Full wwPDB EM Validation Report

Aug 7, 2026 – 01:05 AM JST

PDB ID	:	9LK5 / pdb_00009lk5
EMDB ID	:	EMD-63168
Title	:	The structure of Lhcb8-C2S2 PSII-LHCII supercomplex from Arabidopsis thaliana
Authors	:	Zhou, Q.; Caferri, R.; Shan, J.Y.; Amelii, A.; Bassi, R.; Liu, Z.F.
Deposited on	:	2025-01-16
Resolution	:	3.00 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:

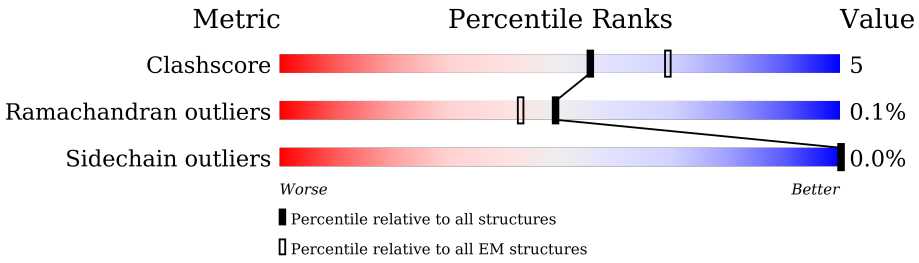
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

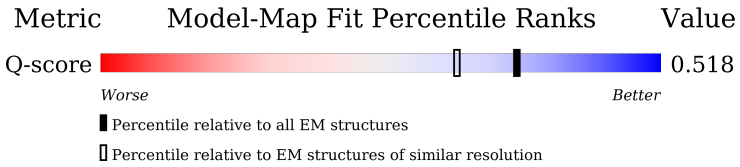
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	A	353	86% 9% 5%
1	a	353	86% 8% 5%
2	B	508	88% 8%
2	b	508	87% 10%

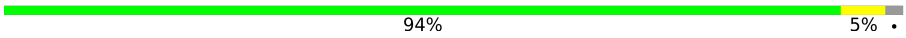
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Mol	Chain	Length	Quality of chain
3	C	473	88% 7% 5%
3	c	473	88% 7% 5%
4	D	353	88% 8%
4	d	353	88% 8%
5	E	83	78% 7% 14%
5	e	83	76% 10% 14%
6	F	39	72% 23%
6	f	39	72% 23%
7	G	267	74% 8% 18%
7	N	267	73% 9% 18%
7	g	267	75% 7% 18%
7	n	267	73% 9% 18%
8	H	73	74% 7% 19%
8	h	73	67% 14% 19%
9	I	36	86% 8% 6%
9	i	36	86% 8% 6%
10	J	40	15% 72% 28%
10	j	40	15% 70% 28%
11	K	61	57% 39%
11	k	61	57% 39%
12	L	38	84% 13%
12	l	38	79% 16%
13	M	34	82% 12% 6%
13	m	34	82% 12% 6%
14	O	332	53% 6% 40%

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Mol	Chain	Length	Quality of chain
14	o	332	
15	S	280	
15	s	280	
16	T	33	
16	t	33	
17	U	103	
17	u	103	
18	W	133	
18	w	133	
19	X	116	
19	x	116	
20	Y	265	
20	y	265	
21	Z	62	
21	z	62	
22	R	286	
22	r	286	

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
27	BCT	A	407	-	-	X	-
27	BCT	a	408	-	-	X	-
33	PL9	D	406	-	X	-	-
33	PL9	d	406	-	X	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 71232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	335	Total	C	N	O	S	0	0
			2623	1712	431	467	13		
1	a	335	Total	C	N	O	S	0	0
			2623	1712	431	467	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	489	Total	C	N	O	S	0	0
			3829	2506	647	664	12		
2	b	489	Total	C	N	O	S	0	0
			3829	2506	647	664	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3480	2285	582	602	11		
3	c	449	Total	C	N	O	S	0	0
			3480	2285	582	602	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		
4	d	339	Total	C	N	O	S	0	0
			2696	1783	441	460	12		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	71	Total 576	C 377	N 93	O 106	0	0
5	e	71	Total 576	C 377	N 93	O 106	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total 235	C 156	N 41	O 37	S 1	0	0
6	f	30	Total 235	C 156	N 41	O 37	S 1	0	0

- Molecule 7 is a protein called Chlorophyll a-b binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	219	Total 1666	C 1078	N 273	O 310	S 5	0	0
7	N	219	Total 1666	C 1078	N 273	O 310	S 5	0	0
7	g	219	Total 1666	C 1078	N 273	O 310	S 5	0	0
7	n	219	Total 1666	C 1078	N 273	O 310	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total 438	C 289	N 68	O 79	S 2	0	0
8	h	59	Total 438	C 289	N 68	O 79	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total 277	C 190	N 43	O 43	S 1	0	0
9	i	34	Total 277	C 190	N 43	O 43	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	29	Total	C	N	O	0	0
			219	152	33	34		
10	j	29	Total	C	N	O	0	0
			219	152	33	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			301	211	44	45	1		
11	k	37	Total	C	N	O	S	0	0
			301	211	44	45	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	37	Total	C	N	O	0	0
			309	204	48	57		
12	l	37	Total	C	N	O	0	0
			309	204	48	57		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total	C	N	O	0	0
			250	172	36	42		
13	m	32	Total	C	N	O	0	0
			250	172	36	42		

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		
14	o	198	Total	C	N	O	S	0	0
			1523	974	240	305	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	s	221	Total	C	N	O	S	0	0
			1705	1111	277	313	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
16	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 17 is a protein called Photosystem II 5 kDa protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	23	Total	C	N	O	S	0	0
			179	114	31	31	3		
17	u	23	Total	C	N	O	S	0	0
			179	114	31	31	3		

- Molecule 18 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	54	Total	C	N	O	S	0	0
			427	282	61	83	1		
18	w	54	Total	C	N	O	S	0	0
			427	282	61	83	1		

- Molecule 19 is a protein called (thale cress) hypothetical protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	38	Total	C	N	O	0	0
			267	176	42	49		
19	x	38	Total	C	N	O	0	0
			267	176	42	49		

- Molecule 20 is a protein called Chlorophyll a-b binding protein 2.2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		
20	y	220	Total	C	N	O	S	0	0
			1699	1107	273	314	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		
21	z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		

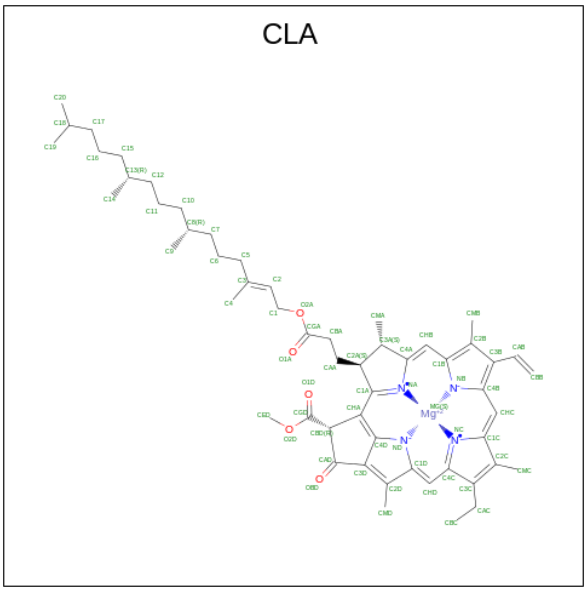
- Molecule 22 is a protein called Chlorophyll a-b binding protein CP29.3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	220	Total	C	N	O	S	0	0
			1718	1124	274	316	4		
22	R	220	Total	C	N	O	S	0	0
			1718	1124	274	316	4		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	277	GLY	-	expression tag	UNP Q9S7W1
r	278	GLY	-	expression tag	UNP Q9S7W1
r	279	GLY	-	expression tag	UNP Q9S7W1
r	280	GLY	-	expression tag	UNP Q9S7W1
r	281	HIS	-	expression tag	UNP Q9S7W1
r	282	HIS	-	expression tag	UNP Q9S7W1
r	283	HIS	-	expression tag	UNP Q9S7W1
r	284	HIS	-	expression tag	UNP Q9S7W1
r	285	HIS	-	expression tag	UNP Q9S7W1
r	286	HIS	-	expression tag	UNP Q9S7W1
R	277	GLY	-	expression tag	UNP Q9S7W1
R	278	GLY	-	expression tag	UNP Q9S7W1
R	279	GLY	-	expression tag	UNP Q9S7W1
R	280	GLY	-	expression tag	UNP Q9S7W1
R	281	HIS	-	expression tag	UNP Q9S7W1
R	282	HIS	-	expression tag	UNP Q9S7W1
R	283	HIS	-	expression tag	UNP Q9S7W1
R	284	HIS	-	expression tag	UNP Q9S7W1
R	285	HIS	-	expression tag	UNP Q9S7W1
R	286	HIS	-	expression tag	UNP Q9S7W1

- Molecule 23 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
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	G	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	G	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	N	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	N	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	N	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	S	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	S	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	Y	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	Y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	Y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	Y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	Y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	g	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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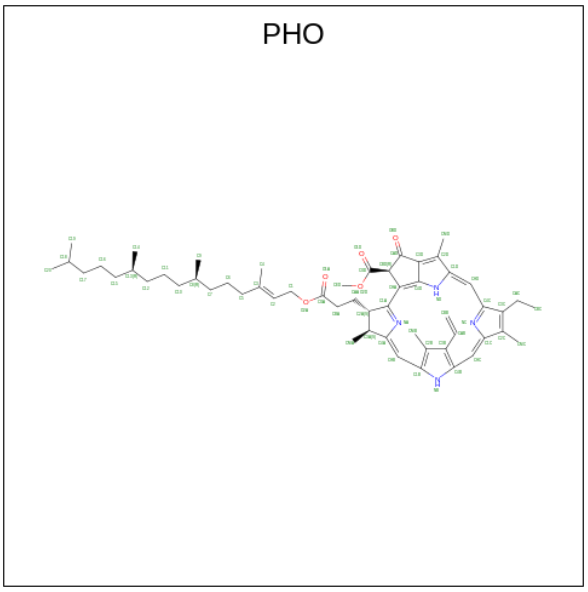
Mol	Chain	Residues	Atoms					AltConf
23	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	n	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	y	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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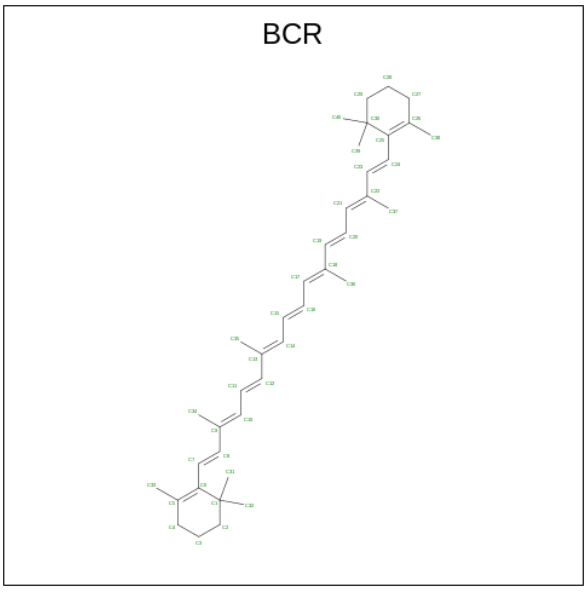
Mol	Chain	Residues	Atoms					AltConf
23	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	y	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



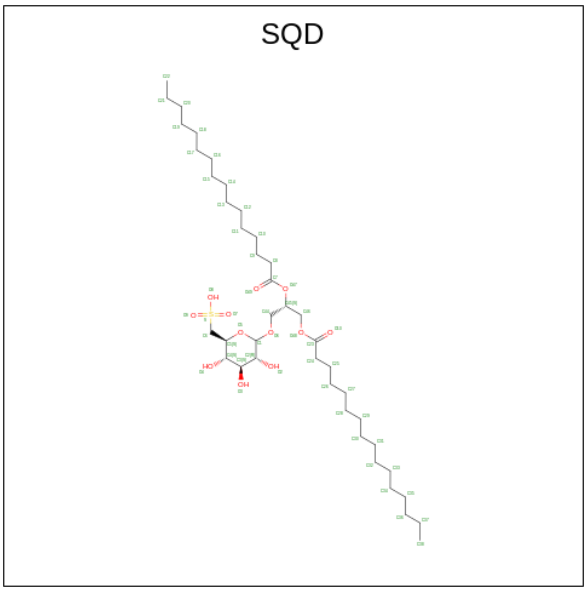
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	N	O	0
			64	55	4	5	
24	D	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	
24	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



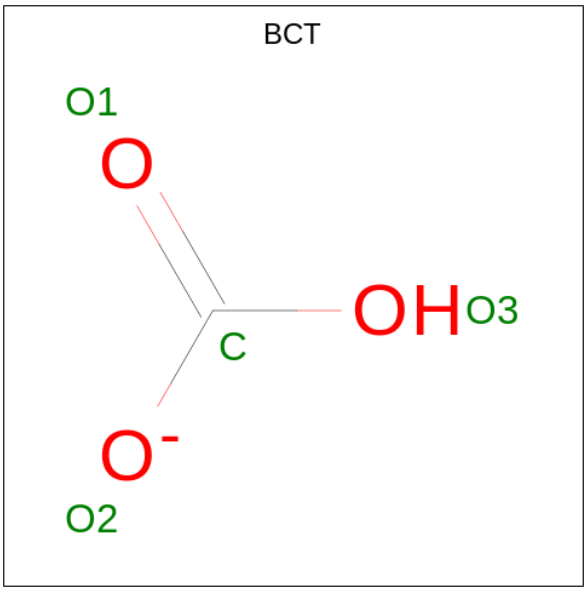
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 40 40	0
25	H	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	a	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	b	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	c	1	Total C 40 40	0
25	d	1	Total C 40 40	0
25	h	1	Total C 40 40	0
25	k	1	Total C 40 40	0
25	z	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



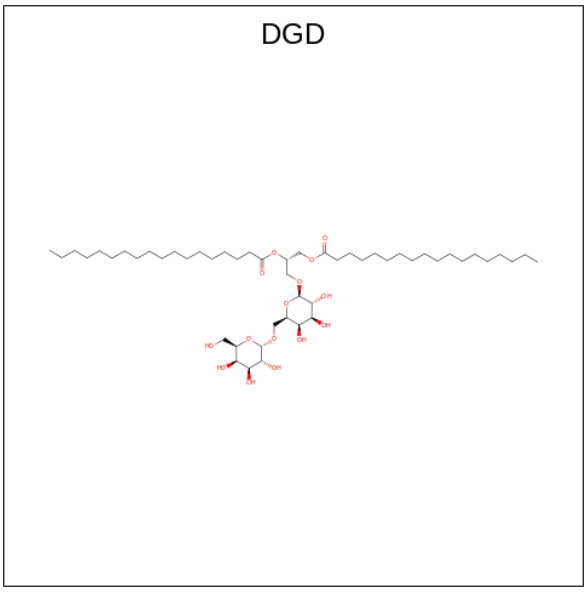
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			50	37	12	1	
26	B	1	Total	C	O	S	0
			54	41	12	1	
26	C	1	Total	C	O	S	0
			45	32	12	1	
26	L	1	Total	C	O	S	0
			54	41	12	1	
26	a	1	Total	C	O	S	0
			50	37	12	1	
26	b	1	Total	C	O	S	0
			54	41	12	1	
26	c	1	Total	C	O	S	0
			45	32	12	1	
26	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			4	1	3	
27	a	1	Total	C	O	0
			4	1	3	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			59	44	15	

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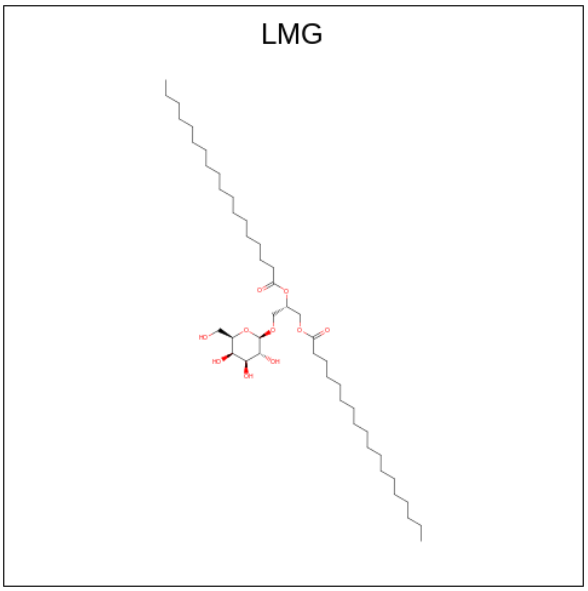
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Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C O 59 44 15	0
28	B	1	Total C O 56 41 15	0
28	C	1	Total C O 55 40 15	0
28	D	1	Total C O 62 47 15	0
28	b	1	Total C O 56 41 15	0
28	c	1	Total C O 55 40 15	0
28	d	1	Total C O 62 47 15	0

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

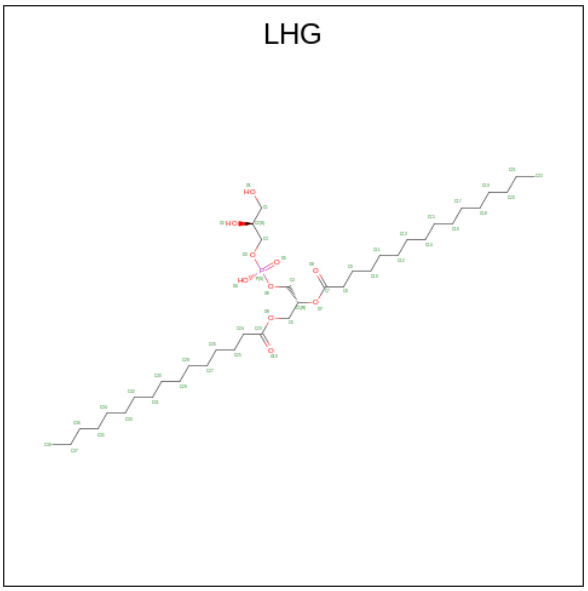
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total Fe 1 1	0
29	a	1	Total Fe 1 1	0

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			51	41	10	
30	B	1	Total	C	O	0
			40	30	10	
30	C	1	Total	C	O	0
			48	38	10	
30	C	1	Total	C	O	0
			50	40	10	
30	D	1	Total	C	O	0
			46	36	10	
30	S	1	Total	C	O	0
			55	45	10	
30	W	1	Total	C	O	0
			51	41	10	
30	a	1	Total	C	O	0
			48	38	10	
30	b	1	Total	C	O	0
			40	30	10	
30	b	1	Total	C	O	0
			51	41	10	
30	c	1	Total	C	O	0
			50	40	10	
30	d	1	Total	C	O	0
			46	36	10	
30	s	1	Total	C	O	0
			55	45	10	
30	w	1	Total	C	O	0
			51	41	10	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



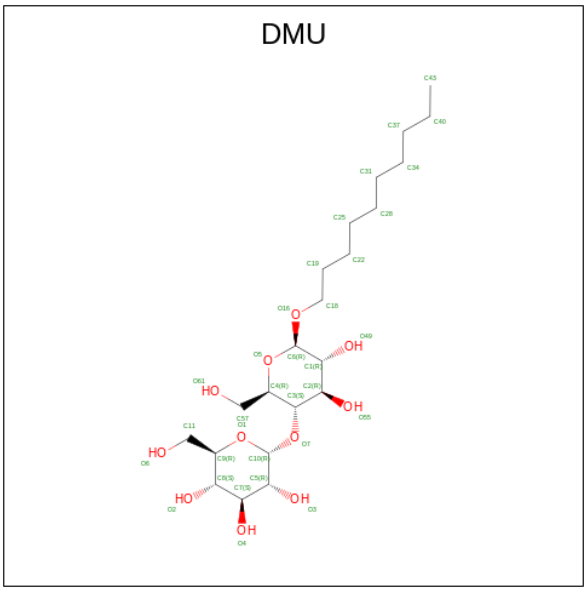
Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	O	P	0
			49	38	10	1	
31	B	1	Total	C	O	P	0
			46	35	10	1	
31	B	1	Total	C	O	P	0
			40	29	10	1	
31	C	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	G	1	Total	C	O	P	0
			46	35	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	
31	N	1	Total	C	O	P	0
			49	38	10	1	
31	S	1	Total	C	O	P	0
			49	38	10	1	
31	W	1	Total	C	O	P	0
			49	38	10	1	
31	Y	1	Total	C	O	P	0
			49	38	10	1	
31	b	1	Total	C	O	P	0
			49	38	10	1	

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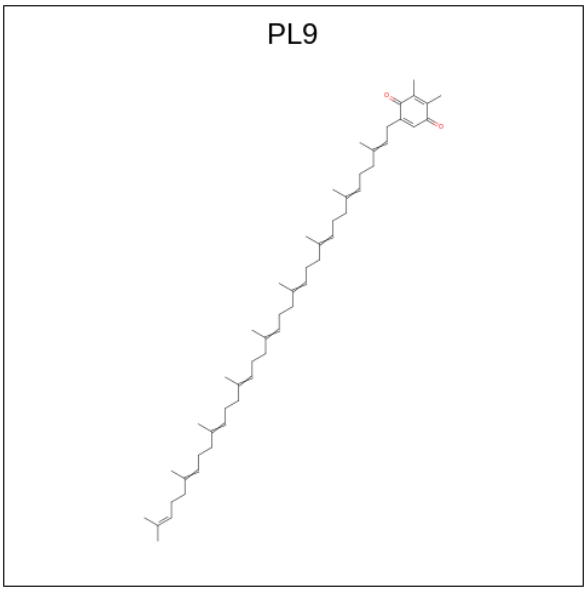
Mol	Chain	Residues	Atoms				AltConf
31	b	1	Total	C	O	P	0
			46	35	10	1	
31	b	1	Total	C	O	P	0
			40	29	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	c	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	d	1	Total	C	O	P	0
			49	38	10	1	
31	g	1	Total	C	O	P	0
			46	35	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	l	1	Total	C	O	P	0
			49	38	10	1	
31	r	1	Total	C	O	P	0
			42	31	10	1	
31	s	1	Total	C	O	P	0
			49	38	10	1	
31	n	1	Total	C	O	P	0
			49	38	10	1	
31	y	1	Total	C	O	P	0
			49	38	10	1	
31	R	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 32 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



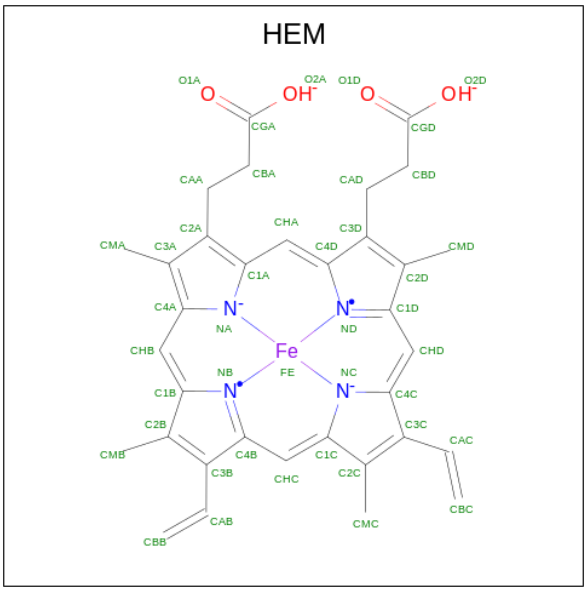
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			33	22	11	
32	C	1	Total	C	O	0
			33	22	11	
32	S	1	Total	C	O	0
			33	22	11	
32	c	1	Total	C	O	0
			33	22	11	
32	c	1	Total	C	O	0
			33	22	11	
32	s	1	Total	C	O	0
			33	22	11	

- 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	D	1	Total	C	O	0
			55	53	2	
33	d	1	Total	C	O	0
			55	53	2	

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



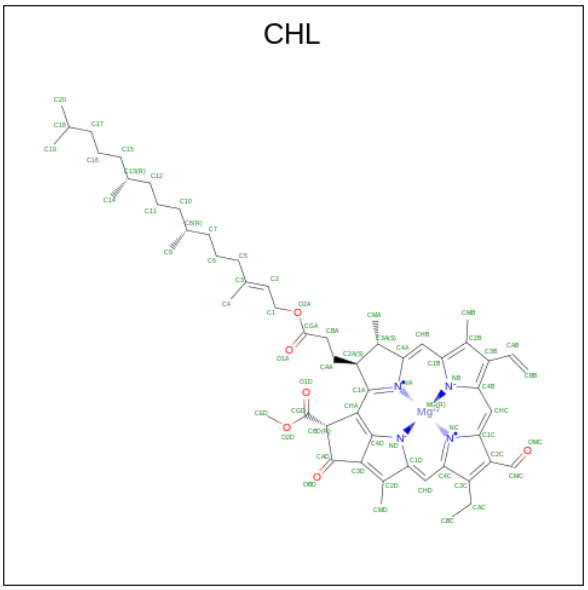
Mol	Chain	Residues	Atoms					AltConf
34	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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

- Molecule 35 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
35	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	G	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	G	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	G	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
35	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	N	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
35	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	N	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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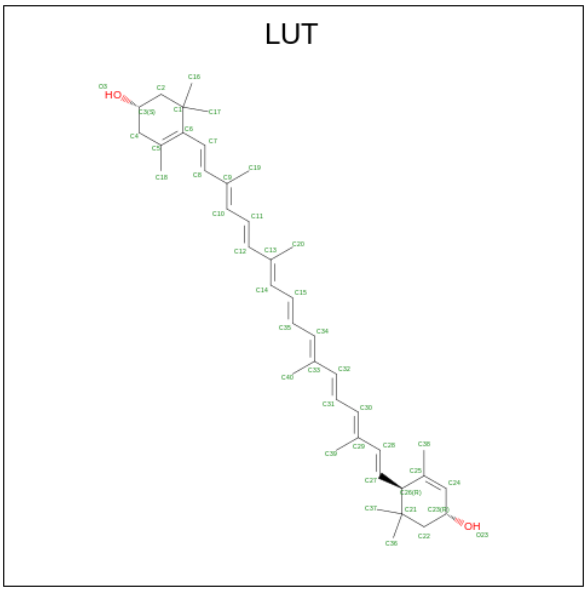
Mol	Chain	Residues	Atoms					AltConf
35	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	S	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	Y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	Y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
35	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	g	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	g	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	g	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
35	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	r	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
35	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
35	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
35	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	R	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
35	R	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



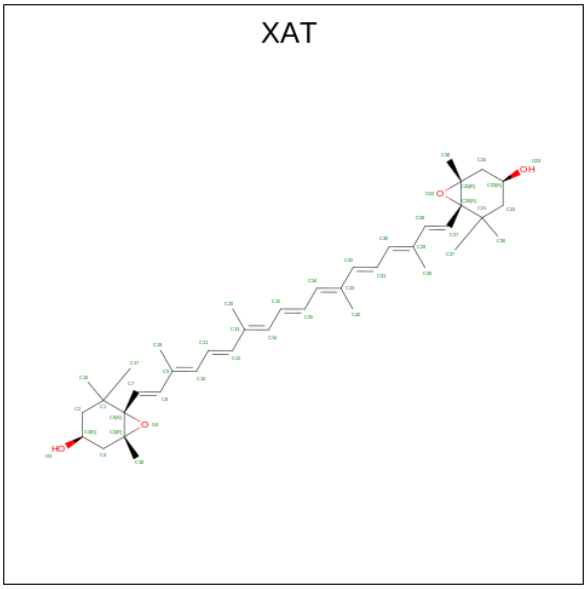
Mol	Chain	Residues	Atoms			AltConf
36	G	1	Total	C	O	0
			42	40	2	
36	G	1	Total	C	O	0
			42	40	2	
36	N	1	Total	C	O	0
			42	40	2	
36	N	1	Total	C	O	0
			42	40	2	
36	S	1	Total	C	O	0
			42	40	2	
36	S	1	Total	C	O	0
			42	40	2	
36	Y	1	Total	C	O	0
			42	40	2	
36	Y	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	g	1	Total	C	O	0
			42	40	2	
36	r	1	Total	C	O	0
			42	40	2	
36	s	1	Total	C	O	0
			42	40	2	
36	s	1	Total	C	O	0
			42	40	2	
36	n	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms	AltConf
36	n	1	Total C O 42 40 2	0
36	y	1	Total C O 42 40 2	0
36	y	1	Total C O 42 40 2	0
36	R	1	Total C O 42 40 2	0

- Molecule 37 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



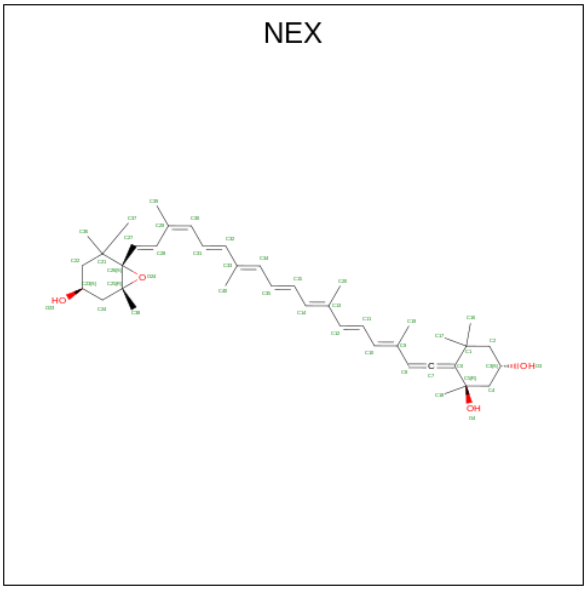
Mol	Chain	Residues	Atoms	AltConf
37	G	1	Total C O 44 40 4	0
37	G	1	Total C O 44 40 4	0
37	Y	1	Total C O 44 40 4	0
37	g	1	Total C O 44 40 4	0
37	g	1	Total C O 44 40 4	0
37	r	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
37	y	1	Total C O 44 40 4	0
37	R	1	Total C O 44 40 4	0

- Molecule 38 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: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



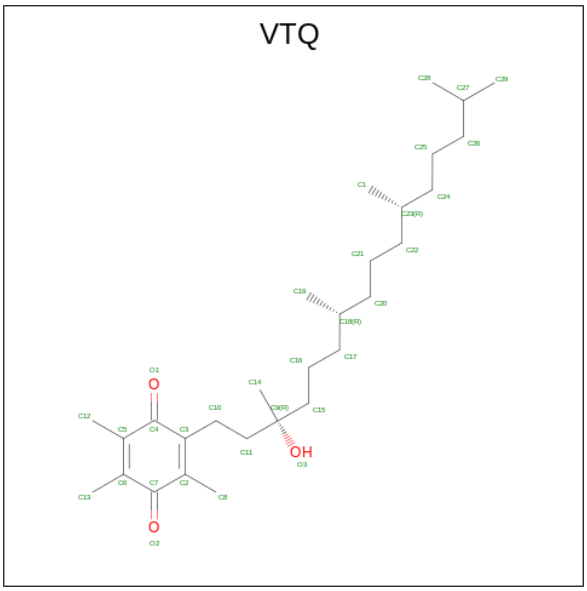
Mol	Chain	Residues	Atoms	AltConf
38	G	1	Total C O 44 40 4	0
38	N	1	Total C O 44 40 4	0
38	S	1	Total C O 44 40 4	0
38	Y	1	Total C O 44 40 4	0
38	g	1	Total C O 44 40 4	0
38	r	1	Total C O 44 40 4	0
38	s	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
38	n	1	Total C O 44 40 4	0
38	R	1	Total C O 44 40 4	0
38	R	1	Total C O 44 40 4	0

- Molecule 39 is RRR-ALPHA-TOCOPHERYLQUINONE (CCD ID: VTQ) (formula: $C_{29}H_{50}O_3$).



Mol	Chain	Residues	Atoms	AltConf
39	W	1	Total C O 32 29 3	0
39	w	1	Total C O 32 29 3	0

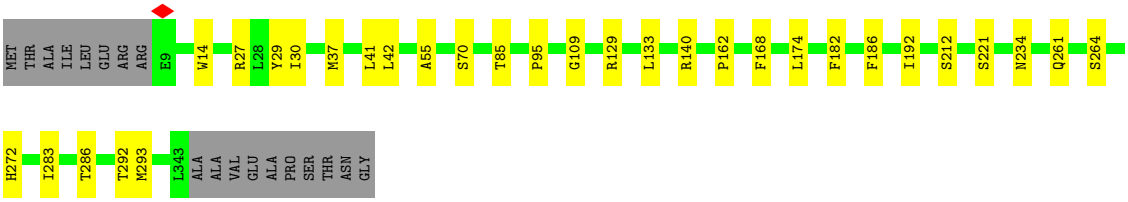
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

Chain A:

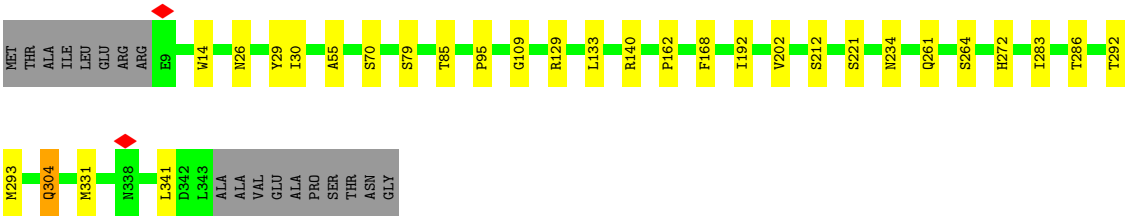




• Molecule 1: Photosystem II protein D1

Chain a:

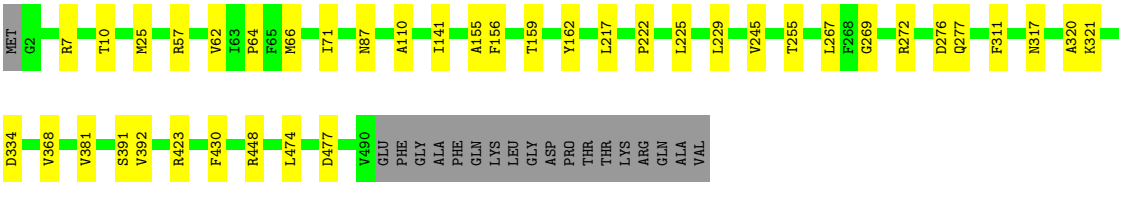




• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:

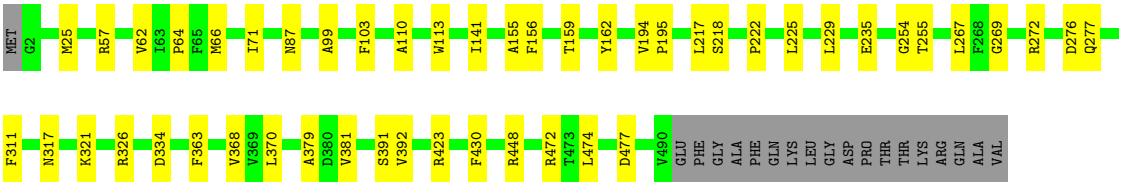




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

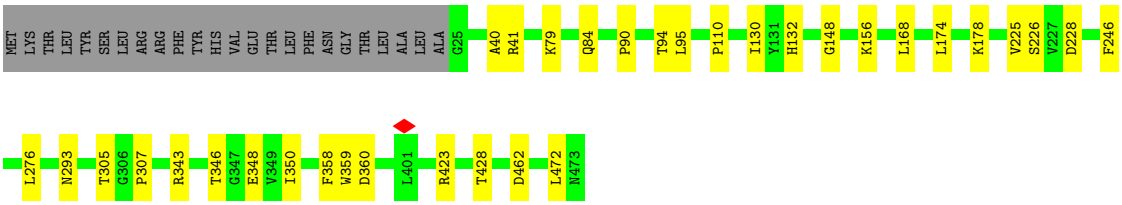




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

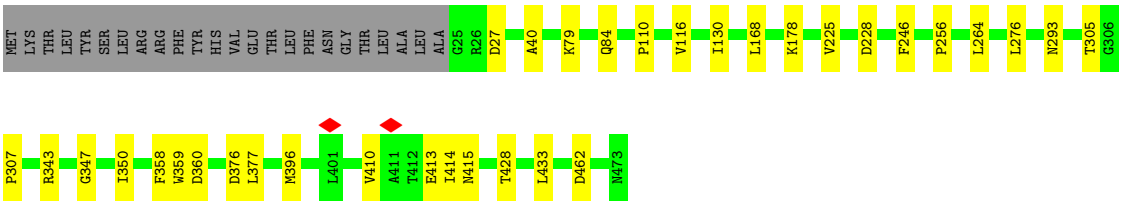




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

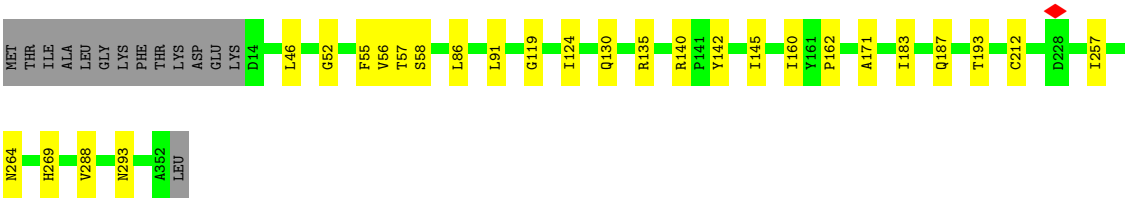




• Molecule 4: Photosystem II D2 protein

Chain D:

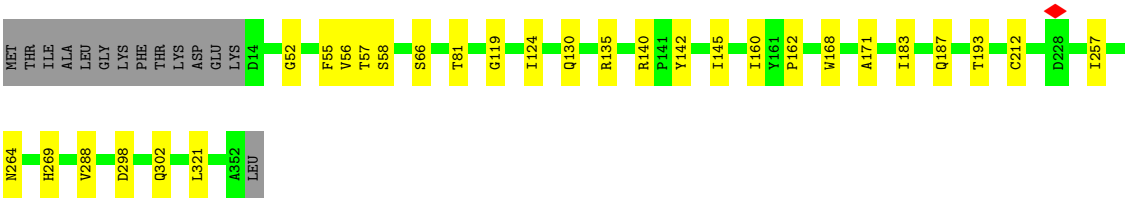




• Molecule 4: Photosystem II D2 protein

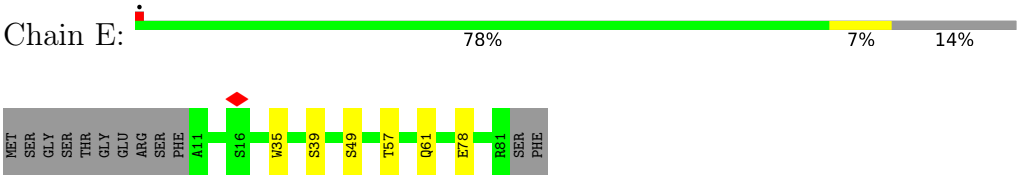
Chain d:





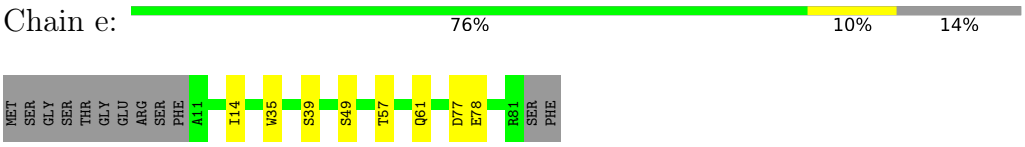
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



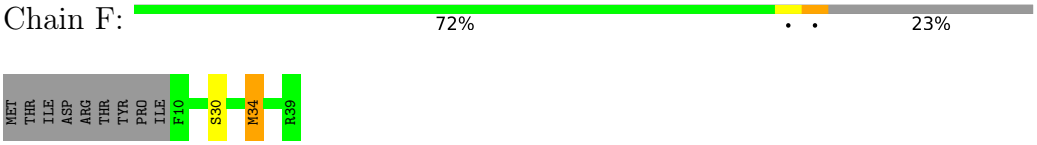
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



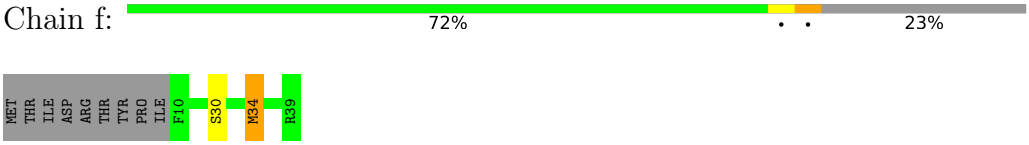
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



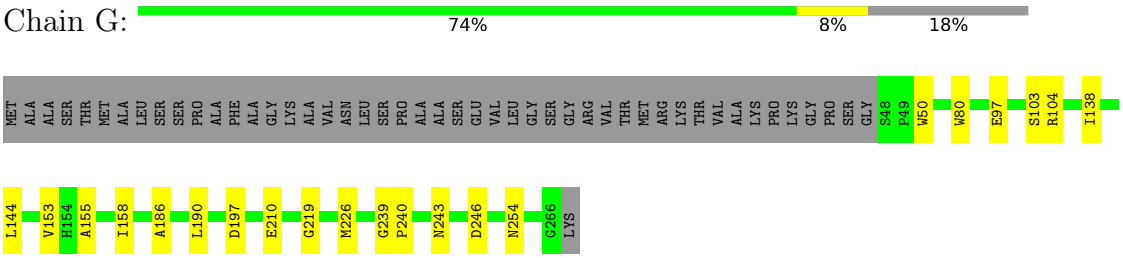
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



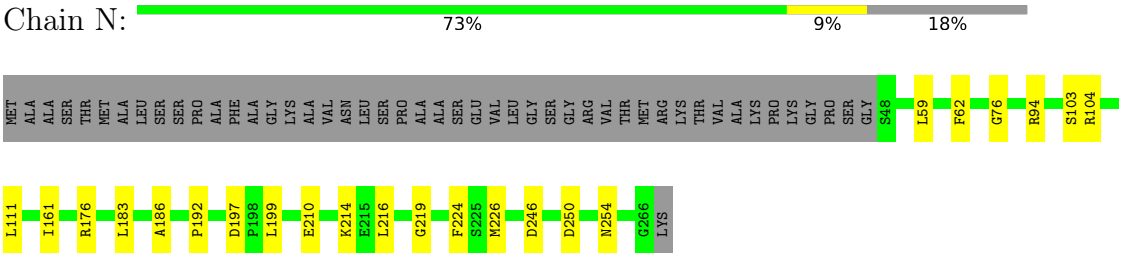
• Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

Chain G:



• Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

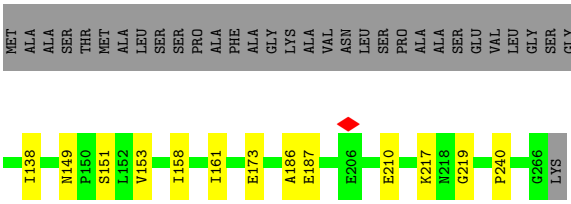
Chain N:



• Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic

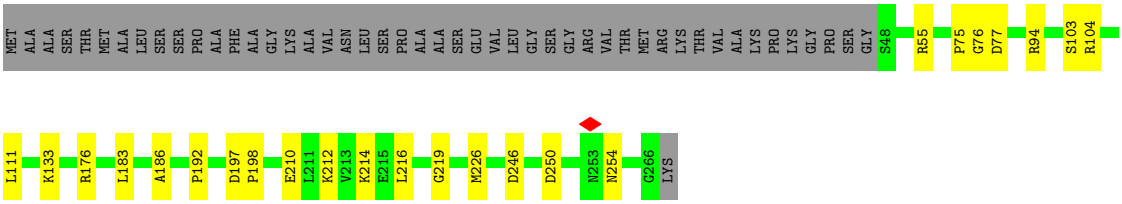
Chain g:





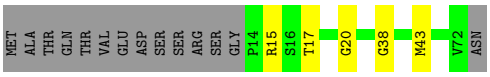
• Molecule 7: Chlorophyll a-b binding protein 2, chloroplastic





• Molecule 8: Photosystem II reaction center protein H



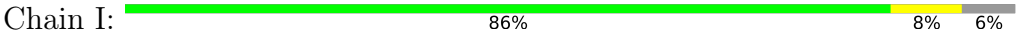


• Molecule 8: Photosystem II reaction center protein H



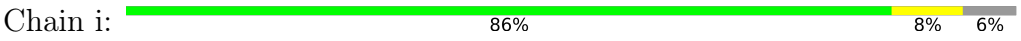


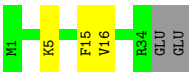
• Molecule 9: Photosystem II reaction center protein I





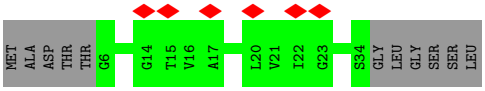
• Molecule 9: Photosystem II reaction center protein I





• Molecule 10: Photosystem II reaction center protein J

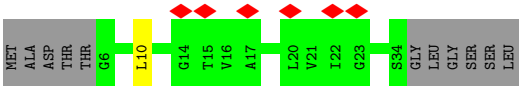




• Molecule 10: Photosystem II reaction center protein J

Chain j:

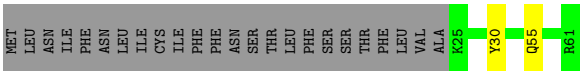




• Molecule 11: Photosystem II reaction center protein K

Chain K:





• Molecule 11: Photosystem II reaction center protein K

Chain k:

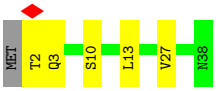




• Molecule 12: Photosystem II reaction center protein L

Chain L:

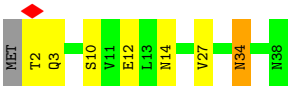




• Molecule 12: Photosystem II reaction center protein L

Chain l:

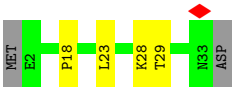




• Molecule 13: Photosystem II reaction center protein M

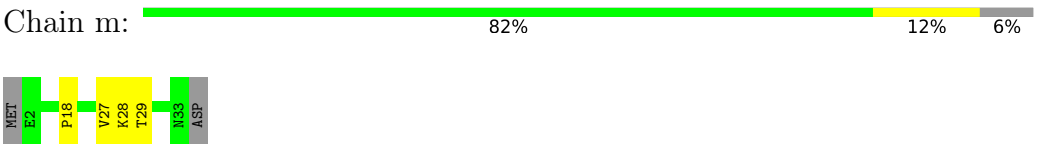
Chain M:





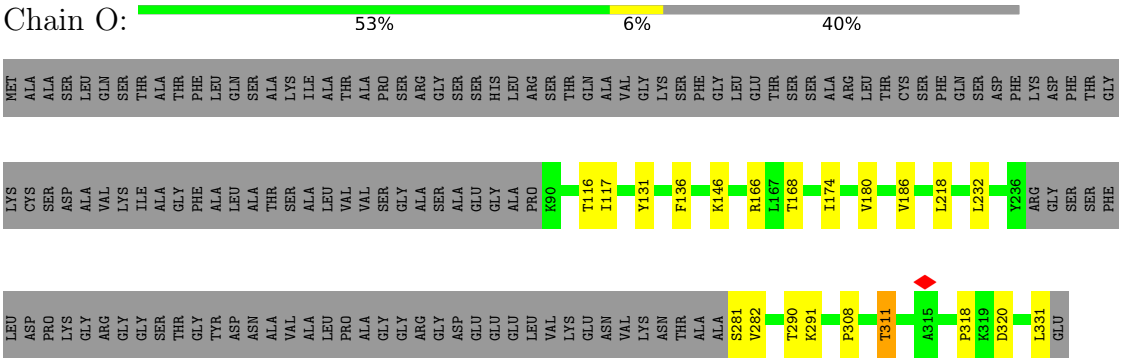
• Molecule 13: Photosystem II reaction center protein M

Chain m:



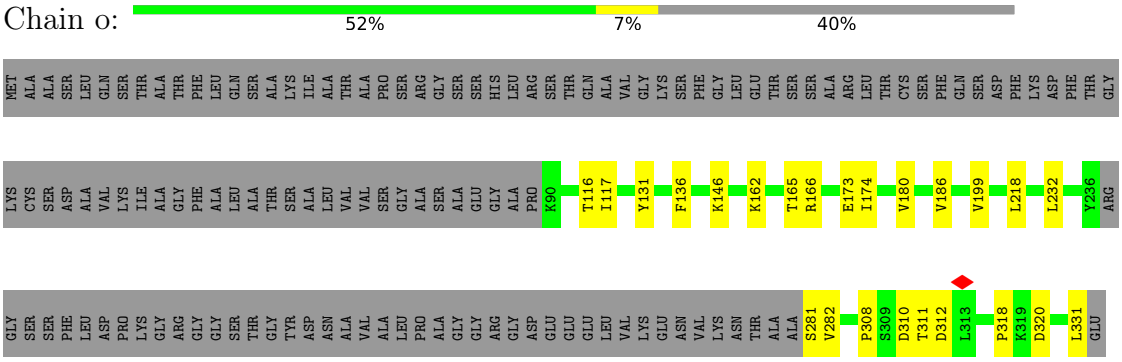
• Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O:



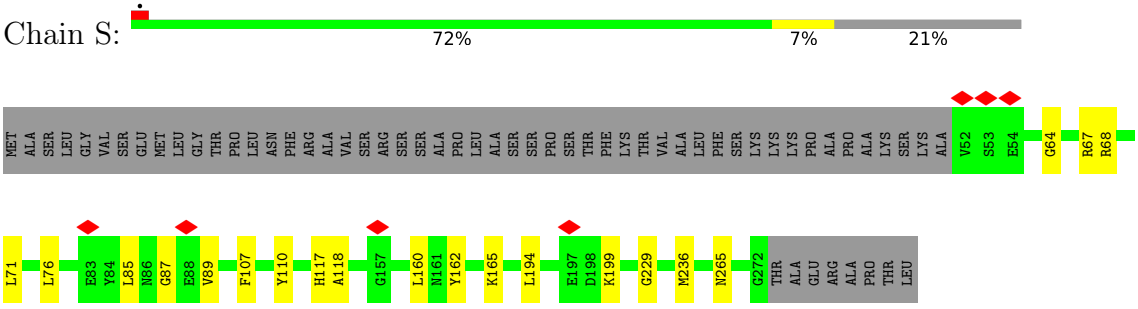
• Molecule 14: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain o:



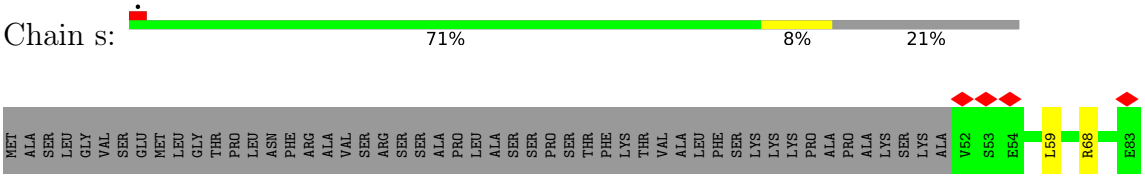
• Molecule 15: Chlorophyll a-b binding protein CP26, chloroplastic

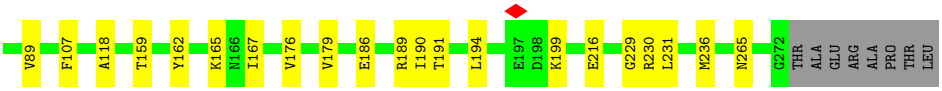
Chain S:



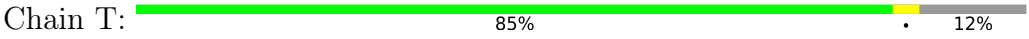
• Molecule 15: Chlorophyll a-b binding protein CP26, chloroplastic

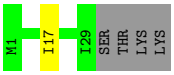
Chain s:



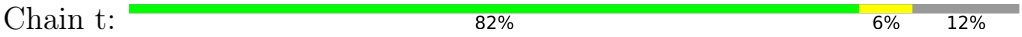


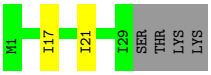
• Molecule 16: Photosystem II reaction center protein T





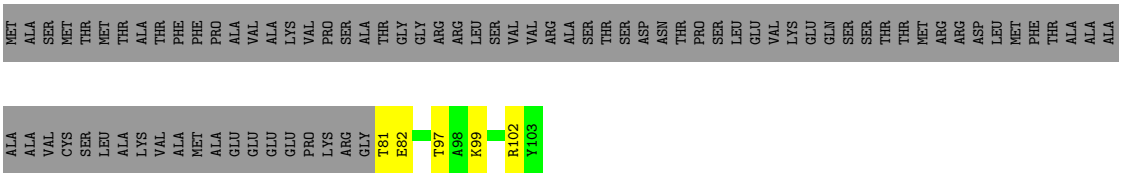
• Molecule 16: Photosystem II reaction center protein T





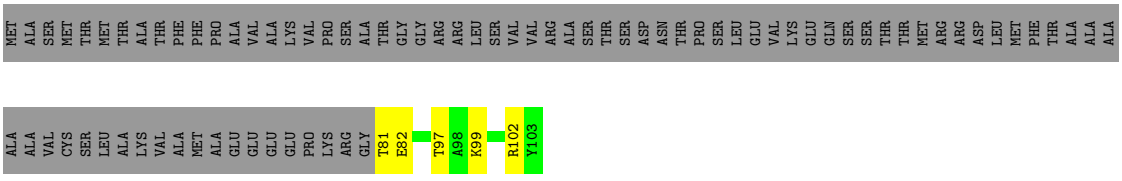
• Molecule 17: Photosystem II 5 kDa protein, chloroplastic





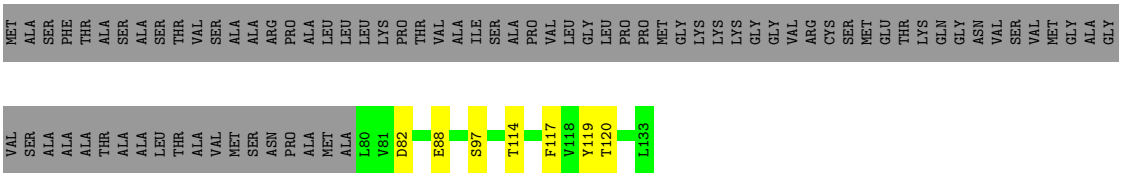
• Molecule 17: Photosystem II 5 kDa protein, chloroplastic





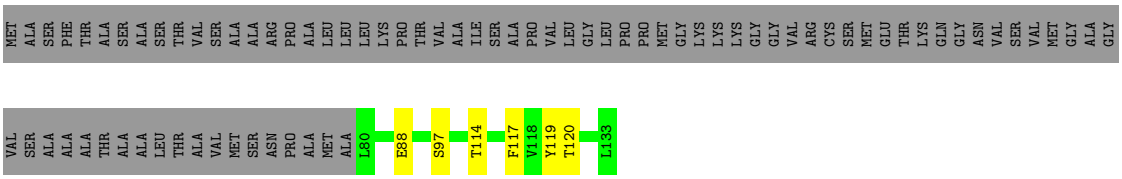
• Molecule 18: Photosystem II reaction center W protein, chloroplastic



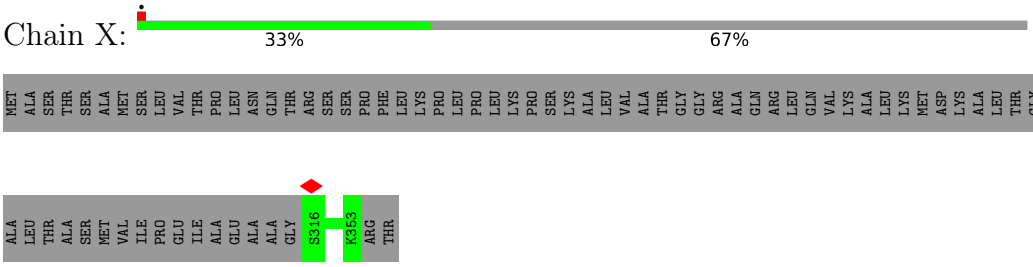


• Molecule 18: Photosystem II reaction center W protein, chloroplastic

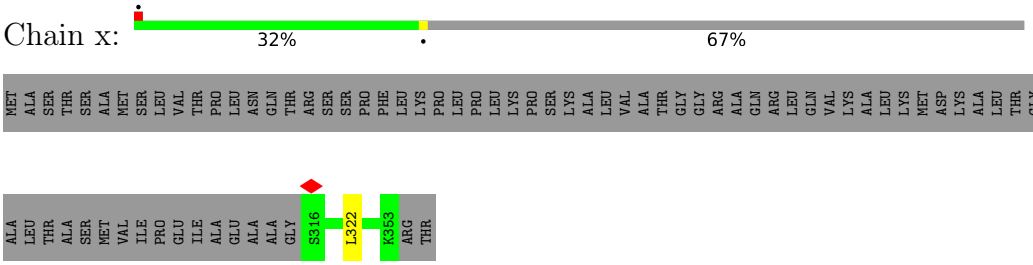




• Molecule 19: (thale cress) hypothetical protein

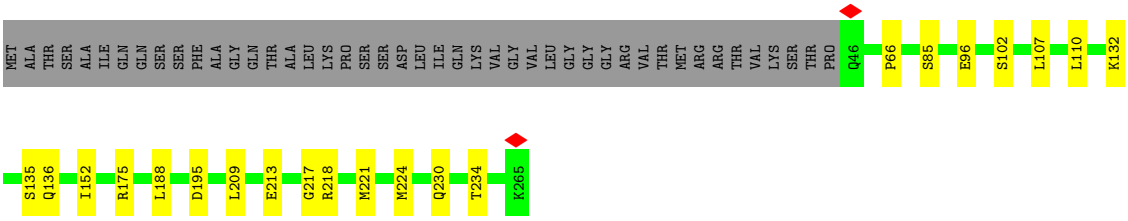


• Molecule 19: (thale cress) hypothetical protein



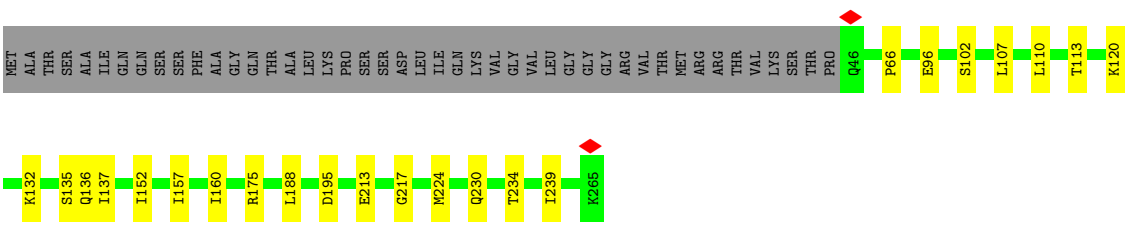
• Molecule 20: Chlorophyll a-b binding protein 2.2, chloroplastic





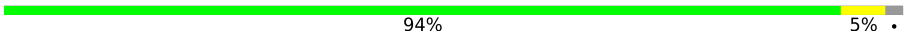
• Molecule 20: Chlorophyll a-b binding protein 2.2, chloroplastic

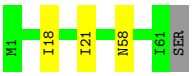




• Molecule 21: Photosystem II reaction center protein Z

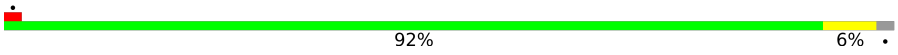
Chain Z:

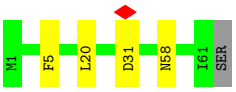




• Molecule 21: Photosystem II reaction center protein Z

Chain z:

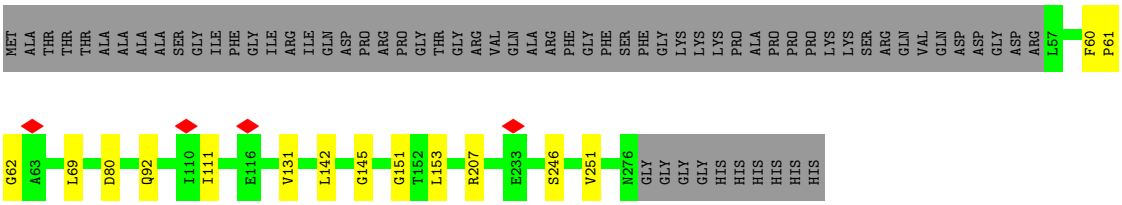




• Molecule 22: Chlorophyll a-b binding protein CP29.3, chloroplastic

Chain r:

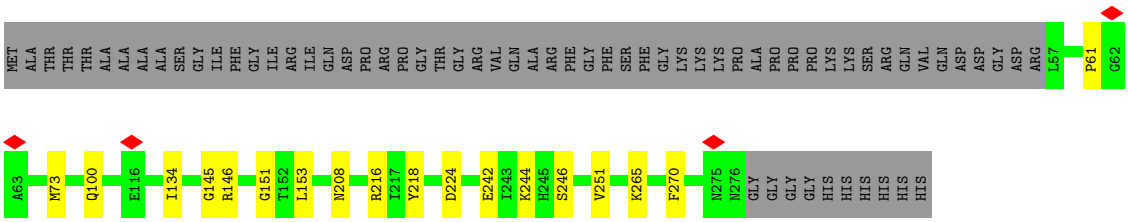




• Molecule 22: Chlorophyll a-b binding protein CP29.3, chloroplastic

Chain R:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104217	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	28.356	Depositor
Minimum map value	-16.319	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	1.048	Depositor
Recommended contour level	3	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: DGD, PHO, PL9, LUT, LMG, SQD, CLA, LHG, DMU, BCT, BCR, HEM, FE2, NEX, VTQ, CHL, XAT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/2704	0.54	0/3687
1	a	0.27	0/2704	0.56	1/3687 (0.0%)
2	B	0.22	0/3959	0.44	0/5394
2	b	0.22	0/3959	0.46	0/5394
3	C	0.23	0/3595	0.49	0/4899
3	c	0.23	0/3595	0.49	0/4899
4	D	0.24	0/2789	0.51	0/3803
4	d	0.24	0/2789	0.49	0/3803
5	E	0.30	0/593	0.79	1/808 (0.1%)
5	e	0.30	0/593	0.84	4/808 (0.5%)
6	F	0.31	0/241	0.78	2/327 (0.6%)
6	f	0.32	0/241	0.81	1/327 (0.3%)
7	G	0.23	0/1716	0.47	1/2336 (0.0%)
7	N	0.23	0/1716	0.47	0/2336
7	g	0.25	0/1716	0.55	1/2336 (0.0%)
7	n	0.22	0/1716	0.44	0/2336
8	H	0.29	0/447	0.52	0/608
8	h	0.30	0/447	0.58	0/608
9	I	0.28	0/285	0.58	0/385
9	i	0.28	0/285	0.56	0/385
10	J	0.23	0/225	0.43	0/306
10	j	0.23	0/225	0.42	0/306
11	K	0.47	0/312	0.86	0/428
11	k	0.44	0/312	0.89	0/428
12	L	0.23	0/317	0.52	0/431
12	l	0.29	0/317	0.62	0/431
13	M	0.41	0/254	0.69	0/348
13	m	0.35	0/254	0.71	0/348
14	O	0.23	0/1556	0.62	4/2104 (0.2%)
14	o	0.26	0/1556	0.66	4/2104 (0.2%)
15	S	0.26	0/1750	0.57	0/2376

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	s	0.25	0/1750	0.54	0/2376
16	T	0.23	0/246	0.53	0/333
16	t	0.29	0/246	0.65	0/333
17	U	0.13	0/181	0.39	0/242
17	u	0.12	0/181	0.40	0/242
18	W	0.24	0/438	0.54	0/594
18	w	0.22	0/438	0.47	0/594
19	X	0.25	0/270	0.48	0/367
19	x	0.25	0/270	0.49	0/367
20	Y	0.23	0/1753	0.51	0/2385
20	y	0.23	0/1753	0.51	0/2385
21	Z	0.30	0/468	0.64	0/641
21	z	0.33	0/468	0.71	0/641
22	R	0.25	0/1766	0.58	0/2403
22	r	0.23	0/1766	0.52	0/2403
All	All	0.25	0/55162	0.54	19/75082 (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
3	c	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	34	MET	CB-CG-SD	-6.43	93.41	112.70
14	O	311	THR	CA-C-N	6.36	133.69	121.54
14	O	311	THR	C-N-CA	6.36	133.69	121.54
14	o	311	THR	CA-C-N	6.21	133.40	121.54
14	o	311	THR	C-N-CA	6.21	133.40	121.54
7	g	173	GLU	CA-CB-CG	6.12	126.34	114.10
5	e	78	GLU	N-CA-CB	6.09	119.77	110.44
5	e	78	GLU	CA-CB-CG	5.96	126.01	114.10
5	E	78	GLU	N-CA-CB	5.93	120.08	110.40
7	G	197	ASP	CB-CA-C	5.85	120.27	111.14
6	F	34	MET	CA-CB-CG	5.71	125.52	114.10
5	e	77	ASP	CA-C-N	-5.62	112.21	122.38
5	e	77	ASP	C-N-CA	-5.62	112.21	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	218	LEU	CA-C-N	5.59	132.21	121.54
14	O	218	LEU	C-N-CA	5.59	132.21	121.54
14	o	218	LEU	CA-C-N	5.50	132.06	121.54
14	o	218	LEU	C-N-CA	5.50	132.06	121.54
1	a	304	GLN	CA-CB-CG	5.47	125.05	114.10
6	F	34	MET	CB-CG-SD	-5.05	97.54	112.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	413	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2527	22	0
1	a	2623	0	2527	24	0
2	B	3829	0	3707	30	0
2	b	3829	0	3707	36	0
3	C	3480	0	3409	27	0
3	c	3480	0	3409	28	0
4	D	2696	0	2585	22	0
4	d	2696	0	2585	25	0
5	E	576	0	559	3	0
5	e	576	0	559	4	0
6	F	235	0	242	1	0
6	f	235	0	242	1	0
7	G	1666	0	1593	12	0
7	N	1666	0	1593	19	0
7	g	1666	0	1593	12	0
7	n	1666	0	1593	18	0
8	H	438	0	465	4	0
8	h	438	0	465	8	0
9	I	277	0	289	3	0
9	i	277	0	289	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	219	0	231	0	0
10	j	219	0	231	1	0
11	K	301	0	313	2	0
11	k	301	0	313	2	0
12	L	309	0	298	5	0
12	l	309	0	298	6	0
13	M	250	0	273	5	0
13	m	250	0	273	4	0
14	O	1523	0	1504	11	0
14	o	1523	0	1504	12	0
15	S	1705	0	1681	14	0
15	s	1705	0	1681	15	0
16	T	239	0	255	1	0
16	t	239	0	255	2	0
17	U	179	0	190	3	0
17	u	179	0	190	3	0
18	W	427	0	405	6	0
18	w	427	0	405	5	0
19	X	267	0	292	0	0
19	x	267	0	292	1	0
20	Y	1699	0	1630	17	0
20	y	1699	0	1630	17	0
21	Z	458	0	490	2	0
21	z	458	0	490	4	0
22	R	1718	0	1691	13	0
22	r	1718	0	1691	11	0
23	A	175	0	170	6	0
23	B	1040	0	1152	23	0
23	C	810	0	854	21	0
23	D	195	0	216	9	0
23	G	448	0	429	9	0
23	N	435	0	396	7	0
23	R	511	0	493	11	0
23	S	415	0	313	8	0
23	Y	466	0	454	15	0
23	a	125	0	131	5	0
23	b	1040	0	1152	22	0
23	c	810	0	854	16	0
23	d	245	0	255	8	0
23	g	448	0	429	9	0
23	n	435	0	396	8	0
23	r	511	0	493	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	s	415	0	313	6	0
23	y	466	0	454	12	0
24	A	64	0	74	3	0
24	D	64	0	74	5	0
24	a	128	0	148	4	0
25	A	40	0	56	1	0
25	B	120	0	168	8	0
25	C	120	0	168	10	0
25	D	40	0	56	1	0
25	H	40	0	56	3	0
25	K	40	0	56	1	0
25	a	40	0	56	4	0
25	b	120	0	168	11	0
25	c	80	0	112	6	0
25	d	40	0	56	1	0
25	h	40	0	56	2	0
25	k	40	0	56	3	0
25	z	40	0	56	2	0
26	A	50	0	67	0	0
26	B	54	0	78	3	0
26	C	45	0	54	2	0
26	L	54	0	78	1	0
26	a	50	0	67	2	0
26	b	54	0	78	3	0
26	c	45	0	54	1	0
26	l	54	0	78	4	0
27	A	4	0	0	2	0
27	a	4	0	0	2	0
28	A	59	0	76	1	0
28	B	115	0	146	4	0
28	C	55	0	68	2	0
28	D	62	0	82	3	0
28	b	56	0	70	0	0
28	c	55	0	68	2	0
28	d	62	0	82	5	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	B	91	0	122	6	0
30	C	98	0	139	2	0
30	D	46	0	62	1	0
30	S	55	0	86	0	0
30	W	51	0	75	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	48	0	66	0	0
30	b	91	0	122	6	0
30	c	50	0	73	0	0
30	d	46	0	62	0	0
30	s	55	0	86	0	0
30	w	51	0	75	0	0
31	B	135	0	192	3	0
31	C	49	0	74	2	0
31	D	98	0	148	4	0
31	G	46	0	65	2	0
31	L	98	0	148	4	0
31	N	49	0	74	2	0
31	R	42	0	57	1	0
31	S	49	0	74	3	0
31	W	49	0	74	1	0
31	Y	49	0	74	3	0
31	b	135	0	192	3	0
31	c	98	0	148	2	0
31	d	98	0	148	7	0
31	g	46	0	65	4	0
31	l	98	0	148	3	0
31	n	49	0	74	1	0
31	r	42	0	57	1	0
31	s	49	0	74	2	0
31	y	49	0	74	3	0
32	C	66	0	84	2	0
32	S	33	0	42	1	0
32	c	66	0	84	2	0
32	s	33	0	42	1	0
33	D	55	0	80	2	0
33	d	55	0	80	0	0
34	F	43	0	30	1	0
34	f	43	0	30	1	0
35	G	325	0	286	7	0
35	N	338	0	305	9	0
35	R	153	0	119	2	0
35	S	184	0	125	5	0
35	Y	365	0	354	13	0
35	g	325	0	286	8	0
35	n	338	0	305	11	0
35	r	153	0	119	2	0
35	s	184	0	125	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	y	365	0	354	15	0
36	G	84	0	112	6	0
36	N	84	0	112	9	0
36	R	42	0	56	4	0
36	S	84	0	112	6	0
36	Y	84	0	112	7	0
36	g	84	0	112	5	0
36	n	84	0	112	7	0
36	r	42	0	56	3	0
36	s	84	0	112	4	0
36	y	84	0	112	7	0
37	G	88	0	112	4	0
37	R	44	0	56	1	0
37	Y	44	0	56	5	0
37	g	88	0	112	6	0
37	r	44	0	56	2	0
37	y	44	0	56	6	0
38	G	44	0	56	1	0
38	N	44	0	56	3	0
38	R	88	0	112	6	0
38	S	44	0	56	1	0
38	Y	44	0	56	1	0
38	g	44	0	56	1	0
38	n	44	0	56	1	0
38	r	44	0	56	1	0
38	s	44	0	56	1	0
39	W	32	0	50	0	0
39	w	32	0	50	0	0
All	All	71232	0	71854	714	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 5.

All (714) 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)
23:Y:311:CLA:HAB	36:Y:316:LUT:H32	1.62	0.80
3:c:276:LEU:HD21	23:c:508:CLA:HAB	1.69	0.75
23:s:609:CLA:HAB	36:s:614:LUT:H32	1.70	0.74
3:C:276:LEU:HD21	23:C:509:CLA:HAB	1.69	0.74
23:n:602:CLA:HAB	36:n:616:LUT:H32	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:514:CLA:HBB1	25:C:515:BCR:H24C	1.70	0.73
23:n:610:CLA:HAB	36:n:615:LUT:H32	1.69	0.73
35:G:601:CHL:H52	35:Y:310:CHL:HBB1	1.69	0.73
7:n:226:MET:HE2	36:n:616:LUT:H10	1.70	0.73
23:y:311:CLA:HAB	36:y:316:LUT:H32	1.71	0.72
15:S:236:MET:HE1	36:S:316:LUT:H10	1.72	0.72
23:c:513:CLA:HBB1	25:z:101:BCR:H24C	1.71	0.72
23:G:610:CLA:HAB	36:G:615:LUT:H32	1.72	0.70
23:S:310:CLA:HAB	36:S:315:LUT:H32	1.75	0.68
20:y:213:GLU:OE1	23:y:311:CLA:NB	2.27	0.68
22:R:61:PRO:HG3	23:R:302:CLA:H3A	1.76	0.68
20:Y:213:GLU:OE1	23:Y:311:CLA:NB	2.27	0.67
6:F:30:SER:O	6:F:34:MET:HB3	1.95	0.67
2:b:254:GLY:HA3	28:d:410:DGD:HB51	1.77	0.66
23:A:402:CLA:HAB	23:D:403:CLA:H72	1.78	0.66
35:g:601:CHL:H52	35:y:310:CHL:HBB1	1.79	0.65
7:n:183:LEU:HD13	35:n:608:CHL:HAB	1.79	0.64
7:N:183:LEU:HD13	35:N:608:CHL:HAB	1.79	0.63
20:Y:224:MET:HE2	36:Y:317:LUT:H10	1.80	0.62
23:g:610:CLA:HAB	36:g:615:LUT:H32	1.80	0.62
22:r:61:PRO:HG3	23:r:601:CLA:H3A	1.82	0.61
1:A:272:HIS:CE1	27:A:407:BCT:O3	2.52	0.61
2:B:277:GLN:HB3	17:U:99:LYS:HG3	1.82	0.61
3:c:178:LYS:HB2	23:c:502:CLA:H172	1.83	0.61
37:Y:301:XAT:H32	31:Y:319:LHG:H191	1.82	0.60
2:b:225:LEU:O	2:b:229:LEU:HB2	2.01	0.60
1:a:272:HIS:CE1	27:a:408:BCT:O3	2.53	0.60
12:L:13:LEU:H	13:M:29:THR:HG21	1.67	0.60
20:y:224:MET:HE2	36:y:317:LUT:H10	1.84	0.59
1:a:331:MET:HE2	4:d:321:LEU:HB3	1.83	0.59
8:h:29:GLU:HB2	8:h:32:LYS:HG3	1.85	0.59
1:a:304:GLN:NE2	3:c:415:ASN:OD1	2.35	0.59
37:y:301:XAT:H32	31:y:318:LHG:H191	1.85	0.59
4:D:119:GLY:HA3	24:D:402:PHO:H92	1.85	0.58
7:G:144:LEU:HB3	7:G:155:ALA:HB3	1.85	0.58
7:G:226:MET:HG2	36:G:616:LUT:H12	1.85	0.58
23:N:610:CLA:HAB	36:N:615:LUT:H32	1.84	0.58
23:g:602:CLA:H102	23:y:304:CLA:H41	1.86	0.58
37:G:617:XAT:H222	35:N:601:CHL:HMC	1.86	0.58
31:D:407:LHG:H291	16:T:17:ILE:HG23	1.86	0.57
7:N:226:MET:HG2	36:N:616:LUT:H12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:y:137:ILE:HG21	20:y:157:ILE:HD13	1.86	0.57
23:b:614:CLA:H8	23:b:615:CLA:HAB	1.87	0.57
24:a:403:PHO:H92	4:d:119:GLY:HA3	1.87	0.57
7:n:76:GLY:HA3	7:n:216:LEU:HD23	1.87	0.57
27:a:408:BCT:O2	4:d:269:HIS:CE1	2.57	0.57
2:b:391:SER:OG	2:b:392:VAL:N	2.38	0.57
15:s:236:MET:HG2	36:s:615:LUT:H14	1.87	0.57
23:B:612:CLA:H8	23:B:613:CLA:HAB	1.87	0.56
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.88	0.56
23:c:513:CLA:H101	25:z:101:BCR:H23C	1.87	0.56
1:A:212:SER:HB2	4:D:212:CYS:HB2	1.87	0.56
31:d:407:LHG:H311	16:t:21:ILE:HD11	1.85	0.56
35:G:601:CHL:HMC	37:G:620:XAT:H242	1.88	0.56
27:A:407:BCT:O2	4:D:269:HIS:CE1	2.57	0.56
35:g:601:CHL:HMC	37:g:620:XAT:H242	1.88	0.56
3:C:178:LYS:HB2	23:C:503:CLA:H172	1.86	0.56
7:N:246:ASP:O	7:N:254:ASN:ND2	2.38	0.56
23:C:514:CLA:H101	25:C:515:BCR:H23C	1.88	0.56
7:G:239:GLY:O	7:G:243:ASN:ND2	2.39	0.56
23:B:608:CLA:HAB	4:D:124:ILE:HG23	1.87	0.55
2:B:141:ILE:HG13	2:B:217:LEU:HD21	1.89	0.55
37:g:617:XAT:H222	35:n:601:CHL:HMC	1.88	0.55
14:o:146:LYS:HE3	14:o:320:ASP:H	1.72	0.55
7:n:246:ASP:O	7:n:254:ASN:ND2	2.38	0.55
2:b:269:GLY:O	2:b:448:ARG:NH1	2.40	0.55
31:d:407:LHG:H291	16:t:17:ILE:HG23	1.87	0.55
23:A:404:CLA:H3A	30:C:501:LMG:H122	1.88	0.55
8:H:17:THR:HG23	8:H:20:GLY:H	1.70	0.55
22:R:208:ASN:HA	22:R:216:ARG:HE	1.71	0.55
1:a:212:SER:HB2	4:d:212:CYS:HB2	1.88	0.55
7:G:103:SER:HB2	7:G:219:GLY:HA3	1.89	0.55
26:L:103:SQD:H441	26:L:103:SQD:H102	1.88	0.55
3:c:305:THR:HG22	3:c:307:PRO:HD2	1.88	0.54
23:b:609:CLA:H161	23:b:615:CLA:H171	1.89	0.54
31:L:101:LHG:H331	13:M:18:PRO:HB3	1.89	0.54
7:n:55:ARG:NH1	7:n:77:ASP:OD2	2.41	0.54
24:D:402:PHO:HHC	23:D:403:CLA:H11	1.88	0.54
14:O:281:SER:HB2	14:O:308:PRO:HG3	1.90	0.54
37:Y:301:XAT:H30	31:Y:319:LHG:H211	1.89	0.54
23:b:615:CLA:H12	23:b:615:CLA:H2A	1.90	0.54
23:B:610:CLA:H43	23:B:612:CLA:H51	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:17:THR:HG23	8:h:20:GLY:H	1.72	0.54
2:B:391:SER:OG	2:B:392:VAL:N	2.40	0.54
2:b:222:PRO:HB3	8:h:38:GLY:H	1.73	0.54
23:b:609:CLA:H12	30:b:622:LMG:H121	1.90	0.54
2:B:269:GLY:O	2:B:448:ARG:NH1	2.41	0.53
23:B:607:CLA:H12	30:B:620:LMG:H121	1.90	0.53
14:O:166:ARG:NH2	18:W:88:GLU:OE1	2.41	0.53
20:y:132:LYS:HA	35:y:308:CHL:HED3	1.91	0.53
23:n:603:CLA:HBB1	35:n:609:CHL:H161	1.91	0.53
23:b:612:CLA:H43	23:b:614:CLA:H51	1.90	0.53
23:B:613:CLA:H12	23:B:613:CLA:H2A	1.89	0.53
7:N:76:GLY:HA3	7:N:216:LEU:HD23	1.90	0.53
2:b:272:ARG:NH1	2:b:276:ASP:OD2	2.41	0.53
9:i:5:LYS:NZ	18:w:97:SER:OG	2.42	0.53
2:B:311:PHE:O	2:B:317:ASN:ND2	2.42	0.53
2:B:222:PRO:HB3	8:H:38:GLY:H	1.72	0.53
2:B:255:THR:HG21	23:B:602:CLA:HED1	1.91	0.53
2:b:25:MET:HE3	25:b:619:BCR:H23C	1.91	0.53
23:Y:304:CLA:H91	35:Y:310:CHL:H121	1.90	0.53
23:R:309:CLA:H43	23:R:313:CLA:H122	1.91	0.52
2:b:311:PHE:O	2:b:317:ASN:ND2	2.42	0.52
23:r:608:CLA:H43	23:r:612:CLA:H122	1.91	0.52
1:A:192:ILE:HA	1:A:293:MET:HE1	1.91	0.52
7:G:138:ILE:HG21	7:G:158:ILE:HD13	1.91	0.52
2:b:141:ILE:HG13	2:b:217:LEU:HD21	1.92	0.52
23:b:606:CLA:HBB1	23:b:615:CLA:HBC2	1.92	0.52
23:C:512:CLA:HBC2	11:K:55:GLN:HG3	1.91	0.52
4:D:130:GLN:NE2	24:D:402:PHO:OBD	2.43	0.52
7:N:210:GLU:HG2	7:N:214:LYS:HE2	1.91	0.52
7:n:250:ASP:OD1	7:n:254:ASN:ND2	2.43	0.52
7:n:103:SER:HB3	7:n:219:GLY:HA3	1.90	0.52
14:O:311:THR:HB	14:O:318:PRO:HG3	1.91	0.52
26:C:521:SQD:H112	23:S:311:CLA:HBB1	1.91	0.51
2:b:235:GLU:OE2	2:b:472:ARG:NH1	2.40	0.51
3:c:27:ASP:N	3:c:27:ASP:OD1	2.43	0.51
15:s:194:LEU:HB2	35:s:607:CHL:HMC	1.91	0.51
23:B:604:CLA:HBB1	23:B:613:CLA:HBC2	1.93	0.51
11:k:30:TYR:OH	21:z:58:ASN:ND2	2.42	0.51
31:n:618:LHG:H311	31:n:618:LHG:H122	1.93	0.51
23:B:607:CLA:H161	23:B:613:CLA:H171	1.92	0.51
25:C:515:BCR:HC42	25:C:519:BCR:HC42	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:10:SER:OG	13:m:28:LYS:NZ	2.43	0.51
31:l:102:LHG:H331	13:m:18:PRO:HB3	1.92	0.51
23:g:602:CLA:H92	23:g:603:CLA:HHB	1.91	0.51
24:a:403:PHO:OBD	4:d:130:GLN:NE2	2.43	0.51
22:r:145:GLY:HA3	22:r:246:SER:HB2	1.93	0.51
20:y:113:THR:HG23	20:y:239:ILE:HD11	1.93	0.51
2:B:71:ILE:HD11	23:B:606:CLA:H2A	1.93	0.51
1:a:304:GLN:HE22	3:c:414:ILE:HG12	1.75	0.51
23:B:602:CLA:H42	28:D:410:DGD:HB22	1.92	0.51
14:o:281:SER:HB2	14:o:308:PRO:HG3	1.92	0.51
28:B:624:DGD:HB91	28:B:624:DGD:HA91	1.93	0.51
2:b:477:ASP:OD1	2:b:477:ASP:N	2.44	0.51
7:N:161:ILE:HG12	35:N:605:CHL:HBC2	1.93	0.50
20:Y:175:ARG:NH2	35:Y:310:CHL:O1D	2.45	0.50
2:B:57:ARG:NH1	2:B:317:ASN:OD1	2.44	0.50
20:Y:132:LYS:HA	35:Y:308:CHL:HED3	1.93	0.50
2:b:64:PRO:HB3	2:b:267:LEU:HB3	1.94	0.50
7:g:103:SER:HB2	7:g:219:GLY:HA3	1.94	0.50
12:l:27:VAL:HG11	31:l:102:LHG:H201	1.92	0.50
4:d:52:GLY:HA2	4:d:56:VAL:HB	1.94	0.50
22:R:145:GLY:HA3	22:R:246:SER:HB2	1.93	0.50
2:B:474:LEU:O	4:D:135:ARG:NH1	2.44	0.50
3:c:130:ILE:HD11	25:c:518:BCR:H21C	1.94	0.50
1:A:29:TYR:O	1:A:129:ARG:NH1	2.45	0.50
28:B:624:DGD:O3D	14:o:162:LYS:NZ	2.43	0.50
4:D:124:ILE:HD11	28:D:410:DGD:HAH2	1.94	0.50
1:a:85:THR:HA	1:a:109:GLY:HA3	1.94	0.50
12:l:12:GLU:HB2	13:m:29:THR:HG23	1.94	0.50
1:a:95:PRO:HA	23:a:404:CLA:HED3	1.93	0.49
7:g:85:LEU:HD11	23:y:304:CLA:H12	1.94	0.49
8:h:67:LEU:HD21	19:x:322:LEU:HD13	1.93	0.49
23:A:401:CLA:H192	23:D:401:CLA:H161	1.93	0.49
2:B:57:ARG:NH2	2:B:334:ASP:OD1	2.45	0.49
25:B:617:BCR:H383	31:l:103:LHG:H291	1.94	0.49
9:I:5:LYS:NZ	18:W:97:SER:OG	2.45	0.49
13:M:28:LYS:HB2	13:m:27:VAL:HG12	1.94	0.49
3:c:343:ARG:NH1	3:c:347:GLY:O	2.45	0.49
7:g:138:ILE:HG21	7:g:158:ILE:HD13	1.93	0.49
24:a:403:PHO:H152	23:d:402:CLA:HMB2	1.94	0.49
20:y:102:SER:HB3	20:y:217:GLY:HA3	1.94	0.49
37:y:301:XAT:H30	31:y:318:LHG:H211	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:R:308:CHL:H101	35:R:308:CHL:HAB	1.95	0.49
1:A:133:LEU:HD23	4:D:257:ILE:HG12	1.94	0.49
2:B:25:MET:HE3	25:B:617:BCR:H23C	1.94	0.49
7:G:240:PRO:HB3	36:G:615:LUT:H41	1.94	0.49
17:U:81:THR:OG1	17:U:82:GLU:N	2.45	0.49
7:g:240:PRO:HB3	36:g:615:LUT:H41	1.92	0.49
20:y:175:ARG:NH2	35:y:310:CHL:O1D	2.45	0.49
22:R:146:ARG:NE	22:R:242:GLU:OE2	2.45	0.49
3:C:225:VAL:O	3:C:293:ASN:ND2	2.44	0.49
4:D:55:PHE:O	5:E:49:SER:OG	2.31	0.49
2:b:87:ASN:ND2	30:b:601:LMG:O4	2.43	0.49
2:b:255:THR:HG21	23:b:604:CLA:HED1	1.94	0.49
3:c:228:ASP:OD1	3:c:228:ASP:N	2.45	0.49
22:r:151:GLY:HA2	37:r:614:XAT:H181	1.93	0.49
2:B:156:PHE:HB3	2:B:162:TYR:HB3	1.94	0.49
15:S:194:LEU:HB2	35:S:308:CHL:HMC	1.94	0.49
2:b:113:TRP:NE1	26:b:602:SQD:O3	2.45	0.49
23:A:404:CLA:H92	9:I:16:VAL:HG11	1.94	0.49
20:Y:102:SER:HB3	20:Y:217:GLY:HA3	1.93	0.49
2:b:57:ARG:NH1	2:b:317:ASN:OD1	2.44	0.49
15:s:190:ILE:HG23	15:s:191:THR:HG23	1.95	0.49
3:C:79:LYS:HD2	3:C:84:GLN:HG2	1.95	0.49
31:D:408:LHG:H342	31:D:408:LHG:H131	1.94	0.49
5:E:35:TRP:O	5:E:39:SER:HB3	2.12	0.49
15:S:117:HIS:HD2	36:S:316:LUT:H15	1.78	0.49
14:o:166:ARG:NH2	18:w:88:GLU:OE2	2.45	0.49
1:A:292:THR:HG22	3:C:428:THR:HG23	1.94	0.49
23:A:401:CLA:H152	23:D:401:CLA:H102	1.95	0.49
15:S:68:ARG:NH1	31:S:318:LHG:O1	2.45	0.49
23:b:610:CLA:H172	23:b:611:CLA:H18	1.95	0.49
1:A:27:ARG:HA	3:C:472:LEU:HD11	1.95	0.49
1:A:85:THR:HA	1:A:109:GLY:HA3	1.95	0.49
2:B:272:ARG:NH1	2:B:276:ASP:OD2	2.45	0.49
12:L:10:SER:OG	13:M:28:LYS:NZ	2.42	0.49
23:a:404:CLA:H92	9:i:16:VAL:HG11	1.94	0.49
35:s:607:CHL:H12	36:s:614:LUT:H383	1.95	0.49
2:B:87:ASN:ND2	30:B:623:LMG:O4	2.42	0.48
7:N:59:LEU:HB3	7:N:62:PHE:HB2	1.95	0.48
7:N:176:ARG:NH2	35:N:609:CHL:O1D	2.46	0.48
15:S:160:LEU:HD22	23:S:305:CLA:HED1	1.95	0.48
4:d:55:PHE:O	5:e:49:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:118:ALA:HB1	15:S:229:GLY:HA3	1.95	0.48
20:Y:218:ARG:HA	20:Y:221:MET:HG3	1.95	0.48
1:A:95:PRO:HA	23:A:404:CLA:HED3	1.95	0.48
3:C:40:ALA:HB2	23:C:509:CLA:H2A	1.94	0.48
11:K:30:TYR:OH	21:Z:58:ASN:ND2	2.47	0.48
15:S:89:VAL:HG21	15:S:107:PHE:HE2	1.77	0.48
20:Y:230:GLN:O	20:Y:234:THR:OG1	2.29	0.48
2:b:57:ARG:NH2	2:b:334:ASP:OD1	2.47	0.48
23:b:610:CLA:HAB	4:d:124:ILE:HG23	1.96	0.48
4:D:160:ILE:HG21	4:D:288:VAL:HG22	1.95	0.48
23:S:303:CLA:H3A	23:S:303:CLA:HBA2	1.61	0.48
2:b:474:LEU:O	4:d:135:ARG:NH1	2.46	0.48
31:d:408:LHG:H342	31:d:408:LHG:H131	1.95	0.48
23:y:304:CLA:H91	35:y:310:CHL:H121	1.94	0.48
31:C:518:LHG:H242	23:Y:312:CLA:H43	1.96	0.48
23:N:602:CLA:HAB	36:N:616:LUT:H32	1.95	0.48
3:c:462:ASP:OD1	3:c:462:ASP:N	2.47	0.48
4:d:193:THR:HG23	23:d:403:CLA:HBC2	1.95	0.48
5:e:35:TRP:O	5:e:39:SER:HB3	2.13	0.48
26:l:101:SQD:H102	26:l:101:SQD:H441	1.94	0.48
15:s:186:GLU:HA	15:s:189:ARG:HG2	1.94	0.48
7:n:210:GLU:HG2	7:n:214:LYS:HE2	1.96	0.48
3:C:148:GLY:O	3:C:156:LYS:NZ	2.45	0.48
12:l:2:THR:OG1	12:l:3:GLN:N	2.47	0.48
2:b:71:ILE:HD11	23:b:608:CLA:H2A	1.95	0.48
3:c:225:VAL:O	3:c:293:ASN:ND2	2.45	0.48
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.95	0.48
1:A:140:ARG:NH2	31:D:408:LHG:O5	2.47	0.48
23:S:310:CLA:HBA2	23:S:310:CLA:H3A	1.51	0.48
15:s:176:VAL:HA	15:s:179:VAL:HG12	1.95	0.48
23:g:613:CLA:H12	23:g:614:CLA:HED2	1.95	0.47
2:B:64:PRO:HB3	2:B:267:LEU:HB3	1.96	0.47
7:G:246:ASP:OD1	7:G:254:ASN:ND2	2.47	0.47
15:S:110:TYR:HB3	23:S:303:CLA:HHB	1.95	0.47
1:a:133:LEU:HD23	4:d:257:ILE:HG12	1.96	0.47
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.96	0.47
3:C:462:ASP:OD1	3:C:462:ASP:N	2.47	0.47
24:D:402:PHO:H41	24:D:402:PHO:H61	1.60	0.47
4:d:81:THR:OG1	4:d:168:TRP:O	2.30	0.47
28:d:410:DGD:HG11	8:h:62:ASN:ND2	2.29	0.47
7:g:108:LEU:HB3	23:g:604:CLA:HBB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:251:VAL:HG21	31:R:317:LHG:H261	1.96	0.47
35:S:306:CHL:HMC	35:S:307:CHL:C4C	2.45	0.47
1:a:261:GLN:HE22	1:a:264:SER:H	1.62	0.47
2:b:321:LYS:NZ	2:b:363:PHE:O	2.48	0.47
35:N:607:CHL:HAA2	37:Y:301:XAT:H241	1.95	0.47
23:Y:303:CLA:HBA2	23:Y:303:CLA:H3A	1.51	0.47
1:a:140:ARG:NH2	31:d:408:LHG:O5	2.47	0.47
7:n:176:ARG:NH2	35:n:609:CHL:O1D	2.47	0.47
20:y:107:LEU:HB3	23:y:305:CLA:HBB2	1.96	0.47
2:B:7:ARG:NH2	31:B:622:LHG:O5	2.48	0.47
23:B:614:CLA:H8	23:B:614:CLA:H52	1.71	0.47
3:C:130:ILE:HD11	25:C:519:BCR:H21C	1.97	0.47
31:b:624:LHG:O4	4:d:142:TYR:OH	2.33	0.47
35:r:607:CHL:H101	35:r:607:CHL:HAB	1.97	0.47
15:s:231:LEU:HD21	23:s:611:CLA:HBC2	1.96	0.47
38:R:301:NEX:H15	38:R:301:NEX:H201	1.78	0.47
23:C:507:CLA:HBB2	23:C:508:CLA:H62	1.97	0.47
4:D:52:GLY:HA2	4:D:56:VAL:HB	1.96	0.47
2:b:156:PHE:HB3	2:b:162:TYR:HB3	1.95	0.47
25:b:619:BCR:H322	30:b:622:LMG:H111	1.97	0.47
4:d:124:ILE:HD11	28:d:410:DGD:HAH2	1.97	0.47
23:s:609:CLA:HED2	23:s:609:CLA:H2A	1.96	0.47
3:c:168:LEU:HD13	23:c:507:CLA:H43	1.97	0.47
22:R:151:GLY:HA2	37:R:315:XAT:H181	1.96	0.47
2:B:320:ALA:HB1	4:D:293:ASN:HD22	1.80	0.47
4:D:162:PRO:HB3	4:D:171:ALA:HB2	1.96	0.47
4:d:162:PRO:HB3	4:d:171:ALA:HB2	1.97	0.47
23:s:602:CLA:HBA2	23:s:602:CLA:H3A	1.61	0.47
18:w:117:PHE:HA	18:w:120:THR:HG22	1.97	0.47
35:n:601:CHL:H61	35:n:601:CHL:H41	1.79	0.47
3:C:168:LEU:HD13	23:C:508:CLA:H43	1.97	0.47
3:c:79:LYS:HD2	3:c:84:GLN:HG2	1.96	0.47
7:N:250:ASP:OD1	7:N:254:ASN:ND2	2.48	0.46
18:W:117:PHE:HA	18:W:120:THR:HG22	1.97	0.46
15:s:68:ARG:NH1	31:s:617:LHG:O1	2.47	0.46
25:c:518:BCR:H24C	25:c:518:BCR:H371	1.75	0.46
2:B:477:ASP:OD1	2:B:477:ASP:N	2.49	0.46
23:Y:311:CLA:H52	36:Y:316:LUT:H30	1.97	0.46
1:a:341:LEU:HD21	3:c:410:VAL:HG11	1.97	0.46
22:R:218:TYR:HB3	23:R:310:CLA:HED2	1.97	0.46
7:G:186:ALA:HB2	35:G:608:CHL:HBC1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:94:ARG:HH21	20:Y:66:PRO:HG3	1.80	0.46
14:O:232:LEU:HA	14:O:282:VAL:HA	1.97	0.46
17:U:97:THR:HA	17:U:102:ARG:HH21	1.80	0.46
31:Y:319:LHG:HC91	31:Y:319:LHG:H321	1.96	0.46
23:G:613:CLA:H12	23:G:614:CLA:HED2	1.97	0.46
23:r:609:CLA:H52	36:r:613:LUT:H30	1.98	0.46
20:y:135:SER:HB3	35:y:308:CHL:HED2	1.97	0.46
23:N:610:CLA:H3A	23:N:610:CLA:HBA2	1.65	0.46
1:a:292:THR:HG22	3:c:428:THR:HG23	1.98	0.46
23:R:303:CLA:HBA2	23:R:303:CLA:H3A	1.57	0.46
23:S:304:CLA:H2A	23:S:304:CLA:HED2	1.98	0.46
1:a:29:TYR:O	1:a:129:ARG:NH1	2.45	0.46
7:g:186:ALA:HB2	35:g:608:CHL:HBC1	1.97	0.46
7:N:186:ALA:HA	7:N:192:PRO:HB3	1.98	0.46
4:d:160:ILE:HG21	4:d:288:VAL:HG22	1.98	0.46
7:g:50:TRP:NE1	7:g:210:GLU:OE2	2.49	0.46
14:o:136:PHE:HB2	14:o:174:ILE:HB	1.98	0.46
2:b:368:VAL:HB	2:b:381:VAL:HB	1.98	0.46
3:c:40:ALA:HB2	23:c:508:CLA:H2A	1.96	0.46
3:c:116:VAL:HG22	25:c:518:BCR:H323	1.98	0.46
3:c:396:MET:HE3	3:c:396:MET:HB3	1.83	0.46
35:y:310:CHL:HBA2	35:y:310:CHL:H3A	1.62	0.46
2:b:370:LEU:HD12	2:b:379:ALA:HB3	1.98	0.45
23:B:601:CLA:HAC1	25:H:101:BCR:H383	1.98	0.45
4:D:193:THR:HG23	23:D:403:CLA:HBC2	1.97	0.45
28:D:410:DGD:O5D	28:D:410:DGD:O4D	2.31	0.45
12:L:27:VAL:HG11	31:L:101:LHG:H201	1.98	0.45
31:L:102:LHG:H291	25:b:619:BCR:H383	1.98	0.45
11:k:29:ALA:HB1	21:z:5:PHE:HE2	1.80	0.45
7:n:94:ARG:HH21	20:y:66:PRO:HG3	1.80	0.45
3:C:174:LEU:HG	23:C:503:CLA:H171	1.98	0.45
23:b:609:CLA:HBB1	30:b:622:LMG:H191	1.99	0.45
7:g:149:ASN:OD1	7:g:151:SER:OG	2.33	0.45
14:O:146:LYS:HE3	14:O:320:ASP:H	1.82	0.45
23:r:610:CLA:H2A	23:r:610:CLA:HED3	1.98	0.45
22:R:244:LYS:NZ	23:R:311:CLA:O1D	2.46	0.45
38:N:617:NEX:H15	38:N:617:NEX:H201	1.81	0.45
25:a:405:BCR:H11C	25:a:405:BCR:H341	1.84	0.45
26:C:521:SQD:H442	31:S:318:LHG:HC12	1.99	0.45
38:Y:318:NEX:H15	38:Y:318:NEX:H201	1.78	0.45
23:c:507:CLA:HMA1	23:c:507:CLA:H2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:n:610:CLA:HBA2	23:n:610:CLA:H3A	1.65	0.45
38:n:617:NEX:H11	38:n:617:NEX:H191	1.82	0.45
31:y:318:LHG:HC91	31:y:318:LHG:H321	1.98	0.45
15:S:64:GLY:H	15:S:87:GLY:HA3	1.81	0.45
1:a:283:ILE:HA	1:a:286:THR:HG22	1.98	0.45
23:a:401:CLA:H192	23:d:401:CLA:H161	1.97	0.45
23:r:603:CLA:H62	23:r:603:CLA:H41	1.72	0.45
20:y:120:LYS:HE2	20:y:120:LYS:HB2	1.78	0.45
14:O:136:PHE:HB2	14:O:174:ILE:HB	1.99	0.45
23:b:618:CLA:H93	23:b:618:CLA:H41	1.99	0.45
3:c:246:PHE:HD2	32:c:522:DMU:H23	1.81	0.45
28:d:410:DGD:HG11	8:h:62:ASN:HD22	1.82	0.45
36:g:615:LUT:H35	36:g:615:LUT:H401	1.81	0.45
35:y:308:CHL:H3A	35:y:308:CHL:HBA1	1.71	0.45
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.99	0.45
23:c:510:CLA:H41	31:d:408:LHG:H151	1.99	0.45
22:R:73:MET:HE1	22:R:134:ILE:HG12	1.99	0.45
25:H:101:BCR:H20C	25:H:101:BCR:H361	1.84	0.45
3:C:246:PHE:HD2	32:C:523:DMU:H23	1.82	0.44
23:a:401:CLA:H152	23:d:401:CLA:H102	1.98	0.44
2:b:277:GLN:HB3	17:u:99:LYS:HG3	1.99	0.44
37:g:620:XAT:H15	37:g:620:XAT:H201	1.80	0.44
38:s:616:NEX:H15	38:s:616:NEX:H201	1.80	0.44
1:A:283:ILE:HA	1:A:286:THR:HG22	1.98	0.44
3:C:110:PRO:HB3	32:C:520:DMU:H1	1.99	0.44
25:b:620:BCR:H24C	25:b:620:BCR:H371	1.82	0.44
20:y:195:ASP:OD1	36:y:316:LUT:O23	2.35	0.44
23:C:504:CLA:H202	23:C:504:CLA:H162	1.87	0.44
38:N:617:NEX:H11	38:N:617:NEX:H191	1.86	0.44
2:b:62:VAL:HG12	2:b:66:MET:HE2	2.00	0.44
25:b:620:BCR:H15C	25:b:620:BCR:H351	1.82	0.44
4:d:187:GLN:HB2	23:d:403:CLA:HBC1	1.99	0.44
1:A:261:GLN:HE22	1:A:264:SER:H	1.66	0.44
25:A:405:BCR:H15C	25:A:405:BCR:H351	1.87	0.44
26:B:625:SQD:O8	8:H:15:ARG:NH1	2.46	0.44
31:C:518:LHG:H321	31:C:518:LHG:H352	1.81	0.44
23:G:603:CLA:H93	23:Y:304:CLA:H102	2.00	0.44
1:a:202:VAL:HG23	23:a:401:CLA:HMB2	1.99	0.44
2:b:334:ASP:OD1	2:b:334:ASP:N	2.50	0.44
7:n:104:ARG:NH1	35:n:608:CHL:OBD	2.48	0.44
23:G:602:CLA:H102	23:Y:304:CLA:H41	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:111:LEU:HG	23:N:604:CLA:HBC2	1.99	0.44
14:O:180:VAL:HA	14:O:186:VAL:HG12	1.99	0.44
20:Y:96:GLU:HA	20:Y:188:LEU:HD21	2.00	0.44
2:b:423:ARG:NH2	2:b:430:PHE:O	2.51	0.44
23:b:617:CLA:H71	31:b:623:LHG:H362	1.99	0.44
31:b:624:LHG:H271	31:b:624:LHG:H242	1.85	0.44
36:n:616:LUT:H15	36:n:616:LUT:H201	1.86	0.44
2:B:423:ARG:NH2	2:B:430:PHE:O	2.50	0.44
30:C:501:LMG:H381	28:C:517:DGD:HB51	1.99	0.44
23:c:511:CLA:H171	21:z:20:LEU:HD12	2.00	0.44
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	2.00	0.44
7:g:80:TRP:HZ3	23:g:602:CLA:HBC2	1.83	0.44
7:n:111:LEU:HG	23:n:604:CLA:HBC2	1.99	0.44
35:y:302:CHL:H143	35:y:302:CHL:H161	1.89	0.44
2:B:368:VAL:HB	2:B:381:VAL:HB	2.00	0.44
30:B:620:LMG:H341	30:B:620:LMG:H372	1.84	0.44
31:B:627:LHG:H151	31:B:627:LHG:H121	1.85	0.44
20:Y:136:GLN:HE22	23:Y:305:CLA:HED2	1.82	0.44
1:a:14:TRP:HB3	18:w:119:TYR:HB2	2.00	0.44
20:y:96:GLU:HA	20:y:188:LEU:HD21	2.00	0.44
20:y:136:GLN:HE22	23:y:305:CLA:HED2	1.82	0.44
3:C:307:PRO:HB3	3:C:358:PHE:HB3	1.99	0.44
23:C:508:CLA:HMA1	23:C:508:CLA:H2	1.99	0.44
38:G:618:NEX:H15	38:G:618:NEX:H201	1.70	0.44
12:L:2:THR:OG1	12:L:3:GLN:N	2.51	0.44
35:Y:302:CHL:H143	35:Y:302:CHL:H161	1.89	0.44
35:Y:308:CHL:H3A	35:Y:308:CHL:HBA1	1.72	0.44
3:c:307:PRO:HB3	3:c:358:PHE:HB3	1.99	0.44
12:l:34:ASN:ND2	12:l:34:ASN:H	2.15	0.44
35:n:607:CHL:HAA2	37:y:301:XAT:H241	1.99	0.44
25:b:619:BCR:H11C	25:b:619:BCR:H341	1.86	0.44
14:o:116:THR:OG1	14:o:117:ILE:N	2.51	0.44
35:r:607:CHL:H92	35:r:607:CHL:H61	1.87	0.44
3:C:90:PRO:O	3:C:94:THR:OG1	2.36	0.43
7:N:199:LEU:HD12	36:N:615:LUT:H222	2.00	0.43
35:N:601:CHL:HBA1	35:N:601:CHL:H3A	1.78	0.43
2:b:326:ARG:NH2	4:d:298:ASP:OD2	2.48	0.43
15:s:118:ALA:HB1	15:s:229:GLY:HA3	1.99	0.43
23:y:312:CLA:H92	23:y:312:CLA:H61	1.85	0.43
2:B:25:MET:HG2	25:B:617:BCR:H23C	2.00	0.43
23:B:603:CLA:H3A	23:B:603:CLA:HBA2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D:403:CLA:H192	30:D:409:LMG:H222	2.00	0.43
33:D:406:PL9:H38	12:L:27:VAL:HG13	2.00	0.43
15:S:67:ARG:NH2	15:S:85:LEU:O	2.46	0.43
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.80	0.43
37:g:620:XAT:H31	37:g:620:XAT:H391	1.85	0.43
38:R:316:NEX:H35	38:R:316:NEX:H401	1.91	0.43
25:B:619:BCR:H11C	25:B:619:BCR:H341	1.85	0.43
23:C:511:CLA:HBA1	23:C:511:CLA:H3A	1.78	0.43
35:Y:308:CHL:H93	35:Y:308:CHL:H61	1.85	0.43
23:b:605:CLA:H61	23:b:605:CLA:H41	1.77	0.43
7:n:197:ASP:OD1	36:n:615:LUT:O23	2.36	0.43
25:K:101:BCR:H15C	25:K:101:BCR:H351	1.87	0.43
23:N:611:CLA:HBA1	23:N:611:CLA:H3A	1.72	0.43
25:a:405:BCR:H24C	25:a:405:BCR:H371	1.86	0.43
26:b:602:SQD:H462	25:b:621:BCR:H393	2.00	0.43
23:r:602:CLA:H3A	23:r:602:CLA:HBA2	1.57	0.43
15:s:162:TYR:HB3	15:s:165:LYS:HE2	1.99	0.43
37:y:301:XAT:H31	37:y:301:XAT:H391	1.90	0.43
2:B:225:LEU:O	2:B:229:LEU:HB2	2.18	0.43
4:D:142:TYR:HA	4:D:145:ILE:HD12	2.00	0.43
7:G:80:TRP:HZ3	23:G:602:CLA:HBC2	1.84	0.43
23:G:610:CLA:HBA2	23:G:610:CLA:H3A	1.72	0.43
35:S:306:CHL:HBA1	35:S:306:CHL:HED3	2.01	0.43
22:r:251:VAL:HG21	31:r:616:LHG:H261	2.00	0.43
23:R:310:CLA:H52	36:R:314:LUT:H30	2.00	0.43
20:Y:85:SER:O	20:Y:85:SER:OG	2.33	0.43
21:Z:18:ILE:HA	21:Z:21:ILE:HG22	2.01	0.43
3:c:360:ASP:O	28:c:515:DGD:O2E	2.34	0.43
38:R:316:NEX:H191	38:R:316:NEX:H11	1.76	0.43
1:A:14:TRP:HB3	18:W:119:TYR:HB2	2.00	0.43
1:A:182:PHE:O	1:A:186:PHE:HB2	2.19	0.43
24:A:403:PHO:H8	24:A:403:PHO:H122	1.82	0.43
25:C:515:BCR:H20C	25:C:515:BCR:H361	1.91	0.43
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	2.00	0.43
36:G:615:LUT:H15	36:G:615:LUT:H201	1.91	0.43
36:N:616:LUT:H15	36:N:616:LUT:H201	1.87	0.43
23:b:616:CLA:H52	26:l:101:SQD:H281	2.00	0.43
3:c:264:LEU:HD21	25:c:514:BCR:H322	1.99	0.43
3:c:377:LEU:HB2	14:o:173:GLU:HG3	2.01	0.43
36:r:613:LUT:H11	36:r:613:LUT:H191	1.86	0.43
36:r:613:LUT:H31	36:r:613:LUT:H391	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:R:314:LUT:H15	36:R:314:LUT:H201	1.86	0.43
2:B:155:ALA:O	2:B:159:THR:OG1	2.37	0.43
36:s:615:LUT:H35	36:s:615:LUT:H401	1.86	0.43
2:B:10:THR:O	22:R:100:GLN:NE2	2.52	0.43
37:G:620:XAT:H31	37:G:620:XAT:H391	1.85	0.43
23:Y:304:CLA:HAB	35:Y:310:CHL:H162	2.00	0.43
2:b:103:PHE:HB2	23:b:608:CLA:H61	1.99	0.43
15:s:159:THR:OG1	15:s:167:ILE:O	2.36	0.43
2:B:334:ASP:OD1	2:B:334:ASP:N	2.49	0.43
23:B:607:CLA:HBB1	30:B:620:LMG:H191	2.00	0.43
7:N:104:ARG:NH1	35:N:608:CHL:OBD	2.46	0.43
35:S:306:CHL:HBC2	35:S:307:CHL:HHD	2.01	0.43
25:a:405:BCR:H15C	25:a:405:BCR:H351	1.86	0.43
8:h:63:SER:HB3	8:h:72:VAL:HG12	2.01	0.43
21:z:31:ASP:OD1	21:z:31:ASP:N	2.51	0.43
20:Y:107:LEU:HB3	23:Y:305:CLA:HBB2	2.01	0.42
23:b:618:CLA:H61	23:b:618:CLA:H102	1.61	0.42
4:d:58:SER:OG	4:d:66:SER:OG	2.32	0.42
14:o:180:VAL:HA	14:o:186:VAL:HG12	2.00	0.42
22:r:207:ARG:NH2	23:r:608:CLA:O1D	2.48	0.42
35:n:608:CHL:H51	35:n:608:CHL:H11	1.84	0.42
24:A:403:PHO:H152	24:A:403:PHO:H111	1.90	0.42
2:B:321:LYS:HE3	2:B:321:LYS:HB3	1.85	0.42
23:B:611:CLA:HAB	23:B:613:CLA:HMA3	2.01	0.42
23:C:510:CLA:H3A	23:C:510:CLA:HBA1	1.61	0.42
4:D:183:ILE:HG23	23:D:403:CLA:HAC1	2.00	0.42
23:D:401:CLA:H61	23:D:401:CLA:H2	1.75	0.42
5:E:57:THR:O	5:E:61:GLN:NE2	2.46	0.42
7:N:216:LEU:HD12	7:N:216:LEU:HA	1.91	0.42
14:O:116:THR:OG1	14:O:117:ILE:N	2.52	0.42
20:Y:195:ASP:OD1	36:Y:316:LUT:O23	2.36	0.42
23:s:603:CLA:H2A	23:s:603:CLA:HED2	2.01	0.42
7:n:186:ALA:HA	7:n:192:PRO:HB3	2.00	0.42
3:C:343:ARG:HB3	14:O:168:THR:HB	2.01	0.42
7:G:97:GLU:HG2	7:G:190:LEU:HD13	2.01	0.42
1:a:55:ALA:HB3	1:a:70:SER:HB2	2.02	0.42
25:b:621:BCR:H351	25:b:621:BCR:H15C	1.83	0.42
35:g:601:CHL:HBA1	35:g:601:CHL:H3A	1.78	0.42
37:r:614:XAT:H35	37:r:614:XAT:H401	1.85	0.42
25:B:619:BCR:H15C	25:B:619:BCR:H351	1.83	0.42
35:N:601:CHL:HED3	31:N:618:LHG:H142	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:265:ASN:HD21	32:S:319:DMU:H14	1.84	0.42
37:Y:301:XAT:H31	37:Y:301:XAT:H391	1.90	0.42
1:a:79:SER:OG	4:d:302:GLN:NE2	2.49	0.42
2:b:155:ALA:O	2:b:159:THR:OG1	2.36	0.42
6:f:30:SER:O	6:f:34:MET:HB2	2.19	0.42
23:g:602:CLA:H141	23:g:602:CLA:H162	1.84	0.42
38:r:615:NEX:H191	38:r:615:NEX:H11	1.75	0.42
23:B:611:CLA:H202	23:B:611:CLA:H162	1.93	0.42
7:G:50:TRP:NE1	7:G:210:GLU:OE2	2.52	0.42
7:N:111:LEU:HD13	23:N:612:CLA:HBB2	2.02	0.42
3:c:256:PRO:HA	23:c:506:CLA:HED3	2.01	0.42
23:c:509:CLA:H11	23:c:509:CLA:H51	1.89	0.42
28:c:515:DGD:HBE1	28:c:515:DGD:HB82	1.88	0.42
23:d:401:CLA:H2	23:d:401:CLA:H61	1.72	0.42
14:o:131:TYR:HB3	14:o:331:LEU:HD12	2.02	0.42
22:r:142:LEU:HD23	22:r:142:LEU:HA	1.82	0.42
17:u:97:THR:HA	17:u:102:ARG:HH21	1.85	0.42
3:C:293:ASN:O	3:C:423:ARG:NH1	2.50	0.42
33:D:406:PL9:H212	31:L:101:LHG:H222	2.02	0.42
23:g:602:CLA:H42	36:g:616:LUT:H373	2.01	0.42
35:g:609:CHL:H43	35:n:601:CHL:H12	2.02	0.42
23:y:311:CLA:H52	36:y:316:LUT:H30	2.02	0.42
25:B:617:BCR:H322	30:B:620:LMG:H111	2.02	0.42
3:C:226:SER:O	3:C:226:SER:OG	2.32	0.42
25:H:101:BCR:H15C	25:H:101:BCR:H351	1.90	0.42
35:Y:309:CHL:H122	35:Y:309:CHL:HBA1	2.02	0.42
2:b:99:ALA:HB1	23:b:608:CLA:H72	2.02	0.42
3:c:350:ILE:HG21	3:c:359:TRP:HB2	2.01	0.42
3:c:376:ASP:OD1	3:c:376:ASP:N	2.47	0.42
14:o:310:ASP:H	14:o:318:PRO:HB3	1.85	0.42
15:s:89:VAL:HG21	15:s:107:PHE:HE2	1.84	0.42
15:s:265:ASN:HD21	32:s:618:DMU:H14	1.85	0.42
36:y:317:LUT:H11	36:y:317:LUT:H191	1.89	0.42
4:D:187:GLN:HB2	23:D:403:CLA:HBC1	2.02	0.42
7:N:197:ASP:OD1	36:N:615:LUT:O23	2.38	0.42
20:Y:135:SER:HB3	35:Y:308:CHL:HED2	2.01	0.42
37:Y:301:XAT:H11	37:Y:301:XAT:H191	1.84	0.42
24:a:403:PHO:H143	23:d:403:CLA:H162	2.02	0.42
31:c:516:LHG:H152	31:c:516:LHG:H122	1.86	0.42
25:d:405:BCR:H351	25:d:405:BCR:H15C	1.82	0.42
23:n:612:CLA:HBB1	36:n:615:LUT:C14	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:y:316:LUT:H35	36:y:316:LUT:H401	1.86	0.42
8:H:43:MET:HE2	8:H:43:MET:HB3	1.84	0.42
23:S:314:CLA:HBC1	36:S:315:LUT:H162	2.01	0.42
35:Y:310:CHL:H3A	35:Y:310:CHL:HBA2	1.62	0.42
23:c:502:CLA:H142	23:c:503:CLA:H3A	2.02	0.42
4:d:183:ILE:HG23	23:d:403:CLA:HAC1	2.01	0.42
14:o:232:LEU:HA	14:o:282:VAL:HA	2.01	0.42
22:r:92:GLN:HG3	22:r:111:ILE:HD11	2.02	0.42
17:u:81:THR:OG1	17:u:82:GLU:N	2.45	0.42
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.86	0.42
26:B:625:SQD:H81	1:a:26:ASN:HB3	2.01	0.42
15:S:199:LYS:HA	35:S:308:CHL:HBC1	2.02	0.42
3:c:433:LEU:HD22	23:c:502:CLA:HMC3	2.02	0.42
23:c:503:CLA:H142	23:c:509:CLA:H42	2.02	0.42
4:d:142:TYR:HA	4:d:145:ILE:HD12	2.02	0.42
18:w:114:THR:HG23	23:y:313:CLA:H61	2.02	0.42
7:n:111:LEU:HD13	23:n:612:CLA:HBB2	2.01	0.42
35:y:308:CHL:H61	35:y:308:CHL:H93	1.84	0.42
22:R:153:LEU:HG	23:R:305:CLA:HBC2	2.00	0.42
23:R:311:CLA:H2A	23:R:311:CLA:HED3	2.02	0.42
23:B:606:CLA:H122	28:B:624:DGD:HAW2	2.02	0.41
3:C:132:HIS:HE1	23:C:514:CLA:HMA3	1.85	0.41
4:D:57:THR:OG1	4:D:58:SER:N	2.52	0.41
23:G:602:CLA:H91	23:G:602:CLA:H112	1.82	0.41
25:b:621:BCR:H11C	25:b:621:BCR:H341	1.87	0.41
14:o:165:THR:HG21	14:o:199:VAL:HG22	2.02	0.41
22:r:60:PHE:HB3	22:r:62:GLY:H	1.85	0.41
22:r:69:LEU:HD11	22:r:80:ASP:HB2	2.01	0.41
37:y:301:XAT:H15	37:y:301:XAT:H201	1.89	0.41
23:C:503:CLA:H142	23:C:504:CLA:H3A	2.02	0.41
13:M:23:LEU:HD13	26:l:101:SQD:H162	2.01	0.41
18:W:82:ASP:OD1	18:W:82:ASP:N	2.53	0.41
2:b:218:SER:HB2	22:r:131:VAL:HG21	2.02	0.41
26:l:101:SQD:H112	26:l:101:SQD:H81	1.87	0.41
7:n:75:PRO:HG3	7:n:212:LYS:HD3	2.02	0.41
20:y:110:LEU:HD13	23:y:313:CLA:HBB2	2.02	0.41
35:y:302:CHL:HBA1	35:y:302:CHL:H3A	1.77	0.41
35:y:308:CHL:H142	35:y:308:CHL:H111	1.89	0.41
22:R:265:LYS:HE3	22:R:270:PHE:HD1	1.85	0.41
28:A:408:DGD:HBT1	30:b:601:LMG:H362	2.01	0.41
31:B:621:LHG:H312	31:B:621:LHG:H281	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:625:SQD:H91	1:a:30:ILE:HD11	2.02	0.41
23:N:612:CLA:HBB1	36:N:615:LUT:C14	2.50	0.41
35:Y:302:CHL:HBA1	35:Y:302:CHL:H3A	1.79	0.41
2:b:194:VAL:HA	2:b:195:PRO:HD3	1.92	0.41
15:s:59:LEU:HD21	15:s:216:GLU:HG3	2.00	0.41
36:R:314:LUT:H11	36:R:314:LUT:H191	1.91	0.41
3:C:360:ASP:O	28:C:517:DGD:O2E	2.35	0.41
20:Y:110:LEU:HD13	23:Y:313:CLA:HBB2	2.03	0.41
23:b:608:CLA:H143	23:b:608:CLA:H111	1.90	0.41
3:c:110:PRO:HB3	32:c:519:DMU:H1	2.01	0.41
5:e:57:THR:O	5:e:61:GLN:NE2	2.49	0.41
1:A:37:MET:HE3	1:A:41:LEU:HD12	2.01	0.41
23:B:614:CLA:H93	23:B:614:CLA:H111	1.93	0.41
23:C:511:CLA:H93	23:C:511:CLA:H61	1.94	0.41
4:D:86:LEU:HD13	4:D:91:LEU:HD11	2.03	0.41
35:G:601:CHL:HBC1	31:G:619:LHG:HC11	2.03	0.41
31:S:318:LHG:H112	31:S:318:LHG:HC81	1.91	0.41
20:Y:218:ARG:HB3	23:Y:303:CLA:HBC3	2.02	0.41
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.03	0.41
31:g:619:LHG:H302	31:g:619:LHG:H271	1.91	0.41
35:n:606:CHL:HMC	35:n:607:CHL:C4C	2.50	0.41
20:y:230:GLN:O	20:y:234:THR:OG1	2.34	0.41
23:R:303:CLA:H41	23:R:303:CLA:H61	1.83	0.41
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.01	0.41
23:C:514:CLA:HBB1	25:C:515:BCR:H371	2.03	0.41
25:C:515:BCR:H15C	25:C:515:BCR:H351	1.82	0.41
7:G:104:ARG:NH1	35:G:608:CHL:OBD	2.54	0.41
23:G:602:CLA:H141	23:G:602:CLA:H162	1.85	0.41
36:S:316:LUT:H15	36:S:316:LUT:H201	1.86	0.41
36:S:316:LUT:H35	36:S:316:LUT:H401	1.92	0.41
35:Y:309:CHL:H121	35:Y:309:CHL:H162	1.92	0.41
23:b:616:CLA:H93	23:b:616:CLA:H111	1.92	0.41
35:g:601:CHL:H41	35:g:601:CHL:H61	1.87	0.41
38:g:618:NEX:H35	38:g:618:NEX:H401	1.88	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.89	0.41
2:B:245:VAL:HG22	23:B:612:CLA:H201	2.01	0.41
23:B:614:CLA:H141	23:B:614:CLA:H162	1.92	0.41
28:B:624:DGD:HBF2	28:B:624:DGD:HBE1	1.96	0.41
23:C:502:CLA:H92	23:C:502:CLA:H62	1.91	0.41
25:D:405:BCR:H15C	25:D:405:BCR:H351	1.82	0.41
36:N:615:LUT:H35	36:N:615:LUT:H401	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:131:TYR:HB3	14:O:331:LEU:HD12	2.02	0.41
31:W:201:LHG:H122	31:W:201:LHG:H152	1.86	0.41
25:a:405:BCR:HC41	9:i:15:PHE:HE1	1.86	0.41
2:b:25:MET:HG2	25:b:619:BCR:H23C	2.03	0.41
28:d:410:DGD:HBN1	28:d:410:DGD:HBW2	1.87	0.41
8:h:47:MET:HG2	25:h:101:BCR:H312	2.02	0.41
25:h:101:BCR:H371	25:h:101:BCR:H24C	1.77	0.41
25:k:101:BCR:H371	25:k:101:BCR:H24C	1.89	0.41
20:y:160:ILE:HG12	35:y:306:CHL:HAC1	2.03	0.41
35:y:309:CHL:HBA1	35:y:309:CHL:H122	2.03	0.41
22:R:224:ASP:OD1	36:R:314:LUT:O23	2.37	0.41
38:R:301:NEX:H191	38:R:301:NEX:H11	1.83	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.93	0.41
23:B:612:CLA:H93	23:B:612:CLA:H62	1.87	0.41
38:N:617:NEX:H35	38:N:617:NEX:H401	1.89	0.41
26:a:406:SQD:H292	31:d:408:LHG:H383	2.03	0.41
38:R:316:NEX:H15	38:R:316:NEX:H201	1.77	0.41
2:B:110:ALA:HB2	25:B:619:BCR:H17C	2.01	0.41
23:B:604:CLA:H12	23:B:604:CLA:H51	1.85	0.41
30:B:620:LMG:H312	30:B:620:LMG:H342	1.92	0.41
3:C:95:LEU:HD12	3:C:178:LYS:HG2	2.02	0.41
23:C:511:CLA:H41	31:D:408:LHG:H151	2.03	0.41
23:G:613:CLA:H93	31:G:619:LHG:H132	2.03	0.41
7:N:103:SER:HB3	7:N:219:GLY:HA3	2.01	0.41
36:N:616:LUT:H35	36:N:616:LUT:H401	1.96	0.41
38:S:317:NEX:H35	38:S:317:NEX:H401	1.86	0.41
1:a:234:ASN:HB2	4:d:264:ASN:HD22	1.86	0.41
7:g:161:ILE:HG12	35:g:605:CHL:HAC1	2.02	0.41
31:g:619:LHG:H362	37:g:620:XAT:H371	2.01	0.41
15:s:230:ARG:HB3	23:s:602:CLA:HBC3	2.03	0.41
36:y:317:LUT:H15	36:y:317:LUT:H201	1.86	0.41
1:A:30:ILE:HD11	26:b:602:SQD:H91	2.02	0.41
1:A:221:SER:HA	4:D:140:ARG:HB2	2.03	0.41
36:G:615:LUT:H11	36:G:615:LUT:H191	1.94	0.41
1:a:221:SER:HA	4:d:140:ARG:HB2	2.03	0.41
23:b:616:CLA:H52	23:b:616:CLA:H8	1.84	0.41
23:c:509:CLA:H3A	23:c:509:CLA:HBA1	1.61	0.41
23:c:513:CLA:H93	23:c:513:CLA:H61	1.93	0.41
31:c:516:LHG:O3	31:c:516:LHG:O1	2.39	0.41
26:c:520:SQD:H442	31:s:617:LHG:HC12	2.03	0.41
4:d:57:THR:OG1	4:d:58:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:78:TYR:OH	7:g:217:LYS:NZ	2.44	0.41
31:g:619:LHG:H382	37:g:620:XAT:H28	2.02	0.41
25:k:101:BCR:H11C	25:k:101:BCR:H341	1.96	0.41
15:s:199:LYS:HA	35:s:607:CHL:HBC1	2.03	0.41
23:n:611:CLA:H3A	23:n:611:CLA:HBA1	1.72	0.41
35:R:307:CHL:HAB	23:R:313:CLA:H191	2.03	0.41
1:A:234:ASN:HB3	4:D:264:ASN:HD22	1.86	0.40
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.89	0.40
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.80	0.40
4:D:46:LEU:HD23	4:D:46:LEU:HA	1.97	0.40
37:G:617:XAT:H31	37:G:617:XAT:H391	1.85	0.40
35:N:608:CHL:H51	35:N:608:CHL:H11	1.85	0.40
36:Y:316:LUT:H15	36:Y:316:LUT:H201	1.92	0.40
23:g:603:CLA:H93	23:y:304:CLA:H102	2.03	0.40
7:n:198:PRO:HD2	36:n:615:LUT:H23	2.03	0.40
3:C:228:ASP:OD1	3:C:228:ASP:N	2.54	0.40
25:C:519:BCR:H15C	25:C:519:BCR:H351	1.84	0.40
36:G:616:LUT:H35	36:G:616:LUT:H401	1.91	0.40
15:S:71:LEU:HB2	15:S:76:LEU:HD22	2.04	0.40
2:b:110:ALA:HB2	25:b:621:BCR:H17C	2.02	0.40
30:b:622:LMG:H352	30:b:622:LMG:H382	1.93	0.40
12:l:14:ASN:OD1	12:l:14:ASN:N	2.54	0.40
22:r:153:LEU:HG	23:r:604:CLA:HBC2	2.03	0.40
37:y:301:XAT:H22	35:y:302:CHL:HMC	2.02	0.40
35:y:307:CHL:H42	38:R:301:NEX:H35	2.03	0.40
1:A:55:ALA:HB3	1:A:70:SER:HB2	2.02	0.40
1:A:174:LEU:HD22	24:A:403:PHO:H151	2.02	0.40
23:C:509:CLA:H141	23:C:509:CLA:H161	1.91	0.40
24:D:402:PHO:HBA2	24:D:402:PHO:H3A	1.79	0.40
9:I:13:ILE:HD12	9:I:13:ILE:HA	1.93	0.40
36:Y:316:LUT:H35	36:Y:316:LUT:H401	1.86	0.40
36:Y:317:LUT:H35	36:Y:317:LUT:H401	1.84	0.40
5:e:14:ILE:HD13	10:j:10:LEU:HB2	2.03	0.40
36:g:616:LUT:H31	36:g:616:LUT:H391	1.99	0.40
7:n:133:LYS:HE3	7:n:133:LYS:HB2	1.80	0.40
3:C:346:THR:OG1	3:C:348:GLU:OE1	2.32	0.40
35:G:601:CHL:H3A	35:G:601:CHL:HBA1	1.77	0.40
15:S:162:TYR:HB3	15:S:165:LYS:HE2	2.03	0.40
18:W:114:THR:HG23	23:Y:313:CLA:H61	2.04	0.40
20:Y:209:LEU:HB3	23:Y:311:CLA:H3A	2.04	0.40
26:a:406:SQD:H151	31:d:408:LHG:H352	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:321:LYS:HE3	2:b:321:LYS:HB3	1.88	0.40
7:g:187:GLU:H	7:g:187:GLU:HG2	1.75	0.40
35:n:601:CHL:HBA1	35:n:601:CHL:H3A	1.81	0.40
23:R:310:CLA:H151	23:R:310:CLA:H111	1.98	0.40
23:B:616:CLA:H141	23:B:616:CLA:H162	1.93	0.40
3:C:41:ARG:NH1	23:C:512:CLA:OBD	2.54	0.40
35:G:601:CHL:H61	35:G:601:CHL:H41	1.86	0.40
7:N:224:PHE:HZ	31:N:618:LHG:H172	1.85	0.40
14:O:290:THR:HG22	14:O:291:LYS:H	1.86	0.40
23:b:610:CLA:H41	23:b:610:CLA:H62	1.80	0.40
25:c:518:BCR:H11C	25:c:518:BCR:H341	1.89	0.40
35:g:601:CHL:HBC1	31:g:619:LHG:HC11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/353 (94%)	314 (94%)	19 (6%)	0	100	100
1	a	333/353 (94%)	315 (95%)	18 (5%)	0	100	100
2	B	487/508 (96%)	467 (96%)	20 (4%)	0	100	100
2	b	487/508 (96%)	469 (96%)	18 (4%)	0	100	100
3	C	447/473 (94%)	432 (97%)	15 (3%)	0	100	100
3	c	447/473 (94%)	434 (97%)	13 (3%)	0	100	100
4	D	337/353 (96%)	327 (97%)	10 (3%)	0	100	100
4	d	337/353 (96%)	329 (98%)	8 (2%)	0	100	100
5	E	69/83 (83%)	65 (94%)	4 (6%)	0	100	100
5	e	69/83 (83%)	63 (91%)	6 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	28/39 (72%)	26 (93%)	2 (7%)	0	100	100
6	f	28/39 (72%)	27 (96%)	1 (4%)	0	100	100
7	G	217/267 (81%)	206 (95%)	10 (5%)	1 (0%)	24	60
7	N	217/267 (81%)	207 (95%)	10 (5%)	0	100	100
7	g	217/267 (81%)	208 (96%)	8 (4%)	1 (0%)	24	60
7	n	217/267 (81%)	204 (94%)	13 (6%)	0	100	100
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	55 (96%)	2 (4%)	0	100	100
9	I	32/36 (89%)	32 (100%)	0	0	100	100
9	i	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
10	J	27/40 (68%)	27 (100%)	0	0	100	100
10	j	27/40 (68%)	27 (100%)	0	0	100	100
11	K	35/61 (57%)	35 (100%)	0	0	100	100
11	k	35/61 (57%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
13	m	30/34 (88%)	29 (97%)	1 (3%)	0	100	100
14	O	194/332 (58%)	180 (93%)	14 (7%)	0	100	100
14	o	194/332 (58%)	176 (91%)	17 (9%)	1 (0%)	24	60
15	S	219/280 (78%)	200 (91%)	19 (9%)	0	100	100
15	s	219/280 (78%)	206 (94%)	13 (6%)	0	100	100
16	T	27/33 (82%)	26 (96%)	1 (4%)	0	100	100
16	t	27/33 (82%)	27 (100%)	0	0	100	100
17	U	21/103 (20%)	19 (90%)	2 (10%)	0	100	100
17	u	21/103 (20%)	19 (90%)	2 (10%)	0	100	100
18	W	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
18	w	52/133 (39%)	51 (98%)	1 (2%)	0	100	100
19	X	36/116 (31%)	36 (100%)	0	0	100	100
19	x	36/116 (31%)	36 (100%)	0	0	100	100
20	Y	218/265 (82%)	211 (97%)	6 (3%)	1 (0%)	24	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	y	218/265 (82%)	209 (96%)	8 (4%)	1 (0%)	24 60
21	Z	59/62 (95%)	59 (100%)	0	0	100 100
21	z	59/62 (95%)	59 (100%)	0	0	100 100
22	R	218/286 (76%)	210 (96%)	8 (4%)	0	100 100
22	r	218/286 (76%)	209 (96%)	9 (4%)	0	100 100
All	All	6790/8470 (80%)	6501 (96%)	284 (4%)	5 (0%)	49 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	o	312	ASP
20	y	152	ILE
20	Y	152	ILE
7	g	153	VAL
7	G	153	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	272/285 (95%)	272 (100%)	0	100 100
1	a	272/285 (95%)	272 (100%)	0	100 100
2	B	387/402 (96%)	387 (100%)	0	100 100
2	b	387/402 (96%)	387 (100%)	0	100 100
3	C	352/373 (94%)	352 (100%)	0	100 100
3	c	352/373 (94%)	352 (100%)	0	100 100
4	D	271/283 (96%)	271 (100%)	0	100 100
4	d	271/283 (96%)	271 (100%)	0	100 100
5	E	63/73 (86%)	63 (100%)	0	100 100
5	e	63/73 (86%)	63 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	25/34 (74%)	25 (100%)	0	100	100
6	f	25/34 (74%)	25 (100%)	0	100	100
7	G	167/201 (83%)	167 (100%)	0	100	100
7	N	167/201 (83%)	167 (100%)	0	100	100
7	g	167/201 (83%)	167 (100%)	0	100	100
7	n	167/201 (83%)	167 (100%)	0	100	100
8	H	49/61 (80%)	49 (100%)	0	100	100
8	h	49/61 (80%)	49 (100%)	0	100	100
9	I	31/33 (94%)	31 (100%)	0	100	100
9	i	31/33 (94%)	31 (100%)	0	100	100
10	J	22/30 (73%)	22 (100%)	0	100	100
10	j	22/30 (73%)	22 (100%)	0	100	100
11	K	32/55 (58%)	32 (100%)	0	100	100
11	k	32/55 (58%)	32 (100%)	0	100	100
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	34 (97%)	1 (3%)	37	70
13	M	28/30 (93%)	28 (100%)	0	100	100
13	m	28/30 (93%)	28 (100%)	0	100	100
14	O	170/268 (63%)	170 (100%)	0	100	100
14	o	170/268 (63%)	170 (100%)	0	100	100
15	S	172/219 (78%)	172 (100%)	0	100	100
15	s	172/219 (78%)	172 (100%)	0	100	100
16	T	26/30 (87%)	26 (100%)	0	100	100
16	t	26/30 (87%)	26 (100%)	0	100	100
17	U	19/82 (23%)	19 (100%)	0	100	100
17	u	19/82 (23%)	19 (100%)	0	100	100
18	W	47/102 (46%)	47 (100%)	0	100	100
18	w	47/102 (46%)	47 (100%)	0	100	100
19	X	32/92 (35%)	32 (100%)	0	100	100
19	x	32/92 (35%)	32 (100%)	0	100	100
20	Y	173/209 (83%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	y	173/209 (83%)	173 (100%)	0	100	100
21	Z	53/54 (98%)	53 (100%)	0	100	100
21	z	53/54 (98%)	53 (100%)	0	100	100
22	R	178/226 (79%)	178 (100%)	0	100	100
22	r	178/226 (79%)	178 (100%)	0	100	100
All	All	5542/6758 (82%)	5541 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	108	ASN
1	A	181	ASN
1	A	187	GLN
1	A	261	GLN
1	A	325	ASN
1	A	335	ASN
2	B	182	ASN
3	C	418	ASN
4	D	187	GLN
4	D	251	ASN
5	E	53	ASN
7	G	102	HIS
7	N	262	ASN
14	O	113	GLN
15	S	265	ASN
20	Y	164	GLN
21	Z	58	ASN
1	a	75	ASN
1	a	181	ASN
1	a	304	GLN
2	b	182	ASN
4	d	187	GLN
4	d	251	ASN

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Mol	Chain	Res	Type
4	d	264	ASN
5	e	53	ASN
7	g	154	HIS
7	g	156	GLN
7	g	243	ASN
14	o	307	GLN
22	r	126	GLN
21	z	58	ASN
7	n	165	GLN
7	n	218	ASN
7	n	262	ASN
20	y	164	GLN
20	y	198	ASN
22	R	126	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 338 ligands modelled in this entry, 2 are monoatomic - leaving 336 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	$\#\|Z\|>2$
25	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.71	13 (23%)
32	DMU	c	522	-	34,34,34	0.58	0	45,45,45	0.81	1 (2%)
23	CLA	B	609	2	69,73,73	1.26	7 (10%)	83,113,113	1.20	5 (6%)
23	CLA	B	612	2	69,73,73	1.22	8 (11%)	83,113,113	1.37	6 (7%)
35	CHL	g	607	-	47,51,74	1.46	7 (14%)	52,86,114	1.50	7 (13%)
31	LHG	l	103	-	48,48,48	0.97	2 (4%)	51,54,54	0.93	3 (5%)
39	VTQ	W	202	-	30,32,32	0.42	0	39,44,44	0.50	0
35	CHL	n	607	-	50,54,74	1.43	7 (14%)	56,90,114	1.58	9 (16%)
31	LHG	R	317	23	41,41,48	1.01	2 (4%)	44,47,54	1.05	3 (6%)
23	CLA	C	503	3	69,73,73	1.25	7 (10%)	83,113,113	1.34	6 (7%)
23	CLA	c	509	3	69,73,73	1.26	7 (10%)	83,113,113	1.20	5 (6%)
35	CHL	y	308	-	70,74,74	1.20	8 (11%)	80,114,114	1.36	9 (11%)
23	CLA	g	603	7	69,73,73	1.26	7 (10%)	83,113,113	1.25	8 (9%)
23	CLA	y	303	20	65,69,73	1.28	7 (10%)	78,108,113	1.20	5 (6%)
35	CHL	y	302	20	70,74,74	1.20	8 (11%)	80,114,114	1.24	7 (8%)
31	LHG	D	408	-	48,48,48	0.94	2 (4%)	51,54,54	1.10	2 (3%)
25	BCR	B	619	-	41,41,41	0.68	0	56,56,56	1.73	11 (19%)
30	LMG	a	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.01	3 (5%)
31	LHG	L	102	-	48,48,48	0.97	2 (4%)	51,54,54	0.93	2 (3%)
35	CHL	y	307	-	54,58,74	1.38	7 (12%)	59,94,114	1.45	8 (13%)
23	CLA	b	611	2	69,73,73	1.26	7 (10%)	83,113,113	1.19	5 (6%)
35	CHL	G	606	-	47,51,74	1.47	7 (14%)	52,86,114	1.45	10 (19%)
23	CLA	S	314	15	45,49,73	1.51	8 (17%)	54,84,113	1.47	8 (14%)
31	LHG	n	618	23	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
23	CLA	y	313	20	64,68,73	1.30	7 (10%)	77,107,113	1.29	10 (12%)
23	CLA	A	402	-	54,58,73	1.43	7 (12%)	65,95,113	1.42	7 (10%)
23	CLA	g	613	7	62,66,73	1.32	6 (9%)	74,104,113	1.27	4 (5%)
35	CHL	N	608	-	70,74,74	1.21	8 (11%)	80,114,114	1.22	7 (8%)
35	CHL	R	308	-	65,69,74	1.27	8 (12%)	74,108,114	1.31	9 (12%)
28	DGD	B	624	-	60,60,67	0.89	2 (3%)	74,74,81	0.91	2 (2%)
35	CHL	G	601	7	70,74,74	1.24	7 (10%)	80,114,114	1.28	7 (8%)
31	LHG	B	622	-	45,45,48	0.96	2 (4%)	48,51,54	0.99	3 (6%)
35	CHL	g	608	-	70,74,74	1.20	8 (11%)	80,114,114	1.16	5 (6%)
28	DGD	d	410	-	63,63,67	0.90	2 (3%)	77,77,81	0.94	2 (2%)
26	SQD	b	602	-	53,54,54	1.20	4 (7%)	62,65,65	3.65	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	XAT	G	617	-	39,47,47	0.87	0	54,74,74	2.51	16 (29%)
23	CLA	y	314	20	69,73,73	1.25	7 (10%)	83,113,113	1.23	4 (4%)
23	CLA	R	303	22	64,68,73	1.31	10 (15%)	77,107,113	1.18	5 (6%)
38	NEX	n	617	-	38,46,46	0.87	1 (2%)	50,70,70	2.23	16 (32%)
31	LHG	s	617	23	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
23	CLA	b	609	-	69,73,73	1.25	8 (11%)	83,113,113	1.20	5 (6%)
35	CHL	y	310	20	70,74,74	1.27	10 (14%)	80,114,114	1.36	9 (11%)
23	CLA	G	602	7	69,73,73	1.26	9 (13%)	83,113,113	1.11	4 (4%)
24	PHO	D	402	-	58,69,69	1.19	3 (5%)	56,99,99	1.74	8 (14%)
35	CHL	Y	307	-	54,58,74	1.39	7 (12%)	59,94,114	1.47	8 (13%)
23	CLA	B	601	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	7 (8%)
37	XAT	g	620	-	39,47,47	0.92	0	54,74,74	2.47	18 (33%)
33	PL9	d	406	-	55,55,55	4.32	23 (41%)	68,69,69	3.64	33 (48%)
35	CHL	S	308	-	53,57,74	1.38	6 (11%)	59,93,114	1.41	10 (16%)
28	DGD	A	408	-	60,60,67	0.91	2 (3%)	74,74,81	0.96	3 (4%)
39	VTQ	w	201	-	30,32,32	0.42	0	39,44,44	0.50	0
23	CLA	n	613	7	64,68,73	1.30	6 (9%)	77,107,113	1.31	7 (9%)
36	LUT	g	615	-	42,43,43	0.73	0	51,60,60	1.53	9 (17%)
31	LHG	g	619	23	45,45,48	0.96	2 (4%)	48,51,54	1.04	3 (6%)
25	BCR	C	519	-	41,41,41	0.67	0	56,56,56	1.96	15 (26%)
23	CLA	b	618	2	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
36	LUT	S	315	-	42,43,43	0.74	0	51,60,60	1.60	11 (21%)
26	SQD	L	103	-	53,54,54	1.18	4 (7%)	62,65,65	1.10	6 (9%)
23	CLA	S	313	15	59,63,73	1.35	7 (11%)	71,101,113	1.30	3 (4%)
23	CLA	G	611	31	64,68,73	1.29	8 (12%)	77,107,113	1.23	5 (6%)
28	DGD	B	626	-	57,57,67	0.96	2 (3%)	71,71,81	1.04	4 (5%)
23	CLA	c	513	3	69,73,73	1.25	8 (11%)	83,113,113	1.23	8 (9%)
23	CLA	C	506	3	62,66,73	1.29	7 (11%)	74,104,113	1.29	8 (10%)
35	CHL	y	306	20	55,59,74	1.36	7 (12%)	62,96,114	1.34	9 (14%)
23	CLA	Y	304	20	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
23	CLA	r	602	22	64,68,73	1.31	9 (14%)	77,107,113	1.18	6 (7%)
23	CLA	C	512	3	69,73,73	1.27	6 (8%)	83,113,113	1.29	5 (6%)
27	BCT	A	407	29	2,3,3	0.87	0	2,3,3	3.25	2 (100%)
36	LUT	y	316	-	42,43,43	0.72	0	51,60,60	1.52	10 (19%)
31	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LHG	d	408	-	48,48,48	0.94	2 (4%)	51,54,54	1.10	2 (3%)
26	SQD	l	101	-	53,54,54	1.19	4 (7%)	62,65,65	1.09	4 (6%)
36	LUT	G	615	-	42,43,43	0.73	0	51,60,60	1.54	10 (19%)
23	CLA	n	612	7	49,53,73	1.50	7 (14%)	59,89,113	1.44	6 (10%)
25	BCR	H	101	-	41,41,41	0.71	0	56,56,56	1.56	7 (12%)
38	NEX	S	317	-	38,46,46	0.86	1 (2%)	50,70,70	2.26	17 (34%)
23	CLA	G	610	7	68,72,73	1.23	7 (10%)	81,111,113	1.20	7 (8%)
25	BCR	A	405	-	41,41,41	0.68	0	56,56,56	1.69	12 (21%)
23	CLA	B	615	2	69,73,73	1.23	7 (10%)	83,113,113	1.34	9 (10%)
23	CLA	b	606	2	69,73,73	1.26	7 (10%)	83,113,113	1.33	6 (7%)
37	XAT	R	315	-	39,47,47	0.88	0	54,74,74	2.51	19 (35%)
23	CLA	b	613	2	69,73,73	1.23	8 (11%)	83,113,113	1.19	6 (7%)
23	CLA	d	404	4	69,73,73	1.23	6 (8%)	83,113,113	1.23	5 (6%)
28	DGD	b	625	-	57,57,67	0.95	2 (3%)	71,71,81	1.06	4 (5%)
32	DMU	c	519	-	34,34,34	0.54	0	45,45,45	1.50	5 (11%)
23	CLA	R	312	22	69,73,73	1.26	7 (10%)	83,113,113	1.28	6 (7%)
23	CLA	b	612	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
35	CHL	n	606	-	50,54,74	1.44	7 (14%)	56,90,114	1.39	10 (17%)
23	CLA	C	502	3	69,73,73	1.27	8 (11%)	83,113,113	1.14	6 (7%)
38	NEX	s	616	-	38,46,46	0.89	1 (2%)	50,70,70	2.35	20 (40%)
23	CLA	r	601	22	53,57,73	1.45	7 (13%)	62,93,113	1.32	5 (8%)
23	CLA	n	614	7	45,49,73	1.51	7 (15%)	54,84,113	1.34	5 (9%)
23	CLA	n	603	7	63,67,73	1.31	7 (11%)	75,105,113	1.31	6 (8%)
38	NEX	G	618	-	38,46,46	0.88	1 (2%)	50,70,70	2.34	16 (32%)
23	CLA	N	603	7	63,67,73	1.33	7 (11%)	75,105,113	1.35	6 (8%)
24	PHO	a	403	-	58,69,69	1.19	4 (6%)	56,99,99	1.73	8 (14%)
25	BCR	z	101	-	41,41,41	0.71	0	56,56,56	1.63	9 (16%)
35	CHL	Y	306	20	55,59,74	1.37	7 (12%)	62,96,114	1.32	9 (14%)
25	BCR	K	101	-	41,41,41	0.65	0	56,56,56	1.80	16 (28%)
30	LMG	b	601	-	40,40,55	1.06	2 (5%)	48,48,63	1.00	2 (4%)
23	CLA	s	609	15	49,53,73	1.48	8 (16%)	59,89,113	1.41	9 (15%)
23	CLA	N	613	7	64,68,73	1.30	6 (9%)	77,107,113	1.30	7 (9%)
23	CLA	R	310	22	69,73,73	1.26	8 (11%)	83,113,113	1.22	5 (6%)
31	LHG	C	518	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
23	CLA	y	305	-	54,58,73	1.42	10 (18%)	65,95,113	1.35	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	509	3	69,73,73	1.25	9 (13%)	83,113,113	1.24	7 (8%)
23	CLA	N	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.37	7 (10%)
23	CLA	c	507	-	69,73,73	1.23	7 (10%)	83,113,113	1.31	7 (8%)
34	HEM	F	101	6,5	50,50,50	1.48	7 (14%)	66,82,82	1.33	7 (10%)
30	LMG	b	622	-	51,51,55	0.94	2 (3%)	59,59,63	0.99	3 (5%)
33	PL9	D	406	-	55,55,55	4.31	22 (40%)	68,69,69	3.66	33 (48%)
35	CHL	G	609	7	65,69,74	1.29	7 (10%)	74,108,114	1.47	8 (10%)
23	CLA	S	310	15	49,53,73	1.48	7 (14%)	59,89,113	1.31	8 (13%)
23	CLA	B	610	-	69,73,73	1.23	8 (11%)	83,113,113	1.27	6 (7%)
23	CLA	C	510	3	69,73,73	1.27	9 (13%)	83,113,113	1.21	5 (6%)
37	XAT	G	620	-	39,47,47	0.91	0	54,74,74	2.47	17 (31%)
35	CHL	N	607	-	50,54,74	1.44	7 (14%)	56,90,114	1.55	8 (14%)
35	CHL	g	606	-	47,51,74	1.44	6 (12%)	52,86,114	1.41	7 (13%)
23	CLA	s	603	15	49,53,73	1.49	7 (14%)	59,89,113	1.42	5 (8%)
23	CLA	s	610	31	46,50,73	1.50	8 (17%)	55,85,113	1.37	4 (7%)
23	CLA	C	507	3	55,59,73	1.38	9 (16%)	66,96,113	1.56	8 (12%)
37	XAT	Y	301	-	39,47,47	0.91	0	54,74,74	2.56	18 (33%)
35	CHL	R	306	-	50,54,74	1.44	6 (12%)	56,90,114	1.38	7 (12%)
35	CHL	N	605	7	52,56,74	1.37	7 (13%)	58,92,114	1.59	10 (17%)
23	CLA	r	612	22	69,73,73	1.26	9 (13%)	83,113,113	1.25	8 (9%)
23	CLA	b	616	2	69,73,73	1.25	8 (11%)	83,113,113	1.21	9 (10%)
25	BCR	a	405	-	41,41,41	0.69	0	56,56,56	1.70	11 (19%)
26	SQD	a	406	-	49,50,54	1.24	4 (8%)	58,61,65	1.05	5 (8%)
30	LMG	s	619	-	55,55,55	0.90	2 (3%)	63,63,63	0.98	4 (6%)
35	CHL	N	609	7	70,74,74	1.23	7 (10%)	80,114,114	1.41	9 (11%)
37	XAT	g	617	-	39,47,47	0.89	0	54,74,74	2.51	16 (29%)
23	CLA	A	401	1	69,73,73	1.26	8 (11%)	83,113,113	1.20	4 (4%)
23	CLA	d	401	-	69,73,73	1.23	7 (10%)	83,113,113	1.29	7 (8%)
35	CHL	y	309	-	70,74,74	1.22	8 (11%)	80,114,114	1.24	8 (10%)
23	CLA	g	611	31	64,68,73	1.30	7 (10%)	77,107,113	1.23	4 (5%)
25	BCR	B	618	-	41,41,41	0.68	0	56,56,56	1.83	17 (30%)
31	LHG	N	618	23	48,48,48	0.92	2 (4%)	51,54,54	1.05	4 (7%)
23	CLA	y	311	20	64,68,73	1.29	9 (14%)	77,107,113	1.24	8 (10%)
23	CLA	R	309	22	62,66,73	1.32	7 (11%)	74,104,113	1.22	6 (8%)
31	LHG	b	626	-	39,39,48	1.03	2 (5%)	42,45,54	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	CHL	n	605	7	52,56,74	1.37	6 (11%)	58,92,114	1.56	9 (15%)
38	NEX	N	617	-	38,46,46	0.87	1 (2%)	50,70,70	2.23	15 (30%)
31	LHG	G	619	23	45,45,48	0.96	2 (4%)	48,51,54	1.05	3 (6%)
23	CLA	s	602	15	50,54,73	1.46	8 (16%)	60,90,113	1.28	5 (8%)
36	LUT	n	616	-	42,43,43	0.76	0	51,60,60	1.54	13 (25%)
23	CLA	S	304	15	49,53,73	1.48	6 (12%)	59,89,113	1.41	4 (6%)
23	CLA	Y	314	20	69,73,73	1.25	7 (10%)	83,113,113	1.23	4 (4%)
36	LUT	n	615	-	42,43,43	0.72	0	51,60,60	1.53	11 (21%)
35	CHL	s	605	-	50,54,74	1.46	8 (16%)	56,90,114	1.44	5 (8%)
31	LHG	B	621	-	48,48,48	0.93	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	Y	313	20	64,68,73	1.30	7 (10%)	77,107,113	1.30	8 (10%)
35	CHL	r	606	-	50,54,74	1.43	7 (14%)	56,90,114	1.34	6 (10%)
23	CLA	y	312	31	64,68,73	1.30	7 (10%)	77,107,113	1.26	5 (6%)
23	CLA	s	604	-	54,58,73	1.41	9 (16%)	65,95,113	1.34	6 (9%)
36	LUT	s	614	-	42,43,43	0.74	0	51,60,60	1.59	11 (21%)
23	CLA	B	602	2	69,73,73	1.25	8 (11%)	83,113,113	1.16	7 (8%)
35	CHL	r	607	-	65,69,74	1.26	7 (10%)	74,108,114	1.27	8 (10%)
23	CLA	g	610	7	68,72,73	1.24	6 (8%)	81,111,113	1.13	3 (3%)
23	CLA	d	402	-	54,58,73	1.44	8 (14%)	65,95,113	1.36	6 (9%)
32	DMU	s	618	-	34,34,34	0.54	0	45,45,45	0.98	1 (2%)
23	CLA	S	311	31	46,50,73	1.50	7 (15%)	55,85,113	1.32	5 (9%)
25	BCR	b	620	-	41,41,41	0.68	0	56,56,56	1.83	17 (30%)
35	CHL	Y	309	-	70,74,74	1.22	8 (11%)	80,114,114	1.24	8 (10%)
23	CLA	R	311	31	45,49,73	1.52	7 (15%)	54,84,113	1.41	4 (7%)
25	BCR	b	619	-	41,41,41	0.70	0	56,56,56	1.68	12 (21%)
23	CLA	G	603	7	69,73,73	1.25	6 (8%)	83,113,113	1.25	7 (8%)
35	CHL	N	601	7	70,74,74	1.21	7 (10%)	80,114,114	1.30	9 (11%)
35	CHL	Y	308	-	70,74,74	1.20	8 (11%)	80,114,114	1.36	9 (11%)
30	LMG	B	623	-	40,40,55	1.06	2 (5%)	48,48,63	0.99	2 (4%)
23	CLA	a	404	1	64,68,73	1.28	7 (10%)	77,107,113	1.27	7 (9%)
23	CLA	s	608	15	49,53,73	1.49	7 (14%)	59,89,113	1.36	7 (11%)
23	CLA	r	603	22	64,68,73	1.29	8 (12%)	77,107,113	1.27	5 (6%)
23	CLA	C	511	3	69,73,73	1.25	7 (10%)	83,113,113	1.27	5 (6%)
32	DMU	C	520	-	34,34,34	0.54	0	45,45,45	1.48	5 (11%)
23	CLA	B	611	2	69,73,73	1.24	9 (13%)	83,113,113	1.19	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	504	-	64,68,73	1.30	7 (10%)	77,107,113	1.23	3 (3%)
23	CLA	B	616	2	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
36	LUT	Y	317	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
35	CHL	n	601	7	70,74,74	1.20	7 (10%)	80,114,114	1.31	7 (8%)
23	CLA	b	603	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	8 (9%)
23	CLA	G	612	7	49,53,73	1.48	6 (12%)	59,89,113	1.39	7 (11%)
26	SQD	c	520	-	44,45,54	1.31	4 (9%)	53,56,65	3.95	8 (15%)
23	CLA	b	615	2	69,73,73	1.25	8 (11%)	83,113,113	1.24	5 (6%)
32	DMU	S	319	-	34,34,34	0.53	0	45,45,45	0.97	2 (4%)
31	LHG	B	627	-	39,39,48	1.03	2 (5%)	42,45,54	0.97	2 (4%)
23	CLA	b	604	2	69,73,73	1.25	8 (11%)	83,113,113	1.17	7 (8%)
30	LMG	W	203	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	3 (5%)
23	CLA	r	610	31	45,49,73	1.52	7 (15%)	54,84,113	1.42	4 (7%)
23	CLA	r	609	22	69,73,73	1.24	8 (11%)	83,113,113	1.16	7 (8%)
35	CHL	G	608	-	70,74,74	1.21	7 (10%)	80,114,114	1.17	5 (6%)
35	CHL	G	605	7	50,54,74	1.45	8 (16%)	56,90,114	1.34	8 (14%)
31	LHG	W	201	-	48,48,48	0.93	2 (4%)	51,54,54	1.03	3 (5%)
23	CLA	c	511	3	69,73,73	1.26	7 (10%)	83,113,113	1.25	4 (4%)
23	CLA	n	604	-	54,58,73	1.41	8 (14%)	65,95,113	1.33	6 (9%)
23	CLA	C	508	-	69,73,73	1.24	6 (8%)	83,113,113	1.32	7 (8%)
23	CLA	C	504	3	69,73,73	1.25	6 (8%)	83,113,113	1.20	4 (4%)
30	LMG	B	620	-	51,51,55	0.94	2 (3%)	59,59,63	0.98	3 (5%)
38	NEX	Y	318	-	38,46,46	0.92	1 (2%)	50,70,70	3.98	18 (36%)
23	CLA	S	312	15	49,53,73	1.47	7 (14%)	59,89,113	1.50	7 (11%)
23	CLA	b	605	2	69,73,73	1.24	8 (11%)	83,113,113	1.20	6 (7%)
23	CLA	B	606	2	69,73,73	1.25	8 (11%)	83,113,113	1.21	6 (7%)
36	LUT	R	314	-	42,43,43	0.73	0	51,60,60	1.60	10 (19%)
23	CLA	B	613	2	69,73,73	1.24	7 (10%)	83,113,113	1.24	5 (6%)
23	CLA	G	614	7	46,50,73	1.50	7 (15%)	55,85,113	1.30	7 (12%)
23	CLA	S	303	15	50,54,73	1.46	8 (16%)	60,90,113	1.30	4 (6%)
30	LMG	w	202	-	51,51,55	0.94	2 (3%)	59,59,63	1.03	3 (5%)
30	LMG	d	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.98	2 (3%)
36	LUT	Y	316	-	42,43,43	0.71	0	51,60,60	1.48	9 (17%)
23	CLA	s	613	15	45,49,73	1.50	8 (17%)	54,84,113	1.45	7 (12%)
23	CLA	s	612	15	59,63,73	1.36	7 (11%)	71,101,113	1.29	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	R	305	-	52,56,73	1.43	8 (15%)	62,92,113	1.36	7 (11%)
23	CLA	s	611	15	49,53,73	1.51	7 (14%)	59,89,113	1.41	8 (13%)
36	LUT	G	616	-	42,43,43	0.76	0	51,60,60	1.58	12 (23%)
25	BCR	c	518	-	41,41,41	0.67	0	56,56,56	1.82	13 (23%)
38	NEX	R	301	-	38,46,46	0.91	1 (2%)	50,70,70	4.00	18 (36%)
23	CLA	c	503	3	69,73,73	1.25	7 (10%)	83,113,113	1.19	5 (6%)
35	CHL	R	307	-	50,54,74	1.44	7 (14%)	56,90,114	1.35	7 (12%)
23	CLA	G	604	-	53,57,73	1.42	8 (15%)	62,93,113	1.34	6 (9%)
35	CHL	n	609	7	70,74,74	1.23	7 (10%)	80,114,114	1.40	8 (10%)
23	CLA	c	512	3	60,64,73	1.33	6 (10%)	72,102,113	1.35	6 (8%)
31	LHG	b	624	-	45,45,48	0.96	2 (4%)	48,51,54	0.98	2 (4%)
28	DGD	c	515	-	56,56,67	0.92	2 (3%)	70,70,81	1.01	3 (4%)
35	CHL	r	605	-	50,54,74	1.44	6 (12%)	56,90,114	1.38	7 (12%)
25	BCR	b	621	-	41,41,41	0.68	0	56,56,56	1.72	10 (17%)
23	CLA	b	617	2	69,73,73	1.23	7 (10%)	83,113,113	1.34	8 (9%)
31	LHG	y	318	23	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
31	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	D	403	4	69,73,73	1.28	9 (13%)	83,113,113	1.21	6 (7%)
35	CHL	g	609	7	65,69,74	1.27	8 (12%)	74,108,114	1.22	7 (9%)
23	CLA	C	513	3	60,64,73	1.33	5 (8%)	72,102,113	1.33	7 (9%)
23	CLA	c	505	3	62,66,73	1.29	7 (11%)	74,104,113	1.28	7 (9%)
23	CLA	c	508	3	69,73,73	1.25	8 (11%)	83,113,113	1.23	7 (8%)
28	DGD	C	517	-	56,56,67	0.92	2 (3%)	70,70,81	1.02	3 (4%)
23	CLA	a	401	1	69,73,73	1.25	8 (11%)	83,113,113	1.21	4 (4%)
23	CLA	y	315	20	49,53,73	1.48	8 (16%)	59,89,113	1.31	5 (8%)
35	CHL	s	607	-	53,57,74	1.38	6 (11%)	59,93,114	1.34	10 (16%)
31	LHG	Y	319	23	48,48,48	0.92	2 (4%)	51,54,54	0.97	2 (3%)
23	CLA	S	305	-	54,58,73	1.43	9 (16%)	65,95,113	1.36	7 (10%)
35	CHL	N	606	-	50,54,74	1.44	8 (16%)	56,90,114	1.41	12 (21%)
23	CLA	Y	303	20	65,69,73	1.29	6 (9%)	78,108,113	1.21	5 (6%)
24	PHO	a	402	-	58,69,69	1.21	5 (8%)	56,99,99	1.83	7 (12%)
23	CLA	B	603	2	69,73,73	1.24	7 (10%)	83,113,113	1.20	6 (7%)
23	CLA	b	608	2	69,73,73	1.24	8 (11%)	83,113,113	1.21	6 (7%)
34	HEM	f	101	6,5	50,50,50	1.48	7 (14%)	66,82,82	1.32	7 (10%)
23	CLA	y	304	20	69,73,73	1.28	7 (10%)	83,113,113	1.31	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	LUT	s	615	-	42,43,43	0.73	0	51,60,60	1.47	8 (15%)
23	CLA	Y	305	-	54,58,73	1.42	10 (18%)	65,95,113	1.38	7 (10%)
23	CLA	Y	315	20	49,53,73	1.47	6 (12%)	59,89,113	1.32	5 (8%)
35	CHL	S	307	-	47,51,74	1.45	6 (12%)	52,86,114	1.53	7 (13%)
31	LHG	S	318	23	48,48,48	0.92	2 (4%)	51,54,54	0.99	2 (3%)
25	BCR	D	405	-	41,41,41	0.67	0	56,56,56	1.99	15 (26%)
23	CLA	B	604	2	69,73,73	1.27	7 (10%)	83,113,113	1.32	5 (6%)
35	CHL	G	607	-	47,51,74	1.46	7 (14%)	52,86,114	1.46	6 (11%)
23	CLA	c	506	3	55,59,73	1.40	8 (14%)	66,96,113	1.36	7 (10%)
27	BCT	a	408	29	2,3,3	0.87	0	2,3,3	3.26	2 (100%)
36	LUT	y	317	-	42,43,43	0.74	0	51,60,60	1.50	10 (19%)
23	CLA	R	304	22	64,68,73	1.29	8 (12%)	77,107,113	1.31	5 (6%)
25	BCR	c	514	-	41,41,41	0.69	0	56,56,56	1.72	14 (25%)
23	CLA	n	611	31	64,68,73	1.30	6 (9%)	77,107,113	1.33	7 (9%)
23	CLA	b	607	2	69,73,73	1.25	7 (10%)	83,113,113	1.39	7 (8%)
23	CLA	r	611	22	69,73,73	1.26	7 (10%)	83,113,113	1.24	4 (4%)
36	LUT	N	616	-	42,43,43	0.75	0	51,60,60	1.49	11 (21%)
35	CHL	S	302	15	50,54,74	1.43	7 (14%)	56,90,114	1.46	6 (10%)
25	BCR	k	101	-	41,41,41	0.65	0	56,56,56	1.84	15 (26%)
23	CLA	N	611	31	64,68,73	1.30	6 (9%)	77,107,113	1.33	7 (9%)
23	CLA	B	608	2	69,73,73	1.24	8 (11%)	83,113,113	1.24	7 (8%)
30	LMG	c	521	-	50,50,55	0.97	2 (4%)	58,58,63	1.07	4 (6%)
23	CLA	R	302	22	53,57,73	1.45	7 (13%)	62,93,113	1.31	5 (8%)
31	LHG	c	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
35	CHL	Y	310	20	70,74,74	1.27	9 (12%)	80,114,114	1.37	8 (10%)
23	CLA	C	505	-	64,68,73	1.29	6 (9%)	77,107,113	1.24	4 (5%)
32	DMU	C	523	-	34,34,34	0.59	0	45,45,45	0.81	1 (2%)
26	SQD	A	406	-	49,50,54	1.24	4 (8%)	58,61,65	1.05	5 (8%)
25	BCR	h	101	-	41,41,41	0.70	0	56,56,56	1.59	9 (16%)
38	NEX	g	618	-	38,46,46	0.88	1 (2%)	50,70,70	2.45	16 (32%)
23	CLA	g	612	7	49,53,73	1.48	8 (16%)	59,89,113	1.37	4 (6%)
23	CLA	N	610	7	63,67,73	1.28	7 (11%)	75,105,113	1.23	7 (9%)
23	CLA	C	514	3	69,73,73	1.26	8 (11%)	83,113,113	1.24	8 (9%)
35	CHL	g	605	7	50,54,74	1.44	8 (16%)	56,90,114	1.34	8 (14%)
38	NEX	R	316	-	38,46,46	0.86	1 (2%)	50,70,70	2.30	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	A	404	1	64,68,73	1.27	7 (10%)	77,107,113	1.27	8 (10%)
38	NEX	r	615	-	38,46,46	0.90	1 (2%)	50,70,70	2.31	18 (36%)
23	CLA	c	501	3	69,73,73	1.27	9 (13%)	83,113,113	1.17	6 (7%)
23	CLA	g	602	7	69,73,73	1.25	7 (10%)	83,113,113	1.12	4 (4%)
26	SQD	B	625	-	53,54,54	1.20	4 (7%)	62,65,65	3.67	8 (12%)
23	CLA	Y	311	20	64,68,73	1.28	8 (12%)	77,107,113	1.18	6 (7%)
23	CLA	N	614	7	45,49,73	1.52	6 (13%)	54,84,113	1.33	5 (9%)
23	CLA	r	604	-	52,56,73	1.44	7 (13%)	62,92,113	1.37	6 (9%)
23	CLA	g	614	7	46,50,73	1.49	7 (15%)	55,85,113	1.31	7 (12%)
23	CLA	b	614	2	69,73,73	1.23	8 (11%)	83,113,113	1.36	6 (7%)
37	XAT	y	301	-	39,47,47	0.91	0	54,74,74	2.56	17 (31%)
31	LHG	b	623	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	G	613	7	62,66,73	1.32	7 (11%)	74,104,113	1.25	4 (5%)
23	CLA	n	610	7	63,67,73	1.28	7 (11%)	75,105,113	1.20	7 (9%)
25	BCR	d	405	-	41,41,41	0.67	0	56,56,56	1.99	15 (26%)
35	CHL	g	601	7	70,74,74	1.23	7 (10%)	80,114,114	1.28	8 (10%)
25	BCR	B	617	-	41,41,41	0.70	0	56,56,56	1.66	12 (21%)
30	LMG	C	501	-	48,48,55	0.95	2 (4%)	56,56,63	1.06	4 (7%)
23	CLA	N	612	7	49,53,73	1.51	7 (14%)	59,89,113	1.46	6 (10%)
23	CLA	S	309	15	49,53,73	1.51	7 (14%)	59,89,113	1.33	4 (6%)
23	CLA	n	602	7	65,69,73	1.27	8 (12%)	78,108,113	1.35	8 (10%)
36	LUT	g	616	-	42,43,43	0.75	0	51,60,60	1.62	11 (21%)
24	PHO	A	403	-	58,69,69	1.22	5 (8%)	56,99,99	1.85	7 (12%)
37	XAT	r	614	-	39,47,47	0.89	0	54,74,74	2.49	17 (31%)
23	CLA	D	404	4	69,73,73	1.24	6 (8%)	83,113,113	1.23	4 (4%)
23	CLA	N	602	7	65,69,73	1.28	8 (12%)	78,108,113	1.34	9 (11%)
23	CLA	g	604	-	53,57,73	1.42	9 (16%)	62,93,113	1.33	6 (9%)
23	CLA	b	610	2	69,73,73	1.23	7 (10%)	83,113,113	1.23	7 (8%)
23	CLA	D	401	-	69,73,73	1.24	8 (11%)	83,113,113	1.27	7 (8%)
30	LMG	C	522	-	50,50,55	0.96	2 (4%)	58,58,63	1.08	4 (6%)
31	LHG	l	102	-	48,48,48	0.91	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	B	605	2	69,73,73	1.25	7 (10%)	83,113,113	1.37	7 (8%)
35	CHL	S	306	-	50,54,74	1.47	6 (12%)	56,90,114	1.50	9 (16%)
31	LHG	r	616	23	41,41,48	1.00	2 (4%)	44,47,54	1.05	3 (6%)
23	CLA	c	510	3	69,73,73	1.26	7 (10%)	83,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LMG	D	409	-	46,46,55	0.99	2 (4%)	54,54,63	0.97	2 (3%)
26	SQD	C	521	-	44,45,54	1.31	4 (9%)	53,56,65	3.96	8 (15%)
35	CHL	n	608	-	70,74,74	1.22	8 (11%)	80,114,114	1.19	6 (7%)
36	LUT	S	316	-	42,43,43	0.77	0	51,60,60	1.48	8 (15%)
31	LHG	D	407	-	48,48,48	0.93	2 (4%)	51,54,54	0.94	2 (3%)
35	CHL	Y	302	20	70,74,74	1.21	8 (11%)	80,114,114	1.25	7 (8%)
31	LHG	c	517	-	48,48,48	0.92	2 (4%)	51,54,54	0.98	2 (3%)
23	CLA	d	403	4	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
36	LUT	r	613	-	42,43,43	0.73	0	51,60,60	1.67	11 (21%)
25	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.61	9 (16%)
30	LMG	S	301	-	55,55,55	0.90	2 (3%)	63,63,63	0.97	4 (6%)
23	CLA	Y	312	31	64,68,73	1.30	7 (10%)	77,107,113	1.27	5 (6%)
23	CLA	B	614	2	69,73,73	1.25	8 (11%)	83,113,113	1.20	9 (10%)
35	CHL	s	601	15	50,54,74	1.44	7 (14%)	56,90,114	1.47	5 (8%)
23	CLA	c	502	3	69,73,73	1.25	7 (10%)	83,113,113	1.34	6 (7%)
23	CLA	B	607	-	69,73,73	1.26	8 (11%)	83,113,113	1.20	5 (6%)
36	LUT	N	615	-	42,43,43	0.72	0	51,60,60	1.48	9 (17%)
23	CLA	R	313	22	69,73,73	1.25	7 (10%)	83,113,113	1.22	8 (9%)
28	DGD	D	410	-	63,63,67	0.90	2 (3%)	77,77,81	0.92	2 (2%)
35	CHL	s	606	-	47,51,74	1.46	6 (12%)	52,86,114	1.56	8 (15%)
23	CLA	r	608	22	62,66,73	1.31	7 (11%)	74,104,113	1.22	5 (6%)

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
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
32	DMU	c	522	-	-	5/19/59/59	0/2/2/2
23	CLA	B	609	2	-	14/39/115/115	-
23	CLA	B	612	2	-	18/39/115/115	-
35	CHL	g	607	-	-	7/14/90/117	-
31	LHG	l	103	-	-	18/53/53/53	-
39	VTQ	W	202	-	-	3/25/49/49	0/1/1/1
35	CHL	n	607	-	-	11/17/93/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	R	317	23	-	8/46/46/53	-
23	CLA	C	503	3	-	13/39/115/115	-
23	CLA	c	509	3	-	11/39/115/115	-
35	CHL	y	308	-	-	22/41/117/117	-
23	CLA	g	603	7	-	8/39/115/115	-
23	CLA	y	303	20	-	18/35/111/115	-
35	CHL	y	302	20	-	16/41/117/117	-
31	LHG	D	408	-	-	7/53/53/53	-
25	BCR	B	619	-	-	6/29/63/63	0/2/2/2
30	LMG	a	407	-	-	2/43/63/70	0/1/1/1
31	LHG	L	102	-	-	18/53/53/53	-
35	CHL	y	307	-	-	10/22/98/117	-
23	CLA	b	611	2	-	13/39/115/115	-
35	CHL	G	606	-	-	8/14/90/117	-
23	CLA	S	314	15	-	8/10/86/115	-
31	LHG	n	618	23	-	10/53/53/53	-
23	CLA	y	313	20	-	9/33/109/115	-
23	CLA	A	402	-	-	7/21/97/115	-
23	CLA	g	613	7	-	13/31/107/115	-
35	CHL	N	608	-	-	10/41/117/117	-
35	CHL	R	308	-	-	13/35/111/117	-
28	DGD	B	624	-	-	7/48/88/95	0/2/2/2
35	CHL	G	601	7	-	20/41/117/117	-
31	LHG	B	622	-	-	11/50/50/53	-
35	CHL	g	608	-	-	18/41/117/117	-
28	DGD	d	410	-	-	9/51/91/95	0/2/2/2
26	SQD	b	602	-	-	20/49/69/69	0/1/1/1
37	XAT	G	617	-	-	1/31/93/93	0/4/4/4
23	CLA	y	314	20	-	15/39/115/115	-
23	CLA	R	303	22	-	15/33/109/115	-
38	NEX	n	617	-	-	5/27/83/83	0/3/3/3
31	LHG	s	617	23	-	9/53/53/53	-
23	CLA	b	609	-	-	16/39/115/115	-
35	CHL	y	310	20	-	21/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	G	602	7	-	20/39/115/115	-
24	PHO	D	402	-	-	6/37/103/103	0/5/6/6
35	CHL	Y	307	-	-	10/22/98/117	-
23	CLA	B	601	-	-	15/39/115/115	-
37	XAT	g	620	-	-	0/31/93/93	0/4/4/4
33	PL9	d	406	-	-	25/53/73/73	0/1/1/1
35	CHL	S	308	-	-	12/21/97/117	-
28	DGD	A	408	-	-	8/48/88/95	0/2/2/2
39	VTQ	w	201	-	-	3/25/49/49	0/1/1/1
23	CLA	n	613	7	-	14/33/109/115	-
36	LUT	g	615	-	-	3/29/67/67	0/2/2/2
31	LHG	g	619	23	-	10/50/50/53	-
25	BCR	C	519	-	-	0/29/63/63	0/2/2/2
23	CLA	b	618	2	-	14/39/115/115	-
36	LUT	S	315	-	-	2/29/67/67	0/2/2/2
26	SQD	L	103	-	-	15/49/69/69	0/1/1/1
23	CLA	S	313	15	-	11/27/103/115	-
23	CLA	G	611	31	-	5/33/109/115	-
28	DGD	B	626	-	-	13/45/85/95	0/2/2/2
23	CLA	c	513	3	-	9/39/115/115	-
23	CLA	C	506	3	-	13/31/107/115	-
35	CHL	y	306	20	-	13/23/99/117	-
23	CLA	Y	304	20	-	13/39/115/115	-
23	CLA	r	602	22	-	18/33/109/115	-
23	CLA	C	512	3	-	16/39/115/115	-
36	LUT	y	316	-	-	2/29/67/67	0/2/2/2
31	LHG	d	407	-	-	12/53/53/53	-
31	LHG	d	408	-	-	9/53/53/53	-
26	SQD	l	101	-	-	17/49/69/69	0/1/1/1
36	LUT	G	615	-	-	2/29/67/67	0/2/2/2
23	CLA	n	612	7	-	10/15/91/115	-
25	BCR	H	101	-	-	7/29/63/63	0/2/2/2
38	NEX	S	317	-	-	4/27/83/83	0/3/3/3
23	CLA	G	610	7	-	13/38/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	A	405	-	-	2/29/63/63	0/2/2/2
23	CLA	B	615	2	-	16/39/115/115	-
23	CLA	b	606	2	-	11/39/115/115	-
37	XAT	R	315	-	-	1/31/93/93	0/4/4/4
23	CLA	b	613	2	-	12/39/115/115	-
23	CLA	d	404	4	-	17/39/115/115	-
28	DGD	b	625	-	-	12/45/85/95	0/2/2/2
32	DMU	c	519	-	-	6/19/59/59	0/2/2/2
23	CLA	R	312	22	-	14/39/115/115	-
23	CLA	b	612	-	-	11/39/115/115	-
35	CHL	n	606	-	-	7/17/93/117	-
23	CLA	C	502	3	-	14/39/115/115	-
38	NEX	s	616	-	-	2/27/83/83	0/3/3/3
23	CLA	r	601	22	-	13/20/96/115	-
23	CLA	n	614	7	-	5/10/86/115	-
23	CLA	n	603	7	-	12/32/108/115	-
38	NEX	G	618	-	-	3/27/83/83	0/3/3/3
23	CLA	N	603	7	-	13/32/108/115	-
24	PHO	a	403	-	-	7/37/103/103	0/5/6/6
25	BCR	z	101	-	-	0/29/63/63	0/2/2/2
35	CHL	Y	306	20	-	13/23/99/117	-
25	BCR	K	101	-	-	4/29/63/63	0/2/2/2
30	LMG	b	601	-	-	3/35/55/70	0/1/1/1
23	CLA	s	609	15	-	6/15/91/115	-
23	CLA	N	613	7	-	14/33/109/115	-
23	CLA	R	310	22	-	11/39/115/115	-
31	LHG	C	518	-	-	11/53/53/53	-
23	CLA	y	305	-	-	9/21/97/115	-
23	CLA	C	509	3	-	11/39/115/115	-
23	CLA	N	604	-	-	7/21/97/115	-
23	CLA	c	507	-	-	10/39/115/115	-
34	HEM	F	101	6,5	-	5/14/54/54	-
30	LMG	b	622	-	-	7/46/66/70	0/1/1/1
33	PL9	D	406	-	-	26/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CHL	G	609	7	-	12/35/111/117	-
23	CLA	S	310	15	-	9/15/91/115	-
23	CLA	B	610	-	-	11/39/115/115	-
23	CLA	C	510	3	-	11/39/115/115	-
37	XAT	G	620	-	-	0/31/93/93	0/4/4/4
35	CHL	N	607	-	-	11/17/93/117	-
35	CHL	g	606	-	-	4/14/90/117	-
23	CLA	s	603	15	-	7/15/91/115	-
23	CLA	s	610	31	-	6/12/88/115	-
23	CLA	C	507	3	-	5/23/99/115	-
37	XAT	Y	301	-	-	0/31/93/93	0/4/4/4
35	CHL	R	306	-	-	7/17/93/117	-
35	CHL	N	605	7	-	12/20/96/117	-
23	CLA	r	612	22	-	11/39/115/115	-
23	CLA	b	616	2	-	18/39/115/115	-
25	BCR	a	405	-	-	2/29/63/63	0/2/2/2
26	SQD	a	406	-	-	8/45/65/69	0/1/1/1
30	LMG	s	619	-	-	5/50/70/70	0/1/1/1
35	CHL	N	609	7	-	16/41/117/117	-
37	XAT	g	617	-	-	2/31/93/93	0/4/4/4
23	CLA	A	401	1	-	10/39/115/115	-
23	CLA	d	401	-	-	14/39/115/115	-
35	CHL	y	309	-	-	13/41/117/117	-
23	CLA	g	611	31	-	6/33/109/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
31	LHG	N	618	23	-	9/53/53/53	-
23	CLA	y	311	20	-	8/33/109/115	-
23	CLA	R	309	22	-	7/31/107/115	-
31	LHG	b	626	-	-	13/44/44/53	-
35	CHL	n	605	7	-	12/20/96/117	-
38	NEX	N	617	-	-	4/27/83/83	0/3/3/3
31	LHG	G	619	23	-	11/50/50/53	-
23	CLA	s	602	15	-	10/17/93/115	-
36	LUT	n	616	-	-	1/29/67/67	0/2/2/2
23	CLA	S	304	15	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	Y	314	20	-	13/39/115/115	-
36	LUT	n	615	-	-	3/29/67/67	0/2/2/2
35	CHL	s	605	-	-	8/17/93/117	-
31	LHG	B	621	-	-	11/53/53/53	-
23	CLA	Y	313	20	-	9/33/109/115	-
35	CHL	r	606	-	-	7/17/93/117	-
23	CLA	y	312	31	-	10/33/109/115	-
23	CLA	s	604	-	-	5/21/97/115	-
36	LUT	s	614	-	-	2/29/67/67	0/2/2/2
23	CLA	B	602	2	-	15/39/115/115	-
35	CHL	r	607	-	-	13/35/111/117	-
23	CLA	g	610	7	-	15/38/114/115	-
23	CLA	d	402	-	-	12/21/97/115	-
32	DMU	s	618	-	-	5/19/59/59	0/2/2/2
23	CLA	S	311	31	-	6/12/88/115	-
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
35	CHL	Y	309	-	-	14/41/117/117	-
23	CLA	R	311	31	-	7/10/86/115	-
25	BCR	b	619	-	-	6/29/63/63	0/2/2/2
23	CLA	G	603	7	-	9/39/115/115	-
35	CHL	N	601	7	-	11/41/117/117	-
35	CHL	Y	308	-	-	24/41/117/117	-
30	LMG	B	623	-	-	3/35/55/70	0/1/1/1
23	CLA	a	404	1	-	14/33/109/115	-
23	CLA	s	608	15	-	6/15/91/115	-
23	CLA	r	603	22	-	8/33/109/115	-
23	CLA	C	511	3	-	15/39/115/115	-
32	DMU	C	520	-	-	7/19/59/59	0/2/2/2
23	CLA	B	611	2	-	11/39/115/115	-
23	CLA	c	504	-	-	5/33/109/115	-
23	CLA	B	616	2	-	12/39/115/115	-
36	LUT	Y	317	-	-	1/29/67/67	0/2/2/2
35	CHL	n	601	7	-	16/41/117/117	-
23	CLA	b	603	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	G	612	7	-	9/15/91/115	-
26	SQD	c	520	-	-	2/40/60/69	0/1/1/1
23	CLA	b	615	2	-	15/39/115/115	-
32	DMU	S	319	-	-	4/19/59/59	0/2/2/2
31	LHG	B	627	-	-	13/44/44/53	-
23	CLA	b	604	2	-	12/39/115/115	-
30	LMG	W	203	-	-	7/46/66/70	0/1/1/1
23	CLA	r	610	31	-	6/10/86/115	-
23	CLA	r	609	22	-	12/39/115/115	-
35	CHL	G	608	-	-	17/41/117/117	-
35	CHL	G	605	7	-	12/17/93/117	-
31	LHG	W	201	-	-	9/53/53/53	-
23	CLA	c	511	3	-	13/39/115/115	-
23	CLA	n	604	-	-	6/21/97/115	-
23	CLA	C	508	-	-	12/39/115/115	-
23	CLA	C	504	3	-	19/39/115/115	-
30	LMG	B	620	-	-	9/46/66/70	0/1/1/1
38	NEX	Y	318	-	-	3/27/83/83	0/3/3/3
23	CLA	S	312	15	-	6/15/91/115	-
23	CLA	b	605	2	-	16/39/115/115	-
23	CLA	B	606	2	-	9/39/115/115	-
36	LUT	R	314	-	-	2/29/67/67	0/2/2/2
23	CLA	B	613	2	-	15/39/115/115	-
23	CLA	G	614	7	-	7/12/88/115	-
23	CLA	S	303	15	-	8/17/93/115	-
30	LMG	w	202	-	-	7/46/66/70	0/1/1/1
30	LMG	d	409	-	-	3/41/61/70	0/1/1/1
36	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
23	CLA	s	613	15	-	8/10/86/115	-
23	CLA	s	612	15	-	11/27/103/115	-
23	CLA	R	305	-	-	10/19/95/115	-
23	CLA	s	611	15	-	4/15/91/115	-
36	LUT	G	616	-	-	1/29/67/67	0/2/2/2
25	BCR	c	518	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	NEX	R	301	-	-	4/27/83/83	0/3/3/3
23	CLA	c	503	3	-	18/39/115/115	-
35	CHL	R	307	-	-	7/17/93/117	-
23	CLA	G	604	-	-	11/20/96/115	-
35	CHL	n	609	7	-	15/41/117/117	-
23	CLA	c	512	3	-	8/29/105/115	-
31	LHG	b	624	-	-	9/50/50/53	-
28	DGD	c	515	-	-	4/44/84/95	0/2/2/2
35	CHL	r	605	-	-	7/17/93/117	-
25	BCR	b	621	-	-	4/29/63/63	0/2/2/2
23	CLA	b	617	2	-	20/39/115/115	-
31	LHG	y	318	23	-	12/53/53/53	-
31	LHG	L	101	-	-	8/53/53/53	-
23	CLA	D	403	4	-	7/39/115/115	-
35	CHL	g	609	7	-	14/35/111/117	-
23	CLA	C	513	3	-	8/29/105/115	-
23	CLA	c	505	3	-	15/31/107/115	-
23	CLA	c	508	3	-	13/39/115/115	-
28	DGD	C	517	-	-	4/44/84/95	0/2/2/2
23	CLA	a	401	1	-	10/39/115/115	-
23	CLA	y	315	20	-	6/15/91/115	-
35	CHL	s	607	-	-	14/21/97/117	-
31	LHG	Y	319	23	-	12/53/53/53	-
23	CLA	S	305	-	-	7/21/97/115	-
35	CHL	N	606	-	-	9/17/93/117	-
23	CLA	Y	303	20	-	18/35/111/115	-
24	PHO	a	402	-	-	14/37/103/103	0/5/6/6
23	CLA	B	603	2	-	19/39/115/115	-
23	CLA	b	608	2	-	12/39/115/115	-
34	HEM	f	101	6,5	-	5/14/54/54	-
23	CLA	y	304	20	-	13/39/115/115	-
36	LUT	s	615	-	-	3/29/67/67	0/2/2/2
23	CLA	Y	305	-	-	9/21/97/115	-
23	CLA	Y	315	20	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CHL	S	307	-	-	7/14/90/117	-
31	LHG	S	318	23	-	10/53/53/53	-
25	BCR	D	405	-	-	7/29/63/63	0/2/2/2
23	CLA	B	604	2	-	11/39/115/115	-
35	CHL	G	607	-	-	6/14/90/117	-
23	CLA	c	506	3	-	8/23/99/115	-
36	LUT	y	317	-	-	1/29/67/67	0/2/2/2
23	CLA	R	304	22	-	9/33/109/115	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
23	CLA	n	611	31	-	11/33/109/115	-
23	CLA	b	607	2	-	13/39/115/115	-
23	CLA	r	611	22	-	12/39/115/115	-
36	LUT	N	616	-	-	1/29/67/67	0/2/2/2
35	CHL	S	302	15	-	9/17/93/117	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	N	611	31	-	11/33/109/115	-
23	CLA	B	608	2	-	14/39/115/115	-
30	LMG	c	521	-	-	9/45/65/70	0/1/1/1
23	CLA	R	302	22	-	12/20/96/115	-
31	LHG	c	516	-	-	9/53/53/53	-
35	CHL	Y	310	20	-	20/41/117/117	-
23	CLA	C	505	-	-	7/33/109/115	-
32	DMU	C	523	-	-	6/19/59/59	0/2/2/2
26	SQD	A	406	-	-	5/45/65/69	0/1/1/1
25	BCR	h	101	-	-	7/29/63/63	0/2/2/2
38	NEX	g	618	-	-	2/27/83/83	0/3/3/3
23	CLA	g	612	7	-	9/15/91/115	-
23	CLA	N	610	7	-	9/32/108/115	-
23	CLA	C	514	3	-	7/39/115/115	-
35	CHL	g	605	7	-	12/17/93/117	-
38	NEX	R	316	-	-	5/27/83/83	0/3/3/3
23	CLA	A	404	1	-	14/33/109/115	-
38	NEX	r	615	-	-	5/27/83/83	0/3/3/3
23	CLA	c	501	3	-	14/39/115/115	-
23	CLA	g	602	7	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	B	625	-	-	19/49/69/69	0/1/1/1
23	CLA	Y	311	20	-	8/33/109/115	-
23	CLA	N	614	7	-	5/10/86/115	-
23	CLA	r	604	-	-	10/19/95/115	-
23	CLA	g	614	7	-	7/12/88/115	-
23	CLA	b	614	2	-	18/39/115/115	-
37	XAT	y	301	-	-	0/31/93/93	0/4/4/4
31	LHG	b	623	-	-	11/53/53/53	-
23	CLA	G	613	7	-	14/31/107/115	-
23	CLA	n	610	7	-	10/32/108/115	-
25	BCR	d	405	-	-	7/29/63/63	0/2/2/2
35	CHL	g	601	7	-	19/41/117/117	-
25	BCR	B	617	-	-	6/29/63/63	0/2/2/2
30	LMG	C	501	-	-	5/43/63/70	0/1/1/1
23	CLA	N	612	7	-	9/15/91/115	-
23	CLA	S	309	15	-	10/15/91/115	-
23	CLA	n	602	7	-	10/35/111/115	-
36	LUT	g	616	-	-	0/29/67/67	0/2/2/2
24	PHO	A	403	-	-	13/37/103/103	0/5/6/6
37	XAT	r	614	-	-	1/31/93/93	0/4/4/4
23	CLA	D	404	4	-	18/39/115/115	-
23	CLA	N	602	7	-	13/35/111/115	-
23	CLA	g	604	-	-	9/20/96/115	-
23	CLA	b	610	2	-	18/39/115/115	-
23	CLA	D	401	-	-	16/39/115/115	-
30	LMG	C	522	-	-	9/45/65/70	0/1/1/1
31	LHG	l	102	-	-	9/53/53/53	-
23	CLA	B	605	2	-	13/39/115/115	-
35	CHL	S	306	-	-	10/17/93/117	-
31	LHG	r	616	23	-	6/46/46/53	-
23	CLA	c	510	3	-	15/39/115/115	-
30	LMG	D	409	-	-	3/41/61/70	0/1/1/1
26	SQD	C	521	-	-	2/40/60/69	0/1/1/1
35	CHL	n	608	-	-	10/41/117/117	-
36	LUT	S	316	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	D	407	-	-	11/53/53/53	-
35	CHL	Y	302	20	-	17/41/117/117	-
31	LHG	c	517	-	-	12/53/53/53	-
23	CLA	d	403	4	-	11/39/115/115	-
36	LUT	r	613	-	-	2/29/67/67	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
30	LMG	S	301	-	-	5/50/70/70	0/1/1/1
23	CLA	Y	312	31	-	11/33/109/115	-
23	CLA	B	614	2	-	23/39/115/115	-
35	CHL	s	601	15	-	8/17/93/117	-
23	CLA	c	502	3	-	13/39/115/115	-
23	CLA	B	607	-	-	15/39/115/115	-
36	LUT	N	615	-	-	2/29/67/67	0/2/2/2
23	CLA	R	313	22	-	11/39/115/115	-
28	DGD	D	410	-	-	4/51/91/95	0/2/2/2
35	CHL	s	606	-	-	6/14/90/117	-
23	CLA	r	608	22	-	9/31/107/115	-

