Full wwPDB EM Validation Report ⓘ

Jun 3, 2026 – 04:36 PM JST

PDB ID	:	9UAS / pdb_00009uas
EMDB ID	:	EMD-63994
Title	:	PSI-LHCE-LHCII from Euglena gracilis
Authors	:	Feng, Y.
Deposited on	:	2025-04-01
Resolution	:	2.35 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:

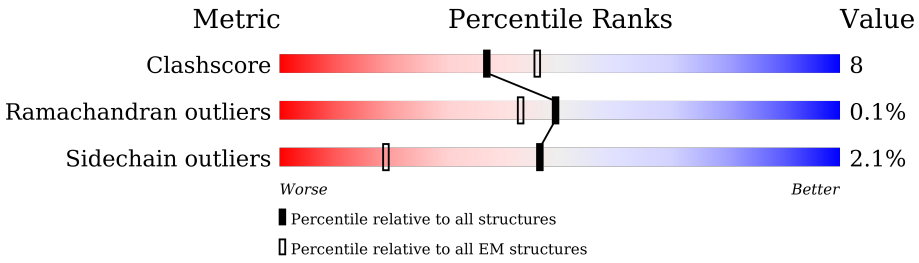
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.49

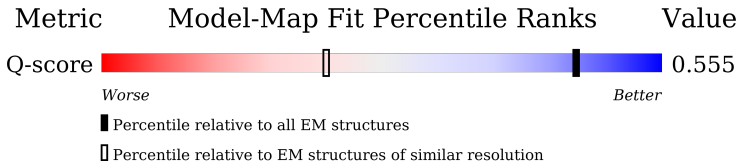
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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.





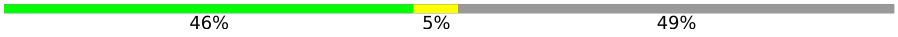
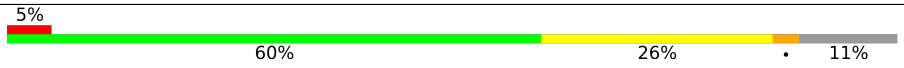
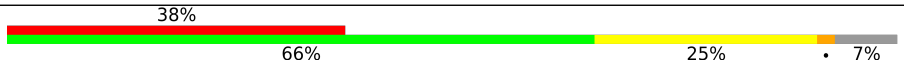
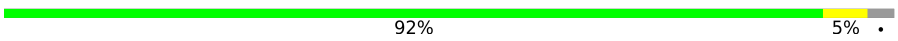
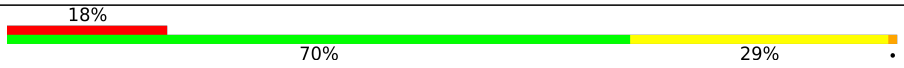
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4607 (1.85 - 2.85)

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	B	734	86% 13%
2	C	81	89% 10%
3	D	193	90% 9%
4	E	158	33% 7% 60%

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Mol	Chain	Length	Quality of chain
5	F	325	
6	G	184	
6	P	184	
7	H	185	
8	I	184	
8	N	184	
9	J	39	
10	K	184	
10	Q	184	
11	L	187	
11	R	187	
12	M	31	
13	O	177	
14	S	180	
15	T	173	
16	U	209	
17	V	196	
18	W	228	
19	X	223	
20	A	756	

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 60137 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 I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	732	5868	3859	985	1009	15	0	0

- Molecule 2 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	80	596	363	104	118	11	0	0

- Molecule 3 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	190	1489	948	254	285	2	0	0

- Molecule 4 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	63	509	324	86	99	0	0

- Molecule 5 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	166	1262	811	210	239	2	0	0

- Molecule 6 is a protein called Lhce5.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	175	1323	853	224	242	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	164	Total	C	N	O	S	0	0
			1243	803	209	227	4		

- Molecule 7 is a protein called Lhce7.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	173	Total	C	N	O	S	0	0
			1342	862	233	242	5		

- Molecule 8 is a protein called Lhce5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	165	Total	C	N	O	S	0	0
			1242	801	212	225	4		
8	N	170	Total	C	N	O	S	0	0
			1271	819	215	233	4		

- Molecule 9 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

- Molecule 10 is a protein called LhcE6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	182	Total	C	N	O	S	0	0
			1444	939	246	253	6		
10	Q	182	Total	C	N	O	S	0	0
			1440	938	245	251	6		

- Molecule 11 is a protein called Lhce8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	178	Total	C	N	O	S	0	0
			1364	876	237	247	4		
11	R	174	Total	C	N	O	S	0	0
			1331	852	232	243	4		

- Molecule 12 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			242	162	37	42	1		

- Molecule 13 is a protein called LhcE7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	175	Total	C	N	O	S	0	0
			1359	870	234	250	5		

- Molecule 14 is a protein called Lhce10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	172	Total	C	N	O	S	0	0
			1327	858	219	246	4		

- Molecule 15 is a protein called Lhce11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	167	Total	C	N	O	S	0	0
			1283	824	221	231	7		

- Molecule 16 is a protein called LhcbM4.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 17 is a protein called LhcbM4.10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	196	Total	C	N	O	S	0	0
			1513	990	253	265	5		

- Molecule 18 is a protein called LhcbM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

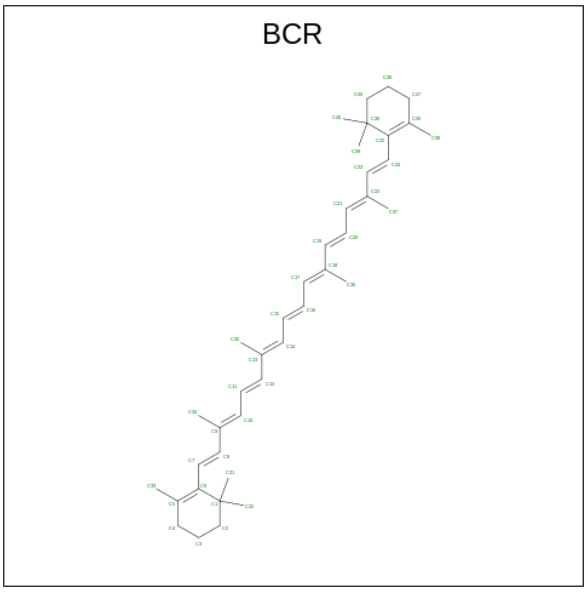
- Molecule 19 is a protein called LhcbM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	223	Total	C	N	O	S	0	0
			1688	1093	284	306	5		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	740	Total	C	N	O	S	0	0
			5872	3855	992	1004	21		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



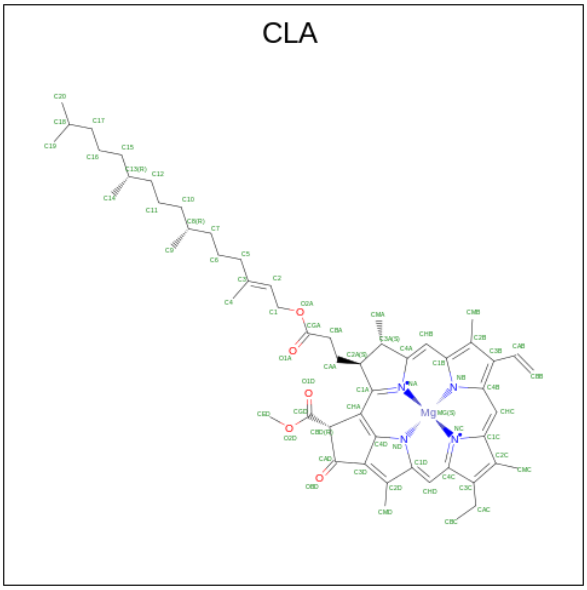
Mol	Chain	Residues	Atoms		AltConf
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	J	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
21	M	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 56 46 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	J	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	N	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	R	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	S	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	T	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	U	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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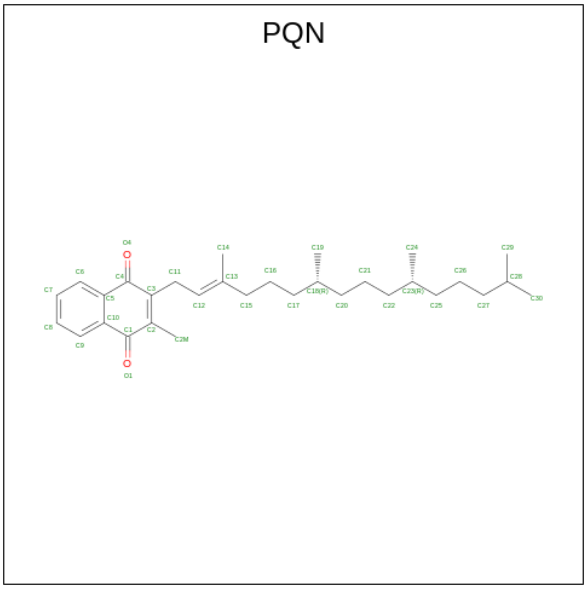
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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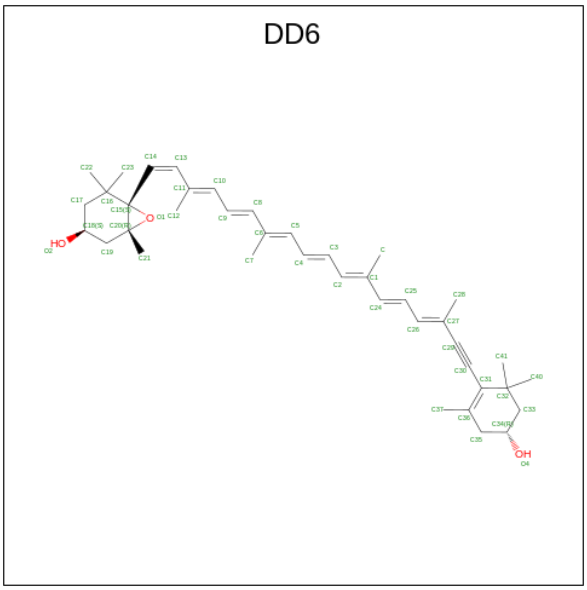
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			33	31	2	
23	A	1	Total	C	O	0
			33	31	2	

- Molecule 24 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



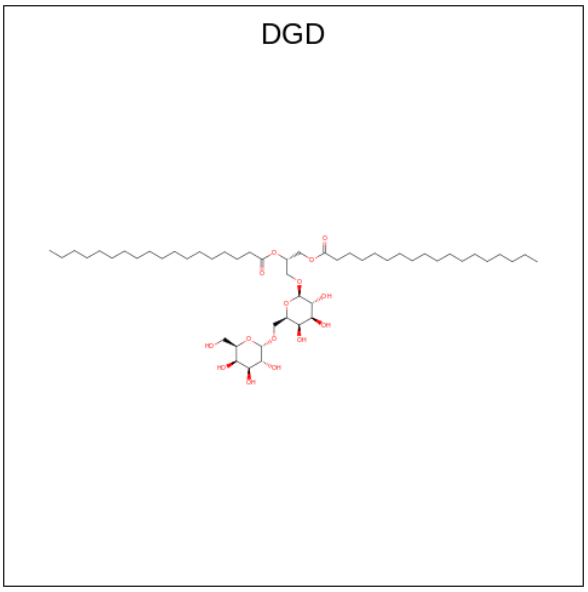
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total	C	O	0
			43	40	3	
24	F	1	Total	C	O	0
			43	40	3	
24	G	1	Total	C	O	0
			43	40	3	
24	G	1	Total	C	O	0
			43	40	3	
24	H	1	Total	C	O	0
			43	40	3	
24	H	1	Total	C	O	0
			43	40	3	
24	I	1	Total	C	O	0
			43	40	3	
24	I	1	Total	C	O	0
			43	40	3	
24	J	1	Total	C	O	0
			43	40	3	
24	K	1	Total	C	O	0
			43	40	3	
24	K	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	L	1	Total	C	O	0
			43	40	3	
24	N	1	Total	C	O	0
			43	40	3	
24	N	1	Total	C	O	0
			43	40	3	
24	O	1	Total	C	O	0
			43	40	3	
24	O	1	Total	C	O	0
			43	40	3	
24	P	1	Total	C	O	0
			43	40	3	
24	P	1	Total	C	O	0
			43	40	3	
24	Q	1	Total	C	O	0
			43	40	3	
24	Q	1	Total	C	O	0
			43	40	3	

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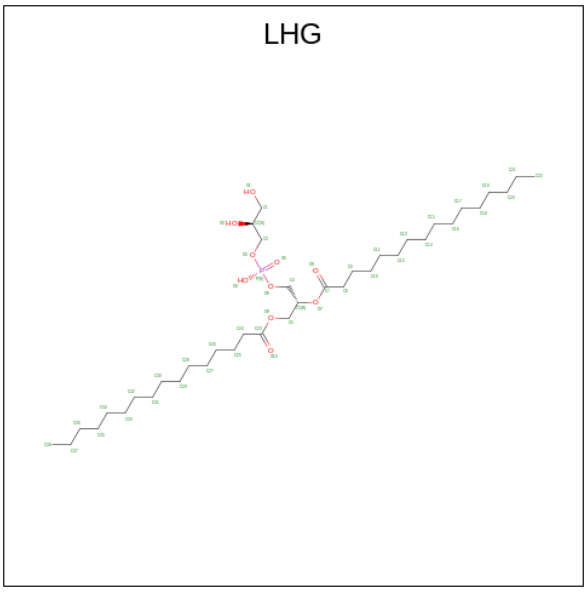
Mol	Chain	Residues	Atoms			AltConf
24	R	1	Total	C	O	0
			43	40	3	
24	R	1	Total	C	O	0
			43	40	3	
24	S	1	Total	C	O	0
			43	40	3	
24	S	1	Total	C	O	0
			43	40	3	
24	T	1	Total	C	O	0
			43	40	3	
24	T	1	Total	C	O	0
			43	40	3	
24	U	1	Total	C	O	0
			43	40	3	
24	U	1	Total	C	O	0
			43	40	3	
24	V	1	Total	C	O	0
			43	40	3	
24	V	1	Total	C	O	0
			43	40	3	
24	W	1	Total	C	O	0
			43	40	3	
24	W	1	Total	C	O	0
			43	40	3	
24	W	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	X	1	Total	C	O	0
			43	40	3	
24	A	1	Total	C	O	0
			43	40	3	
24	A	1	Total	C	O	0
			43	40	3	
24	A	1	Total	C	O	0
			43	40	3	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total 66	C 51	O 15	0
25	F	1	Total 34	C 29	O 5	0
25	O	1	Total 60	C 45	O 15	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



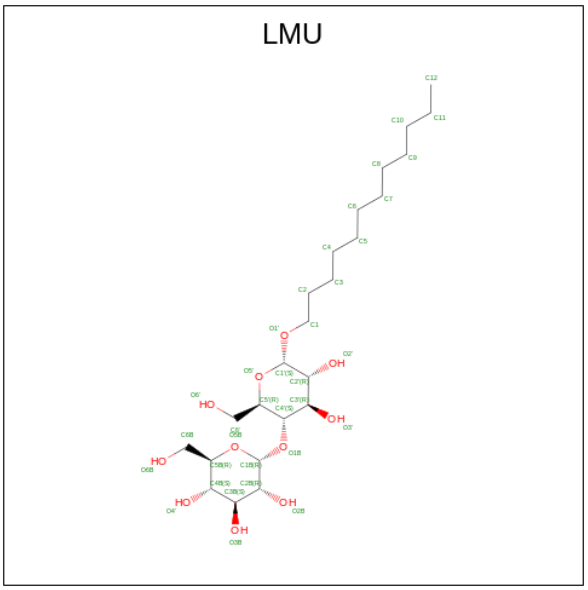
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			42	31	10	1	
26	G	1	Total	C	O	P	0
			32	21	10	1	
26	H	1	Total	C	O	P	0
			27	16	10	1	
26	K	1	Total	C	O	P	0
			39	28	10	1	
26	K	1	Total	C	O	P	0
			33	22	10	1	
26	L	1	Total	C	O	P	0
			42	31	10	1	
26	N	1	Total	C	O	P	0
			28	17	10	1	
26	N	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			34	23	10	1	
26	O	1	Total	C	O	P	0
			49	38	10	1	
26	O	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			42	31	10	1	
26	P	1	Total	C	O	P	0
			40	29	10	1	
26	Q	1	Total	C	O	P	0
			44	33	10	1	
26	R	1	Total	C	O	P	0
			42	31	10	1	
26	S	1	Total	C	O	P	0
			32	21	10	1	
26	T	1	Total	C	O	P	0
			42	31	10	1	
26	U	1	Total	C	O	P	0
			25	16	8	1	
26	W	1	Total	C	O	P	0
			42	31	10	1	
26	X	1	Total	C	O	P	0
			42	31	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			19	14	5	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			15	14	1	
27	F	1	Total	C	O	0
			21	15	6	
27	F	1	Total	C	O	0
			21	15	6	
27	G	1	Total	C	O	0
			21	15	6	

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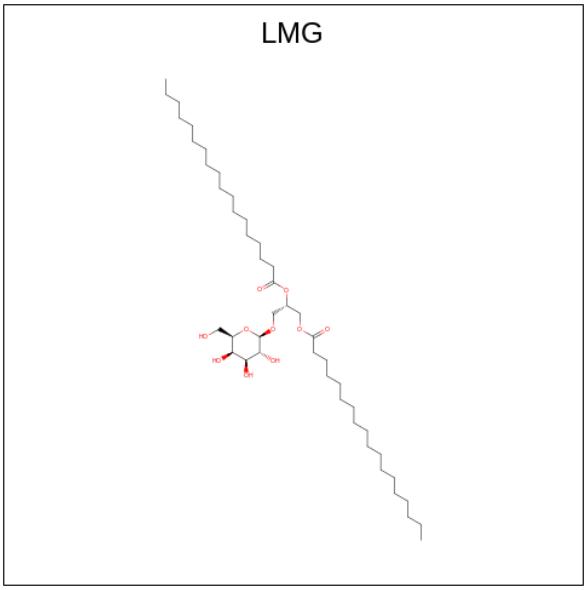
Mol	Chain	Residues	Atoms			AltConf
27	H	1	Total	C	O	0
			21	15	6	
27	H	1	Total	C	O	0
			24	18	6	
27	H	1	Total	C	O	0
			33	23	10	
27	J	1	Total	C	O	0
			34	24	10	
27	K	1	Total	C	O	0
			33	23	10	
27	L	1	Total	C	O	0
			24	18	6	
27	L	1	Total	C	O	0
			27	21	6	
27	L	1	Total	C	O	0
			34	24	10	
27	M	1	Total	C	O	0
			24	18	6	
27	O	1	Total	C	O	0
			24	18	6	
27	O	1	Total	C	O	0
			35	24	11	
27	O	1	Total	C	O	0
			26	22	4	
27	O	1	Total	C	O	0
			35	24	11	
27	T	1	Total	C	O	0
			21	15	6	
27	T	1	Total	C	O	0
			24	18	6	
27	T	1	Total	C	O	0
			24	18	6	
27	U	1	Total	C	O	0
			35	24	11	
27	U	1	Total	C	O	0
			35	24	11	
27	U	1	Total	C	O	0
			24	18	6	
27	W	1	Total	C	O	0
			24	18	6	
27	X	1	Total	C	O	0
			24	18	6	

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Mol	Chain	Residues	Atoms	AltConf
27	X	1	Total C O 35 24 11	0
27	A	1	Total C O 24 18 6	0
27	A	1	Total C O 35 24 11	0
27	A	1	Total C O 21 15 6	0
27	A	1	Total C O 24 18 6	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



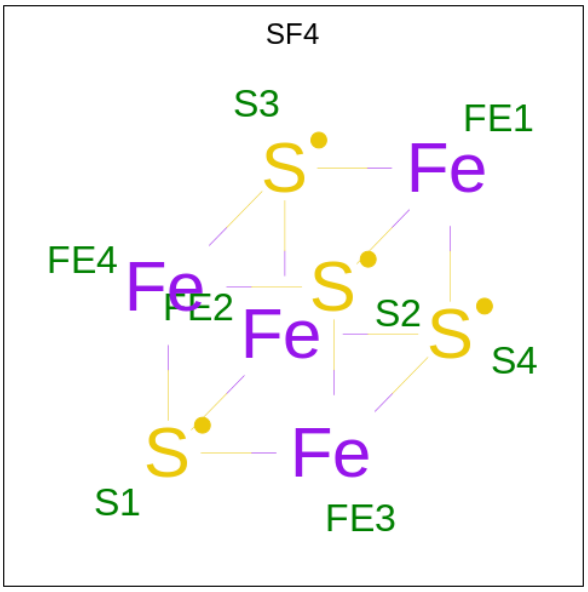
Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C O 43 33 10	0
28	B	1	Total C O 53 43 10	0
28	F	1	Total C O 42 32 10	0
28	G	1	Total C O 46 36 10	0
28	H	1	Total C O 43 33 10	0
28	H	1	Total C O 40 30 10	0

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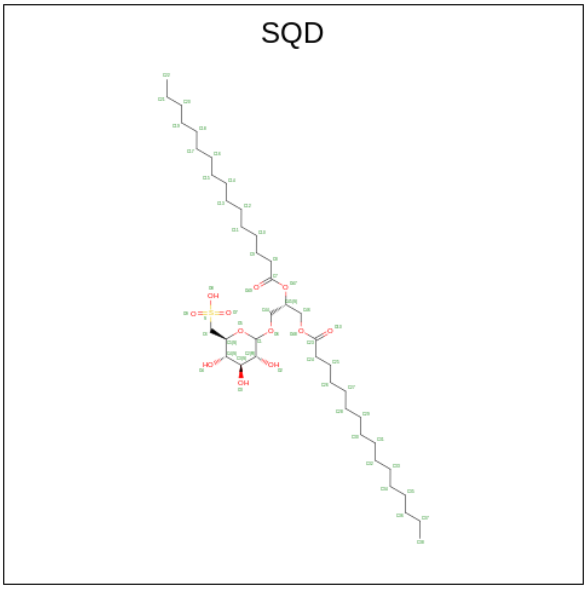
Mol	Chain	Residues	Atoms	AltConf
28	H	1	Total C O 37 27 10	0
28	I	1	Total C O 37 27 10	0
28	I	1	Total C O 50 41 9	0
28	J	1	Total C O 55 45 10	0
28	K	1	Total C O 43 33 10	0
28	K	1	Total C O 49 39 10	0
28	K	1	Total C O 43 33 10	0
28	L	1	Total C O 51 41 10	0
28	N	1	Total C O 44 34 10	0
28	Q	1	Total C O 37 27 10	0
28	T	1	Total C O 41 31 10	0
28	U	1	Total C O 53 43 10	0
28	U	1	Total C O 49 39 10	0
28	W	1	Total C O 48 38 10	0
28	A	1	Total C O 41 31 10	0

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



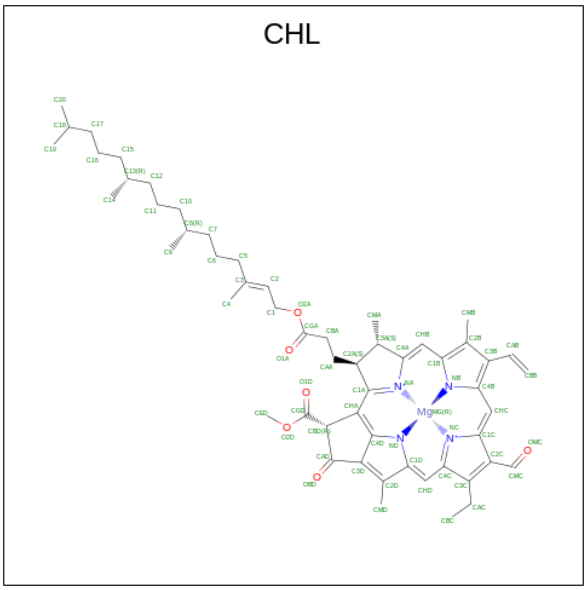
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	F	1	Total	C	O	S	0
			42	29	12	1	
30	K	1	Total	C	O	S	0
			43	30	12	1	
30	O	1	Total	C	O	S	0
			42	29	12	1	
30	V	1	Total	C	O	S	0
			27	16	10	1	

- Molecule 31 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



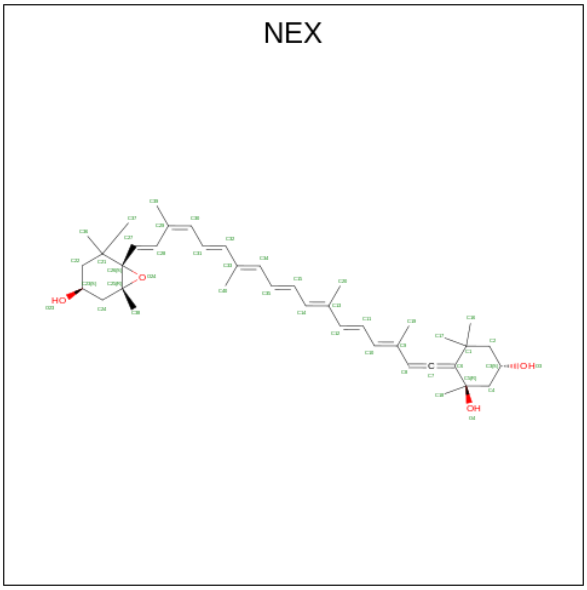
Mol	Chain	Residues	Atoms					AltConf
31	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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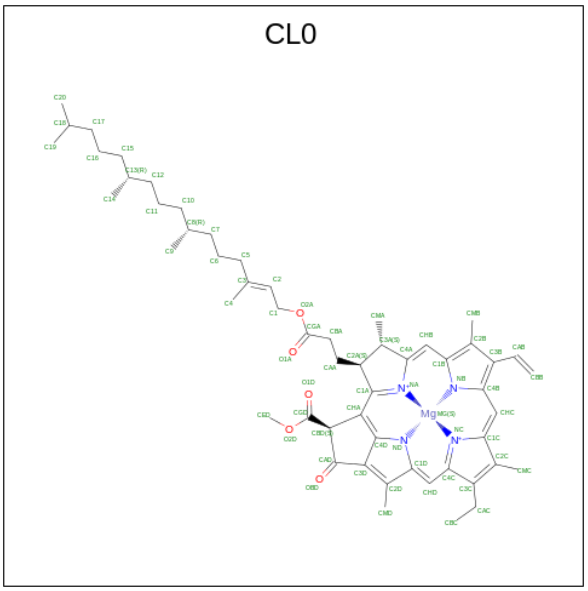
Mol	Chain	Residues	Atoms					AltConf
31	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 32 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
32	U	1	Total	C	O	0
			44	40	4	
32	V	1	Total	C	O	0
			44	40	4	

- Molecule 33 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



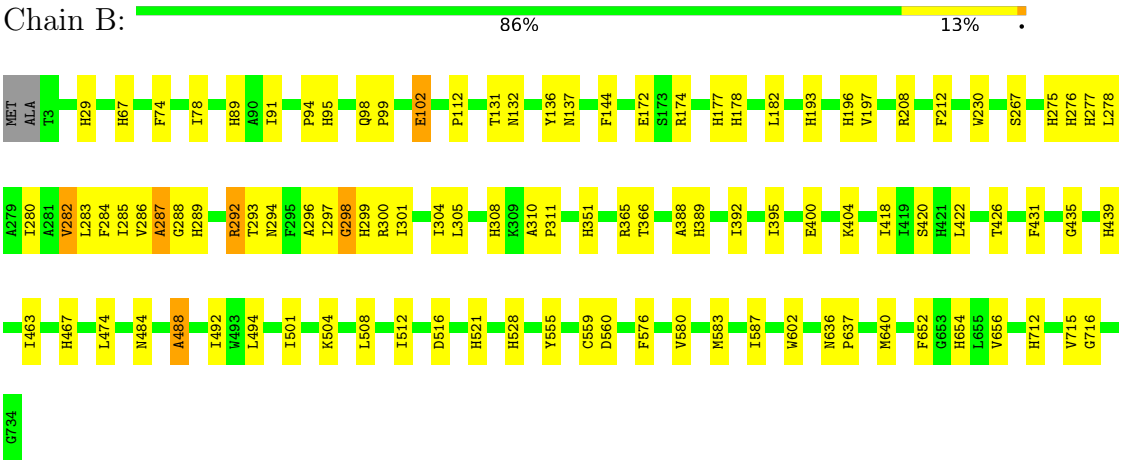
Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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.

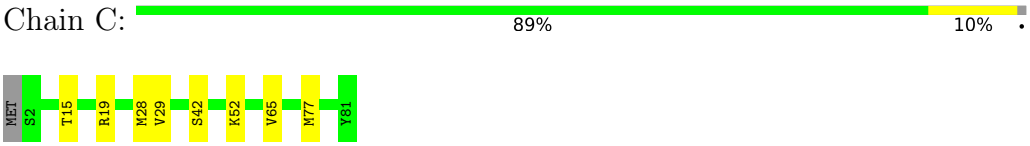
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



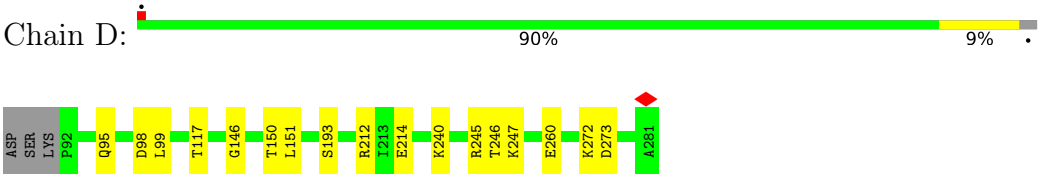
• Molecule 2: Photosystem I iron-sulfur center

Chain C:



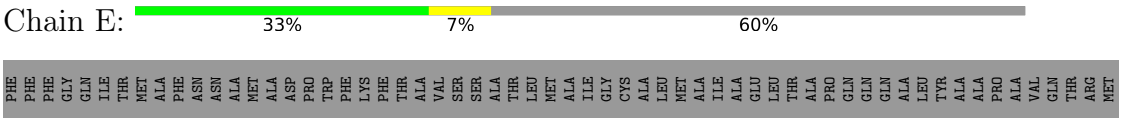
• Molecule 3: PsaD

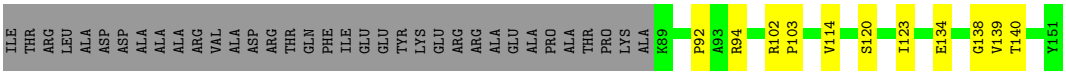
Chain D:



• Molecule 4: PsaE

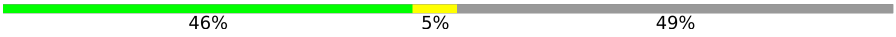
Chain E:

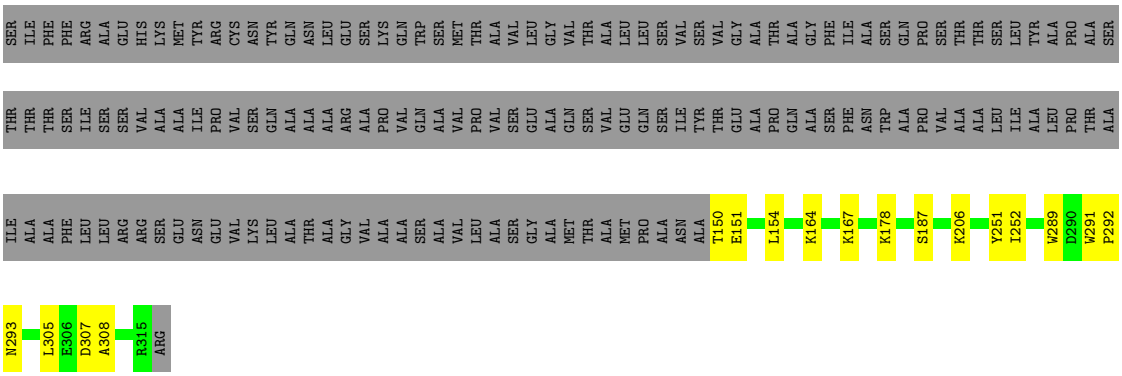




• Molecule 5: PsaF

Chain F:





• Molecule 6: Lhce5.7

Chain G:

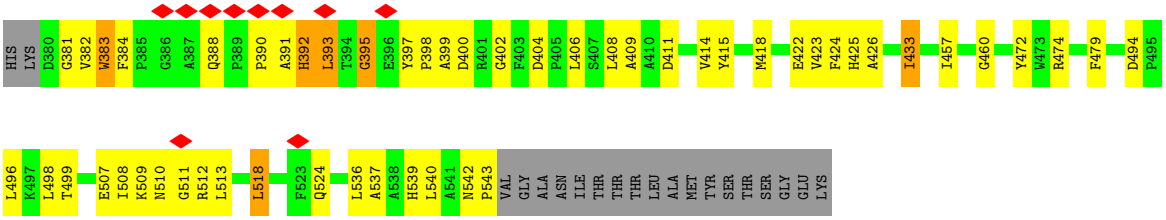




• Molecule 6: Lhce5.7

Chain P:

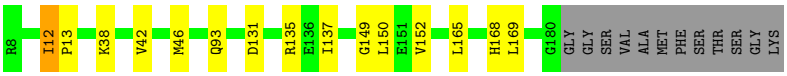




• Molecule 7: Lhce7.3

Chain H:





• Molecule 8: Lhce5

Chain I:



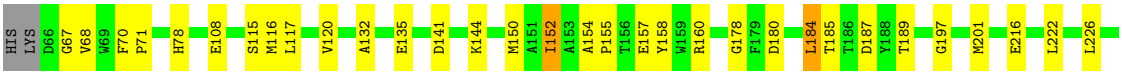


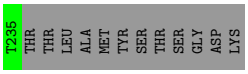


• Molecule 8: Lhce5

Chain N:







• Molecule 9: PsaJ

Chain J:





• Molecule 10: LhcE6

Chain K:

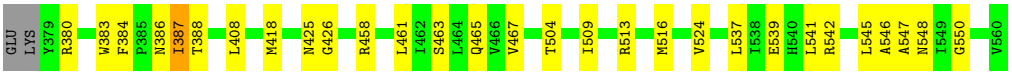




• Molecule 10: LhcE6

Chain Q:

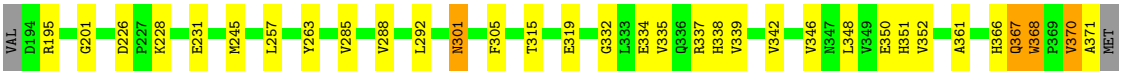


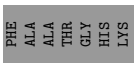


• Molecule 11: Lhce8

Chain L:



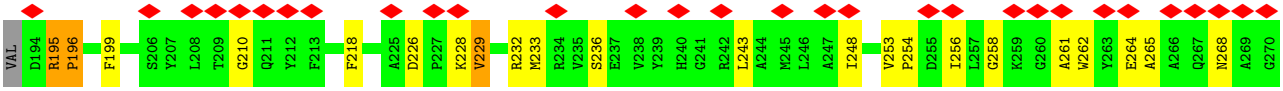


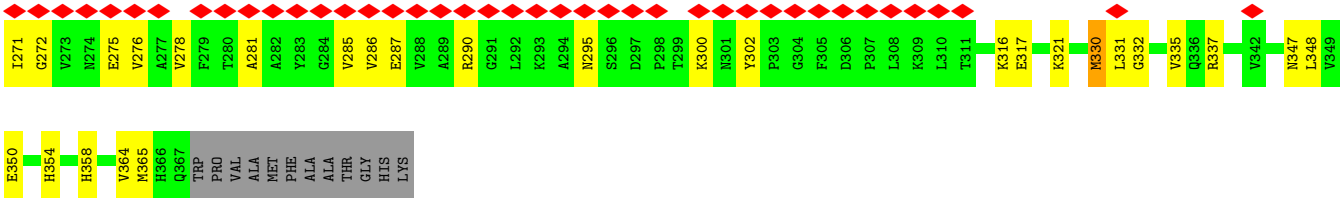


• Molecule 11: Lhce8

Chain R:







• Molecule 12: PsaM

Chain M:





• Molecule 13: LhcE7

Chain O:





• Molecule 14: Lhce10

Chain S:





• Molecule 15: Lhce11

Chain T:

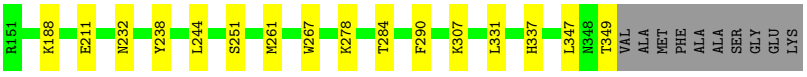




• Molecule 16: LhcbM4.6

Chain U:

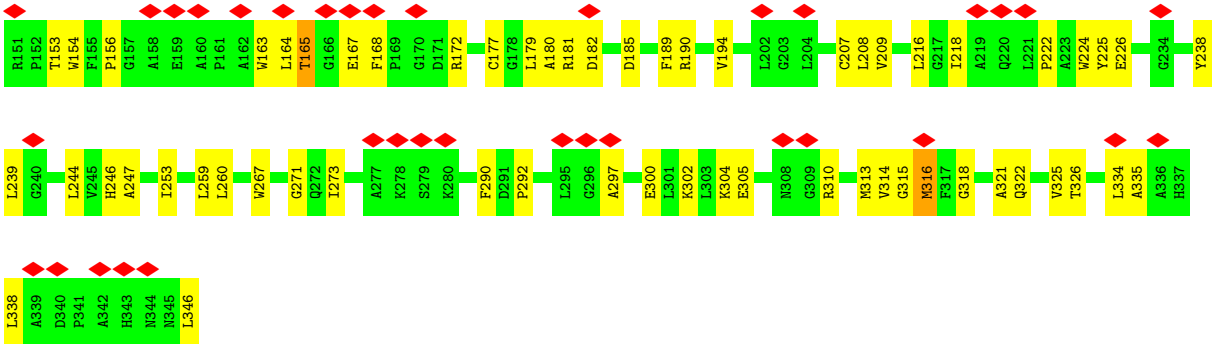




• Molecule 17: LhcbM4.10

Chain V:

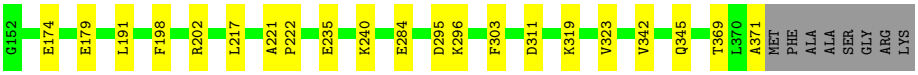




• Molecule 18: LhcbM2

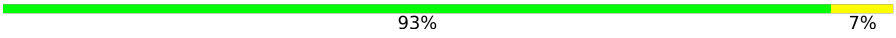
Chain W:





• Molecule 19: LhcbM8

Chain X:





• Molecule 20: PsaA

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51871	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 ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	496.64, 496.64, 496.64	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LMU, CLA, LHG, CL0, CHL, LMG, BCR, NEX, PQN, DD6, SF4, SQD

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	B	0.35	1/6078 (0.0%)	0.49	4/8287 (0.0%)
2	C	0.33	0/606	0.53	0/819
3	D	0.14	0/1525	0.38	0/2065
4	E	0.13	0/521	0.31	0/707
5	F	0.17	0/1288	0.46	0/1747
6	G	0.17	0/1360	0.39	0/1855
6	P	0.41	0/1279	0.68	1/1744 (0.1%)
7	H	0.32	0/1381	0.52	3/1876 (0.2%)
8	I	0.31	0/1278	0.56	0/1741
8	N	0.24	0/1307	0.46	0/1784
9	J	0.14	0/314	0.32	0/429
10	K	0.21	0/1492	0.49	0/2035
10	Q	0.20	0/1489	0.48	0/2034
11	L	0.35	0/1401	0.58	2/1910 (0.1%)
11	R	0.16	0/1365	0.41	0/1858
12	M	0.13	0/246	0.32	0/332
13	O	0.20	0/1397	0.46	0/1898
14	S	0.26	0/1370	0.46	0/1865
15	T	0.16	0/1320	0.40	0/1784
16	U	0.15	0/1566	0.37	0/2141
17	V	0.14	0/1566	0.33	0/2141
18	W	0.16	0/1719	0.38	0/2343
19	X	0.17	0/1731	0.37	0/2351
20	A	0.35	0/6073	0.49	1/8279 (0.0%)
All	All	0.27	1/39672 (0.0%)	0.47	11/54025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	ALA	CA-C	-6.82	1.46	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	395	GLY	N-CA-C	-9.42	102.67	114.92
1	B	298	GLY	N-CA-C	8.87	120.52	111.56
1	B	287	ALA	N-CA-C	-6.79	102.39	111.96
7	H	149	GLY	O-C-N	-6.78	115.67	122.18
7	H	152	VAL	CB-CA-C	-5.83	104.18	112.22
1	B	282	VAL	N-CA-C	-5.81	97.26	109.34
11	L	361	ALA	N-CA-C	5.73	117.61	111.36
11	L	332	GLY	O-C-N	-5.67	116.24	122.24
20	A	446	ILE	O-C-N	-5.62	116.41	121.91
7	H	150	LEU	N-CA-C	5.60	118.15	111.71
1	B	292	ARG	N-CA-C	5.53	117.67	110.43

There are no chirality outliers.

There are no planarity outliers.

