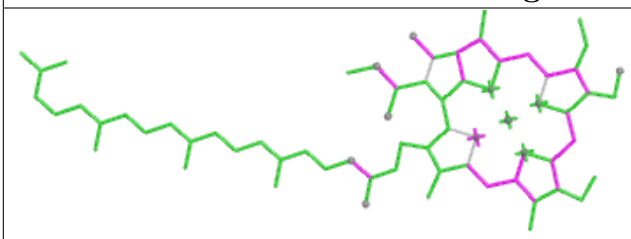


Torsions

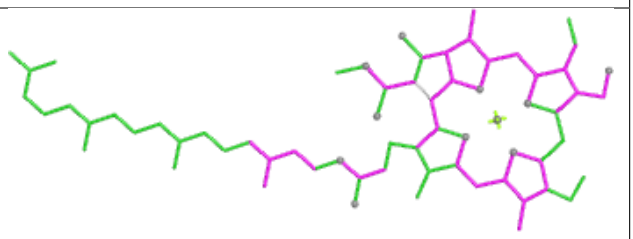


Rings

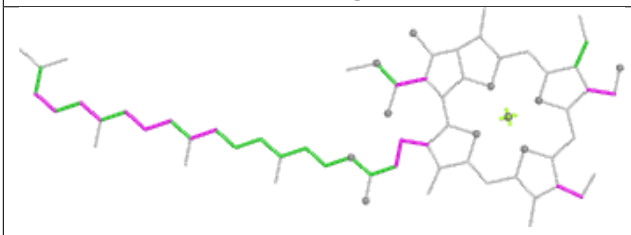
Ligand CHL U 315



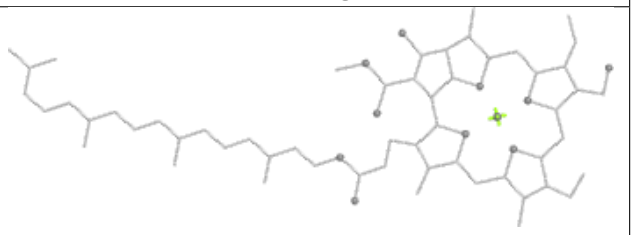
Bond lengths



Bond angles

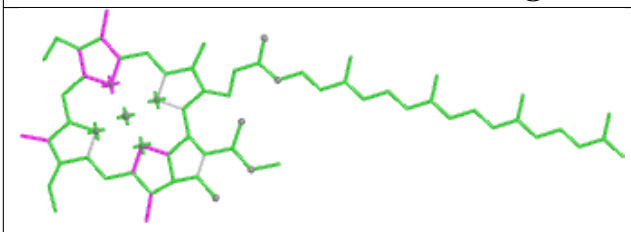


Torsions

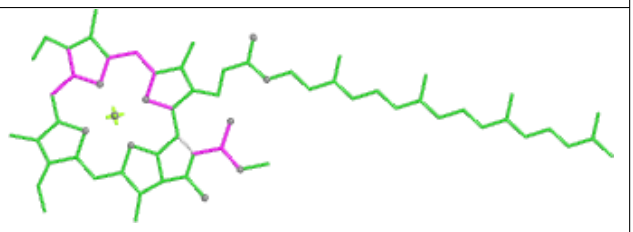


Rings

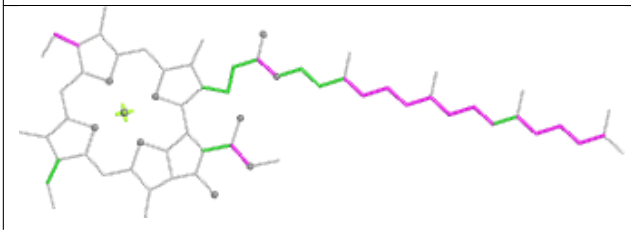
Ligand CLA C 508



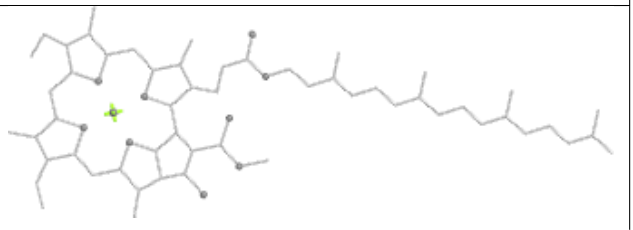
Bond lengths



Bond angles

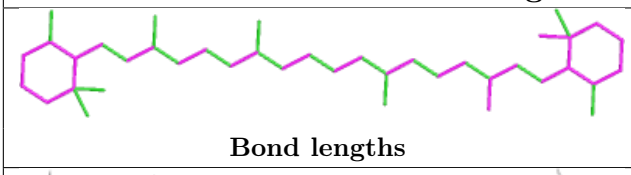


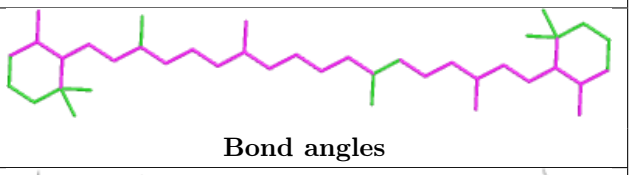
Torsions

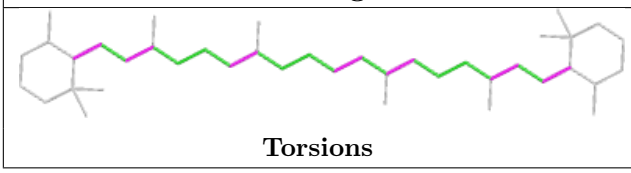


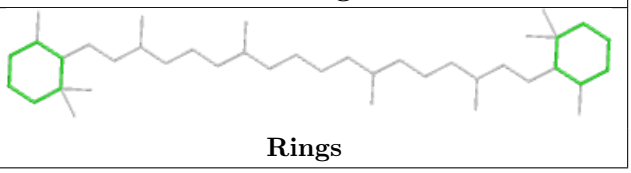
Rings

Ligand BCR d 403

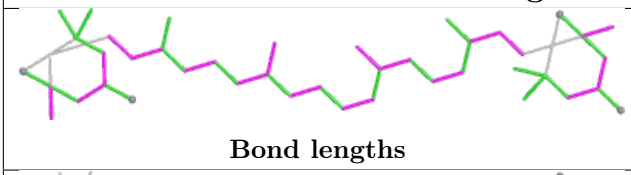

Bond lengths

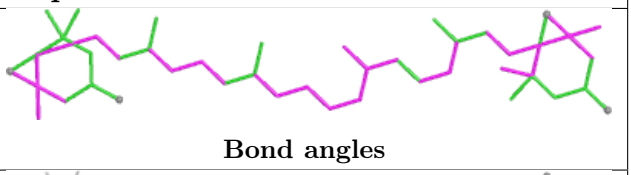

Bond angles

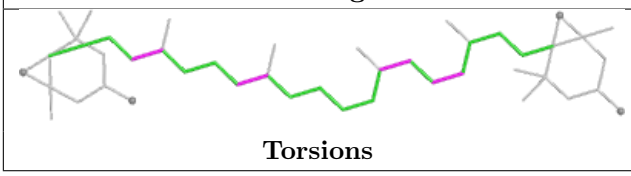

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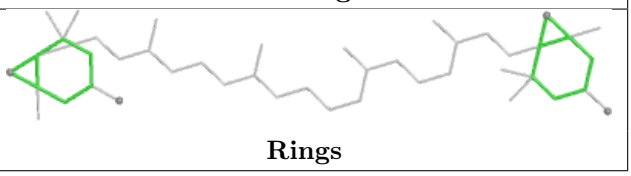

Rings

Ligand XAT p 312

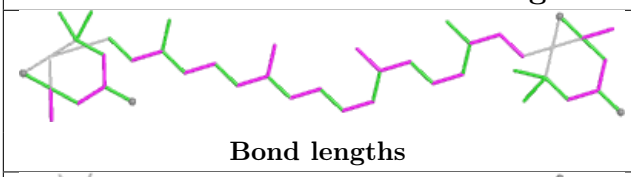

Bond lengths

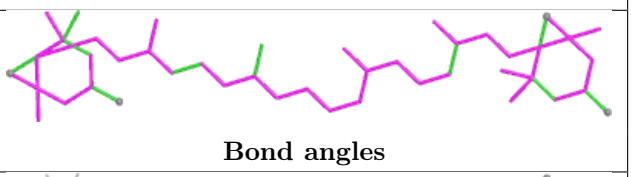

Bond angles

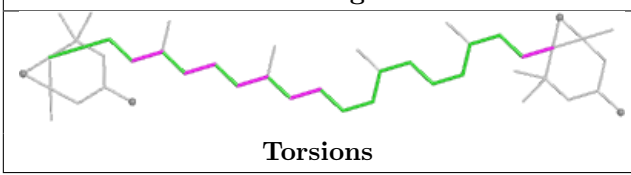

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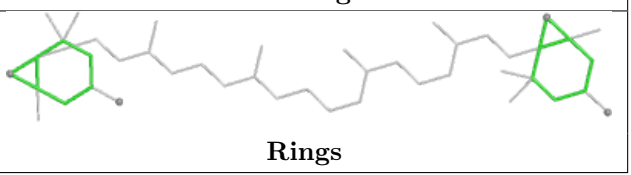

Rings

Ligand XAT r 612

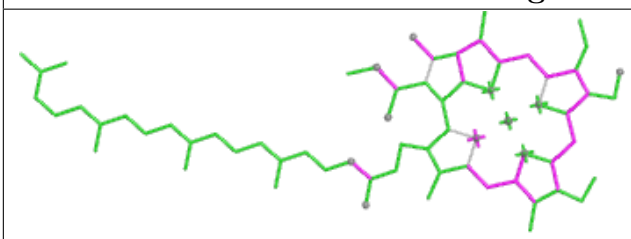

Bond lengths

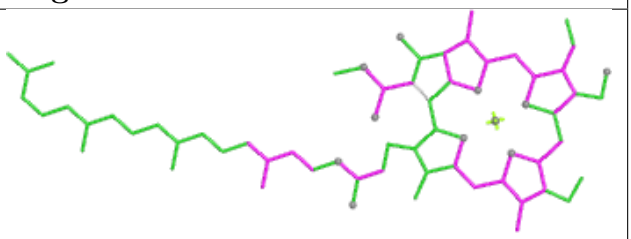

Bond angles

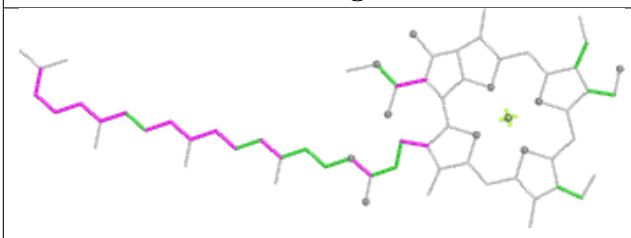

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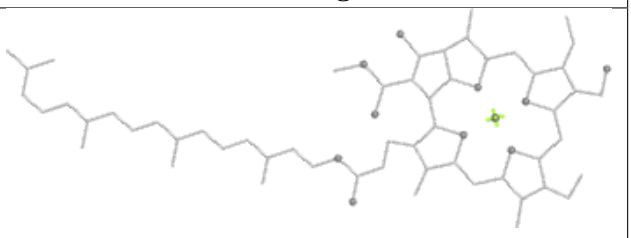

Rings

Ligand CHL g 311

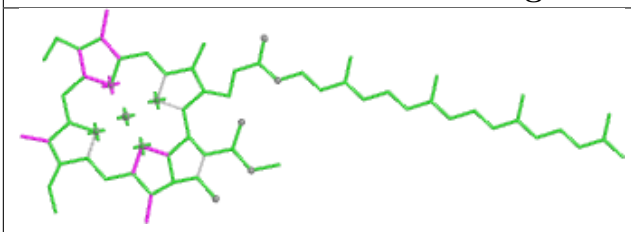

Bond lengths


Bond angles

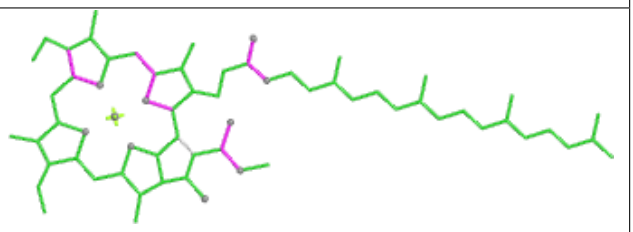

Torsions


Rings

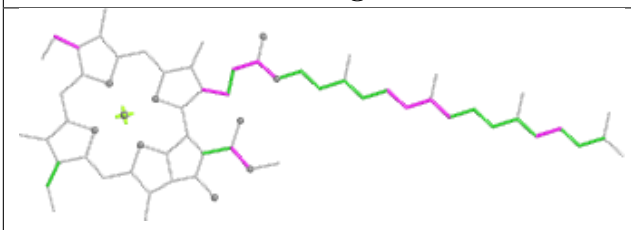
Ligand CLA P 303



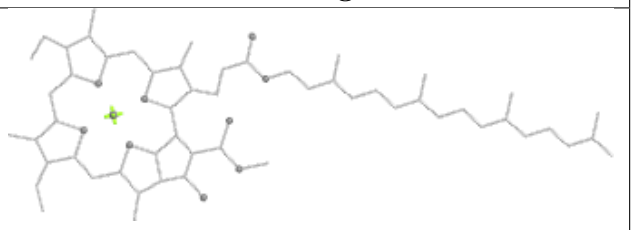
Bond lengths



Bond angles

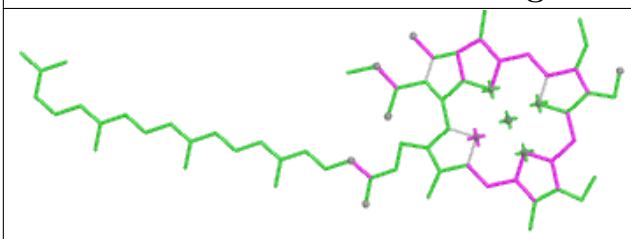


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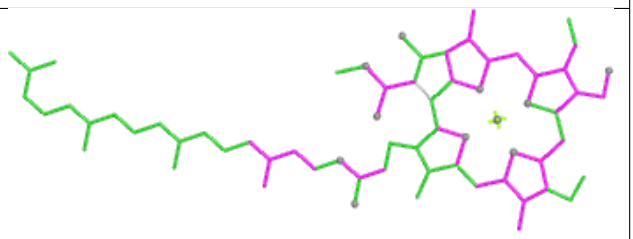


Rings

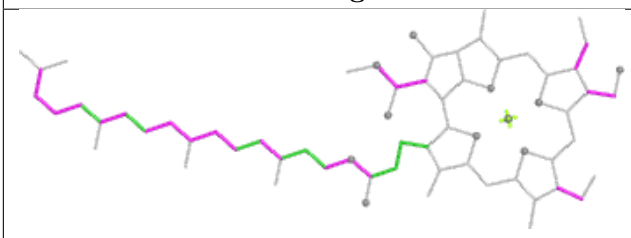
Ligand CHL n 318



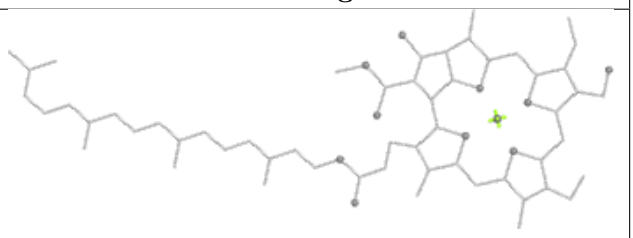
Bond lengths



Bond angles

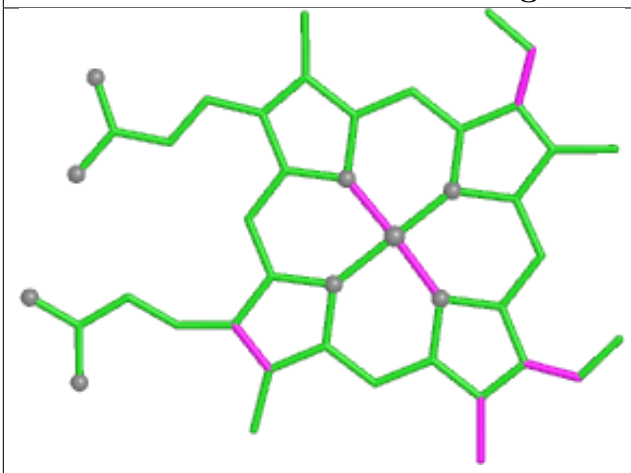


Torsions

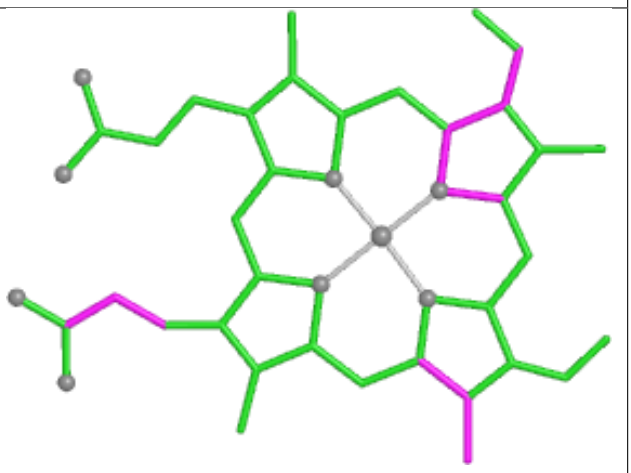


Rings

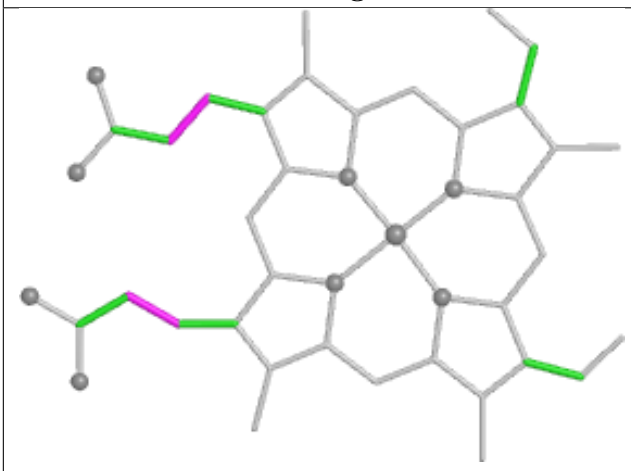
Ligand HEM E 101



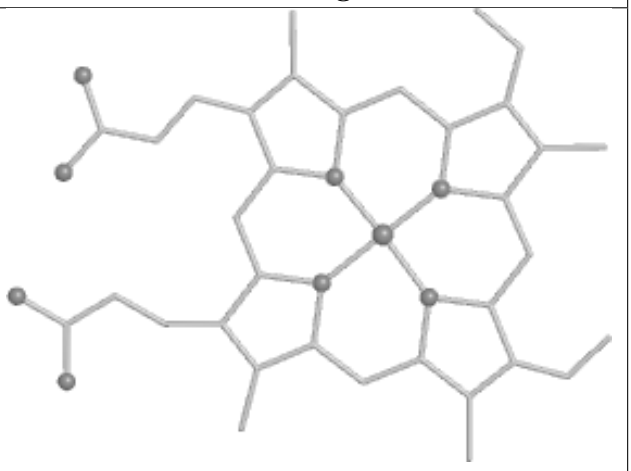
Bond lengths



Bond angles

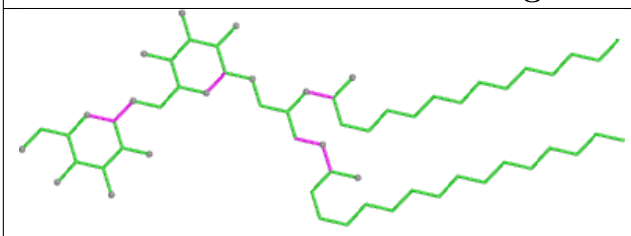


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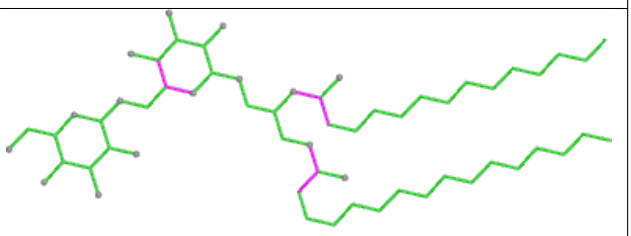


Rings

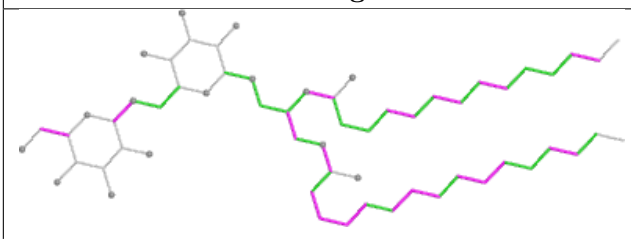
Ligand DGD J 101



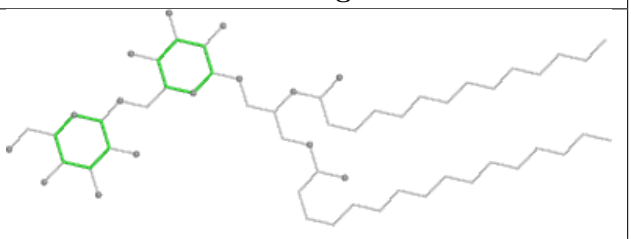
Bond lengths



Bond angles

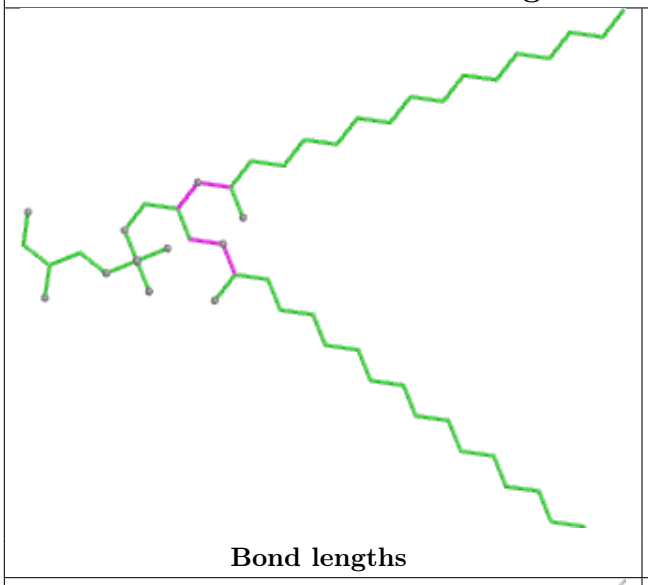


Torsions

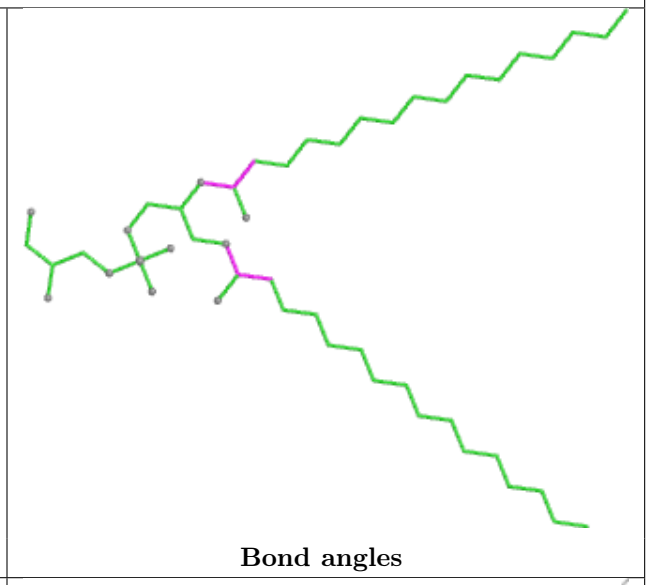


Rings

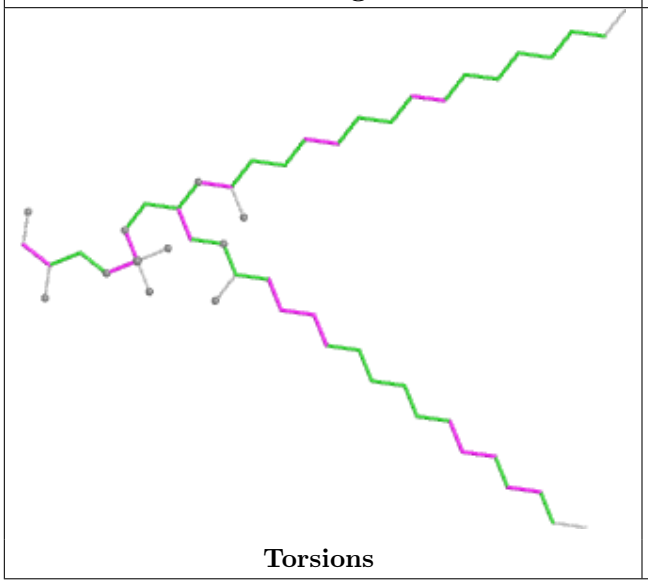
Ligand LHG V 312



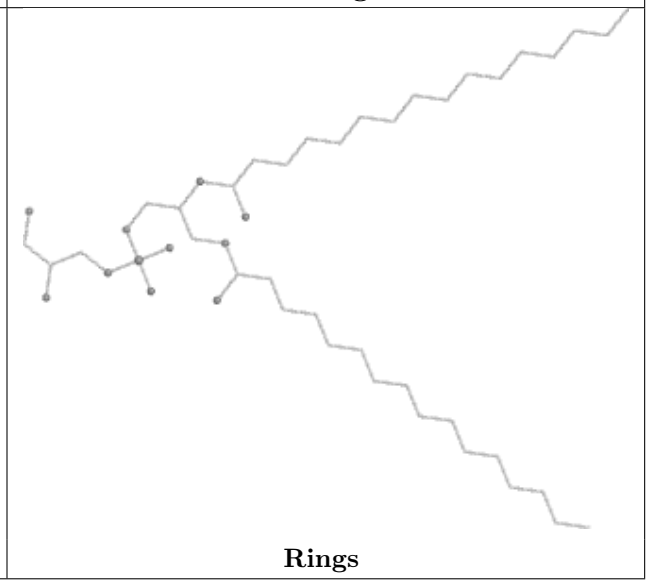
Bond lengths



Bond angles

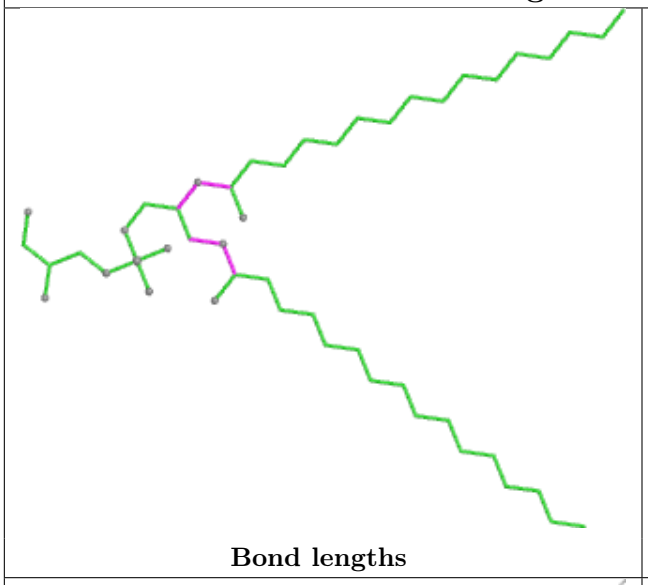


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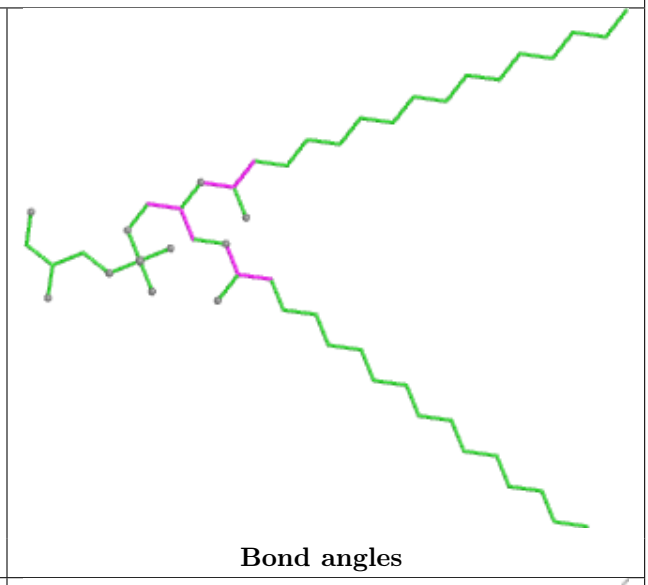


Rings

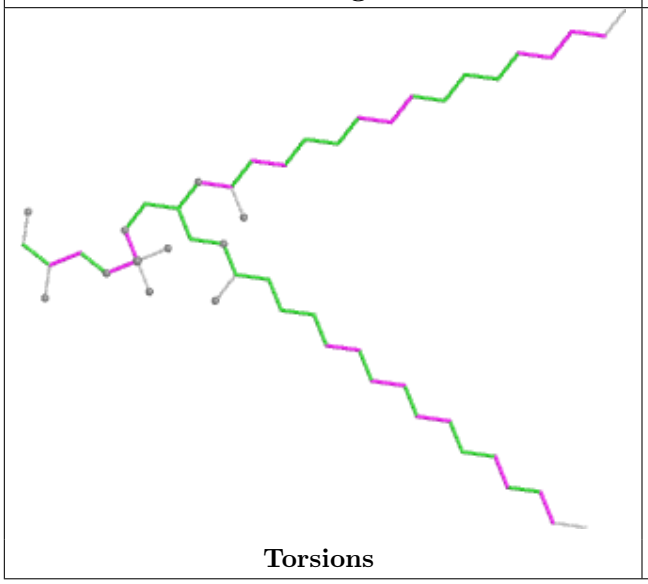
Ligand LHG d 406



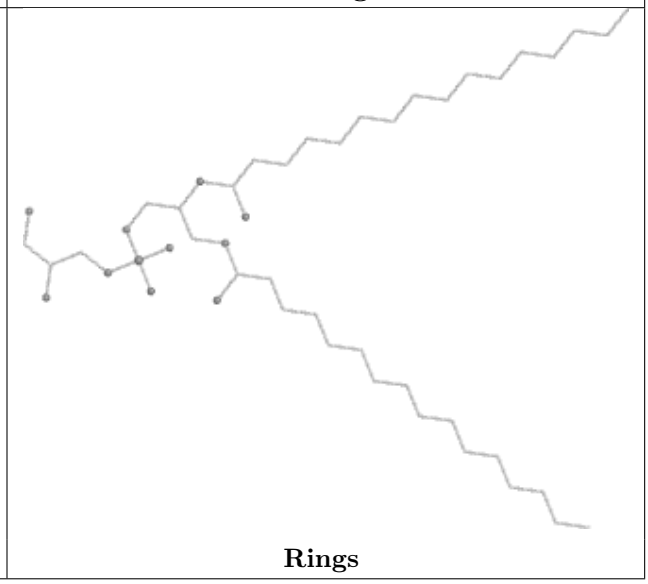
Bond lengths



Bond angles

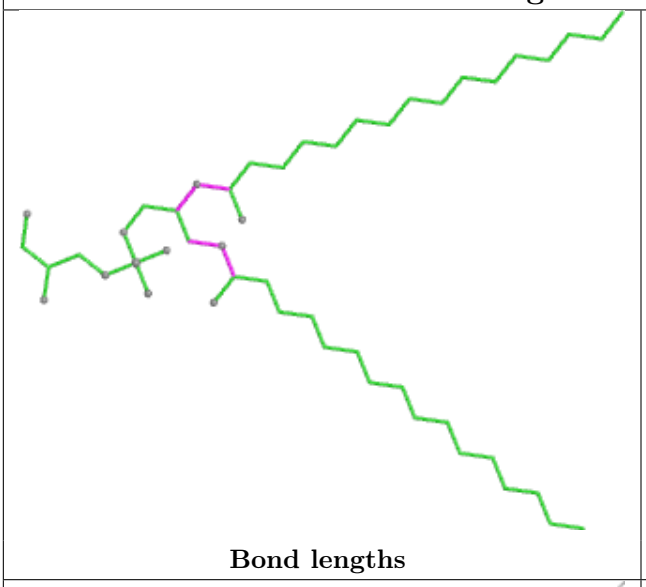


Torsions

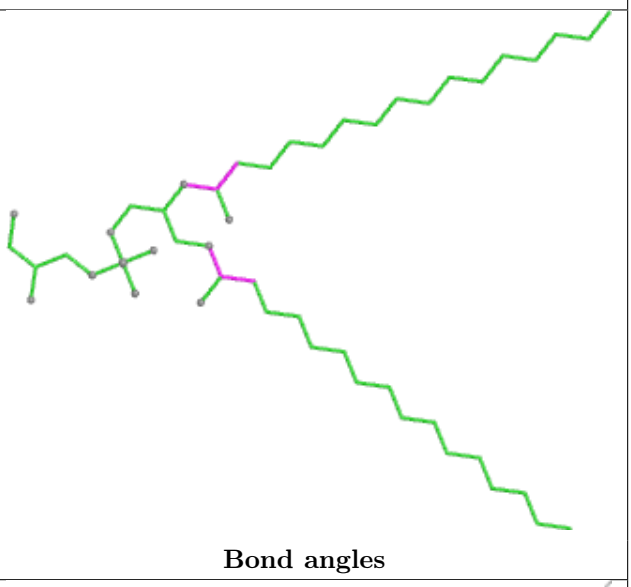


Rings

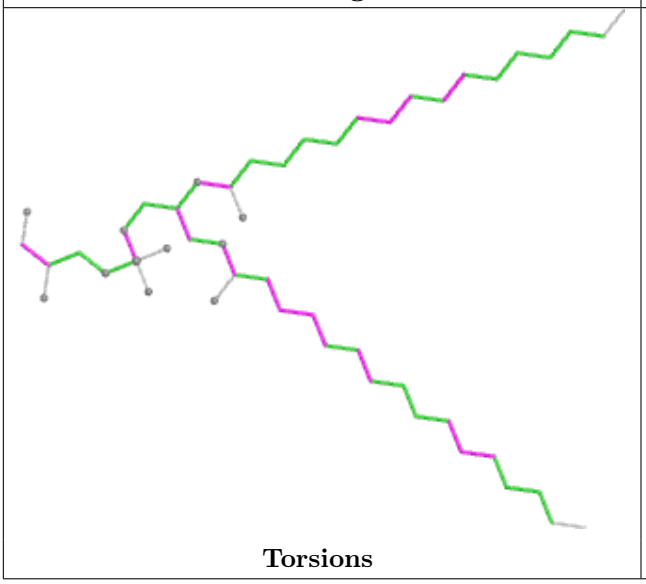
Ligand LHG 6 311



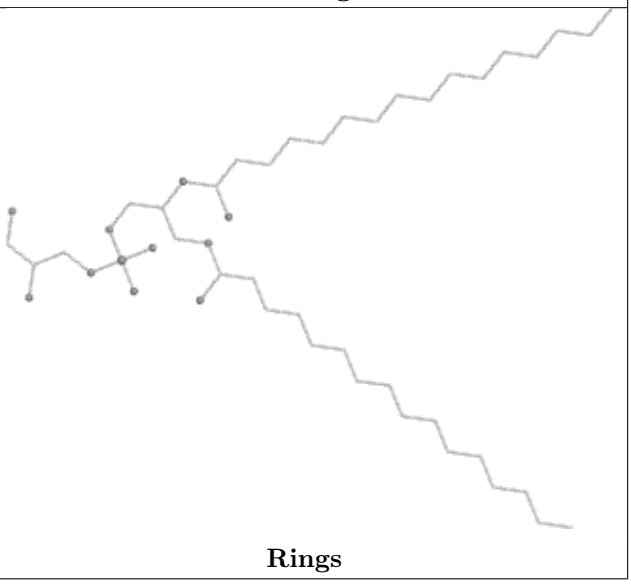
Bond lengths



Bond angles

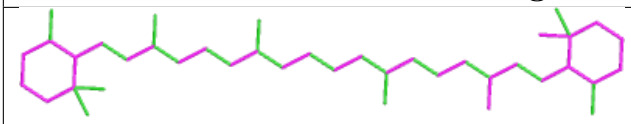


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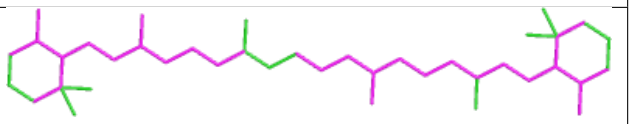


Rings

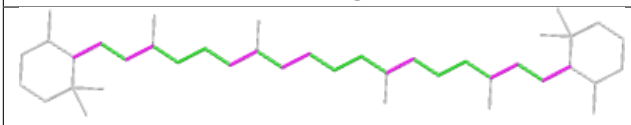
Ligand BCR t 101



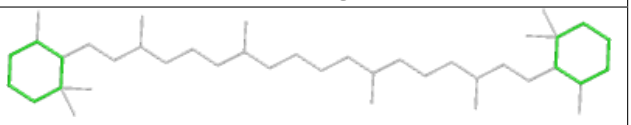
Bond lengths



Bond angles

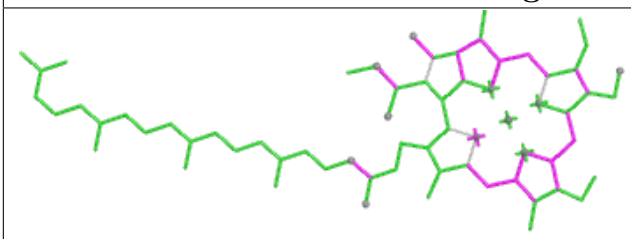


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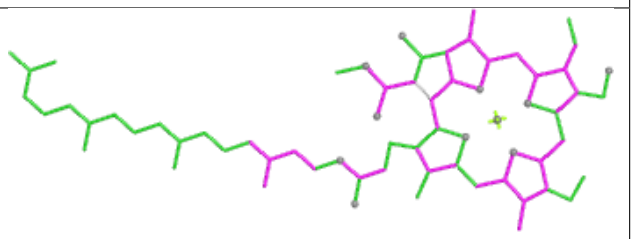


Rings

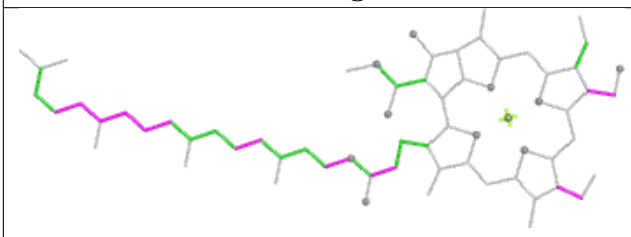
Ligand CHL N 313



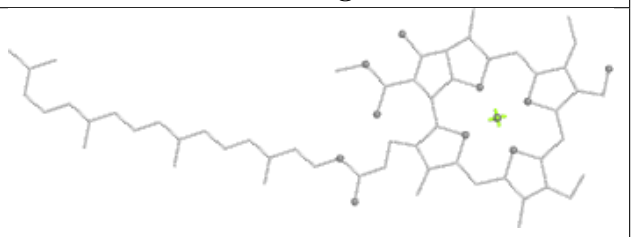
Bond lengths



Bond angles

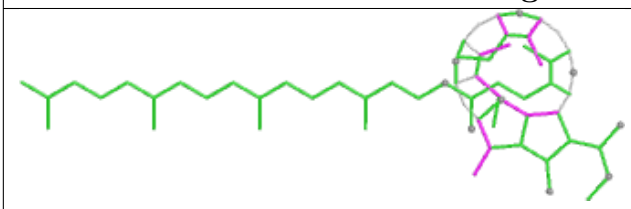


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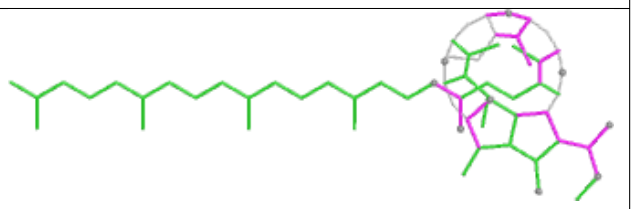


Rings

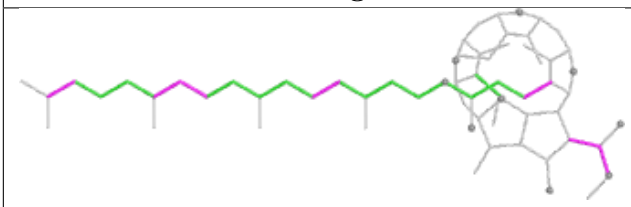
Ligand PHO D 401



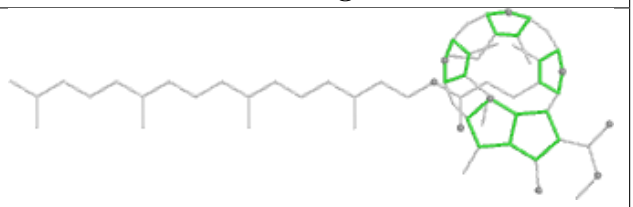
Bond lengths



Bond angles

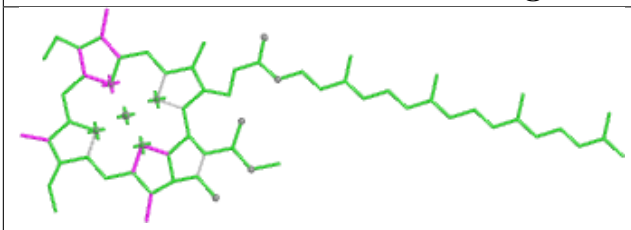


Torsions

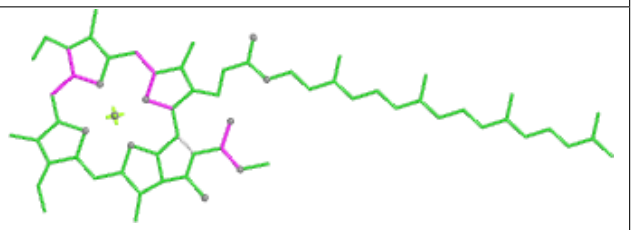


Rings

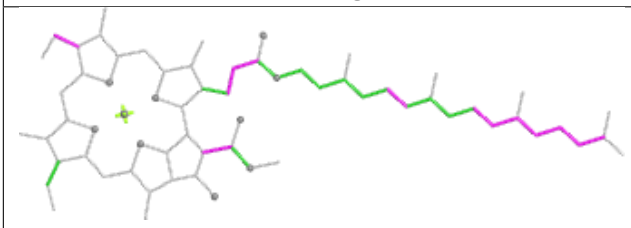
Ligand CLA B 603



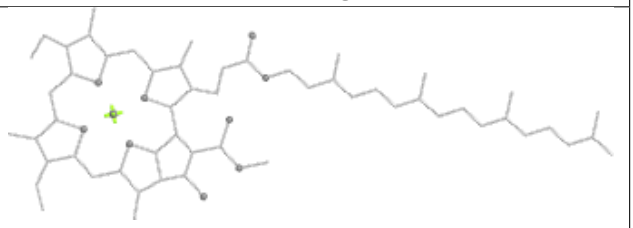
Bond lengths



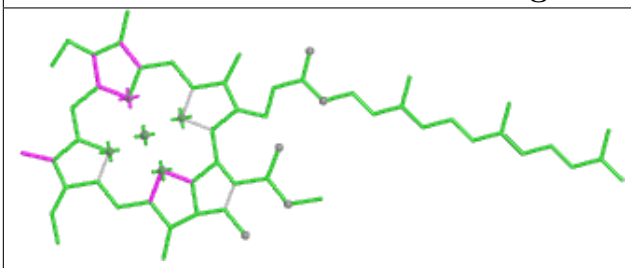
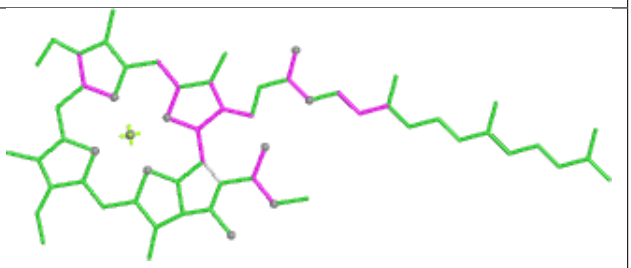
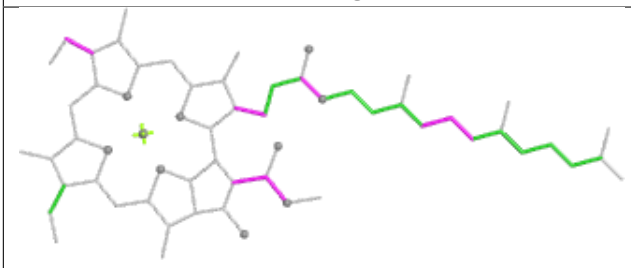
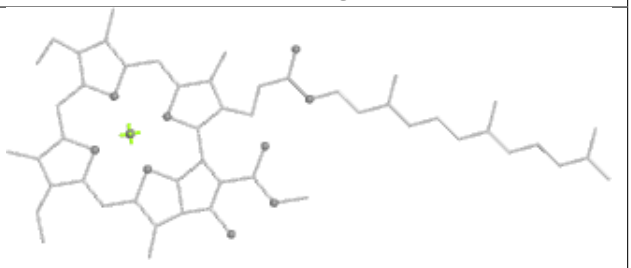
Bond angles

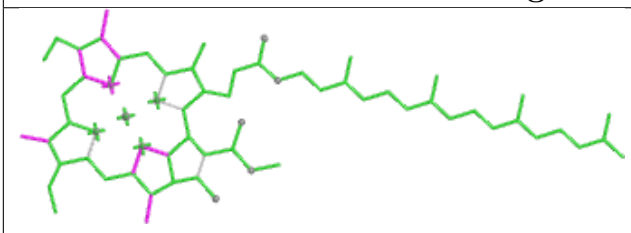
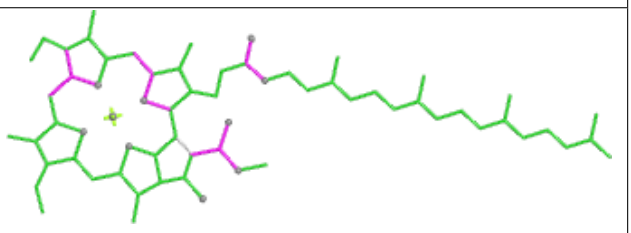
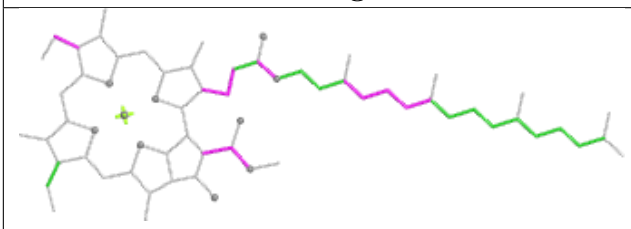
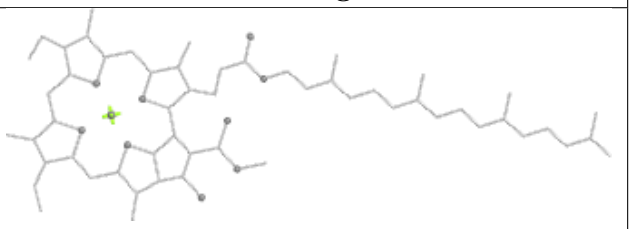


Torsions

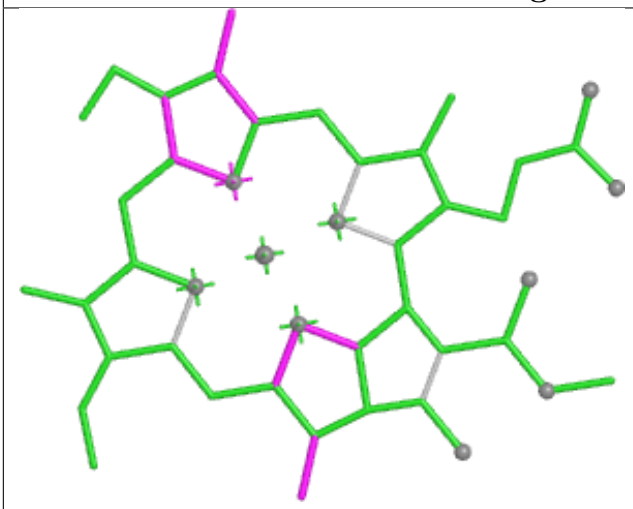


Rings

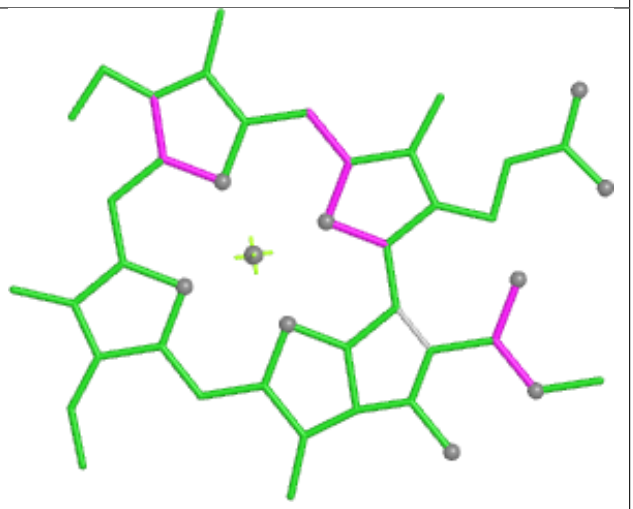
Ligand CLA r 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

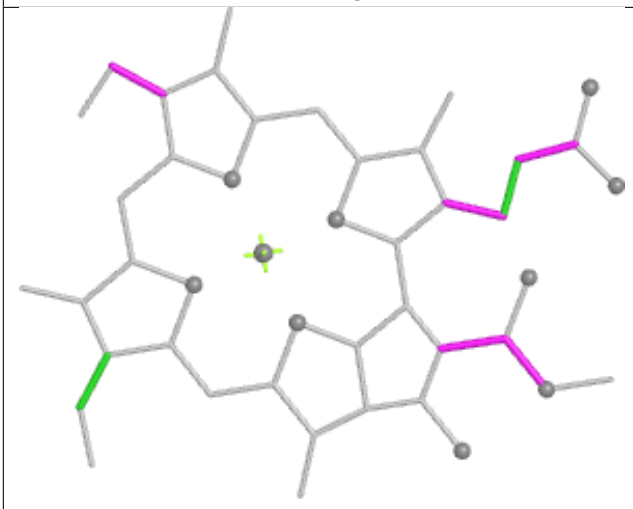
Ligand CLA r 610



Bond lengths



Bond angles

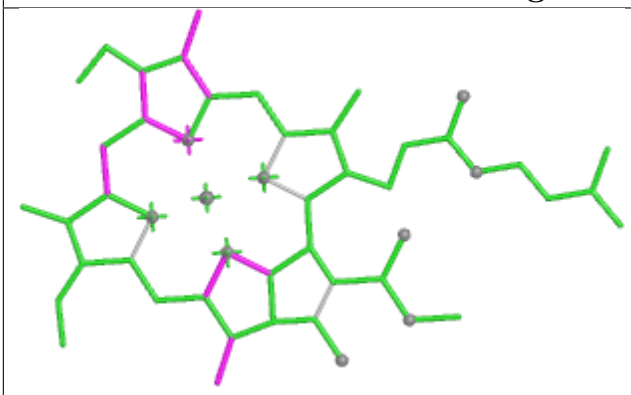


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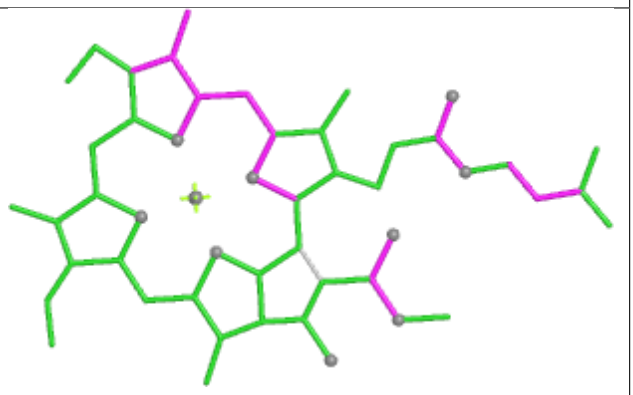


Rings

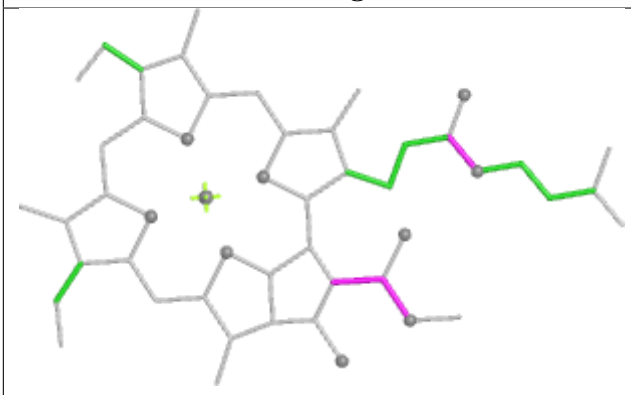
Ligand CLA n 303



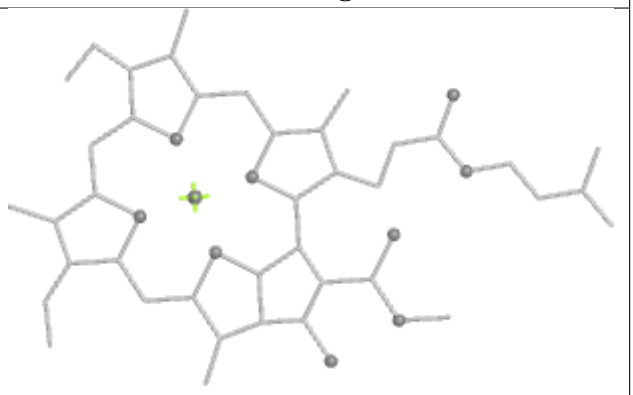
Bond lengths



Bond angles

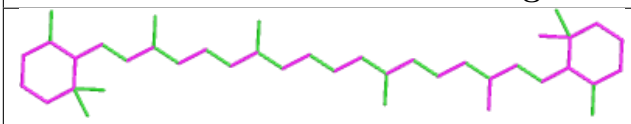


Torsions

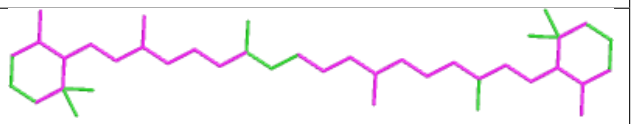


Rings

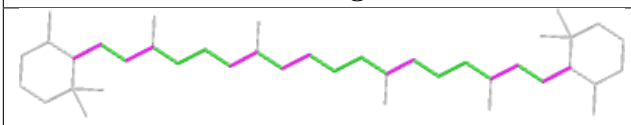
Ligand BCR T 101



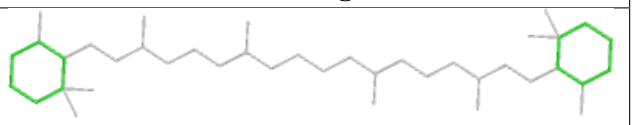
Bond lengths



Bond angles

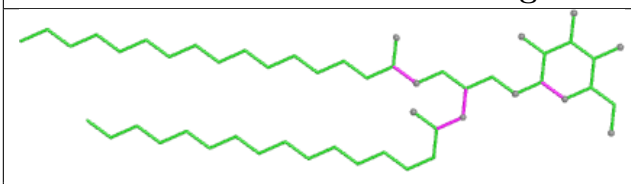


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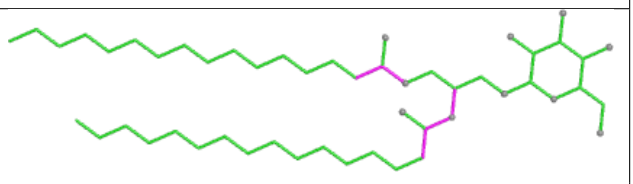


Rings

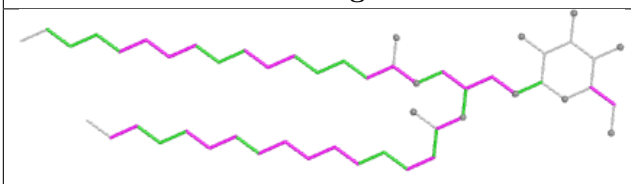
Ligand LMG C 502



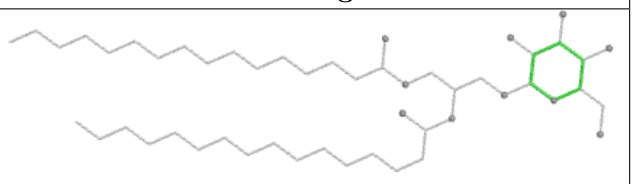
Bond lengths



Bond angles

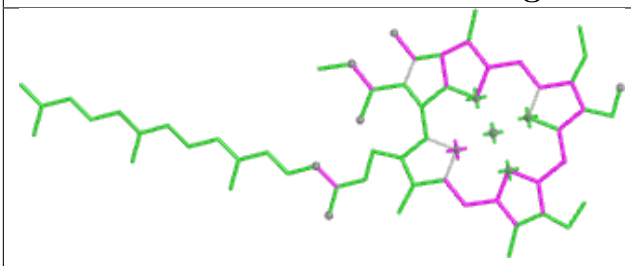


Torsions

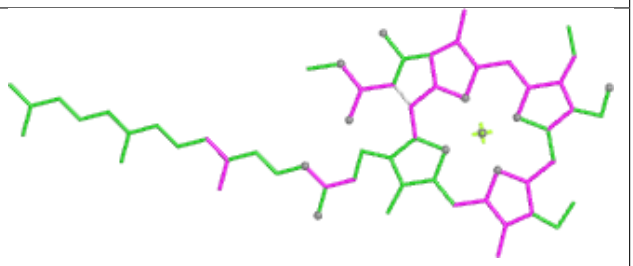


Rings

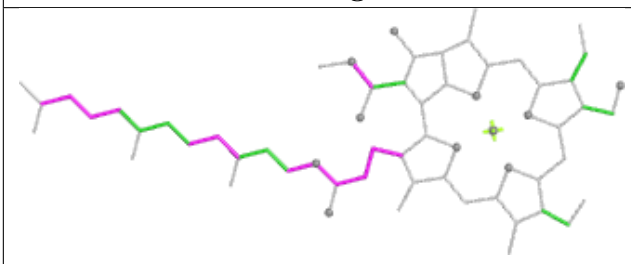
Ligand CHL R 317



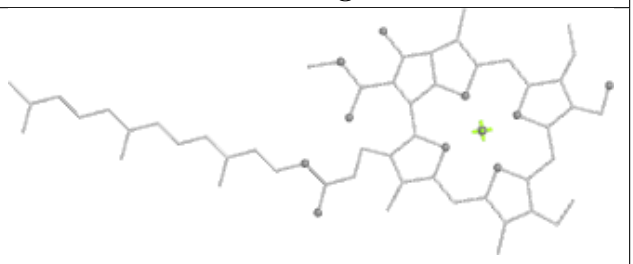
Bond lengths



Bond angles

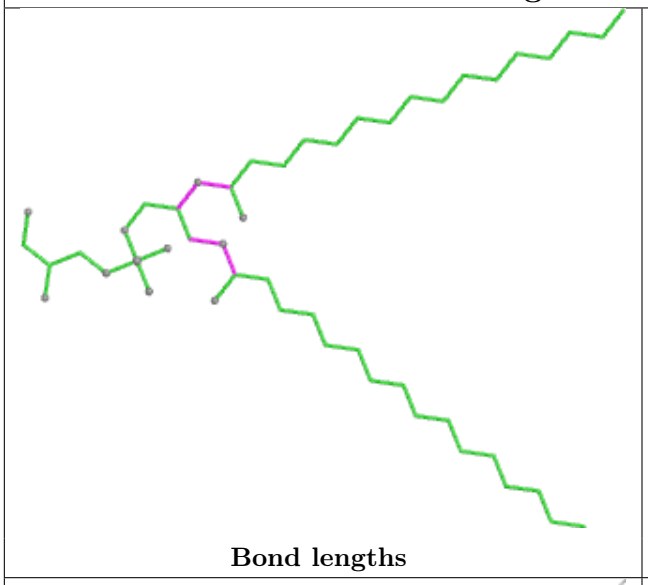


Torsions

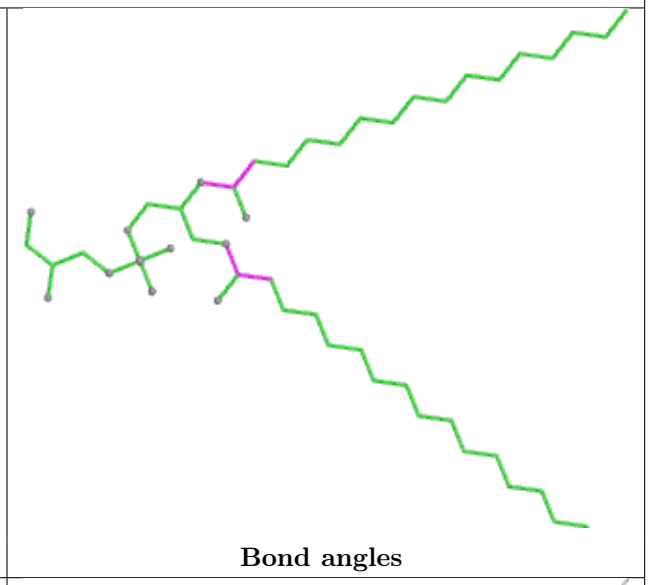


Rings

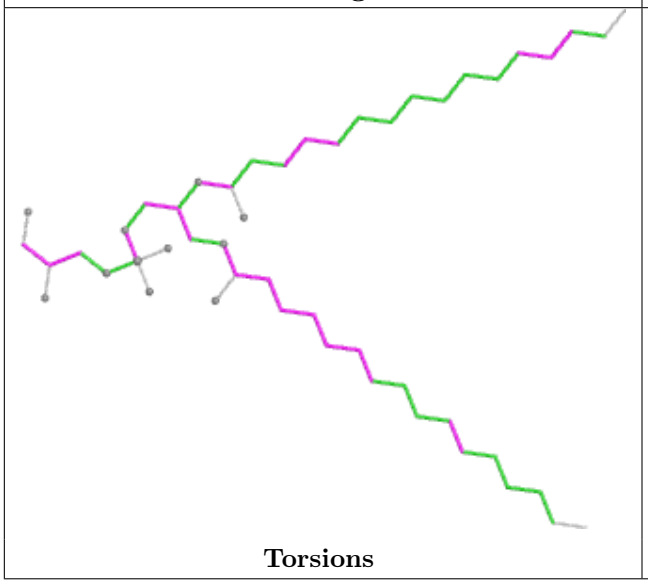
Ligand LHG P 313



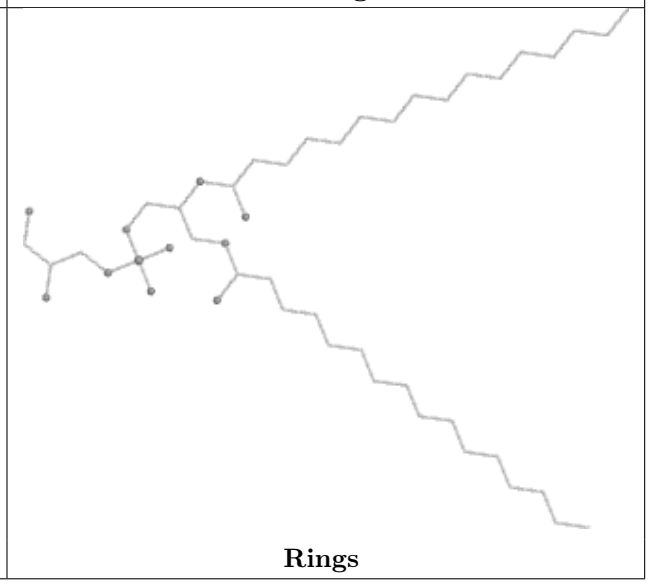
Bond lengths



Bond angles

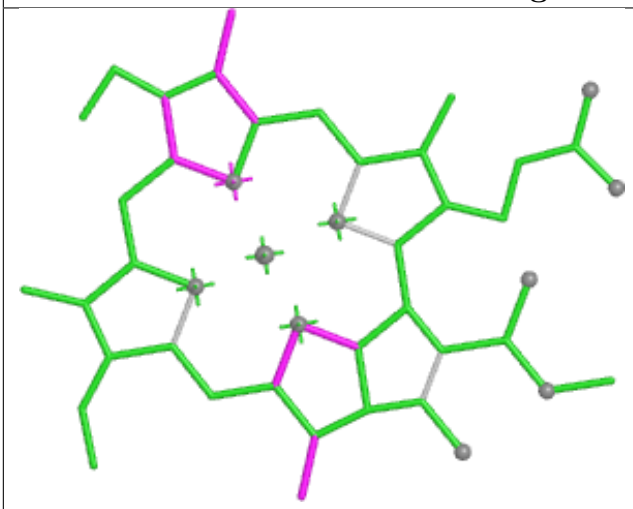


Torsions

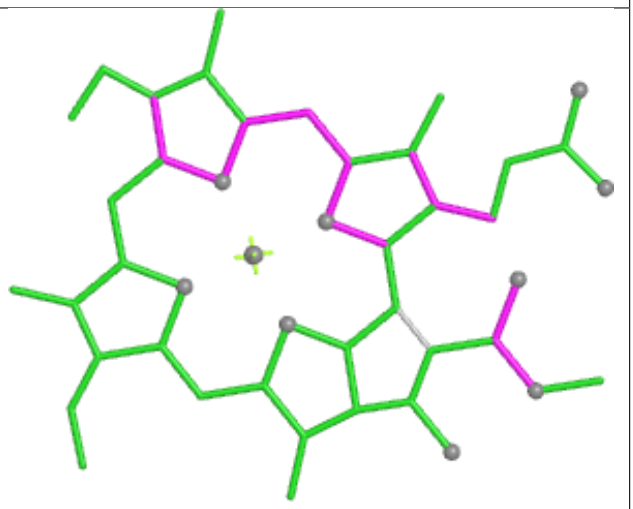


Rings

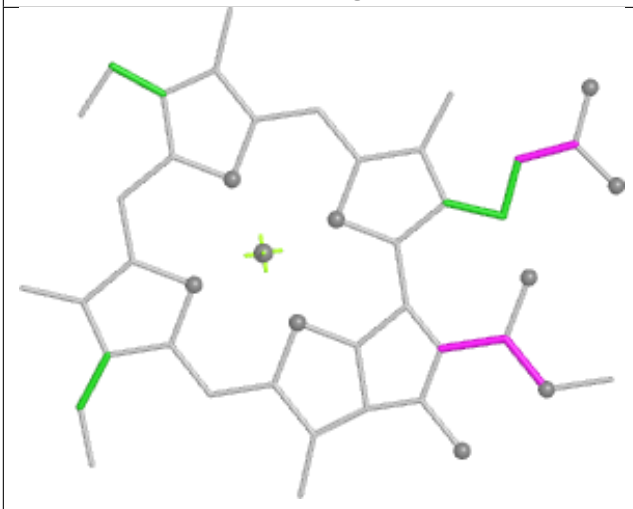
Ligand CLA s 302



Bond lengths



Bond angles

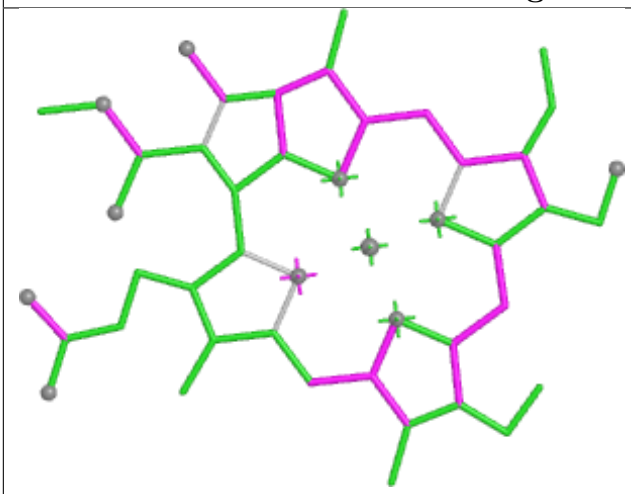


Torsions

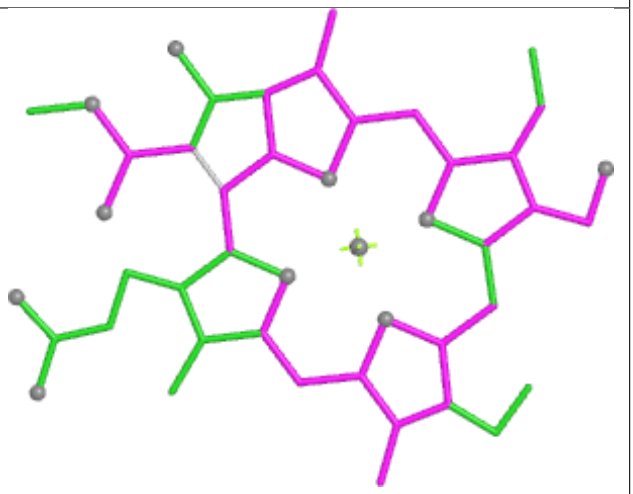


Rings

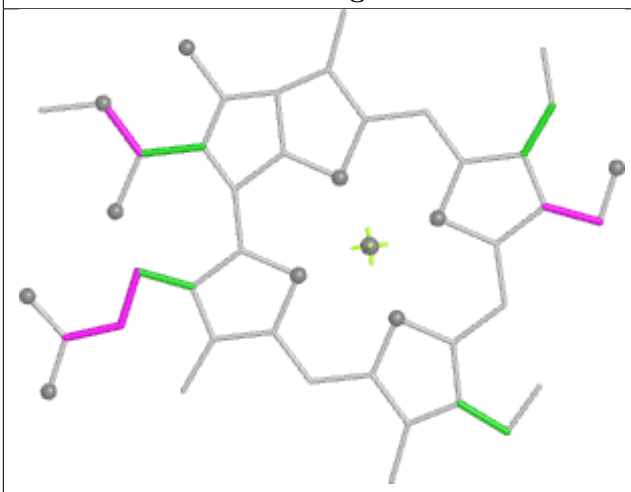
Ligand CHL S 313



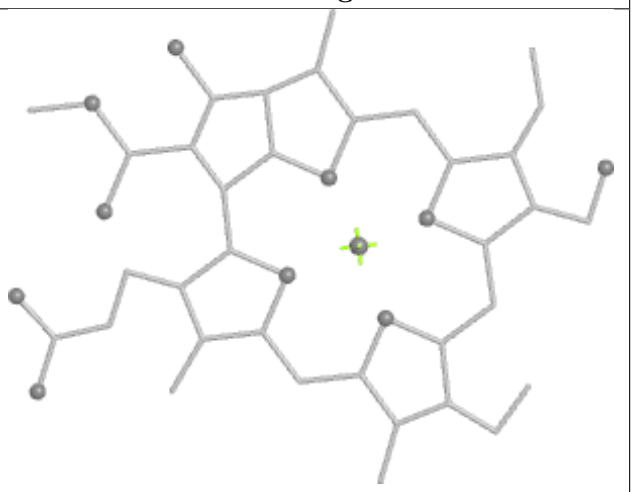
Bond lengths



Bond angles

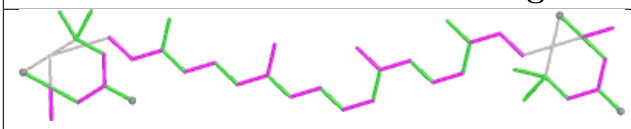


Torsions

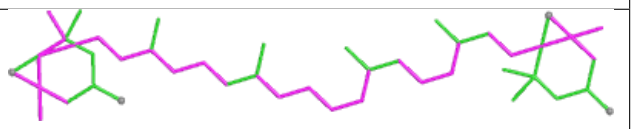


Rings

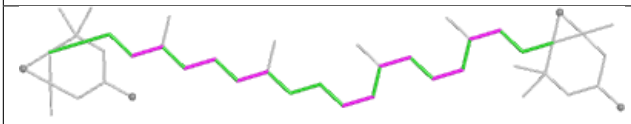
Ligand XAT v 311



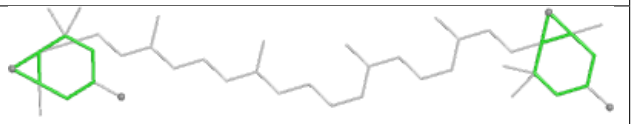
Bond lengths



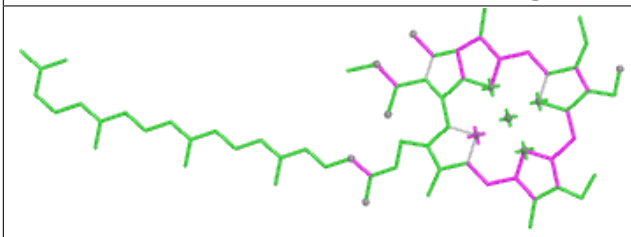
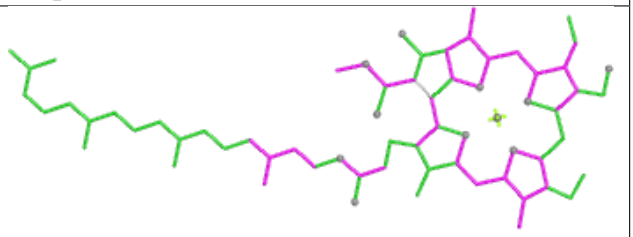
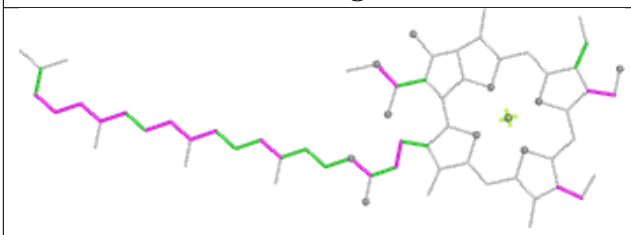
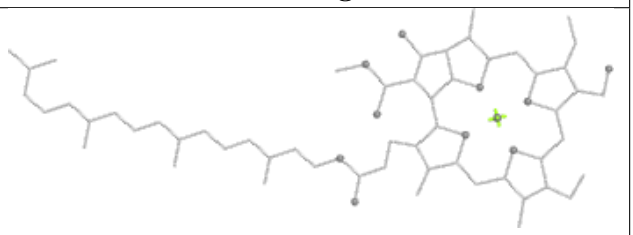
Bond angles

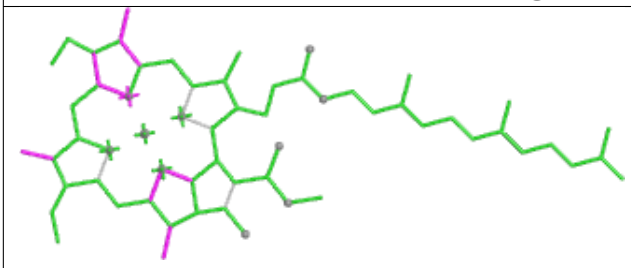
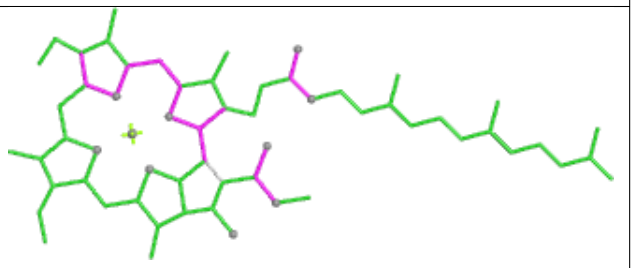
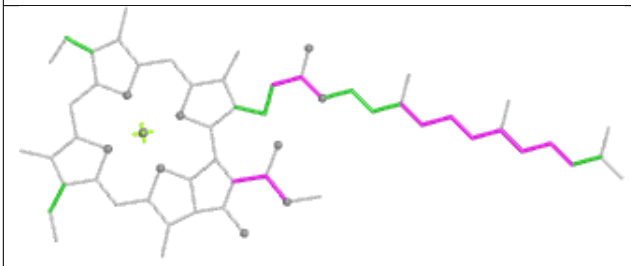
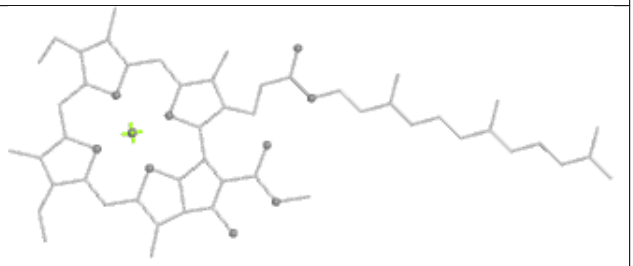


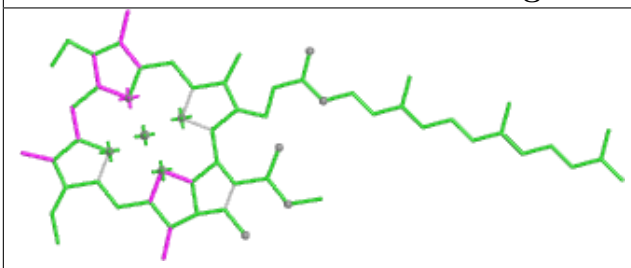
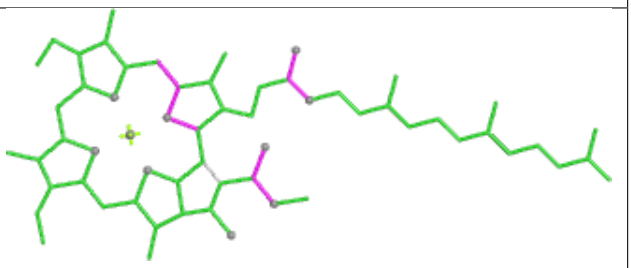
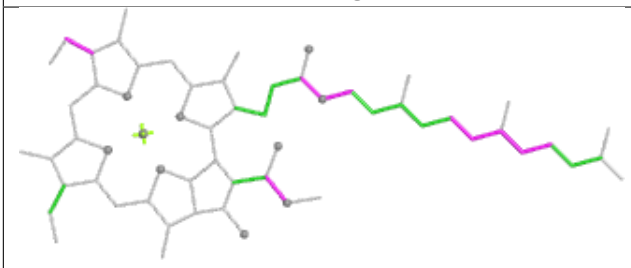
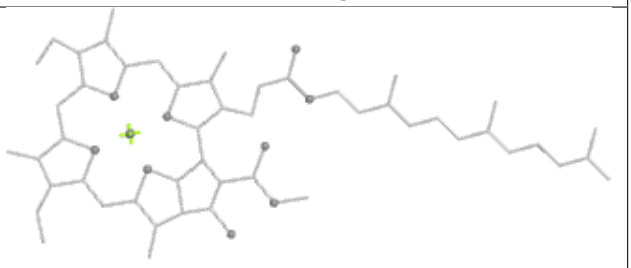
Torsions

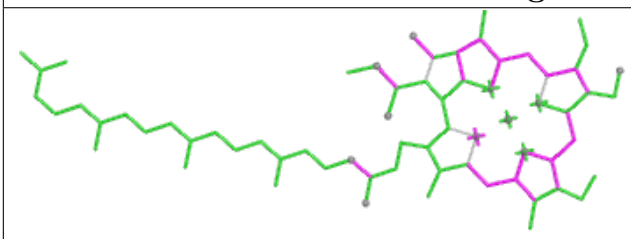
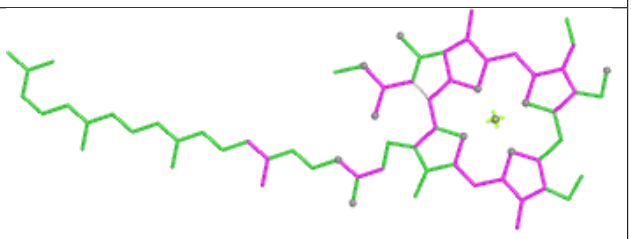
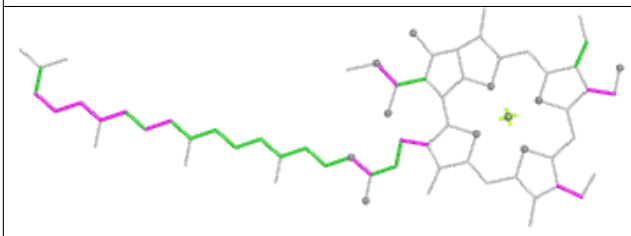
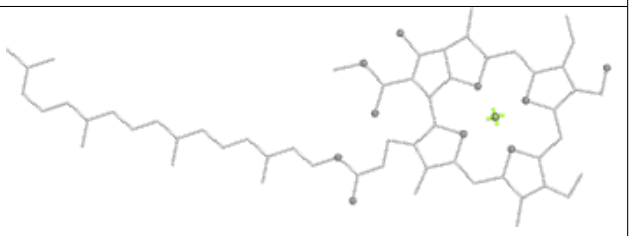


Rings

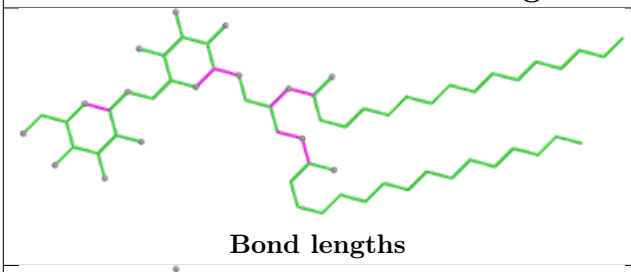
Ligand CHL p 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

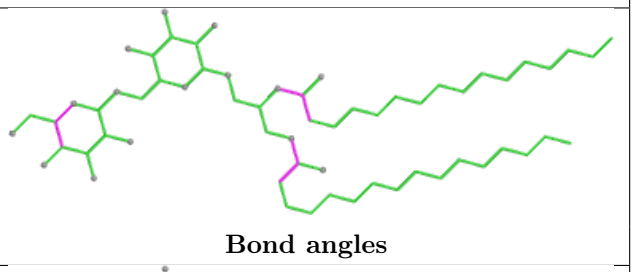
Ligand CLA U 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 4 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

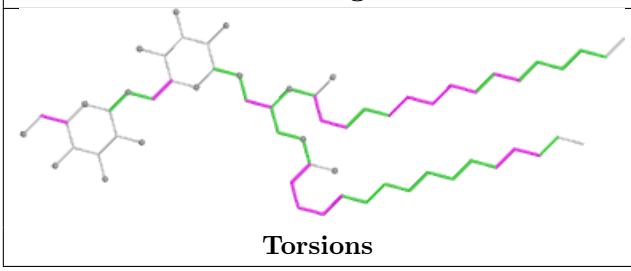
Ligand DGD b 601



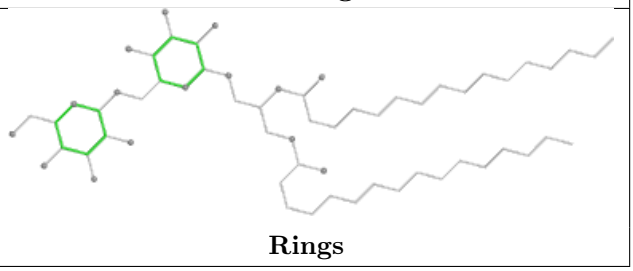
Bond lengths



Bond angles

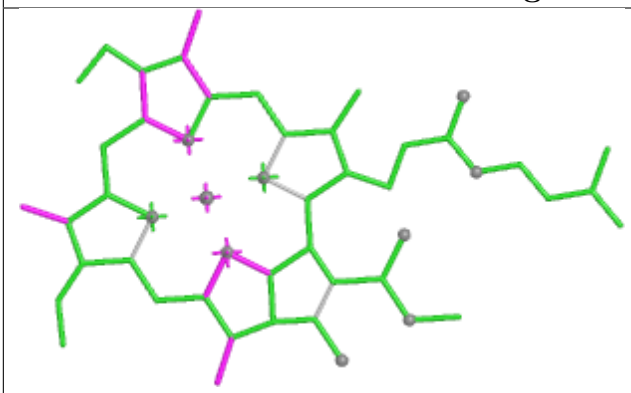


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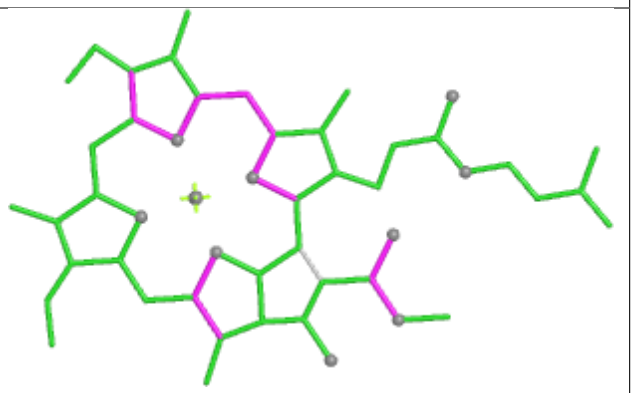


Rings

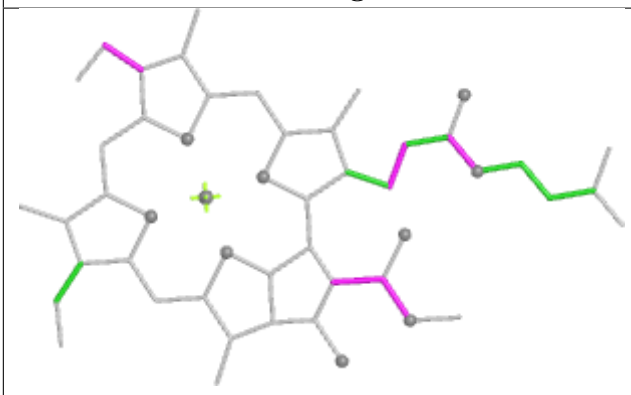
Ligand CLA A 406



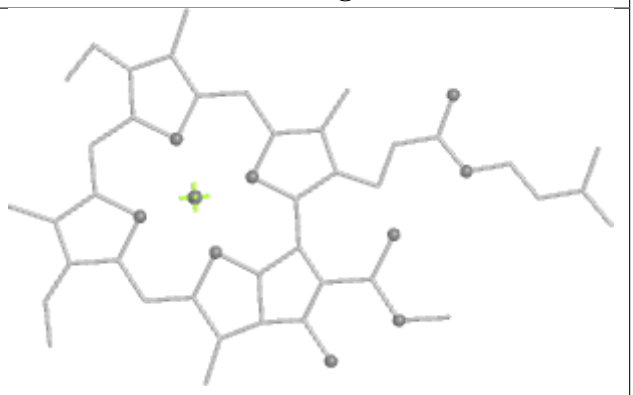
Bond lengths



Bond angles

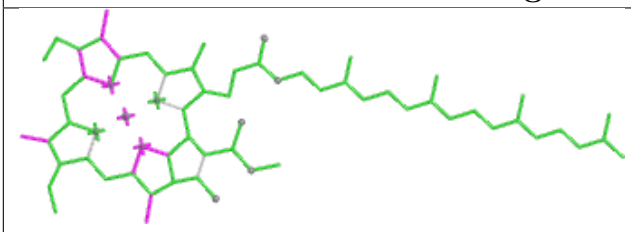


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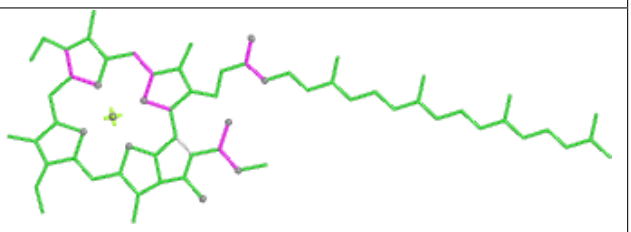


Rings

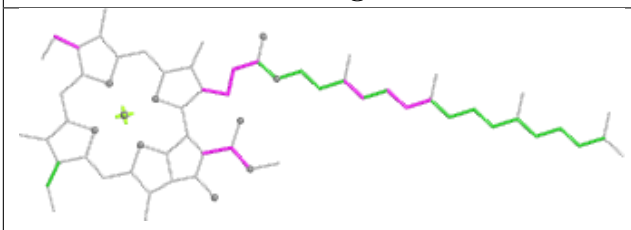
Ligand CLA C 514



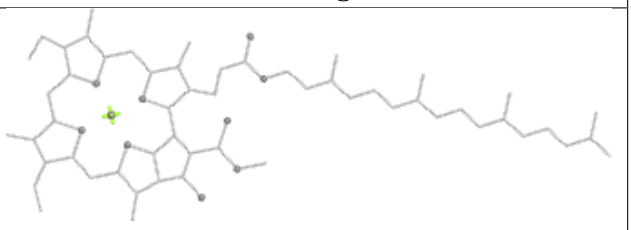
Bond lengths



Bond angles



Torsions

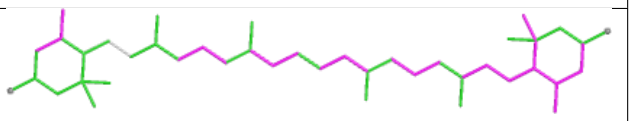


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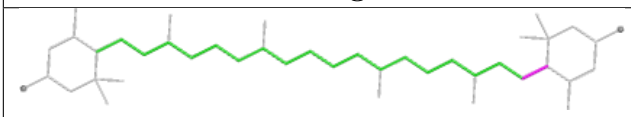
Ligand LUT u 309



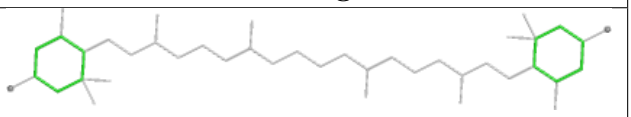
Bond lengths



Bond angles

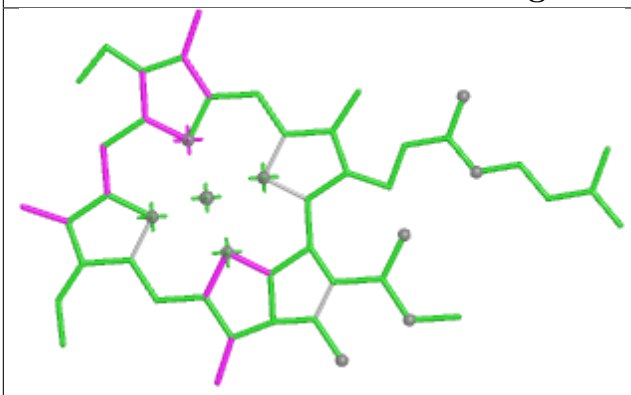


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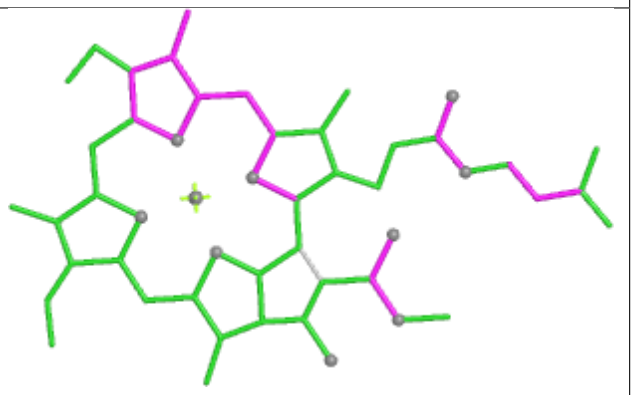


Rings

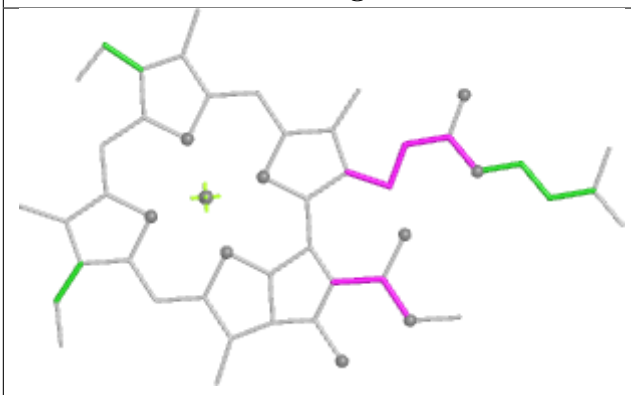
Ligand CLA 6 304



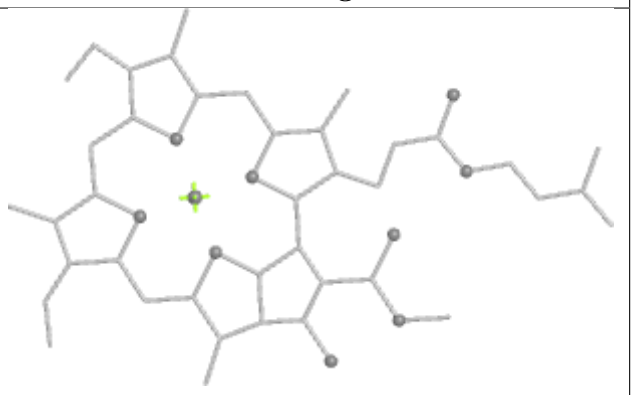
Bond lengths



Bond angles

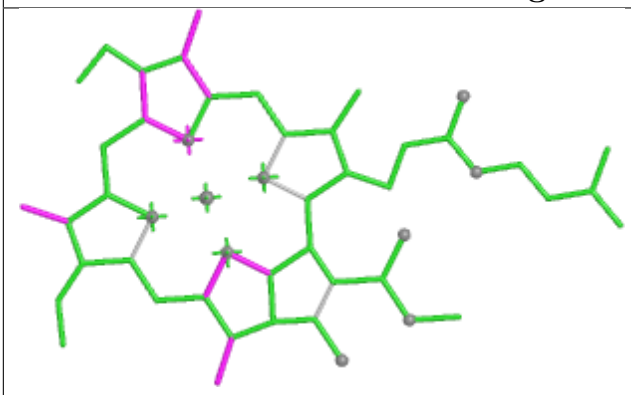


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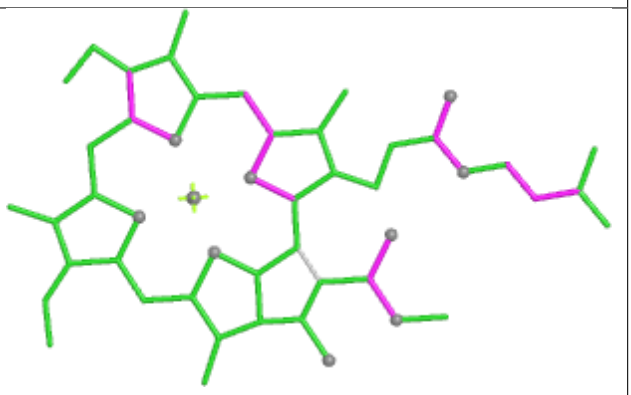


Rings

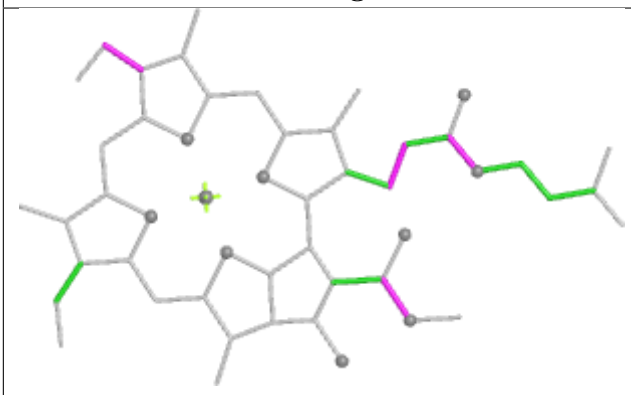
Ligand CLA 5 303



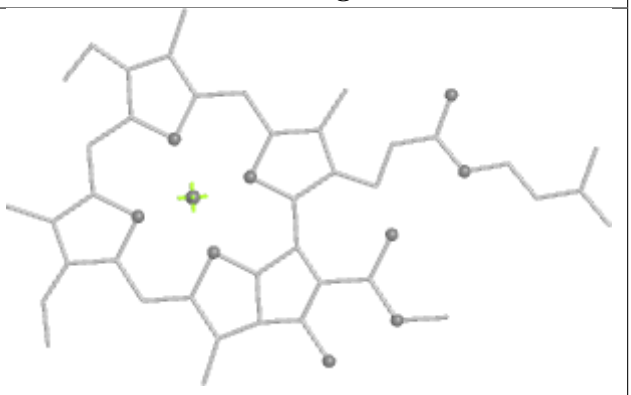
Bond lengths



Bond angles

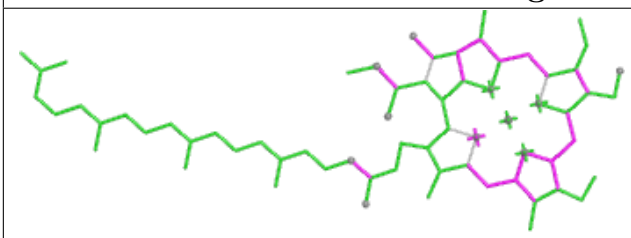


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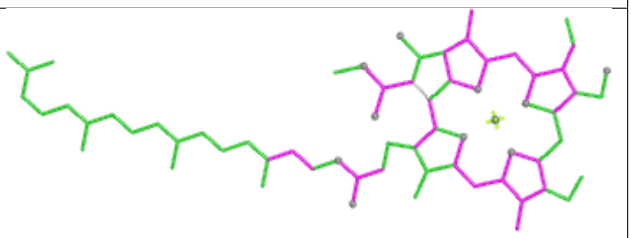


Rings

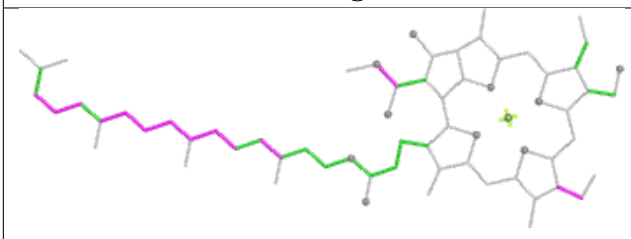
Ligand CHL 5 317



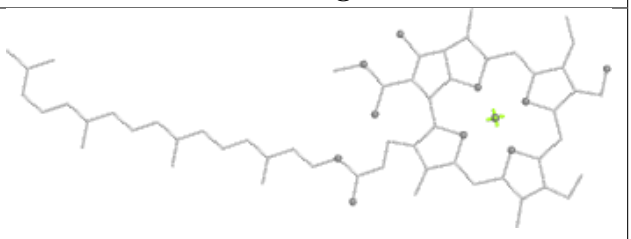
Bond lengths



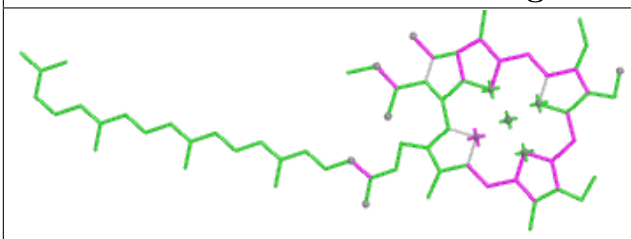
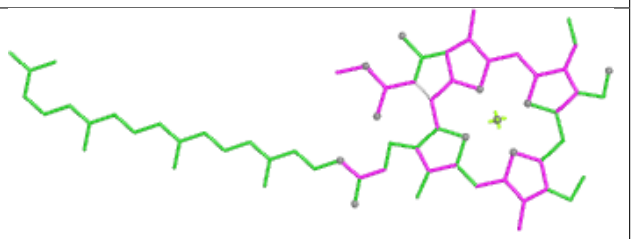
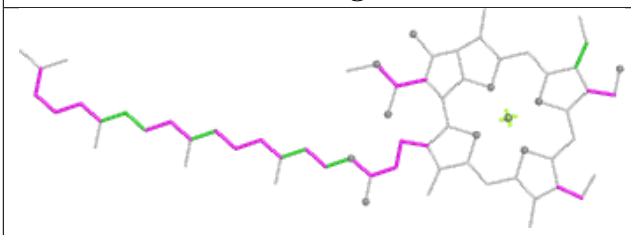
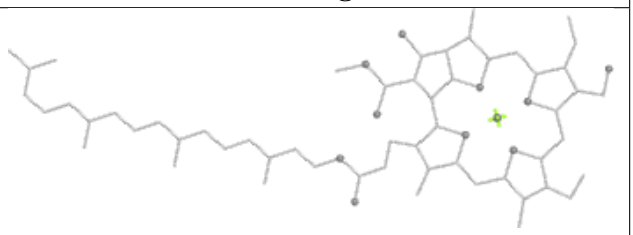
Bond angles

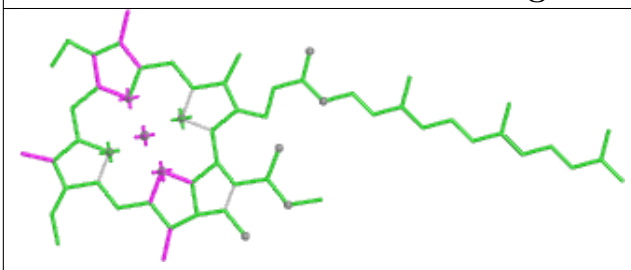
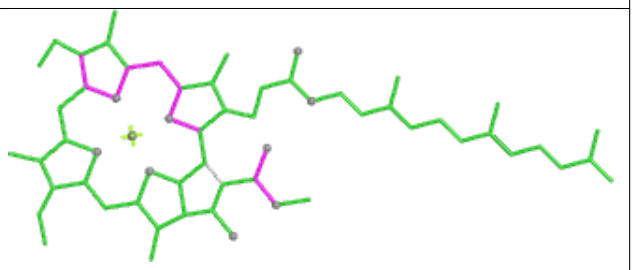
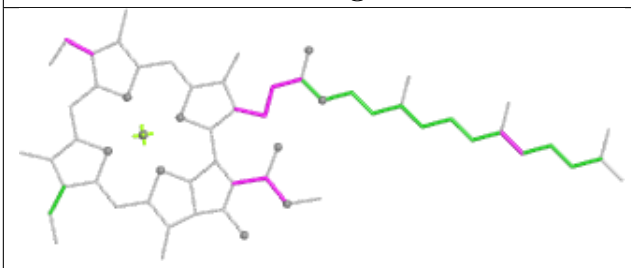
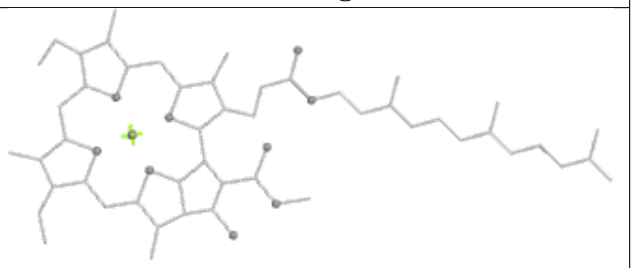


Torsions

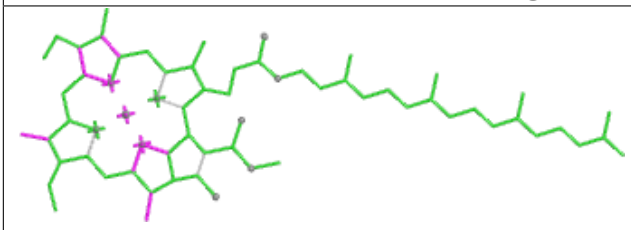


Rings

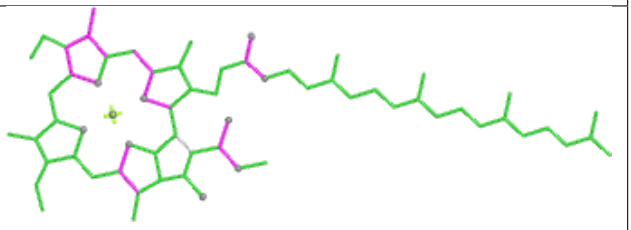
Ligand CHL n 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

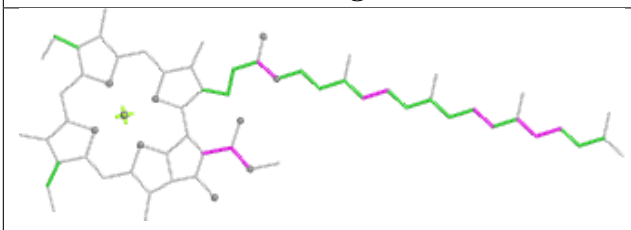
Ligand CLA B 617



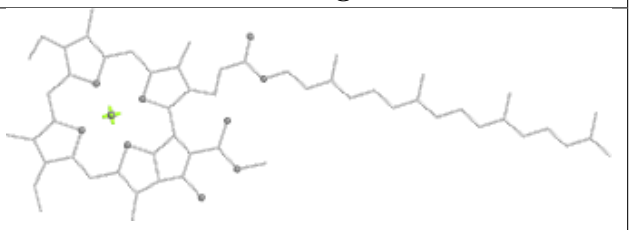
Bond lengths



Bond angles

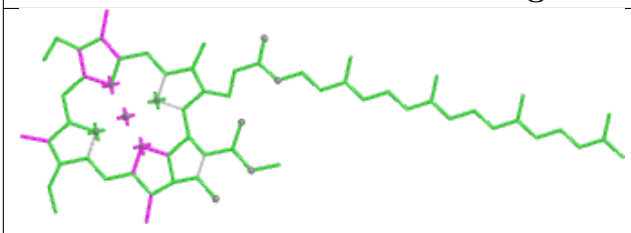


Torsions

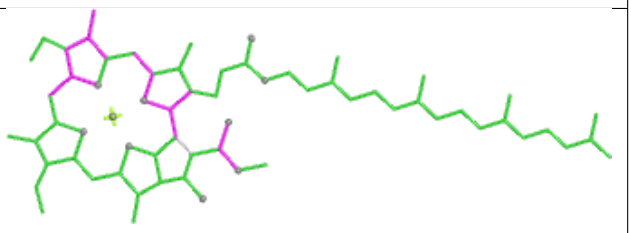


Rings

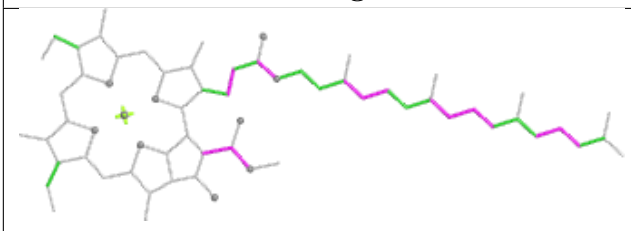
Ligand CLA b 614



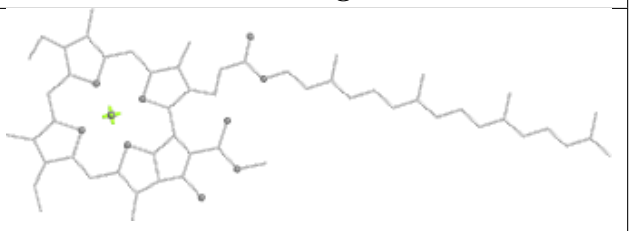
Bond lengths



Bond angles

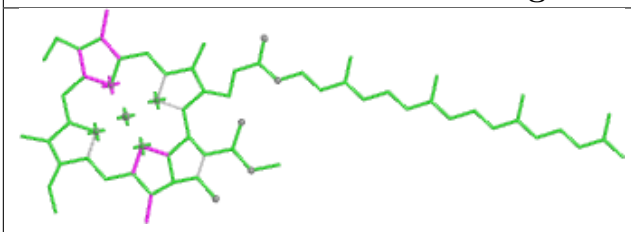


Torsions

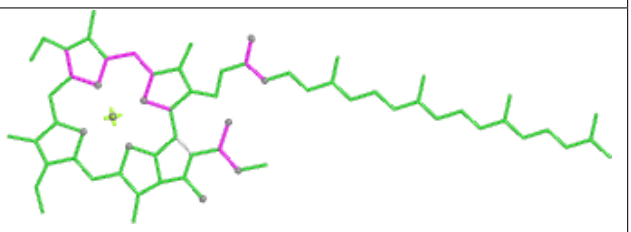


Rings

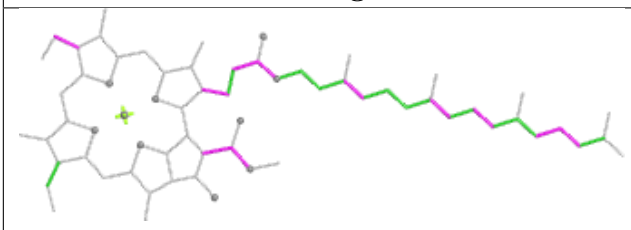
Ligand CLA 5 302



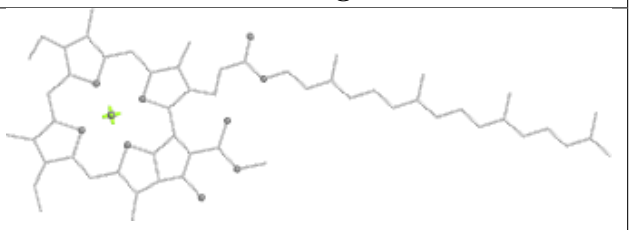
Bond lengths



Bond angles

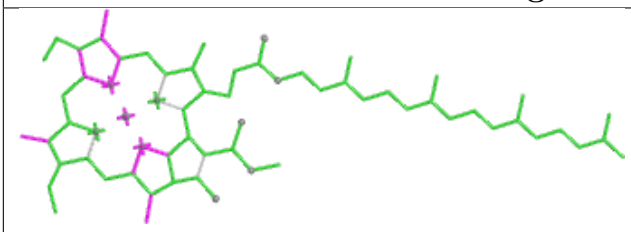


Torsions

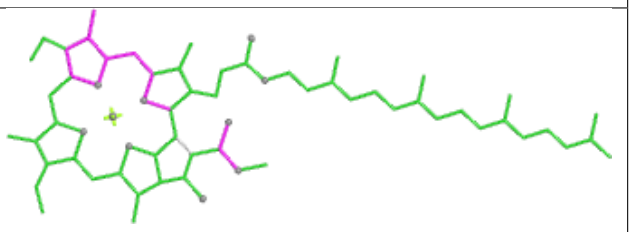


Rings

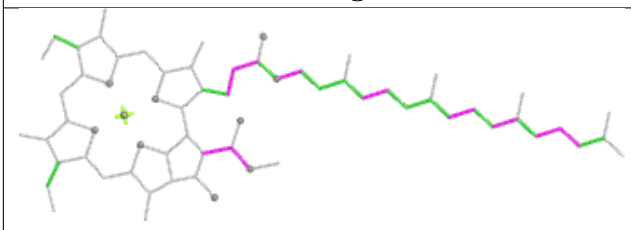
Ligand CLA b 609



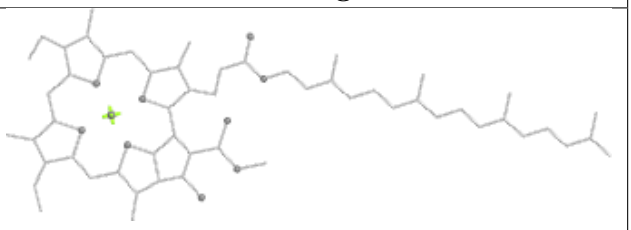
Bond lengths



Bond angles

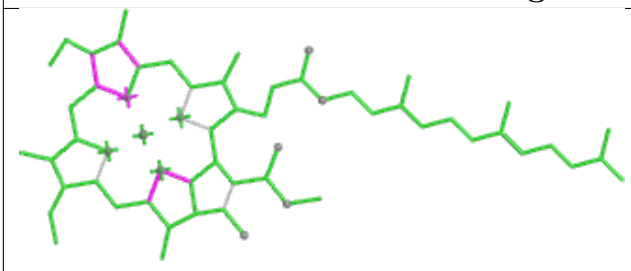


Torsions

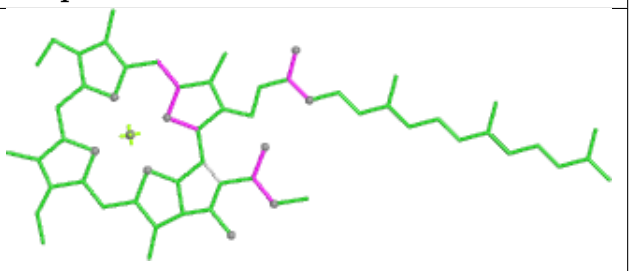


Rings

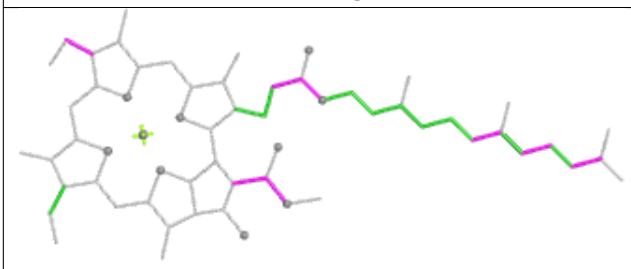
Ligand CLA q 306



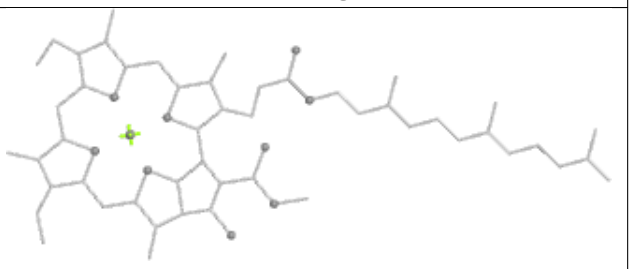
Bond lengths



Bond angles

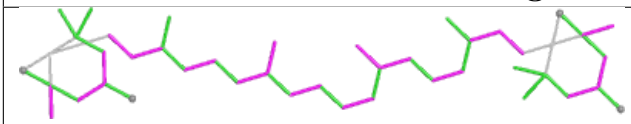


Torsions

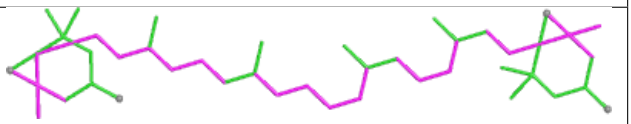


Rings

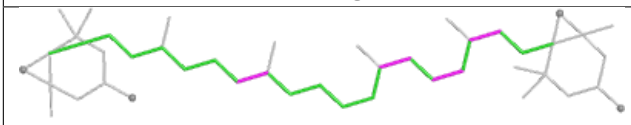
Ligand XAT u 311



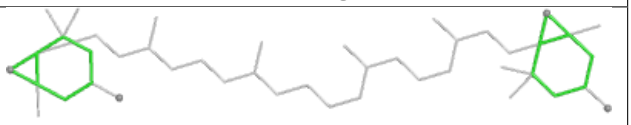
Bond lengths



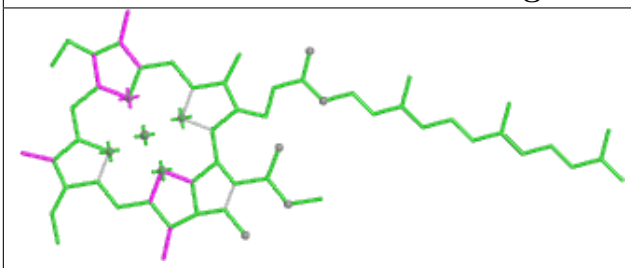
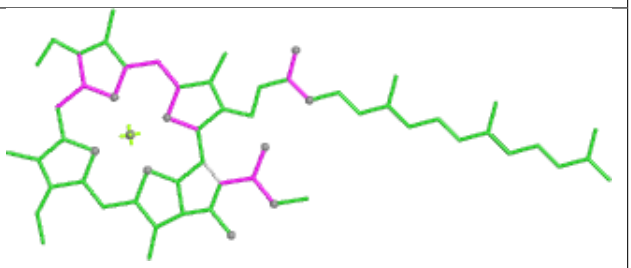
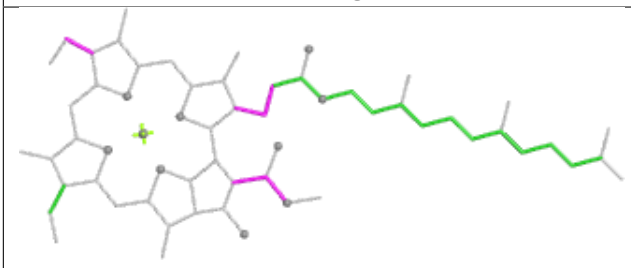
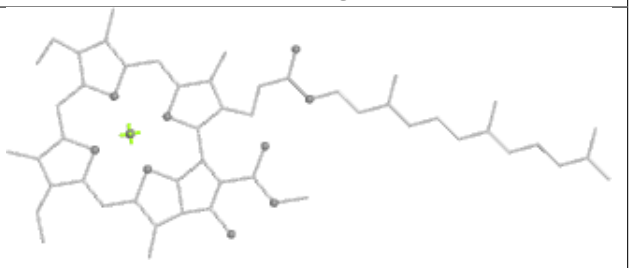
Bond angles

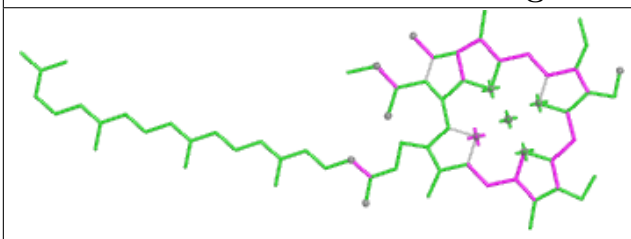
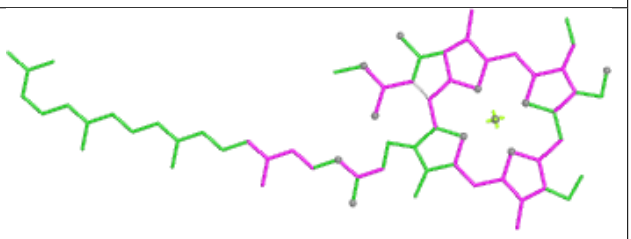
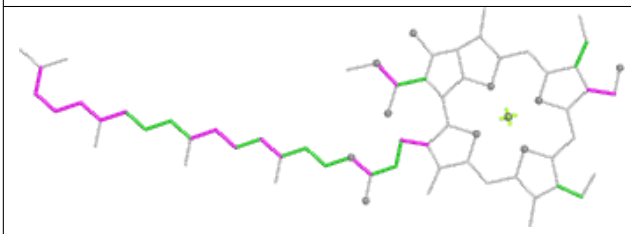
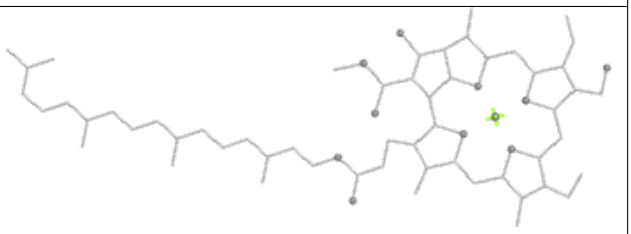


Torsions

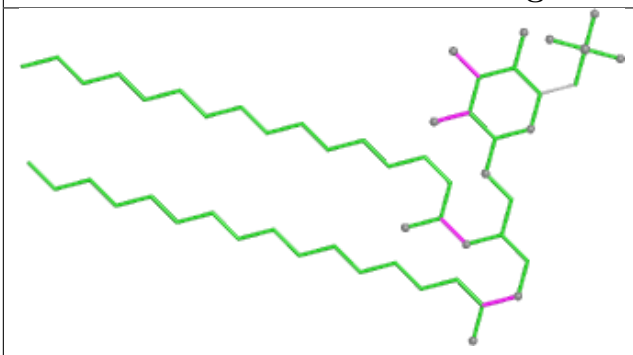


Rings

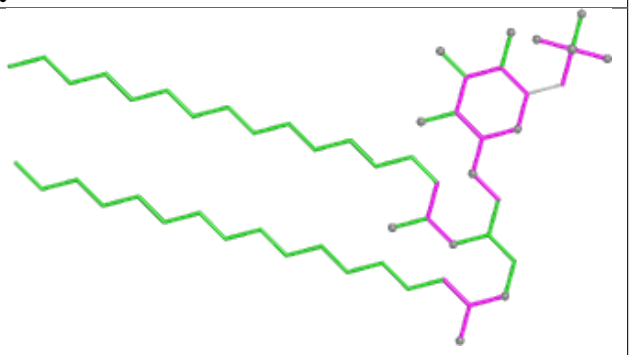
Ligand CLA U 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL u 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

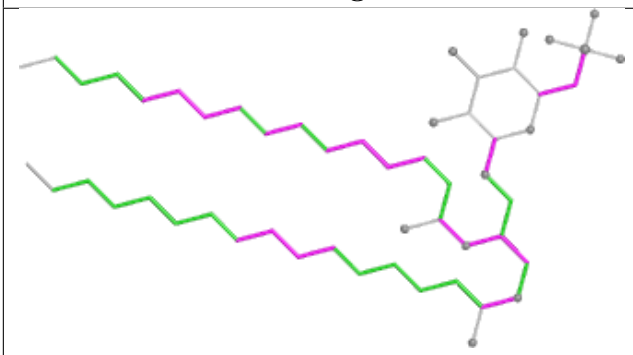
Ligand SQD L 102



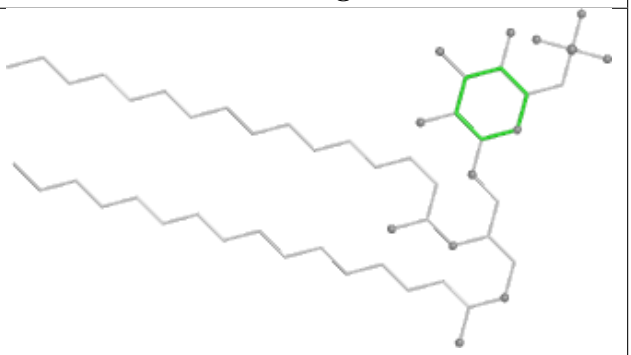
Bond lengths



Bond angles

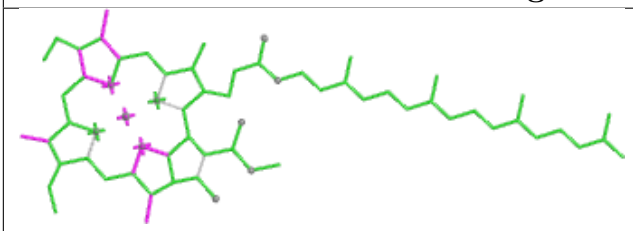


Torsions

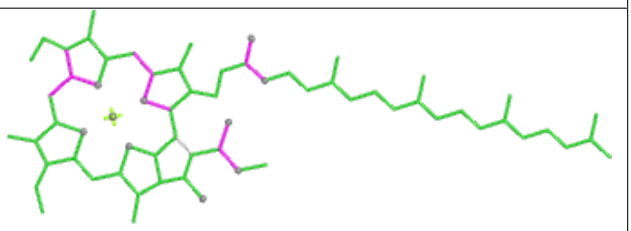


Rings

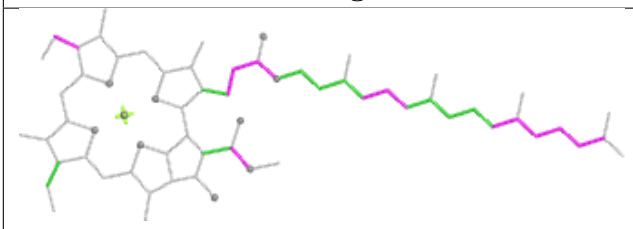
Ligand CLA b 602



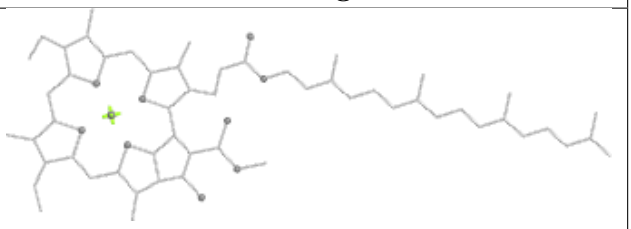
Bond lengths



Bond angles

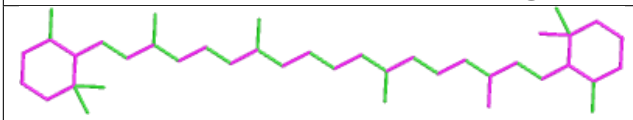


Torsions

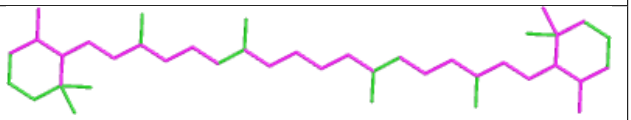


Rings

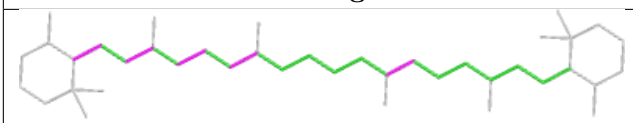
Ligand BCR B 618



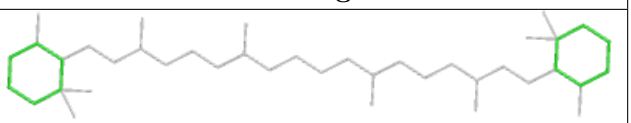
Bond lengths



Bond angles

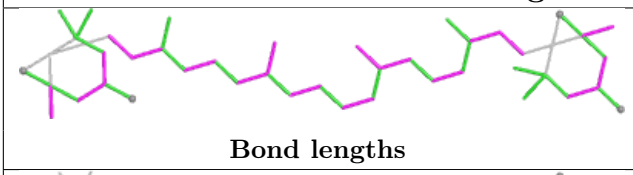


Torsions

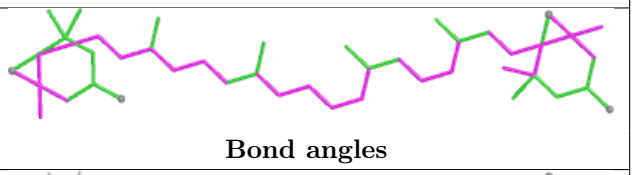


Rings

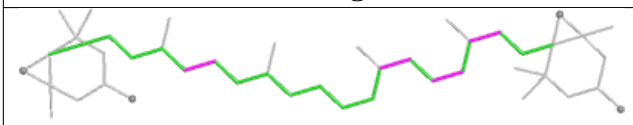
Ligand XAT 2 311



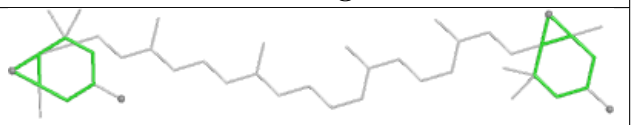
Bond lengths



Bond angles

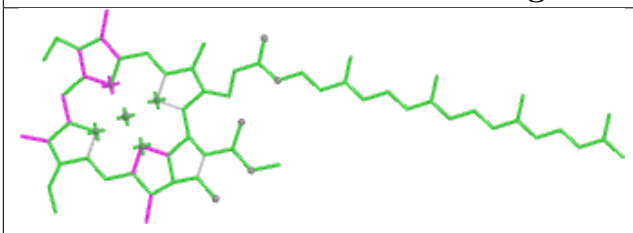


Torsions

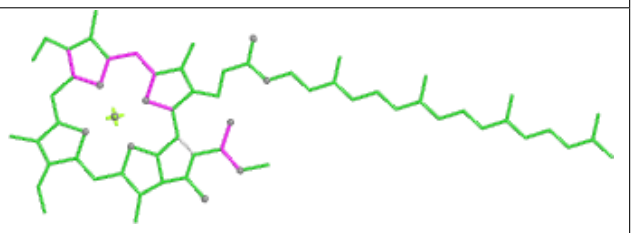


Rings

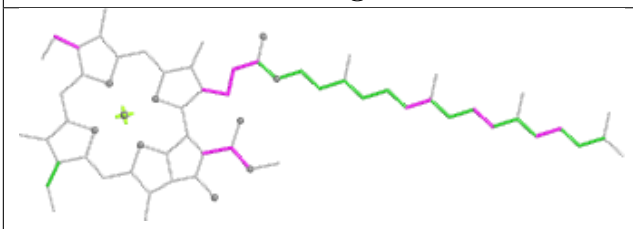
Ligand CLA v 301



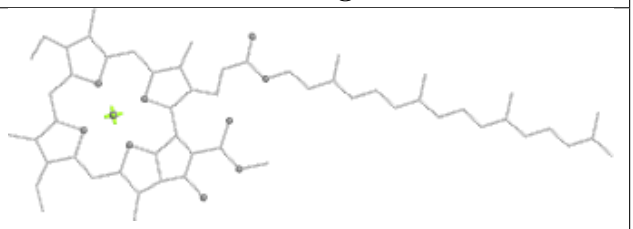
Bond lengths



Bond angles

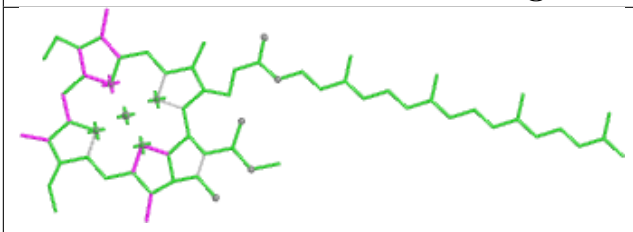


Torsions

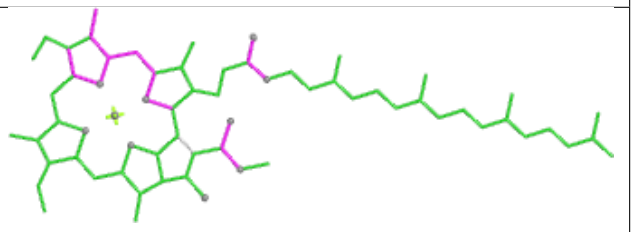


Rings

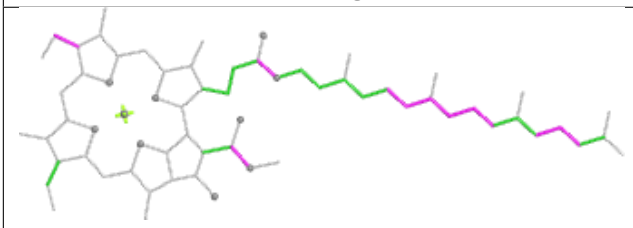
Ligand CLA b 612



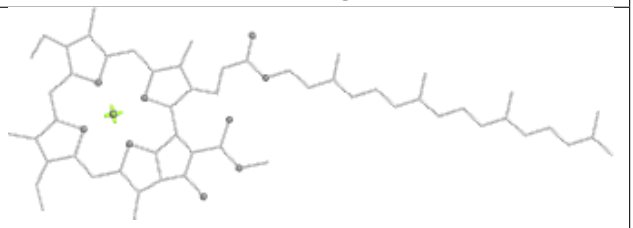
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Bond angles

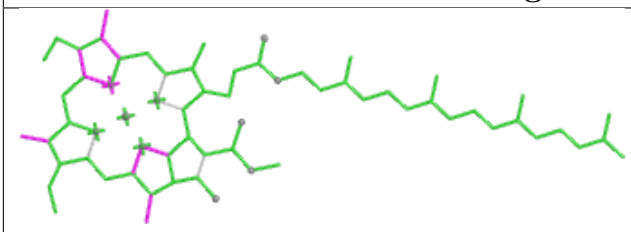


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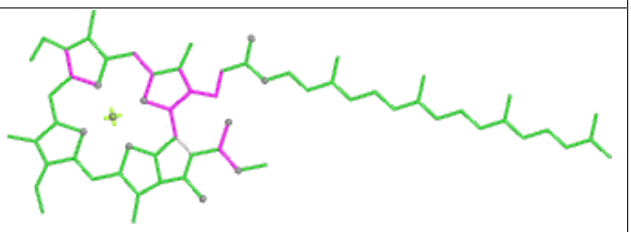


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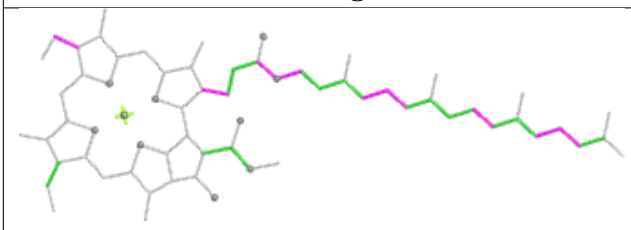
Ligand CLA C 515



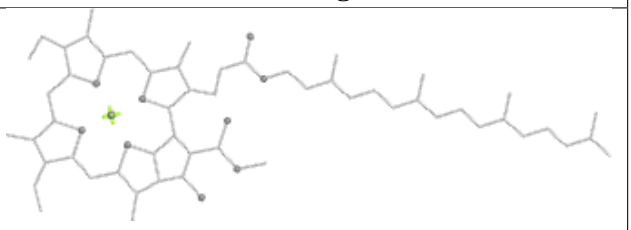
Bond lengths



Bond angles



Torsions



Rings

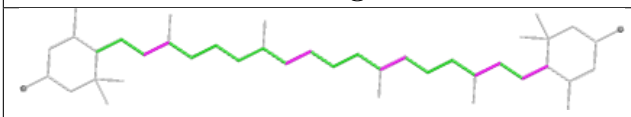
Ligand LUT S 311



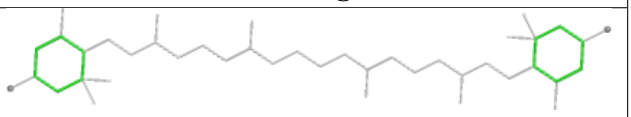
Bond lengths



Bond angles

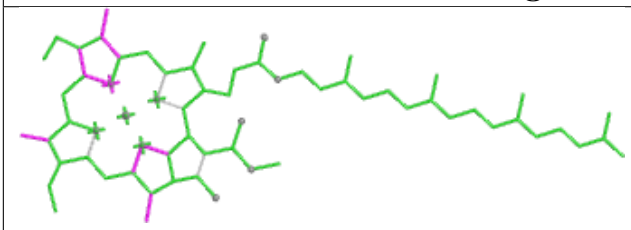


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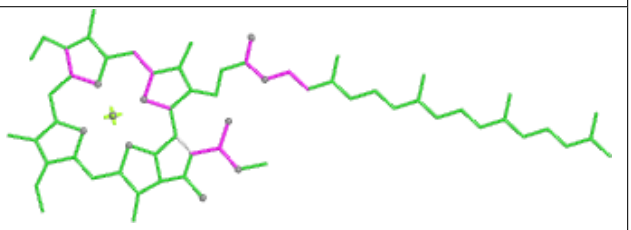


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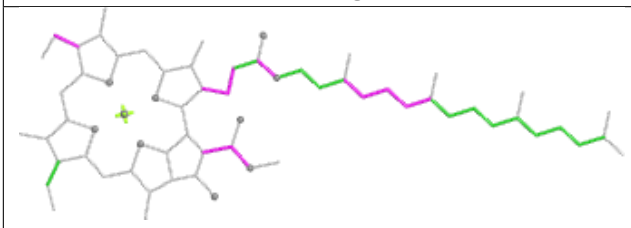
Ligand CLA B 607



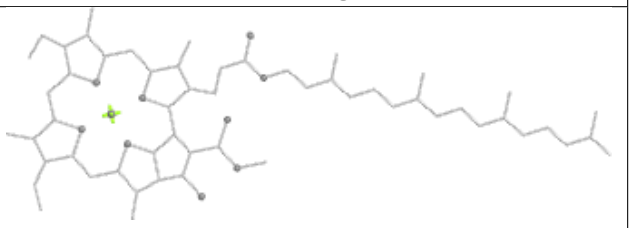
Bond lengths



Bond angles

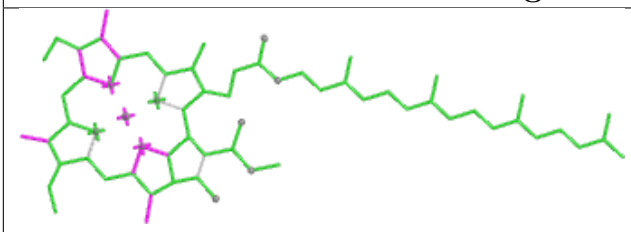


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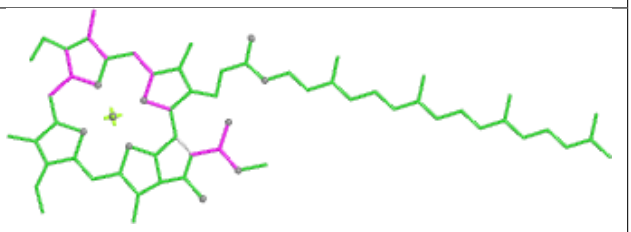


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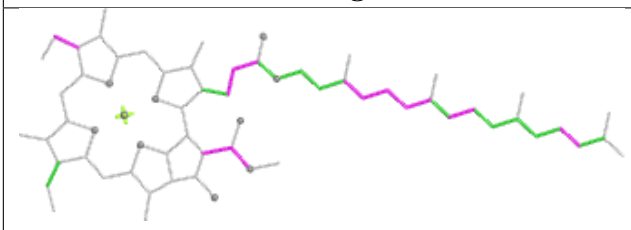
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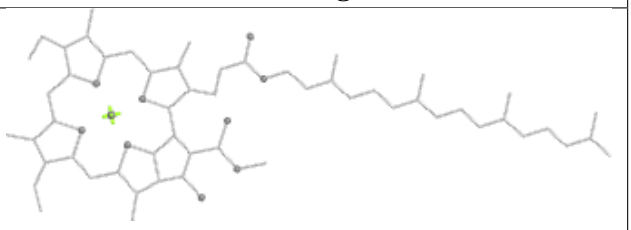
Bond lengths



Bond angles

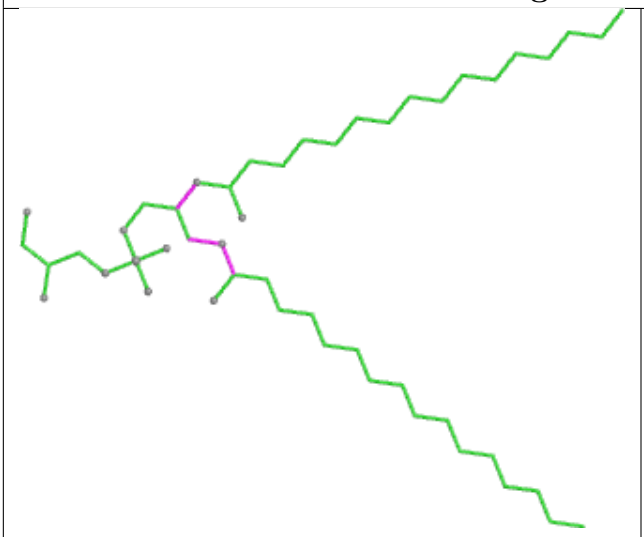


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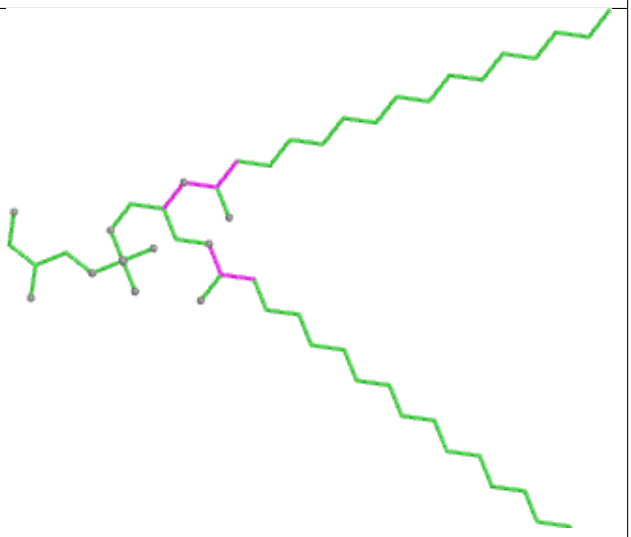


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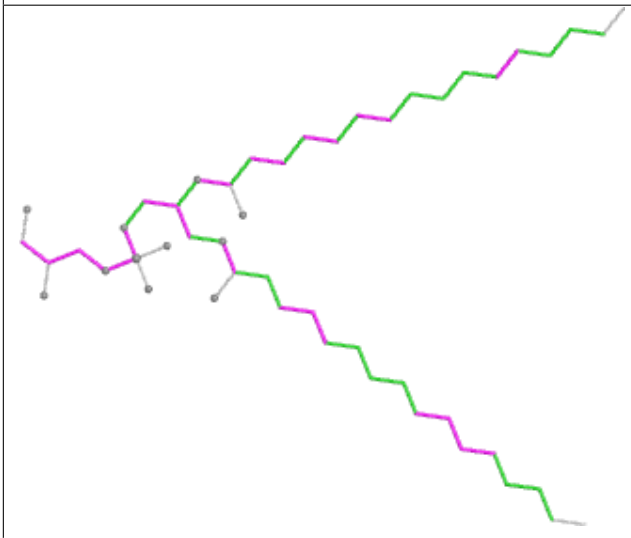
Ligand LHG l 101



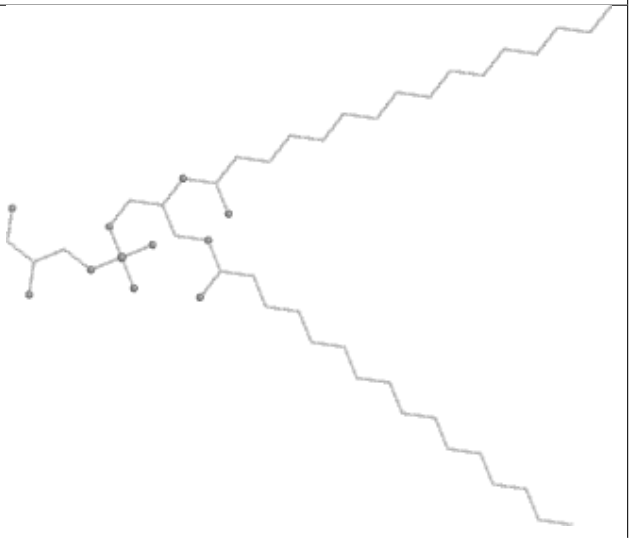
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Bond angles