All (1723) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	406	PL9	C23-C24	10.33	1.57	1.33
33	D	406	PL9	C23-C24	10.29	1.57	1.33
33	d	406	PL9	C38-C39	10.14	1.57	1.33
33	D	406	PL9	C38-C39	10.02	1.57	1.33
33	d	406	PL9	C18-C19	9.68	1.56	1.33
33	D	406	PL9	C18-C19	9.67	1.56	1.33
33	D	406	PL9	C28-C29	9.55	1.55	1.33
33	d	406	PL9	C28-C29	9.53	1.55	1.33
33	D	406	PL9	C33-C34	9.09	1.54	1.33
33	d	406	PL9	C43-C44	9.06	1.54	1.33
33	d	406	PL9	C33-C34	9.04	1.54	1.33
33	D	406	PL9	C43-C44	9.02	1.54	1.33
33	D	406	PL9	C8-C9	8.80	1.54	1.33
33	d	406	PL9	C8-C9	8.78	1.54	1.33
33	D	406	PL9	C13-C14	7.99	1.52	1.33
33	d	406	PL9	C13-C14	7.97	1.52	1.33
33	d	406	PL9	C48-C49	7.57	1.54	1.32
33	D	406	PL9	C48-C49	7.57	1.54	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	406	PL9	O1-C4	7.48	1.39	1.23
33	d	406	PL9	O1-C4	7.48	1.39	1.23
33	d	406	PL9	C3-C4	-6.34	1.39	1.49
33	D	406	PL9	C3-C4	-6.34	1.39	1.49
33	D	406	PL9	O2-C1	5.71	1.39	1.24
33	d	406	PL9	O2-C1	5.70	1.39	1.24
33	D	406	PL9	C6-C1	-5.50	1.38	1.48
33	d	406	PL9	C6-C1	-5.49	1.38	1.48
26	b	602	SQD	O8-S	5.00	1.65	1.47
26	C	521	SQD	O8-S	4.98	1.65	1.47
26	c	520	SQD	O8-S	4.98	1.65	1.47
26	B	625	SQD	O8-S	4.97	1.65	1.47
24	A	403	PHO	C4D-ND	-4.81	1.31	1.38
24	a	402	PHO	C4D-ND	-4.77	1.31	1.38
24	a	403	PHO	C4D-ND	-4.66	1.32	1.38
26	L	103	SQD	O8-S	4.62	1.63	1.47
26	a	406	SQD	O8-S	4.61	1.63	1.47
26	A	406	SQD	O8-S	4.60	1.63	1.47
26	l	101	SQD	O8-S	4.60	1.63	1.47
24	D	402	PHO	C4D-ND	-4.59	1.32	1.38
23	R	302	CLA	C1D-ND	4.53	1.43	1.37
31	L	102	LHG	O7-C7	4.50	1.47	1.34
31	l	103	LHG	O7-C7	4.50	1.47	1.34
28	d	410	DGD	O1G-C1A	4.32	1.46	1.33
24	A	403	PHO	C1B-C2B	4.31	1.44	1.39
23	S	309	CLA	C1D-ND	4.29	1.43	1.37
24	a	402	PHO	C1B-C2B	4.29	1.44	1.39
33	d	406	PL9	C7-C3	4.27	1.55	1.51
28	C	517	DGD	O2G-C1B	4.27	1.46	1.34
31	L	102	LHG	O8-C23	4.27	1.45	1.33
30	C	522	LMG	O8-C28	4.27	1.45	1.33
30	b	601	LMG	O8-C28	4.27	1.45	1.33
30	B	623	LMG	O8-C28	4.27	1.45	1.33
28	b	625	DGD	O2G-C1B	4.26	1.46	1.34
26	l	101	SQD	O48-C23	4.26	1.45	1.33
28	d	410	DGD	O2G-C1B	4.26	1.46	1.34
31	B	627	LHG	O8-C23	4.26	1.45	1.33
30	c	521	LMG	O8-C28	4.25	1.45	1.33
28	B	626	DGD	O2G-C1B	4.25	1.46	1.34
26	B	625	SQD	O48-C23	4.25	1.45	1.33
31	l	103	LHG	O8-C23	4.25	1.45	1.33
28	D	410	DGD	O1G-C1A	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	408	LHG	O7-C7	4.24	1.46	1.34
31	b	626	LHG	O8-C23	4.23	1.45	1.33
26	a	406	SQD	O48-C23	4.23	1.45	1.33
28	c	515	DGD	O2G-C1B	4.23	1.46	1.34
30	b	622	LMG	O8-C28	4.22	1.45	1.33
30	S	301	LMG	O8-C28	4.22	1.45	1.33
30	w	202	LMG	O8-C28	4.22	1.45	1.33
30	B	620	LMG	O8-C28	4.22	1.45	1.33
23	Y	311	CLA	C1D-ND	4.22	1.43	1.37
31	D	407	LHG	O8-C23	4.22	1.45	1.33
30	W	203	LMG	O8-C28	4.21	1.45	1.33
26	A	406	SQD	O47-C7	4.21	1.46	1.34
30	s	619	LMG	O8-C28	4.21	1.45	1.33
31	d	408	LHG	O8-C23	4.21	1.45	1.33
31	d	408	LHG	O7-C7	4.21	1.46	1.34
26	C	521	SQD	O48-C23	4.21	1.45	1.33
26	b	602	SQD	O48-C23	4.21	1.45	1.33
28	A	408	DGD	O1G-C1A	4.21	1.45	1.33
26	c	520	SQD	O48-C23	4.20	1.45	1.33
28	C	517	DGD	O1G-C1A	4.20	1.45	1.33
31	R	317	LHG	O8-C23	4.20	1.45	1.33
30	D	409	LMG	O8-C28	4.20	1.45	1.33
26	A	406	SQD	O48-C23	4.20	1.45	1.33
31	d	407	LHG	O8-C23	4.20	1.45	1.33
26	a	406	SQD	O47-C7	4.20	1.46	1.34
31	D	408	LHG	O8-C23	4.20	1.45	1.33
26	C	521	SQD	O47-C7	4.19	1.46	1.34
28	b	625	DGD	O1G-C1A	4.19	1.45	1.33
31	g	619	LHG	O7-C7	4.19	1.46	1.34
28	B	624	DGD	O1G-C1A	4.19	1.45	1.33
28	D	410	DGD	O2G-C1B	4.19	1.46	1.34
31	C	518	LHG	O8-C23	4.18	1.45	1.33
33	D	406	PL9	C7-C3	4.18	1.55	1.51
26	c	520	SQD	O47-C7	4.18	1.46	1.34
31	r	616	LHG	O8-C23	4.18	1.45	1.33
30	d	409	LMG	O8-C28	4.18	1.45	1.33
30	b	601	LMG	O7-C10	4.18	1.46	1.34
28	c	515	DGD	O1G-C1A	4.18	1.45	1.33
31	W	201	LHG	O8-C23	4.18	1.45	1.33
28	B	626	DGD	O1G-C1A	4.17	1.45	1.33
23	r	601	CLA	C1D-ND	4.17	1.42	1.37
31	c	516	LHG	O8-C23	4.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	407	LMG	O8-C28	4.17	1.45	1.33
30	D	409	LMG	O7-C10	4.17	1.46	1.34
30	d	409	LMG	O7-C10	4.17	1.46	1.34
26	B	625	SQD	O47-C7	4.17	1.46	1.34
23	y	311	CLA	C1D-ND	4.17	1.42	1.37
30	B	623	LMG	O7-C10	4.16	1.46	1.34
31	b	623	LHG	O7-C7	4.16	1.46	1.34
30	c	521	LMG	O7-C10	4.15	1.46	1.34
31	c	517	LHG	O8-C23	4.14	1.45	1.33
31	B	621	LHG	O7-C7	4.14	1.46	1.34
31	c	516	LHG	O7-C7	4.14	1.46	1.34
31	s	617	LHG	O7-C7	4.14	1.46	1.34
31	Y	319	LHG	O8-C23	4.14	1.45	1.33
26	b	602	SQD	O47-C7	4.14	1.46	1.34
26	L	103	SQD	O48-C23	4.14	1.45	1.33
30	a	407	LMG	O7-C10	4.14	1.46	1.34
31	b	624	LHG	O7-C7	4.13	1.46	1.34
30	b	622	LMG	O7-C10	4.13	1.46	1.34
31	B	622	LHG	O7-C7	4.13	1.46	1.34
31	b	624	LHG	O8-C23	4.13	1.45	1.33
31	s	617	LHG	O8-C23	4.13	1.45	1.33
31	y	318	LHG	O8-C23	4.13	1.45	1.33
30	C	501	LMG	O8-C28	4.13	1.45	1.33
31	N	618	LHG	O8-C23	4.12	1.45	1.33
31	G	619	LHG	O7-C7	4.12	1.45	1.34
31	b	623	LHG	O8-C23	4.12	1.45	1.33
30	W	203	LMG	O7-C10	4.12	1.45	1.34
31	S	318	LHG	O8-C23	4.12	1.45	1.33
31	B	622	LHG	O8-C23	4.12	1.45	1.33
31	n	618	LHG	O8-C23	4.11	1.45	1.33
28	A	408	DGD	O2G-C1B	4.11	1.45	1.34
31	B	621	LHG	O8-C23	4.11	1.45	1.33
31	G	619	LHG	O8-C23	4.11	1.45	1.33
31	W	201	LHG	O7-C7	4.11	1.45	1.34
30	C	522	LMG	O7-C10	4.11	1.45	1.34
26	l	101	SQD	O47-C7	4.10	1.45	1.34
30	w	202	LMG	O7-C10	4.10	1.45	1.34
31	r	616	LHG	O7-C7	4.10	1.45	1.34
31	S	318	LHG	O7-C7	4.10	1.45	1.34
31	R	317	LHG	O7-C7	4.09	1.45	1.34
30	B	620	LMG	O7-C10	4.09	1.45	1.34
30	C	501	LMG	O7-C10	4.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	403	PHO	C1B-C2B	4.08	1.44	1.39
31	y	318	LHG	O7-C7	4.08	1.45	1.34
31	Y	319	LHG	O7-C7	4.08	1.45	1.34
23	s	611	CLA	C1D-ND	4.08	1.42	1.37
23	C	512	CLA	C1D-ND	4.07	1.42	1.37
23	R	310	CLA	C1D-ND	4.07	1.42	1.37
31	g	619	LHG	O8-C23	4.07	1.45	1.33
31	d	407	LHG	O7-C7	4.07	1.45	1.34
31	D	407	LHG	O7-C7	4.07	1.45	1.34
31	L	101	LHG	O8-C23	4.07	1.45	1.33
30	s	619	LMG	O7-C10	4.07	1.45	1.34
30	S	301	LMG	O7-C10	4.06	1.45	1.34
28	B	624	DGD	O2G-C1B	4.06	1.45	1.34
23	N	612	CLA	C1D-ND	4.06	1.42	1.37
23	r	602	CLA	C1D-ND	4.06	1.42	1.37
31	l	102	LHG	O7-C7	4.05	1.45	1.34
24	D	402	PHO	C1B-C2B	4.05	1.44	1.39
31	L	101	LHG	O7-C7	4.04	1.45	1.34
31	l	102	LHG	O8-C23	4.03	1.45	1.33
31	N	618	LHG	O7-C7	4.03	1.45	1.34
31	c	517	LHG	O7-C7	4.02	1.45	1.34
23	Y	303	CLA	C1D-ND	4.00	1.42	1.37
31	B	627	LHG	O7-C7	4.00	1.45	1.34
35	G	606	CHL	C1D-ND	3.99	1.42	1.37
31	b	626	LHG	O7-C7	3.99	1.45	1.34
31	n	618	LHG	O7-C7	3.99	1.45	1.34
23	S	303	CLA	C1D-ND	3.98	1.42	1.37
31	C	518	LHG	O7-C7	3.98	1.45	1.34
26	L	103	SQD	O47-C7	3.98	1.45	1.34
23	Y	313	CLA	C1D-ND	3.98	1.42	1.37
23	R	312	CLA	C1D-ND	3.97	1.42	1.37
23	R	303	CLA	C1D-ND	3.97	1.42	1.37
23	n	612	CLA	C1D-ND	3.96	1.42	1.37
23	N	614	CLA	C1D-ND	3.95	1.42	1.37
23	y	313	CLA	C1D-ND	3.95	1.42	1.37
35	G	605	CHL	C1D-ND	3.95	1.42	1.37
23	r	609	CLA	C1D-ND	3.94	1.42	1.37
23	N	610	CLA	C1D-ND	3.94	1.42	1.37
23	G	614	CLA	C1D-ND	3.93	1.42	1.37
23	R	309	CLA	C1D-ND	3.93	1.42	1.37
23	g	610	CLA	C1D-ND	3.93	1.42	1.37
23	n	610	CLA	C1D-ND	3.93	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	s	608	CLA	C1D-ND	3.93	1.42	1.37
23	s	603	CLA	C1D-ND	3.92	1.42	1.37
35	g	606	CHL	C1D-ND	3.92	1.42	1.37
23	n	614	CLA	C1D-ND	3.92	1.42	1.37
35	N	605	CHL	C1D-ND	3.92	1.42	1.37
23	n	602	CLA	C1D-ND	3.91	1.42	1.37
23	C	505	CLA	C1D-ND	3.91	1.42	1.37
23	y	303	CLA	C1D-ND	3.91	1.42	1.37
23	Y	312	CLA	C1D-ND	3.91	1.42	1.37
23	S	312	CLA	C1D-ND	3.90	1.42	1.37
23	g	614	CLA	C1D-ND	3.90	1.42	1.37
35	N	601	CHL	C1D-ND	3.90	1.42	1.37
34	F	101	HEM	FE-NB	3.89	2.06	1.94
23	g	612	CLA	C1D-ND	3.89	1.42	1.37
23	s	602	CLA	C1D-ND	3.88	1.42	1.37
34	f	101	HEM	FE-ND	3.88	2.06	1.94
23	C	508	CLA	C1D-ND	3.88	1.42	1.37
23	r	610	CLA	C1D-ND	3.88	1.42	1.37
23	G	613	CLA	C1D-ND	3.88	1.42	1.37
23	N	602	CLA	C1D-ND	3.88	1.42	1.37
23	c	504	CLA	C1D-ND	3.87	1.42	1.37
23	y	304	CLA	C4B-NB	3.87	1.42	1.37
34	f	101	HEM	FE-NB	3.87	2.06	1.94
23	A	402	CLA	C1D-ND	3.87	1.42	1.37
23	c	503	CLA	C1D-ND	3.87	1.42	1.37
23	G	603	CLA	C1D-ND	3.86	1.42	1.37
23	c	509	CLA	C1D-ND	3.86	1.42	1.37
34	F	101	HEM	FE-ND	3.86	2.06	1.94
23	G	602	CLA	C1D-ND	3.86	1.42	1.37
23	G	611	CLA	C1D-ND	3.86	1.42	1.37
35	y	308	CHL	C1D-ND	3.86	1.42	1.37
23	b	606	CLA	C1D-ND	3.86	1.42	1.37
23	R	311	CLA	C1D-ND	3.85	1.42	1.37
23	b	607	CLA	C1D-ND	3.85	1.42	1.37
23	c	501	CLA	C1D-ND	3.85	1.42	1.37
23	g	611	CLA	C1D-ND	3.85	1.42	1.37
23	G	612	CLA	C1D-ND	3.85	1.42	1.37
23	r	608	CLA	C1D-ND	3.85	1.42	1.37
23	S	304	CLA	C1D-ND	3.85	1.42	1.37
23	B	601	CLA	C1D-ND	3.84	1.42	1.37
23	Y	315	CLA	C1D-ND	3.84	1.42	1.37
23	C	510	CLA	C1D-ND	3.84	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	g	602	CLA	C1D-ND	3.84	1.42	1.37
23	y	312	CLA	C1D-ND	3.84	1.42	1.37
23	C	513	CLA	C1D-ND	3.84	1.42	1.37
23	r	611	CLA	C1D-ND	3.84	1.42	1.37
23	A	401	CLA	C1D-ND	3.84	1.42	1.37
23	g	613	CLA	C1D-ND	3.84	1.42	1.37
23	B	604	CLA	C1D-ND	3.83	1.42	1.37
23	S	314	CLA	C1D-ND	3.83	1.42	1.37
35	s	601	CHL	C1D-ND	3.83	1.42	1.37
23	n	611	CLA	C1D-ND	3.83	1.42	1.37
23	b	603	CLA	C1D-ND	3.83	1.42	1.37
23	a	401	CLA	C1D-ND	3.83	1.42	1.37
35	Y	302	CHL	C1D-ND	3.83	1.42	1.37
23	G	610	CLA	C1D-ND	3.83	1.42	1.37
35	Y	307	CHL	C1D-ND	3.82	1.42	1.37
23	s	612	CLA	C1D-ND	3.82	1.42	1.37
23	c	511	CLA	C1D-ND	3.82	1.42	1.37
35	n	606	CHL	C1D-ND	3.82	1.42	1.37
23	N	603	CLA	C1D-ND	3.82	1.42	1.37
23	c	507	CLA	C1D-ND	3.82	1.42	1.37
23	C	509	CLA	C1D-ND	3.82	1.42	1.37
23	s	610	CLA	C1D-ND	3.82	1.42	1.37
23	y	315	CLA	C1D-ND	3.82	1.42	1.37
23	B	615	CLA	C1D-ND	3.82	1.42	1.37
23	B	605	CLA	C1D-ND	3.81	1.42	1.37
35	s	605	CHL	C1D-ND	3.81	1.42	1.37
23	c	512	CLA	C1D-ND	3.81	1.42	1.37
35	G	601	CHL	C1D-ND	3.81	1.42	1.37
23	n	613	CLA	C1D-ND	3.80	1.42	1.37
23	C	502	CLA	C1D-ND	3.80	1.42	1.37
23	y	305	CLA	C1D-ND	3.80	1.42	1.37
23	S	309	CLA	C4B-NB	3.80	1.42	1.37
23	d	401	CLA	C1D-ND	3.80	1.42	1.37
23	d	402	CLA	C1D-ND	3.80	1.42	1.37
35	s	606	CHL	C1D-ND	3.80	1.42	1.37
23	n	603	CLA	C1D-ND	3.80	1.42	1.37
35	N	609	CHL	C1D-ND	3.80	1.42	1.37
35	S	302	CHL	C1D-ND	3.79	1.42	1.37
23	s	613	CLA	C1D-ND	3.79	1.42	1.37
23	D	404	CLA	C1D-ND	3.79	1.42	1.37
23	a	404	CLA	C1D-ND	3.79	1.42	1.37
23	C	504	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C1D-ND	3.79	1.42	1.37
23	S	310	CLA	C1D-ND	3.78	1.42	1.37
23	b	611	CLA	C1D-ND	3.78	1.42	1.37
23	r	612	CLA	C1D-ND	3.78	1.42	1.37
35	G	607	CHL	C1D-ND	3.78	1.42	1.37
23	S	311	CLA	C1D-ND	3.78	1.42	1.37
23	N	613	CLA	C1D-ND	3.78	1.42	1.37
23	Y	304	CLA	C1D-ND	3.78	1.42	1.37
23	N	604	CLA	C1D-ND	3.78	1.42	1.37
23	G	604	CLA	C1D-ND	3.78	1.42	1.37
23	Y	305	CLA	C1D-ND	3.78	1.42	1.37
23	b	615	CLA	C1D-ND	3.77	1.42	1.37
35	g	607	CHL	C1D-ND	3.77	1.42	1.37
23	s	609	CLA	C1D-ND	3.77	1.42	1.37
23	y	314	CLA	C1D-ND	3.77	1.42	1.37
35	G	609	CHL	C1D-ND	3.77	1.42	1.37
23	r	604	CLA	C1D-ND	3.77	1.42	1.37
23	d	404	CLA	C1D-ND	3.77	1.42	1.37
35	G	608	CHL	C1D-ND	3.76	1.42	1.37
24	D	402	PHO	C3B-C4B	3.76	1.45	1.41
23	B	607	CLA	C1D-ND	3.76	1.42	1.37
23	g	604	CLA	C1D-ND	3.76	1.42	1.37
23	S	313	CLA	C1D-ND	3.76	1.42	1.37
35	N	606	CHL	C1D-ND	3.76	1.42	1.37
35	N	608	CHL	C1D-ND	3.76	1.42	1.37
35	Y	308	CHL	C1D-ND	3.76	1.42	1.37
23	Y	314	CLA	C1D-ND	3.76	1.42	1.37
35	S	308	CHL	C1D-ND	3.76	1.42	1.37
23	b	617	CLA	C1D-ND	3.75	1.42	1.37
23	C	514	CLA	C1D-ND	3.75	1.42	1.37
23	r	601	CLA	C4B-NB	3.75	1.42	1.37
23	B	614	CLA	C1D-ND	3.75	1.42	1.37
23	N	611	CLA	C1D-ND	3.75	1.42	1.37
35	Y	310	CHL	C1D-ND	3.75	1.42	1.37
23	y	304	CLA	C1D-ND	3.75	1.42	1.37
35	n	607	CHL	C1D-ND	3.75	1.42	1.37
35	n	608	CHL	C1D-ND	3.75	1.42	1.37
23	s	604	CLA	C1D-ND	3.75	1.42	1.37
23	c	513	CLA	C1D-ND	3.74	1.42	1.37
23	B	616	CLA	C1D-ND	3.74	1.42	1.37
23	c	508	CLA	C1D-ND	3.74	1.42	1.37
23	n	604	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	C1D-ND	3.74	1.42	1.37
35	r	605	CHL	C1D-ND	3.73	1.42	1.37
35	s	607	CHL	C1D-ND	3.73	1.42	1.37
23	b	618	CLA	C1D-ND	3.73	1.42	1.37
35	R	307	CHL	C1D-ND	3.73	1.42	1.37
35	n	609	CHL	C1D-ND	3.73	1.42	1.37
23	C	503	CLA	C1D-ND	3.73	1.42	1.37
35	g	609	CHL	C1D-ND	3.73	1.42	1.37
23	R	305	CLA	C1D-ND	3.73	1.42	1.37
23	B	613	CLA	C1D-ND	3.72	1.42	1.37
35	y	302	CHL	C1D-ND	3.72	1.42	1.37
35	Y	306	CHL	C1D-ND	3.72	1.42	1.37
23	B	609	CLA	C1D-ND	3.72	1.42	1.37
35	n	601	CHL	C1D-ND	3.72	1.42	1.37
23	Y	304	CLA	C4B-NB	3.72	1.42	1.37
35	Y	309	CHL	C1D-ND	3.72	1.42	1.37
35	N	607	CHL	C1D-ND	3.71	1.42	1.37
35	R	306	CHL	C1D-ND	3.71	1.42	1.37
35	S	306	CHL	C1D-ND	3.71	1.42	1.37
35	y	306	CHL	C1D-ND	3.71	1.42	1.37
23	D	401	CLA	C1D-ND	3.71	1.42	1.37
35	g	605	CHL	C1D-ND	3.71	1.42	1.37
35	y	309	CHL	C1D-ND	3.71	1.42	1.37
35	S	307	CHL	C1D-ND	3.70	1.42	1.37
23	b	609	CLA	C1D-ND	3.70	1.42	1.37
23	c	506	CLA	C1D-ND	3.70	1.42	1.37
35	g	601	CHL	C1D-ND	3.70	1.42	1.37
23	B	611	CLA	C1D-ND	3.70	1.42	1.37
23	s	611	CLA	C4B-NB	3.70	1.42	1.37
35	r	606	CHL	C1D-ND	3.69	1.42	1.37
35	R	308	CHL	C1D-ND	3.69	1.42	1.37
23	b	616	CLA	C1D-ND	3.68	1.42	1.37
23	b	612	CLA	C1D-ND	3.68	1.42	1.37
35	y	310	CHL	C1D-ND	3.68	1.42	1.37
23	N	603	CLA	C4B-NB	3.68	1.42	1.37
23	C	510	CLA	C4B-NB	3.67	1.42	1.37
23	C	502	CLA	C4B-NB	3.67	1.42	1.37
23	B	610	CLA	C1D-ND	3.67	1.42	1.37
23	b	608	CLA	C1D-ND	3.67	1.42	1.37
35	y	307	CHL	C1D-ND	3.67	1.42	1.37
23	B	603	CLA	C1D-ND	3.67	1.42	1.37
23	B	606	CLA	C1D-ND	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C4B-NB	3.67	1.42	1.37
23	d	402	CLA	C4B-NB	3.66	1.42	1.37
35	g	608	CHL	C1D-ND	3.66	1.42	1.37
23	g	603	CLA	C1D-ND	3.66	1.42	1.37
23	b	604	CLA	C1D-ND	3.66	1.42	1.37
23	n	612	CLA	C4B-NB	3.65	1.42	1.37
23	C	506	CLA	C1D-ND	3.65	1.42	1.37
23	S	305	CLA	C1D-ND	3.64	1.42	1.37
23	b	613	CLA	C1D-ND	3.64	1.42	1.37
35	n	605	CHL	C1D-ND	3.64	1.42	1.37
23	r	603	CLA	C1D-ND	3.64	1.42	1.37
23	C	507	CLA	C1D-ND	3.64	1.42	1.37
23	c	505	CLA	C1D-ND	3.64	1.42	1.37
23	B	602	CLA	C1D-ND	3.64	1.42	1.37
23	R	304	CLA	C1D-ND	3.63	1.42	1.37
35	r	607	CHL	C1D-ND	3.62	1.42	1.37
23	R	313	CLA	C1D-ND	3.62	1.42	1.37
23	S	305	CLA	C4B-NB	3.61	1.42	1.37
23	b	605	CLA	C1D-ND	3.61	1.42	1.37
23	N	612	CLA	C4B-NB	3.61	1.42	1.37
23	c	509	CLA	C4B-NB	3.61	1.42	1.37
23	c	510	CLA	C1D-ND	3.61	1.42	1.37
23	G	613	CLA	C4B-NB	3.60	1.42	1.37
23	R	311	CLA	C4B-NB	3.60	1.42	1.37
35	S	308	CHL	C4B-NB	3.60	1.42	1.37
23	c	501	CLA	C4B-NB	3.58	1.42	1.37
23	C	514	CLA	C4B-NB	3.57	1.42	1.37
23	g	613	CLA	C4B-NB	3.57	1.42	1.37
23	N	613	CLA	C4B-NB	3.57	1.42	1.37
23	s	604	CLA	C4B-NB	3.57	1.42	1.37
23	b	610	CLA	C1D-ND	3.57	1.42	1.37
23	C	511	CLA	C1D-ND	3.56	1.42	1.37
35	g	605	CHL	C4B-NB	3.56	1.42	1.37
23	g	603	CLA	C4B-NB	3.56	1.42	1.37
23	b	611	CLA	C4B-NB	3.55	1.42	1.37
23	s	608	CLA	C4B-NB	3.55	1.42	1.37
24	a	403	PHO	C3B-C4B	3.55	1.45	1.41
35	S	306	CHL	C4B-NB	3.55	1.42	1.37
23	n	613	CLA	C4B-NB	3.54	1.42	1.37
23	S	313	CLA	C4B-NB	3.54	1.42	1.37
23	r	604	CLA	C4B-NB	3.54	1.42	1.37
23	B	609	CLA	C4B-NB	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	r	611	CLA	C4B-NB	3.53	1.42	1.37
23	s	612	CLA	C4B-NB	3.53	1.42	1.37
23	R	305	CLA	C4B-NB	3.53	1.42	1.37
35	s	607	CHL	C4B-NB	3.53	1.42	1.37
23	B	607	CLA	C4B-NB	3.52	1.42	1.37
23	B	601	CLA	C4B-NB	3.52	1.42	1.37
23	R	302	CLA	C4B-NB	3.52	1.42	1.37
23	G	603	CLA	C4B-NB	3.51	1.42	1.37
35	G	606	CHL	C4B-NB	3.51	1.42	1.37
23	b	603	CLA	C4B-NB	3.51	1.42	1.37
23	n	603	CLA	C4B-NB	3.50	1.42	1.37
23	Y	314	CLA	C4B-NB	3.50	1.42	1.37
35	R	306	CHL	C4B-NB	3.50	1.42	1.37
23	D	404	CLA	C4B-NB	3.50	1.42	1.37
35	y	306	CHL	C4B-NB	3.49	1.42	1.37
23	r	610	CLA	C4B-NB	3.49	1.42	1.37
35	G	605	CHL	C4B-NB	3.49	1.42	1.37
35	s	605	CHL	C4B-NB	3.48	1.42	1.37
23	c	513	CLA	C4B-NB	3.48	1.42	1.37
35	Y	309	CHL	C4B-NB	3.48	1.42	1.37
23	s	610	CLA	C4B-NB	3.48	1.42	1.37
23	R	313	CLA	C4B-NB	3.48	1.42	1.37
23	N	614	CLA	C4B-NB	3.48	1.42	1.37
23	r	612	CLA	C4B-NB	3.48	1.42	1.37
35	R	307	CHL	C4B-NB	3.48	1.42	1.37
23	c	511	CLA	C4B-NB	3.47	1.42	1.37
23	s	603	CLA	C4B-NB	3.47	1.42	1.37
23	R	303	CLA	C4B-NB	3.47	1.42	1.37
35	y	309	CHL	C4B-NB	3.47	1.42	1.37
23	S	311	CLA	C4B-NB	3.47	1.42	1.37
23	n	611	CLA	C4B-NB	3.47	1.42	1.37
23	A	402	CLA	C4B-NB	3.47	1.42	1.37
23	B	608	CLA	C1D-ND	3.46	1.42	1.37
35	n	606	CHL	C4B-NB	3.46	1.42	1.37
35	Y	306	CHL	C4B-NB	3.46	1.42	1.37
23	B	612	CLA	C1D-ND	3.46	1.42	1.37
23	y	305	CLA	C4B-NB	3.46	1.42	1.37
35	N	606	CHL	C4B-NB	3.46	1.42	1.37
23	y	314	CLA	C4B-NB	3.46	1.42	1.37
23	s	602	CLA	C4B-NB	3.45	1.42	1.37
23	S	310	CLA	C4B-NB	3.44	1.42	1.37
23	R	304	CLA	C4B-NB	3.44	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C4B-NB	3.44	1.42	1.37
35	r	605	CHL	C4B-NB	3.44	1.42	1.37
23	S	314	CLA	C4B-NB	3.43	1.42	1.37
23	d	404	CLA	C4B-NB	3.43	1.42	1.37
23	r	603	CLA	C4B-NB	3.43	1.42	1.37
23	b	609	CLA	C4B-NB	3.43	1.42	1.37
23	c	505	CLA	C4B-NB	3.43	1.42	1.37
23	C	512	CLA	C4B-NB	3.43	1.42	1.37
23	g	611	CLA	C4B-NB	3.43	1.42	1.37
23	Y	305	CLA	C4B-NB	3.43	1.42	1.37
23	G	612	CLA	C4B-NB	3.42	1.42	1.37
23	S	304	CLA	C4B-NB	3.42	1.42	1.37
23	c	504	CLA	C4B-NB	3.42	1.42	1.37
23	B	606	CLA	C4B-NB	3.42	1.42	1.37
23	N	604	CLA	C4B-NB	3.42	1.42	1.37
23	b	608	CLA	C4B-NB	3.42	1.42	1.37
23	R	312	CLA	C4B-NB	3.42	1.42	1.37
23	g	612	CLA	C4B-NB	3.42	1.42	1.37
23	C	506	CLA	C4B-NB	3.41	1.42	1.37
23	G	604	CLA	C4B-NB	3.41	1.42	1.37
23	n	614	CLA	C4B-NB	3.41	1.42	1.37
23	b	610	CLA	C4B-NB	3.41	1.42	1.37
23	C	505	CLA	C4B-NB	3.41	1.42	1.37
23	C	502	CLA	C3B-C4B	3.40	1.50	1.42
23	Y	315	CLA	C4B-NB	3.40	1.42	1.37
35	Y	310	CHL	C4B-NB	3.40	1.42	1.37
23	g	604	CLA	C4B-NB	3.40	1.42	1.37
23	y	315	CLA	C4B-NB	3.40	1.42	1.37
23	d	403	CLA	C1D-ND	3.40	1.42	1.37
23	g	614	CLA	C4B-NB	3.40	1.42	1.37
23	s	609	CLA	C4B-NB	3.40	1.42	1.37
23	G	614	CLA	C4B-NB	3.40	1.42	1.37
23	C	503	CLA	C4B-NB	3.39	1.42	1.37
35	g	608	CHL	C4B-NB	3.39	1.42	1.37
23	C	513	CLA	C4B-NB	3.39	1.42	1.37
35	G	609	CHL	C4B-NB	3.38	1.41	1.37
23	c	503	CLA	C4B-NB	3.38	1.41	1.37
23	C	509	CLA	C4B-NB	3.38	1.41	1.37
23	R	309	CLA	C4B-NB	3.38	1.41	1.37
23	N	611	CLA	C4B-NB	3.37	1.41	1.37
23	s	613	CLA	C4B-NB	3.37	1.41	1.37
23	b	617	CLA	C4B-NB	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	609	CHL	C4B-NB	3.37	1.41	1.37
23	B	611	CLA	C4B-NB	3.37	1.41	1.37
23	S	303	CLA	C4B-NB	3.37	1.41	1.37
23	c	512	CLA	C4B-NB	3.37	1.41	1.37
23	b	614	CLA	C1D-ND	3.36	1.41	1.37
23	c	508	CLA	C4B-NB	3.36	1.41	1.37
35	y	307	CHL	C4B-NB	3.36	1.41	1.37
23	B	605	CLA	C4B-NB	3.36	1.41	1.37
35	r	607	CHL	C4B-NB	3.35	1.41	1.37
23	c	502	CLA	C4B-NB	3.35	1.41	1.37
23	B	602	CLA	C4B-NB	3.34	1.41	1.37
23	C	504	CLA	C4B-NB	3.34	1.41	1.37
23	D	403	CLA	C1D-ND	3.34	1.41	1.37
23	b	607	CLA	C4B-NB	3.34	1.41	1.37
23	B	613	CLA	C4B-NB	3.34	1.41	1.37
35	N	608	CHL	C4B-NB	3.34	1.41	1.37
23	B	604	CLA	C4B-NB	3.34	1.41	1.37
23	B	614	CLA	C4B-NB	3.33	1.41	1.37
23	c	510	CLA	C4B-NB	3.33	1.41	1.37
23	r	608	CLA	C4B-NB	3.33	1.41	1.37
23	b	616	CLA	C4B-NB	3.33	1.41	1.37
23	N	602	CLA	C3B-C4B	3.33	1.50	1.42
23	C	511	CLA	C4B-NB	3.33	1.41	1.37
23	G	611	CLA	C4B-NB	3.33	1.41	1.37
35	R	308	CHL	C4B-NB	3.33	1.41	1.37
35	G	608	CHL	C4B-NB	3.33	1.41	1.37
35	Y	307	CHL	C4B-NB	3.33	1.41	1.37
23	r	602	CLA	C4B-NB	3.32	1.41	1.37
35	n	608	CHL	C4B-NB	3.32	1.41	1.37
23	b	615	CLA	C4B-NB	3.32	1.41	1.37
23	S	312	CLA	C4B-NB	3.32	1.41	1.37
23	b	604	CLA	C4B-NB	3.32	1.41	1.37
23	y	304	CLA	C3B-C4B	3.32	1.50	1.42
23	b	605	CLA	C4B-NB	3.31	1.41	1.37
23	A	402	CLA	C4D-ND	-3.31	1.33	1.37
23	y	312	CLA	C4B-NB	3.31	1.41	1.37
35	S	307	CHL	C4B-NB	3.31	1.41	1.37
23	n	604	CLA	C4B-NB	3.31	1.41	1.37
23	y	313	CLA	C4B-NB	3.31	1.41	1.37
23	B	615	CLA	C4B-NB	3.30	1.41	1.37
24	A	403	PHO	C3B-C4B	3.30	1.45	1.41
23	B	603	CLA	C4B-NB	3.30	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C4B-NB	3.30	1.41	1.37
23	R	310	CLA	C4B-NB	3.29	1.41	1.37
35	y	310	CHL	C4B-NB	3.29	1.41	1.37
24	a	402	PHO	C3B-C4B	3.29	1.45	1.41
23	d	403	CLA	C4B-NB	3.29	1.41	1.37
35	S	302	CHL	C4B-NB	3.28	1.41	1.37
23	y	303	CLA	C4B-NB	3.28	1.41	1.37
23	Y	312	CLA	C4B-NB	3.27	1.41	1.37
35	n	605	CHL	C4B-NB	3.27	1.41	1.37
23	N	602	CLA	C4B-NB	3.27	1.41	1.37
34	f	101	HEM	CAC-C3C	3.27	1.56	1.47
34	F	101	HEM	CAC-C3C	3.26	1.56	1.47
23	a	404	CLA	C4B-NB	3.25	1.41	1.37
23	b	614	CLA	C4B-NB	3.25	1.41	1.37
35	y	302	CHL	C4B-NB	3.25	1.41	1.37
23	d	402	CLA	C4D-ND	-3.25	1.33	1.37
23	Y	313	CLA	C4B-NB	3.25	1.41	1.37
23	b	606	CLA	C4B-NB	3.25	1.41	1.37
23	c	506	CLA	C4B-NB	3.25	1.41	1.37
23	D	401	CLA	C4B-NB	3.25	1.41	1.37
23	c	501	CLA	C3B-C4B	3.24	1.50	1.42
23	r	609	CLA	C4B-NB	3.24	1.41	1.37
35	g	606	CHL	C4B-NB	3.23	1.41	1.37
35	r	606	CHL	C4B-NB	3.23	1.41	1.37
35	g	607	CHL	C4B-NB	3.23	1.41	1.37
35	n	601	CHL	C4B-NB	3.22	1.41	1.37
23	a	401	CLA	C4B-NB	3.22	1.41	1.37
35	s	601	CHL	C4B-NB	3.22	1.41	1.37
35	G	607	CHL	C4B-NB	3.22	1.41	1.37
35	s	606	CHL	C4B-NB	3.21	1.41	1.37
23	A	404	CLA	C4B-NB	3.21	1.41	1.37
23	D	403	CLA	C3B-C4B	3.21	1.50	1.42
35	Y	302	CHL	C4B-NB	3.21	1.41	1.37
35	N	607	CHL	C4B-NB	3.20	1.41	1.37
23	Y	303	CLA	C4D-ND	-3.19	1.33	1.37
23	A	401	CLA	C4B-NB	3.19	1.41	1.37
23	C	509	CLA	C4D-ND	-3.19	1.33	1.37
23	G	610	CLA	C4B-NB	3.19	1.41	1.37
23	Y	303	CLA	C4B-NB	3.19	1.41	1.37
23	B	612	CLA	C4B-NB	3.18	1.41	1.37
23	n	602	CLA	C4B-NB	3.18	1.41	1.37
23	b	618	CLA	C4B-NB	3.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	602	CLA	C4D-ND	-3.18	1.33	1.37
23	Y	304	CLA	C3B-C4B	3.18	1.50	1.42
23	C	514	CLA	C3B-C4B	3.17	1.50	1.42
35	Y	308	CHL	C4B-NB	3.17	1.41	1.37
35	N	609	CHL	C4B-NB	3.17	1.41	1.37
23	d	401	CLA	C4B-NB	3.16	1.41	1.37
35	y	308	CHL	C4B-NB	3.16	1.41	1.37
23	c	508	CLA	C4D-ND	-3.16	1.33	1.37
35	n	609	CHL	C4B-NB	3.16	1.41	1.37
23	B	616	CLA	C4B-NB	3.15	1.41	1.37
23	b	612	CLA	C4D-ND	-3.15	1.33	1.37
34	f	101	HEM	CAB-C3B	3.15	1.56	1.47
35	y	307	CHL	C3B-C4B	3.14	1.50	1.42
34	F	101	HEM	CAB-C3B	3.14	1.56	1.47
23	s	602	CLA	C4D-ND	-3.14	1.33	1.37
23	B	610	CLA	C4D-ND	-3.14	1.33	1.37
23	S	303	CLA	C4D-ND	-3.14	1.33	1.37
23	S	305	CLA	C4D-ND	-3.13	1.33	1.37
23	N	613	CLA	C4D-ND	-3.13	1.33	1.37
35	N	605	CHL	C4B-NB	3.13	1.41	1.37
35	S	306	CHL	C4D-ND	-3.11	1.33	1.37
23	S	310	CLA	C3B-C4B	3.11	1.50	1.42
35	N	601	CHL	C4B-NB	3.11	1.41	1.37
35	n	607	CHL	C4B-NB	3.11	1.41	1.37
23	b	603	CLA	C4D-ND	-3.11	1.33	1.37
23	c	513	CLA	C3B-C4B	3.11	1.50	1.42
35	Y	307	CHL	C3B-C4B	3.11	1.50	1.42
23	n	613	CLA	C4D-ND	-3.11	1.33	1.37
23	C	510	CLA	C3B-C4B	3.11	1.50	1.42
23	y	303	CLA	C4D-ND	-3.11	1.33	1.37
23	B	606	CLA	C4D-ND	-3.10	1.33	1.37
23	b	612	CLA	C4B-NB	3.10	1.41	1.37
23	s	611	CLA	C3B-C4B	3.10	1.50	1.42
23	b	608	CLA	C4D-ND	-3.10	1.33	1.37
23	c	504	CLA	C4D-ND	-3.10	1.33	1.37
23	c	509	CLA	C3B-C4B	3.09	1.50	1.42
23	B	605	CLA	C4D-ND	-3.09	1.33	1.37
35	g	601	CHL	C4B-NB	3.09	1.41	1.37
23	S	310	CLA	C4D-ND	-3.08	1.33	1.37
23	B	610	CLA	C4B-NB	3.08	1.41	1.37
23	s	604	CLA	C4D-ND	-3.07	1.33	1.37
23	B	608	CLA	C4D-ND	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C4D-ND	-3.07	1.33	1.37
23	C	514	CLA	C4D-ND	-3.07	1.33	1.37
23	y	312	CLA	C4D-ND	-3.06	1.33	1.37
23	c	513	CLA	C4D-ND	-3.06	1.33	1.37
23	n	612	CLA	C3B-C4B	3.06	1.49	1.42
23	N	603	CLA	C4D-ND	-3.06	1.33	1.37
23	C	505	CLA	C4D-ND	-3.06	1.33	1.37
23	C	507	CLA	C4B-NB	3.06	1.41	1.37
38	Y	318	NEX	C7-C8	-3.06	1.26	1.32
23	g	603	CLA	C4D-ND	-3.06	1.33	1.37
23	g	613	CLA	C4D-ND	-3.06	1.33	1.37
23	Y	314	CLA	C4D-ND	-3.05	1.33	1.37
23	C	503	CLA	C4D-ND	-3.05	1.33	1.37
23	D	404	CLA	C4D-ND	-3.05	1.33	1.37
23	C	507	CLA	C4D-ND	-3.05	1.33	1.37
23	c	506	CLA	C4D-ND	-3.05	1.33	1.37
23	d	403	CLA	C4D-ND	-3.05	1.33	1.37
23	N	612	CLA	C3B-C4B	3.05	1.49	1.42
23	r	612	CLA	C4D-ND	-3.05	1.33	1.37
23	y	314	CLA	C4D-ND	-3.05	1.33	1.37
23	B	614	CLA	C4D-ND	-3.04	1.33	1.37
23	B	607	CLA	C4D-ND	-3.04	1.33	1.37
23	B	611	CLA	C4D-ND	-3.04	1.33	1.37
23	g	602	CLA	C4D-ND	-3.04	1.33	1.37
23	N	610	CLA	C4B-NB	3.04	1.41	1.37
23	y	311	CLA	C4B-NB	3.04	1.41	1.37
23	D	401	CLA	C4D-ND	-3.04	1.33	1.37
23	G	613	CLA	C4D-ND	-3.04	1.33	1.37
23	B	601	CLA	C4D-ND	-3.04	1.33	1.37
23	s	609	CLA	C3B-C4B	3.04	1.49	1.42
23	d	403	CLA	C3B-C4B	3.03	1.49	1.42
23	a	404	CLA	C4D-ND	-3.03	1.33	1.37
23	n	610	CLA	C4B-NB	3.03	1.41	1.37
23	b	607	CLA	C4D-ND	-3.03	1.33	1.37
35	G	609	CHL	C4D-ND	-3.03	1.33	1.37
35	y	309	CHL	C4D-ND	-3.02	1.33	1.37
23	D	403	CLA	C4D-ND	-3.02	1.33	1.37
35	G	601	CHL	C4B-NB	3.02	1.41	1.37
23	Y	303	CLA	C3B-C4B	3.02	1.49	1.42
23	b	611	CLA	C4D-ND	-3.02	1.33	1.37
23	r	609	CLA	C4D-ND	-3.02	1.33	1.37
23	c	501	CLA	C4D-ND	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	s	609	CLA	C4D-ND	-3.01	1.33	1.37
23	b	610	CLA	C4D-ND	-3.01	1.33	1.37
23	g	610	CLA	C4D-ND	-3.01	1.33	1.37
23	y	303	CLA	C3B-C4B	3.01	1.49	1.42
23	a	401	CLA	C4D-ND	-3.00	1.33	1.37
23	Y	312	CLA	C4D-ND	-3.00	1.33	1.37
23	b	609	CLA	C4D-ND	-3.00	1.33	1.37
23	A	401	CLA	C4D-ND	-3.00	1.33	1.37
35	G	606	CHL	C3B-C4B	3.00	1.49	1.42
23	S	311	CLA	C4D-ND	-3.00	1.33	1.37
35	g	607	CHL	C4D-ND	-3.00	1.33	1.37
35	N	601	CHL	C3B-C4B	3.00	1.49	1.42
23	y	315	CLA	C4D-ND	-3.00	1.33	1.37
23	N	603	CLA	C3B-C4B	3.00	1.49	1.42
23	A	404	CLA	C4D-ND	-3.00	1.33	1.37
23	B	609	CLA	C4D-ND	-3.00	1.33	1.37
23	R	313	CLA	C4D-ND	-2.99	1.33	1.37
23	c	512	CLA	C4D-ND	-2.99	1.33	1.37
23	c	502	CLA	C4D-ND	-2.99	1.33	1.37
23	N	611	CLA	C4D-ND	-2.99	1.33	1.37
23	r	608	CLA	C4D-ND	-2.99	1.33	1.37
35	Y	309	CHL	C4D-ND	-2.99	1.33	1.37
23	G	602	CLA	C3B-C4B	2.99	1.49	1.42
23	R	305	CLA	C4D-ND	-2.98	1.33	1.37
35	N	609	CHL	C4D-ND	-2.98	1.33	1.37
23	d	404	CLA	C4D-ND	-2.98	1.33	1.37
23	n	604	CLA	C4D-ND	-2.98	1.33	1.37
23	d	401	CLA	C4D-ND	-2.98	1.33	1.37
23	Y	305	CLA	C4D-ND	-2.98	1.33	1.37
35	r	607	CHL	C4D-ND	-2.98	1.33	1.37
23	N	604	CLA	C4D-ND	-2.97	1.33	1.37
23	d	402	CLA	C3B-C4B	2.97	1.49	1.42
23	Y	313	CLA	C4D-ND	-2.97	1.33	1.37
23	r	604	CLA	C4D-ND	-2.97	1.33	1.37
23	C	508	CLA	C4B-NB	2.97	1.41	1.37
26	A	406	SQD	C6-S	-2.97	1.66	1.77
26	a	406	SQD	C6-S	-2.97	1.66	1.77
23	N	614	CLA	C4D-ND	-2.97	1.33	1.37
23	Y	315	CLA	C4D-ND	-2.96	1.33	1.37
35	n	606	CHL	C3B-C4B	2.96	1.49	1.42
23	c	503	CLA	C4D-ND	-2.96	1.33	1.37
23	C	502	CLA	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	303	CLA	C4D-ND	-2.96	1.33	1.37
35	y	309	CHL	C3B-C4B	2.96	1.49	1.42
23	S	314	CLA	C4D-ND	-2.96	1.33	1.37
23	b	616	CLA	C4D-ND	-2.96	1.33	1.37
35	N	605	CHL	C3B-C4B	2.95	1.49	1.42
23	c	507	CLA	C4B-NB	2.95	1.41	1.37
35	Y	306	CHL	C4D-ND	-2.95	1.33	1.37
35	N	608	CHL	C4D-ND	-2.95	1.33	1.37
26	L	103	SQD	C6-S	-2.94	1.66	1.77
23	C	504	CLA	C4D-ND	-2.94	1.33	1.37
23	y	305	CLA	C4D-ND	-2.94	1.33	1.37
23	G	602	CLA	C4B-NB	2.94	1.41	1.37
35	G	607	CHL	C4D-ND	-2.94	1.33	1.37
35	n	609	CHL	C4D-ND	-2.94	1.33	1.37
23	n	602	CLA	C3B-C4B	2.94	1.49	1.42
23	Y	311	CLA	C4D-ND	-2.94	1.33	1.37
23	b	605	CLA	C4D-ND	-2.94	1.33	1.37
23	c	510	CLA	C4D-ND	-2.94	1.33	1.37
23	n	602	CLA	C4D-ND	-2.94	1.33	1.37
23	R	310	CLA	C4D-ND	-2.94	1.33	1.37
23	b	615	CLA	C4D-ND	-2.93	1.33	1.37
35	N	606	CHL	C4D-ND	-2.93	1.33	1.37
23	c	505	CLA	C4D-ND	-2.93	1.33	1.37
35	N	606	CHL	C3B-C4B	2.93	1.49	1.42
23	b	606	CLA	C4D-ND	-2.93	1.33	1.37
23	B	607	CLA	C3B-C4B	2.93	1.49	1.42
35	n	606	CHL	C4D-ND	-2.93	1.33	1.37
23	B	604	CLA	C4D-ND	-2.93	1.33	1.37
23	S	313	CLA	C4D-ND	-2.92	1.33	1.37
23	R	309	CLA	C4D-ND	-2.92	1.33	1.37
23	g	610	CLA	C3B-C4B	2.92	1.49	1.42
35	G	608	CHL	C4D-ND	-2.92	1.33	1.37
35	y	306	CHL	C4D-ND	-2.92	1.33	1.37
23	n	610	CLA	C4D-ND	-2.92	1.33	1.37
23	g	604	CLA	C4D-ND	-2.92	1.33	1.37
23	n	614	CLA	C4D-ND	-2.92	1.33	1.37
35	s	606	CHL	C4D-ND	-2.92	1.33	1.37
23	B	603	CLA	C4D-ND	-2.92	1.33	1.37
23	N	610	CLA	C4D-ND	-2.92	1.33	1.37
23	b	614	CLA	C4D-ND	-2.92	1.33	1.37
26	l	101	SQD	C6-S	-2.92	1.66	1.77
23	n	603	CLA	C4D-ND	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	313	CLA	C4D-ND	-2.91	1.33	1.37
35	g	605	CHL	C4D-ND	-2.91	1.33	1.37
23	C	506	CLA	C4D-ND	-2.91	1.33	1.37
23	b	609	CLA	C3B-C4B	2.91	1.49	1.42
35	y	302	CHL	C3B-C4B	2.91	1.49	1.42
23	c	511	CLA	C4D-ND	-2.91	1.33	1.37
23	g	602	CLA	C4B-NB	2.91	1.41	1.37
34	f	101	HEM	FE-NA	2.91	2.05	1.95
23	G	604	CLA	C4D-ND	-2.91	1.33	1.37
23	C	513	CLA	C4D-ND	-2.91	1.33	1.37
23	R	311	CLA	C4D-ND	-2.91	1.33	1.37
35	s	605	CHL	C3B-C4B	2.91	1.49	1.42
35	n	608	CHL	C4D-ND	-2.91	1.33	1.37
35	r	605	CHL	C3B-C4B	2.91	1.49	1.42
23	r	610	CLA	C4D-ND	-2.91	1.33	1.37
23	B	616	CLA	C4D-ND	-2.90	1.33	1.37
23	N	610	CLA	C3B-C4B	2.90	1.49	1.42
35	n	601	CHL	C3B-C4B	2.90	1.49	1.42
23	C	510	CLA	C4D-ND	-2.90	1.33	1.37
35	S	302	CHL	C3B-C4B	2.90	1.49	1.42
23	c	509	CLA	C4D-ND	-2.90	1.33	1.37
34	F	101	HEM	FE-NA	2.90	2.04	1.95
23	s	603	CLA	C4D-ND	-2.90	1.33	1.37
35	R	306	CHL	C3B-C4B	2.90	1.49	1.42
38	R	301	NEX	C7-C8	-2.90	1.27	1.32
23	G	604	CLA	C3B-C4B	2.90	1.49	1.42
35	g	605	CHL	C3B-C4B	2.90	1.49	1.42
23	C	511	CLA	C4D-ND	-2.90	1.33	1.37
35	n	607	CHL	C3B-C4B	2.89	1.49	1.42
23	c	508	CLA	C3B-C4B	2.89	1.49	1.42
23	G	603	CLA	C4D-ND	-2.89	1.33	1.37
23	s	613	CLA	C4D-ND	-2.89	1.33	1.37
23	G	611	CLA	C4D-ND	-2.89	1.33	1.37
35	G	609	CHL	C3B-C4B	2.89	1.49	1.42
35	y	307	CHL	C4D-ND	-2.89	1.33	1.37
35	R	307	CHL	C4D-ND	-2.89	1.33	1.37
23	G	610	CLA	C4D-ND	-2.89	1.33	1.37
23	g	614	CLA	C4D-ND	-2.89	1.33	1.37
35	n	607	CHL	C4D-ND	-2.89	1.33	1.37
23	n	611	CLA	C4D-ND	-2.89	1.33	1.37
35	Y	302	CHL	C3B-C4B	2.89	1.49	1.42
35	Y	309	CHL	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	Y	307	CHL	C4D-ND	-2.88	1.33	1.37
23	G	614	CLA	C3B-C4B	2.88	1.49	1.42
23	S	312	CLA	C3B-C4B	2.88	1.49	1.42
23	G	603	CLA	C3B-C4B	2.88	1.49	1.42
35	s	601	CHL	C3B-C4B	2.88	1.49	1.42
35	S	307	CHL	C3B-C4B	2.88	1.49	1.42
23	s	602	CLA	C3B-C4B	2.88	1.49	1.42
23	n	610	CLA	C3B-C4B	2.88	1.49	1.42
35	R	306	CHL	C4D-ND	-2.88	1.33	1.37
23	B	612	CLA	C3B-C4B	2.88	1.49	1.42
23	y	313	CLA	C3B-C4B	2.88	1.49	1.42
23	r	602	CLA	C4D-ND	-2.88	1.33	1.37
23	y	304	CLA	C4D-ND	-2.88	1.33	1.37
23	g	602	CLA	C3B-C4B	2.88	1.49	1.42
23	C	507	CLA	C3B-C4B	2.87	1.49	1.42
23	B	602	CLA	C4D-ND	-2.87	1.33	1.37
23	s	612	CLA	C4D-ND	-2.87	1.33	1.37
23	B	614	CLA	C3B-C4B	2.87	1.49	1.42
23	B	613	CLA	C4D-ND	-2.87	1.33	1.37
23	b	618	CLA	C3B-C4B	2.87	1.49	1.42
35	R	308	CHL	C4D-ND	-2.87	1.33	1.37
23	s	603	CLA	C3B-C4B	2.87	1.49	1.42
23	B	615	CLA	C3B-C4B	2.87	1.49	1.42
23	s	610	CLA	C4D-ND	-2.86	1.33	1.37
35	n	605	CHL	C3B-C4B	2.86	1.49	1.42
23	N	602	CLA	C4D-ND	-2.86	1.33	1.37
23	b	618	CLA	C4D-ND	-2.86	1.33	1.37
23	S	311	CLA	C3B-C4B	2.86	1.49	1.42
23	A	404	CLA	C3B-C4B	2.85	1.49	1.42
23	y	311	CLA	C4D-ND	-2.85	1.33	1.37
35	Y	310	CHL	C4D-ND	-2.85	1.33	1.37
23	r	610	CLA	C3B-C4B	2.85	1.49	1.42
23	B	616	CLA	C3B-C4B	2.85	1.49	1.42
23	B	612	CLA	C4D-ND	-2.85	1.33	1.37
35	N	607	CHL	C4D-ND	-2.85	1.33	1.37
35	y	306	CHL	C3B-C4B	2.85	1.49	1.42
35	s	607	CHL	C3B-C4B	2.85	1.49	1.42
23	b	617	CLA	C3B-C4B	2.85	1.49	1.42
23	b	614	CLA	C3B-C4B	2.85	1.49	1.42
35	N	607	CHL	C3B-C4B	2.85	1.49	1.42
23	G	614	CLA	C4D-ND	-2.85	1.33	1.37
35	r	606	CHL	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	303	CLA	C3B-C4B	2.85	1.49	1.42
23	y	315	CLA	C3B-C4B	2.85	1.49	1.42
35	S	308	CHL	C3B-C4B	2.85	1.49	1.42
23	B	609	CLA	C3B-C4B	2.85	1.49	1.42
35	s	605	CHL	C4D-ND	-2.85	1.33	1.37
23	s	608	CLA	C3B-C4B	2.84	1.49	1.42
23	Y	312	CLA	C3B-C4B	2.84	1.49	1.42
35	G	605	CHL	C4D-ND	-2.84	1.33	1.37
23	N	604	CLA	C3B-C4B	2.84	1.49	1.42
23	n	613	CLA	C3B-C4B	2.84	1.49	1.42
23	C	512	CLA	C3B-C4B	2.84	1.49	1.42
23	r	601	CLA	C3B-C4B	2.84	1.49	1.42
23	y	312	CLA	C3B-C4B	2.84	1.49	1.42
23	b	604	CLA	C4D-ND	-2.84	1.33	1.37
23	R	302	CLA	C3B-C4B	2.84	1.49	1.42
23	C	511	CLA	C3B-C4B	2.84	1.49	1.42
23	C	509	CLA	C3B-C4B	2.83	1.49	1.42
23	b	608	CLA	C3B-C4B	2.83	1.49	1.42
23	G	612	CLA	C3B-C4B	2.83	1.49	1.42
23	c	507	CLA	C4D-ND	-2.83	1.33	1.37
35	n	609	CHL	C3B-C4B	2.83	1.49	1.42
33	d	406	PL9	C36-C34	2.83	1.57	1.51
23	C	513	CLA	C3B-C4B	2.83	1.49	1.42
23	n	603	CLA	C3B-C4B	2.83	1.49	1.42
23	S	304	CLA	C4D-ND	-2.83	1.33	1.37
23	r	611	CLA	C4D-ND	-2.83	1.33	1.37
35	S	307	CHL	C4D-ND	-2.83	1.33	1.37
23	C	508	CLA	C4D-ND	-2.83	1.33	1.37
23	N	611	CLA	C3B-C4B	2.83	1.49	1.42
35	r	605	CHL	C4D-ND	-2.83	1.33	1.37
23	b	605	CLA	C3B-C4B	2.83	1.49	1.42
23	g	611	CLA	C4D-ND	-2.83	1.33	1.37
23	a	404	CLA	C3B-C4B	2.83	1.49	1.42
35	s	601	CHL	C4D-ND	-2.82	1.33	1.37
23	R	309	CLA	C3B-C4B	2.82	1.49	1.42
23	b	611	CLA	C3B-C4B	2.82	1.49	1.42
23	Y	305	CLA	C3B-C4B	2.82	1.49	1.42
23	b	616	CLA	C3B-C4B	2.82	1.49	1.42
35	G	605	CHL	C3B-C4B	2.82	1.49	1.42
33	D	406	PL9	C36-C34	2.82	1.57	1.51
23	B	603	CLA	C3B-C4B	2.82	1.49	1.42
23	c	510	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C3B-C4B	2.82	1.49	1.42
35	s	606	CHL	C3B-C4B	2.82	1.49	1.42
35	S	306	CHL	C3B-C4B	2.82	1.49	1.42
23	R	305	CLA	C3B-C4B	2.82	1.49	1.42
35	g	606	CHL	C3B-C4B	2.82	1.49	1.42
23	R	311	CLA	C3B-C4B	2.82	1.49	1.42
35	Y	306	CHL	C3B-C4B	2.81	1.49	1.42
23	R	312	CLA	C3B-C4B	2.81	1.49	1.42
23	N	612	CLA	C4D-ND	-2.81	1.33	1.37
35	S	308	CHL	C4D-ND	-2.81	1.33	1.37
23	s	610	CLA	C3B-C4B	2.81	1.49	1.42
35	g	607	CHL	C3B-C4B	2.81	1.49	1.42
23	R	304	CLA	C4D-ND	-2.81	1.33	1.37
35	s	607	CHL	C4D-ND	-2.81	1.33	1.37
23	g	612	CLA	C3B-C4B	2.81	1.49	1.42
23	C	504	CLA	C3B-C4B	2.81	1.49	1.42
35	Y	308	CHL	C3B-C4B	2.81	1.49	1.42
23	r	603	CLA	C4D-ND	-2.81	1.33	1.37
23	R	304	CLA	C3B-C4B	2.81	1.49	1.42
35	y	308	CHL	C4D-ND	-2.80	1.33	1.37
23	r	603	CLA	C3B-C4B	2.80	1.49	1.42
23	n	611	CLA	C3B-C4B	2.80	1.49	1.42
23	S	309	CLA	C1B-C2B	2.80	1.49	1.43
23	Y	315	CLA	C3B-C4B	2.80	1.49	1.42
35	n	608	CHL	C3B-C4B	2.80	1.49	1.42
23	g	604	CLA	C3B-C4B	2.80	1.49	1.42
35	y	310	CHL	C4D-ND	-2.80	1.33	1.37
23	s	604	CLA	C3B-C4B	2.80	1.49	1.42
23	n	614	CLA	C3B-C4B	2.80	1.49	1.42
35	R	307	CHL	C3B-C4B	2.80	1.49	1.42
23	S	305	CLA	C3B-C4B	2.80	1.49	1.42
23	c	512	CLA	C3B-C4B	2.80	1.49	1.42
23	r	609	CLA	C3B-C4B	2.80	1.49	1.42
23	c	511	CLA	C3B-C4B	2.80	1.49	1.42
23	b	613	CLA	C3B-C4B	2.79	1.49	1.42
23	g	614	CLA	C3B-C4B	2.79	1.49	1.42
23	n	604	CLA	C3B-C4B	2.79	1.49	1.42
35	Y	310	CHL	C3B-C4B	2.79	1.49	1.42
35	r	607	CHL	C3B-C4B	2.79	1.49	1.42
23	C	512	CLA	C4D-ND	-2.79	1.33	1.37
23	R	312	CLA	C4D-ND	-2.79	1.33	1.37
35	g	606	CHL	C4D-ND	-2.79	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	614	CLA	C3B-C4B	2.79	1.49	1.42
23	n	612	CLA	C4D-ND	-2.79	1.33	1.37
23	b	604	CLA	C3B-C4B	2.79	1.49	1.42
35	y	308	CHL	C3B-C4B	2.79	1.49	1.42
23	B	611	CLA	C3B-C4B	2.79	1.49	1.42
23	s	608	CLA	C4D-ND	-2.79	1.33	1.37
23	r	611	CLA	C3B-C4B	2.78	1.49	1.42
23	C	506	CLA	C3B-C4B	2.78	1.49	1.42
23	B	602	CLA	C3B-C4B	2.78	1.49	1.42
23	y	305	CLA	C3B-C4B	2.78	1.49	1.42
23	r	604	CLA	C3B-C4B	2.78	1.49	1.42
23	N	613	CLA	C3B-C4B	2.78	1.49	1.42
35	g	608	CHL	C4D-ND	-2.78	1.33	1.37
35	G	607	CHL	C3B-C4B	2.78	1.49	1.42
23	Y	311	CLA	C3B-C4B	2.78	1.49	1.42
23	c	503	CLA	C3B-C4B	2.78	1.49	1.42
35	g	608	CHL	C3B-C4B	2.78	1.49	1.42
35	N	608	CHL	C3B-C4B	2.77	1.49	1.42
23	r	608	CLA	C3B-C4B	2.77	1.49	1.42
23	Y	313	CLA	C3B-C4B	2.77	1.49	1.42
23	s	611	CLA	C4D-ND	-2.77	1.33	1.37
23	y	311	CLA	C3B-C4B	2.77	1.49	1.42
38	r	615	NEX	C7-C8	-2.77	1.27	1.32
35	G	601	CHL	C4D-ND	-2.77	1.33	1.37
23	r	612	CLA	C3B-C4B	2.77	1.49	1.42
23	b	607	CLA	C1B-C2B	2.77	1.49	1.43
23	c	506	CLA	C3B-C4B	2.76	1.49	1.42
35	r	606	CHL	C3B-C4B	2.76	1.49	1.42
23	S	314	CLA	C3B-C4B	2.76	1.49	1.42
23	G	613	CLA	C3B-C4B	2.76	1.49	1.42
23	s	613	CLA	C3B-C4B	2.76	1.49	1.42
35	N	609	CHL	C3B-C4B	2.76	1.49	1.42
23	g	603	CLA	C3B-C4B	2.76	1.49	1.42
35	G	608	CHL	C3B-C4B	2.76	1.49	1.42
23	B	601	CLA	C3B-C4B	2.76	1.49	1.42
23	S	304	CLA	C3B-C4B	2.76	1.49	1.42
23	D	401	CLA	C3B-C4B	2.75	1.49	1.42
23	b	610	CLA	C3B-C4B	2.75	1.49	1.42
23	y	314	CLA	C3B-C4B	2.75	1.49	1.42
23	R	303	CLA	C3B-C4B	2.75	1.49	1.42
23	A	401	CLA	C3B-C4B	2.75	1.49	1.42
23	c	504	CLA	C3B-C4B	2.75	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	d	406	PL9	C41-C39	2.75	1.57	1.51
23	g	612	CLA	C4D-ND	-2.74	1.33	1.37
23	D	404	CLA	C3B-C4B	2.74	1.49	1.42
23	b	603	CLA	C3B-C4B	2.74	1.49	1.42
23	c	510	CLA	CMD-C2D	-2.74	1.45	1.50
23	c	505	CLA	C3B-C4B	2.74	1.49	1.42
23	r	601	CLA	C4D-ND	-2.74	1.33	1.37
23	R	302	CLA	C4D-ND	-2.73	1.33	1.37
35	g	601	CHL	C4D-ND	-2.73	1.33	1.37
23	g	611	CLA	C3B-C4B	2.73	1.49	1.42
35	G	606	CHL	C4D-ND	-2.73	1.33	1.37
38	s	616	NEX	C7-C8	-2.73	1.27	1.32
35	y	310	CHL	CMB-C2B	-2.73	1.45	1.50
23	G	611	CLA	C3B-C4B	2.73	1.49	1.42
23	d	401	CLA	C3B-C4B	2.73	1.49	1.42
23	G	612	CLA	C4D-ND	-2.73	1.33	1.37
23	S	309	CLA	C4D-ND	-2.73	1.33	1.37
23	g	613	CLA	C3B-C4B	2.72	1.49	1.42
35	G	601	CHL	C3B-C4B	2.72	1.49	1.42
23	Y	304	CLA	C4D-ND	-2.72	1.33	1.37
23	Y	314	CLA	C3B-C4B	2.72	1.49	1.42
23	B	605	CLA	C1B-C2B	2.72	1.49	1.43
23	g	603	CLA	C1B-C2B	2.72	1.49	1.43
23	d	404	CLA	C3B-C4B	2.71	1.49	1.42
23	r	602	CLA	C3B-C4B	2.71	1.49	1.42
23	g	610	CLA	C4B-NB	2.71	1.41	1.37
33	D	406	PL9	C41-C39	2.71	1.56	1.51
23	A	401	CLA	C1B-C2B	2.71	1.49	1.43
23	s	612	CLA	C3B-C4B	2.71	1.49	1.42
35	n	605	CHL	C4D-ND	-2.71	1.34	1.37
35	n	601	CHL	C4D-ND	-2.70	1.34	1.37
23	B	613	CLA	C3B-C4B	2.70	1.49	1.42
23	G	613	CLA	C1B-C2B	2.70	1.49	1.43
23	b	615	CLA	C3B-C4B	2.70	1.49	1.42
23	S	312	CLA	C4D-ND	-2.70	1.34	1.37
35	g	601	CHL	C3B-C4B	2.70	1.49	1.42
23	R	313	CLA	C3B-C4B	2.70	1.49	1.42
35	y	310	CHL	C3B-C4B	2.70	1.49	1.42
23	S	309	CLA	C3B-C4B	2.70	1.49	1.42
23	C	505	CLA	C3B-C4B	2.69	1.49	1.42
35	S	302	CHL	C4D-ND	-2.69	1.34	1.37
38	G	618	NEX	C7-C8	-2.69	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	N	613	CLA	C1B-C2B	2.69	1.49	1.43
23	Y	314	CLA	C1B-C2B	2.69	1.49	1.43
23	a	401	CLA	C3B-C4B	2.68	1.49	1.42
35	Y	302	CHL	C4D-ND	-2.68	1.34	1.37
23	y	314	CLA	C1B-C2B	2.68	1.49	1.43
35	Y	310	CHL	CMB-C2B	-2.68	1.45	1.50
23	g	613	CLA	C1B-C2B	2.68	1.49	1.43
23	S	313	CLA	C1B-C2B	2.68	1.49	1.43
35	Y	308	CHL	C4D-ND	-2.68	1.34	1.37
35	G	608	CHL	C1B-C2B	2.68	1.49	1.43
23	B	608	CLA	C3B-C4B	2.67	1.49	1.42
23	C	505	CLA	C1B-C2B	2.66	1.49	1.43
23	B	615	CLA	C4D-ND	-2.66	1.34	1.37
35	g	601	CHL	C1B-C2B	2.66	1.49	1.43
23	c	504	CLA	C1B-C2B	2.66	1.49	1.43
23	n	613	CLA	C1B-C2B	2.66	1.49	1.43
23	B	605	CLA	C3B-C4B	2.66	1.49	1.42
23	b	617	CLA	C4D-ND	-2.66	1.34	1.37
23	N	614	CLA	C1B-C2B	2.66	1.49	1.43
23	s	612	CLA	C1B-C2B	2.66	1.49	1.43
23	R	311	CLA	C1B-C2B	2.66	1.49	1.43
23	c	502	CLA	C1B-C2B	2.66	1.49	1.43
23	A	402	CLA	C3B-C4B	2.66	1.49	1.42
23	C	503	CLA	C1B-C2B	2.66	1.49	1.43
23	b	611	CLA	C1B-C2B	2.66	1.49	1.43
35	R	308	CHL	C3B-C4B	2.65	1.49	1.42
35	Y	306	CHL	C1B-C2B	2.65	1.49	1.43
35	g	609	CHL	C3B-C4B	2.65	1.49	1.42
23	a	401	CLA	C1B-C2B	2.65	1.49	1.43
23	r	610	CLA	C1B-C2B	2.65	1.49	1.43
23	R	310	CLA	C1B-C2B	2.65	1.49	1.43
23	s	608	CLA	C1B-C2B	2.64	1.49	1.43
23	S	313	CLA	C3B-C4B	2.64	1.49	1.42
23	r	602	CLA	C1B-C2B	2.64	1.49	1.43
35	g	608	CHL	C1B-C2B	2.64	1.49	1.43
23	C	504	CLA	C1B-C2B	2.64	1.49	1.43
23	g	602	CLA	C1B-C2B	2.63	1.49	1.43
23	R	303	CLA	C1B-C2B	2.63	1.49	1.43
35	G	605	CHL	C1B-C2B	2.63	1.49	1.43
35	g	609	CHL	CMB-C2B	-2.63	1.45	1.50
35	y	306	CHL	C1B-C2B	2.63	1.49	1.43
35	s	606	CHL	C1B-C2B	2.63	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	605	CHL	C1B-C2B	2.62	1.49	1.43
35	r	606	CHL	C1B-C2B	2.62	1.49	1.43
35	y	308	CHL	C1B-C2B	2.62	1.49	1.43
23	y	312	CLA	C1B-C2B	2.62	1.49	1.43
35	G	601	CHL	C1B-C2B	2.62	1.49	1.43
34	F	101	HEM	FE-NC	2.62	2.04	1.95
23	r	601	CLA	C1B-C2B	2.62	1.49	1.43
34	f	101	HEM	FE-NC	2.62	2.04	1.95
23	B	609	CLA	C1B-C2B	2.62	1.49	1.43
35	S	306	CHL	C1B-C2B	2.62	1.49	1.43
23	c	503	CLA	C1B-C2B	2.62	1.49	1.43
23	B	604	CLA	C1B-C2B	2.61	1.49	1.43
33	d	406	PL9	C21-C19	2.61	1.56	1.51
23	S	314	CLA	C1B-C2B	2.61	1.49	1.43
23	c	502	CLA	C3B-C4B	2.61	1.48	1.42
23	G	614	CLA	C1B-C2B	2.61	1.49	1.43
23	g	614	CLA	C1B-C2B	2.61	1.49	1.43
23	Y	312	CLA	C1B-C2B	2.61	1.49	1.43
23	n	614	CLA	C1B-C2B	2.61	1.49	1.43
35	y	302	CHL	C4D-ND	-2.61	1.34	1.37
35	g	606	CHL	C1B-C2B	2.61	1.49	1.43
23	b	606	CLA	C1B-C2B	2.61	1.49	1.43
23	g	611	CLA	C1B-C2B	2.61	1.49	1.43
35	S	308	CHL	C1B-C2B	2.61	1.49	1.43
23	r	608	CLA	C1B-C2B	2.60	1.49	1.43
35	R	306	CHL	C1B-C2B	2.60	1.49	1.43
35	r	605	CHL	C1B-C2B	2.60	1.49	1.43
23	Y	313	CLA	C1B-C2B	2.60	1.49	1.43
23	c	507	CLA	C1B-C2B	2.60	1.49	1.43
23	s	610	CLA	C1B-C2B	2.60	1.49	1.43
23	C	508	CLA	C1B-C2B	2.60	1.49	1.43
23	R	302	CLA	C1B-C2B	2.59	1.49	1.43
35	n	605	CHL	C1B-C2B	2.59	1.49	1.43
35	R	307	CHL	C1B-C2B	2.59	1.49	1.43
26	b	602	SQD	C6-S	-2.59	1.67	1.77
23	R	310	CLA	C3B-C4B	2.59	1.48	1.42
23	R	309	CLA	C1B-C2B	2.59	1.49	1.43
23	n	603	CLA	C1B-C2B	2.59	1.49	1.43
35	Y	308	CHL	C1B-C2B	2.59	1.49	1.43
33	D	406	PL9	C21-C19	2.59	1.56	1.51
23	g	612	CLA	C1B-C2B	2.59	1.49	1.43
23	s	613	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	S	302	CHL	C1B-C2B	2.59	1.49	1.43
23	b	618	CLA	C1B-C2B	2.59	1.49	1.43
35	s	601	CHL	C1B-C2B	2.58	1.49	1.43
35	r	607	CHL	C1B-C2B	2.58	1.49	1.43
35	s	605	CHL	C1B-C2B	2.58	1.49	1.43
23	N	603	CLA	C1B-C2B	2.58	1.49	1.43
23	G	602	CLA	C1B-C2B	2.58	1.49	1.43
23	S	312	CLA	C1B-C2B	2.58	1.49	1.43
23	n	611	CLA	C1B-C2B	2.58	1.49	1.43
35	n	601	CHL	C1B-C2B	2.58	1.49	1.43
35	N	606	CHL	C1B-C2B	2.58	1.49	1.43
23	C	511	CLA	C1B-C2B	2.58	1.49	1.43
23	G	612	CLA	C1B-C2B	2.58	1.49	1.43
23	S	303	CLA	C1B-C2B	2.57	1.49	1.43
35	G	607	CHL	C1B-C2B	2.57	1.49	1.43
35	n	606	CHL	C1B-C2B	2.57	1.49	1.43
26	B	625	SQD	C6-S	-2.57	1.67	1.77
38	g	618	NEX	C7-C8	-2.57	1.27	1.32
23	G	611	CLA	C1B-C2B	2.57	1.49	1.43
23	c	512	CLA	C1B-C2B	2.57	1.49	1.43
23	r	611	CLA	C1B-C2B	2.57	1.49	1.43
35	S	307	CHL	C1B-C2B	2.57	1.49	1.43
23	b	612	CLA	C1B-C2B	2.57	1.49	1.43
26	c	520	SQD	C6-S	-2.57	1.67	1.77
23	s	603	CLA	C1B-C2B	2.56	1.49	1.43
23	S	311	CLA	C1B-C2B	2.56	1.49	1.43
23	d	404	CLA	C1B-C2B	2.56	1.49	1.43
23	N	611	CLA	C1B-C2B	2.56	1.49	1.43
23	y	315	CLA	C1B-C2B	2.56	1.49	1.43
23	S	305	CLA	CMB-C2B	-2.56	1.45	1.50
23	C	503	CLA	C3B-C4B	2.56	1.48	1.42
35	G	606	CHL	C1B-C2B	2.55	1.49	1.43
35	N	601	CHL	C4D-ND	-2.55	1.34	1.37
23	d	403	CLA	C1B-C2B	2.55	1.49	1.43
35	N	605	CHL	C1B-C2B	2.55	1.49	1.43
23	D	404	CLA	C1B-C2B	2.55	1.49	1.43
35	g	607	CHL	C1B-C2B	2.55	1.49	1.43
23	b	612	CLA	C3B-C4B	2.55	1.48	1.42
35	s	607	CHL	C1B-C2B	2.55	1.49	1.43
23	Y	311	CLA	C4B-NB	2.55	1.40	1.37
23	c	510	CLA	C1B-C2B	2.55	1.49	1.43
23	b	604	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1B-C2B	2.55	1.49	1.43
23	B	601	CLA	C1B-C2B	2.55	1.49	1.43
23	S	304	CLA	C1B-C2B	2.54	1.49	1.43
26	C	521	SQD	C6-S	-2.54	1.68	1.77
23	r	603	CLA	C1B-C2B	2.54	1.49	1.43
23	B	611	CLA	C1B-C2B	2.54	1.49	1.43
35	R	308	CHL	C1B-C2B	2.54	1.49	1.43
23	b	610	CLA	C1B-C2B	2.54	1.49	1.43
23	c	505	CLA	C1B-C2B	2.54	1.49	1.43
35	y	302	CHL	C1B-C2B	2.54	1.49	1.43
38	R	316	NEX	C7-C8	-2.54	1.27	1.32
23	A	404	CLA	C1B-C2B	2.54	1.49	1.43
35	Y	302	CHL	C1B-C2B	2.54	1.49	1.43
35	y	309	CHL	C1B-C2B	2.54	1.49	1.43
23	B	610	CLA	C3B-C4B	2.54	1.48	1.42
23	C	510	CLA	C1B-C2B	2.54	1.49	1.43
23	R	304	CLA	C1B-C2B	2.54	1.49	1.43
23	c	507	CLA	C3B-C4B	2.53	1.48	1.42
23	b	603	CLA	C1B-C2B	2.53	1.49	1.43
35	n	607	CHL	C1B-C2B	2.53	1.49	1.43
23	C	513	CLA	C1B-C2B	2.53	1.49	1.43
23	b	607	CLA	C3B-C4B	2.53	1.48	1.42
23	Y	315	CLA	C1B-C2B	2.53	1.49	1.43
23	B	602	CLA	C1B-C2B	2.53	1.49	1.43
35	Y	309	CHL	C1B-C2B	2.53	1.49	1.43
23	C	511	CLA	CMD-C2D	-2.53	1.45	1.50
23	R	312	CLA	C1B-C2B	2.53	1.49	1.43
35	N	605	CHL	C4D-ND	-2.53	1.34	1.37
23	B	616	CLA	C1B-C2B	2.53	1.49	1.43
23	G	610	CLA	C3B-C4B	2.52	1.48	1.42
23	G	610	CLA	C1B-C2B	2.52	1.49	1.43
23	N	610	CLA	C1B-C2B	2.52	1.49	1.43
23	N	612	CLA	C1B-C2B	2.52	1.49	1.43
35	g	609	CHL	C4D-ND	-2.52	1.34	1.37
23	a	404	CLA	C1B-C2B	2.52	1.49	1.43
23	c	509	CLA	C1B-C2B	2.52	1.49	1.43
35	N	601	CHL	C1B-C2B	2.52	1.49	1.43
23	Y	305	CLA	CMB-C2B	-2.51	1.45	1.50
23	B	610	CLA	C1B-C2B	2.51	1.49	1.43
23	C	514	CLA	C1B-C2B	2.51	1.49	1.43
35	Y	307	CHL	C1B-C2B	2.51	1.49	1.43
23	b	613	CLA	C1B-C2B	2.51	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	n	610	CLA	C1B-C2B	2.51	1.49	1.43
23	n	602	CLA	C1B-C2B	2.51	1.49	1.43
23	C	508	CLA	C3B-C4B	2.50	1.48	1.42
23	C	512	CLA	C1B-C2B	2.50	1.49	1.43
35	y	307	CHL	C1B-C2B	2.50	1.49	1.43
23	G	604	CLA	C1B-C2B	2.49	1.49	1.43
23	g	610	CLA	C1B-C2B	2.49	1.49	1.43
23	r	609	CLA	C1B-C2B	2.49	1.49	1.43
35	N	609	CHL	C1B-C2B	2.49	1.49	1.43
35	n	609	CHL	C1B-C2B	2.49	1.49	1.43
23	c	513	CLA	C1B-C2B	2.49	1.49	1.43
23	C	506	CLA	C1B-C2B	2.49	1.49	1.43
23	G	603	CLA	C1B-C2B	2.48	1.49	1.43
23	S	310	CLA	C1B-C2B	2.48	1.49	1.43
23	n	612	CLA	C1B-C2B	2.48	1.49	1.43
23	s	611	CLA	C1B-C2B	2.48	1.49	1.43
23	b	614	CLA	C1B-C2B	2.48	1.49	1.43
33	D	406	PL9	C7-C8	2.47	1.54	1.50
35	N	607	CHL	C1B-C2B	2.47	1.49	1.43
23	y	313	CLA	C1B-C2B	2.47	1.49	1.43
23	D	403	CLA	CMC-C2C	-2.47	1.45	1.50
23	y	303	CLA	C1B-C2B	2.46	1.49	1.43
23	Y	304	CLA	C1B-C2B	2.46	1.49	1.43
23	A	402	CLA	C1B-C2B	2.46	1.49	1.43
23	b	605	CLA	C1B-C2B	2.46	1.49	1.43
38	S	317	NEX	C7-C8	-2.45	1.27	1.32
23	y	305	CLA	CMB-C2B	-2.45	1.45	1.50
23	B	604	CLA	C3B-C4B	2.45	1.48	1.42
23	D	403	CLA	C1B-C2B	2.45	1.49	1.43
23	B	603	CLA	C1B-C2B	2.44	1.49	1.43
23	d	401	CLA	C1B-C2B	2.44	1.49	1.43
33	d	406	PL9	C7-C8	2.44	1.54	1.50
23	d	403	CLA	CMC-C2C	-2.44	1.45	1.50
35	G	609	CHL	C1B-C2B	2.44	1.49	1.43
23	y	304	CLA	C1B-C2B	2.44	1.49	1.43
23	B	606	CLA	C1B-C2B	2.44	1.49	1.43
23	s	602	CLA	C1B-C2B	2.44	1.49	1.43
23	b	606	CLA	C3B-C4B	2.43	1.48	1.42
23	B	615	CLA	C1B-C2B	2.43	1.49	1.43
23	r	612	CLA	C1B-C2B	2.43	1.49	1.43
23	Y	303	CLA	C1B-C2B	2.43	1.49	1.43
23	r	604	CLA	C1B-C2B	2.42	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	401	CLA	CMC-C2C	-2.42	1.45	1.50
35	N	608	CHL	C1B-C2B	2.42	1.48	1.43
23	B	612	CLA	C1B-C2B	2.42	1.48	1.43
23	b	615	CLA	C1B-C2B	2.42	1.48	1.43
23	b	617	CLA	C1B-C2B	2.42	1.48	1.43
23	s	609	CLA	C1B-C2B	2.41	1.48	1.43
38	n	617	NEX	C7-C8	-2.41	1.27	1.32
23	D	401	CLA	C1B-C2B	2.41	1.48	1.43
23	c	506	CLA	C1B-C2B	2.41	1.48	1.43
23	R	305	CLA	C1B-C2B	2.41	1.48	1.43
23	A	401	CLA	CMC-C2C	-2.40	1.45	1.50
23	R	313	CLA	CMB-C2B	-2.40	1.45	1.50
23	Y	311	CLA	C1B-C2B	2.39	1.48	1.43
23	b	616	CLA	C1B-C2B	2.39	1.48	1.43
23	B	613	CLA	C1B-C2B	2.39	1.48	1.43
23	b	608	CLA	C1B-C2B	2.39	1.48	1.43
23	B	614	CLA	C1B-C2B	2.39	1.48	1.43
23	b	606	CLA	CMB-C2B	-2.38	1.45	1.50
38	N	617	NEX	C7-C8	-2.38	1.28	1.32
23	g	604	CLA	C1B-C2B	2.37	1.48	1.43
23	n	604	CLA	CMB-C2B	-2.37	1.45	1.50
35	n	608	CHL	C1B-C2B	2.37	1.48	1.43
23	y	311	CLA	C1B-C2B	2.36	1.48	1.43
23	R	313	CLA	C1B-C2B	2.36	1.48	1.43
23	B	608	CLA	CMB-C2B	-2.36	1.45	1.50
23	S	310	CLA	CHC-C1C	2.36	1.43	1.38
23	B	608	CLA	C1B-C2B	2.35	1.48	1.43
23	D	403	CLA	CMD-C2D	-2.35	1.45	1.50
23	s	604	CLA	C1B-C2B	2.35	1.48	1.43
23	g	604	CLA	CMB-C2B	-2.35	1.45	1.50
23	C	506	CLA	CMD-C2D	-2.34	1.45	1.50
35	r	607	CHL	CMD-C2D	-2.34	1.45	1.50
23	d	402	CLA	C1B-C2B	2.34	1.48	1.43
23	D	403	CLA	CHC-C1C	2.34	1.43	1.38
23	C	502	CLA	C1B-C2B	2.33	1.48	1.43
23	N	602	CLA	C1B-C2B	2.33	1.48	1.43
23	c	505	CLA	CMD-C2D	-2.32	1.45	1.50
23	N	602	CLA	CHC-C1C	2.32	1.43	1.38
23	B	604	CLA	CMB-C2B	-2.32	1.45	1.50
23	C	507	CLA	C1B-C2B	2.32	1.48	1.43
23	c	506	CLA	CMB-C2B	-2.32	1.45	1.50
23	B	607	CLA	C1B-C2B	2.32	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C1B-C2B	2.32	1.48	1.43
23	b	609	CLA	CMB-C2B	-2.31	1.45	1.50
23	c	501	CLA	C1B-C2B	2.31	1.48	1.43
23	B	605	CLA	CMD-C2D	-2.30	1.45	1.50
23	N	604	CLA	CMB-C2B	-2.30	1.45	1.50
23	n	604	CLA	C1B-C2B	2.30	1.48	1.43
23	d	403	CLA	CMD-C2D	-2.29	1.45	1.50
23	B	607	CLA	CMB-C2B	-2.29	1.45	1.50
23	N	604	CLA	C1B-C2B	2.29	1.48	1.43
23	s	609	CLA	CHC-C1C	2.27	1.43	1.38
23	b	614	CLA	CMD-C2D	-2.27	1.46	1.50
35	G	609	CHL	CMB-C2B	-2.27	1.46	1.50
23	C	507	CLA	CMB-C2B	-2.27	1.46	1.50
23	B	612	CLA	CMD-C2D	-2.27	1.46	1.50
23	r	604	CLA	CMB-C2B	-2.25	1.46	1.50
23	r	612	CLA	CMB-C2B	-2.25	1.46	1.50
23	b	618	CLA	CMC-C2C	-2.25	1.46	1.50
23	d	402	CLA	CMB-C2B	-2.25	1.46	1.50
23	B	604	CLA	CMD-C2D	-2.25	1.46	1.50
23	B	608	CLA	CMD-C2D	-2.24	1.46	1.50
23	d	403	CLA	CHC-C1C	2.24	1.43	1.38
23	B	603	CLA	CMD-C2D	-2.24	1.46	1.50
23	R	305	CLA	CMB-C2B	-2.23	1.46	1.50
23	a	401	CLA	CMD-C2D	-2.23	1.46	1.50
23	y	305	CLA	C1B-C2B	2.23	1.48	1.43
23	b	614	CLA	CMC-C2C	-2.23	1.46	1.50
23	b	610	CLA	CMD-C2D	-2.23	1.46	1.50
33	D	406	PL9	C5-C4	-2.23	1.39	1.47
35	y	310	CHL	C1B-C2B	2.23	1.48	1.43
35	Y	310	CHL	C1B-C2B	2.23	1.48	1.43
23	b	607	CLA	CMD-C2D	-2.22	1.46	1.50
33	d	406	PL9	C5-C4	-2.22	1.39	1.47
23	B	616	CLA	CMC-C2C	-2.22	1.46	1.50
35	N	601	CHL	CHC-C1C	2.22	1.43	1.38
24	A	403	PHO	C1D-C2D	2.22	1.42	1.39
23	c	508	CLA	CMB-C2B	-2.22	1.46	1.50
23	b	605	CLA	CMB-C2B	-2.22	1.46	1.50
23	b	605	CLA	CMD-C2D	-2.21	1.46	1.50
33	D	406	PL9	C26-C24	2.21	1.55	1.51
35	g	609	CHL	C1B-C2B	2.21	1.48	1.43
33	d	406	PL9	C26-C24	2.21	1.55	1.51
35	Y	309	CHL	CHC-C1C	2.21	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	s	607	CHL	CHC-C1C	2.21	1.43	1.38
23	c	501	CLA	CMD-C2D	-2.21	1.46	1.50
23	C	509	CLA	CMB-C2B	-2.21	1.46	1.50
23	y	311	CLA	CHC-C1C	2.21	1.43	1.38
23	B	616	CLA	CHC-C1C	2.20	1.43	1.38
23	A	401	CLA	CMD-C2D	-2.20	1.46	1.50
23	N	611	CLA	CMD-C2D	-2.20	1.46	1.50
23	B	603	CLA	CMB-C2B	-2.20	1.46	1.50
23	r	602	CLA	MG-NB	-2.20	2.01	2.05
23	C	502	CLA	CMD-C2D	-2.20	1.46	1.50
35	Y	307	CHL	CMD-C2D	-2.20	1.46	1.50
35	g	609	CHL	MG-NA	2.20	2.11	2.06
23	c	508	CLA	C1B-C2B	2.20	1.48	1.43
35	R	308	CHL	CMD-C2D	-2.20	1.46	1.50
23	R	303	CLA	MG-NB	-2.20	2.01	2.05
23	Y	305	CLA	C1B-C2B	2.19	1.48	1.43
35	y	309	CHL	CHC-C1C	2.19	1.43	1.38
35	n	609	CHL	CMB-C2B	-2.19	1.46	1.50
23	b	606	CLA	CMD-C2D	-2.19	1.46	1.50
23	c	502	CLA	CMB-C2B	-2.19	1.46	1.50
23	b	614	CLA	CHC-C1C	2.19	1.43	1.38
23	G	604	CLA	CMB-C2B	-2.19	1.46	1.50
35	N	609	CHL	CMB-C2B	-2.19	1.46	1.50
35	n	601	CHL	CHC-C1C	2.19	1.43	1.38
23	R	310	CLA	MG-NB	-2.18	2.01	2.05
23	s	604	CLA	CMB-C2B	-2.18	1.46	1.50
23	B	612	CLA	CMC-C2C	-2.18	1.46	1.50
23	C	503	CLA	CMB-C2B	-2.18	1.46	1.50
23	b	616	CLA	CMD-C2D	-2.17	1.46	1.50
23	b	604	CLA	CHC-C1C	2.17	1.42	1.38
23	r	602	CLA	CHC-C1C	2.17	1.42	1.38
35	S	308	CHL	CHC-C1C	2.17	1.42	1.38
23	B	601	CLA	CMD-C2D	-2.17	1.46	1.50
23	C	509	CLA	C1B-C2B	2.17	1.48	1.43
23	B	616	CLA	MG-NB	-2.16	2.01	2.05
23	D	401	CLA	CMD-C2D	-2.16	1.46	1.50
23	G	604	CLA	CHC-C1C	2.16	1.42	1.38
35	N	608	CHL	CHC-C1C	2.16	1.42	1.38
23	n	611	CLA	CMD-C2D	-2.16	1.46	1.50
35	y	307	CHL	CMD-C2D	-2.16	1.46	1.50
35	Y	310	CHL	CMD-C2D	-2.16	1.46	1.50
34	F	101	HEM	CMC-C2C	2.16	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	n	606	CHL	CHC-C1C	2.15	1.42	1.38
23	B	606	CLA	CMC-C2C	-2.15	1.46	1.50
23	R	309	CLA	CHC-C1C	2.15	1.42	1.38
23	b	618	CLA	CHC-C1C	2.15	1.42	1.38
35	g	608	CHL	CMD-C2D	-2.15	1.46	1.50
23	b	610	CLA	CMB-C2B	-2.15	1.46	1.50
35	n	608	CHL	CHC-C1C	2.15	1.42	1.38
23	b	616	CLA	CMB-C2B	-2.15	1.46	1.50
23	b	608	CLA	CMC-C2C	-2.15	1.46	1.50
23	b	613	CLA	CMC-C2C	-2.15	1.46	1.50
23	R	303	CLA	CHC-C1C	2.15	1.42	1.38
23	c	511	CLA	CMB-C2B	-2.15	1.46	1.50
23	B	614	CLA	CMB-C2B	-2.14	1.46	1.50
23	b	618	CLA	MG-NB	-2.14	2.01	2.05
23	B	612	CLA	CHC-C1C	2.14	1.42	1.38
23	Y	311	CLA	MG-NB	-2.14	2.01	2.05
35	G	607	CHL	CHC-C1C	2.14	1.42	1.38
23	B	602	CLA	CHC-C1C	2.14	1.42	1.38
23	y	304	CLA	CMD-C2D	-2.14	1.46	1.50
23	c	513	CLA	CHC-C1C	2.14	1.42	1.38
35	R	308	CHL	CMB-C2B	-2.13	1.46	1.50
35	s	601	CHL	CHC-C1C	2.13	1.42	1.38
35	G	601	CHL	CMD-C2D	-2.13	1.46	1.50
23	b	612	CLA	CMC-C2C	-2.13	1.46	1.50
23	R	310	CLA	CMB-C2B	-2.13	1.46	1.50
23	n	602	CLA	CHC-C1C	2.13	1.42	1.38
35	n	608	CHL	CMB-C2B	-2.13	1.46	1.50
23	B	606	CLA	CMD-C2D	-2.13	1.46	1.50
23	s	608	CLA	CHC-C1C	2.13	1.42	1.38
35	g	608	CHL	CHC-C1C	2.13	1.42	1.38
35	N	606	CHL	CMD-C2D	-2.13	1.46	1.50
35	G	608	CHL	CMD-C2D	-2.13	1.46	1.50
35	G	606	CHL	CHC-C1C	2.13	1.42	1.38
23	S	314	CLA	CMD-C2D	-2.13	1.46	1.50
23	g	603	CLA	CMB-C2B	-2.13	1.46	1.50
23	b	607	CLA	CMB-C2B	-2.13	1.46	1.50
23	B	607	CLA	CMD-C2D	-2.13	1.46	1.50
35	Y	308	CHL	CMD-C2D	-2.13	1.46	1.50
35	N	606	CHL	CHC-C1C	2.12	1.42	1.38
35	G	608	CHL	CHC-C1C	2.12	1.42	1.38
23	B	611	CLA	CMC-C2C	-2.12	1.46	1.50
23	A	404	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	611	CLA	CHC-C1C	2.12	1.42	1.38
35	N	607	CHL	CHC-C1C	2.12	1.42	1.38
23	A	402	CLA	CMB-C2B	-2.12	1.46	1.50
23	b	603	CLA	CMD-C2D	-2.12	1.46	1.50
23	B	610	CLA	CMC-C2C	-2.12	1.46	1.50
35	r	605	CHL	CHC-C1C	2.12	1.42	1.38
23	b	618	CLA	CMD-C2D	-2.12	1.46	1.50
23	C	507	CLA	MG-NB	-2.11	2.01	2.05
23	Y	304	CLA	CMD-C2D	-2.11	1.46	1.50
23	y	312	CLA	CHC-C1C	2.11	1.42	1.38
23	S	313	CLA	CMB-C2B	-2.11	1.46	1.50
23	C	504	CLA	CMD-C2D	-2.11	1.46	1.50
23	b	615	CLA	CMB-C2B	-2.11	1.46	1.50
35	r	606	CHL	CHC-C1C	2.11	1.42	1.38
23	b	616	CLA	CHC-C1C	2.11	1.42	1.38
23	N	610	CLA	CMD-C2D	-2.11	1.46	1.50
23	d	401	CLA	CMB-C2B	-2.11	1.46	1.50
23	R	303	CLA	CMC-C2C	-2.11	1.46	1.50
23	c	503	CLA	CMD-C2D	-2.11	1.46	1.50
23	C	510	CLA	CMD-C2D	-2.11	1.46	1.50
23	d	402	CLA	CHC-C1C	2.11	1.42	1.38
35	y	302	CHL	CHC-C1C	2.11	1.42	1.38
23	r	603	CLA	CMD-C2D	-2.11	1.46	1.50
35	y	308	CHL	CMD-C2D	-2.11	1.46	1.50
23	S	305	CLA	MG-NB	-2.11	2.01	2.05
35	N	605	CHL	CHC-C1C	2.11	1.42	1.38
35	R	306	CHL	CHC-C1C	2.11	1.42	1.38
23	c	510	CLA	CHC-C1C	2.11	1.42	1.38
23	R	304	CLA	CMD-C2D	-2.10	1.46	1.50
23	Y	312	CLA	CHC-C1C	2.10	1.42	1.38
23	C	514	CLA	CMD-C2D	-2.10	1.46	1.50
23	S	314	CLA	CMB-C2B	-2.10	1.46	1.50
35	N	601	CHL	CMD-C2D	-2.10	1.46	1.50
35	g	601	CHL	CMB-C2B	-2.10	1.46	1.50
23	B	606	CLA	CMB-C2B	-2.10	1.46	1.50
23	B	613	CLA	CMB-C2B	-2.10	1.46	1.50
23	b	609	CLA	CMD-C2D	-2.10	1.46	1.50
35	y	306	CHL	CHC-C1C	2.10	1.42	1.38
35	g	601	CHL	CMD-C2D	-2.10	1.46	1.50
23	N	610	CLA	CHC-C1C	2.10	1.42	1.38
23	g	611	CLA	CHC-C1C	2.10	1.42	1.38
23	Y	315	CLA	CMD-C2D	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	302	CLA	CMD-C2D	-2.10	1.46	1.50
35	n	607	CHL	CHC-C1C	2.10	1.42	1.38
23	y	315	CLA	CMD-C2D	-2.10	1.46	1.50
35	n	608	CHL	CMD-C2D	-2.10	1.46	1.50
23	G	612	CLA	CMD-C2D	-2.10	1.46	1.50
35	y	310	CHL	CMD-C2D	-2.10	1.46	1.50
35	S	302	CHL	CHC-C1C	2.09	1.42	1.38
23	c	505	CLA	CMB-C2B	-2.09	1.46	1.50
35	Y	302	CHL	CMD-C2D	-2.09	1.46	1.50
23	d	402	CLA	CMD-C2D	-2.09	1.46	1.50
23	g	602	CLA	CMD-C2D	-2.09	1.46	1.50
23	c	506	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	608	CLA	CMB-C2B	-2.09	1.46	1.50
35	n	601	CHL	CMD-C2D	-2.09	1.46	1.50
34	f	101	HEM	CMC-C2C	2.09	1.55	1.50
24	a	402	PHO	C1D-C2D	2.09	1.41	1.39
35	Y	302	CHL	CHC-C1C	2.09	1.42	1.38
23	B	616	CLA	CMD-C2D	-2.09	1.46	1.50
23	G	610	CLA	CMD-C2D	-2.09	1.46	1.50
23	s	608	CLA	CMD-C2D	-2.09	1.46	1.50
35	s	605	CHL	CHC-C1C	2.09	1.42	1.38
23	b	611	CLA	CMD-C2D	-2.09	1.46	1.50
35	n	606	CHL	CMD-C2D	-2.09	1.46	1.50
23	B	609	CLA	CMD-C2D	-2.09	1.46	1.50
35	N	608	CHL	CMB-C2B	-2.09	1.46	1.50
23	y	311	CLA	CMD-C2D	-2.09	1.46	1.50
35	R	308	CHL	CHC-C1C	2.09	1.42	1.38
23	Y	303	CLA	CMC-C2C	-2.09	1.46	1.50
35	S	306	CHL	CMB-C2B	-2.09	1.46	1.50
23	r	608	CLA	CHC-C1C	2.09	1.42	1.38
23	G	611	CLA	CMD-C2D	-2.09	1.46	1.50
23	R	311	CLA	CHC-C1C	2.09	1.42	1.38
23	S	309	CLA	CMD-C2D	-2.09	1.46	1.50
23	c	508	CLA	CMC-C2C	-2.09	1.46	1.50
23	d	401	CLA	CMD-C2D	-2.09	1.46	1.50
23	s	602	CLA	CMB-C2B	-2.09	1.46	1.50
23	B	614	CLA	CHC-C1C	2.09	1.42	1.38
23	r	612	CLA	MG-NB	-2.09	2.01	2.05
23	G	613	CLA	CMD-C2D	-2.08	1.46	1.50
23	n	610	CLA	CMD-C2D	-2.08	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.08	1.46	1.50
23	Y	305	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	501	CLA	CMB-C2B	-2.08	1.46	1.50
23	G	614	CLA	CHC-C1C	2.08	1.42	1.38
23	s	613	CLA	CMB-C2B	-2.08	1.46	1.50
35	Y	308	CHL	CMB-C2B	-2.08	1.46	1.50
23	G	602	CLA	CMD-C2D	-2.08	1.46	1.50
23	c	513	CLA	CMD-C2D	-2.08	1.46	1.50
23	b	608	CLA	CMD-C2D	-2.08	1.46	1.50
35	N	609	CHL	CMD-C2D	-2.08	1.46	1.50
35	R	307	CHL	CHC-C1C	2.08	1.42	1.38
23	r	609	CLA	CHC-C1C	2.08	1.42	1.38
23	r	611	CLA	CHC-C1C	2.08	1.42	1.38
23	s	613	CLA	CMD-C2D	-2.08	1.46	1.50
23	R	303	CLA	CMD-C2D	-2.08	1.46	1.50
23	R	312	CLA	CHC-C1C	2.08	1.42	1.38
35	y	302	CHL	CMD-C2D	-2.08	1.46	1.50
23	r	610	CLA	CHC-C1C	2.08	1.42	1.38
23	y	311	CLA	MG-NB	-2.08	2.01	2.05
23	Y	313	CLA	CMD-C2D	-2.08	1.46	1.50
23	s	612	CLA	CMD-C2D	-2.08	1.46	1.50
23	g	611	CLA	CMD-C2D	-2.08	1.46	1.50
23	D	401	CLA	CMB-C2B	-2.08	1.46	1.50
23	g	614	CLA	CMD-C2D	-2.08	1.46	1.50
23	c	501	CLA	CHC-C1C	2.07	1.42	1.38
23	b	613	CLA	CMD-C2D	-2.07	1.46	1.50
23	R	303	CLA	CMB-C2B	-2.07	1.46	1.50
23	N	604	CLA	CHC-C1C	2.07	1.42	1.38
23	n	603	CLA	CMB-C2B	-2.07	1.46	1.50
35	N	608	CHL	CMD-C2D	-2.07	1.46	1.50
35	G	605	CHL	CMD-C2D	-2.07	1.46	1.50
23	b	609	CLA	CHC-C1C	2.07	1.42	1.38
23	c	509	CLA	CMB-C2B	-2.07	1.46	1.50
23	a	404	CLA	CHC-C1C	2.07	1.42	1.38
35	n	609	CHL	CMD-C2D	-2.07	1.46	1.50
23	C	507	CLA	CMD-C2D	-2.07	1.46	1.50
23	R	309	CLA	CMD-C2D	-2.07	1.46	1.50
23	S	303	CLA	CMB-C2B	-2.07	1.46	1.50
35	s	601	CHL	CMD-C2D	-2.07	1.46	1.50
35	y	307	CHL	CHC-C1C	2.07	1.42	1.38
23	C	506	CLA	CMB-C2B	-2.07	1.46	1.50
23	C	512	CLA	CMB-C2B	-2.07	1.46	1.50
35	Y	309	CHL	CMD-C2D	-2.07	1.46	1.50
23	c	506	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	y	313	CLA	CMD-C2D	-2.07	1.46	1.50
23	S	305	CLA	CHC-C1C	2.07	1.42	1.38
23	B	613	CLA	CMD-C2D	-2.07	1.46	1.50
23	C	509	CLA	CMC-C2C	-2.07	1.46	1.50
23	C	514	CLA	CHC-C1C	2.07	1.42	1.38
35	r	607	CHL	CHC-C1C	2.07	1.42	1.38
24	a	403	PHO	C1D-C2D	2.06	1.41	1.39
35	Y	308	CHL	CHC-C1C	2.06	1.42	1.38
23	b	612	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	613	CLA	CMB-C2B	-2.06	1.46	1.50
23	B	609	CLA	CMB-C2B	-2.06	1.46	1.50
23	g	613	CLA	CMD-C2D	-2.06	1.46	1.50
35	Y	309	CHL	CMB-C2B	-2.06	1.46	1.50
23	r	603	CLA	CHC-C1C	2.06	1.42	1.38
23	n	603	CLA	CMD-C2D	-2.06	1.46	1.50
23	y	305	CLA	CMC-C2C	-2.06	1.46	1.50
23	G	614	CLA	CMD-C2D	-2.06	1.46	1.50
23	y	304	CLA	CMB-C2B	-2.06	1.46	1.50
23	R	305	CLA	CMD-C2D	-2.06	1.46	1.50
35	y	308	CHL	CMB-C2B	-2.06	1.46	1.50
23	g	604	CLA	CHC-C1C	2.06	1.42	1.38
23	B	602	CLA	CMB-C2B	-2.06	1.46	1.50
23	s	609	CLA	CMD-C2D	-2.06	1.46	1.50
35	S	307	CHL	CHC-C1C	2.06	1.42	1.38
23	b	611	CLA	CMB-C2B	-2.06	1.46	1.50
23	y	315	CLA	CHC-C1C	2.06	1.42	1.38
23	S	313	CLA	CMD-C2D	-2.06	1.46	1.50
35	y	309	CHL	CMD-C2D	-2.06	1.46	1.50
23	B	611	CLA	CMB-C2B	-2.06	1.46	1.50
23	N	604	CLA	CMD-C2D	-2.06	1.46	1.50
23	c	509	CLA	CMD-C2D	-2.06	1.46	1.50
23	r	608	CLA	CMD-C2D	-2.06	1.46	1.50
23	R	302	CLA	CHC-C1C	2.06	1.42	1.38
23	Y	312	CLA	CMD-C2D	-2.06	1.46	1.50
23	B	614	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	503	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	510	CLA	CMB-C2B	-2.06	1.46	1.50
23	Y	313	CLA	CMC-C2C	-2.06	1.46	1.50
35	G	607	CHL	CMD-C2D	-2.06	1.46	1.50
33	d	406	PL9	C31-C29	2.06	1.55	1.51
23	R	304	CLA	CMB-C2B	-2.06	1.46	1.50
23	R	313	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	g	614	CLA	CHC-C1C	2.06	1.42	1.38
23	B	610	CLA	CMD-C2D	-2.05	1.46	1.50
23	r	609	CLA	CMD-C2D	-2.05	1.46	1.50
35	S	302	CHL	CMD-C2D	-2.05	1.46	1.50
23	b	615	CLA	CMD-C2D	-2.05	1.46	1.50
23	S	304	CLA	CMB-C2B	-2.05	1.46	1.50
23	B	610	CLA	MG-NB	-2.05	2.01	2.05
23	C	511	CLA	CHC-C1C	2.05	1.42	1.38
23	A	404	CLA	CMD-C2D	-2.05	1.46	1.50
23	a	404	CLA	CMD-C2D	-2.05	1.46	1.50
35	g	606	CHL	CMD-C2D	-2.05	1.46	1.50
35	Y	307	CHL	CHC-C1C	2.05	1.42	1.38
23	n	602	CLA	CMD-C2D	-2.05	1.46	1.50
23	R	310	CLA	CMD-C2D	-2.05	1.46	1.50
35	y	310	CHL	MG-NB	-2.05	2.01	2.05
23	g	603	CLA	CMD-C2D	-2.05	1.46	1.50
23	r	612	CLA	CMD-C2D	-2.05	1.46	1.50
35	r	606	CHL	CMD-C2D	-2.05	1.46	1.50
35	y	306	CHL	CMD-C2D	-2.05	1.46	1.50
23	c	507	CLA	CMD-C2D	-2.05	1.46	1.50
23	s	612	CLA	CMB-C2B	-2.05	1.46	1.50
35	Y	306	CHL	CHC-C1C	2.05	1.42	1.38
35	y	310	CHL	CHC-C1C	2.05	1.42	1.38
23	Y	314	CLA	CMD-C2D	-2.05	1.46	1.50
23	N	603	CLA	CMB-C2B	-2.05	1.46	1.50
35	g	607	CHL	CMD-C2D	-2.05	1.46	1.50
23	B	601	CLA	CHC-C1C	2.05	1.42	1.38
33	D	406	PL9	C31-C29	2.05	1.55	1.51
23	B	601	CLA	CMB-C2B	-2.05	1.46	1.50
23	g	610	CLA	CMD-C2D	-2.05	1.46	1.50
23	r	602	CLA	CMC-C2C	-2.05	1.46	1.50
35	N	607	CHL	CMD-C2D	-2.05	1.46	1.50
23	C	502	CLA	CHC-C1C	2.05	1.42	1.38
23	C	502	CLA	CMB-C2B	-2.05	1.46	1.50
23	G	603	CLA	CMD-C2D	-2.05	1.46	1.50
23	r	602	CLA	CMB-C2B	-2.05	1.46	1.50
35	G	601	CHL	CMB-C2B	-2.05	1.46	1.50
23	n	604	CLA	CMD-C2D	-2.05	1.46	1.50
35	y	310	CHL	C1B-NB	-2.04	1.35	1.37
23	a	401	CLA	CMB-C2B	-2.04	1.46	1.50
23	y	314	CLA	CMD-C2D	-2.04	1.46	1.50
23	D	404	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	304	CLA	CMB-C2B	-2.04	1.46	1.50
23	B	615	CLA	CMD-C2D	-2.04	1.46	1.50
33	d	406	PL9	C37-C38	2.04	1.57	1.50
35	Y	310	CHL	CHC-C1C	2.04	1.42	1.38
23	y	314	CLA	CMB-C2B	-2.04	1.46	1.50
35	y	308	CHL	CHC-C1C	2.04	1.42	1.38
35	G	606	CHL	CMD-C2D	-2.04	1.46	1.50
23	G	602	CLA	CMC-C2C	-2.04	1.46	1.50
35	n	607	CHL	CMD-C2D	-2.04	1.46	1.50
23	b	612	CLA	MG-NB	-2.04	2.01	2.05
23	g	612	CLA	CMD-C2D	-2.04	1.46	1.50
35	y	309	CHL	CMB-C2B	-2.04	1.46	1.50
23	c	507	CLA	CMB-C2B	-2.04	1.46	1.50
23	N	602	CLA	CMD-C2D	-2.04	1.46	1.50
23	r	601	CLA	CMD-C2D	-2.04	1.46	1.50
23	n	613	CLA	CMD-C2D	-2.04	1.46	1.50
24	a	402	PHO	C3B-C2B	-2.04	1.37	1.40
23	B	615	CLA	CMB-C2B	-2.04	1.46	1.50
23	D	403	CLA	CMB-C2B	-2.04	1.46	1.50
23	c	502	CLA	CMD-C2D	-2.04	1.46	1.50
23	r	610	CLA	CMD-C2D	-2.04	1.46	1.50
23	n	602	CLA	CMC-C2C	-2.04	1.46	1.50
23	Y	305	CLA	CMC-C2C	-2.04	1.46	1.50
23	s	602	CLA	CMD-C2D	-2.04	1.46	1.50
23	C	509	CLA	CHC-C1C	2.04	1.42	1.38
23	C	509	CLA	CMD-C2D	-2.04	1.46	1.50
23	r	601	CLA	CHC-C1C	2.04	1.42	1.38
23	r	604	CLA	CMD-C2D	-2.04	1.46	1.50
35	y	302	CHL	CMB-C2B	-2.04	1.46	1.50
23	b	615	CLA	CHC-C1C	2.04	1.42	1.38
23	A	401	CLA	CMB-C2B	-2.03	1.46	1.50
23	s	603	CLA	CMD-C2D	-2.03	1.46	1.50
35	g	609	CHL	CMD-C2D	-2.03	1.46	1.50
23	r	603	CLA	CMB-C2B	-2.03	1.46	1.50
23	y	315	CLA	CMB-C2B	-2.03	1.46	1.50
23	y	303	CLA	CHC-C1C	2.03	1.42	1.38
23	C	510	CLA	CMC-C2C	-2.03	1.46	1.50
23	N	603	CLA	CMD-C2D	-2.03	1.46	1.50
23	S	305	CLA	C1B-C2B	2.03	1.48	1.43
23	r	612	CLA	CHC-C1C	2.03	1.42	1.38
35	G	605	CHL	CHC-C1C	2.03	1.42	1.38
23	A	402	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	S	303	CLA	CMD-C2D	-2.03	1.46	1.50
23	n	604	CLA	CHC-C1C	2.03	1.42	1.38
23	r	609	CLA	CMC-C2C	-2.03	1.46	1.50
23	s	610	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	604	CLA	CMD-C2D	-2.03	1.46	1.50
23	N	612	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	604	CLA	CMB-C2B	-2.03	1.46	1.50
35	N	605	CHL	CMD-C2D	-2.03	1.46	1.50
23	Y	305	CLA	MG-NB	-2.03	2.01	2.05
23	b	603	CLA	CMB-C2B	-2.03	1.46	1.50
23	b	617	CLA	CMD-C2D	-2.03	1.46	1.50
23	B	602	CLA	CMD-C2D	-2.03	1.46	1.50
23	B	607	CLA	CHC-C1C	2.03	1.42	1.38
23	c	504	CLA	CMB-C2B	-2.03	1.46	1.50
23	N	602	CLA	CMC-C2C	-2.03	1.46	1.50
35	s	606	CHL	CHC-C1C	2.03	1.42	1.38
23	B	611	CLA	CMD-C2D	-2.03	1.46	1.50
23	c	504	CLA	CMD-C2D	-2.03	1.46	1.50
23	b	603	CLA	CHC-C1C	2.03	1.42	1.38
23	S	311	CLA	CHC-C1C	2.03	1.42	1.38
23	G	602	CLA	CHC-C1C	2.02	1.42	1.38
23	g	602	CLA	CMC-C2C	-2.02	1.46	1.50
24	A	403	PHO	C3B-C2B	-2.02	1.37	1.40
23	Y	311	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	501	CLA	CMC-C2C	-2.02	1.46	1.50
23	y	303	CLA	CMD-C2D	-2.02	1.46	1.50
23	s	603	CLA	CHC-C1C	2.02	1.42	1.38
23	s	610	CLA	CMB-C2B	-2.02	1.46	1.50
23	S	312	CLA	CHC-C1C	2.02	1.42	1.38
23	c	513	CLA	CMC-C2C	-2.02	1.46	1.50
35	G	609	CHL	CMD-C2D	-2.02	1.46	1.50
23	s	604	CLA	CHC-C1C	2.02	1.42	1.38
35	Y	302	CHL	CMB-C2B	-2.02	1.46	1.50
23	s	602	CLA	CHC-C1C	2.02	1.42	1.38
23	Y	305	CLA	CHC-C1C	2.02	1.42	1.38
23	C	507	CLA	CHC-C1C	2.02	1.42	1.38
23	y	312	CLA	CMD-C2D	-2.02	1.46	1.50
35	s	605	CHL	CMD-C2D	-2.02	1.46	1.50
23	N	613	CLA	CMD-C2D	-2.02	1.46	1.50
23	Y	311	CLA	CMB-C2B	-2.02	1.46	1.50
23	s	611	CLA	CMD-C2D	-2.02	1.46	1.50
23	y	311	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	605	CHL	CMB-C2B	-2.02	1.46	1.50
23	g	604	CLA	MG-NB	-2.02	2.01	2.05
23	c	511	CLA	CMD-C2D	-2.02	1.46	1.50
35	g	605	CHL	CMB-C2B	-2.02	1.46	1.50
23	G	610	CLA	CMB-C2B	-2.02	1.46	1.50
23	C	505	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	617	CLA	CMB-C2B	-2.02	1.46	1.50
23	s	609	CLA	CMB-C2B	-2.02	1.46	1.50
23	s	613	CLA	CHC-C1C	2.02	1.42	1.38
23	n	614	CLA	CHC-C1C	2.02	1.42	1.38
35	Y	310	CHL	MG-NB	-2.02	2.01	2.05
23	y	313	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	608	CLA	MG-NB	-2.01	2.01	2.05
23	S	312	CLA	CMD-C2D	-2.01	1.46	1.50
23	B	611	CLA	CHC-C1C	2.01	1.42	1.38
23	S	311	CLA	CMD-C2D	-2.01	1.46	1.50
35	Y	306	CHL	CMD-C2D	-2.01	1.46	1.50
35	g	605	CHL	CMD-C2D	-2.01	1.46	1.50
23	y	305	CLA	CHC-C1C	2.01	1.42	1.38
23	y	305	CLA	MG-NB	-2.01	2.01	2.05
23	G	613	CLA	CMB-C2B	-2.01	1.46	1.50
23	S	310	CLA	CMC-C2C	-2.01	1.46	1.50
35	R	307	CHL	CMD-C2D	-2.01	1.46	1.50
23	Y	314	CLA	CMB-C2B	-2.01	1.46	1.50
23	y	305	CLA	CMD-C2D	-2.01	1.46	1.50
33	d	406	PL9	C42-C43	2.01	1.57	1.50
23	S	309	CLA	CHC-C1C	2.01	1.42	1.38
23	d	404	CLA	CMD-C2D	-2.01	1.46	1.50
23	S	305	CLA	CMD-C2D	-2.01	1.46	1.50
23	N	614	CLA	CHC-C1C	2.01	1.42	1.38
23	g	612	CLA	CMC-C2C	-2.01	1.46	1.50
23	S	303	CLA	CHC-C1C	2.01	1.42	1.38
23	c	508	CLA	CHC-C1C	2.01	1.42	1.38
35	g	605	CHL	CHC-C1C	2.01	1.42	1.38
23	C	514	CLA	CMC-C2C	-2.01	1.46	1.50
23	C	510	CLA	CHC-C1C	2.01	1.42	1.38
23	R	305	CLA	CHC-C1C	2.01	1.42	1.38
23	G	602	CLA	CMB-C2B	-2.01	1.46	1.50
23	R	304	CLA	CHC-C1C	2.01	1.42	1.38
23	G	604	CLA	CMD-C2D	-2.01	1.46	1.50
23	c	512	CLA	CMD-C2D	-2.01	1.46	1.50
23	s	604	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	311	CLA	CMD-C2D	-2.00	1.46	1.50
35	g	607	CHL	CMB-C2B	-2.00	1.46	1.50
23	n	610	CLA	CHC-C1C	2.00	1.42	1.38
23	n	614	CLA	CMD-C2D	-2.00	1.46	1.50
23	N	612	CLA	CMB-C2B	-2.00	1.46	1.50
35	s	605	CHL	CMB-C2B	-2.00	1.46	1.50
23	R	312	CLA	CMD-C2D	-2.00	1.46	1.50
23	g	612	CLA	CHC-C1C	2.00	1.42	1.38
33	D	406	PL9	C42-C43	2.00	1.56	1.50
23	r	611	CLA	CMB-C2B	-2.00	1.46	1.50
23	n	612	CLA	CMB-C2B	-2.00	1.46	1.50
35	g	608	CHL	CMB-C2B	-2.00	1.46	1.50
23	G	611	CLA	CMB-C2B	-2.00	1.46	1.50
23	c	503	CLA	CMB-C2B	-2.00	1.46	1.50
23	s	604	CLA	CMC-C2C	-2.00	1.46	1.50
23	D	401	CLA	MG-NB	-2.00	2.01	2.05
23	b	605	CLA	CMC-C2C	-2.00	1.46	1.50
23	g	604	CLA	CMD-C2D	-2.00	1.46	1.50
35	n	605	CHL	CHC-C1C	2.00	1.42	1.38
23	B	605	CLA	CMB-C2B	-2.00	1.46	1.50
23	s	611	CLA	CMB-C2B	-2.00	1.46	1.50
23	n	612	CLA	CMD-C2D	-2.00	1.46	1.50
23	S	314	CLA	CHC-C1C	2.00	1.42	1.38
23	s	610	CLA	CHC-C1C	2.00	1.42	1.38
35	N	606	CHL	CMB-C2B	-2.00	1.46	1.50