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	B	5868	0	5667	91	0
2	C	596	0	571	6	0
3	D	1489	0	1462	9	0
4	E	509	0	489	5	0
5	F	1262	0	1293	10	0
6	G	1323	0	1305	15	0
6	P	1243	0	1218	39	0
7	H	1342	0	1315	9	0
8	I	1242	0	1213	25	0
8	N	1271	0	1245	27	0
9	J	305	0	314	4	0
10	K	1444	0	1391	17	0
10	Q	1440	0	1388	26	0
11	L	1364	0	1346	27	0
11	R	1331	0	1315	45	0
12	M	242	0	258	8	0
13	O	1359	0	1328	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	S	1327	0	1271	18	0
15	T	1283	0	1238	6	0
16	U	1517	0	1466	14	0
17	V	1513	0	1467	56	0
18	W	1669	0	1647	15	0
19	X	1688	0	1693	10	0
20	A	5872	0	5735	55	0
21	A	160	0	224	8	0
21	B	240	0	336	21	0
21	J	40	0	56	1	0
21	M	40	0	56	3	0
22	A	2638	0	2742	77	0
22	B	2341	0	2395	78	0
22	F	165	0	154	6	0
22	G	571	0	498	10	0
22	H	698	0	626	10	0
22	I	567	0	490	17	0
22	J	50	0	39	1	0
22	K	765	0	758	33	0
22	L	703	0	694	30	0
22	N	570	0	504	19	0
22	O	651	0	585	20	0
22	P	446	0	326	10	0
22	Q	738	0	655	20	0
22	R	678	0	653	29	0
22	S	621	0	530	14	0
22	T	625	0	603	10	0
22	U	676	0	586	14	0
22	V	625	0	548	32	0
22	W	733	0	694	18	0
22	X	741	0	716	7	0
23	A	33	0	46	2	0
23	B	33	0	46	1	0
24	A	129	0	0	0	0
24	B	43	0	0	1	0
24	F	43	0	0	0	0
24	G	86	0	0	0	0
24	H	86	0	0	0	0
24	I	86	0	0	0	0
24	J	43	0	0	0	0
24	K	86	0	0	0	0
24	L	129	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	N	86	0	0	0	0
24	O	86	0	0	0	0
24	P	86	0	0	0	0
24	Q	86	0	0	1	0
24	R	86	0	0	0	0
24	S	86	0	0	1	0
24	T	86	0	0	0	0
24	U	86	0	0	0	0
24	V	86	0	0	0	0
24	W	129	0	0	0	0
24	X	172	0	0	0	0
25	B	66	0	96	6	0
25	F	34	0	50	2	0
25	O	60	0	81	3	0
26	A	98	0	148	3	0
26	B	69	0	81	8	0
26	G	32	0	34	0	0
26	H	27	0	24	0	0
26	K	72	0	84	3	0
26	L	42	0	57	3	0
26	N	71	0	82	2	0
26	O	168	0	228	4	0
26	P	40	0	53	1	0
26	Q	44	0	61	1	0
26	R	42	0	57	3	0
26	S	32	0	34	2	0
26	T	42	0	57	1	0
26	U	25	0	21	0	0
26	W	42	0	57	2	0
26	X	42	0	57	0	0
27	A	104	0	142	2	0
27	B	165	0	233	10	0
27	F	42	0	52	1	0
27	G	21	0	26	0	0
27	H	78	0	103	2	0
27	J	34	0	44	0	0
27	K	33	0	42	2	0
27	L	85	0	110	6	0
27	M	24	0	35	1	0
27	O	120	0	155	4	0
27	T	69	0	96	2	0
27	U	94	0	127	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	W	24	0	35	0	0
27	X	59	0	81	0	0
28	A	41	0	52	0	0
28	B	96	0	138	4	0
28	F	42	0	54	3	0
28	G	46	0	65	0	0
28	H	120	0	150	2	0
28	I	87	0	117	1	0
28	J	55	0	86	1	0
28	K	135	0	183	3	0
28	L	51	0	75	0	0
28	N	44	0	61	1	0
28	Q	37	0	44	2	0
28	T	41	0	52	2	0
28	U	102	0	150	4	0
28	W	48	0	69	3	0
29	B	8	0	0	0	0
29	C	16	0	0	0	0
30	F	42	0	48	2	0
30	K	43	0	50	1	0
30	O	42	0	48	8	0
30	V	27	0	25	1	0
31	U	92	0	62	7	0
31	V	92	0	62	14	0
31	W	178	0	171	10	0
31	X	46	0	31	0	0
32	U	44	0	56	4	0
32	V	44	0	56	9	0
33	A	65	0	72	6	0
All	All	60137	0	57815	901	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (901) 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:B:840:PQN:H291	25:B:847:DGD:HBT1	1.23	1.10
31:V:605:CHL:HAB	31:V:606:CHL:OMC	1.50	1.08
8:N:184:LEU:HD12	22:N:607:CLA:H42	1.41	1.01
6:P:391:ALA:HB2	6:P:404:ASP:HB3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:THR:HB	12:M:1:MET:HE1	1.46	0.94
28:F:408:LMG:H122	22:W:402:CLA:HAB	1.55	0.89
13:O:135:PHE:HE2	30:O:302:SQD:H82	1.38	0.89
13:O:135:PHE:CE2	30:O:302:SQD:H82	2.09	0.88
11:L:315:THR:HG21	22:L:408:CLA:H12	1.54	0.87
22:L:404:CLA:HMC1	22:L:417:CLA:HBB2	1.57	0.87
33:A:802:CL0:H2	33:A:802:CL0:H15	1.57	0.85
1:B:293:THR:HG22	1:B:294:ASN:H	1.41	0.85
31:V:605:CHL:CAB	31:V:606:CHL:OMC	2.24	0.84
17:V:273:ILE:HG21	32:V:616:NEX:H172	1.60	0.83
22:V:604:CLA:C1C	32:V:616:NEX:H222	2.08	0.83
22:L:404:CLA:CMC	22:L:417:CLA:CBB	2.57	0.83
8:I:222:LEU:HD11	22:I:611:CLA:HBC2	1.62	0.82
14:S:223:VAL:HG21	22:S:610:CLA:HAC2	1.62	0.81
22:V:604:CLA:CHC	32:V:616:NEX:H362	2.12	0.80
11:R:233:MET:HE1	22:R:602:CLA:H3A	1.63	0.79
22:B:833:CLA:H203	31:U:408:CHL:HMD1	1.67	0.77
22:A:828:CLA:HED1	22:A:836:CLA:HAB	1.65	0.76
22:L:404:CLA:HMC1	22:L:417:CLA:CBB	2.16	0.76
12:M:20:PHE:CD2	22:O:311:CLA:H42	2.21	0.75
28:K:601:LMG:H302	22:K:613:CLA:HMA2	1.69	0.75
20:A:408:HIS:HE1	22:A:831:CLA:NA	1.85	0.74
6:P:388:GLN:O	6:P:390:PRO:HD3	1.87	0.74
22:B:822:CLA:HAB	22:B:829:CLA:HMD1	1.69	0.74
8:I:65:LYS:HE2	8:I:65:LYS:H	1.53	0.74
1:B:95:HIS:HE1	22:B:809:CLA:NB	1.83	0.73
8:I:158:TYR:CE2	22:K:607:CLA:HBA1	2.24	0.73
22:A:819:CLA:HBB1	22:A:819:CLA:HHC	1.69	0.73
11:L:315:THR:CG2	22:L:408:CLA:H12	2.18	0.73
31:V:605:CHL:CMC	31:V:606:CHL:C4C	2.67	0.73
22:L:404:CLA:HMC3	22:L:417:CLA:CBB	2.18	0.72
17:V:305:GLU:OE2	22:V:609:CLA:NB	2.22	0.72
6:P:383:TRP:HE3	6:P:384:PHE:H	1.35	0.72
3:D:212:ARG:NH2	3:D:214:GLU:OE2	2.23	0.72
1:B:292:ARG:HD3	1:B:300:ARG:HD3	1.70	0.72
1:B:389:HIS:HE1	22:B:828:CLA:NA	1.88	0.71
8:I:193:GLU:OE2	22:I:607:CLA:NB	2.24	0.71
11:R:195:ARG:HH21	11:R:210:GLY:H	1.38	0.71
20:A:121:ILE:HG13	20:A:122:VAL:HG13	1.72	0.71
1:B:230:TRP:HB2	22:B:815:CLA:H12	1.72	0.70
31:V:605:CHL:C1C	31:V:606:CHL:HBC2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:335:VAL:HG11	22:R:610:CLA:HAC2	1.71	0.70
8:N:68:VAL:HG12	8:N:70:PHE:H	1.57	0.70
1:B:292:ARG:HD3	1:B:300:ARG:CD	2.22	0.69
5:F:307:ASP:OD2	5:F:308:ALA:N	2.25	0.69
28:H:319:LMG:H132	30:K:621:SQD:H121	1.75	0.69
8:N:160:ARG:NH2	22:N:606:CLA:O1D	2.25	0.69
17:V:334:LEU:HD11	22:V:613:CLA:HBB1	1.75	0.69
1:B:178:HIS:CD2	22:B:812:CLA:NB	2.61	0.69
10:K:390:PRO:HG2	10:K:393:LEU:HD12	1.74	0.69
20:A:94:HIS:HE1	22:A:809:CLA:NA	1.91	0.68
22:N:610:CLA:HBA1	22:N:610:CLA:HBD	1.75	0.68
11:R:232:ARG:HB3	11:R:295:ASN:HD22	1.58	0.68
22:R:604:CLA:H3A	22:R:605:CLA:H152	1.74	0.68
1:B:282:VAL:HG13	24:B:841:DD6:C7	2.23	0.67
22:K:613:CLA:H42	22:L:417:CLA:OBD	1.94	0.67
22:A:811:CLA:HBD	22:A:811:CLA:HBA1	1.77	0.67
1:B:292:ARG:HH21	1:B:296:ALA:HA	1.60	0.67
10:Q:418:MET:HE1	22:Q:604:CLA:H43	1.75	0.67
1:B:287:ALA:O	1:B:289:HIS:N	2.27	0.67
6:P:537:ALA:O	6:P:540:LEU:HB3	1.95	0.67
11:R:229:VAL:HA	11:R:232:ARG:HG2	1.76	0.67
22:A:822:CLA:H171	22:A:832:CLA:HBC1	1.77	0.67
8:I:65:LYS:HE2	8:I:65:LYS:N	2.09	0.66
2:C:15:THR:HG22	2:C:28:MET:HE2	1.78	0.66
17:V:315:GLY:HA2	22:V:612:CLA:HBB1	1.76	0.66
22:Q:610:CLA:NB	26:Q:616:LHG:O4	2.29	0.66
28:N:615:LMG:H211	22:O:315:CLA:HBB1	1.76	0.66
1:B:94:PRO:HB3	27:B:854:LMU:H51	1.78	0.66
22:G:603:CLA:H93	22:K:603:CLA:H112	1.78	0.66
10:K:496:PRO:HA	27:K:620:LMU:H3'	1.77	0.66
6:P:381:GLY:HA3	22:P:608:CLA:HBB1	1.77	0.66
12:M:24:LYS:HE3	27:M:102:LMU:H6E	1.79	0.65
11:R:272:GLY:H	11:R:275:GLU:HB2	1.61	0.65
10:Q:425:ASN:HD22	22:Q:604:CLA:HBB2	1.61	0.65
28:T:616:LMG:H371	22:A:816:CLA:H141	1.76	0.65
20:A:704:HIS:HE1	22:A:841:CLA:C4D	2.10	0.65
26:B:851:LHG:H131	27:L:419:LMU:H12	1.78	0.65
6:P:411:ASP:HB3	6:P:414:VAL:HG12	1.79	0.65
22:V:604:CLA:NC	32:V:616:NEX:H222	2.11	0.64
6:P:399:ALA:O	22:P:602:CLA:HED1	1.96	0.64
22:N:606:CLA:HHC	22:N:606:CLA:HBB1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:233:MET:CE	22:R:602:CLA:H3A	2.28	0.64
13:O:135:PHE:CZ	30:O:302:SQD:H111	2.34	0.63
6:P:391:ALA:HB2	6:P:404:ASP:CB	2.25	0.63
20:A:704:HIS:HE1	22:A:841:CLA:ND	1.97	0.63
6:P:474:ARG:HH12	22:P:606:CLA:HED1	1.62	0.63
6:G:426:ALA:HB1	6:G:511:GLY:HA3	1.81	0.63
13:O:100:LEU:CD2	22:V:603:CLA:H43	2.27	0.63
22:W:412:CLA:H8	22:W:413:CLA:C4D	2.26	0.63
10:K:544:PRO:HB2	10:K:545:LEU:HD13	1.81	0.62
20:A:329:HIS:HD2	22:A:824:CLA:NB	1.97	0.62
1:B:144:PHE:HB2	28:B:856:LMG:H222	1.80	0.62
19:X:301:HIS:CD2	22:X:413:CLA:NC	2.67	0.62
22:A:840:CLA:H122	21:A:849:BCR:H312	1.82	0.62
11:L:231:GLU:N	11:L:231:GLU:OE1	2.31	0.62
17:V:156:PRO:HG2	22:V:601:CLA:HBB1	1.82	0.62
1:B:287:ALA:C	1:B:289:HIS:H	2.08	0.61
5:F:293:ASN:ND2	22:W:410:CLA:O1A	2.31	0.61
31:V:605:CHL:C2C	31:V:606:CHL:HBC2	2.29	0.61
22:B:833:CLA:H203	31:U:408:CHL:CMD	2.29	0.61
31:V:605:CHL:HAB	31:V:606:CHL:CMC	2.27	0.61
22:K:607:CLA:HHC	22:K:607:CLA:HBB1	1.82	0.61
11:R:302:TYR:OH	11:R:316:LYS:NZ	2.28	0.61
22:B:859:CLA:HBA1	22:B:859:CLA:HBD	1.83	0.61
7:H:12:ILE:HG13	7:H:13:PRO:HD2	1.82	0.61
8:I:195:LYS:HB3	22:I:608:CLA:HMD2	1.83	0.61
15:T:372:LEU:HB2	15:T:374:MET:HE2	1.83	0.61
27:H:321:LMU:H123	22:A:824:CLA:H203	1.82	0.61
19:X:211:LYS:H	22:X:419:CLA:HBB1	1.65	0.61
11:R:253:VAL:HG11	22:R:604:CLA:HAC2	1.83	0.60
8:I:154:ALA:HA	22:I:606:CLA:HAB	1.82	0.60
1:B:196:HIS:HE1	22:B:814:CLA:C1C	2.05	0.60
8:I:201:MET:HE1	22:I:602:CLA:HAB	1.84	0.60
30:O:302:SQD:O7	10:Q:545:LEU:HB2	2.01	0.60
1:B:560:ASP:OD1	2:C:52:LYS:NZ	2.30	0.60
7:H:42:VAL:O	7:H:46:MET:HG2	2.01	0.60
22:P:608:CLA:HBD	22:P:609:CLA:HMD3	1.84	0.59
17:V:335:ALA:HA	17:V:338:LEU:HD12	1.84	0.59
11:R:261:ALA:O	11:R:265:ALA:N	2.29	0.59
11:R:233:MET:HA	11:R:236:SER:HB3	1.85	0.59
19:X:257:LYS:HA	19:X:257:LYS:HE2	1.82	0.59
27:L:420:LMU:H51	22:A:834:CLA:HBB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:334:GLU:O	11:L:334:GLU:HG3	2.02	0.59
22:Q:607:CLA:HBB1	11:R:199:PHE:CE1	2.38	0.59
17:V:322:GLN:NE2	22:V:612:CLA:O1D	2.36	0.59
18:W:179:GLU:OE2	18:W:179:GLU:N	2.30	0.59
22:A:839:CLA:HBC2	27:A:854:LMU:H91	1.85	0.59
17:V:179:LEU:HD13	22:V:602:CLA:H42	1.85	0.59
22:B:829:CLA:HBB1	22:B:829:CLA:HMB1	1.85	0.59
7:H:38:LYS:HE2	7:H:38:LYS:HA	1.85	0.58
14:S:208:ILE:HD12	14:S:208:ILE:H	1.68	0.58
17:V:165:THR:OG1	17:V:167:GLU:OE2	2.20	0.58
17:V:207:CYS:HG	17:V:224:TRP:CD1	2.22	0.58
31:V:605:CHL:HMC	31:V:606:CHL:C1C	2.34	0.58
8:I:150:MET:HE1	28:K:601:LMG:H172	1.85	0.58
13:O:106:VAL:O	13:O:110:MET:HG2	2.03	0.58
6:G:446:ALA:HB3	6:G:449:GLU:HG2	1.86	0.58
13:O:177:ASP:OD1	13:O:177:ASP:N	2.36	0.57
6:P:460:GLY:C	10:Q:461:LEU:HD21	2.29	0.57
13:O:179:PRO:HD3	10:Q:386:ASN:O	2.03	0.57
1:B:275:HIS:HE1	22:B:815:CLA:C4D	2.18	0.57
8:I:64:HIS:N	8:I:65:LYS:HZ3	2.02	0.57
1:B:193:HIS:HB2	22:B:813:CLA:CHC	2.34	0.57
1:B:712:HIS:HE1	22:B:838:CLA:ND	2.02	0.57
22:V:612:CLA:H62	22:V:612:CLA:H193	1.86	0.57
22:B:802:CLA:HMB2	22:A:804:CLA:OBD	2.05	0.57
22:R:610:CLA:HAB	22:R:610:CLA:H121	1.87	0.57
11:R:226:ASP:HB3	11:R:229:VAL:HB	1.86	0.57
21:B:801:BCR:HC8	21:B:801:BCR:H331	1.86	0.57
31:V:605:CHL:HMC	31:V:606:CHL:NC	2.20	0.57
8:N:154:ALA:HB3	8:N:155:PRO:HD3	1.87	0.57
1:B:463:ILE:HD11	22:B:834:CLA:H2	1.87	0.56
10:K:523:GLU:OE2	22:K:617:CLA:NA	2.38	0.56
8:N:184:LEU:HG	22:N:607:CLA:H11	1.87	0.56
8:N:197:GLY:O	8:N:201:MET:HG3	2.05	0.56
22:G:608:CLA:H71	22:G:609:CLA:C4D	2.35	0.56
11:R:331:LEU:HD21	22:R:615:CLA:H52	1.86	0.56
17:V:346:LEU:HD22	22:V:612:CLA:H43	1.87	0.56
1:B:654:HIS:NE2	22:B:802:CLA:NA	2.53	0.56
13:O:195:GLU:OE2	27:O:301:LMU:C2'	2.52	0.56
6:P:539:HIS:HA	6:P:542:ASN:CG	2.31	0.56
10:Q:461:LEU:O	10:Q:465:GLN:HG2	2.06	0.56
22:U:406:CLA:H2	31:U:407:CHL:HBD	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:150:THR:OG1	5:F:151:GLU:N	2.33	0.56
3:D:150:THR:OG1	3:D:151:LEU:N	2.39	0.56
1:B:174:ARG:O	1:B:178:HIS:HB2	2.06	0.56
6:P:393:LEU:HD11	6:P:402:GLY:HA2	1.88	0.56
6:P:542:ASN:HB2	6:P:543:PRO:HD2	1.88	0.56
1:B:29:HIS:HE1	22:B:803:CLA:NB	2.00	0.56
10:Q:504:THR:HG22	22:Q:609:CLA:HHB	1.87	0.56
20:A:37:ARG:HH22	20:A:62:HIS:HA	1.70	0.56
17:V:325:VAL:HG23	17:V:326:THR:HG23	1.88	0.56
11:R:248:ILE:HA	11:R:330:MET:HE1	1.87	0.55
1:B:488:ALA:HB2	16:U:232:ASN:OD1	2.06	0.55
8:I:183:LYS:HE2	8:I:183:LYS:N	2.20	0.55
1:B:292:ARG:NH1	1:B:292:ARG:HB3	2.21	0.55
1:B:293:THR:HG22	1:B:294:ASN:N	2.17	0.55
7:H:168:HIS:CD2	22:H:312:CLA:NC	2.74	0.55
14:S:164:MET:HB3	15:T:337:MET:HE3	1.88	0.55
4:E:134:GLU:OE2	4:E:138:GLY:HA2	2.07	0.55
9:J:37:ARG:NH2	22:J:102:CLA:O1D	2.31	0.55
14:S:220:GLY:O	14:S:224:GLN:HG3	2.07	0.55
19:X:258:ASP:OD1	19:X:259:GLU:N	2.39	0.55
31:V:605:CHL:C2C	31:V:606:CHL:CBC	2.85	0.55
22:B:830:CLA:O1A	5:F:305:LEU:HD11	2.06	0.55
6:P:433:ILE:HG12	6:P:518:LEU:HD22	1.88	0.55
26:B:851:LHG:H292	27:B:854:LMU:H12	1.89	0.54
8:N:144:LYS:HG3	13:O:149:ASN:ND2	2.22	0.54
22:O:305:CLA:HBA2	26:O:318:LHG:H251	1.89	0.54
10:K:521:GLY:O	10:K:525:GLN:HG3	2.07	0.54
6:P:398:PRO:O	6:P:399:ALA:C	2.51	0.54
6:P:391:ALA:C	6:P:392:HIS:CG	2.85	0.54
20:A:201:HIS:CD2	22:A:815:CLA:NB	2.74	0.54
10:Q:539:GLU:HG3	10:Q:547:ALA:HB1	1.90	0.54
33:A:802:CL0:CGD	33:A:802:CL0:H8	2.38	0.54
8:I:132:ALA:N	8:I:135:GLU:OE2	2.40	0.54
22:K:609:CLA:HMB2	22:A:844:CLA:H11	1.89	0.54
22:L:408:CLA:CGA	22:L:408:CLA:H3A	2.38	0.54
10:Q:548:ASN:HD21	28:Q:602:LMG:HC8	1.71	0.54
1:B:283:LEU:C	1:B:285:ILE:N	2.66	0.54
22:L:408:CLA:H43	22:L:410:CLA:H11	1.90	0.54
13:O:180:ASP:OD2	13:O:181:ARG:N	2.40	0.54
6:G:494:ASP:OD2	6:G:499:THR:OG1	2.22	0.53
22:L:404:CLA:CMC	22:L:417:CLA:HBB2	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:178:GLY:HA2	22:N:607:CLA:HED1	1.90	0.53
20:A:75:SER:OG	20:A:181:TYR:HB2	2.08	0.53
1:B:102:GLU:N	1:B:102:GLU:OE1	2.41	0.53
16:U:251:SER:HB3	22:U:401:CLA:HBD	1.89	0.53
20:A:491:HIS:HE1	22:A:836:CLA:NB	2.05	0.53
8:I:195:LYS:HE3	22:I:608:CLA:C3D	2.39	0.53
10:K:543:HIS:HB3	10:K:546:ALA:HB3	1.89	0.53
1:B:712:HIS:HE1	22:B:838:CLA:C4D	2.21	0.53
26:R:614:LHG:H112	26:R:614:LHG:H291	1.89	0.53
17:V:267:TRP:HH2	32:V:616:NEX:C19	2.21	0.53
21:B:801:BCR:H331	23:A:843:PQN:H193	1.90	0.53
26:N:614:LHG:O3	26:N:614:LHG:O1	2.24	0.53
13:O:184:PRO:HB3	22:Q:601:CLA:HBC2	1.89	0.53
22:Q:607:CLA:HBB1	11:R:199:PHE:HE1	1.74	0.53
11:L:335:VAL:O	11:L:339:VAL:HG23	2.09	0.53
22:P:602:CLA:HMB1	22:P:602:CLA:HBB1	1.90	0.53
11:R:354:HIS:HB2	11:R:358:HIS:CE1	2.43	0.53
8:N:216:GLU:N	8:N:216:GLU:OE1	2.41	0.53
1:B:431:PHE:HZ	21:B:801:BCR:H341	1.74	0.53
13:O:227:THR:O	13:O:231:GLU:HG2	2.09	0.53
22:R:605:CLA:O2A	22:R:605:CLA:H2A	2.09	0.52
33:A:802:CL0:H2	33:A:802:CL0:CBB	2.36	0.52
5:F:164:LYS:HA	5:F:167:LYS:HE2	1.90	0.52
11:L:351:HIS:CD2	22:L:412:CLA:NC	2.78	0.52
10:Q:458:ARG:NH2	11:R:364:VAL:O	2.39	0.52
18:W:303:PHE:HE1	22:W:409:CLA:HBA2	1.75	0.52
22:W:414:CLA:H202	22:W:415:CLA:HBC1	1.91	0.52
31:W:407:CHL:C3C	31:W:408:CHL:HBC3	2.39	0.52
10:K:486:LYS:HD2	10:K:486:LYS:N	2.24	0.52
11:L:301:ASN:OD1	11:L:301:ASN:N	2.39	0.52
11:L:315:THR:HG22	22:L:408:CLA:HHB	1.91	0.52
6:P:395:GLY:HA2	6:P:400:ASP:HB3	1.90	0.52
1:B:292:ARG:HG3	1:B:299:HIS:N	2.25	0.52
1:B:528:HIS:CD2	22:B:836:CLA:NB	2.77	0.52
22:B:806:CLA:H43	27:B:855:LMU:H111	1.92	0.52
6:G:530:GLU:OE1	6:G:530:GLU:N	2.43	0.52
15:T:261:LYS:H	27:A:857:LMU:H2'	1.74	0.52
28:W:401:LMG:H341	31:W:408:CHL:C4	2.39	0.52
20:A:308:ALA:HB2	22:A:822:CLA:HBC2	1.92	0.52
6:P:542:ASN:O	6:P:543:PRO:C	2.52	0.51
1:B:467:HIS:CD2	22:B:833:CLA:ND	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:189:THR:HG22	22:I:607:CLA:HHB	1.91	0.51
33:A:802:CL0:H13	22:A:852:CLA:OBD	2.09	0.51
1:B:278:LEU:O	1:B:278:LEU:HG	2.09	0.51
1:B:418:ILE:HG23	22:B:836:CLA:HBB2	1.91	0.51
6:G:546:ALA:HB1	22:G:610:CLA:HED1	1.92	0.51
17:V:224:TRP:CZ3	31:V:606:CHL:HMA1	2.45	0.51
1:B:512:ILE:HG22	1:B:516:ASP:OD2	2.10	0.51
6:P:457:ILE:HG23	10:Q:461:LEU:HD12	1.92	0.51
10:Q:425:ASN:ND2	22:Q:604:CLA:HBB2	2.24	0.51
31:V:605:CHL:HBC2	31:V:606:CHL:HBC3	1.92	0.51
1:B:285:ILE:HG22	1:B:285:ILE:O	2.10	0.51
30:O:302:SQD:H132	22:O:308:CLA:CBC	2.41	0.51
6:P:382:VAL:HG22	6:P:383:TRP:CD2	2.45	0.51
20:A:57:HIS:HE1	22:A:806:CLA:NB	2.05	0.51
20:A:199:ASN:HB3	22:A:821:CLA:HMD1	1.93	0.51
6:P:539:HIS:O	6:P:540:LEU:C	2.54	0.51
11:R:236:SER:HB2	22:R:606:CLA:HED3	1.91	0.51
17:V:189:PHE:CD2	22:V:602:CLA:H12	2.46	0.51
30:O:302:SQD:H132	22:O:308:CLA:HBC2	1.93	0.51
10:K:492:PRO:HB3	22:K:606:CLA:HBC2	1.92	0.51
14:S:104:THR:O	14:S:108:MET:HG2	2.11	0.50
22:A:806:CLA:HBD	22:A:813:CLA:H2	1.92	0.50
1:B:299:HIS:HD1	1:B:304:ILE:HD11	1.76	0.50
21:B:843:BCR:H311	22:Q:613:CLA:HBB2	1.94	0.50
6:P:414:VAL:HG22	6:P:418:MET:SD	2.51	0.50
17:V:318:GLY:O	17:V:322:GLN:HG3	2.12	0.50
1:B:559:CYS:SG	20:A:578:PRO:HG3	2.51	0.50
16:U:267:TRP:HH2	32:U:418:NEX:C19	2.24	0.50
22:B:815:CLA:CHA	22:B:815:CLA:HBA1	2.41	0.50
11:L:348:LEU:HD13	22:L:412:CLA:HBC2	1.93	0.50
25:O:304:DGD:O1A	25:O:304:DGD:HE5	2.11	0.50
6:P:494:ASP:OD2	6:P:499:THR:OG1	2.29	0.50
14:S:72:VAL:HG11	14:S:77:ALA:HB3	1.92	0.50
16:U:188:LYS:HZ1	22:U:405:CLA:HBA1	1.75	0.50
26:K:616:LHG:O1	26:K:616:LHG:O3	2.26	0.50
22:S:610:CLA:HBA1	22:S:610:CLA:HBD	1.92	0.50
10:Q:524:VAL:HG11	22:Q:612:CLA:HAC2	1.94	0.50
22:V:601:CLA:HAA2	22:V:601:CLA:HED2	1.93	0.50
20:A:37:ARG:H	20:A:37:ARG:HD2	1.77	0.50
20:A:408:HIS:HE1	22:A:831:CLA:C4A	2.24	0.50
1:B:521:HIS:CD2	22:B:835:CLA:NB	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:50:TRP:O	20:A:51:ASN:HB2	2.12	0.50
1:B:283:LEU:O	1:B:285:ILE:N	2.46	0.49
22:L:408:CLA:H51	22:L:410:CLA:HMA3	1.92	0.49
8:N:158:TYR:CE2	22:O:309:CLA:HBA1	2.47	0.49
14:S:204:LYS:O	14:S:208:ILE:HD12	2.11	0.49
31:U:407:CHL:O2A	32:U:418:NEX:H403	2.12	0.49
13:O:229:LEU:HD13	22:O:314:CLA:HBC2	1.94	0.49
22:V:604:CLA:C1B	32:V:616:NEX:H383	2.42	0.49
11:R:243:LEU:HD13	22:R:606:CLA:HMD3	1.94	0.49
16:U:267:TRP:HH2	32:U:418:NEX:H191	1.78	0.49
1:B:297:ILE:HG13	22:B:819:CLA:HED2	1.93	0.49
11:L:370:VAL:HG22	11:L:371:ALA:N	2.27	0.49
12:M:20:PHE:CE2	22:O:311:CLA:H11	2.47	0.49
13:O:163:GLU:HG2	22:O:309:CLA:C1B	2.42	0.49
20:A:29:TRP:HH2	22:A:806:CLA:H42	1.76	0.49
22:B:830:CLA:HMB1	22:B:830:CLA:HBB1	1.94	0.49
26:B:851:LHG:H112	27:L:419:LMU:H1'	1.94	0.49
19:X:174:ALA:HB2	19:X:181:PHE:HD2	1.77	0.49
17:V:225:TYR:HA	31:V:606:CHL:CMA	2.42	0.49
22:F:403:CLA:H142	9:J:20:VAL:HG13	1.95	0.49
22:A:825:CLA:H141	26:A:846:LHG:H192	1.93	0.49
22:B:809:CLA:CMA	27:B:854:LMU:H71	2.42	0.49
28:W:401:LMG:H341	31:W:408:CHL:H42	1.95	0.49
6:G:511:GLY:O	6:G:515:MET:HG3	2.13	0.49
8:N:189:THR:HG22	22:N:607:CLA:HHB	1.94	0.49
1:B:292:ARG:HD3	1:B:300:ARG:HD2	1.95	0.49
3:D:272:LYS:HG3	3:D:273:ASP:OD2	2.13	0.49
5:F:251:TYR:CE2	22:F:404:CLA:HBA1	2.48	0.49
11:L:346:VAL:O	11:L:350:GLU:HG2	2.13	0.49
22:X:404:CLA:H13	22:X:408:CLA:H112	1.93	0.49
20:A:57:HIS:HE1	22:A:806:CLA:C4B	2.26	0.49
8:I:173:ASP:OD1	8:I:174:ARG:N	2.45	0.48
28:K:601:LMG:O5	28:K:601:LMG:O4	2.28	0.48
22:N:606:CLA:H121	22:O:315:CLA:HAB	1.94	0.48
17:V:313:MET:HE1	22:V:602:CLA:HHC	1.94	0.48
17:V:321:ALA:O	17:V:325:VAL:HG22	2.13	0.48
1:B:292:ARG:HA	1:B:297:ILE:O	2.13	0.48
22:K:605:CLA:H151	22:K:605:CLA:H112	1.53	0.48
22:R:601:CLA:O1A	26:R:614:LHG:O2	2.31	0.48
14:S:164:MET:HE2	14:S:164:MET:HA	1.94	0.48
1:B:29:HIS:HE1	22:B:803:CLA:C4B	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:F:407:SQD:H151	22:X:403:CLA:H93	1.95	0.48
18:W:284:GLU:O	18:W:296:LYS:NZ	2.39	0.48
1:B:292:ARG:HG2	1:B:298:GLY:CA	2.44	0.48
22:K:604:CLA:HED3	22:K:607:CLA:H43	1.95	0.48
11:R:347:ASN:HB3	22:R:610:CLA:HED2	1.95	0.48
22:B:809:CLA:H43	11:L:352:VAL:HG21	1.94	0.48
8:N:116:MET:O	8:N:120:VAL:HG23	2.14	0.48
22:V:608:CLA:HBA2	22:V:608:CLA:H3A	1.61	0.48
22:B:823:CLA:H171	22:B:823:CLA:H13	1.63	0.48
26:B:851:LHG:H252	27:B:854:LMU:H22	1.96	0.48
17:V:267:TRP:O	17:V:271:GLY:N	2.41	0.48
17:V:267:TRP:CD1	17:V:273:ILE:HA	2.49	0.48
1:B:172:GLU:OE2	1:B:301:ILE:HG13	2.13	0.48
11:R:254:PRO:O	11:R:258:GLY:N	2.47	0.48
26:W:420:LHG:HC81	26:W:420:LHG:H111	1.56	0.48
22:A:832:CLA:H62	26:A:846:LHG:H131	1.96	0.48
22:B:834:CLA:H142	22:B:839:CLA:H193	1.95	0.48
22:K:605:CLA:H3A	22:K:605:CLA:HBA2	1.45	0.48
13:O:195:GLU:OE2	27:O:301:LMU:H2'	2.13	0.48
6:P:496:LEU:HB2	6:P:498:LEU:HD23	1.95	0.48
19:X:197:GLU:OE1	19:X:197:GLU:N	2.41	0.48
1:B:308:HIS:HE1	22:B:821:CLA:ND	2.09	0.48
1:B:435:GLY:HA3	22:B:832:CLA:HAB	1.96	0.48
22:L:411:CLA:H2	22:L:411:CLA:H61	1.67	0.48
17:V:222:PRO:HB3	17:V:226:GLU:HB2	1.95	0.48
22:A:803:CLA:H142	21:A:851:BCR:H23C	1.96	0.48
1:B:98:GLN:HB3	1:B:99:PRO:HD3	1.96	0.47
1:B:576:PHE:O	1:B:580:VAL:HG23	2.14	0.47
22:L:402:CLA:H41	22:L:402:CLA:H61	1.48	0.47
20:A:370:HIS:CD2	22:A:828:CLA:NC	2.81	0.47
1:B:277:HIS:HA	1:B:280:ILE:HG12	1.95	0.47
1:B:286:VAL:HG12	1:B:286:VAL:O	2.14	0.47
22:B:831:CLA:H62	22:B:831:CLA:H2	1.67	0.47
6:P:424:PHE:O	6:P:425:HIS:C	2.54	0.47
22:P:605:CLA:HBA1	22:P:605:CLA:H3A	1.50	0.47
26:B:851:LHG:H262	27:B:854:LMU:H22	1.96	0.47
22:K:604:CLA:H143	22:K:604:CLA:H162	1.76	0.47
1:B:193:HIS:HB2	22:B:813:CLA:C1C	2.44	0.47
7:H:169:LEU:HD11	22:H:312:CLA:HMC2	1.96	0.47
8:I:78:HIS:NE2	8:I:90:ASP:OD2	2.41	0.47
6:P:397:TYR:O	6:P:400:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:216:LEU:HB3	17:V:218:ILE:HG12	1.97	0.47
17:V:325:VAL:HG21	22:V:612:CLA:HMD2	1.97	0.47
27:O:301:LMU:H102	22:O:312:CLA:H2	1.97	0.47
31:V:605:CHL:CMC	31:V:606:CHL:NC	2.77	0.47
20:A:393:HIS:HE1	22:A:829:CLA:C1D	2.15	0.47
1:B:74:PHE:O	1:B:78:ILE:HG12	2.14	0.47
22:F:404:CLA:H91	22:W:410:CLA:H143	1.96	0.47
11:L:305:PHE:CE2	26:O:321:LHG:H361	2.49	0.47
22:S:608:CLA:NB	26:S:613:LHG:O4	2.48	0.47
20:A:178:TRP:HB2	22:A:813:CLA:CMC	2.45	0.47
1:B:283:LEU:C	1:B:285:ILE:H	2.21	0.47
22:B:806:CLA:H2	22:B:806:CLA:H61	1.63	0.47
22:B:816:CLA:H3A	22:B:816:CLA:HBA2	1.46	0.47
22:B:822:CLA:O1A	21:B:844:BCR:H14C	2.15	0.47
22:B:834:CLA:H41	22:B:834:CLA:H61	1.67	0.47
25:B:847:DGD:HB82	25:B:847:DGD:HBE1	1.49	0.47
28:B:856:LMG:H342	28:B:856:LMG:H202	1.97	0.47
5:F:289:TRP:HE1	30:F:407:SQD:H462	1.79	0.47
25:F:401:DGD:HAF2	25:F:401:DGD:HAV2	1.63	0.47
22:F:403:CLA:H162	22:F:403:CLA:H122	1.62	0.47
8:I:155:PRO:HG2	22:K:607:CLA:H72	1.96	0.47
8:N:67:GLY:HA3	22:N:601:CLA:HED2	1.96	0.47
22:R:601:CLA:H171	22:R:601:CLA:H13	1.65	0.47
16:U:337:HIS:CD2	22:U:415:CLA:NC	2.82	0.47
17:V:154:TRP:CE3	22:V:601:CLA:HAA1	2.50	0.47
17:V:273:ILE:HD11	22:V:607:CLA:HAB	1.97	0.47
22:N:610:CLA:HBA1	22:N:610:CLA:CBD	2.43	0.47
11:R:228:LYS:H	11:R:228:LYS:HD3	1.80	0.47
18:W:319:LYS:O	18:W:323:VAL:HG23	2.14	0.47
6:G:455:ASP:OD1	6:G:455:ASP:N	2.46	0.47
22:G:608:CLA:H121	22:G:609:CLA:C4B	2.45	0.47
22:H:311:CLA:HBB1	22:H:311:CLA:H8	1.97	0.47
6:P:422:GLU:O	6:P:423:VAL:C	2.56	0.47
20:A:274:ASP:N	20:A:274:ASP:OD1	2.47	0.47
20:A:506:THR:HG22	20:A:507:THR:HG22	1.96	0.47
12:M:13:LEU:HD21	21:M:101:BCR:H281	1.96	0.47
22:O:308:CLA:H2	10:Q:550:GLY:O	2.15	0.47
15:T:261:LYS:HE2	15:T:261:LYS:HA	1.96	0.46
27:T:618:LMU:H12	22:A:812:CLA:H42	1.96	0.46
22:L:408:CLA:O1D	22:L:408:CLA:H2A	2.15	0.46
8:N:132:ALA:HB3	8:N:135:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:118:GLY:HA2	13:O:208:MET:HE2	1.97	0.46
17:V:189:PHE:HD2	22:V:602:CLA:H12	1.79	0.46
31:W:407:CHL:C1C	31:W:408:CHL:HBC2	2.45	0.46
1:B:351:HIS:HE1	22:B:825:CLA:C1B	2.13	0.46
30:O:302:SQD:H241	30:O:302:SQD:H462	1.47	0.46
11:R:350:GLU:HB3	11:R:358:HIS:CG	2.50	0.46
22:R:604:CLA:HHB	22:R:605:CLA:H152	1.97	0.46
17:V:267:TRP:HH2	32:V:616:NEX:H192	1.79	0.46
18:W:311:ASP:N	18:W:311:ASP:OD2	2.48	0.46
6:P:507:GLU:CD	22:P:607:CLA:NB	2.72	0.46
10:Q:463:SER:O	10:Q:467:VAL:HG23	2.16	0.46
22:Q:605:CLA:H61	22:Q:605:CLA:H2	1.59	0.46
11:R:365:MET:HE3	11:R:365:MET:HA	1.97	0.46
7:H:131:ASP:OD2	7:H:135:ARG:NH1	2.47	0.46
8:I:183:LYS:HE2	8:I:183:LYS:H	1.81	0.46
11:L:285:VAL:HG22	17:V:259:LEU:HA	1.98	0.46
8:N:222:LEU:O	8:N:226:LEU:HB2	2.16	0.46
11:R:264:GLU:O	11:R:268:ASN:ND2	2.48	0.46
31:V:605:CHL:CMC	31:V:606:CHL:C3C	2.93	0.46
22:A:822:CLA:H141	22:A:822:CLA:H162	1.74	0.46
22:B:807:CLA:H8	22:B:807:CLA:HBB1	1.98	0.46
25:B:847:DGD:HBW1	25:B:847:DGD:HBG3	1.97	0.46
6:G:418:MET:HE1	22:G:602:CLA:H43	1.96	0.46
22:I:611:CLA:HAC2	28:I:615:LMG:H401	1.97	0.46
22:S:605:CLA:H8	22:S:605:CLA:C2C	2.46	0.46
17:V:260:LEU:HD12	17:V:260:LEU:H	1.81	0.46
18:W:191:LEU:HD13	22:W:404:CLA:H42	1.97	0.46
1:B:132:ASN:HB2	12:M:1:MET:HE2	1.97	0.46
1:B:636:ASN:HB2	1:B:637:PRO:HD2	1.97	0.46
11:L:366:HIS:O	11:L:367:GLN:C	2.58	0.46
11:R:262:TRP:CH2	11:R:337:ARG:HD3	2.50	0.46
28:J:101:LMG:H232	28:J:101:LMG:H262	1.77	0.46
22:K:604:CLA:HMD3	22:K:607:CLA:ND	2.30	0.46
22:K:613:CLA:H2	22:K:613:CLA:H61	1.68	0.46
6:P:382:VAL:HG22	6:P:383:TRP:H	1.80	0.46
11:R:300:LYS:HD3	11:R:300:LYS:HA	1.80	0.46
20:A:730:HIS:HE1	22:A:842:CLA:C4D	2.29	0.46
1:B:395:ILE:HD12	1:B:555:TYR:HD1	1.81	0.46
1:B:422:LEU:O	1:B:426:THR:HG23	2.16	0.46
22:B:818:CLA:HBB1	22:B:818:CLA:HMB3	1.97	0.46
22:B:829:CLA:HBA2	22:B:829:CLA:H3A	1.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:508:GLU:OE2	22:K:608:CLA:NB	2.48	0.46
11:R:287:GLU:HG2	11:R:290:ARG:HH12	1.80	0.46
16:U:278:LYS:HD2	16:U:278:LYS:N	2.31	0.46
17:V:290:PHE:O	17:V:292:PRO:HD3	2.15	0.46
20:A:91:MET:HE2	20:A:91:MET:HA	1.98	0.46
1:B:292:ARG:HB3	1:B:292:ARG:CZ	2.45	0.46
27:B:854:LMU:H51	27:B:854:LMU:H22	1.82	0.46
13:O:135:PHE:CE2	30:O:302:SQD:H111	2.51	0.46
6:P:472:TYR:CE2	22:Q:608:CLA:HBA1	2.50	0.46
18:W:217:LEU:HB3	22:W:406:CLA:HMC2	1.97	0.46
21:B:845:BCR:H15C	21:B:845:BCR:H351	1.72	0.45
22:G:603:CLA:H101	22:K:603:CLA:C15	2.46	0.45
22:K:604:CLA:H91	22:K:604:CLA:H111	1.62	0.45
13:O:74:LEU:HD13	13:O:79:ALA:HB3	1.98	0.45
11:R:195:ARG:O	11:R:196:PRO:C	2.58	0.45
11:R:248:ILE:CA	11:R:330:MET:HE1	2.47	0.45
14:S:98:LEU:HD13	22:S:602:CLA:H42	1.98	0.45
17:V:247:ALA:HB1	17:V:253:ILE:HD11	1.97	0.45
20:A:37:ARG:H	20:A:37:ARG:CD	2.29	0.45
1:B:144:PHE:HD1	28:B:856:LMG:H242	1.81	0.45
27:K:620:LMU:H102	26:L:416:LHG:H141	1.98	0.45
22:L:408:CLA:HMB2	22:L:408:CLA:H2	1.98	0.45
14:S:184:GLU:C	14:S:185:LYS:HD2	2.41	0.45
18:W:371:ALA:HB2	31:W:422:CHL:HAA2	1.97	0.45
20:A:520:LYS:HE2	20:A:520:LYS:HB3	1.77	0.45
22:A:814:CLA:H161	22:A:814:CLA:H141	1.67	0.45
21:B:844:BCR:HC42	28:U:402:LMG:H182	1.99	0.45
11:L:288:VAL:O	11:L:292:LEU:HG	2.16	0.45
13:O:105:LYS:HD2	13:O:105:LYS:HA	1.65	0.45
10:Q:541:LEU:HD23	10:Q:541:LEU:HA	1.73	0.45
11:R:271:ILE:HD11	11:R:276:VAL:HG22	1.98	0.45
20:A:343:GLU:OE1	20:A:343:GLU:N	2.48	0.45
22:A:817:CLA:H141	22:A:817:CLA:H161	1.64	0.45
1:B:474:LEU:HD11	5:F:154:LEU:HD23	1.97	0.45
27:B:858:LMU:H52	27:B:858:LMU:H81	1.76	0.45
3:D:240:LYS:HE3	3:D:240:LYS:HB3	1.66	0.45
22:A:844:CLA:HBA1	22:A:844:CLA:H3A	1.45	0.45
22:B:835:CLA:HBB1	22:B:835:CLA:HMB3	1.97	0.45
10:K:474:ARG:HG3	22:K:606:CLA:CHD	2.47	0.45
22:S:605:CLA:H62	22:S:605:CLA:H41	1.75	0.45
20:A:338:HIS:CD2	22:A:825:CLA:ND	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ARG:HB3	1:B:602:TRP:CZ3	2.51	0.45
22:B:806:CLA:H141	22:B:806:CLA:H162	1.72	0.45
21:B:846:BCR:H15C	21:B:846:BCR:H351	1.85	0.45
26:B:851:LHG:H262	27:B:854:LMU:C2	2.46	0.45
8:N:70:PHE:CG	8:N:71:PRO:HD2	2.52	0.45
6:P:406:LEU:HB2	6:P:408:LEU:HG	1.98	0.45
19:X:101:LEU:HD11	19:X:260:THR:HG23	1.99	0.45
22:A:842:CLA:O1A	26:A:845:LHG:H131	2.17	0.45
22:B:810:CLA:H61	22:B:810:CLA:H92	1.70	0.45
25:B:847:DGD:O2D	25:B:847:DGD:HG31	2.16	0.45
4:E:94:ARG:HB3	4:E:94:ARG:NH1	2.32	0.45
6:G:539:HIS:CD2	22:G:611:CLA:NC	2.85	0.45
22:K:609:CLA:CHB	22:A:844:CLA:H42	2.46	0.45
13:O:183:TYR:HB3	22:O:310:CLA:HED2	1.98	0.45
6:P:510:ASN:O	6:P:513:LEU:HG	2.16	0.45
11:R:317:GLU:O	11:R:321:LYS:HG3	2.17	0.45
22:R:611:CLA:H3A	22:R:611:CLA:HBA2	1.48	0.45
14:S:210:ASN:ND2	22:S:609:CLA:NB	2.65	0.45
20:A:522:ALA:O	20:A:523:MET:HE2	2.17	0.45
22:B:805:CLA:H203	22:B:805:CLA:H161	1.84	0.45
8:I:193:GLU:HG3	22:I:607:CLA:C1B	2.47	0.45
26:N:616:LHG:H122	26:N:616:LHG:H152	1.83	0.45
13:O:171:PHE:CE2	10:Q:383:TRP:CH2	3.05	0.45
22:Q:611:CLA:H2	22:Q:611:CLA:H62	1.62	0.45
22:R:604:CLA:C3A	22:R:605:CLA:H152	2.45	0.45
22:W:404:CLA:H142	22:W:404:CLA:H112	1.78	0.45
31:W:407:CHL:C2C	31:W:408:CHL:HBC3	2.46	0.45
22:L:409:CLA:H143	27:L:419:LMU:H121	1.98	0.45
8:N:189:THR:HG21	22:N:607:CLA:H12	1.98	0.45
22:R:601:CLA:H52	26:R:614:LHG:H101	1.99	0.45
22:T:604:CLA:H142	22:T:604:CLA:H111	1.76	0.45
17:V:310:ARG:O	17:V:314:VAL:HG23	2.17	0.45
22:A:817:CLA:H62	22:A:817:CLA:H102	1.79	0.45
1:B:583:MET:O	1:B:587:ILE:HG12	2.17	0.45
17:V:297:ALA:HB1	17:V:302:LYS:HE3	1.98	0.45
22:B:804:CLA:H61	22:B:804:CLA:H2	1.67	0.44
18:W:303:PHE:CE2	22:W:409:CLA:NC	2.85	0.44
10:K:487:TYR:CE1	11:L:201:GLY:HA3	2.53	0.44
11:L:368:TRP:CH2	11:L:370:VAL:HA	2.53	0.44
8:N:115:SER:CB	8:N:201:MET:HG2	2.48	0.44
10:Q:426:GLY:HA2	10:Q:516:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:604:CLA:HMB1	22:R:605:CLA:H162	1.98	0.44
14:S:75:PRO:HD3	22:S:601:CLA:HMA1	2.00	0.44
1:B:656:VAL:HG23	1:B:716:GLY:HA2	1.98	0.44
2:C:29:VAL:HG12	3:D:245:ARG:HB3	2.00	0.44
11:L:245:MET:SD	22:L:408:CLA:HAB	2.57	0.44
10:Q:546:ALA:HB2	28:Q:602:LMG:HC5	1.99	0.44
20:A:169:PHE:O	20:A:172:VAL:HG22	2.17	0.44
22:A:824:CLA:H91	22:A:824:CLA:H111	1.60	0.44
1:B:89:HIS:CD2	22:B:807:CLA:NA	2.85	0.44
1:B:276:HIS:O	1:B:280:ILE:HG23	2.16	0.44
22:K:607:CLA:HHC	22:K:607:CLA:CBB	2.47	0.44
8:N:150:MET:HE3	8:N:150:MET:HB3	1.80	0.44
17:V:168:PHE:CE2	17:V:190:ARG:HD2	2.52	0.44
17:V:180:ALA:HB2	22:V:602:CLA:HAA2	1.99	0.44
19:X:207:LEU:O	19:X:209:HIS:N	2.51	0.44
21:B:801:BCR:H331	21:B:801:BCR:C8	2.48	0.44
22:B:839:CLA:HBA1	26:B:848:LHG:HC41	2.00	0.44
21:B:843:BCR:H24C	21:B:843:BCR:H371	1.61	0.44
22:H:305:CLA:HBA2	22:H:305:CLA:H3A	1.79	0.44
22:I:601:CLA:H61	22:I:601:CLA:H2	1.79	0.44
10:K:549:ILE:HG21	22:K:611:CLA:H42	1.98	0.44
10:Q:384:PHE:HD2	10:Q:387:ILE:HD13	1.82	0.44
11:R:253:VAL:HA	11:R:256:ILE:HD12	1.98	0.44
28:U:402:LMG:H392	28:U:402:LMG:H362	1.81	0.44
22:U:415:CLA:H3A	22:U:415:CLA:HBA2	1.44	0.44
20:A:14:ARG:HG2	20:A:15:VAL:H	1.82	0.44
22:A:833:CLA:H162	22:A:833:CLA:H121	1.77	0.44
1:B:420:SER:HB2	22:A:841:CLA:HED2	1.99	0.44
21:B:844:BCR:H15C	21:B:844:BCR:H351	1.82	0.44
6:P:509:LYS:HA	6:P:512:ARG:HD2	1.99	0.44
22:T:605:CLA:H62	22:T:605:CLA:H41	1.67	0.44
22:U:404:CLA:HMB1	22:U:404:CLA:HBB1	2.00	0.44
22:B:820:CLA:H62	22:B:820:CLA:H41	1.53	0.44
7:H:131:ASP:O	7:H:135:ARG:HG3	2.18	0.44
22:K:613:CLA:H42	11:L:370:VAL:HG23	2.00	0.44
22:L:417:CLA:H202	22:L:417:CLA:H162	1.83	0.44
11:R:196:PRO:HB2	22:R:601:CLA:HED2	2.00	0.44
11:R:232:ARG:HG3	11:R:233:MET:N	2.32	0.44
14:S:113:VAL:HG12	14:S:117:ARG:HD2	1.99	0.44
31:W:407:CHL:CBC	31:W:408:CHL:HBC3	2.48	0.44
20:A:51:ASN:N	20:A:51:ASN:HD22	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:820:CLA:HAB	22:A:820:CLA:H8	2.00	0.44
22:A:832:CLA:H41	22:A:832:CLA:H61	1.78	0.44
1:B:652:PHE:O	1:B:656:VAL:HG22	2.17	0.44
22:B:828:CLA:H162	22:B:828:CLA:H141	1.78	0.44
25:B:847:DGD:HA51	25:B:847:DGD:HA21	1.40	0.44
10:Q:542:ARG:HH11	10:Q:542:ARG:HG2	1.83	0.44
22:T:605:CLA:H162	22:T:605:CLA:H192	1.74	0.44
22:T:611:CLA:HBA1	22:T:611:CLA:H3A	1.44	0.44
2:C:77:MET:HE3	2:C:77:MET:HB3	1.90	0.44
22:H:313:CLA:H62	22:H:313:CLA:H41	1.87	0.44
11:L:228:LYS:HB3	11:L:228:LYS:HE3	1.80	0.44
6:P:536:LEU:HD12	6:P:536:LEU:HA	1.81	0.44
22:P:606:CLA:HBA1	22:P:606:CLA:H3A	1.68	0.44
16:U:290:PHE:CE2	22:U:409:CLA:NC	2.86	0.44
28:U:423:LMG:H142	28:U:423:LMG:H111	1.79	0.44
17:V:267:TRP:CH2	32:V:616:NEX:H192	2.53	0.44
22:V:609:CLA:H62	22:V:609:CLA:H41	1.85	0.44
22:A:824:CLA:H141	22:A:828:CLA:H151	2.00	0.44
8:I:154:ALA:HB3	8:I:155:PRO:HD3	2.00	0.43
8:I:222:LEU:CD1	22:I:611:CLA:HBC2	2.42	0.43
11:L:263:TYR:CD2	11:L:337:ARG:HD2	2.52	0.43
22:W:402:CLA:H41	22:W:402:CLA:H62	1.72	0.43
20:A:626:LYS:HE2	20:A:626:LYS:N	2.33	0.43
22:A:814:CLA:H41	22:A:814:CLA:H62	1.70	0.43
22:F:404:CLA:H62	22:F:404:CLA:H41	1.74	0.43
6:P:409:ALA:HB1	6:P:415:TYR:HD1	1.82	0.43
14:S:103:ALA:O	14:S:106:GLU:HG3	2.18	0.43
17:V:238:TYR:CD1	17:V:239:LEU:HG	2.53	0.43
22:X:419:CLA:H3A	22:X:419:CLA:HBA1	1.62	0.43
20:A:204:GLY:O	20:A:208:LEU:HB2	2.18	0.43
20:A:320:HIS:HE1	22:A:823:CLA:C4A	2.32	0.43
1:B:136:TYR:CZ	12:M:7:GLN:HB3	2.53	0.43
1:B:178:HIS:O	1:B:182:LEU:HB3	2.18	0.43
22:B:833:CLA:H192	22:B:833:CLA:H162	1.69	0.43
13:O:163:GLU:HG2	22:O:309:CLA:NB	2.32	0.43
6:G:383:TRP:O	22:G:601:CLA:NA	2.51	0.43
25:O:304:DGD:HA52	25:O:304:DGD:HA81	1.31	0.43
10:Q:509:ILE:HG22	10:Q:513:ARG:HE	1.84	0.43
22:R:601:CLA:H41	22:R:601:CLA:H62	1.44	0.43
16:U:238:TYR:HB3	16:U:244:LEU:HD13	1.99	0.43
17:V:224:TRP:HE3	17:V:225:TYR:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:409:CLA:H162	22:X:409:CLA:H122	1.73	0.43
22:A:805:CLA:H92	22:A:805:CLA:H62	1.73	0.43
22:A:852:CLA:H161	22:A:852:CLA:H141	1.79	0.43
1:B:91:ILE:HD12	1:B:112:PRO:HB2	2.00	0.43
1:B:208:ARG:O	1:B:212:PHE:HB3	2.18	0.43
22:B:824:CLA:HAA2	22:B:825:CLA:OBD	2.18	0.43
25:B:847:DGD:HE61	25:B:847:DGD:HE1	1.68	0.43
3:D:95:GLN:OE1	3:D:95:GLN:N	2.49	0.43
22:L:410:CLA:HMA1	22:L:410:CLA:H2	2.01	0.43
22:U:411:CLA:H92	22:U:411:CLA:H61	1.71	0.43
17:V:238:TYR:HB3	17:V:244:LEU:HD12	2.01	0.43
22:W:411:CLA:H41	22:W:411:CLA:H62	1.77	0.43
22:B:827:CLA:H92	22:B:827:CLA:H61	1.81	0.43
22:H:307:CLA:H61	22:H:307:CLA:H2	1.67	0.43
8:N:141:ASP:OD1	8:N:144:LYS:HB3	2.18	0.43
22:N:603:CLA:H141	22:N:603:CLA:H161	1.78	0.43
22:N:603:CLA:H142	22:N:603:CLA:H112	1.86	0.43
22:O:313:CLA:H161	22:O:313:CLA:H141	1.66	0.43
22:O:313:CLA:H92	22:O:313:CLA:H61	1.77	0.43
18:W:174:GLU:N	18:W:174:GLU:OE1	2.51	0.43
20:A:671:MET:HE3	20:A:671:MET:HB3	1.76	0.43
21:A:849:BCR:H24C	21:A:849:BCR:H371	1.77	0.43
1:B:439:HIS:HE1	22:B:832:CLA:C1A	2.16	0.43
12:M:20:PHE:CG	22:O:311:CLA:H42	2.53	0.43
13:O:189:LEU:HD12	13:O:191:LEU:HD11	2.00	0.43
22:U:405:CLA:H51	27:U:421:LMU:H82	2.00	0.43
22:V:603:CLA:H112	22:V:603:CLA:H72	1.89	0.43
22:W:406:CLA:H101	22:W:409:CLA:H151	2.01	0.43
22:A:801:CLA:H62	22:A:801:CLA:H41	1.77	0.43
21:B:801:BCR:H12C	23:A:843:PQN:H291	2.01	0.43
22:B:804:CLA:H162	22:B:804:CLA:H141	1.75	0.43
10:K:508:GLU:HG3	22:K:608:CLA:C1B	2.49	0.43
26:K:616:LHG:H272	26:K:616:LHG:H242	1.80	0.43
22:O:313:CLA:H111	22:O:313:CLA:H71	1.56	0.43
11:R:195:ARG:NH2	11:R:210:GLY:H	2.13	0.43
22:R:601:CLA:H111	22:R:601:CLA:H72	1.59	0.43
22:R:615:CLA:HBA1	22:R:615:CLA:H3A	1.80	0.43
17:V:224:TRP:CE3	17:V:225:TYR:HB3	2.54	0.43
22:V:604:CLA:H93	22:V:604:CLA:H62	1.71	0.43
22:B:817:CLA:H141	22:B:817:CLA:H161	1.83	0.43
27:H:301:LMU:H31	28:H:322:LMG:H112	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:614:LHG:H271	26:T:614:LHG:H242	1.86	0.43
22:V:601:CLA:HED2	22:V:601:CLA:HBD	1.69	0.43
22:A:844:CLA:H61	22:A:844:CLA:H92	1.80	0.43
1:B:308:HIS:HE1	22:B:821:CLA:C4D	2.31	0.43
22:B:830:CLA:H201	22:W:410:CLA:H91	2.01	0.43
6:G:464:MET:CE	7:H:93:GLN:HG3	2.48	0.43
22:G:608:CLA:H62	22:G:608:CLA:H41	1.49	0.43
22:K:605:CLA:H112	22:K:605:CLA:H91	1.76	0.43
13:O:82:PRO:HG2	13:O:85:LEU:HD12	2.01	0.43
22:R:607:CLA:H91	22:R:607:CLA:H111	1.77	0.43
17:V:238:TYR:HD1	17:V:239:LEU:HG	1.83	0.43
20:A:681:PHE:HZ	22:A:842:CLA:HBC2	1.83	0.43
22:A:840:CLA:H112	22:A:840:CLA:H143	1.74	0.43
25:F:401:DGD:HA32	9:J:42:ILE:HG22	2.01	0.42
22:O:308:CLA:HBA2	22:O:308:CLA:H3A	1.85	0.42
6:P:524:GLN:OE1	22:P:610:CLA:C1A	2.67	0.42
22:V:612:CLA:H111	22:V:612:CLA:H91	1.81	0.42
20:A:418:ASP:O	20:A:422:ASN:ND2	2.48	0.42
33:A:802:CL0:CMB	22:A:852:CLA:OBD	2.66	0.42
21:A:848:BCR:H11C	21:A:848:BCR:H341	1.80	0.42
1:B:67:HIS:HE1	22:B:806:CLA:C4D	2.32	0.42
4:E:92:PRO:HB2	4:E:114:VAL:HG21	2.02	0.42
28:F:408:LMG:H132	27:U:424:LMU:H21	2.01	0.42
22:I:601:CLA:CHA	22:I:601:CLA:HBA1	2.50	0.42
22:I:603:CLA:H2	22:I:603:CLA:H61	1.76	0.42
13:O:194:GLU:OE1	13:O:194:GLU:N	2.52	0.42
6:P:426:ALA:HB1	6:P:511:GLY:HA3	2.00	0.42
22:Q:610:CLA:H112	22:Q:610:CLA:H172	2.01	0.42
11:R:348:LEU:HD13	22:R:611:CLA:HBC2	2.01	0.42
22:T:605:CLA:H92	22:T:605:CLA:H61	1.74	0.42
17:V:209:VAL:HG21	22:V:604:CLA:HAC2	2.01	0.42
22:A:812:CLA:H61	22:A:812:CLA:H2	1.81	0.42
6:G:415:TYR:O	6:G:419:ARG:HG3	2.19	0.42
22:L:402:CLA:HBA2	26:L:416:LHG:HC81	2.00	0.42
22:S:608:CLA:C1B	26:S:613:LHG:HC32	2.50	0.42
22:W:409:CLA:H61	22:W:409:CLA:H2	1.72	0.42
22:A:808:CLA:H151	22:A:808:CLA:H112	1.44	0.42
22:A:827:CLA:HAA2	22:A:828:CLA:OBD	2.20	0.42
1:B:504:LYS:HA	1:B:504:LYS:HD3	1.86	0.42
21:B:801:BCR:H15C	21:B:801:BCR:H351	1.67	0.42
28:F:408:LMG:H152	28:F:408:LMG:H182	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:F:409:LMU:H12	27:F:409:LMU:H41	1.84	0.42
22:K:604:CLA:HMD1	22:K:607:CLA:C1D	2.49	0.42
10:Q:408:LEU:HD13	22:Q:604:CLA:H42	2.00	0.42
22:S:605:CLA:H3A	22:S:605:CLA:HBA2	1.43	0.42
22:S:607:CLA:HAB	24:S:611:DD6:C24	2.49	0.42
22:T:608:CLA:CED	22:T:608:CLA:H2A	2.49	0.42
18:W:295:ASP:OD1	18:W:296:LYS:N	2.52	0.42
33:A:802:CL0:H40	22:A:804:CLA:O1D	2.20	0.42
22:A:838:CLA:H41	22:A:838:CLA:H61	1.66	0.42
6:G:433:ILE:HD13	6:G:518:LEU:HG	2.01	0.42
11:L:231:GLU:H	11:L:231:GLU:CD	2.26	0.42
22:L:408:CLA:HBB1	22:L:408:CLA:HMB1	2.01	0.42
10:Q:516:MET:HG2	24:Q:614:DD6:C5	2.50	0.42
22:Q:603:CLA:HBB1	22:Q:603:CLA:HMB3	2.00	0.42
11:R:281:ALA:O	11:R:285:VAL:HG23	2.19	0.42
22:S:606:CLA:HBA1	22:S:606:CLA:H3A	1.83	0.42
22:T:605:CLA:H142	22:T:605:CLA:H111	1.83	0.42
16:U:211:GLU:HB3	16:U:331:LEU:HD12	2.02	0.42
18:W:345:GLN:OE1	18:W:345:GLN:N	2.52	0.42
21:A:851:BCR:H361	21:A:851:BCR:H20C	1.77	0.42
21:B:842:BCR:H20C	21:B:842:BCR:H361	1.91	0.42
2:C:15:THR:O	2:C:19:ARG:HG3	2.18	0.42
4:E:120:SER:HB3	4:E:123:ILE:HG12	2.00	0.42
8:I:224:ALA:C	8:I:226:LEU:N	2.76	0.42
22:Q:604:CLA:H61	22:Q:604:CLA:H41	1.76	0.42
17:V:208:LEU:HD23	17:V:208:LEU:HA	1.86	0.42
22:B:816:CLA:H161	22:B:816:CLA:H121	1.68	0.42
22:H:308:CLA:HBB1	22:H:310:CLA:H3A	2.02	0.42
8:I:186:THR:O	8:I:190:LYS:HG3	2.20	0.42
22:I:603:CLA:H92	22:I:603:CLA:H62	1.91	0.42
26:O:321:LHG:HC62	26:O:321:LHG:H241	1.75	0.42
20:A:183:LYS:HE3	20:A:183:LYS:HB3	1.84	0.42
20:A:544:HIS:CD2	22:A:840:CLA:NB	2.86	0.42
20:A:613:LYS:HG2	22:A:838:CLA:HBC1	2.02	0.42
1:B:712:HIS:CE1	22:B:838:CLA:C4D	3.03	0.42
10:K:547:ALA:HB1	22:K:611:CLA:HED1	2.02	0.42
22:N:610:CLA:HBA1	22:N:610:CLA:CHA	2.49	0.42
15:T:304:LEU:HD11	22:T:607:CLA:HAC1	2.02	0.42
17:V:163:TRP:CD1	17:V:164:LEU:HG	2.55	0.42
17:V:290:PHE:CE1	22:V:607:CLA:NC	2.88	0.42
1:B:400:GLU:O	1:B:404:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:822:CLA:H51	22:B:823:CLA:H143	2.01	0.42
22:K:604:CLA:CMD	22:K:607:CLA:C1D	2.97	0.42
21:M:101:BCR:H24C	21:M:101:BCR:H371	1.79	0.42
8:N:178:GLY:HA2	22:N:607:CLA:CED	2.50	0.42
22:V:604:CLA:HHC	32:V:616:NEX:H362	1.96	0.42
18:W:235:GLU:HG2	18:W:240:LYS:HB3	2.02	0.42
22:A:814:CLA:H102	22:A:814:CLA:H61	1.83	0.42
1:B:137:ASN:HB3	28:B:856:LMG:H132	2.01	0.42
8:N:108:GLU:HG3	22:N:602:CLA:C1B	2.49	0.42
14:S:168:TYR:HB2	22:T:606:CLA:HAB	2.01	0.42
22:A:842:CLA:H141	22:A:842:CLA:H161	1.60	0.42
5:F:291:TRP:CG	5:F:292:PRO:HD3	2.55	0.41
22:H:311:CLA:H141	22:H:311:CLA:H161	1.87	0.41
13:O:171:PHE:HE2	10:Q:383:TRP:CH2	2.37	0.41
16:U:307:LYS:HB3	22:U:412:CLA:HMD1	2.01	0.41
16:U:347:LEU:HD23	16:U:347:LEU:HA	1.89	0.41
17:V:181:ARG:NH2	30:V:618:SQD:O8	2.53	0.41
31:W:407:CHL:C2C	31:W:408:CHL:CBC	2.97	0.41
22:A:805:CLA:H142	22:A:805:CLA:H112	1.79	0.41
22:A:815:CLA:H141	22:A:815:CLA:H162	1.90	0.41
22:B:824:CLA:H142	22:B:824:CLA:H111	1.78	0.41
21:B:844:BCR:H341	21:B:844:BCR:H11C	1.81	0.41
13:O:191:LEU:HD22	27:O:301:LMU:H72	2.01	0.41
6:P:479:PHE:HB3	26:P:601:LHG:O4	2.21	0.41
31:W:407:CHL:HAB	31:W:408:CHL:OMC	2.20	0.41
26:W:420:LHG:H131	26:W:420:LHG:H102	1.77	0.41
20:A:51:ASN:HA	20:A:54:ALA:HB3	2.02	0.41
21:A:848:BCR:H371	21:A:848:BCR:H24C	1.79	0.41
22:G:608:CLA:H121	22:G:609:CLA:CHC	2.50	0.41
11:L:226:ASP:OD2	11:L:226:ASP:C	2.64	0.41
22:L:412:CLA:H3A	22:L:412:CLA:HBA2	1.71	0.41
8:N:189:THR:CG2	22:N:607:CLA:HHB	2.51	0.41
22:Q:608:CLA:HBA1	22:Q:608:CLA:H3A	1.94	0.41
22:T:608:CLA:H2A	22:T:608:CLA:HED3	2.01	0.41
17:V:207:CYS:HB3	17:V:224:TRP:HD1	1.85	0.41
17:V:267:TRP:CE2	17:V:273:ILE:HG23	2.56	0.41
22:A:804:CLA:H142	22:A:804:CLA:H111	1.77	0.41
22:A:852:CLA:H91	22:A:852:CLA:H111	1.79	0.41
8:I:111:HIS:CE1	22:I:603:CLA:C4A	2.95	0.41
22:I:606:CLA:HED3	10:K:481:TRP:CZ3	2.56	0.41
22:L:406:CLA:H111	22:L:406:CLA:H72	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:408:CLA:CGA	22:L:408:CLA:C3A	2.99	0.41
22:P:603:CLA:HMD1	22:P:606:CLA:C1D	2.50	0.41
20:A:233:ASN:OD1	20:A:233:ASN:C	2.63	0.41
20:A:494:ALA:N	20:A:495:PRO:HD2	2.36	0.41
22:A:830:CLA:HBA1	22:A:830:CLA:HBD	2.02	0.41
1:B:516:ASP:N	1:B:516:ASP:OD1	2.54	0.41
1:B:640:MET:HE2	1:B:640:MET:HB2	1.83	0.41
6:G:440:GLU:OE2	6:G:446:ALA:HA	2.20	0.41
22:K:617:CLA:H92	22:K:617:CLA:H62	1.74	0.41
14:S:74:PHE:CD1	14:S:75:PRO:HD2	2.55	0.41
15:T:353:GLY:H	15:T:358:GLU:CD	2.27	0.41
31:U:407:CHL:CBA	32:U:418:NEX:H403	2.50	0.41
17:V:316:MET:HE2	17:V:316:MET:HB2	1.87	0.41
31:W:422:CHL:H141	19:X:221:ILE:HG13	2.01	0.41
22:A:807:CLA:H3A	22:A:807:CLA:HBA1	1.47	0.41
21:A:851:BCR:H24C	21:A:851:BCR:H371	1.81	0.41
22:B:809:CLA:HMA1	27:B:854:LMU:H71	2.01	0.41
26:K:616:LHG:HC82	26:K:616:LHG:H281	2.02	0.41
11:L:319:GLU:HG3	22:L:408:CLA:C1B	2.51	0.41
8:N:157:GLU:OE2	22:N:606:CLA:C1C	2.67	0.41
6:P:392:HIS:CD2	6:P:409:ALA:O	2.74	0.41
11:R:218:PHE:HB3	22:R:602:CLA:CAD	2.50	0.41
28:W:401:LMG:H342	28:W:401:LMG:H311	1.69	0.41
22:W:411:CLA:H142	22:W:411:CLA:H111	1.79	0.41
20:A:354:SER:OG	20:A:409:ALA:HB2	2.21	0.41
22:A:827:CLA:HBA2	22:A:827:CLA:H3A	1.69	0.41
21:A:849:BCR:H11C	21:A:849:BCR:H341	1.84	0.41
2:C:29:VAL:HG21	3:D:247:LYS:HG2	2.01	0.41
3:D:98:ASP:OD2	3:D:99:LEU:N	2.54	0.41
11:L:257:LEU:HA	27:L:419:LMU:H6D	2.01	0.41
22:L:404:CLA:H2	22:L:404:CLA:H61	1.75	0.41
11:R:233:MET:HE2	22:R:602:CLA:H12	2.03	0.41
14:S:150:ASN:HB2	14:S:152:GLU:OE2	2.20	0.41
16:U:188:LYS:NZ	22:U:405:CLA:HBA1	2.34	0.41
20:A:233:ASN:HA	20:A:234:PRO:HD3	1.91	0.41
22:A:816:CLA:H151	22:A:816:CLA:H112	1.66	0.41
22:B:823:CLA:H62	22:B:823:CLA:H41	1.85	0.41
22:B:834:CLA:HBB1	22:B:834:CLA:HMB3	2.02	0.41
8:N:180:ASP:OD2	8:N:185:THR:OG1	2.38	0.41
11:R:286:VAL:O	11:R:290:ARG:HG3	2.20	0.41
16:U:261:MET:HE3	16:U:261:MET:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:U:408:CHL:HMA2	28:U:423:LMG:O2	2.21	0.41
17:V:314:VAL:HG12	22:V:612:CLA:HBB2	2.03	0.41
22:W:412:CLA:H121	22:W:413:CLA:C4B	2.50	0.41
20:A:200:HIS:CE1	22:A:814:CLA:NA	2.88	0.41
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.93	0.41
1:B:310:ALA:HA	1:B:311:PRO:HD3	1.94	0.41
1:B:494:LEU:HD12	1:B:494:LEU:HA	1.86	0.41
22:B:813:CLA:H2	22:B:813:CLA:H61	1.59	0.41
22:B:824:CLA:HMA1	21:B:845:BCR:H14C	2.03	0.41
22:B:825:CLA:H122	21:B:844:BCR:H373	2.03	0.41
21:B:843:BCR:H24C	21:B:843:BCR:H402	1.73	0.41
26:B:851:LHG:H161	26:B:851:LHG:H192	1.84	0.41
8:I:79:LEU:HD11	8:I:90:ASP:HB2	2.03	0.41
10:K:525:GLN:HG2	22:K:611:CLA:C1D	2.50	0.41
22:K:608:CLA:H41	22:K:608:CLA:H62	1.87	0.41
8:N:117:LEU:HD22	22:N:604:CLA:HAB	2.03	0.41
13:O:117:HIS:HE1	22:O:307:CLA:C4D	2.34	0.41
11:R:195:ARG:HB2	11:R:195:ARG:HH11	1.86	0.41
22:R:607:CLA:H52	22:R:607:CLA:HBB1	2.03	0.41
14:S:136:ALA:O	14:S:139:THR:OG1	2.38	0.41
27:T:618:LMU:H31	27:T:618:LMU:H62	1.73	0.41
22:U:401:CLA:HBA1	22:U:401:CLA:H3A	1.89	0.41
19:X:268:LYS:HD3	22:X:411:CLA:HAA2	2.02	0.41
20:A:88:LEU:HD23	20:A:88:LEU:HA	1.90	0.41
20:A:339:LYS:HB2	20:A:339:LYS:HE2	1.94	0.41
1:B:177:HIS:HE1	22:B:811:CLA:C4A	2.34	0.41
22:B:830:CLA:HBC3	22:B:830:CLA:HHD	2.03	0.41
6:G:447:TRP:CE2	6:G:448:PHE:HD2	2.39	0.41
11:L:338:HIS:HB3	11:L:368:TRP:HZ3	1.85	0.41
22:L:409:CLA:NC	26:L:416:LHG:HC41	2.36	0.41
21:M:101:BCR:H11C	21:M:101:BCR:H341	1.85	0.41
10:Q:537:LEU:HD13	22:Q:613:CLA:HBC2	2.02	0.41
22:S:605:CLA:O1D	22:S:605:CLA:H2A	2.21	0.41
17:V:182:ASP:HB3	17:V:185:ASP:CG	2.46	0.41
17:V:190:ARG:O	17:V:194:VAL:HG23	2.21	0.41
17:V:246:HIS:HB2	22:V:617:CLA:C1B	2.51	0.41
17:V:300:GLU:O	17:V:304:LYS:HG3	2.21	0.41
20:A:609:HIS:NE2	22:A:838:CLA:HBC3	2.36	0.41
21:B:801:BCR:H272	22:B:831:CLA:HBB2	2.03	0.40
21:B:842:BCR:H341	21:B:842:BCR:H11C	1.82	0.40
10:K:545:LEU:H	10:K:545:LEU:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:R:243:LEU:HD11	22:R:606:CLA:HBC3	2.03	0.40
22:S:604:CLA:H112	22:S:604:CLA:H91	1.82	0.40
28:T:616:LMG:HC1	28:T:616:LMG:HC8	1.79	0.40
22:U:404:CLA:H92	22:U:404:CLA:H61	1.66	0.40
18:W:198:PHE:O	18:W:202:ARG:HG3	2.21	0.40
1:B:388:ALA:O	1:B:392:ILE:HG13	2.19	0.40
22:B:832:CLA:H12	9:J:42:ILE:HD12	2.04	0.40
4:E:102:ARG:HA	4:E:103:PRO:HD3	1.98	0.40
22:H:308:CLA:H92	22:H:308:CLA:H61	1.79	0.40
27:L:420:LMU:H51	27:L:420:LMU:H22	1.82	0.40
26:O:321:LHG:H372	26:O:321:LHG:H342	1.84	0.40
11:R:332:GLY:HA2	11:R:335:VAL:HG12	2.02	0.40
22:R:607:CLA:H92	22:R:607:CLA:H61	1.70	0.40
21:B:801:BCR:H24C	21:B:801:BCR:H371	1.90	0.40
3:D:117:THR:O	3:D:146:GLY:HA3	2.22	0.40
7:H:165:LEU:HD13	22:H:312:CLA:HBC2	2.03	0.40
22:I:611:CLA:HBA2	22:I:611:CLA:H3A	1.67	0.40
25:O:304:DGD:HB71	25:O:304:DGD:HB41	1.13	0.40
22:B:859:CLA:H142	22:B:859:CLA:H111	1.79	0.40
22:K:607:CLA:H93	22:K:607:CLA:H111	1.79	0.40
8:N:152:ILE:HA	8:N:152:ILE:HD13	1.85	0.40
13:O:240:ASN:OD1	13:O:243:THR:HG23	2.22	0.40
22:Q:608:CLA:HHC	22:Q:608:CLA:HBB1	2.03	0.40
17:V:153:THR:HA	17:V:172:ARG:O	2.22	0.40
22:W:406:CLA:H92	22:W:406:CLA:H62	1.92	0.40
20:A:37:ARG:NH2	20:A:62:HIS:O	2.54	0.40
1:B:293:THR:CG2	1:B:294:ASN:H	2.22	0.40
1:B:484:ASN:ND2	31:U:408:CHL:OBD	2.54	0.40
22:B:834:CLA:H51	22:B:834:CLA:H11	1.87	0.40
5:F:252:ILE:HD13	22:F:404:CLA:C1D	2.32	0.40
21:J:103:BCR:H24C	21:J:103:BCR:H371	1.92	0.40
22:K:608:CLA:H3A	22:K:608:CLA:CGA	2.51	0.40
22:U:420:CLA:HBA2	22:U:420:CLA:H3A	1.30	0.40
18:W:221:ALA:HB3	18:W:222:PRO:HD3	2.04	0.40
20:A:180:HIS:HE1	22:A:812:CLA:C1A	2.34	0.40
20:A:502:LEU:HD23	20:A:502:LEU:HA	1.87	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	B	730/734 (100%)	698 (96%)	29 (4%)	3 (0%)	30	34
2	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	D	188/193 (97%)	182 (97%)	6 (3%)	0	100	100
4	E	61/158 (39%)	61 (100%)	0	0	100	100
5	F	164/325 (50%)	161 (98%)	3 (2%)	0	100	100
6	G	173/184 (94%)	169 (98%)	4 (2%)	0	100	100
6	P	162/184 (88%)	146 (90%)	16 (10%)	0	100	100
7	H	171/185 (92%)	165 (96%)	6 (4%)	0	100	100
8	I	163/184 (89%)	160 (98%)	3 (2%)	0	100	100
8	N	168/184 (91%)	155 (92%)	13 (8%)	0	100	100
9	J	35/39 (90%)	35 (100%)	0	0	100	100
10	K	180/184 (98%)	175 (97%)	5 (3%)	0	100	100
10	Q	180/184 (98%)	168 (93%)	12 (7%)	0	100	100
11	L	176/187 (94%)	167 (95%)	8 (4%)	1 (1%)	21	24
11	R	172/187 (92%)	163 (95%)	8 (5%)	1 (1%)	21	24
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	O	173/177 (98%)	160 (92%)	12 (7%)	1 (1%)	21	24
14	S	170/180 (94%)	166 (98%)	4 (2%)	0	100	100
15	T	165/173 (95%)	158 (96%)	7 (4%)	0	100	100
16	U	197/209 (94%)	186 (94%)	11 (6%)	0	100	100
17	V	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
18	W	218/228 (96%)	209 (96%)	9 (4%)	0	100	100
19	X	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
20	A	738/756 (98%)	715 (97%)	22 (3%)	1 (0%)	48	59
All	All	4906/5366 (91%)	4700 (96%)	199 (4%)	7 (0%)	49	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	R	196	PRO
1	B	288	GLY
1	B	284	PHE
11	L	367	GLN
1	B	488	ALA
13	O	184	PRO
20	A	122	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	B	608/609 (100%)	600 (99%)	8 (1%)	61	76
2	C	69/70 (99%)	67 (97%)	2 (3%)	37	49
3	D	157/160 (98%)	154 (98%)	3 (2%)	50	65
4	E	54/124 (44%)	52 (96%)	2 (4%)	30	40
5	F	132/251 (53%)	129 (98%)	3 (2%)	44	58
6	G	133/140 (95%)	132 (99%)	1 (1%)	73	84
6	P	124/140 (89%)	118 (95%)	6 (5%)	23	29
7	H	141/149 (95%)	139 (99%)	2 (1%)	59	73
8	I	120/136 (88%)	114 (95%)	6 (5%)	22	27
8	N	124/136 (91%)	120 (97%)	4 (3%)	34	46
9	J	34/36 (94%)	34 (100%)	0	100	100
10	K	144/146 (99%)	139 (96%)	5 (4%)	32	42
10	Q	144/146 (99%)	141 (98%)	3 (2%)	47	61
11	L	139/145 (96%)	134 (96%)	5 (4%)	31	41
11	R	136/145 (94%)	132 (97%)	4 (3%)	37	49
12	M	26/26 (100%)	26 (100%)	0	100	100
13	O	143/144 (99%)	138 (96%)	5 (4%)	32	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	S	133/137 (97%)	130 (98%)	3 (2%)	44 58
15	T	126/131 (96%)	125 (99%)	1 (1%)	73 84
16	U	152/158 (96%)	150 (99%)	2 (1%)	61 76
17	V	151/151 (100%)	148 (98%)	3 (2%)	48 63
18	W	167/172 (97%)	165 (99%)	2 (1%)	63 77
19	X	173/173 (100%)	171 (99%)	2 (1%)	63 77
20	A	621/636 (98%)	612 (99%)	9 (1%)	59 73
All	All	3951/4261 (93%)	3870 (98%)	81 (2%)	46 61

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	GLU
1	B	197	VAL
1	B	267	SER
1	B	366	THR
1	B	492	ILE
1	B	501	ILE
1	B	508	LEU
1	B	715	VAL
2	C	42	SER
2	C	65	VAL
3	D	193	SER
3	D	246	THR
3	D	260	GLU
4	E	139	VAL
4	E	140	THR
5	F	178	LYS
5	F	187	SER
5	F	206	LYS
6	G	438	VAL
7	H	12	ILE
7	H	137	ILE
8	I	120	VAL
8	I	123	ILE
8	I	124	VAL
8	I	145	LEU
8	I	152	ILE
8	I	185	THR
10	K	434	VAL

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Mol	Chain	Res	Type
10	K	471	GLU
10	K	523	GLU
10	K	528	VAL
10	K	545	LEU
11	L	195	ARG
11	L	301	ASN
11	L	342	VAL
11	L	368	TRP
11	L	370	VAL
8	N	78	HIS
8	N	152	ILE
8	N	184	LEU
8	N	187	ASP
13	O	80	THR
13	O	102	LYS
13	O	108	GLN
13	O	177	ASP
13	O	211	MET
6	P	383	TRP
6	P	392	HIS
6	P	393	LEU
6	P	433	ILE
6	P	508	ILE
6	P	518	LEU
10	Q	380	ARG
10	Q	387	ILE
10	Q	388	THR
11	R	195	ARG
11	R	229	VAL
11	R	278	VAL
11	R	330	MET
14	S	78	THR
14	S	168	TYR
14	S	203	THR
15	T	281	PHE
16	U	284	THR
16	U	349	THR
17	V	165	THR
17	V	177	CYS
17	V	316	MET
18	W	342	VAL
18	W	369	THR

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Mol	Chain	Res	Type
19	X	306	THR
19	X	320	ASP
20	A	75	SER
20	A	111	VAL
20	A	307	LEU
20	A	328	SER
20	A	395	TYR
20	A	414	VAL
20	A	506	THR
20	A	622	VAL
20	A	628	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	672	GLN
1	B	704	GLN
6	G	378	HIS
6	G	524	GLN
6	G	542	ASN
7	H	93	GLN
7	H	139	ASN
7	H	153	GLN
10	K	425	ASN
10	K	511	ASN
10	K	525	GLN
11	L	211	GLN
11	L	336	GLN
8	N	196	ASN
13	O	203	ASN
13	O	217	GLN
13	O	235	HIS
10	Q	425	ASN
10	Q	511	ASN
10	Q	525	GLN
10	Q	526	ASN
11	R	268	ASN
11	R	336	GLN
14	S	210	ASN
14	S	224	GLN
14	S	225	HIS
15	T	386	ASN

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Mol	Chain	Res	Type
17	V	232	ASN
17	V	322	GLN
19	X	123	HIS
19	X	200	ASN
19	X	204	ASN
20	A	34	HIS
20	A	51	ASN
20	A	116	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