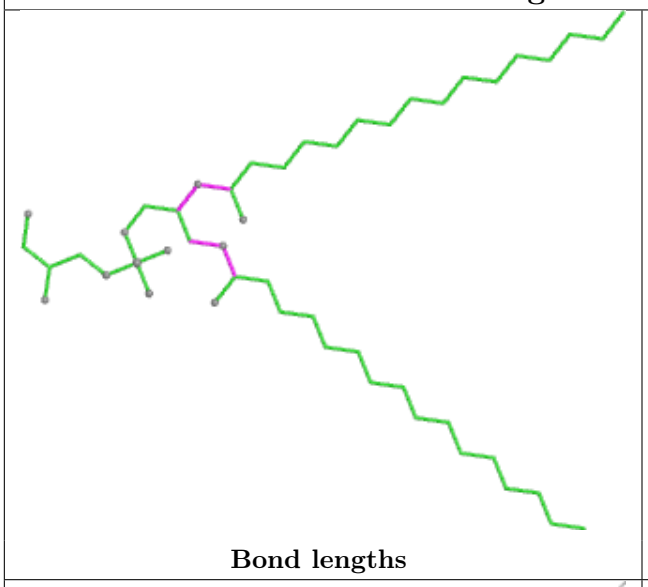


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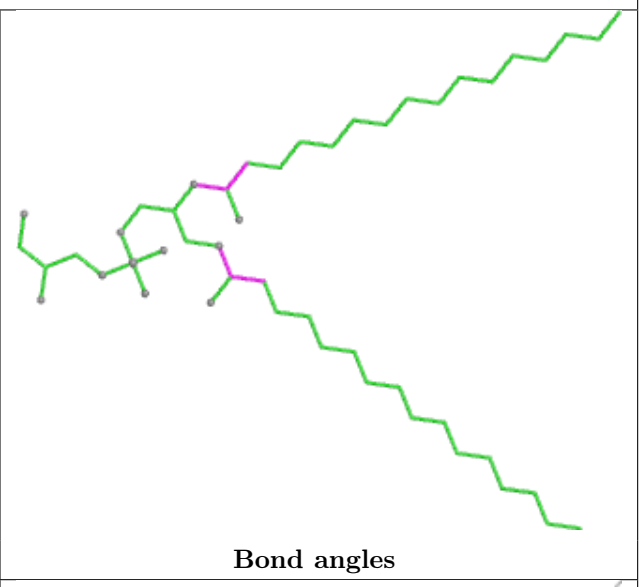


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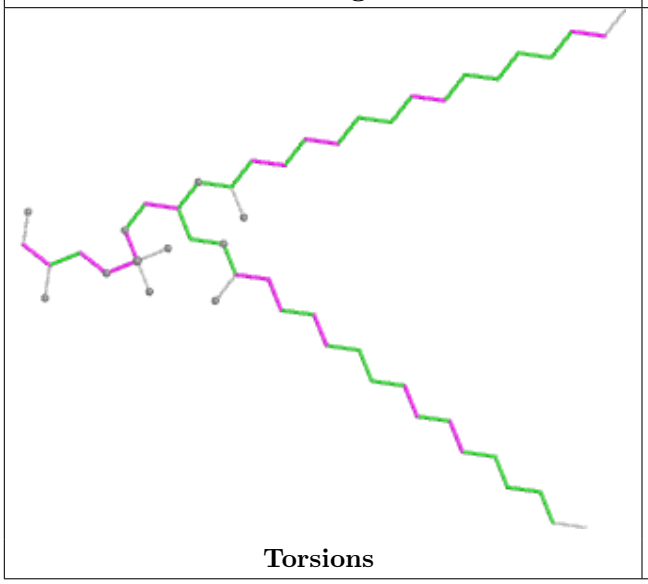
Ligand LHG 4 312



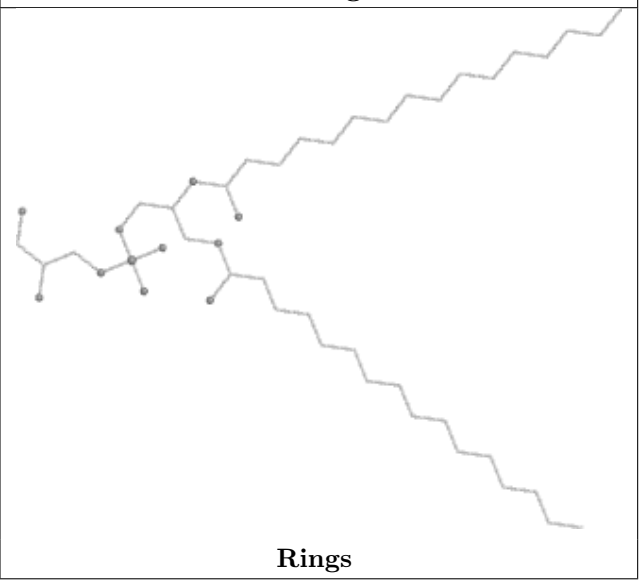
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Bond angles

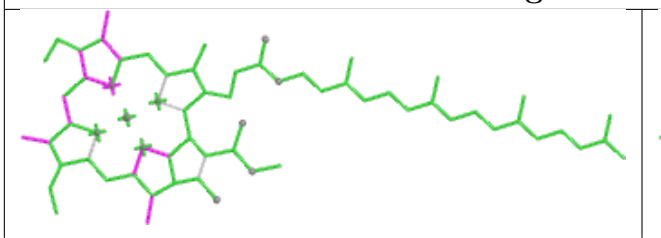


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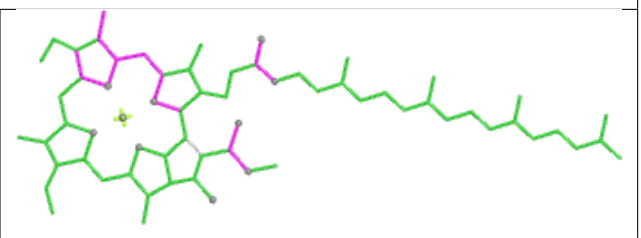


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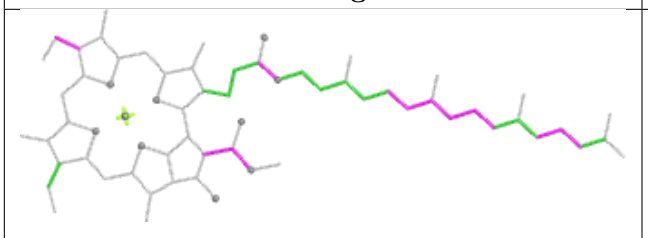
Ligand CLA B 612



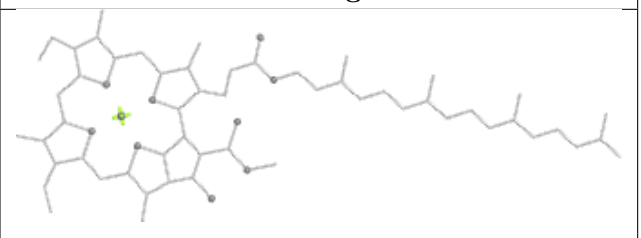
Bond lengths



Bond angles

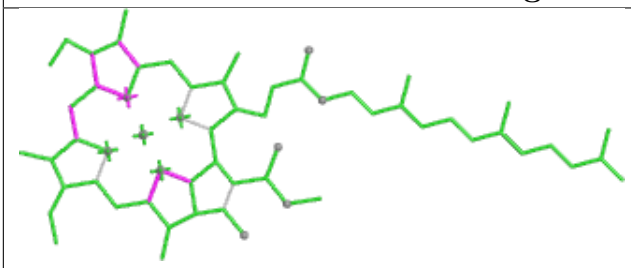


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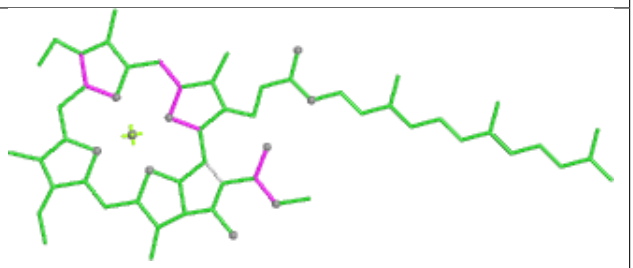


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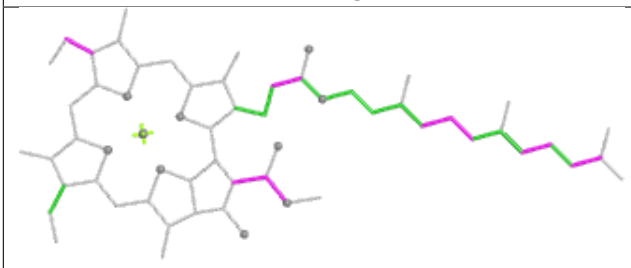
Ligand CLA R 304



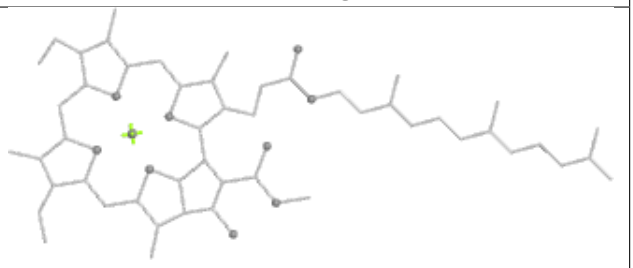
Bond lengths



Bond angles

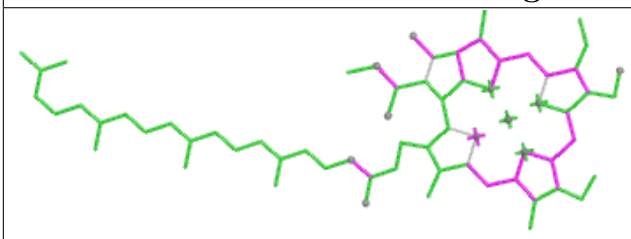


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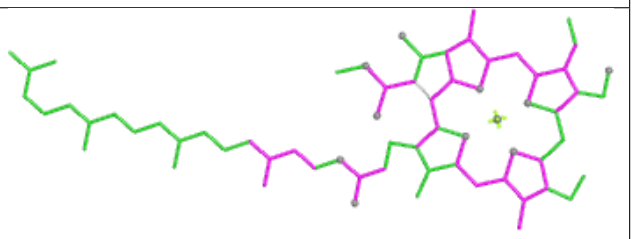


Rings

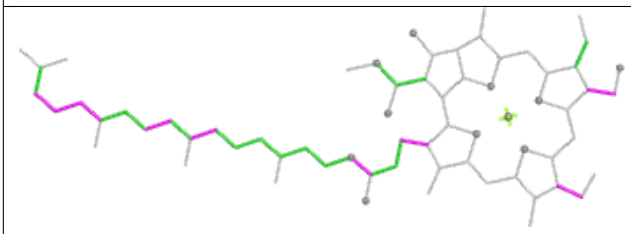
Ligand CHL U 316



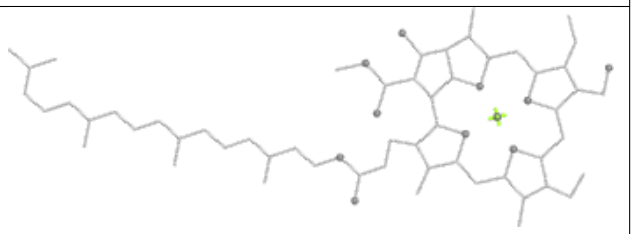
Bond lengths



Bond angles

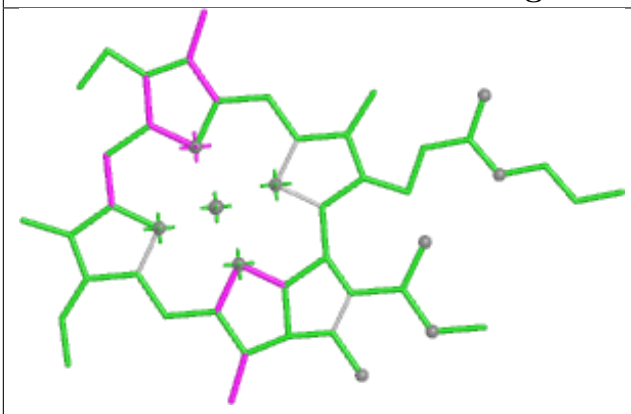


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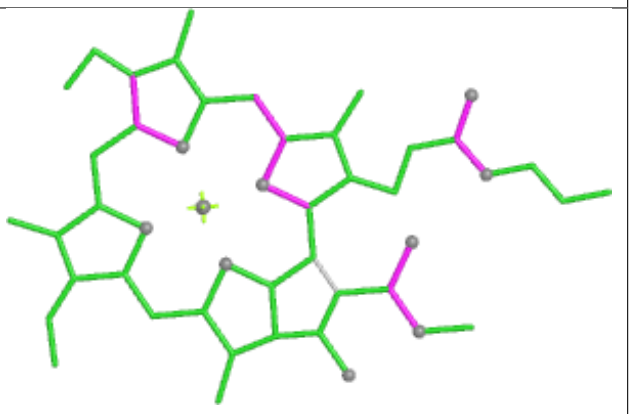


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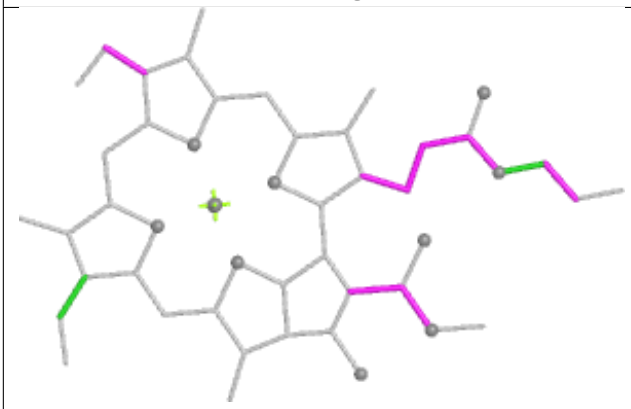
Ligand CLA P 309



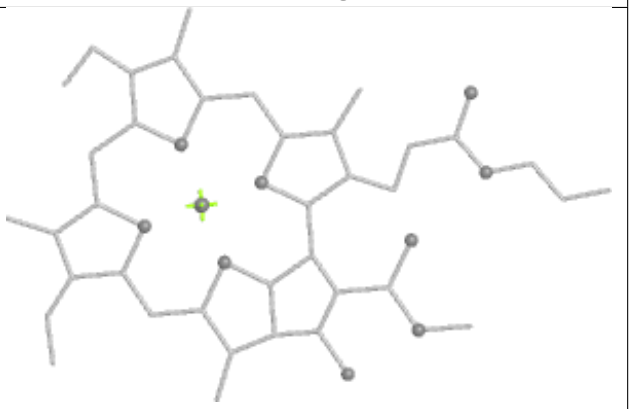
Bond lengths



Bond angles

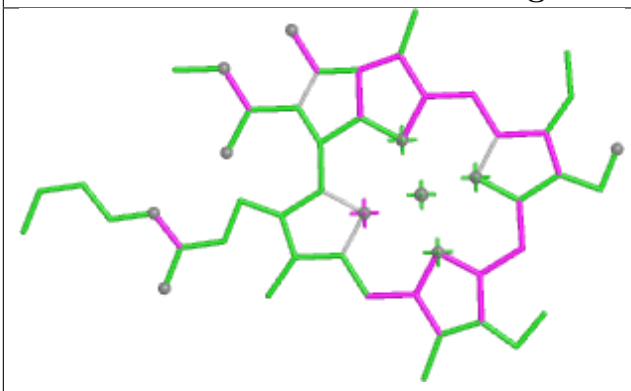


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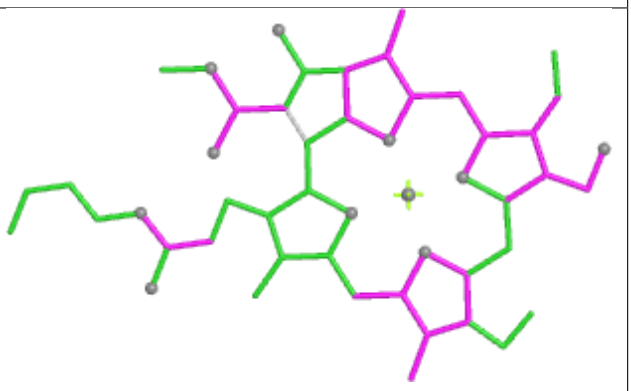


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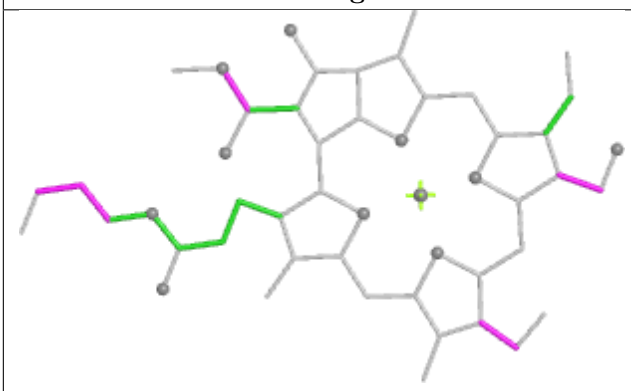
Ligand CHL 1 315



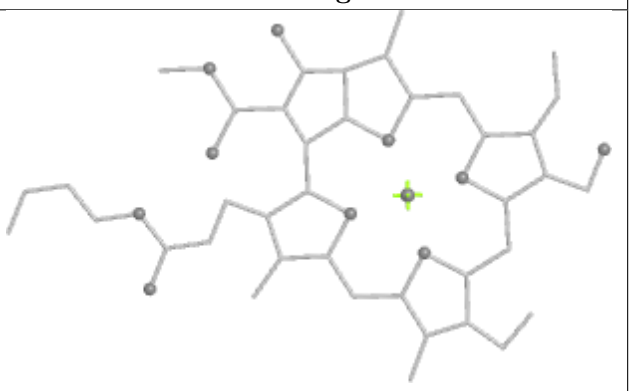
Bond lengths



Bond angles

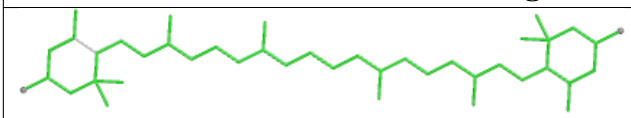


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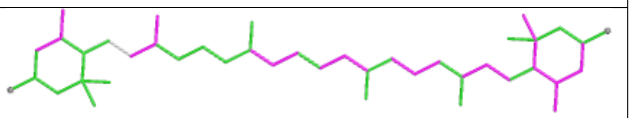


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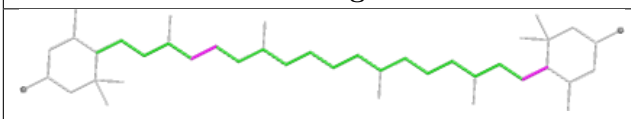
Ligand LUT U 310



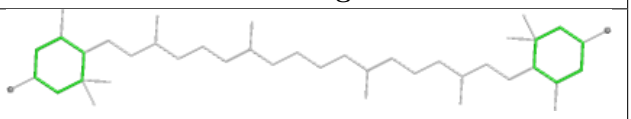
Bond lengths



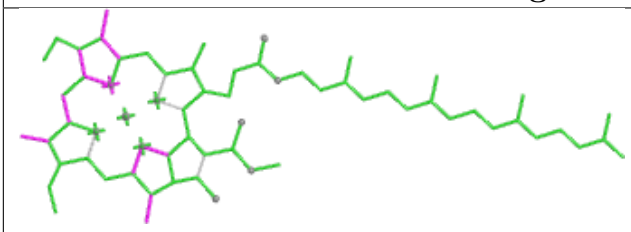
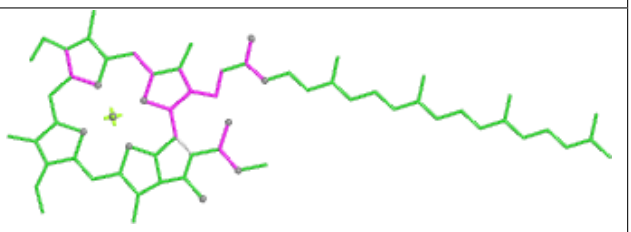
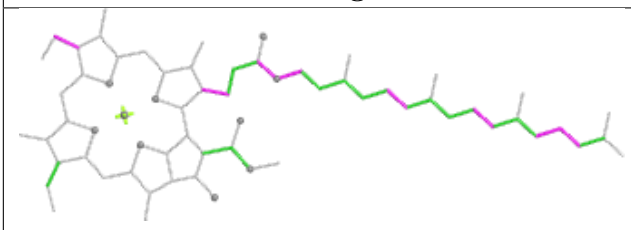
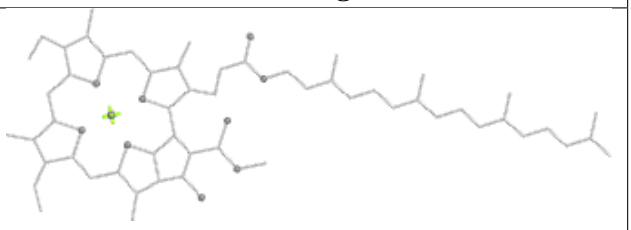
Bond angles

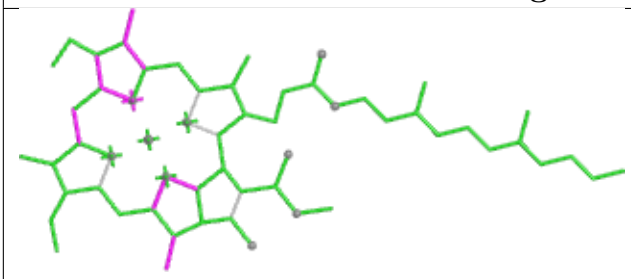
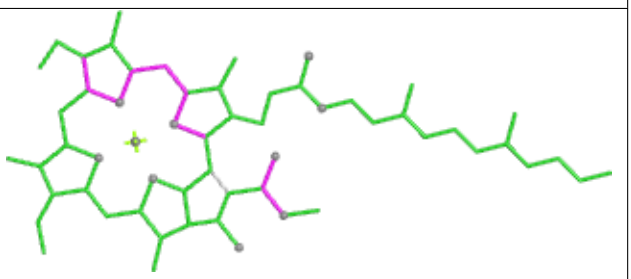
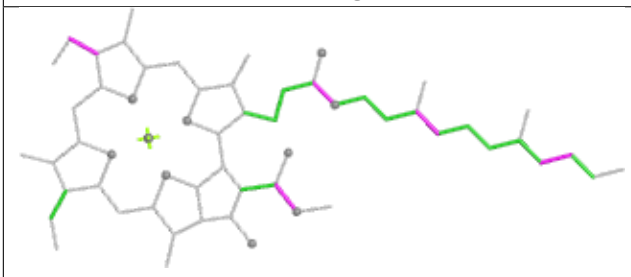
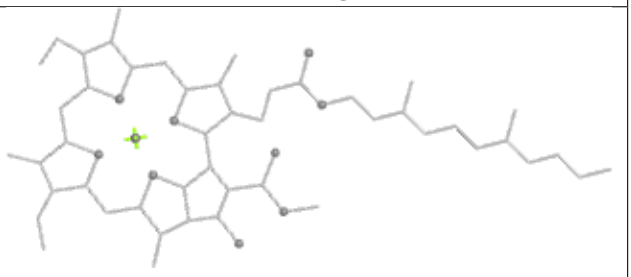


Torsions

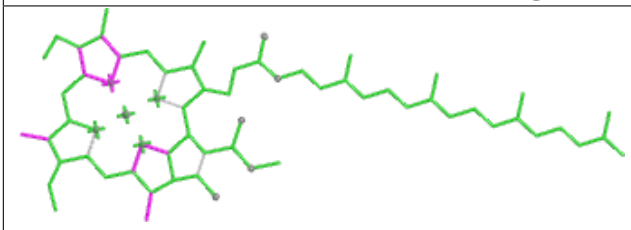


Rings

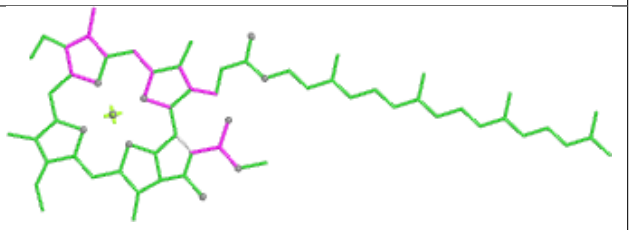
Ligand CLA c 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

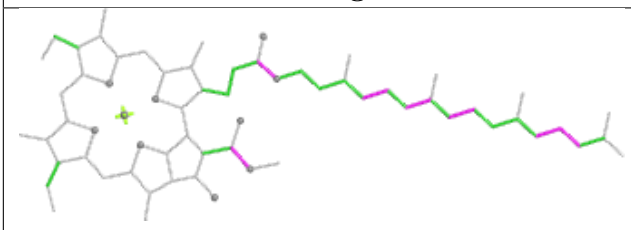
Ligand CLA x 201



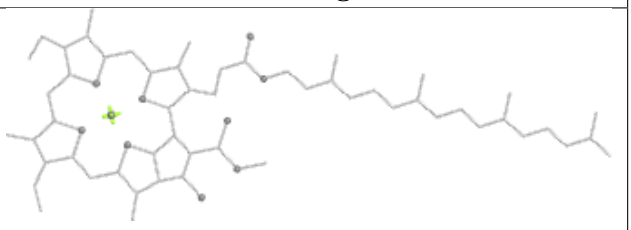
Bond lengths



Bond angles

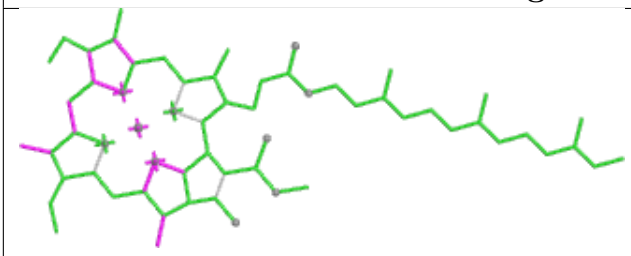


Torsions

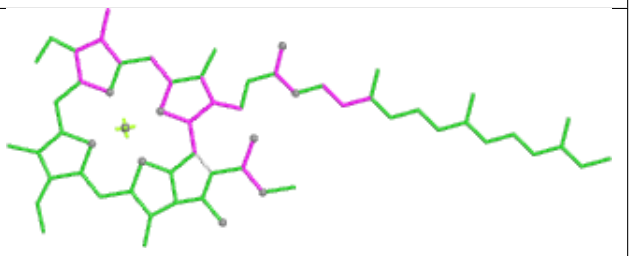


Rings

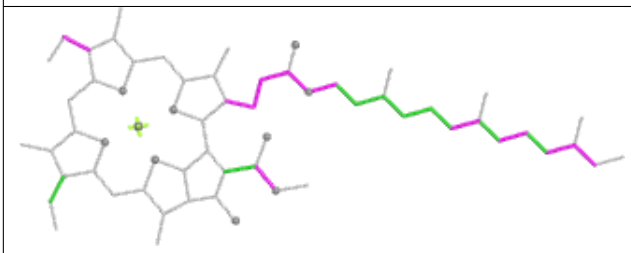
Ligand CLA S 301



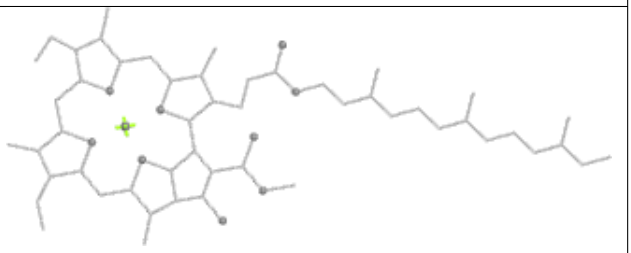
Bond lengths



Bond angles

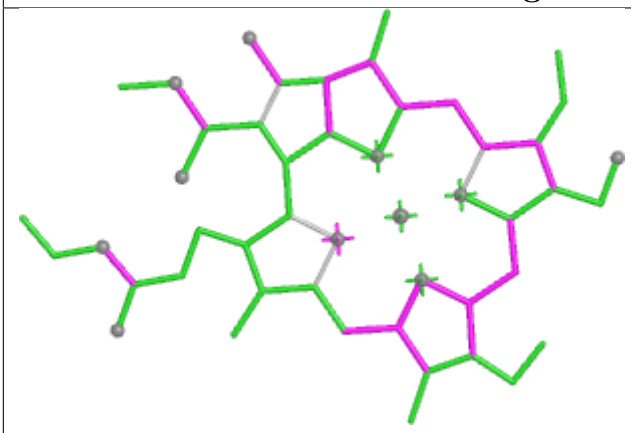


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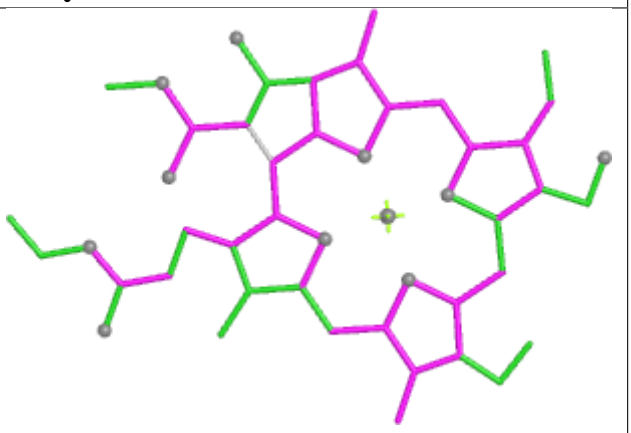


Rings

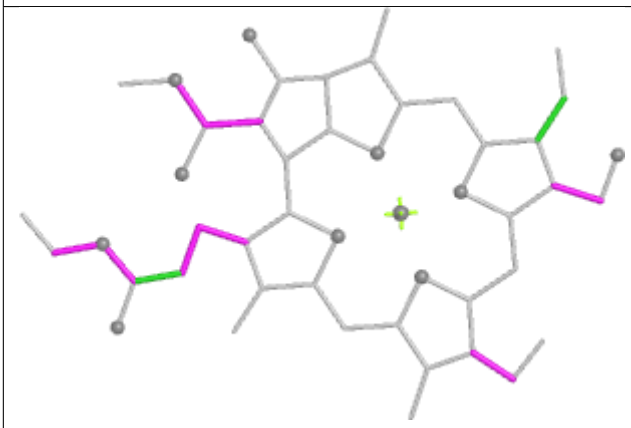
Ligand CHL Q 312



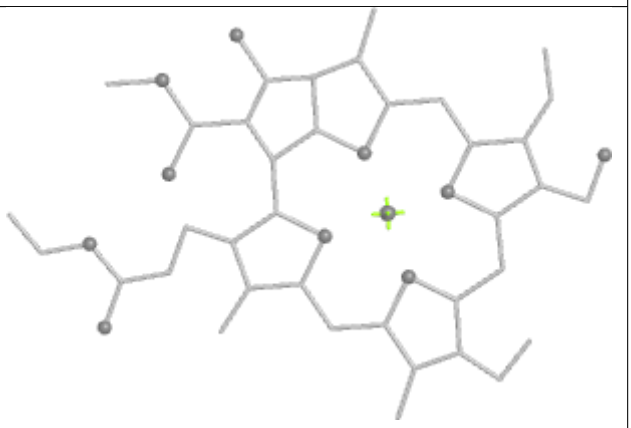
Bond lengths



Bond angles

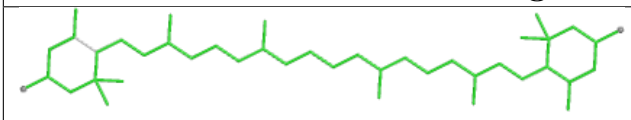


Torsions

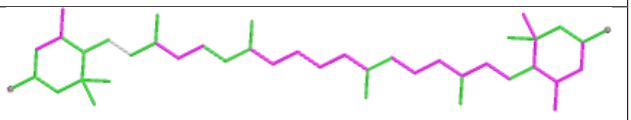


Rings

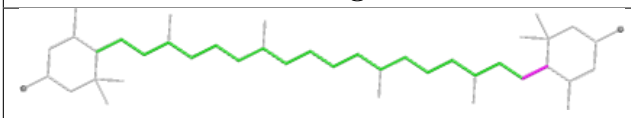
Ligand LUT 4 309



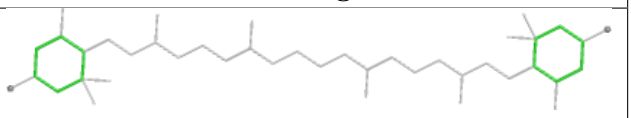
Bond lengths



Bond angles

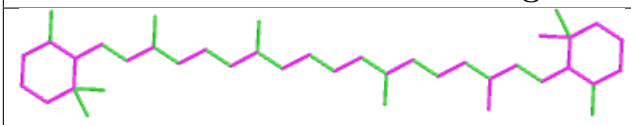


Torsions

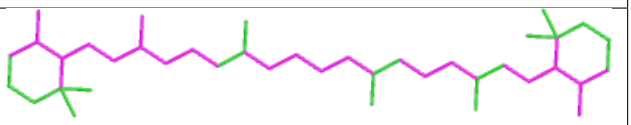


Rings

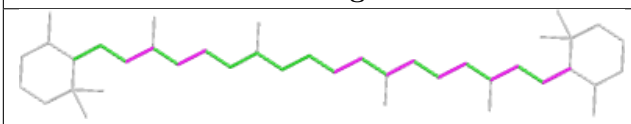
Ligand BCR C 518



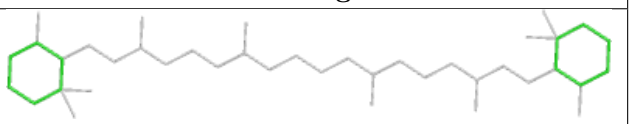
Bond lengths



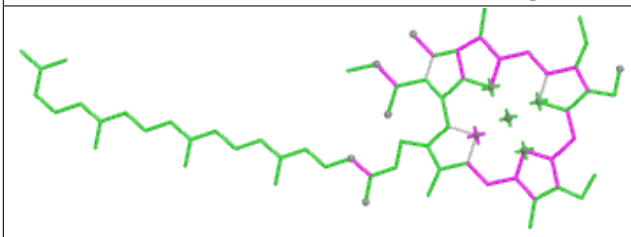
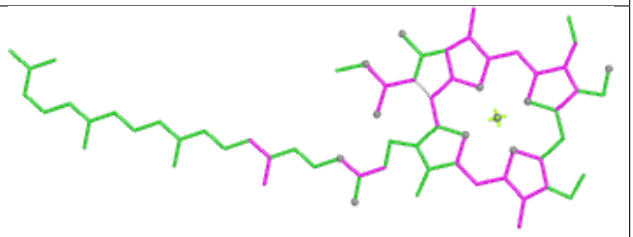
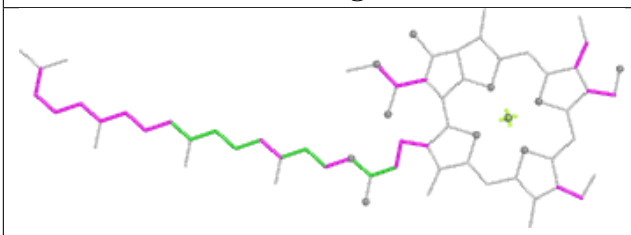
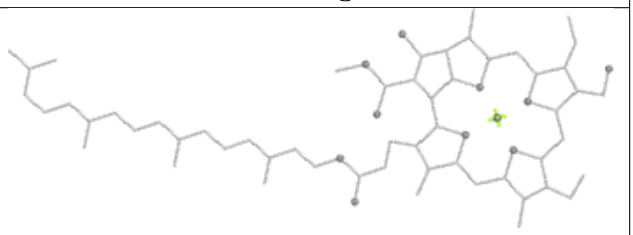
Bond angles

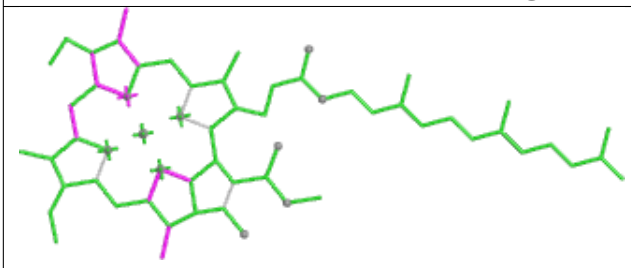
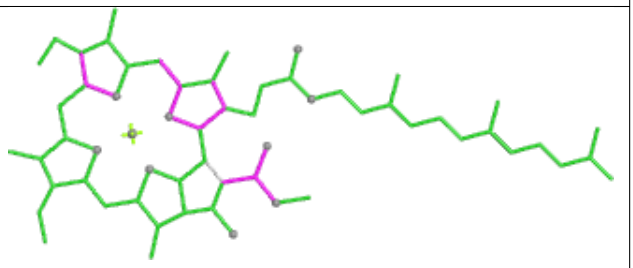
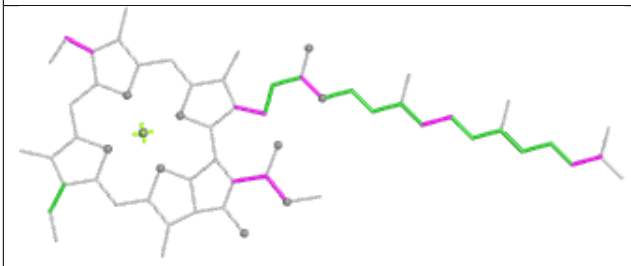
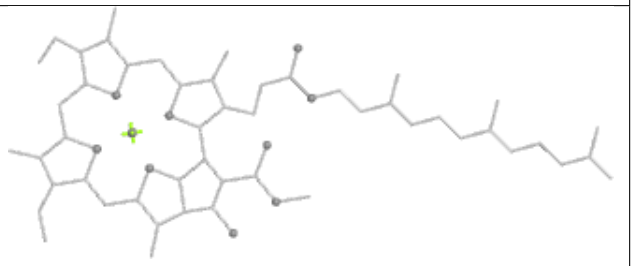


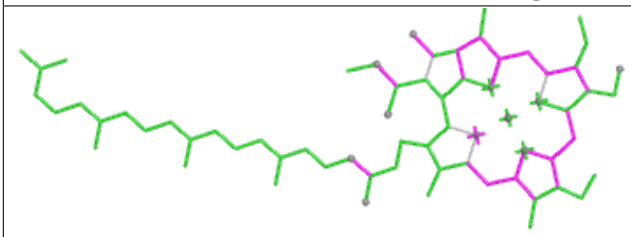
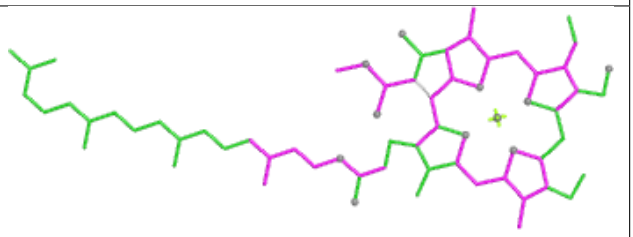
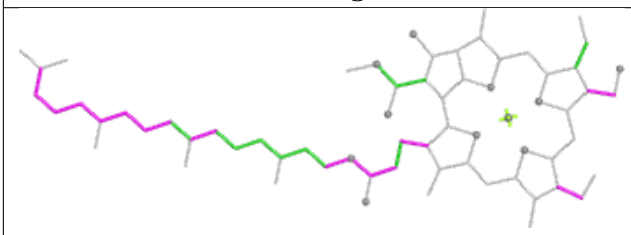
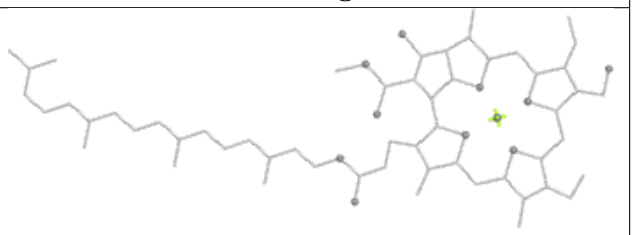
Torsions

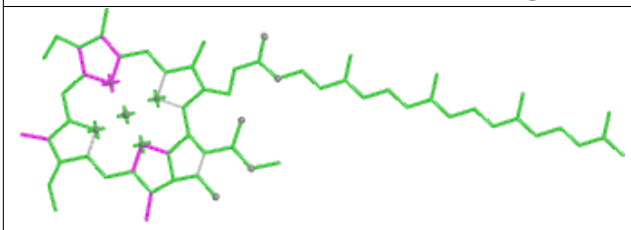
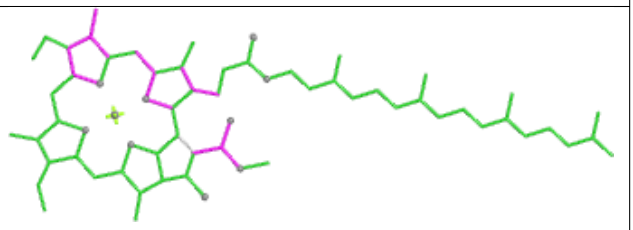
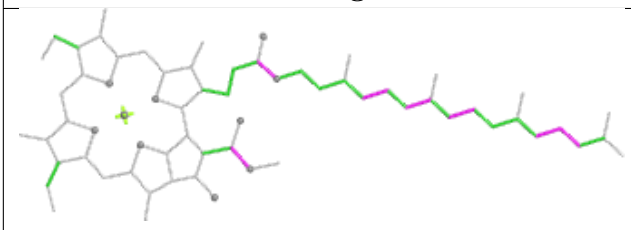
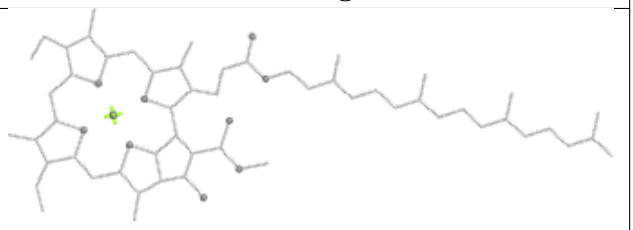


Rings

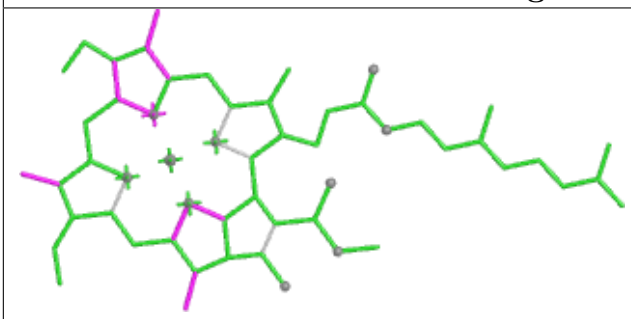
Ligand CHL P 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

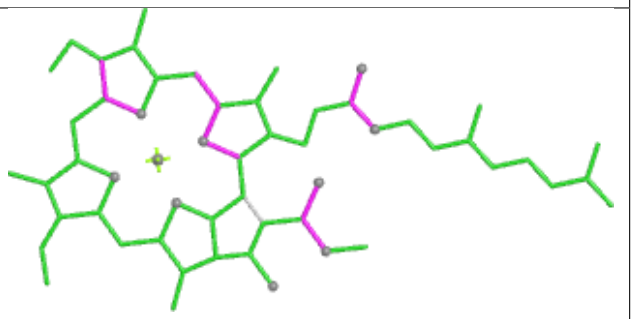
Ligand CHL 1 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA X 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

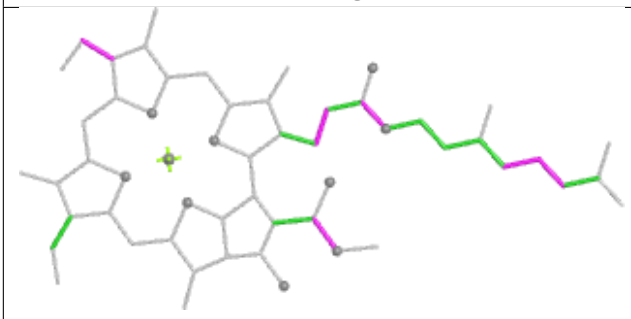
Ligand CLA S 308



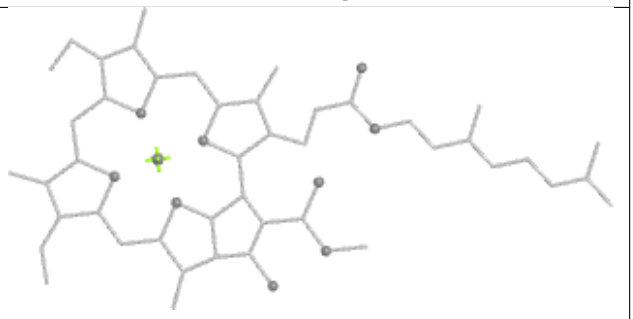
Bond lengths



Bond angles

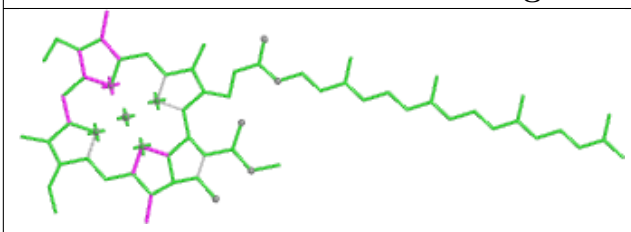


Torsions

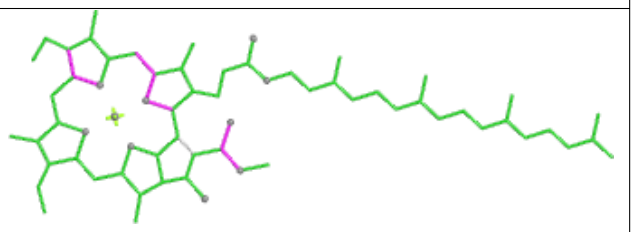


Rings

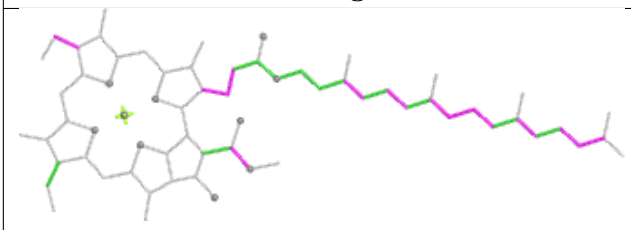
Ligand CLA R 307



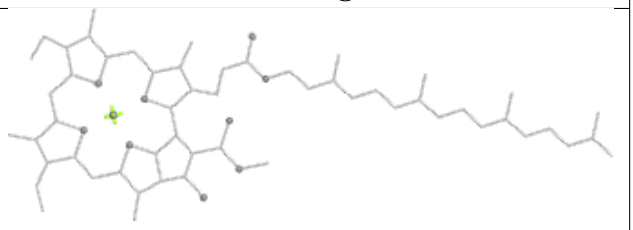
Bond lengths



Bond angles

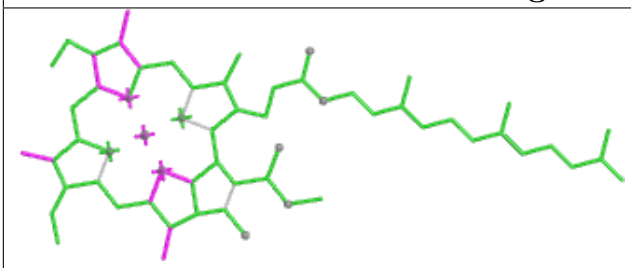


Torsions

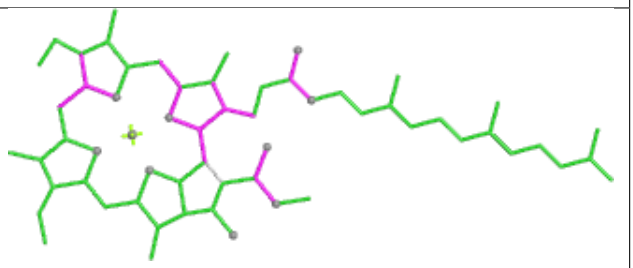


Rings

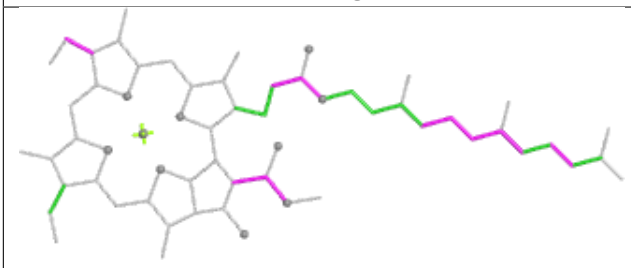
Ligand CLA 1 306



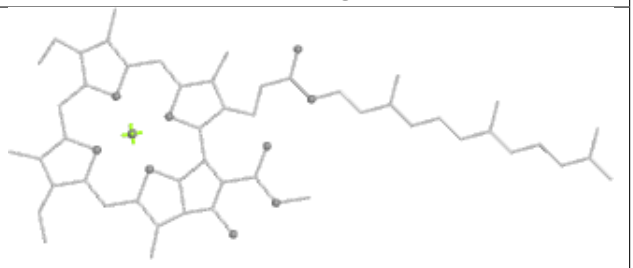
Bond lengths



Bond angles

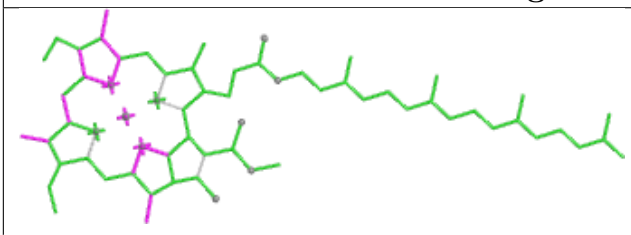


Torsions

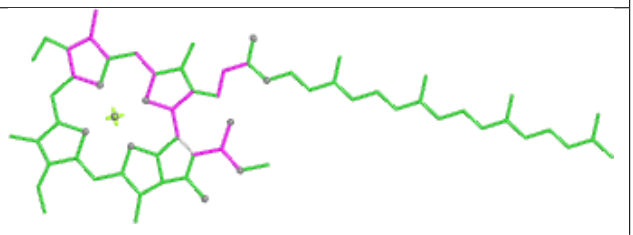


Rings

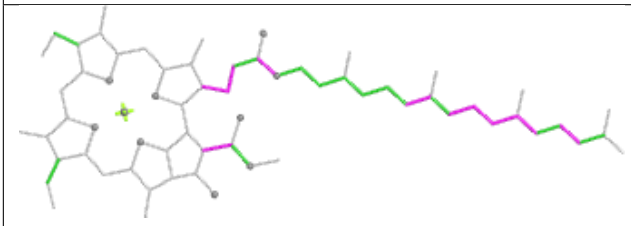
Ligand CLA b 613



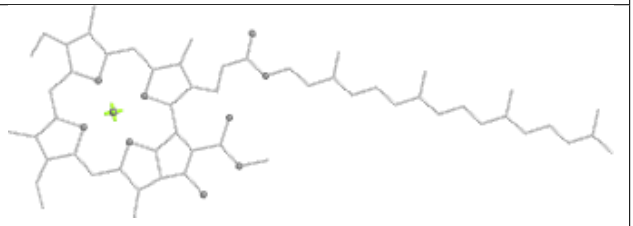
Bond lengths



Bond angles



Torsions

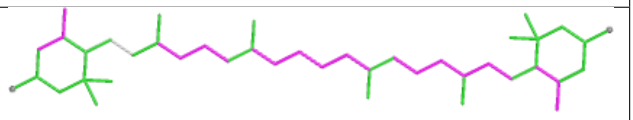


Rings

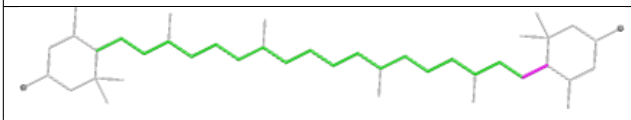
Ligand LUT r 611



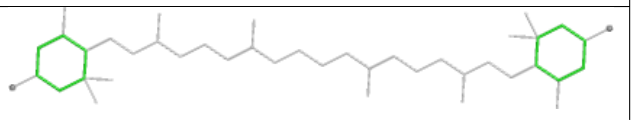
Bond lengths



Bond angles

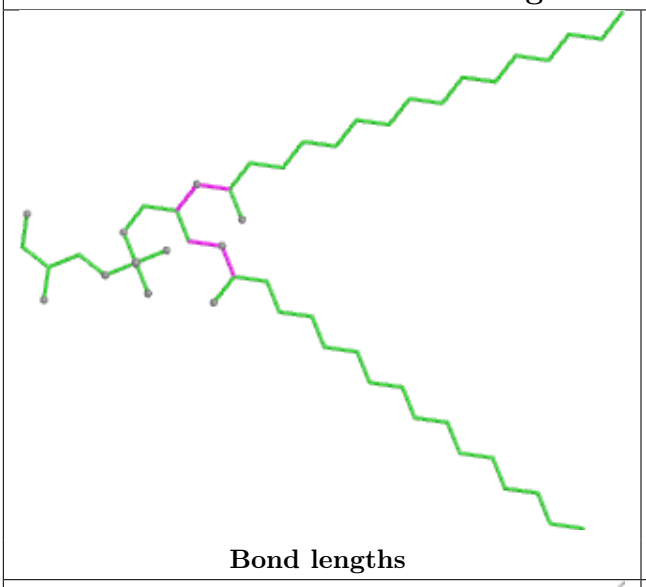


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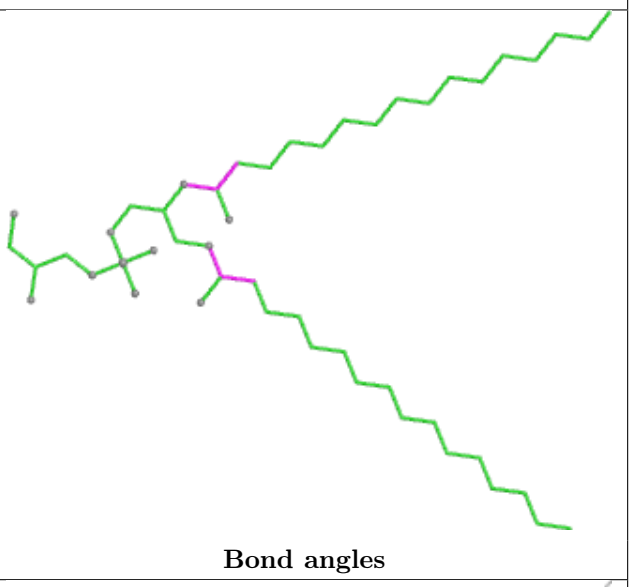


Rings

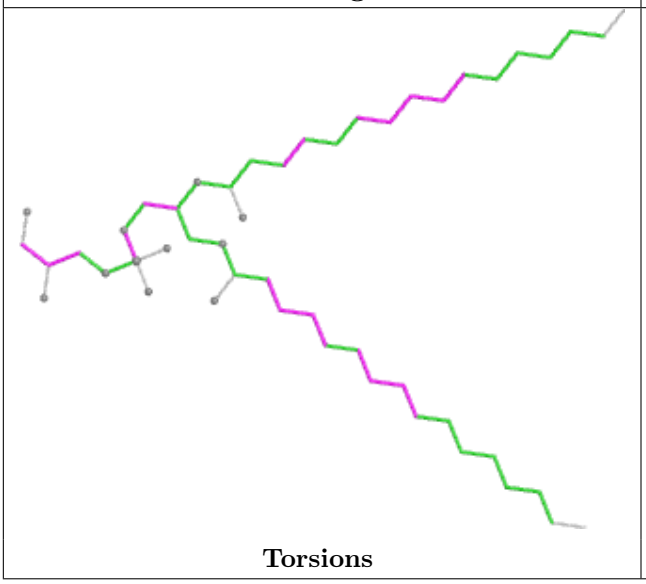
Ligand LHG n 312



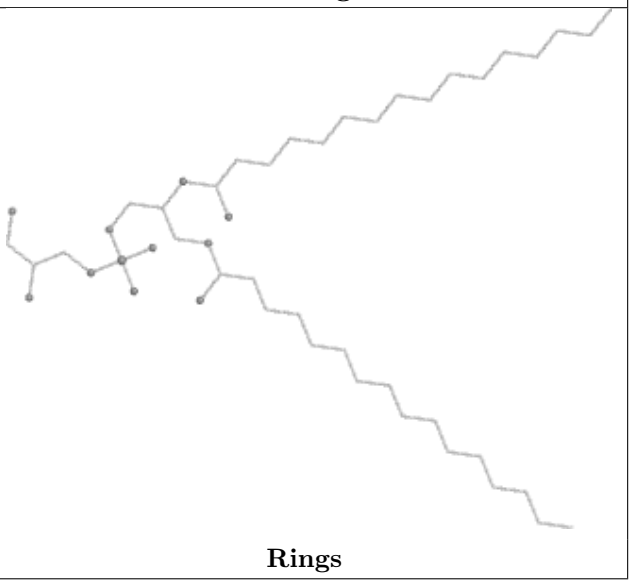
Bond lengths



Bond angles



Torsions

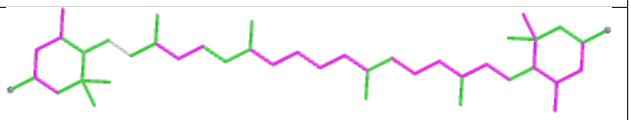


Rings

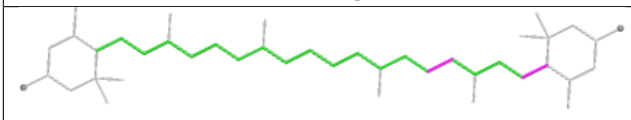
Ligand LUT P 311



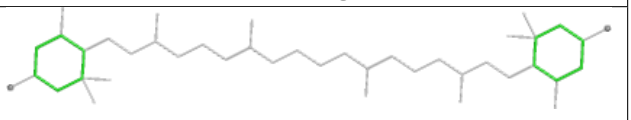
Bond lengths



Bond angles

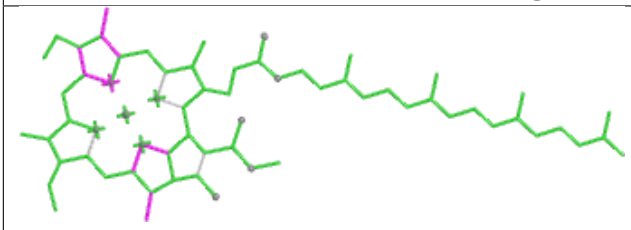


Torsions

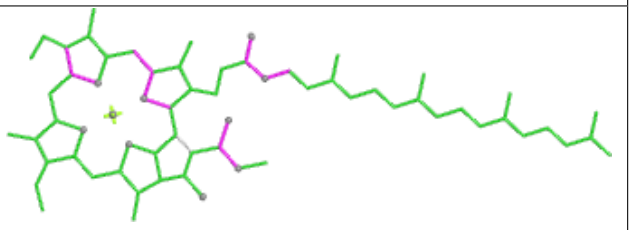


Rings

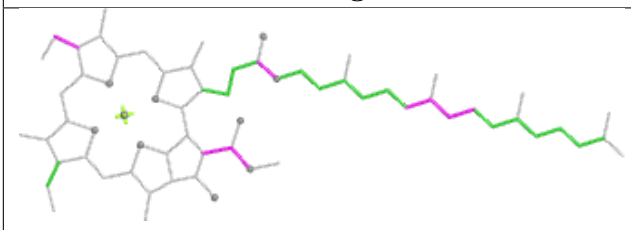
Ligand CLA 3 302



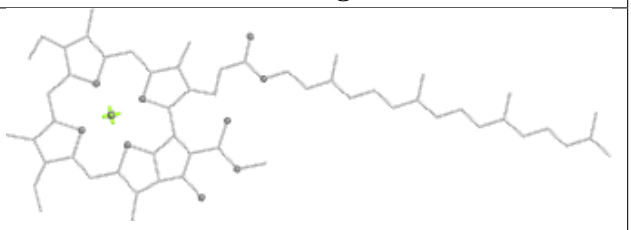
Bond lengths



Bond angles

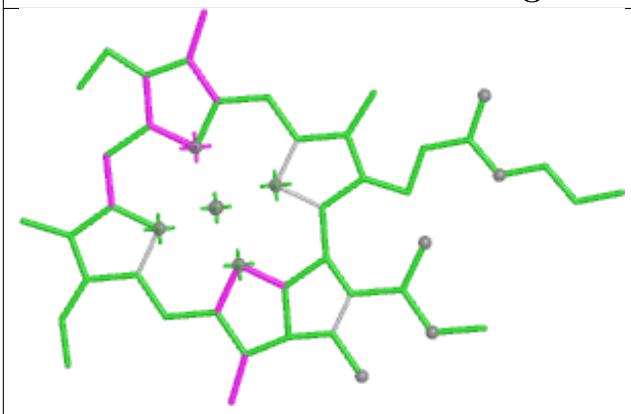


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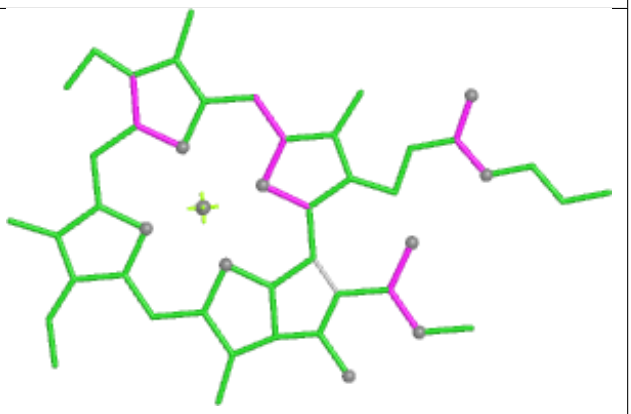


Rings

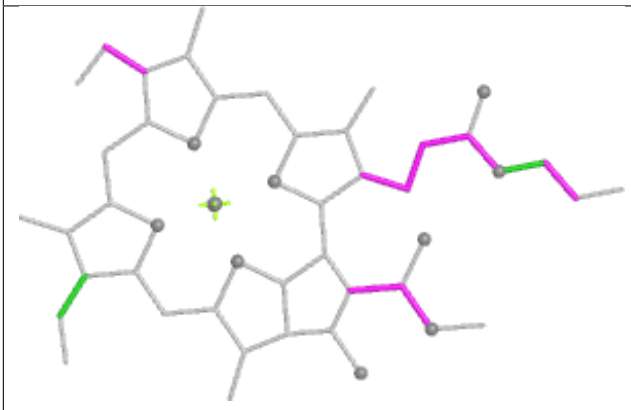
Ligand CLA N 308



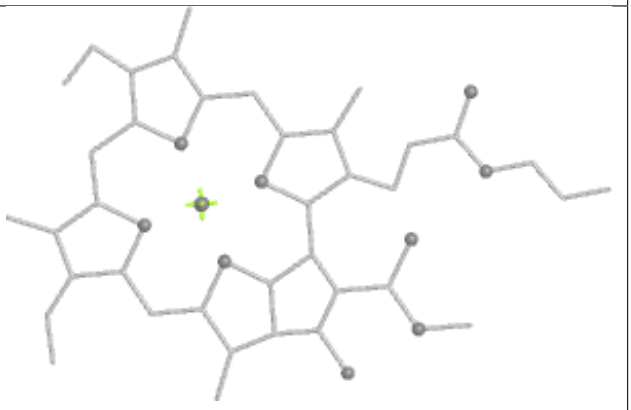
Bond lengths



Bond angles

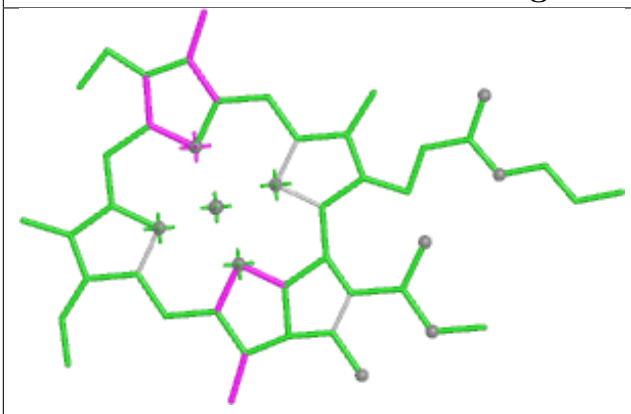


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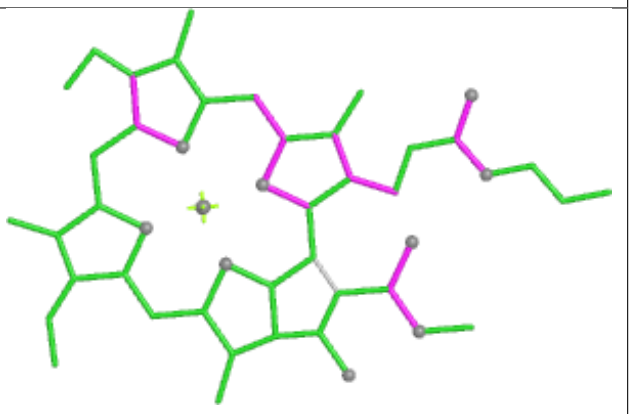


Rings

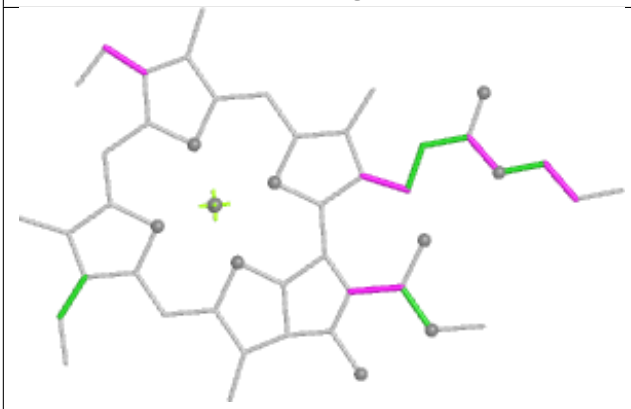
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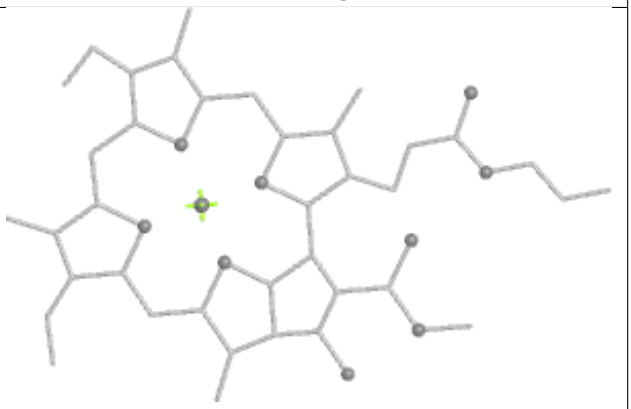
Bond lengths



Bond angles

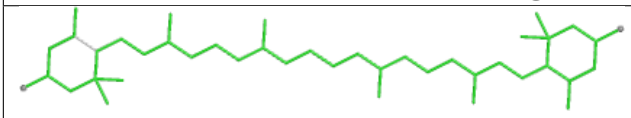


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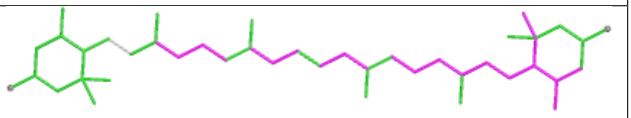


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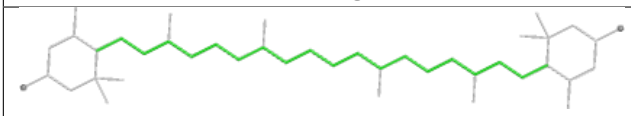
Ligand LUT n 309



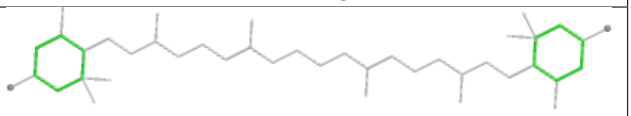
Bond lengths



Bond angles

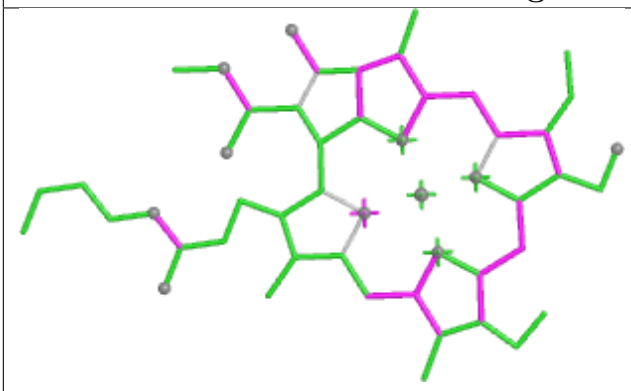


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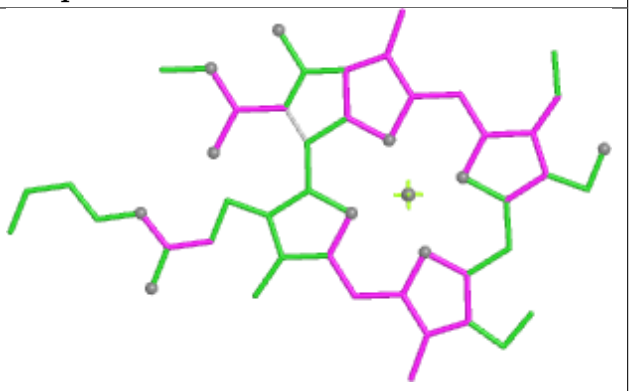


Rings

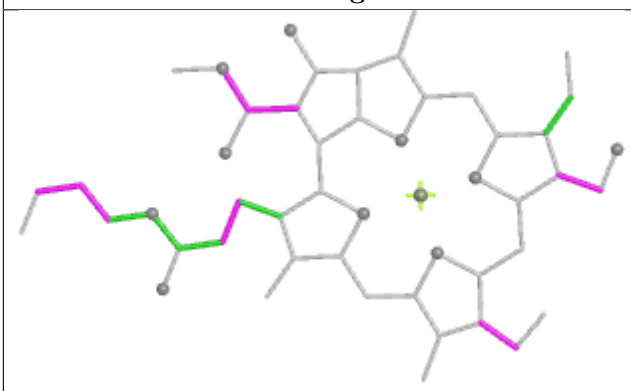
Ligand CHL q 313



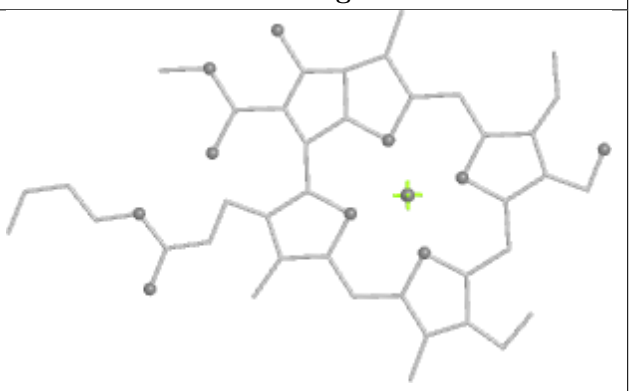
Bond lengths



Bond angles

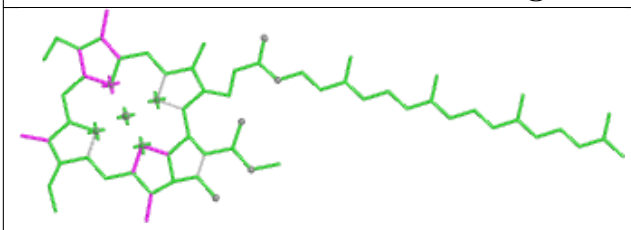


Torsions

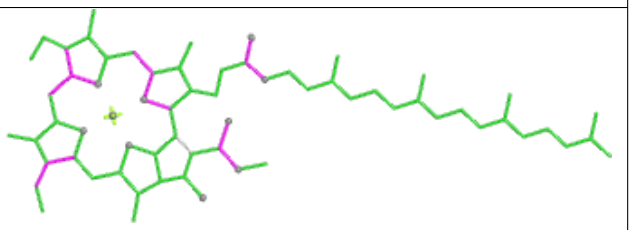


Rings

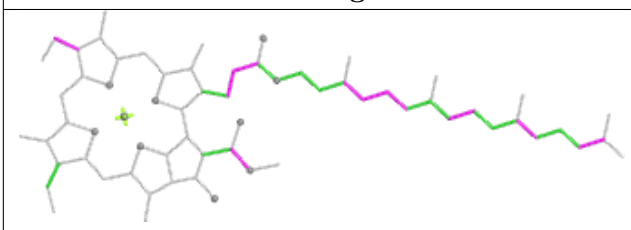
Ligand CLA u 307



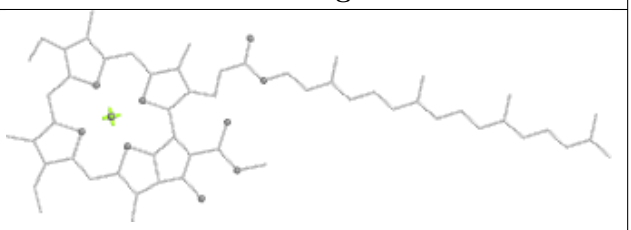
Bond lengths



Bond angles

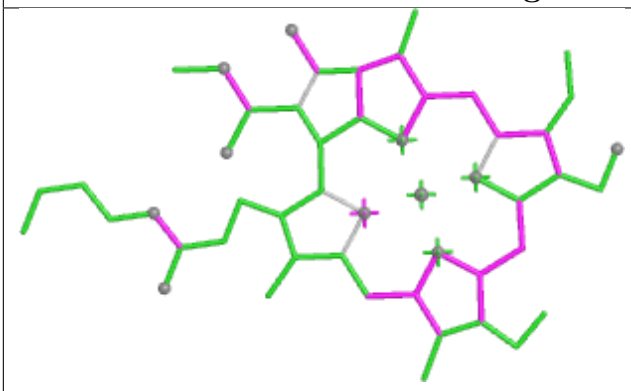


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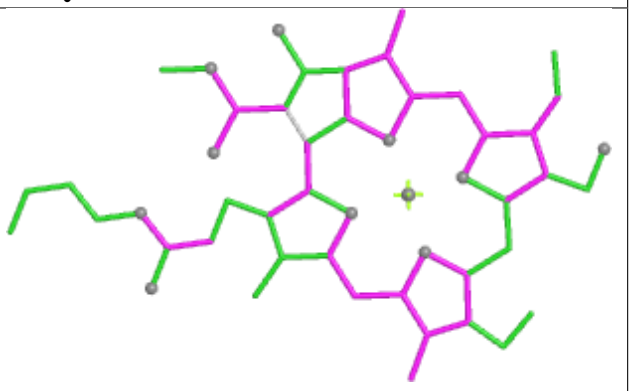


Rings

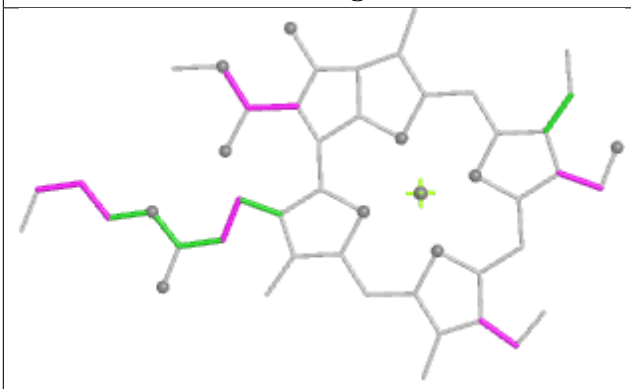
Ligand CHL Q 313



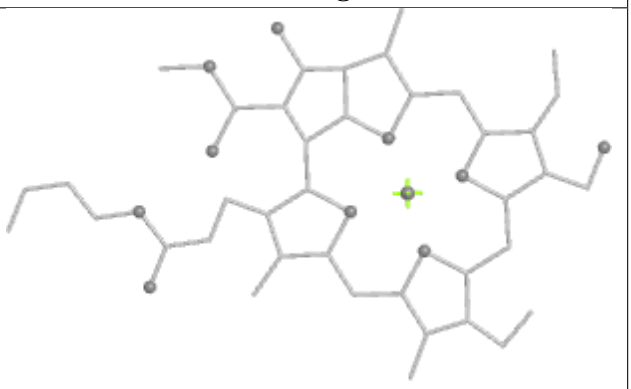
Bond lengths



Bond angles

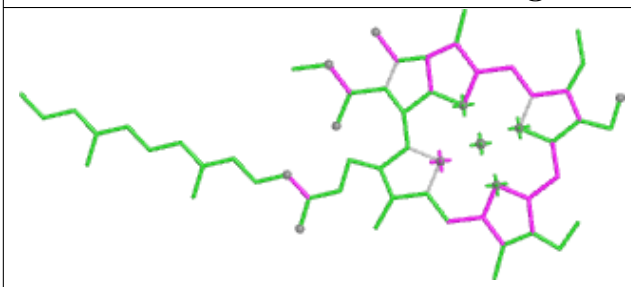


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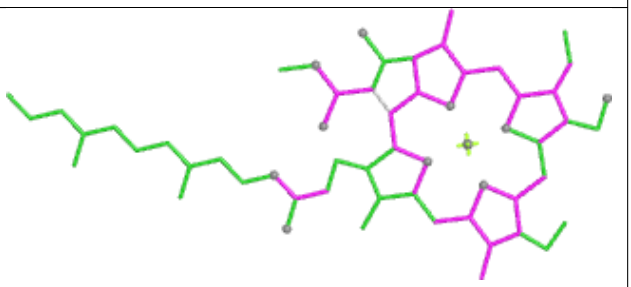


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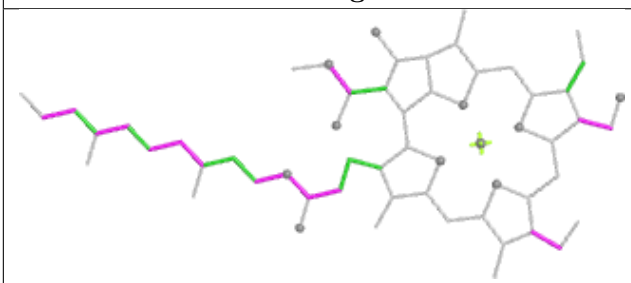
Ligand CHL S 315



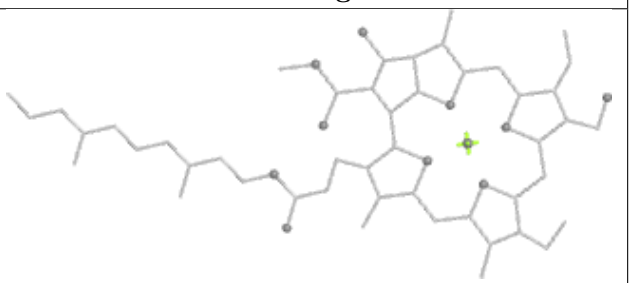
Bond lengths



Bond angles

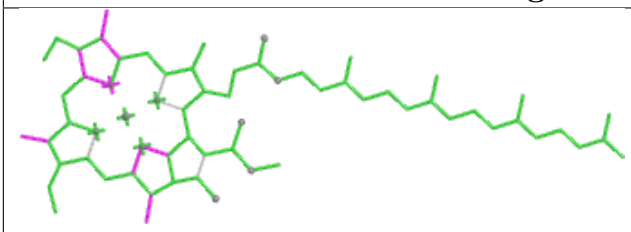


Torsions

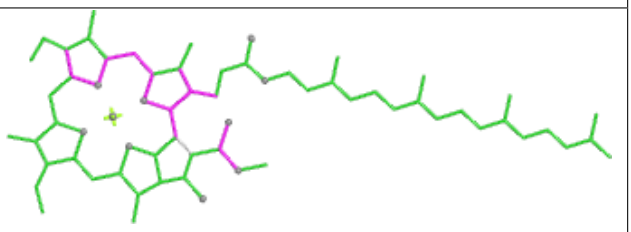


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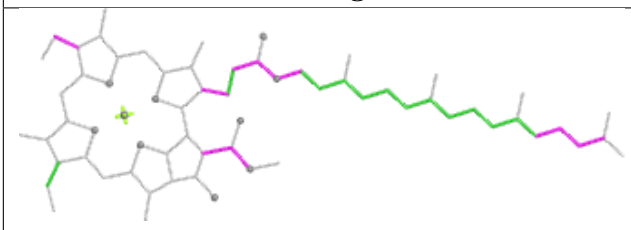
Ligand CLA b 611



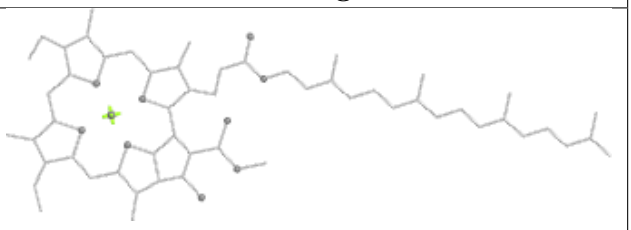
Bond lengths



Bond angles

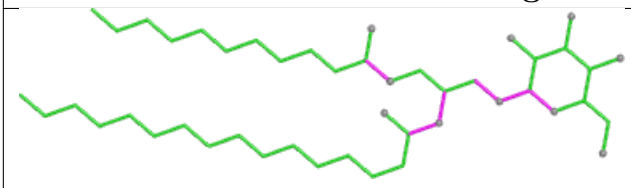


Torsions

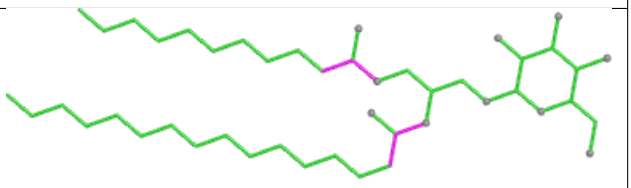


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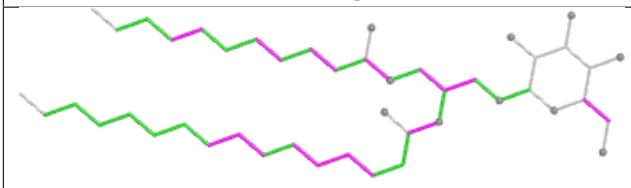
Ligand LMG d 407



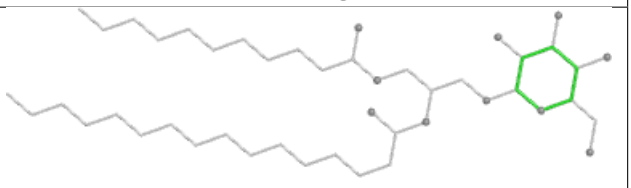
Bond lengths



Bond angles

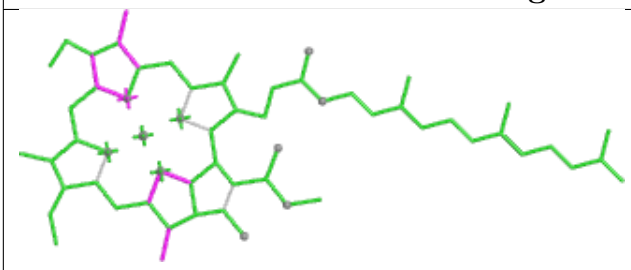


Torsions

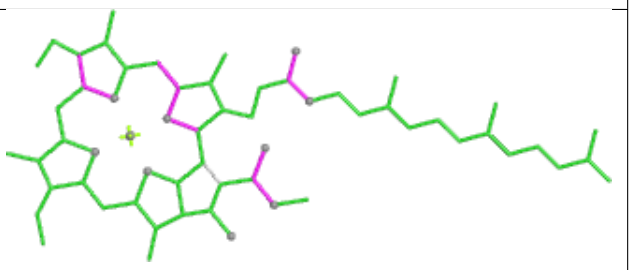


Rings

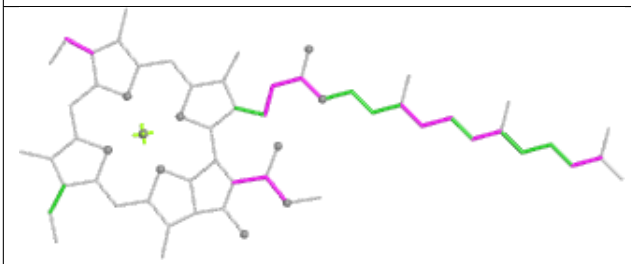
Ligand CLA 3 306



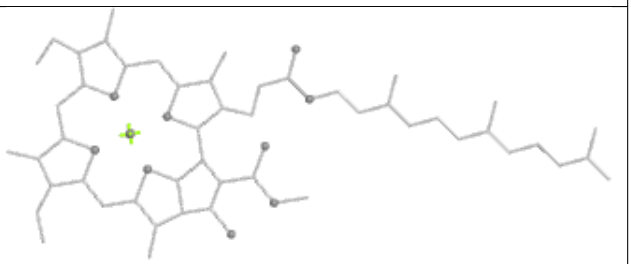
Bond lengths



Bond angles

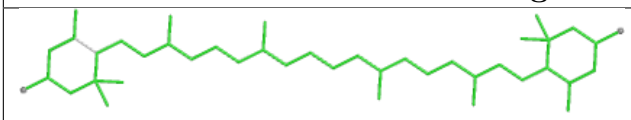


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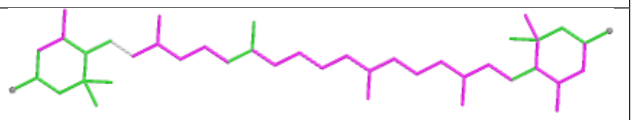


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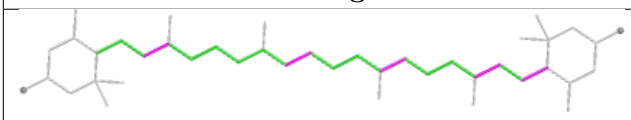
Ligand LUT s 311



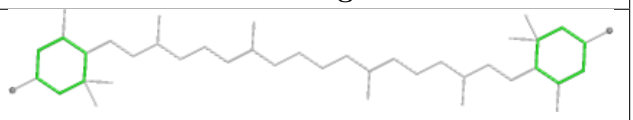
Bond lengths



Bond angles

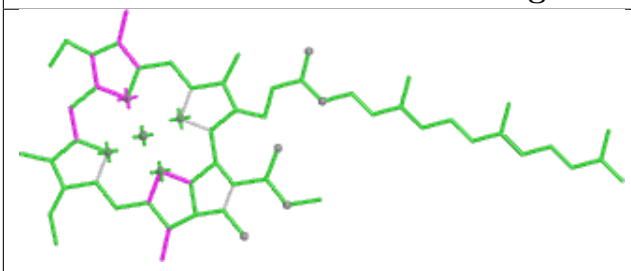


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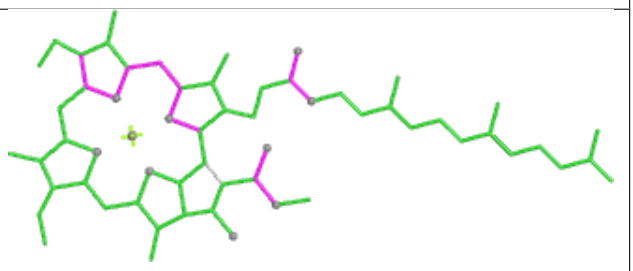


Rings

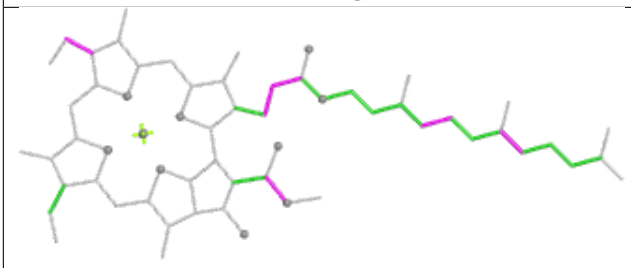
Ligand CLA 2 307



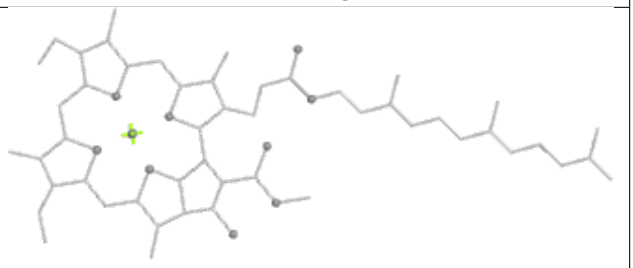
Bond lengths



Bond angles

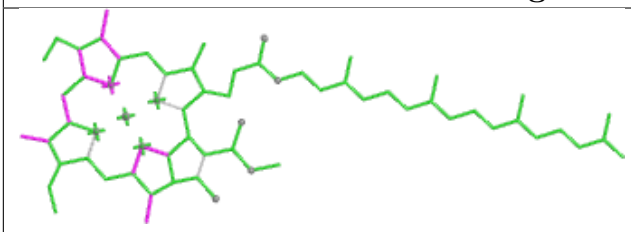


Torsions

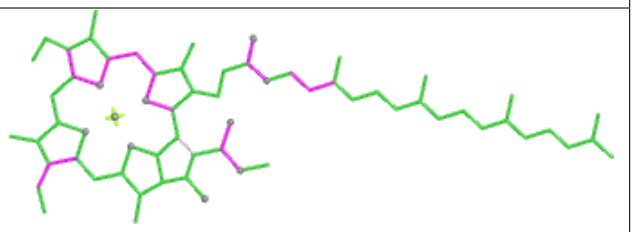


Rings

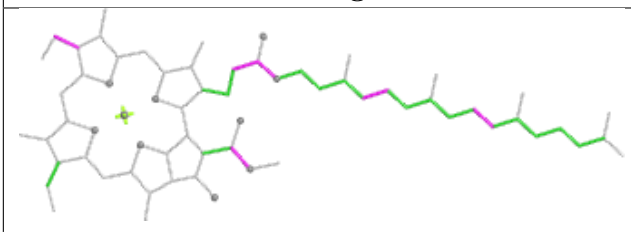
Ligand CLA 4 307



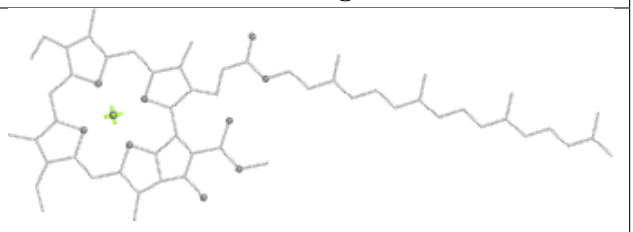
Bond lengths



Bond angles

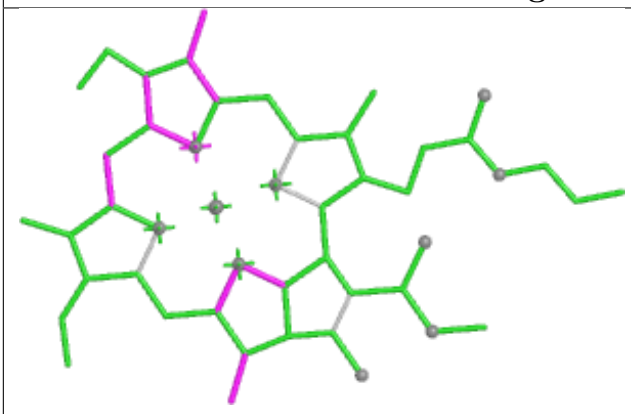


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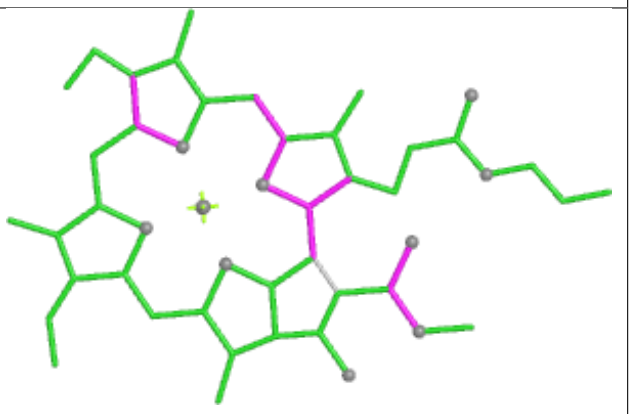


Rings

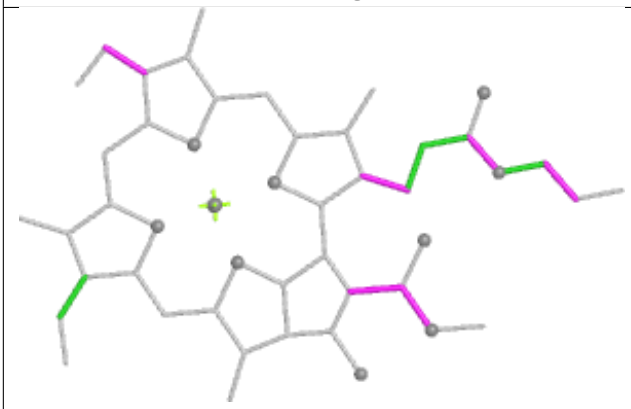
Ligand CLA 4 308



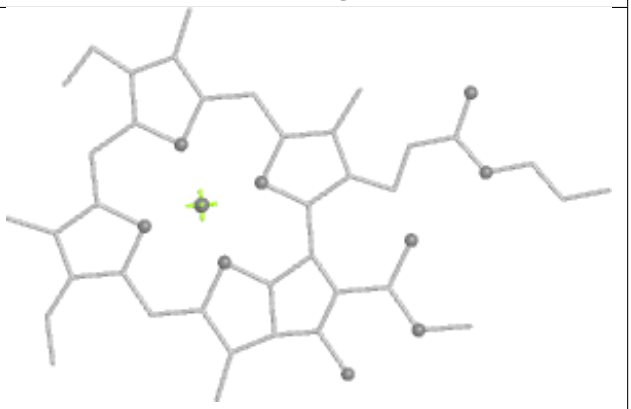
Bond lengths



Bond angles

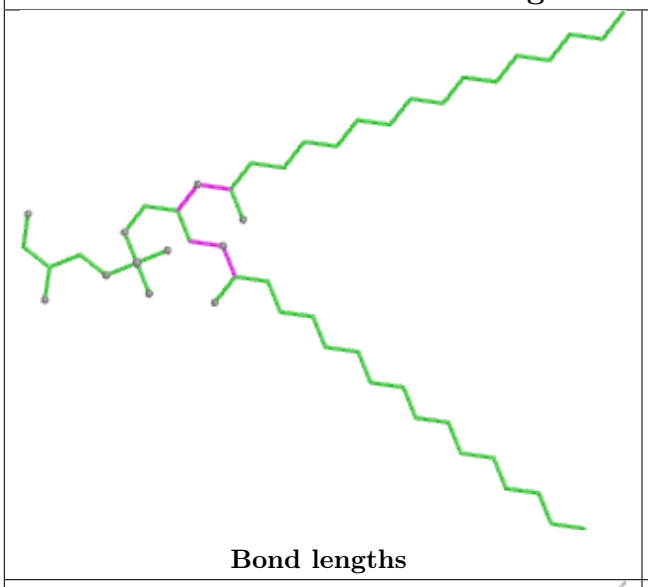


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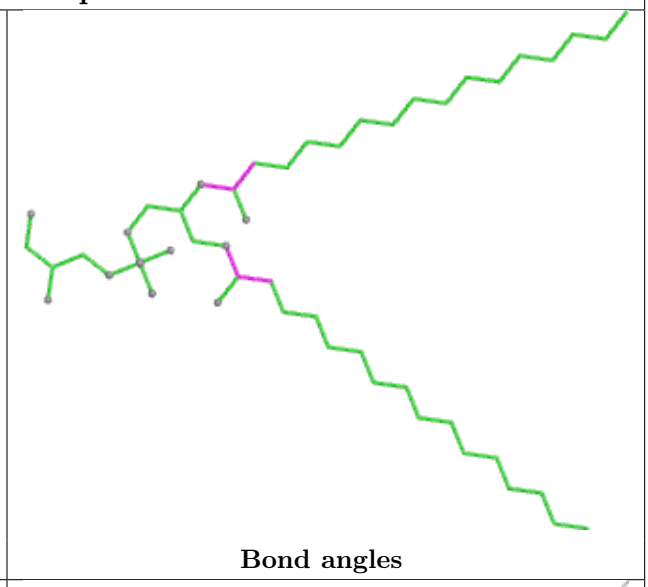


Rings

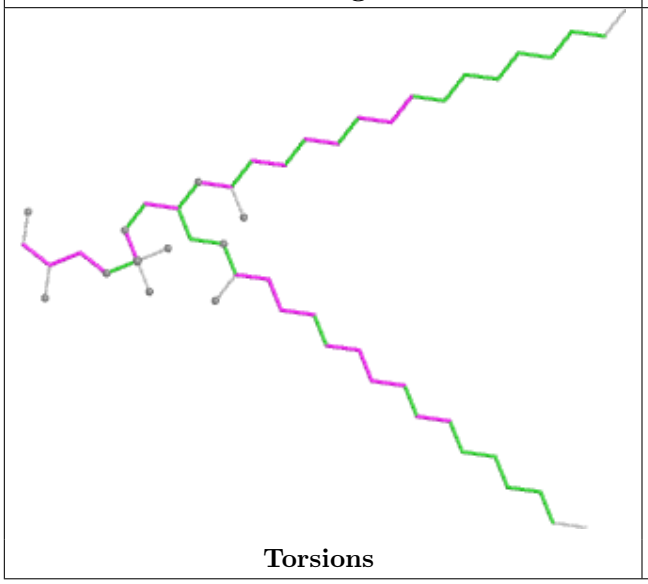
Ligand LHG q 310



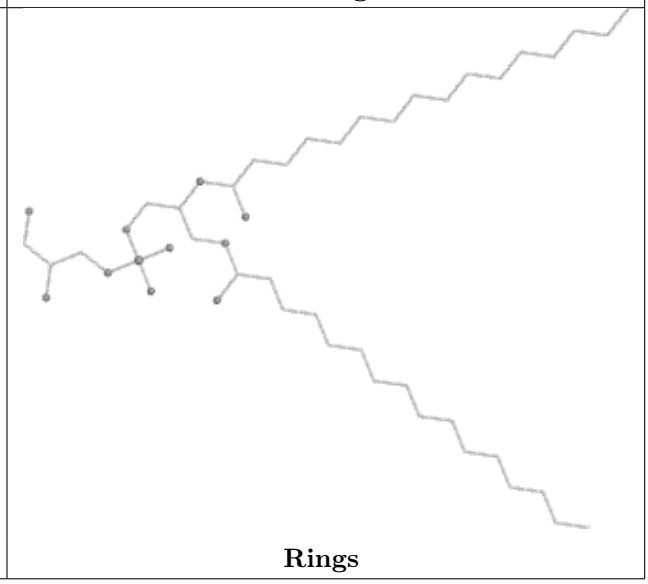
Bond lengths



Bond angles

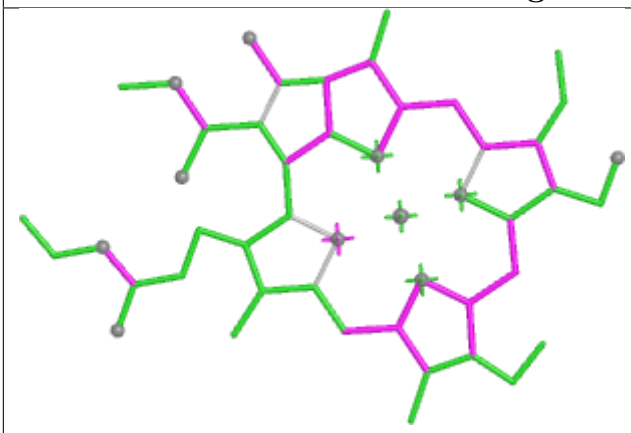


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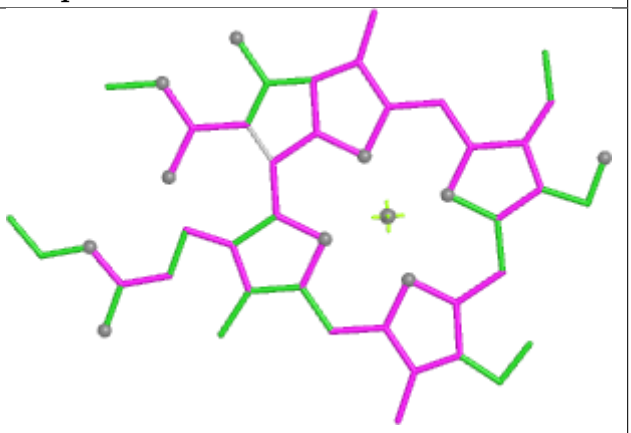


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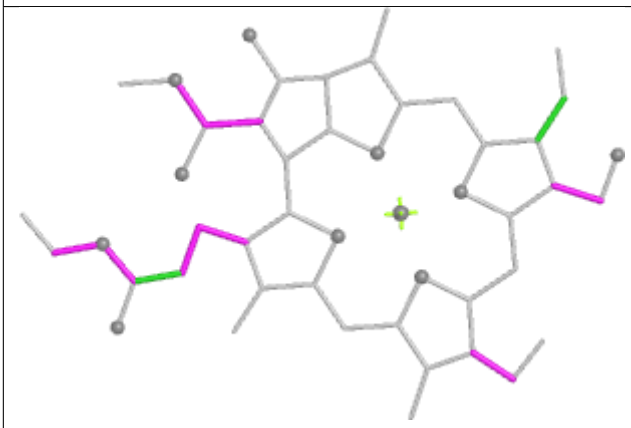
Ligand CHL q 312



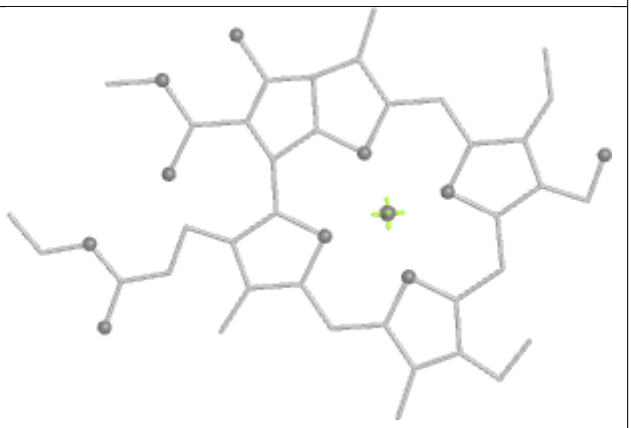
Bond lengths



Bond angles

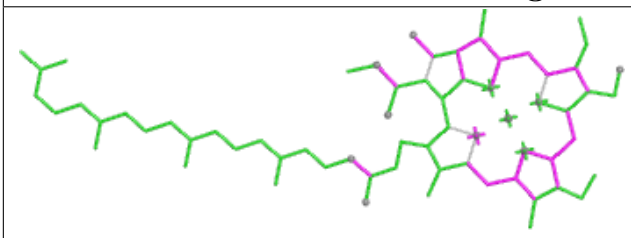


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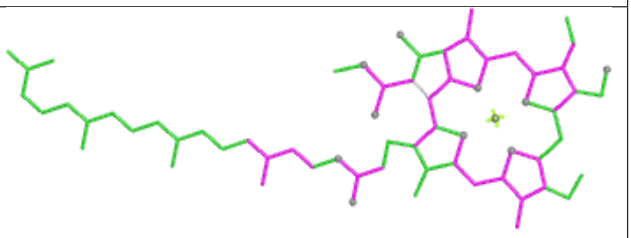


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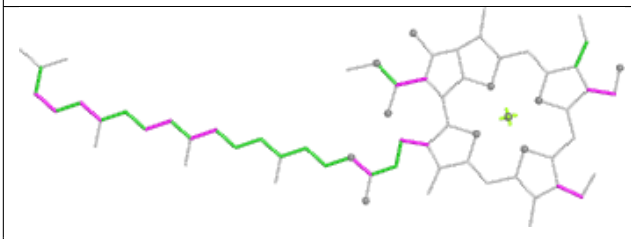
Ligand CHL u 317



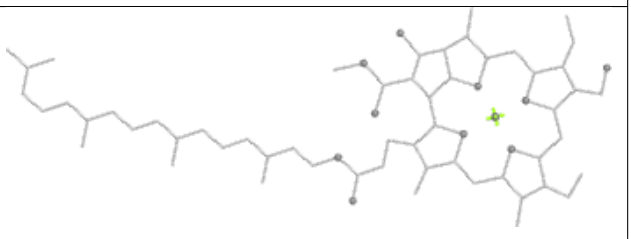
Bond lengths



Bond angles

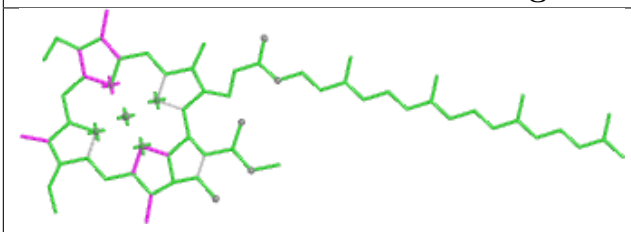


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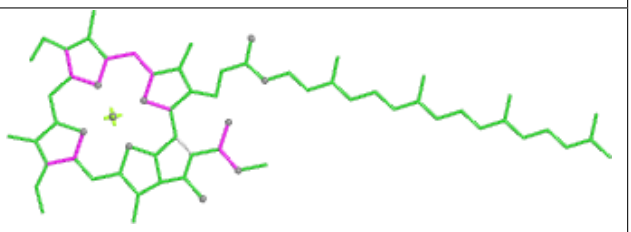


Rings

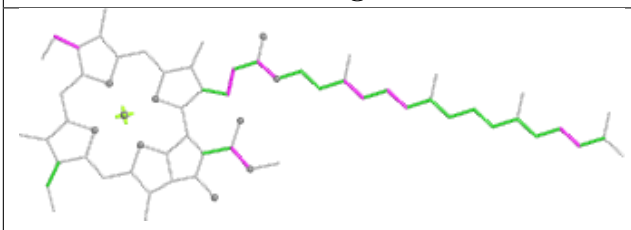
Ligand CLA c 505



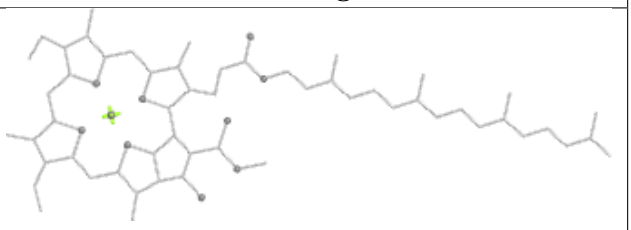
Bond lengths



Bond angles

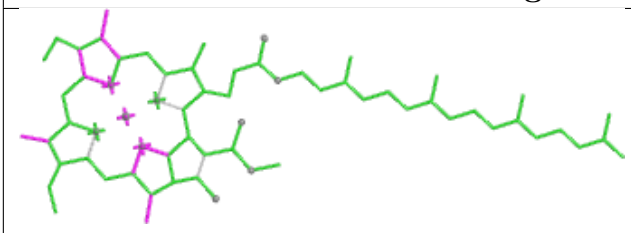


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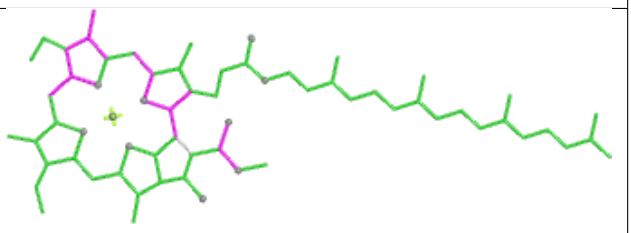


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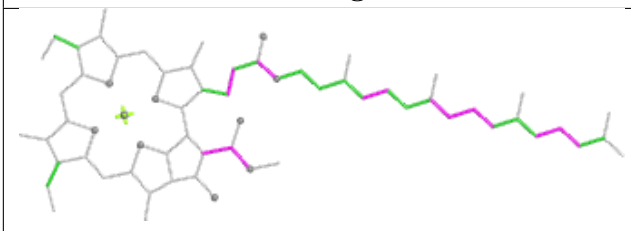
Ligand CLA B 614



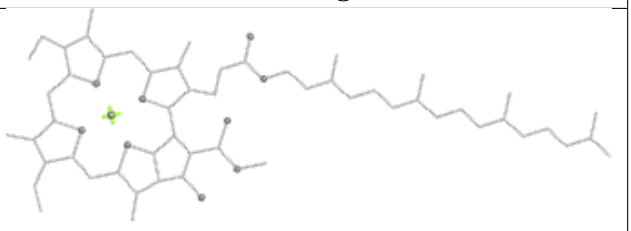
Bond lengths



Bond angles

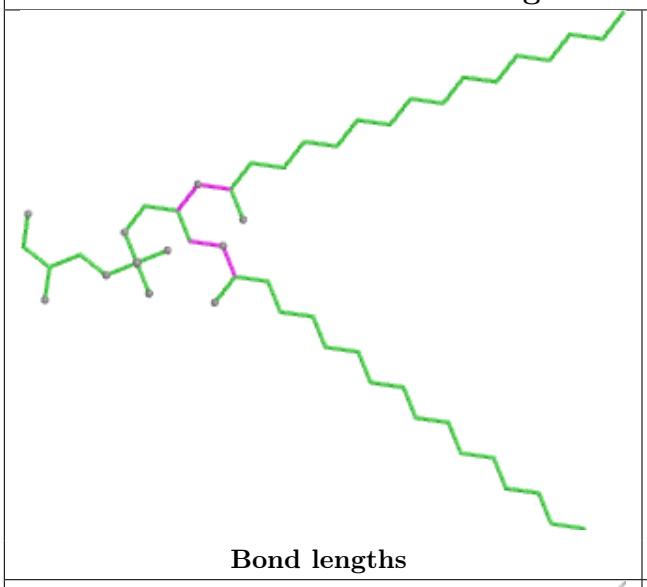


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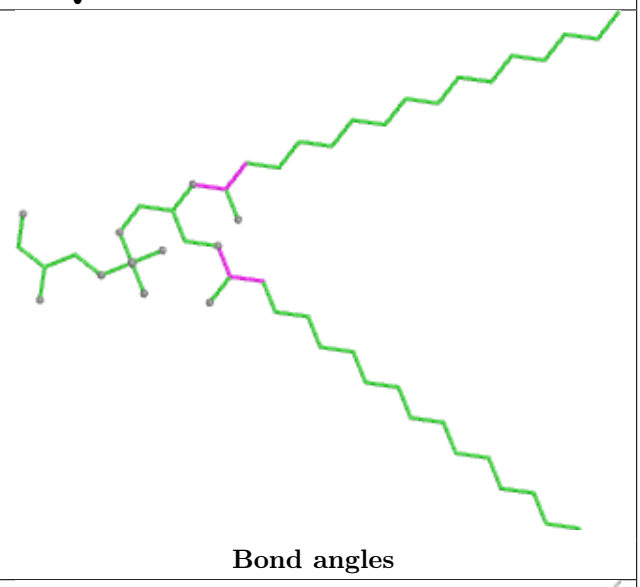


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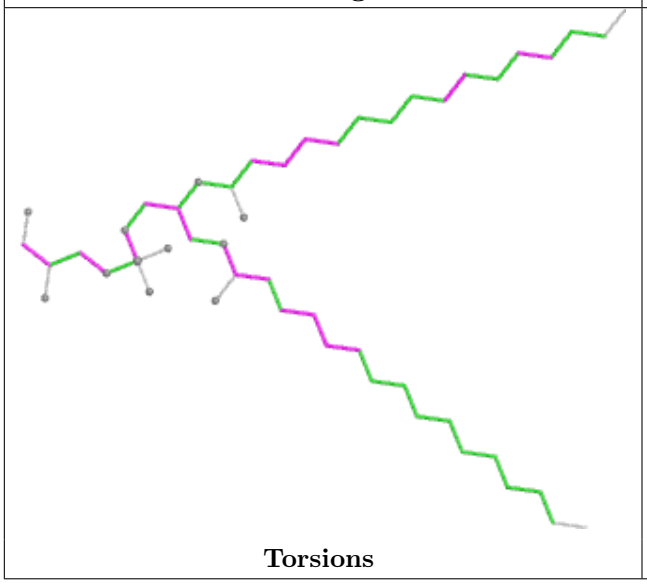
Ligand LHG Q 310



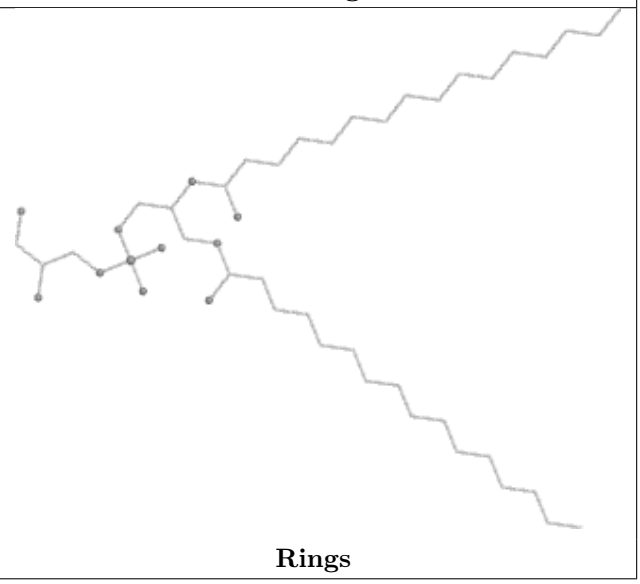
Bond lengths



Bond angles

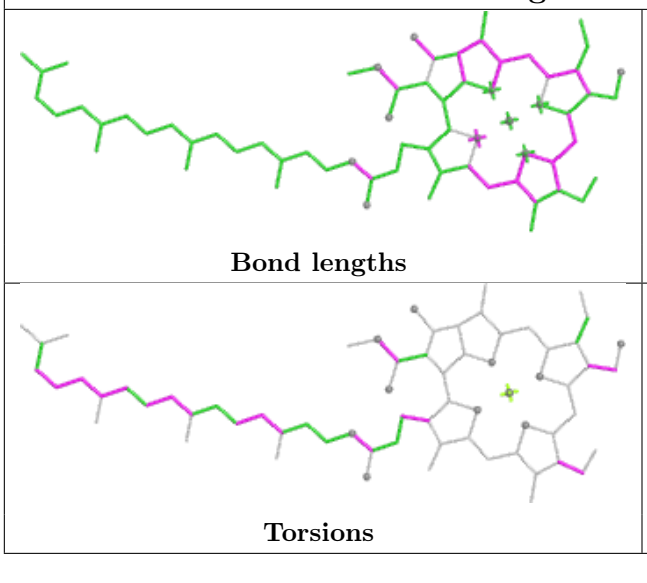


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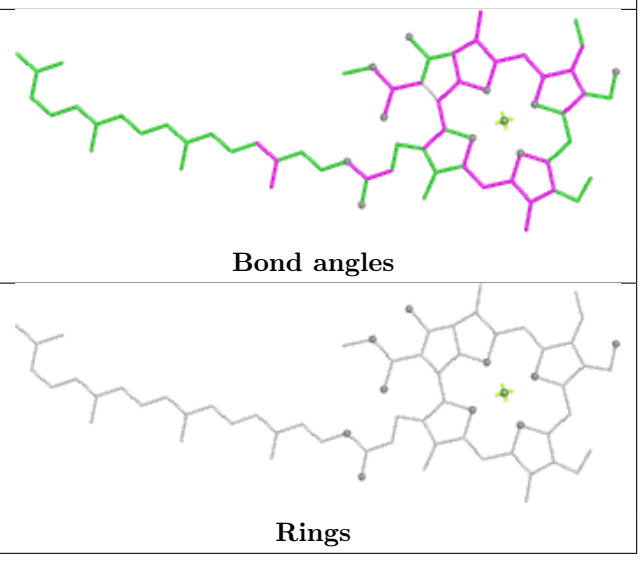


Rings

Ligand CHL 5 318



Bond lengths

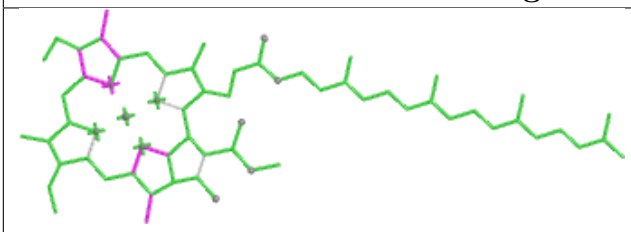


Bond angles

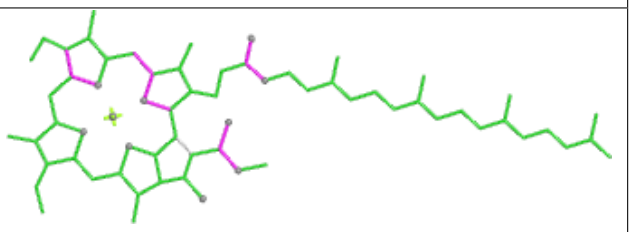
Torsions

Rings

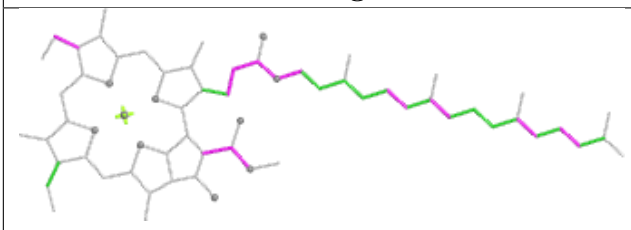
Ligand CLA G 302



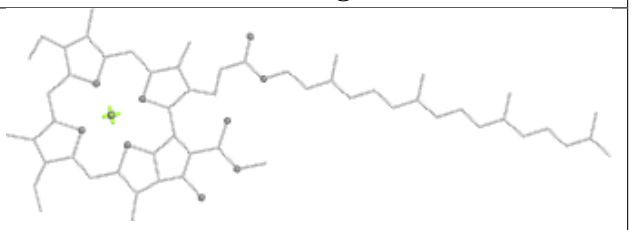
Bond lengths



Bond angles

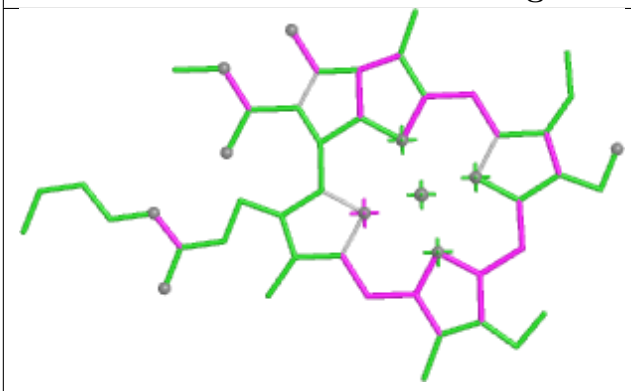


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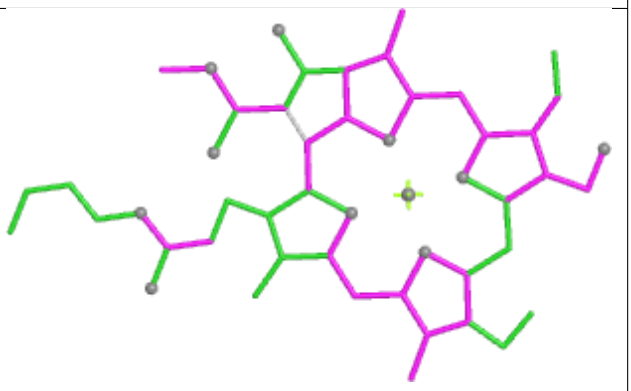


Rings

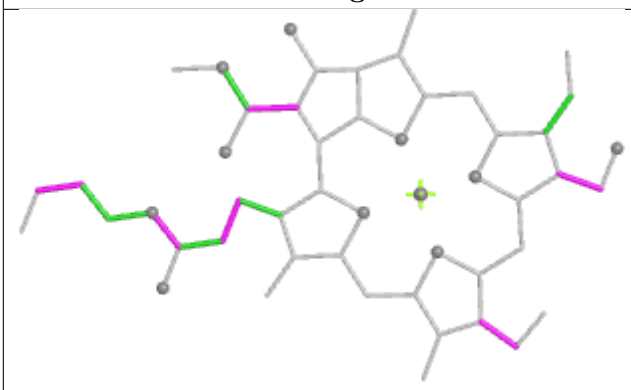
Ligand CHL u 315



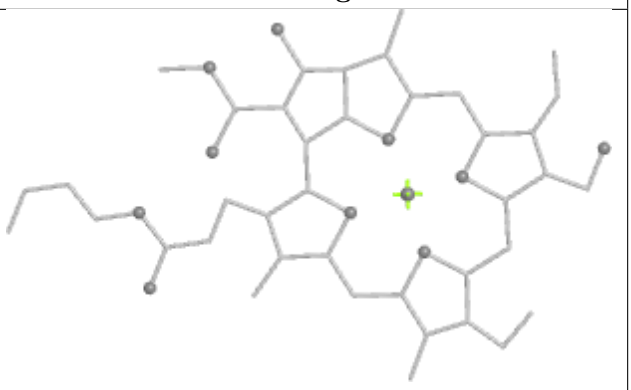
Bond lengths



Bond angles

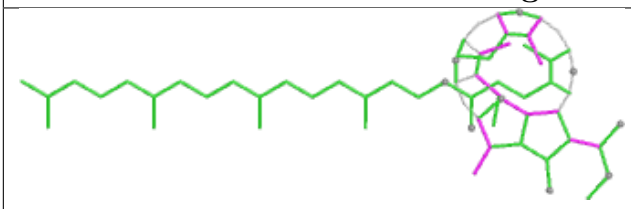


Torsions

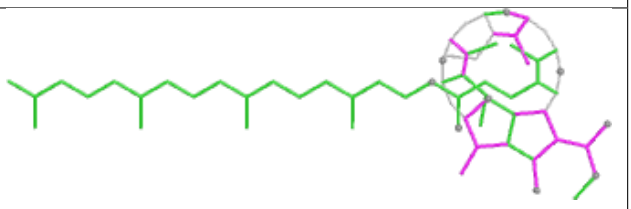


Rings

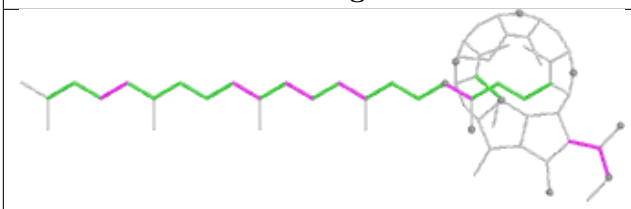
Ligand PHO A 407



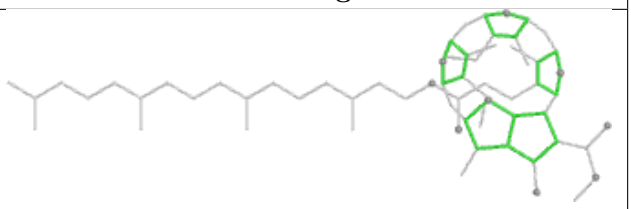
Bond lengths



Bond angles

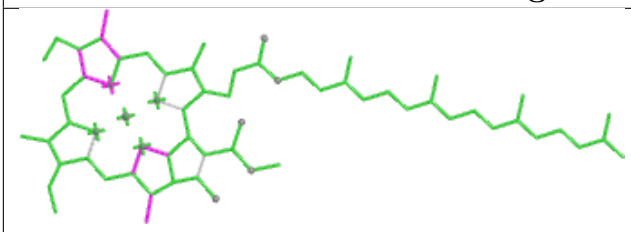


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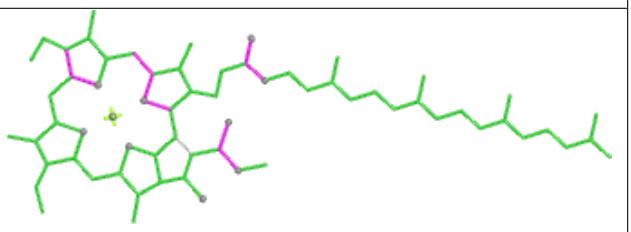


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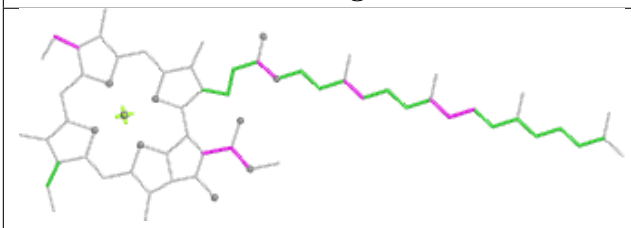
Ligand CLA 6 303



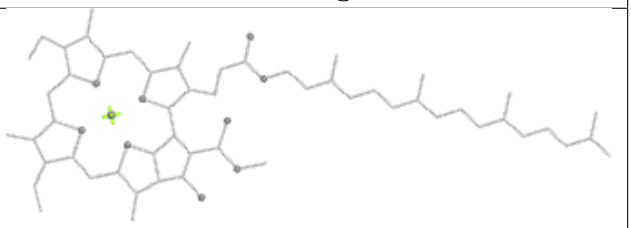
Bond lengths



Bond angles

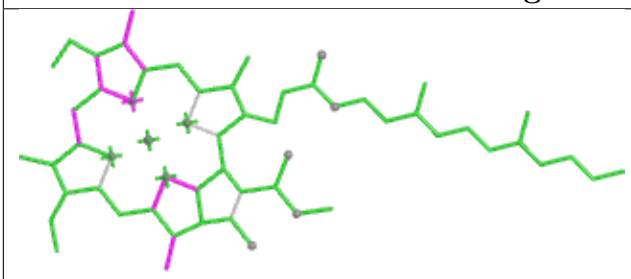


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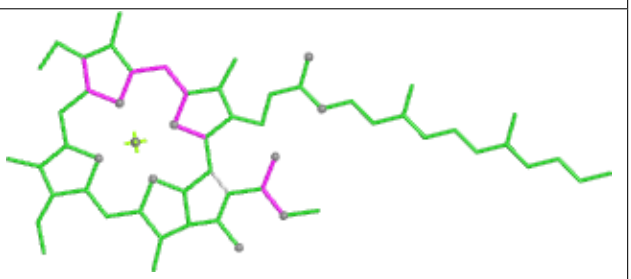


Rings

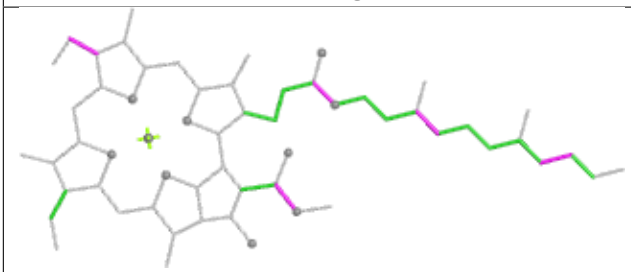
Ligand CLA R 306



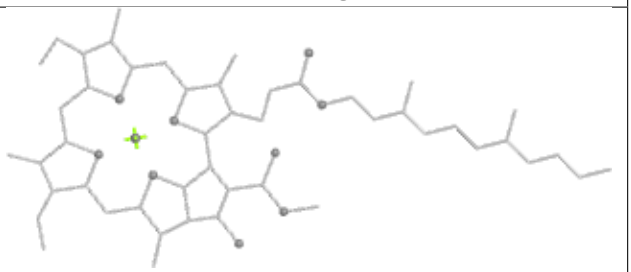
Bond lengths



Bond angles

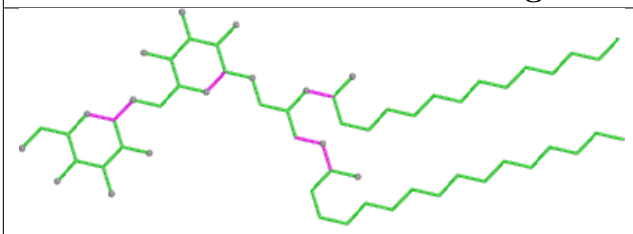


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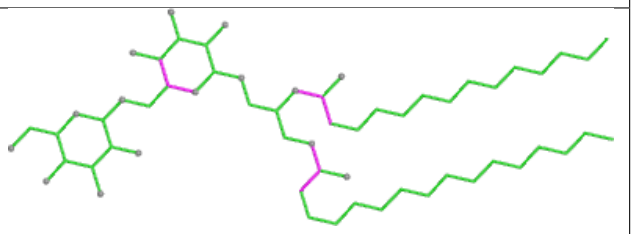


Rings

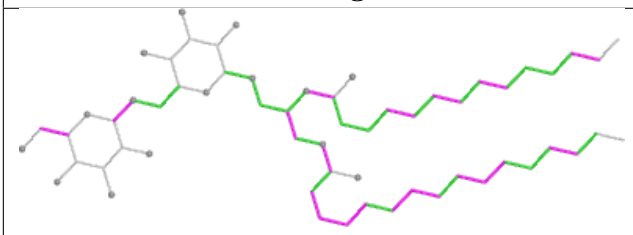
Ligand DGD c 519



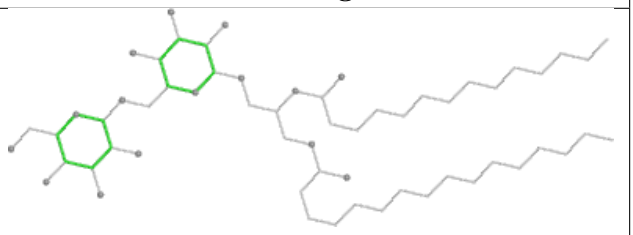
Bond lengths



Bond angles

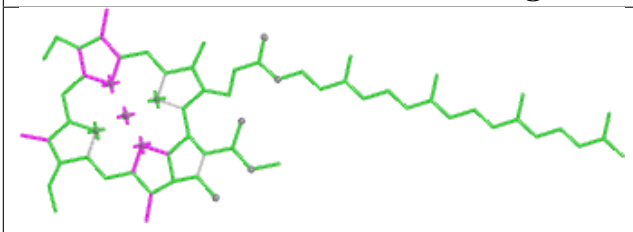


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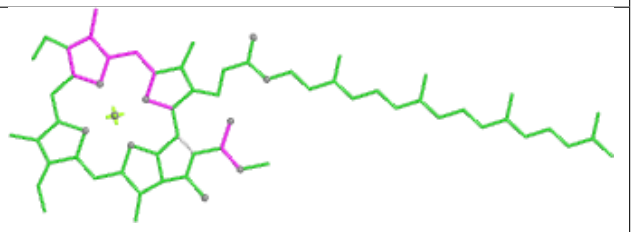


Rings

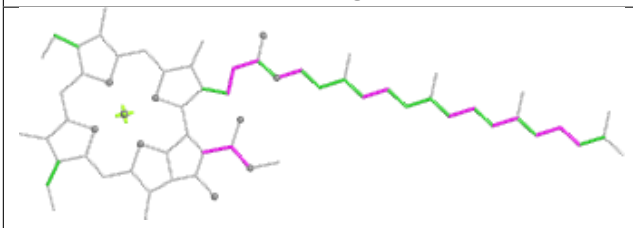
Ligand CLA B 609



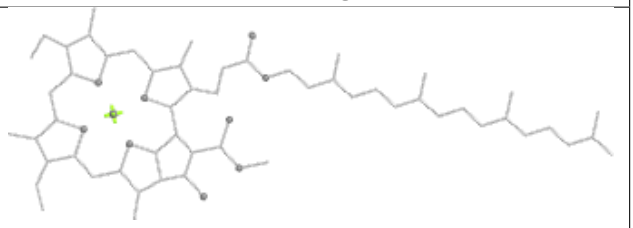
Bond lengths



Bond angles

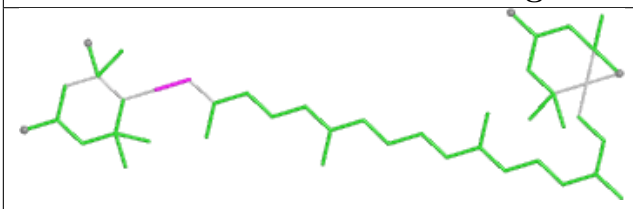


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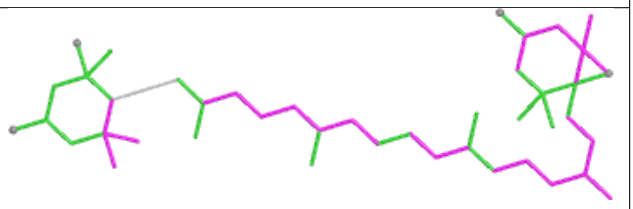


Rings

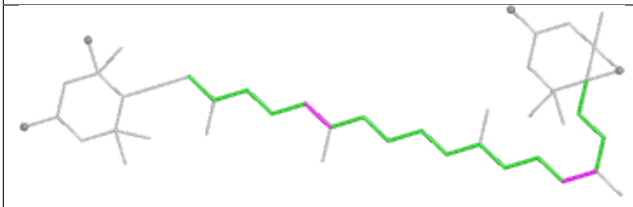
Ligand NEX v 319



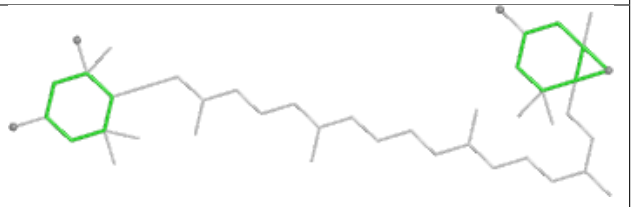
Bond lengths



Bond angles

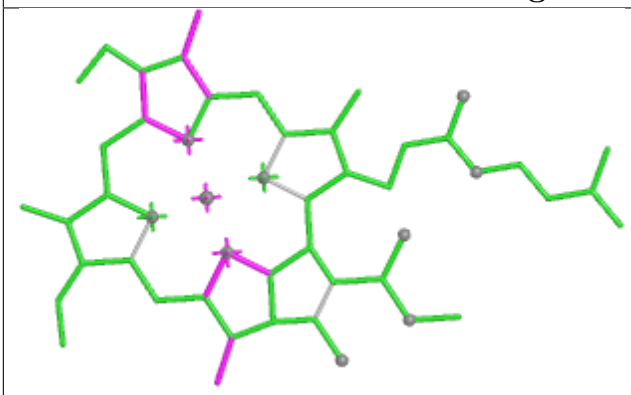


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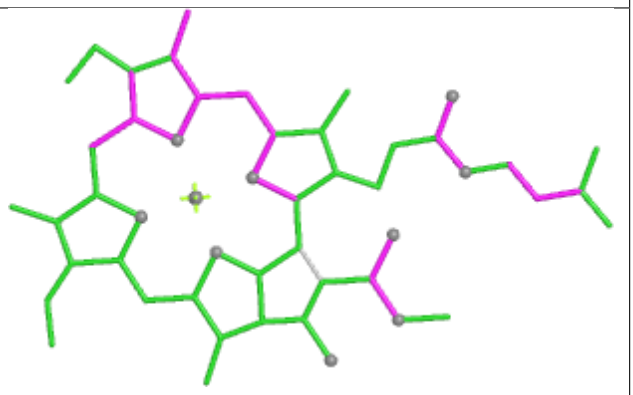


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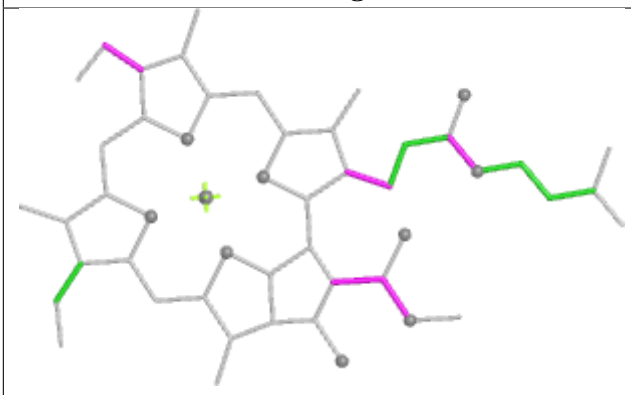
Ligand CLA 4 303



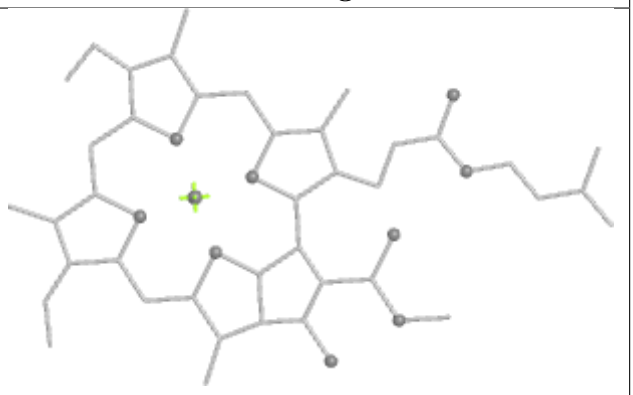
Bond lengths



Bond angles

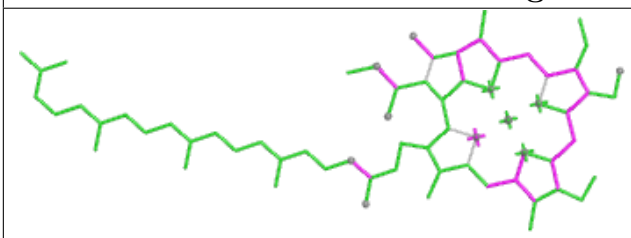


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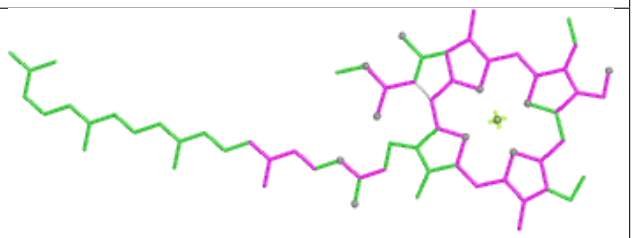


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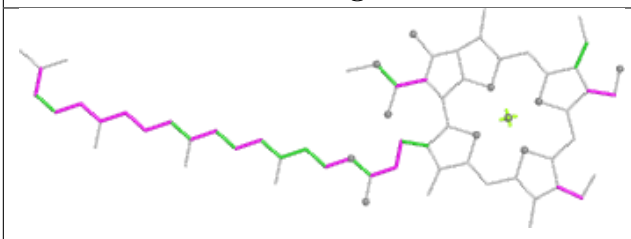
Ligand CHL n 313



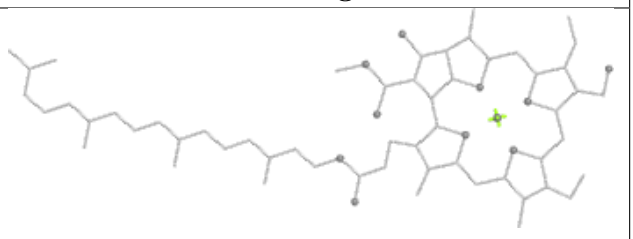
Bond lengths



Bond angles

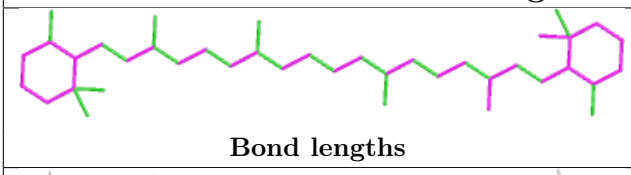


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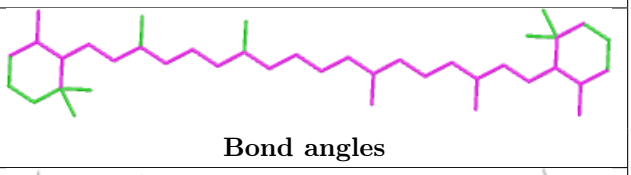


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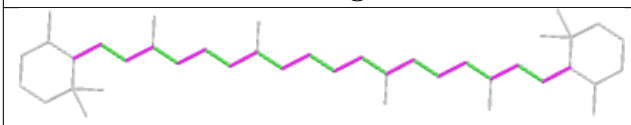
Ligand BCR c 515



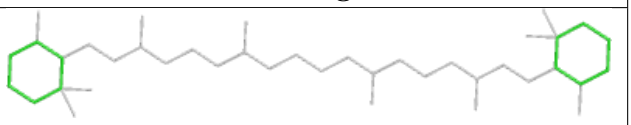
Bond lengths



Bond angles

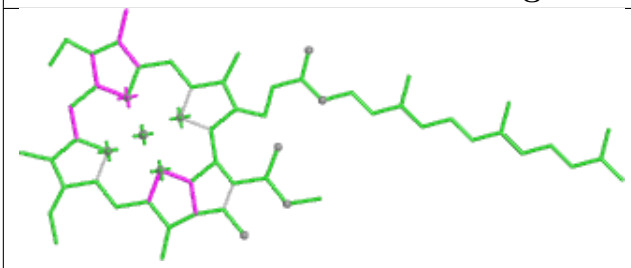


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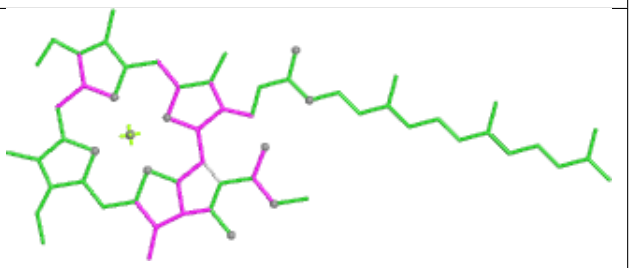