All (2385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	625	SQD	O9-S-C6	-20.17	82.96	106.94
26	C	521	SQD	O9-S-C6	-20.02	83.14	106.94
26	c	520	SQD	O9-S-C6	-19.99	83.18	106.94
26	b	602	SQD	O9-S-C6	-19.91	83.27	106.94
38	R	301	NEX	C17-C1-C6	-17.45	94.86	110.47
38	Y	318	NEX	C17-C1-C6	-17.35	94.94	110.47
26	C	521	SQD	O8-S-O9	-11.90	82.21	111.27
26	c	520	SQD	O8-S-O9	-11.86	82.29	111.27
26	b	602	SQD	O8-S-O9	-11.63	82.86	111.27
26	B	625	SQD	O8-S-O9	-11.52	83.12	111.27
26	B	625	SQD	O7-S-C6	9.73	118.51	106.94
38	R	301	NEX	C16-C1-C6	9.72	119.17	110.47
26	b	602	SQD	O7-S-C6	9.63	118.38	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	521	SQD	O7-S-C6	9.53	118.27	106.94
26	c	520	SQD	O7-S-C6	9.52	118.25	106.94
38	Y	318	NEX	C16-C1-C6	9.38	118.87	110.47
24	A	403	PHO	C4D-CHA-CBD	-9.33	104.30	108.52
38	g	618	NEX	O24-C25-C24	9.28	120.36	113.38
38	s	616	NEX	O24-C25-C24	9.27	120.35	113.38
24	a	402	PHO	C4D-CHA-CBD	-9.25	104.33	108.52
33	D	406	PL9	C7-C8-C9	-9.19	111.50	126.79
33	d	406	PL9	C7-C8-C9	-9.16	111.55	126.79
26	B	625	SQD	O9-S-O7	-8.98	82.88	113.95
38	N	617	NEX	O24-C25-C24	8.93	120.09	113.38
26	b	602	SQD	O9-S-O7	-8.91	83.12	113.95
38	Y	318	NEX	C17-C1-C16	-8.76	81.63	108.53
26	C	521	SQD	O9-S-O7	-8.76	83.64	113.95
38	R	301	NEX	C17-C1-C16	-8.76	81.65	108.53
26	c	520	SQD	O9-S-O7	-8.75	83.68	113.95
38	n	617	NEX	O24-C25-C24	8.73	119.94	113.38
38	G	618	NEX	O24-C25-C24	8.68	119.90	113.38
38	R	316	NEX	O24-C25-C24	8.62	119.86	113.38
38	Y	318	NEX	O24-C25-C24	8.45	119.73	113.38
38	r	615	NEX	O24-C25-C24	8.40	119.69	113.38
38	R	301	NEX	O24-C25-C24	8.38	119.68	113.38
24	D	402	PHO	C4D-CHA-CBD	-8.33	104.75	108.52
24	a	403	PHO	C4D-CHA-CBD	-8.25	104.78	108.52
26	c	520	SQD	O8-S-C6	8.19	118.80	105.74
38	S	317	NEX	O24-C25-C24	8.19	119.53	113.38
26	C	521	SQD	O8-S-C6	8.18	118.77	105.74
37	y	301	XAT	O24-C25-C24	8.09	119.46	113.38
26	b	602	SQD	O8-S-C6	8.08	118.61	105.74
26	B	625	SQD	O8-S-C6	8.02	118.52	105.74
37	Y	301	XAT	O24-C25-C24	7.86	119.29	113.38
37	Y	301	XAT	O4-C5-C4	7.85	119.28	113.38
37	y	301	XAT	O4-C5-C4	7.84	119.27	113.38
37	g	617	XAT	O24-C25-C24	7.70	119.17	113.38
37	G	617	XAT	O24-C25-C24	7.67	119.14	113.38
35	G	609	CHL	C4A-NA-C1A	7.65	110.14	106.71
23	b	618	CLA	C4A-NA-C1A	7.64	110.14	106.71
23	B	616	CLA	C4A-NA-C1A	7.27	109.97	106.71
37	R	315	XAT	O4-C5-C4	7.22	118.81	113.38
35	Y	310	CHL	C4A-NA-C1A	7.22	109.95	106.71
35	N	609	CHL	C4A-NA-C1A	7.14	109.92	106.71
37	G	617	XAT	O4-C5-C4	7.09	118.71	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	r	614	XAT	O24-C25-C24	7.09	118.71	113.38
35	y	310	CHL	C4A-NA-C1A	7.07	109.89	106.71
23	b	614	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	B	612	CLA	C4A-NA-C1A	7.05	109.88	106.71
37	g	620	XAT	O24-C25-C24	7.02	118.66	113.38
23	C	503	CLA	C4A-NA-C1A	7.00	109.85	106.71
37	G	620	XAT	O24-C25-C24	6.99	118.64	113.38
23	c	502	CLA	C4A-NA-C1A	6.98	109.84	106.71
37	r	614	XAT	O4-C5-C4	6.96	118.61	113.38
23	b	607	CLA	C4A-NA-C1A	6.95	109.83	106.71
38	Y	318	NEX	C2-C1-C6	6.93	115.95	109.21
33	D	406	PL9	C17-C18-C19	-6.87	111.12	127.66
37	g	617	XAT	O4-C5-C4	6.86	118.54	113.38
33	d	406	PL9	C17-C18-C19	-6.84	111.19	127.66
35	n	609	CHL	C4A-NA-C1A	6.83	109.78	106.71
23	C	508	CLA	C4A-NA-C1A	6.81	109.77	106.71
23	n	611	CLA	C4A-NA-C1A	6.78	109.75	106.71
35	n	607	CHL	C4A-NA-C1A	6.72	109.73	106.71
23	c	507	CLA	C4A-NA-C1A	6.72	109.72	106.71
23	N	611	CLA	C4A-NA-C1A	6.71	109.72	106.71
38	R	301	NEX	C2-C1-C6	6.68	115.71	109.21
37	R	315	XAT	O24-C25-C24	6.66	118.39	113.38
23	B	605	CLA	C4A-NA-C1A	6.64	109.69	106.71
35	y	308	CHL	C4A-NA-C1A	6.55	109.65	106.71
23	s	612	CLA	C4A-NA-C1A	6.51	109.63	106.71
35	Y	308	CHL	C4A-NA-C1A	6.47	109.62	106.71
35	N	607	CHL	C4A-NA-C1A	6.45	109.61	106.71
23	S	313	CLA	C4A-NA-C1A	6.42	109.59	106.71
23	b	606	CLA	C4A-NA-C1A	6.33	109.55	106.71
23	r	611	CLA	C4A-NA-C1A	6.29	109.53	106.71
23	C	511	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	d	401	CLA	C4A-NA-C1A	6.28	109.53	106.71
23	B	604	CLA	C4A-NA-C1A	6.27	109.52	106.71
33	D	406	PL9	C15-C14-C13	-6.24	107.66	123.68
33	d	406	PL9	C15-C14-C13	-6.24	107.67	123.68
23	R	310	CLA	C4A-NA-C1A	6.23	109.51	106.71
33	D	406	PL9	C12-C13-C14	-6.23	112.66	127.66
35	s	606	CHL	C4A-NA-C1A	6.21	109.50	106.71
33	D	406	PL9	C11-C9-C8	-6.20	108.56	121.12
33	d	406	PL9	C22-C23-C24	-6.20	112.74	127.66
23	D	401	CLA	C4A-NA-C1A	6.19	109.49	106.71
33	d	406	PL9	C12-C13-C14	-6.19	112.75	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	406	PL9	C11-C9-C8	-6.18	108.62	121.12
23	G	613	CLA	C4A-NA-C1A	6.17	109.48	106.71
33	D	406	PL9	C22-C23-C24	-6.17	112.81	127.66
23	G	611	CLA	C4A-NA-C1A	6.16	109.47	106.71
23	C	507	CLA	C4A-NA-C1A	6.15	109.47	106.71
23	g	611	CLA	C4A-NA-C1A	6.11	109.45	106.71
23	C	505	CLA	C4A-NA-C1A	6.10	109.45	106.71
23	C	510	CLA	C4A-NA-C1A	6.07	109.44	106.71
33	D	406	PL9	C27-C28-C29	-6.07	113.06	127.66
23	c	504	CLA	C4A-NA-C1A	6.06	109.43	106.71
23	g	613	CLA	C4A-NA-C1A	6.06	109.43	106.71
33	d	406	PL9	C27-C28-C29	-6.05	113.10	127.66
23	b	617	CLA	C4A-NA-C1A	6.05	109.42	106.71
23	b	615	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	c	512	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	y	314	CLA	C4A-NA-C1A	6.03	109.42	106.71
23	c	509	CLA	C4A-NA-C1A	6.03	109.42	106.71
35	g	607	CHL	C4A-NA-C1A	6.02	109.41	106.71
23	Y	312	CLA	C4A-NA-C1A	6.01	109.41	106.71
23	c	510	CLA	C4A-NA-C1A	6.01	109.41	106.71
23	c	511	CLA	C4A-NA-C1A	5.98	109.40	106.71
23	Y	314	CLA	C4A-NA-C1A	5.98	109.39	106.71
23	B	613	CLA	C4A-NA-C1A	5.97	109.39	106.71
23	y	312	CLA	C4A-NA-C1A	5.97	109.39	106.71
23	R	312	CLA	C4A-NA-C1A	5.97	109.39	106.71
33	d	406	PL9	C32-C33-C34	-5.96	113.30	127.66
23	d	404	CLA	C4A-NA-C1A	5.96	109.39	106.71
23	c	506	CLA	C4A-NA-C1A	5.95	109.38	106.71
23	s	604	CLA	C4A-NA-C1A	5.94	109.38	106.71
23	R	304	CLA	C4A-NA-C1A	5.93	109.37	106.71
23	B	615	CLA	C4A-NA-C1A	5.93	109.37	106.71
33	d	406	PL9	C37-C38-C39	-5.92	113.40	127.66
23	B	609	CLA	C4A-NA-C1A	5.92	109.37	106.71
33	D	406	PL9	C32-C33-C34	-5.92	113.42	127.66
33	D	406	PL9	C37-C38-C39	-5.91	113.42	127.66
23	r	604	CLA	C4A-NA-C1A	5.91	109.36	106.71
23	C	512	CLA	C4A-NA-C1A	5.90	109.36	106.71
23	D	404	CLA	C4A-NA-C1A	5.89	109.35	106.71
23	R	305	CLA	C4A-NA-C1A	5.83	109.33	106.71
23	b	612	CLA	C4A-NA-C1A	5.82	109.32	106.71
23	b	611	CLA	C4A-NA-C1A	5.82	109.32	106.71
23	n	613	CLA	C4A-NA-C1A	5.82	109.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	C4A-NA-C1A	5.80	109.31	106.71
35	Y	307	CHL	C4A-NA-C1A	5.79	109.31	106.71
35	n	605	CHL	C4A-NA-C1A	5.79	109.31	106.71
35	S	307	CHL	C4A-NA-C1A	5.78	109.30	106.71
35	n	601	CHL	C4A-NA-C1A	5.77	109.30	106.71
23	N	612	CLA	C4A-NA-C1A	5.77	109.30	106.71
33	d	406	PL9	C42-C43-C44	-5.76	113.78	127.66
37	g	620	XAT	O4-C5-C4	5.76	117.71	113.38
23	N	613	CLA	C4A-NA-C1A	5.75	109.29	106.71
23	b	608	CLA	C4A-NA-C1A	5.74	109.29	106.71
23	r	601	CLA	C4A-NA-C1A	5.74	109.29	106.71
35	s	601	CHL	C4A-NA-C1A	5.73	109.28	106.71
33	D	406	PL9	C42-C43-C44	-5.73	113.87	127.66
35	N	601	CHL	C4A-NA-C1A	5.71	109.27	106.71
35	s	605	CHL	C4A-NA-C1A	5.71	109.27	106.71
23	r	608	CLA	C4A-NA-C1A	5.71	109.27	106.71
35	S	302	CHL	C4A-NA-C1A	5.70	109.27	106.71
23	s	610	CLA	C4A-NA-C1A	5.69	109.26	106.71
23	b	609	CLA	C4A-NA-C1A	5.67	109.26	106.71
23	B	606	CLA	C4A-NA-C1A	5.66	109.25	106.71
23	Y	304	CLA	C4A-NA-C1A	5.66	109.25	106.71
23	d	403	CLA	C4A-NA-C1A	5.66	109.25	106.71
35	y	307	CHL	C4A-NA-C1A	5.66	109.25	106.71
23	S	312	CLA	C4A-NA-C1A	5.64	109.24	106.71
23	D	403	CLA	C4A-NA-C1A	5.64	109.24	106.71
23	C	513	CLA	C4A-NA-C1A	5.61	109.23	106.71
23	a	404	CLA	C4A-NA-C1A	5.61	109.23	106.71
23	A	404	CLA	C4A-NA-C1A	5.61	109.23	106.71
38	g	618	NEX	C11-C10-C9	-5.58	119.35	127.31
33	D	406	PL9	C36-C34-C33	-5.58	109.83	121.12
35	N	605	CHL	C4A-NA-C1A	5.57	109.21	106.71
23	r	610	CLA	C4A-NA-C1A	5.57	109.21	106.71
33	D	406	PL9	C16-C14-C13	-5.56	109.86	121.12
23	b	613	CLA	C4A-NA-C1A	5.55	109.20	106.71
35	G	607	CHL	C4A-NA-C1A	5.55	109.20	106.71
35	R	308	CHL	C4A-NA-C1A	5.55	109.20	106.71
23	B	611	CLA	C4A-NA-C1A	5.54	109.20	106.71
37	G	620	XAT	O4-C5-C4	5.54	117.55	113.38
23	B	610	CLA	C4A-NA-C1A	5.54	109.20	106.71
23	R	309	CLA	C4A-NA-C1A	5.53	109.19	106.71
23	C	504	CLA	C4A-NA-C1A	5.52	109.19	106.71
33	d	406	PL9	C16-C14-C13	-5.52	109.95	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	N	603	CLA	C4A-NA-C1A	5.49	109.17	106.71
23	R	302	CLA	C4A-NA-C1A	5.49	109.17	106.71
23	R	311	CLA	C4A-NA-C1A	5.48	109.17	106.71
33	d	406	PL9	C10-C9-C8	-5.47	109.64	123.68
23	s	603	CLA	C4A-NA-C1A	5.47	109.17	106.71
33	D	406	PL9	C10-C9-C8	-5.46	109.67	123.68
23	N	604	CLA	C4A-NA-C1A	5.46	109.16	106.71
23	S	303	CLA	C4A-NA-C1A	5.46	109.16	106.71
23	r	603	CLA	C4A-NA-C1A	5.44	109.15	106.71
32	C	520	DMU	O7-C10-C5	5.44	122.19	108.10
38	R	301	NEX	C17-C1-C2	-5.43	84.65	109.05
33	D	406	PL9	C46-C44-C43	-5.43	110.13	121.12
38	Y	318	NEX	C17-C1-C2	-5.43	84.67	109.05
23	n	612	CLA	C4A-NA-C1A	5.43	109.15	106.71
23	G	604	CLA	C4A-NA-C1A	5.42	109.14	106.71
23	r	612	CLA	C4A-NA-C1A	5.41	109.14	106.71
33	d	406	PL9	C36-C34-C33	-5.40	110.18	121.12
23	d	402	CLA	C4A-NA-C1A	5.38	109.13	106.71
33	d	406	PL9	C46-C44-C43	-5.38	110.23	121.12
23	R	303	CLA	C4A-NA-C1A	5.36	109.12	106.71
35	g	601	CHL	C4A-NA-C1A	5.35	109.11	106.71
35	Y	302	CHL	C4A-NA-C1A	5.34	109.11	106.71
23	c	503	CLA	C4A-NA-C1A	5.33	109.10	106.71
23	y	304	CLA	C4A-NA-C1A	5.32	109.10	106.71
23	A	402	CLA	C4A-NA-C1A	5.30	109.09	106.71
32	C	520	DMU	C10-O7-C3	5.29	131.05	117.96
23	r	602	CLA	C4A-NA-C1A	5.28	109.08	106.71
23	b	610	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	D	405	BCR	C28-C27-C26	-5.26	104.69	114.08
24	A	403	PHO	C2B-C1B-NB	-5.26	105.90	109.53
23	a	401	CLA	C4A-NA-C1A	5.25	109.07	106.71
25	d	405	BCR	C28-C27-C26	-5.25	104.70	114.08
23	s	608	CLA	C4A-NA-C1A	5.25	109.07	106.71
33	d	406	PL9	C35-C34-C33	-5.25	110.21	123.68
23	S	311	CLA	C4A-NA-C1A	5.24	109.06	106.71
35	G	601	CHL	C4A-NA-C1A	5.24	109.06	106.71
24	a	402	PHO	C2B-C1B-NB	-5.23	105.91	109.53
35	y	302	CHL	C4A-NA-C1A	5.23	109.06	106.71
23	n	602	CLA	C4A-NA-C1A	5.22	109.06	106.71
23	A	401	CLA	C4A-NA-C1A	5.22	109.05	106.71
23	S	305	CLA	C4A-NA-C1A	5.20	109.05	106.71
35	Y	309	CHL	C4A-NA-C1A	5.20	109.05	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	406	PL9	C35-C34-C33	-5.20	110.34	123.68
23	Y	313	CLA	C4A-NA-C1A	5.20	109.04	106.71
23	n	603	CLA	C4A-NA-C1A	5.19	109.04	106.71
35	r	607	CHL	C4A-NA-C1A	5.19	109.04	106.71
25	k	101	BCR	C3-C4-C5	-5.19	104.82	114.08
23	S	304	CLA	C4A-NA-C1A	5.17	109.03	106.71
38	g	618	NEX	C15-C14-C13	-5.16	119.94	127.31
33	D	406	PL9	C41-C39-C38	-5.16	110.67	121.12
32	c	519	DMU	C10-O7-C3	5.16	130.73	117.96
23	y	303	CLA	C4A-NA-C1A	5.15	109.02	106.71
23	g	602	CLA	C4A-NA-C1A	5.14	109.02	106.71
38	G	618	NEX	C15-C14-C13	-5.11	120.02	127.31
23	g	604	CLA	C4A-NA-C1A	5.11	109.00	106.71
23	n	604	CLA	C4A-NA-C1A	5.10	109.00	106.71
23	c	501	CLA	C4A-NA-C1A	5.08	108.99	106.71
37	G	620	XAT	C38-C25-C26	-5.08	113.74	122.26
35	y	309	CHL	C4A-NA-C1A	5.08	108.99	106.71
23	Y	303	CLA	C4A-NA-C1A	5.07	108.98	106.71
33	d	406	PL9	C45-C44-C43	-5.06	110.69	123.68
24	a	403	PHO	C2D-C1D-ND	-5.06	106.03	109.53
23	G	612	CLA	C4A-NA-C1A	5.06	108.98	106.71
23	y	305	CLA	C4A-NA-C1A	5.06	108.98	106.71
37	G	620	XAT	C18-C5-C6	-5.06	113.78	122.26
33	D	406	PL9	C45-C44-C43	-5.04	110.75	123.68
23	R	313	CLA	C4A-NA-C1A	5.04	108.97	106.71
37	g	620	XAT	C38-C25-C26	-5.03	113.83	122.26
23	g	612	CLA	C4A-NA-C1A	5.03	108.97	106.71
23	Y	305	CLA	C4A-NA-C1A	5.02	108.97	106.71
23	g	603	CLA	C4A-NA-C1A	5.02	108.96	106.71
37	R	315	XAT	C38-C25-C26	-5.01	113.86	122.26
37	g	620	XAT	C18-C5-C6	-5.01	113.86	122.26
23	S	314	CLA	C4A-NA-C1A	5.01	108.96	106.71
32	c	519	DMU	O7-C10-C5	5.01	121.08	108.10
23	s	602	CLA	C4A-NA-C1A	4.98	108.95	106.71
33	d	406	PL9	C41-C39-C38	-4.98	111.04	121.12
23	s	609	CLA	C4A-NA-C1A	4.96	108.94	106.71
23	s	613	CLA	C4A-NA-C1A	4.96	108.94	106.71
23	b	605	CLA	C4A-NA-C1A	4.96	108.94	106.71
38	S	317	NEX	C11-C10-C9	-4.96	120.24	127.31
23	B	603	CLA	C4A-NA-C1A	4.94	108.93	106.71
35	N	608	CHL	C4A-NA-C1A	4.94	108.93	106.71
23	s	611	CLA	C4A-NA-C1A	4.93	108.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	G	620	XAT	O4-C5-C18	4.92	120.95	115.06
25	K	101	BCR	C3-C4-C5	-4.90	105.32	114.08
23	y	315	CLA	C4A-NA-C1A	4.89	108.91	106.71
23	r	609	CLA	C4A-NA-C1A	4.89	108.91	106.71
33	D	406	PL9	C40-C39-C38	-4.89	111.14	123.68
35	S	306	CHL	C4A-NA-C1A	4.88	108.90	106.71
23	Y	315	CLA	C4A-NA-C1A	4.87	108.90	106.71
23	G	602	CLA	C4A-NA-C1A	4.86	108.89	106.71
37	G	617	XAT	C38-C25-C26	-4.85	114.13	122.26
37	g	620	XAT	O4-C5-C18	4.85	120.86	115.06
23	y	313	CLA	C4A-NA-C1A	4.84	108.88	106.71
37	R	315	XAT	C6-C7-C8	-4.83	115.77	125.99
37	g	617	XAT	C38-C25-C26	-4.82	114.19	122.26
37	r	614	XAT	C18-C5-C6	-4.80	114.22	122.26
38	G	618	NEX	C11-C10-C9	-4.80	120.46	127.31
25	D	405	BCR	C7-C8-C9	-4.79	118.99	126.23
24	A	403	PHO	C2D-C1D-ND	-4.79	106.22	109.53
23	G	610	CLA	C4A-NA-C1A	4.78	108.86	106.71
37	r	614	XAT	C38-C25-C26	-4.77	114.26	122.26
25	C	519	BCR	C7-C8-C9	-4.76	119.05	126.23
37	r	614	XAT	O4-C5-C18	4.75	120.75	115.06
23	B	608	CLA	C4A-NA-C1A	4.75	108.84	106.71
25	d	405	BCR	C7-C8-C9	-4.75	119.06	126.23
37	r	614	XAT	C6-C7-C8	-4.73	115.99	125.99
37	g	617	XAT	C18-C5-C6	-4.73	114.34	122.26
33	d	406	PL9	C40-C39-C38	-4.72	111.56	123.68
23	c	508	CLA	C4A-NA-C1A	4.72	108.83	106.71
24	D	402	PHO	C2D-C1D-ND	-4.71	106.27	109.53
23	N	602	CLA	C4A-NA-C1A	4.71	108.82	106.71
38	r	615	NEX	C11-C10-C9	-4.70	120.60	127.31
37	R	315	XAT	O24-C25-C38	4.70	120.69	115.06
35	N	605	CHL	O2D-CGD-O1D	-4.70	114.65	123.84
37	R	315	XAT	C18-C5-C6	-4.69	114.39	122.26
33	D	406	PL9	C21-C19-C18	-4.69	111.62	121.12
23	C	502	CLA	C4A-NA-C1A	4.68	108.81	106.71
23	S	309	CLA	C4A-NA-C1A	4.67	108.81	106.71
23	C	509	CLA	C4A-NA-C1A	4.67	108.81	106.71
24	a	402	PHO	C2D-C1D-ND	-4.66	106.31	109.53
24	a	403	PHO	C2B-C1B-NB	-4.65	106.32	109.53
23	g	610	CLA	C4A-NA-C1A	4.65	108.80	106.71
31	D	408	LHG	O7-C7-C8	4.65	121.52	111.50
37	y	301	XAT	C18-C5-C6	-4.64	114.48	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	406	PL9	C20-C19-C18	-4.64	111.77	123.68
23	b	603	CLA	C4A-NA-C1A	4.64	108.79	106.71
31	d	408	LHG	O7-C7-C8	4.64	121.50	111.50
37	Y	301	XAT	C18-C5-C6	-4.64	114.49	122.26
35	G	606	CHL	C4A-NA-C1A	4.64	108.79	106.71
33	d	406	PL9	C20-C19-C18	-4.63	111.79	123.68
33	d	406	PL9	C21-C19-C18	-4.63	111.74	121.12
33	D	406	PL9	C30-C29-C28	-4.63	111.81	123.68
33	d	406	PL9	C30-C29-C28	-4.61	111.84	123.68
37	G	617	XAT	C18-C5-C6	-4.61	114.53	122.26
35	G	608	CHL	C4A-NA-C1A	4.61	108.78	106.71
35	R	306	CHL	C4A-NA-C1A	4.60	108.77	106.71
23	B	601	CLA	C4A-NA-C1A	4.60	108.77	106.71
33	d	406	PL9	C31-C29-C28	-4.59	111.82	121.12
37	R	315	XAT	O4-C5-C18	4.59	120.55	115.06
35	n	608	CHL	C4A-NA-C1A	4.56	108.75	106.71
37	Y	301	XAT	C38-C25-C26	-4.55	114.63	122.26
33	D	406	PL9	C47-C48-C49	-4.55	112.20	127.75
24	D	402	PHO	C2B-C1B-NB	-4.52	106.40	109.53
37	y	301	XAT	C38-C25-C26	-4.52	114.68	122.26
35	r	605	CHL	C4A-NA-C1A	4.52	108.74	106.71
33	d	406	PL9	C47-C48-C49	-4.49	112.41	127.75
38	n	617	NEX	C38-C25-C26	-4.49	114.74	122.26
33	D	406	PL9	C26-C24-C23	-4.49	112.04	121.12
23	C	514	CLA	C4A-NA-C1A	4.48	108.72	106.71
33	D	406	PL9	C45-C44-C46	-4.47	107.75	115.27
23	C	507	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
38	R	316	NEX	C11-C10-C9	-4.47	120.94	127.31
38	r	615	NEX	C38-C25-C26	-4.47	114.78	122.26
33	d	406	PL9	C45-C44-C46	-4.46	107.76	115.27
38	S	317	NEX	C38-C25-C26	-4.46	114.78	122.26
38	Y	318	NEX	C38-C25-C26	-4.46	114.78	122.26
37	G	620	XAT	O24-C25-C38	4.46	120.40	115.06
33	d	406	PL9	C26-C24-C23	-4.46	112.10	121.12
37	g	620	XAT	O24-C25-C38	4.46	120.39	115.06
25	c	518	BCR	C28-C27-C26	-4.45	106.13	114.08
38	R	316	NEX	C15-C14-C13	-4.45	120.96	127.31
25	C	519	BCR	C28-C27-C26	-4.44	106.15	114.08
23	G	603	CLA	C4A-NA-C1A	4.43	108.70	106.71
33	D	406	PL9	C31-C29-C28	-4.42	112.18	121.12
23	n	614	CLA	C4A-NA-C1A	4.42	108.69	106.71
38	R	316	NEX	C38-C25-C26	-4.41	114.86	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	R	301	NEX	C38-C25-C26	-4.41	114.87	122.26
38	N	617	NEX	C38-C25-C26	-4.37	114.94	122.26
33	d	406	PL9	C25-C24-C23	-4.36	112.49	123.68
31	n	618	LHG	O7-C7-C8	4.35	120.89	111.50
23	N	614	CLA	C4A-NA-C1A	4.35	108.66	106.71
23	g	614	CLA	C4A-NA-C1A	4.35	108.66	106.71
33	D	406	PL9	C25-C24-C23	-4.35	112.53	123.68
38	s	616	NEX	C27-C28-C29	-4.34	118.79	125.53
37	G	617	XAT	O24-C25-C38	4.34	120.26	115.06
23	c	513	CLA	C4A-NA-C1A	4.34	108.66	106.71
35	r	606	CHL	C4A-NA-C1A	4.33	108.65	106.71
23	S	310	CLA	C4A-NA-C1A	4.33	108.65	106.71
38	g	618	NEX	C38-C25-C26	-4.33	115.01	122.26
37	g	617	XAT	O24-C25-C38	4.32	120.23	115.06
38	r	615	NEX	C15-C14-C13	-4.31	121.16	127.31
37	g	617	XAT	O4-C5-C18	4.30	120.21	115.06
23	c	505	CLA	C4A-NA-C1A	4.30	108.64	106.71
38	s	616	NEX	C38-C25-C26	-4.27	115.10	122.26
37	r	614	XAT	C26-C27-C28	-4.26	116.98	125.99
28	C	517	DGD	O2G-C1B-C2B	4.26	120.67	111.50
23	n	610	CLA	C4A-NA-C1A	4.24	108.61	106.71
37	g	617	XAT	C15-C14-C13	-4.24	121.27	127.31
35	N	606	CHL	C4A-NA-C1A	4.24	108.61	106.71
31	N	618	LHG	O7-C7-C8	4.23	120.61	111.50
35	R	307	CHL	C4A-NA-C1A	4.22	108.60	106.71
38	G	618	NEX	C38-C25-C26	-4.20	115.21	122.26
38	s	616	NEX	C11-C10-C9	-4.20	121.31	127.31
25	C	519	BCR	C24-C23-C22	-4.19	119.90	126.23
35	g	605	CHL	C4A-NA-C1A	4.19	108.59	106.71
37	G	620	XAT	C15-C14-C13	-4.18	121.34	127.31
37	y	301	XAT	O4-C5-C18	4.18	120.06	115.06
25	c	518	BCR	C24-C23-C22	-4.17	119.93	126.23
23	C	506	CLA	C4A-NA-C1A	4.17	108.58	106.71
36	r	613	LUT	C7-C8-C9	-4.17	119.94	126.23
38	Y	318	NEX	C15-C14-C13	-4.16	121.37	127.31
23	n	602	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
28	b	625	DGD	O2G-C1B-C2B	4.14	120.43	111.50
38	R	301	NEX	C15-C14-C13	-4.14	121.40	127.31
37	Y	301	XAT	O4-C5-C18	4.14	120.01	115.06
37	R	315	XAT	C26-C27-C28	-4.13	117.25	125.99
32	c	519	DMU	C10-O1-C9	4.13	121.80	113.69
35	n	605	CHL	O2D-CGD-O1D	-4.13	115.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	G	617	XAT	O4-C5-C18	4.13	120.00	115.06
23	G	614	CLA	C4A-NA-C1A	4.13	108.56	106.71
28	c	515	DGD	O2G-C1B-C2B	4.12	120.39	111.50
25	H	101	BCR	C16-C17-C18	-4.12	121.43	127.31
35	g	608	CHL	C4A-NA-C1A	4.11	108.56	106.71
38	s	616	NEX	C15-C14-C13	-4.11	121.45	127.31
25	C	516	BCR	C15-C14-C13	-4.10	121.45	127.31
31	g	619	LHG	O7-C7-C8	4.10	120.34	111.50
23	N	610	CLA	C4A-NA-C1A	4.10	108.55	106.71
25	h	101	BCR	C16-C17-C18	-4.10	121.46	127.31
25	c	514	BCR	C15-C14-C13	-4.10	121.46	127.31
37	g	620	XAT	C15-C14-C13	-4.10	121.46	127.31
31	G	619	LHG	O7-C7-C8	4.08	120.30	111.50
37	r	614	XAT	O24-C25-C38	4.08	119.95	115.06
26	l	101	SQD	O47-C7-C8	4.08	120.29	111.50
23	N	602	CLA	O2D-CGD-CBD	4.08	118.51	111.27
33	d	406	PL9	C51-C49-C48	-4.07	110.89	122.65
36	g	615	LUT	C35-C34-C33	-4.05	121.53	127.31
38	R	301	NEX	O24-C25-C38	4.04	119.90	115.06
25	B	618	BCR	C15-C14-C13	-4.04	121.55	127.31
28	A	408	DGD	O2G-C1B-C2B	4.03	120.20	111.50
33	D	406	PL9	C51-C49-C48	-4.03	110.99	122.65
37	G	617	XAT	C15-C14-C13	-4.03	121.56	127.31
37	Y	301	XAT	C35-C34-C33	-4.03	121.56	127.31
35	y	306	CHL	C4A-NA-C1A	4.03	108.52	106.71
27	a	408	BCT	O2-C-O1	4.02	129.98	119.55
23	c	513	CLA	CAA-C2A-C3A	-4.02	101.77	112.78
25	b	620	BCR	C15-C14-C13	-4.02	121.58	127.31
27	A	407	BCT	O2-C-O1	4.02	129.97	119.55
38	S	317	NEX	C27-C28-C29	-4.02	119.30	125.53
28	B	626	DGD	O2G-C1B-C2B	4.01	120.14	111.50
37	y	301	XAT	C26-C27-C28	-3.99	117.56	125.99
33	d	406	PL9	C50-C49-C48	-3.99	111.13	122.65
30	W	203	LMG	O7-C10-C11	3.98	120.09	111.50
33	D	406	PL9	C50-C49-C48	-3.98	111.13	122.65
23	N	602	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
25	k	101	BCR	C16-C17-C18	-3.98	121.63	127.31
30	C	522	LMG	O7-C10-C11	3.98	120.08	111.50
35	n	606	CHL	C4A-NA-C1A	3.98	108.49	106.71
37	g	617	XAT	C6-C7-C8	-3.98	117.58	125.99
35	g	606	CHL	C4A-NA-C1A	3.97	108.49	106.71
38	Y	318	NEX	O24-C25-C38	3.97	119.81	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	C4A-NA-C1A	3.97	108.49	106.71
25	h	101	BCR	C20-C21-C22	-3.97	121.65	127.31
26	a	406	SQD	O47-C7-C8	3.96	120.03	111.50
30	w	202	LMG	O7-C10-C11	3.96	120.03	111.50
25	H	101	BCR	C20-C21-C22	-3.95	121.67	127.31
38	n	617	NEX	C15-C14-C13	-3.95	121.67	127.31
38	N	617	NEX	C35-C34-C33	-3.95	121.68	127.31
38	N	617	NEX	C27-C28-C29	-3.94	119.41	125.53
37	y	301	XAT	C35-C34-C33	-3.94	121.68	127.31
38	r	615	NEX	C27-C28-C29	-3.94	119.42	125.53
37	g	620	XAT	C6-C7-C8	-3.93	117.68	125.99
31	r	616	LHG	O7-C7-C8	3.93	119.98	111.50
30	c	521	LMG	O7-C10-C11	3.93	119.97	111.50
37	G	620	XAT	C6-C7-C8	-3.93	117.69	125.99
25	D	405	BCR	C11-C10-C9	-3.92	121.71	127.31
38	S	317	NEX	O24-C25-C38	3.92	119.75	115.06
37	Y	301	XAT	C26-C27-C28	-3.91	117.72	125.99
25	h	101	BCR	C24-C23-C22	-3.91	120.33	126.23
25	H	101	BCR	C24-C23-C22	-3.91	120.33	126.23
25	b	619	BCR	C15-C14-C13	-3.91	121.73	127.31
25	K	101	BCR	C16-C17-C18	-3.91	121.73	127.31
38	R	301	NEX	C15-C35-C34	-3.90	115.48	123.47
37	G	617	XAT	C6-C7-C8	-3.90	117.75	125.99
26	A	406	SQD	O47-C7-C8	3.90	119.90	111.50
35	Y	306	CHL	C4A-NA-C1A	3.89	108.46	106.71
31	W	201	LHG	O7-C7-C8	3.89	119.89	111.50
25	B	617	BCR	C15-C14-C13	-3.89	121.76	127.31
25	d	405	BCR	C15-C14-C13	-3.89	121.76	127.31
25	D	405	BCR	C15-C14-C13	-3.89	121.77	127.31
23	n	602	CLA	O2D-CGD-CBD	3.89	118.17	111.27
38	R	316	NEX	C27-C28-C29	-3.88	119.51	125.53
25	d	405	BCR	C11-C10-C9	-3.88	121.77	127.31
35	G	605	CHL	C4A-NA-C1A	3.87	108.45	106.71
37	G	620	XAT	C26-C27-C28	-3.87	117.82	125.99
25	C	515	BCR	C7-C8-C9	-3.86	120.40	126.23
30	b	622	LMG	O7-C10-C11	3.86	119.82	111.50
23	b	603	CLA	CAA-C2A-C3A	-3.86	102.22	112.78
25	C	519	BCR	C15-C14-C13	-3.85	121.81	127.31
31	R	317	LHG	O7-C7-C8	3.85	119.80	111.50
25	C	519	BCR	C20-C21-C22	-3.85	121.82	127.31
38	r	615	NEX	O24-C25-C38	3.85	119.67	115.06
25	d	405	BCR	C24-C23-C22	-3.85	120.42	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	n	615	LUT	C35-C34-C33	-3.85	121.82	127.31
38	R	301	NEX	C11-C10-C9	-3.84	121.82	127.31
23	B	601	CLA	CAA-C2A-C3A	-3.84	102.26	112.78
31	c	516	LHG	O7-C7-C8	3.84	119.78	111.50
36	R	314	LUT	C7-C8-C9	-3.84	120.43	126.23
28	d	410	DGD	O2G-C1B-C2B	3.83	119.76	111.50
31	B	622	LHG	O7-C7-C8	3.83	119.76	111.50
25	z	101	BCR	C7-C8-C9	-3.83	120.45	126.23
30	B	620	LMG	O7-C10-C11	3.83	119.75	111.50
38	g	618	NEX	C31-C30-C29	-3.83	121.85	127.31
23	C	507	CLA	CMB-C2B-C1B	-3.82	119.55	125.37
38	N	617	NEX	C15-C14-C13	-3.82	121.86	127.31
25	B	617	BCR	C3-C4-C5	-3.82	107.25	114.08
31	b	624	LHG	O7-C7-C8	3.82	119.73	111.50
23	C	514	CLA	CAA-C2A-C3A	-3.82	102.32	112.78
38	n	617	NEX	C35-C34-C33	-3.81	121.87	127.31
30	D	409	LMG	O7-C10-C11	3.80	119.70	111.50
30	d	409	LMG	O7-C10-C11	3.80	119.69	111.50
26	L	103	SQD	O47-C7-C8	3.80	119.69	111.50
25	b	619	BCR	C3-C4-C5	-3.80	107.30	114.08
31	y	318	LHG	O7-C7-C8	3.80	119.68	111.50
36	s	614	LUT	C35-C34-C33	-3.78	121.91	127.31
36	G	615	LUT	C35-C34-C33	-3.78	121.91	127.31
23	B	614	CLA	C4A-NA-C1A	3.78	108.40	106.71
38	N	617	NEX	O24-C25-C38	3.77	119.58	115.06
31	Y	319	LHG	O7-C7-C8	3.77	119.63	111.50
38	R	316	NEX	O24-C25-C38	3.77	119.57	115.06
26	c	520	SQD	O47-C7-C8	3.76	119.61	111.50
25	D	405	BCR	C24-C23-C22	-3.76	120.55	126.23
37	g	620	XAT	C26-C27-C28	-3.76	118.04	125.99
38	Y	318	NEX	C15-C35-C34	-3.76	115.77	123.47
30	C	501	LMG	O7-C10-C11	3.75	119.58	111.50
25	z	101	BCR	C15-C14-C13	-3.75	121.96	127.31
23	Y	311	CLA	C4A-NA-C1A	3.75	108.39	106.71
38	n	617	NEX	O24-C25-C38	3.74	119.54	115.06
25	c	514	BCR	C11-C10-C9	-3.73	121.98	127.31
25	C	516	BCR	C11-C10-C9	-3.72	122.00	127.31
23	S	314	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
23	C	507	CLA	O2D-CGD-CBD	3.71	117.85	111.27
31	c	517	LHG	O7-C7-C8	3.70	119.48	111.50
25	b	621	BCR	C33-C5-C6	-3.69	120.39	124.53
38	R	301	NEX	C27-C28-C29	-3.68	119.81	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	S	317	NEX	C15-C14-C13	-3.68	122.06	127.31
25	d	405	BCR	C27-C26-C25	-3.68	117.39	122.73
31	b	623	LHG	O7-C7-C8	3.68	119.43	111.50
25	K	101	BCR	C15-C14-C13	-3.68	122.06	127.31
31	B	621	LHG	O7-C7-C8	3.68	119.42	111.50
30	b	601	LMG	O7-C10-C11	3.67	119.42	111.50
25	k	101	BCR	C15-C14-C13	-3.67	122.07	127.31
25	C	515	BCR	C15-C14-C13	-3.66	122.08	127.31
36	n	616	LUT	C35-C34-C33	-3.66	122.09	127.31
26	C	521	SQD	O47-C7-C8	3.66	119.39	111.50
36	r	613	LUT	C35-C34-C33	-3.66	122.09	127.31
38	Y	318	NEX	C27-C28-C29	-3.66	119.86	125.53
25	B	619	BCR	C33-C5-C6	-3.66	120.42	124.53
25	B	619	BCR	C16-C17-C18	-3.66	122.09	127.31
25	c	514	BCR	C7-C8-C9	-3.65	120.71	126.23
25	D	405	BCR	C27-C26-C25	-3.65	117.43	122.73
31	s	617	LHG	O7-C7-C8	3.65	119.36	111.50
30	a	407	LMG	O7-C10-C11	3.63	119.33	111.50
36	Y	316	LUT	C35-C34-C33	-3.63	122.13	127.31
28	D	410	DGD	O2G-C1B-C2B	3.63	119.32	111.50
36	N	615	LUT	C35-C34-C33	-3.63	122.13	127.31
25	c	518	BCR	C7-C8-C9	-3.62	120.76	126.23
30	B	623	LMG	O7-C10-C11	3.62	119.31	111.50
25	A	405	BCR	C16-C17-C18	-3.61	122.15	127.31
25	b	619	BCR	C16-C17-C18	-3.61	122.15	127.31
37	Y	301	XAT	O24-C25-C38	3.61	119.38	115.06
25	C	516	BCR	C7-C8-C9	-3.60	120.79	126.23
36	g	616	LUT	C15-C14-C13	-3.60	122.17	127.31
25	c	518	BCR	C15-C14-C13	-3.59	122.19	127.31
25	B	618	BCR	C24-C23-C22	-3.59	120.81	126.23
37	G	617	XAT	C26-C27-C28	-3.59	118.41	125.99
25	a	405	BCR	C16-C17-C18	-3.59	122.19	127.31
25	A	405	BCR	C15-C14-C13	-3.58	122.20	127.31
38	g	618	NEX	C15-C35-C34	-3.58	116.14	123.47
37	Y	301	XAT	C11-C10-C9	-3.58	122.20	127.31
38	G	618	NEX	C27-C28-C29	-3.57	119.99	125.53
31	l	102	LHG	O7-C7-C8	3.57	119.19	111.50
25	a	405	BCR	C7-C8-C9	-3.57	120.84	126.23
37	y	301	XAT	C11-C10-C9	-3.57	122.22	127.31
25	A	405	BCR	C7-C8-C9	-3.57	120.85	126.23
25	b	621	BCR	C15-C14-C13	-3.56	122.22	127.31
25	B	617	BCR	C16-C17-C18	-3.56	122.23	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	519	BCR	C11-C10-C9	-3.56	122.23	127.31
37	y	301	XAT	O24-C25-C38	3.56	119.32	115.06
36	R	314	LUT	C35-C34-C33	-3.56	122.23	127.31
36	S	316	LUT	C10-C11-C12	-3.55	112.12	123.22
34	f	101	HEM	C3B-C2B-C1B	3.55	109.12	106.49
36	y	316	LUT	C35-C34-C33	-3.55	122.24	127.31
25	a	405	BCR	C15-C14-C13	-3.55	122.24	127.31
23	s	613	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
38	g	618	NEX	C27-C28-C29	-3.55	120.02	125.53
31	S	318	LHG	O7-C7-C8	3.55	119.14	111.50
25	b	620	BCR	C24-C23-C22	-3.54	120.88	126.23
23	b	616	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
23	b	604	CLA	CAA-C2A-C3A	-3.54	103.09	112.78
38	g	618	NEX	O24-C25-C38	3.54	119.29	115.06
38	G	618	NEX	O24-C25-C38	3.53	119.29	115.06
31	L	101	LHG	O7-C7-C8	3.53	119.11	111.50
36	S	315	LUT	C35-C34-C33	-3.53	122.28	127.31
25	B	619	BCR	C15-C14-C13	-3.52	122.28	127.31
23	B	602	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
25	c	518	BCR	C20-C21-C22	-3.52	122.28	127.31
28	B	624	DGD	O2G-C1B-C2B	3.52	119.09	111.50
31	d	407	LHG	O7-C7-C8	3.52	119.08	111.50
31	D	407	LHG	O7-C7-C8	3.52	119.08	111.50
25	b	621	BCR	C16-C17-C18	-3.52	122.29	127.31
23	B	614	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
34	F	101	HEM	C3B-C2B-C1B	3.50	109.08	106.49
37	g	617	XAT	C31-C30-C29	-3.50	122.32	127.31
25	b	620	BCR	C3-C4-C5	-3.50	107.84	114.08
25	B	618	BCR	C3-C4-C5	-3.49	107.84	114.08
38	s	616	NEX	O24-C25-C38	3.49	119.24	115.06
25	B	619	BCR	C24-C23-C22	-3.49	120.96	126.23
32	C	520	DMU	O3-C5-C10	3.49	118.52	110.05
23	c	505	CLA	CAA-C2A-C3A	-3.48	103.25	112.78
36	S	316	LUT	C15-C14-C13	-3.48	122.35	127.31
25	C	519	BCR	C16-C17-C18	-3.48	122.35	127.31
24	A	403	PHO	C4D-ND-C1D	3.47	112.36	108.83
38	S	317	NEX	C39-C29-C30	-3.47	118.06	122.92
38	s	616	NEX	C39-C29-C30	-3.47	118.06	122.92
36	s	615	LUT	C35-C34-C33	-3.46	122.37	127.31
23	b	604	CLA	C4A-NA-C1A	3.46	108.26	106.71
25	a	405	BCR	C11-C10-C9	-3.45	122.38	127.31
23	b	617	CLA	O2D-CGD-O1D	-3.45	117.09	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	g	617	XAT	C11-C10-C9	-3.45	122.39	127.31
37	y	301	XAT	C35-C15-C14	-3.44	116.42	123.47
23	D	404	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
23	G	603	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
38	s	616	NEX	C35-C34-C33	-3.43	122.41	127.31
23	d	404	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
25	b	619	BCR	C20-C21-C22	-3.43	122.41	127.31
30	S	301	LMG	O7-C10-C11	3.43	118.89	111.50
24	a	402	PHO	C4D-ND-C1D	3.43	112.31	108.83
37	Y	301	XAT	C35-C15-C14	-3.42	116.47	123.47
30	s	619	LMG	O7-C10-C11	3.41	118.85	111.50
25	b	619	BCR	C11-C10-C9	-3.41	122.45	127.31
23	B	612	CLA	CMB-C2B-C1B	-3.40	120.18	125.37
36	s	614	LUT	C35-C15-C14	-3.40	116.51	123.47
37	g	620	XAT	C11-C10-C9	-3.39	122.47	127.31
23	a	404	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
23	B	605	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
38	Y	318	NEX	C16-C1-C2	3.39	124.28	109.05
36	g	616	LUT	C35-C34-C33	-3.39	122.47	127.31
25	A	405	BCR	C11-C10-C9	-3.39	122.47	127.31
25	b	621	BCR	C24-C23-C22	-3.39	121.11	126.23
35	g	606	CHL	CMB-C2B-C1B	-3.39	120.21	125.37
25	C	516	BCR	C3-C4-C5	-3.39	108.03	114.08
25	z	101	BCR	C16-C17-C18	-3.38	122.48	127.31
23	B	615	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
25	c	514	BCR	C3-C4-C5	-3.38	108.04	114.08
23	y	311	CLA	CMB-C2B-C1B	-3.38	120.22	125.37
36	R	314	LUT	C15-C14-C13	-3.38	122.48	127.31
32	c	519	DMU	O3-C5-C10	3.38	118.25	110.05
38	n	617	NEX	C27-C28-C29	-3.38	120.29	125.53
31	C	518	LHG	O7-C7-C8	3.38	118.78	111.50
38	R	301	NEX	C16-C1-C2	3.38	124.21	109.05
25	A	405	BCR	C3-C4-C5	-3.37	108.05	114.08
23	b	607	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
25	c	518	BCR	C16-C17-C18	-3.37	122.50	127.31
36	Y	317	LUT	C35-C34-C33	-3.37	122.50	127.31
31	L	102	LHG	O7-C7-C8	3.37	118.76	111.50
25	b	620	BCR	C28-C27-C26	-3.36	108.07	114.08
37	G	617	XAT	C31-C30-C29	-3.36	122.51	127.31
37	G	620	XAT	C11-C10-C9	-3.36	122.51	127.31
25	a	405	BCR	C3-C4-C5	-3.36	108.09	114.08
25	C	515	BCR	C11-C10-C9	-3.35	122.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	s	608	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	s	611	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	A	404	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
25	B	617	BCR	C11-C10-C9	-3.35	122.54	127.31
25	B	618	BCR	C28-C27-C26	-3.34	108.12	114.08
25	B	617	BCR	C20-C21-C22	-3.33	122.55	127.31
23	N	610	CLA	CMB-C2B-C1B	-3.33	120.30	125.37
25	C	515	BCR	C16-C17-C18	-3.33	122.56	127.31
31	l	103	LHG	O7-C7-C8	3.32	118.66	111.50
36	G	616	LUT	C15-C14-C13	-3.32	122.57	127.31
37	g	620	XAT	C31-C30-C29	-3.32	122.57	127.31
25	z	101	BCR	C11-C10-C9	-3.32	122.57	127.31
33	d	406	PL9	C10-C9-C11	-3.32	109.69	115.27
25	d	405	BCR	C38-C26-C27	3.32	119.99	113.62
23	s	609	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	B	602	CLA	C4A-NA-C1A	3.31	108.19	106.71
25	B	619	BCR	C28-C27-C26	-3.31	108.17	114.08
23	y	311	CLA	C4A-NA-C1A	3.30	108.19	106.71
37	g	617	XAT	C26-C27-C28	-3.30	119.02	125.99
32	S	319	DMU	C10-O1-C9	3.30	120.16	113.69
25	D	405	BCR	C38-C26-C27	3.29	119.94	113.62
25	k	101	BCR	C11-C10-C9	-3.29	122.61	127.31
25	b	619	BCR	C7-C8-C9	-3.29	121.26	126.23
37	G	620	XAT	C31-C30-C29	-3.28	122.62	127.31
25	b	620	BCR	C20-C21-C22	-3.28	122.63	127.31
38	G	618	NEX	C31-C30-C29	-3.28	122.63	127.31
37	Y	301	XAT	C24-C23-C22	-3.28	104.44	110.77
37	R	315	XAT	C35-C34-C33	-3.28	122.63	127.31
33	D	406	PL9	C10-C9-C11	-3.28	109.76	115.27
38	Y	318	NEX	C11-C10-C9	-3.28	122.63	127.31
23	S	309	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
32	s	618	DMU	C10-O1-C9	3.27	120.11	113.69
36	r	613	LUT	C15-C14-C13	-3.27	122.64	127.31
23	C	506	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
23	n	613	CLA	CBA-CAA-C2A	3.27	123.50	113.86
37	R	315	XAT	C15-C14-C13	-3.26	122.66	127.31
25	b	621	BCR	C28-C27-C26	-3.26	108.26	114.08
25	B	618	BCR	C20-C21-C22	-3.25	122.68	127.31
23	B	610	CLA	CMB-C2B-C1B	-3.24	120.43	125.37
23	b	617	CLA	CHB-C4A-NA	3.24	129.00	124.51
23	N	613	CLA	CBA-CAA-C2A	3.24	123.44	113.86
35	S	308	CHL	O2D-CGD-O1D	-3.24	117.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	CMB-C2B-C1B	-3.24	120.44	125.37
23	C	512	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
38	S	317	NEX	C35-C34-C33	-3.23	122.70	127.31
38	n	617	NEX	C11-C10-C9	-3.23	122.71	127.31
31	b	626	LHG	O7-C7-C8	3.22	118.45	111.50
37	R	315	XAT	C24-C23-C22	-3.22	104.55	110.77
23	N	603	CLA	CAA-C2A-C3A	-3.22	103.96	112.78
25	h	101	BCR	C10-C11-C12	-3.22	113.18	123.22
25	d	405	BCR	C16-C17-C18	-3.22	122.72	127.31
36	N	615	LUT	C35-C15-C14	-3.21	116.89	123.47
25	B	619	BCR	C7-C8-C9	-3.21	121.38	126.23
23	b	612	CLA	CMB-C2B-C1B	-3.21	120.48	125.37
25	H	101	BCR	C10-C11-C12	-3.21	113.20	123.22
36	Y	317	LUT	C15-C14-C13	-3.21	122.73	127.31
23	b	614	CLA	CMB-C2B-C1B	-3.21	120.48	125.37
35	Y	302	CHL	O2D-CGD-O1D	-3.21	117.57	123.84
37	r	614	XAT	C15-C14-C13	-3.20	122.74	127.31
37	r	614	XAT	C24-C23-C22	-3.20	104.60	110.77
23	B	615	CLA	CHB-C4A-NA	3.19	128.93	124.51
35	y	302	CHL	O2D-CGD-O1D	-3.19	117.60	123.84
23	R	311	CLA	CAA-C2A-C3A	-3.19	108.66	116.10
36	n	616	LUT	C15-C14-C13	-3.19	122.76	127.31
37	r	614	XAT	C35-C34-C33	-3.18	122.77	127.31
25	b	621	BCR	C7-C8-C9	-3.18	121.42	126.23
36	r	613	LUT	C11-C10-C9	-3.18	122.77	127.31
23	d	403	CLA	CMB-C2B-C1B	-3.18	120.53	125.37
32	C	520	DMU	C10-O1-C9	3.18	119.93	113.69
37	G	617	XAT	C11-C10-C9	-3.18	122.78	127.31
38	G	618	NEX	C15-C35-C34	-3.18	116.97	123.47
23	D	403	CLA	C3B-C4B-NB	-3.17	107.58	110.52
36	r	613	LUT	C18-C5-C6	-3.17	120.97	124.53
25	D	405	BCR	C16-C17-C18	-3.16	122.80	127.31
23	R	312	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
31	B	627	LHG	O7-C7-C8	3.16	118.32	111.50
38	N	617	NEX	C39-C29-C30	-3.16	118.50	122.92
25	C	515	BCR	C20-C21-C22	-3.16	122.80	127.31
25	B	619	BCR	C11-C10-C9	-3.16	122.80	127.31
37	y	301	XAT	C24-C23-C22	-3.15	104.69	110.77
25	b	620	BCR	C11-C10-C9	-3.15	122.81	127.31
36	y	317	LUT	C35-C34-C33	-3.14	122.83	127.31
38	Y	318	NEX	C31-C30-C29	-3.13	122.84	127.31
23	B	605	CLA	CGD-CBD-CAD	-3.13	100.59	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	z	101	BCR	C20-C21-C22	-3.13	122.84	127.31
23	s	609	CLA	CMB-C2B-C1B	-3.13	120.60	125.37
25	b	621	BCR	C20-C21-C22	-3.13	122.84	127.31
23	B	605	CLA	O2D-CGD-CBD	3.13	116.83	111.27
36	n	615	LUT	C35-C15-C14	-3.13	117.07	123.47
25	B	617	BCR	C7-C8-C9	-3.13	121.51	126.23
36	G	616	LUT	C10-C11-C12	-3.13	113.46	123.22
23	C	509	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	Y	315	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
35	G	607	CHL	CHD-C1D-ND	-3.12	121.59	124.45
34	F	101	HEM	C1B-NB-C4B	3.12	108.29	105.07
23	r	610	CLA	CAA-C2A-C3A	-3.12	108.82	116.10
24	D	402	PHO	CMB-C2B-C3B	3.11	130.50	124.68
25	B	618	BCR	C11-C10-C9	-3.11	122.87	127.31
37	y	301	XAT	C7-C8-C9	-3.11	120.71	125.53
35	G	609	CHL	CHD-C1D-ND	-3.10	121.60	124.45
23	c	508	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
23	c	511	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	g	614	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	a	403	PHO	C4D-ND-C1D	3.09	111.97	108.83
23	Y	311	CLA	CMB-C2B-C1B	-3.09	120.67	125.37
23	Y	305	CLA	CMB-C2B-C1B	-3.07	120.69	125.37
23	C	508	CLA	CHB-C4A-NA	3.07	128.76	124.51
23	N	614	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
37	g	620	XAT	C35-C34-C33	-3.07	122.93	127.31
38	r	615	NEX	C39-C29-C30	-3.07	118.62	122.92
36	S	315	LUT	C35-C15-C14	-3.07	117.19	123.47
23	n	614	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	c	507	CLA	CHB-C4A-NA	3.06	128.75	124.51
37	Y	301	XAT	C7-C8-C9	-3.06	120.78	125.53
35	N	608	CHL	O2D-CGD-O1D	-3.06	117.86	123.84
23	G	614	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
23	r	611	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
35	N	607	CHL	CHB-C4A-NA	3.05	128.74	124.51
36	Y	316	LUT	C35-C15-C14	-3.05	117.22	123.47
34	f	101	HEM	C1B-NB-C4B	3.05	108.22	105.07
36	Y	317	LUT	C7-C8-C9	-3.05	121.63	126.23
37	G	620	XAT	C35-C34-C33	-3.05	122.96	127.31
33	D	406	PL9	C35-C34-C36	-3.05	110.14	115.27
26	b	602	SQD	O8-S-O7	3.05	118.72	111.27
35	S	308	CHL	CMB-C2B-C1B	-3.05	120.73	125.37
33	D	406	PL9	C30-C29-C31	-3.04	110.15	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	619	BCR	C20-C21-C22	-3.04	122.97	127.31
23	R	312	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	S	312	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	b	607	CLA	O2D-CGD-CBD	3.04	116.67	111.27
36	G	616	LUT	C7-C8-C9	-3.03	121.66	126.23
37	G	617	XAT	C4-C3-C2	-3.03	104.92	110.77
35	N	609	CHL	CAA-C2A-C3A	-3.03	104.49	112.78
23	c	508	CLA	CMB-C2B-C1B	-3.02	120.76	125.37
23	R	302	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
37	R	315	XAT	C10-C11-C12	-3.02	113.78	123.22
35	y	309	CHL	O2D-CGD-O1D	-3.02	117.93	123.84
35	n	609	CHL	CAA-C2A-C3A	-3.02	104.51	112.78
38	R	301	NEX	C31-C30-C29	-3.02	123.00	127.31
23	b	615	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	S	312	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
33	d	406	PL9	C30-C29-C31	-3.02	110.20	115.27
23	y	315	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
36	N	616	LUT	C15-C14-C13	-3.01	123.01	127.31
23	b	616	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
35	g	609	CHL	C4A-NA-C1A	3.01	108.06	106.71
23	N	610	CLA	CHB-C4A-NA	3.01	128.67	124.51
25	b	620	BCR	C7-C8-C9	-3.01	121.69	126.23
26	c	520	SQD	O8-S-O7	3.01	118.62	111.27
23	Y	304	CLA	CHB-C4A-NA	3.01	128.67	124.51
36	y	317	LUT	C7-C8-C9	-3.00	121.70	126.23
25	D	405	BCR	C20-C21-C22	-3.00	123.02	127.31
35	n	607	CHL	CHB-C4A-NA	3.00	128.66	124.51
25	B	618	BCR	C7-C8-C9	-3.00	121.70	126.23
23	B	614	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
23	S	312	CLA	CMB-C2B-C1B	-3.00	120.81	125.37
23	G	610	CLA	CHB-C4A-NA	3.00	128.65	124.51
36	y	316	LUT	C35-C15-C14	-2.99	117.34	123.47
23	b	614	CLA	CHB-C4A-NA	2.99	128.65	124.51
23	B	612	CLA	CHB-C4A-NA	2.99	128.65	124.51
25	d	405	BCR	C20-C21-C22	-2.99	123.04	127.31
37	y	301	XAT	C15-C14-C13	-2.99	123.05	127.31
37	y	301	XAT	C6-C7-C8	-2.99	119.68	125.99
31	L	101	LHG	O8-C23-C24	2.99	121.28	111.91
36	n	615	LUT	C11-C10-C9	-2.99	123.05	127.31
23	y	304	CLA	CHB-C4A-NA	2.99	128.64	124.51
35	s	606	CHL	CAA-C2A-C3A	-2.99	106.80	114.26
35	Y	309	CHL	O2D-CGD-O1D	-2.99	118.00	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	625	SQD	O8-S-O7	2.98	118.57	111.27
26	C	521	SQD	O8-S-O7	2.98	118.56	111.27
23	N	612	CLA	CHB-C4A-NA	2.98	128.64	124.51
25	b	620	BCR	C16-C17-C18	-2.98	123.06	127.31
23	n	603	CLA	CAA-C2A-C3A	-2.98	104.63	112.78
25	c	518	BCR	C11-C10-C9	-2.98	123.06	127.31
38	R	316	NEX	C39-C29-C30	-2.98	118.75	122.92
36	S	315	LUT	C30-C31-C32	-2.97	113.93	123.22
23	A	402	CLA	CAA-C2A-C3A	-2.97	104.64	112.78
23	B	613	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	C	506	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	r	608	CLA	CHB-C4A-NA	2.97	128.62	124.51
37	Y	301	XAT	C6-C7-C8	-2.97	119.71	125.99
25	b	621	BCR	C11-C10-C9	-2.97	123.07	127.31
35	N	605	CHL	O2D-CGD-CBD	2.97	116.54	111.27
25	H	101	BCR	C15-C14-C13	-2.97	123.07	127.31
25	c	514	BCR	C15-C16-C17	-2.97	117.40	123.47
23	r	604	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
35	g	609	CHL	CHB-C4A-NA	2.96	128.61	124.51
37	r	614	XAT	C4-C3-C2	-2.96	105.05	110.77
25	h	101	BCR	C15-C14-C13	-2.96	123.08	127.31
36	y	317	LUT	C15-C14-C13	-2.96	123.08	127.31
35	n	605	CHL	CMB-C2B-C1B	-2.96	120.86	125.37
35	g	609	CHL	CHD-C1D-ND	-2.96	121.73	124.45
35	s	607	CHL	O2D-CGD-O1D	-2.96	118.05	123.84
37	r	614	XAT	C10-C11-C12	-2.96	113.99	123.22
23	R	305	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	b	607	CLA	CGD-CBD-CAD	-2.96	101.16	110.73
23	S	304	CLA	CHB-C4A-NA	2.95	128.59	124.51
23	Y	305	CLA	CHB-C1B-NB	2.95	127.38	124.26
23	n	614	CLA	CAA-C2A-C3A	-2.95	109.22	116.10
35	G	606	CHL	CMB-C2B-C1B	-2.95	120.88	125.37
23	b	607	CLA	CHB-C4A-NA	2.95	128.59	124.51
35	G	608	CHL	O2D-CGD-O1D	-2.95	118.07	123.84
23	S	305	CLA	CMB-C2B-C1B	-2.95	120.88	125.37
38	g	618	NEX	C35-C34-C33	-2.95	123.10	127.31
35	N	609	CHL	O2D-CGD-O1D	-2.95	118.08	123.84
23	g	613	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
35	n	608	CHL	O2D-CGD-O1D	-2.95	118.08	123.84
23	S	312	CLA	CHB-C4A-NA	2.94	128.58	124.51
23	S	305	CLA	CHB-C1B-NB	2.94	127.37	124.26
23	r	601	CLA	O2D-CGD-O1D	-2.94	118.08	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	S	308	CHL	CHD-C1D-ND	-2.94	121.75	124.45
35	g	608	CHL	O2D-CGD-O1D	-2.94	118.09	123.84
35	g	607	CHL	CHD-C1D-ND	-2.94	121.75	124.45
23	n	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
25	C	516	BCR	C15-C16-C17	-2.94	117.46	123.47
23	c	505	CLA	CHB-C4A-NA	2.94	128.57	124.51
23	s	603	CLA	CHB-C4A-NA	2.94	128.57	124.51
35	Y	306	CHL	O2D-CGD-O1D	-2.94	118.10	123.84
23	N	614	CLA	CAA-C2A-C3A	-2.93	109.25	116.10
35	R	307	CHL	CHD-C1D-ND	-2.93	121.76	124.45
37	g	617	XAT	C35-C34-C33	-2.93	123.12	127.31
23	c	506	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
36	S	315	LUT	C10-C11-C12	-2.93	114.08	123.22
37	G	620	XAT	C4-C3-C2	-2.93	105.12	110.77
24	A	403	PHO	C1C-C2C-C3C	-2.93	106.17	108.61
35	y	306	CHL	O2D-CGD-O1D	-2.92	118.12	123.84
25	B	618	BCR	C16-C17-C18	-2.92	123.14	127.31
23	y	313	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
35	y	308	CHL	O2D-CGD-O1D	-2.92	118.13	123.84
38	r	615	NEX	C11-C12-C13	-2.92	118.21	126.42
35	n	609	CHL	O2D-CGD-O1D	-2.92	118.13	123.84
31	b	623	LHG	O8-C23-C24	2.92	121.06	111.91
38	G	618	NEX	C39-C29-C30	-2.91	118.84	122.92
37	Y	301	XAT	C15-C14-C13	-2.91	123.15	127.31
31	B	621	LHG	O8-C23-C24	2.91	121.05	111.91
35	S	306	CHL	CHB-C4A-NA	2.91	128.54	124.51
23	y	311	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	l	102	LHG	O8-C23-C24	2.91	121.04	111.91
23	C	511	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	C	513	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
38	R	316	NEX	C24-C23-C22	-2.91	105.16	110.77
24	a	402	PHO	C1C-C2C-C3C	-2.91	106.19	108.61
23	g	610	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	n	612	CLA	CHB-C4A-NA	2.90	128.53	124.51
23	N	610	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
35	Y	308	CHL	O2D-CGD-O1D	-2.90	118.16	123.84
36	N	616	LUT	C10-C11-C12	-2.90	114.16	123.22
37	g	617	XAT	C4-C3-C2	-2.90	105.17	110.77
23	S	309	CLA	CHB-C4A-NA	2.90	128.52	124.51
23	S	313	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
35	R	308	CHL	O2D-CGD-O1D	-2.90	118.17	123.84
23	s	612	CLA	O2D-CGD-O1D	-2.90	118.17	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	s	603	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	N	603	CLA	CHB-C4A-NA	2.90	128.52	124.51
38	n	617	NEX	C26-C27-C28	-2.89	119.88	125.99
23	y	303	CLA	CHB-C4A-NA	2.89	128.51	124.51
23	c	509	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	D	402	PHO	C4D-ND-C1D	2.89	111.77	108.83
23	g	603	CLA	CHB-C4A-NA	2.89	128.51	124.51
35	G	607	CHL	O2D-CGD-O1D	-2.89	118.19	123.84
23	S	304	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	S	310	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	b	619	BCR	C1-C6-C5	-2.89	118.55	122.61
23	c	513	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
35	r	605	CHL	CMB-C2B-C1B	-2.88	120.99	125.37
23	Y	313	CLA	CHB-C4A-NA	2.88	128.49	124.51
35	y	306	CHL	CHD-C1D-ND	-2.88	121.81	124.45
36	g	615	LUT	C7-C8-C9	-2.88	121.89	126.23
23	N	612	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
38	r	615	NEX	C24-C23-C22	-2.87	105.22	110.77
23	B	601	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	r	604	CLA	CHB-C4A-NA	2.87	128.48	124.51
35	G	606	CHL	O2D-CGD-O1D	-2.87	118.23	123.84
23	C	508	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	B	612	CLA	CMB-C2B-C3B	2.87	133.53	126.59
23	n	610	CLA	CHB-C4A-NA	2.87	128.48	124.51
23	B	603	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	a	405	BCR	C20-C21-C22	-2.87	123.22	127.31
35	Y	306	CHL	CHD-C1D-ND	-2.87	121.82	124.45
36	R	314	LUT	C11-C10-C9	-2.86	123.22	127.31
23	G	612	CLA	CHB-C4A-NA	2.86	128.47	124.51
36	s	614	LUT	C30-C31-C32	-2.86	114.29	123.22
35	G	609	CHL	O2D-CGD-O1D	-2.86	118.24	123.84
33	d	406	PL9	C35-C34-C36	-2.86	110.46	115.27
37	g	620	XAT	C4-C3-C2	-2.86	105.25	110.77
23	d	402	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
37	R	315	XAT	C4-C3-C2	-2.86	105.25	110.77
23	B	605	CLA	CHB-C4A-NA	2.86	128.46	124.51
35	R	306	CHL	CMB-C2B-C1B	-2.86	121.02	125.37
23	b	605	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
23	Y	311	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	d	401	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	g	612	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	S	303	CLA	O2D-CGD-O1D	-2.85	118.27	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	612	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	C	510	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	B	617	BCR	C1-C6-C5	-2.85	118.60	122.61
23	y	313	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	C	504	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	y	316	LUT	C38-C25-C24	-2.85	117.47	123.56
23	c	503	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	C	503	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
36	g	615	LUT	C15-C14-C13	-2.85	123.25	127.31
23	c	502	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
23	C	514	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	c	510	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	c	512	CLA	CAA-C2A-C3A	-2.84	104.99	112.78
23	Y	313	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	R	312	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	k	101	BCR	C24-C23-C22	-2.84	121.94	126.23
23	Y	314	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	C	519	BCR	C3-C4-C5	-2.84	109.01	114.08
35	r	607	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
36	s	615	LUT	C38-C25-C24	-2.84	117.48	123.56
36	g	615	LUT	C35-C15-C14	-2.84	117.67	123.47
23	n	612	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
36	N	616	LUT	C38-C25-C24	-2.83	117.49	123.56
23	N	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
35	s	607	CHL	CHD-C1D-ND	-2.83	121.85	124.45
23	C	513	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	s	611	CLA	CHB-C4A-NA	2.83	128.43	124.51
38	n	617	NEX	C39-C29-C30	-2.83	118.96	122.92
23	s	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	h	101	BCR	C38-C26-C25	-2.83	121.35	124.53
36	S	316	LUT	C38-C25-C24	-2.83	117.51	123.56
23	b	603	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
35	g	609	CHL	O2D-CGD-O1D	-2.82	118.32	123.84
23	r	610	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	y	305	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
36	g	616	LUT	C38-C25-C24	-2.82	117.52	123.56
23	B	606	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	Y	303	CLA	CHB-C4A-NA	2.82	128.41	124.51
35	S	307	CHL	CHB-C4A-NA	2.82	128.41	124.51
36	G	616	LUT	C38-C25-C24	-2.82	117.53	123.56
23	G	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	C	503	CLA	CHB-C4A-NA	2.82	128.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	R	305	CLA	CHB-C4A-NA	2.81	128.40	124.51
23	b	612	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	C	516	BCR	C21-C20-C19	-2.81	114.44	123.22
35	n	607	CHL	O2D-CGD-O1D	-2.81	118.34	123.84
23	Y	305	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
35	Y	309	CHL	C3B-C4B-NB	-2.81	107.91	110.52
23	c	512	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
36	g	615	LUT	C11-C10-C9	-2.80	123.31	127.31
23	R	304	CLA	CHB-C4A-NA	2.80	128.39	124.51
36	Y	316	LUT	C38-C25-C24	-2.80	117.56	123.56
35	r	605	CHL	CHD-C1D-ND	-2.80	121.88	124.45
36	G	615	LUT	C35-C15-C14	-2.80	117.73	123.47
23	b	608	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	R	309	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	B	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	G	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	g	612	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	C	507	CLA	CMB-C2B-C3B	2.80	133.37	126.59
23	y	303	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	r	609	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	B	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
35	G	605	CHL	O2D-CGD-O1D	-2.80	118.37	123.84
23	b	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
35	Y	310	CHL	C2A-C1A-CHA	2.80	128.75	123.86
23	G	610	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
24	a	403	PHO	C1C-C2C-C3C	-2.80	106.29	108.61
35	N	606	CHL	O2D-CGD-O1D	-2.79	118.38	123.84
23	B	610	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
37	Y	301	XAT	C31-C30-C29	-2.79	123.32	127.31
25	z	101	BCR	C24-C23-C22	-2.79	122.01	126.23
23	G	603	CLA	CHB-C4A-NA	2.79	128.37	124.51
35	S	306	CHL	O2D-CGD-O1D	-2.79	118.38	123.84
35	y	310	CHL	C2A-C1A-CHA	2.79	128.74	123.86
25	c	514	BCR	C21-C20-C19	-2.79	114.51	123.22
23	D	401	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	R	311	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
35	s	606	CHL	OMC-CMC-C2C	-2.79	119.38	125.69
25	C	516	BCR	C16-C17-C18	-2.79	123.33	127.31
23	N	611	CLA	CHB-C4A-NA	2.79	128.37	124.51
35	N	605	CHL	CMB-C2B-C1B	-2.79	121.13	125.37
38	G	618	NEX	C35-C34-C33	-2.79	123.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	s	614	LUT	C38-C25-C24	-2.79	117.60	123.56
35	n	609	CHL	CHD-C1D-ND	-2.78	121.89	124.45
25	c	514	BCR	C16-C17-C18	-2.78	123.34	127.31
23	C	502	CLA	C3B-C4B-NB	-2.78	107.93	110.52
38	R	301	NEX	C26-C27-C28	-2.78	120.11	125.99
35	R	306	CHL	CHD-C1D-ND	-2.78	121.90	124.45
37	G	617	XAT	C15-C35-C34	-2.78	117.78	123.47
36	s	614	LUT	C10-C11-C12	-2.78	114.54	123.22
37	y	301	XAT	C31-C30-C29	-2.78	123.34	127.31
23	B	613	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	R	313	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
35	S	308	CHL	C2A-C1A-CHA	2.78	128.72	123.86
23	b	609	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
38	G	618	NEX	C11-C12-C13	-2.78	118.62	126.42
36	r	613	LUT	C31-C30-C29	-2.78	123.35	127.31
23	c	502	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	r	603	CLA	CHB-C4A-NA	2.77	128.35	124.51
35	y	310	CHL	O2D-CGD-O1D	-2.77	118.41	123.84
23	d	401	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	b	615	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	c	512	CLA	CHB-C4A-NA	2.77	128.34	124.51
38	g	618	NEX	C24-C23-C22	-2.77	105.42	110.77
23	c	501	CLA	C3B-C4B-NB	-2.77	107.95	110.52
23	N	610	CLA	CMB-C2B-C3B	2.77	133.29	126.59
35	S	307	CHL	O2D-CGD-O1D	-2.77	118.43	123.84
25	k	101	BCR	C7-C8-C9	-2.76	122.06	126.23
23	Y	311	CLA	CHB-C4A-NA	2.76	128.34	124.51
23	b	618	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	B	608	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	b	618	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	G	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
35	g	605	CHL	O2D-CGD-O1D	-2.76	118.44	123.84
23	n	603	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	n	604	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	s	613	CLA	CAA-C2A-C3A	-2.75	109.67	116.10
23	y	311	CLA	CHB-C1B-NB	2.75	127.17	124.26
36	S	316	LUT	C19-C9-C8	2.75	122.42	118.08
23	B	607	CLA	CHB-C4A-NA	2.75	128.32	124.51
36	y	316	LUT	C30-C31-C32	-2.75	114.63	123.22
35	s	606	CHL	CHB-C4A-NA	2.75	128.32	124.51
35	S	302	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
23	n	611	CLA	CHB-C4A-NA	2.75	128.31	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	n	605	CHL	OMC-CMC-C2C	-2.75	119.47	125.69
23	Y	303	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	g	603	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	C	509	CLA	CHB-C1B-NB	2.75	127.16	124.26
37	g	617	XAT	C24-C23-C22	-2.75	105.47	110.77
25	A	405	BCR	C20-C21-C22	-2.74	123.39	127.31
23	b	604	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	C	506	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	r	612	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
36	G	615	LUT	C7-C8-C9	-2.74	122.09	126.23
23	b	614	CLA	CMB-C2B-C3B	2.74	133.22	126.59
23	c	509	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	a	403	PHO	CMB-C2B-C3B	2.74	129.80	124.68
23	r	602	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
23	y	305	CLA	CMB-C2B-C1B	-2.73	121.20	125.37
36	N	616	LUT	C7-C8-C9	-2.73	122.11	126.23
23	n	602	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	a	401	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
36	G	615	LUT	C15-C14-C13	-2.73	123.41	127.31
35	N	607	CHL	O2D-CGD-O1D	-2.73	118.50	123.84
38	Y	318	NEX	C26-C27-C28	-2.73	120.22	125.99
36	y	317	LUT	C38-C25-C24	-2.73	117.72	123.56
23	y	314	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	N	602	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	N	612	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
24	A	403	PHO	C4B-NB-C1B	2.73	113.05	108.83
36	g	615	LUT	C38-C25-C24	-2.73	117.72	123.56
23	D	401	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
35	Y	310	CHL	O2D-CGD-O1D	-2.73	118.51	123.84
23	y	305	CLA	CHB-C1B-NB	2.72	127.14	124.26
35	N	605	CHL	OMC-CMC-C2C	-2.72	119.53	125.69
23	b	610	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	A	405	BCR	C33-C5-C6	-2.72	121.47	124.53
38	R	316	NEX	C11-C12-C13	-2.72	118.78	126.42
35	Y	308	CHL	CHB-C4A-NA	2.72	128.27	124.51
23	C	510	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
30	C	522	LMG	O8-C28-C29	2.72	120.44	111.91
23	d	404	CLA	CHB-C4A-NA	2.72	128.27	124.51
24	a	402	PHO	C4B-NB-C1B	2.71	113.03	108.83
23	G	613	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	s	610	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
38	R	316	NEX	C31-C30-C29	-2.71	123.44	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	404	CLA	CHB-C4A-NA	2.71	128.26	124.51
30	c	521	LMG	O8-C28-C29	2.71	120.42	111.91
37	G	617	XAT	C35-C34-C33	-2.71	123.44	127.31
23	B	610	CLA	CMB-C2B-C3B	2.71	133.15	126.59
23	B	602	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	c	505	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
36	Y	317	LUT	C38-C25-C24	-2.71	117.76	123.56
35	y	309	CHL	C3B-C4B-NB	-2.71	108.00	110.52
25	C	515	BCR	C24-C23-C22	-2.71	122.14	126.23
38	R	316	NEX	C15-C35-C34	-2.71	117.93	123.47
35	G	601	CHL	O2D-CGD-O1D	-2.71	118.54	123.84
37	r	614	XAT	C31-C30-C29	-2.71	123.45	127.31
23	y	311	CLA	CMB-C2B-C3B	2.70	133.14	126.59
38	G	618	NEX	C24-C23-C22	-2.70	105.55	110.77
36	r	613	LUT	C38-C25-C24	-2.70	117.77	123.56
23	s	602	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	S	314	CLA	CAA-C2A-C3A	-2.70	109.79	116.10
23	g	604	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	G	611	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	y	304	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
26	B	625	SQD	O47-C7-C8	2.70	117.31	111.50
35	r	606	CHL	CHD-C1D-ND	-2.70	121.98	124.45
25	H	101	BCR	C38-C26-C25	-2.70	121.50	124.53
23	S	303	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	b	602	SQD	O48-C23-C24	2.69	120.36	111.91
36	G	615	LUT	C38-C25-C24	-2.69	117.80	123.56
23	C	505	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
35	g	601	CHL	O2D-CGD-O1D	-2.69	118.57	123.84
23	A	402	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
38	s	616	NEX	C17-C1-C6	-2.69	108.06	110.47
35	s	607	CHL	C2A-C1A-CHA	2.69	128.56	123.86
36	n	616	LUT	C38-C25-C24	-2.69	117.81	123.56
23	C	513	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	s	608	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	n	615	LUT	C38-C25-C24	-2.69	117.81	123.56
23	c	508	CLA	CHB-C1B-NB	2.68	127.10	124.26
23	B	612	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	C	512	CLA	CHB-C4A-NA	2.68	128.22	124.51
35	n	601	CHL	O2D-CGD-O1D	-2.68	118.59	123.84
23	N	611	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
25	K	101	BCR	C30-C25-C26	-2.68	118.84	122.61
25	c	514	BCR	C33-C5-C6	-2.68	121.52	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	402	CLA	CHB-C4A-NA	2.68	128.22	124.51
38	R	301	NEX	C24-C23-C22	-2.68	105.60	110.77
23	A	401	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
36	N	615	LUT	C30-C31-C32	-2.68	114.86	123.22
25	a	405	BCR	C33-C5-C6	-2.68	121.52	124.53
23	b	609	CLA	CHB-C4A-NA	2.68	128.21	124.51
23	n	602	CLA	CMB-C2B-C1B	-2.67	121.30	125.37
30	C	522	LMG	C8-O7-C10	-2.67	111.21	117.79
35	n	606	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
24	D	402	PHO	C1C-C2C-C3C	-2.67	106.39	108.61
23	G	602	CLA	CHB-C4A-NA	2.67	128.21	124.51
35	N	606	CHL	OMC-CMC-C2C	-2.67	119.64	125.69
38	S	317	NEX	C24-C23-C22	-2.67	105.61	110.77
33	d	406	PL9	C7-C3-C4	2.67	119.05	116.88
23	N	613	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
36	N	615	LUT	C38-C25-C24	-2.67	117.84	123.56
25	K	101	BCR	C11-C10-C9	-2.67	123.50	127.31
38	Y	318	NEX	C39-C29-C30	-2.67	119.18	122.92
23	g	602	CLA	CHB-C4A-NA	2.67	128.20	124.51
31	L	102	LHG	O8-C23-C24	2.67	120.28	111.91
23	n	611	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	b	614	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
35	s	606	CHL	O2D-CGD-O1D	-2.67	118.62	123.84
36	n	615	LUT	C30-C31-C32	-2.67	114.89	123.22
23	A	404	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	y	311	CLA	CHB-C4A-NA	2.67	128.20	124.51
23	b	612	CLA	CMB-C2B-C3B	2.67	133.04	126.59
23	b	612	CLA	CHB-C4A-NA	2.66	128.20	124.51
36	R	314	LUT	C38-C25-C24	-2.66	117.86	123.56
23	r	608	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
23	c	507	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
25	C	516	BCR	C33-C5-C6	-2.66	121.54	124.53
31	l	103	LHG	O8-C23-C24	2.66	120.27	111.91
23	c	507	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
23	B	616	CLA	CHB-C4A-NA	2.66	128.19	124.51
35	g	606	CHL	OMC-CMC-C2C	-2.66	119.67	125.69
38	g	618	NEX	C39-C29-C30	-2.66	119.20	122.92
35	y	308	CHL	CHB-C4A-NA	2.66	128.19	124.51
35	n	605	CHL	CHD-C1D-ND	-2.66	122.01	124.45
23	g	611	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
35	n	606	CHL	CMB-C2B-C1B	-2.66	121.32	125.37
23	C	504	CLA	CHB-C4A-NA	2.66	128.19	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	g	610	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
23	B	610	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
35	g	606	CHL	CMB-C2B-C3B	2.66	133.02	126.59
23	A	402	CLA	CBA-CAA-C2A	2.66	121.70	113.86
23	B	616	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
38	n	617	NEX	C16-C1-C6	2.65	112.85	110.47
26	B	625	SQD	O48-C23-C24	2.65	120.24	111.91
25	k	101	BCR	C16-C15-C14	-2.65	118.04	123.47
23	s	613	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	B	606	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	n	604	CLA	CHB-C1B-NB	2.65	127.06	124.26
35	y	307	CHL	CMB-C2B-C1B	-2.65	121.33	125.37
23	C	514	CLA	CHB-C4A-NA	2.65	128.18	124.51
35	s	601	CHL	O2D-CGD-O1D	-2.65	118.66	123.84
23	R	304	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
23	s	603	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
38	Y	318	NEX	C24-C23-C22	-2.65	105.66	110.77
38	n	617	NEX	C31-C30-C29	-2.65	123.53	127.31
23	B	613	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
35	S	306	CHL	OMC-CMC-C2C	-2.65	119.70	125.69
36	G	615	LUT	C11-C10-C9	-2.65	123.53	127.31
23	b	606	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	c	518	BCR	C29-C30-C25	2.65	114.55	110.48
38	R	301	NEX	C39-C29-C30	-2.64	119.22	122.92
23	g	602	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
35	y	307	CHL	O2D-CGD-O1D	-2.64	118.67	123.84
23	c	513	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	B	610	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	b	608	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	B	604	CLA	CHB-C4A-NA	2.64	128.16	124.51
31	W	201	LHG	C5-O7-C7	-2.64	111.30	117.79
35	N	606	CHL	CMB-C2B-C1B	-2.64	121.35	125.37
23	a	404	CLA	CHB-C4A-NA	2.64	128.16	124.51
38	r	615	NEX	C35-C34-C33	-2.64	123.55	127.31
23	S	314	CLA	CMA-C3A-C2A	-2.64	109.94	116.10
25	C	519	BCR	C15-C16-C17	-2.64	118.07	123.47
38	r	615	NEX	C16-C1-C6	2.64	112.83	110.47
30	a	407	LMG	O8-C28-C29	2.64	120.18	111.91
23	S	314	CLA	CHB-C4A-NA	2.63	128.16	124.51
23	b	604	CLA	C3B-C4B-NB	-2.63	108.07	110.52
23	S	310	CLA	CMB-C2B-C1B	-2.63	121.36	125.37
23	C	514	CLA	CBA-CAA-C2A	2.63	121.63	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	CHB-C4A-NA	2.63	128.15	124.51
35	n	601	CHL	CHD-C1D-ND	-2.63	122.03	124.45
35	g	607	CHL	O2D-CGD-O1D	-2.63	118.69	123.84
36	Y	316	LUT	C30-C31-C32	-2.63	115.00	123.22
35	g	605	CHL	CHD-C1D-ND	-2.63	122.04	124.45
35	Y	307	CHL	CMB-C2B-C1B	-2.63	121.36	125.37
35	Y	307	CHL	O2D-CGD-O1D	-2.63	118.70	123.84
35	n	605	CHL	CHB-C4A-NA	2.63	128.15	124.51
31	c	516	LHG	C5-O7-C7	-2.63	111.32	117.79
23	d	403	CLA	CMB-C2B-C3B	2.63	132.95	126.59
23	C	505	CLA	CHB-C4A-NA	2.63	128.14	124.51
23	N	604	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
38	R	316	NEX	C35-C34-C33	-2.63	123.56	127.31
23	N	602	CLA	CMB-C2B-C1B	-2.63	121.37	125.37
26	b	602	SQD	O47-C7-C8	2.62	117.16	111.50
23	N	603	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
25	a	405	BCR	C24-C23-C22	-2.62	122.27	126.23
25	d	405	BCR	C29-C30-C25	2.62	114.52	110.48
31	c	516	LHG	O8-C23-C24	2.62	120.14	111.91
23	C	502	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
35	Y	307	CHL	CHD-C1D-ND	-2.62	122.04	124.45
30	s	619	LMG	C7-O1-C1	-2.62	108.62	113.74
23	B	609	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	Y	304	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
35	S	307	CHL	CAA-C2A-C3A	-2.62	107.71	114.26
36	g	616	LUT	C7-C8-C9	-2.62	122.28	126.23
23	c	504	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	y	312	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
35	N	601	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
23	D	403	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
36	g	616	LUT	C10-C11-C12	-2.62	115.05	123.22
25	b	620	BCR	C15-C16-C17	-2.62	118.12	123.47
23	n	613	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	S	304	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
25	B	618	BCR	C15-C16-C17	-2.61	118.12	123.47
35	S	307	CHL	OMC-CMC-C2C	-2.61	119.78	125.69
37	G	620	XAT	C15-C35-C34	-2.61	118.12	123.47
35	Y	310	CHL	CHD-C1D-ND	-2.61	122.05	124.45
23	b	606	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
35	n	606	CHL	CHD-C1D-ND	-2.61	122.05	124.45
23	C	508	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
30	B	620	LMG	O8-C28-C29	2.61	120.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	G	609	CHL	CAA-C2A-C3A	-2.61	105.63	112.78
34	F	101	HEM	C4A-NA-C1A	2.61	107.90	105.35
26	l	101	SQD	O7-S-C6	2.61	110.04	106.94
23	d	403	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	R	309	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	s	610	CLA	CAA-C2A-C3A	-2.60	107.75	114.26
23	B	604	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	B	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	K	101	BCR	C38-C26-C27	2.60	118.62	113.62
23	B	602	CLA	C3B-C4B-NB	-2.60	108.10	110.52
31	W	201	LHG	O8-C23-C24	2.60	120.07	111.91
26	l	101	SQD	O48-C23-C24	2.60	120.07	111.91
23	b	615	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
25	D	405	BCR	C29-C30-C25	2.60	114.48	110.48
23	R	303	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	g	612	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
35	s	601	CHL	OMC-CMC-C2C	-2.60	119.81	125.69
23	r	610	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	b	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
35	N	609	CHL	CHD-C1D-ND	-2.60	122.07	124.45
38	n	617	NEX	C24-C23-C22	-2.60	105.76	110.77
31	s	617	LHG	O8-C23-C24	2.59	120.05	111.91
38	r	615	NEX	C31-C30-C29	-2.59	123.61	127.31
23	n	613	CLA	CHB-C4A-NA	2.59	128.10	124.51
23	c	503	CLA	CHB-C4A-NA	2.59	128.09	124.51
35	s	606	CHL	CHD-C1D-ND	-2.59	122.07	124.45
23	N	604	CLA	CHB-C1B-NB	2.59	127.00	124.26
36	Y	316	LUT	C15-C14-C13	-2.59	123.61	127.31
23	r	601	CLA	CHB-C4A-NA	2.59	128.09	124.51
38	g	618	NEX	C26-C27-C28	-2.59	120.52	125.99
35	G	609	CHL	C2A-C1A-CHA	2.59	128.38	123.86
23	G	612	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
35	G	601	CHL	CHD-C1D-ND	-2.59	122.08	124.45
35	s	605	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
25	c	514	BCR	C24-C23-C22	-2.59	122.33	126.23
23	C	511	CLA	CHB-C4A-NA	2.59	128.09	124.51
33	D	406	PL9	C7-C3-C4	2.59	118.98	116.88
35	g	605	CHL	OMC-CMC-C2C	-2.59	119.84	125.69
23	S	305	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
23	n	613	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
37	g	620	XAT	C15-C35-C34	-2.58	118.18	123.47
24	D	402	PHO	C6-C5-C3	2.58	120.22	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	R	308	CHL	CHB-C4A-NA	2.58	128.08	124.51
31	D	408	LHG	O8-C23-C24	2.58	120.01	111.91
23	N	602	CLA	CHB-C1B-NB	2.58	126.99	124.26
36	y	316	LUT	C10-C11-C12	-2.58	115.16	123.22
25	k	101	BCR	C38-C26-C27	2.58	118.57	113.62
28	B	626	DGD	C1D-O6D-C5D	2.58	118.75	113.69
35	r	606	CHL	OMC-CMC-C2C	-2.58	119.86	125.69
35	y	307	CHL	CHD-C1D-ND	-2.58	122.08	124.45
35	G	605	CHL	OMC-CMC-C2C	-2.58	119.86	125.69
23	b	611	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	s	609	CLA	O2D-CGD-CBD	2.58	115.85	111.27
23	Y	304	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	b	610	CLA	CHB-C4A-NA	2.58	128.07	124.51
23	C	502	CLA	CHB-C1B-NB	2.57	126.98	124.26
34	F	101	HEM	C4D-ND-C1D	2.57	107.73	105.07
30	C	501	LMG	O8-C28-C29	2.57	119.98	111.91
23	c	501	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
28	A	408	DGD	O1G-C1A-C2A	2.57	119.98	111.91
25	k	101	BCR	C30-C25-C26	-2.57	118.99	122.61
23	c	506	CLA	CMB-C2B-C1B	-2.57	121.45	125.37
23	R	311	CLA	CHB-C4A-NA	2.57	128.06	124.51
35	R	306	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
35	G	605	CHL	CHD-C1D-ND	-2.57	122.09	124.45
31	d	408	LHG	O8-C23-C24	2.57	119.97	111.91
35	n	605	CHL	O2D-CGD-CBD	2.57	115.83	111.27
35	s	605	CHL	CHD-C1D-ND	-2.56	122.10	124.45
35	N	609	CHL	O2D-CGD-CBD	2.56	115.83	111.27
23	N	604	CLA	CHB-C4A-NA	2.56	128.06	124.51
24	a	403	PHO	C6-C5-C3	2.56	120.18	113.45
23	s	604	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
35	S	302	CHL	OMC-CMC-C2C	-2.56	119.89	125.69
24	D	402	PHO	C4B-NB-C1B	2.56	112.79	108.83
36	S	315	LUT	C38-C25-C24	-2.56	118.08	123.56
35	N	605	CHL	CHB-C4A-NA	2.56	128.05	124.51
36	R	314	LUT	C31-C30-C29	-2.56	123.66	127.31
25	c	518	BCR	C1-C6-C5	-2.56	119.01	122.61
30	W	203	LMG	O8-C28-C29	2.56	119.94	111.91
23	Y	312	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	Y	315	CLA	CHB-C4A-NA	2.56	128.05	124.51
35	Y	308	CHL	OMC-CMC-C2C	-2.56	119.90	125.69
23	B	601	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	Y	314	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	k	101	BCR	C38-C26-C25	-2.56	121.66	124.53
23	b	613	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	D	405	BCR	C3-C4-C5	-2.55	109.52	114.08
35	G	606	CHL	OMC-CMC-C2C	-2.55	119.91	125.69
30	D	409	LMG	O8-C28-C29	2.55	119.92	111.91
23	s	613	CLA	CMA-C3A-C2A	-2.55	110.14	116.10
35	g	606	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
38	N	617	NEX	C24-C23-C22	-2.55	105.85	110.77
23	B	615	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
23	c	504	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
35	r	606	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
35	R	307	CHL	O2D-CGD-O1D	-2.55	118.85	123.84
34	f	101	HEM	C4A-NA-C1A	2.55	107.84	105.35
23	c	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	d	409	LMG	O8-C28-C29	2.55	119.90	111.91
25	d	405	BCR	C3-C4-C5	-2.55	109.53	114.08
23	C	509	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	G	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	S	310	CLA	CHB-C4A-NA	2.54	128.03	124.51
34	f	101	HEM	C4D-ND-C1D	2.54	107.70	105.07
30	w	202	LMG	O8-C28-C29	2.54	119.89	111.91
23	y	312	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	c	521	LMG	C8-O7-C10	-2.54	111.53	117.79
23	c	508	CLA	CHB-C4A-NA	2.54	128.03	124.51
35	y	310	CHL	CHD-C1D-ND	-2.54	122.12	124.45
23	y	315	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	N	613	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
35	g	601	CHL	OMC-CMC-C2C	-2.54	119.95	125.69
23	B	608	CLA	CHB-C1B-NB	2.54	126.94	124.26
23	s	612	CLA	CHB-C4A-NA	2.54	128.02	124.51
28	c	515	DGD	O1G-C1A-C2A	2.54	119.87	111.91
35	r	605	CHL	O2D-CGD-O1D	-2.54	118.88	123.84
23	g	611	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	S	310	CLA	C3B-C4B-NB	-2.53	108.16	110.52
23	y	314	CLA	CHB-C4A-NA	2.53	128.02	124.51
23	B	611	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
36	y	316	LUT	C7-C8-C9	-2.53	122.41	126.23
35	g	606	CHL	CHD-C1D-ND	-2.53	122.13	124.45
23	C	507	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	N	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
38	g	618	NEX	C11-C12-C13	-2.53	119.31	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	g	616	LUT	C11-C10-C9	-2.53	123.70	127.31
23	Y	311	CLA	CMB-C2B-C3B	2.53	132.72	126.59
23	c	510	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
28	C	517	DGD	O1G-C1A-C2A	2.53	119.83	111.91
23	N	602	CLA	C3B-C4B-NB	-2.53	108.17	110.52
37	R	315	XAT	C19-C9-C8	2.52	122.06	118.08
35	g	601	CHL	CHD-C1D-ND	-2.52	122.13	124.45
37	R	315	XAT	C31-C30-C29	-2.52	123.71	127.31
31	S	318	LHG	O8-C23-C24	2.52	119.83	111.91
25	A	405	BCR	C24-C23-C22	-2.52	122.42	126.23
23	r	603	CLA	CAA-C2A-C3A	-2.52	105.87	112.78
35	N	609	CHL	CHB-C4A-NA	2.52	128.00	124.51
38	S	317	NEX	C16-C1-C6	2.52	112.73	110.47
35	N	608	CHL	C3B-C4B-NB	-2.52	108.18	110.52
23	S	312	CLA	CMB-C2B-C3B	2.52	132.69	126.59
23	r	609	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
35	G	601	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
23	b	613	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
38	r	615	NEX	C2-C1-C6	2.52	111.66	109.21
35	n	608	CHL	C3B-C4B-NB	-2.51	108.18	110.52
35	g	609	CHL	CHB-C1B-NB	2.51	126.92	124.26
36	Y	317	LUT	C36-C21-C26	2.51	113.35	109.55
23	y	304	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
23	S	313	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	a	401	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	R	304	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	b	617	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
23	r	611	CLA	CHB-C4A-NA	2.51	127.98	124.51
35	y	308	CHL	OMC-CMC-C2C	-2.51	120.02	125.69
35	N	601	CHL	CMB-C2B-C1B	-2.50	121.56	125.37
35	y	302	CHL	OMC-CMC-C2C	-2.50	120.03	125.69
36	S	315	LUT	C15-C14-C13	-2.50	123.74	127.31
25	b	620	BCR	C33-C5-C4	2.50	118.42	113.62
35	n	605	CHL	CMB-C2B-C3B	2.50	132.65	126.59
35	s	601	CHL	C3B-C4B-NB	-2.50	108.19	110.52
36	N	616	LUT	C11-C10-C9	-2.50	123.74	127.31
38	s	616	NEX	C24-C23-C22	-2.50	105.94	110.77
30	b	601	LMG	O8-C28-C29	2.50	119.76	111.91
30	b	622	LMG	O8-C28-C29	2.50	119.76	111.91
25	k	101	BCR	C10-C11-C12	-2.50	115.41	123.22
23	Y	313	CLA	C2A-C1A-CHA	2.50	128.23	123.86
23	C	507	CLA	CHB-C1B-NB	2.50	126.90	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	z	101	BCR	C33-C5-C6	-2.50	121.72	124.53
35	S	307	CHL	CHD-C1D-ND	-2.50	122.16	124.45
23	R	302	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	s	604	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
23	C	509	CLA	CMB-C2B-C3B	2.50	132.63	126.59
30	B	623	LMG	O8-C28-C29	2.50	119.74	111.91
23	B	614	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	s	604	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	g	613	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	G	613	CLA	CHB-C4A-NA	2.49	127.96	124.51
35	r	607	CHL	CHB-C4A-NA	2.49	127.96	124.51
36	y	317	LUT	C11-C10-C9	-2.49	123.75	127.31
23	d	403	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	s	609	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	c	514	BCR	C33-C5-C4	2.49	118.40	113.62
23	b	616	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	C	516	BCR	C33-C5-C4	2.49	118.40	113.62
35	Y	302	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
23	n	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	c	506	CLA	CHB-C4A-NA	2.49	127.95	124.51
36	G	615	LUT	C10-C11-C12	-2.49	115.46	123.22
35	N	601	CHL	OMC-CMC-C2C	-2.49	120.06	125.69
23	S	311	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
23	y	304	CLA	CHB-C1B-NB	2.48	126.89	124.26
23	D	403	CLA	CHB-C4A-NA	2.48	127.95	124.51
36	N	615	LUT	C11-C10-C9	-2.48	123.77	127.31
25	K	101	BCR	C24-C23-C22	-2.48	122.49	126.23
28	b	625	DGD	C1D-O6D-C5D	2.48	118.55	113.69
30	S	301	LMG	C7-O1-C1	-2.48	108.90	113.74
23	y	304	CLA	C2A-C1A-CHA	2.48	128.19	123.86
23	R	309	CLA	C3B-C4B-NB	-2.47	108.22	110.52
28	B	626	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
23	N	612	CLA	C2A-C1A-CHA	2.47	128.19	123.86
25	b	620	BCR	C38-C26-C25	-2.47	121.75	124.53
35	y	307	CHL	OMC-CMC-C2C	-2.47	120.09	125.69
38	N	617	NEX	C11-C10-C9	-2.47	123.78	127.31
23	R	313	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	C	519	BCR	C29-C30-C25	2.47	114.29	110.48
23	s	609	CLA	CMB-C2B-C3B	2.47	132.57	126.59
24	a	403	PHO	C4B-NB-C1B	2.47	112.65	108.83
23	y	313	CLA	C2A-C1A-CHA	2.47	128.18	123.86
25	K	101	BCR	C2-C1-C6	2.47	114.28	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	619	LHG	O8-C23-C24	2.47	119.66	111.91
23	Y	312	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	C	502	CLA	CHB-C4A-NA	2.47	127.92	124.51
35	s	601	CHL	CHD-C1D-ND	-2.47	122.19	124.45
36	s	615	LUT	C15-C14-C13	-2.47	123.79	127.31
23	b	609	CLA	CHB-C1B-NB	2.47	126.87	124.26
25	a	405	BCR	C33-C5-C4	2.47	118.35	113.62
23	R	310	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	A	401	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	B	618	BCR	C33-C5-C4	2.46	118.35	113.62
36	s	615	LUT	C10-C11-C12	-2.46	115.53	123.22
23	R	313	CLA	CHB-C1B-NB	2.46	126.86	124.26
25	B	618	BCR	C38-C26-C25	-2.46	121.76	124.53
38	r	615	NEX	C17-C1-C6	-2.46	108.27	110.47
23	g	614	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	G	610	CLA	CHC-C4B-NB	2.46	126.86	124.26
23	R	313	CLA	O2D-CGD-CBD	2.46	115.64	111.27
26	A	406	SQD	O48-C23-C24	2.46	119.62	111.91
35	Y	307	CHL	OMC-CMC-C2C	-2.46	120.13	125.69
36	g	616	LUT	C31-C30-C29	-2.46	123.80	127.31
35	S	308	CHL	CAA-C2A-C3A	-2.46	106.05	112.78
23	c	501	CLA	CHB-C1B-NB	2.46	126.86	124.26
23	S	309	CLA	O2D-CGD-CBD	2.45	115.63	111.27
35	y	302	CHL	C3B-C4B-NB	-2.45	108.24	110.52
36	N	615	LUT	C15-C14-C13	-2.45	123.81	127.31
25	A	405	BCR	C33-C5-C4	2.45	118.33	113.62
23	N	614	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	h	101	BCR	C16-C15-C14	-2.45	118.45	123.47
25	K	101	BCR	C23-C24-C25	-2.45	120.32	127.20
23	n	604	CLA	CMB-C2B-C1B	-2.45	121.64	125.37
35	S	308	CHL	CMB-C2B-C3B	2.45	132.51	126.59
30	s	619	LMG	O8-C28-C29	2.45	119.58	111.91
23	n	614	CLA	CHB-C4A-NA	2.44	127.89	124.51
35	n	608	CHL	CHB-C1B-NB	2.44	126.84	124.26
35	Y	302	CHL	CHB-C4A-NA	2.44	127.89	124.51
23	B	603	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	g	604	CLA	CHB-C1B-NB	2.44	126.84	124.26
35	y	306	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
23	b	612	CLA	CAA-C2A-C3A	-2.44	106.10	112.78
23	G	604	CLA	CHB-C4A-NA	2.44	127.89	124.51
25	D	405	BCR	C30-C25-C26	-2.44	119.18	122.61
36	s	614	LUT	C15-C14-C13	-2.44	123.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	r	614	XAT	C19-C9-C8	2.44	121.92	118.08
31	g	619	LHG	O8-C23-C24	2.44	119.56	111.91
23	r	612	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	G	603	CLA	O2D-CGD-CBD	2.44	115.60	111.27
35	N	608	CHL	CHD-C1D-ND	-2.44	122.21	124.45
30	C	501	LMG	C8-O7-C10	-2.44	111.79	117.79
38	R	316	NEX	C26-C27-C28	-2.44	120.84	125.99
23	C	513	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
38	S	317	NEX	C11-C12-C13	-2.44	119.57	126.42
36	g	616	LUT	C3-C4-C5	-2.43	107.01	111.85
23	r	603	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	r	609	CLA	CHB-C1B-NB	2.43	126.83	124.26
23	n	612	CLA	C2A-C1A-CHA	2.43	128.11	123.86
23	s	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
35	s	607	CHL	OMC-CMC-C2C	-2.43	120.19	125.69
35	Y	306	CHL	CHB-C4A-NA	2.43	127.87	124.51
28	d	410	DGD	O1G-C1A-C2A	2.43	119.53	111.91
23	n	610	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
25	C	519	BCR	C27-C26-C25	-2.43	119.21	122.73
25	H	101	BCR	C16-C15-C14	-2.43	118.50	123.47
35	y	306	CHL	CHB-C4A-NA	2.43	127.87	124.51
23	B	614	CLA	C3B-C4B-NB	-2.42	108.27	110.52
25	d	405	BCR	C30-C25-C26	-2.42	119.20	122.61
36	Y	317	LUT	C11-C10-C9	-2.42	123.85	127.31
23	c	513	CLA	C3B-C4B-NB	-2.42	108.27	110.52
23	B	607	CLA	CHB-C1B-NB	2.42	126.82	124.26
25	C	516	BCR	C24-C23-C22	-2.42	122.58	126.23
23	r	612	CLA	CHB-C1B-NB	2.42	126.82	124.26
23	Y	312	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
35	n	607	CHL	CAA-C2A-C3A	-2.42	106.15	112.78
35	n	601	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
35	N	606	CHL	CHD-C1D-ND	-2.42	122.23	124.45
36	y	316	LUT	C15-C14-C13	-2.42	123.86	127.31
30	S	301	LMG	O8-C28-C29	2.42	119.50	111.91
23	s	609	CLA	CHB-C1B-NB	2.42	126.82	124.26
35	s	607	CHL	CHB-C1B-NB	2.42	126.82	124.26
36	G	616	LUT	C15-C35-C34	-2.42	118.52	123.47
36	Y	316	LUT	C7-C8-C9	-2.42	122.58	126.23
35	N	608	CHL	CHB-C1B-NB	2.42	126.81	124.26
25	K	101	BCR	C16-C15-C14	-2.42	118.53	123.47
23	c	505	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
35	r	607	CHL	CHD-C1D-ND	-2.41	122.24	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	621	BCR	C33-C5-C4	2.41	118.25	113.62
36	Y	316	LUT	C10-C11-C12	-2.41	115.69	123.22
23	d	402	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	b	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
35	S	302	CHL	CHD-C1D-ND	-2.41	122.24	124.45
23	c	507	CLA	C2A-C1A-CHA	2.41	128.07	123.86
35	N	605	CHL	CMB-C2B-C3B	2.41	132.42	126.59
36	n	616	LUT	C10-C11-C12	-2.41	115.70	123.22
35	n	601	CHL	C3B-C4B-NB	-2.41	108.28	110.52
23	R	310	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
36	R	314	LUT	C18-C5-C6	-2.41	121.82	124.53
26	L	103	SQD	O48-C23-C24	2.41	119.46	111.91
23	r	601	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
23	n	602	CLA	CMB-C2B-C3B	2.41	132.41	126.59
23	B	603	CLA	C3B-C4B-NB	-2.40	108.28	110.52
35	s	607	CHL	C3B-C4B-NB	-2.40	108.28	110.52
23	y	305	CLA	CHB-C4A-NA	2.40	127.84	124.51
26	L	103	SQD	C1-O5-C5	2.40	118.41	113.69
23	C	508	CLA	C2A-C1A-CHA	2.40	128.06	123.86
38	s	616	NEX	C2-C1-C6	2.40	111.55	109.21
23	B	602	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	s	611	CLA	C2A-C1A-CHA	2.40	128.06	123.86
23	b	616	CLA	C3B-C4B-NB	-2.40	108.29	110.52
36	N	616	LUT	C31-C30-C29	-2.40	123.89	127.31
38	S	317	NEX	C26-C27-C28	-2.40	120.92	125.99
31	n	618	LHG	C5-O7-C7	-2.40	111.88	117.79
35	s	607	CHL	C2A-C3A-C4A	-2.40	97.99	101.87
36	G	616	LUT	C35-C34-C33	-2.40	123.89	127.31
23	b	605	CLA	CHB-C4A-NA	2.40	127.83	124.51
35	n	608	CHL	CHD-C1D-ND	-2.40	122.25	124.45
35	n	609	CHL	O2D-CGD-CBD	2.40	115.53	111.27
25	B	619	BCR	C33-C5-C4	2.40	118.22	113.62
26	a	406	SQD	O48-C23-C24	2.40	119.43	111.91
32	c	522	DMU	C1-C2-C3	2.40	115.15	109.68
23	B	615	CLA	O2D-CGD-CBD	2.40	115.53	111.27
28	B	624	DGD	O1G-C1A-C2A	2.40	119.42	111.91
35	g	609	CHL	O2D-CGD-CBD	2.39	115.52	111.27
25	b	620	BCR	C38-C26-C27	2.39	118.21	113.62
31	c	517	LHG	O8-C23-C24	2.39	119.42	111.91
31	C	518	LHG	O8-C23-C24	2.39	119.41	111.91
35	n	606	CHL	CHB-C4A-NA	2.39	127.82	124.51
31	R	317	LHG	O8-C23-C24	2.39	119.41	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Y	306	CHL	OMC-CMC-C2C	-2.39	120.29	125.69
23	b	617	CLA	O2D-CGD-CBD	2.39	115.51	111.27
23	Y	303	CLA	CMB-C2B-C1B	-2.39	121.73	125.37
36	S	316	LUT	C8-C9-C10	-2.39	115.28	118.94
35	y	302	CHL	CHB-C4A-NA	2.38	127.81	124.51
37	g	617	XAT	C15-C35-C34	-2.38	118.59	123.47
23	b	605	CLA	C3B-C4B-NB	-2.38	108.30	110.52
35	Y	302	CHL	C3B-C4B-NB	-2.38	108.30	110.52
23	Y	305	CLA	CHB-C4A-NA	2.38	127.81	124.51
23	B	608	CLA	CBA-CAA-C2A	2.38	120.89	113.86
23	C	506	CLA	CHC-C4B-NB	2.38	126.78	124.26
35	S	302	CHL	C3B-C4B-NB	-2.38	108.31	110.52
35	R	308	CHL	C3B-C4B-NB	-2.38	108.31	110.52
32	C	523	DMU	C1-C2-C3	2.38	115.11	109.68
25	B	618	BCR	C38-C26-C27	2.38	118.18	113.62
23	b	610	CLA	CBA-CAA-C2A	2.38	120.88	113.86
23	C	514	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	B	608	CLA	CHB-C4A-NA	2.38	127.80	124.51
31	b	626	LHG	O8-C23-C24	2.38	119.36	111.91
23	b	610	CLA	C3B-C4B-NB	-2.37	108.31	110.52
38	r	615	NEX	C26-C27-C28	-2.37	120.98	125.99
23	S	311	CLA	CHB-C4A-NA	2.37	127.79	124.51
35	G	608	CHL	CHB-C4A-NA	2.37	127.79	124.51
36	n	616	LUT	C7-C8-C9	-2.37	122.65	126.23
23	R	303	CLA	CHB-C4A-NA	2.37	127.79	124.51
35	r	606	CHL	CHB-C4A-NA	2.37	127.79	124.51
35	r	607	CHL	C3B-C4B-NB	-2.37	108.32	110.52
23	y	312	CLA	C3B-C4B-NB	-2.37	108.32	110.52
31	N	618	LHG	C5-O7-C7	-2.37	111.96	117.79
23	c	508	CLA	CMB-C2B-C3B	2.37	132.32	126.59
30	W	203	LMG	C8-O7-C10	-2.37	111.97	117.79
36	Y	317	LUT	C3-C4-C5	-2.37	107.14	111.85
35	g	607	CHL	CAA-C2A-C3A	-2.37	108.35	114.26
23	G	614	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	Y	312	CLA	C3B-C4B-NB	-2.36	108.32	110.52
25	b	620	BCR	C33-C5-C6	-2.36	121.87	124.53
23	R	303	CLA	C3B-C4B-NB	-2.36	108.32	110.52
23	r	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	C	506	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
37	G	617	XAT	C24-C23-C22	-2.36	106.22	110.77
23	d	402	CLA	CHB-C1B-NB	2.36	126.75	124.26
23	B	609	CLA	C3B-C4B-NB	-2.36	108.33	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	605	CHL	CHD-C1D-ND	-2.36	122.29	124.45
25	c	518	BCR	C15-C16-C17	-2.36	118.64	123.47
35	n	606	CHL	OMC-CMC-C2C	-2.36	120.36	125.69
36	g	616	LUT	C15-C35-C34	-2.36	118.64	123.47
25	k	101	BCR	C21-C20-C19	-2.36	115.86	123.22
23	Y	313	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
23	N	602	CLA	CMB-C2B-C3B	2.35	132.29	126.59
35	R	306	CHL	CMB-C2B-C3B	2.35	132.29	126.59
23	S	314	CLA	O2D-CGD-CBD	2.35	115.45	111.27
35	r	605	CHL	CMB-C2B-C3B	2.35	132.28	126.59
23	r	612	CLA	O2D-CGD-CBD	2.35	115.44	111.27
23	C	511	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
38	N	617	NEX	C26-C27-C28	-2.35	121.03	125.99
35	N	608	CHL	CHB-C4A-NA	2.35	127.76	124.51
35	S	306	CHL	CHD-C1D-ND	-2.35	122.30	124.45
31	r	616	LHG	O8-C23-C24	2.35	119.28	111.91
25	b	620	BCR	C30-C25-C26	-2.35	119.31	122.61
35	G	606	CHL	CMB-C2B-C3B	2.35	132.27	126.59
35	G	601	CHL	CHC-C1C-NC	2.34	127.76	124.20
25	B	618	BCR	C30-C25-C26	-2.34	119.31	122.61
23	g	604	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	S	311	CLA	C3B-C4B-NB	-2.34	108.34	110.52
23	c	506	CLA	CHB-C1B-NB	2.34	126.73	124.26
35	g	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
25	K	101	BCR	C38-C26-C25	-2.34	121.90	124.53
38	N	617	NEX	C16-C1-C6	2.34	112.56	110.47
31	R	317	LHG	C5-O7-C7	-2.34	112.04	117.79
35	Y	308	CHL	CAA-CBA-CGA	-2.34	106.42	113.25
28	D	410	DGD	O1G-C1A-C2A	2.34	119.24	111.91
25	k	101	BCR	C2-C1-C6	2.34	114.08	110.48
35	Y	308	CHL	C3B-C4B-NB	-2.34	108.35	110.52
30	w	202	LMG	C8-O7-C10	-2.34	112.04	117.79
36	n	615	LUT	C7-C8-C9	-2.33	122.71	126.23
23	S	311	CLA	CAA-C2A-C3A	-2.33	108.43	114.26
35	g	608	CHL	C3B-C4B-NB	-2.33	108.35	110.52
23	G	604	CLA	C3B-C4B-NB	-2.33	108.35	110.52
25	c	518	BCR	C21-C20-C19	-2.33	115.94	123.22
25	K	101	BCR	C21-C20-C19	-2.33	115.95	123.22
35	g	605	CHL	C3B-C4B-NB	-2.33	108.36	110.52
35	g	607	CHL	CHB-C4A-NA	2.33	127.73	124.51
23	d	403	CLA	C3B-C4B-NB	-2.33	108.36	110.52
35	n	608	CHL	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	S	315	LUT	C39-C29-C28	2.32	121.74	118.08
35	S	306	CHL	C3C-C4C-NC	-2.32	107.97	110.57
35	S	308	CHL	OMC-CMC-C2C	-2.32	120.44	125.69
36	s	614	LUT	C39-C29-C28	2.32	121.73	118.08
38	r	615	NEX	C15-C35-C34	-2.32	118.72	123.47
35	N	609	CHL	C2A-C1A-CHA	2.32	127.91	123.86
35	n	607	CHL	C2A-C1A-CHA	2.32	127.91	123.86
25	c	518	BCR	C27-C26-C25	-2.32	119.37	122.73
35	y	309	CHL	OMC-CMC-C2C	-2.31	120.46	125.69
35	Y	307	CHL	CHB-C4A-NA	2.31	127.71	124.51
26	L	103	SQD	O7-S-C6	2.31	109.69	106.94
35	G	606	CHL	CHB-C4A-NA	2.31	127.71	124.51
23	R	302	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
35	r	607	CHL	O2A-CGA-O1A	-2.31	117.76	123.59
37	g	617	XAT	C27-C28-C29	-2.31	121.95	125.53
23	n	612	CLA	CHB-C1B-NB	2.31	126.70	124.26
36	y	317	LUT	C36-C21-C26	2.31	113.04	109.55
35	g	605	CHL	CHB-C4A-NA	2.31	127.70	124.51
35	y	309	CHL	CHB-C4A-NA	2.31	127.70	124.51
35	R	306	CHL	CHB-C4A-NA	2.31	127.70	124.51
35	S	308	CHL	C2A-C3A-C4A	-2.31	98.14	101.87
28	b	625	DGD	C2G-O2G-C1B	-2.31	112.12	117.79
35	n	609	CHL	C2A-C1A-CHA	2.30	127.89	123.86
23	r	602	CLA	C3B-C4B-NB	-2.30	108.38	110.52
23	s	603	CLA	C2A-C1A-CHA	2.30	127.89	123.86
25	B	618	BCR	C33-C5-C6	-2.30	121.94	124.53
36	n	616	LUT	C30-C31-C32	-2.30	116.03	123.22
38	s	616	NEX	C15-C35-C34	-2.30	118.76	123.47
23	Y	313	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
35	n	607	CHL	O2D-CGD-CBD	2.30	115.36	111.27
23	n	610	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
23	N	604	CLA	C3B-C4B-NB	-2.30	108.38	110.52
38	R	316	NEX	C4-C3-C2	-2.30	106.33	110.77
23	S	305	CLA	CHB-C4A-NA	2.30	127.69	124.51
35	N	601	CHL	CHD-C1D-ND	-2.30	122.34	124.45
35	n	601	CHL	CHB-C4A-NA	2.30	127.69	124.51
31	d	407	LHG	O8-C23-C24	2.30	119.11	111.91
23	R	313	CLA	CHD-C1D-ND	-2.29	122.34	124.45
35	Y	309	CHL	CHB-C4A-NA	2.29	127.68	124.51
35	R	308	CHL	CHD-C1D-ND	-2.29	122.35	124.45
23	G	604	CLA	CHB-C1B-NB	2.29	126.69	124.26
36	s	615	LUT	C35-C15-C14	-2.29	118.78	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	G	608	CHL	CHD-C1D-ND	-2.29	122.35	124.45
25	B	619	BCR	C29-C30-C25	2.29	114.01	110.48
36	G	616	LUT	C3-C4-C5	-2.29	107.29	111.85
23	C	506	CLA	CHB-C1B-NB	2.29	126.68	124.26
31	B	627	LHG	O8-C23-C24	2.29	119.10	111.91
36	G	616	LUT	C11-C10-C9	-2.29	124.04	127.31
35	g	601	CHL	CHC-C1C-NC	2.29	127.68	124.20
36	s	614	LUT	C20-C13-C12	2.29	121.69	118.08
35	G	601	CHL	C2A-C1A-CHA	2.29	127.86	123.86
23	y	313	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
37	Y	301	XAT	C30-C31-C32	-2.29	116.08	123.22
35	y	308	CHL	CHD-C1D-ND	-2.29	122.35	124.45
23	N	603	CLA	C2A-C1A-CHA	2.29	127.86	123.86
36	N	616	LUT	C15-C35-C34	-2.29	118.79	123.47
35	G	606	CHL	CHD-C1D-ND	-2.29	122.35	124.45
28	A	408	DGD	C2G-O2G-C1B	-2.28	112.17	117.79
35	N	607	CHL	C2A-C1A-CHA	2.28	127.85	123.86
23	S	312	CLA	C2A-C1A-CHA	2.28	127.85	123.86
35	g	601	CHL	C2A-C1A-CHA	2.28	127.85	123.86
23	b	617	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
25	K	101	BCR	C7-C8-C9	-2.28	122.79	126.23
35	n	609	CHL	CHB-C4A-NA	2.28	127.67	124.51
31	D	407	LHG	O8-C23-C24	2.28	119.06	111.91
38	G	618	NEX	C26-C27-C28	-2.28	121.17	125.99
23	B	608	CLA	C3B-C4B-NB	-2.28	108.40	110.52
23	n	604	CLA	C3B-C4B-NB	-2.28	108.40	110.52
25	a	405	BCR	C1-C6-C5	-2.28	119.40	122.61
23	D	401	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
36	n	616	LUT	C16-C1-C6	-2.28	106.60	110.30
36	g	616	LUT	C16-C1-C6	-2.28	106.61	110.30
35	n	606	CHL	C2A-C1A-CHA	2.28	127.84	123.86
23	Y	311	CLA	CHB-C1B-NB	2.28	126.67	124.26
38	S	317	NEX	C28-C29-C30	2.28	122.43	118.94
35	g	608	CHL	CHD-C1D-ND	-2.28	122.36	124.45
38	s	616	NEX	C11-C12-C13	-2.27	120.03	126.42
23	A	404	CLA	C3B-C4B-NB	-2.27	108.41	110.52
25	K	101	BCR	C27-C26-C25	-2.27	119.43	122.73
32	C	520	DMU	C1-C2-C3	2.27	114.87	109.68
23	Y	304	CLA	C2A-C1A-CHA	2.27	127.83	123.86
25	A	405	BCR	C1-C6-C5	-2.27	119.41	122.61
23	r	612	CLA	C3B-C4B-NB	-2.27	108.41	110.52
35	R	307	CHL	CHB-C4A-NA	2.27	127.65	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	s	605	CHL	CHB-C4A-NA	2.27	127.65	124.51
25	C	519	BCR	C21-C20-C19	-2.27	116.14	123.22
36	n	616	LUT	C36-C21-C26	2.27	112.98	109.55
35	Y	310	CHL	C3B-C4B-NB	-2.27	108.41	110.52
23	S	310	CLA	CMB-C2B-C3B	2.27	132.08	126.59
25	d	405	BCR	C15-C16-C17	-2.27	118.83	123.47
23	g	614	CLA	CAA-C2A-C3A	-2.27	108.60	114.26
36	r	613	LUT	C1-C6-C5	-2.27	119.42	122.61
25	C	519	BCR	C31-C1-C6	-2.27	106.62	110.30
23	s	604	CLA	CHB-C1B-NB	2.26	126.65	124.26
23	b	605	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	b	619	BCR	C24-C23-C22	-2.26	122.82	126.23
23	N	610	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
25	B	617	BCR	C24-C23-C22	-2.26	122.82	126.23
23	s	602	CLA	CHB-C1B-NB	2.26	126.65	124.26
36	r	613	LUT	C35-C15-C14	-2.26	118.84	123.47
35	y	307	CHL	CHB-C4A-NA	2.26	127.64	124.51
36	y	316	LUT	C20-C13-C12	2.26	121.64	118.08
23	b	611	CLA	C3B-C4B-NB	-2.26	108.42	110.52
35	G	607	CHL	C3B-C4B-NB	-2.26	108.42	110.52
23	s	609	CLA	C3B-C4B-NB	-2.26	108.42	110.52
37	G	620	XAT	C7-C8-C9	-2.26	122.03	125.53
23	g	603	CLA	C2A-C1A-CHA	2.26	127.81	123.86
35	N	606	CHL	CHB-C4A-NA	2.26	127.63	124.51
36	S	315	LUT	C11-C10-C9	-2.26	124.09	127.31
35	y	307	CHL	CMB-C2B-C3B	2.25	132.05	126.59
35	r	605	CHL	CHB-C4A-NA	2.25	127.62	124.51
23	n	610	CLA	CMB-C2B-C3B	2.25	132.04	126.59
34	F	101	HEM	CAB-C3B-C2B	-2.25	121.19	128.60
35	y	307	CHL	C3B-C4B-NB	-2.25	108.43	110.52
23	y	312	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	R	310	CLA	C3B-C4B-NB	-2.25	108.43	110.52
27	a	408	BCT	O3-C-O1	-2.25	113.71	119.55
23	g	602	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	c	512	CLA	CMB-C2B-C1B	-2.25	121.95	125.37
36	S	315	LUT	C20-C13-C12	2.25	121.62	118.08
35	G	607	CHL	CHB-C4A-NA	2.25	127.62	124.51
25	b	621	BCR	C29-C30-C25	2.25	113.94	110.48
25	d	405	BCR	C33-C5-C6	-2.24	122.01	124.53
35	N	607	CHL	CHD-C1D-ND	-2.24	122.39	124.45
23	C	506	CLA	CMB-C2B-C1B	-2.24	121.95	125.37
35	y	302	CHL	CHD-C1D-ND	-2.24	122.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	y	313	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	L	101	LHG	O8-C23-O10	-2.24	117.93	123.59
34	f	101	HEM	CAB-C3B-C2B	-2.24	121.21	128.60
32	c	519	DMU	C1-C2-C3	2.24	114.80	109.68
35	n	607	CHL	CHD-C1D-ND	-2.24	122.39	124.45
23	B	608	CLA	CHC-C4B-NB	2.24	126.63	124.26
35	Y	307	CHL	CMB-C2B-C3B	2.24	132.01	126.59
31	y	318	LHG	O8-C23-C24	2.24	118.94	111.91
35	y	308	CHL	C3B-C4B-NB	-2.24	108.44	110.52
26	L	103	SQD	O8-S-C6	2.24	109.31	105.74
23	N	611	CLA	C3B-C4B-NB	-2.24	108.44	110.52
23	S	310	CLA	CHB-C1B-NB	2.24	126.63	124.26
25	k	101	BCR	C23-C24-C25	-2.24	120.92	127.20
23	B	603	CLA	CHB-C1B-NB	2.24	126.63	124.26
23	r	602	CLA	O2D-CGD-CBD	2.24	115.24	111.27
26	a	406	SQD	O8-S-C6	2.24	109.31	105.74
25	c	514	BCR	C1-C6-C5	-2.24	119.46	122.61
35	R	307	CHL	C3B-C4B-NB	-2.24	108.44	110.52
36	n	615	LUT	C20-C13-C12	2.24	121.60	118.08
30	a	407	LMG	C8-O7-C10	-2.24	112.29	117.79
23	Y	313	CLA	CHA-C1A-NA	-2.23	121.28	126.40
25	c	518	BCR	C10-C11-C12	-2.23	116.25	123.22
23	G	603	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
23	B	616	CLA	C3B-C4B-NB	-2.23	108.44	110.52
23	b	618	CLA	C3B-C4B-NB	-2.23	108.44	110.52
26	A	406	SQD	O8-S-C6	2.23	109.30	105.74
25	C	516	BCR	C1-C6-C5	-2.23	119.47	122.61
23	R	312	CLA	C3B-C4B-NB	-2.23	108.45	110.52
23	d	401	CLA	CMB-C2B-C1B	-2.23	121.97	125.37
23	B	614	CLA	CHB-C1B-NB	2.23	126.62	124.26
27	A	407	BCT	O3-C-O1	-2.23	113.77	119.55
23	d	403	CLA	O2D-CGD-CBD	2.23	115.22	111.27
23	B	615	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	b	604	CLA	CHC-C4B-NB	2.23	126.61	124.26
23	y	313	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
23	a	404	CLA	C3B-C4B-NB	-2.22	108.45	110.52
36	G	615	LUT	C30-C31-C32	-2.22	116.28	123.22
25	b	620	BCR	C1-C6-C5	-2.22	119.48	122.61
23	C	513	CLA	CMB-C2B-C3B	2.22	131.97	126.59
36	S	316	LUT	C15-C35-C34	-2.22	118.92	123.47
35	G	608	CHL	C3B-C4B-NB	-2.22	108.45	110.52
35	G	601	CHL	C2D-C1D-ND	-2.22	108.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	CHD-C1D-ND	-2.22	122.41	124.45
36	G	616	LUT	C16-C1-C6	-2.22	106.70	110.30
23	C	510	CLA	C3B-C4B-NB	-2.22	108.46	110.52
23	D	401	CLA	O2D-CGD-CBD	2.22	115.21	111.27
38	s	616	NEX	C31-C30-C29	-2.22	124.14	127.31
23	s	613	CLA	O2D-CGD-CBD	2.22	115.21	111.27
25	D	405	BCR	C33-C5-C6	-2.22	122.04	124.53
23	R	305	CLA	O2D-CGD-CBD	2.21	115.20	111.27
36	n	615	LUT	C10-C11-C12	-2.21	116.31	123.22
23	G	603	CLA	C2A-C1A-CHA	2.21	127.73	123.86
23	B	616	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
26	c	520	SQD	O48-C23-C24	2.21	118.85	111.91
35	G	605	CHL	CHB-C4A-NA	2.21	127.57	124.51
23	b	609	CLA	C3B-C4B-NB	-2.21	108.46	110.52
35	N	601	CHL	CMB-C2B-C3B	2.21	131.94	126.59
23	G	614	CLA	CAA-C2A-C3A	-2.21	108.74	114.26
23	r	612	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
23	y	303	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
35	S	308	CHL	CHB-C1B-NB	2.21	126.60	124.26
23	G	610	CLA	C3B-C4B-NB	-2.21	108.47	110.52
36	s	614	LUT	C11-C10-C9	-2.21	124.16	127.31
35	R	308	CHL	CHC-C4B-NB	2.21	126.59	124.26
25	D	405	BCR	C15-C16-C17	-2.21	118.95	123.47
38	S	317	NEX	C4-C3-C2	-2.21	106.51	110.77
23	A	401	CLA	CHC-C4B-NB	2.21	126.59	124.26
35	G	605	CHL	C3B-C4B-NB	-2.21	108.47	110.52
36	n	615	LUT	C39-C29-C28	2.21	121.55	118.08
23	Y	304	CLA	CHB-C1B-NB	2.21	126.59	124.26
23	B	607	CLA	C3B-C4B-NB	-2.21	108.47	110.52
31	Y	319	LHG	O8-C23-C24	2.20	118.83	111.91
36	N	616	LUT	C16-C1-C6	-2.20	106.72	110.30
25	C	515	BCR	C33-C5-C6	-2.20	122.05	124.53
38	s	616	NEX	C16-C1-C6	2.20	112.44	110.47
23	B	615	CLA	C3B-C4B-NB	-2.20	108.47	110.52
36	n	616	LUT	C3-C4-C5	-2.20	107.47	111.85
23	g	604	CLA	C3B-C4B-NB	-2.20	108.47	110.52
35	N	607	CHL	C3B-C4B-NB	-2.20	108.47	110.52
23	Y	303	CLA	CMB-C2B-C3B	2.20	131.91	126.59
35	Y	302	CHL	CHD-C1D-ND	-2.20	122.43	124.45
31	N	618	LHG	O8-C23-C24	2.20	118.81	111.91
25	B	618	BCR	C1-C6-C5	-2.20	119.52	122.61
23	G	612	CLA	C2A-C1A-CHA	2.20	127.70	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	401	CLA	O2D-CGD-CBD	2.20	115.17	111.27
35	Y	308	CHL	CAA-C2A-C1A	-2.20	104.78	111.97
23	C	504	CLA	C3B-C4B-NB	-2.19	108.48	110.52
35	S	307	CHL	C3B-C4B-NB	-2.19	108.48	110.52
25	B	617	BCR	C33-C5-C4	2.19	117.83	113.62
26	a	406	SQD	O9-S-C6	2.19	109.55	106.94
35	Y	308	CHL	CHD-C1D-ND	-2.19	122.44	124.45
36	r	613	LUT	C18-C5-C4	2.19	118.42	114.36
35	y	308	CHL	CAA-CBA-CGA	-2.19	106.85	113.25
23	s	611	CLA	CHB-C1B-NB	2.19	126.58	124.26
23	s	608	CLA	C3B-C4B-NB	-2.19	108.48	110.52
35	N	601	CHL	C3B-C4B-NB	-2.19	108.48	110.52
36	Y	317	LUT	C35-C15-C14	-2.19	118.99	123.47
23	b	617	CLA	C3B-C4B-NB	-2.19	108.48	110.52
36	N	615	LUT	C7-C8-C9	-2.19	122.93	126.23
36	S	315	LUT	C19-C9-C8	2.19	121.53	118.08
23	R	304	CLA	C3B-C4B-NB	-2.19	108.48	110.52
23	B	614	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
35	Y	309	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
35	Y	306	CHL	O2A-CGA-O1A	-2.19	118.07	123.59
35	r	607	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
23	A	404	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
31	l	102	LHG	O8-C23-O10	-2.19	118.08	123.59
26	C	521	SQD	O48-C23-C24	2.19	118.77	111.91
35	n	607	CHL	OMC-CMC-C2C	-2.18	120.75	125.69
23	G	604	CLA	CMB-C2B-C1B	-2.18	122.04	125.37
23	N	613	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
26	l	101	SQD	O8-S-C6	2.18	109.22	105.74
25	C	515	BCR	C1-C6-C5	-2.18	119.54	122.61
36	N	615	LUT	C39-C29-C28	2.18	121.51	118.08
36	s	615	LUT	C11-C10-C9	-2.18	124.20	127.31
23	g	604	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
35	R	307	CHL	OMC-CMC-C2C	-2.18	120.76	125.69
31	n	618	LHG	O8-C23-C24	2.18	118.75	111.91
38	r	615	NEX	C4-C3-C2	-2.18	106.56	110.77
23	Y	305	CLA	C3B-C4B-NB	-2.18	108.49	110.52
38	s	616	NEX	C30-C31-C32	-2.18	116.42	123.22
23	n	614	CLA	C3B-C4B-NB	-2.18	108.50	110.52
36	N	615	LUT	C10-C11-C12	-2.18	116.42	123.22
23	R	313	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
23	r	604	CLA	O2D-CGD-CBD	2.18	115.13	111.27
25	b	619	BCR	C15-C16-C17	-2.17	119.02	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	n	606	CHL	CMB-C2B-C3B	2.17	131.85	126.59
26	A	406	SQD	O9-S-C6	2.17	109.52	106.94
35	s	605	CHL	C3B-C4B-NB	-2.17	108.50	110.52
36	g	615	LUT	C10-C11-C12	-2.17	116.43	123.22
36	n	615	LUT	C15-C14-C13	-2.17	124.21	127.31
23	N	612	CLA	CHB-C1B-NB	2.17	126.56	124.26
23	C	511	CLA	O2D-CGD-CBD	2.17	115.13	111.27
38	G	618	NEX	C17-C1-C6	-2.17	108.53	110.47
23	c	509	CLA	C3B-C4B-NB	-2.17	108.50	110.52
23	b	618	CLA	C2A-C1A-CHA	2.17	127.66	123.86
23	c	502	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	g	614	CLA	C3B-C4B-NB	-2.17	108.50	110.52
35	N	607	CHL	CAA-C2A-C3A	-2.17	106.83	112.78
35	y	308	CHL	CAA-C2A-C1A	-2.17	104.86	111.97
23	B	606	CLA	CHB-C1B-NB	2.17	126.56	124.26
25	b	619	BCR	C33-C5-C4	2.17	117.79	113.62
23	r	608	CLA	C3B-C4B-NB	-2.17	108.50	110.52
38	N	617	NEX	C31-C30-C29	-2.17	124.21	127.31
23	g	603	CLA	CHC-C4B-NB	2.17	126.55	124.26
23	s	608	CLA	O2A-CGA-O1A	-2.17	117.89	123.30
35	G	609	CHL	OMC-CMC-C2C	-2.17	120.78	125.69
23	s	611	CLA	CHA-C1A-NA	-2.17	121.43	126.40
36	s	614	LUT	C7-C8-C9	-2.17	122.96	126.23
23	C	514	CLA	CHB-C1B-NB	2.17	126.55	124.26
35	y	306	CHL	C3B-C4B-NB	-2.17	108.50	110.52
23	A	402	CLA	CAA-C2A-C1A	2.17	119.08	111.97
36	G	616	LUT	C20-C13-C12	2.17	121.49	118.08
38	n	617	NEX	C30-C31-C32	-2.17	116.45	123.22
23	r	611	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
35	G	607	CHL	CAA-C2A-C3A	-2.17	108.84	114.26
23	Y	313	CLA	CMB-C2B-C3B	2.17	131.84	126.59
23	r	609	CLA	C3B-C4B-NB	-2.17	108.50	110.52
35	y	310	CHL	C3B-C4B-NB	-2.17	108.50	110.52
23	B	602	CLA	CHC-C4B-NB	2.17	126.55	124.26
23	y	311	CLA	C3B-C4B-NB	-2.17	108.51	110.52
35	R	308	CHL	O2D-CGD-CBD	2.17	115.12	111.27
23	b	616	CLA	CHB-C1B-NB	2.16	126.55	124.26
36	y	317	LUT	C35-C15-C14	-2.16	119.04	123.47
23	g	613	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
25	z	101	BCR	C30-C25-C26	-2.16	119.57	122.61
23	n	610	CLA	C3B-C4B-NB	-2.16	108.51	110.52
35	Y	309	CHL	CHB-C1B-NB	2.16	126.55	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
35	y	310	CHL	CMB-C2B-C1B	-2.16	122.08	125.37
37	G	617	XAT	C27-C28-C29	-2.16	122.18	125.53
23	b	607	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	b	608	CLA	CHB-C1B-NB	2.16	126.54	124.26
35	y	309	CHL	CHB-C1B-NB	2.16	126.54	124.26
35	y	306	CHL	O2A-CGA-O1A	-2.16	118.14	123.59
23	c	513	CLA	CBA-CAA-C2A	2.16	120.23	113.86
23	b	608	CLA	C3B-C4B-NB	-2.16	108.52	110.52
23	c	503	CLA	C3B-C4B-NB	-2.16	108.52	110.52
23	C	512	CLA	C2A-C1A-CHA	2.15	127.63	123.86
35	s	607	CHL	CHB-C4A-NA	2.15	127.49	124.51
35	y	310	CHL	CHB-C4A-NA	2.15	127.49	124.51
25	b	620	BCR	C8-C7-C6	-2.15	121.15	127.20
23	B	614	CLA	C2A-C1A-CHA	2.15	127.62	123.86
23	b	616	CLA	C2A-C1A-CHA	2.15	127.62	123.86
23	b	617	CLA	C2A-C1A-CHA	2.15	127.62	123.86
35	y	306	CHL	C2A-C1A-CHA	2.15	127.62	123.86
25	B	618	BCR	C8-C7-C6	-2.15	121.16	127.20
24	a	402	PHO	CMB-C2B-C3B	2.15	128.70	124.68
23	Y	315	CLA	C3B-C4B-NB	-2.15	108.52	110.52
38	N	617	NEX	C2-C1-C6	2.15	111.30	109.21
23	g	603	CLA	CHA-C1A-NA	-2.15	121.47	126.40
34	F	101	HEM	CAC-C3C-C4C	-2.15	119.70	124.90
26	L	103	SQD	O9-S-C6	2.15	109.50	106.94
36	G	616	LUT	C30-C31-C32	-2.15	116.51	123.22
38	R	316	NEX	C2-C1-C6	2.15	111.30	109.21
36	N	616	LUT	C20-C13-C12	2.15	121.46	118.08
36	g	615	LUT	C30-C31-C32	-2.15	116.51	123.22
38	g	618	NEX	C17-C1-C6	-2.15	108.55	110.47
23	a	404	CLA	CMB-C2B-C1B	-2.15	122.10	125.37
23	b	616	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
34	f	101	HEM	CAC-C3C-C4C	-2.15	119.71	124.90
23	y	315	CLA	C3B-C4B-NB	-2.15	108.52	110.52
35	Y	307	CHL	C3B-C4B-NB	-2.15	108.52	110.52
35	g	606	CHL	CHB-C4A-NA	2.15	127.48	124.51
36	y	317	LUT	C1-C2-C3	2.15	118.49	113.64
28	C	517	DGD	C2G-O2G-C1B	-2.14	112.51	117.79
35	g	607	CHL	C3B-C4B-NB	-2.14	108.53	110.52
37	y	301	XAT	C30-C31-C32	-2.14	116.53	123.22
23	b	606	CLA	C2A-C1A-CHA	2.14	127.61	123.86
23	n	611	CLA	C3B-C4B-NB	-2.14	108.53	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	CHB-C1B-NB	2.14	126.53	124.26
23	c	505	CLA	CHC-C4B-NB	2.14	126.53	124.26
25	B	617	BCR	C15-C16-C17	-2.14	119.09	123.47
23	c	506	CLA	C3B-C4B-NB	-2.14	108.53	110.52
23	n	613	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	y	304	CLA	CHA-C1A-NA	-2.14	121.49	126.40
23	b	611	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	B	615	CLA	C2A-C1A-CHA	2.14	127.60	123.86
25	z	101	BCR	C1-C6-C5	-2.14	119.60	122.61
23	c	510	CLA	O2D-CGD-CBD	2.14	115.07	111.27
37	R	315	XAT	C15-C35-C34	-2.14	119.09	123.47
23	N	614	CLA	C3B-C4B-NB	-2.14	108.53	110.52
37	g	620	XAT	C7-C8-C9	-2.14	122.21	125.53
35	Y	310	CHL	CHB-C4A-NA	2.14	127.47	124.51
33	D	406	PL9	C53-C6-C1	2.14	119.36	114.99
31	r	616	LHG	C5-O7-C7	-2.14	112.53	117.79
35	G	609	CHL	C3B-C4B-NB	-2.14	108.53	110.52
35	g	607	CHL	C2A-C1A-CHA	2.14	127.59	123.86
23	C	512	CLA	CHD-C1D-ND	-2.14	122.49	124.45
36	Y	317	LUT	C16-C1-C6	-2.14	106.83	110.30
38	s	616	NEX	C26-C27-C28	-2.13	121.48	125.99
36	r	613	LUT	C30-C31-C32	-2.13	116.56	123.22
23	B	613	CLA	C3B-C4B-NB	-2.13	108.53	110.52
23	Y	305	CLA	CMB-C2B-C3B	2.13	131.76	126.59
37	Y	301	XAT	C27-C28-C29	-2.13	122.22	125.53
35	Y	306	CHL	C2A-C1A-CHA	2.13	127.59	123.86
23	n	602	CLA	CHB-C1B-NB	2.13	126.52	124.26
23	B	604	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
31	n	618	LHG	O7-C7-O9	-2.13	118.55	123.70
23	N	610	CLA	CHB-C1B-NB	2.13	126.51	124.26
36	Y	316	LUT	C39-C29-C28	2.13	121.44	118.08
35	S	306	CHL	C2D-C1D-ND	-2.13	108.53	110.10
30	B	620	LMG	C8-O7-C10	-2.13	112.54	117.79
23	B	611	CLA	CHB-C1B-NB	2.13	126.51	124.26
31	B	622	LHG	O8-C23-C24	2.13	118.59	111.91
35	N	606	CHL	CMB-C2B-C3B	2.13	131.75	126.59
25	C	516	BCR	C37-C22-C23	2.13	121.43	118.08
38	s	616	NEX	C28-C29-C30	2.13	122.21	118.94
36	R	314	LUT	C10-C11-C12	-2.13	116.57	123.22
23	C	508	CLA	C3B-C4B-NB	-2.13	108.54	110.52
23	R	310	CLA	CHC-C4B-NB	2.13	126.51	124.26
23	D	403	CLA	O2D-CGD-CBD	2.13	115.05	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	F	101	HEM	C4C-NC-C1C	2.13	107.43	105.35
25	C	519	BCR	C1-C6-C5	-2.13	119.62	122.61
24	A	403	PHO	CMB-C2B-C3B	2.13	128.66	124.68
23	A	404	CLA	CHB-C1B-NB	2.13	126.51	124.26
35	s	606	CHL	C2A-C1A-CHA	2.13	127.58	123.86
23	c	505	CLA	CHB-C1B-NB	2.12	126.51	124.26
36	G	615	LUT	C20-C13-C12	2.12	121.42	118.08
36	y	316	LUT	C39-C29-C28	2.12	121.42	118.08
25	c	514	BCR	C20-C21-C22	-2.12	124.28	127.31
35	y	310	CHL	CHA-C1A-NA	-2.12	121.54	126.40
36	n	616	LUT	C11-C10-C9	-2.12	124.28	127.31
25	b	619	BCR	C4-C5-C6	-2.12	119.65	122.73
23	s	611	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
23	y	313	CLA	CMB-C2B-C3B	2.12	131.73	126.59
23	B	616	CLA	C2A-C1A-CHA	2.12	127.57	123.86
30	S	301	LMG	O1-C1-C2	2.12	111.61	108.30
25	K	101	BCR	C10-C11-C12	-2.12	116.60	123.22
35	y	309	CHL	O2A-CGA-O1A	-2.12	118.24	123.59
23	G	614	CLA	C3B-C4B-NB	-2.12	108.55	110.52
23	R	312	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	G	610	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	r	603	CLA	C3B-C4B-NB	-2.12	108.55	110.52
35	S	302	CHL	CHB-C4A-NA	2.12	127.44	124.51
33	d	406	PL9	C53-C6-C1	2.12	119.31	114.99
38	G	618	NEX	O24-C25-C26	-2.11	57.21	58.96
36	n	616	LUT	C35-C15-C14	-2.11	119.14	123.47
36	R	314	LUT	C16-C1-C6	-2.11	106.87	110.30
23	y	305	CLA	C3B-C4B-NB	-2.11	108.56	110.52
23	B	604	CLA	C2A-C1A-CHA	2.11	127.55	123.86
35	N	605	CHL	O1D-CGD-CBD	2.11	128.80	124.48
25	B	617	BCR	C4-C5-C6	-2.11	119.67	122.73
23	r	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
25	b	620	BCR	C4-C5-C6	-2.11	119.67	122.73
31	b	624	LHG	O8-C23-C24	2.11	118.53	111.91
23	s	608	CLA	O2D-CGD-CBD	2.11	115.02	111.27
38	S	317	NEX	O24-C25-C26	-2.11	57.21	58.96
23	d	401	CLA	CHB-C1B-NB	2.11	126.49	124.26
35	y	309	CHL	CHD-C1D-ND	-2.11	122.52	124.45
30	s	619	LMG	O1-C1-C2	2.11	111.59	108.30
23	D	404	CLA	O2D-CGD-CBD	2.11	115.01	111.27
23	r	612	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	c	507	CLA	C3B-C4B-NB	-2.11	108.56	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	618	BCR	C4-C5-C6	-2.10	119.67	122.73
23	B	609	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	y	314	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	g	614	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	d	402	CLA	CHD-C1D-ND	-2.10	122.52	124.45
38	S	317	NEX	C30-C31-C32	-2.10	116.65	123.22
37	G	620	XAT	O24-C25-C26	-2.10	57.22	58.96
35	G	606	CHL	CHB-C1B-NB	2.10	126.48	124.26
23	b	606	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
23	c	502	CLA	C2A-C1A-CHA	2.10	127.53	123.86
30	C	522	LMG	C4-C3-C2	2.10	114.49	110.82
31	B	621	LHG	O8-C23-O10	-2.10	118.29	123.59
25	K	101	BCR	C37-C22-C23	2.10	121.39	118.08
30	b	622	LMG	C8-O7-C10	-2.10	112.62	117.79
23	a	404	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	G	614	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	G	602	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
35	Y	310	CHL	CHA-C1A-NA	-2.10	121.59	126.40
23	S	305	CLA	CMB-C2B-C3B	2.10	131.67	126.59
23	G	614	CLA	CHD-C1D-ND	-2.10	122.53	124.45
35	N	606	CHL	C2A-C1A-CHA	2.10	127.53	123.86
23	B	615	CLA	C3A-C2A-C1A	2.10	104.48	101.34
35	n	606	CHL	CHB-C1B-NB	2.10	126.48	124.26
35	Y	309	CHL	CHD-C1D-ND	-2.10	122.53	124.45
26	A	406	SQD	O7-S-C6	2.10	109.43	106.94
23	b	605	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	b	615	CLA	C3B-C4B-NB	-2.09	108.57	110.52
34	f	101	HEM	C4C-NC-C1C	2.09	107.40	105.35
23	b	618	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
23	B	603	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	c	512	CLA	CMB-C2B-C3B	2.09	131.66	126.59
23	y	315	CLA	CHB-C1B-NB	2.09	126.47	124.26
23	G	613	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
35	n	609	CHL	OMC-CMC-C2C	-2.09	120.95	125.69
35	G	605	CHL	CHB-C1B-NB	2.09	126.47	124.26
36	g	616	LUT	C30-C31-C32	-2.09	116.69	123.22
23	B	611	CLA	C3B-C4B-NB	-2.09	108.58	110.52
23	C	510	CLA	C2A-C1A-CHA	2.09	127.51	123.86
35	R	308	CHL	O2A-CGA-O1A	-2.09	118.32	123.59
31	b	623	LHG	O8-C23-O10	-2.09	118.32	123.59
38	g	618	NEX	C2-C1-C6	2.09	111.24	109.21
23	b	613	CLA	C3B-C4B-NB	-2.09	108.58	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	606	CHL	CHB-C1B-NB	2.09	126.47	124.26
38	N	617	NEX	C19-C9-C10	-2.09	120.00	122.92
25	C	515	BCR	C30-C25-C26	-2.08	119.68	122.61
23	d	404	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	n	611	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	b	610	CLA	CHC-C4B-NB	2.08	126.46	124.26
35	r	607	CHL	O2D-CGD-CBD	2.08	114.97	111.27
35	g	601	CHL	CHB-C4A-NA	2.08	127.39	124.51
38	n	617	NEX	O24-C25-C26	-2.08	57.24	58.96
38	Y	318	NEX	O24-C25-C26	-2.08	57.24	58.96
23	C	514	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
31	B	622	LHG	C5-O7-C7	-2.08	112.67	117.79
35	G	606	CHL	C2A-C1A-CHA	2.08	127.50	123.86
35	Y	306	CHL	C3B-C4B-NB	-2.08	108.59	110.52
37	g	620	XAT	O24-C25-C26	-2.08	57.24	58.96
25	c	514	BCR	C37-C22-C23	2.08	121.35	118.08
35	Y	309	CHL	O2A-CGA-O1A	-2.08	118.35	123.59
23	D	403	CLA	CHB-C1B-NB	2.08	126.45	124.26
23	G	610	CLA	CHB-C1B-NB	2.08	126.45	124.26
23	r	604	CLA	CHB-C1B-NB	2.08	126.45	124.26
23	S	303	CLA	CHB-C1B-NB	2.07	126.45	124.26
23	B	606	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
38	R	316	NEX	C17-C1-C6	-2.07	108.62	110.47
26	a	406	SQD	O7-S-C6	2.07	109.40	106.94
23	B	606	CLA	C3B-C4B-NB	-2.07	108.59	110.52
36	y	316	LUT	C11-C10-C9	-2.07	124.35	127.31
36	N	616	LUT	C35-C15-C14	-2.07	119.23	123.47
23	C	513	CLA	C2B-C1B-NB	2.07	111.62	110.23
25	k	101	BCR	C27-C26-C25	-2.07	119.72	122.73
36	n	616	LUT	C19-C9-C8	2.07	121.34	118.08
38	N	617	NEX	O24-C25-C26	-2.07	57.25	58.96
32	S	319	DMU	C1-C2-C3	2.07	114.41	109.68
36	Y	317	LUT	C31-C30-C29	-2.07	124.36	127.31
35	N	601	CHL	CHB-C4A-NA	2.07	127.37	124.51
35	g	609	CHL	CHC-C4B-NB	2.07	126.45	124.26
38	s	616	NEX	O24-C25-C26	-2.07	57.25	58.96
23	C	503	CLA	C2A-C1A-CHA	2.07	127.47	123.86
23	d	402	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
36	R	314	LUT	C30-C31-C32	-2.07	116.77	123.22
23	C	508	CLA	CHC-C4B-NB	2.07	126.44	124.26
35	Y	306	CHL	CHB-C1B-NB	2.07	126.44	124.26
23	N	602	CLA	CHD-C1D-ND	-2.07	122.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	n	602	CLA	C3B-C4B-NB	-2.07	108.60	110.52
37	r	614	XAT	O24-C25-C26	-2.07	57.25	58.96
35	N	607	CHL	OMC-CMC-C2C	-2.06	121.02	125.69
23	B	601	CLA	C3B-C4B-NB	-2.06	108.60	110.52
35	n	607	CHL	C3B-C4B-NB	-2.06	108.60	110.52
31	G	619	LHG	C5-O7-C7	-2.06	112.71	117.79
37	R	315	XAT	C8-C9-C10	-2.06	115.78	118.94
25	B	619	BCR	C16-C15-C14	-2.06	119.25	123.47
38	g	618	NEX	C20-C13-C14	-2.06	120.03	122.92
25	h	101	BCR	C34-C9-C8	2.06	121.33	118.08
25	A	405	BCR	C16-C15-C14	-2.06	119.25	123.47
23	a	401	CLA	CHC-C4B-NB	2.06	126.44	124.26
23	s	611	CLA	O2A-CGA-O1A	-2.06	118.16	123.30
35	Y	310	CHL	CMB-C2B-C1B	-2.06	122.23	125.37
23	g	611	CLA	C3B-C4B-NB	-2.06	108.60	110.52
23	S	305	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	D	401	CLA	CHB-C1B-NB	2.06	126.44	124.26
23	S	310	CLA	O2D-CGD-CBD	2.06	114.92	111.27
36	G	615	LUT	C31-C30-C29	-2.06	124.37	127.31
23	g	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	D	405	BCR	C10-C11-C12	-2.06	116.80	123.22
35	R	306	CHL	O2A-CGA-O1A	-2.06	118.17	123.30
23	Y	315	CLA	CHB-C1B-NB	2.06	126.44	124.26
23	g	603	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	G	611	CLA	C3B-C4B-NB	-2.06	108.61	110.52
23	g	603	CLA	CAA-C2A-C3A	-2.06	107.15	112.78
35	s	607	CHL	C4A-NA-C1A	2.06	107.63	106.71
23	c	511	CLA	C2A-C1A-CHA	2.05	127.45	123.86
23	c	509	CLA	C2A-C1A-CHA	2.05	127.45	123.86
36	S	316	LUT	C18-C5-C6	-2.05	122.22	124.53
35	g	605	CHL	O2A-CGA-O1A	-2.05	118.18	123.30
23	n	603	CLA	C2A-C1A-CHA	2.05	127.45	123.86
35	N	609	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
23	c	513	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
23	c	507	CLA	CHC-C4B-NB	2.05	126.43	124.26
23	c	513	CLA	CHB-C1B-NB	2.05	126.43	124.26
38	R	301	NEX	O24-C25-C26	-2.05	57.26	58.96
23	c	502	CLA	CHC-C4B-NB	2.05	126.43	124.26
23	s	613	CLA	C3B-C4B-NB	-2.05	108.61	110.52
36	y	317	LUT	C16-C1-C6	-2.05	106.97	110.30
23	Y	314	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	d	404	CLA	O2D-CGD-CBD	2.05	114.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	s	609	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
36	n	616	LUT	C31-C30-C29	-2.05	124.39	127.31
23	b	603	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	r	602	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	N	604	CLA	CMB-C2B-C3B	2.05	131.55	126.59
23	y	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	b	610	CLA	CHB-C1B-NB	2.05	126.42	124.26
23	S	314	CLA	C3B-C4B-NB	-2.05	108.62	110.52
23	N	611	CLA	CHB-C1B-NB	2.05	126.42	124.26
36	g	615	LUT	C39-C29-C28	2.05	121.30	118.08
35	y	308	CHL	C2A-C1A-CHA	2.05	127.44	123.86
23	r	604	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
36	S	316	LUT	C11-C10-C9	2.05	130.23	127.31
23	B	601	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	a	404	CLA	O2D-CGD-CBD	2.05	114.90	111.27
35	G	606	CHL	O2D-CGD-CBD	2.04	114.90	111.27
25	C	519	BCR	C38-C26-C27	2.04	117.54	113.62
35	y	302	CHL	O2D-CGD-CBD	2.04	114.90	111.27
37	R	315	XAT	O24-C25-C26	-2.04	57.27	58.96
23	G	612	CLA	CHC-C4B-NB	2.04	126.42	124.26
38	n	617	NEX	C15-C35-C34	-2.04	119.29	123.47
25	d	405	BCR	C10-C11-C12	-2.04	116.84	123.22
23	N	611	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
35	Y	308	CHL	C2A-C1A-CHA	2.04	127.43	123.86
23	c	501	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	r	609	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
35	y	310	CHL	CBA-CAA-C2A	2.04	119.88	113.86
23	B	601	CLA	CBA-CAA-C2A	2.04	119.88	113.86
23	s	608	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	b	613	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
23	n	611	CLA	C2A-C1A-CHA	2.04	127.42	123.86
35	N	606	CHL	C3B-C4B-NB	-2.04	108.62	110.52
25	h	101	BCR	C20-C19-C18	-2.04	120.69	126.42
36	N	616	LUT	C3-C4-C5	-2.04	107.80	111.85
35	G	605	CHL	O2A-CGA-O1A	-2.04	118.22	123.30
38	G	618	NEX	C2-C1-C6	2.04	111.19	109.21
35	G	609	CHL	C1D-CHD-C4C	-2.04	121.67	126.06
35	Y	302	CHL	O2D-CGD-CBD	2.03	114.88	111.27
37	G	620	XAT	O4-C5-C6	-2.03	57.28	58.96
36	s	615	LUT	C30-C31-C32	-2.03	116.87	123.22
23	b	608	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
35	N	605	CHL	O2A-CGA-O1A	-2.03	118.46	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	r	606	CHL	C3B-C4B-NB	-2.03	108.63	110.52
38	r	615	NEX	O24-C25-C26	-2.03	57.28	58.96
30	C	501	LMG	C7-O1-C1	-2.03	109.77	113.74
31	g	619	LHG	C5-O7-C7	-2.03	112.79	117.79
38	S	317	NEX	C15-C35-C34	-2.03	119.31	123.47
35	S	308	CHL	CHB-C4A-NA	2.03	127.32	124.51
23	r	601	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
31	l	103	LHG	O8-C23-O10	-2.03	118.47	123.59
23	B	612	CLA	C2A-C1A-CHA	2.03	127.41	123.86
35	s	606	CHL	C3B-C4B-NB	-2.03	108.63	110.52
36	s	614	LUT	C19-C9-C8	2.03	121.28	118.08
36	Y	317	LUT	C1-C2-C3	2.03	118.23	113.64
35	N	609	CHL	CMB-C2B-C1B	-2.03	122.28	125.37
30	c	521	LMG	C4-C3-C2	2.03	114.36	110.82
23	C	509	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	b	604	CLA	C2A-C1A-CHA	2.03	127.41	123.86
23	N	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
38	n	617	NEX	C19-C9-C10	-2.03	120.08	122.92
35	y	306	CHL	CHB-C1B-NB	2.03	126.40	124.26
23	G	603	CLA	CHA-C1A-NA	-2.03	121.75	126.40
28	c	515	DGD	C2G-O2G-C1B	-2.03	112.80	117.79
28	b	625	DGD	O1G-C1A-C2A	2.03	118.27	111.91
23	C	503	CLA	CHC-C4B-NB	2.03	126.40	124.26
23	N	603	CLA	CHB-C1B-NB	2.03	126.40	124.26
35	R	307	CHL	CHC-C4B-NB	2.03	126.40	124.26
23	C	502	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
25	b	619	BCR	C21-C20-C19	-2.03	116.89	123.22
25	B	617	BCR	C21-C20-C19	-2.03	116.90	123.22
23	G	612	CLA	CHA-C1A-NA	-2.02	121.76	126.40
23	R	305	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
37	R	315	XAT	O4-C5-C6	-2.02	57.28	58.96
23	N	611	CLA	C2A-C1A-CHA	2.02	127.40	123.86
28	B	626	DGD	O1G-C1A-C2A	2.02	118.25	111.91
23	b	603	CLA	C3B-C4B-NB	-2.02	108.64	110.52
36	n	615	LUT	C1-C2-C3	2.02	118.21	113.64
23	n	603	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	C	507	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	B	614	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
36	Y	316	LUT	C20-C13-C12	2.02	121.26	118.08
23	n	613	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	y	303	CLA	CMB-C2B-C3B	2.02	131.48	126.59
35	N	606	CHL	CAA-C2A-C3A	-2.02	107.25	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	y	313	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
37	g	620	XAT	O4-C5-C6	-2.02	57.29	58.96
23	b	607	CLA	C11-C12-C13	-2.02	109.39	115.92
35	S	306	CHL	CHC-C4B-NB	2.02	126.39	124.26
25	C	516	BCR	C20-C21-C22	-2.02	124.43	127.31
35	R	308	CHL	CAA-C2A-C3A	-2.02	107.25	112.78
23	S	314	CLA	CHD-C1D-ND	-2.02	122.60	124.45
38	s	616	NEX	C4-C3-C2	-2.02	106.88	110.77
37	g	620	XAT	C27-C28-C29	-2.02	122.40	125.53
23	R	305	CLA	CHB-C1B-NB	2.02	126.39	124.26
23	c	506	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	b	614	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
36	y	317	LUT	C31-C30-C29	-2.02	124.43	127.31
23	R	313	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
35	n	605	CHL	O2A-CGA-O1A	-2.02	118.50	123.59
23	y	313	CLA	CHB-C1B-NB	2.02	126.39	124.26
23	G	611	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	B	602	CLA	C2A-C1A-CHA	2.01	127.38	123.86
23	A	404	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
23	b	618	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	c	514	BCR	C36-C18-C19	2.01	121.25	118.08
23	c	503	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
37	Y	301	XAT	C4-C3-C2	-2.01	106.89	110.77
31	N	618	LHG	O7-C7-O9	-2.01	118.84	123.70
35	r	605	CHL	O2A-CGA-O1A	-2.01	118.29	123.30
35	s	607	CHL	CMB-C2B-C1B	-2.01	122.31	125.37
23	R	305	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
35	N	606	CHL	O2A-CGA-O1A	-2.01	118.29	123.30
25	a	405	BCR	C16-C15-C14	-2.01	119.36	123.47
23	n	611	CLA	CHB-C1B-NB	2.01	126.39	124.26
23	b	616	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
23	s	602	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	R	303	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	B	605	CLA	C11-C12-C13	-2.01	109.43	115.92
23	C	505	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
35	N	601	CHL	C3C-C4C-NC	-2.01	108.32	110.57
35	n	606	CHL	C3B-C4B-NB	-2.01	108.65	110.52
35	g	601	CHL	C2D-C1D-ND	-2.01	108.62	110.10
25	A	405	BCR	C21-C20-C19	-2.01	116.95	123.22
23	R	302	CLA	O2D-CGD-CBD	2.01	114.83	111.27
23	A	404	CLA	CMB-C2B-C3B	2.01	131.45	126.59
37	r	614	XAT	O4-C5-C6	-2.01	57.30	58.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	G	616	LUT	C31-C30-C29	-2.01	124.45	127.31
35	N	608	CHL	OMC-CMC-C2C	-2.01	121.15	125.69
36	s	615	LUT	C19-C9-C8	2.01	121.24	118.08
23	b	603	CLA	CHB-C1B-NB	2.01	126.38	124.26
37	y	301	XAT	C27-C28-C29	-2.00	122.42	125.53
23	b	603	CLA	CBA-CAA-C2A	2.00	119.78	113.86
23	A	402	CLA	CHB-C1B-NB	2.00	126.38	124.26
35	S	306	CHL	C3B-C4B-NB	-2.00	108.66	110.52
23	R	309	CLA	CHC-C4B-NB	2.00	126.38	124.26
23	B	616	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
35	g	605	CHL	CHB-C1B-NB	2.00	126.38	124.26
23	c	508	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
36	S	315	LUT	C7-C8-C9	-2.00	123.21	126.23
23	D	401	CLA	CMB-C2B-C3B	2.00	131.44	126.59
23	b	606	CLA	CBC-CAC-C3C	2.00	117.95	112.43
23	d	401	CLA	CHD-C1D-ND	-2.00	122.61	124.45
23	R	309	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
35	n	601	CHL	CMB-C2B-C1B	-2.00	122.32	125.37
23	r	609	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	s	604	CLA	CMB-C2B-C3B	2.00	131.43	126.59

There are no chirality outliers.

All (3166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	401	CLA	CBD-CGD-O2D-CED
23	A	402	CLA	C1A-C2A-CAA-CBA
23	A	402	CLA	C2B-C3B-CAB-CBB
23	A	402	CLA	C4B-C3B-CAB-CBB
23	A	402	CLA	CHA-CBD-CGD-O1D
23	A	402	CLA	CHA-CBD-CGD-O2D
23	A	404	CLA	CHA-CBD-CGD-O1D
23	A	404	CLA	CHA-CBD-CGD-O2D
23	A	404	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	C2B-C3B-CAB-CBB
23	B	601	CLA	C4B-C3B-CAB-CBB
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C2-C3-C5-C6
23	B	602	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C3A-C2A-CAA-CBA
23	B	604	CLA	CHA-CBD-CGD-O1D
23	B	604	CLA	CHA-CBD-CGD-O2D
23	B	605	CLA	C11-C10-C8-C9
23	B	606	CLA	C2B-C3B-CAB-CBB
23	B	606	CLA	C4B-C3B-CAB-CBB
23	B	607	CLA	CBD-CGD-O2D-CED
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	608	CLA	C2B-C3B-CAB-CBB
23	B	608	CLA	C4B-C3B-CAB-CBB
23	B	609	CLA	C2B-C3B-CAB-CBB
23	B	609	CLA	C4B-C3B-CAB-CBB
23	B	609	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	C1A-C2A-CAA-CBA
23	B	613	CLA	C2B-C3B-CAB-CBB
23	B	613	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	C1A-C2A-CAA-CBA
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	C4B-C3B-CAB-CBB
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	C1A-C2A-CAA-CBA
23	C	506	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	D	401	CLA	CHA-CBD-CGD-O1D
23	D	401	CLA	CHA-CBD-CGD-O2D
23	D	404	CLA	CHA-CBD-CGD-O1D
23	D	404	CLA	CHA-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O1D
23	G	610	CLA	C1A-C2A-CAA-CBA
23	G	610	CLA	C3A-C2A-CAA-CBA
23	G	613	CLA	CHA-CBD-CGD-O1D
23	G	613	CLA	CHA-CBD-CGD-O2D
23	G	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	G	614	CLA	C3A-C2A-CAA-CBA
23	N	610	CLA	C3A-C2A-CAA-CBA
23	N	611	CLA	C1A-C2A-CAA-CBA
23	N	611	CLA	C4B-C3B-CAB-CBB
23	N	613	CLA	C1A-C2A-CAA-CBA
23	N	613	CLA	CHA-CBD-CGD-O1D
23	N	613	CLA	CHA-CBD-CGD-O2D
23	S	303	CLA	C3A-C2A-CAA-CBA
23	S	304	CLA	C4B-C3B-CAB-CBB
23	S	305	CLA	CHA-CBD-CGD-O1D
23	S	305	CLA	CHA-CBD-CGD-O2D
23	S	309	CLA	C2B-C3B-CAB-CBB
23	S	309	CLA	C4B-C3B-CAB-CBB
23	S	309	CLA	CHA-CBD-CGD-O1D
23	S	309	CLA	CHA-CBD-CGD-O2D
23	S	309	CLA	CAD-CBD-CGD-O1D
23	S	310	CLA	C1A-C2A-CAA-CBA
23	S	310	CLA	C3A-C2A-CAA-CBA
23	S	310	CLA	C2A-CAA-CBA-CGA
23	S	311	CLA	C2B-C3B-CAB-CBB
23	S	311	CLA	C4B-C3B-CAB-CBB
23	S	311	CLA	CHA-CBD-CGD-O1D
23	S	311	CLA	CHA-CBD-CGD-O2D
23	S	312	CLA	CBD-CGD-O2D-CED
23	S	313	CLA	CHA-CBD-CGD-O1D
23	S	313	CLA	CHA-CBD-CGD-O2D
23	S	314	CLA	CHA-CBD-CGD-O1D
23	S	314	CLA	CHA-CBD-CGD-O2D
23	S	314	CLA	CAD-CBD-CGD-O1D
23	S	314	CLA	CAD-CBD-CGD-O2D
23	Y	303	CLA	C1A-C2A-CAA-CBA
23	Y	303	CLA	C3A-C2A-CAA-CBA
23	Y	311	CLA	CBD-CGD-O2D-CED
23	Y	313	CLA	CBD-CGD-O2D-CED
23	Y	314	CLA	C6-C7-C8-C9
23	a	401	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CHA-CBD-CGD-O1D
23	a	404	CLA	CHA-CBD-CGD-O2D
23	a	404	CLA	CAD-CBD-CGD-O1D
23	b	603	CLA	C1A-C2A-CAA-CBA
23	b	603	CLA	C2B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	b	603	CLA	CHA-CBD-CGD-O1D
23	b	603	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	C1A-C2A-CAA-CBA
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	605	CLA	C3A-C2A-CAA-CBA
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	C11-C10-C8-C9
23	b	608	CLA	C2B-C3B-CAB-CBB
23	b	608	CLA	C4B-C3B-CAB-CBB
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	610	CLA	C2B-C3B-CAB-CBB
23	b	610	CLA	C4B-C3B-CAB-CBB
23	b	611	CLA	C2B-C3B-CAB-CBB
23	b	611	CLA	C4B-C3B-CAB-CBB
23	b	611	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	CHA-CBD-CGD-O2D
23	b	611	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	615	CLA	C2B-C3B-CAB-CBB
23	b	615	CLA	C4B-C3B-CAB-CBB
23	b	616	CLA	C1A-C2A-CAA-CBA
23	b	616	CLA	CHA-CBD-CGD-O1D
23	b	616	CLA	CHA-CBD-CGD-O2D
23	b	617	CLA	C4B-C3B-CAB-CBB
23	b	617	CLA	CHA-CBD-CGD-O1D
23	b	617	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	C1A-C2A-CAA-CBA
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	d	401	CLA	CHA-CBD-CGD-O1D
23	d	401	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	C1A-C2A-CAA-CBA
23	d	402	CLA	C4B-C3B-CAB-CBB
23	d	402	CLA	CHA-CBD-CGD-O1D
23	d	402	CLA	CHA-CBD-CGD-O2D
23	d	404	CLA	CHA-CBD-CGD-O1D
23	d	404	CLA	CHA-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O1D
23	g	610	CLA	C3A-C2A-CAA-CBA
23	g	613	CLA	CHA-CBD-CGD-O1D
23	g	613	CLA	CHA-CBD-CGD-O2D
23	g	614	CLA	C1A-C2A-CAA-CBA
23	g	614	CLA	C3A-C2A-CAA-CBA
23	g	614	CLA	CBD-CGD-O2D-CED
23	r	601	CLA	C1A-C2A-CAA-CBA
23	r	601	CLA	C3A-C2A-CAA-CBA
23	r	601	CLA	C2B-C3B-CAB-CBB
23	r	601	CLA	C4B-C3B-CAB-CBB
23	r	601	CLA	CHA-CBD-CGD-O1D
23	r	601	CLA	CHA-CBD-CGD-O2D
23	r	602	CLA	C1A-C2A-CAA-CBA
23	r	602	CLA	C3A-C2A-CAA-CBA
23	r	602	CLA	C2B-C3B-CAB-CBB
23	r	602	CLA	C4B-C3B-CAB-CBB
23	r	602	CLA	CHA-CBD-CGD-O1D
23	r	602	CLA	CHA-CBD-CGD-O2D
23	r	611	CLA	C2B-C3B-CAB-CBB
23	r	611	CLA	C4B-C3B-CAB-CBB
23	r	611	CLA	CBD-CGD-O2D-CED
23	r	612	CLA	CHA-CBD-CGD-O1D
23	r	612	CLA	CHA-CBD-CGD-O2D
23	s	602	CLA	C3A-C2A-CAA-CBA
23	s	602	CLA	C2B-C3B-CAB-CBB
23	s	602	CLA	C4B-C3B-CAB-CBB
23	s	604	CLA	CHA-CBD-CGD-O1D
23	s	604	CLA	CHA-CBD-CGD-O2D
23	s	608	CLA	C2B-C3B-CAB-CBB
23	s	608	CLA	C4B-C3B-CAB-CBB
23	s	610	CLA	C2B-C3B-CAB-CBB
23	s	610	CLA	C4B-C3B-CAB-CBB
23	s	610	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	s	610	CLA	CHA-CBD-CGD-O2D
23	s	611	CLA	CBD-CGD-O2D-CED
23	s	612	CLA	CHA-CBD-CGD-O1D
23	s	612	CLA	CHA-CBD-CGD-O2D
23	s	613	CLA	CHA-CBD-CGD-O1D
23	s	613	CLA	CHA-CBD-CGD-O2D
23	s	613	CLA	CAD-CBD-CGD-O1D
23	n	603	CLA	C2B-C3B-CAB-CBB
23	n	603	CLA	C4B-C3B-CAB-CBB
23	n	610	CLA	C3A-C2A-CAA-CBA
23	n	611	CLA	C1A-C2A-CAA-CBA
23	n	611	CLA	C4B-C3B-CAB-CBB
23	n	613	CLA	C1A-C2A-CAA-CBA
23	n	613	CLA	CHA-CBD-CGD-O1D
23	n	613	CLA	CHA-CBD-CGD-O2D
23	y	303	CLA	C1A-C2A-CAA-CBA
23	y	303	CLA	C3A-C2A-CAA-CBA
23	y	311	CLA	CBD-CGD-O2D-CED
23	y	313	CLA	CBD-CGD-O2D-CED
23	R	302	CLA	C1A-C2A-CAA-CBA
23	R	302	CLA	C3A-C2A-CAA-CBA
23	R	302	CLA	C2B-C3B-CAB-CBB
23	R	302	CLA	C4B-C3B-CAB-CBB
23	R	302	CLA	CHA-CBD-CGD-O1D
23	R	303	CLA	C1A-C2A-CAA-CBA
23	R	303	CLA	C3A-C2A-CAA-CBA
23	R	303	CLA	CHA-CBD-CGD-O1D
23	R	303	CLA	CHA-CBD-CGD-O2D
23	R	312	CLA	C2B-C3B-CAB-CBB
23	R	312	CLA	C4B-C3B-CAB-CBB
23	R	312	CLA	CBD-CGD-O2D-CED
23	R	313	CLA	CHA-CBD-CGD-O1D
23	R	313	CLA	CHA-CBD-CGD-O2D
25	B	617	BCR	C21-C22-C23-C24
25	B	617	BCR	C37-C22-C23-C24
25	D	405	BCR	C5-C6-C7-C8
25	D	405	BCR	C7-C8-C9-C34
25	H	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C1-C6-C7-C8
25	b	619	BCR	C21-C22-C23-C24
25	b	619	BCR	C37-C22-C23-C24
25	b	619	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	d	405	BCR	C5-C6-C7-C8
25	d	405	BCR	C7-C8-C9-C34
25	h	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C7-C8-C9-C10
25	k	101	BCR	C7-C8-C9-C34
26	B	625	SQD	C5-C6-S-O7
26	C	521	SQD	C5-C6-S-O9
26	L	103	SQD	O5-C5-C6-S
26	b	602	SQD	C5-C6-S-O8
26	c	520	SQD	C5-C6-S-O9
26	l	101	SQD	C2-C1-O6-C44
26	l	101	SQD	O5-C5-C6-S
28	A	408	DGD	C2B-C1B-O2G-C2G
28	A	408	DGD	O1B-C1B-O2G-C2G
28	B	626	DGD	O1B-C1B-O2G-C2G
28	b	625	DGD	O1B-C1B-O2G-C2G
30	C	522	LMG	C11-C10-O7-C8
30	c	521	LMG	C11-C10-O7-C8
31	B	621	LHG	C4-O6-P-O4
31	B	627	LHG	C3-O3-P-O5
31	B	627	LHG	C4-O6-P-O3
31	B	627	LHG	C4-O6-P-O4
31	B	627	LHG	C4-O6-P-O5
31	C	518	LHG	C3-O3-P-O5
31	C	518	LHG	C4-O6-P-O5
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C4-O6-P-O3
31	D	408	LHG	C4-O6-P-O4
31	G	619	LHG	O2-C2-C3-O3
31	G	619	LHG	C3-O3-P-O5
31	G	619	LHG	C4-O6-P-O4
31	L	101	LHG	C3-O3-P-O4
31	L	102	LHG	C4-O6-P-O3
31	L	102	LHG	C4-O6-P-O4
31	L	102	LHG	C4-O6-P-O5
31	L	102	LHG	O6-C4-C5-O7
31	N	618	LHG	C4-O6-P-O4
31	S	318	LHG	C3-O3-P-O5
31	S	318	LHG	C4-O6-P-O4
31	S	318	LHG	C4-O6-P-O5
31	Y	319	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
31	Y	319	LHG	C4-O6-P-O4
31	b	623	LHG	C4-O6-P-O4
31	b	624	LHG	C3-O3-P-O6
31	b	624	LHG	C4-O6-P-O4
31	b	626	LHG	C4-O6-P-O4
31	b	626	LHG	C4-O6-P-O5
31	c	517	LHG	C3-O3-P-O5
31	c	517	LHG	C4-O6-P-O3
31	c	517	LHG	C4-O6-P-O5
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C4-O6-P-O3
31	d	408	LHG	C4-O6-P-O4
31	g	619	LHG	O2-C2-C3-O3
31	g	619	LHG	C3-O3-P-O5
31	g	619	LHG	C4-O6-P-O4
31	l	102	LHG	C3-O3-P-O4
31	l	103	LHG	C3-O3-P-O5
31	l	103	LHG	C4-O6-P-O3
31	l	103	LHG	C4-O6-P-O4
31	l	103	LHG	C4-O6-P-O5
31	l	103	LHG	O6-C4-C5-O7
31	r	616	LHG	C3-O3-P-O6
31	r	616	LHG	C4-O6-P-O3
31	s	617	LHG	C3-O3-P-O5
31	s	617	LHG	C4-O6-P-O4
31	s	617	LHG	C4-O6-P-O5
31	n	618	LHG	C4-O6-P-O4
31	y	318	LHG	C3-O3-P-O4
31	y	318	LHG	C4-O6-P-O4
32	C	520	DMU	C1-C6-O16-C18
32	C	520	DMU	O5-C6-O16-C18
32	C	520	DMU	C5-C10-O7-C3
32	c	519	DMU	C5-C10-O7-C3
33	D	406	PL9	C12-C11-C9-C8
33	D	406	PL9	C9-C11-C12-C13
33	D	406	PL9	C12-C13-C14-C16
33	D	406	PL9	C13-C14-C16-C17
33	D	406	PL9	C17-C18-C19-C20
33	D	406	PL9	C17-C18-C19-C21
33	D	406	PL9	C22-C23-C24-C25
33	D	406	PL9	C27-C28-C29-C30
33	D	406	PL9	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
33	D	406	PL9	C34-C36-C37-C38
33	D	406	PL9	C37-C38-C39-C40
33	D	406	PL9	C37-C38-C39-C41
33	D	406	PL9	C42-C43-C44-C45
33	d	406	PL9	C12-C11-C9-C8
33	d	406	PL9	C9-C11-C12-C13
33	d	406	PL9	C12-C13-C14-C16
33	d	406	PL9	C13-C14-C16-C17
33	d	406	PL9	C17-C18-C19-C20
33	d	406	PL9	C17-C18-C19-C21
33	d	406	PL9	C22-C23-C24-C25
33	d	406	PL9	C27-C28-C29-C30
33	d	406	PL9	C32-C33-C34-C35
33	d	406	PL9	C37-C38-C39-C40
33	d	406	PL9	C37-C38-C39-C41
33	d	406	PL9	C42-C43-C44-C45
35	G	601	CHL	C2B-C3B-CAB-CBB
35	G	601	CHL	C4B-C3B-CAB-CBB
35	G	601	CHL	C1C-C2C-CMC-OMC
35	G	601	CHL	C3C-C2C-CMC-OMC
35	G	601	CHL	CHA-CBD-CGD-O1D
35	G	601	CHL	CHA-CBD-CGD-O2D
35	G	605	CHL	C1A-C2A-CAA-CBA
35	G	605	CHL	C3A-C2A-CAA-CBA
35	G	605	CHL	C2B-C3B-CAB-CBB
35	G	605	CHL	C4B-C3B-CAB-CBB
35	G	605	CHL	C1C-C2C-CMC-OMC
35	G	605	CHL	C3C-C2C-CMC-OMC
35	G	605	CHL	CHA-CBD-CGD-O1D
35	G	605	CHL	CHA-CBD-CGD-O2D
35	G	606	CHL	C1A-C2A-CAA-CBA
35	G	606	CHL	C1C-C2C-CMC-OMC
35	G	606	CHL	C3C-C2C-CMC-OMC
35	G	606	CHL	CHA-CBD-CGD-O1D
35	G	606	CHL	CHA-CBD-CGD-O2D
35	G	607	CHL	C1C-C2C-CMC-OMC
35	G	607	CHL	C3C-C2C-CMC-OMC
35	G	607	CHL	CBD-CGD-O2D-CED
35	G	608	CHL	C1A-C2A-CAA-CBA
35	G	608	CHL	C1C-C2C-CMC-OMC
35	G	608	CHL	C3C-C2C-CMC-OMC
35	G	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	G	609	CHL	C1C-C2C-CMC-OMC
35	G	609	CHL	C3C-C2C-CMC-OMC
35	N	601	CHL	C1C-C2C-CMC-OMC
35	N	601	CHL	C3C-C2C-CMC-OMC
35	N	601	CHL	CHA-CBD-CGD-O1D
35	N	601	CHL	CHA-CBD-CGD-O2D
35	N	605	CHL	C1C-C2C-CMC-OMC
35	N	605	CHL	C3C-C2C-CMC-OMC
35	N	605	CHL	CAD-CBD-CGD-O1D
35	N	605	CHL	CAD-CBD-CGD-O2D
35	N	606	CHL	C1A-C2A-CAA-CBA
35	N	606	CHL	C1C-C2C-CMC-OMC
35	N	606	CHL	C3C-C2C-CMC-OMC
35	N	607	CHL	C1A-C2A-CAA-CBA
35	N	607	CHL	C1C-C2C-CMC-OMC
35	N	607	CHL	C3C-C2C-CMC-OMC
35	N	608	CHL	C1C-C2C-CMC-OMC
35	N	608	CHL	C3C-C2C-CMC-OMC
35	N	609	CHL	C1C-C2C-CMC-OMC
35	N	609	CHL	C3C-C2C-CMC-OMC
35	S	302	CHL	C1C-C2C-CMC-OMC
35	S	302	CHL	C3C-C2C-CMC-OMC
35	S	306	CHL	C1C-C2C-CMC-OMC
35	S	306	CHL	C3C-C2C-CMC-OMC
35	S	307	CHL	C1A-C2A-CAA-CBA
35	S	307	CHL	C3A-C2A-CAA-CBA
35	S	307	CHL	C1C-C2C-CMC-OMC
35	S	307	CHL	C3C-C2C-CMC-OMC
35	S	308	CHL	C1C-C2C-CMC-OMC
35	S	308	CHL	C3C-C2C-CMC-OMC
35	S	308	CHL	CHA-CBD-CGD-O1D
35	S	308	CHL	CHA-CBD-CGD-O2D
35	S	308	CHL	CAD-CBD-CGD-O1D
35	S	308	CHL	CBD-CGD-O2D-CED
35	Y	302	CHL	C1C-C2C-CMC-OMC
35	Y	302	CHL	C3C-C2C-CMC-OMC
35	Y	302	CHL	CHA-CBD-CGD-O1D
35	Y	302	CHL	CHA-CBD-CGD-O2D
35	Y	306	CHL	C1A-C2A-CAA-CBA
35	Y	306	CHL	C2A-CAA-CBA-CGA
35	Y	306	CHL	C1C-C2C-CMC-OMC
35	Y	306	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
35	Y	307	CHL	C1A-C2A-CAA-CBA
35	Y	307	CHL	C1C-C2C-CMC-OMC
35	Y	307	CHL	C3C-C2C-CMC-OMC
35	Y	308	CHL	O1A-CGA-O2A-C1
35	Y	308	CHL	C2B-C3B-CAB-CBB
35	Y	308	CHL	C4B-C3B-CAB-CBB
35	Y	308	CHL	C1C-C2C-CMC-OMC
35	Y	308	CHL	C3C-C2C-CMC-OMC
35	Y	309	CHL	C1C-C2C-CMC-OMC
35	Y	309	CHL	C3C-C2C-CMC-OMC
35	Y	310	CHL	C1A-C2A-CAA-CBA
35	Y	310	CHL	C3A-C2A-CAA-CBA
35	Y	310	CHL	C2B-C3B-CAB-CBB
35	Y	310	CHL	C4B-C3B-CAB-CBB
35	Y	310	CHL	C1C-C2C-CMC-OMC
35	Y	310	CHL	C3C-C2C-CMC-OMC
35	g	601	CHL	C2B-C3B-CAB-CBB
35	g	601	CHL	C4B-C3B-CAB-CBB
35	g	601	CHL	C1C-C2C-CMC-OMC
35	g	601	CHL	C3C-C2C-CMC-OMC
35	g	601	CHL	CHA-CBD-CGD-O1D
35	g	601	CHL	CHA-CBD-CGD-O2D
35	g	605	CHL	C1A-C2A-CAA-CBA
35	g	605	CHL	C3A-C2A-CAA-CBA
35	g	605	CHL	C2B-C3B-CAB-CBB
35	g	605	CHL	C4B-C3B-CAB-CBB
35	g	605	CHL	C1C-C2C-CMC-OMC
35	g	605	CHL	C3C-C2C-CMC-OMC
35	g	605	CHL	CHA-CBD-CGD-O1D
35	g	605	CHL	CHA-CBD-CGD-O2D
35	g	606	CHL	C1A-C2A-CAA-CBA
35	g	606	CHL	C1C-C2C-CMC-OMC
35	g	606	CHL	C3C-C2C-CMC-OMC
35	g	607	CHL	C2B-C3B-CAB-CBB
35	g	607	CHL	C4B-C3B-CAB-CBB
35	g	607	CHL	C1C-C2C-CMC-OMC
35	g	607	CHL	C3C-C2C-CMC-OMC
35	g	608	CHL	C1A-C2A-CAA-CBA
35	g	608	CHL	C1C-C2C-CMC-OMC
35	g	608	CHL	C3C-C2C-CMC-OMC
35	g	608	CHL	CBD-CGD-O2D-CED
35	g	609	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
35	g	609	CHL	C4B-C3B-CAB-CBB
35	g	609	CHL	C1C-C2C-CMC-OMC
35	g	609	CHL	C3C-C2C-CMC-OMC
35	r	605	CHL	C1C-C2C-CMC-OMC
35	r	606	CHL	C1C-C2C-CMC-OMC
35	r	606	CHL	C3C-C2C-CMC-OMC
35	r	607	CHL	C1C-C2C-CMC-OMC
35	r	607	CHL	C3C-C2C-CMC-OMC
35	s	601	CHL	C1C-C2C-CMC-OMC
35	s	601	CHL	C3C-C2C-CMC-OMC
35	s	605	CHL	C1C-C2C-CMC-OMC
35	s	606	CHL	C1A-C2A-CAA-CBA
35	s	606	CHL	C3A-C2A-CAA-CBA
35	s	606	CHL	C2B-C3B-CAB-CBB
35	s	606	CHL	C4B-C3B-CAB-CBB
35	s	606	CHL	C1C-C2C-CMC-OMC
35	s	606	CHL	C3C-C2C-CMC-OMC
35	s	607	CHL	C1A-C2A-CAA-CBA
35	s	607	CHL	C1C-C2C-CMC-OMC
35	s	607	CHL	C3C-C2C-CMC-OMC
35	n	601	CHL	C1C-C2C-CMC-OMC
35	n	601	CHL	C3C-C2C-CMC-OMC
35	n	601	CHL	CHA-CBD-CGD-O1D
35	n	601	CHL	CHA-CBD-CGD-O2D
35	n	605	CHL	C1C-C2C-CMC-OMC
35	n	605	CHL	C3C-C2C-CMC-OMC
35	n	605	CHL	CHA-CBD-CGD-O1D
35	n	605	CHL	CAD-CBD-CGD-O1D
35	n	605	CHL	CAD-CBD-CGD-O2D
35	n	606	CHL	C1A-C2A-CAA-CBA
35	n	606	CHL	C1C-C2C-CMC-OMC
35	n	606	CHL	C3C-C2C-CMC-OMC
35	n	607	CHL	C1A-C2A-CAA-CBA
35	n	607	CHL	C1C-C2C-CMC-OMC
35	n	607	CHL	C3C-C2C-CMC-OMC
35	n	608	CHL	C1C-C2C-CMC-OMC
35	n	608	CHL	C3C-C2C-CMC-OMC
35	n	609	CHL	C1C-C2C-CMC-OMC
35	n	609	CHL	C3C-C2C-CMC-OMC
35	y	302	CHL	C1C-C2C-CMC-OMC
35	y	302	CHL	C3C-C2C-CMC-OMC
35	y	302	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
35	y	302	CHL	CHA-CBD-CGD-O2D
35	y	306	CHL	C1A-C2A-CAA-CBA
35	y	306	CHL	C1C-C2C-CMC-OMC
35	y	306	CHL	C3C-C2C-CMC-OMC
35	y	307	CHL	C1A-C2A-CAA-CBA
35	y	307	CHL	C1C-C2C-CMC-OMC
35	y	307	CHL	C3C-C2C-CMC-OMC
35	y	308	CHL	O1A-CGA-O2A-C1
35	y	308	CHL	C2B-C3B-CAB-CBB
35	y	308	CHL	C4B-C3B-CAB-CBB
35	y	308	CHL	C1C-C2C-CMC-OMC
35	y	308	CHL	C3C-C2C-CMC-OMC
35	y	309	CHL	C1C-C2C-CMC-OMC
35	y	309	CHL	C3C-C2C-CMC-OMC
35	y	310	CHL	C1A-C2A-CAA-CBA
35	y	310	CHL	C3A-C2A-CAA-CBA
35	y	310	CHL	C2B-C3B-CAB-CBB
35	y	310	CHL	C4B-C3B-CAB-CBB
35	y	310	CHL	C1C-C2C-CMC-OMC
35	y	310	CHL	C3C-C2C-CMC-OMC
35	R	306	CHL	C1C-C2C-CMC-OMC
35	R	307	CHL	C1C-C2C-CMC-OMC
35	R	307	CHL	C3C-C2C-CMC-OMC
35	R	308	CHL	C1C-C2C-CMC-OMC
35	R	308	CHL	C3C-C2C-CMC-OMC
36	N	615	LUT	C1-C6-C7-C8
36	Y	316	LUT	C1-C6-C7-C8
36	r	613	LUT	C7-C8-C9-C10
36	r	613	LUT	C7-C8-C9-C19
36	s	614	LUT	C1-C6-C7-C8
36	n	615	LUT	C1-C6-C7-C8
36	y	316	LUT	C1-C6-C7-C8
36	R	314	LUT	C7-C8-C9-C19
38	S	317	NEX	C11-C12-C13-C20
38	r	615	NEX	C11-C12-C13-C20
38	n	617	NEX	C31-C32-C33-C40
23	A	401	CLA	O1D-CGD-O2D-CED
23	g	603	CLA	O1D-CGD-O2D-CED
23	r	611	CLA	O1D-CGD-O2D-CED
23	R	312	CLA	O1D-CGD-O2D-CED
23	Y	313	CLA	O1D-CGD-O2D-CED
23	a	401	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	g	610	CLA	O1D-CGD-O2D-CED
23	y	313	CLA	O1D-CGD-O2D-CED
35	s	607	CHL	O1D-CGD-O2D-CED
23	A	404	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	G	610	CLA	CBD-CGD-O2D-CED
23	G	614	CLA	CBD-CGD-O2D-CED
23	N	602	CLA	CBD-CGD-O2D-CED
23	N	610	CLA	CBD-CGD-O2D-CED
23	S	303	CLA	CBD-CGD-O2D-CED
23	S	304	CLA	CBD-CGD-O2D-CED
23	S	313	CLA	CBD-CGD-O2D-CED
23	S	314	CLA	CBD-CGD-O2D-CED
23	Y	315	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	CBD-CGD-O2D-CED
23	c	502	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
23	g	603	CLA	CBD-CGD-O2D-CED
23	g	610	CLA	CBD-CGD-O2D-CED
23	g	613	CLA	CBD-CGD-O2D-CED
23	s	612	CLA	CBD-CGD-O2D-CED
23	s	613	CLA	CBD-CGD-O2D-CED
23	n	602	CLA	CBD-CGD-O2D-CED
23	n	610	CLA	CBD-CGD-O2D-CED
23	y	315	CLA	CBD-CGD-O2D-CED
35	N	608	CHL	CBD-CGD-O2D-CED
35	S	306	CHL	CBD-CGD-O2D-CED
35	Y	302	CHL	CBD-CGD-O2D-CED
35	Y	308	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	Y	309	CHL	CBD-CGD-O2D-CED
35	s	607	CHL	CBD-CGD-O2D-CED
35	y	302	CHL	CBD-CGD-O2D-CED
35	y	308	CHL	CBD-CGD-O2D-CED
35	y	309	CHL	CBD-CGD-O2D-CED
23	Y	312	CLA	O1A-CGA-O2A-C1
23	g	611	CLA	O1A-CGA-O2A-C1
23	R	309	CLA	O1A-CGA-O2A-C1
23	B	607	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	O1D-CGD-O2D-CED
23	G	610	CLA	O1D-CGD-O2D-CED
23	N	610	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	O1D-CGD-O2D-CED
35	S	306	CHL	O1D-CGD-O2D-CED
23	C	504	CLA	O1D-CGD-O2D-CED
23	S	312	CLA	O1D-CGD-O2D-CED
23	Y	311	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
23	s	611	CLA	O1D-CGD-O2D-CED
35	G	607	CHL	O1D-CGD-O2D-CED
35	g	608	CHL	O1D-CGD-O2D-CED
32	C	520	DMU	O6-C11-C9-C8
33	D	406	PL9	C47-C48-C49-C50
33	D	406	PL9	C47-C48-C49-C51
33	d	406	PL9	C47-C48-C49-C50
33	d	406	PL9	C47-C48-C49-C51
23	B	610	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
23	D	404	CLA	CBD-CGD-O2D-CED
23	G	603	CLA	CBD-CGD-O2D-CED
23	G	613	CLA	CBD-CGD-O2D-CED
23	N	604	CLA	CBD-CGD-O2D-CED
23	N	612	CLA	CBD-CGD-O2D-CED
23	N	614	CLA	CBD-CGD-O2D-CED
23	Y	305	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	d	404	CLA	CBD-CGD-O2D-CED
23	r	608	CLA	CBD-CGD-O2D-CED
23	r	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	s	602	CLA	CBD-CGD-O2D-CED
23	s	603	CLA	CBD-CGD-O2D-CED
23	s	609	CLA	CBD-CGD-O2D-CED
23	n	614	CLA	CBD-CGD-O2D-CED
23	y	305	CLA	CBD-CGD-O2D-CED
23	R	302	CLA	CBD-CGD-O2D-CED
23	R	311	CLA	CBD-CGD-O2D-CED
35	N	605	CHL	CBD-CGD-O2D-CED
35	Y	306	CHL	CBD-CGD-O2D-CED
35	n	608	CHL	CBD-CGD-O2D-CED
35	y	306	CHL	CBD-CGD-O2D-CED
23	B	607	CLA	O1A-CGA-O2A-C1
23	B	613	CLA	O1A-CGA-O2A-C1
23	G	604	CLA	O1A-CGA-O2A-C1
23	G	611	CLA	O1A-CGA-O2A-C1
23	N	603	CLA	O1A-CGA-O2A-C1
23	N	611	CLA	O1A-CGA-O2A-C1
23	Y	313	CLA	O1A-CGA-O2A-C1
23	b	609	CLA	O1A-CGA-O2A-C1
23	b	615	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	O1A-CGA-O2A-C1
23	g	602	CLA	O1A-CGA-O2A-C1
23	g	604	CLA	O1A-CGA-O2A-C1
23	r	608	CLA	O1A-CGA-O2A-C1
23	n	603	CLA	O1A-CGA-O2A-C1
23	n	611	CLA	O1A-CGA-O2A-C1
23	y	312	CLA	O1A-CGA-O2A-C1
24	A	403	PHO	O1A-CGA-O2A-C1
24	a	402	PHO	O1A-CGA-O2A-C1
35	S	308	CHL	O1A-CGA-O2A-C1
35	Y	307	CHL	O1A-CGA-O2A-C1
35	r	607	CHL	O1A-CGA-O2A-C1
35	y	307	CHL	O1A-CGA-O2A-C1
35	R	308	CHL	O1A-CGA-O2A-C1
23	C	507	CLA	O1D-CGD-O2D-CED
23	b	611	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
23	g	614	CLA	O1D-CGD-O2D-CED
23	y	311	CLA	O1D-CGD-O2D-CED
35	G	608	CHL	O1D-CGD-O2D-CED
35	S	308	CHL	O1D-CGD-O2D-CED
23	S	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	b	618	CLA	CBD-CGD-O2D-CED
23	r	601	CLA	CBD-CGD-O2D-CED
23	S	303	CLA	O1D-CGD-O2D-CED
30	C	522	LMG	O9-C10-O7-C8
30	c	521	LMG	O9-C10-O7-C8
23	G	610	CLA	O1A-CGA-O2A-C1
23	n	610	CLA	O1D-CGD-O2D-CED
23	B	613	CLA	C3-C5-C6-C7
23	C	503	CLA	C3-C5-C6-C7
23	C	512	CLA	C3-C5-C6-C7
23	D	401	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
23	b	618	CLA	C3-C5-C6-C7
23	c	507	CLA	C3-C5-C6-C7
23	c	511	CLA	C3-C5-C6-C7
23	d	401	CLA	C3-C5-C6-C7
23	g	602	CLA	C3-C5-C6-C7
23	r	609	CLA	C3-C5-C6-C7
23	R	310	CLA	C3-C5-C6-C7
24	D	402	PHO	C3-C5-C6-C7
24	a	403	PHO	C3-C5-C6-C7
35	G	609	CHL	C3-C5-C6-C7
35	Y	308	CHL	C3-C5-C6-C7
35	g	609	CHL	C3-C5-C6-C7
35	r	607	CHL	C3-C5-C6-C7
35	n	609	CHL	C3-C5-C6-C7
35	y	308	CHL	C3-C5-C6-C7
23	B	607	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	CBA-CGA-O2A-C1
23	C	503	CLA	CBA-CGA-O2A-C1
23	G	604	CLA	CBA-CGA-O2A-C1
23	N	603	CLA	CBA-CGA-O2A-C1
23	Y	312	CLA	CBA-CGA-O2A-C1
23	b	609	CLA	CBA-CGA-O2A-C1
23	b	615	CLA	CBA-CGA-O2A-C1
23	c	502	CLA	CBA-CGA-O2A-C1
23	d	404	CLA	CBA-CGA-O2A-C1
23	g	602	CLA	CBA-CGA-O2A-C1
23	g	604	CLA	CBA-CGA-O2A-C1
23	g	611	CLA	CBA-CGA-O2A-C1
23	n	613	CLA	CBA-CGA-O2A-C1
23	y	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	y	313	CLA	CBA-CGA-O2A-C1
23	R	309	CLA	CBA-CGA-O2A-C1
24	A	403	PHO	CBA-CGA-O2A-C1
24	a	402	PHO	CBA-CGA-O2A-C1
35	Y	307	CHL	CBA-CGA-O2A-C1
35	r	607	CHL	CBA-CGA-O2A-C1
35	y	307	CHL	CBA-CGA-O2A-C1
35	y	308	CHL	CBA-CGA-O2A-C1
35	R	308	CHL	CBA-CGA-O2A-C1
28	B	626	DGD	C2B-C1B-O2G-C2G
28	b	625	DGD	C2B-C1B-O2G-C2G
23	A	404	CLA	O1D-CGD-O2D-CED
23	C	508	CLA	CBD-CGD-O2D-CED
23	n	602	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	r	603	CLA	C4-C3-C5-C6
23	R	304	CLA	C4-C3-C5-C6
33	D	406	PL9	C25-C24-C26-C27
33	d	406	PL9	C25-C24-C26-C27
35	n	601	CHL	C4-C3-C5-C6
32	c	519	DMU	O6-C11-C9-C8
23	r	603	CLA	C2-C3-C5-C6
35	n	601	CHL	C2-C3-C5-C6
23	n	604	CLA	CBD-CGD-O2D-CED
35	G	605	CHL	CBD-CGD-O2D-CED
35	g	605	CHL	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	608	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C2A-CAA-CBA-CGA
23	g	602	CLA	C2A-CAA-CBA-CGA
23	g	604	CLA	C2A-CAA-CBA-CGA
23	r	602	CLA	C2A-CAA-CBA-CGA
35	S	308	CHL	C2A-CAA-CBA-CGA
35	Y	307	CHL	C2A-CAA-CBA-CGA
35	y	307	CHL	C2A-CAA-CBA-CGA
23	g	613	CLA	O1D-CGD-O2D-CED
35	y	308	CHL	O1D-CGD-O2D-CED
23	B	604	CLA	C3-C5-C6-C7
23	b	606	CLA	C3-C5-C6-C7
23	c	502	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
35	N	609	CHL	C3-C5-C6-C7
35	Y	310	CHL	C3-C5-C6-C7
35	y	310	CHL	C3-C5-C6-C7
35	R	308	CHL	C3-C5-C6-C7
23	G	610	CLA	CBA-CGA-O2A-C1
23	G	611	CLA	CBA-CGA-O2A-C1
23	N	611	CLA	CBA-CGA-O2A-C1
23	N	613	CLA	CBA-CGA-O2A-C1
23	S	305	CLA	CBA-CGA-O2A-C1
23	Y	313	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
23	r	608	CLA	CBA-CGA-O2A-C1
23	n	603	CLA	CBA-CGA-O2A-C1
23	n	611	CLA	CBA-CGA-O2A-C1
35	S	308	CHL	CBA-CGA-O2A-C1
35	Y	308	CHL	CBA-CGA-O2A-C1
35	s	607	CHL	CBA-CGA-O2A-C1
32	C	520	DMU	O6-C11-C9-O1
23	B	614	CLA	O1D-CGD-O2D-CED
23	C	512	CLA	O1D-CGD-O2D-CED
23	Y	315	CLA	O1D-CGD-O2D-CED
23	c	502	CLA	O1D-CGD-O2D-CED
33	D	406	PL9	C7-C8-C9-C10
33	d	406	PL9	C7-C8-C9-C10
23	b	605	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
23	C	510	CLA	O1D-CGD-O2D-CED
23	a	404	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	O1D-CGD-O2D-CED
23	c	508	CLA	O1D-CGD-O2D-CED
23	s	613	CLA	O1D-CGD-O2D-CED
35	N	608	CHL	O1D-CGD-O2D-CED
35	Y	308	CHL	O1D-CGD-O2D-CED
32	C	523	DMU	O6-C11-C9-C8
32	c	522	DMU	O6-C11-C9-C8
23	C	503	CLA	O1A-CGA-O2A-C1
23	C	505	CLA	O1A-CGA-O2A-C1
23	G	602	CLA	O1A-CGA-O2A-C1
23	S	305	CLA	O1A-CGA-O2A-C1
23	Y	303	CLA	O1A-CGA-O2A-C1
23	c	504	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	n	613	CLA	O1A-CGA-O2A-C1
23	y	313	CLA	O1A-CGA-O2A-C1
35	s	607	CHL	O1A-CGA-O2A-C1
23	G	614	CLA	O1D-CGD-O2D-CED
23	s	612	CLA	O1D-CGD-O2D-CED
23	y	315	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED
23	G	602	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	s	610	CLA	CBD-CGD-O2D-CED
23	n	612	CLA	CBD-CGD-O2D-CED
35	S	302	CHL	CBD-CGD-O2D-CED
35	n	605	CHL	CBD-CGD-O2D-CED
23	B	605	CLA	O1D-CGD-O2D-CED
23	N	602	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C3-C5-C6-C7
23	C	508	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
23	C	505	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	CBA-CGA-O2A-C1
35	G	608	CHL	CBA-CGA-O2A-C1
35	g	608	CHL	CBA-CGA-O2A-C1
35	n	605	CHL	CBA-CGA-O2A-C1
23	c	502	CLA	O1A-CGA-O2A-C1
23	d	404	CLA	O1A-CGA-O2A-C1
23	y	303	CLA	O1A-CGA-O2A-C1
23	S	313	CLA	O1D-CGD-O2D-CED
26	B	625	SQD	C8-C7-O47-C45
23	S	314	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	CBD-CGD-O2D-CED
23	b	603	CLA	CBD-CGD-O2D-CED
32	c	519	DMU	O6-C11-C9-O1
35	G	608	CHL	O1A-CGA-O2A-C1
23	c	509	CLA	O1D-CGD-O2D-CED
35	y	309	CHL	O1D-CGD-O2D-CED
23	d	403	CLA	C3-C5-C6-C7
23	G	602	CLA	CBA-CGA-O2A-C1
23	Y	303	CLA	CBA-CGA-O2A-C1
23	y	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	S	304	CLA	O1D-CGD-O2D-CED
23	N	613	CLA	O1A-CGA-O2A-C1
24	D	402	PHO	C4-C3-C5-C6
24	a	403	PHO	C4-C3-C5-C6
33	D	406	PL9	C40-C39-C41-C42
33	d	406	PL9	C40-C39-C41-C42
23	R	304	CLA	C2-C3-C5-C6
24	D	402	PHO	C2-C3-C5-C6
24	a	403	PHO	C2-C3-C5-C6
35	R	308	CHL	CBD-CGD-O2D-CED
23	G	604	CLA	C2A-CAA-CBA-CGA
23	N	603	CLA	C2A-CAA-CBA-CGA
23	Y	313	CLA	C2A-CAA-CBA-CGA
23	R	303	CLA	C2A-CAA-CBA-CGA
32	s	618	DMU	C4-C3-O7-C10
32	C	523	DMU	O6-C11-C9-O1
32	c	522	DMU	O6-C11-C9-O1
35	g	608	CHL	O1A-CGA-O2A-C1
30	C	522	LMG	O6-C1-O1-C7
30	W	203	LMG	O6-C1-O1-C7
30	c	521	LMG	O6-C1-O1-C7
30	w	202	LMG	O6-C1-O1-C7
35	Y	309	CHL	O1D-CGD-O2D-CED
33	d	406	PL9	C34-C36-C37-C38
23	C	506	CLA	CBA-CGA-O2A-C1
23	y	305	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	O1D-CGD-O2D-CED
23	N	614	CLA	O1D-CGD-O2D-CED
23	b	612	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	O1D-CGD-O2D-CED
23	n	614	CLA	O1D-CGD-O2D-CED
35	Y	302	CHL	O1D-CGD-O2D-CED
35	y	302	CHL	O1D-CGD-O2D-CED
35	n	605	CHL	O1A-CGA-O2A-C1
26	b	602	SQD	C8-C7-O47-C45
23	G	603	CLA	O1D-CGD-O2D-CED
23	N	604	CLA	O1D-CGD-O2D-CED
23	s	602	CLA	O1D-CGD-O2D-CED
23	y	305	CLA	O1D-CGD-O2D-CED
31	G	619	LHG	C1-C2-C3-O3
31	g	619	LHG	C1-C2-C3-O3
32	S	319	DMU	C4-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C3-C5-C6-C7
23	b	607	CLA	C3-C5-C6-C7
23	r	610	CLA	O1D-CGD-O2D-CED
23	s	603	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	CBA-CGA-O2A-C1
23	B	603	CLA	CBA-CGA-O2A-C1
23	B	616	CLA	CBA-CGA-O2A-C1
23	G	613	CLA	CBA-CGA-O2A-C1
23	Y	305	CLA	CBA-CGA-O2A-C1
23	b	604	CLA	CBA-CGA-O2A-C1
23	b	605	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CBA-CGA-O2A-C1
23	g	613	CLA	CBA-CGA-O2A-C1
35	N	605	CHL	CBA-CGA-O2A-C1
23	Y	314	CLA	CBD-CGD-O2D-CED
35	s	601	CHL	CBD-CGD-O2D-CED
31	b	623	LHG	C7-C8-C9-C10
23	R	310	CLA	C10-C11-C12-C13
24	a	403	PHO	C15-C16-C17-C18
35	Y	310	CHL	C13-C15-C16-C17
35	n	608	CHL	C15-C16-C17-C18
35	y	310	CHL	C13-C15-C16-C17
28	d	410	DGD	O1G-C1G-C2G-O2G
23	B	616	CLA	O1A-CGA-O2A-C1
23	B	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	G	602	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	g	602	CLA	C6-C7-C8-C9
23	y	314	CLA	C6-C7-C8-C9
35	Y	309	CHL	C11-C10-C8-C9
35	y	309	CHL	C11-C10-C8-C9
23	D	404	CLA	O1D-CGD-O2D-CED
23	G	613	CLA	O1D-CGD-O2D-CED
23	d	404	CLA	O1D-CGD-O2D-CED
23	r	608	CLA	O1D-CGD-O2D-CED
23	R	302	CLA	O1D-CGD-O2D-CED
23	y	303	CLA	CBD-CGD-O2D-CED
23	G	602	CLA	C2A-CAA-CBA-CGA
23	r	604	CLA	C2A-CAA-CBA-CGA
23	R	305	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	B	619	BCR	C37-C22-C23-C24
25	K	101	BCR	C7-C8-C9-C34
25	b	621	BCR	C37-C22-C23-C24
25	d	405	BCR	C37-C22-C23-C24
35	n	608	CHL	O1D-CGD-O2D-CED
23	B	603	CLA	O1A-CGA-O2A-C1
23	b	605	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C5-C6-C7-C8
23	B	608	CLA	C5-C6-C7-C8
23	B	615	CLA	C10-C11-C12-C13
23	c	508	CLA	C5-C6-C7-C8
23	r	609	CLA	C10-C11-C12-C13
35	N	608	CHL	C15-C16-C17-C18
35	g	601	CHL	C13-C15-C16-C17
35	g	608	CHL	C15-C16-C17-C18
35	r	607	CHL	C10-C11-C12-C13
23	R	311	CLA	O1D-CGD-O2D-CED
23	Y	314	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
23	y	314	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	C	510	CLA	C10-C11-C12-C13
23	C	510	CLA	C13-C15-C16-C17
23	D	404	CLA	C13-C15-C16-C17
23	Y	303	CLA	C10-C11-C12-C13
23	b	608	CLA	C10-C11-C12-C13
23	b	612	CLA	C13-C15-C16-C17
23	b	616	CLA	C8-C10-C11-C12
24	D	402	PHO	C15-C16-C17-C18
35	G	608	CHL	C15-C16-C17-C18
28	B	624	DGD	C1B-C2B-C3B-C4B
30	b	622	LMG	C28-C29-C30-C31
31	B	621	LHG	C7-C8-C9-C10
31	G	619	LHG	C23-C24-C25-C26
23	N	612	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	C10-C11-C12-C13
23	C	504	CLA	C10-C11-C12-C13
23	C	509	CLA	C5-C6-C7-C8
23	b	604	CLA	C5-C6-C7-C8
23	b	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C10-C11-C12-C13
23	c	503	CLA	C10-C11-C12-C13
23	c	509	CLA	C13-C15-C16-C17
23	d	403	CLA	C10-C11-C12-C13
35	G	601	CHL	C13-C15-C16-C17
35	R	308	CHL	C5-C6-C7-C8
39	W	202	VTQ	C15-C16-C17-C18
39	W	202	VTQ	C23-C24-C25-C26
39	w	201	VTQ	C23-C24-C25-C26
31	d	408	LHG	C7-C8-C9-C10
35	Y	306	CHL	O1D-CGD-O2D-CED
23	y	311	CLA	C5-C6-C7-C8
24	A	403	PHO	C15-C16-C17-C18
35	Y	302	CHL	C13-C15-C16-C17
23	b	617	CLA	O1D-CGD-O2D-CED
35	N	605	CHL	O1D-CGD-O2D-CED
35	y	306	CHL	O1D-CGD-O2D-CED
26	B	625	SQD	O49-C7-O47-C45
26	b	602	SQD	O49-C7-O47-C45
23	Y	312	CLA	C8-C10-C11-C12
35	G	601	CHL	C5-C6-C7-C8
23	Y	305	CLA	O1D-CGD-O2D-CED
30	B	620	LMG	C28-C29-C30-C31
23	B	616	CLA	CBD-CGD-O2D-CED
23	G	604	CLA	CBD-CGD-O2D-CED
23	S	309	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	n	611	CLA	CBD-CGD-O2D-CED
35	s	607	CHL	O2A-C1-C2-C3
23	B	612	CLA	C5-C6-C7-C8
24	a	402	PHO	C10-C11-C12-C13
24	a	402	PHO	C15-C16-C17-C18
35	g	601	CHL	C5-C6-C7-C8
35	y	302	CHL	C13-C15-C16-C17
23	b	618	CLA	C6-C7-C8-C10
23	r	611	CLA	C6-C7-C8-C10
35	Y	310	CHL	C11-C12-C13-C15
23	B	602	CLA	O1A-CGA-O2A-C1
23	G	613	CLA	O1A-CGA-O2A-C1
23	Y	314	CLA	O1A-CGA-O2A-C1
23	Y	303	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C2A-CAA-CBA-CGA
23	n	610	CLA	C2A-CAA-CBA-CGA
23	y	313	CLA	C2A-CAA-CBA-CGA
35	y	306	CHL	C2A-CAA-CBA-CGA
23	s	609	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	C5-C6-C7-C8
23	B	611	CLA	C13-C15-C16-C17
23	Y	311	CLA	C5-C6-C7-C8
23	b	607	CLA	C5-C6-C7-C8
23	b	613	CLA	C13-C15-C16-C17
23	b	614	CLA	C5-C6-C7-C8
23	c	509	CLA	C10-C11-C12-C13
23	d	404	CLA	C5-C6-C7-C8
23	r	609	CLA	C15-C16-C17-C18
23	y	312	CLA	C8-C10-C11-C12
24	A	403	PHO	C10-C11-C12-C13
24	a	403	PHO	C13-C15-C16-C17
35	Y	308	CHL	C13-C15-C16-C17
35	y	308	CHL	C13-C15-C16-C17
39	w	201	VTQ	C15-C16-C17-C18
23	C	506	CLA	O1A-CGA-O2A-C1
23	Y	305	CLA	O1A-CGA-O2A-C1
23	b	604	CLA	O1A-CGA-O2A-C1
35	N	605	CHL	O1A-CGA-O2A-C1
26	l	101	SQD	O5-C1-O6-C44
32	c	519	DMU	O5-C6-O16-C18
24	D	402	PHO	C13-C15-C16-C17
23	B	615	CLA	O1D-CGD-O2D-CED
23	S	310	CLA	O1D-CGD-O2D-CED
33	D	406	PL9	C39-C41-C42-C43
33	d	406	PL9	C39-C41-C42-C43
31	B	622	LHG	C23-C24-C25-C26
35	N	601	CHL	C15-C16-C17-C18
35	n	609	CHL	C5-C6-C7-C8
23	D	404	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
23	y	305	CLA	O1A-CGA-O2A-C1
23	y	314	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	C13-C15-C16-C17
23	C	511	CLA	C15-C16-C17-C18
23	Y	313	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	r	611	CLA	C5-C6-C7-C8
23	y	303	CLA	C10-C11-C12-C13
23	y	313	CLA	C10-C11-C12-C13
35	Y	308	CHL	C8-C10-C11-C12
35	Y	310	CHL	C5-C6-C7-C8
35	r	607	CHL	C5-C6-C7-C8
35	n	601	CHL	C15-C16-C17-C18
23	C	508	CLA	O1D-CGD-O2D-CED
23	b	618	CLA	O1D-CGD-O2D-CED
23	r	601	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	C8-C10-C11-C12
23	b	608	CLA	C8-C10-C11-C12
23	c	503	CLA	C13-C15-C16-C17
23	c	510	CLA	C15-C16-C17-C18
35	N	609	CHL	C5-C6-C7-C8
35	y	308	CHL	C8-C10-C11-C12
35	y	310	CHL	C5-C6-C7-C8
35	R	308	CHL	C10-C11-C12-C13
31	B	621	LHG	C3-O3-P-O6
31	B	621	LHG	C4-O6-P-O3
31	B	622	LHG	C3-O3-P-O6
31	D	407	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	G	619	LHG	C4-O6-P-O3
31	L	101	LHG	C3-O3-P-O6
31	N	618	LHG	C4-O6-P-O3
31	S	318	LHG	C4-O6-P-O3
31	W	201	LHG	C4-O6-P-O3
31	Y	319	LHG	C3-O3-P-O6
31	Y	319	LHG	C4-O6-P-O3
31	b	623	LHG	C3-O3-P-O6
31	b	623	LHG	C4-O6-P-O3
31	b	624	LHG	C4-O6-P-O3
31	b	626	LHG	C4-O6-P-O3
31	c	516	LHG	C4-O6-P-O3
31	d	407	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O3
31	g	619	LHG	C4-O6-P-O3
31	l	102	LHG	C3-O3-P-O6
31	s	617	LHG	C4-O6-P-O3
31	n	618	LHG	C4-O6-P-O3
31	y	318	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
31	y	318	LHG	C4-O6-P-O3
31	D	408	LHG	C7-C8-C9-C10
23	C	509	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C5-C6-C7-C8
23	b	615	CLA	C8-C10-C11-C12
23	c	508	CLA	C8-C10-C11-C12
23	n	604	CLA	O1D-CGD-O2D-CED
23	g	603	CLA	C4-C3-C5-C6
23	R	309	CLA	C5-C6-C7-C8
23	R	312	CLA	C8-C10-C11-C12
35	g	609	CHL	C5-C6-C7-C8
35	G	605	CHL	O1D-CGD-O2D-CED
23	C	502	CLA	C2A-CAA-CBA-CGA
23	y	303	CLA	C2A-CAA-CBA-CGA
35	Y	308	CHL	C2A-CAA-CBA-CGA
23	B	605	CLA	C16-C17-C18-C19
23	B	608	CLA	C16-C17-C18-C19
23	y	311	CLA	C11-C12-C13-C15
35	g	605	CHL	O1D-CGD-O2D-CED
23	A	401	CLA	CBA-CGA-O2A-C1
23	a	401	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	C8-C10-C11-C12
35	Y	310	CHL	C15-C16-C17-C18
31	g	619	LHG	C23-C24-C25-C26
31	n	618	LHG	C11-C12-C13-C14
23	n	603	CLA	CBD-CGD-O2D-CED
28	d	410	DGD	C4B-C5B-C6B-C7B
31	B	621	LHG	C15-C16-C17-C18
35	g	601	CHL	C2C-C3C-CAC-CBC
23	B	602	CLA	C16-C17-C18-C20
23	D	401	CLA	C16-C17-C18-C19
23	G	602	CLA	C16-C17-C18-C19
23	b	604	CLA	C16-C17-C18-C20
23	d	401	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
23	r	602	CLA	C11-C12-C13-C14
35	Y	308	CHL	C16-C17-C18-C20
23	r	602	CLA	CBA-CGA-O2A-C1
23	R	303	CLA	CBA-CGA-O2A-C1
31	D	407	LHG	C30-C31-C32-C33
31	b	623	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	L	102	LHG	O9-C7-O7-C5
31	l	103	LHG	O9-C7-O7-C5
31	D	408	LHG	C11-C12-C13-C14
31	d	408	LHG	C11-C12-C13-C14
35	G	601	CHL	C2C-C3C-CAC-CBC
31	B	622	LHG	O2-C2-C3-O3
26	l	101	SQD	C17-C18-C19-C20
23	C	511	CLA	C3-C5-C6-C7
23	c	510	CLA	C3-C5-C6-C7
23	b	605	CLA	O1D-CGD-O2D-CED
35	S	302	CHL	O1D-CGD-O2D-CED
26	B	625	SQD	C2-C1-O6-C44
26	L	103	SQD	C2-C1-O6-C44
26	b	602	SQD	C2-C1-O6-C44
32	c	519	DMU	C1-C6-O16-C18
23	N	610	CLA	CBA-CGA-O2A-C1
23	C	509	CLA	O1A-CGA-O2A-C1
23	c	508	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C16-C17-C18-C19
23	D	401	CLA	C16-C17-C18-C20
23	Y	311	CLA	C11-C12-C13-C15
23	b	607	CLA	C16-C17-C18-C19
35	Y	310	CHL	C16-C17-C18-C20
35	y	308	CHL	C16-C17-C18-C20
35	y	310	CHL	C16-C17-C18-C20
23	B	603	CLA	O1D-CGD-O2D-CED
23	s	610	CLA	O1D-CGD-O2D-CED
23	B	611	CLA	C4-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	N	611	CLA	C4-C3-C5-C6
23	b	613	CLA	C4-C3-C5-C6
23	n	611	CLA	C4-C3-C5-C6
23	B	611	CLA	C2-C3-C5-C6
23	g	603	CLA	C2-C3-C5-C6
23	B	609	CLA	C11-C12-C13-C14
23	B	612	CLA	C6-C7-C8-C9
23	B	613	CLA	C6-C7-C8-C9
23	B	614	CLA	C6-C7-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	611	CLA	C11-C12-C13-C14
23	b	618	CLA	C11-C10-C8-C9
23	y	304	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	R	312	CLA	C14-C13-C15-C16
35	y	310	CHL	C11-C12-C13-C14
23	G	602	CLA	O1D-CGD-O2D-CED
23	n	612	CLA	O1D-CGD-O2D-CED
30	d	409	LMG	C28-C29-C30-C31
26	c	520	SQD	C10-C11-C12-C13
31	N	618	LHG	C11-C12-C13-C14
23	B	603	CLA	C13-C15-C16-C17
23	B	613	CLA	C8-C10-C11-C12
23	A	401	CLA	C2A-CAA-CBA-CGA
23	C	506	CLA	C2A-CAA-CBA-CGA
23	N	610	CLA	C2A-CAA-CBA-CGA
23	a	401	CLA	C2A-CAA-CBA-CGA
23	c	505	CLA	C2A-CAA-CBA-CGA
23	n	603	CLA	C2A-CAA-CBA-CGA
35	N	608	CHL	C2A-CAA-CBA-CGA
35	n	607	CHL	C2A-CAA-CBA-CGA
31	D	407	LHG	O1-C1-C2-C3
31	d	407	LHG	O1-C1-C2-C3
25	D	405	BCR	C7-C8-C9-C10
38	S	317	NEX	C11-C12-C13-C14
23	b	610	CLA	C3-C5-C6-C7
23	B	601	CLA	C8-C10-C11-C12
31	L	102	LHG	C8-C7-O7-C5
31	l	103	LHG	C8-C7-O7-C5
30	c	521	LMG	C13-C14-C15-C16
31	L	102	LHG	C24-C25-C26-C27
31	l	103	LHG	C24-C25-C26-C27
28	A	408	DGD	C1B-C2B-C3B-C4B
30	s	619	LMG	C19-C20-C21-C22
31	L	102	LHG	C28-C29-C30-C31
31	l	103	LHG	C28-C29-C30-C31
23	A	401	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C4B-C3B-CAB-CBB
23	B	603	CLA	C4B-C3B-CAB-CBB
23	B	607	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	C4B-C3B-CAB-CBB
23	D	404	CLA	C4B-C3B-CAB-CBB
23	G	602	CLA	C4B-C3B-CAB-CBB
23	G	611	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	G	612	CLA	C4B-C3B-CAB-CBB
23	G	613	CLA	C4B-C3B-CAB-CBB
23	N	603	CLA	C4B-C3B-CAB-CBB
23	N	612	CLA	C4B-C3B-CAB-CBB
23	N	614	CLA	C4B-C3B-CAB-CBB
23	S	303	CLA	C4B-C3B-CAB-CBB
23	S	313	CLA	C4B-C3B-CAB-CBB
23	S	314	CLA	C4B-C3B-CAB-CBB
23	Y	315	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	b	605	CLA	C4B-C3B-CAB-CBB
23	b	607	CLA	C4B-C3B-CAB-CBB
23	b	609	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	c	505	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
23	c	511	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
23	d	404	CLA	C4B-C3B-CAB-CBB
23	g	602	CLA	C4B-C3B-CAB-CBB
23	g	603	CLA	C4B-C3B-CAB-CBB
23	g	611	CLA	C4B-C3B-CAB-CBB
23	g	612	CLA	C4B-C3B-CAB-CBB
23	g	614	CLA	C4B-C3B-CAB-CBB
23	r	603	CLA	C4B-C3B-CAB-CBB
23	r	608	CLA	C4B-C3B-CAB-CBB
23	r	610	CLA	C4B-C3B-CAB-CBB
23	r	612	CLA	C4B-C3B-CAB-CBB
23	s	603	CLA	C4B-C3B-CAB-CBB
23	s	612	CLA	C4B-C3B-CAB-CBB
23	s	613	CLA	C4B-C3B-CAB-CBB
23	n	612	CLA	C4B-C3B-CAB-CBB
23	n	614	CLA	C4B-C3B-CAB-CBB
23	y	315	CLA	C4B-C3B-CAB-CBB
23	R	303	CLA	C4B-C3B-CAB-CBB
23	R	304	CLA	C4B-C3B-CAB-CBB
23	R	309	CLA	C4B-C3B-CAB-CBB
23	R	310	CLA	C4B-C3B-CAB-CBB
23	R	311	CLA	C4B-C3B-CAB-CBB
23	R	313	CLA	C4B-C3B-CAB-CBB
35	G	607	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
35	G	608	CHL	C4B-C3B-CAB-CBB
35	G	609	CHL	C4B-C3B-CAB-CBB
35	N	607	CHL	C4B-C3B-CAB-CBB
35	N	608	CHL	C4B-C3B-CAB-CBB
35	S	306	CHL	C4B-C3B-CAB-CBB
35	S	307	CHL	C4B-C3B-CAB-CBB
35	Y	302	CHL	C4B-C3B-CAB-CBB
35	Y	306	CHL	C4B-C3B-CAB-CBB
35	Y	309	CHL	C4B-C3B-CAB-CBB
35	g	608	CHL	C4B-C3B-CAB-CBB
35	r	606	CHL	C4B-C3B-CAB-CBB
35	r	607	CHL	C4B-C3B-CAB-CBB
35	s	601	CHL	C4B-C3B-CAB-CBB
35	n	607	CHL	C4B-C3B-CAB-CBB
35	n	608	CHL	C4B-C3B-CAB-CBB
35	y	302	CHL	C4B-C3B-CAB-CBB
35	y	306	CHL	C4B-C3B-CAB-CBB
35	y	309	CHL	C4B-C3B-CAB-CBB
35	R	307	CHL	C4B-C3B-CAB-CBB
35	R	308	CHL	C4B-C3B-CAB-CBB
23	C	511	CLA	C16-C17-C18-C20
23	b	604	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C20
23	d	401	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C19
23	g	602	CLA	C16-C17-C18-C19
23	g	602	CLA	C16-C17-C18-C20
23	y	311	CLA	C11-C12-C13-C14
23	R	303	CLA	C11-C12-C13-C14
26	B	625	SQD	O5-C1-O6-C44
26	b	602	SQD	O5-C1-O6-C44
23	A	404	CLA	C5-C6-C7-C8
23	b	618	CLA	C5-C6-C7-C8
23	y	312	CLA	C5-C6-C7-C8
23	R	312	CLA	C5-C6-C7-C8
35	G	606	CHL	CBD-CGD-O2D-CED
23	C	513	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
30	S	301	LMG	C19-C20-C21-C22
31	C	518	LHG	C14-C15-C16-C17
23	G	602	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	r	608	CLA	C5-C6-C7-C8
24	A	403	PHO	C5-C6-C7-C8
24	a	402	PHO	C5-C6-C7-C8
35	G	609	CHL	C5-C6-C7-C8
23	g	610	CLA	C15-C16-C17-C18
31	c	517	LHG	C14-C15-C16-C17
23	B	614	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
23	n	610	CLA	CBA-CGA-O2A-C1
28	B	626	DGD	C2A-C1A-O1G-C1G
28	b	625	DGD	C2A-C1A-O1G-C1G
23	A	402	CLA	C3A-C2A-CAA-CBA
23	B	608	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	C3A-C2A-CAA-CBA
23	C	508	CLA	C3A-C2A-CAA-CBA
23	D	403	CLA	C3A-C2A-CAA-CBA
23	N	603	CLA	C3A-C2A-CAA-CBA
23	N	612	CLA	C3A-C2A-CAA-CBA
23	N	613	CLA	C3A-C2A-CAA-CBA
23	S	312	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	615	CLA	C3A-C2A-CAA-CBA
23	c	507	CLA	C3A-C2A-CAA-CBA
23	d	403	CLA	C3A-C2A-CAA-CBA
23	r	611	CLA	C3A-C2A-CAA-CBA
23	s	608	CLA	C3A-C2A-CAA-CBA
23	n	603	CLA	C3A-C2A-CAA-CBA
23	n	612	CLA	C3A-C2A-CAA-CBA
23	n	613	CLA	C3A-C2A-CAA-CBA
23	R	312	CLA	C3A-C2A-CAA-CBA
35	N	607	CHL	C3A-C2A-CAA-CBA
35	Y	306	CHL	C3A-C2A-CAA-CBA
35	Y	307	CHL	C3A-C2A-CAA-CBA
35	r	605	CHL	C3A-C2A-CAA-CBA
35	n	607	CHL	C3A-C2A-CAA-CBA
35	y	306	CHL	C3A-C2A-CAA-CBA
35	y	307	CHL	C3A-C2A-CAA-CBA
35	R	306	CHL	C3A-C2A-CAA-CBA
35	Y	302	CHL	C10-C11-C12-C13
32	C	523	DMU	C19-C18-O16-C6
31	Y	319	LHG	C30-C31-C32-C33
23	D	404	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C16-C17-C18-C19
23	G	602	CLA	C16-C17-C18-C20
23	r	602	CLA	C11-C12-C13-C15
23	R	303	CLA	C11-C12-C13-C15
35	y	310	CHL	C16-C17-C18-C19
26	B	625	SQD	C9-C10-C11-C12
28	C	517	DGD	C3B-C4B-C5B-C6B
26	l	101	SQD	O6-C44-C45-C46
32	S	319	DMU	C18-C19-C22-C25
32	s	618	DMU	C18-C19-C22-C25
23	g	612	CLA	CBD-CGD-O2D-CED
23	r	604	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	C3-C5-C6-C7
23	Y	304	CLA	C3-C5-C6-C7
23	C	513	CLA	C4-C3-C5-C6
23	N	613	CLA	C4-C3-C5-C6
23	b	610	CLA	C4-C3-C5-C6
23	B	614	CLA	C2-C3-C5-C6
23	C	513	CLA	C2-C3-C5-C6
23	N	613	CLA	C2-C3-C5-C6
23	b	613	CLA	C2-C3-C5-C6
23	r	612	CLA	C2-C3-C5-C6
23	R	313	CLA	C2-C3-C5-C6
35	n	605	CHL	O1D-CGD-O2D-CED
23	C	511	CLA	O1D-CGD-O2D-CED
30	C	522	LMG	C30-C31-C32-C33
31	b	624	LHG	C28-C29-C30-C31
23	a	401	CLA	O1A-CGA-O2A-C1
23	Y	311	CLA	C11-C12-C13-C14
23	A	401	CLA	C2B-C3B-CAB-CBB
23	B	602	CLA	C2B-C3B-CAB-CBB
23	B	603	CLA	C2B-C3B-CAB-CBB
23	B	607	CLA	C2B-C3B-CAB-CBB
23	B	615	CLA	C2B-C3B-CAB-CBB
23	C	503	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB
23	C	508	CLA	C2B-C3B-CAB-CBB
23	D	404	CLA	C2B-C3B-CAB-CBB
23	G	602	CLA	C2B-C3B-CAB-CBB
23	G	611	CLA	C2B-C3B-CAB-CBB
23	G	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	G	613	CLA	C2B-C3B-CAB-CBB
23	N	603	CLA	C2B-C3B-CAB-CBB
23	N	611	CLA	C2B-C3B-CAB-CBB
23	N	614	CLA	C2B-C3B-CAB-CBB
23	S	303	CLA	C2B-C3B-CAB-CBB
23	S	304	CLA	C2B-C3B-CAB-CBB
23	S	313	CLA	C2B-C3B-CAB-CBB
23	S	314	CLA	C2B-C3B-CAB-CBB
23	Y	315	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	b	605	CLA	C2B-C3B-CAB-CBB
23	b	607	CLA	C2B-C3B-CAB-CBB
23	b	609	CLA	C2B-C3B-CAB-CBB
23	b	617	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
23	c	504	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C2B-C3B-CAB-CBB
23	d	402	CLA	C2B-C3B-CAB-CBB
23	d	404	CLA	C2B-C3B-CAB-CBB
23	g	602	CLA	C2B-C3B-CAB-CBB
23	g	603	CLA	C2B-C3B-CAB-CBB
23	g	611	CLA	C2B-C3B-CAB-CBB
23	g	612	CLA	C2B-C3B-CAB-CBB
23	g	614	CLA	C2B-C3B-CAB-CBB
23	r	603	CLA	C2B-C3B-CAB-CBB
23	r	604	CLA	C2B-C3B-CAB-CBB
23	r	608	CLA	C2B-C3B-CAB-CBB
23	r	610	CLA	C2B-C3B-CAB-CBB
23	r	612	CLA	C2B-C3B-CAB-CBB
23	s	603	CLA	C2B-C3B-CAB-CBB
23	s	612	CLA	C2B-C3B-CAB-CBB
23	s	613	CLA	C2B-C3B-CAB-CBB
23	n	611	CLA	C2B-C3B-CAB-CBB
23	n	614	CLA	C2B-C3B-CAB-CBB
23	y	315	CLA	C2B-C3B-CAB-CBB
23	R	303	CLA	C2B-C3B-CAB-CBB
23	R	304	CLA	C2B-C3B-CAB-CBB
23	R	305	CLA	C2B-C3B-CAB-CBB
23	R	309	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	R	310	CLA	C2B-C3B-CAB-CBB
23	R	311	CLA	C2B-C3B-CAB-CBB
23	R	313	CLA	C2B-C3B-CAB-CBB
35	G	607	CHL	C2B-C3B-CAB-CBB
35	G	608	CHL	C2B-C3B-CAB-CBB
35	G	609	CHL	C2B-C3B-CAB-CBB
35	N	607	CHL	C2B-C3B-CAB-CBB
35	N	608	CHL	C2B-C3B-CAB-CBB
35	S	306	CHL	C2B-C3B-CAB-CBB
35	S	307	CHL	C2B-C3B-CAB-CBB
35	Y	302	CHL	C2B-C3B-CAB-CBB
35	Y	306	CHL	C2B-C3B-CAB-CBB
35	Y	309	CHL	C2B-C3B-CAB-CBB
35	g	608	CHL	C2B-C3B-CAB-CBB
35	r	606	CHL	C2B-C3B-CAB-CBB
35	r	607	CHL	C2B-C3B-CAB-CBB
35	s	601	CHL	C2B-C3B-CAB-CBB
35	n	607	CHL	C2B-C3B-CAB-CBB
35	n	608	CHL	C2B-C3B-CAB-CBB
35	y	302	CHL	C2B-C3B-CAB-CBB
35	y	306	CHL	C2B-C3B-CAB-CBB
35	y	309	CHL	C2B-C3B-CAB-CBB
35	R	307	CHL	C2B-C3B-CAB-CBB
35	R	308	CHL	C2B-C3B-CAB-CBB
23	G	602	CLA	C8-C10-C11-C12
30	C	522	LMG	C14-C15-C16-C17
31	c	517	LHG	C26-C27-C28-C29
23	B	601	CLA	O1D-CGD-O2D-CED
30	C	501	LMG	C37-C38-C39-C40
31	y	318	LHG	C30-C31-C32-C33
23	A	401	CLA	O1A-CGA-O2A-C1
23	r	602	CLA	O1A-CGA-O2A-C1
23	R	303	CLA	O1A-CGA-O2A-C1
23	g	610	CLA	C10-C11-C12-C13
30	b	622	LMG	C36-C37-C38-C39
30	B	620	LMG	C32-C33-C34-C35
23	B	603	CLA	C8-C10-C11-C12
23	b	603	CLA	C8-C10-C11-C12
35	n	609	CHL	C8-C10-C11-C12
23	N	610	CLA	O1A-CGA-O2A-C1
28	B	626	DGD	O1A-C1A-O1G-C1G
28	b	625	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
30	C	522	LMG	C13-C14-C15-C16
31	L	102	LHG	C23-C24-C25-C26
25	A	405	BCR	C23-C24-C25-C26
25	A	405	BCR	C23-C24-C25-C30
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	B	617	BCR	C23-C24-C25-C26
25	B	617	BCR	C23-C24-C25-C30
25	B	619	BCR	C23-C24-C25-C26
25	B	619	BCR	C23-C24-C25-C30
25	D	405	BCR	C1-C6-C7-C8
25	H	101	BCR	C1-C6-C7-C8
25	H	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	a	405	BCR	C23-C24-C25-C26
25	a	405	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C26
25	b	621	BCR	C23-C24-C25-C26
25	b	621	BCR	C23-C24-C25-C30
25	c	518	BCR	C1-C6-C7-C8
25	c	518	BCR	C5-C6-C7-C8
25	d	405	BCR	C1-C6-C7-C8
25	h	101	BCR	C1-C6-C7-C8
25	h	101	BCR	C5-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
36	N	615	LUT	C5-C6-C7-C8
36	S	315	LUT	C1-C6-C7-C8
36	S	315	LUT	C5-C6-C7-C8
36	S	316	LUT	C1-C6-C7-C8
36	S	316	LUT	C5-C6-C7-C8
36	Y	316	LUT	C5-C6-C7-C8
36	s	614	LUT	C5-C6-C7-C8
36	n	615	LUT	C5-C6-C7-C8
36	y	316	LUT	C5-C6-C7-C8
30	c	521	LMG	C30-C31-C32-C33
23	C	514	CLA	CBA-CGA-O2A-C1
23	g	610	CLA	CBA-CGA-O2A-C1
23	C	503	CLA	C15-C16-C17-C18
23	R	310	CLA	C15-C16-C17-C18
35	N	609	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	y	310	CHL	C15-C16-C17-C18
31	N	618	LHG	C8-C7-O7-C5
23	r	604	CLA	O2A-C1-C2-C3
23	B	608	CLA	CBD-CGD-O2D-CED
23	r	612	CLA	C4-C3-C5-C6
23	b	603	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C6-C7-C8-C10
23	B	607	CLA	C11-C10-C8-C7
23	B	609	CLA	C11-C12-C13-C15
23	B	613	CLA	C6-C7-C8-C10
23	Y	304	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16
23	b	611	CLA	C11-C12-C13-C15
23	b	617	CLA	C11-C12-C13-C15
23	b	617	CLA	C12-C13-C15-C16
23	c	512	CLA	C2-C3-C5-C6
23	g	602	CLA	C6-C7-C8-C10
23	n	611	CLA	C2-C3-C5-C6
23	y	304	CLA	C6-C7-C8-C10
23	R	312	CLA	C6-C7-C8-C10
23	R	312	CLA	C12-C13-C15-C16
35	y	310	CHL	C11-C12-C13-C15
23	B	614	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	O1A-CGA-O2A-C1
23	n	610	CLA	O1A-CGA-O2A-C1
23	B	616	CLA	C5-C6-C7-C8
23	a	404	CLA	C5-C6-C7-C8
39	w	201	VTQ	C18-C20-C21-C22
23	b	607	CLA	C16-C17-C18-C20
31	b	626	LHG	O9-C7-O7-C5
31	n	618	LHG	O9-C7-O7-C5
23	C	507	CLA	CBA-CGA-O2A-C1
23	c	506	CLA	CBA-CGA-O2A-C1
23	y	304	CLA	CBA-CGA-O2A-C1
31	Y	319	LHG	C24-C23-O8-C6
26	L	103	SQD	C26-C27-C28-C29
23	A	402	CLA	C2A-CAA-CBA-CGA
23	N	602	CLA	C2A-CAA-CBA-CGA
23	Y	314	CLA	C2A-CAA-CBA-CGA
23	n	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	y	314	CLA	C2A-CAA-CBA-CGA
35	N	607	CHL	C2A-CAA-CBA-CGA
23	B	615	CLA	C15-C16-C17-C18
23	G	611	CLA	C10-C11-C12-C13
23	Y	303	CLA	CBD-CGD-O2D-CED
23	R	313	CLA	C15-C16-C17-C18
35	y	302	CHL	C10-C11-C12-C13
26	B	625	SQD	C31-C32-C33-C34
31	D	407	LHG	C10-C11-C12-C13
23	g	610	CLA	O1A-CGA-O2A-C1
23	Y	304	CLA	CBA-CGA-O2A-C1
23	R	312	CLA	CBA-CGA-O2A-C1
23	Y	313	CLA	C11-C12-C13-C14
26	L	103	SQD	O5-C1-O6-C44
26	L	103	SQD	C15-C16-C17-C18
31	G	619	LHG	C11-C10-C9-C8
26	a	406	SQD	C23-C24-C25-C26
31	l	103	LHG	C23-C24-C25-C26
26	l	101	SQD	C8-C7-O47-C45
31	B	627	LHG	C8-C7-O7-C5
31	b	626	LHG	C8-C7-O7-C5
31	n	618	LHG	C8-C7-O7-C5
23	B	607	CLA	C8-C10-C11-C12
23	r	602	CLA	CBD-CGD-O2D-CED
26	l	101	SQD	O49-C7-O47-C45
31	B	627	LHG	O9-C7-O7-C5
31	N	618	LHG	O9-C7-O7-C5
35	Y	309	CHL	C3-C5-C6-C7
23	d	404	CLA	C15-C16-C17-C18
26	B	625	SQD	O47-C45-C46-O48
26	b	602	SQD	O47-C45-C46-O48
28	B	624	DGD	O1G-C1G-C2G-O2G
28	D	410	DGD	O1G-C1G-C2G-O2G
30	b	601	LMG	O7-C8-C9-O8
31	N	618	LHG	O7-C5-C6-O8
31	Y	319	LHG	O7-C5-C6-O8
31	y	318	LHG	O7-C5-C6-O8
23	b	608	CLA	CBD-CGD-O2D-CED
23	y	313	CLA	C11-C12-C13-C14
35	y	308	CHL	C16-C17-C18-C19
23	D	401	CLA	C4-C3-C5-C6
23	c	512	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	d	403	CLA	C4-C3-C5-C6
23	n	613	CLA	C4-C3-C5-C6
23	R	303	CLA	C4-C3-C5-C6
23	R	313	CLA	C4-C3-C5-C6
23	N	611	CLA	C2-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
31	d	407	LHG	C10-C11-C12-C13
23	Y	304	CLA	C6-C7-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	b	617	CLA	C11-C12-C13-C14
23	b	617	CLA	C14-C13-C15-C16
23	r	611	CLA	C6-C7-C8-C9
23	R	312	CLA	C6-C7-C8-C9
35	Y	310	CHL	C11-C12-C13-C14
35	R	308	CHL	O1D-CGD-O2D-CED
23	N	611	CLA	CBD-CGD-O2D-CED
23	S	313	CLA	C3-C5-C6-C7
35	y	309	CHL	C3-C5-C6-C7
23	G	613	CLA	C2A-CAA-CBA-CGA
23	N	604	CLA	C2A-CAA-CBA-CGA
23	g	613	CLA	C2A-CAA-CBA-CGA
35	r	606	CHL	C2A-CAA-CBA-CGA
35	n	606	CHL	C2A-CAA-CBA-CGA
35	n	608	CHL	C2A-CAA-CBA-CGA
35	y	308	CHL	C2A-CAA-CBA-CGA
26	l	101	SQD	C25-C26-C27-C28
28	c	515	DGD	C3B-C4B-C5B-C6B
31	g	619	LHG	C11-C10-C9-C8
23	r	611	CLA	CBA-CGA-O2A-C1
35	G	601	CHL	C8-C10-C11-C12
26	l	101	SQD	C26-C27-C28-C29
25	d	405	BCR	C7-C8-C9-C10
38	r	615	NEX	C11-C12-C13-C14
38	n	617	NEX	C31-C32-C33-C34
23	C	514	CLA	O1A-CGA-O2A-C1
23	A	404	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	B	613	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	503	CLA	C1A-C2A-CAA-CBA
23	C	508	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C1A-C2A-CAA-CBA
23	D	403	CLA	C1A-C2A-CAA-CBA
23	D	404	CLA	C1A-C2A-CAA-CBA
23	G	604	CLA	C1A-C2A-CAA-CBA
23	N	603	CLA	C1A-C2A-CAA-CBA
23	N	610	CLA	C1A-C2A-CAA-CBA
23	N	612	CLA	C1A-C2A-CAA-CBA
23	S	303	CLA	C1A-C2A-CAA-CBA
23	S	305	CLA	C1A-C2A-CAA-CBA
23	S	312	CLA	C1A-C2A-CAA-CBA
23	Y	311	CLA	C1A-C2A-CAA-CBA
23	Y	312	CLA	C1A-C2A-CAA-CBA
23	Y	315	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	b	605	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C1A-C2A-CAA-CBA
23	b	615	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	502	CLA	C1A-C2A-CAA-CBA
23	c	503	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	d	401	CLA	C1A-C2A-CAA-CBA
23	d	403	CLA	C1A-C2A-CAA-CBA
23	g	604	CLA	C1A-C2A-CAA-CBA
23	g	610	CLA	C1A-C2A-CAA-CBA
23	r	608	CLA	C1A-C2A-CAA-CBA
23	r	609	CLA	C1A-C2A-CAA-CBA
23	r	611	CLA	C1A-C2A-CAA-CBA
23	r	612	CLA	C1A-C2A-CAA-CBA
23	s	602	CLA	C1A-C2A-CAA-CBA
23	s	603	CLA	C1A-C2A-CAA-CBA
23	s	608	CLA	C1A-C2A-CAA-CBA
23	s	609	CLA	C1A-C2A-CAA-CBA
23	n	603	CLA	C1A-C2A-CAA-CBA
23	n	610	CLA	C1A-C2A-CAA-CBA
23	n	612	CLA	C1A-C2A-CAA-CBA
23	y	311	CLA	C1A-C2A-CAA-CBA
23	y	312	CLA	C1A-C2A-CAA-CBA
23	y	315	CLA	C1A-C2A-CAA-CBA
23	R	309	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	R	310	CLA	C1A-C2A-CAA-CBA
23	R	312	CLA	C1A-C2A-CAA-CBA
23	R	313	CLA	C1A-C2A-CAA-CBA
28	B	624	DGD	O6E-C5E-C6E-O5E
35	r	605	CHL	C1A-C2A-CAA-CBA
35	r	607	CHL	C1A-C2A-CAA-CBA
35	n	608	CHL	C1A-C2A-CAA-CBA
35	R	306	CHL	C1A-C2A-CAA-CBA
35	R	308	CHL	C1A-C2A-CAA-CBA
23	B	605	CLA	C16-C17-C18-C20
23	B	608	CLA	C16-C17-C18-C20
23	Y	313	CLA	C11-C12-C13-C15
23	c	511	CLA	C16-C17-C18-C19
35	Y	310	CHL	C16-C17-C18-C19
23	G	610	CLA	C15-C16-C17-C18
38	R	301	NEX	C33-C34-C35-C15
23	Y	314	CLA	O1D-CGD-O2D-CED
23	G	610	CLA	C10-C11-C12-C13
23	b	609	CLA	C8-C10-C11-C12
35	g	601	CHL	C8-C10-C11-C12
35	n	609	CHL	C10-C11-C12-C13
31	R	317	LHG	C3-O3-P-O6
35	s	601	CHL	O1D-CGD-O2D-CED
23	Y	312	CLA	C5-C6-C7-C8
23	B	608	CLA	CBA-CGA-O2A-C1
31	B	627	LHG	O6-C4-C5-C6
31	C	518	LHG	O6-C4-C5-C6
31	L	102	LHG	O6-C4-C5-C6
31	c	517	LHG	O6-C4-C5-C6
31	l	103	LHG	O6-C4-C5-C6
30	D	409	LMG	C28-C29-C30-C31
30	b	601	LMG	O6-C5-C6-O5
35	Y	308	CHL	C16-C17-C18-C19
30	B	623	LMG	O6-C5-C6-O5
31	B	622	LHG	C11-C10-C9-C8
31	y	318	LHG	C24-C23-O8-C6
23	S	311	CLA	C3A-C2A-CAA-CBA
35	g	606	CHL	C3A-C2A-CAA-CBA
35	Y	302	CHL	C8-C10-C11-C12
32	C	520	DMU	C18-C19-C22-C25
30	w	202	LMG	C11-C10-O7-C8
23	c	506	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	y	304	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C8-C10-C11-C12
23	n	604	CLA	C2A-CAA-CBA-CGA
23	c	510	CLA	C16-C17-C18-C19
26	B	625	SQD	C44-C45-C46-O48
26	L	103	SQD	O6-C44-C45-C46
26	l	101	SQD	C11-C10-C9-C8
31	N	618	LHG	C4-C5-C6-O8
31	S	318	LHG	C4-C5-C6-O8
31	b	626	LHG	C4-C5-C6-O8
31	n	618	LHG	C4-C5-C6-O8
31	b	624	LHG	C11-C10-C9-C8
23	C	507	CLA	O1A-CGA-O2A-C1
30	C	522	LMG	C8-C7-O1-C1
30	c	521	LMG	C8-C7-O1-C1
35	g	601	CHL	C4C-C3C-CAC-CBC
23	c	502	CLA	C15-C16-C17-C18
23	g	611	CLA	C10-C11-C12-C13
28	b	625	DGD	C1A-C2A-C3A-C4A
23	y	303	CLA	O1D-CGD-O2D-CED
26	b	602	SQD	C12-C13-C14-C15
30	c	521	LMG	C14-C15-C16-C17
30	D	409	LMG	O6-C5-C6-O5
35	S	308	CHL	O2A-C1-C2-C3
23	B	610	CLA	C15-C16-C17-C18
30	W	203	LMG	C11-C10-O7-C8
31	W	201	LHG	C8-C7-O7-C5
28	B	626	DGD	O6E-C5E-C6E-O5E
28	b	625	DGD	O6E-C5E-C6E-O5E
30	d	409	LMG	O6-C5-C6-O5
23	b	616	CLA	C4-C3-C5-C6
30	B	620	LMG	C17-C18-C19-C20
31	b	623	LHG	C27-C28-C29-C30
32	S	319	DMU	C2-C3-O7-C10
23	R	312	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	CBA-CGA-O2A-C1
23	c	501	CLA	CBA-CGA-O2A-C1
23	R	313	CLA	CBA-CGA-O2A-C1
35	N	601	CHL	CBA-CGA-O2A-C1
35	G	601	CHL	C4C-C3C-CAC-CBC
23	r	609	CLA	CBD-CGD-O2D-CED
23	g	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	c	516	LHG	C13-C14-C15-C16
30	C	522	LMG	O6-C5-C6-O5
30	c	521	LMG	O6-C5-C6-O5
23	B	608	CLA	O1A-CGA-O2A-C1
23	c	503	CLA	C15-C16-C17-C18
35	G	601	CHL	C2-C1-O2A-CGA
35	y	308	CHL	C2-C1-O2A-CGA
32	s	618	DMU	C2-C3-O7-C10
32	s	618	DMU	C3-C4-C57-O61
23	G	604	CLA	O1D-CGD-O2D-CED
31	C	518	LHG	C10-C11-C12-C13
23	n	611	CLA	O1D-CGD-O2D-CED
30	b	622	LMG	C17-C18-C19-C20
31	G	619	LHG	C30-C31-C32-C33
23	A	404	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
31	b	623	LHG	C24-C23-O8-C6
31	c	517	LHG	C24-C23-O8-C6
23	Y	304	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	C16-C17-C18-C19
23	G	612	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	r	611	CLA	O1A-CGA-O2A-C1
23	d	402	CLA	CBD-CGD-O2D-CED
28	B	626	DGD	C1A-C2A-C3A-C4A
23	b	613	CLA	C10-C11-C12-C13
30	B	623	LMG	O7-C8-C9-O8
31	n	618	LHG	O7-C5-C6-O8
23	B	616	CLA	O1D-CGD-O2D-CED
28	d	410	DGD	CBB-CCB-CDB-CEB
31	Y	319	LHG	O10-C23-O8-C6
23	y	313	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C12-C13-C15
23	B	609	CLA	C12-C13-C15-C16
23	B	611	CLA	C12-C13-C15-C16
23	B	612	CLA	C6-C7-C8-C10
23	B	616	CLA	C11-C10-C8-C7
23	C	502	CLA	C11-C10-C8-C7
23	C	504	CLA	C12-C13-C15-C16
23	C	508	CLA	C6-C7-C8-C10
23	C	510	CLA	C12-C13-C15-C16
23	C	512	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C12-C13-C15-C16
23	G	603	CLA	C12-C13-C15-C16
23	N	602	CLA	C6-C7-C8-C10
23	Y	304	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C10-C8-C7
23	b	611	CLA	C12-C13-C15-C16
23	b	613	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	b	616	CLA	C2-C3-C5-C6
23	b	618	CLA	C11-C10-C8-C7
23	c	507	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C10
23	n	602	CLA	C6-C7-C8-C10
23	y	303	CLA	C11-C12-C13-C15
33	D	406	PL9	C28-C29-C31-C32
33	d	406	PL9	C28-C29-C31-C32
35	G	608	CHL	C12-C13-C15-C16
35	N	609	CHL	C6-C7-C8-C10
35	Y	309	CHL	C11-C10-C8-C7
35	g	608	CHL	C12-C13-C15-C16
35	y	309	CHL	C11-C10-C8-C7
31	W	201	LHG	C13-C14-C15-C16
23	B	601	CLA	C11-C12-C13-C14
23	B	603	CLA	C11-C10-C8-C9
23	B	606	CLA	C11-C12-C13-C14
23	B	607	CLA	C11-C10-C8-C9
23	B	609	CLA	C14-C13-C15-C16
23	B	611	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C10-C8-C9
23	B	612	CLA	C14-C13-C15-C16
23	C	502	CLA	C11-C10-C8-C9
23	C	504	CLA	C6-C7-C8-C9
23	C	508	CLA	C6-C7-C8-C9
23	C	512	CLA	C6-C7-C8-C9
23	N	602	CLA	C6-C7-C8-C9
23	b	603	CLA	C11-C12-C13-C14
23	b	608	CLA	C14-C13-C15-C16
23	b	609	CLA	C11-C10-C8-C9
23	b	611	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C14-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C9
23	c	503	CLA	C6-C7-C8-C9
23	c	507	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	r	609	CLA	C6-C7-C8-C9
23	n	602	CLA	C6-C7-C8-C9
23	y	304	CLA	C11-C12-C13-C14
23	R	310	CLA	C6-C7-C8-C9
35	G	608	CHL	C14-C13-C15-C16
35	g	608	CHL	C14-C13-C15-C16
23	b	610	CLA	CBA-CGA-O2A-C1
23	d	402	CLA	CBA-CGA-O2A-C1
31	B	621	LHG	C24-C23-O8-C6
35	y	306	CHL	CBA-CGA-O2A-C1
35	y	309	CHL	C2A-CAA-CBA-CGA
35	N	601	CHL	O1A-CGA-O2A-C1
26	b	602	SQD	C9-C10-C11-C12
25	B	619	BCR	C21-C22-C23-C24
25	H	101	BCR	C7-C8-C9-C10
36	R	314	LUT	C7-C8-C9-C10
23	B	614	CLA	C3-C5-C6-C7
23	S	309	CLA	O1D-CGD-O2D-CED
35	N	609	CHL	C10-C11-C12-C13
30	C	501	LMG	C11-C10-O7-C8
23	R	304	CLA	CBA-CGA-O2A-C1
31	C	518	LHG	C24-C23-O8-C6
35	Y	310	CHL	CBA-CGA-O2A-C1
35	n	601	CHL	CBA-CGA-O2A-C1
23	C	505	CLA	CBD-CGD-O2D-CED
35	r	607	CHL	CBD-CGD-O2D-CED
23	B	605	CLA	C4B-C3B-CAB-CBB
23	B	611	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C4B-C3B-CAB-CBB
23	C	512	CLA	C4B-C3B-CAB-CBB
23	C	514	CLA	C4B-C3B-CAB-CBB
23	D	401	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
23	G	603	CLA	C4B-C3B-CAB-CBB
23	G	604	CLA	C4B-C3B-CAB-CBB
23	G	614	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	N	604	CLA	C4B-C3B-CAB-CBB
23	N	613	CLA	C4B-C3B-CAB-CBB
23	S	305	CLA	C4B-C3B-CAB-CBB
23	Y	312	CLA	C4B-C3B-CAB-CBB
23	Y	314	CLA	C4B-C3B-CAB-CBB
23	a	401	CLA	C4B-C3B-CAB-CBB
23	b	616	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	C4B-C3B-CAB-CBB
23	d	401	CLA	C4B-C3B-CAB-CBB
23	g	604	CLA	C4B-C3B-CAB-CBB
23	g	610	CLA	C4B-C3B-CAB-CBB
23	g	613	CLA	C4B-C3B-CAB-CBB
23	r	604	CLA	C4B-C3B-CAB-CBB
23	r	609	CLA	C4B-C3B-CAB-CBB
23	n	604	CLA	C4B-C3B-CAB-CBB
23	y	303	CLA	C4B-C3B-CAB-CBB
23	y	305	CLA	C4B-C3B-CAB-CBB
23	y	312	CLA	C4B-C3B-CAB-CBB
23	y	314	CLA	C4B-C3B-CAB-CBB
23	R	305	CLA	C4B-C3B-CAB-CBB
35	S	302	CHL	C4B-C3B-CAB-CBB
35	s	605	CHL	C4B-C3B-CAB-CBB
35	s	607	CHL	C4B-C3B-CAB-CBB
35	n	601	CHL	C4B-C3B-CAB-CBB
35	n	609	CHL	C4B-C3B-CAB-CBB
23	C	512	CLA	C16-C17-C18-C20
28	A	408	DGD	O6D-C1D-O3G-C3G
23	b	617	CLA	C5-C6-C7-C8
31	B	622	LHG	O6-C4-C5-C6
23	B	608	CLA	C3-C5-C6-C7
23	b	609	CLA	C3-C5-C6-C7
33	D	406	PL9	C24-C26-C27-C28
33	d	406	PL9	C24-C26-C27-C28
26	B	625	SQD	C23-C24-C25-C26
23	b	618	CLA	CBA-CGA-O2A-C1
35	Y	306	CHL	CBA-CGA-O2A-C1
24	a	402	PHO	CBD-CGD-O2D-CED
23	b	605	CLA	C8-C10-C11-C12
23	D	401	CLA	C2-C3-C5-C6
23	n	613	CLA	C2-C3-C5-C6
23	C	502	CLA	C10-C11-C12-C13
23	b	614	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
35	Y	308	CHL	C10-C11-C12-C13
23	r	612	CLA	CBA-CGA-O2A-C1
23	g	612	CLA	O1D-CGD-O2D-CED
23	n	603	CLA	O1D-CGD-O2D-CED
23	A	404	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C3A-C2A-CAA-CBA
23	C	510	CLA	C3A-C2A-CAA-CBA
23	N	611	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	c	509	CLA	C3A-C2A-CAA-CBA
23	d	402	CLA	C3A-C2A-CAA-CBA
23	n	611	CLA	C3A-C2A-CAA-CBA
35	Y	308	CHL	C3A-C2A-CAA-CBA
35	g	608	CHL	C3A-C2A-CAA-CBA
35	n	601	CHL	C3A-C2A-CAA-CBA
32	S	319	DMU	C19-C18-O16-C6
32	c	522	DMU	C19-C18-O16-C6
32	s	618	DMU	C19-C18-O16-C6
23	r	603	CLA	C3-C5-C6-C7
23	B	604	CLA	C15-C16-C17-C18
23	b	610	CLA	C13-C15-C16-C17
35	y	308	CHL	C5-C6-C7-C8
23	c	510	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	C15-C16-C17-C18
26	b	602	SQD	C44-C45-C46-O48
28	B	624	DGD	O1G-C1G-C2G-C3G
28	C	517	DGD	O1G-C1G-C2G-C3G
28	D	410	DGD	O1G-C1G-C2G-C3G
28	d	410	DGD	O1G-C1G-C2G-C3G
30	b	601	LMG	C7-C8-C9-O8
31	y	318	LHG	C4-C5-C6-O8
23	C	502	CLA	O1A-CGA-O2A-C1
30	C	501	LMG	C13-C14-C15-C16
23	d	404	CLA	C3-C5-C6-C7
23	R	313	CLA	O1A-CGA-O2A-C1
23	b	612	CLA	C15-C16-C17-C18
23	g	602	CLA	C13-C15-C16-C17
23	c	505	CLA	C4-C3-C5-C6
23	n	603	CLA	C4-C3-C5-C6
23	r	603	CLA	CBA-CGA-O2A-C1
30	W	203	LMG	C38-C39-C40-C41
28	B	626	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
31	B	621	LHG	C27-C28-C29-C30
23	r	604	CLA	O1D-CGD-O2D-CED
35	y	302	CHL	C8-C10-C11-C12
31	l	102	LHG	C4-O6-P-O3
35	r	605	CHL	C3C-C2C-CMC-OMC
35	s	605	CHL	C3C-C2C-CMC-OMC
35	R	306	CHL	C3C-C2C-CMC-OMC
23	c	501	CLA	O1A-CGA-O2A-C1
31	c	517	LHG	O10-C23-O8-C6
31	y	318	LHG	O10-C23-O8-C6
31	L	102	LHG	C11-C10-C9-C8
23	R	304	CLA	C3-C5-C6-C7
23	S	312	CLA	C2A-CAA-CBA-CGA
23	R	302	CLA	C2A-CAA-CBA-CGA
31	B	621	LHG	O6-C4-C5-O7
31	b	626	LHG	O6-C4-C5-O7
23	C	511	CLA	O1A-CGA-O2A-C1
23	b	610	CLA	O1A-CGA-O2A-C1
23	C	509	CLA	C16-C17-C18-C20
30	w	202	LMG	C38-C39-C40-C41
31	L	102	LHG	C33-C34-C35-C36
23	C	506	CLA	CAA-CBA-CGA-O2A
23	c	505	CLA	CAA-CBA-CGA-O2A
23	B	605	CLA	C2B-C3B-CAB-CBB
23	B	614	CLA	C2B-C3B-CAB-CBB
23	C	512	CLA	C2B-C3B-CAB-CBB
23	G	604	CLA	C2B-C3B-CAB-CBB
23	G	614	CLA	C2B-C3B-CAB-CBB
23	N	612	CLA	C2B-C3B-CAB-CBB
23	Y	312	CLA	C2B-C3B-CAB-CBB
23	Y	314	CLA	C2B-C3B-CAB-CBB
23	b	616	CLA	C2B-C3B-CAB-CBB
23	c	511	CLA	C2B-C3B-CAB-CBB
23	g	604	CLA	C2B-C3B-CAB-CBB
23	g	610	CLA	C2B-C3B-CAB-CBB
23	g	613	CLA	C2B-C3B-CAB-CBB
23	r	609	CLA	C2B-C3B-CAB-CBB
23	n	604	CLA	C2B-C3B-CAB-CBB
23	n	612	CLA	C2B-C3B-CAB-CBB
23	y	312	CLA	C2B-C3B-CAB-CBB
23	y	314	CLA	C2B-C3B-CAB-CBB
35	S	302	CHL	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
35	s	605	CHL	C2B-C3B-CAB-CBB
23	B	607	CLA	C3-C5-C6-C7
26	b	602	SQD	C23-C24-C25-C26
26	l	101	SQD	O47-C45-C46-O48
30	W	203	LMG	O1-C7-C8-O7
30	w	202	LMG	O1-C7-C8-O7
31	b	626	LHG	O7-C5-C6-O8
35	G	606	CHL	O1D-CGD-O2D-CED
23	n	610	CLA	C11-C12-C13-C14
26	L	103	SQD	C8-C7-O47-C45
30	s	619	LMG	C11-C10-O7-C8
23	B	605	CLA	C8-C10-C11-C12
23	b	607	CLA	C8-C10-C11-C12
26	L	103	SQD	O49-C7-O47-C45
30	W	203	LMG	O9-C10-O7-C8
30	w	202	LMG	O9-C10-O7-C8
31	W	201	LHG	O9-C7-O7-C5
23	N	603	CLA	C4-C3-C5-C6
35	N	609	CHL	C2-C1-O2A-CGA
35	g	601	CHL	C2-C1-O2A-CGA
35	G	601	CHL	C10-C11-C12-C13
23	B	614	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C11-C10-C8-C9
23	C	503	CLA	C6-C7-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	D	401	CLA	C11-C12-C13-C14
23	N	613	CLA	C6-C7-C8-C9
23	Y	304	CLA	C11-C12-C13-C14
23	b	605	CLA	C11-C10-C8-C9
23	b	617	CLA	C6-C7-C8-C9
23	c	501	CLA	C11-C10-C8-C9
23	c	502	CLA	C6-C7-C8-C9
23	d	401	CLA	C11-C12-C13-C14
23	n	613	CLA	C6-C7-C8-C9
31	l	103	LHG	C33-C34-C35-C36
31	b	623	LHG	O10-C23-O8-C6
35	Y	310	CHL	O1A-CGA-O2A-C1
23	s	602	CLA	C2A-CAA-CBA-CGA
35	Y	309	CHL	C2A-CAA-CBA-CGA
35	R	307	CHL	C2A-CAA-CBA-CGA
23	c	508	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
35	Y	307	CHL	O2A-C1-C2-C3
35	y	307	CHL	O2A-C1-C2-C3
25	H	101	BCR	C23-C24-C25-C26
36	G	615	LUT	C1-C6-C7-C8
36	g	615	LUT	C5-C6-C7-C8
36	s	615	LUT	C1-C6-C7-C8
36	s	615	LUT	C5-C6-C7-C8
23	B	611	CLA	C10-C11-C12-C13
31	b	624	LHG	C31-C32-C33-C34
23	d	402	CLA	O1A-CGA-O2A-C1
35	y	306	CHL	O1A-CGA-O2A-C1
23	r	604	CLA	CBA-CGA-O2A-C1
23	S	311	CLA	C1A-C2A-CAA-CBA
25	b	621	BCR	C21-C22-C23-C24
25	h	101	BCR	C7-C8-C9-C10
23	d	403	CLA	C15-C16-C17-C18
26	B	625	SQD	C15-C16-C17-C18
23	B	608	CLA	O1D-CGD-O2D-CED
30	C	501	LMG	O9-C10-O7-C8
30	s	619	LMG	O9-C10-O7-C8
26	l	101	SQD	C32-C33-C34-C35
23	n	613	CLA	C8-C10-C11-C12
31	b	623	LHG	O6-C4-C5-C6
31	b	626	LHG	O6-C4-C5-C6
23	A	401	CLA	C11-C12-C13-C15
23	B	601	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C10-C8-C7
23	B	610	CLA	C12-C13-C15-C16
23	B	612	CLA	C11-C10-C8-C7
23	B	612	CLA	C12-C13-C15-C16
23	B	615	CLA	C12-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C12-C13-C15
23	D	401	CLA	C11-C12-C13-C15
23	D	404	CLA	C11-C12-C13-C15
23	N	603	CLA	C2-C3-C5-C6
23	N	613	CLA	C6-C7-C8-C10
23	Y	303	CLA	C6-C7-C8-C10
23	a	401	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C12-C13-C15
23	b	605	CLA	C11-C10-C8-C7
23	b	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	b	615	CLA	C6-C7-C8-C10
23	b	617	CLA	C6-C7-C8-C10
23	c	501	CLA	C11-C10-C8-C7
23	c	503	CLA	C6-C7-C8-C10
23	c	503	CLA	C12-C13-C15-C16
23	d	401	CLA	C11-C12-C13-C15
23	r	609	CLA	C6-C7-C8-C10
23	n	603	CLA	C2-C3-C5-C6
23	n	613	CLA	C6-C7-C8-C10
23	y	303	CLA	C6-C7-C8-C10
23	y	304	CLA	C11-C12-C13-C15
23	R	310	CLA	C6-C7-C8-C10
33	D	406	PL9	C43-C44-C46-C47
33	d	406	PL9	C43-C44-C46-C47
35	G	601	CHL	C11-C12-C13-C15
35	G	609	CHL	C6-C7-C8-C10
35	Y	302	CHL	C11-C12-C13-C15
35	Y	308	CHL	C11-C10-C8-C7
35	g	601	CHL	C11-C12-C13-C15
35	g	609	CHL	C6-C7-C8-C10
35	n	609	CHL	C6-C7-C8-C10
23	c	501	CLA	C10-C11-C12-C13
36	Y	317	LUT	C29-C30-C31-C32
36	y	317	LUT	C29-C30-C31-C32
37	r	614	XAT	C29-C30-C31-C32
37	R	315	XAT	C29-C30-C31-C32
28	b	625	DGD	C3A-C4A-C5A-C6A
31	S	318	LHG	C27-C28-C29-C30
23	a	404	CLA	CBA-CGA-O2A-C1
23	N	613	CLA	C5-C6-C7-C8
31	l	103	LHG	C11-C10-C9-C8
23	B	612	CLA	C3-C5-C6-C7
23	C	509	CLA	C16-C17-C18-C19
23	B	614	CLA	C5-C6-C7-C8
39	W	202	VTQ	C18-C20-C21-C22
23	B	601	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
23	N	611	CLA	O1D-CGD-O2D-CED
23	b	612	CLA	C8-C10-C11-C12
35	g	601	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	c	517	LHG	C10-C11-C12-C13
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	606	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	D	404	CLA	CAD-CBD-CGD-O2D
23	G	614	CLA	CAD-CBD-CGD-O2D
23	N	610	CLA	CAD-CBD-CGD-O2D
23	N	614	CLA	CAD-CBD-CGD-O2D
23	Y	315	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O2D
23	g	610	CLA	CAD-CBD-CGD-O2D
23	g	614	CLA	CAD-CBD-CGD-O2D
23	r	609	CLA	CAD-CBD-CGD-O2D
23	r	611	CLA	CAD-CBD-CGD-O2D
23	s	613	CLA	CAD-CBD-CGD-O2D
23	n	602	CLA	CAD-CBD-CGD-O2D
23	n	610	CLA	CAD-CBD-CGD-O2D
23	n	614	CLA	CAD-CBD-CGD-O2D
23	y	305	CLA	CAD-CBD-CGD-O2D
23	y	315	CLA	CAD-CBD-CGD-O2D
23	R	309	CLA	CAD-CBD-CGD-O2D
23	R	310	CLA	CAD-CBD-CGD-O2D
35	S	302	CHL	CAD-CBD-CGD-O2D
35	r	605	CHL	CAD-CBD-CGD-O2D
35	R	306	CHL	CAD-CBD-CGD-O2D
23	Y	303	CLA	O1D-CGD-O2D-CED
30	B	620	LMG	C35-C36-C37-C38
23	b	617	CLA	C10-C11-C12-C13
26	B	625	SQD	C11-C10-C9-C8
32	c	519	DMU	C18-C19-C22-C25
31	B	621	LHG	O10-C23-O8-C6
23	b	606	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	CBA-CGA-O2A-C1
23	C	506	CLA	C4-C3-C5-C6
23	G	602	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	B	620	LMG	O6-C1-O1-C7
30	b	622	LMG	O6-C1-O1-C7
28	c	515	DGD	O1G-C1G-C2G-C3G
30	W	203	LMG	O1-C7-C8-C9
31	B	627	LHG	C4-C5-C6-O8
31	Y	319	LHG	C4-C5-C6-O8
31	s	617	LHG	C4-C5-C6-O8
23	b	618	CLA	O1A-CGA-O2A-C1
31	c	516	LHG	C8-C7-O7-C5
31	B	622	LHG	O6-C4-C5-O7
31	B	627	LHG	O6-C4-C5-O7
31	C	518	LHG	O6-C4-C5-O7
23	B	601	CLA	C10-C11-C12-C13
23	g	604	CLA	O2A-C1-C2-C3
23	d	402	CLA	O1D-CGD-O2D-CED
34	F	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4B-C3B-CAB-CBB
23	B	604	CLA	CBD-CGD-O2D-CED
23	r	604	CLA	O1A-CGA-O2A-C1
23	G	612	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
23	B	612	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	G	603	CLA	CHA-CBD-CGD-O1D
23	G	612	CLA	CHA-CBD-CGD-O1D
23	N	602	CLA	CHA-CBD-CGD-O1D
23	Y	314	CLA	CHA-CBD-CGD-O1D
23	Y	314	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	g	612	CLA	CHA-CBD-CGD-O1D
23	g	612	CLA	CHA-CBD-CGD-O2D
23	s	602	CLA	CHA-CBD-CGD-O1D
23	s	602	CLA	CHA-CBD-CGD-O2D
23	R	302	CLA	CHA-CBD-CGD-O2D
35	s	607	CHL	CHA-CBD-CGD-O1D
35	s	607	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
35	n	605	CHL	CHA-CBD-CGD-O2D
23	y	304	CLA	C3-C5-C6-C7
23	a	404	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	O1A-CGA-O2A-C1
23	R	304	CLA	O1A-CGA-O2A-C1
31	C	518	LHG	O10-C23-O8-C6
35	Y	306	CHL	O1A-CGA-O2A-C1
35	n	601	CHL	O1A-CGA-O2A-C1
23	R	305	CLA	O2A-C1-C2-C3
35	y	308	CHL	C10-C11-C12-C13
26	a	406	SQD	O6-C44-C45-O47
26	l	101	SQD	O6-C44-C45-O47
30	B	620	LMG	O7-C8-C9-O8
30	b	622	LMG	O7-C8-C9-O8
31	B	627	LHG	O7-C5-C6-O8
23	y	304	CLA	CBD-CGD-O2D-CED
23	r	603	CLA	O1A-CGA-O2A-C1
31	l	102	LHG	C13-C14-C15-C16
23	r	602	CLA	O1D-CGD-O2D-CED
31	Y	319	LHG	C17-C18-C19-C20
23	r	612	CLA	O1A-CGA-O2A-C1
23	G	602	CLA	C2-C3-C5-C6
31	c	516	LHG	O9-C7-O7-C5
23	B	610	CLA	C14-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C9
23	b	612	CLA	C14-C13-C15-C16
35	G	601	CHL	C11-C12-C13-C14
35	Y	308	CHL	C11-C10-C8-C9
35	g	601	CHL	C11-C12-C13-C14
35	y	308	CHL	C11-C10-C8-C9
35	r	607	CHL	O1D-CGD-O2D-CED
23	B	601	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
23	r	609	CLA	O1D-CGD-O2D-CED
28	D	410	DGD	C4B-C5B-C6B-C7B
31	L	101	LHG	C13-C14-C15-C16
23	Y	314	CLA	C5-C6-C7-C8
26	l	101	SQD	C4-C5-C6-S
23	c	508	CLA	C16-C17-C18-C19
35	N	606	CHL	C2A-CAA-CBA-CGA
23	b	613	CLA	O1A-CGA-O2A-C1
25	D	405	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
38	R	316	NEX	C11-C12-C13-C20
30	a	407	LMG	O6-C5-C6-O5
25	d	405	BCR	C21-C22-C23-C24
31	L	101	LHG	C30-C31-C32-C33
23	B	607	CLA	C1A-C2A-CAA-CBA
23	C	504	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C1A-C2A-CAA-CBA
23	G	602	CLA	C1A-C2A-CAA-CBA
23	N	602	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C1A-C2A-CAA-CBA
23	c	504	CLA	C1A-C2A-CAA-CBA
23	c	506	CLA	C1A-C2A-CAA-CBA
23	g	602	CLA	C1A-C2A-CAA-CBA
23	n	602	CLA	C1A-C2A-CAA-CBA
35	N	605	CHL	C1A-C2A-CAA-CBA
35	Y	308	CHL	C1A-C2A-CAA-CBA
35	n	601	CHL	C1A-C2A-CAA-CBA
35	n	605	CHL	C1A-C2A-CAA-CBA
23	B	611	CLA	CBA-CGA-O2A-C1
31	C	518	LHG	C4-O6-P-O3
31	G	619	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	c	517	LHG	C3-O3-P-O6
31	R	317	LHG	C4-O6-P-O3
23	C	505	CLA	O1D-CGD-O2D-CED
23	r	602	CLA	C4-C3-C5-C6
23	Y	312	CLA	C3-C5-C6-C7
23	d	403	CLA	C2-C3-C5-C6
23	R	303	CLA	C2-C3-C5-C6
23	C	510	CLA	C4B-C3B-CAB-CBB
23	Y	304	CLA	C4B-C3B-CAB-CBB
23	c	501	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C4B-C3B-CAB-CBB
23	s	611	CLA	C4B-C3B-CAB-CBB
31	B	621	LHG	C3-O3-P-O4
31	B	622	LHG	C3-O3-P-O5
31	D	407	LHG	C4-O6-P-O4
31	G	619	LHG	C4-O6-P-O5
31	W	201	LHG	C4-O6-P-O5
31	b	623	LHG	C3-O3-P-O4
31	b	624	LHG	C3-O3-P-O4
31	c	516	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
31	d	407	LHG	C4-O6-P-O4
31	g	619	LHG	C4-O6-P-O5
31	l	102	LHG	C4-O6-P-O4
31	r	616	LHG	C3-O3-P-O4
31	r	616	LHG	C4-O6-P-O4
31	R	317	LHG	C3-O3-P-O4
23	b	610	CLA	C16-C17-C18-C19
23	R	302	CLA	O2A-C1-C2-C3
35	G	608	CHL	C5-C6-C7-C8
23	c	503	CLA	CBA-CGA-O2A-C1
35	y	310	CHL	CBA-CGA-O2A-C1
24	A	403	PHO	CBD-CGD-O2D-CED
31	W	201	LHG	O6-C4-C5-C6
30	c	521	LMG	C12-C13-C14-C15
23	r	609	CLA	C2A-CAA-CBA-CGA
23	Y	303	CLA	C3-C5-C6-C7
23	c	501	CLA	C3-C5-C6-C7
28	d	410	DGD	C3B-C4B-C5B-C6B
31	b	624	LHG	C32-C33-C34-C35
23	B	614	CLA	C16-C17-C18-C20
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	604	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	b	603	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	611	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	616	CLA	CAD-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	g	612	CLA	CAD-CBD-CGD-O1D
23	s	602	CLA	CAD-CBD-CGD-O1D
26	B	625	SQD	C5-C6-S-O9
26	b	602	SQD	C5-C6-S-O9
35	G	606	CHL	CAD-CBD-CGD-O1D
35	Y	302	CHL	CAD-CBD-CGD-O1D
35	s	607	CHL	CAD-CBD-CGD-O1D
35	y	302	CHL	CAD-CBD-CGD-O1D
35	g	608	CHL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	s	612	CLA	C3-C5-C6-C7
23	y	303	CLA	C3-C5-C6-C7
23	b	606	CLA	C15-C16-C17-C18
23	y	312	CLA	C10-C11-C12-C13
32	c	522	DMU	C22-C25-C28-C31
31	B	622	LHG	C1-C2-C3-O3
23	Y	312	CLA	C10-C11-C12-C13
31	g	619	LHG	C24-C25-C26-C27
23	B	603	CLA	C16-C17-C18-C19
23	B	607	CLA	C12-C13-C15-C16
23	B	615	CLA	C6-C7-C8-C10
23	D	403	CLA	C11-C12-C13-C15
23	D	404	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C10-C8-C7
23	Y	303	CLA	C11-C12-C13-C15
23	b	610	CLA	C12-C13-C15-C16
23	b	612	CLA	C11-C10-C8-C7
23	g	610	CLA	C6-C7-C8-C10
24	A	403	PHO	C6-C7-C8-C10
24	a	402	PHO	C6-C7-C8-C10
31	L	101	LHG	O6-C4-C5-O7
31	W	201	LHG	O6-C4-C5-O7
31	b	623	LHG	O6-C4-C5-O7
31	c	516	LHG	O6-C4-C5-O7
31	c	517	LHG	O6-C4-C5-O7
35	y	302	CHL	C11-C12-C13-C15
35	y	308	CHL	C11-C10-C8-C7
31	b	626	LHG	C10-C11-C12-C13
26	B	625	SQD	C7-C8-C9-C10
31	d	407	LHG	C9-C10-C11-C12
23	g	610	CLA	C2A-CAA-CBA-CGA
23	N	610	CLA	C11-C12-C13-C14
30	B	623	LMG	C7-C8-C9-O8
26	B	625	SQD	O6-C44-C45-O47
26	L	103	SQD	O6-C44-C45-O47
26	b	602	SQD	O6-C44-C45-O47
28	B	626	DGD	O1G-C1G-C2G-O2G
28	b	625	DGD	O1G-C1G-C2G-O2G
31	S	318	LHG	O7-C5-C6-O8
23	B	611	CLA	O1A-CGA-O2A-C1
23	c	503	CLA	O1A-CGA-O2A-C1
23	D	401	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	b	617	CLA	C8-C10-C11-C12
31	l	102	LHG	C30-C31-C32-C33
35	y	310	CHL	O1A-CGA-O2A-C1
23	d	401	CLA	C4-C3-C5-C6
35	g	609	CHL	C4-C3-C5-C6
23	C	513	CLA	CBA-CGA-O2A-C1
31	c	516	LHG	C14-C15-C16-C17
23	D	401	CLA	C14-C13-C15-C16
23	D	404	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	G	602	CLA	C11-C10-C8-C9
23	G	603	CLA	C14-C13-C15-C16
23	Y	303	CLA	C6-C7-C8-C9
23	b	617	CLA	C11-C10-C8-C9
23	c	503	CLA	C14-C13-C15-C16
23	y	303	CLA	C6-C7-C8-C9
23	y	303	CLA	C11-C12-C13-C14
24	D	402	PHO	C11-C12-C13-C14
35	G	609	CHL	C6-C7-C8-C9
35	Y	302	CHL	C11-C12-C13-C14
35	y	302	CHL	C11-C12-C13-C14
23	C	513	CLA	O1A-CGA-O2A-C1
23	y	305	CLA	C2A-CAA-CBA-CGA
31	d	407	LHG	O1-C1-C2-O2
31	D	408	LHG	C23-C24-C25-C26
26	b	602	SQD	C29-C30-C31-C32
23	y	304	CLA	O1D-CGD-O2D-CED
23	y	314	CLA	C5-C6-C7-C8
26	l	101	SQD	C10-C11-C12-C13
23	A	404	CLA	C2B-C3B-CAB-CBB
23	B	604	CLA	C2B-C3B-CAB-CBB
23	B	611	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C2B-C3B-CAB-CBB
23	C	511	CLA	C2B-C3B-CAB-CBB
23	C	514	CLA	C2B-C3B-CAB-CBB
23	D	401	CLA	C2B-C3B-CAB-CBB
23	D	403	CLA	C2B-C3B-CAB-CBB
23	G	603	CLA	C2B-C3B-CAB-CBB
23	G	610	CLA	C2B-C3B-CAB-CBB
23	N	604	CLA	C2B-C3B-CAB-CBB
23	N	613	CLA	C2B-C3B-CAB-CBB
23	S	305	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	Y	304	CLA	C2B-C3B-CAB-CBB
23	Y	305	CLA	C2B-C3B-CAB-CBB
23	a	401	CLA	C2B-C3B-CAB-CBB
23	a	404	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
23	b	613	CLA	C2B-C3B-CAB-CBB
23	b	618	CLA	C2B-C3B-CAB-CBB
23	c	510	CLA	C2B-C3B-CAB-CBB
23	d	401	CLA	C2B-C3B-CAB-CBB
23	s	604	CLA	C2B-C3B-CAB-CBB
23	n	613	CLA	C2B-C3B-CAB-CBB
23	y	303	CLA	C2B-C3B-CAB-CBB
23	y	305	CLA	C2B-C3B-CAB-CBB
31	L	102	LHG	O2-C2-C3-O3
35	N	609	CHL	C2B-C3B-CAB-CBB
35	s	607	CHL	C2B-C3B-CAB-CBB
35	n	601	CHL	C2B-C3B-CAB-CBB
35	n	609	CHL	C2B-C3B-CAB-CBB
35	G	601	CHL	C4-C3-C5-C6
31	d	407	LHG	C28-C29-C30-C31
23	G	604	CLA	C1-C2-C3-C4
23	g	604	CLA	C1-C2-C3-C4
23	r	601	CLA	C1-C2-C3-C4
23	R	302	CLA	C1-C2-C3-C4
35	Y	307	CHL	C1-C2-C3-C4
35	y	307	CHL	C1-C2-C3-C4
23	N	603	CLA	C3-C5-C6-C7
26	B	625	SQD	C44-C45-O47-C7
26	b	602	SQD	C44-C45-O47-C7
31	L	102	LHG	C6-C5-O7-C7
31	l	103	LHG	C6-C5-O7-C7
31	B	621	LHG	O6-C4-C5-C6
31	c	516	LHG	O6-C4-C5-C6
23	N	612	CLA	C2A-CAA-CBA-CGA
23	s	609	CLA	C2A-CAA-CBA-CGA
35	Y	310	CHL	C2A-CAA-CBA-CGA
35	y	310	CHL	C2A-CAA-CBA-CGA
26	L	103	SQD	C11-C10-C9-C8
31	d	407	LHG	C30-C31-C32-C33
30	S	301	LMG	O9-C10-O7-C8
35	g	607	CHL	O1D-CGD-O2D-CED
23	a	404	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	G	613	CLA	C2-C1-O2A-CGA
23	g	613	CLA	C2-C1-O2A-CGA
35	Y	308	CHL	C2-C1-O2A-CGA
35	r	607	CHL	C2-C1-O2A-CGA
28	B	626	DGD	C4D-C5D-C6D-O5D
28	b	625	DGD	C4D-C5D-C6D-O5D
26	L	103	SQD	C32-C33-C34-C35
23	C	504	CLA	O1A-CGA-O2A-C1
25	H	101	BCR	C23-C24-C25-C30
36	G	615	LUT	C5-C6-C7-C8
36	g	615	LUT	C1-C6-C7-C8
23	C	504	CLA	CBA-CGA-O2A-C1
30	S	301	LMG	C11-C10-O7-C8
23	b	609	CLA	C5-C6-C7-C8
28	A	408	DGD	O2G-C2G-C3G-O3G
30	C	522	LMG	C12-C13-C14-C15
31	B	622	LHG	C4-O6-P-O3
31	B	627	LHG	C3-O3-P-O6
31	C	518	LHG	C3-O3-P-O6
31	D	408	LHG	C3-O3-P-O6
31	L	102	LHG	C3-O3-P-O6
31	N	618	LHG	C3-O3-P-O6
31	S	318	LHG	C3-O3-P-O6
31	W	201	LHG	C3-O3-P-O6
31	b	626	LHG	C3-O3-P-O6
31	c	516	LHG	C3-O3-P-O6
31	d	408	LHG	C3-O3-P-O6
31	g	619	LHG	C3-O3-P-O6
31	l	103	LHG	C3-O3-P-O6
31	s	617	LHG	C3-O3-P-O6
31	n	618	LHG	C3-O3-P-O6
24	a	402	PHO	O1D-CGD-O2D-CED
26	b	602	SQD	C11-C10-C9-C8
23	B	614	CLA	C16-C17-C18-C19
35	g	607	CHL	CBD-CGD-O2D-CED
31	d	408	LHG	C23-C24-C25-C26
26	a	406	SQD	O6-C44-C45-C46
28	A	408	DGD	C1G-C2G-C3G-O3G
30	B	620	LMG	C7-C8-C9-O8
30	b	622	LMG	C7-C8-C9-O8
30	w	202	LMG	O1-C7-C8-C9
31	l	102	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C6-C7-C8-C10
23	c	505	CLA	C2-C3-C5-C6
23	c	507	CLA	C11-C12-C13-C15
23	A	401	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	510	CLA	C14-C13-C15-C16
23	a	401	CLA	C11-C12-C13-C14
23	b	618	CLA	C6-C7-C8-C9
23	c	509	CLA	C14-C13-C15-C16
35	N	609	CHL	C6-C7-C8-C9
35	g	609	CHL	C6-C7-C8-C9
35	n	609	CHL	C6-C7-C8-C9
23	b	603	CLA	C10-C11-C12-C13
23	b	606	CLA	O1D-CGD-O2D-CED
25	D	405	BCR	C9-C10-C11-C12
25	H	101	BCR	C9-C10-C11-C12
25	d	405	BCR	C9-C10-C11-C12
38	Y	318	NEX	C33-C34-C35-C15
23	B	603	CLA	C16-C17-C18-C20
23	b	610	CLA	C16-C17-C18-C20
23	B	604	CLA	O1D-CGD-O2D-CED
31	L	101	LHG	C10-C11-C12-C13
31	B	627	LHG	C14-C15-C16-C17
35	g	608	CHL	C16-C17-C18-C20
23	b	611	CLA	CBA-CGA-O2A-C1
23	R	305	CLA	CBA-CGA-O2A-C1
25	K	101	BCR	C7-C8-C9-C10
23	G	604	CLA	O2A-C1-C2-C3
31	D	407	LHG	C9-C10-C11-C12
31	y	318	LHG	C17-C18-C19-C20
30	C	501	LMG	O6-C5-C6-O5
23	b	611	CLA	O1A-CGA-O2A-C1
28	B	626	DGD	O6D-C5D-C6D-O5D
23	R	305	CLA	O1A-CGA-O2A-C1
35	n	609	CHL	CBA-CGA-O2A-C1
23	A	404	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C4B-C3B-CAB-CBB
23	B	616	CLA	C4B-C3B-CAB-CBB
23	C	511	CLA	C4B-C3B-CAB-CBB
23	G	610	CLA	C4B-C3B-CAB-CBB
23	N	602	CLA	C4B-C3B-CAB-CBB
23	Y	305	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	a	404	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	b	613	CLA	C4B-C3B-CAB-CBB
23	b	618	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
23	c	510	CLA	C4B-C3B-CAB-CBB
23	s	604	CLA	C4B-C3B-CAB-CBB
23	n	613	CLA	C4B-C3B-CAB-CBB
35	N	609	CHL	C4B-C3B-CAB-CBB
23	y	312	CLA	C11-C12-C13-C15
25	h	101	BCR	C9-C10-C11-C12
36	g	615	LUT	C29-C30-C31-C32
36	s	615	LUT	C29-C30-C31-C32
23	C	502	CLA	C15-C16-C17-C18
35	S	306	CHL	CAA-CBA-CGA-O2A
23	B	606	CLA	CBD-CGD-O2D-CED
28	c	515	DGD	C4B-C5B-C6B-C7B
31	W	201	LHG	C14-C15-C16-C17
32	C	523	DMU	C22-C25-C28-C31
23	d	404	CLA	C8-C10-C11-C12
23	C	506	CLA	C2-C3-C5-C6
23	d	401	CLA	C2-C3-C5-C6
23	B	616	CLA	C8-C10-C11-C12
23	C	503	CLA	C2-C1-O2A-CGA
23	c	502	CLA	C2-C1-O2A-CGA
35	n	609	CHL	C2-C1-O2A-CGA
35	R	308	CHL	C2-C1-O2A-CGA
31	R	317	LHG	C11-C12-C13-C14
32	C	523	DMU	O5-C4-C57-O61
23	B	601	CLA	C2A-CAA-CBA-CGA
23	S	303	CLA	C2A-CAA-CBA-CGA
23	Y	305	CLA	C2A-CAA-CBA-CGA
23	s	612	CLA	C2A-CAA-CBA-CGA
23	n	612	CLA	C2A-CAA-CBA-CGA
23	R	313	CLA	C2A-CAA-CBA-CGA
28	d	410	DGD	CAB-CBB-CCB-CDB
23	B	612	CLA	C3A-C2A-CAA-CBA
23	C	514	CLA	C3A-C2A-CAA-CBA
23	b	614	CLA	C3A-C2A-CAA-CBA
23	c	505	CLA	C3A-C2A-CAA-CBA
35	G	601	CHL	C3A-C2A-CAA-CBA
35	N	606	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	S	308	CHL	C3A-C2A-CAA-CBA
35	Y	302	CHL	C3A-C2A-CAA-CBA
35	n	606	CHL	C3A-C2A-CAA-CBA
35	y	302	CHL	C3A-C2A-CAA-CBA
35	y	308	CHL	C3A-C2A-CAA-CBA
23	Y	312	CLA	C11-C12-C13-C15
26	b	602	SQD	C24-C25-C26-C27
35	n	606	CHL	CAA-CBA-CGA-O1A
35	g	609	CHL	C2-C3-C5-C6
23	n	613	CLA	C3-C5-C6-C7
31	D	408	LHG	C12-C13-C14-C15
28	D	410	DGD	O2G-C1B-C2B-C3B
31	D	407	LHG	O7-C7-C8-C9
23	B	615	CLA	C6-C7-C8-C9
23	Y	303	CLA	C11-C12-C13-C14
23	b	616	CLA	C11-C10-C8-C9
23	y	314	CLA	C11-C10-C8-C9
35	Y	302	CHL	C14-C13-C15-C16
38	G	618	NEX	C39-C29-C30-C31
38	N	617	NEX	C39-C29-C30-C31
38	S	317	NEX	C39-C29-C30-C31
38	Y	318	NEX	C39-C29-C30-C31
38	g	618	NEX	C39-C29-C30-C31
38	r	615	NEX	C39-C29-C30-C31
38	s	616	NEX	C39-C29-C30-C31
38	n	617	NEX	C39-C29-C30-C31
38	R	301	NEX	C39-C29-C30-C31
38	R	316	NEX	C39-C29-C30-C31
28	b	625	DGD	O6D-C5D-C6D-O5D
23	B	606	CLA	C3-C5-C6-C7
23	S	309	CLA	CAA-CBA-CGA-O1A
35	S	306	CHL	C2A-CAA-CBA-CGA
23	b	616	CLA	C16-C17-C18-C20
35	g	608	CHL	C16-C17-C18-C19
31	B	627	LHG	C10-C11-C12-C13
23	D	403	CLA	C15-C16-C17-C18
23	b	610	CLA	CBD-CGD-O2D-CED
23	g	612	CLA	CAA-CBA-CGA-O1A
23	B	612	CLA	C1A-C2A-CAA-CBA
23	C	510	CLA	C1A-C2A-CAA-CBA
23	b	614	CLA	C1A-C2A-CAA-CBA
23	b	618	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C1A-C2A-CAA-CBA
23	d	404	CLA	C1A-C2A-CAA-CBA
23	g	611	CLA	C1A-C2A-CAA-CBA
35	G	601	CHL	C1A-C2A-CAA-CBA
35	N	608	CHL	C1A-C2A-CAA-CBA
35	S	306	CHL	C1A-C2A-CAA-CBA
35	Y	302	CHL	C1A-C2A-CAA-CBA
35	y	302	CHL	C1A-C2A-CAA-CBA
35	y	308	CHL	C1A-C2A-CAA-CBA
32	C	520	DMU	O16-C18-C19-C22
23	Y	314	CLA	C6-C7-C8-C10
23	c	501	CLA	C15-C16-C17-C18
35	n	609	CHL	O1A-CGA-O2A-C1
36	n	616	LUT	C29-C30-C31-C32
23	B	606	CLA	O1D-CGD-O2D-CED
28	B	626	DGD	O1G-C1A-C2A-C3A
35	N	606	CHL	CAA-CBA-CGA-O1A
35	G	601	CHL	C3-C5-C6-C7
23	S	313	CLA	C2A-CAA-CBA-CGA
23	R	310	CLA	C2A-CAA-CBA-CGA
31	D	407	LHG	O1-C1-C2-O2
23	N	613	CLA	C8-C10-C11-C12
35	N	607	CHL	CAA-CBA-CGA-O2A
30	B	620	LMG	O9-C10-O7-C8
23	r	601	CLA	O2A-C1-C2-C3
35	N	609	CHL	CBA-CGA-O2A-C1
26	a	406	SQD	C15-C16-C17-C18
35	G	605	CHL	CAA-CBA-CGA-O1A
35	N	607	CHL	CAA-CBA-CGA-O1A
23	C	511	CLA	C4-C3-C5-C6
35	G	609	CHL	C4-C3-C5-C6
35	g	601	CHL	C4-C3-C5-C6
23	C	510	CLA	C2B-C3B-CAB-CBB
23	N	602	CLA	C2B-C3B-CAB-CBB
23	Y	303	CLA	C2B-C3B-CAB-CBB
23	c	501	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
23	c	509	CLA	C2B-C3B-CAB-CBB
23	s	611	CLA	C2B-C3B-CAB-CBB
23	g	612	CLA	CAA-CBA-CGA-O2A
35	G	605	CHL	CAA-CBA-CGA-O2A
31	b	624	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	B	612	CLA	C8-C10-C11-C12
26	b	602	SQD	C7-C8-C9-C10
30	w	202	LMG	C10-C11-C12-C13
31	R	317	LHG	O9-C7-O7-C5
38	G	618	NEX	C28-C29-C30-C31
38	N	617	NEX	C28-C29-C30-C31
38	S	317	NEX	C28-C29-C30-C31
38	Y	318	NEX	C28-C29-C30-C31
38	g	618	NEX	C28-C29-C30-C31
38	r	615	NEX	C28-C29-C30-C31
38	s	616	NEX	C28-C29-C30-C31
38	n	617	NEX	C28-C29-C30-C31
38	R	301	NEX	C28-C29-C30-C31
38	R	316	NEX	C28-C29-C30-C31
31	s	617	LHG	O7-C5-C6-O8
31	d	407	LHG	O7-C7-C8-C9
23	G	612	CLA	CAA-CBA-CGA-O1A
35	S	306	CHL	CAA-CBA-CGA-O1A
35	g	605	CHL	CAA-CBA-CGA-O1A
24	A	403	PHO	C8-C10-C11-C12
23	b	610	CLA	O1D-CGD-O2D-CED
23	B	607	CLA	C5-C6-C7-C8
23	b	614	CLA	C13-C15-C16-C17
23	B	612	CLA	C13-C15-C16-C17
23	c	502	CLA	C5-C6-C7-C8
24	A	403	PHO	O1D-CGD-O2D-CED
23	c	503	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
23	B	613	CLA	C2-C1-O2A-CGA
23	G	603	CLA	C2-C1-O2A-CGA
23	N	611	CLA	C2-C1-O2A-CGA
23	Y	314	CLA	C2-C1-O2A-CGA
23	b	609	CLA	C2-C1-O2A-CGA
23	b	615	CLA	C2-C1-O2A-CGA
23	r	602	CLA	C2-C1-O2A-CGA
23	s	604	CLA	C2-C1-O2A-CGA
23	n	611	CLA	C2-C1-O2A-CGA
23	y	314	CLA	C2-C1-O2A-CGA
23	S	309	CLA	CAA-CBA-CGA-O2A
35	n	606	CHL	CAA-CBA-CGA-O2A
35	n	607	CHL	CAA-CBA-CGA-O2A
23	y	314	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	r	601	CLA	CAA-CBA-CGA-O2A
23	R	302	CLA	CAA-CBA-CGA-O2A
28	b	625	DGD	O1G-C1A-C2A-C3A
24	a	402	PHO	C8-C10-C11-C12
35	N	606	CHL	CAA-CBA-CGA-O2A
35	n	607	CHL	CAA-CBA-CGA-O1A
26	B	625	SQD	O47-C7-C8-C9
23	r	612	CLA	C2A-CAA-CBA-CGA
23	G	612	CLA	CAA-CBA-CGA-O2A
34	F	101	HEM	CAD-CBD-CGD-O2D
31	d	407	LHG	C23-C24-C25-C26
30	a	407	LMG	C33-C34-C35-C36
25	B	619	BCR	C1-C6-C7-C8
25	B	619	BCR	C5-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C30
36	G	616	LUT	C1-C6-C7-C8
36	N	616	LUT	C1-C6-C7-C8
23	b	614	CLA	C8-C10-C11-C12
26	L	103	SQD	C25-C26-C27-C28
34	f	101	HEM	CAA-CBA-CGA-O2A
23	C	503	CLA	C5-C6-C7-C8
23	b	609	CLA	C10-C11-C12-C13
30	D	409	LMG	C21-C22-C23-C24
36	Y	316	LUT	C29-C30-C31-C32
38	R	301	NEX	C29-C30-C31-C32
23	C	504	CLA	C4-C3-C5-C6
35	N	609	CHL	C4-C3-C5-C6
25	D	405	BCR	C21-C22-C23-C24
38	R	316	NEX	C11-C12-C13-C14
35	Y	308	CHL	C5-C6-C7-C8
28	A	408	DGD	O2G-C1B-C2B-C3B
23	G	613	CLA	C3-C5-C6-C7
23	g	613	CLA	C3-C5-C6-C7
23	S	304	CLA	CAA-CBA-CGA-O2A
35	R	307	CHL	CAA-CBA-CGA-O2A
35	s	605	CHL	O1D-CGD-O2D-CED
35	N	609	CHL	O1A-CGA-O2A-C1
35	G	608	CHL	C13-C15-C16-C17
35	n	601	CHL	C13-C15-C16-C17
31	d	408	LHG	C12-C13-C14-C15
26	b	602	SQD	O47-C7-C8-C9
23	B	608	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	a	401	CLA	C10-C11-C12-C13
35	Y	308	CHL	C15-C16-C17-C18
31	l	102	LHG	O6-C4-C5-O7
23	S	310	CLA	CAA-CBA-CGA-O2A
34	F	101	HEM	CAA-CBA-CGA-O2A
34	f	101	HEM	CAD-CBD-CGD-O2D
35	g	605	CHL	CAA-CBA-CGA-O2A
35	r	606	CHL	CAA-CBA-CGA-O2A
23	r	601	CLA	O1A-CGA-O2A-C1
31	B	622	LHG	C28-C29-C30-C31
35	S	302	CHL	CAA-CBA-CGA-O2A
23	Y	303	CLA	C4B-C3B-CAB-CBB
23	G	610	CLA	C16-C17-C18-C19
23	b	606	CLA	C13-C15-C16-C17
31	Y	319	LHG	O6-C4-C5-C6
31	y	318	LHG	O6-C4-C5-C6
23	B	608	CLA	C4-C3-C5-C6
23	s	608	CLA	O1D-CGD-O2D-CED
33	d	406	PL9	C44-C46-C47-C48
23	B	614	CLA	C11-C10-C8-C7
23	D	401	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C7
30	S	301	LMG	C29-C28-O8-C9
30	s	619	LMG	C29-C28-O8-C9
23	B	604	CLA	C13-C15-C16-C17
35	y	308	CHL	C15-C16-C17-C18
38	n	617	NEX	C33-C34-C35-C15
35	s	601	CHL	CAA-CBA-CGA-O2A
23	B	607	CLA	C10-C11-C12-C13
26	A	406	SQD	O6-C44-C45-O47
28	B	624	DGD	O2G-C2G-C3G-O3G
23	c	501	CLA	C5-C6-C7-C8
23	N	604	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	C5-C6-C7-C8
23	d	401	CLA	C13-C15-C16-C17
31	n	618	LHG	C13-C14-C15-C16
35	r	605	CHL	CAA-CBA-CGA-O2A
23	r	601	CLA	CBA-CGA-O2A-C1
23	R	303	CLA	CAA-CBA-CGA-O2A
33	D	406	PL9	C35-C34-C36-C37
35	n	609	CHL	C4-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C2-C3-C5-C6
23	r	602	CLA	C2-C3-C5-C6
35	G	601	CHL	C2-C3-C5-C6
35	N	609	CHL	C2-C3-C5-C6
23	y	312	CLA	C11-C12-C13-C14
23	D	401	CLA	C5-C6-C7-C8
23	N	604	CLA	CBA-CGA-O2A-C1
31	L	102	LHG	O7-C7-C8-C9
31	C	518	LHG	C11-C12-C13-C14
23	C	508	CLA	C11-C12-C13-C14
23	D	403	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	g	610	CLA	C6-C7-C8-C9
24	A	403	PHO	C6-C7-C8-C9
24	a	402	PHO	C6-C7-C8-C9
24	a	403	PHO	C6-C7-C8-C9
24	a	403	PHO	C11-C12-C13-C14
23	n	612	CLA	CAA-CBA-CGA-O2A
23	C	506	CLA	C3A-C2A-CAA-CBA
23	b	618	CLA	C3A-C2A-CAA-CBA
35	G	608	CHL	C3A-C2A-CAA-CBA
35	N	601	CHL	C3A-C2A-CAA-CBA
35	g	601	CHL	C3A-C2A-CAA-CBA
31	l	103	LHG	O2-C2-C3-O3
23	b	614	CLA	CAA-CBA-CGA-O2A
23	g	602	CLA	CAA-CBA-CGA-O2A
35	S	302	CHL	CAA-CBA-CGA-O1A
23	A	404	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O2D
23	C	514	CLA	CAD-CBD-CGD-O2D
23	G	604	CLA	CAD-CBD-CGD-O2D
23	G	610	CLA	CAD-CBD-CGD-O2D
23	N	602	CLA	CAD-CBD-CGD-O2D
23	S	303	CLA	CAD-CBD-CGD-O2D
23	S	309	CLA	CAD-CBD-CGD-O2D
23	S	310	CLA	CAD-CBD-CGD-O2D
23	S	312	CLA	CAD-CBD-CGD-O2D
23	Y	303	CLA	CAD-CBD-CGD-O2D
23	Y	305	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	Y	311	CLA	CAD-CBD-CGD-O2D
23	Y	313	CLA	CAD-CBD-CGD-O2D
23	a	404	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
23	g	602	CLA	CAD-CBD-CGD-O2D
23	g	604	CLA	CAD-CBD-CGD-O2D
23	r	608	CLA	CAD-CBD-CGD-O2D
23	s	608	CLA	CAD-CBD-CGD-O2D
23	y	303	CLA	CAD-CBD-CGD-O2D
23	y	311	CLA	CAD-CBD-CGD-O2D
23	y	313	CLA	CAD-CBD-CGD-O2D
24	a	402	PHO	CAD-CBD-CGD-O2D
35	G	609	CHL	CAD-CBD-CGD-O2D
35	Y	306	CHL	CAD-CBD-CGD-O2D
35	Y	307	CHL	CAD-CBD-CGD-O2D
35	g	607	CHL	CAD-CBD-CGD-O2D
35	y	306	CHL	CAD-CBD-CGD-O2D
35	y	307	CHL	CAD-CBD-CGD-O2D
23	b	616	CLA	C16-C17-C18-C19
35	y	310	CHL	C10-C11-C12-C13
30	b	622	LMG	O9-C10-O7-C8
31	d	408	LHG	C13-C14-C15-C16
23	s	609	CLA	CAA-CBA-CGA-O2A
35	R	306	CHL	CAA-CBA-CGA-O2A
23	B	615	CLA	CAA-CBA-CGA-O2A
23	r	602	CLA	CAA-CBA-CGA-O2A
26	A	406	SQD	O47-C7-C8-C9
23	C	502	CLA	C3-C5-C6-C7
23	S	304	CLA	CAA-CBA-CGA-O1A
23	S	310	CLA	CAA-CBA-CGA-O1A
35	r	605	CHL	CAA-CBA-CGA-O1A
35	G	609	CHL	C2-C3-C5-C6
28	B	624	DGD	O1G-C1A-C2A-C3A
31	N	618	LHG	C24-C25-C26-C27
37	G	617	XAT	C31-C32-C33-C34
37	g	617	XAT	C31-C32-C33-C34
31	b	626	LHG	C14-C15-C16-C17
23	C	509	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	l	101	SQD	C44-C45-C46-O48
28	B	624	DGD	C1G-C2G-C3G-O3G
28	B	626	DGD	O1G-C1G-C2G-C3G
28	b	625	DGD	O1G-C1G-C2G-C3G
38	G	618	NEX	O24-C26-C27-C28
38	N	617	NEX	O24-C26-C27-C28
38	r	615	NEX	O24-C26-C27-C28
38	R	316	NEX	O24-C26-C27-C28
35	s	601	CHL	CAA-CBA-CGA-O1A
35	R	307	CHL	CAA-CBA-CGA-O1A
23	s	612	CLA	CBA-CGA-O2A-C1
35	s	605	CHL	CBD-CGD-O2D-CED
35	S	307	CHL	O1D-CGD-O2D-CED
31	Y	319	LHG	O6-C4-C5-O7
31	y	318	LHG	O6-C4-C5-O7
23	G	602	CLA	C5-C6-C7-C8
23	G	602	CLA	CAA-CBA-CGA-O2A
23	b	617	CLA	CAA-CBA-CGA-O2A
23	d	402	CLA	CAA-CBA-CGA-O2A
31	s	617	LHG	O8-C23-C24-C25
34	F	101	HEM	CAD-CBD-CGD-O1D
34	f	101	HEM	CAA-CBA-CGA-O1A
35	R	306	CHL	CAA-CBA-CGA-O1A
31	d	408	LHG	C32-C33-C34-C35
23	b	615	CLA	C5-C6-C7-C8
23	B	602	CLA	O2A-C1-C2-C3
23	C	506	CLA	O2A-C1-C2-C3
23	G	602	CLA	O2A-C1-C2-C3
23	c	505	CLA	O2A-C1-C2-C3
23	S	313	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	C5-C6-C7-C8
31	D	407	LHG	C23-C24-C25-C26
23	g	603	CLA	CAA-CBA-CGA-O2A
35	r	606	CHL	CAA-CBA-CGA-O1A
23	g	610	CLA	C16-C17-C18-C19
23	b	616	CLA	C13-C15-C16-C17
23	Y	312	CLA	C11-C12-C13-C14
31	l	102	LHG	C27-C28-C29-C30
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	G	603	CLA	CHA-CBD-CGD-O2D
23	G	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	N	602	CLA	CHA-CBD-CGD-O2D
23	N	603	CLA	CHA-CBD-CGD-O1D
23	S	304	CLA	CHA-CBD-CGD-O2D
23	S	310	CLA	CHA-CBD-CGD-O2D
23	Y	304	CLA	CHA-CBD-CGD-O1D
23	Y	304	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	r	604	CLA	CHA-CBD-CGD-O1D
23	r	604	CLA	CHA-CBD-CGD-O2D
23	r	610	CLA	CHA-CBD-CGD-O1D
23	r	610	CLA	CHA-CBD-CGD-O2D
23	s	603	CLA	CHA-CBD-CGD-O1D
23	s	603	CLA	CHA-CBD-CGD-O2D
23	n	603	CLA	CHA-CBD-CGD-O2D
23	n	612	CLA	CHA-CBD-CGD-O2D
23	y	304	CLA	CHA-CBD-CGD-O1D
23	y	314	CLA	CHA-CBD-CGD-O1D
23	y	314	CLA	CHA-CBD-CGD-O2D
23	R	305	CLA	CHA-CBD-CGD-O1D
23	R	305	CLA	CHA-CBD-CGD-O2D
23	R	311	CLA	CHA-CBD-CGD-O1D
23	R	311	CLA	CHA-CBD-CGD-O2D
35	N	605	CHL	CHA-CBD-CGD-O1D
35	N	605	CHL	CHA-CBD-CGD-O2D
35	N	607	CHL	CHA-CBD-CGD-O1D
35	N	607	CHL	CHA-CBD-CGD-O2D
35	Y	308	CHL	CHA-CBD-CGD-O1D
35	Y	308	CHL	CHA-CBD-CGD-O2D
35	g	609	CHL	CHA-CBD-CGD-O1D
35	g	609	CHL	CHA-CBD-CGD-O2D
35	n	607	CHL	CHA-CBD-CGD-O1D
35	n	607	CHL	CHA-CBD-CGD-O2D
23	s	609	CLA	CAA-CBA-CGA-O1A
35	s	605	CHL	CAA-CBA-CGA-O1A
23	y	303	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	C4B-C5B-C6B-C7B
31	R	317	LHG	C10-C11-C12-C13
23	b	613	CLA	C3-C5-C6-C7
34	F	101	HEM	CAA-CBA-CGA-O1A
23	C	502	CLA	CAA-CBA-CGA-O2A
23	c	501	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	L	103	SQD	O47-C7-C8-C9
26	a	406	SQD	O47-C7-C8-C9
23	B	602	CLA	C10-C11-C12-C13
35	Y	309	CHL	C13-C15-C16-C17
23	N	603	CLA	CAA-CBA-CGA-O2A
31	S	318	LHG	O8-C23-C24-C25
31	l	103	LHG	O7-C7-C8-C9
35	N	601	CHL	CAA-CBA-CGA-O2A
23	y	311	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C5-C6-C7-C8
23	n	610	CLA	C5-C6-C7-C8
23	B	609	CLA	CBA-CGA-O2A-C1
23	B	609	CLA	O1A-CGA-O2A-C1
23	g	613	CLA	CAA-CBA-CGA-O2A
26	C	521	SQD	O47-C7-C8-C9
34	f	101	HEM	CAD-CBD-CGD-O1D
23	B	605	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	609	CLA	C12-C13-C15-C16
35	Y	310	CHL	C6-C7-C8-C10
35	n	609	CHL	C2-C3-C5-C6
35	y	310	CHL	C6-C7-C8-C10
31	G	619	LHG	C34-C35-C36-C37
23	Y	303	CLA	CAA-CBA-CGA-O2A
23	d	404	CLA	CAA-CBA-CGA-O2A
23	B	607	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
23	d	401	CLA	C14-C13-C15-C16
24	A	403	PHO	C11-C10-C8-C9
24	a	402	PHO	C11-C10-C8-C9
35	Y	309	CHL	O1A-CGA-O2A-C1
35	Y	309	CHL	CBA-CGA-O2A-C1
35	g	608	CHL	CAA-CBA-CGA-O2A
26	A	406	SQD	C5-C6-S-O8
26	L	103	SQD	C4-C5-C6-S
26	a	406	SQD	C5-C6-S-O8
23	s	612	CLA	O1A-CGA-O2A-C1
30	S	301	LMG	O10-C28-O8-C9
31	R	317	LHG	C8-C7-O7-C5
23	B	603	CLA	C2A-CAA-CBA-CGA
23	G	610	CLA	C2A-CAA-CBA-CGA
23	b	605	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	G	602	CLA	CAA-CBA-CGA-O1A
23	B	612	CLA	CAA-CBA-CGA-O2A
35	n	605	CHL	CAA-CBA-CGA-O2A
23	n	612	CLA	CAA-CBA-CGA-O1A
37	g	617	XAT	C31-C32-C33-C40
23	c	513	CLA	C16-C17-C18-C19
33	d	406	PL9	C20-C19-C21-C22
23	S	313	CLA	O1A-CGA-O2A-C1
28	d	410	DGD	O1A-C1A-O1G-C1G
23	b	617	CLA	CAA-CBA-CGA-O1A
23	d	402	CLA	CAA-CBA-CGA-O1A
28	d	410	DGD	C2A-C1A-O1G-C1G
35	N	606	CHL	O1D-CGD-O2D-CED
23	R	310	CLA	C8-C10-C11-C12
35	g	609	CHL	C10-C11-C12-C13
23	B	609	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	Y	305	CLA	C1A-C2A-CAA-CBA
23	y	305	CLA	C1A-C2A-CAA-CBA
23	R	305	CLA	C1A-C2A-CAA-CBA
35	N	601	CHL	C1A-C2A-CAA-CBA
35	g	601	CHL	C1A-C2A-CAA-CBA
23	g	602	CLA	CAA-CBA-CGA-O1A
23	R	303	CLA	CAA-CBA-CGA-O1A
35	s	605	CHL	CAA-CBA-CGA-O2A
30	B	620	LMG	C11-C10-O7-C8
30	s	619	LMG	O10-C28-O8-C9
23	Y	304	CLA	C2-C1-O2A-CGA
23	y	304	CLA	C2-C1-O2A-CGA
23	r	602	CLA	CAA-CBA-CGA-O1A
23	N	612	CLA	CAA-CBA-CGA-O2A
26	B	625	SQD	O6-C44-C45-C46
26	b	602	SQD	O6-C44-C45-C46
23	n	602	CLA	CAA-CBA-CGA-O2A
35	G	608	CHL	CAA-CBA-CGA-O2A
32	c	522	DMU	C25-C28-C31-C34
23	Y	311	CLA	C2A-CAA-CBA-CGA
23	b	615	CLA	C2A-CAA-CBA-CGA
23	B	612	CLA	CAA-CBA-CGA-O1A
23	Y	303	CLA	CAA-CBA-CGA-O1A
23	b	614	CLA	CAA-CBA-CGA-O1A
23	c	505	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	G	613	CLA	CAA-CBA-CGA-O2A
23	C	504	CLA	C5-C6-C7-C8
23	b	603	CLA	C5-C6-C7-C8
23	c	508	CLA	C13-C15-C16-C17
24	a	402	PHO	C13-C15-C16-C17
31	c	517	LHG	C11-C12-C13-C14
23	C	502	CLA	C4B-C3B-CAB-CBB
31	L	102	LHG	C3-O3-P-O5
31	b	626	LHG	C3-O3-P-O5
23	B	615	CLA	CAA-CBA-CGA-O1A
23	d	404	CLA	CAA-CBA-CGA-O1A
23	y	303	CLA	CAA-CBA-CGA-O1A
31	L	102	LHG	O9-C7-C8-C9
31	S	318	LHG	O10-C23-C24-C25
25	h	101	BCR	C23-C24-C25-C26
23	c	501	CLA	CAA-CBA-CGA-O1A
26	A	406	SQD	O49-C7-C8-C9
26	a	406	SQD	O49-C7-C8-C9
31	s	617	LHG	O10-C23-C24-C25
26	B	625	SQD	C16-C17-C18-C19
23	Y	304	CLA	CAA-CBA-CGA-O2A
23	r	603	CLA	CAA-CBA-CGA-O2A
31	B	622	LHG	C26-C27-C28-C29
23	B	613	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	CAA-CBA-CGA-O1A
23	C	506	CLA	CAA-CBA-CGA-O1A
23	g	603	CLA	CAA-CBA-CGA-O1A
23	G	613	CLA	C5-C6-C7-C8
35	Y	310	CHL	C10-C11-C12-C13
31	R	317	LHG	C11-C10-C9-C8
23	b	610	CLA	C8-C10-C11-C12
23	y	314	CLA	CBD-CGD-O2D-CED
32	C	523	DMU	C25-C28-C31-C34
30	W	203	LMG	O6-C5-C6-O5
35	N	601	CHL	CAA-CBA-CGA-O1A
33	D	406	PL9	C30-C29-C31-C32
33	d	406	PL9	C35-C34-C36-C37
23	R	305	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	G	612	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	n	602	CLA	CAD-CBD-CGD-O1D
23	R	311	CLA	CAD-CBD-CGD-O1D
26	A	406	SQD	C5-C6-S-O7
26	a	406	SQD	C5-C6-S-O7
26	l	101	SQD	C46-C45-O47-C7
35	g	609	CHL	CAD-CBD-CGD-O1D
35	N	606	CHL	CBD-CGD-O2D-CED
23	b	606	CLA	O1A-CGA-O2A-C1
23	N	603	CLA	CAA-CBA-CGA-O1A
23	g	613	CLA	CAA-CBA-CGA-O1A
23	N	602	CLA	CAA-CBA-CGA-O2A
23	B	602	CLA	C15-C16-C17-C18
23	b	609	CLA	C14-C13-C15-C16
35	N	609	CHL	C11-C12-C13-C14
28	B	626	DGD	C2B-C3B-C4B-C5B
28	d	410	DGD	C5A-C6A-C7A-C8A
23	B	604	CLA	O1A-CGA-O2A-C1
23	y	304	CLA	CAA-CBA-CGA-O2A
35	y	306	CHL	CAA-CBA-CGA-O2A
35	y	310	CHL	CAA-CBA-CGA-O2A
28	A	408	DGD	C2A-C3A-C4A-C5A
31	r	616	LHG	C11-C10-C9-C8
23	C	504	CLA	C8-C10-C11-C12
23	S	313	CLA	C5-C6-C7-C8
35	G	609	CHL	O1D-CGD-O2D-CED
23	b	603	CLA	O1A-CGA-O2A-C1
23	n	604	CLA	O1A-CGA-O2A-C1
23	C	514	CLA	C2A-CAA-CBA-CGA
26	b	602	SQD	C16-C17-C18-C19
23	A	404	CLA	CAA-CBA-CGA-O2A
23	C	511	CLA	CAA-CBA-CGA-O2A
35	N	608	CHL	CAA-CBA-CGA-O2A
23	s	612	CLA	C5-C6-C7-C8
24	A	403	PHO	C13-C15-C16-C17
31	r	616	LHG	C11-C12-C13-C14
30	d	409	LMG	C10-C11-C12-C13
33	D	406	PL9	C20-C19-C21-C22
23	A	401	CLA	C10-C11-C12-C13
23	B	610	CLA	C11-C10-C8-C7
23	c	503	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	y	314	CLA	C6-C7-C8-C10
23	y	314	CLA	C11-C10-C8-C7
24	A	403	PHO	C11-C10-C8-C7
24	a	402	PHO	C11-C10-C8-C7
35	g	601	CHL	C2-C3-C5-C6
35	s	607	CHL	C3A-C2A-CAA-CBA
23	N	602	CLA	CAA-CBA-CGA-O1A
23	n	602	CLA	CAA-CBA-CGA-O1A
23	N	612	CLA	CAA-CBA-CGA-O1A
31	n	618	LHG	C29-C30-C31-C32
23	R	304	CLA	CAA-CBA-CGA-O2A
35	Y	306	CHL	CAA-CBA-CGA-O2A
35	Y	309	CHL	CAA-CBA-CGA-O2A
35	Y	310	CHL	CAA-CBA-CGA-O2A
35	n	608	CHL	CAA-CBA-CGA-O2A
35	y	309	CHL	CAA-CBA-CGA-O2A
23	r	612	CLA	C15-C16-C17-C18
36	n	615	LUT	C11-C12-C13-C14
23	A	404	CLA	CAA-CBA-CGA-O1A
23	y	304	CLA	CAA-CBA-CGA-O1A
31	l	103	LHG	O9-C7-C8-C9
35	g	608	CHL	CAA-CBA-CGA-O1A
35	y	309	CHL	CAA-CBA-CGA-O1A
35	y	310	CHL	CAA-CBA-CGA-O1A
38	N	617	NEX	C33-C34-C35-C15
23	a	404	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	O1G-C1A-C2A-C3A
35	N	605	CHL	CAA-CBA-CGA-O2A
35	n	601	CHL	CAA-CBA-CGA-O2A
26	L	103	SQD	O49-C7-C8-C9
33	D	406	PL9	C44-C46-C47-C48
23	B	614	CLA	CAA-CBA-CGA-O2A
23	G	613	CLA	CAA-CBA-CGA-O1A
35	G	608	CHL	CAA-CBA-CGA-O1A
23	c	513	CLA	C16-C17-C18-C20
31	L	101	LHG	C27-C28-C29-C30
35	y	309	CHL	C13-C15-C16-C17
23	R	304	CLA	CAA-CBA-CGA-O1A
35	n	601	CHL	CAA-CBA-CGA-O1A
28	c	515	DGD	O1G-C1A-C2A-C3A