436 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	DD6	H	314	-	39,45,45	1.99	3 (7%)	52,67,67	1.88	12 (23%)
22	CLA	O	315	13	54,58,73	1.43	9 (16%)	65,95,113	1.36	8 (12%)
22	CLA	B	838	1	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
29	SF4	C	101	2	0,12,12	-	-	-		
24	DD6	P	612	-	39,45,45	2.04	2 (5%)	52,67,67	2.96	18 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	O	314	13	49,53,73	1.48	8 (16%)	59,89,113	1.40	5 (8%)
22	CLA	L	407	-	61,65,73	1.33	8 (13%)	73,103,113	1.33	5 (6%)
27	LMU	T	618	-	24,24,36	0.44	0	29,29,47	0.66	0
22	CLA	A	828	20	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
22	CLA	L	411	11	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	G	602	6	64,68,73	1.30	8 (12%)	77,107,113	1.33	8 (10%)
27	LMU	X	418	-	24,24,36	0.43	0	29,29,47	0.55	0
26	LHG	L	416	22	41,41,48	1.17	6 (14%)	44,47,54	0.99	2 (4%)
22	CLA	W	402	18	59,63,73	1.35	8 (13%)	71,101,113	1.31	7 (9%)
24	DD6	V	614	-	39,45,45	2.00	3 (7%)	52,67,67	2.03	13 (25%)
28	LMG	U	423	-	49,49,55	0.73	0	57,57,63	1.31	3 (5%)
22	CLA	S	602	14	64,68,73	1.30	7 (10%)	77,107,113	1.33	8 (10%)
28	LMG	H	319	-	40,40,55	0.81	0	48,48,63	1.21	3 (6%)
22	CLA	B	830	1	69,73,73	1.24	10 (14%)	83,113,113	1.34	9 (10%)
22	CLA	X	410	26	64,68,73	1.31	7 (10%)	77,107,113	1.30	6 (7%)
22	CLA	B	812	1	69,73,73	1.26	7 (10%)	83,113,113	1.29	8 (9%)
30	SQD	K	621	-	42,43,54	0.42	1 (2%)	51,54,65	0.53	0
24	DD6	J	105	-	39,45,45	1.96	2 (5%)	52,67,67	1.88	13 (25%)
22	CLA	B	835	1	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
24	DD6	B	841	-	39,45,45	1.99	3 (7%)	52,67,67	1.99	13 (25%)
22	CLA	L	404	-	60,64,73	1.35	8 (13%)	72,102,113	1.36	6 (8%)
22	CLA	S	606	14	54,58,73	1.42	7 (12%)	65,95,113	1.38	6 (9%)
32	NEX	V	616	-	38,46,46	0.37	1 (2%)	50,70,70	0.70	2 (4%)
22	CLA	A	841	20	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
21	BCR	A	849	-	41,41,41	0.73	0	56,56,56	1.89	13 (23%)
27	LMU	B	853	-	19,19,36	0.46	0	23,23,47	0.44	0
22	CLA	V	602	17	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	B	810	-	60,64,73	1.34	8 (13%)	72,102,113	1.33	5 (6%)
22	CLA	B	808	1	59,63,73	1.36	8 (13%)	71,101,113	1.34	4 (5%)
27	LMU	M	102	-	24,24,36	0.44	0	29,29,47	0.61	0
27	LMU	X	421	-	36,36,36	0.40	0	47,47,47	0.67	1 (2%)
22	CLA	B	809	1	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
22	CLA	B	821	1	64,68,73	1.31	8 (12%)	77,107,113	1.31	5 (6%)
24	DD6	G	612	-	39,45,45	2.00	3 (7%)	52,67,67	1.81	11 (21%)
22	CLA	B	831	1	69,73,73	1.24	7 (10%)	83,113,113	1.26	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	U	412	26	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
27	LMU	O	322	-	36,36,36	0.49	0	47,47,47	1.09	5 (10%)
22	CLA	Q	617	10	56,60,73	1.39	8 (14%)	67,97,113	1.40	6 (8%)
22	CLA	B	823	-	69,73,73	1.25	7 (10%)	83,113,113	1.28	4 (4%)
22	CLA	P	610	6	45,49,73	1.54	7 (15%)	54,84,113	1.54	7 (12%)
22	CLA	W	414	18	69,73,73	1.27	8 (11%)	83,113,113	1.27	8 (9%)
21	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.80	13 (23%)
22	CLA	O	308	-	65,69,73	1.29	8 (12%)	78,108,113	1.30	7 (8%)
22	CLA	H	302	7	49,53,73	1.49	8 (16%)	59,89,113	1.42	5 (8%)
28	LMG	J	101	-	55,55,55	0.70	0	63,63,63	1.35	7 (11%)
22	CLA	V	612	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	6 (7%)
22	CLA	I	607	8	59,63,73	1.35	8 (13%)	71,101,113	1.35	7 (9%)
24	DD6	U	416	-	39,45,45	2.01	3 (7%)	52,67,67	1.80	11 (21%)
22	CLA	A	807	20	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
22	CLA	H	310	7	49,53,73	1.48	8 (16%)	59,89,113	1.42	6 (10%)
22	CLA	S	601	14	49,53,73	1.49	7 (14%)	59,89,113	1.46	4 (6%)
27	LMU	A	857	-	24,24,36	0.45	0	29,29,47	0.66	0
22	CLA	K	608	10	69,73,73	1.24	9 (13%)	83,113,113	1.29	8 (9%)
21	BCR	B	843	-	41,41,41	0.71	0	56,56,56	3.38	24 (42%)
22	CLA	F	403	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
26	LHG	O	323	-	42,42,48	1.18	6 (14%)	45,48,54	0.95	2 (4%)
22	CLA	N	602	8	64,68,73	1.30	8 (12%)	77,107,113	1.33	7 (9%)
22	CLA	K	613	-	57,61,73	1.38	8 (14%)	68,98,113	1.35	6 (8%)
22	CLA	N	601	8	49,53,73	1.48	8 (16%)	59,89,113	1.41	4 (6%)
24	DD6	W	417	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	11 (21%)
28	LMG	F	408	-	42,42,55	0.85	1 (2%)	50,50,63	1.32	4 (8%)
27	LMU	H	320	-	24,24,36	0.44	0	29,29,47	0.59	0
22	CLA	B	826	1	62,66,73	1.32	7 (11%)	74,104,113	1.33	5 (6%)
28	LMG	K	601	-	43,43,55	0.77	0	51,51,63	1.27	4 (7%)
22	CLA	V	611	-	49,53,73	1.50	8 (16%)	59,89,113	1.43	4 (6%)
24	DD6	S	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	12 (23%)
22	CLA	T	608	26	64,68,73	1.30	7 (10%)	77,107,113	1.31	5 (6%)
26	LHG	H	316	22	26,26,48	1.40	6 (23%)	29,32,54	1.16	2 (6%)
22	CLA	A	822	-	69,73,73	1.24	7 (10%)	83,113,113	1.26	6 (7%)
24	DD6	Q	614	-	39,45,45	1.97	3 (7%)	52,67,67	1.79	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	DD6	I	613	-	39,45,45	2.05	3 (7%)	52,67,67	1.90	16 (30%)
22	CLA	R	603	-	60,64,73	1.35	8 (13%)	72,102,113	1.35	6 (8%)
26	LHG	S	613	22	31,31,48	1.32	6 (19%)	34,37,54	1.12	3 (8%)
22	CLA	I	601	8	69,73,73	1.27	9 (13%)	83,113,113	1.25	6 (7%)
24	DD6	N	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.87	13 (25%)
22	CLA	P	603	6	49,53,73	1.49	6 (12%)	59,89,113	1.30	4 (6%)
22	CLA	R	601	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	A	818	20	57,61,73	1.37	8 (14%)	68,98,113	1.37	8 (11%)
22	CLA	U	405	16	61,65,73	1.34	8 (13%)	73,103,113	1.33	4 (5%)
22	CLA	G	608	26	64,68,73	1.30	7 (10%)	77,107,113	1.35	6 (7%)
22	CLA	A	830	20	69,73,73	1.24	8 (11%)	83,113,113	1.25	6 (7%)
27	LMU	T	617	-	24,24,36	0.42	0	29,29,47	0.66	0
22	CLA	L	408	11	64,68,73	1.30	10 (15%)	77,107,113	1.43	11 (14%)
22	CLA	A	811	20	61,65,73	1.33	8 (13%)	73,103,113	1.40	10 (13%)
31	CHL	U	408	-	45,54,74	3.24	13 (28%)	35,90,114	1.52	6 (17%)
22	CLA	Q	603	10	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
22	CLA	A	815	20	69,73,73	1.25	7 (10%)	83,113,113	1.29	8 (9%)
28	LMG	G	616	-	46,46,55	0.81	0	54,54,63	1.29	7 (12%)
24	DD6	P	613	-	39,45,45	2.03	3 (7%)	52,67,67	1.94	18 (34%)
22	CLA	W	411	18	64,68,73	1.29	8 (12%)	77,107,113	1.28	7 (9%)
27	LMU	J	104	-	34,35,36	0.36	0	42,45,47	0.89	2 (4%)
22	CLA	G	610	6	49,53,73	1.48	7 (14%)	59,89,113	1.43	5 (8%)
24	DD6	G	613	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	16 (30%)
24	DD6	I	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.72	10 (19%)
28	LMG	N	615	-	44,44,55	0.78	0	52,52,63	1.26	4 (7%)
26	LHG	K	619	-	32,32,48	1.31	6 (18%)	35,38,54	1.10	2 (5%)
27	LMU	L	420	-	35,35,36	0.37	0	43,45,47	0.81	2 (4%)
24	DD6	R	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.85	12 (23%)
28	LMG	B	856	-	53,53,55	0.72	0	61,61,63	1.37	7 (11%)
22	CLA	A	808	20	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
22	CLA	W	413	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	X	413	19	49,53,73	1.49	6 (12%)	59,89,113	1.42	4 (6%)
22	CLA	A	803	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	10 (12%)
28	LMG	W	401	-	48,48,55	0.73	0	56,56,63	1.33	8 (14%)
22	CLA	N	608	26	49,53,73	1.49	8 (16%)	59,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	811	1	49,53,73	1.48	7 (14%)	59,89,113	1.47	6 (10%)
22	CLA	T	605	-	69,73,73	1.26	9 (13%)	83,113,113	1.25	6 (7%)
22	CLA	B	828	1	69,73,73	1.25	9 (13%)	83,113,113	1.28	9 (10%)
22	CLA	G	609	-	49,53,73	1.48	8 (16%)	59,89,113	1.42	6 (10%)
22	CLA	Q	609	10	64,68,73	1.29	9 (14%)	77,107,113	1.27	5 (6%)
22	CLA	P	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.44	6 (10%)
22	CLA	H	303	7	64,68,73	1.31	9 (14%)	77,107,113	1.30	6 (7%)
22	CLA	V	609	17	61,65,73	1.34	8 (13%)	73,103,113	1.34	6 (8%)
22	CLA	J	102	9	54,58,73	1.41	8 (14%)	65,95,113	1.40	5 (7%)
24	DD6	N	613	-	39,45,45	2.00	3 (7%)	52,67,67	1.86	15 (28%)
26	LHG	O	318	22	33,33,48	1.29	6 (18%)	36,39,54	1.06	3 (8%)
21	BCR	B	845	-	41,41,41	0.68	0	56,56,56	1.90	15 (26%)
22	CLA	K	602	10	64,68,73	1.30	9 (14%)	77,107,113	1.30	7 (9%)
22	CLA	O	307	13	49,53,73	1.48	8 (16%)	59,89,113	1.42	5 (8%)
27	LMU	W	421	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	R	615	11	69,73,73	1.27	7 (10%)	83,113,113	1.28	6 (7%)
32	NEX	U	418	-	38,46,46	0.35	1 (2%)	50,70,70	0.67	2 (4%)
22	CLA	B	827	1	69,73,73	1.24	8 (11%)	83,113,113	1.20	7 (8%)
22	CLA	A	814	20	69,73,73	1.24	7 (10%)	83,113,113	1.27	5 (6%)
22	CLA	X	403	19	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
22	CLA	I	608	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)
22	CLA	V	617	-	49,53,73	1.50	7 (14%)	59,89,113	1.44	4 (6%)
27	LMU	O	320	-	27,27,36	0.53	0	28,31,47	0.82	2 (7%)
22	CLA	B	802	1	69,73,73	1.26	12 (17%)	83,113,113	1.31	7 (8%)
22	CLA	A	819	20	62,66,73	1.32	9 (14%)	74,104,113	1.46	8 (10%)
22	CLA	A	827	-	66,70,73	1.27	7 (10%)	79,109,113	1.30	7 (8%)
22	CLA	A	813	20	69,73,73	1.25	7 (10%)	83,113,113	1.20	6 (7%)
27	LMU	L	418	-	24,24,36	0.48	0	29,29,47	0.74	0
22	CLA	K	617	10	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
22	CLA	O	313	13	69,73,73	1.26	8 (11%)	83,113,113	1.26	4 (4%)
22	CLA	R	607	11	64,68,73	1.32	9 (14%)	77,107,113	1.32	7 (9%)
22	CLA	F	404	-	59,63,73	1.35	7 (11%)	71,101,113	1.37	7 (9%)
22	CLA	O	319	13	49,53,73	1.48	7 (14%)	59,89,113	1.45	6 (10%)
22	CLA	B	819	1	57,61,73	1.42	7 (12%)	68,98,113	1.38	4 (5%)
27	LMU	B	857	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	5 (6%)
26	LHG	O	321	-	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
22	CLA	K	610	10	60,64,73	1.34	8 (13%)	72,102,113	1.32	5 (6%)
22	CLA	H	311	7	69,73,73	1.27	7 (10%)	83,113,113	1.29	8 (9%)
22	CLA	U	420	16	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	P	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	X	419	19	49,53,73	1.50	8 (16%)	59,89,113	1.41	5 (8%)
22	CLA	G	603	6	60,64,73	1.34	9 (15%)	72,102,113	1.33	8 (11%)
22	CLA	H	312	7	49,53,73	1.49	7 (14%)	59,89,113	1.40	5 (8%)
31	CHL	V	606	-	45,54,74	3.26	13 (28%)	35,90,114	1.50	6 (17%)
22	CLA	L	405	-	49,53,73	1.50	9 (18%)	59,89,113	1.46	4 (6%)
22	CLA	V	610	-	49,53,73	1.50	6 (12%)	59,89,113	1.42	7 (11%)
31	CHL	W	407	-	45,54,74	3.25	12 (26%)	35,90,114	1.61	6 (17%)
24	DD6	X	415	-	39,45,45	1.94	2 (5%)	52,67,67	1.71	10 (19%)
28	LMG	U	402	-	53,53,55	0.72	0	61,61,63	1.31	4 (6%)
31	CHL	U	407	-	45,54,74	3.24	14 (31%)	35,90,114	1.57	6 (17%)
27	LMU	F	409	-	21,21,36	0.49	0	26,26,47	0.57	0
24	DD6	L	415	-	39,45,45	2.01	2 (5%)	52,67,67	1.96	17 (32%)
22	CLA	I	611	8	49,53,73	1.53	8 (16%)	59,89,113	1.45	9 (15%)
22	CLA	V	604	-	60,64,73	1.35	8 (13%)	72,102,113	1.33	6 (8%)
22	CLA	A	829	20	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)
22	CLA	W	410	18	64,68,73	1.29	8 (12%)	77,107,113	1.32	6 (7%)
21	BCR	A	850	-	41,41,41	0.71	0	56,56,56	1.97	12 (21%)
24	DD6	K	615	-	39,45,45	1.95	2 (5%)	52,67,67	1.69	11 (21%)
24	DD6	X	414	-	39,45,45	1.97	3 (7%)	52,67,67	1.81	12 (23%)
22	CLA	A	821	20	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
22	CLA	V	603	17	61,65,73	1.34	7 (11%)	73,103,113	1.31	4 (5%)
27	LMU	T	615	-	21,21,36	0.47	0	26,26,47	0.59	0
22	CLA	T	606	15	54,58,73	1.41	6 (11%)	65,95,113	1.38	6 (9%)
22	CLA	K	604	-	68,72,73	1.26	8 (11%)	81,111,113	1.28	5 (6%)
22	CLA	V	601	17	49,53,73	1.51	6 (12%)	59,89,113	1.44	5 (8%)
22	CLA	G	611	6	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	U	409	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	6 (10%)
22	CLA	B	820	1	57,61,73	1.39	7 (12%)	68,98,113	1.50	5 (7%)
22	CLA	B	818	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	W	404	18	69,73,73	1.25	7 (10%)	83,113,113	1.28	5 (6%)
24	DD6	T	612	-	39,45,45	2.03	3 (7%)	52,67,67	1.84	13 (25%)
22	CLA	N	606	8	69,73,73	1.28	7 (10%)	83,113,113	1.26	7 (8%)
22	CLA	L	406	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	K	607	10	61,65,73	1.31	9 (14%)	73,103,113	1.48	9 (12%)
22	CLA	Q	612	10	69,73,73	1.24	7 (10%)	83,113,113	1.28	4 (4%)
22	CLA	S	605	-	64,68,73	1.30	9 (14%)	77,107,113	1.43	7 (9%)
22	CLA	B	837	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
22	CLA	A	816	20	65,69,73	1.29	11 (16%)	78,108,113	1.42	10 (12%)
27	LMU	F	402	-	21,21,36	0.46	0	26,26,47	0.69	0
22	CLA	F	405	5	49,53,73	1.49	8 (16%)	59,89,113	1.38	4 (6%)
22	CLA	B	824	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	7 (8%)
22	CLA	T	604	15	69,73,73	1.24	7 (10%)	83,113,113	1.29	6 (7%)
22	CLA	A	812	20	61,65,73	1.32	8 (13%)	73,103,113	1.30	6 (8%)
22	CLA	X	405	-	60,64,73	1.34	8 (13%)	72,102,113	1.34	6 (8%)
26	LHG	W	420	22	41,41,48	1.19	6 (14%)	44,47,54	0.89	2 (4%)
22	CLA	I	606	8	65,69,73	1.30	9 (13%)	78,108,113	1.29	5 (6%)
22	CLA	U	410	16	59,63,73	1.35	8 (13%)	71,101,113	1.33	5 (7%)
26	LHG	P	601	-	39,39,48	1.20	6 (15%)	42,45,54	0.98	2 (4%)
22	CLA	Q	610	26	69,73,73	1.26	9 (13%)	83,113,113	1.25	5 (6%)
22	CLA	G	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)
22	CLA	G	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	6 (10%)
26	LHG	G	614	22	31,31,48	1.32	6 (19%)	34,37,54	1.06	2 (5%)
22	CLA	L	417	11	69,73,73	1.27	7 (10%)	83,113,113	1.30	5 (6%)
22	CLA	W	415	18	49,53,73	1.53	9 (18%)	59,89,113	1.45	8 (13%)
22	CLA	K	612	10	49,53,73	1.48	8 (16%)	59,89,113	1.39	7 (11%)
22	CLA	B	836	1	55,59,73	1.40	8 (14%)	66,96,113	1.37	5 (7%)
22	CLA	W	405	18	64,68,73	1.31	7 (10%)	77,107,113	1.29	6 (7%)
22	CLA	U	406	-	60,64,73	1.35	7 (11%)	72,102,113	1.33	6 (8%)
22	CLA	Q	606	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
22	CLA	I	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
22	CLA	A	809	20	57,61,73	1.38	8 (14%)	68,98,113	1.36	7 (10%)
22	CLA	B	859	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	6 (7%)
22	CLA	Q	601	-	49,53,73	1.51	9 (18%)	59,89,113	1.43	5 (8%)
22	CLA	R	605	-	69,73,73	1.27	8 (11%)	83,113,113	1.29	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	R	609	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	7 (12%)
22	CLA	K	609	26	64,68,73	1.29	8 (12%)	77,107,113	1.30	4 (5%)
25	DGD	F	401	-	33,33,67	1.08	2 (6%)	35,35,81	1.31	4 (11%)
22	CLA	B	814	1	49,53,73	1.47	8 (16%)	59,89,113	1.42	7 (11%)
26	LHG	X	420	22	41,41,48	1.19	6 (14%)	44,47,54	0.99	2 (4%)
22	CLA	B	834	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
26	LHG	N	614	22	27,27,48	1.38	6 (22%)	30,33,54	1.10	2 (6%)
22	CLA	T	602	15	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	W	409	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
22	CLA	A	838	20	56,60,73	1.39	9 (16%)	67,97,113	1.43	9 (13%)
22	CLA	X	404	19	64,68,73	1.31	7 (10%)	77,107,113	1.27	6 (7%)
22	CLA	W	406	-	60,64,73	1.34	8 (13%)	72,102,113	1.32	5 (6%)
22	CLA	A	842	20	69,73,73	1.26	7 (10%)	83,113,113	1.30	6 (7%)
22	CLA	B	804	1	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
27	LMU	B	849	-	24,24,36	0.45	0	29,29,47	0.65	0
31	CHL	W	408	-	65,74,74	2.71	13 (20%)	59,114,114	1.30	7 (11%)
22	CLA	S	603	14	49,53,73	1.48	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	H	309	26	59,63,73	1.37	8 (13%)	71,101,113	1.34	6 (8%)
27	LMU	H	301	-	21,21,36	0.49	0	26,26,47	0.72	0
22	CLA	G	607	-	64,68,73	1.29	8 (12%)	77,107,113	1.27	5 (6%)
31	CHL	V	605	-	45,54,74	3.25	14 (31%)	35,90,114	1.56	6 (17%)
22	CLA	X	411	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	7 (11%)
26	LHG	O	324	-	41,41,48	1.18	5 (12%)	44,47,54	0.97	2 (4%)
22	CLA	Q	611	10	59,63,73	1.36	8 (13%)	71,101,113	1.33	7 (9%)
22	CLA	B	817	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
22	CLA	A	834	20	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
21	BCR	M	101	-	41,41,41	0.75	0	56,56,56	2.02	16 (28%)
24	DD6	S	611	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
22	CLA	A	836	20	69,73,73	1.25	7 (10%)	83,113,113	1.26	6 (7%)
22	CLA	A	805	20	65,69,73	1.29	7 (10%)	78,108,113	1.30	7 (8%)
22	CLA	A	801	-	69,73,73	1.23	11 (15%)	83,113,113	1.36	10 (12%)
22	CLA	O	311	26	64,68,73	1.29	7 (10%)	77,107,113	1.29	6 (7%)
21	BCR	B	842	-	41,41,41	0.72	0	56,56,56	1.99	15 (26%)
22	CLA	V	607	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	R	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.40	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	837	20	54,58,73	1.42	9 (16%)	65,95,113	1.39	8 (12%)
28	LMG	L	401	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
22	CLA	H	305	7	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
22	CLA	X	407	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
28	LMG	H	317	-	43,43,55	0.79	1 (2%)	51,51,63	1.31	7 (13%)
22	CLA	N	609	8	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)
26	LHG	B	851	-	41,41,48	1.17	6 (14%)	44,47,54	0.99	3 (6%)
22	CLA	R	608	26	58,62,73	1.38	8 (13%)	69,99,113	1.32	5 (7%)
22	CLA	A	824	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	S	604	-	64,68,73	1.31	8 (12%)	77,107,113	1.30	6 (7%)
22	CLA	P	608	-	49,53,73	1.51	8 (16%)	59,89,113	1.44	6 (10%)
22	CLA	A	852	-	69,73,73	1.25	7 (10%)	83,113,113	1.23	6 (7%)
22	CLA	B	829	-	49,53,73	1.44	11 (22%)	59,89,113	1.53	5 (8%)
22	CLA	G	601	6	49,53,73	1.48	7 (14%)	59,89,113	1.45	5 (8%)
22	CLA	L	409	26	64,68,73	1.30	9 (14%)	77,107,113	1.30	5 (6%)
22	CLA	Q	608	10	54,58,73	1.42	7 (12%)	65,95,113	1.38	7 (10%)
22	CLA	A	831	20	69,73,73	1.24	8 (11%)	83,113,113	1.29	6 (7%)
22	CLA	I	602	8	64,68,73	1.31	8 (12%)	77,107,113	1.32	8 (10%)
22	CLA	N	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
22	CLA	B	816	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
24	DD6	X	416	-	39,45,45	2.01	2 (5%)	52,67,67	2.23	15 (28%)
22	CLA	B	825	1	69,73,73	1.25	6 (8%)	83,113,113	1.30	7 (8%)
28	LMG	I	614	-	37,37,55	0.85	0	45,45,63	1.27	5 (11%)
22	CLA	B	839	26	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
22	CLA	H	306	-	59,63,73	1.36	9 (15%)	71,101,113	1.34	5 (7%)
24	DD6	X	401	-	39,45,45	1.98	3 (7%)	52,67,67	1.83	11 (21%)
28	LMG	I	615	-	49,50,55	0.75	0	54,57,63	1.38	4 (7%)
22	CLA	S	607	14	64,68,73	1.31	7 (10%)	77,107,113	1.29	5 (6%)
22	CLA	T	607	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	8 (10%)
24	DD6	A	858	-	39,45,45	1.97	2 (5%)	52,67,67	2.54	18 (34%)
27	LMU	U	424	-	24,24,36	0.42	0	29,29,47	0.58	0
22	CLA	N	611	-	43,48,73	1.56	7 (16%)	52,82,113	1.52	7 (13%)
24	DD6	L	413	-	39,45,45	2.00	3 (7%)	52,67,67	1.78	12 (23%)
26	LHG	N	616	-	42,42,48	1.17	6 (14%)	45,48,54	0.98	2 (4%)
22	CLA	X	409	19	69,73,73	1.25	8 (11%)	83,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LMG	Q	602	-	37,37,55	0.84	1 (2%)	45,45,63	1.28	5 (11%)
24	DD6	H	315	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
22	CLA	A	817	20	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
28	LMG	K	622	-	43,43,55	0.80	0	51,51,63	1.27	5 (9%)
27	LMU	A	854	-	36,36,36	0.42	0	47,47,47	0.69	1 (2%)
22	CLA	K	611	10	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
27	LMU	L	419	-	27,27,36	0.41	0	30,30,47	0.75	0
24	DD6	Q	615	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	14 (26%)
26	LHG	U	419	22	24,24,48	1.42	5 (20%)	27,29,54	1.22	2 (7%)
31	CHL	X	406	-	45,54,74	3.28	13 (28%)	35,90,114	1.58	6 (17%)
24	DD6	A	859	-	39,45,45	2.07	3 (7%)	52,67,67	1.88	13 (25%)
28	LMG	K	618	-	49,49,55	0.76	0	57,57,63	1.31	7 (12%)
22	CLA	L	410	11	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
26	LHG	B	848	22	26,26,48	1.33	5 (19%)	29,32,54	1.15	2 (6%)
22	CLA	T	609	15	49,53,73	1.48	8 (16%)	59,89,113	1.44	7 (11%)
28	LMG	H	322	-	37,37,55	0.85	0	45,45,63	1.23	4 (8%)
23	PQN	B	840	-	34,34,34	1.61	2 (5%)	42,45,45	1.07	3 (7%)
22	CLA	U	403	16	49,53,73	1.50	7 (14%)	59,89,113	1.47	6 (10%)
28	LMG	B	852	-	43,43,55	0.84	0	51,51,63	1.27	4 (7%)
27	LMU	O	303	-	36,36,36	0.42	0	47,47,47	0.71	1 (2%)
26	LHG	A	845	-	48,48,48	1.10	6 (12%)	51,54,54	0.94	3 (5%)
22	CLA	L	402	11	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
22	CLA	R	602	-	64,68,73	1.31	8 (12%)	77,107,113	1.28	5 (6%)
22	CLA	Q	613	10	49,53,73	1.48	8 (16%)	59,89,113	1.46	7 (11%)
22	CLA	B	805	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
22	CLA	X	412	19	69,73,73	1.27	8 (11%)	83,113,113	1.27	6 (7%)
22	CLA	O	306	13	64,68,73	1.30	8 (12%)	77,107,113	1.29	7 (9%)
22	CLA	T	610	-	49,53,73	1.49	6 (12%)	59,89,113	1.41	4 (6%)
22	CLA	H	313	7	62,66,73	1.33	7 (11%)	74,104,113	1.32	6 (8%)
22	CLA	S	609	14	59,63,73	1.36	6 (10%)	71,101,113	1.31	6 (8%)
24	DD6	T	613	-	39,45,45	1.98	3 (7%)	52,67,67	1.73	11 (21%)
22	CLA	R	606	11	61,65,73	1.34	6 (9%)	73,103,113	1.29	6 (8%)
22	CLA	T	601	15	49,53,73	1.48	8 (16%)	59,89,113	1.45	4 (6%)
22	CLA	I	609	8	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)
22	CLA	P	606	6	49,53,73	1.47	8 (16%)	59,89,113	1.43	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	820	20	69,73,73	1.25	8 (11%)	83,113,113	1.27	9 (10%)
22	CLA	A	825	20	65,69,73	1.27	6 (9%)	78,108,113	1.29	6 (7%)
22	CLA	O	312	13	64,68,73	1.29	8 (12%)	77,107,113	1.32	9 (11%)
21	BCR	A	851	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
22	CLA	A	839	20	69,73,73	1.24	6 (8%)	83,113,113	1.38	8 (9%)
22	CLA	P	607	6	49,53,73	1.49	9 (18%)	59,89,113	1.43	5 (8%)
22	CLA	V	608	17	59,63,73	1.35	7 (11%)	71,101,113	1.31	6 (8%)
22	CLA	A	844	26	59,63,73	1.36	9 (15%)	71,101,113	1.39	7 (9%)
22	CLA	W	403	18	56,60,73	1.41	9 (16%)	67,97,113	1.39	7 (10%)
25	DGD	O	304	-	61,61,67	0.87	3 (4%)	75,75,81	1.14	8 (10%)
22	CLA	B	806	1	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	S	614	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	5 (8%)
24	DD6	W	416	-	39,45,45	1.97	3 (7%)	52,67,67	1.80	11 (21%)
22	CLA	T	603	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	6 (7%)
22	CLA	Q	605	-	60,64,73	1.34	7 (11%)	72,102,113	1.34	8 (11%)
22	CLA	A	840	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	A	833	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
22	CLA	K	606	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	6 (9%)
22	CLA	N	610	8	59,63,73	1.36	7 (11%)	71,101,113	1.43	8 (11%)
27	LMU	B	858	-	14,14,36	0.31	0	13,13,47	0.58	0
25	DGD	B	847	-	67,67,67	0.83	2 (2%)	81,81,81	1.01	5 (6%)
22	CLA	X	408	19	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
28	LMG	A	855	-	41,41,55	0.84	0	49,49,63	1.26	5 (10%)
22	CLA	U	413	16	49,53,73	1.49	7 (14%)	59,89,113	1.47	6 (10%)
22	CLA	R	610	11	69,73,73	1.27	7 (10%)	83,113,113	1.24	7 (8%)
22	CLA	N	607	-	64,68,73	1.31	7 (10%)	77,107,113	1.28	6 (7%)
22	CLA	R	611	11	49,53,73	1.50	7 (14%)	59,89,113	1.41	5 (8%)
24	DD6	R	613	-	39,45,45	2.01	3 (7%)	52,67,67	2.01	18 (34%)
22	CLA	B	803	1	60,64,73	1.34	6 (10%)	72,102,113	1.34	7 (9%)
22	CLA	W	419	18	49,53,73	1.49	7 (14%)	59,89,113	1.44	4 (6%)
24	DD6	L	414	-	39,45,45	2.01	3 (7%)	52,67,67	1.80	15 (28%)
22	CLA	S	610	14	49,53,73	1.50	7 (14%)	59,89,113	1.51	5 (8%)
22	CLA	A	832	20	56,60,73	1.39	8 (14%)	67,97,113	1.36	6 (8%)
28	LMG	T	616	-	41,41,55	0.84	0	49,49,63	1.24	3 (6%)
27	LMU	B	855	-	24,24,36	0.45	0	29,29,47	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	I	610	8	49,53,73	1.49	9 (18%)	59,89,113	1.44	5 (8%)
22	CLA	T	611	15	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
22	CLA	H	307	7	64,68,73	1.31	7 (10%)	77,107,113	1.29	4 (5%)
22	CLA	P	602	6	49,53,73	1.47	10 (20%)	59,89,113	1.48	6 (10%)
22	CLA	N	603	8	69,73,73	1.26	8 (11%)	83,113,113	1.26	7 (8%)
22	CLA	U	415	16	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)
24	DD6	O	316	-	39,45,45	1.96	3 (7%)	52,67,67	1.72	12 (23%)
27	LMU	G	615	-	21,21,36	0.46	0	26,26,47	0.51	0
22	CLA	B	822	1	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	Q	618	-	49,53,73	1.50	7 (14%)	59,89,113	1.41	4 (6%)
22	CLA	V	613	-	49,53,73	1.51	6 (12%)	59,89,113	1.48	4 (6%)
24	DD6	V	615	-	39,45,45	1.94	3 (7%)	52,67,67	1.87	13 (25%)
21	BCR	J	103	-	41,41,41	0.68	0	56,56,56	1.78	12 (21%)
22	CLA	L	403	11	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
22	CLA	A	835	20	65,69,73	1.29	8 (12%)	78,108,113	1.29	6 (7%)
22	CLA	U	414	16	65,69,73	1.30	8 (12%)	78,108,113	1.31	5 (6%)
27	LMU	B	850	-	24,24,36	0.44	0	29,29,47	0.55	0
26	LHG	Q	616	22	43,43,48	1.16	6 (13%)	46,49,54	0.94	2 (4%)
22	CLA	I	603	8	60,64,73	1.36	8 (13%)	72,102,113	1.31	7 (9%)
27	LMU	H	321	-	34,34,36	0.48	0	44,44,47	0.79	2 (4%)
22	CLA	K	603	10	64,68,73	1.30	8 (12%)	77,107,113	1.30	6 (7%)
30	SQD	O	302	-	41,42,54	0.43	1 (2%)	50,53,65	0.52	1 (2%)
24	DD6	U	417	-	39,45,45	1.93	3 (7%)	52,67,67	1.87	15 (28%)
22	CLA	B	813	1	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
22	CLA	U	411	16	61,65,73	1.32	7 (11%)	73,103,113	1.31	6 (8%)
22	CLA	L	412	11	49,53,73	1.49	8 (16%)	59,89,113	1.38	5 (8%)
22	CLA	H	308	7	64,68,73	1.29	7 (10%)	77,107,113	1.29	6 (7%)
24	DD6	W	418	-	39,45,45	2.02	3 (7%)	52,67,67	1.89	14 (26%)
26	LHG	K	616	22	38,38,48	1.22	5 (13%)	41,44,54	1.03	3 (7%)
22	CLA	N	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
27	LMU	A	853	-	24,24,36	0.43	0	29,29,47	0.57	0
22	CLA	S	608	26	49,53,73	1.50	7 (14%)	59,89,113	1.42	6 (10%)
30	SQD	V	618	-	26,27,54	0.52	1 (3%)	33,36,65	0.45	0
21	BCR	B	846	-	41,41,41	0.71	0	56,56,56	1.82	17 (30%)
22	CLA	A	810	20	69,73,73	1.24	7 (10%)	83,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	U	401	-	59,63,73	1.36	8 (13%)	71,101,113	1.34	7 (9%)
24	DD6	F	406	-	39,45,45	2.01	3 (7%)	52,67,67	1.89	16 (30%)
22	CLA	A	806	20	69,73,73	1.25	7 (10%)	83,113,113	1.26	6 (7%)
22	CLA	A	804	-	69,73,73	1.25	7 (10%)	83,113,113	1.21	5 (6%)
22	CLA	X	417	19	54,58,73	1.42	6 (11%)	65,95,113	1.41	8 (12%)
22	CLA	P	609	-	49,53,73	1.49	9 (18%)	59,89,113	1.41	4 (6%)
22	CLA	G	606	6	69,73,73	1.26	8 (11%)	83,113,113	1.23	5 (6%)
22	CLA	I	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	7 (11%)
29	SF4	B	860	20,1	0,12,12	-	-	-		
22	CLA	A	823	20	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
27	LMU	K	620	-	34,34,36	0.50	0	44,44,47	1.04	5 (11%)
21	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.81	10 (17%)
22	CLA	K	605	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	4 (4%)
22	CLA	P	611	6	49,53,73	1.50	6 (12%)	59,89,113	1.48	5 (8%)
22	CLA	O	309	13	54,58,73	1.40	9 (16%)	65,95,113	1.41	5 (7%)
24	DD6	O	317	-	39,45,45	2.01	3 (7%)	52,67,67	1.79	14 (26%)
22	CLA	S	615	-	55,59,73	1.40	8 (14%)	66,96,113	1.39	6 (9%)
26	LHG	A	846	22	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
22	CLA	U	404	16	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	X	402	19	59,63,73	1.35	7 (11%)	71,101,113	1.36	7 (9%)
27	LMU	O	301	-	24,24,36	0.44	0	29,29,47	0.57	0
27	LMU	U	422	-	36,36,36	0.44	0	47,47,47	0.79	2 (4%)
21	BCR	B	801	-	41,41,41	0.69	0	56,56,56	1.96	16 (28%)
27	LMU	U	421	-	36,36,36	0.41	0	47,47,47	0.65	1 (2%)
33	CL0	A	802	20	63,73,73	2.83	21 (33%)	61,113,113	1.91	12 (19%)
27	LMU	A	856	-	21,21,36	0.46	0	26,26,47	0.50	0
26	LHG	T	614	22	41,41,48	1.19	6 (14%)	44,47,54	0.98	2 (4%)
22	CLA	Q	604	10	69,73,73	1.25	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	Q	607	-	49,53,73	1.49	7 (14%)	59,89,113	1.42	5 (8%)
31	CHL	W	422	-	65,74,74	2.67	13 (20%)	59,114,114	1.27	6 (10%)
22	CLA	B	815	1	56,60,73	1.39	9 (16%)	67,97,113	1.32	6 (8%)
24	DD6	K	614	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	15 (28%)
29	SF4	C	102	2	0,12,12	-	-	-		
22	CLA	H	304	7	49,53,73	1.48	8 (16%)	59,89,113	1.43	7 (11%)
22	CLA	O	310	13	64,68,73	1.29	9 (14%)	77,107,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SQD	F	407	-	41,42,54	0.42	1 (2%)	50,53,65	0.49	1 (2%)
23	PQN	A	843	-	34,34,34	1.59	2 (5%)	42,45,45	1.08	3 (7%)
26	LHG	R	614	22	41,41,48	1.18	6 (14%)	44,47,54	0.96	2 (4%)
24	DD6	A	847	-	39,45,45	1.98	3 (7%)	52,67,67	1.85	15 (28%)
22	CLA	B	807	1	69,73,73	1.24	9 (13%)	83,113,113	1.24	5 (6%)
22	CLA	H	318	7	49,53,73	1.49	7 (14%)	59,89,113	1.44	5 (8%)
27	LMU	B	854	-	24,24,36	0.46	0	29,29,47	0.81	1 (3%)
22	CLA	O	305	13	54,58,73	1.40	8 (14%)	65,95,113	1.41	8 (12%)
22	CLA	B	832	1	66,70,73	1.27	8 (12%)	79,109,113	1.34	7 (8%)
22	CLA	B	833	1	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
22	CLA	W	412	26	64,68,73	1.31	9 (14%)	77,107,113	1.32	6 (7%)

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
24	DD6	H	314	-	-	1/26/80/80	0/3/3/3
22	CLA	O	315	13	-	4/21/97/115	-
22	CLA	B	838	1	-	7/15/91/115	-
29	SF4	C	101	2	-	-	0/6/5/5
24	DD6	P	612	-	-	6/26/80/80	0/3/3/3
22	CLA	O	314	13	-	1/15/91/115	-
22	CLA	L	407	-	-	11/30/106/115	-
27	LMU	T	618	-	-	1/15/35/61	0/1/1/2
22	CLA	A	828	20	-	8/39/115/115	-
22	CLA	L	411	11	-	14/39/115/115	-
22	CLA	G	602	6	-	4/33/109/115	-
27	LMU	X	418	-	-	1/15/35/61	0/1/1/2
26	LHG	L	416	22	-	20/46/46/53	-
22	CLA	W	402	18	-	2/27/103/115	-
24	DD6	V	614	-	-	1/26/80/80	0/3/3/3
28	LMG	U	423	-	-	20/44/64/70	0/1/1/1
22	CLA	S	602	14	-	9/33/109/115	-
28	LMG	H	319	-	-	19/35/55/70	0/1/1/1
22	CLA	B	830	1	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	X	410	26	-	12/33/109/115	-
22	CLA	B	812	1	-	18/39/115/115	-
30	SQD	K	621	-	-	5/38/58/69	0/1/1/1
24	DD6	J	105	-	-	3/26/80/80	0/3/3/3
22	CLA	B	835	1	-	11/39/115/115	-
24	DD6	B	841	-	-	1/26/80/80	0/3/3/3
22	CLA	L	404	-	-	12/29/105/115	-
22	CLA	S	606	14	-	4/21/97/115	-
32	NEX	V	616	-	-	4/27/83/83	0/3/3/3
22	CLA	A	841	20	-	12/39/115/115	-
21	BCR	A	849	-	-	0/29/63/63	0/2/2/2
27	LMU	B	853	-	-	0/10/27/61	0/1/1/2
22	CLA	V	602	17	-	8/39/115/115	-
22	CLA	B	810	-	-	4/29/105/115	-
22	CLA	B	808	1	-	7/27/103/115	-
27	LMU	M	102	-	-	4/15/35/61	0/1/1/2
27	LMU	X	421	-	-	3/21/61/61	0/2/2/2
22	CLA	B	809	1	-	3/39/115/115	-
22	CLA	B	821	1	-	11/33/109/115	-
24	DD6	G	612	-	-	0/26/80/80	0/3/3/3
22	CLA	B	831	1	-	7/39/115/115	-
22	CLA	U	412	26	-	3/15/91/115	-
27	LMU	O	322	-	-	5/21/61/61	0/2/2/2
22	CLA	Q	617	10	-	5/24/100/115	-
22	CLA	B	823	-	-	10/39/115/115	-
22	CLA	P	610	6	-	5/10/86/115	-
22	CLA	W	414	18	-	10/39/115/115	-
21	BCR	B	844	-	-	1/29/63/63	0/2/2/2
22	CLA	O	308	-	-	14/35/111/115	-
22	CLA	H	302	7	-	4/15/91/115	-
28	LMG	J	101	-	-	23/50/70/70	0/1/1/1
22	CLA	V	612	-	-	15/39/115/115	-
22	CLA	I	607	8	-	4/27/103/115	-
24	DD6	U	416	-	-	1/26/80/80	0/3/3/3
22	CLA	A	807	20	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	H	310	7	-	3/15/91/115	-
22	CLA	S	601	14	-	6/15/91/115	-
27	LMU	A	857	-	-	3/15/35/61	0/1/1/2
22	CLA	K	608	10	-	11/39/115/115	-
21	BCR	B	843	-	-	4/29/63/63	0/2/2/2
22	CLA	F	403	-	-	11/39/115/115	-
26	LHG	O	323	-	-	19/47/47/53	-
22	CLA	N	602	8	-	5/33/109/115	-
22	CLA	K	613	-	-	5/25/101/115	-
22	CLA	N	601	8	-	6/15/91/115	-
24	DD6	W	417	-	-	1/26/80/80	0/3/3/3
28	LMG	F	408	-	-	18/37/57/70	0/1/1/1
27	LMU	H	320	-	-	2/15/35/61	0/1/1/2
22	CLA	B	826	1	-	10/31/107/115	-
28	LMG	K	601	-	-	24/38/58/70	0/1/1/1
22	CLA	V	611	-	-	5/15/91/115	-
24	DD6	S	612	-	-	1/26/80/80	0/3/3/3
22	CLA	T	608	26	-	4/33/109/115	-
26	LHG	H	316	22	-	5/31/31/53	-
22	CLA	A	822	-	-	8/39/115/115	-
24	DD6	Q	614	-	-	1/26/80/80	0/3/3/3
24	DD6	I	613	-	-	0/26/80/80	0/3/3/3
22	CLA	R	603	-	-	10/29/105/115	-
26	LHG	S	613	22	-	13/36/36/53	-
22	CLA	I	601	8	-	15/39/115/115	-
24	DD6	N	612	-	-	0/26/80/80	0/3/3/3
22	CLA	P	603	6	-	5/15/91/115	-
22	CLA	R	601	-	-	19/39/115/115	-
22	CLA	A	818	20	-	4/25/101/115	-
22	CLA	U	405	16	-	5/30/106/115	-
22	CLA	G	608	26	-	16/33/109/115	-
22	CLA	A	830	20	-	13/39/115/115	-
27	LMU	T	617	-	-	3/15/35/61	0/1/1/2
22	CLA	L	408	11	-	6/33/109/115	-
22	CLA	A	811	20	-	10/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CHL	U	408	-	-	1/15/113/137	-
22	CLA	Q	603	10	-	4/15/91/115	-
22	CLA	A	815	20	-	6/39/115/115	-
28	LMG	G	616	-	-	21/41/61/70	0/1/1/1
24	DD6	P	613	-	-	4/26/80/80	0/3/3/3
22	CLA	W	411	18	-	10/33/109/115	-
27	LMU	J	104	-	-	9/21/57/61	0/2/2/2
22	CLA	G	610	6	-	5/15/91/115	-
24	DD6	G	613	-	-	1/26/80/80	0/3/3/3
24	DD6	I	612	-	-	0/26/80/80	0/3/3/3
28	LMG	N	615	-	-	24/39/59/70	0/1/1/1
26	LHG	K	619	-	-	19/37/37/53	-
27	LMU	L	420	-	-	4/21/57/61	1/2/2/2
24	DD6	R	612	-	-	1/26/80/80	0/3/3/3
28	LMG	B	856	-	-	26/48/68/70	0/1/1/1
22	CLA	A	808	20	-	12/39/115/115	-
22	CLA	W	413	-	-	6/15/91/115	-
22	CLA	X	413	19	-	3/15/91/115	-
22	CLA	A	803	-	-	12/39/115/115	-
28	LMG	W	401	-	-	19/43/63/70	0/1/1/1
22	CLA	N	608	26	-	7/15/91/115	-
22	CLA	B	811	1	-	2/15/91/115	-
22	CLA	T	605	-	-	15/39/115/115	-
22	CLA	B	828	1	-	15/39/115/115	-
22	CLA	G	609	-	-	4/15/91/115	-
22	CLA	Q	609	10	-	9/33/109/115	-
22	CLA	P	605	-	-	8/15/91/115	-
22	CLA	H	303	7	-	11/33/109/115	-
22	CLA	V	609	17	-	8/30/106/115	-
22	CLA	J	102	9	-	7/21/97/115	-
24	DD6	N	613	-	-	4/26/80/80	0/3/3/3
26	LHG	O	318	22	-	16/38/38/53	-
21	BCR	B	845	-	-	2/29/63/63	0/2/2/2
22	CLA	K	602	10	-	11/33/109/115	-
22	CLA	O	307	13	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	W	421	-	-	4/15/35/61	0/1/1/2
22	CLA	R	615	11	-	13/39/115/115	-
32	NEX	U	418	-	-	4/27/83/83	0/3/3/3
22	CLA	B	827	1	-	9/39/115/115	-
22	CLA	A	814	20	-	9/39/115/115	-
22	CLA	X	403	19	-	9/39/115/115	-
22	CLA	I	608	-	-	5/15/91/115	-
22	CLA	V	617	-	-	10/15/91/115	-
27	LMU	O	320	-	-	1/17/35/61	0/2/2/2
22	CLA	B	802	1	-	6/39/115/115	-
22	CLA	A	819	20	-	11/31/107/115	-
22	CLA	A	827	-	-	5/36/112/115	-
22	CLA	A	813	20	-	10/39/115/115	-
27	LMU	L	418	-	-	0/15/35/61	0/1/1/2
22	CLA	K	617	10	-	12/39/115/115	-
22	CLA	O	313	13	-	14/39/115/115	-
22	CLA	R	607	11	-	17/33/109/115	-
22	CLA	F	404	-	-	10/27/103/115	-
22	CLA	O	319	13	-	1/15/91/115	-
22	CLA	B	819	1	-	9/25/101/115	-
27	LMU	B	857	-	-	4/21/61/61	0/2/2/2
22	CLA	A	826	-	-	8/39/115/115	-
26	LHG	O	321	-	-	30/53/53/53	-
22	CLA	K	610	10	-	8/29/105/115	-
22	CLA	H	311	7	-	16/39/115/115	-
22	CLA	U	420	16	-	9/15/91/115	-
22	CLA	P	604	-	-	6/15/91/115	-
22	CLA	X	419	19	-	9/15/91/115	-
22	CLA	G	603	6	-	10/29/105/115	-
22	CLA	H	312	7	-	3/15/91/115	-
31	CHL	V	606	-	-	1/15/113/137	-
22	CLA	L	405	-	-	3/15/91/115	-
22	CLA	V	610	-	-	4/15/91/115	-
31	CHL	W	407	-	-	2/15/113/137	-
24	DD6	X	415	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	U	402	-	-	25/48/68/70	0/1/1/1
31	CHL	U	407	-	-	0/15/113/137	-
27	LMU	F	409	-	-	4/12/32/61	0/1/1/2
24	DD6	L	415	-	-	3/26/80/80	0/3/3/3
22	CLA	I	611	8	-	6/15/91/115	-
22	CLA	V	604	-	-	9/29/105/115	-
22	CLA	A	829	20	-	15/39/115/115	-
22	CLA	W	410	18	-	10/33/109/115	-
21	BCR	A	850	-	-	4/29/63/63	0/2/2/2
24	DD6	K	615	-	-	0/26/80/80	0/3/3/3
24	DD6	X	414	-	-	1/26/80/80	0/3/3/3
22	CLA	A	821	20	-	15/39/115/115	-
22	CLA	V	603	17	-	11/30/106/115	-
27	LMU	T	615	-	-	0/12/32/61	0/1/1/2
22	CLA	T	606	15	-	5/21/97/115	-
22	CLA	K	604	-	-	19/37/113/115	-
22	CLA	V	601	17	-	6/15/91/115	-
22	CLA	G	611	6	-	5/15/91/115	-
22	CLA	U	409	-	-	6/15/91/115	-
22	CLA	B	820	1	-	8/25/101/115	-
22	CLA	B	818	-	-	12/39/115/115	-
22	CLA	W	404	18	-	10/39/115/115	-
24	DD6	T	612	-	-	1/26/80/80	0/3/3/3
22	CLA	N	606	8	-	13/39/115/115	-
22	CLA	L	406	-	-	10/39/115/115	-
22	CLA	K	607	10	-	9/30/106/115	-
22	CLA	Q	612	10	-	15/39/115/115	-
22	CLA	S	605	-	-	14/33/109/115	-
22	CLA	B	837	-	-	3/15/91/115	-
22	CLA	A	816	20	-	14/35/111/115	-
27	LMU	F	402	-	-	1/12/32/61	0/1/1/2
22	CLA	F	405	5	-	7/15/91/115	-
22	CLA	B	824	-	-	11/39/115/115	-
22	CLA	T	604	15	-	18/39/115/115	-
22	CLA	A	812	20	-	10/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	X	405	-	-	8/29/105/115	-
26	LHG	W	420	22	-	22/46/46/53	-
22	CLA	I	606	8	-	12/35/111/115	-
22	CLA	U	410	16	-	7/27/103/115	-
26	LHG	P	601	-	-	23/44/44/53	-
22	CLA	Q	610	26	-	16/39/115/115	-
22	CLA	G	605	-	-	3/15/91/115	-
22	CLA	G	604	-	-	0/15/91/115	-
26	LHG	G	614	22	-	13/36/36/53	-
22	CLA	L	417	11	-	8/39/115/115	-
22	CLA	W	415	18	-	6/15/91/115	-
22	CLA	K	612	10	-	2/15/91/115	-
22	CLA	B	836	1	-	2/23/99/115	-
22	CLA	W	405	18	-	3/33/109/115	-
22	CLA	U	406	-	-	7/29/105/115	-
22	CLA	Q	606	-	-	7/15/91/115	-
22	CLA	I	604	-	-	1/15/91/115	-
22	CLA	A	809	20	-	1/25/101/115	-
22	CLA	B	859	-	-	12/39/115/115	-
22	CLA	Q	601	-	-	6/15/91/115	-
22	CLA	R	605	-	-	15/39/115/115	-
22	CLA	R	609	-	-	3/10/86/115	-
22	CLA	K	609	26	-	13/33/109/115	-
25	DGD	F	401	-	-	19/35/35/95	-
22	CLA	B	814	1	-	6/15/91/115	-
26	LHG	X	420	22	-	28/46/46/53	-
22	CLA	B	834	1	-	7/39/115/115	-
26	LHG	N	614	22	-	9/32/32/53	-
22	CLA	T	602	15	-	9/39/115/115	-
22	CLA	W	409	-	-	10/39/115/115	-
22	CLA	A	838	20	-	7/24/100/115	-
22	CLA	X	404	19	-	8/33/109/115	-
22	CLA	W	406	-	-	2/29/105/115	-
22	CLA	A	842	20	-	12/39/115/115	-
22	CLA	B	804	1	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	B	849	-	-	2/15/35/61	0/1/1/2
31	CHL	W	408	-	-	4/39/137/137	-
22	CLA	S	603	14	-	3/15/91/115	-
22	CLA	H	309	26	-	10/27/103/115	-
27	LMU	H	301	-	-	2/12/32/61	0/1/1/2
22	CLA	G	607	-	-	3/33/109/115	-
31	CHL	V	605	-	-	0/15/113/137	-
22	CLA	X	411	-	-	3/15/91/115	-
26	LHG	O	324	-	-	25/46/46/53	-
22	CLA	Q	611	10	-	9/27/103/115	-
22	CLA	B	817	1	-	15/39/115/115	-
22	CLA	A	834	20	-	5/15/91/115	-
21	BCR	M	101	-	-	2/29/63/63	0/2/2/2
24	DD6	S	611	-	-	1/26/80/80	0/3/3/3
22	CLA	A	836	20	-	12/39/115/115	-
22	CLA	A	805	20	-	9/35/111/115	-
22	CLA	A	801	-	-	15/39/115/115	-
22	CLA	O	311	26	-	9/33/109/115	-
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
22	CLA	V	607	-	-	3/15/91/115	-
22	CLA	R	604	-	-	5/15/91/115	-
22	CLA	A	837	20	-	6/21/97/115	-
28	LMG	L	401	-	-	20/46/66/70	0/1/1/1
22	CLA	H	305	7	-	11/33/109/115	-
22	CLA	X	407	-	-	4/39/115/115	-
28	LMG	H	317	-	-	13/38/58/70	0/1/1/1
22	CLA	N	609	8	-	4/15/91/115	-
26	LHG	B	851	-	-	22/46/46/53	-
22	CLA	R	608	26	-	10/26/102/115	-
22	CLA	A	824	20	-	25/39/115/115	-
22	CLA	S	604	-	-	9/33/109/115	-
22	CLA	P	608	-	-	9/15/91/115	-
22	CLA	A	852	-	-	14/39/115/115	-
22	CLA	B	829	-	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	G	601	6	-	6/15/91/115	-
22	CLA	L	409	26	-	6/33/109/115	-
22	CLA	Q	608	10	-	3/21/97/115	-
22	CLA	A	831	20	-	6/39/115/115	-
22	CLA	I	602	8	-	3/33/109/115	-
22	CLA	N	604	-	-	6/15/91/115	-
22	CLA	B	816	1	-	13/39/115/115	-
24	DD6	X	416	-	-	5/26/80/80	0/3/3/3
22	CLA	B	825	1	-	10/39/115/115	-
28	LMG	I	614	-	-	10/32/52/70	0/1/1/1
22	CLA	B	839	26	-	3/39/115/115	-
22	CLA	H	306	-	-	10/27/103/115	-
24	DD6	X	401	-	-	0/26/80/80	0/3/3/3
28	LMG	I	615	-	-	26/46/62/70	0/1/1/1
22	CLA	S	607	14	-	9/33/109/115	-
22	CLA	T	607	15	-	9/33/109/115	-
24	DD6	A	858	-	-	5/26/80/80	0/3/3/3
27	LMU	U	424	-	-	2/15/35/61	0/1/1/2
22	CLA	N	611	-	-	4/10/82/115	-
24	DD6	L	413	-	-	1/26/80/80	0/3/3/3
26	LHG	N	616	-	-	23/47/47/53	-
22	CLA	X	409	19	-	10/39/115/115	-
28	LMG	Q	602	-	-	11/32/52/70	0/1/1/1
24	DD6	H	315	-	-	1/26/80/80	0/3/3/3
22	CLA	A	817	20	-	16/39/115/115	-
28	LMG	K	622	-	-	15/38/58/70	0/1/1/1
27	LMU	A	854	-	-	3/21/61/61	0/2/2/2
22	CLA	K	611	10	-	11/39/115/115	-
27	LMU	L	419	-	-	6/21/34/61	1/1/1/2
24	DD6	Q	615	-	-	0/26/80/80	0/3/3/3
26	LHG	U	419	22	-	15/28/28/53	-
31	CHL	X	406	-	-	0/15/113/137	-
24	DD6	A	859	-	-	1/26/80/80	0/3/3/3
28	LMG	K	618	-	-	24/44/64/70	0/1/1/1
22	CLA	L	410	11	-	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	B	848	22	-	10/31/31/53	-
22	CLA	T	609	15	-	5/15/91/115	-
28	LMG	H	322	-	-	15/32/52/70	0/1/1/1
23	PQN	B	840	-	-	0/23/43/43	0/2/2/2
22	CLA	U	403	16	-	8/15/91/115	-
28	LMG	B	852	-	-	15/38/58/70	0/1/1/1
27	LMU	O	303	-	-	2/21/61/61	0/2/2/2
26	LHG	A	845	-	-	25/53/53/53	-
22	CLA	L	402	11	-	17/39/115/115	-
22	CLA	R	602	-	-	12/33/109/115	-
22	CLA	Q	613	10	-	6/15/91/115	-
22	CLA	B	805	1	-	7/39/115/115	-
22	CLA	X	412	19	-	12/39/115/115	-
22	CLA	O	306	13	-	7/33/109/115	-
22	CLA	T	610	-	-	7/15/91/115	-
22	CLA	H	313	7	-	10/31/107/115	-
22	CLA	S	609	14	-	9/27/103/115	-
24	DD6	T	613	-	-	1/26/80/80	0/3/3/3
22	CLA	R	606	11	-	12/30/106/115	-
22	CLA	T	601	15	-	5/15/91/115	-
22	CLA	I	609	8	-	4/15/91/115	-
22	CLA	P	606	6	-	6/15/91/115	-
22	CLA	A	820	20	-	12/39/115/115	-
22	CLA	A	825	20	-	17/35/111/115	-
22	CLA	O	312	13	-	8/33/109/115	-
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
22	CLA	A	839	20	-	6/39/115/115	-
22	CLA	P	607	6	-	4/15/91/115	-
22	CLA	V	608	17	-	8/27/103/115	-
22	CLA	A	844	26	-	12/27/103/115	-
22	CLA	W	403	18	-	7/24/100/115	-
25	DGD	O	304	-	-	31/49/89/95	0/2/2/2
22	CLA	B	806	1	-	13/39/115/115	-
22	CLA	S	614	-	-	0/15/91/115	-
24	DD6	W	416	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	T	603	15	-	8/33/109/115	-
22	CLA	Q	605	-	-	3/29/105/115	-
22	CLA	A	840	20	-	16/39/115/115	-
22	CLA	A	833	20	-	6/39/115/115	-
22	CLA	K	606	-	-	1/21/97/115	-
22	CLA	N	610	8	-	18/27/103/115	-
27	LMU	B	858	-	-	2/12/12/61	-
25	DGD	B	847	-	-	33/55/95/95	0/2/2/2
22	CLA	X	408	19	-	12/39/115/115	-
28	LMG	A	855	-	-	12/36/56/70	0/1/1/1
22	CLA	U	413	16	-	5/15/91/115	-
22	CLA	R	610	11	-	12/39/115/115	-
22	CLA	N	607	-	-	14/33/109/115	-
22	CLA	R	611	11	-	6/15/91/115	-
24	DD6	R	613	-	-	1/26/80/80	0/3/3/3
22	CLA	B	803	1	-	7/29/105/115	-
22	CLA	W	419	18	-	6/15/91/115	-
24	DD6	L	414	-	-	2/26/80/80	0/3/3/3
22	CLA	S	610	14	-	4/15/91/115	-
22	CLA	A	832	20	-	5/24/100/115	-
28	LMG	T	616	-	-	16/36/56/70	0/1/1/1
27	LMU	B	855	-	-	2/15/35/61	0/1/1/2
22	CLA	I	610	8	-	8/15/91/115	-
22	CLA	T	611	15	-	15/39/115/115	-
22	CLA	H	307	7	-	11/33/109/115	-
22	CLA	P	602	6	-	10/15/91/115	-
22	CLA	N	603	8	-	10/39/115/115	-
22	CLA	U	415	16	-	7/15/91/115	-
24	DD6	O	316	-	-	1/26/80/80	0/3/3/3
27	LMU	G	615	-	-	0/12/32/61	0/1/1/2
22	CLA	B	822	1	-	10/39/115/115	-
22	CLA	Q	618	-	-	9/15/91/115	-
22	CLA	V	613	-	-	11/15/91/115	-
24	DD6	V	615	-	-	3/26/80/80	0/3/3/3
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	L	403	11	-	5/33/109/115	-
22	CLA	A	835	20	-	9/35/111/115	-
22	CLA	U	414	16	-	14/35/111/115	-
27	LMU	B	850	-	-	3/15/35/61	0/1/1/2
26	LHG	Q	616	22	-	15/48/48/53	-
22	CLA	I	603	8	-	9/29/105/115	-
27	LMU	H	321	-	-	1/19/56/61	0/2/2/2
22	CLA	K	603	10	-	7/33/109/115	-
30	SQD	O	302	-	-	5/37/57/69	0/1/1/1
24	DD6	U	417	-	-	1/26/80/80	0/3/3/3
22	CLA	B	813	1	-	10/39/115/115	-
22	CLA	U	411	16	-	7/30/106/115	-
22	CLA	L	412	11	-	5/15/91/115	-
22	CLA	H	308	7	-	6/33/109/115	-
24	DD6	W	418	-	-	1/26/80/80	0/3/3/3
26	LHG	K	616	22	-	18/43/43/53	-
22	CLA	N	605	-	-	1/15/91/115	-
27	LMU	A	853	-	-	0/15/35/61	0/1/1/2
22	CLA	S	608	26	-	9/15/91/115	-
30	SQD	V	618	-	-	4/19/39/69	0/1/1/1
21	BCR	B	846	-	-	6/29/63/63	0/2/2/2
22	CLA	A	810	20	-	10/39/115/115	-
22	CLA	U	401	-	-	9/27/103/115	-
24	DD6	F	406	-	-	7/26/80/80	0/3/3/3
22	CLA	A	806	20	-	10/39/115/115	-
22	CLA	A	804	-	-	6/39/115/115	-
22	CLA	X	417	19	-	5/21/97/115	-
22	CLA	P	609	-	-	8/15/91/115	-
22	CLA	G	606	6	-	12/39/115/115	-
22	CLA	I	605	-	-	2/15/91/115	-
29	SF4	B	860	20,1	-	-	0/6/5/5
22	CLA	A	823	20	-	5/15/91/115	-
27	LMU	K	620	-	-	6/19/56/61	0/2/2/2
21	BCR	A	848	-	-	0/29/63/63	0/2/2/2
22	CLA	K	605	-	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	611	6	-	6/15/91/115	-
22	CLA	O	309	13	-	4/21/97/115	-
24	DD6	O	317	-	-	0/26/80/80	0/3/3/3
22	CLA	S	615	-	-	4/23/99/115	-
26	LHG	A	846	22	-	27/53/53/53	-
22	CLA	U	404	16	-	14/39/115/115	-
22	CLA	X	402	19	-	11/27/103/115	-
27	LMU	O	301	-	-	1/15/35/61	0/1/1/2
27	LMU	U	422	-	-	5/21/61/61	0/2/2/2
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
27	LMU	U	421	-	-	7/21/61/61	0/2/2/2
33	CL0	A	802	20	-	8/37/135/135	-
27	LMU	A	856	-	-	0/12/32/61	0/1/1/2
26	LHG	T	614	22	-	27/46/46/53	-
22	CLA	Q	604	10	-	16/39/115/115	-
22	CLA	Q	607	-	-	5/15/91/115	-
31	CHL	W	422	-	-	9/39/137/137	-
22	CLA	B	815	1	-	3/24/100/115	-
24	DD6	K	614	-	-	0/26/80/80	0/3/3/3
29	SF4	C	102	2	-	-	0/6/5/5
22	CLA	H	304	7	-	6/15/91/115	-
22	CLA	O	310	13	-	9/33/109/115	-
30	SQD	F	407	-	-	2/37/57/69	0/1/1/1
23	PQN	A	843	-	-	4/23/43/43	0/2/2/2
26	LHG	R	614	22	-	20/46/46/53	-
24	DD6	A	847	-	-	1/26/80/80	0/3/3/3
22	CLA	B	807	1	-	15/39/115/115	-
22	CLA	H	318	7	-	6/15/91/115	-
27	LMU	B	854	-	-	3/15/35/61	0/1/1/2
22	CLA	O	305	13	-	4/21/97/115	-
22	CLA	B	832	1	-	12/36/112/115	-
22	CLA	B	833	1	-	9/39/115/115	-
22	CLA	W	412	26	-	5/33/109/115	-