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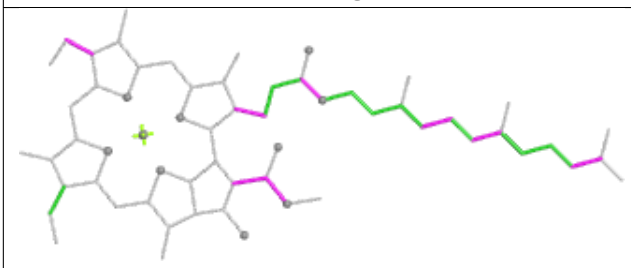
Ligand CLA N 305



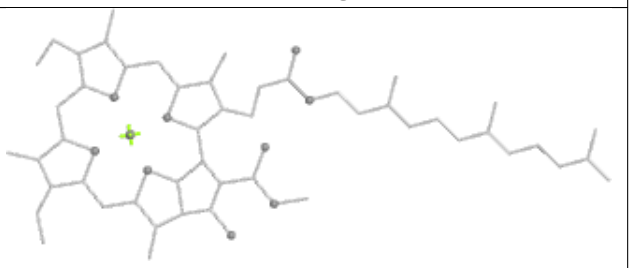
Bond lengths



Bond angles

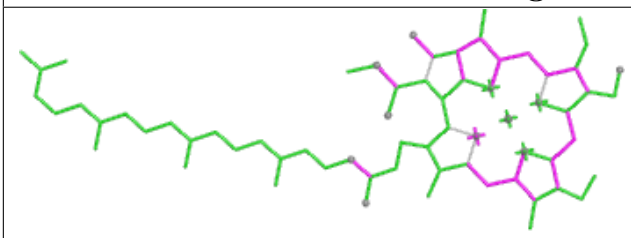


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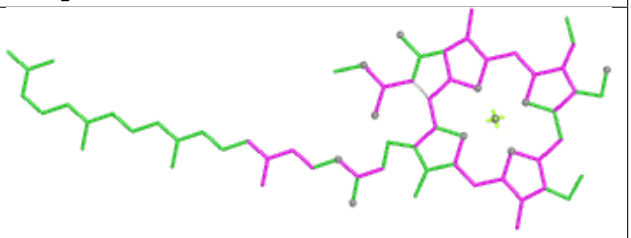


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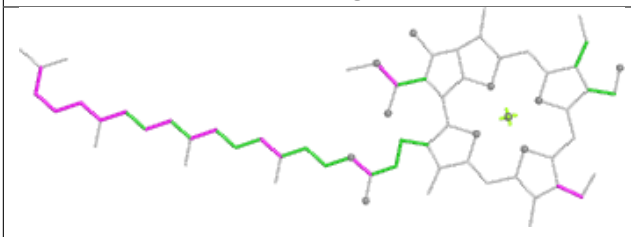
Ligand CHL q 311



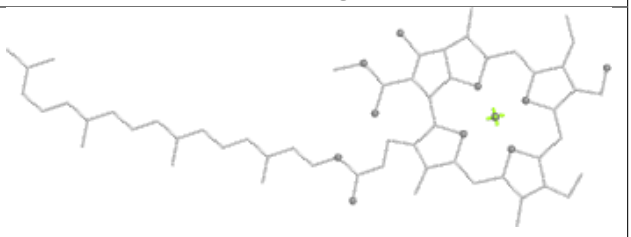
Bond lengths



Bond angles

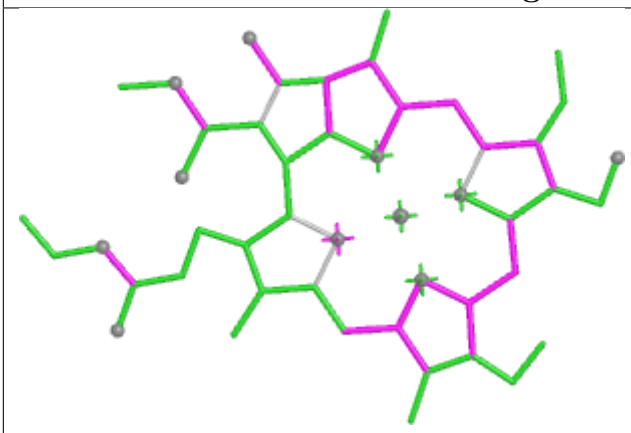


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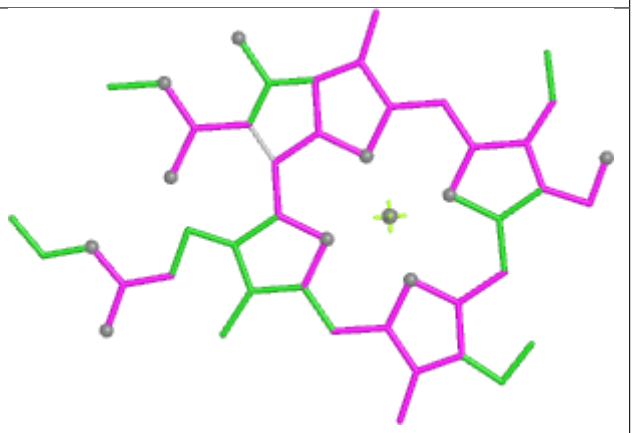


Rings

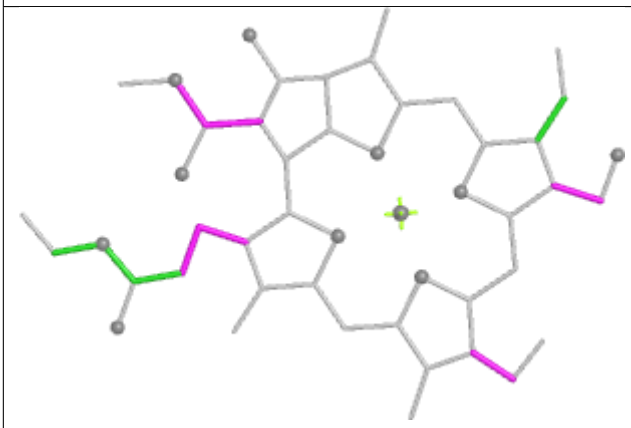
Ligand CHL N 314



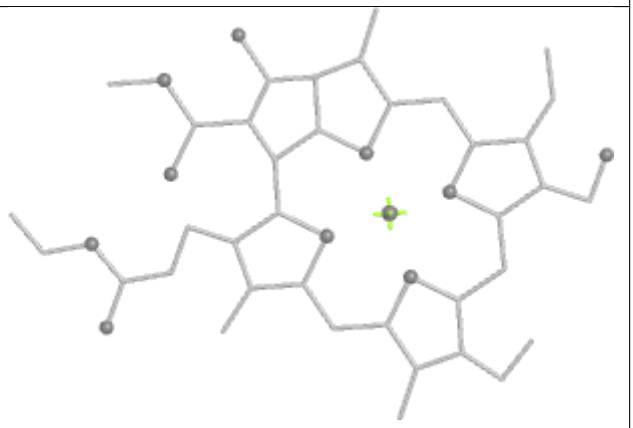
Bond lengths



Bond angles

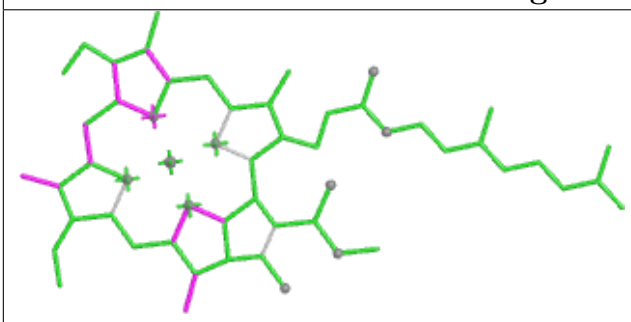


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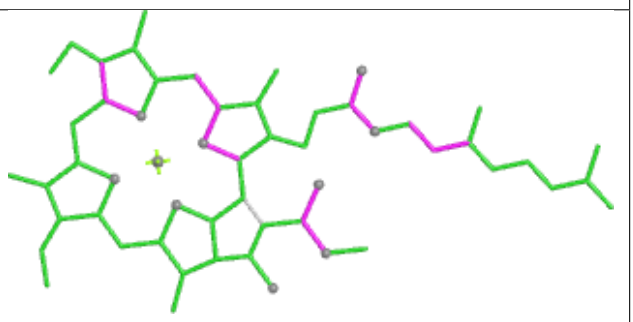


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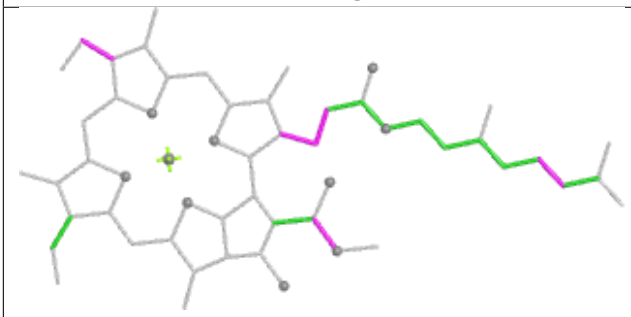
Ligand CLA s 305



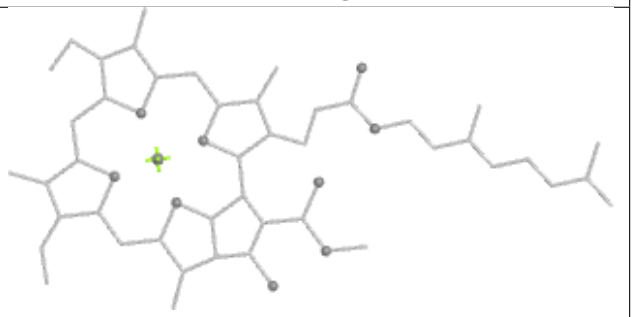
Bond lengths



Bond angles

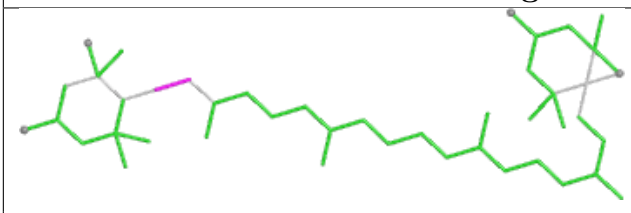


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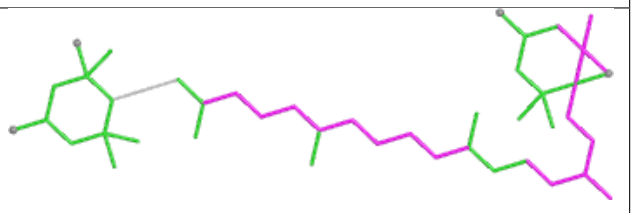


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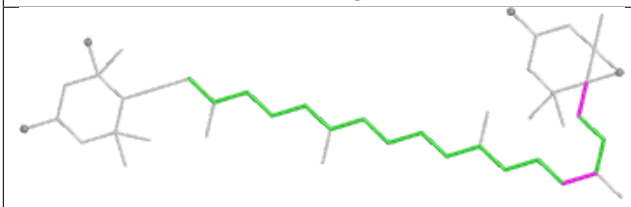
Ligand NEX U 318



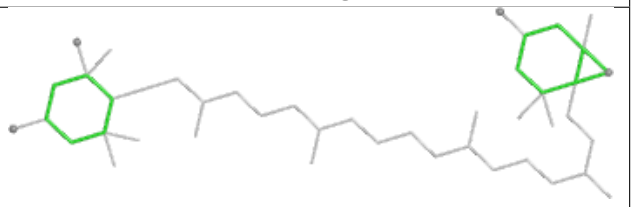
Bond lengths



Bond angles



Torsions

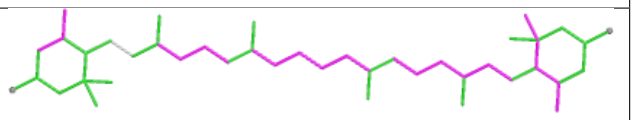


Rings

Ligand LUT R 312



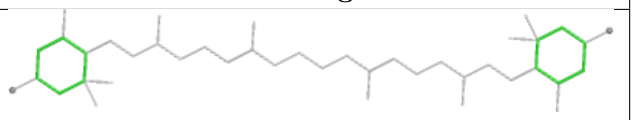
Bond lengths



Bond angles

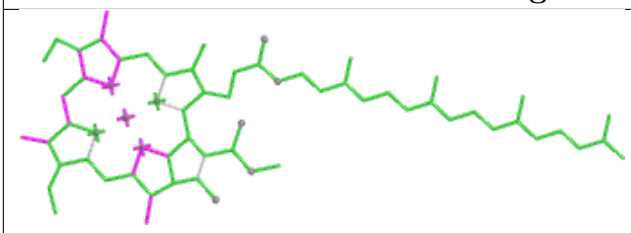


Torsions

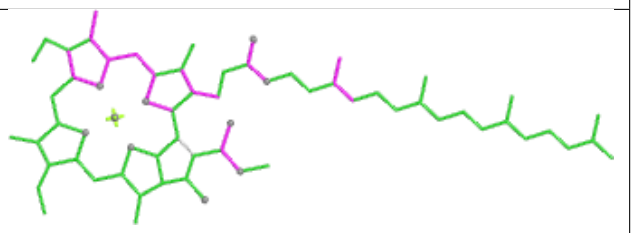


Rings

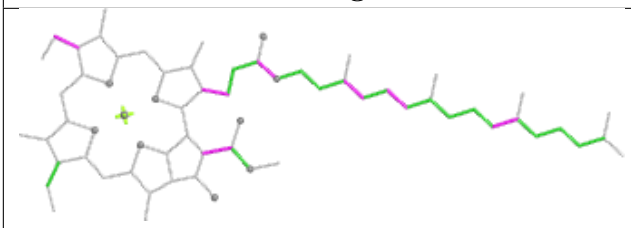
Ligand CLA c 509



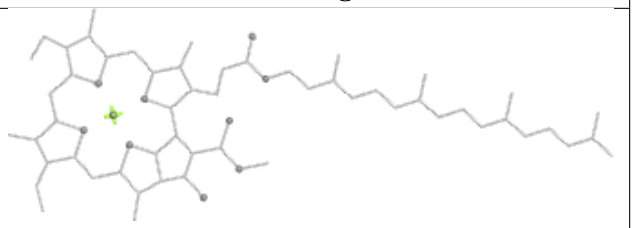
Bond lengths



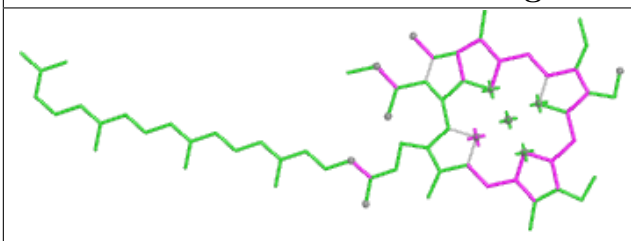
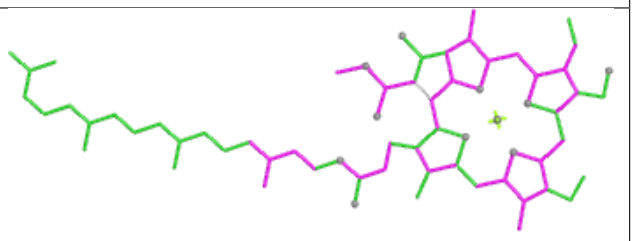
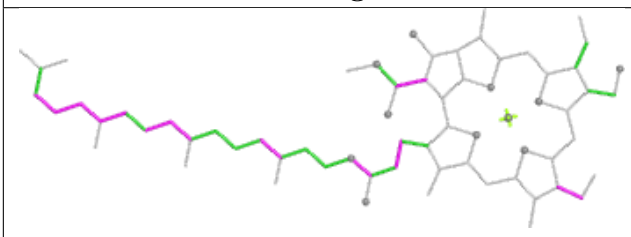
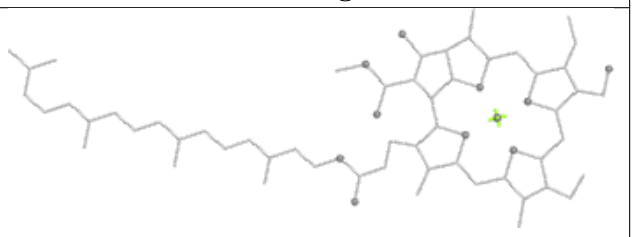
Bond angles

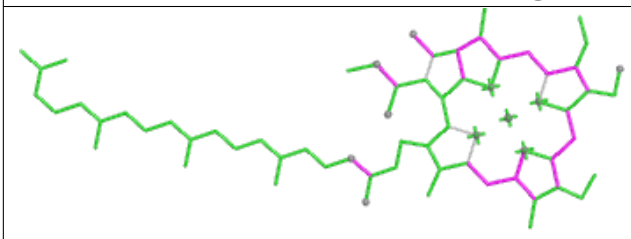
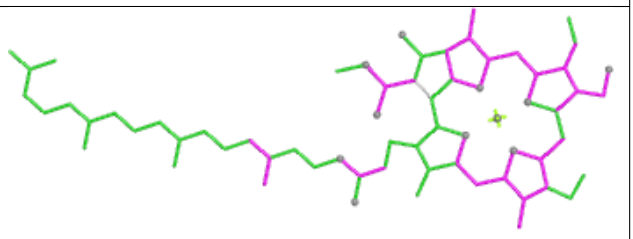
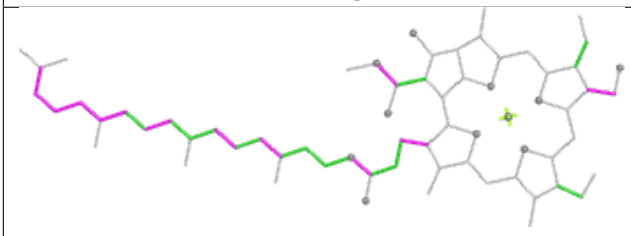
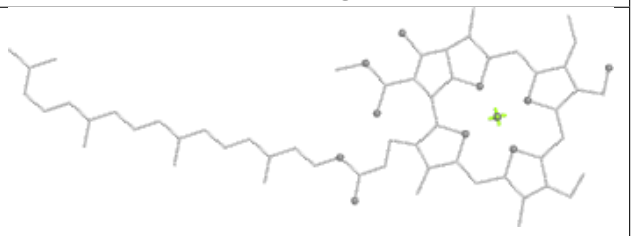


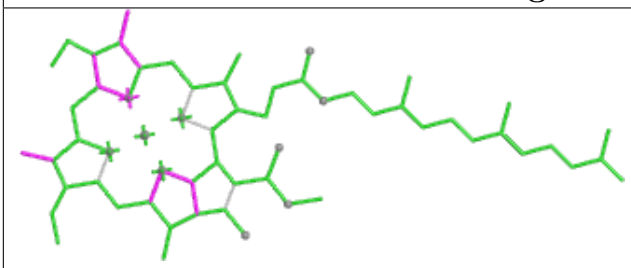
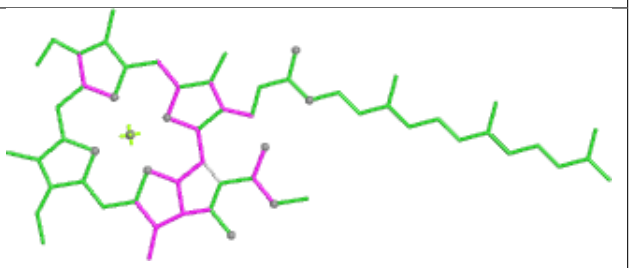
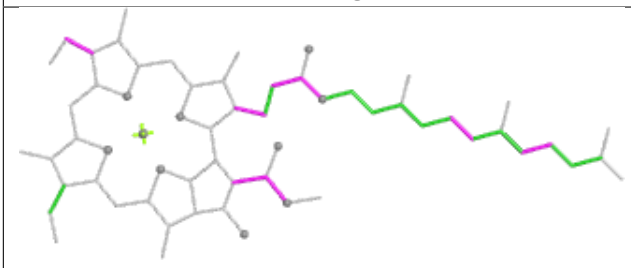
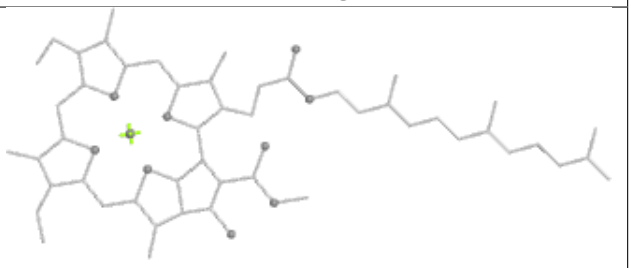
Torsions

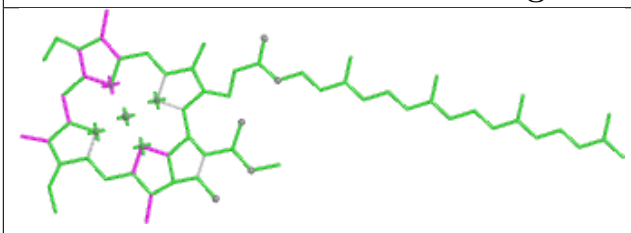
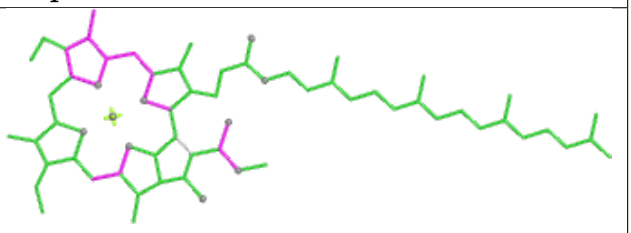
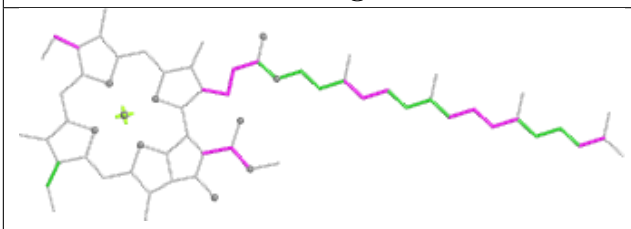
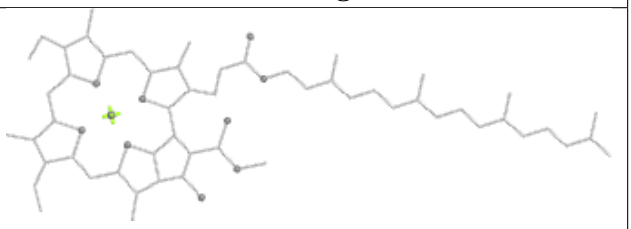


Rings

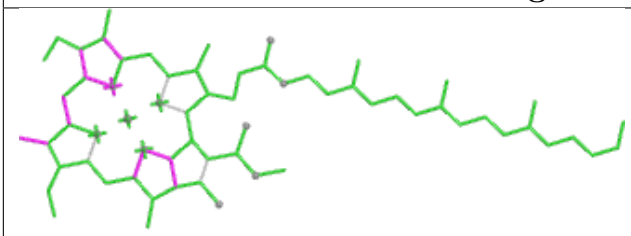
Ligand CHL P 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

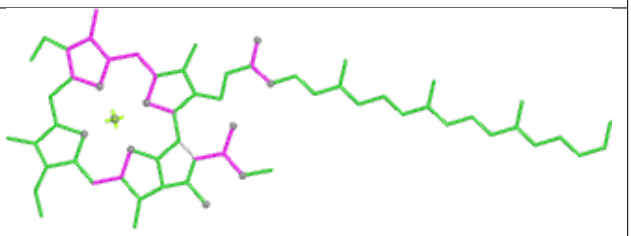
Ligand CLA 5 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

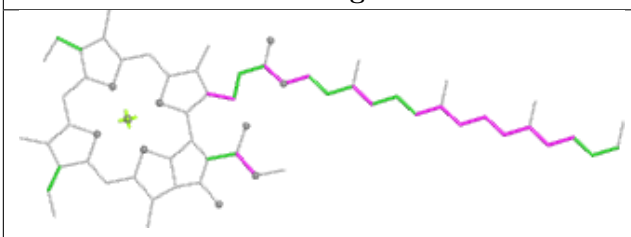
Ligand CLA 6 305



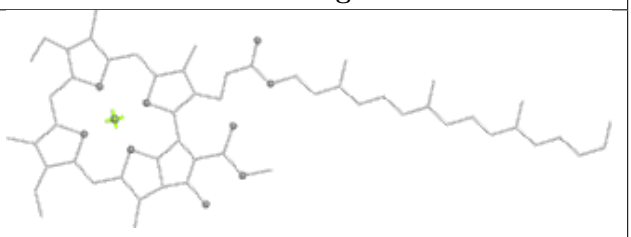
Bond lengths



Bond angles

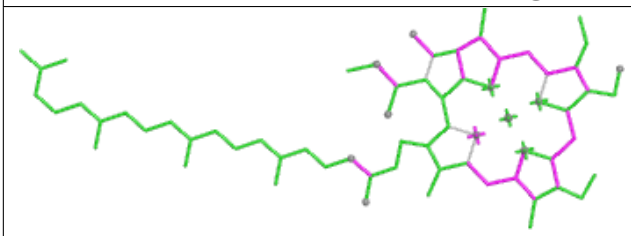


Torsions

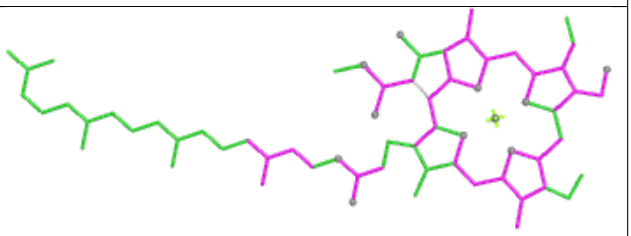


Rings

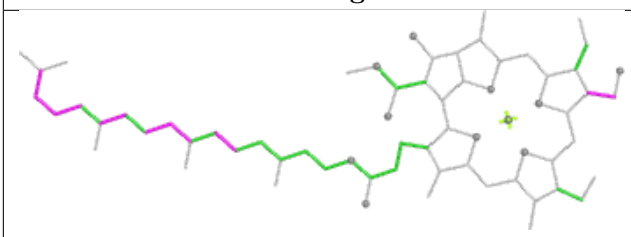
Ligand CHL v 317



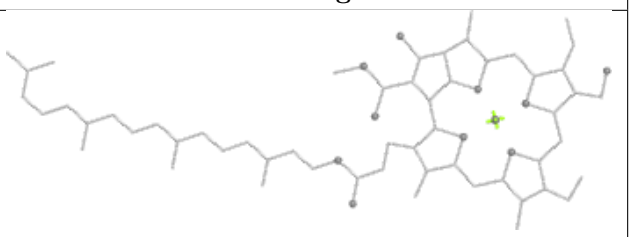
Bond lengths



Bond angles

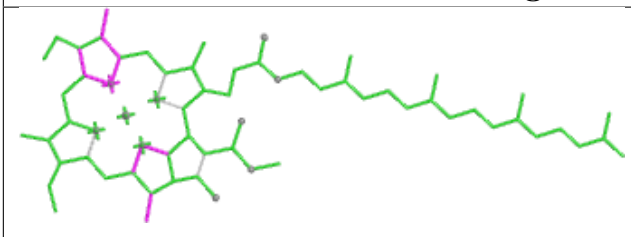


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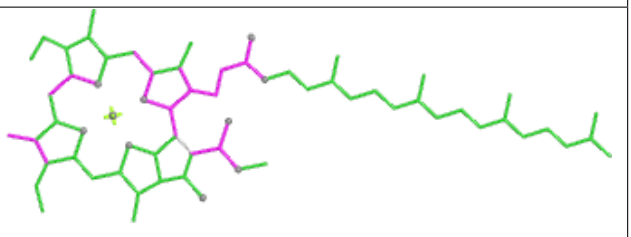


Rings

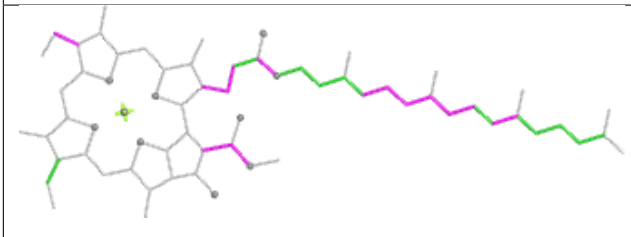
Ligand CLA B 605



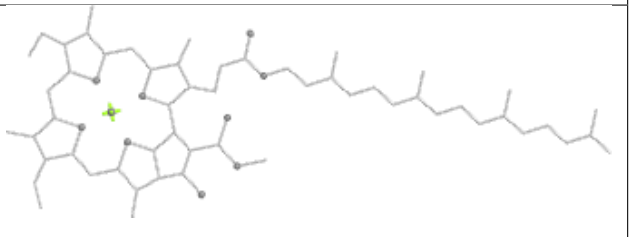
Bond lengths



Bond angles

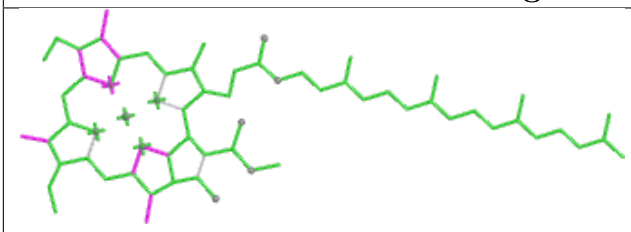


Torsions

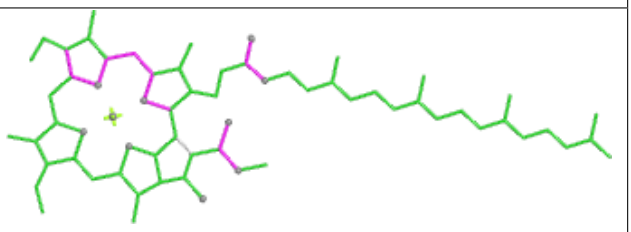


Rings

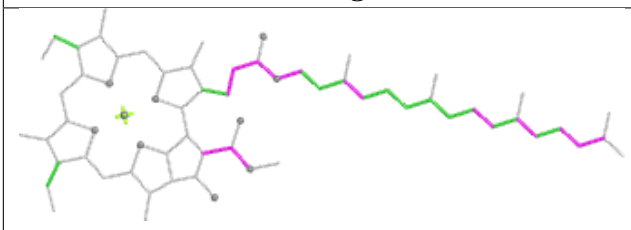
Ligand CLA N 302



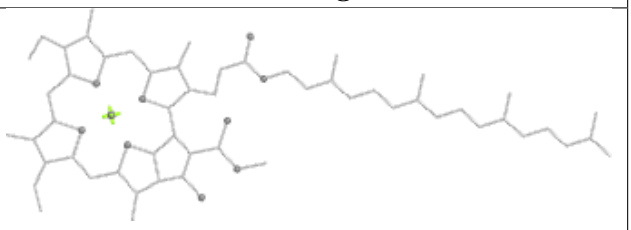
Bond lengths



Bond angles

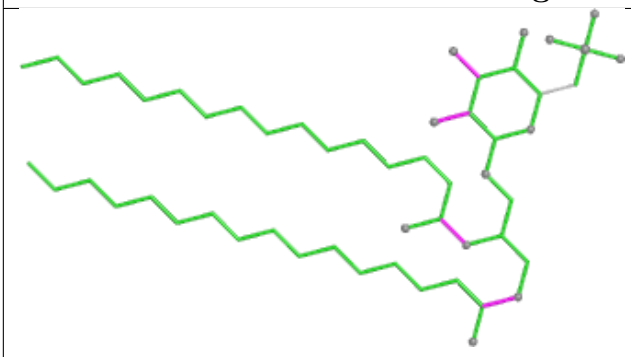


Torsions

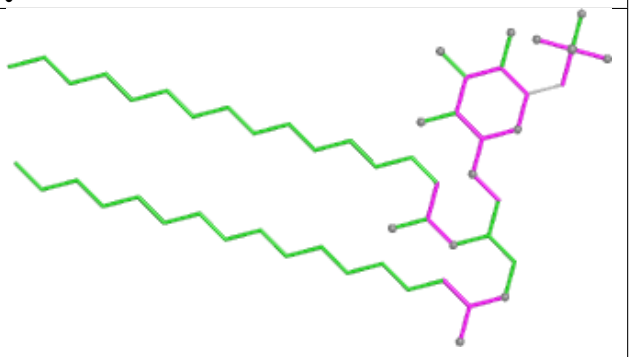


Rings

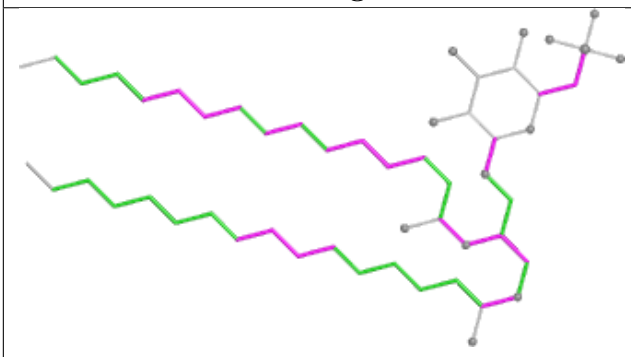
Ligand SQD l 102



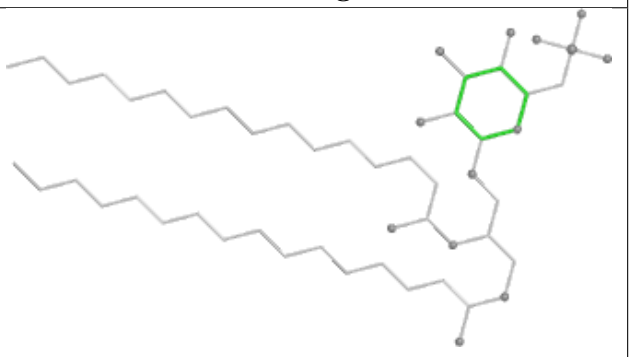
Bond lengths



Bond angles

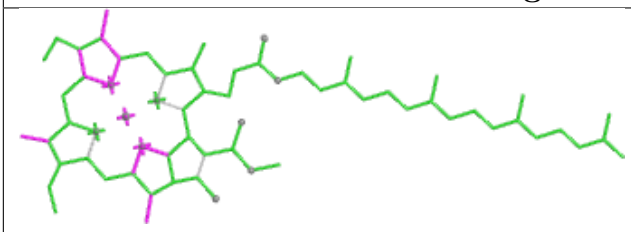


Torsions

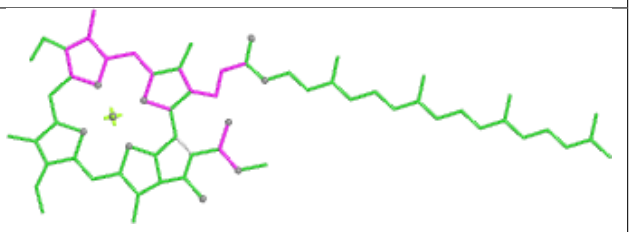


Rings

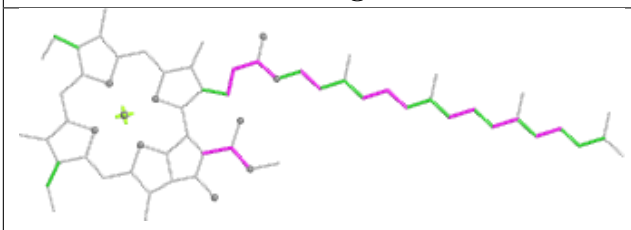
Ligand CLA A 404



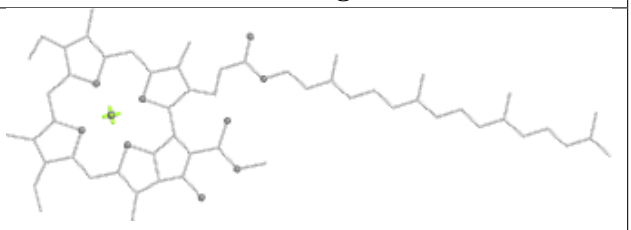
Bond lengths



Bond angles

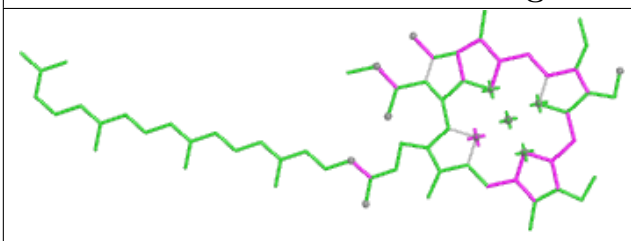


Torsions

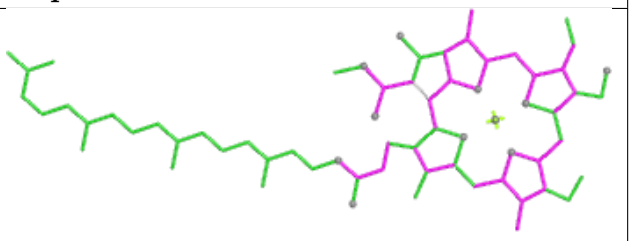


Rings

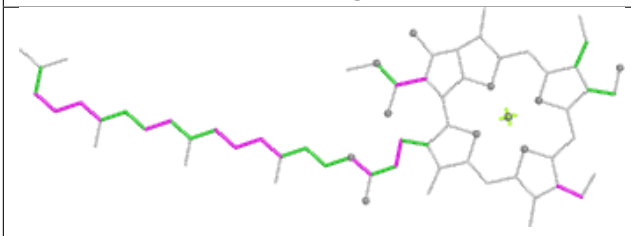
Ligand CHL p 317



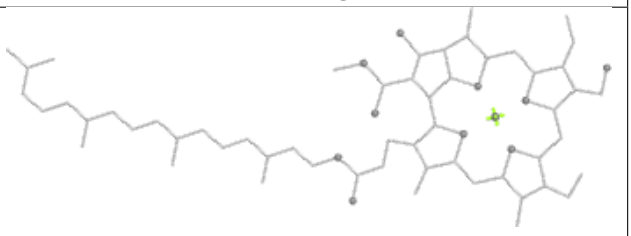
Bond lengths



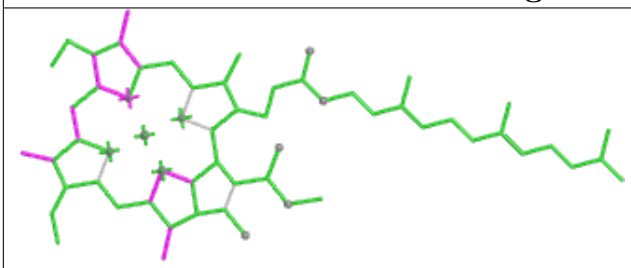
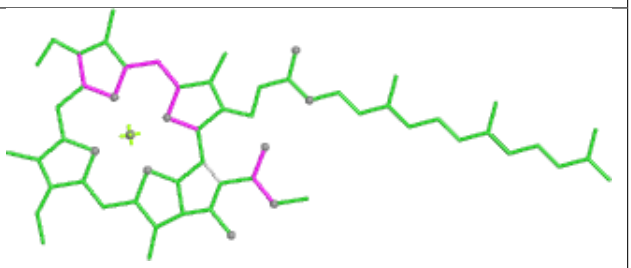
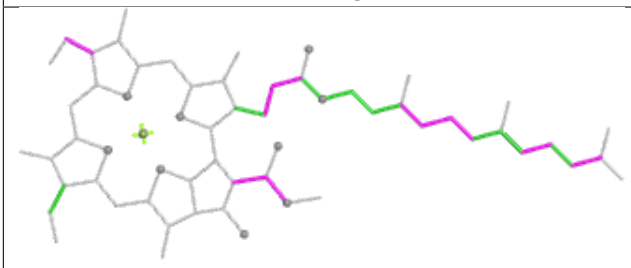
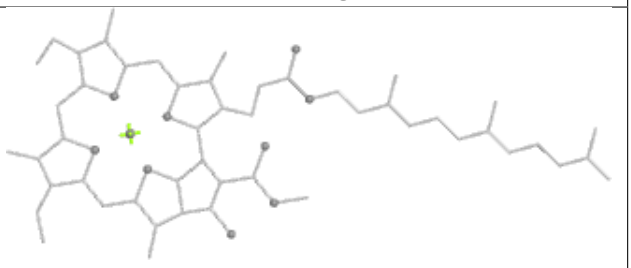
Bond angles

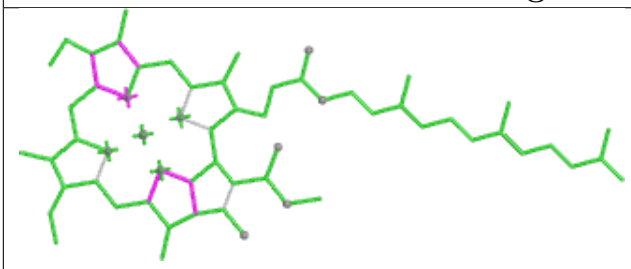
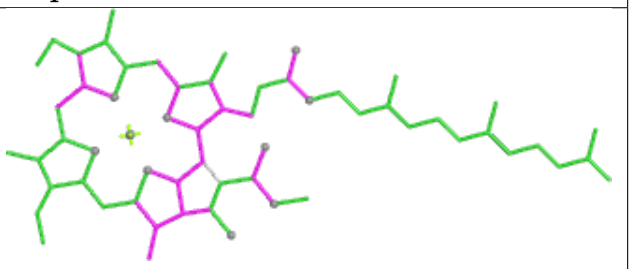
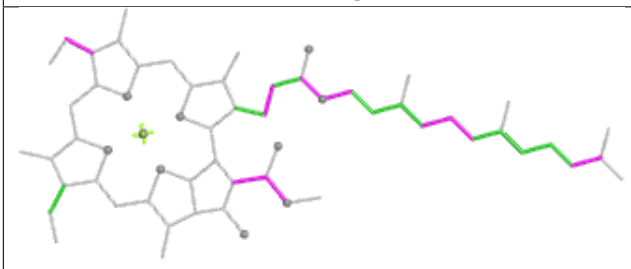
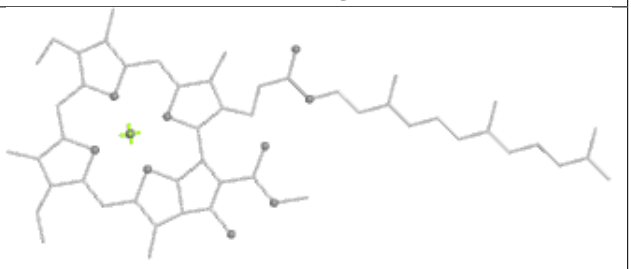


Torsions

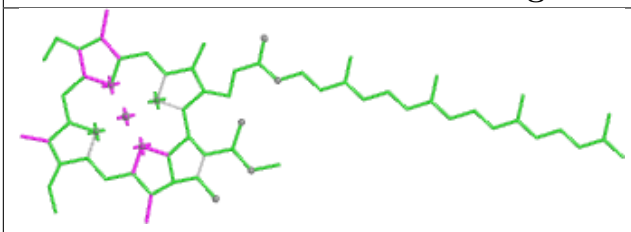


Rings

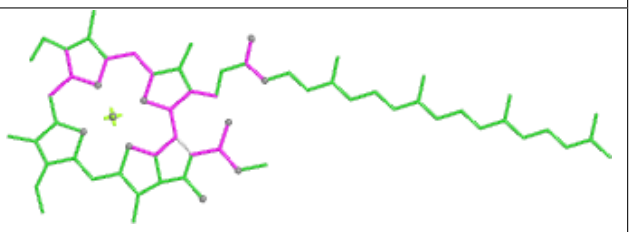
Ligand CLA P 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

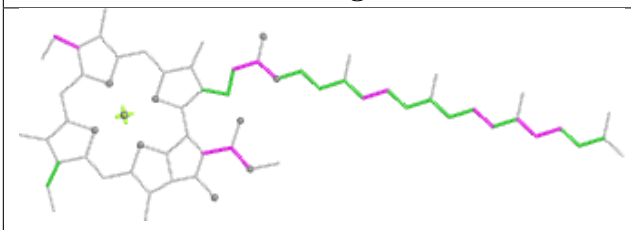
Ligand CLA b 617



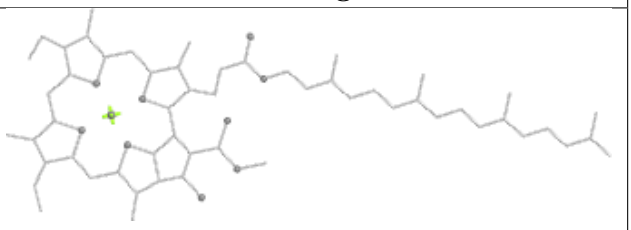
Bond lengths



Bond angles

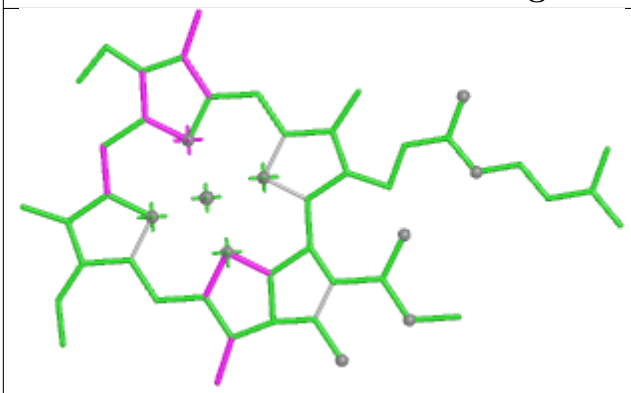


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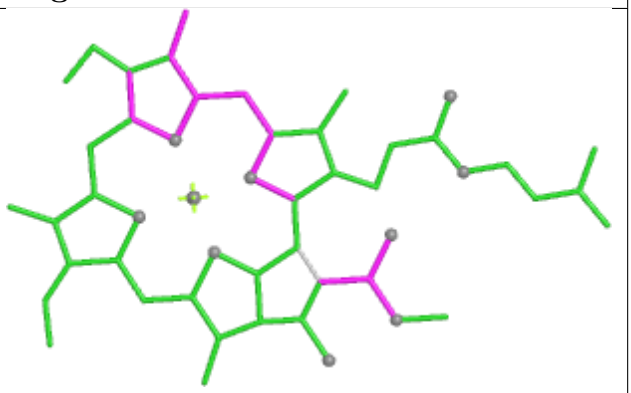


Rings

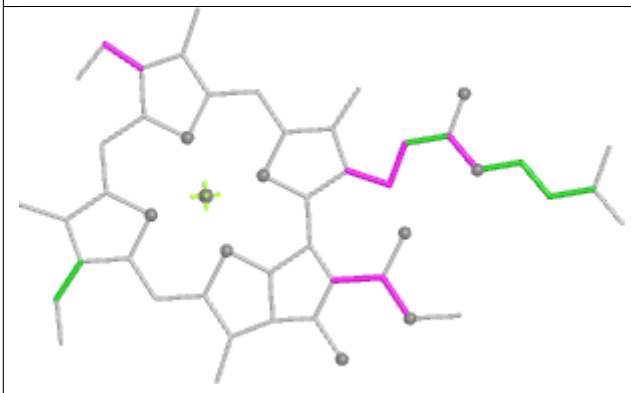
Ligand CLA g 303



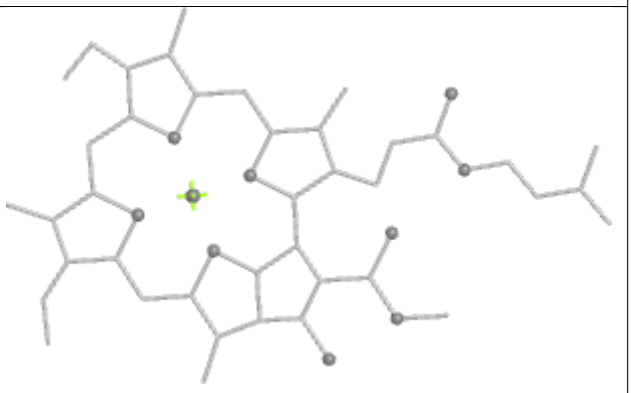
Bond lengths



Bond angles

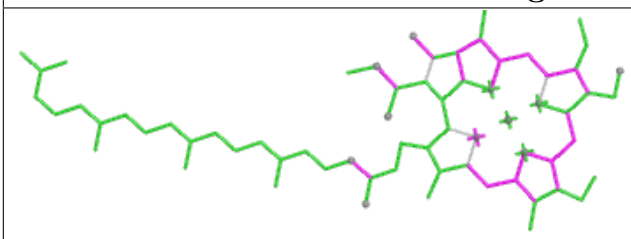


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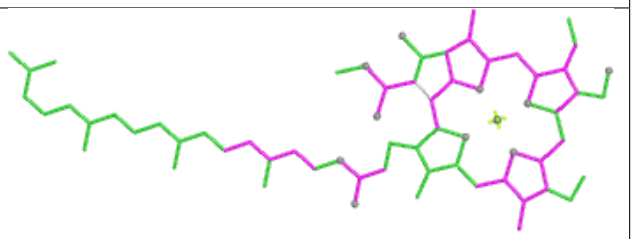


Rings

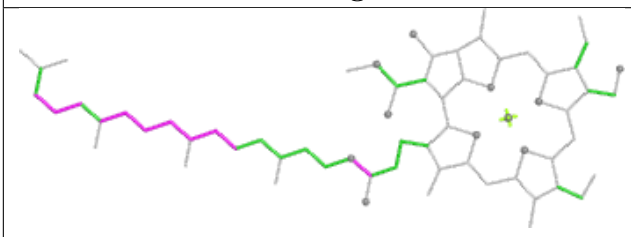
Ligand CHL 1 313



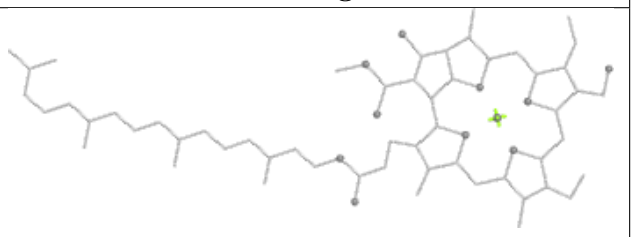
Bond lengths



Bond angles

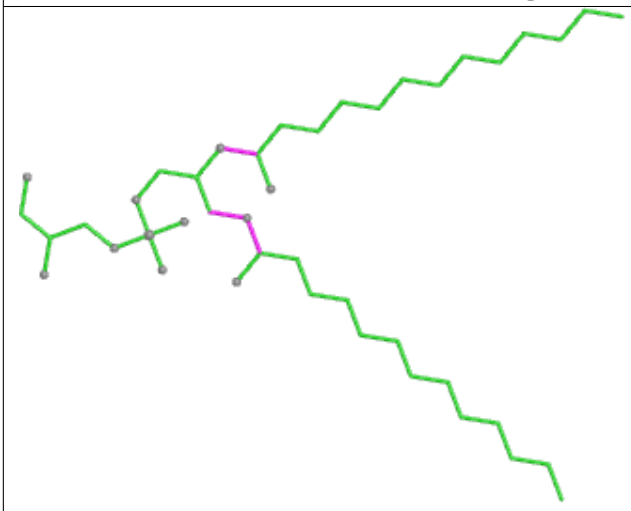


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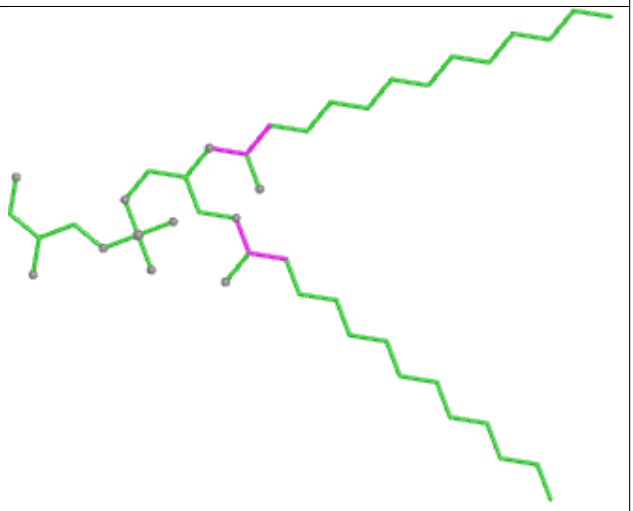


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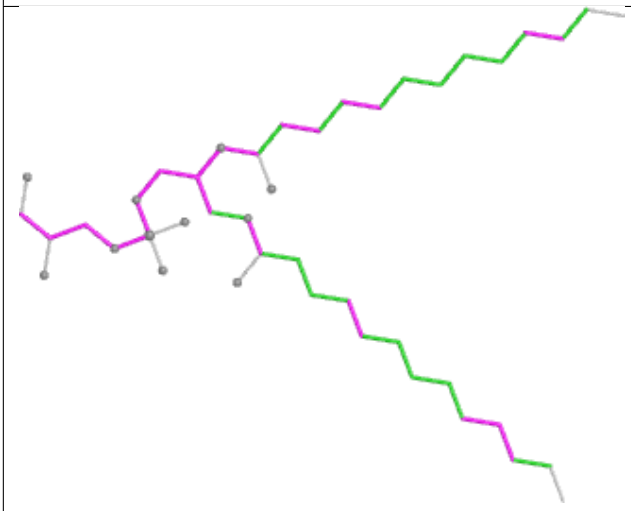
Ligand LHG A 413



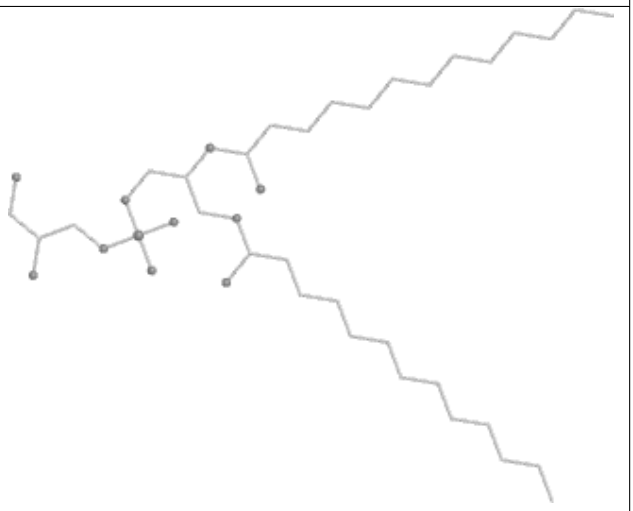
Bond lengths



Bond angles

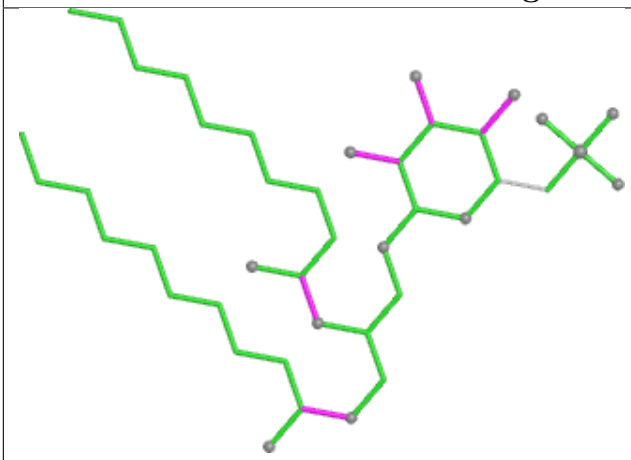


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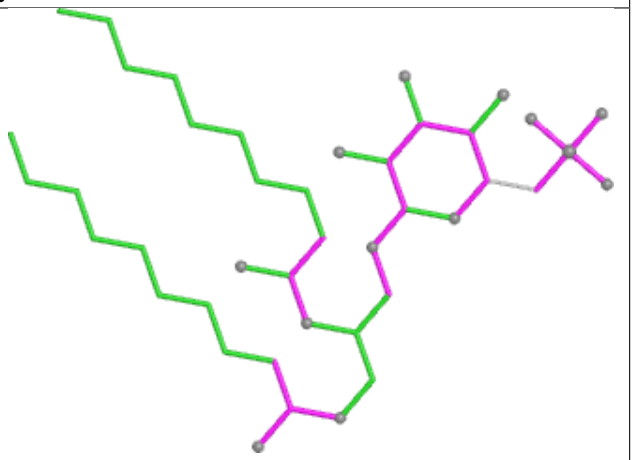


Rings

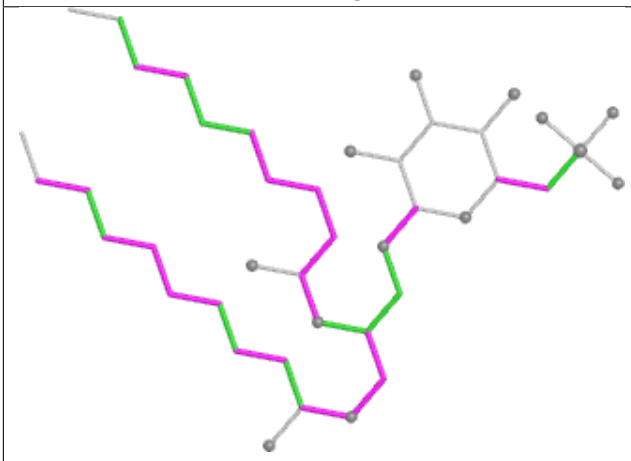
Ligand SQD m 101



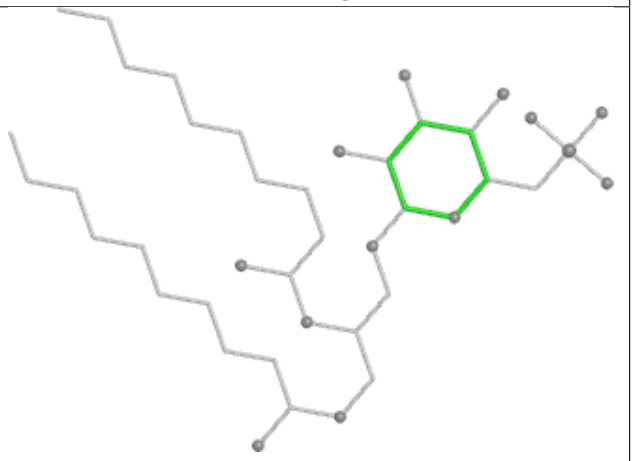
Bond lengths



Bond angles

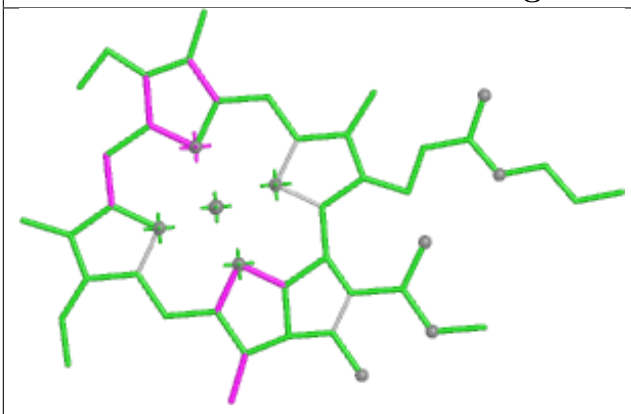


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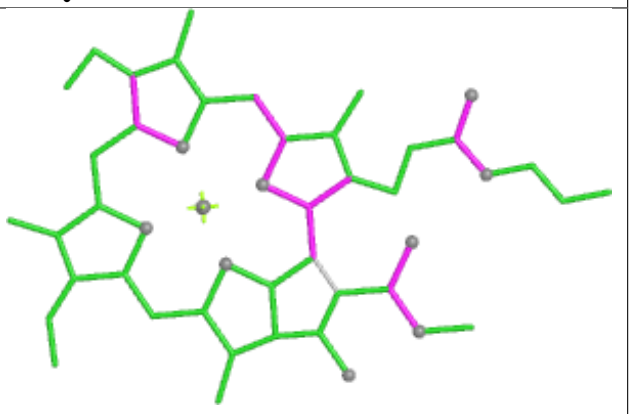


Rings

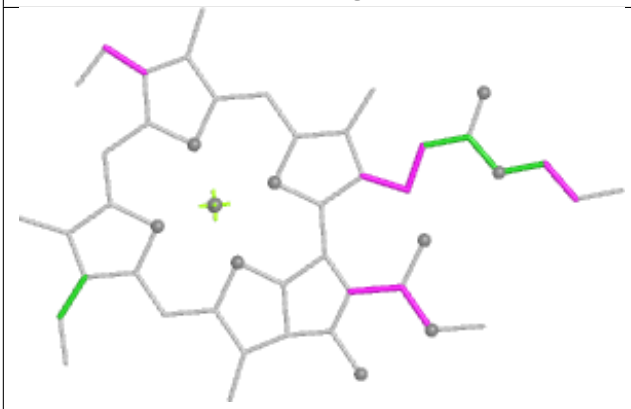
Ligand CLA Q 308



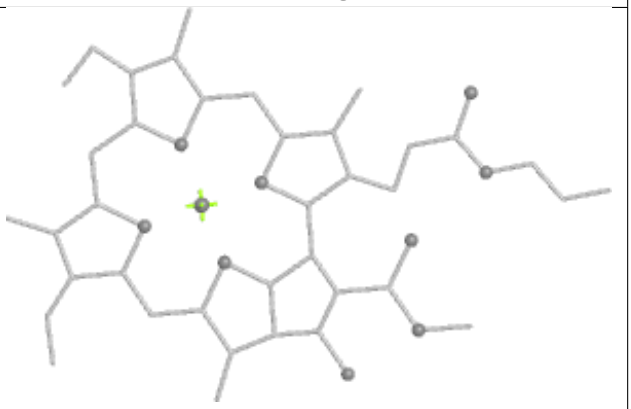
Bond lengths



Bond angles

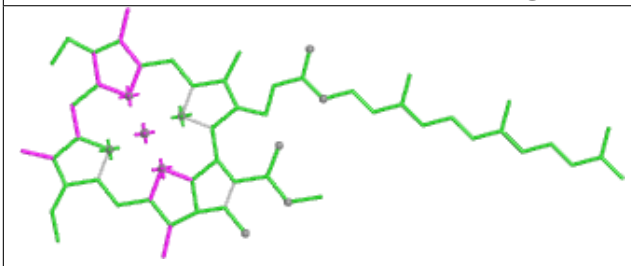


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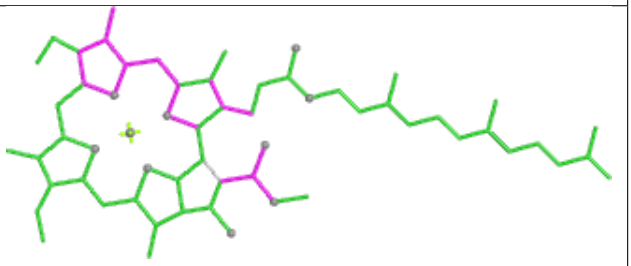


Rings

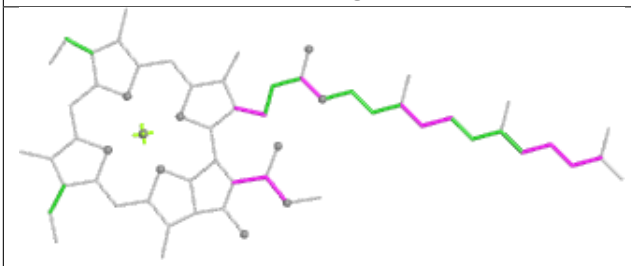
Ligand CLA A 408



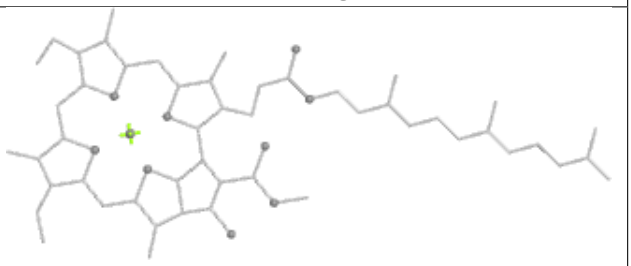
Bond lengths



Bond angles

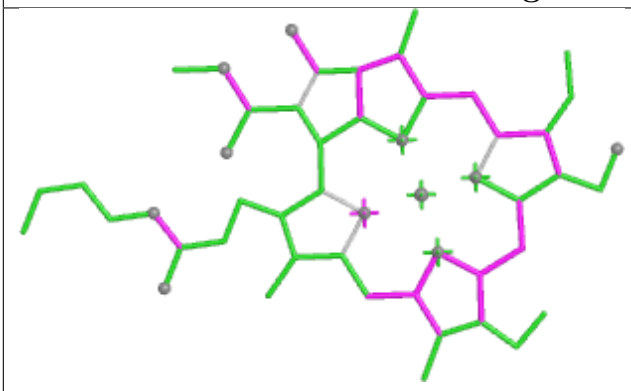


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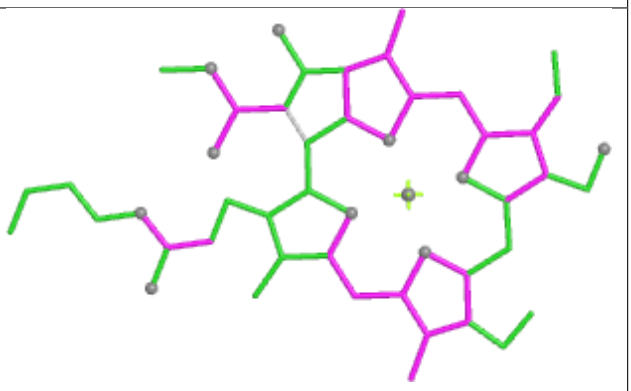


Rings

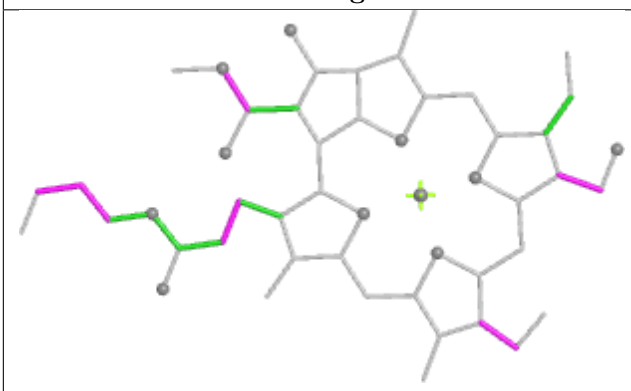
Ligand CHL G 313



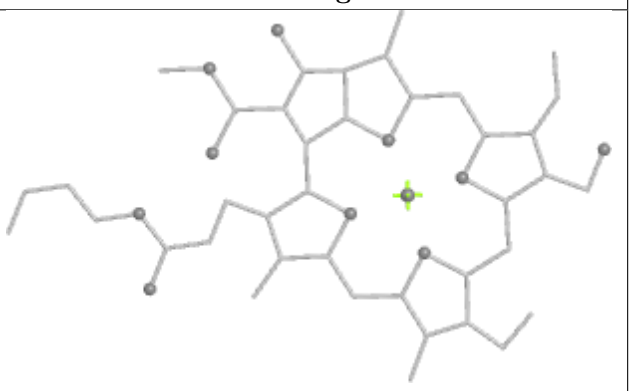
Bond lengths



Bond angles

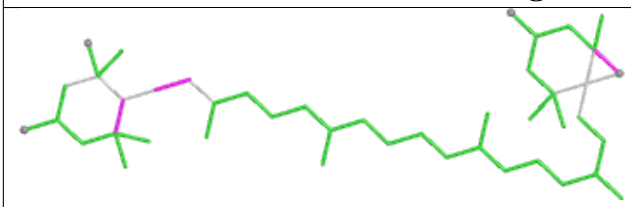


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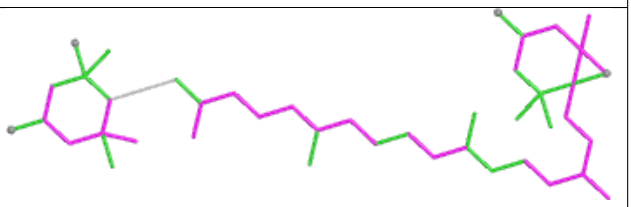


Rings

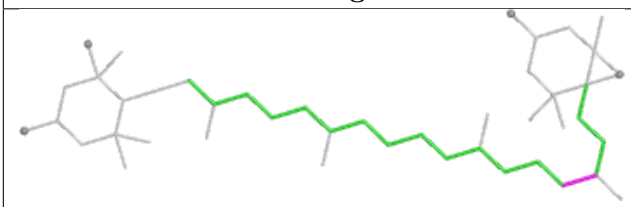
Ligand NEX r 617



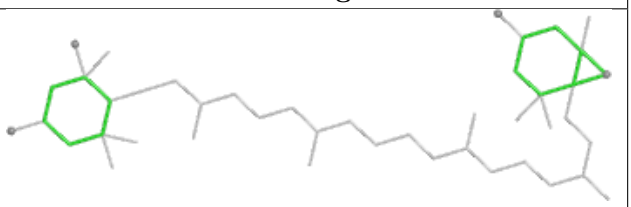
Bond lengths



Bond angles

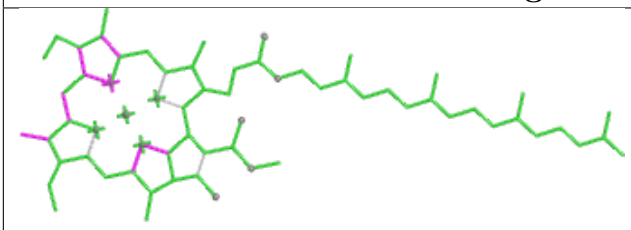


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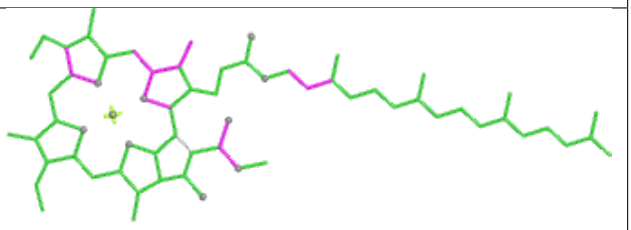


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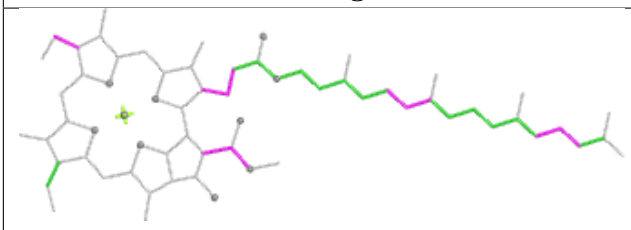
Ligand CLA P 305



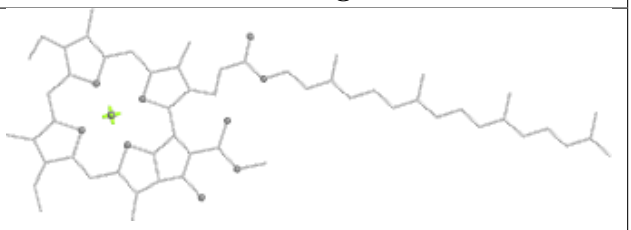
Bond lengths



Bond angles

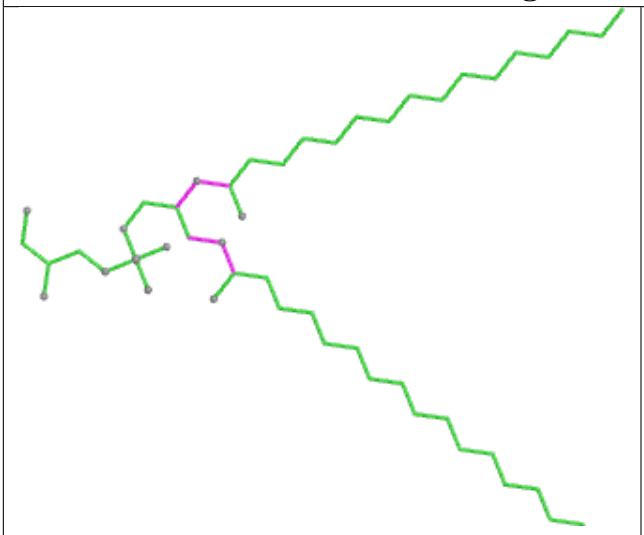


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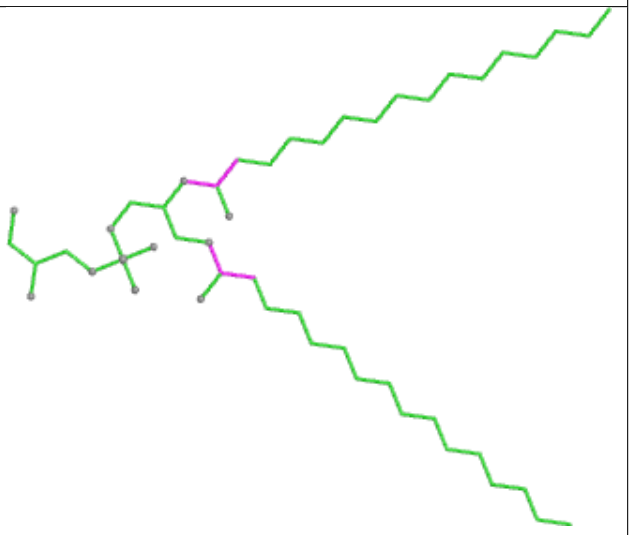


Rings

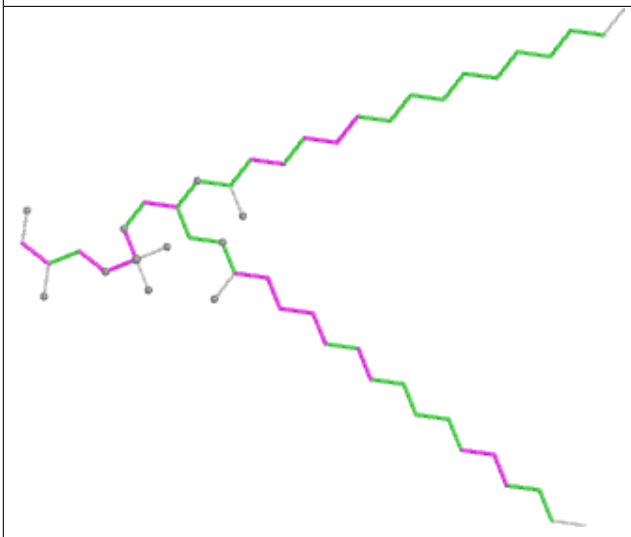
Ligand LHG G 310



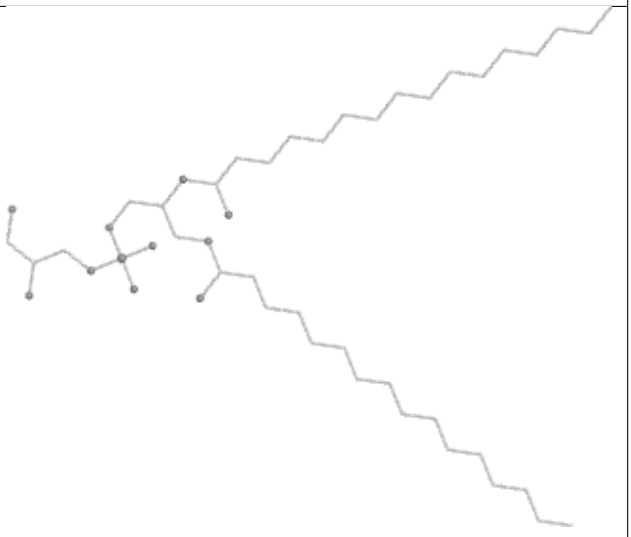
Bond lengths



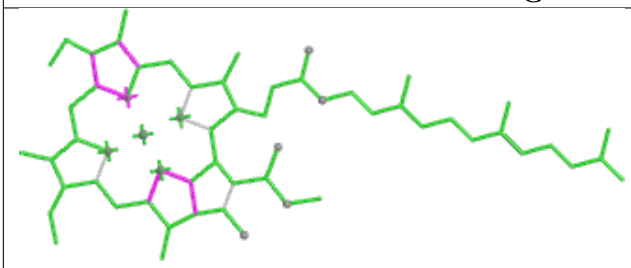
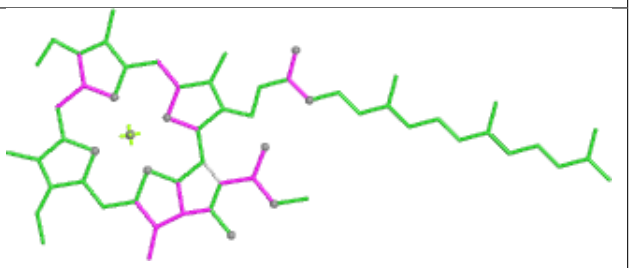
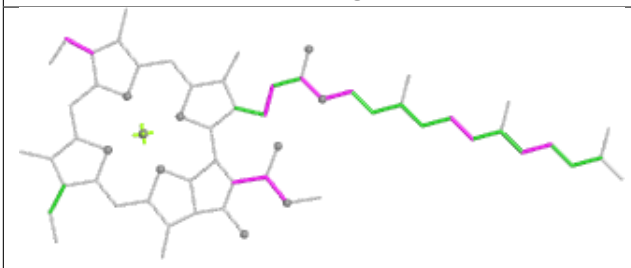
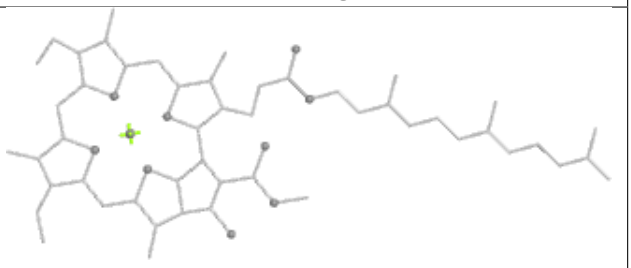
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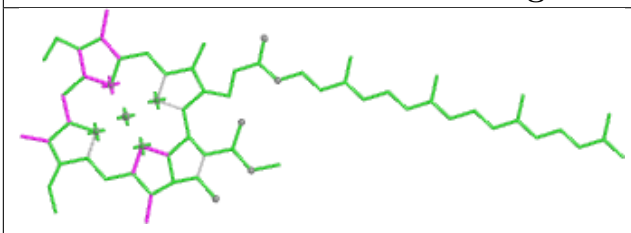
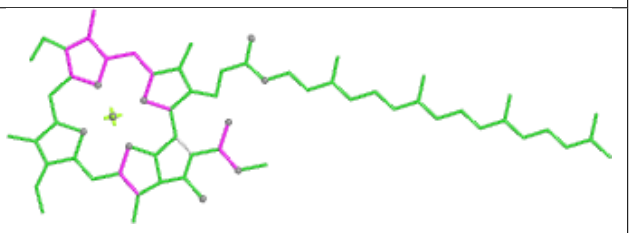
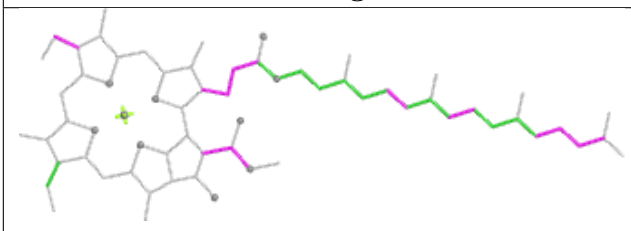
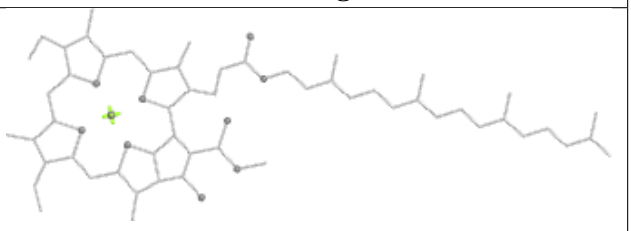


Torsions

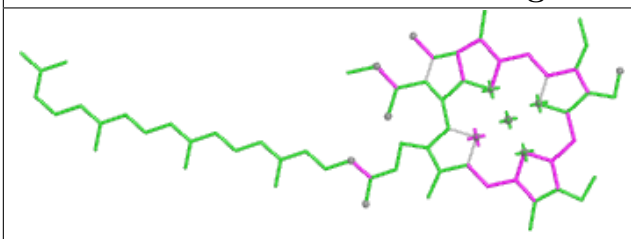


Rings

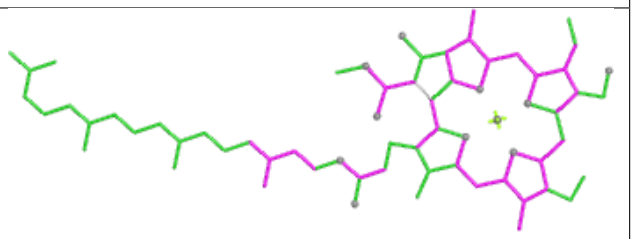
Ligand CLA P 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA n 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

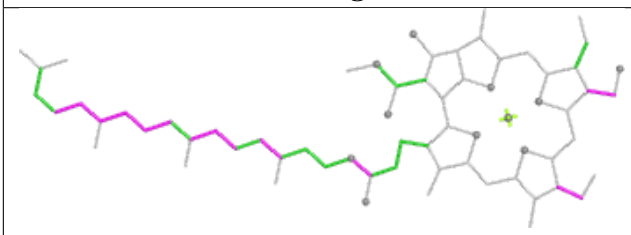
Ligand CHL v 313



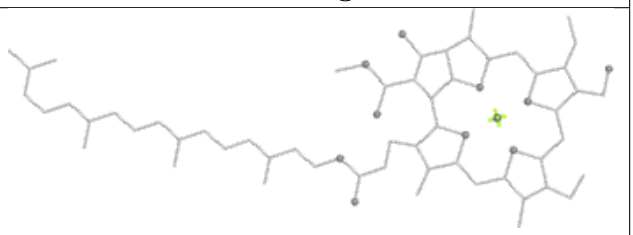
Bond lengths



Bond angles

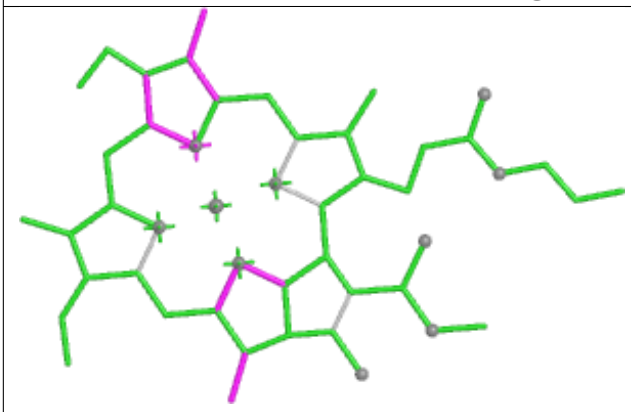


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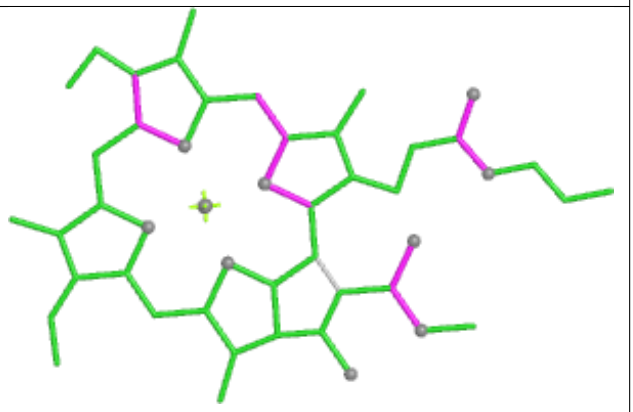


Rings

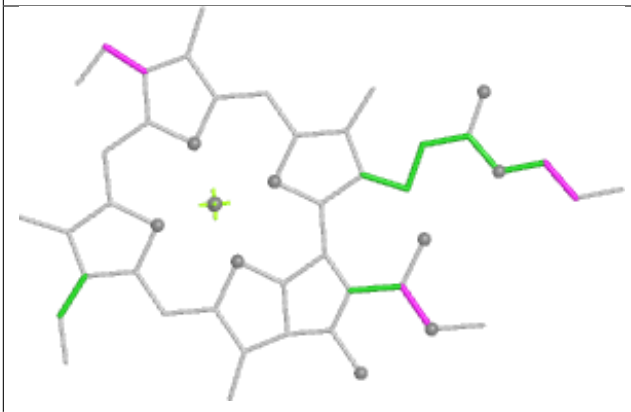
Ligand CLA 5 308



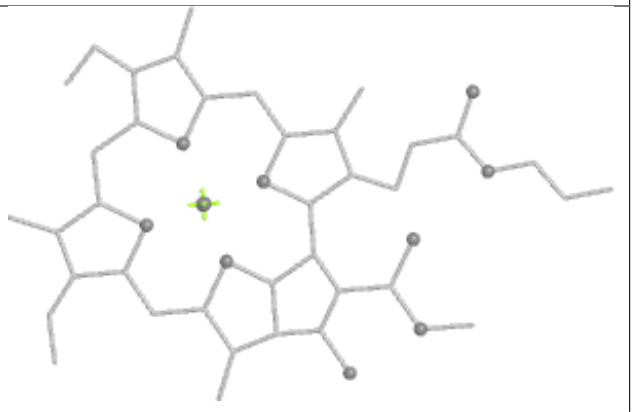
Bond lengths



Bond angles

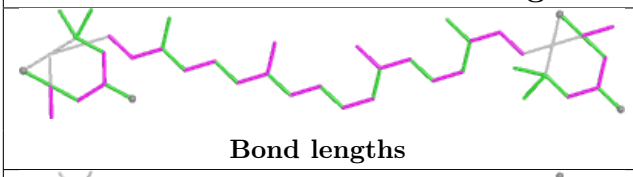


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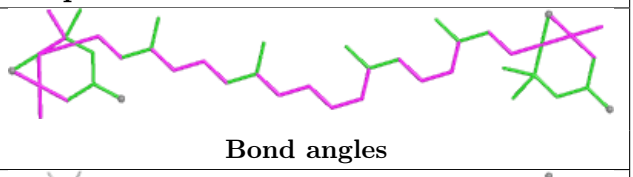


Rings

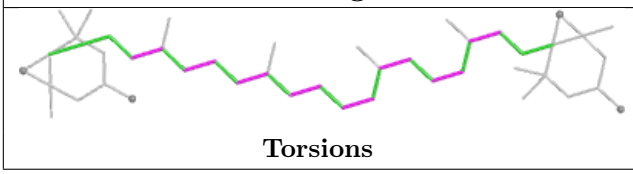
Ligand XAT q 309



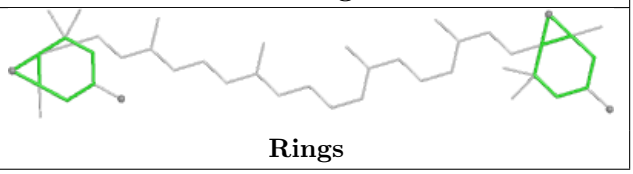
Bond lengths



Bond angles

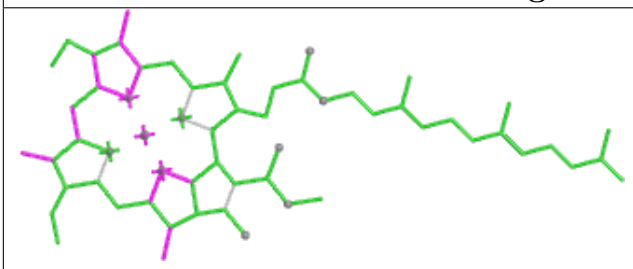


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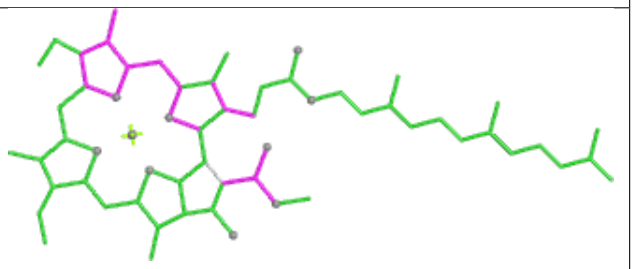


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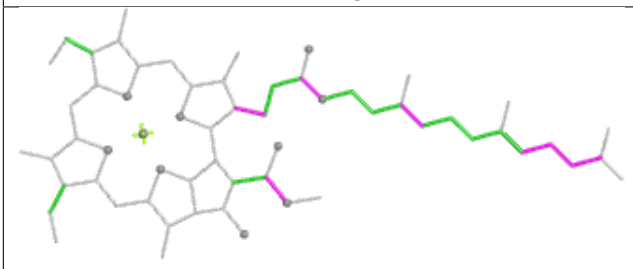
Ligand CLA a 408



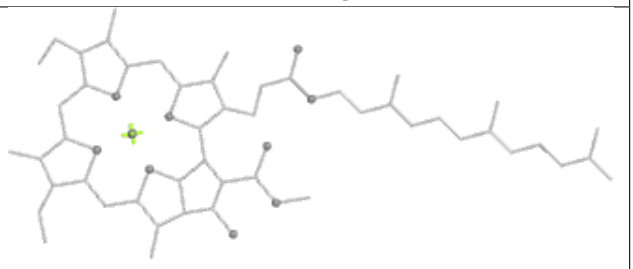
Bond lengths



Bond angles

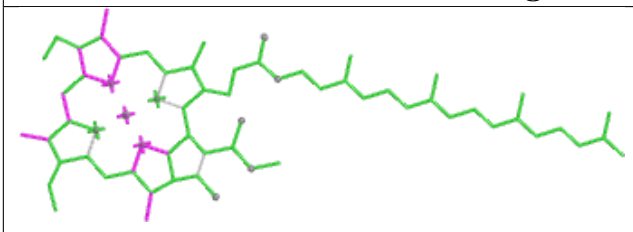


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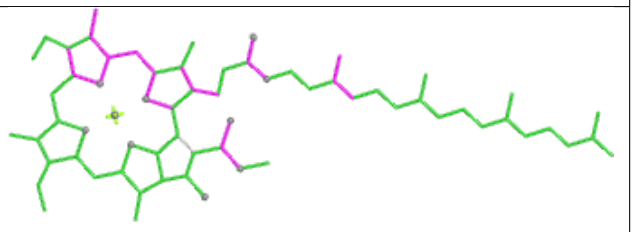


Rings

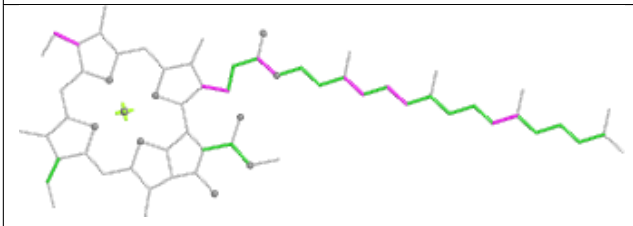
Ligand CLA C 510



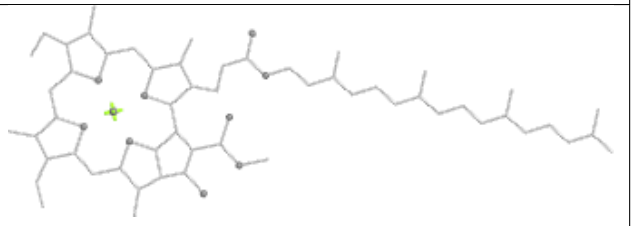
Bond lengths



Bond angles

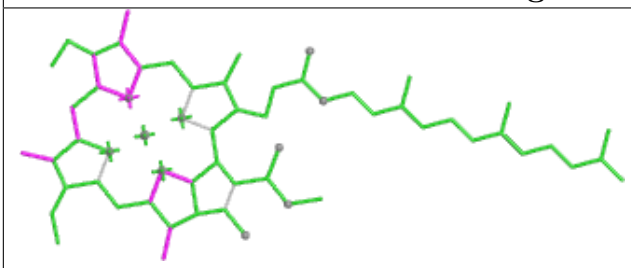


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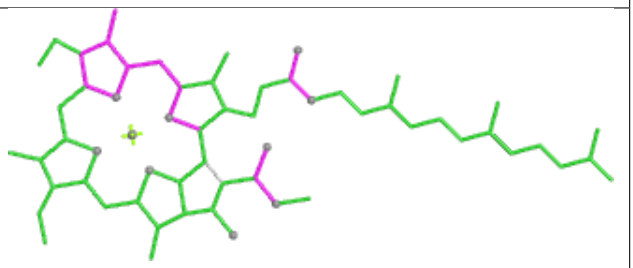


Rings

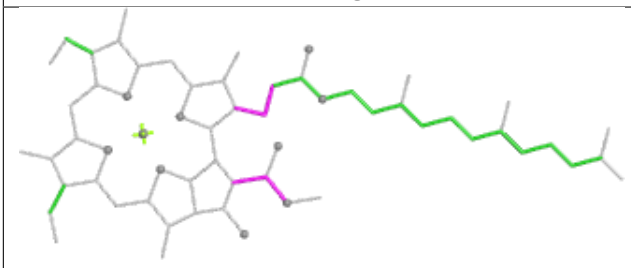
Ligand CLA u 304



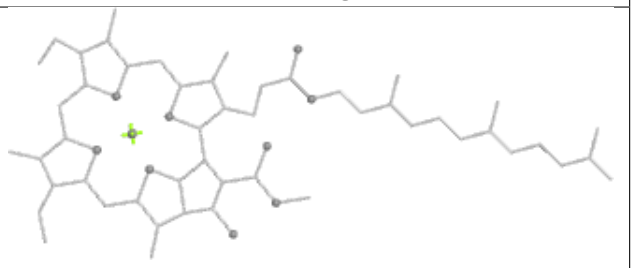
Bond lengths



Bond angles

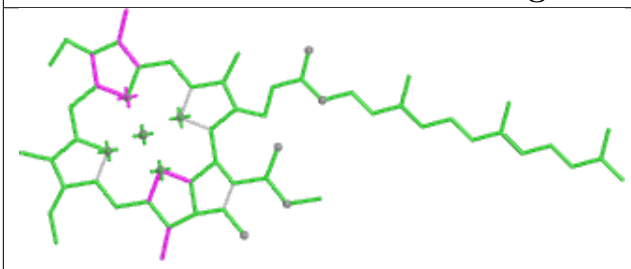


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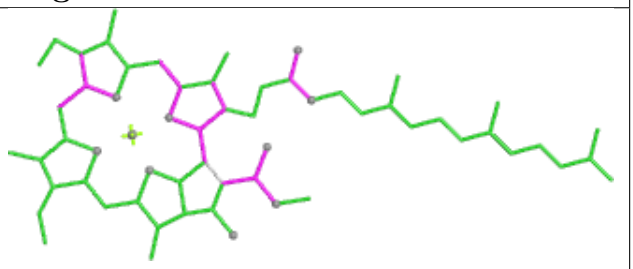


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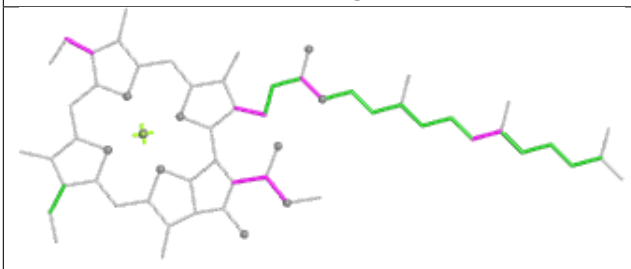
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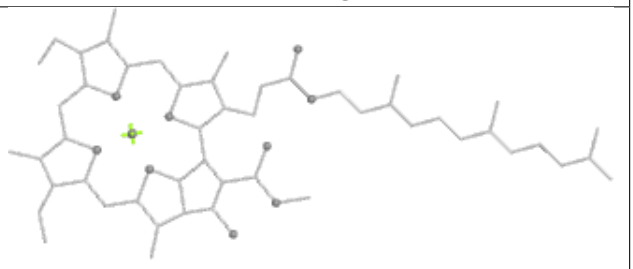
Bond lengths



Bond angles

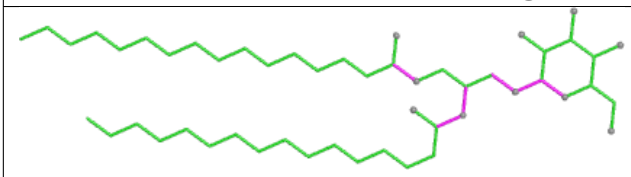


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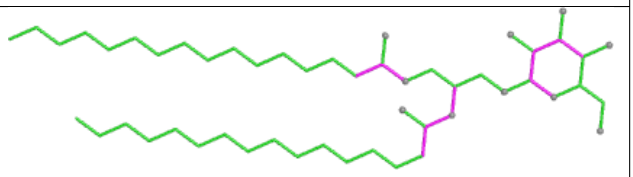


Rings

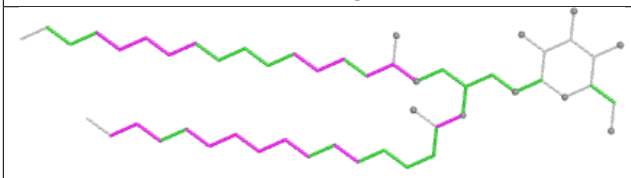
Ligand LMG B 621



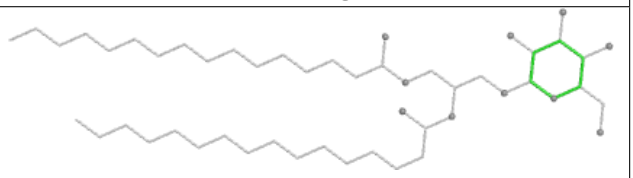
Bond lengths



Bond angles

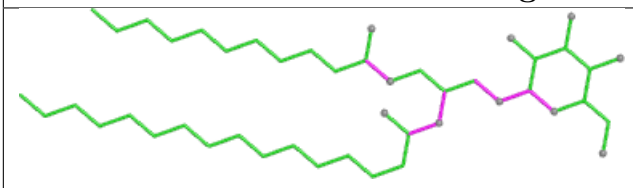


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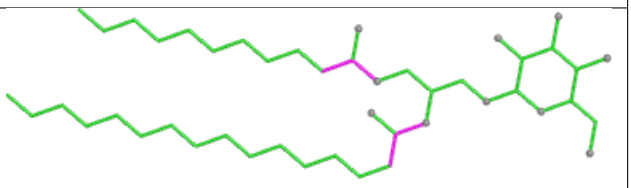


Rings

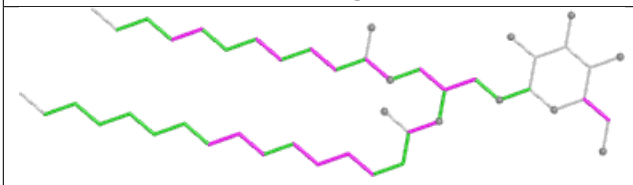
Ligand LMG D 408



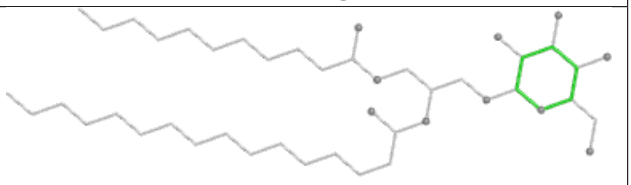
Bond lengths



Bond angles

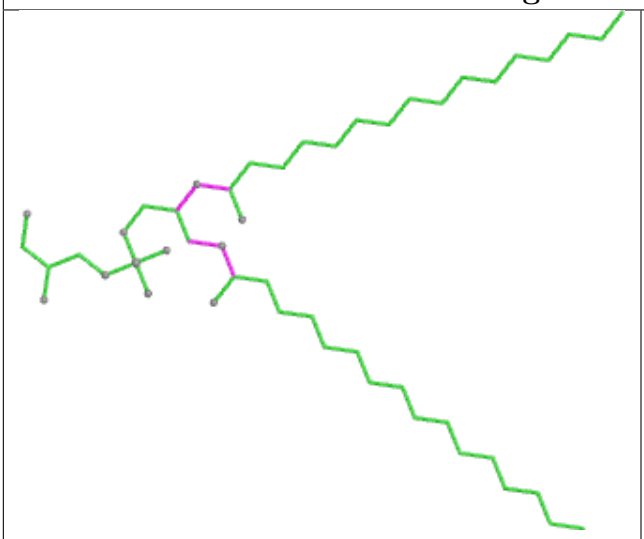


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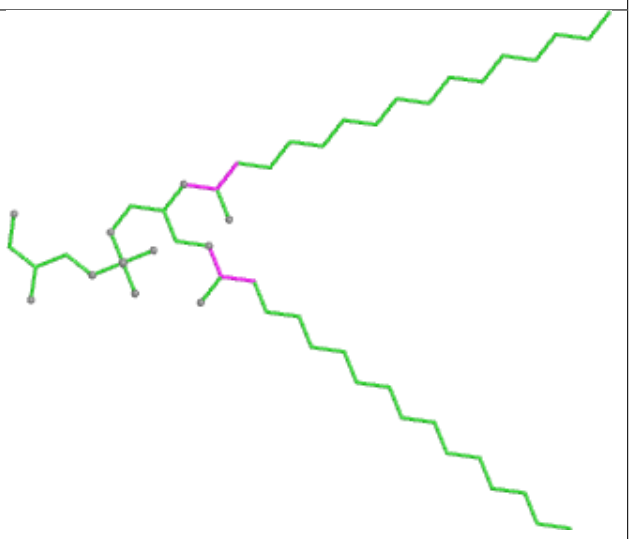


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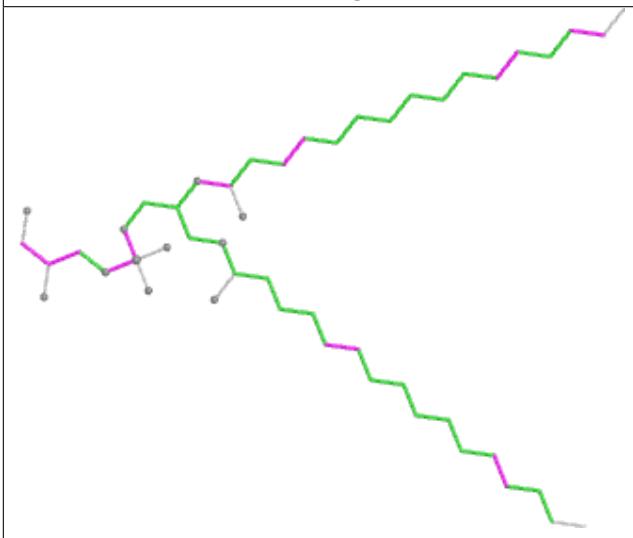
Ligand LHG C 524



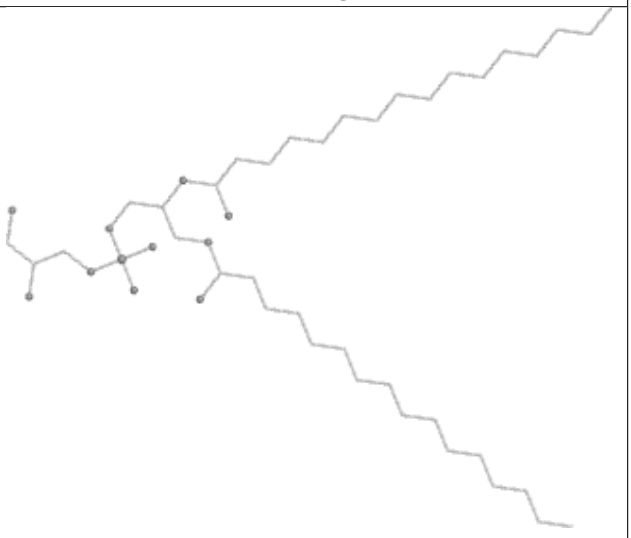
Bond lengths



Bond angles

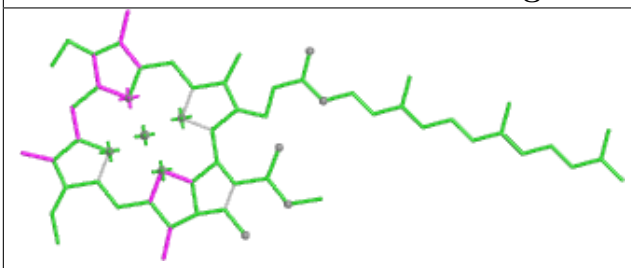


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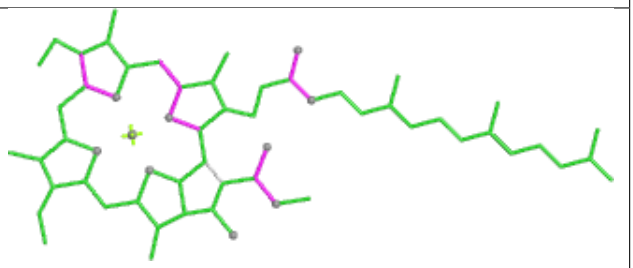


Rings

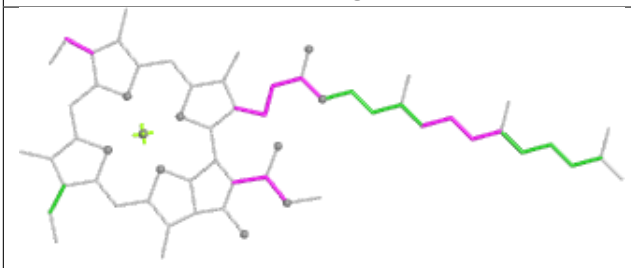
Ligand CLA N 307



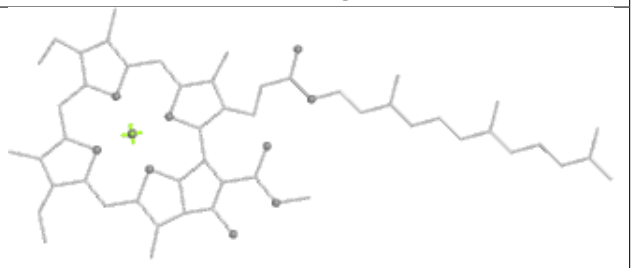
Bond lengths



Bond angles

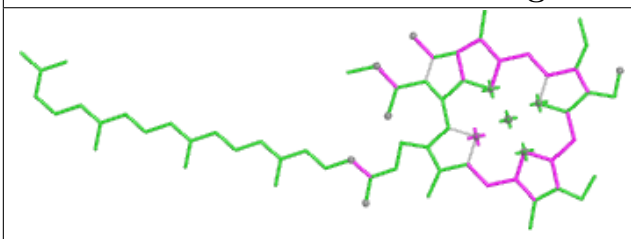


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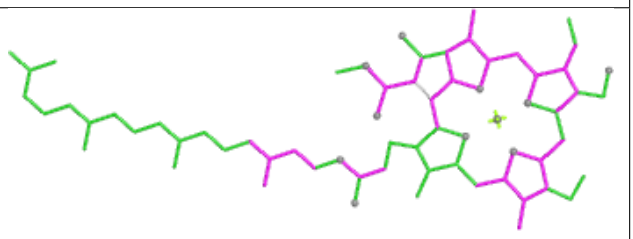


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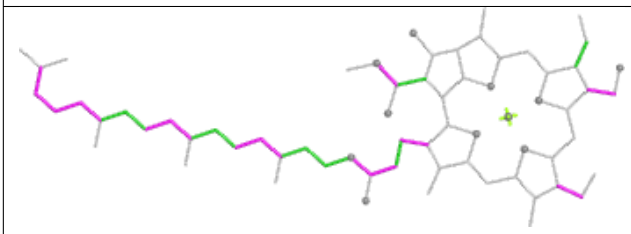
Ligand CHL 6 301



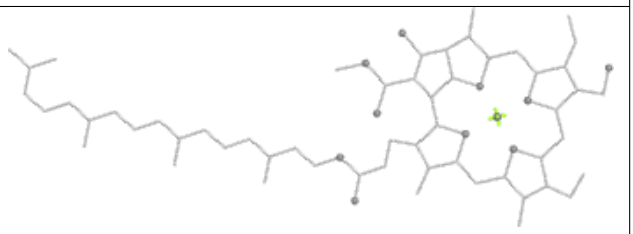
Bond lengths



Bond angles

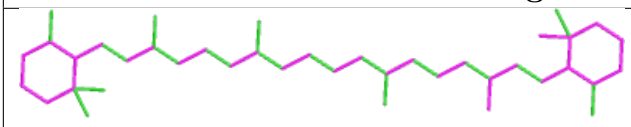


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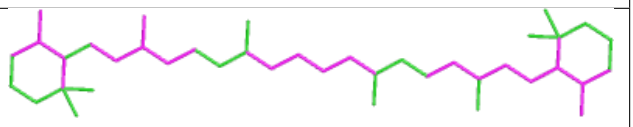


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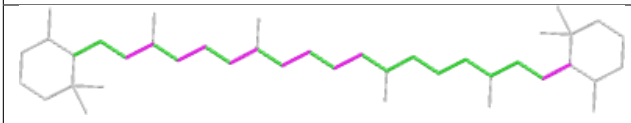
Ligand BCR x 202



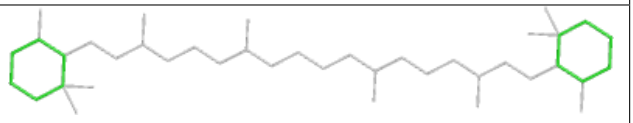
Bond lengths



Bond angles

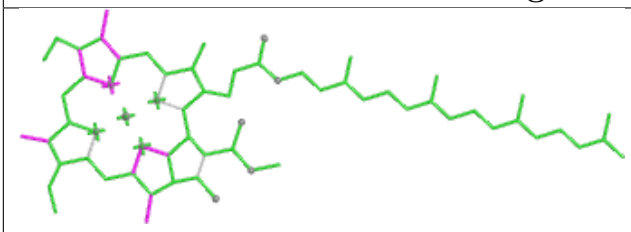


Torsions

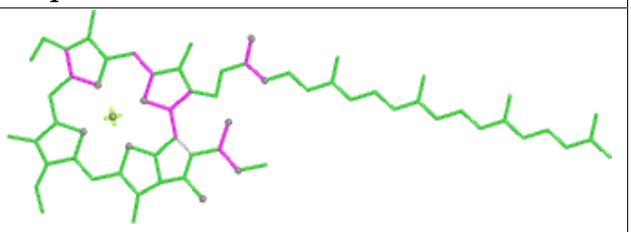


Rings

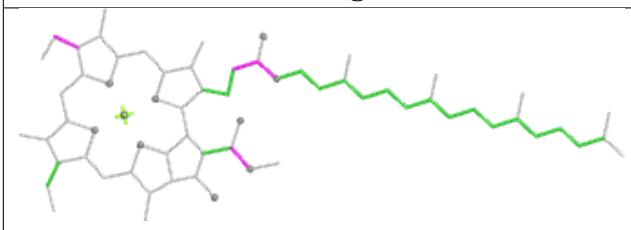
Ligand CLA p 303



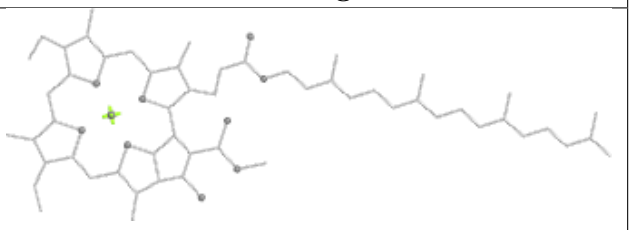
Bond lengths



Bond angles

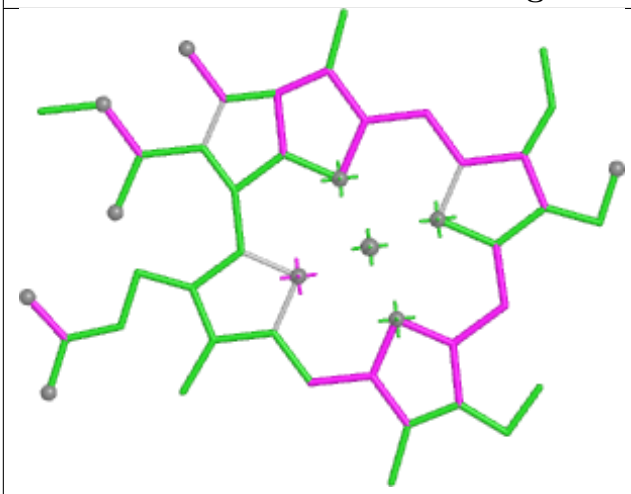


Torsions



Rings

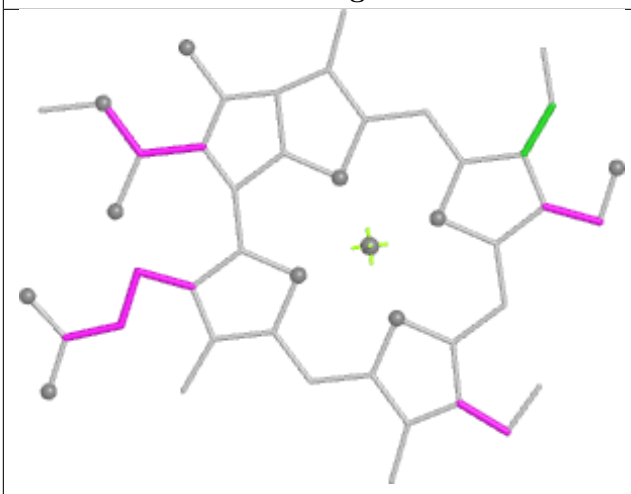
Ligand CHL S 316



Bond lengths



Bond angles

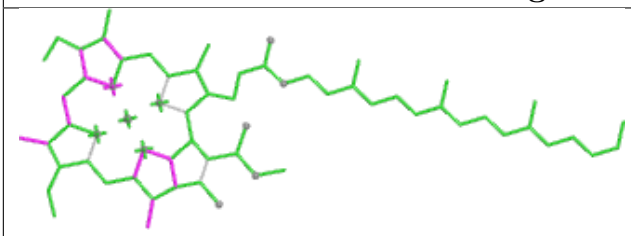


Torsions

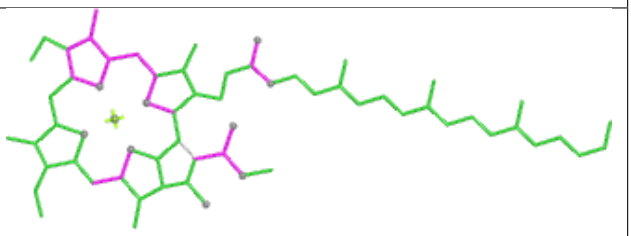


Rings

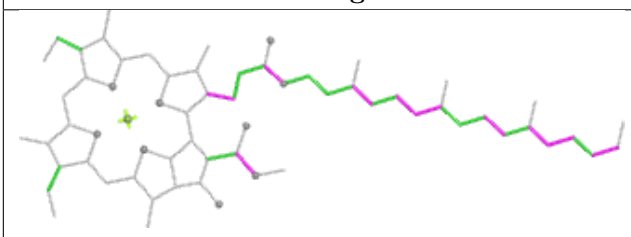
Ligand CLA 3 304



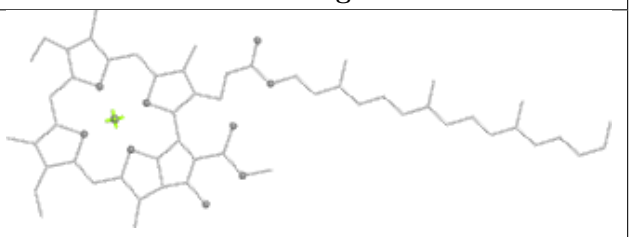
Bond lengths



Bond angles

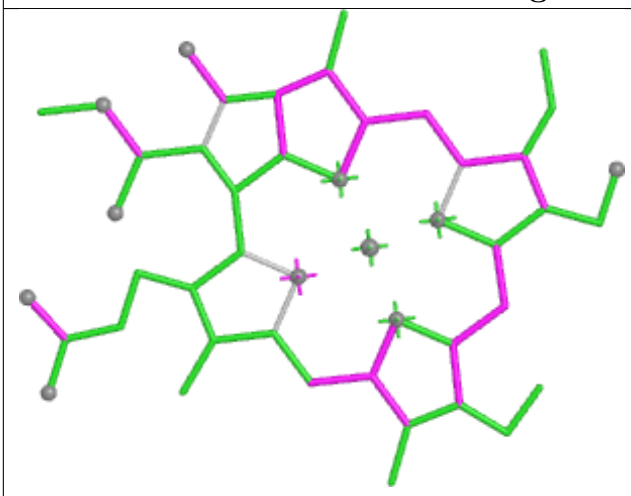


Torsions

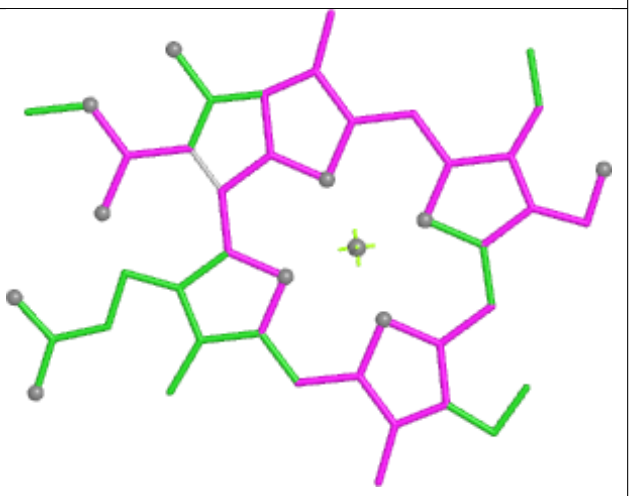


Rings

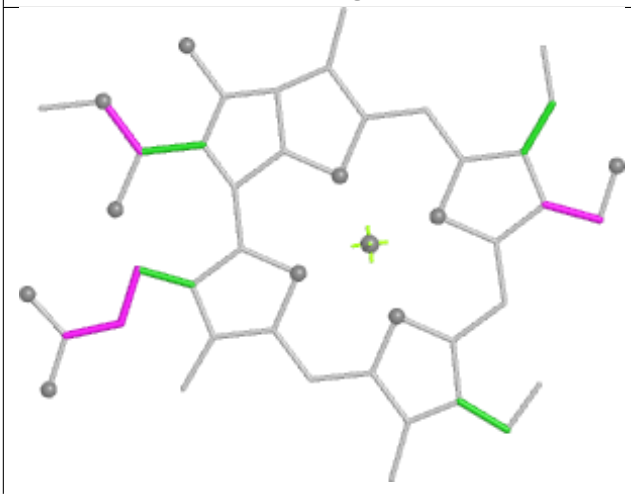
Ligand CHL s 313



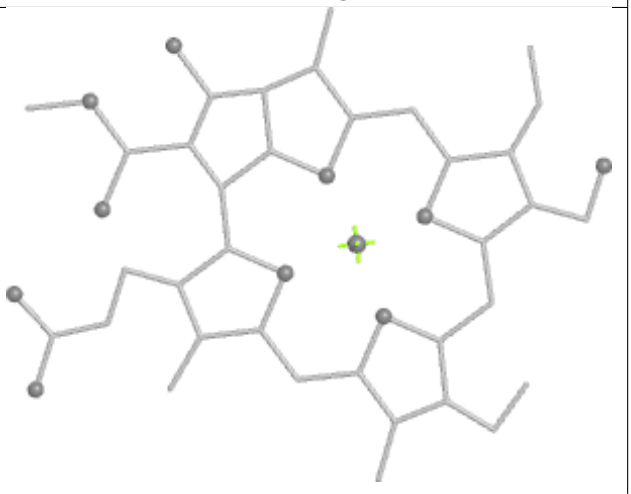
Bond lengths



Bond angles

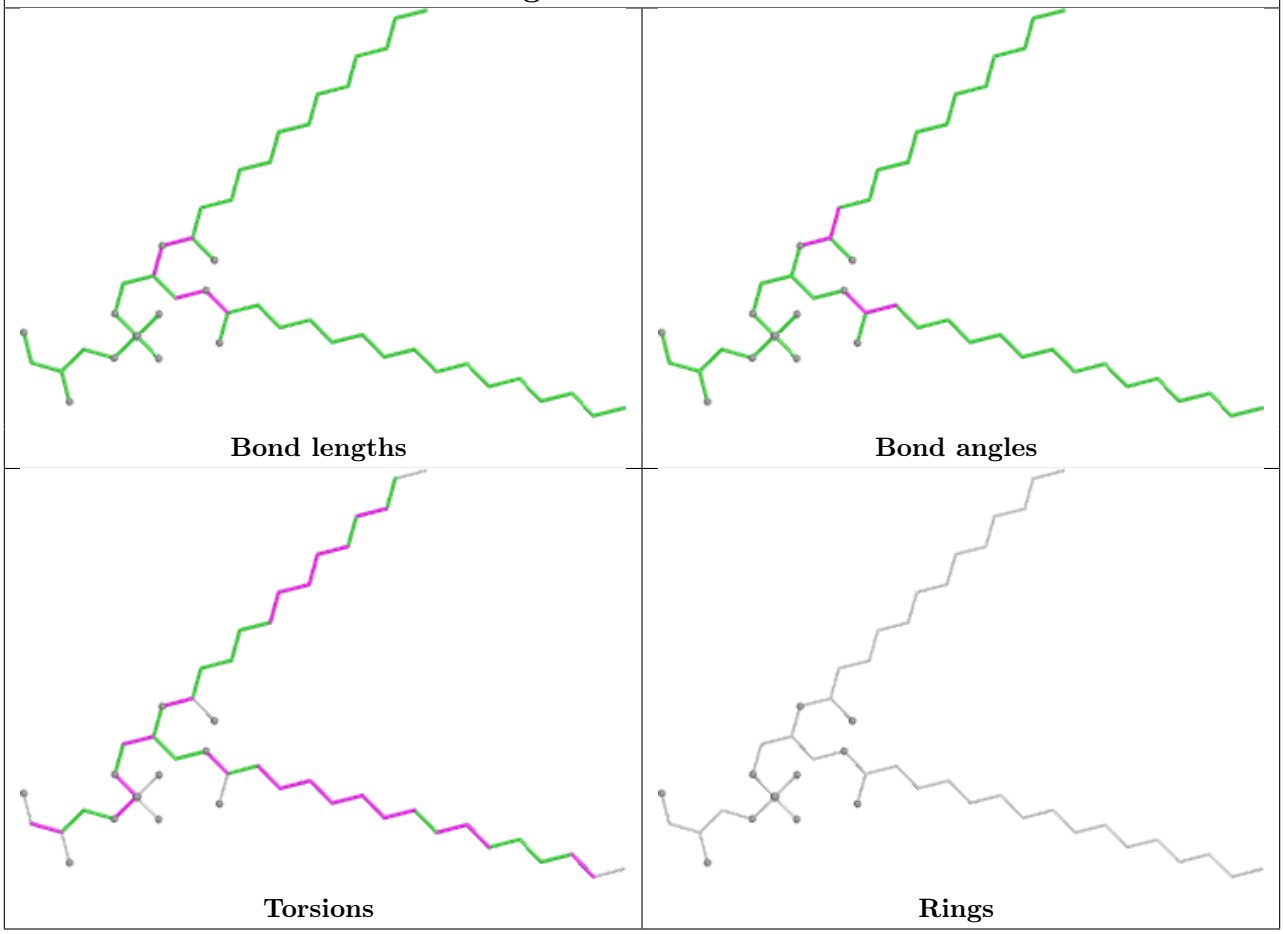


Torsions

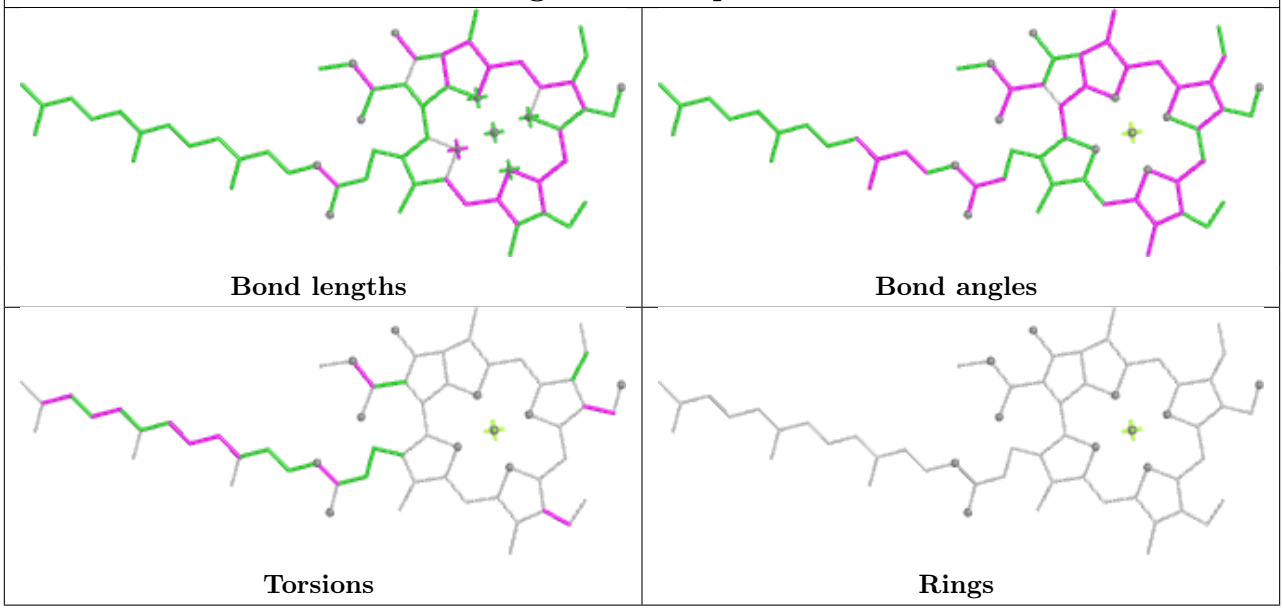


Rings

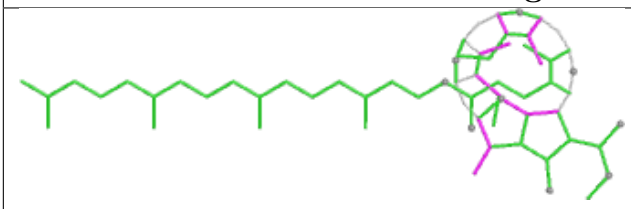
Ligand LHG D 406



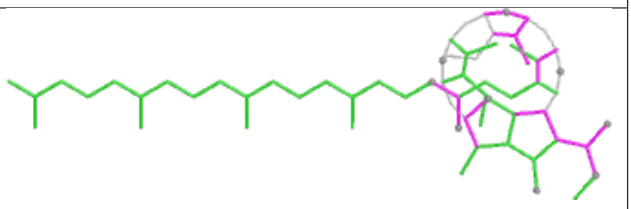
Ligand CHL q 315



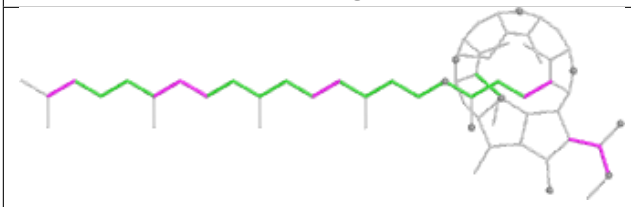
Ligand PHO d 401



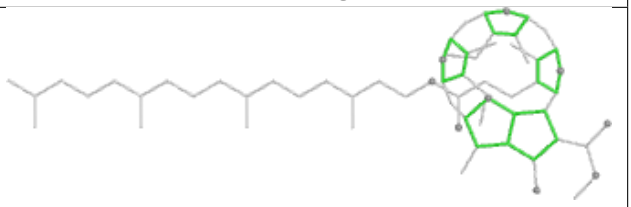
Bond lengths



Bond angles

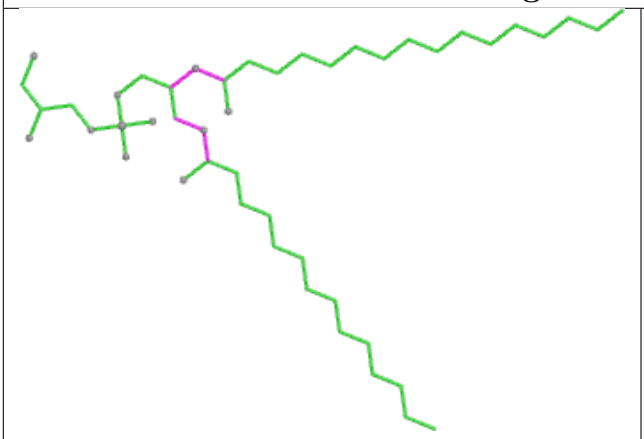


Torsions

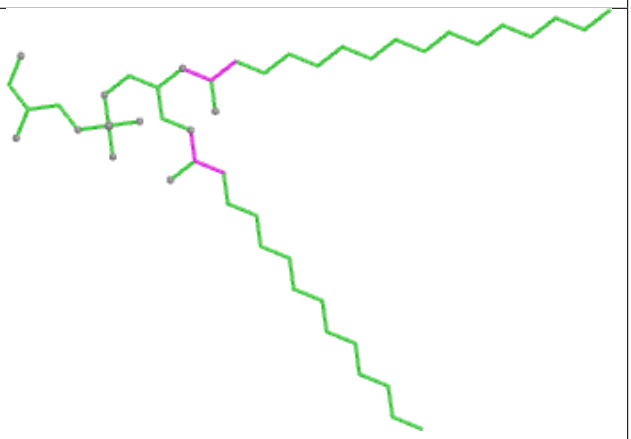


Rings

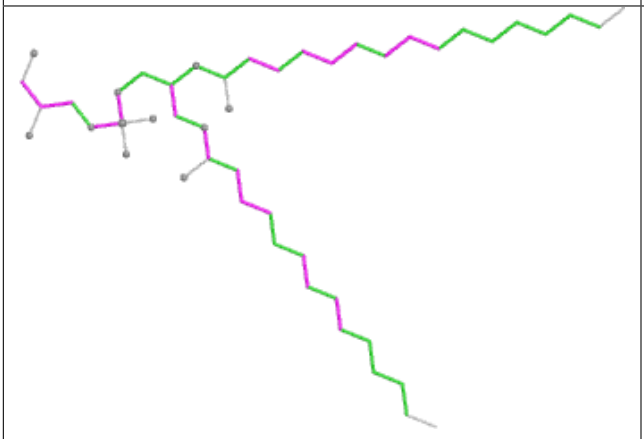
Ligand LHG B 622



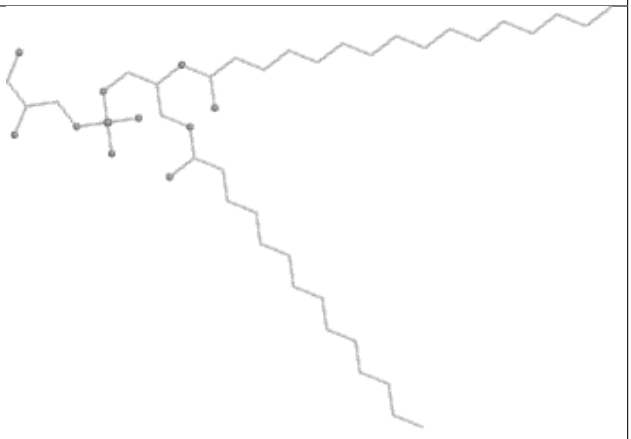
Bond lengths



Bond angles

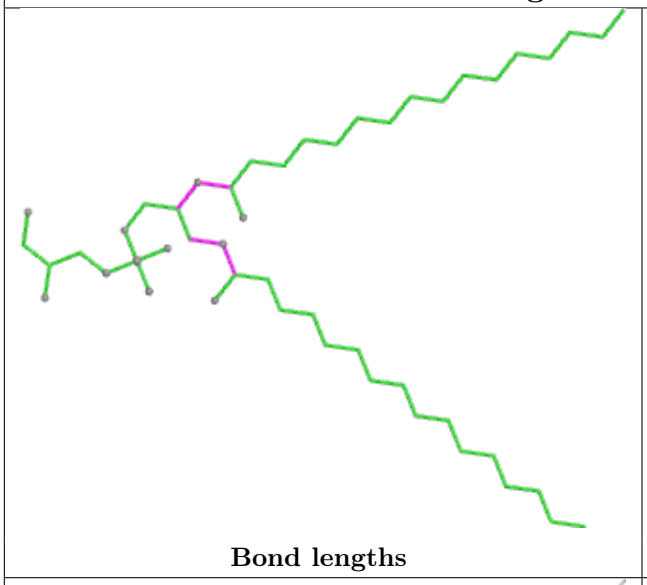


Torsions

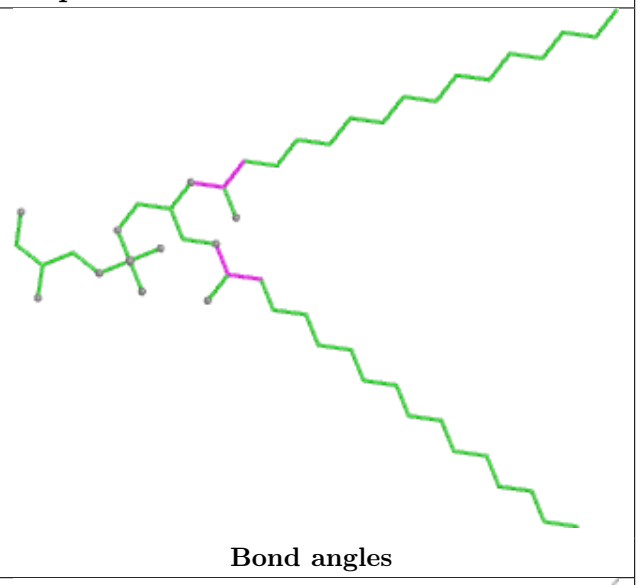


Rings

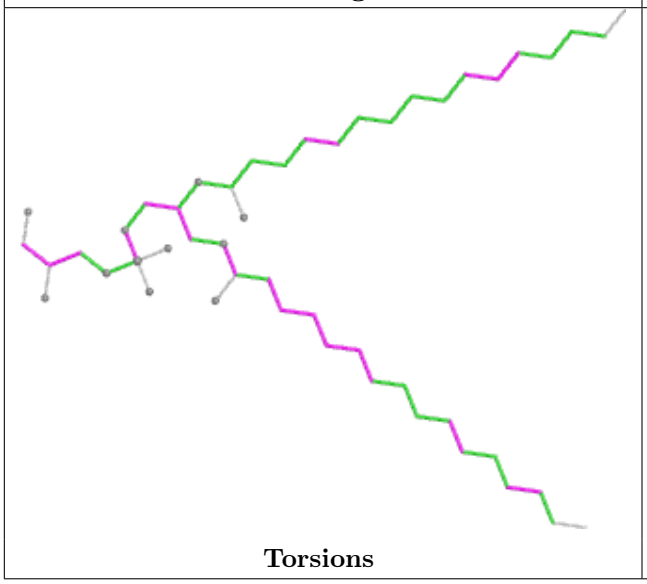
Ligand LHG p 313



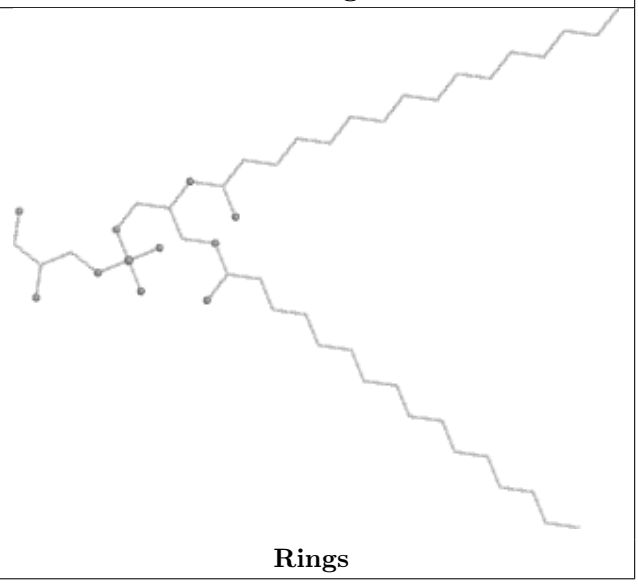
Bond lengths



Bond angles

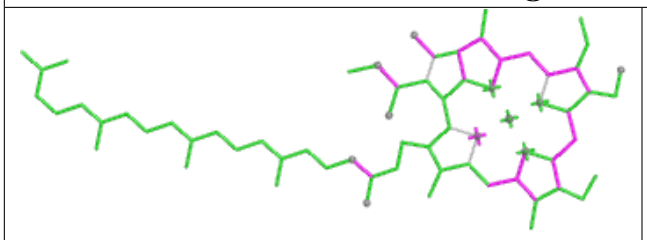


Torsions

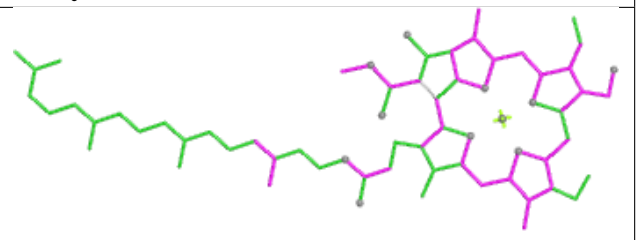


Rings

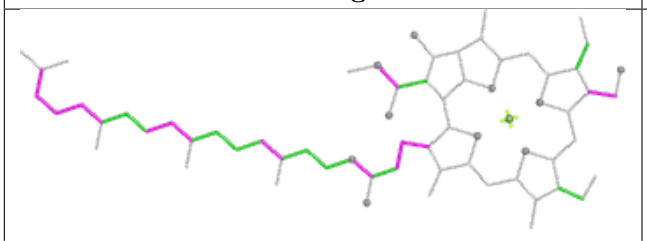
Ligand CHL Q 315



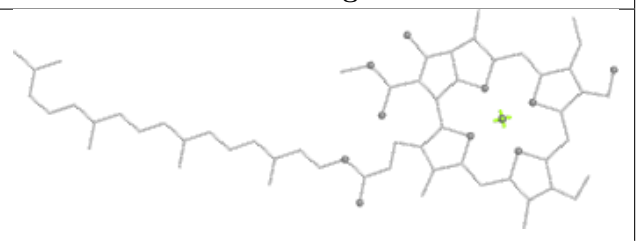
Bond lengths



Bond angles

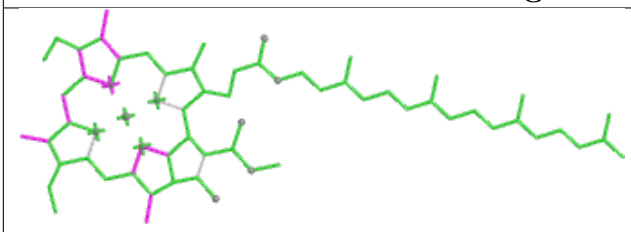


Torsions

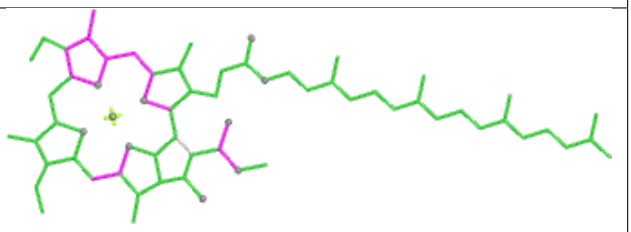


Rings

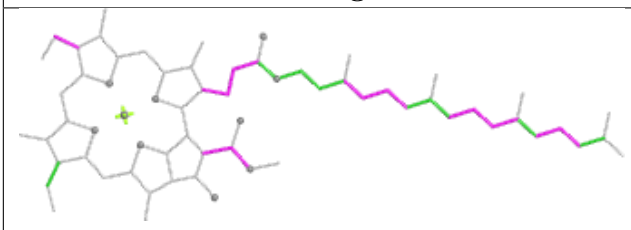
Ligand CLA P 302



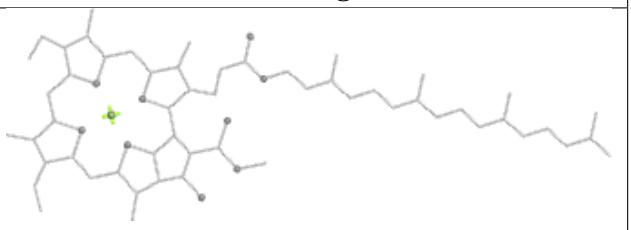
Bond lengths



Bond angles

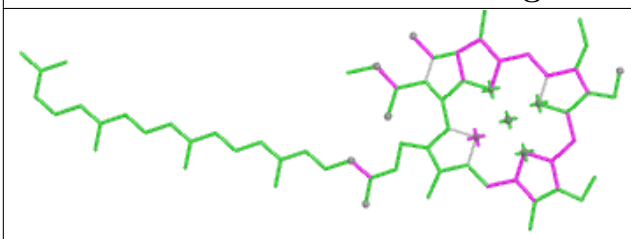


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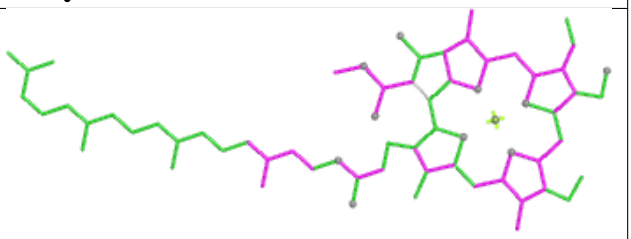