There are no ring outliers.

260 monomers are involved in 465 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	516	BCR	1	0
32	c	522	DMU	1	0
23	B	612	CLA	4	0
31	l	103	LHG	1	0
35	n	607	CHL	2	0
31	R	317	LHG	1	0
23	C	503	CLA	3	0
23	c	509	CLA	3	0
35	y	308	CHL	5	0
23	g	603	CLA	2	0
35	y	302	CHL	3	0
31	D	408	LHG	3	0
25	B	619	BCR	4	0
31	L	102	LHG	1	0
35	y	307	CHL	1	0
23	b	611	CLA	1	0
23	S	314	CLA	1	0
31	n	618	LHG	1	0
23	y	313	CLA	2	0
23	A	402	CLA	1	0
23	g	613	CLA	1	0
35	N	608	CHL	3	0
35	R	308	CHL	1	0
28	B	624	DGD	4	0
35	G	601	CHL	5	0
31	B	622	LHG	1	0
35	g	608	CHL	1	0
28	d	410	DGD	5	0
26	b	602	SQD	3	0
37	G	617	XAT	2	0
23	R	303	CLA	2	0
38	n	617	NEX	1	0
31	s	617	LHG	2	0
23	b	609	CLA	3	0
35	y	310	CHL	4	0
23	G	602	CLA	4	0
24	D	402	PHO	5	0
23	B	601	CLA	1	0
37	g	620	XAT	5	0
35	S	308	CHL	2	0
28	A	408	DGD	1	0
36	g	615	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	g	619	LHG	4	0
25	C	519	BCR	3	0
23	b	618	CLA	2	0
36	S	315	LUT	2	0
26	L	103	SQD	1	0
23	c	513	CLA	3	0
35	y	306	CHL	1	0
23	Y	304	CLA	4	0
23	r	602	CLA	1	0
23	C	512	CLA	2	0
27	A	407	BCT	2	0
36	y	316	LUT	4	0
31	d	407	LHG	2	0
31	d	408	LHG	5	0
26	l	101	SQD	4	0
36	G	615	LUT	4	0
23	n	612	CLA	2	0
25	H	101	BCR	3	0
38	S	317	NEX	1	0
23	G	610	CLA	2	0
25	A	405	BCR	1	0
23	b	606	CLA	1	0
37	R	315	XAT	1	0
32	c	519	DMU	1	0
23	b	612	CLA	1	0
35	n	606	CHL	1	0
23	C	502	CLA	1	0
38	s	616	NEX	1	0
23	r	601	CLA	1	0
23	n	603	CLA	1	0
38	G	618	NEX	1	0
24	a	403	PHO	4	0
25	z	101	BCR	2	0
25	K	101	BCR	1	0
30	b	601	LMG	2	0
23	s	609	CLA	2	0
23	R	310	CLA	3	0
31	C	518	LHG	2	0
23	y	305	CLA	2	0
23	C	509	CLA	3	0
23	N	604	CLA	1	0
23	c	507	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	F	101	HEM	1	0
30	b	622	LMG	4	0
33	D	406	PL9	2	0
23	S	310	CLA	2	0
23	B	610	CLA	1	0
23	C	510	CLA	1	0
37	G	620	XAT	2	0
35	N	607	CHL	1	0
23	s	603	CLA	1	0
23	C	507	CLA	1	0
37	Y	301	XAT	5	0
35	N	605	CHL	1	0
23	r	612	CLA	1	0
23	b	616	CLA	3	0
25	a	405	BCR	4	0
26	a	406	SQD	2	0
35	N	609	CHL	1	0
37	g	617	XAT	1	0
23	A	401	CLA	2	0
23	d	401	CLA	3	0
35	y	309	CHL	1	0
31	N	618	LHG	2	0
23	y	311	CLA	3	0
23	R	309	CLA	1	0
38	N	617	NEX	3	0
31	G	619	LHG	2	0
23	s	602	CLA	2	0
36	n	616	LUT	3	0
23	S	304	CLA	1	0
36	n	615	LUT	4	0
31	B	621	LHG	1	0
23	Y	313	CLA	2	0
23	y	312	CLA	1	0
36	s	614	LUT	2	0
23	B	602	CLA	2	0
35	r	607	CHL	2	0
23	g	610	CLA	1	0
23	d	402	CLA	1	0
32	s	618	DMU	1	0
23	S	311	CLA	1	0
25	b	620	BCR	2	0
35	Y	309	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	R	311	CLA	2	0
25	b	619	BCR	5	0
23	G	603	CLA	1	0
35	N	601	CHL	3	0
35	Y	308	CHL	4	0
30	B	623	LMG	1	0
23	a	404	CLA	2	0
23	r	603	CLA	1	0
23	C	511	CLA	3	0
32	C	520	DMU	1	0
23	B	611	CLA	2	0
23	B	616	CLA	1	0
36	Y	317	LUT	2	0
35	n	601	CHL	4	0
26	c	520	SQD	1	0
23	b	615	CLA	4	0
32	S	319	DMU	1	0
31	B	627	LHG	1	0
23	b	604	CLA	1	0
23	r	610	CLA	1	0
23	r	609	CLA	1	0
35	G	608	CHL	2	0
31	W	201	LHG	1	0
23	c	511	CLA	1	0
23	n	604	CLA	1	0
23	C	508	CLA	3	0
23	C	504	CLA	2	0
30	B	620	LMG	5	0
38	Y	318	NEX	1	0
23	b	605	CLA	1	0
23	B	606	CLA	2	0
36	R	314	LUT	4	0
23	B	613	CLA	5	0
23	G	614	CLA	1	0
23	S	303	CLA	2	0
36	Y	316	LUT	5	0
23	R	305	CLA	1	0
23	s	611	CLA	1	0
36	G	616	LUT	2	0
25	c	518	BCR	4	0
38	R	301	NEX	3	0
23	c	503	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	R	307	CHL	1	0
35	n	609	CHL	2	0
31	b	624	LHG	2	0
28	c	515	DGD	2	0
25	b	621	BCR	4	0
23	b	617	CLA	1	0
31	y	318	LHG	3	0
31	L	101	LHG	3	0
23	D	403	CLA	6	0
35	g	609	CHL	1	0
23	c	508	CLA	2	0
28	C	517	DGD	2	0
23	a	401	CLA	3	0
35	s	607	CHL	3	0
31	Y	319	LHG	3	0
23	S	305	CLA	1	0
23	Y	303	CLA	2	0
23	B	603	CLA	1	0
23	b	608	CLA	4	0
34	f	101	HEM	1	0
23	y	304	CLA	4	0
36	s	615	LUT	2	0
23	Y	305	CLA	2	0
35	S	307	CHL	2	0
31	S	318	LHG	3	0
25	D	405	BCR	1	0
23	B	604	CLA	2	0
23	c	506	CLA	1	0
27	a	408	BCT	2	0
36	y	317	LUT	3	0
25	c	514	BCR	2	0
23	n	611	CLA	1	0
36	N	616	LUT	4	0
25	k	101	BCR	3	0
23	N	611	CLA	1	0
23	B	608	CLA	1	0
23	R	302	CLA	1	0
31	c	516	LHG	2	0
35	Y	310	CHL	5	0
32	C	523	DMU	1	0
25	h	101	BCR	2	0
38	g	618	NEX	1	0

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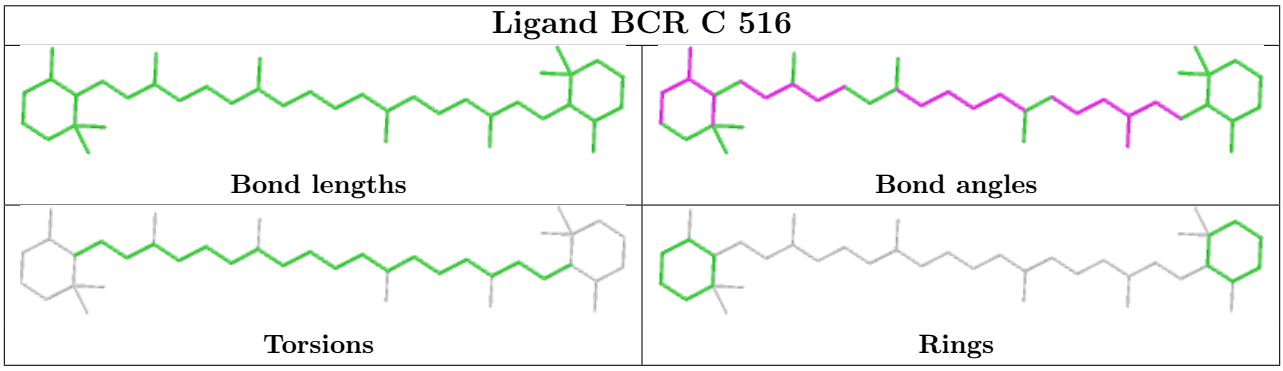
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	N	610	CLA	2	0
23	C	514	CLA	4	0
35	g	605	CHL	1	0
38	R	316	NEX	3	0
23	A	404	CLA	3	0
38	r	615	NEX	1	0
23	g	602	CLA	5	0
26	B	625	SQD	3	0
23	Y	311	CLA	4	0
23	r	604	CLA	1	0
23	g	614	CLA	1	0
23	b	614	CLA	2	0
37	y	301	XAT	6	0
31	b	623	LHG	1	0
23	G	613	CLA	2	0
23	n	610	CLA	2	0
25	d	405	BCR	1	0
35	g	601	CHL	5	0
25	B	617	BCR	4	0
30	C	501	LMG	2	0
23	N	612	CLA	2	0
23	n	602	CLA	1	0
36	g	616	LUT	2	0
24	A	403	PHO	3	0
37	r	614	XAT	2	0
23	N	602	CLA	1	0
23	g	604	CLA	1	0
23	b	610	CLA	3	0
23	D	401	CLA	3	0
31	l	102	LHG	2	0
35	S	306	CHL	3	0
31	r	616	LHG	1	0
23	c	510	CLA	1	0
30	D	409	LMG	1	0
26	C	521	SQD	2	0
35	n	608	CHL	3	0
36	S	316	LUT	4	0
31	D	407	LHG	1	0
35	Y	302	CHL	2	0
23	d	403	CLA	4	0
36	r	613	LUT	3	0
25	C	515	BCR	7	0

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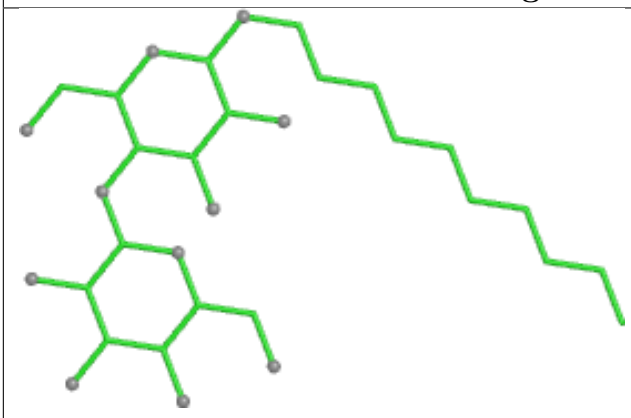
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Y	312	CLA	1	0
23	B	614	CLA	3	0
23	c	502	CLA	3	0
23	B	607	CLA	3	0
36	N	615	LUT	5	0
23	R	313	CLA	2	0
28	D	410	DGD	3	0
23	r	608	CLA	2	0

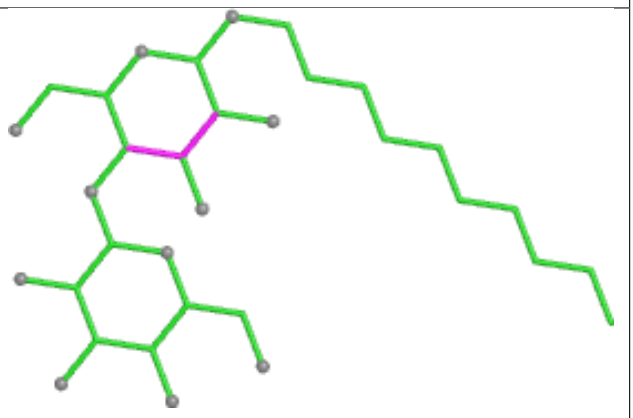
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



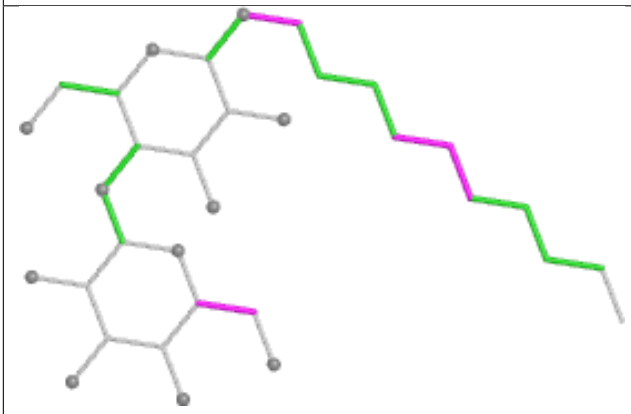
Ligand DMU c 522



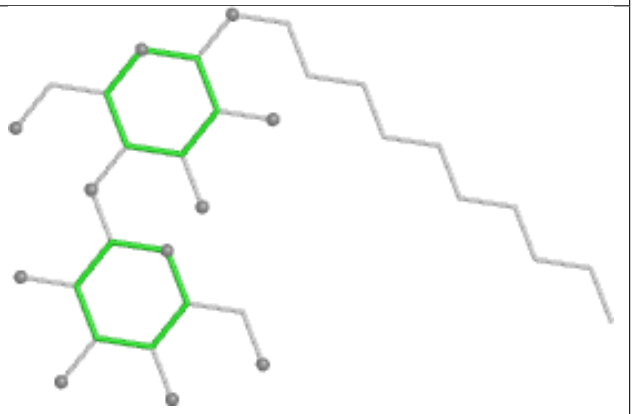
Bond lengths



Bond angles

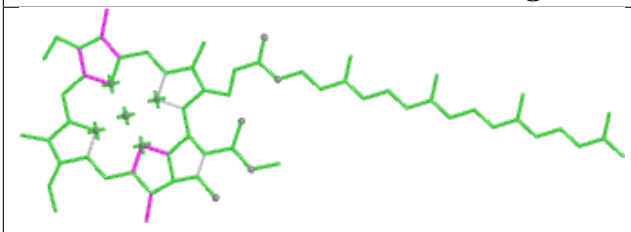


Torsions

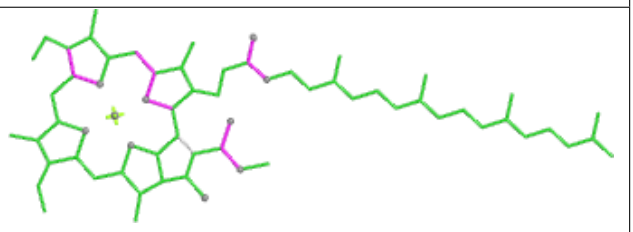


Rings

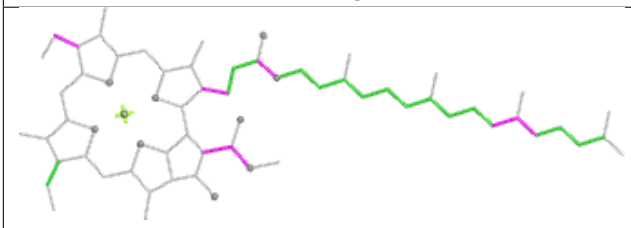
Ligand CLA B 609



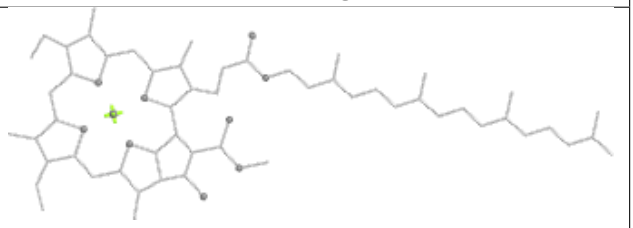
Bond lengths



Bond angles

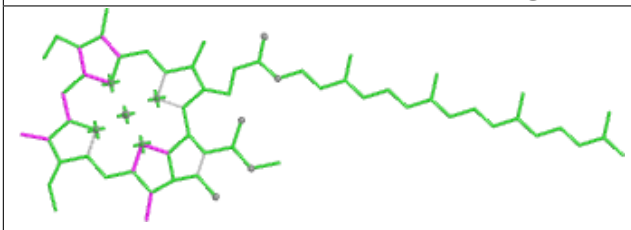


Torsions

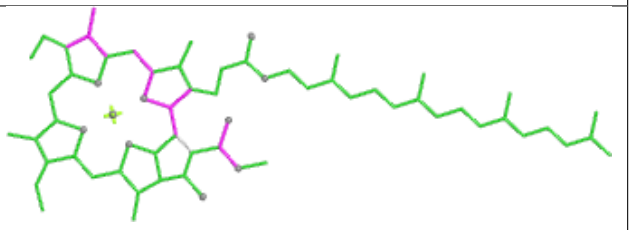


Rings

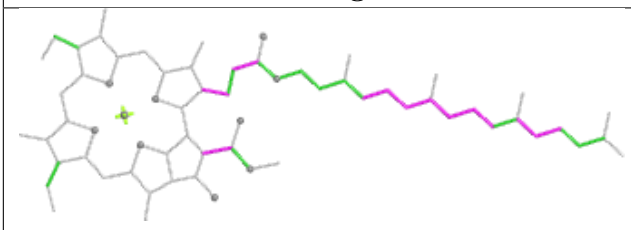
Ligand CLA B 612



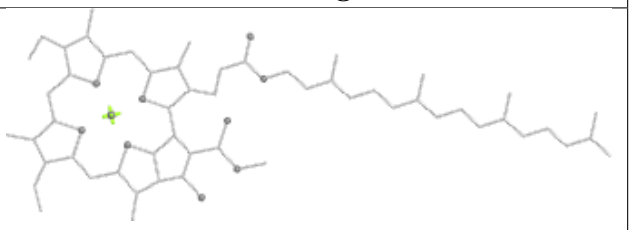
Bond lengths



Bond angles

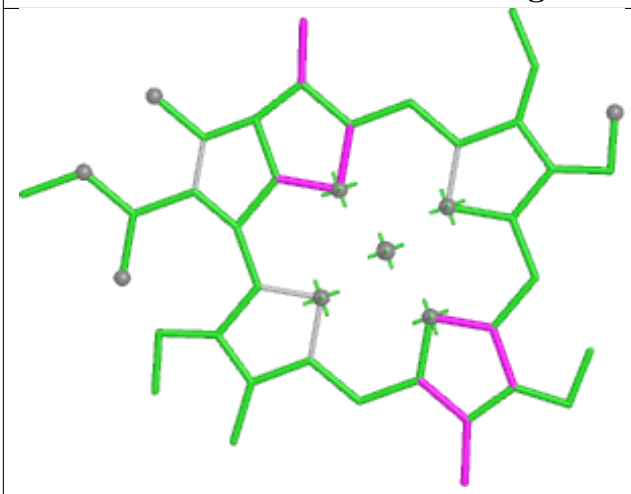


Torsions

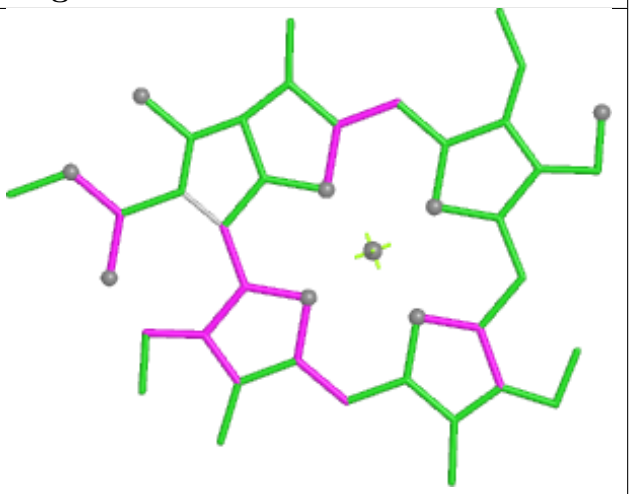


Rings

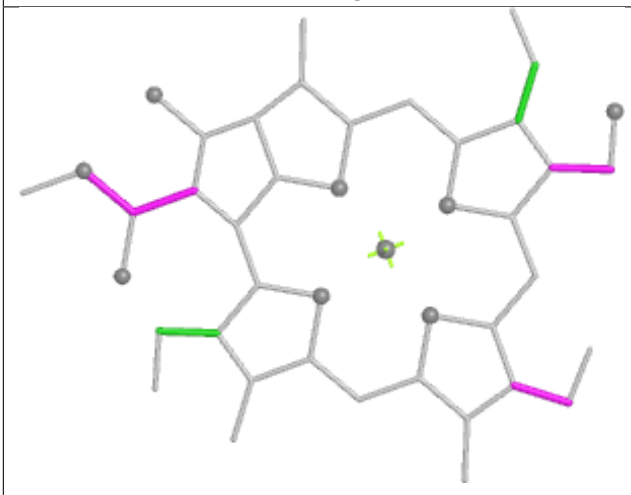
Ligand CHL g 607



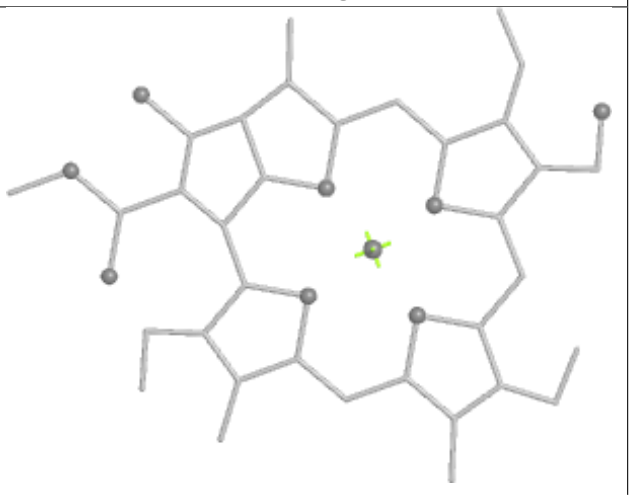
Bond lengths



Bond angles

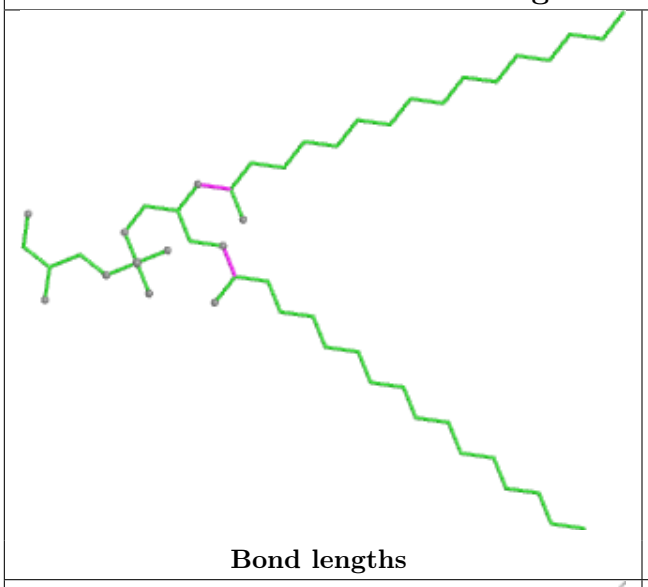


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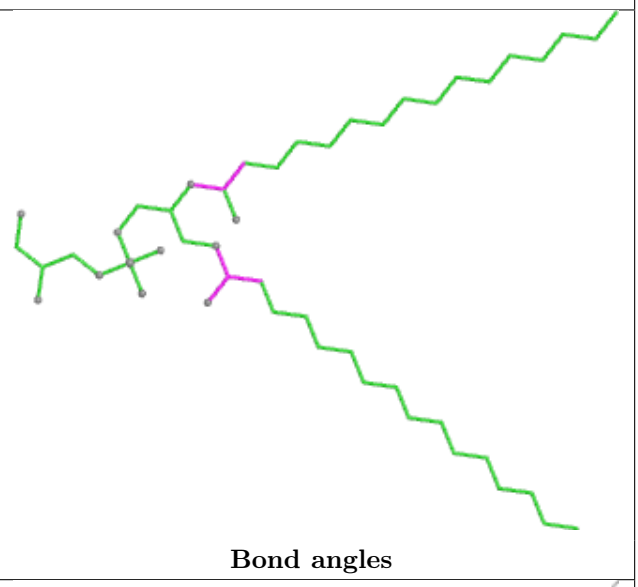


Rings

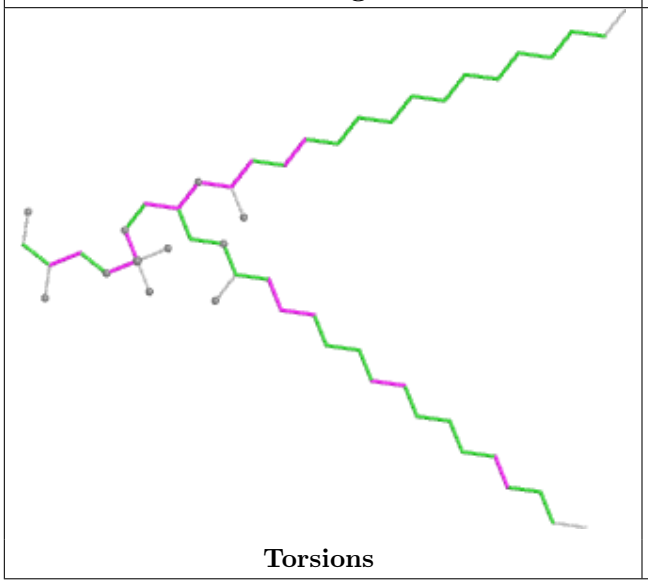
Ligand LHG l 103



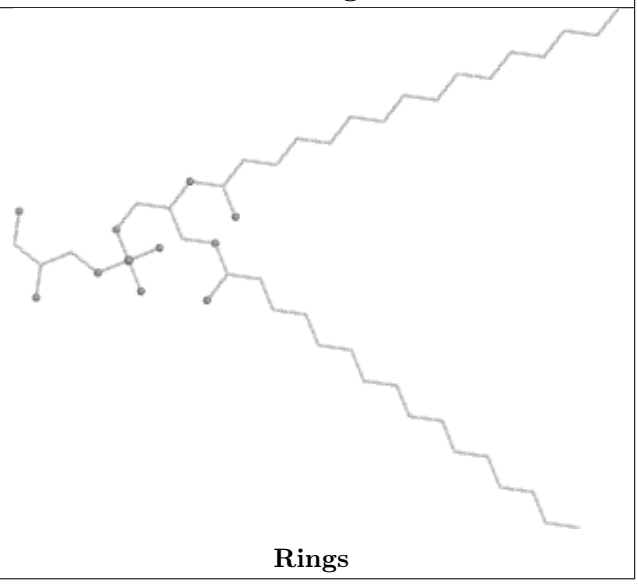
Bond lengths



Bond angles



Torsions



Rings

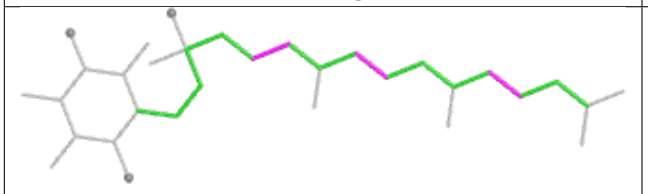
Ligand VTQ W 202



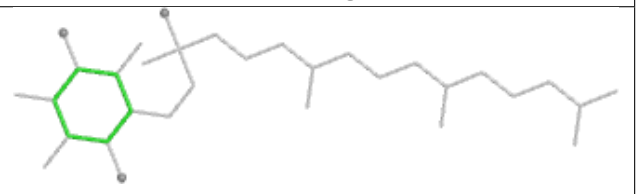
Bond lengths



Bond angles

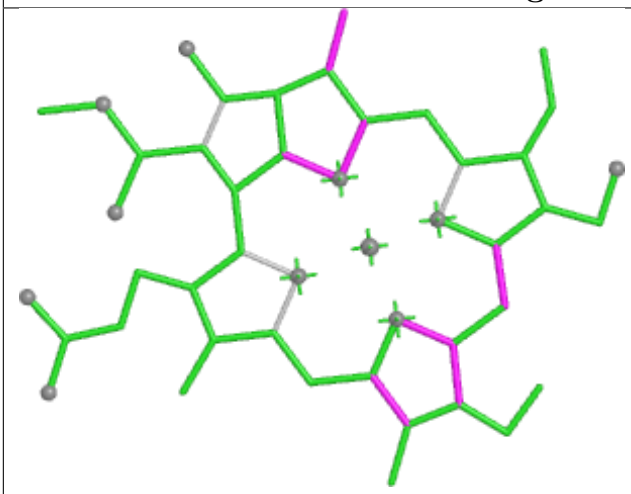


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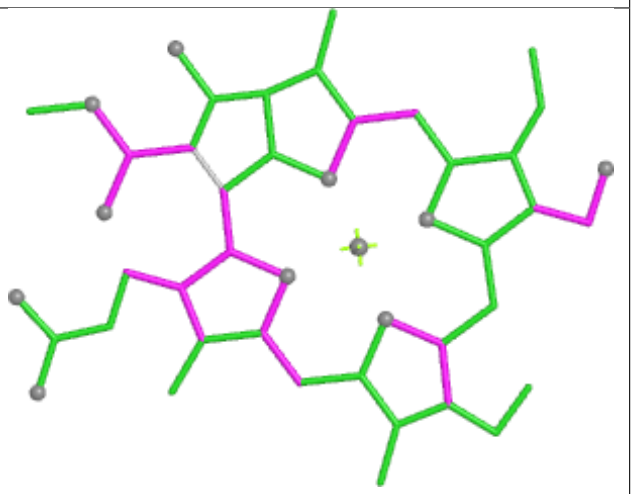


Rings

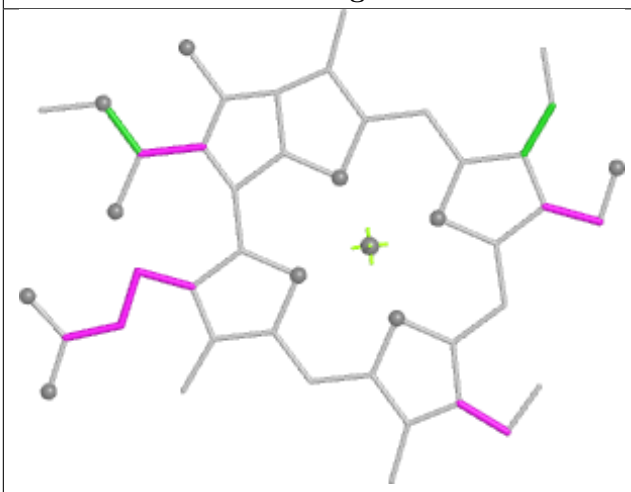
Ligand CHL n 607



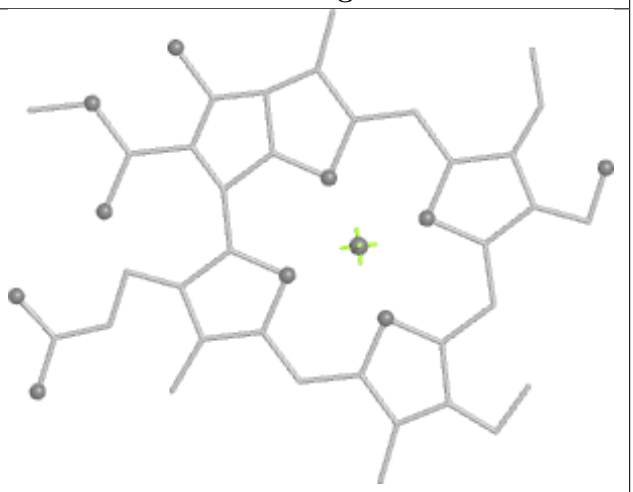
Bond lengths



Bond angles

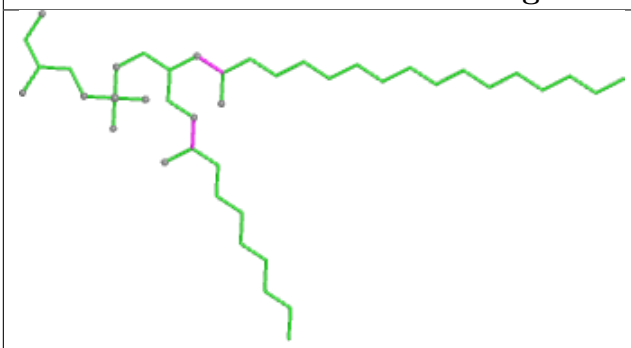


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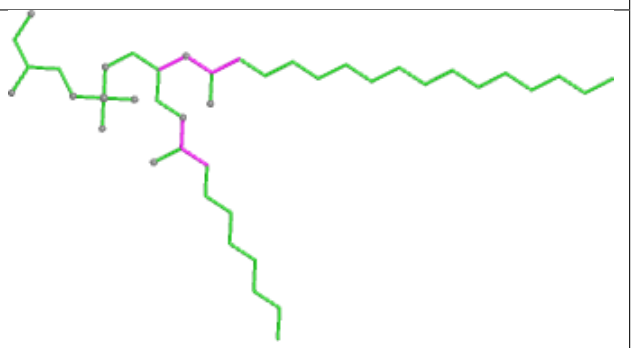


Rings

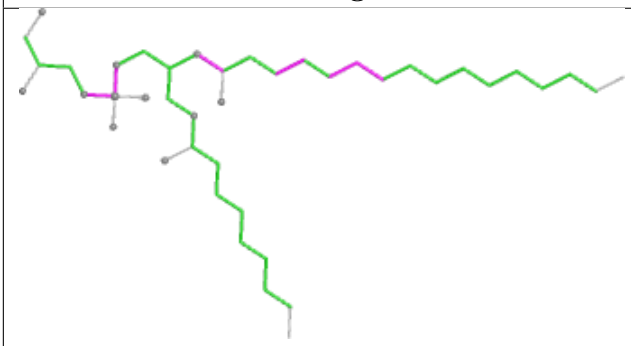
Ligand LHG R 317



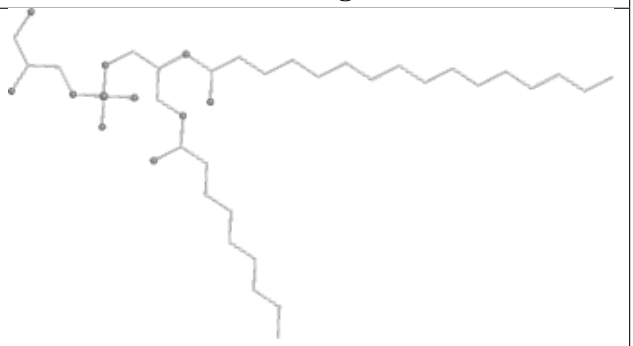
Bond lengths



Bond angles

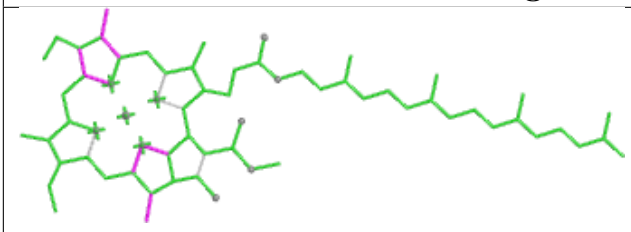


Torsions

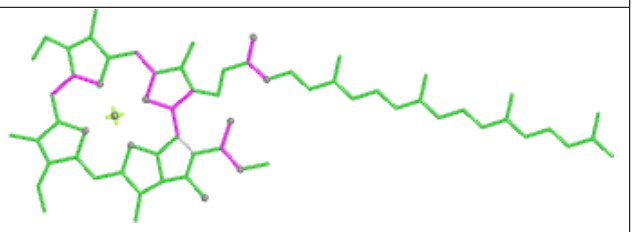


Rings

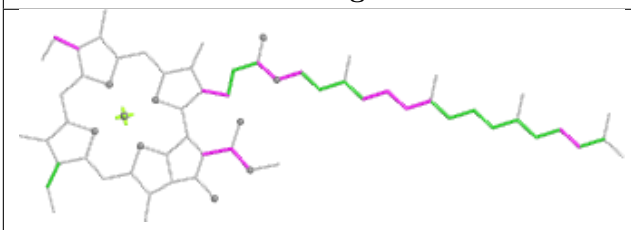
Ligand CLA C 503



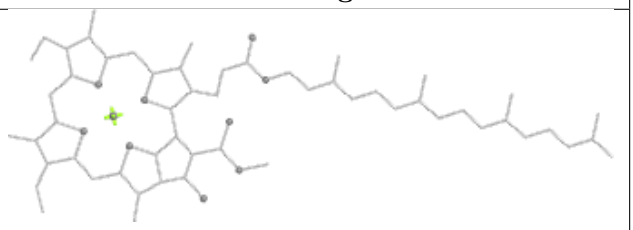
Bond lengths



Bond angles

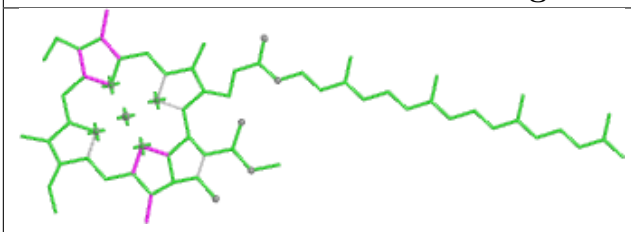


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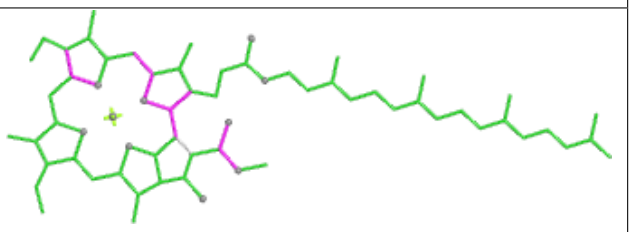


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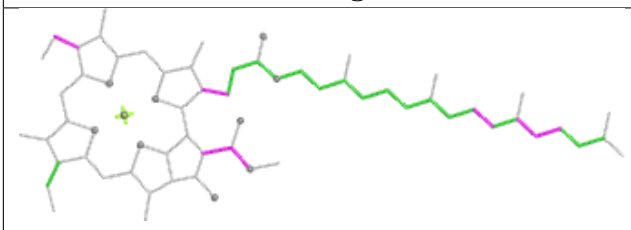
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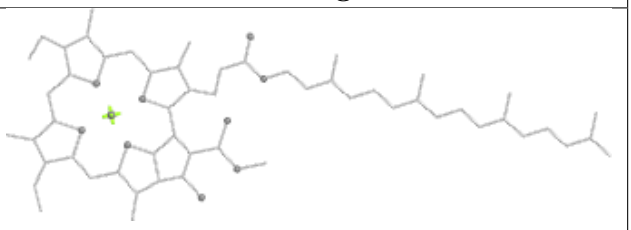
Bond lengths



Bond angles

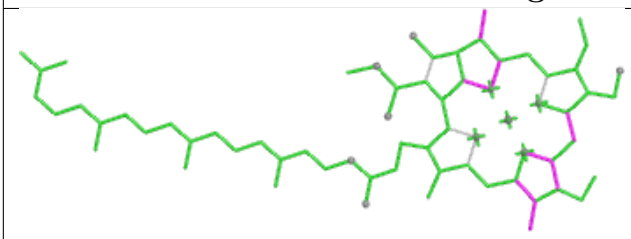


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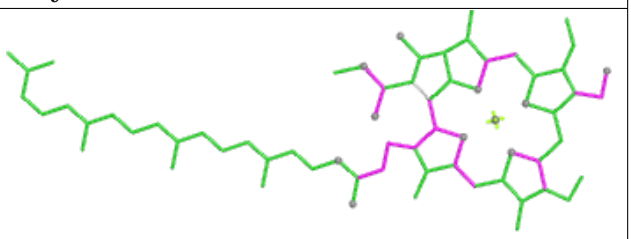


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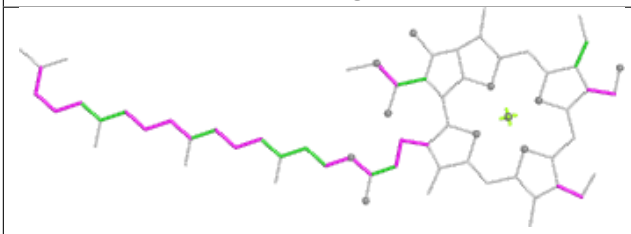
Ligand CHL y 308



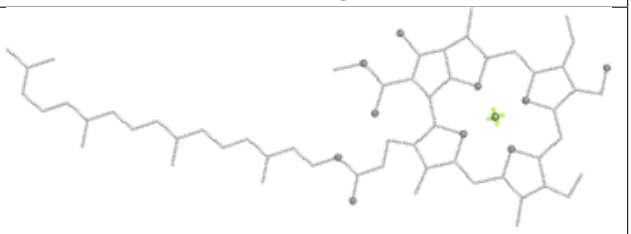
Bond lengths



Bond angles

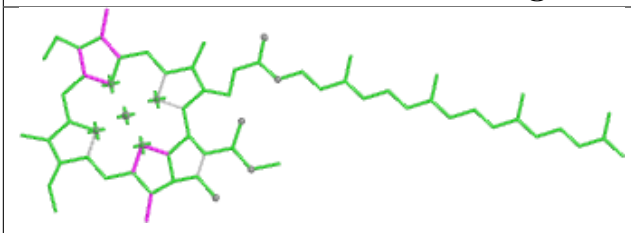


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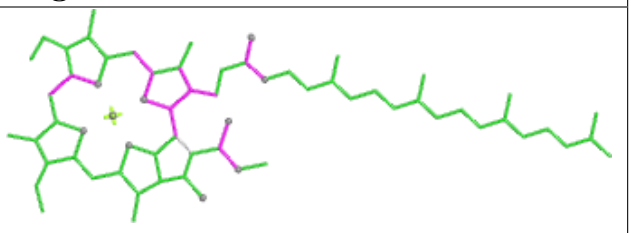


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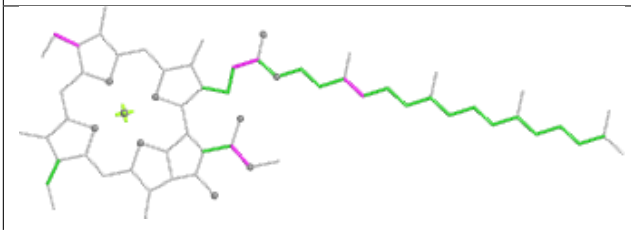
Ligand CLA g 603



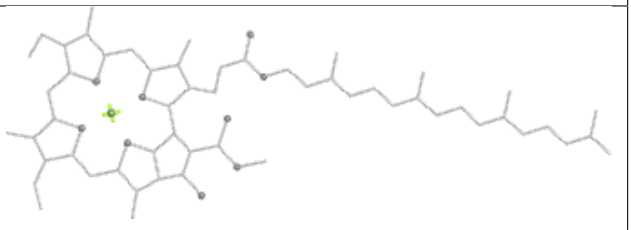
Bond lengths



Bond angles

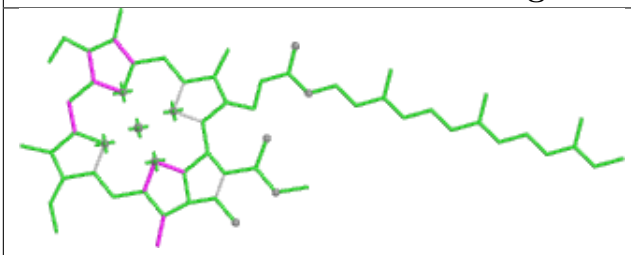


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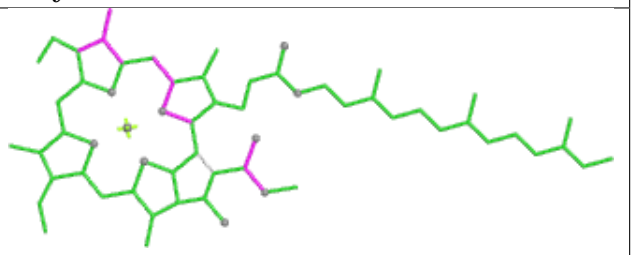


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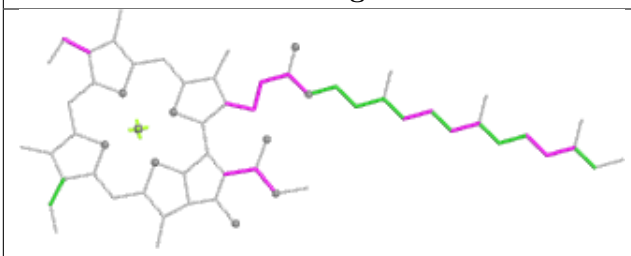
Ligand CLA y 303



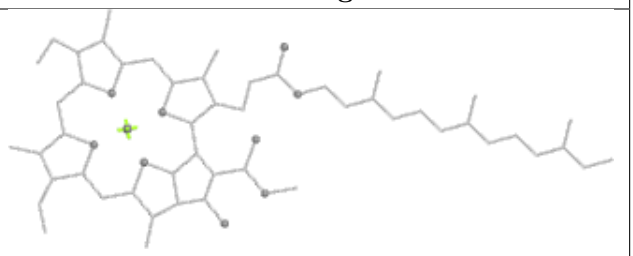
Bond lengths



Bond angles

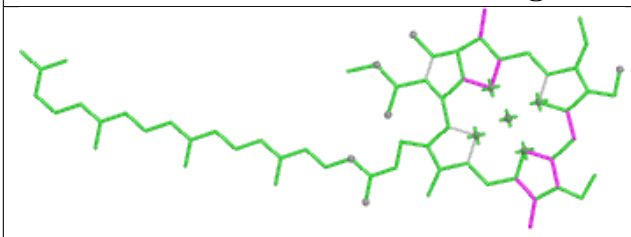


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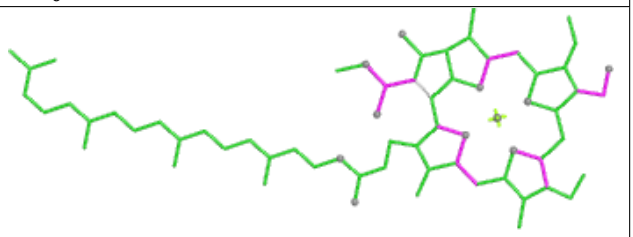


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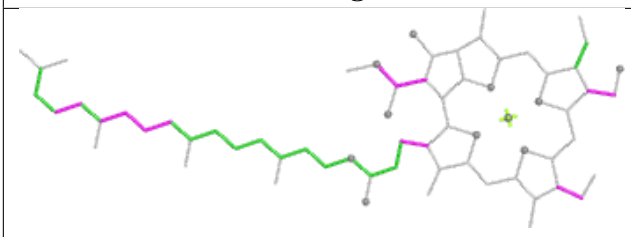
Ligand CHL y 302



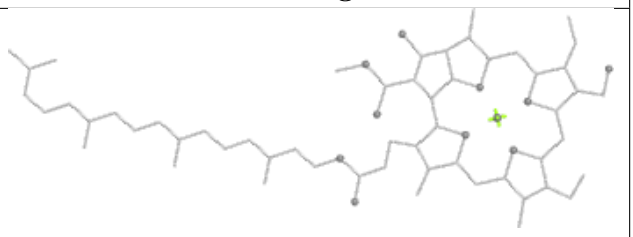
Bond lengths



Bond angles

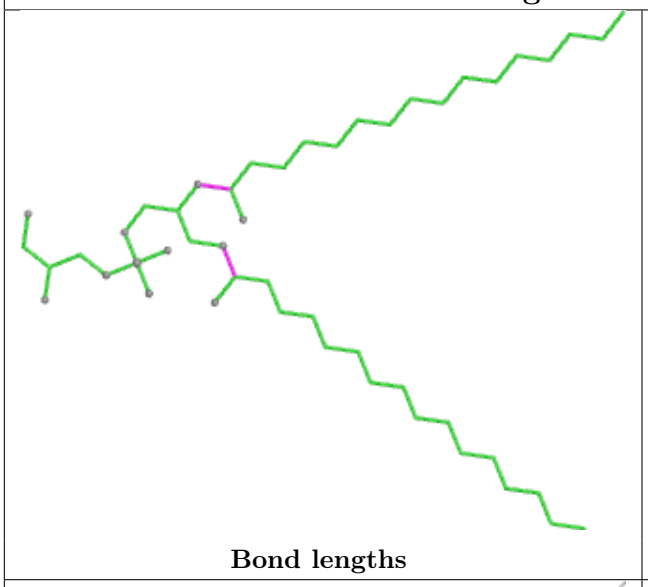


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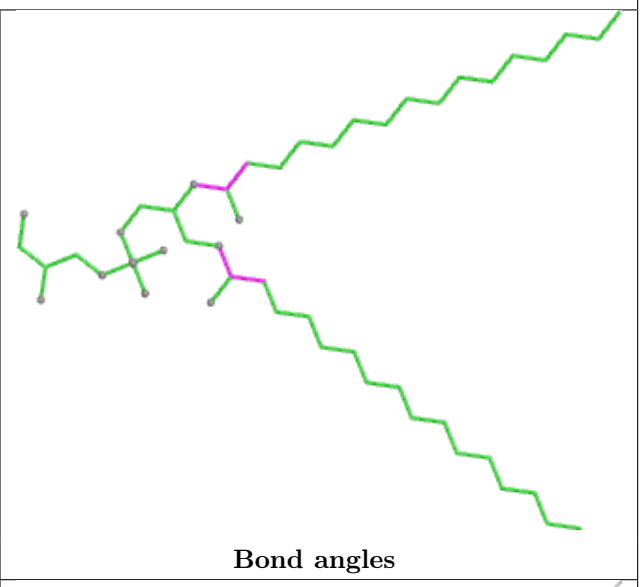


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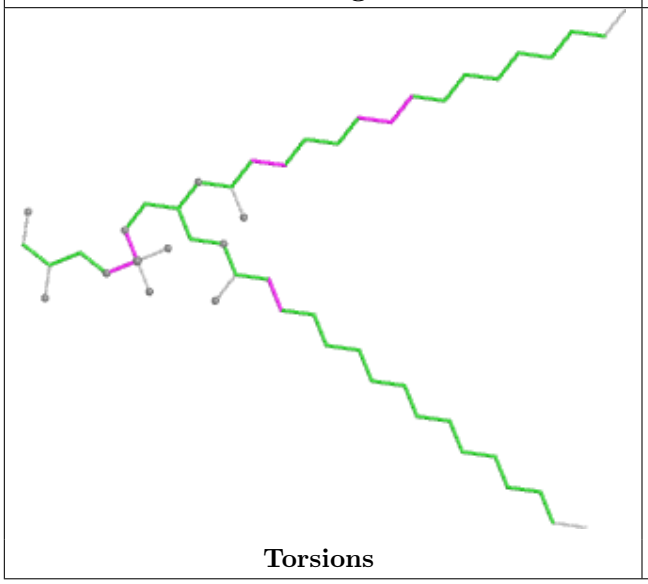
Ligand LHG D 408



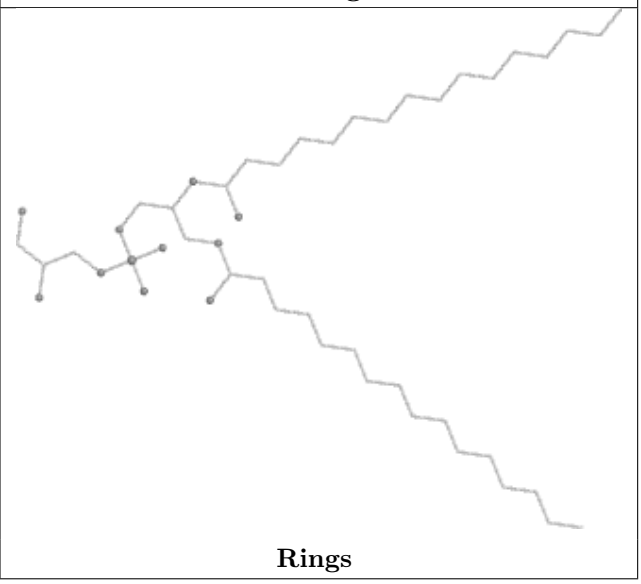
Bond lengths



Bond angles



Torsions

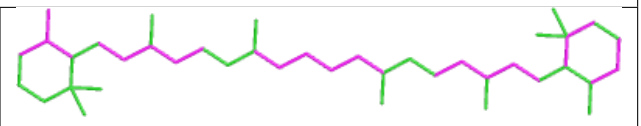


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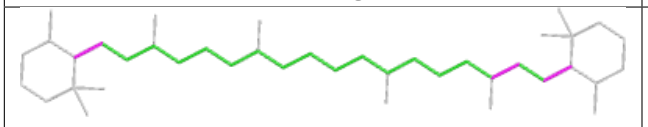
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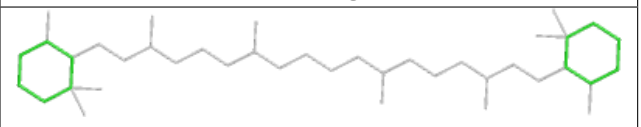
Bond lengths



Bond angles

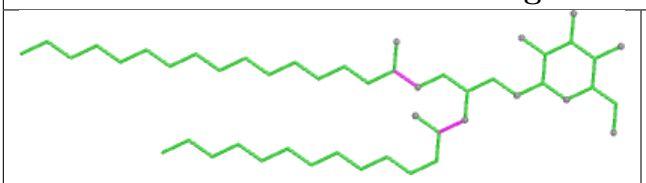


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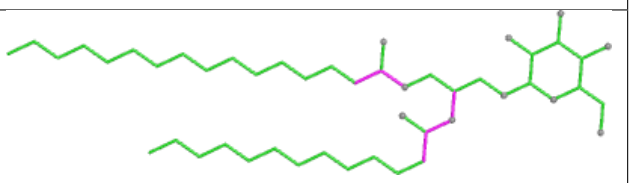


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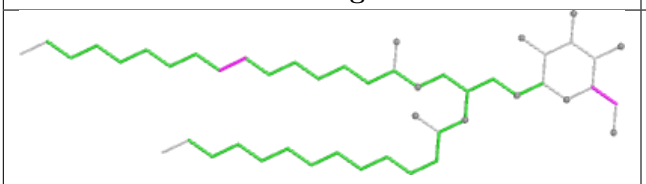
Ligand LMG a 407



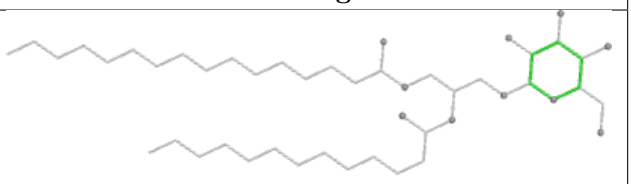
Bond lengths



Bond angles

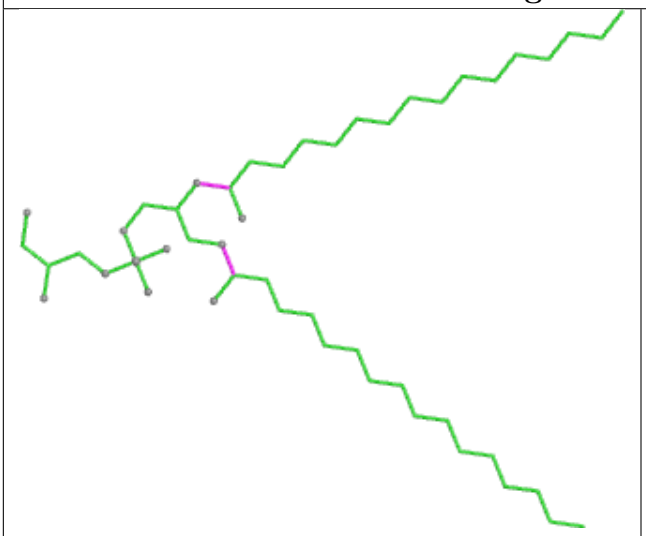


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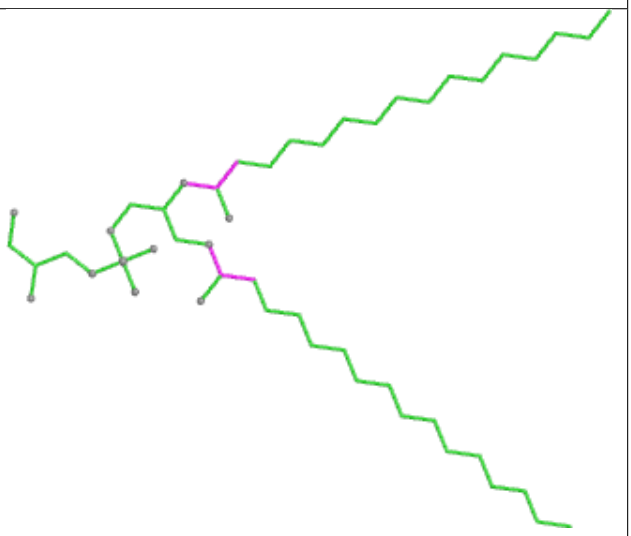


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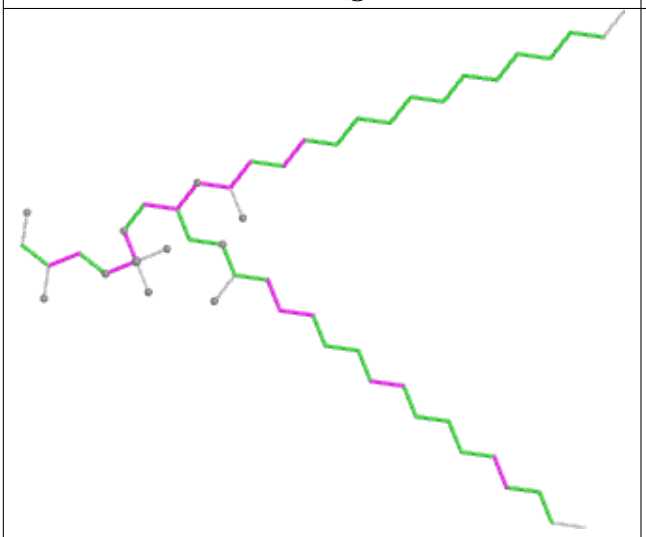
Ligand LHG L 102



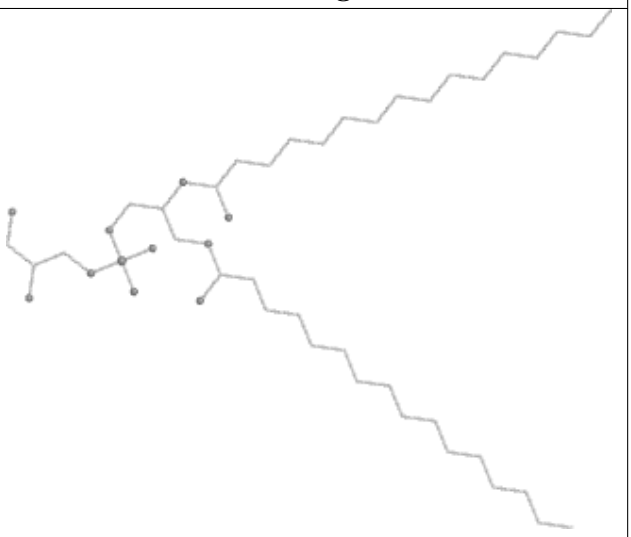
Bond lengths



Bond angles

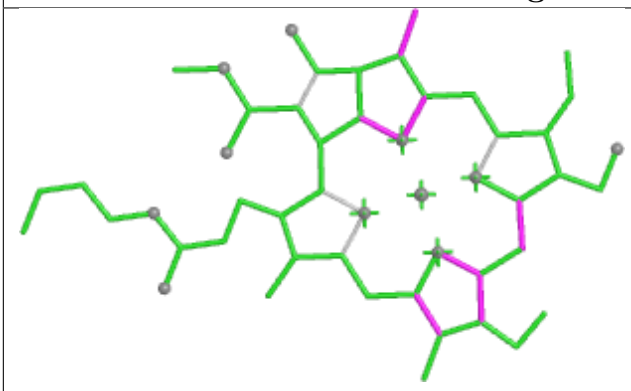


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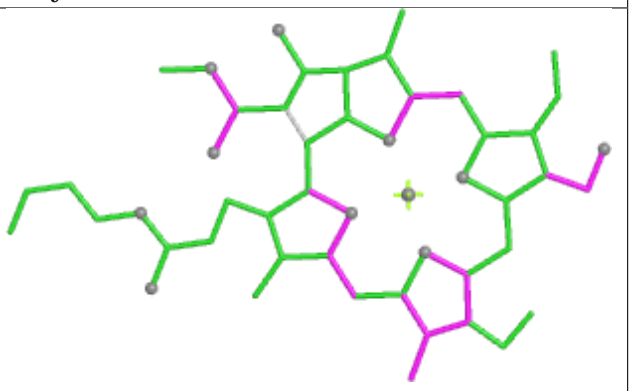


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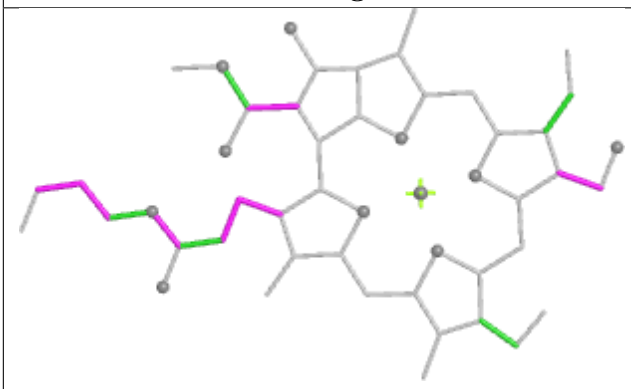
Ligand CHL y 307



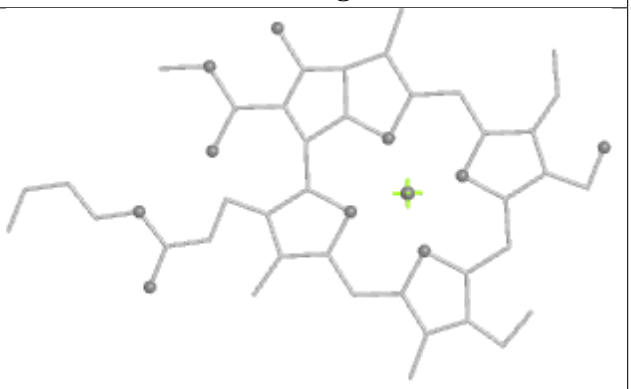
Bond lengths



Bond angles

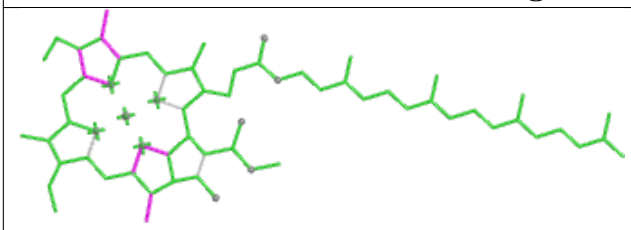


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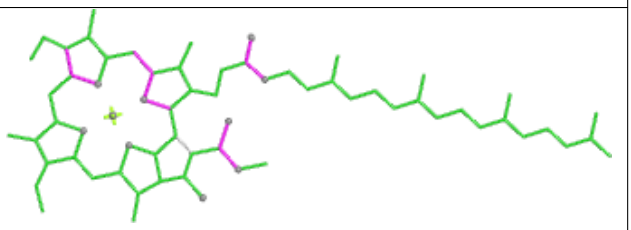


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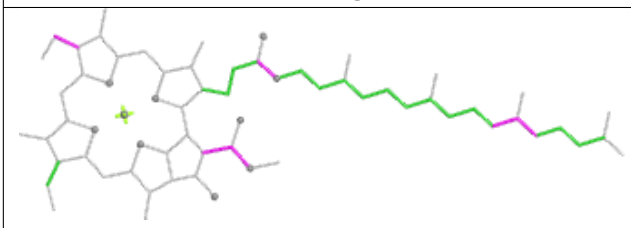
Ligand CLA b 611



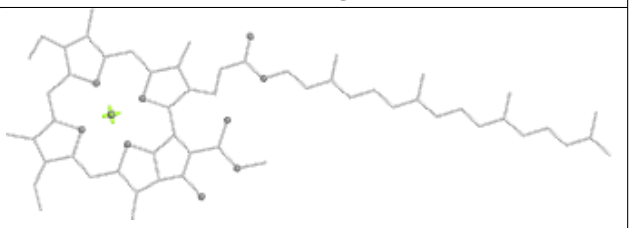
Bond lengths



Bond angles

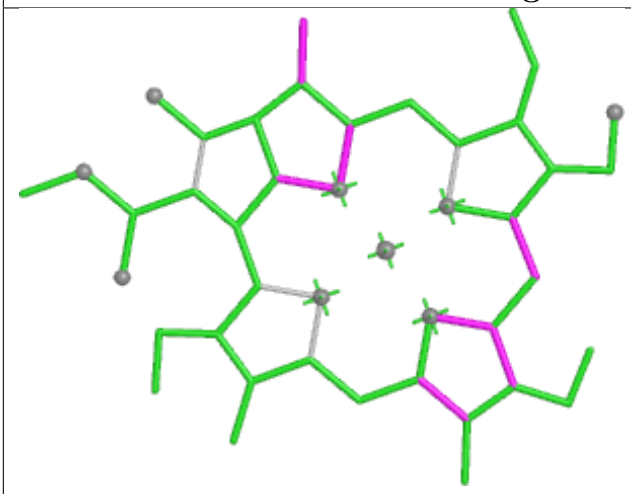


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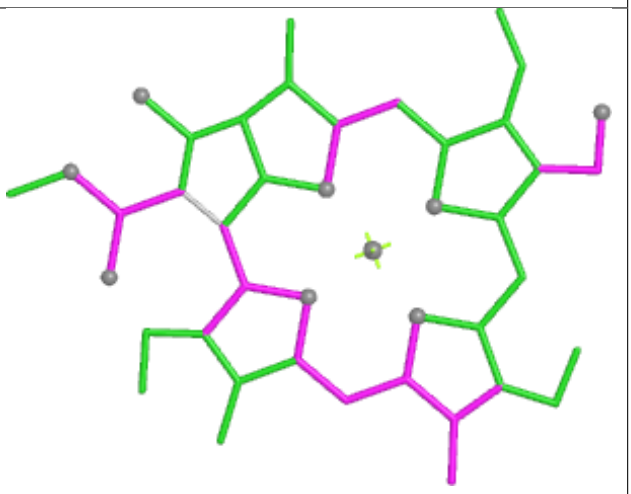


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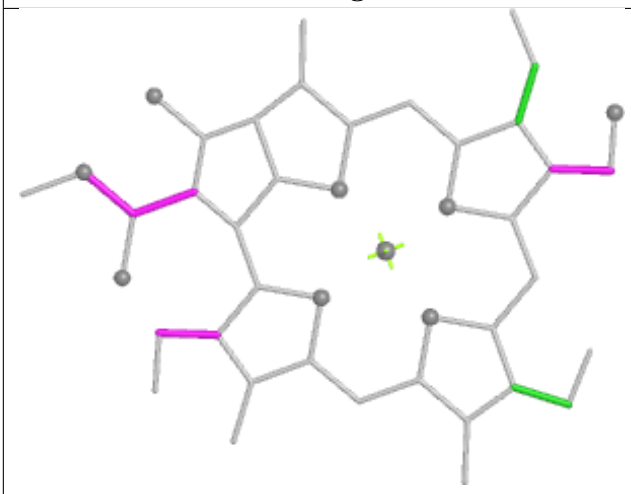
Ligand CHL G 606



Bond lengths



Bond angles

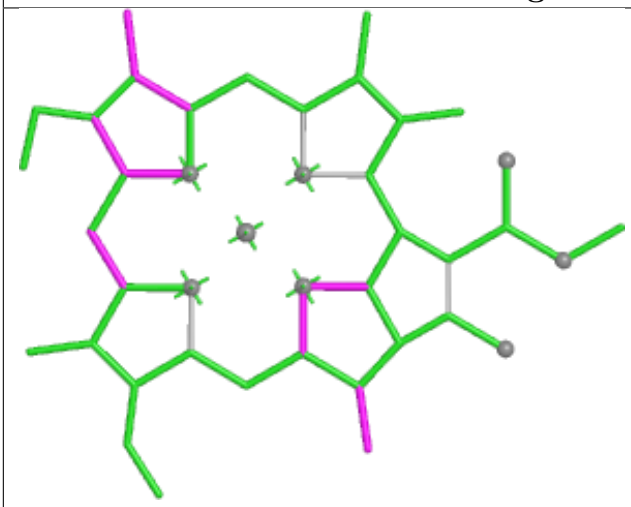


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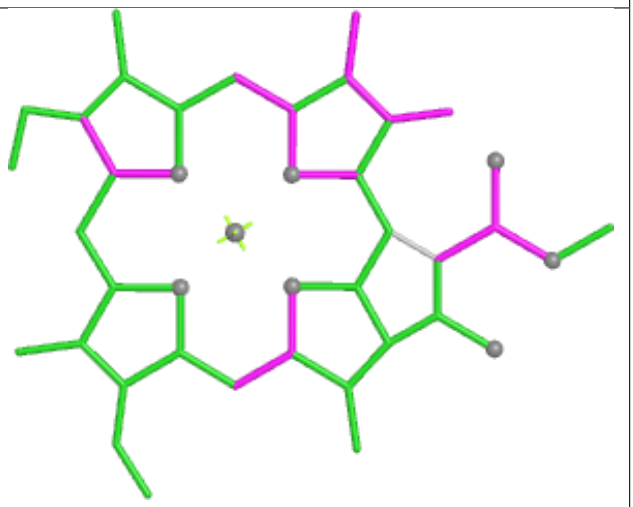


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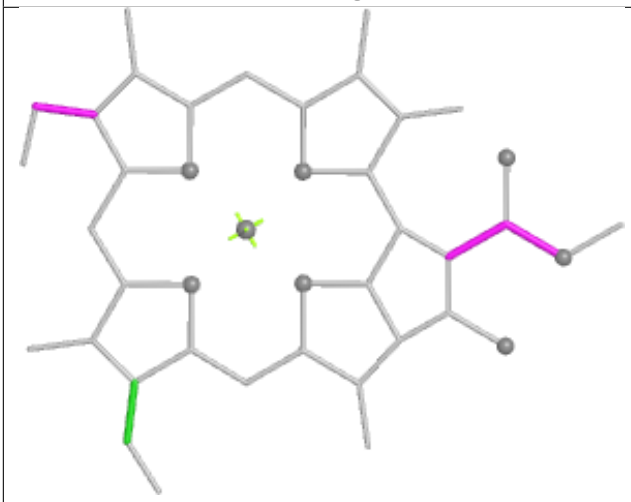
Ligand CLA S 314



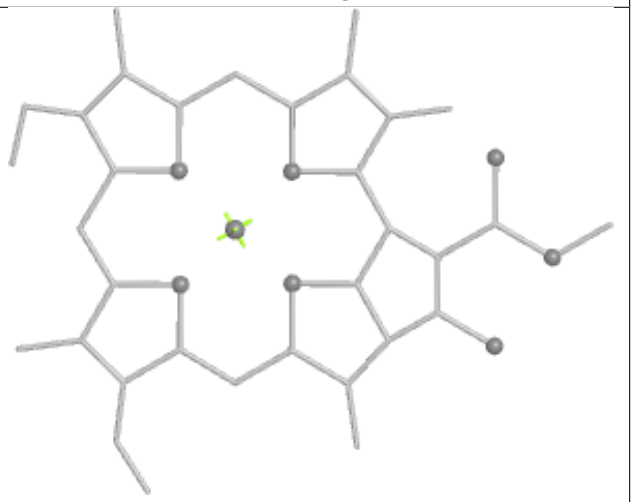
Bond lengths



Bond angles

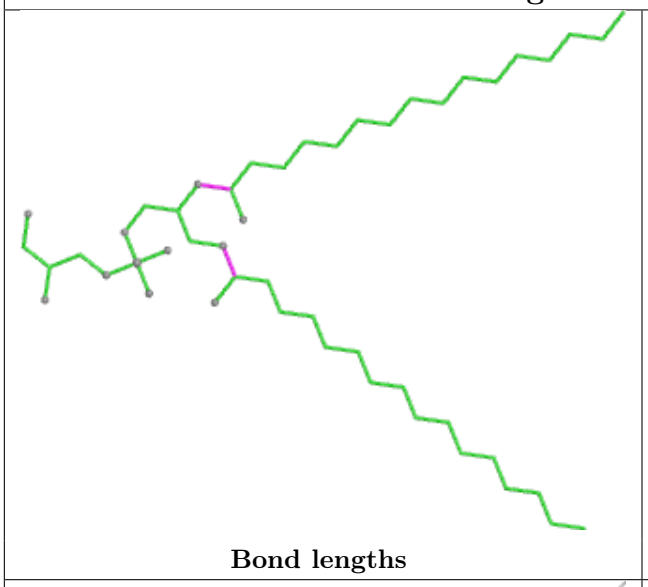


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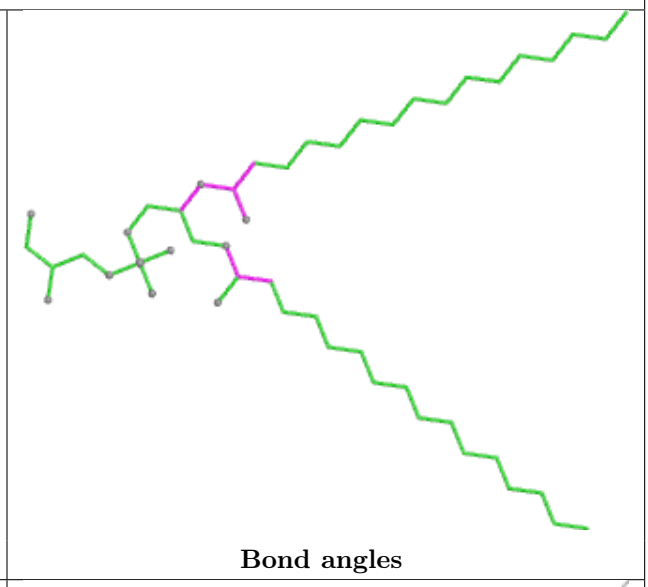


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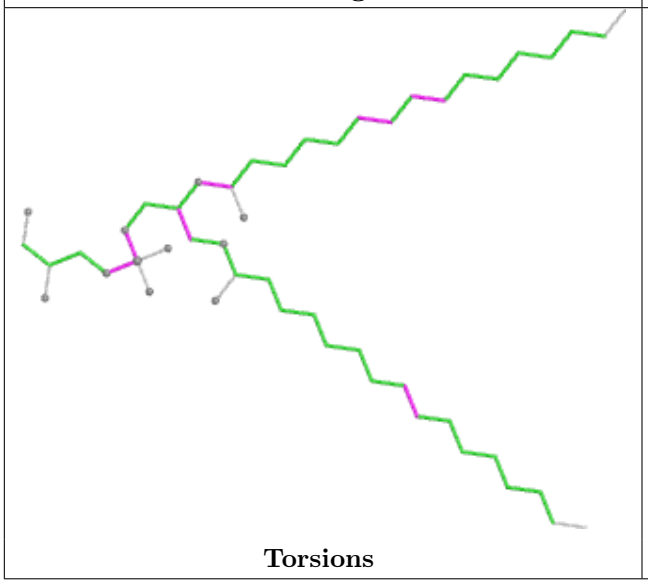
Ligand LHG n 618



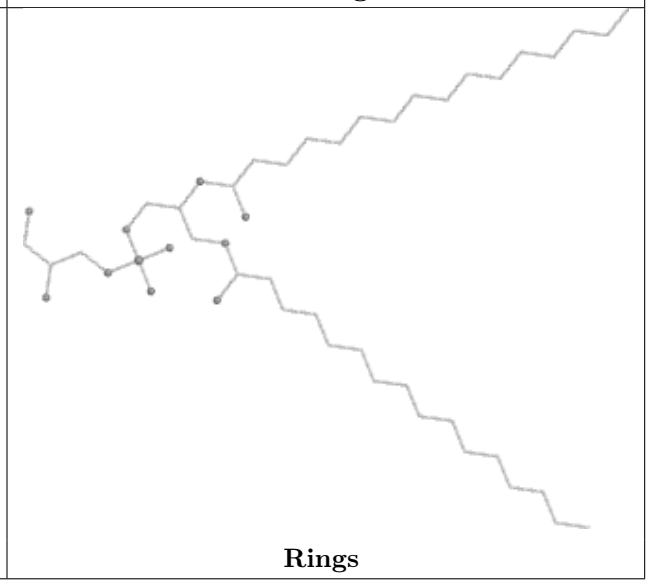
Bond lengths



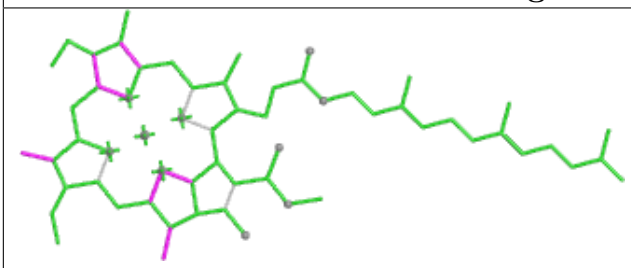
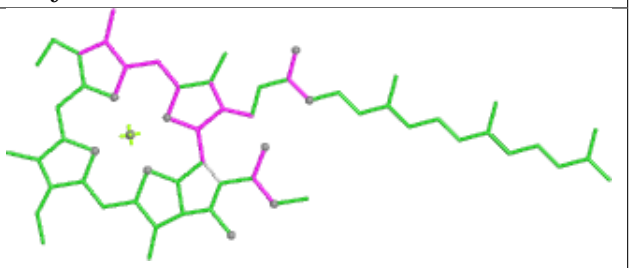
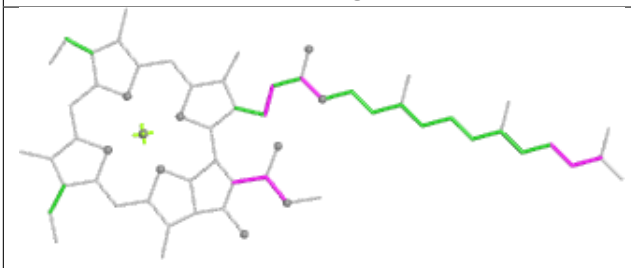
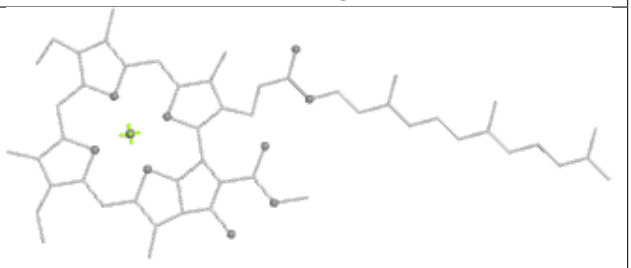
Bond angles

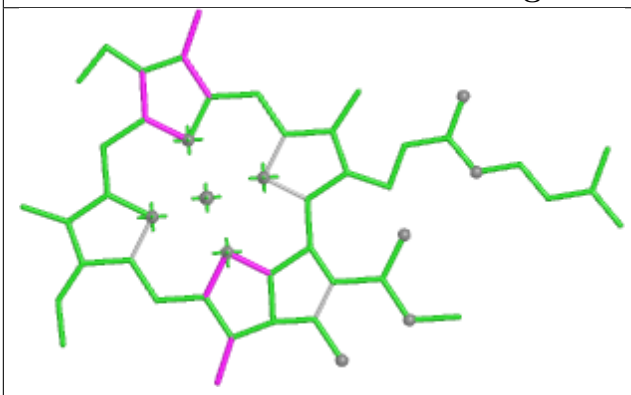
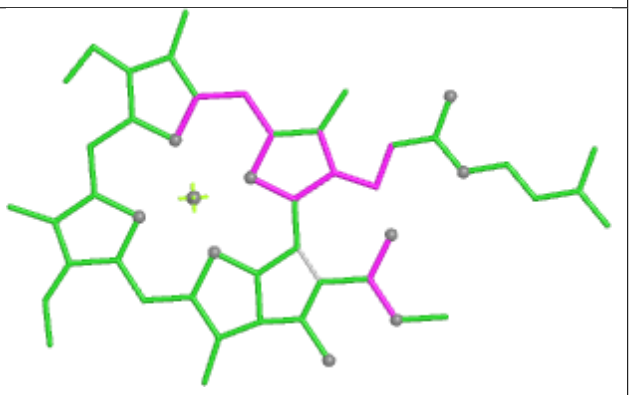
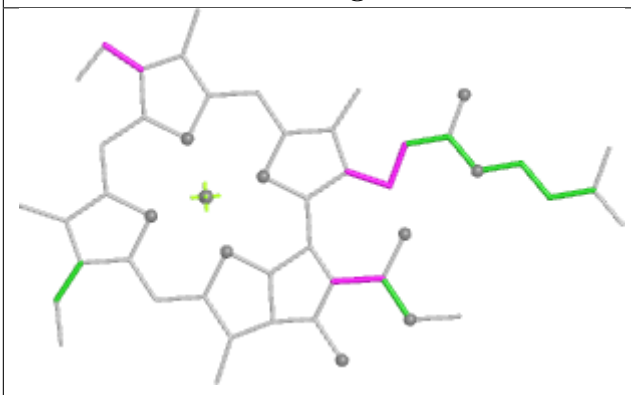
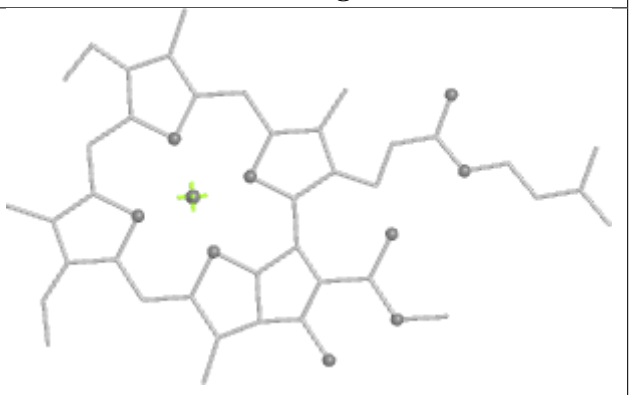


Torsions

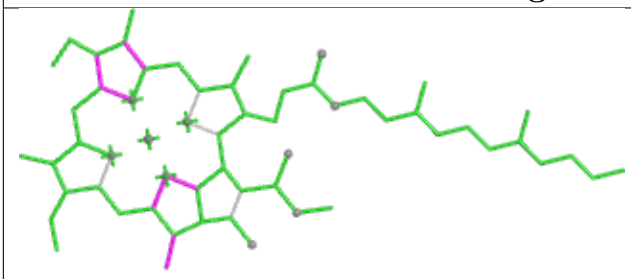


Rings

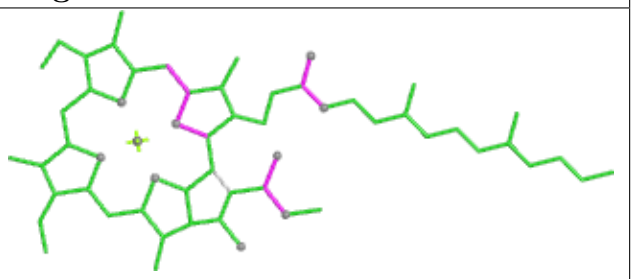
Ligand CLA y 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

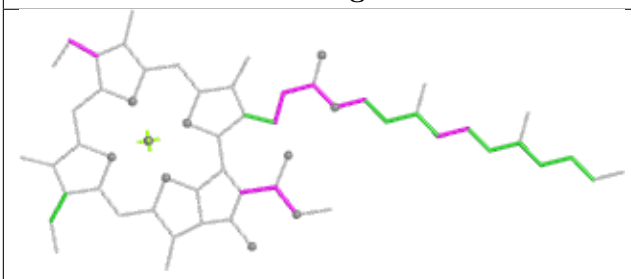
Ligand CLA g 613



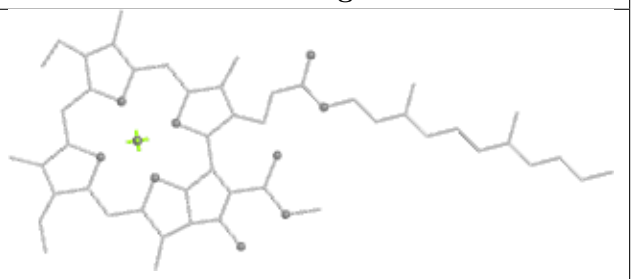
Bond lengths



Bond angles

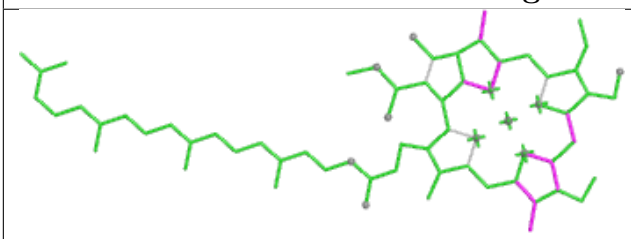


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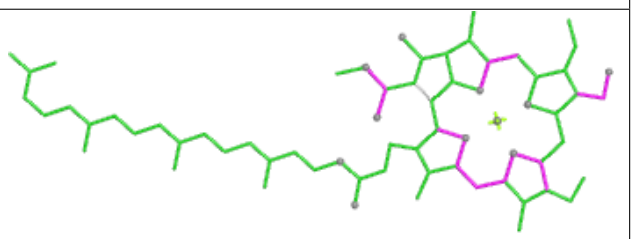


Rings

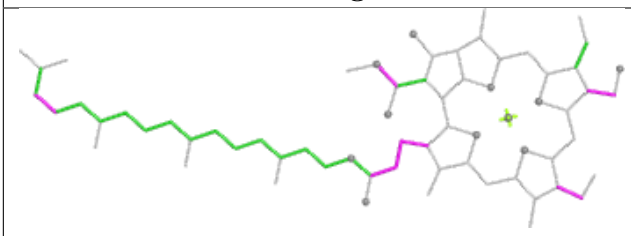
Ligand CHL N 608



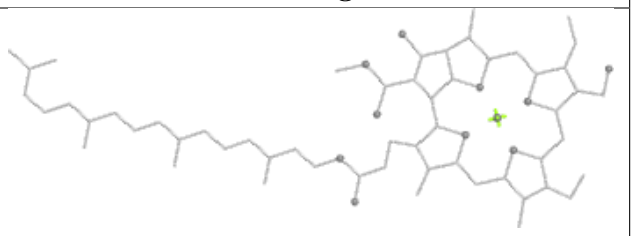
Bond lengths



Bond angles

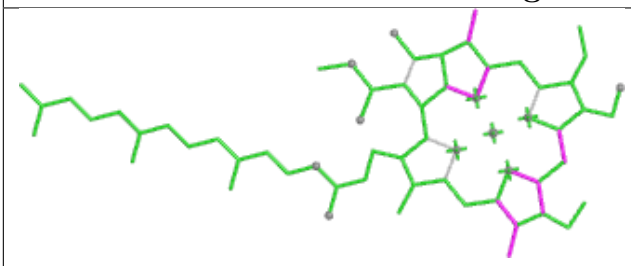


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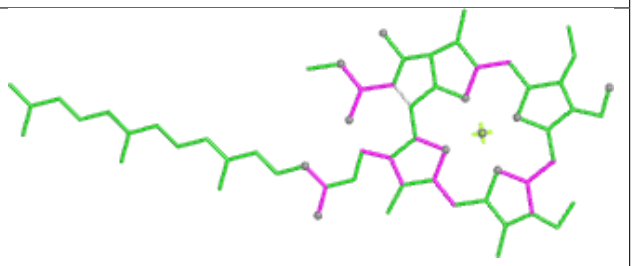


Rings

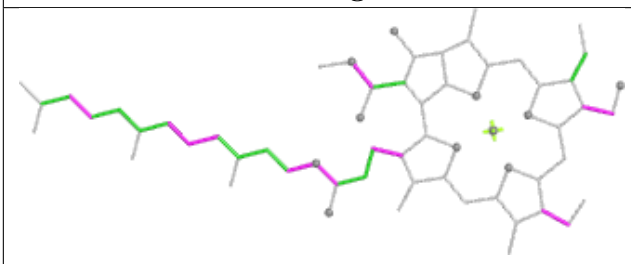
Ligand CHL R 308



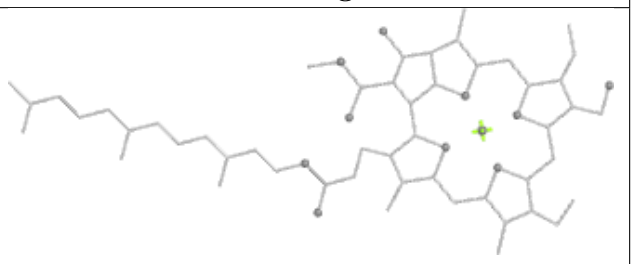
Bond lengths



Bond angles

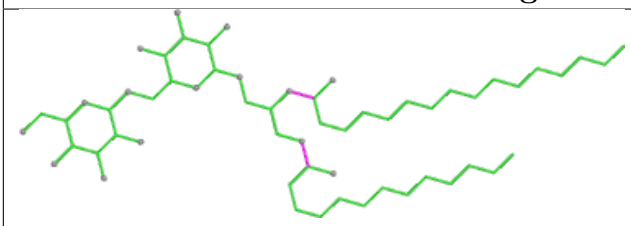


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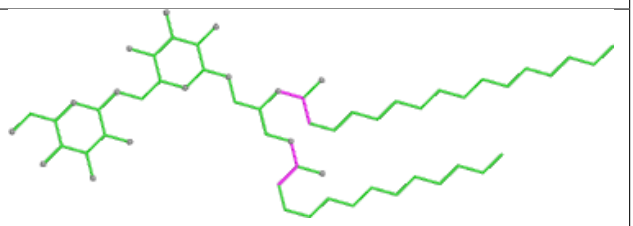


Rings

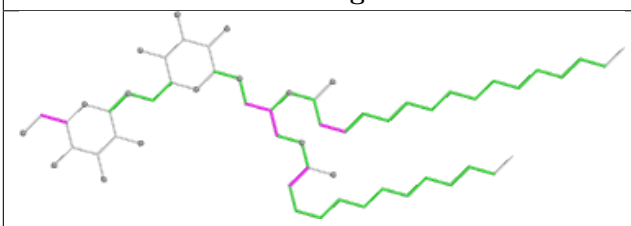
Ligand DGD B 624



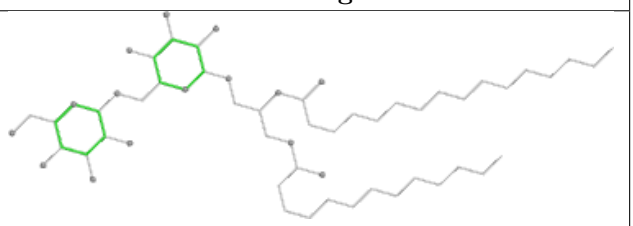
Bond lengths



Bond angles

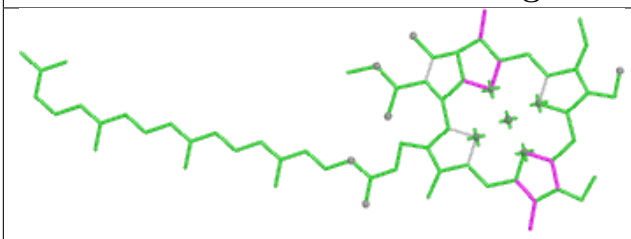


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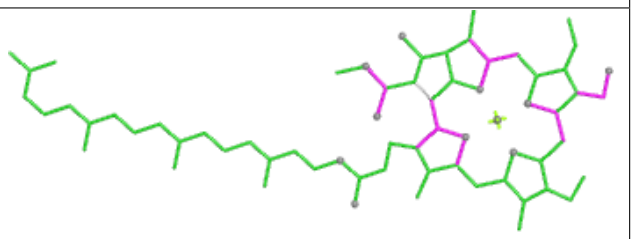


Rings

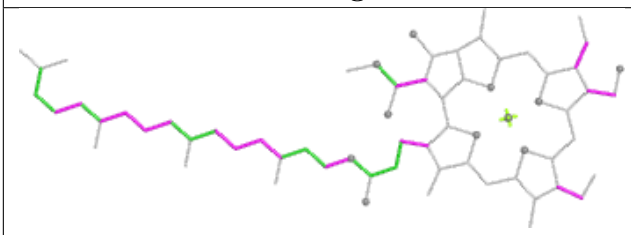
Ligand CHL G 601



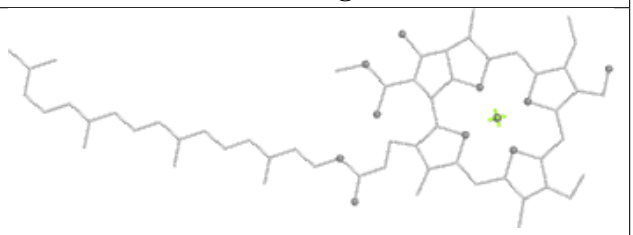
Bond lengths



Bond angles

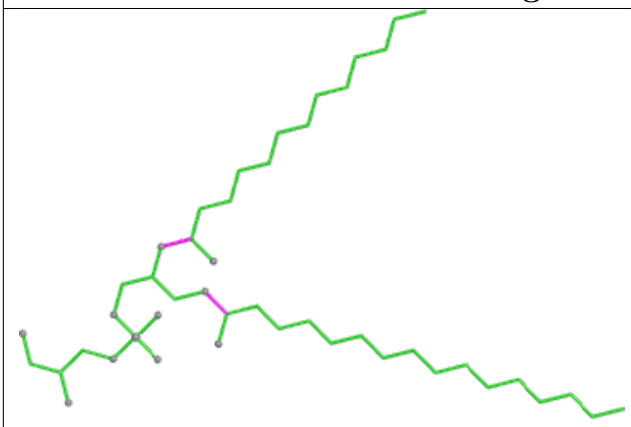


Torsions

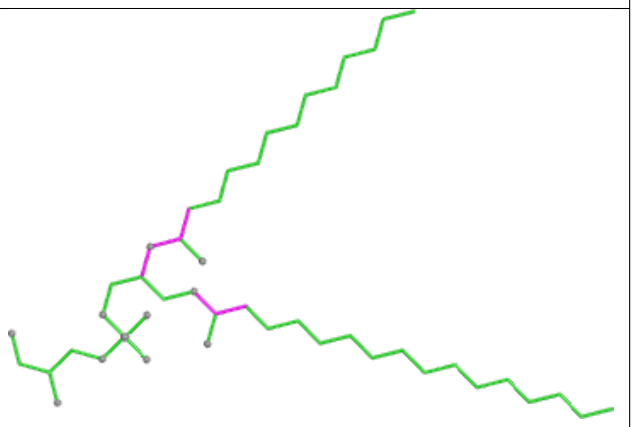


Rings

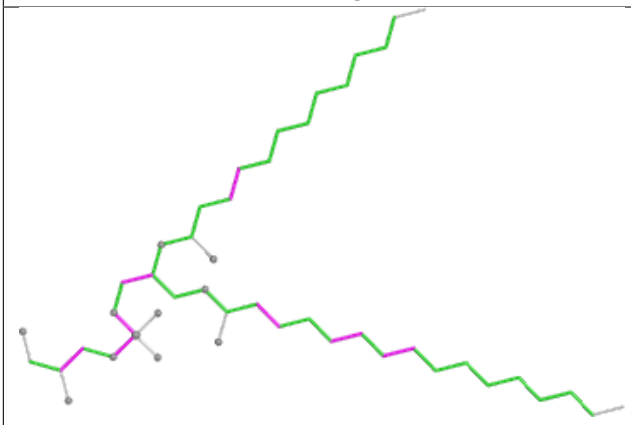
Ligand LHG B 622



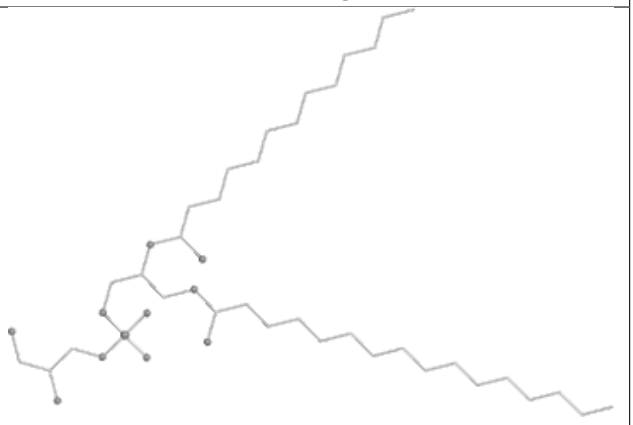
Bond lengths



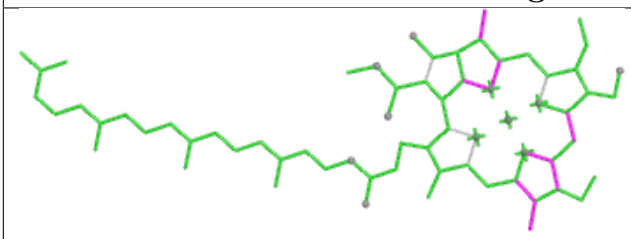
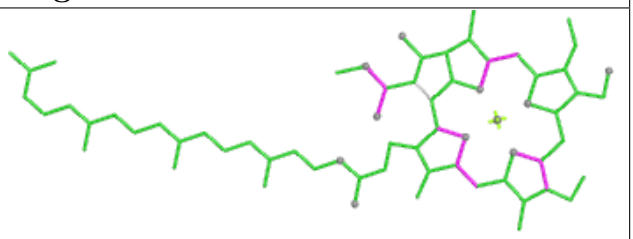
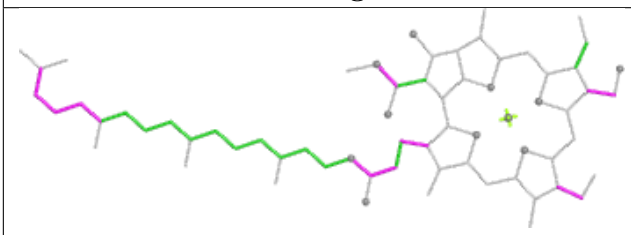
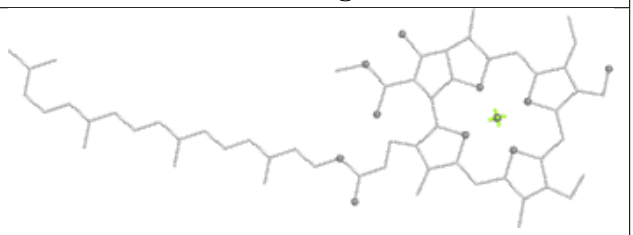
Bond angles

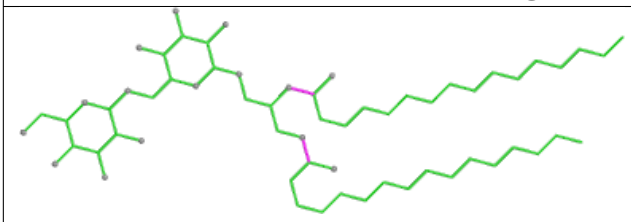
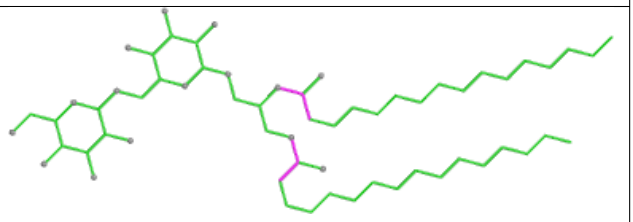
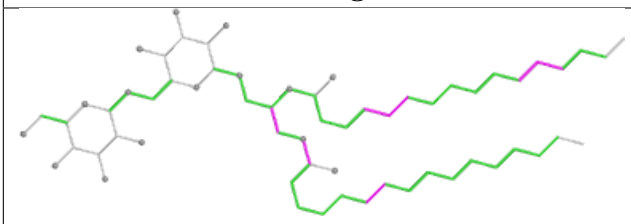
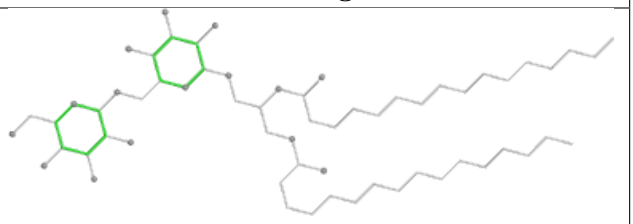


Torsions

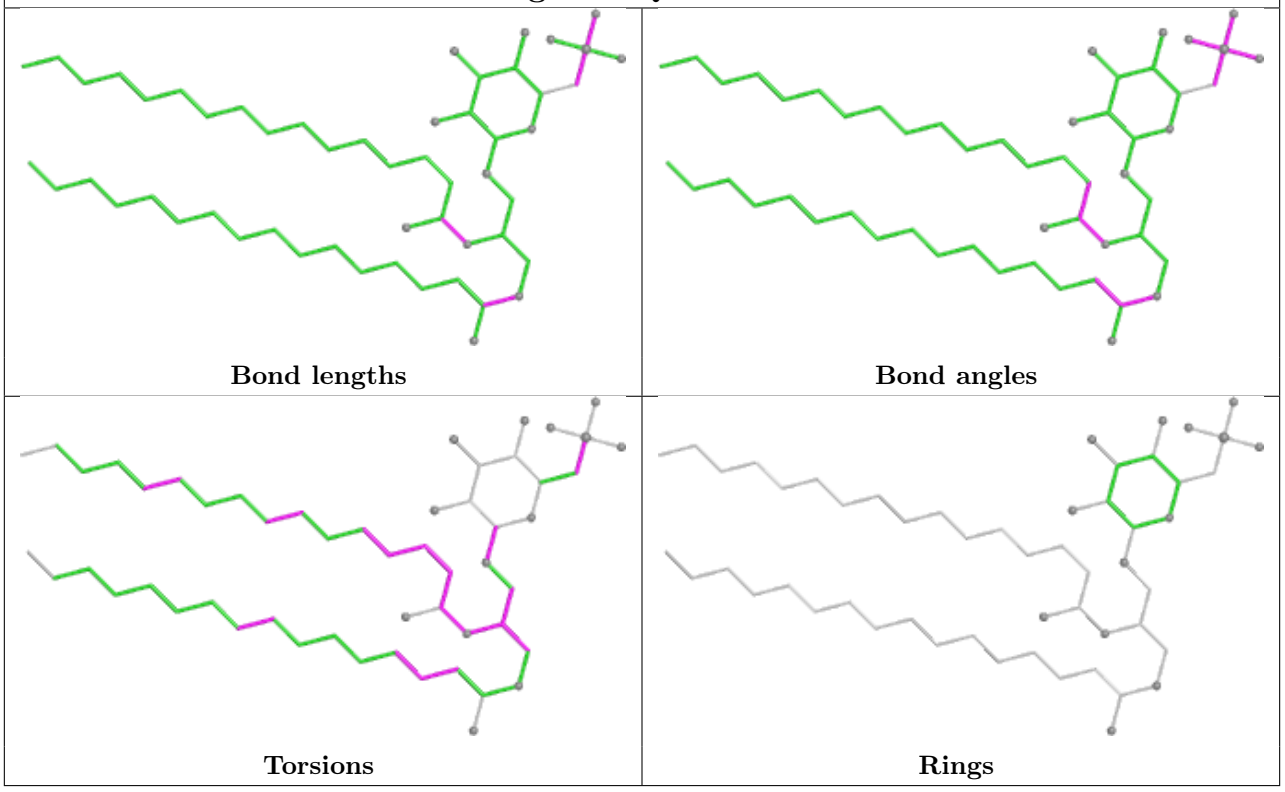


Rings

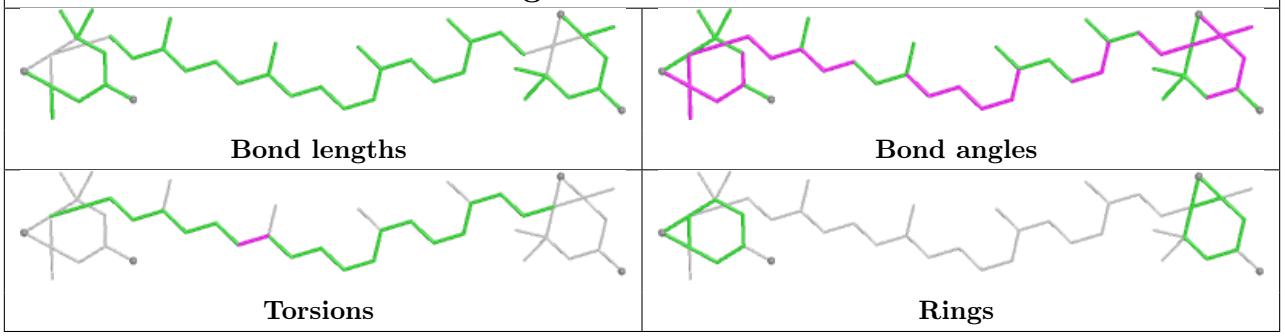
Ligand CHL g 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD d 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

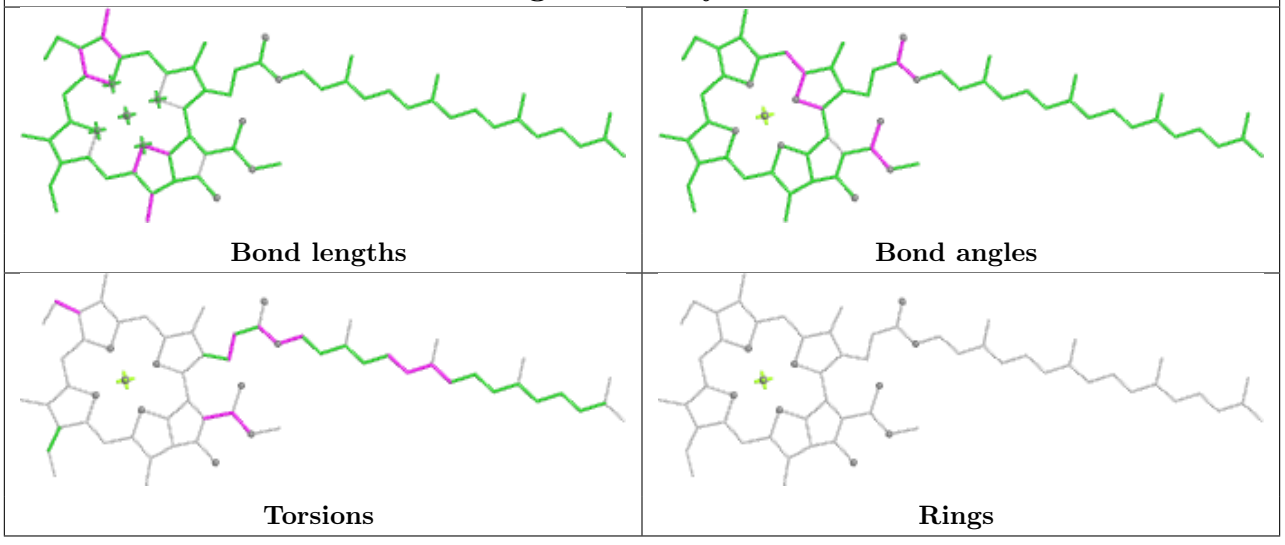
Ligand SQD b 602



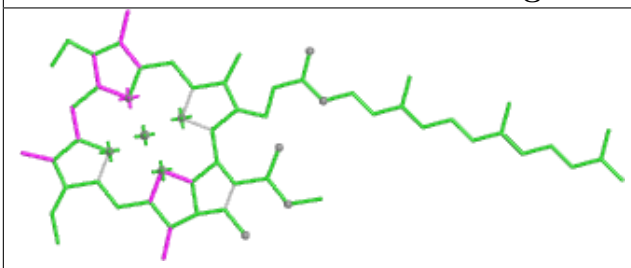
Ligand XAT G 617



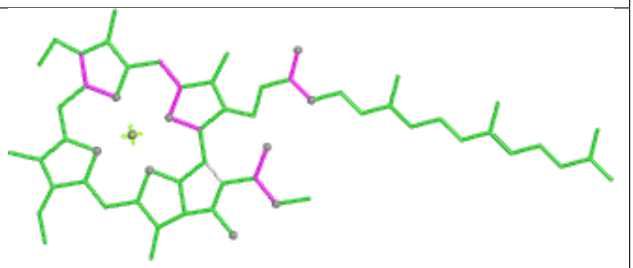
Ligand CLA y 314



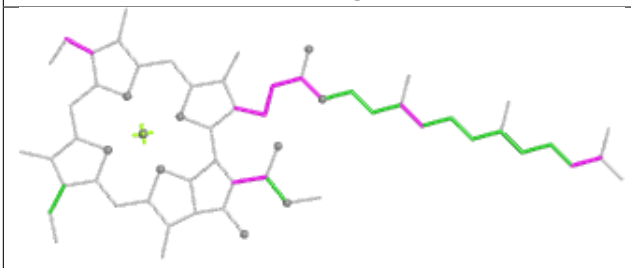
Ligand CLA R 303



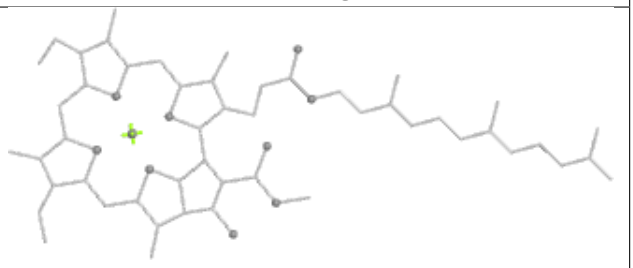
Bond lengths



Bond angles

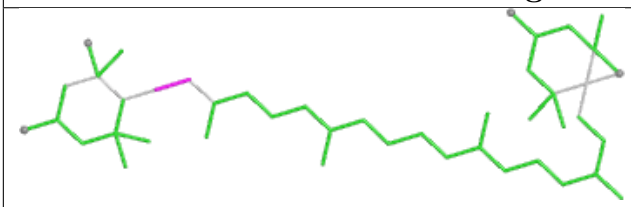


Torsions

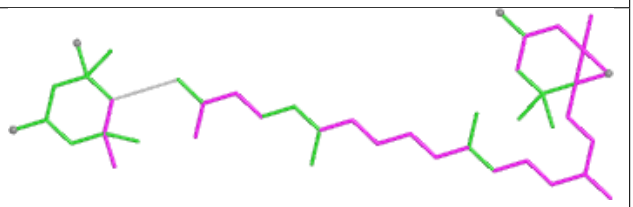


Rings

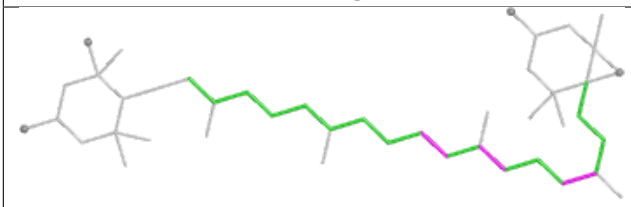
Ligand NEX n 617



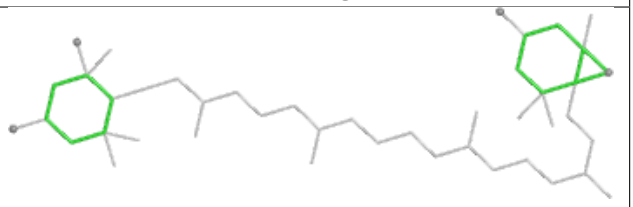
Bond lengths



Bond angles

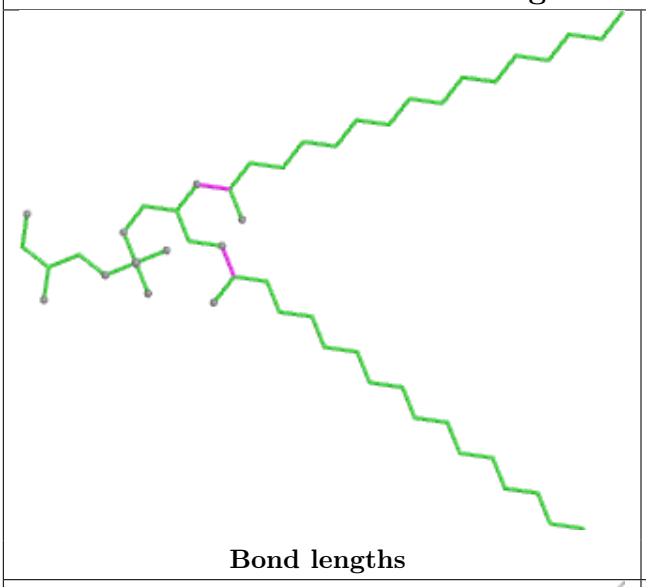


Torsions

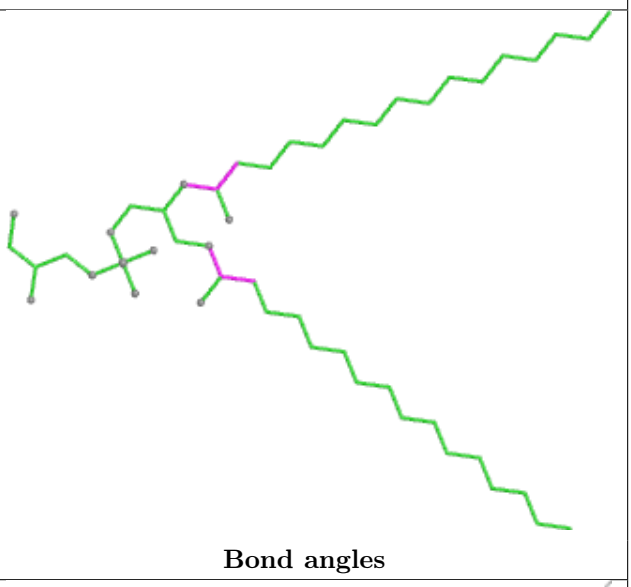


Rings

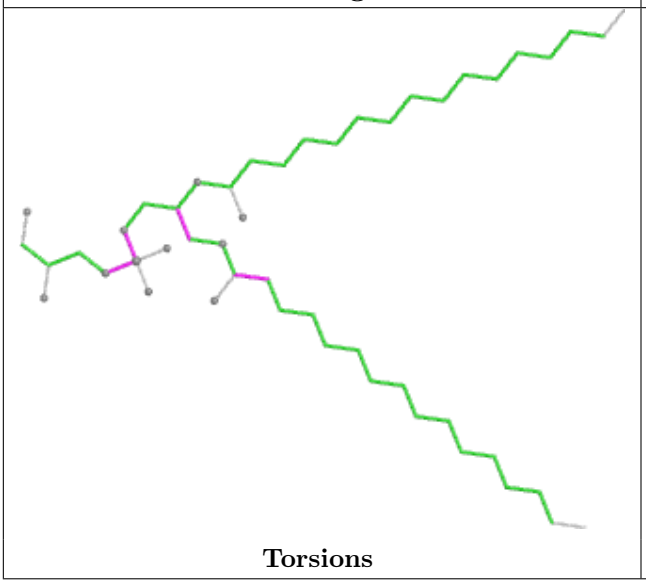
Ligand LHG s 617



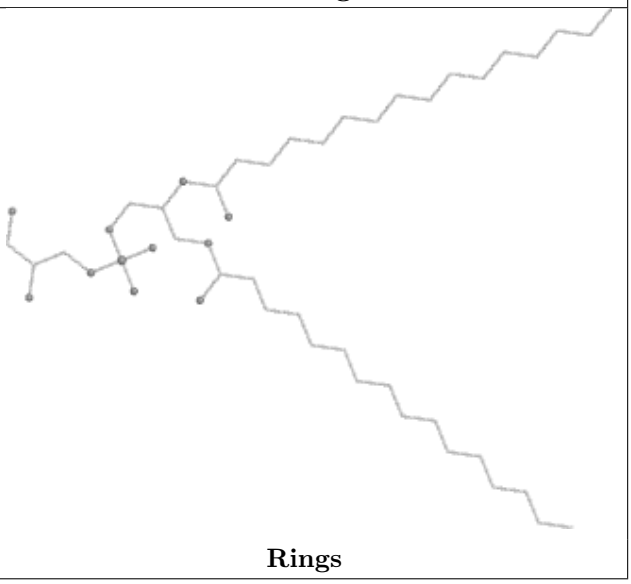
Bond lengths



Bond angles

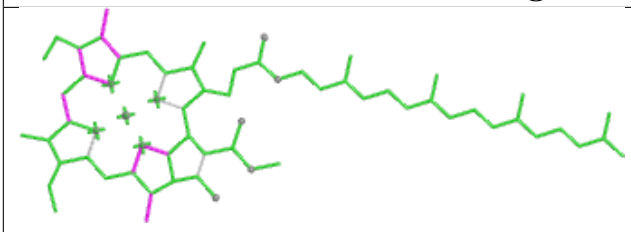


Torsions

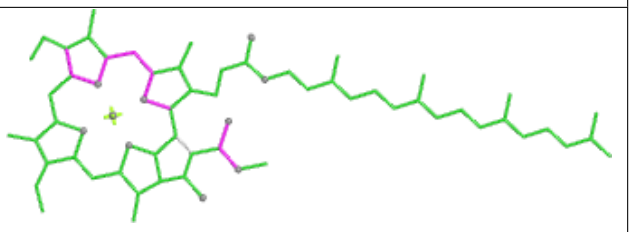


Rings

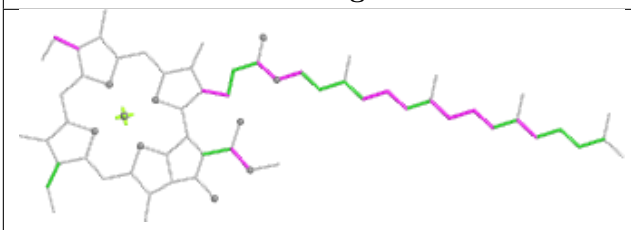
Ligand CLA b 609



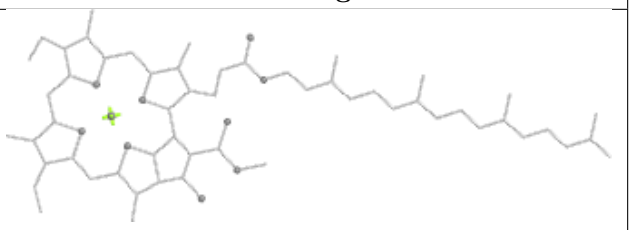
Bond lengths



Bond angles

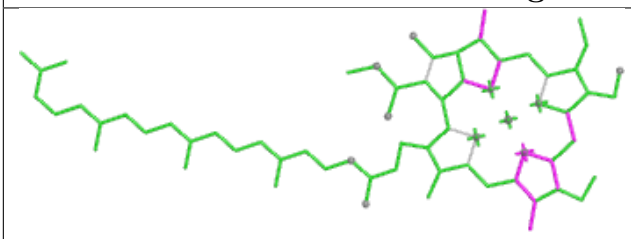


Torsions

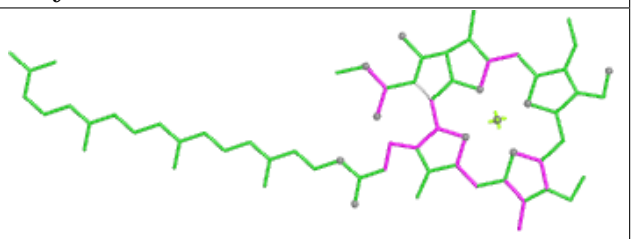


Rings

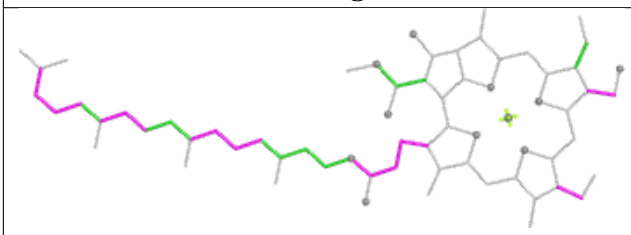
Ligand CHL y 310



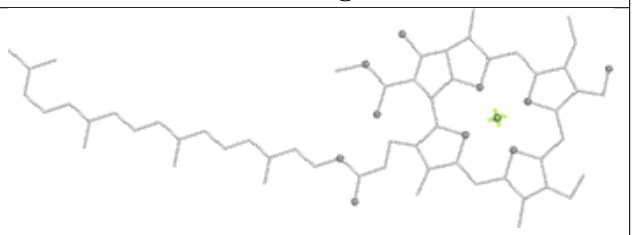
Bond lengths



Bond angles

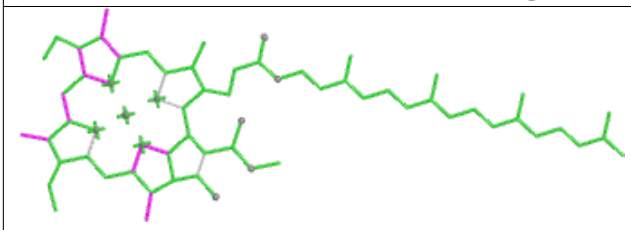


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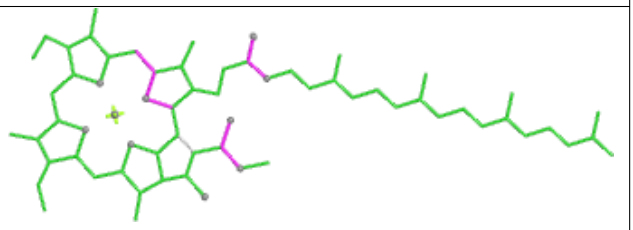