All (2588) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	W	408	CHL	C4C-NC	15.74	1.49	1.35
31	X	406	CHL	C4C-NC	15.66	1.49	1.35
31	W	407	CHL	C4C-NC	15.51	1.49	1.35
31	V	605	CHL	C4C-NC	15.34	1.48	1.35
31	U	407	CHL	C4C-NC	15.32	1.48	1.35
31	V	606	CHL	C4C-NC	15.27	1.48	1.35
31	U	408	CHL	C4C-NC	15.20	1.48	1.35
31	W	422	CHL	C4C-NC	15.12	1.48	1.35
24	A	859	DD6	C29-C27	-8.82	1.25	1.42
24	I	613	DD6	C29-C27	-8.81	1.25	1.42
24	W	418	DD6	C29-C27	-8.76	1.25	1.42
24	P	612	DD6	C29-C27	-8.75	1.25	1.42
24	Q	615	DD6	C29-C27	-8.72	1.25	1.42
24	G	613	DD6	C29-C27	-8.71	1.25	1.42
24	P	613	DD6	C29-C27	-8.70	1.25	1.42
24	T	612	DD6	C29-C27	-8.69	1.25	1.42
24	O	317	DD6	C29-C27	-8.64	1.25	1.42
24	L	413	DD6	C29-C27	-8.64	1.25	1.42
24	H	315	DD6	C29-C27	-8.63	1.25	1.42
24	R	613	DD6	C29-C27	-8.63	1.25	1.42
24	S	612	DD6	C29-C27	-8.61	1.26	1.42
24	U	416	DD6	C29-C27	-8.61	1.26	1.42
24	V	614	DD6	C29-C27	-8.60	1.26	1.42
24	L	414	DD6	C29-C27	-8.60	1.26	1.42
24	R	612	DD6	C29-C27	-8.59	1.26	1.42
24	X	401	DD6	C29-C27	-8.59	1.26	1.42
24	T	613	DD6	C29-C27	-8.58	1.26	1.42
24	F	406	DD6	C29-C27	-8.58	1.26	1.42
24	L	415	DD6	C29-C27	-8.58	1.26	1.42
24	B	841	DD6	C29-C27	-8.57	1.26	1.42
24	K	614	DD6	C29-C27	-8.57	1.26	1.42
24	W	416	DD6	C29-C27	-8.57	1.26	1.42
24	H	314	DD6	C29-C27	-8.56	1.26	1.42
24	G	612	DD6	C29-C27	-8.55	1.26	1.42
24	A	847	DD6	C29-C27	-8.54	1.26	1.42
24	N	613	DD6	C29-C27	-8.52	1.26	1.42
33	A	802	CL0	C3B-C4B	8.52	1.48	1.41
24	I	612	DD6	C29-C27	-8.51	1.26	1.42
24	S	611	DD6	C29-C27	-8.50	1.26	1.42
24	X	416	DD6	C29-C27	-8.50	1.26	1.42
24	Q	614	DD6	C29-C27	-8.49	1.26	1.42
24	N	612	DD6	C29-C27	-8.46	1.26	1.42
24	W	417	DD6	C29-C27	-8.42	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	858	DD6	C29-C27	-8.40	1.26	1.42
24	X	414	DD6	C29-C27	-8.39	1.26	1.42
24	O	316	DD6	C29-C27	-8.36	1.26	1.42
24	J	105	DD6	C29-C27	-8.35	1.26	1.42
24	V	615	DD6	C29-C27	-8.35	1.26	1.42
24	X	415	DD6	C29-C27	-8.35	1.26	1.42
24	K	615	DD6	C29-C27	-8.29	1.26	1.42
24	U	417	DD6	C29-C27	-8.23	1.26	1.42
24	A	859	DD6	C30-C31	-7.92	1.25	1.42
24	P	612	DD6	C30-C31	-7.92	1.25	1.42
24	P	613	DD6	C30-C31	-7.90	1.25	1.42
24	N	612	DD6	C30-C31	-7.89	1.25	1.42
24	G	613	DD6	C30-C31	-7.85	1.26	1.42
24	Q	615	DD6	C30-C31	-7.84	1.26	1.42
24	L	414	DD6	C30-C31	-7.83	1.26	1.42
24	T	612	DD6	C30-C31	-7.83	1.26	1.42
24	O	317	DD6	C30-C31	-7.83	1.26	1.42
24	I	613	DD6	C30-C31	-7.78	1.26	1.42
24	S	611	DD6	C30-C31	-7.78	1.26	1.42
24	X	416	DD6	C30-C31	-7.78	1.26	1.42
24	S	612	DD6	C30-C31	-7.78	1.26	1.42
24	L	415	DD6	C30-C31	-7.77	1.26	1.42
24	R	613	DD6	C30-C31	-7.77	1.26	1.42
24	G	612	DD6	C30-C31	-7.76	1.26	1.42
24	V	614	DD6	C30-C31	-7.74	1.26	1.42
24	U	416	DD6	C30-C31	-7.74	1.26	1.42
24	A	847	DD6	C30-C31	-7.73	1.26	1.42
24	R	612	DD6	C30-C31	-7.72	1.26	1.42
24	F	406	DD6	C30-C31	-7.71	1.26	1.42
24	B	841	DD6	C30-C31	-7.71	1.26	1.42
24	I	612	DD6	C30-C31	-7.70	1.26	1.42
23	B	840	PQN	C3-C2	7.69	1.49	1.35
24	N	613	DD6	C30-C31	-7.69	1.26	1.42
24	Q	614	DD6	C30-C31	-7.67	1.26	1.42
24	H	314	DD6	C30-C31	-7.67	1.26	1.42
24	L	413	DD6	C30-C31	-7.66	1.26	1.42
24	K	615	DD6	C30-C31	-7.66	1.26	1.42
24	W	418	DD6	C30-C31	-7.65	1.26	1.42
24	H	315	DD6	C30-C31	-7.65	1.26	1.42
24	T	613	DD6	C30-C31	-7.63	1.26	1.42
24	O	316	DD6	C30-C31	-7.63	1.26	1.42
24	X	414	DD6	C30-C31	-7.62	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	614	DD6	C30-C31	-7.61	1.26	1.42
24	X	401	DD6	C30-C31	-7.61	1.26	1.42
23	A	843	PQN	C3-C2	7.61	1.49	1.35
24	J	105	DD6	C30-C31	-7.60	1.26	1.42
24	W	416	DD6	C30-C31	-7.59	1.26	1.42
24	A	858	DD6	C30-C31	-7.56	1.26	1.42
24	W	417	DD6	C30-C31	-7.55	1.26	1.42
24	V	615	DD6	C30-C31	-7.52	1.26	1.42
24	X	415	DD6	C30-C31	-7.48	1.26	1.42
33	A	802	CL0	C1B-C2B	7.43	1.48	1.39
24	U	417	DD6	C30-C31	-7.37	1.27	1.42
31	V	606	CHL	MG-NB	-7.28	1.91	2.05
31	W	408	CHL	MG-NB	-7.15	1.91	2.05
31	U	408	CHL	MG-NB	-7.14	1.91	2.05
31	V	605	CHL	MG-NB	-7.05	1.91	2.05
31	W	407	CHL	MG-NB	-7.00	1.91	2.05
31	W	422	CHL	MG-NB	-6.98	1.91	2.05
31	U	407	CHL	MG-NB	-6.98	1.92	2.05
33	A	802	CL0	C1A-CHA	6.95	1.48	1.40
31	X	406	CHL	MG-NB	-6.92	1.92	2.05
33	A	802	CL0	C1D-C2D	6.85	1.47	1.39
31	W	408	CHL	C1B-C2B	6.58	1.47	1.39
31	W	422	CHL	C1B-C2B	6.52	1.47	1.39
31	W	407	CHL	C1B-C2B	6.51	1.47	1.39
31	X	406	CHL	C1B-C2B	6.46	1.47	1.39
31	V	606	CHL	C1B-C2B	6.44	1.47	1.39
31	V	605	CHL	C1B-C2B	6.43	1.47	1.39
31	U	407	CHL	C1B-C2B	6.33	1.47	1.39
31	U	408	CHL	C1B-C2B	6.29	1.47	1.39
31	W	407	CHL	MG-ND	-5.84	1.94	2.05
31	X	406	CHL	MG-ND	-5.76	1.94	2.05
31	W	408	CHL	MG-ND	-5.74	1.94	2.05
31	U	407	CHL	MG-ND	-5.72	1.94	2.05
31	W	422	CHL	MG-ND	-5.71	1.94	2.05
31	V	605	CHL	MG-ND	-5.69	1.94	2.05
31	U	408	CHL	MG-ND	-5.66	1.94	2.05
31	V	606	CHL	MG-ND	-5.64	1.94	2.05
33	A	802	CL0	CHB-C4A	-5.57	1.32	1.38
33	A	802	CL0	C3A-C2A	-5.44	1.49	1.54
23	B	840	PQN	C10-C5	4.89	1.48	1.40
31	U	407	CHL	C3B-C4B	4.81	1.45	1.41
23	A	843	PQN	C10-C5	4.80	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	606	CHL	C3B-C4B	4.73	1.45	1.41
31	U	408	CHL	C3B-C4B	4.69	1.45	1.41
31	V	605	CHL	C3B-C4B	4.69	1.45	1.41
31	X	406	CHL	C3B-C4B	4.68	1.45	1.41
31	W	407	CHL	C3B-C4B	4.53	1.45	1.41
33	A	802	CL0	CHB-C1B	4.50	1.46	1.39
33	A	802	CL0	C3D-C2D	4.46	1.47	1.39
31	W	422	CHL	C3B-C4B	4.43	1.44	1.41
33	A	802	CL0	C3C-C2C	4.38	1.46	1.36
33	A	802	CL0	O2D-CGD	4.32	1.43	1.33
31	W	408	CHL	C3B-C4B	4.29	1.44	1.41
31	U	408	CHL	CHB-C4A	-4.26	1.33	1.38
25	F	401	DGD	O1G-C1A	4.25	1.45	1.33
31	V	606	CHL	CHB-C4A	-4.21	1.33	1.38
22	I	611	CLA	C1D-ND	4.21	1.43	1.37
33	A	802	CL0	O2A-CGA	4.20	1.45	1.33
22	W	415	CLA	C1D-ND	4.20	1.42	1.37
31	U	407	CHL	CHB-C4A	-4.19	1.33	1.38
33	A	802	CL0	C3B-C2B	4.14	1.46	1.40
31	V	605	CHL	CHB-C4A	-4.12	1.33	1.38
31	X	406	CHL	CHB-C4A	-4.12	1.33	1.38
22	P	603	CLA	C1D-ND	4.11	1.42	1.37
22	B	820	CLA	C1D-ND	4.10	1.42	1.37
22	A	803	CLA	C1D-ND	4.10	1.42	1.37
31	W	422	CHL	CHB-C4A	-4.06	1.33	1.38
22	A	839	CLA	C1D-ND	4.05	1.42	1.37
31	W	407	CHL	CHB-C4A	-4.05	1.33	1.38
22	A	838	CLA	C1D-ND	4.04	1.42	1.37
22	P	611	CLA	C1D-ND	4.01	1.42	1.37
25	O	304	DGD	O1G-C1A	4.01	1.45	1.33
31	W	408	CHL	CHB-C4A	-4.00	1.33	1.38
22	P	608	CLA	C1D-ND	4.00	1.42	1.37
22	B	819	CLA	C1D-ND	3.99	1.42	1.37
22	B	826	CLA	C1D-ND	3.99	1.42	1.37
22	X	417	CLA	C1D-ND	3.98	1.42	1.37
22	V	601	CLA	C1D-ND	3.98	1.42	1.37
25	B	847	DGD	O1G-C1A	3.98	1.45	1.33
22	P	610	CLA	C1D-ND	3.97	1.42	1.37
22	R	610	CLA	C1D-ND	3.97	1.42	1.37
22	V	613	CLA	C1D-ND	3.96	1.42	1.37
22	R	606	CLA	C1D-ND	3.96	1.42	1.37
31	U	408	CHL	C1A-CHA	-3.95	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	409	CLA	C1D-ND	3.94	1.42	1.37
22	U	404	CLA	C1D-ND	3.94	1.42	1.37
22	Q	618	CLA	C1D-ND	3.94	1.42	1.37
22	I	603	CLA	C1D-ND	3.94	1.42	1.37
22	R	611	CLA	C1D-ND	3.94	1.42	1.37
25	F	401	DGD	O2G-C1B	3.93	1.45	1.34
22	B	859	CLA	C1D-ND	3.93	1.42	1.37
22	I	609	CLA	C1D-ND	3.93	1.42	1.37
22	Q	608	CLA	C1D-ND	3.93	1.42	1.37
22	S	608	CLA	C1D-ND	3.93	1.42	1.37
22	A	840	CLA	C1D-ND	3.93	1.42	1.37
22	P	604	CLA	C1D-ND	3.93	1.42	1.37
22	T	607	CLA	C1D-ND	3.93	1.42	1.37
22	I	601	CLA	C1D-ND	3.93	1.42	1.37
22	S	610	CLA	C1D-ND	3.92	1.42	1.37
22	B	804	CLA	C1D-ND	3.92	1.42	1.37
22	U	414	CLA	C1D-ND	3.92	1.42	1.37
22	V	604	CLA	C1D-ND	3.92	1.42	1.37
22	V	609	CLA	C1D-ND	3.92	1.42	1.37
22	R	607	CLA	C1D-ND	3.91	1.42	1.37
22	S	602	CLA	C1D-ND	3.91	1.42	1.37
22	V	607	CLA	C1D-ND	3.91	1.42	1.37
22	B	816	CLA	C1D-ND	3.91	1.42	1.37
22	R	605	CLA	C1D-ND	3.91	1.42	1.37
22	R	615	CLA	C1D-ND	3.91	1.42	1.37
22	X	404	CLA	C1D-ND	3.91	1.42	1.37
22	O	315	CLA	C1D-ND	3.91	1.42	1.37
22	Q	613	CLA	C1D-ND	3.91	1.42	1.37
22	B	836	CLA	C1D-ND	3.91	1.42	1.37
22	H	302	CLA	C1D-ND	3.91	1.42	1.37
22	N	602	CLA	C1D-ND	3.91	1.42	1.37
22	N	603	CLA	C1D-ND	3.90	1.42	1.37
22	W	414	CLA	C1D-ND	3.90	1.42	1.37
22	H	307	CLA	C1D-ND	3.90	1.42	1.37
22	H	311	CLA	C1D-ND	3.90	1.42	1.37
22	A	829	CLA	C1D-ND	3.90	1.42	1.37
22	A	826	CLA	C1D-ND	3.90	1.42	1.37
31	V	605	CHL	C1A-CHA	-3.90	1.35	1.40
22	B	806	CLA	C1D-ND	3.90	1.42	1.37
22	U	405	CLA	C1D-ND	3.90	1.42	1.37
22	G	604	CLA	C1D-ND	3.90	1.42	1.37
22	N	609	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	842	CLA	C1D-ND	3.89	1.42	1.37
22	S	609	CLA	C1D-ND	3.89	1.42	1.37
22	G	602	CLA	C1D-ND	3.89	1.42	1.37
22	A	815	CLA	C1D-ND	3.89	1.42	1.37
22	H	313	CLA	C1D-ND	3.89	1.42	1.37
22	L	417	CLA	C1D-ND	3.89	1.42	1.37
22	B	821	CLA	C1D-ND	3.89	1.42	1.37
22	K	611	CLA	C1D-ND	3.88	1.42	1.37
22	R	609	CLA	C1D-ND	3.88	1.42	1.37
22	V	603	CLA	C1D-ND	3.88	1.42	1.37
22	O	319	CLA	C1D-ND	3.88	1.42	1.37
22	R	603	CLA	C1D-ND	3.88	1.42	1.37
22	X	412	CLA	C1D-ND	3.88	1.42	1.37
22	T	611	CLA	C1D-ND	3.87	1.42	1.37
22	X	408	CLA	C1D-ND	3.87	1.42	1.37
22	L	405	CLA	C1D-ND	3.87	1.42	1.37
22	R	608	CLA	C1D-ND	3.87	1.42	1.37
22	V	617	CLA	C1D-ND	3.87	1.42	1.37
22	W	419	CLA	C1D-ND	3.87	1.42	1.37
22	S	606	CLA	C1D-ND	3.87	1.42	1.37
22	K	604	CLA	C1D-ND	3.87	1.42	1.37
22	N	606	CLA	C1D-ND	3.87	1.42	1.37
22	U	413	CLA	C1D-ND	3.87	1.42	1.37
22	A	841	CLA	C1D-ND	3.87	1.42	1.37
22	U	403	CLA	C1D-ND	3.87	1.42	1.37
22	A	844	CLA	C1D-ND	3.86	1.42	1.37
22	K	613	CLA	C1D-ND	3.86	1.42	1.37
22	V	602	CLA	C1D-ND	3.86	1.42	1.37
22	I	602	CLA	C1D-ND	3.86	1.42	1.37
22	U	415	CLA	C1D-ND	3.86	1.42	1.37
22	V	611	CLA	C1D-ND	3.86	1.42	1.37
22	A	824	CLA	C1D-ND	3.86	1.42	1.37
22	V	612	CLA	C1D-ND	3.86	1.42	1.37
22	B	834	CLA	C1D-ND	3.86	1.42	1.37
31	V	606	CHL	C3A-C2A	-3.86	1.51	1.54
22	N	610	CLA	C1D-ND	3.86	1.42	1.37
22	U	412	CLA	C1D-ND	3.86	1.42	1.37
22	X	411	CLA	C1D-ND	3.85	1.42	1.37
22	W	403	CLA	C1D-ND	3.85	1.42	1.37
22	H	318	CLA	C1D-ND	3.85	1.42	1.37
22	N	601	CLA	C1D-ND	3.85	1.42	1.37
22	R	602	CLA	C1D-ND	3.85	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	419	CLA	C1D-ND	3.85	1.42	1.37
22	H	303	CLA	C1D-ND	3.85	1.42	1.37
22	X	407	CLA	C1D-ND	3.85	1.42	1.37
22	B	817	CLA	C1D-ND	3.85	1.42	1.37
22	N	611	CLA	C1D-ND	3.84	1.42	1.37
22	S	607	CLA	C1D-ND	3.84	1.42	1.37
22	F	405	CLA	C1D-ND	3.84	1.42	1.37
22	V	610	CLA	C1D-ND	3.84	1.42	1.37
22	K	612	CLA	C1D-ND	3.84	1.42	1.37
22	X	403	CLA	C1D-ND	3.84	1.42	1.37
22	U	411	CLA	C1D-ND	3.84	1.42	1.37
22	T	606	CLA	C1D-ND	3.84	1.42	1.37
22	U	401	CLA	C1D-ND	3.84	1.42	1.37
22	A	833	CLA	C1D-ND	3.84	1.42	1.37
22	B	825	CLA	C1D-ND	3.84	1.42	1.37
22	B	815	CLA	C1D-ND	3.84	1.42	1.37
22	R	601	CLA	C1D-ND	3.84	1.42	1.37
22	X	413	CLA	C1D-ND	3.84	1.42	1.37
31	W	422	CHL	C1A-CHA	-3.84	1.35	1.40
22	X	410	CLA	C1D-ND	3.84	1.42	1.37
22	G	609	CLA	C1D-ND	3.83	1.42	1.37
22	G	611	CLA	C1D-ND	3.83	1.42	1.37
22	T	602	CLA	C1D-ND	3.83	1.42	1.37
22	H	304	CLA	C1D-ND	3.83	1.42	1.37
22	W	412	CLA	C1D-ND	3.83	1.42	1.37
22	A	827	CLA	C1D-ND	3.83	1.42	1.37
22	B	832	CLA	C1D-ND	3.83	1.42	1.37
22	H	309	CLA	C1D-ND	3.83	1.42	1.37
22	A	807	CLA	C1D-ND	3.83	1.42	1.37
22	O	313	CLA	C1D-ND	3.83	1.42	1.37
22	S	614	CLA	C1D-ND	3.83	1.42	1.37
22	F	403	CLA	C1D-ND	3.83	1.42	1.37
22	A	813	CLA	C1D-ND	3.83	1.42	1.37
22	L	409	CLA	C1D-ND	3.82	1.42	1.37
22	A	817	CLA	C1D-ND	3.82	1.42	1.37
31	V	606	CHL	C1A-CHA	-3.82	1.35	1.40
22	V	608	CLA	C1D-ND	3.82	1.42	1.37
22	B	812	CLA	C1D-ND	3.82	1.42	1.37
22	W	404	CLA	C1D-ND	3.82	1.42	1.37
22	B	808	CLA	C1D-ND	3.82	1.42	1.37
22	N	604	CLA	C1D-ND	3.82	1.42	1.37
22	A	831	CLA	C1D-ND	3.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	308	CLA	C1D-ND	3.82	1.42	1.37
22	Q	611	CLA	C1D-ND	3.82	1.42	1.37
22	U	406	CLA	C1D-ND	3.82	1.42	1.37
22	S	601	CLA	C1D-ND	3.82	1.42	1.37
22	R	604	CLA	C1D-ND	3.81	1.42	1.37
22	B	828	CLA	C1D-ND	3.81	1.42	1.37
22	B	835	CLA	C1D-ND	3.81	1.42	1.37
22	H	305	CLA	C1D-ND	3.81	1.42	1.37
22	G	601	CLA	C1D-ND	3.81	1.42	1.37
22	A	818	CLA	C1D-ND	3.81	1.42	1.37
22	Q	601	CLA	C1D-ND	3.81	1.42	1.37
22	T	610	CLA	C1D-ND	3.81	1.42	1.37
22	N	607	CLA	C1D-ND	3.81	1.42	1.37
22	O	308	CLA	C1D-ND	3.81	1.42	1.37
22	X	405	CLA	C1D-ND	3.81	1.42	1.37
22	A	808	CLA	C1D-ND	3.81	1.42	1.37
22	B	837	CLA	C1D-ND	3.81	1.42	1.37
22	B	809	CLA	C1D-ND	3.80	1.42	1.37
22	G	603	CLA	C1D-ND	3.80	1.42	1.37
22	B	839	CLA	C1D-ND	3.80	1.42	1.37
22	O	312	CLA	C1D-ND	3.80	1.42	1.37
22	B	818	CLA	C1D-ND	3.80	1.42	1.37
22	A	832	CLA	C1D-ND	3.80	1.42	1.37
22	I	610	CLA	C1D-ND	3.80	1.42	1.37
22	B	831	CLA	C1D-ND	3.80	1.42	1.37
22	L	410	CLA	C1D-ND	3.80	1.42	1.37
22	O	314	CLA	C1D-ND	3.80	1.42	1.37
22	T	609	CLA	C1D-ND	3.80	1.42	1.37
22	I	604	CLA	C1D-ND	3.79	1.42	1.37
22	N	605	CLA	C1D-ND	3.79	1.42	1.37
22	P	607	CLA	C1D-ND	3.79	1.42	1.37
22	A	837	CLA	C1D-ND	3.79	1.42	1.37
22	A	809	CLA	C1D-ND	3.79	1.42	1.37
22	I	606	CLA	C1D-ND	3.79	1.42	1.37
22	A	828	CLA	C1D-ND	3.79	1.42	1.37
22	G	606	CLA	C1D-ND	3.79	1.42	1.37
22	K	603	CLA	C1D-ND	3.79	1.42	1.37
22	Q	605	CLA	C1D-ND	3.79	1.42	1.37
22	P	605	CLA	C1D-ND	3.79	1.42	1.37
22	Q	603	CLA	C1D-ND	3.79	1.42	1.37
22	L	407	CLA	C1D-ND	3.79	1.42	1.37
22	A	804	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	605	CLA	C1D-ND	3.78	1.42	1.37
22	W	405	CLA	C1D-ND	3.78	1.42	1.37
22	Q	606	CLA	C1D-ND	3.78	1.42	1.37
22	O	307	CLA	C1D-ND	3.78	1.42	1.37
22	K	609	CLA	C1D-ND	3.78	1.42	1.37
22	L	404	CLA	C1D-ND	3.78	1.42	1.37
33	A	802	CL0	CHC-C4B	3.78	1.45	1.39
22	B	805	CLA	C1D-ND	3.78	1.42	1.37
22	L	412	CLA	C1D-ND	3.78	1.42	1.37
22	B	813	CLA	C1D-ND	3.78	1.42	1.37
22	T	604	CLA	C1D-ND	3.78	1.42	1.37
22	B	838	CLA	C1D-ND	3.78	1.42	1.37
22	S	615	CLA	C1D-ND	3.78	1.42	1.37
22	J	102	CLA	C1D-ND	3.78	1.42	1.37
22	U	420	CLA	C1D-ND	3.78	1.42	1.37
22	A	825	CLA	C1D-ND	3.78	1.42	1.37
22	Q	617	CLA	C1D-ND	3.77	1.42	1.37
25	O	304	DGD	O2G-C1B	3.77	1.44	1.34
22	Q	607	CLA	C1D-ND	3.77	1.42	1.37
22	A	835	CLA	C1D-ND	3.77	1.42	1.37
22	B	803	CLA	C1D-ND	3.77	1.42	1.37
22	Q	604	CLA	C1D-ND	3.77	1.42	1.37
31	W	407	CHL	C1A-CHA	-3.77	1.35	1.40
31	U	408	CHL	C3A-C2A	-3.77	1.51	1.54
22	G	607	CLA	C1D-ND	3.77	1.42	1.37
22	B	822	CLA	C1D-ND	3.77	1.42	1.37
22	W	411	CLA	C1D-ND	3.77	1.42	1.37
22	L	411	CLA	C1D-ND	3.77	1.42	1.37
22	P	609	CLA	C1D-ND	3.77	1.42	1.37
22	S	604	CLA	C1D-ND	3.77	1.42	1.37
22	W	410	CLA	C1D-ND	3.77	1.42	1.37
22	W	413	CLA	C1D-ND	3.77	1.42	1.37
22	K	606	CLA	C1D-ND	3.77	1.42	1.37
22	K	605	CLA	C1D-ND	3.76	1.42	1.37
22	T	603	CLA	C1D-ND	3.76	1.42	1.37
22	X	402	CLA	C1D-ND	3.76	1.42	1.37
22	H	310	CLA	C1D-ND	3.76	1.42	1.37
22	A	806	CLA	C1D-ND	3.76	1.42	1.37
22	U	410	CLA	C1D-ND	3.76	1.42	1.37
22	B	827	CLA	C1D-ND	3.76	1.42	1.37
22	Q	610	CLA	C1D-ND	3.76	1.42	1.37
22	I	607	CLA	C1D-ND	3.76	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	823	CLA	C1D-ND	3.75	1.42	1.37
22	B	824	CLA	C1D-ND	3.75	1.42	1.37
22	H	306	CLA	C1D-ND	3.75	1.42	1.37
22	B	833	CLA	C1D-ND	3.75	1.42	1.37
22	O	311	CLA	C1D-ND	3.75	1.42	1.37
22	W	406	CLA	C1D-ND	3.75	1.42	1.37
31	X	406	CHL	C1A-CHA	-3.75	1.35	1.40
22	T	608	CLA	C1D-ND	3.74	1.42	1.37
22	K	602	CLA	C1D-ND	3.74	1.42	1.37
22	K	617	CLA	C1D-ND	3.74	1.42	1.37
22	A	836	CLA	C1D-ND	3.74	1.42	1.37
31	W	408	CHL	C1A-CHA	-3.74	1.35	1.40
22	N	606	CLA	C4B-NB	3.74	1.42	1.37
22	W	402	CLA	C1D-ND	3.74	1.42	1.37
22	O	310	CLA	C1D-ND	3.74	1.42	1.37
22	F	404	CLA	C1D-ND	3.74	1.42	1.37
22	K	610	CLA	C1D-ND	3.74	1.42	1.37
22	L	406	CLA	C1D-ND	3.73	1.42	1.37
22	B	823	CLA	C1D-ND	3.73	1.42	1.37
22	O	306	CLA	C1D-ND	3.73	1.42	1.37
22	O	309	CLA	C1D-ND	3.73	1.42	1.37
22	H	312	CLA	C1D-ND	3.73	1.42	1.37
22	L	403	CLA	C1D-ND	3.73	1.42	1.37
22	S	603	CLA	C1D-ND	3.73	1.42	1.37
22	U	409	CLA	C1D-ND	3.72	1.42	1.37
22	B	811	CLA	C1D-ND	3.72	1.42	1.37
22	A	810	CLA	C1D-ND	3.72	1.42	1.37
22	A	812	CLA	C1D-ND	3.72	1.42	1.37
22	A	852	CLA	C1D-ND	3.72	1.42	1.37
33	A	802	CL0	CHD-C1D	3.72	1.45	1.39
22	G	610	CLA	C1D-ND	3.72	1.42	1.37
22	N	608	CLA	C1D-ND	3.72	1.42	1.37
22	A	834	CLA	C1D-ND	3.72	1.42	1.37
22	A	811	CLA	C1D-ND	3.71	1.42	1.37
22	Q	609	CLA	C1D-ND	3.71	1.42	1.37
31	U	407	CHL	C1A-CHA	-3.71	1.35	1.40
22	A	830	CLA	C1D-ND	3.71	1.42	1.37
22	L	402	CLA	C1D-ND	3.70	1.42	1.37
22	G	608	CLA	C1D-ND	3.70	1.42	1.37
22	A	805	CLA	C1D-ND	3.70	1.42	1.37
22	B	807	CLA	C1D-ND	3.70	1.42	1.37
31	X	406	CHL	C3A-C2A	-3.69	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	814	CLA	C1D-ND	3.69	1.42	1.37
22	I	605	CLA	C1D-ND	3.69	1.42	1.37
25	B	847	DGD	O2G-C1B	3.69	1.44	1.34
22	A	822	CLA	C1D-ND	3.68	1.42	1.37
22	A	821	CLA	C1D-ND	3.68	1.42	1.37
22	G	605	CLA	C1D-ND	3.68	1.42	1.37
22	B	810	CLA	C1D-ND	3.67	1.42	1.37
31	U	407	CHL	C3A-C2A	-3.67	1.51	1.54
22	A	820	CLA	C1D-ND	3.67	1.42	1.37
22	Q	612	CLA	C1D-ND	3.66	1.42	1.37
22	L	408	CLA	C4D-ND	-3.66	1.32	1.37
22	B	814	CLA	C1D-ND	3.66	1.42	1.37
22	T	601	CLA	C1D-ND	3.66	1.42	1.37
22	O	305	CLA	C1D-ND	3.64	1.42	1.37
33	A	802	CL0	C4D-CHA	3.63	1.45	1.40
33	A	802	CL0	CHD-C4C	3.63	1.46	1.39
22	S	605	CLA	C1D-ND	3.62	1.42	1.37
22	O	315	CLA	C4B-NB	3.60	1.42	1.37
22	B	838	CLA	C4B-NB	3.60	1.42	1.37
22	P	602	CLA	C1D-ND	3.59	1.42	1.37
22	K	608	CLA	C4D-ND	-3.59	1.32	1.37
22	B	830	CLA	C4D-ND	-3.58	1.32	1.37
22	A	803	CLA	C4B-NB	3.58	1.42	1.37
22	W	409	CLA	C1D-ND	3.57	1.42	1.37
22	A	801	CLA	C4D-ND	-3.57	1.32	1.37
22	V	601	CLA	C4B-NB	3.56	1.42	1.37
22	S	609	CLA	C4B-NB	3.56	1.42	1.37
22	P	606	CLA	C1D-ND	3.55	1.42	1.37
22	V	613	CLA	C4B-NB	3.54	1.42	1.37
22	W	405	CLA	C4B-NB	3.54	1.42	1.37
31	V	605	CHL	C3A-C2A	-3.54	1.51	1.54
22	I	608	CLA	C1D-ND	3.53	1.42	1.37
22	R	610	CLA	C4B-NB	3.52	1.42	1.37
22	P	608	CLA	C4B-NB	3.52	1.42	1.37
22	A	842	CLA	C4B-NB	3.52	1.42	1.37
22	B	819	CLA	C4B-NB	3.52	1.42	1.37
22	A	819	CLA	C4D-ND	-3.51	1.32	1.37
22	B	820	CLA	C4B-NB	3.51	1.42	1.37
22	B	825	CLA	C4B-NB	3.51	1.42	1.37
22	H	311	CLA	C4B-NB	3.51	1.42	1.37
22	X	404	CLA	C4B-NB	3.51	1.42	1.37
22	I	601	CLA	C4B-NB	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	601	CLA	C4B-NB	3.50	1.42	1.37
31	W	422	CHL	C3A-C2A	-3.49	1.51	1.54
22	A	819	CLA	C1D-ND	3.49	1.42	1.37
22	P	610	CLA	C4B-NB	3.49	1.42	1.37
22	P	609	CLA	C4B-NB	3.48	1.42	1.37
22	X	419	CLA	C4B-NB	3.48	1.42	1.37
22	R	608	CLA	C4B-NB	3.47	1.42	1.37
22	U	403	CLA	C4B-NB	3.47	1.42	1.37
22	V	611	CLA	C4B-NB	3.47	1.42	1.37
22	B	802	CLA	C4D-ND	-3.46	1.32	1.37
22	U	415	CLA	C4B-NB	3.46	1.42	1.37
33	A	802	CL0	OBD-CAD	3.45	1.27	1.22
22	Q	610	CLA	C4B-NB	3.45	1.42	1.37
22	A	806	CLA	C4B-NB	3.45	1.42	1.37
22	V	617	CLA	C4B-NB	3.44	1.42	1.37
22	P	603	CLA	C4B-NB	3.44	1.42	1.37
22	F	405	CLA	C4B-NB	3.44	1.42	1.37
22	Q	618	CLA	C4B-NB	3.44	1.42	1.37
22	W	415	CLA	C4B-NB	3.43	1.42	1.37
22	V	612	CLA	C4B-NB	3.43	1.42	1.37
22	S	610	CLA	C4B-NB	3.43	1.42	1.37
22	T	606	CLA	C4B-NB	3.42	1.42	1.37
22	V	610	CLA	C4B-NB	3.42	1.42	1.37
22	B	833	CLA	C4B-NB	3.41	1.42	1.37
22	X	412	CLA	C4B-NB	3.41	1.42	1.37
22	T	610	CLA	C4B-NB	3.41	1.42	1.37
22	A	834	CLA	C4B-NB	3.41	1.42	1.37
22	W	414	CLA	C4B-NB	3.41	1.42	1.37
22	B	829	CLA	C4D-ND	-3.41	1.33	1.37
22	H	307	CLA	C4B-NB	3.40	1.42	1.37
22	T	605	CLA	C4B-NB	3.40	1.42	1.37
22	S	608	CLA	C4B-NB	3.40	1.42	1.37
22	H	309	CLA	C4B-NB	3.40	1.42	1.37
22	A	816	CLA	C1D-ND	3.40	1.42	1.37
22	P	607	CLA	C4B-NB	3.40	1.42	1.37
22	R	615	CLA	C4B-NB	3.40	1.42	1.37
31	W	407	CHL	C3A-C2A	-3.39	1.51	1.54
22	G	606	CLA	C4B-NB	3.39	1.42	1.37
22	S	606	CLA	C4B-NB	3.39	1.42	1.37
22	K	610	CLA	C4B-NB	3.39	1.42	1.37
22	X	410	CLA	C4B-NB	3.39	1.42	1.37
22	F	403	CLA	C4B-NB	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	611	CLA	C4B-NB	3.39	1.42	1.37
22	A	820	CLA	C4B-NB	3.39	1.42	1.37
22	O	313	CLA	C4B-NB	3.39	1.41	1.37
22	H	313	CLA	C4B-NB	3.38	1.41	1.37
22	R	606	CLA	C4B-NB	3.38	1.41	1.37
22	R	607	CLA	C4B-NB	3.38	1.41	1.37
22	R	611	CLA	C4B-NB	3.38	1.41	1.37
22	G	603	CLA	C4B-NB	3.38	1.41	1.37
22	A	824	CLA	C4B-NB	3.38	1.41	1.37
22	N	604	CLA	C4B-NB	3.38	1.41	1.37
22	B	803	CLA	C4B-NB	3.38	1.41	1.37
22	I	608	CLA	C4B-NB	3.38	1.41	1.37
22	A	804	CLA	C4B-NB	3.37	1.41	1.37
22	A	852	CLA	C4B-NB	3.37	1.41	1.37
22	T	603	CLA	C4B-NB	3.37	1.41	1.37
22	V	603	CLA	C4B-NB	3.37	1.41	1.37
22	A	816	CLA	C4D-ND	-3.37	1.33	1.37
22	B	806	CLA	C4B-NB	3.37	1.41	1.37
22	B	828	CLA	C4B-NB	3.37	1.41	1.37
22	Q	607	CLA	C4B-NB	3.37	1.41	1.37
22	I	606	CLA	C4B-NB	3.37	1.41	1.37
33	A	802	CL0	CHC-C1C	3.36	1.45	1.39
22	N	608	CLA	C4B-NB	3.36	1.41	1.37
22	O	307	CLA	C4B-NB	3.36	1.41	1.37
22	U	406	CLA	C4B-NB	3.36	1.41	1.37
22	T	601	CLA	C4B-NB	3.36	1.41	1.37
22	I	603	CLA	C4B-NB	3.36	1.41	1.37
22	H	302	CLA	C4B-NB	3.35	1.41	1.37
22	R	609	CLA	C4B-NB	3.35	1.41	1.37
22	B	837	CLA	C4B-NB	3.35	1.41	1.37
22	V	602	CLA	C4B-NB	3.35	1.41	1.37
22	W	403	CLA	C4B-NB	3.35	1.41	1.37
22	S	605	CLA	C4D-ND	-3.35	1.33	1.37
22	B	821	CLA	C4B-NB	3.35	1.41	1.37
22	Q	605	CLA	C4B-NB	3.35	1.41	1.37
22	R	605	CLA	C4B-NB	3.35	1.41	1.37
22	L	409	CLA	C4B-NB	3.34	1.41	1.37
22	N	603	CLA	C4B-NB	3.34	1.41	1.37
22	B	817	CLA	C4B-NB	3.34	1.41	1.37
22	A	809	CLA	C4B-NB	3.34	1.41	1.37
22	B	826	CLA	C4B-NB	3.34	1.41	1.37
22	H	318	CLA	C4B-NB	3.34	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	608	CLA	C4B-NB	3.34	1.41	1.37
22	A	836	CLA	C4B-NB	3.34	1.41	1.37
22	B	807	CLA	C4B-NB	3.33	1.41	1.37
22	K	604	CLA	C4B-NB	3.33	1.41	1.37
22	B	835	CLA	C4B-NB	3.33	1.41	1.37
22	V	604	CLA	C4B-NB	3.33	1.41	1.37
22	K	613	CLA	C4B-NB	3.33	1.41	1.37
22	A	829	CLA	C4B-NB	3.33	1.41	1.37
22	A	837	CLA	C4B-NB	3.33	1.41	1.37
22	K	602	CLA	C4B-NB	3.33	1.41	1.37
22	W	406	CLA	C4B-NB	3.33	1.41	1.37
22	B	812	CLA	C4B-NB	3.33	1.41	1.37
22	B	831	CLA	C4B-NB	3.33	1.41	1.37
22	R	601	CLA	C4B-NB	3.33	1.41	1.37
22	R	604	CLA	C4B-NB	3.33	1.41	1.37
22	V	607	CLA	C4B-NB	3.33	1.41	1.37
22	X	417	CLA	C4B-NB	3.32	1.41	1.37
22	B	859	CLA	C4B-NB	3.32	1.41	1.37
22	S	607	CLA	C4B-NB	3.32	1.41	1.37
22	A	831	CLA	C4B-NB	3.32	1.41	1.37
22	G	611	CLA	C4B-NB	3.32	1.41	1.37
22	U	405	CLA	C4B-NB	3.32	1.41	1.37
22	L	417	CLA	C4B-NB	3.32	1.41	1.37
22	A	839	CLA	C4B-NB	3.32	1.41	1.37
22	A	814	CLA	C4B-NB	3.31	1.41	1.37
22	A	807	CLA	C4B-NB	3.31	1.41	1.37
22	R	602	CLA	C4B-NB	3.31	1.41	1.37
22	I	611	CLA	C4B-NB	3.31	1.41	1.37
22	S	601	CLA	C4B-NB	3.31	1.41	1.37
22	S	604	CLA	C4B-NB	3.31	1.41	1.37
22	S	615	CLA	C4B-NB	3.31	1.41	1.37
22	N	607	CLA	C4B-NB	3.31	1.41	1.37
22	B	815	CLA	C4B-NB	3.30	1.41	1.37
22	Q	606	CLA	C4B-NB	3.30	1.41	1.37
22	A	805	CLA	C4B-NB	3.30	1.41	1.37
22	I	605	CLA	C4B-NB	3.30	1.41	1.37
22	W	412	CLA	C4B-NB	3.30	1.41	1.37
22	B	814	CLA	C4B-NB	3.30	1.41	1.37
22	V	609	CLA	C4B-NB	3.30	1.41	1.37
22	B	836	CLA	C4B-NB	3.30	1.41	1.37
22	A	841	CLA	C4B-NB	3.30	1.41	1.37
22	U	420	CLA	C4B-NB	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	609	CLA	C4B-NB	3.29	1.41	1.37
22	W	419	CLA	C4B-NB	3.29	1.41	1.37
22	L	412	CLA	C4B-NB	3.29	1.41	1.37
22	T	608	CLA	C4B-NB	3.29	1.41	1.37
22	B	824	CLA	C4B-NB	3.29	1.41	1.37
22	F	404	CLA	C4B-NB	3.29	1.41	1.37
22	G	604	CLA	C4B-NB	3.29	1.41	1.37
22	H	312	CLA	C4B-NB	3.29	1.41	1.37
22	L	405	CLA	C4B-NB	3.29	1.41	1.37
22	X	413	CLA	C4B-NB	3.29	1.41	1.37
22	L	411	CLA	C4B-NB	3.29	1.41	1.37
22	U	414	CLA	C4B-NB	3.29	1.41	1.37
22	P	611	CLA	C4B-NB	3.28	1.41	1.37
22	U	413	CLA	C4B-NB	3.28	1.41	1.37
22	V	608	CLA	C4B-NB	3.28	1.41	1.37
22	G	609	CLA	C4B-NB	3.28	1.41	1.37
22	U	409	CLA	C4B-NB	3.28	1.41	1.37
22	Q	603	CLA	C4B-NB	3.28	1.41	1.37
22	U	410	CLA	C4B-NB	3.28	1.41	1.37
22	H	310	CLA	C4B-NB	3.28	1.41	1.37
22	A	823	CLA	C4B-NB	3.28	1.41	1.37
22	K	606	CLA	C4B-NB	3.27	1.41	1.37
22	K	611	CLA	C4B-NB	3.27	1.41	1.37
22	X	409	CLA	C4B-NB	3.27	1.41	1.37
22	I	604	CLA	C4B-NB	3.27	1.41	1.37
22	B	809	CLA	C4B-NB	3.27	1.41	1.37
22	B	808	CLA	C4B-NB	3.27	1.41	1.37
22	N	610	CLA	C4B-NB	3.27	1.41	1.37
22	Q	617	CLA	C4B-NB	3.26	1.41	1.37
22	S	603	CLA	C4B-NB	3.26	1.41	1.37
22	T	611	CLA	C4B-NB	3.26	1.41	1.37
22	A	830	CLA	C4B-NB	3.26	1.41	1.37
22	B	822	CLA	C4B-NB	3.26	1.41	1.37
22	O	305	CLA	C4B-NB	3.26	1.41	1.37
22	W	409	CLA	C4B-NB	3.26	1.41	1.37
22	B	810	CLA	C4B-NB	3.26	1.41	1.37
22	A	810	CLA	C4B-NB	3.26	1.41	1.37
22	U	401	CLA	C4B-NB	3.25	1.41	1.37
22	L	407	CLA	C4B-NB	3.25	1.41	1.37
22	B	816	CLA	C4B-NB	3.25	1.41	1.37
22	P	604	CLA	C4B-NB	3.25	1.41	1.37
22	G	601	CLA	C4B-NB	3.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	606	CLA	C4B-NB	3.25	1.41	1.37
22	O	319	CLA	C4B-NB	3.25	1.41	1.37
22	B	805	CLA	C4B-NB	3.24	1.41	1.37
22	A	835	CLA	C4B-NB	3.24	1.41	1.37
22	B	823	CLA	C4B-NB	3.24	1.41	1.37
22	O	311	CLA	C4B-NB	3.24	1.41	1.37
22	I	607	CLA	C4B-NB	3.24	1.41	1.37
22	H	305	CLA	C4B-NB	3.24	1.41	1.37
22	W	410	CLA	C4B-NB	3.24	1.41	1.37
22	N	609	CLA	C4B-NB	3.24	1.41	1.37
22	B	811	CLA	C4B-NB	3.24	1.41	1.37
22	B	818	CLA	C4B-NB	3.24	1.41	1.37
22	U	411	CLA	C4B-NB	3.24	1.41	1.37
22	A	833	CLA	C4B-NB	3.24	1.41	1.37
22	B	804	CLA	C4B-NB	3.23	1.41	1.37
22	B	813	CLA	C4B-NB	3.23	1.41	1.37
22	W	413	CLA	C4B-NB	3.23	1.41	1.37
22	K	605	CLA	C4B-NB	3.23	1.41	1.37
22	H	306	CLA	C4B-NB	3.23	1.41	1.37
22	L	406	CLA	C4B-NB	3.23	1.41	1.37
22	O	308	CLA	C4B-NB	3.23	1.41	1.37
22	T	602	CLA	C4B-NB	3.23	1.41	1.37
22	X	402	CLA	C4B-NB	3.23	1.41	1.37
22	A	828	CLA	C4B-NB	3.23	1.41	1.37
22	A	818	CLA	C4B-NB	3.22	1.41	1.37
22	G	608	CLA	C4B-NB	3.22	1.41	1.37
22	L	410	CLA	C4B-NB	3.22	1.41	1.37
22	X	405	CLA	C4B-NB	3.22	1.41	1.37
22	A	813	CLA	C4B-NB	3.22	1.41	1.37
22	K	612	CLA	C4B-NB	3.22	1.41	1.37
22	L	403	CLA	C4B-NB	3.22	1.41	1.37
22	A	844	CLA	C4B-NB	3.22	1.41	1.37
22	X	403	CLA	C4B-NB	3.22	1.41	1.37
22	A	815	CLA	C4B-NB	3.22	1.41	1.37
22	U	412	CLA	C4B-NB	3.22	1.41	1.37
22	Q	611	CLA	C4B-NB	3.21	1.41	1.37
22	A	812	CLA	C4B-NB	3.21	1.41	1.37
22	S	614	CLA	C4B-NB	3.21	1.41	1.37
22	X	407	CLA	C4B-NB	3.21	1.41	1.37
22	A	822	CLA	C4B-NB	3.21	1.41	1.37
22	A	840	CLA	C4B-NB	3.21	1.41	1.37
22	W	411	CLA	C4B-NB	3.21	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	832	CLA	C4B-NB	3.21	1.41	1.37
22	N	606	CLA	C3B-C4B	3.21	1.50	1.42
22	H	303	CLA	C4B-NB	3.21	1.41	1.37
22	Q	609	CLA	C4B-NB	3.20	1.41	1.37
22	R	603	CLA	C4B-NB	3.20	1.41	1.37
22	A	811	CLA	C4B-NB	3.20	1.41	1.37
22	L	402	CLA	C4B-NB	3.20	1.41	1.37
22	A	821	CLA	C4B-NB	3.19	1.41	1.37
22	A	838	CLA	C4B-NB	3.19	1.41	1.37
22	K	607	CLA	C4D-ND	-3.19	1.33	1.37
22	T	604	CLA	C4B-NB	3.18	1.41	1.37
22	W	402	CLA	C4B-NB	3.18	1.41	1.37
22	O	309	CLA	C4B-NB	3.18	1.41	1.37
22	A	826	CLA	C4B-NB	3.18	1.41	1.37
22	G	610	CLA	C4B-NB	3.18	1.41	1.37
22	N	605	CLA	C4B-NB	3.18	1.41	1.37
22	X	411	CLA	C4B-NB	3.18	1.41	1.37
22	H	304	CLA	C4B-NB	3.18	1.41	1.37
22	I	610	CLA	C4B-NB	3.18	1.41	1.37
22	X	408	CLA	C4B-NB	3.18	1.41	1.37
22	J	102	CLA	C4B-NB	3.18	1.41	1.37
22	B	832	CLA	C4B-NB	3.18	1.41	1.37
22	U	404	CLA	C4B-NB	3.18	1.41	1.37
22	B	839	CLA	C4B-NB	3.18	1.41	1.37
22	L	404	CLA	C4B-NB	3.17	1.41	1.37
22	O	310	CLA	C4B-NB	3.17	1.41	1.37
22	W	404	CLA	C4B-NB	3.17	1.41	1.37
22	T	607	CLA	C4B-NB	3.17	1.41	1.37
22	T	609	CLA	C4B-NB	3.17	1.41	1.37
22	K	607	CLA	C1D-ND	3.16	1.41	1.37
22	K	617	CLA	C4B-NB	3.16	1.41	1.37
22	A	825	CLA	C4B-NB	3.16	1.41	1.37
22	N	601	CLA	C4B-NB	3.16	1.41	1.37
22	K	609	CLA	C4B-NB	3.16	1.41	1.37
22	A	817	CLA	C4B-NB	3.16	1.41	1.37
22	O	314	CLA	C4B-NB	3.16	1.41	1.37
22	G	605	CLA	C4B-NB	3.16	1.41	1.37
22	I	602	CLA	C4B-NB	3.16	1.41	1.37
22	H	308	CLA	C4B-NB	3.15	1.41	1.37
22	P	605	CLA	C4B-NB	3.15	1.41	1.37
22	Q	612	CLA	C4B-NB	3.15	1.41	1.37
22	K	603	CLA	C4B-NB	3.15	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	827	CLA	C4B-NB	3.15	1.41	1.37
22	G	607	CLA	C4B-NB	3.14	1.41	1.37
22	B	827	CLA	C4B-NB	3.14	1.41	1.37
22	O	312	CLA	C4B-NB	3.14	1.41	1.37
22	Q	613	CLA	C4B-NB	3.14	1.41	1.37
22	Q	604	CLA	C4B-NB	3.13	1.41	1.37
22	N	602	CLA	C4B-NB	3.13	1.41	1.37
22	B	829	CLA	C1D-ND	3.12	1.41	1.37
22	T	606	CLA	C3B-C4B	3.12	1.50	1.42
22	S	602	CLA	C4B-NB	3.12	1.41	1.37
22	B	834	CLA	C4B-NB	3.11	1.41	1.37
22	O	306	CLA	C4B-NB	3.10	1.41	1.37
22	P	602	CLA	C4D-ND	-3.10	1.33	1.37
22	Q	608	CLA	C3B-C4B	3.09	1.50	1.42
22	A	808	CLA	C4B-NB	3.09	1.41	1.37
22	O	306	CLA	C4D-ND	-3.08	1.33	1.37
22	U	403	CLA	C3B-C4B	3.07	1.50	1.42
22	X	410	CLA	C3B-C4B	3.06	1.49	1.42
22	G	602	CLA	C4B-NB	3.06	1.41	1.37
22	K	608	CLA	C1D-ND	3.05	1.41	1.37
22	H	311	CLA	C3B-C4B	3.05	1.49	1.42
22	A	842	CLA	C3B-C4B	3.05	1.49	1.42
22	B	802	CLA	C1D-ND	3.05	1.41	1.37
31	W	422	CHL	C3B-C2B	-3.04	1.36	1.40
22	W	405	CLA	C3B-C4B	3.04	1.49	1.42
22	G	606	CLA	C3B-C4B	3.03	1.49	1.42
22	B	830	CLA	C1D-ND	3.03	1.41	1.37
22	X	404	CLA	C3B-C4B	3.03	1.49	1.42
22	P	603	CLA	C3B-C4B	3.02	1.49	1.42
22	L	417	CLA	C4D-ND	-3.02	1.33	1.37
22	P	602	CLA	C4B-NB	3.01	1.41	1.37
22	X	403	CLA	C4D-ND	-3.01	1.33	1.37
22	Q	604	CLA	C4D-ND	-3.01	1.33	1.37
22	A	811	CLA	C4D-ND	-3.01	1.33	1.37
22	H	307	CLA	C3B-C4B	3.00	1.49	1.42
22	Q	618	CLA	C3B-C4B	3.00	1.49	1.42
22	A	837	CLA	C4D-ND	-3.00	1.33	1.37
22	P	607	CLA	C3B-C4B	3.00	1.49	1.42
22	R	611	CLA	C4D-ND	-3.00	1.33	1.37
22	K	603	CLA	C4D-ND	-3.00	1.33	1.37
22	P	611	CLA	C3B-C4B	3.00	1.49	1.42
22	A	809	CLA	C4D-ND	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	601	CLA	C3B-C4B	3.00	1.49	1.42
22	X	412	CLA	C3B-C4B	3.00	1.49	1.42
22	I	602	CLA	C4D-ND	-3.00	1.33	1.37
31	U	407	CHL	C3B-C2B	-3.00	1.36	1.40
22	W	414	CLA	C3B-C4B	3.00	1.49	1.42
22	S	608	CLA	C3B-C4B	2.99	1.49	1.42
22	T	602	CLA	C4D-ND	-2.99	1.33	1.37
22	H	312	CLA	C3B-C4B	2.99	1.49	1.42
22	A	832	CLA	C4D-ND	-2.99	1.33	1.37
22	X	411	CLA	C4D-ND	-2.99	1.33	1.37
22	L	408	CLA	C1D-ND	2.99	1.41	1.37
22	A	813	CLA	C4D-ND	-2.99	1.33	1.37
31	W	407	CHL	C3B-C2B	-2.99	1.36	1.40
22	G	605	CLA	C4D-ND	-2.99	1.33	1.37
22	L	410	CLA	C4D-ND	-2.99	1.33	1.37
22	Q	610	CLA	C3B-C4B	2.99	1.49	1.42
22	U	404	CLA	C4D-ND	-2.98	1.33	1.37
22	W	403	CLA	C3B-C4B	2.98	1.49	1.42
22	W	409	CLA	C4D-ND	-2.98	1.33	1.37
22	S	606	CLA	C3B-C4B	2.98	1.49	1.42
22	A	834	CLA	C4D-ND	-2.98	1.33	1.37
22	Q	607	CLA	C3B-C4B	2.98	1.49	1.42
22	R	608	CLA	C3B-C4B	2.97	1.49	1.42
22	P	607	CLA	C4D-ND	-2.97	1.33	1.37
22	A	819	CLA	C4B-NB	2.97	1.41	1.37
22	F	404	CLA	C4D-ND	-2.97	1.33	1.37
22	Q	611	CLA	C4D-ND	-2.97	1.33	1.37
22	L	404	CLA	C4D-ND	-2.97	1.33	1.37
22	H	308	CLA	C3B-C4B	2.97	1.49	1.42
22	I	601	CLA	C4D-ND	-2.97	1.33	1.37
22	K	604	CLA	C4D-ND	-2.97	1.33	1.37
22	V	617	CLA	C3B-C4B	2.97	1.49	1.42
22	V	610	CLA	C3B-C4B	2.96	1.49	1.42
22	G	608	CLA	C4D-ND	-2.96	1.33	1.37
22	N	607	CLA	C3B-C4B	2.96	1.49	1.42
22	P	610	CLA	C3B-C4B	2.96	1.49	1.42
22	S	607	CLA	C3B-C4B	2.96	1.49	1.42
22	X	419	CLA	C3B-C4B	2.96	1.49	1.42
22	A	819	CLA	C3B-C4B	2.96	1.49	1.42
22	I	601	CLA	C3B-C4B	2.96	1.49	1.42
22	B	805	CLA	C4D-ND	-2.96	1.33	1.37
22	X	410	CLA	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	804	CLA	C4D-ND	-2.96	1.33	1.37
22	A	827	CLA	C4D-ND	-2.96	1.33	1.37
31	U	408	CHL	C3B-C2B	-2.96	1.36	1.40
22	K	617	CLA	C4D-ND	-2.96	1.33	1.37
22	B	820	CLA	C3B-C4B	2.96	1.49	1.42
22	H	305	CLA	C4D-ND	-2.95	1.33	1.37
22	H	313	CLA	C4D-ND	-2.95	1.33	1.37
22	K	606	CLA	C4D-ND	-2.95	1.33	1.37
22	H	303	CLA	C4D-ND	-2.95	1.33	1.37
22	A	812	CLA	C4D-ND	-2.95	1.33	1.37
22	N	602	CLA	C4D-ND	-2.95	1.33	1.37
22	L	405	CLA	C4D-ND	-2.95	1.33	1.37
22	Q	603	CLA	C4D-ND	-2.95	1.33	1.37
22	W	403	CLA	C4D-ND	-2.95	1.33	1.37
22	H	302	CLA	C3B-C4B	2.95	1.49	1.42
22	T	610	CLA	C4D-ND	-2.95	1.33	1.37
22	V	603	CLA	C3B-C4B	2.94	1.49	1.42
22	P	605	CLA	C4D-ND	-2.94	1.33	1.37
22	T	609	CLA	C4D-ND	-2.94	1.33	1.37
22	A	820	CLA	C4D-ND	-2.94	1.33	1.37
22	V	611	CLA	C3B-C4B	2.94	1.49	1.42
22	K	610	CLA	C4D-ND	-2.94	1.33	1.37
22	A	844	CLA	C4D-ND	-2.94	1.33	1.37
22	S	615	CLA	C3B-C4B	2.94	1.49	1.42
22	N	604	CLA	C4D-ND	-2.94	1.33	1.37
22	J	102	CLA	C4D-ND	-2.94	1.33	1.37
22	R	602	CLA	C3B-C4B	2.94	1.49	1.42
22	B	835	CLA	C4D-ND	-2.94	1.33	1.37
22	R	602	CLA	C4D-ND	-2.94	1.33	1.37
22	A	810	CLA	C4D-ND	-2.94	1.33	1.37
22	B	807	CLA	C4D-ND	-2.94	1.33	1.37
22	X	413	CLA	C4D-ND	-2.94	1.33	1.37
22	B	822	CLA	C4D-ND	-2.94	1.33	1.37
22	B	825	CLA	C4D-ND	-2.94	1.33	1.37
22	V	613	CLA	C4D-ND	-2.94	1.33	1.37
22	A	808	CLA	C4D-ND	-2.94	1.33	1.37
22	F	403	CLA	C4D-ND	-2.94	1.33	1.37
22	A	815	CLA	C4D-ND	-2.94	1.33	1.37
22	X	409	CLA	C3B-C4B	2.93	1.49	1.42
22	N	601	CLA	C4D-ND	-2.93	1.33	1.37
22	H	310	CLA	C4D-ND	-2.93	1.33	1.37
22	P	608	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	405	CLA	C3B-C4B	2.93	1.49	1.42
22	N	608	CLA	C3B-C4B	2.93	1.49	1.42
22	R	603	CLA	C3B-C4B	2.93	1.49	1.42
22	R	605	CLA	C3B-C4B	2.93	1.49	1.42
22	V	609	CLA	C3B-C4B	2.93	1.49	1.42
22	A	801	CLA	C1D-ND	2.93	1.41	1.37
22	I	609	CLA	C4D-ND	-2.93	1.33	1.37
22	B	821	CLA	C4D-ND	-2.93	1.33	1.37
22	P	608	CLA	C3B-C4B	2.93	1.49	1.42
22	W	412	CLA	C4D-ND	-2.93	1.33	1.37
22	R	610	CLA	C3B-C4B	2.93	1.49	1.42
22	G	602	CLA	C4D-ND	-2.93	1.33	1.37
22	X	405	CLA	C4D-ND	-2.93	1.33	1.37
22	N	611	CLA	C4D-ND	-2.93	1.33	1.37
22	V	613	CLA	C3B-C4B	2.93	1.49	1.42
22	H	307	CLA	C4D-ND	-2.93	1.33	1.37
22	B	811	CLA	C4D-ND	-2.93	1.33	1.37
22	L	412	CLA	C4D-ND	-2.93	1.33	1.37
22	U	406	CLA	C3B-C4B	2.93	1.49	1.42
22	X	402	CLA	C4D-ND	-2.92	1.33	1.37
22	A	828	CLA	C4D-ND	-2.92	1.33	1.37
22	W	405	CLA	C4D-ND	-2.92	1.33	1.37
22	A	836	CLA	C4D-ND	-2.92	1.33	1.37
22	H	309	CLA	C3B-C4B	2.92	1.49	1.42
22	H	312	CLA	C4D-ND	-2.92	1.33	1.37
22	N	605	CLA	C4D-ND	-2.92	1.33	1.37
22	L	409	CLA	C3B-C4B	2.92	1.49	1.42
22	A	825	CLA	C4D-ND	-2.92	1.33	1.37
22	T	601	CLA	C4D-ND	-2.92	1.33	1.37
22	X	417	CLA	C4D-ND	-2.92	1.33	1.37
22	R	606	CLA	C3B-C4B	2.92	1.49	1.42
22	U	420	CLA	C3B-C4B	2.92	1.49	1.42
22	B	818	CLA	C4D-ND	-2.92	1.33	1.37
22	G	610	CLA	C4D-ND	-2.92	1.33	1.37
22	A	852	CLA	C4D-ND	-2.92	1.33	1.37
22	B	812	CLA	C4D-ND	-2.92	1.33	1.37
22	R	607	CLA	C4D-ND	-2.92	1.33	1.37
22	B	827	CLA	C4D-ND	-2.92	1.33	1.37
22	W	410	CLA	C4D-ND	-2.91	1.33	1.37
22	B	811	CLA	C3B-C4B	2.91	1.49	1.42
22	T	611	CLA	C3B-C4B	2.91	1.49	1.42
22	U	405	CLA	C3B-C4B	2.91	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	803	CLA	C4D-ND	-2.91	1.33	1.37
22	A	834	CLA	C3B-C4B	2.91	1.49	1.42
22	K	602	CLA	C4D-ND	-2.91	1.33	1.37
22	N	610	CLA	C4D-ND	-2.91	1.33	1.37
22	R	604	CLA	C3B-C4B	2.91	1.49	1.42
22	U	415	CLA	C3B-C4B	2.91	1.49	1.42
22	W	404	CLA	C4D-ND	-2.91	1.33	1.37
22	I	607	CLA	C3B-C4B	2.91	1.49	1.42
22	P	604	CLA	C3B-C4B	2.91	1.49	1.42
22	R	608	CLA	C4D-ND	-2.91	1.33	1.37
22	B	838	CLA	C4D-ND	-2.91	1.33	1.37
22	O	311	CLA	C4D-ND	-2.91	1.33	1.37
22	T	607	CLA	C4D-ND	-2.91	1.33	1.37
22	A	836	CLA	C3B-C4B	2.91	1.49	1.42
22	S	603	CLA	C3B-C4B	2.91	1.49	1.42
22	X	407	CLA	C4D-ND	-2.91	1.33	1.37
22	Q	601	CLA	C3B-C4B	2.90	1.49	1.42
22	Q	613	CLA	C3B-C4B	2.90	1.49	1.42
22	A	837	CLA	C3B-C4B	2.90	1.49	1.42
22	R	601	CLA	C3B-C4B	2.90	1.49	1.42
22	A	805	CLA	C4D-ND	-2.90	1.33	1.37
22	W	406	CLA	C4D-ND	-2.90	1.33	1.37
22	H	311	CLA	C4D-ND	-2.90	1.33	1.37
22	T	609	CLA	C3B-C4B	2.90	1.49	1.42
22	O	305	CLA	C4D-ND	-2.90	1.33	1.37
22	A	833	CLA	C4D-ND	-2.90	1.33	1.37
22	I	611	CLA	C4D-ND	-2.90	1.33	1.37
22	K	605	CLA	C4D-ND	-2.90	1.33	1.37
22	K	613	CLA	C3B-C4B	2.90	1.49	1.42
22	T	604	CLA	C4D-ND	-2.90	1.33	1.37
22	A	842	CLA	C4D-ND	-2.90	1.33	1.37
22	O	307	CLA	C3B-C4B	2.90	1.49	1.42
31	X	406	CHL	C3B-C2B	-2.90	1.36	1.40
22	B	824	CLA	C3B-C4B	2.90	1.49	1.42
22	O	315	CLA	C3B-C4B	2.90	1.49	1.42
22	A	824	CLA	C3B-C4B	2.90	1.49	1.42
22	S	601	CLA	C3B-C4B	2.90	1.49	1.42
22	H	318	CLA	C4D-ND	-2.90	1.33	1.37
22	I	605	CLA	C4D-ND	-2.90	1.33	1.37
22	X	408	CLA	C3B-C4B	2.89	1.49	1.42
22	B	836	CLA	C4D-ND	-2.89	1.33	1.37
22	L	406	CLA	C4D-ND	-2.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	610	CLA	C3B-C4B	2.89	1.49	1.42
22	I	608	CLA	C3B-C4B	2.89	1.49	1.42
22	X	417	CLA	C3B-C4B	2.89	1.49	1.42
22	L	402	CLA	C4D-ND	-2.89	1.33	1.37
22	B	828	CLA	C4D-ND	-2.89	1.33	1.37
22	K	611	CLA	C3B-C4B	2.89	1.49	1.42
22	R	609	CLA	C3B-C4B	2.89	1.49	1.42
22	I	603	CLA	C4D-ND	-2.89	1.33	1.37
22	U	412	CLA	C4D-ND	-2.89	1.33	1.37
22	A	817	CLA	C3B-C4B	2.89	1.49	1.42
22	A	823	CLA	C4D-ND	-2.89	1.33	1.37
22	G	601	CLA	C4D-ND	-2.89	1.33	1.37
22	A	822	CLA	C4D-ND	-2.89	1.33	1.37
22	A	807	CLA	C4D-ND	-2.89	1.33	1.37
22	Q	617	CLA	C4D-ND	-2.89	1.33	1.37
22	Q	609	CLA	C3B-C4B	2.89	1.49	1.42
22	F	403	CLA	C3B-C4B	2.89	1.49	1.42
22	V	610	CLA	C4D-ND	-2.89	1.33	1.37
22	L	405	CLA	C3B-C4B	2.89	1.49	1.42
22	R	615	CLA	C3B-C4B	2.89	1.49	1.42
22	A	803	CLA	C3B-C4B	2.89	1.49	1.42
22	R	601	CLA	C4D-ND	-2.89	1.33	1.37
22	B	818	CLA	C3B-C4B	2.89	1.49	1.42
22	T	607	CLA	C3B-C4B	2.89	1.49	1.42
22	R	604	CLA	C4D-ND	-2.88	1.33	1.37
22	N	611	CLA	C3B-C4B	2.88	1.49	1.42
22	H	306	CLA	C4D-ND	-2.88	1.33	1.37
22	B	859	CLA	C3B-C4B	2.88	1.49	1.42
22	N	609	CLA	C3B-C4B	2.88	1.49	1.42
22	T	603	CLA	C3B-C4B	2.88	1.49	1.42
22	B	819	CLA	C4D-ND	-2.88	1.33	1.37
22	S	610	CLA	C3B-C4B	2.88	1.49	1.42
22	V	607	CLA	C3B-C4B	2.88	1.49	1.42
22	N	607	CLA	C4D-ND	-2.88	1.33	1.37
22	S	607	CLA	C4D-ND	-2.88	1.33	1.37
22	B	828	CLA	C3B-C4B	2.88	1.49	1.42
22	L	406	CLA	C3B-C4B	2.88	1.49	1.42
22	X	408	CLA	C4D-ND	-2.88	1.33	1.37
22	F	404	CLA	C3B-C4B	2.88	1.49	1.42
22	A	821	CLA	C4D-ND	-2.88	1.33	1.37
22	K	609	CLA	C4D-ND	-2.88	1.33	1.37
22	S	610	CLA	C4D-ND	-2.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	612	CLA	C4D-ND	-2.88	1.33	1.37
22	B	822	CLA	C3B-C4B	2.88	1.49	1.42
22	X	413	CLA	C3B-C4B	2.88	1.49	1.42
22	A	840	CLA	C4D-ND	-2.88	1.33	1.37
22	Q	605	CLA	C3B-C4B	2.88	1.49	1.42
22	Q	608	CLA	C4D-ND	-2.88	1.33	1.37
22	O	309	CLA	C3B-C4B	2.88	1.49	1.42
22	T	608	CLA	C3B-C4B	2.88	1.49	1.42
22	B	815	CLA	C4D-ND	-2.88	1.33	1.37
22	B	816	CLA	C4D-ND	-2.88	1.33	1.37
22	I	610	CLA	C4D-ND	-2.88	1.33	1.37
22	O	315	CLA	C4D-ND	-2.88	1.33	1.37
22	N	605	CLA	C3B-C4B	2.88	1.49	1.42
22	S	609	CLA	C3B-C4B	2.88	1.49	1.42
31	W	408	CHL	C3B-C2B	-2.87	1.36	1.40
22	B	823	CLA	C4D-ND	-2.87	1.33	1.37
22	I	605	CLA	C3B-C4B	2.87	1.49	1.42
22	V	612	CLA	C3B-C4B	2.87	1.49	1.42
22	H	302	CLA	C4D-ND	-2.87	1.33	1.37
22	O	314	CLA	C4D-ND	-2.87	1.33	1.37
22	I	609	CLA	C3B-C4B	2.87	1.49	1.42
22	W	419	CLA	C4D-ND	-2.87	1.33	1.37
22	T	604	CLA	C3B-C4B	2.87	1.49	1.42
22	O	312	CLA	C3B-C4B	2.87	1.49	1.42
22	O	308	CLA	C4D-ND	-2.87	1.33	1.37
22	L	411	CLA	C3B-C4B	2.87	1.49	1.42
22	Q	603	CLA	C3B-C4B	2.87	1.49	1.42
22	G	604	CLA	C4D-ND	-2.87	1.33	1.37
22	L	403	CLA	C4D-ND	-2.87	1.33	1.37
22	X	412	CLA	C4D-ND	-2.87	1.33	1.37
22	P	609	CLA	C4D-ND	-2.87	1.33	1.37
22	I	606	CLA	C3B-C4B	2.87	1.49	1.42
22	S	602	CLA	C4D-ND	-2.87	1.33	1.37
22	H	305	CLA	C3B-C4B	2.87	1.49	1.42
22	I	611	CLA	C3B-C4B	2.87	1.49	1.42
22	A	831	CLA	C4D-ND	-2.87	1.33	1.37
22	B	809	CLA	C4D-ND	-2.87	1.33	1.37
22	A	838	CLA	C4D-ND	-2.87	1.33	1.37
31	V	605	CHL	C3B-C2B	-2.87	1.36	1.40
22	B	834	CLA	C3B-C4B	2.87	1.49	1.42
22	W	414	CLA	C4D-ND	-2.87	1.33	1.37
22	H	313	CLA	C3B-C4B	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	808	CLA	C4D-ND	-2.86	1.33	1.37
22	B	839	CLA	C4D-ND	-2.86	1.33	1.37
22	O	314	CLA	C3B-C4B	2.86	1.49	1.42
22	B	804	CLA	C4D-ND	-2.86	1.33	1.37
22	I	606	CLA	C4D-ND	-2.86	1.33	1.37
22	O	312	CLA	C4D-ND	-2.86	1.33	1.37
22	T	605	CLA	C4D-ND	-2.86	1.33	1.37
22	U	411	CLA	C3B-C4B	2.86	1.49	1.42
22	G	611	CLA	C4D-ND	-2.86	1.33	1.37
22	N	606	CLA	C4D-ND	-2.86	1.33	1.37
22	B	839	CLA	C3B-C4B	2.86	1.49	1.42
22	G	604	CLA	C3B-C4B	2.86	1.49	1.42
22	W	409	CLA	C3B-C4B	2.86	1.49	1.42
22	P	606	CLA	C3B-C4B	2.86	1.49	1.42
22	B	833	CLA	C3B-C4B	2.86	1.49	1.42
22	L	403	CLA	C3B-C4B	2.86	1.49	1.42
22	A	822	CLA	C3B-C4B	2.86	1.49	1.42
22	S	614	CLA	C3B-C4B	2.86	1.49	1.42
22	V	608	CLA	C4D-ND	-2.86	1.33	1.37
22	X	419	CLA	C4D-ND	-2.86	1.33	1.37
22	A	817	CLA	C4D-ND	-2.86	1.33	1.37
22	A	830	CLA	C3B-C4B	2.86	1.49	1.42
22	G	607	CLA	C3B-C4B	2.86	1.49	1.42
22	R	611	CLA	C3B-C4B	2.86	1.49	1.42
22	N	601	CLA	C3B-C4B	2.86	1.49	1.42
22	A	814	CLA	C3B-C4B	2.86	1.49	1.42
22	I	604	CLA	C4D-ND	-2.86	1.33	1.37
22	L	411	CLA	C4D-ND	-2.86	1.33	1.37
22	I	603	CLA	C3B-C4B	2.85	1.49	1.42
22	A	809	CLA	C3B-C4B	2.85	1.49	1.42
22	B	806	CLA	C4D-ND	-2.85	1.33	1.37
22	R	605	CLA	C4D-ND	-2.85	1.33	1.37
22	S	606	CLA	C4D-ND	-2.85	1.33	1.37
22	A	839	CLA	C4D-ND	-2.85	1.33	1.37
22	A	825	CLA	C3B-C4B	2.85	1.49	1.42
22	W	413	CLA	C4D-ND	-2.85	1.33	1.37
22	B	812	CLA	C3B-C4B	2.85	1.49	1.42
22	A	829	CLA	C3B-C4B	2.85	1.49	1.42
22	B	814	CLA	C4D-ND	-2.85	1.33	1.37
22	T	606	CLA	C4D-ND	-2.85	1.33	1.37
22	B	837	CLA	C3B-C4B	2.85	1.49	1.42
22	A	827	CLA	C3B-C4B	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	823	CLA	C3B-C4B	2.85	1.49	1.42
22	G	611	CLA	C3B-C4B	2.85	1.49	1.42
22	L	410	CLA	C3B-C4B	2.85	1.49	1.42
22	H	309	CLA	C4D-ND	-2.85	1.33	1.37
22	A	818	CLA	C4D-ND	-2.85	1.33	1.37
22	L	404	CLA	C3B-C4B	2.85	1.49	1.42
22	G	603	CLA	C3B-C4B	2.85	1.49	1.42
22	A	852	CLA	C3B-C4B	2.85	1.49	1.42
22	G	606	CLA	C4D-ND	-2.85	1.33	1.37
22	Q	601	CLA	C4D-ND	-2.85	1.33	1.37
22	B	859	CLA	C4D-ND	-2.85	1.33	1.37
22	N	608	CLA	C4D-ND	-2.85	1.33	1.37
22	A	832	CLA	C3B-C4B	2.85	1.49	1.42
22	O	305	CLA	C3B-C4B	2.85	1.49	1.42
22	B	831	CLA	C4D-ND	-2.85	1.33	1.37
22	G	609	CLA	C4D-ND	-2.85	1.33	1.37
22	H	308	CLA	C4D-ND	-2.85	1.33	1.37
22	U	409	CLA	C4D-ND	-2.85	1.33	1.37
22	P	605	CLA	C3B-C4B	2.85	1.49	1.42
22	W	419	CLA	C3B-C4B	2.85	1.49	1.42
22	R	615	CLA	C4D-ND	-2.85	1.33	1.37
22	B	821	CLA	C3B-C4B	2.85	1.49	1.42
22	O	310	CLA	C4D-ND	-2.85	1.33	1.37
22	U	413	CLA	C4D-ND	-2.85	1.33	1.37
22	H	318	CLA	C3B-C4B	2.85	1.49	1.42
22	Q	618	CLA	C4D-ND	-2.85	1.33	1.37
22	W	406	CLA	C3B-C4B	2.84	1.49	1.42
22	U	405	CLA	C4D-ND	-2.84	1.33	1.37
22	U	406	CLA	C4D-ND	-2.84	1.33	1.37
22	Q	609	CLA	C4D-ND	-2.84	1.33	1.37
22	A	806	CLA	C4D-ND	-2.84	1.33	1.37
22	K	610	CLA	C3B-C4B	2.84	1.49	1.42
22	B	833	CLA	C4D-ND	-2.84	1.33	1.37
22	P	604	CLA	C4D-ND	-2.84	1.33	1.37
22	U	401	CLA	C4D-ND	-2.84	1.33	1.37
22	Q	611	CLA	C3B-C4B	2.84	1.49	1.42
22	B	825	CLA	C3B-C4B	2.84	1.49	1.42
22	G	610	CLA	C3B-C4B	2.84	1.49	1.42
22	W	411	CLA	C3B-C4B	2.84	1.49	1.42
31	V	606	CHL	C3B-C2B	-2.84	1.36	1.40
22	B	838	CLA	C3B-C4B	2.84	1.49	1.42
22	B	804	CLA	C3B-C4B	2.84	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	407	CLA	C3B-C4B	2.84	1.49	1.42
22	A	811	CLA	C3B-C4B	2.84	1.49	1.42
22	N	602	CLA	C3B-C4B	2.84	1.49	1.42
22	Q	610	CLA	C4D-ND	-2.84	1.33	1.37
22	B	831	CLA	C3B-C4B	2.84	1.49	1.42
22	N	604	CLA	C3B-C4B	2.84	1.49	1.42
22	A	833	CLA	C3B-C4B	2.84	1.49	1.42
22	B	814	CLA	C3B-C4B	2.84	1.49	1.42
22	Q	607	CLA	C4D-ND	-2.84	1.33	1.37
22	V	602	CLA	C4D-ND	-2.84	1.33	1.37
26	U	419	LHG	C26-C25	-2.84	1.35	1.51
22	K	602	CLA	C3B-C4B	2.84	1.49	1.42
22	U	414	CLA	C3B-C4B	2.84	1.49	1.42
22	B	810	CLA	C4D-ND	-2.83	1.33	1.37
22	B	817	CLA	C3B-C4B	2.83	1.49	1.42
22	U	410	CLA	C3B-C4B	2.83	1.49	1.42
22	A	826	CLA	C4D-ND	-2.83	1.33	1.37
22	K	606	CLA	C3B-C4B	2.83	1.49	1.42
22	X	405	CLA	C3B-C4B	2.83	1.49	1.42
22	T	608	CLA	C4D-ND	-2.83	1.33	1.37
22	A	831	CLA	C3B-C4B	2.83	1.49	1.42
26	H	316	LHG	C26-C25	-2.83	1.35	1.51
22	X	402	CLA	C3B-C4B	2.83	1.49	1.42
22	S	615	CLA	C4D-ND	-2.83	1.33	1.37
22	U	410	CLA	C4D-ND	-2.83	1.33	1.37
22	V	601	CLA	C4D-ND	-2.83	1.33	1.37
22	H	306	CLA	C3B-C4B	2.83	1.49	1.42
22	K	604	CLA	C3B-C4B	2.83	1.49	1.42
22	S	603	CLA	C4D-ND	-2.83	1.33	1.37
22	H	304	CLA	C3B-C4B	2.83	1.49	1.42
22	V	604	CLA	C4D-ND	-2.83	1.33	1.37
22	N	603	CLA	C3B-C4B	2.83	1.49	1.42
22	P	609	CLA	C3B-C4B	2.83	1.49	1.42
22	S	604	CLA	C4D-ND	-2.83	1.33	1.37
22	G	609	CLA	C3B-C4B	2.83	1.49	1.42
22	U	414	CLA	C4D-ND	-2.83	1.33	1.37
22	A	815	CLA	C3B-C4B	2.83	1.49	1.42
22	B	835	CLA	C3B-C4B	2.83	1.49	1.42
26	X	420	LHG	C26-C25	-2.83	1.35	1.51
22	U	420	CLA	C4D-ND	-2.83	1.33	1.37
22	U	412	CLA	C3B-C4B	2.83	1.49	1.42
22	L	407	CLA	C4D-ND	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	609	CLA	C4D-ND	-2.83	1.33	1.37
26	L	416	LHG	C26-C25	-2.83	1.35	1.51
22	S	604	CLA	C3B-C4B	2.83	1.49	1.42
22	I	604	CLA	C3B-C4B	2.83	1.49	1.42
22	O	319	CLA	C3B-C4B	2.83	1.49	1.42
22	B	827	CLA	C3B-C4B	2.82	1.49	1.42
22	O	319	CLA	C4D-ND	-2.82	1.33	1.37
22	U	401	CLA	C3B-C4B	2.82	1.49	1.42
22	W	410	CLA	C3B-C4B	2.82	1.49	1.42
22	A	806	CLA	C3B-C4B	2.82	1.49	1.42
22	W	413	CLA	C3B-C4B	2.82	1.49	1.42
22	X	411	CLA	C3B-C4B	2.82	1.49	1.42
22	W	404	CLA	C3B-C4B	2.82	1.49	1.42
22	Q	606	CLA	C4D-ND	-2.82	1.33	1.37
22	V	609	CLA	C4D-ND	-2.82	1.33	1.37
22	V	602	CLA	C3B-C4B	2.82	1.49	1.42
26	P	601	LHG	C26-C25	-2.82	1.35	1.51
22	S	605	CLA	C4B-NB	2.82	1.41	1.37
22	T	601	CLA	C3B-C4B	2.82	1.49	1.42
22	A	823	CLA	C3B-C4B	2.82	1.49	1.42
22	N	610	CLA	C1B-C2B	2.82	1.49	1.43
22	Q	617	CLA	C3B-C4B	2.82	1.49	1.42
22	O	313	CLA	C4D-ND	-2.82	1.33	1.37
22	O	311	CLA	C3B-C4B	2.82	1.49	1.42
22	O	310	CLA	C3B-C4B	2.82	1.49	1.42
22	A	828	CLA	C3B-C4B	2.82	1.49	1.42
22	T	605	CLA	C3B-C4B	2.82	1.49	1.42
22	A	835	CLA	C4D-ND	-2.82	1.33	1.37
26	N	614	LHG	C26-C25	-2.82	1.35	1.51
26	T	614	LHG	C26-C25	-2.82	1.35	1.51
22	G	605	CLA	C3B-C4B	2.82	1.49	1.42
26	B	851	LHG	C26-C25	-2.82	1.35	1.51
22	W	415	CLA	C3B-C4B	2.81	1.49	1.42
22	V	604	CLA	C3B-C4B	2.81	1.49	1.42
22	A	804	CLA	C3B-C4B	2.81	1.49	1.42
22	U	403	CLA	C4D-ND	-2.81	1.33	1.37
22	V	612	CLA	C4D-ND	-2.81	1.33	1.37
26	O	323	LHG	C26-C25	-2.81	1.35	1.51
26	Q	616	LHG	C26-C25	-2.81	1.35	1.51
22	B	810	CLA	C3B-C4B	2.81	1.49	1.42
22	K	612	CLA	C3B-C4B	2.81	1.49	1.42
22	O	308	CLA	C3B-C4B	2.81	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	607	CLA	C1B-C2B	2.81	1.49	1.43
26	O	318	LHG	C26-C25	-2.81	1.35	1.51
22	A	814	CLA	C4D-ND	-2.81	1.33	1.37
22	I	602	CLA	C3B-C4B	2.81	1.49	1.42
22	U	409	CLA	C3B-C4B	2.81	1.49	1.42
22	B	813	CLA	C3B-C4B	2.81	1.49	1.42
26	O	324	LHG	C26-C25	-2.81	1.35	1.51
22	I	607	CLA	C4D-ND	-2.81	1.33	1.37
22	V	607	CLA	C4D-ND	-2.81	1.33	1.37
26	A	845	LHG	C26-C25	-2.81	1.35	1.51
22	K	603	CLA	C3B-C4B	2.81	1.49	1.42
22	W	402	CLA	C3B-C4B	2.81	1.49	1.42
22	H	304	CLA	C4D-ND	-2.81	1.33	1.37
22	K	613	CLA	C4D-ND	-2.81	1.33	1.37
22	R	610	CLA	C4D-ND	-2.81	1.33	1.37
22	S	602	CLA	C3B-C4B	2.81	1.49	1.42
22	S	614	CLA	C4D-ND	-2.81	1.33	1.37
26	R	614	LHG	C26-C25	-2.81	1.35	1.51
22	B	808	CLA	C3B-C4B	2.81	1.49	1.42
22	Q	606	CLA	C3B-C4B	2.81	1.49	1.42
22	S	601	CLA	C4D-ND	-2.81	1.33	1.37
26	K	619	LHG	C26-C25	-2.81	1.35	1.51
22	R	603	CLA	C4D-ND	-2.81	1.33	1.37
22	A	810	CLA	C3B-C4B	2.80	1.49	1.42
22	O	313	CLA	C3B-C4B	2.80	1.49	1.42
22	W	412	CLA	C3B-C4B	2.80	1.49	1.42
26	K	616	LHG	C26-C25	-2.80	1.35	1.51
22	A	808	CLA	C3B-C4B	2.80	1.49	1.42
22	B	826	CLA	C3B-C4B	2.80	1.49	1.42
22	K	609	CLA	C3B-C4B	2.80	1.49	1.42
22	A	824	CLA	C4D-ND	-2.80	1.33	1.37
22	A	826	CLA	C3B-C4B	2.80	1.49	1.42
22	A	820	CLA	C3B-C4B	2.80	1.49	1.42
22	K	612	CLA	C4D-ND	-2.80	1.33	1.37
22	W	402	CLA	C4D-ND	-2.80	1.33	1.37
22	B	834	CLA	C4D-ND	-2.80	1.33	1.37
22	O	309	CLA	C4D-ND	-2.80	1.33	1.37
22	B	815	CLA	C3B-C4B	2.80	1.49	1.42
26	W	420	LHG	C26-C25	-2.80	1.35	1.51
22	H	310	CLA	C3B-C4B	2.80	1.49	1.42
22	U	404	CLA	C3B-C4B	2.80	1.49	1.42
26	O	321	LHG	C26-C25	-2.80	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	616	LHG	C26-C25	-2.80	1.35	1.51
22	K	605	CLA	C3B-C4B	2.80	1.49	1.42
22	A	821	CLA	C3B-C4B	2.80	1.49	1.42
22	K	611	CLA	C4D-ND	-2.80	1.33	1.37
26	A	846	LHG	C26-C25	-2.79	1.35	1.51
22	V	611	CLA	C4D-ND	-2.79	1.33	1.37
22	L	417	CLA	C3B-C4B	2.79	1.49	1.42
22	T	603	CLA	C4D-ND	-2.79	1.33	1.37
22	N	609	CLA	C4D-ND	-2.79	1.33	1.37
26	S	613	LHG	C26-C25	-2.79	1.35	1.51
22	X	409	CLA	C4D-ND	-2.79	1.33	1.37
22	U	413	CLA	C3B-C4B	2.79	1.49	1.42
22	X	403	CLA	C3B-C4B	2.79	1.49	1.42
26	G	614	LHG	C26-C25	-2.79	1.35	1.51
22	B	826	CLA	C4D-ND	-2.79	1.33	1.37
22	A	844	CLA	C3B-C4B	2.79	1.49	1.42
22	Q	612	CLA	C3B-C4B	2.79	1.49	1.42
22	Q	605	CLA	C4D-ND	-2.79	1.33	1.37
22	R	609	CLA	C4D-ND	-2.79	1.33	1.37
22	G	601	CLA	C3B-C4B	2.79	1.49	1.42
22	U	415	CLA	C4D-ND	-2.79	1.33	1.37
22	A	807	CLA	C3B-C4B	2.79	1.49	1.42
22	B	824	CLA	C4D-ND	-2.78	1.33	1.37
22	I	610	CLA	C3B-C4B	2.78	1.49	1.42
22	S	609	CLA	C1B-C2B	2.78	1.49	1.43
22	A	835	CLA	C3B-C4B	2.78	1.49	1.42
22	B	832	CLA	C4D-ND	-2.78	1.33	1.37
22	B	806	CLA	C3B-C4B	2.78	1.49	1.42
22	A	813	CLA	C3B-C4B	2.78	1.49	1.42
22	B	802	CLA	MG-NB	-2.78	2.00	2.05
22	B	817	CLA	C4D-ND	-2.78	1.33	1.37
22	T	602	CLA	C3B-C4B	2.78	1.49	1.42
22	F	405	CLA	C4D-ND	-2.78	1.33	1.37
22	B	807	CLA	C3B-C4B	2.78	1.49	1.42
22	L	412	CLA	C3B-C4B	2.77	1.49	1.42
22	X	404	CLA	C4D-ND	-2.77	1.33	1.37
22	G	608	CLA	C3B-C4B	2.77	1.49	1.42
22	B	813	CLA	C4D-ND	-2.77	1.33	1.37
22	I	608	CLA	C4D-ND	-2.77	1.33	1.37
22	H	303	CLA	C3B-C4B	2.77	1.49	1.42
22	T	611	CLA	C4D-ND	-2.77	1.33	1.37
22	B	816	CLA	C3B-C4B	2.77	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	803	CLA	C3B-C4B	2.77	1.49	1.42
22	B	809	CLA	C3B-C4B	2.76	1.49	1.42
22	A	839	CLA	C3B-C4B	2.76	1.49	1.42
22	P	611	CLA	C1B-C2B	2.76	1.49	1.43
22	B	805	CLA	C3B-C4B	2.76	1.49	1.42
22	U	411	CLA	C4D-ND	-2.76	1.33	1.37
22	A	830	CLA	C4D-ND	-2.76	1.33	1.37
22	K	617	CLA	C3B-C4B	2.76	1.49	1.42
22	V	612	CLA	C1B-C2B	2.76	1.49	1.43
22	B	832	CLA	C3B-C4B	2.76	1.49	1.42
22	K	607	CLA	C3B-C4B	2.76	1.49	1.42
22	V	608	CLA	C3B-C4B	2.76	1.49	1.42
22	L	409	CLA	C4D-ND	-2.75	1.33	1.37
22	V	602	CLA	C1B-C2B	2.75	1.49	1.43
22	L	407	CLA	C3B-C4B	2.75	1.49	1.42
22	L	408	CLA	C3B-C4B	2.75	1.49	1.42
22	A	838	CLA	C3B-C4B	2.75	1.49	1.42
22	G	607	CLA	C4D-ND	-2.75	1.33	1.37
22	A	812	CLA	C3B-C4B	2.75	1.49	1.42
22	Q	613	CLA	C4D-ND	-2.75	1.33	1.37
22	S	608	CLA	C4D-ND	-2.75	1.33	1.37
22	O	306	CLA	C3B-C4B	2.75	1.49	1.42
22	B	837	CLA	C4D-ND	-2.74	1.33	1.37
22	P	603	CLA	C1B-C2B	2.74	1.49	1.43
22	L	402	CLA	C3B-C4B	2.74	1.49	1.42
22	V	603	CLA	C4D-ND	-2.74	1.33	1.37
22	B	819	CLA	C3B-C4B	2.74	1.49	1.42
22	A	841	CLA	C3B-C4B	2.74	1.49	1.42
22	R	606	CLA	C4D-ND	-2.74	1.33	1.37
22	R	615	CLA	C1B-C2B	2.73	1.49	1.43
22	S	601	CLA	C1B-C2B	2.73	1.49	1.43
22	Q	604	CLA	C3B-C4B	2.73	1.49	1.42
22	A	841	CLA	C4D-ND	-2.73	1.33	1.37
22	A	805	CLA	C3B-C4B	2.73	1.49	1.42
22	A	818	CLA	C3B-C4B	2.73	1.49	1.42
22	B	819	CLA	C1B-C2B	2.73	1.49	1.43
22	S	602	CLA	C1B-C2B	2.73	1.49	1.43
22	V	617	CLA	C4D-ND	-2.72	1.33	1.37
22	G	603	CLA	C4D-ND	-2.72	1.33	1.37
22	J	102	CLA	C3B-C4B	2.72	1.49	1.42
22	G	602	CLA	C3B-C4B	2.72	1.49	1.42
22	R	602	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	829	CLA	C4D-ND	-2.72	1.34	1.37
22	N	610	CLA	C3B-C4B	2.71	1.49	1.42
22	P	602	CLA	C3B-C4B	2.71	1.49	1.42
22	R	607	CLA	C3B-C4B	2.71	1.49	1.42
22	V	608	CLA	C1B-C2B	2.71	1.49	1.43
22	V	610	CLA	C1B-C2B	2.71	1.49	1.43
22	X	412	CLA	C1B-C2B	2.71	1.49	1.43
22	O	307	CLA	C4D-ND	-2.70	1.34	1.37
22	B	820	CLA	C4D-ND	-2.70	1.34	1.37
22	P	603	CLA	C4D-ND	-2.70	1.34	1.37
22	O	310	CLA	C1B-C2B	2.70	1.49	1.43