Rings

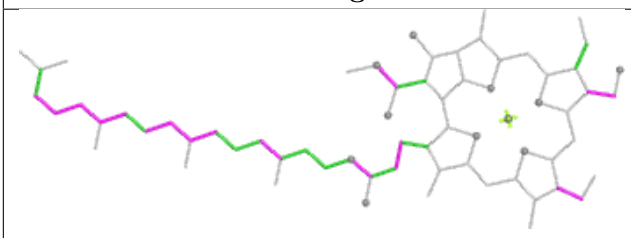
Ligand CHL Q 314



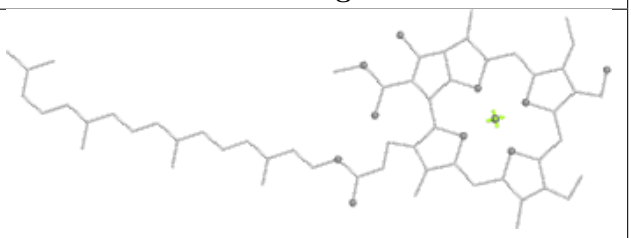
Bond lengths



Bond angles

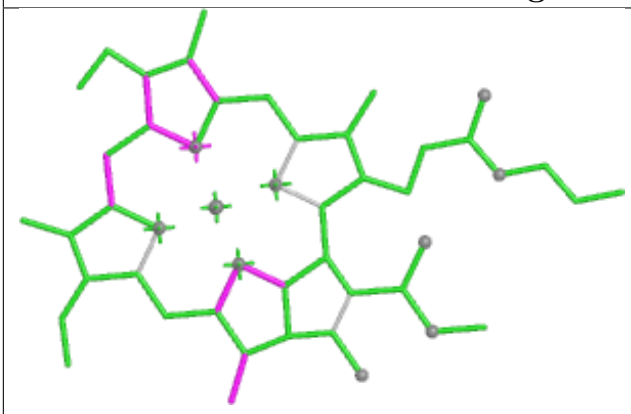


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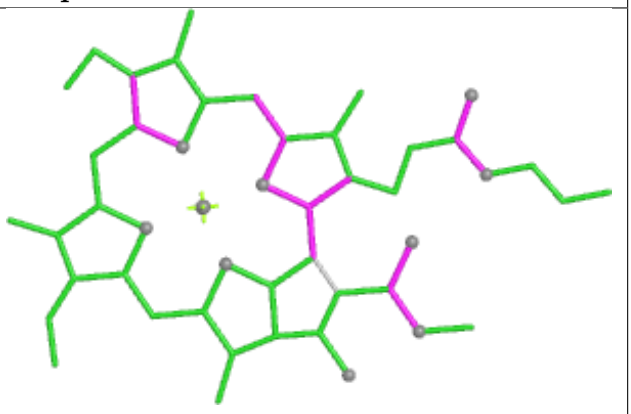


Rings

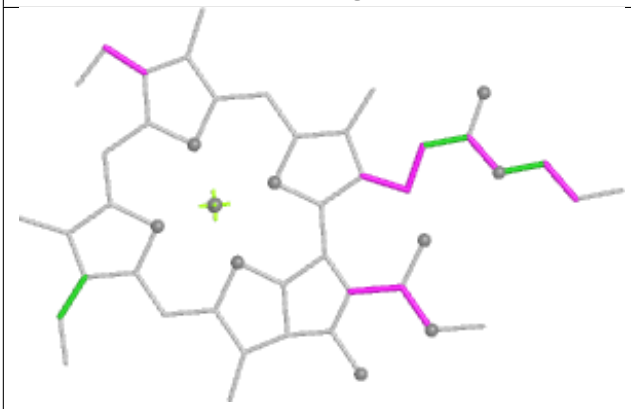
Ligand CLA q 308



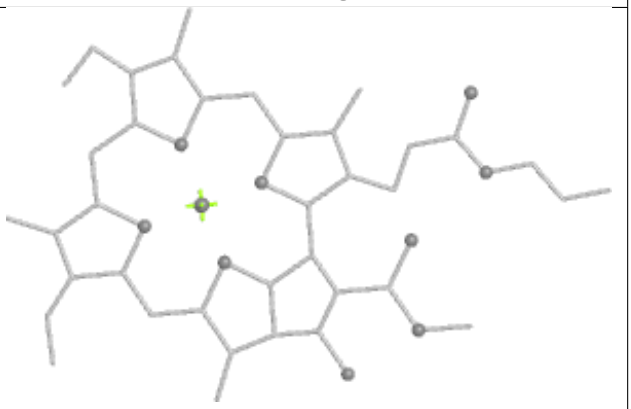
Bond lengths



Bond angles

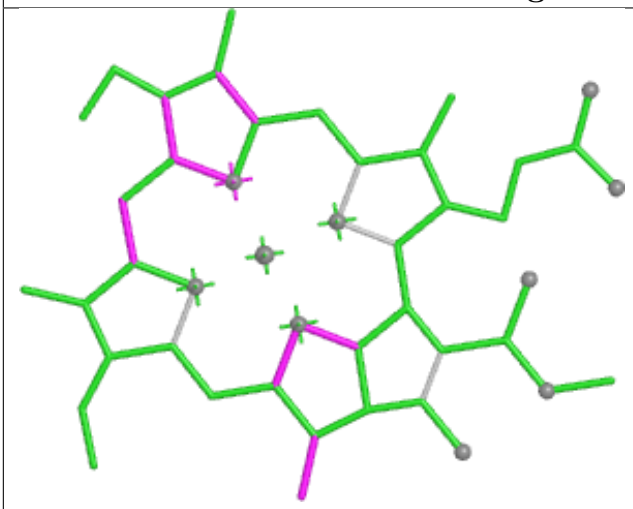


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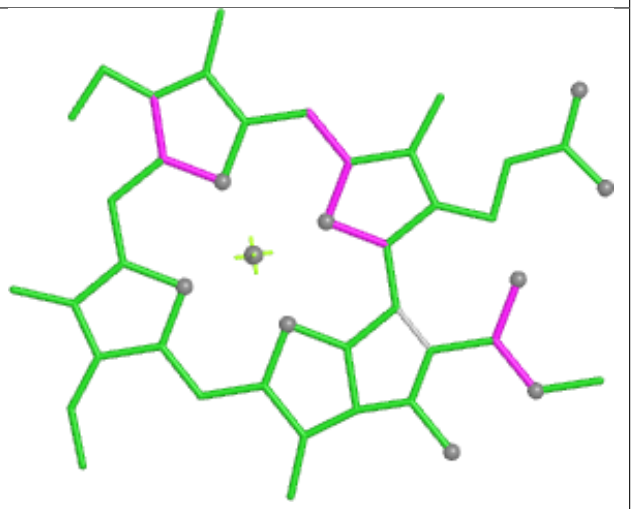


Rings

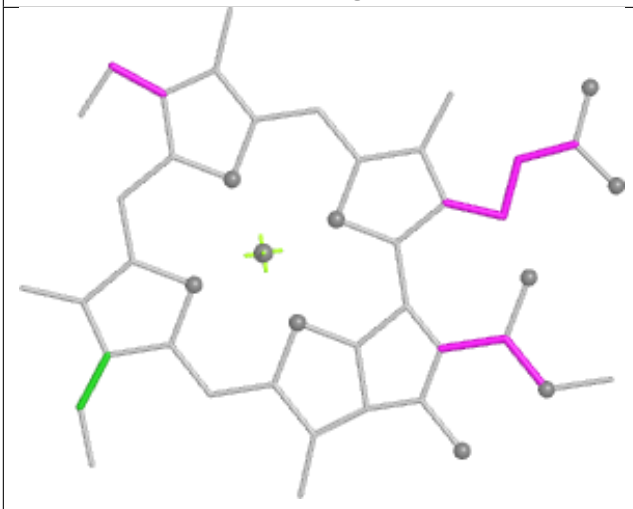
Ligand CLA S 304



Bond lengths



Bond angles

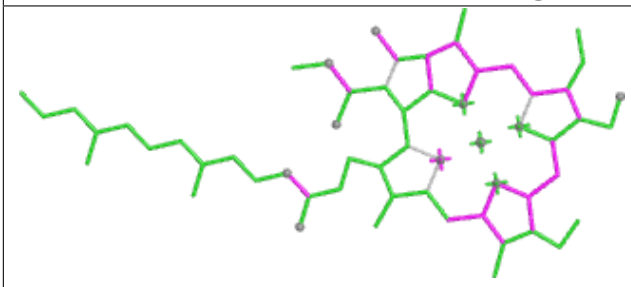


Torsions

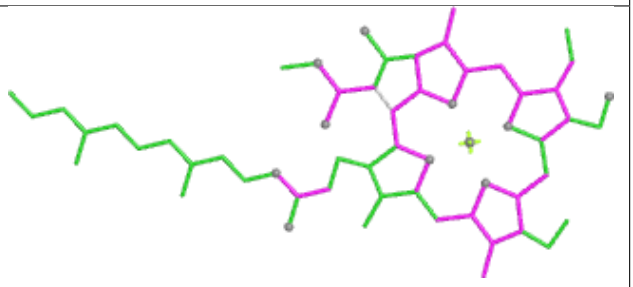


Rings

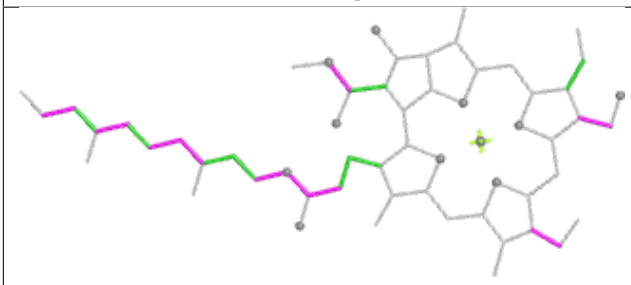
Ligand CHL s 315



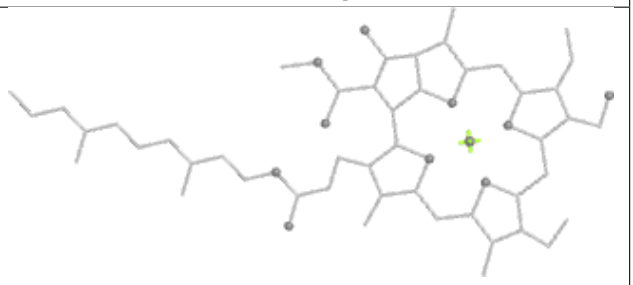
Bond lengths



Bond angles

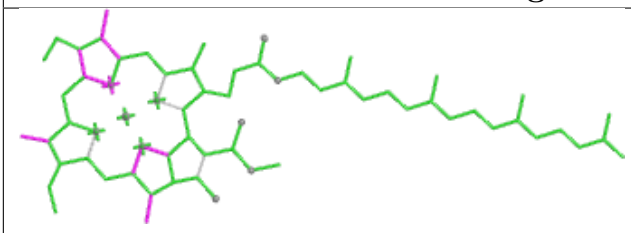


Torsions

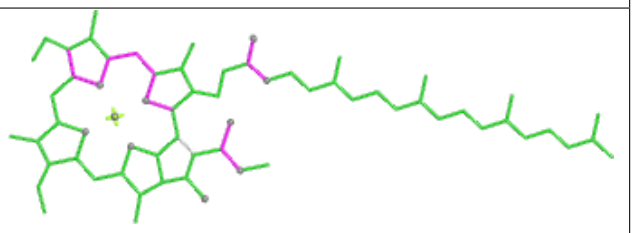


Rings

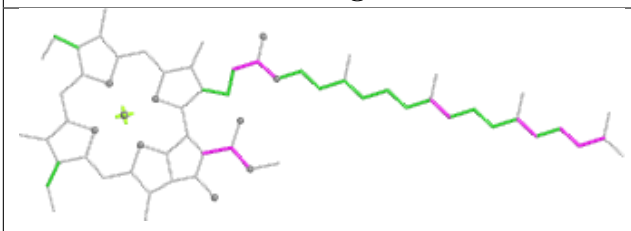
Ligand CLA n 302



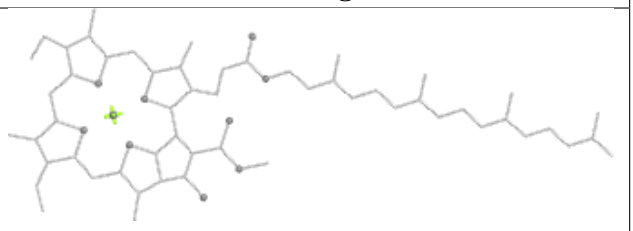
Bond lengths



Bond angles

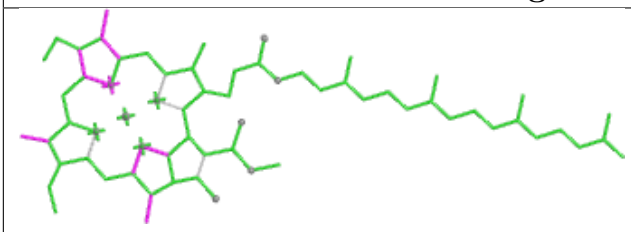


Torsions

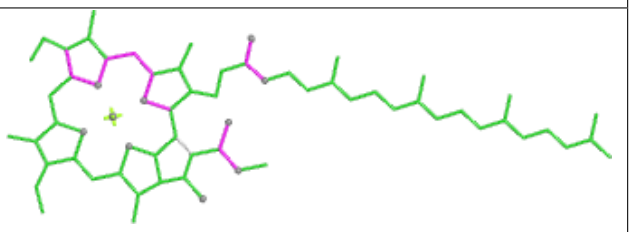


Rings

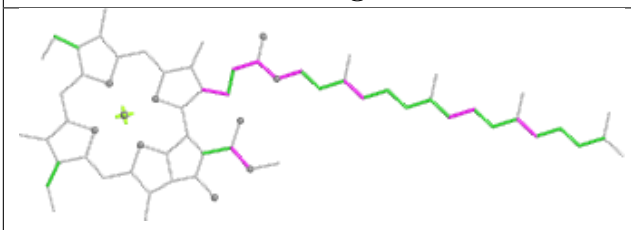
Ligand CLA 2 302



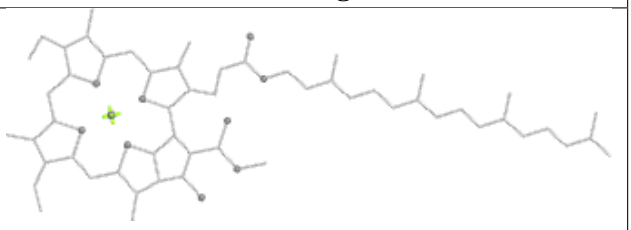
Bond lengths



Bond angles

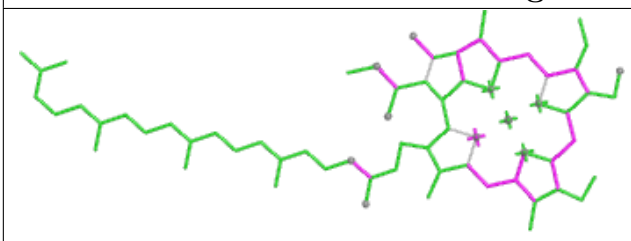


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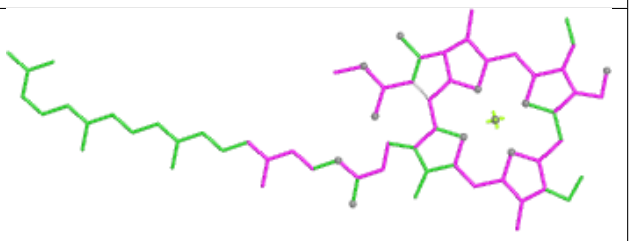


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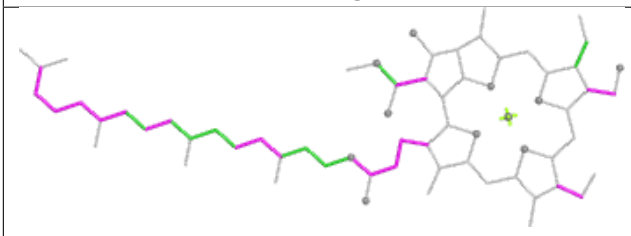
Ligand CHL u 316



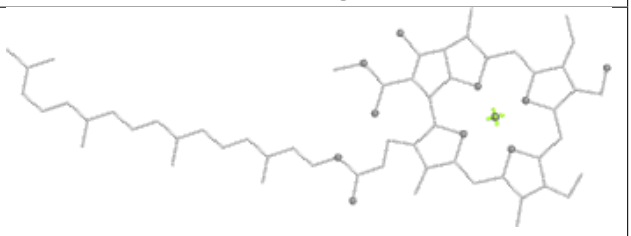
Bond lengths



Bond angles

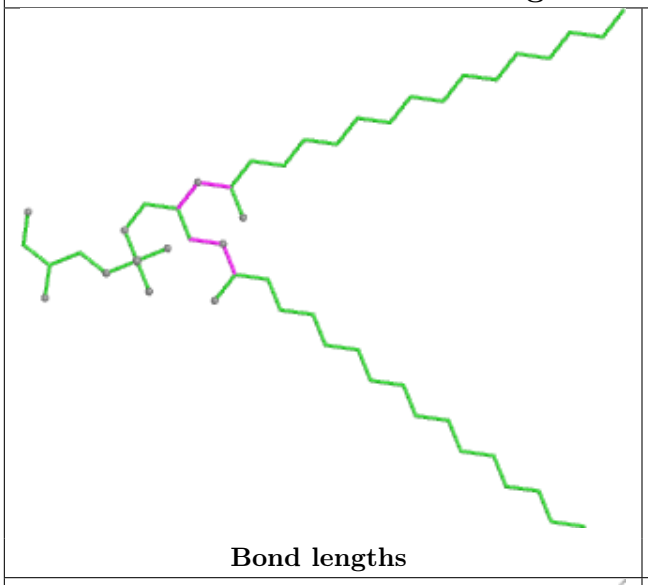


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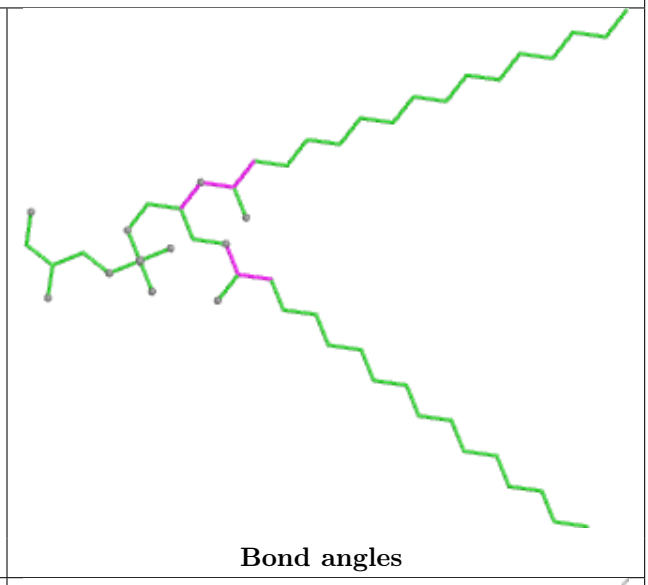


Rings

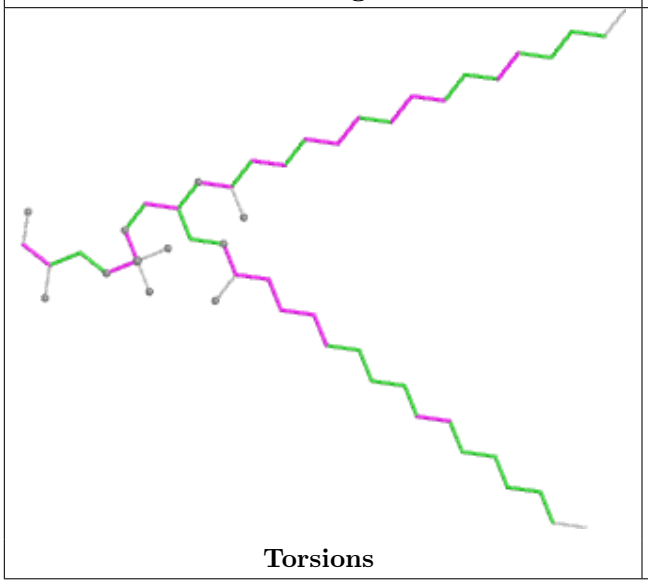
Ligand LHG u 312



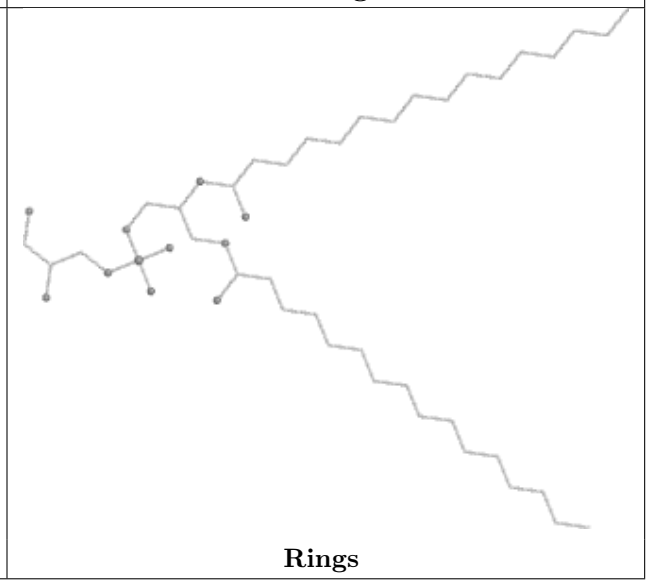
Bond lengths



Bond angles

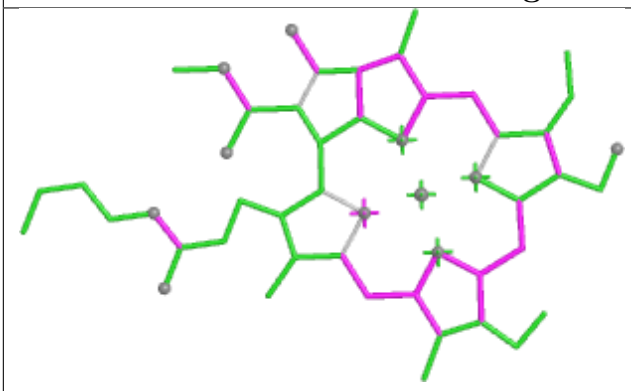


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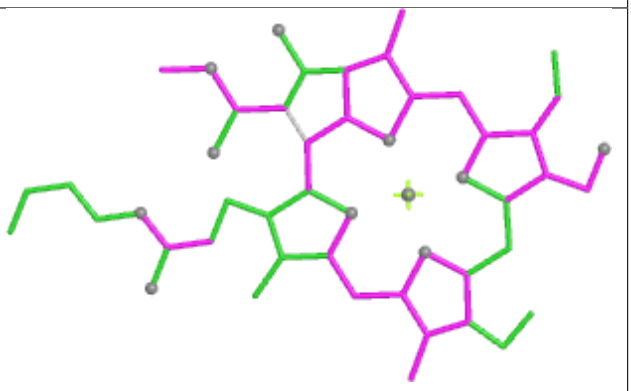


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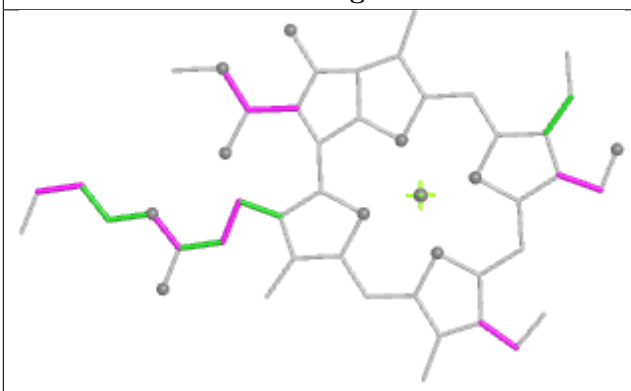
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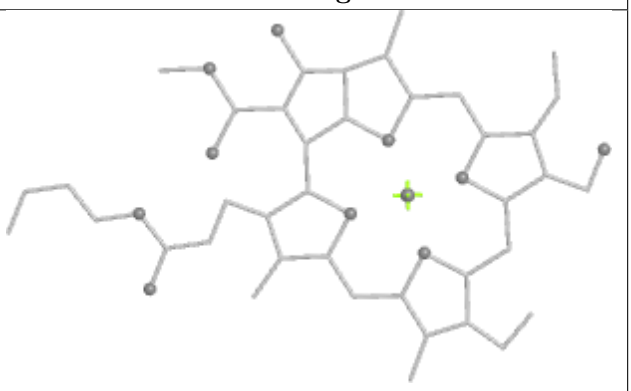
Bond lengths



Bond angles

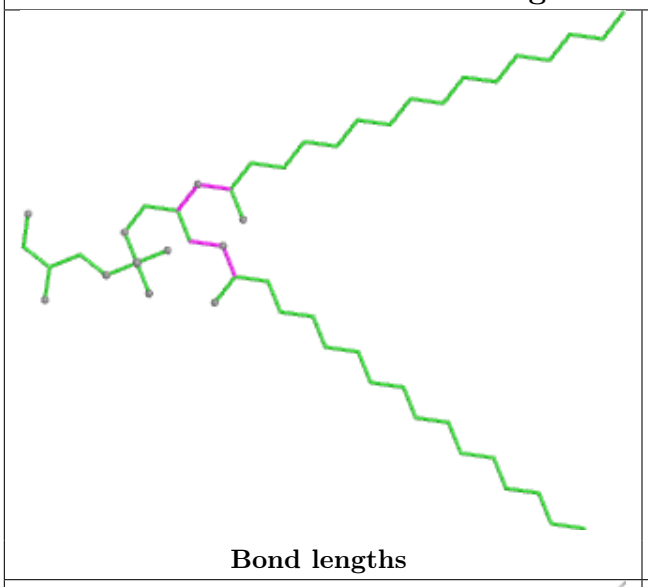


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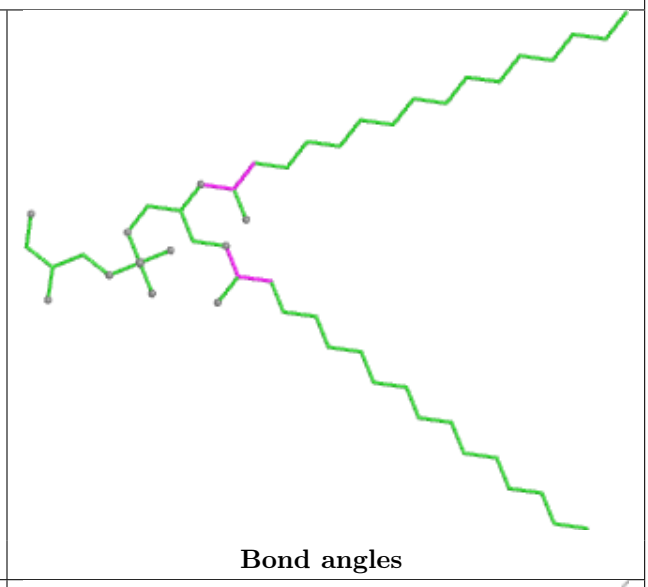


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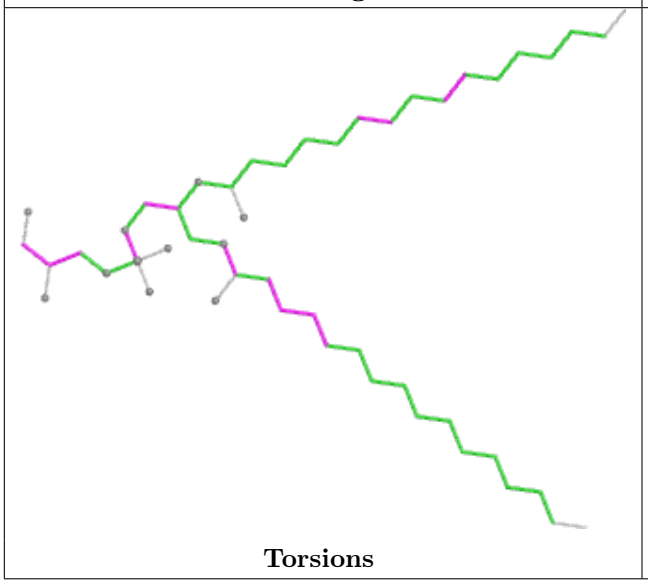
Ligand LHG c 521



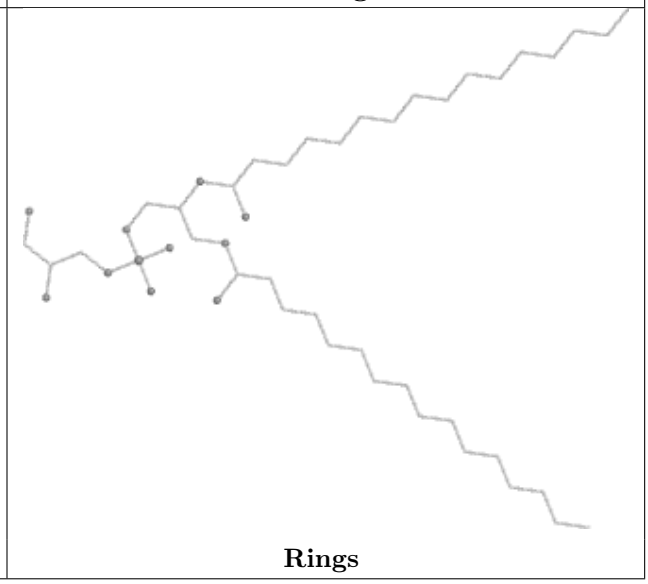
Bond lengths



Bond angles

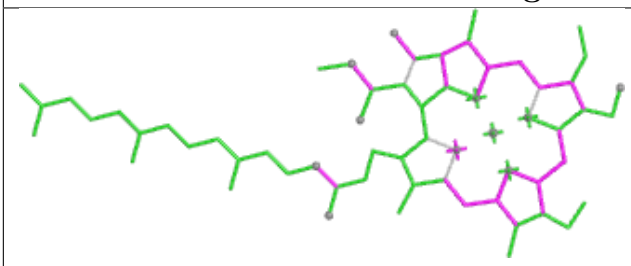


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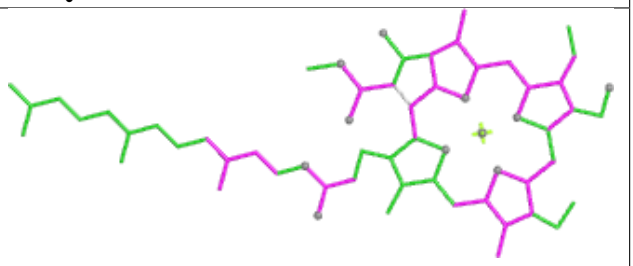


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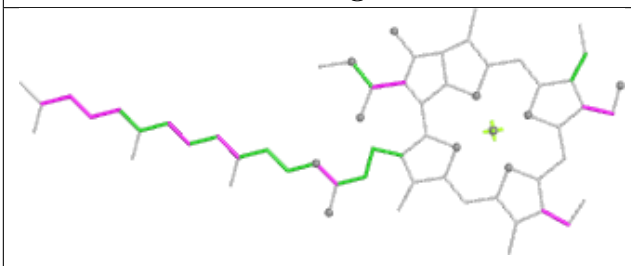
Ligand CHL Q 316



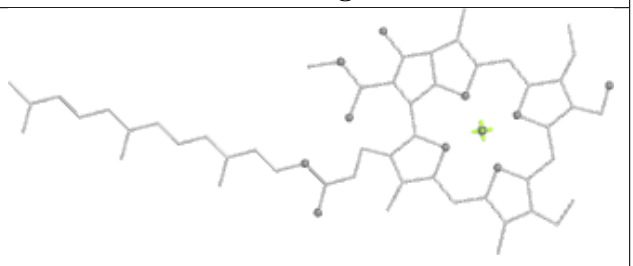
Bond lengths



Bond angles

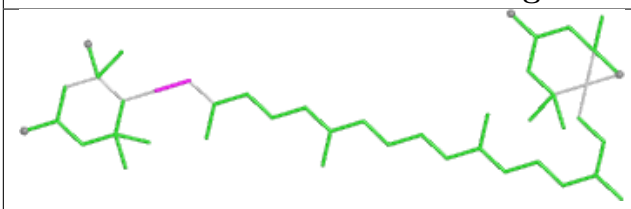


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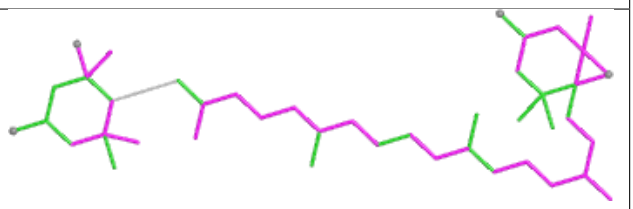


Rings

Ligand NEX P 301



Bond lengths



Bond angles

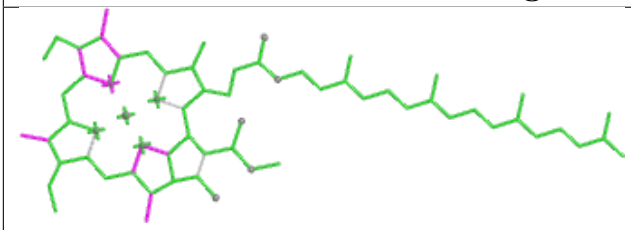


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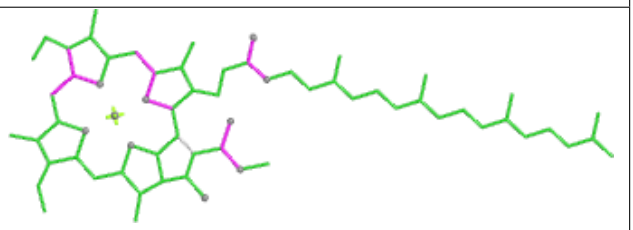


Rings

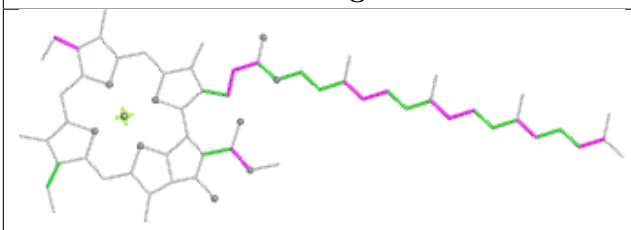
Ligand CLA U 307



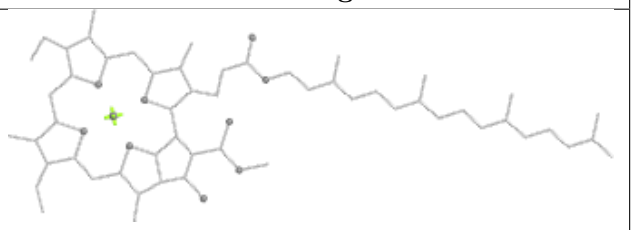
Bond lengths



Bond angles

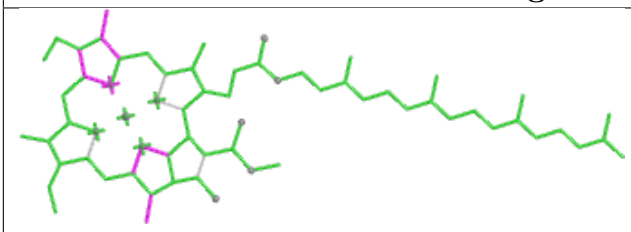


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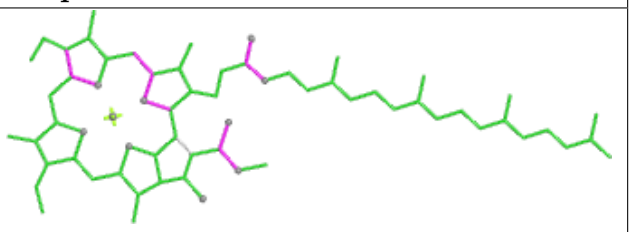


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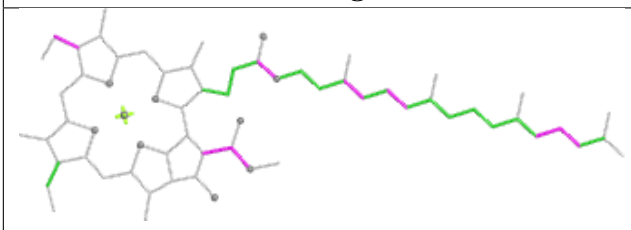
Ligand CLA q 302



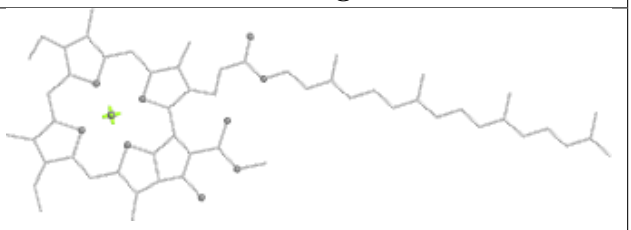
Bond lengths



Bond angles

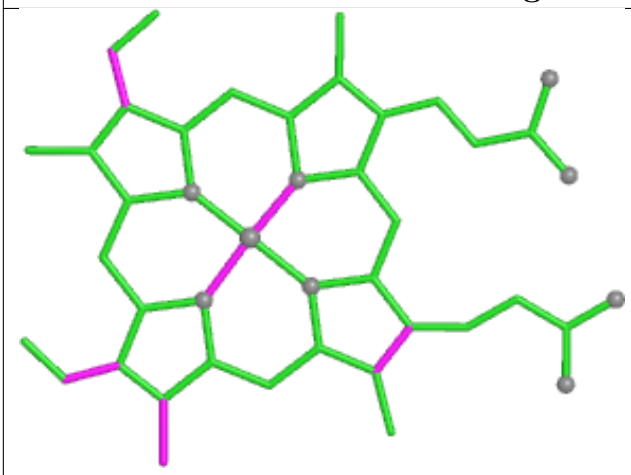


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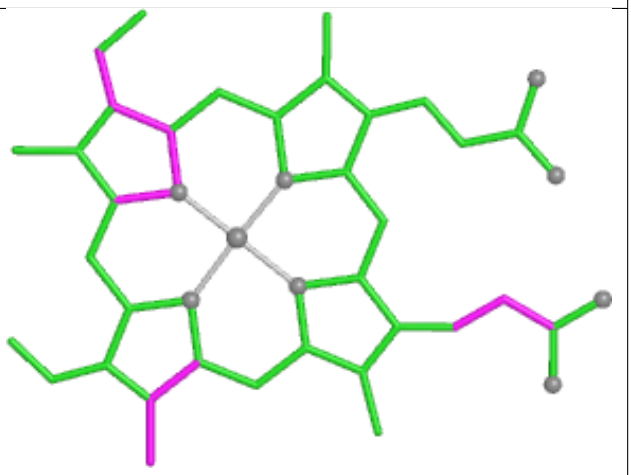


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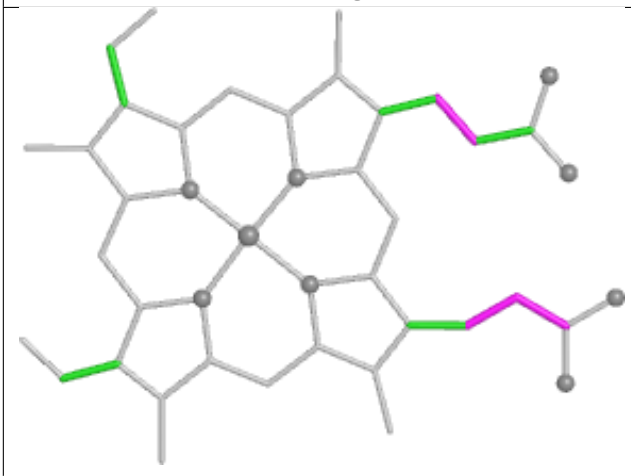
Ligand HEM e 101



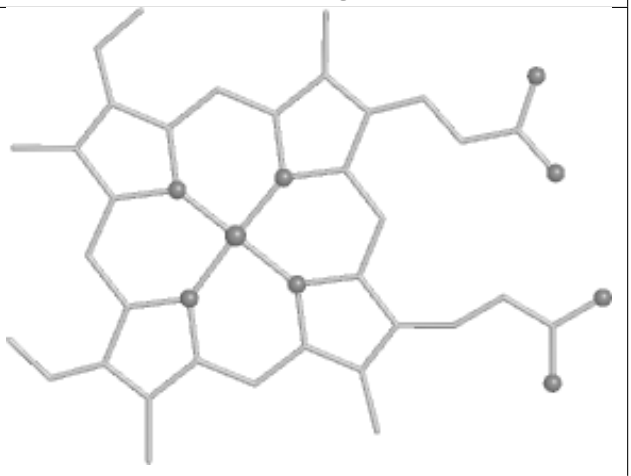
Bond lengths



Bond angles

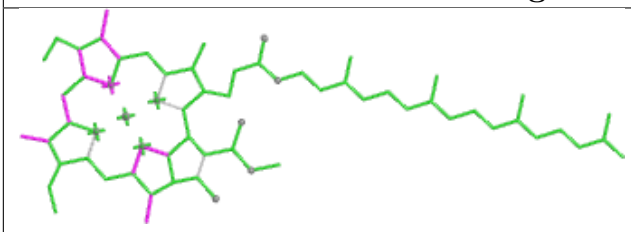


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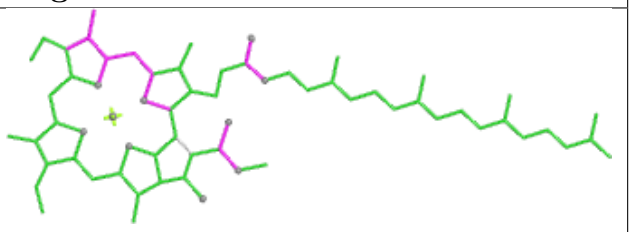


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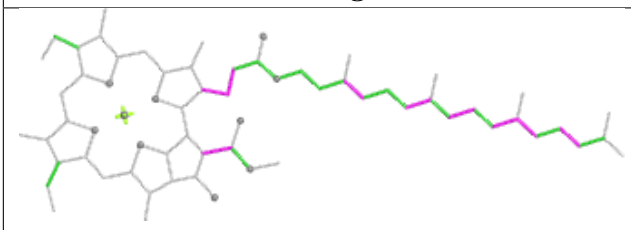
Ligand CLA g 301



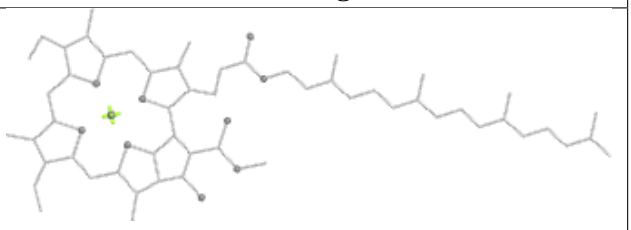
Bond lengths



Bond angles



Torsions

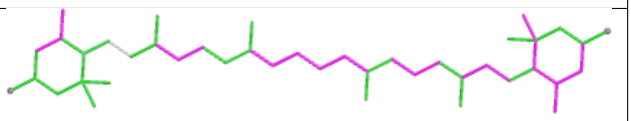


Rings

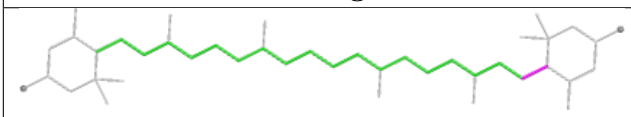
Ligand LUT 1 309



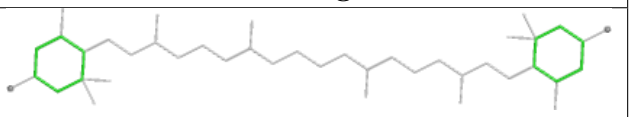
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Bond angles

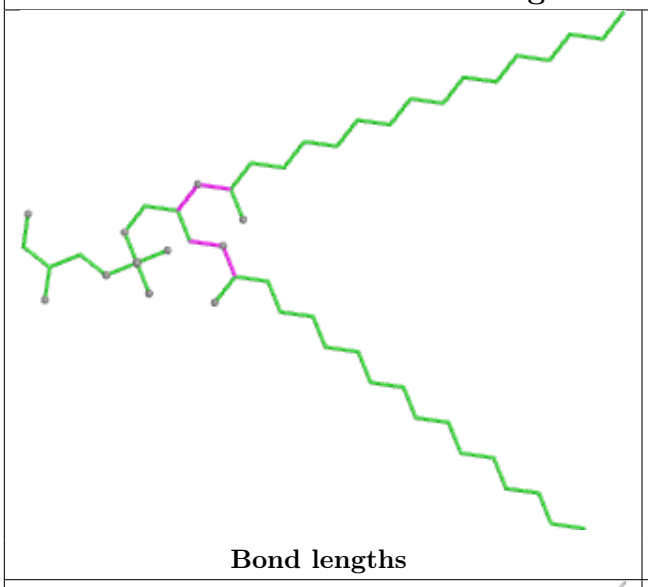


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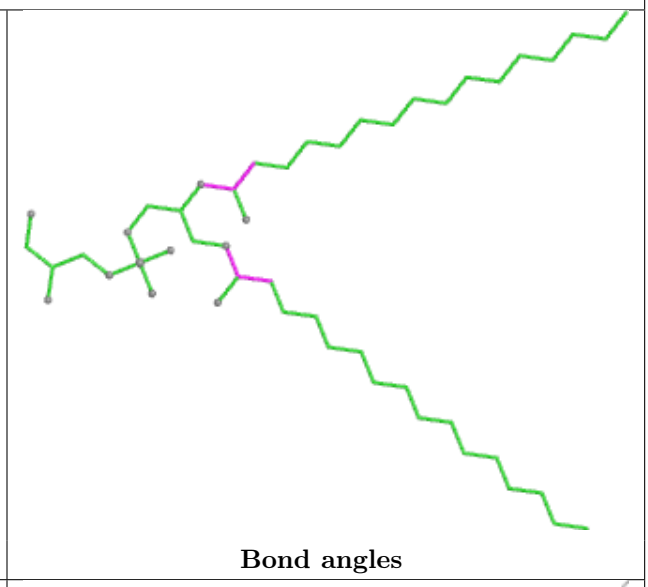


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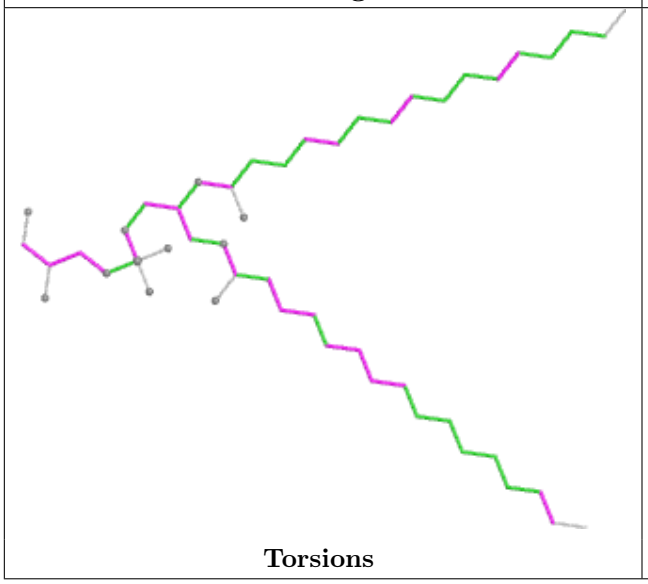
Ligand LHG 2 312



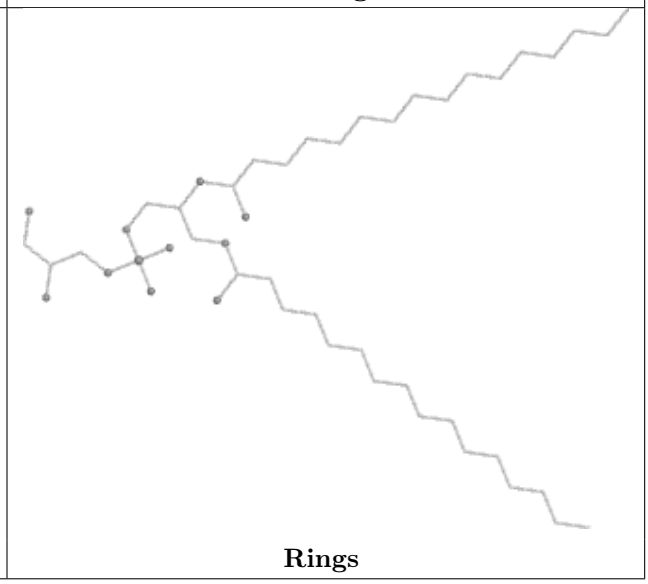
Bond lengths



Bond angles

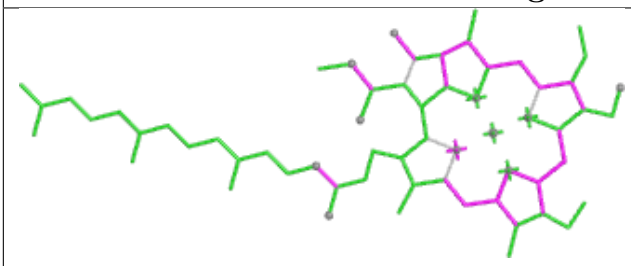


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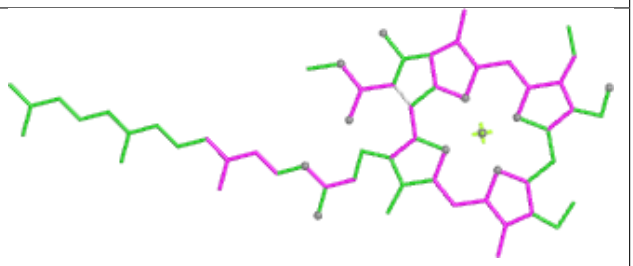


Rings

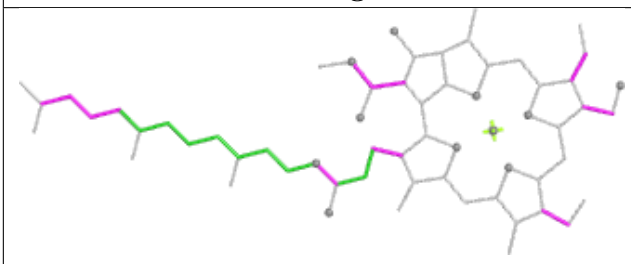
Ligand CHL 6 317



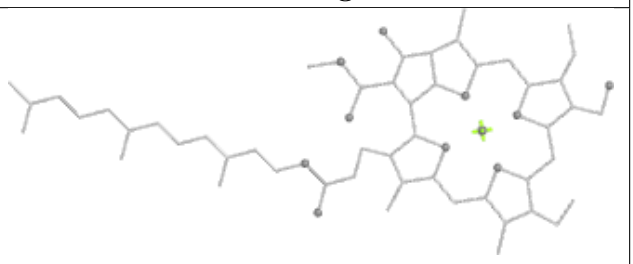
Bond lengths



Bond angles

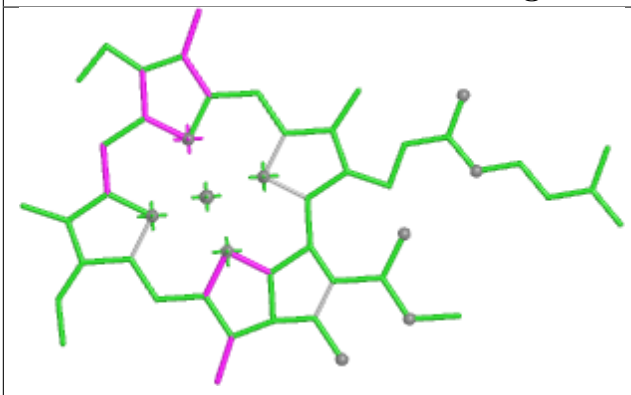


Torsions

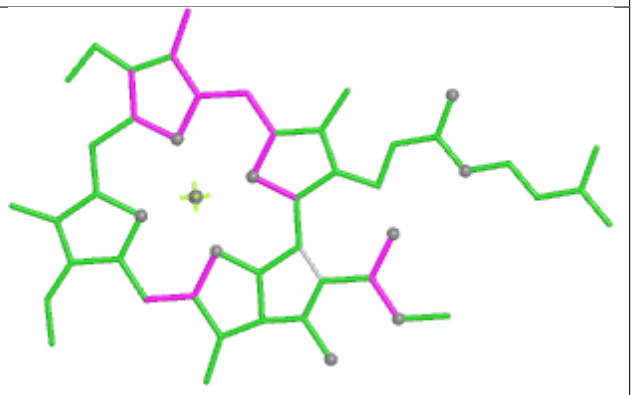


Rings

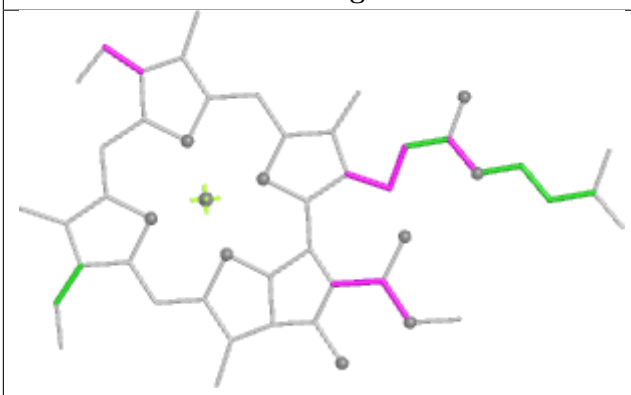
Ligand CLA G 303



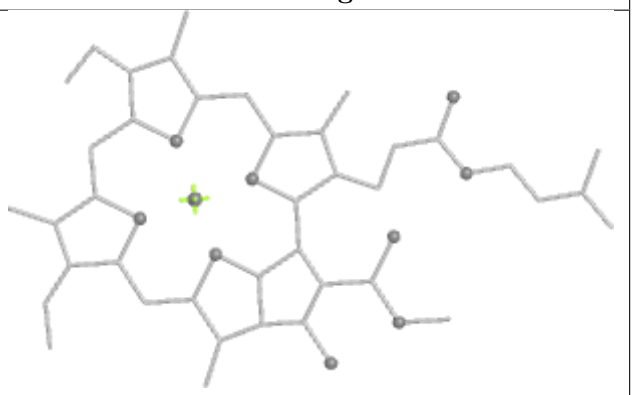
Bond lengths



Bond angles

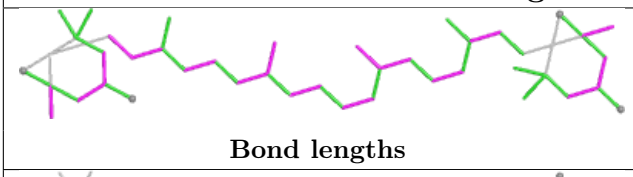


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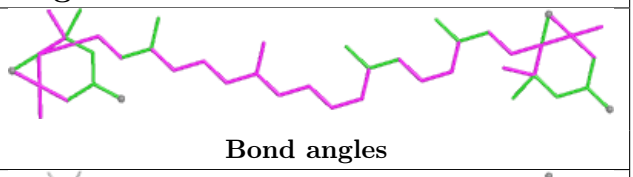


Rings

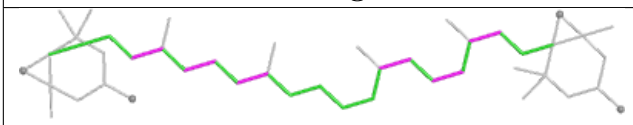
Ligand XAT g 309



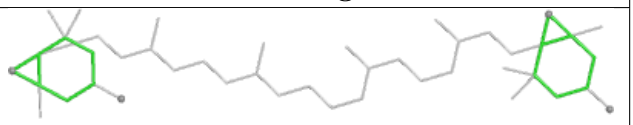
Bond lengths



Bond angles

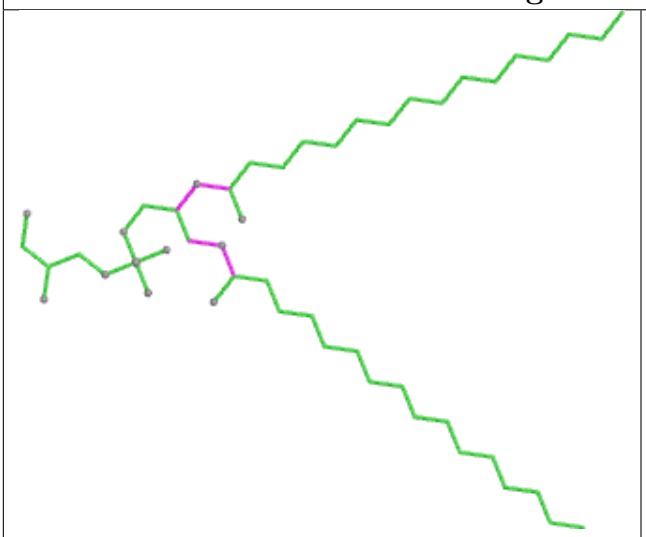


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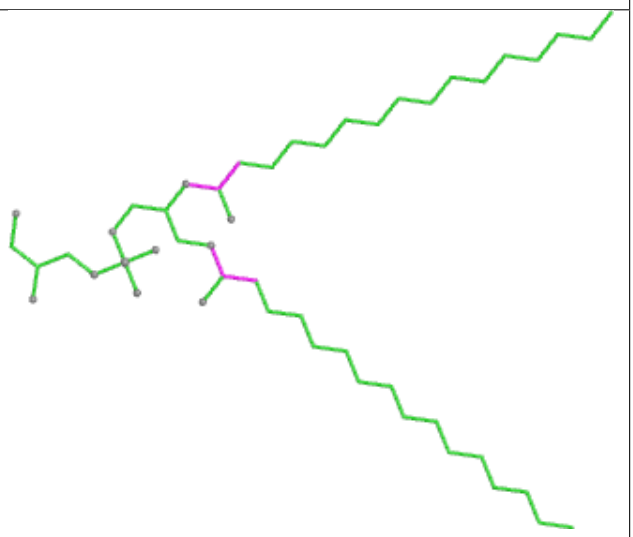


Rings

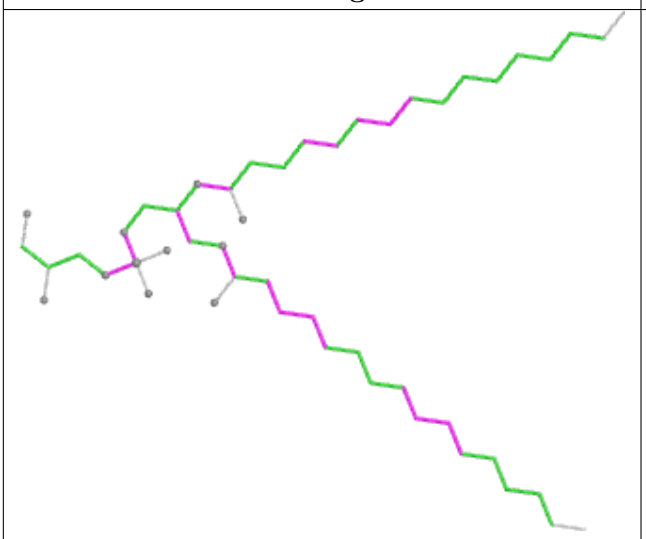
Ligand LHG v 312



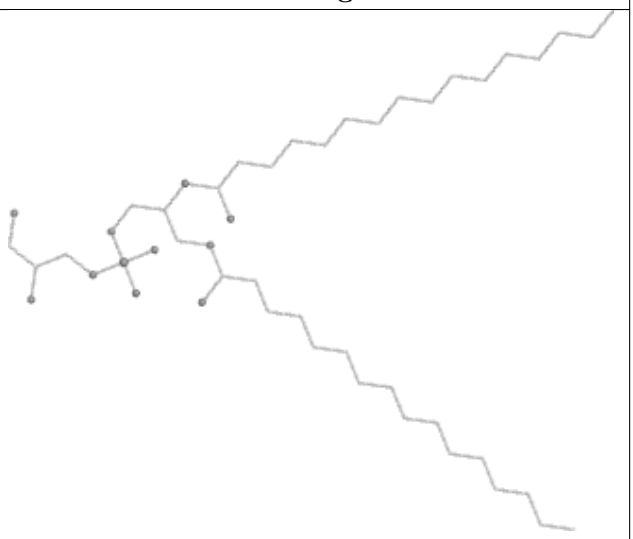
Bond lengths



Bond angles

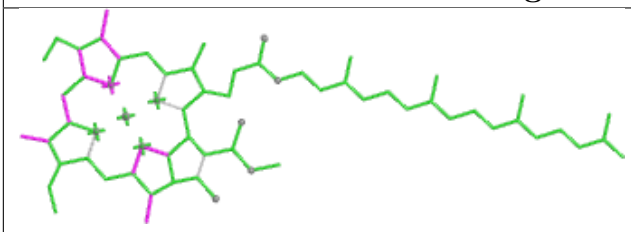


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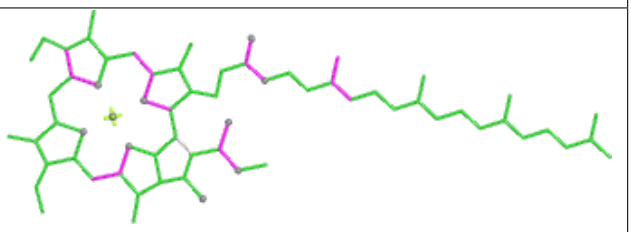


Rings

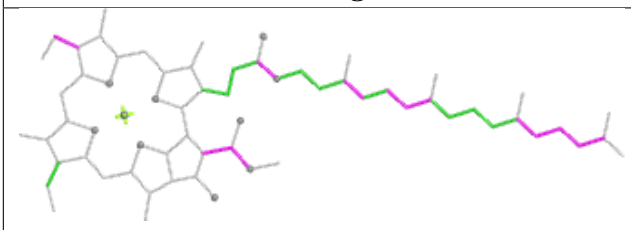
Ligand CLA B 610



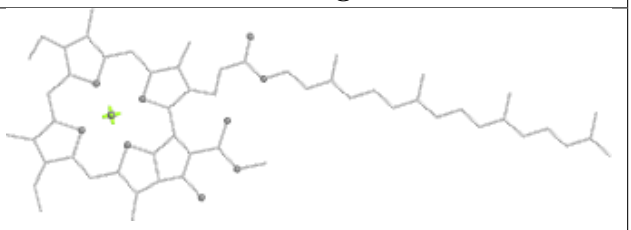
Bond lengths



Bond angles

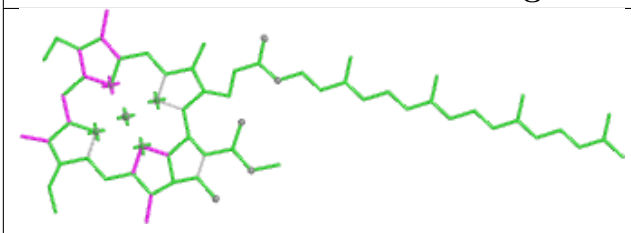


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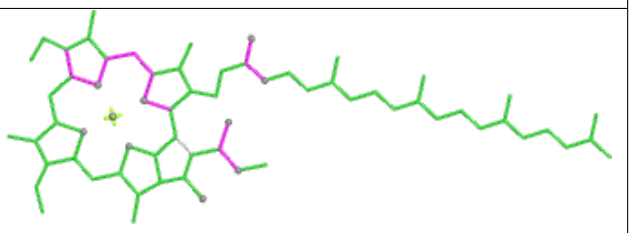


Rings

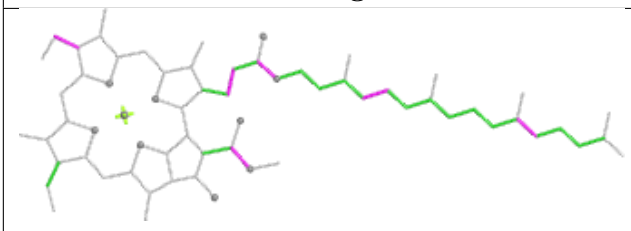
Ligand CLA V 307



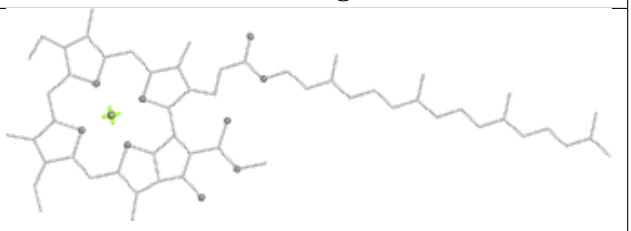
Bond lengths



Bond angles

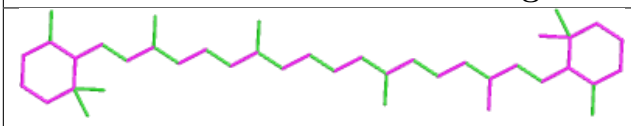


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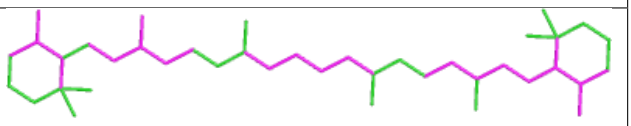


Rings

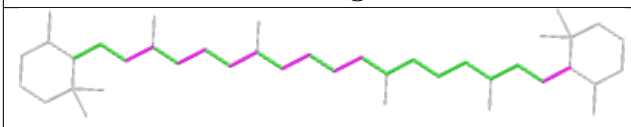
Ligand BCR X 201



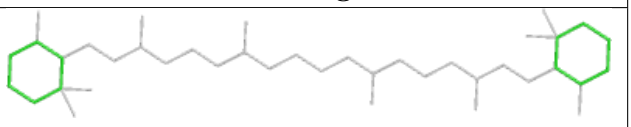
Bond lengths



Bond angles

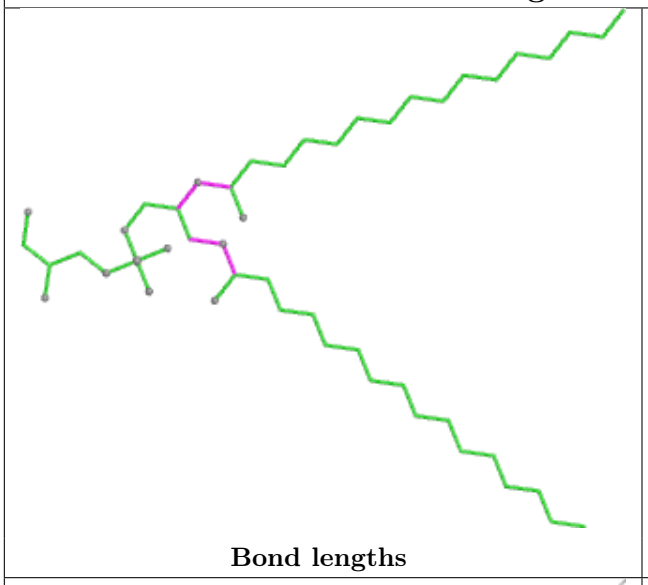


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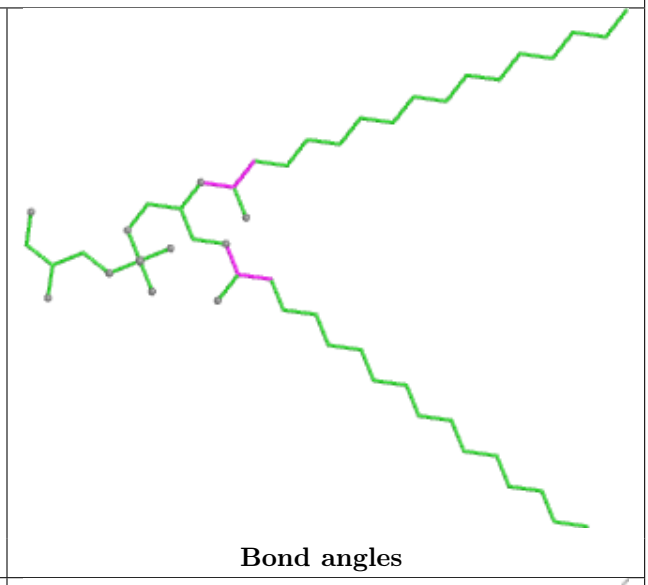


Rings

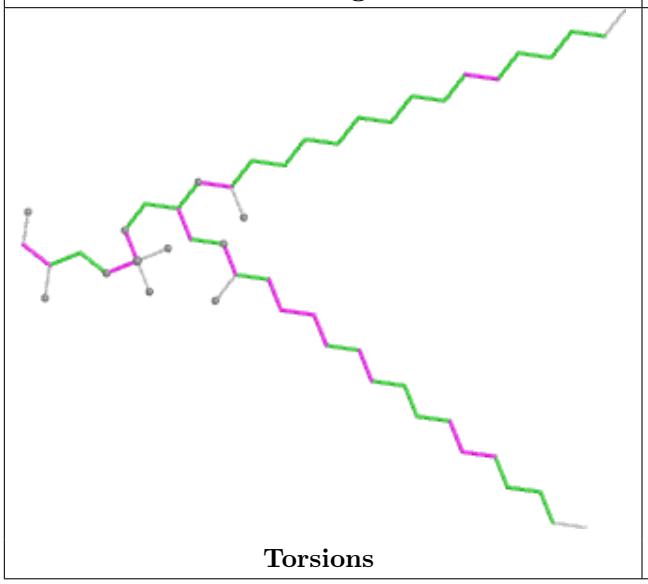
Ligand LHG 3 310



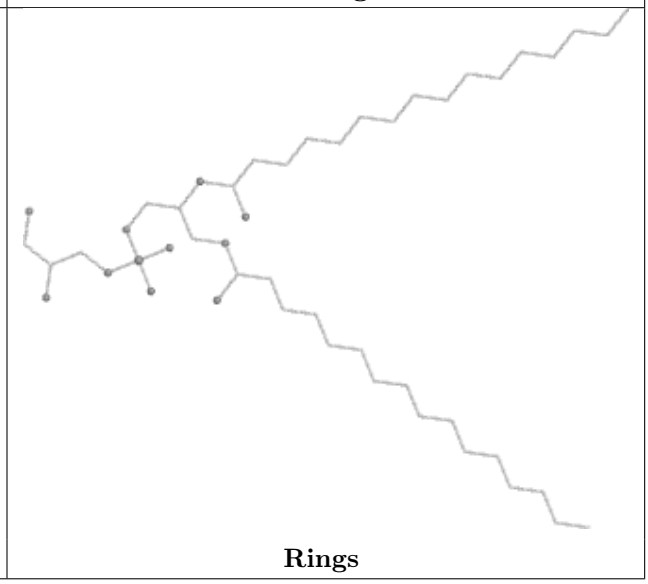
Bond lengths



Bond angles

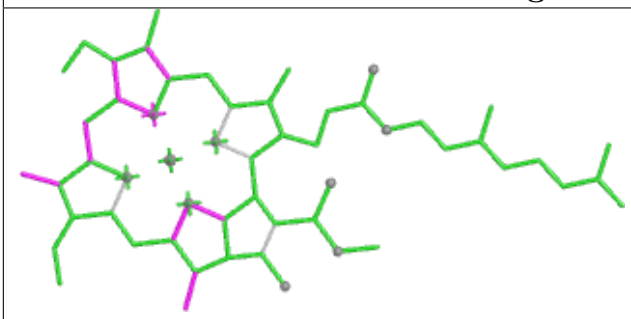


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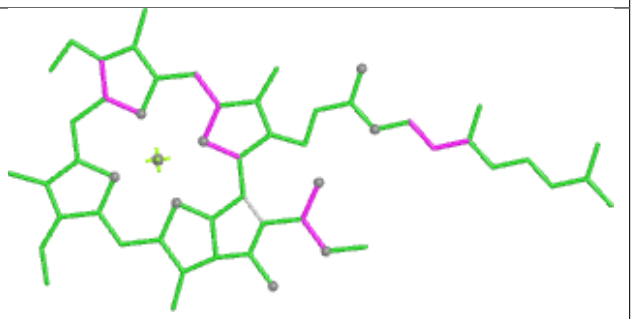


Rings

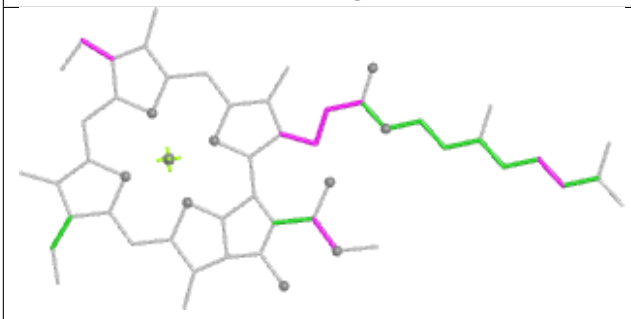
Ligand CLA S 305



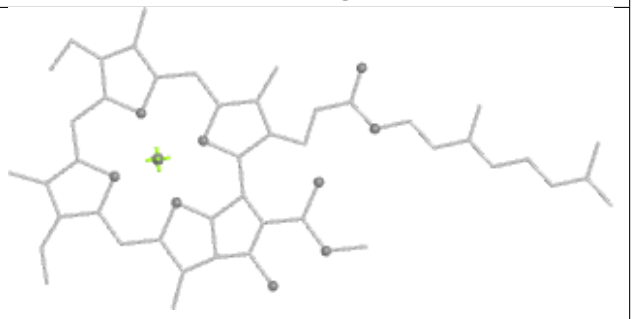
Bond lengths



Bond angles

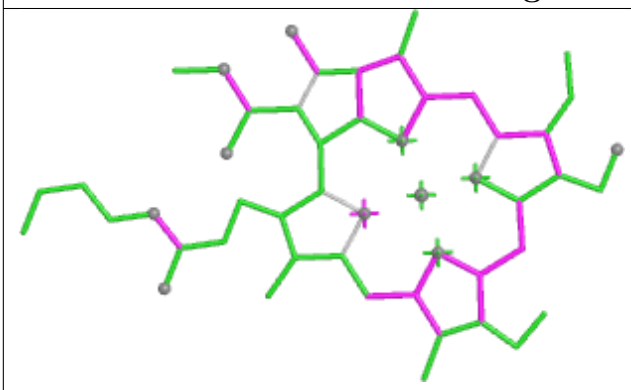


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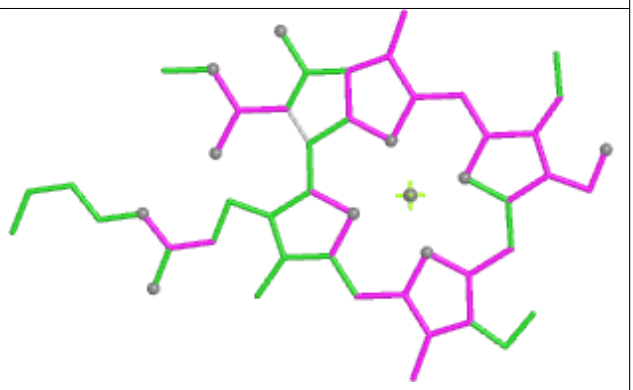


Rings

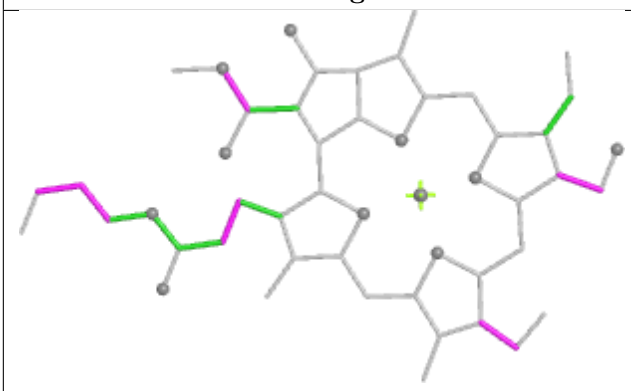
Ligand CHL V 315



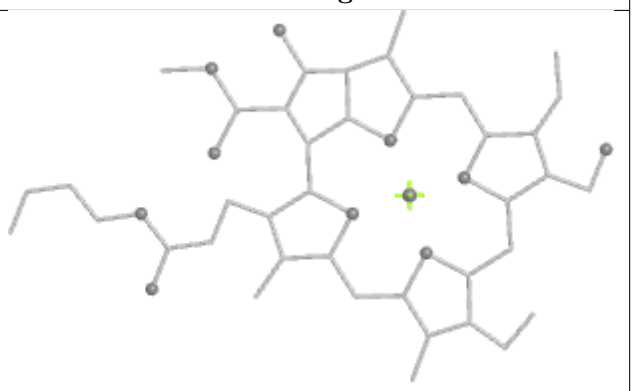
Bond lengths



Bond angles

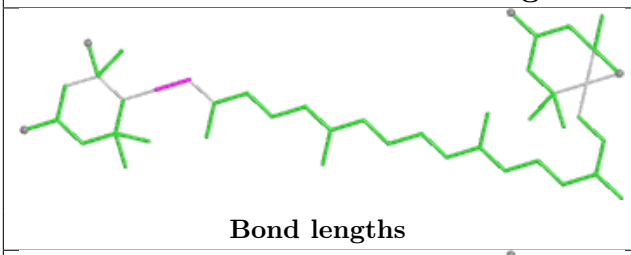


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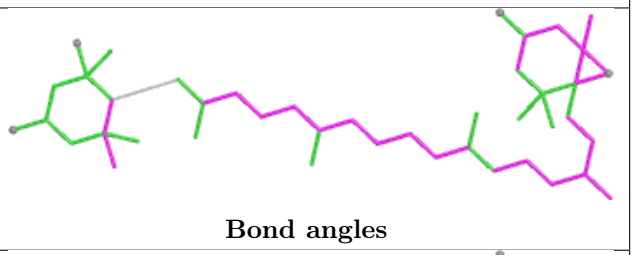


Rings

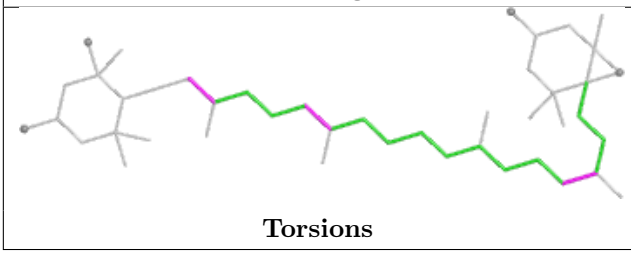
Ligand NEX V 319



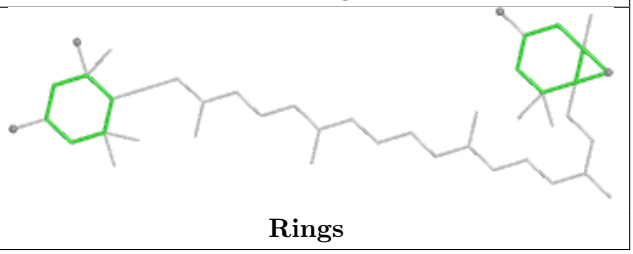
Bond lengths



Bond angles

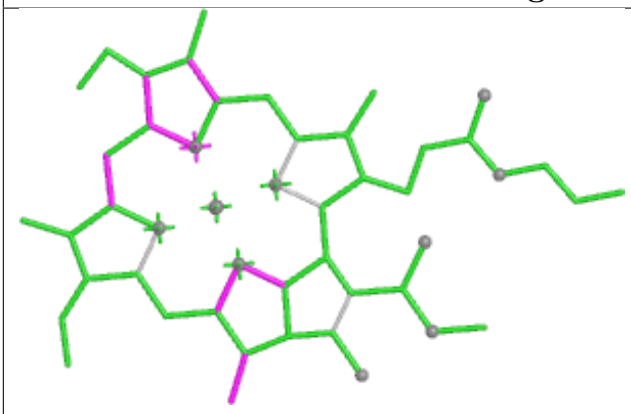


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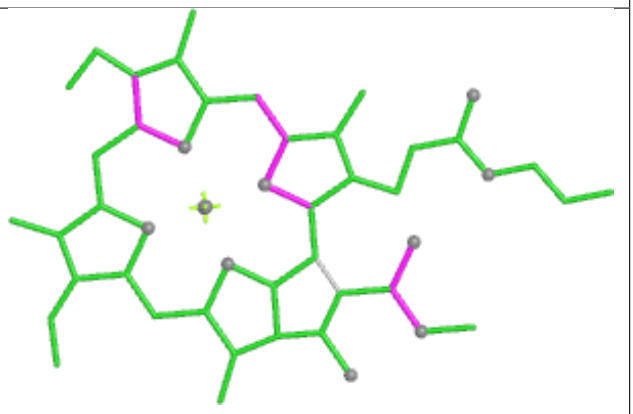


Rings

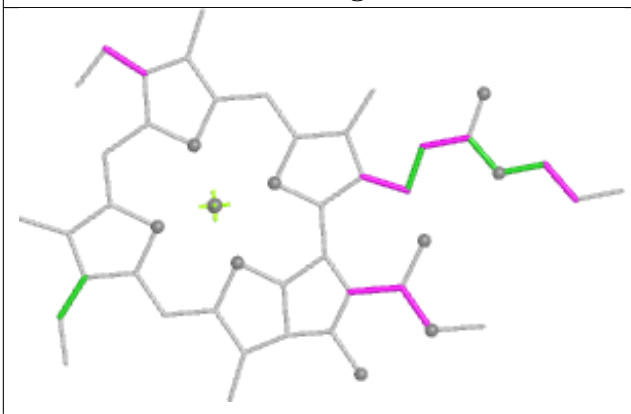
Ligand CLA v 308



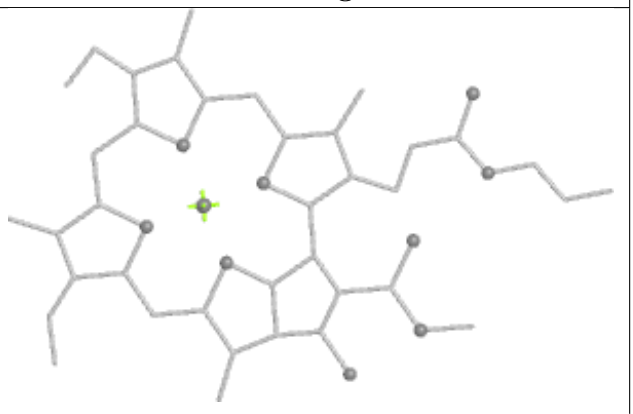
Bond lengths



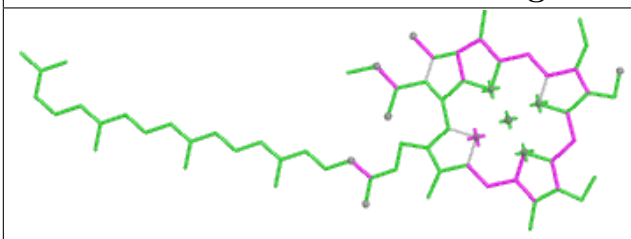
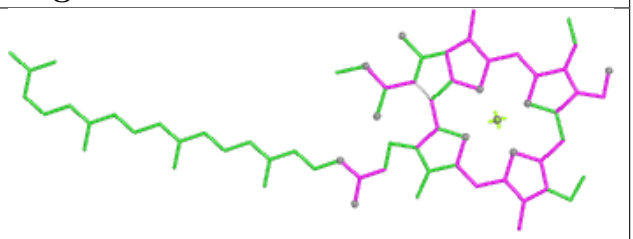
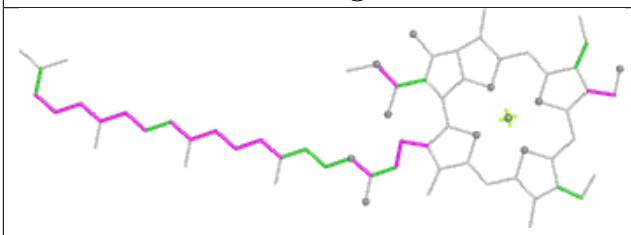
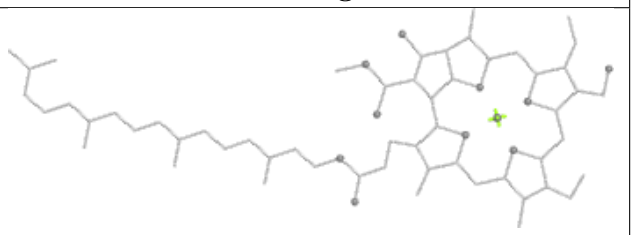
Bond angles

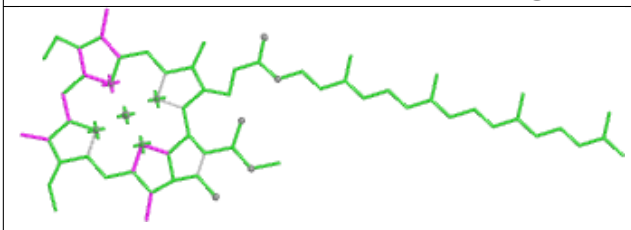
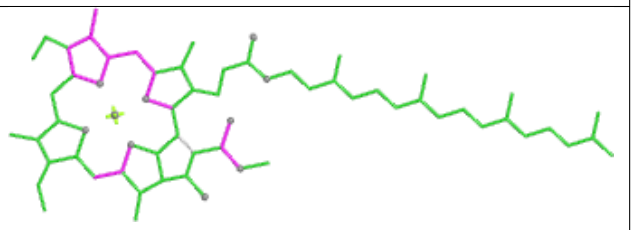
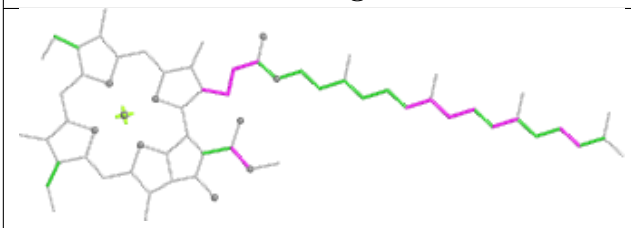
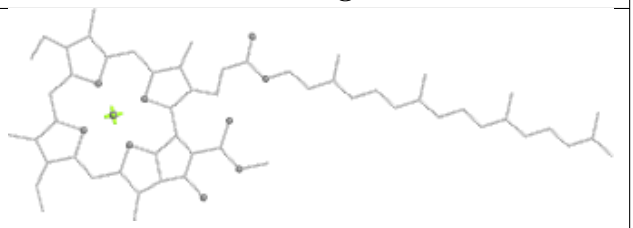


Torsions

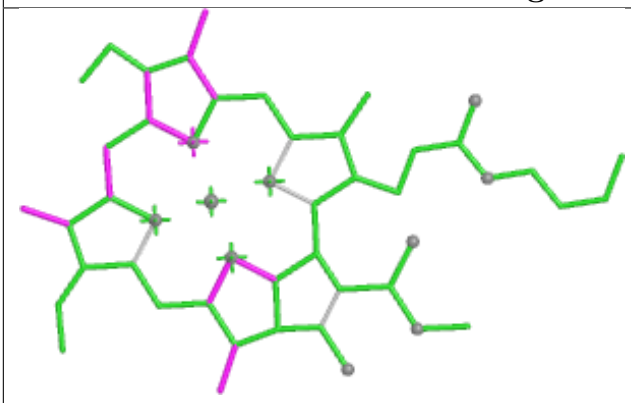


Rings

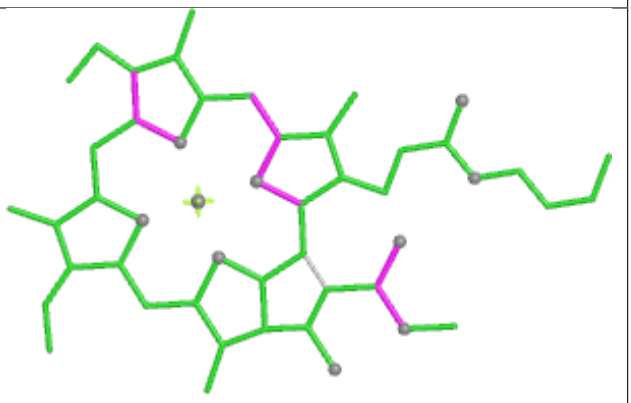
Ligand CHL g 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

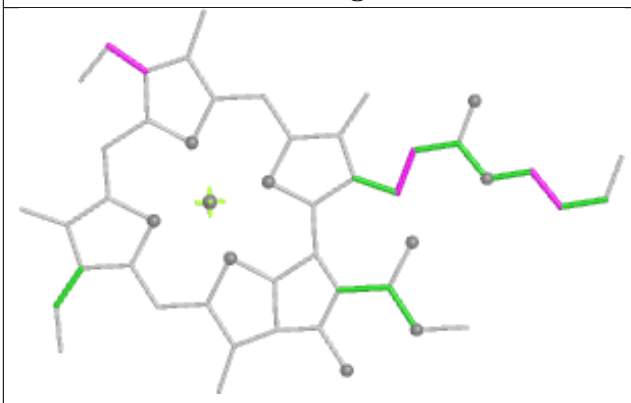
Ligand CLA S 309



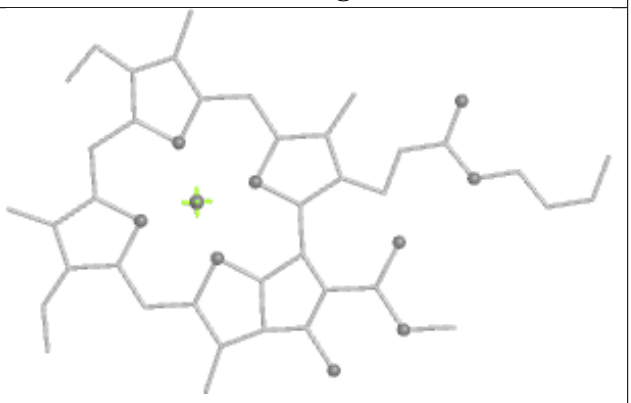
Bond lengths



Bond angles

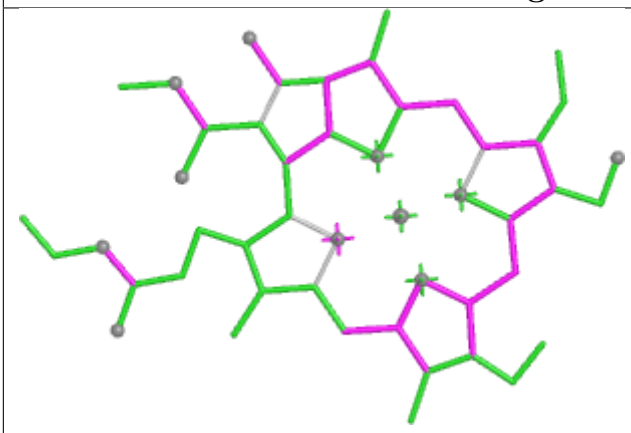


Torsions

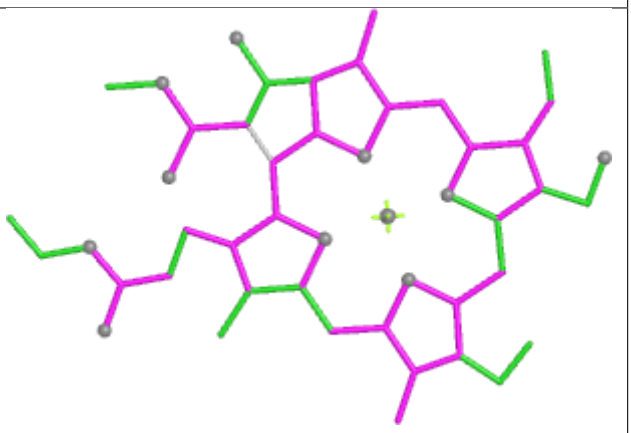


Rings

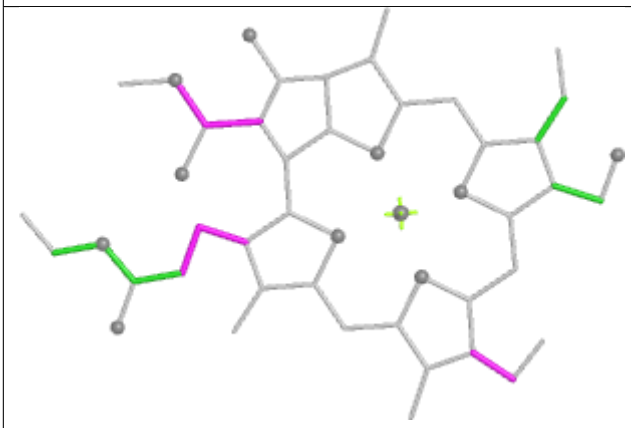
Ligand CHL 3 312



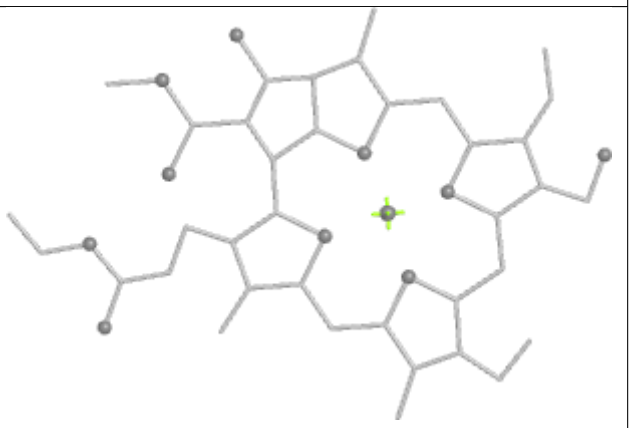
Bond lengths



Bond angles

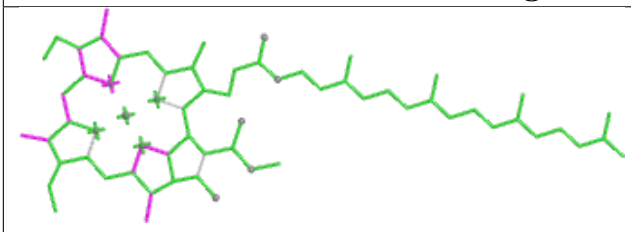


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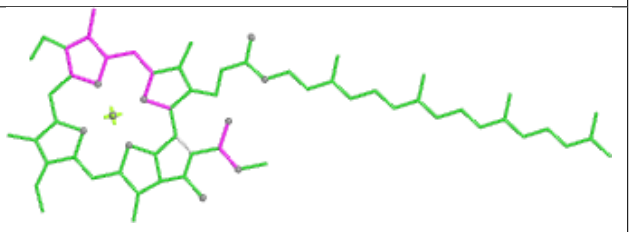


Rings

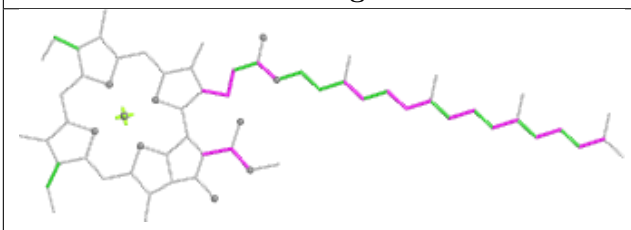
Ligand CLA G 301



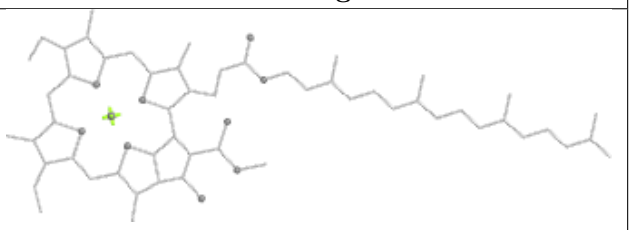
Bond lengths



Bond angles

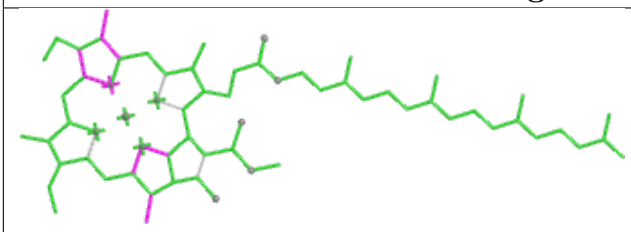


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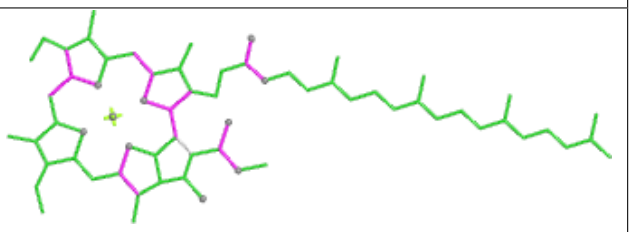


Rings

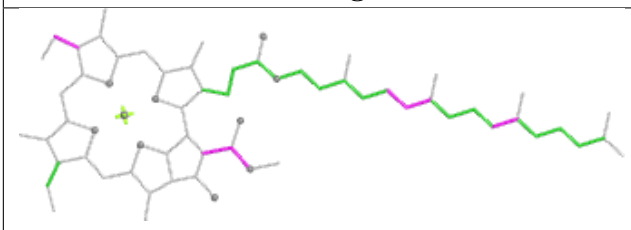
Ligand CLA b 616



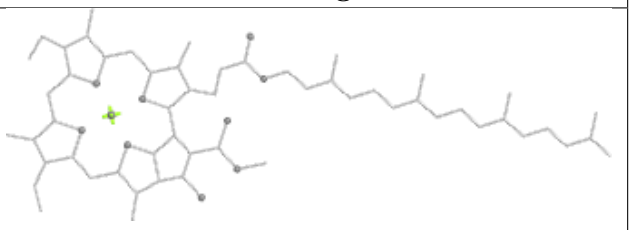
Bond lengths



Bond angles



Torsions

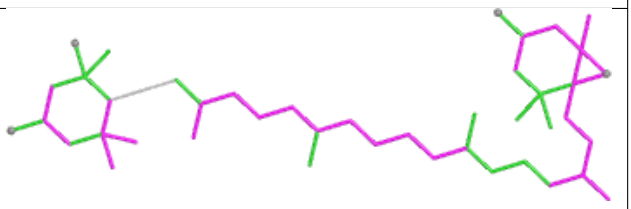


Rings

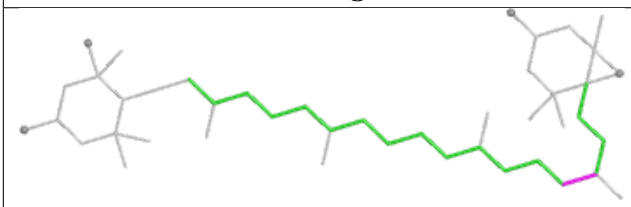
Ligand NEX u 320



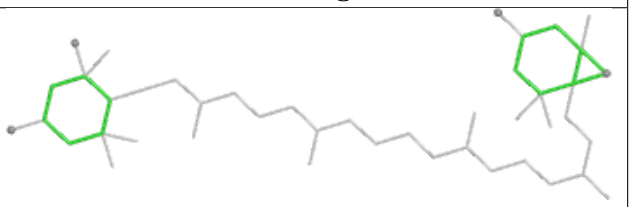
Bond lengths



Bond angles

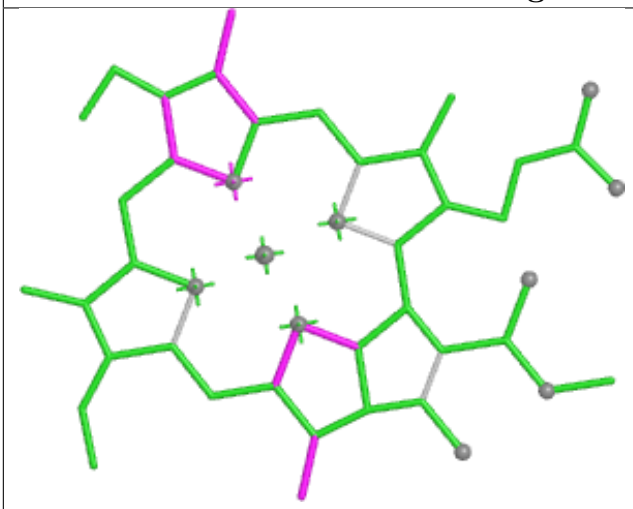


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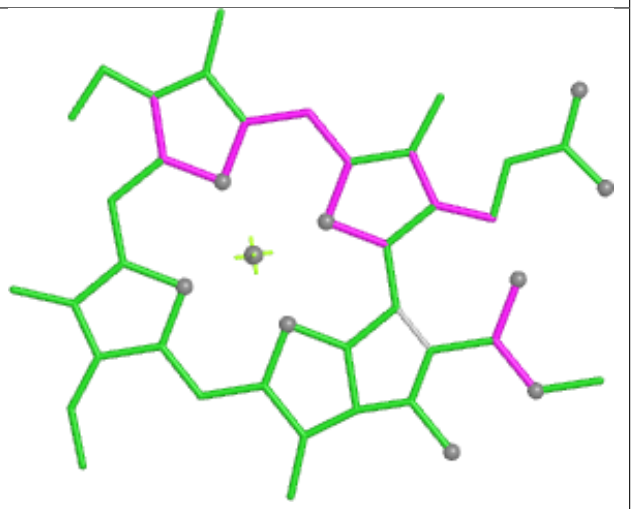


Rings

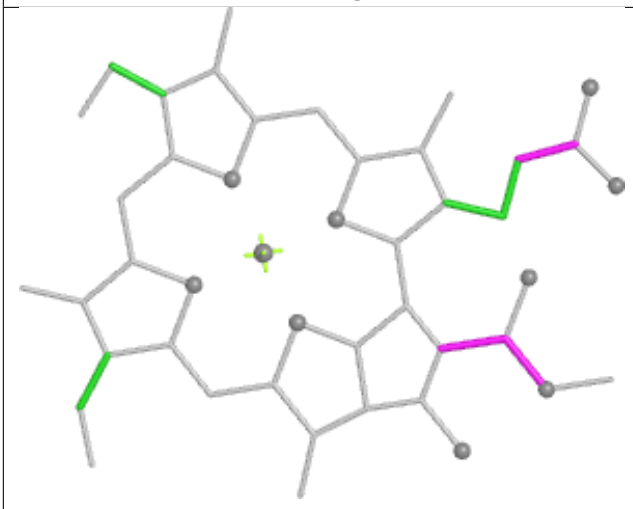
Ligand CLA S 302



Bond lengths



Bond angles

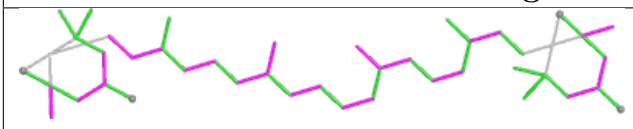


Torsions

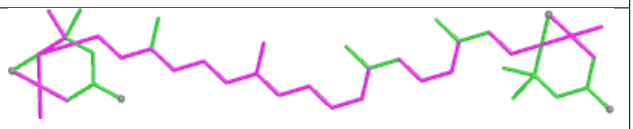


Rings

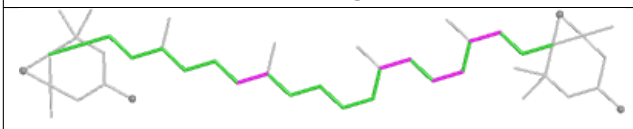
Ligand XAT U 311



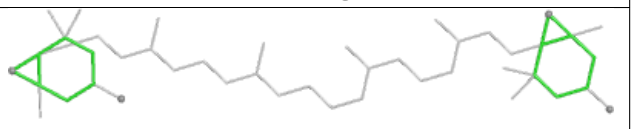
Bond lengths



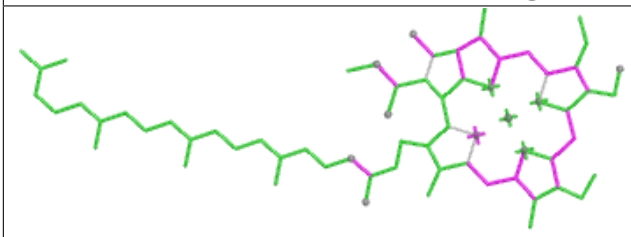
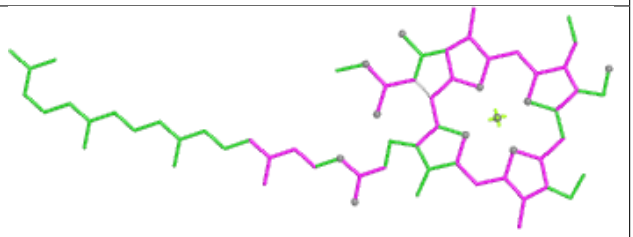
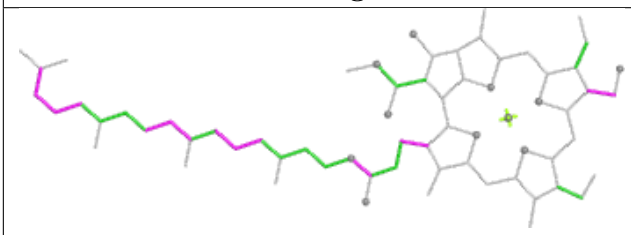
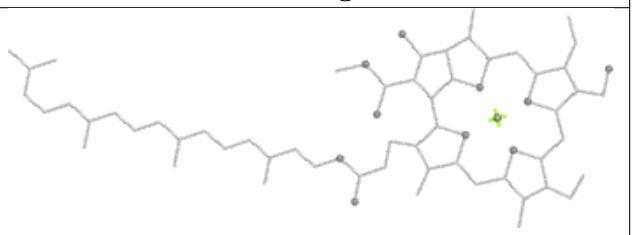
Bond angles

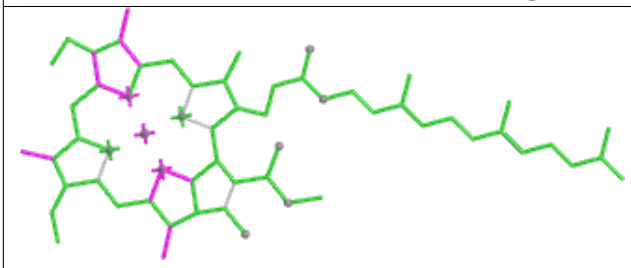
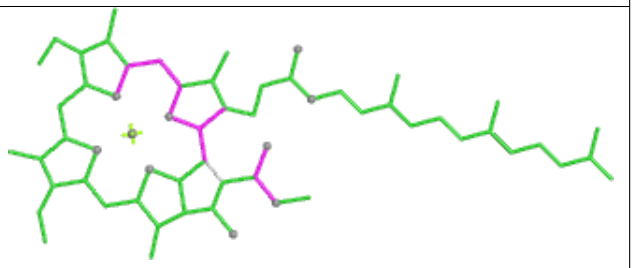
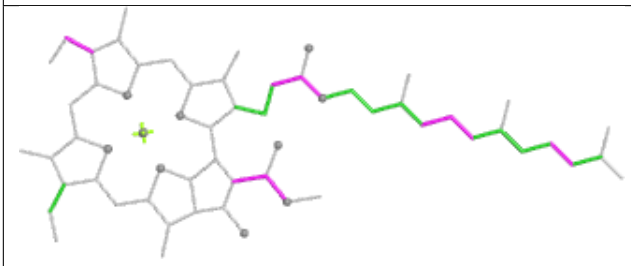
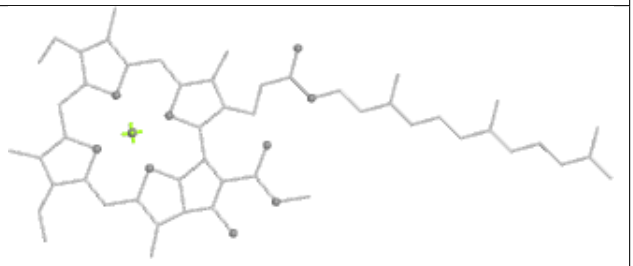


Torsions

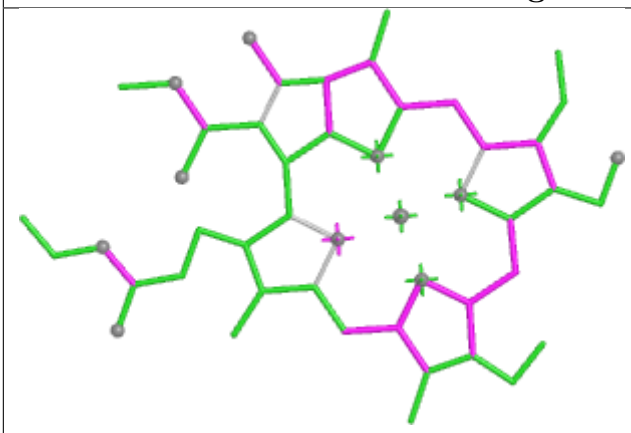


Rings

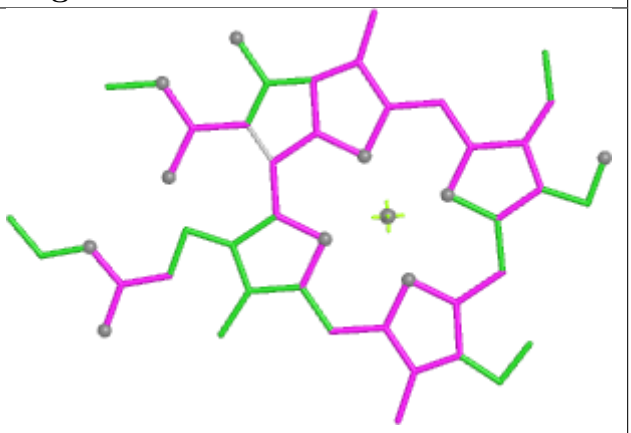
Ligand CHL V 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

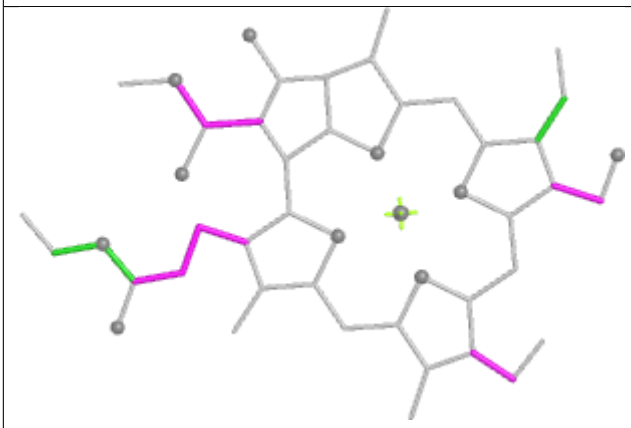
Ligand CHL g 312



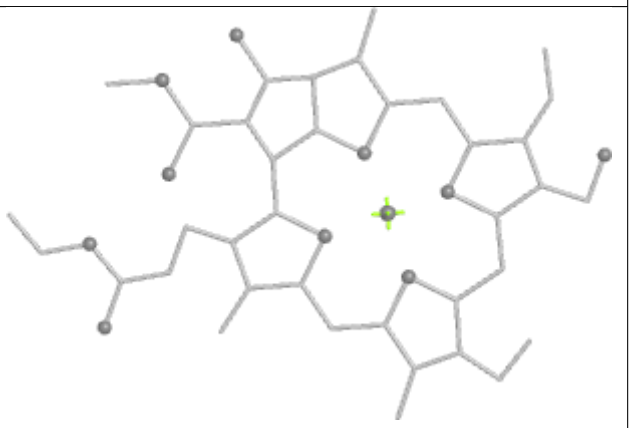
Bond lengths



Bond angles

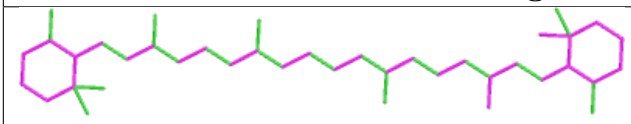


Torsions

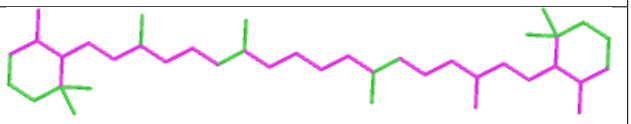


Rings

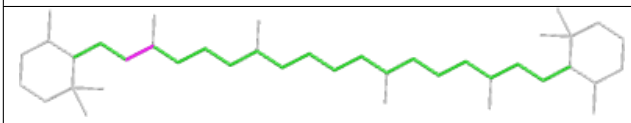
Ligand BCR a 409



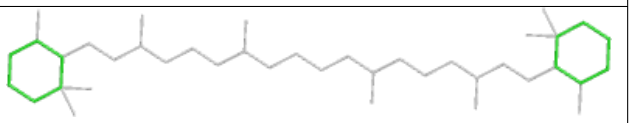
Bond lengths



Bond angles

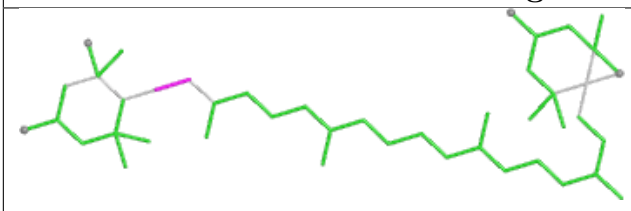


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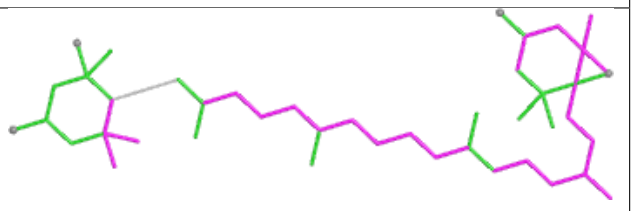


Rings

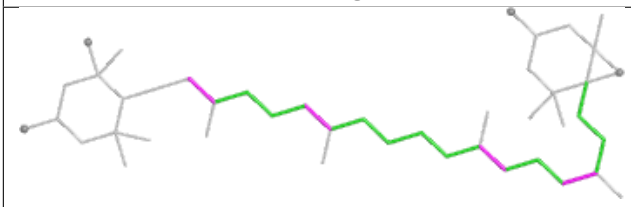
Ligand NEX 5 319



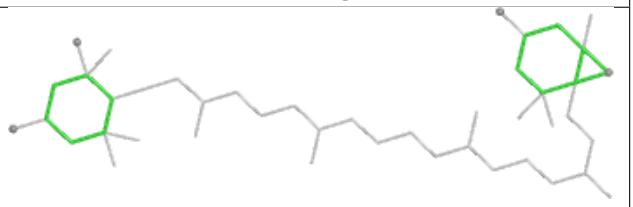
Bond lengths



Bond angles

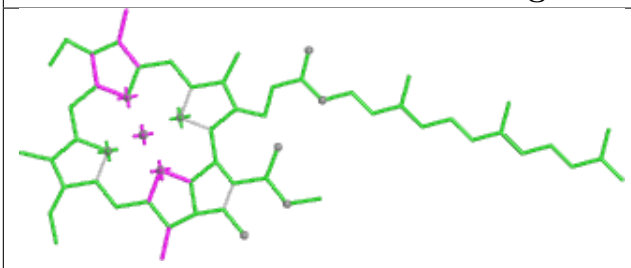


Torsions

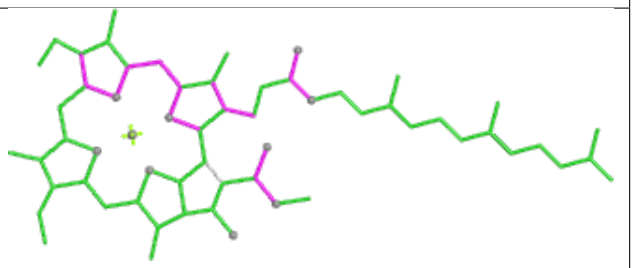


Rings

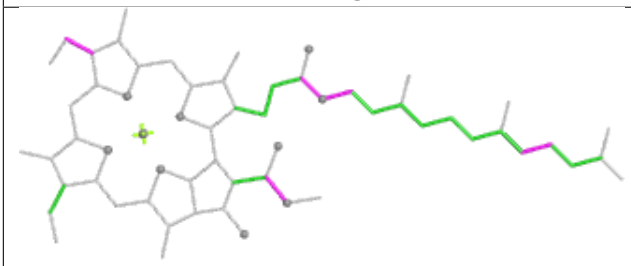
Ligand CLA 4 305



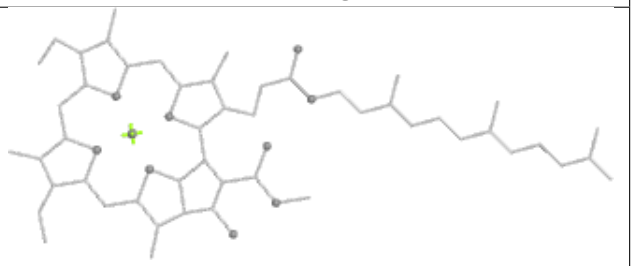
Bond lengths



Bond angles

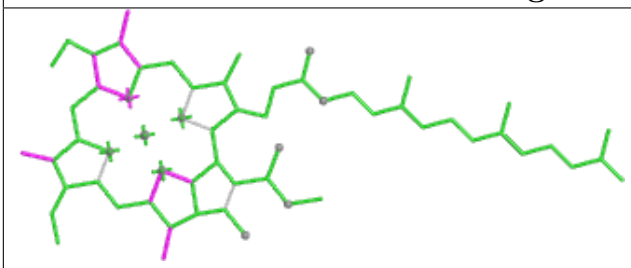


Torsions

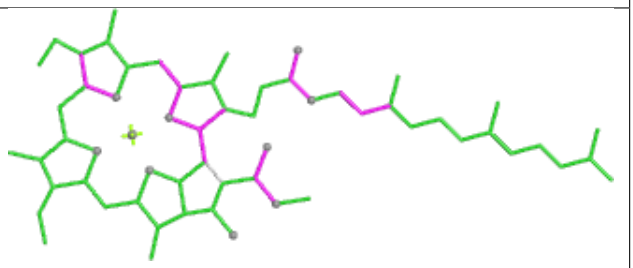


Rings

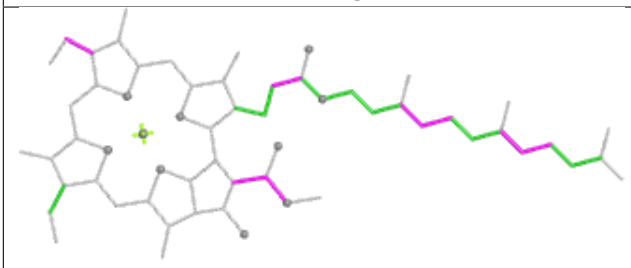
Ligand CLA v 306



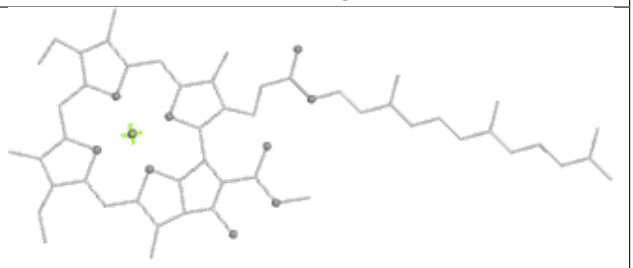
Bond lengths



Bond angles

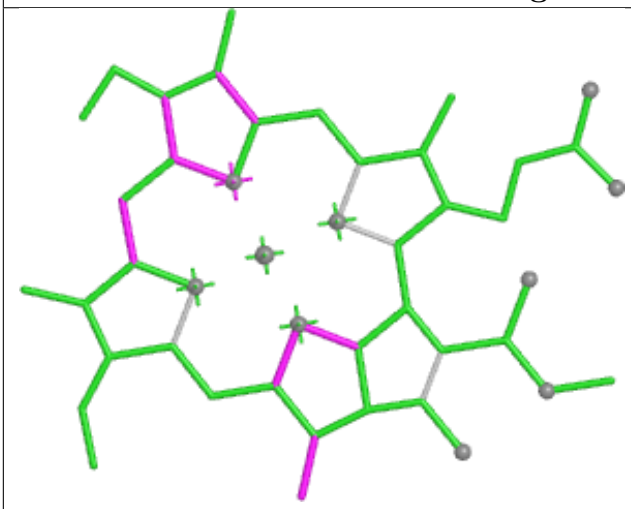


Torsions

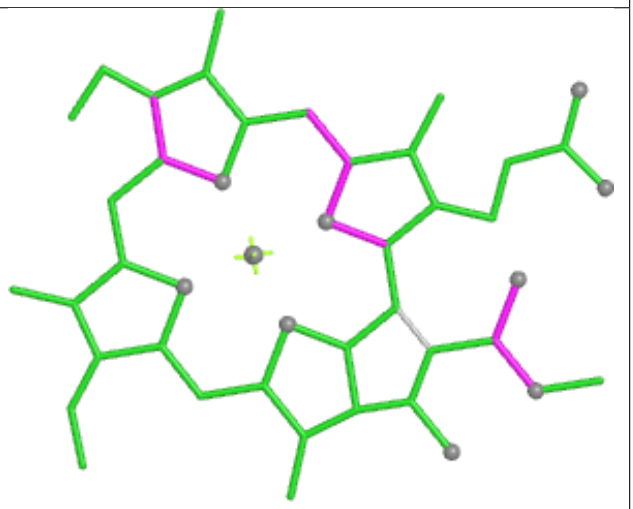


Rings

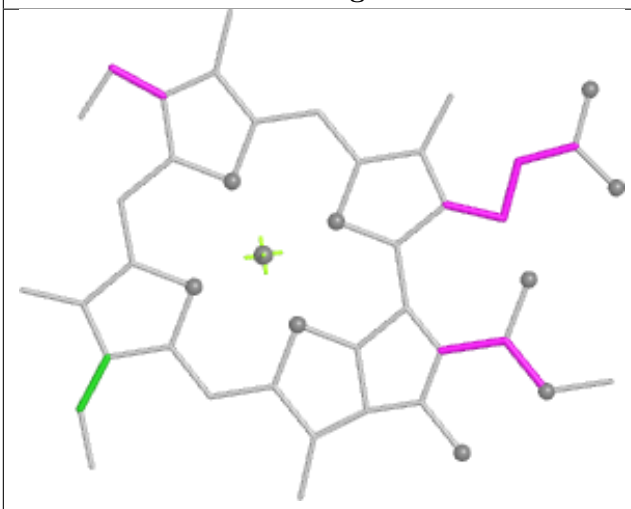
Ligand CLA s 304



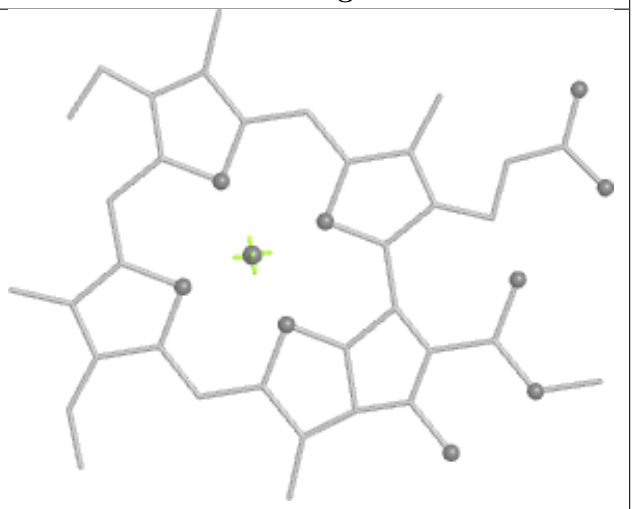
Bond lengths



Bond angles

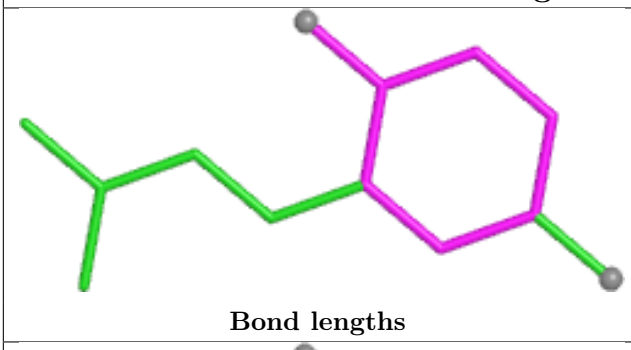


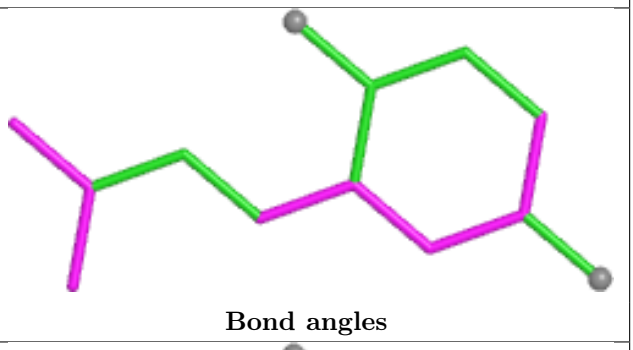
Torsions

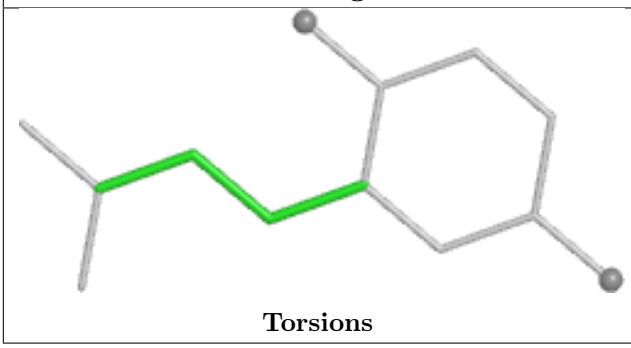


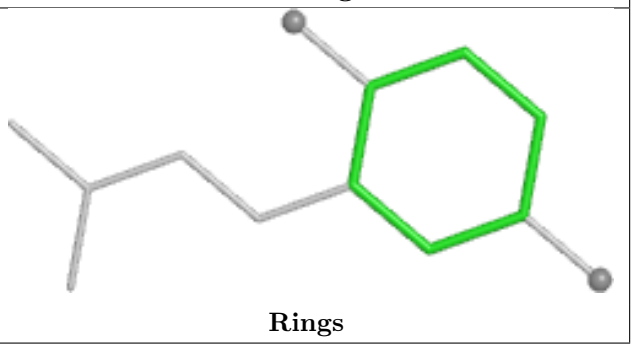
Rings

Ligand PL9 a 411

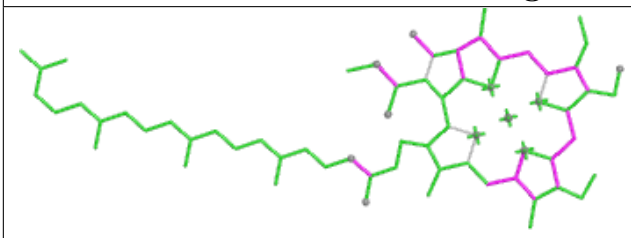

Bond lengths

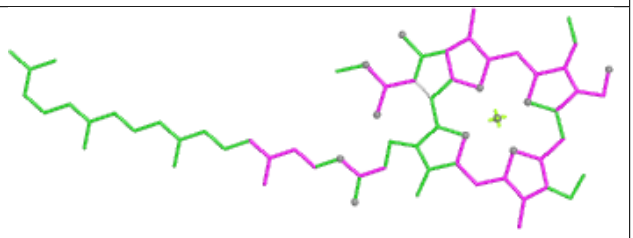

Bond angles

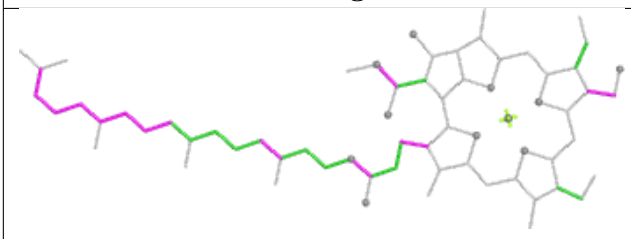

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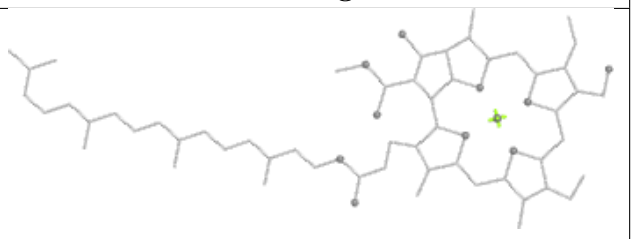

Rings

Ligand CHL R 315

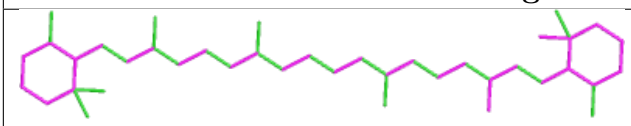

Bond lengths

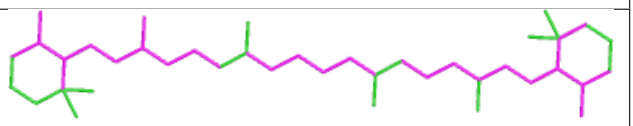

Bond angles

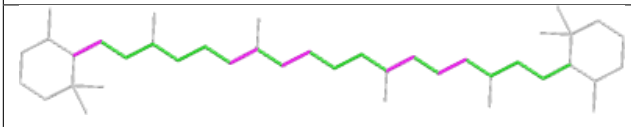

Torsions

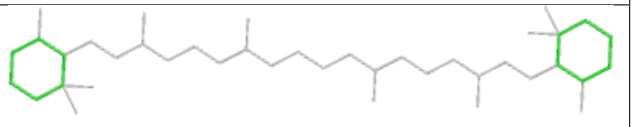

Rings

Ligand BCR C 516

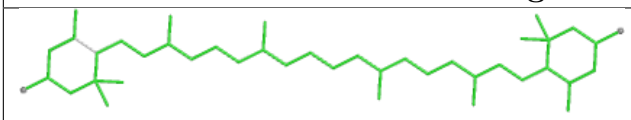

Bond lengths


Bond angles

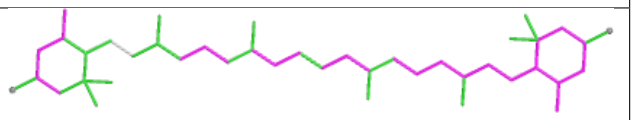

Torsions


Rings

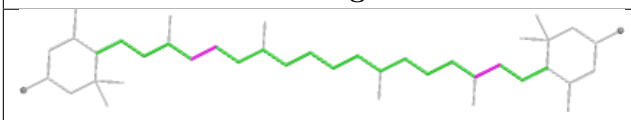
Ligand LUT n 310



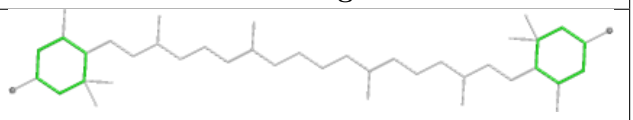
Bond lengths



Bond angles

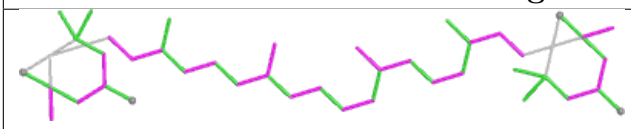


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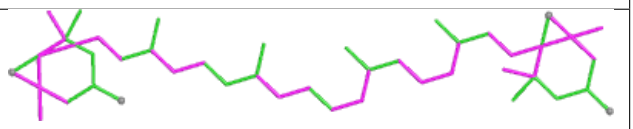


Rings

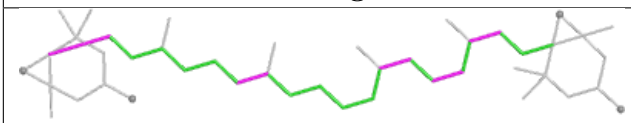
Ligand XAT 6 310



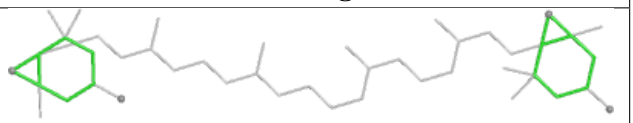
Bond lengths



Bond angles

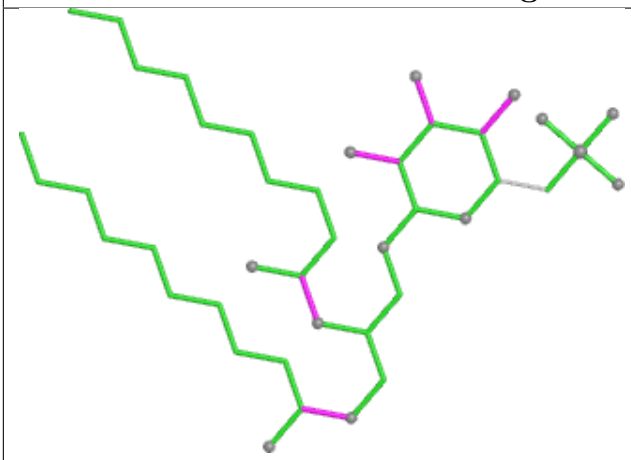


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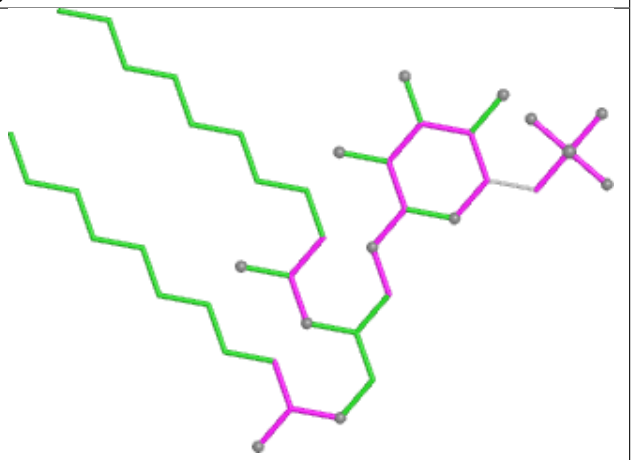


Rings

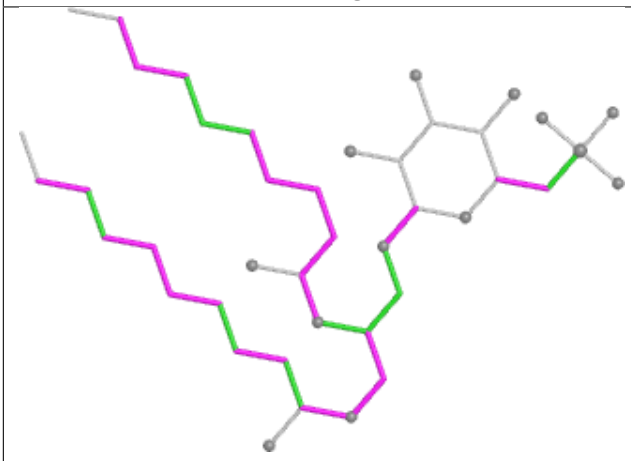
Ligand SQD M 101



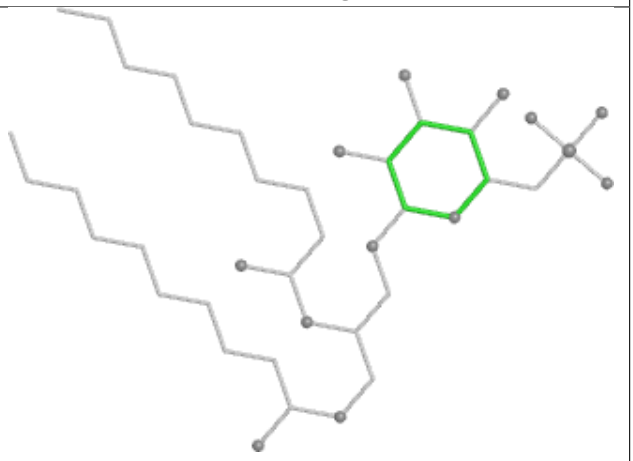
Bond lengths



Bond angles

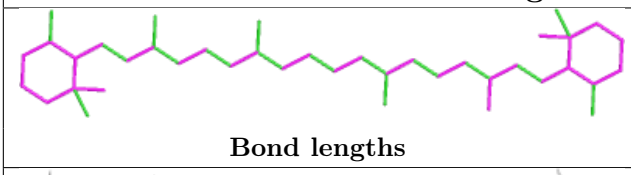


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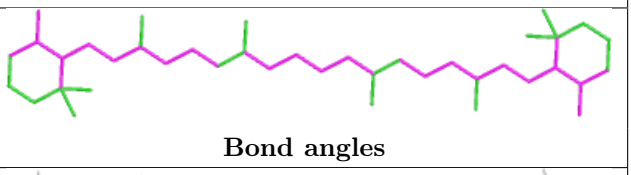


Rings

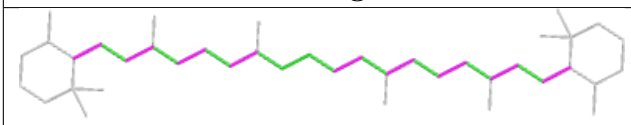
Ligand BCR k 101



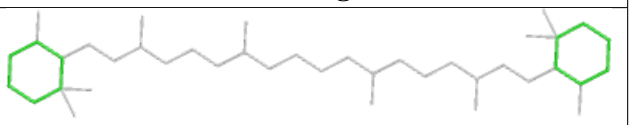
Bond lengths



Bond angles

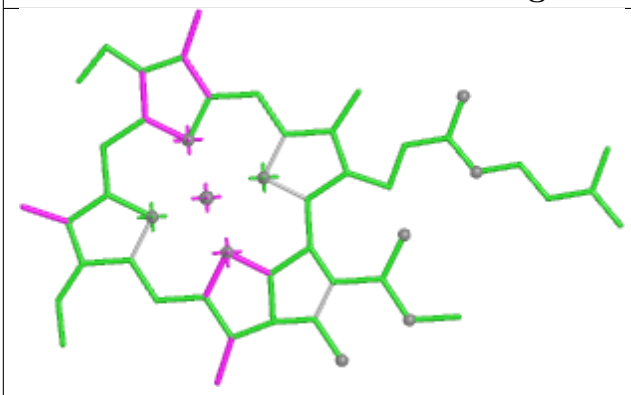


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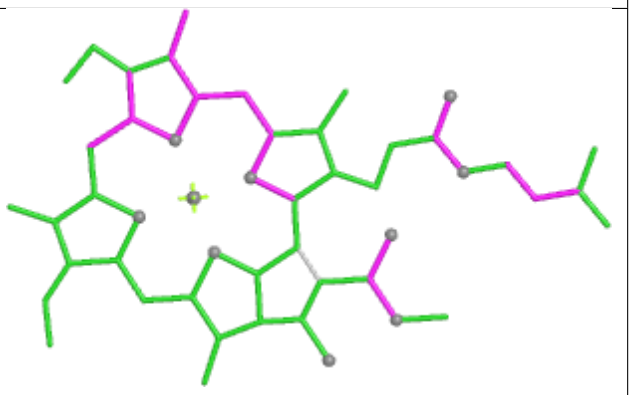


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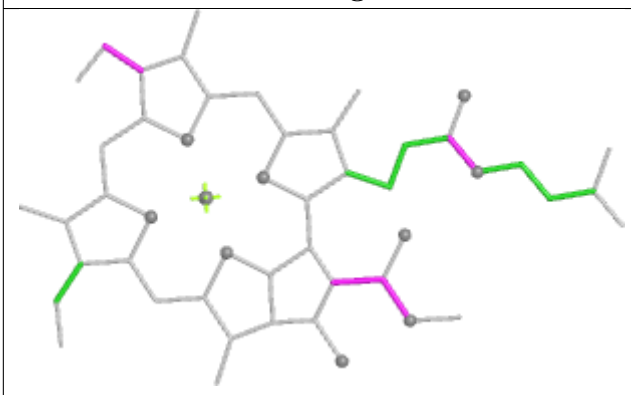
Ligand CLA 1 303



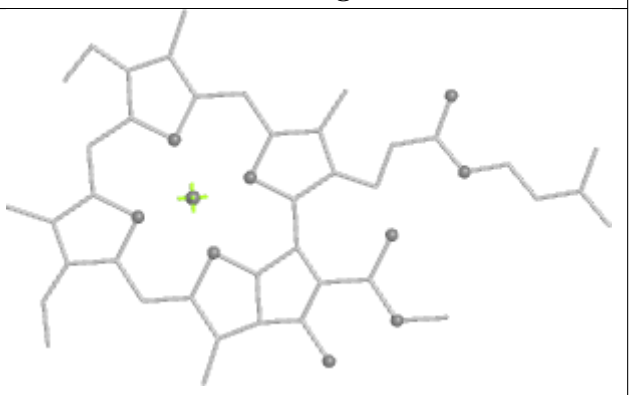
Bond lengths



Bond angles

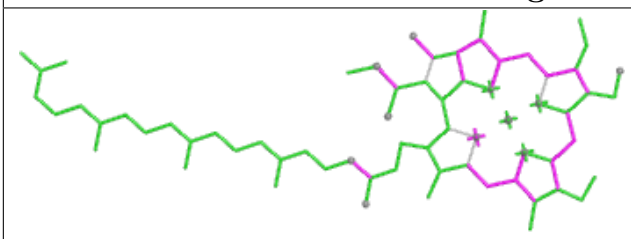


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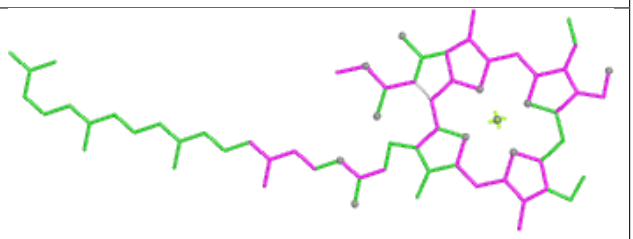


Rings

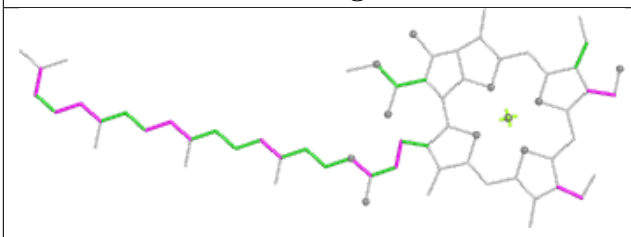
Ligand CHL v 316



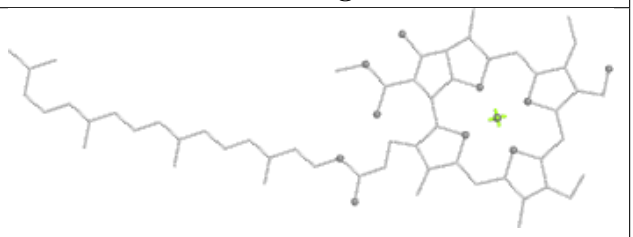
Bond lengths



Bond angles

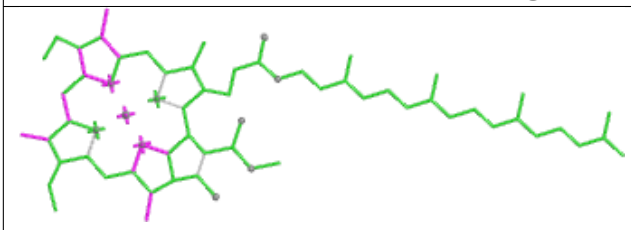


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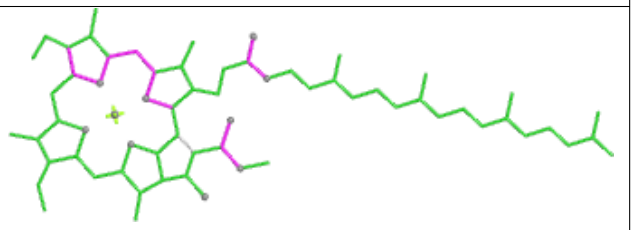