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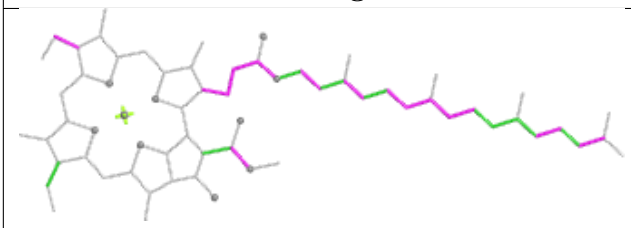
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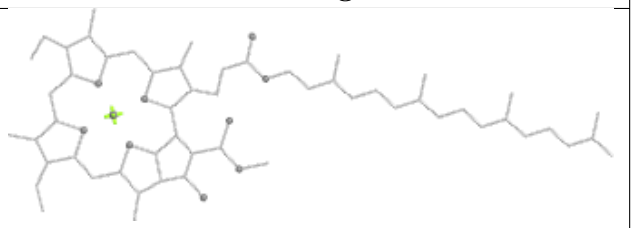
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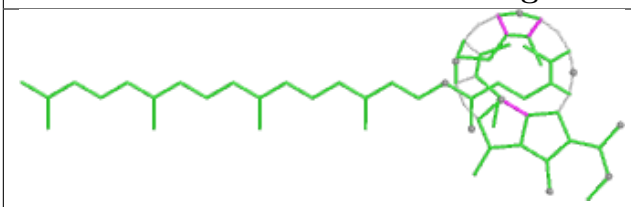


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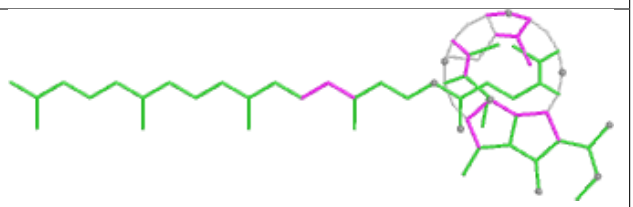


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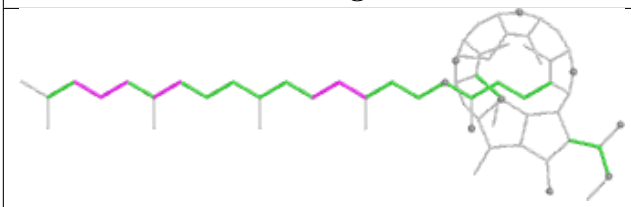
Ligand PHO D 402



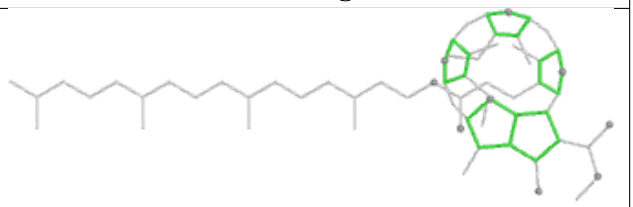
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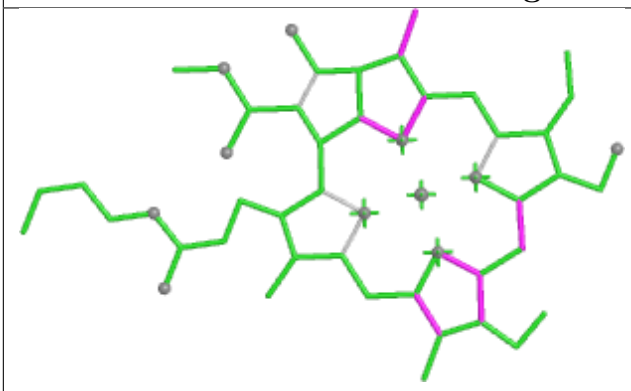


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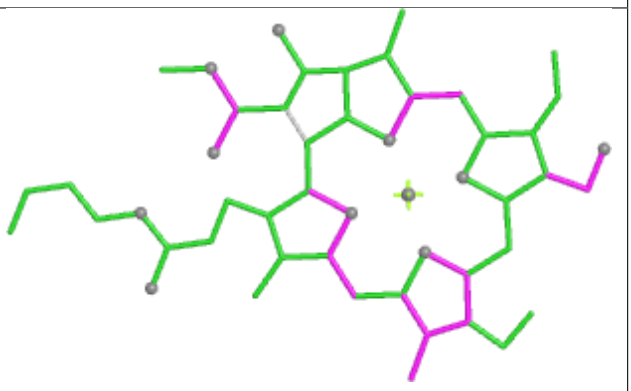


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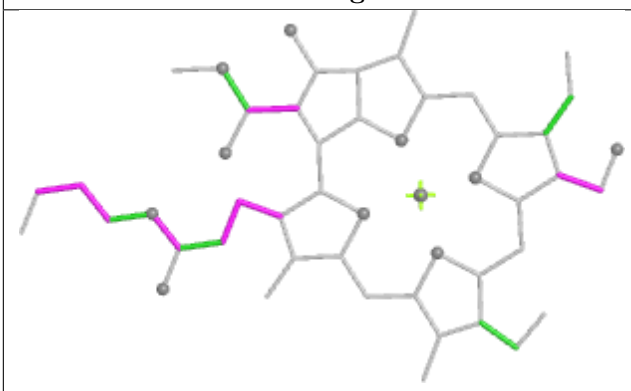
Ligand CHL Y 307



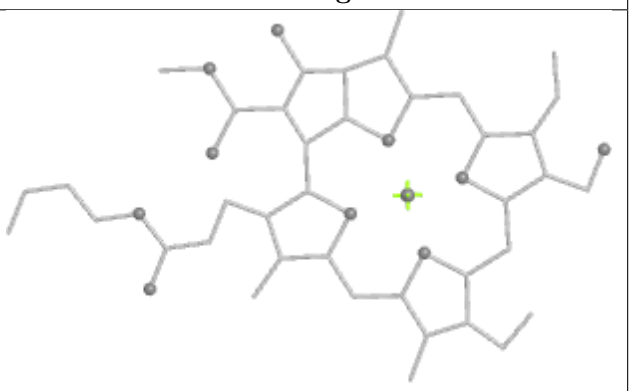
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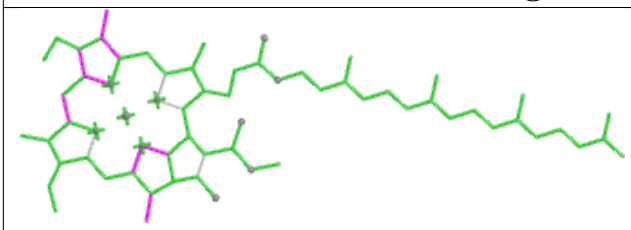


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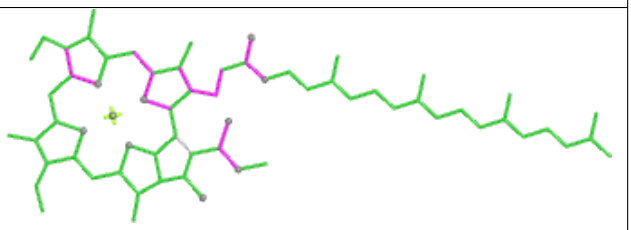


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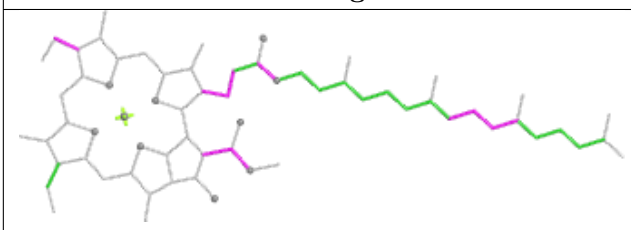
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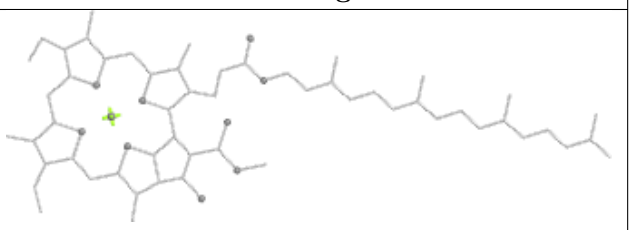
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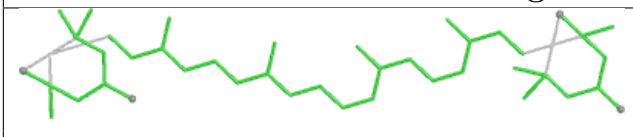


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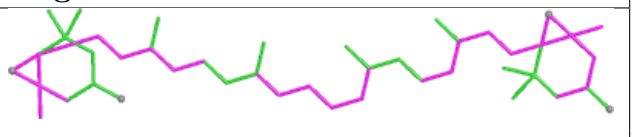


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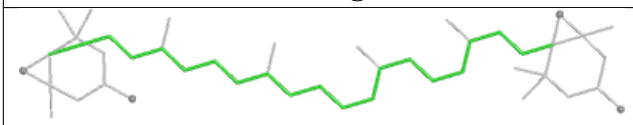
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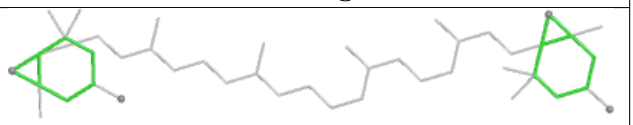
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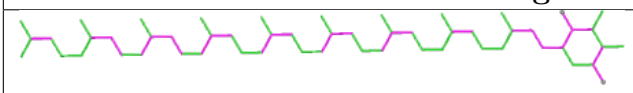


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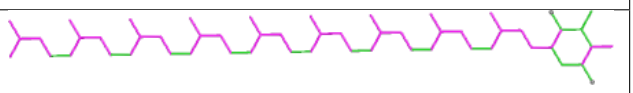


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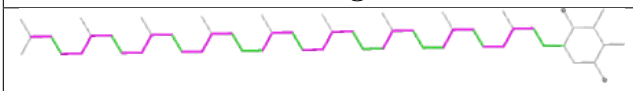
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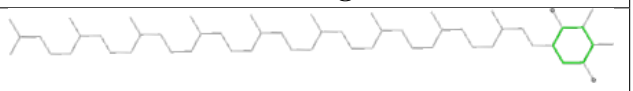
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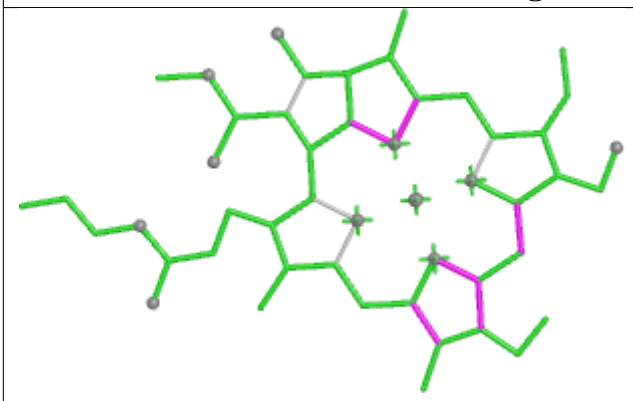


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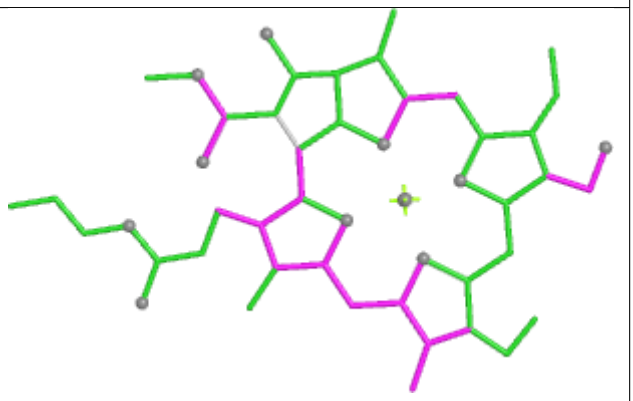


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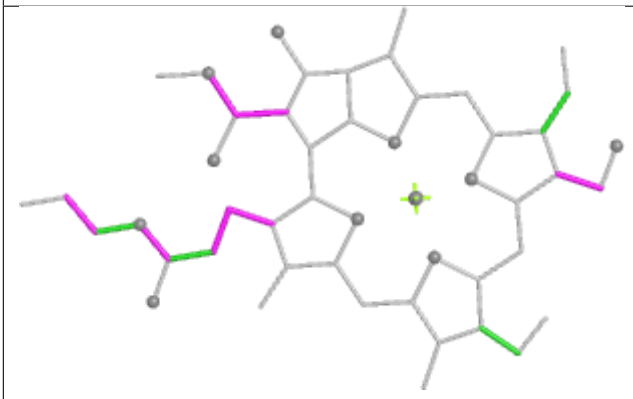
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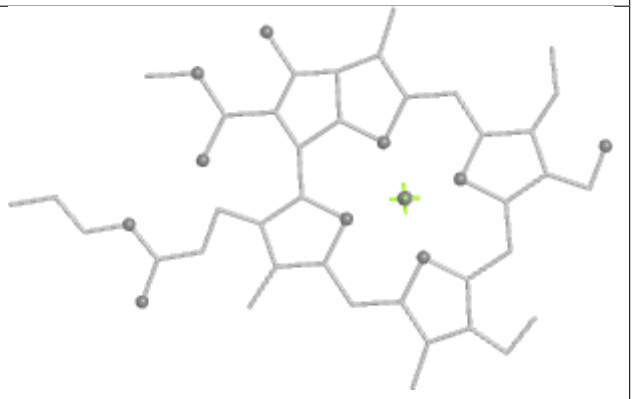
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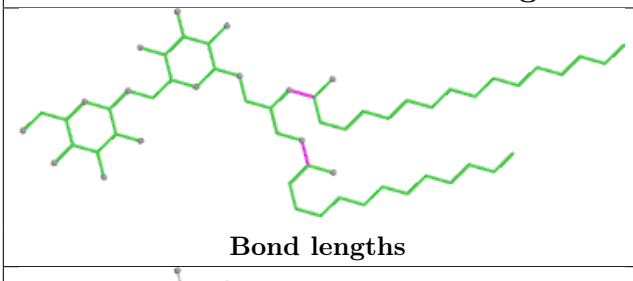


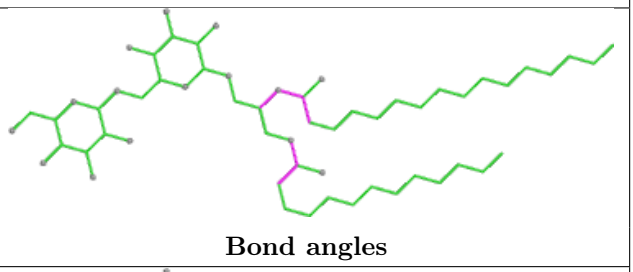
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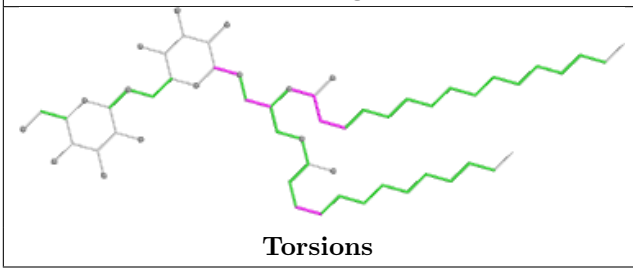


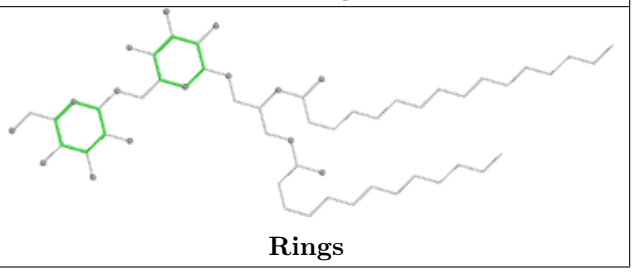
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Ligand DGD A 408

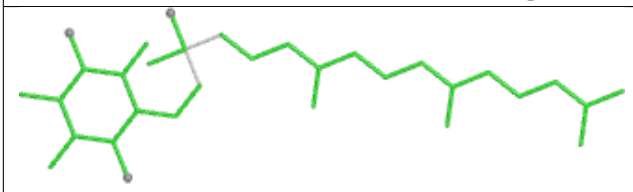

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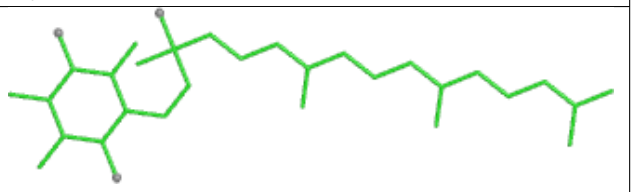

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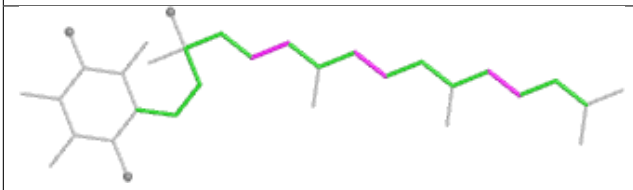

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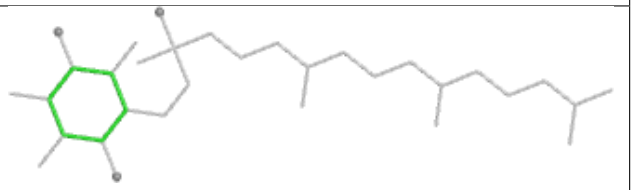

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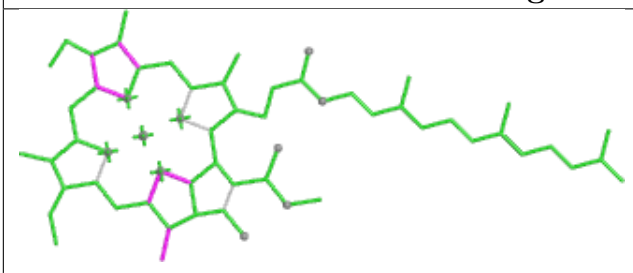

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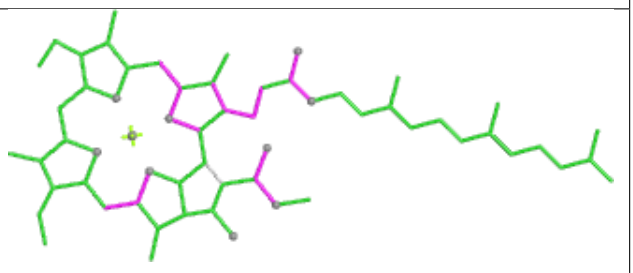

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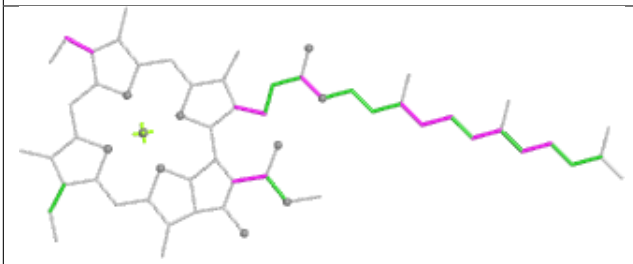

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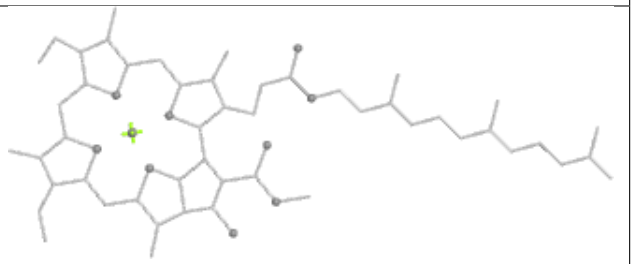

Rings

Ligand CLA n 613

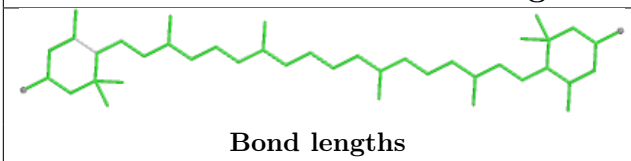

Bond lengths


Bond angles

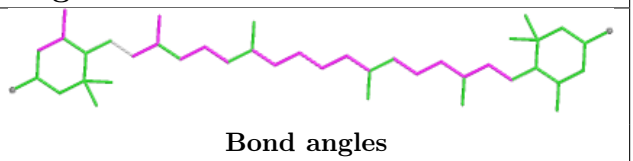

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Rings

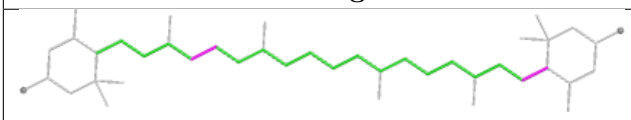
Ligand LUT g 615



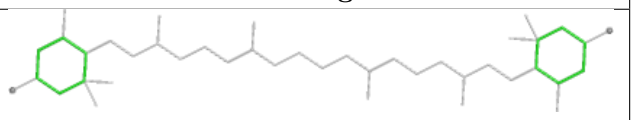
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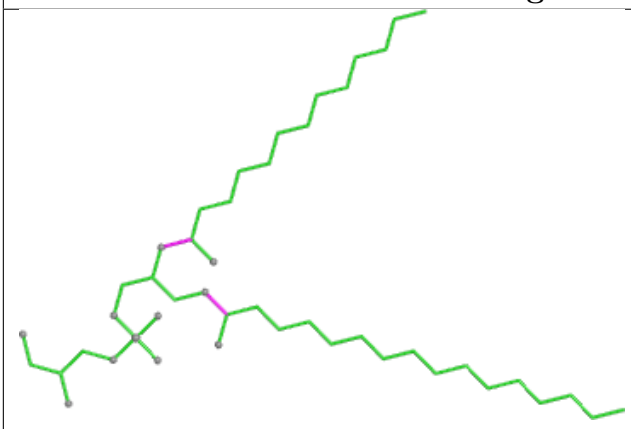


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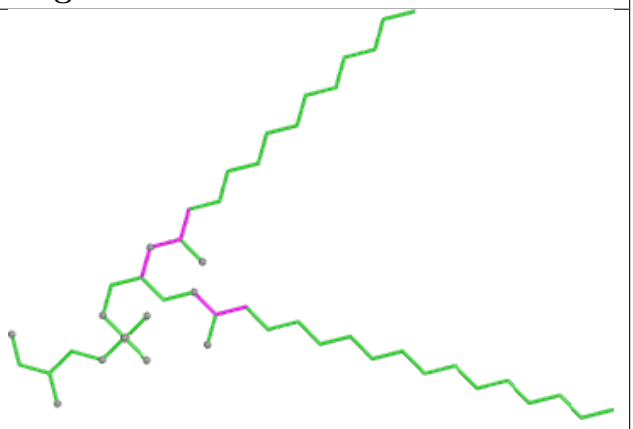


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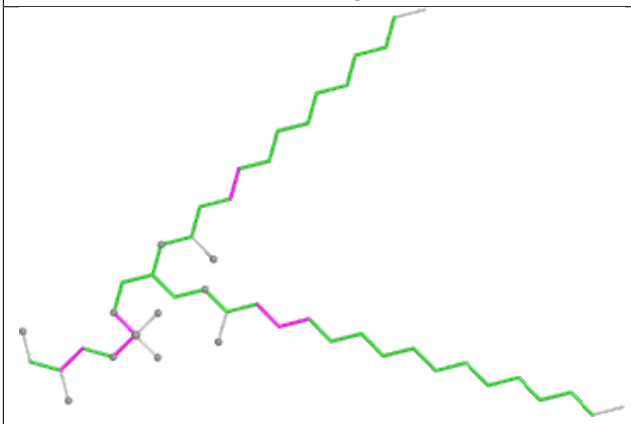
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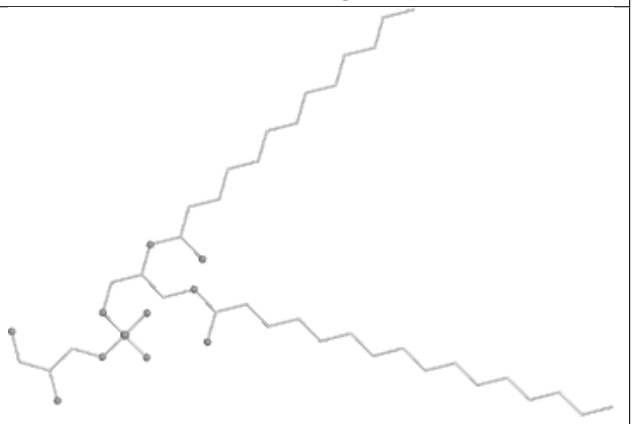
Bond lengths



Bond angles

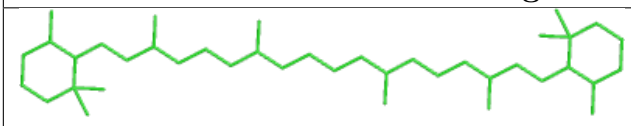


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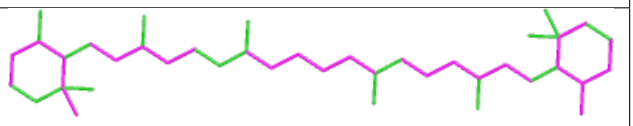


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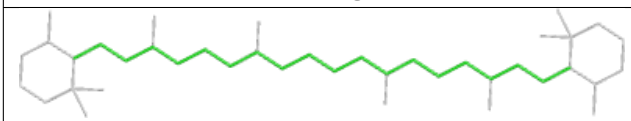
Ligand BCR C 519



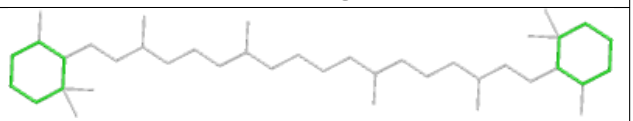
Bond lengths



Bond angles

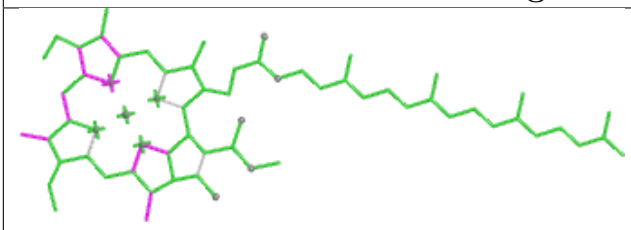


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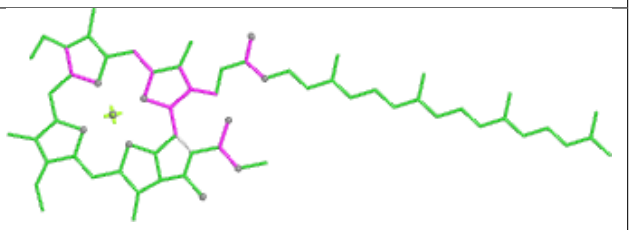


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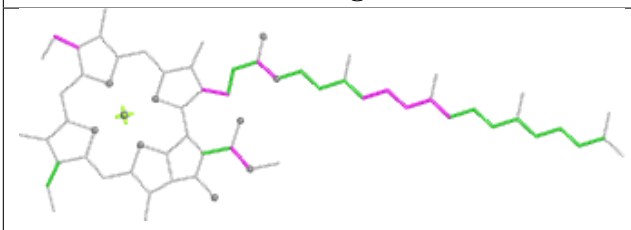
Ligand CLA b 618



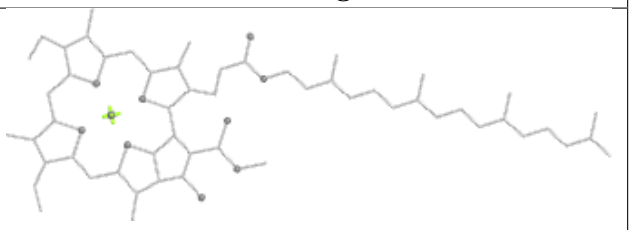
Bond lengths



Bond angles

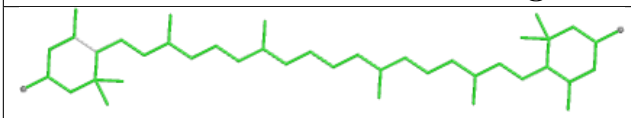


Torsions

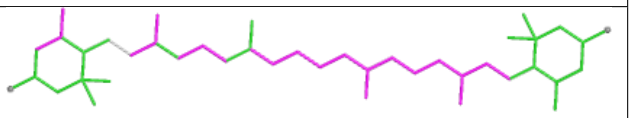


Rings

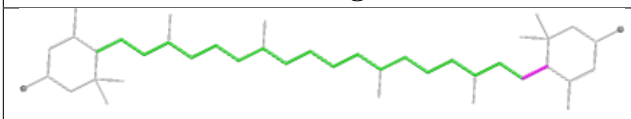
Ligand LUT S 315



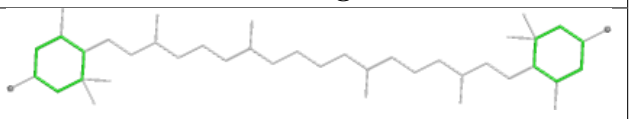
Bond lengths



Bond angles

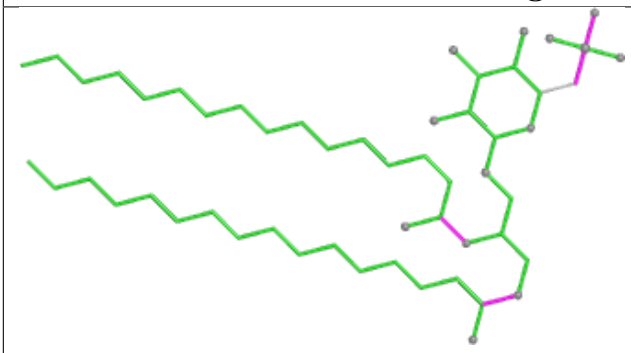


Torsions

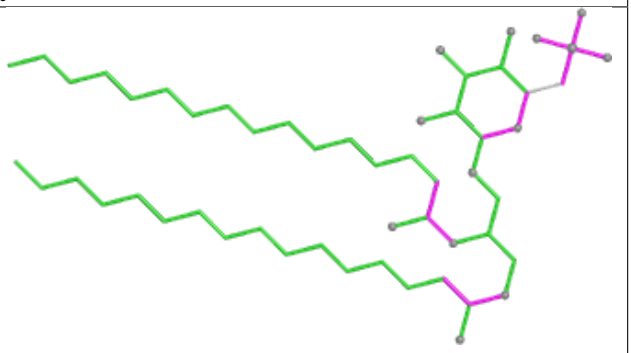


Rings

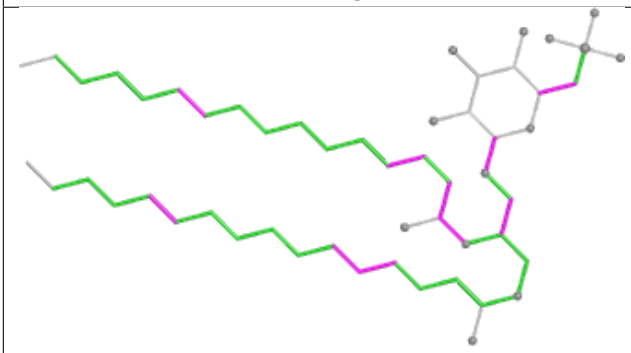
Ligand SQD L 103



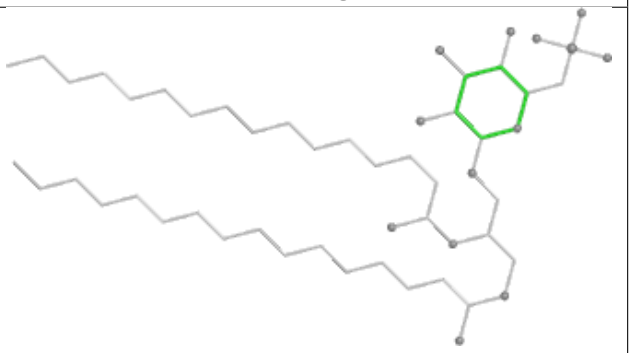
Bond lengths



Bond angles

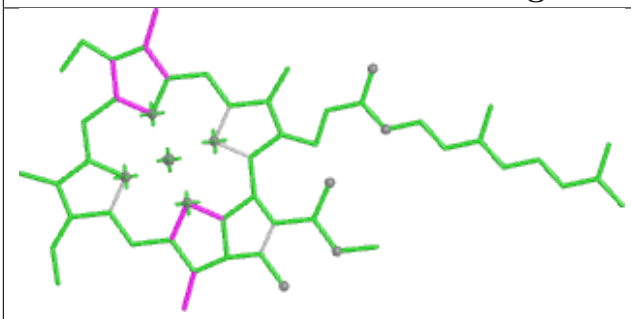


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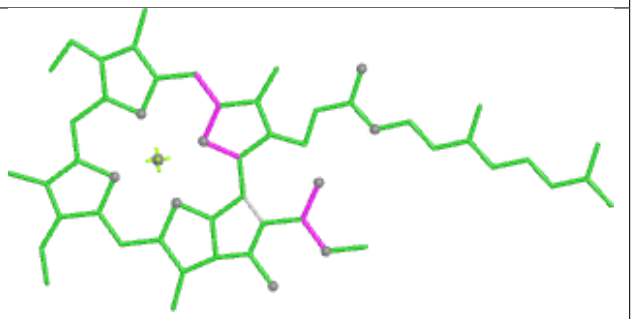


Rings

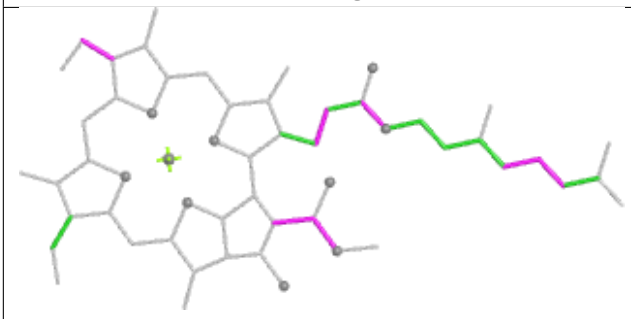
Ligand CLA S 313



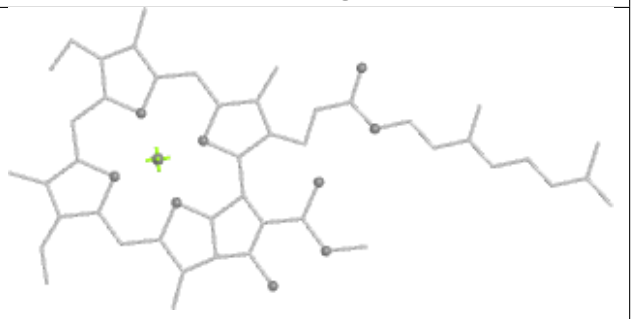
Bond lengths



Bond angles

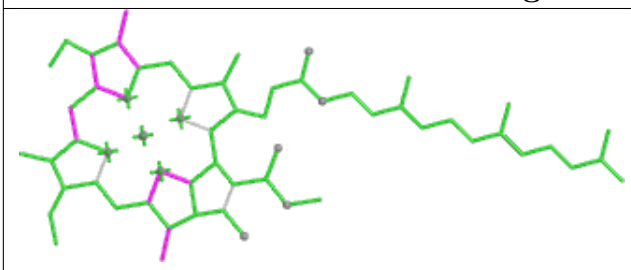


Torsions

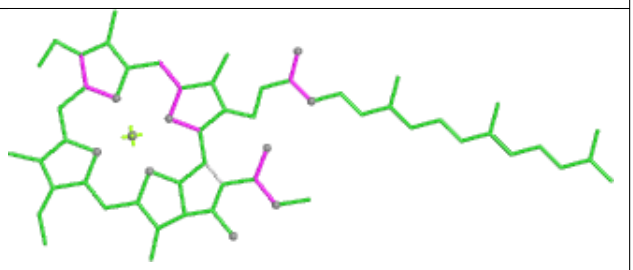


Rings

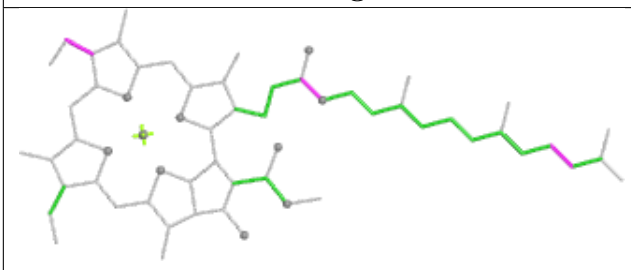
Ligand CLA G 611



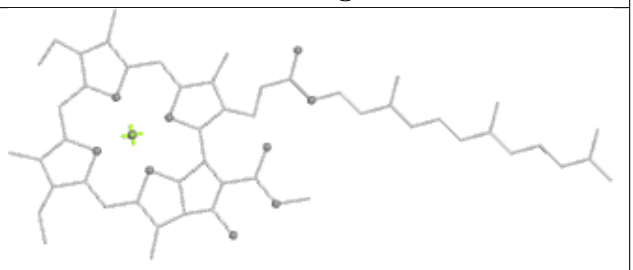
Bond lengths



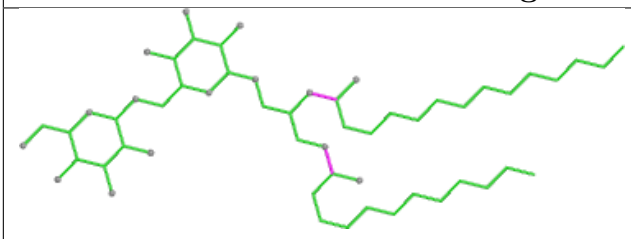
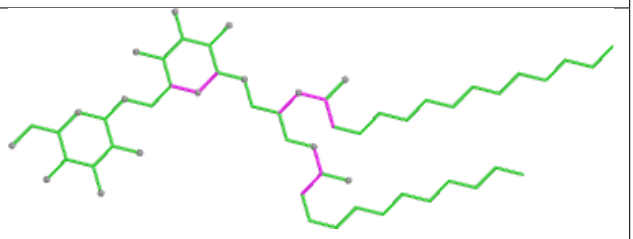
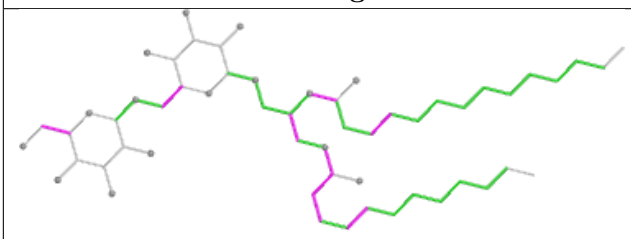
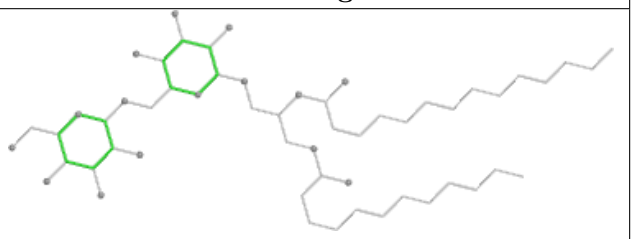
Bond angles

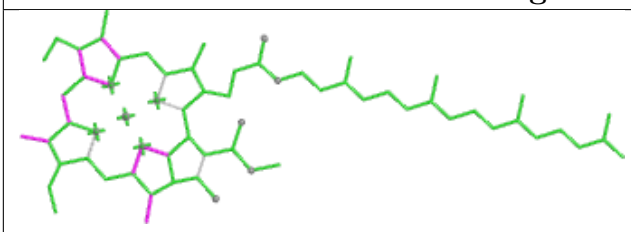
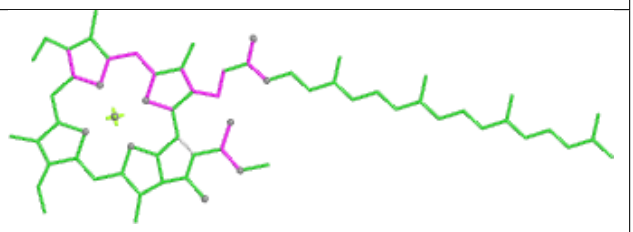
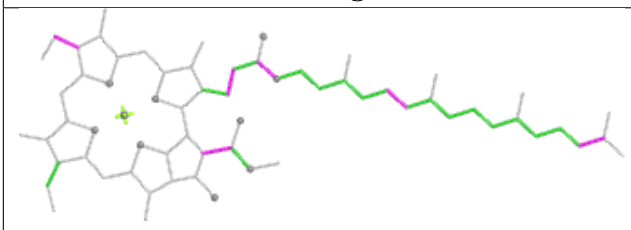
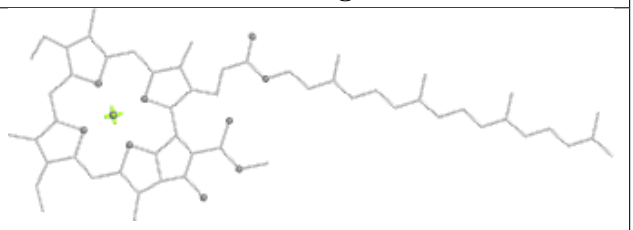


Torsions

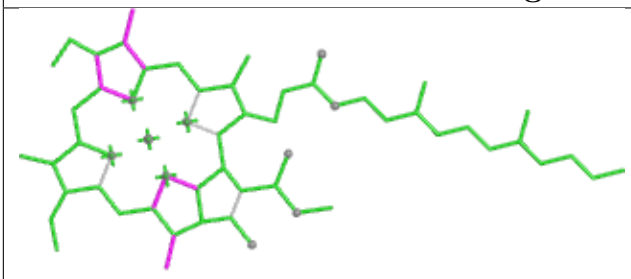


Rings

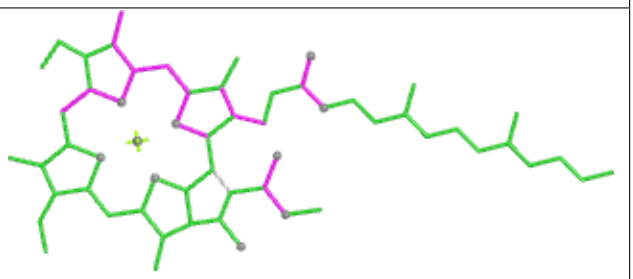
Ligand DGD B 626	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

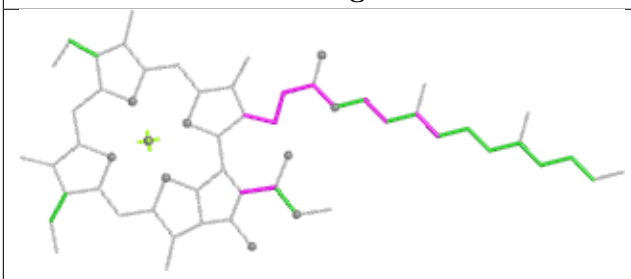
Ligand CLA C 506



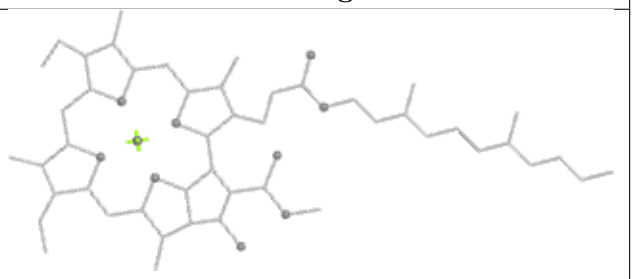
Bond lengths



Bond angles

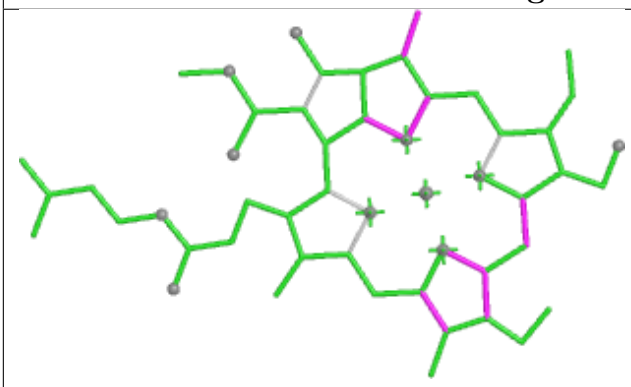


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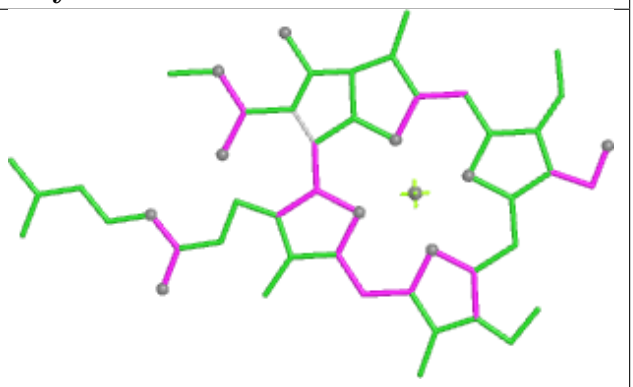


Rings

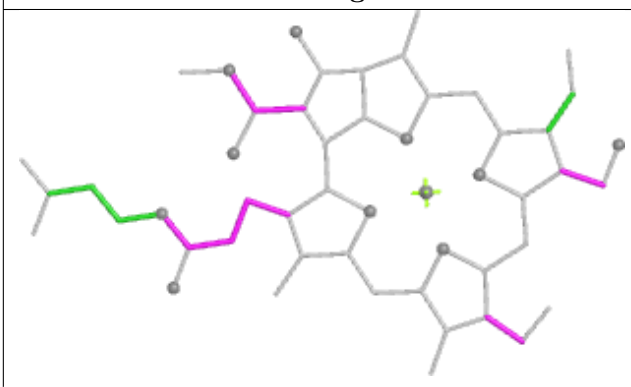
Ligand CHL y 306



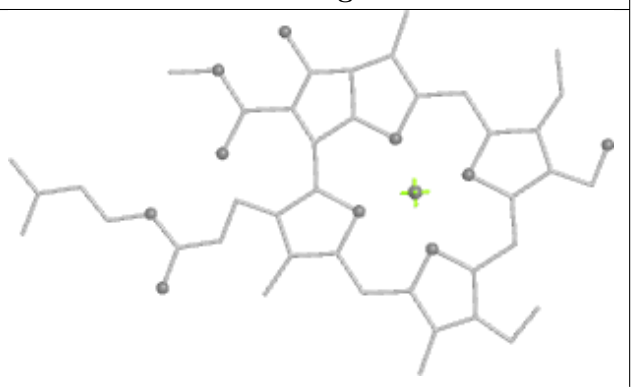
Bond lengths



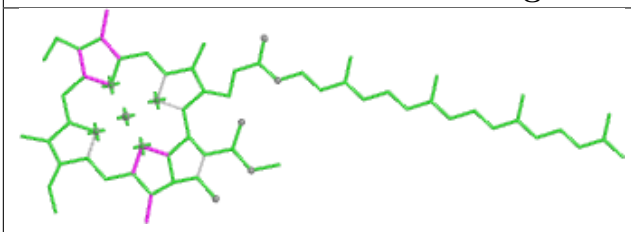
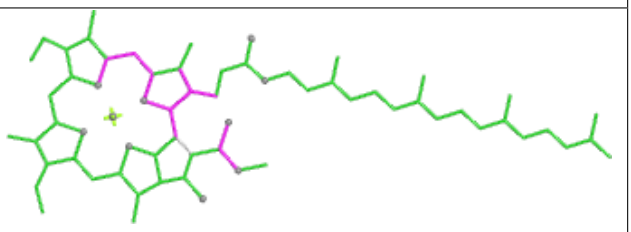
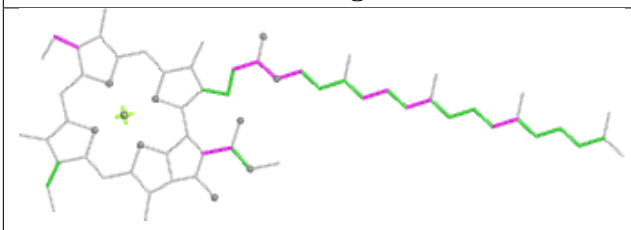
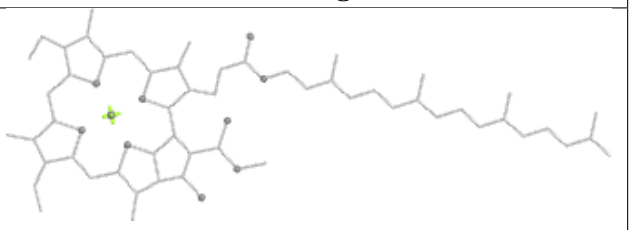
Bond angles

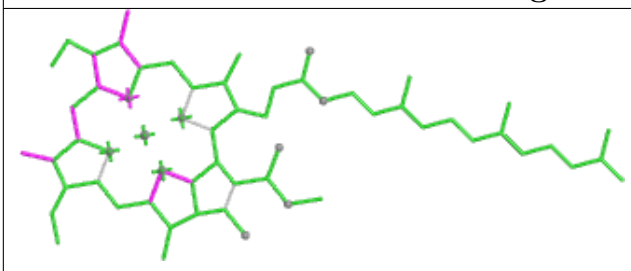
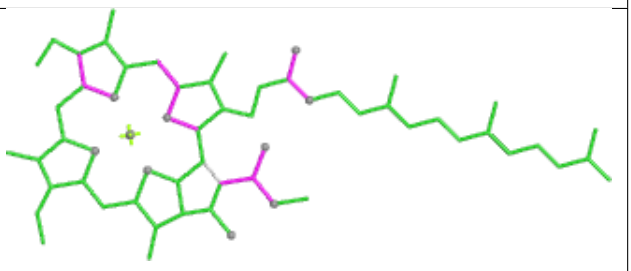
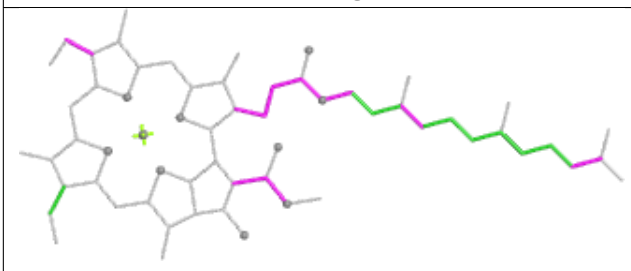
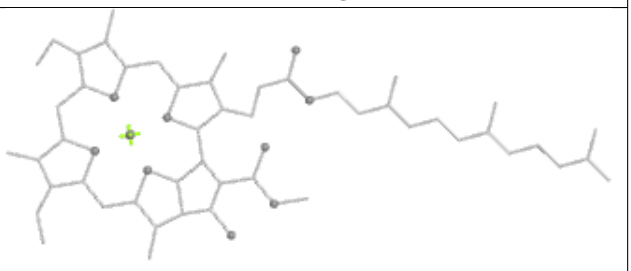


Torsions

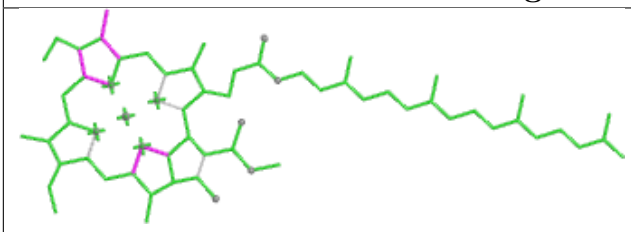


Rings

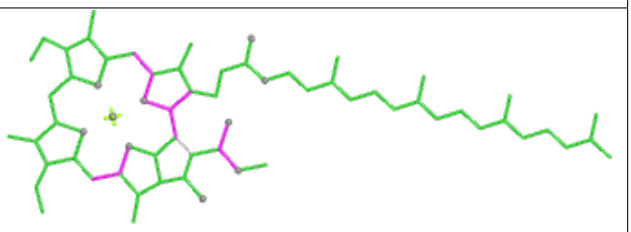
Ligand CLA Y 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

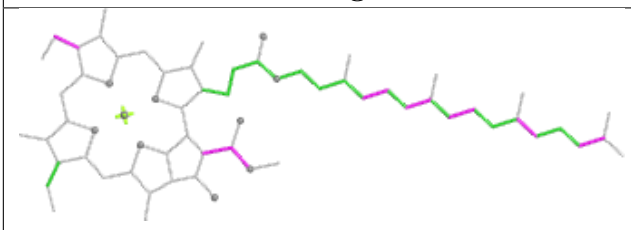
Ligand CLA C 512



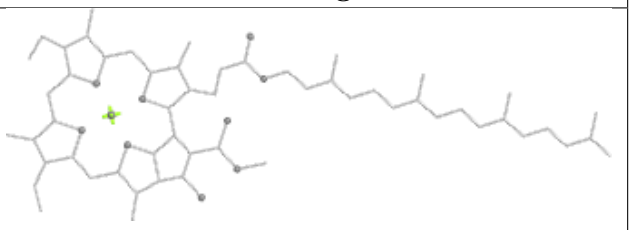
Bond lengths



Bond angles



Torsions



Rings

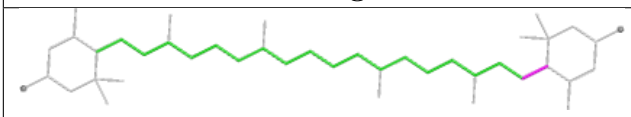
Ligand LUT y 316



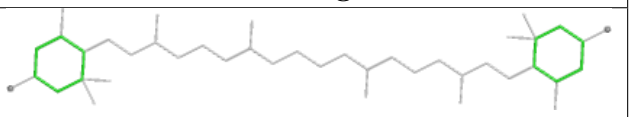
Bond lengths



Bond angles

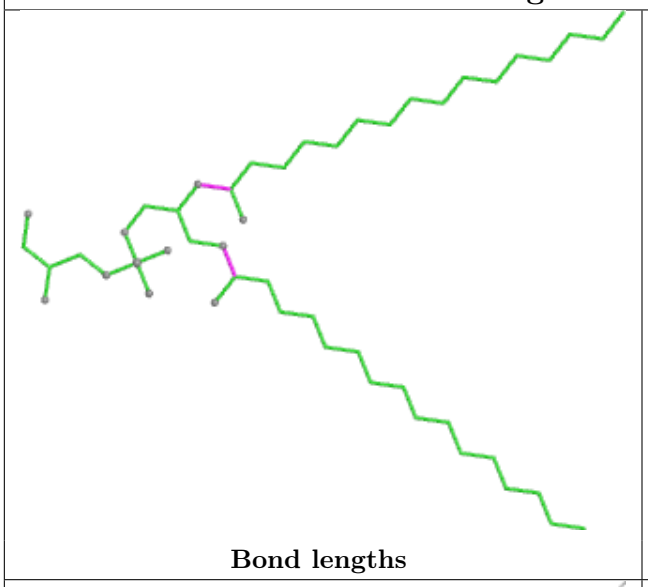


Torsions

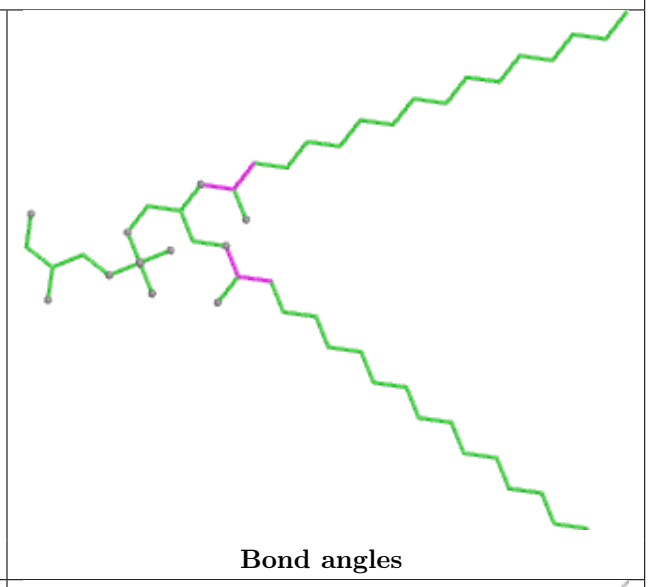


Rings

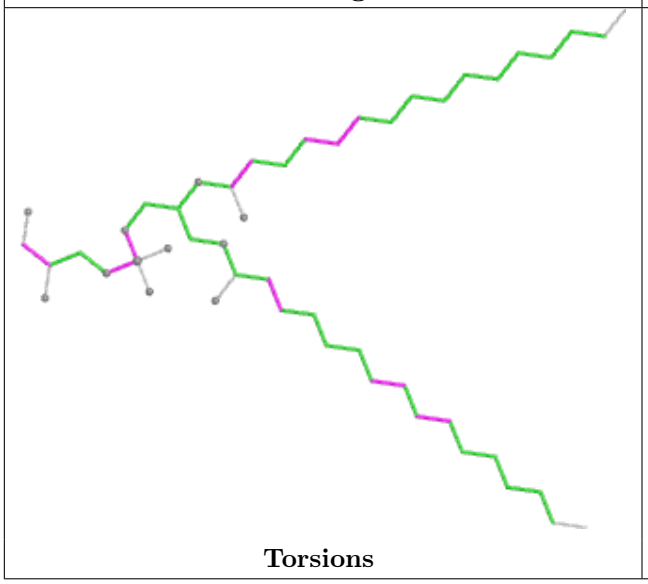
Ligand LHG d 407



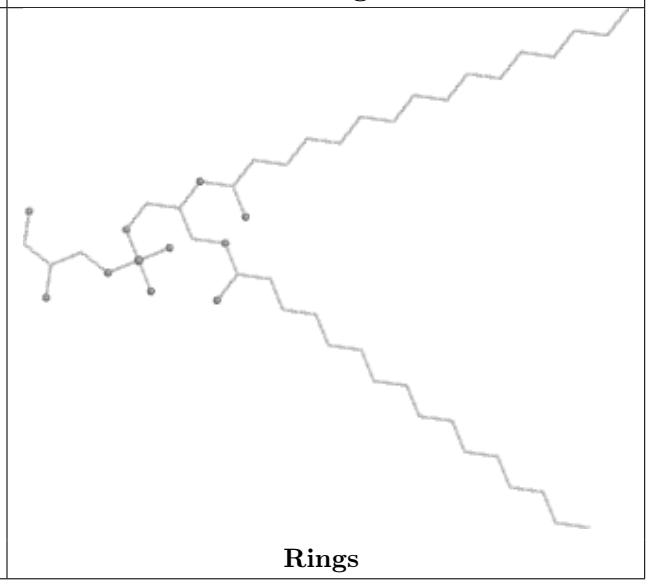
Bond lengths



Bond angles

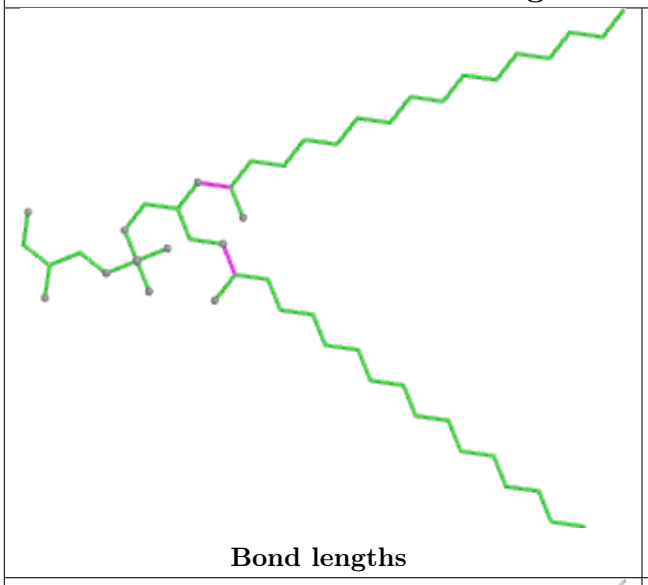


Torsions

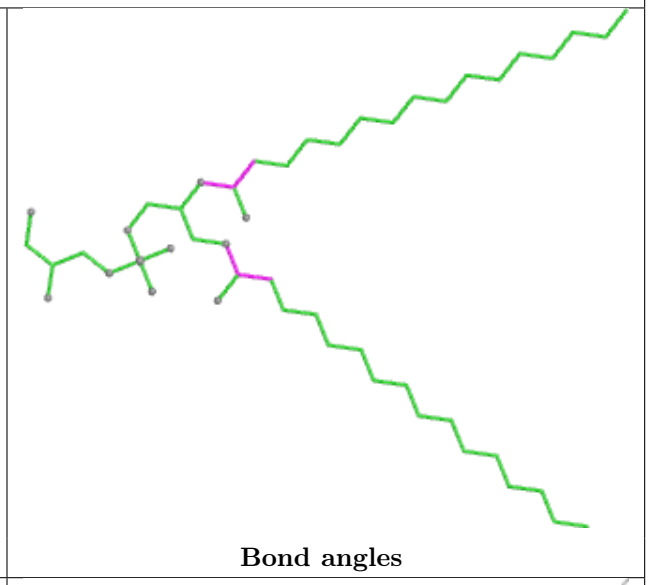


Rings

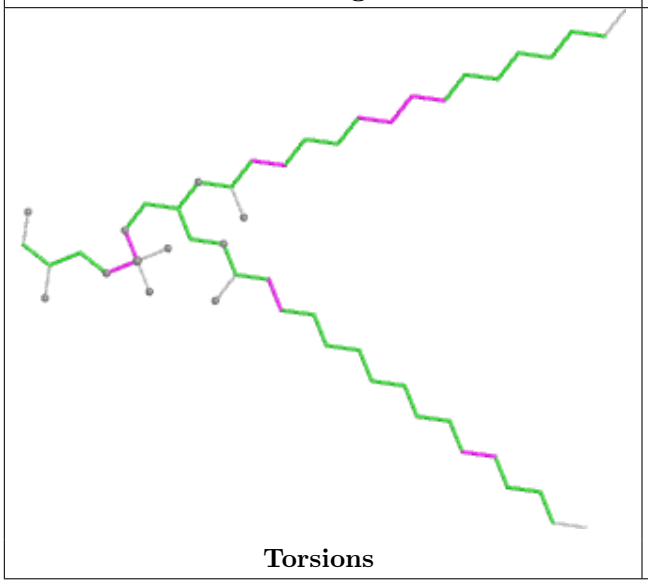
Ligand LHG d 408



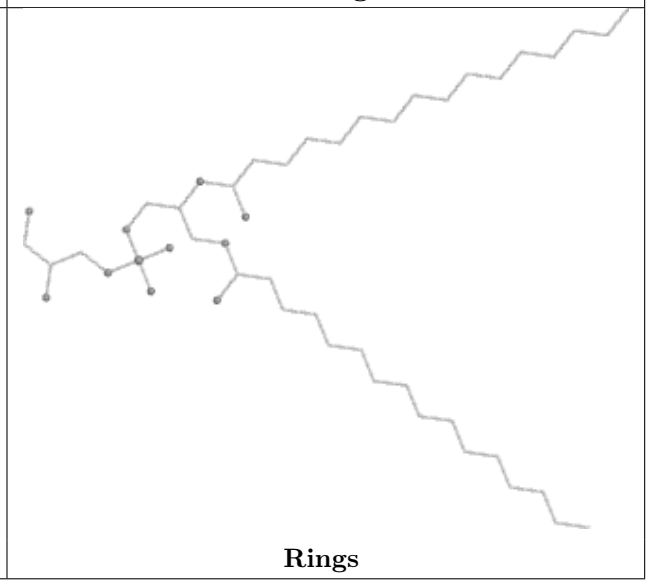
Bond lengths



Bond angles

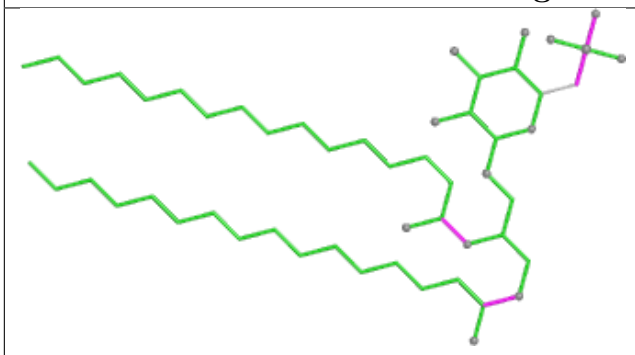


Torsions

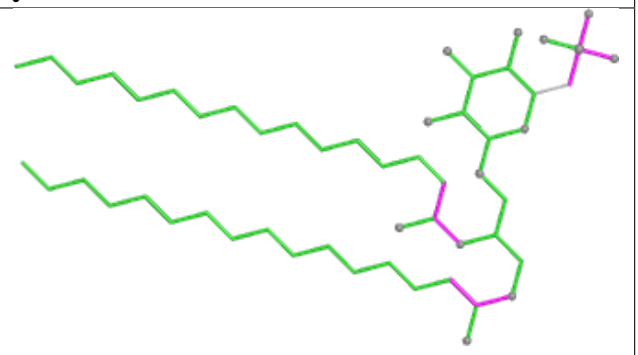


Rings

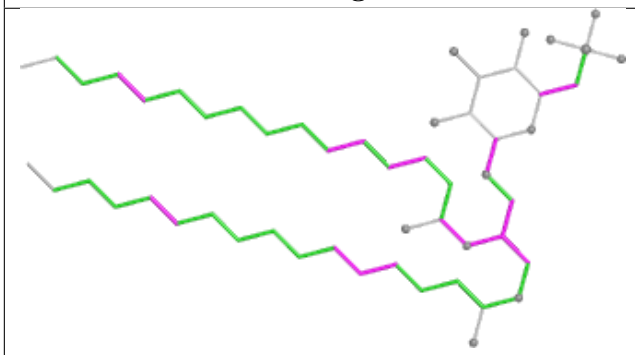
Ligand SQD l 101



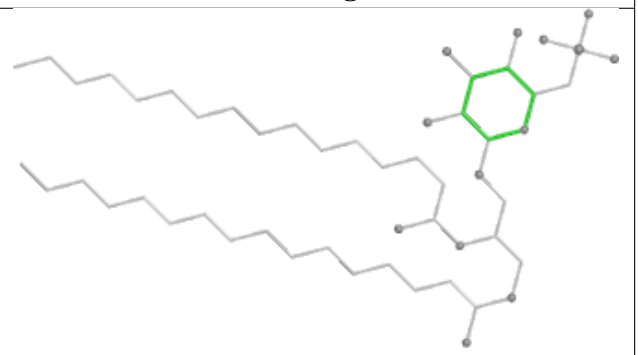
Bond lengths



Bond angles



Torsions

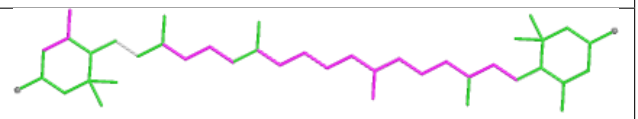


Rings

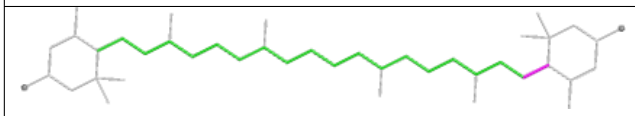
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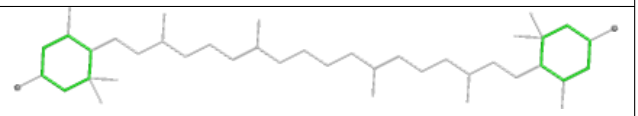
Bond lengths



Bond angles

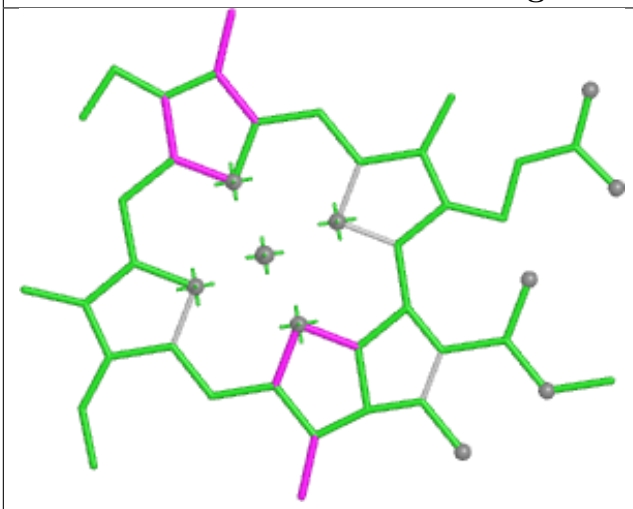


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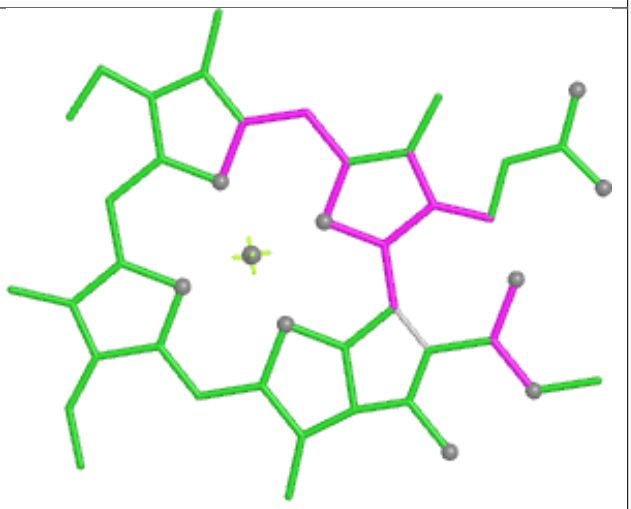


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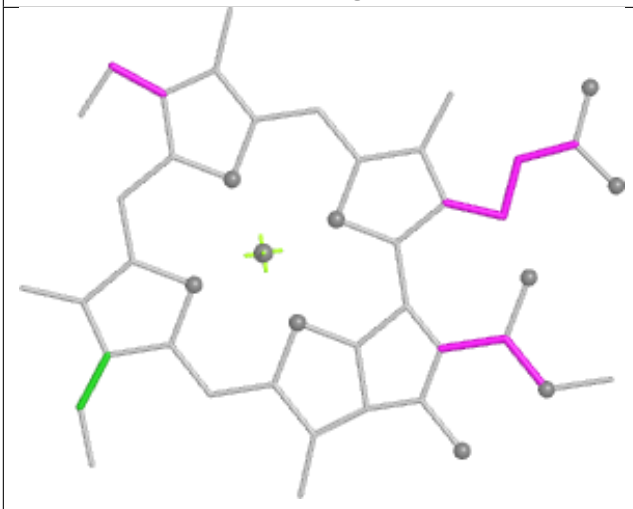
Ligand CLA n 612



Bond lengths



Bond angles

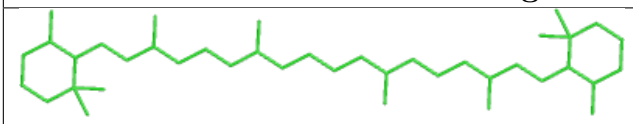


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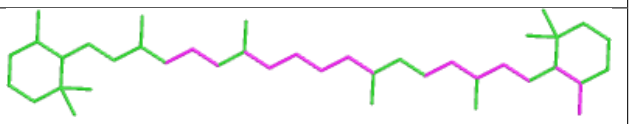


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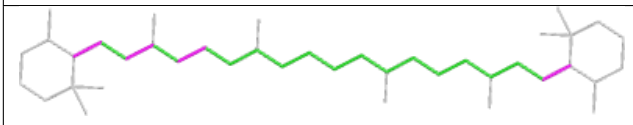
Ligand BCR H 101



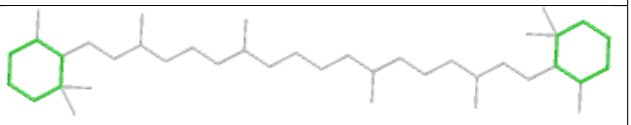
Bond lengths



Bond angles

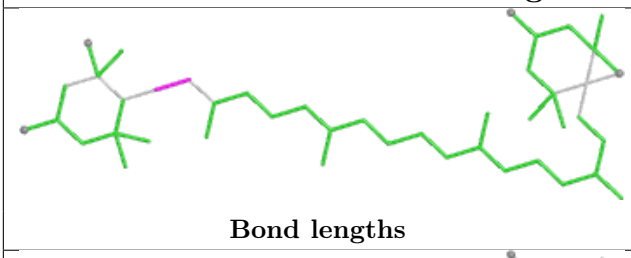


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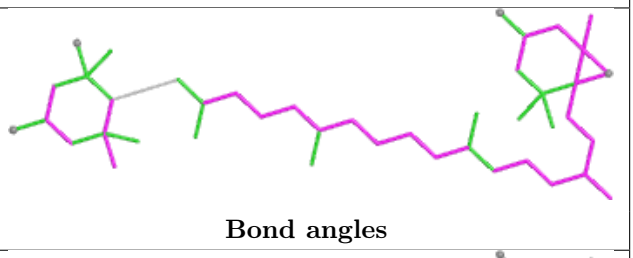


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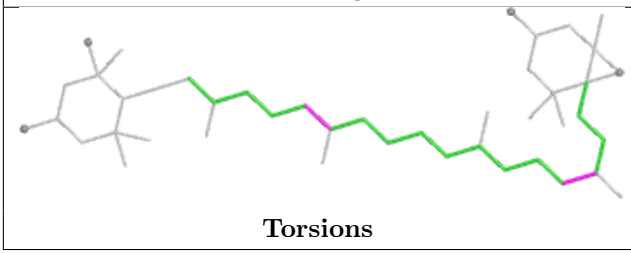
Ligand NEX S 317



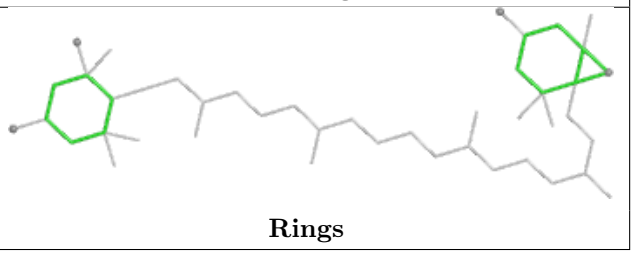
Bond lengths



Bond angles

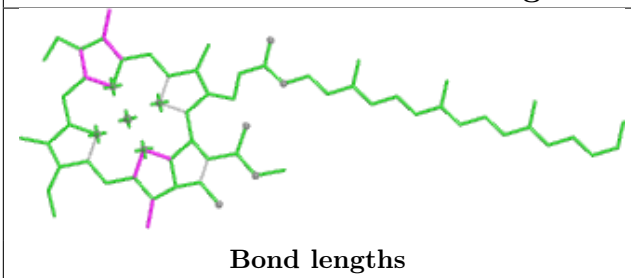


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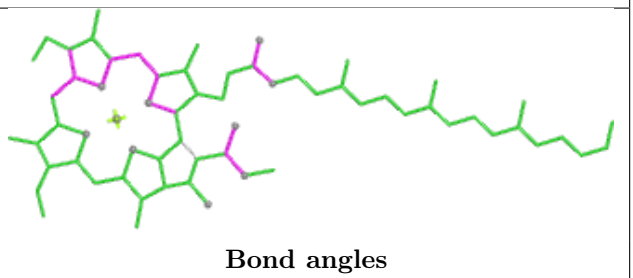


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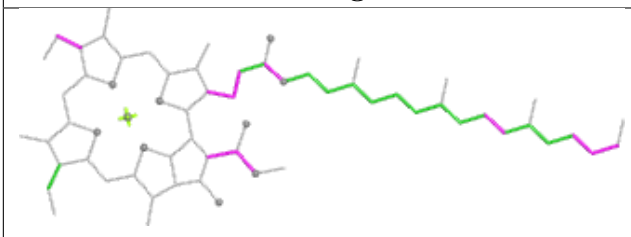
Ligand CLA G 610



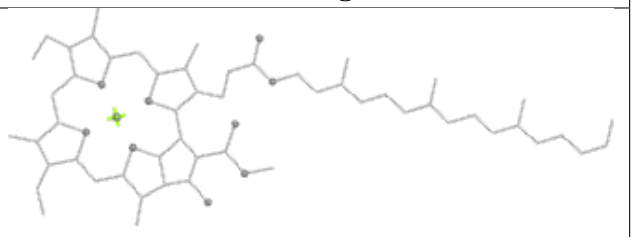
Bond lengths



Bond angles

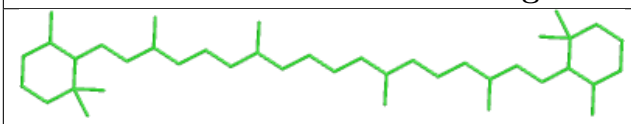


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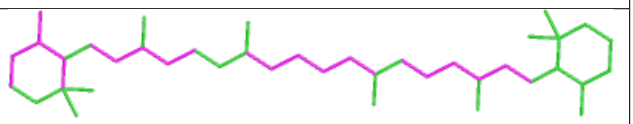


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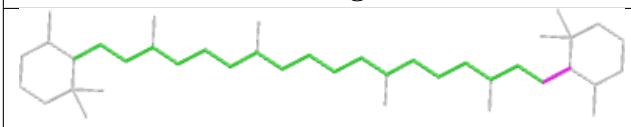
Ligand BCR A 405



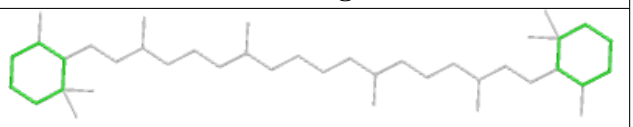
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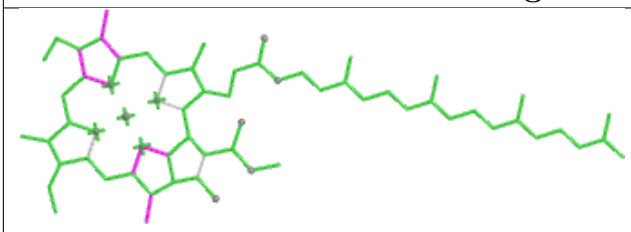


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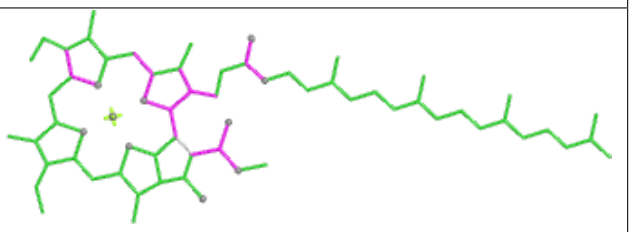


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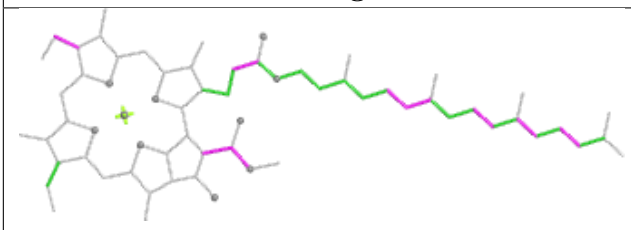
Ligand CLA B 615



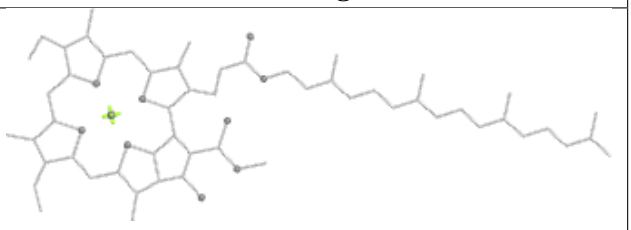
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Bond angles

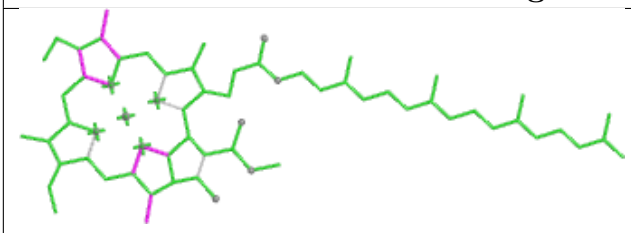


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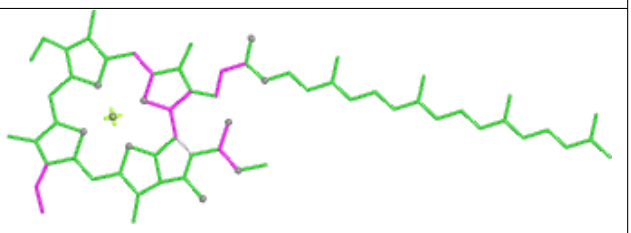


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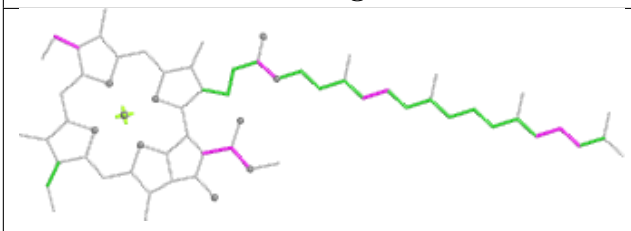
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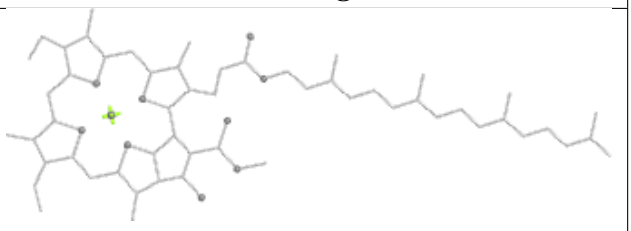
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Bond angles

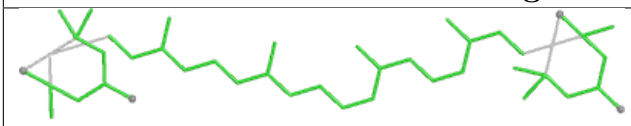


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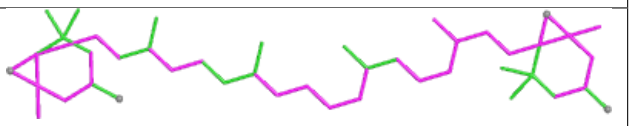


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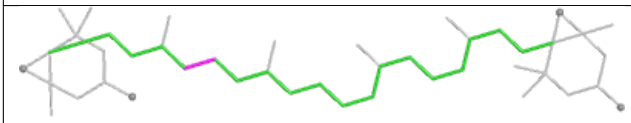
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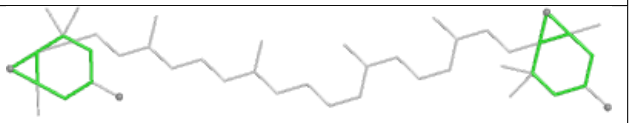
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Bond angles

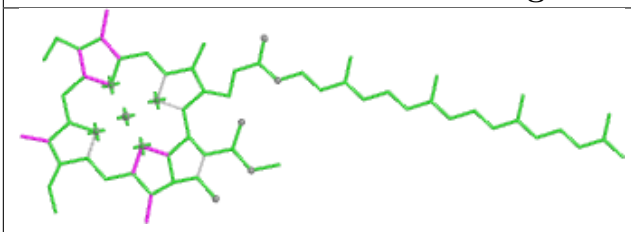


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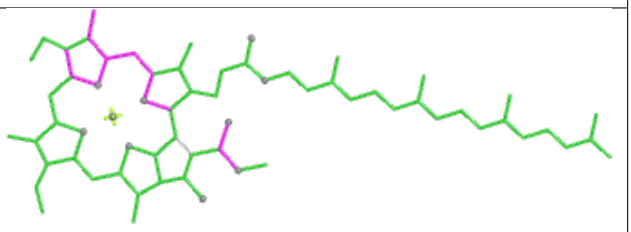


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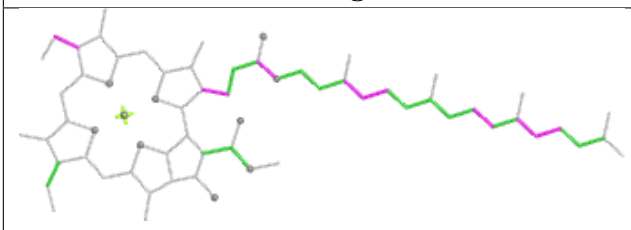
Ligand CLA b 613



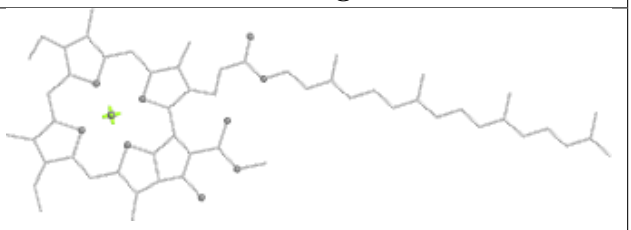
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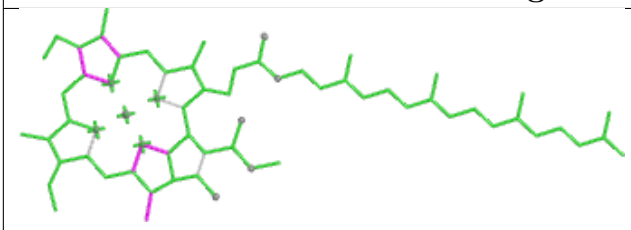


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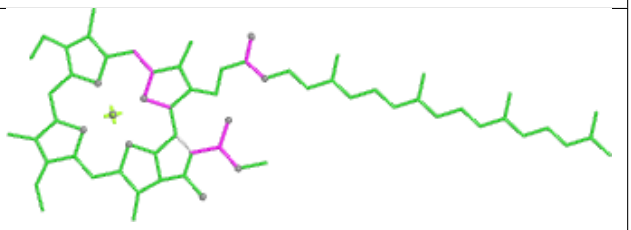


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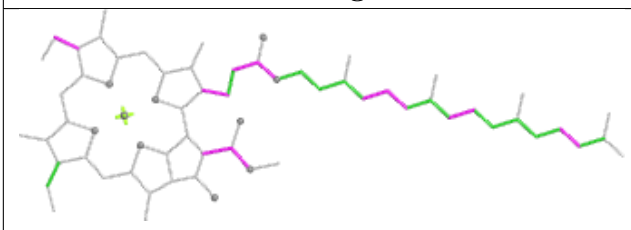
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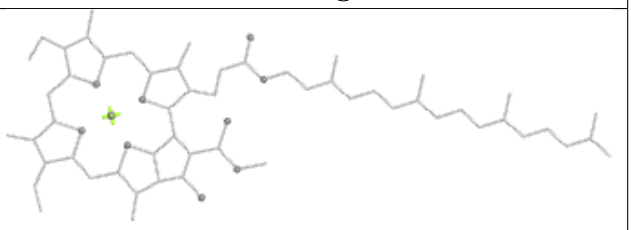
Bond lengths



Bond angles

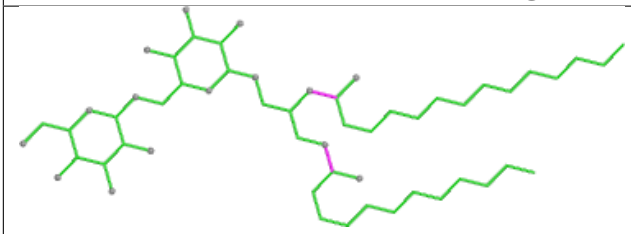


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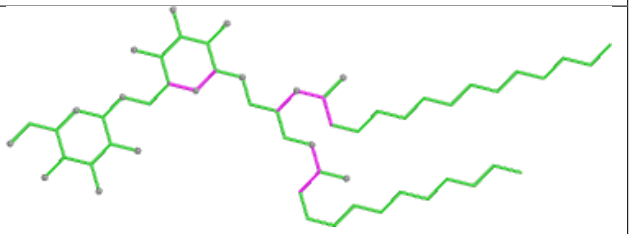


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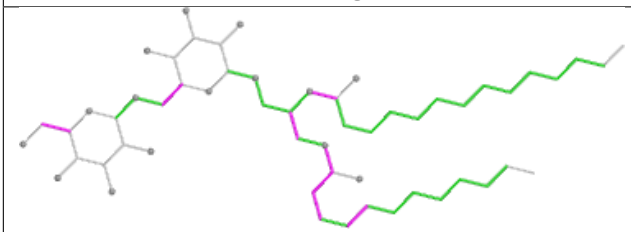
Ligand DGD b 625



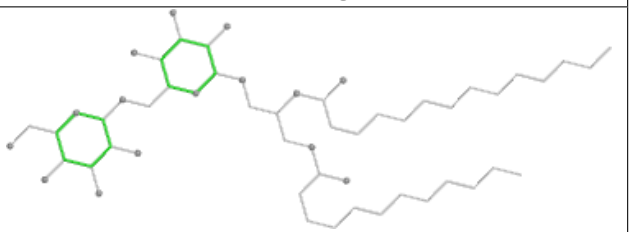
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Bond angles

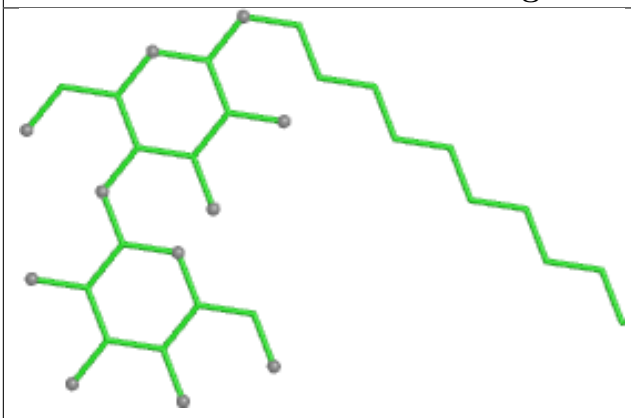


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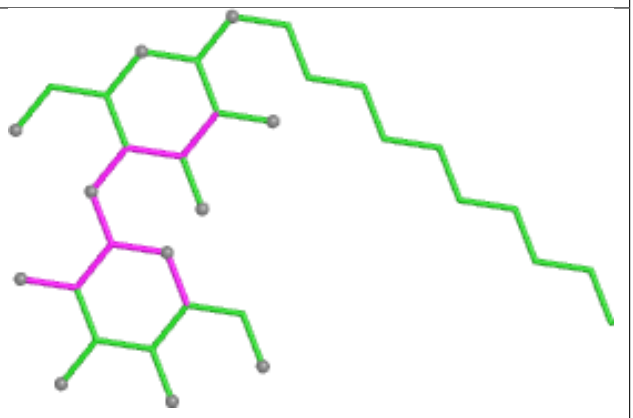


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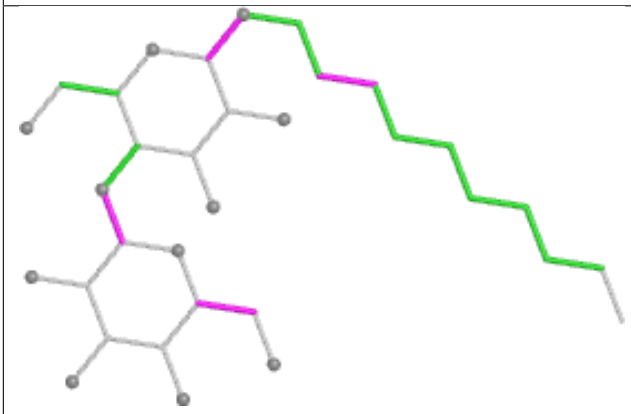
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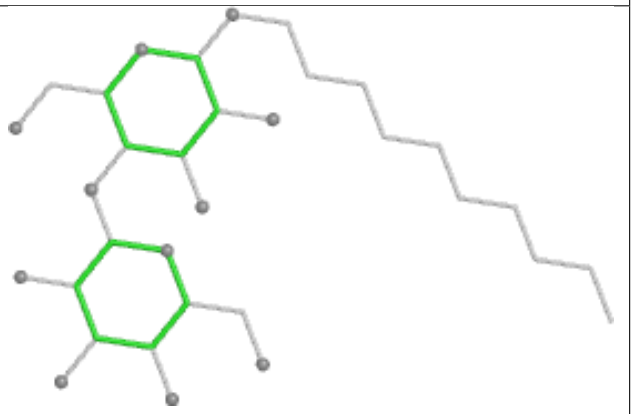
Bond lengths



Bond angles

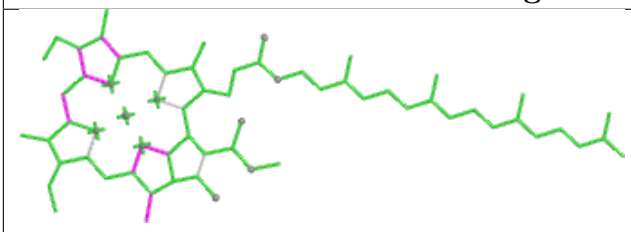


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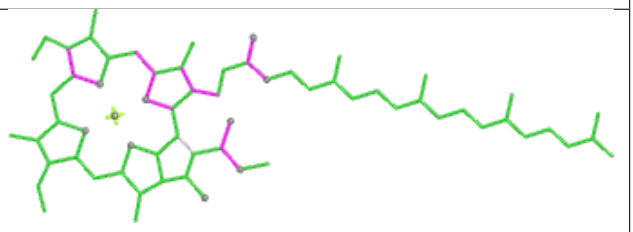


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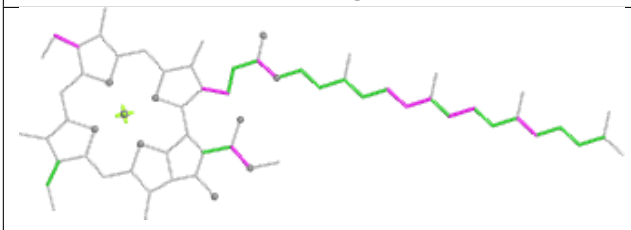
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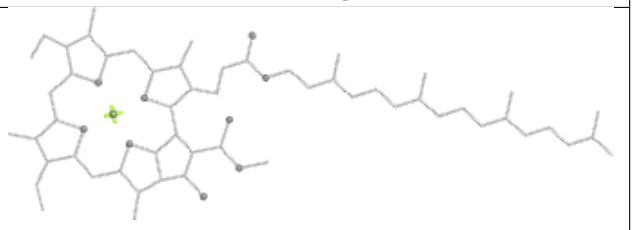
Bond lengths



Bond angles

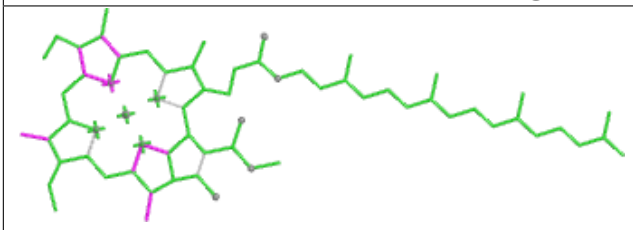


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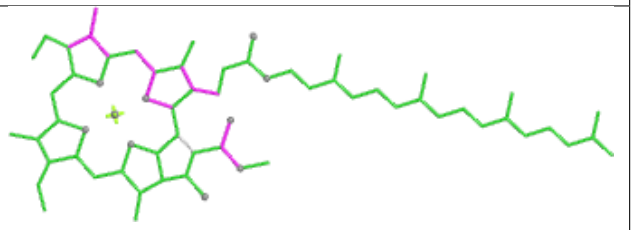


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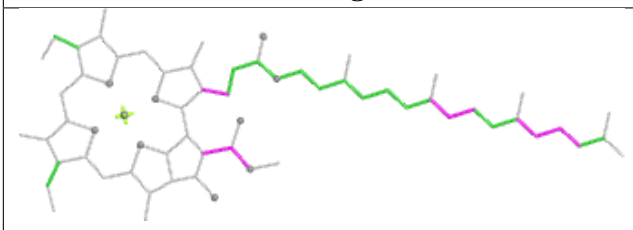
Ligand CLA b 612



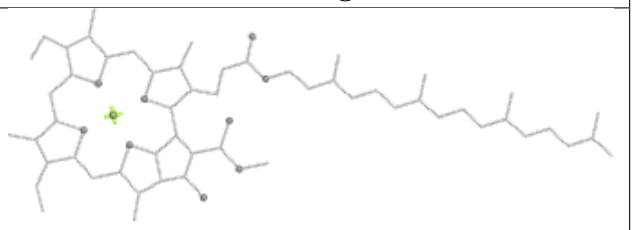
Bond lengths



Bond angles

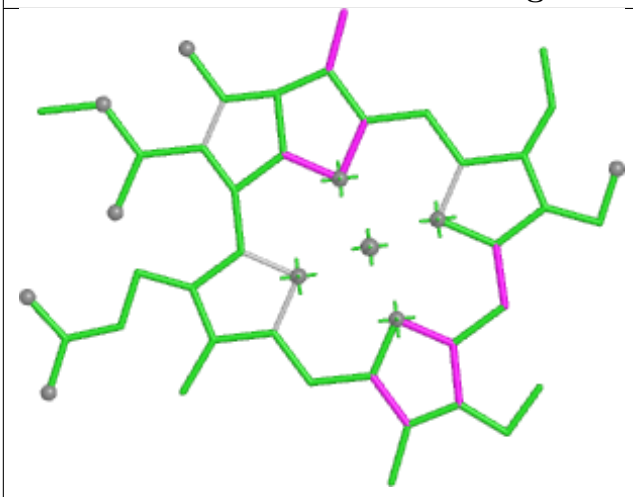


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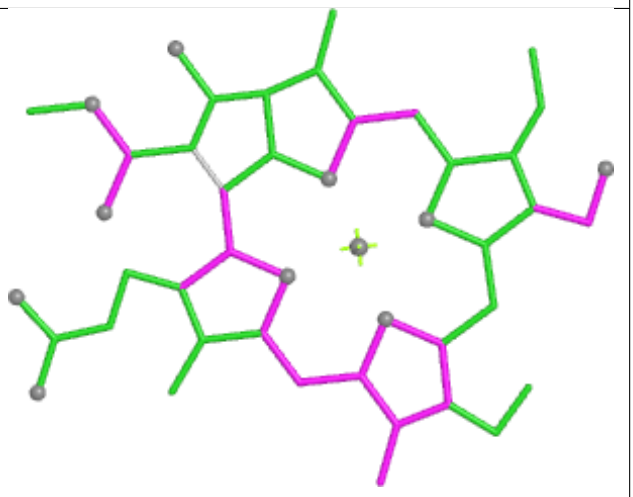


Rings

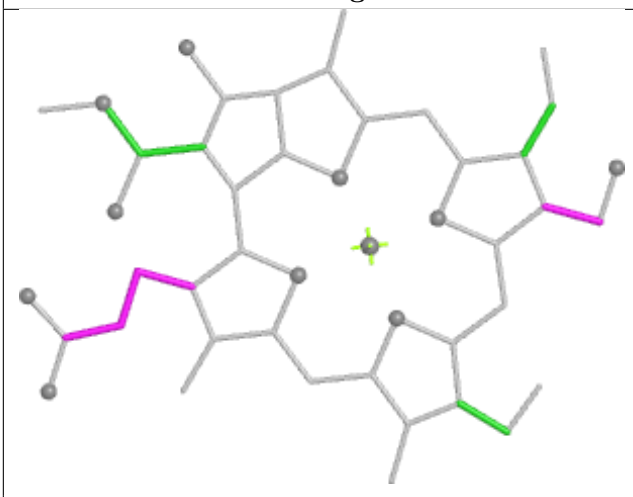
Ligand CHL n 606



Bond lengths



Bond angles

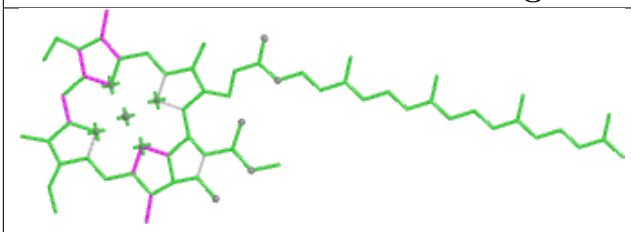


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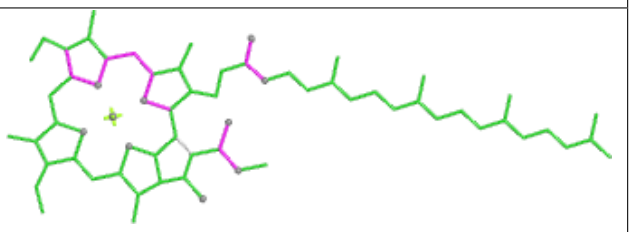


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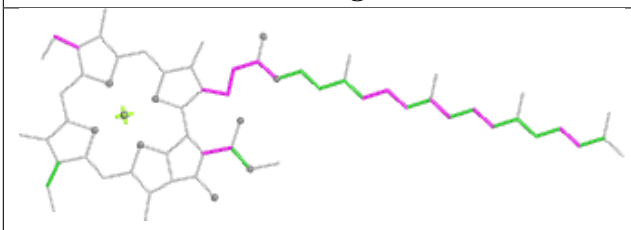
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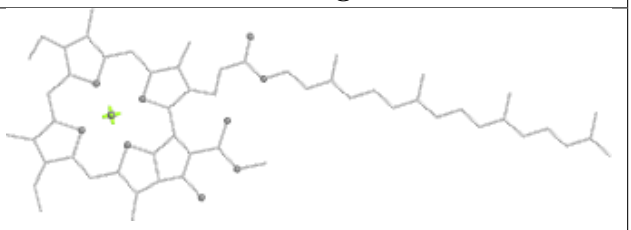
Bond lengths



Bond angles



Torsions

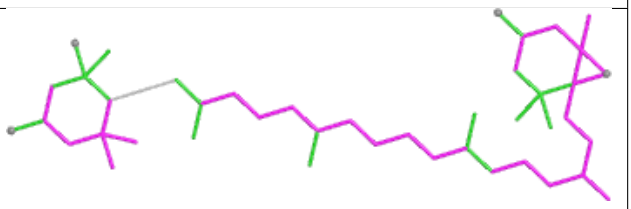


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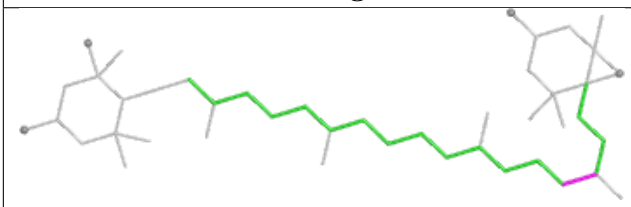
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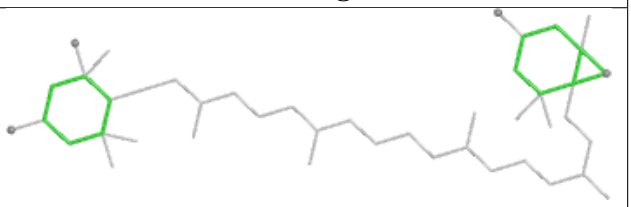
Bond lengths



Bond angles

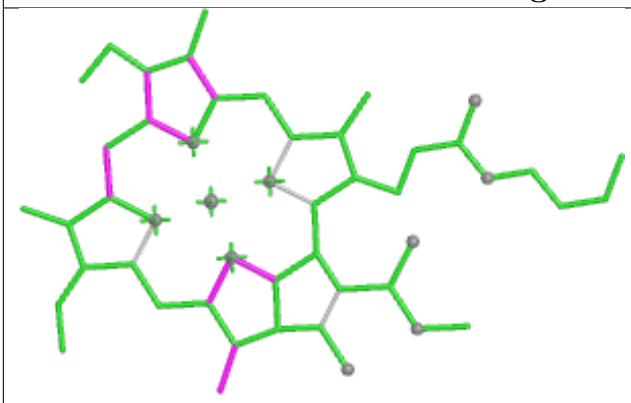


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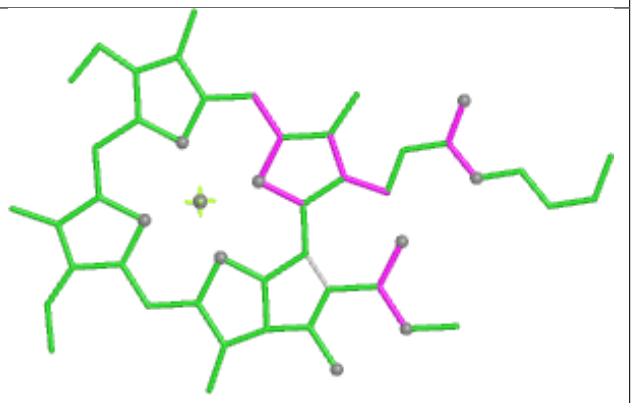


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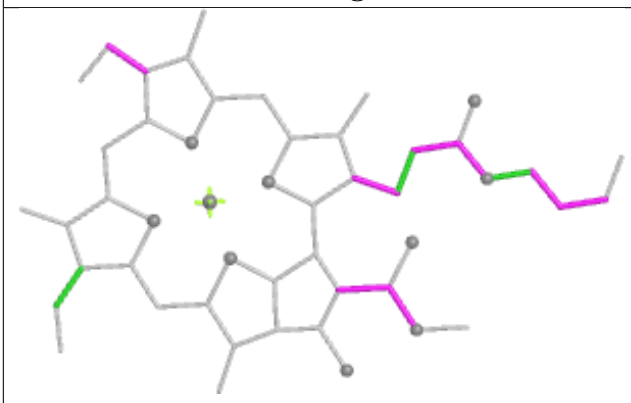
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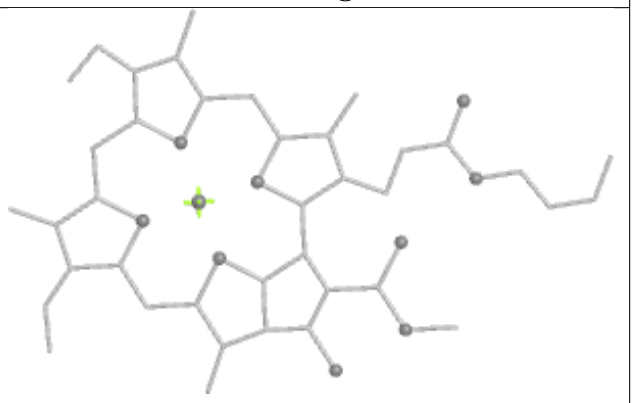
Bond lengths



Bond angles

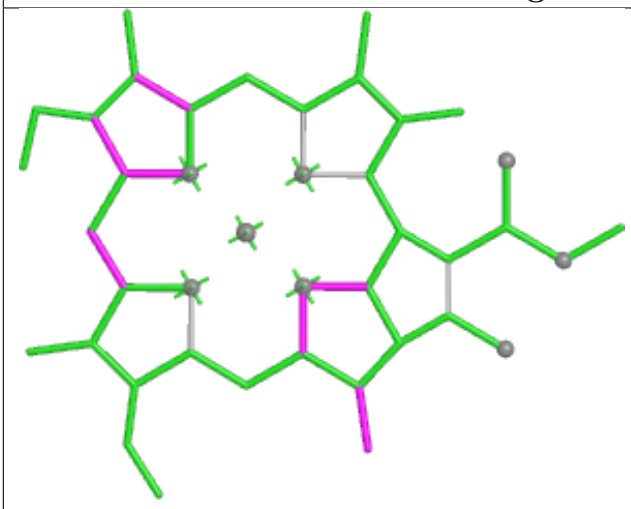


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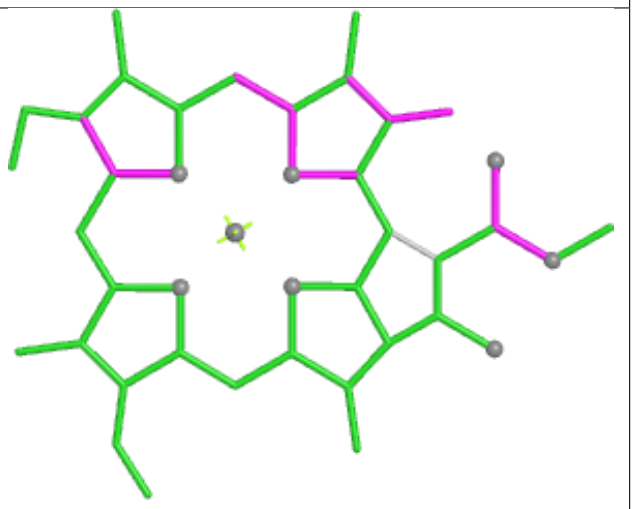


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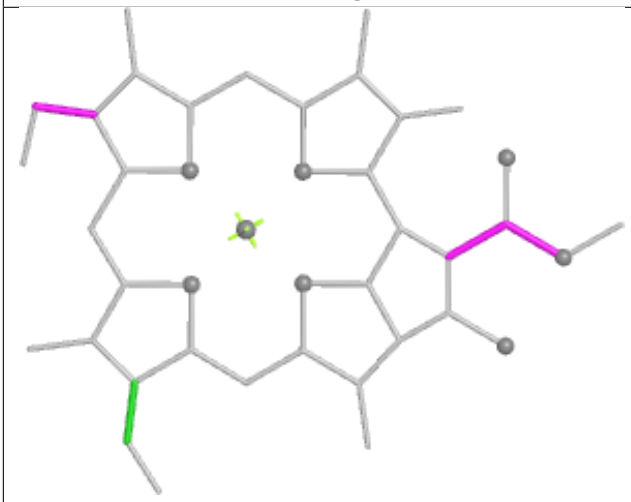
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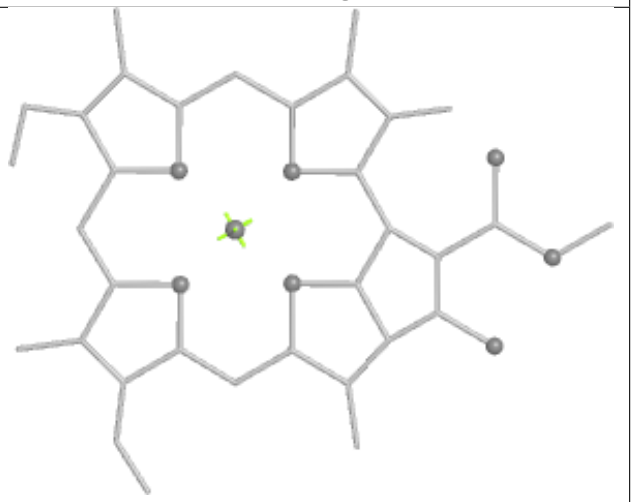
Bond lengths



Bond angles

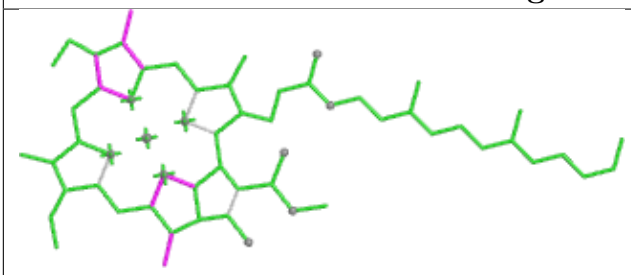


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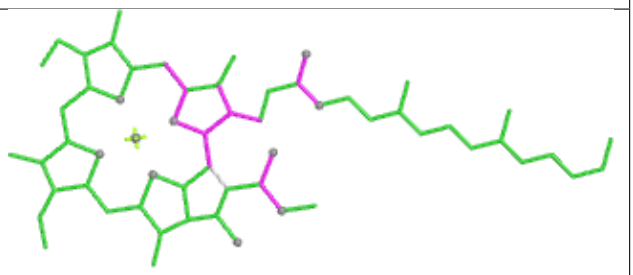


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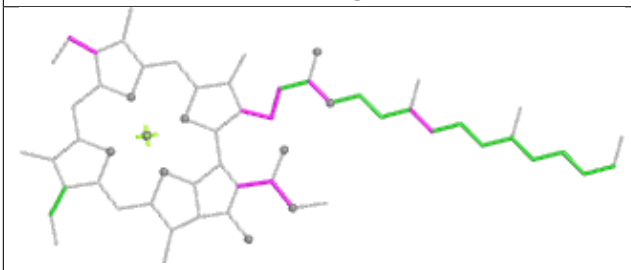
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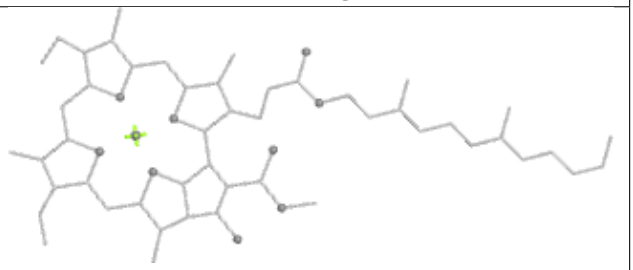
Bond lengths



Bond angles

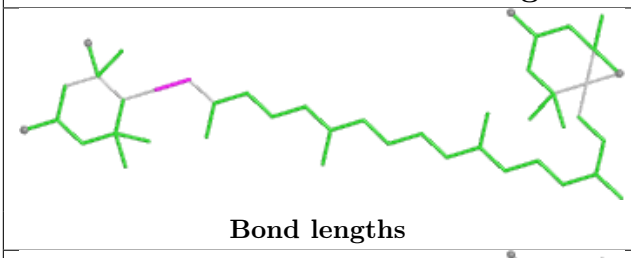


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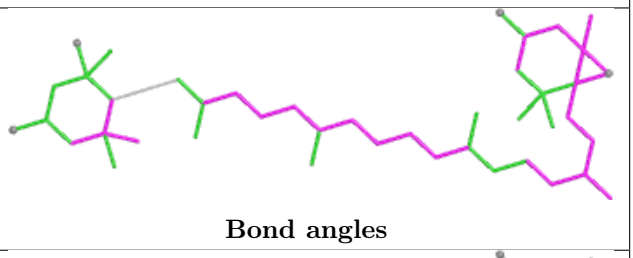


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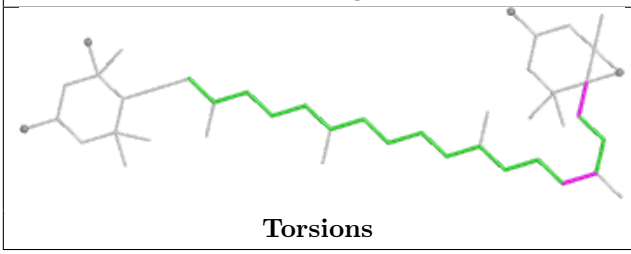
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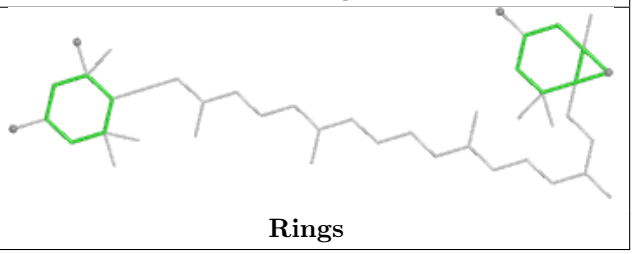
Bond lengths



Bond angles

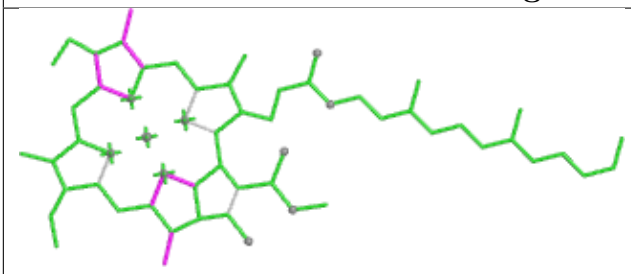


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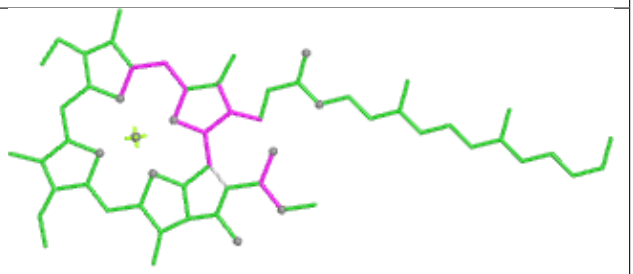


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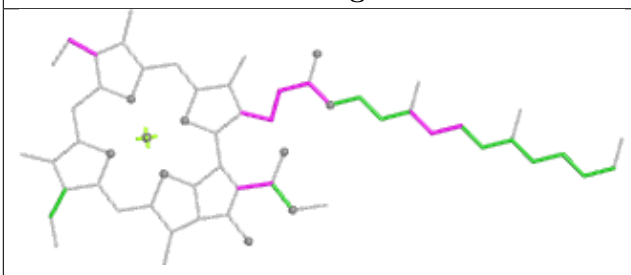
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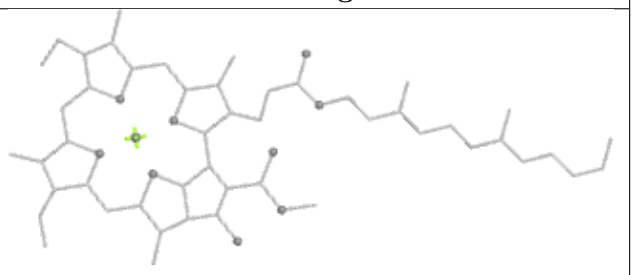
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Bond angles

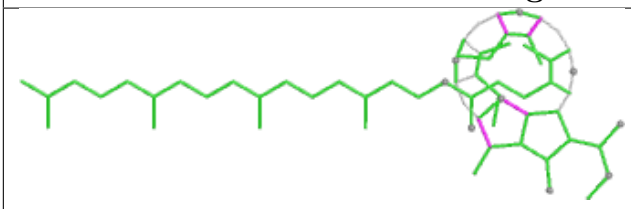


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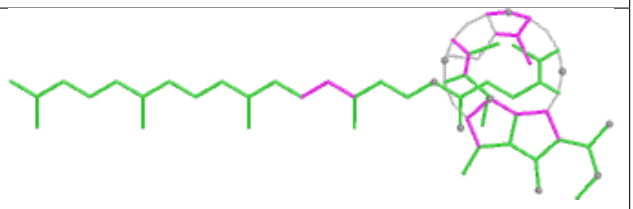


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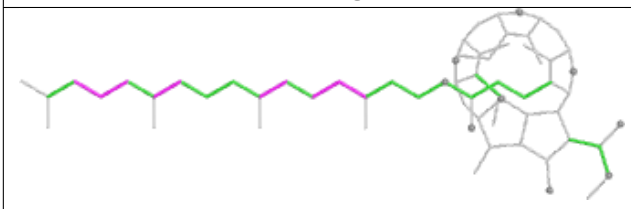
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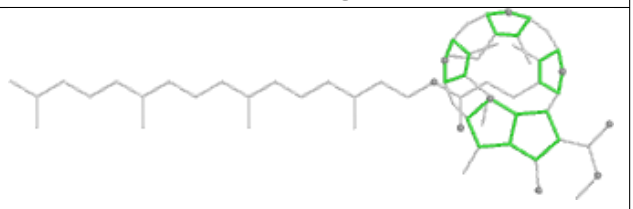
Bond lengths



Bond angles

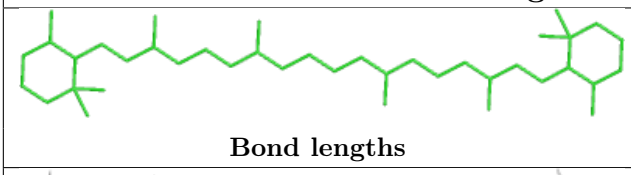


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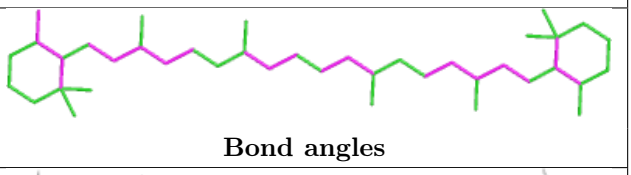


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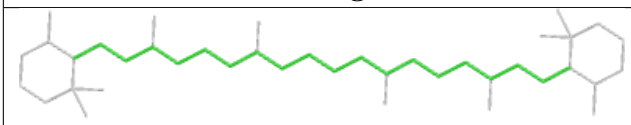
Ligand BCR z 101



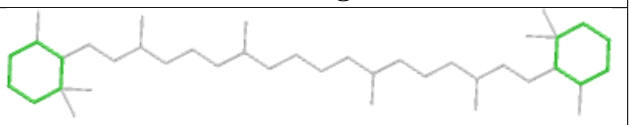
Bond lengths



Bond angles

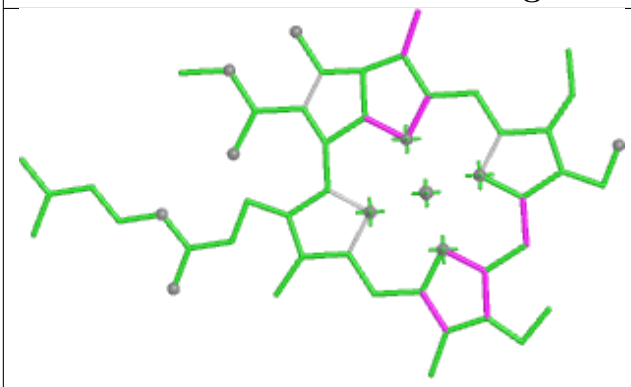


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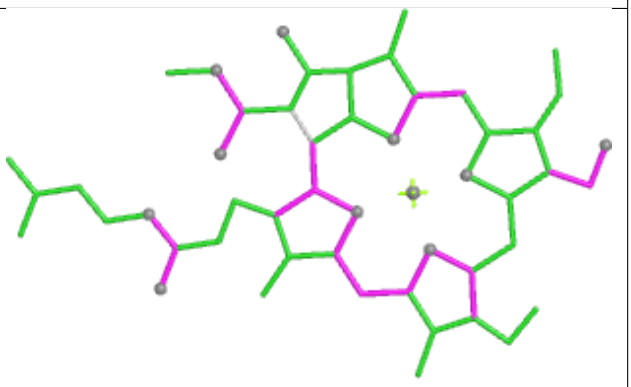


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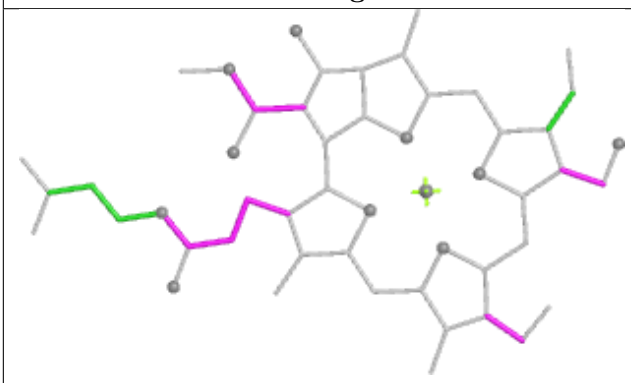
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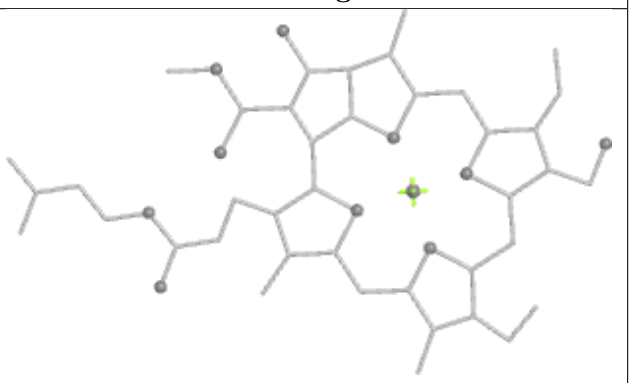
Bond lengths



Bond angles

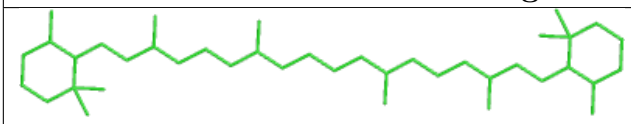


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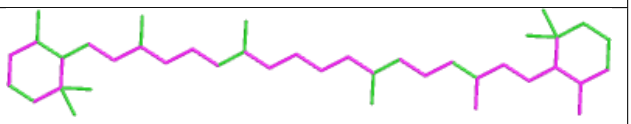


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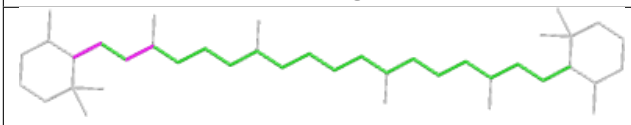
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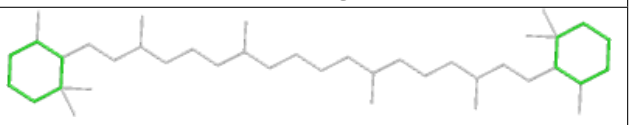
Bond lengths



Bond angles

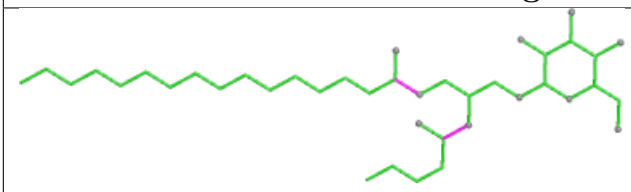


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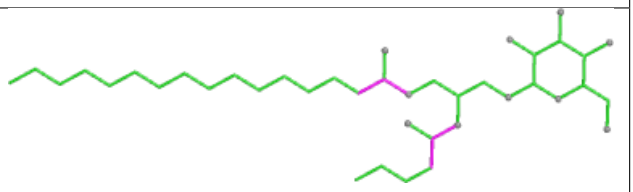


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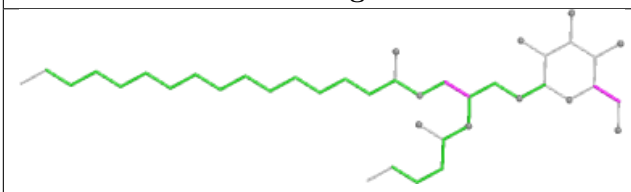
Ligand LMG b 601



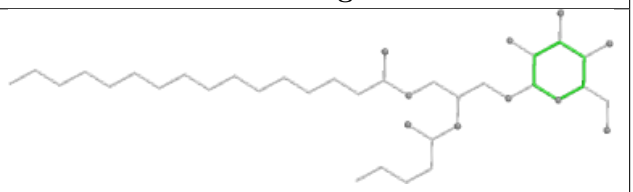
Bond lengths



Bond angles

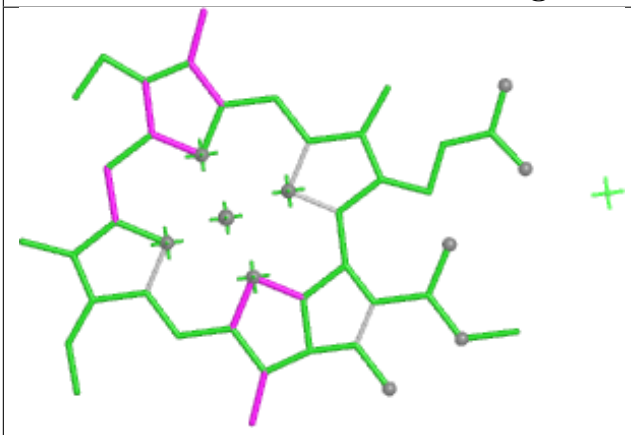


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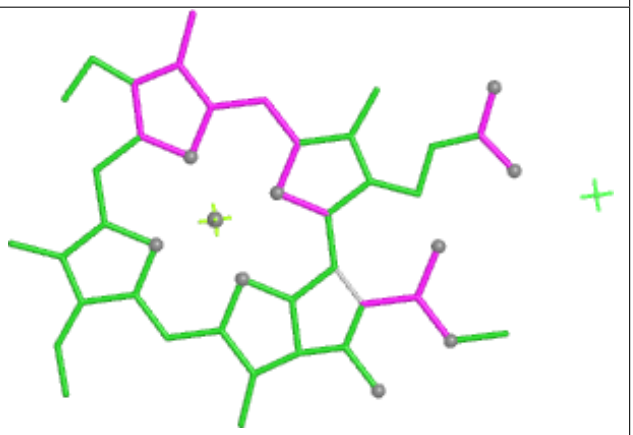


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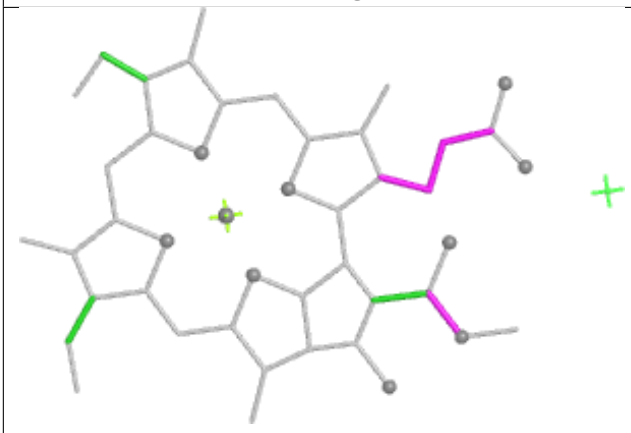
Ligand CLA s 609



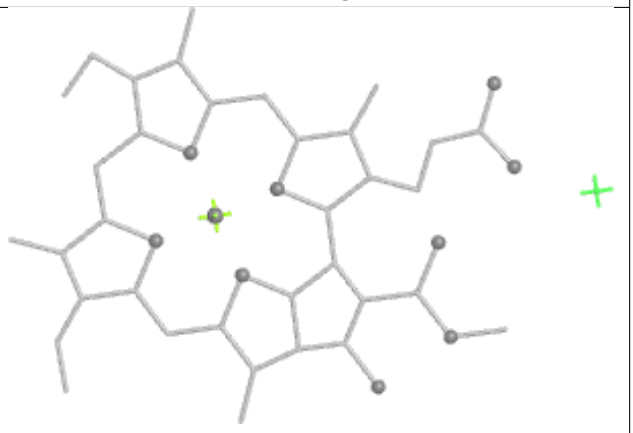
Bond lengths



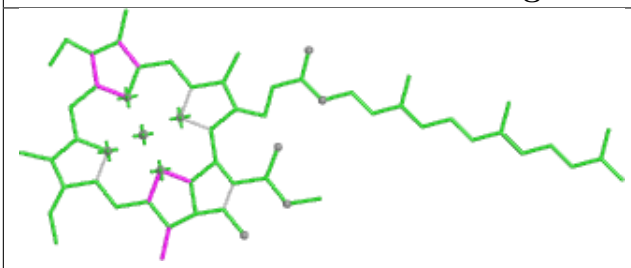
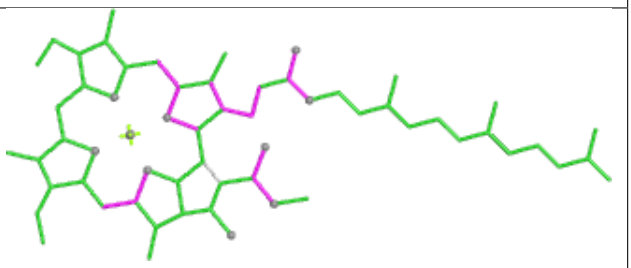
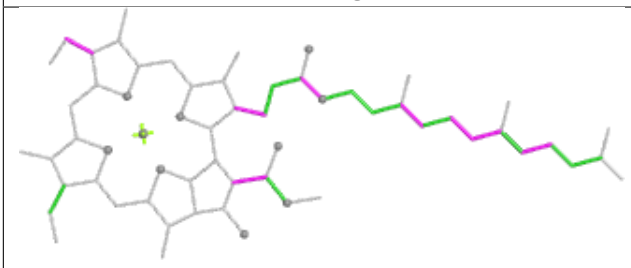
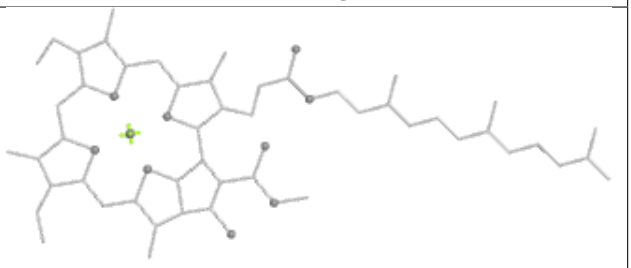
Bond angles

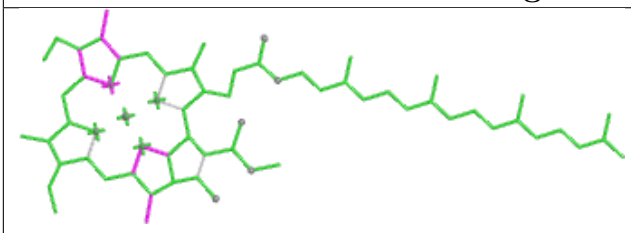
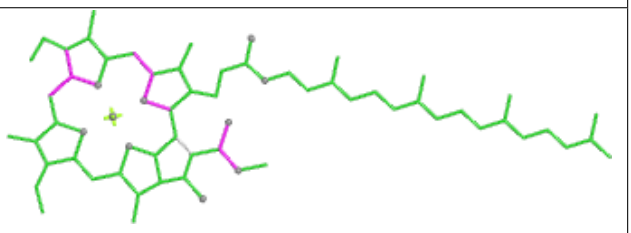
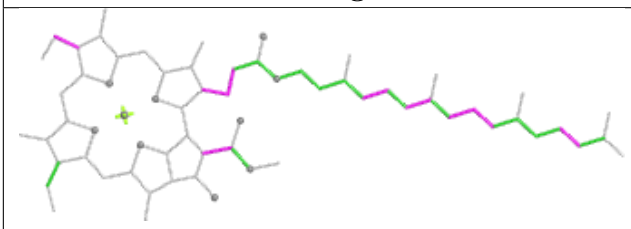
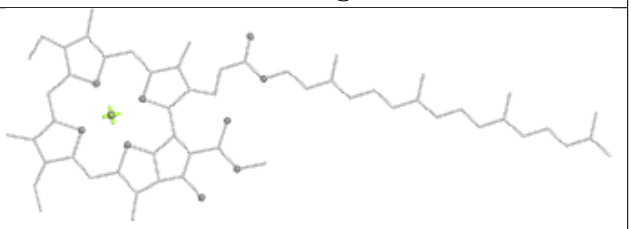


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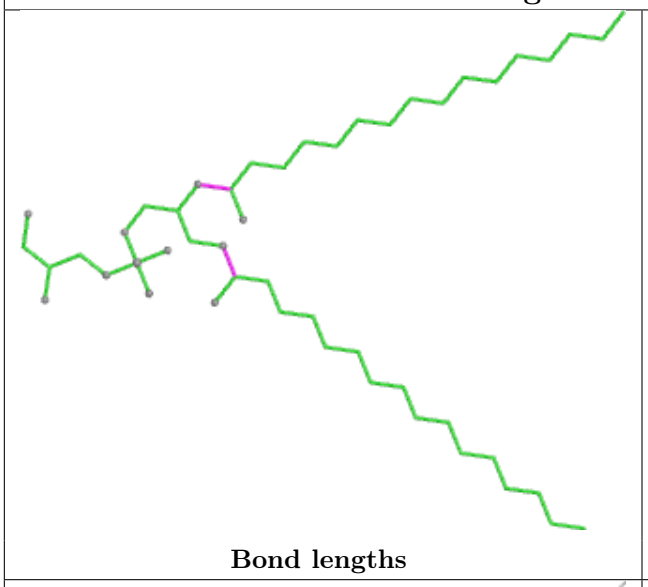


Rings

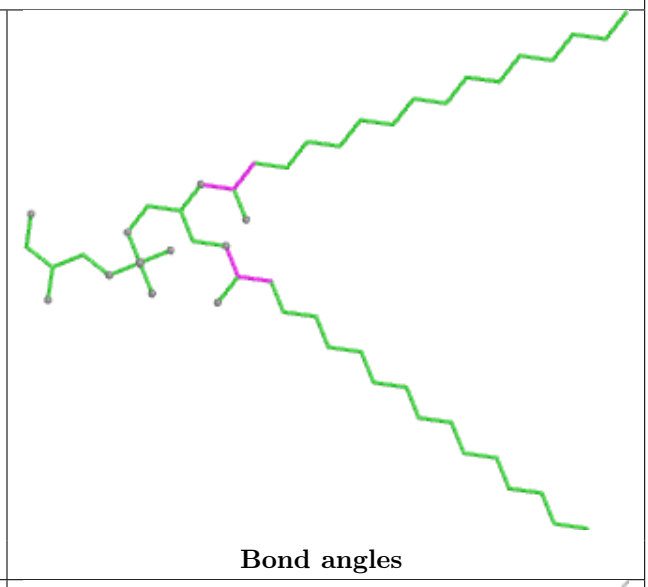
Ligand CLA N 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

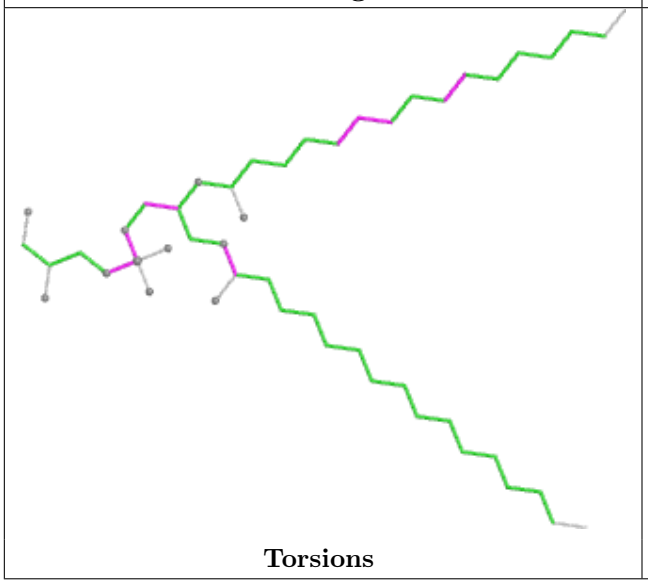
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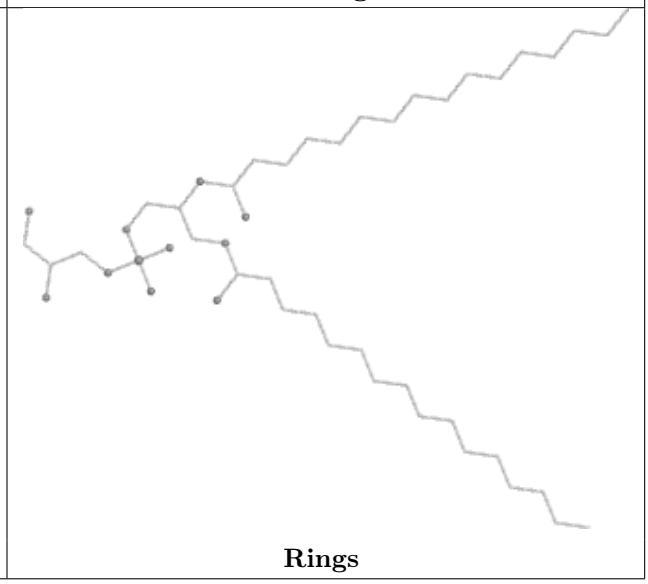
Bond lengths



Bond angles

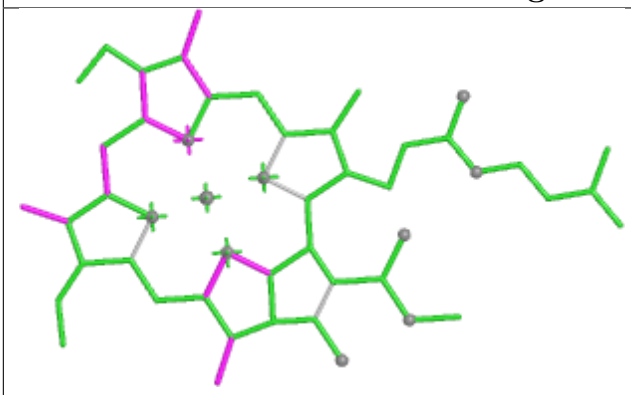


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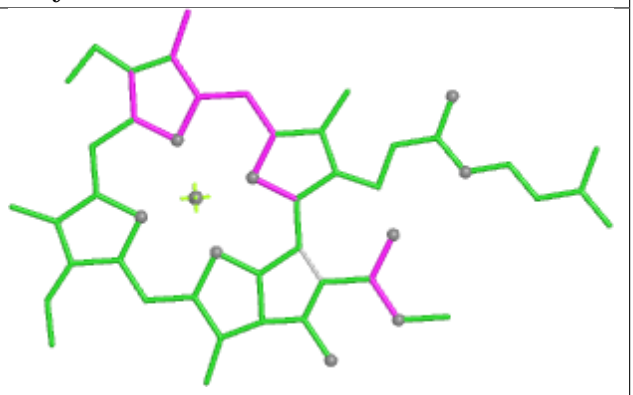


Rings

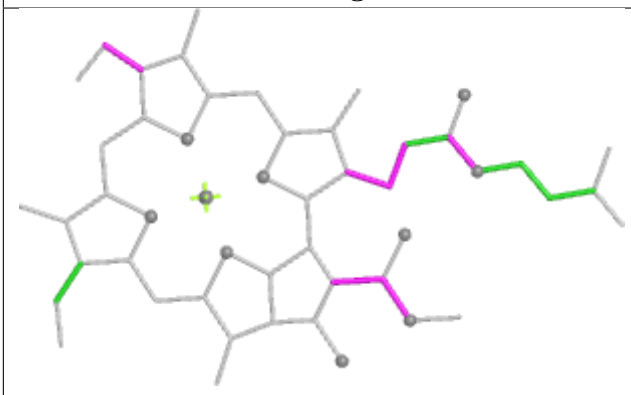
Ligand CLA y 305



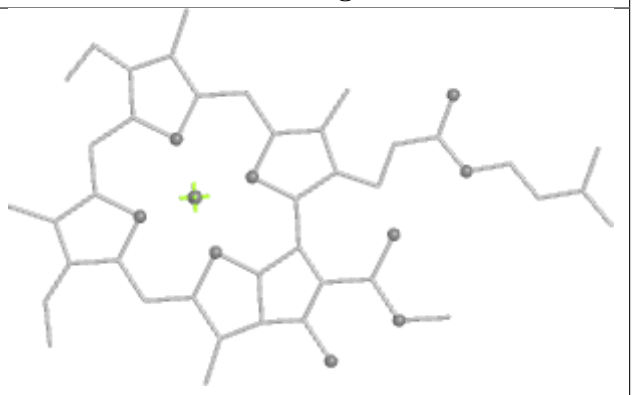
Bond lengths



Bond angles

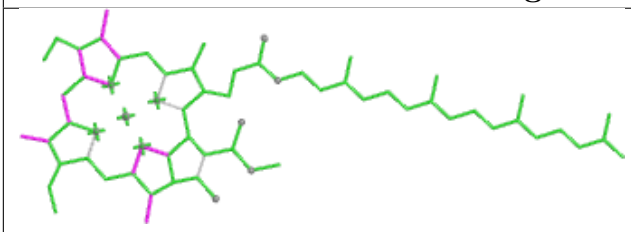


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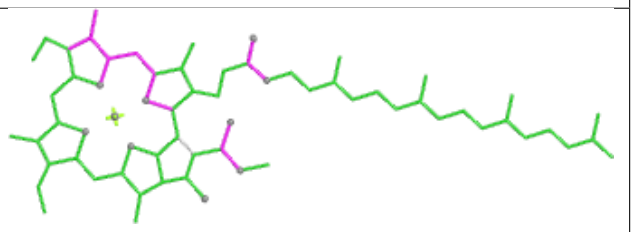


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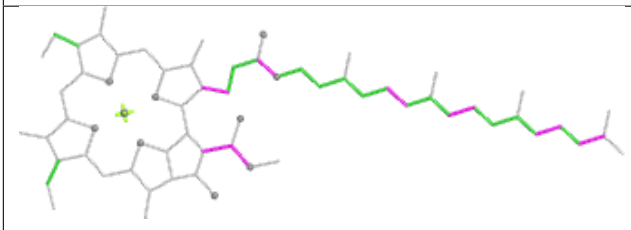
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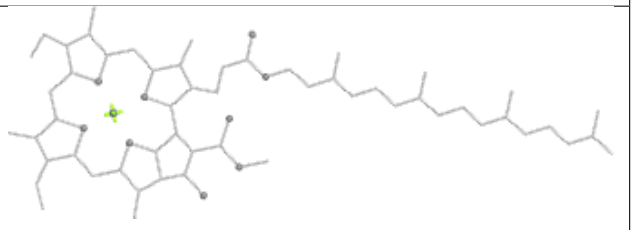
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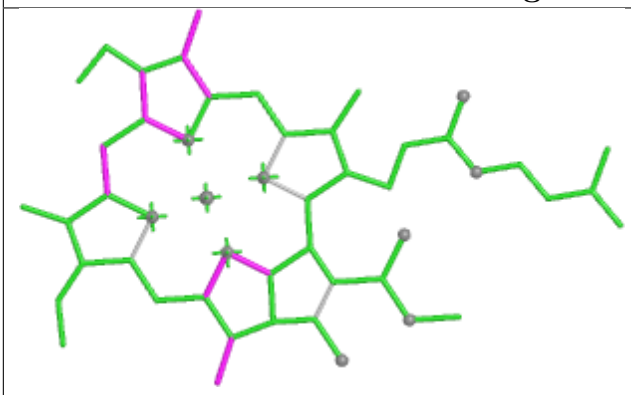


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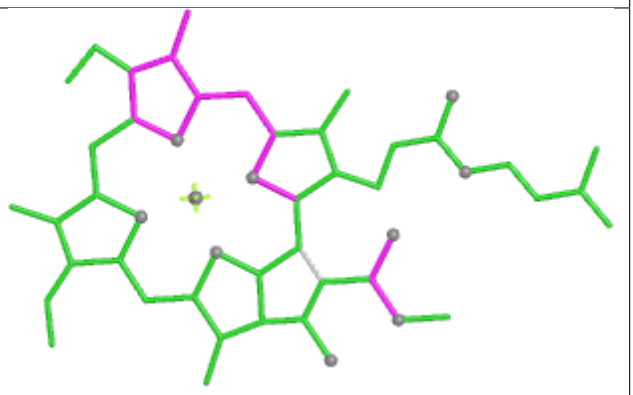


Rings

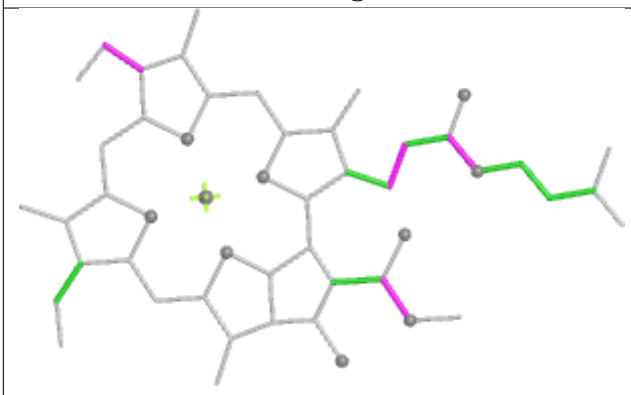
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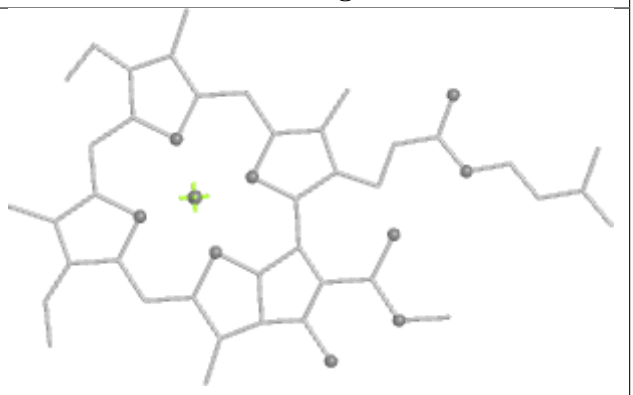
Bond lengths



Bond angles

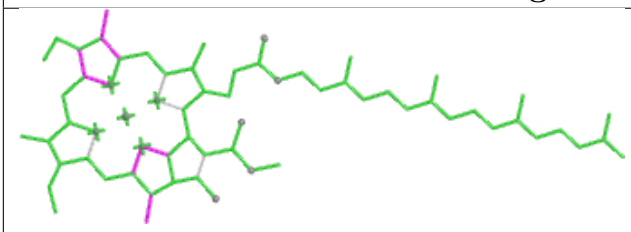


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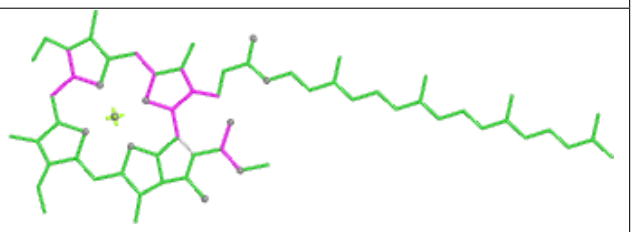


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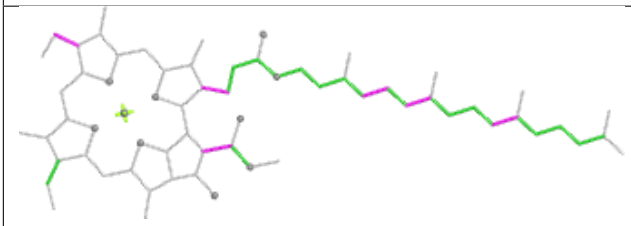
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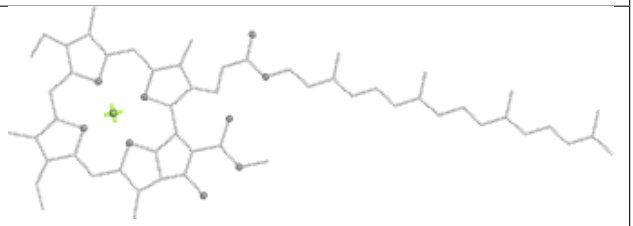
Bond lengths



Bond angles

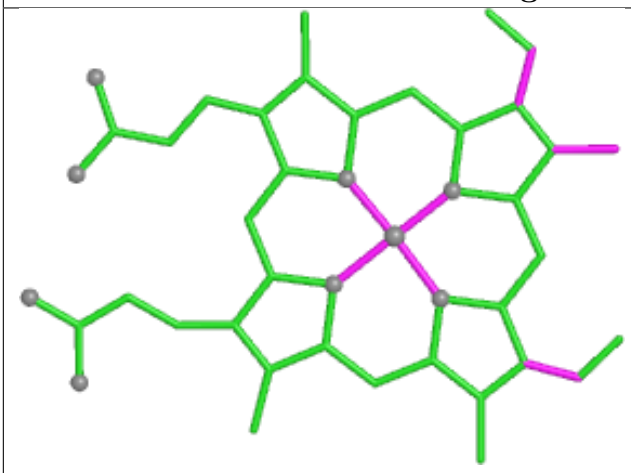


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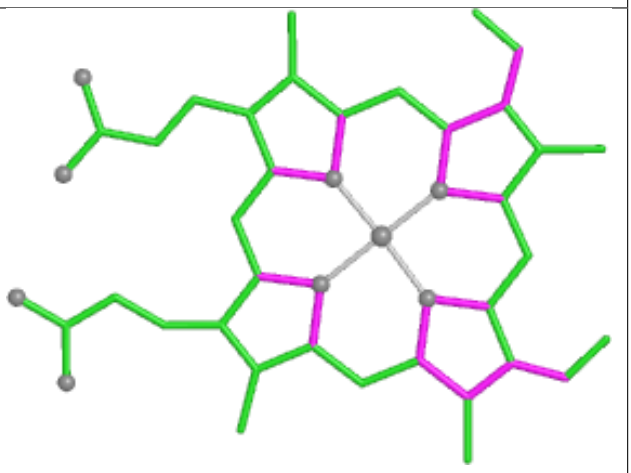


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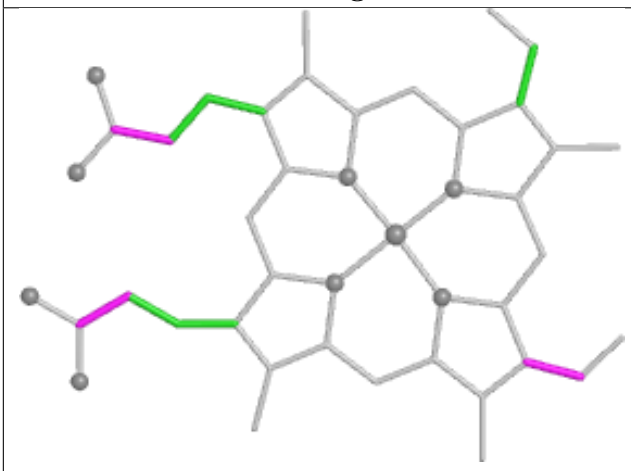
Ligand HEM F 101



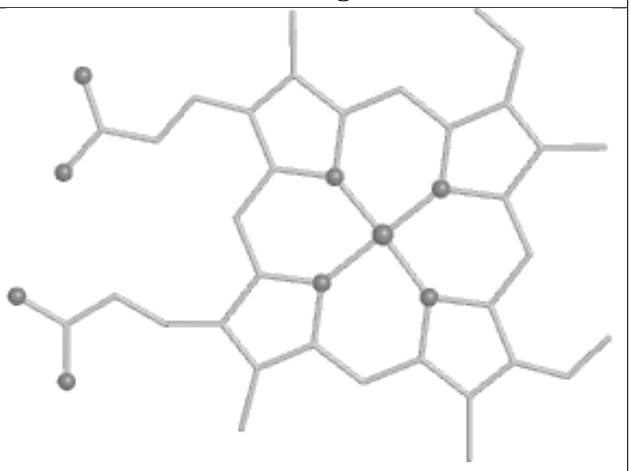
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Bond angles

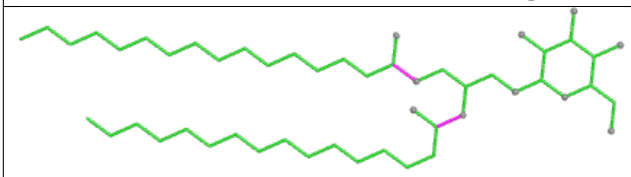


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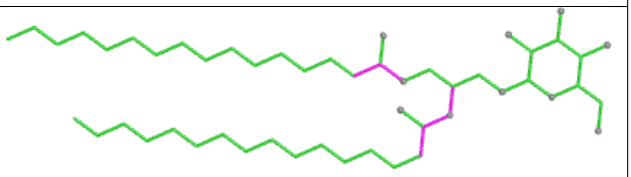


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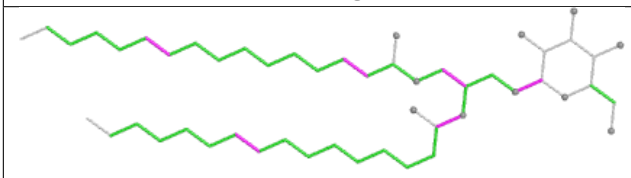
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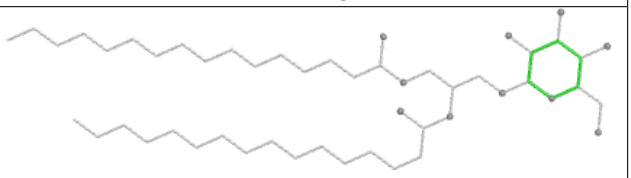
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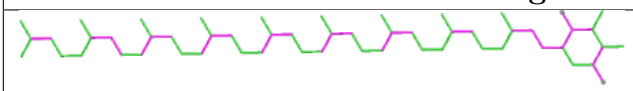


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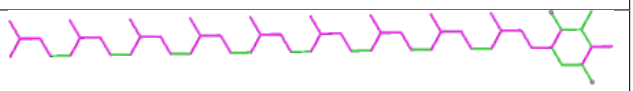


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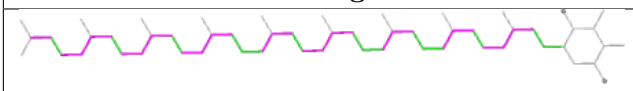
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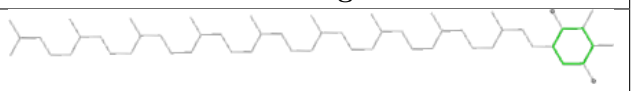
Bond lengths



Bond angles

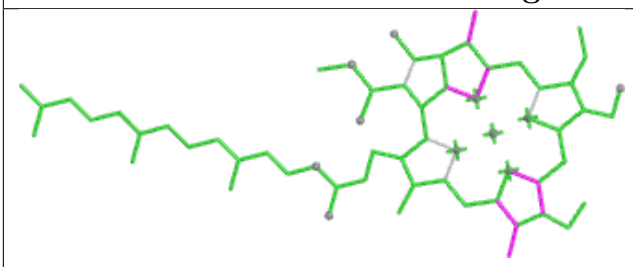


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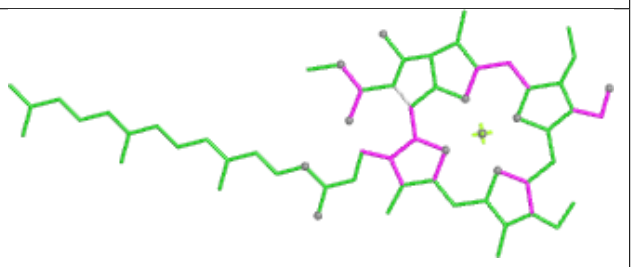


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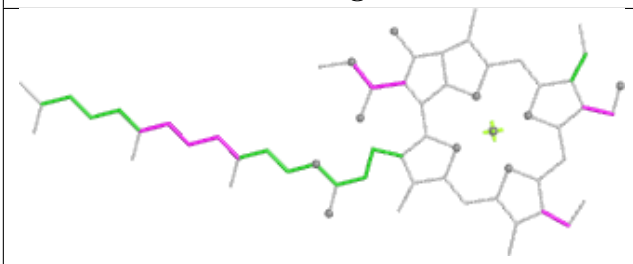
Ligand CHL G 609



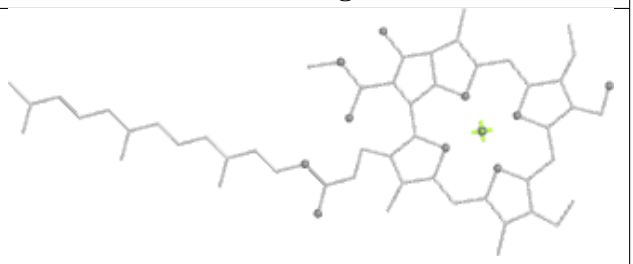
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Bond angles

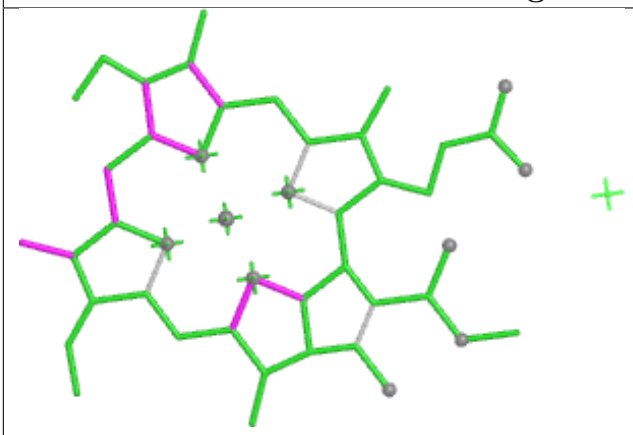


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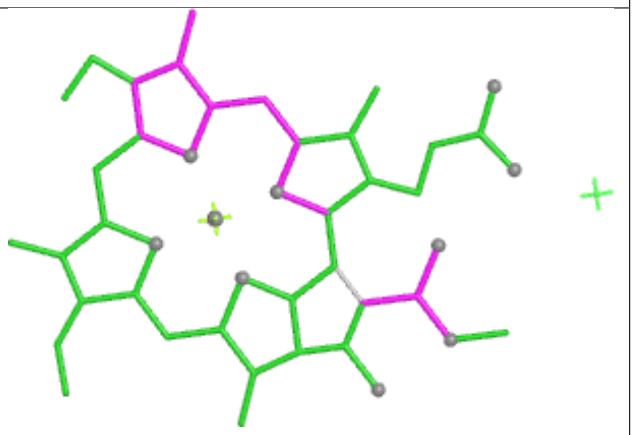


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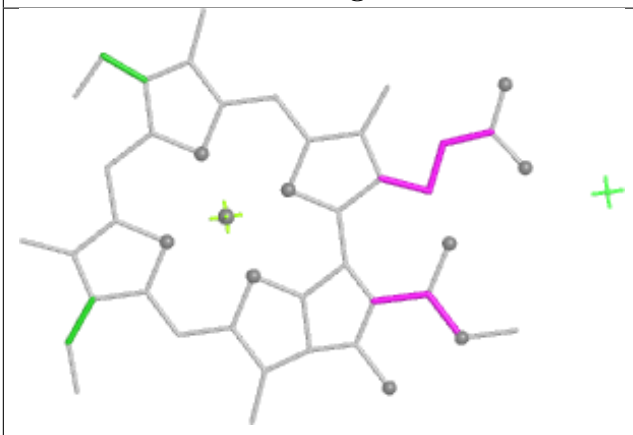
Ligand CLA S 310



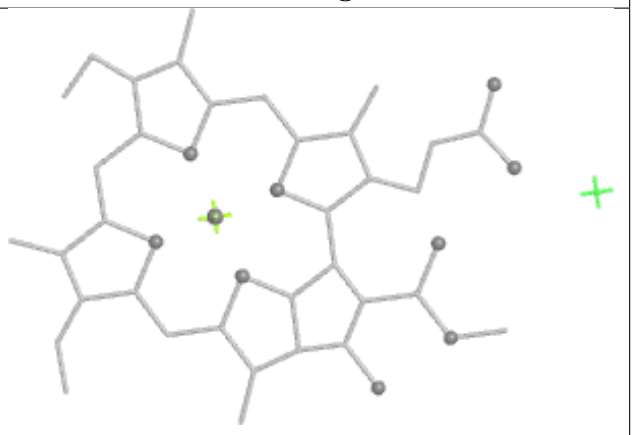
Bond lengths



Bond angles

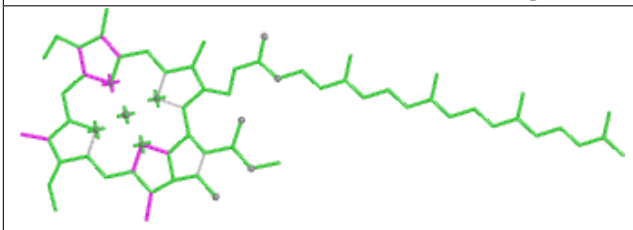


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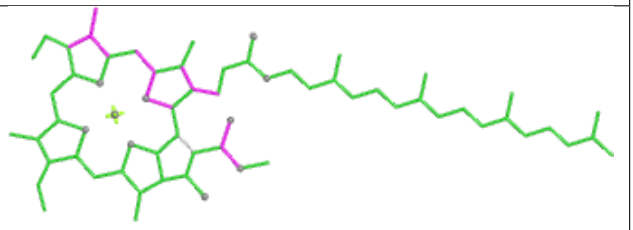


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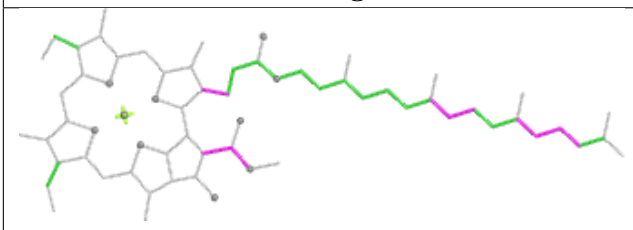
Ligand CLA B 610



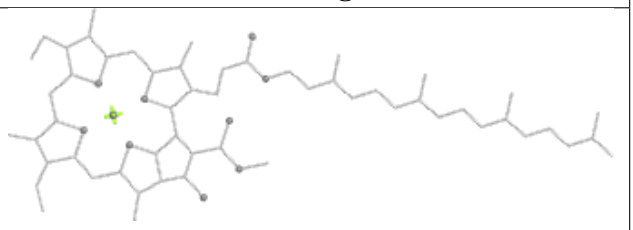
Bond lengths



Bond angles

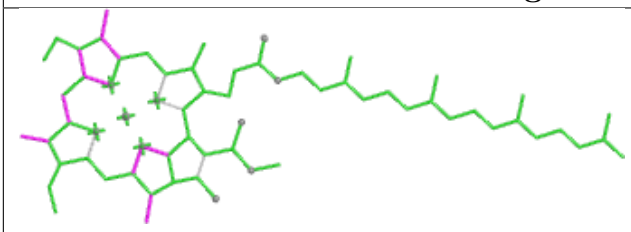


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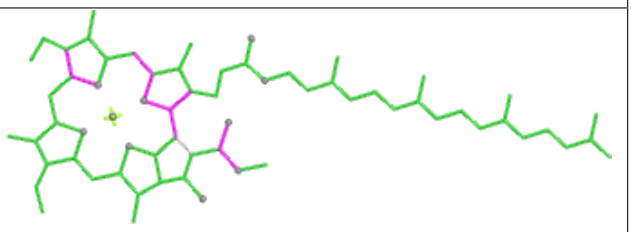


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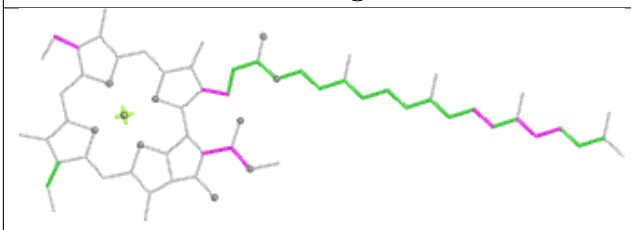
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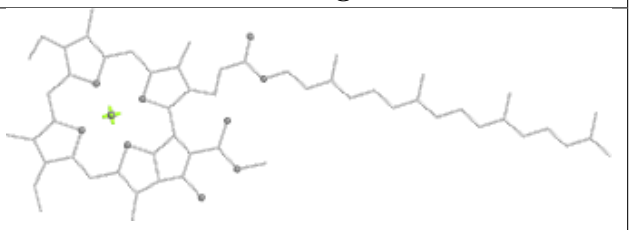
Bond lengths



Bond angles



Torsions

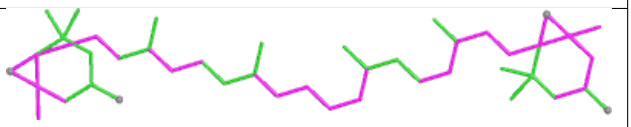


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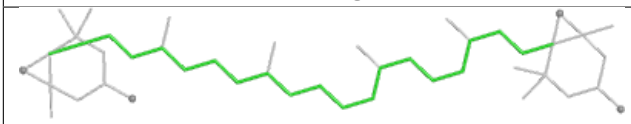
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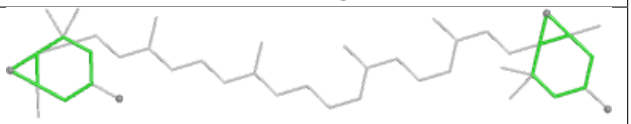
Bond lengths



Bond angles

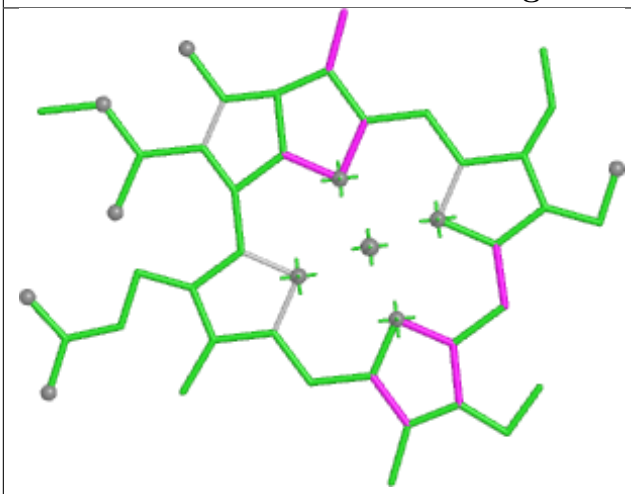


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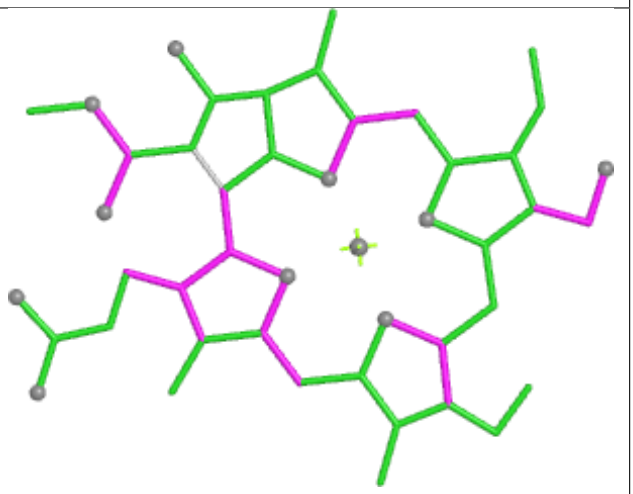


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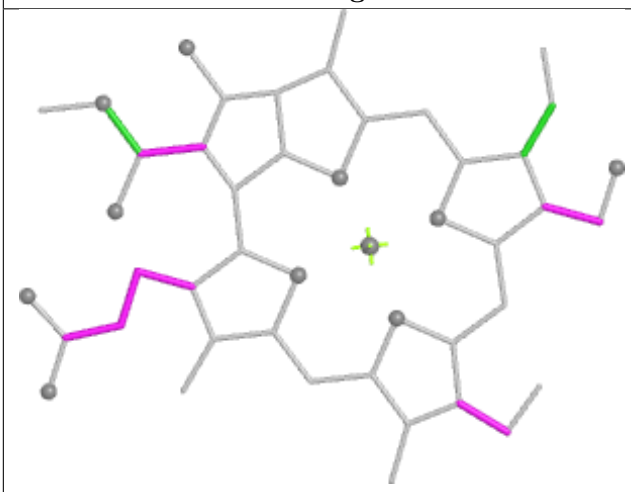
Ligand CHL N 607



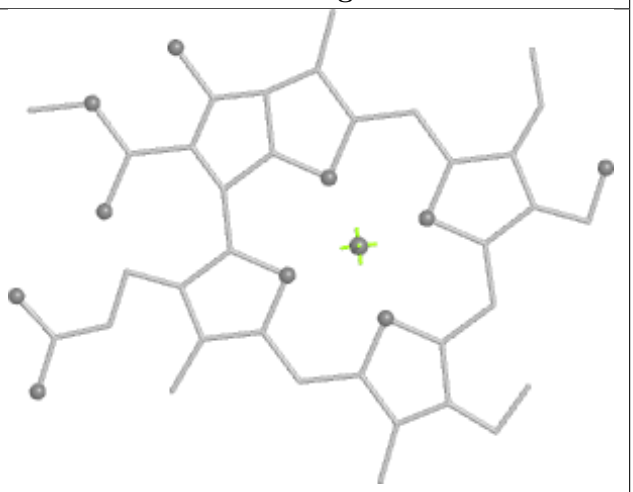
Bond lengths



Bond angles

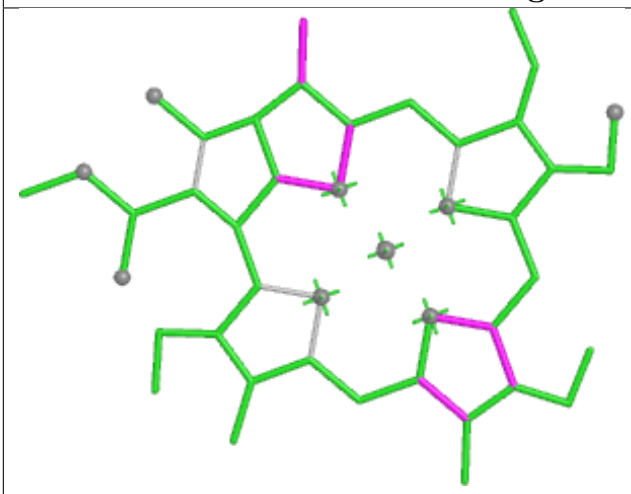


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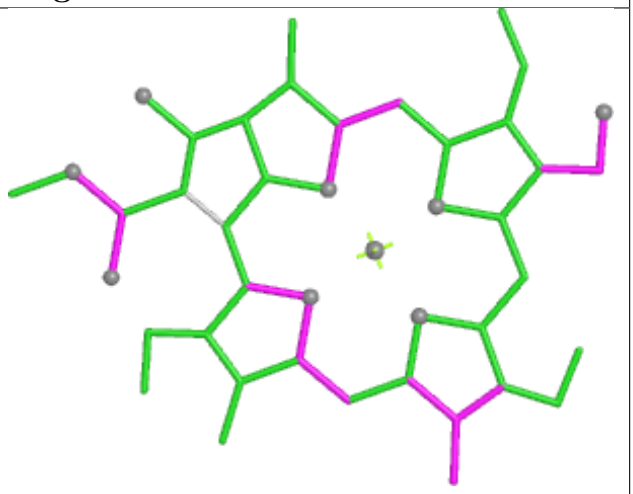


Rings

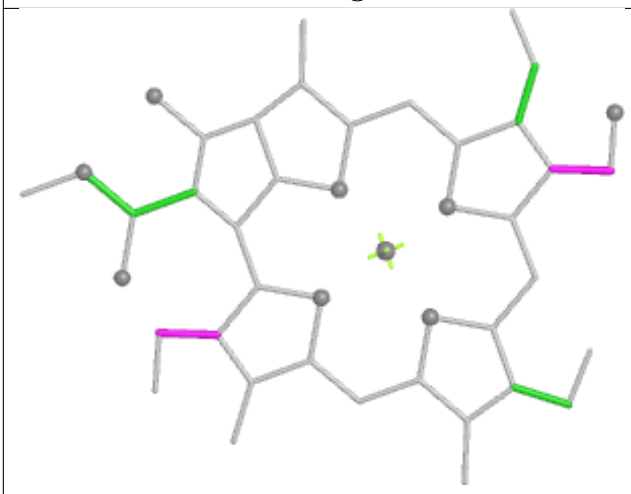
Ligand CHL g 606



Bond lengths



Bond angles

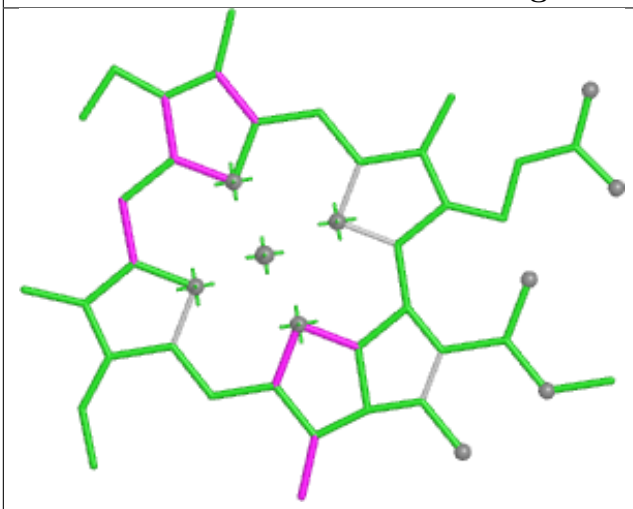


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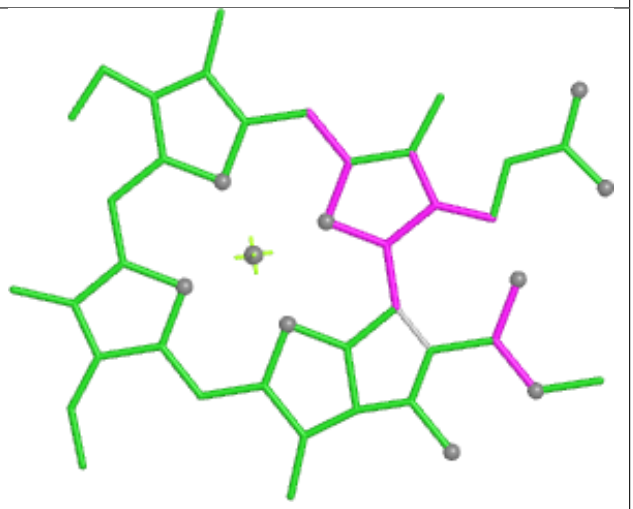


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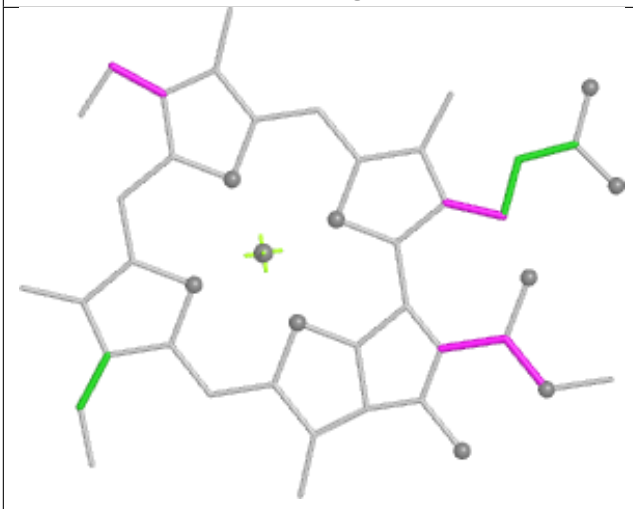
Ligand CLA s 603



Bond lengths



Bond angles

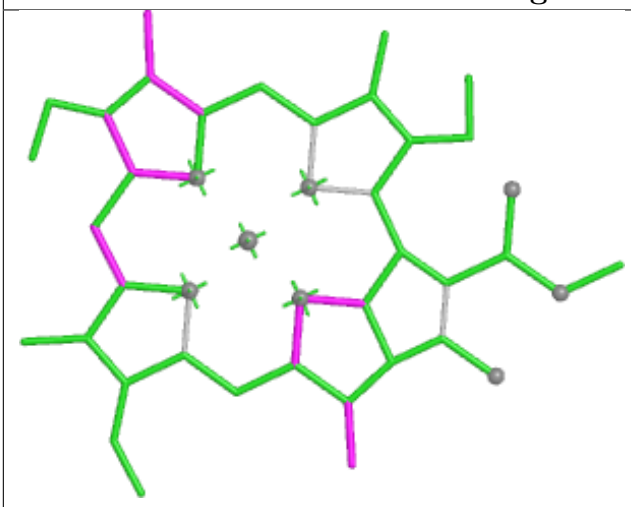


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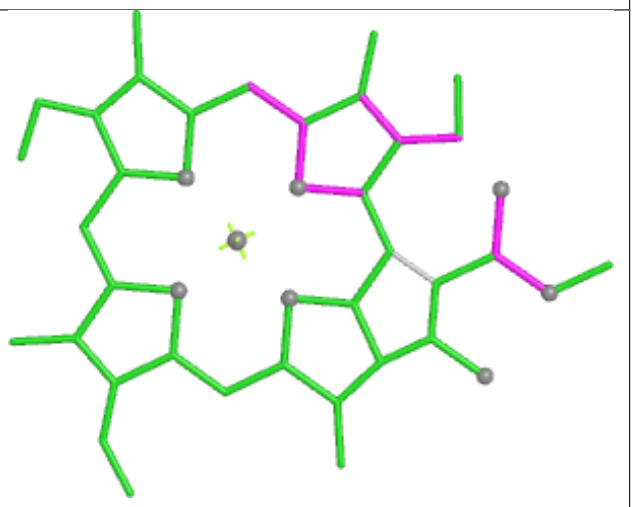


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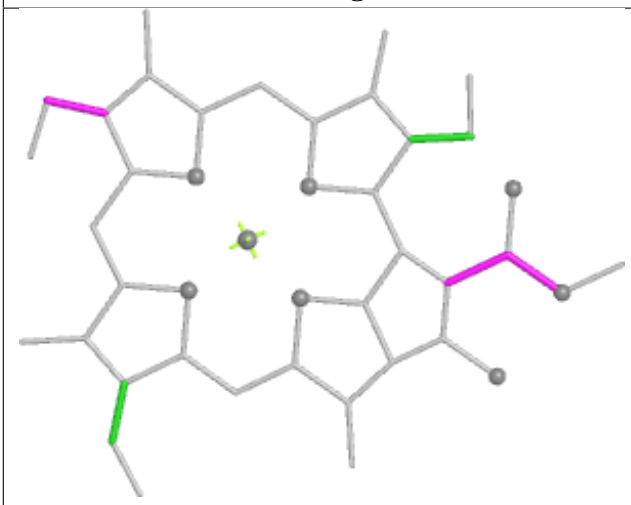
Ligand CLA s 610



Bond lengths



Bond angles

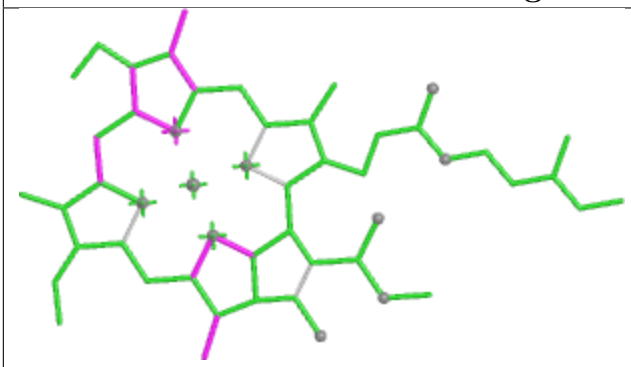


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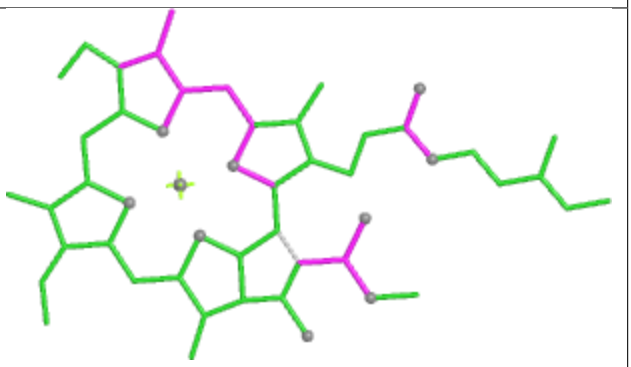