22	P	611	CLA	C4D-ND	-2.70	1.34	1.37
22	T	611	CLA	C1B-C2B	2.70	1.49	1.43
22	X	402	CLA	C1B-C2B	2.70	1.49	1.43
22	R	611	CLA	C1B-C2B	2.69	1.49	1.43
22	U	413	CLA	C1B-C2B	2.69	1.49	1.43
22	A	806	CLA	C1B-C2B	2.69	1.49	1.43
22	B	811	CLA	C1B-C2B	2.69	1.49	1.43
22	V	617	CLA	C1B-C2B	2.69	1.49	1.43
22	L	405	CLA	C1B-C2B	2.69	1.49	1.43
22	N	603	CLA	C4D-ND	-2.69	1.34	1.37
22	I	604	CLA	C1B-C2B	2.68	1.49	1.43
22	U	414	CLA	C1B-C2B	2.68	1.49	1.43
22	T	610	CLA	C1B-C2B	2.68	1.49	1.43
22	P	610	CLA	C4D-ND	-2.68	1.34	1.37
22	H	305	CLA	C1B-C2B	2.68	1.49	1.43
22	V	604	CLA	C1B-C2B	2.68	1.49	1.43
22	Q	601	CLA	C1B-C2B	2.68	1.49	1.43
22	A	831	CLA	C1B-C2B	2.68	1.49	1.43
22	I	609	CLA	C1B-C2B	2.68	1.49	1.43
22	R	601	CLA	C1B-C2B	2.68	1.49	1.43
22	A	841	CLA	C1B-C2B	2.68	1.49	1.43
22	W	411	CLA	C4D-ND	-2.68	1.34	1.37
22	I	610	CLA	C1B-C2B	2.67	1.49	1.43
22	V	613	CLA	C1B-C2B	2.67	1.49	1.43
22	Q	606	CLA	C1B-C2B	2.67	1.49	1.43
22	J	102	CLA	C1B-C2B	2.67	1.49	1.43
22	O	319	CLA	C1B-C2B	2.67	1.49	1.43
22	P	608	CLA	C1B-C2B	2.67	1.49	1.43
22	N	611	CLA	C1B-C2B	2.67	1.49	1.43
22	A	840	CLA	C3B-C4B	2.67	1.49	1.42
22	X	411	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	604	CLA	C1B-C2B	2.67	1.49	1.43
22	K	605	CLA	C1B-C2B	2.67	1.49	1.43
22	A	824	CLA	C1B-C2B	2.67	1.49	1.43
31	W	408	CHL	C1C-NC	2.67	1.37	1.35
22	X	413	CLA	C1B-C2B	2.66	1.49	1.43
22	Q	618	CLA	C1B-C2B	2.66	1.49	1.43
22	W	412	CLA	C1B-C2B	2.66	1.49	1.43
22	L	407	CLA	C1B-C2B	2.66	1.49	1.43
22	N	604	CLA	C1B-C2B	2.66	1.49	1.43
22	W	415	CLA	C4D-ND	-2.66	1.34	1.37
22	O	313	CLA	C1B-C2B	2.66	1.49	1.43
22	U	406	CLA	C1B-C2B	2.66	1.49	1.43
22	U	420	CLA	C1B-C2B	2.66	1.49	1.43
22	K	606	CLA	C1B-C2B	2.65	1.49	1.43
22	S	608	CLA	C1B-C2B	2.65	1.49	1.43
22	V	609	CLA	C1B-C2B	2.65	1.49	1.43
22	A	839	CLA	C1B-C2B	2.65	1.49	1.43
22	N	607	CLA	C1B-C2B	2.65	1.49	1.43
22	Q	603	CLA	C1B-C2B	2.65	1.49	1.43
22	U	412	CLA	C1B-C2B	2.65	1.49	1.43
22	L	417	CLA	C1B-C2B	2.65	1.49	1.43
22	A	840	CLA	C1B-C2B	2.65	1.49	1.43
22	A	833	CLA	C1B-C2B	2.65	1.49	1.43
22	B	810	CLA	C1B-C2B	2.65	1.49	1.43
22	F	403	CLA	C1B-C2B	2.65	1.49	1.43
22	P	606	CLA	C1B-C2B	2.65	1.49	1.43
22	P	610	CLA	C1B-C2B	2.65	1.49	1.43
22	R	609	CLA	C1B-C2B	2.65	1.49	1.43
22	R	608	CLA	C1B-C2B	2.64	1.49	1.43
22	P	606	CLA	C4D-ND	-2.64	1.34	1.37
22	U	401	CLA	C1B-C2B	2.64	1.49	1.43
22	R	605	CLA	C1B-C2B	2.64	1.49	1.43
31	V	606	CHL	C1C-C2C	2.64	1.49	1.45
22	H	310	CLA	C1B-C2B	2.64	1.49	1.43
22	H	312	CLA	C1B-C2B	2.64	1.49	1.43
22	T	601	CLA	C1B-C2B	2.64	1.49	1.43
22	U	410	CLA	C1B-C2B	2.64	1.49	1.43
22	A	814	CLA	C1B-C2B	2.64	1.49	1.43
22	A	805	CLA	C1B-C2B	2.64	1.49	1.43
22	A	821	CLA	C1B-C2B	2.64	1.49	1.43
22	G	611	CLA	C1B-C2B	2.64	1.49	1.43
22	A	835	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	414	CLA	C1B-C2B	2.64	1.49	1.43
22	T	609	CLA	C1B-C2B	2.64	1.49	1.43
22	A	813	CLA	C1B-C2B	2.64	1.49	1.43
22	H	311	CLA	C1B-C2B	2.64	1.49	1.43
22	P	605	CLA	C1B-C2B	2.64	1.49	1.43
22	R	603	CLA	C1B-C2B	2.64	1.49	1.43
22	I	608	CLA	C1B-C2B	2.64	1.49	1.43
22	T	605	CLA	C1B-C2B	2.64	1.49	1.43
22	V	611	CLA	C1B-C2B	2.64	1.49	1.43
22	A	844	CLA	C1B-C2B	2.64	1.49	1.43
22	G	602	CLA	C1B-C2B	2.64	1.49	1.43
22	G	604	CLA	C1B-C2B	2.63	1.49	1.43
22	X	419	CLA	C1B-C2B	2.63	1.49	1.43
22	R	610	CLA	C1B-C2B	2.63	1.49	1.43
22	T	608	CLA	C1B-C2B	2.63	1.49	1.43
22	B	818	CLA	C1B-C2B	2.63	1.49	1.43
22	P	604	CLA	C1B-C2B	2.63	1.49	1.43
22	Q	617	CLA	C1B-C2B	2.63	1.49	1.43
22	B	825	CLA	C1B-C2B	2.63	1.49	1.43
22	N	608	CLA	C1B-C2B	2.63	1.49	1.43
22	V	607	CLA	C1B-C2B	2.63	1.49	1.43
22	B	833	CLA	C1B-C2B	2.63	1.49	1.43
22	Q	607	CLA	C1B-C2B	2.63	1.49	1.43
22	H	309	CLA	C1B-C2B	2.63	1.49	1.43
22	B	816	CLA	C1B-C2B	2.63	1.49	1.43
22	X	407	CLA	C1B-C2B	2.63	1.49	1.43
22	L	409	CLA	C1B-C2B	2.62	1.49	1.43
22	W	419	CLA	C1B-C2B	2.62	1.49	1.43
22	A	807	CLA	C1B-C2B	2.62	1.49	1.43
22	I	605	CLA	C1B-C2B	2.62	1.49	1.43
22	X	403	CLA	C1B-C2B	2.62	1.49	1.43
22	I	606	CLA	C1B-C2B	2.62	1.49	1.43
22	R	604	CLA	C1B-C2B	2.62	1.49	1.43
22	K	611	CLA	C1B-C2B	2.62	1.49	1.43
22	N	601	CLA	C1B-C2B	2.62	1.49	1.43
22	I	602	CLA	C1B-C2B	2.62	1.49	1.43
22	H	303	CLA	C1B-C2B	2.62	1.49	1.43
22	O	311	CLA	C1B-C2B	2.62	1.49	1.43
22	L	406	CLA	C1B-C2B	2.62	1.49	1.43
22	A	818	CLA	C1B-C2B	2.62	1.49	1.43
22	A	801	CLA	C3B-C4B	2.62	1.48	1.42
22	N	609	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	601	CLA	C1B-C2B	2.62	1.49	1.43
22	F	404	CLA	C1B-C2B	2.62	1.49	1.43
22	U	415	CLA	C1B-C2B	2.62	1.49	1.43
22	U	409	CLA	C1B-C2B	2.62	1.49	1.43
22	B	831	CLA	C1B-C2B	2.62	1.49	1.43
22	A	808	CLA	C1B-C2B	2.62	1.49	1.43
22	R	606	CLA	C1B-C2B	2.61	1.49	1.43
22	A	823	CLA	C1B-C2B	2.61	1.49	1.43
22	B	809	CLA	C1B-C2B	2.61	1.49	1.43
22	I	603	CLA	C1B-C2B	2.61	1.49	1.43
22	O	305	CLA	C1B-C2B	2.61	1.49	1.43
22	Q	612	CLA	C1B-C2B	2.61	1.49	1.43
22	W	415	CLA	C1B-C2B	2.61	1.49	1.43
22	U	404	CLA	C1B-C2B	2.61	1.49	1.43
22	X	405	CLA	C1B-C2B	2.61	1.49	1.43
22	B	826	CLA	C1B-C2B	2.61	1.49	1.43
22	B	803	CLA	C1B-C2B	2.61	1.49	1.43
22	B	832	CLA	C1B-C2B	2.61	1.49	1.43
22	B	839	CLA	C1B-C2B	2.61	1.49	1.43
22	A	803	CLA	C1B-C2B	2.61	1.49	1.43
22	B	836	CLA	C3B-C4B	2.61	1.48	1.42
22	N	605	CLA	C1B-C2B	2.61	1.49	1.43
22	G	610	CLA	C1B-C2B	2.61	1.49	1.43
22	B	804	CLA	C1B-C2B	2.61	1.49	1.43
22	I	607	CLA	C1B-C2B	2.61	1.49	1.43
22	K	613	CLA	C1B-C2B	2.61	1.49	1.43
22	W	413	CLA	C1B-C2B	2.61	1.49	1.43
22	O	314	CLA	C1B-C2B	2.61	1.49	1.43
22	Q	610	CLA	C1B-C2B	2.61	1.49	1.43
31	W	422	CHL	C1C-NC	2.61	1.37	1.35
22	B	821	CLA	C1B-C2B	2.61	1.49	1.43
33	A	802	CL0	CHA-CBD	-2.60	1.48	1.51
22	B	808	CLA	C1B-C2B	2.60	1.49	1.43
22	V	603	CLA	C1B-C2B	2.60	1.49	1.43
22	A	837	CLA	C1B-C2B	2.60	1.49	1.43
22	B	837	CLA	C1B-C2B	2.60	1.49	1.43
22	U	405	CLA	C1B-C2B	2.60	1.49	1.43
22	O	309	CLA	C1B-C2B	2.60	1.49	1.43
22	B	823	CLA	C1B-C2B	2.60	1.49	1.43
22	H	302	CLA	C1B-C2B	2.60	1.49	1.43
22	B	859	CLA	C1B-C2B	2.60	1.49	1.43
22	P	609	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	615	CLA	C1B-C2B	2.60	1.49	1.43
22	G	608	CLA	C1B-C2B	2.60	1.49	1.43
22	L	411	CLA	C1B-C2B	2.60	1.49	1.43
22	S	614	CLA	C1B-C2B	2.60	1.49	1.43
22	X	409	CLA	C1B-C2B	2.60	1.49	1.43
22	B	824	CLA	C1B-C2B	2.60	1.49	1.43
22	O	308	CLA	C1B-C2B	2.60	1.49	1.43
22	L	404	CLA	C1B-C2B	2.60	1.49	1.43
22	A	832	CLA	C1B-C2B	2.60	1.49	1.43
22	H	318	CLA	C1B-C2B	2.60	1.49	1.43
22	B	807	CLA	C1B-C2B	2.59	1.49	1.43
22	A	810	CLA	C1B-C2B	2.59	1.49	1.43
22	A	829	CLA	C1B-C2B	2.59	1.49	1.43
22	Q	605	CLA	C1B-C2B	2.59	1.49	1.43
22	N	603	CLA	C1B-C2B	2.59	1.49	1.43
22	X	410	CLA	C1B-C2B	2.59	1.49	1.43
22	O	307	CLA	C1B-C2B	2.59	1.49	1.43
22	T	603	CLA	C1B-C2B	2.59	1.49	1.43
31	V	605	CHL	C1C-NC	2.59	1.37	1.35
22	I	601	CLA	C1B-C2B	2.59	1.49	1.43
22	A	852	CLA	C1B-C2B	2.59	1.49	1.43
22	S	607	CLA	C1B-C2B	2.59	1.49	1.43
22	S	610	CLA	C1B-C2B	2.59	1.49	1.43
22	H	306	CLA	C1B-C2B	2.59	1.49	1.43
22	W	409	CLA	C1B-C2B	2.59	1.49	1.43
22	N	606	CLA	C1B-C2B	2.59	1.49	1.43
22	X	408	CLA	C1B-C2B	2.59	1.49	1.43
22	A	827	CLA	C1B-C2B	2.59	1.49	1.43
22	F	405	CLA	C1B-C2B	2.58	1.49	1.43
22	K	612	CLA	C1B-C2B	2.58	1.49	1.43
22	B	806	CLA	C1B-C2B	2.58	1.49	1.43
22	U	403	CLA	C1B-C2B	2.58	1.49	1.43
22	A	815	CLA	C1B-C2B	2.58	1.49	1.43
22	N	602	CLA	C1B-C2B	2.58	1.49	1.43
22	G	609	CLA	C1B-C2B	2.58	1.49	1.43
22	W	406	CLA	C1B-C2B	2.58	1.49	1.43
22	G	607	CLA	C1B-C2B	2.58	1.49	1.43
22	H	307	CLA	C1B-C2B	2.58	1.49	1.43
22	U	411	CLA	C1B-C2B	2.58	1.49	1.43
22	B	830	CLA	MG-NB	-2.58	2.00	2.05
22	G	605	CLA	C1B-C2B	2.58	1.49	1.43
22	L	402	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	315	CLA	C1B-C2B	2.58	1.49	1.43
22	Q	611	CLA	C1B-C2B	2.58	1.49	1.43
22	W	403	CLA	C1B-C2B	2.58	1.49	1.43
22	A	809	CLA	C1B-C2B	2.58	1.49	1.43
22	T	602	CLA	C1B-C2B	2.58	1.49	1.43
22	S	606	CLA	C1B-C2B	2.58	1.49	1.43
22	X	417	CLA	C1B-C2B	2.58	1.49	1.43
22	H	313	CLA	C1B-C2B	2.58	1.49	1.43
22	K	617	CLA	C1B-C2B	2.58	1.49	1.43
22	A	817	CLA	C1B-C2B	2.58	1.49	1.43
22	W	405	CLA	C1B-C2B	2.58	1.49	1.43
22	B	812	CLA	C1B-C2B	2.58	1.49	1.43
22	P	607	CLA	C1B-C2B	2.57	1.49	1.43
22	B	836	CLA	C1B-C2B	2.57	1.49	1.43
22	G	601	CLA	C1B-C2B	2.57	1.49	1.43
22	W	404	CLA	C1B-C2B	2.57	1.49	1.43
22	A	828	CLA	C1B-C2B	2.57	1.49	1.43
22	K	608	CLA	C3B-C4B	2.57	1.48	1.42
22	A	826	CLA	C1B-C2B	2.57	1.49	1.43
22	B	805	CLA	C1B-C2B	2.57	1.49	1.43
22	T	607	CLA	C1B-C2B	2.57	1.49	1.43
22	L	412	CLA	C1B-C2B	2.57	1.49	1.43
22	O	312	CLA	C1B-C2B	2.57	1.49	1.43
22	B	822	CLA	C1B-C2B	2.57	1.49	1.43
22	L	403	CLA	C1B-C2B	2.57	1.49	1.43
22	B	817	CLA	C1B-C2B	2.56	1.49	1.43
22	B	838	CLA	C1B-C2B	2.56	1.49	1.43
22	H	308	CLA	C1B-C2B	2.56	1.49	1.43
22	K	609	CLA	C1B-C2B	2.56	1.49	1.43
22	K	610	CLA	C1B-C2B	2.56	1.49	1.43
22	S	603	CLA	C1B-C2B	2.56	1.49	1.43
22	B	835	CLA	C1B-C2B	2.56	1.49	1.43
22	Q	604	CLA	C1B-C2B	2.55	1.49	1.43
22	B	828	CLA	C1B-C2B	2.55	1.49	1.43
22	W	411	CLA	C1B-C2B	2.55	1.49	1.43
22	Q	608	CLA	C1B-C2B	2.55	1.49	1.43
22	X	404	CLA	C1B-C2B	2.55	1.49	1.43
22	A	822	CLA	C1B-C2B	2.55	1.49	1.43
22	L	410	CLA	C1B-C2B	2.55	1.49	1.43
31	X	406	CHL	C1C-NC	2.54	1.37	1.35
22	B	814	CLA	C1B-C2B	2.54	1.49	1.43
22	K	602	CLA	C1B-C2B	2.54	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Q	609	CLA	C1B-C2B	2.54	1.49	1.43
22	A	811	CLA	C1B-C2B	2.54	1.49	1.43
22	A	812	CLA	C1B-C2B	2.54	1.49	1.43
22	K	604	CLA	C1B-C2B	2.54	1.49	1.43
22	T	606	CLA	C1B-C2B	2.54	1.49	1.43
22	P	602	CLA	C1B-C2B	2.54	1.49	1.43
22	A	838	CLA	C1B-C2B	2.54	1.49	1.43
22	O	306	CLA	C1B-C2B	2.54	1.49	1.43
22	G	603	CLA	C1B-C2B	2.54	1.49	1.43
22	A	836	CLA	C1B-C2B	2.54	1.49	1.43
22	H	304	CLA	C1B-C2B	2.53	1.49	1.43
22	K	608	CLA	CMD-C2D	-2.53	1.45	1.50
22	B	827	CLA	C1B-C2B	2.53	1.49	1.43
22	K	603	CLA	C1B-C2B	2.53	1.49	1.43
22	B	813	CLA	C1B-C2B	2.53	1.49	1.43
22	G	606	CLA	C1B-C2B	2.53	1.49	1.43
31	U	408	CHL	C1C-C2C	2.53	1.49	1.45
22	W	402	CLA	C1B-C2B	2.53	1.49	1.43
22	T	604	CLA	C1B-C2B	2.52	1.49	1.43
22	B	815	CLA	C1B-C2B	2.51	1.49	1.43
22	A	834	CLA	C1B-C2B	2.51	1.49	1.43
22	K	607	CLA	C4B-NB	2.51	1.40	1.37
22	A	842	CLA	C1B-C2B	2.51	1.49	1.43
22	B	834	CLA	C1B-C2B	2.50	1.49	1.43
22	W	410	CLA	C1B-C2B	2.50	1.49	1.43
33	A	802	CL0	C3D-C4D	-2.50	1.37	1.41
31	W	407	CHL	C1C-NC	2.50	1.37	1.35
22	B	802	CLA	CMD-C2D	-2.49	1.45	1.50
22	Q	613	CLA	C1B-C2B	2.49	1.49	1.43
22	A	825	CLA	C1B-C2B	2.48	1.49	1.43
22	A	830	CLA	C1B-C2B	2.48	1.49	1.43
22	B	820	CLA	C1B-C2B	2.48	1.49	1.43
22	L	408	CLA	CHC-C1C	2.47	1.43	1.38
22	A	804	CLA	C1B-C2B	2.47	1.49	1.43
26	K	616	LHG	O8-C6	-2.47	1.39	1.45
22	I	611	CLA	C1B-C2B	2.46	1.49	1.43
22	A	803	CLA	CHC-C1C	2.46	1.43	1.38
22	K	608	CLA	C4B-NB	2.45	1.40	1.37
22	L	408	CLA	C4B-NB	2.45	1.40	1.37
22	P	607	CLA	CHC-C1C	2.45	1.43	1.38
26	T	614	LHG	O8-C6	-2.44	1.39	1.45
22	A	839	CLA	CHC-C1C	2.44	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	802	CLA	MG-ND	-2.44	2.00	2.05
26	O	324	LHG	O7-C7	2.44	1.41	1.34
26	G	614	LHG	O8-C6	-2.44	1.39	1.45
26	U	419	LHG	O7-C7	2.43	1.41	1.34
26	W	420	LHG	O7-C7	2.43	1.41	1.34
22	B	830	CLA	C4B-NB	2.43	1.40	1.37
22	A	816	CLA	MG-NB	-2.43	2.01	2.05
26	Q	616	LHG	O8-C6	-2.42	1.39	1.45
31	W	407	CHL	CHC-C4B	-2.41	1.35	1.39
26	A	846	LHG	O8-C6	-2.40	1.39	1.45
22	A	816	CLA	C4B-NB	2.40	1.40	1.37
26	A	845	LHG	O8-C6	-2.40	1.39	1.45
26	O	318	LHG	O8-C6	-2.40	1.39	1.45
22	S	605	CLA	C3B-C4B	2.39	1.48	1.42
26	W	420	LHG	O8-C6	-2.39	1.39	1.45
31	V	605	CHL	CHC-C4B	-2.39	1.35	1.39
26	O	323	LHG	O8-C23	2.38	1.40	1.33
22	B	829	CLA	CMD-C2D	-2.38	1.45	1.50
26	O	321	LHG	O8-C23	2.38	1.40	1.33
22	B	829	CLA	C4B-NB	2.38	1.40	1.37
26	R	614	LHG	O8-C6	-2.37	1.39	1.45
31	X	406	CHL	CHB-C1B	-2.37	1.35	1.39
22	L	408	CLA	CMD-C2D	-2.37	1.45	1.50
31	X	406	CHL	C1C-C2C	2.37	1.49	1.45
22	B	830	CLA	CMD-C2D	-2.37	1.45	1.50
31	U	408	CHL	CHB-C1B	-2.36	1.35	1.39
26	U	419	LHG	O8-C6	-2.36	1.39	1.45
22	B	813	CLA	CHC-C1C	2.36	1.43	1.38
22	S	605	CLA	C1B-C2B	2.36	1.48	1.43
26	P	601	LHG	O8-C23	2.36	1.40	1.33
22	A	819	CLA	CHC-C1C	2.36	1.43	1.38
33	A	802	CL0	CBD-CGD	-2.36	1.49	1.52
22	A	816	CLA	CMD-C2D	-2.36	1.45	1.50
22	B	802	CLA	CMB-C2B	-2.36	1.45	1.50
31	X	406	CHL	CHC-C4B	-2.35	1.35	1.39
22	K	608	CLA	CMB-C2B	-2.35	1.45	1.50
22	A	820	CLA	C1B-C2B	2.35	1.48	1.43
26	X	420	LHG	O8-C23	2.35	1.40	1.33
22	K	607	CLA	MG-NB	-2.35	2.01	2.05
31	W	408	CHL	CHB-C1B	-2.35	1.35	1.39
26	X	420	LHG	O8-C6	-2.35	1.39	1.45
26	L	416	LHG	O8-C23	2.34	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	830	CLA	C3B-C4B	2.34	1.48	1.42
31	U	407	CHL	CHC-C4B	-2.34	1.35	1.39
26	O	324	LHG	O8-C6	-2.34	1.39	1.45
22	I	607	CLA	CHC-C1C	2.33	1.43	1.38
22	B	802	CLA	C4B-NB	2.33	1.40	1.37
26	K	619	LHG	O8-C23	2.33	1.40	1.33
22	R	604	CLA	CHC-C1C	2.33	1.43	1.38
26	K	619	LHG	O8-C6	-2.33	1.39	1.45
26	B	848	LHG	O8-C23	2.33	1.40	1.33
26	B	848	LHG	O8-C6	-2.33	1.39	1.45
22	K	607	CLA	CMB-C2B	-2.33	1.45	1.50
22	K	607	CLA	CMD-C2D	-2.33	1.45	1.50
26	B	851	LHG	O8-C23	2.32	1.40	1.33
26	N	614	LHG	O7-C7	2.32	1.40	1.34
26	O	318	LHG	O7-C7	2.32	1.40	1.34
26	O	321	LHG	O8-C6	-2.32	1.39	1.45
22	B	830	CLA	CMB-C2B	-2.32	1.45	1.50
22	B	829	CLA	C3B-C4B	2.32	1.48	1.42
22	S	605	CLA	MG-NB	-2.32	2.01	2.05
26	S	613	LHG	O8-C23	2.32	1.40	1.33
22	S	607	CLA	CHC-C1C	2.32	1.43	1.38
26	B	851	LHG	O8-C6	-2.32	1.39	1.45
26	K	619	LHG	O7-C7	2.32	1.40	1.34
26	O	324	LHG	O8-C23	2.32	1.40	1.33
26	P	601	LHG	O8-C6	-2.32	1.39	1.45
26	O	323	LHG	O8-C6	-2.32	1.39	1.45
22	A	819	CLA	CMB-C2B	-2.32	1.45	1.50
22	A	801	CLA	CMD-C2D	-2.32	1.45	1.50
26	L	416	LHG	O8-C6	-2.32	1.39	1.45
22	K	608	CLA	CMC-C2C	-2.32	1.45	1.50
26	Q	616	LHG	O7-C7	2.31	1.40	1.34
26	B	851	LHG	O7-C7	2.31	1.40	1.34
22	H	312	CLA	CHC-C1C	2.31	1.43	1.38
22	I	608	CLA	CMD-C2D	-2.31	1.45	1.50
26	W	420	LHG	O8-C23	2.31	1.40	1.33
26	A	846	LHG	O8-C23	2.31	1.40	1.33
31	V	606	CHL	CHB-C1B	-2.31	1.35	1.39
26	N	614	LHG	O8-C23	2.31	1.40	1.33
22	B	814	CLA	CHC-C1C	2.31	1.43	1.38
26	Q	616	LHG	O8-C23	2.31	1.40	1.33
26	G	614	LHG	O7-C7	2.30	1.40	1.34
22	O	306	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	829	CLA	CMB-C2B	-2.30	1.45	1.50
26	U	419	LHG	O8-C23	2.30	1.40	1.33
26	S	613	LHG	O8-C6	-2.30	1.39	1.45
26	O	323	LHG	O7-C7	2.30	1.40	1.34
26	H	316	LHG	O8-C23	2.30	1.40	1.33
22	S	606	CLA	CHC-C1C	2.30	1.43	1.38
22	P	611	CLA	CHC-C1C	2.30	1.43	1.38
26	N	616	LHG	O7-C7	2.30	1.40	1.34
26	O	318	LHG	O8-C23	2.30	1.40	1.33
31	W	422	CHL	CHC-C4B	-2.29	1.35	1.39
26	H	316	LHG	O8-C6	-2.29	1.39	1.45
22	B	822	CLA	CHC-C1C	2.29	1.43	1.38
26	G	614	LHG	O8-C23	2.29	1.40	1.33
26	A	845	LHG	O7-C7	2.29	1.40	1.34
22	L	408	CLA	CMB-C2B	-2.29	1.45	1.50
26	R	614	LHG	O7-C7	2.29	1.40	1.34
26	N	616	LHG	O8-C23	2.29	1.40	1.33
22	N	607	CLA	CHC-C1C	2.29	1.43	1.38
26	R	614	LHG	O8-C23	2.29	1.40	1.33
22	A	816	CLA	C1B-NB	-2.28	1.35	1.37
22	B	825	CLA	CHC-C1C	2.28	1.43	1.38
26	T	614	LHG	O8-C23	2.28	1.40	1.33
22	B	836	CLA	MG-NB	-2.28	2.01	2.05
31	V	606	CHL	C1C-NC	2.28	1.37	1.35
26	X	420	LHG	O7-C7	2.28	1.40	1.34
22	V	609	CLA	CHC-C1C	2.28	1.43	1.38
22	Q	607	CLA	CHC-C1C	2.28	1.43	1.38
22	L	408	CLA	MG-NB	-2.28	2.01	2.05
22	S	608	CLA	CHC-C1C	2.27	1.43	1.38
26	N	614	LHG	O8-C6	-2.27	1.40	1.45
28	F	408	LMG	C4-C5	2.27	1.57	1.53
22	T	611	CLA	CHC-C1C	2.27	1.43	1.38
26	H	316	LHG	O7-C7	2.27	1.40	1.34
26	B	848	LHG	O7-C7	2.27	1.40	1.34
22	H	308	CLA	CHC-C1C	2.27	1.43	1.38
22	O	309	CLA	CHC-C1C	2.27	1.43	1.38
31	U	407	CHL	C1C-NC	2.27	1.37	1.35
24	F	406	DD6	O1-C20	-2.27	1.43	1.46
22	A	801	CLA	C1B-C2B	2.27	1.48	1.43
31	V	605	CHL	C1C-C2C	2.27	1.49	1.45
22	H	309	CLA	CHC-C1C	2.27	1.43	1.38
26	S	613	LHG	O7-C7	2.27	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	859	CLA	CHC-C1C	2.27	1.43	1.38
22	B	820	CLA	CHC-C1C	2.27	1.43	1.38
22	V	611	CLA	CHC-C1C	2.26	1.43	1.38
26	N	616	LHG	O8-C6	-2.26	1.40	1.45
22	S	605	CLA	CMD-C2D	-2.26	1.46	1.50
24	Q	615	DD6	O1-C20	-2.26	1.43	1.46
22	B	802	CLA	CMC-C2C	-2.26	1.46	1.50
31	U	408	CHL	C1C-NC	2.26	1.37	1.35
22	B	812	CLA	CHC-C1C	2.26	1.43	1.38
26	A	846	LHG	O7-C7	2.26	1.40	1.34
26	P	601	LHG	O7-C5	-2.26	1.40	1.46
31	W	408	CHL	CHC-C4B	-2.26	1.36	1.39
22	G	609	CLA	CHC-C1C	2.26	1.43	1.38
22	A	806	CLA	CHC-C1C	2.26	1.43	1.38
31	V	606	CHL	CHC-C4B	-2.25	1.36	1.39
31	W	422	CHL	C1C-C2C	2.25	1.49	1.45
22	P	604	CLA	CHC-C1C	2.25	1.43	1.38
26	T	614	LHG	O7-C7	2.25	1.40	1.34
26	O	321	LHG	O7-C7	2.25	1.40	1.34
22	A	811	CLA	CHC-C1C	2.25	1.43	1.38
22	L	417	CLA	MG-NB	-2.25	2.01	2.05
22	N	606	CLA	CHC-C1C	2.25	1.43	1.38
26	A	845	LHG	O8-C23	2.25	1.39	1.33
26	P	601	LHG	O7-C7	2.25	1.40	1.34
22	U	405	CLA	CHC-C1C	2.25	1.43	1.38
22	W	415	CLA	CHC-C1C	2.25	1.43	1.38
26	L	416	LHG	O7-C7	2.25	1.40	1.34
22	R	606	CLA	CHC-C1C	2.25	1.43	1.38
22	I	608	CLA	CHC-C1C	2.24	1.43	1.38
22	V	613	CLA	CHC-C1C	2.24	1.43	1.38
22	X	411	CLA	CHC-C1C	2.24	1.43	1.38
22	L	412	CLA	CHC-C1C	2.24	1.43	1.38
22	H	311	CLA	CHC-C1C	2.24	1.43	1.38
22	T	602	CLA	CHC-C1C	2.24	1.43	1.38
22	T	607	CLA	CHC-C1C	2.24	1.43	1.38
22	A	801	CLA	CMC-C2C	-2.24	1.46	1.50
22	R	608	CLA	CHC-C1C	2.24	1.43	1.38
22	V	607	CLA	CHC-C1C	2.24	1.43	1.38
22	I	611	CLA	CHC-C1C	2.24	1.43	1.38
22	R	605	CLA	CHC-C1C	2.24	1.43	1.38
22	B	802	CLA	C3B-C4B	2.24	1.48	1.42
31	V	605	CHL	CHB-C1B	-2.24	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	611	CLA	CHC-C1C	2.24	1.43	1.38
22	U	409	CLA	CHC-C1C	2.24	1.43	1.38
22	P	606	CLA	MG-NB	-2.24	2.01	2.05
22	Q	601	CLA	CHC-C1C	2.24	1.43	1.38
22	Q	618	CLA	CHC-C1C	2.24	1.43	1.38
24	A	859	DD6	O1-C20	-2.24	1.43	1.46
22	N	609	CLA	CHC-C1C	2.24	1.43	1.38
22	W	406	CLA	CHC-C1C	2.24	1.43	1.38
22	O	311	CLA	CHC-C1C	2.24	1.43	1.38
22	W	403	CLA	CHC-C1C	2.24	1.43	1.38
22	A	830	CLA	CHC-C1C	2.24	1.43	1.38
22	L	409	CLA	CHC-C1C	2.23	1.43	1.38
22	R	602	CLA	CHC-C1C	2.23	1.43	1.38
24	H	315	DD6	O1-C20	-2.23	1.43	1.46
22	V	602	CLA	CHC-C1C	2.23	1.43	1.38
22	A	829	CLA	CHC-C1C	2.23	1.43	1.38
22	B	803	CLA	CHC-C1C	2.23	1.43	1.38
22	L	403	CLA	CHC-C1C	2.23	1.43	1.38
22	R	601	CLA	CHC-C1C	2.23	1.43	1.38
22	A	801	CLA	MG-NB	-2.23	2.01	2.05
22	A	834	CLA	CHC-C1C	2.23	1.43	1.38
22	N	604	CLA	CHC-C1C	2.23	1.43	1.38
22	A	828	CLA	CHC-C1C	2.23	1.43	1.38
22	G	608	CLA	MG-NB	-2.23	2.01	2.05
22	A	816	CLA	C3B-C4B	2.23	1.48	1.42
22	O	315	CLA	CHC-C1C	2.23	1.43	1.38
22	A	840	CLA	MG-NB	-2.23	2.01	2.05
26	K	616	LHG	O7-C5	-2.23	1.41	1.46
26	B	848	LHG	O7-C5	-2.23	1.41	1.46
22	V	604	CLA	CHC-C1C	2.23	1.43	1.38
22	X	409	CLA	CHC-C1C	2.23	1.43	1.38
22	P	606	CLA	CMD-C2D	-2.23	1.46	1.50
22	X	413	CLA	CHC-C1C	2.23	1.43	1.38
22	Q	604	CLA	MG-NB	-2.23	2.01	2.05
22	B	835	CLA	CHC-C1C	2.23	1.43	1.38
22	A	804	CLA	CHC-C1C	2.23	1.43	1.38
22	P	603	CLA	CHC-C1C	2.22	1.43	1.38
22	A	837	CLA	CHC-C1C	2.22	1.43	1.38
22	K	617	CLA	MG-NB	-2.22	2.01	2.05
22	S	604	CLA	CHC-C1C	2.22	1.43	1.38
22	U	410	CLA	CHC-C1C	2.22	1.43	1.38
22	U	406	CLA	CHC-C1C	2.22	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	611	DD6	O1-C20	-2.22	1.43	1.46
26	K	616	LHG	O8-C23	2.22	1.39	1.33
22	B	815	CLA	CHC-C1C	2.22	1.43	1.38
22	H	318	CLA	CHC-C1C	2.22	1.43	1.38
26	A	846	LHG	O7-C5	-2.22	1.41	1.46
26	N	614	LHG	O7-C5	-2.22	1.41	1.46
22	B	807	CLA	CHC-C1C	2.22	1.43	1.38
22	O	306	CLA	CHC-C1C	2.22	1.43	1.38
22	U	420	CLA	CHC-C1C	2.22	1.43	1.38
22	Q	604	CLA	CHC-C1C	2.22	1.43	1.38
22	B	816	CLA	CHC-C1C	2.22	1.43	1.38
22	B	833	CLA	CHC-C1C	2.22	1.43	1.38
22	G	610	CLA	CHC-C1C	2.22	1.43	1.38
22	V	601	CLA	CHC-C1C	2.22	1.43	1.38
22	B	815	CLA	MG-NB	-2.22	2.01	2.05
22	L	406	CLA	CMD-C2D	-2.22	1.46	1.50
22	K	610	CLA	CHC-C1C	2.22	1.43	1.38
22	P	610	CLA	CHC-C1C	2.22	1.43	1.38
22	N	605	CLA	CHC-C1C	2.22	1.43	1.38
22	W	413	CLA	CHC-C1C	2.22	1.43	1.38
22	A	807	CLA	CHC-C1C	2.22	1.43	1.38
22	A	827	CLA	CHC-C1C	2.22	1.43	1.38
22	I	611	CLA	MG-NB	-2.22	2.01	2.05
22	B	818	CLA	CHC-C1C	2.22	1.43	1.38
22	L	405	CLA	CHC-C1C	2.21	1.43	1.38
22	O	308	CLA	CHC-C1C	2.21	1.43	1.38
22	A	844	CLA	CMC-C2C	-2.21	1.46	1.50
22	L	406	CLA	CHC-C1C	2.21	1.43	1.38
22	V	610	CLA	CHC-C1C	2.21	1.43	1.38
22	N	602	CLA	CHC-C1C	2.21	1.43	1.38
22	R	603	CLA	CHC-C1C	2.21	1.43	1.38
22	A	852	CLA	CHC-C1C	2.21	1.43	1.38
22	B	827	CLA	CHC-C1C	2.21	1.43	1.38
22	U	401	CLA	CHC-C1C	2.21	1.43	1.38
22	B	831	CLA	CHC-C1C	2.21	1.43	1.38
22	O	314	CLA	CHC-C1C	2.21	1.43	1.38
26	R	614	LHG	O7-C5	-2.21	1.41	1.46
22	S	605	CLA	CMC-C2C	-2.21	1.46	1.50
22	B	824	CLA	CHC-C1C	2.21	1.43	1.38
22	K	603	CLA	CHC-C1C	2.21	1.43	1.38
22	Q	610	CLA	CHC-C1C	2.21	1.43	1.38
22	T	607	CLA	MG-NB	-2.21	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	612	CLA	CHC-C1C	2.21	1.43	1.38
22	P	602	CLA	CMD-C2D	-2.21	1.46	1.50
22	I	602	CLA	CHC-C1C	2.21	1.43	1.38
22	A	826	CLA	CHC-C1C	2.21	1.43	1.38
22	G	602	CLA	CHC-C1C	2.21	1.43	1.38
22	A	832	CLA	CHC-C1C	2.21	1.43	1.38
22	K	611	CLA	CHC-C1C	2.20	1.43	1.38
22	B	839	CLA	CHC-C1C	2.20	1.43	1.38
22	P	605	CLA	CHC-C1C	2.20	1.43	1.38
22	A	810	CLA	CHC-C1C	2.20	1.43	1.38
22	Q	609	CLA	CHC-C1C	2.20	1.43	1.38
22	T	609	CLA	CHC-C1C	2.20	1.43	1.38
22	X	407	CLA	CHC-C1C	2.20	1.43	1.38
22	A	817	CLA	CHC-C1C	2.20	1.43	1.38
22	R	609	CLA	CHC-C1C	2.20	1.43	1.38
26	G	614	LHG	O7-C5	-2.20	1.41	1.46
22	G	601	CLA	CHC-C1C	2.20	1.43	1.38
22	W	410	CLA	CHC-C1C	2.20	1.43	1.38
22	T	609	CLA	MG-NB	-2.20	2.01	2.05
22	T	604	CLA	CHC-C1C	2.20	1.43	1.38
22	V	603	CLA	CHC-C1C	2.20	1.43	1.38
22	A	814	CLA	CHC-C1C	2.20	1.43	1.38
22	V	617	CLA	CHC-C1C	2.20	1.43	1.38
22	L	410	CLA	CHC-C1C	2.20	1.43	1.38
24	T	612	DD6	O1-C20	-2.20	1.43	1.46
22	K	617	CLA	CHC-C1C	2.20	1.43	1.38
22	A	809	CLA	CHC-C1C	2.20	1.43	1.38
22	K	606	CLA	CHC-C1C	2.20	1.43	1.38
22	B	808	CLA	CHC-C1C	2.20	1.43	1.38
22	B	829	CLA	C1B-C2B	2.20	1.48	1.43
22	F	405	CLA	CHC-C1C	2.20	1.43	1.38
31	V	605	CHL	C4D-CHA	-2.20	1.36	1.40
22	K	608	CLA	MG-NB	-2.20	2.01	2.05
22	I	606	CLA	CHC-C1C	2.20	1.43	1.38
22	P	602	CLA	CHC-C1C	2.20	1.43	1.38
22	T	605	CLA	CHC-C1C	2.20	1.43	1.38
22	G	602	CLA	MG-NB	-2.20	2.01	2.05
22	H	313	CLA	CHC-C1C	2.20	1.43	1.38
22	A	823	CLA	CHC-C1C	2.20	1.43	1.38
22	Q	603	CLA	CHC-C1C	2.19	1.43	1.38
22	U	415	CLA	CHC-C1C	2.19	1.43	1.38
22	S	614	CLA	CHC-C1C	2.19	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	416	LHG	O7-C5	-2.19	1.41	1.46
22	N	602	CLA	MG-NB	-2.19	2.01	2.05
22	W	412	CLA	CHC-C1C	2.19	1.43	1.38
22	A	801	CLA	C4B-NB	2.19	1.40	1.37
22	L	408	CLA	CMC-C2C	-2.19	1.46	1.50
24	G	613	DD6	O1-C20	-2.19	1.43	1.46
22	T	601	CLA	CHC-C1C	2.19	1.43	1.38
22	I	610	CLA	CHC-C1C	2.19	1.43	1.38
22	A	819	CLA	CMD-C2D	-2.19	1.46	1.50
22	A	820	CLA	CHC-C1C	2.19	1.43	1.38
22	A	831	CLA	CHC-C1C	2.19	1.43	1.38
31	U	407	CHL	CHB-C1B	-2.19	1.36	1.39
22	B	828	CLA	CHC-C1C	2.19	1.43	1.38
22	W	411	CLA	CHC-C1C	2.19	1.43	1.38
22	H	306	CLA	CHC-C1C	2.19	1.43	1.38
22	L	402	CLA	CHC-C1C	2.19	1.43	1.38
26	K	616	LHG	O7-C7	2.19	1.40	1.34
22	U	414	CLA	CHC-C1C	2.19	1.43	1.38
26	T	614	LHG	O7-C5	-2.19	1.41	1.46
22	H	302	CLA	CHC-C1C	2.19	1.43	1.38
22	X	405	CLA	CHC-C1C	2.19	1.43	1.38
22	X	408	CLA	CHC-C1C	2.19	1.43	1.38
26	X	420	LHG	O7-C5	-2.19	1.41	1.46
22	Q	617	CLA	CHC-C1C	2.19	1.43	1.38
22	S	603	CLA	CHC-C1C	2.19	1.43	1.38
22	H	303	CLA	CHC-C1C	2.19	1.43	1.38
22	W	402	CLA	CHC-C1C	2.19	1.43	1.38
22	A	805	CLA	CHC-C1C	2.19	1.43	1.38
22	O	313	CLA	CHC-C1C	2.19	1.43	1.38
26	Q	616	LHG	O7-C5	-2.19	1.41	1.46
22	F	404	CLA	CHC-C1C	2.19	1.43	1.38
26	A	845	LHG	O7-C5	-2.19	1.41	1.46
31	U	408	CHL	CHC-C4B	-2.18	1.36	1.39
22	B	834	CLA	CHC-C1C	2.18	1.43	1.38
31	W	422	CHL	CHB-C1B	-2.18	1.36	1.39
22	S	610	CLA	CHC-C1C	2.18	1.43	1.38
22	U	412	CLA	CHC-C1C	2.18	1.43	1.38
22	A	833	CLA	CHC-C1C	2.18	1.43	1.38
22	G	604	CLA	CHC-C1C	2.18	1.43	1.38
22	S	609	CLA	CHC-C1C	2.18	1.43	1.38
31	W	408	CHL	C1C-C2C	2.18	1.49	1.45
22	B	811	CLA	CHC-C1C	2.18	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	822	CLA	CHC-C1C	2.18	1.43	1.38
22	R	610	CLA	CHC-C1C	2.18	1.43	1.38
22	X	404	CLA	CHC-C1C	2.18	1.43	1.38
22	A	842	CLA	CHC-C1C	2.18	1.43	1.38
22	G	611	CLA	CHC-C1C	2.18	1.43	1.38
22	I	603	CLA	CHC-C1C	2.18	1.43	1.38
22	B	830	CLA	CMC-C2C	-2.18	1.46	1.50
22	A	824	CLA	CHC-C1C	2.18	1.42	1.38
26	K	619	LHG	O7-C5	-2.18	1.41	1.46
22	I	601	CLA	CHC-C1C	2.18	1.42	1.38
22	O	305	CLA	CHC-C1C	2.18	1.42	1.38
24	O	317	DD6	O1-C20	-2.18	1.43	1.46
22	S	605	CLA	CMB-C2B	-2.18	1.46	1.50
26	O	321	LHG	O7-C5	-2.18	1.41	1.46
22	J	102	CLA	CHC-C1C	2.18	1.42	1.38
22	R	615	CLA	CHC-C1C	2.18	1.42	1.38
22	W	415	CLA	MG-NB	-2.18	2.01	2.05
22	O	319	CLA	CHC-C1C	2.17	1.42	1.38
22	H	305	CLA	CHC-C1C	2.17	1.42	1.38
22	I	605	CLA	CHC-C1C	2.17	1.42	1.38
22	A	815	CLA	CHC-C1C	2.17	1.42	1.38
22	T	608	CLA	CHC-C1C	2.17	1.42	1.38
22	T	603	CLA	CHC-C1C	2.17	1.42	1.38
22	X	412	CLA	CHC-C1C	2.17	1.42	1.38
22	A	808	CLA	CHC-C1C	2.17	1.42	1.38
26	H	316	LHG	O7-C5	-2.17	1.41	1.46
22	Q	608	CLA	CHC-C1C	2.17	1.42	1.38
22	A	809	CLA	MG-NB	-2.17	2.01	2.05
22	K	602	CLA	CHC-C1C	2.17	1.42	1.38
22	U	403	CLA	CHC-C1C	2.17	1.42	1.38
22	U	411	CLA	CHC-C1C	2.17	1.42	1.38
22	X	402	CLA	CHC-C1C	2.17	1.42	1.38
22	B	805	CLA	CHC-C1C	2.17	1.42	1.38
22	B	823	CLA	CHC-C1C	2.17	1.42	1.38
22	L	411	CLA	CHC-C1C	2.17	1.42	1.38
22	N	609	CLA	MG-NB	-2.17	2.01	2.05
22	K	612	CLA	MG-NB	-2.17	2.01	2.05
22	N	607	CLA	MG-NB	-2.17	2.01	2.05
22	A	835	CLA	CHC-C1C	2.17	1.42	1.38
22	A	808	CLA	MG-NB	-2.17	2.01	2.05
22	G	605	CLA	CHC-C1C	2.17	1.42	1.38
22	L	407	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	613	CLA	CHC-C1C	2.17	1.42	1.38
22	Q	605	CLA	CHC-C1C	2.17	1.42	1.38
22	W	409	CLA	CHC-C1C	2.17	1.42	1.38
22	W	413	CLA	MG-NB	-2.16	2.01	2.05
26	N	616	LHG	O7-C5	-2.16	1.41	1.46
26	S	613	LHG	O7-C5	-2.16	1.41	1.46
22	H	305	CLA	MG-NB	-2.16	2.01	2.05
22	W	404	CLA	MG-NB	-2.16	2.01	2.05
22	B	820	CLA	CMD-C2D	-2.16	1.46	1.50
22	A	816	CLA	C1B-C2B	2.16	1.48	1.43
22	B	810	CLA	CHC-C1C	2.16	1.42	1.38
22	H	304	CLA	MG-NB	-2.16	2.01	2.05
22	A	820	CLA	MG-NB	-2.16	2.01	2.05
24	W	418	DD6	O1-C20	-2.16	1.43	1.46
22	B	805	CLA	MG-NB	-2.16	2.01	2.05
22	L	403	CLA	MG-NB	-2.16	2.01	2.05
22	O	307	CLA	CHC-C1C	2.16	1.42	1.38
22	B	809	CLA	CHC-C1C	2.16	1.42	1.38
22	B	839	CLA	MG-NB	-2.16	2.01	2.05
22	B	829	CLA	MG-NB	-2.16	2.01	2.05
22	L	410	CLA	MG-NB	-2.16	2.01	2.05
22	L	404	CLA	CHC-C1C	2.16	1.42	1.38
22	G	606	CLA	CHC-C1C	2.16	1.42	1.38
22	X	403	CLA	MG-NB	-2.16	2.01	2.05
22	Q	606	CLA	CHC-C1C	2.16	1.42	1.38
22	A	825	CLA	CHC-C1C	2.16	1.42	1.38
22	A	801	CLA	CMB-C2B	-2.16	1.46	1.50
22	A	838	CLA	MG-NB	-2.16	2.01	2.05
22	W	410	CLA	MG-NB	-2.16	2.01	2.05
22	H	304	CLA	CHC-C1C	2.16	1.42	1.38
22	A	841	CLA	CHC-C1C	2.16	1.42	1.38
31	W	408	CHL	C3A-C2A	-2.15	1.52	1.54
22	B	804	CLA	CHC-C1C	2.15	1.42	1.38
22	T	610	CLA	CHC-C1C	2.15	1.42	1.38
31	U	407	CHL	C4D-CHA	-2.15	1.36	1.40
24	H	314	DD6	O1-C20	-2.15	1.43	1.46
22	A	819	CLA	CMC-C2C	-2.15	1.46	1.50
22	K	612	CLA	CHC-C1C	2.15	1.42	1.38
22	L	407	CLA	CHC-C1C	2.15	1.42	1.38
22	A	813	CLA	CHC-C1C	2.15	1.42	1.38
22	O	312	CLA	CHC-C1C	2.15	1.42	1.38
22	K	602	CLA	MG-NB	-2.15	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	826	CLA	CHC-C1C	2.15	1.42	1.38
24	P	613	DD6	O1-C20	-2.15	1.43	1.46
22	T	602	CLA	MG-NB	-2.15	2.01	2.05
22	G	608	CLA	CHC-C1C	2.15	1.42	1.38
22	I	604	CLA	CHC-C1C	2.15	1.42	1.38
22	N	601	CLA	CHC-C1C	2.15	1.42	1.38
22	P	606	CLA	CHC-C1C	2.15	1.42	1.38
22	N	603	CLA	CHC-C1C	2.15	1.42	1.38
22	N	611	CLA	CHC-C1C	2.15	1.42	1.38
26	B	851	LHG	O7-C5	-2.15	1.41	1.46
22	O	305	CLA	MG-NB	-2.15	2.01	2.05
22	W	419	CLA	CHC-C1C	2.15	1.42	1.38
30	V	618	SQD	O8-S	2.15	1.55	1.47
22	N	608	CLA	CHC-C1C	2.15	1.42	1.38
22	B	837	CLA	CHC-C1C	2.15	1.42	1.38
22	G	607	CLA	CHC-C1C	2.15	1.42	1.38
22	N	608	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	834	CLA	MG-NB	-2.15	2.01	2.05
22	K	605	CLA	CHC-C1C	2.15	1.42	1.38
22	P	607	CLA	MG-NB	-2.15	2.01	2.05
22	L	417	CLA	CHC-C1C	2.15	1.42	1.38
22	K	609	CLA	MG-NB	-2.15	2.01	2.05
22	N	603	CLA	MG-NB	-2.15	2.01	2.05
22	H	303	CLA	MG-NB	-2.15	2.01	2.05
22	P	602	CLA	MG-NB	-2.15	2.01	2.05
22	U	404	CLA	CHC-C1C	2.14	1.42	1.38
22	K	607	CLA	CMC-C2C	-2.14	1.46	1.50
22	J	102	CLA	MG-NB	-2.14	2.01	2.05
22	G	603	CLA	MG-NB	-2.14	2.01	2.05
31	U	407	CHL	C1C-C2C	2.14	1.49	1.45
22	S	602	CLA	CHC-C1C	2.14	1.42	1.38
22	B	821	CLA	MG-NB	-2.14	2.01	2.05
22	A	818	CLA	MG-NB	-2.14	2.01	2.05
22	P	609	CLA	CHC-C1C	2.14	1.42	1.38
22	A	804	CLA	MG-NB	-2.14	2.01	2.05
22	R	607	CLA	CMB-C2B	-2.14	1.46	1.50
22	B	838	CLA	CHC-C1C	2.14	1.42	1.38
22	I	609	CLA	CHC-C1C	2.14	1.42	1.38
24	X	414	DD6	O1-C20	-2.14	1.43	1.46
22	B	835	CLA	MG-NB	-2.14	2.01	2.05
22	B	802	CLA	C1B-C2B	2.14	1.48	1.43
22	X	407	CLA	MG-NB	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	821	CLA	CHC-C1C	2.14	1.42	1.38
22	A	844	CLA	CHC-C1C	2.14	1.42	1.38
22	I	602	CLA	MG-NB	-2.14	2.01	2.05
22	K	603	CLA	MG-NB	-2.14	2.01	2.05
22	K	610	CLA	MG-NB	-2.14	2.01	2.05
22	B	817	CLA	CHC-C1C	2.14	1.42	1.38
22	O	310	CLA	CMD-C2D	-2.14	1.46	1.50
22	G	603	CLA	CHC-C1C	2.14	1.42	1.38
22	T	603	CLA	MG-NB	-2.14	2.01	2.05
22	U	404	CLA	MG-NB	-2.14	2.01	2.05
24	B	841	DD6	O1-C20	-2.14	1.43	1.46
22	B	810	CLA	MG-NB	-2.13	2.01	2.05
22	H	318	CLA	MG-NB	-2.13	2.01	2.05
22	I	607	CLA	MG-NB	-2.13	2.01	2.05
22	N	605	CLA	MG-NB	-2.13	2.01	2.05
22	R	607	CLA	CHC-C1C	2.13	1.42	1.38
22	W	412	CLA	MG-NB	-2.13	2.01	2.05
24	V	615	DD6	O1-C20	-2.13	1.43	1.46
22	S	601	CLA	CHC-C1C	2.13	1.42	1.38
22	X	419	CLA	CHC-C1C	2.13	1.42	1.38
26	O	318	LHG	O7-C5	-2.13	1.41	1.46
22	S	604	CLA	MG-NB	-2.13	2.01	2.05
22	A	812	CLA	CHC-C1C	2.13	1.42	1.38
24	G	612	DD6	O1-C20	-2.13	1.43	1.46
24	R	612	DD6	O1-C20	-2.13	1.43	1.46
22	Q	613	CLA	CHC-C1C	2.13	1.42	1.38
22	B	816	CLA	MG-NB	-2.13	2.01	2.05
22	K	605	CLA	MG-NB	-2.13	2.01	2.05
22	A	822	CLA	MG-NB	-2.13	2.01	2.05
22	U	413	CLA	CHC-C1C	2.13	1.42	1.38
22	Q	617	CLA	MG-NB	-2.13	2.01	2.05
22	O	319	CLA	MG-NB	-2.13	2.01	2.05
22	B	806	CLA	CHC-C1C	2.13	1.42	1.38
22	L	412	CLA	MG-NB	-2.13	2.01	2.05
22	W	414	CLA	CHC-C1C	2.13	1.42	1.38
22	X	410	CLA	CHC-C1C	2.13	1.42	1.38
22	B	806	CLA	MG-NB	-2.13	2.01	2.05
22	I	603	CLA	MG-NB	-2.13	2.01	2.05
22	L	402	CLA	MG-NB	-2.13	2.01	2.05
22	B	829	CLA	CMC-C2C	-2.13	1.46	1.50
22	A	836	CLA	CHC-C1C	2.12	1.42	1.38
22	G	607	CLA	MG-NB	-2.12	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	312	CLA	MG-NB	-2.12	2.01	2.05
22	H	307	CLA	CHC-C1C	2.12	1.42	1.38
22	V	608	CLA	CHC-C1C	2.12	1.42	1.38
22	O	308	CLA	MG-NB	-2.12	2.01	2.05
22	N	610	CLA	CMB-C2B	-2.12	1.46	1.50
26	K	619	LHG	P-O6	2.12	1.67	1.59
22	A	820	CLA	CMB-C2B	-2.12	1.46	1.50
22	I	608	CLA	MG-NB	-2.12	2.01	2.05
22	W	404	CLA	CHC-C1C	2.12	1.42	1.38
22	H	304	CLA	CMD-C2D	-2.12	1.46	1.50
22	F	403	CLA	CHC-C1C	2.12	1.42	1.38
22	S	615	CLA	CHC-C1C	2.12	1.42	1.38
24	V	614	DD6	O1-C20	-2.12	1.43	1.46
22	G	609	CLA	CMD-C2D	-2.12	1.46	1.50
22	A	838	CLA	CHC-C1C	2.12	1.42	1.38
22	A	821	CLA	CHC-C1C	2.12	1.42	1.38
22	X	402	CLA	MG-NB	-2.12	2.01	2.05
22	H	310	CLA	CHC-C1C	2.12	1.42	1.38
22	P	608	CLA	CHC-C1C	2.12	1.42	1.38
22	A	816	CLA	CMB-C2B	-2.12	1.46	1.50
22	A	817	CLA	MG-NB	-2.12	2.01	2.05
22	A	833	CLA	MG-NB	-2.12	2.01	2.05
22	B	802	CLA	C1B-NB	-2.11	1.35	1.37
22	N	604	CLA	MG-NB	-2.11	2.01	2.05
24	N	613	DD6	O1-C20	-2.11	1.43	1.46
22	U	413	CLA	MG-NB	-2.11	2.01	2.05
22	T	606	CLA	CHC-C1C	2.11	1.42	1.38
22	K	609	CLA	CHC-C1C	2.11	1.42	1.38
22	R	603	CLA	CMD-C2D	-2.11	1.46	1.50
22	U	412	CLA	MG-NB	-2.11	2.01	2.05
22	W	409	CLA	MG-NB	-2.11	2.01	2.05
24	K	614	DD6	O1-C20	-2.11	1.43	1.46
22	A	834	CLA	MG-NB	-2.11	2.01	2.05
22	G	603	CLA	CMD-C2D	-2.11	1.46	1.50
25	O	304	DGD	O5D-C1E	2.11	1.43	1.40
22	R	603	CLA	MG-NB	-2.11	2.01	2.05
22	I	611	CLA	CMB-C2B	-2.11	1.46	1.50
30	O	302	SQD	O8-S	2.11	1.55	1.47
22	Q	611	CLA	CHC-C1C	2.11	1.42	1.38
24	Q	614	DD6	O1-C20	-2.11	1.43	1.46
22	A	832	CLA	MG-NB	-2.11	2.01	2.05
22	B	830	CLA	C1B-C2B	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	607	CLA	C1B-C2B	2.11	1.48	1.43
22	Q	606	CLA	MG-NB	-2.11	2.01	2.05
22	I	605	CLA	MG-NB	-2.11	2.01	2.05
30	K	621	SQD	O8-S	2.10	1.55	1.47
22	W	411	CLA	MG-NB	-2.10	2.01	2.05
22	A	816	CLA	CMC-C2C	-2.10	1.46	1.50
22	L	404	CLA	CMD-C2D	-2.10	1.46	1.50
22	W	405	CLA	CMD-C2D	-2.10	1.46	1.50
22	G	605	CLA	MG-NB	-2.10	2.01	2.05
22	Q	609	CLA	MG-NB	-2.10	2.01	2.05
22	A	810	CLA	MG-NB	-2.10	2.01	2.05
22	A	815	CLA	MG-NB	-2.10	2.01	2.05
22	A	829	CLA	MG-NB	-2.10	2.01	2.05
22	G	601	CLA	MG-NB	-2.10	2.01	2.05
22	I	610	CLA	MG-NB	-2.10	2.01	2.05
22	A	811	CLA	MG-NB	-2.10	2.01	2.05
30	F	407	SQD	O8-S	2.10	1.55	1.47
24	N	612	DD6	O1-C20	-2.10	1.43	1.46
24	X	401	DD6	O1-C20	-2.10	1.43	1.46
22	X	417	CLA	CHC-C1C	2.10	1.42	1.38
22	T	601	CLA	MG-NB	-2.10	2.01	2.05
22	L	406	CLA	MG-NB	-2.10	2.01	2.05
22	S	603	CLA	MG-NB	-2.10	2.01	2.05
22	K	608	CLA	C1B-C2B	2.10	1.48	1.43
22	K	604	CLA	CHC-C1C	2.10	1.42	1.38
22	R	601	CLA	MG-NB	-2.10	2.01	2.05
22	K	604	CLA	CMD-C2D	-2.09	1.46	1.50
22	O	314	CLA	MG-NB	-2.09	2.01	2.05
22	U	409	CLA	MG-NB	-2.09	2.01	2.05
24	I	613	DD6	O1-C20	-2.09	1.43	1.46
22	L	408	CLA	C1B-C2B	2.09	1.48	1.43
22	G	604	CLA	MG-NB	-2.09	2.01	2.05
22	U	420	CLA	MG-NB	-2.09	2.01	2.05
22	R	608	CLA	MG-NB	-2.09	2.01	2.05
22	W	406	CLA	MG-NB	-2.09	2.01	2.05
26	O	323	LHG	P-O6	2.09	1.67	1.59
22	X	403	CLA	CHC-C1C	2.09	1.42	1.38
26	O	321	LHG	P-O6	2.09	1.67	1.59
22	B	817	CLA	MG-NB	-2.09	2.01	2.05
22	O	307	CLA	MG-NB	-2.09	2.01	2.05
22	T	608	CLA	MG-NB	-2.09	2.01	2.05
26	B	851	LHG	P-O6	2.09	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	807	CLA	CMC-C2C	-2.09	1.46	1.50
22	T	602	CLA	CMD-C2D	-2.09	1.46	1.50
26	H	316	LHG	P-O6	2.09	1.67	1.59
26	N	616	LHG	P-O6	2.09	1.67	1.59
22	X	411	CLA	MG-NB	-2.09	2.01	2.05
22	O	313	CLA	MG-NB	-2.09	2.01	2.05
26	N	614	LHG	P-O6	2.09	1.67	1.59
22	A	840	CLA	CHC-C1C	2.09	1.42	1.38
22	S	601	CLA	MG-NB	-2.09	2.01	2.05
22	A	807	CLA	MG-NB	-2.09	2.01	2.05
26	P	601	LHG	P-O6	2.09	1.67	1.59
26	O	323	LHG	O7-C5	-2.09	1.41	1.46
31	W	407	CHL	CHB-C1B	-2.08	1.36	1.39
22	Q	601	CLA	CMD-C2D	-2.08	1.46	1.50
22	X	407	CLA	CMD-C2D	-2.08	1.46	1.50
22	X	405	CLA	MG-NB	-2.08	2.01	2.05
22	B	818	CLA	MG-NB	-2.08	2.01	2.05
22	V	609	CLA	MG-NB	-2.08	2.01	2.05
22	B	807	CLA	CMD-C2D	-2.08	1.46	1.50
22	P	602	CLA	CMC-C2C	-2.08	1.46	1.50
22	O	310	CLA	CHC-C1C	2.08	1.42	1.38
22	Q	612	CLA	CHC-C1C	2.08	1.42	1.38
22	X	405	CLA	CMB-C2B	-2.08	1.46	1.50
22	H	305	CLA	CMD-C2D	-2.08	1.46	1.50
22	N	608	CLA	MG-NB	-2.08	2.01	2.05
22	I	602	CLA	CMD-C2D	-2.08	1.46	1.50
22	U	410	CLA	MG-NB	-2.08	2.01	2.05
22	Q	611	CLA	MG-NB	-2.08	2.01	2.05
22	K	606	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	833	CLA	CMD-C2D	-2.08	1.46	1.50
22	V	612	CLA	MG-NB	-2.08	2.01	2.05
22	A	835	CLA	MG-NB	-2.08	2.01	2.05
22	A	818	CLA	CHC-C1C	2.08	1.42	1.38
22	B	830	CLA	C1B-NB	-2.08	1.35	1.37
22	B	828	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	838	CLA	CMB-C2B	-2.08	1.46	1.50
22	F	405	CLA	CMD-C2D	-2.08	1.46	1.50
22	F	405	CLA	MG-NB	-2.08	2.01	2.05
22	W	402	CLA	MG-NB	-2.08	2.01	2.05
22	K	610	CLA	CMD-C2D	-2.07	1.46	1.50
22	P	607	CLA	CMC-C2C	-2.07	1.46	1.50
22	A	844	CLA	MG-NB	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	603	CLA	CMD-C2D	-2.07	1.46	1.50
22	V	608	CLA	MG-NB	-2.07	2.01	2.05
22	X	404	CLA	CMD-C2D	-2.07	1.46	1.50
22	P	605	CLA	MG-NB	-2.07	2.01	2.05
26	O	324	LHG	P-O6	2.07	1.67	1.59
22	A	816	CLA	CHC-C1C	2.07	1.42	1.38
24	O	316	DD6	O1-C20	-2.07	1.43	1.46
22	B	804	CLA	MG-NB	-2.07	2.01	2.05
22	B	814	CLA	MG-NB	-2.07	2.01	2.05
22	O	309	CLA	MG-NB	-2.07	2.01	2.05
22	P	604	CLA	MG-NB	-2.07	2.01	2.05
22	U	415	CLA	MG-NB	-2.07	2.01	2.05
22	L	404	CLA	MG-NB	-2.07	2.01	2.05
22	R	607	CLA	MG-NB	-2.07	2.01	2.05
22	K	611	CLA	MG-NB	-2.07	2.01	2.05
22	B	822	CLA	MG-NB	-2.07	2.01	2.05
22	K	606	CLA	MG-NB	-2.07	2.01	2.05
22	U	414	CLA	MG-NB	-2.07	2.01	2.05
22	A	828	CLA	MG-NB	-2.07	2.01	2.05
24	R	613	DD6	O1-C20	-2.07	1.43	1.46
22	L	411	CLA	MG-NB	-2.07	2.01	2.05
22	Q	605	CLA	CMD-C2D	-2.07	1.46	1.50
22	X	409	CLA	MG-NB	-2.07	2.01	2.05
22	K	613	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	824	CLA	CMB-C2B	-2.07	1.46	1.50
22	I	609	CLA	MG-NB	-2.07	2.01	2.05
22	A	823	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	819	CLA	CHC-C1C	2.07	1.42	1.38
22	A	840	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	811	CLA	MG-NB	-2.06	2.01	2.05
22	B	832	CLA	CHC-C1C	2.06	1.42	1.38
22	I	605	CLA	CMD-C2D	-2.06	1.46	1.50
24	U	416	DD6	O1-C20	-2.06	1.43	1.46
22	B	829	CLA	MG-ND	-2.06	2.01	2.05
22	Q	613	CLA	MG-NB	-2.06	2.01	2.05
26	R	614	LHG	P-O6	2.06	1.67	1.59
22	G	607	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	817	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	841	CLA	MG-NB	-2.06	2.01	2.05
22	R	605	CLA	CMD-C2D	-2.06	1.46	1.50
22	K	613	CLA	MG-NB	-2.06	2.01	2.05
26	U	419	LHG	P-O6	2.06	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	T	604	CLA	MG-NB	-2.06	2.01	2.05
22	B	837	CLA	CMB-C2B	-2.06	1.46	1.50
22	U	401	CLA	MG-NB	-2.06	2.01	2.05
24	L	414	DD6	O1-C20	-2.06	1.43	1.46
22	B	804	CLA	CMD-C2D	-2.06	1.46	1.50
22	T	605	CLA	MG-NB	-2.06	2.01	2.05
22	W	419	CLA	MG-NB	-2.06	2.01	2.05
22	S	614	CLA	MG-NB	-2.06	2.01	2.05
22	L	409	CLA	CMD-C2D	-2.06	1.46	1.50
22	G	606	CLA	CMD-C2D	-2.06	1.46	1.50
22	R	607	CLA	CMC-C2C	-2.06	1.46	1.50
22	H	308	CLA	MG-NB	-2.06	2.01	2.05
22	H	310	CLA	CMD-C2D	-2.06	1.46	1.50
22	K	603	CLA	CMB-C2B	-2.06	1.46	1.50
24	S	612	DD6	O1-C20	-2.06	1.43	1.46
26	S	613	LHG	P-O6	2.06	1.67	1.59
22	H	311	CLA	CMB-C2B	-2.06	1.46	1.50
26	G	614	LHG	P-O6	2.06	1.67	1.59
22	V	612	CLA	CMB-C2B	-2.06	1.46	1.50
22	H	310	CLA	MG-NB	-2.06	2.01	2.05
22	R	615	CLA	MG-NB	-2.06	2.01	2.05
22	O	307	CLA	CMD-C2D	-2.05	1.46	1.50
22	Q	603	CLA	CMD-C2D	-2.05	1.46	1.50
22	W	409	CLA	CMB-C2B	-2.05	1.46	1.50
22	G	611	CLA	MG-NB	-2.05	2.01	2.05
22	Q	603	CLA	MG-NB	-2.05	2.01	2.05
24	I	612	DD6	O1-C20	-2.05	1.43	1.46
22	S	607	CLA	MG-NB	-2.05	2.01	2.05
22	A	826	CLA	MG-NB	-2.05	2.01	2.05
22	A	827	CLA	MG-NB	-2.05	2.01	2.05
22	B	834	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	835	CLA	CMD-C2D	-2.05	1.46	1.50
22	F	403	CLA	MG-NB	-2.05	2.01	2.05
22	S	606	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	822	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	827	CLA	CMD-C2D	-2.05	1.46	1.50
22	L	412	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	831	CLA	MG-NB	-2.05	2.01	2.05
22	S	602	CLA	MG-NB	-2.05	2.01	2.05
22	Q	611	CLA	CMD-C2D	-2.05	1.46	1.50
32	V	616	NEX	C1-C6	-2.05	1.51	1.54
22	V	611	CLA	MG-NB	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	405	CLA	CMB-C2B	-2.05	1.46	1.50
22	O	309	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	838	CLA	MG-NB	-2.05	2.01	2.05
22	A	841	CLA	CMB-C2B	-2.05	1.46	1.50
22	N	605	CLA	CMD-C2D	-2.05	1.46	1.50
22	S	603	CLA	CMD-C2D	-2.05	1.46	1.50
24	W	417	DD6	O1-C20	-2.05	1.43	1.46
22	R	609	CLA	MG-NB	-2.05	2.01	2.05
22	A	838	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	806	CLA	CMD-C2D	-2.05	1.46	1.50
22	H	306	CLA	MG-NB	-2.05	2.01	2.05
22	L	405	CLA	MG-NB	-2.05	2.01	2.05
22	B	819	CLA	CMB-C2B	-2.05	1.46	1.50
22	B	837	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	813	CLA	MG-NB	-2.05	2.01	2.05
22	O	308	CLA	CMD-C2D	-2.05	1.46	1.50
22	A	830	CLA	CMD-C2D	-2.05	1.46	1.50
26	O	318	LHG	P-O6	2.05	1.67	1.59
22	N	601	CLA	MG-NB	-2.05	2.01	2.05
22	O	309	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	812	CLA	MG-NB	-2.05	2.01	2.05
22	K	617	CLA	CMD-C2D	-2.05	1.46	1.50
26	X	420	LHG	P-O6	2.05	1.67	1.59
22	I	604	CLA	MG-NB	-2.05	2.01	2.05
22	S	608	CLA	MG-NB	-2.05	2.01	2.05
22	U	405	CLA	MG-NB	-2.05	2.01	2.05
22	S	615	CLA	CMD-C2D	-2.05	1.46	1.50
22	W	403	CLA	MG-NB	-2.04	2.01	2.05
22	P	609	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	808	CLA	MG-NB	-2.04	2.01	2.05
22	O	312	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	819	CLA	C1B-C2B	2.04	1.48	1.43
22	V	604	CLA	MG-NB	-2.04	2.01	2.05
22	Q	613	CLA	CMB-C2B	-2.04	1.46	1.50
22	A	812	CLA	CMD-C2D	-2.04	1.46	1.50
24	W	416	DD6	O1-C20	-2.04	1.43	1.46
22	I	606	CLA	CMD-C2D	-2.04	1.46	1.50
22	Q	610	CLA	CMD-C2D	-2.04	1.46	1.50
22	P	608	CLA	MG-NB	-2.04	2.01	2.05
22	Q	612	CLA	CMD-C2D	-2.04	1.46	1.50
26	A	845	LHG	P-O6	2.04	1.67	1.59
22	O	315	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	617	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	833	CLA	MG-NB	-2.04	2.01	2.05
22	I	601	CLA	MG-NB	-2.04	2.01	2.05
22	A	801	CLA	C1B-NB	-2.04	1.35	1.37
22	B	813	CLA	CMB-C2B	-2.04	1.46	1.50
22	X	412	CLA	CMB-C2B	-2.04	1.46	1.50
22	G	605	CLA	CMB-C2B	-2.04	1.46	1.50
22	K	609	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	836	CLA	CMB-C2B	-2.04	1.46	1.50
24	U	417	DD6	O1-C20	-2.04	1.43	1.46
22	F	403	CLA	CMD-C2D	-2.04	1.46	1.50
22	L	411	CLA	CMD-C2D	-2.04	1.46	1.50
22	Q	609	CLA	CMB-C2B	-2.04	1.46	1.50
22	T	611	CLA	MG-NB	-2.04	2.01	2.05
22	U	409	CLA	CMD-C2D	-2.04	1.46	1.50
22	X	411	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	832	CLA	CMD-C2D	-2.04	1.46	1.50
22	H	303	CLA	CMB-C2B	-2.04	1.46	1.50
22	V	604	CLA	CMB-C2B	-2.04	1.46	1.50
22	F	404	CLA	CMD-C2D	-2.04	1.46	1.50
22	X	403	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	827	CLA	MG-NB	-2.04	2.01	2.05
22	B	816	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	818	CLA	CMD-C2D	-2.04	1.46	1.50
22	H	309	CLA	MG-NB	-2.04	2.01	2.05
22	A	830	CLA	MG-NB	-2.04	2.01	2.05
22	B	821	CLA	CMB-C2B	-2.04	1.46	1.50
22	G	606	CLA	CMB-C2B	-2.04	1.46	1.50
22	A	831	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	859	CLA	CMD-C2D	-2.04	1.46	1.50
22	H	307	CLA	CMB-C2B	-2.04	1.46	1.50
22	B	802	CLA	CHC-C1C	2.04	1.42	1.38
22	I	606	CLA	MG-NB	-2.03	2.01	2.05
22	U	410	CLA	CMD-C2D	-2.03	1.46	1.50
26	A	846	LHG	P-O6	2.03	1.67	1.59
22	A	837	CLA	MG-NB	-2.03	2.01	2.05
22	A	818	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	805	CLA	CMD-C2D	-2.03	1.46	1.50
22	I	610	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	808	CLA	CMD-C2D	-2.03	1.46	1.50
22	R	604	CLA	MG-NB	-2.03	2.01	2.05
26	T	614	LHG	P-O6	2.03	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	409	CLA	CMD-C2D	-2.03	1.46	1.50
22	G	602	CLA	CMD-C2D	-2.03	1.46	1.50
26	B	848	LHG	P-O6	2.03	1.67	1.59
22	B	809	CLA	CMD-C2D	-2.03	1.46	1.50
22	Q	601	CLA	CMB-C2B	-2.03	1.46	1.50
22	W	412	CLA	CMB-C2B	-2.03	1.46	1.50
22	P	609	CLA	MG-NB	-2.03	2.01	2.05
26	W	420	LHG	O7-C5	-2.03	1.41	1.46
28	H	317	LMG	O7-C8	-2.03	1.41	1.46
22	O	313	CLA	CMD-C2D	-2.03	1.46	1.50
22	P	609	CLA	CMD-C2D	-2.03	1.46	1.50
22	X	419	CLA	CMD-C2D	-2.03	1.46	1.50
22	R	605	CLA	MG-NB	-2.03	2.01	2.05
22	G	610	CLA	MG-NB	-2.03	2.01	2.05
22	Q	617	CLA	CMD-C2D	-2.03	1.46	1.50
22	U	412	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	831	CLA	CMB-C2B	-2.03	1.46	1.50
22	X	408	CLA	MG-NB	-2.03	2.01	2.05
22	O	310	CLA	CMB-C2B	-2.03	1.46	1.50
22	P	605	CLA	CMD-C2D	-2.03	1.46	1.50
22	W	403	CLA	CMB-C2B	-2.03	1.46	1.50
22	Q	610	CLA	MG-NB	-2.03	2.01	2.05
24	L	413	DD6	O1-C20	-2.03	1.43	1.46
22	B	824	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	814	CLA	CMD-C2D	-2.03	1.46	1.50
22	H	309	CLA	CMD-C2D	-2.03	1.46	1.50
22	L	402	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	821	CLA	CMD-C2D	-2.03	1.46	1.50
22	H	306	CLA	CMB-C2B	-2.03	1.46	1.50
22	A	812	CLA	MG-NB	-2.03	2.01	2.05
22	B	810	CLA	CMD-C2D	-2.03	1.46	1.50
22	H	313	CLA	CMD-C2D	-2.03	1.46	1.50
22	O	314	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	835	CLA	CMD-C2D	-2.03	1.46	1.50
22	K	612	CLA	CMD-C2D	-2.03	1.46	1.50
22	W	402	CLA	CMD-C2D	-2.03	1.46	1.50
22	W	413	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	838	CLA	CMD-C2D	-2.03	1.46	1.50
22	U	415	CLA	CMB-C2B	-2.03	1.46	1.50
22	W	406	CLA	CMB-C2B	-2.03	1.46	1.50
22	H	312	CLA	MG-NB	-2.03	2.01	2.05
22	B	815	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	817	CLA	CMB-C2B	-2.02	1.46	1.50
22	A	829	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	852	CLA	MG-NB	-2.02	2.01	2.05
22	I	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	R	602	CLA	CMD-C2D	-2.02	1.46	1.50
22	T	607	CLA	CMB-C2B	-2.02	1.46	1.50
22	G	609	CLA	MG-NB	-2.02	2.01	2.05
22	W	405	CLA	MG-NB	-2.02	2.01	2.05
22	X	419	CLA	MG-NB	-2.02	2.01	2.05
22	T	605	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	818	CLA	CMB-C2B	-2.02	1.46	1.50
22	W	415	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	806	CLA	CMD-C2D	-2.02	1.46	1.50
24	A	847	DD6	O1-C20	-2.02	1.43	1.46
22	B	807	CLA	CMB-C2B	-2.02	1.46	1.50
22	P	608	CLA	CMC-C2C	-2.02	1.46	1.50
22	Q	618	CLA	MG-NB	-2.02	2.01	2.05
22	R	611	CLA	MG-NB	-2.02	2.01	2.05
22	B	828	CLA	MG-NB	-2.02	2.01	2.05
22	V	611	CLA	CMD-C2D	-2.02	1.46	1.50
22	N	611	CLA	MG-NB	-2.02	2.01	2.05
22	W	414	CLA	CMD-C2D	-2.02	1.46	1.50
22	X	412	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	842	CLA	CMB-C2B	-2.02	1.46	1.50
22	A	844	CLA	CMD-C2D	-2.02	1.46	1.50
22	L	409	CLA	MG-NB	-2.02	2.01	2.05
22	A	821	CLA	MG-NB	-2.02	2.01	2.05
22	A	832	CLA	CMD-C2D	-2.02	1.46	1.50
22	N	606	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	837	CLA	MG-NB	-2.02	2.01	2.05
22	K	602	CLA	CMD-C2D	-2.02	1.46	1.50
22	O	306	CLA	CMD-C2D	-2.02	1.46	1.50
22	O	315	CLA	CMB-C2B	-2.02	1.46	1.50
22	G	604	CLA	CMD-C2D	-2.02	1.46	1.50
22	P	610	CLA	CMD-C2D	-2.02	1.46	1.50
22	V	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	813	CLA	CMD-C2D	-2.02	1.46	1.50
22	B	808	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	814	CLA	CMD-C2D	-2.02	1.46	1.50
22	I	609	CLA	CMD-C2D	-2.02	1.46	1.50
22	L	403	CLA	CMD-C2D	-2.02	1.46	1.50
22	N	609	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	305	CLA	CMD-C2D	-2.02	1.46	1.50
22	L	405	CLA	CMD-C2D	-2.02	1.46	1.50
22	L	409	CLA	CMB-C2B	-2.02	1.46	1.50
22	H	302	CLA	MG-NB	-2.02	2.01	2.05
22	R	610	CLA	CMD-C2D	-2.02	1.46	1.50
22	T	605	CLA	CMD-C2D	-2.02	1.46	1.50
22	K	604	CLA	MG-NB	-2.02	2.01	2.05
22	O	310	CLA	MG-NB	-2.02	2.01	2.05
22	B	816	CLA	CMB-C2B	-2.02	1.46	1.50
22	N	603	CLA	CMD-C2D	-2.02	1.46	1.50
22	T	601	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	838	CLA	CMB-C2B	-2.02	1.46	1.50
22	A	803	CLA	MG-NB	-2.02	2.01	2.05
22	R	601	CLA	CMD-C2D	-2.02	1.46	1.50
22	W	410	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	826	CLA	CMD-C2D	-2.02	1.46	1.50
22	I	607	CLA	CMC-C2C	-2.02	1.46	1.50
22	J	102	CLA	CMD-C2D	-2.02	1.46	1.50
22	S	615	CLA	CMB-C2B	-2.02	1.46	1.50
22	R	602	CLA	MG-NB	-2.02	2.01	2.05
22	O	315	CLA	CMD-C2D	-2.01	1.46	1.50
22	P	607	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	836	CLA	CHC-C1C	2.01	1.42	1.38
22	V	602	CLA	MG-NB	-2.01	2.01	2.05
22	H	302	CLA	CMB-C2B	-2.01	1.46	1.50
22	S	614	CLA	CMD-C2D	-2.01	1.46	1.50
24	T	613	DD6	O1-C20	-2.01	1.43	1.46
22	B	823	CLA	MG-NB	-2.01	2.01	2.05
22	Q	601	CLA	MG-NB	-2.01	2.01	2.05
22	B	828	CLA	CMD-C2D	-2.01	1.46	1.50
22	X	410	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	808	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	821	CLA	CMB-C2B	-2.01	1.46	1.50
26	Q	616	LHG	P-O6	2.01	1.67	1.59
22	B	859	CLA	MG-NB	-2.01	2.01	2.05
22	U	406	CLA	MG-NB	-2.01	2.01	2.05
32	U	418	NEX	C1-C6	-2.01	1.51	1.54
22	H	306	CLA	CMD-C2D	-2.01	1.46	1.50
22	R	608	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	824	CLA	MG-NB	-2.01	2.01	2.05
22	I	608	CLA	CMB-C2B	-2.01	1.46	1.50
22	U	403	CLA	CMD-C2D	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	U	414	CLA	CMB-C2B	-2.01	1.46	1.50
22	I	606	CLA	CMB-C2B	-2.01	1.46	1.50
22	I	610	CLA	CMB-C2B	-2.01	1.46	1.50
22	X	408	CLA	CMD-C2D	-2.01	1.46	1.50
22	Q	608	CLA	CMB-C2B	-2.01	1.46	1.50
22	W	414	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	801	CLA	CHC-C1C	2.01	1.42	1.38
22	I	601	CLA	CMB-C2B	-2.01	1.46	1.50
22	I	601	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	833	CLA	CMD-C2D	-2.01	1.46	1.50
22	Q	607	CLA	MG-NB	-2.01	2.01	2.05
28	Q	602	LMG	O7-C8	-2.01	1.41	1.46
22	I	604	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	837	CLA	CMD-C2D	-2.01	1.46	1.50
22	V	617	CLA	MG-NB	-2.01	2.01	2.05
22	B	809	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	859	CLA	CMB-C2B	-2.01	1.46	1.50
22	N	602	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	809	CLA	CMD-C2D	-2.01	1.46	1.50
22	P	602	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	807	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	811	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	832	CLA	MG-NB	-2.01	2.01	2.05
22	B	815	CLA	CMD-C2D	-2.01	1.46	1.50
22	S	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	U	401	CLA	CMB-C2B	-2.01	1.46	1.50
22	W	412	CLA	CMD-C2D	-2.01	1.46	1.50
22	N	610	CLA	CHC-C1C	2.01	1.42	1.38
22	H	303	CLA	CMD-C2D	-2.01	1.46	1.50
22	O	311	CLA	CMD-C2D	-2.01	1.46	1.50
22	Q	606	CLA	CMB-C2B	-2.01	1.46	1.50
22	V	609	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	834	CLA	CMB-C2B	-2.01	1.46	1.50
22	N	601	CLA	CMD-C2D	-2.01	1.46	1.50
22	N	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	V	607	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	803	CLA	CMC-C2C	-2.01	1.46	1.50
22	K	602	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	823	CLA	CMB-C2B	-2.01	1.46	1.50
22	U	405	CLA	CMD-C2D	-2.01	1.46	1.50
22	W	403	CLA	CMD-C2D	-2.01	1.46	1.50
26	W	420	LHG	P-O6	2.00	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	836	CLA	CMB-C2B	-2.00	1.46	1.50
22	A	805	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	824	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	834	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	841	CLA	CMD-C2D	-2.00	1.46	1.50
22	Q	610	CLA	CMB-C2B	-2.00	1.46	1.50
22	U	404	CLA	CMD-C2D	-2.00	1.46	1.50
22	W	415	CLA	CMB-C2B	-2.00	1.46	1.50
22	X	409	CLA	CMD-C2D	-2.00	1.46	1.50
22	L	407	CLA	CMD-C2D	-2.00	1.46	1.50
22	S	610	CLA	CMB-C2B	-2.00	1.46	1.50
22	U	420	CLA	CMD-C2D	-2.00	1.46	1.50
22	W	411	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	803	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	837	CLA	CMB-C2B	-2.00	1.46	1.50
26	L	416	LHG	P-O6	2.00	1.67	1.59
22	B	804	CLA	CMB-C2B	-2.00	1.46	1.50
22	T	609	CLA	CMD-C2D	-2.00	1.46	1.50
22	B	829	CLA	CHC-C1C	2.00	1.42	1.38
22	B	839	CLA	CMD-C2D	-2.00	1.46	1.50
22	G	603	CLA	CMB-C2B	-2.00	1.46	1.50
22	Q	609	CLA	CMD-C2D	-2.00	1.46	1.50
22	L	402	CLA	CMD-C2D	-2.00	1.46	1.50
22	U	411	CLA	MG-NB	-2.00	2.01	2.05
22	B	826	CLA	CMD-C2D	-2.00	1.46	1.50