Rings

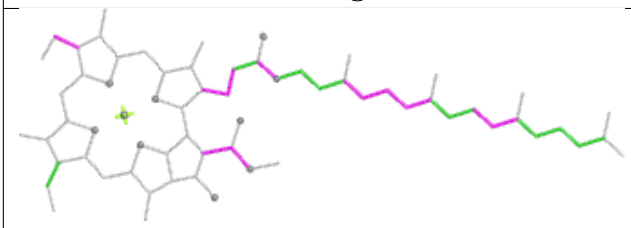
Ligand CLA C 505



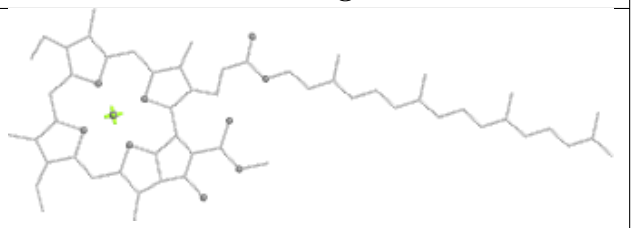
Bond lengths



Bond angles

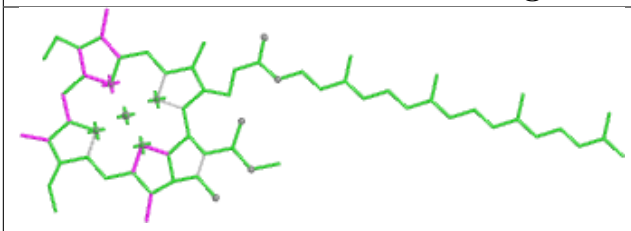


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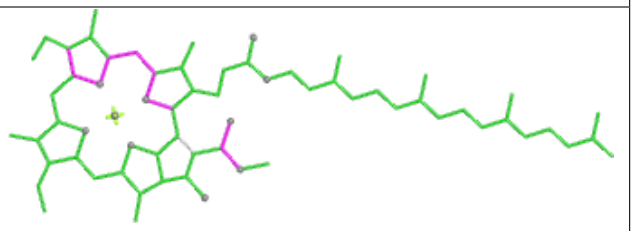


Rings

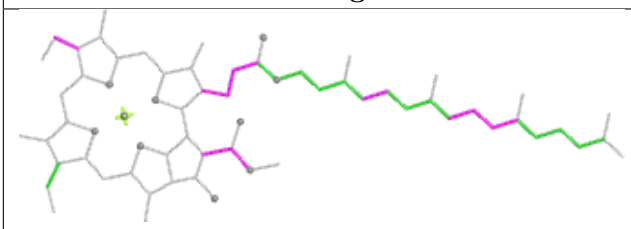
Ligand CLA V 301



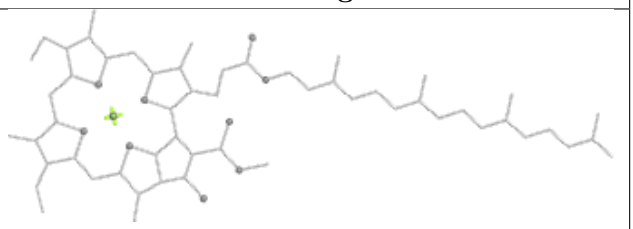
Bond lengths



Bond angles

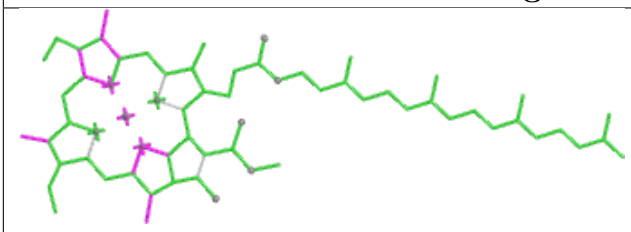


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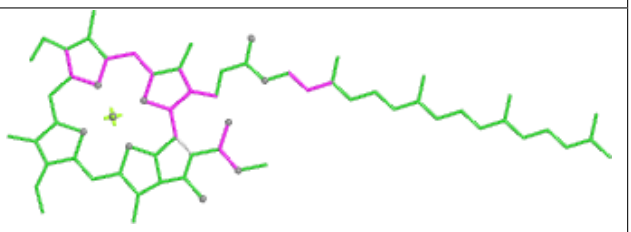


Rings

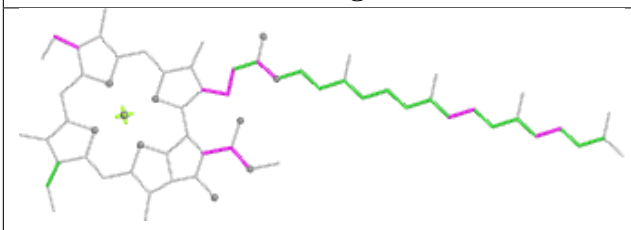
Ligand CLA A 405



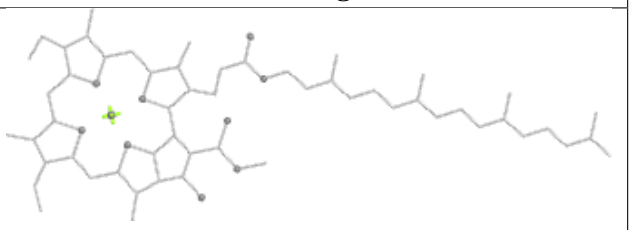
Bond lengths



Bond angles

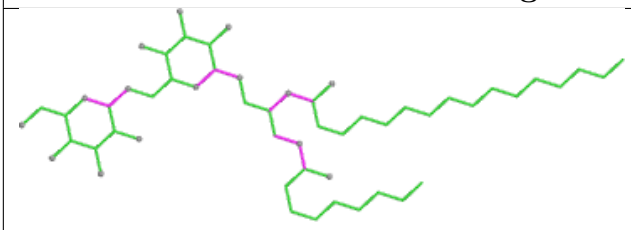


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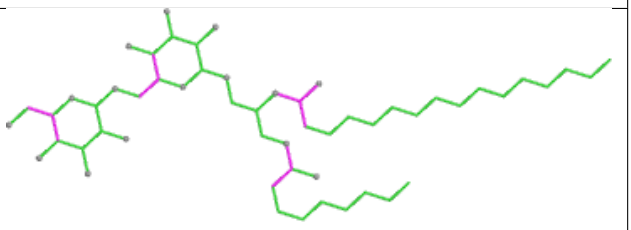


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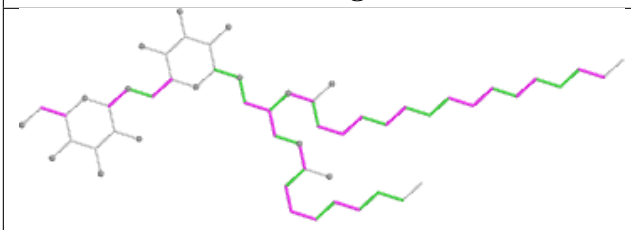
Ligand DGD C 519



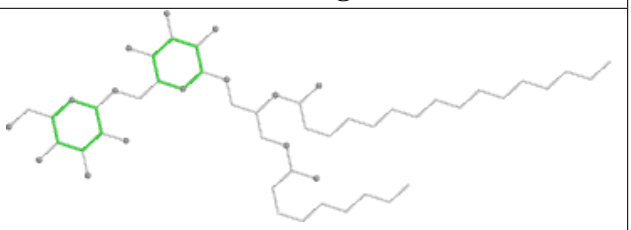
Bond lengths



Bond angles

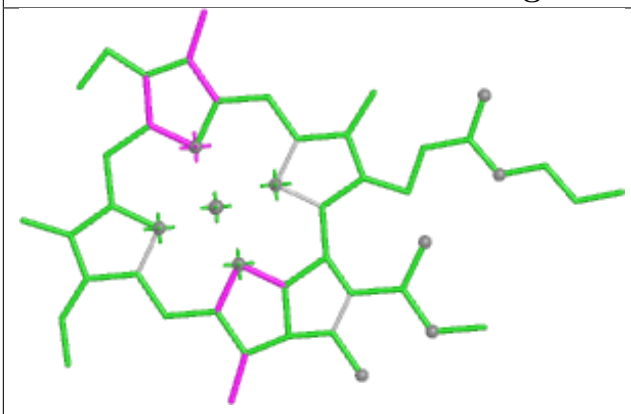


Torsions

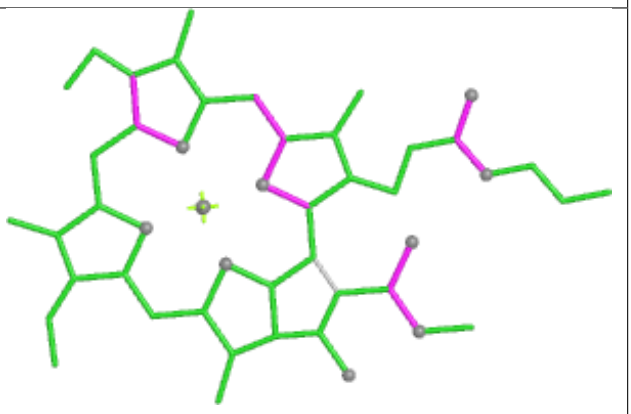


Rings

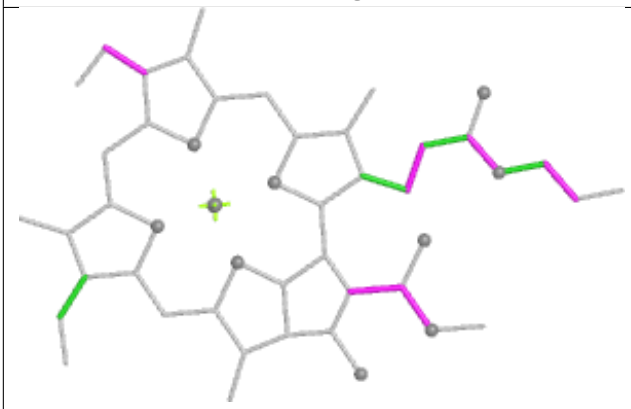
Ligand CLA U 308



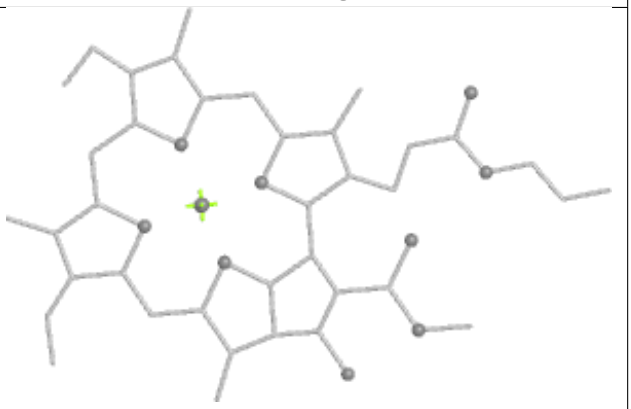
Bond lengths



Bond angles

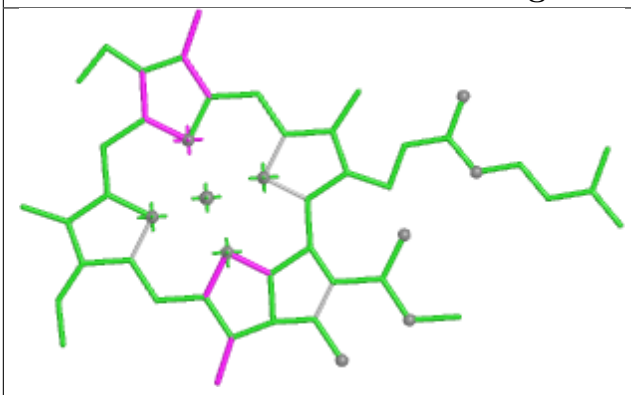


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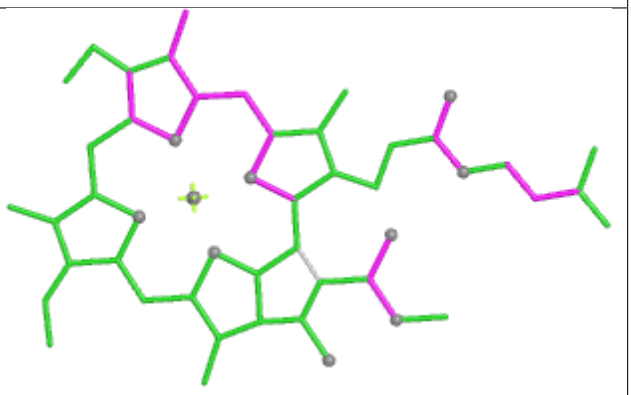


Rings

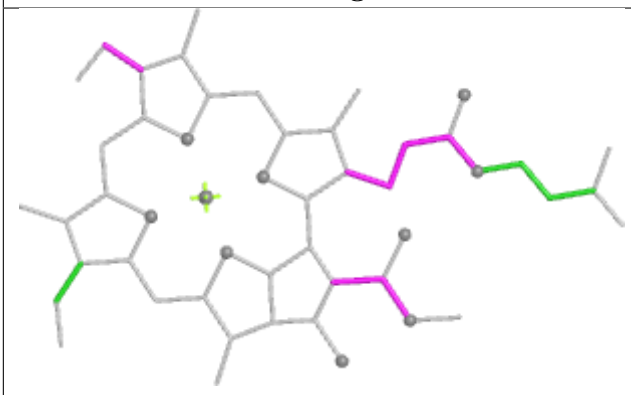
Ligand CLA 3 303



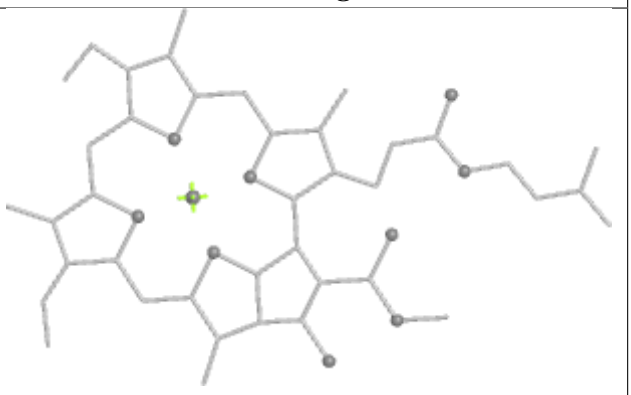
Bond lengths



Bond angles

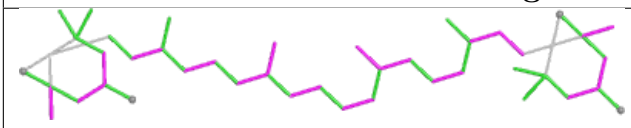


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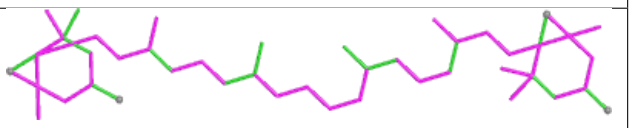


Rings

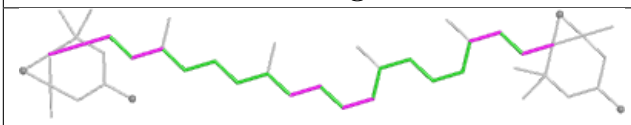
Ligand XAT R 313



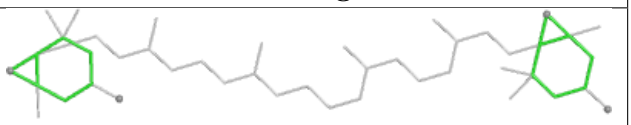
Bond lengths



Bond angles

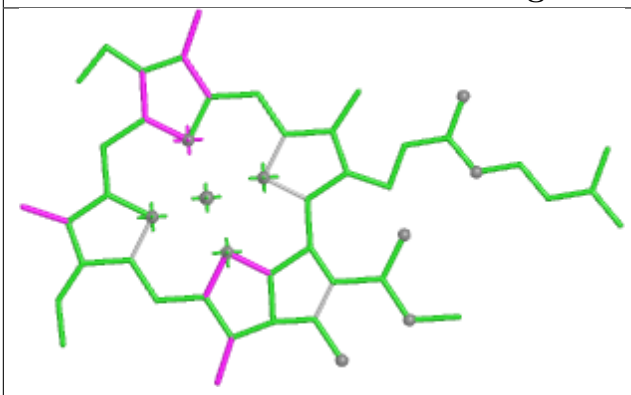


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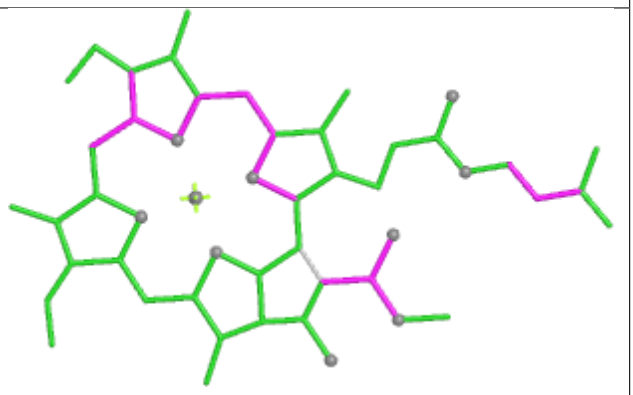


Rings

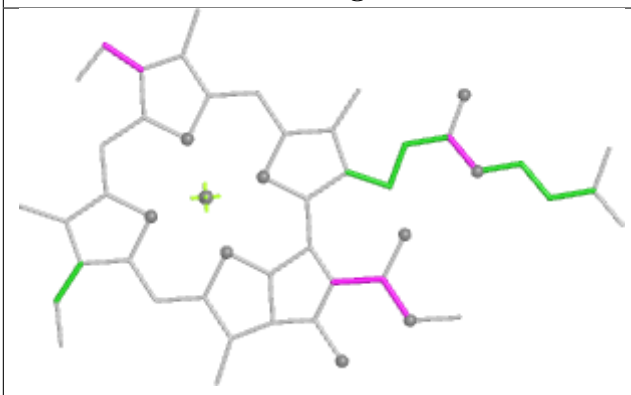
Ligand CLA u 303



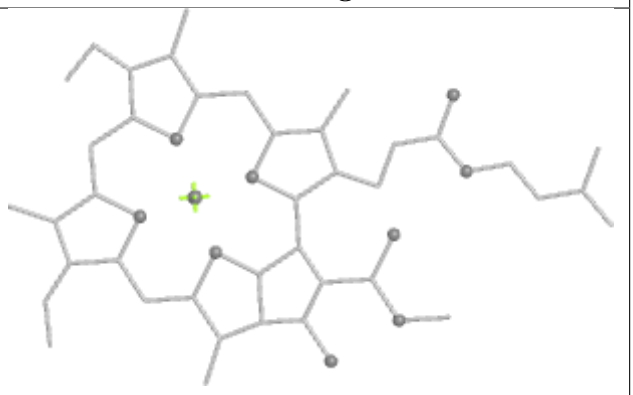
Bond lengths



Bond angles

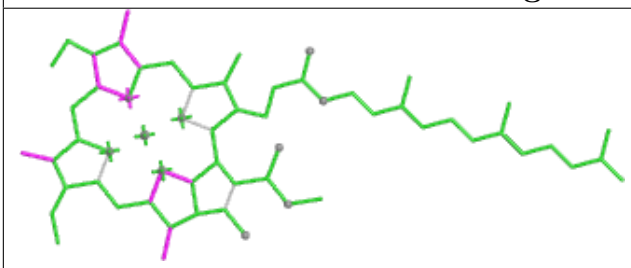


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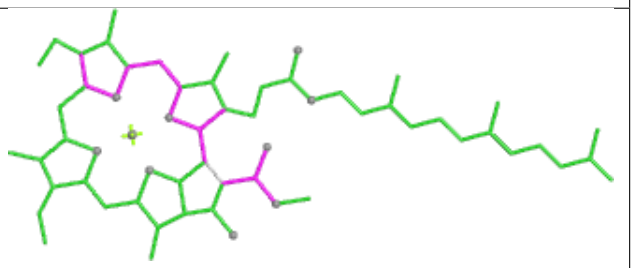


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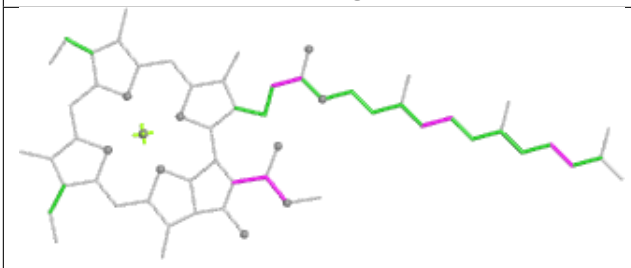
Ligand CLA V 306



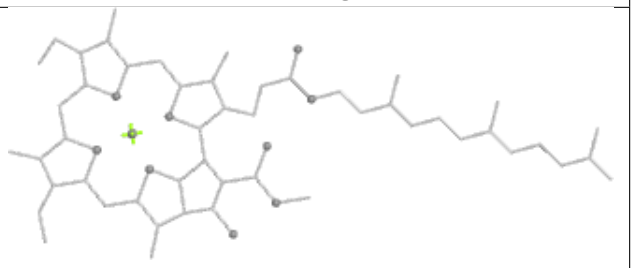
Bond lengths



Bond angles

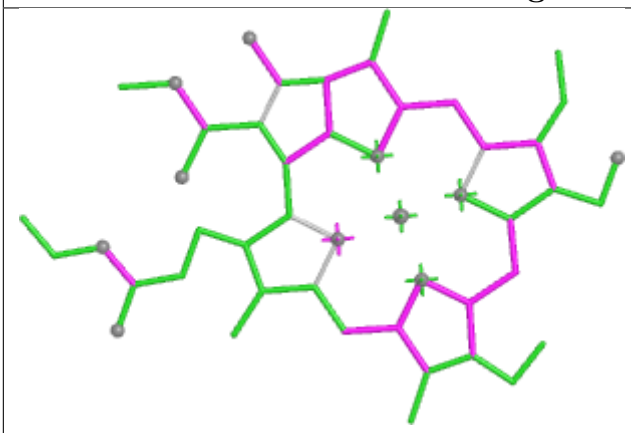


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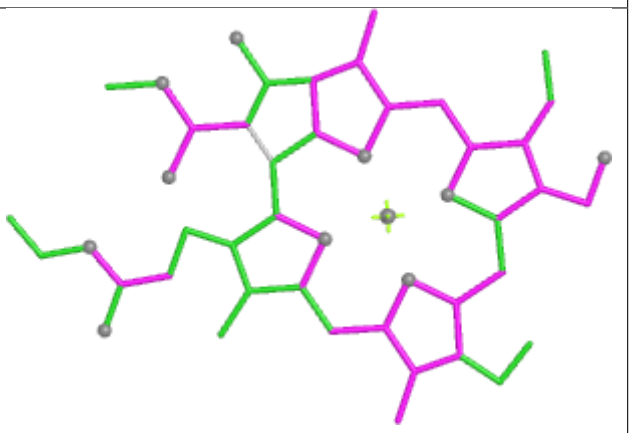


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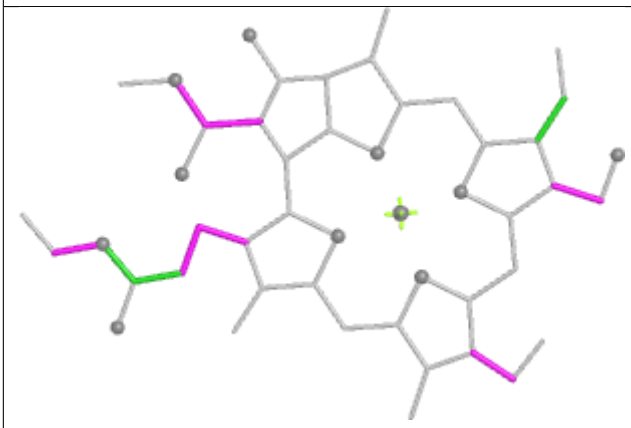
Ligand CHL 5 314



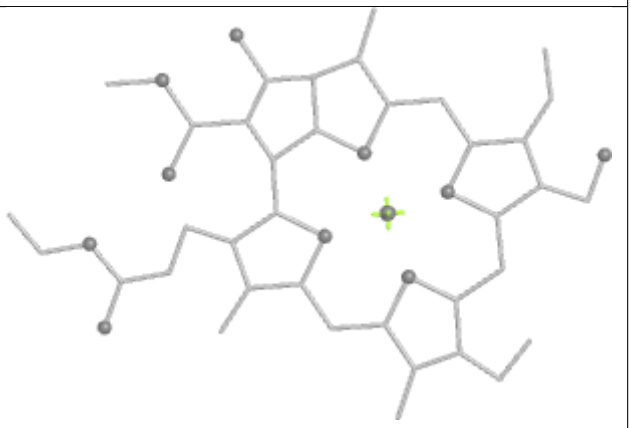
Bond lengths



Bond angles

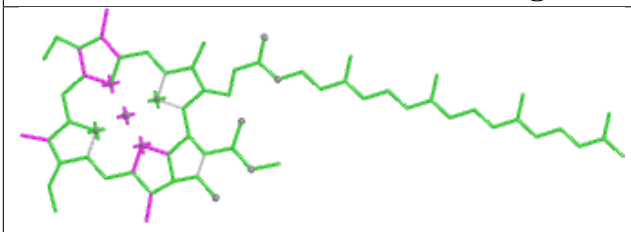


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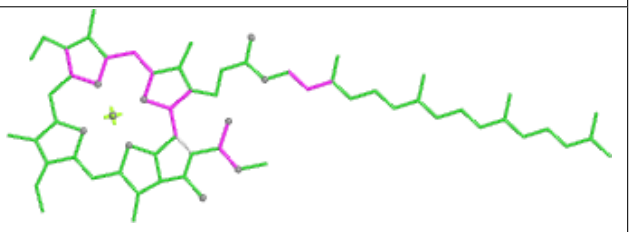


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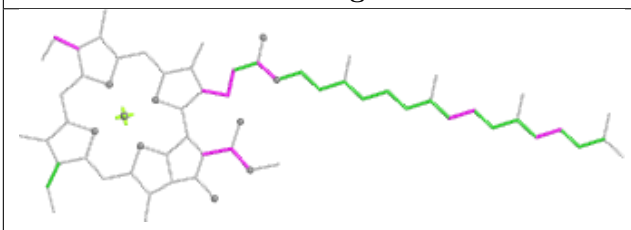
Ligand CLA a 405



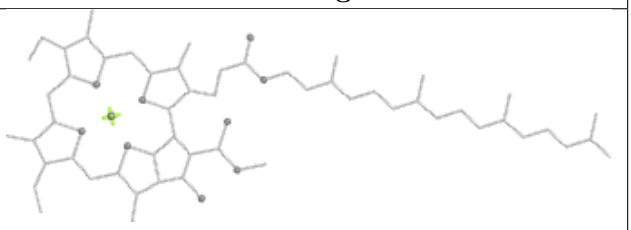
Bond lengths



Bond angles

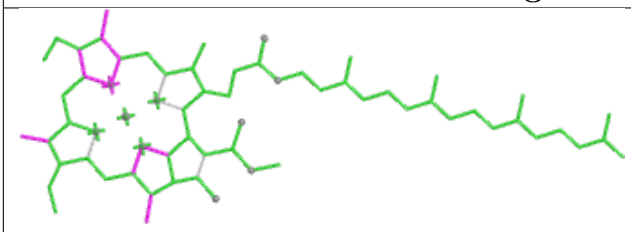


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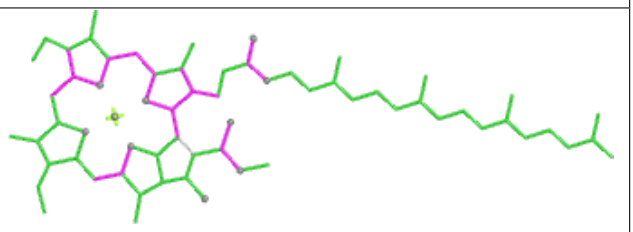


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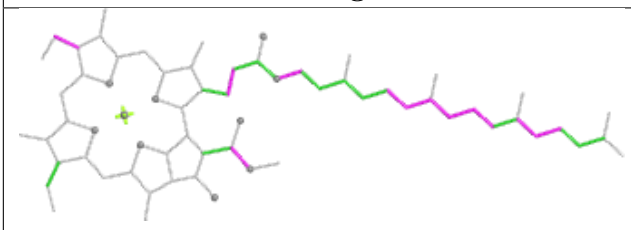
Ligand CLA C 509



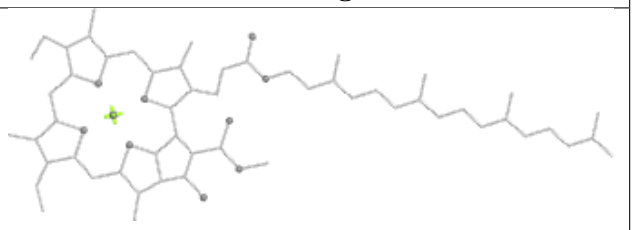
Bond lengths



Bond angles

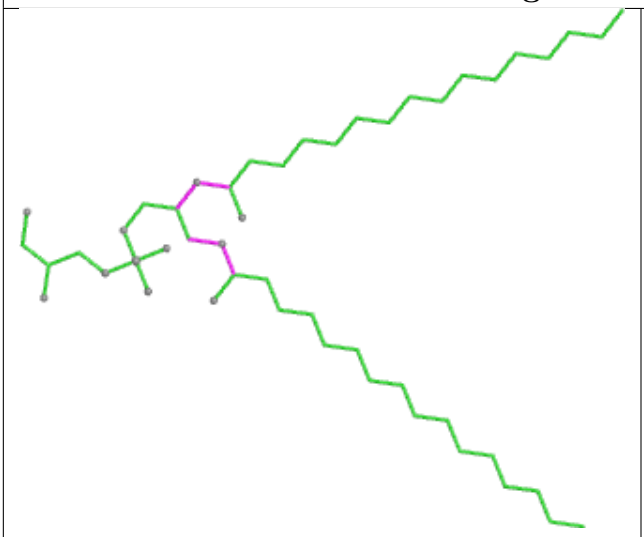


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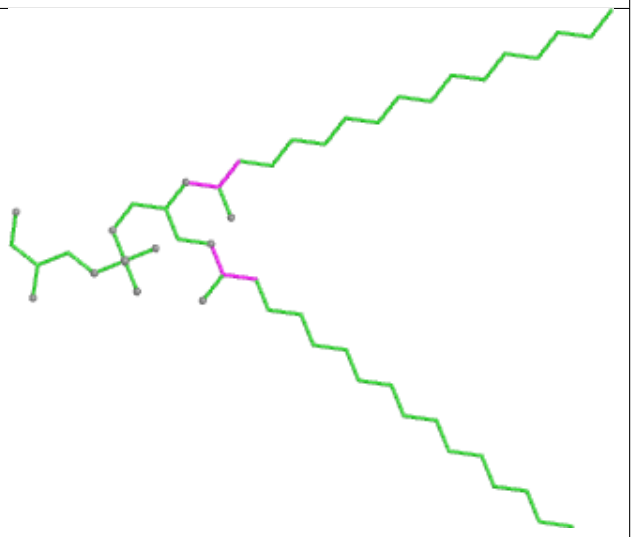


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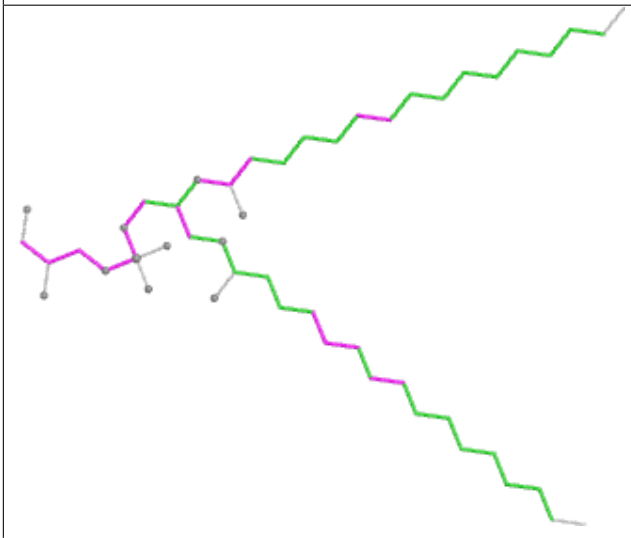
Ligand LHG B 623



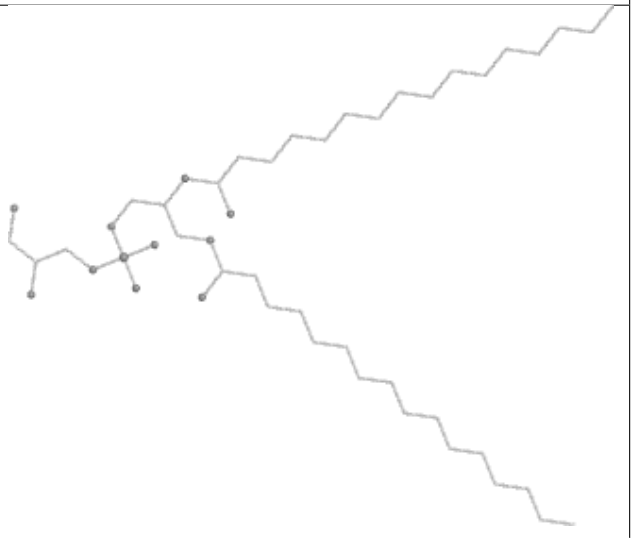
Bond lengths



Bond angles

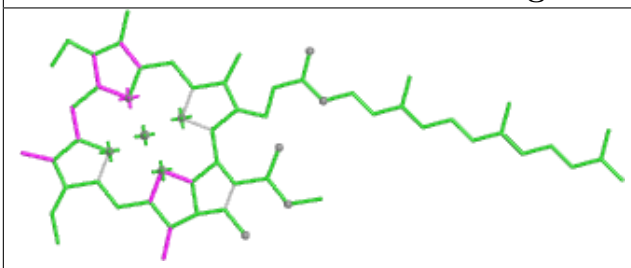


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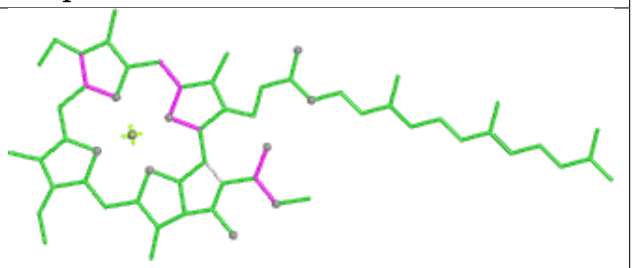


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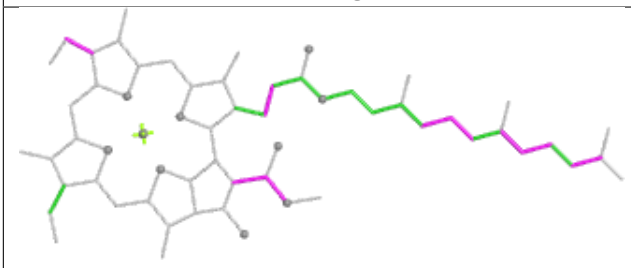
Ligand CLA q 305



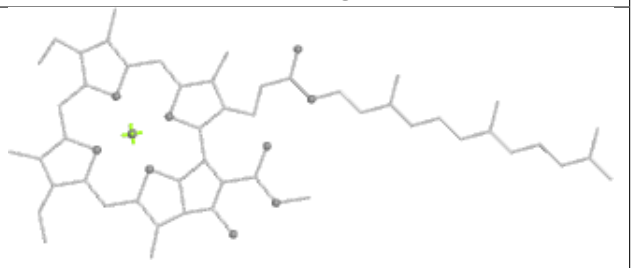
Bond lengths



Bond angles

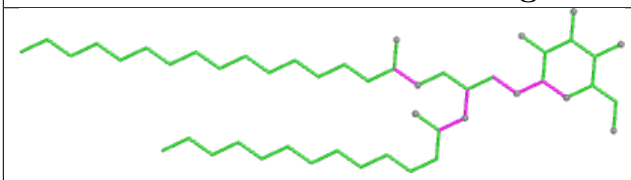


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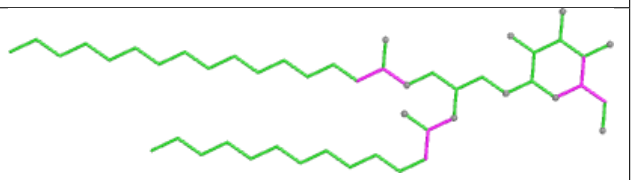


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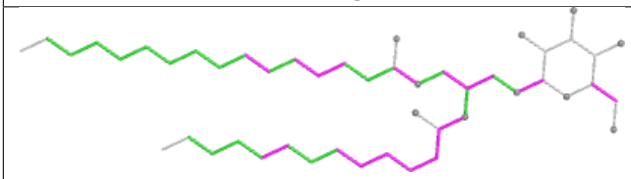
Ligand LMG w 201



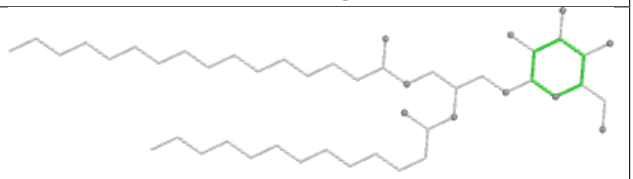
Bond lengths



Bond angles

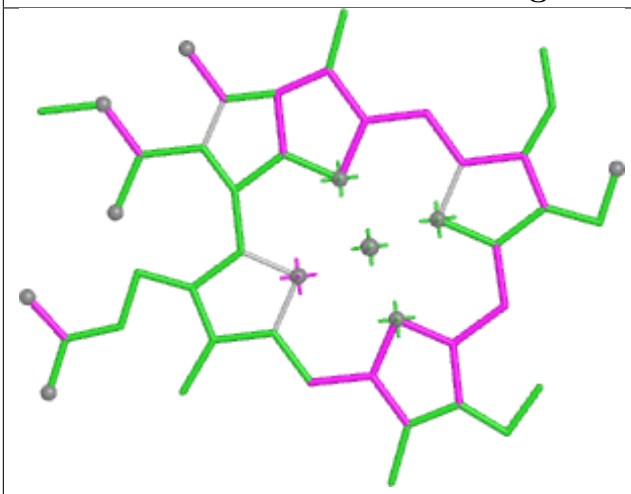


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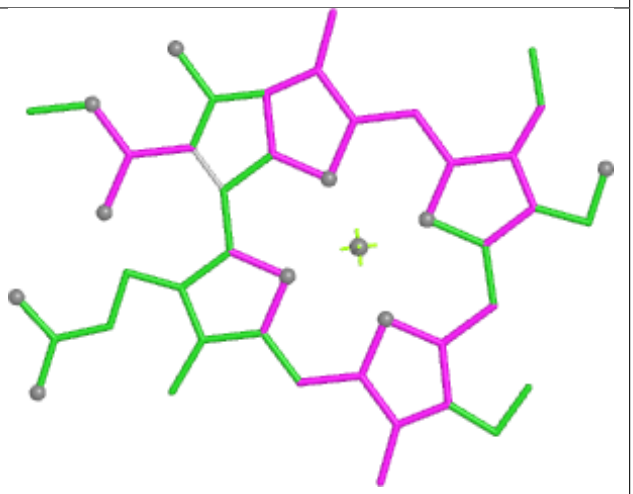


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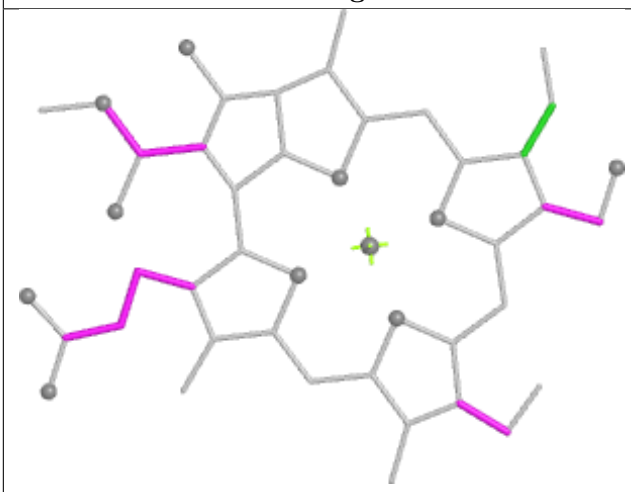
Ligand CHL s 316



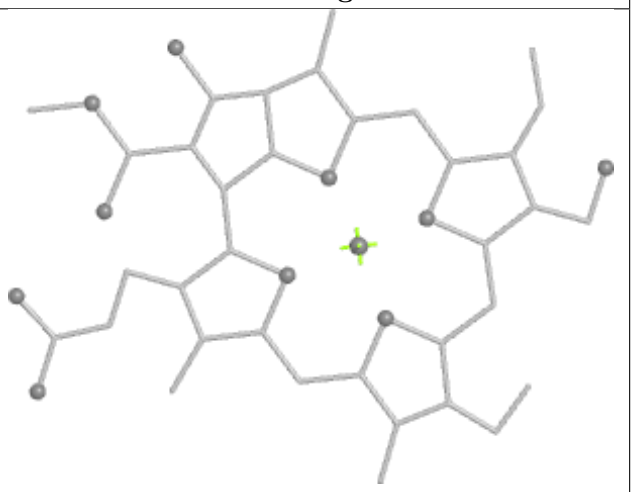
Bond lengths



Bond angles

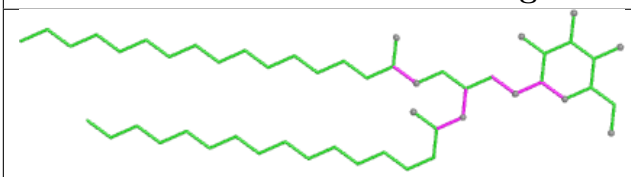


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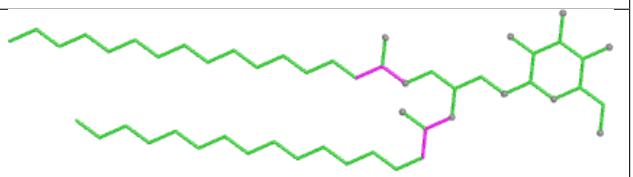


Rings

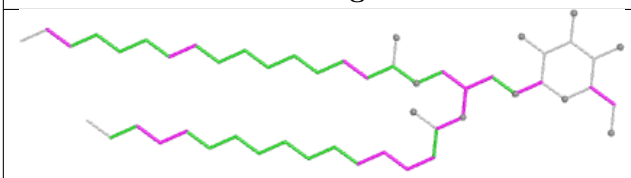
Ligand LMG C 521



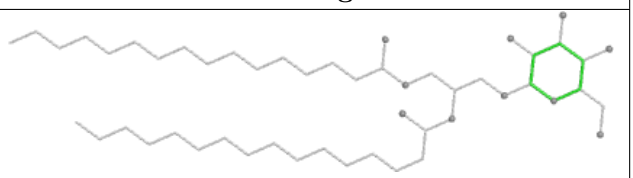
Bond lengths



Bond angles

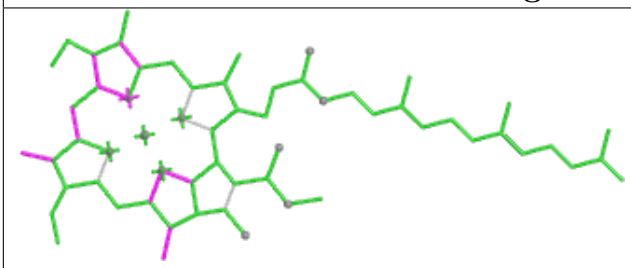


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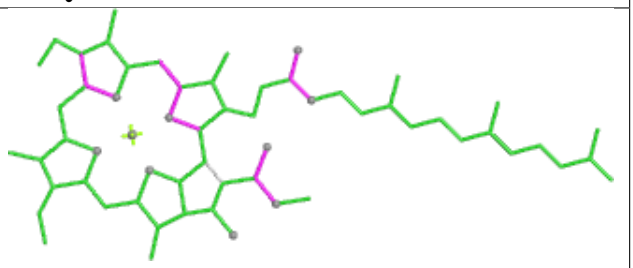


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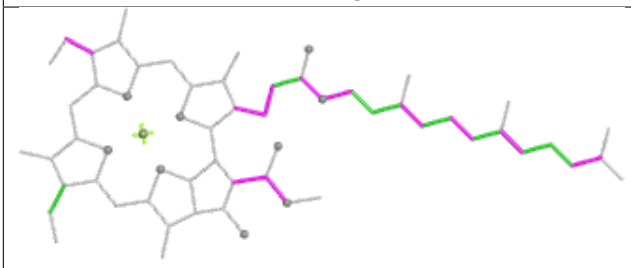
Ligand CLA Q 305



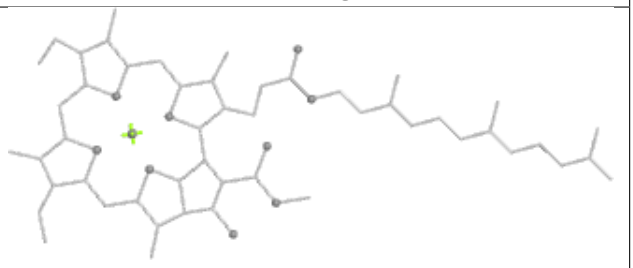
Bond lengths



Bond angles

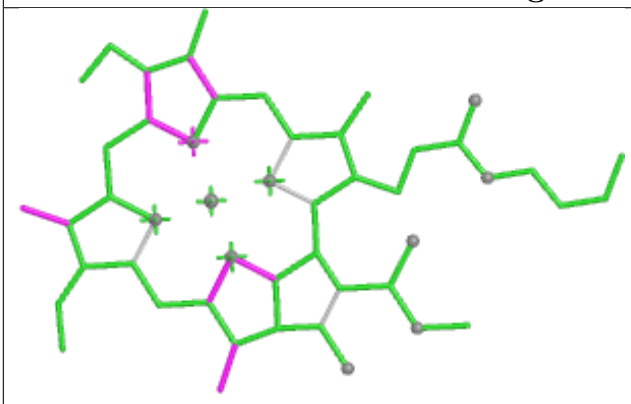


Torsions

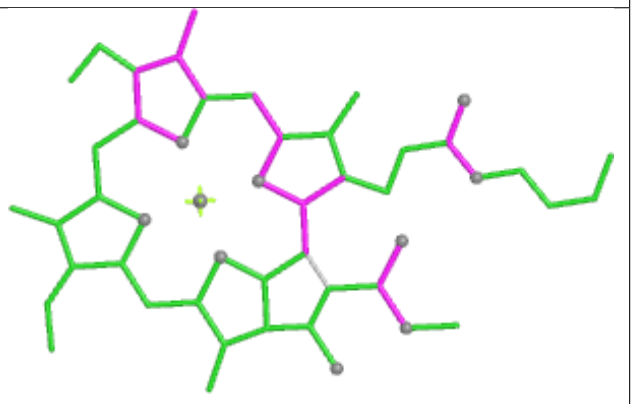


Rings

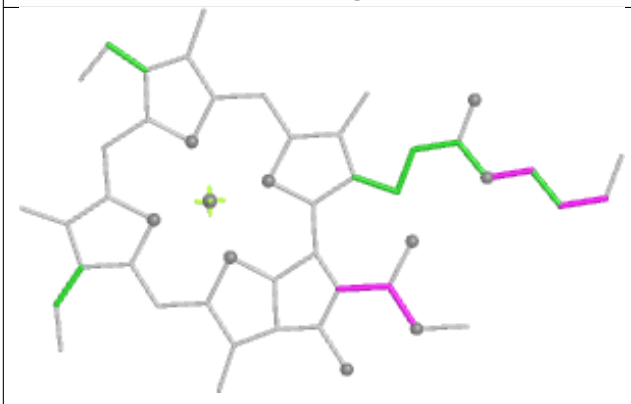
Ligand CLA S 307



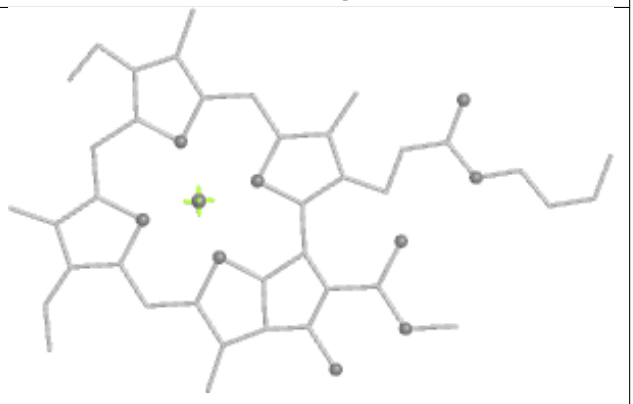
Bond lengths



Bond angles

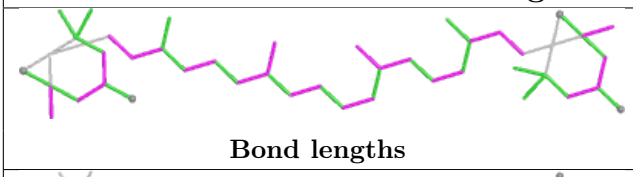


Torsions

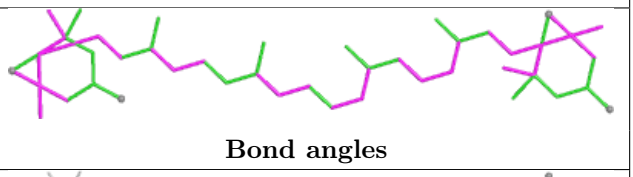


Rings

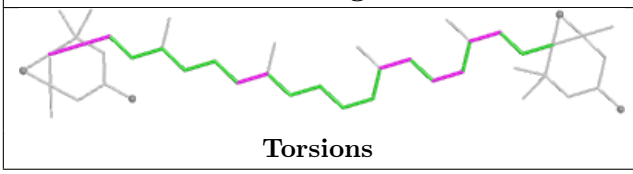
Ligand XAT 3 309



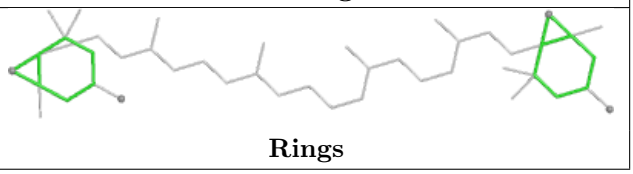
Bond lengths



Bond angles

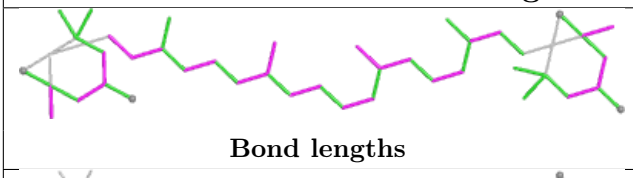


Torsions

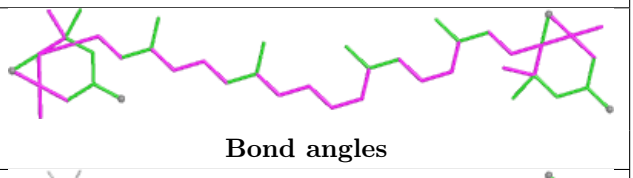


Rings

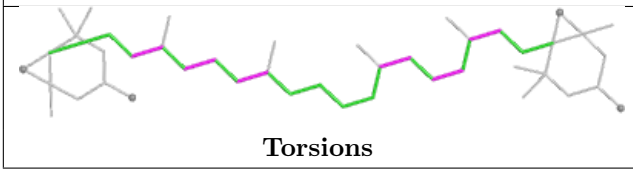
Ligand XAT G 309



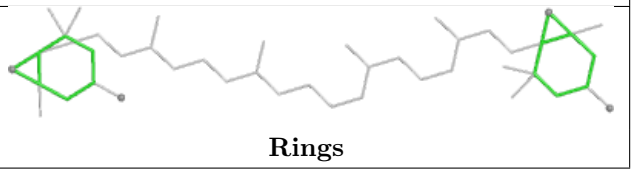
Bond lengths



Bond angles

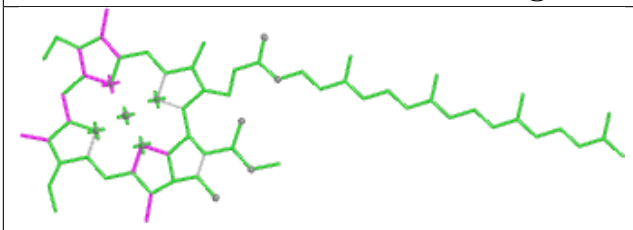


Torsions

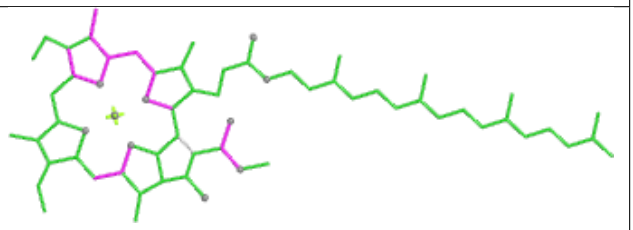


Rings

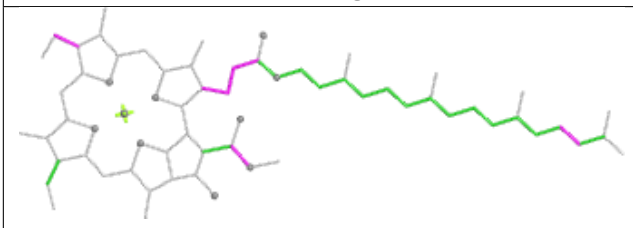
Ligand CLA 1 301



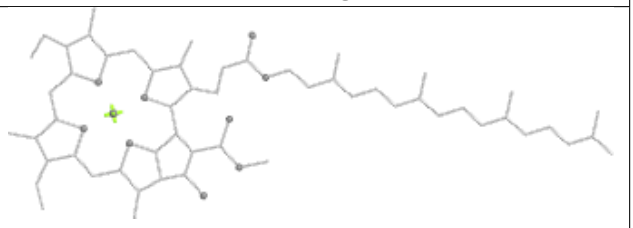
Bond lengths



Bond angles

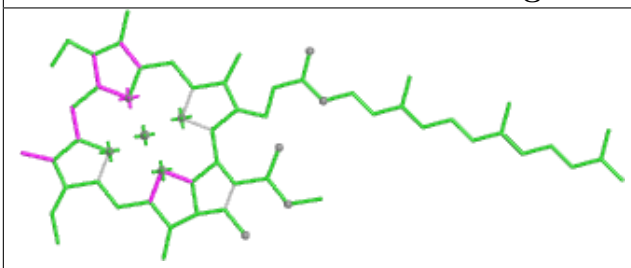


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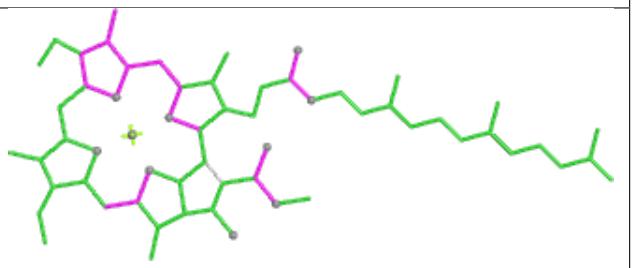


Rings

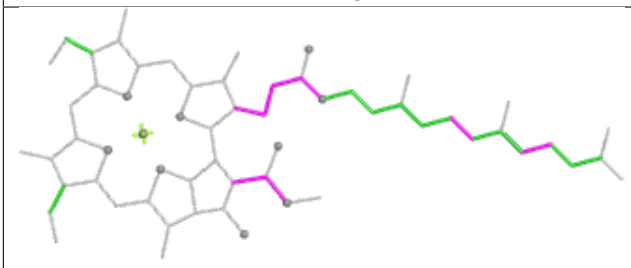
Ligand CLA V 304



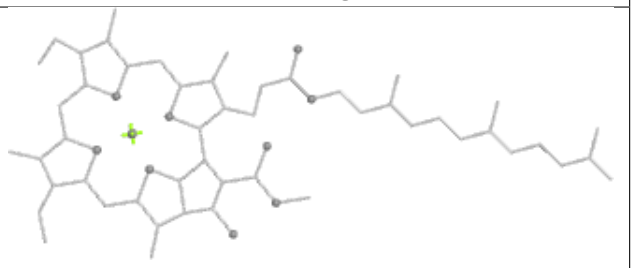
Bond lengths



Bond angles

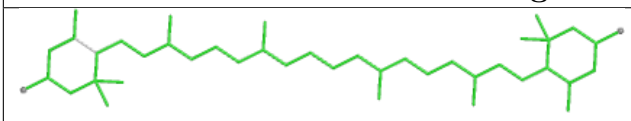


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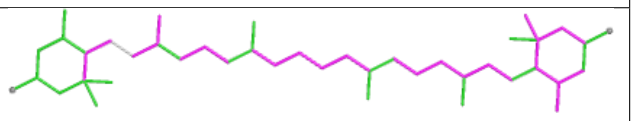


Rings

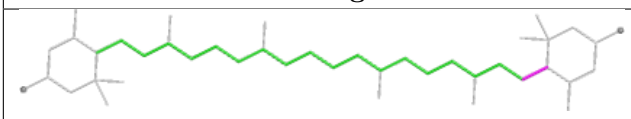
Ligand LUT s 310



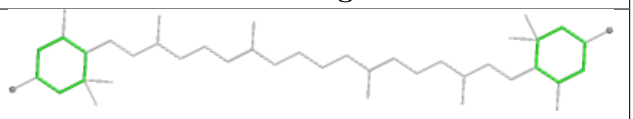
Bond lengths



Bond angles

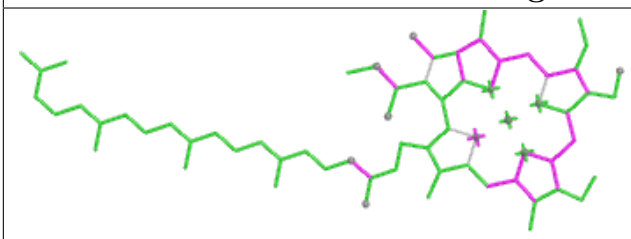


Torsions

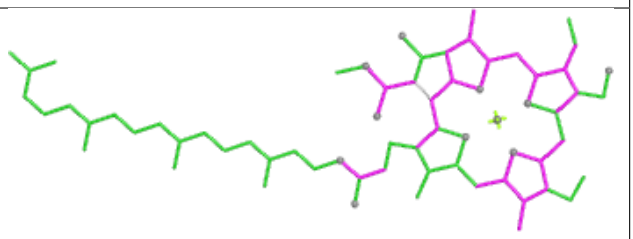


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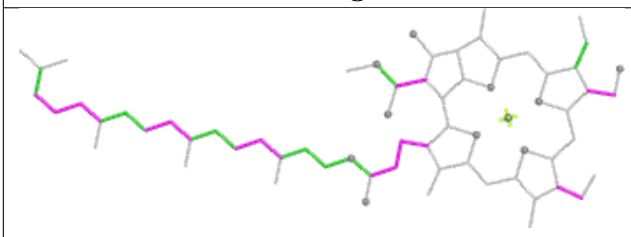
Ligand CHL 5 316



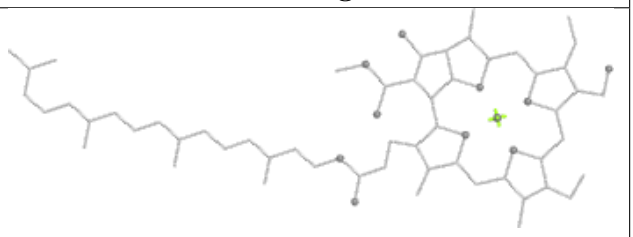
Bond lengths



Bond angles

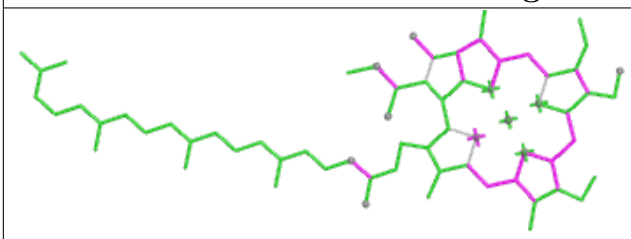


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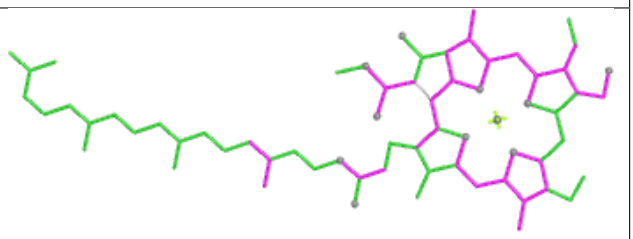


Rings

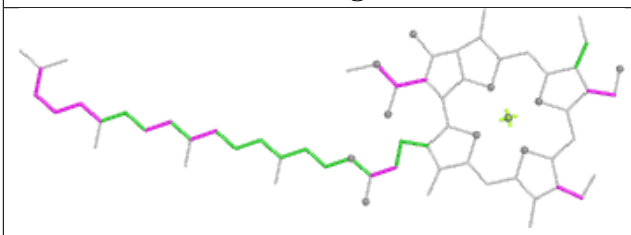
Ligand CHL N 316



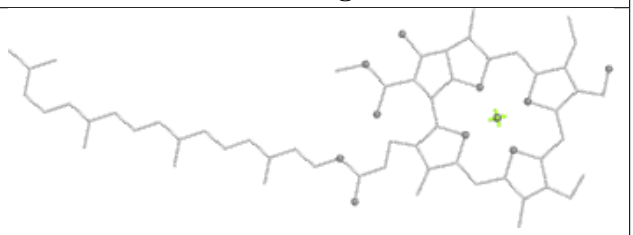
Bond lengths



Bond angles

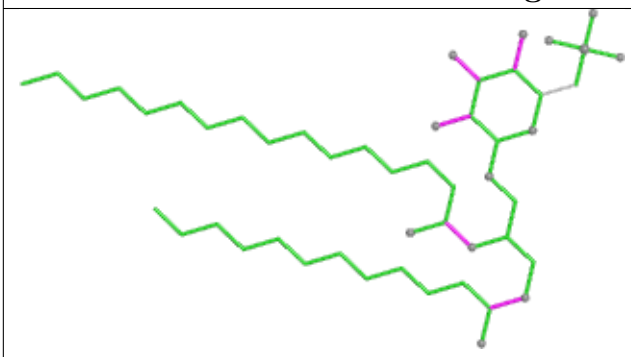


Torsions

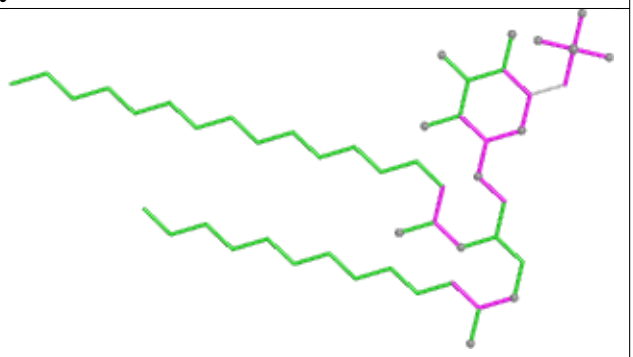


Rings

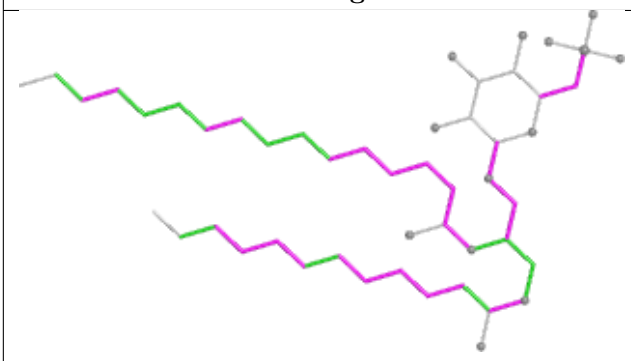
Ligand SQD C 501



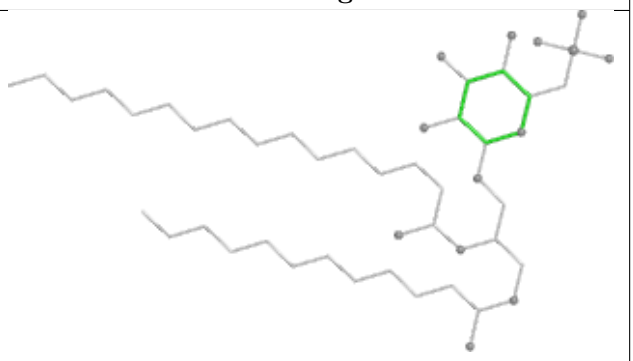
Bond lengths



Bond angles

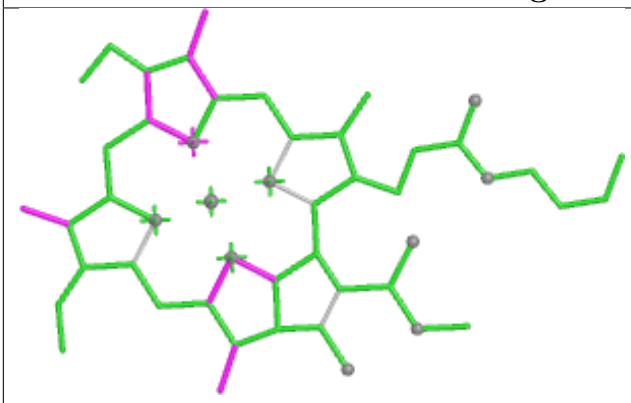


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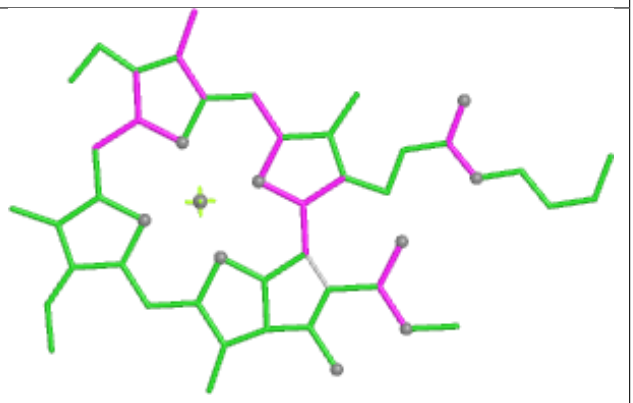


Rings

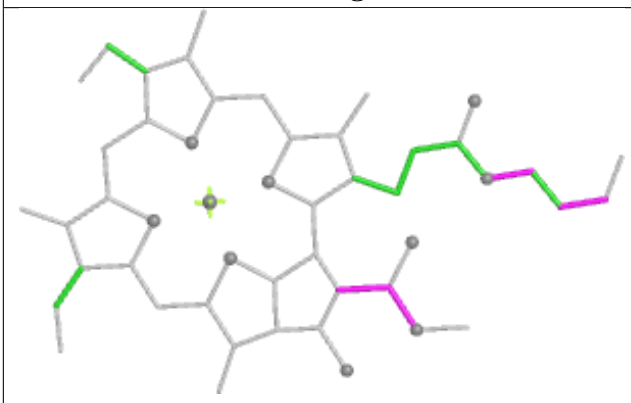
Ligand CLA s 307



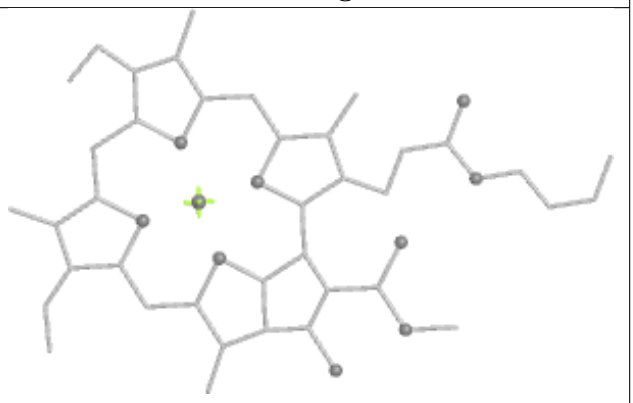
Bond lengths



Bond angles

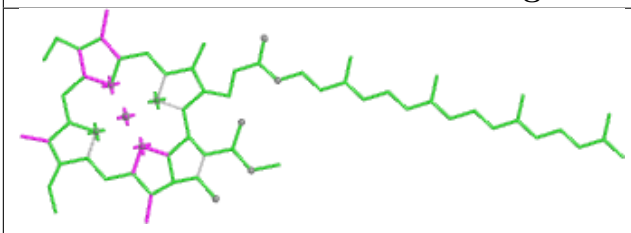


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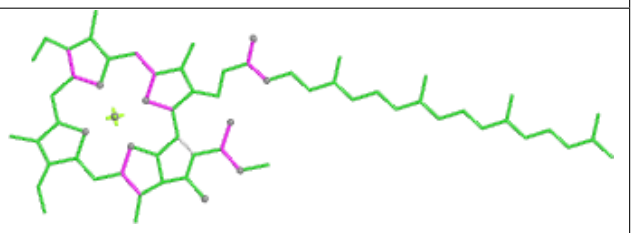


Rings

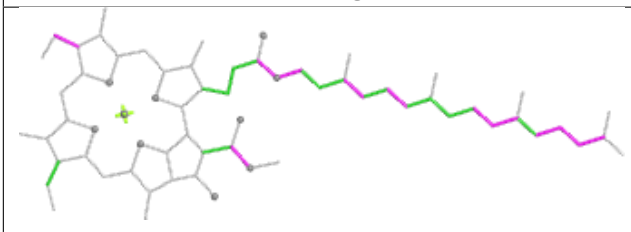
Ligand CLA D 403



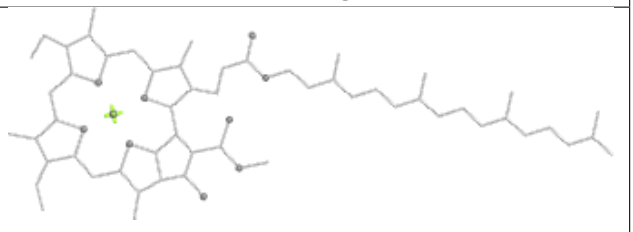
Bond lengths



Bond angles

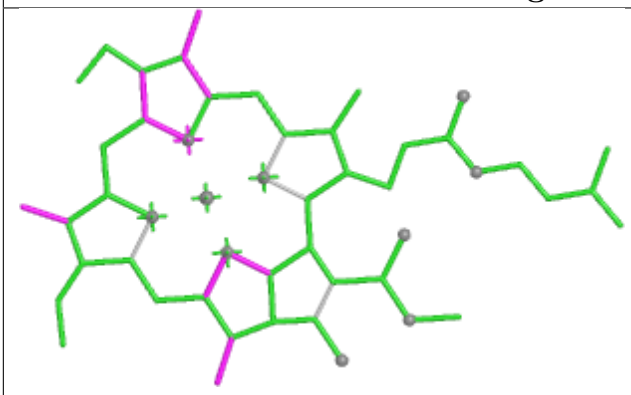


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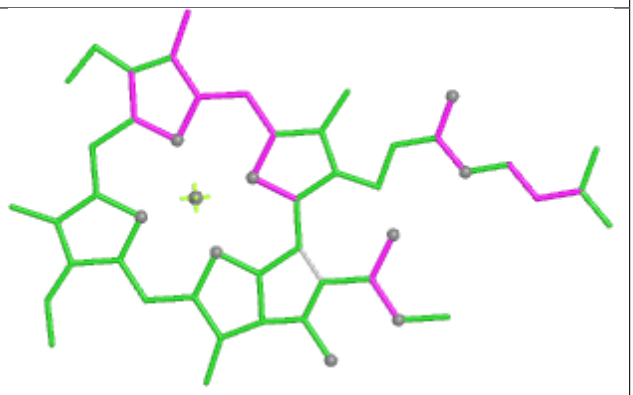


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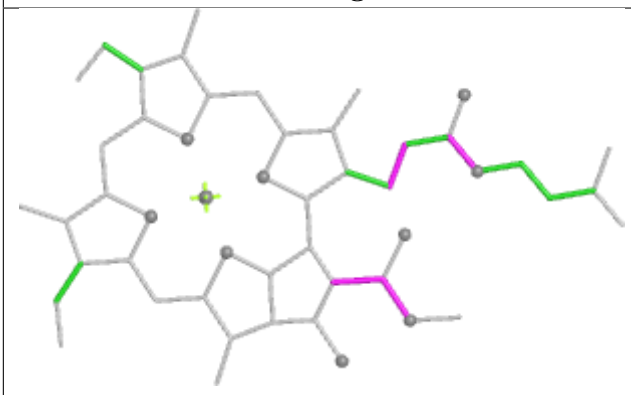
Ligand CLA S 303



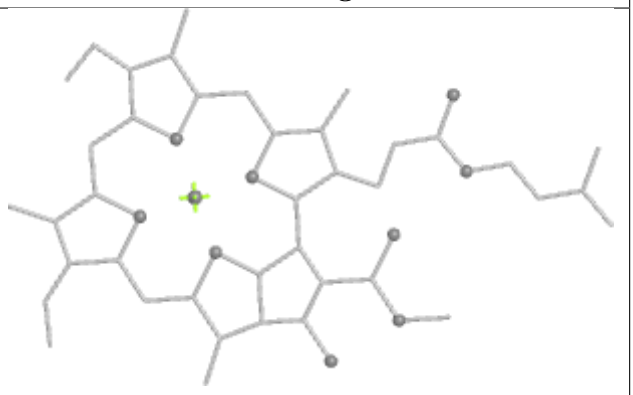
Bond lengths



Bond angles

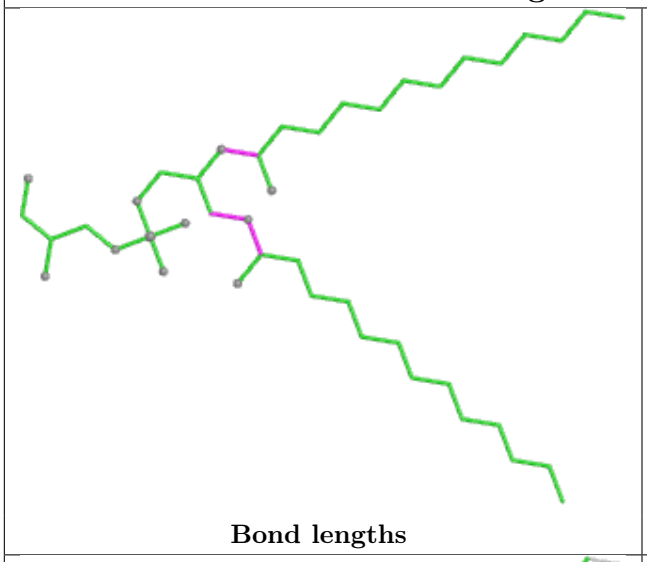


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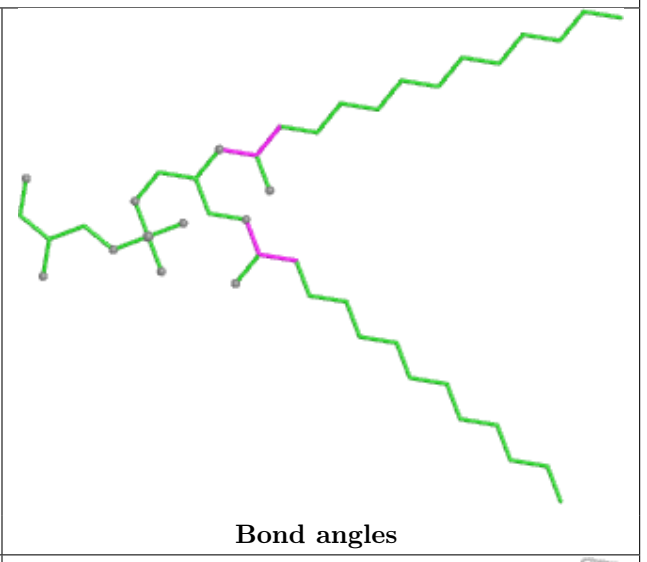


Rings

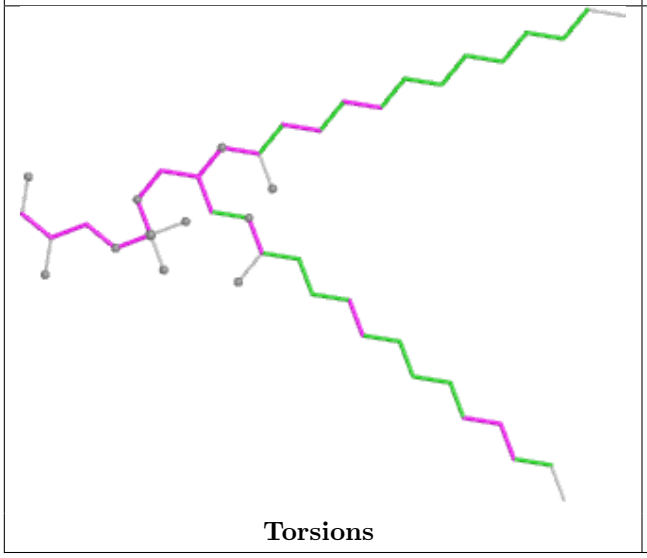
Ligand LHG a 415



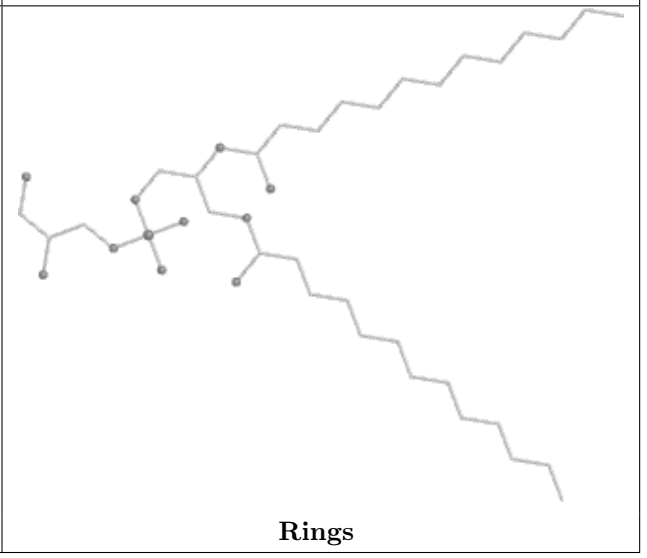
Bond lengths



Bond angles

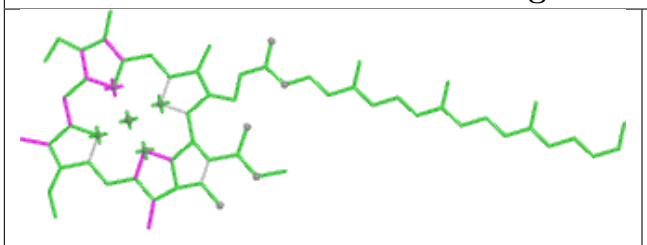


Torsions

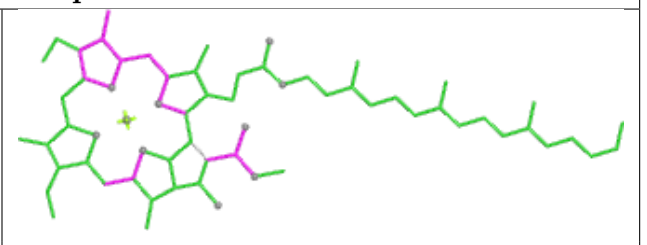


Rings

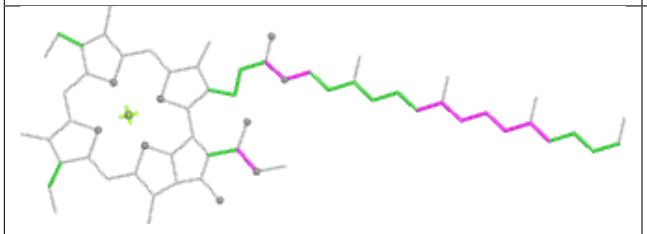
Ligand CLA q 304



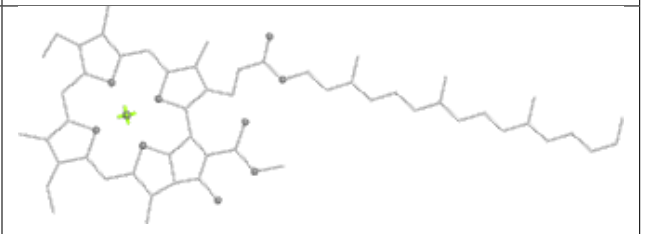
Bond lengths



Bond angles

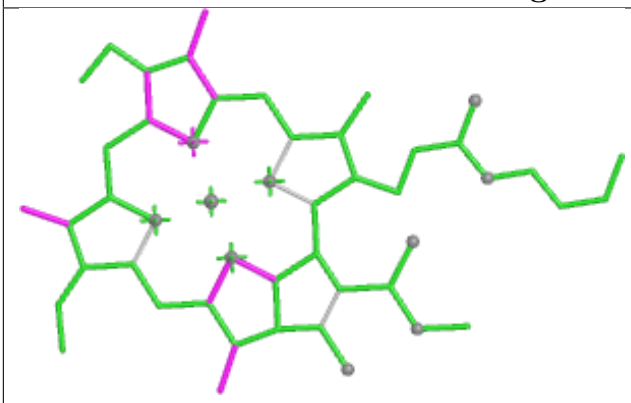


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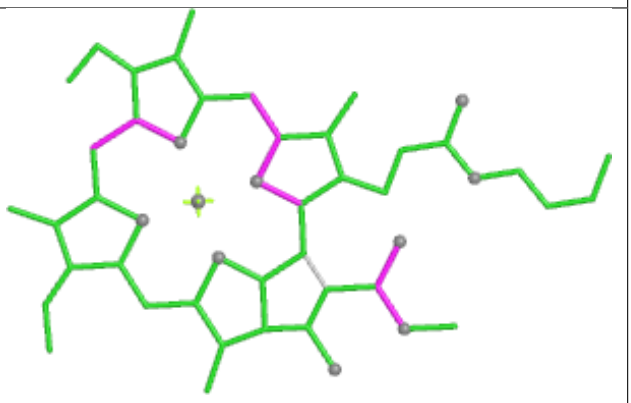


Rings

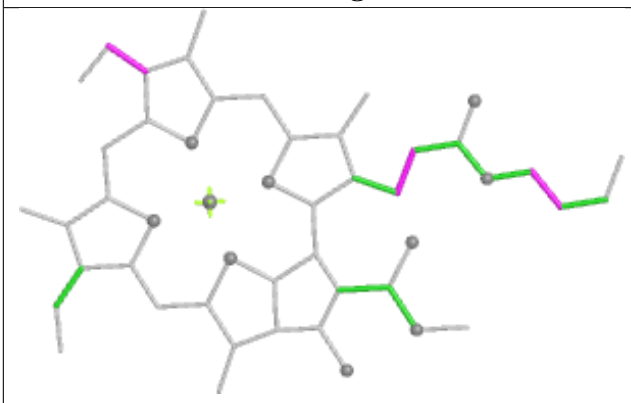
Ligand CLA s 309



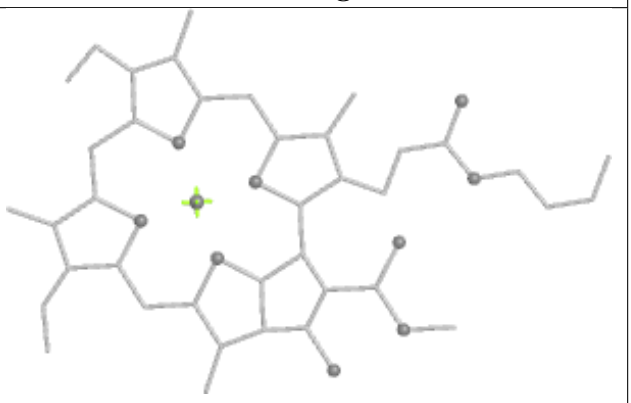
Bond lengths



Bond angles

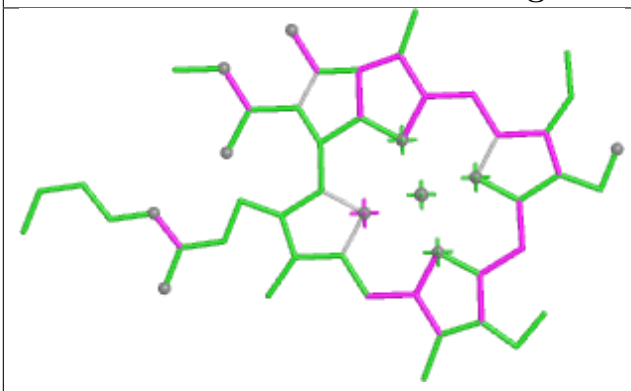


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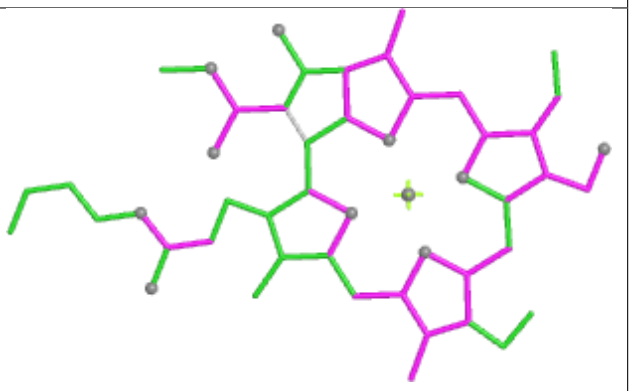


Rings

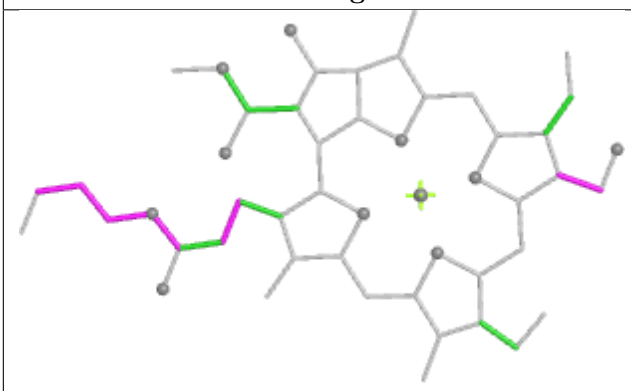
Ligand CHL v 315



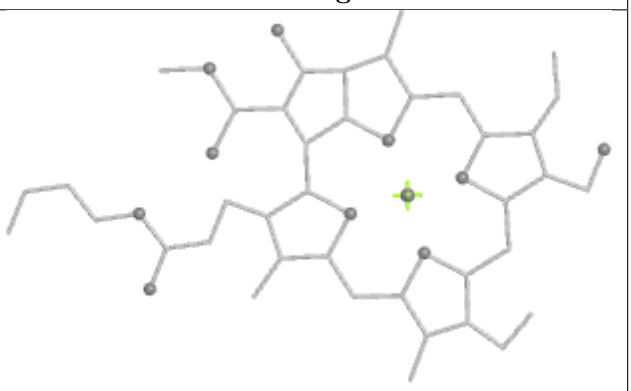
Bond lengths



Bond angles

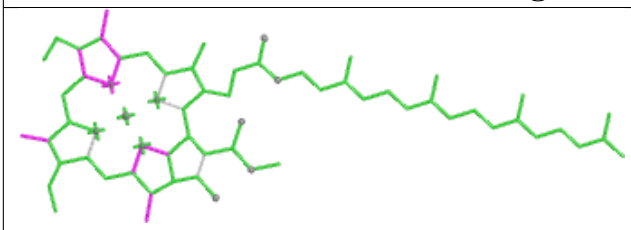


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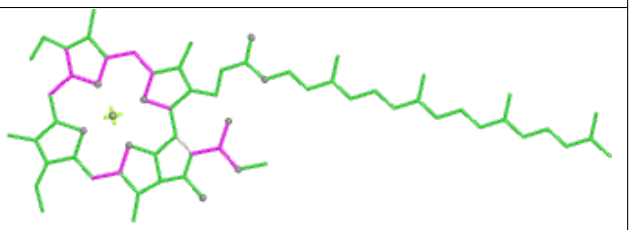


Rings

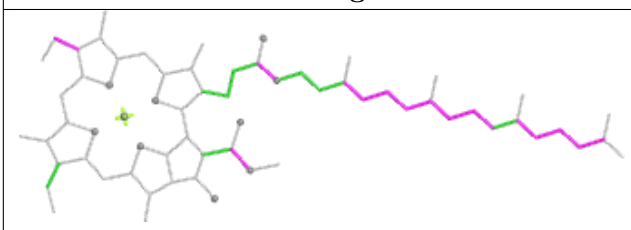
Ligand CLA c 507



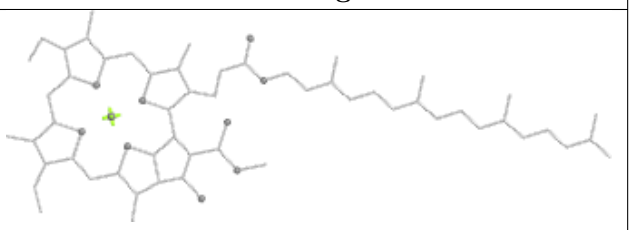
Bond lengths



Bond angles

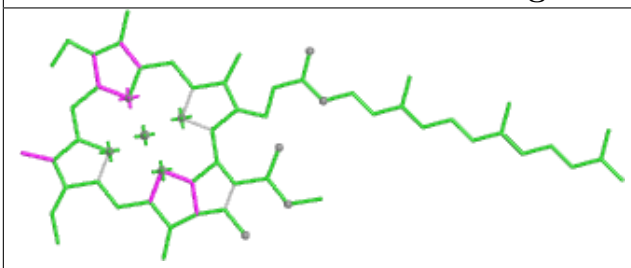


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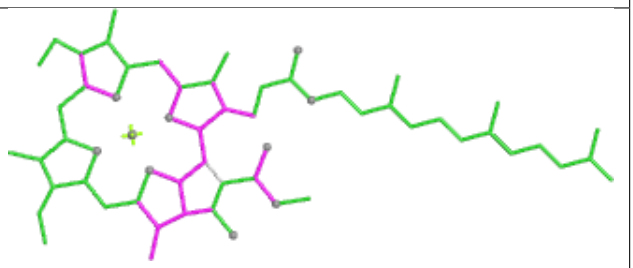


Rings

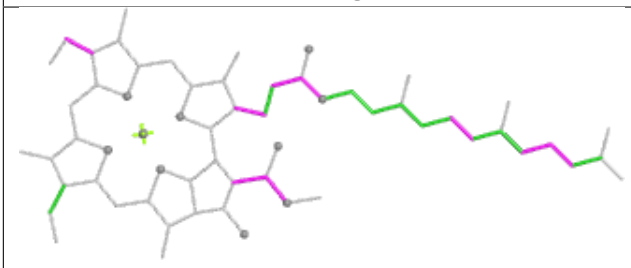
Ligand CLA 2 305



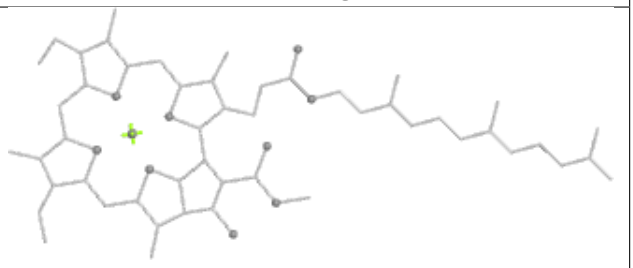
Bond lengths



Bond angles

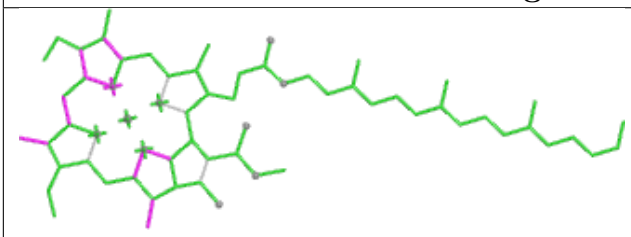


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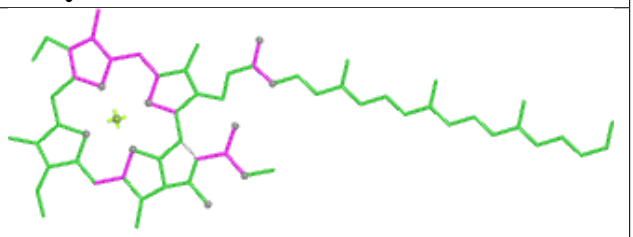


Rings

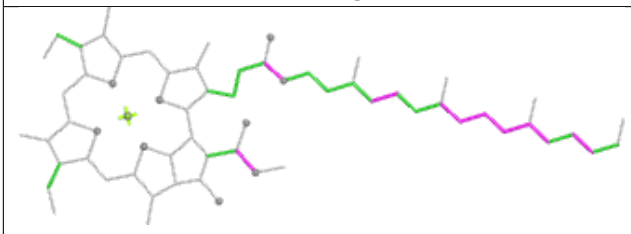
Ligand CLA Q 304



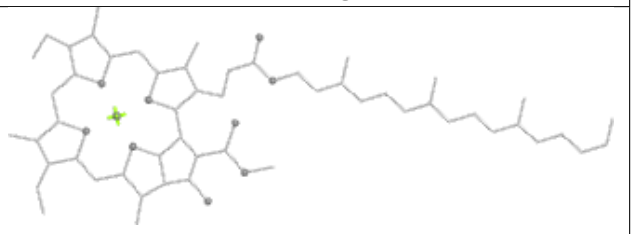
Bond lengths



Bond angles

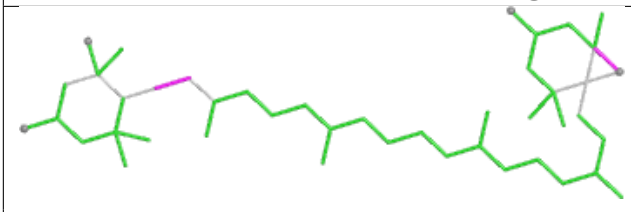


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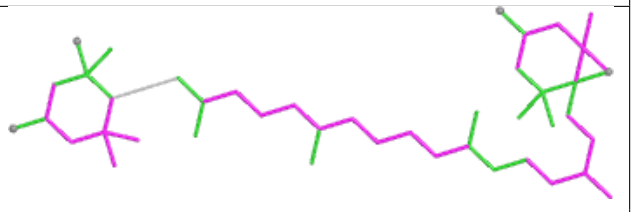


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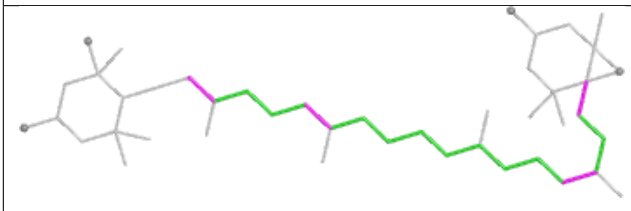
Ligand NEX n 319



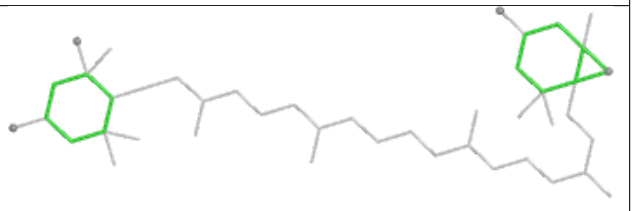
Bond lengths



Bond angles

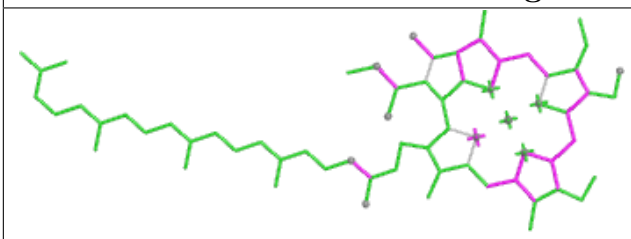


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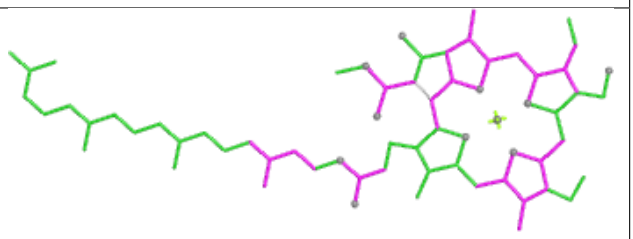


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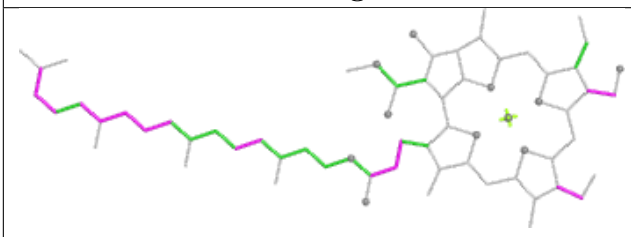
Ligand CHL P 314



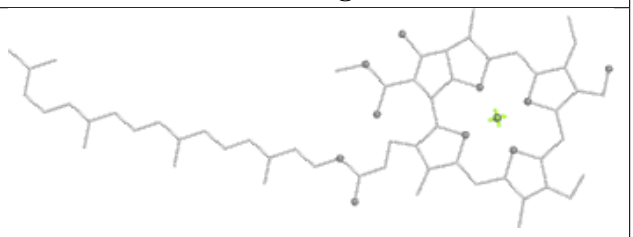
Bond lengths



Bond angles

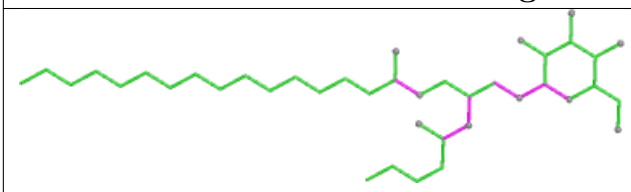


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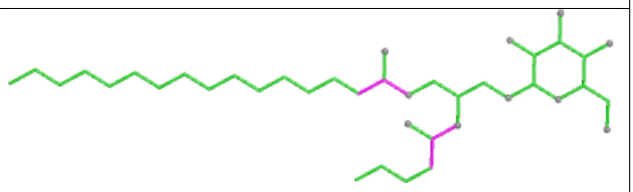


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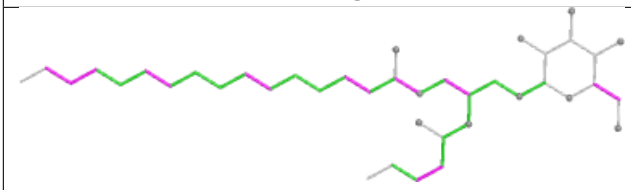
Ligand LMG A 411



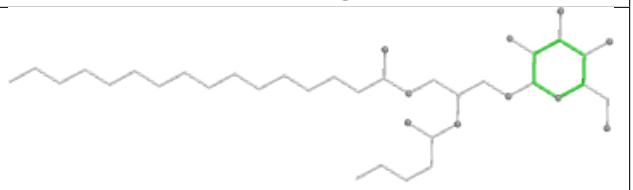
Bond lengths



Bond angles

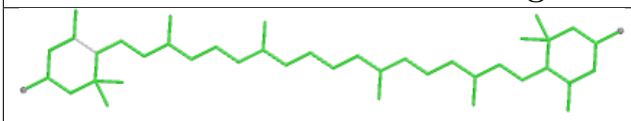


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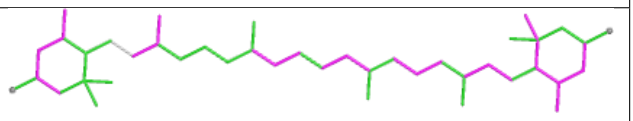


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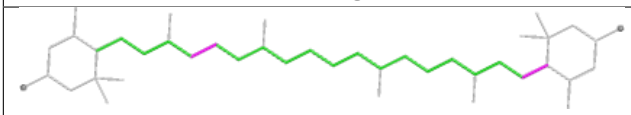
Ligand LUT u 310



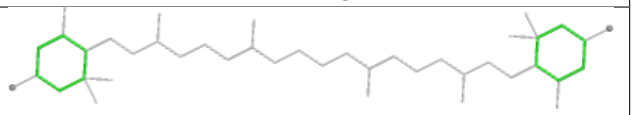
Bond lengths



Bond angles

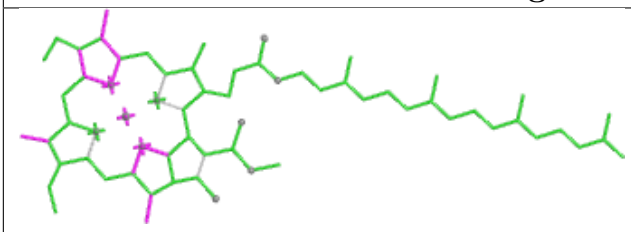


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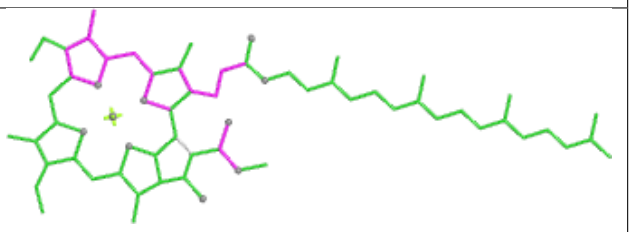


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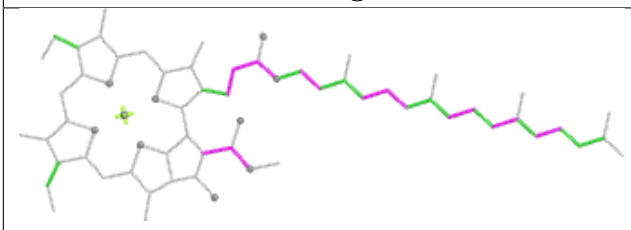
Ligand CLA a 404



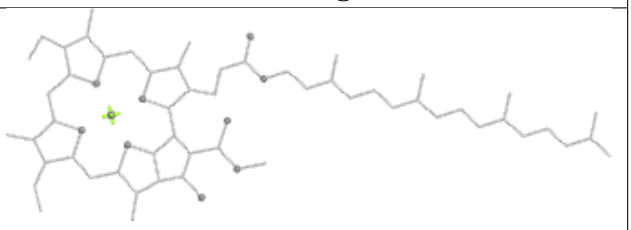
Bond lengths



Bond angles

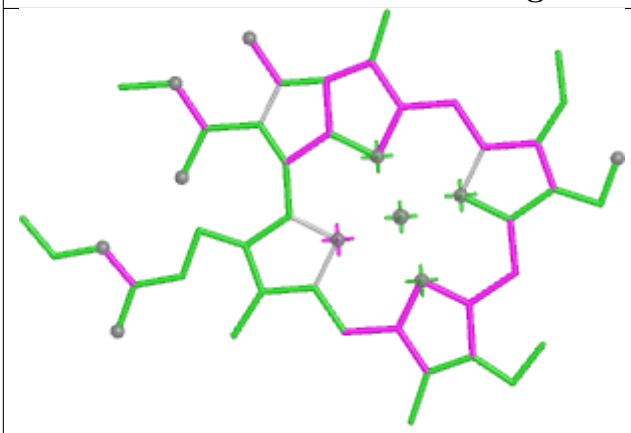


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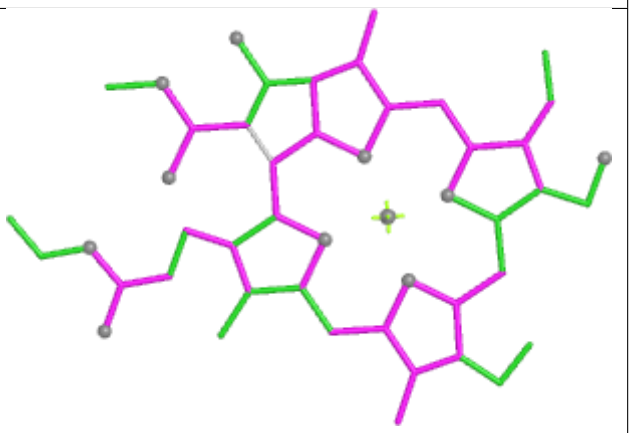


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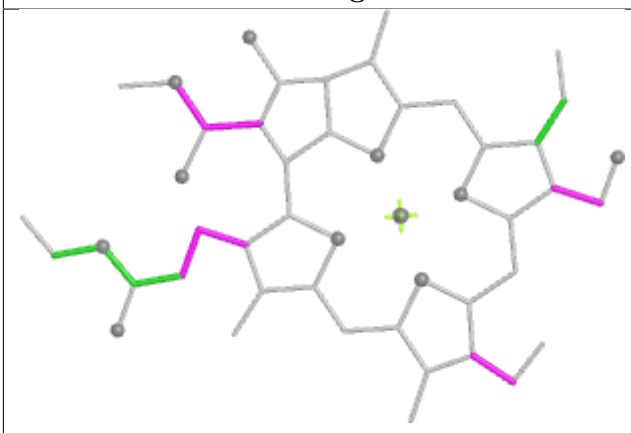
Ligand CHL n 314



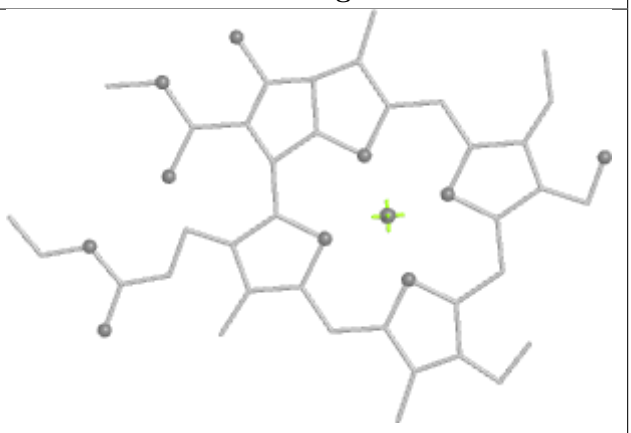
Bond lengths



Bond angles

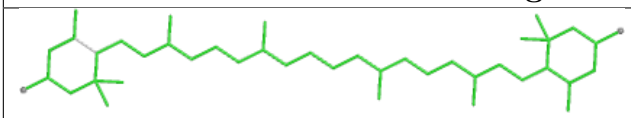


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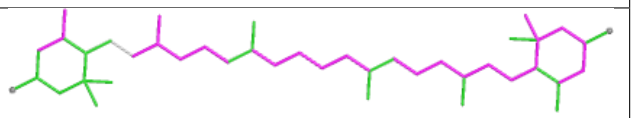


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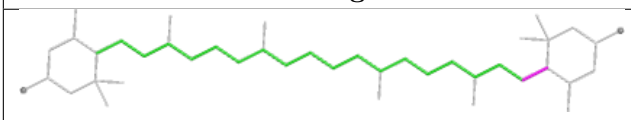
Ligand LUT P 310



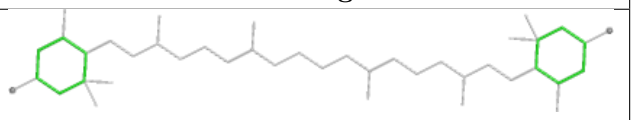
Bond lengths



Bond angles

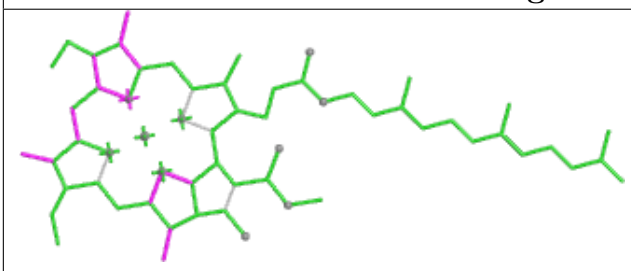


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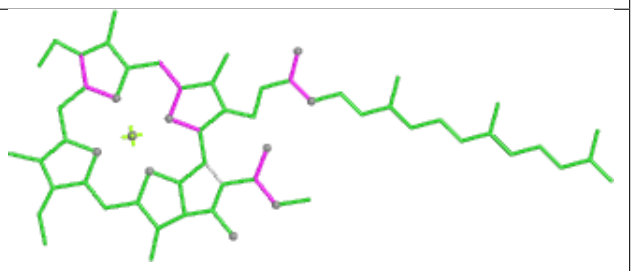


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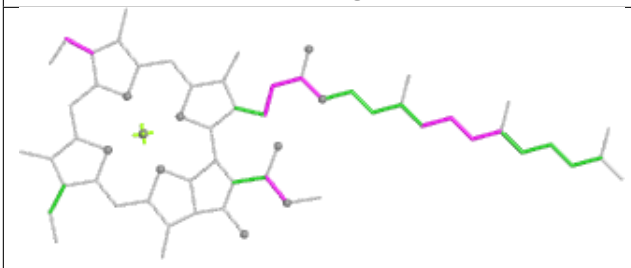
Ligand CLA n 307



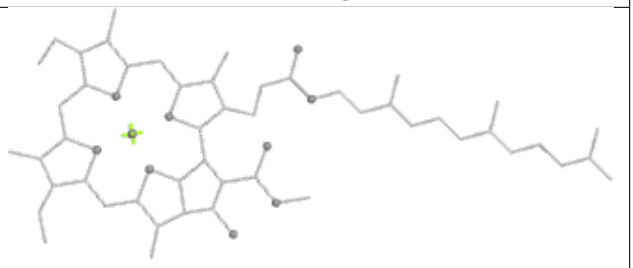
Bond lengths



Bond angles

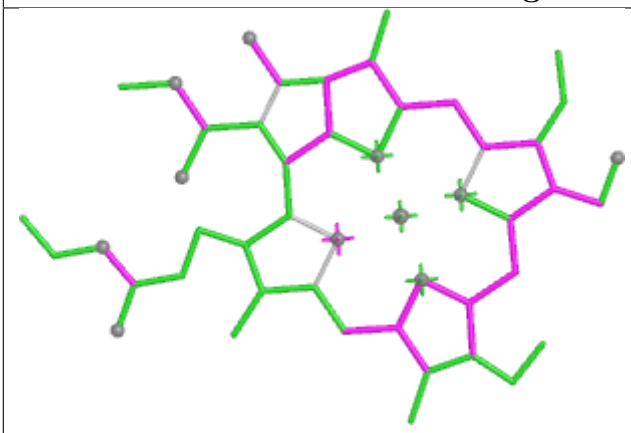


Torsions

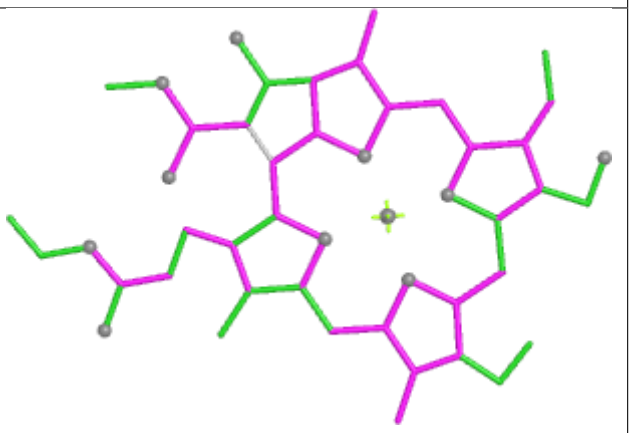


Rings

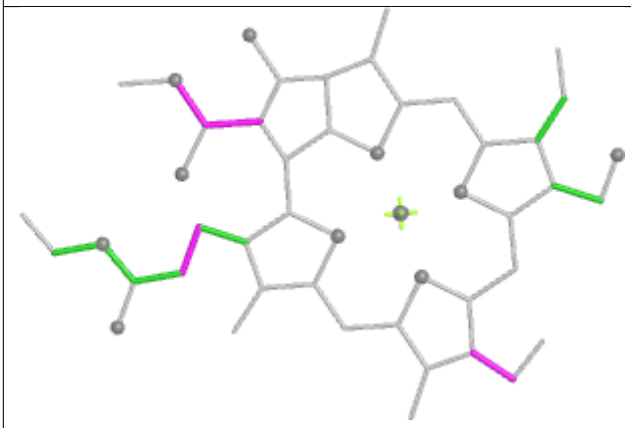
Ligand CHL G 312



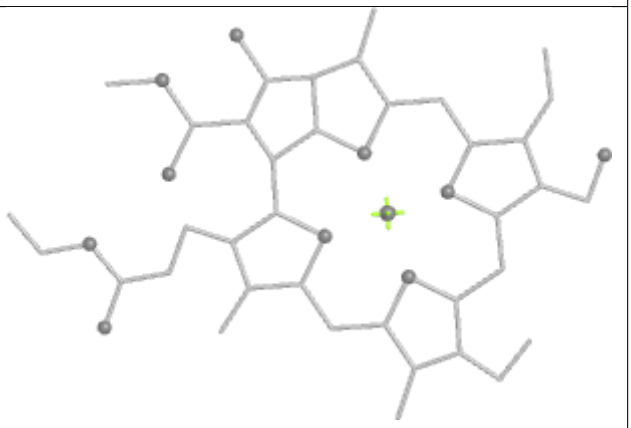
Bond lengths



Bond angles

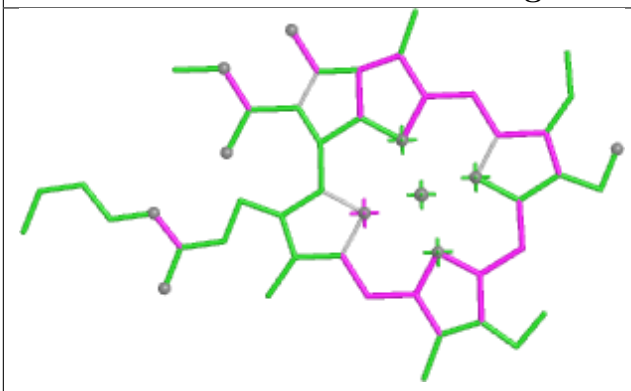


Torsions

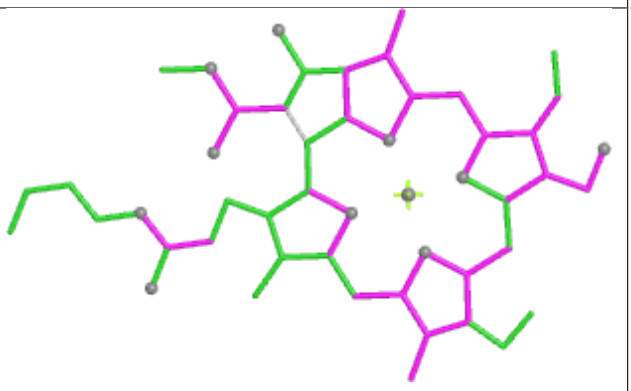


Rings

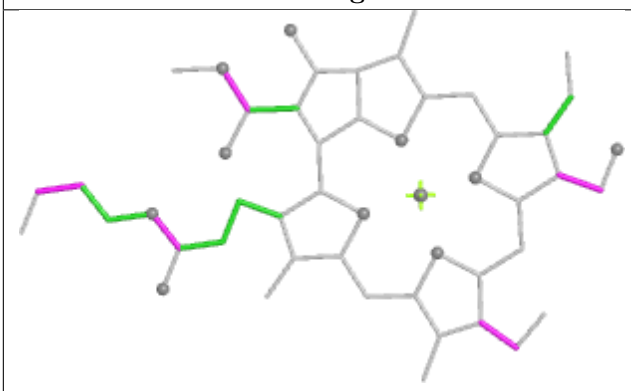
Ligand CHL P 316



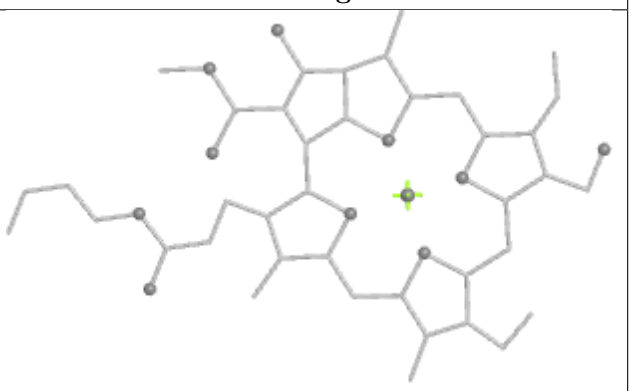
Bond lengths



Bond angles

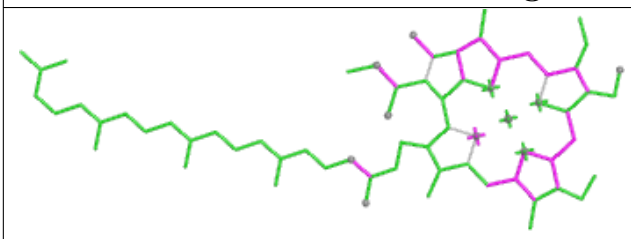


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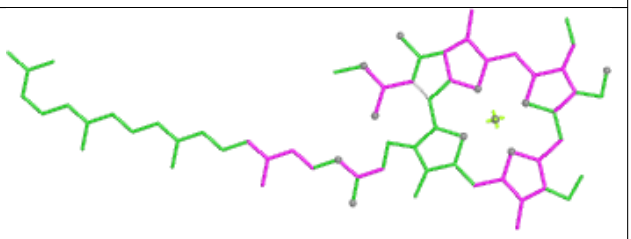


Rings

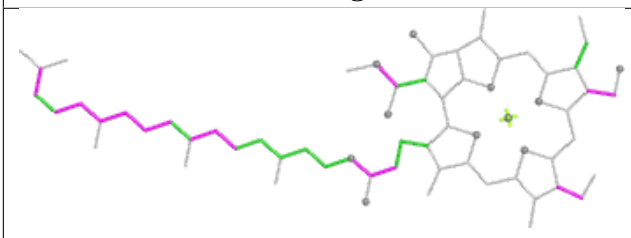
Ligand CHL V 313



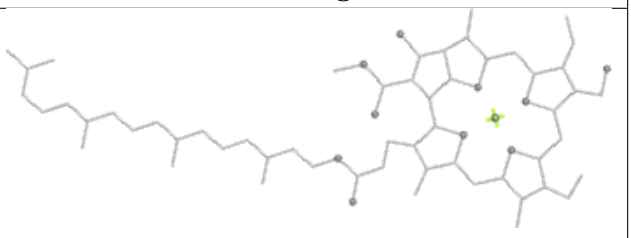
Bond lengths



Bond angles

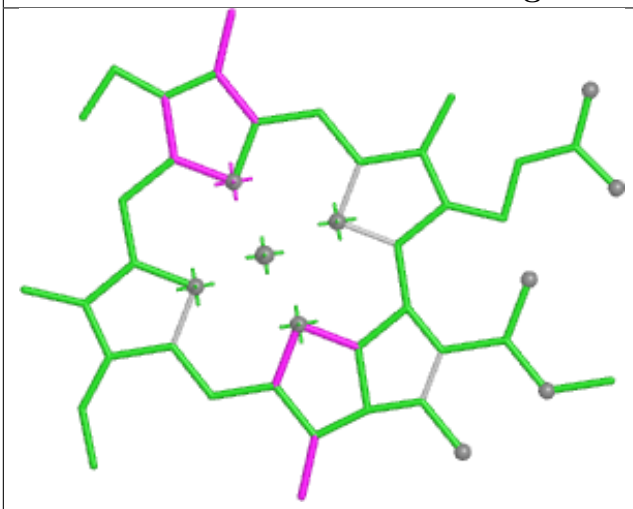


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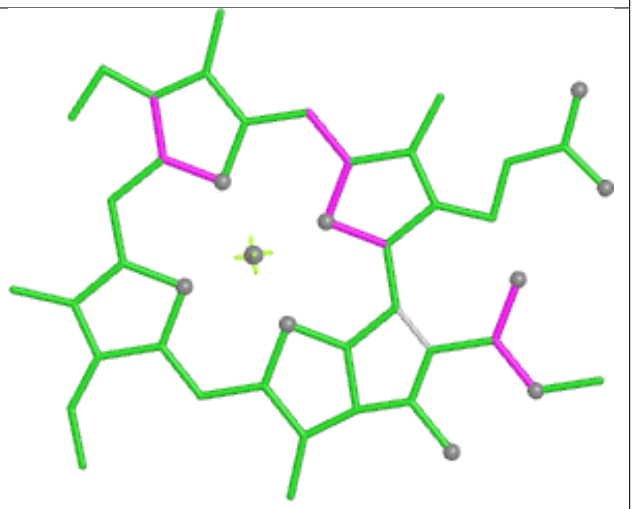


Rings

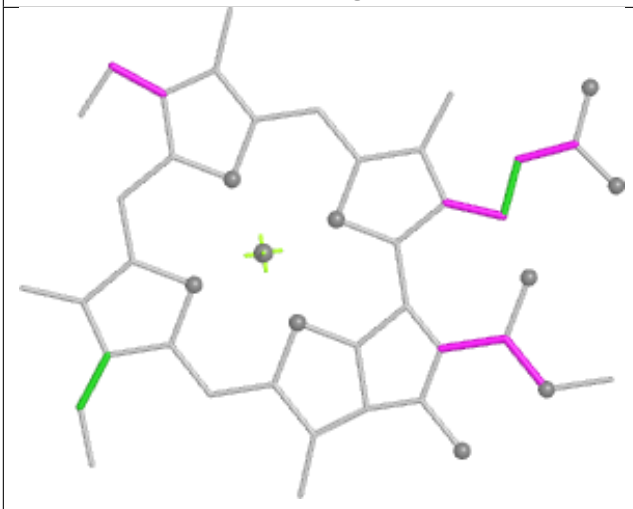
Ligand CLA R 311



Bond lengths



Bond angles

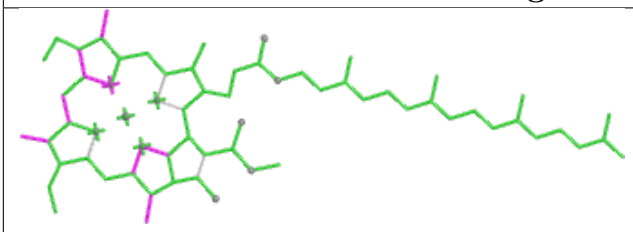


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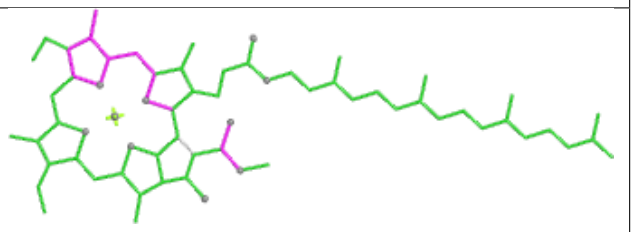


Rings

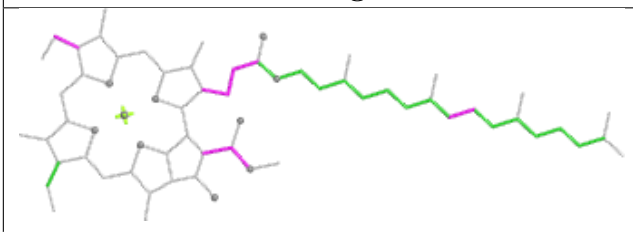
Ligand CLA u 301



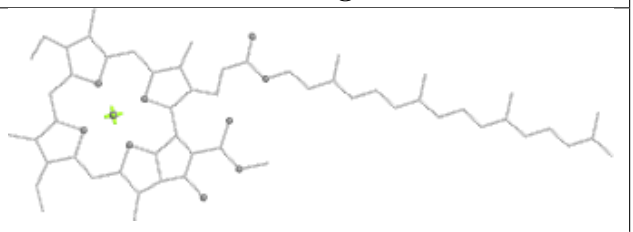
Bond lengths



Bond angles

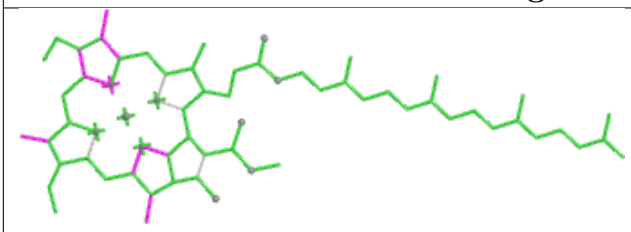


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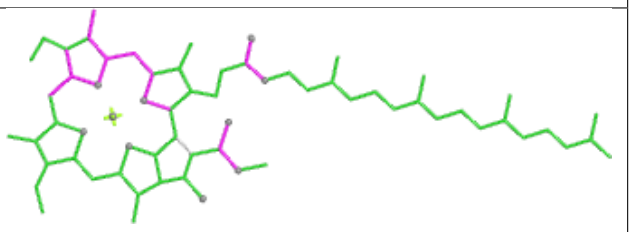


Rings

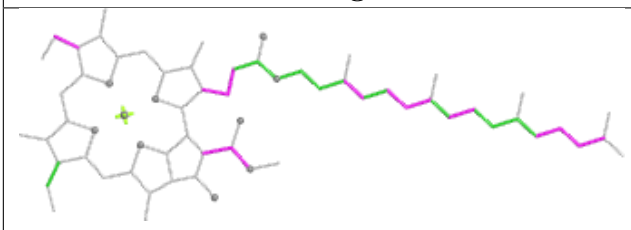
Ligand CLA b 604



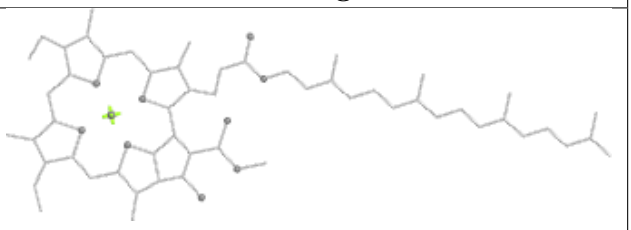
Bond lengths



Bond angles

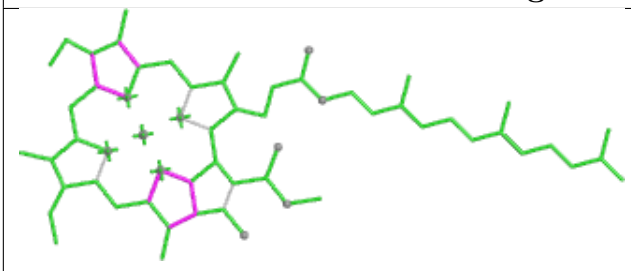


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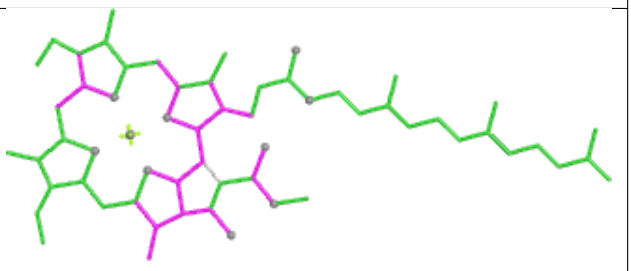


Rings

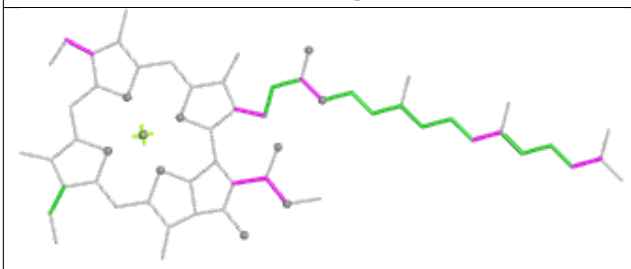
Ligand CLA n 305



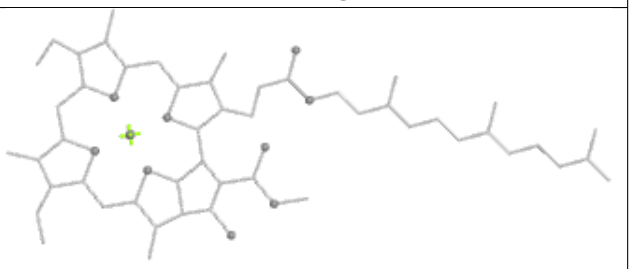
Bond lengths



Bond angles

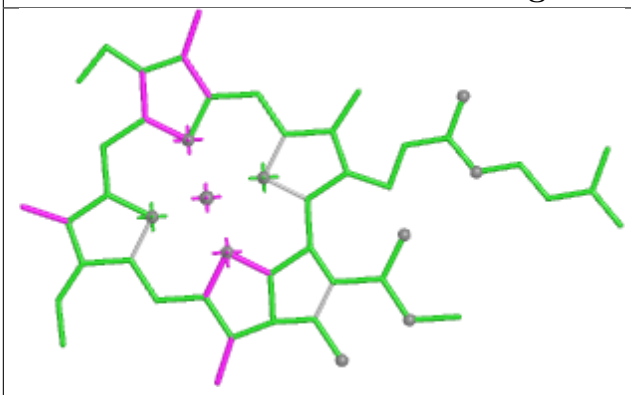


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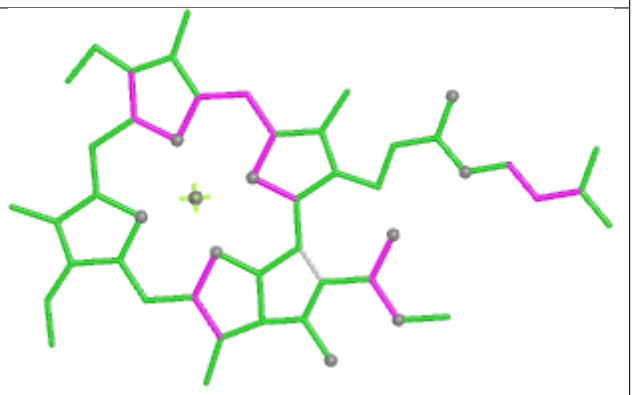


Rings

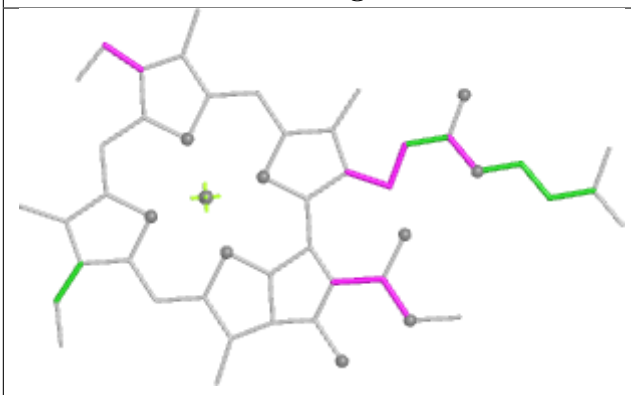
Ligand CLA a 406



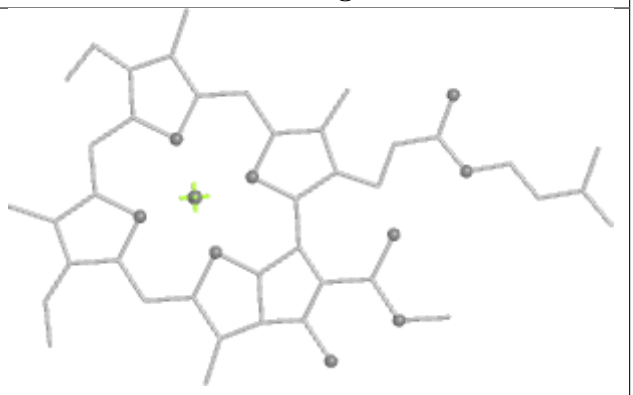
Bond lengths



Bond angles

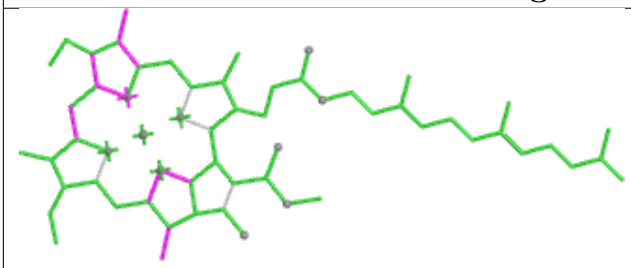


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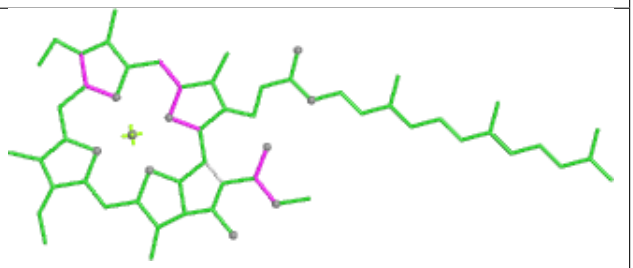


Rings

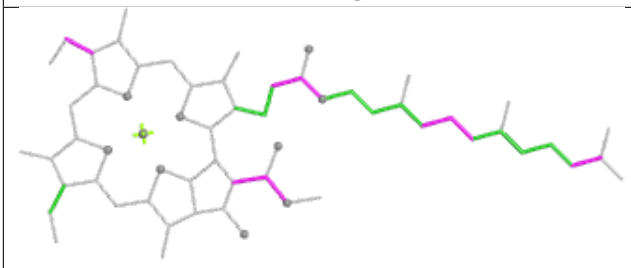
Ligand CLA r 603



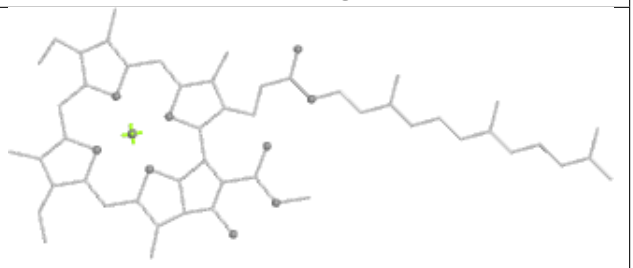
Bond lengths



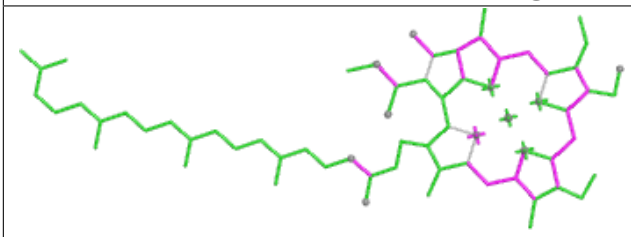
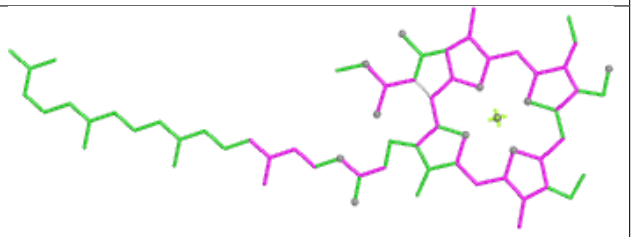
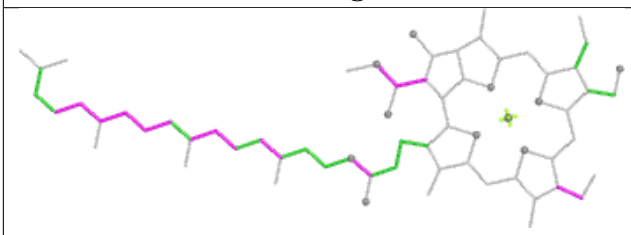
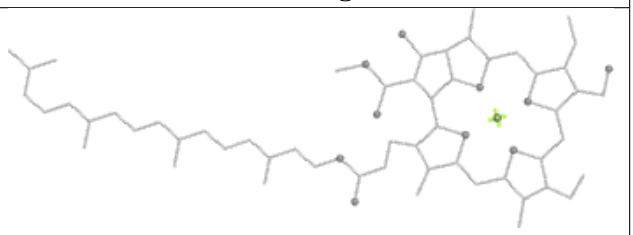
Bond angles

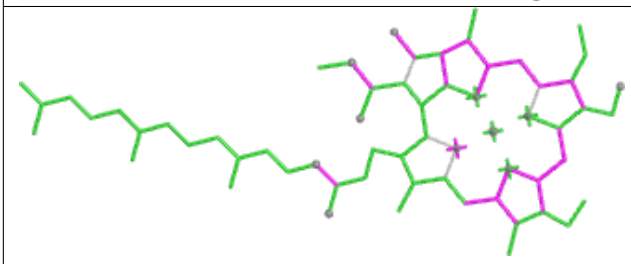
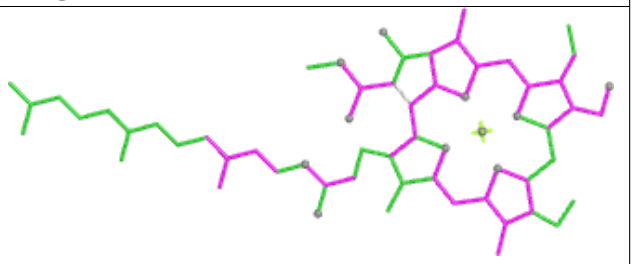
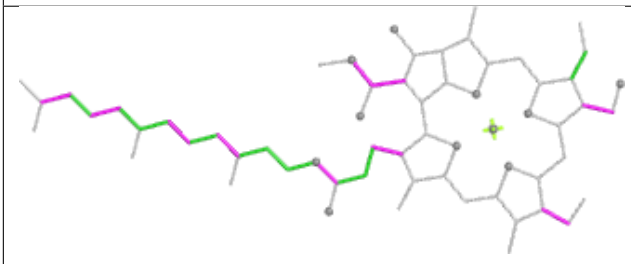
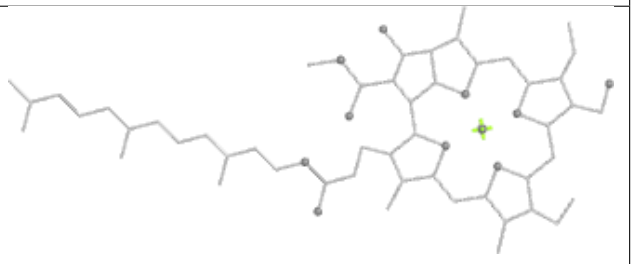


Torsions

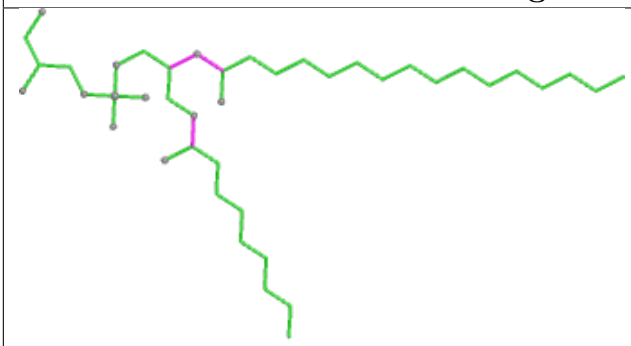


Rings

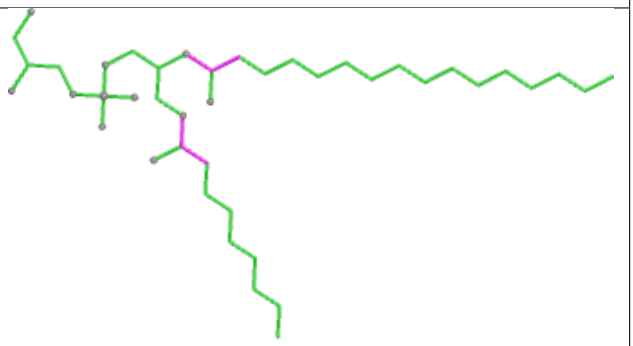
Ligand CHL 6 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL g 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