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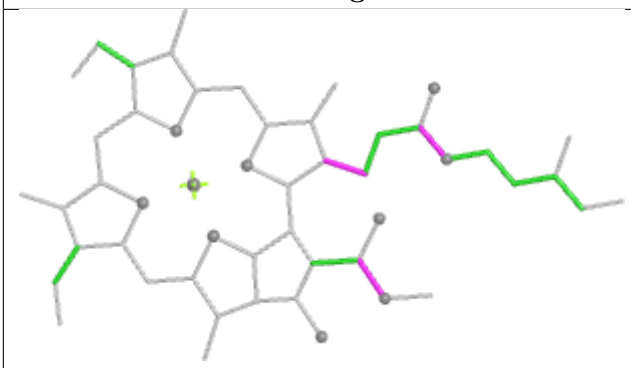
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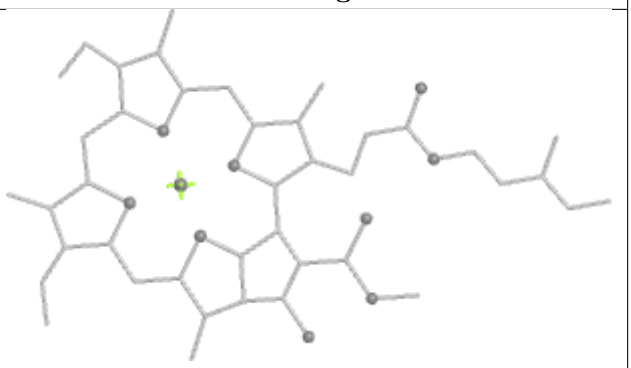
Bond lengths



Bond angles

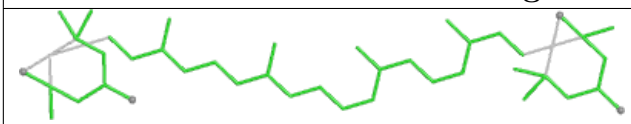


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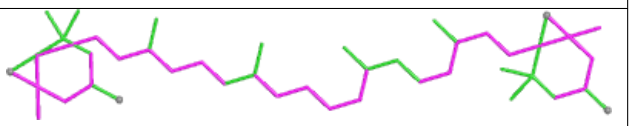


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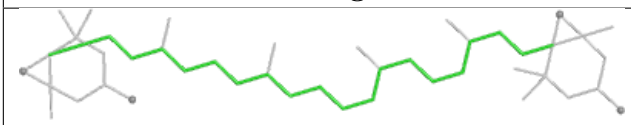
Ligand XAT Y 301



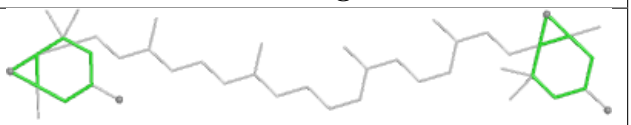
Bond lengths



Bond angles

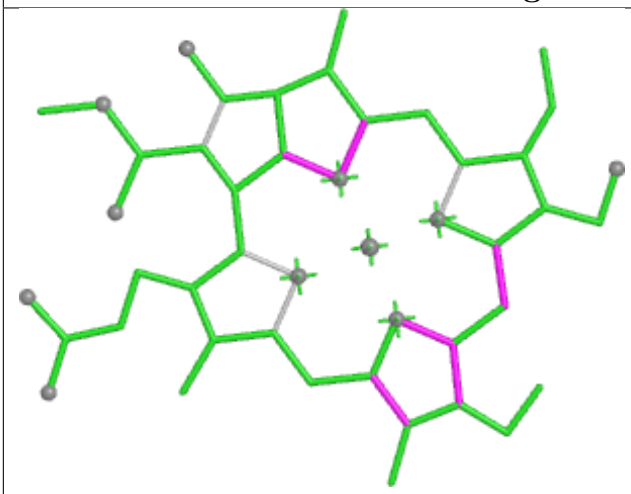


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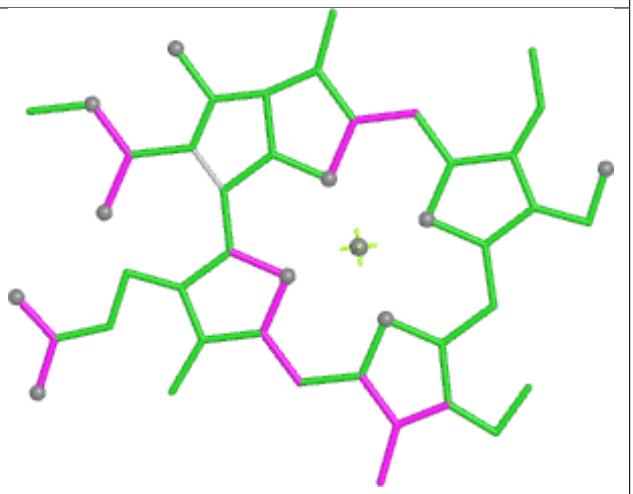


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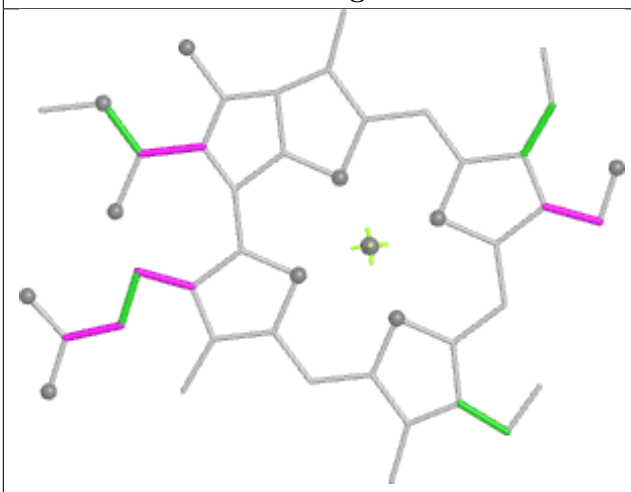
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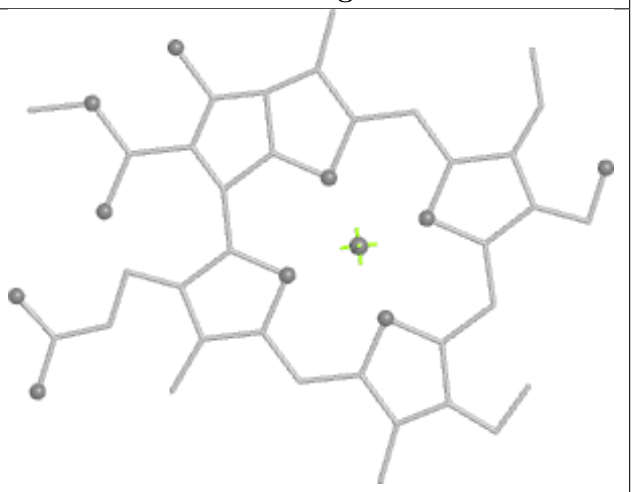
Bond lengths



Bond angles

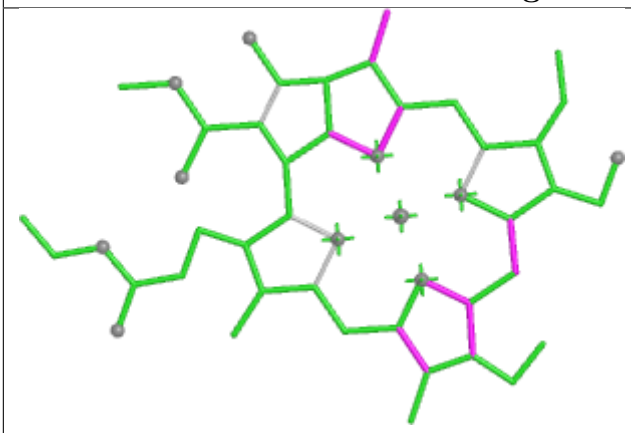


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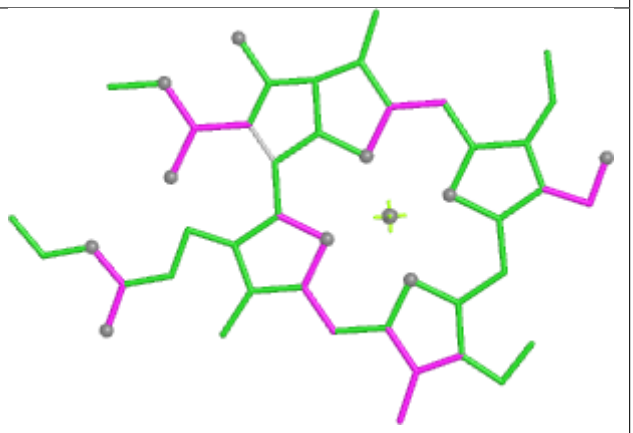


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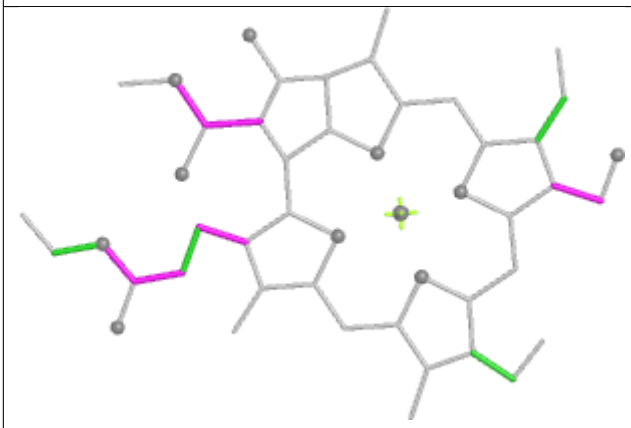
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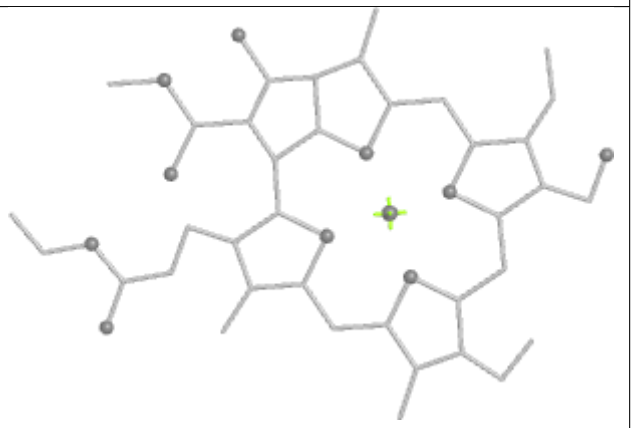
Bond lengths



Bond angles

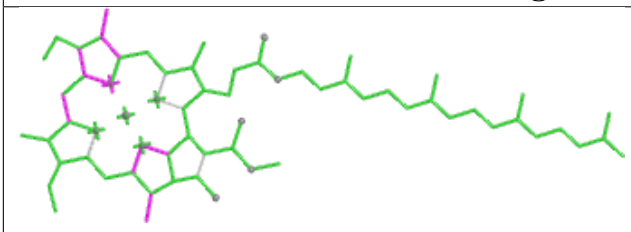


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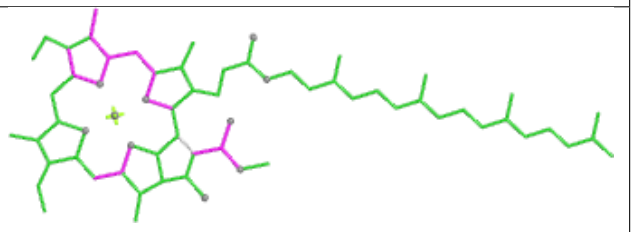


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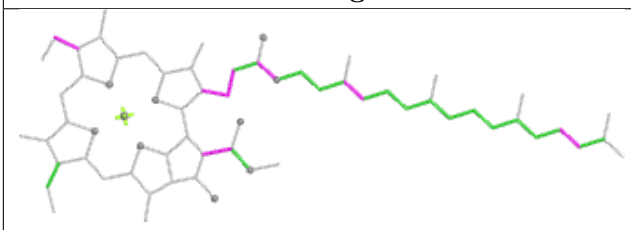
Ligand CLA r 612



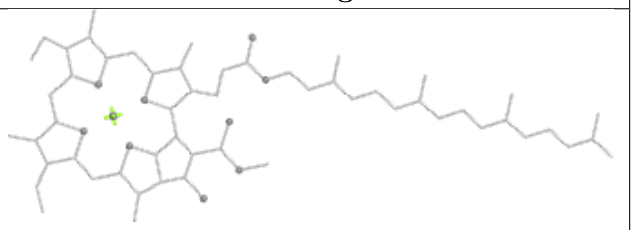
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Bond angles

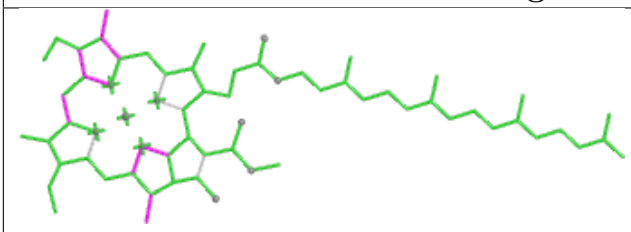


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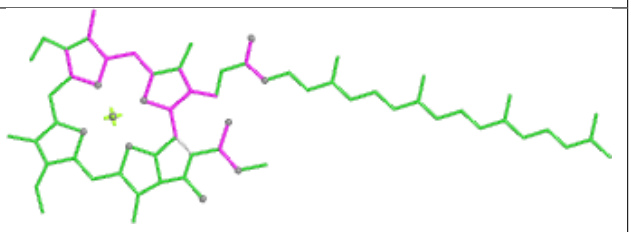


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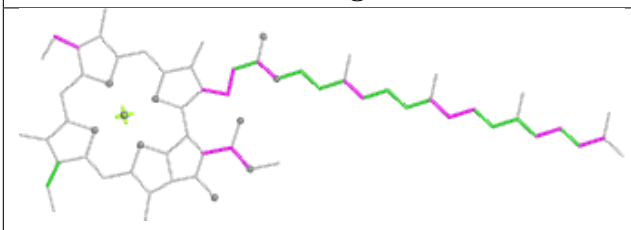
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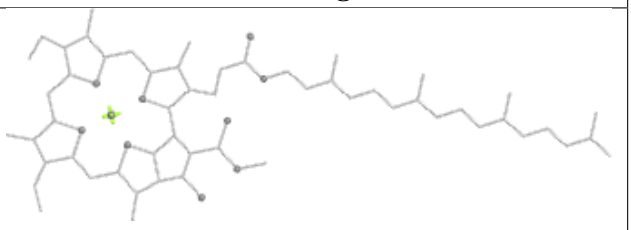
Bond lengths



Bond angles



Torsions

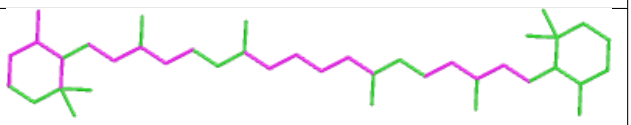


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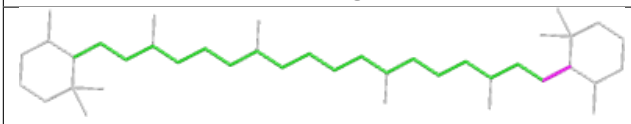
Ligand BCR a 405



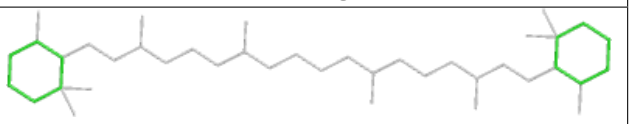
Bond lengths



Bond angles

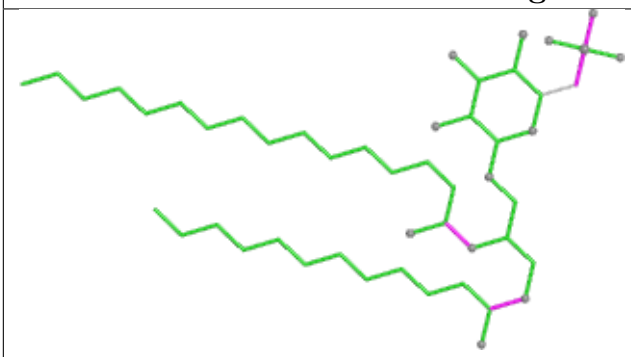


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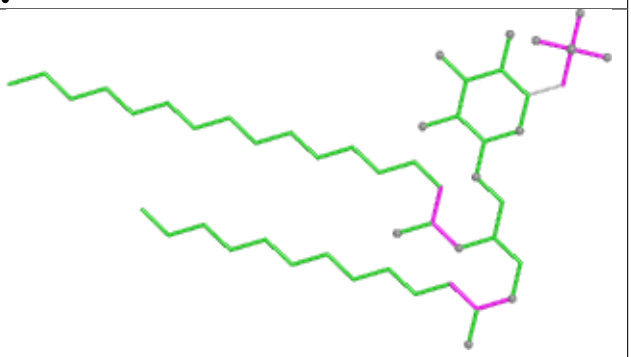


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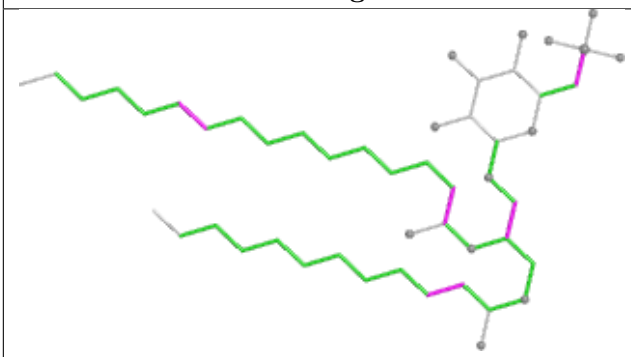
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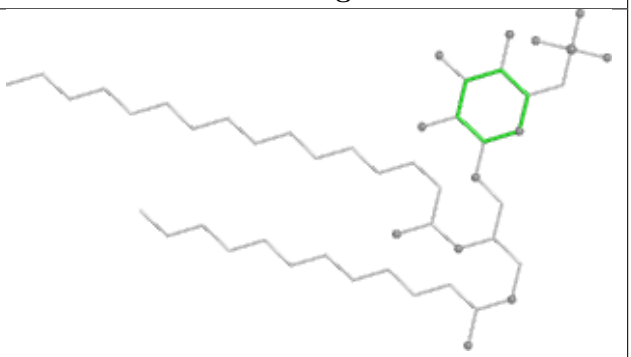
Bond lengths



Bond angles

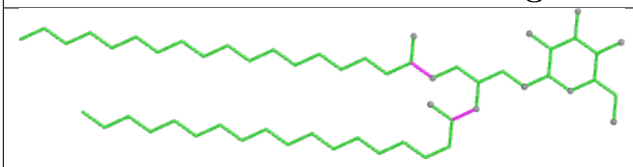


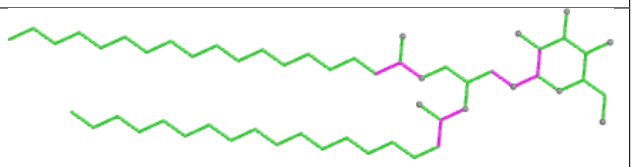
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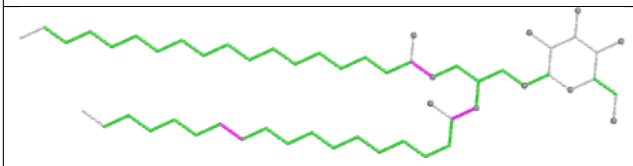


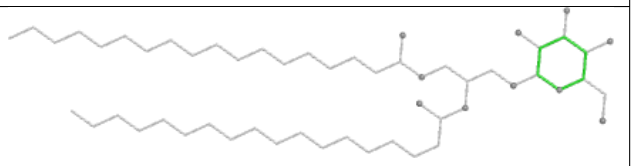
Rings

Ligand LMG s 619

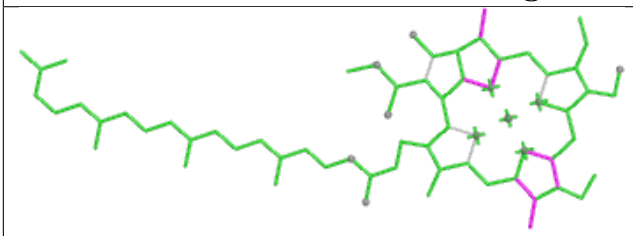

Bond lengths

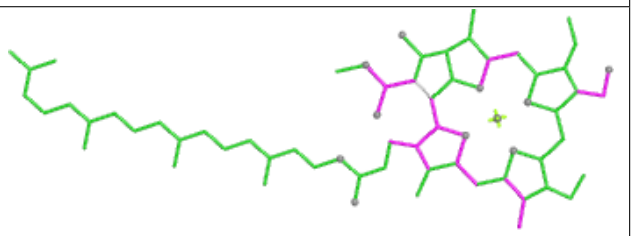

Bond angles

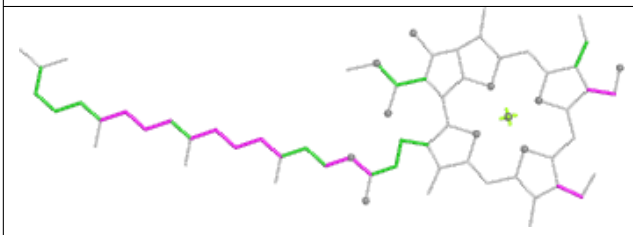

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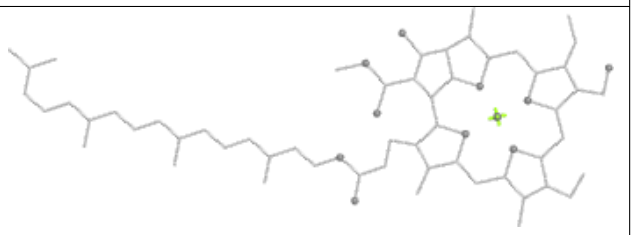

Rings

Ligand CHL N 609

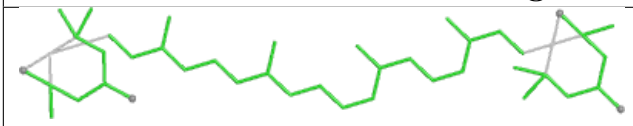

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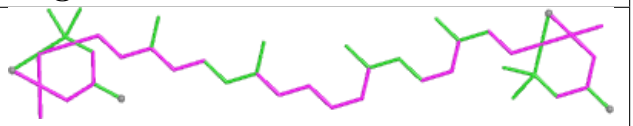

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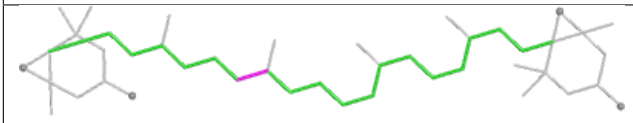

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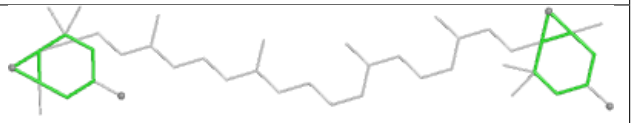

Rings

Ligand XAT g 617

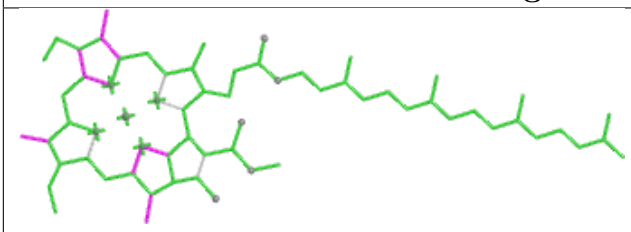

Bond lengths


Bond angles

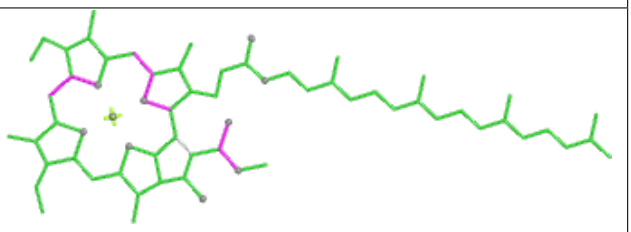

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Rings

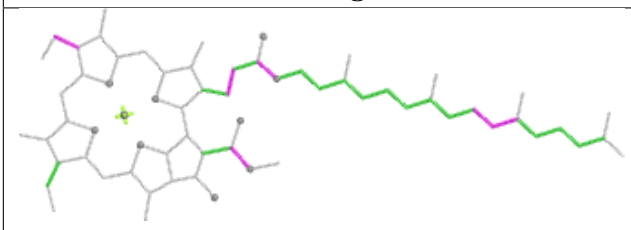
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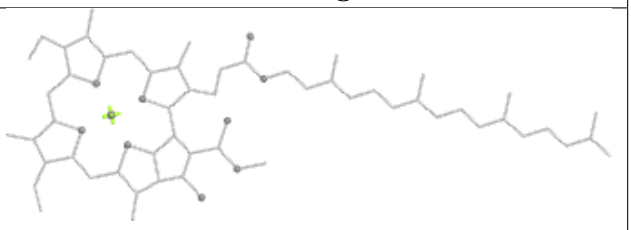
Bond lengths



Bond angles

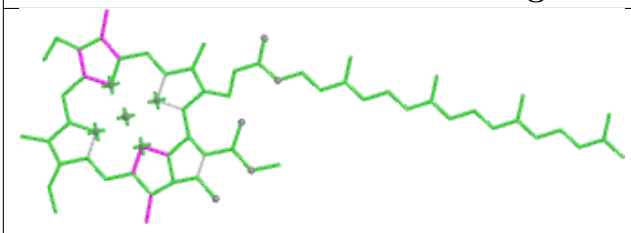


Torsions

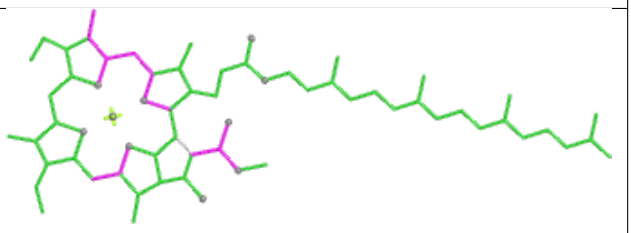


Rings

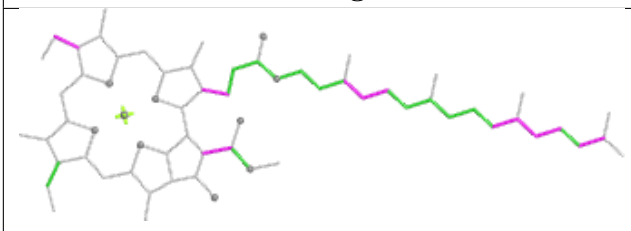
Ligand CLA d 401



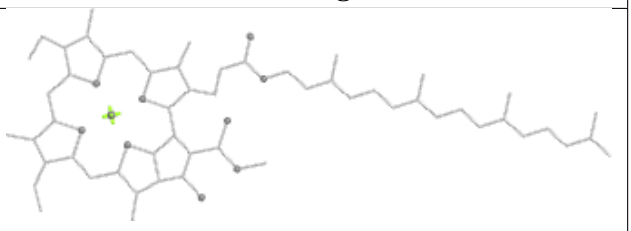
Bond lengths



Bond angles

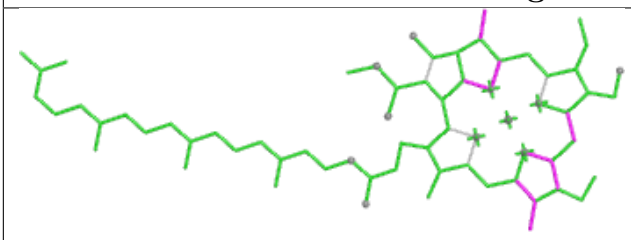


Torsions

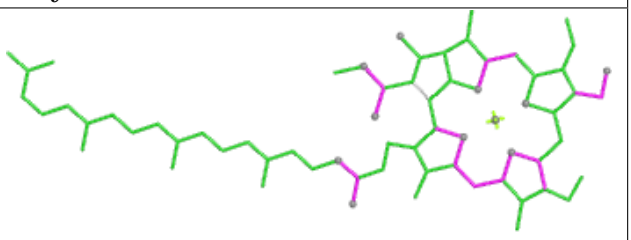


Rings

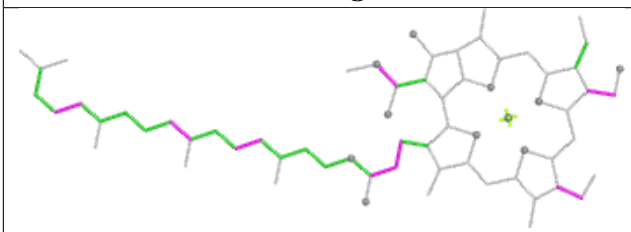
Ligand CHL y 309



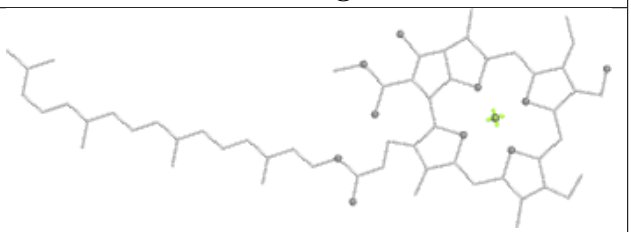
Bond lengths



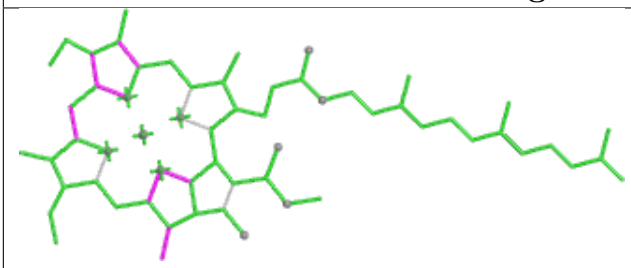
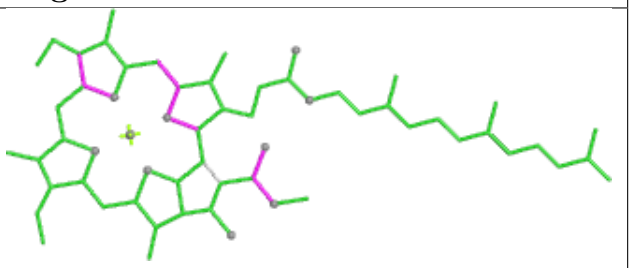
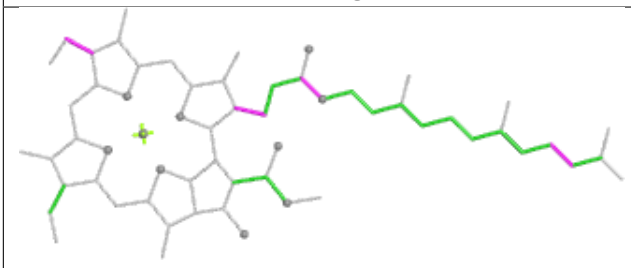
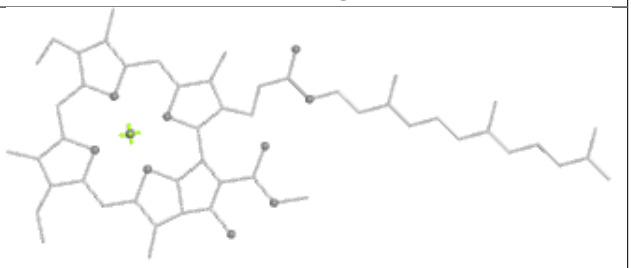
Bond angles

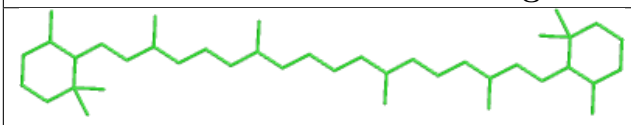
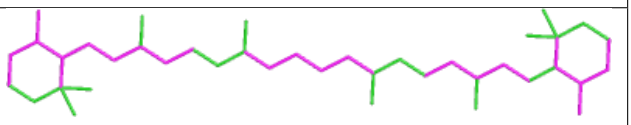
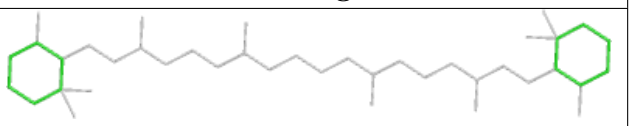


Torsions

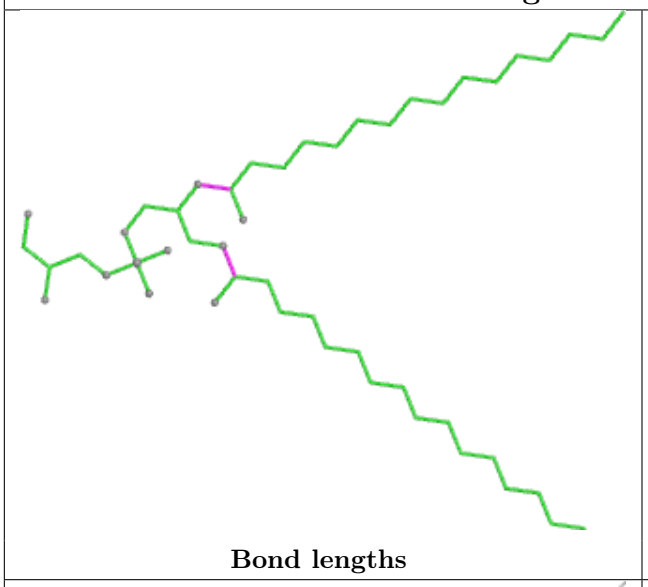


Rings

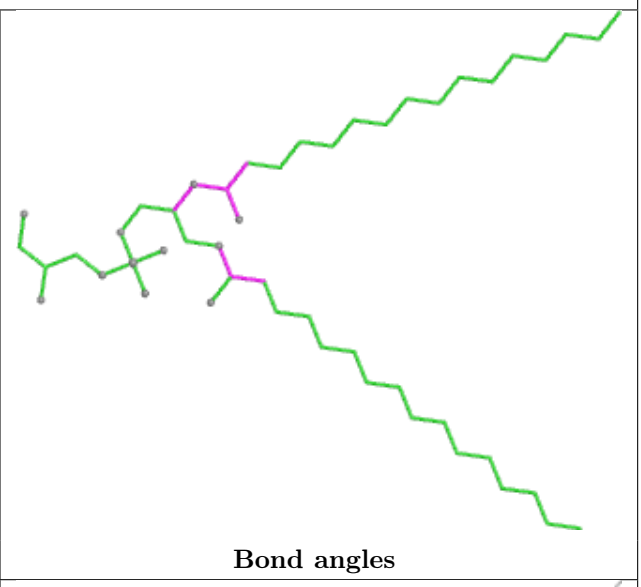
Ligand CLA g 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

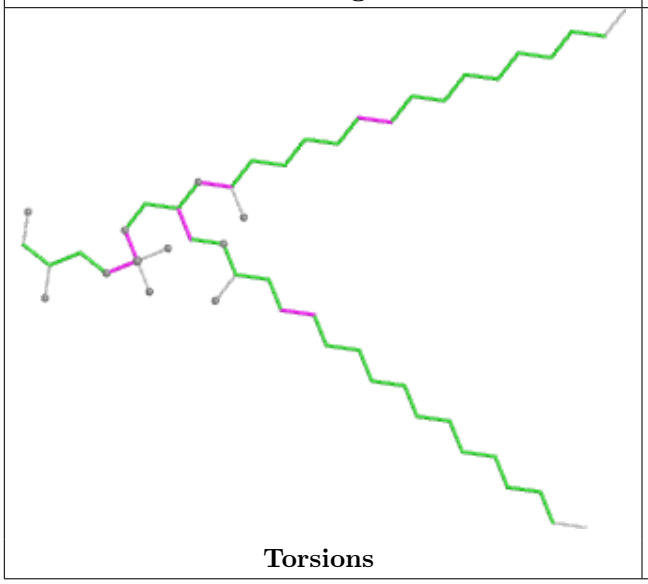
Ligand LHG N 618



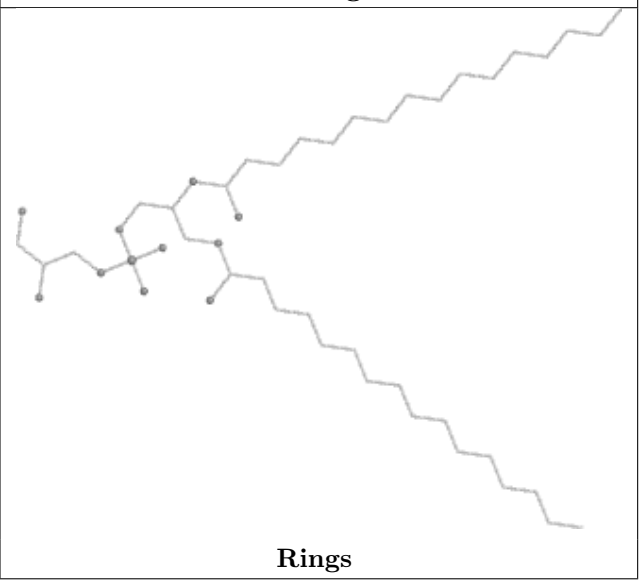
Bond lengths



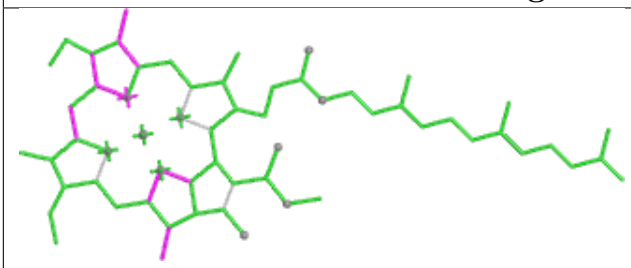
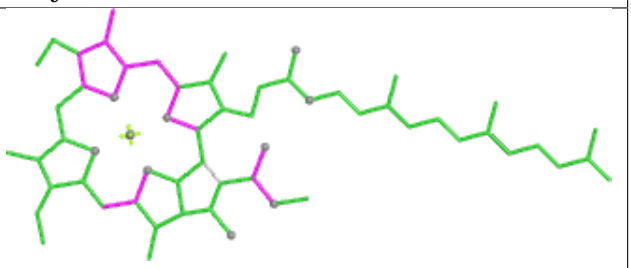
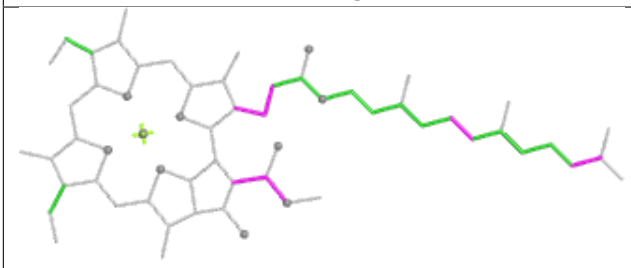
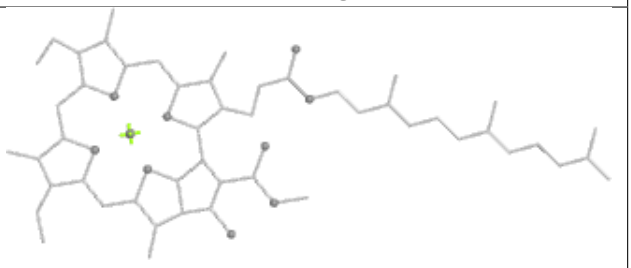
Bond angles

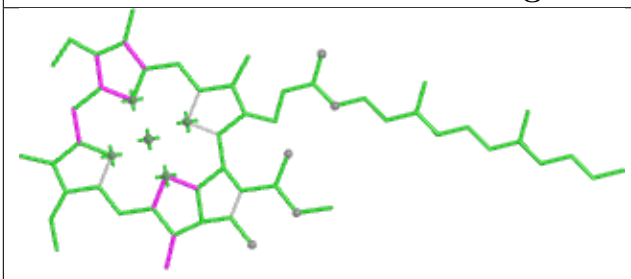
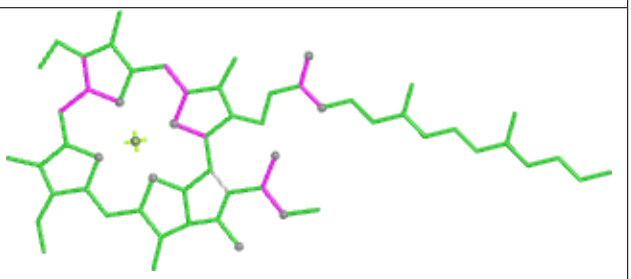
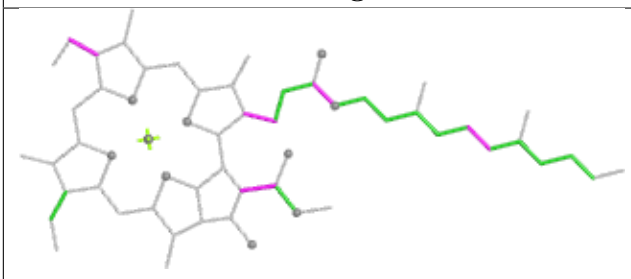
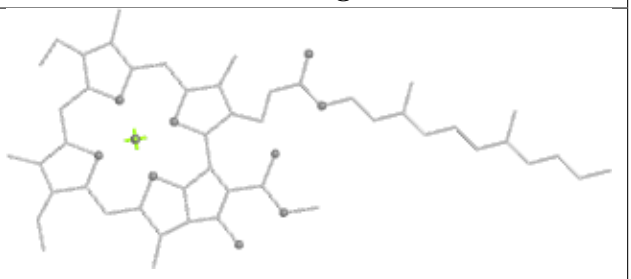


Torsions

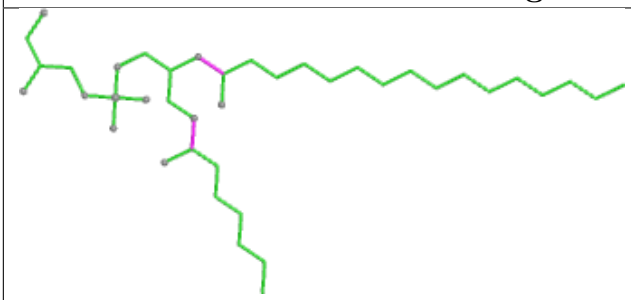


Rings

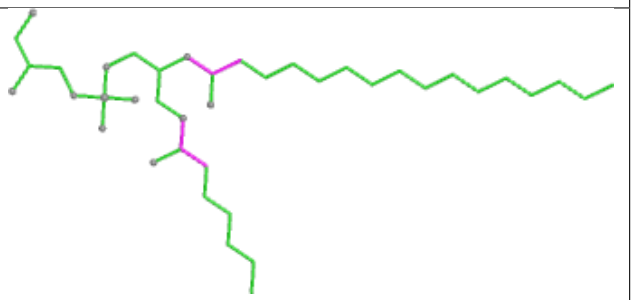
Ligand CLA y 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

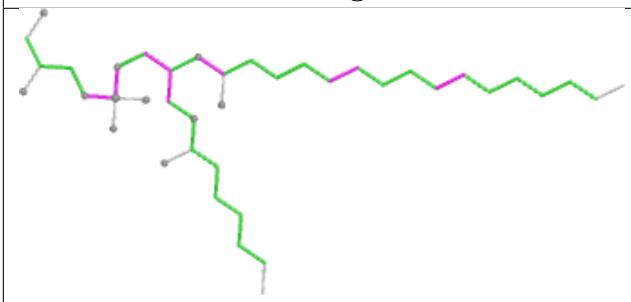
Ligand LHG b 626



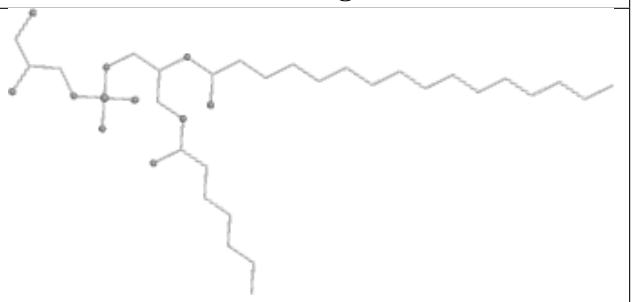
Bond lengths



Bond angles

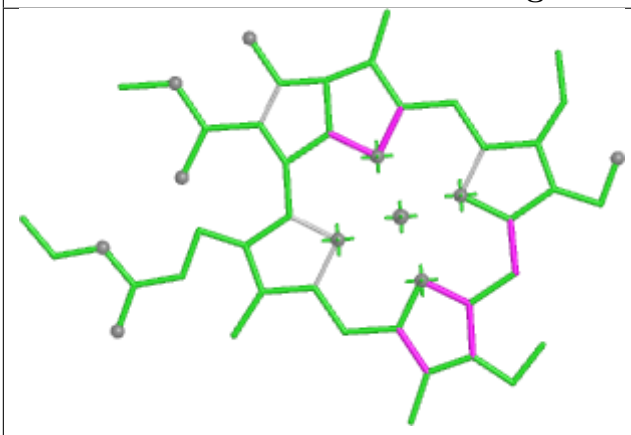


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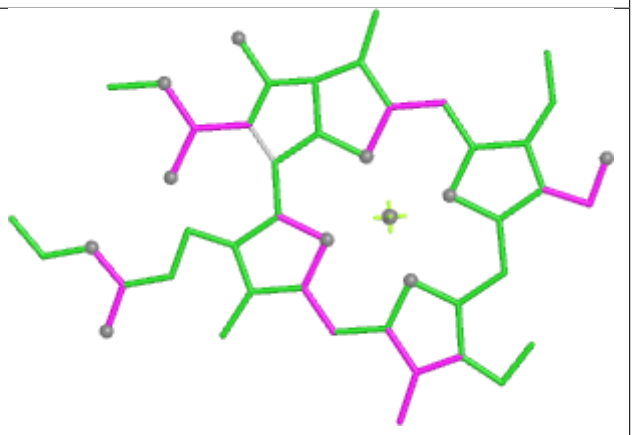


Rings

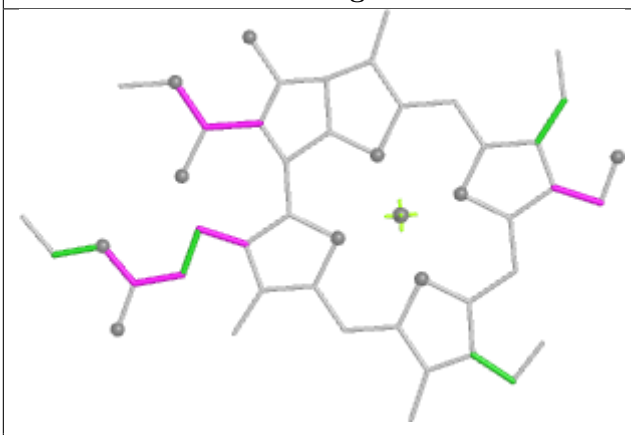
Ligand CHL n 605



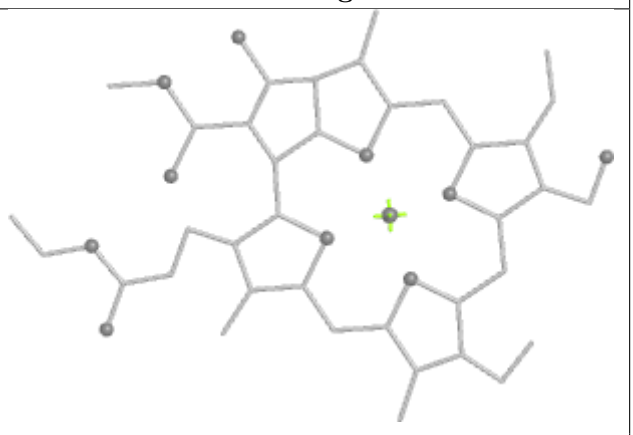
Bond lengths



Bond angles

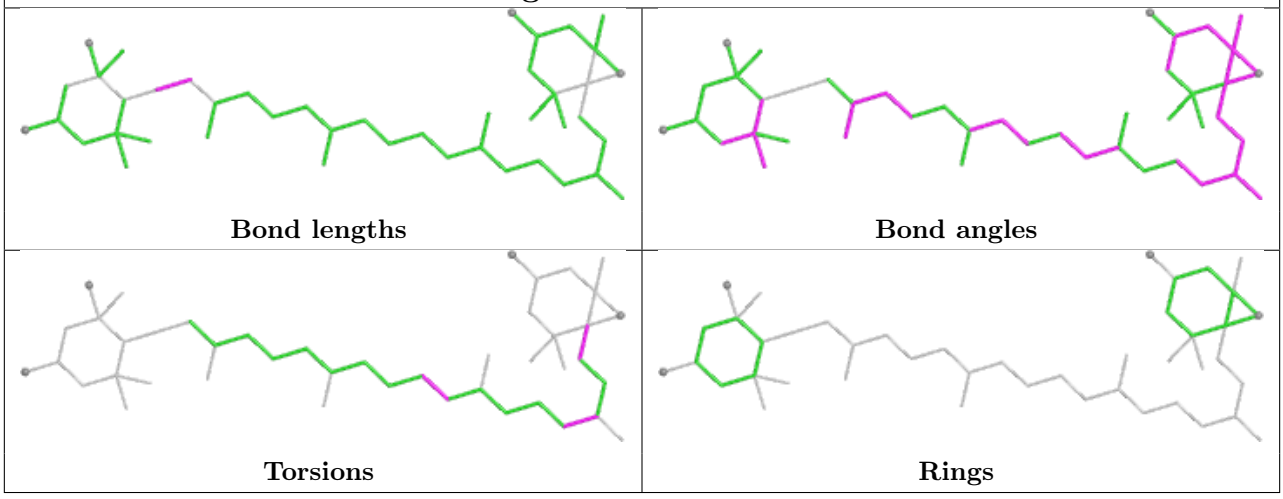


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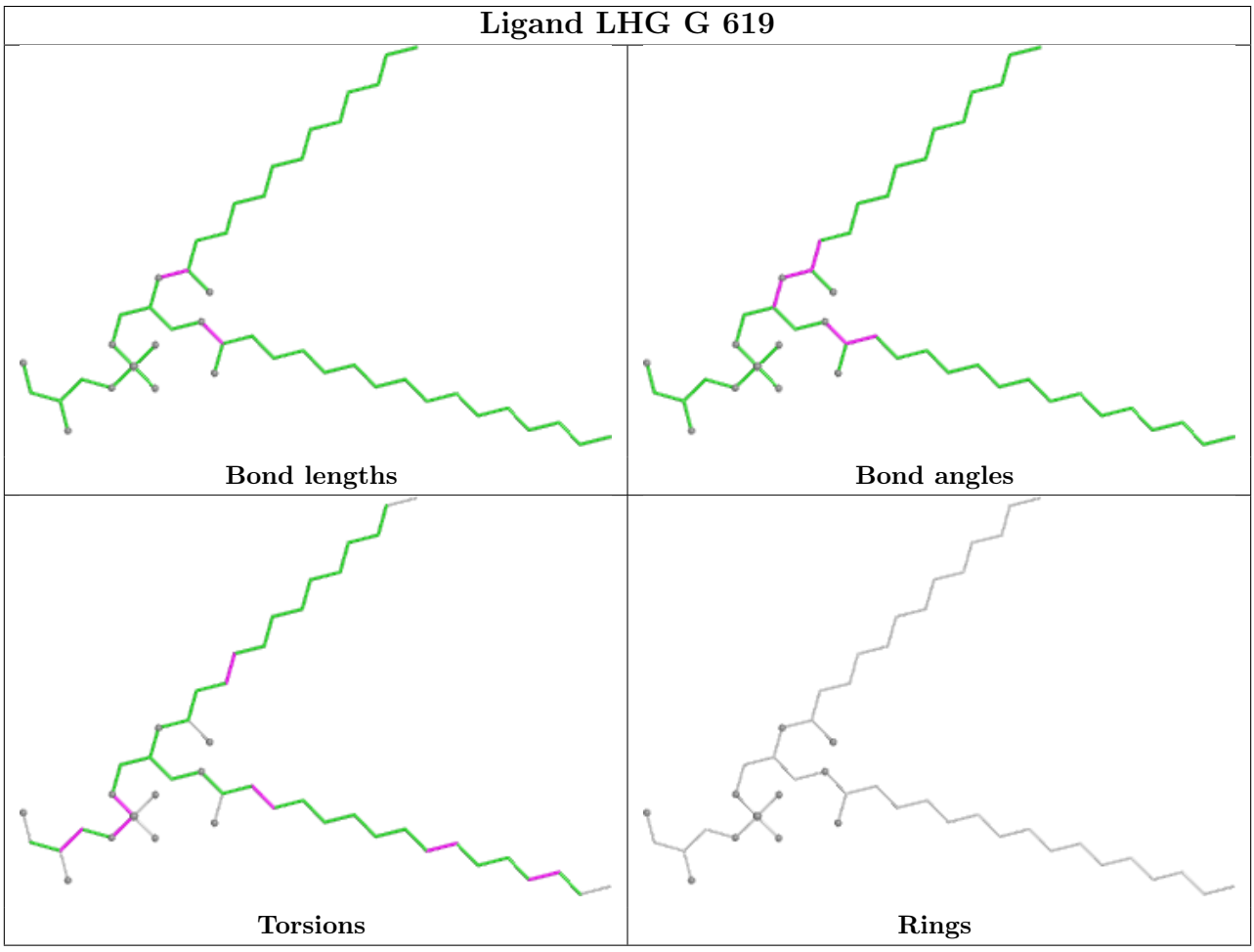


Rings

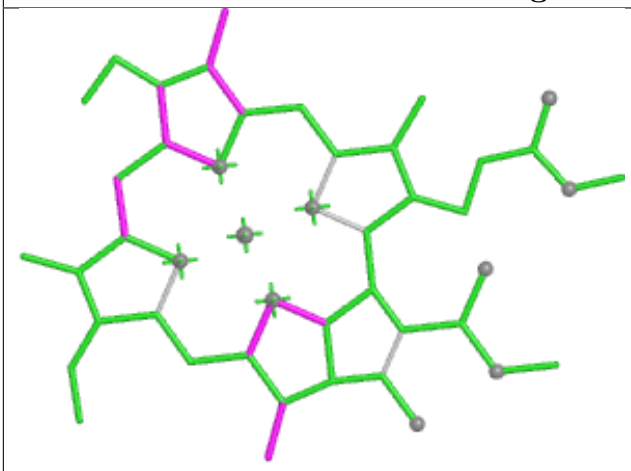
Ligand NEX N 617



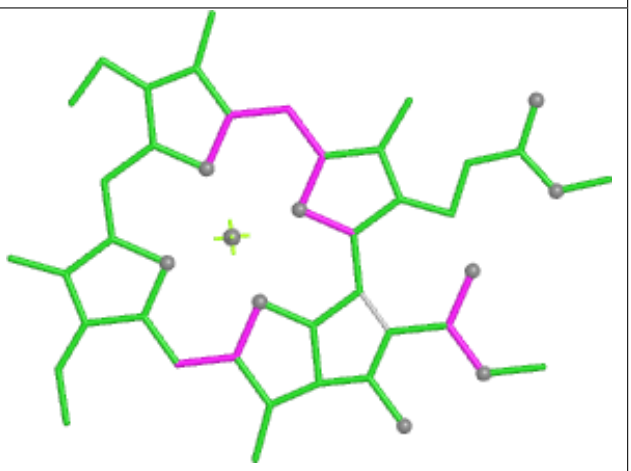
Ligand LHG G 619



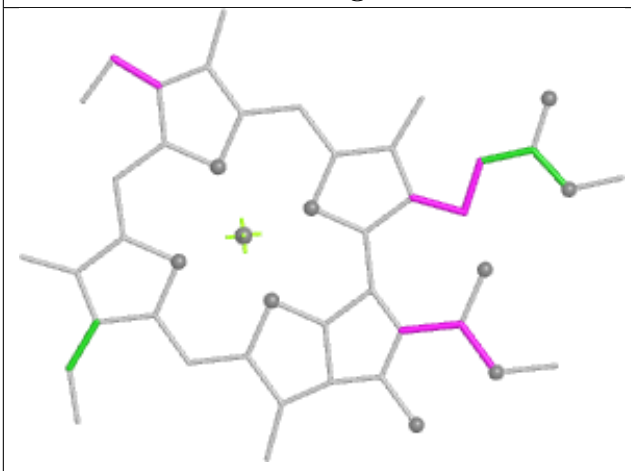
Ligand CLA s 602



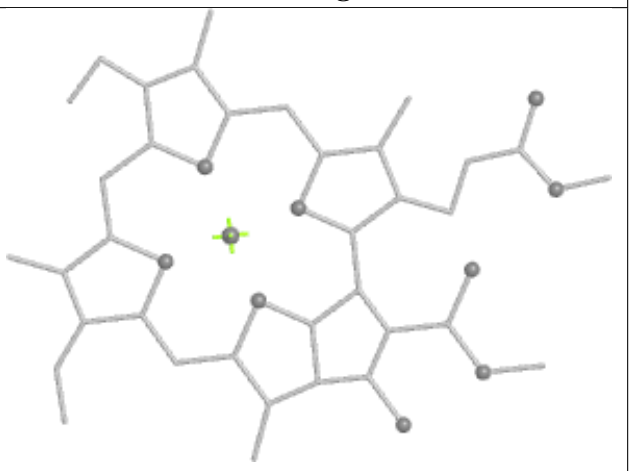
Bond lengths



Bond angles



Torsions

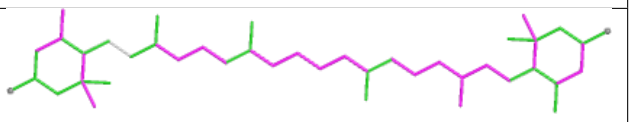


Rings

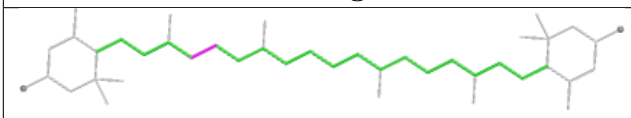
Ligand LUT n 616



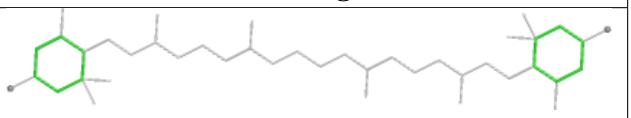
Bond lengths



Bond angles

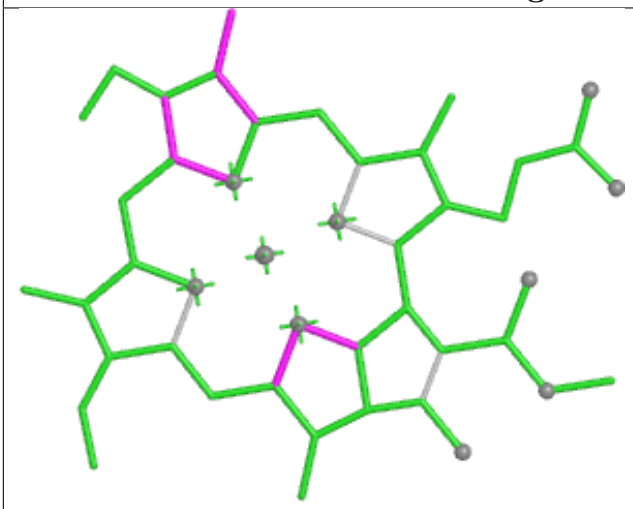


Torsions

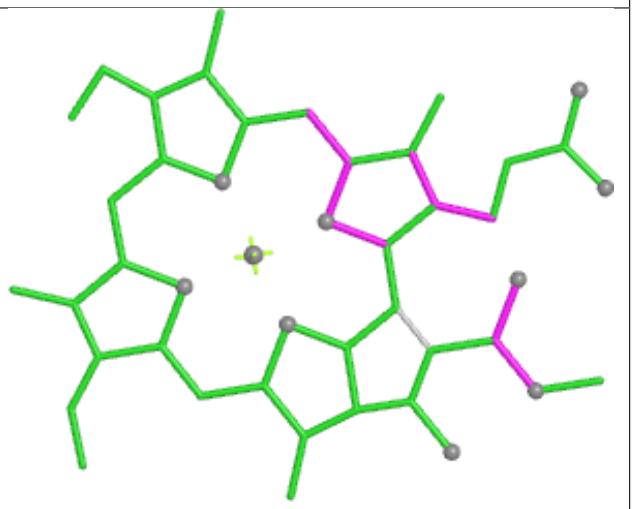


Rings

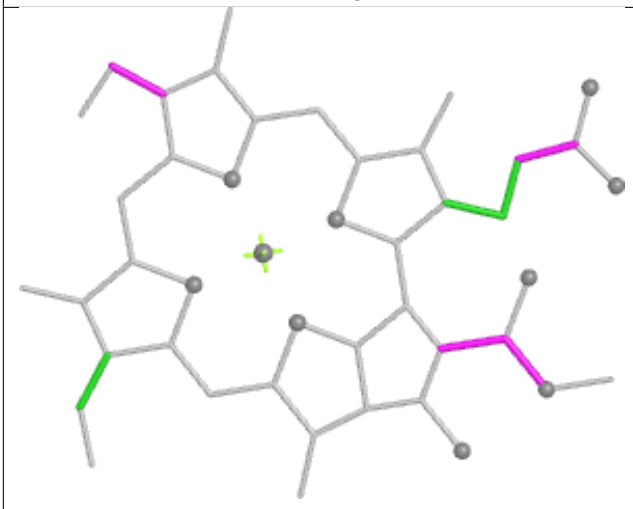
Ligand CLA S 304



Bond lengths



Bond angles

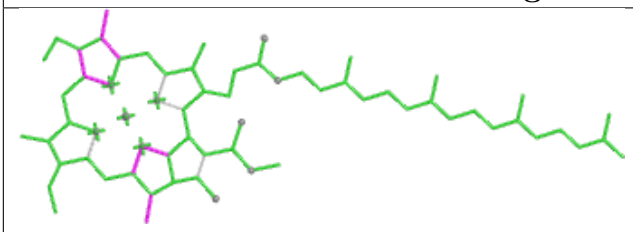


Torsions

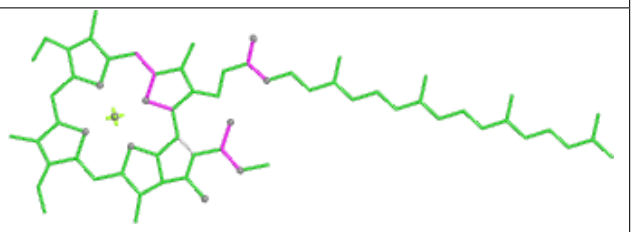


Rings

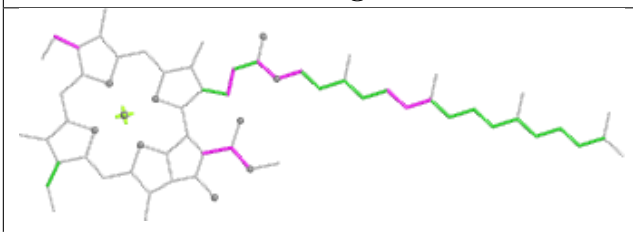
Ligand CLA Y 314



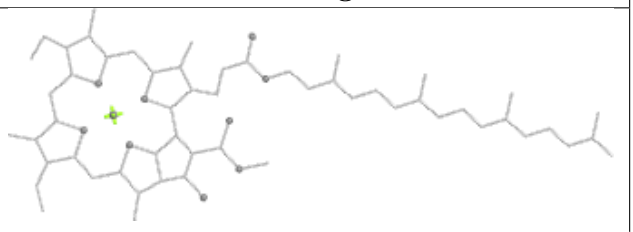
Bond lengths



Bond angles

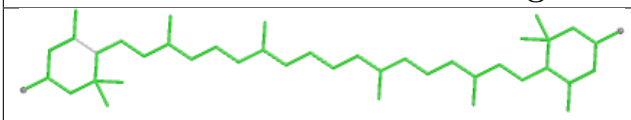


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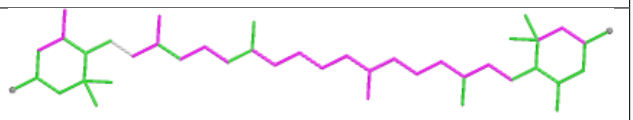


Rings

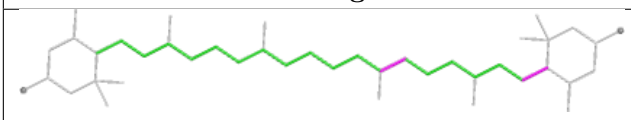
Ligand LUT n 615



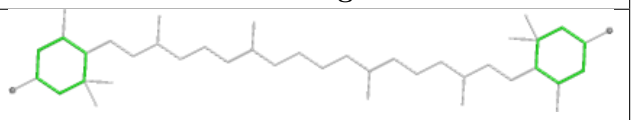
Bond lengths



Bond angles

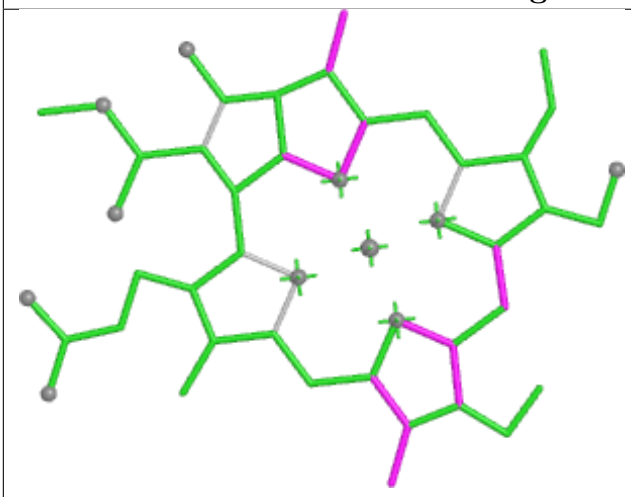


Torsions

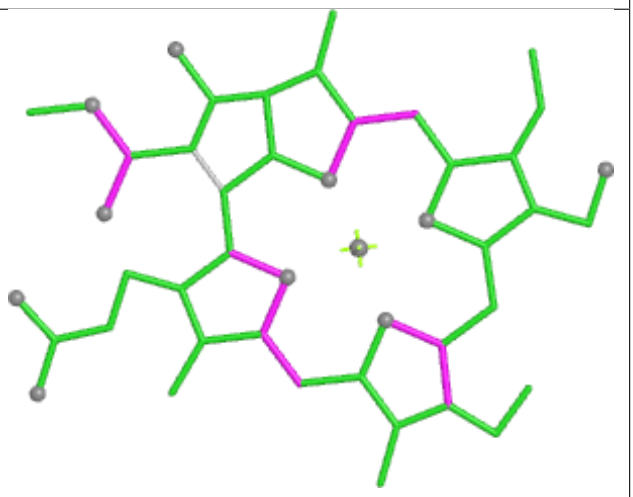


Rings

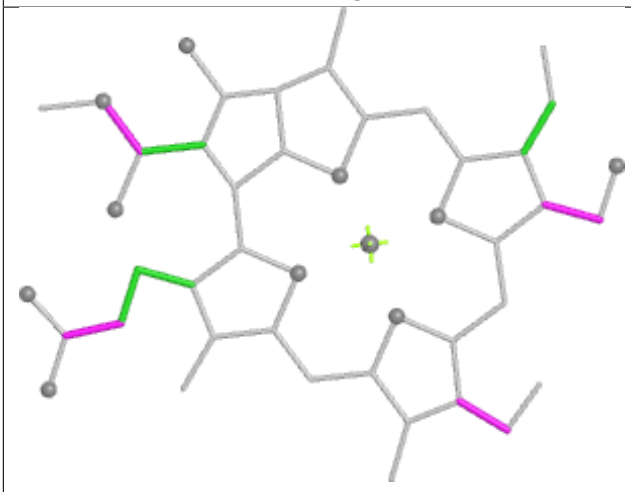
Ligand CHL s 605



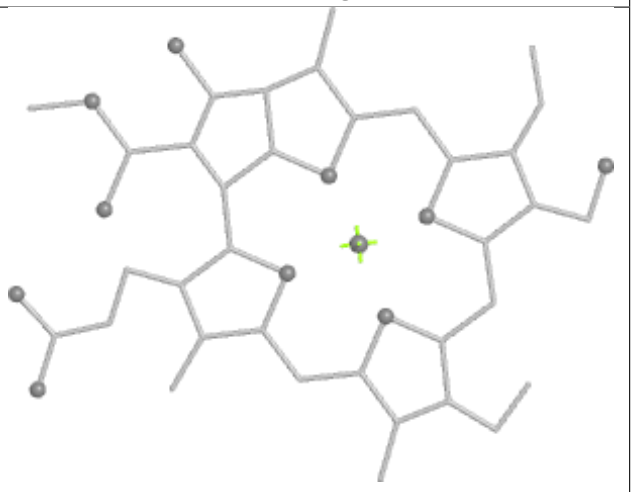
Bond lengths



Bond angles

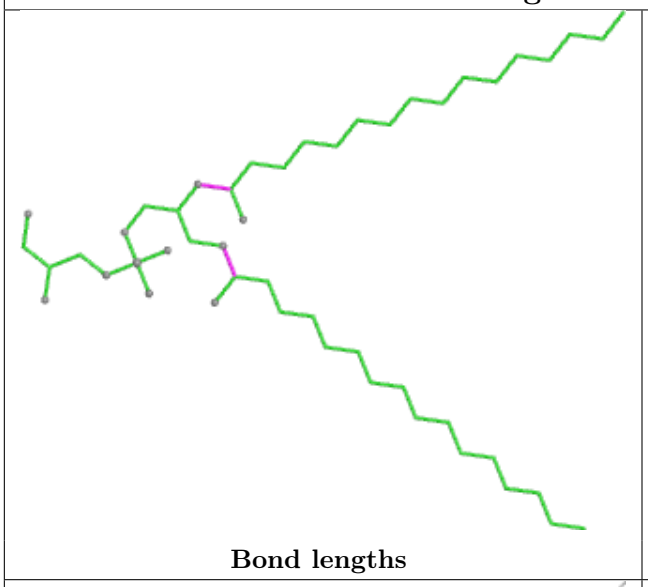


Torsions

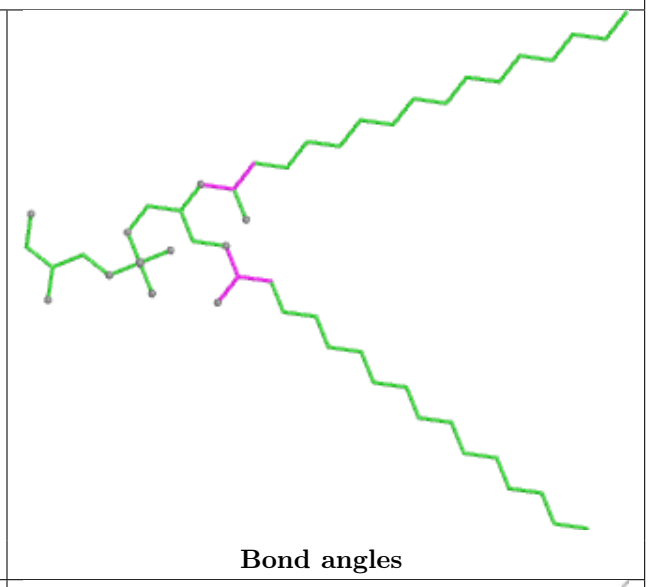


Rings

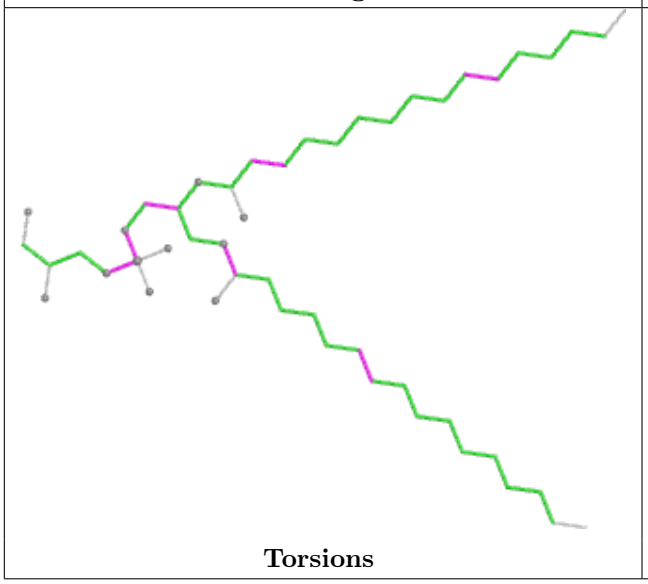
Ligand LHG B 621



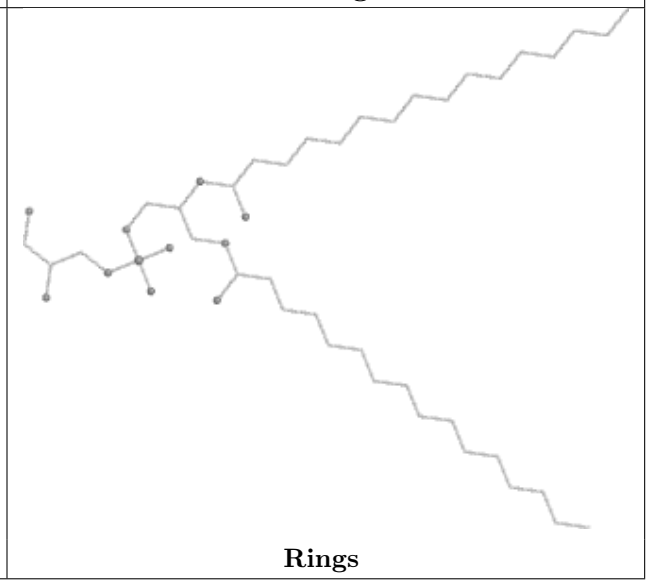
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Bond angles

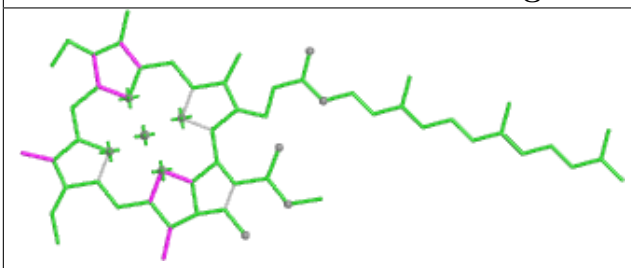


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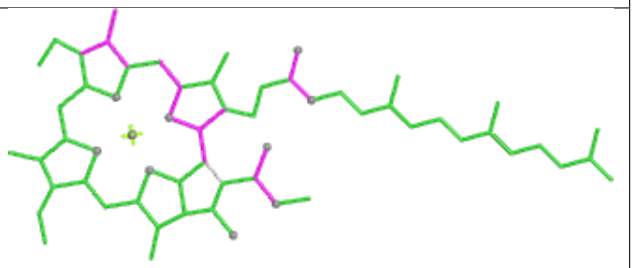


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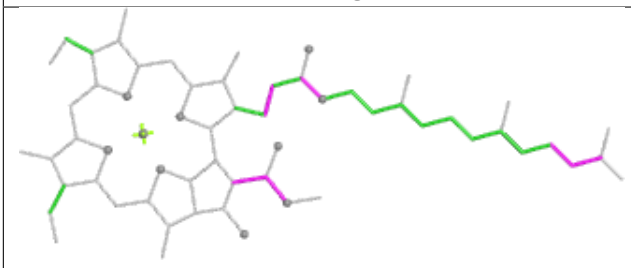
Ligand CLA Y 313



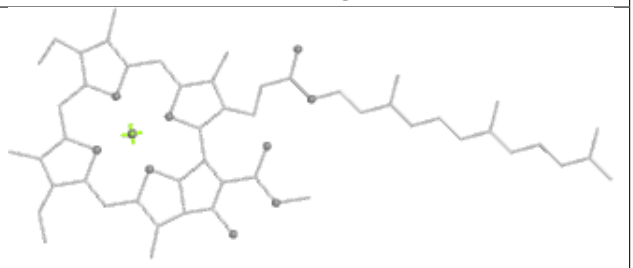
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Bond angles

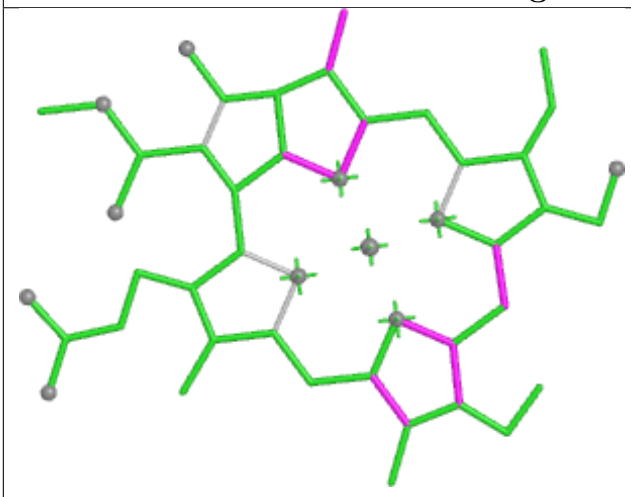


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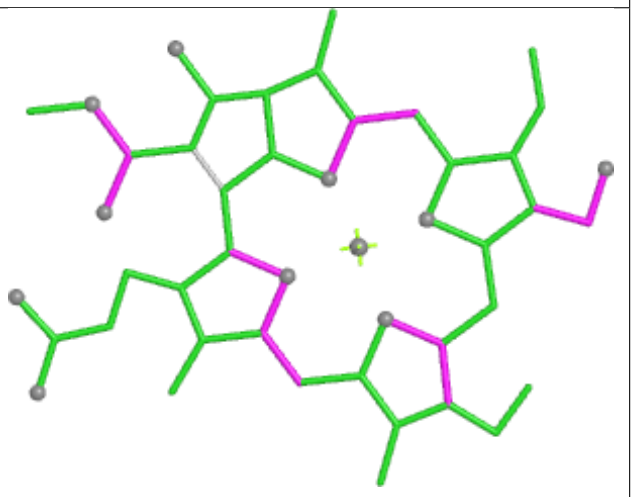


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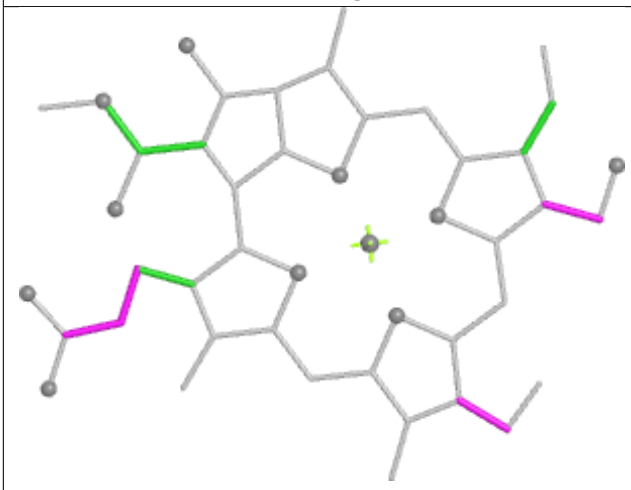
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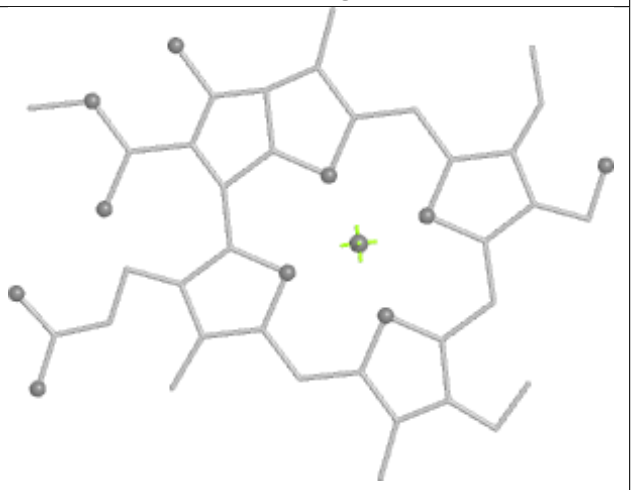
Bond lengths



Bond angles

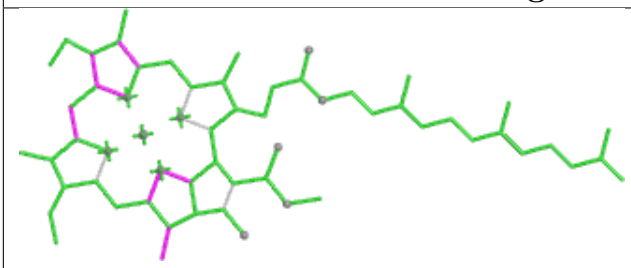


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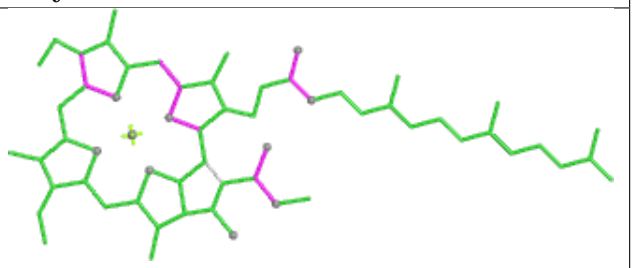


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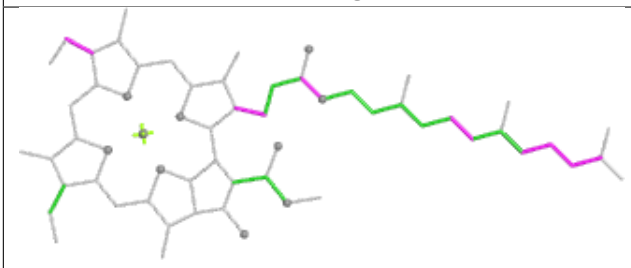
Ligand CLA y 312



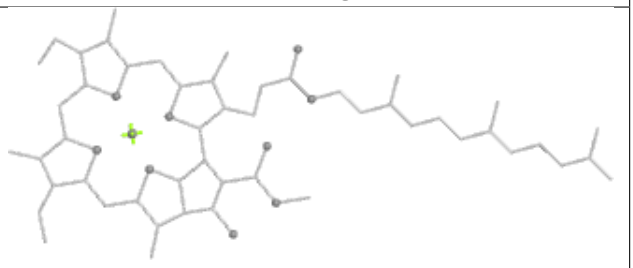
Bond lengths



Bond angles

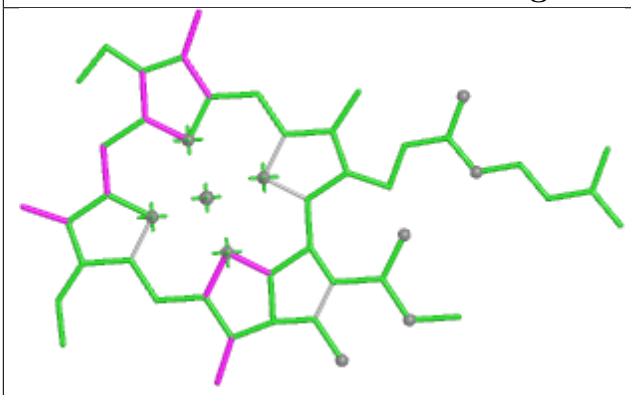


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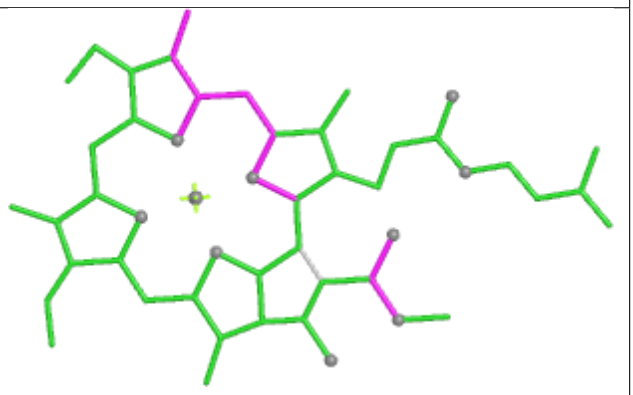


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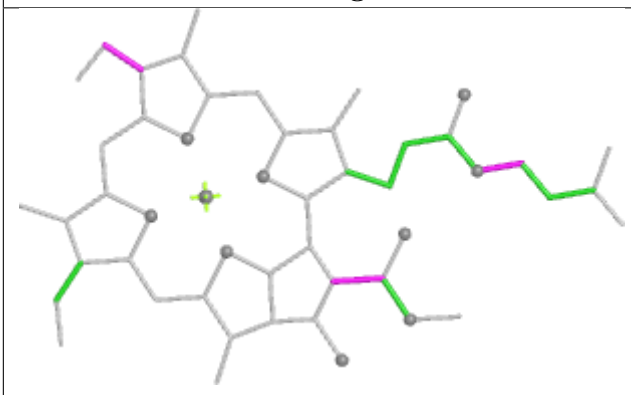
Ligand CLA s 604



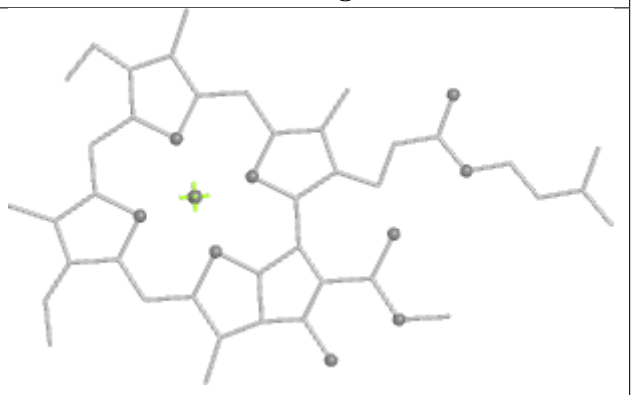
Bond lengths



Bond angles

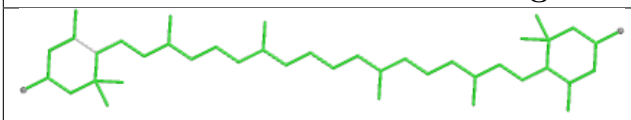


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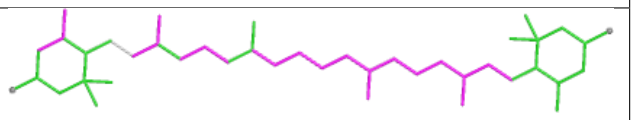


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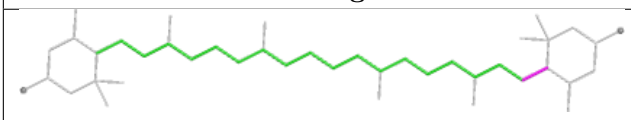
Ligand LUT s 614



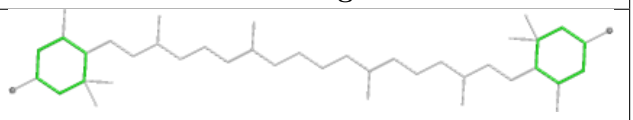
Bond lengths



Bond angles

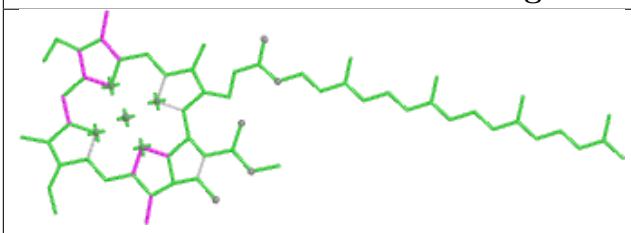


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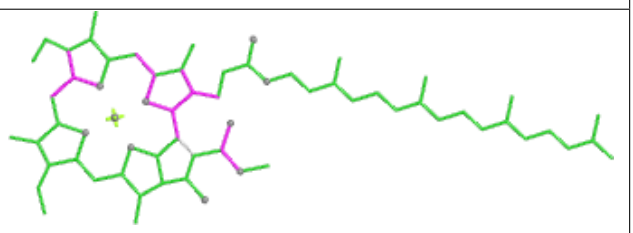


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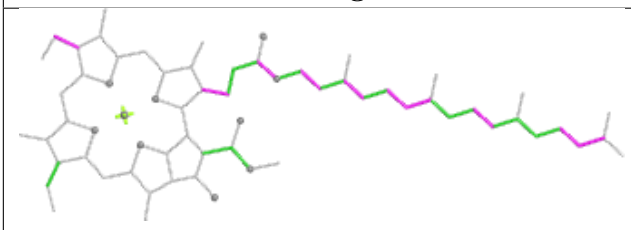
Ligand CLA B 602



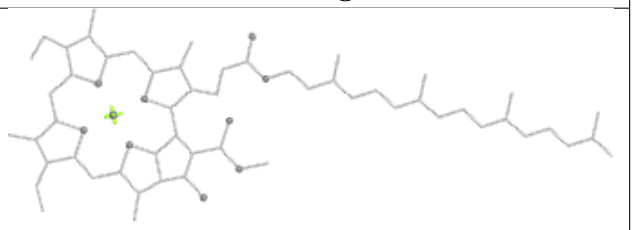
Bond lengths



Bond angles

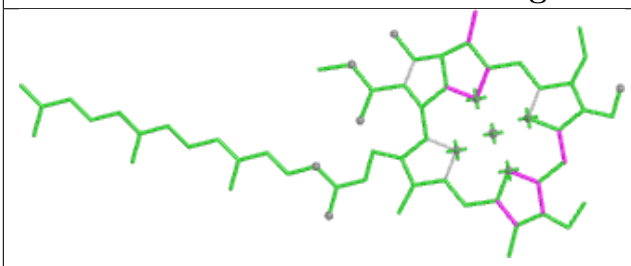


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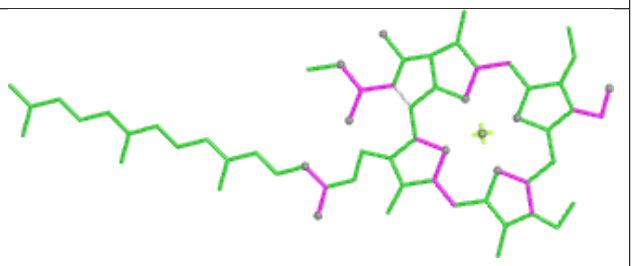


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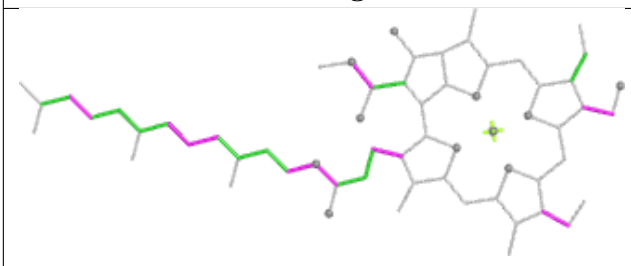
Ligand CHL r 607



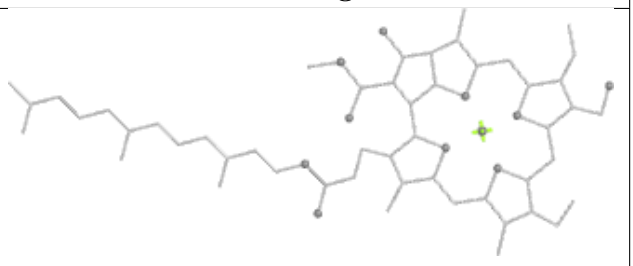
Bond lengths



Bond angles

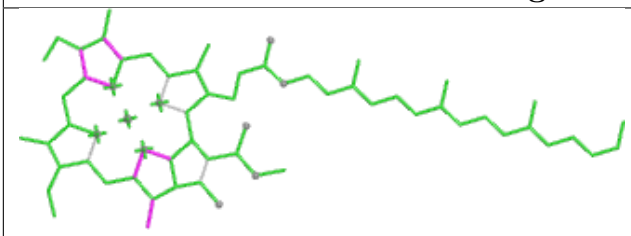


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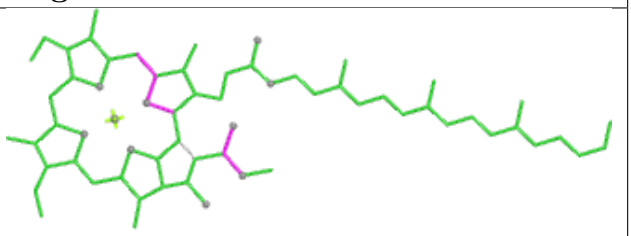


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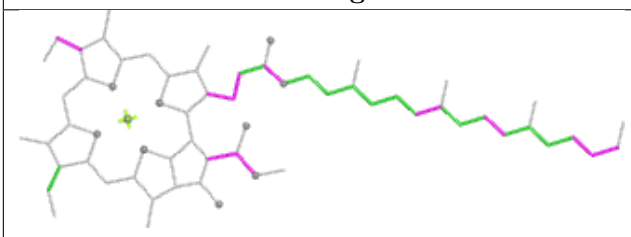
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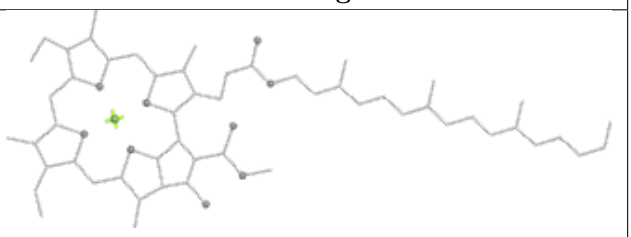
Bond lengths



Bond angles

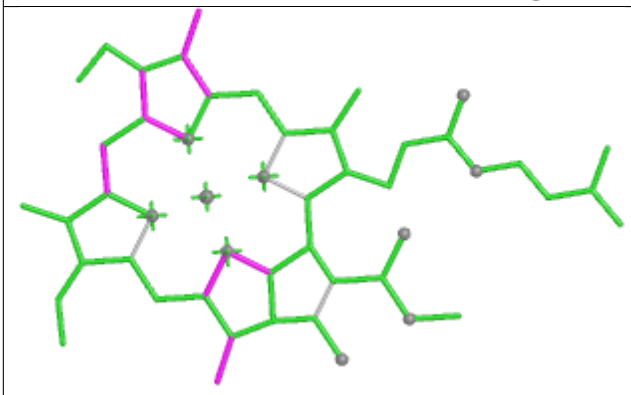


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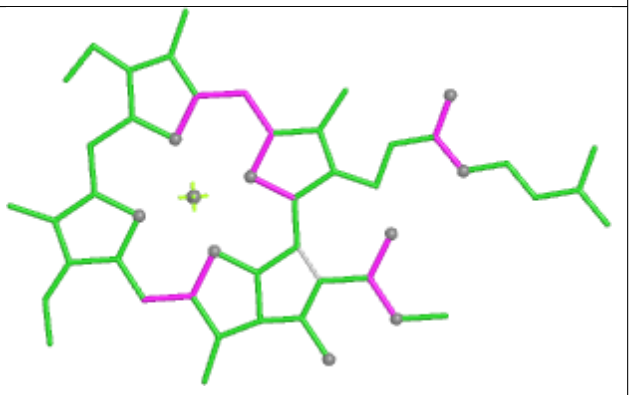


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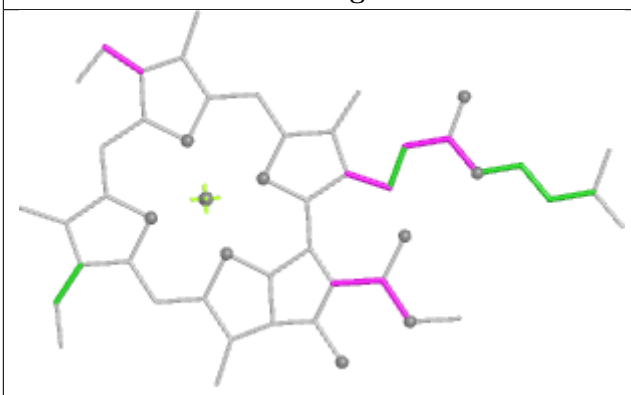
Ligand CLA d 402



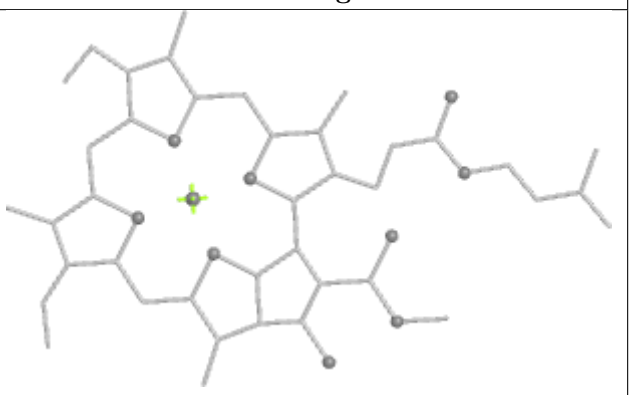
Bond lengths



Bond angles

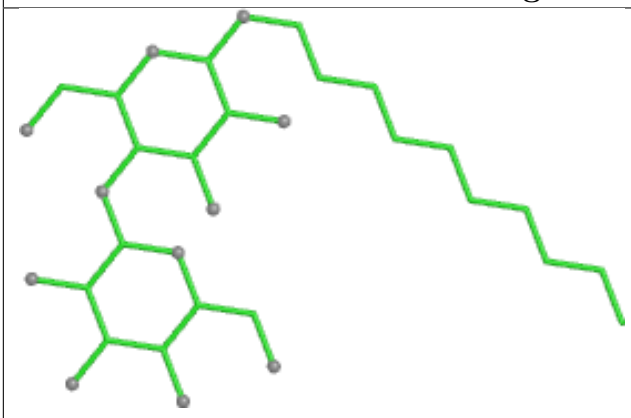


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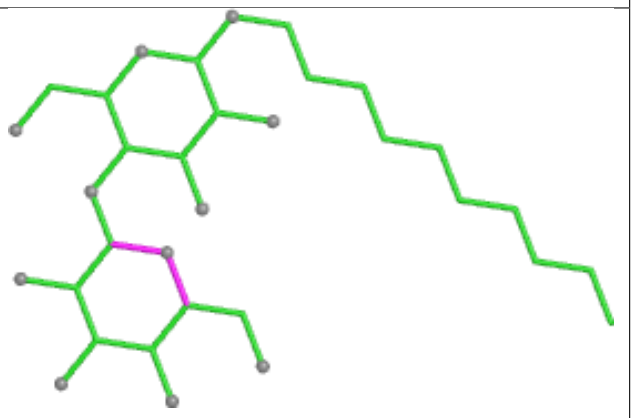


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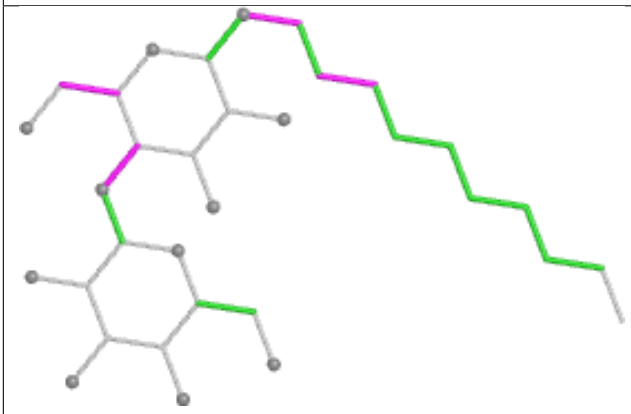
Ligand DMU s 618



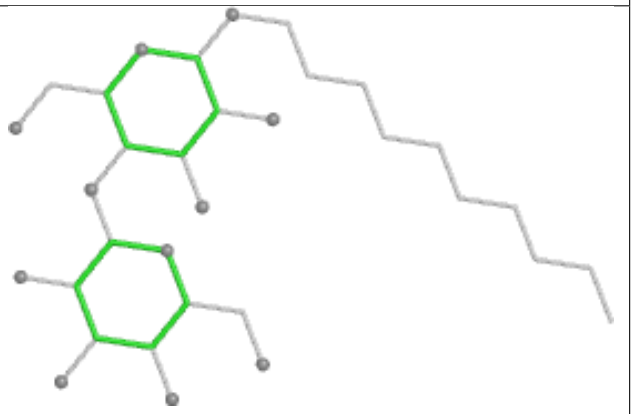
Bond lengths



Bond angles

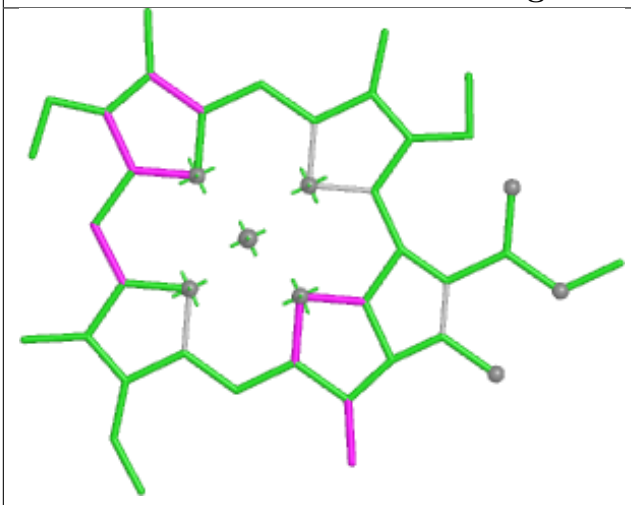


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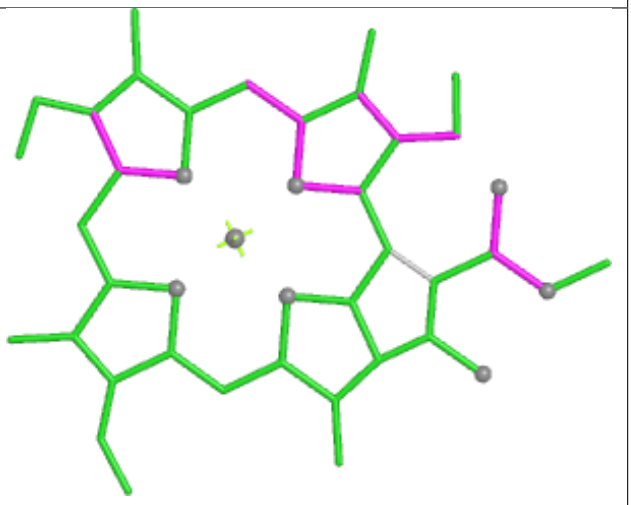


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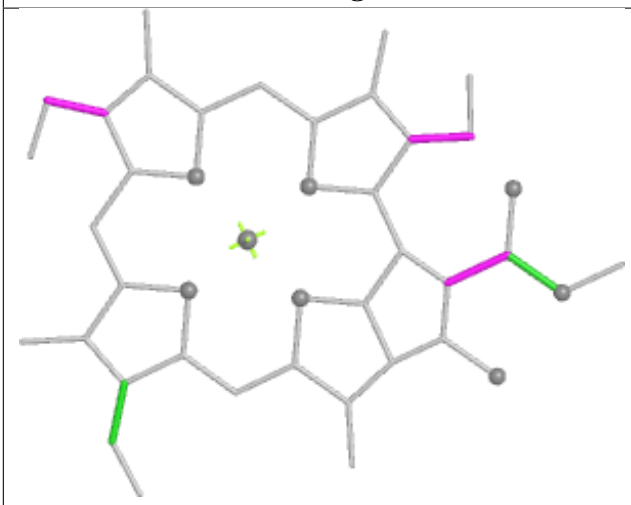
Ligand CLA S 311



Bond lengths



Bond angles



Torsions

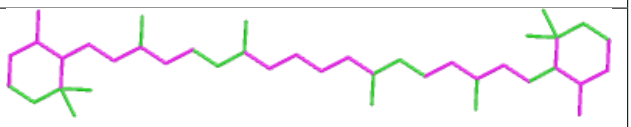


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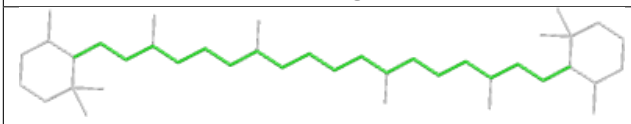
Ligand BCR b 620



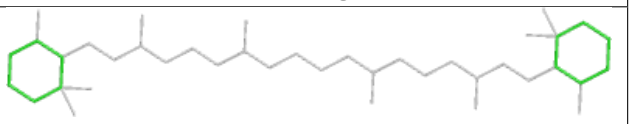
Bond lengths



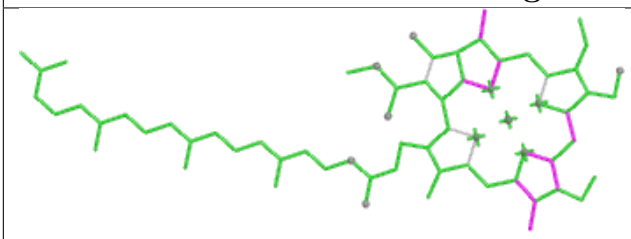
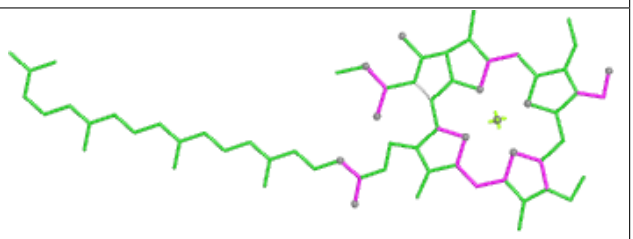
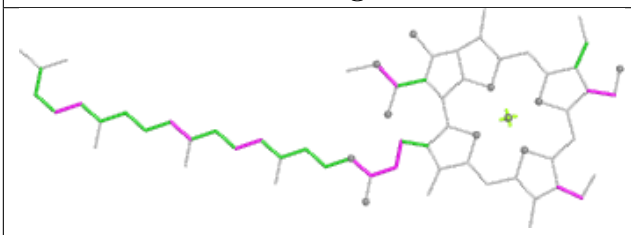
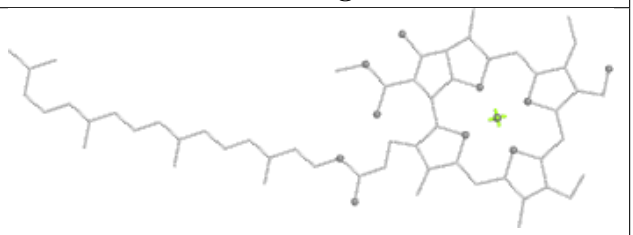
Bond angles

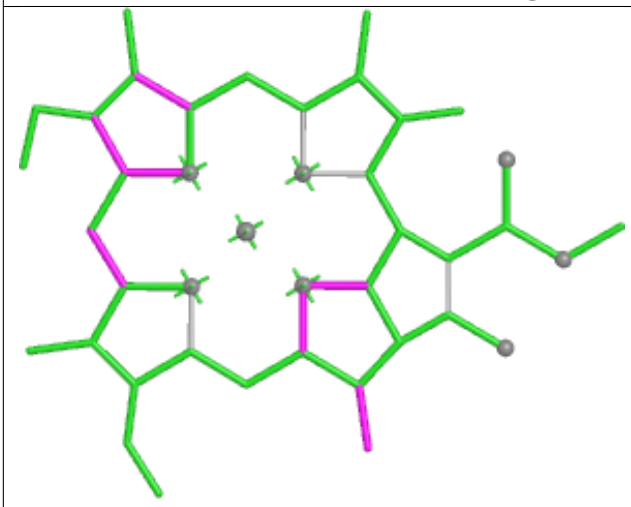
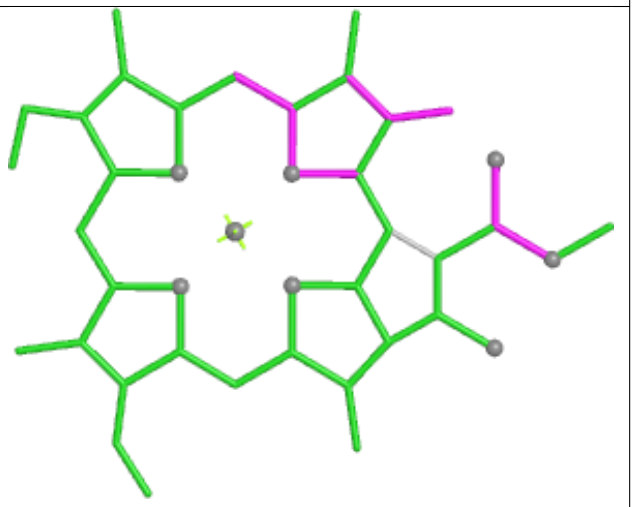
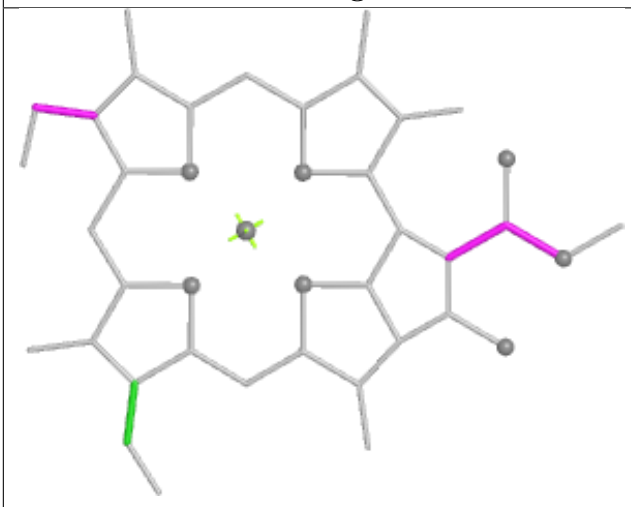
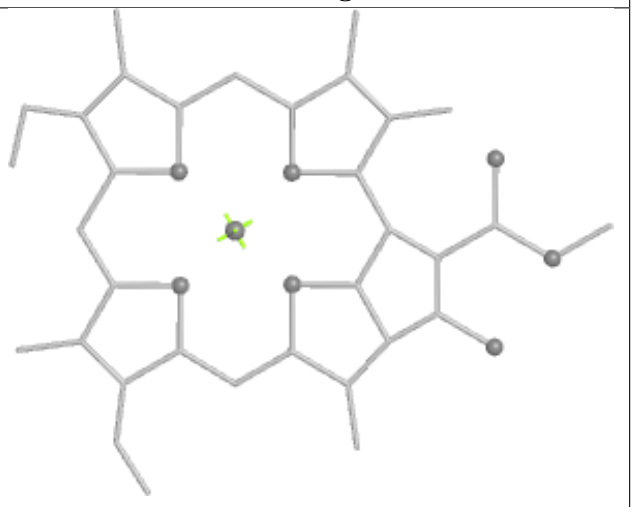


Torsions

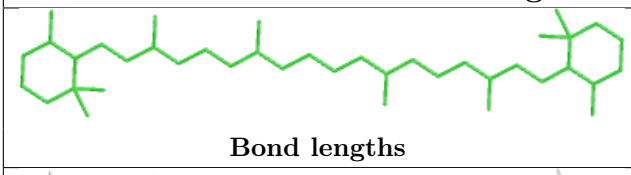


Rings

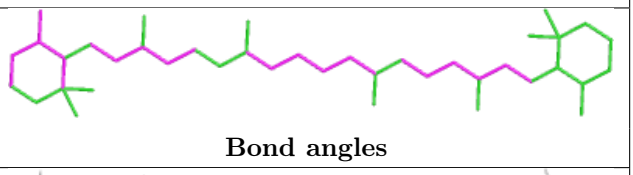
Ligand CHL Y 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

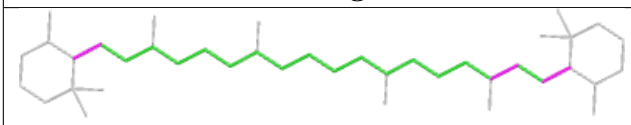
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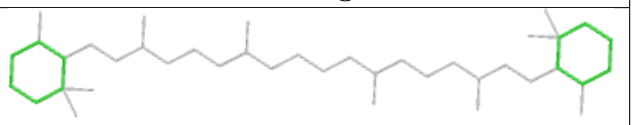
Bond lengths



Bond angles

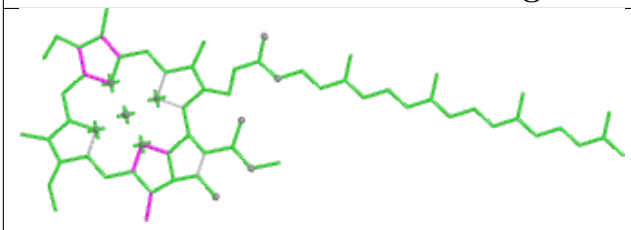


Torsions

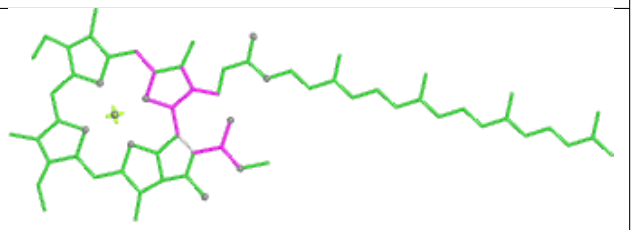


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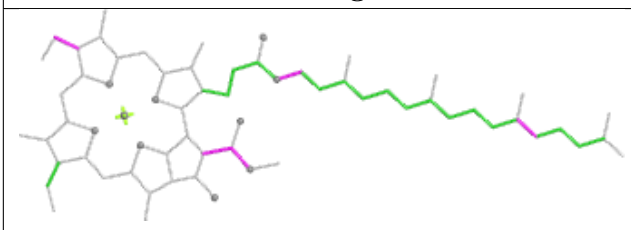
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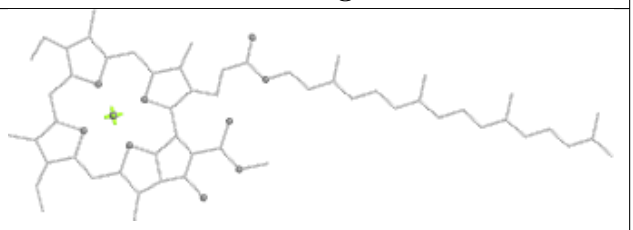
Bond lengths



Bond angles

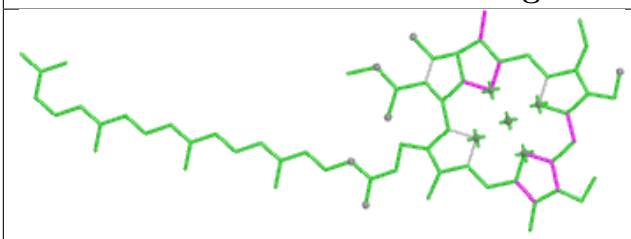


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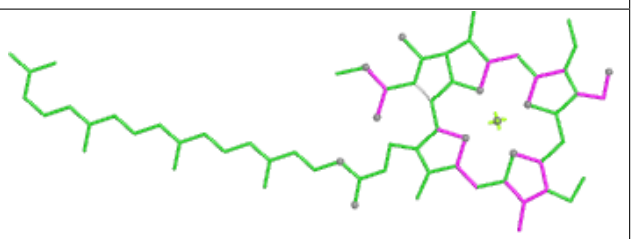


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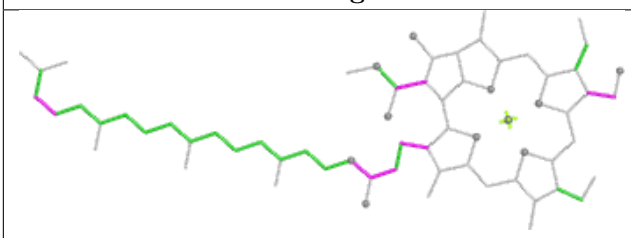
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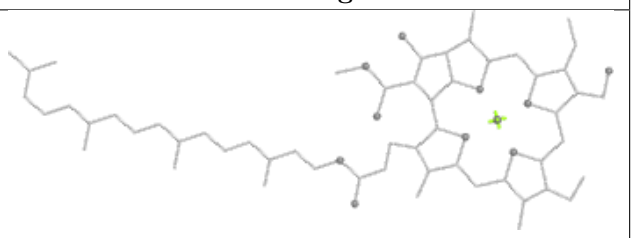
Bond lengths



Bond angles

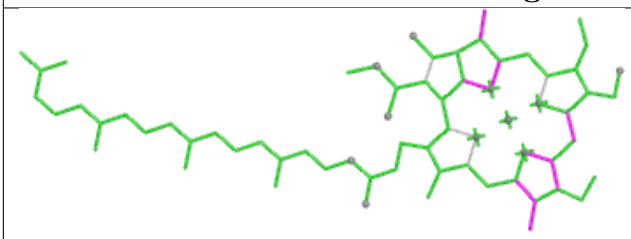


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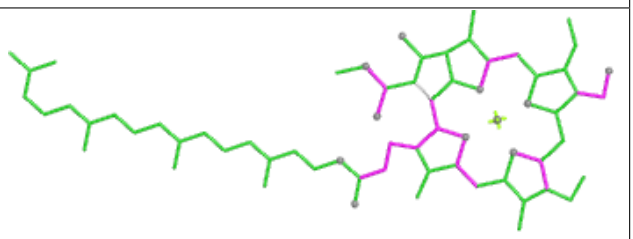


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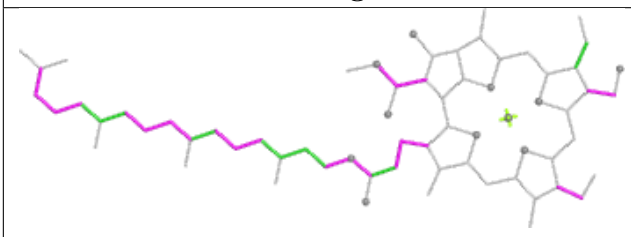
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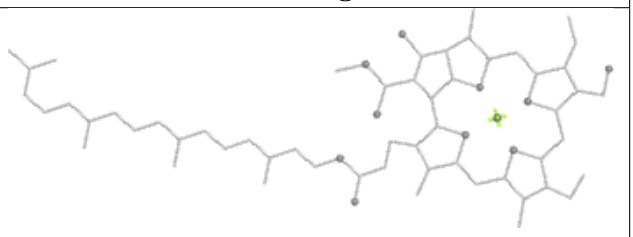
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Bond angles

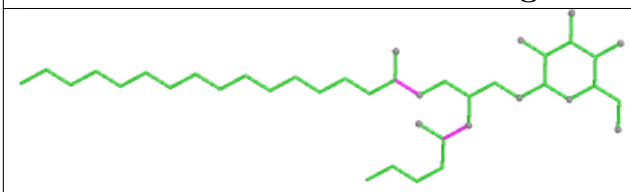


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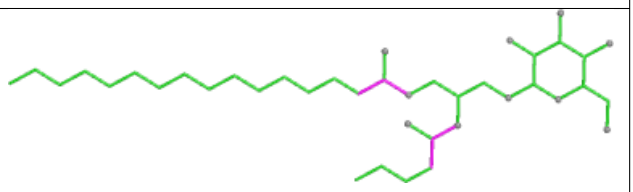


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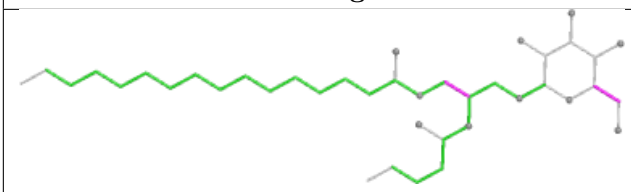
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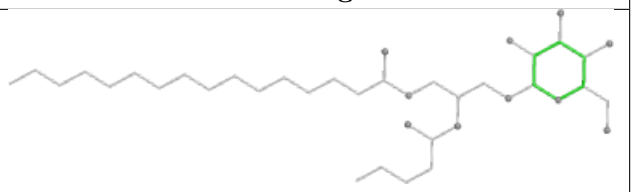
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Bond angles

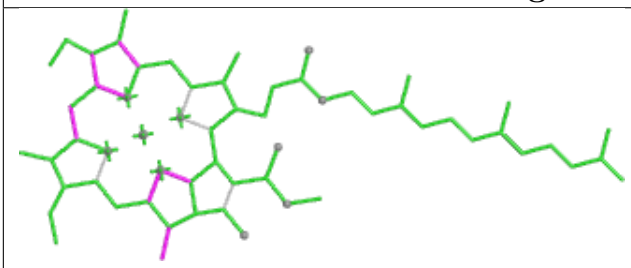


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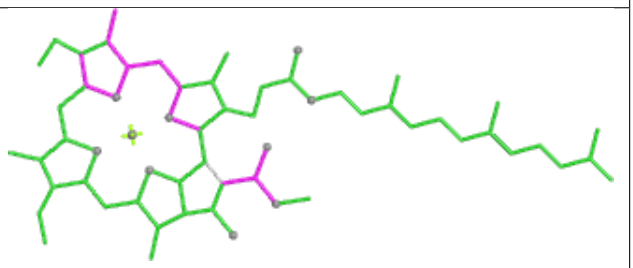


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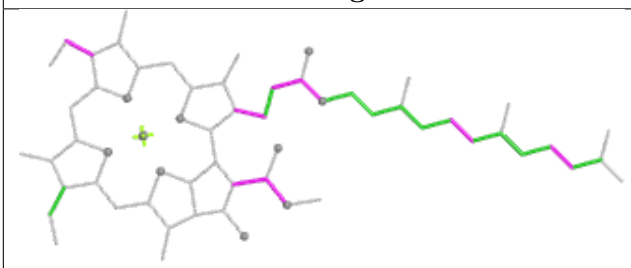
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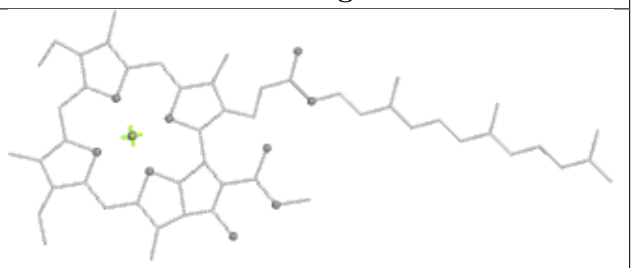
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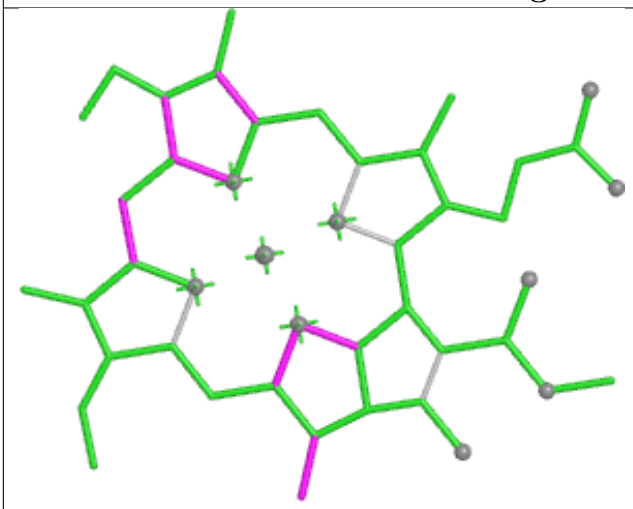


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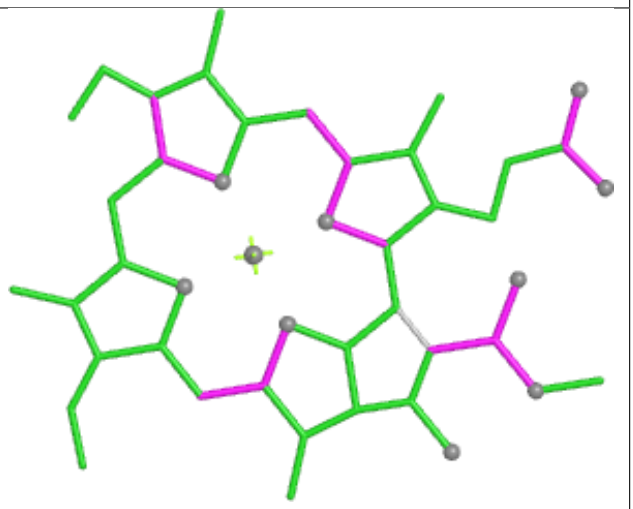


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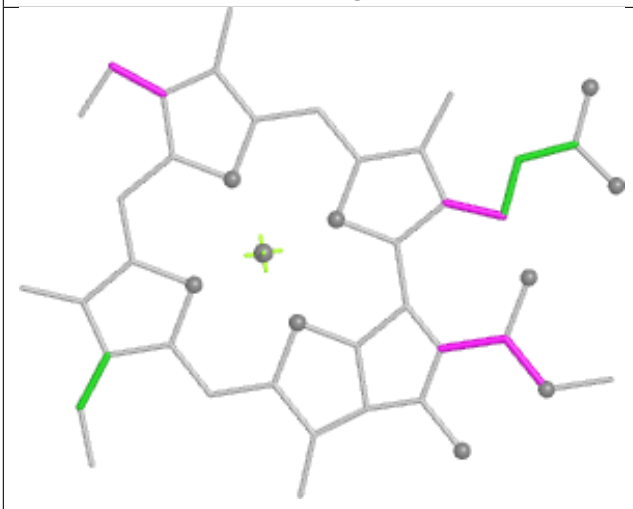
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Bond lengths



Bond angles

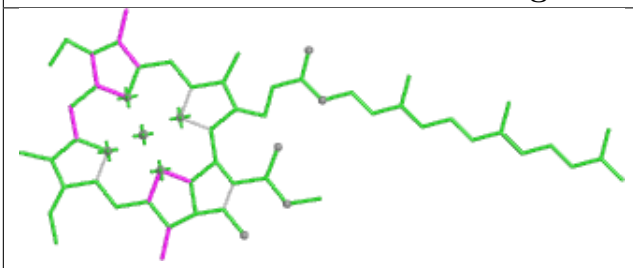


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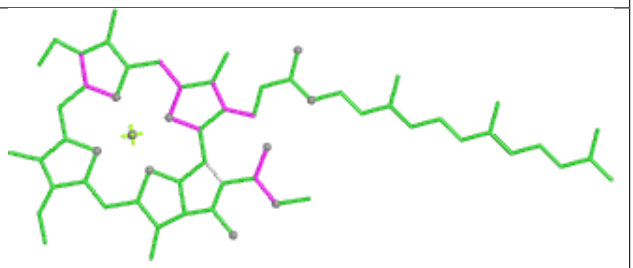


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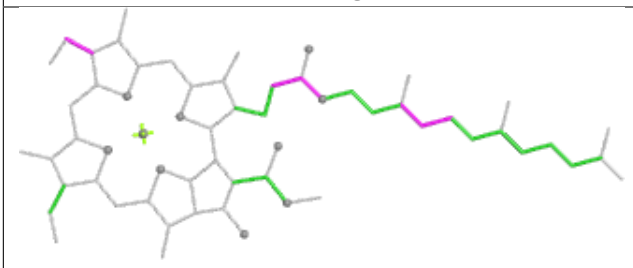
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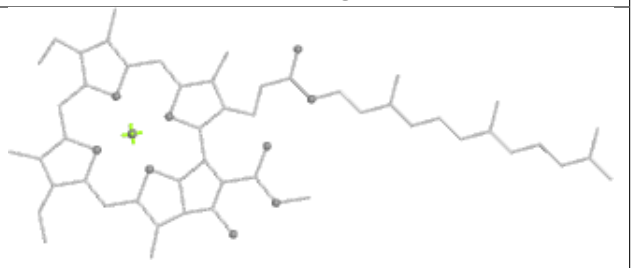
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Bond angles

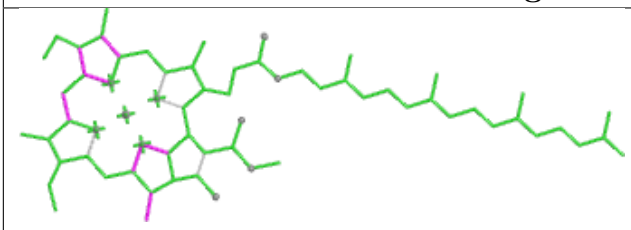


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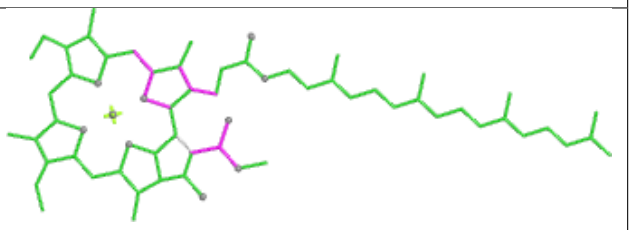


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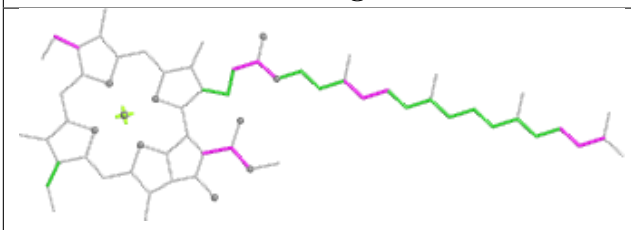
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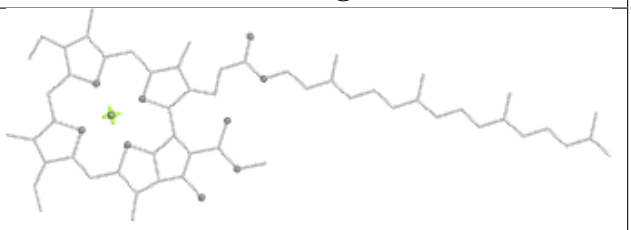
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Bond angles

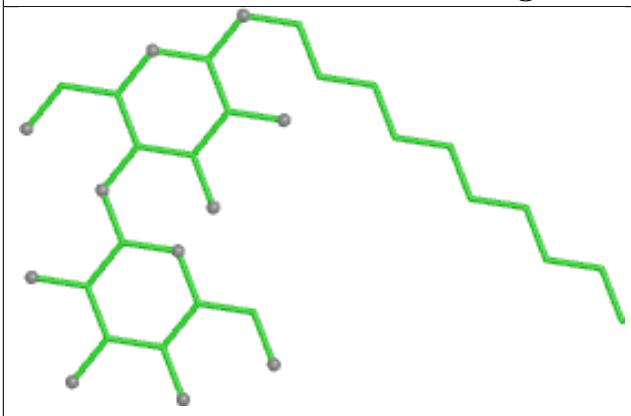


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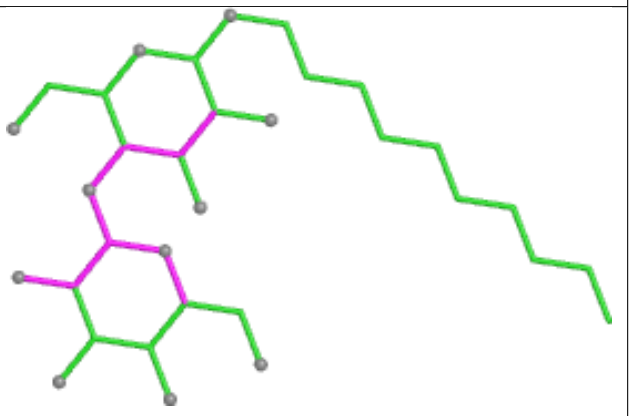


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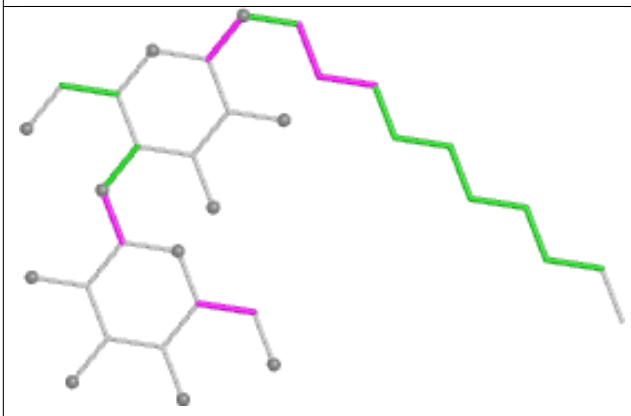
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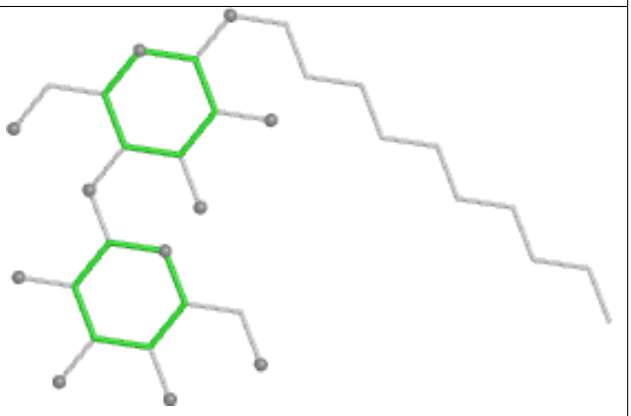
Bond lengths



Bond angles

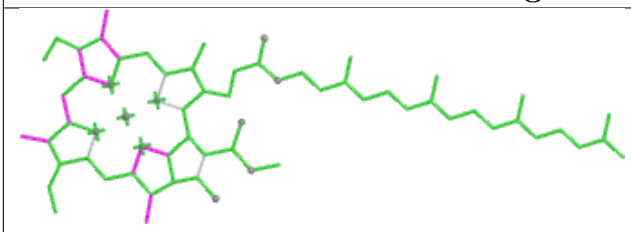


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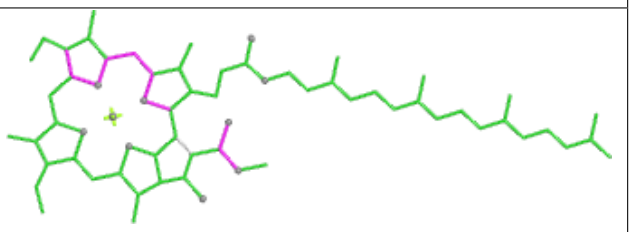


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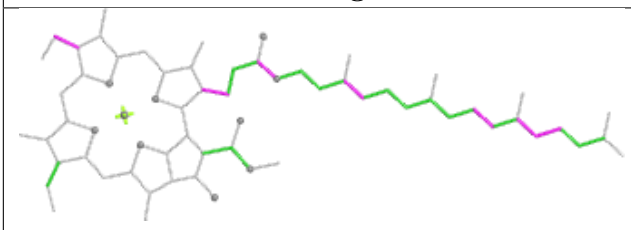
Ligand CLA B 611



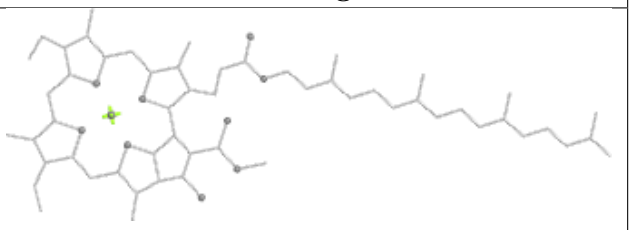
Bond lengths



Bond angles

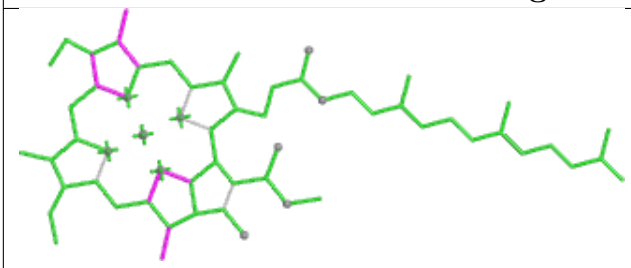


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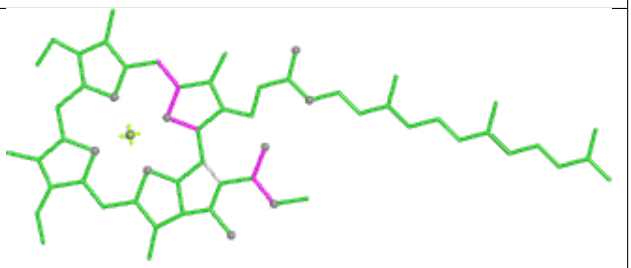


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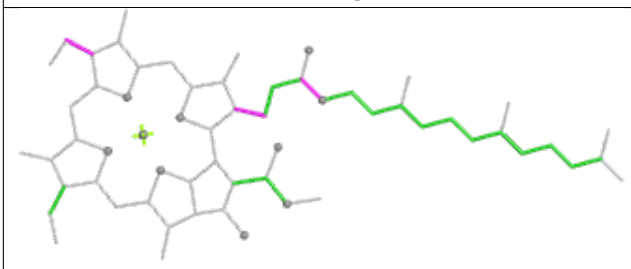
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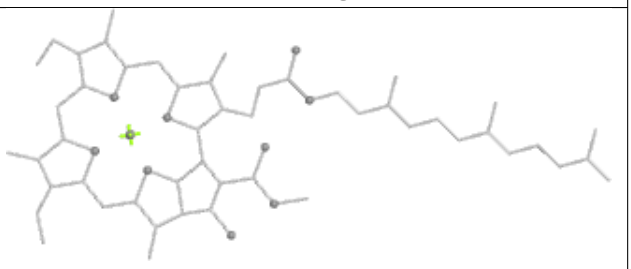
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Bond angles

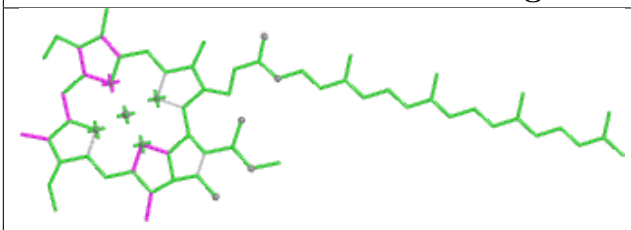


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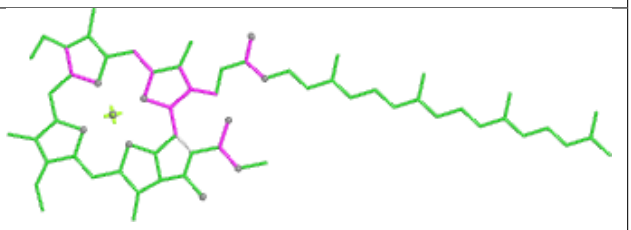


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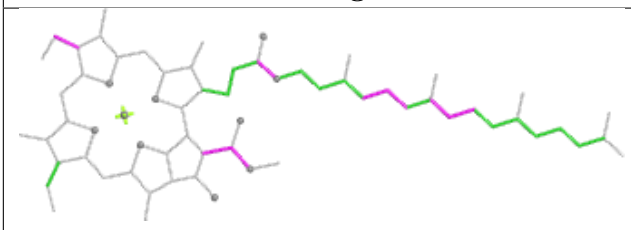
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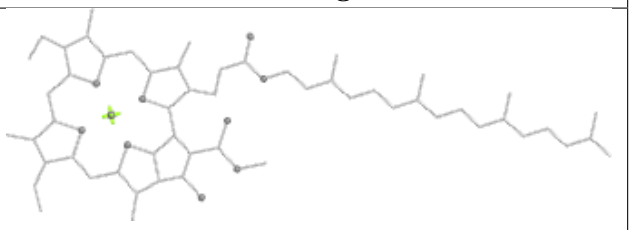
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Bond angles

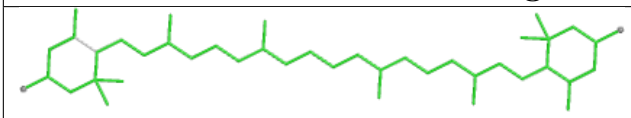


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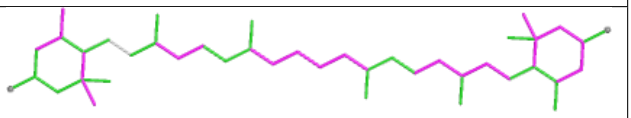


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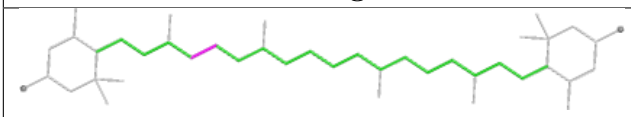
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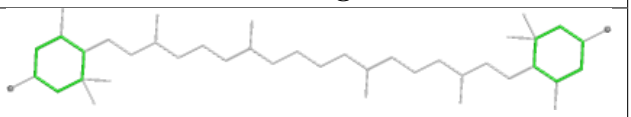
Bond lengths



Bond angles

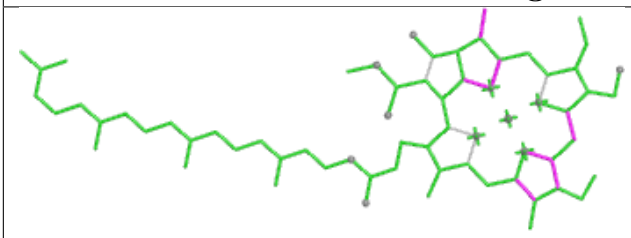


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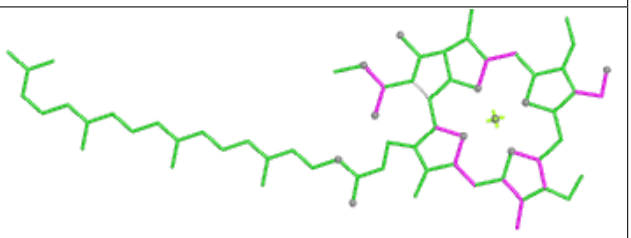


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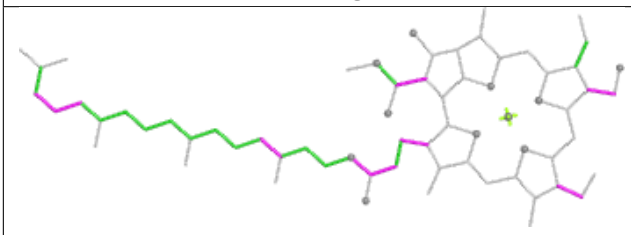
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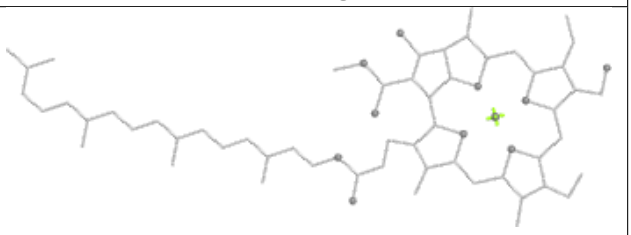
Bond lengths



Bond angles

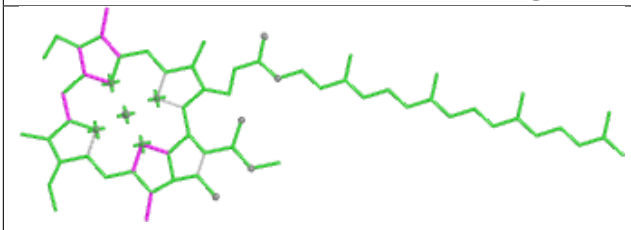


Torsions

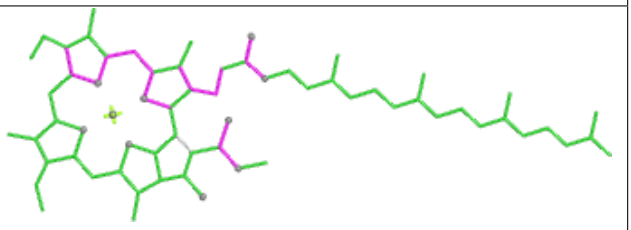


Rings

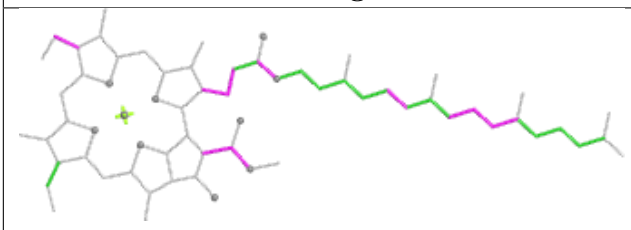
Ligand CLA b 603



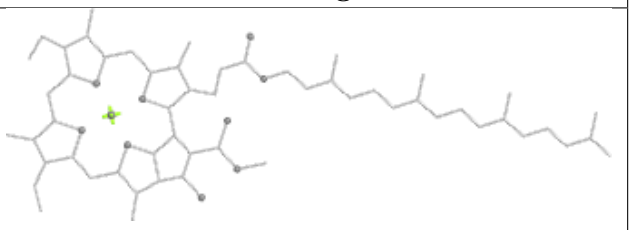
Bond lengths



Bond angles

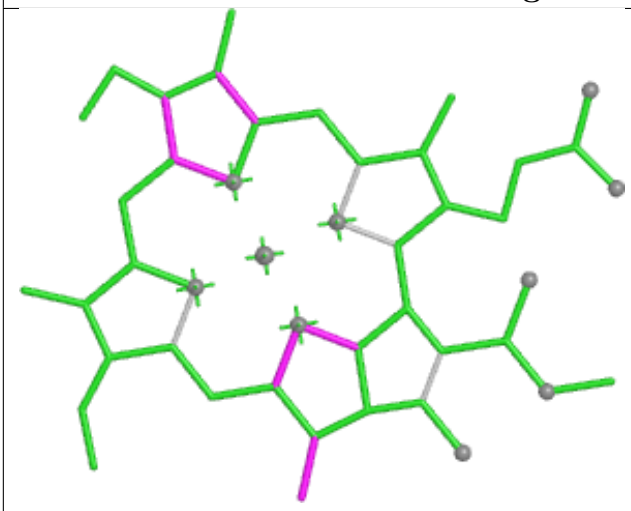


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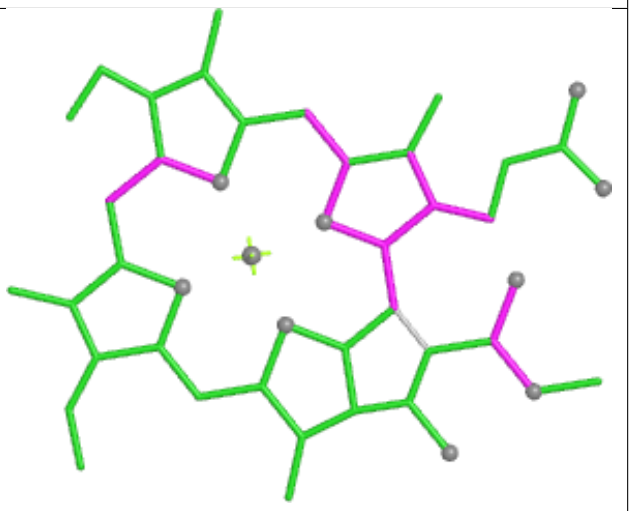


Rings

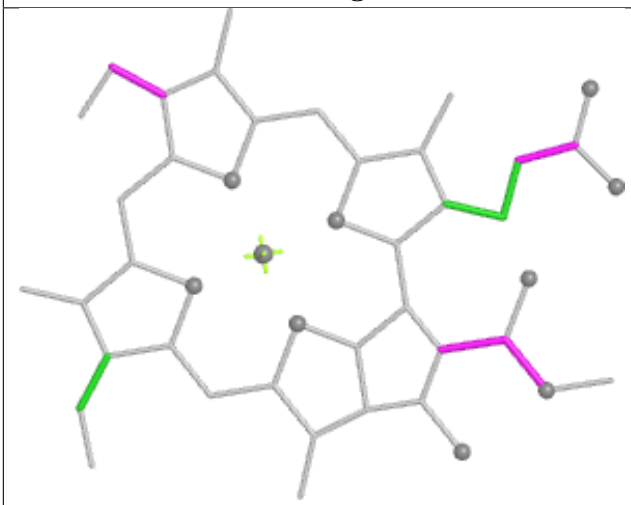
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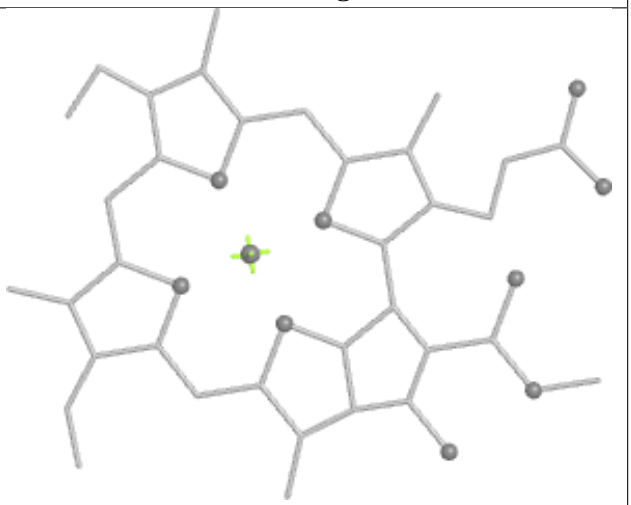
Bond lengths



Bond angles

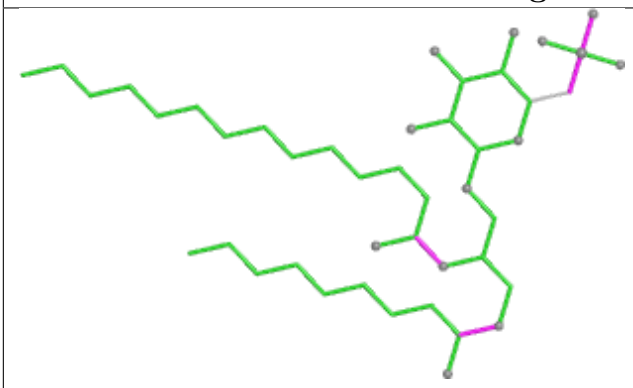


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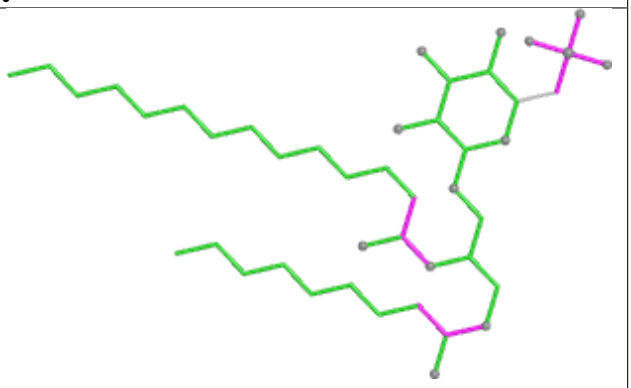


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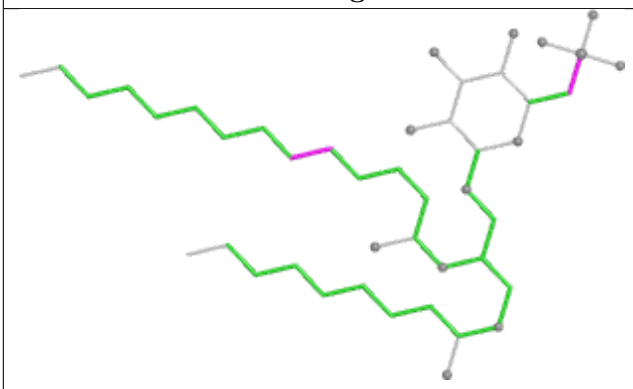
Ligand SQD c 520



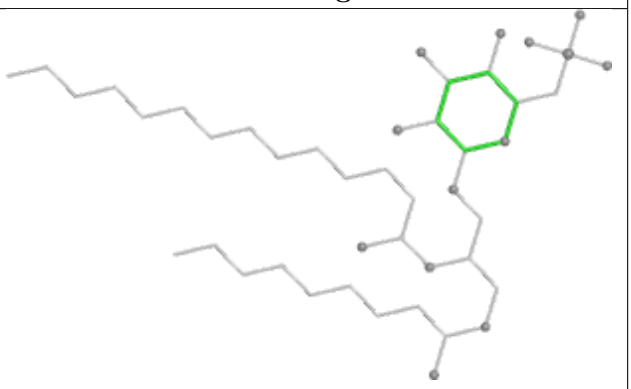
Bond lengths



Bond angles

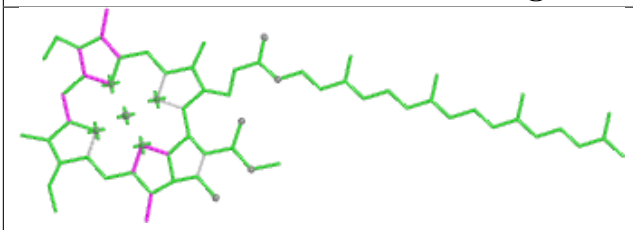


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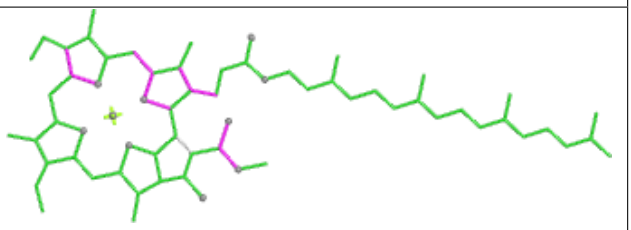


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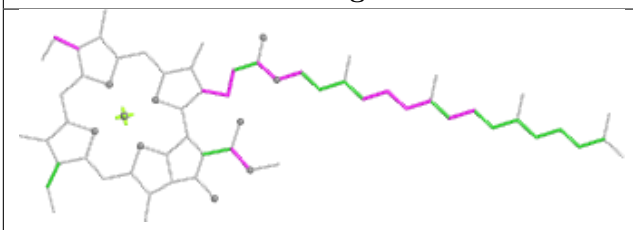
Ligand CLA b 615



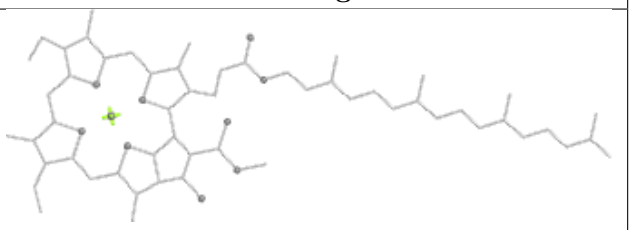
Bond lengths



Bond angles

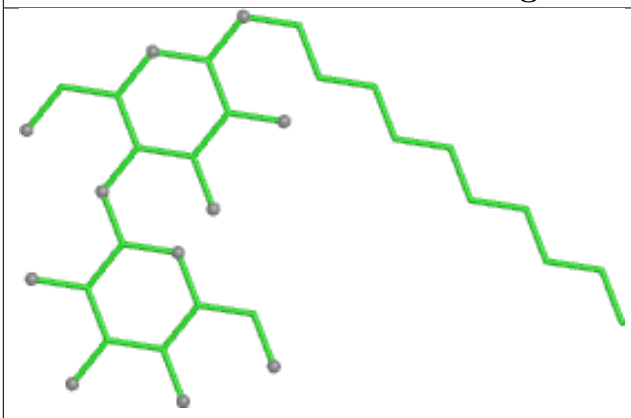


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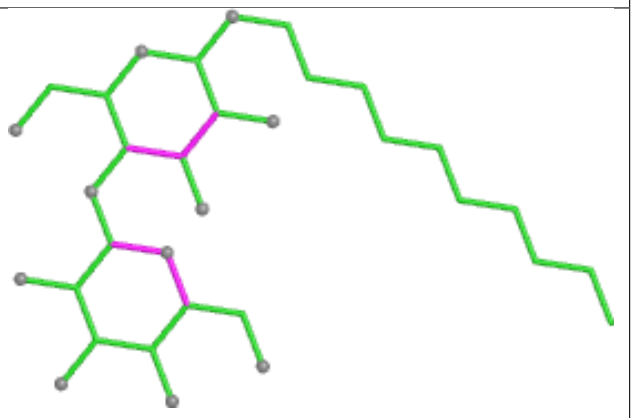


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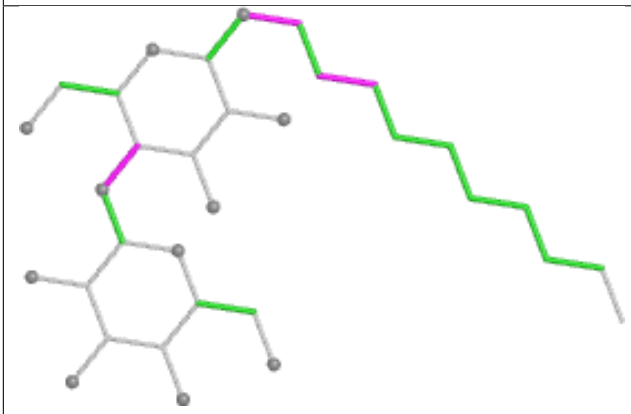
Ligand DMU S 319



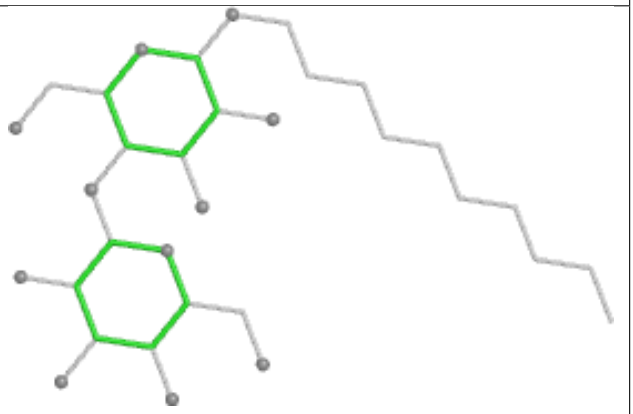
Bond lengths



Bond angles

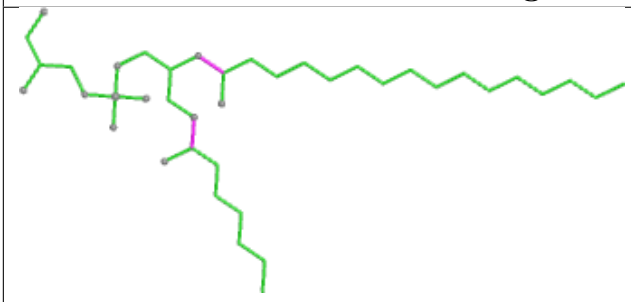


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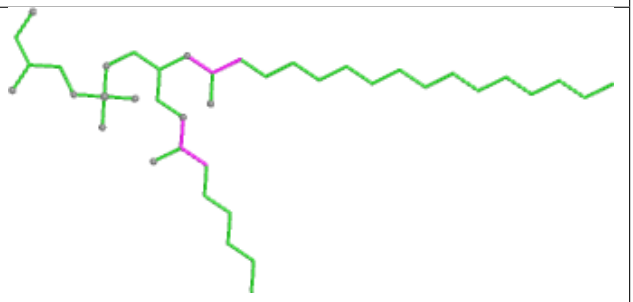


Rings

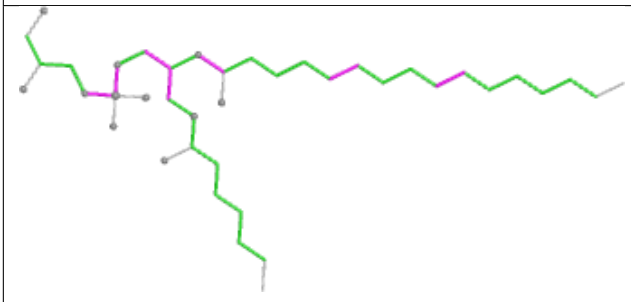
Ligand LHG B 627



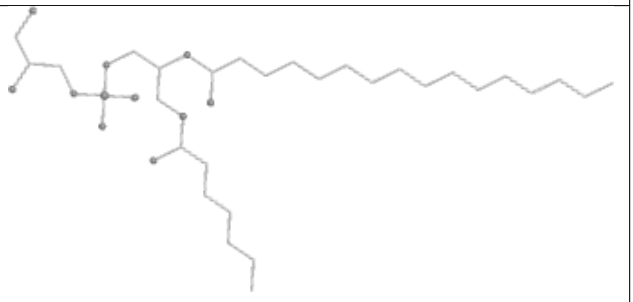
Bond lengths



Bond angles

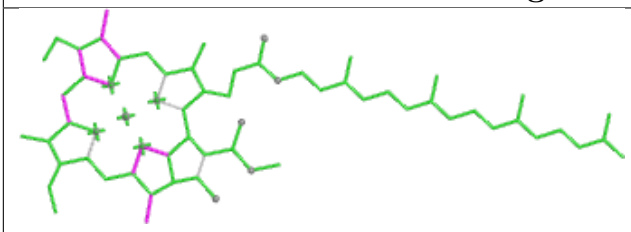


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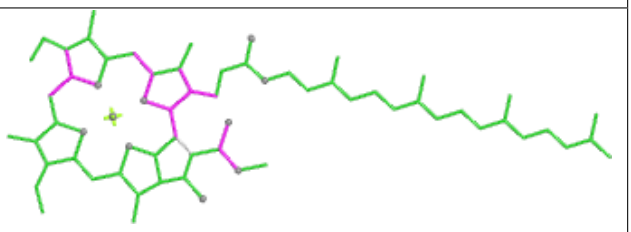


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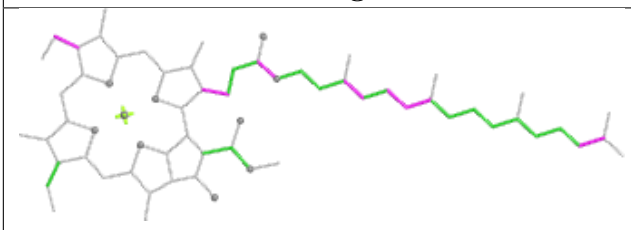
Ligand CLA b 604



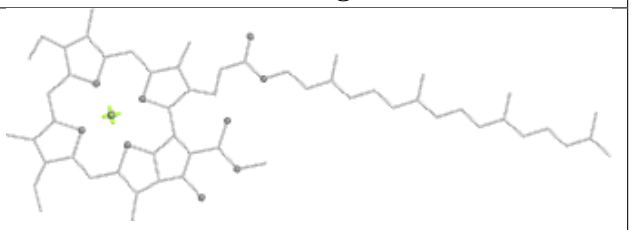
Bond lengths



Bond angles



Torsions

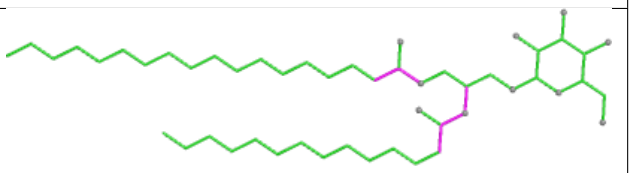


Rings

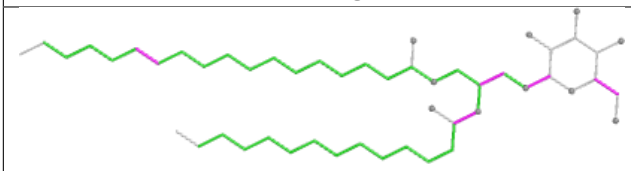
Ligand LMG W 203



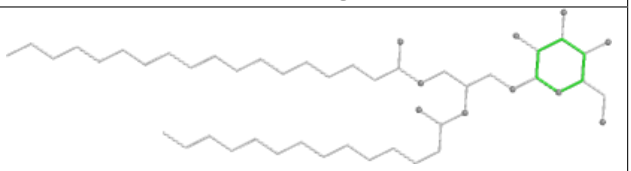
Bond lengths



Bond angles

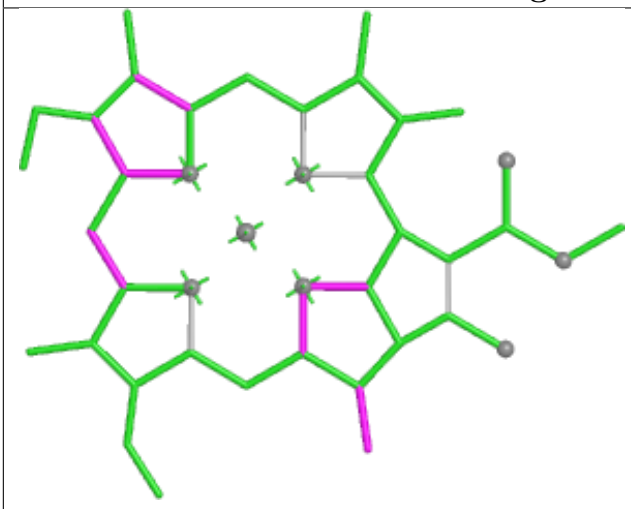


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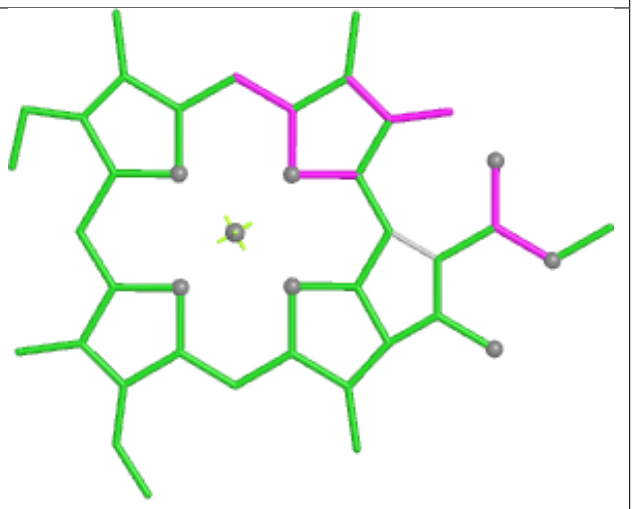


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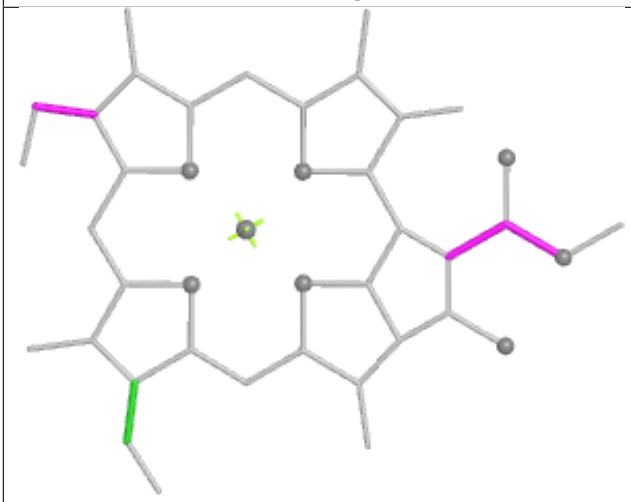
Ligand CLA r 610



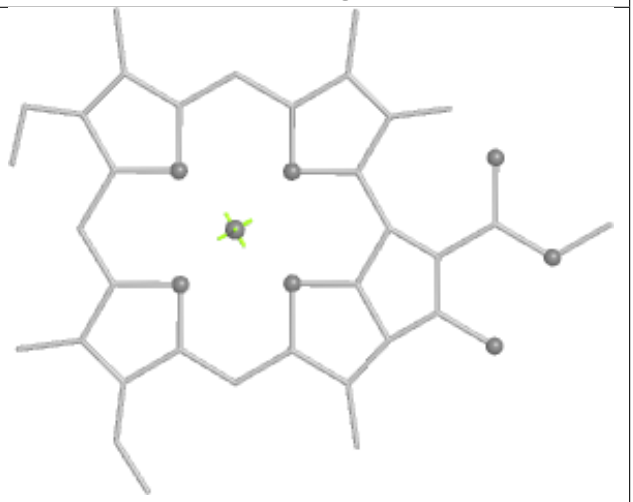
Bond lengths



Bond angles

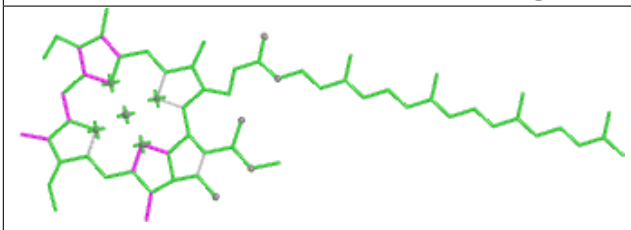


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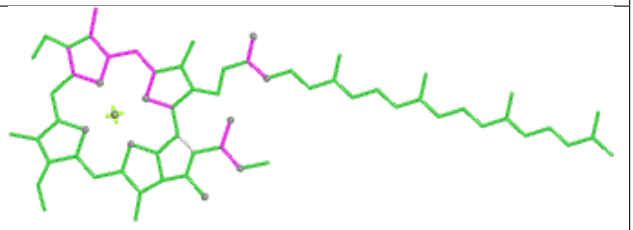


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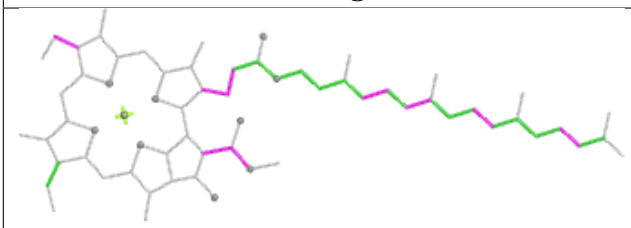
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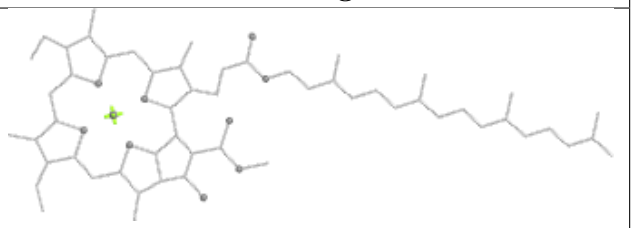
Bond lengths



Bond angles

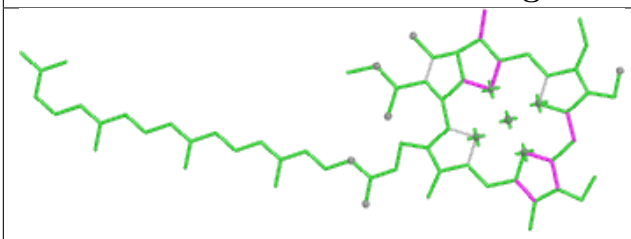


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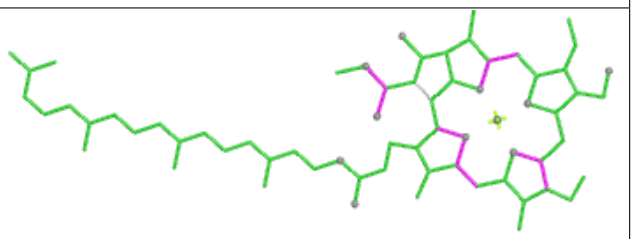


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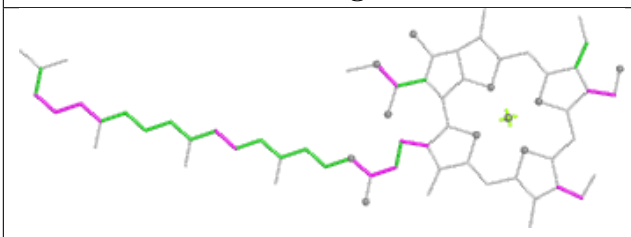
Ligand CHL G 608



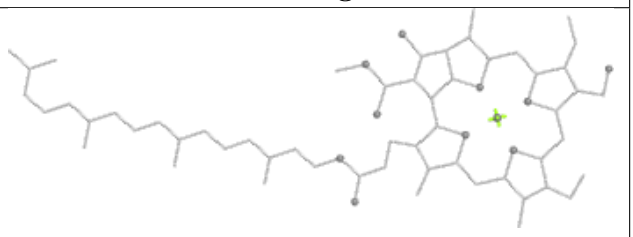
Bond lengths



Bond angles

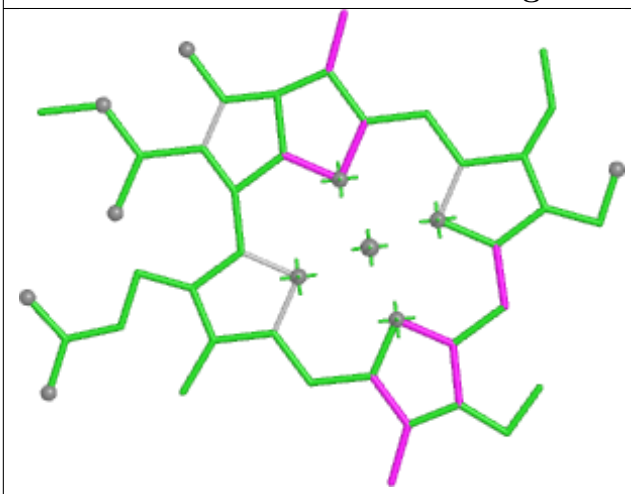


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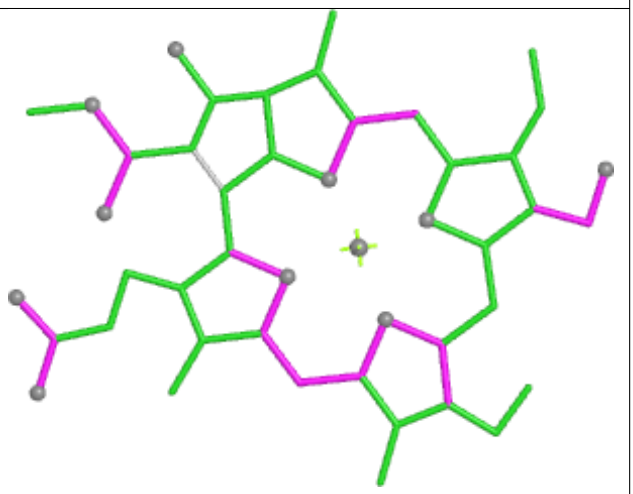


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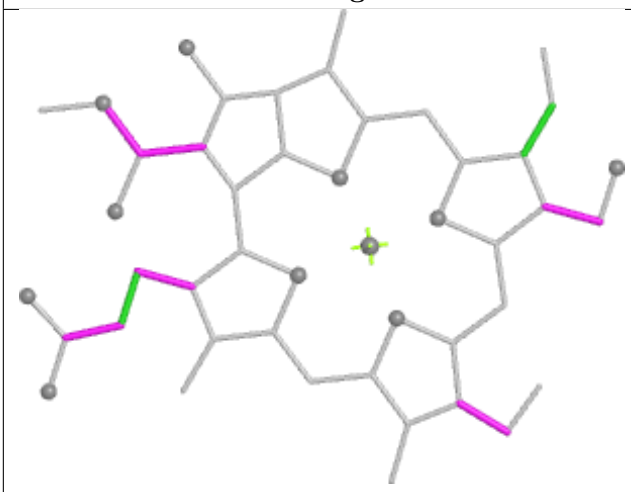
Ligand CHL G 605



Bond lengths



Bond angles

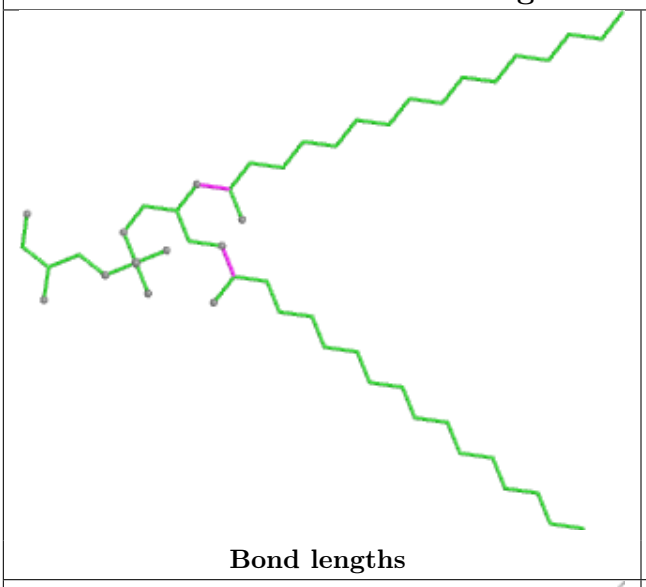


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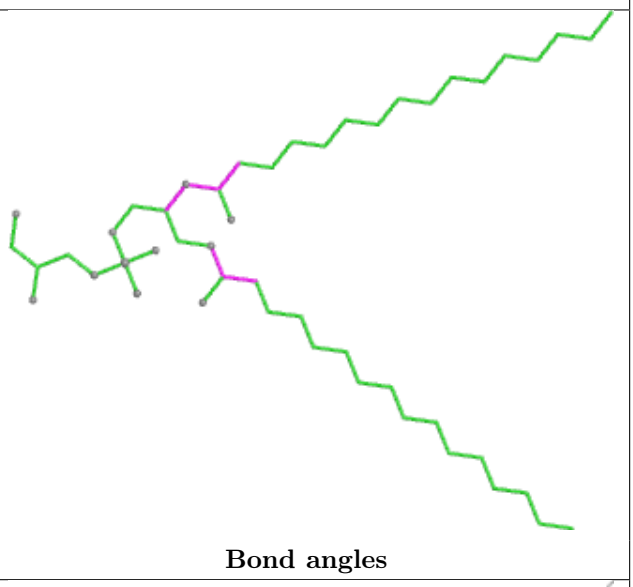


Rings

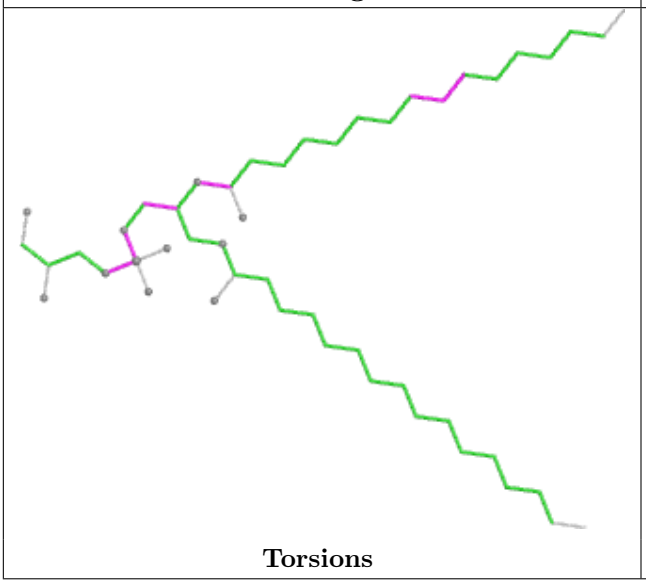
Ligand LHG W 201



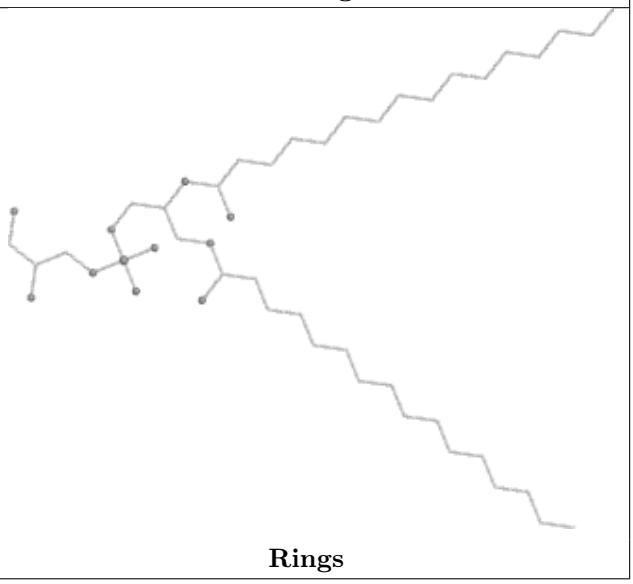
Bond lengths



Bond angles

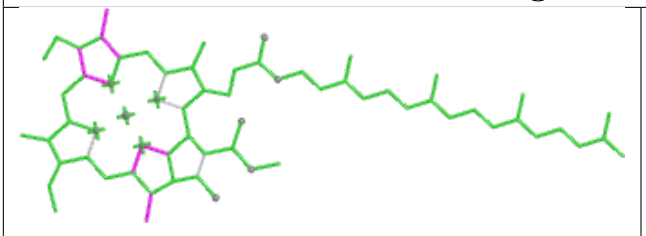


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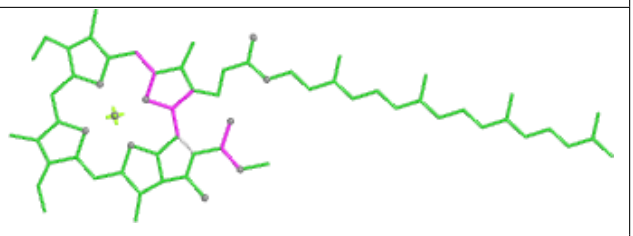


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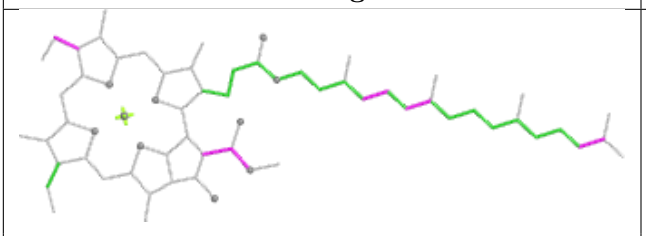
Ligand CLA c 511



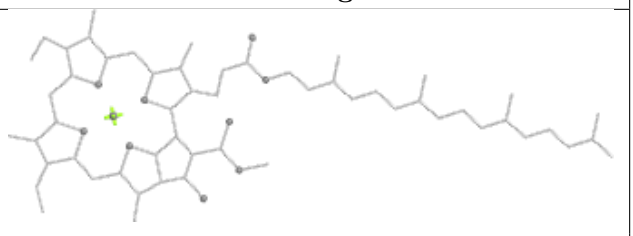
Bond lengths



Bond angles

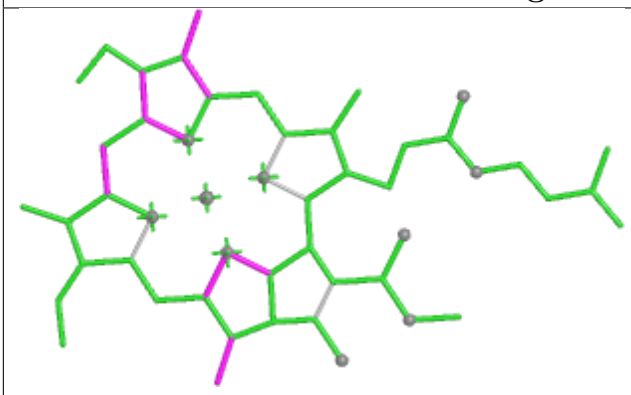


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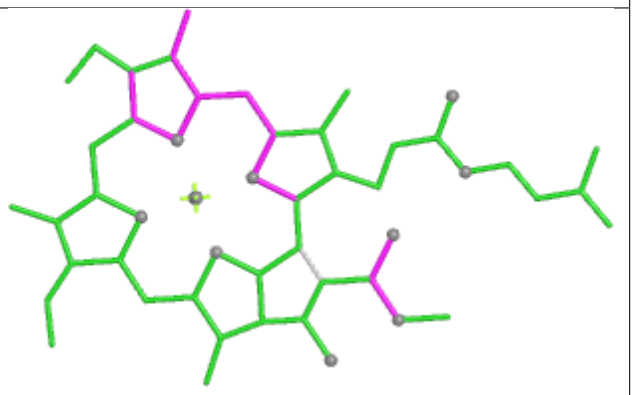


Rings

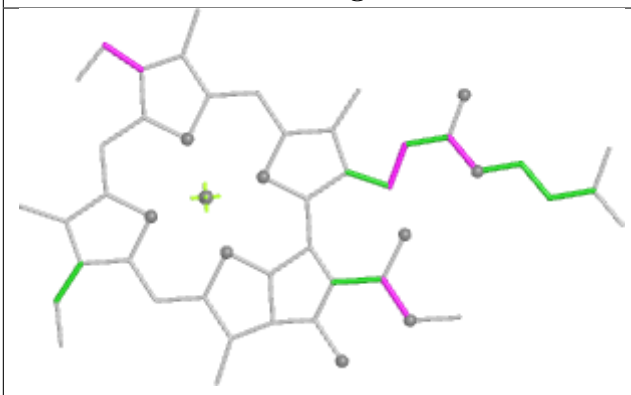
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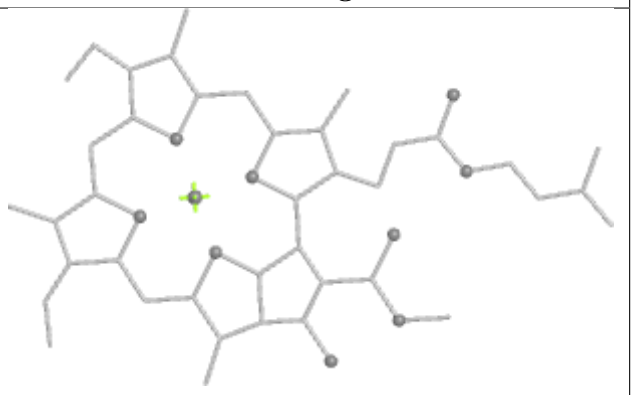
Bond lengths



Bond angles

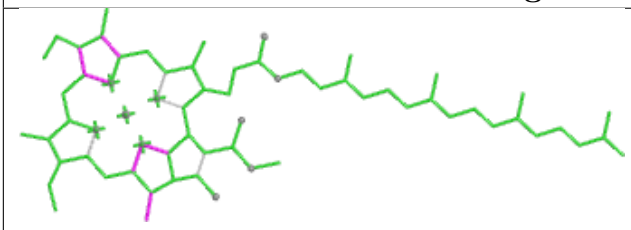


Torsions

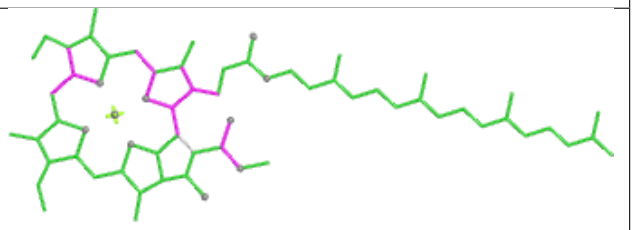


Rings

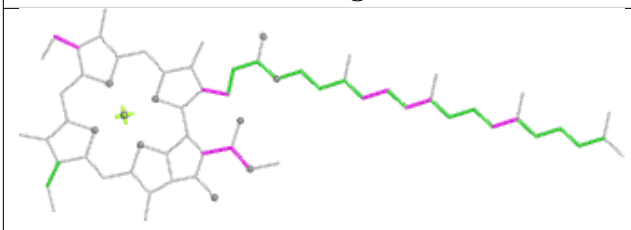
Ligand CLA C 508



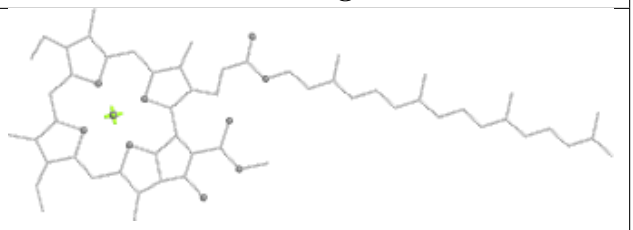
Bond lengths



Bond angles

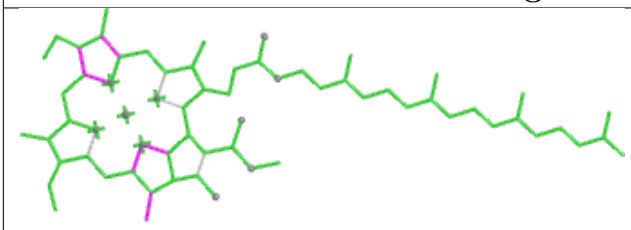


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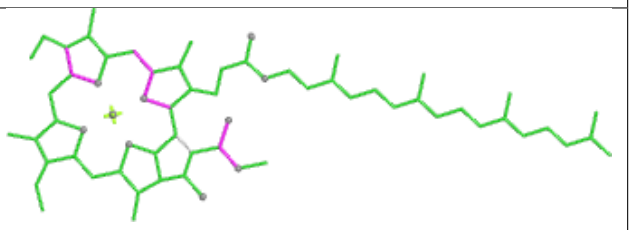