All (2716) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	843	BCR	C40-C30-C25	-13.35	88.64	110.30
24	P	612	DD6	C9-C10-C11	-9.93	113.14	127.31
24	P	612	DD6	C4-C5-C6	-9.08	114.35	127.31
24	X	416	DD6	C4-C5-C6	-8.39	115.34	127.31
21	B	843	BCR	C40-C30-C39	-8.38	82.82	108.53
24	A	858	DD6	C4-C5-C6	-7.70	116.32	127.31
24	P	612	DD6	C14-C13-C11	-7.43	114.00	125.53
22	A	839	CLA	C4A-NA-C1A	7.36	110.02	106.71
22	B	820	CLA	C4A-NA-C1A	7.31	109.99	106.71
22	B	829	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	B	804	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	K	607	CLA	C4A-NA-C1A	7.18	109.93	106.71
22	P	611	CLA	C4A-NA-C1A	7.17	109.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	613	CLA	C4A-NA-C1A	7.16	109.93	106.71
22	B	819	CLA	C4A-NA-C1A	7.07	109.88	106.71
22	B	835	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	A	807	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	N	610	CLA	C4A-NA-C1A	7.03	109.87	106.71
24	A	858	DD6	C9-C10-C11	-7.03	117.28	127.31
22	R	607	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	P	602	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	I	609	CLA	C4A-NA-C1A	6.93	109.82	106.71
22	O	310	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	B	802	CLA	C4A-NA-C1A	6.85	109.78	106.71
22	B	824	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	L	409	CLA	C4A-NA-C1A	6.76	109.75	106.71
22	U	403	CLA	C4A-NA-C1A	6.76	109.75	106.71
22	A	844	CLA	C4A-NA-C1A	6.76	109.74	106.71
22	L	417	CLA	C4A-NA-C1A	6.74	109.74	106.71
22	A	841	CLA	C4A-NA-C1A	6.74	109.73	106.71
22	B	837	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	809	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	U	413	CLA	C4A-NA-C1A	6.72	109.72	106.71
22	L	405	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	A	821	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	A	838	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	P	610	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	S	601	CLA	C4A-NA-C1A	6.69	109.72	106.71
22	O	309	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	X	408	CLA	C4A-NA-C1A	6.67	109.70	106.71
22	L	404	CLA	C4A-NA-C1A	6.67	109.70	106.71
22	B	817	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	Q	603	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	B	826	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	A	814	CLA	C4A-NA-C1A	6.65	109.70	106.71
22	B	838	CLA	C4A-NA-C1A	6.65	109.69	106.71
22	X	413	CLA	C4A-NA-C1A	6.65	109.69	106.71
22	K	611	CLA	C4A-NA-C1A	6.64	109.69	106.71
22	V	609	CLA	C4A-NA-C1A	6.64	109.69	106.71
22	B	803	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	B	821	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	L	402	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	O	313	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	Q	617	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	T	606	CLA	C4A-NA-C1A	6.61	109.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	836	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	U	414	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	V	604	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	S	605	CLA	C4A-NA-C1A	6.58	109.66	106.71
22	A	801	CLA	C4A-NA-C1A	6.58	109.66	106.71
22	B	825	CLA	C4A-NA-C1A	6.58	109.66	106.71
21	B	843	BCR	C39-C30-C25	6.57	120.95	110.30
22	I	608	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	V	611	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	B	823	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	B	806	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	H	311	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	X	411	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	F	403	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	A	831	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	A	819	CLA	C4A-NA-C1A	6.55	109.65	106.71
22	V	617	CLA	C4A-NA-C1A	6.55	109.65	106.71
22	G	608	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	N	602	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	P	608	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	N	606	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	W	410	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	A	840	CLA	C4A-NA-C1A	6.54	109.64	106.71
22	O	319	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	I	605	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	T	604	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	U	401	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	B	807	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	G	605	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	U	412	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	T	608	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	N	605	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	V	612	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	A	826	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	X	412	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	X	402	CLA	C4A-NA-C1A	6.51	109.64	106.71
24	A	858	DD6	C3-C2-C1	-6.51	118.01	127.31
22	B	805	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	H	318	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	K	605	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	K	606	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	S	615	CLA	C4A-NA-C1A	6.51	109.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	H	308	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	W	405	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	A	828	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	S	606	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	T	601	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	R	603	CLA	C4A-NA-C1A	6.49	109.63	106.71
22	S	614	CLA	C4A-NA-C1A	6.49	109.63	106.71
22	B	811	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	H	309	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	W	414	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	X	419	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	B	808	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	I	610	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	A	816	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	I	606	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	J	102	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	O	305	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	P	606	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	W	404	CLA	C4A-NA-C1A	6.47	109.62	106.71
22	N	611	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	T	611	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	K	609	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	N	608	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	X	403	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	H	305	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	K	608	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	T	610	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	L	406	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	S	602	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	W	419	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	A	833	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	B	818	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	Q	610	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	R	605	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	H	307	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	R	611	CLA	C4A-NA-C1A	6.45	109.60	106.71
22	P	607	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	X	410	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	R	615	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	G	601	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	P	605	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	W	412	CLA	C4A-NA-C1A	6.42	109.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	H	313	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	S	604	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	I	601	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	V	602	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	B	810	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	B	816	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	G	611	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	Q	612	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	A	810	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	R	609	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	B	832	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	O	312	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	X	405	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	Q	608	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	B	833	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	L	410	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	U	406	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	P	604	CLA	C4A-NA-C1A	6.38	109.58	106.71
22	G	610	CLA	C4A-NA-C1A	6.38	109.58	106.71
22	I	604	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	Q	606	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	F	404	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	Q	601	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	V	601	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	P	609	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	A	823	CLA	C4A-NA-C1A	6.36	109.56	106.71
22	U	420	CLA	C4A-NA-C1A	6.36	109.56	106.71
22	A	805	CLA	C4A-NA-C1A	6.36	109.56	106.71
22	A	806	CLA	C4A-NA-C1A	6.36	109.56	106.71
22	K	613	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	H	306	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	A	824	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	A	835	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	G	604	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	K	604	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	R	601	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	S	607	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	U	409	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	O	311	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	B	839	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	L	408	CLA	C4A-NA-C1A	6.33	109.55	106.71
24	R	613	DD6	C3-C2-C1	-6.32	118.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Q	609	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	A	829	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	N	601	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	W	406	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	N	604	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	A	815	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	B	812	CLA	C4A-NA-C1A	6.31	109.55	106.71
22	O	308	CLA	C4A-NA-C1A	6.31	109.55	106.71
22	W	403	CLA	C4A-NA-C1A	6.31	109.54	106.71
22	R	608	CLA	C4A-NA-C1A	6.31	109.54	106.71
22	I	607	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	V	607	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	A	834	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	Q	618	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	H	302	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	A	836	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	A	842	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	U	404	CLA	C4A-NA-C1A	6.29	109.54	106.71
22	K	603	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	X	407	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	V	610	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	X	409	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	G	607	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	A	827	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	H	303	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	U	410	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	A	837	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	G	606	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	L	407	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	H	310	CLA	C4A-NA-C1A	6.27	109.53	106.71
22	K	617	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	W	413	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	G	602	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	K	602	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	S	608	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	Q	607	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	U	411	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	T	605	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	T	607	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	U	405	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	T	609	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	V	608	CLA	C4A-NA-C1A	6.24	109.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	802	CL0	C1C-C2C-C3C	-6.24	103.42	108.61
22	B	822	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	A	809	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	Q	611	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	L	411	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	B	859	CLA	C4A-NA-C1A	6.23	109.50	106.71
22	V	603	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	B	834	CLA	C4A-NA-C1A	6.20	109.50	106.71
22	S	609	CLA	C4A-NA-C1A	6.20	109.50	106.71
22	A	817	CLA	C4A-NA-C1A	6.20	109.50	106.71
22	N	607	CLA	C4A-NA-C1A	6.20	109.49	106.71
22	A	852	CLA	C4A-NA-C1A	6.20	109.49	106.71
22	A	822	CLA	C4A-NA-C1A	6.19	109.49	106.71
22	K	610	CLA	C4A-NA-C1A	6.19	109.49	106.71
22	Q	604	CLA	C4A-NA-C1A	6.18	109.49	106.71
22	X	404	CLA	C4A-NA-C1A	6.18	109.49	106.71
22	A	808	CLA	C4A-NA-C1A	6.18	109.48	106.71
22	F	405	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	T	602	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	W	415	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	B	828	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	I	602	CLA	C4A-NA-C1A	6.16	109.48	106.71
22	A	825	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	L	403	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	T	603	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	U	415	CLA	C4A-NA-C1A	6.14	109.47	106.71
21	A	851	BCR	C7-C8-C9	-6.13	116.97	126.23
22	O	306	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	O	315	CLA	C4A-NA-C1A	6.11	109.45	106.71
22	Q	613	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	A	832	CLA	C4A-NA-C1A	6.10	109.45	106.71
22	W	411	CLA	C4A-NA-C1A	6.08	109.44	106.71
22	B	831	CLA	C4A-NA-C1A	6.08	109.44	106.71
22	N	603	CLA	C4A-NA-C1A	6.07	109.43	106.71
22	N	609	CLA	C4A-NA-C1A	6.07	109.43	106.71
22	A	812	CLA	C4A-NA-C1A	6.06	109.43	106.71
22	R	606	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	H	312	CLA	C4A-NA-C1A	6.02	109.41	106.71
22	S	610	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	O	314	CLA	C4A-NA-C1A	6.00	109.40	106.71
33	A	802	CL0	CHA-C1A-C2A	-5.99	119.24	133.31
22	Q	605	CLA	C4A-NA-C1A	5.99	109.40	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	R	604	CLA	C4A-NA-C1A	5.98	109.40	106.71
22	A	818	CLA	C4A-NA-C1A	5.98	109.39	106.71
22	A	811	CLA	C4A-NA-C1A	5.97	109.39	106.71
22	W	402	CLA	C4A-NA-C1A	5.96	109.39	106.71
22	R	602	CLA	C4A-NA-C1A	5.96	109.39	106.71
24	P	613	DD6	C3-C2-C1	-5.96	118.81	127.31
22	S	603	CLA	C4A-NA-C1A	5.95	109.38	106.71
22	X	417	CLA	C4A-NA-C1A	5.94	109.38	106.71
22	W	409	CLA	C4A-NA-C1A	5.93	109.37	106.71
22	G	609	CLA	C4A-NA-C1A	5.93	109.37	106.71
22	G	603	CLA	C4A-NA-C1A	5.92	109.37	106.71
21	B	843	BCR	C24-C23-C22	-5.91	117.31	126.23
22	R	610	CLA	C4A-NA-C1A	5.89	109.35	106.71
22	I	611	CLA	C4A-NA-C1A	5.87	109.35	106.71
22	B	814	CLA	C4A-NA-C1A	5.83	109.33	106.71
22	A	803	CLA	C4A-NA-C1A	5.81	109.32	106.71
24	J	105	DD6	C9-C10-C11	-5.78	119.06	127.31
22	H	304	CLA	C4A-NA-C1A	5.77	109.30	106.71
22	B	830	CLA	C4A-NA-C1A	5.77	109.30	106.71
22	K	612	CLA	C4A-NA-C1A	5.74	109.29	106.71
22	O	307	CLA	C4A-NA-C1A	5.74	109.29	106.71
21	B	843	BCR	C40-C30-C29	-5.71	86.06	108.91
22	I	603	CLA	C4A-NA-C1A	5.69	109.27	106.71
21	A	850	BCR	C24-C23-C22	-5.69	117.64	126.23
21	B	843	BCR	C7-C8-C9	-5.62	117.74	126.23
22	B	815	CLA	C4A-NA-C1A	5.62	109.23	106.71
22	L	412	CLA	C4A-NA-C1A	5.59	109.22	106.71
22	A	804	CLA	C4A-NA-C1A	5.55	109.20	106.71
22	A	820	CLA	C4A-NA-C1A	5.53	109.19	106.71
22	A	813	CLA	C4A-NA-C1A	5.53	109.19	106.71
22	P	603	CLA	C4A-NA-C1A	5.42	109.14	106.71
21	B	801	BCR	C11-C10-C9	-5.40	119.60	127.31
21	B	801	BCR	C7-C8-C9	-5.36	118.14	126.23
21	B	801	BCR	C15-C14-C13	-5.34	119.68	127.31
24	A	847	DD6	C4-C5-C6	-5.34	119.69	127.31
22	B	827	CLA	C4A-NA-C1A	5.32	109.10	106.71
24	B	841	DD6	C3-C2-C1	-5.29	119.77	127.31
24	L	415	DD6	C3-C2-C1	-5.25	119.82	127.31
21	B	843	BCR	C30-C25-C26	-5.24	115.23	122.61
24	T	612	DD6	C3-C2-C1	-5.23	119.85	127.31
21	M	101	BCR	C20-C21-C22	-5.22	119.86	127.31
24	P	612	DD6	C4-C3-C2	-5.21	112.79	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	850	BCR	C20-C21-C22	-5.21	119.87	127.31
24	G	613	DD6	C3-C2-C1	-5.20	119.88	127.31
24	J	105	DD6	C4-C5-C6	-5.19	119.90	127.31
21	B	843	BCR	C3-C4-C5	-5.18	104.83	114.08
24	V	614	DD6	C4-C5-C6	-5.15	119.95	127.31
24	I	613	DD6	C3-C2-C1	-5.15	119.96	127.31
22	B	813	CLA	C4A-NA-C1A	5.14	109.02	106.71
22	A	830	CLA	C4A-NA-C1A	5.12	109.01	106.71
24	V	614	DD6	C21-C20-C19	5.07	119.98	114.28
21	A	851	BCR	C28-C27-C26	-5.07	105.03	114.08
24	W	418	DD6	C21-C20-C19	5.04	119.95	114.28
21	M	101	BCR	C16-C17-C18	-5.01	120.16	127.31
24	V	614	DD6	O1-C20-C19	-5.01	109.62	113.38
24	S	611	DD6	C3-C2-C1	-4.99	120.19	127.31
24	H	314	DD6	C21-C20-C19	4.99	119.89	114.28
24	Q	615	DD6	C21-C20-C19	4.99	119.89	114.28
33	A	802	CL0	C1B-CHB-C4A	4.99	124.44	121.39
24	N	613	DD6	C3-C2-C1	-4.96	120.23	127.31
24	I	613	DD6	C21-C20-C19	4.96	119.86	114.28
24	L	414	DD6	C3-C2-C1	-4.95	120.24	127.31
24	R	613	DD6	C21-C20-C19	4.95	119.85	114.28
21	B	845	BCR	C15-C14-C13	-4.94	120.25	127.31
24	U	416	DD6	C21-C20-C19	4.93	119.83	114.28
24	O	317	DD6	C21-C20-C19	4.92	119.81	114.28
24	G	613	DD6	C21-C20-C19	4.90	119.79	114.28
24	X	401	DD6	C4-C5-C6	-4.89	120.33	127.31
24	N	612	DD6	C21-C20-C19	4.88	119.77	114.28
24	K	614	DD6	C21-C20-C19	4.86	119.75	114.28
24	Q	615	DD6	C3-C2-C1	-4.85	120.39	127.31
24	L	415	DD6	C9-C10-C11	-4.82	120.43	127.31
24	H	315	DD6	C21-C20-C19	4.82	119.70	114.28
31	W	407	CHL	CHC-C1C-C2C	-4.81	118.98	126.66
24	A	858	DD6	C21-C20-C19	4.81	119.69	114.28
24	S	612	DD6	C21-C20-C19	4.80	119.69	114.28
24	N	613	DD6	C21-C20-C19	4.80	119.68	114.28
24	T	612	DD6	C21-C20-C19	4.79	119.67	114.28
24	W	418	DD6	C3-C2-C1	-4.79	120.47	127.31
24	A	859	DD6	C3-C2-C1	-4.79	120.48	127.31
31	W	408	CHL	C1B-CHB-C4A	4.77	124.31	121.39
24	F	406	DD6	C21-C20-C19	4.77	119.64	114.28
24	P	613	DD6	C21-C20-C19	4.77	119.64	114.28
24	S	611	DD6	C21-C20-C19	4.75	119.63	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	L	414	DD6	C21-C20-C19	4.75	119.62	114.28
24	X	401	DD6	C21-C20-C19	4.74	119.62	114.28
24	O	317	DD6	C3-C2-C1	-4.74	120.54	127.31
24	W	417	DD6	O1-C20-C19	-4.73	109.83	113.38
24	F	406	DD6	C4-C5-C6	-4.73	120.56	127.31
21	B	842	BCR	C15-C14-C13	-4.72	120.57	127.31
24	V	615	DD6	C21-C20-C19	4.72	119.59	114.28
24	R	612	DD6	C21-C20-C19	4.72	119.59	114.28
24	U	417	DD6	C37-C36-C31	-4.69	117.98	124.35
31	W	422	CHL	CHC-C1C-C2C	-4.68	119.18	126.66
31	W	408	CHL	CHC-C1C-C2C	-4.68	119.19	126.66
24	X	414	DD6	C21-C20-C19	4.67	119.53	114.28
31	X	406	CHL	CHC-C1C-C2C	-4.67	119.21	126.66
31	U	407	CHL	CHC-C1C-C2C	-4.67	119.21	126.66
24	W	416	DD6	C21-C20-C19	4.64	119.50	114.28
24	L	415	DD6	C21-C20-C19	4.63	119.48	114.28
31	W	422	CHL	C1B-CHB-C4A	4.61	124.21	121.39
31	V	605	CHL	CHC-C1C-C2C	-4.61	119.30	126.66
21	M	101	BCR	C24-C23-C22	-4.57	119.33	126.23
21	A	849	BCR	C15-C14-C13	-4.54	120.83	127.31
24	H	314	DD6	C4-C5-C6	-4.53	120.84	127.31
24	K	614	DD6	C37-C36-C31	-4.51	118.22	124.35
21	B	846	BCR	C16-C17-C18	-4.50	120.89	127.31
24	B	841	DD6	C21-C20-C19	4.50	119.34	114.28
24	A	847	DD6	C21-C20-C19	4.49	119.33	114.28
31	W	407	CHL	C1B-CHB-C4A	4.48	124.14	121.39
31	U	408	CHL	CHC-C1C-C2C	-4.48	119.50	126.66
21	B	846	BCR	C24-C23-C22	-4.46	119.49	126.23
24	I	612	DD6	C21-C20-C19	4.43	119.26	114.28
24	L	413	DD6	C21-C20-C19	4.41	119.24	114.28
24	Q	615	DD6	C37-C36-C31	-4.40	118.37	124.35
24	N	612	DD6	C4-C5-C6	-4.39	121.04	127.31
31	V	606	CHL	CHC-C1C-C2C	-4.39	119.65	126.66
24	A	859	DD6	C4-C5-C6	-4.38	121.06	127.31
24	L	415	DD6	C4-C5-C6	-4.37	121.08	127.31
24	X	414	DD6	C4-C5-C6	-4.37	121.08	127.31
24	G	612	DD6	C21-C20-C19	4.36	119.18	114.28
22	A	819	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
24	W	417	DD6	C21-C20-C19	4.33	119.15	114.28
21	A	850	BCR	C16-C17-C18	-4.28	121.20	127.31
31	U	407	CHL	C1B-CHB-C4A	4.28	124.01	121.39
24	P	612	DD6	C9-C8-C6	-4.28	114.40	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	415	DD6	C21-C20-C19	4.24	119.05	114.28
31	X	406	CHL	C1B-CHB-C4A	4.24	123.99	121.39
24	B	841	DD6	C4-C5-C6	-4.24	121.26	127.31
24	P	612	DD6	C13-C11-C10	4.23	125.44	118.94
31	V	605	CHL	C1B-CHB-C4A	4.23	123.98	121.39
24	R	612	DD6	C3-C2-C1	-4.22	121.28	127.31
24	W	416	DD6	C4-C5-C6	-4.22	121.28	127.31
24	K	615	DD6	C21-C20-C19	4.22	119.03	114.28
24	U	417	DD6	C21-C20-C19	4.22	119.03	114.28
25	F	401	DGD	O2G-C1B-C2B	4.22	120.59	111.50
24	K	615	DD6	C4-C5-C6	-4.22	121.29	127.31
24	P	612	DD6	C21-C20-C19	4.21	119.02	114.28
24	F	406	DD6	C14-C13-C11	-4.20	119.01	125.53
24	B	841	DD6	C9-C10-C11	-4.18	121.34	127.31
24	X	416	DD6	C8-C6-C5	4.18	125.36	118.94
24	B	841	DD6	O1-C20-C19	-4.18	110.24	113.38
24	Q	614	DD6	C21-C20-C19	4.17	118.97	114.28
21	A	848	BCR	C33-C5-C6	-4.17	119.85	124.53
24	N	613	DD6	C9-C10-C11	-4.17	121.36	127.31
24	Q	614	DD6	O1-C20-C19	-4.15	110.26	113.38
24	R	612	DD6	C4-C5-C6	-4.14	121.40	127.31
26	L	416	LHG	O7-C7-C8	4.13	120.40	111.50
33	A	802	CL0	O2D-CGD-O1D	-4.12	115.78	123.84
24	A	859	DD6	C21-C20-C19	4.12	118.92	114.28
24	T	613	DD6	C21-C20-C19	4.11	118.91	114.28
26	N	616	LHG	O7-C7-C8	4.11	120.36	111.50
24	I	612	DD6	O1-C20-C19	-4.11	110.30	113.38
26	U	419	LHG	O7-C7-C8	4.10	120.34	111.50
24	L	413	DD6	C4-C5-C6	-4.10	121.46	127.31
21	A	851	BCR	C20-C21-C22	-4.09	121.47	127.31
26	O	324	LHG	O7-C7-C8	4.09	120.31	111.50
26	S	613	LHG	O7-C7-C8	4.08	120.30	111.50
22	A	819	CLA	C3B-C4B-NB	-4.08	106.73	110.52
24	K	614	DD6	C4-C5-C6	-4.07	121.50	127.31
26	A	845	LHG	O7-C7-C8	4.07	120.27	111.50
24	O	316	DD6	C21-C20-C19	4.06	118.85	114.28
31	U	408	CHL	C1B-CHB-C4A	4.06	123.88	121.39
22	S	605	CLA	C1-C2-C3	-4.06	119.02	126.04
24	A	858	DD6	C-C1-C2	-4.06	117.24	122.92
21	B	842	BCR	C33-C5-C6	-4.05	119.98	124.53
21	B	843	BCR	C16-C17-C18	-4.05	121.53	127.31
26	X	420	LHG	O7-C7-C8	4.05	120.22	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	619	LHG	O7-C7-C8	4.04	120.21	111.50
24	H	315	DD6	C3-C2-C1	-4.04	121.55	127.31
26	H	316	LHG	O7-C7-C8	4.03	120.19	111.50
24	G	613	DD6	C37-C36-C31	-4.03	118.87	124.35
21	A	848	BCR	C16-C17-C18	-4.03	121.56	127.31
26	T	614	LHG	O7-C7-C8	4.01	120.14	111.50
24	U	417	DD6	O1-C20-C19	-4.00	110.38	113.38
24	X	415	DD6	C4-C5-C6	-3.99	121.61	127.31
24	X	415	DD6	O1-C20-C19	-3.99	110.38	113.38
21	B	844	BCR	C7-C8-C9	-3.99	120.20	126.23
24	G	612	DD6	C4-C5-C6	-3.99	121.62	127.31
26	B	851	LHG	O7-C7-C8	3.99	120.10	111.50
26	A	846	LHG	O7-C7-C8	3.98	120.09	111.50
21	A	850	BCR	C38-C26-C25	-3.98	120.06	124.53
24	V	614	DD6	C9-C10-C11	-3.98	121.63	127.31
26	K	616	LHG	O7-C7-C8	3.97	120.06	111.50
21	A	851	BCR	C16-C17-C18	-3.97	121.64	127.31
26	G	614	LHG	O7-C7-C8	3.96	120.04	111.50
24	S	612	DD6	C4-C5-C6	-3.96	121.66	127.31
24	Q	614	DD6	C4-C5-C6	-3.95	121.67	127.31
21	A	849	BCR	C16-C17-C18	-3.95	121.67	127.31
24	R	612	DD6	C9-C10-C11	-3.95	121.67	127.31
24	U	416	DD6	C4-C5-C6	-3.95	121.67	127.31
26	O	321	LHG	O7-C7-C8	3.95	120.01	111.50
24	H	315	DD6	C37-C36-C31	-3.94	118.99	124.35
24	N	613	DD6	C37-C36-C31	-3.94	118.99	124.35
31	V	606	CHL	C1B-CHB-C4A	3.94	123.80	121.39
21	A	849	BCR	C24-C23-C22	-3.93	120.30	126.23
24	X	416	DD6	C12-C11-C13	3.91	124.24	118.08
24	V	615	DD6	C4-C5-C6	-3.91	121.73	127.31
24	S	612	DD6	C3-C2-C1	-3.90	121.74	127.31
24	P	612	DD6	C25-C24-C1	-3.90	115.46	126.42
21	B	845	BCR	C24-C23-C22	-3.89	120.35	126.23
21	B	845	BCR	C11-C10-C9	-3.89	121.76	127.31
21	A	848	BCR	C11-C10-C9	-3.88	121.77	127.31
26	B	848	LHG	O7-C7-C8	3.88	119.86	111.50
24	G	612	DD6	C37-C36-C31	-3.87	119.08	124.35
24	A	858	DD6	C-C1-C24	3.87	124.17	118.08
26	O	318	LHG	O7-C7-C8	3.87	119.84	111.50
24	L	413	DD6	C3-C2-C1	-3.87	121.79	127.31
21	A	849	BCR	C20-C21-C22	-3.86	121.80	127.31
21	A	848	BCR	C7-C8-C9	-3.85	120.42	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	323	LHG	O7-C7-C8	3.85	119.79	111.50
22	A	839	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
24	G	612	DD6	O1-C20-C19	-3.84	110.49	113.38
24	W	417	DD6	C4-C5-C6	-3.84	121.83	127.31
24	X	416	DD6	C14-C13-C11	3.83	131.47	125.53
24	W	416	DD6	C3-C2-C1	-3.83	121.85	127.31
21	J	103	BCR	C15-C14-C13	-3.83	121.85	127.31
24	V	615	DD6	C3-C2-C1	-3.82	121.85	127.31
21	B	844	BCR	C11-C10-C9	-3.82	121.86	127.31
21	A	851	BCR	C15-C14-C13	-3.81	121.87	127.31
33	A	802	CL0	O2D-CGD-CBD	3.81	115.83	111.00
26	P	601	LHG	O7-C7-C8	3.81	119.72	111.50
26	N	614	LHG	O7-C7-C8	3.80	119.70	111.50
26	Q	616	LHG	O7-C7-C8	3.80	119.70	111.50
24	X	416	DD6	C21-C20-C19	3.80	118.56	114.28
26	R	614	LHG	O7-C7-C8	3.79	119.68	111.50
24	Q	615	DD6	C15-C14-C13	-3.79	117.97	125.99
24	P	612	DD6	C37-C36-C31	-3.79	119.20	124.35
24	W	418	DD6	O1-C20-C19	-3.79	110.54	113.38
21	B	845	BCR	C3-C4-C5	-3.79	107.32	114.08
21	B	842	BCR	C24-C23-C22	-3.78	120.52	126.23
21	B	844	BCR	C15-C14-C13	-3.78	121.91	127.31
24	U	417	DD6	C4-C5-C6	-3.76	121.94	127.31
24	T	613	DD6	C3-C2-C1	-3.75	121.95	127.31
24	R	613	DD6	C15-C14-C13	-3.74	118.08	125.99
24	O	316	DD6	C37-C36-C31	-3.73	119.28	124.35
21	B	842	BCR	C16-C17-C18	-3.73	121.99	127.31
24	T	612	DD6	C37-C36-C31	-3.73	119.28	124.35
24	A	847	DD6	C9-C10-C11	-3.72	122.00	127.31
21	M	101	BCR	C15-C14-C13	-3.71	122.01	127.31
24	J	105	DD6	C37-C36-C31	-3.71	119.31	124.35
24	Q	614	DD6	C3-C2-C1	-3.70	122.03	127.31
21	B	844	BCR	C16-C17-C18	-3.70	122.03	127.31
24	V	614	DD6	C3-C2-C1	-3.69	122.04	127.31
24	H	314	DD6	C37-C36-C31	-3.69	119.34	124.35
24	F	406	DD6	C37-C36-C31	-3.68	119.34	124.35
24	O	316	DD6	O1-C20-C19	-3.68	110.62	113.38
24	W	418	DD6	C4-C5-C6	-3.68	122.06	127.31
21	B	845	BCR	C7-C8-C9	-3.68	120.68	126.23
21	A	848	BCR	C24-C23-C22	-3.67	120.68	126.23
21	B	842	BCR	C11-C10-C9	-3.67	122.08	127.31
24	S	611	DD6	C15-C14-C13	-3.67	118.24	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	842	BCR	C30-C25-C26	-3.66	117.45	122.61
24	V	614	DD6	C37-C36-C31	-3.66	119.37	124.35
21	A	848	BCR	C15-C14-C13	-3.66	122.09	127.31
21	A	850	BCR	C15-C14-C13	-3.65	122.10	127.31
24	V	614	DD6	C15-C14-C13	-3.65	118.28	125.99
24	H	314	DD6	C3-C2-C1	-3.64	122.11	127.31
24	T	613	DD6	O1-C20-C19	-3.63	110.65	113.38
22	K	607	CLA	C3B-C4B-NB	-3.63	107.15	110.52
24	L	413	DD6	C37-C36-C31	-3.62	119.42	124.35
21	A	850	BCR	C33-C5-C6	-3.60	120.48	124.53
25	O	304	DGD	O2G-C1B-C2B	3.60	119.26	111.50
21	B	843	BCR	C15-C14-C13	-3.60	122.17	127.31
24	X	414	DD6	C3-C2-C1	-3.60	122.17	127.31
24	R	612	DD6	C37-C36-C31	-3.60	119.46	124.35
24	W	416	DD6	C37-C36-C31	-3.59	119.47	124.35
24	X	401	DD6	C9-C10-C11	-3.59	122.19	127.31
21	B	846	BCR	C20-C21-C22	-3.59	122.19	127.31
22	A	816	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
24	V	615	DD6	C37-C36-C31	-3.58	119.48	124.35
21	A	851	BCR	C27-C26-C25	-3.58	117.54	122.73
24	N	612	DD6	C3-C2-C1	-3.58	122.21	127.31
21	B	844	BCR	C24-C23-C22	-3.57	120.83	126.23
21	B	801	BCR	C28-C27-C26	-3.57	107.70	114.08
21	B	842	BCR	C20-C21-C22	-3.57	122.22	127.31
21	B	843	BCR	C39-C30-C29	3.56	123.16	108.91
22	A	831	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
21	B	844	BCR	C33-C5-C6	-3.55	120.54	124.53
21	A	849	BCR	C38-C26-C25	-3.55	120.55	124.53
24	I	613	DD6	C15-C14-C13	-3.54	118.51	125.99
24	X	401	DD6	C3-C2-C1	-3.54	122.26	127.31
24	V	615	DD6	O1-C20-C19	-3.53	110.73	113.38
22	B	820	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
21	M	101	BCR	C7-C8-C9	-3.53	120.91	126.23
24	P	612	DD6	C-C1-C2	-3.52	117.99	122.92
24	L	414	DD6	C37-C36-C31	-3.52	119.56	124.35
26	W	420	LHG	O7-C7-C8	3.52	119.09	111.50
24	H	315	DD6	C15-C14-C13	-3.52	118.56	125.99
21	J	103	BCR	C16-C17-C18	-3.51	122.30	127.31
24	I	613	DD6	C37-C36-C31	-3.51	119.58	124.35
24	P	612	DD6	C7-C6-C5	-3.51	118.01	122.92
24	H	314	DD6	C15-C14-C13	-3.50	118.58	125.99
24	A	858	DD6	O1-C20-C19	-3.50	110.75	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	W	418	DD6	C37-C36-C31	-3.50	119.59	124.35
24	N	612	DD6	C37-C36-C31	-3.50	119.59	124.35
24	O	317	DD6	C15-C14-C13	-3.50	118.60	125.99
24	G	613	DD6	C15-C14-C13	-3.49	118.61	125.99
24	A	858	DD6	C9-C8-C6	-3.49	116.62	126.42
24	Q	614	DD6	C37-C36-C31	-3.48	119.62	124.35
24	H	314	DD6	O1-C20-C19	-3.47	110.78	113.38
22	A	816	CLA	CAA-CBA-CGA	-3.46	103.14	113.25
24	T	612	DD6	C15-C14-C13	-3.46	118.67	125.99
24	U	416	DD6	C3-C2-C1	-3.46	122.37	127.31
21	B	843	BCR	C33-C5-C4	3.46	120.26	113.62
21	A	849	BCR	C11-C10-C9	-3.46	122.37	127.31
24	X	401	DD6	C37-C36-C31	-3.46	119.65	124.35
24	X	415	DD6	C37-C36-C31	-3.45	119.66	124.35
22	B	802	CLA	C3B-C4B-NB	-3.45	107.32	110.52
21	M	101	BCR	C33-C5-C6	-3.44	120.67	124.53
27	O	322	LMU	C1-O1'-C1'	-3.44	108.14	113.84
24	X	414	DD6	C37-C36-C31	-3.44	119.68	124.35
24	B	841	DD6	C37-C36-C31	-3.44	119.68	124.35
28	I	615	LMG	C6-C5-C4	-3.43	108.76	113.54
22	A	816	CLA	C3B-C4B-NB	-3.42	107.34	110.52
22	L	408	CLA	C3B-C4B-NB	-3.41	107.36	110.52
25	B	847	DGD	O2G-C1B-C2B	3.41	118.84	111.50
24	X	416	DD6	C10-C9-C8	-3.40	112.60	123.22
21	B	846	BCR	C33-C5-C6	-3.40	120.71	124.53
24	T	613	DD6	C4-C5-C6	-3.39	122.47	127.31
24	U	416	DD6	C9-C10-C11	-3.39	122.47	127.31
21	A	851	BCR	C34-C9-C10	-3.39	118.17	122.92
24	K	615	DD6	O1-C20-C19	-3.39	110.84	113.38
24	T	612	DD6	O1-C20-C19	-3.38	110.84	113.38
22	I	611	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
24	T	613	DD6	C37-C36-C31	-3.38	119.76	124.35
21	B	846	BCR	C15-C14-C13	-3.37	122.49	127.31
24	X	416	DD6	C37-C36-C31	-3.37	119.77	124.35
24	A	859	DD6	C37-C36-C31	-3.36	119.78	124.35
24	L	415	DD6	C37-C36-C31	-3.35	119.80	124.35
24	A	859	DD6	C15-C14-C13	-3.34	118.92	125.99
24	N	612	DD6	C9-C10-C11	-3.34	122.54	127.31
21	J	103	BCR	C33-C5-C6	-3.34	120.78	124.53
24	I	612	DD6	C4-C5-C6	-3.34	122.55	127.31
24	P	613	DD6	C4-C5-C6	-3.33	122.55	127.31
24	L	415	DD6	C14-C13-C11	-3.33	120.36	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	J	103	BCR	C3-C4-C5	-3.33	108.13	114.08
22	A	824	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
24	J	105	DD6	C3-C2-C1	-3.32	122.57	127.31
21	J	103	BCR	C28-C27-C26	-3.32	108.15	114.08
24	A	858	DD6	C37-C36-C31	-3.32	119.84	124.35
24	S	612	DD6	O1-C20-C19	-3.32	110.89	113.38
22	Q	613	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
24	V	615	DD6	C15-C14-C13	-3.31	118.99	125.99
24	G	612	DD6	C3-C2-C1	-3.31	122.59	127.31
22	B	830	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
21	M	101	BCR	C11-C10-C9	-3.31	122.59	127.31
24	P	613	DD6	C37-C36-C31	-3.31	119.85	124.35
22	S	610	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
24	P	612	DD6	C12-C11-C10	-3.29	118.31	122.92
24	G	613	DD6	C4-C5-C6	-3.29	122.61	127.31
24	S	612	DD6	C37-C36-C31	-3.29	119.88	124.35
22	B	824	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
22	B	828	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
21	A	851	BCR	C24-C23-C22	-3.28	121.28	126.23
24	W	417	DD6	C3-C2-C1	-3.28	122.63	127.31
24	S	612	DD6	C15-C14-C13	-3.27	119.09	125.99
24	O	316	DD6	C3-C2-C1	-3.27	122.65	127.31
21	B	843	BCR	C34-C9-C10	-3.27	118.35	122.92
21	B	845	BCR	C28-C27-C26	-3.26	108.25	114.08
21	A	848	BCR	C38-C26-C25	-3.26	120.87	124.53
22	B	803	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
22	U	403	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
24	X	416	DD6	C37-C36-C35	3.23	120.35	114.36
24	O	316	DD6	C9-C10-C11	-3.23	122.69	127.31
24	N	613	DD6	C4-C5-C6	-3.23	122.70	127.31
31	U	407	CHL	CHA-C1A-C2A	-3.23	125.72	133.31
24	W	418	DD6	C15-C14-C13	-3.23	119.17	125.99
24	W	416	DD6	C9-C10-C11	-3.23	122.70	127.31
24	K	614	DD6	C15-C14-C13	-3.22	119.18	125.99
24	L	414	DD6	C15-C14-C13	-3.22	119.19	125.99
22	S	609	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
21	B	846	BCR	C3-C4-C5	-3.21	108.34	114.08
24	S	612	DD6	C9-C10-C11	-3.21	122.73	127.31
28	U	402	LMG	O6-C1-O1	-3.21	102.37	109.97
24	V	615	DD6	C9-C10-C11	-3.21	122.73	127.31
22	P	608	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
21	A	849	BCR	C7-C8-C9	-3.21	121.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	848	BCR	C20-C21-C22	-3.21	122.73	127.31
21	M	101	BCR	C30-C25-C26	-3.21	118.10	122.61
21	J	103	BCR	C11-C10-C9	-3.20	122.74	127.31
24	X	414	DD6	O1-C20-C19	-3.20	110.98	113.38
24	I	612	DD6	C3-C2-C1	-3.20	122.74	127.31
25	B	847	DGD	O1G-C1A-C2A	3.20	121.95	111.91
31	V	605	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
24	X	416	DD6	C7-C6-C5	-3.20	118.45	122.92
21	B	842	BCR	C7-C8-C9	-3.19	121.42	126.23
22	P	610	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
24	W	417	DD6	C37-C36-C31	-3.18	120.02	124.35
22	A	810	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
21	J	103	BCR	C7-C8-C9	-3.18	121.43	126.23
22	A	838	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
24	X	416	DD6	C4-C3-C2	-3.18	116.96	123.47
22	A	835	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
24	N	612	DD6	C15-C14-C13	-3.17	119.28	125.99
21	B	845	BCR	C38-C26-C25	-3.17	120.96	124.53
21	A	849	BCR	C33-C5-C6	-3.17	120.97	124.53
21	A	851	BCR	C38-C26-C27	3.16	119.69	113.62
22	B	804	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
31	X	406	CHL	CHA-C1A-C2A	-3.15	125.90	133.31
24	O	317	DD6	C4-C5-C6	-3.15	122.81	127.31
31	W	407	CHL	CHA-C1A-C2A	-3.14	125.93	133.31
22	B	835	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
22	A	806	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
24	O	316	DD6	C4-C5-C6	-3.14	122.83	127.31
25	O	304	DGD	O1G-C1A-C2A	3.14	121.75	111.91
22	B	819	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
31	W	408	CHL	CHA-C1A-C2A	-3.14	125.94	133.31
21	B	843	BCR	C37-C22-C21	-3.14	118.53	122.92
25	F	401	DGD	O1G-C1A-C2A	3.13	121.74	111.91
22	B	830	CLA	C3B-C4B-NB	-3.13	107.61	110.52
24	K	614	DD6	C3-C2-C1	-3.13	122.85	127.31
22	G	603	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
22	A	842	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	H	313	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	W	415	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
21	B	842	BCR	C3-C4-C5	-3.11	108.52	114.08
24	A	847	DD6	C37-C36-C31	-3.11	120.12	124.35
24	F	406	DD6	C-C1-C2	-3.10	118.57	122.92
22	T	608	CLA	O2D-CGD-O1D	-3.10	117.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	612	DD6	O1-C20-C19	-3.10	111.05	113.38
24	R	612	DD6	C15-C14-C13	-3.10	119.43	125.99
28	F	408	LMG	O6-C5-C4	3.10	115.33	109.69
22	U	405	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	L	408	CLA	CHD-C1D-ND	-3.10	121.61	124.45
21	B	844	BCR	C20-C21-C22	-3.09	122.89	127.31
22	B	832	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	I	613	DD6	C4-C5-C6	-3.09	122.89	127.31
24	I	613	DD6	C9-C10-C11	-3.09	122.90	127.31
22	A	816	CLA	O2D-CGD-CBD	3.09	116.76	111.27
22	B	836	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	L	414	DD6	C4-C5-C6	-3.09	122.90	127.31
24	J	105	DD6	C21-C20-C19	3.09	117.75	114.28
21	A	849	BCR	C3-C4-C5	-3.08	108.57	114.08
24	H	314	DD6	C9-C10-C11	-3.08	122.91	127.31
22	A	801	CLA	C3B-C4B-NB	-3.08	107.66	110.52
21	B	842	BCR	C28-C27-C26	-3.08	108.58	114.08
24	S	611	DD6	C4-C5-C6	-3.07	122.92	127.31
22	A	811	CLA	CAA-C2A-C3A	-3.07	104.36	112.78
22	B	831	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	U	416	DD6	C15-C14-C13	-3.07	119.50	125.99
22	B	817	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
22	A	833	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	I	613	DD6	C37-C36-C35	3.07	120.04	114.36
24	X	414	DD6	C15-C14-C13	-3.07	119.50	125.99
22	A	844	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	P	612	DD6	C8-C6-C5	3.07	123.65	118.94
28	H	319	LMG	O6-C1-O1	-3.06	102.72	109.97
24	R	613	DD6	C3-C4-C5	-3.06	117.20	123.47
24	Q	615	DD6	C4-C5-C6	-3.06	122.94	127.31
31	W	422	CHL	CHA-C1A-C2A	-3.06	126.13	133.31
24	I	612	DD6	C37-C36-C31	-3.05	120.20	124.35
22	B	827	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	A	827	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	X	414	DD6	C9-C10-C11	-3.05	122.96	127.31
22	O	307	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	R	613	DD6	C4-C5-C6	-3.05	122.96	127.31
22	B	815	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
21	B	843	BCR	C38-C26-C27	3.04	119.46	113.62
24	N	613	DD6	C15-C14-C13	-3.04	119.56	125.99
22	Q	604	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	B	812	CLA	O2D-CGD-O1D	-3.04	117.89	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	813	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	I	603	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	U	417	DD6	C3-C2-C1	-3.04	122.98	127.31
24	T	612	DD6	C3-C4-C5	-3.04	117.25	123.47
22	S	614	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
24	L	413	DD6	C9-C10-C11	-3.03	122.98	127.31
24	K	615	DD6	C3-C2-C1	-3.03	122.98	127.31
24	U	416	DD6	C37-C36-C31	-3.03	120.23	124.35
31	U	408	CHL	CHA-C1A-C2A	-3.03	126.19	133.31
24	L	413	DD6	C15-C14-C13	-3.03	119.59	125.99
22	B	811	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	B	814	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
21	A	851	BCR	C33-C5-C6	-3.02	121.13	124.53
22	Q	618	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	A	808	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	A	828	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	B	807	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	N	605	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	A	821	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	B	806	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
28	W	401	LMG	O6-C1-O1	-3.02	102.83	109.97
22	V	617	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
22	X	410	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
24	B	841	DD6	C25-C26-C27	-3.01	117.83	126.58
22	A	840	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	G	612	DD6	C15-C14-C13	-3.01	119.62	125.99
22	A	852	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
21	J	103	BCR	C24-C23-C22	-3.01	121.68	126.23
22	A	801	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	A	830	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	A	814	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
24	H	315	DD6	O1-C20-C21	-3.00	111.46	115.06
22	L	412	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	F	401	DGD	C2G-O2G-C1B	-3.00	110.40	117.79
22	A	825	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	I	612	DD6	C9-C10-C11	-3.00	123.03	127.31
22	A	823	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
22	B	834	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
22	P	611	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
22	T	604	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
22	T	601	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
22	O	312	CLA	O2D-CGD-O1D	-3.00	117.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	416	DD6	C3-C2-C1	-2.99	123.04	127.31
22	F	405	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
24	W	416	DD6	C33-C34-C35	-2.99	106.21	110.30
22	J	102	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	Q	605	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
24	P	612	DD6	O1-C20-C21	-2.99	111.47	115.06
22	A	817	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	B	841	DD6	C15-C14-C13	-2.99	119.68	125.99
22	A	809	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
31	V	606	CHL	CHA-C1A-C2A	-2.99	126.30	133.31
22	G	602	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
24	X	415	DD6	C3-C2-C1	-2.98	123.05	127.31
24	A	859	DD6	C9-C10-C11	-2.98	123.05	127.31
22	U	406	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	X	404	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	I	602	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	K	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	P	606	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	Q	604	CLA	C3B-C4B-NB	-2.98	107.75	110.52
24	R	613	DD6	C37-C36-C35	2.98	119.87	114.36
21	B	843	BCR	C33-C5-C6	-2.98	121.19	124.53
22	L	407	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	W	403	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	T	610	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
24	R	613	DD6	O1-C20-C19	-2.98	111.15	113.38
22	I	608	CLA	C3B-C4B-NB	-2.97	107.76	110.52
22	U	415	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
22	A	807	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	B	823	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	G	605	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	A	826	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
22	A	834	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
24	K	615	DD6	C37-C36-C31	-2.97	120.32	124.35
23	A	843	PQN	C14-C13-C15	2.97	120.26	115.27
22	L	417	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
22	B	838	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
21	B	842	BCR	C27-C26-C25	-2.96	118.43	122.73
22	W	409	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	B	809	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	S	601	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
24	P	613	DD6	C9-C10-C11	-2.96	123.08	127.31
22	G	609	CLA	O2D-CGD-O1D	-2.96	118.05	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	T	602	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
21	B	801	BCR	C3-C4-C5	-2.96	108.79	114.08
22	W	404	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	K	608	CLA	CHD-C1D-ND	-2.96	121.73	124.45
22	T	605	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	B	859	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	S	615	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	L	409	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
22	B	825	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
22	K	608	CLA	C3B-C4B-NB	-2.95	107.78	110.52
22	B	826	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	Q	607	CLA	C3B-C4B-NB	-2.95	107.78	110.52
22	N	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	B	810	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	B	829	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	N	604	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	W	405	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	V	602	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
24	K	614	DD6	C37-C36-C35	2.94	119.81	114.36
24	I	612	DD6	C15-C14-C13	-2.94	119.77	125.99
22	W	419	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
21	A	849	BCR	C33-C5-C4	2.94	119.26	113.62
22	R	606	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	K	617	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	T	603	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	U	413	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	A	837	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
24	X	401	DD6	C15-C14-C13	-2.93	119.79	125.99
22	H	311	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	O	309	CLA	C3B-C4B-NB	-2.93	107.80	110.52
22	G	604	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
22	B	816	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	K	611	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	X	419	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	Q	603	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	L	406	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	X	409	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	X	408	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	B	820	CLA	CHB-C4A-NA	2.92	128.56	124.51
22	U	409	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	B	821	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	O	306	CLA	O2D-CGD-O1D	-2.92	118.12	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	602	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	G	607	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	K	613	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	B	833	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	V	613	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	K	612	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	K	603	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	A	820	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
24	F	406	DD6	C25-C24-C1	-2.92	118.22	126.42
24	G	612	DD6	C9-C10-C11	-2.91	123.15	127.31
22	S	603	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	U	412	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	I	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	A	812	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	O	315	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	O	311	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	T	609	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	Q	614	DD6	C9-C10-C11	-2.91	123.16	127.31
22	P	607	CLA	C3B-C4B-NB	-2.91	107.82	110.52
21	B	845	BCR	C15-C16-C17	-2.91	117.52	123.47
22	U	420	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
22	A	813	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
22	A	818	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	N	606	CLA	C3B-C4B-NB	-2.90	107.82	110.52
22	K	610	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	O	310	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	H	309	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	B	813	CLA	C3B-C4B-NB	-2.90	107.83	110.52
22	W	403	CLA	C3B-C4B-NB	-2.90	107.83	110.52
22	L	405	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
21	B	843	BCR	C4-C5-C6	-2.90	118.53	122.73
22	A	836	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
22	B	837	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
22	R	603	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
22	Q	606	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	A	832	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	B	818	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	A	837	CLA	C3B-C4B-NB	-2.89	107.83	110.52
22	G	608	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	H	305	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	L	403	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	V	601	CLA	O2D-CGD-O1D	-2.89	118.18	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	850	BCR	C7-C8-C9	-2.89	121.87	126.23
24	A	858	DD6	C7-C6-C5	-2.89	118.87	122.92
22	P	604	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	R	604	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	S	610	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	O	314	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	Q	614	DD6	C15-C14-C13	-2.89	119.89	125.99
22	A	811	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
28	B	852	LMG	O6-C1-O1	-2.88	103.14	109.97
22	F	404	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	U	404	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	X	405	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	K	614	DD6	O1-C20-C19	-2.88	111.22	113.38
22	H	307	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	A	831	CLA	O2D-CGD-CBD	2.88	116.39	111.27
21	B	801	BCR	C24-C23-C22	-2.88	121.89	126.23
21	B	801	BCR	C15-C16-C17	-2.88	117.58	123.47
24	K	614	DD6	C9-C10-C11	-2.88	123.21	127.31
21	M	101	BCR	C38-C26-C27	2.88	119.14	113.62
22	R	615	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	B	802	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
22	N	602	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	A	804	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	I	607	CLA	C1-C2-C3	-2.86	121.09	126.04
22	L	411	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	Q	611	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	Q	601	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	L	406	CLA	C3B-C4B-NB	-2.86	107.86	110.52
24	P	613	DD6	C15-C14-C13	-2.86	119.94	125.99
22	H	306	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	T	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	U	410	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	T	606	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	L	404	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	A	842	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
22	O	308	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	W	413	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	H	303	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
22	S	608	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	N	611	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	I	610	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	U	411	CLA	O2D-CGD-O1D	-2.85	118.26	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	H	315	DD6	O1-C20-C19	-2.85	111.24	113.38
22	G	608	CLA	C11-C10-C8	-2.85	106.71	115.92
22	G	601	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	G	611	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	K	603	CLA	C3B-C4B-NB	-2.85	107.87	110.52
24	R	613	DD6	O1-C20-C21	-2.85	111.64	115.06
22	X	413	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	H	310	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	W	412	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	R	613	DD6	C10-C9-C8	-2.85	114.34	123.22
22	X	402	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	N	607	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	Q	610	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	O	309	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	T	613	DD6	C15-C14-C13	-2.84	119.98	125.99
22	N	610	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
22	V	607	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	N	610	CLA	CHB-C4A-NA	2.84	128.44	124.51
27	J	104	LMU	C6B-C5B-C4B	-2.84	109.58	113.54
22	H	309	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	A	822	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	H	315	DD6	C4-C5-C6	-2.84	123.26	127.31
24	A	858	DD6	C12-C11-C10	-2.84	118.95	122.92
22	H	312	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	B	803	CLA	C3B-C4B-NB	-2.84	107.88	110.52
22	W	411	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	I	605	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
22	L	410	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
22	X	407	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
22	Q	612	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	B	805	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	I	607	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	S	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	V	608	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	X	403	CLA	C3B-C4B-NB	-2.83	107.89	110.52
22	W	410	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	A	859	DD6	C4-C3-C2	-2.83	117.68	123.47
22	P	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	H	306	CLA	C3B-C4B-NB	-2.83	107.89	110.52
24	N	613	DD6	C21-C20-C15	-2.83	117.52	122.26
24	A	847	DD6	C14-C13-C11	-2.83	121.14	125.53
22	N	609	CLA	O2D-CGD-O1D	-2.83	118.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	809	CLA	C3B-C4B-NB	-2.83	107.89	110.52
24	V	615	DD6	C33-C34-C35	-2.82	106.44	110.30
21	M	101	BCR	C28-C27-C26	-2.82	109.04	114.08
22	S	607	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	V	611	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	R	608	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	V	604	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	V	609	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	Q	613	CLA	C3B-C4B-NB	-2.82	107.90	110.52
21	A	851	BCR	C29-C30-C25	2.82	114.82	110.48
24	U	416	DD6	O1-C20-C19	-2.82	111.27	113.38
22	A	815	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
22	W	410	CLA	C3B-C4B-NB	-2.81	107.90	110.52
22	A	842	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
22	I	608	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	W	402	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	W	406	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	R	611	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	U	406	CLA	C3B-C4B-NB	-2.81	107.91	110.52
24	G	612	DD6	C33-C34-C35	-2.81	106.46	110.30
22	H	318	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	B	840	PQN	C14-C13-C15	2.81	119.99	115.27
24	X	416	DD6	C21-C20-C15	-2.81	117.56	122.26
22	B	822	CLA	C3B-C4B-NB	-2.81	107.91	110.52
24	Q	615	DD6	C37-C36-C35	2.81	119.55	114.36
21	B	843	BCR	C27-C26-C25	-2.81	118.66	122.73
22	F	403	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	O	317	DD6	O1-C20-C21	-2.80	111.70	115.06
22	K	605	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	N	607	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	S	605	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	J	105	DD6	C14-C13-C11	-2.80	121.18	125.53
22	B	822	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	S	606	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	V	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	K	605	CLA	C3B-C4B-NB	-2.80	107.92	110.52
22	N	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	V	610	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	L	413	DD6	O1-C20-C19	-2.80	111.28	113.38
24	A	859	DD6	O1-C20-C19	-2.80	111.28	113.38
22	K	602	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	L	408	CLA	C6-C5-C3	-2.80	106.12	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	606	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	P	609	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
24	A	858	DD6	C8-C6-C5	2.79	123.23	118.94
24	U	417	DD6	C9-C10-C11	-2.79	123.33	127.31
24	W	416	DD6	C14-C13-C11	-2.79	121.20	125.53
22	X	403	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	I	607	CLA	C3B-C4B-NB	-2.79	107.93	110.52
22	Q	608	CLA	C3B-C4B-NB	-2.79	107.93	110.52
22	G	605	CLA	C3B-C4B-NB	-2.79	107.93	110.52
24	P	612	DD6	C24-C1-C2	2.79	123.22	118.94
22	A	836	CLA	C3B-C4B-NB	-2.79	107.93	110.52
22	O	305	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	W	414	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	U	417	DD6	C-C1-C2	-2.79	119.02	122.92
22	A	839	CLA	CHB-C4A-NA	2.78	128.36	124.51
24	S	611	DD6	C37-C36-C35	2.78	119.51	114.36
22	X	411	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
24	N	612	DD6	C21-C20-C15	-2.78	117.59	122.26
22	V	610	CLA	C3B-C4B-NB	-2.78	107.93	110.52
22	R	607	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	R	609	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	R	602	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	X	406	CHL	C3D-C4D-CHA	2.78	112.77	108.54
22	V	612	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	G	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	K	609	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	W	411	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	H	308	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	I	606	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	B	839	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	V	609	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	A	841	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	W	412	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	W	413	CLA	C3B-C4B-NB	-2.78	107.94	110.52
22	R	605	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
22	A	803	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
33	A	802	CL0	C1C-CHC-C4B	2.77	124.92	115.73
22	P	610	CLA	CHB-C4A-NA	2.77	128.35	124.51
22	N	611	CLA	C3B-C4B-NB	-2.77	107.94	110.52
22	A	810	CLA	C3B-C4B-NB	-2.77	107.94	110.52
22	R	610	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	O	313	CLA	O2D-CGD-O1D	-2.77	118.42	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	H	304	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	U	415	CLA	C3B-C4B-NB	-2.77	107.95	110.52
24	F	406	DD6	C21-C20-C15	-2.77	117.62	122.26
22	O	306	CLA	C3B-C4B-NB	-2.77	107.95	110.52
22	Q	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	I	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
28	Q	602	LMG	O6-C1-O1	-2.77	103.42	109.97
22	T	602	CLA	C3B-C4B-NB	-2.77	107.95	110.52
22	V	617	CLA	C3B-C4B-NB	-2.77	107.95	110.52
22	X	410	CLA	C3B-C4B-NB	-2.77	107.95	110.52
22	N	606	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
24	W	418	DD6	C37-C36-C35	2.77	119.48	114.36
22	Q	606	CLA	C3B-C4B-NB	-2.77	107.95	110.52
22	U	412	CLA	C3B-C4B-NB	-2.77	107.95	110.52
22	Q	610	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	H	303	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	S	608	CLA	C3B-C4B-NB	-2.76	107.95	110.52
22	A	801	CLA	C2D-C1D-ND	-2.76	108.07	110.10
28	L	401	LMG	O6-C1-O1	-2.76	103.43	109.97
24	J	105	DD6	C12-C11-C10	-2.76	119.05	122.92
22	P	607	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
28	K	618	LMG	O6-C1-O1	-2.76	103.44	109.97
33	A	802	CL0	O2A-CGA-O1A	-2.76	116.63	123.59
21	B	844	BCR	C38-C26-C25	-2.76	121.43	124.53
24	R	613	DD6	C37-C36-C31	-2.76	120.60	124.35
22	X	412	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	W	414	CLA	C3B-C4B-NB	-2.76	107.96	110.52
22	K	609	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	L	415	DD6	C21-C20-C15	-2.76	117.64	122.26
22	H	302	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	Q	607	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
24	O	316	DD6	C33-C34-C35	-2.75	106.53	110.30
22	Q	609	CLA	C3B-C4B-NB	-2.75	107.96	110.52
21	B	843	BCR	C2-C1-C6	2.75	114.72	110.48
24	Q	615	DD6	C33-C34-C35	-2.75	106.54	110.30
24	X	401	DD6	C14-C13-C11	-2.75	121.27	125.53
28	I	614	LMG	O6-C1-O1	-2.75	103.47	109.97
28	I	615	LMG	O6-C1-O1	-2.75	103.47	109.97
22	P	605	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	X	407	CLA	C3B-C4B-NB	-2.75	107.97	110.52
21	B	843	BCR	C8-C9-C10	2.75	123.16	118.94
22	N	601	CLA	O2D-CGD-O1D	-2.75	118.47	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	T	606	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	U	414	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
24	V	615	DD6	C37-C36-C35	2.75	119.44	114.36
22	U	403	CLA	C3B-C4B-NB	-2.75	107.97	110.52
22	A	822	CLA	C3B-C4B-NB	-2.74	107.97	110.52
21	A	850	BCR	C38-C26-C27	2.74	118.88	113.62
22	U	401	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	Q	601	CLA	C3B-C4B-NB	-2.74	107.97	110.52
21	M	101	BCR	C27-C26-C25	-2.74	118.75	122.73
22	B	859	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
22	A	827	CLA	C3B-C4B-NB	-2.74	107.97	110.52
22	T	607	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	G	608	CLA	C3B-C4B-NB	-2.74	107.98	110.52
21	B	801	BCR	C11-C12-C13	-2.74	118.73	126.42
22	A	807	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	O	319	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	F	403	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	H	307	CLA	C3B-C4B-NB	-2.73	107.98	110.52
21	B	801	BCR	C38-C26-C25	-2.73	121.46	124.53
22	O	311	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	U	420	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	I	606	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	I	601	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	A	829	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	B	837	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	S	615	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	T	611	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	U	411	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	B	859	CLA	C3B-C4B-NB	-2.73	107.98	110.52
22	G	606	CLA	C3B-C4B-NB	-2.73	107.98	110.52
24	G	613	DD6	C37-C36-C35	2.73	119.41	114.36
24	A	847	DD6	C4-C3-C2	-2.73	117.89	123.47
24	Q	615	DD6	O1-C20-C21	-2.73	111.79	115.06
22	Q	617	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
22	N	608	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
21	J	103	BCR	C20-C21-C22	-2.72	123.42	127.31
24	T	612	DD6	C4-C5-C6	-2.72	123.42	127.31
22	Q	612	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	A	824	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	W	404	CLA	C3B-C4B-NB	-2.72	107.99	110.52
31	W	422	CHL	C3D-C4D-CHA	2.72	112.67	108.54
22	P	605	CLA	O2D-CGD-O1D	-2.72	118.52	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	I	613	DD6	C32-C31-C36	-2.72	118.79	122.63
22	B	812	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	Q	617	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	T	608	CLA	C3B-C4B-NB	-2.72	107.99	110.52
22	R	609	CLA	CAA-C2A-C3A	-2.72	109.75	116.10
22	B	829	CLA	C3B-C4B-NB	-2.72	108.00	110.52
24	K	615	DD6	C15-C14-C13	-2.71	120.25	125.99
21	B	845	BCR	C20-C21-C22	-2.71	123.44	127.31
22	V	602	CLA	C3B-C4B-NB	-2.71	108.00	110.52
22	L	402	CLA	C3B-C4B-NB	-2.71	108.00	110.52
21	A	851	BCR	C8-C9-C10	2.71	123.10	118.94
22	V	612	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	L	402	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
22	L	409	CLA	C3B-C4B-NB	-2.71	108.00	110.52
22	X	412	CLA	C3B-C4B-NB	-2.71	108.00	110.52
24	Q	614	DD6	C33-C34-C35	-2.71	106.60	110.30
22	O	305	CLA	C1-C2-C3	-2.71	122.37	126.75
24	U	417	DD6	C15-C14-C13	-2.71	120.27	125.99
22	Q	608	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
24	O	317	DD6	C33-C34-C35	-2.70	106.61	110.30
22	U	401	CLA	C3B-C4B-NB	-2.70	108.01	110.52
26	K	619	LHG	O8-C23-C24	2.70	120.38	111.91
22	P	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	P	604	CLA	C3B-C4B-NB	-2.70	108.01	110.52
27	O	322	LMU	O1B-C4'-C3'	2.70	114.45	107.28
24	W	417	DD6	C15-C14-C13	-2.70	120.29	125.99
26	B	848	LHG	O8-C23-C24	2.70	120.37	111.91
28	T	616	LMG	O6-C1-O1	-2.69	103.59	109.97
22	B	825	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	L	417	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	O	310	CLA	CHB-C4A-NA	2.69	128.24	124.51
22	R	601	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	F	406	DD6	C9-C10-C11	-2.69	123.47	127.31
22	N	608	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	R	605	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	R	608	CLA	C3B-C4B-NB	-2.69	108.02	110.52
28	J	101	LMG	O6-C1-O1	-2.69	103.60	109.97
22	B	839	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	K	613	CLA	C3B-C4B-NB	-2.69	108.02	110.52
24	A	847	DD6	C15-C14-C13	-2.69	120.31	125.99
22	X	417	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
22	T	604	CLA	C3B-C4B-NB	-2.69	108.02	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	U	416	DD6	C14-C13-C11	-2.69	121.36	125.53
22	U	410	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	A	823	CLA	C3B-C4B-NB	-2.69	108.02	110.52
22	S	610	CLA	CHB-C4A-NA	2.69	128.22	124.51
22	G	609	CLA	C3B-C4B-NB	-2.68	108.03	110.52
22	L	407	CLA	C3B-C4B-NB	-2.68	108.03	110.52
26	O	318	LHG	O8-C23-C24	2.68	120.33	111.91
22	B	808	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	R	613	DD6	C32-C31-C36	-2.68	118.85	122.63
22	G	607	CLA	C3B-C4B-NB	-2.68	108.03	110.52
22	O	314	CLA	C3B-C4B-NB	-2.68	108.03	110.52
24	X	415	DD6	C9-C10-C11	-2.68	123.49	127.31
22	G	606	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	B	859	CLA	CHB-C4A-NA	2.68	128.22	124.51
31	W	408	CHL	C3D-C4D-CHA	2.68	112.61	108.54
24	F	406	DD6	C3-C2-C1	-2.67	123.49	127.31
21	B	842	BCR	C33-C5-C4	2.67	118.75	113.62
22	Q	613	CLA	CHB-C4A-NA	2.67	128.21	124.51
33	A	802	CL0	CMD-C2D-C3D	2.67	129.68	124.68
22	B	816	CLA	C3B-C4B-NB	-2.67	108.04	110.52
28	A	855	LMG	O6-C1-O1	-2.67	103.65	109.97
24	W	417	DD6	C33-C34-C35	-2.67	106.65	110.30
22	B	808	CLA	C3B-C4B-NB	-2.67	108.04	110.52
22	N	602	CLA	C3B-C4B-NB	-2.67	108.04	110.52
22	R	615	CLA	C3B-C4B-NB	-2.67	108.04	110.52
22	V	611	CLA	C3B-C4B-NB	-2.67	108.04	110.52
24	R	612	DD6	C14-C13-C11	-2.67	121.39	125.53
24	I	613	DD6	C3-C4-C5	-2.67	118.01	123.47
23	B	840	PQN	C11-C12-C13	-2.67	122.35	126.79
24	Q	615	DD6	C10-C9-C8	-2.67	114.90	123.22
31	W	407	CHL	C3D-C4D-CHA	2.67	112.59	108.54
22	K	607	CLA	CHD-C1D-ND	-2.66	122.01	124.45
24	P	613	DD6	C3-C4-C5	-2.66	118.02	123.47
24	Q	615	DD6	C3-C4-C5	-2.66	118.02	123.47
22	S	604	CLA	C3B-C4B-NB	-2.66	108.05	110.52
22	G	610	CLA	C3B-C4B-NB	-2.66	108.05	110.52
26	O	321	LHG	O8-C23-C24	2.66	120.26	111.91
22	B	809	CLA	C3B-C4B-NB	-2.66	108.05	110.52
22	S	606	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	N	612	DD6	C33-C34-C35	-2.66	106.66	110.30
22	W	406	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	A	847	DD6	O1-C20-C19	-2.66	111.39	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	V	605	CHL	C3D-C4D-CHA	2.66	112.58	108.54
24	X	416	DD6	C13-C11-C10	-2.66	114.86	118.94
22	L	403	CLA	C3B-C4B-NB	-2.66	108.05	110.52
22	W	409	CLA	C3B-C4B-NB	-2.66	108.05	110.52
24	O	317	DD6	C37-C36-C31	-2.66	120.74	124.35
22	A	808	CLA	C3B-C4B-NB	-2.66	108.05	110.52
21	A	850	BCR	C11-C10-C9	-2.66	123.52	127.31
24	W	416	DD6	O1-C20-C19	-2.65	111.39	113.38
22	X	408	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	A	858	DD6	C21-C20-C15	-2.65	117.81	122.26
22	S	609	CLA	C3B-C4B-NB	-2.65	108.06	110.52
22	S	610	CLA	C3B-C4B-NB	-2.65	108.06	110.52
26	H	316	LHG	O8-C23-C24	2.65	120.21	111.91
22	A	839	CLA	O1D-CGD-CBD	2.65	129.90	124.48
21	B	843	BCR	C23-C22-C21	2.65	123.00	118.94
22	T	607	CLA	C3B-C4B-NB	-2.64	108.06	110.52
24	G	613	DD6	C9-C10-C11	-2.64	123.54	127.31
26	U	419	LHG	O8-C23-C24	2.64	120.20	111.91
22	V	617	CLA	CHB-C4A-NA	2.64	128.17	124.51
28	N	615	LMG	O6-C1-O1	-2.64	103.72	109.97
31	U	407	CHL	C3D-C4D-CHA	2.64	112.56	108.54
22	O	309	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	A	828	CLA	C3B-C4B-NB	-2.64	108.06	110.52
22	B	833	CLA	C3B-C4B-NB	-2.64	108.07	110.52
28	H	317	LMG	O6-C1-O1	-2.64	103.72	109.97
24	W	416	DD6	C15-C14-C13	-2.64	120.42	125.99
22	I	604	CLA	C3B-C4B-NB	-2.64	108.07	110.52
24	B	841	DD6	C25-C24-C1	-2.63	119.01	126.42
22	K	607	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
22	W	419	CLA	C3B-C4B-NB	-2.63	108.07	110.52
27	K	620	LMU	C1-O1'-C1'	-2.63	109.47	113.84
22	A	817	CLA	C3B-C4B-NB	-2.63	108.07	110.52
22	V	608	CLA	C3B-C4B-NB	-2.63	108.08	110.52
22	B	810	CLA	C3B-C4B-NB	-2.63	108.08	110.52
27	L	420	LMU	C1B-O1B-C4'	-2.63	111.46	117.96
33	A	802	CL0	C4D-CHA-CBD	-2.63	106.18	108.89
22	I	605	CLA	C3B-C4B-NB	-2.63	108.08	110.52
22	N	604	CLA	C3B-C4B-NB	-2.62	108.08	110.52
26	S	613	LHG	O8-C23-C24	2.62	120.14	111.91
22	S	614	CLA	C3B-C4B-NB	-2.62	108.08	110.52
22	U	409	CLA	CHB-C4A-NA	2.62	128.14	124.51
22	B	832	CLA	C3B-C4B-NB	-2.62	108.08	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	K	601	LMG	O6-C1-O1	-2.62	103.77	109.97
24	K	615	DD6	C9-C10-C11	-2.62	123.57	127.31
22	G	611	CLA	C3B-C4B-NB	-2.62	108.09	110.52
26	P	601	LHG	O8-C23-C24	2.62	120.12	111.91
22	A	806	CLA	C3B-C4B-NB	-2.62	108.09	110.52
24	L	415	DD6	C15-C14-C13	-2.62	120.46	125.99
22	N	611	CLA	CBD-CHA-C1A	2.62	131.58	128.50
22	B	824	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	L	404	CLA	C3B-C4B-NB	-2.62	108.09	110.52
24	X	401	DD6	C21-C20-C15	-2.61	117.88	122.26
24	R	613	DD6	C25-C24-C1	-2.61	119.07	126.42
24	B	841	DD6	C33-C34-C35	-2.61	106.72	110.30
22	K	606	CLA	C1-C2-C3	-2.61	122.52	126.75
22	H	311	CLA	C3B-C4B-NB	-2.61	108.09	110.52
22	L	411	CLA	C3B-C4B-NB	-2.61	108.09	110.52
26	Q	616	LHG	O8-C23-C24	2.61	120.10	111.91
24	S	611	DD6	C9-C10-C11	-2.61	123.58	127.31
22	T	605	CLA	C3B-C4B-NB	-2.61	108.09	110.52
22	B	805	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	I	610	CLA	C3B-C4B-NB	-2.61	108.10	110.52
22	S	605	CLA	C3B-C4B-NB	-2.61	108.10	110.52
24	I	612	DD6	C33-C34-C35	-2.61	106.74	110.30
22	A	821	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	I	602	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	I	607	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
22	U	403	CLA	CHB-C4A-NA	2.60	128.11	124.51
27	K	620	LMU	C1B-O1B-C4'	-2.60	111.31	115.33
26	L	416	LHG	O8-C23-C24	2.60	120.07	111.91
22	O	319	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	T	604	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	B	804	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	A	813	CLA	C3B-C4B-NB	-2.60	108.10	110.52
22	H	302	CLA	C3B-C4B-NB	-2.60	108.11	110.52
22	B	804	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	F	404	CLA	CHB-C4A-NA	2.59	128.09	124.51
28	U	423	LMG	O6-C1-O1	-2.59	103.84	109.97
22	V	613	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	A	838	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	B	809	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	X	417	CLA	C1-C2-C3	-2.59	122.57	126.75
24	W	416	DD6	C21-C20-C15	-2.59	117.93	122.26
22	B	814	CLA	C3B-C4B-NB	-2.59	108.12	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	U	408	CHL	C3D-C4D-CHA	2.59	112.47	108.54
24	U	417	DD6	C21-C20-C15	-2.59	117.93	122.26
26	T	614	LHG	O8-C23-C24	2.59	120.02	111.91
22	G	604	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	U	417	DD6	C28-C27-C29	2.58	121.95	116.84
22	B	828	CLA	CMB-C2B-C1B	-2.58	121.44	125.37
22	O	305	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	L	409	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	T	610	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	X	402	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	P	606	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	A	811	CLA	C3B-C4B-NB	-2.58	108.12	110.52
24	A	847	DD6	C3-C2-C1	-2.58	123.63	127.31
22	U	409	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	X	411	CLA	C3B-C4B-NB	-2.58	108.12	110.52
22	A	819	CLA	CHB-C1B-NB	2.58	126.98	124.26
26	N	614	LHG	O8-C23-C24	2.58	119.99	111.91
26	A	846	LHG	O8-C23-C24	2.58	119.99	111.91
22	L	405	CLA	C3B-C4B-NB	-2.57	108.13	110.52
31	X	406	CHL	C4C-CHD-C1D	2.57	124.25	115.73
24	W	418	DD6	C9-C10-C11	-2.57	123.64	127.31
22	G	601	CLA	C3B-C4B-NB	-2.57	108.13	110.52
26	O	323	LHG	O8-C23-C24	2.57	119.98	111.91
22	B	830	CLA	CHB-C1B-NB	2.57	126.98	124.26
22	A	830	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
23	A	843	PQN	C11-C12-C13	-2.57	122.51	126.79
22	A	825	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	B	823	CLA	C3B-C4B-NB	-2.57	108.13	110.52
22	L	404	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	R	601	CLA	C3B-C4B-NB	-2.57	108.13	110.52
26	R	614	LHG	O8-C23-C24	2.57	119.96	111.91
27	A	854	LMU	C1B-O1B-C4'	-2.57	111.62	117.96
22	X	409	CLA	C3B-C4B-NB	-2.56	108.14	110.52
26	W	420	LHG	O8-C23-C24	2.56	119.95	111.91
22	K	610	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	V	601	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	X	408	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	L	408	CLA	C1-C2-C3	-2.56	121.61	126.04
22	P	602	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	N	616	LHG	O8-C23-C24	2.56	119.94	111.91