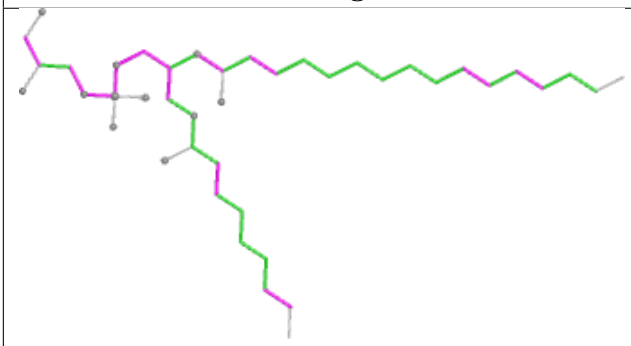
Ligand LHG r 613



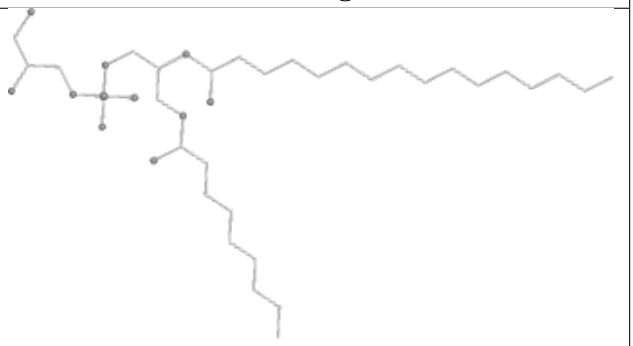
Bond lengths



Bond angles

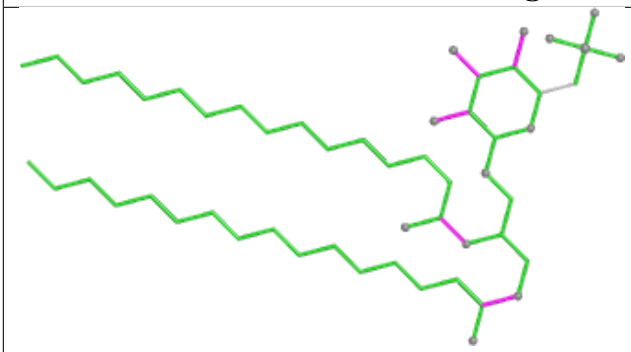


Torsions

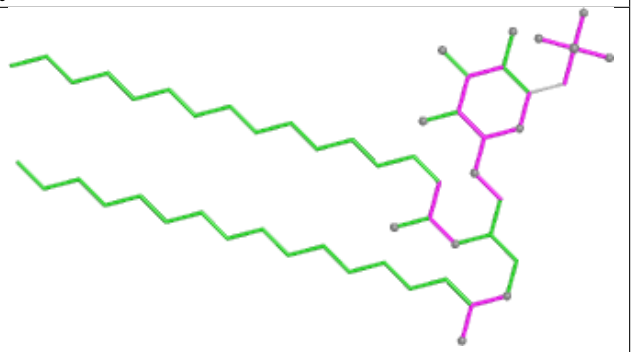


Rings

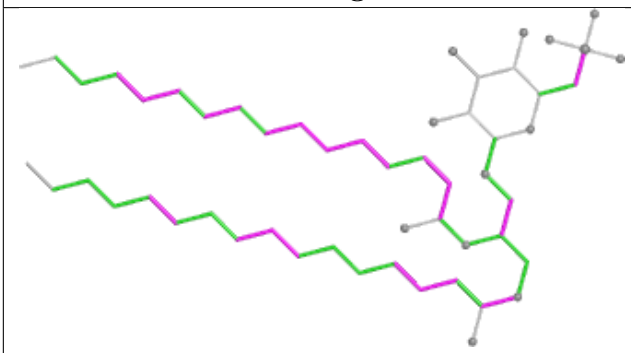
Ligand SQD A 412



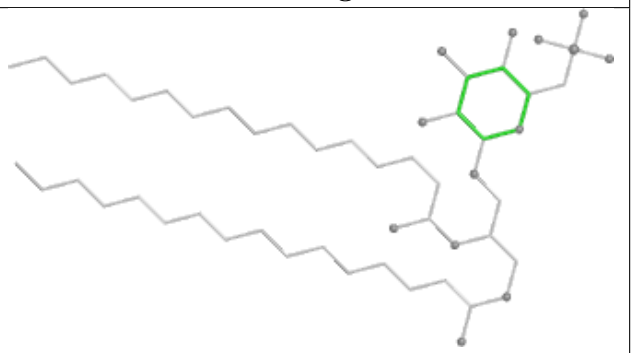
Bond lengths



Bond angles

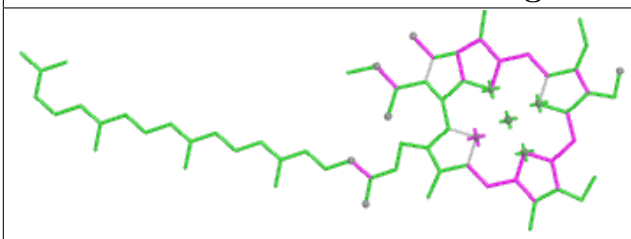


Torsions

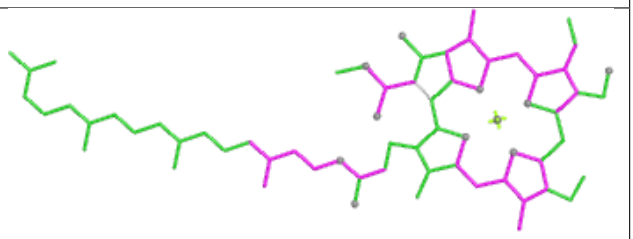


Rings

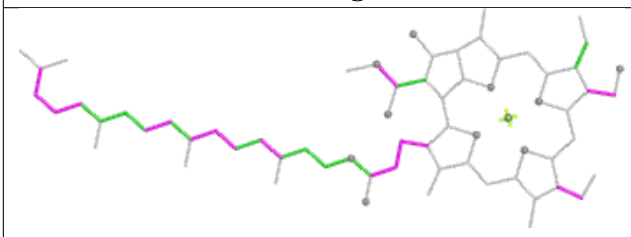
Ligand CHL P 318



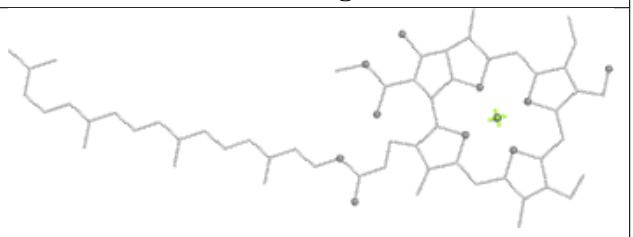
Bond lengths



Bond angles

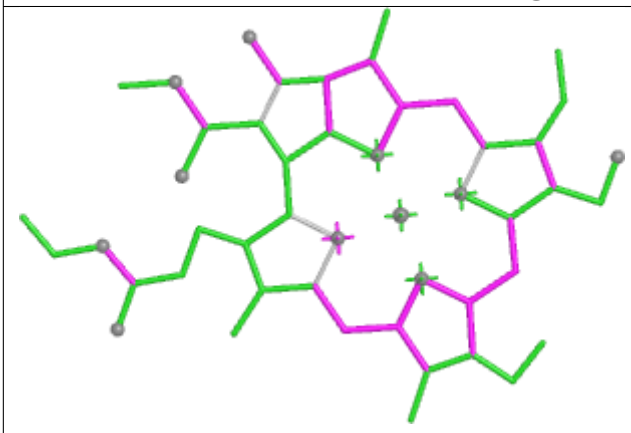


Torsions

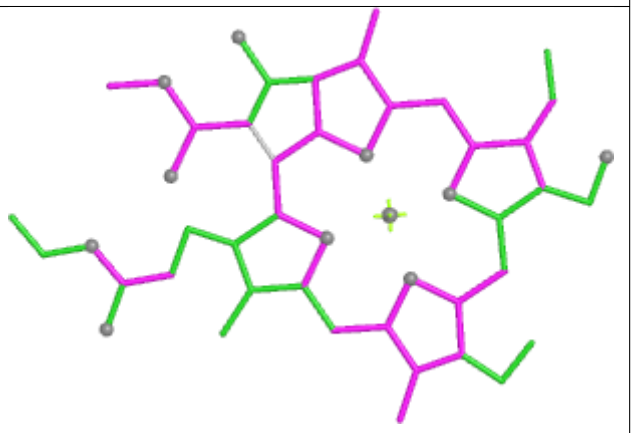


Rings

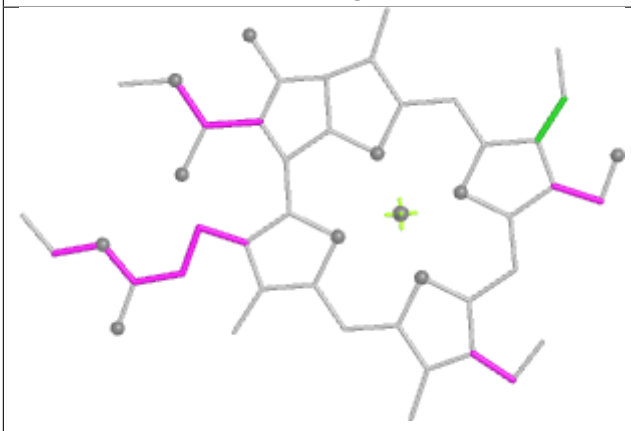
Ligand CHL 1 314



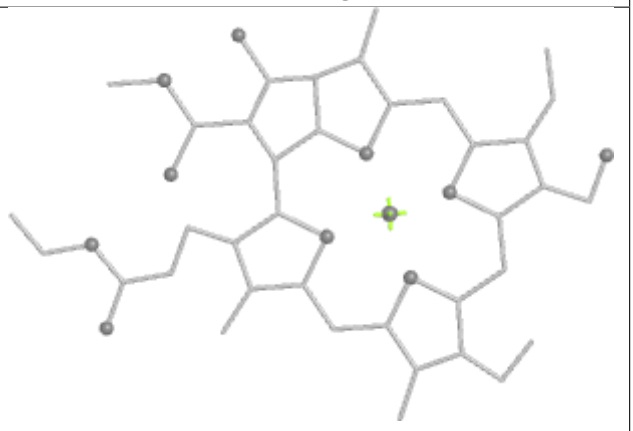
Bond lengths



Bond angles

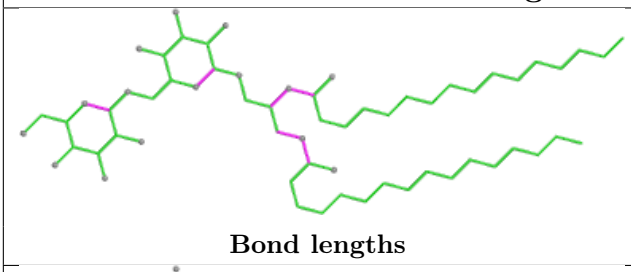


Torsions

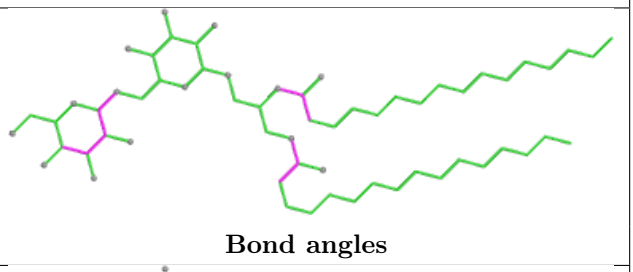


Rings

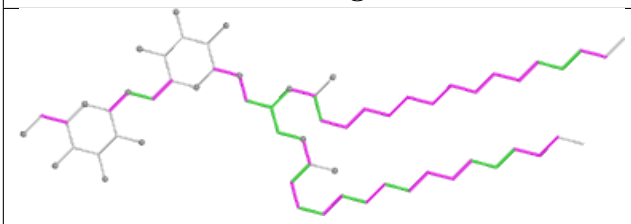
Ligand DGD c 518



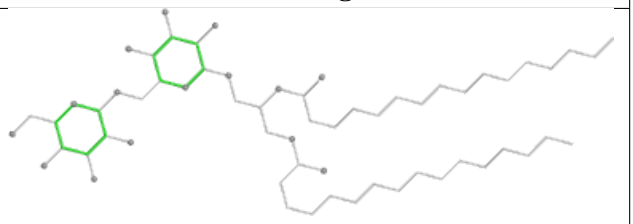
Bond lengths



Bond angles

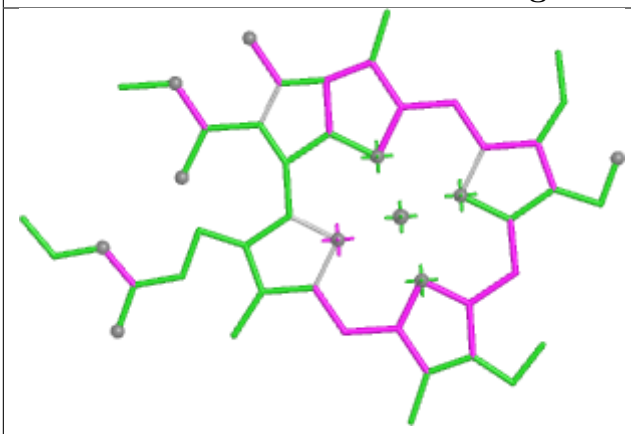


Torsions

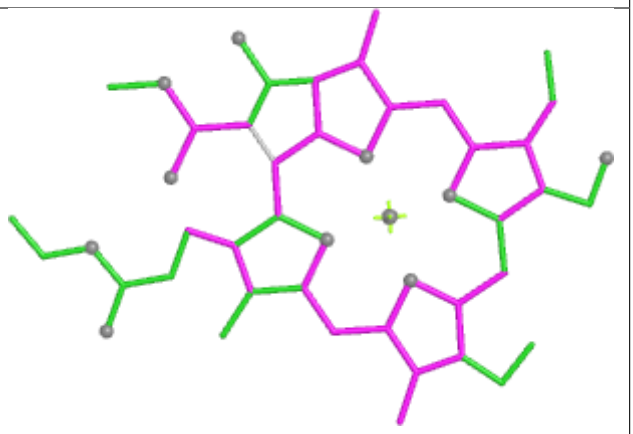


Rings

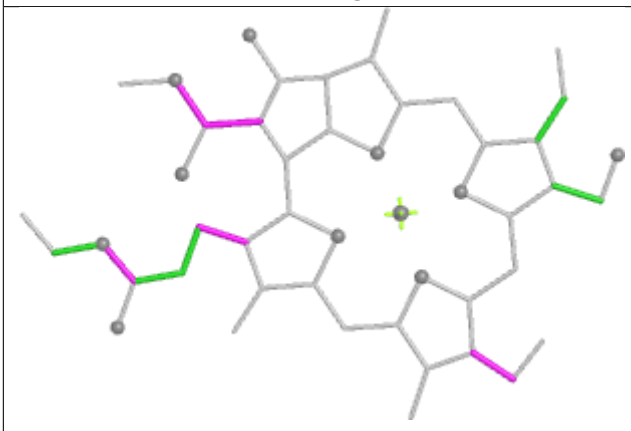
Ligand CHL r 619



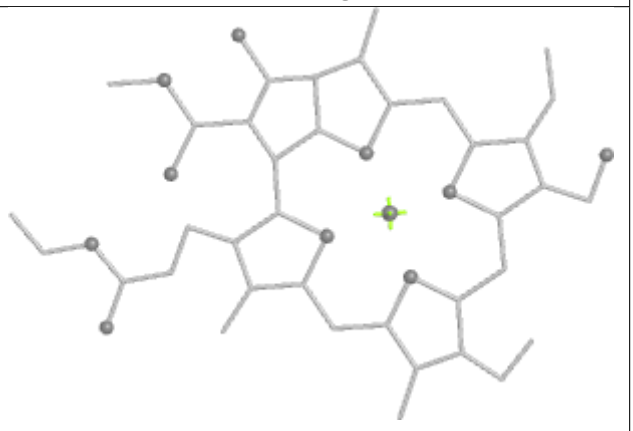
Bond lengths



Bond angles

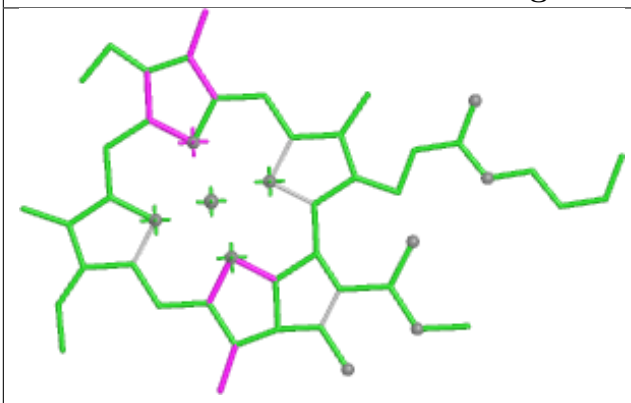


Torsions

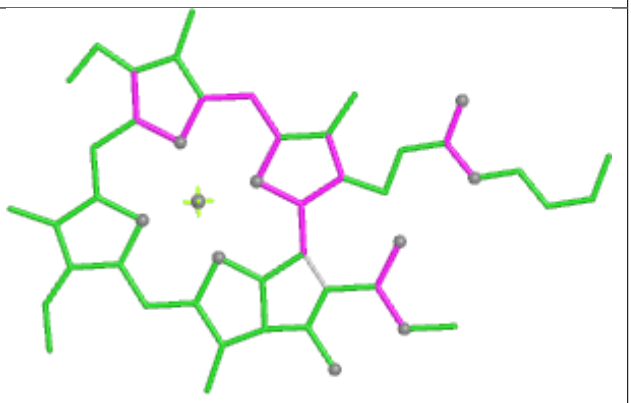


Rings

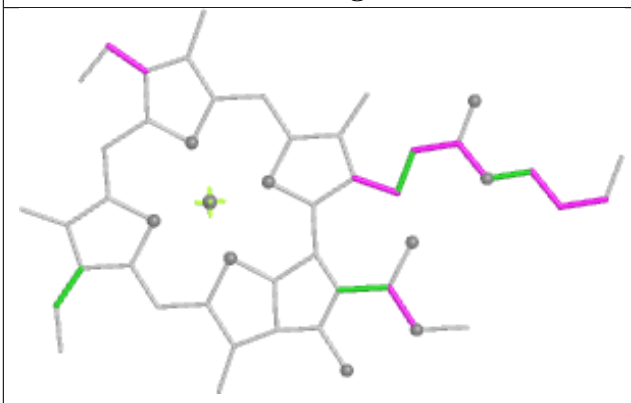
Ligand CLA r 607



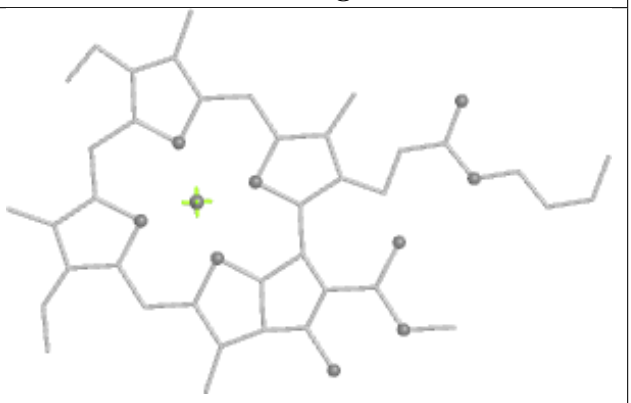
Bond lengths



Bond angles

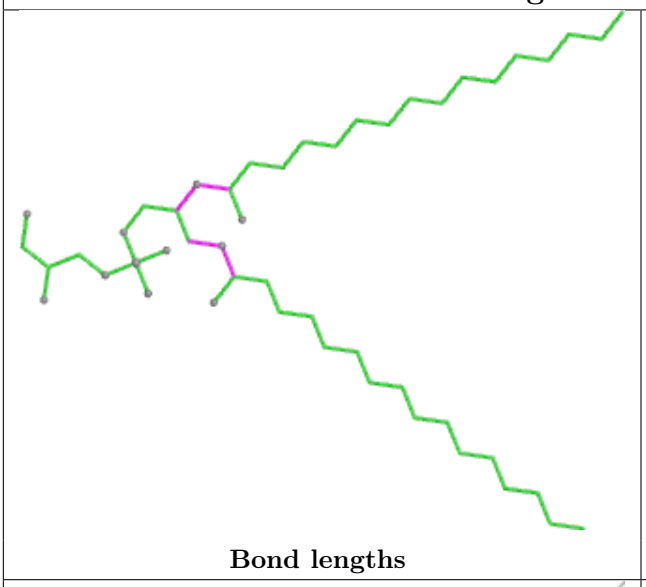


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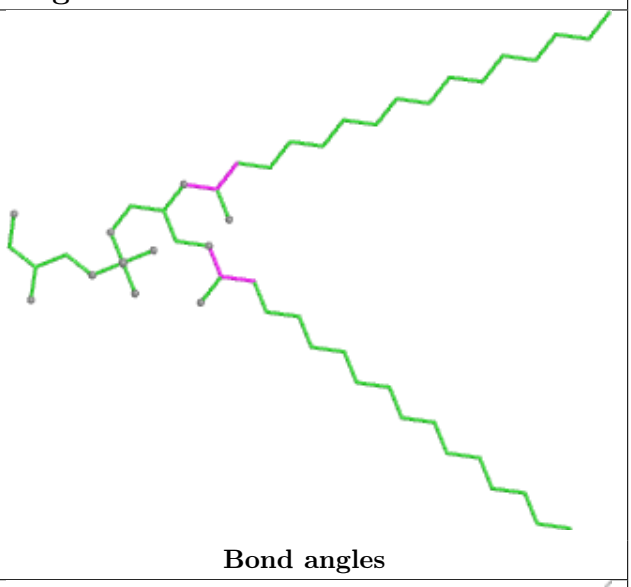


Rings

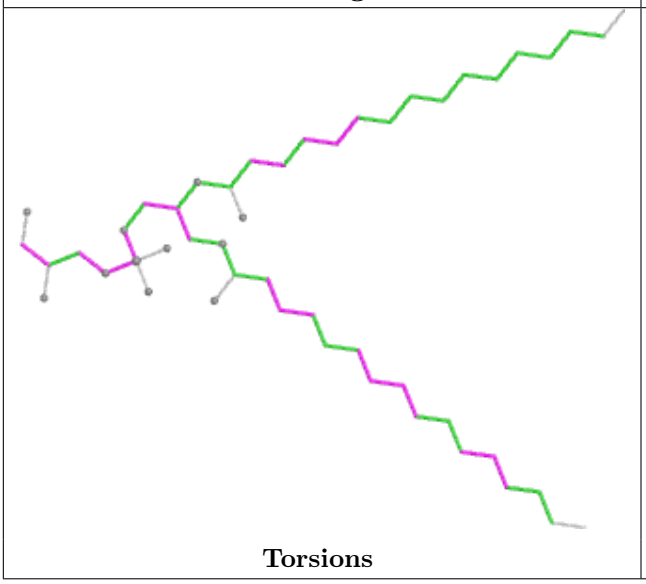
Ligand LHG g 310



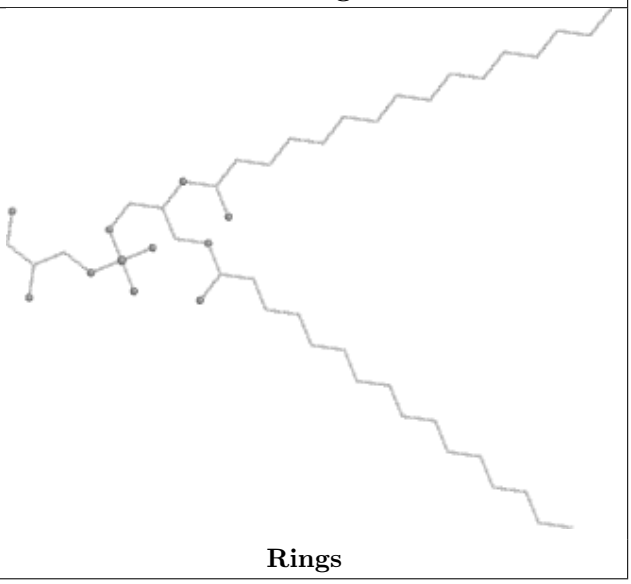
Bond lengths



Bond angles

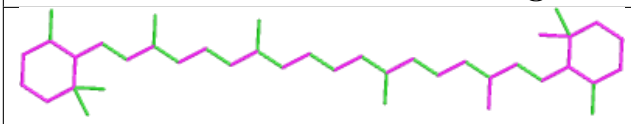


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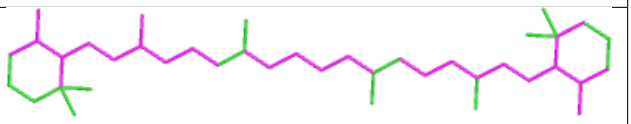


Rings

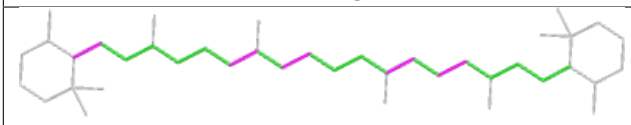
Ligand BCR z 101



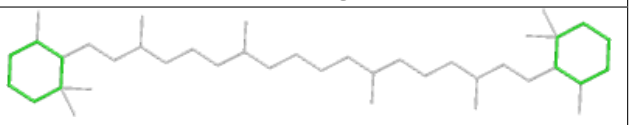
Bond lengths



Bond angles

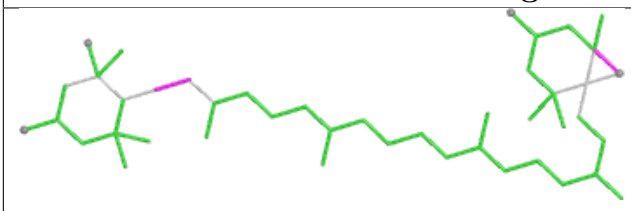


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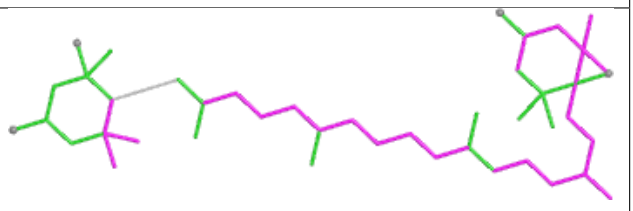


Rings

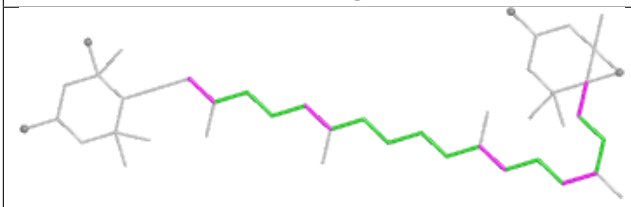
Ligand NEX N 318



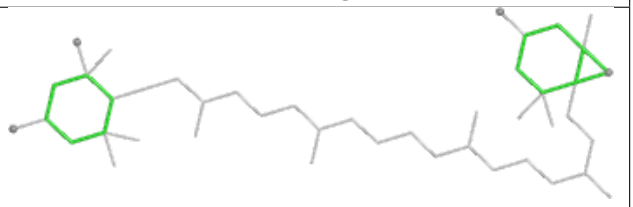
Bond lengths



Bond angles

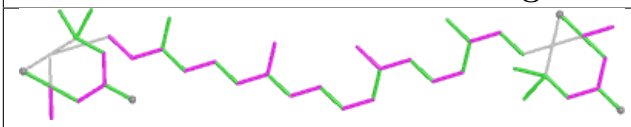


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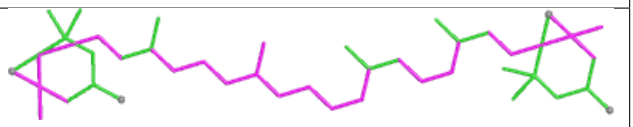


Rings

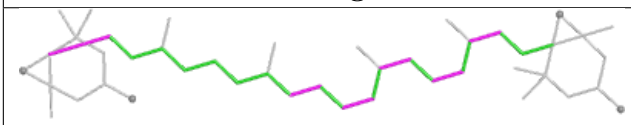
Ligand XAT N 311



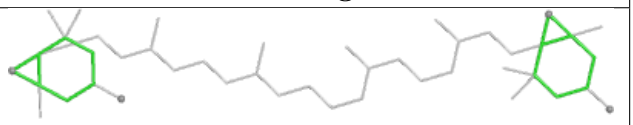
Bond lengths



Bond angles

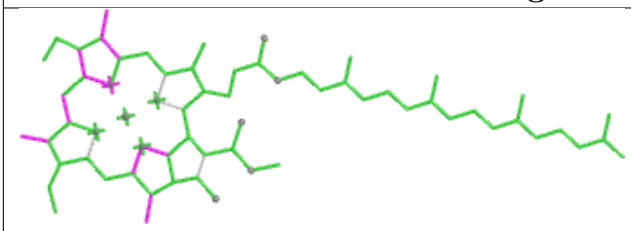


Torsions

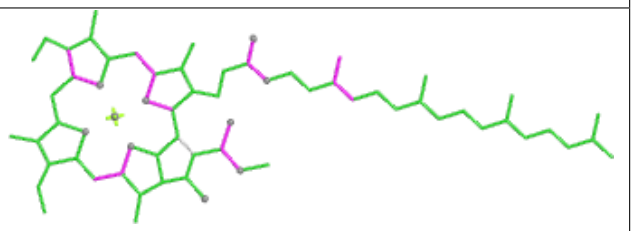


Rings

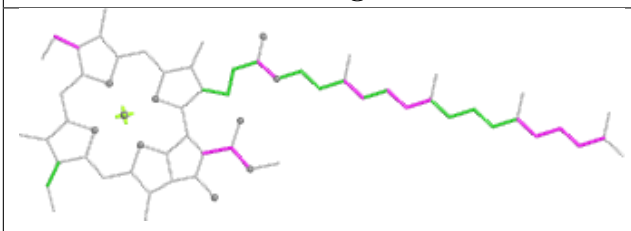
Ligand CLA b 610



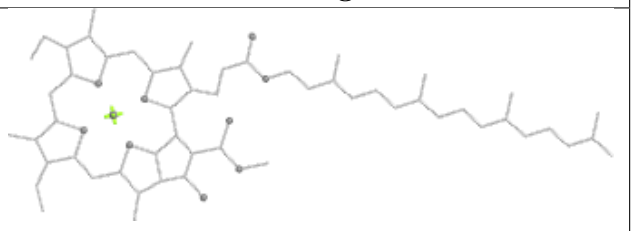
Bond lengths



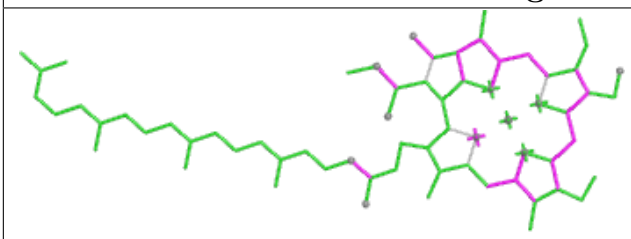
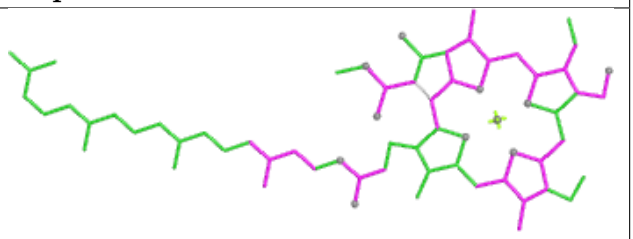
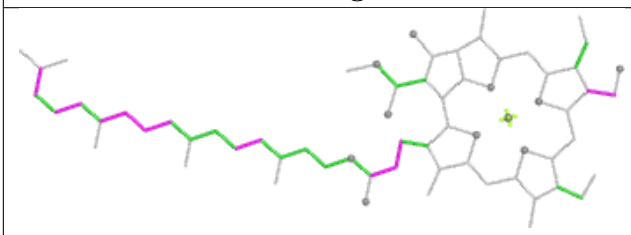
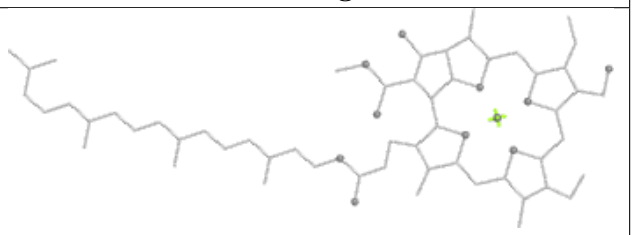
Bond angles

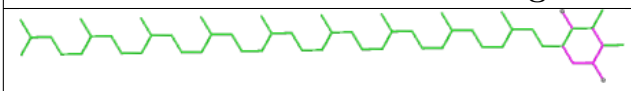
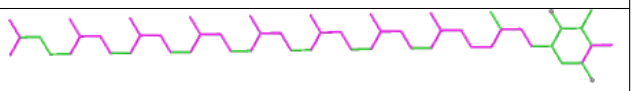
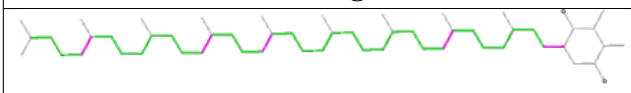
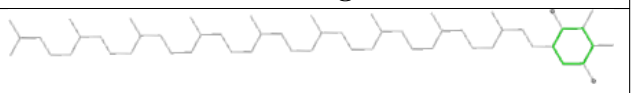


Torsions

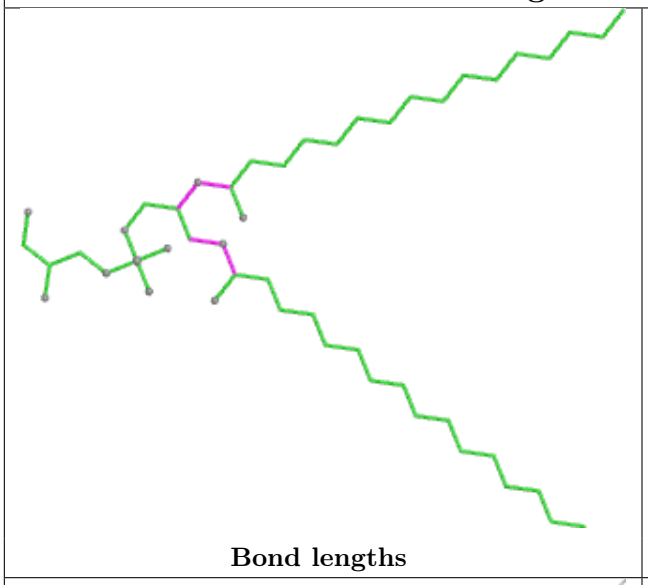


Rings

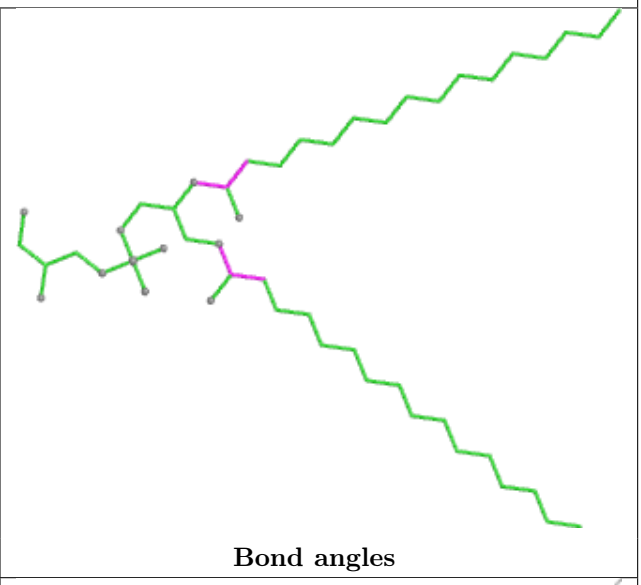
Ligand CHL p 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PL9 D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

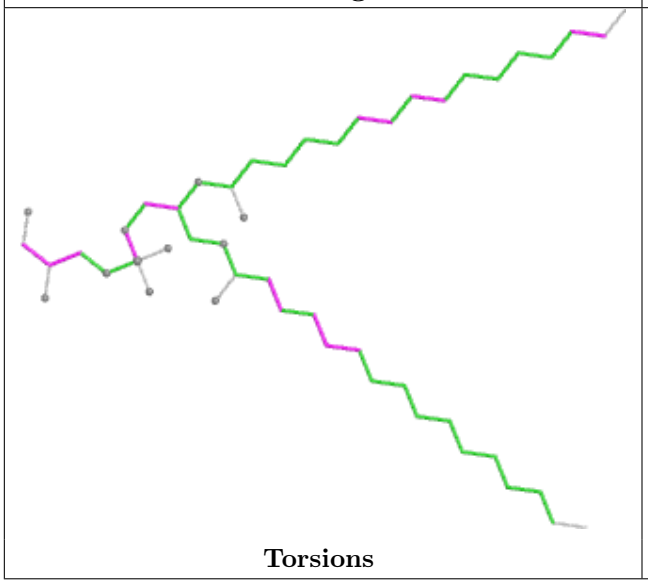
Ligand LHG 1 312



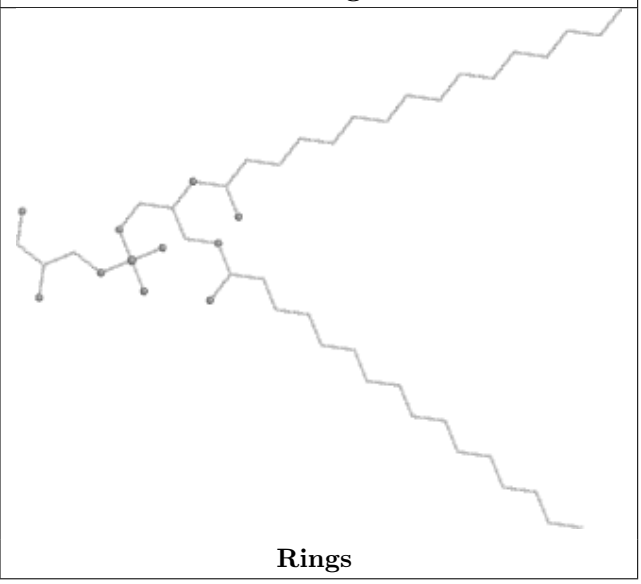
Bond lengths



Bond angles

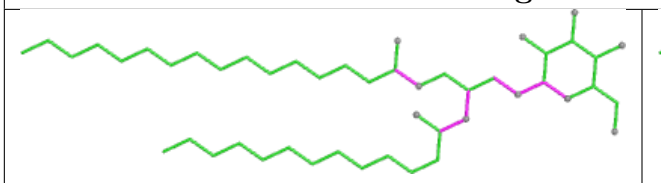


Torsions

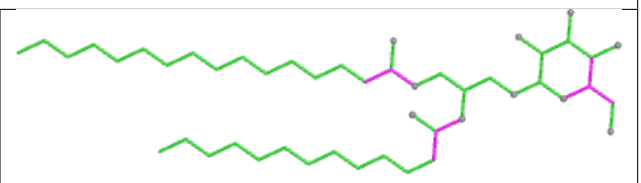


Rings

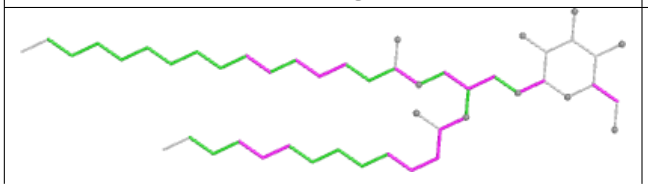
Ligand LMG W 201



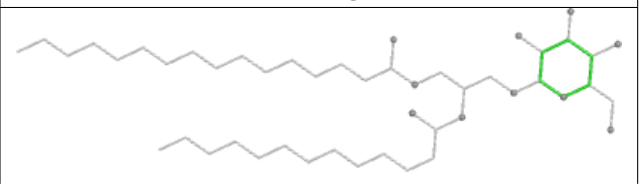
Bond lengths



Bond angles

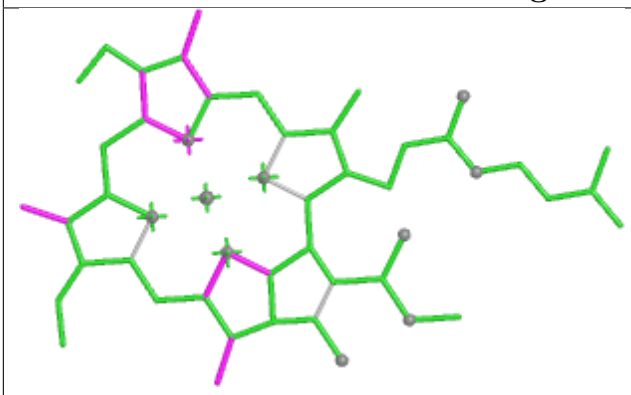


Torsions

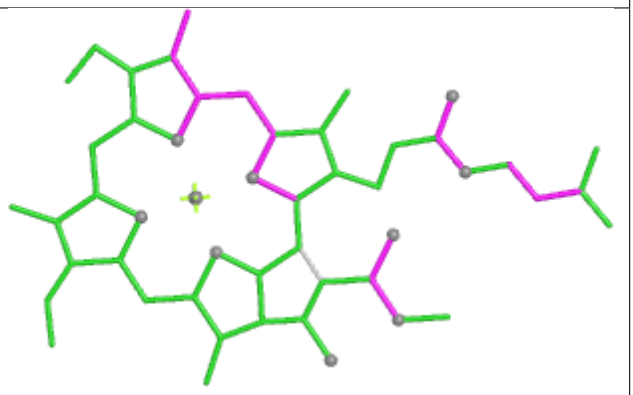


Rings

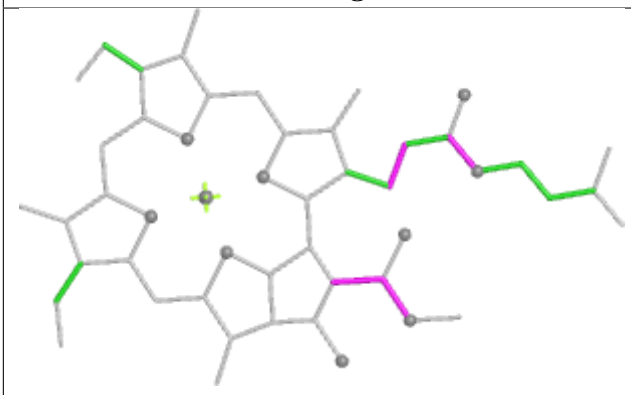
Ligand CLA s 303



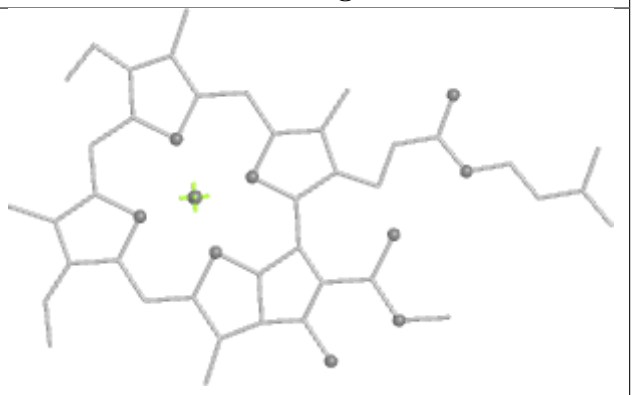
Bond lengths



Bond angles

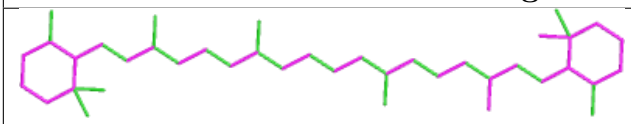


Torsions

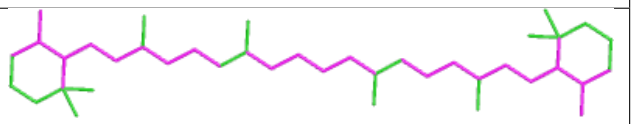


Rings

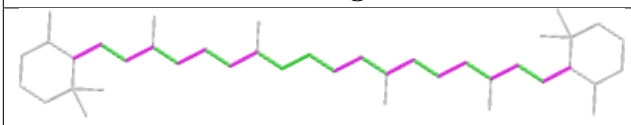
Ligand BCR K 101



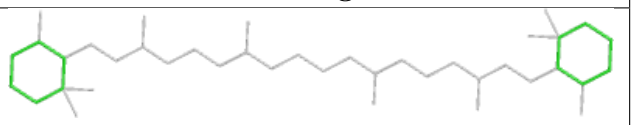
Bond lengths



Bond angles

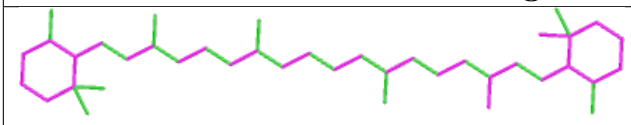


Torsions

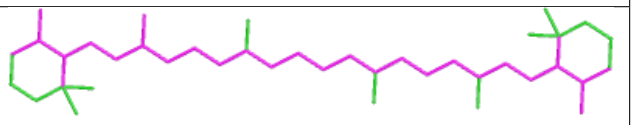


Rings

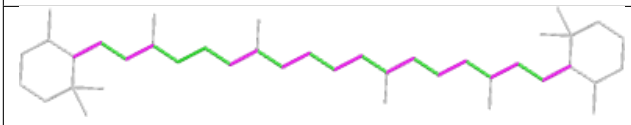
Ligand BCR B 619



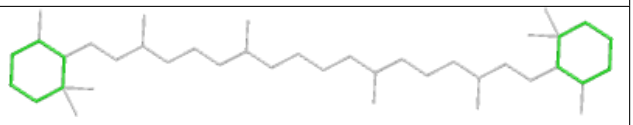
Bond lengths



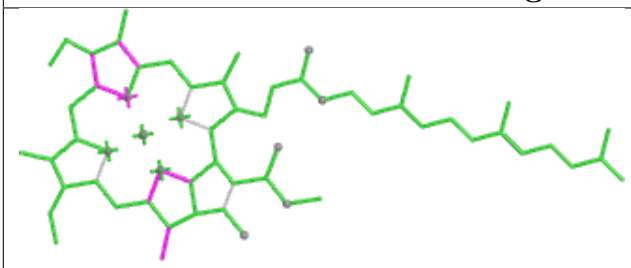
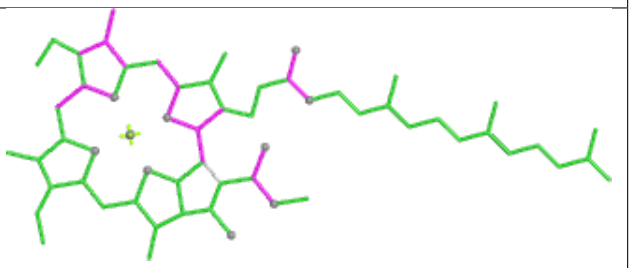
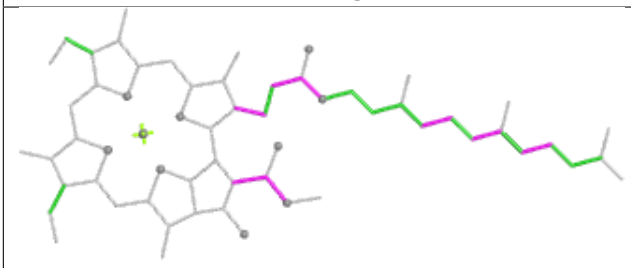
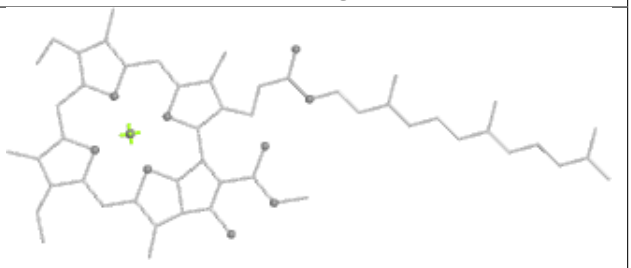
Bond angles

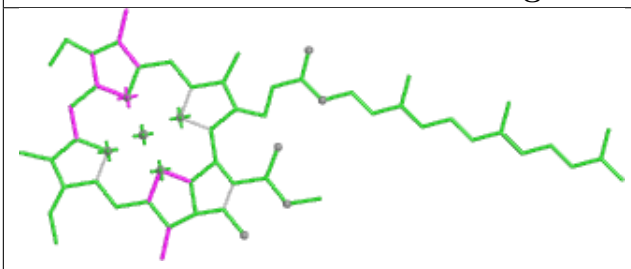
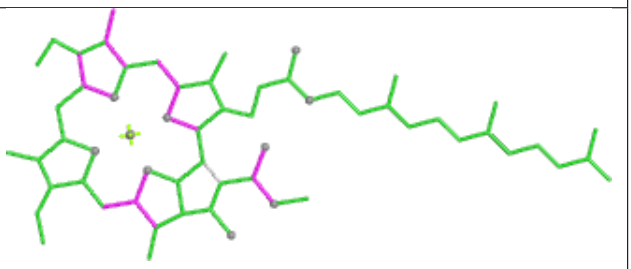
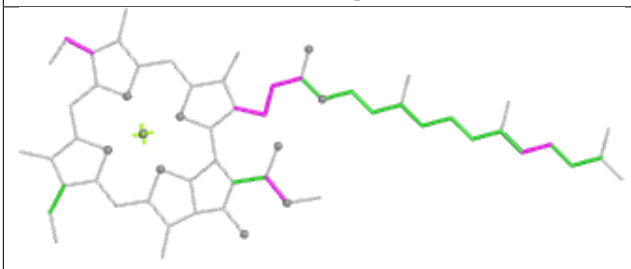
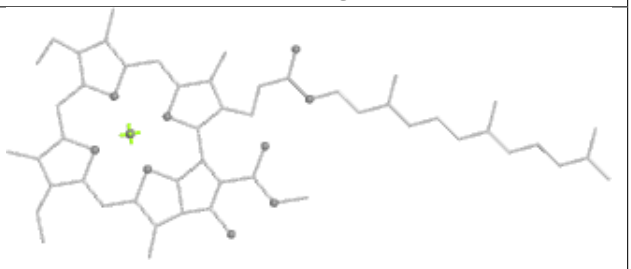


Torsions

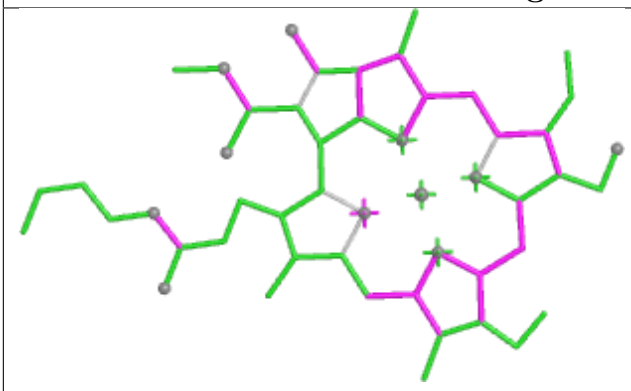


Rings

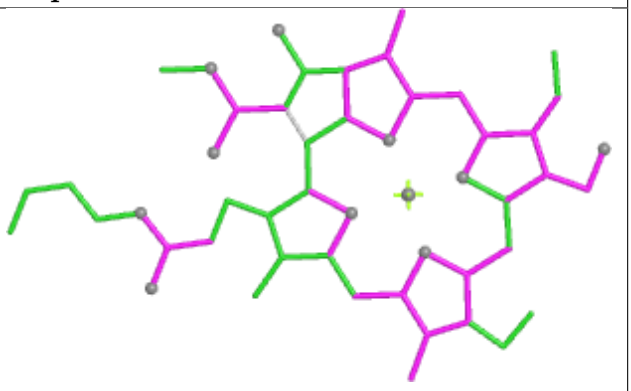
Ligand CLA P 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

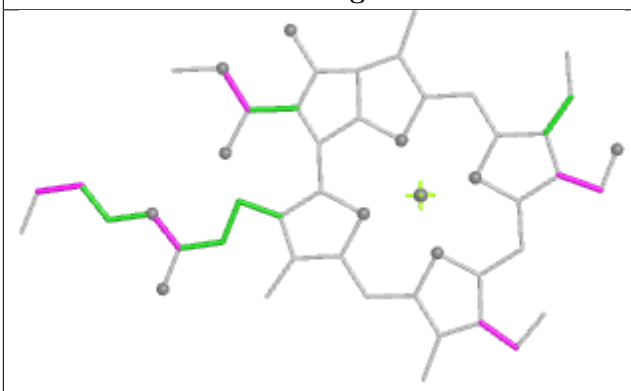
Ligand CHL p 316



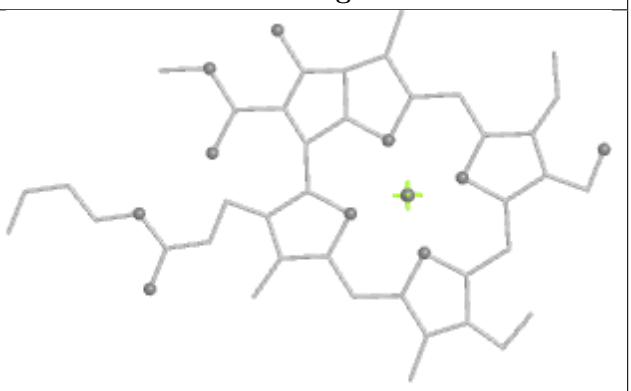
Bond lengths



Bond angles

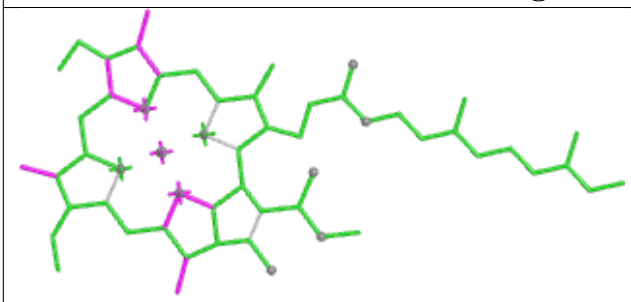


Torsions

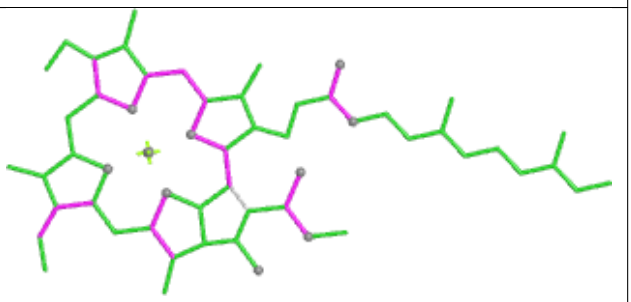


Rings

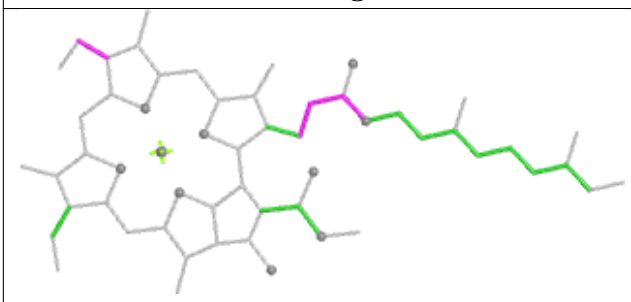
Ligand CLA s 306



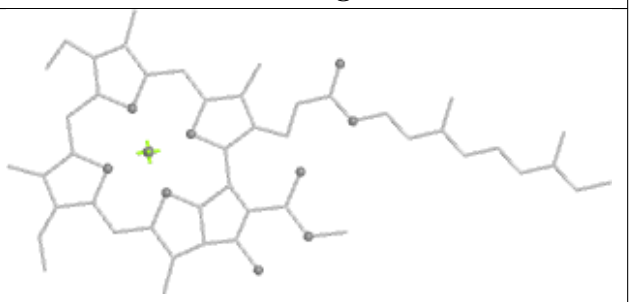
Bond lengths



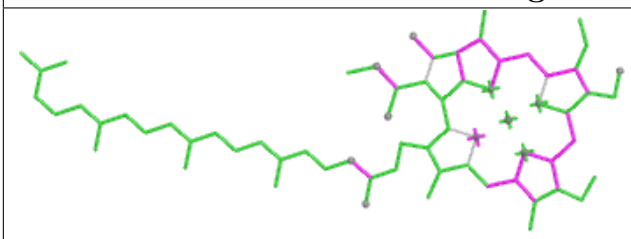
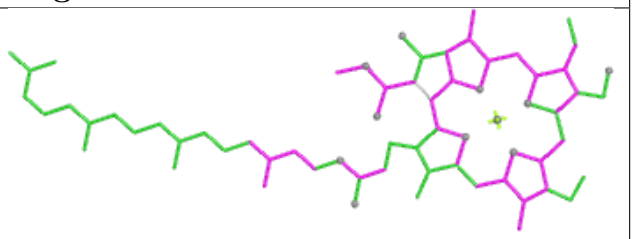
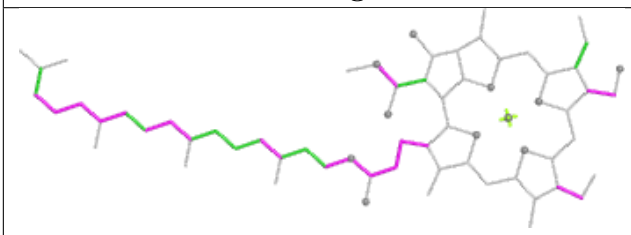
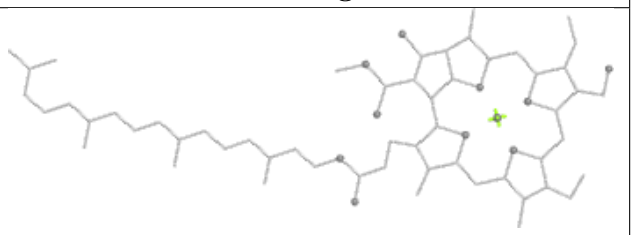
Bond angles

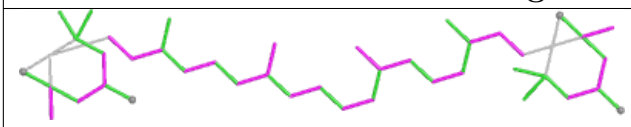
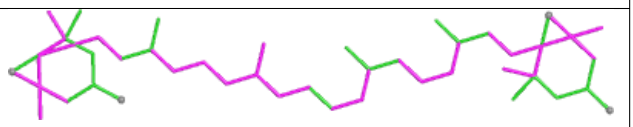
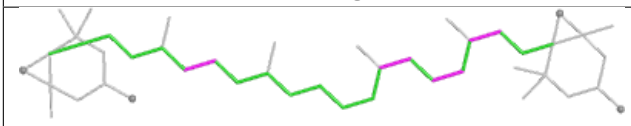
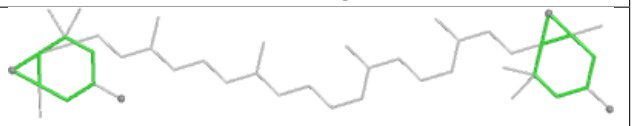


Torsions

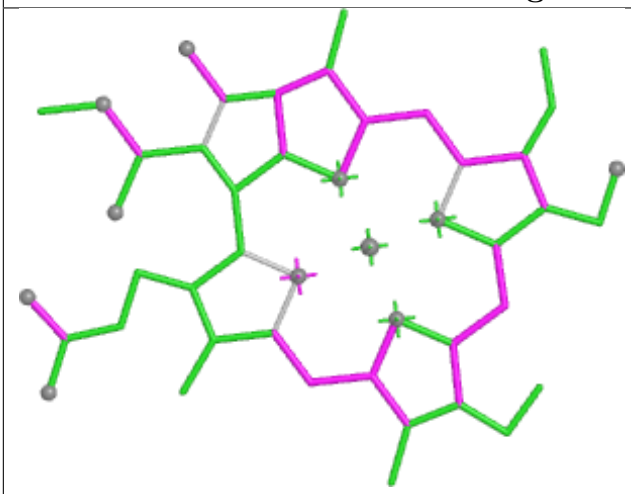


Rings

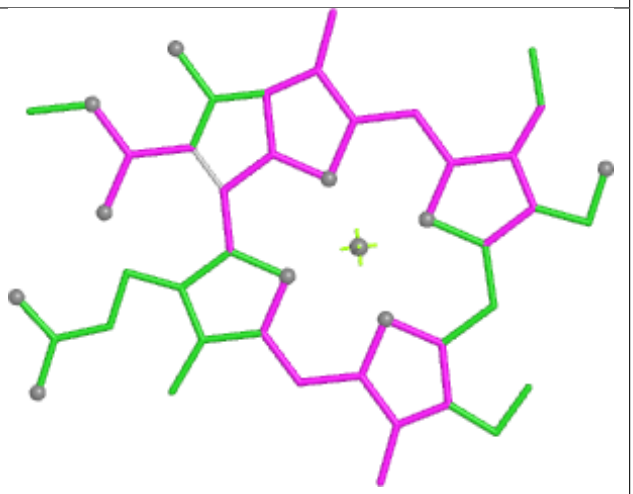
Ligand CHL g 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 5 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

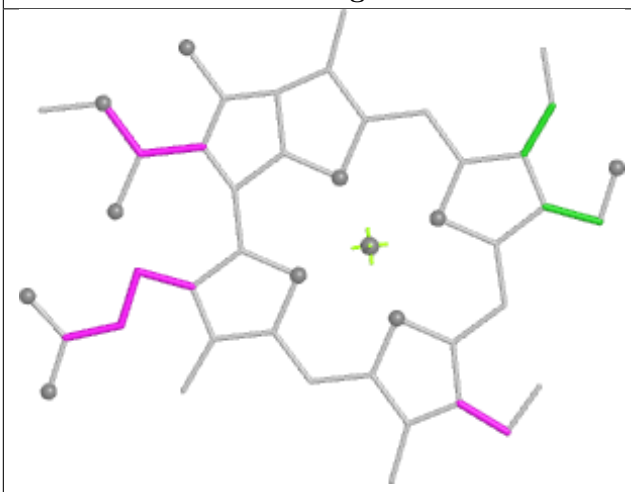
Ligand CHL S 314



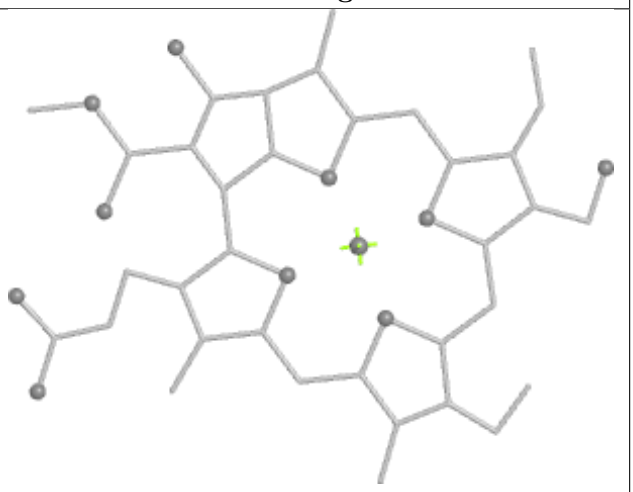
Bond lengths



Bond angles

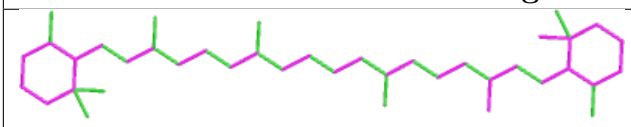


Torsions

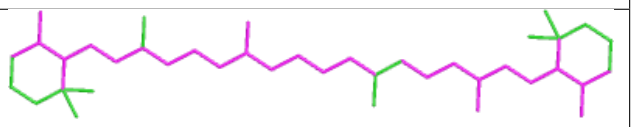


Rings

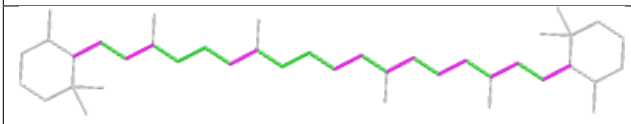
Ligand BCR D 404



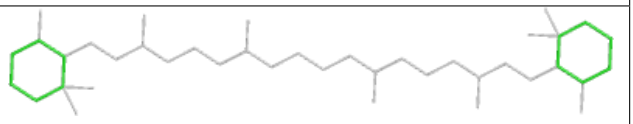
Bond lengths



Bond angles

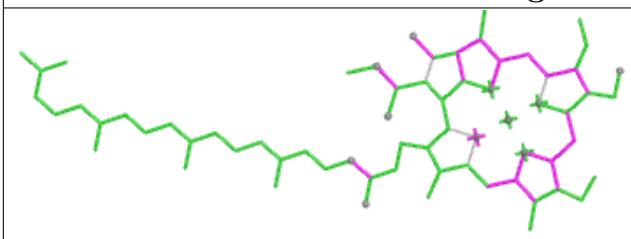


Torsions

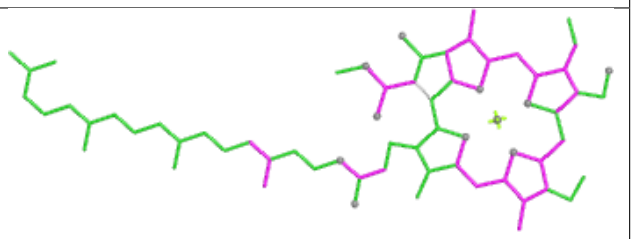


Rings

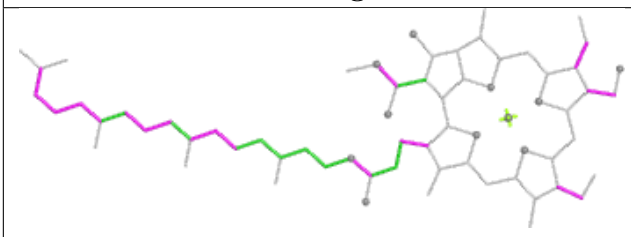
Ligand CHL v 318



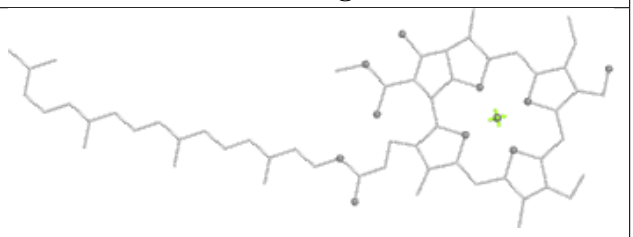
Bond lengths



Bond angles

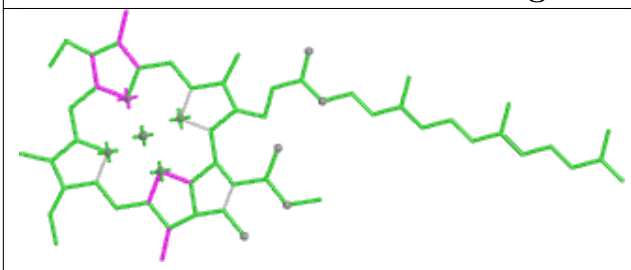


Torsions

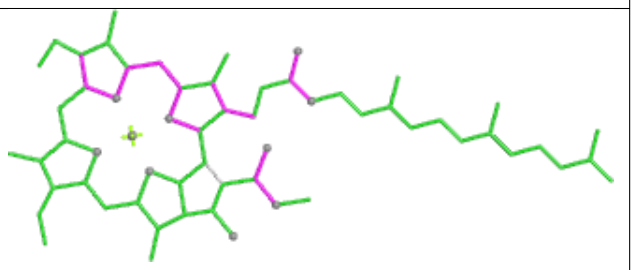


Rings

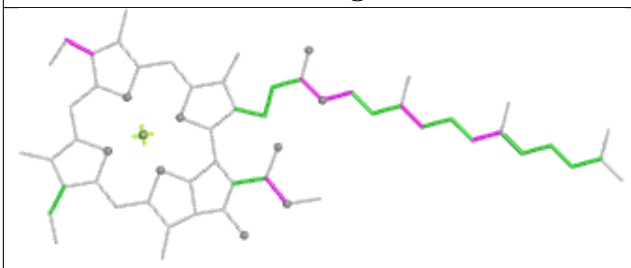
Ligand CLA 1 305



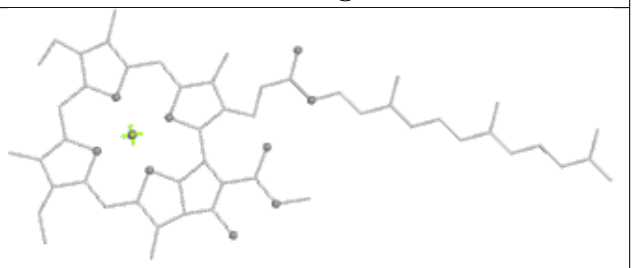
Bond lengths



Bond angles



Torsions



Rings

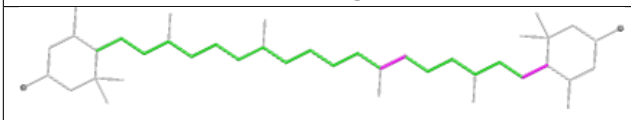
Ligand LUT U 309



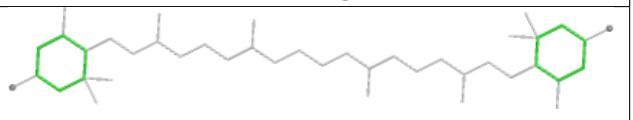
Bond lengths



Bond angles

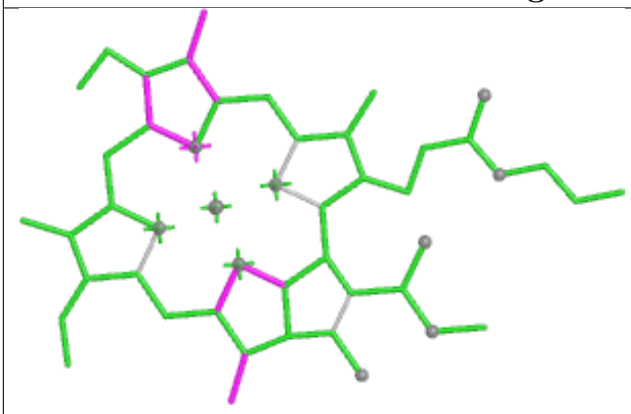


Torsions

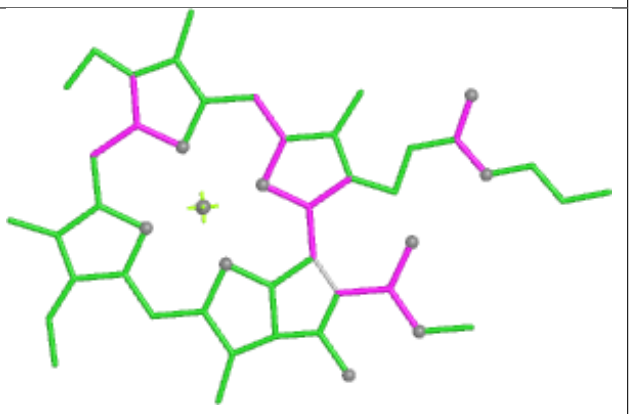


Rings

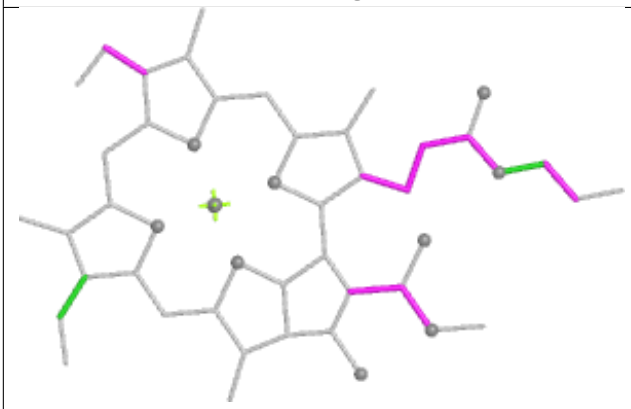
Ligand CLA n 308



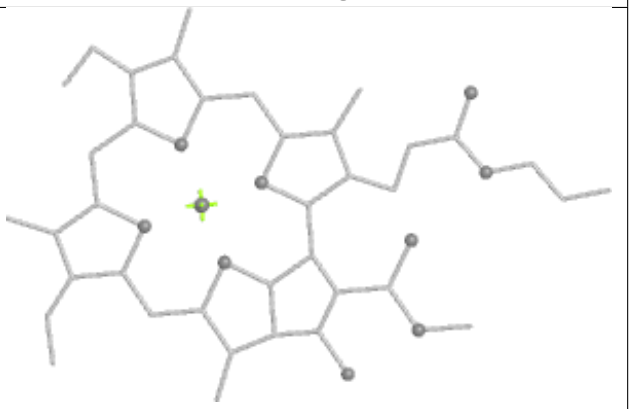
Bond lengths



Bond angles

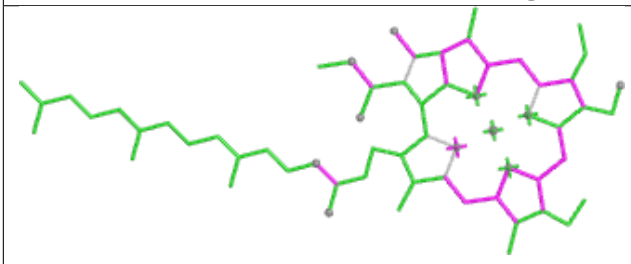


Torsions

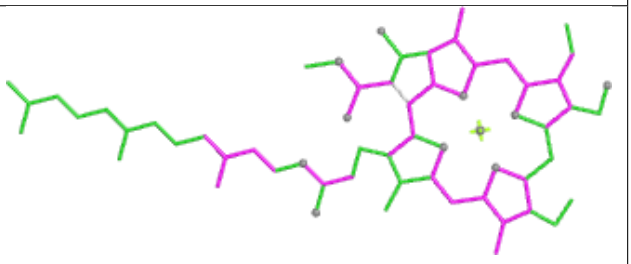


Rings

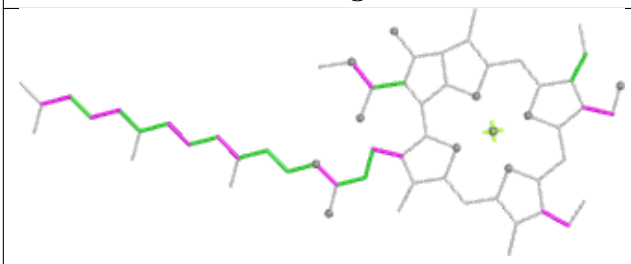
Ligand CHL G 316



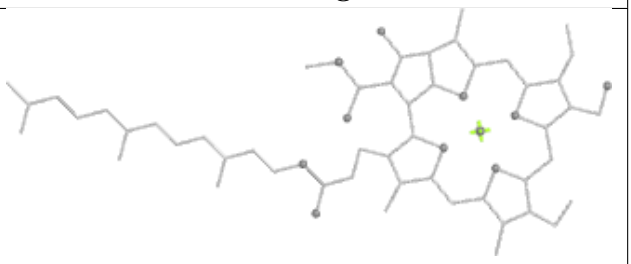
Bond lengths



Bond angles

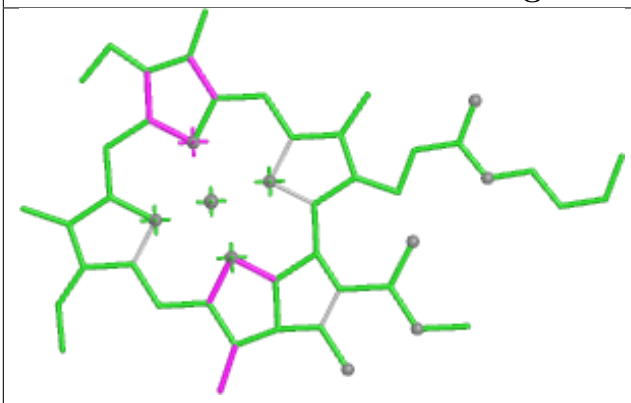


Torsions

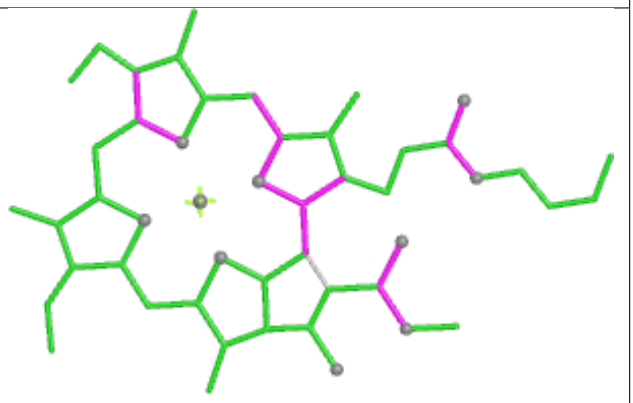


Rings

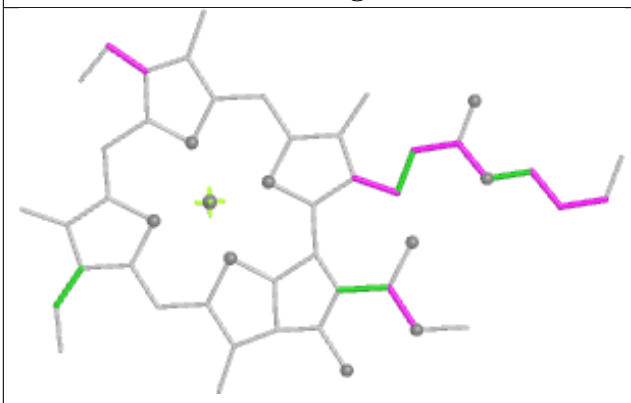
Ligand CLA R 308



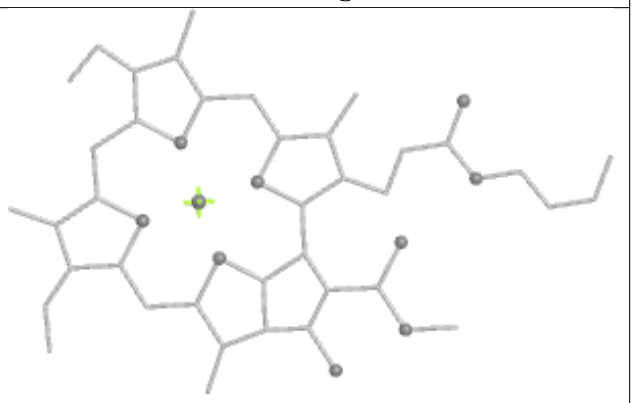
Bond lengths



Bond angles

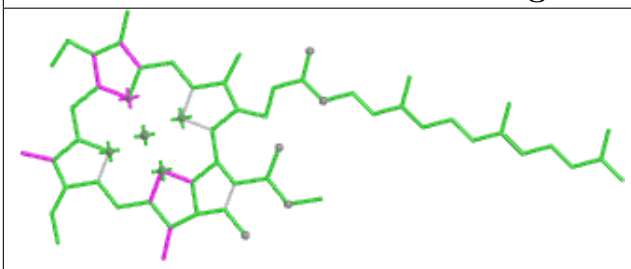


Torsions

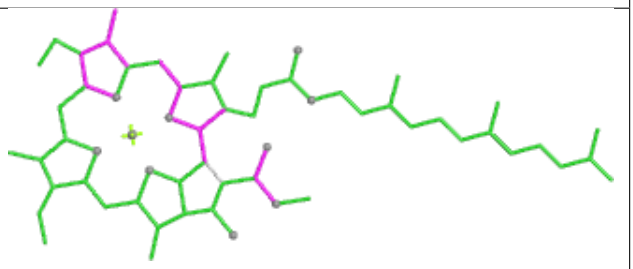


Rings

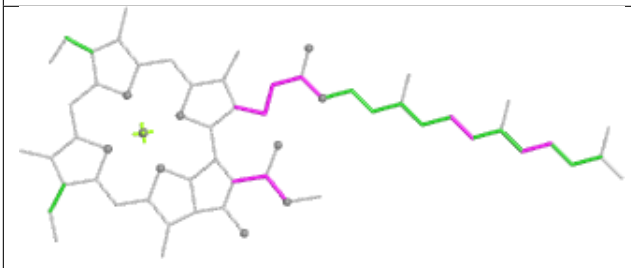
Ligand CLA 5 306



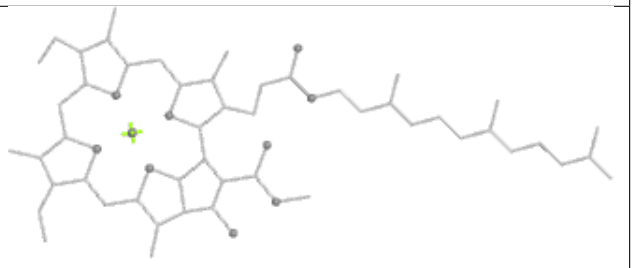
Bond lengths



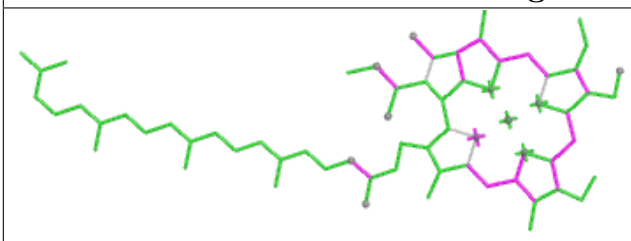
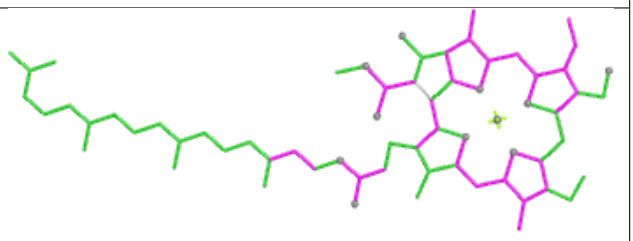
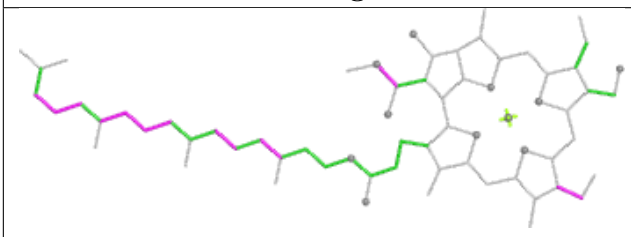
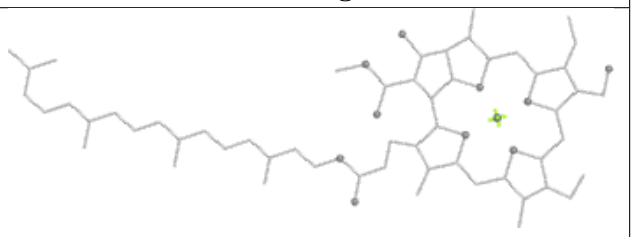
Bond angles

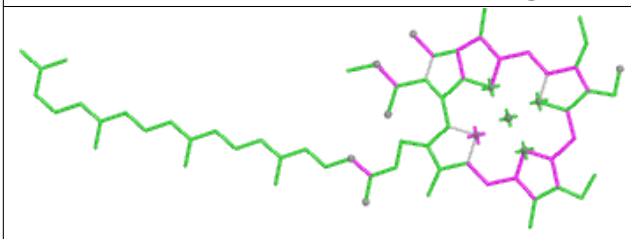
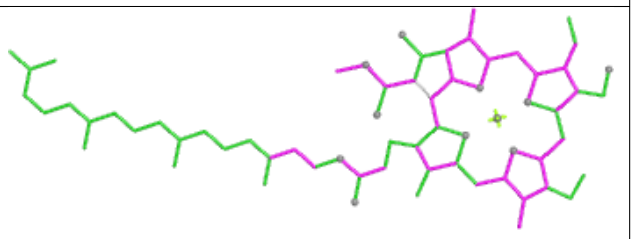
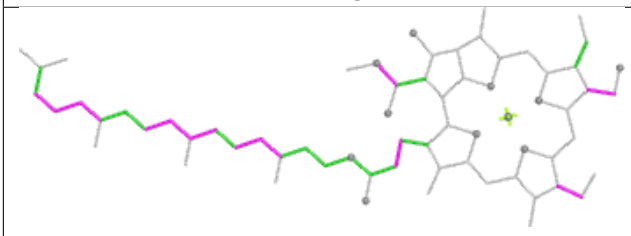
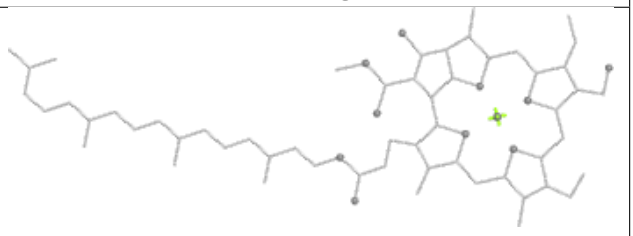


Torsions

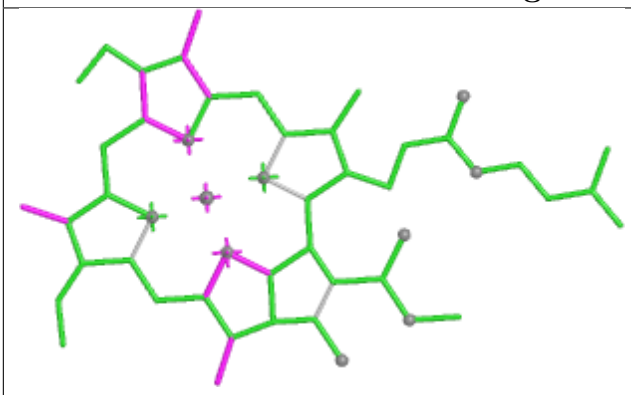


Rings

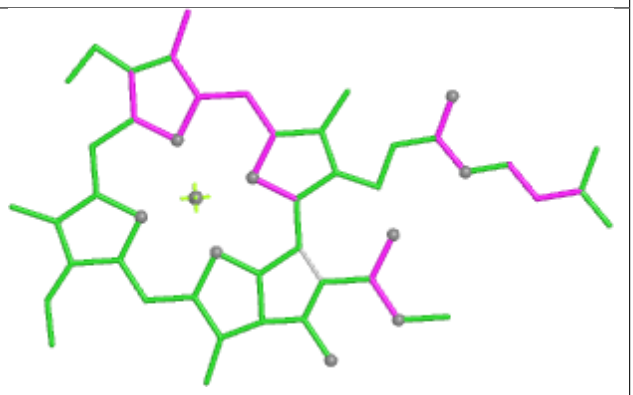
Ligand CHL 2 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL G 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

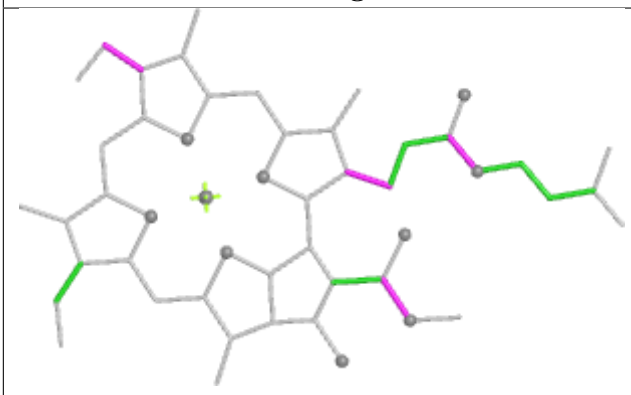
Ligand CLA V 303



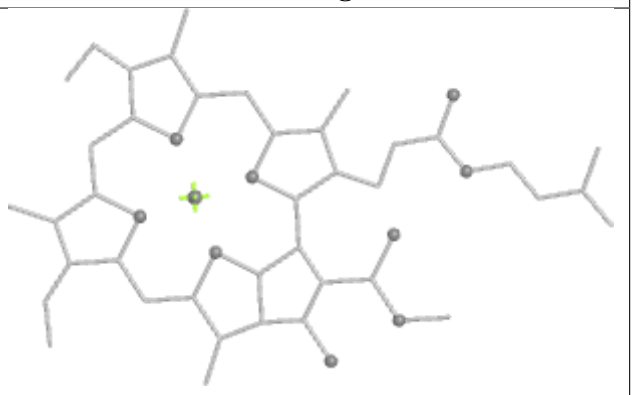
Bond lengths



Bond angles

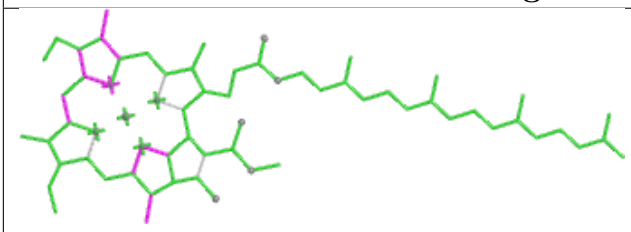


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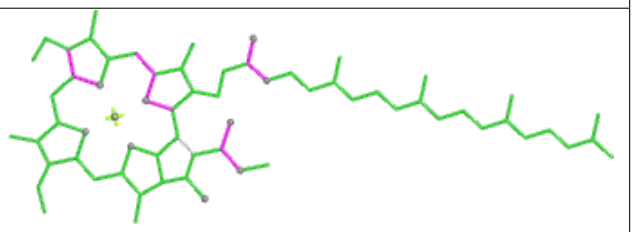


Rings

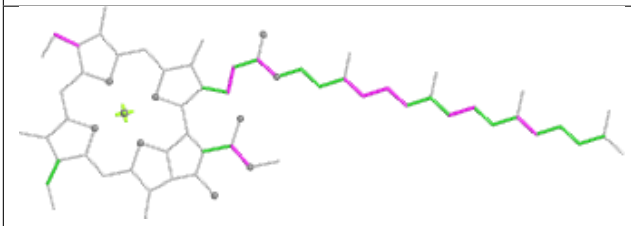
Ligand CLA G 307



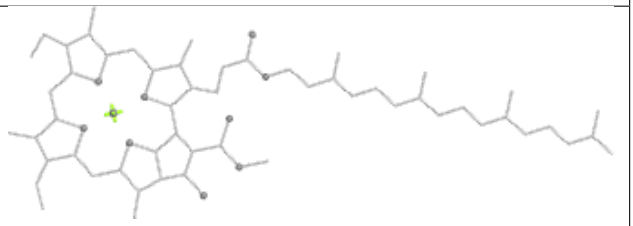
Bond lengths



Bond angles

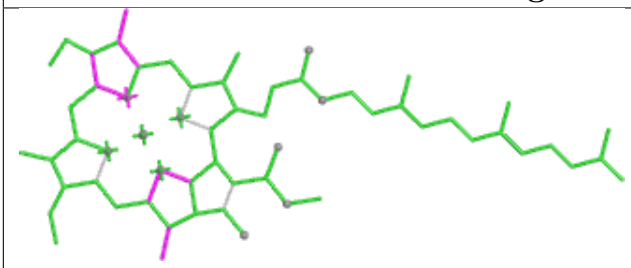


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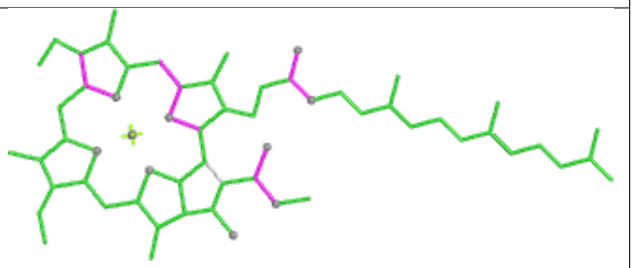


Rings

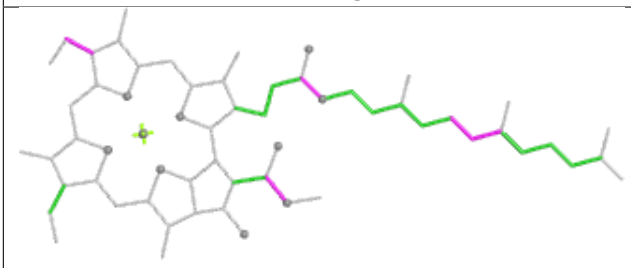
Ligand CLA v 305



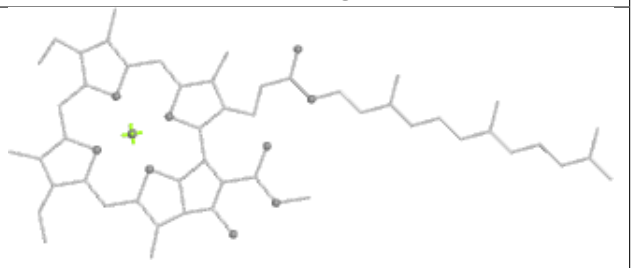
Bond lengths



Bond angles

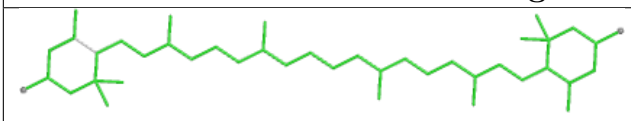


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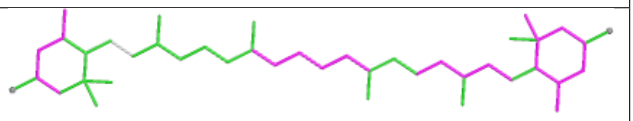


Rings

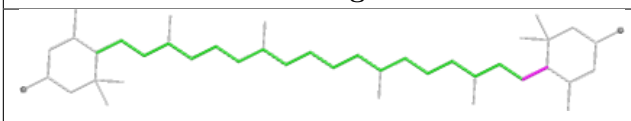
Ligand LUT 5 310



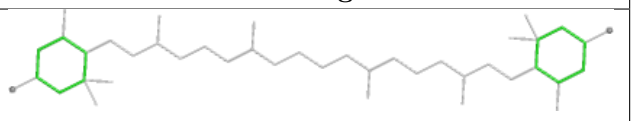
Bond lengths



Bond angles

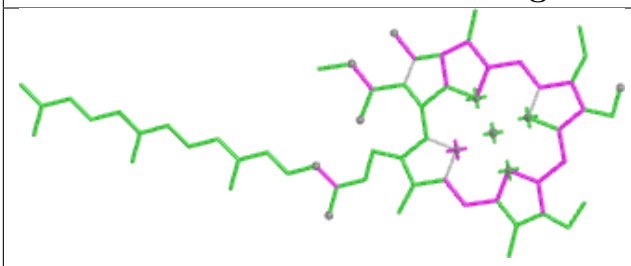


Torsions

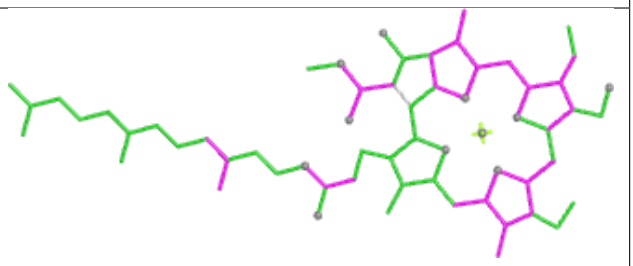


Rings

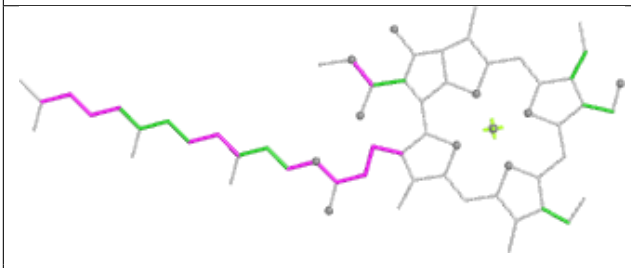
Ligand CHL r 616



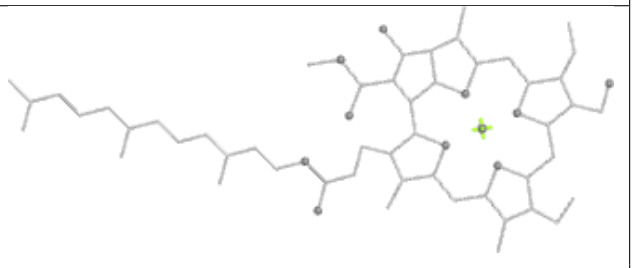
Bond lengths



Bond angles

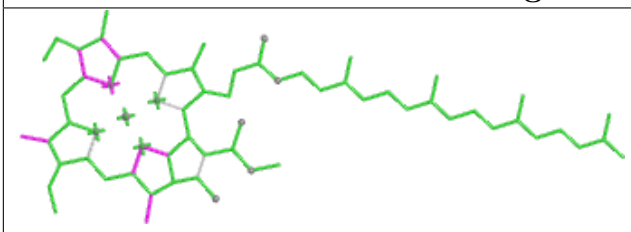


Torsions

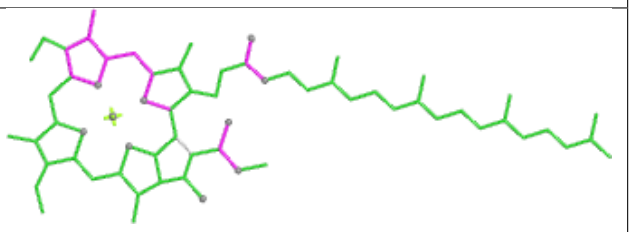


Rings

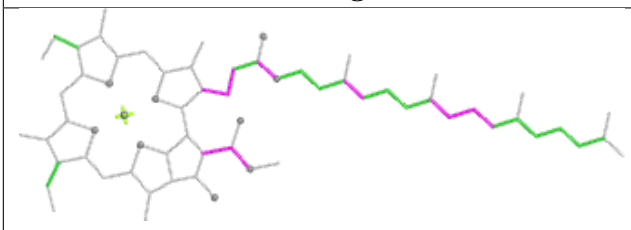
Ligand CLA B 608



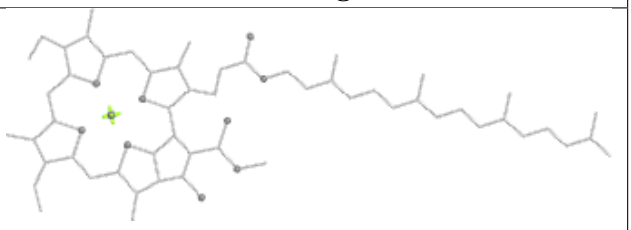
Bond lengths



Bond angles

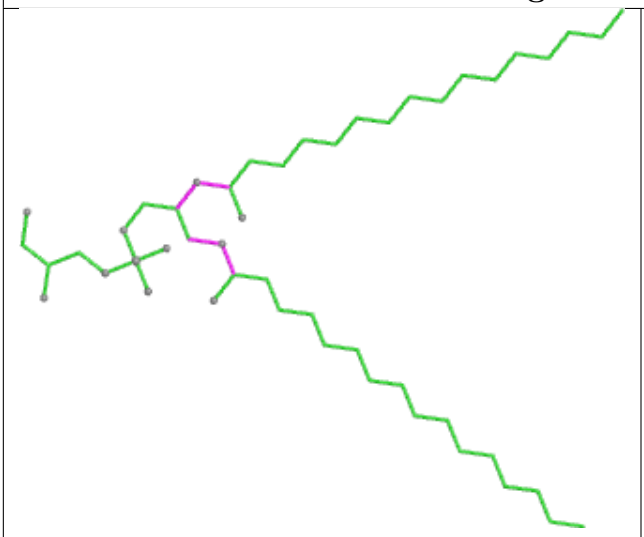


Torsions

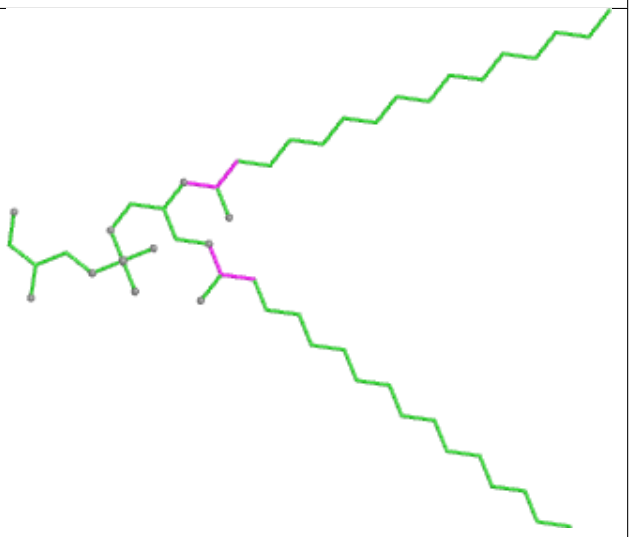


Rings

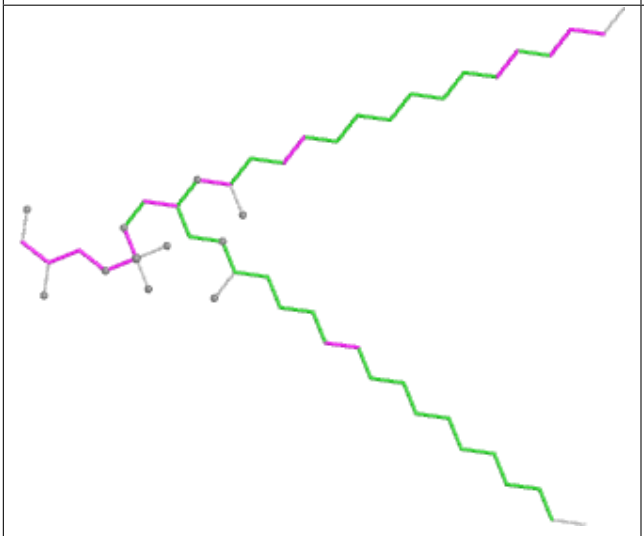
Ligand LHG c 523



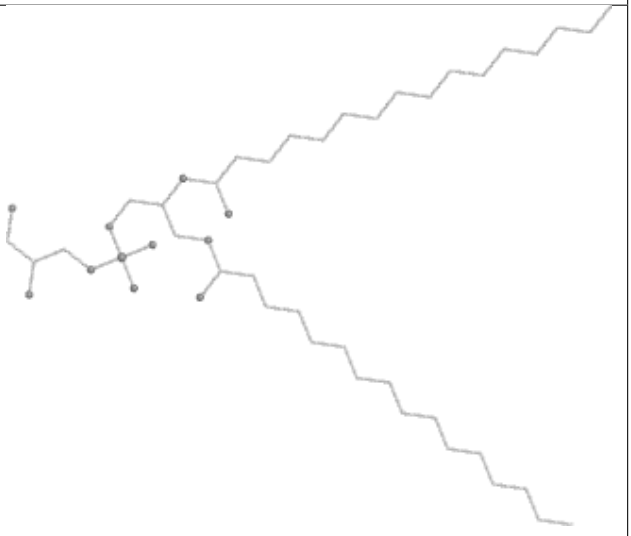
Bond lengths



Bond angles

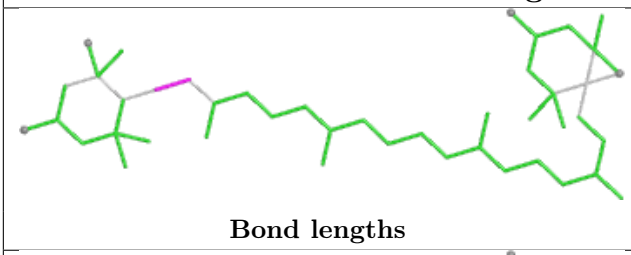


Torsions

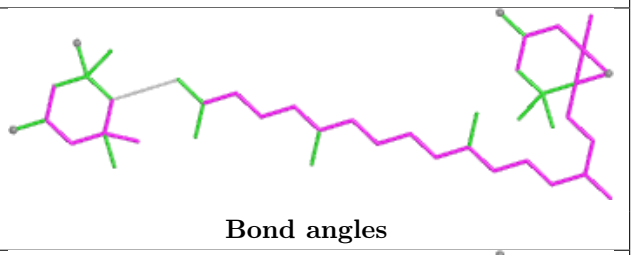


Rings

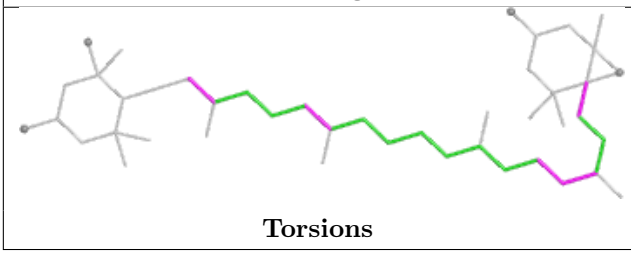
Ligand NEX u 319



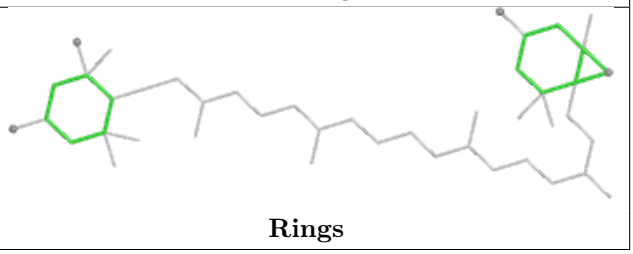
Bond lengths



Bond angles

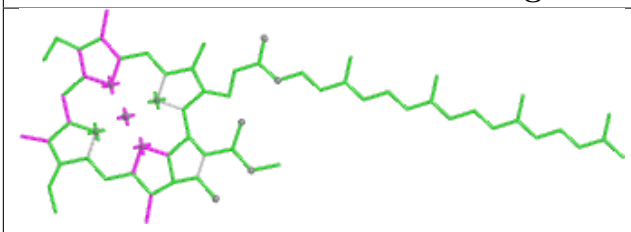


Torsions

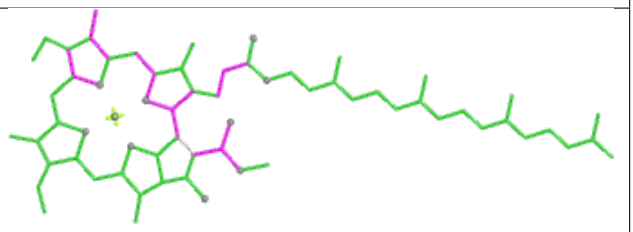


Rings

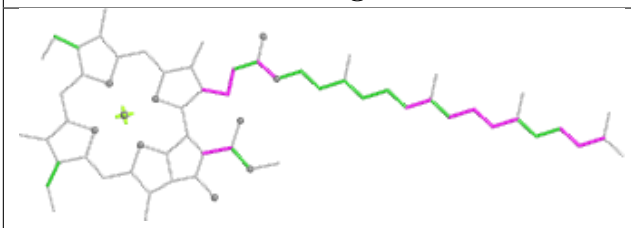
Ligand CLA B 613



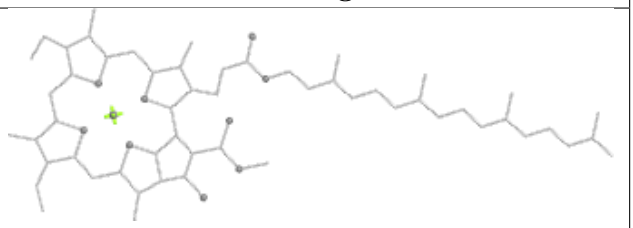
Bond lengths



Bond angles

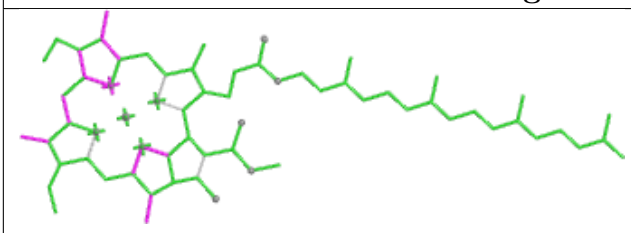


Torsions

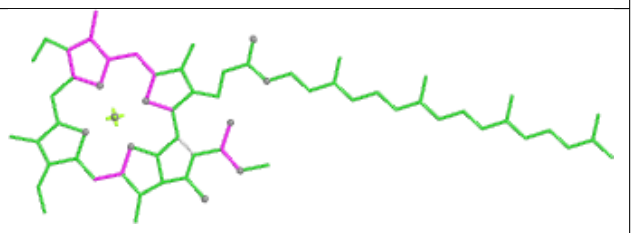


Rings

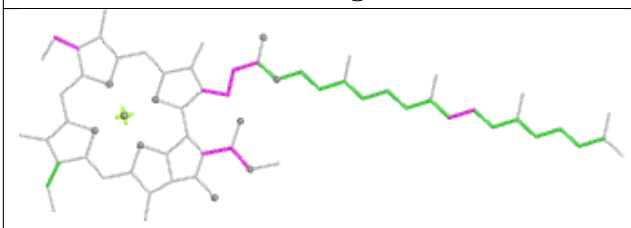
Ligand CLA U 301



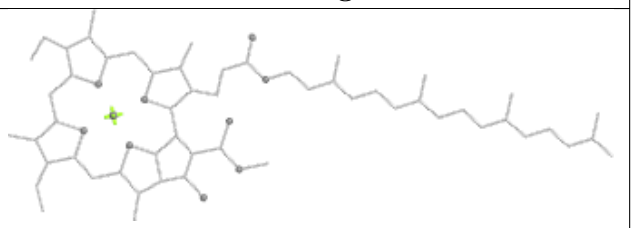
Bond lengths



Bond angles

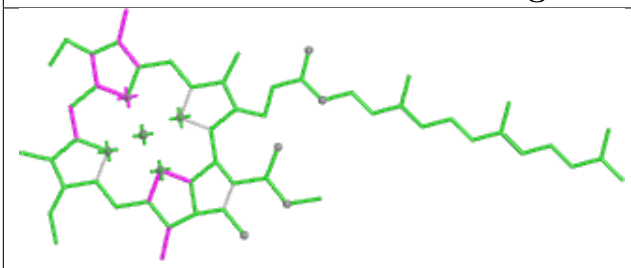


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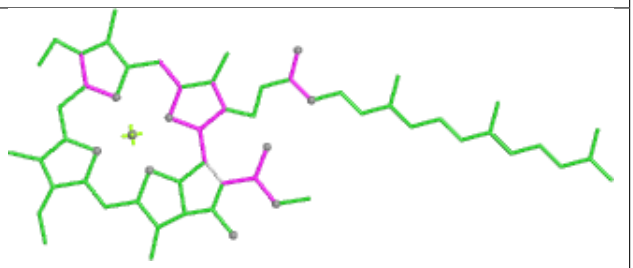


Rings

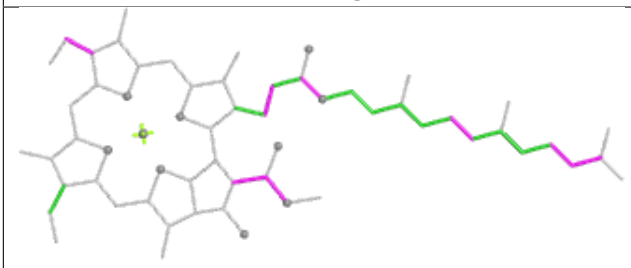
Ligand CLA 3 305



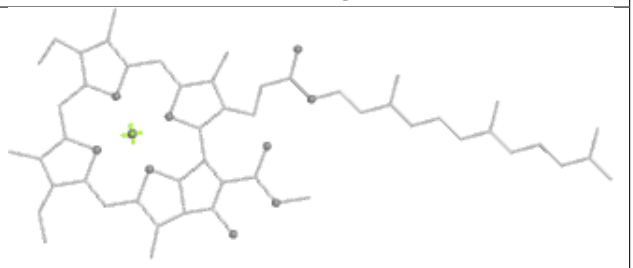
Bond lengths



Bond angles

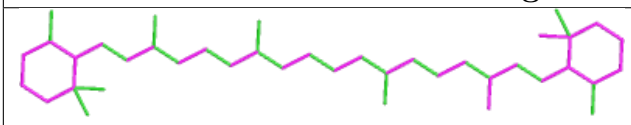


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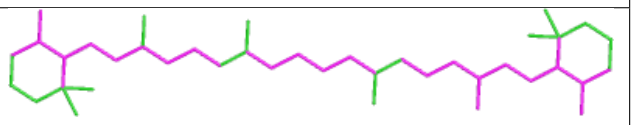


Rings

Ligand BCR A 409



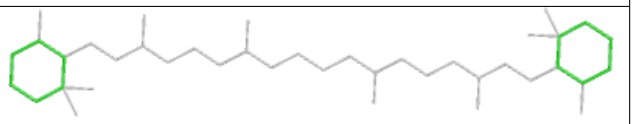
Bond lengths



Bond angles

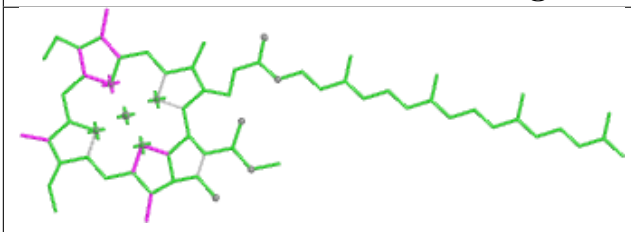


Torsions

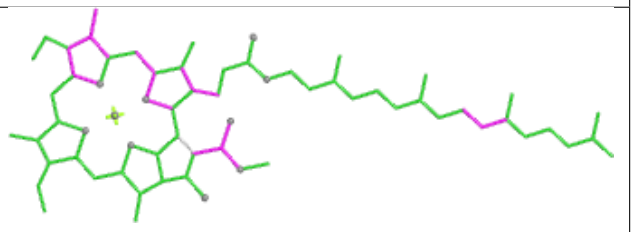


Rings

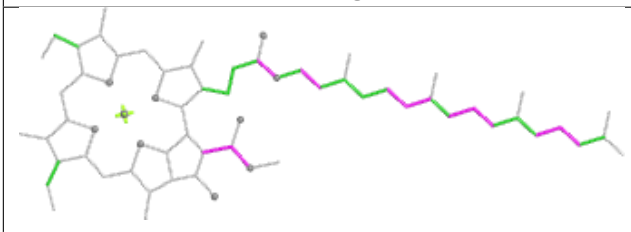
Ligand CLA c 510



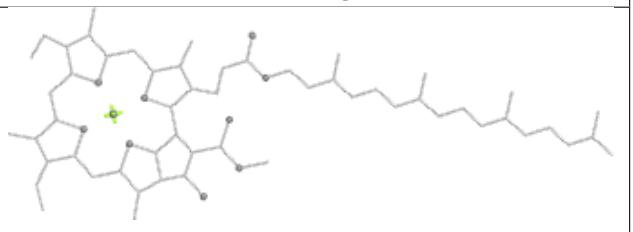
Bond lengths



Bond angles

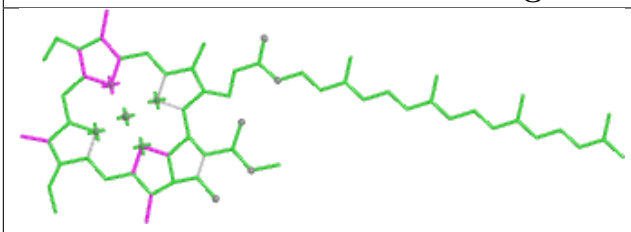


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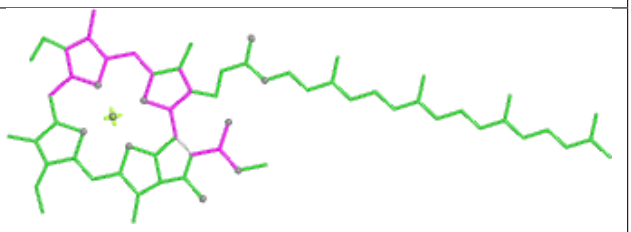


Rings

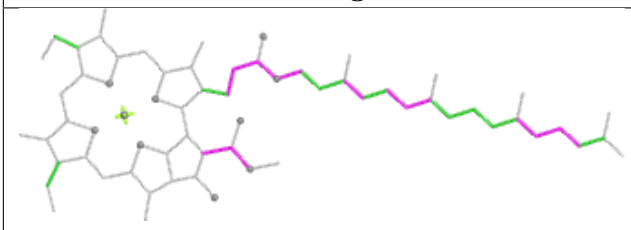
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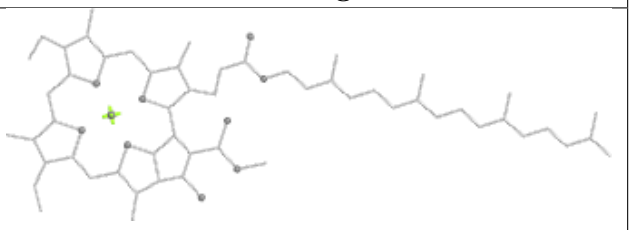
Bond lengths



Bond angles

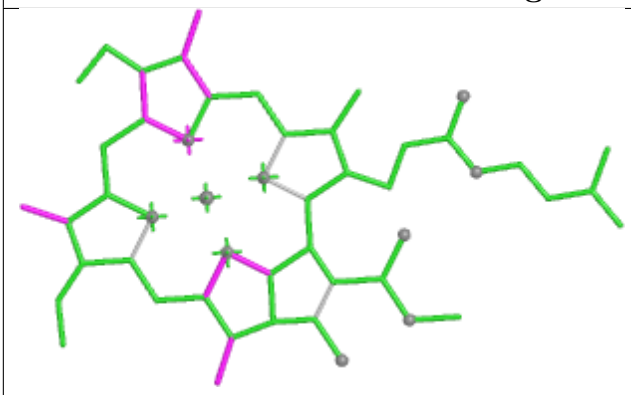


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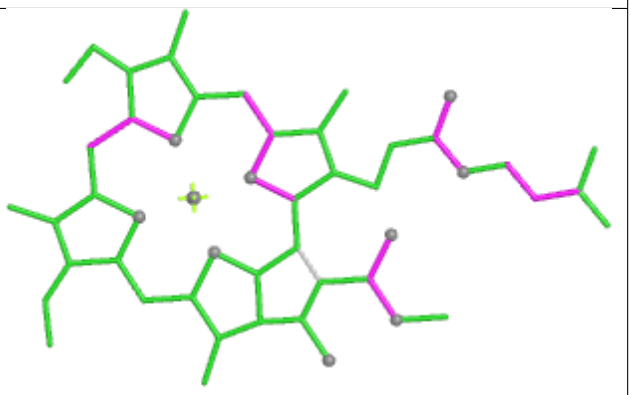


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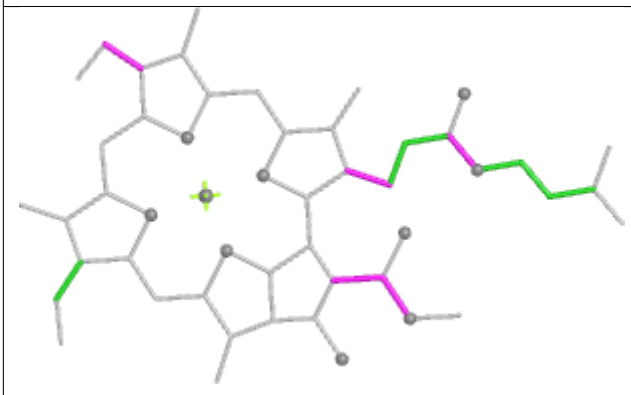
Ligand CLA P 304



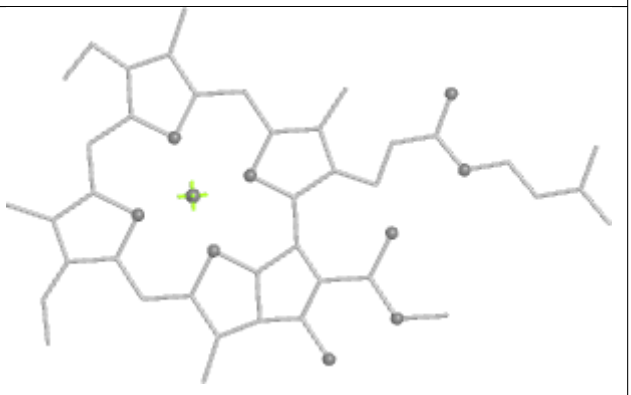
Bond lengths



Bond angles

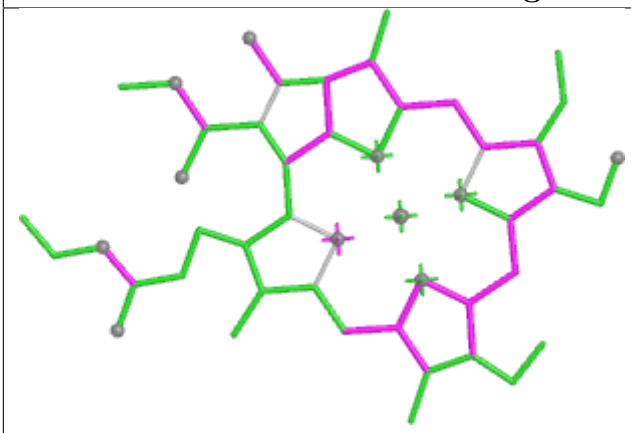


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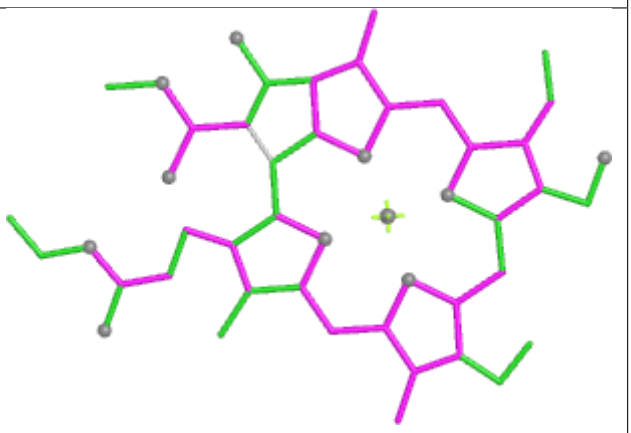


Rings

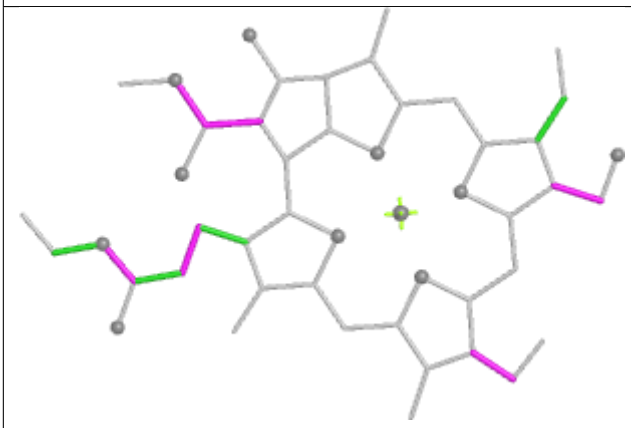
Ligand CHL V 314



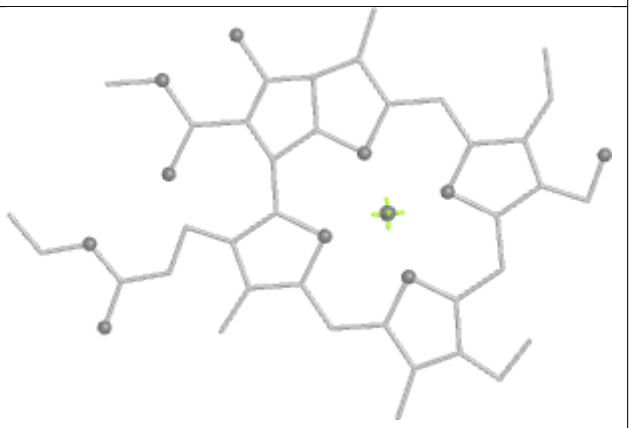
Bond lengths



Bond angles

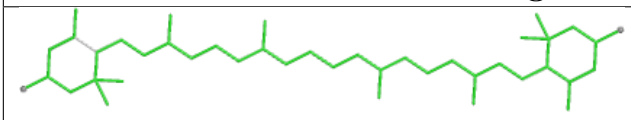


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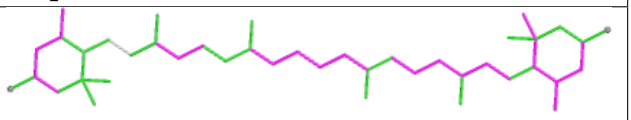


Rings

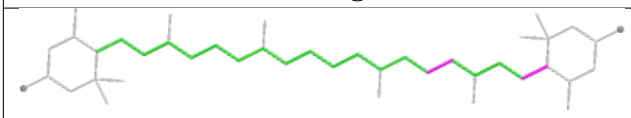
Ligand LUT p 311



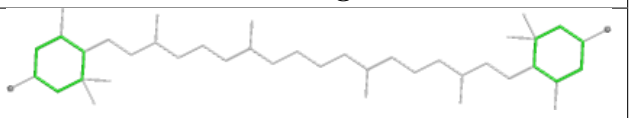
Bond lengths



Bond angles

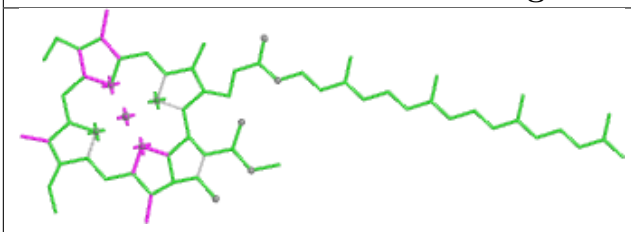


Torsions

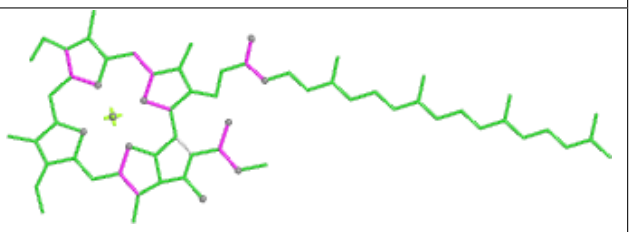


Rings

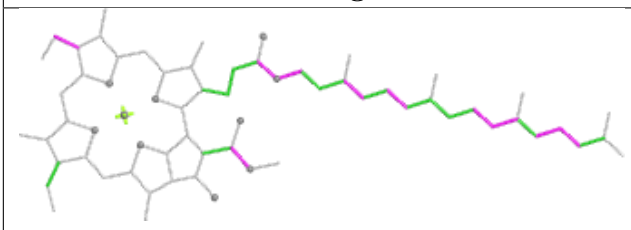
Ligand CLA d 402



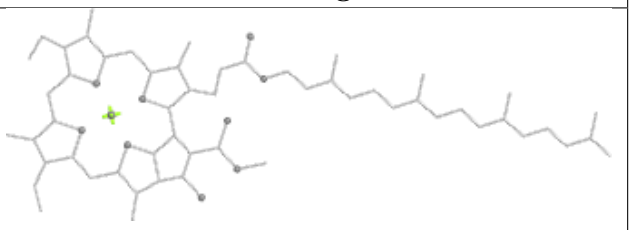
Bond lengths



Bond angles

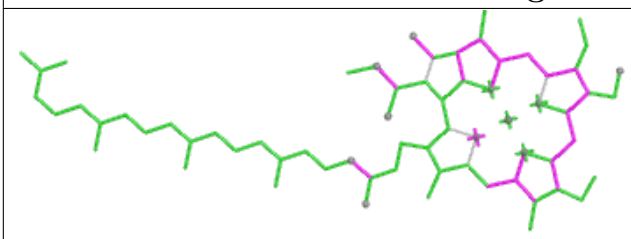


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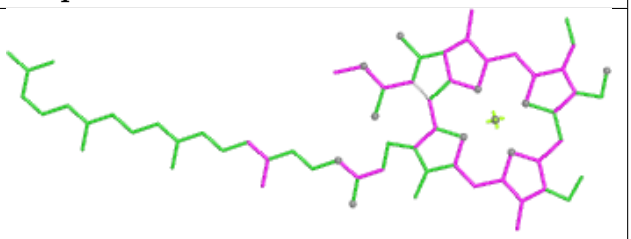


Rings

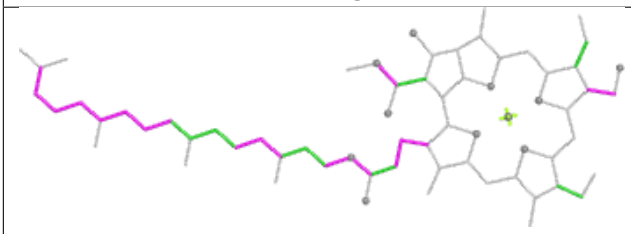
Ligand CHL q 314



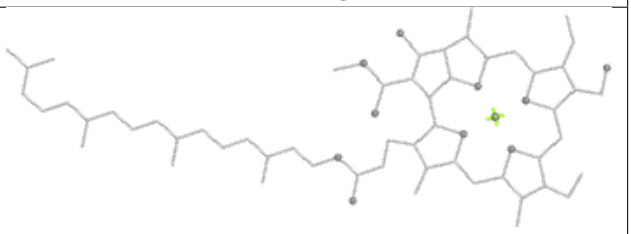
Bond lengths



Bond angles

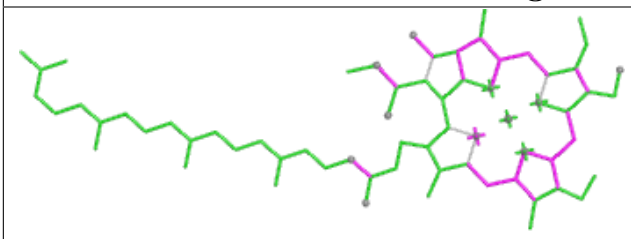


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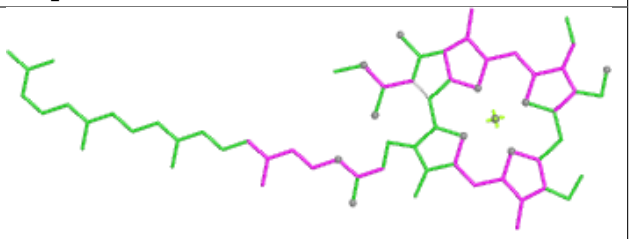


Rings

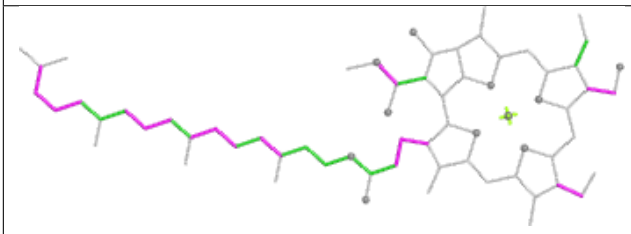
Ligand CHL p 318



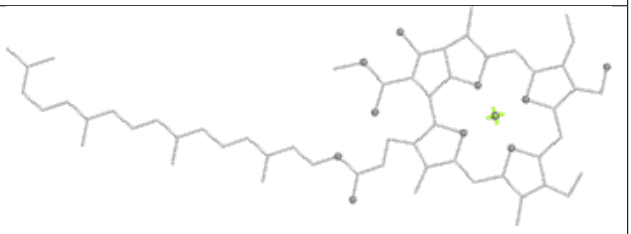
Bond lengths



Bond angles

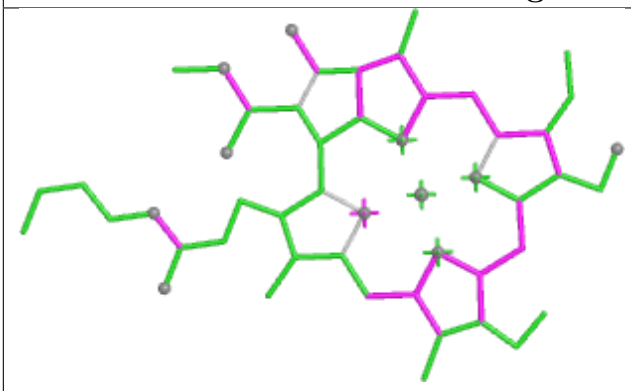


Torsions

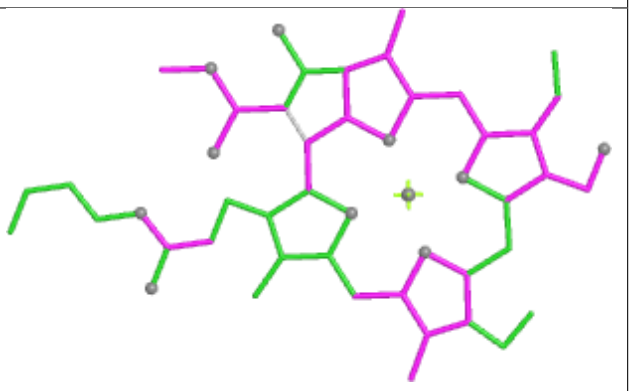


Rings

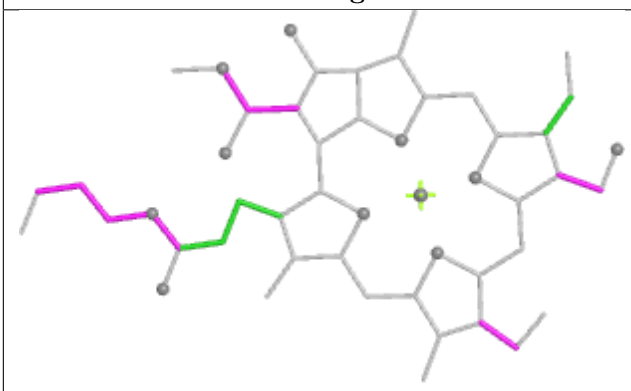
Ligand CHL n 315



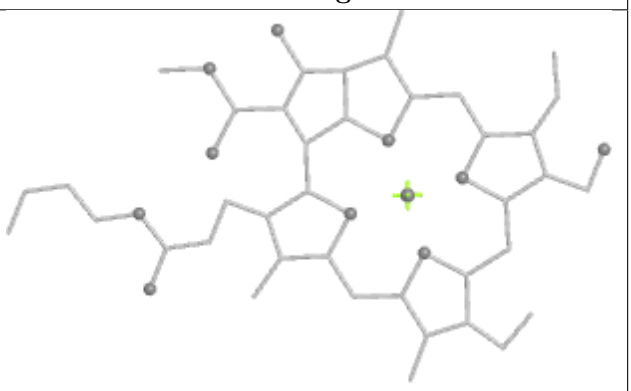
Bond lengths



Bond angles

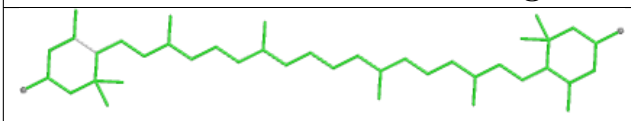


Torsions

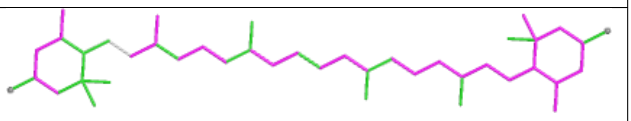


Rings

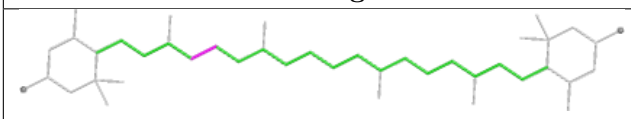
Ligand LUT N 310



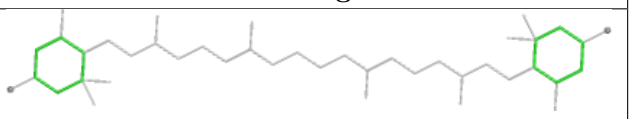
Bond lengths



Bond angles

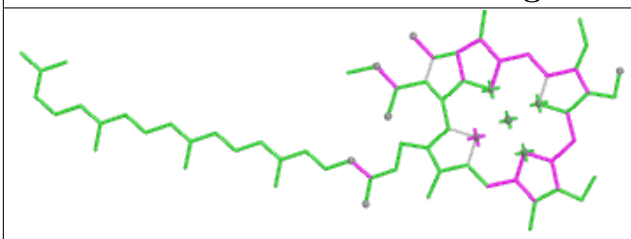


Torsions

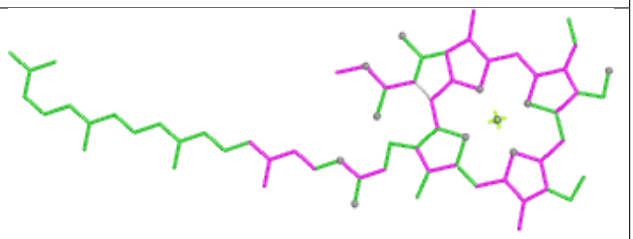


Rings

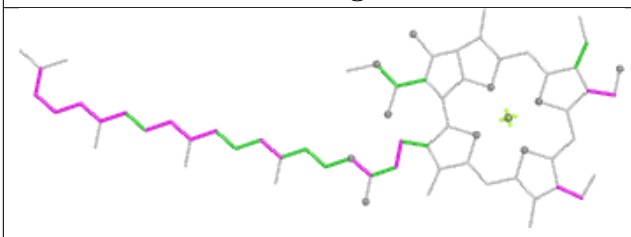
Ligand CHL V 316



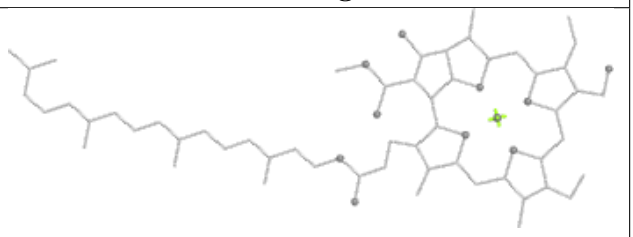
Bond lengths



Bond angles

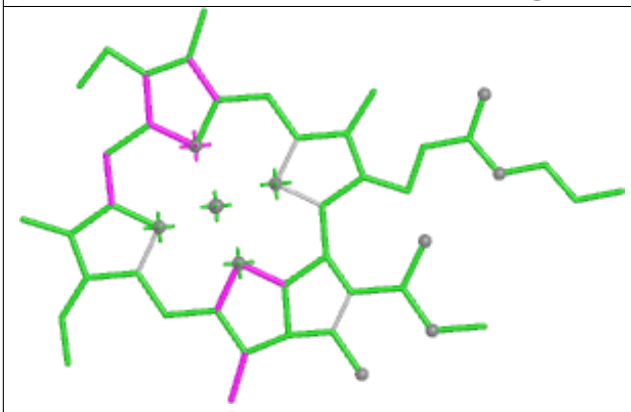


Torsions

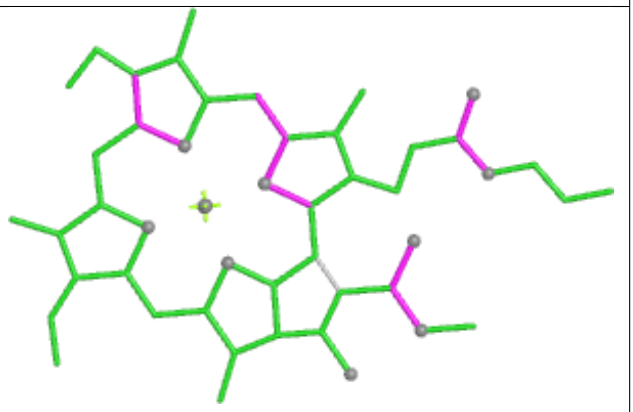


Rings

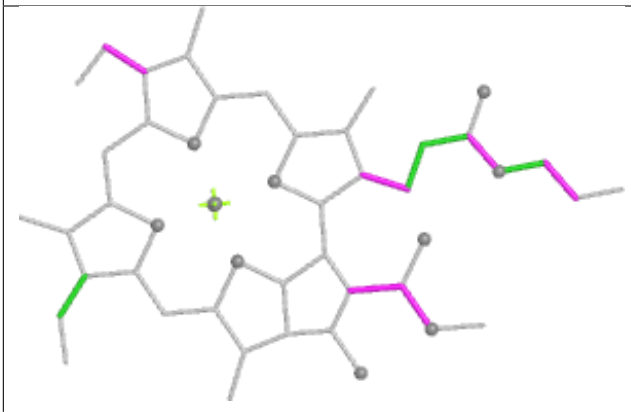
Ligand CLA 6 309



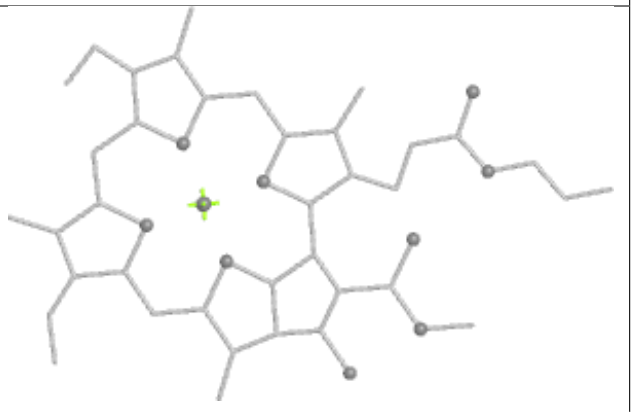
Bond lengths



Bond angles

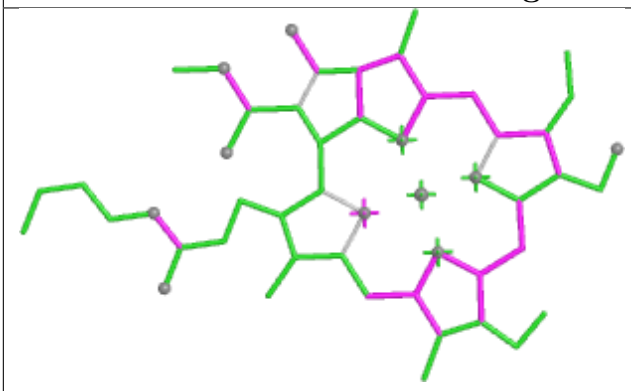


Torsions

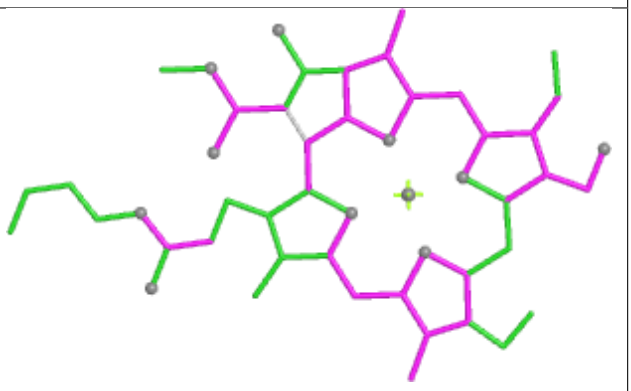


Rings

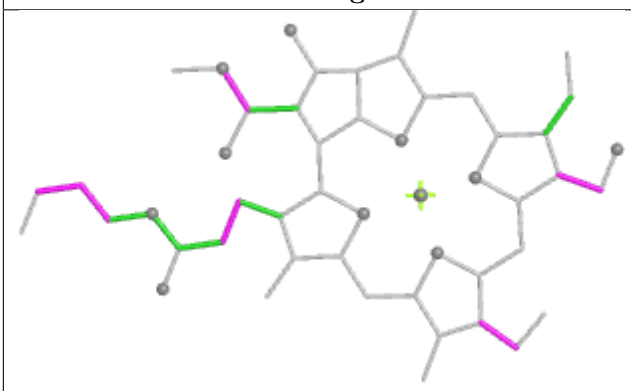
Ligand CHL N 315



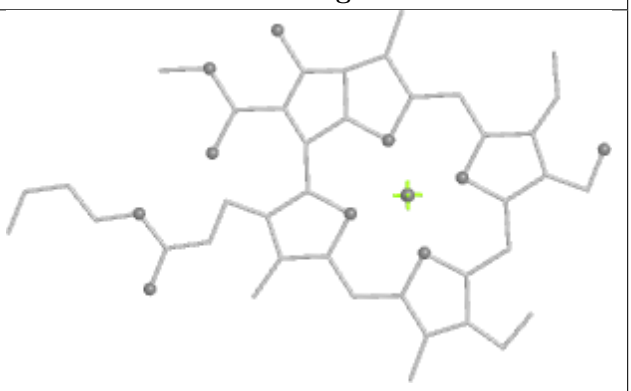
Bond lengths



Bond angles

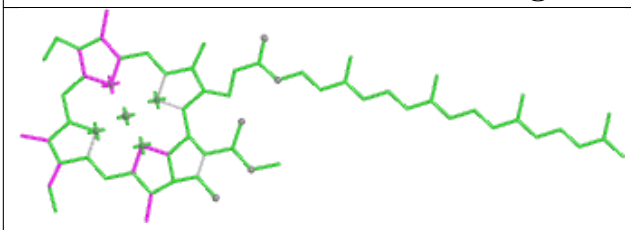


Torsions

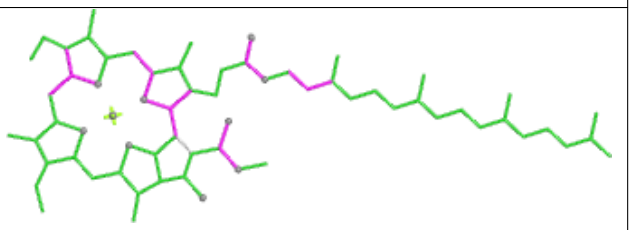


Rings

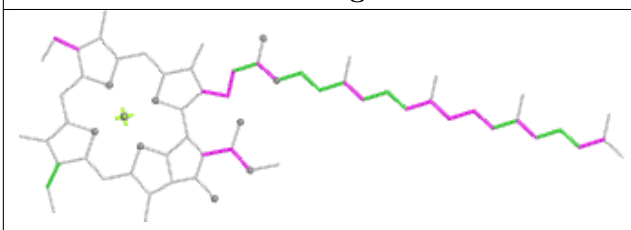
Ligand CLA c 503



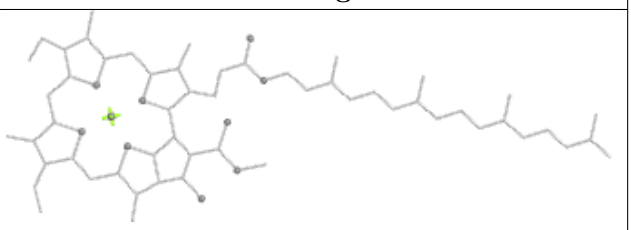
Bond lengths



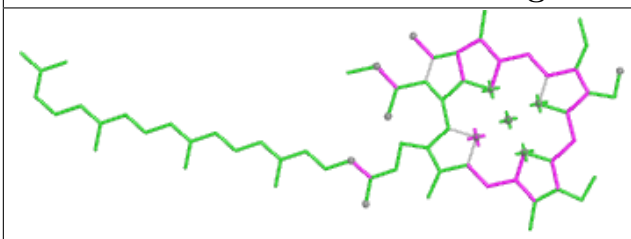
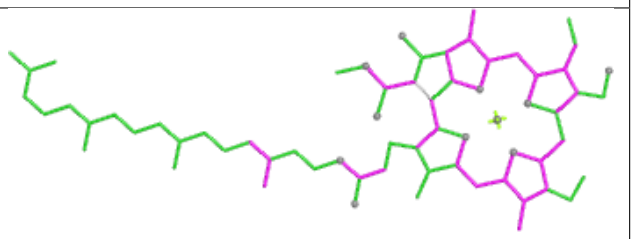
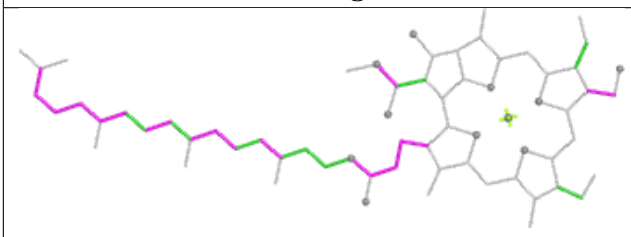
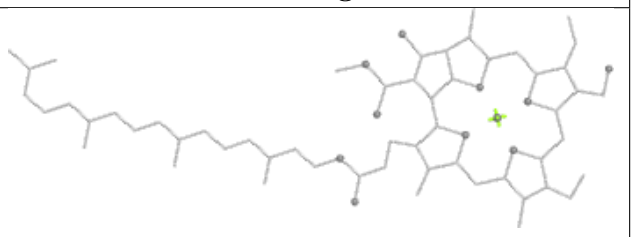
Bond angles