Rings

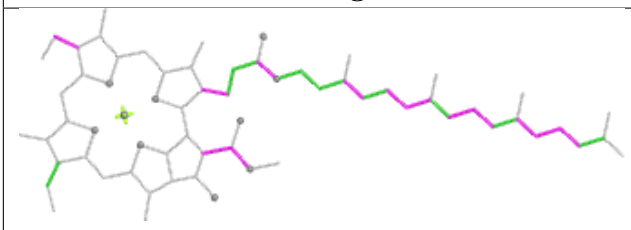
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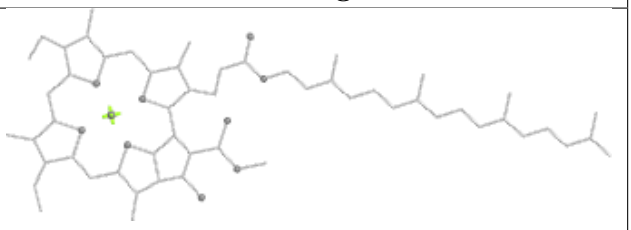
Bond lengths



Bond angles

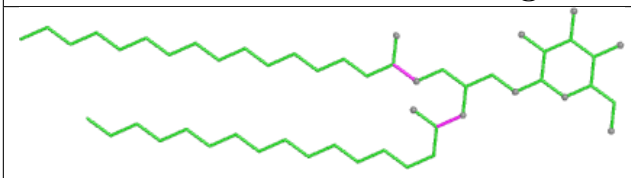


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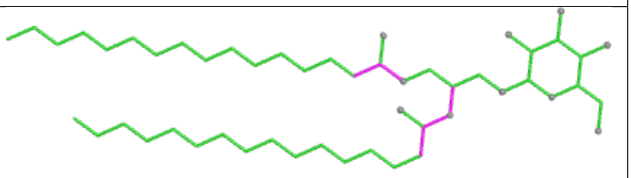


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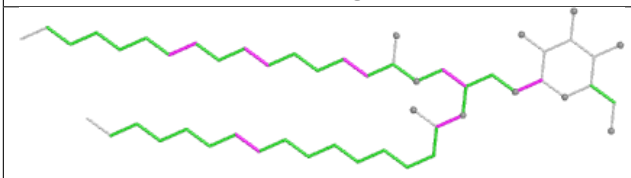
Ligand LMG B 620



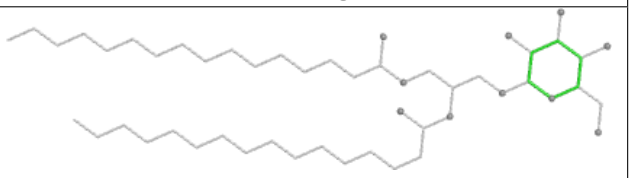
Bond lengths



Bond angles

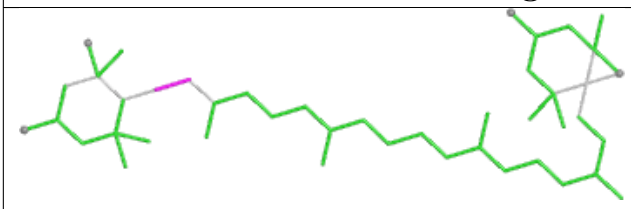


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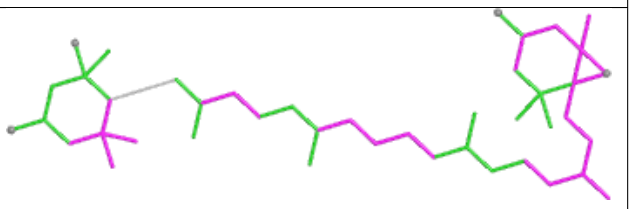


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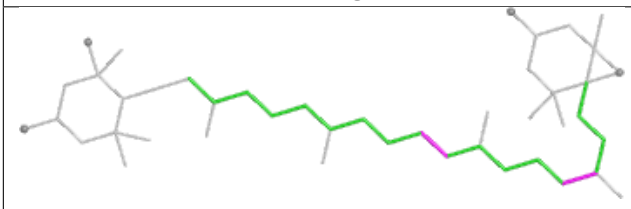
Ligand NEX Y 318



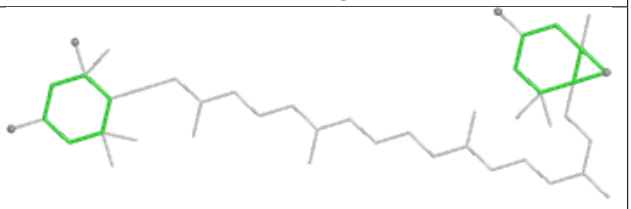
Bond lengths



Bond angles

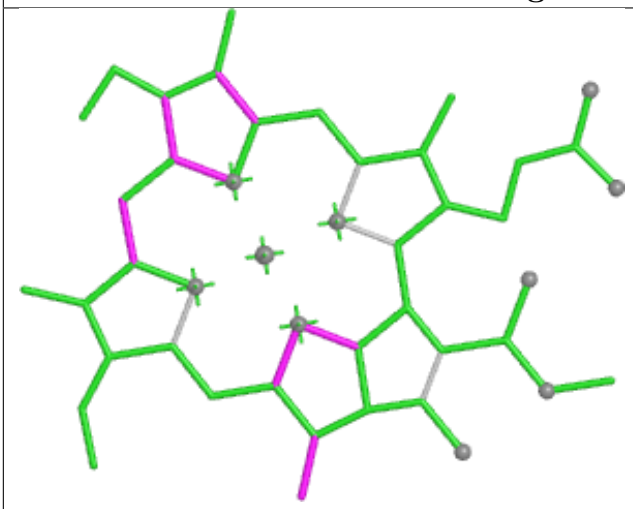


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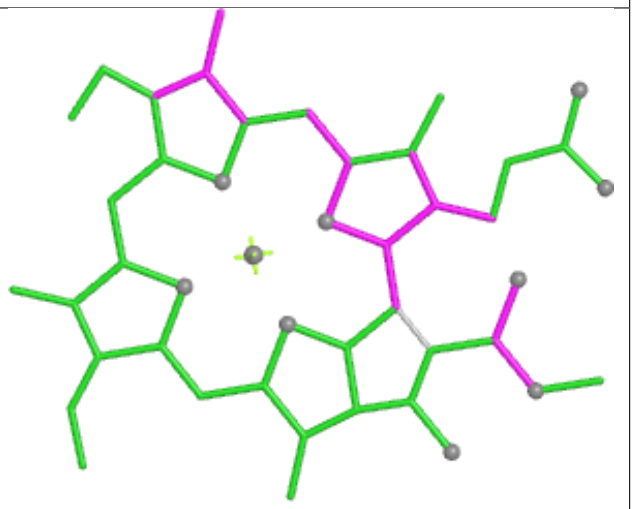


Rings

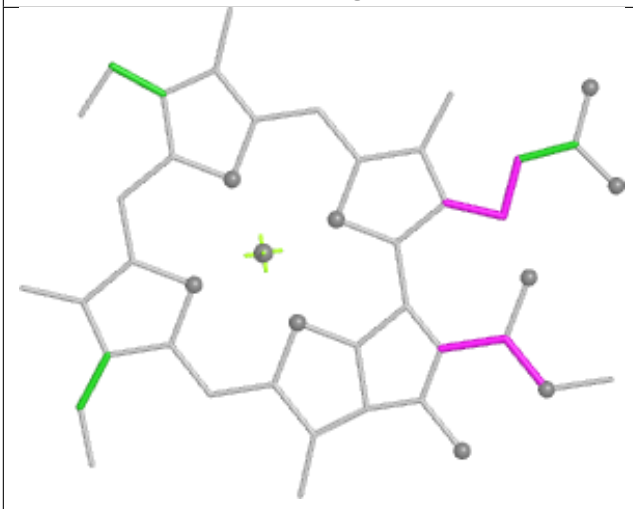
Ligand CLA S 312



Bond lengths



Bond angles

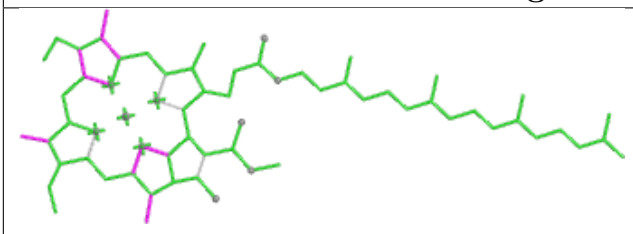


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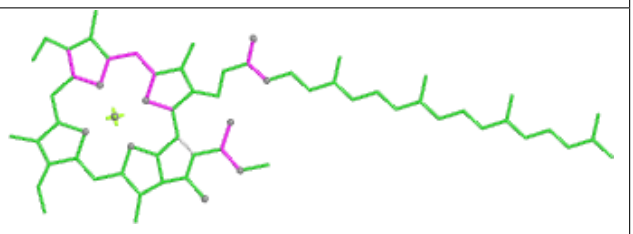


Rings

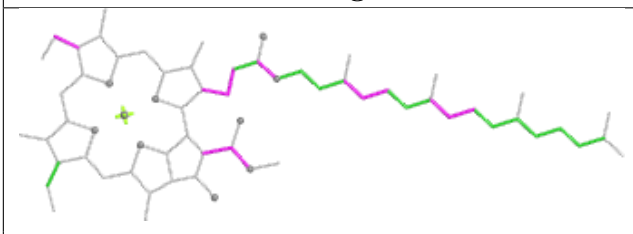
Ligand CLA b 605



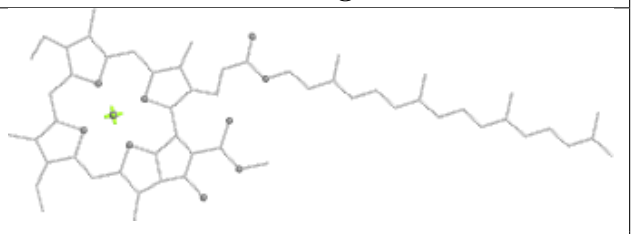
Bond lengths



Bond angles

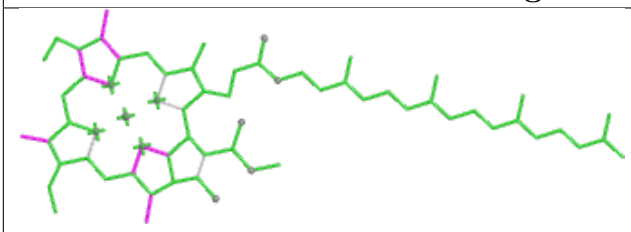


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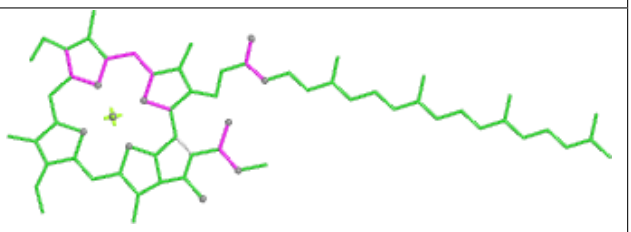


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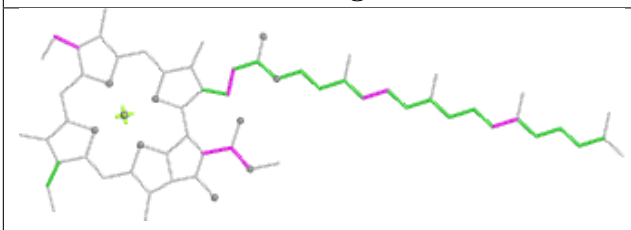
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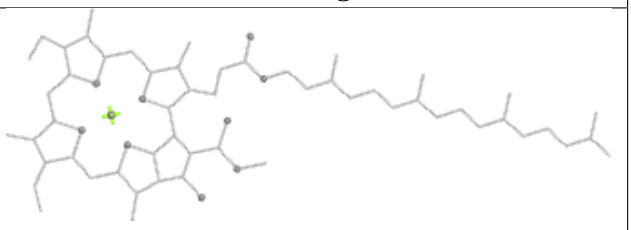
Bond lengths



Bond angles



Torsions

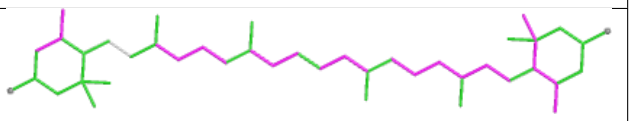


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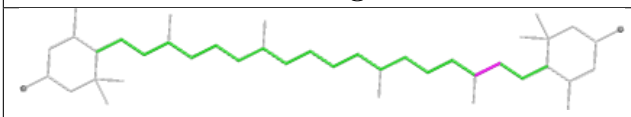
Ligand LUT R 314



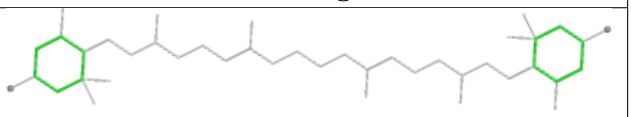
Bond lengths



Bond angles

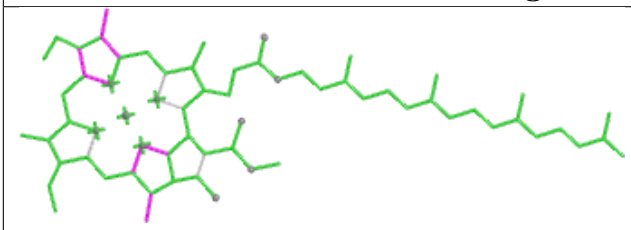


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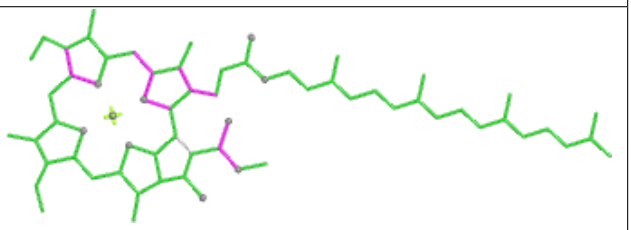


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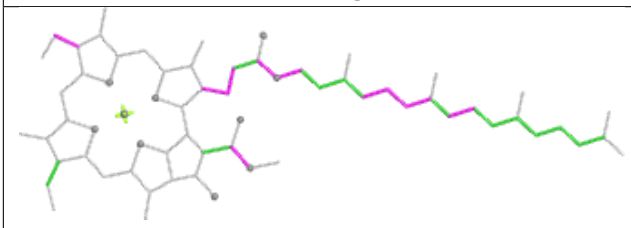
Ligand CLA B 613



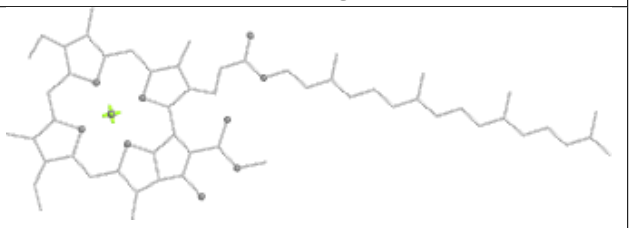
Bond lengths



Bond angles

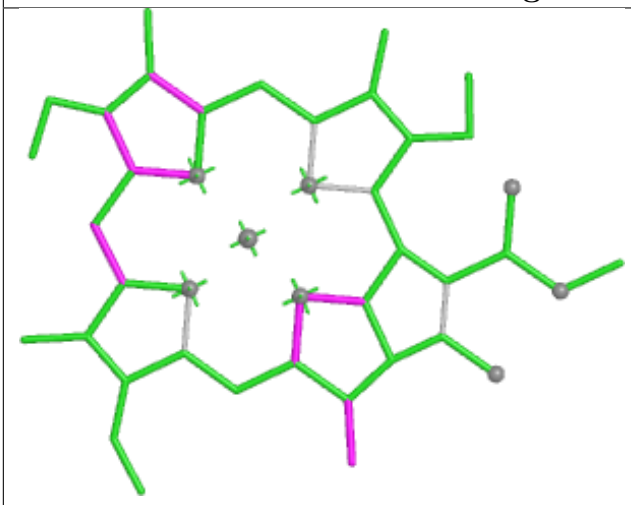


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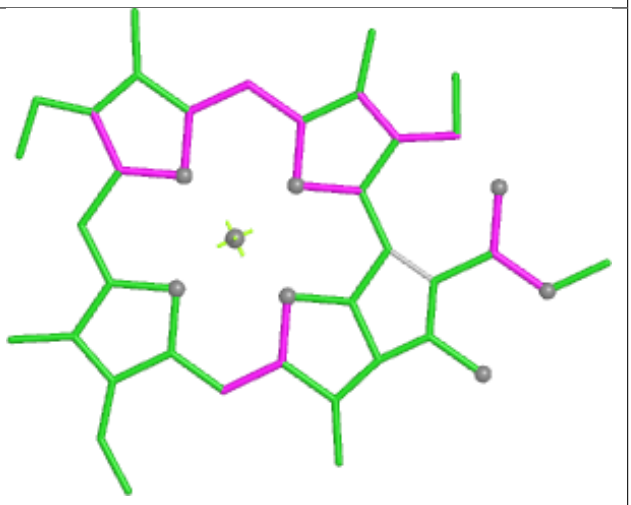


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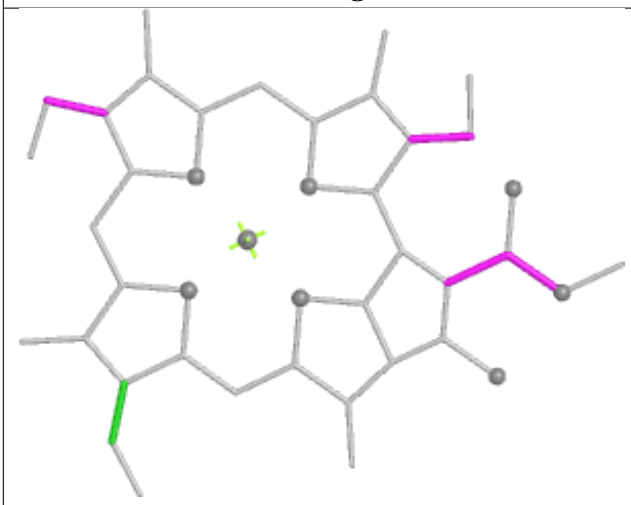
Ligand CLA G 614



Bond lengths



Bond angles

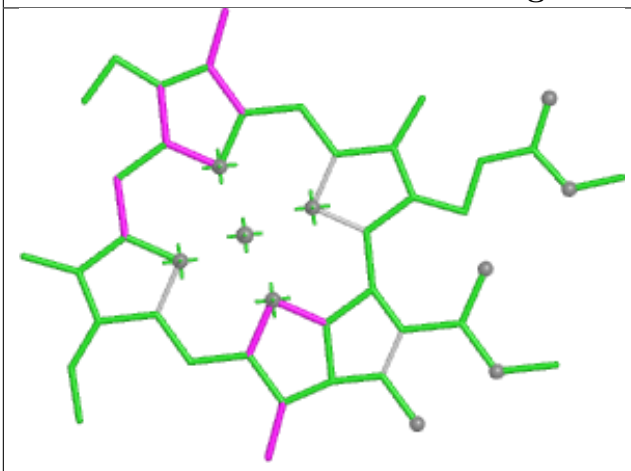


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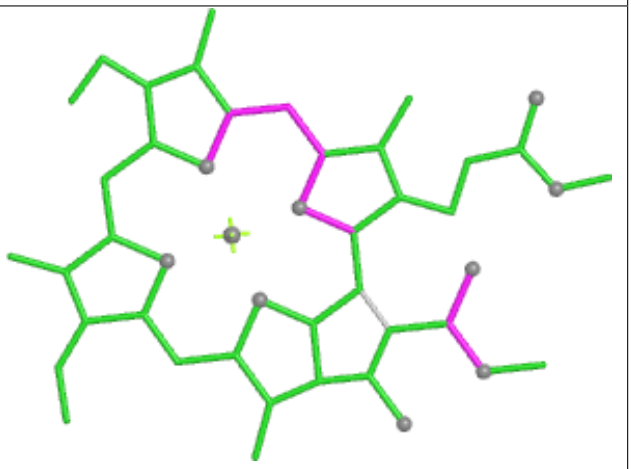


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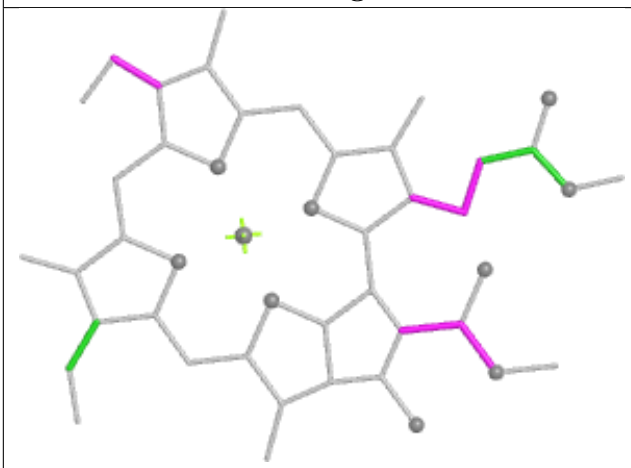
Ligand CLA S 303



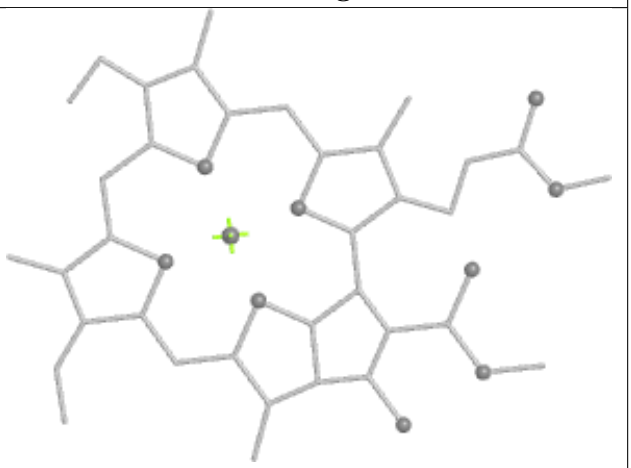
Bond lengths



Bond angles



Torsions

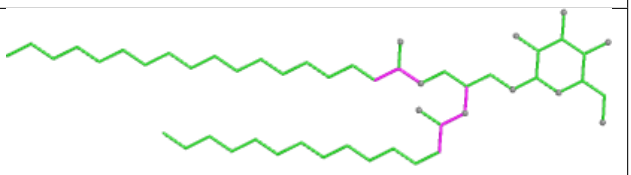


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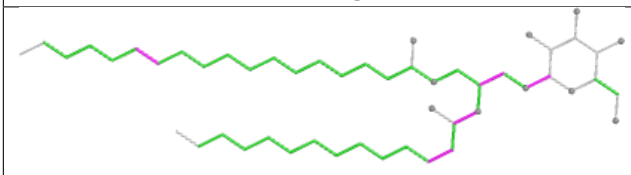
Ligand LMG w 202



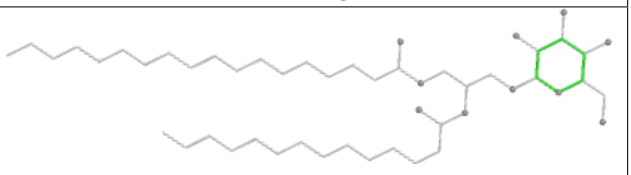
Bond lengths



Bond angles

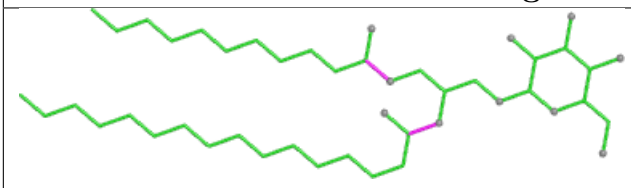


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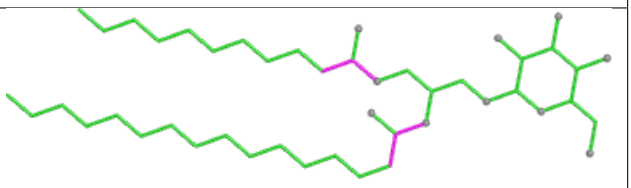


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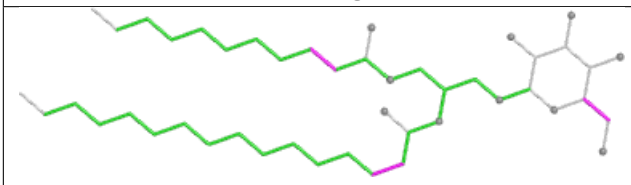
Ligand LMG d 409



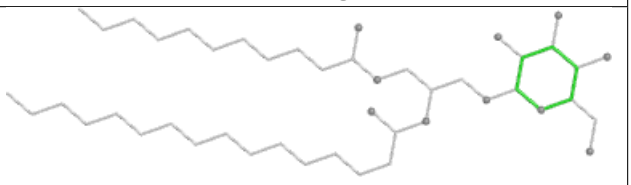
Bond lengths



Bond angles

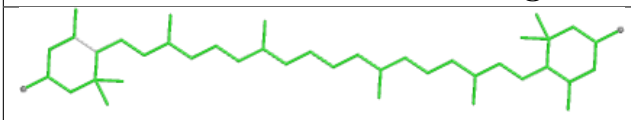


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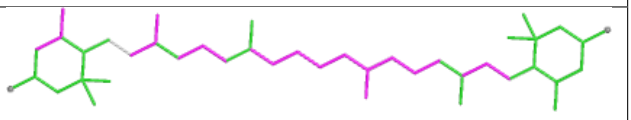


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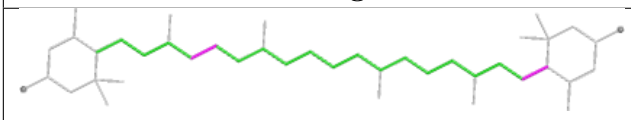
Ligand LUT Y 316



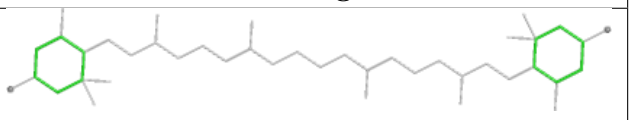
Bond lengths



Bond angles

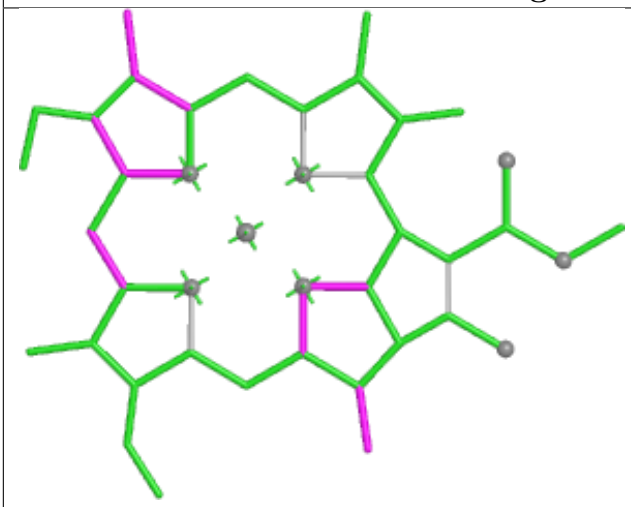


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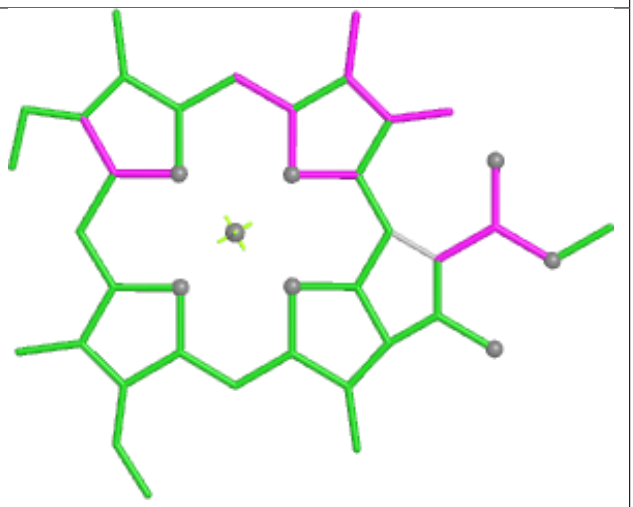


Rings

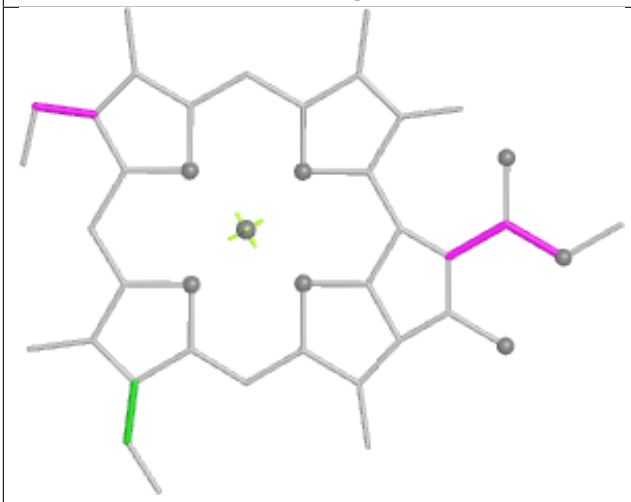
Ligand CLA s 613



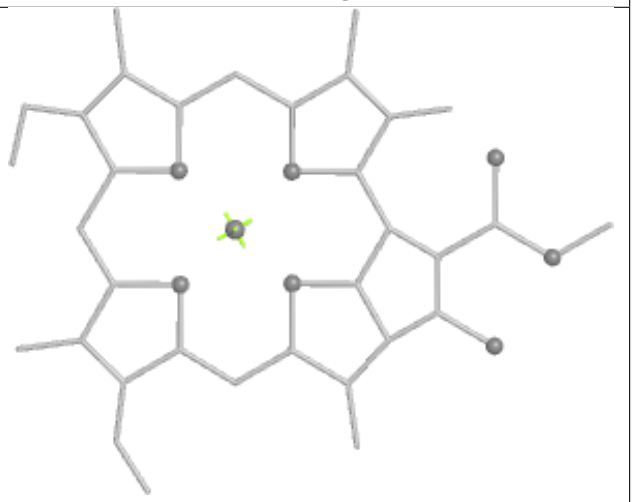
Bond lengths



Bond angles

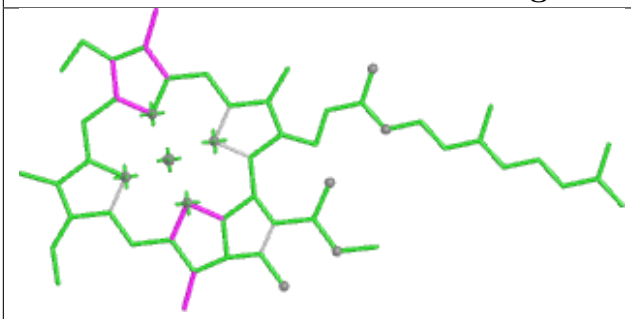


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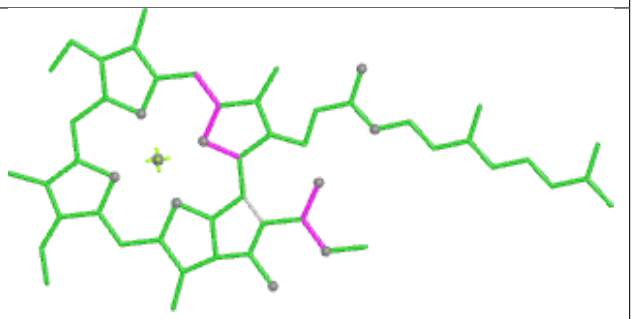


Rings

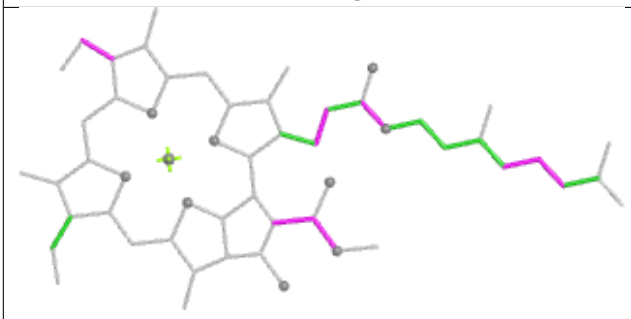
Ligand CLA s 612



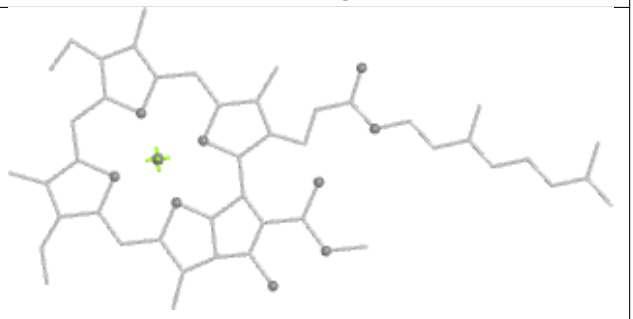
Bond lengths



Bond angles

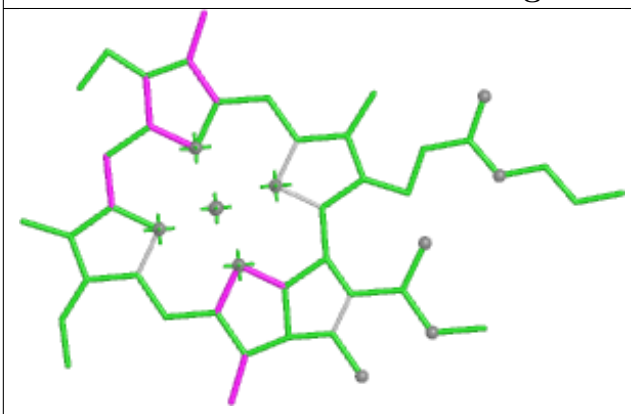


Torsions

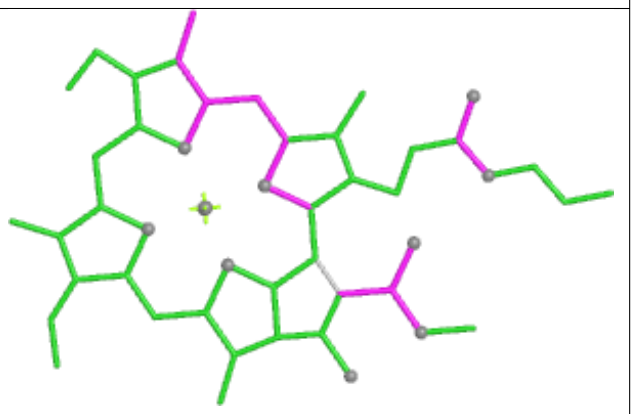


Rings

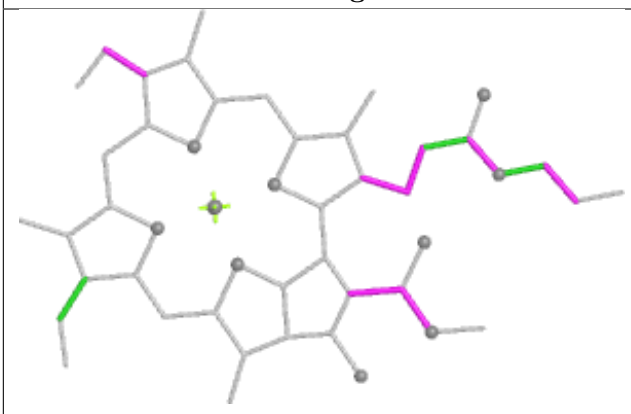
Ligand CLA R 305



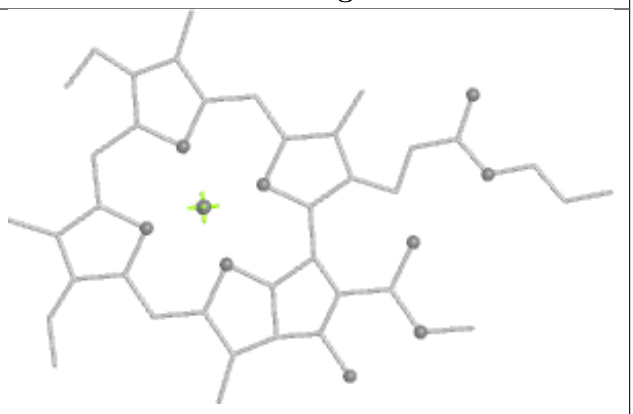
Bond lengths



Bond angles

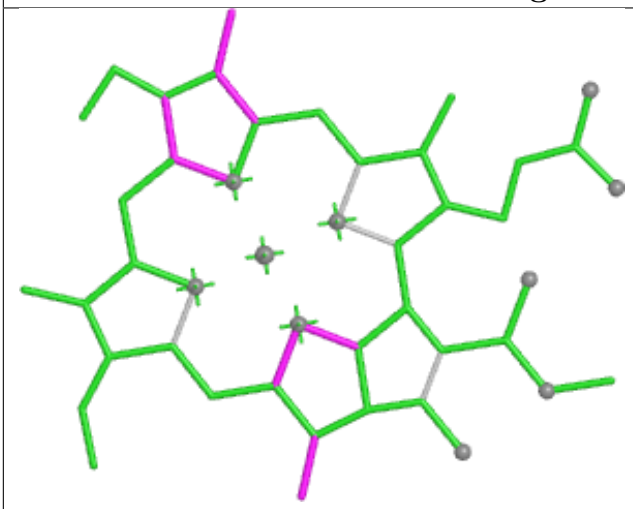


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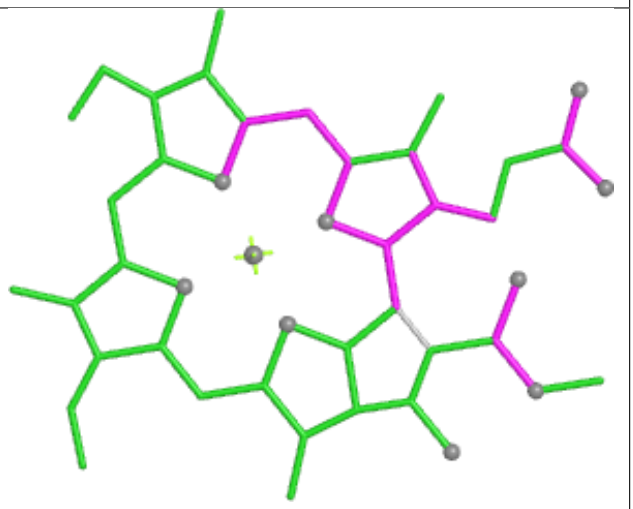


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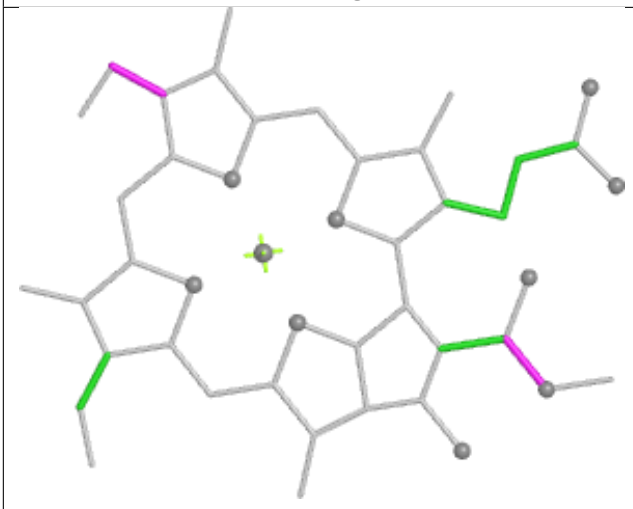
Ligand CLA s 611



Bond lengths



Bond angles

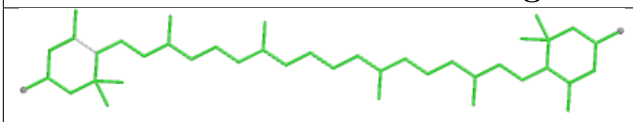


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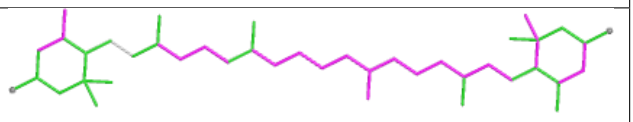


Rings

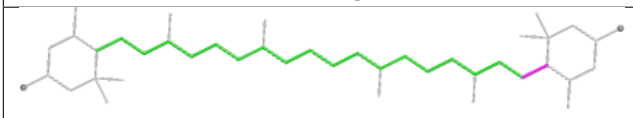
Ligand LUT G 616



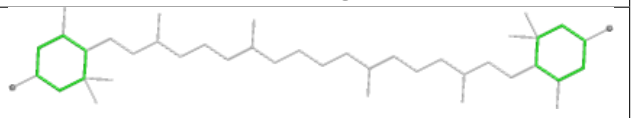
Bond lengths



Bond angles

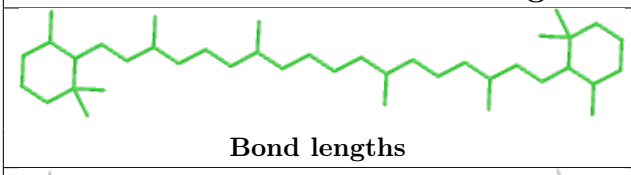


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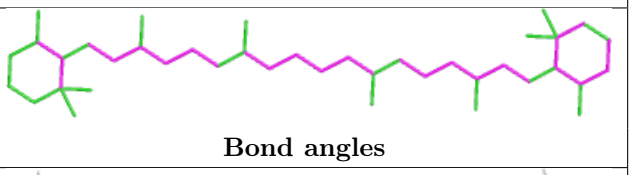


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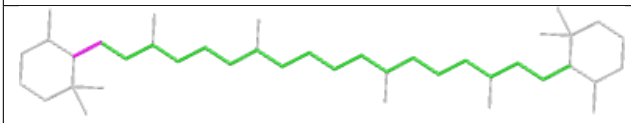
Ligand BCR c 518



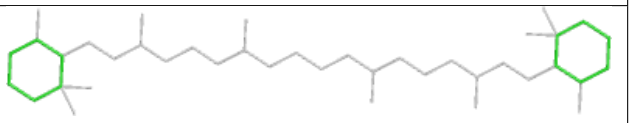
Bond lengths



Bond angles



Torsions



Rings

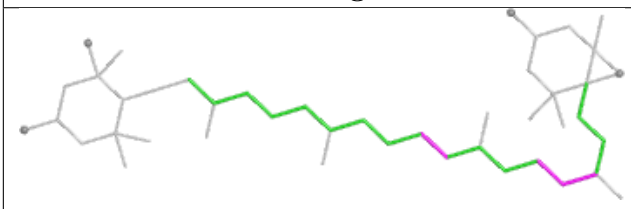
Ligand NEX R 301



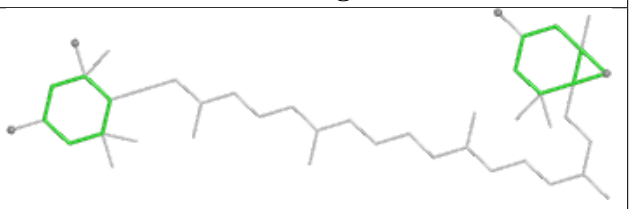
Bond lengths



Bond angles

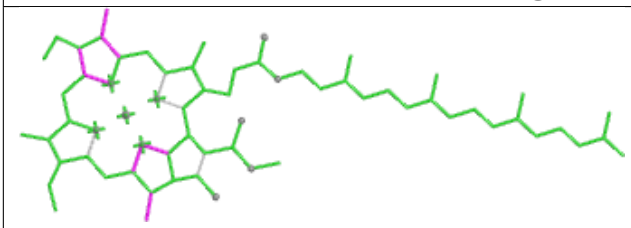


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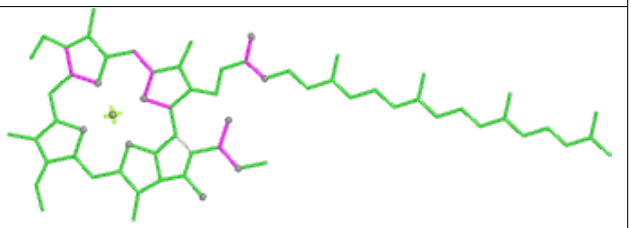


Rings

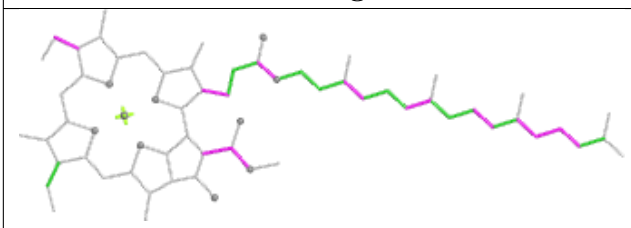
Ligand CLA c 503



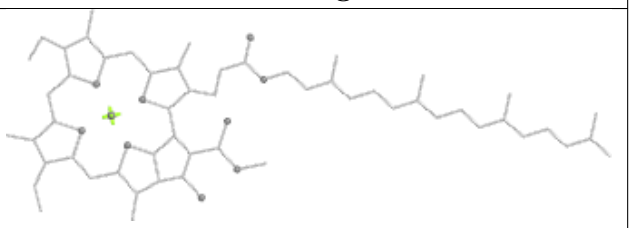
Bond lengths



Bond angles

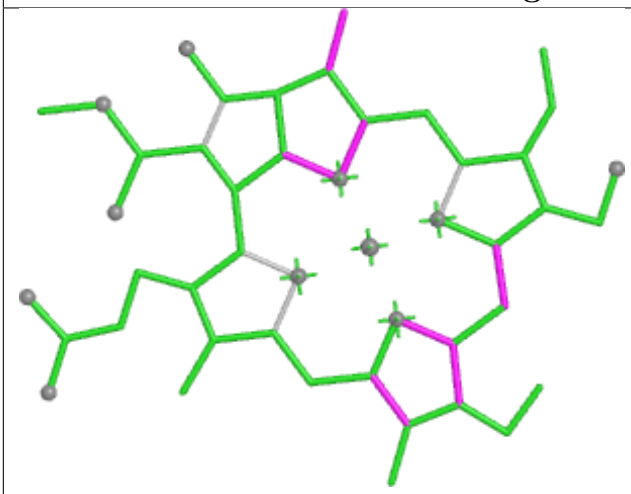


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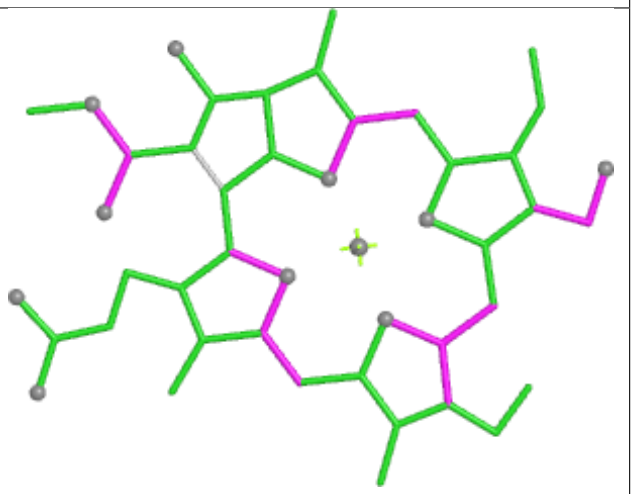


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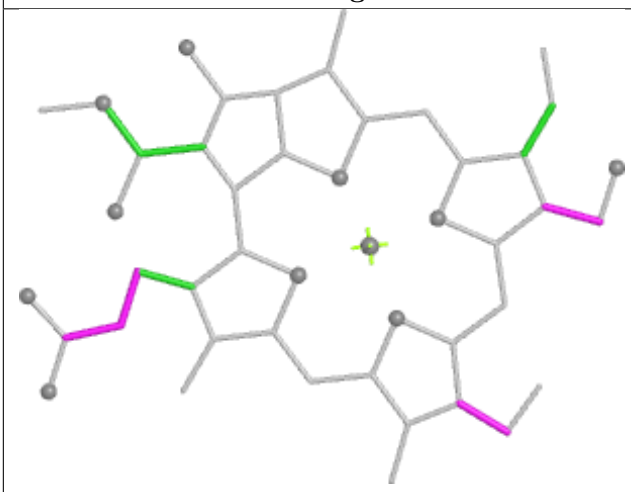
Ligand CHL R 307



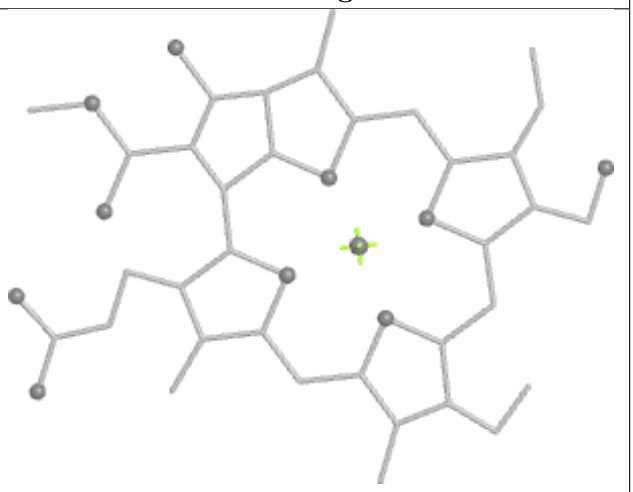
Bond lengths



Bond angles

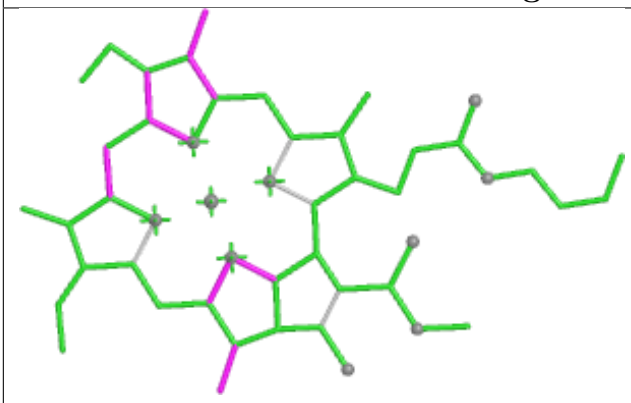


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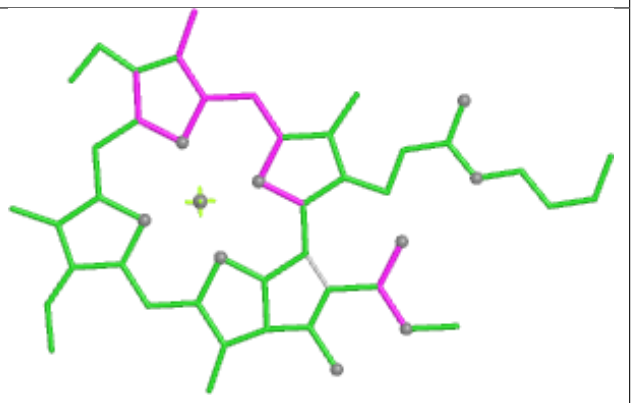


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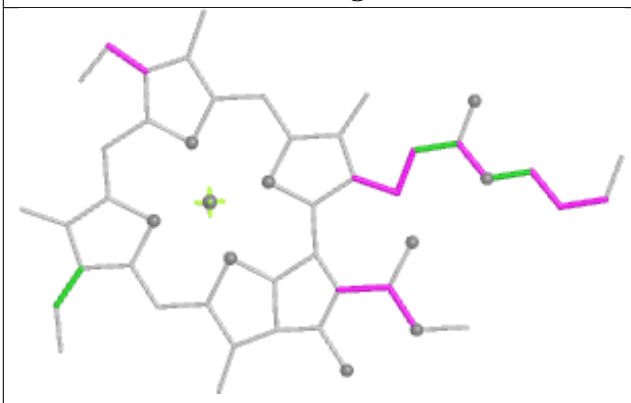
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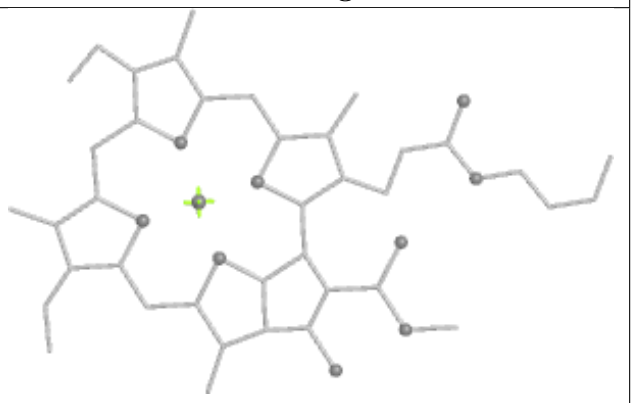
Bond lengths



Bond angles

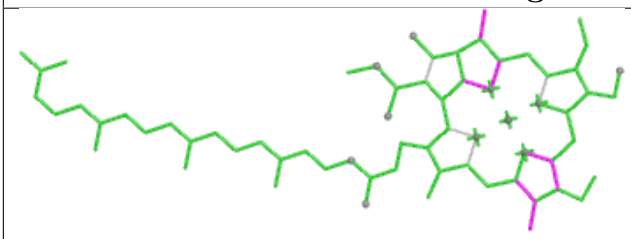


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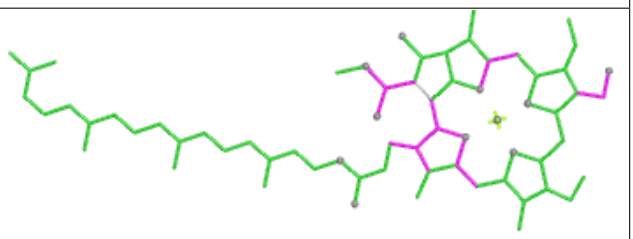


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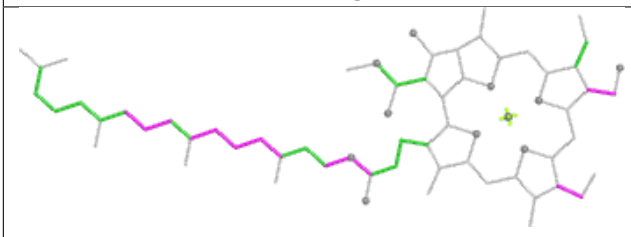
Ligand CHL n 609



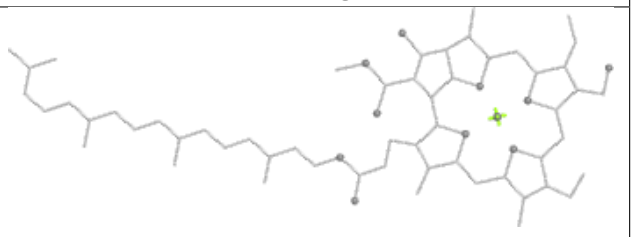
Bond lengths



Bond angles

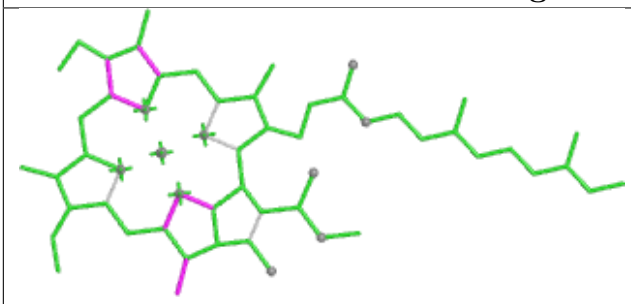


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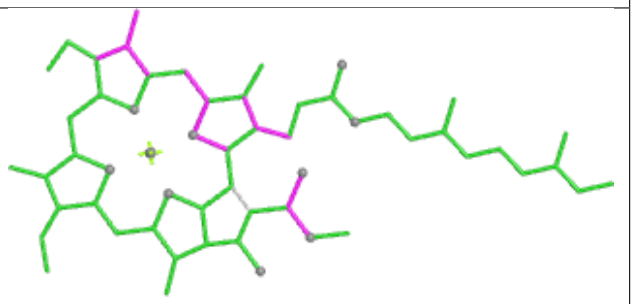


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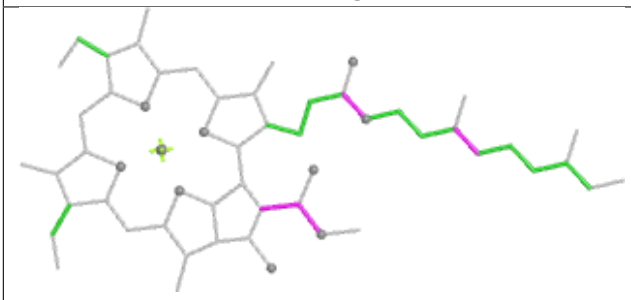
Ligand CLA c 512



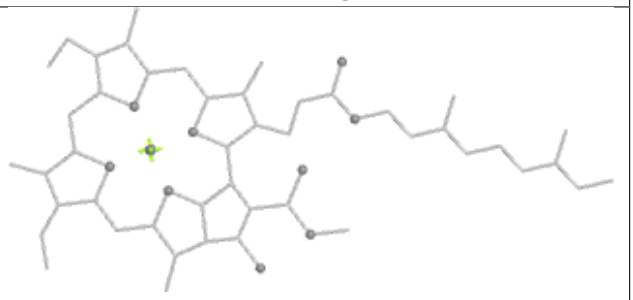
Bond lengths



Bond angles

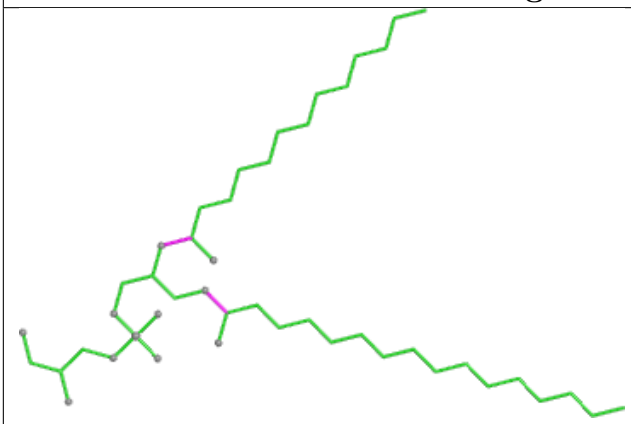


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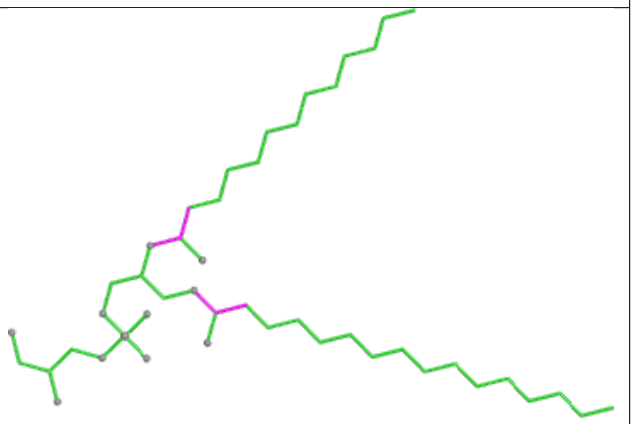


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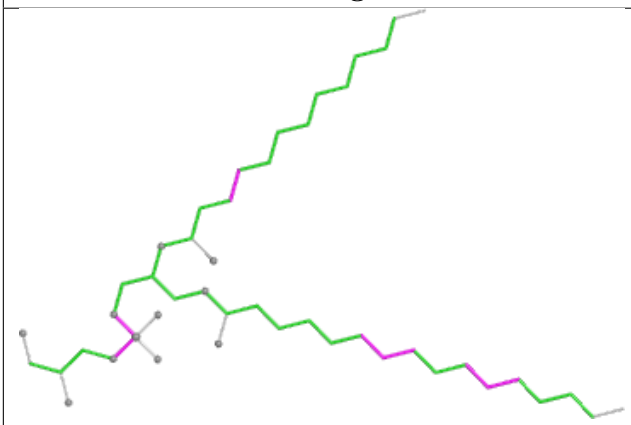
Ligand LHG b 624



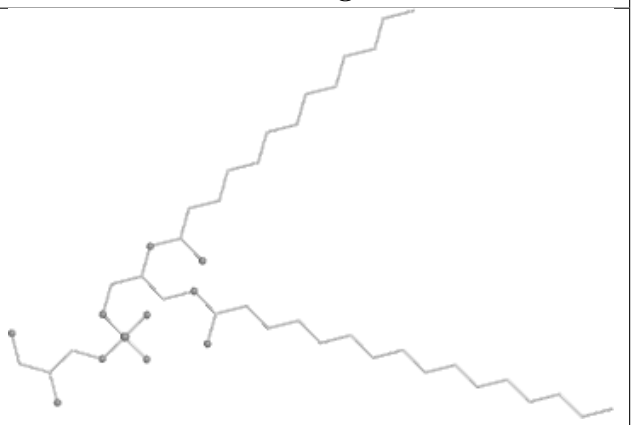
Bond lengths



Bond angles

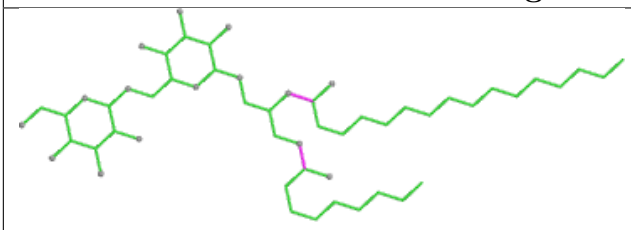


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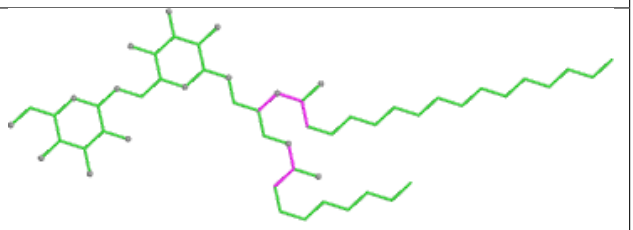


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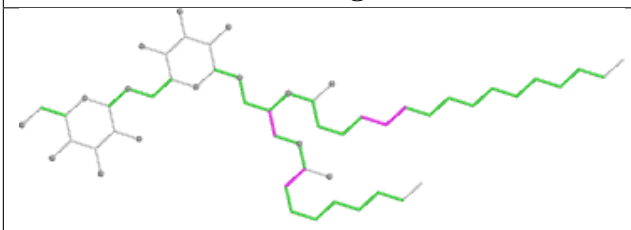
Ligand DGD c 515



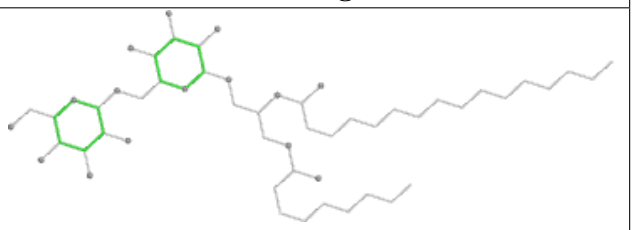
Bond lengths



Bond angles

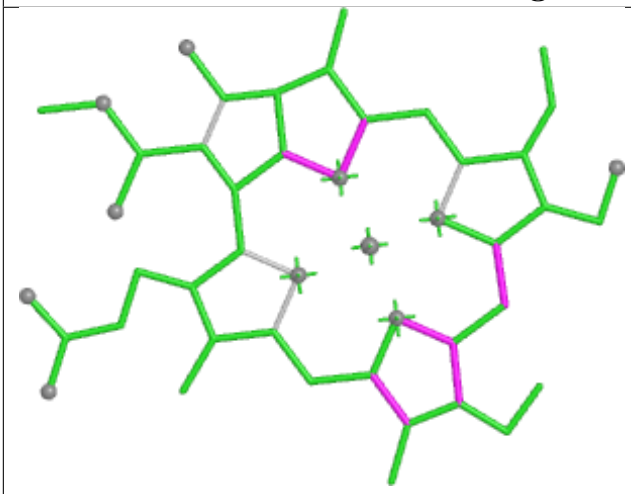


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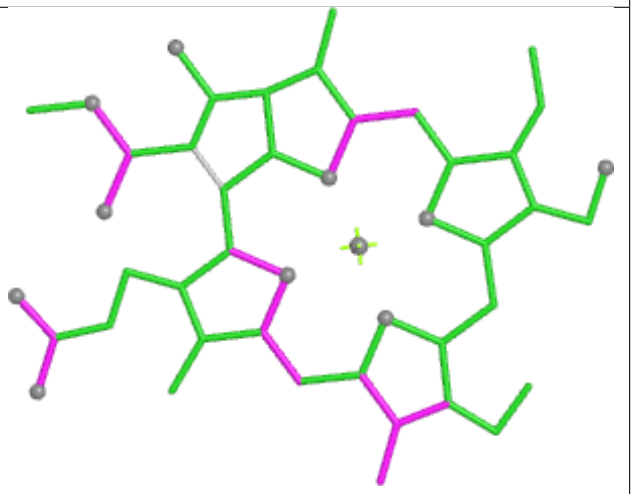


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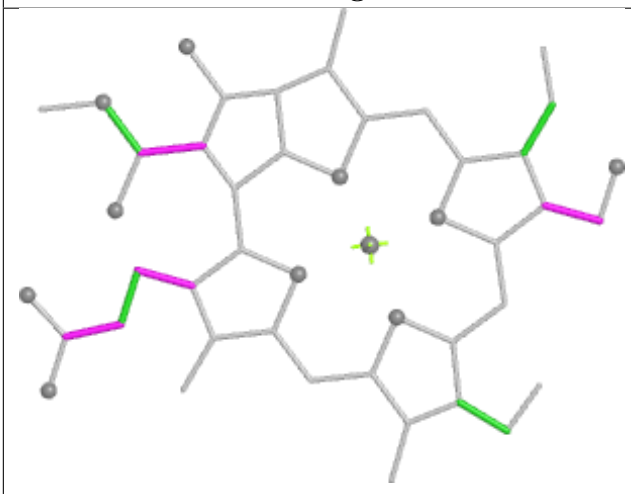
Ligand CHL r 605



Bond lengths



Bond angles

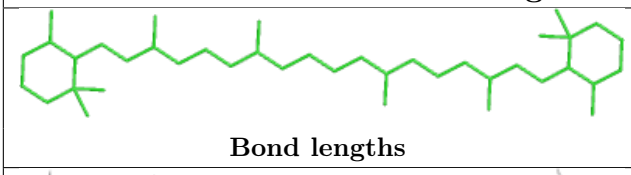


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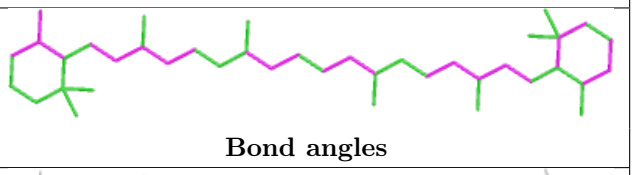


Rings

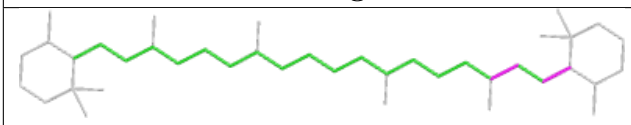
Ligand BCR b 621



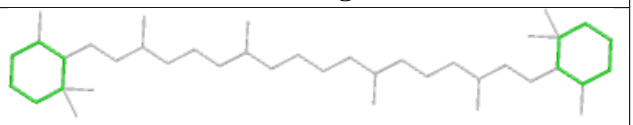
Bond lengths



Bond angles

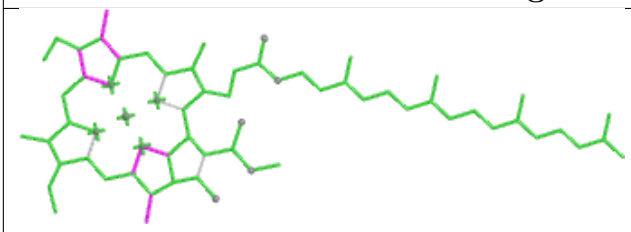


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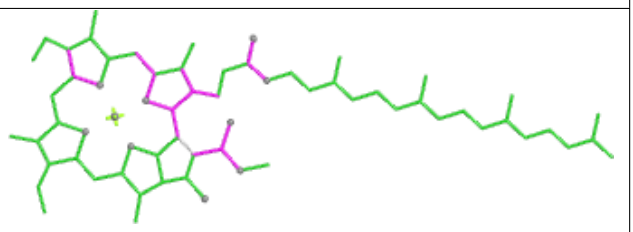


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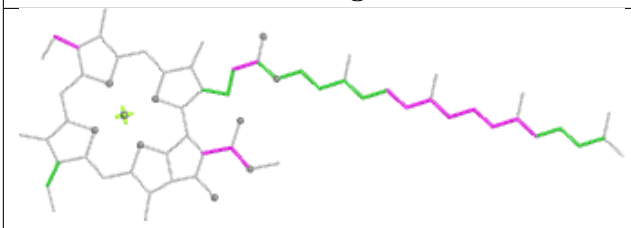
Ligand CLA b 617



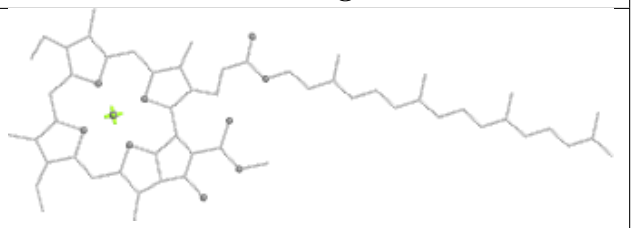
Bond lengths



Bond angles

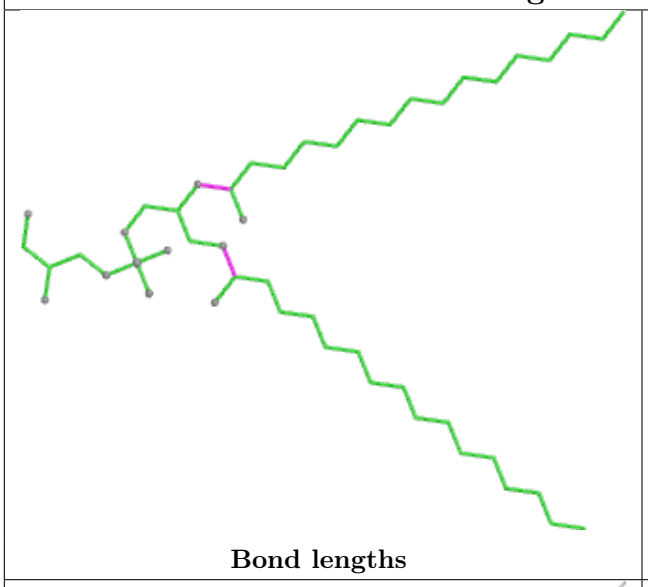


Torsions

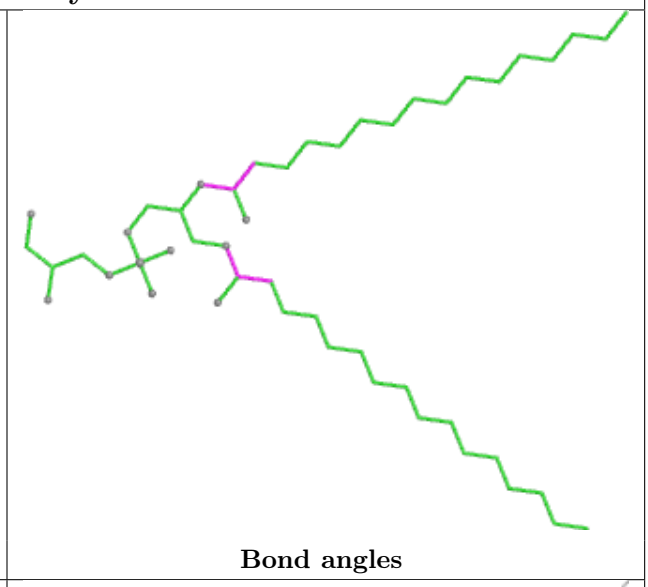


Rings

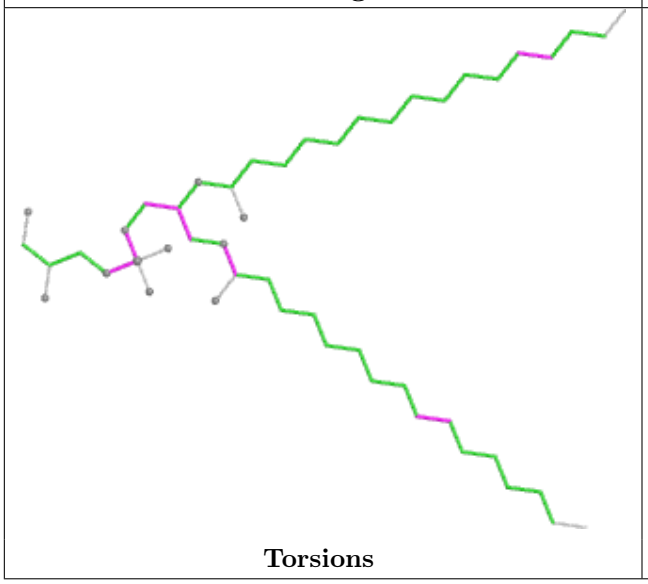
Ligand LHG y 318



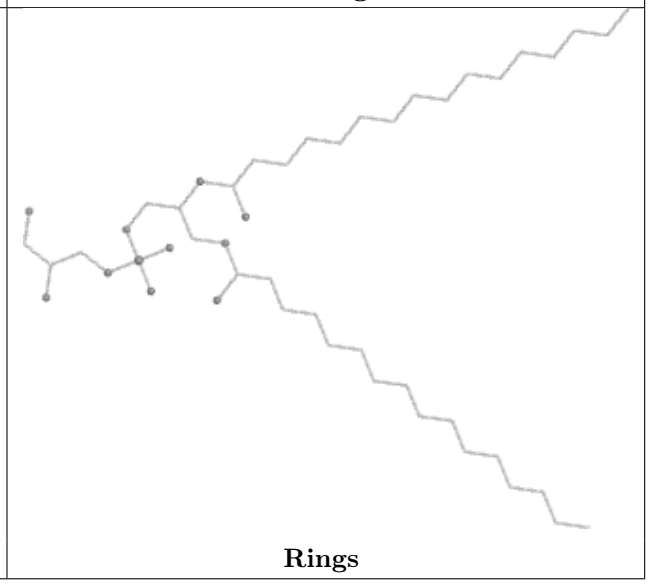
Bond lengths



Bond angles

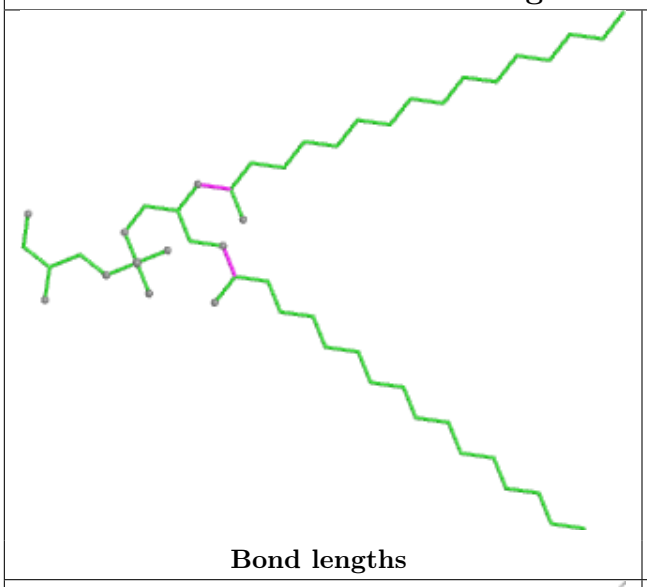


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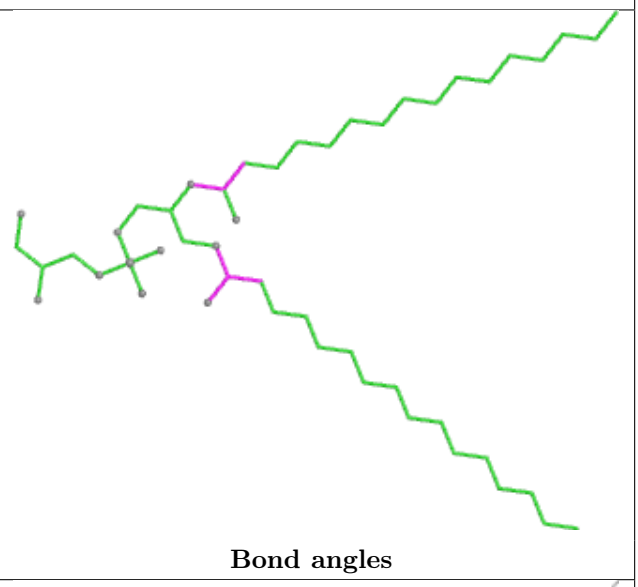


Rings

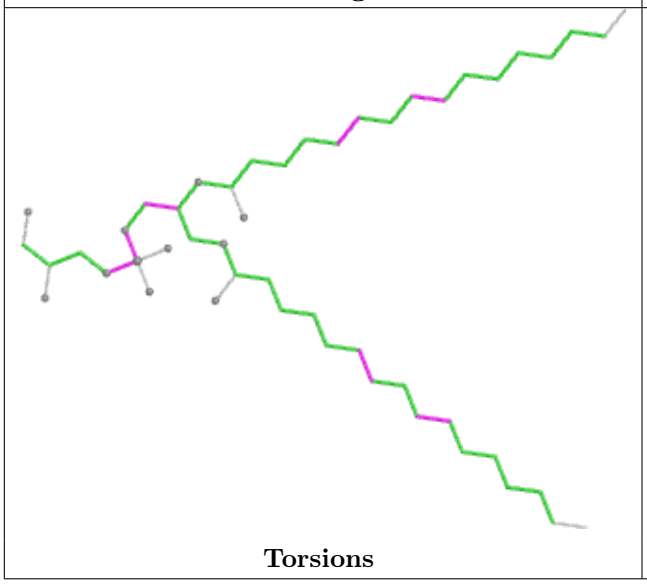
Ligand LHG L 101



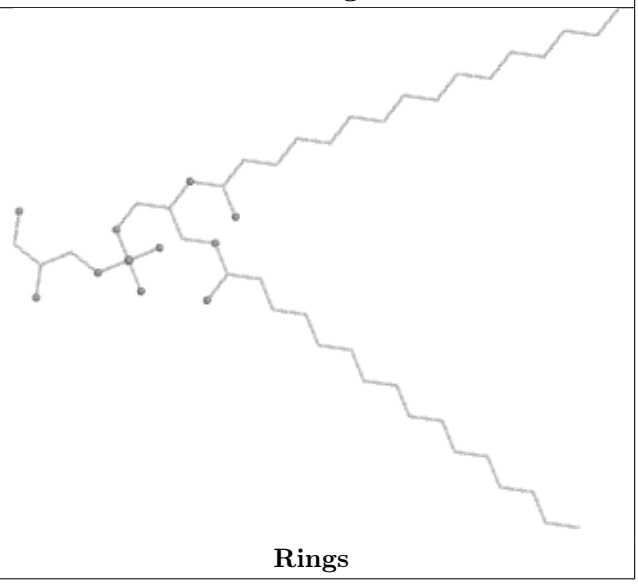
Bond lengths



Bond angles

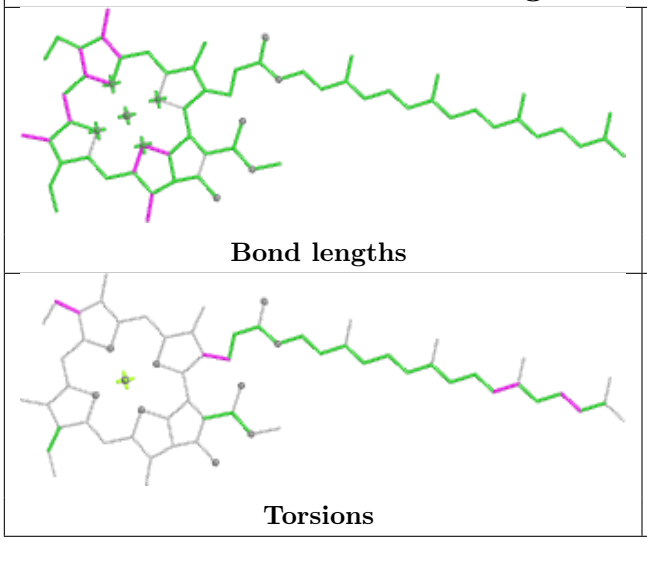


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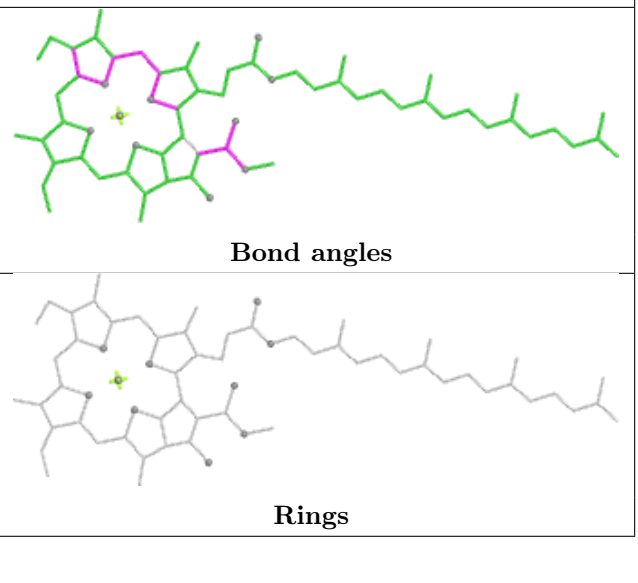


Rings

Ligand CLA D 403



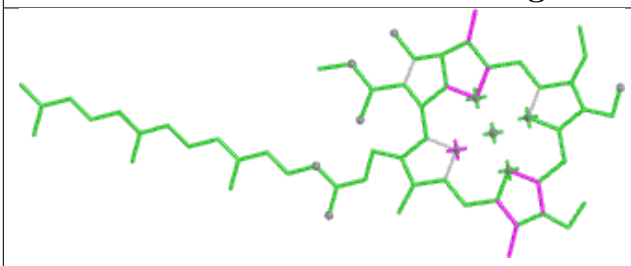
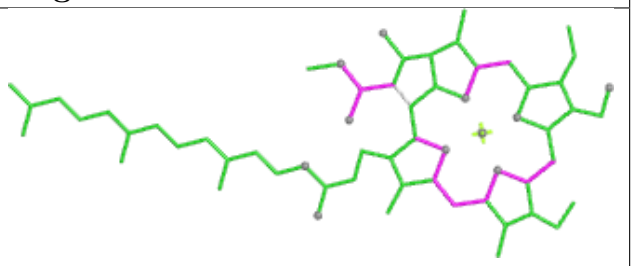
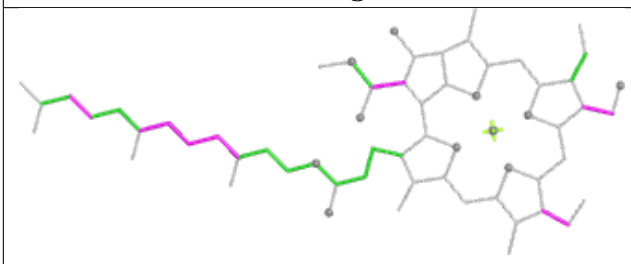
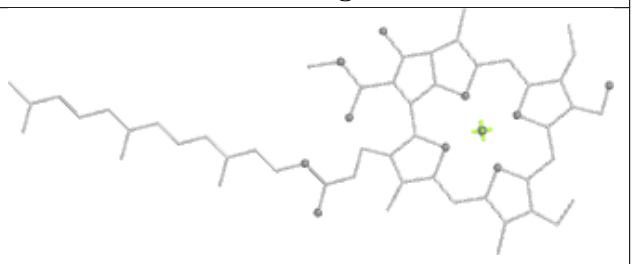
Bond lengths

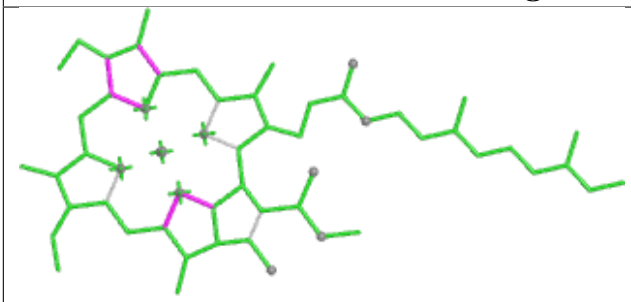
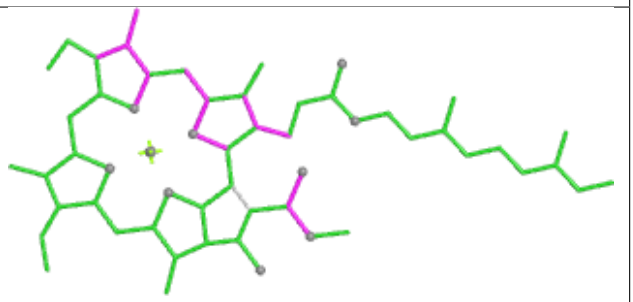
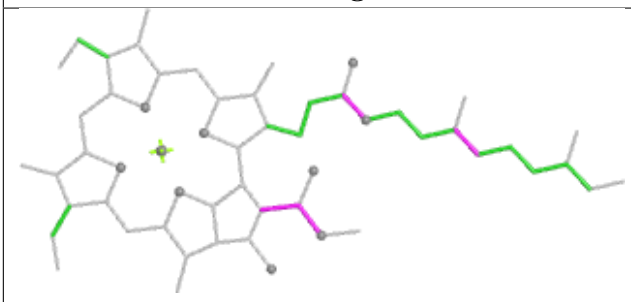
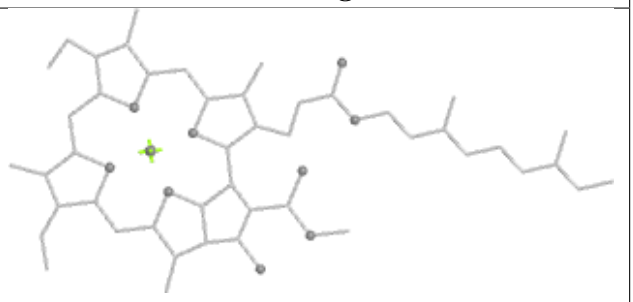


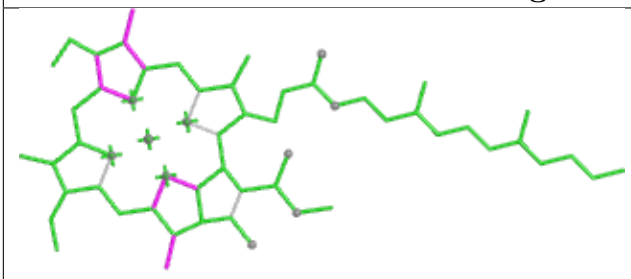
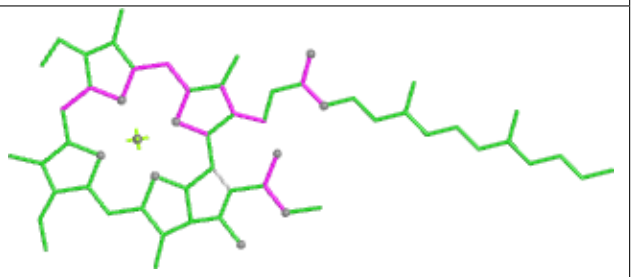
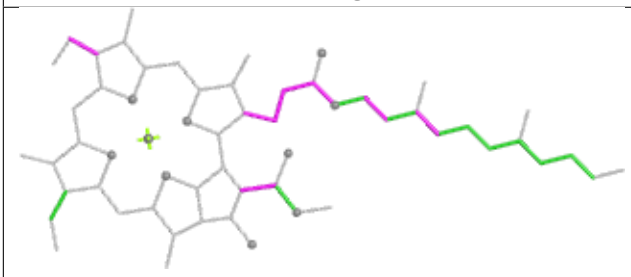
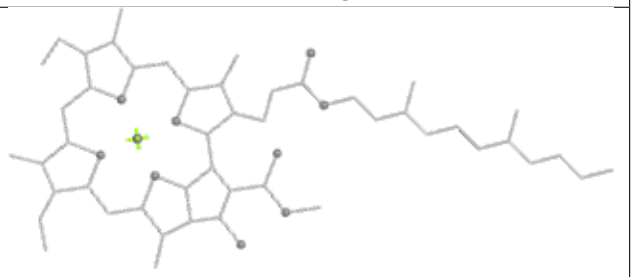
Bond angles

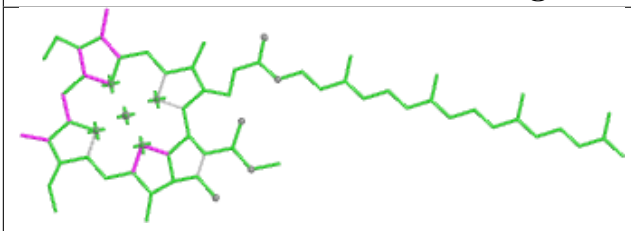
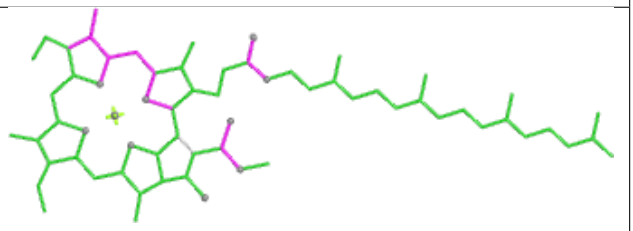
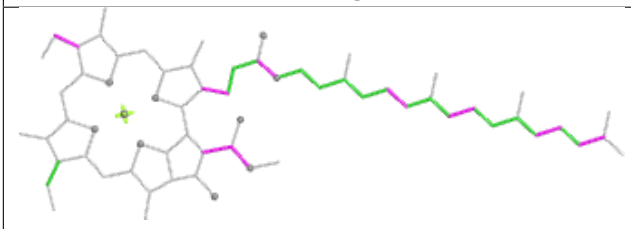
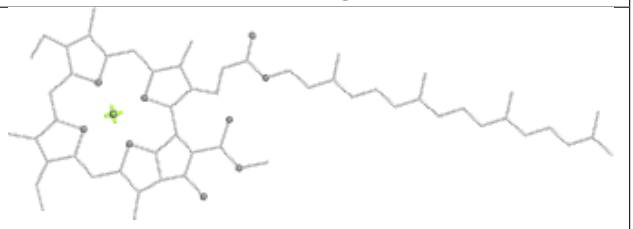
Torsions

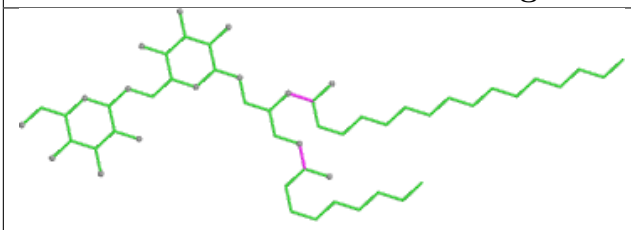
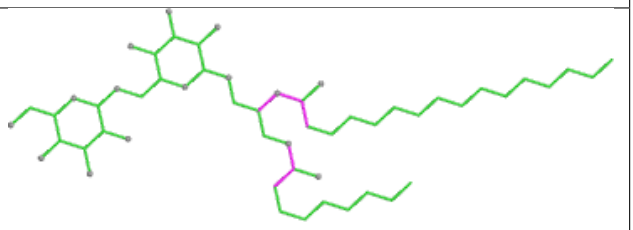
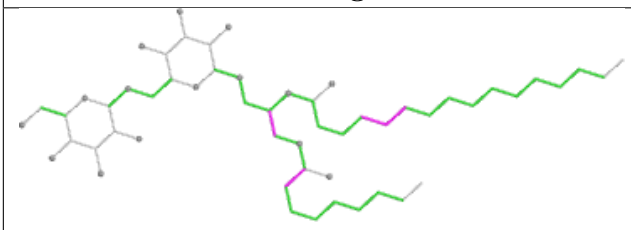
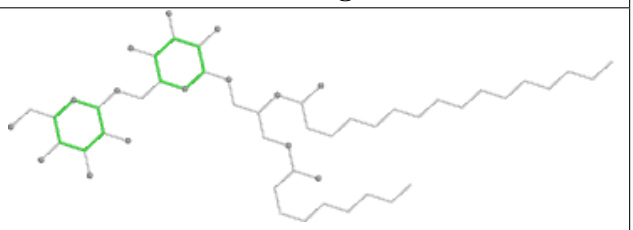
Rings

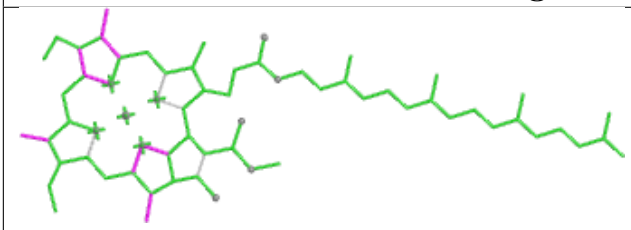
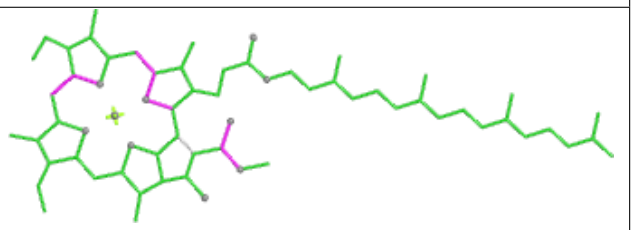
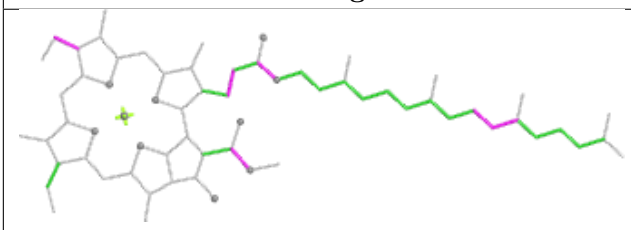
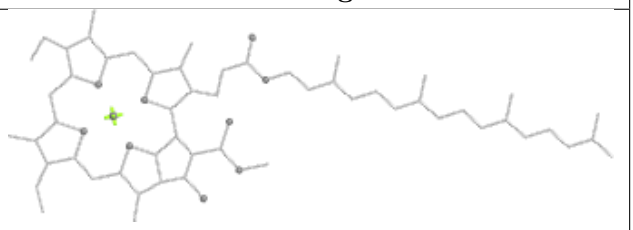
Ligand CHL g 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

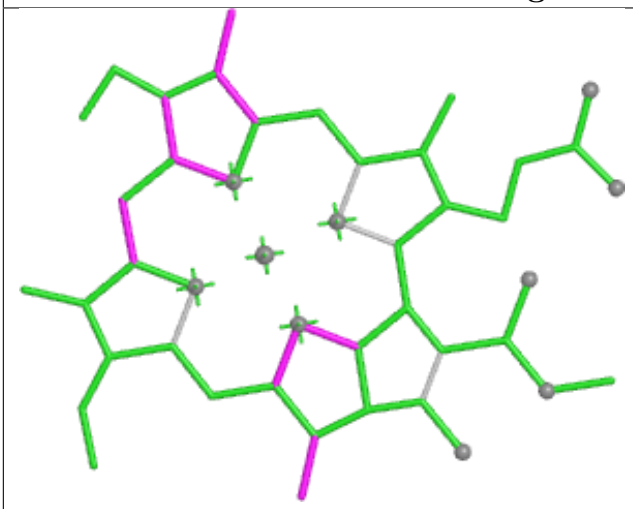
Ligand CLA c 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

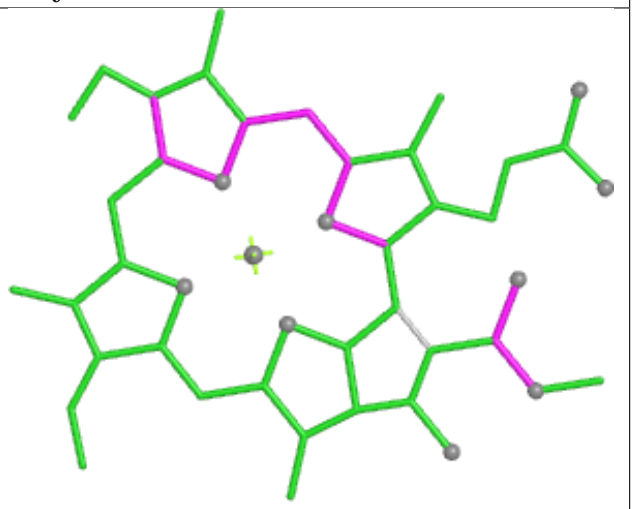
Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

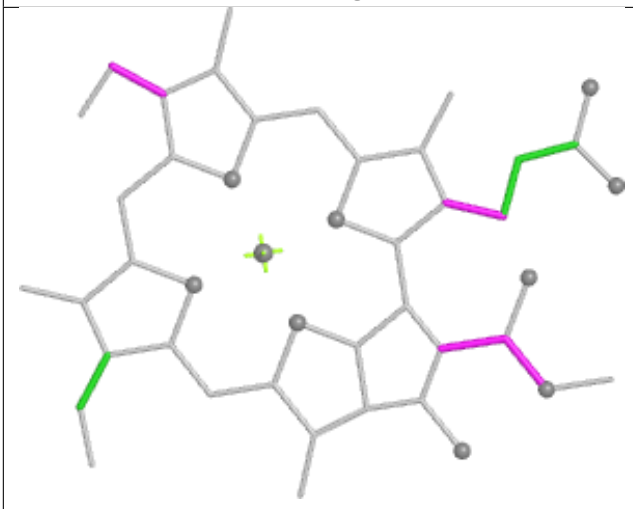
Ligand CLA y 315



Bond lengths



Bond angles

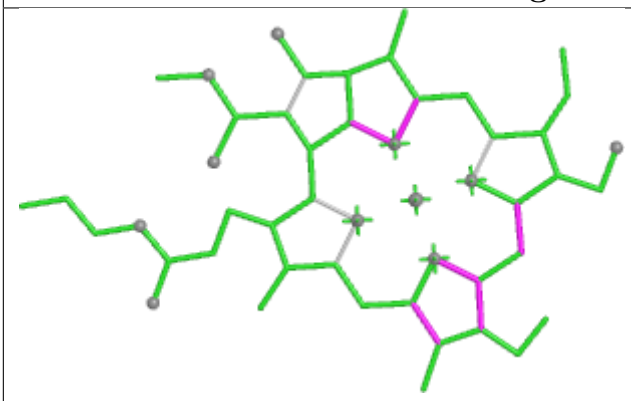


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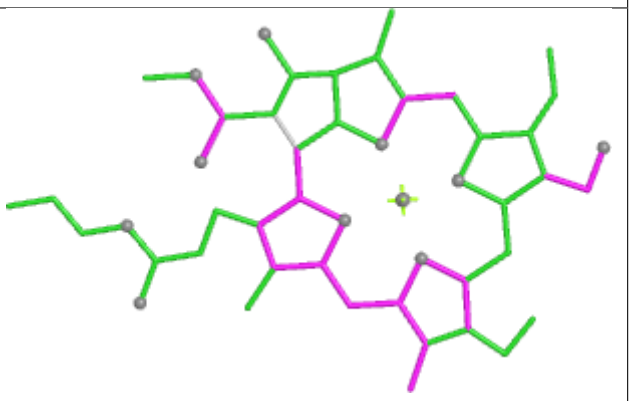


Rings

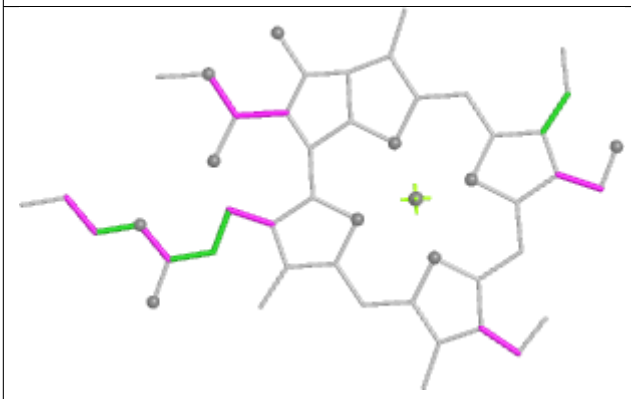
Ligand CHL s 607



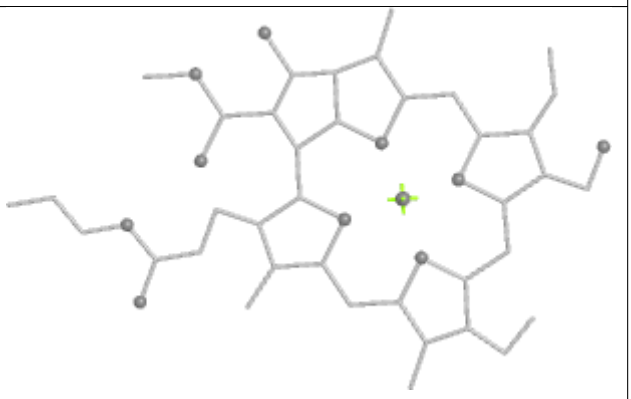
Bond lengths



Bond angles

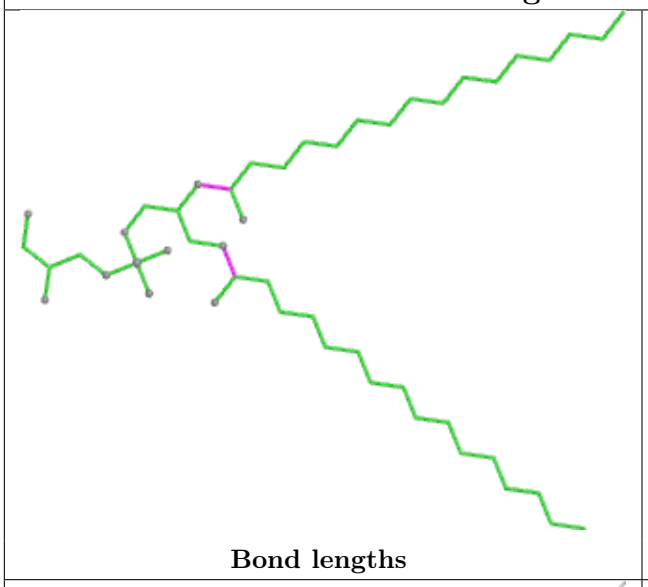


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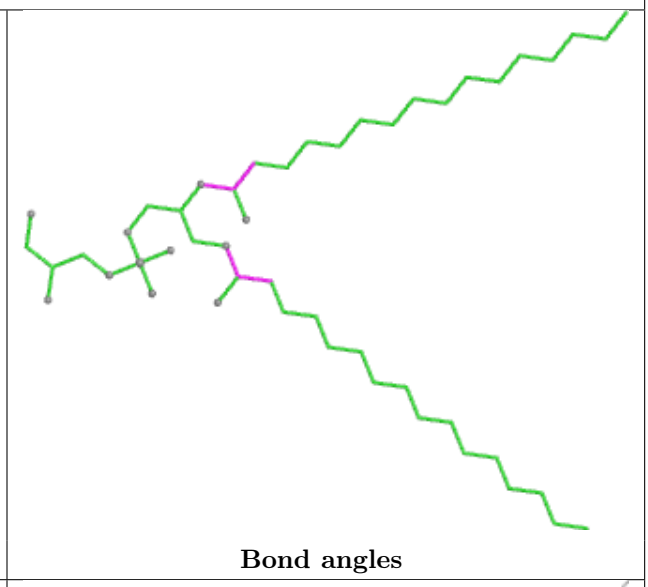


Rings

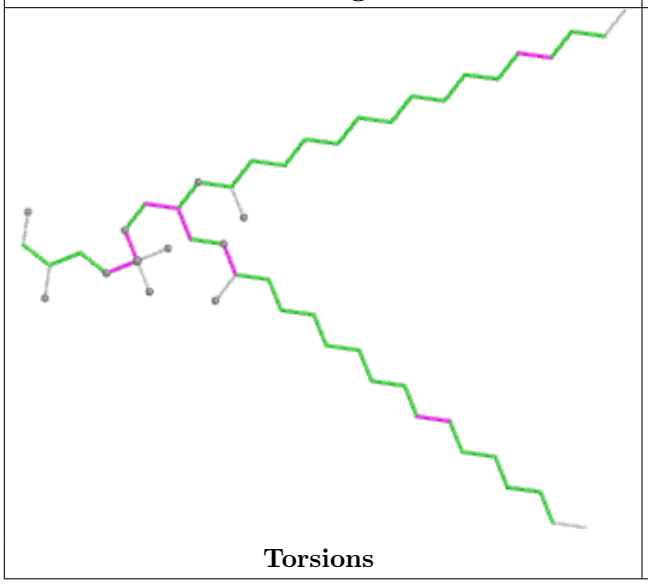
Ligand LHG Y 319



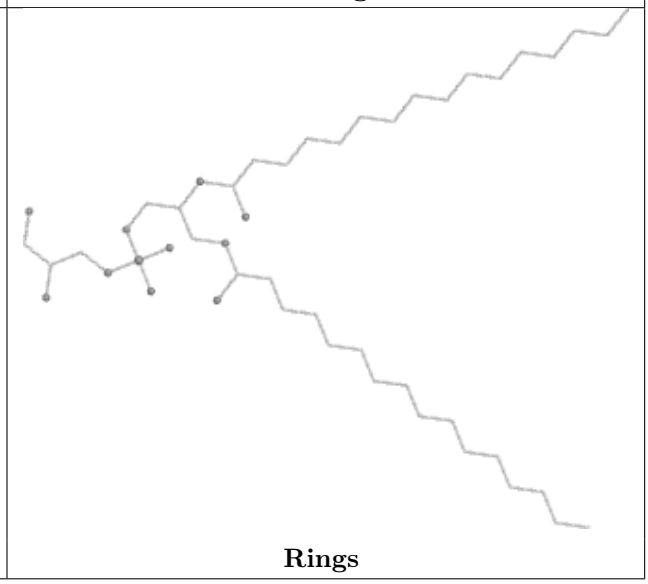
Bond lengths



Bond angles

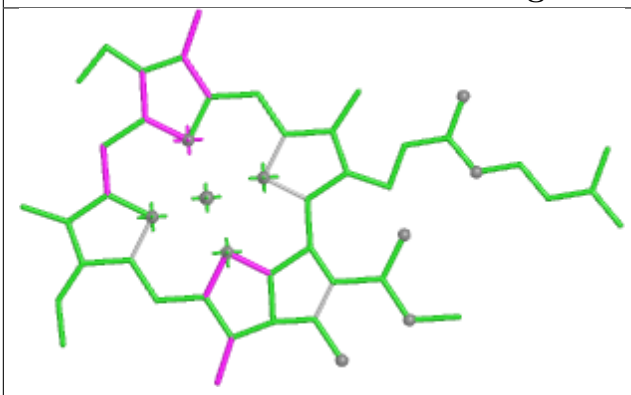


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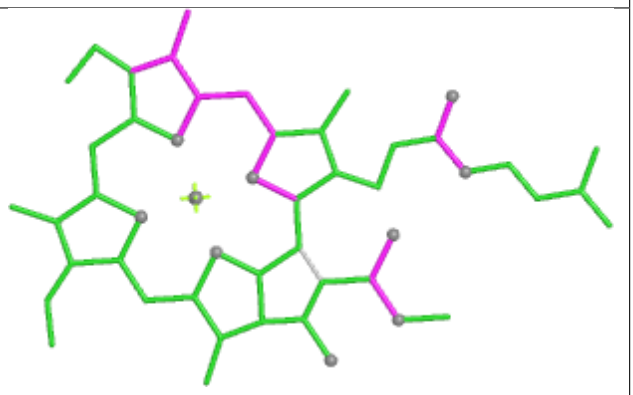


Rings

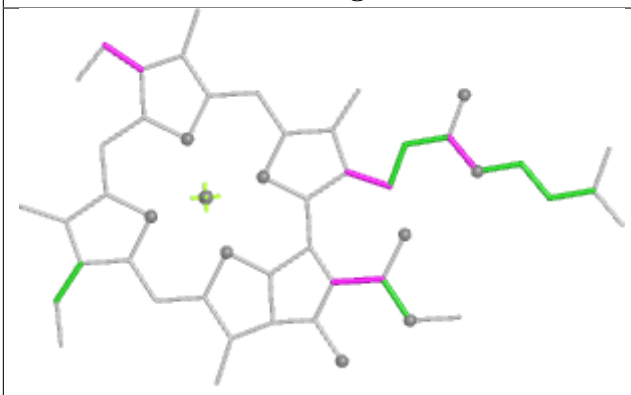
Ligand CLA S 305



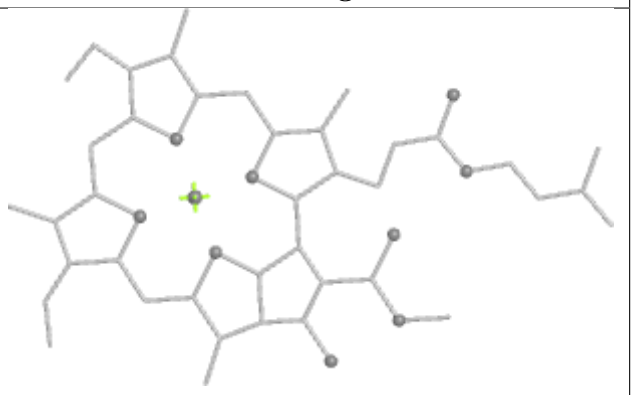
Bond lengths



Bond angles

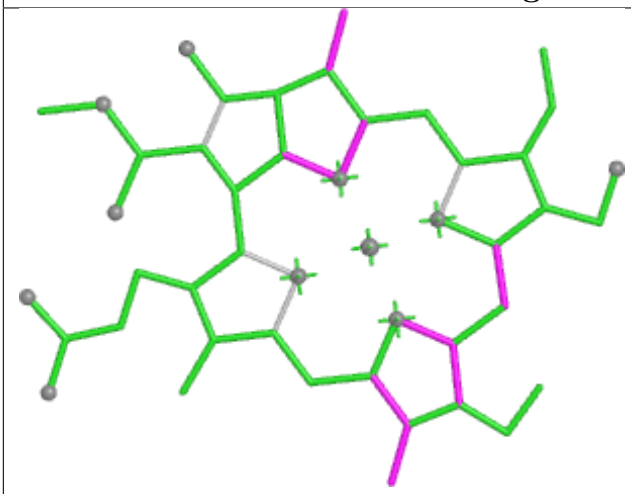


Torsions

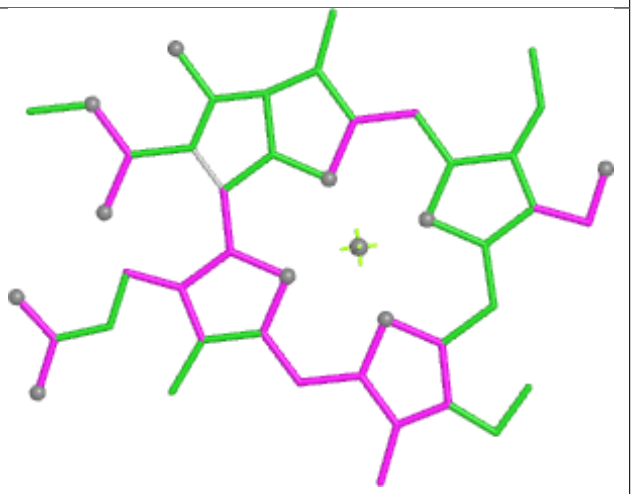


Rings

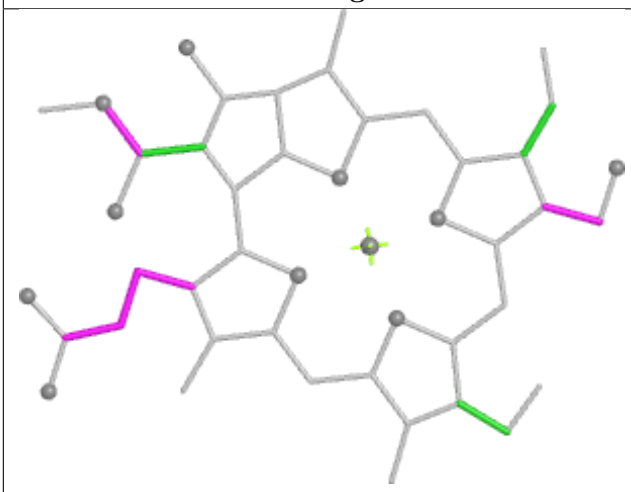
Ligand CHL N 606



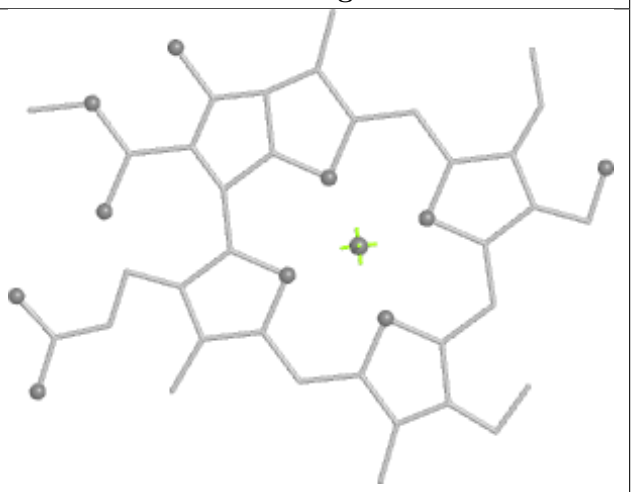
Bond lengths



Bond angles

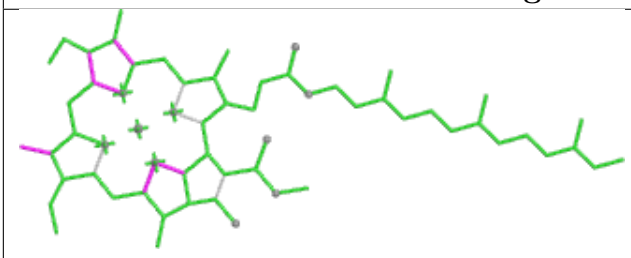


Torsions

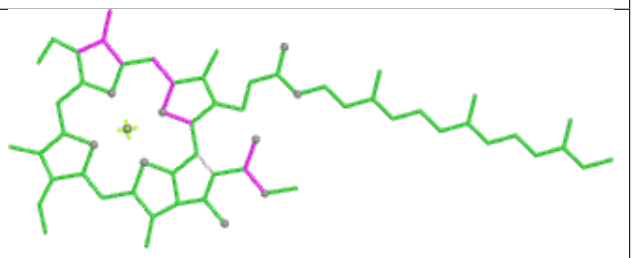


Rings

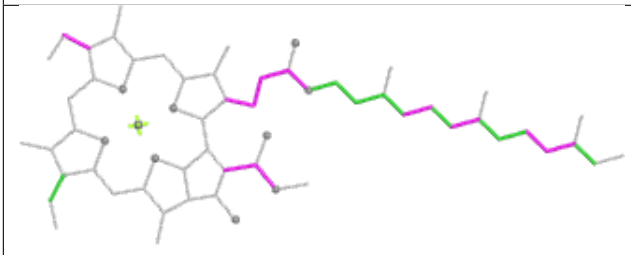
Ligand CLA Y 303



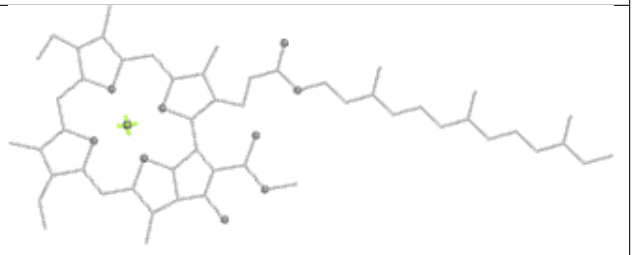
Bond lengths



Bond angles

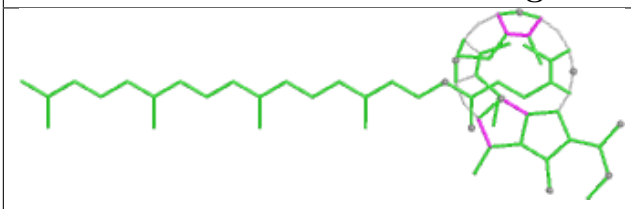


Torsions

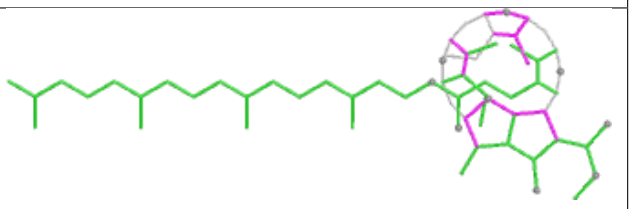


Rings

Ligand PHO a 402



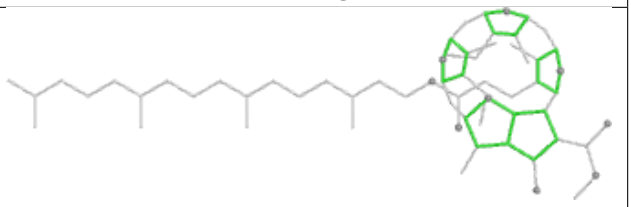
Bond lengths



Bond angles

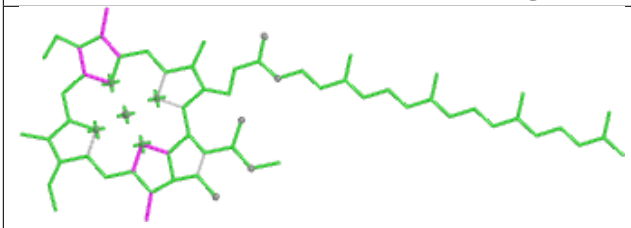


Torsions

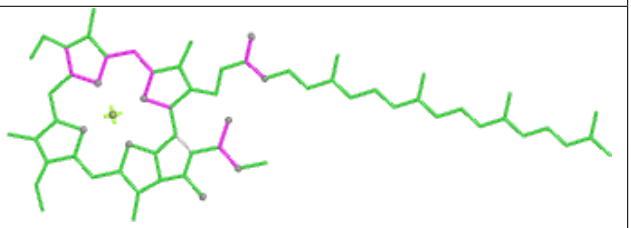


Rings

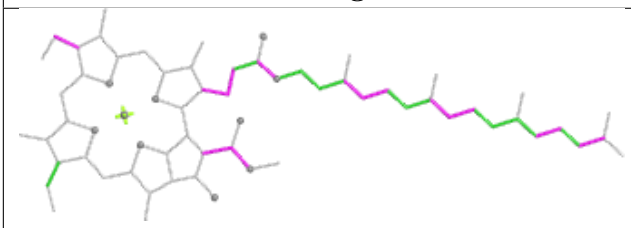
Ligand CLA B 603



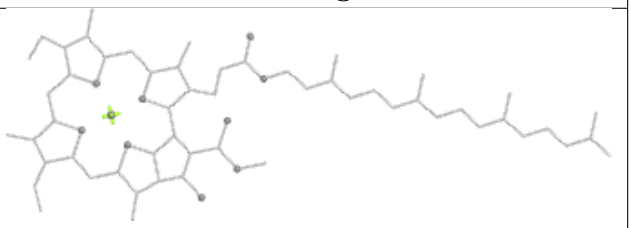
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Bond angles

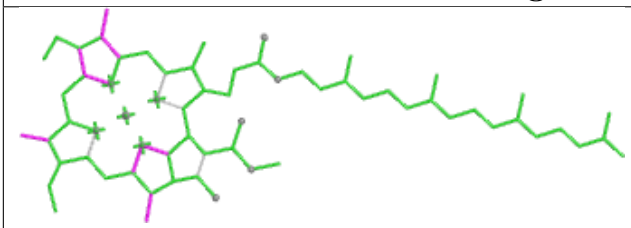


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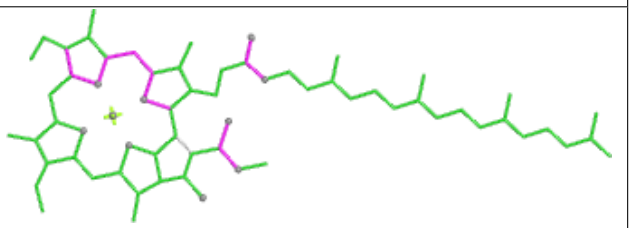


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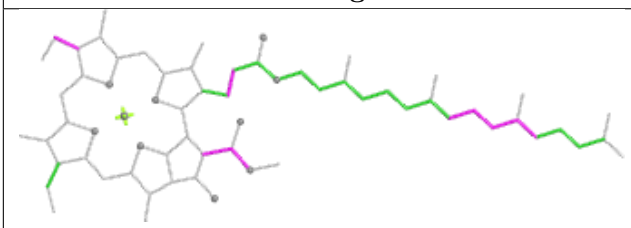
Ligand CLA b 608



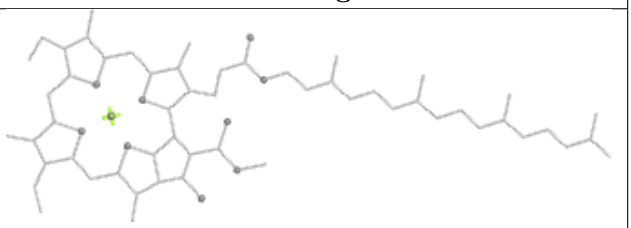
Bond lengths



Bond angles

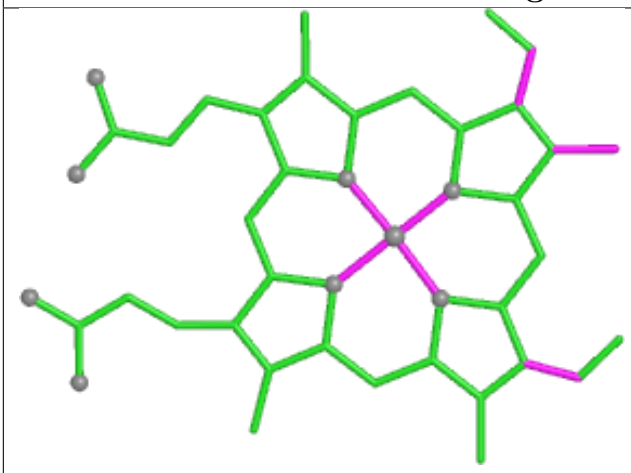


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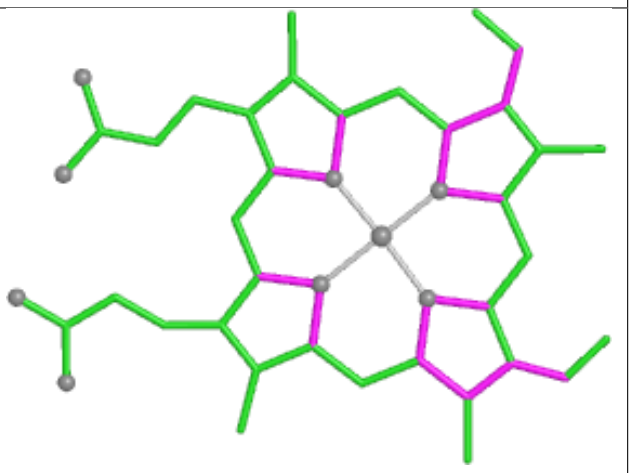


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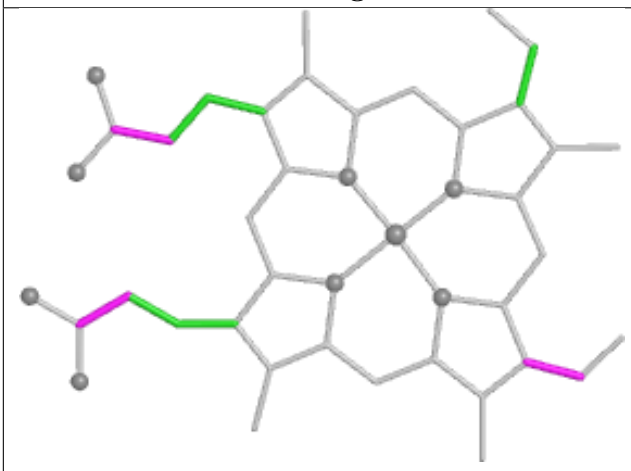
Ligand HEM f 101



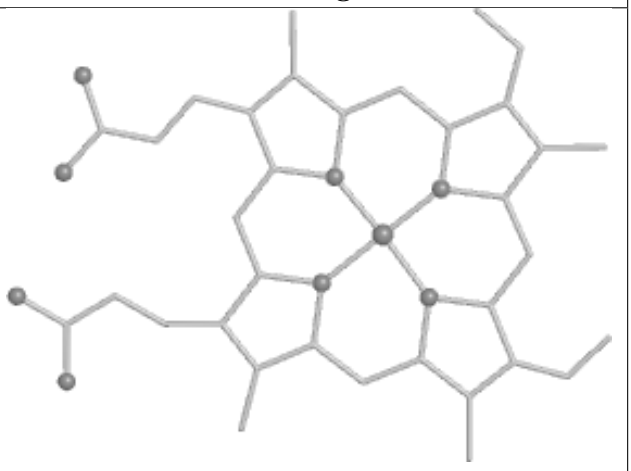
Bond lengths



Bond angles

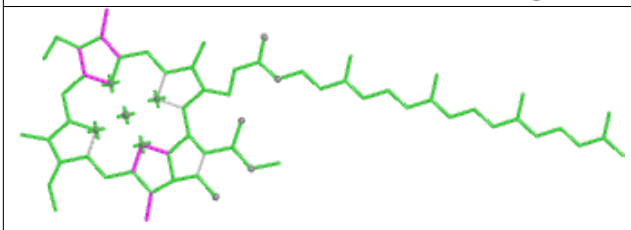


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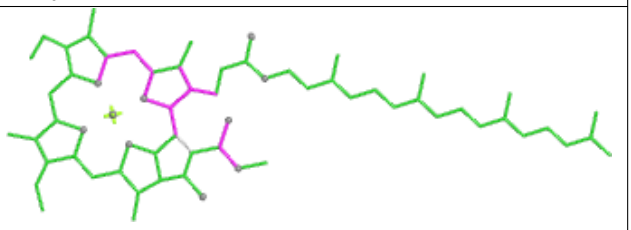


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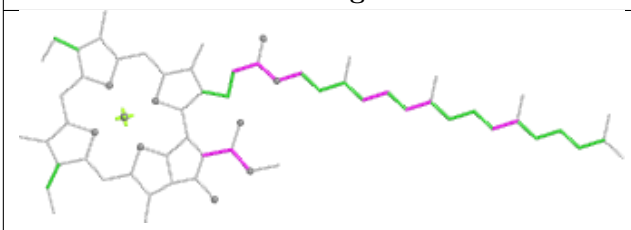
Ligand CLA y 304



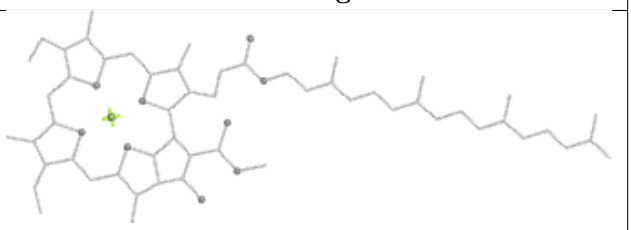
Bond lengths



Bond angles

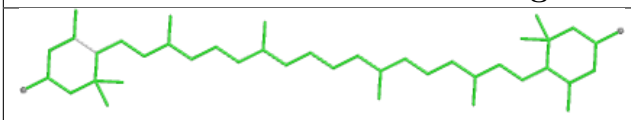


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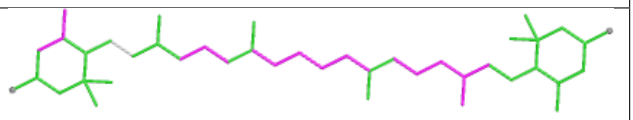


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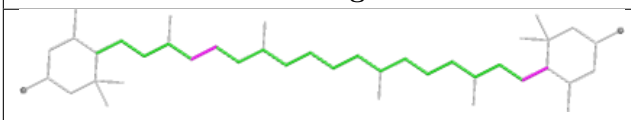
Ligand LUT s 615



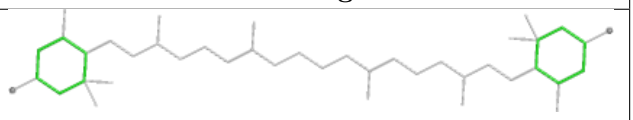
Bond lengths



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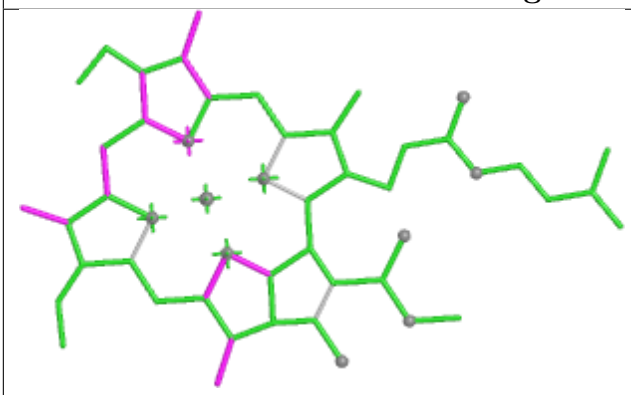


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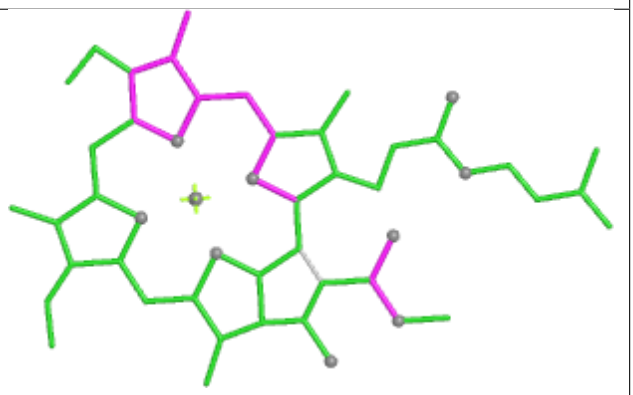


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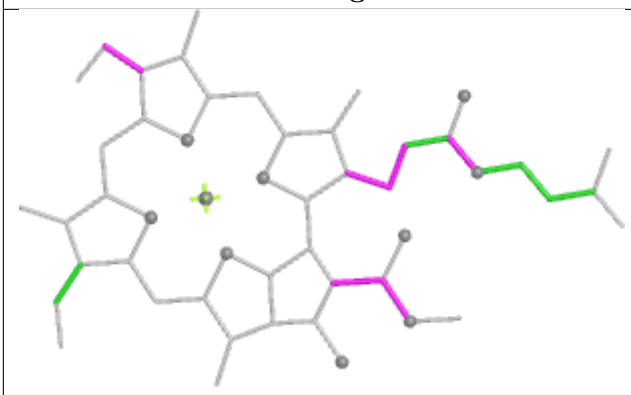
Ligand CLA Y 305



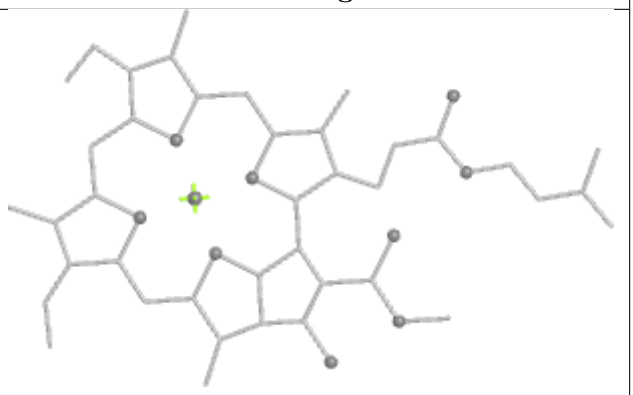
Bond lengths



Bond angles

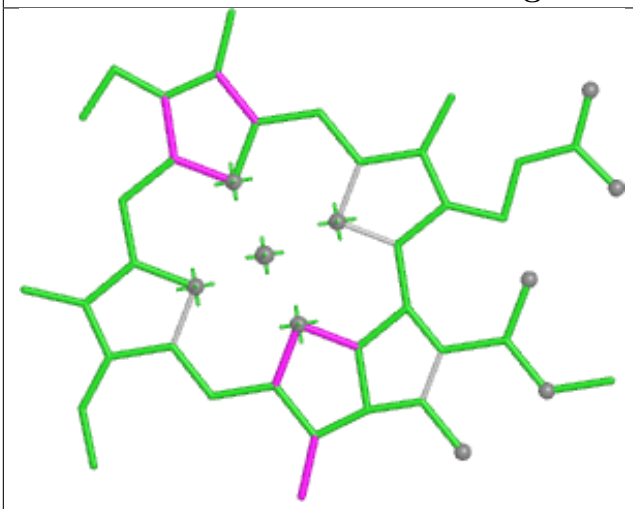


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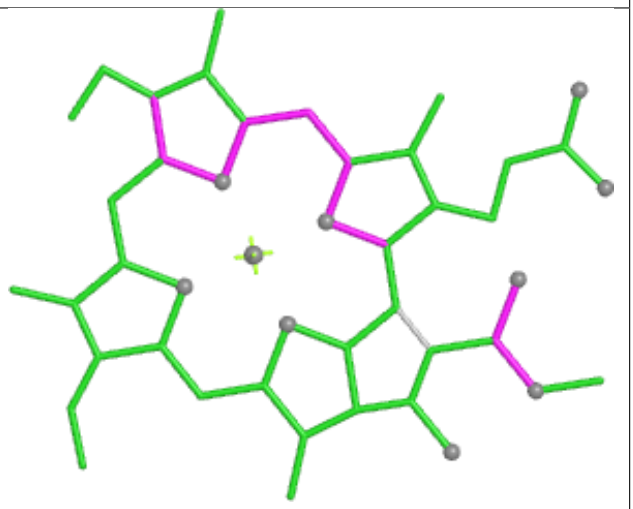


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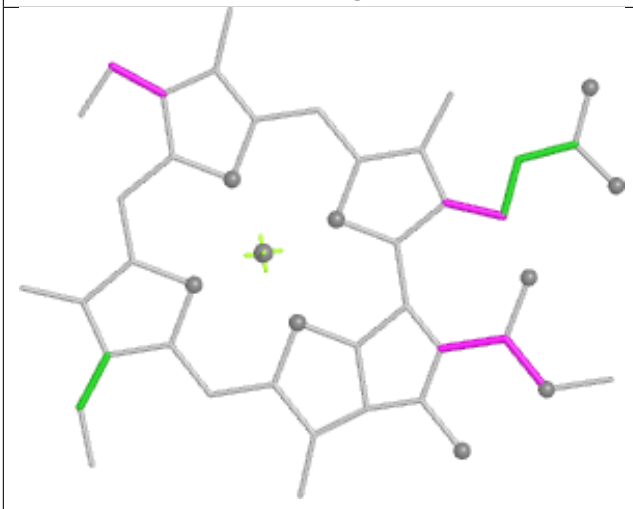
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Bond lengths



Bond angles

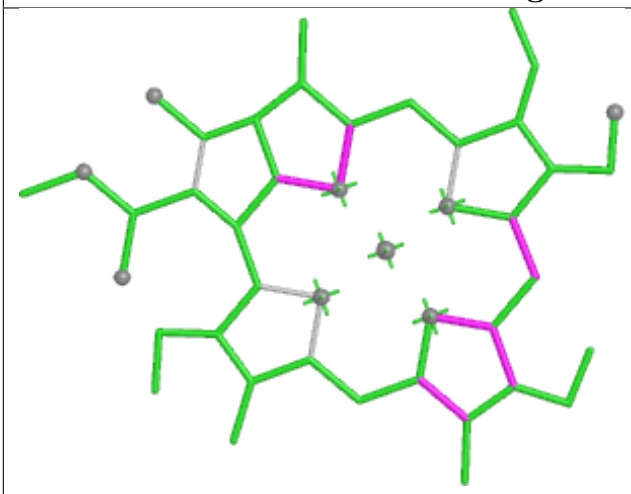


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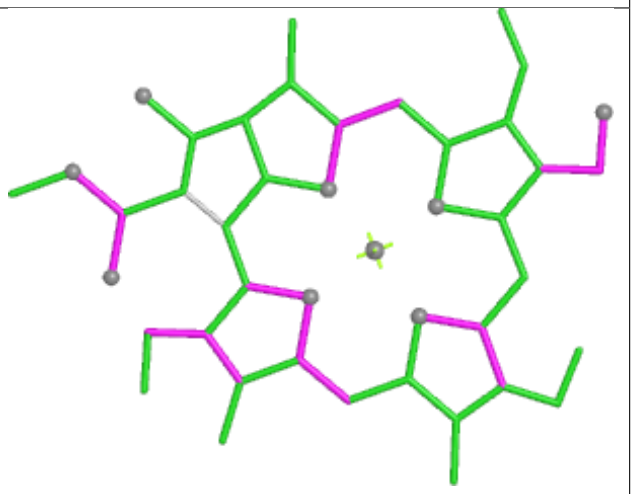


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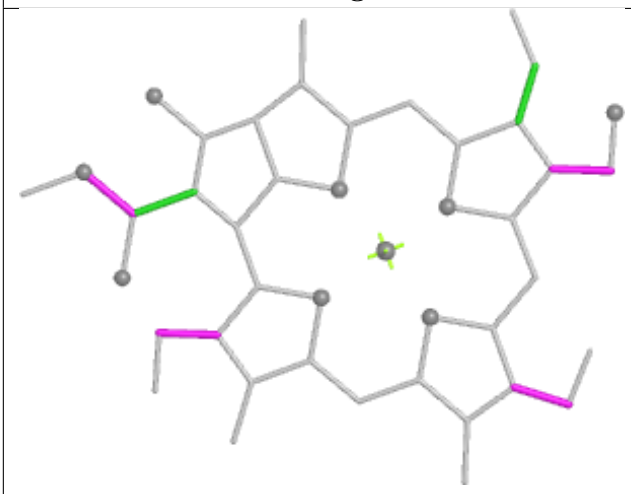
Ligand CHL S 307



Bond lengths



Bond angles

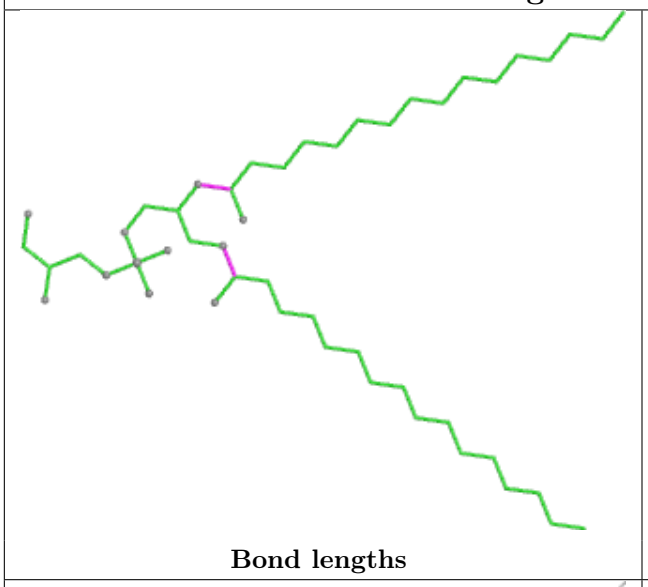


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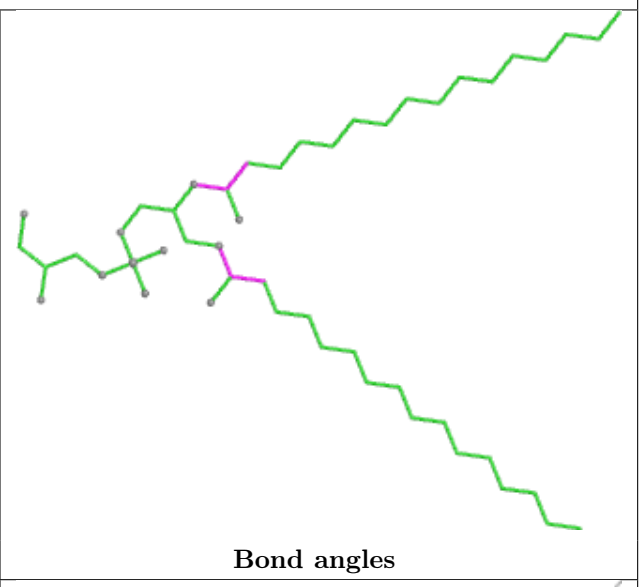


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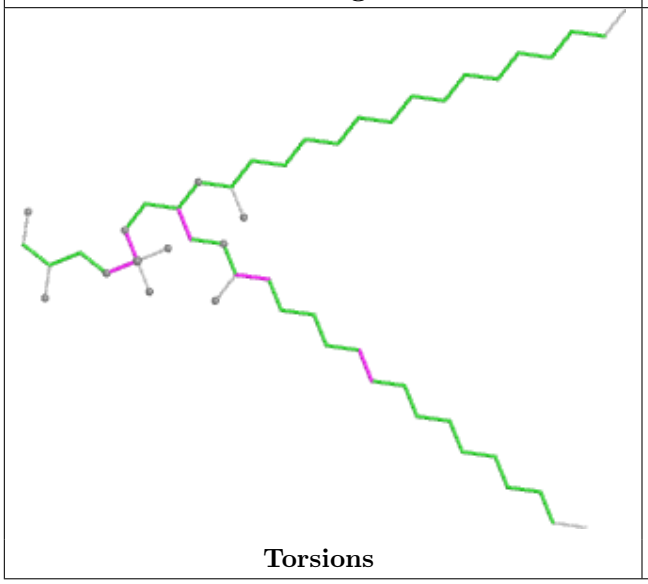
Ligand LHG S 318



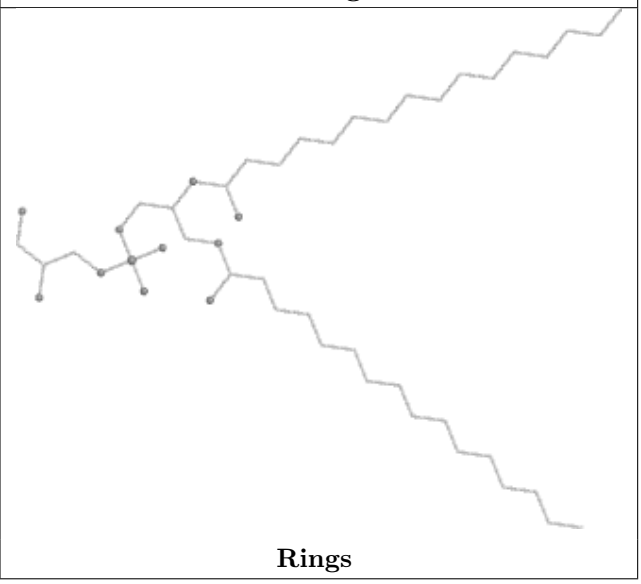
Bond lengths



Bond angles



Torsions

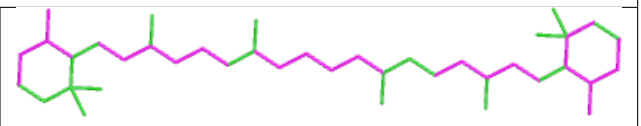


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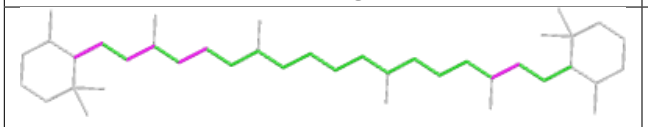
Ligand BCR D 405



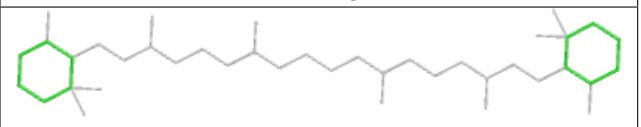
Bond lengths



Bond angles

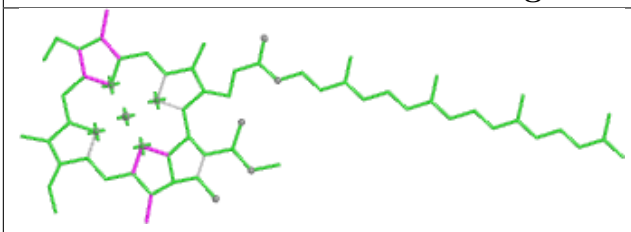


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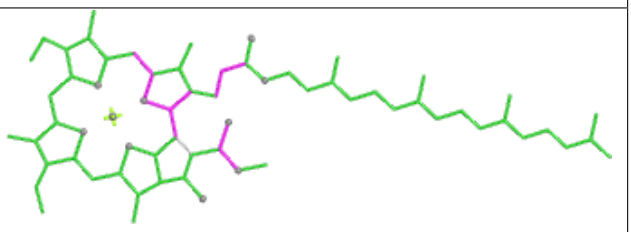


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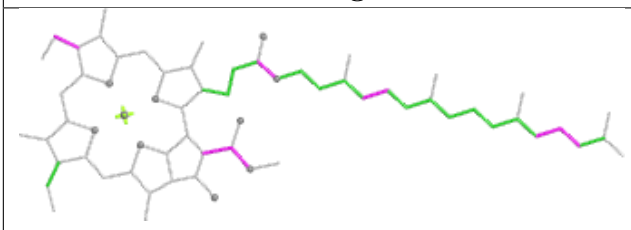
Ligand CLA B 604



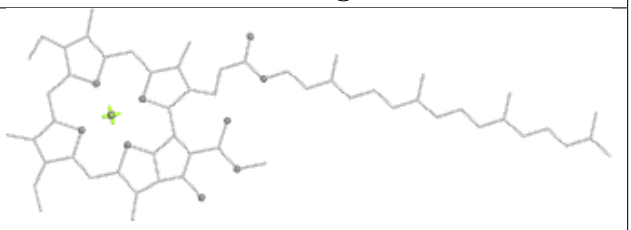
Bond lengths



Bond angles

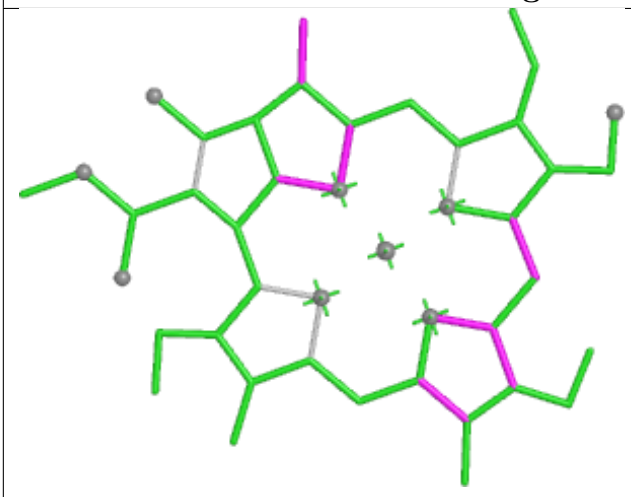


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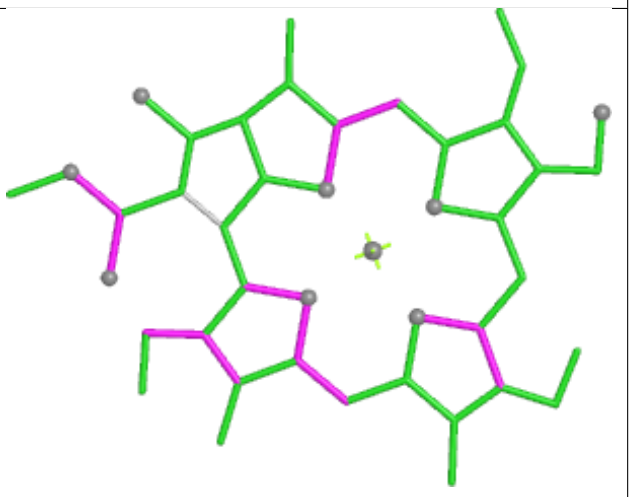


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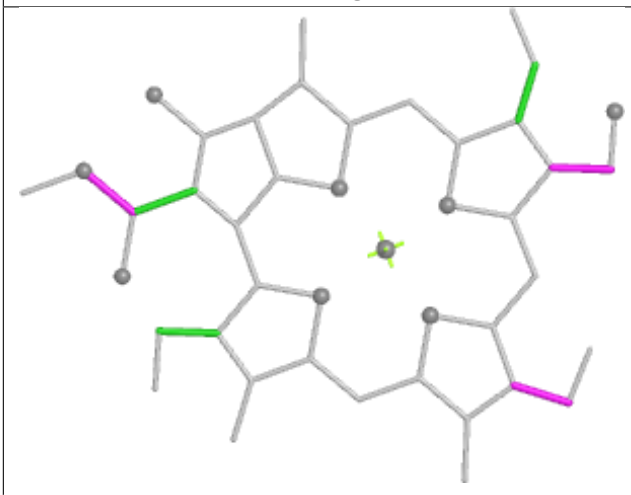
Ligand CHL G 607



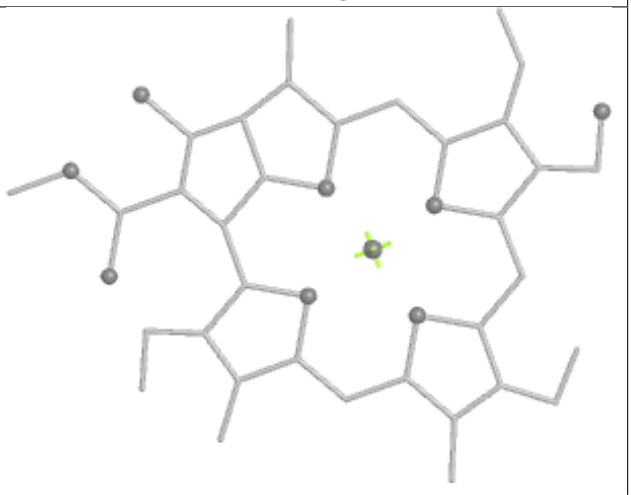
Bond lengths



Bond angles

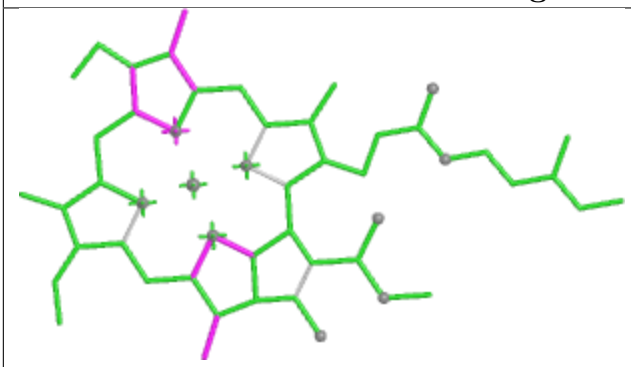


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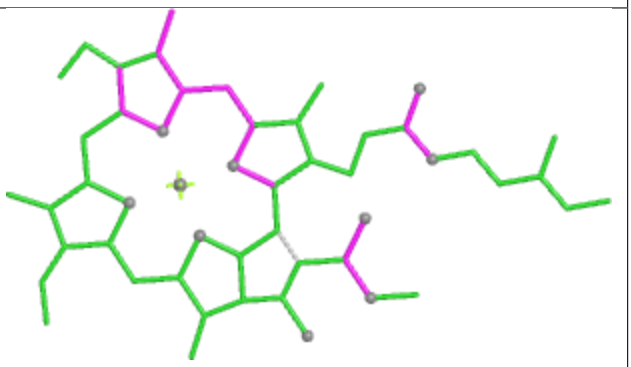


Rings

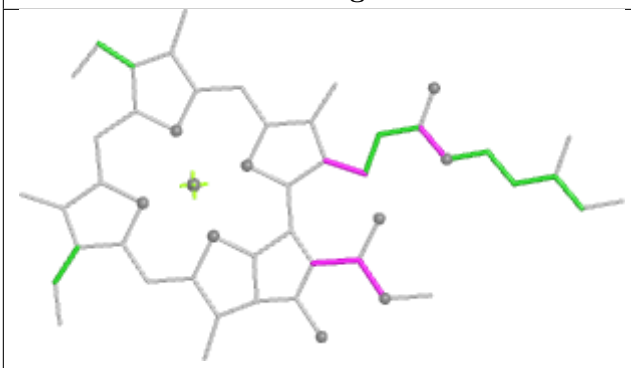
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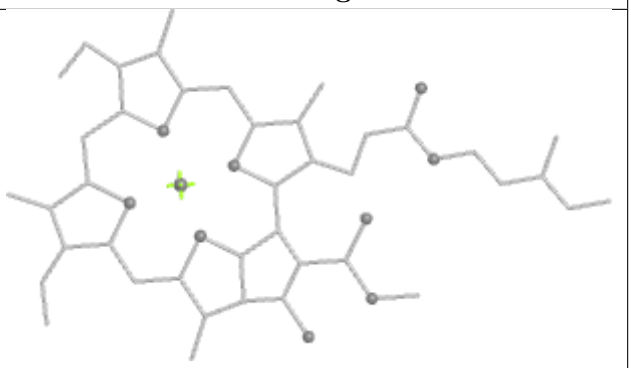
Bond lengths



Bond angles

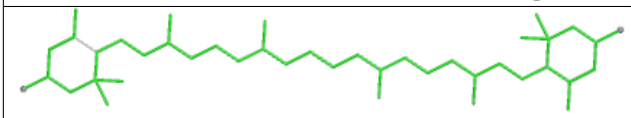


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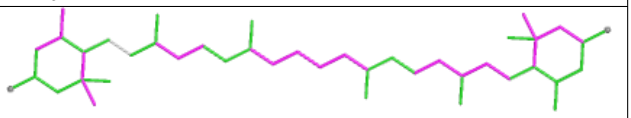


Rings

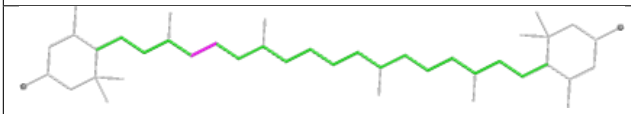
Ligand LUT y 317



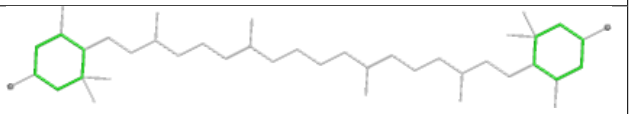
Bond lengths



Bond angles

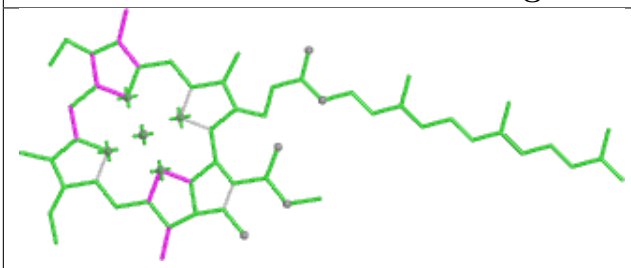


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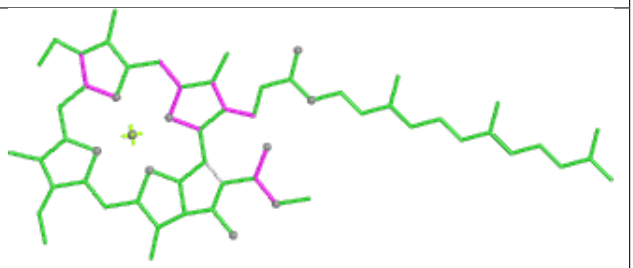


Rings

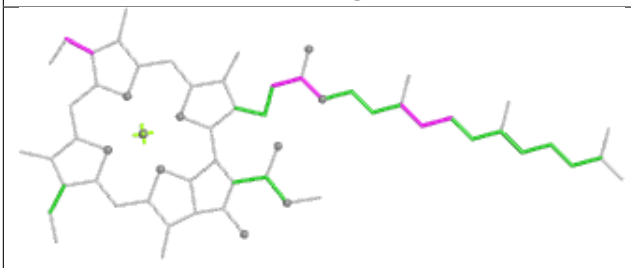
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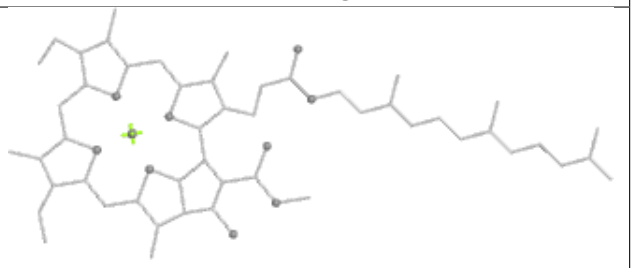
Bond lengths



Bond angles

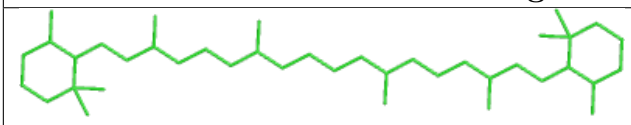


Torsions

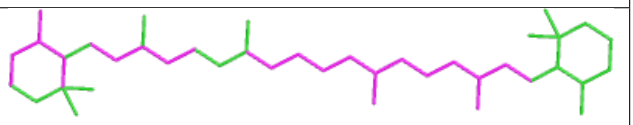


Rings

Ligand BCR c 514



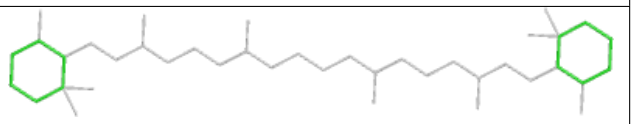
Bond lengths



Bond angles

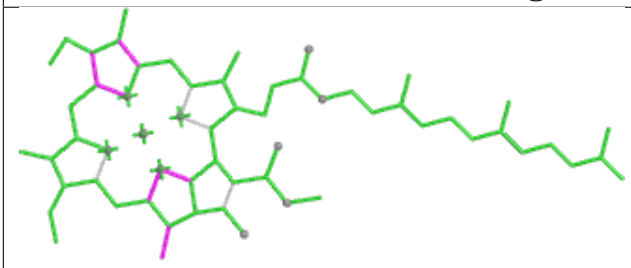


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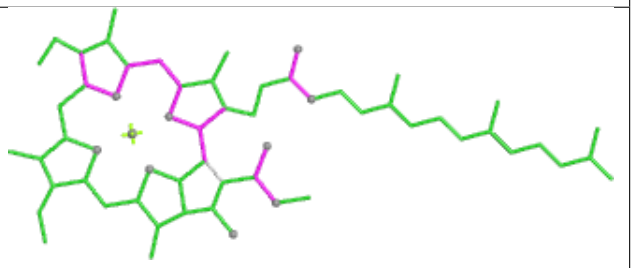


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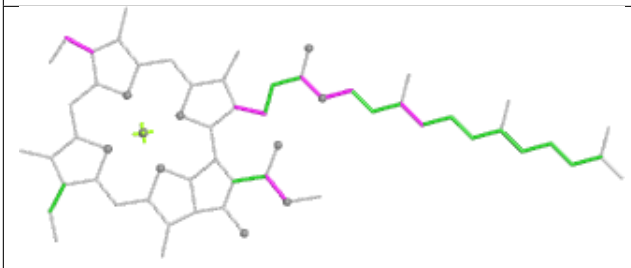
Ligand CLA n 611



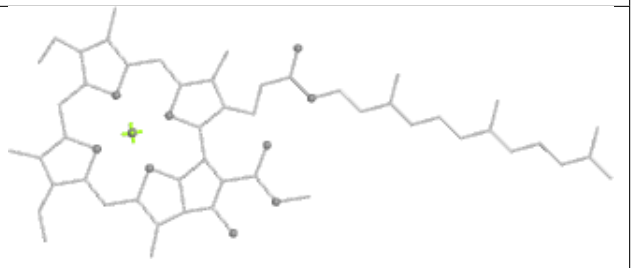
Bond lengths



Bond angles

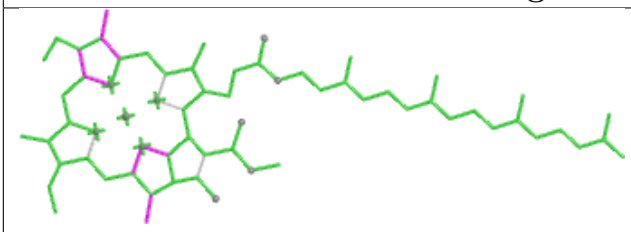


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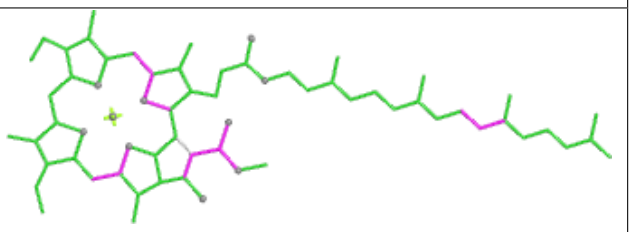


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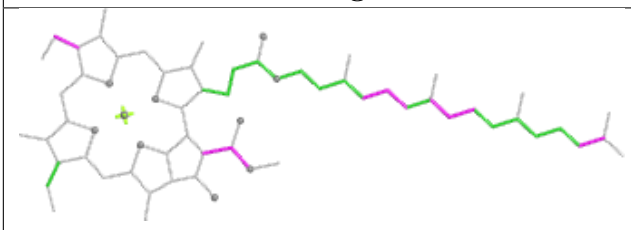
Ligand CLA b 607



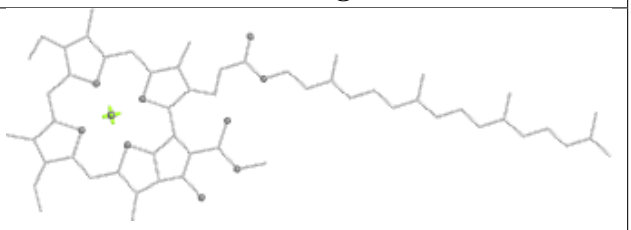
Bond lengths



Bond angles

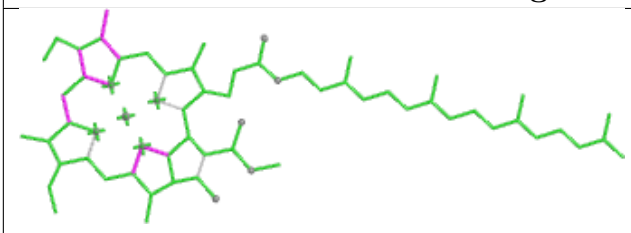


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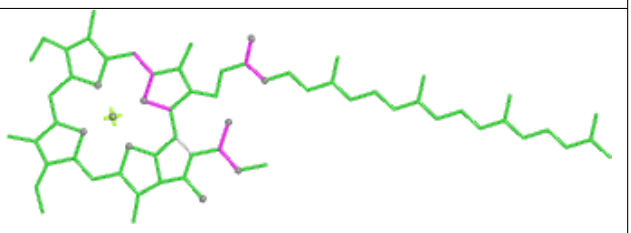


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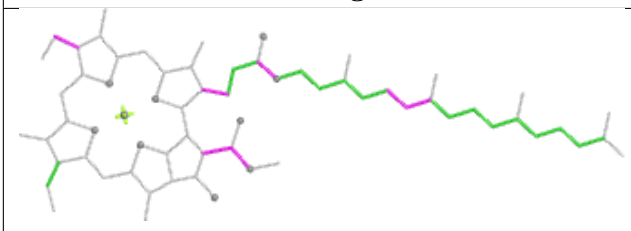
Ligand CLA r 611



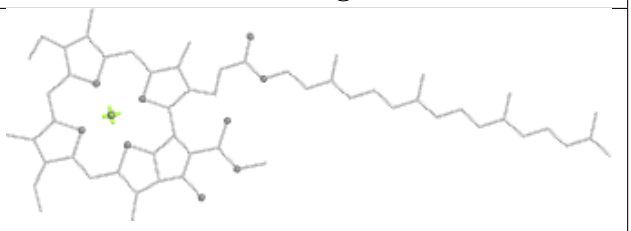
Bond lengths



Bond angles

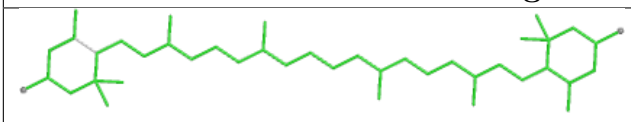


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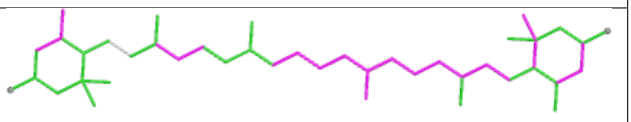


Rings

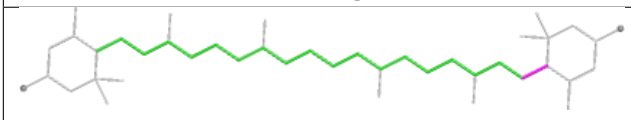
Ligand LUT N 616



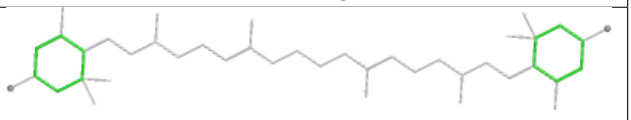
Bond lengths



Bond angles

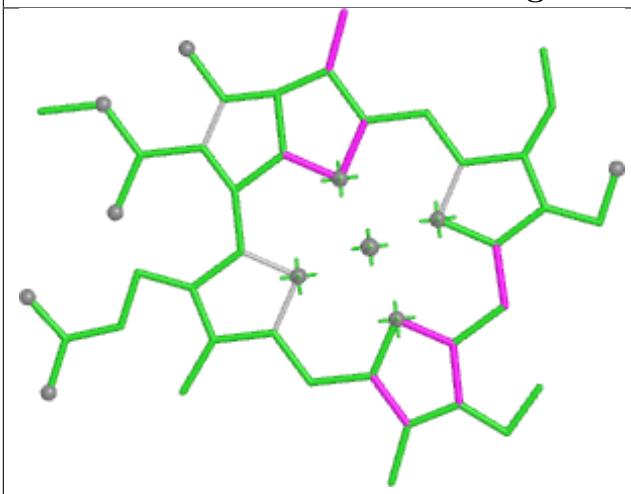


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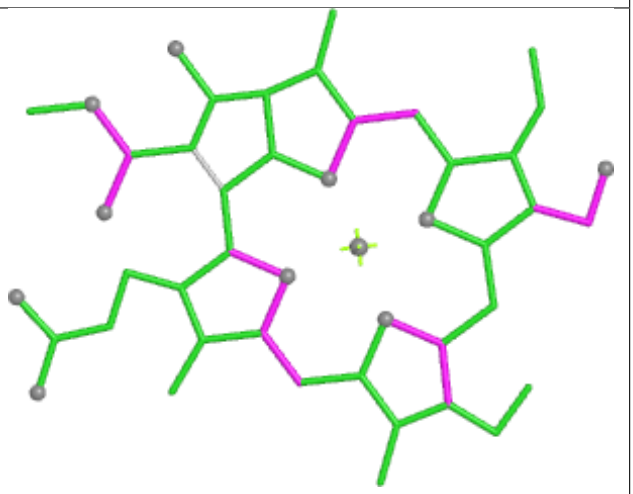


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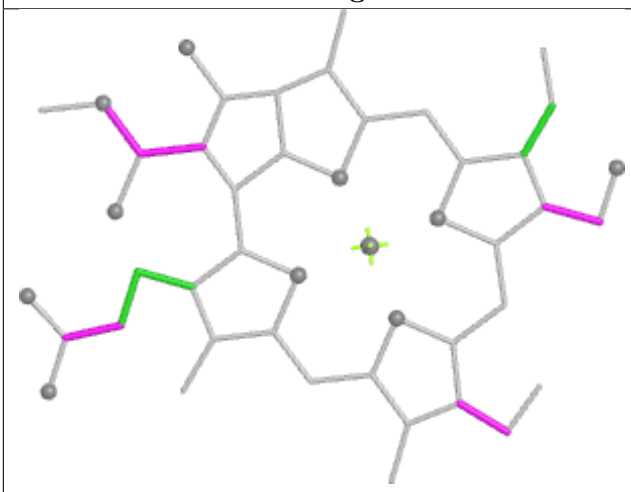
Ligand CHL S 302



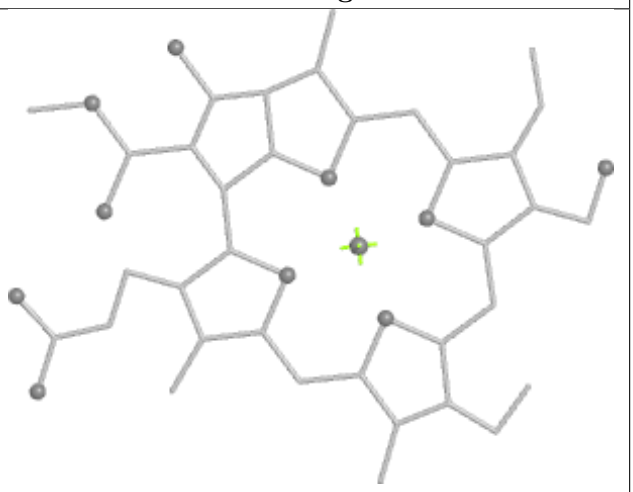
Bond lengths



Bond angles



Torsions

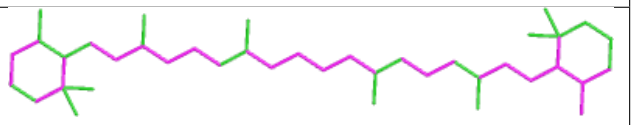


Rings

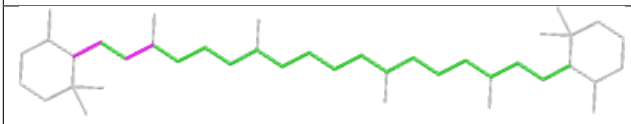
Ligand BCR k 101



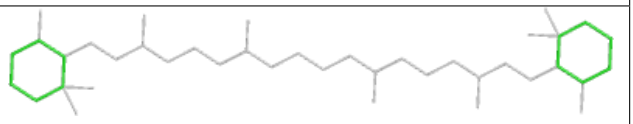
Bond lengths



Bond angles

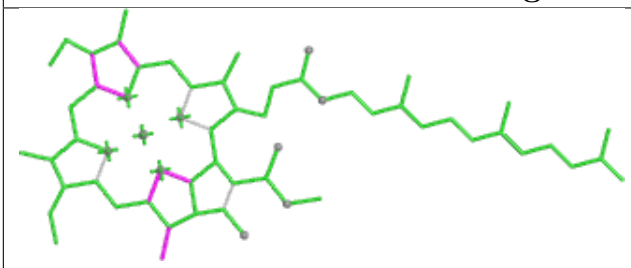


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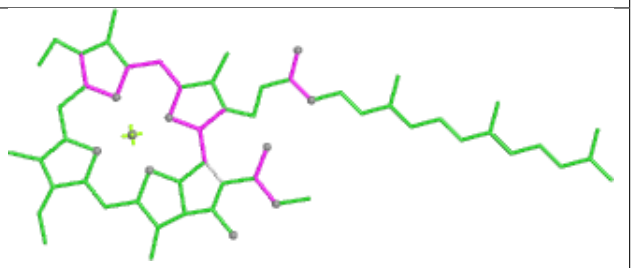


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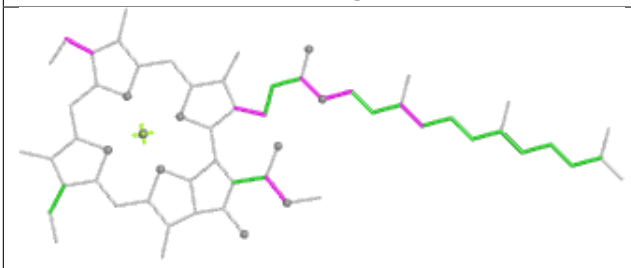
Ligand CLA N 611



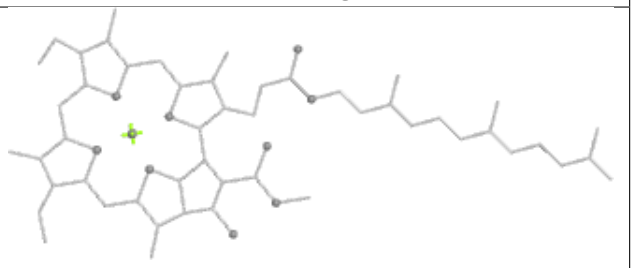
Bond lengths



Bond angles

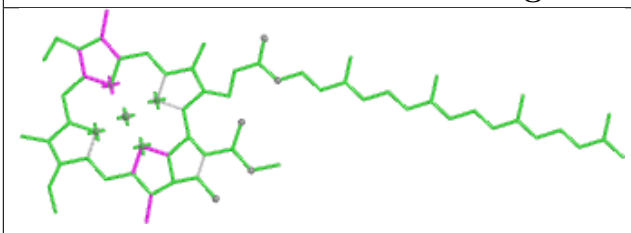


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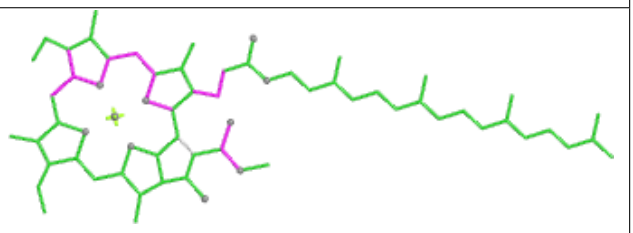


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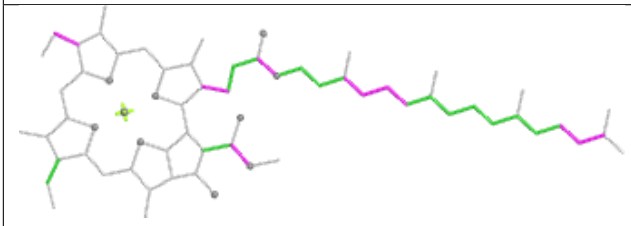
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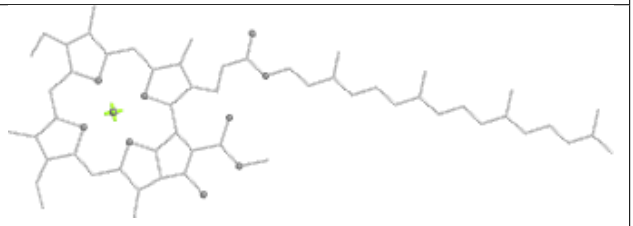
Bond lengths



Bond angles

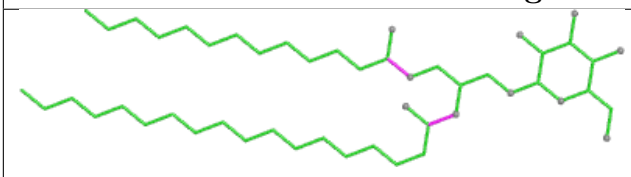


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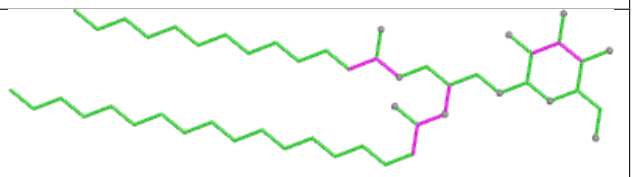


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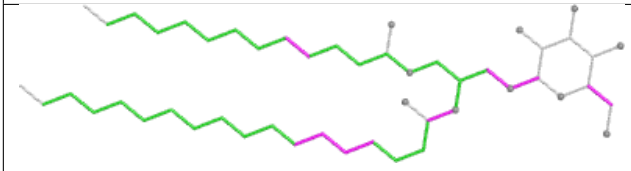
Ligand LMG c 521



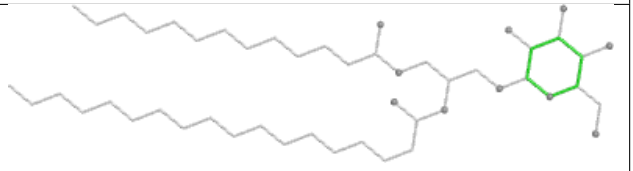
Bond lengths



Bond angles

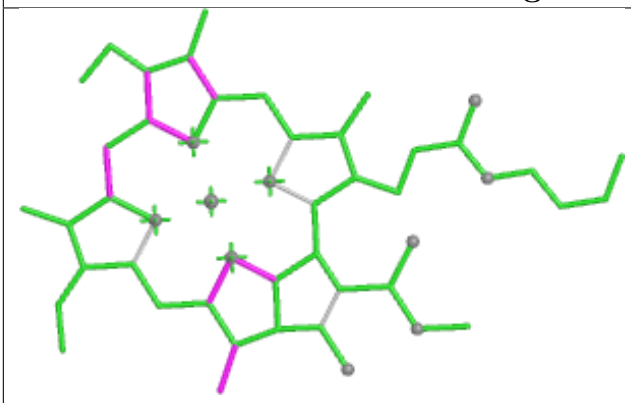


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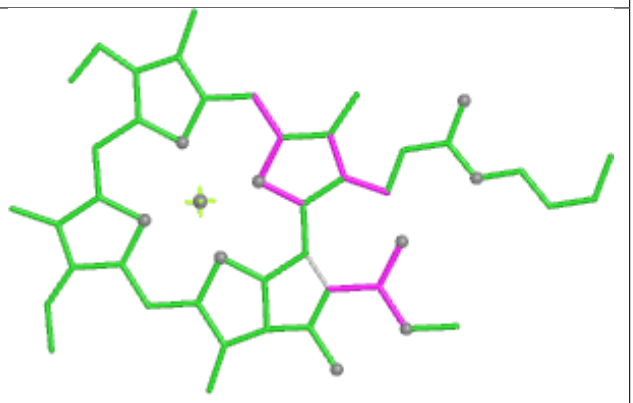


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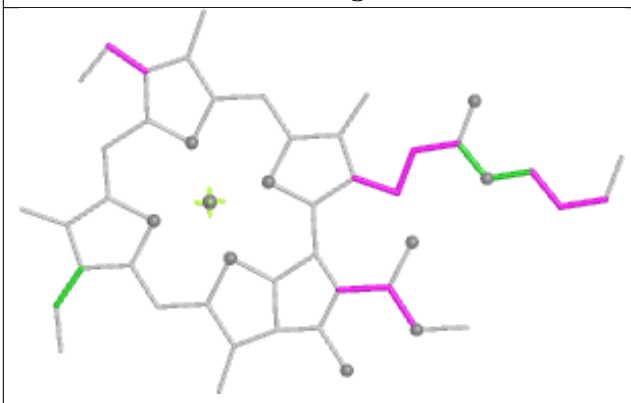
Ligand CLA R 302



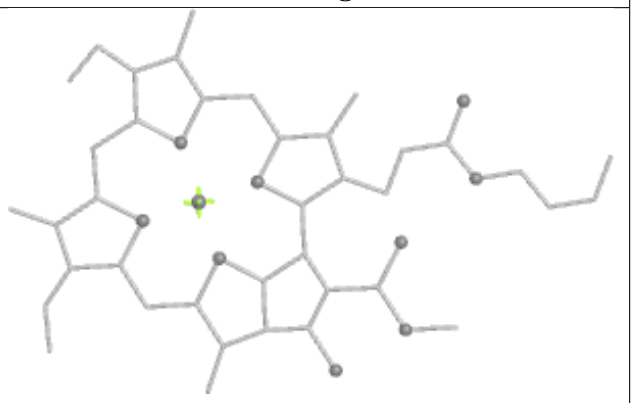
Bond lengths



Bond angles

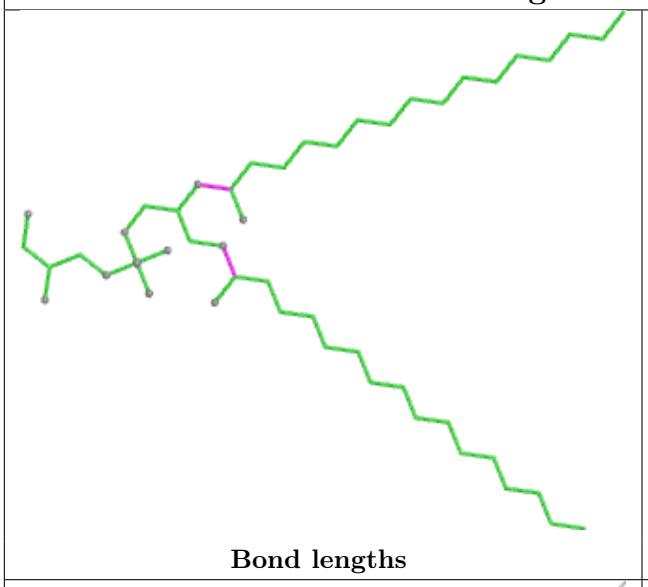


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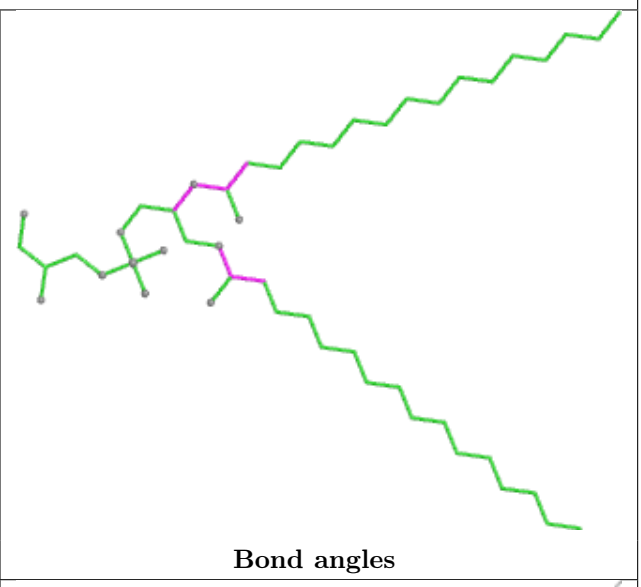


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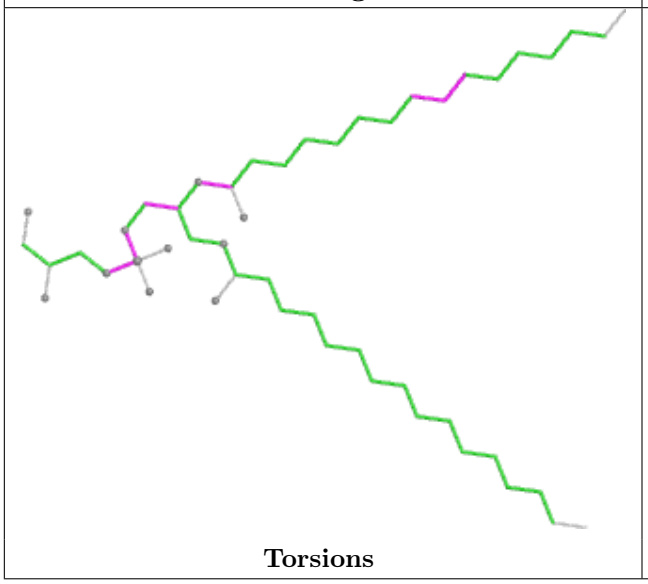
Ligand LHG c 516



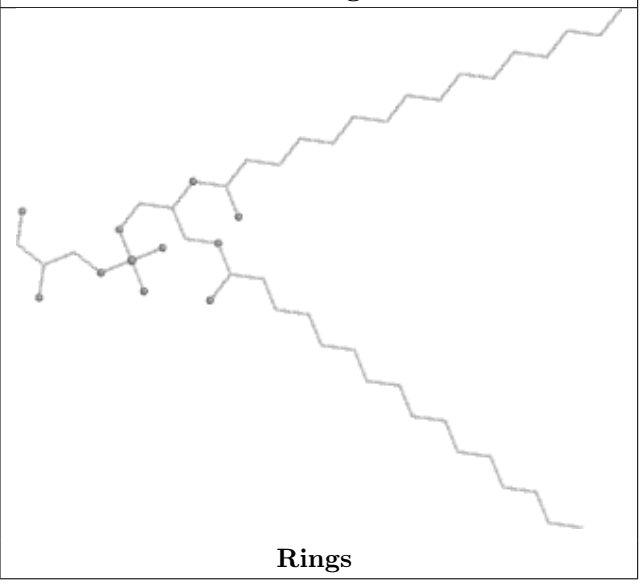
Bond lengths



Bond angles

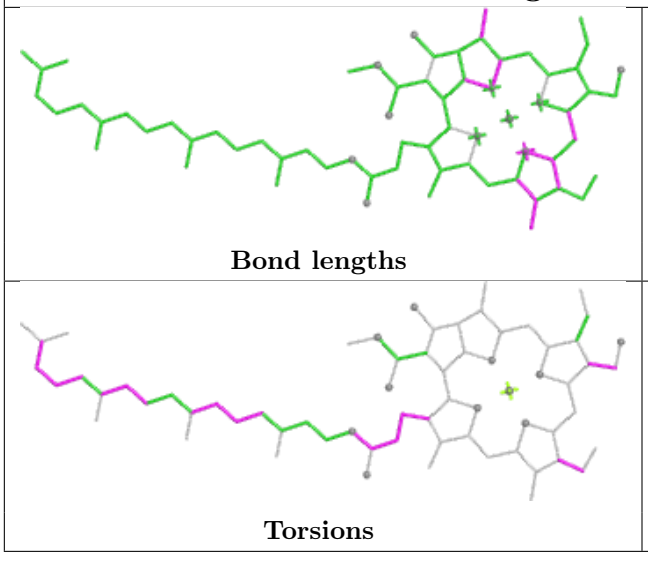


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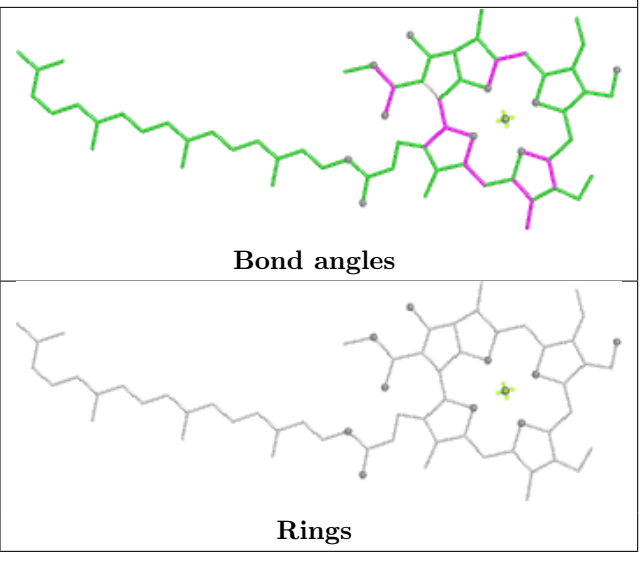