22	K	602	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	U	414	CLA	C3B-C4B-NB	-2.56	108.14	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	616	LHG	O8-C23-C24	2.56	119.94	111.91
22	O	308	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	P	602	CLA	C3B-C4B-NB	-2.56	108.14	110.52
22	B	811	CLA	CHB-C4A-NA	2.55	128.04	124.51
26	A	845	LHG	O8-C23-C24	2.55	119.92	111.91
24	L	414	DD6	O1-C20-C21	-2.55	112.00	115.06
22	B	825	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	G	613	DD6	C3-C4-C5	-2.55	118.25	123.47
22	A	824	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	T	601	CLA	C3B-C4B-NB	-2.55	108.15	110.52
31	W	408	CHL	C4C-CHD-C1D	2.55	124.18	115.73
22	K	607	CLA	CHB-C1B-NB	2.55	126.95	124.26
22	I	611	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	J	102	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	K	611	CLA	C3B-C4B-NB	-2.55	108.15	110.52
22	I	605	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	A	836	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	Q	618	CLA	C3B-C4B-NB	-2.54	108.15	110.52
22	A	838	CLA	C3B-C4B-NB	-2.54	108.15	110.52
22	N	605	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	A	805	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	K	611	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	I	601	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	A	805	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
26	X	420	LHG	O8-C23-C24	2.54	119.89	111.91
31	W	407	CHL	C4C-CHD-C1D	2.54	124.15	115.73
22	A	825	CLA	CHB-C4A-NA	2.54	128.03	124.51
21	A	850	BCR	C28-C27-C26	-2.54	109.54	114.08
22	A	815	CLA	C3B-C4B-NB	-2.54	108.16	110.52
28	G	616	LMG	O6-C1-O1	-2.54	103.96	109.97
22	H	309	CLA	CHB-C4A-NA	2.54	128.02	124.51
24	I	613	DD6	C21-C20-C15	-2.54	118.01	122.26
21	B	845	BCR	C16-C17-C18	-2.54	123.69	127.31
22	H	307	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	A	833	CLA	C3B-C4B-NB	-2.54	108.16	110.52
31	V	606	CHL	C3D-C4D-CHA	2.54	112.40	108.54
31	V	605	CHL	C4C-CHD-C1D	2.54	124.13	115.73
22	B	824	CLA	C3B-C4B-NB	-2.54	108.16	110.52
24	W	418	DD6	C21-C20-C15	-2.54	118.01	122.26
22	G	602	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	H	312	CLA	C3B-C4B-NB	-2.54	108.16	110.52
22	R	603	CLA	C3B-C4B-NB	-2.54	108.16	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	842	BCR	C38-C26-C27	2.54	118.49	113.62
22	A	801	CLA	O1D-CGD-CBD	2.54	129.67	124.48
22	K	606	CLA	C3B-C4B-NB	-2.53	108.16	110.52
22	A	839	CLA	C3B-C4B-NB	-2.53	108.16	110.52
22	P	610	CLA	O2D-CGD-CBD	2.53	115.77	111.27
21	B	845	BCR	C2-C1-C6	2.53	114.38	110.48
22	L	405	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	P	610	CLA	C3B-C4B-NB	-2.53	108.17	110.52
24	P	613	DD6	C25-C26-C27	-2.53	119.23	126.58
22	B	836	CLA	CHC-C4B-NB	2.53	126.94	124.26
22	A	819	CLA	O2D-CGD-CBD	2.53	115.77	111.27
22	N	605	CLA	C3B-C4B-NB	-2.53	108.17	110.52
24	U	417	DD6	C37-C36-C35	2.53	119.04	114.36
22	H	311	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	A	821	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	V	615	DD6	C21-C20-C15	-2.53	118.02	122.26
22	A	831	CLA	C3B-C4B-NB	-2.53	108.17	110.52
24	A	859	DD6	C33-C34-C35	-2.53	106.84	110.30
22	B	823	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	J	103	BCR	C38-C26-C25	-2.53	121.69	124.53
24	P	613	DD6	C14-C13-C11	-2.53	121.61	125.53
24	J	105	DD6	C9-C8-C6	-2.53	119.32	126.42
27	J	104	LMU	C1B-O1B-C4'	-2.53	111.71	117.96
22	U	413	CLA	CHB-C4A-NA	2.53	128.00	124.51
24	X	414	DD6	C33-C34-C35	-2.53	106.85	110.30
28	H	322	LMG	O6-C1-O1	-2.52	104.00	109.97
22	B	807	CLA	C3B-C4B-NB	-2.52	108.17	110.52
22	S	601	CLA	C3B-C4B-NB	-2.52	108.17	110.52
22	L	406	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	X	419	CLA	C3B-C4B-NB	-2.52	108.18	110.52
24	X	416	DD6	O1-C20-C21	-2.52	112.04	115.06
22	B	805	CLA	C3B-C4B-NB	-2.52	108.18	110.52
22	K	605	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	B	830	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
22	A	834	CLA	C3B-C4B-NB	-2.52	108.18	110.52
22	N	606	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	A	811	CLA	CMB-C2B-C1B	-2.52	121.54	125.37
22	B	821	CLA	C3B-C4B-NB	-2.51	108.18	110.52
22	V	602	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	T	611	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	O	310	CLA	C3B-C4B-NB	-2.51	108.18	110.52
31	U	407	CHL	C4C-CHD-C1D	2.51	124.05	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	821	CLA	C1-C2-C3	-2.51	121.70	126.04
22	S	607	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	R	605	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	X	413	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	A	828	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	S	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	A	842	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	I	608	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	Q	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	Q	605	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	R	607	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	L	408	CLA	CHB-C1B-NB	2.51	126.91	124.26
22	B	824	CLA	O2D-CGD-CBD	2.51	115.73	111.27
24	S	611	DD6	C37-C36-C31	-2.51	120.94	124.35
24	H	314	DD6	C33-C34-C35	-2.51	106.87	110.30
22	N	601	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	N	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	L	412	CLA	C3B-C4B-NB	-2.51	108.19	110.52
22	W	403	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	V	613	CLA	C3B-C4B-NB	-2.50	108.19	110.52
24	F	406	DD6	C25-C26-C27	-2.50	119.31	126.58
22	A	842	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	T	607	CLA	CMB-C2B-C1B	-2.50	121.56	125.37
28	I	614	LMG	O1-C7-C8	-2.50	104.87	110.90
22	G	608	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	P	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	I	606	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	Q	603	CLA	C3B-C4B-NB	-2.50	108.20	110.52
22	R	607	CLA	C3B-C4B-NB	-2.50	108.20	110.52
22	W	410	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	O	304	DGD	O6D-C1D-C2D	-2.50	105.07	110.35
24	P	612	DD6	C37-C36-C35	2.50	118.98	114.36
22	X	402	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	T	606	CLA	CHB-C4A-NA	2.49	127.96	124.51
31	U	408	CHL	C4C-CHD-C1D	2.49	123.99	115.73
22	P	603	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
24	W	417	DD6	C9-C10-C11	-2.49	123.75	127.31
26	O	324	LHG	O8-C23-C24	2.49	119.73	111.91
22	A	826	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	P	613	DD6	C25-C24-C1	-2.49	119.42	126.42
26	B	851	LHG	O8-C23-C24	2.49	119.73	111.91
22	A	814	CLA	CHB-C4A-NA	2.49	127.96	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	H	318	CLA	C3B-C4B-NB	-2.49	108.20	110.52
22	H	308	CLA	C3B-C4B-NB	-2.49	108.20	110.52
24	H	315	DD6	C33-C34-C35	-2.49	106.90	110.30
22	H	305	CLA	C3B-C4B-NB	-2.49	108.21	110.52
22	U	412	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	L	402	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	O	311	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	P	613	DD6	C33-C34-C35	-2.49	106.90	110.30
33	A	802	CL0	C4C-C3C-C2C	-2.49	103.96	113.64
22	T	603	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	K	613	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	V	607	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	P	608	CLA	C3B-C4B-NB	-2.48	108.21	110.52
22	R	606	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	N	603	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	V	601	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	G	601	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	B	829	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	V	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	A	840	CLA	CHC-C4B-NB	2.48	126.88	124.26
22	O	312	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	S	611	DD6	C3-C4-C5	-2.48	118.40	123.47
28	I	615	LMG	C3-C4-C5	-2.48	107.55	110.77
21	B	844	BCR	C28-C27-C26	-2.48	109.65	114.08
22	I	609	CLA	CHB-C4A-NA	2.48	127.94	124.51
28	K	622	LMG	O6-C1-O1	-2.48	104.11	109.97
22	L	411	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	H	313	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	T	609	CLA	C3B-C4B-NB	-2.48	108.22	110.52
22	A	841	CLA	C3B-C4B-NB	-2.47	108.22	110.52
28	B	856	LMG	C40-C39-C38	-2.47	101.86	114.42
22	X	411	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	A	808	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	H	310	CLA	C3B-C4B-NB	-2.47	108.22	110.52
22	R	602	CLA	C3B-C4B-NB	-2.47	108.22	110.52
22	B	835	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	X	405	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	B	842	BCR	C8-C7-C6	-2.47	120.26	127.20
22	P	605	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	Q	601	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	T	613	DD6	C37-C36-C35	2.47	118.93	114.36
22	X	403	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	X	404	CLA	C3B-C4B-NB	-2.47	108.22	110.52
22	A	805	CLA	C3B-C4B-NB	-2.47	108.22	110.52
22	X	410	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	A	811	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	F	405	CLA	C3B-C4B-NB	-2.47	108.22	110.52
22	W	412	CLA	C11-C10-C8	-2.47	107.94	115.92
22	K	609	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	H	308	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	K	604	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	L	407	CLA	CHB-C4A-NA	2.47	127.92	124.51
27	O	320	LMU	C5'-O5'-C1'	2.47	114.78	111.91
22	B	839	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	O	319	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	T	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	V	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	G	605	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	A	827	CLA	CHB-C4A-NA	2.46	127.92	124.51
24	P	613	DD6	O1-C20-C21	-2.46	112.11	115.06
22	O	313	CLA	C3B-C4B-NB	-2.46	108.23	110.52
24	T	613	DD6	C9-C10-C11	-2.46	123.80	127.31
22	H	302	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	B	816	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	R	603	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	V	606	CHL	C4C-CHD-C1D	2.46	123.88	115.73
24	V	614	DD6	C33-C34-C35	-2.46	106.94	110.30
22	G	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	T	609	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	Q	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	T	601	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	S	612	DD6	C33-C34-C35	-2.46	106.94	110.30
22	B	834	CLA	C3B-C4B-NB	-2.46	108.24	110.52
22	B	807	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	N	601	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	A	844	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	W	402	CLA	C3B-C4B-NB	-2.46	108.24	110.52
22	B	818	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	B	828	CLA	C3B-C4B-NB	-2.45	108.24	110.52
22	B	815	CLA	C3B-C4B-NB	-2.45	108.24	110.52
21	B	846	BCR	C7-C8-C9	-2.45	122.53	126.23
22	R	610	CLA	C3B-C4B-NB	-2.45	108.24	110.52
22	B	834	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	S	604	CLA	CHB-C4A-NA	2.45	127.90	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	837	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	832	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	V	607	CLA	C3B-C4B-NB	-2.45	108.24	110.52
22	A	820	CLA	CHB-C1B-NB	2.45	126.85	124.26
21	B	843	BCR	C29-C30-C25	2.45	114.25	110.48
24	K	614	DD6	C33-C34-C35	-2.45	106.95	110.30
22	B	821	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	U	414	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	X	405	CLA	C3B-C4B-NB	-2.45	108.25	110.52
24	R	612	DD6	C33-C34-C35	-2.45	106.96	110.30
22	U	405	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	R	604	CLA	C3B-C4B-NB	-2.44	108.25	110.52
22	A	835	CLA	C3B-C4B-NB	-2.44	108.25	110.52
22	K	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
28	H	317	LMG	C38-C37-C36	-2.44	102.02	114.42
26	G	614	LHG	O8-C23-C24	2.44	119.57	111.91
22	A	824	CLA	O2D-CGD-CBD	2.44	115.61	111.27
22	H	312	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	R	613	DD6	C25-C26-C27	-2.44	119.50	126.58
22	W	419	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	K	620	LMU	O5'-C5'-C4'	2.44	114.35	109.41
22	I	610	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	S	607	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	B	818	CLA	C3B-C4B-NB	-2.44	108.25	110.52
22	K	617	CLA	C3B-C4B-NB	-2.44	108.25	110.52
22	I	611	CLA	CHB-C1B-NB	2.44	126.84	124.26
22	A	815	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
22	W	412	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	B	804	CLA	CMB-C2B-C1B	-2.44	121.66	125.37
22	B	833	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	X	415	DD6	C33-C34-C35	-2.44	106.97	110.30
31	W	422	CHL	C4C-CHD-C1D	2.43	123.80	115.73
24	X	415	DD6	C15-C14-C13	-2.43	120.85	125.99
22	N	609	CLA	C3B-C4B-NB	-2.43	108.26	110.52
23	A	843	PQN	C2M-C2-C3	-2.43	120.43	124.40
22	V	609	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	V	610	CLA	CHB-C4A-NA	2.43	127.88	124.51
24	J	105	DD6	C13-C11-C10	2.43	122.67	118.94
24	J	105	DD6	C25-C26-C27	-2.43	119.52	126.58
22	U	404	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	G	602	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	S	606	CLA	CHB-C4A-NA	2.43	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J	101	LMG	C40-C39-C38	-2.43	102.08	114.42
22	R	615	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	A	812	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	P	612	DD6	C21-C20-C15	-2.43	118.19	122.26
22	G	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	Q	604	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	S	615	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	A	844	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	X	412	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	A	848	BCR	C33-C5-C4	2.43	118.28	113.62
22	V	612	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	L	414	DD6	C21-C20-C15	-2.43	118.19	122.26
22	A	839	CLA	CMB-C2B-C1B	-2.43	121.67	125.37
22	W	409	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	B	811	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	S	608	CLA	CHB-C4A-NA	2.43	127.87	124.51
33	A	802	CL0	C3D-C4D-CHA	2.43	112.23	108.54
22	N	608	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	Q	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	H	310	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	G	606	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	F	403	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	P	613	DD6	C21-C20-C15	-2.42	118.20	122.26
22	G	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	X	404	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	X	421	LMU	C1B-O1B-C4'	-2.42	111.97	117.96
24	G	613	DD6	C21-C20-C15	-2.42	118.20	122.26
22	H	306	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	Q	607	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	W	404	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	O	315	CLA	C1-C2-C3	-2.42	122.84	126.75
22	J	102	CLA	C1-C2-C3	-2.42	122.84	126.75
21	B	801	BCR	C20-C21-C22	-2.42	123.86	127.31
22	A	833	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	O	316	DD6	C15-C14-C13	-2.42	120.88	125.99
24	X	415	DD6	C21-C20-C15	-2.42	118.21	122.26
22	A	822	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	Q	606	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	U	420	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	A	820	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
22	X	407	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	L	415	DD6	C33-C34-C35	-2.41	107.00	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	601	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	B	837	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	P	608	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	B	808	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	V	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	W	414	CLA	CHB-C4A-NA	2.41	127.85	124.51
28	B	856	LMG	O6-C5-C4	2.41	114.07	109.69
22	P	607	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	A	810	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	O	317	DD6	C10-C9-C8	-2.41	115.69	123.22
22	B	803	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	815	CLA	CHB-C1B-NB	2.41	126.81	124.26
24	A	859	DD6	C25-C24-C1	-2.41	119.65	126.42
22	R	610	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	R	608	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	S	602	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	S	603	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	X	414	DD6	C14-C13-C11	-2.41	121.79	125.53
22	G	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	813	CLA	CHB-C1B-NB	2.41	126.81	124.26
22	H	313	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	R	601	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	L	410	CLA	C3B-C4B-NB	-2.41	108.28	110.52
22	N	609	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	P	611	CLA	C3B-C4B-NB	-2.40	108.28	110.52
22	A	823	CLA	CHB-C4A-NA	2.40	127.84	124.51
22	A	801	CLA	CHB-C1B-NB	2.40	126.80	124.26
24	N	612	DD6	C14-C13-C11	-2.40	121.80	125.53
22	U	404	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
22	Q	611	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	P	613	DD6	O1-C20-C19	-2.40	111.58	113.38
24	N	613	DD6	C3-C4-C5	-2.40	118.55	123.47
24	A	847	DD6	C21-C20-C15	-2.40	118.23	122.26
22	G	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	L	413	DD6	C37-C36-C35	2.40	118.81	114.36
28	U	402	LMG	C40-C39-C38	-2.40	102.23	114.42
22	Q	608	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	A	831	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	B	811	CLA	CMB-C2B-C1B	-2.40	121.71	125.37
22	H	305	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	B	846	BCR	C16-C15-C14	-2.40	118.56	123.47
22	X	417	CLA	CMB-C2B-C1B	-2.40	121.71	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	615	DD6	C33-C34-C35	-2.40	107.02	110.30
28	W	401	LMG	C38-C37-C36	-2.40	102.24	114.42
22	G	607	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	H	304	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	W	406	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	H	303	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	K	610	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	U	410	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	K	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	A	841	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	S	611	DD6	C21-C20-C15	-2.40	118.24	122.26
24	A	858	DD6	C13-C11-C10	2.40	122.62	118.94
22	B	802	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
22	A	835	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	B	846	BCR	C11-C10-C9	-2.40	123.89	127.31
28	B	852	LMG	O1-C7-C8	-2.40	105.12	110.90
22	W	405	CLA	CHB-C4A-NA	2.40	127.82	124.51
22	Q	618	CLA	CHB-C4A-NA	2.39	127.82	124.51
21	A	851	BCR	C36-C18-C17	-2.39	119.57	122.92
32	V	616	NEX	C5-C6-C1	2.39	122.07	119.70
24	L	413	DD6	C21-C20-C15	-2.39	118.25	122.26
24	L	415	DD6	C37-C36-C35	2.39	118.79	114.36
24	A	859	DD6	C25-C26-C27	-2.39	119.64	126.58
24	O	316	DD6	C21-C20-C15	-2.39	118.25	122.26
22	I	602	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	O	316	DD6	C14-C13-C11	-2.39	121.82	125.53
28	K	618	LMG	C40-C39-C38	-2.39	102.30	114.42
22	R	606	CLA	C3B-C4B-NB	-2.39	108.30	110.52
24	J	105	DD6	C7-C6-C5	-2.39	119.58	122.92
22	R	611	CLA	C3B-C4B-NB	-2.39	108.30	110.52
24	U	416	DD6	C21-C20-C15	-2.39	118.26	122.26
24	F	406	DD6	C19-C18-C17	2.39	115.38	110.77
22	O	315	CLA	C3B-C4B-NB	-2.39	108.30	110.52
22	A	803	CLA	CHB-C1B-NB	2.39	126.78	124.26
24	Q	614	DD6	C21-C20-C15	-2.39	118.26	122.26
24	L	414	DD6	C33-C34-C35	-2.39	107.04	110.30
22	B	810	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	A	858	DD6	C15-C14-C13	-2.38	120.95	125.99
24	H	314	DD6	C21-C20-C15	-2.38	118.27	122.26
22	A	807	CLA	CHB-C4A-NA	2.38	127.81	124.51
21	B	846	BCR	C10-C11-C12	-2.38	115.78	123.22
24	S	612	DD6	C21-C20-C15	-2.38	118.27	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	603	CLA	CHB-C1B-NB	2.38	126.78	124.26
24	B	841	DD6	C14-C13-C11	-2.38	121.84	125.53
22	I	604	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	U	411	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	B	822	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	I	601	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	L	417	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	V	609	CLA	C1-C2-C3	-2.38	121.93	126.04
22	O	313	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	O	317	DD6	C21-C20-C15	-2.38	118.28	122.26
22	O	307	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	G	612	DD6	C37-C36-C35	2.38	118.76	114.36
22	A	830	CLA	C3B-C4B-NB	-2.38	108.31	110.52
22	T	609	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
28	I	615	LMG	C38-C37-C36	-2.37	102.37	114.42
24	T	612	DD6	C9-C10-C11	-2.37	123.92	127.31
28	G	616	LMG	C40-C39-C38	-2.37	102.37	114.42
22	R	609	CLA	CHB-C4A-NA	2.37	127.80	124.51
22	X	417	CLA	CHD-C1D-ND	-2.37	122.27	124.45
22	W	415	CLA	C3B-C4B-NB	-2.37	108.31	110.52
22	B	819	CLA	C3B-C4B-NB	-2.37	108.31	110.52
30	F	407	SQD	O8-S-C6	-2.37	101.96	105.74
22	Q	617	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	A	832	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	O	308	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	W	418	DD6	C14-C13-C11	-2.37	121.85	125.53
22	U	401	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	X	417	CLA	CHB-C4A-NA	2.37	127.79	124.51
28	W	401	LMG	C40-C39-C38	-2.37	102.40	114.42
22	A	826	CLA	C3B-C4B-NB	-2.37	108.32	110.52
21	M	101	BCR	C20-C19-C18	-2.37	119.77	126.42
24	K	614	DD6	C21-C20-C15	-2.37	118.29	122.26
27	U	421	LMU	C1B-O1B-C4'	-2.37	112.11	117.96
24	V	614	DD6	C4-C3-C2	-2.37	118.63	123.47
22	G	602	CLA	C1-C2-C3	-2.36	121.95	126.04
22	X	409	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	L	408	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
27	B	854	LMU	C1-O1'-C1'	-2.36	109.92	113.84
22	T	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	O	310	CLA	C1-C2-C3	-2.36	121.96	126.04
22	A	806	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	X	401	DD6	C33-C34-C35	-2.36	107.07	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	U	417	DD6	C33-C34-C35	-2.36	107.07	110.30
27	B	857	LMU	C1B-O1B-C4'	-2.36	112.12	117.96
22	B	827	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	W	413	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	W	417	DD6	C21-C20-C15	-2.36	118.31	122.26
21	B	843	BCR	C38-C26-C25	-2.36	121.88	124.53
22	K	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	N	604	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	A	817	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	B	817	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	L	403	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	K	617	CLA	CMB-C2B-C1B	-2.36	121.78	125.37
24	S	612	DD6	C14-C13-C11	-2.35	121.88	125.53
22	H	318	CLA	CHB-C4A-NA	2.35	127.77	124.51
22	J	102	CLA	CHB-C4A-NA	2.35	127.77	124.51
22	B	834	CLA	CMB-C2B-C1B	-2.35	121.78	125.37
22	A	819	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
25	B	847	DGD	O1G-C1A-O1A	-2.35	117.65	123.59
22	L	410	CLA	CHB-C4A-NA	2.35	127.77	124.51
24	F	406	DD6	C4-C3-C2	-2.35	118.66	123.47
22	N	610	CLA	C3B-C4B-NB	-2.35	108.33	110.52
22	U	403	CLA	O2D-CGD-CBD	2.35	115.44	111.27
22	U	415	CLA	CHB-C4A-NA	2.35	127.75	124.51
22	O	305	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	L	408	CLA	C6-C7-C8	-2.34	108.34	115.92
22	U	406	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	I	612	DD6	C14-C13-C11	-2.34	121.90	125.53
22	B	813	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	U	404	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	A	818	CLA	CMB-C2B-C1B	-2.34	121.81	125.37
22	O	315	CLA	CHB-C4A-NA	2.34	127.74	124.51
22	P	606	CLA	CHB-C4A-NA	2.34	127.74	124.51
22	B	803	CLA	O2D-CGD-CBD	2.34	115.42	111.27
22	V	604	CLA	C3B-C4B-NB	-2.34	108.35	110.52
24	F	406	DD6	C24-C1-C2	2.33	122.52	118.94
22	B	820	CLA	O2D-CGD-CBD	2.33	115.42	111.27
22	P	608	CLA	O2D-CGD-CBD	2.33	115.42	111.27
22	Q	611	CLA	C3B-C4B-NB	-2.33	108.35	110.52
22	N	607	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	O	306	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	K	607	CLA	CHB-C4A-NA	2.33	127.74	124.51
22	G	602	CLA	O2A-CGA-O1A	-2.33	117.71	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	815	CLA	CHB-C4A-NA	2.33	127.73	124.51
28	G	616	LMG	C38-C37-C36	-2.33	102.60	114.42
28	I	614	LMG	O1-C1-C2	-2.33	104.67	108.30
22	W	411	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	X	419	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	A	809	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
22	B	812	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	R	602	CLA	CHD-C1D-ND	-2.33	122.32	124.45
24	R	613	DD6	C-C1-C2	-2.33	119.67	122.92
28	J	101	LMG	C38-C37-C36	-2.32	102.62	114.42
25	O	304	DGD	O1G-C1A-O1A	-2.32	117.73	123.59
24	R	613	DD6	C12-C11-C13	2.32	121.74	118.08
28	K	622	LMG	C38-C37-C36	-2.32	102.64	114.42
24	P	613	DD6	C-C1-C2	-2.32	119.67	122.92
22	K	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
28	B	856	LMG	C38-C37-C36	-2.32	102.64	114.42
22	Q	608	CLA	C1-C2-C3	-2.32	123.00	126.75
22	G	604	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
22	H	308	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
22	O	314	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	W	402	CLA	CHB-C4A-NA	2.32	127.71	124.51
22	H	305	CLA	CMB-C2B-C1B	-2.32	121.84	125.37
24	I	613	DD6	O1-C20-C19	-2.31	111.64	113.38
28	L	401	LMG	C38-C37-C36	-2.31	102.68	114.42
22	P	610	CLA	CAA-C2A-C3A	-2.31	110.70	116.10
22	B	828	CLA	CHB-C1B-NB	2.31	126.71	124.26
22	T	605	CLA	CHB-C4A-NA	2.31	127.71	124.51
22	I	611	CLA	CMB-C2B-C1B	-2.31	121.85	125.37
21	M	101	BCR	C16-C15-C14	-2.31	118.74	123.47
24	K	615	DD6	C21-C20-C15	-2.31	118.39	122.26
27	K	620	LMU	C5'-O5'-C1'	2.31	117.05	112.38
27	U	422	LMU	C1B-O1B-C4'	-2.31	112.25	117.96
22	A	840	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	X	413	CLA	C3B-C4B-NB	-2.31	108.38	110.52
22	A	820	CLA	C3B-C4B-NB	-2.31	108.38	110.52
21	A	849	BCR	C1-C6-C5	-2.31	119.36	122.61
24	O	317	DD6	C3-C4-C5	-2.31	118.75	123.47
24	Q	615	DD6	C21-C20-C15	-2.30	118.40	122.26
22	B	802	CLA	O1D-CGD-CBD	2.30	129.20	124.48
28	I	614	LMG	O3-C3-C2	-2.30	105.02	110.35
22	B	802	CLA	CHC-C4B-NB	2.30	126.70	124.26
24	V	614	DD6	C14-C13-C11	-2.30	121.96	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	403	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
22	T	602	CLA	CHB-C4A-NA	2.30	127.70	124.51
22	A	818	CLA	CHB-C4A-NA	2.30	127.70	124.51
30	O	302	SQD	O8-S-C6	-2.30	102.07	105.74
22	T	607	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	I	613	DD6	C25-C24-C1	-2.30	119.95	126.42
22	R	609	CLA	CMB-C2B-C1B	-2.30	121.87	125.37
22	A	840	CLA	C3B-C4B-NB	-2.30	108.38	110.52
22	A	818	CLA	CHC-C4B-NB	2.30	126.69	124.26
22	A	819	CLA	CHB-C4A-NA	2.30	127.69	124.51
21	B	842	BCR	C15-C16-C17	-2.30	118.77	123.47
22	A	814	CLA	C3B-C4B-NB	-2.30	108.39	110.52
23	B	840	PQN	C2M-C2-C3	-2.29	120.66	124.40
22	B	835	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	S	602	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	A	820	CLA	C1-C2-C3	-2.29	122.08	126.04
28	K	618	LMG	C38-C37-C36	-2.29	102.79	114.42
24	L	413	DD6	C33-C34-C35	-2.29	107.17	110.30
24	A	858	DD6	C37-C36-C35	2.29	118.60	114.36
22	B	826	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	U	416	DD6	C33-C34-C35	-2.29	107.17	110.30
22	W	415	CLA	CHC-C4B-NB	2.29	126.68	124.26
22	S	609	CLA	CHB-C4A-NA	2.29	127.68	124.51
22	B	806	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
22	B	836	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
28	K	622	LMG	O3-C3-C2	-2.29	105.06	110.35
24	P	612	DD6	C28-C27-C29	2.29	121.37	116.84
24	T	612	DD6	O1-C20-C21	-2.29	112.31	115.06
22	O	312	CLA	CMB-C2B-C1B	-2.29	121.89	125.37
21	B	845	BCR	C21-C20-C19	-2.29	116.08	123.22
22	A	830	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	L	415	DD6	C25-C26-C27	-2.29	119.94	126.58
24	U	417	DD6	C14-C13-C11	-2.29	121.98	125.53
31	W	422	CHL	C1A-CHA-C4D	2.28	122.79	118.98
28	U	402	LMG	C38-C37-C36	-2.28	102.83	114.42
22	H	304	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
22	A	832	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
24	A	859	DD6	C37-C36-C35	2.28	118.58	114.36
22	I	609	CLA	CMB-C2B-C1B	-2.28	121.89	125.37
22	B	827	CLA	C3B-C4B-NB	-2.28	108.40	110.52
22	A	816	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
21	B	845	BCR	C38-C26-C27	2.28	117.99	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	607	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	A	834	CLA	CHB-C4A-NA	2.28	127.66	124.51
22	P	606	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
24	L	414	DD6	C3-C4-C5	-2.28	118.81	123.47
22	Q	613	CLA	O1D-CGD-CBD	2.28	129.14	124.48
32	U	418	NEX	C5-C6-C1	2.28	121.95	119.70
24	A	847	DD6	C37-C36-C35	2.28	118.57	114.36
21	A	850	BCR	C37-C22-C21	-2.28	119.73	122.92
22	Q	603	CLA	CMB-C2B-C1B	-2.28	121.90	125.37
22	A	806	CLA	O2D-CGD-CBD	2.27	115.31	111.27
22	W	409	CLA	CHB-C1B-NB	2.27	126.67	124.26
22	Q	609	CLA	CHB-C4A-NA	2.27	127.66	124.51
28	B	856	LMG	C42-C41-C40	-2.27	102.88	114.42
22	S	603	CLA	CMB-C2B-C1B	-2.27	121.91	125.37
22	U	405	CLA	C3B-C4B-NB	-2.27	108.41	110.52
24	R	612	DD6	O1-C20-C21	-2.27	112.33	115.06
24	W	418	DD6	C10-C9-C8	-2.27	116.13	123.22
24	G	613	DD6	C-C1-C2	-2.27	119.74	122.92
28	B	856	LMG	O3-C3-C2	-2.27	105.10	110.35
22	A	813	CLA	CHB-C4A-NA	2.27	127.65	124.51
21	B	845	BCR	C33-C5-C6	-2.27	121.98	124.53
22	R	611	CLA	CHB-C4A-NA	2.27	127.65	124.51
28	L	401	LMG	O3-C3-C2	-2.27	105.11	110.35
22	B	817	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	R	605	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	B	831	CLA	CHB-C4A-NA	2.27	127.65	124.51
28	J	101	LMG	O3-C3-C2	-2.27	105.11	110.35
22	N	605	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
21	A	849	BCR	C8-C7-C6	-2.26	120.84	127.20
24	H	315	DD6	C10-C9-C8	-2.26	116.15	123.22
24	L	414	DD6	C10-C9-C8	-2.26	116.15	123.22
22	N	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	S	602	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
22	A	828	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
28	A	855	LMG	C38-C37-C36	-2.26	102.94	114.42
24	U	416	DD6	C28-C27-C29	2.26	121.32	116.84
24	L	415	DD6	C25-C24-C1	-2.26	120.06	126.42
24	O	317	DD6	O1-C20-C19	-2.26	111.69	113.38
24	U	417	DD6	C40-C32-C31	-2.26	106.88	110.47
22	X	411	CLA	CMB-C2B-C1B	-2.26	121.93	125.37
22	B	806	CLA	CHB-C4A-NA	2.26	127.63	124.51
22	R	602	CLA	CHB-C4A-NA	2.26	127.63	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	A	851	BCR	C30-C25-C26	-2.26	119.44	122.61
22	A	839	CLA	CMB-C2B-C3B	2.26	132.05	126.59
24	O	316	DD6	C37-C36-C35	2.25	118.53	114.36
27	H	321	LMU	C1-O1'-C1'	-2.25	110.10	113.84
28	U	423	LMG	O3-C3-C2	-2.25	105.14	110.35
24	A	858	DD6	C33-C34-C35	-2.25	107.22	110.30
24	W	416	DD6	C37-C36-C35	2.25	118.53	114.36
24	T	612	DD6	C10-C9-C8	-2.25	116.19	123.22
28	H	317	LMG	O3-C3-C2	-2.25	105.15	110.35
27	H	321	LMU	C1B-O1B-C4'	-2.25	111.86	115.33
22	A	803	CLA	C1-C2-C3	-2.25	122.15	126.04
22	A	820	CLA	CHB-C4A-NA	2.25	127.62	124.51
28	J	101	LMG	C42-C41-C40	-2.25	103.02	114.42
21	J	103	BCR	C33-C5-C4	2.25	117.93	113.62
22	B	807	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
21	B	801	BCR	C38-C26-C27	2.25	117.93	113.62
21	B	844	BCR	C3-C4-C5	-2.25	110.07	114.08
32	V	616	NEX	C5-C4-C3	2.25	114.40	111.75
24	T	612	DD6	C21-C20-C15	-2.25	118.50	122.26
24	X	414	DD6	C21-C20-C15	-2.24	118.50	122.26
22	P	603	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	X	414	DD6	O1-C20-C21	-2.24	112.37	115.06
24	H	315	DD6	C37-C36-C35	2.24	118.51	114.36
31	W	408	CHL	C1A-CHA-C4D	2.24	122.72	118.98
22	K	608	CLA	C3C-C4C-NC	-2.24	108.06	110.57
22	I	605	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	N	611	CLA	CHD-C1D-ND	-2.24	122.39	124.45
22	O	307	CLA	C3B-C4B-NB	-2.24	108.44	110.52
28	B	856	LMG	O2-C2-C1	-2.24	104.61	110.05
22	S	609	CLA	O2D-CGD-CBD	2.24	115.25	111.27
24	S	611	DD6	O1-C20-C19	-2.24	111.70	113.38
22	A	805	CLA	CHD-C1D-ND	-2.24	122.40	124.45
22	B	824	CLA	CMB-C2B-C1B	-2.24	121.96	125.37
31	W	407	CHL	C1A-CHA-C4D	2.24	122.72	118.98
28	G	616	LMG	O1-C7-C8	-2.24	105.50	110.90
22	W	415	CLA	CHB-C4A-NA	2.24	127.60	124.51
21	B	801	BCR	C16-C17-C18	-2.24	124.12	127.31
28	F	408	LMG	C1-C2-C3	-2.24	105.34	110.00
24	V	615	DD6	C34-C35-C36	-2.23	107.40	111.85
22	A	812	CLA	C3B-C4B-NB	-2.23	108.44	110.52
22	O	309	CLA	C1-C2-C3	-2.23	123.14	126.75
22	B	812	CLA	O2A-CGA-O1A	-2.23	117.95	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	H	304	CLA	CHB-C1B-NB	2.23	126.62	124.26
22	A	820	CLA	CHD-C1D-ND	-2.23	122.40	124.45
24	H	315	DD6	C3-C4-C5	-2.23	118.90	123.47
24	A	847	DD6	C26-C25-C24	-2.23	116.25	123.22
22	A	818	CLA	C3B-C4B-NB	-2.23	108.44	110.52
22	B	828	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	I	613	DD6	C25-C26-C27	-2.23	120.10	126.58
22	B	828	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
28	J	101	LMG	O1-C7-C8	-2.23	105.52	110.90
21	A	851	BCR	C20-C19-C18	-2.23	120.15	126.42
28	Q	602	LMG	O1-C7-C8	-2.23	105.52	110.90
24	G	613	DD6	C25-C26-C27	-2.23	120.11	126.58
28	H	317	LMG	C40-C39-C38	-2.23	103.12	114.42
24	B	841	DD6	C-C1-C2	-2.23	119.80	122.92
22	A	803	CLA	C3B-C4B-NB	-2.23	108.45	110.52
24	G	613	DD6	C40-C32-C31	-2.23	106.93	110.47
28	K	618	LMG	C42-C41-C40	-2.22	103.13	114.42
21	B	846	BCR	C30-C25-C26	-2.22	119.48	122.61
22	B	814	CLA	CHB-C4A-NA	2.22	127.59	124.51
22	B	831	CLA	CMB-C2B-C1B	-2.22	121.98	125.37
24	N	613	DD6	C25-C24-C1	-2.22	120.17	126.42
28	F	408	LMG	O3-C3-C2	-2.22	105.21	110.35
22	B	814	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
24	G	612	DD6	C21-C20-C15	-2.22	118.54	122.26
24	L	413	DD6	C14-C13-C11	-2.22	122.08	125.53
22	G	603	CLA	C3B-C4B-NB	-2.22	108.45	110.52
22	A	832	CLA	C3B-C4B-NB	-2.22	108.45	110.52
22	B	831	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
22	P	609	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	A	822	CLA	CHB-C1B-NB	2.22	126.61	124.26
22	K	608	CLA	O1D-CGD-CBD	2.22	129.03	124.48
24	L	414	DD6	C37-C36-C35	2.22	118.47	114.36
22	W	415	CLA	CHB-C1B-NB	2.22	126.61	124.26
28	W	401	LMG	O3-C3-C2	-2.22	105.22	110.35
22	B	820	CLA	C3B-C4B-NB	-2.22	108.46	110.52
22	A	809	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	V	603	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	K	612	CLA	C3B-C4B-NB	-2.22	108.46	110.52
24	K	614	DD6	C14-C13-C11	-2.22	122.09	125.53
22	B	839	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
24	F	406	DD6	C37-C36-C35	2.21	118.46	114.36
22	L	412	CLA	CHB-C4A-NA	2.21	127.57	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	825	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
22	G	609	CLA	CHB-C1B-NB	2.21	126.60	124.26
27	U	422	LMU	C1-O1'-C1'	-2.21	110.17	113.84
24	H	314	DD6	C4-C3-C2	-2.21	118.94	123.47
28	T	616	LMG	O3-C3-C2	-2.21	105.24	110.35
22	A	829	CLA	C1-C2-C3	-2.21	122.22	126.04
22	Q	605	CLA	CMB-C2B-C1B	-2.21	122.00	125.37
22	Q	604	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	P	613	DD6	C10-C9-C8	-2.21	116.32	123.22
22	A	835	CLA	O2D-CGD-CBD	2.21	115.19	111.27
22	A	808	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
24	O	317	DD6	C40-C32-C31	-2.21	106.96	110.47
21	A	848	BCR	C28-C27-C26	-2.21	110.14	114.08
22	N	610	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
21	B	844	BCR	C21-C20-C19	-2.21	116.33	123.22
22	A	803	CLA	CHB-C4A-NA	2.20	127.56	124.51
28	K	601	LMG	O3-C3-C2	-2.20	105.25	110.35
22	A	801	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
28	G	616	LMG	C42-C41-C40	-2.20	103.23	114.42
22	B	835	CLA	CMB-C2B-C1B	-2.20	122.01	125.37
21	M	101	BCR	C38-C26-C25	-2.20	122.06	124.53
22	B	830	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
22	S	605	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	B	829	CLA	O1D-CGD-CBD	2.20	128.99	124.48
22	B	825	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	H	309	CLA	CHD-C1D-ND	-2.20	122.43	124.45
22	B	838	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	B	818	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
22	A	837	CLA	CHB-C1B-NB	2.20	126.58	124.26
22	W	415	CLA	O1D-CGD-CBD	2.20	128.98	124.48
22	X	409	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
28	H	322	LMG	O3-C3-C2	-2.20	105.27	110.35
22	U	413	CLA	C3B-C4B-NB	-2.20	108.48	110.52
28	K	618	LMG	O3-C3-C2	-2.20	105.27	110.35
24	G	613	DD6	O1-C20-C21	-2.20	112.42	115.06
22	T	603	CLA	C3B-C4B-NB	-2.20	108.48	110.52
24	I	613	DD6	C14-C13-C11	-2.19	122.12	125.53
24	T	613	DD6	C21-C20-C15	-2.19	118.58	122.26
22	P	607	CLA	CMB-C2B-C1B	-2.19	122.03	125.37
22	B	830	CLA	CHC-C4B-NB	2.19	126.58	124.26
24	K	615	DD6	C14-C13-C11	-2.19	122.13	125.53
24	A	847	DD6	C33-C34-C35	-2.19	107.30	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	847	DGD	C3B-C2B-C1B	-2.19	105.65	113.62
22	B	822	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	F	406	DD6	C33-C34-C35	-2.19	107.31	110.30
22	W	403	CLA	C1-C2-C3	-2.19	122.26	126.04
21	B	846	BCR	C2-C1-C6	2.19	113.85	110.48
22	O	310	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
28	Q	602	LMG	O3-C3-C2	-2.19	105.29	110.35
24	W	418	DD6	C32-C31-C36	-2.19	119.55	122.63
22	A	840	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
22	B	815	CLA	CHB-C4A-NA	2.19	127.54	124.51
22	I	611	CLA	O1D-CGD-CBD	2.19	128.96	124.48
31	X	406	CHL	C1A-CHA-C4D	2.19	122.63	118.98
22	O	308	CLA	CMB-C2B-C1B	-2.19	122.04	125.37
24	U	417	DD6	C-C1-C24	2.18	121.52	118.08
28	I	614	LMG	O2-C2-C1	-2.18	104.74	110.05
24	L	414	DD6	C25-C24-C1	-2.18	120.28	126.42
24	N	613	DD6	C37-C36-C35	2.18	118.40	114.36
22	X	409	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
22	B	832	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
31	V	605	CHL	C1A-CHA-C4D	2.18	122.62	118.98
27	O	322	LMU	C3'-C4'-C5'	-2.18	105.92	110.93
28	N	615	LMG	O3-C3-C2	-2.18	105.31	110.35
28	A	855	LMG	O1-C7-C8	-2.18	105.64	110.90
22	A	813	CLA	CHB-C1B-NB	2.18	126.56	124.26
25	O	304	DGD	O5D-C6D-C5D	2.18	113.08	109.05
22	A	839	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	R	610	CLA	CHD-C1D-ND	-2.18	122.45	124.45
33	A	802	CL0	O1D-CGD-CBD	2.18	128.37	124.74
24	O	316	DD6	C4-C3-C2	-2.18	119.01	123.47
22	A	827	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
24	J	105	DD6	O1-C20-C21	-2.18	112.45	115.06
28	J	101	LMG	O2-C2-C1	-2.18	104.76	110.05
22	V	607	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
22	X	410	CLA	CHB-C1B-NB	2.18	126.56	124.26
22	K	612	CLA	CHB-C4A-NA	2.18	127.52	124.51
24	W	418	DD6	O1-C20-C21	-2.18	112.45	115.06
21	B	846	BCR	C38-C26-C25	-2.18	122.08	124.53
28	N	615	LMG	O1-C7-C8	-2.18	105.65	110.90
22	H	308	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
21	B	801	BCR	C35-C13-C14	-2.18	119.88	122.92
24	L	415	DD6	O1-C20-C21	-2.17	112.45	115.06
24	W	417	DD6	C37-C36-C35	2.17	118.38	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	F	403	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
22	K	610	CLA	CHB-C1B-NB	2.17	126.56	124.26
22	A	803	CLA	C2D-C1D-ND	-2.17	108.50	110.10
22	K	617	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	I	609	CLA	C3B-C4B-NB	-2.17	108.50	110.52
22	A	816	CLA	CHD-C1D-ND	-2.17	122.46	124.45
24	W	417	DD6	C14-C13-C11	-2.17	122.16	125.53
24	P	613	DD6	C37-C36-C35	2.17	118.38	114.36
22	R	604	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	I	603	CLA	CHB-C4A-NA	2.17	127.52	124.51
22	S	604	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
22	S	606	CLA	C1-C2-C3	-2.17	123.24	126.75
28	T	616	LMG	O2-C2-C1	-2.17	104.77	110.05
22	R	611	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	A	803	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	A	833	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	L	410	CLA	CHB-C1B-NB	2.17	126.56	124.26
22	I	602	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	R	612	DD6	C37-C36-C35	2.17	118.38	114.36
24	K	615	DD6	C41-C32-C31	-2.17	107.02	110.47
22	B	817	CLA	C3B-C4B-NB	-2.17	108.50	110.52
28	H	319	LMG	O3-C3-C2	-2.17	105.33	110.35
31	V	606	CHL	C1A-CHA-C4D	2.17	122.60	118.98
28	B	852	LMG	O2-C2-C1	-2.17	104.78	110.05
31	U	407	CHL	C1A-CHA-C4D	2.17	122.60	118.98
24	T	612	DD6	C37-C36-C35	2.17	118.37	114.36
24	T	612	DD6	C14-C13-C11	-2.17	122.17	125.53
22	Q	605	CLA	C3B-C4B-NB	-2.17	108.50	110.52
22	K	612	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
28	B	852	LMG	O3-C3-C2	-2.16	105.34	110.35
28	Q	602	LMG	O2-C2-C1	-2.16	104.79	110.05
22	I	602	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
22	X	405	CLA	CHD-C1D-ND	-2.16	122.47	124.45
31	U	408	CHL	C1A-CHA-C4D	2.16	122.59	118.98
22	V	602	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	O	312	CLA	CHB-C1B-NB	2.16	126.54	124.26
22	S	603	CLA	CHB-C1B-NB	2.16	126.54	124.26
22	A	841	CLA	CHC-C4B-NB	2.16	126.54	124.26
22	A	829	CLA	CHB-C4A-NA	2.16	127.50	124.51
21	B	801	BCR	C4-C5-C6	-2.16	119.60	122.73
28	K	618	LMG	O2-C2-C1	-2.16	104.81	110.05
22	T	604	CLA	O2A-CGA-O1A	-2.16	118.15	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	603	CLA	CHB-C1B-NB	2.16	126.54	124.26
22	F	405	CLA	CHB-C4A-NA	2.16	127.49	124.51
22	A	824	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
22	K	612	CLA	CHD-C1D-ND	-2.16	122.47	124.45
22	A	808	CLA	CHB-C1B-NB	2.16	126.54	124.26
24	S	611	DD6	C25-C24-C1	-2.16	120.36	126.42
28	W	401	LMG	C42-C41-C40	-2.15	103.49	114.42
22	K	617	CLA	CHB-C1B-NB	2.15	126.54	124.26
22	L	412	CLA	CHB-C1B-NB	2.15	126.54	124.26
22	Q	608	CLA	CHB-C1B-NB	2.15	126.54	124.26
21	A	851	BCR	C10-C11-C12	-2.15	116.50	123.22
22	F	404	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
22	A	844	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
22	A	852	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
22	O	308	CLA	CHB-C1B-NB	2.15	126.54	124.26
24	X	401	DD6	C4-C3-C2	-2.15	119.06	123.47
22	N	602	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
22	Q	609	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	R	612	DD6	C21-C20-C15	-2.15	118.66	122.26
28	A	855	LMG	O3-C3-C2	-2.15	105.38	110.35
22	F	404	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	W	409	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
22	Q	605	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	K	604	CLA	CMB-C2B-C1B	-2.15	122.09	125.37
22	I	603	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	A	824	CLA	C1-C2-C3	-2.15	122.33	126.04
22	A	840	CLA	C1-C2-C3	-2.15	122.33	126.04
22	A	815	CLA	CHB-C1B-NB	2.15	126.53	124.26
22	G	603	CLA	CHB-C1B-NB	2.15	126.53	124.26
24	G	612	DD6	C14-C13-C11	-2.15	122.20	125.53
21	B	845	BCR	C33-C5-C4	2.15	117.74	113.62
22	R	607	CLA	CHC-C4B-NB	2.14	126.53	124.26
22	X	402	CLA	CHB-C1B-NB	2.14	126.53	124.26
22	A	816	CLA	CHB-C4A-NA	2.14	127.48	124.51
22	B	816	CLA	CHD-C1D-ND	-2.14	122.48	124.45
24	V	614	DD6	C21-C20-C15	-2.14	118.67	122.26
22	B	826	CLA	CHD-C1D-ND	-2.14	122.49	124.45
22	N	610	CLA	C1-C2-C3	-2.14	122.34	126.04
22	H	318	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
22	R	609	CLA	C3B-C4B-NB	-2.14	108.53	110.52
22	B	834	CLA	CHB-C1B-NB	2.14	126.52	124.26
28	H	317	LMG	O2-C2-C1	-2.14	104.85	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	I	601	CLA	CHB-C1B-NB	2.14	126.52	124.26
28	F	408	LMG	O2-C2-C1	-2.14	104.85	110.05
32	U	418	NEX	C5-C4-C3	2.14	114.28	111.75
21	B	846	BCR	C34-C9-C8	2.14	121.44	118.08
22	T	603	CLA	CHB-C1B-NB	2.14	126.52	124.26
24	R	613	DD6	C21-C20-C15	-2.14	118.68	122.26
22	B	812	CLA	C1-C2-C3	-2.14	122.35	126.04
21	M	101	BCR	C3-C4-C5	-2.13	110.27	114.08
28	K	622	LMG	O2-C2-C1	-2.13	104.86	110.05
22	H	311	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	P	611	CLA	O1D-CGD-CBD	2.13	128.85	124.48
22	S	605	CLA	CHC-C4B-NB	2.13	126.52	124.26
22	A	811	CLA	CHB-C1B-NB	2.13	126.52	124.26
24	O	317	DD6	C25-C26-C27	-2.13	120.39	126.58
22	A	810	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
21	B	801	BCR	C34-C9-C10	-2.13	119.94	122.92
22	B	827	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	L	403	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	A	818	CLA	CHB-C1B-NB	2.13	126.51	124.26
22	T	606	CLA	C1-C2-C3	-2.13	123.30	126.75
28	U	402	LMG	O3-C3-C2	-2.13	105.42	110.35
28	L	401	LMG	O1-C7-C8	-2.13	105.76	110.90
22	A	819	CLA	O1D-CGD-CBD	2.13	128.84	124.48
22	B	815	CLA	CHC-C4B-NB	2.13	126.51	124.26
25	F	401	DGD	O2G-C1B-O1B	-2.13	118.56	123.70
22	A	823	CLA	CHB-C1B-NB	2.13	126.51	124.26
24	K	614	DD6	C40-C32-C31	-2.13	107.08	110.47
24	G	613	DD6	C10-C9-C8	-2.13	116.57	123.22
28	W	401	LMG	O7-C10-O9	-2.13	118.56	123.70
22	B	830	CLA	CHB-C4A-NA	2.13	127.45	124.51
28	H	322	LMG	O2-C2-C1	-2.13	104.88	110.05
22	A	816	CLA	CHB-C1B-NB	2.13	126.51	124.26
28	K	601	LMG	O7-C10-O9	-2.13	118.56	123.70
22	R	601	CLA	CHD-C1D-ND	-2.13	122.50	124.45
22	A	825	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
27	O	303	LMU	C1B-O1B-C4'	-2.12	112.71	117.96
22	O	319	CLA	CHD-C1D-ND	-2.12	122.50	124.45
24	A	847	DD6	O1-C20-C21	-2.12	112.51	115.06
22	G	608	CLA	CHB-C1B-NB	2.12	126.50	124.26
31	W	408	CHL	C1-C2-C3	-2.12	122.37	126.04
24	X	416	DD6	C32-C31-C36	-2.12	119.64	122.63
24	L	414	DD6	C25-C26-C27	-2.12	120.42	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	831	CLA	C3B-C4B-NB	-2.12	108.55	110.52
22	B	838	CLA	C3B-C4B-NB	-2.12	108.55	110.52
22	H	311	CLA	CHB-C1B-NB	2.12	126.50	124.26
22	B	839	CLA	CHB-C1B-NB	2.12	126.50	124.26
22	T	607	CLA	CHB-C1B-NB	2.12	126.50	124.26
22	R	615	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
24	G	613	DD6	C25-C24-C1	-2.12	120.46	126.42
22	B	805	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	X	412	CLA	CHB-C1B-NB	2.12	126.50	124.26
24	V	614	DD6	C37-C36-C35	2.12	118.28	114.36
22	K	612	CLA	CHB-C1B-NB	2.12	126.50	124.26
22	N	603	CLA	CHB-C1B-NB	2.12	126.50	124.26
28	K	601	LMG	O2-C2-C1	-2.12	104.90	110.05
24	W	418	DD6	C3-C4-C5	-2.12	119.14	123.47
24	R	613	DD6	C7-C6-C8	2.12	121.41	118.08
22	W	403	CLA	CHB-C1B-NB	2.12	126.50	124.26
22	B	827	CLA	CHD-C1D-ND	-2.12	122.51	124.45
22	S	606	CLA	CHD-C1D-ND	-2.12	122.51	124.45
22	X	403	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
27	O	322	LMU	O1'-C1'-C2'	2.12	111.61	108.30
22	A	830	CLA	C1-C2-C3	-2.12	122.38	126.04
22	A	810	CLA	O2D-CGD-CBD	2.12	115.03	111.27
22	Q	603	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	V	615	DD6	C25-C26-C27	-2.12	120.44	126.58
22	N	603	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
22	L	408	CLA	CHB-C4A-NA	2.11	127.44	124.51
22	W	402	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	B	837	CLA	CHB-C1B-NB	2.11	126.50	124.26
22	A	818	CLA	C1-C2-C3	-2.11	122.39	126.04
22	K	608	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	K	606	CLA	CHD-C1D-ND	-2.11	122.51	124.45
22	L	410	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	V	603	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
22	G	607	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	W	411	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	A	811	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	U	411	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	N	606	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	T	604	CLA	CHD-C1D-ND	-2.11	122.51	124.45
22	O	306	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	Q	611	CLA	CMB-C2B-C1B	-2.11	122.15	125.37
24	Q	615	DD6	C12-C11-C13	2.11	121.40	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	312	CLA	C3B-C4B-NB	-2.11	108.56	110.52
22	G	603	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
24	N	612	DD6	C37-C36-C35	2.11	118.26	114.36
28	W	401	LMG	O2-C2-C1	-2.11	104.92	110.05
22	I	611	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	A	817	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
22	W	405	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	X	411	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	A	811	CLA	CMB-C2B-C3B	2.11	131.69	126.59
28	A	855	LMG	O2-C2-C1	-2.11	104.93	110.05
22	B	825	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
25	O	304	DGD	C3D-C4D-C5D	2.11	114.00	110.24
22	B	814	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	G	610	CLA	CHB-C1B-NB	2.11	126.49	124.26
22	G	602	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
22	A	820	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
24	I	613	DD6	C10-C9-C8	-2.11	116.64	123.22
24	N	613	DD6	C33-C34-C35	-2.11	107.42	110.30
22	W	415	CLA	C2D-C1D-ND	-2.10	108.55	110.10
22	H	312	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	X	410	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
24	K	614	DD6	C4-C3-C2	-2.10	119.16	123.47
24	V	614	DD6	O1-C20-C21	-2.10	112.53	115.06
22	P	605	CLA	CHD-C1D-ND	-2.10	122.52	124.45
22	V	602	CLA	CHD-C1D-ND	-2.10	122.52	124.45
22	A	801	CLA	CAC-C3C-C4C	2.10	127.54	124.81
22	T	603	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
24	Q	615	DD6	C7-C6-C8	2.10	121.39	118.08
22	O	314	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	O	308	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
22	R	607	CLA	C1-C2-C3	-2.10	122.41	126.04
22	O	305	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
22	A	838	CLA	C1-C2-C3	-2.10	122.41	126.04
22	A	833	CLA	CMB-C2B-C1B	-2.10	122.17	125.37
22	N	611	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	Q	604	CLA	CHC-C4B-NB	2.10	126.48	124.26
22	R	610	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	B	821	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	R	608	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
28	U	423	LMG	O2-C2-C1	-2.10	104.95	110.05
22	A	804	CLA	CHD-C1D-ND	-2.10	122.53	124.45
22	T	602	CLA	CHB-C1B-NB	2.10	126.48	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	829	CLA	C3B-C4B-NB	-2.10	108.57	110.52
24	H	314	DD6	C37-C36-C35	2.10	118.24	114.36
22	G	606	CLA	CHB-C1B-NB	2.10	126.48	124.26
21	B	844	BCR	C33-C5-C4	2.10	117.64	113.62
22	W	410	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	A	833	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	S	608	CLA	O2A-CGA-O1A	-2.09	118.08	123.30
24	X	415	DD6	C14-C13-C11	-2.09	122.28	125.53
22	A	828	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	H	311	CLA	C1-C2-C3	-2.09	122.42	126.04
22	F	403	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	R	613	DD6	C9-C10-C11	-2.09	124.32	127.31
22	S	605	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	T	602	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	O	317	DD6	C-C1-C2	-2.09	119.99	122.92
24	N	612	DD6	C4-C3-C2	-2.09	119.19	123.47
22	B	818	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	Q	605	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	R	610	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
28	N	615	LMG	O2-C2-C1	-2.09	104.97	110.05
22	W	405	CLA	C3B-C4B-NB	-2.09	108.58	110.52
22	B	805	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	A	809	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	X	401	DD6	C7-C6-C5	-2.09	120.00	122.92
28	G	616	LMG	O3-C3-C2	-2.09	105.52	110.35
27	O	320	LMU	C1B-O1B-C4'	-2.09	111.03	115.20
22	Q	613	CLA	C2D-C1D-ND	-2.09	108.56	110.10
22	K	602	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	B	826	CLA	C3B-C4B-NB	-2.09	108.58	110.52
26	A	845	LHG	C26-C25-C24	2.09	120.70	113.19
24	H	315	DD6	C21-C20-C15	-2.09	118.76	122.26
24	H	315	DD6	C9-C10-C11	-2.09	124.33	127.31
22	X	407	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	W	411	CLA	C1-C2-C3	-2.09	122.43	126.04
22	B	835	CLA	CHD-C1D-ND	-2.09	122.53	124.45
22	O	315	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	A	803	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
22	N	607	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
22	N	610	CLA	CHC-C4B-NB	2.09	126.47	124.26
22	A	826	CLA	CMB-C2B-C1B	-2.09	122.19	125.37
22	B	833	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	R	605	CLA	CHD-C1D-ND	-2.08	122.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	847	DD6	C7-C6-C5	-2.08	120.00	122.92
24	L	414	DD6	C9-C10-C11	-2.08	124.34	127.31
22	A	813	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	I	603	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	A	852	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	T	607	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	J	105	DD6	C4-C3-C2	-2.08	119.21	123.47
21	J	103	BCR	C38-C26-C27	2.08	117.62	113.62
22	Q	607	CLA	CHB-C1B-NB	2.08	126.46	124.26
24	L	415	DD6	C41-C32-C31	-2.08	107.16	110.47
22	K	607	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	K	620	LMU	C5'-C4'-C3'	2.08	112.51	109.40
24	V	615	DD6	C14-C13-C11	-2.08	122.30	125.53
22	A	817	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
22	Q	605	CLA	CHB-C1B-NB	2.08	126.46	124.26
22	B	836	CLA	CHB-C4A-NA	2.08	127.39	124.51
22	I	611	CLA	C2D-C1D-ND	-2.08	108.57	110.10
22	N	606	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	A	825	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	W	406	CLA	CHB-C1B-NB	2.08	126.46	124.26
22	L	411	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	S	602	CLA	CHD-C1D-ND	-2.08	122.54	124.45
22	Q	611	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
24	I	613	DD6	O1-C20-C21	-2.08	112.57	115.06
26	S	613	LHG	C26-C25-C24	2.08	120.66	113.19
22	G	602	CLA	CHD-C1D-ND	-2.08	122.55	124.45
22	B	824	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	H	305	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	W	405	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
21	B	843	BCR	C10-C11-C12	-2.08	116.74	123.22
22	T	609	CLA	CHB-C1B-NB	2.08	126.45	124.26
22	U	409	CLA	CHB-C1B-NB	2.08	126.45	124.26
22	K	607	CLA	O2A-C1-C2	-2.08	103.18	108.64
22	S	608	CLA	CHD-C1D-ND	-2.08	122.55	124.45
22	B	835	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	V	608	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	X	405	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	R	603	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	K	608	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
22	K	604	CLA	CHC-C4B-NB	2.07	126.45	124.26
22	A	806	CLA	CHB-C1B-NB	2.07	126.45	124.26
24	B	841	DD6	C37-C36-C35	2.07	118.19	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	602	CLA	C1-C2-C3	-2.07	122.46	126.04
28	H	317	LMG	C42-C41-C40	-2.07	103.91	114.42
21	M	101	BCR	C37-C22-C21	-2.07	120.02	122.92
22	A	829	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	K	607	CLA	O1D-CGD-CBD	2.07	128.72	124.48
22	H	306	CLA	CHB-C1B-NB	2.07	126.45	124.26
22	V	602	CLA	CHC-C4B-NB	2.07	126.45	124.26
22	B	831	CLA	CHB-C1B-NB	2.07	126.45	124.26
22	K	613	CLA	CHB-C1B-NB	2.07	126.45	124.26
28	B	856	LMG	O1-C7-C8	-2.07	105.91	110.90
22	B	819	CLA	CHC-C4B-NB	2.07	126.45	124.26
22	B	804	CLA	C1-C2-C3	-2.07	122.47	126.04
22	B	802	CLA	CHB-C4A-NA	2.07	127.37	124.51
24	R	612	DD6	O1-C20-C19	-2.07	111.83	113.38
24	N	613	DD6	O1-C20-C21	-2.07	112.58	115.06
22	N	607	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
22	V	609	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	H	302	CLA	CHD-C1D-ND	-2.07	122.56	124.45
22	W	412	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	O	307	CLA	CHB-C1B-NB	2.07	126.44	124.26
24	N	613	DD6	C25-C26-C27	-2.06	120.58	126.58
22	W	410	CLA	CHB-C1B-NB	2.06	126.44	124.26
22	A	831	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
22	A	852	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
22	B	859	CLA	CHD-C1D-ND	-2.06	122.56	124.45
28	K	618	LMG	O1-C1-C2	-2.06	105.08	108.30
22	L	403	CLA	CHB-C1B-NB	2.06	126.44	124.26
22	W	404	CLA	CHB-C1B-NB	2.06	126.44	124.26
28	G	616	LMG	O2-C2-C1	-2.06	105.04	110.05
22	O	312	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	A	849	BCR	C4-C5-C6	-2.06	119.74	122.73
28	K	622	LMG	O1-C7-C8	-2.06	105.92	110.90
22	B	831	CLA	CHC-C4B-NB	2.06	126.44	124.26
22	X	407	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	G	603	CLA	O2D-CGD-CBD	2.06	114.93	111.27
22	A	837	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	W	403	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	A	815	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	B	812	CLA	CHB-C1B-NB	2.06	126.44	124.26
22	A	803	CLA	CHC-C4B-NB	2.06	126.44	124.26
28	H	319	LMG	O7-C10-O9	-2.06	118.72	123.70
22	T	606	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	X	412	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
24	Q	615	DD6	C-C1-C2	-2.06	120.04	122.92
22	S	615	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
28	H	317	LMG	O1-C7-C8	-2.06	105.94	110.90
22	N	606	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	A	801	CLA	CHB-C4A-NA	2.06	127.36	124.51
22	R	615	CLA	C1-C2-C3	-2.06	122.49	126.04
24	Q	614	DD6	C37-C36-C35	2.06	118.17	114.36
22	B	816	CLA	CHB-C1B-NB	2.06	126.43	124.26
22	I	606	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	X	403	CLA	CHB-C1B-NB	2.06	126.43	124.26
22	Q	601	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	R	601	CLA	C1-C2-C3	-2.05	122.49	126.04
22	L	408	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	A	822	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
24	Q	614	DD6	C14-C13-C11	-2.05	122.34	125.53
22	X	409	CLA	C1-C2-C3	-2.05	122.49	126.04
22	X	419	CLA	CHB-C1B-NB	2.05	126.43	124.26
22	A	809	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	A	827	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	B	828	CLA	CMB-C2B-C3B	2.05	131.56	126.59
22	L	402	CLA	CHB-C1B-NB	2.05	126.43	124.26
22	T	605	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	A	804	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
22	H	304	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	R	606	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	B	834	CLA	CMB-C2B-C3B	2.05	131.56	126.59
22	A	814	CLA	CHD-C1D-ND	-2.05	122.57	124.45
24	G	613	DD6	C14-C13-C11	-2.05	122.35	125.53
22	X	417	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
24	L	415	DD6	C12-C11-C10	-2.05	120.05	122.92
22	S	607	CLA	CHD-C1D-ND	-2.05	122.57	124.45
24	I	612	DD6	C21-C20-C15	-2.05	118.83	122.26
22	O	311	CLA	CHD-C1D-ND	-2.05	122.57	124.45
24	L	413	DD6	C4-C3-C2	-2.05	119.28	123.47
22	V	604	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
22	P	605	CLA	CHB-C1B-NB	2.05	126.42	124.26
22	A	805	CLA	CHC-C4B-NB	2.05	126.42	124.26
22	A	836	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
22	I	610	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	O	305	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	X	402	CLA	CHD-C1D-ND	-2.04	122.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	N	612	DD6	C28-C27-C29	2.04	120.89	116.84
24	T	613	DD6	C14-C13-C11	-2.04	122.36	125.53
22	I	602	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	P	610	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	U	404	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	V	607	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	N	609	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	H	303	CLA	CHD-C1D-ND	-2.04	122.58	124.45
28	L	401	LMG	O2-C2-C1	-2.04	105.08	110.05
22	H	304	CLA	CMB-C2B-C3B	2.04	131.53	126.59
22	A	801	CLA	CMB-C2B-C1B	-2.04	122.26	125.37
22	A	821	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	B	851	LHG	C26-C25-C24	2.04	120.53	113.19
24	S	612	DD6	C37-C36-C35	2.04	118.14	114.36
22	B	822	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	V	601	CLA	CHB-C1B-NB	2.04	126.42	124.26
24	L	414	DD6	C-C1-C2	-2.04	120.06	122.92
22	U	413	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	X	404	CLA	CHB-C1B-NB	2.04	126.42	124.26
26	K	616	LHG	C26-C25-C24	2.04	120.52	113.19
22	I	611	CLA	CHC-C4B-NB	2.04	126.42	124.26
22	N	602	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	S	609	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	O	315	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	B	809	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
28	Q	602	LMG	O1-C1-C2	-2.04	105.12	108.30
22	F	404	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	A	817	CLA	CHB-C1B-NB	2.04	126.42	124.26
22	A	816	CLA	C2D-C1D-ND	-2.04	108.60	110.10
22	I	602	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	T	607	CLA	CMB-C2B-C3B	2.04	131.52	126.59
22	H	303	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	A	804	CLA	C3B-C4B-NB	-2.04	108.62	110.52
22	U	404	CLA	CMB-C2B-C3B	2.04	131.52	126.59
24	A	858	DD6	C25-C26-C27	-2.04	120.67	126.58
22	T	605	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	U	401	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	S	604	CLA	CHB-C1B-NB	2.04	126.41	124.26
26	O	318	LHG	C26-C25-C24	2.04	120.51	113.19
22	L	406	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	I	605	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
21	B	846	BCR	C8-C7-C6	-2.04	121.48	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	U	403	CLA	CHB-C1B-NB	2.04	126.41	124.26
22	N	603	CLA	C3B-C4B-NB	-2.04	108.63	110.52
22	U	401	CLA	CHD-C1D-ND	-2.03	122.58	124.45
24	K	614	DD6	C26-C25-C24	-2.03	116.87	123.22
25	O	304	DGD	C6D-O5D-C1E	-2.03	109.76	113.74
21	B	844	BCR	C15-C16-C17	-2.03	119.31	123.47
21	B	846	BCR	C38-C26-C27	2.03	117.52	113.62
22	G	603	CLA	CHC-C4B-NB	2.03	126.41	124.26
22	I	605	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	W	414	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	A	807	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	A	837	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	A	852	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	U	414	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	O	311	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	W	414	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	V	608	CLA	CHC-C4B-NB	2.03	126.41	124.26
22	F	403	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	G	601	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	806	CLA	CMB-C2B-C3B	2.03	131.51	126.59
22	H	309	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	I	604	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	V	610	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	Q	617	CLA	C1-C2-C3	-2.03	122.53	126.04
22	X	408	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	R	604	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
22	A	838	CLA	O2D-CGD-CBD	2.03	114.88	111.27
22	B	811	CLA	CMB-C2B-C3B	2.03	131.50	126.59
22	X	417	CLA	CMB-C2B-C3B	2.03	131.50	126.59
22	T	611	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	L	404	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	U	413	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
22	A	805	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
22	F	404	CLA	C2D-C1D-ND	-2.03	108.61	110.10
22	L	408	CLA	C11-C10-C8	-2.03	109.36	115.92
22	A	812	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	A	823	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	L	404	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	A	827	CLA	CHB-C1B-NB	2.03	126.40	124.26
24	T	613	DD6	C33-C34-C35	-2.03	107.53	110.30
22	L	409	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	I	601	CLA	O2A-CGA-O1A	-2.03	118.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	602	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	V	610	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	A	836	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	O	306	CLA	CHC-C4B-NB	2.03	126.40	124.26
22	Q	604	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	B	812	CLA	CMB-C2B-C1B	-2.03	122.28	125.37
27	L	420	LMU	C1-O1'-C1'	-2.03	110.02	113.73
22	R	604	CLA	O2A-CGA-O1A	-2.03	118.25	123.30
22	B	810	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	P	602	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	P	604	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	803	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	B	830	CLA	O2D-CGD-CBD	2.03	114.87	111.27
24	L	415	DD6	C9-C8-C6	-2.03	120.72	126.42
22	X	407	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	B	838	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	G	611	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	Q	617	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	S	615	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	K	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	V	612	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	K	602	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
22	B	838	CLA	CHC-C4B-NB	2.02	126.40	124.26
22	P	604	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	H	311	CLA	CHD-C1D-ND	-2.02	122.59	124.45
24	X	414	DD6	C4-C3-C2	-2.02	119.33	123.47
21	A	850	BCR	C20-C19-C18	-2.02	120.73	126.42
22	T	602	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
22	H	310	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	P	603	CLA	C3B-C4B-NB	-2.02	108.64	110.52
22	H	313	CLA	O2D-CGD-CBD	2.02	114.86	111.27
24	K	614	DD6	O1-C20-C21	-2.02	112.63	115.06
22	A	832	CLA	CMB-C2B-C3B	2.02	131.49	126.59
22	B	813	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	A	812	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	A	844	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	L	411	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	U	415	CLA	CHB-C1B-NB	2.02	126.40	124.26
24	S	611	DD6	C10-C9-C8	-2.02	116.91	123.22
21	B	846	BCR	C28-C27-C26	-2.02	110.47	114.08
22	W	411	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
24	S	611	DD6	C-C1-C2	-2.02	120.09	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	G	604	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	H	305	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	U	406	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	K	617	CLA	CMB-C2B-C3B	2.02	131.48	126.59
22	R	603	CLA	CHB-C1B-NB	2.02	126.39	124.26
22	A	844	CLA	C1-C2-C3	-2.02	122.55	126.04
22	R	604	CLA	CHB-C4A-NA	2.02	127.30	124.51
22	Q	608	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	R	607	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	W	413	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	N	613	DD6	C-C1-C2	-2.02	120.10	122.92
25	B	847	DGD	C2G-O2G-C1B	-2.02	112.82	117.79
24	H	314	DD6	C14-C13-C11	-2.02	122.40	125.53
22	B	814	CLA	CHC-C4B-NB	2.02	126.39	124.26
22	L	411	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	L	417	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	U	420	CLA	CHB-C1B-NB	2.02	126.39	124.26
24	N	613	DD6	C12-C11-C10	-2.02	120.10	122.92
22	N	603	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
22	B	806	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	B	803	CLA	CHB-C1B-NB	2.02	126.39	124.26
22	O	305	CLA	CHB-C1B-NB	2.02	126.39	124.26
22	B	804	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	R	601	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	O	312	CLA	C1-C2-C3	-2.02	122.56	126.04
22	T	609	CLA	CMB-C2B-C3B	2.02	131.47	126.59
28	H	322	LMG	O1-C7-C8	-2.02	106.04	110.90
22	W	414	CLA	C1-C2-C3	-2.02	122.56	126.04
24	A	859	DD6	O1-C20-C21	-2.01	112.64	115.06
24	P	613	DD6	C7-C6-C8	2.01	121.25	118.08
27	O	322	LMU	C1B-O5B-C5B	2.01	117.64	113.69
22	U	401	CLA	CHB-C1B-NB	2.01	126.39	124.26
22	W	402	CLA	CHB-C1B-NB	2.01	126.39	124.26
24	S	612	DD6	C26-C25-C24	-2.01	116.93	123.22
22	B	832	CLA	CHB-C1B-NB	2.01	126.39	124.26
24	L	415	DD6	C-C1-C2	-2.01	120.10	122.92
22	Q	610	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	A	811	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	A	838	CLA	CHB-C1B-NB	2.01	126.39	124.26
22	N	605	CLA	CHB-C1B-NB	2.01	126.39	124.26
22	U	406	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	Q	613	CLA	O2A-CGA-O1A	-2.01	118.29	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	801	BCR	C21-C20-C19	-2.01	116.94	123.22
22	O	306	CLA	CHB-C1B-NB	2.01	126.39	124.26
22	G	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
24	F	406	DD6	C7-C6-C5	-2.01	120.11	122.92
22	B	828	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	U	411	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
22	B	832	CLA	CAA-CBA-CGA	-2.01	107.39	113.25
22	G	609	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	P	608	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
22	O	319	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	K	611	CLA	O1D-CGD-CBD	2.01	128.59	124.48
22	O	312	CLA	CMB-C2B-C3B	2.01	131.45	126.59
22	X	402	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	I	608	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
22	V	610	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
22	S	614	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
22	A	835	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	L	406	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	Q	606	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	Q	611	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	V	612	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	A	828	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	R	609	CLA	CMB-C2B-C3B	2.01	131.45	126.59
22	L	407	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	I	607	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
22	V	604	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
22	W	409	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	A	837	CLA	C1-C2-C3	-2.01	123.51	126.75
22	A	815	CLA	CMB-C2B-C3B	2.01	131.44	126.59
22	K	602	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	A	833	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	A	834	CLA	CHB-C1B-NB	2.01	126.38	124.26
22	U	409	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
22	W	402	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
25	O	304	DGD	C6E-C5E-C4E	-2.00	108.31	113.00
22	B	827	CLA	CHC-C4B-NB	2.00	126.38	124.26
22	I	608	CLA	CHB-C1B-NB	2.00	126.38	124.26
22	P	602	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
22	W	414	CLA	CHD-C1D-ND	-2.00	122.61	124.45
22	R	606	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
22	A	838	CLA	CHC-C4B-NB	2.00	126.38	124.26
22	H	313	CLA	C1-C2-C3	-2.00	122.58	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	807	CLA	C1-C2-C3	-2.00	122.58	126.04
22	S	602	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	U	410	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	T	608	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	X	411	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
22	H	310	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
22	A	834	CLA	CHD-C1D-ND	-2.00	122.61	124.45
22	K	603	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	B	839	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
22	O	315	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
28	W	401	LMG	O1-C7-C8	-2.00	106.07	110.90
22	I	603	CLA	CHC-C4B-NB	2.00	126.38	124.26
22	A	838	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	X	404	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	P	609	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