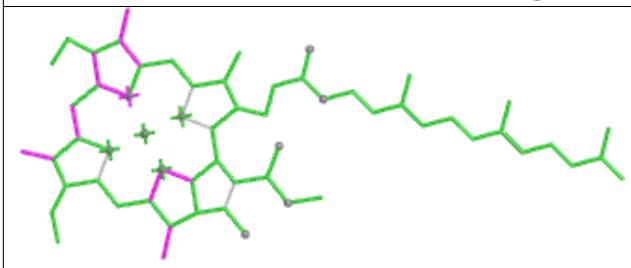
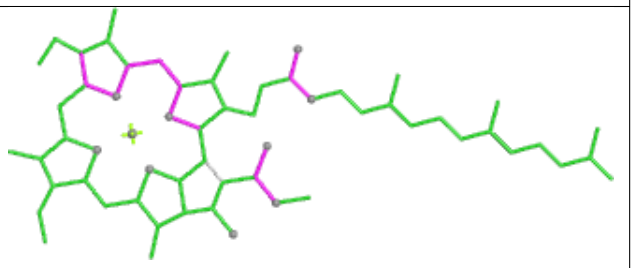
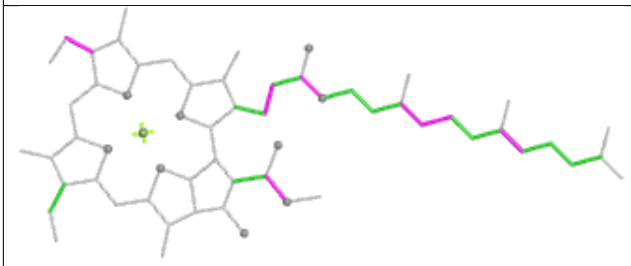
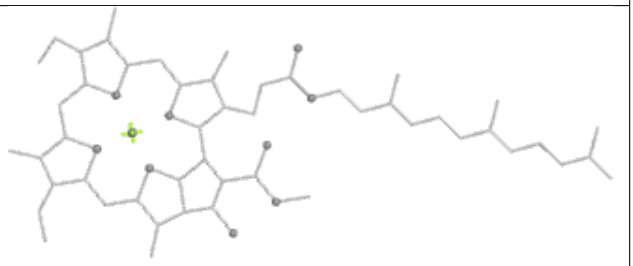


Torsions

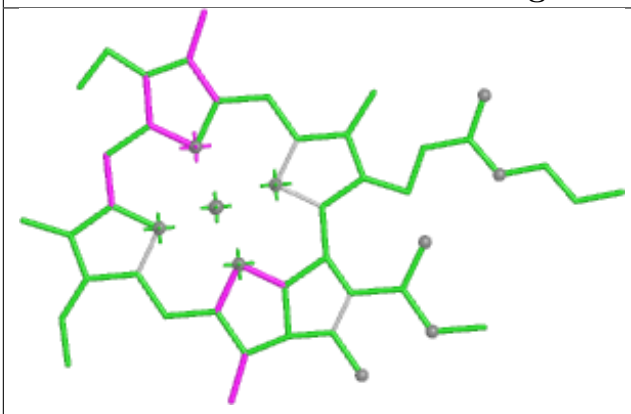


Rings

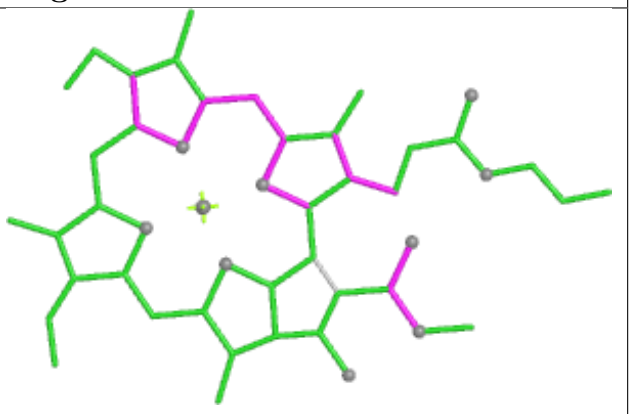
Ligand CHL 6 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

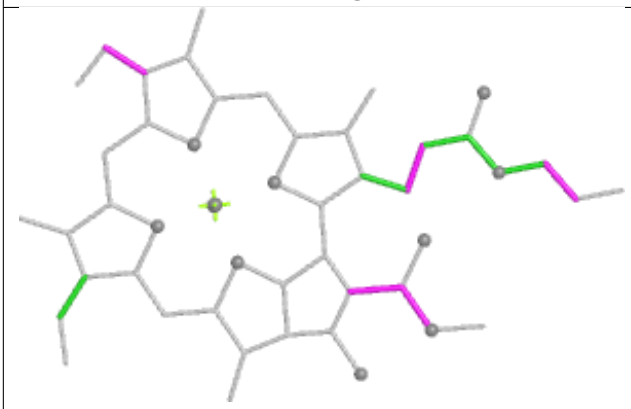
Ligand CLA g 308



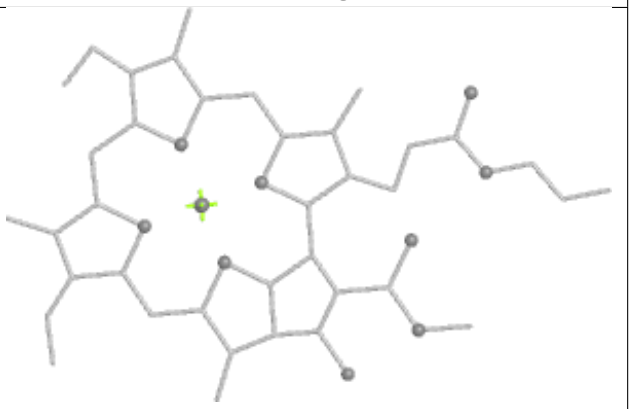
Bond lengths



Bond angles

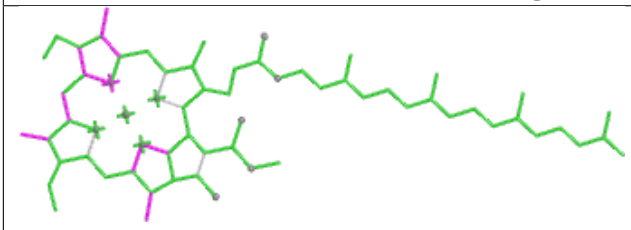


Torsions

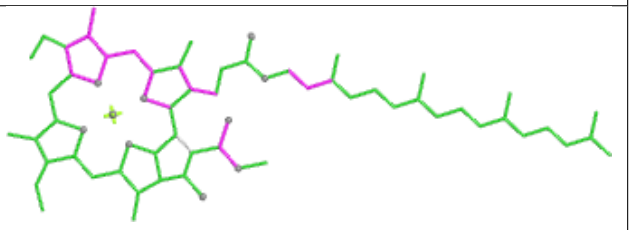


Rings

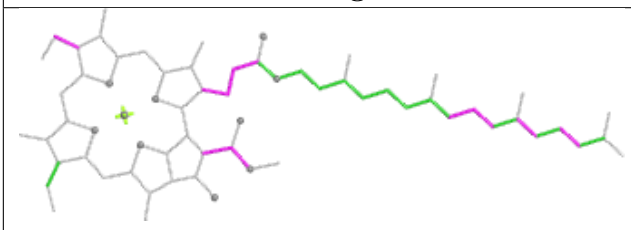
Ligand CLA 2 301



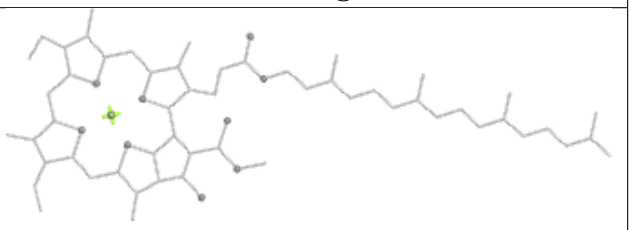
Bond lengths



Bond angles

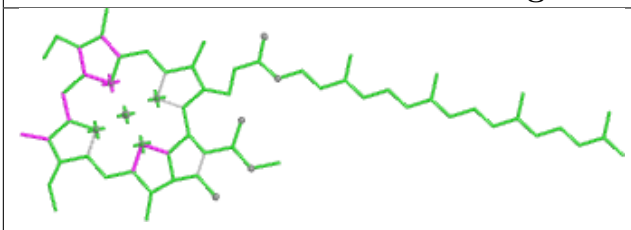


Torsions

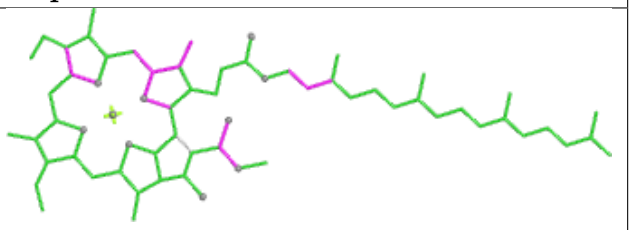


Rings

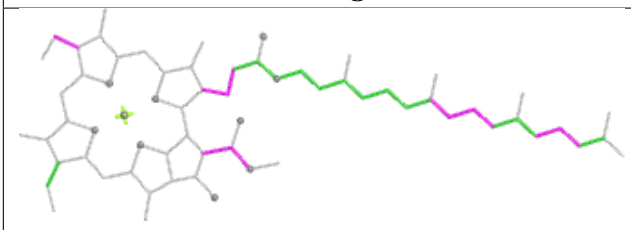
Ligand CLA p 305



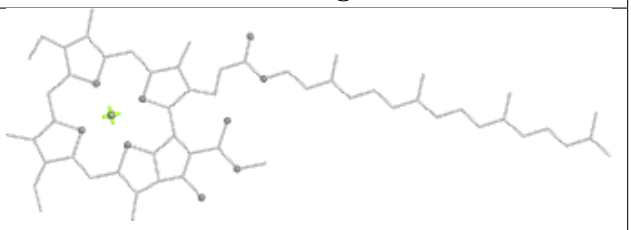
Bond lengths



Bond angles

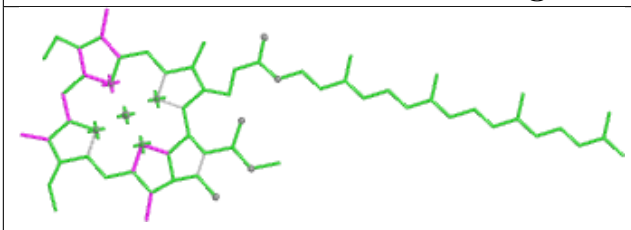


Torsions

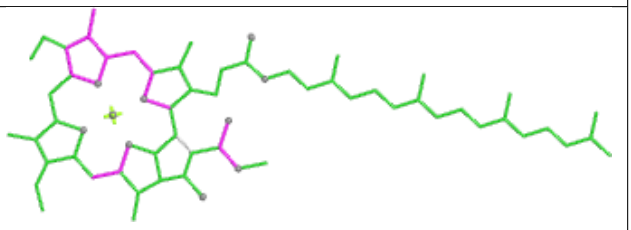


Rings

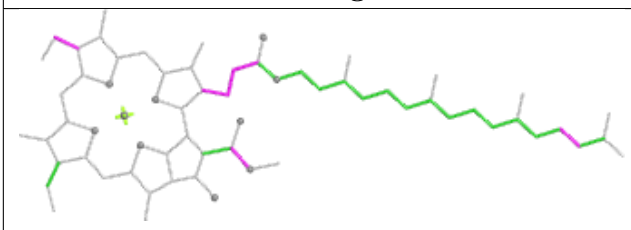
Ligand CLA 4 301



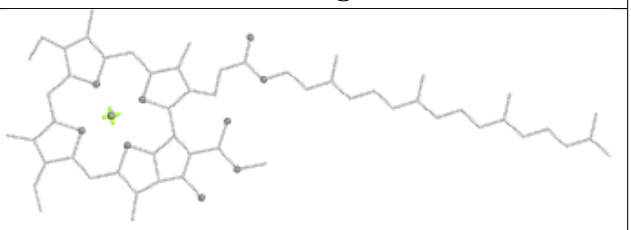
Bond lengths



Bond angles

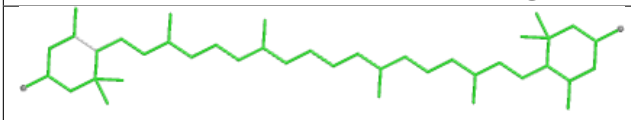


Torsions

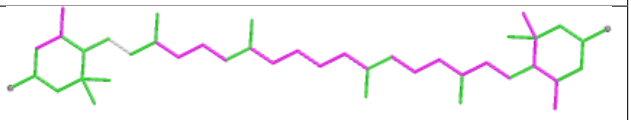


Rings

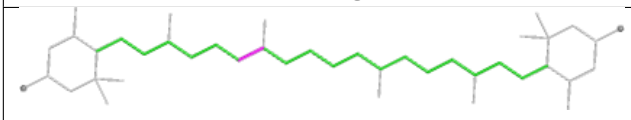
Ligand LUT N 309



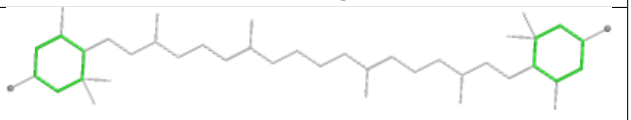
Bond lengths



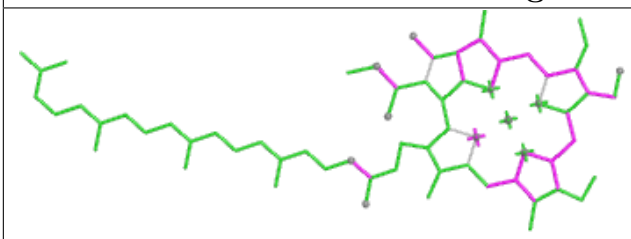
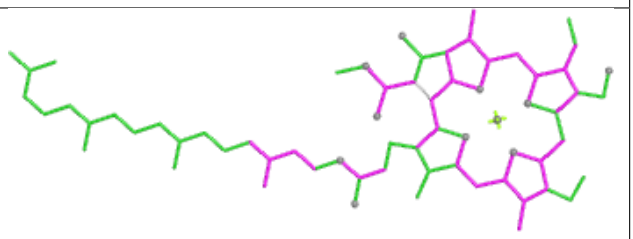
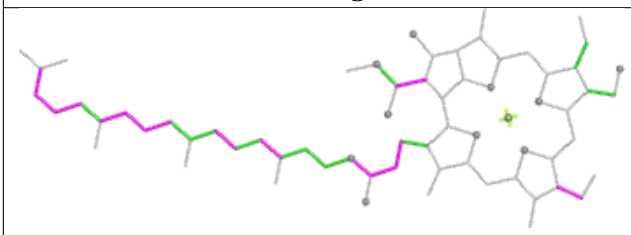
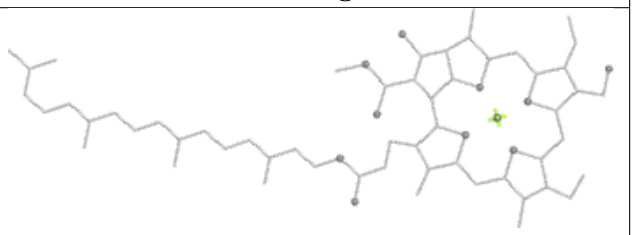
Bond angles

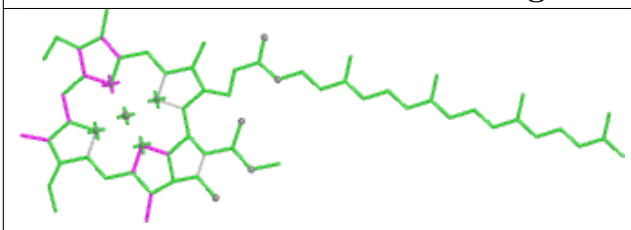
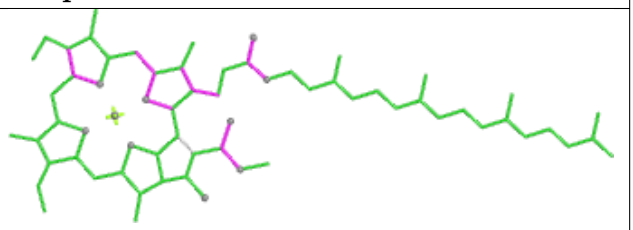
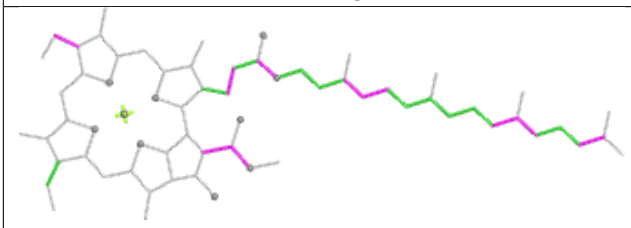
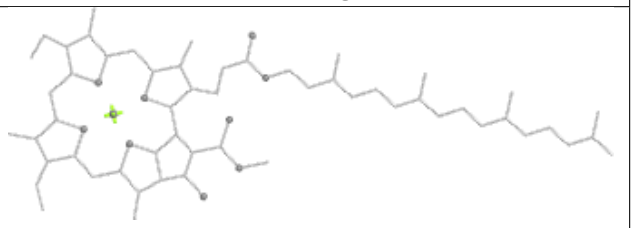


Torsions

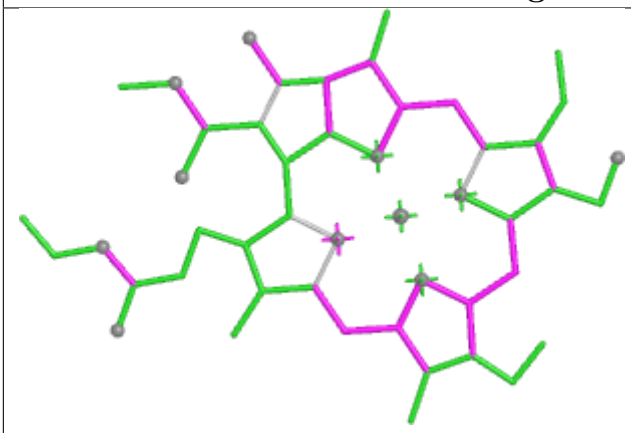


Rings

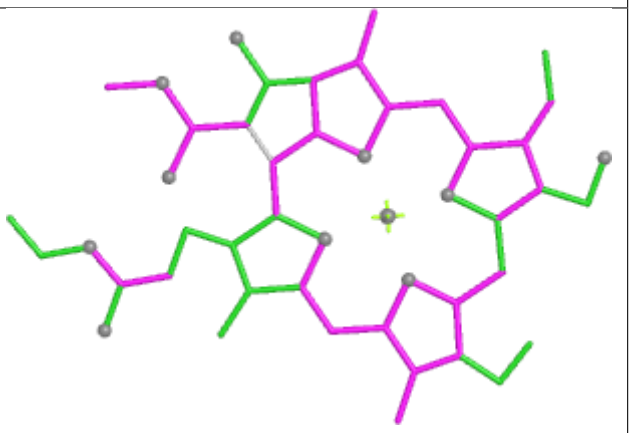
Ligand CHL u 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA q 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

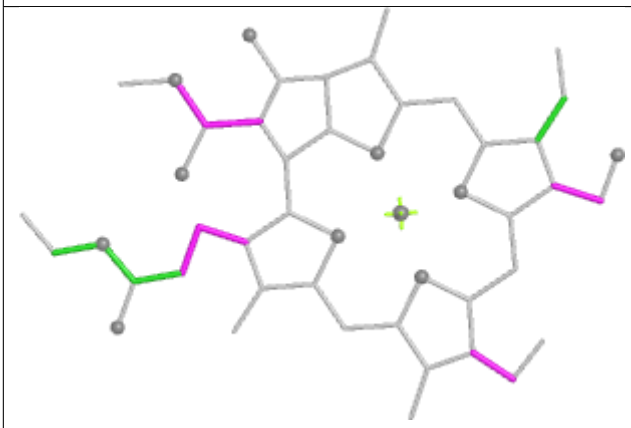
Ligand CHL 4 314



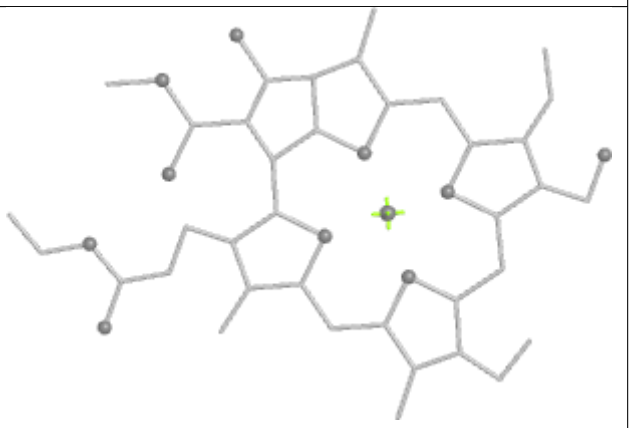
Bond lengths



Bond angles

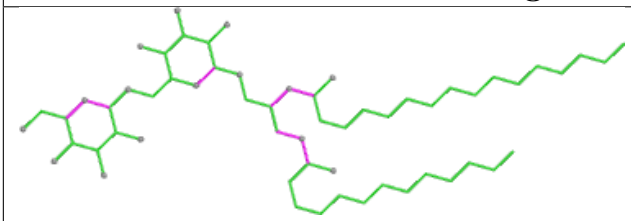


Torsions

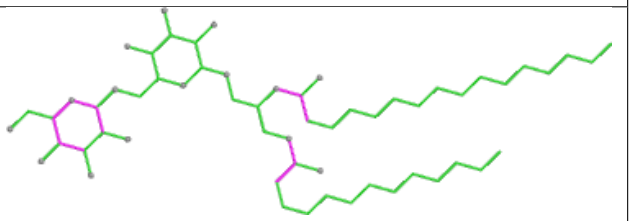


Rings

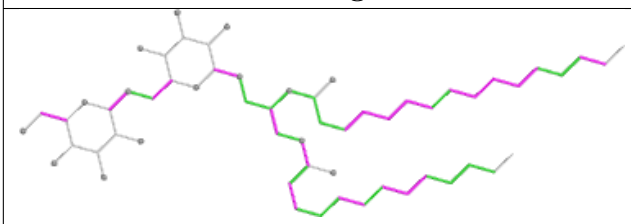
Ligand DGD a 416



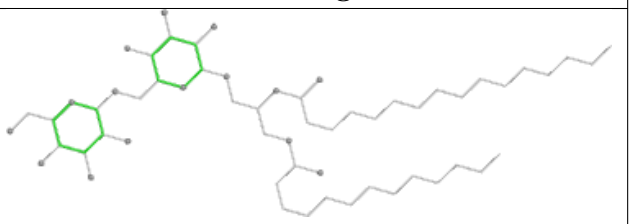
Bond lengths



Bond angles

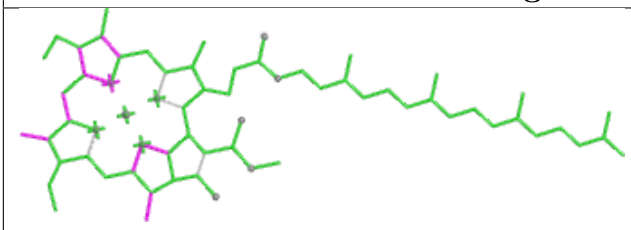


Torsions

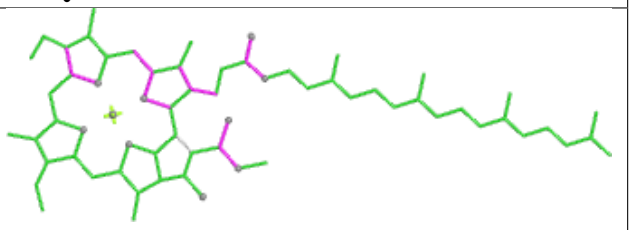


Rings

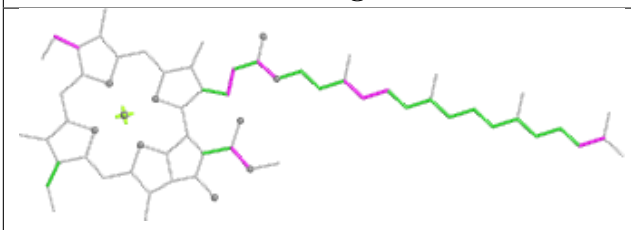
Ligand CLA Q 307



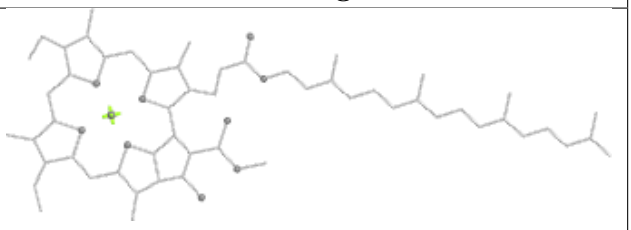
Bond lengths



Bond angles

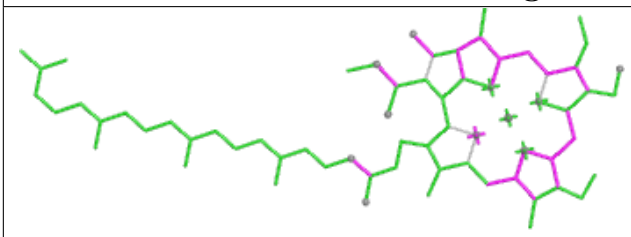


Torsions

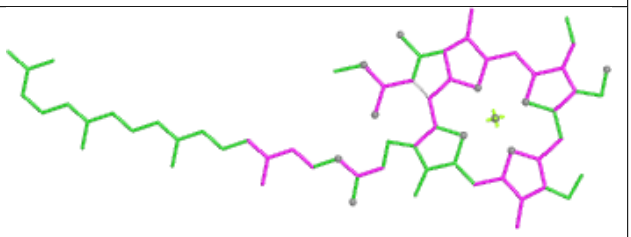


Rings

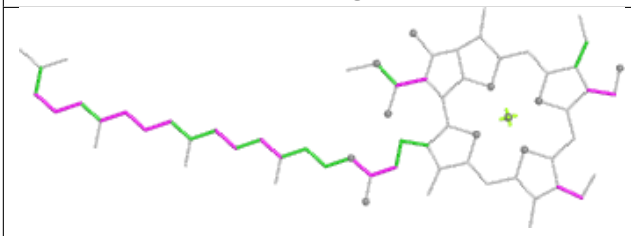
Ligand CHL U 313



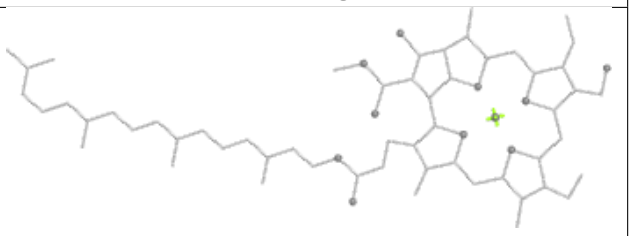
Bond lengths



Bond angles

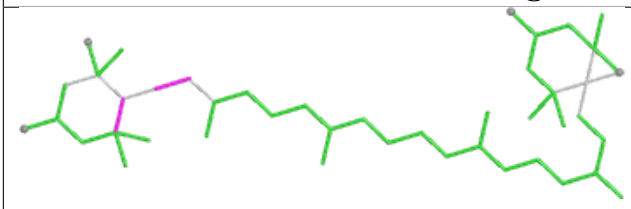


Torsions

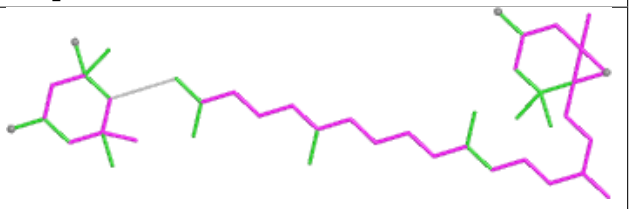


Rings

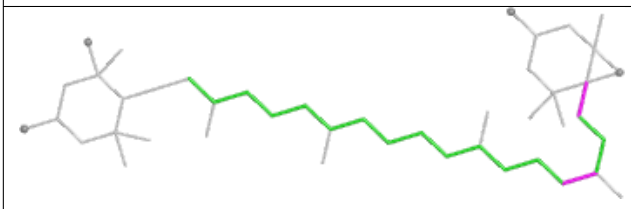
Ligand NEX p 301



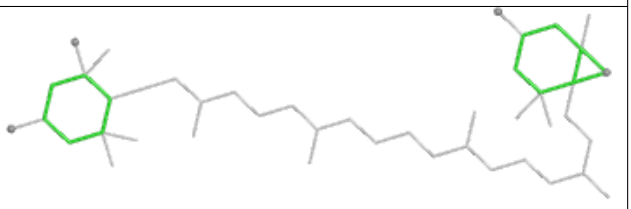
Bond lengths



Bond angles

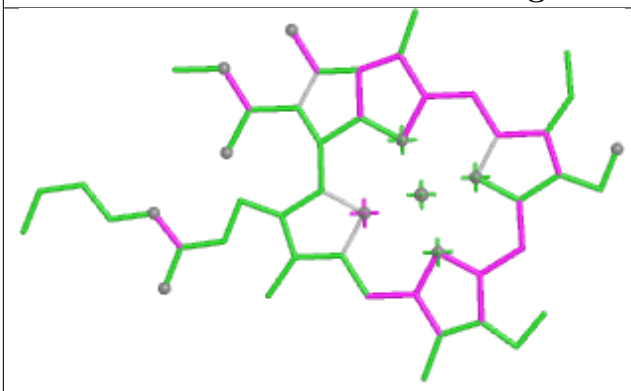


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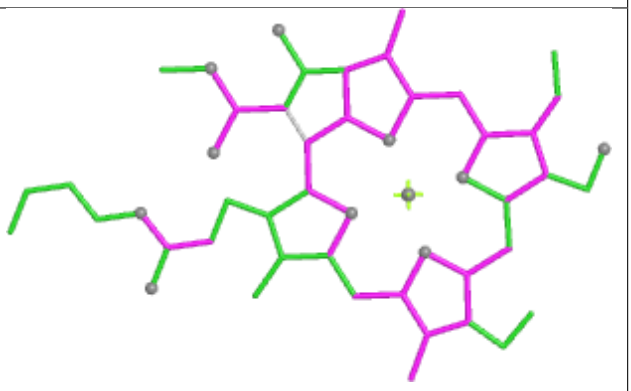


Rings

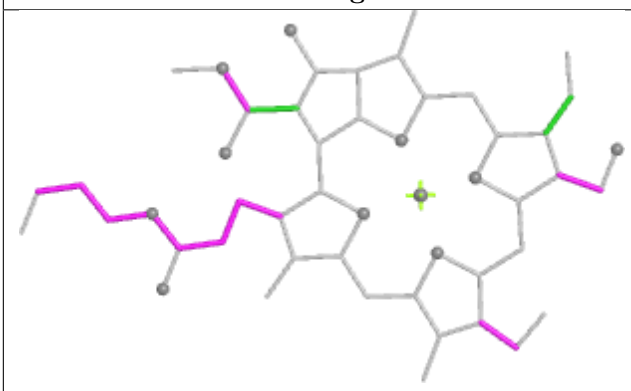
Ligand CHL 3 313



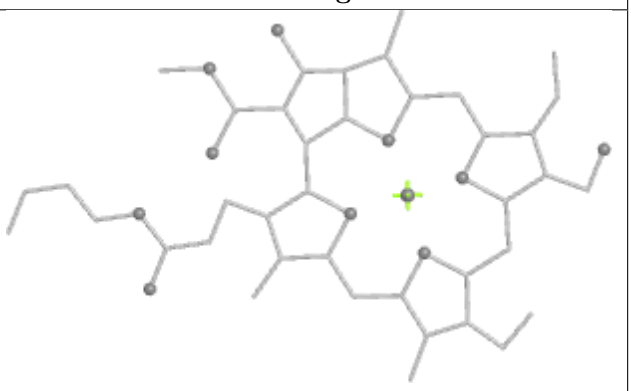
Bond lengths



Bond angles

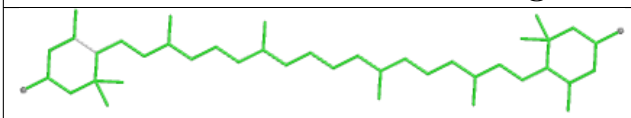


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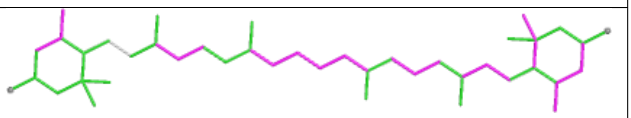


Rings

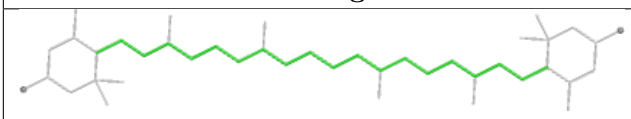
Ligand LUT v 310



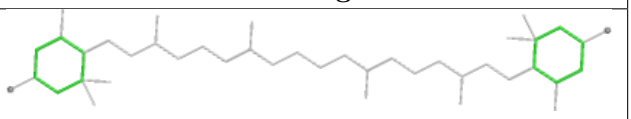
Bond lengths



Bond angles

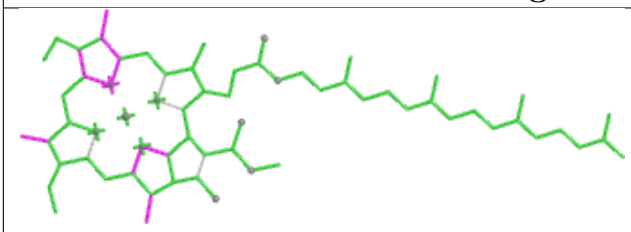


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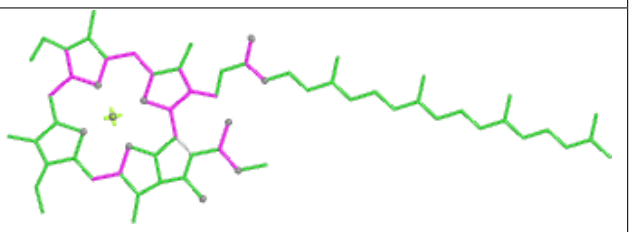


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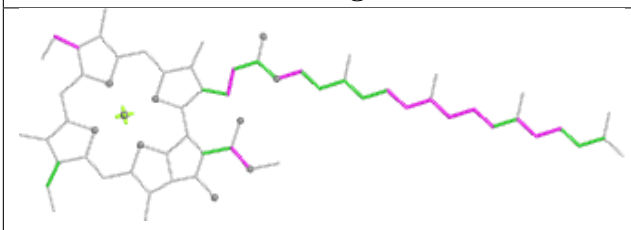
Ligand CLA c 508



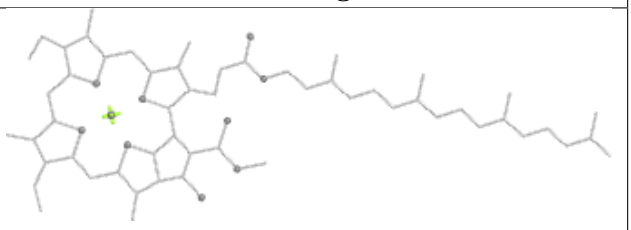
Bond lengths



Bond angles

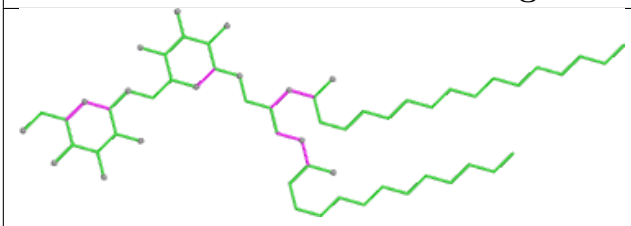


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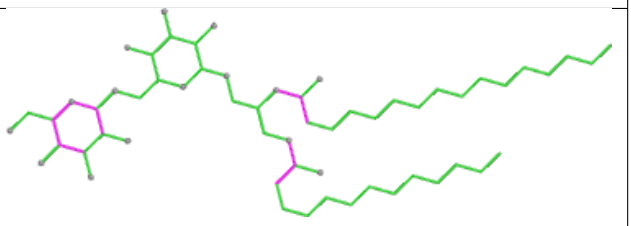


Rings

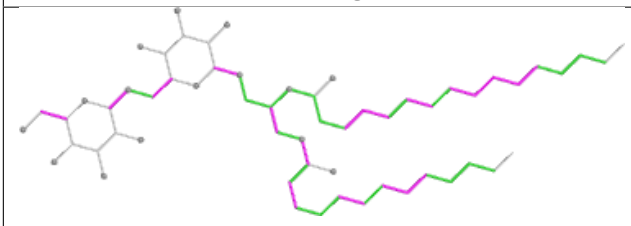
Ligand DGD A 414



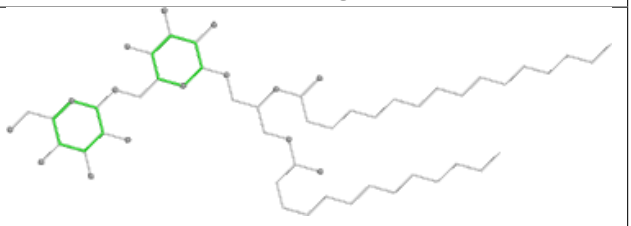
Bond lengths



Bond angles

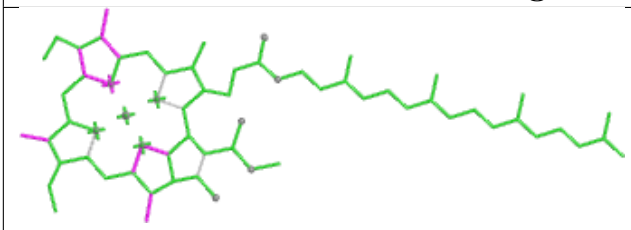


Torsions

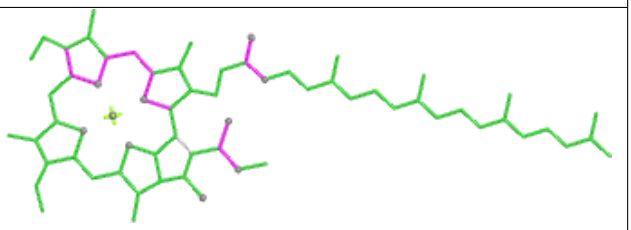


Rings

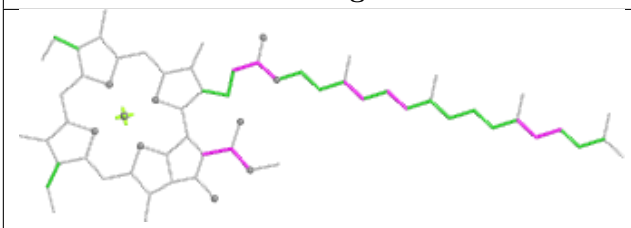
Ligand CLA 4 302



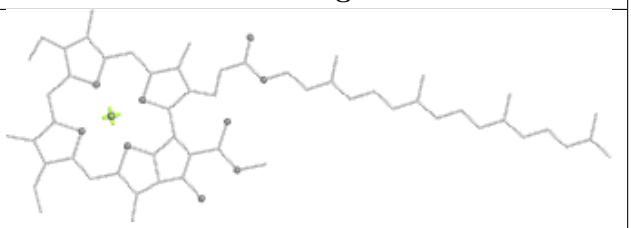
Bond lengths



Bond angles

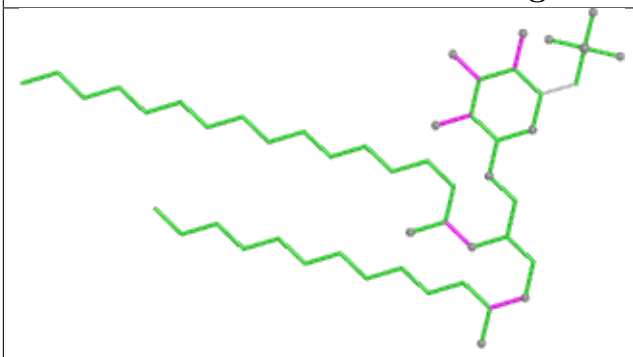


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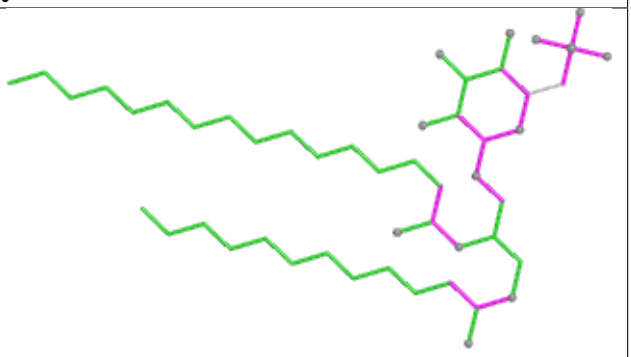


Rings

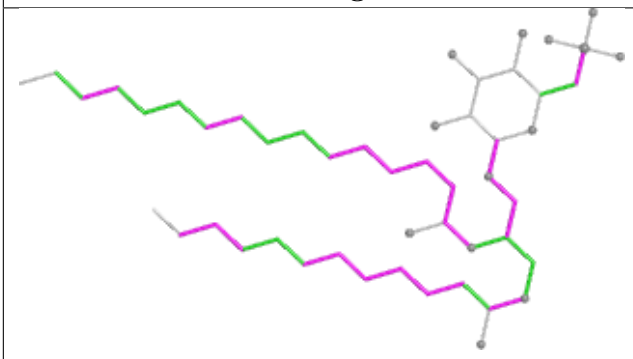
Ligand SQD a 410



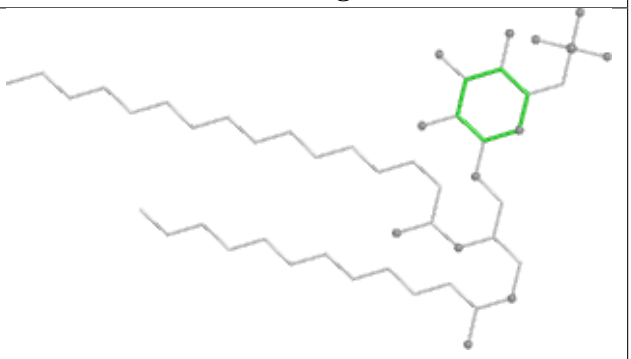
Bond lengths



Bond angles

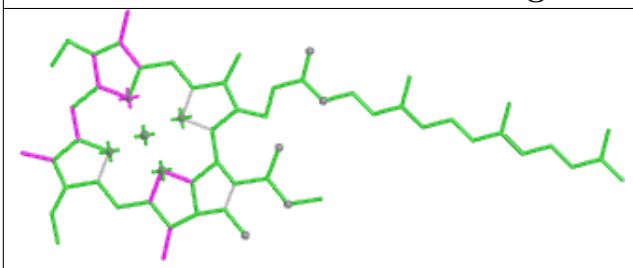


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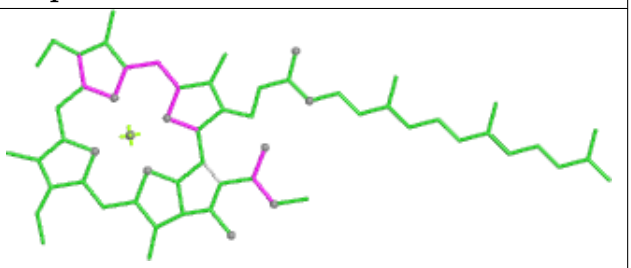


Rings

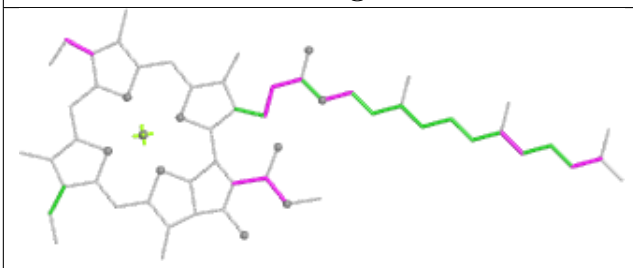
Ligand CLA p 308



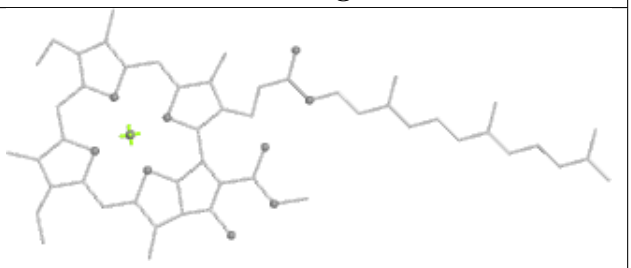
Bond lengths



Bond angles

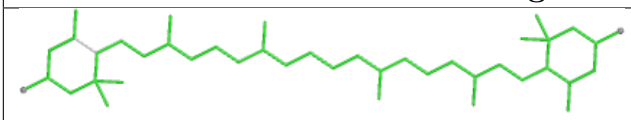


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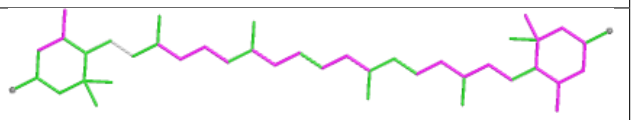


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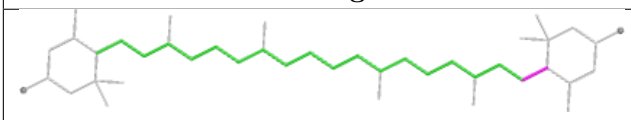
Ligand LUT v 309



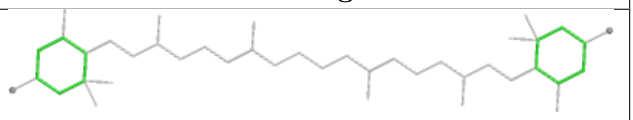
Bond lengths



Bond angles

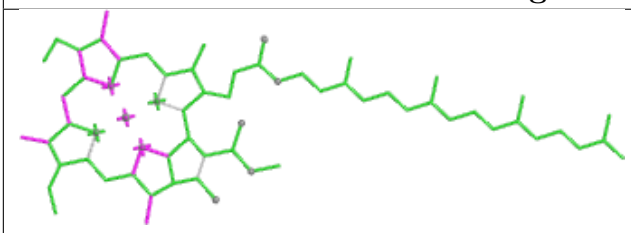


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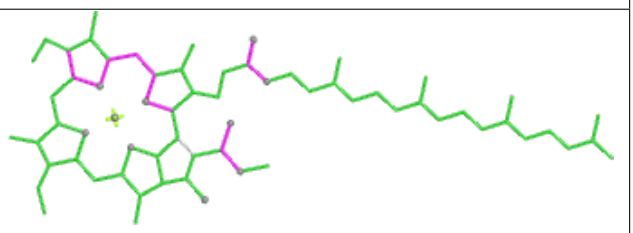


Rings

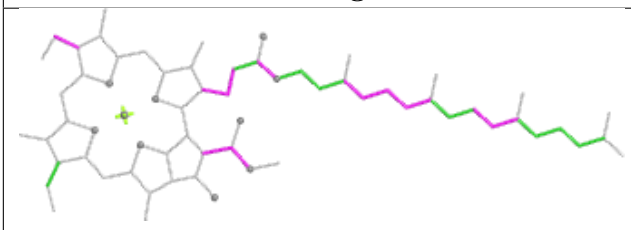
Ligand CLA c 504



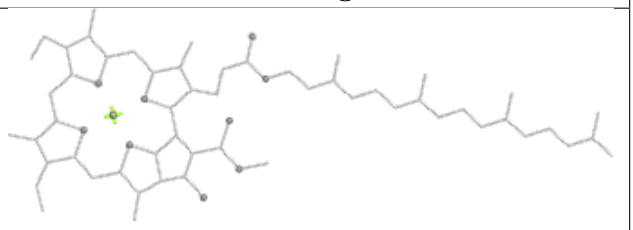
Bond lengths



Bond angles

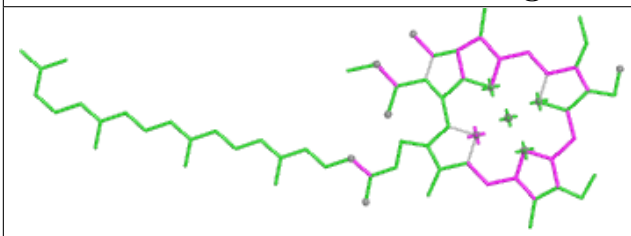


Torsions

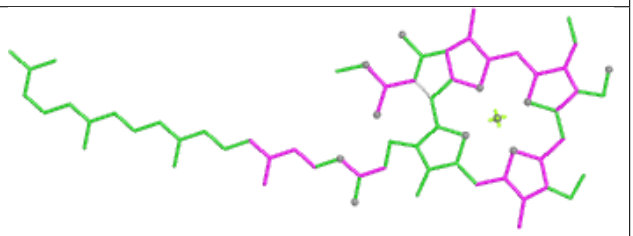


Rings

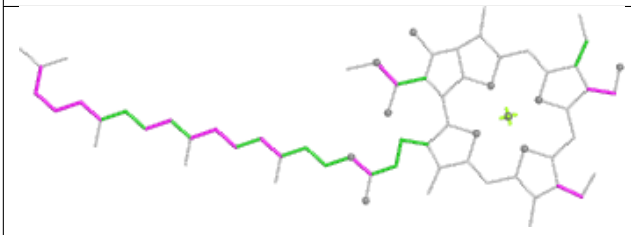
Ligand CHL V 318



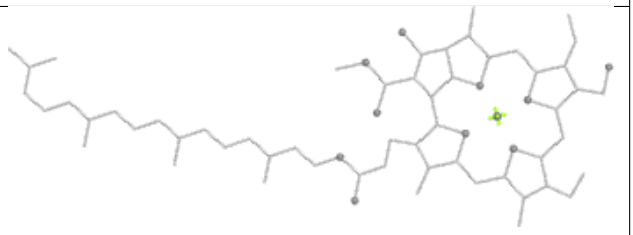
Bond lengths



Bond angles

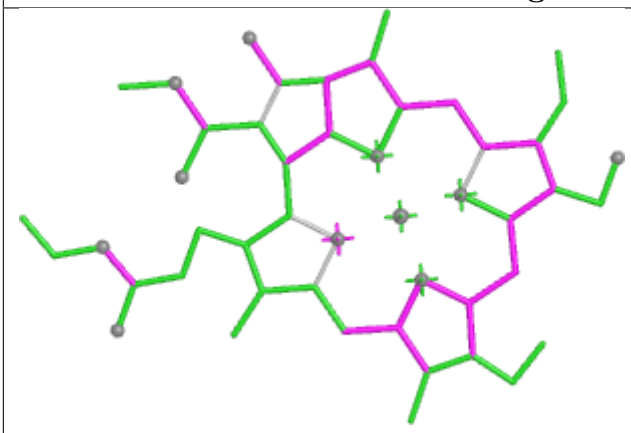


Torsions

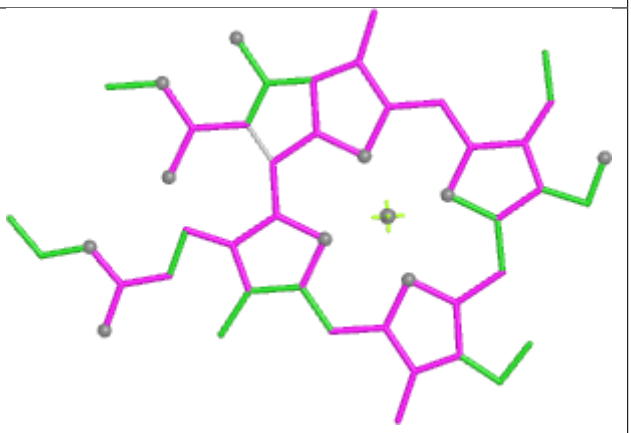


Rings

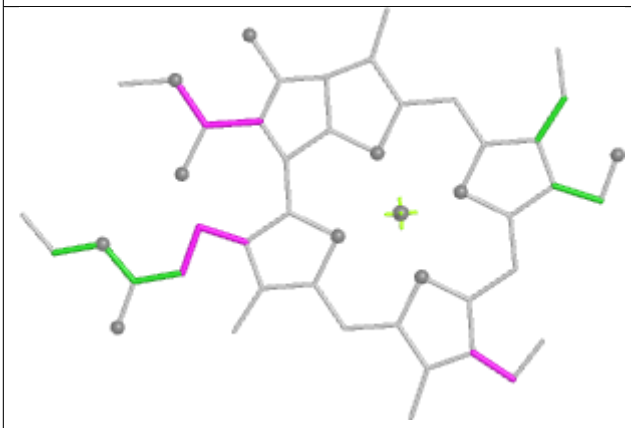
Ligand CHL 6 313



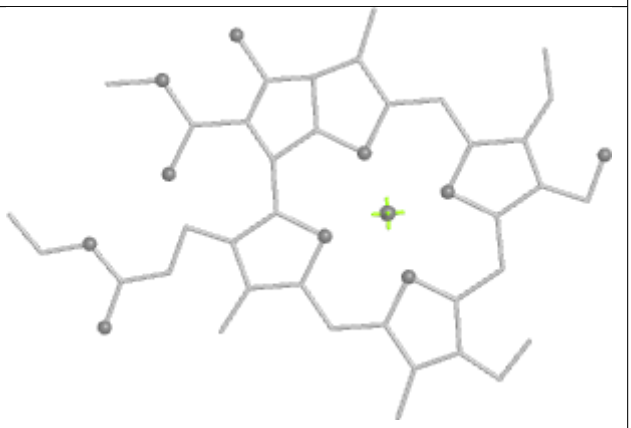
Bond lengths



Bond angles

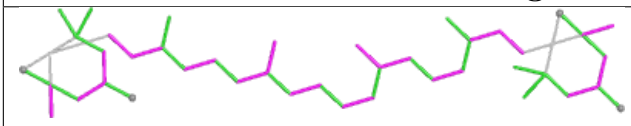


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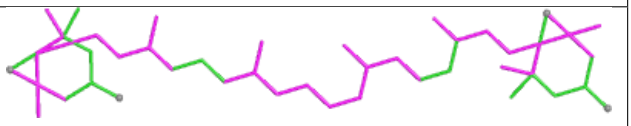


Rings

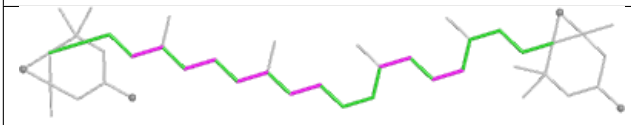
Ligand XAT n 311



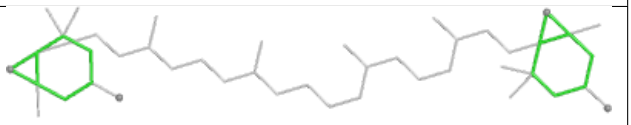
Bond lengths



Bond angles

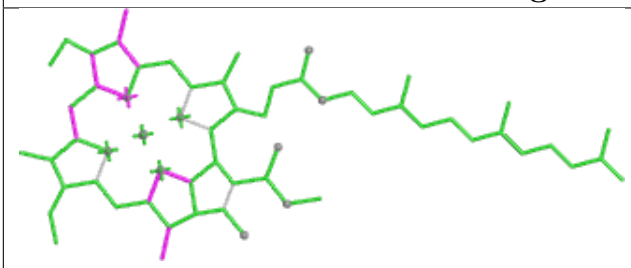


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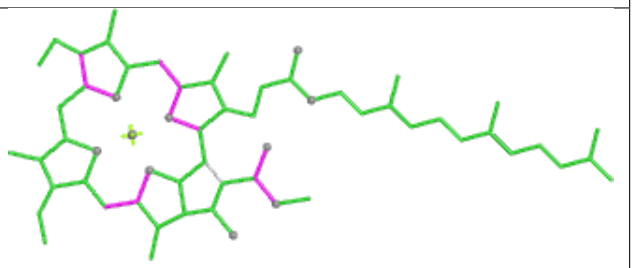


Rings

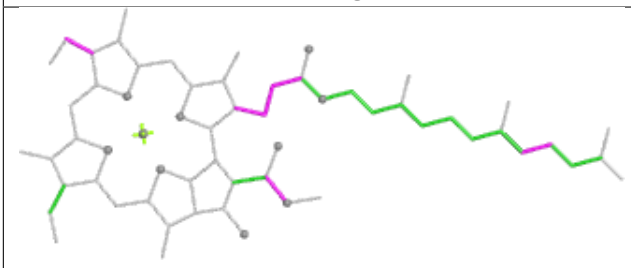
Ligand CLA r 602



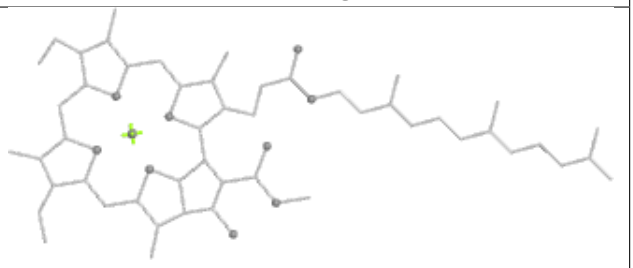
Bond lengths



Bond angles

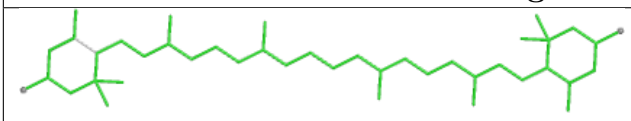


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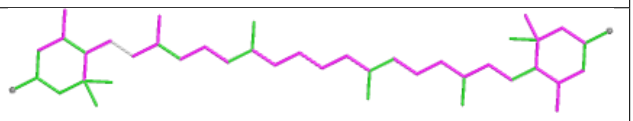


Rings

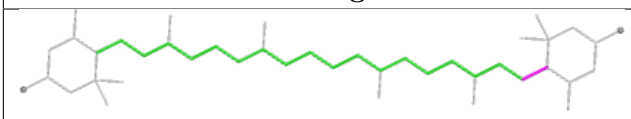
Ligand LUT S 310



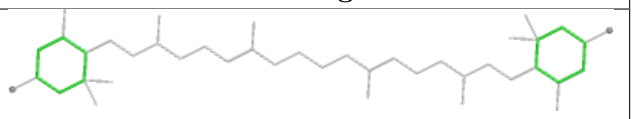
Bond lengths



Bond angles

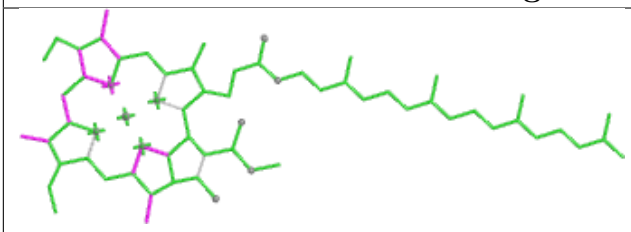


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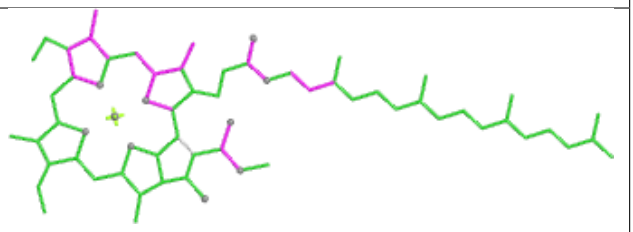


Rings

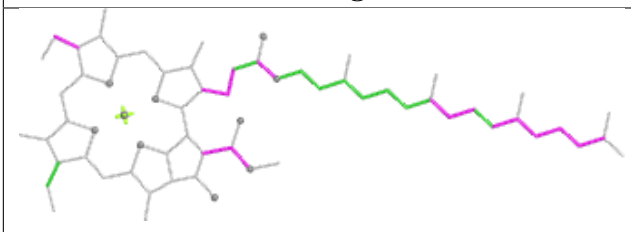
Ligand CLA N 304



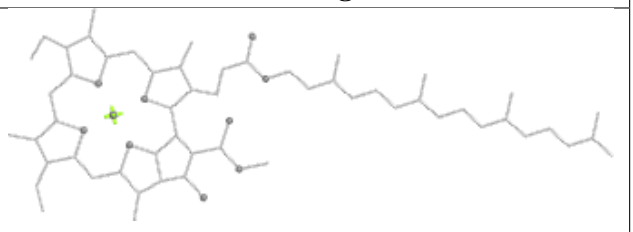
Bond lengths



Bond angles

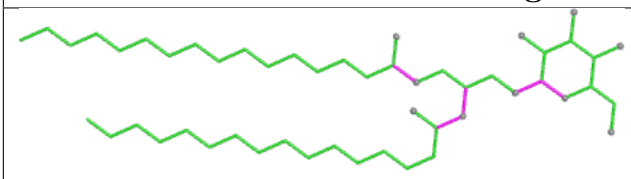


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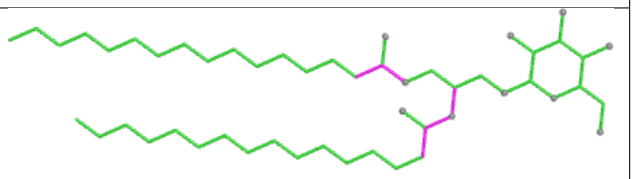


Rings

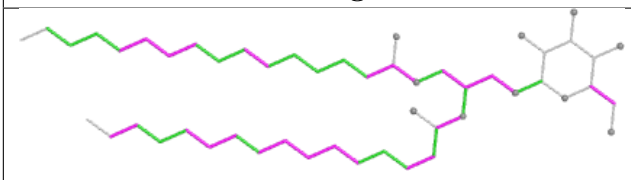
Ligand LMG c 501



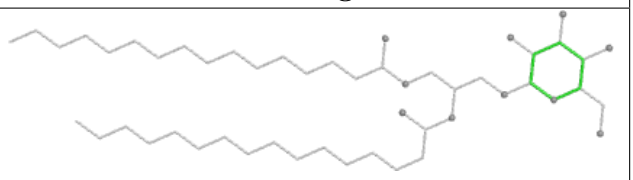
Bond lengths



Bond angles

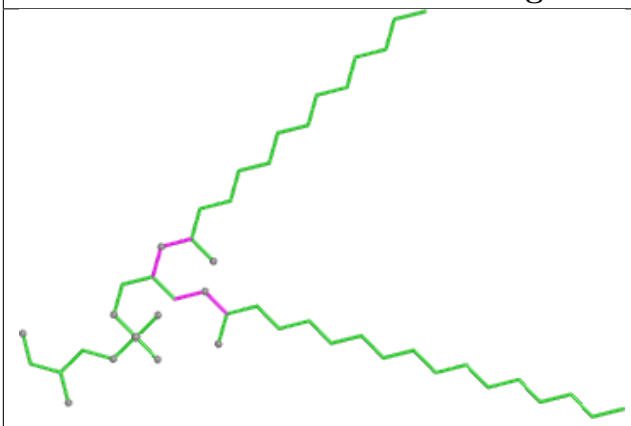


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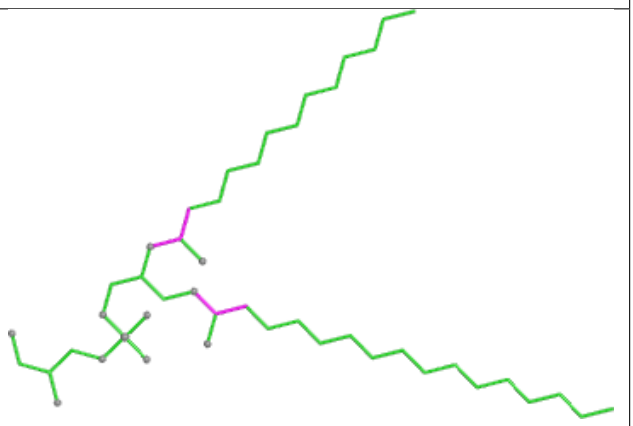


Rings

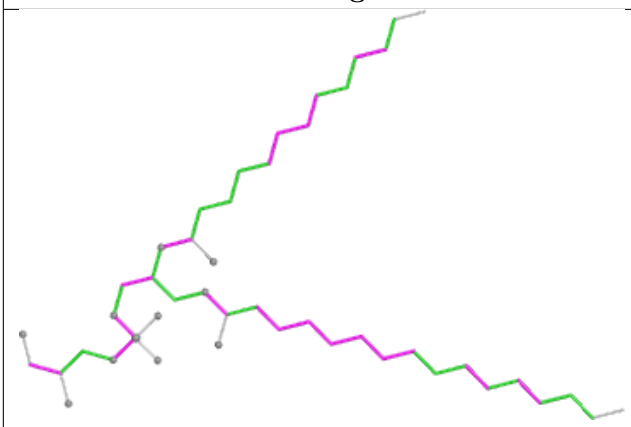
Ligand LHG d 405



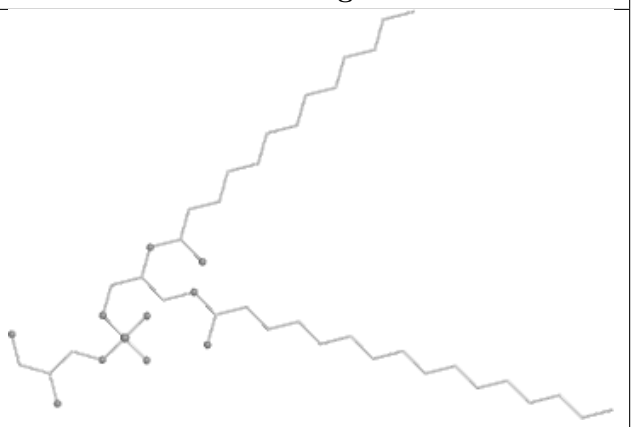
Bond lengths



Bond angles

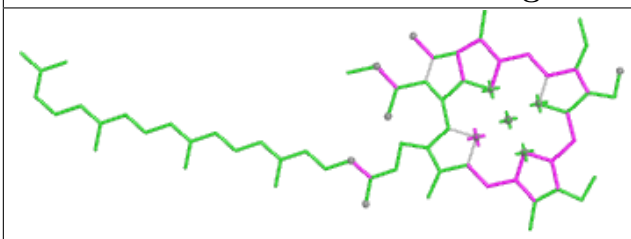


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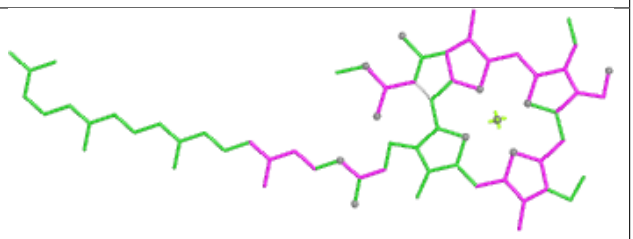


Rings

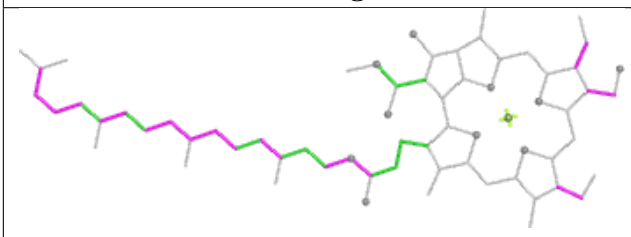
Ligand CHL N 317



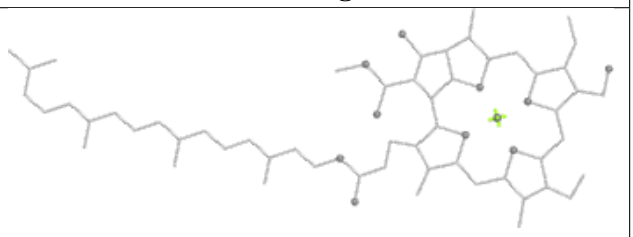
Bond lengths



Bond angles

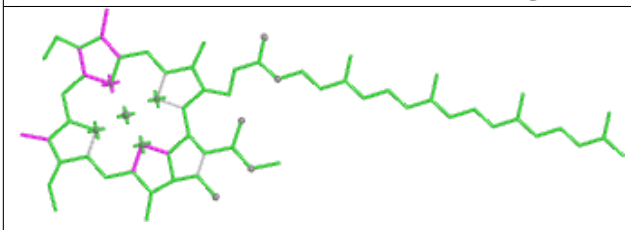


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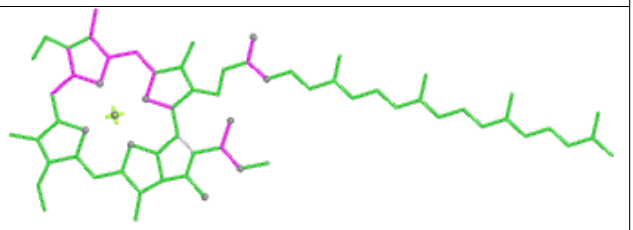


Rings

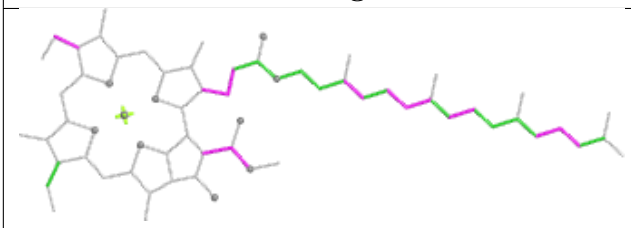
Ligand CLA B 604



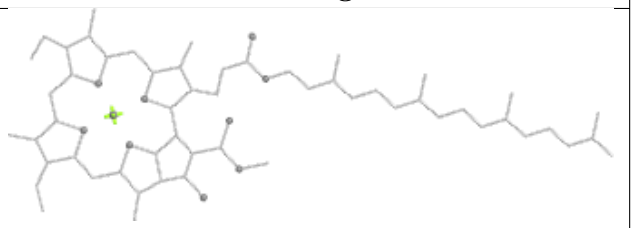
Bond lengths



Bond angles

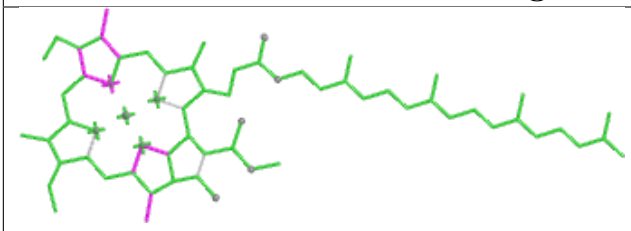


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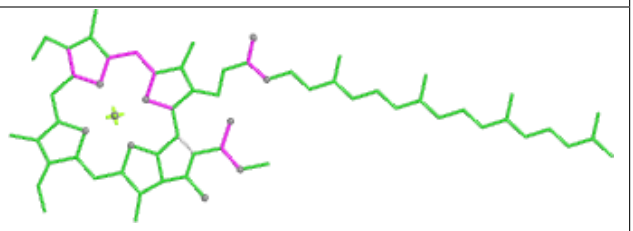


Rings

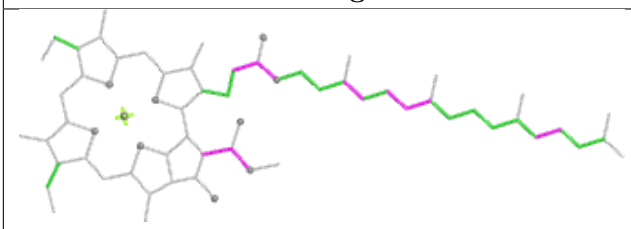
Ligand CLA 1 302



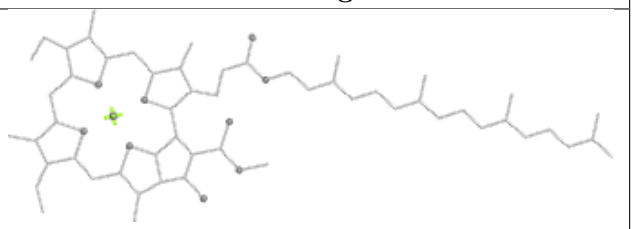
Bond lengths



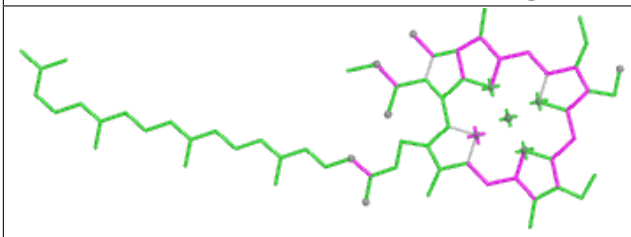
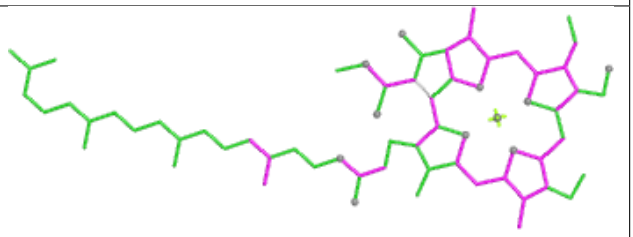
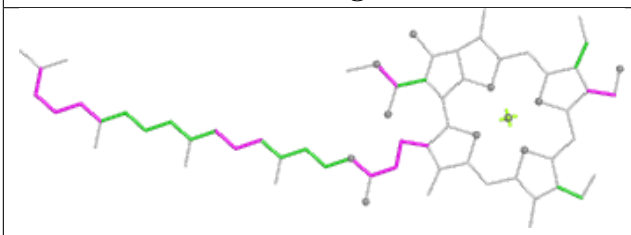
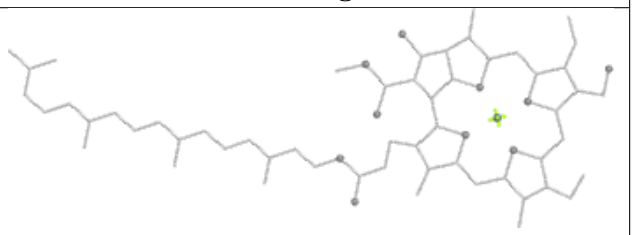
Bond angles

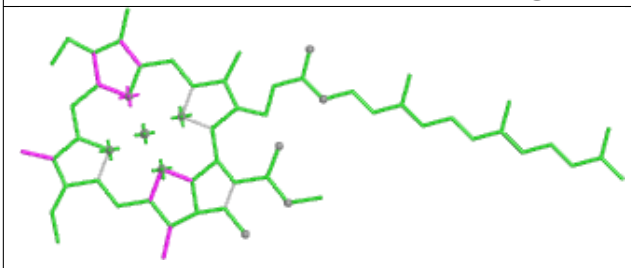
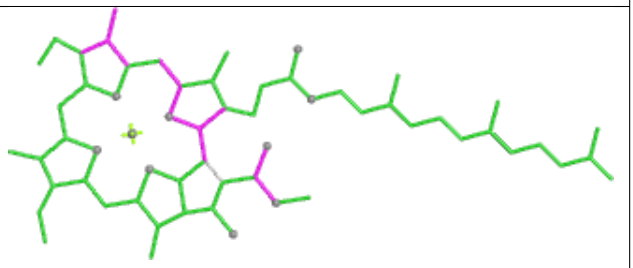
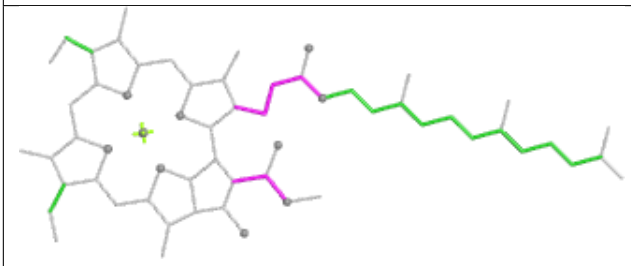
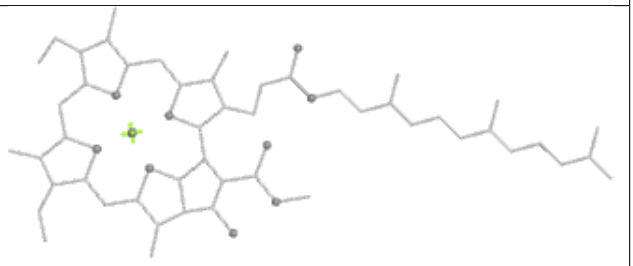


Torsions

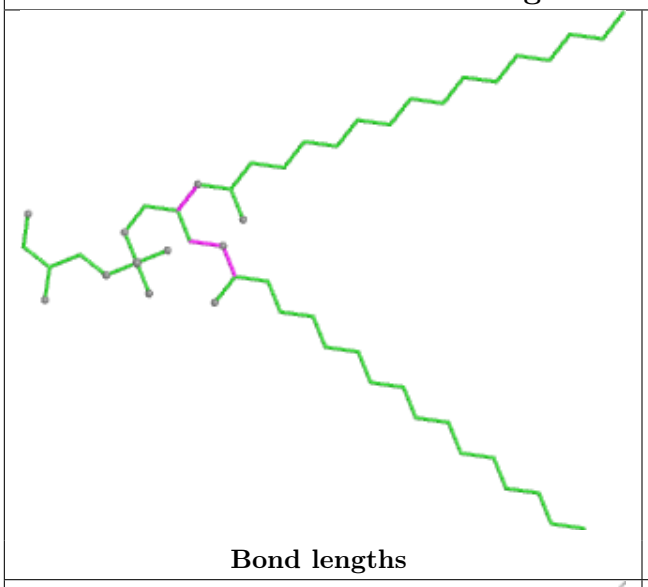


Rings

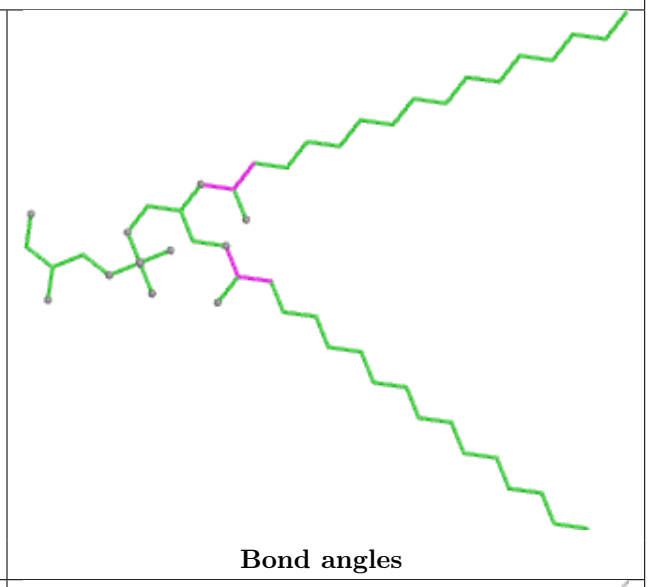
Ligand CHL G 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

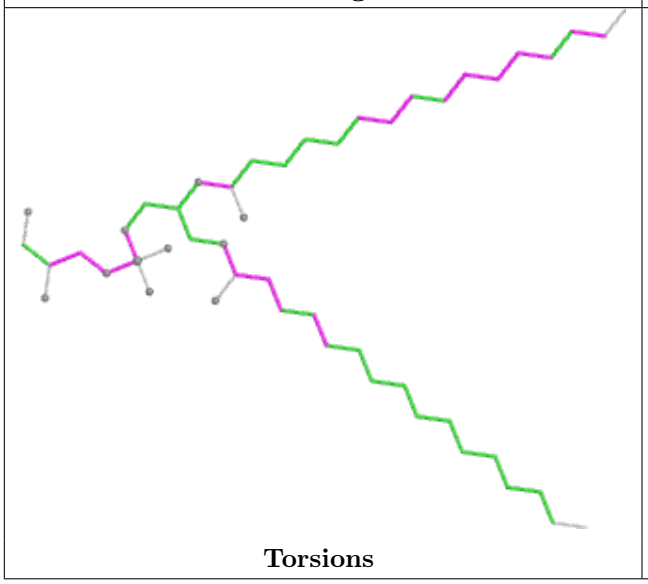
Ligand LHG C 523



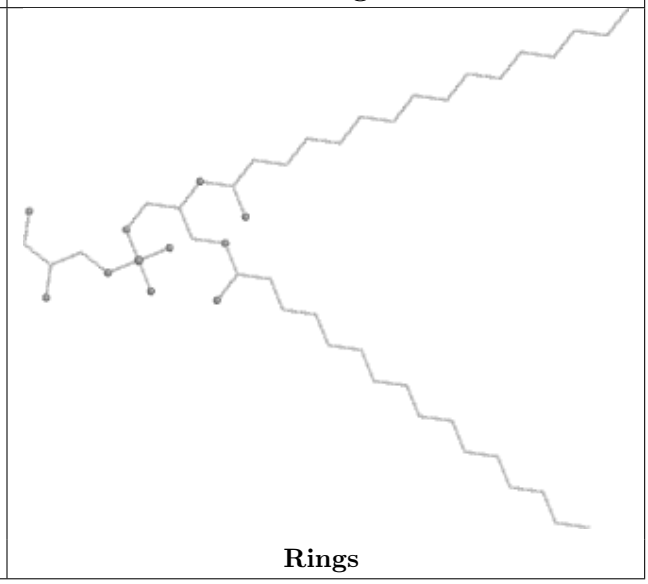
Bond lengths



Bond angles

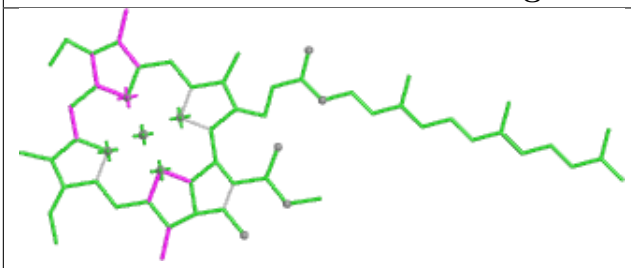


Torsions

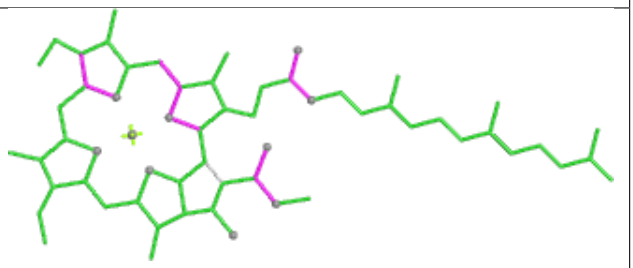


Rings

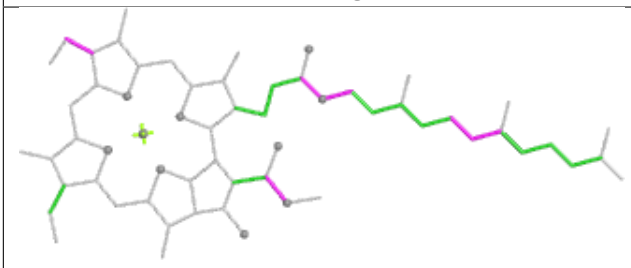
Ligand CLA V 305



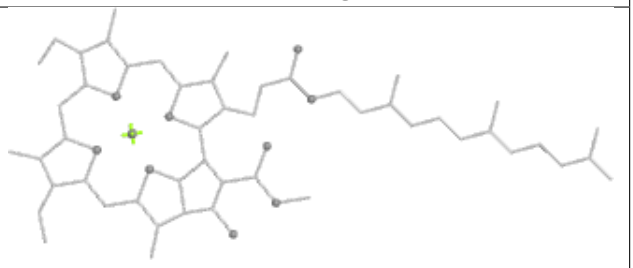
Bond lengths



Bond angles

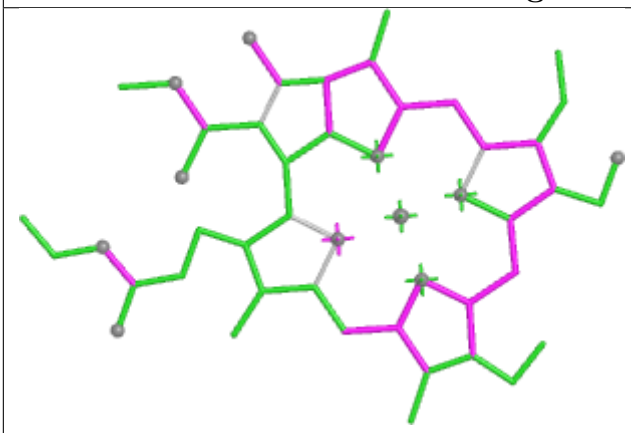


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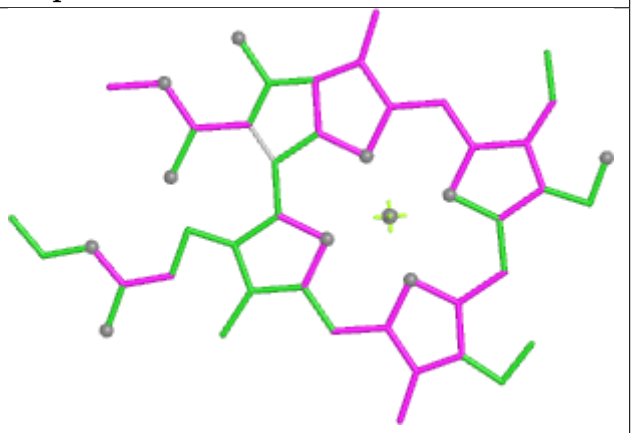


Rings

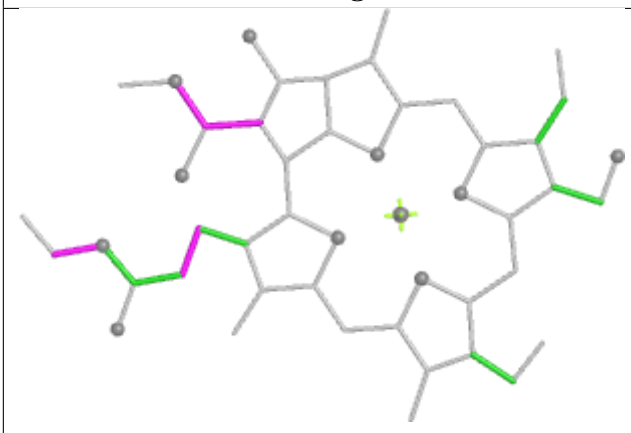
Ligand CHL p 315



Bond lengths



Bond angles

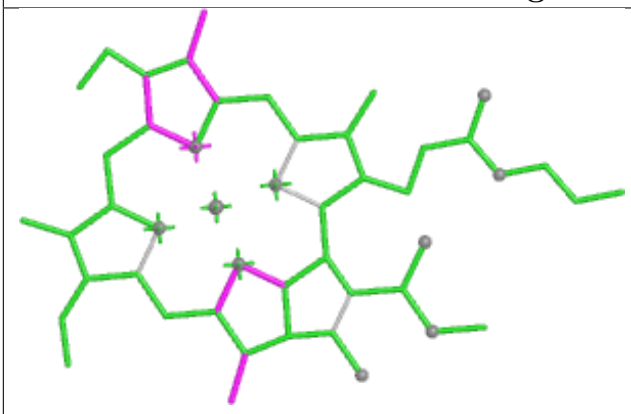


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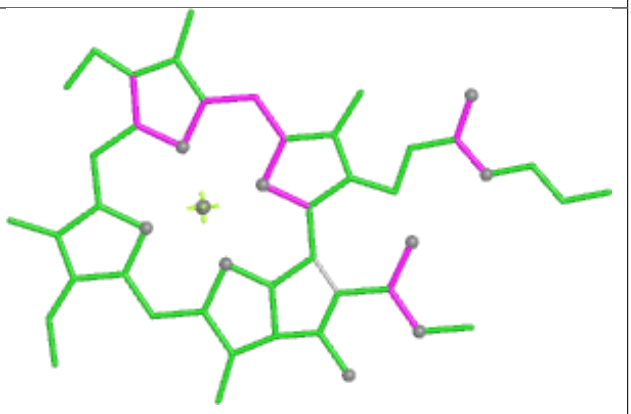


Rings

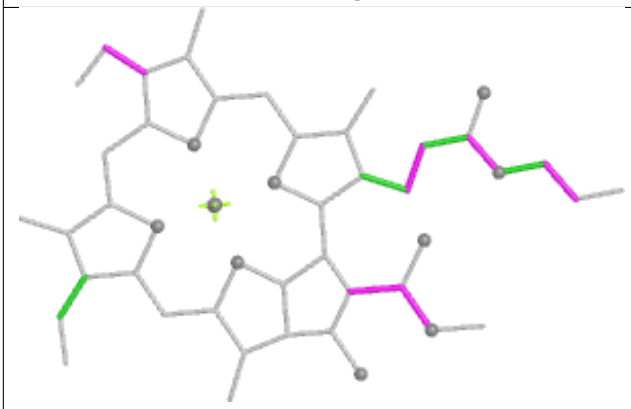
Ligand CLA u 308



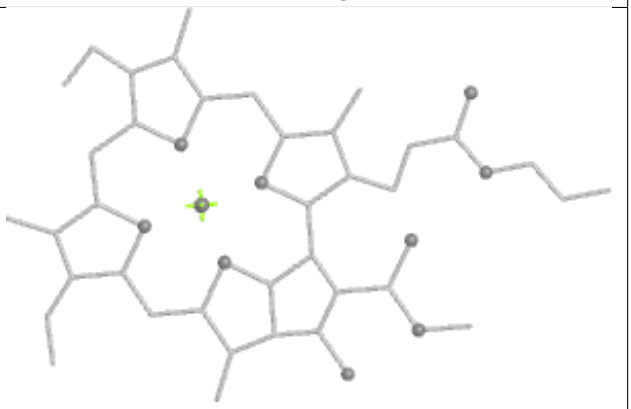
Bond lengths



Bond angles

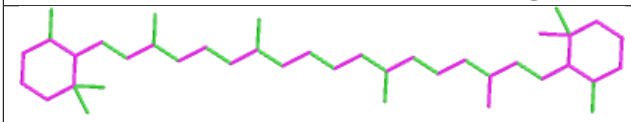


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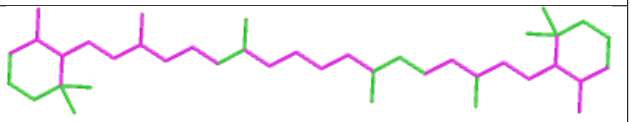


Rings

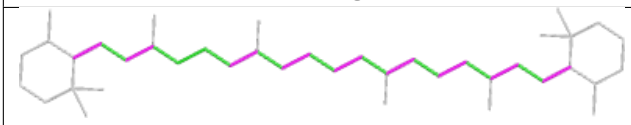
Ligand BCR b 619



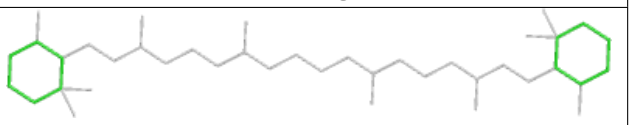
Bond lengths



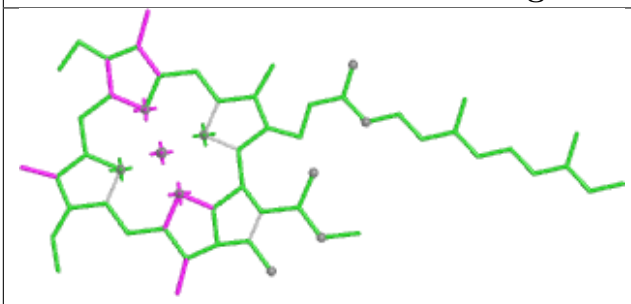
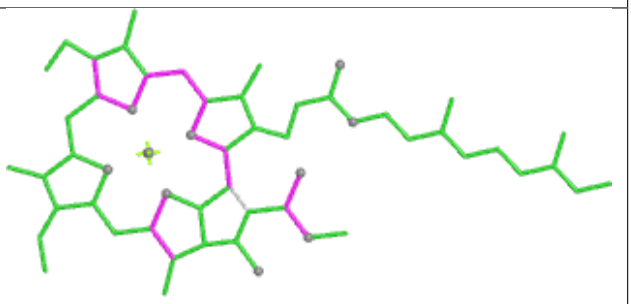
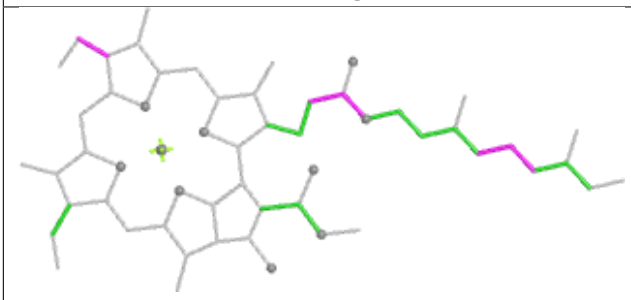
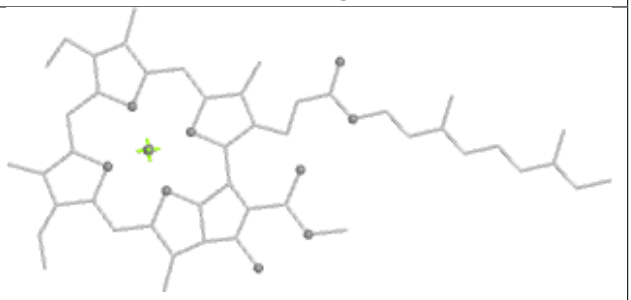
Bond angles

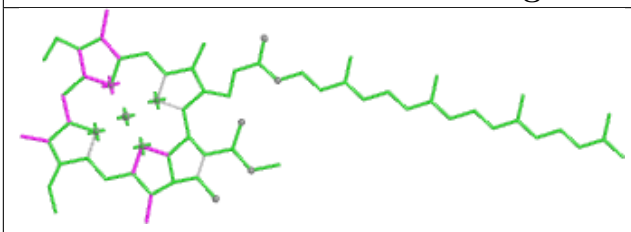
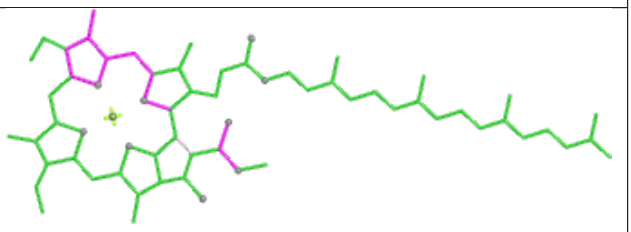
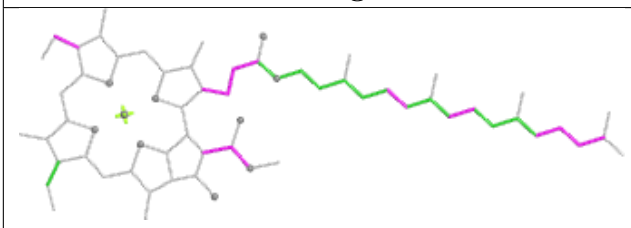
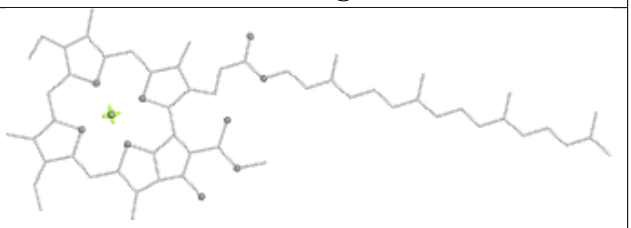


Torsions

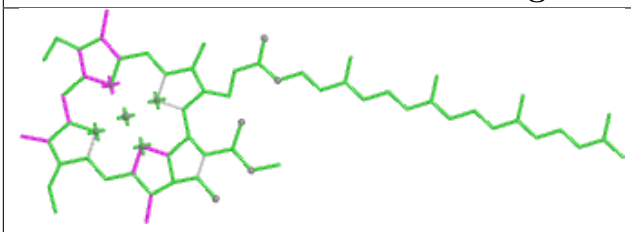


Rings

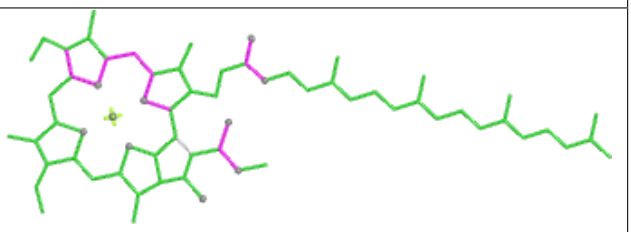
Ligand CLA S 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

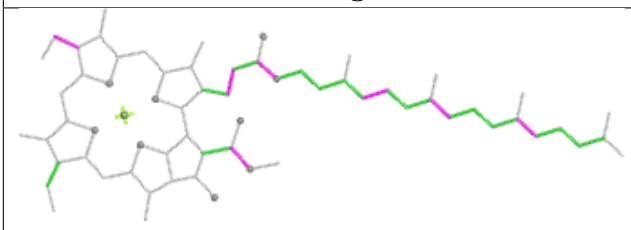
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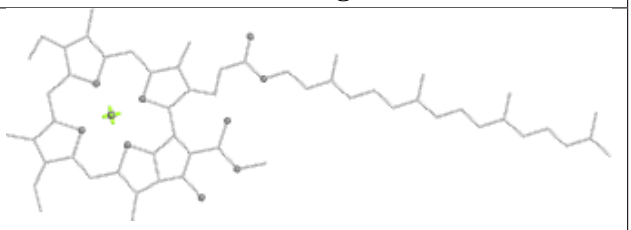
Bond lengths



Bond angles

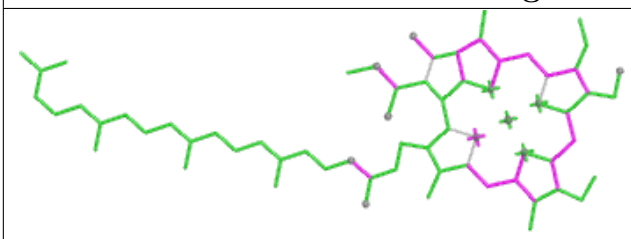


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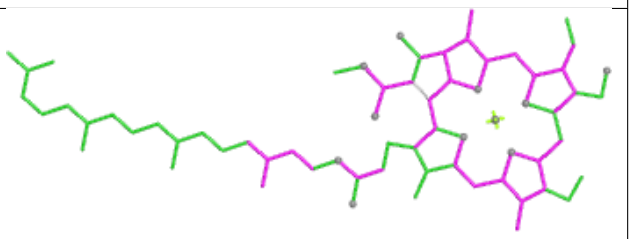


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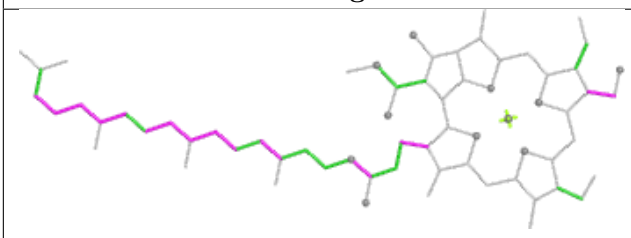
Ligand CHL G 311



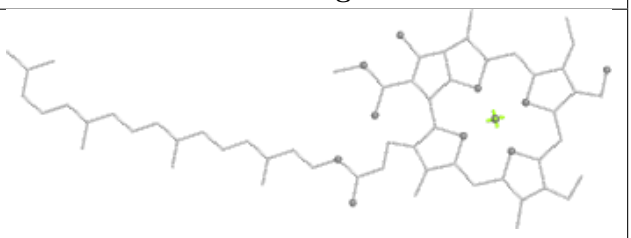
Bond lengths



Bond angles

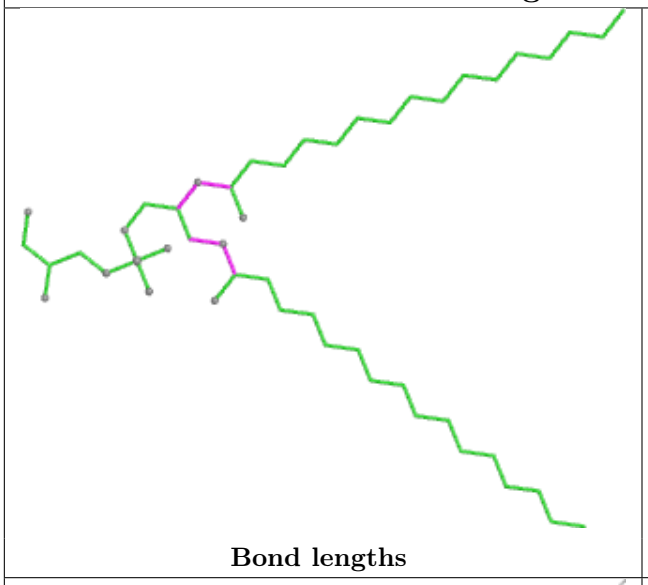


Torsions

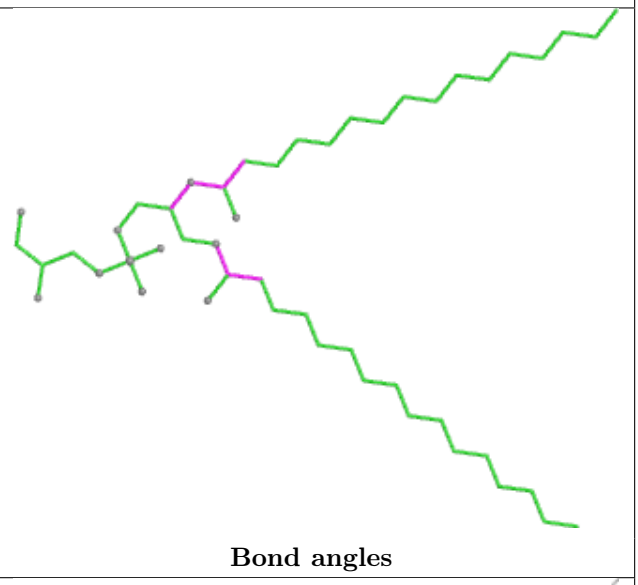


Rings

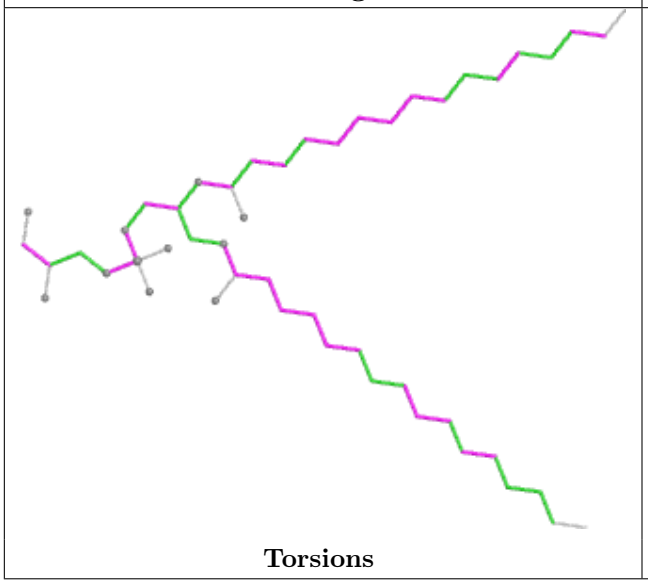
Ligand LHG U 312



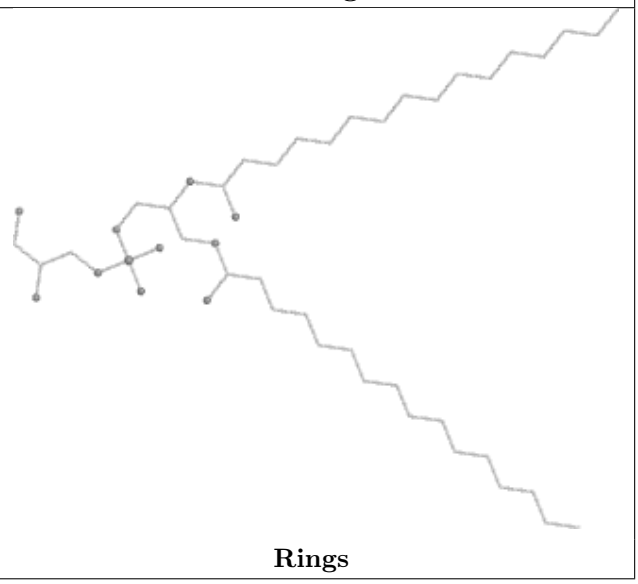
Bond lengths



Bond angles



Torsions



Rings

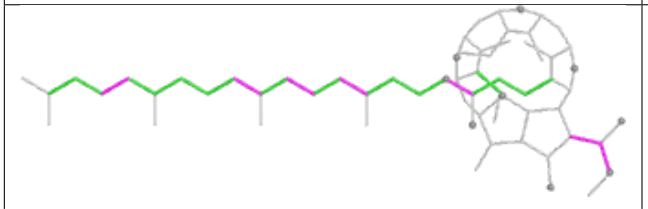
Ligand PHO a 407



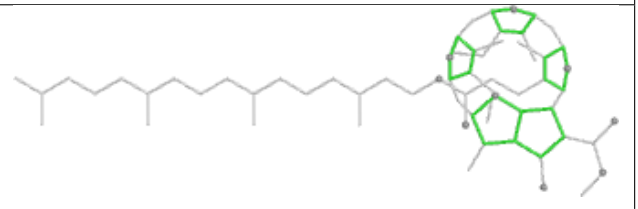
Bond lengths



Bond angles

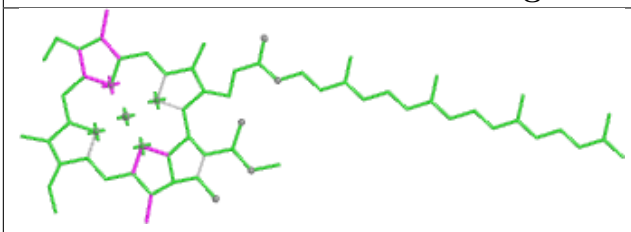


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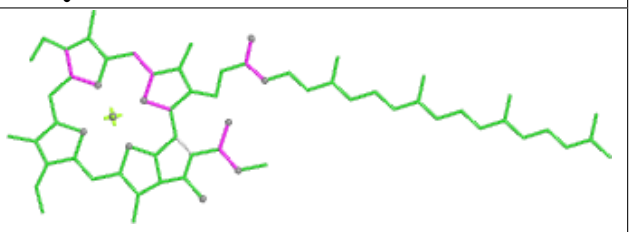


Rings

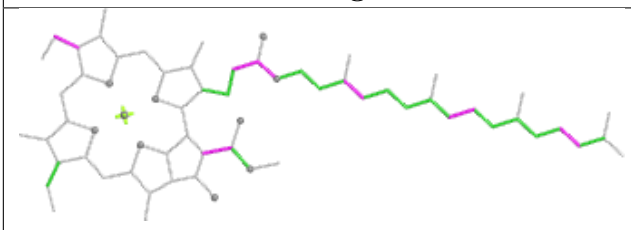
Ligand CLA Q 302



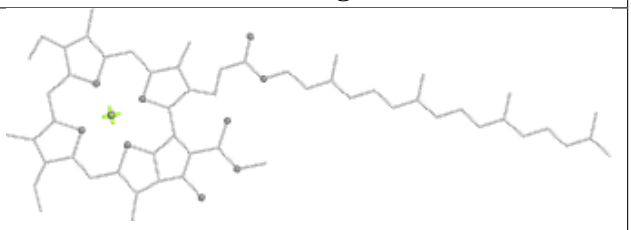
Bond lengths



Bond angles

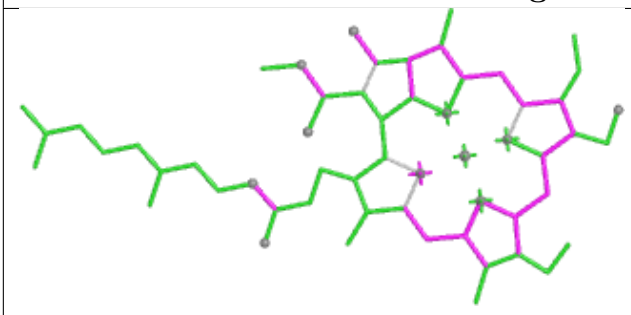


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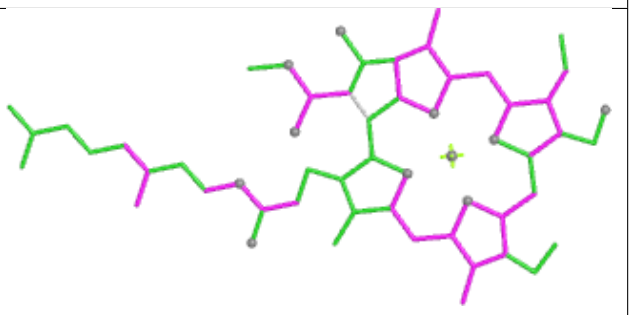


Rings

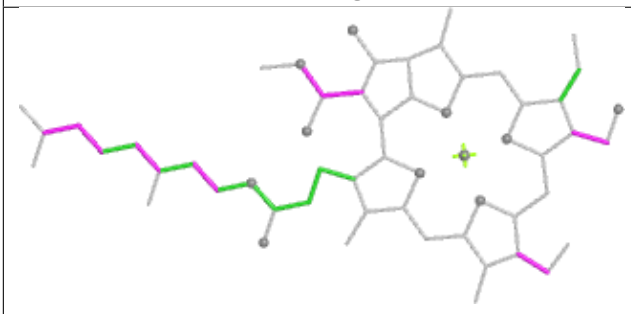
Ligand CHL r 615



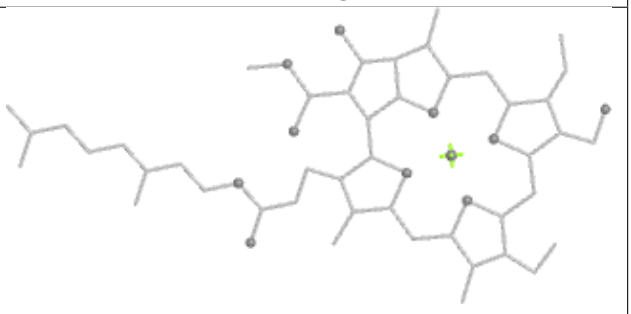
Bond lengths



Bond angles

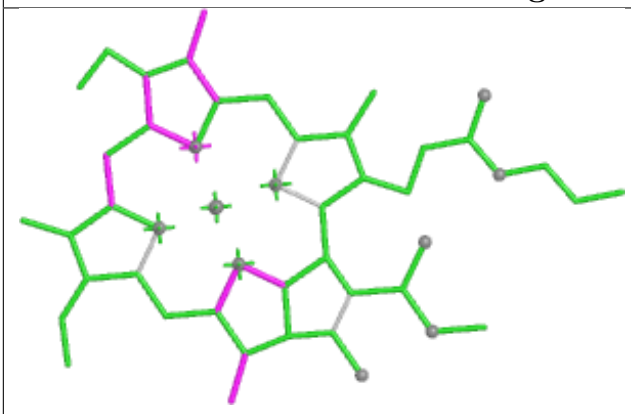


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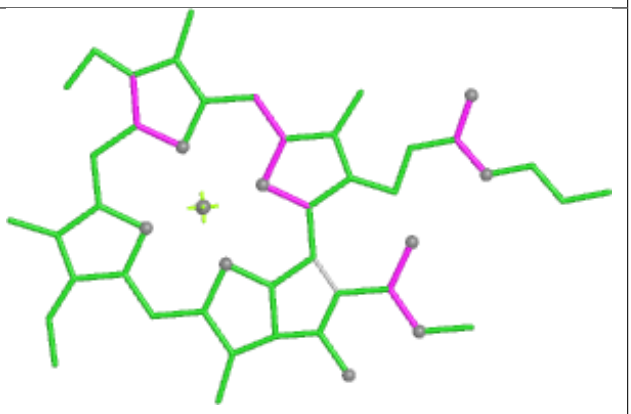


Rings

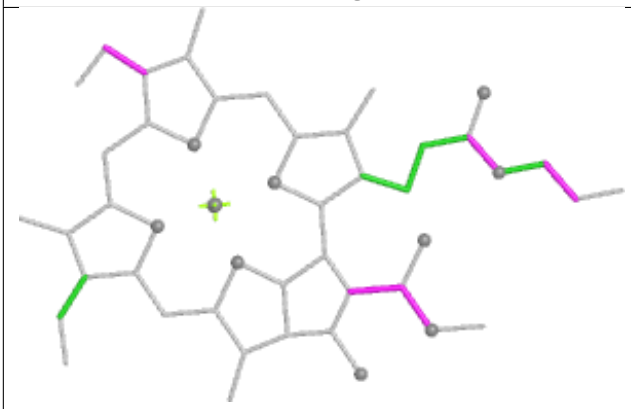
Ligand CLA 2 308



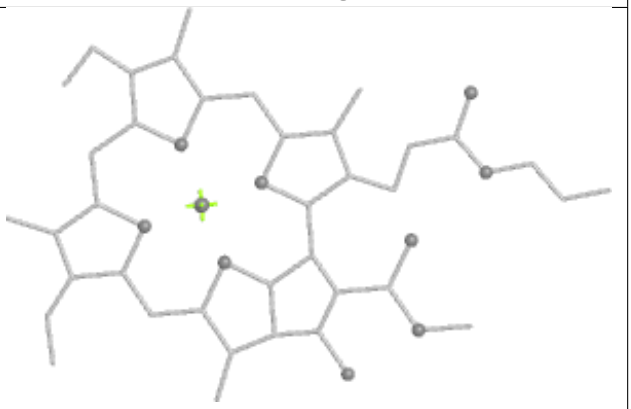
Bond lengths



Bond angles

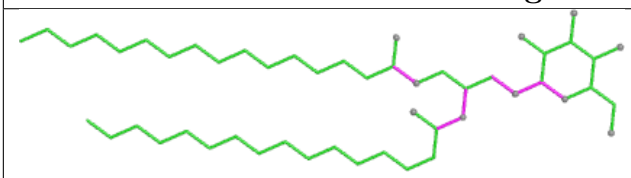


Torsions

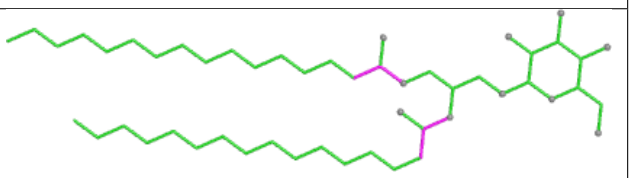


Rings

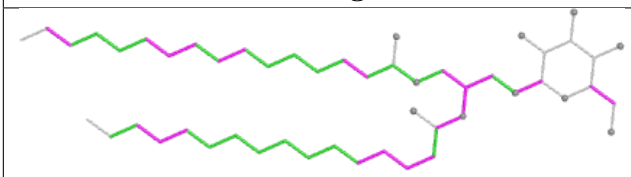
Ligand LMG c 520



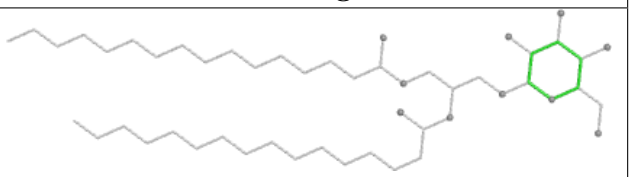
Bond lengths



Bond angles

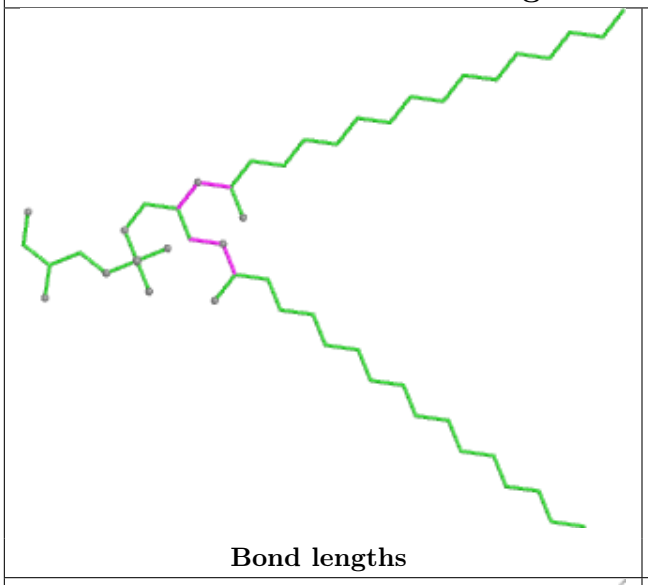


Torsions

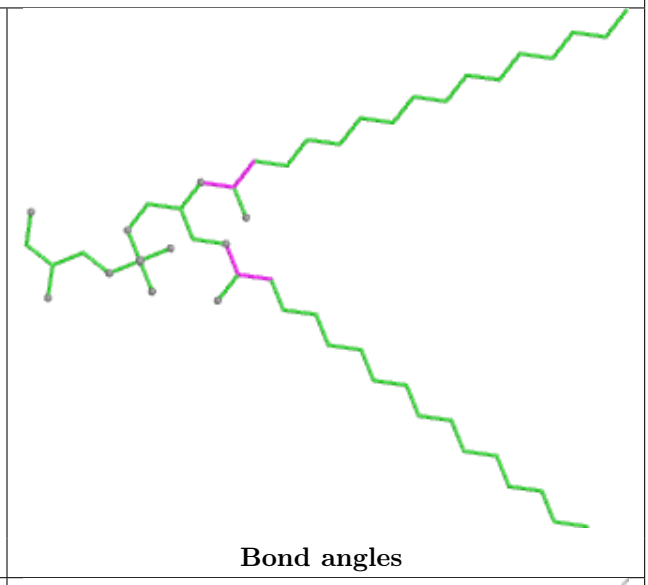


Rings

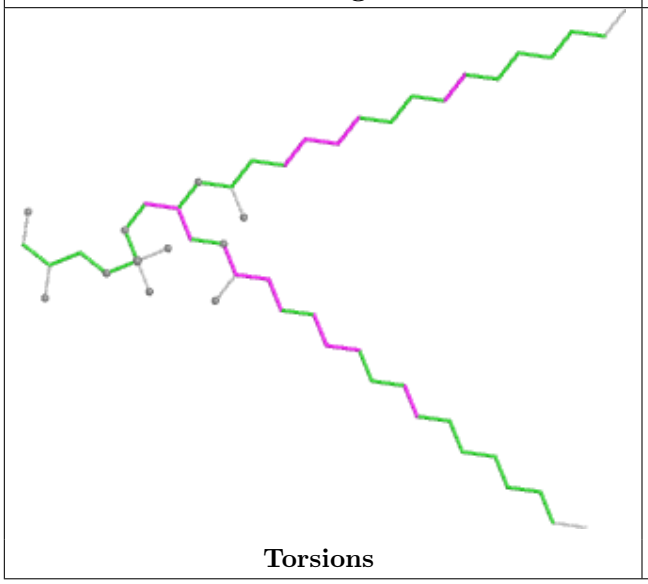
Ligand LHG N 312



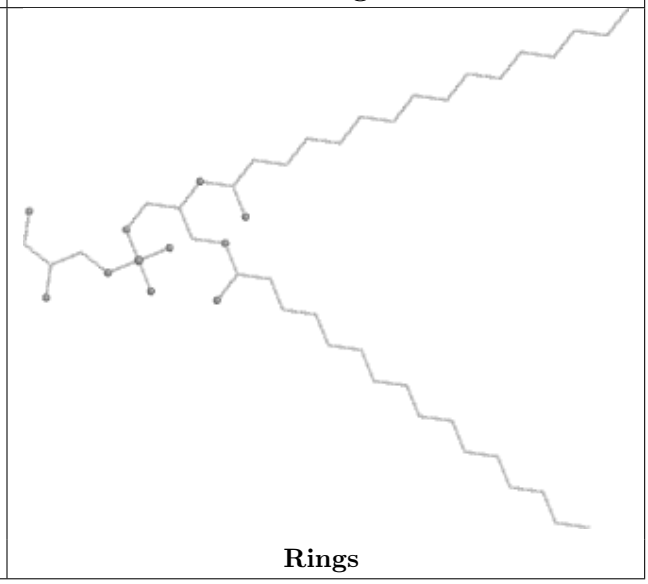
Bond lengths



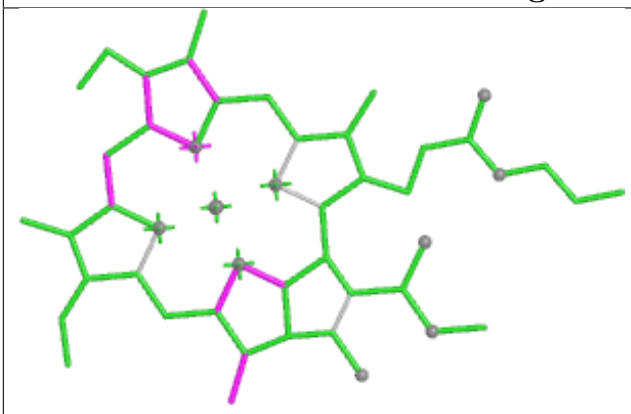
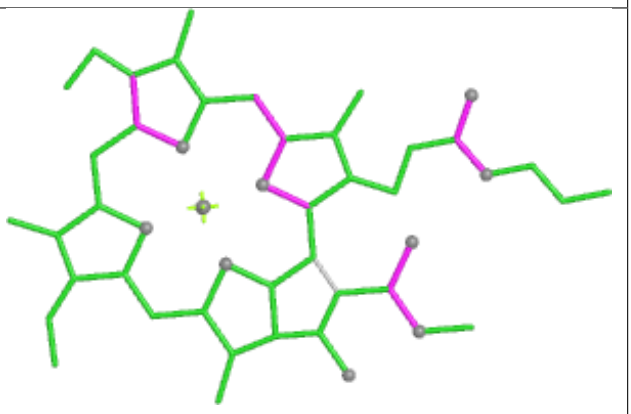
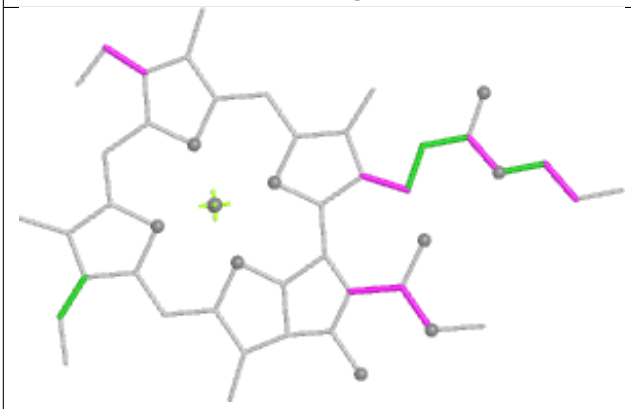
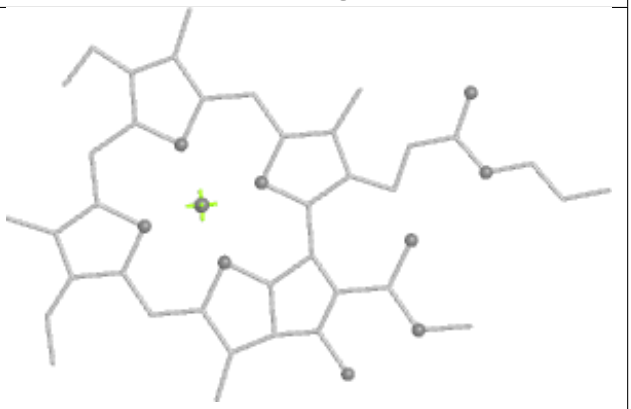
Bond angles

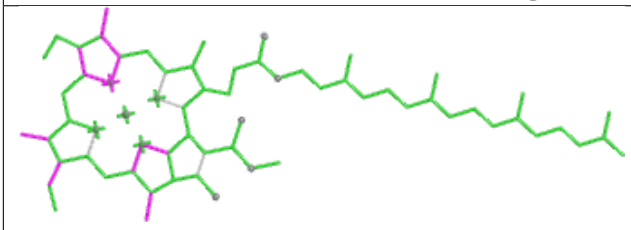
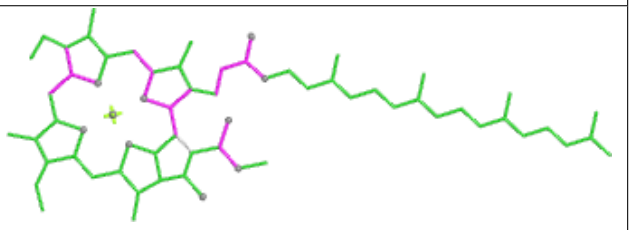
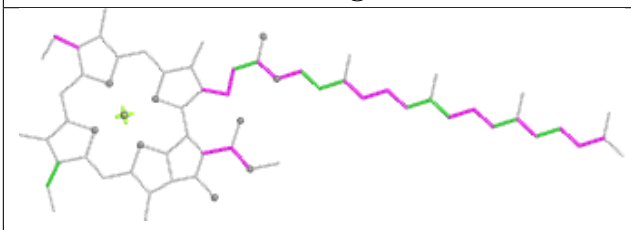
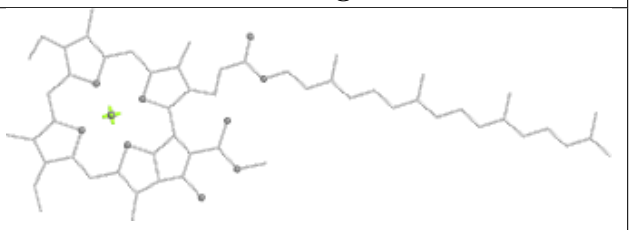


Torsions

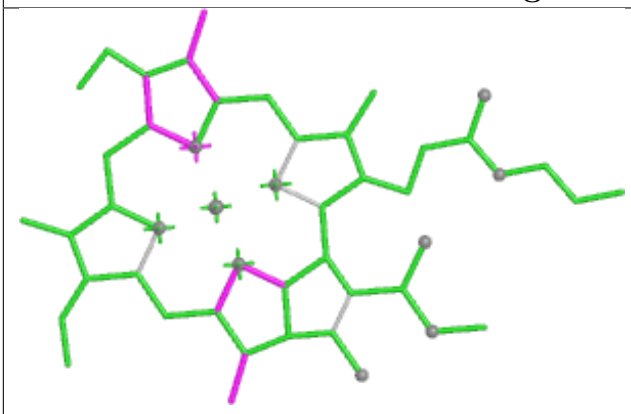


Rings

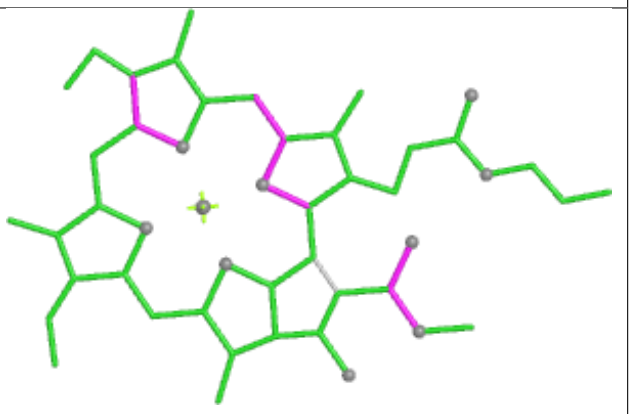
Ligand CLA 3 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

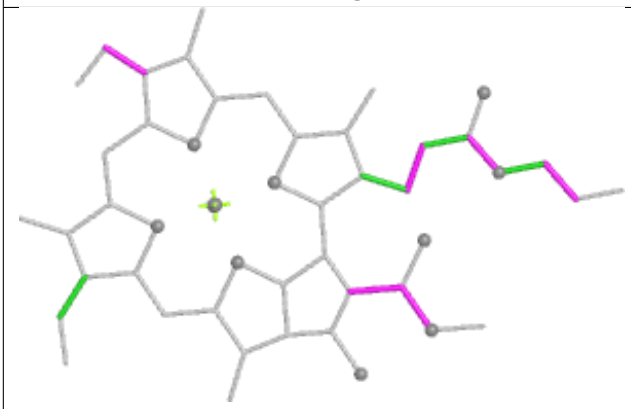
Ligand CLA V 308



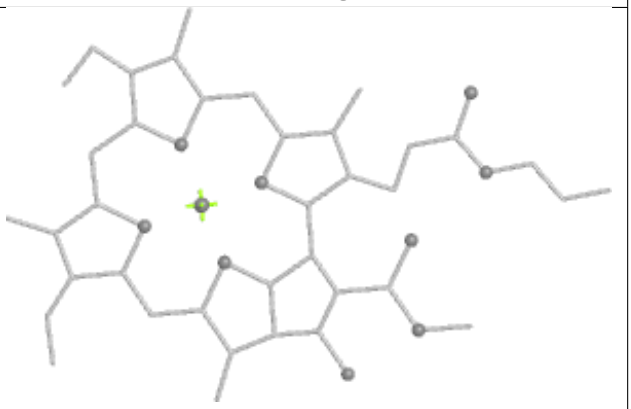
Bond lengths



Bond angles

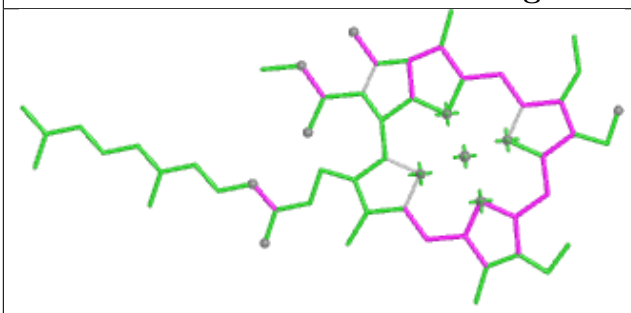


Torsions

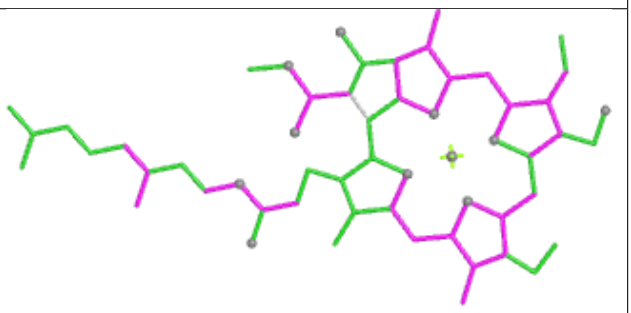


Rings

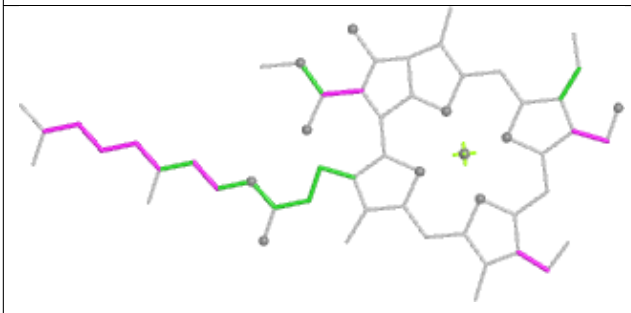
Ligand CHL R 316



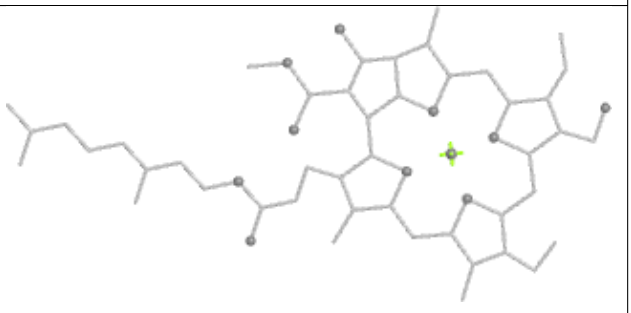
Bond lengths



Bond angles

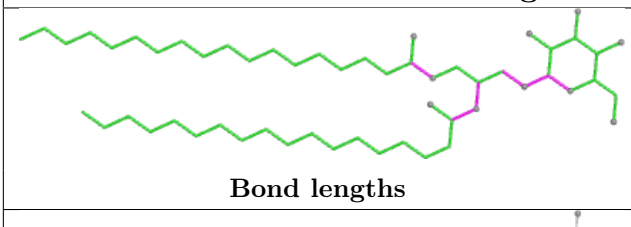


Torsions

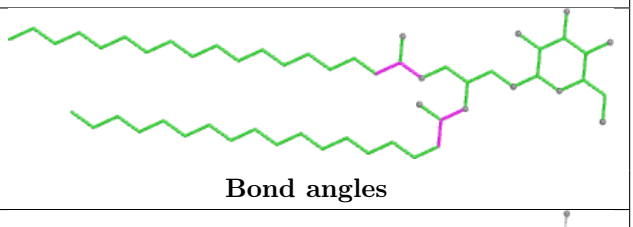


Rings

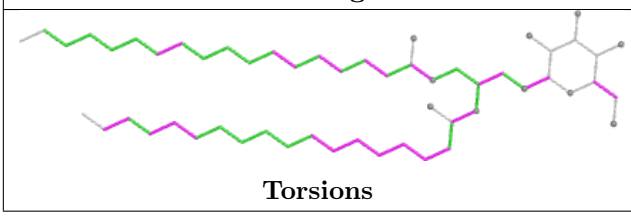
Ligand LMG B 624



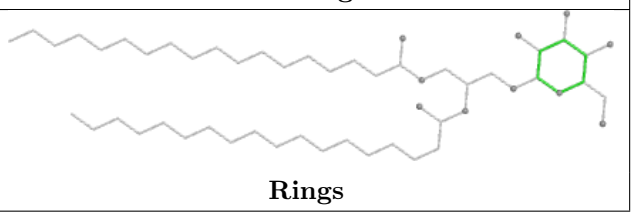
Bond lengths



Bond angles

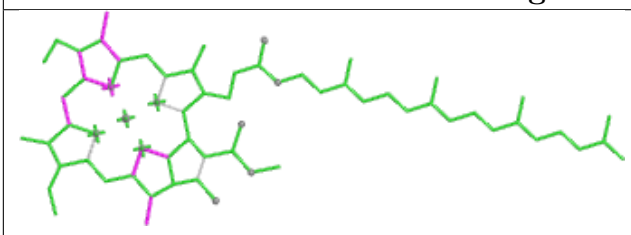


Torsions

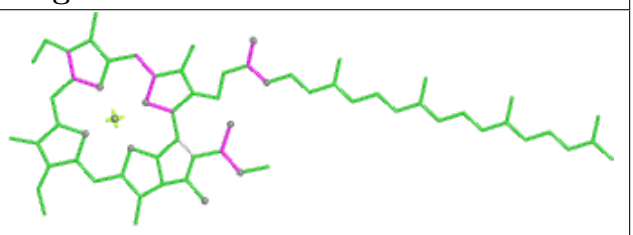


Rings

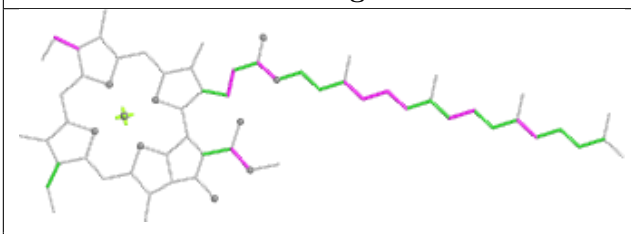
Ligand CLA g 307



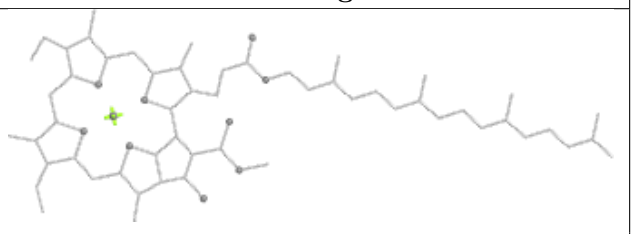
Bond lengths



Bond angles

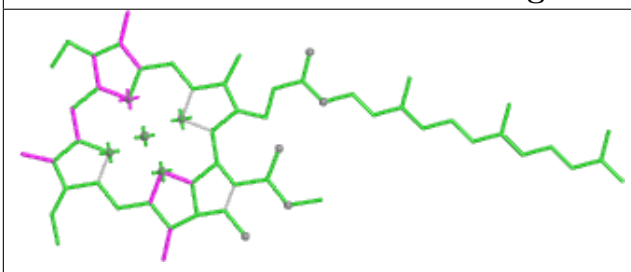


Torsions

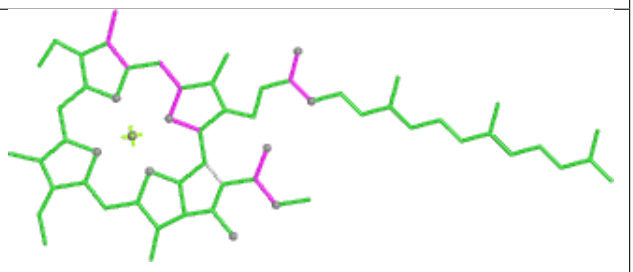


Rings

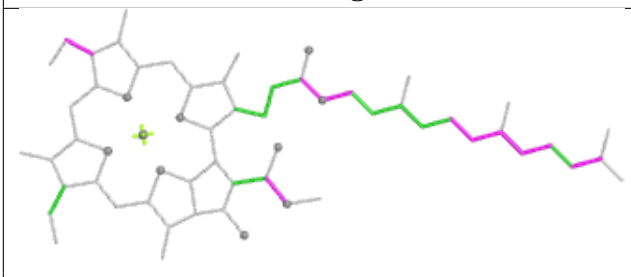
Ligand CLA u 305



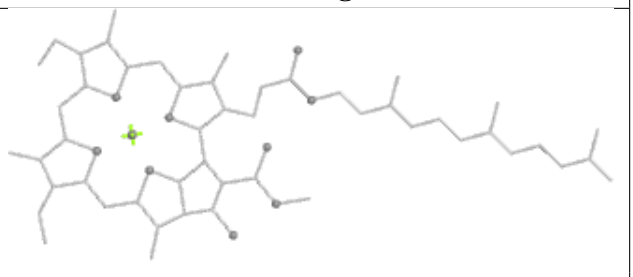
Bond lengths



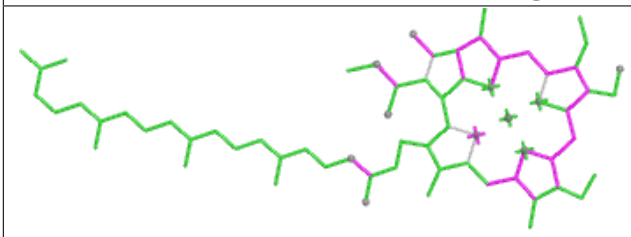
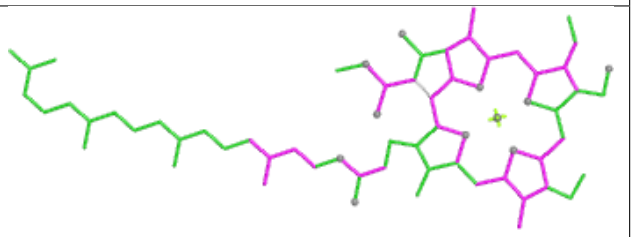
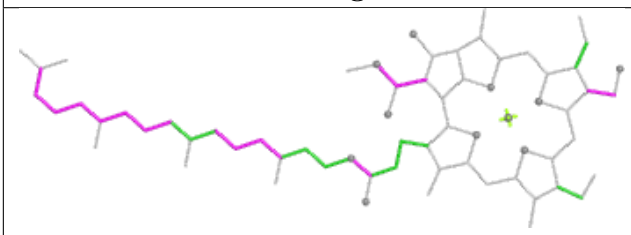
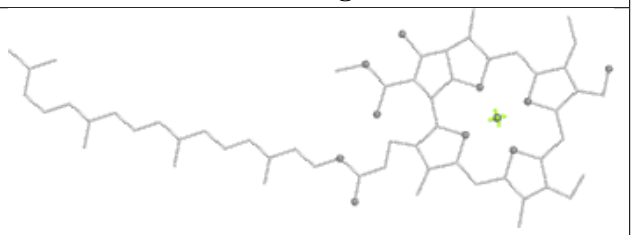
Bond angles