Rings

Ligand CHL Y 310



Bond lengths

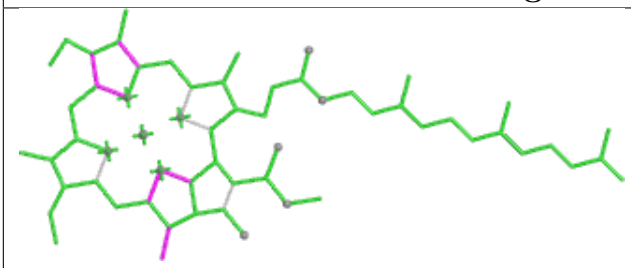


Bond angles

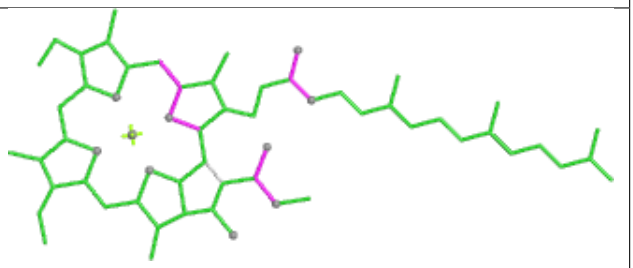
Torsions

Rings

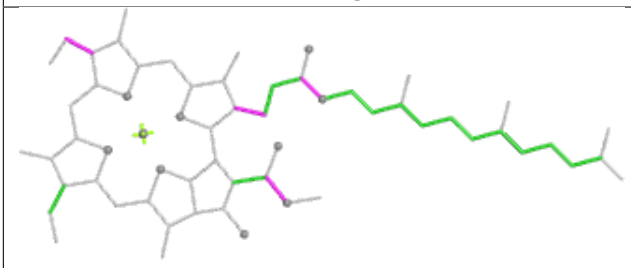
Ligand CLA C 505



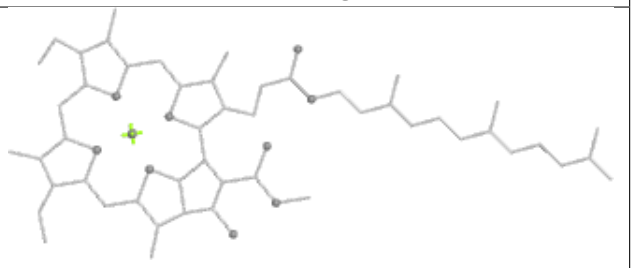
Bond lengths



Bond angles

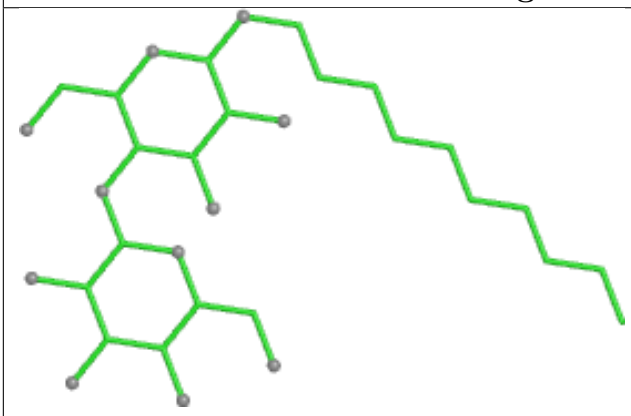


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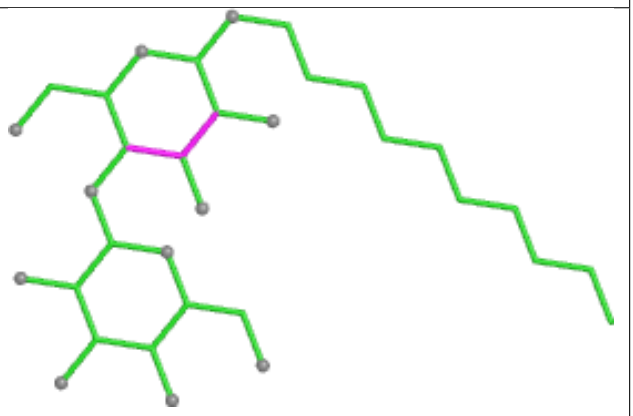


Rings

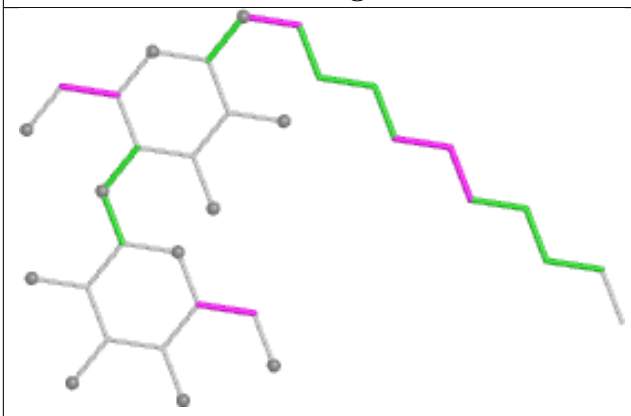
Ligand DMU C 523



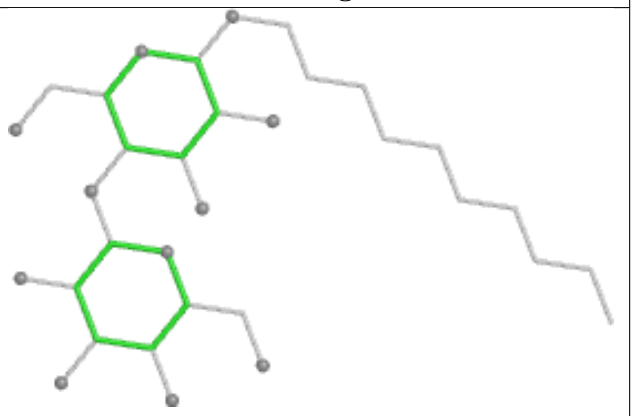
Bond lengths



Bond angles

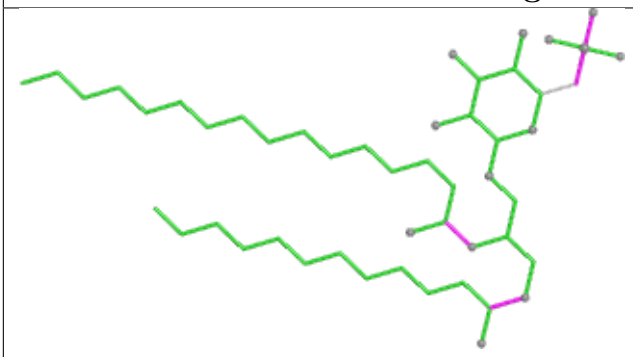


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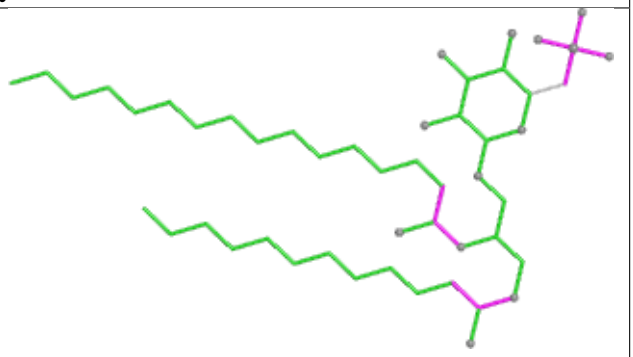


Rings

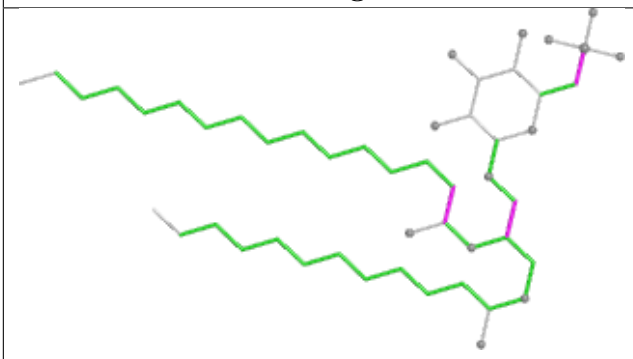
Ligand SQD A 406



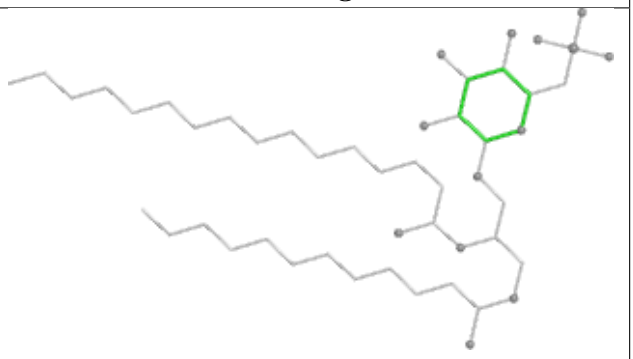
Bond lengths



Bond angles

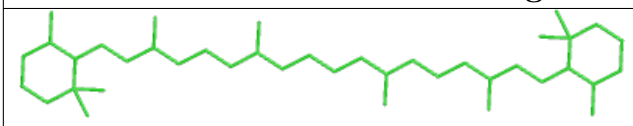


Torsions

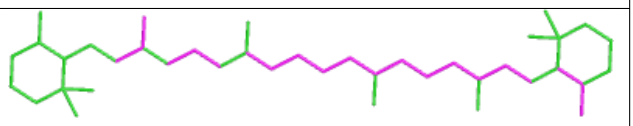


Rings

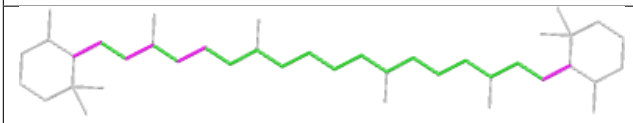
Ligand BCR h 101



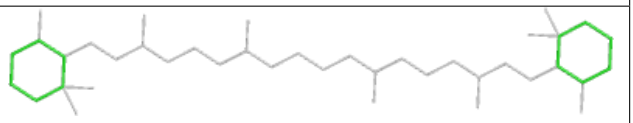
Bond lengths



Bond angles

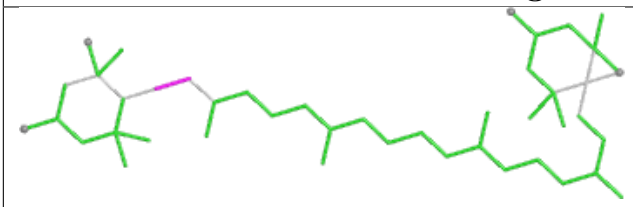


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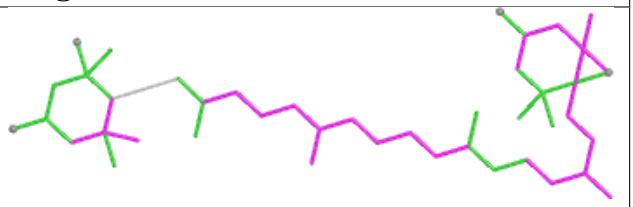


Rings

Ligand NEX g 618



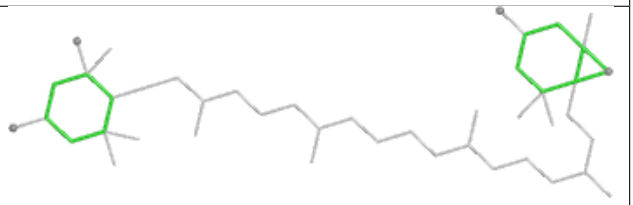
Bond lengths



Bond angles

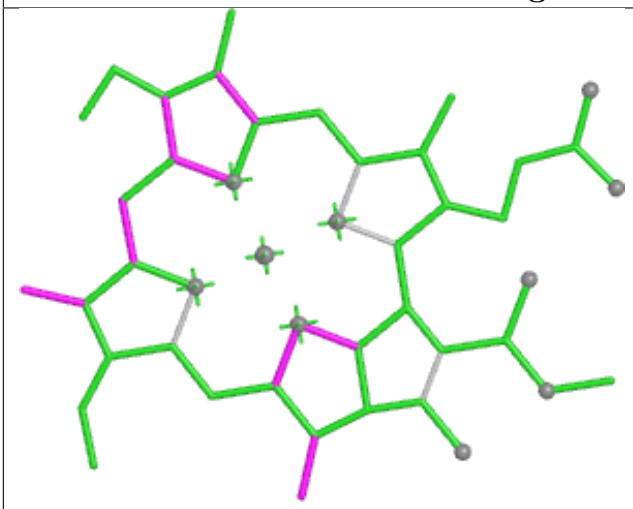


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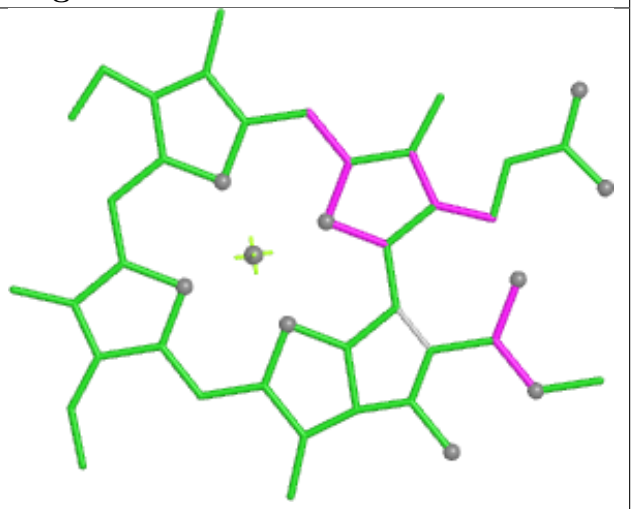


Rings

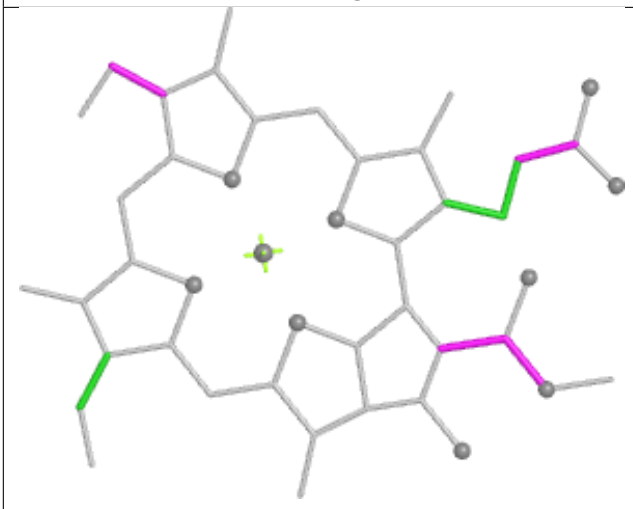
Ligand CLA g 612



Bond lengths



Bond angles

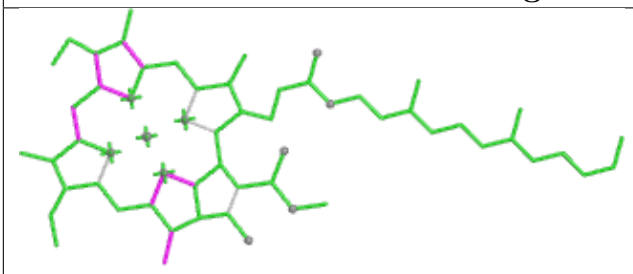


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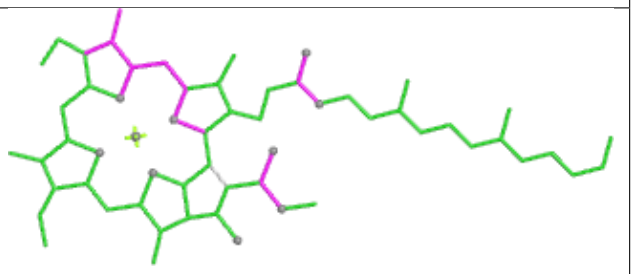


Rings

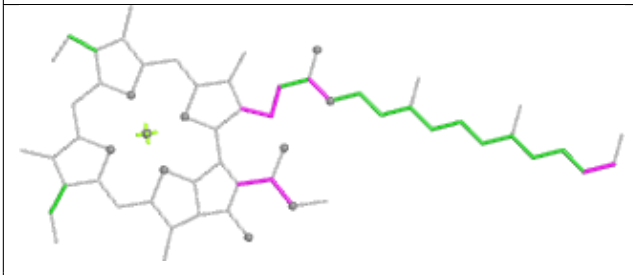
Ligand CLA N 610



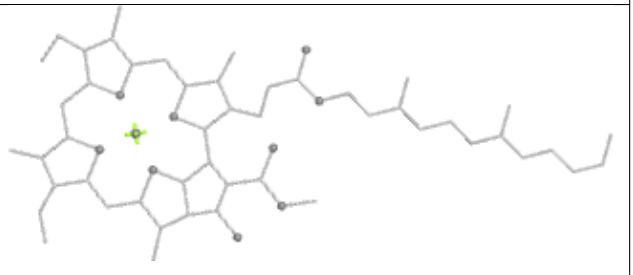
Bond lengths



Bond angles

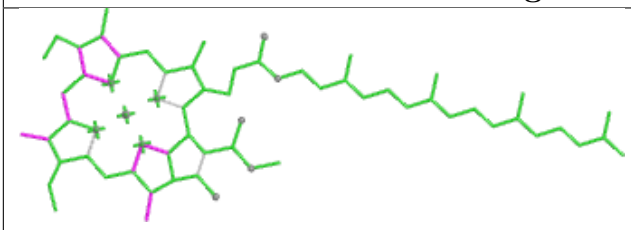


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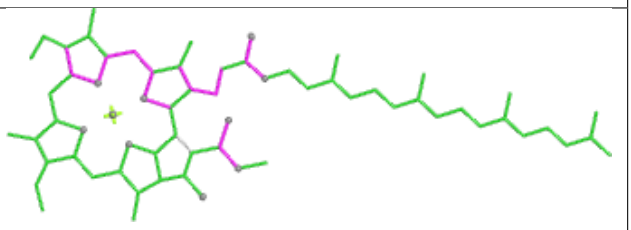


Rings

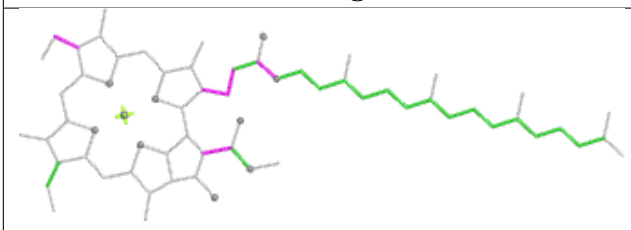
Ligand CLA C 514



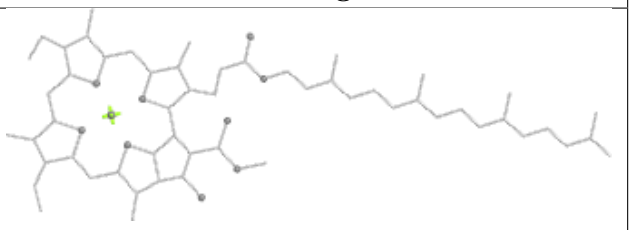
Bond lengths



Bond angles

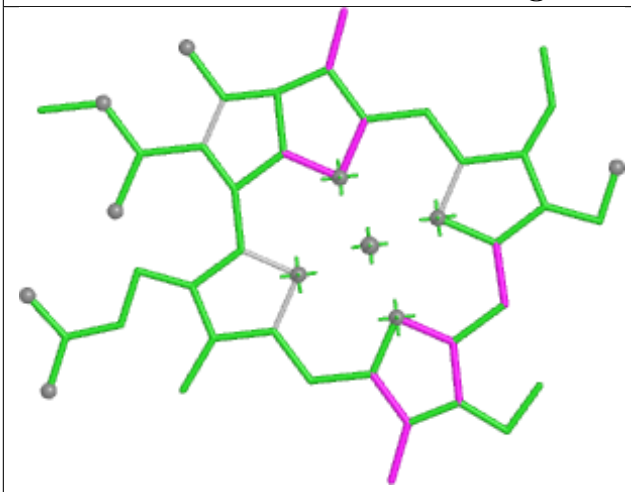


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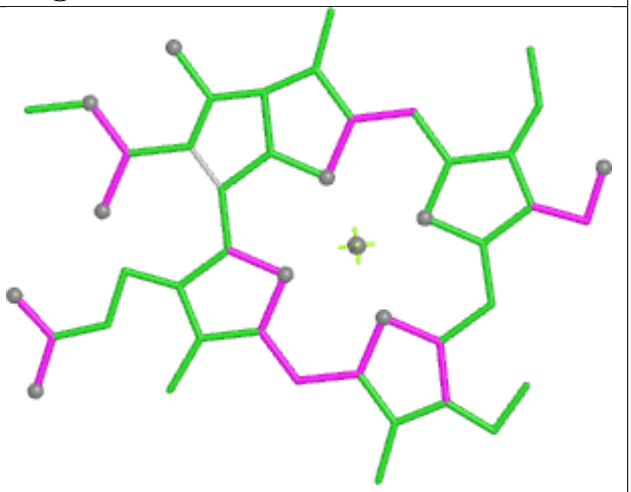


Rings

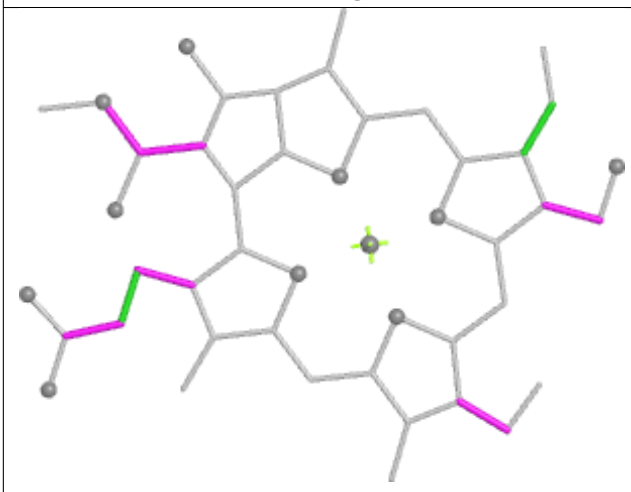
Ligand CHL g 605



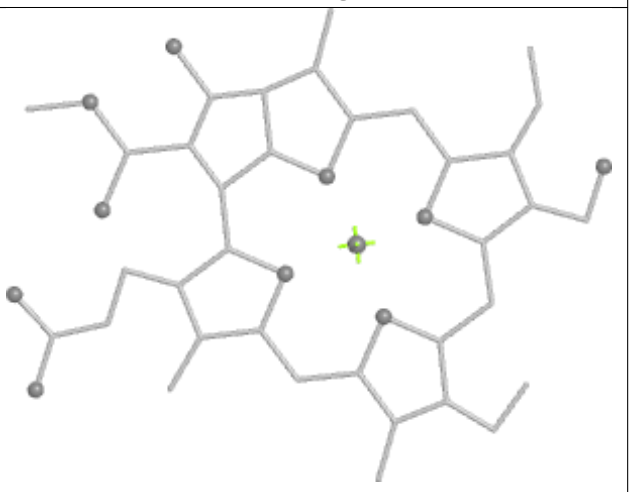
Bond lengths



Bond angles

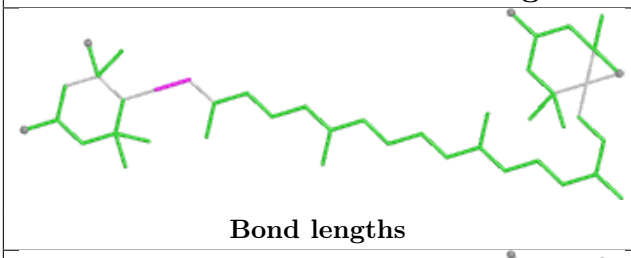


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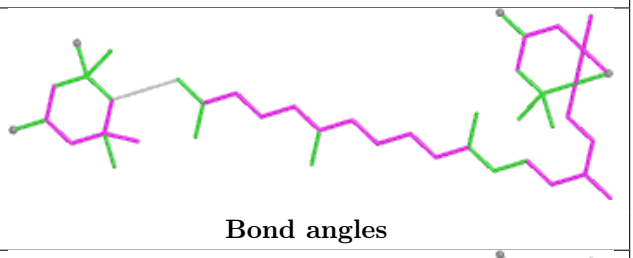


Rings

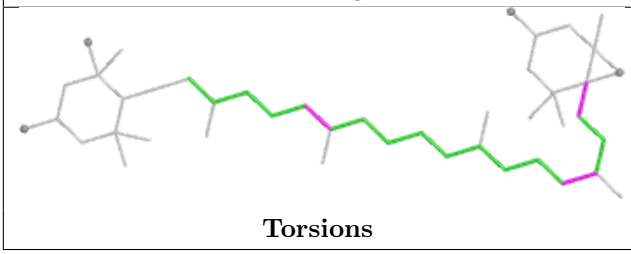
Ligand NEX R 316



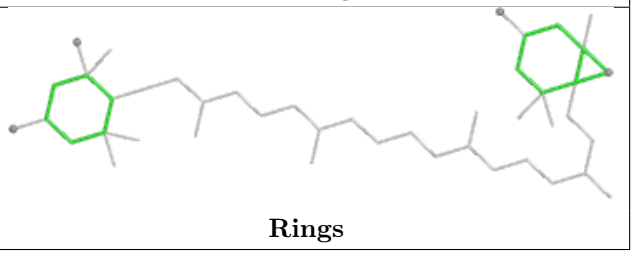
Bond lengths



Bond angles

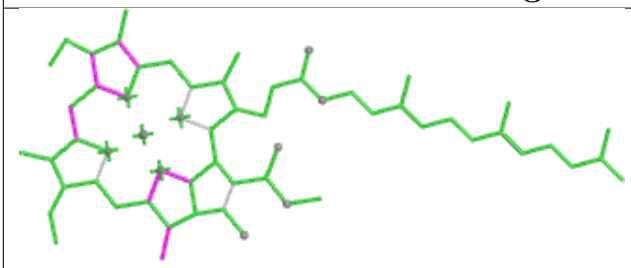


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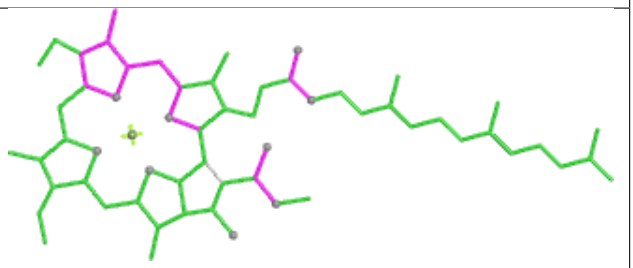


Rings

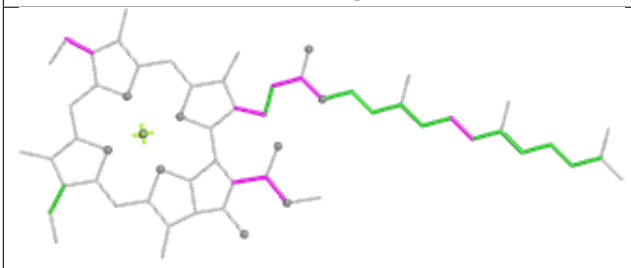
Ligand CLA A 404



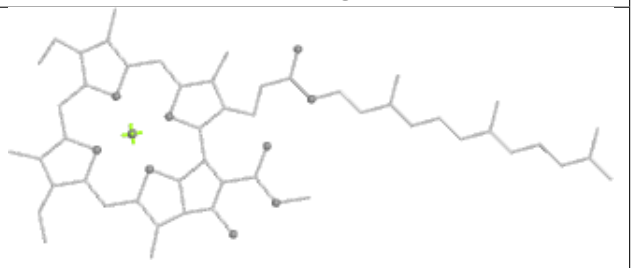
Bond lengths



Bond angles

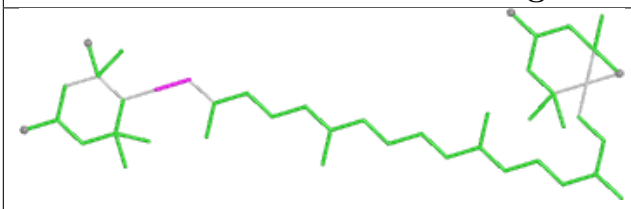


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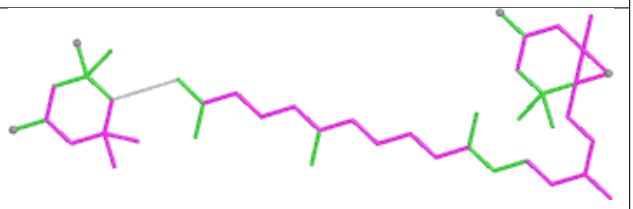


Rings

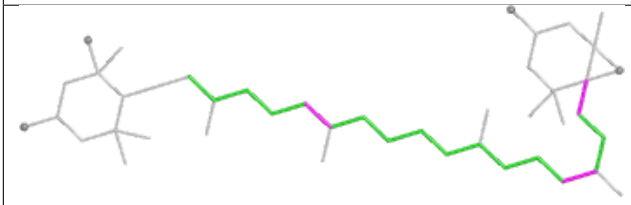
Ligand NEX r 615



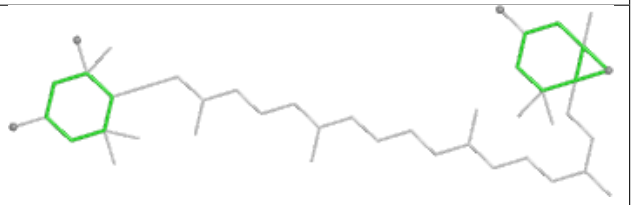
Bond lengths



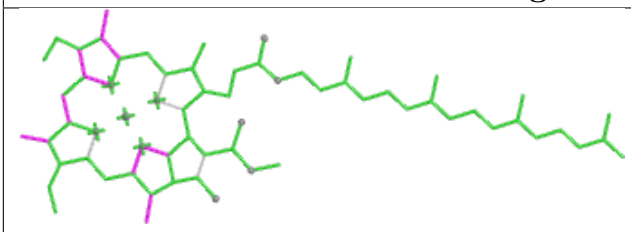
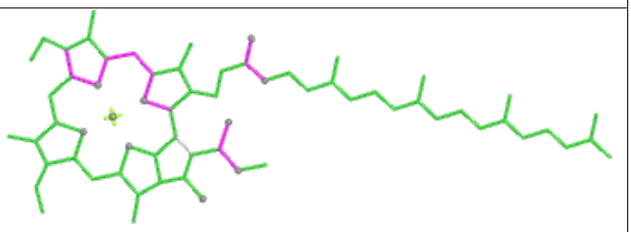
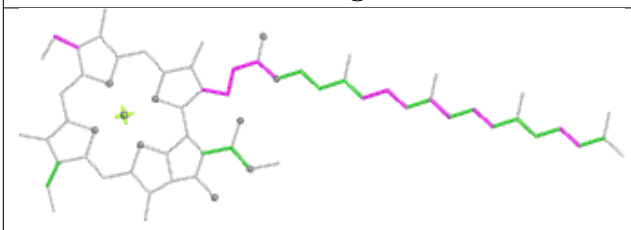
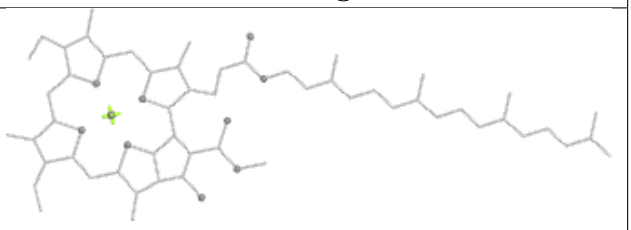
Bond angles

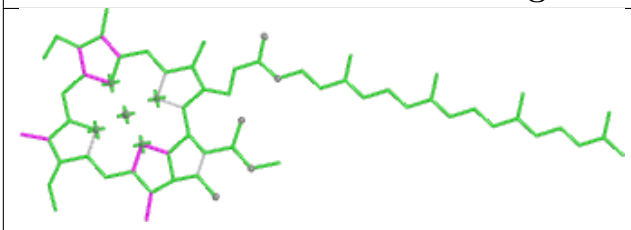
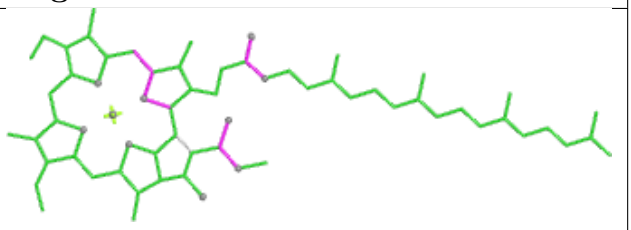
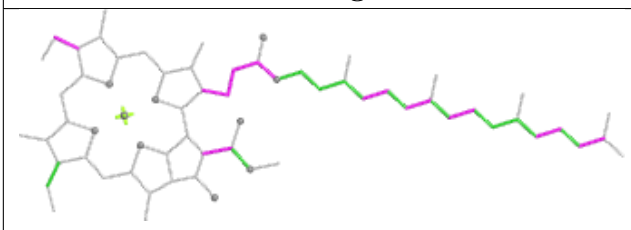
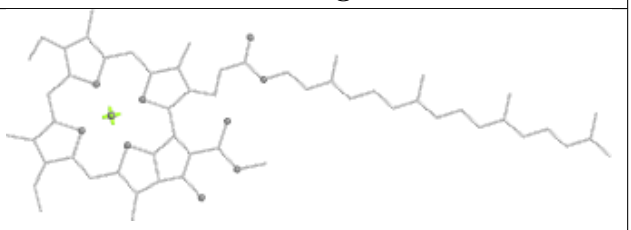


Torsions

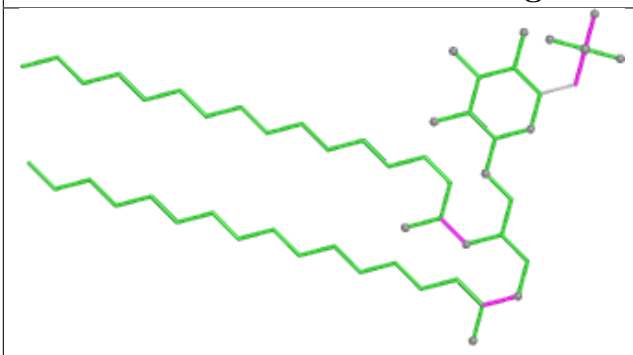


Rings

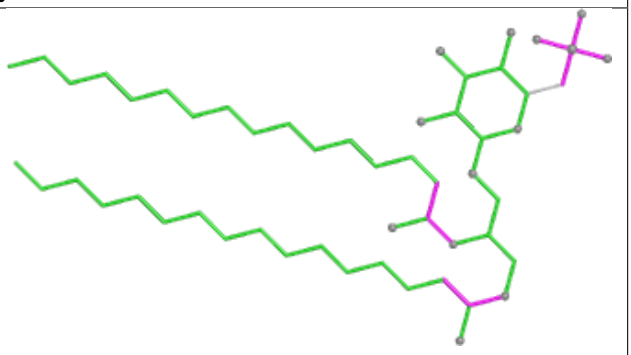
Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

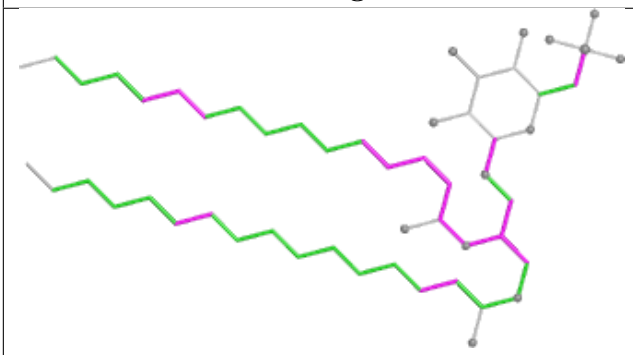
Ligand SQD B 625



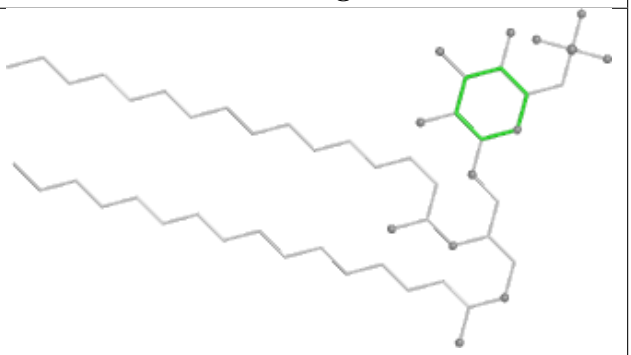
Bond lengths



Bond angles

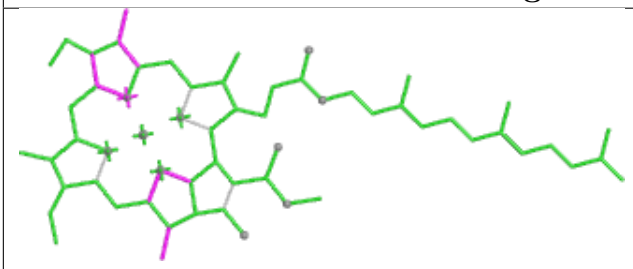


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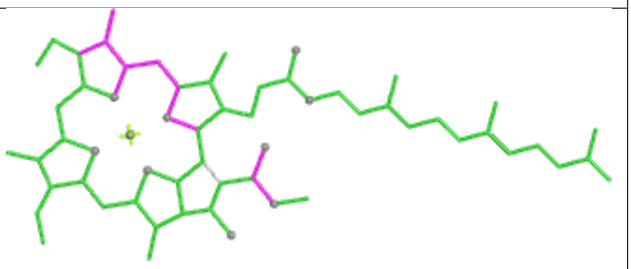


Rings

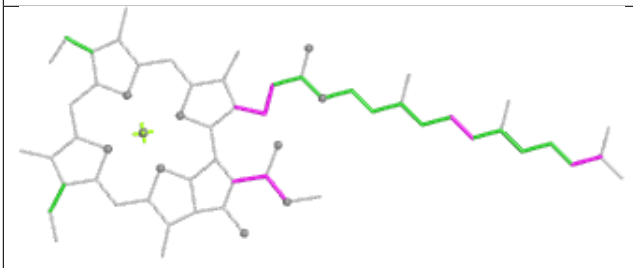
Ligand CLA Y 311



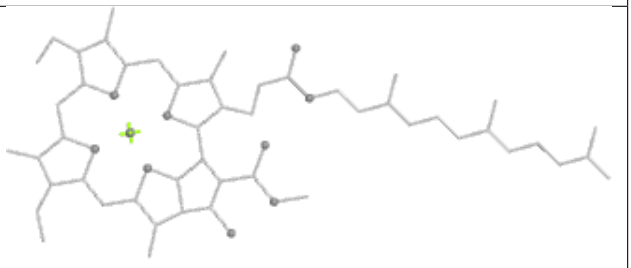
Bond lengths



Bond angles

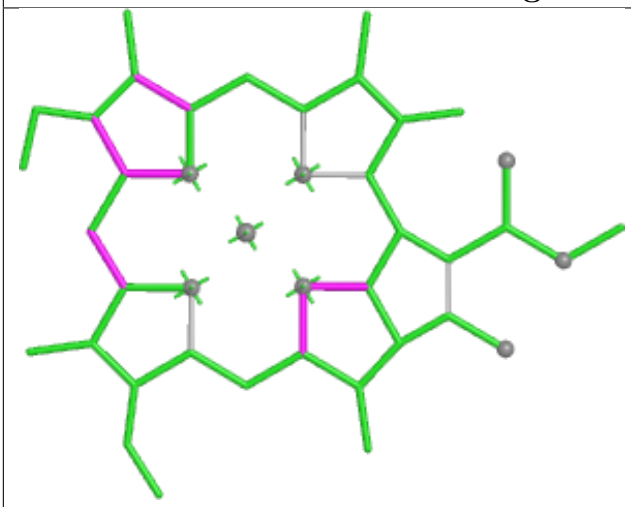


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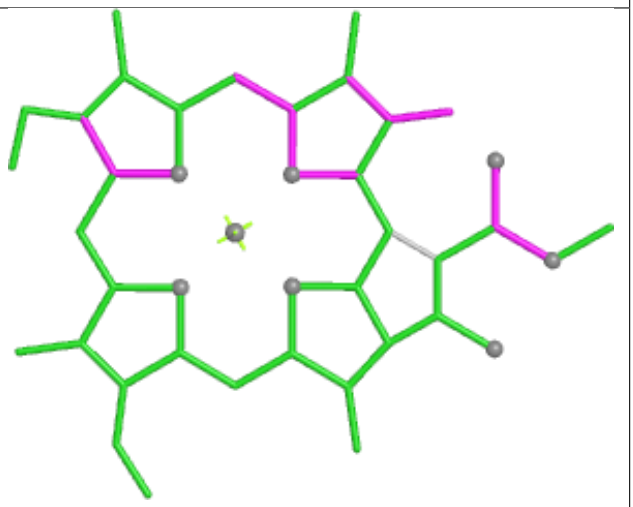


Rings

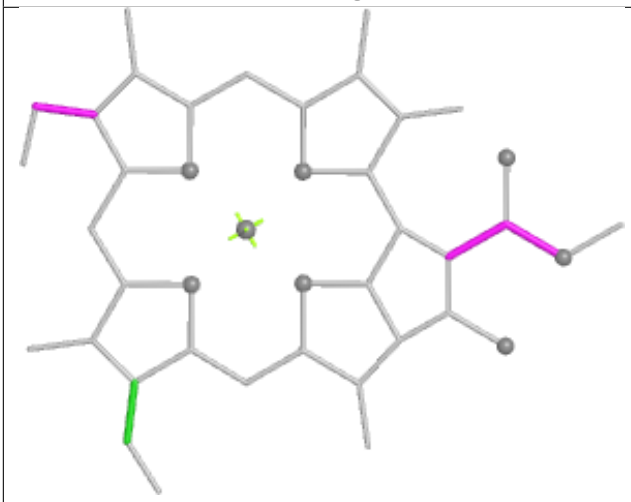
Ligand CLA N 614



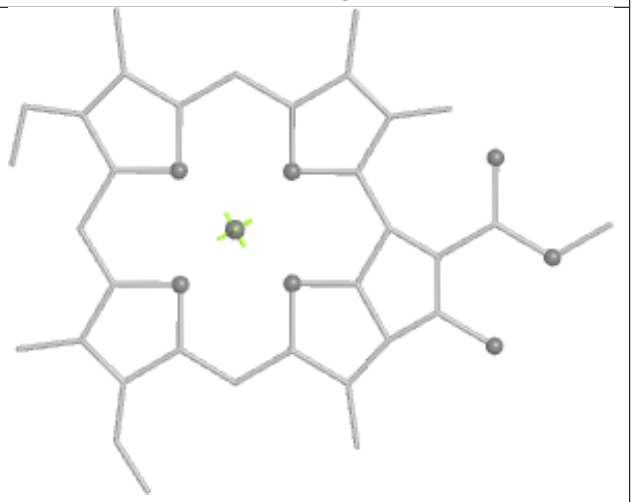
Bond lengths



Bond angles

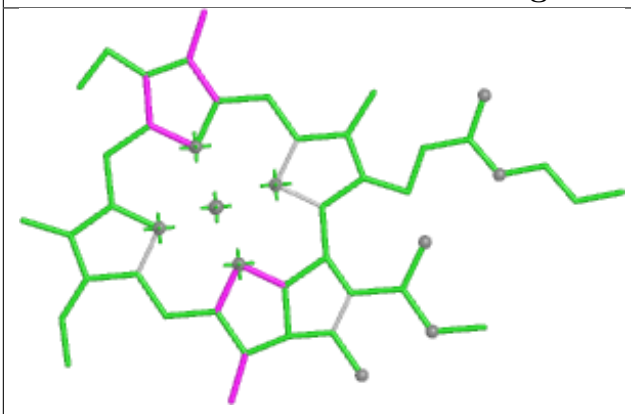


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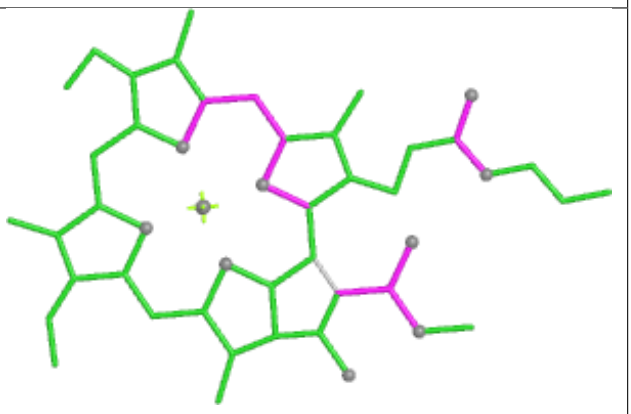


Rings

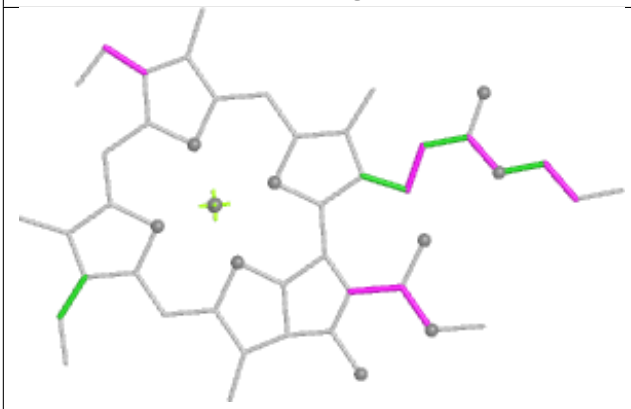
Ligand CLA r 604



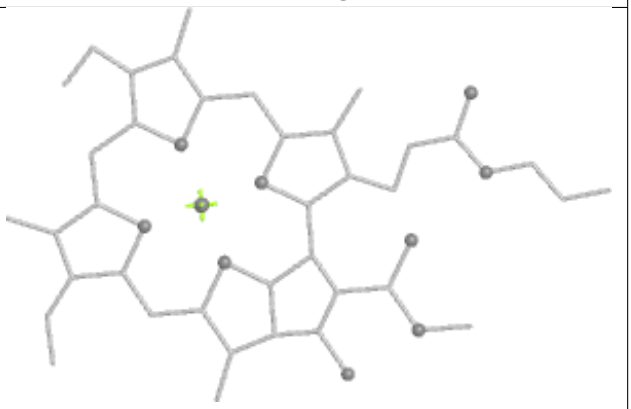
Bond lengths



Bond angles

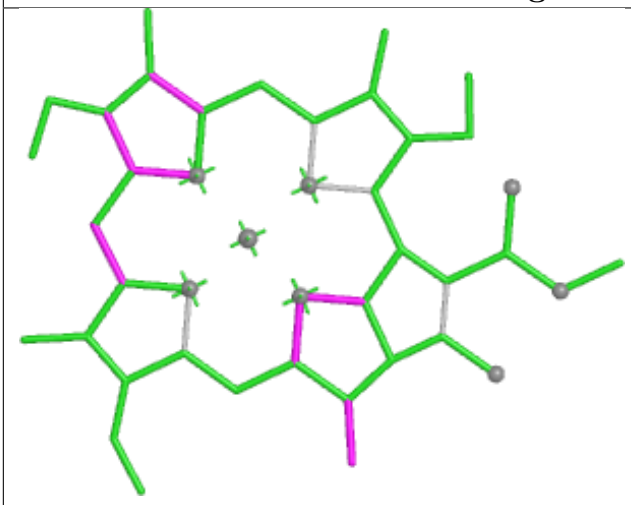


Torsions

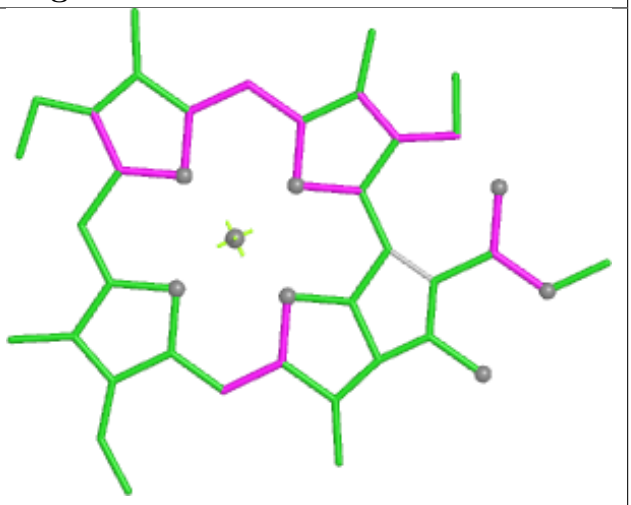


Rings

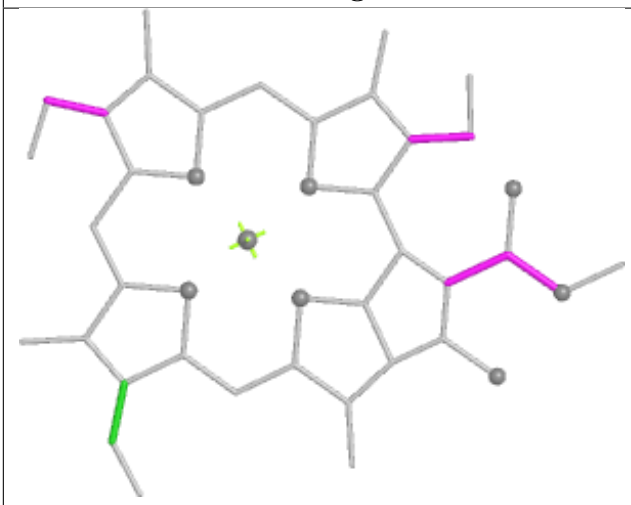
Ligand CLA g 614



Bond lengths



Bond angles

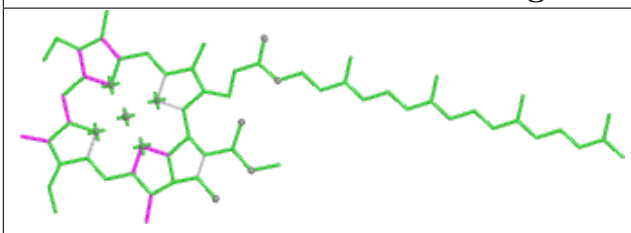


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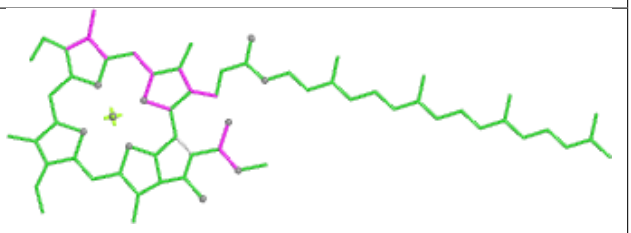


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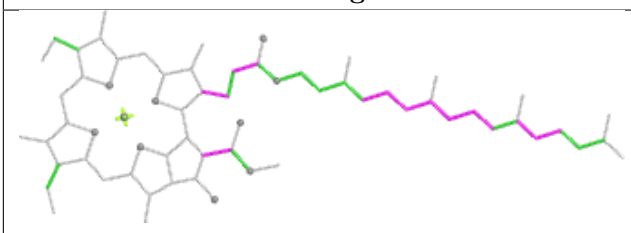
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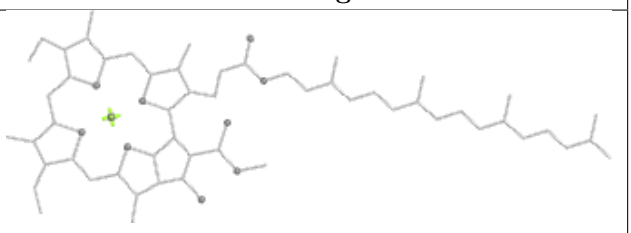
Bond lengths



Bond angles

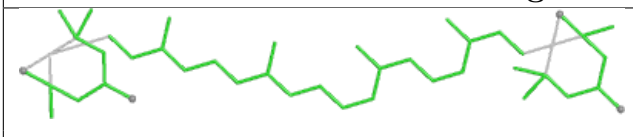


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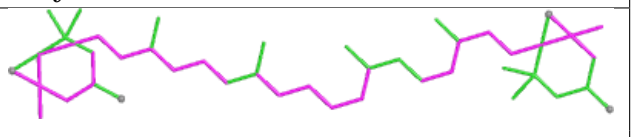


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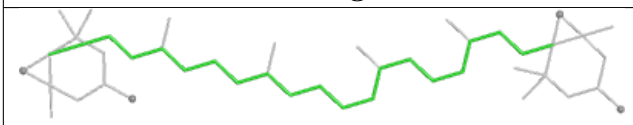
Ligand XAT y 301



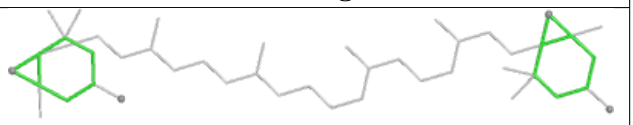
Bond lengths



Bond angles

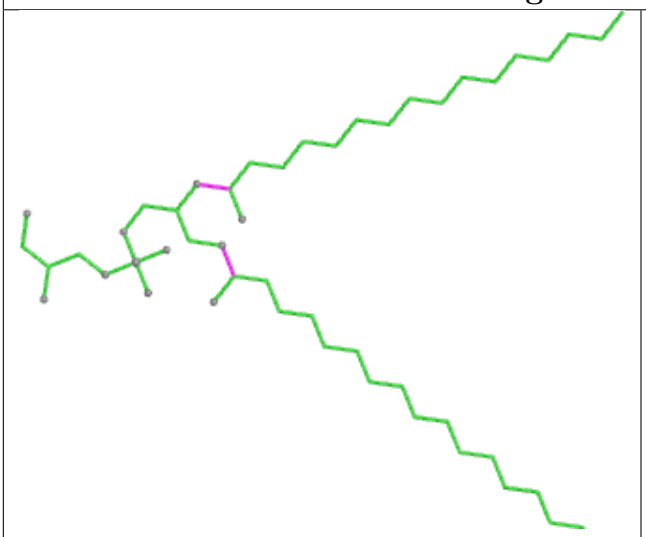


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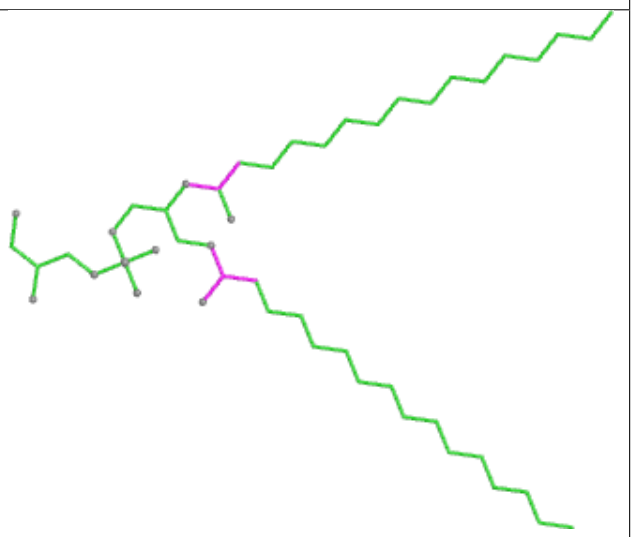


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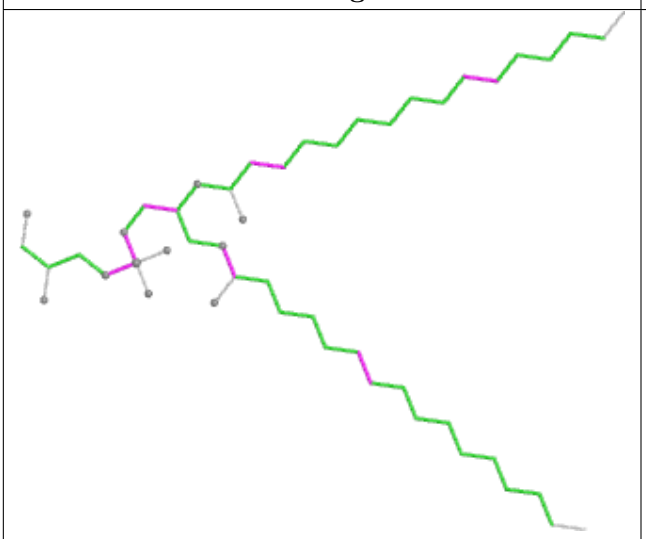
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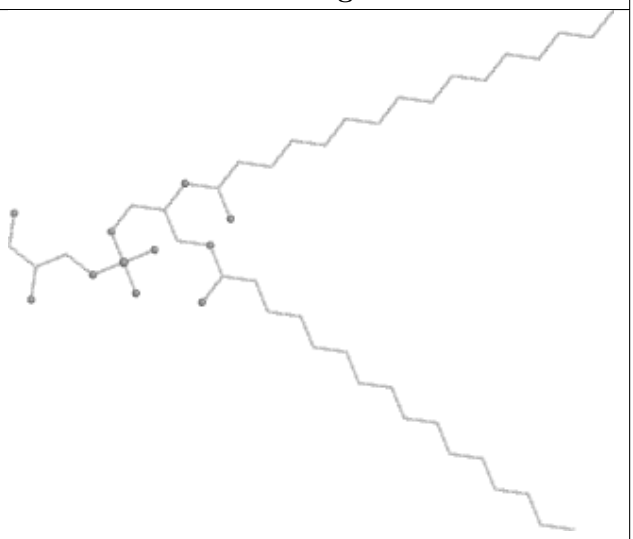
Bond lengths



Bond angles

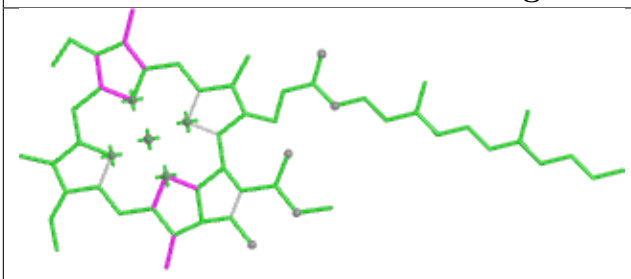


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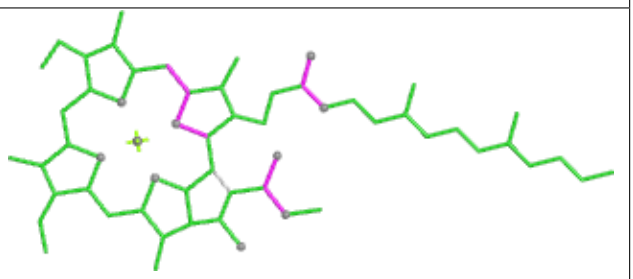


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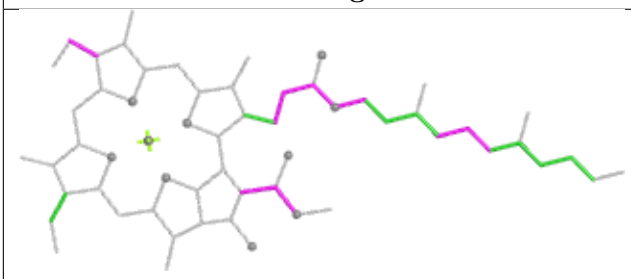
Ligand CLA G 613



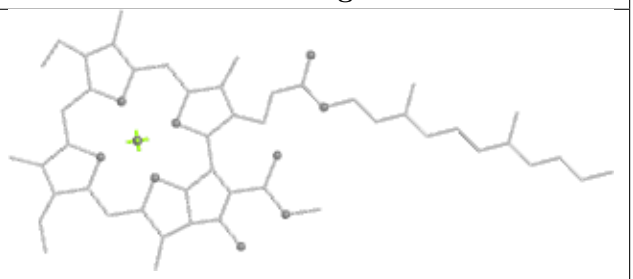
Bond lengths



Bond angles

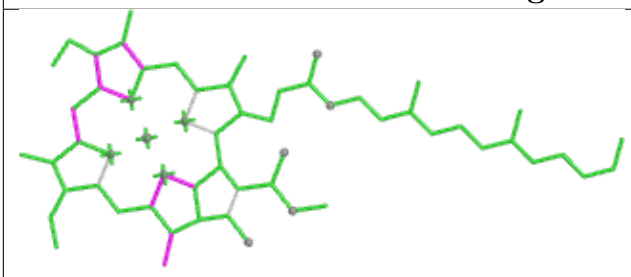


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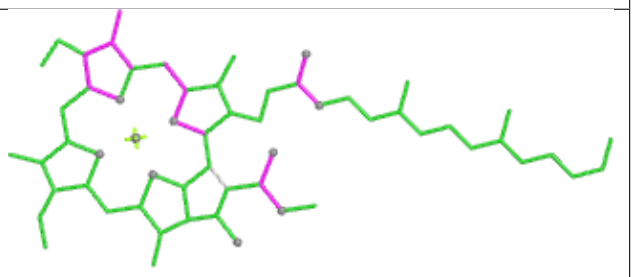


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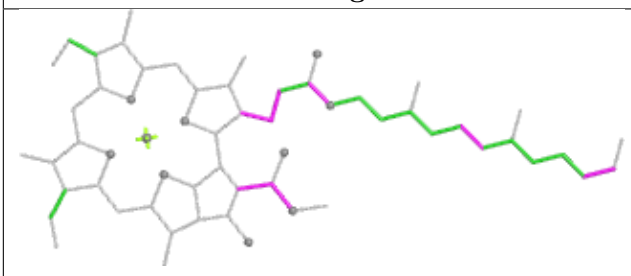
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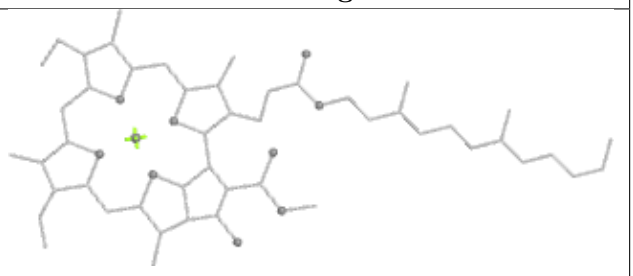
Bond lengths



Bond angles



Torsions

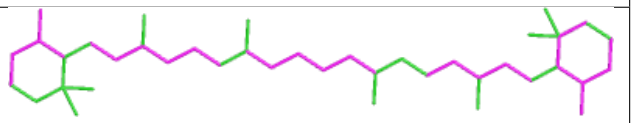


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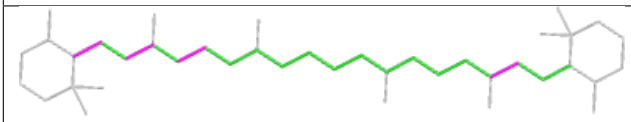
Ligand BCR d 405



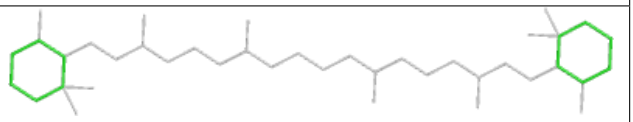
Bond lengths



Bond angles

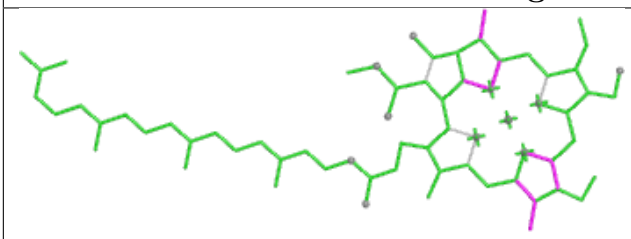


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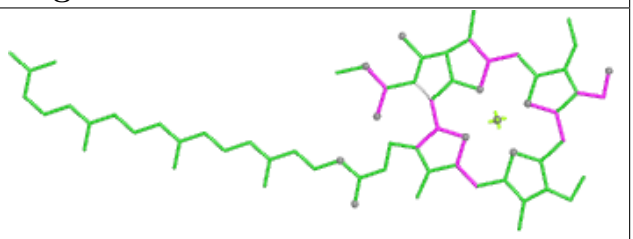


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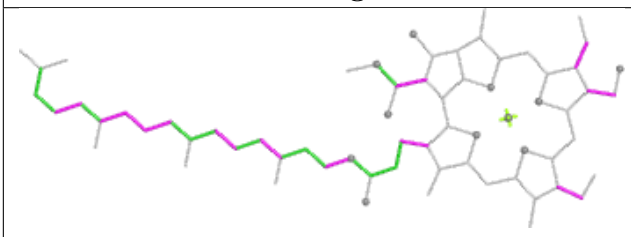
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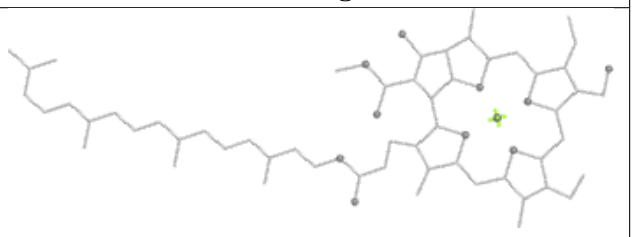
Bond lengths



Bond angles

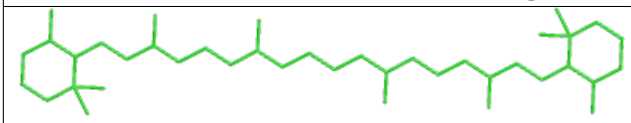


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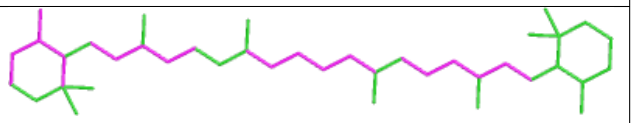


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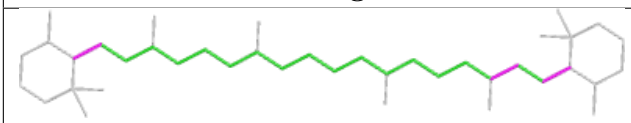
Ligand BCR B 617



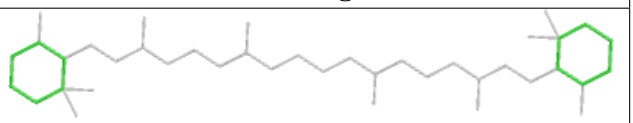
Bond lengths



Bond angles

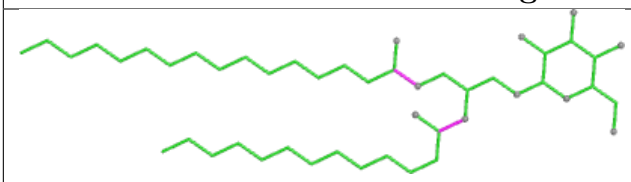


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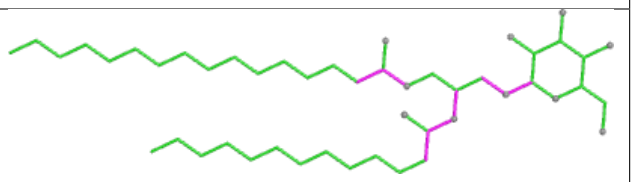


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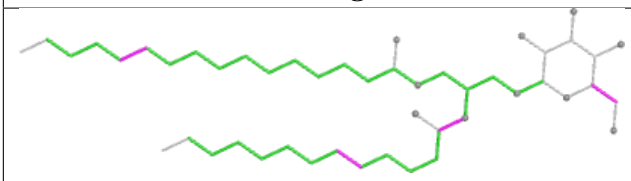
Ligand LMG C 501



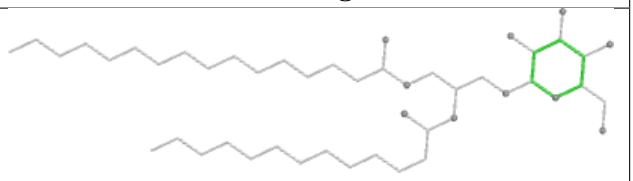
Bond lengths



Bond angles

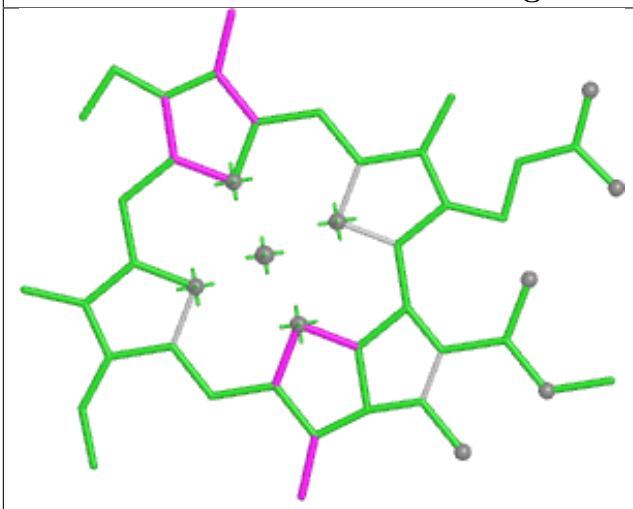


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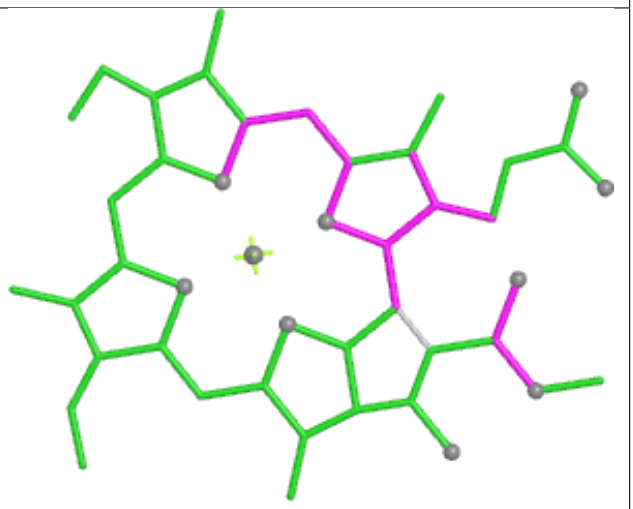


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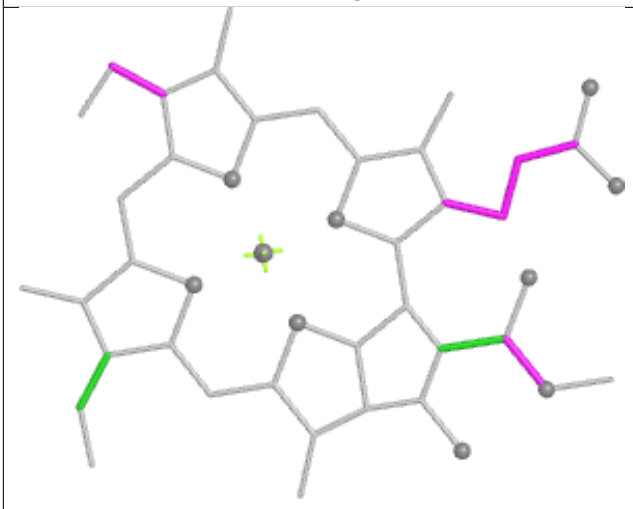
Ligand CLA N 612



Bond lengths



Bond angles

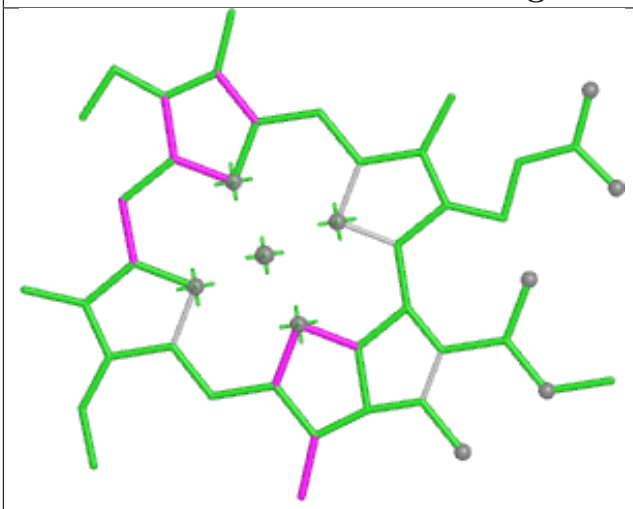


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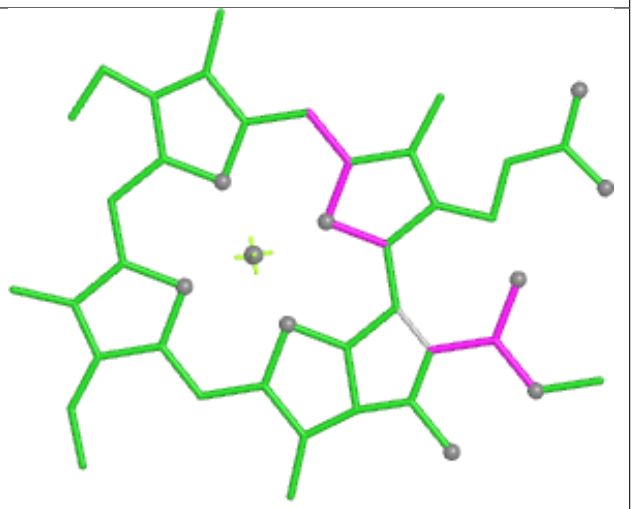


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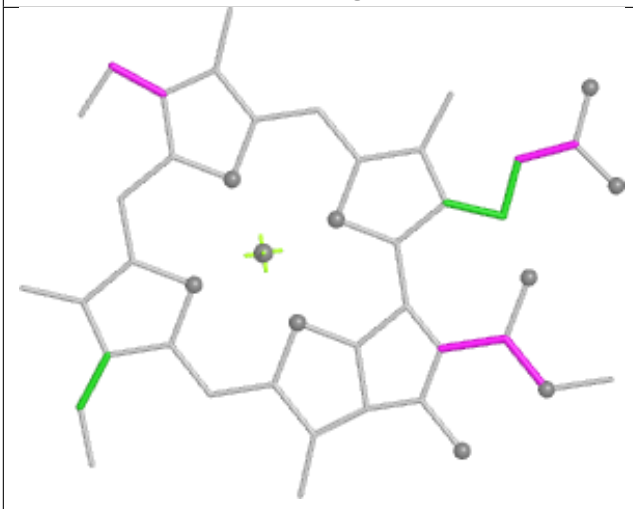
Ligand CLA S 309



Bond lengths



Bond angles

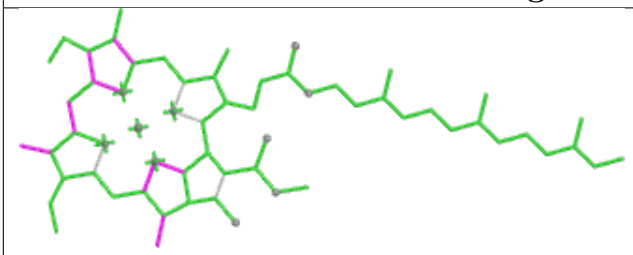


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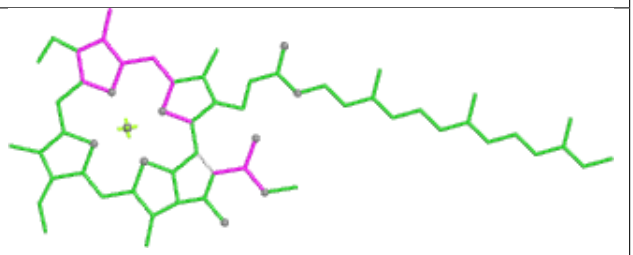


Rings

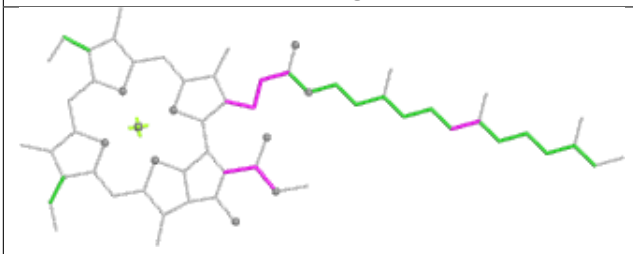
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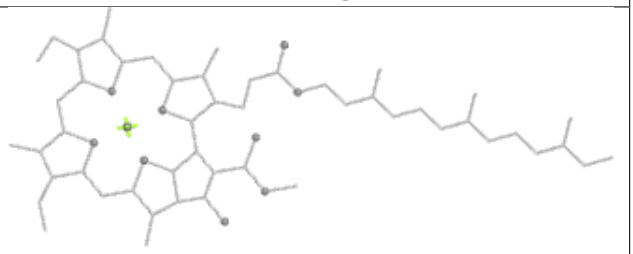
Bond lengths



Bond angles

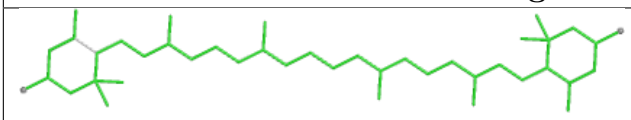


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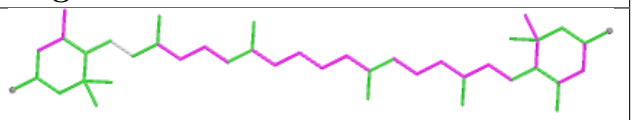


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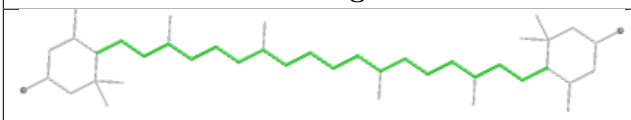
Ligand LUT g 616



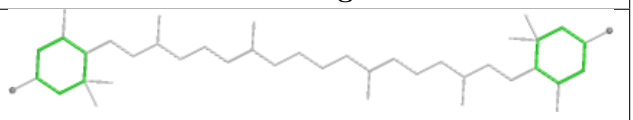
Bond lengths



Bond angles

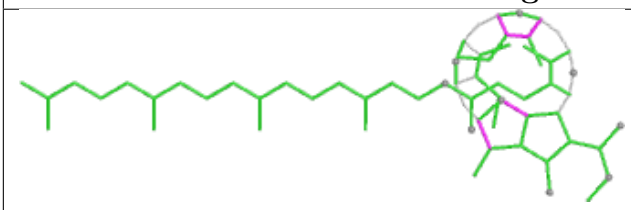


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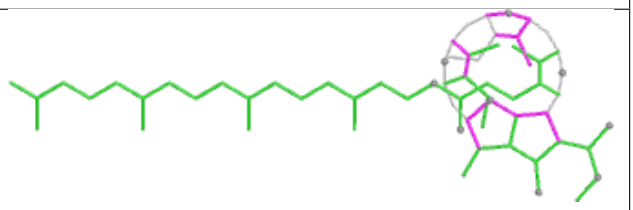


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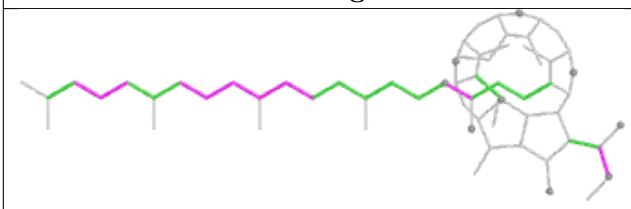
Ligand PHO A 403



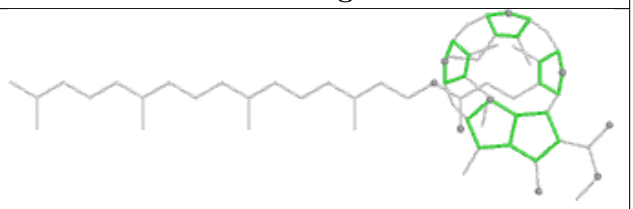
Bond lengths



Bond angles

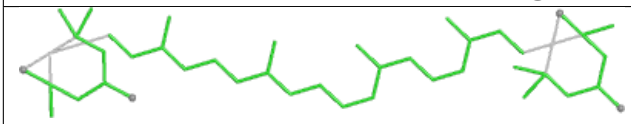


Torsions

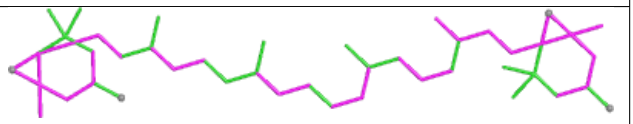


Rings

Ligand XAT r 614



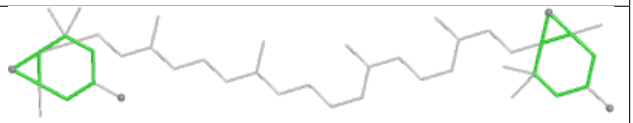
Bond lengths



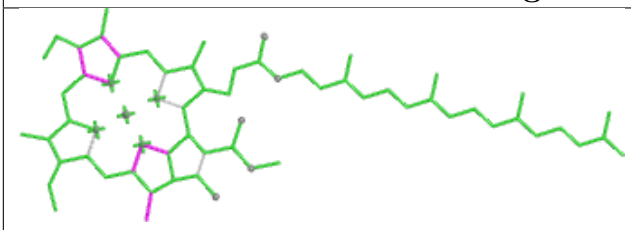
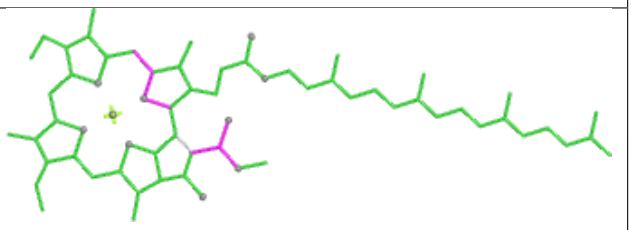
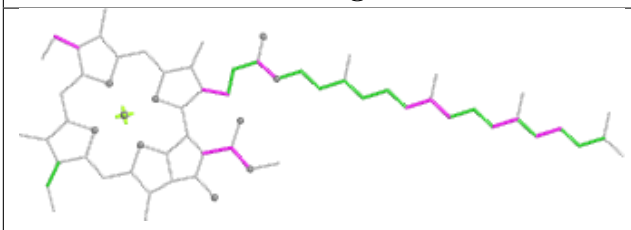
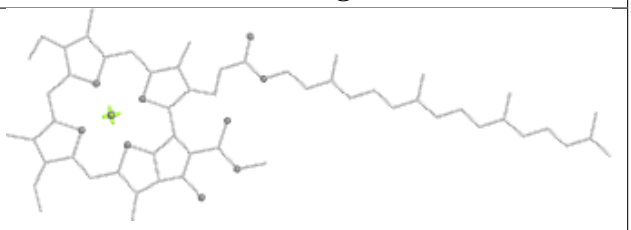
Bond angles

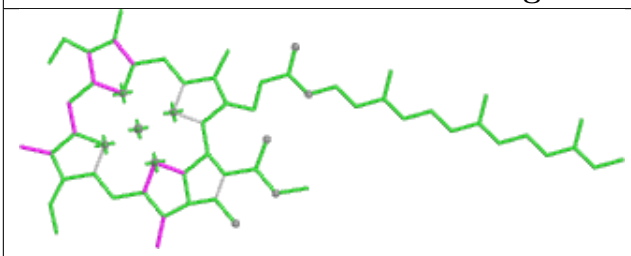
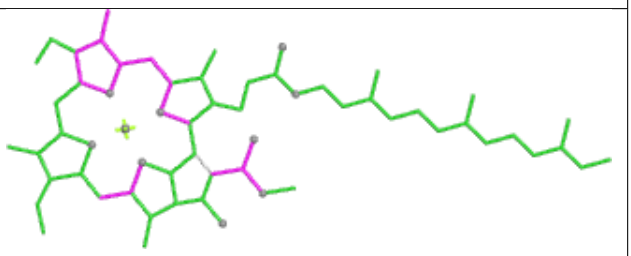
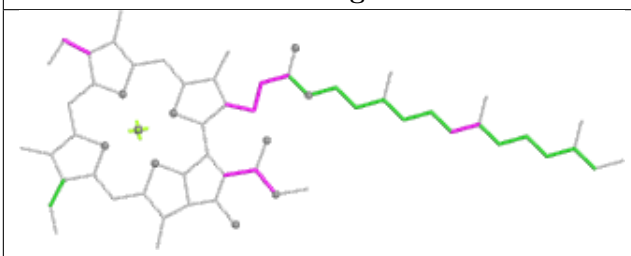
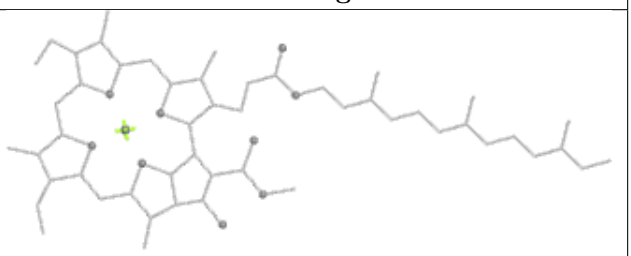


Torsions

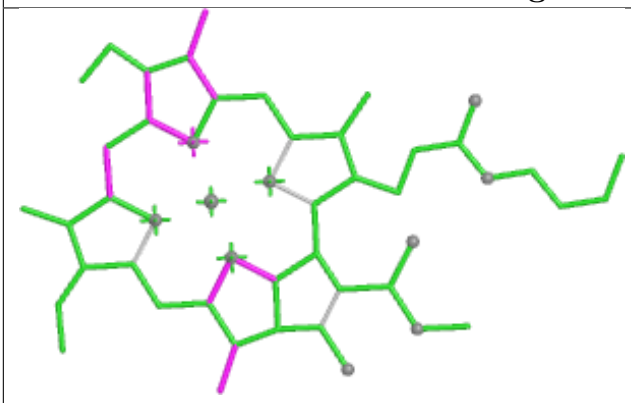


Rings

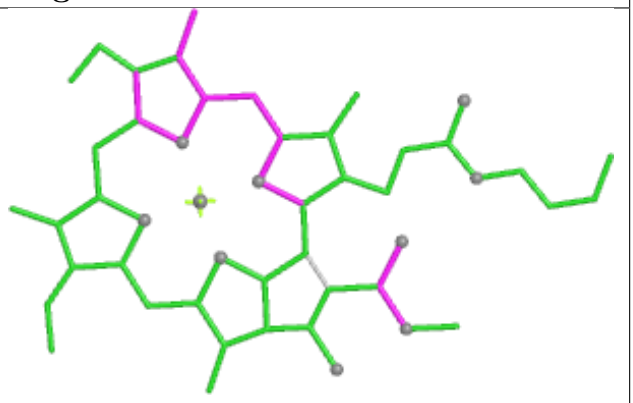
Ligand CLA D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA N 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

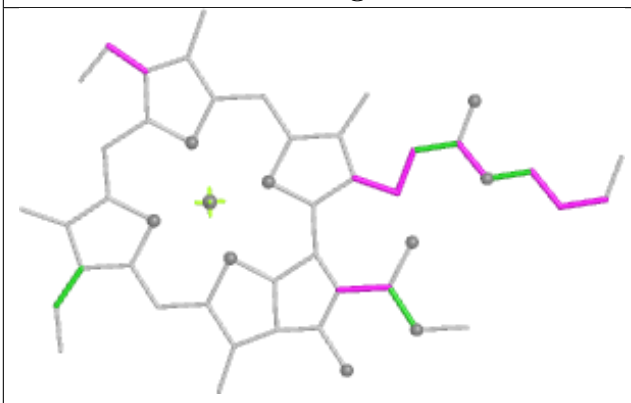
Ligand CLA g 604



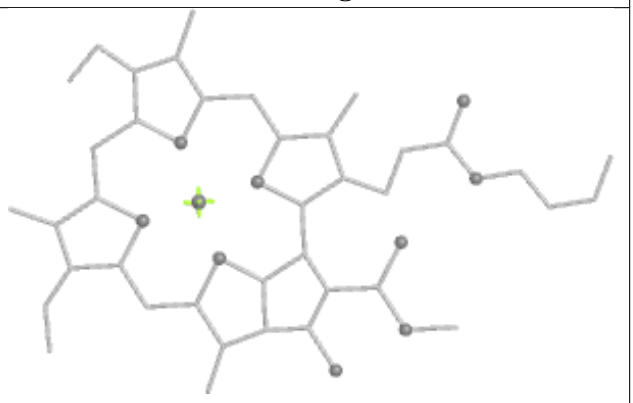
Bond lengths



Bond angles

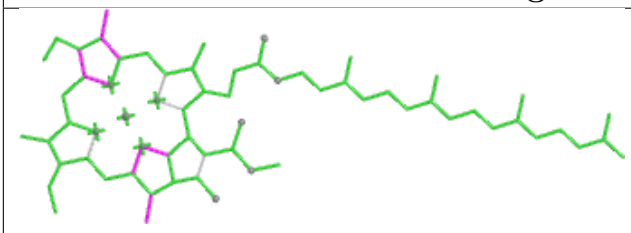


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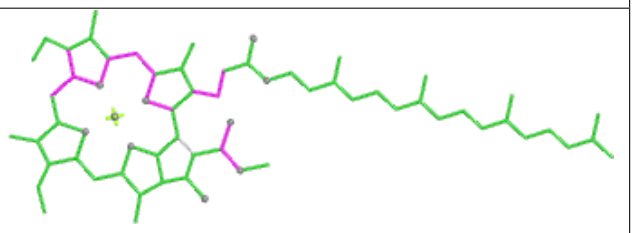


Rings

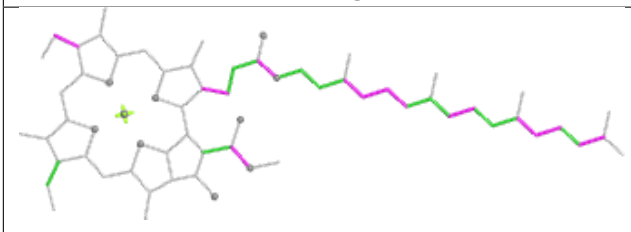
Ligand CLA b 610



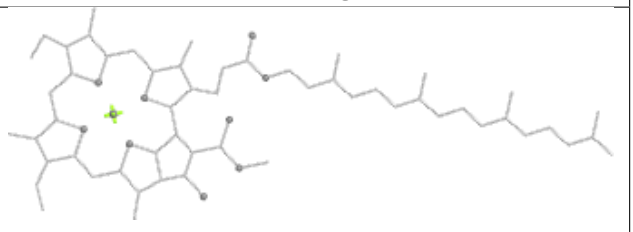
Bond lengths



Bond angles

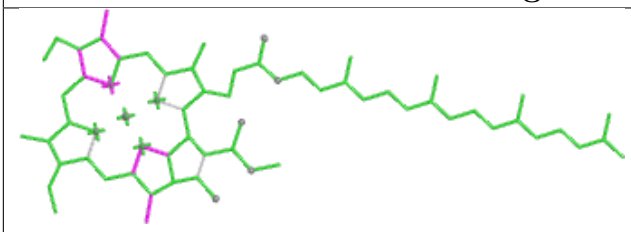


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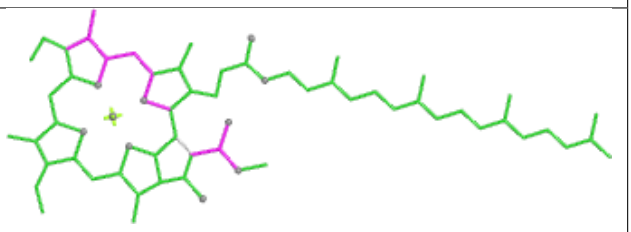


Rings

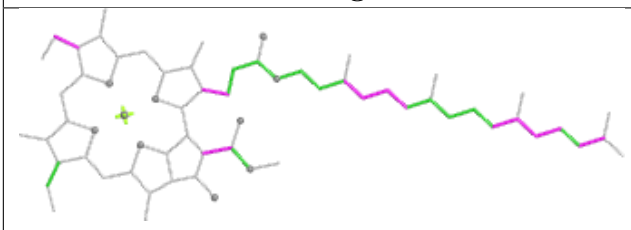
Ligand CLA D 401



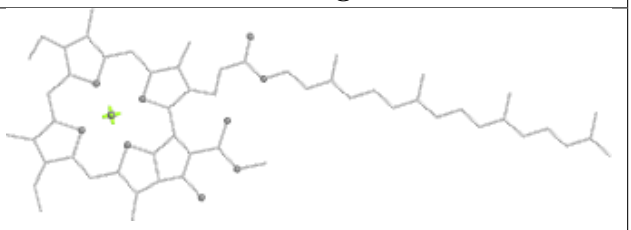
Bond lengths



Bond angles

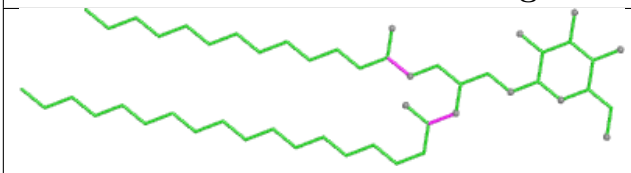


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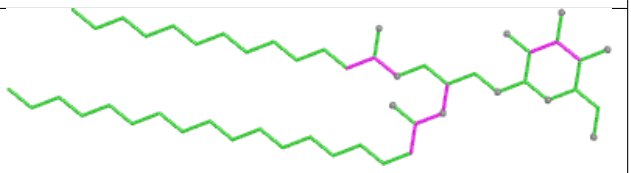


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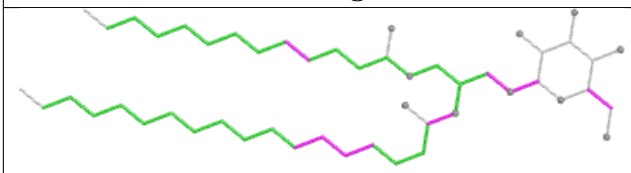
Ligand LMG C 522



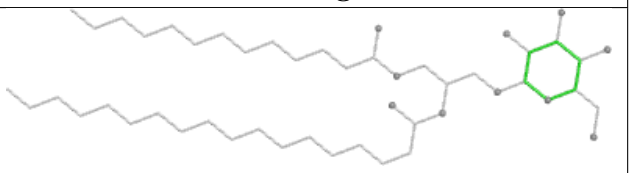
Bond lengths



Bond angles

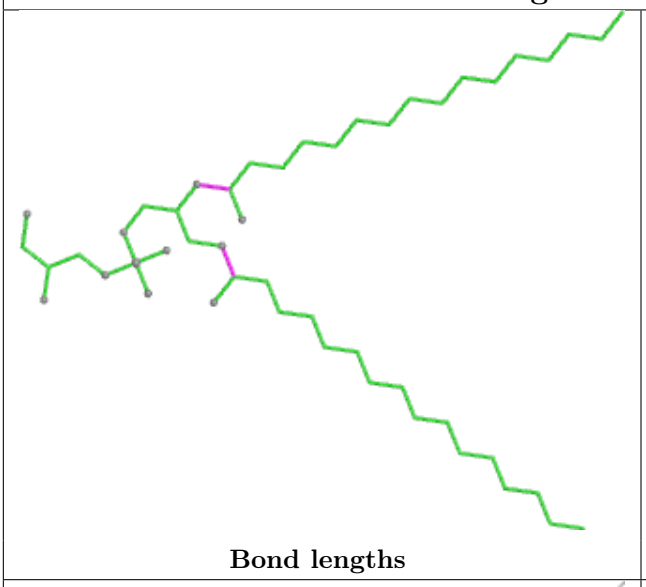


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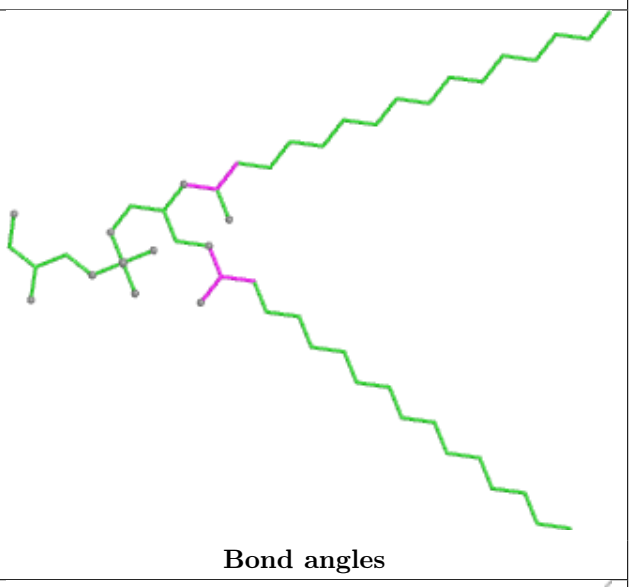


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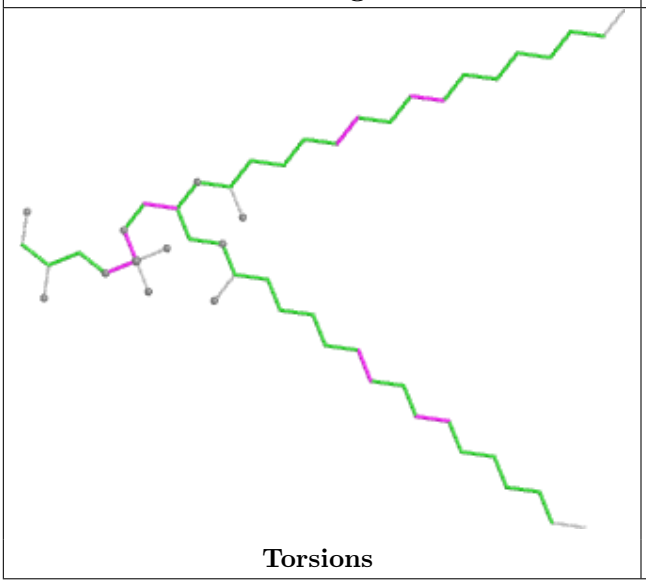
Ligand LHG l 102



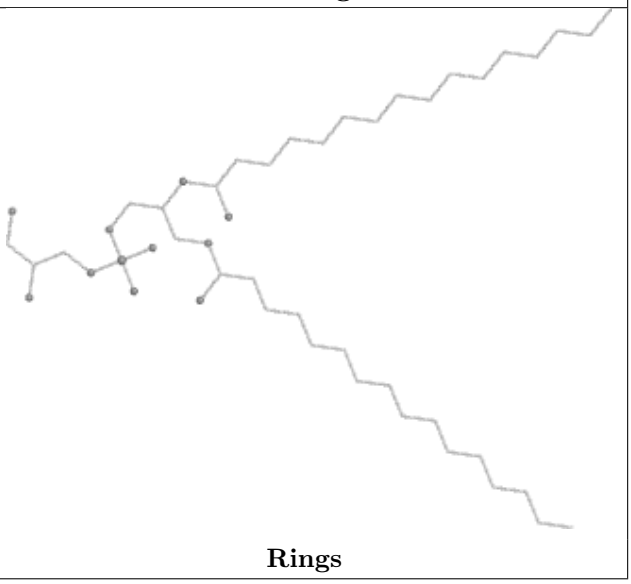
Bond lengths



Bond angles

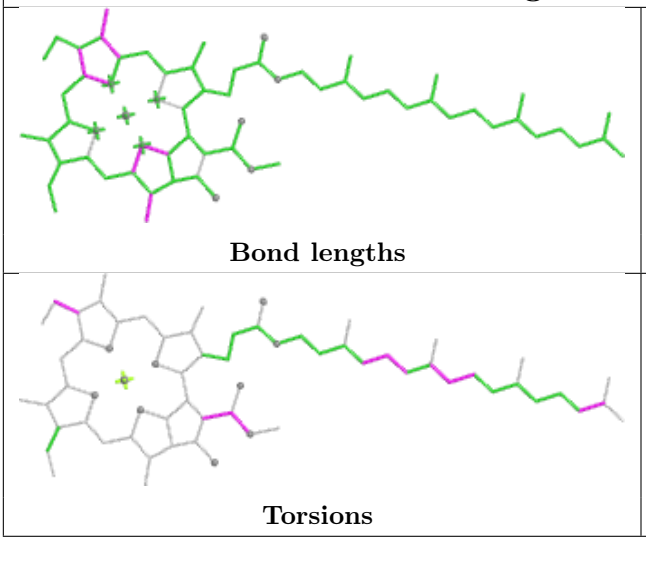


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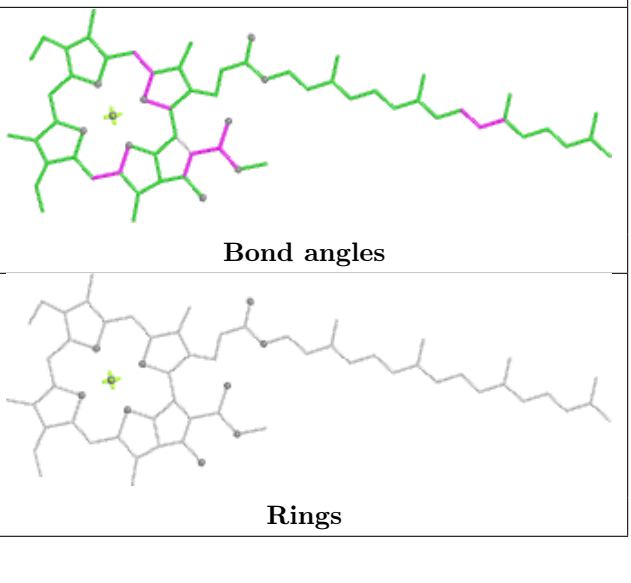


Rings

Ligand CLA B 605



Bond lengths

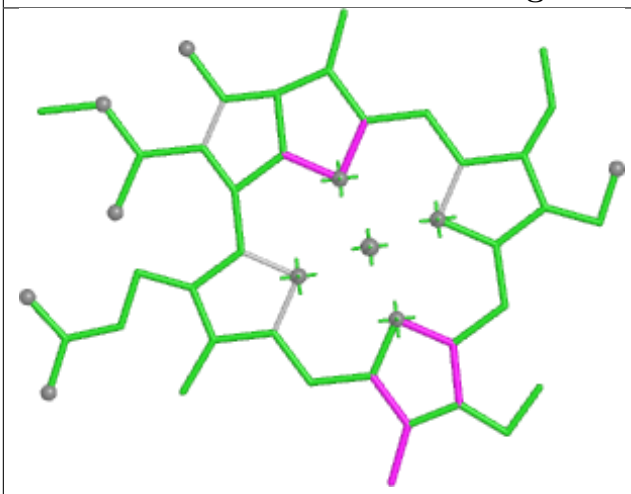


Bond angles

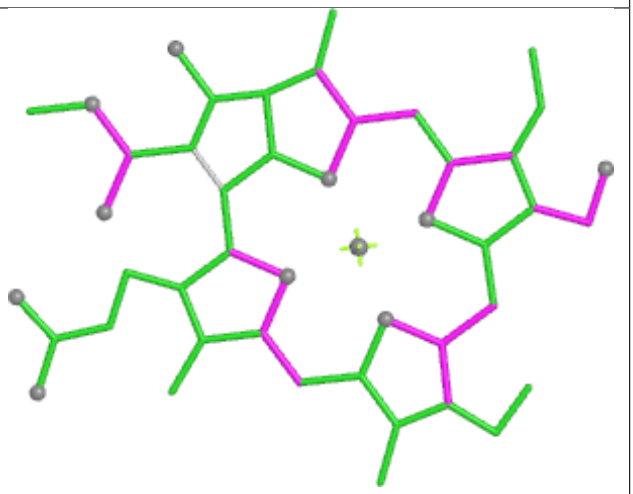
Torsions

Rings

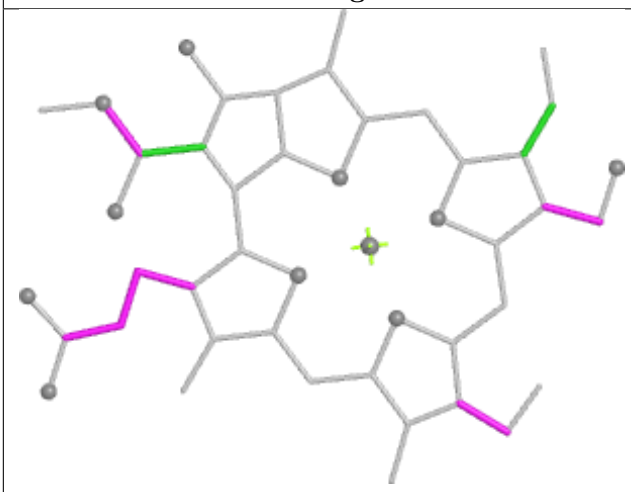
Ligand CHL S 306



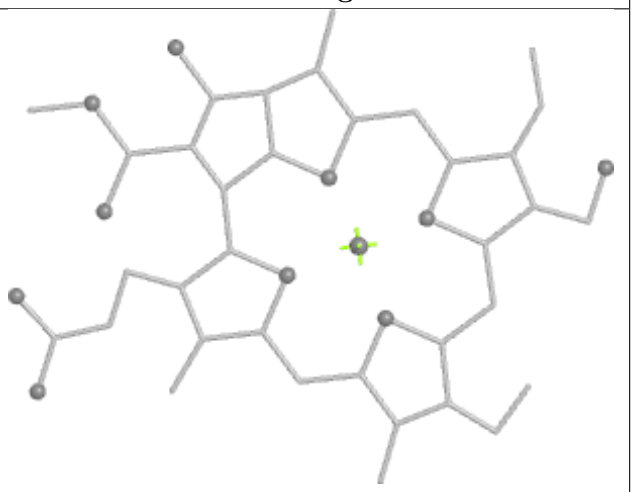
Bond lengths



Bond angles

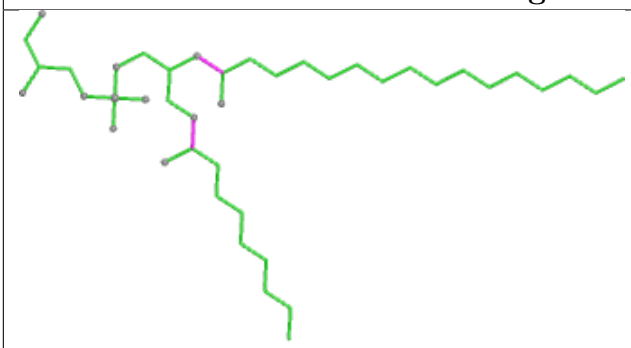


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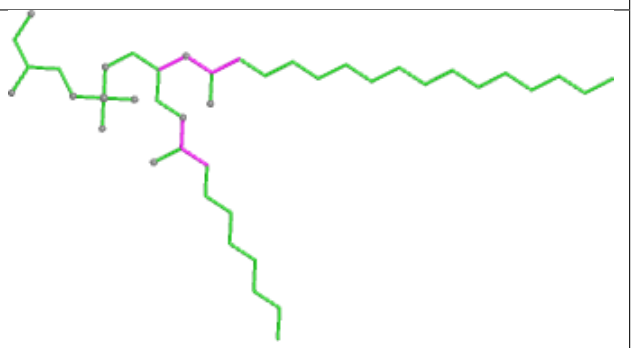


Rings

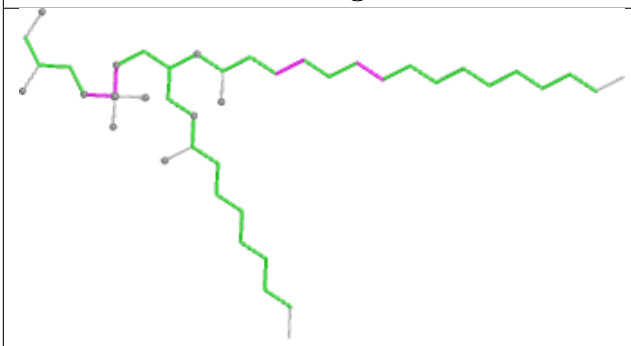
Ligand LHG r 616



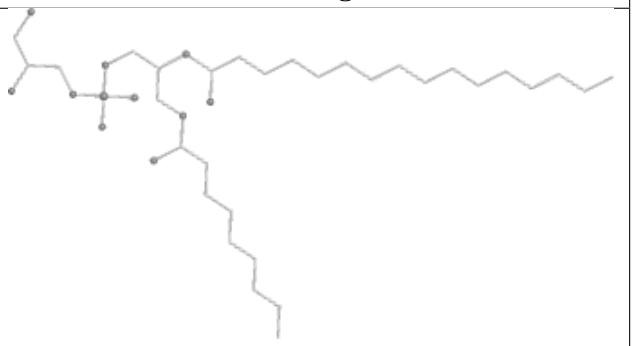
Bond lengths



Bond angles

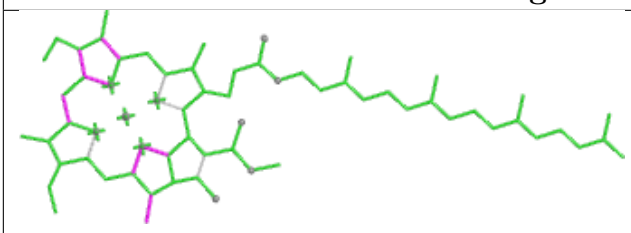


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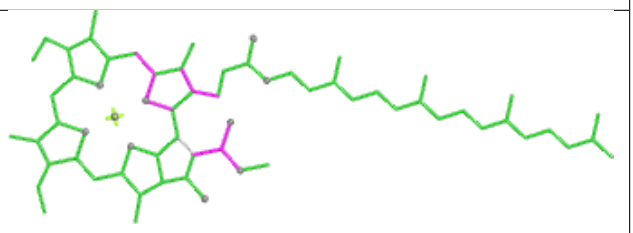


Rings

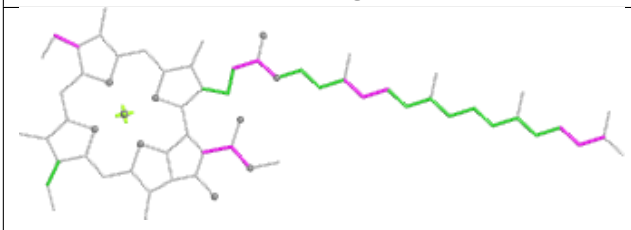
Ligand CLA c 510



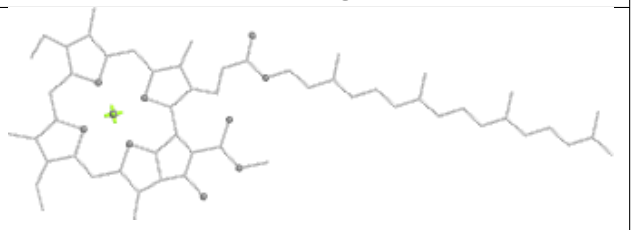
Bond lengths



Bond angles

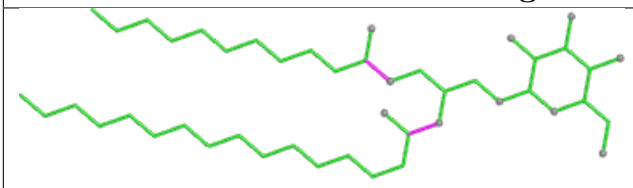


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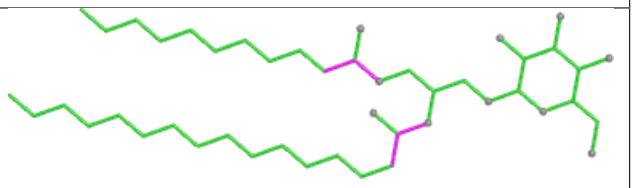


Rings

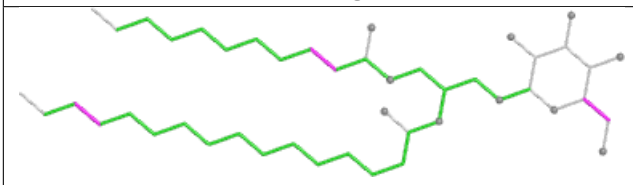
Ligand LMG D 409



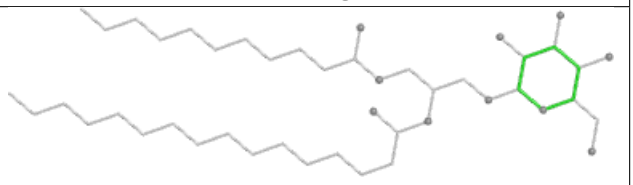
Bond lengths



Bond angles

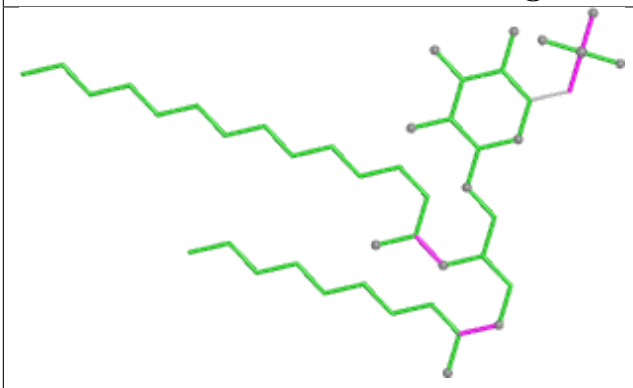


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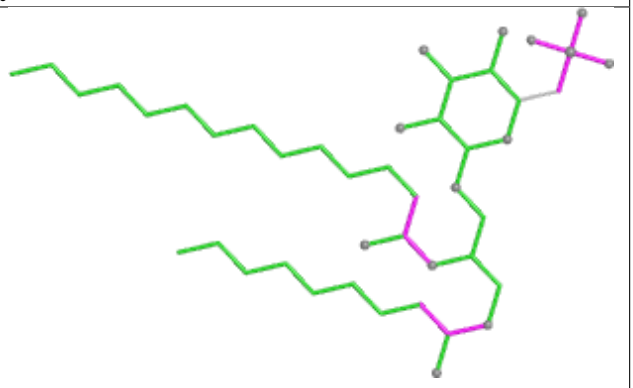


Rings

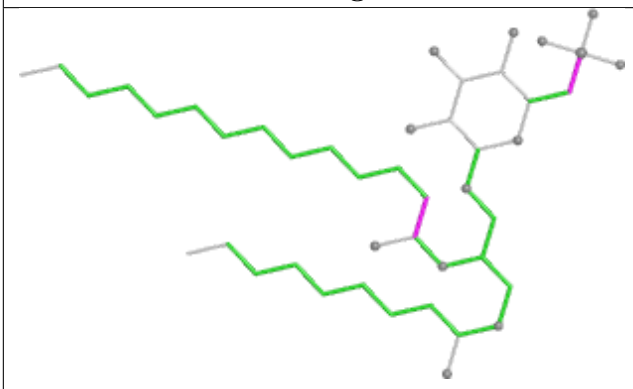
Ligand SQD C 521



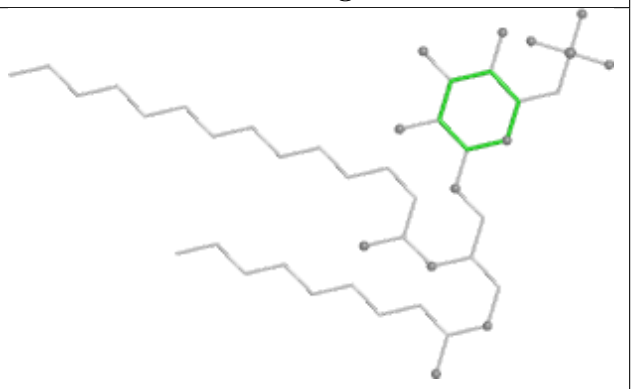
Bond lengths



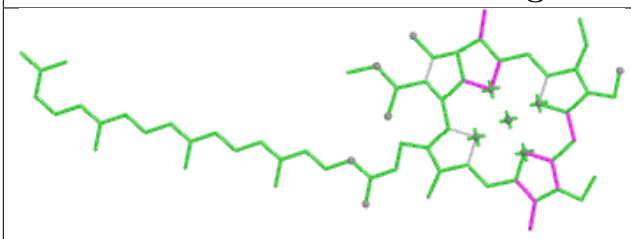
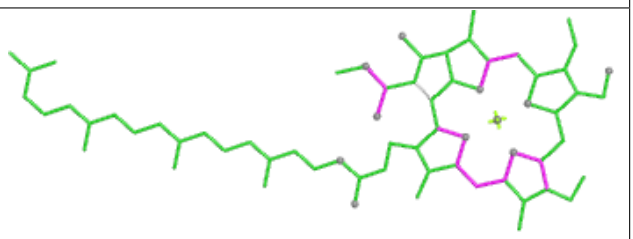
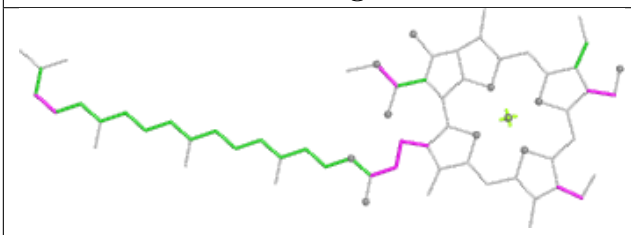
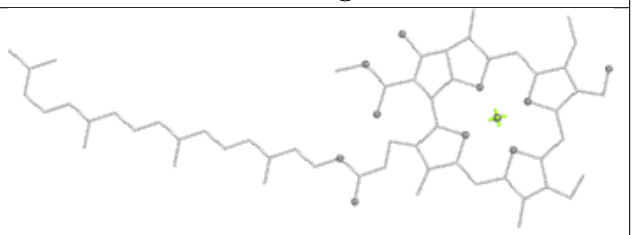
Bond angles

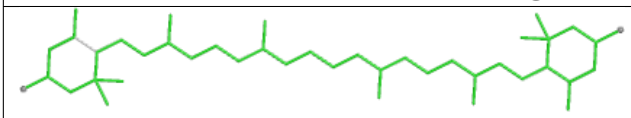
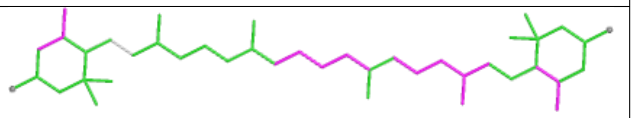
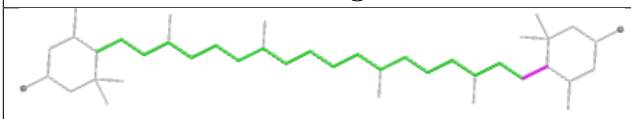
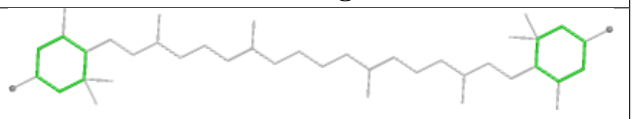


Torsions

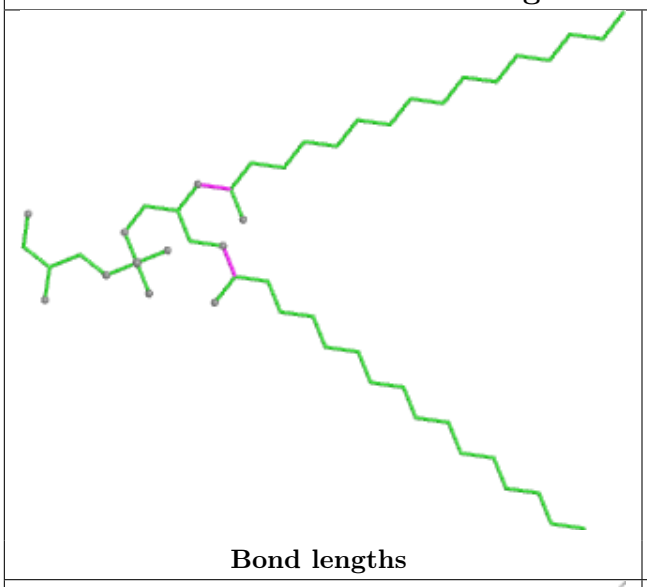


Rings

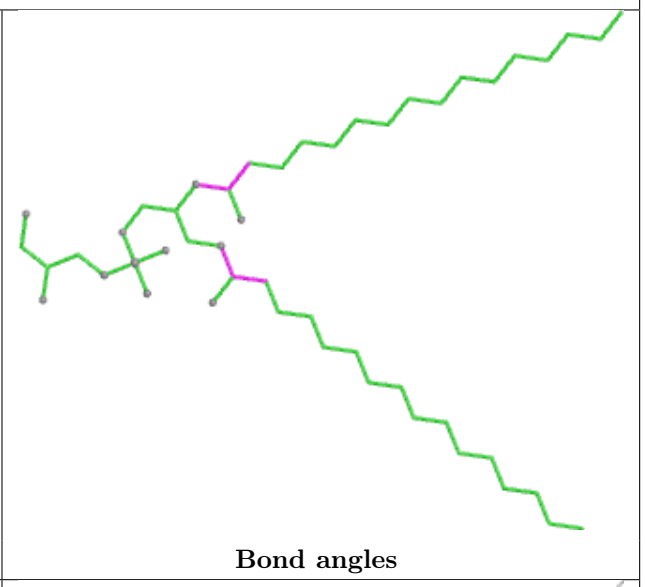
Ligand CHL n 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT S 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

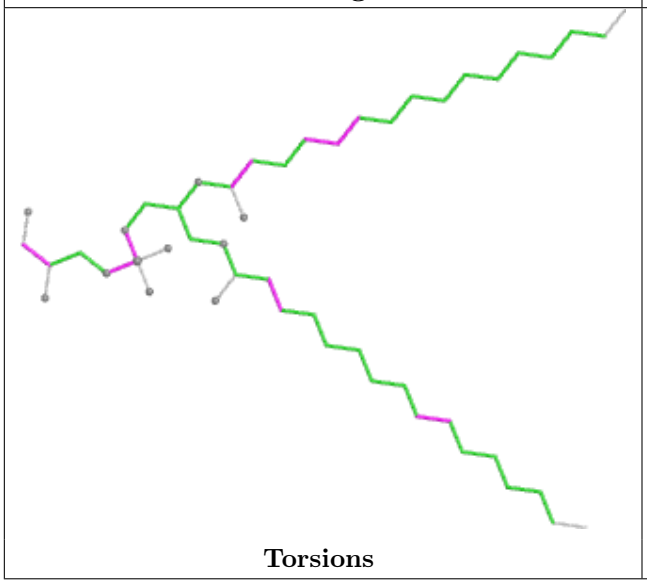
Ligand LHG D 407



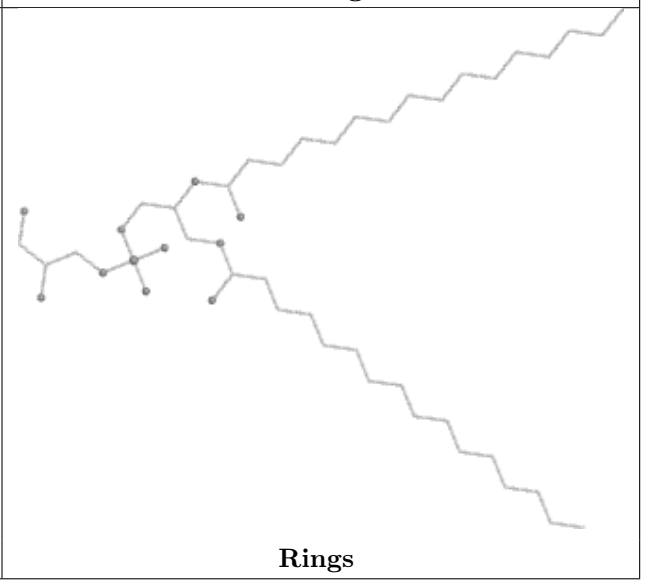
Bond lengths



Bond angles

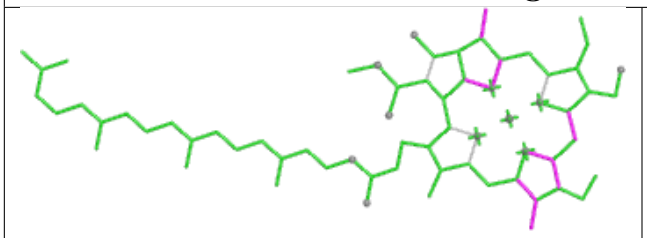


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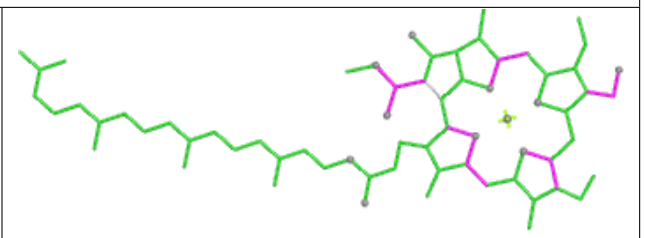


Rings

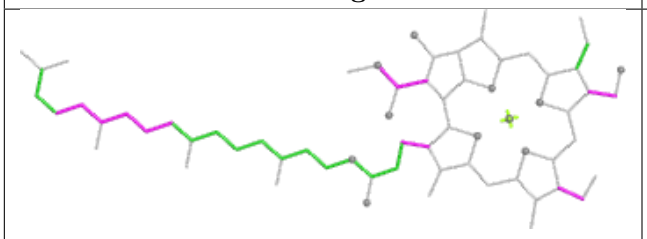
Ligand CHL Y 302



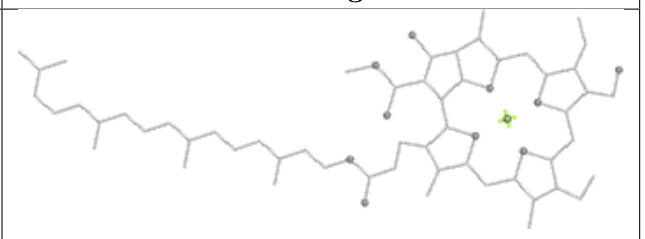
Bond lengths



Bond angles

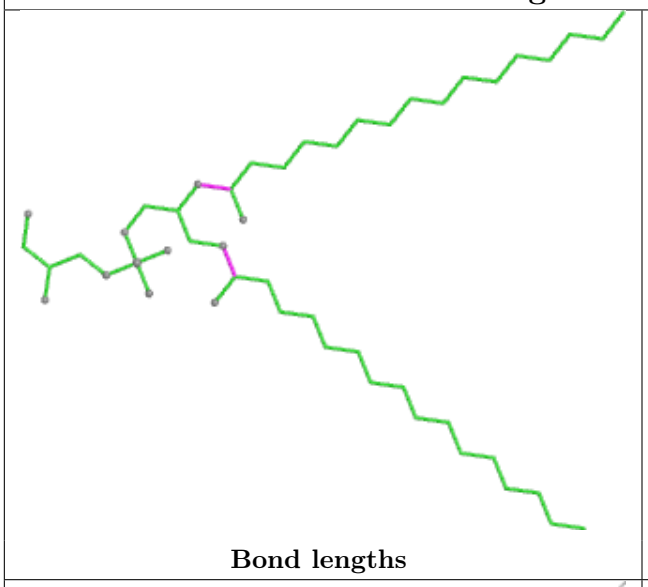


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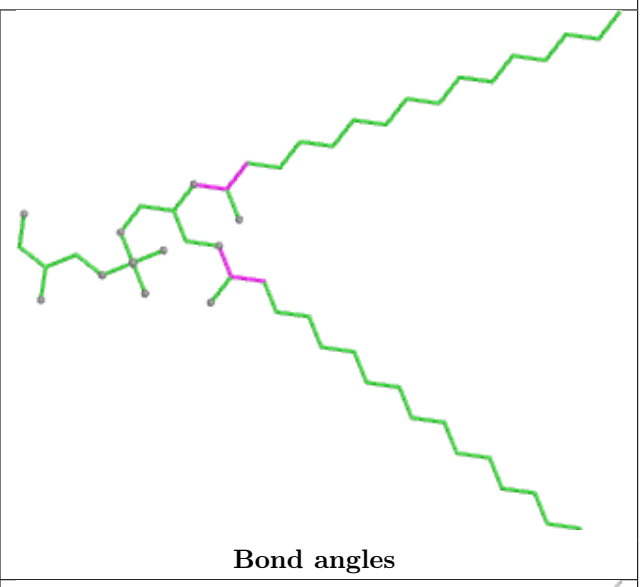


Rings

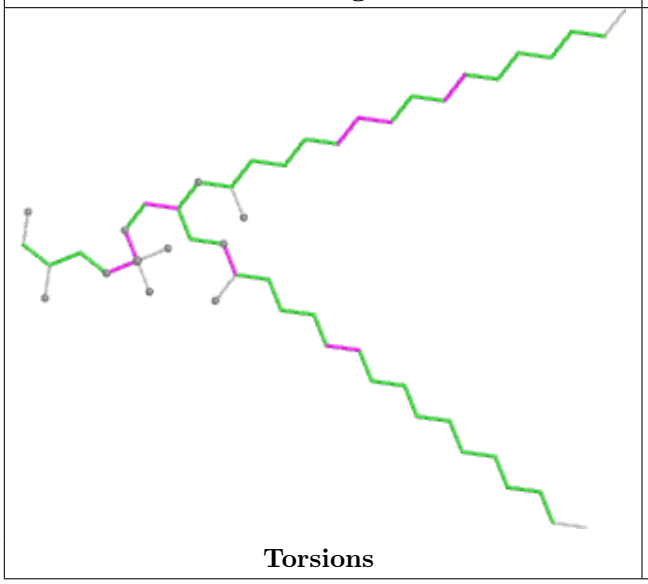
Ligand LHG c 517



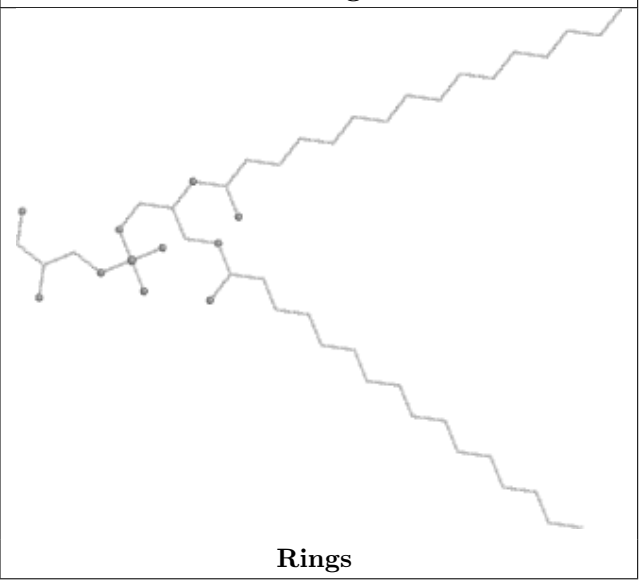
Bond lengths



Bond angles

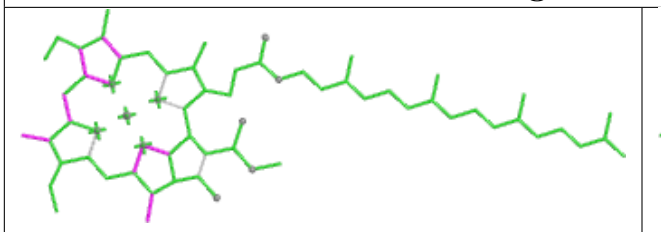


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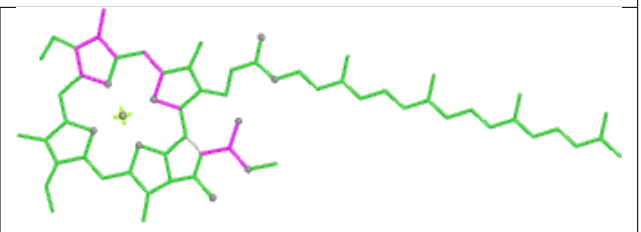


Rings

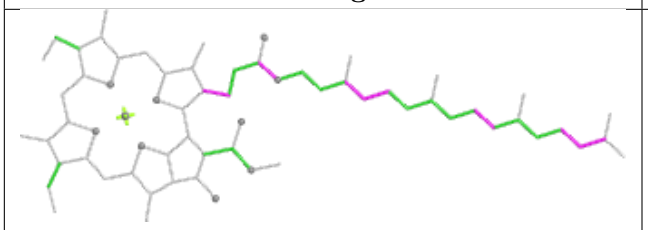
Ligand CLA d 403



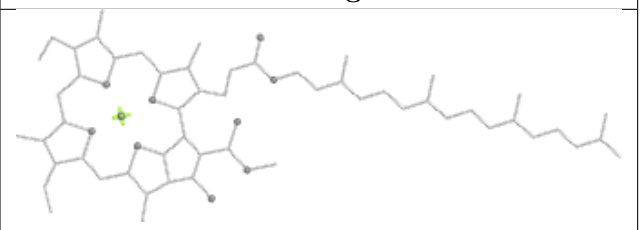
Bond lengths



Bond angles

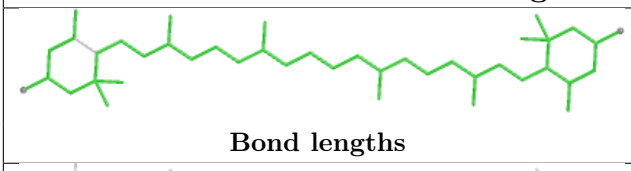


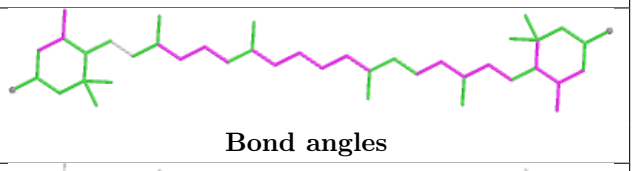
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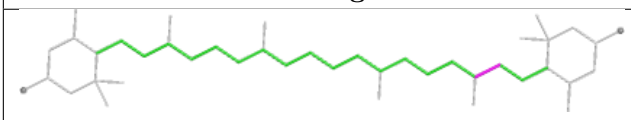


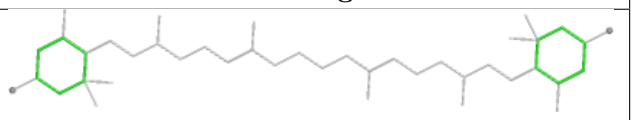
Rings

Ligand LUT r 613


Bond lengths

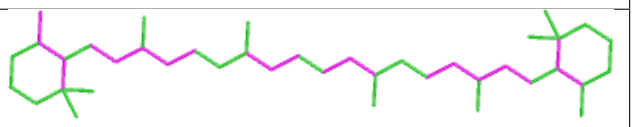

Bond angles

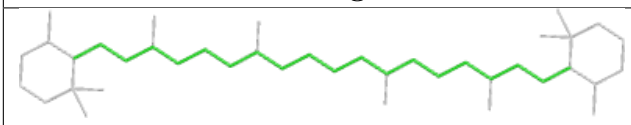

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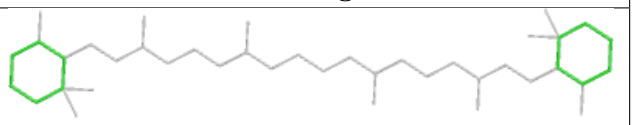

Rings

Ligand BCR C 515

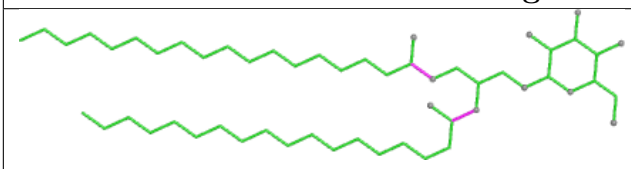

Bond lengths

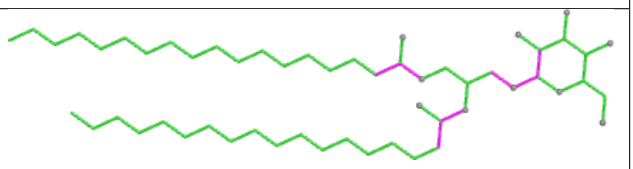

Bond angles

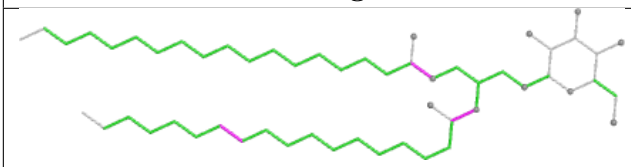

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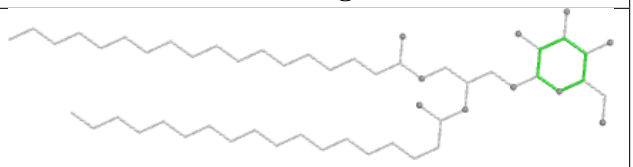

Rings

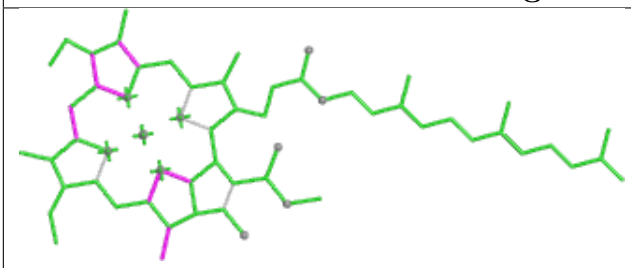
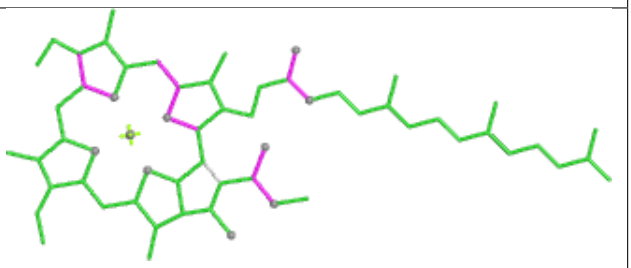
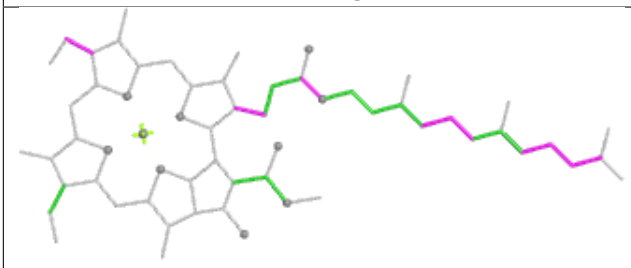
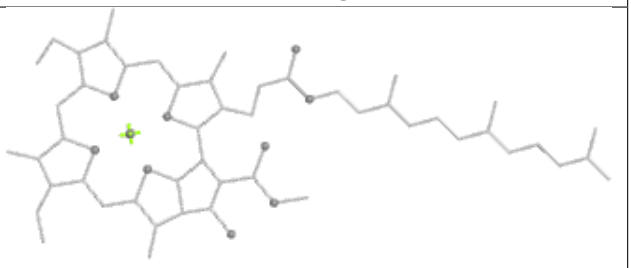
Ligand LMG S 301

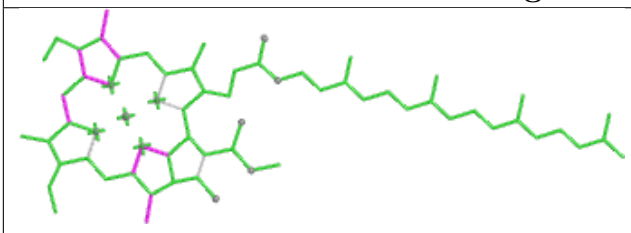
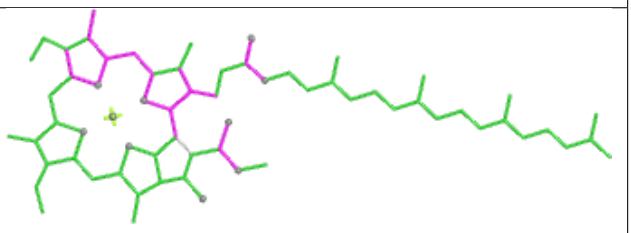
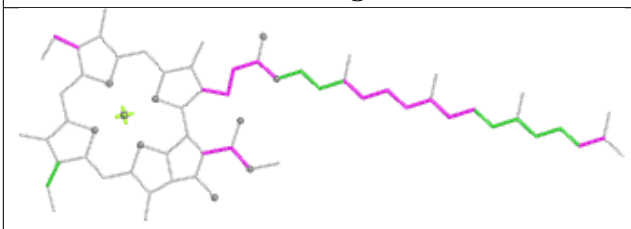
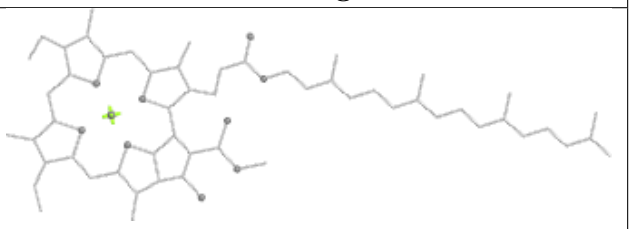

Bond lengths


Bond angles

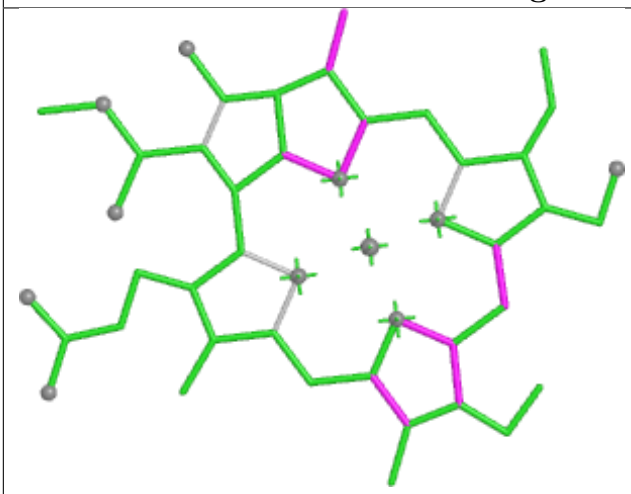

Torsions


Rings

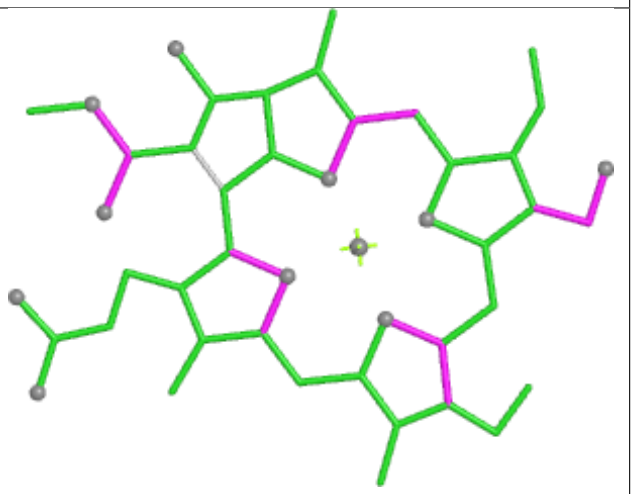
Ligand CLA Y 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

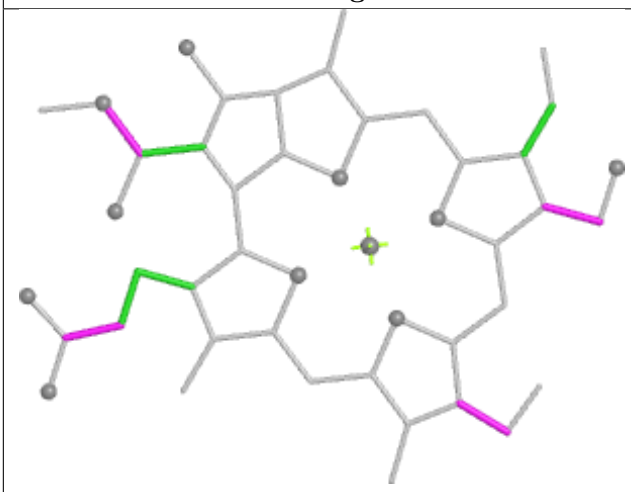
Ligand CHL s 601



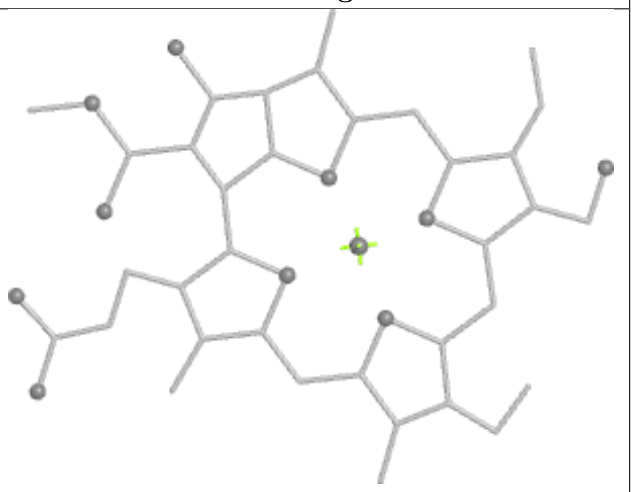
Bond lengths



Bond angles

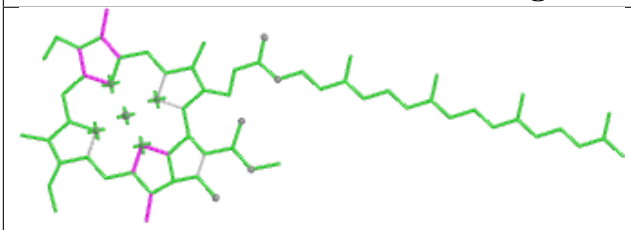


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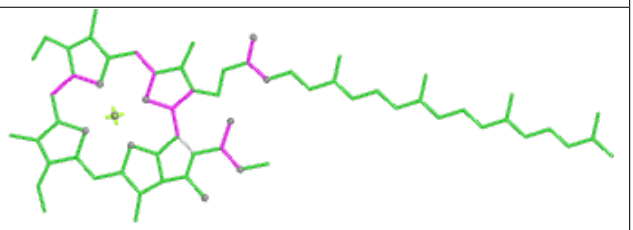


Rings

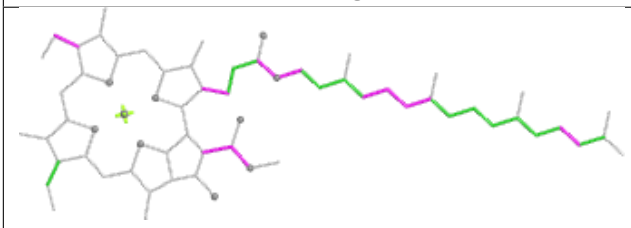
Ligand CLA c 502



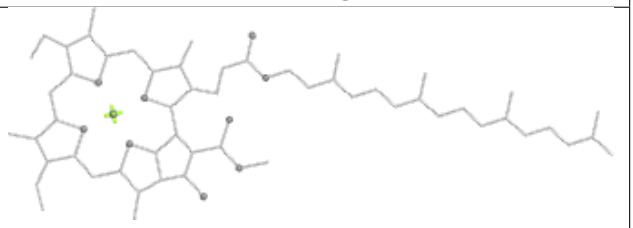
Bond lengths



Bond angles

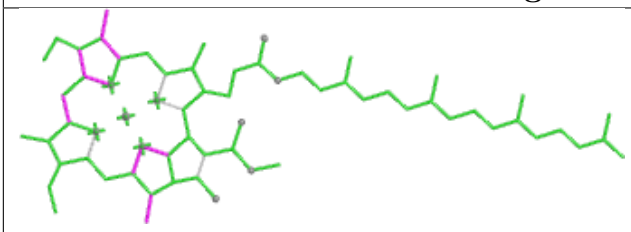


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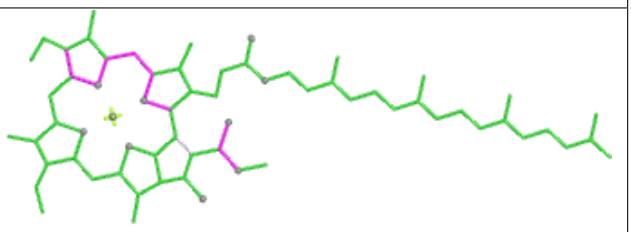


Rings

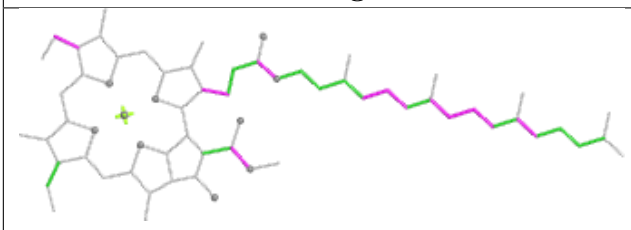
Ligand CLA B 607



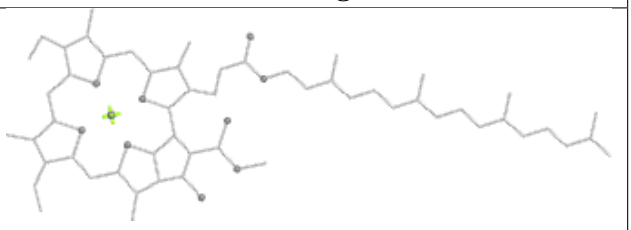
Bond lengths



Bond angles



Torsions

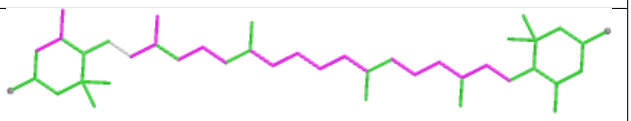


Rings

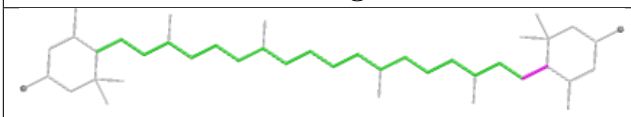
Ligand LUT N 615



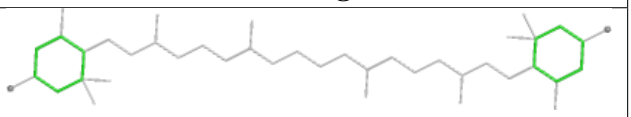
Bond lengths



Bond angles

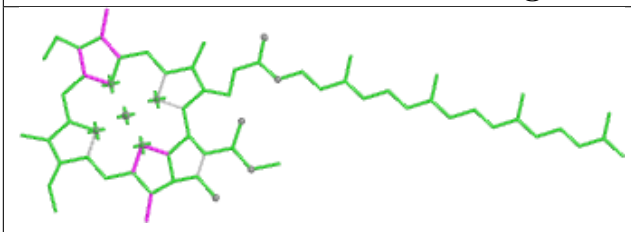


Torsions

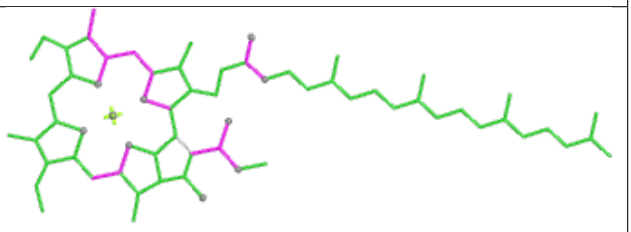


Rings

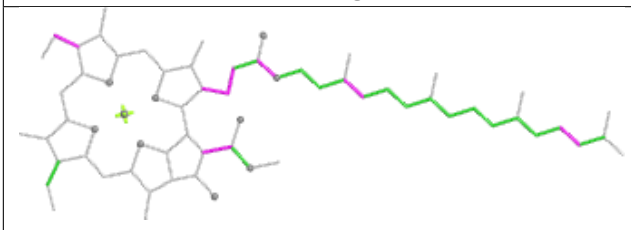
Ligand CLA R 313



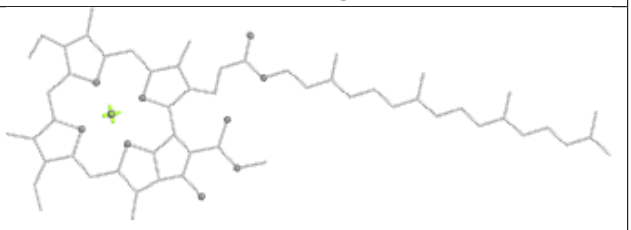
Bond lengths



Bond angles

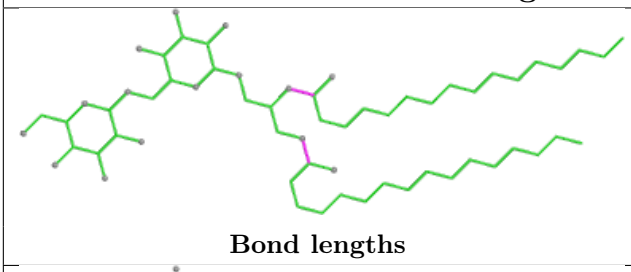


Torsions

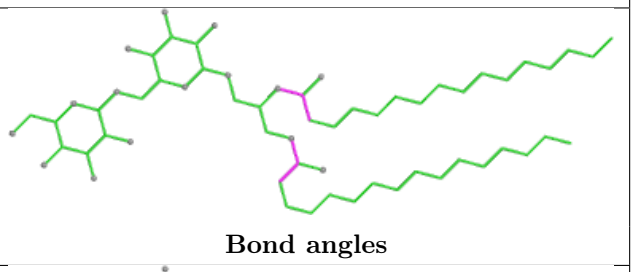


Rings

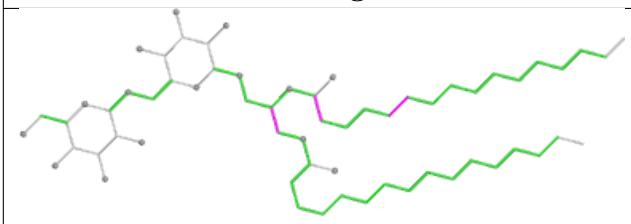
Ligand DGD D 410



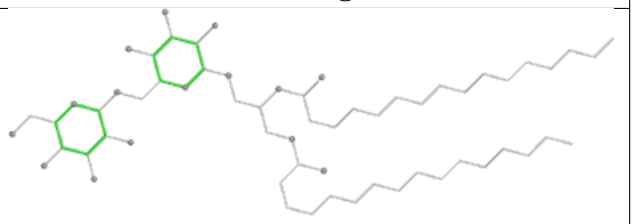
Bond lengths



Bond angles

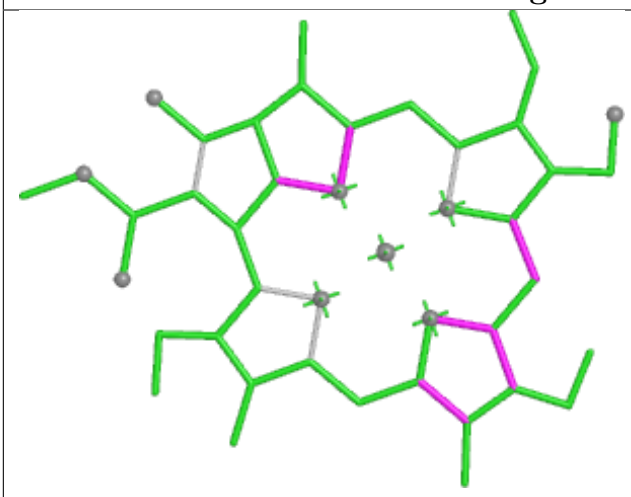


Torsions

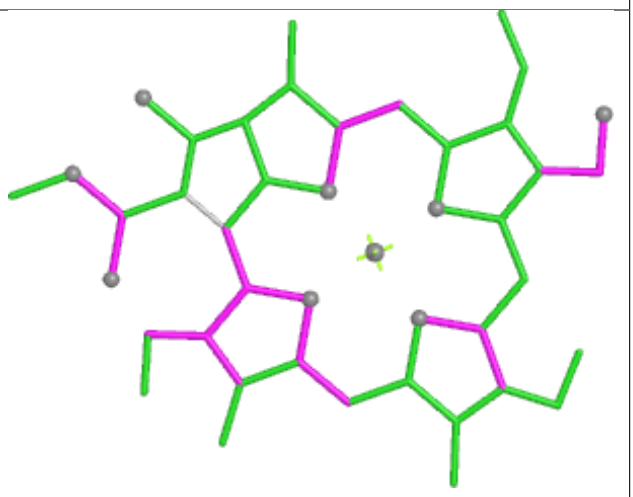


Rings

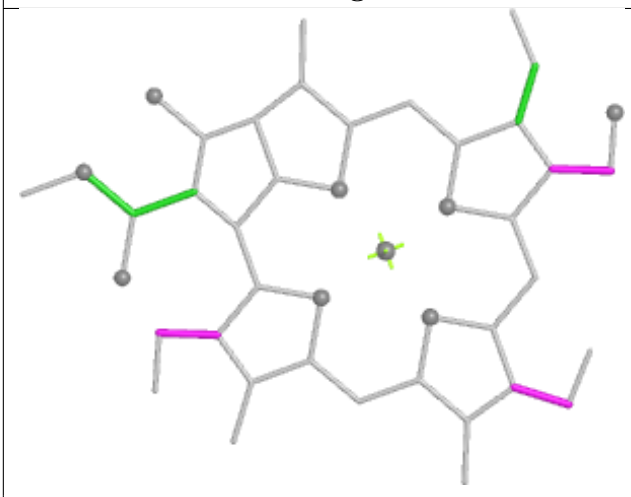
Ligand CHL s 606



Bond lengths



Bond angles

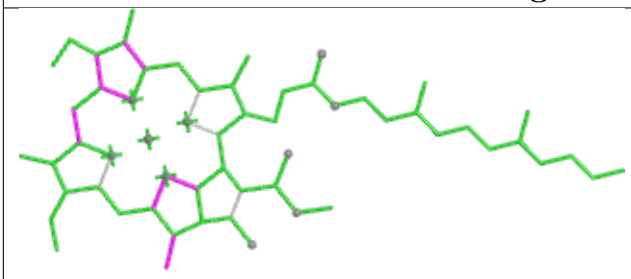


Torsions

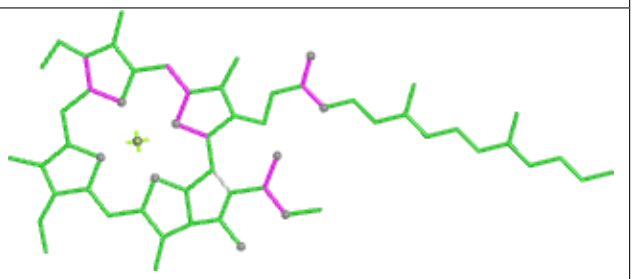


Rings

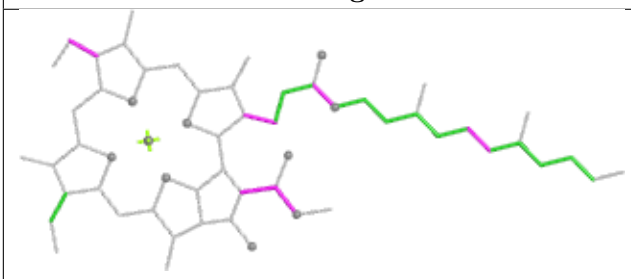
Ligand CLA r 608



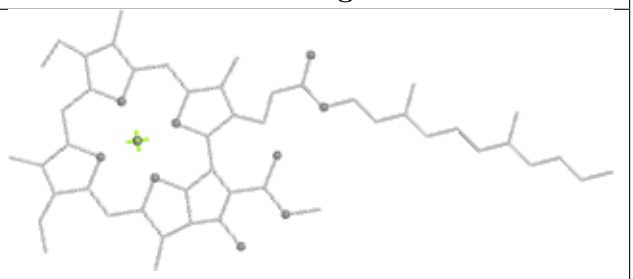
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

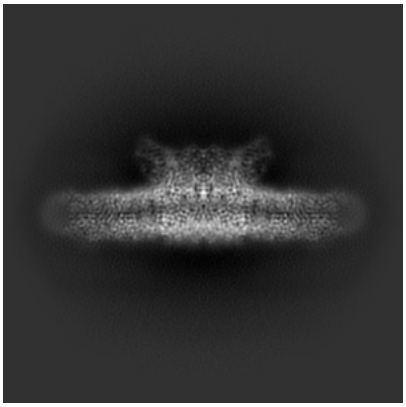
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-63168. These allow visual inspection of the internal detail of the map and identification of artifacts.

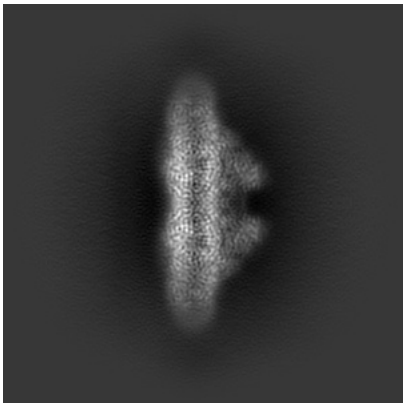
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

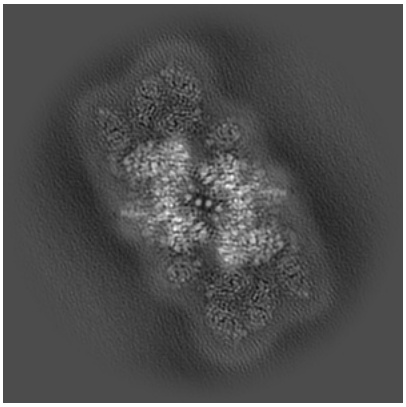
6.1.1 Primary map



X



Y

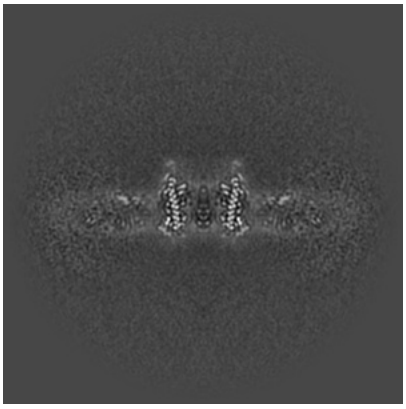


Z

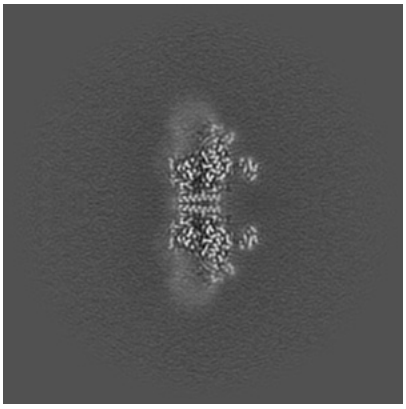
The images above show the map projected in three orthogonal directions.

6.2 Central slices

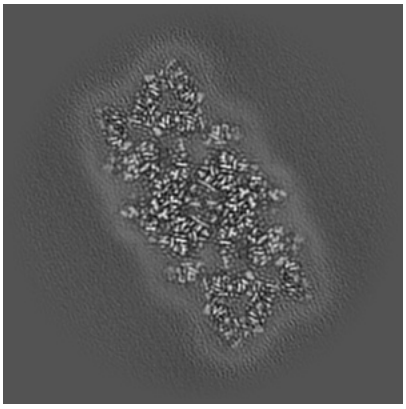
6.2.1 Primary map



X Index: 180



Y Index: 180

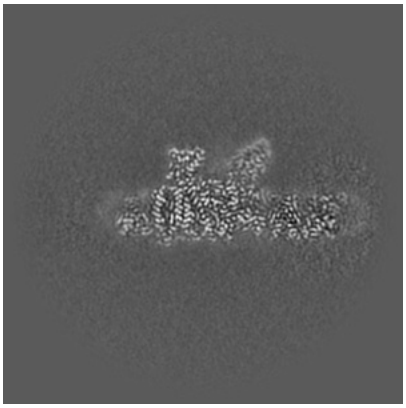


Z Index: 180

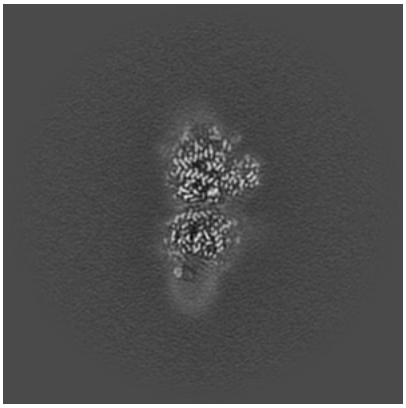
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

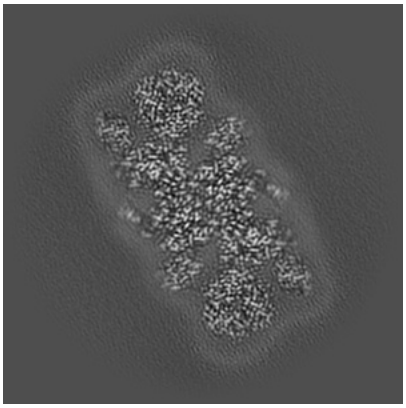
6.3.1 Primary map



X Index: 155



Y Index: 194

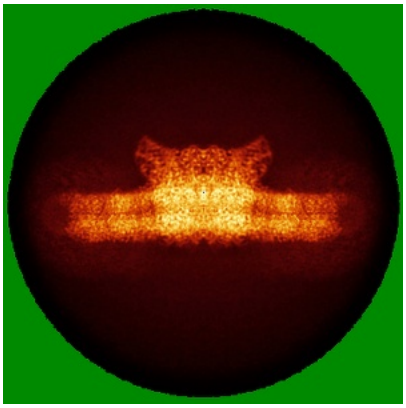


Z Index: 164

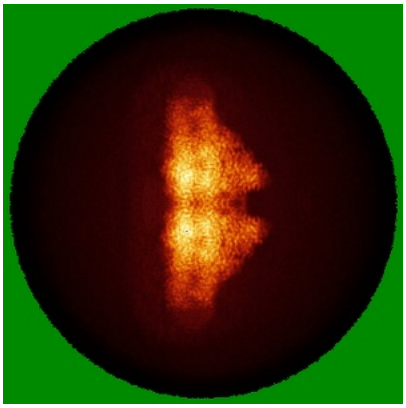
The images above show the largest variance slices of the map in three orthogonal directions.

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

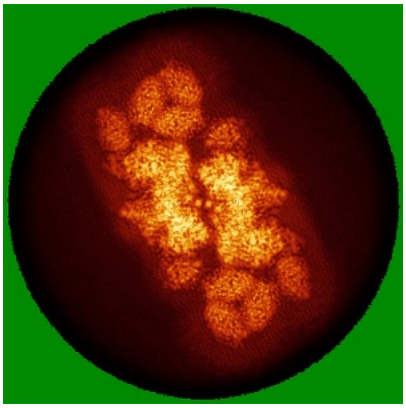
6.4.1 Primary map



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

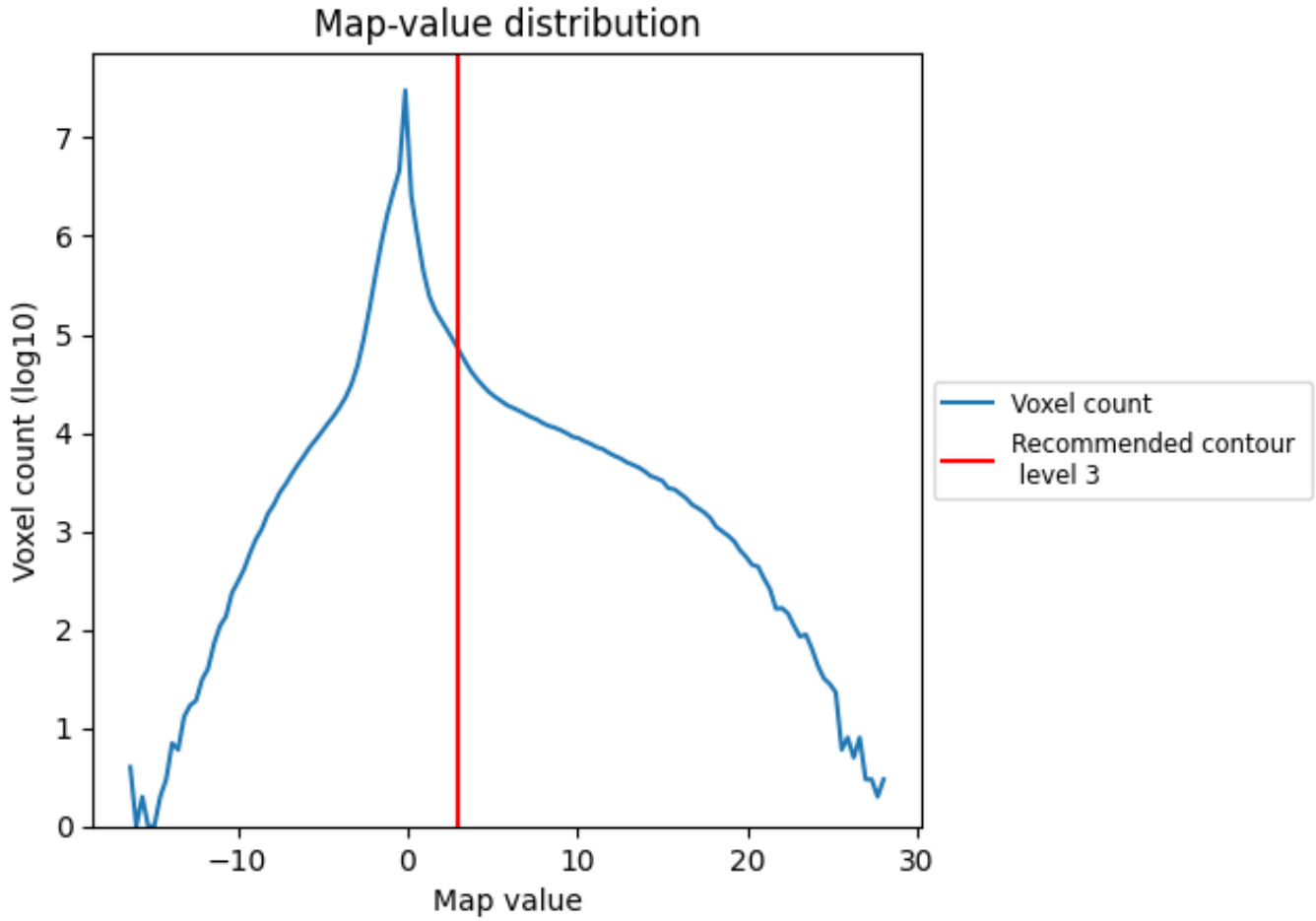
6.6 Mask visualisation (i)

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

7 Map analysis

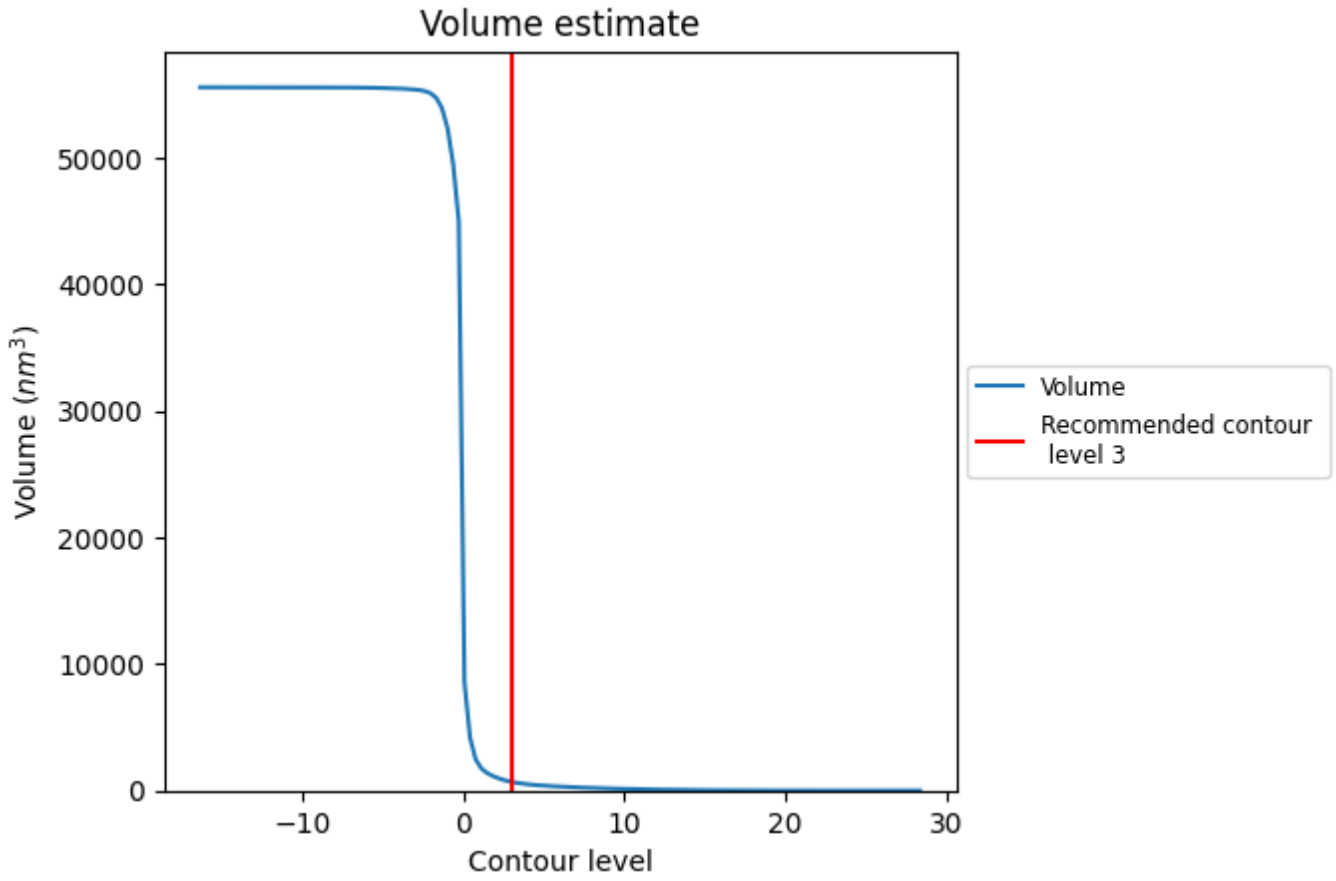
This section contains the results of statistical analysis of the map.

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.

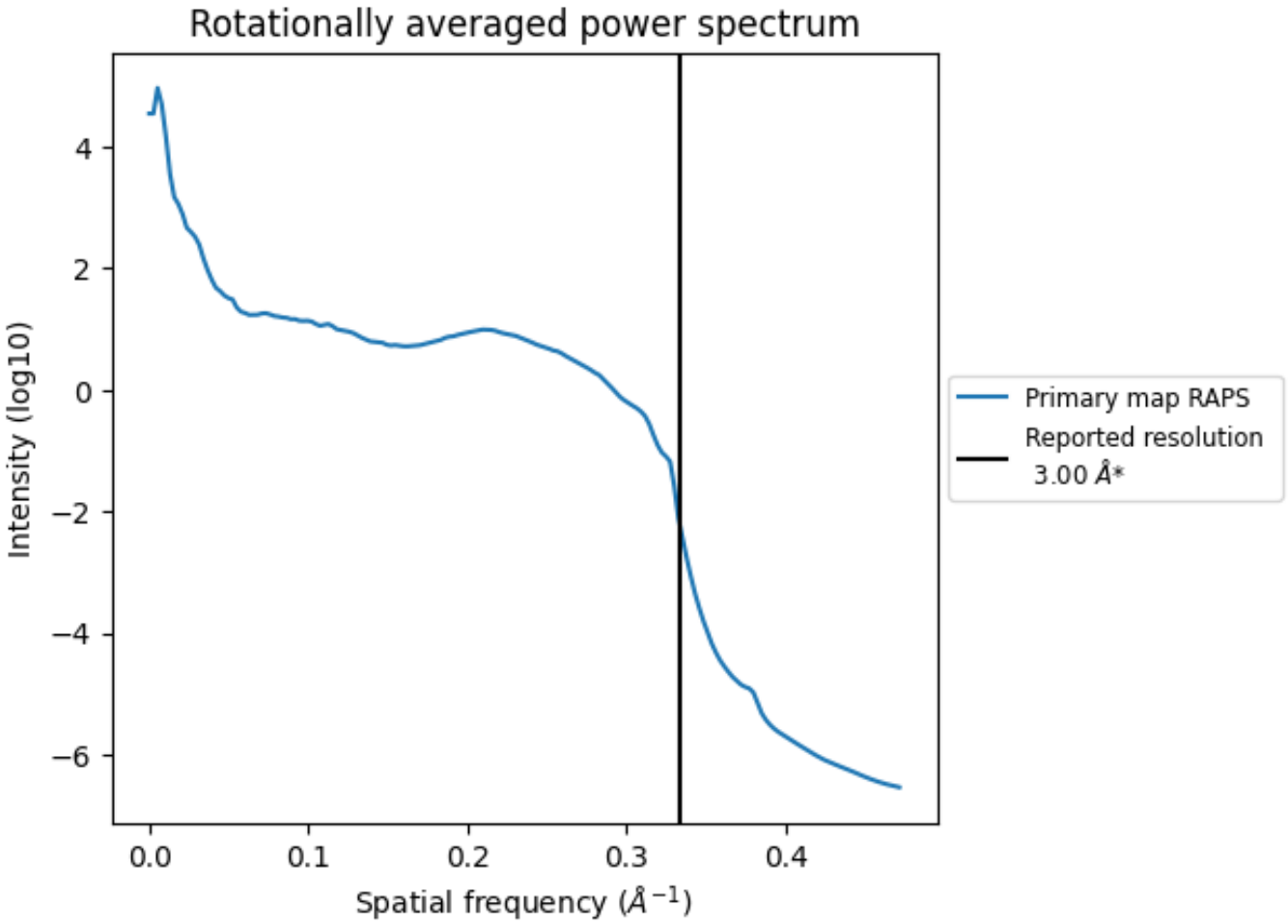
7.2 Volume estimate (i)



The volume at the recommended contour level is 690 nm^3; this corresponds to an approximate mass of 624 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 0.333 Å^{-1}

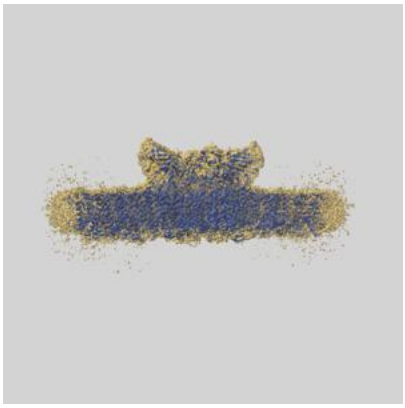
8 Fourier-Shell correlation

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

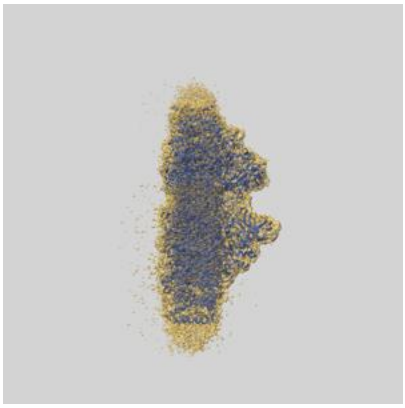
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63168 and PDB model 9LK5. Per-residue inclusion information can be found in section 3 on page 35.

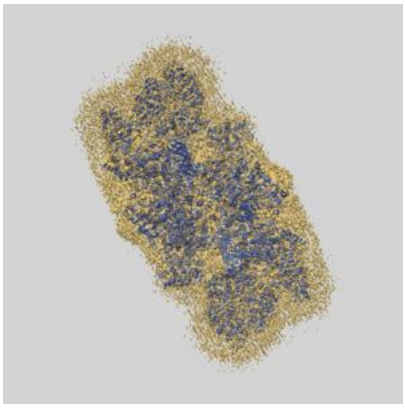
9.1 Map-model overlay



X



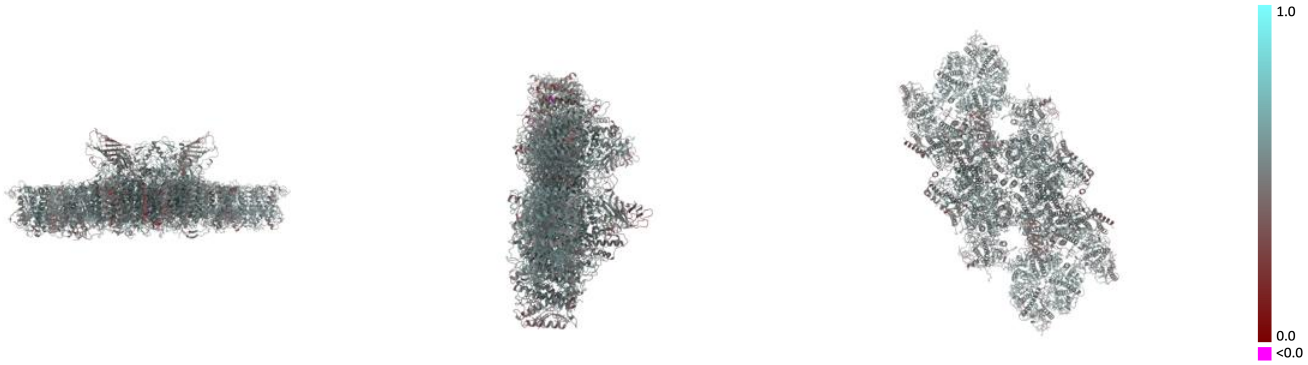
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

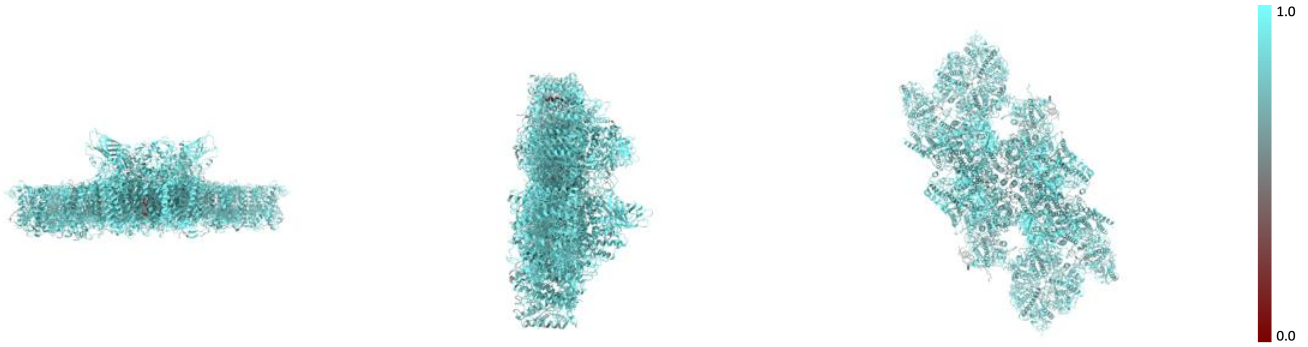
9.2 Q-score mapped to coordinate model (i)



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.

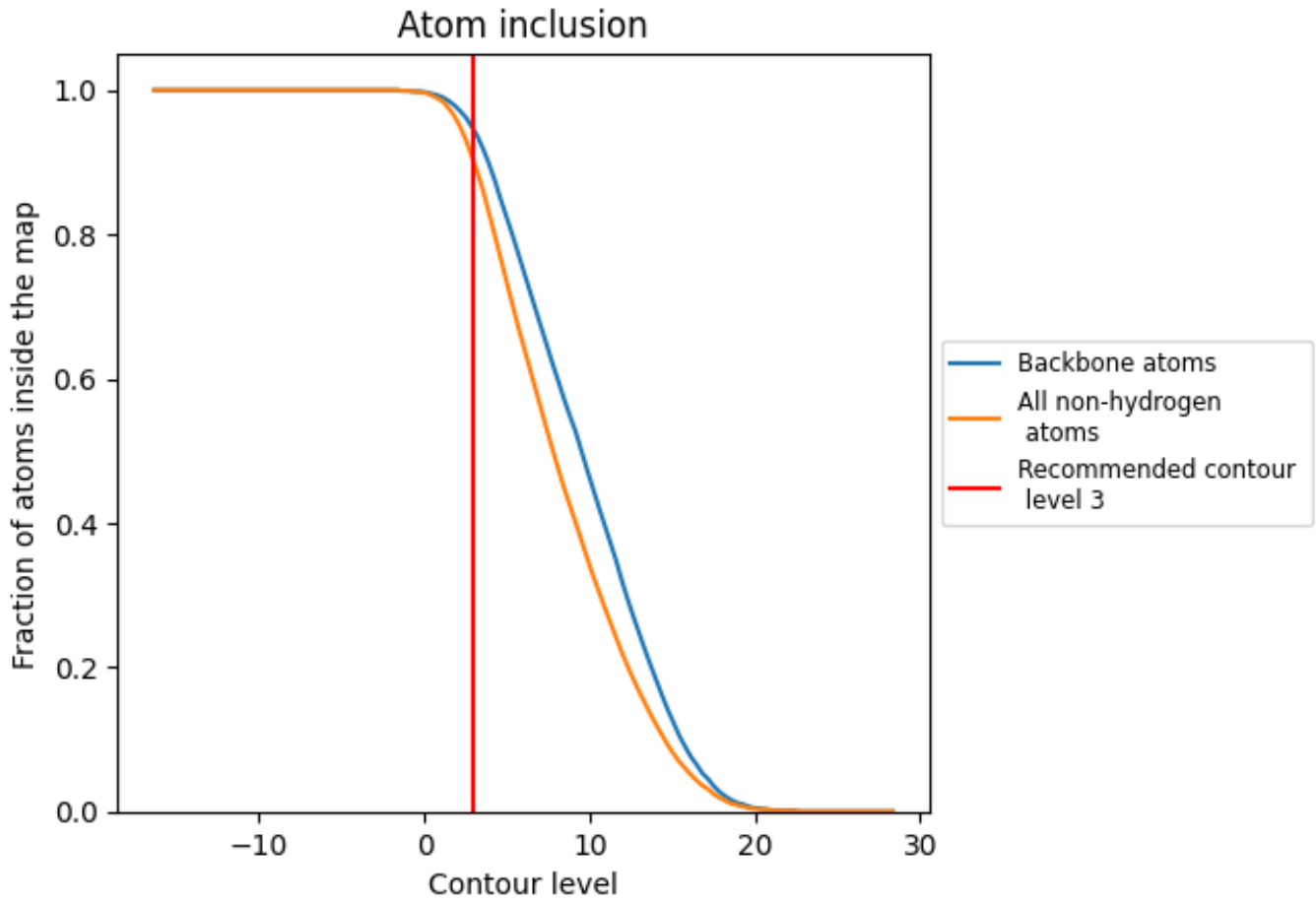
9.3 Atom inclusion mapped to coordinate model (i)



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 (3).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9010	0.5180
A	0.9390	0.5340
B	0.9400	0.5440
C	0.9310	0.5240
D	0.9470	0.5450
E	0.9160	0.4170
F	0.9070	0.4570
G	0.8560	0.5250
H	0.9390	0.5300
I	0.9670	0.5430
J	0.6820	0.3290
K	0.8690	0.4710
L	0.8900	0.5250
M	0.8830	0.4970
N	0.8900	0.5430
O	0.8950	0.4240
R	0.8310	0.4860
S	0.8270	0.4920
T	0.9240	0.5250
U	0.7090	0.4720
W	0.8520	0.5190
X	0.8500	0.4700
Y	0.9070	0.5580
Z	0.8640	0.4290
a	0.9420	0.5360
b	0.9430	0.5440
c	0.9300	0.5240
d	0.9470	0.5440
e	0.9220	0.4190
f	0.9140	0.4560
g	0.8530	0.5240
h	0.9390	0.5280
i	0.9670	0.5490
j	0.6820	0.3310
k	0.8750	0.4720



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Chain	Atom inclusion	Q-score
l	0.8920	0.5270
m	0.8680	0.4860
n	0.8810	0.5410
o	0.8980	0.4230
r	0.8400	0.4830
s	0.8210	0.4920
t	0.9150	0.5270
u	0.7200	0.4620
w	0.8730	0.5140
x	0.8350	0.4650
y	0.9060	0.5560
z	0.8690	0.4320