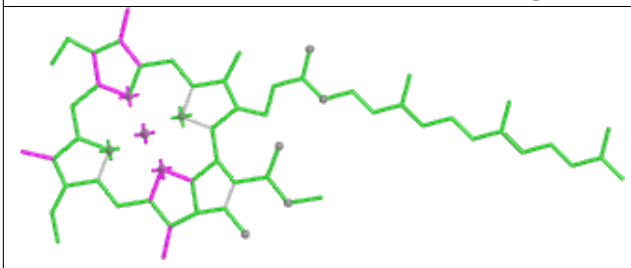
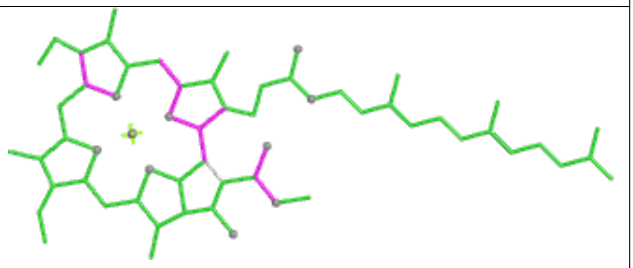
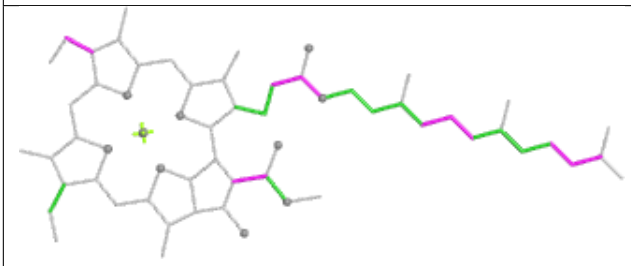
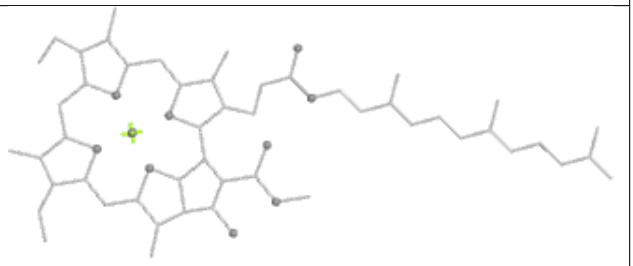


Torsions

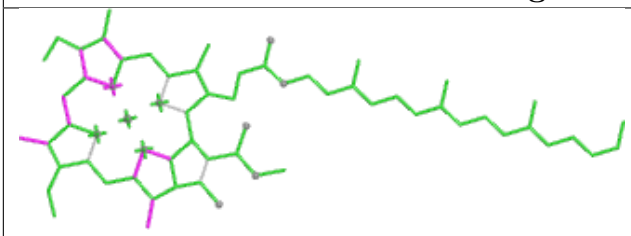


Rings

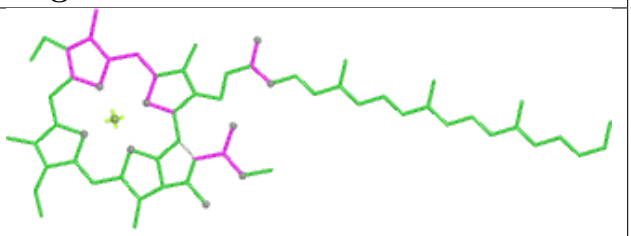
Ligand CHL 5 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA u 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

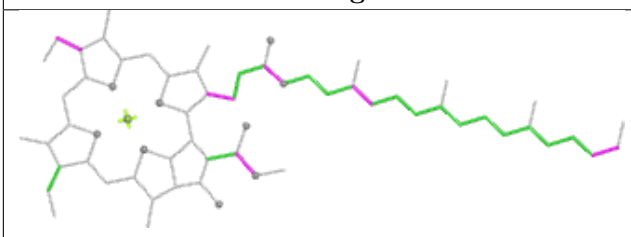
Ligand CLA g 304



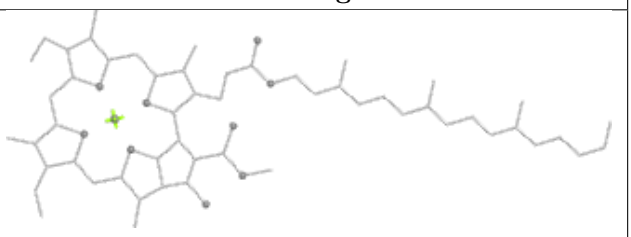
Bond lengths



Bond angles

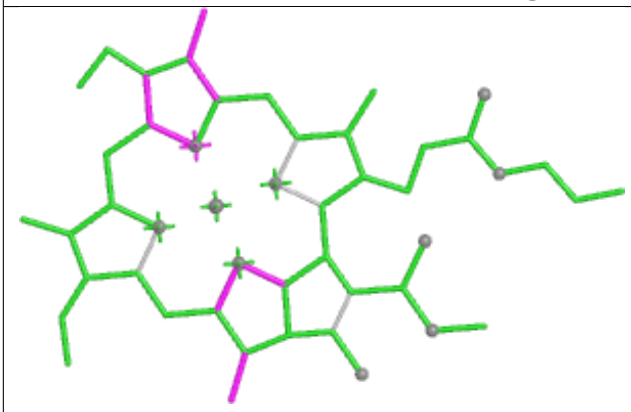


Torsions

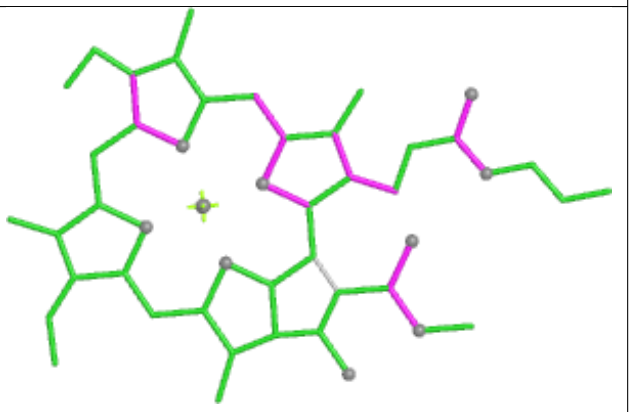


Rings

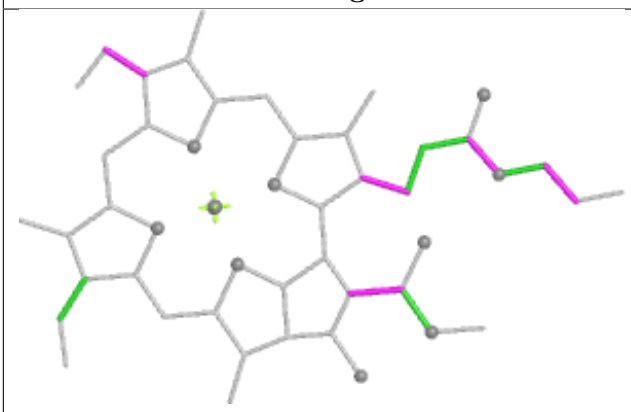
Ligand CLA R 305



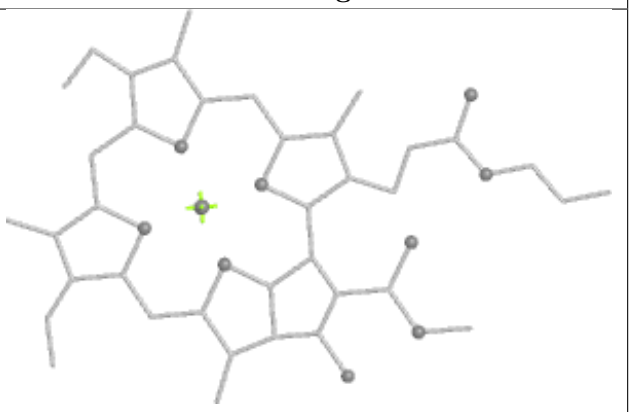
Bond lengths



Bond angles

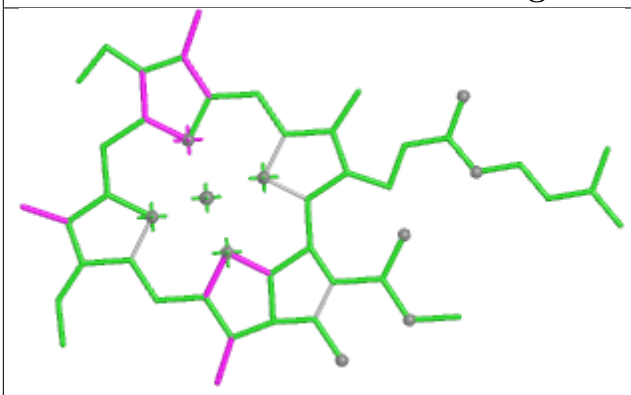


Torsions

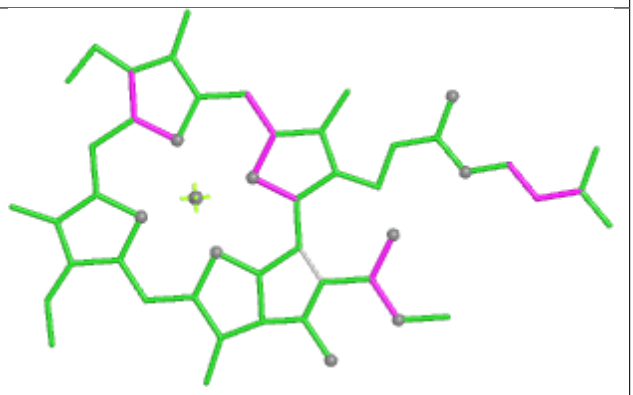


Rings

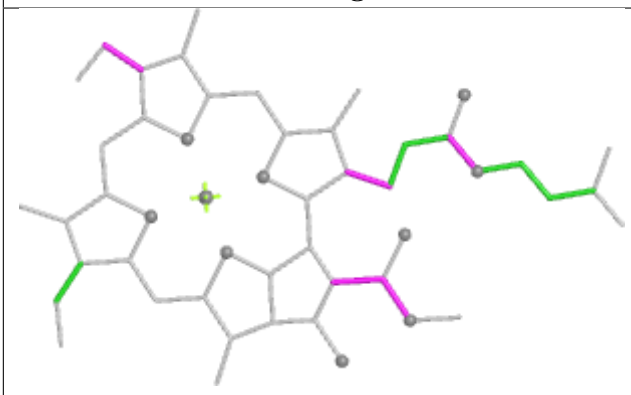
Ligand CLA 2 303



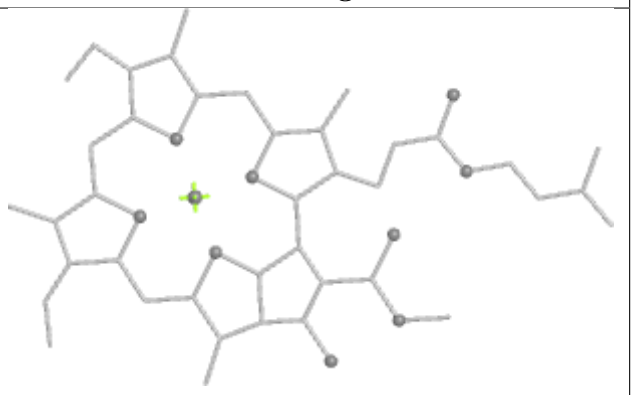
Bond lengths



Bond angles

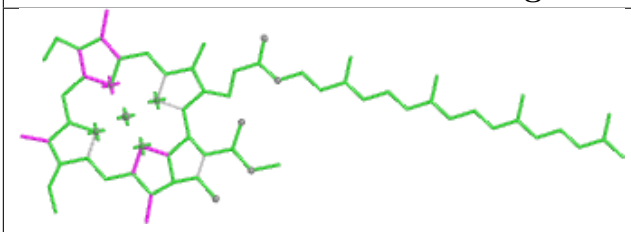


Torsions

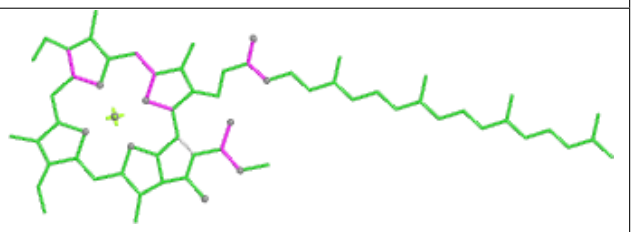


Rings

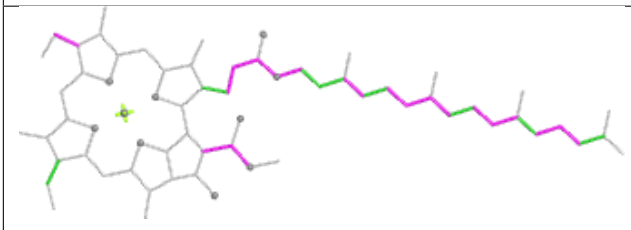
Ligand CLA C 512



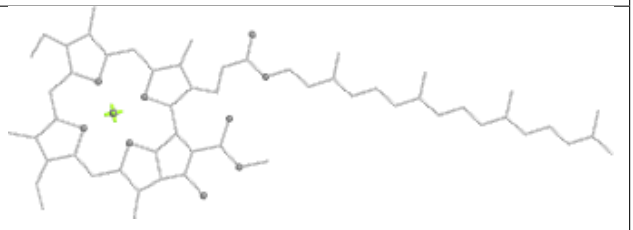
Bond lengths



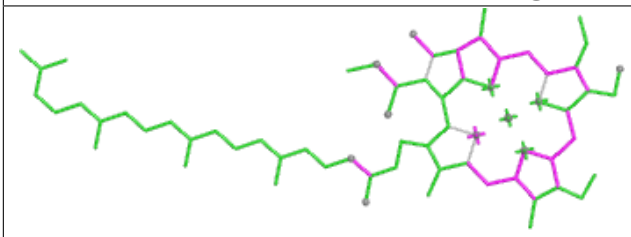
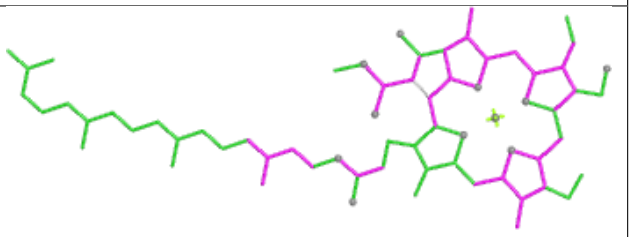
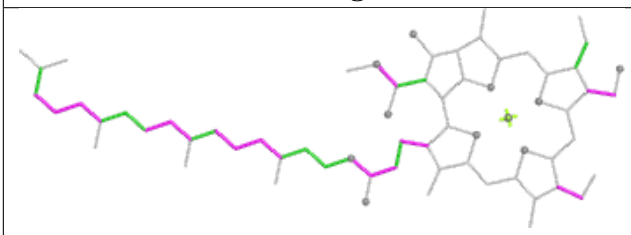
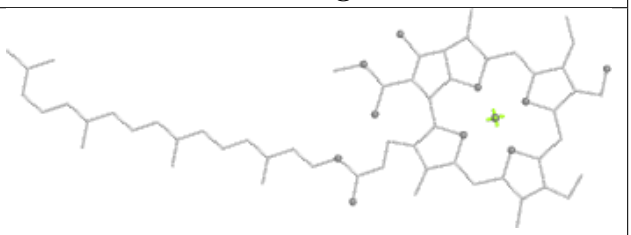
Bond angles

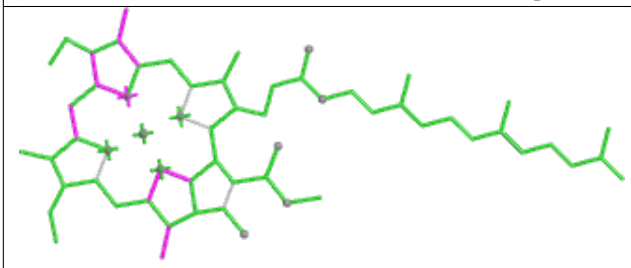
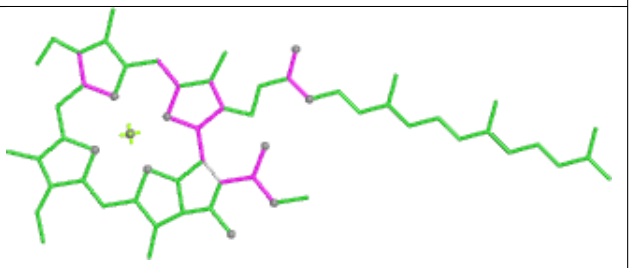
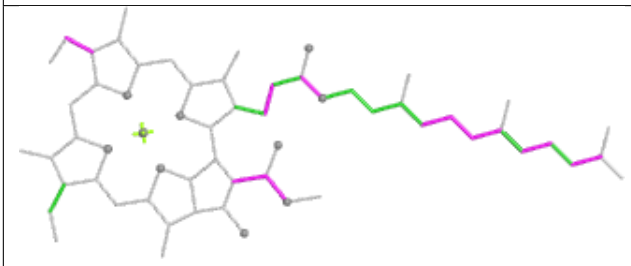
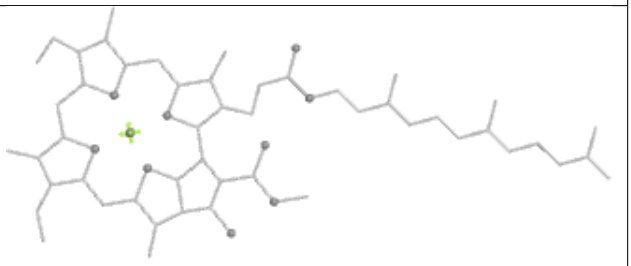


Torsions

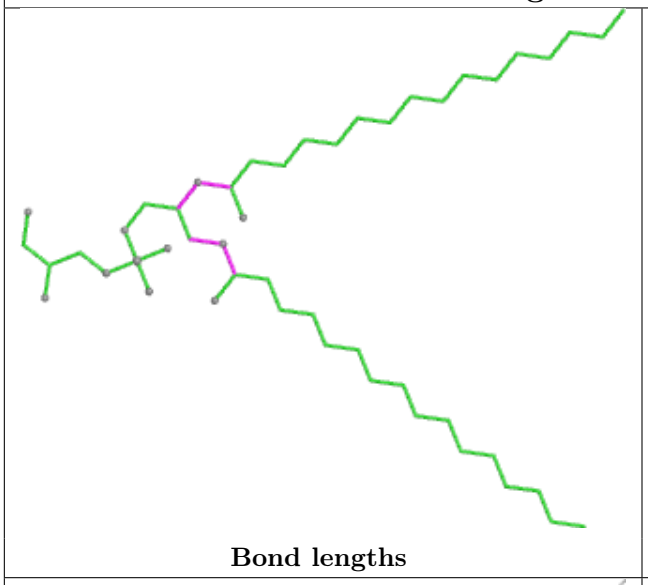


Rings

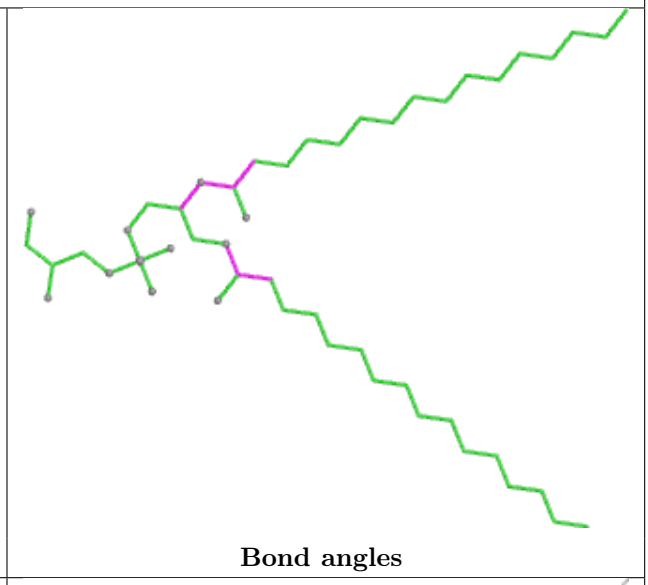
Ligand CHL 1 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

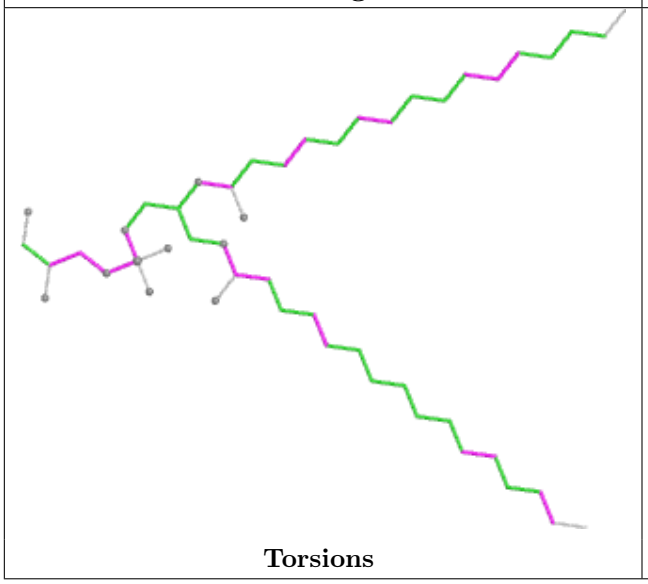
Ligand LHG S 312



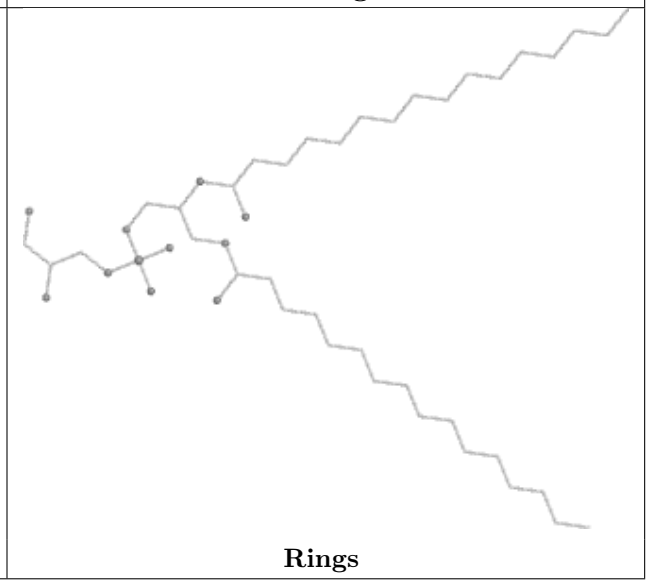
Bond lengths



Bond angles

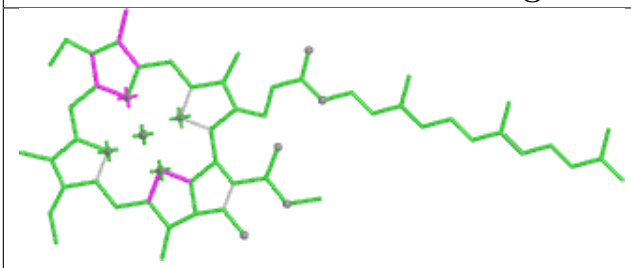


Torsions

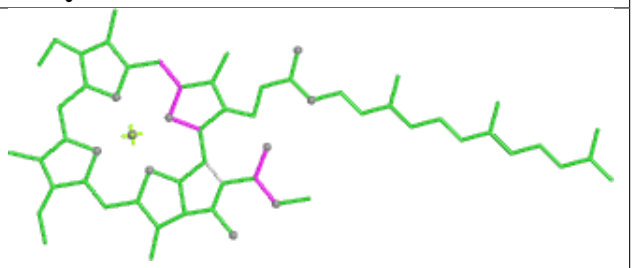


Rings

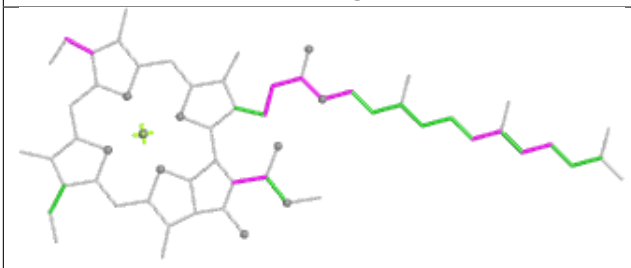
Ligand CLA Q 306



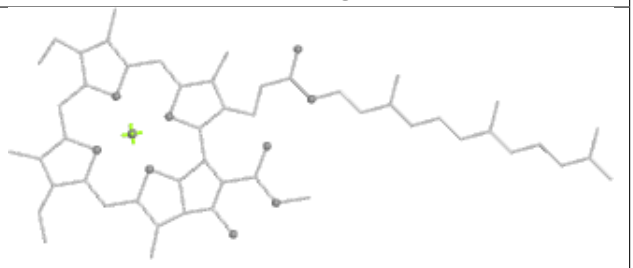
Bond lengths



Bond angles

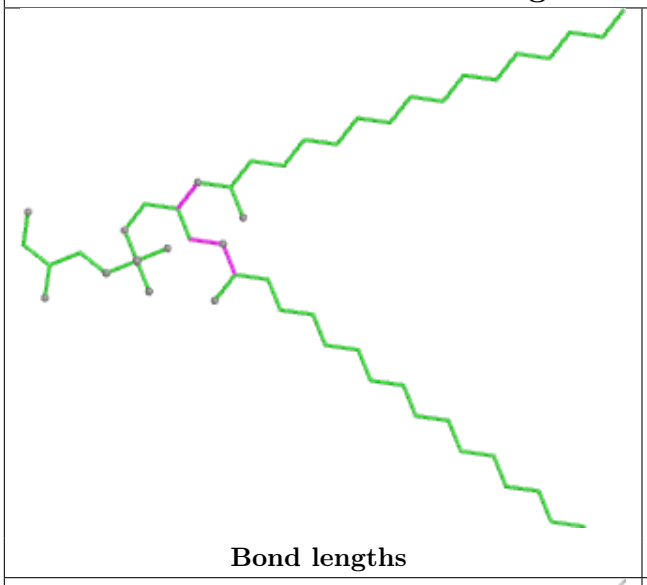


Torsions

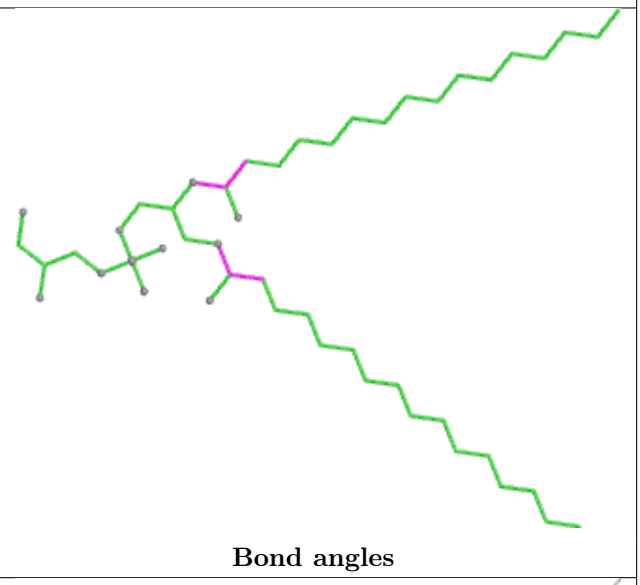


Rings

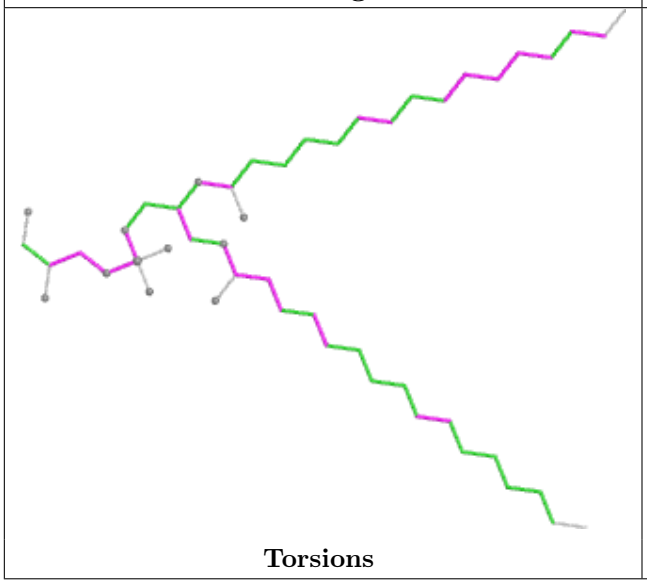
Ligand LHG c 522



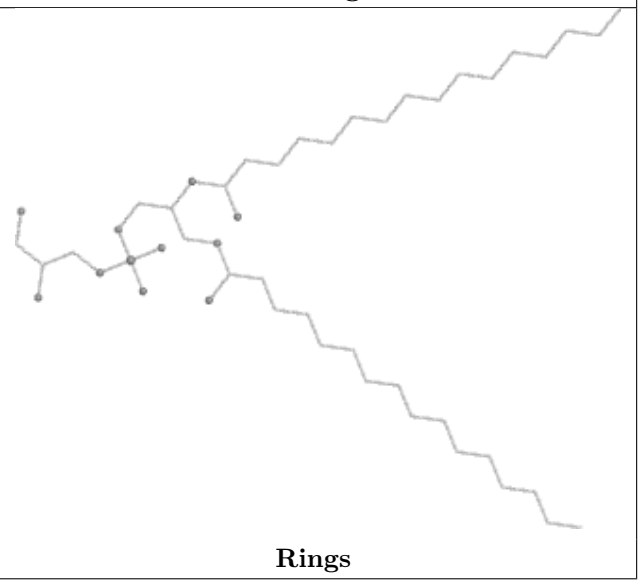
Bond lengths



Bond angles

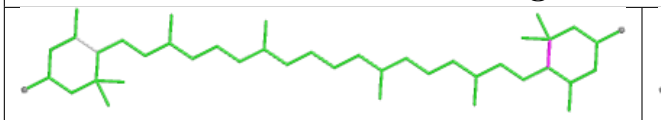


Torsions



Rings

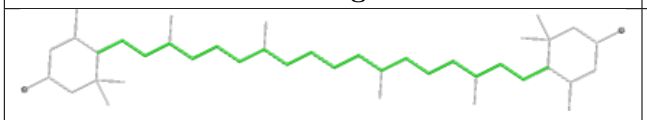
Ligand LUT 4 310



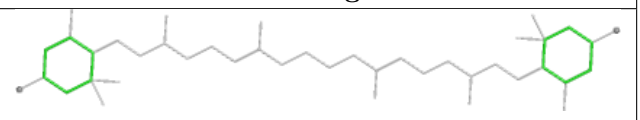
Bond lengths



Bond angles

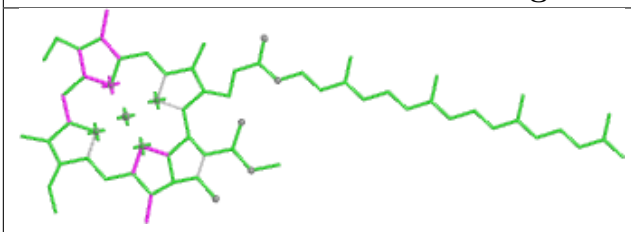


Torsions

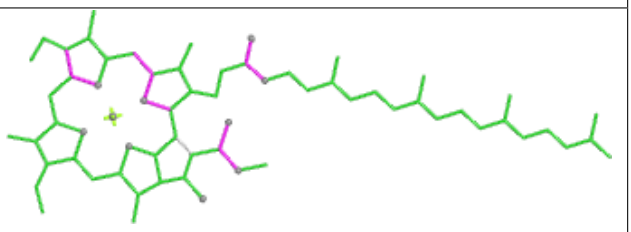


Rings

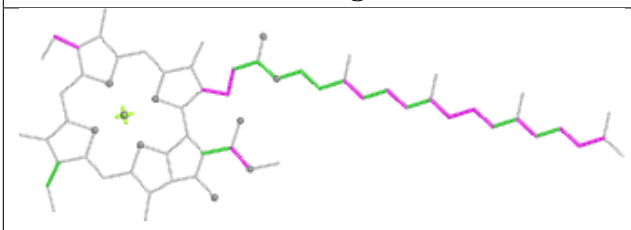
Ligand CLA r 606



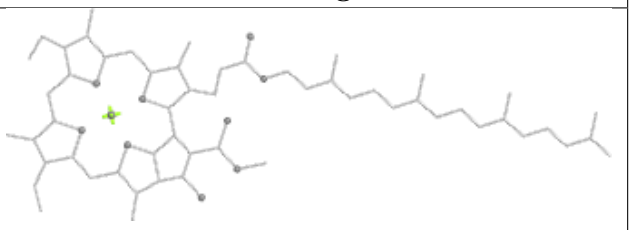
Bond lengths



Bond angles

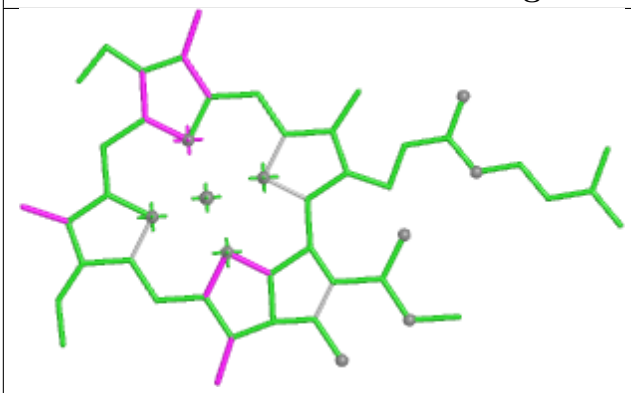


Torsions

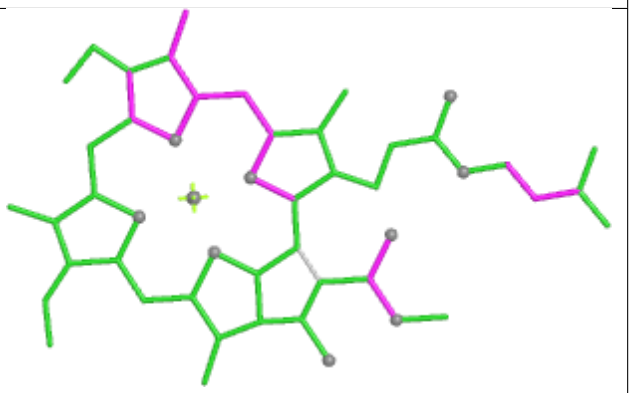


Rings

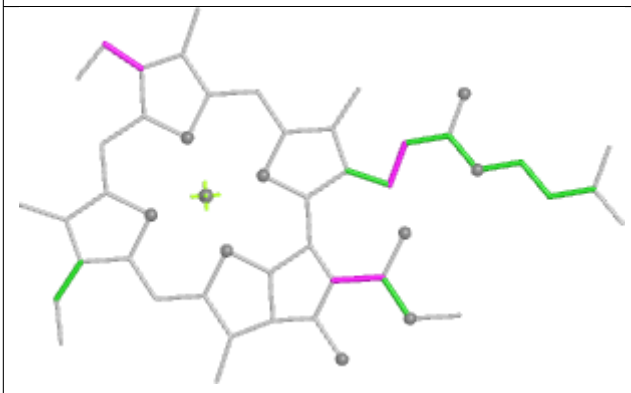
Ligand CLA N 303



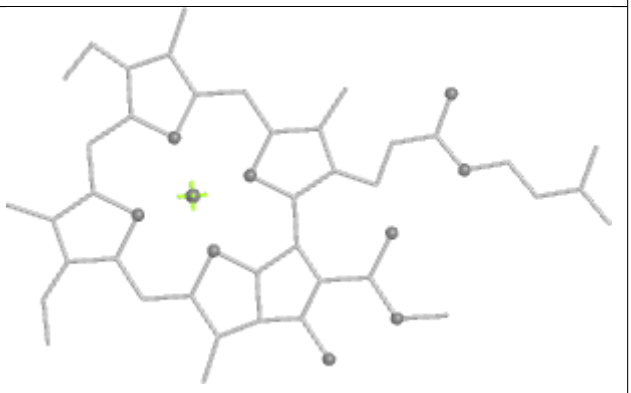
Bond lengths



Bond angles

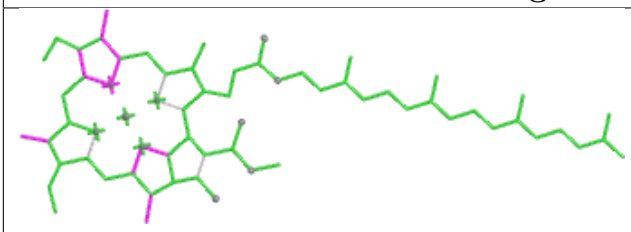


Torsions

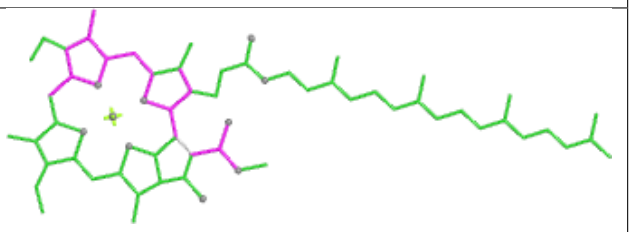


Rings

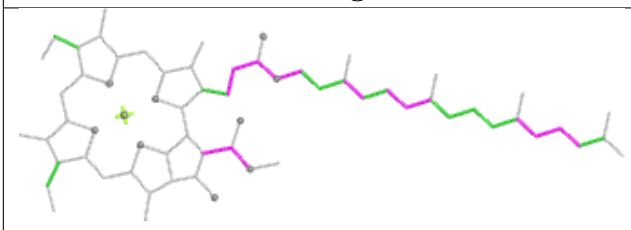
Ligand CLA c 506



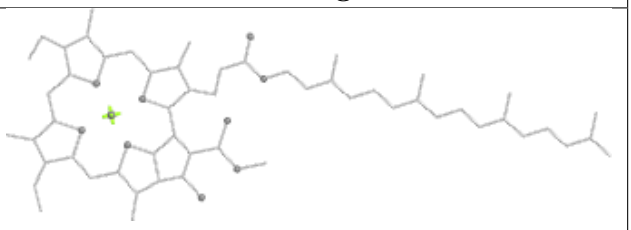
Bond lengths



Bond angles

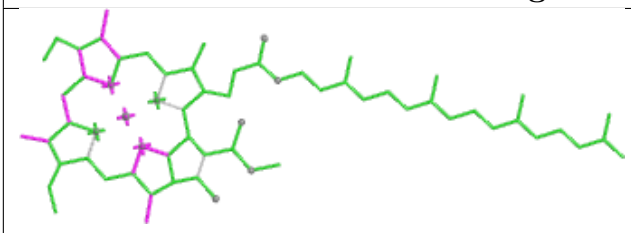


Torsions

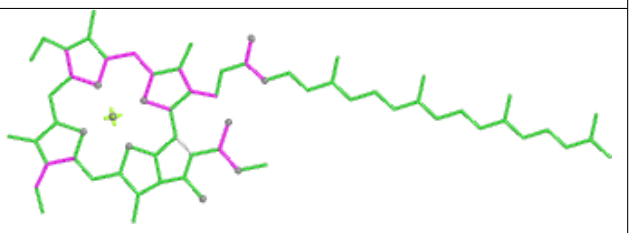


Rings

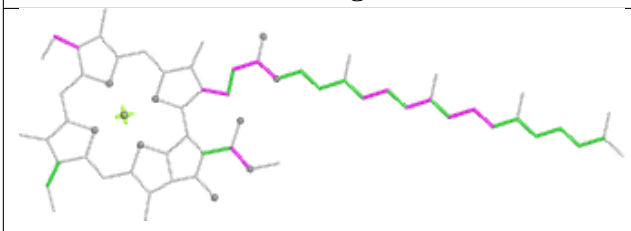
Ligand CLA 1 307



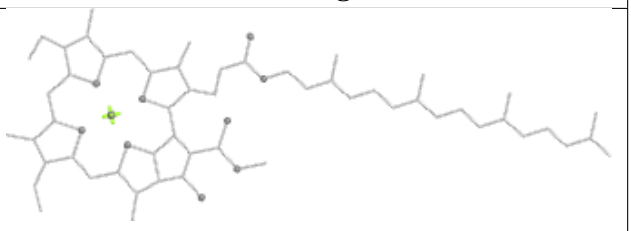
Bond lengths



Bond angles

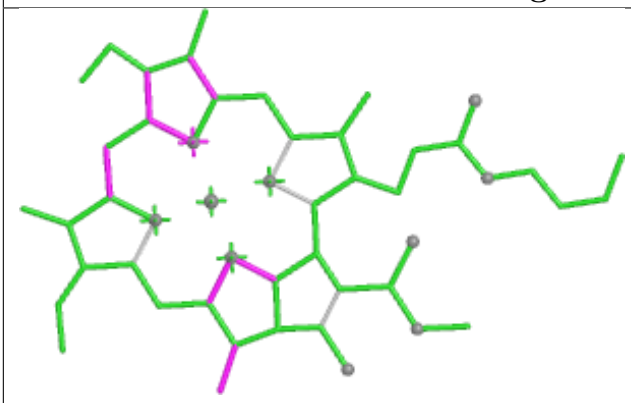


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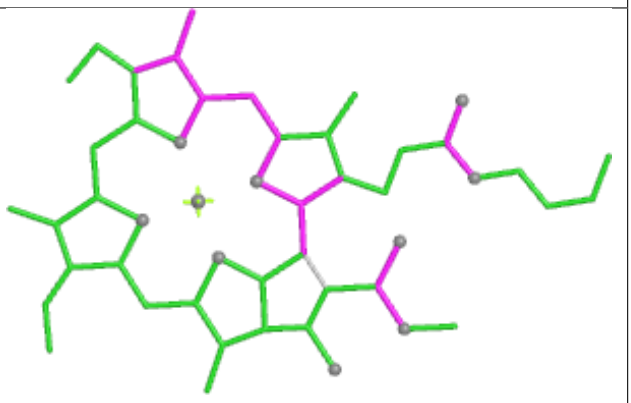


Rings

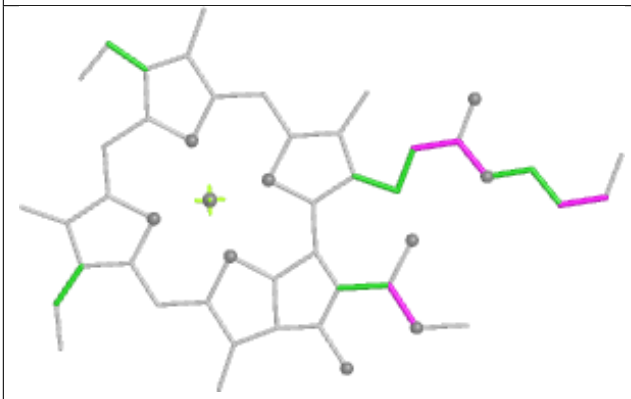
Ligand CLA r 608



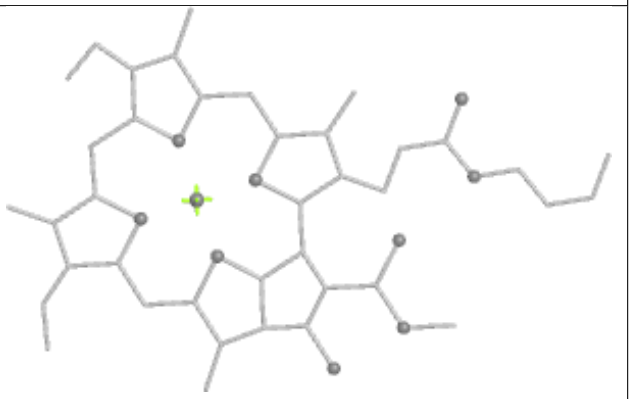
Bond lengths



Bond angles

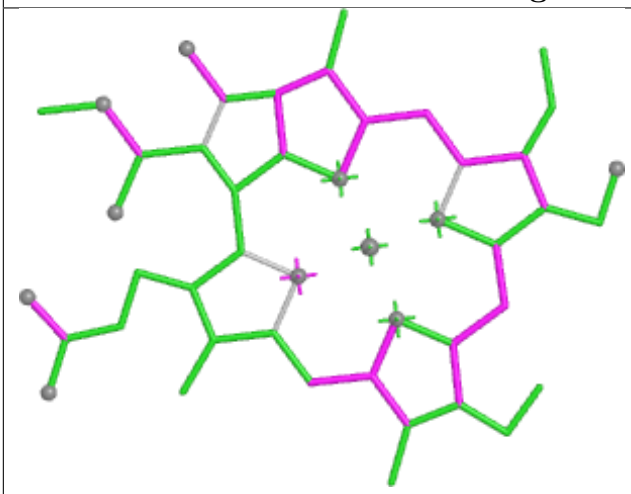


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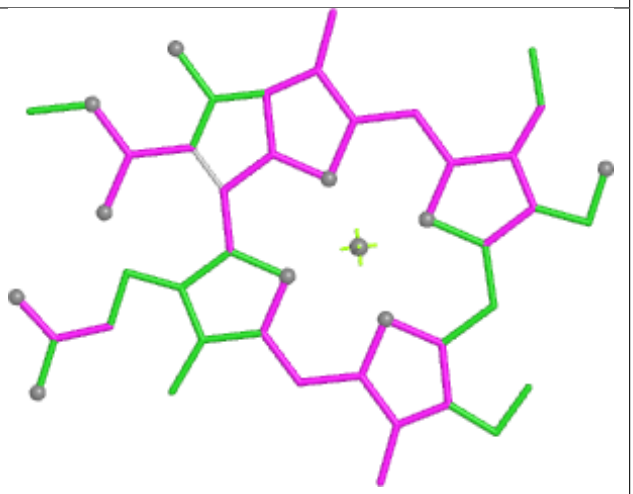


Rings

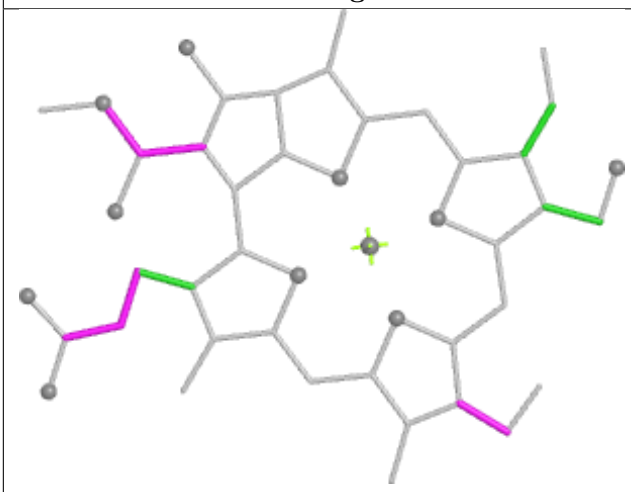
Ligand CHL s 314



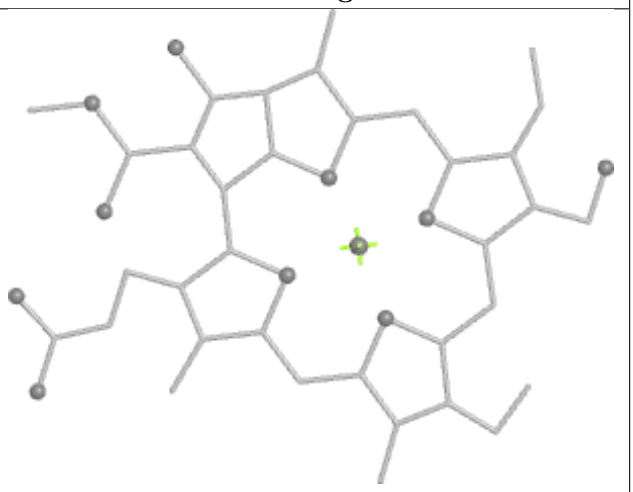
Bond lengths



Bond angles

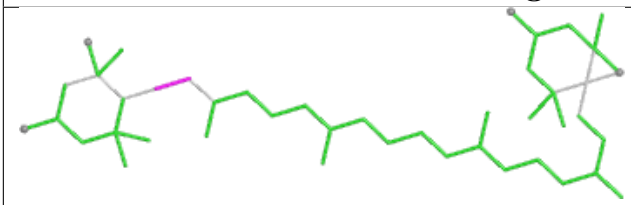


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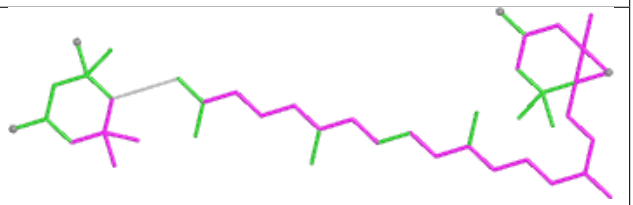


Rings

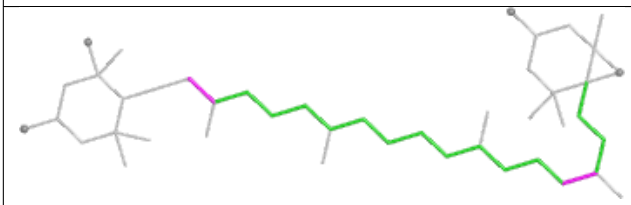
Ligand NEX S 317



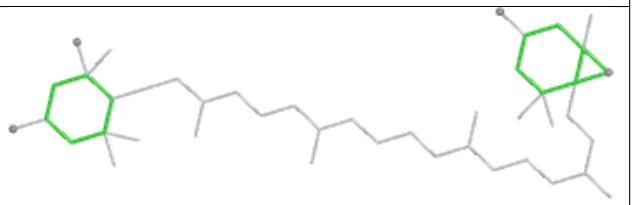
Bond lengths



Bond angles

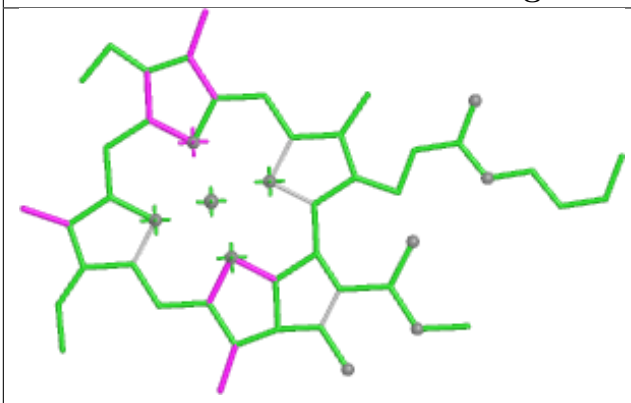


Torsions

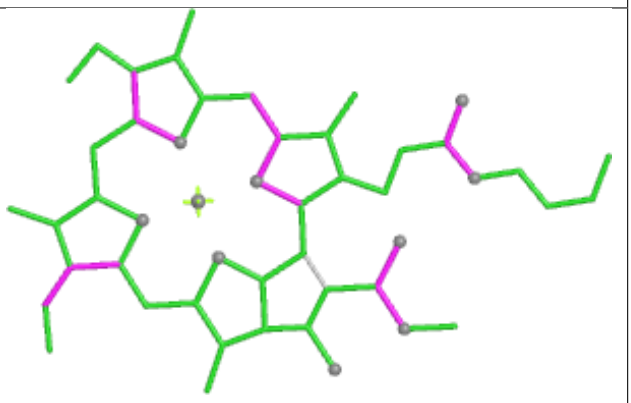


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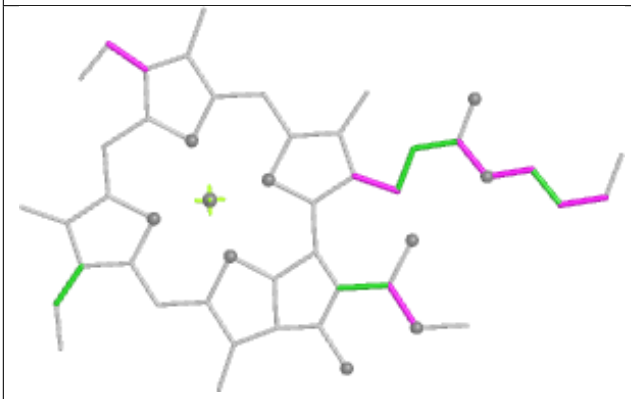
Ligand CLA R 302



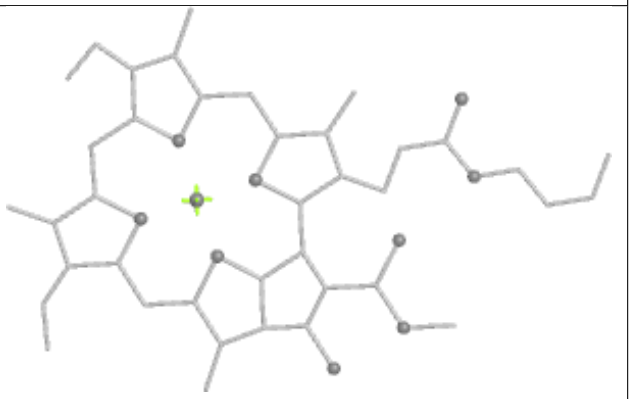
Bond lengths



Bond angles

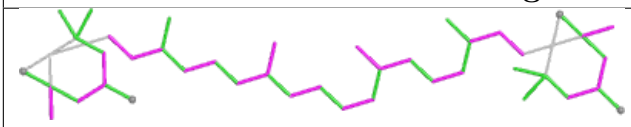


Torsions

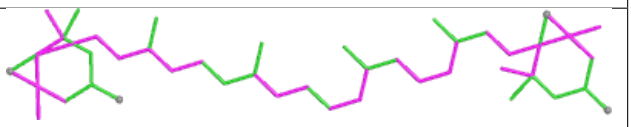


Rings

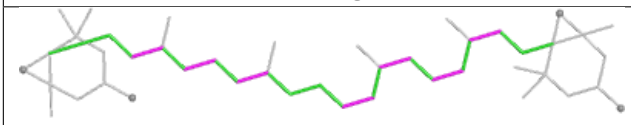
Ligand XAT V 311



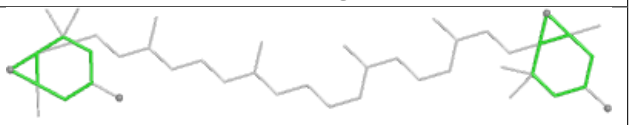
Bond lengths



Bond angles

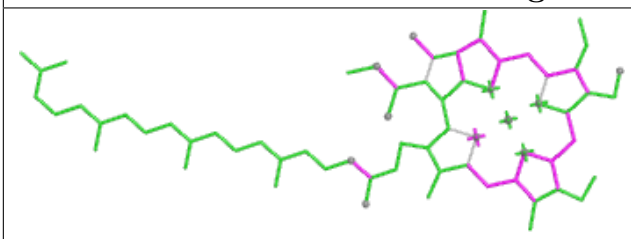


Torsions

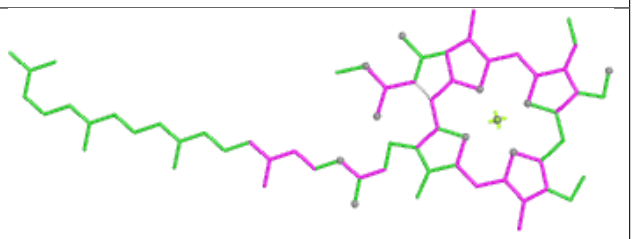


Rings

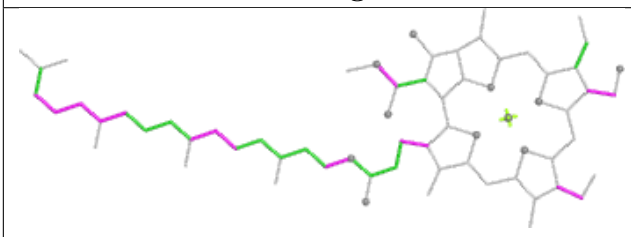
Ligand CHL 1 318



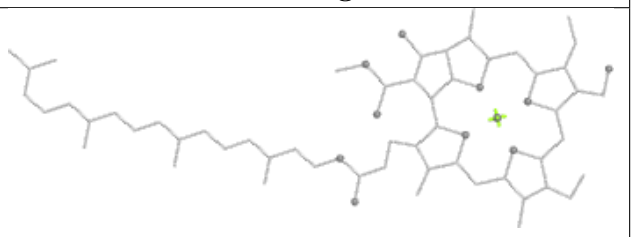
Bond lengths



Bond angles

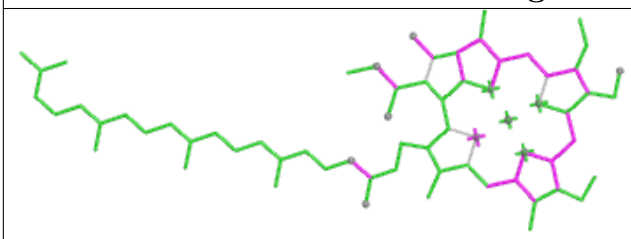


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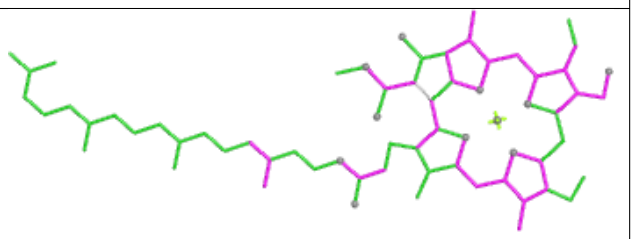


Rings

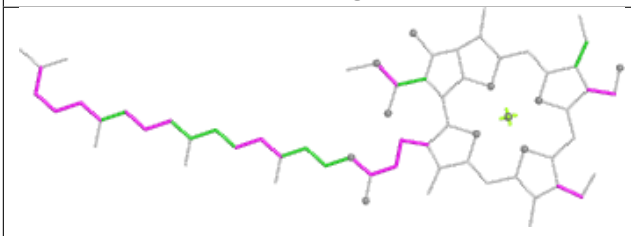
Ligand CHL 3 315



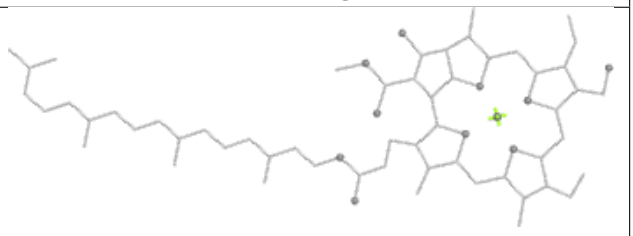
Bond lengths



Bond angles

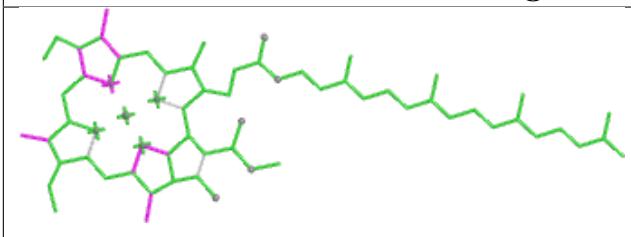


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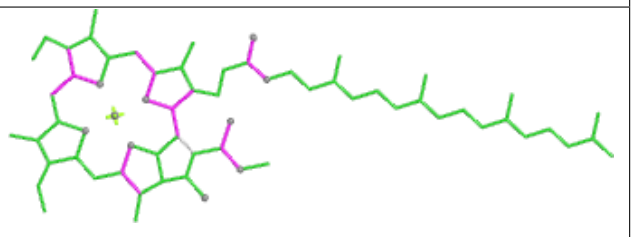


Rings

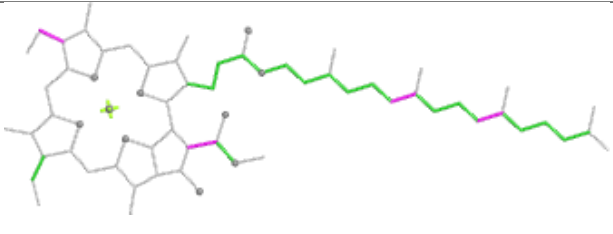
Ligand CLA B 616



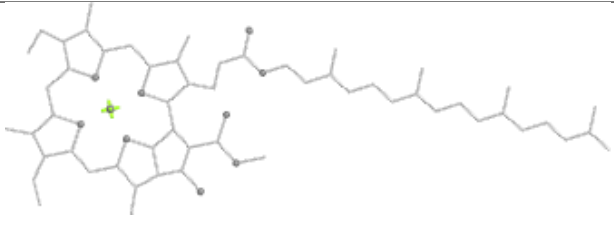
Bond lengths



Bond angles

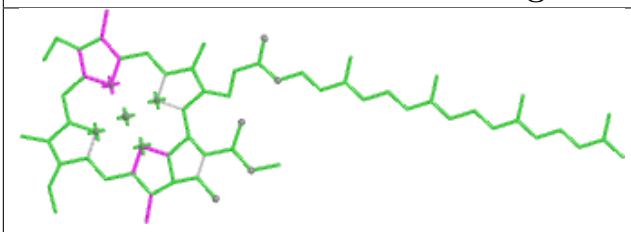


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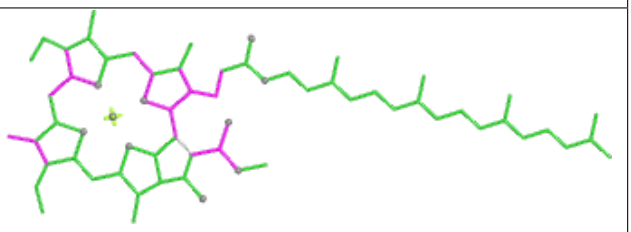


Rings

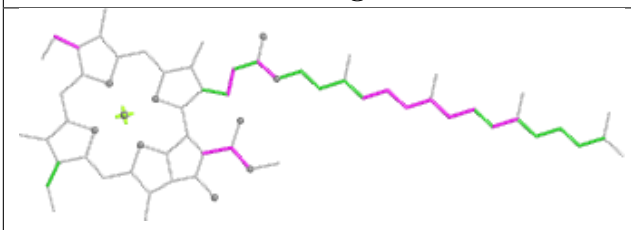
Ligand CLA b 605



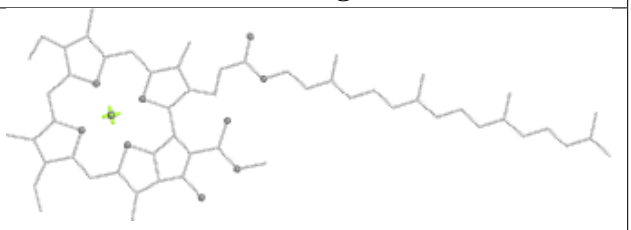
Bond lengths



Bond angles

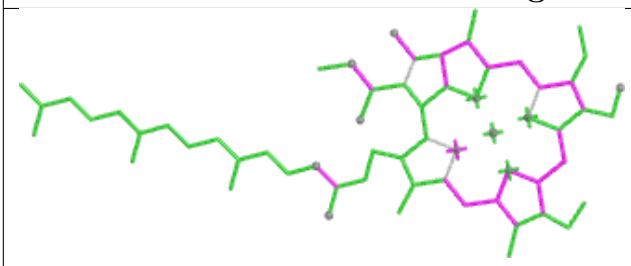


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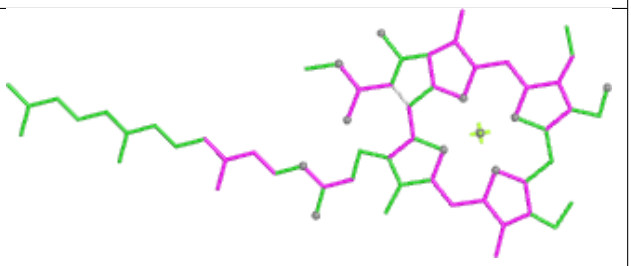


Rings

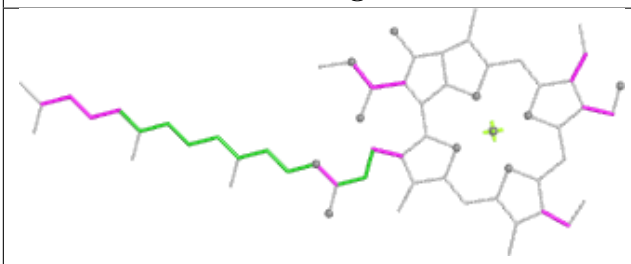
Ligand CHL 3 316



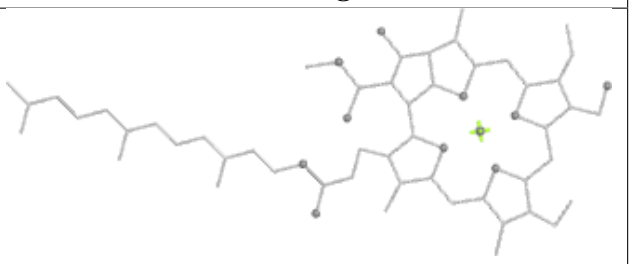
Bond lengths



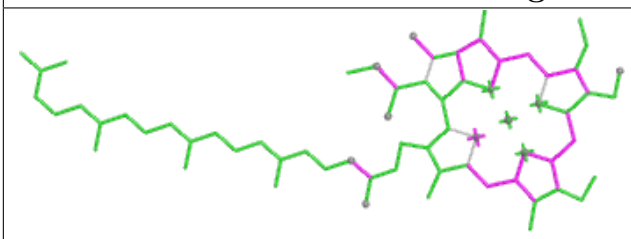
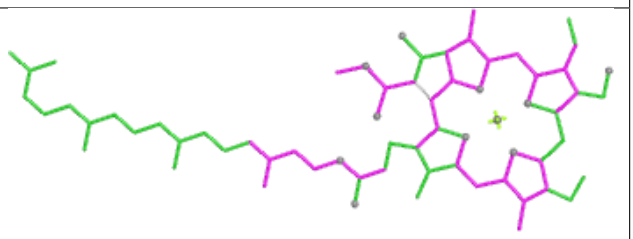
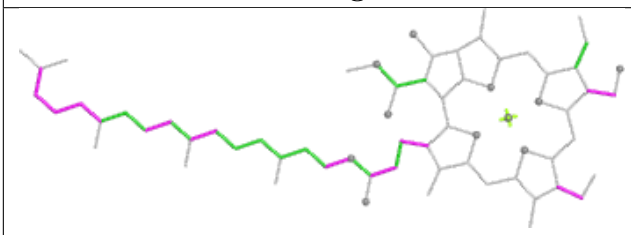
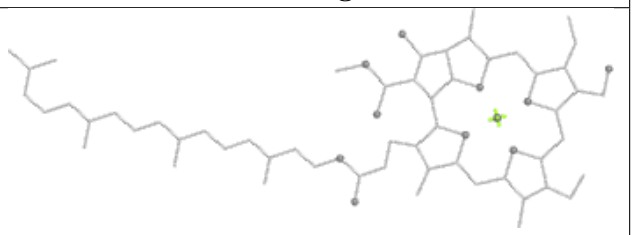
Bond angles

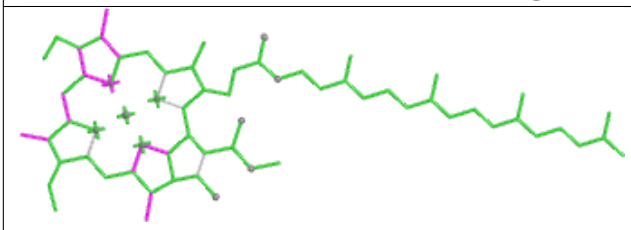
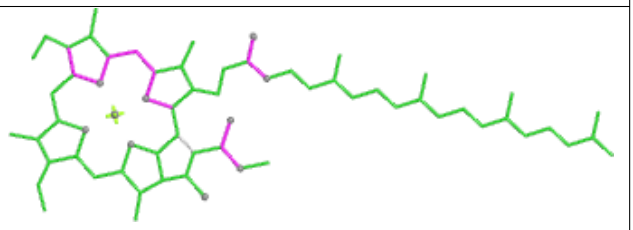
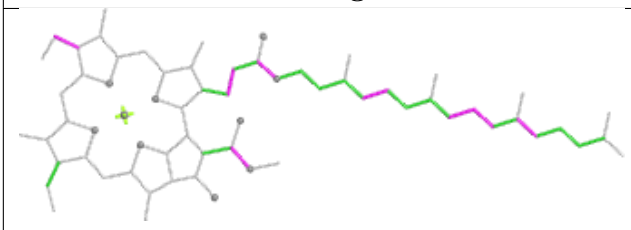
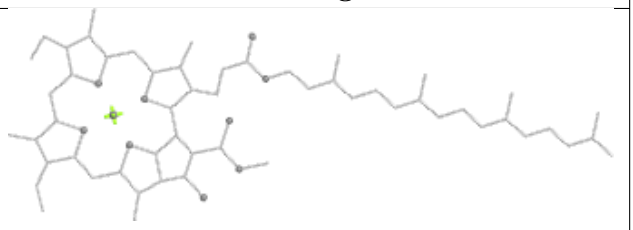


Torsions

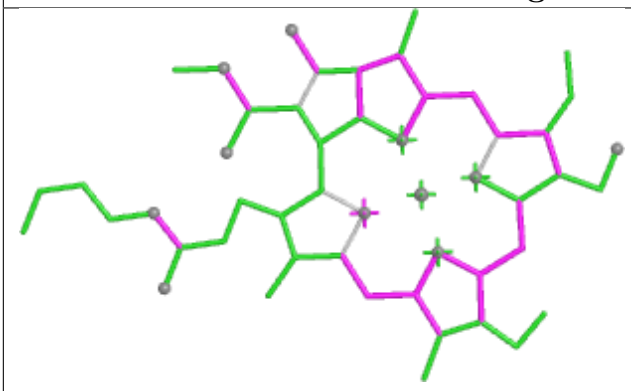


Rings

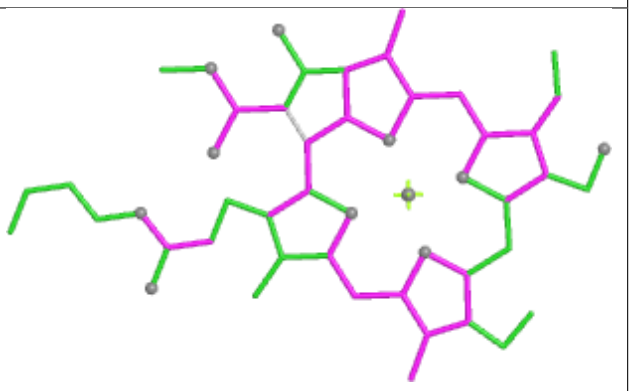
Ligand CHL 4 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA v 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

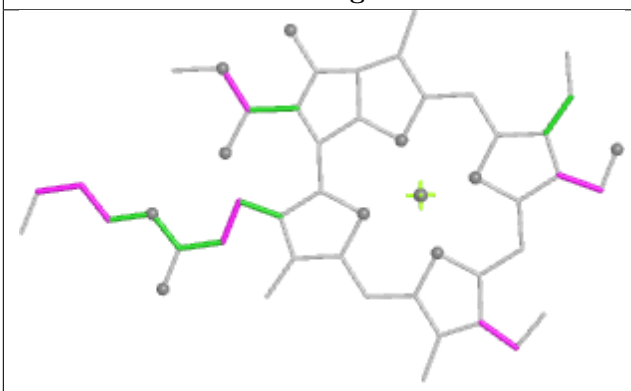
Ligand CHL 5 315



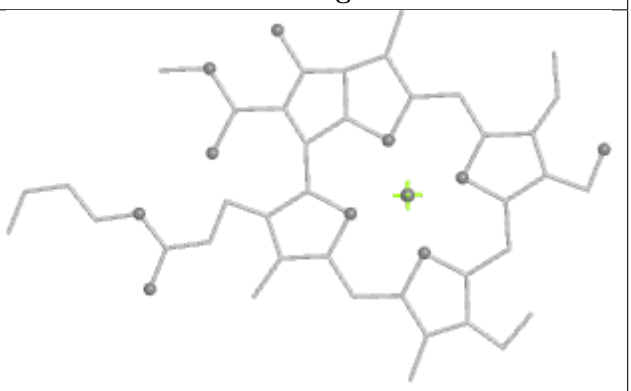
Bond lengths



Bond angles

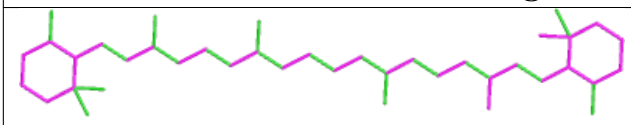


Torsions

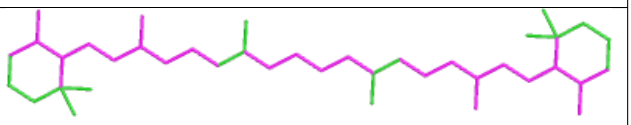


Rings

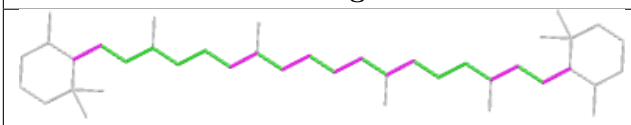
Ligand BCR B 620



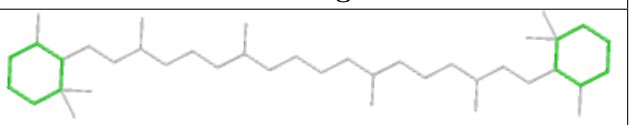
Bond lengths



Bond angles

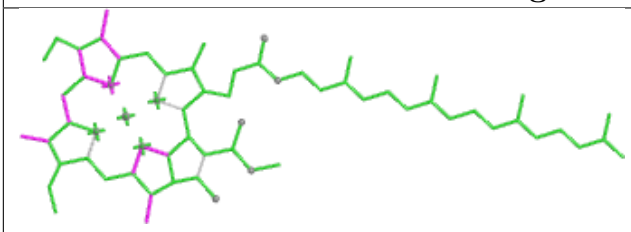


Torsions

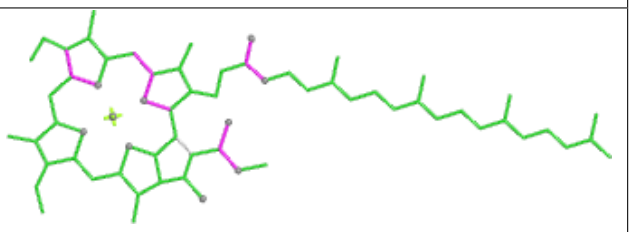


Rings

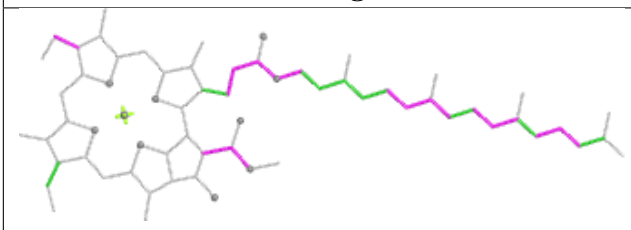
Ligand CLA c 511



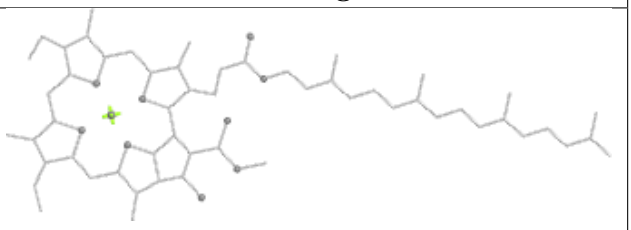
Bond lengths



Bond angles

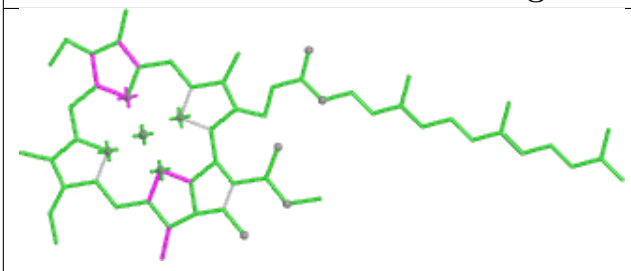


Torsions

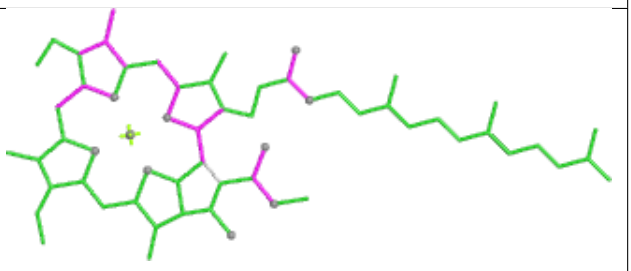


Rings

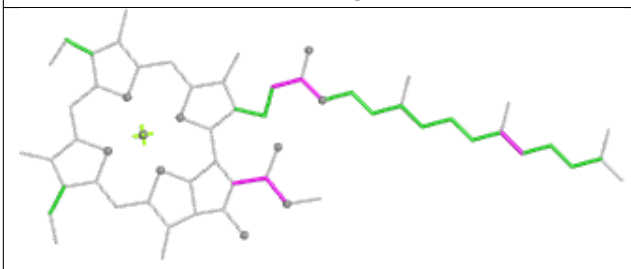
Ligand CLA n 306



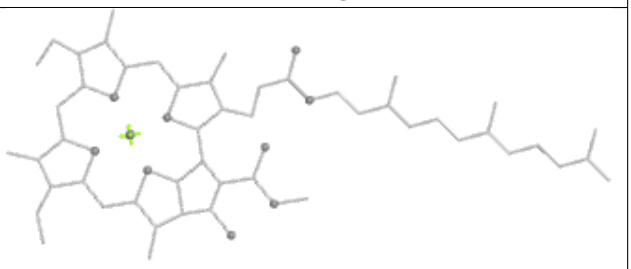
Bond lengths



Bond angles

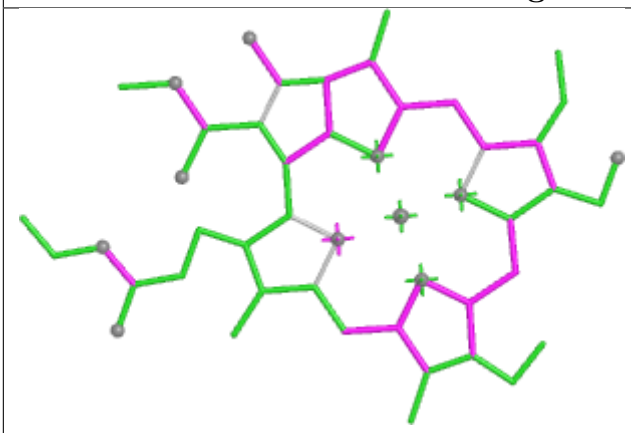


Torsions

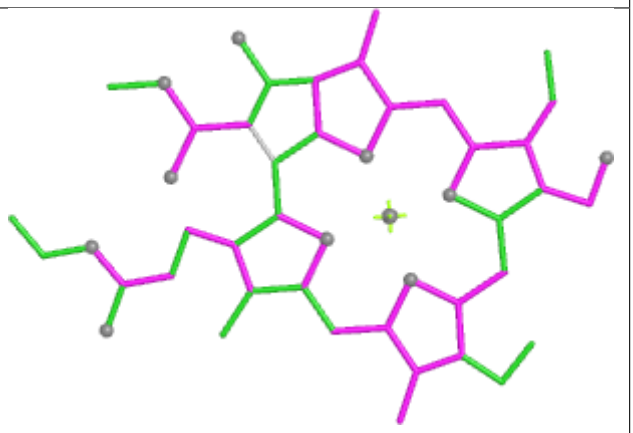


Rings

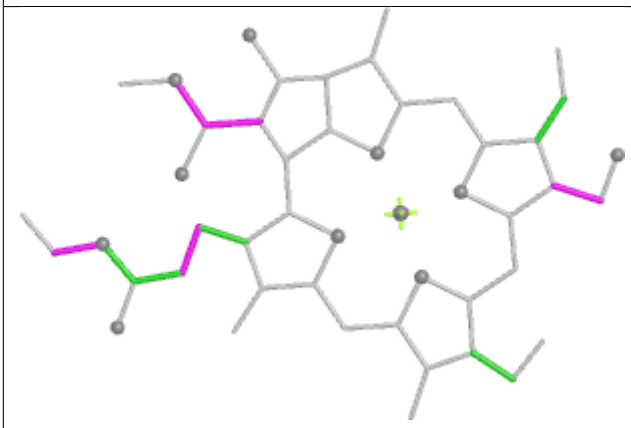
Ligand CHL 2 314



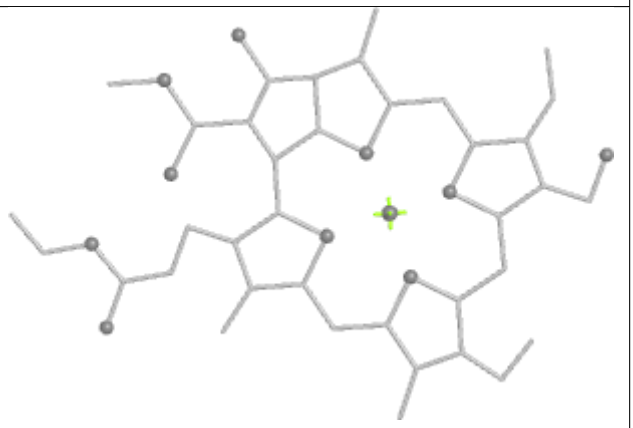
Bond lengths



Bond angles

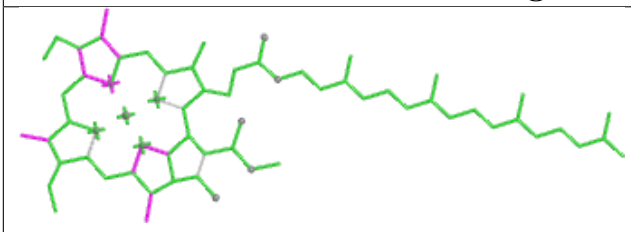


Torsions

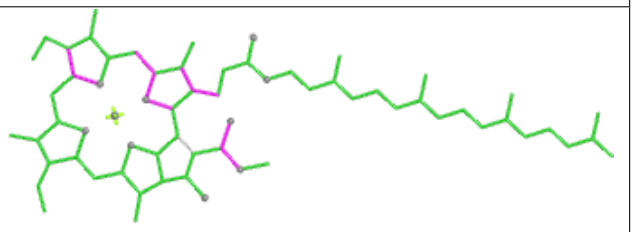


Rings

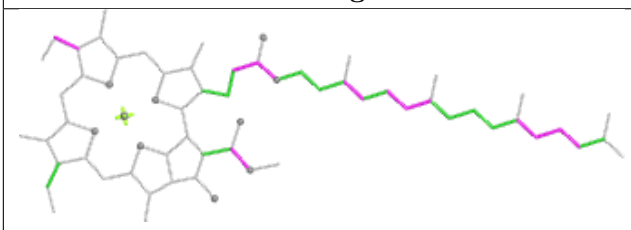
Ligand CLA u 302



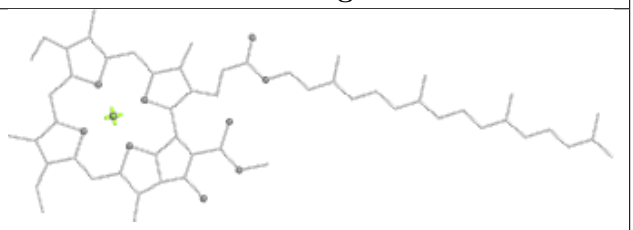
Bond lengths



Bond angles

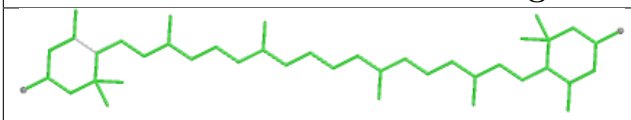


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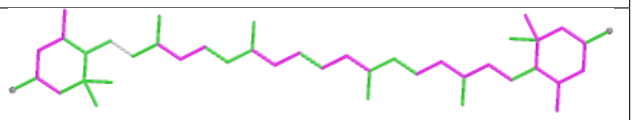


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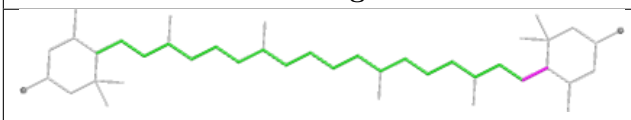
Ligand LUT 2 310



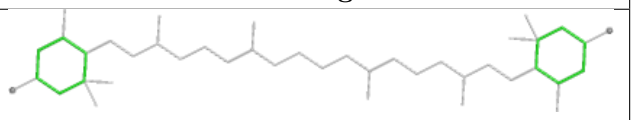
Bond lengths



Bond angles

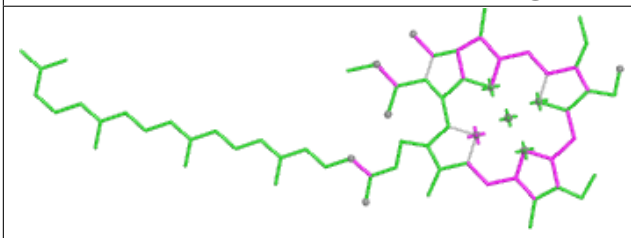


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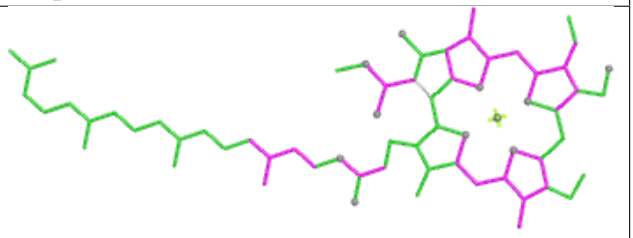


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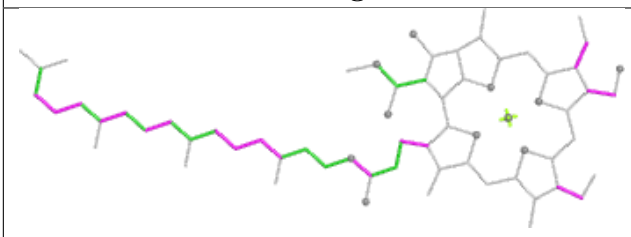
Ligand CHL p 319



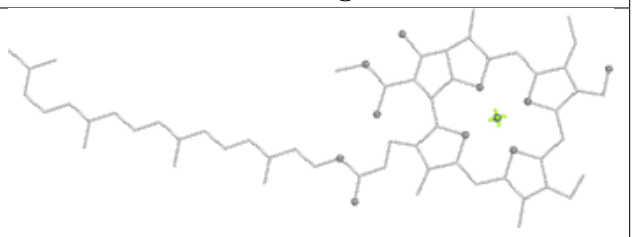
Bond lengths



Bond angles

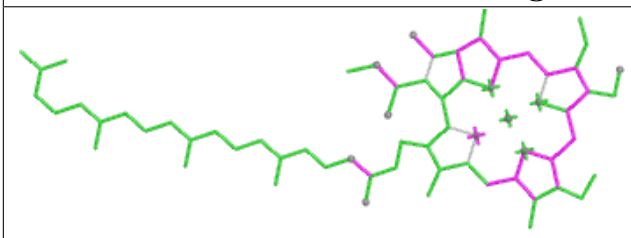


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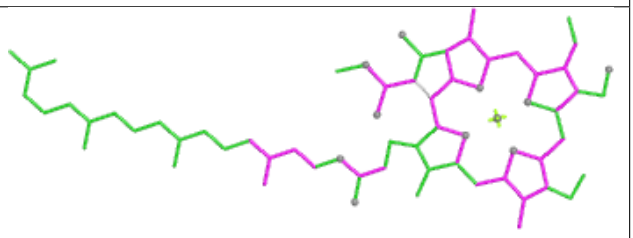


Rings

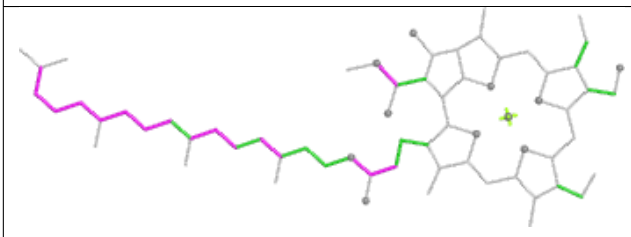
Ligand CHL 2 313



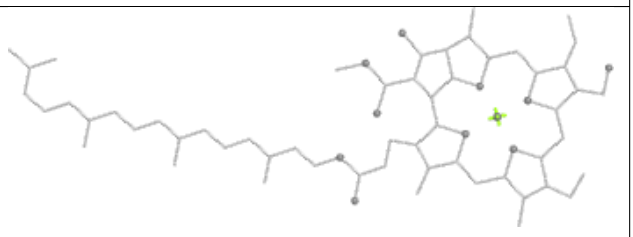
Bond lengths



Bond angles

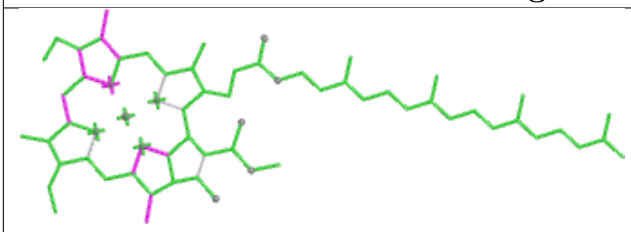


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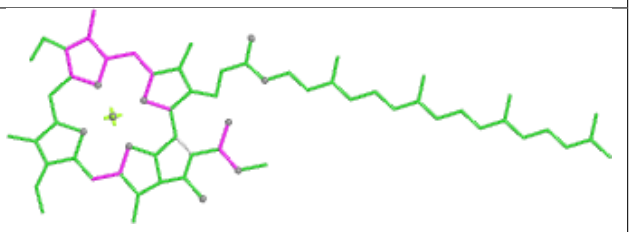


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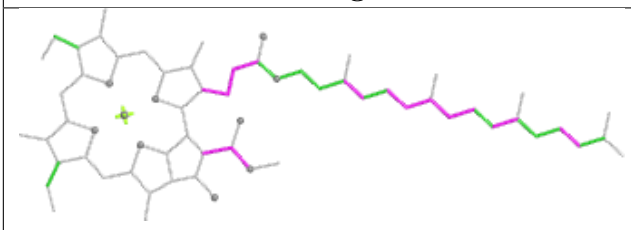
Ligand CLA 6 302



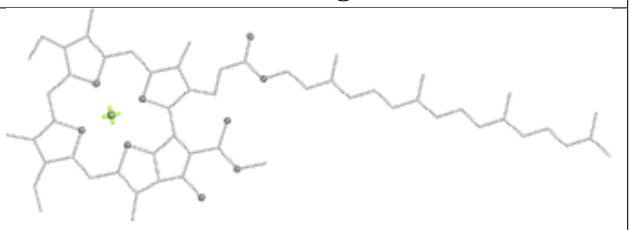
Bond lengths



Bond angles

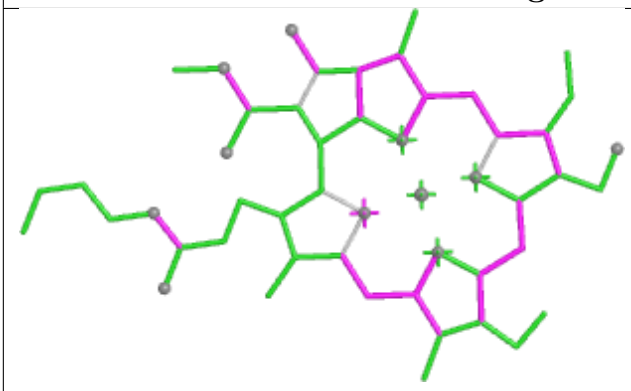


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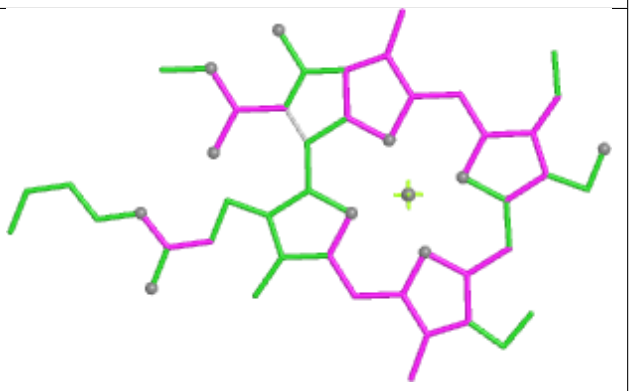


Rings

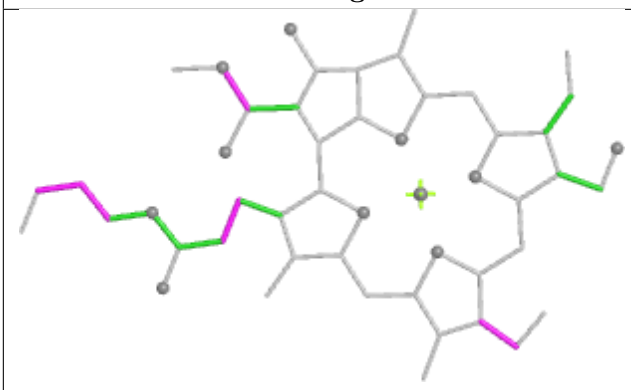
Ligand CHL 2 315



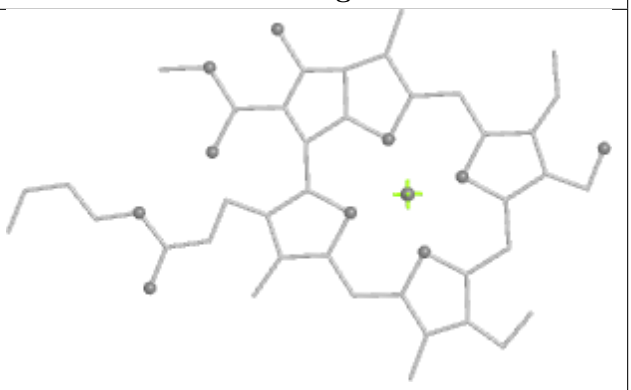
Bond lengths



Bond angles

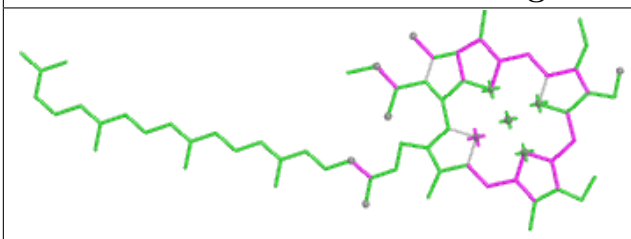


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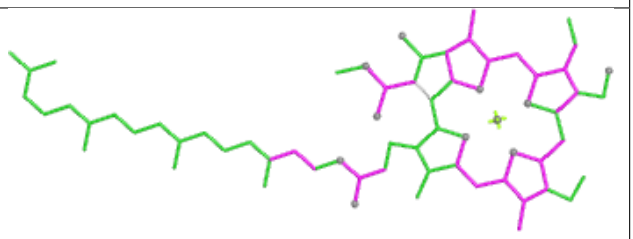


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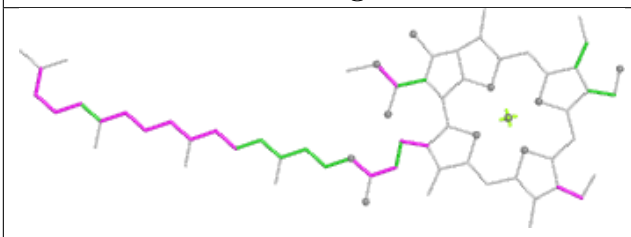
Ligand CHL 4 313



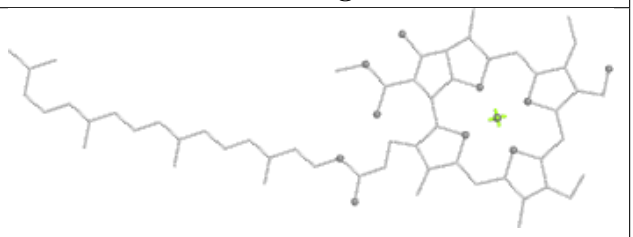
Bond lengths



Bond angles

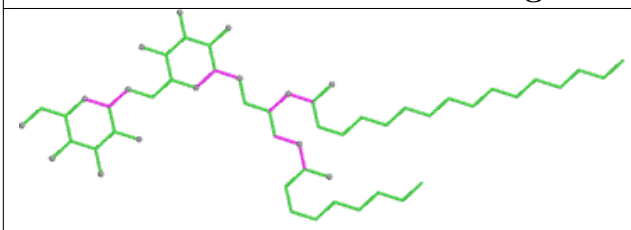


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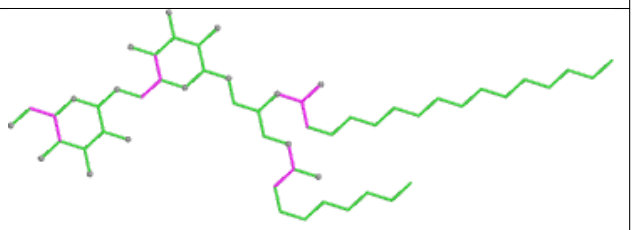


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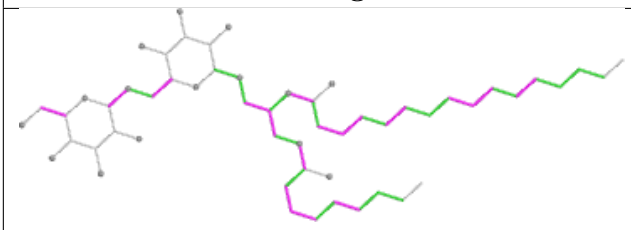
Ligand DGD c 517



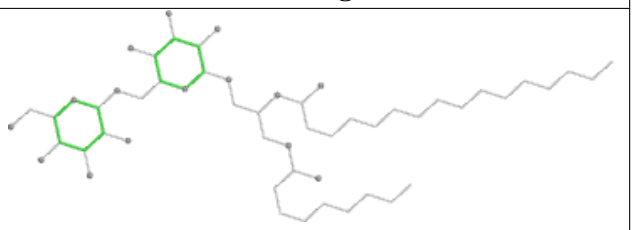
Bond lengths



Bond angles

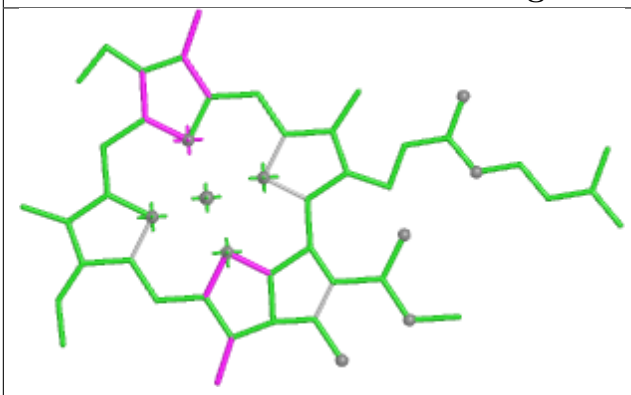


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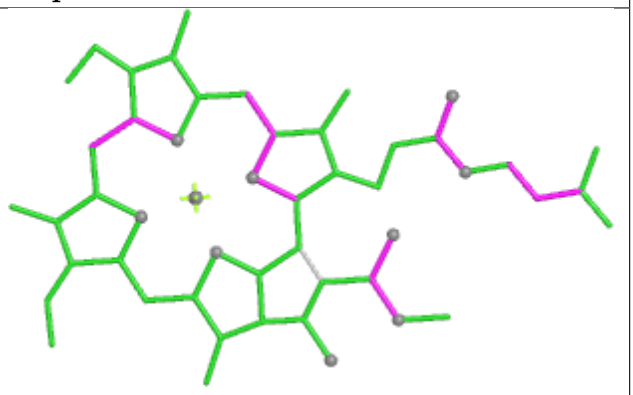


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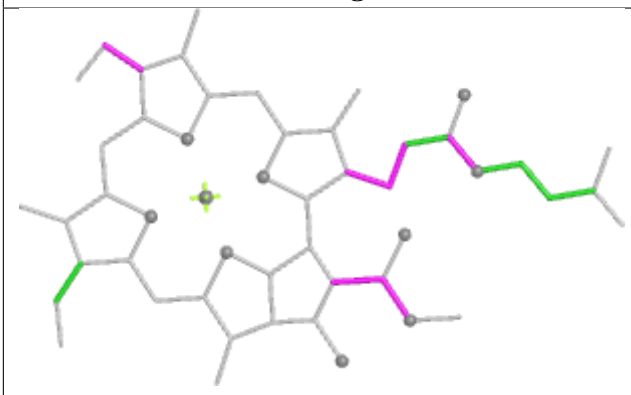
Ligand CLA p 304



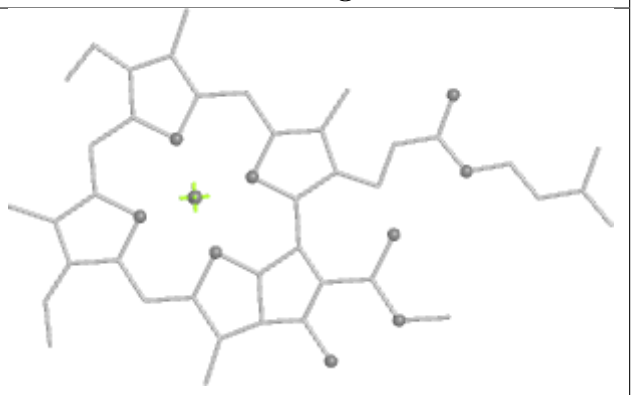
Bond lengths



Bond angles

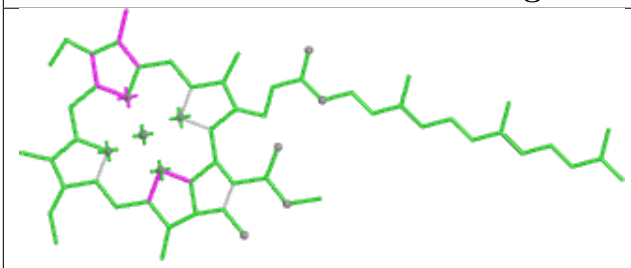


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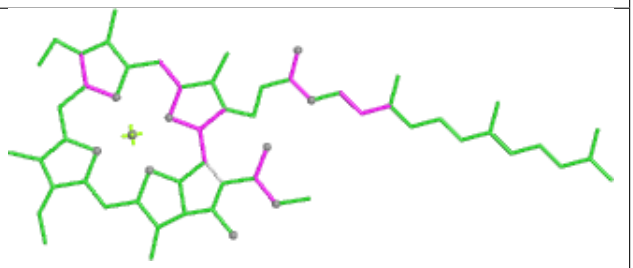


Rings

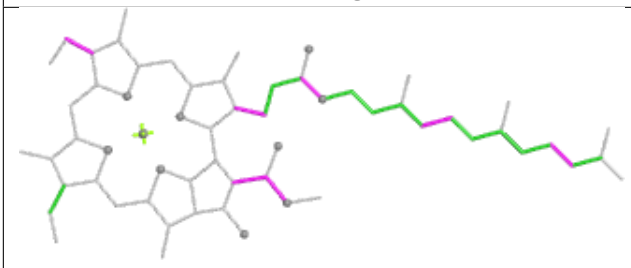
Ligand CLA R 310



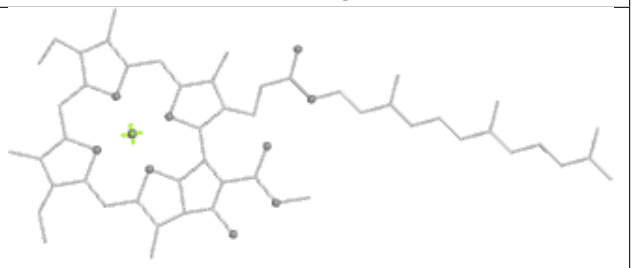
Bond lengths



Bond angles

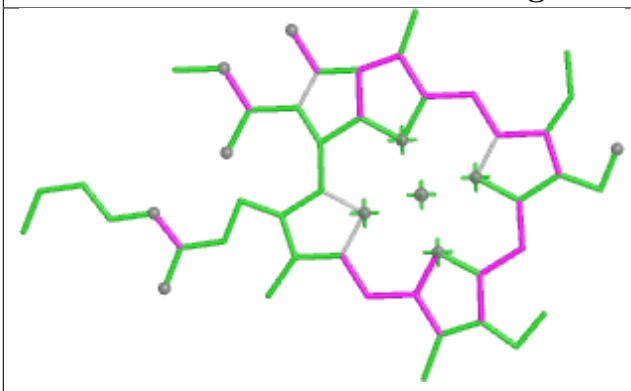


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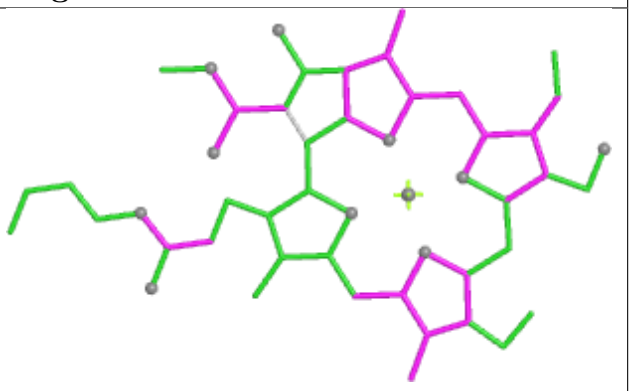


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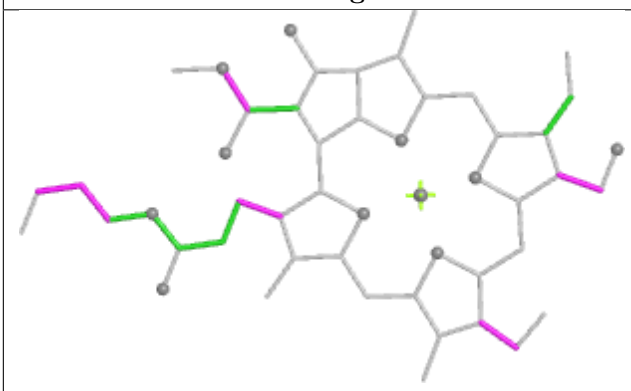
Ligand CHL g 313



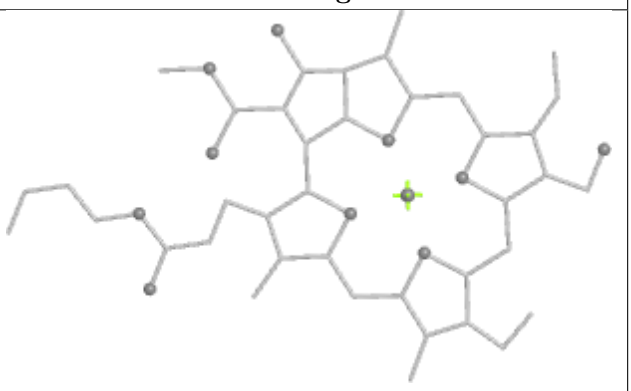
Bond lengths



Bond angles

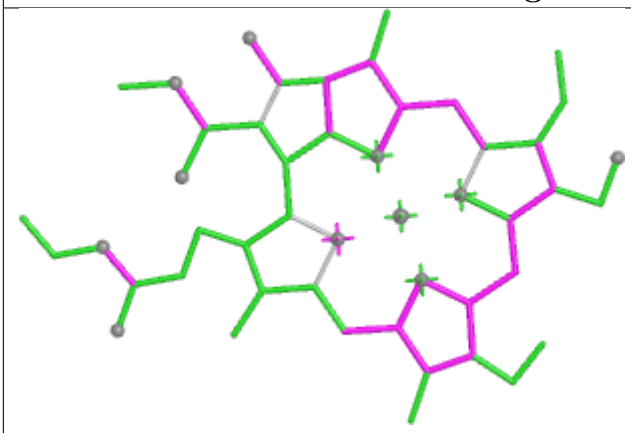


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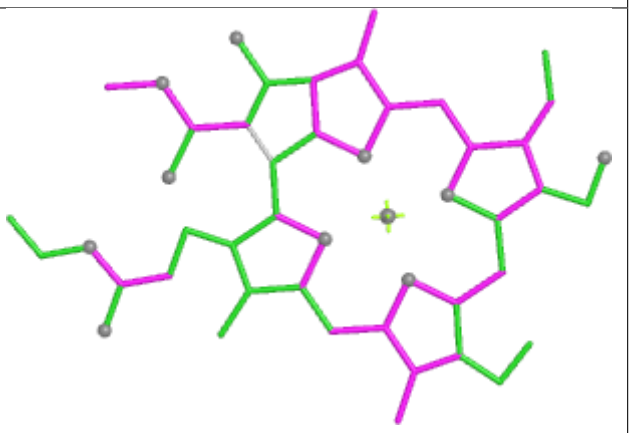


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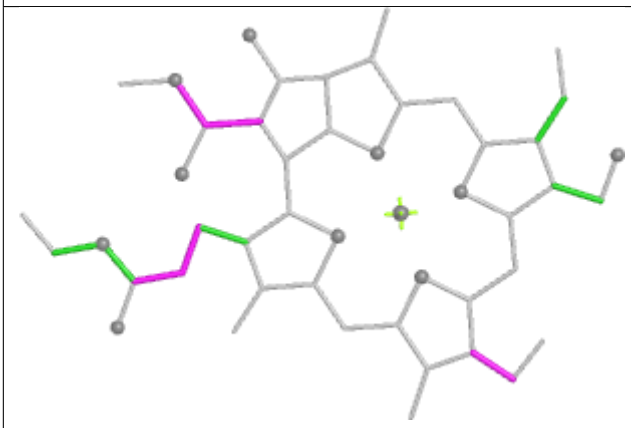
Ligand CHL P 315



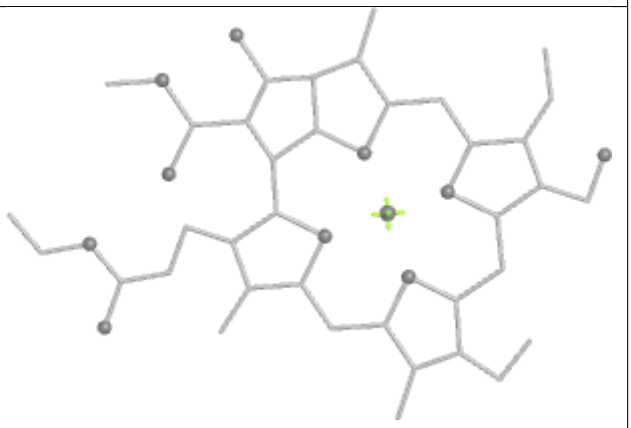
Bond lengths



Bond angles

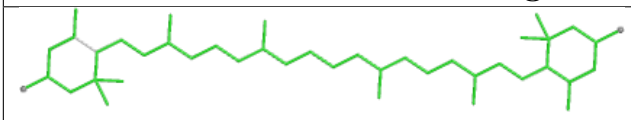


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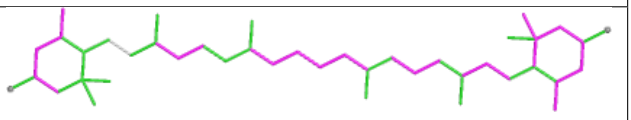


Rings

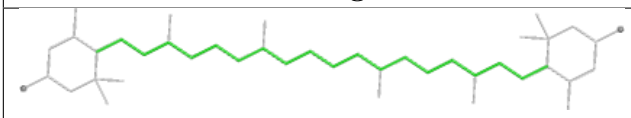
Ligand LUT V 310



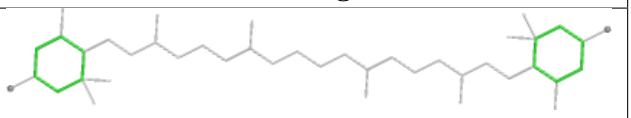
Bond lengths



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.

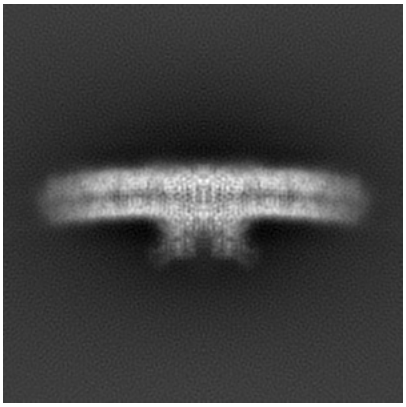
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9957. These allow visual inspection of the internal detail of the map and identification of artifacts.

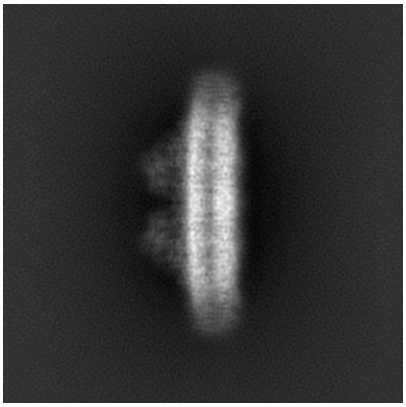
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

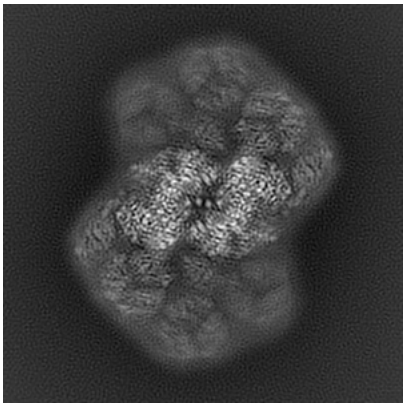
6.1.1 Primary map



X



Y

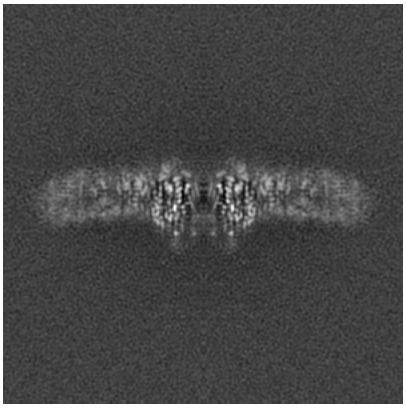


Z

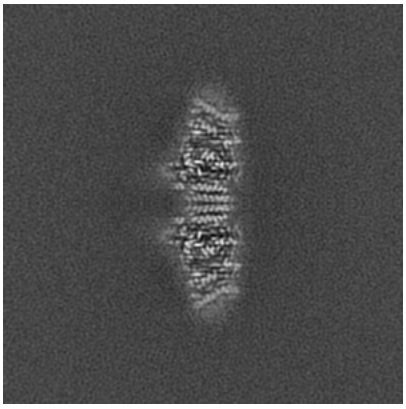
The images above show the map projected in three orthogonal directions.

6.2 Central slices

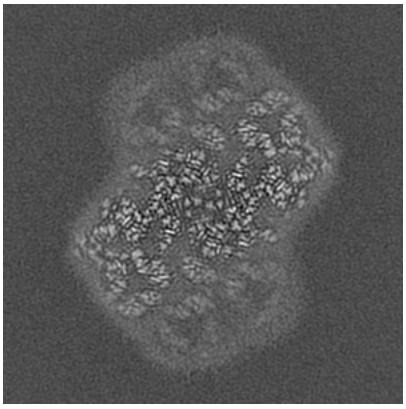
6.2.1 Primary map



X Index: 150



Y Index: 150

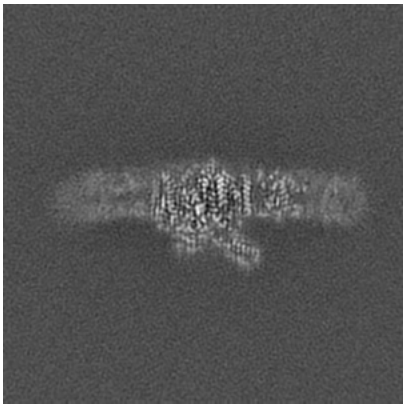


Z Index: 150

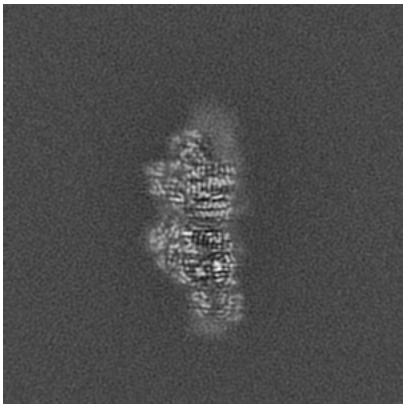
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

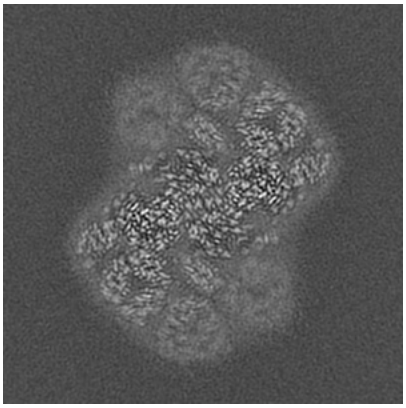
6.3.1 Primary map



X Index: 180



Y Index: 131

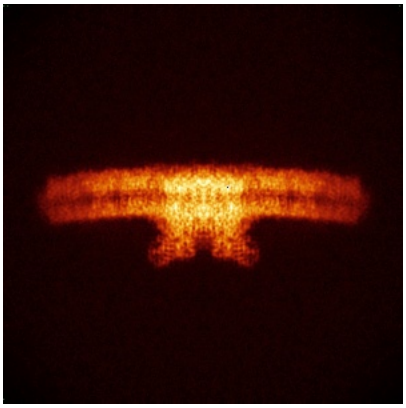


Z Index: 164

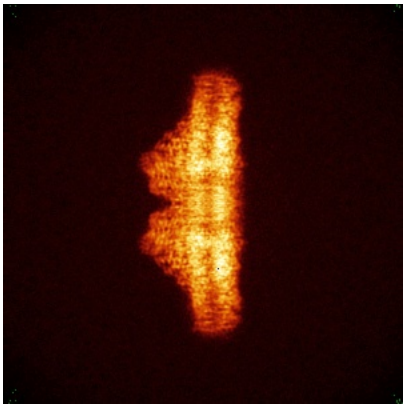
The images above show the largest variance slices of the map in three orthogonal directions.

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

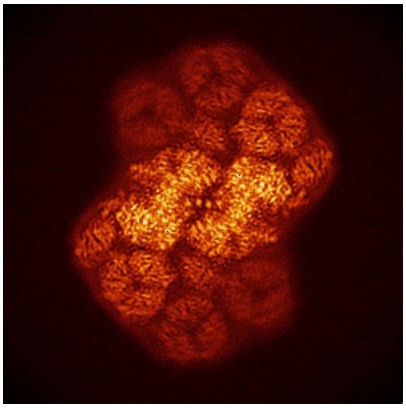
6.4.1 Primary map



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

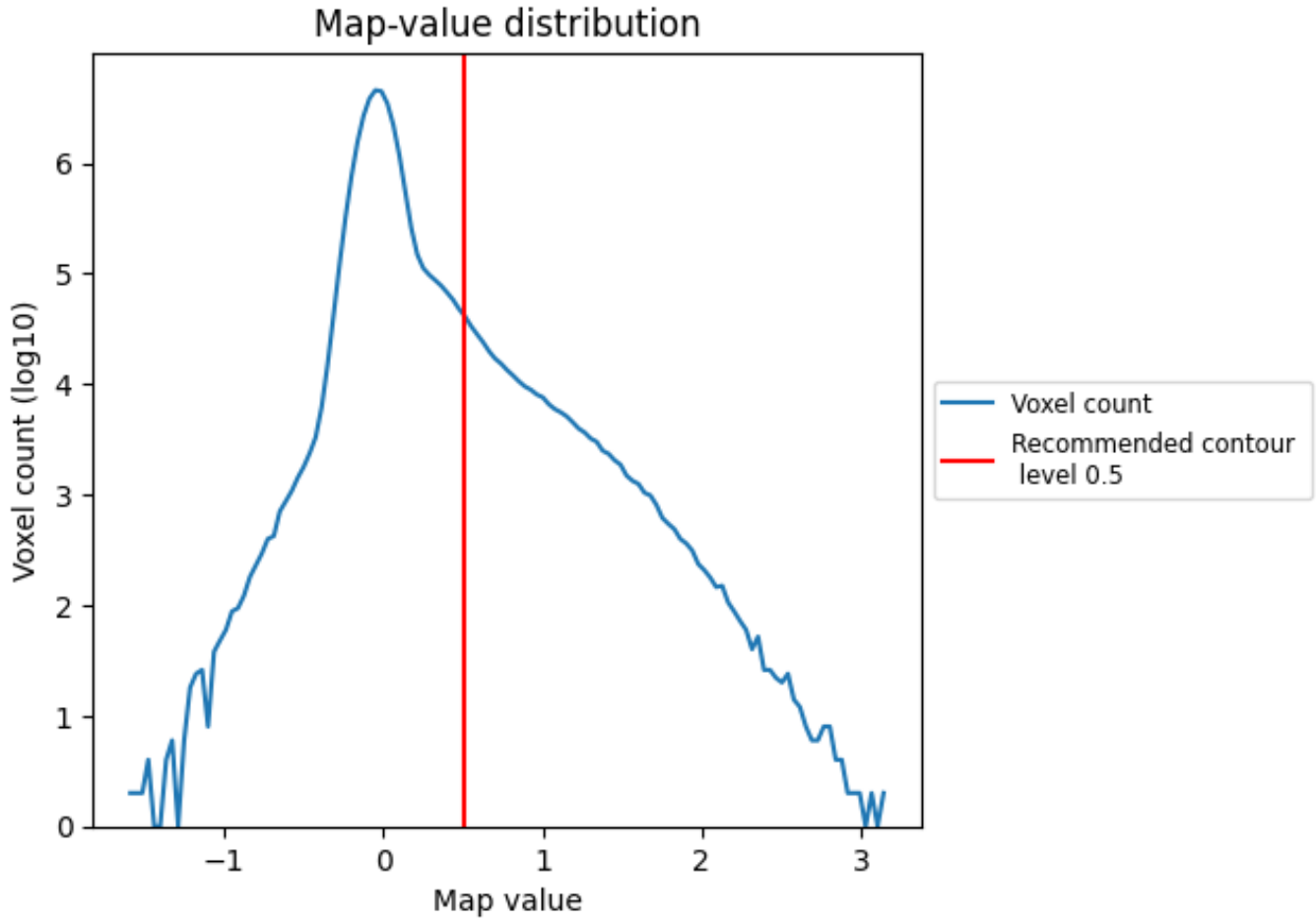
6.6 Mask visualisation (i)

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

7 Map analysis

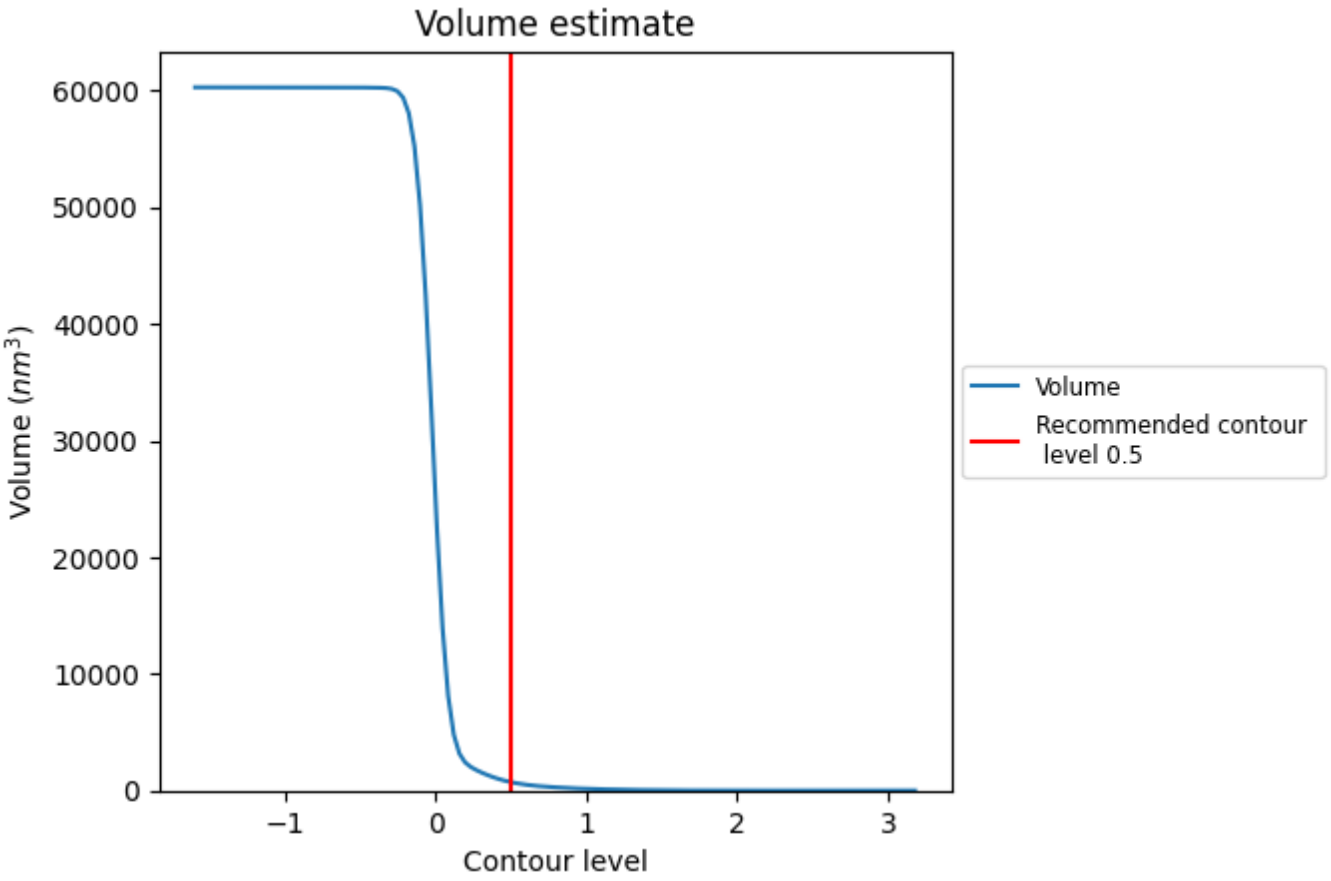
This section contains the results of statistical analysis of the map.

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.

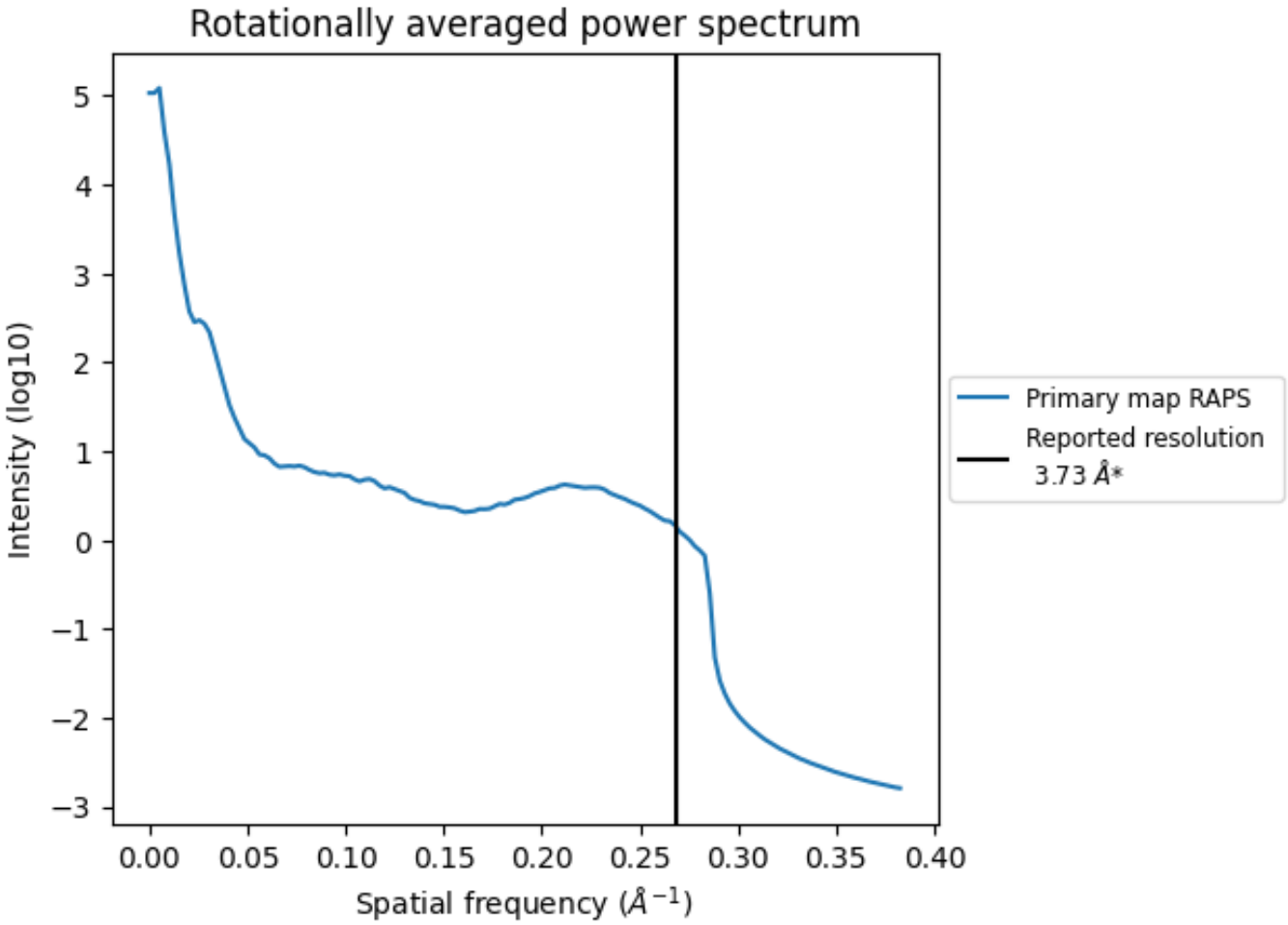
7.2 Volume estimate



The volume at the recommended contour level is 727 nm^3; this corresponds to an approximate mass of 657 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 0.268 Å^{-1}

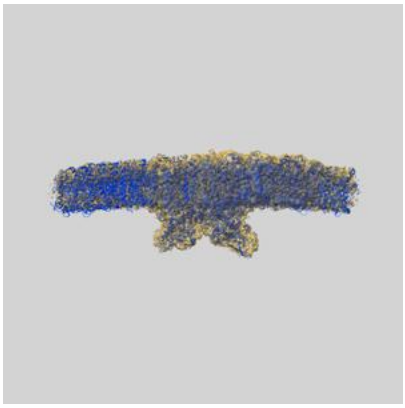
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

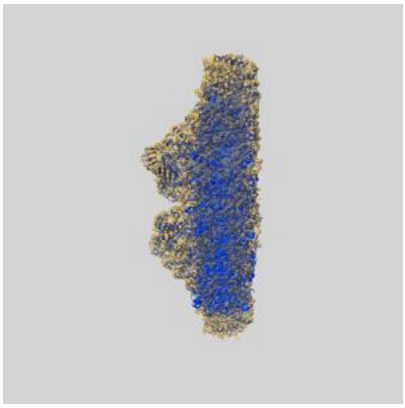
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9957 and PDB model 6KAF. Per-residue inclusion information can be found in section 3 on page 45.

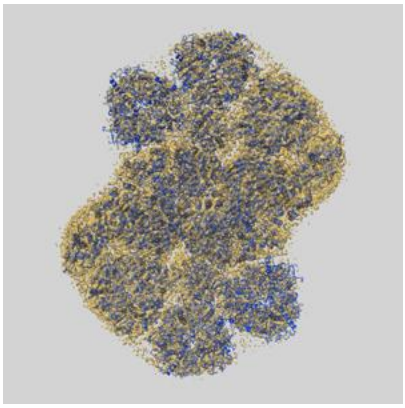
9.1 Map-model overlay



X



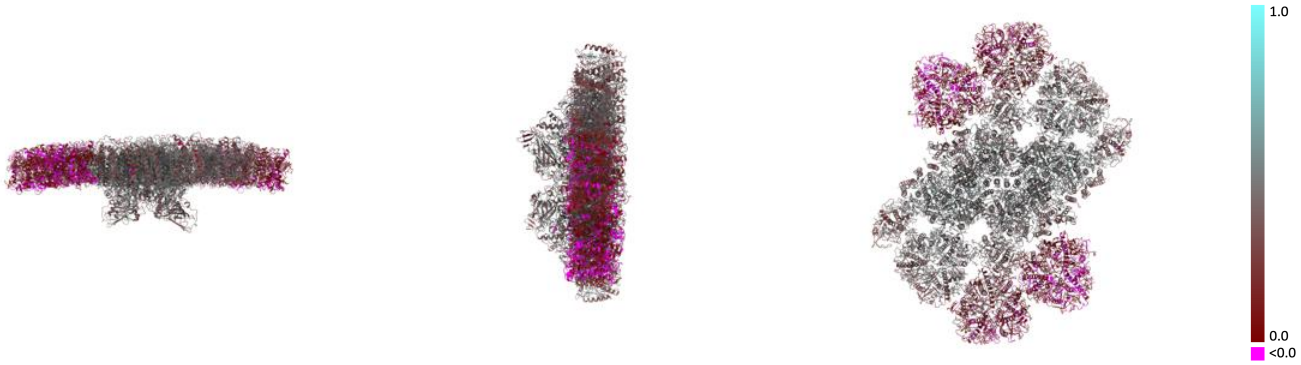
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

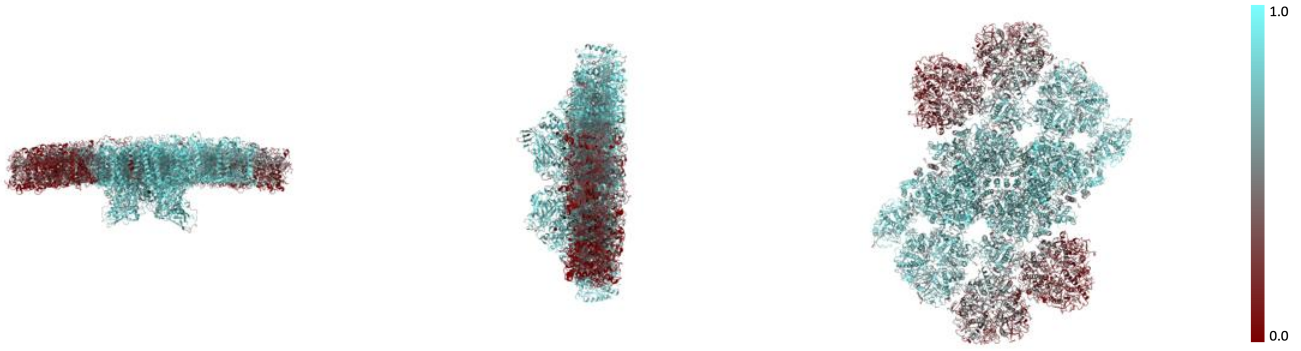
9.2 Q-score mapped to coordinate model (i)



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.

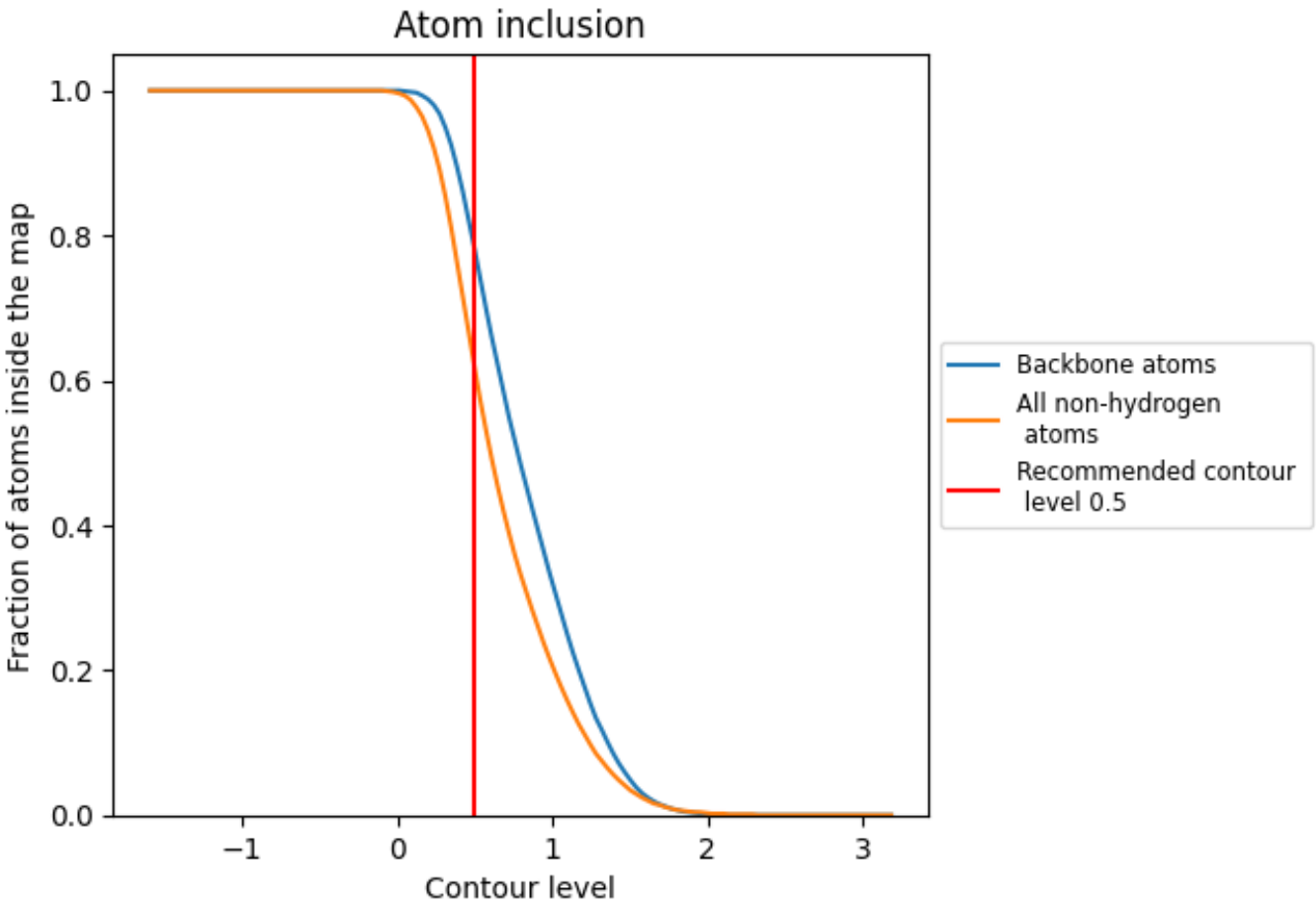
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 62% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.3260
1	0.4690	0.2180
2	0.2680	0.1130
3	0.2680	0.1030
4	0.4800	0.2330
5	0.2690	0.1100
6	0.2770	0.1120
A	0.8490	0.4710
B	0.7780	0.4420
C	0.8260	0.4680
D	0.8310	0.4580
E	0.7560	0.3920
F	0.7560	0.3190
G	0.7130	0.3870
H	0.8090	0.4290
I	0.9010	0.4840
J	0.4170	0.2730
K	0.8150	0.4280
L	0.7390	0.4530
M	0.7010	0.4110
N	0.7720	0.4060
O	0.7120	0.3810
P	0.2560	0.0890
Q	0.1050	0.0300
R	0.6320	0.3760
S	0.7690	0.3680
T	0.6880	0.4350
U	0.7830	0.4490
V	0.2130	0.0700
W	0.7840	0.4360
X	0.6850	0.3900
Y	0.6120	0.3520
Z	0.7730	0.3730
a	0.8460	0.4710
b	0.7770	0.4400



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Chain	Atom inclusion	Q-score
c	0.8220	0.4660
d	0.8320	0.4570
e	0.7540	0.3870
f	0.7600	0.3190
g	0.7080	0.3760
h	0.8160	0.4260
i	0.9010	0.4870
j	0.4120	0.2370
k	0.8150	0.4320
l	0.7360	0.4490
m	0.7010	0.4070
n	0.7640	0.3960
o	0.7120	0.3830
p	0.2400	0.0800
q	0.1080	0.0270
r	0.6390	0.3800
s	0.7680	0.3660
t	0.6880	0.4350
u	0.7850	0.4490
v	0.2150	0.0810
w	0.7790	0.4330
x	0.6850	0.3930
y	0.6120	0.3550
z	0.7630	0.3830