There are no chirality outliers.

All (3517) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	801	BCR	C7-C8-C9-C10
21	B	801	BCR	C7-C8-C9-C34
21	B	842	BCR	C21-C22-C23-C24
21	B	842	BCR	C37-C22-C23-C24
21	B	845	BCR	C21-C22-C23-C24
21	B	845	BCR	C37-C22-C23-C24
21	B	846	BCR	C1-C6-C7-C8
21	B	846	BCR	C21-C22-C23-C24
21	B	846	BCR	C37-C22-C23-C24
21	M	101	BCR	C23-C24-C25-C26
21	A	850	BCR	C37-C22-C23-C24
22	B	804	CLA	C3A-C2A-CAA-CBA
22	B	804	CLA	CHA-CBD-CGD-O1D
22	B	804	CLA	CHA-CBD-CGD-O2D
22	B	804	CLA	CAD-CBD-CGD-O1D
22	B	804	CLA	CAD-CBD-CGD-O2D
22	B	806	CLA	CHA-CBD-CGD-O1D
22	B	806	CLA	CHA-CBD-CGD-O2D
22	B	807	CLA	C2B-C3B-CAB-CBB
22	B	807	CLA	C4B-C3B-CAB-CBB
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	812	CLA	CHA-CBD-CGD-O2D
22	B	812	CLA	CAD-CBD-CGD-O1D
22	B	815	CLA	C1A-C2A-CAA-CBA
22	B	815	CLA	C3A-C2A-CAA-CBA
22	B	816	CLA	C3A-C2A-CAA-CBA
22	B	818	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	C2-C3-C5-C6
22	B	820	CLA	C4-C3-C5-C6
22	B	824	CLA	C3A-C2A-CAA-CBA
22	B	824	CLA	CHA-CBD-CGD-O1D
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	825	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	CHA-CBD-CGD-O1D
22	B	827	CLA	CHA-CBD-CGD-O2D
22	B	828	CLA	CHA-CBD-CGD-O1D
22	B	828	CLA	CHA-CBD-CGD-O2D
22	B	828	CLA	CAD-CBD-CGD-O1D
22	B	829	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	C3A-C2A-CAA-CBA
22	B	830	CLA	C11-C12-C13-C14
22	B	832	CLA	C2-C3-C5-C6
22	B	832	CLA	C4-C3-C5-C6
22	B	833	CLA	C2B-C3B-CAB-CBB
22	B	833	CLA	C4B-C3B-CAB-CBB
22	B	859	CLA	C2B-C3B-CAB-CBB
22	B	859	CLA	C4B-C3B-CAB-CBB
22	G	606	CLA	C1A-C2A-CAA-CBA
22	G	606	CLA	C3A-C2A-CAA-CBA
22	G	608	CLA	C1A-C2A-CAA-CBA
22	G	608	CLA	C3A-C2A-CAA-CBA
22	H	302	CLA	CHA-CBD-CGD-O1D
22	H	302	CLA	CHA-CBD-CGD-O2D
22	H	307	CLA	C1A-C2A-CAA-CBA
22	H	307	CLA	C3A-C2A-CAA-CBA
22	H	309	CLA	C2B-C3B-CAB-CBB
22	H	309	CLA	C4B-C3B-CAB-CBB
22	H	311	CLA	CHA-CBD-CGD-O1D
22	H	311	CLA	CHA-CBD-CGD-O2D
22	H	312	CLA	C1A-C2A-CAA-CBA
22	H	312	CLA	C3A-C2A-CAA-CBA
22	I	601	CLA	C1A-C2A-CAA-CBA
22	I	606	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	I	610	CLA	CHA-CBD-CGD-O1D
22	I	610	CLA	CHA-CBD-CGD-O2D
22	I	611	CLA	C1A-C2A-CAA-CBA
22	I	611	CLA	C3A-C2A-CAA-CBA
22	I	611	CLA	CHA-CBD-CGD-O1D
22	I	611	CLA	CHA-CBD-CGD-O2D
22	J	102	CLA	C1A-C2A-CAA-CBA
22	K	602	CLA	CHA-CBD-CGD-O1D
22	K	602	CLA	CHA-CBD-CGD-O2D
22	K	605	CLA	C1A-C2A-CAA-CBA
22	K	605	CLA	C3A-C2A-CAA-CBA
22	K	605	CLA	CHA-CBD-CGD-O1D
22	K	605	CLA	CHA-CBD-CGD-O2D
22	K	605	CLA	CAD-CBD-CGD-O1D
22	K	605	CLA	C6-C7-C8-C9
22	K	607	CLA	C1A-C2A-CAA-CBA
22	K	607	CLA	C3A-C2A-CAA-CBA
22	K	609	CLA	C1A-C2A-CAA-CBA
22	L	402	CLA	CHA-CBD-CGD-O1D
22	L	402	CLA	CHA-CBD-CGD-O2D
22	L	402	CLA	C2-C3-C5-C6
22	L	402	CLA	C4-C3-C5-C6
22	L	407	CLA	C1A-C2A-CAA-CBA
22	L	407	CLA	C3A-C2A-CAA-CBA
22	L	408	CLA	CBD-CGD-O2D-CED
22	L	409	CLA	CBD-CGD-O2D-CED
22	L	410	CLA	C1A-C2A-CAA-CBA
22	L	411	CLA	CHA-CBD-CGD-O1D
22	L	411	CLA	CHA-CBD-CGD-O2D
22	N	607	CLA	C1A-C2A-CAA-CBA
22	N	610	CLA	CHA-CBD-CGD-O1D
22	N	610	CLA	CHA-CBD-CGD-O2D
22	N	611	CLA	CBD-CGD-O2D-CED
22	O	305	CLA	CHA-CBD-CGD-O1D
22	O	308	CLA	C3A-C2A-CAA-CBA
22	O	309	CLA	C1A-C2A-CAA-CBA
22	O	309	CLA	C3A-C2A-CAA-CBA
22	O	309	CLA	C2B-C3B-CAB-CBB
22	O	309	CLA	C4B-C3B-CAB-CBB
22	O	311	CLA	C2B-C3B-CAB-CBB
22	O	311	CLA	C4B-C3B-CAB-CBB
22	O	313	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	P	602	CLA	C3A-C2A-CAA-CBA
22	P	602	CLA	CBD-CGD-O2D-CED
22	P	606	CLA	C1A-C2A-CAA-CBA
22	P	606	CLA	C3A-C2A-CAA-CBA
22	P	607	CLA	C1A-C2A-CAA-CBA
22	P	611	CLA	C1A-C2A-CAA-CBA
22	P	611	CLA	C3A-C2A-CAA-CBA
22	Q	606	CLA	CHA-CBD-CGD-O1D
22	Q	606	CLA	CHA-CBD-CGD-O2D
22	Q	608	CLA	C1A-C2A-CAA-CBA
22	Q	608	CLA	C3A-C2A-CAA-CBA
22	Q	613	CLA	C1A-C2A-CAA-CBA
22	R	602	CLA	C2-C3-C5-C6
22	R	602	CLA	C4-C3-C5-C6
22	R	606	CLA	C1A-C2A-CAA-CBA
22	R	606	CLA	C3A-C2A-CAA-CBA
22	R	606	CLA	CHA-CBD-CGD-O1D
22	R	606	CLA	CHA-CBD-CGD-O2D
22	R	606	CLA	CBD-CGD-O2D-CED
22	R	607	CLA	CBD-CGD-O2D-CED
22	R	611	CLA	C1A-C2A-CAA-CBA
22	R	611	CLA	C3A-C2A-CAA-CBA
22	R	611	CLA	CHA-CBD-CGD-O1D
22	R	611	CLA	CHA-CBD-CGD-O2D
22	S	605	CLA	C1A-C2A-CAA-CBA
22	S	605	CLA	C3A-C2A-CAA-CBA
22	S	605	CLA	C4-C3-C5-C6
22	S	606	CLA	C1A-C2A-CAA-CBA
22	S	607	CLA	C1A-C2A-CAA-CBA
22	S	608	CLA	C1A-C2A-CAA-CBA
22	S	608	CLA	C3A-C2A-CAA-CBA
22	T	601	CLA	CHA-CBD-CGD-O1D
22	T	601	CLA	CHA-CBD-CGD-O2D
22	T	606	CLA	C1A-C2A-CAA-CBA
22	T	606	CLA	C3A-C2A-CAA-CBA
22	T	608	CLA	CHA-CBD-CGD-O1D
22	T	608	CLA	CHA-CBD-CGD-O2D
22	T	611	CLA	C3A-C2A-CAA-CBA
22	T	611	CLA	CHA-CBD-CGD-O1D
22	T	611	CLA	CHA-CBD-CGD-O2D
22	T	611	CLA	CBD-CGD-O2D-CED
22	U	401	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	U	401	CLA	C3A-C2A-CAA-CBA
22	U	403	CLA	C1A-C2A-CAA-CBA
22	U	403	CLA	C3A-C2A-CAA-CBA
22	U	409	CLA	C1A-C2A-CAA-CBA
22	U	409	CLA	C3A-C2A-CAA-CBA
22	U	410	CLA	C1A-C2A-CAA-CBA
22	U	410	CLA	C3A-C2A-CAA-CBA
22	U	411	CLA	C4-C3-C5-C6
22	U	413	CLA	C1A-C2A-CAA-CBA
22	U	413	CLA	C3A-C2A-CAA-CBA
22	U	413	CLA	CBD-CGD-O2D-CED
22	U	415	CLA	C1A-C2A-CAA-CBA
22	U	415	CLA	C3A-C2A-CAA-CBA
22	U	415	CLA	CBD-CGD-O2D-CED
22	U	420	CLA	C1A-C2A-CAA-CBA
22	U	420	CLA	C3A-C2A-CAA-CBA
22	U	420	CLA	CHA-CBD-CGD-O1D
22	U	420	CLA	CHA-CBD-CGD-O2D
22	U	420	CLA	CBD-CGD-O2D-CED
22	V	601	CLA	CBD-CGD-O2D-CED
22	V	602	CLA	C2B-C3B-CAB-CBB
22	V	602	CLA	C4B-C3B-CAB-CBB
22	V	602	CLA	CBD-CGD-O2D-CED
22	V	604	CLA	CBD-CGD-O2D-CED
22	V	607	CLA	C2A-CAA-CBA-CGA
22	V	607	CLA	CBD-CGD-O2D-CED
22	V	608	CLA	CBD-CGD-O2D-CED
22	V	609	CLA	CBD-CGD-O2D-CED
22	V	612	CLA	CBD-CGD-O2D-CED
22	V	613	CLA	CHA-CBD-CGD-O1D
22	V	613	CLA	CHA-CBD-CGD-O2D
22	V	613	CLA	CAD-CBD-CGD-O1D
22	W	414	CLA	CBD-CGD-O2D-CED
22	W	419	CLA	CHA-CBD-CGD-O1D
22	W	419	CLA	CHA-CBD-CGD-O2D
22	X	402	CLA	C1A-C2A-CAA-CBA
22	X	402	CLA	C3A-C2A-CAA-CBA
22	X	402	CLA	O1A-CGA-O2A-C1
22	X	408	CLA	C1A-C2A-CAA-CBA
22	X	408	CLA	C3A-C2A-CAA-CBA
22	X	409	CLA	CBD-CGD-O2D-CED
22	X	410	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	X	413	CLA	C1A-C2A-CAA-CBA
22	X	413	CLA	C3A-C2A-CAA-CBA
22	X	417	CLA	CHA-CBD-CGD-O1D
22	X	417	CLA	CHA-CBD-CGD-O2D
22	X	417	CLA	CAD-CBD-CGD-O1D
22	X	417	CLA	CAD-CBD-CGD-O2D
22	X	419	CLA	C1A-C2A-CAA-CBA
22	X	419	CLA	C3A-C2A-CAA-CBA
22	X	419	CLA	CBD-CGD-O2D-CED
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	806	CLA	C1A-C2A-CAA-CBA
22	A	806	CLA	C3A-C2A-CAA-CBA
22	A	807	CLA	C1A-C2A-CAA-CBA
22	A	807	CLA	CHA-CBD-CGD-O1D
22	A	807	CLA	CHA-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O1D
22	A	811	CLA	C1A-C2A-CAA-CBA
22	A	817	CLA	C2-C1-O2A-CGA
22	A	818	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	820	CLA	CHA-CBD-CGD-O1D
22	A	820	CLA	CHA-CBD-CGD-O2D
22	A	821	CLA	C1A-C2A-CAA-CBA
22	A	821	CLA	C3A-C2A-CAA-CBA
22	A	823	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	C2-C3-C5-C6
22	A	824	CLA	C4-C3-C5-C6
22	A	825	CLA	C1A-C2A-CAA-CBA
22	A	825	CLA	C3A-C2A-CAA-CBA
22	A	825	CLA	C2B-C3B-CAB-CBB
22	A	825	CLA	C4B-C3B-CAB-CBB
22	A	827	CLA	C3A-C2A-CAA-CBA
22	A	830	CLA	C1A-C2A-CAA-CBA
22	A	830	CLA	C2A-CAA-CBA-CGA
22	A	831	CLA	CHA-CBD-CGD-O1D
22	A	831	CLA	CHA-CBD-CGD-O2D
22	A	832	CLA	C1A-C2A-CAA-CBA
22	A	832	CLA	C3A-C2A-CAA-CBA
22	A	837	CLA	CHA-CBD-CGD-O1D
22	A	837	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	A	838	CLA	C1A-C2A-CAA-CBA
22	A	841	CLA	CHA-CBD-CGD-O1D
22	A	841	CLA	CHA-CBD-CGD-O2D
22	A	852	CLA	C1A-C2A-CAA-CBA
24	F	406	DD6	C5-C6-C8-C9
24	F	406	DD6	C7-C6-C8-C9
24	L	415	DD6	C10-C11-C13-C14
24	L	415	DD6	C12-C11-C13-C14
24	N	613	DD6	C27-C29-C30-C31
24	P	613	DD6	C-C1-C24-C25
24	P	613	DD6	C2-C1-C24-C25
24	P	613	DD6	C13-C14-C15-O1
24	R	613	DD6	C13-C14-C15-O1
24	S	611	DD6	C27-C29-C30-C31
24	T	613	DD6	C27-C29-C30-C31
24	X	416	DD6	C10-C11-C13-C14
24	X	416	DD6	C12-C11-C13-C14
24	A	858	DD6	C13-C14-C15-O1
25	B	847	DGD	O6D-C1D-O3G-C3G
25	B	847	DGD	C2E-C1E-O5D-C6D
25	B	847	DGD	O6E-C1E-O5D-C6D
25	O	304	DGD	O6D-C1D-O3G-C3G
25	O	304	DGD	C2E-C1E-O5D-C6D
25	O	304	DGD	O6E-C1E-O5D-C6D
26	B	848	LHG	O1-C1-C2-C3
26	B	848	LHG	O2-C2-C3-O3
26	B	848	LHG	C3-O3-P-O6
26	B	851	LHG	O2-C2-C3-O3
26	B	851	LHG	C4-O6-P-O3
26	B	851	LHG	C4-O6-P-O5
26	G	614	LHG	C3-O3-P-O5
26	H	316	LHG	C3-O3-P-O5
26	K	616	LHG	O7-C5-C6-O8
26	K	619	LHG	C1-C2-C3-O3
26	K	619	LHG	C3-O3-P-O4
26	K	619	LHG	C3-O3-P-O6
26	K	619	LHG	O6-C4-C5-O7
26	L	416	LHG	C3-O3-P-O5
26	N	614	LHG	C3-O3-P-O5
26	N	616	LHG	C4-O6-P-O3
26	N	616	LHG	C4-O6-P-O4
26	N	616	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
26	N	616	LHG	O9-C7-O7-C5
26	O	318	LHG	C4-O6-P-O3
26	O	318	LHG	C4-O6-P-O4
26	O	321	LHG	O1-C1-C2-O2
26	O	321	LHG	O1-C1-C2-C3
26	O	321	LHG	C3-O3-P-O4
26	O	321	LHG	C3-O3-P-O5
26	O	321	LHG	O10-C23-O8-C6
26	O	321	LHG	C24-C23-O8-C6
26	O	323	LHG	O1-C1-C2-C3
26	O	323	LHG	O2-C2-C3-O3
26	O	323	LHG	C3-O3-P-O5
26	O	323	LHG	C4-O6-P-O5
26	O	324	LHG	O1-C1-C2-C3
26	O	324	LHG	C3-O3-P-O5
26	O	324	LHG	C4-O6-P-O5
26	P	601	LHG	O1-C1-C2-C3
26	P	601	LHG	O7-C5-C6-O8
26	P	601	LHG	C8-C7-O7-C5
26	Q	616	LHG	O1-C1-C2-C3
26	Q	616	LHG	C3-O3-P-O4
26	Q	616	LHG	C3-O3-P-O5
26	Q	616	LHG	C3-O3-P-O6
26	R	614	LHG	C3-O3-P-O4
26	R	614	LHG	C3-O3-P-O5
26	S	613	LHG	O1-C1-C2-C3
26	S	613	LHG	C3-O3-P-O4
26	S	613	LHG	C3-O3-P-O5
26	S	613	LHG	C4-O6-P-O4
26	S	613	LHG	C4-O6-P-O5
26	T	614	LHG	C3-O3-P-O4
26	T	614	LHG	C3-O3-P-O5
26	T	614	LHG	C3-O3-P-O6
26	T	614	LHG	C4-O6-P-O4
26	T	614	LHG	C4-O6-P-O5
26	U	419	LHG	C4-O6-P-O3
26	U	419	LHG	C4-O6-P-O5
26	U	419	LHG	C8-C7-O7-C5
26	W	420	LHG	C3-O3-P-O5
26	W	420	LHG	C4-O6-P-O4
26	W	420	LHG	C4-O6-P-O5
26	X	420	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
26	A	845	LHG	O1-C1-C2-O2
26	A	845	LHG	O1-C1-C2-C3
26	A	846	LHG	C4-O6-P-O3
26	A	846	LHG	C4-O6-P-O4
26	A	846	LHG	C4-O6-P-O5
26	A	846	LHG	C8-C7-O7-C5
27	J	104	LMU	C2-C1-O1'-C1'
27	K	620	LMU	C2-C1-O1'-C1'
27	O	322	LMU	C2-C1-O1'-C1'
27	A	857	LMU	C2-C1-O1'-C1'
28	B	852	LMG	C2-C1-O1-C7
28	B	852	LMG	O6-C1-O1-C7
28	B	856	LMG	O6-C1-O1-C7
28	F	408	LMG	O9-C10-O7-C8
28	H	317	LMG	O6-C1-O1-C7
28	H	317	LMG	O1-C7-C8-O7
28	H	319	LMG	C2-C1-O1-C7
28	H	319	LMG	O6-C1-O1-C7
28	H	319	LMG	O1-C7-C8-O7
28	K	601	LMG	O6-C1-O1-C7
28	K	601	LMG	O9-C10-O7-C8
28	K	601	LMG	C11-C10-O7-C8
28	K	618	LMG	O6-C1-O1-C7
28	L	401	LMG	C2-C1-O1-C7
28	L	401	LMG	O6-C1-O1-C7
28	N	615	LMG	O1-C7-C8-O7
28	N	615	LMG	C11-C10-O7-C8
28	T	616	LMG	C2-C1-O1-C7
28	T	616	LMG	O6-C1-O1-C7
28	T	616	LMG	C8-C7-O1-C1
28	U	402	LMG	C2-C1-O1-C7
28	U	402	LMG	O6-C1-O1-C7
28	U	402	LMG	O9-C10-O7-C8
28	U	402	LMG	C11-C10-O7-C8
28	U	423	LMG	C2-C1-O1-C7
28	U	423	LMG	O6-C1-O1-C7
28	W	401	LMG	C2-C1-O1-C7
28	W	401	LMG	O6-C1-O1-C7
28	W	401	LMG	C11-C10-O7-C8
30	O	302	SQD	O10-C23-O48-C46
30	O	302	SQD	C24-C23-O48-C46
31	W	422	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	W	422	CHL	C4-C3-C5-C6
22	R	606	CLA	O1D-CGD-O2D-CED
22	R	608	CLA	O1D-CGD-O2D-CED
22	I	610	CLA	O1D-CGD-O2D-CED
22	L	408	CLA	O1D-CGD-O2D-CED
22	P	602	CLA	O1D-CGD-O2D-CED
22	R	601	CLA	O1D-CGD-O2D-CED
22	R	609	CLA	O1D-CGD-O2D-CED
22	T	611	CLA	O1D-CGD-O2D-CED
22	U	415	CLA	O1D-CGD-O2D-CED
22	V	608	CLA	O1D-CGD-O2D-CED
22	V	612	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CBD-CGD-O2D-CED
22	B	826	CLA	CBD-CGD-O2D-CED
22	F	403	CLA	CBD-CGD-O2D-CED
22	F	405	CLA	CBD-CGD-O2D-CED
22	G	610	CLA	CBD-CGD-O2D-CED
22	H	307	CLA	CBD-CGD-O2D-CED
22	H	311	CLA	CBD-CGD-O2D-CED
22	I	601	CLA	CBD-CGD-O2D-CED
22	I	607	CLA	CBD-CGD-O2D-CED
22	I	609	CLA	CBD-CGD-O2D-CED
22	I	610	CLA	CBD-CGD-O2D-CED
22	K	605	CLA	CBD-CGD-O2D-CED
22	L	406	CLA	CBD-CGD-O2D-CED
22	N	602	CLA	CBD-CGD-O2D-CED
22	N	607	CLA	CBD-CGD-O2D-CED
22	N	610	CLA	CBD-CGD-O2D-CED
22	Q	606	CLA	CBD-CGD-O2D-CED
22	R	601	CLA	CBD-CGD-O2D-CED
22	R	602	CLA	CBD-CGD-O2D-CED
22	R	604	CLA	CBD-CGD-O2D-CED
22	R	608	CLA	CBD-CGD-O2D-CED
22	R	609	CLA	CBD-CGD-O2D-CED
22	R	610	CLA	CBD-CGD-O2D-CED
22	R	615	CLA	CBD-CGD-O2D-CED
22	S	604	CLA	CBD-CGD-O2D-CED
22	S	605	CLA	CBD-CGD-O2D-CED
22	U	401	CLA	CBD-CGD-O2D-CED
22	U	404	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	U	410	CLA	CBD-CGD-O2D-CED
22	V	610	CLA	CBD-CGD-O2D-CED
22	V	613	CLA	CBD-CGD-O2D-CED
22	V	617	CLA	CBD-CGD-O2D-CED
22	W	410	CLA	CBD-CGD-O2D-CED
22	W	411	CLA	CBD-CGD-O2D-CED
22	A	801	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	CBD-CGD-O2D-CED
22	A	824	CLA	CBD-CGD-O2D-CED
22	A	852	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	O1A-CGA-O2A-C1
22	X	405	CLA	O1A-CGA-O2A-C1
22	A	817	CLA	O1A-CGA-O2A-C1
22	A	824	CLA	O1A-CGA-O2A-C1
26	K	616	LHG	O10-C23-O8-C6
28	H	322	LMG	O10-C28-O8-C9
22	B	821	CLA	O1D-CGD-O2D-CED
22	R	615	CLA	O1D-CGD-O2D-CED
22	U	420	CLA	O1D-CGD-O2D-CED
22	V	601	CLA	O1D-CGD-O2D-CED
27	O	322	LMU	O5B-C1B-O1B-C4'
22	I	609	CLA	O1D-CGD-O2D-CED
22	L	409	CLA	O1D-CGD-O2D-CED
22	R	610	CLA	O1D-CGD-O2D-CED
22	U	413	CLA	O1D-CGD-O2D-CED
22	V	602	CLA	O1D-CGD-O2D-CED
22	V	604	CLA	O1D-CGD-O2D-CED
22	V	607	CLA	O1D-CGD-O2D-CED
22	V	609	CLA	O1D-CGD-O2D-CED
22	W	414	CLA	O1D-CGD-O2D-CED
22	X	409	CLA	O1D-CGD-O2D-CED
22	A	801	CLA	O1D-CGD-O2D-CED
22	X	402	CLA	CBA-CGA-O2A-C1
22	X	405	CLA	CBA-CGA-O2A-C1
26	K	616	LHG	C24-C23-O8-C6
22	B	805	CLA	CBD-CGD-O2D-CED
22	B	822	CLA	CBD-CGD-O2D-CED
22	G	607	CLA	CBD-CGD-O2D-CED
22	H	304	CLA	CBD-CGD-O2D-CED
22	H	318	CLA	CBD-CGD-O2D-CED
22	L	407	CLA	CBD-CGD-O2D-CED
22	L	411	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	N	606	CLA	CBD-CGD-O2D-CED
22	O	308	CLA	CBD-CGD-O2D-CED
22	P	606	CLA	CBD-CGD-O2D-CED
22	Q	604	CLA	CBD-CGD-O2D-CED
22	Q	609	CLA	CBD-CGD-O2D-CED
22	Q	611	CLA	CBD-CGD-O2D-CED
22	Q	618	CLA	CBD-CGD-O2D-CED
22	S	607	CLA	CBD-CGD-O2D-CED
22	T	604	CLA	CBD-CGD-O2D-CED
22	T	606	CLA	CBD-CGD-O2D-CED
22	T	608	CLA	CBD-CGD-O2D-CED
22	U	403	CLA	CBD-CGD-O2D-CED
22	U	411	CLA	CBD-CGD-O2D-CED
22	U	414	CLA	CBD-CGD-O2D-CED
22	W	415	CLA	CBD-CGD-O2D-CED
22	X	405	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	CBD-CGD-O2D-CED
22	A	812	CLA	CBD-CGD-O2D-CED
22	B	817	CLA	O1A-CGA-O2A-C1
22	B	819	CLA	O1A-CGA-O2A-C1
22	O	308	CLA	O1A-CGA-O2A-C1
22	S	605	CLA	O1A-CGA-O2A-C1
22	S	609	CLA	O1A-CGA-O2A-C1
22	T	603	CLA	O1A-CGA-O2A-C1
22	A	805	CLA	O1A-CGA-O2A-C1
26	T	614	LHG	O10-C23-O8-C6
28	N	615	LMG	O10-C28-O8-C9
22	R	607	CLA	O1D-CGD-O2D-CED
22	B	818	CLA	O1D-CGD-O2D-CED
22	N	611	CLA	O1D-CGD-O2D-CED
22	X	419	CLA	O1D-CGD-O2D-CED
22	G	611	CLA	CBD-CGD-O2D-CED
22	O	311	CLA	CBD-CGD-O2D-CED
22	P	610	CLA	CBD-CGD-O2D-CED
22	Q	603	CLA	CBD-CGD-O2D-CED
22	U	404	CLA	O1D-CGD-O2D-CED
22	V	613	CLA	O1D-CGD-O2D-CED
26	O	324	LHG	O9-C7-O7-C5
26	P	601	LHG	O9-C7-O7-C5
26	U	419	LHG	O9-C7-O7-C5
26	A	846	LHG	O9-C7-O7-C5
28	I	615	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
28	N	615	LMG	O9-C10-O7-C8
28	W	401	LMG	O9-C10-O7-C8
22	B	813	CLA	C3-C5-C6-C7
22	B	818	CLA	C3-C5-C6-C7
22	B	819	CLA	C3-C5-C6-C7
22	B	833	CLA	C3-C5-C6-C7
22	G	603	CLA	C3-C5-C6-C7
22	I	603	CLA	C3-C5-C6-C7
22	I	606	CLA	C3-C5-C6-C7
22	K	605	CLA	C3-C5-C6-C7
22	K	611	CLA	C3-C5-C6-C7
22	L	404	CLA	C3-C5-C6-C7
22	L	411	CLA	C3-C5-C6-C7
22	R	601	CLA	C3-C5-C6-C7
22	S	602	CLA	C3-C5-C6-C7
22	S	604	CLA	C3-C5-C6-C7
22	V	604	CLA	C3-C5-C6-C7
22	A	814	CLA	C3-C5-C6-C7
22	B	808	CLA	CBA-CGA-O2A-C1
22	B	817	CLA	CBA-CGA-O2A-C1
22	B	819	CLA	CBA-CGA-O2A-C1
22	K	610	CLA	CBA-CGA-O2A-C1
22	O	308	CLA	CBA-CGA-O2A-C1
22	S	605	CLA	CBA-CGA-O2A-C1
22	T	603	CLA	CBA-CGA-O2A-C1
22	V	603	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	817	CLA	CBA-CGA-O2A-C1
22	A	821	CLA	CBA-CGA-O2A-C1
22	A	824	CLA	CBA-CGA-O2A-C1
28	N	615	LMG	C29-C28-O8-C9
26	N	616	LHG	C8-C7-O7-C5
26	O	324	LHG	C8-C7-O7-C5
28	F	408	LMG	C11-C10-O7-C8
22	F	405	CLA	O1D-CGD-O2D-CED
22	K	605	CLA	O1D-CGD-O2D-CED
22	W	411	CLA	O1D-CGD-O2D-CED
22	L	404	CLA	CBD-CGD-O2D-CED
22	W	409	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	C3-C5-C6-C7
22	B	834	CLA	C4-C3-C5-C6
22	A	811	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	814	CLA	C4-C3-C5-C6
22	B	834	CLA	C2-C3-C5-C6
22	S	605	CLA	C2-C3-C5-C6
22	U	411	CLA	C2-C3-C5-C6
22	B	827	CLA	CBD-CGD-O2D-CED
22	G	608	CLA	CBD-CGD-O2D-CED
22	U	409	CLA	CBD-CGD-O2D-CED
22	B	817	CLA	C2A-CAA-CBA-CGA
22	J	102	CLA	C2A-CAA-CBA-CGA
22	P	604	CLA	C2A-CAA-CBA-CGA
22	T	605	CLA	C2A-CAA-CBA-CGA
22	U	409	CLA	C2A-CAA-CBA-CGA
22	W	419	CLA	C2A-CAA-CBA-CGA
22	X	402	CLA	C2A-CAA-CBA-CGA
22	X	417	CLA	C2A-CAA-CBA-CGA
22	A	818	CLA	C2A-CAA-CBA-CGA
22	A	821	CLA	C2A-CAA-CBA-CGA
22	W	410	CLA	O1D-CGD-O2D-CED
26	B	851	LHG	C24-C25-C26-C27
26	G	614	LHG	C24-C25-C26-C27
26	K	616	LHG	C24-C25-C26-C27
26	O	318	LHG	C24-C25-C26-C27
26	O	321	LHG	C24-C25-C26-C27
26	S	613	LHG	C24-C25-C26-C27
26	T	614	LHG	C24-C25-C26-C27
26	U	419	LHG	C24-C25-C26-C27
26	W	420	LHG	C24-C25-C26-C27
26	X	420	LHG	C24-C25-C26-C27
26	A	845	LHG	C24-C25-C26-C27
26	A	846	LHG	C24-C25-C26-C27
22	Q	605	CLA	C3-C5-C6-C7
33	A	802	CL0	C3-C5-C6-C7
22	B	830	CLA	CBA-CGA-O2A-C1
22	L	404	CLA	CBA-CGA-O2A-C1
22	R	615	CLA	CBA-CGA-O2A-C1
22	S	609	CLA	CBA-CGA-O2A-C1
25	F	401	DGD	C2A-C1A-O1G-C1G
26	T	614	LHG	C24-C23-O8-C6
28	H	322	LMG	C29-C28-O8-C9
25	B	847	DGD	O6E-C5E-C6E-O5E
22	B	802	CLA	O1D-CGD-O2D-CED
22	G	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	I	601	CLA	O1D-CGD-O2D-CED
22	N	602	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	CBD-CGD-O2D-CED
22	B	826	CLA	O1D-CGD-O2D-CED
22	H	307	CLA	O1D-CGD-O2D-CED
22	H	311	CLA	O1D-CGD-O2D-CED
22	Q	606	CLA	O1D-CGD-O2D-CED
22	S	605	CLA	O1D-CGD-O2D-CED
22	V	610	CLA	O1D-CGD-O2D-CED
22	V	617	CLA	O1D-CGD-O2D-CED
22	B	830	CLA	O1A-CGA-O2A-C1
22	K	610	CLA	O1A-CGA-O2A-C1
22	L	404	CLA	O1A-CGA-O2A-C1
22	R	601	CLA	O1A-CGA-O2A-C1
22	R	608	CLA	O1A-CGA-O2A-C1
22	V	603	CLA	O1A-CGA-O2A-C1
26	B	848	LHG	O10-C23-O8-C6
28	H	317	LMG	O10-C28-O8-C9
28	K	618	LMG	O10-C28-O8-C9
28	U	402	LMG	O10-C28-O8-C9
27	J	104	LMU	C4B-C5B-C6B-O6B
22	B	829	CLA	CBD-CGD-O2D-CED
22	N	604	CLA	CBD-CGD-O2D-CED
22	P	608	CLA	CBD-CGD-O2D-CED
22	Q	612	CLA	CBD-CGD-O2D-CED
22	W	404	CLA	CBD-CGD-O2D-CED
22	A	823	CLA	CBD-CGD-O2D-CED
22	A	830	CLA	CBD-CGD-O2D-CED
22	L	406	CLA	O1D-CGD-O2D-CED
22	N	607	CLA	O1D-CGD-O2D-CED
22	U	401	CLA	O1D-CGD-O2D-CED
22	A	824	CLA	O1D-CGD-O2D-CED
26	N	616	LHG	O2-C2-C3-O3
26	O	321	LHG	O2-C2-C3-O3
26	X	420	LHG	O2-C2-C3-O3
22	F	403	CLA	C3-C5-C6-C7
22	G	608	CLA	C3-C5-C6-C7
22	H	303	CLA	C3-C5-C6-C7
22	H	311	CLA	C3-C5-C6-C7
22	L	403	CLA	C3-C5-C6-C7
22	Q	611	CLA	C3-C5-C6-C7
22	U	401	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	X	410	CLA	C3-C5-C6-C7
22	R	601	CLA	CBA-CGA-O2A-C1
22	R	608	CLA	CBA-CGA-O2A-C1
26	B	848	LHG	C24-C23-O8-C6
28	H	317	LMG	C29-C28-O8-C9
28	K	618	LMG	C29-C28-O8-C9
22	A	821	CLA	O1A-CGA-O2A-C1
25	O	304	DGD	O6E-C5E-C6E-O5E
22	I	607	CLA	O1D-CGD-O2D-CED
22	R	602	CLA	O1D-CGD-O2D-CED
25	F	401	DGD	C2B-C1B-O2G-C2G
28	B	856	LMG	C11-C10-O7-C8
28	I	615	LMG	C11-C10-O7-C8
22	R	604	CLA	O1D-CGD-O2D-CED
22	H	309	CLA	CBD-CGD-O2D-CED
22	U	406	CLA	CBD-CGD-O2D-CED
22	V	603	CLA	CBD-CGD-O2D-CED
22	X	410	CLA	CBD-CGD-O2D-CED
22	A	819	CLA	CBD-CGD-O2D-CED
28	H	317	LMG	O6-C5-C6-O5
28	J	101	LMG	O6-C5-C6-O5
28	N	615	LMG	O6-C5-C6-O5
25	B	847	DGD	C4E-C5E-C6E-O5E
26	P	601	LHG	C15-C16-C17-C18
26	Q	616	LHG	C25-C26-C27-C28
22	N	610	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	C4B-C5B-C6B-C7B
27	B	857	LMU	O5'-C5'-C6'-O6'
22	B	813	CLA	O1D-CGD-O2D-CED
22	F	403	CLA	O1D-CGD-O2D-CED
22	S	604	CLA	O1D-CGD-O2D-CED
22	U	410	CLA	O1D-CGD-O2D-CED
22	A	817	CLA	O1D-CGD-O2D-CED
22	A	852	CLA	O1D-CGD-O2D-CED
22	B	820	CLA	C3-C5-C6-C7
22	X	412	CLA	C3-C5-C6-C7
28	A	855	LMG	O6-C5-C6-O5
26	B	851	LHG	C5-C4-O6-P
22	R	615	CLA	O1A-CGA-O2A-C1
25	F	401	DGD	O1A-C1A-O1G-C1G
25	O	304	DGD	C5A-C6A-C7A-C8A
22	G	608	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	R	601	CLA	C4-C3-C5-C6
22	T	605	CLA	C4-C3-C5-C6
22	A	838	CLA	C4-C3-C5-C6
25	O	304	DGD	C4E-C5E-C6E-O5E
22	G	608	CLA	C2-C3-C5-C6
22	R	601	CLA	C2-C3-C5-C6
22	T	605	CLA	C2-C3-C5-C6
22	A	814	CLA	C2-C3-C5-C6
22	N	607	CLA	C2A-CAA-CBA-CGA
28	U	402	LMG	C4-C5-C6-O5
22	A	813	CLA	CBA-CGA-O2A-C1
22	A	835	CLA	CBA-CGA-O2A-C1
28	U	402	LMG	C29-C28-O8-C9
25	B	847	DGD	C8B-C9B-CAB-CBB
22	R	605	CLA	CBD-CGD-O2D-CED
22	L	407	CLA	O1D-CGD-O2D-CED
22	U	414	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	C4D-C5D-C6D-O5D
22	N	606	CLA	O1D-CGD-O2D-CED
22	Q	611	CLA	O1D-CGD-O2D-CED
22	T	606	CLA	O1D-CGD-O2D-CED
22	U	411	CLA	O1D-CGD-O2D-CED
22	W	415	CLA	O1D-CGD-O2D-CED
22	G	601	CLA	CBD-CGD-O2D-CED
22	O	310	CLA	CBD-CGD-O2D-CED
22	H	304	CLA	O1D-CGD-O2D-CED
26	B	848	LHG	C1-C2-C3-O3
26	B	851	LHG	C1-C2-C3-O3
26	L	416	LHG	C1-C2-C3-O3
26	O	323	LHG	C1-C2-C3-O3
25	F	401	DGD	CEA-CFA-CGA-CHA
26	O	323	LHG	C25-C26-C27-C28
22	L	402	CLA	C3-C5-C6-C7
22	S	609	CLA	C3-C5-C6-C7
22	P	606	CLA	O1D-CGD-O2D-CED
22	H	306	CLA	CBA-CGA-O2A-C1
22	J	102	CLA	CBA-CGA-O2A-C1
22	K	602	CLA	CBA-CGA-O2A-C1
22	K	605	CLA	CBA-CGA-O2A-C1
22	N	610	CLA	CBA-CGA-O2A-C1
22	O	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	Q	617	CLA	CBA-CGA-O2A-C1
22	U	406	CLA	CBA-CGA-O2A-C1
22	W	403	CLA	CBA-CGA-O2A-C1
22	A	812	CLA	CBA-CGA-O2A-C1
22	A	825	CLA	CBA-CGA-O2A-C1
26	N	614	LHG	C24-C23-O8-C6
26	P	601	LHG	C24-C23-O8-C6
26	U	419	LHG	C24-C23-O8-C6
22	T	601	CLA	CBD-CGD-O2D-CED
27	J	104	LMU	C4'-C5'-C6'-O6'
28	J	101	LMG	C4-C5-C6-O5
24	F	406	DD6	C11-C10-C9-C8
24	P	612	DD6	C24-C25-C26-C27
22	A	833	CLA	C13-C15-C16-C17
22	A	842	CLA	C15-C16-C17-C18
26	W	420	LHG	C10-C11-C12-C13
25	O	304	DGD	O6D-C5D-C6D-O5D
22	K	608	CLA	C5-C6-C7-C8
22	V	612	CLA	C5-C6-C7-C8
22	X	403	CLA	C10-C11-C12-C13
22	X	409	CLA	C13-C15-C16-C17
22	A	815	CLA	C10-C11-C12-C13
22	A	825	CLA	C8-C10-C11-C12
22	A	840	CLA	C5-C6-C7-C8
31	W	408	CHL	C10-C11-C12-C13
26	O	324	LHG	O2-C2-C3-O3
26	R	614	LHG	O2-C2-C3-O3
22	B	812	CLA	C3-C5-C6-C7
22	H	307	CLA	C3-C5-C6-C7
25	B	847	DGD	C2D-C1D-O3G-C3G
28	B	856	LMG	C2-C1-O1-C7
28	K	601	LMG	C2-C1-O1-C7
28	K	618	LMG	C2-C1-O1-C7
28	N	615	LMG	C2-C1-O1-C7
26	B	851	LHG	O7-C5-C6-O8
22	W	403	CLA	O1A-CGA-O2A-C1
22	A	825	CLA	O1A-CGA-O2A-C1
22	A	835	CLA	O1A-CGA-O2A-C1
22	A	811	CLA	C2-C3-C5-C6
22	B	806	CLA	C14-C13-C15-C16
22	B	807	CLA	C14-C13-C15-C16
22	B	821	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	834	CLA	C14-C13-C15-C16
22	G	606	CLA	C11-C10-C8-C9
22	H	305	CLA	C6-C7-C8-C9
22	H	313	CLA	C11-C10-C8-C9
22	I	601	CLA	C6-C7-C8-C9
22	I	606	CLA	C11-C10-C8-C9
22	K	604	CLA	C11-C10-C8-C9
22	K	604	CLA	C11-C12-C13-C14
22	K	609	CLA	C6-C7-C8-C9
22	L	411	CLA	C14-C13-C15-C16
22	N	606	CLA	C11-C10-C8-C9
22	Q	609	CLA	C6-C7-C8-C9
22	Q	612	CLA	C14-C13-C15-C16
22	R	606	CLA	C6-C7-C8-C9
22	R	607	CLA	C6-C7-C8-C9
22	R	610	CLA	C14-C13-C15-C16
22	S	605	CLA	C11-C10-C8-C9
22	T	603	CLA	C11-C10-C8-C9
22	T	604	CLA	C11-C12-C13-C14
22	T	605	CLA	C6-C7-C8-C9
22	T	607	CLA	C11-C10-C8-C9
22	X	404	CLA	C11-C10-C8-C9
22	A	807	CLA	C14-C13-C15-C16
22	A	808	CLA	C14-C13-C15-C16
22	A	816	CLA	C6-C7-C8-C9
22	A	817	CLA	C14-C13-C15-C16
22	A	825	CLA	C11-C12-C13-C14
22	A	836	CLA	C11-C12-C13-C14
22	A	840	CLA	C11-C12-C13-C14
22	A	841	CLA	C11-C12-C13-C14
22	A	842	CLA	C14-C13-C15-C16
22	B	822	CLA	O1D-CGD-O2D-CED
22	H	318	CLA	O1D-CGD-O2D-CED
22	L	411	CLA	O1D-CGD-O2D-CED
22	T	604	CLA	O1D-CGD-O2D-CED
22	U	403	CLA	O1D-CGD-O2D-CED
22	K	608	CLA	CBD-CGD-O2D-CED
22	T	607	CLA	CBD-CGD-O2D-CED
22	K	609	CLA	C10-C11-C12-C13
22	A	810	CLA	C2A-CAA-CBA-CGA
21	B	801	BCR	C11-C12-C13-C35
21	A	850	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	F	401	DGD	O1B-C1B-O2G-C2G
25	O	304	DGD	C2B-C1B-O2G-C2G
22	K	602	CLA	O1A-CGA-O2A-C1
22	N	610	CLA	O1A-CGA-O2A-C1
26	P	601	LHG	O10-C23-O8-C6
22	B	818	CLA	C15-C16-C17-C18
22	B	834	CLA	C8-C10-C11-C12
22	K	604	CLA	C8-C10-C11-C12
22	A	813	CLA	C13-C15-C16-C17
22	A	830	CLA	C13-C15-C16-C17
22	A	842	CLA	C13-C15-C16-C17
22	Q	609	CLA	O1D-CGD-O2D-CED
22	Q	618	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	A	835	CLA	CBD-CGD-O2D-CED
22	P	611	CLA	C2C-C3C-CAC-CBC
22	G	607	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	C3-C5-C6-C7
22	V	603	CLA	C3-C5-C6-C7
22	W	404	CLA	C3-C5-C6-C7
22	L	407	CLA	C8-C10-C11-C12
22	R	607	CLA	CBA-CGA-O2A-C1
22	S	607	CLA	CBA-CGA-O2A-C1
22	B	839	CLA	C13-C15-C16-C17
22	Q	609	CLA	C5-C6-C7-C8
22	R	601	CLA	C8-C10-C11-C12
22	S	604	CLA	C8-C10-C11-C12
22	T	611	CLA	C5-C6-C7-C8
22	A	807	CLA	C8-C10-C11-C12
22	A	824	CLA	C10-C11-C12-C13
22	A	841	CLA	C13-C15-C16-C17
26	P	601	LHG	C25-C26-C27-C28
26	B	851	LHG	C23-C24-C25-C26
26	G	614	LHG	C23-C24-C25-C26
22	Q	604	CLA	O1D-CGD-O2D-CED
22	T	608	CLA	O1D-CGD-O2D-CED
28	N	615	LMG	C4-C5-C6-O5
22	W	413	CLA	CBD-CGD-O2D-CED
28	T	616	LMG	O6-C5-C6-O5
22	B	806	CLA	C13-C15-C16-C17
22	B	818	CLA	C8-C10-C11-C12
22	B	822	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	824	CLA	C8-C10-C11-C12
22	K	604	CLA	C5-C6-C7-C8
22	L	402	CLA	C10-C11-C12-C13
22	Q	604	CLA	C15-C16-C17-C18
22	R	610	CLA	C8-C10-C11-C12
22	U	404	CLA	C5-C6-C7-C8
22	A	805	CLA	C8-C10-C11-C12
22	A	824	CLA	C8-C10-C11-C12
22	B	805	CLA	O1D-CGD-O2D-CED
26	X	420	LHG	O1-C1-C2-O2
26	O	321	LHG	C7-C8-C9-C10
28	F	408	LMG	C28-C29-C30-C31
28	H	317	LMG	C28-C29-C30-C31
28	H	322	LMG	C10-C11-C12-C13
28	I	615	LMG	C28-C29-C30-C31
27	J	104	LMU	O5B-C5B-C6B-O6B
27	B	857	LMU	C4'-C5'-C6'-O6'
22	L	410	CLA	CBD-CGD-O2D-CED
22	Q	601	CLA	CBD-CGD-O2D-CED
22	B	823	CLA	C5-C6-C7-C8
22	B	835	CLA	C5-C6-C7-C8
22	H	308	CLA	C5-C6-C7-C8
22	L	417	CLA	C5-C6-C7-C8
22	R	610	CLA	C10-C11-C12-C13
22	A	824	CLA	C13-C15-C16-C17
22	B	826	CLA	CBA-CGA-O2A-C1
22	K	617	CLA	CBA-CGA-O2A-C1
26	B	851	LHG	C26-C27-C28-C29
26	N	616	LHG	C12-C13-C14-C15
26	O	318	LHG	C10-C11-C12-C13
26	O	321	LHG	C34-C35-C36-C37
27	U	422	LMU	O5'-C5'-C6'-O6'
22	B	835	CLA	C10-C11-C12-C13
22	K	611	CLA	C8-C10-C11-C12
22	L	417	CLA	C10-C11-C12-C13
22	O	310	CLA	C5-C6-C7-C8
22	R	607	CLA	C8-C10-C11-C12
22	V	612	CLA	C10-C11-C12-C13
22	A	815	CLA	C15-C16-C17-C18
22	X	405	CLA	O1D-CGD-O2D-CED
22	K	612	CLA	CBD-CGD-O2D-CED
22	P	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	O	321	LHG	C32-C33-C34-C35
26	O	321	LHG	C8-C7-O7-C5
28	Q	602	LMG	C11-C10-O7-C8
25	B	847	DGD	C2A-C3A-C4A-C5A
22	X	412	CLA	C8-C10-C11-C12
22	B	807	CLA	C6-C7-C8-C10
22	B	812	CLA	C12-C13-C15-C16
22	H	311	CLA	C6-C7-C8-C10
22	K	604	CLA	C11-C12-C13-C15
22	K	608	CLA	C11-C12-C13-C15
22	O	308	CLA	C11-C12-C13-C15
22	Q	604	CLA	C11-C10-C8-C7
22	R	615	CLA	C12-C13-C15-C16
22	A	801	CLA	C11-C10-C8-C7
22	A	806	CLA	C11-C12-C13-C15
22	A	808	CLA	C11-C12-C13-C15
22	A	813	CLA	C11-C10-C8-C7
22	A	824	CLA	C6-C7-C8-C10
22	A	828	CLA	C6-C7-C8-C10
22	Q	610	CLA	C3-C5-C6-C7
22	K	605	CLA	O1A-CGA-O2A-C1
26	N	614	LHG	O10-C23-O8-C6
22	B	814	CLA	C2A-CAA-CBA-CGA
22	W	415	CLA	C2A-CAA-CBA-CGA
22	O	308	CLA	O1D-CGD-O2D-CED
22	S	607	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	C8-C10-C11-C12
22	B	824	CLA	C10-C11-C12-C13
22	R	607	CLA	C5-C6-C7-C8
22	T	605	CLA	C15-C16-C17-C18
22	A	814	CLA	C13-C15-C16-C17
22	A	841	CLA	C15-C16-C17-C18
27	X	421	LMU	O1'-C1-C2-C3
22	H	306	CLA	O1A-CGA-O2A-C1
22	J	102	CLA	O1A-CGA-O2A-C1
22	O	312	CLA	O1A-CGA-O2A-C1
22	Q	617	CLA	O1A-CGA-O2A-C1
22	U	406	CLA	O1A-CGA-O2A-C1
22	A	813	CLA	O1A-CGA-O2A-C1
26	U	419	LHG	O10-C23-O8-C6
22	B	812	CLA	C10-C11-C12-C13
22	K	602	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	Q	603	CLA	O1D-CGD-O2D-CED
26	R	614	LHG	C25-C26-C27-C28
30	V	618	SQD	O6-C44-C45-O47
22	P	610	CLA	O1D-CGD-O2D-CED
26	K	619	LHG	O2-C2-C3-O3
26	L	416	LHG	O2-C2-C3-O3
26	T	614	LHG	O2-C2-C3-O3
25	O	304	DGD	O1B-C1B-O2G-C2G
22	B	807	CLA	C10-C11-C12-C13
22	R	605	CLA	C15-C16-C17-C18
22	X	410	CLA	C10-C11-C12-C13
22	O	311	CLA	CBA-CGA-O2A-C1
22	N	608	CLA	CBD-CGD-O2D-CED
22	P	604	CLA	CBD-CGD-O2D-CED
22	G	611	CLA	O1D-CGD-O2D-CED
22	O	311	CLA	O1D-CGD-O2D-CED
22	R	607	CLA	O1A-CGA-O2A-C1
22	A	812	CLA	O1A-CGA-O2A-C1
28	B	852	LMG	C28-C29-C30-C31
28	U	402	LMG	C10-C11-C12-C13
22	B	807	CLA	C5-C6-C7-C8
22	B	810	CLA	C5-C6-C7-C8
22	B	812	CLA	C5-C6-C7-C8
22	H	305	CLA	C5-C6-C7-C8
22	N	603	CLA	C15-C16-C17-C18
22	A	829	CLA	C13-C15-C16-C17
22	L	404	CLA	O1D-CGD-O2D-CED
22	W	409	CLA	O1D-CGD-O2D-CED
28	H	317	LMG	C4-C5-C6-O5
28	L	401	LMG	C4-C5-C6-O5
22	K	617	CLA	O1A-CGA-O2A-C1
26	W	420	LHG	C8-C7-O7-C5
28	H	319	LMG	C11-C10-O7-C8
27	J	104	LMU	O1'-C1-C2-C3
22	B	813	CLA	C10-C11-C12-C13
22	B	833	CLA	C13-C15-C16-C17
22	K	604	CLA	C13-C15-C16-C17
22	T	607	CLA	C8-C10-C11-C12
22	V	604	CLA	C5-C6-C7-C8
22	A	816	CLA	C10-C11-C12-C13
26	B	851	LHG	C3-O3-P-O6
26	N	616	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
26	O	323	LHG	C3-O3-P-O6
26	O	324	LHG	C3-O3-P-O6
26	O	324	LHG	C4-O6-P-O3
26	R	614	LHG	C3-O3-P-O6
26	S	613	LHG	C3-O3-P-O6
26	S	613	LHG	C4-O6-P-O3
26	T	614	LHG	C4-O6-P-O3
26	W	420	LHG	C3-O3-P-O6
26	W	420	LHG	C4-O6-P-O3
26	A	845	LHG	C3-O3-P-O6
28	K	618	LMG	C28-C29-C30-C31
22	G	608	CLA	CBA-CGA-O2A-C1
22	X	408	CLA	CBA-CGA-O2A-C1
26	O	318	LHG	C24-C23-O8-C6
26	N	616	LHG	C1-C2-C3-O3
26	T	614	LHG	C1-C2-C3-O3
26	O	321	LHG	O9-C7-O7-C5
26	W	420	LHG	O9-C7-O7-C5
26	T	614	LHG	C30-C31-C32-C33
22	T	602	CLA	C15-C16-C17-C18
22	A	804	CLA	C10-C11-C12-C13
26	S	613	LHG	C11-C10-C9-C8
22	B	806	CLA	C2A-CAA-CBA-CGA
22	B	808	CLA	C2A-CAA-CBA-CGA
22	X	405	CLA	C2A-CAA-CBA-CGA
22	A	805	CLA	C2A-CAA-CBA-CGA
22	A	824	CLA	C2A-CAA-CBA-CGA
22	B	812	CLA	C16-C17-C18-C20
22	L	402	CLA	C16-C17-C18-C20
22	B	810	CLA	CBA-CGA-O2A-C1
22	R	602	CLA	CBA-CGA-O2A-C1
28	U	423	LMG	C28-C29-C30-C31
22	G	608	CLA	O1D-CGD-O2D-CED
26	O	324	LHG	C31-C32-C33-C34
26	W	420	LHG	C11-C10-C9-C8
22	W	403	CLA	CBD-CGD-O2D-CED
22	A	803	CLA	CBD-CGD-O2D-CED
27	J	104	LMU	O5'-C5'-C6'-O6'
22	B	804	CLA	C3-C5-C6-C7
25	B	847	DGD	C5B-C6B-C7B-C8B
25	F	401	DGD	C7A-C8A-C9A-CAA
25	O	304	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
26	K	616	LHG	C26-C27-C28-C29
26	L	416	LHG	C16-C17-C18-C19
26	N	616	LHG	C13-C14-C15-C16
26	O	321	LHG	C27-C28-C29-C30
26	W	420	LHG	C30-C31-C32-C33
27	U	421	LMU	C11-C10-C9-C8
28	B	852	LMG	C13-C14-C15-C16
28	K	601	LMG	C14-C15-C16-C17
28	U	423	LMG	C17-C18-C19-C20
22	B	827	CLA	O1D-CGD-O2D-CED
22	Q	611	CLA	C6-C7-C8-C9
22	X	410	CLA	C11-C12-C13-C15
22	A	806	CLA	C16-C17-C18-C20
22	A	821	CLA	C16-C17-C18-C19
26	A	846	LHG	C24-C23-O8-C6
26	L	416	LHG	C17-C18-C19-C20
26	O	318	LHG	C12-C13-C14-C15
26	O	323	LHG	C26-C27-C28-C29
26	A	845	LHG	C31-C32-C33-C34
27	B	855	LMU	C4-C5-C6-C7
28	B	856	LMG	C32-C33-C34-C35
28	B	856	LMG	C41-C42-C43-C44
28	G	616	LMG	C34-C35-C36-C37
28	L	401	LMG	C31-C32-C33-C34
28	U	402	LMG	C31-C32-C33-C34
26	U	419	LHG	C6-C5-O7-C7
28	I	615	LMG	C7-C8-O7-C10
28	W	401	LMG	C7-C8-O7-C10
22	U	409	CLA	O1D-CGD-O2D-CED
22	A	842	CLA	O1D-CGD-O2D-CED
28	U	402	LMG	O6-C5-C6-O5
22	X	404	CLA	C8-C10-C11-C12
25	B	847	DGD	CCA-CDA-CEA-CFA
26	O	321	LHG	C11-C10-C9-C8
26	Q	616	LHG	C15-C16-C17-C18
26	A	845	LHG	C11-C10-C9-C8
28	H	322	LMG	C30-C31-C32-C33
28	K	601	LMG	C30-C31-C32-C33
26	O	324	LHG	C2-C3-O3-P
27	A	857	LMU	O5'-C5'-C6'-O6'
25	B	847	DGD	C7B-C8B-C9B-CAB
26	P	601	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	J	104	LMU	C2-C3-C4-C5
28	B	856	LMG	C19-C20-C21-C22
28	F	408	LMG	C30-C31-C32-C33
28	I	614	LMG	C32-C33-C34-C35
28	I	615	LMG	C33-C34-C35-C36
26	A	846	LHG	O2-C2-C3-O3
26	G	614	LHG	C9-C10-C11-C12
26	W	420	LHG	C25-C26-C27-C28
28	I	615	LMG	C16-C17-C18-C19
28	T	616	LMG	C34-C35-C36-C37
22	L	417	CLA	C3-C5-C6-C7
22	R	602	CLA	C3-C5-C6-C7
26	K	616	LHG	C23-C24-C25-C26
22	A	823	CLA	O1D-CGD-O2D-CED
22	H	311	CLA	CBA-CGA-O2A-C1
26	G	614	LHG	C24-C23-O8-C6
26	O	318	LHG	C25-C26-C27-C28
26	A	846	LHG	C32-C33-C34-C35
27	F	409	LMU	C5-C6-C7-C8
28	I	615	LMG	C30-C31-C32-C33
28	J	101	LMG	C11-C12-C13-C14
28	J	101	LMG	C13-C14-C15-C16
28	K	601	LMG	C31-C32-C33-C34
28	L	401	LMG	C22-C23-C24-C25
22	A	840	CLA	C10-C11-C12-C13
22	B	826	CLA	O1A-CGA-O2A-C1
22	S	607	CLA	O1A-CGA-O2A-C1
22	H	303	CLA	C11-C12-C13-C15
22	N	610	CLA	C6-C7-C8-C9
22	Q	611	CLA	C6-C7-C8-C10
22	T	602	CLA	C16-C17-C18-C19
22	X	410	CLA	C11-C12-C13-C14
22	A	808	CLA	C16-C17-C18-C19
22	A	824	CLA	C16-C17-C18-C20
22	A	826	CLA	C16-C17-C18-C20
22	A	852	CLA	C16-C17-C18-C20
22	A	830	CLA	C4-C3-C5-C6
25	B	847	DGD	C9A-CAA-CBA-CCA
26	R	614	LHG	C15-C16-C17-C18
26	X	420	LHG	C28-C29-C30-C31
28	G	616	LMG	C41-C42-C43-C44
28	W	401	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	823	CLA	C14-C13-C15-C16
22	B	826	CLA	C6-C7-C8-C9
22	K	617	CLA	C11-C10-C8-C9
22	Q	604	CLA	C14-C13-C15-C16
22	V	603	CLA	C6-C7-C8-C9
22	W	410	CLA	C11-C10-C8-C9
22	A	806	CLA	C11-C12-C13-C14
22	A	830	CLA	C11-C12-C13-C14
22	N	604	CLA	O1D-CGD-O2D-CED
26	O	323	LHG	C7-C8-C9-C10
28	L	401	LMG	C10-C11-C12-C13
26	O	321	LHG	C14-C15-C16-C17
26	A	845	LHG	C14-C15-C16-C17
28	B	852	LMG	C18-C19-C20-C21
28	I	615	LMG	C18-C19-C20-C21
28	J	101	LMG	C18-C19-C20-C21
28	K	601	LMG	C17-C18-C19-C20
28	U	402	LMG	C30-C31-C32-C33
28	U	402	LMG	C33-C34-C35-C36
28	U	423	LMG	C30-C31-C32-C33
28	W	401	LMG	C38-C39-C40-C41
22	H	307	CLA	C5-C6-C7-C8
22	X	408	CLA	C15-C16-C17-C18
22	U	420	CLA	C2A-CAA-CBA-CGA
22	G	608	CLA	O1A-CGA-O2A-C1
22	O	311	CLA	O1A-CGA-O2A-C1
28	K	618	LMG	C36-C37-C38-C39
28	T	616	LMG	C29-C30-C31-C32
28	T	616	LMG	C32-C33-C34-C35
28	U	402	LMG	C18-C19-C20-C21
26	H	316	LHG	O1-C1-C2-C3
26	N	616	LHG	O1-C1-C2-C3
26	T	614	LHG	O1-C1-C2-C3
26	X	420	LHG	O1-C1-C2-C3
22	B	831	CLA	C3-C5-C6-C7
22	O	308	CLA	C3-C5-C6-C7
22	B	807	CLA	C15-C16-C17-C18
22	B	823	CLA	C10-C11-C12-C13
22	I	601	CLA	C5-C6-C7-C8
22	T	605	CLA	C5-C6-C7-C8
22	A	819	CLA	C8-C10-C11-C12
26	A	845	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	L	401	LMG	C17-C18-C19-C20
26	O	324	LHG	C7-C8-C9-C10
26	S	613	LHG	C23-C24-C25-C26
26	U	419	LHG	C23-C24-C25-C26
26	W	420	LHG	C7-C8-C9-C10
28	T	616	LMG	C28-C29-C30-C31
25	B	847	DGD	C6A-C7A-C8A-C9A
25	B	847	DGD	CBA-CCA-CDA-CEA
25	B	847	DGD	CAB-CBB-CCB-CDB
26	B	851	LHG	C15-C16-C17-C18
26	L	416	LHG	C15-C16-C17-C18
26	P	601	LHG	C12-C13-C14-C15
26	Q	616	LHG	C14-C15-C16-C17
27	L	419	LMU	C4-C5-C6-C7
28	H	319	LMG	C31-C32-C33-C34
28	I	615	LMG	C17-C18-C19-C20
28	I	615	LMG	C32-C33-C34-C35
28	J	101	LMG	C17-C18-C19-C20
28	J	101	LMG	C31-C32-C33-C34
28	K	618	LMG	C32-C33-C34-C35
28	K	622	LMG	C34-C35-C36-C37
28	N	615	LMG	C17-C18-C19-C20
28	T	616	LMG	C33-C34-C35-C36
28	U	402	LMG	C15-C16-C17-C18
28	W	401	LMG	C36-C37-C38-C39
22	F	405	CLA	C4B-C3B-CAB-CBB
22	H	306	CLA	C4B-C3B-CAB-CBB
22	H	313	CLA	C4B-C3B-CAB-CBB
22	L	409	CLA	C4B-C3B-CAB-CBB
22	Q	601	CLA	C4B-C3B-CAB-CBB
22	S	610	CLA	C4B-C3B-CAB-CBB
22	U	420	CLA	C4B-C3B-CAB-CBB
22	V	608	CLA	C4B-C3B-CAB-CBB
22	V	612	CLA	C4B-C3B-CAB-CBB
22	A	841	CLA	C4B-C3B-CAB-CBB
22	G	608	CLA	C11-C12-C13-C14
22	L	402	CLA	C16-C17-C18-C19
22	O	312	CLA	C11-C12-C13-C14
22	X	408	CLA	C16-C17-C18-C20
22	A	806	CLA	C16-C17-C18-C19
22	A	824	CLA	C16-C17-C18-C19
22	A	817	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	O	304	DGD	C2B-C3B-C4B-C5B
26	O	321	LHG	C31-C32-C33-C34
26	R	614	LHG	C11-C10-C9-C8
26	W	420	LHG	C34-C35-C36-C37
26	A	845	LHG	C25-C26-C27-C28
22	P	608	CLA	O1D-CGD-O2D-CED
25	B	847	DGD	C9B-CAB-CBB-CCB
26	X	420	LHG	C11-C10-C9-C8
26	A	845	LHG	C28-C29-C30-C31
26	A	846	LHG	C15-C16-C17-C18
28	F	408	LMG	C12-C13-C14-C15
28	G	616	LMG	C14-C15-C16-C17
28	I	615	LMG	C31-C32-C33-C34
28	W	401	LMG	C32-C33-C34-C35
22	R	602	CLA	O1A-CGA-O2A-C1
28	H	322	LMG	C29-C30-C31-C32
22	B	829	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	C3A-C2A-CAA-CBA
22	B	825	CLA	C3A-C2A-CAA-CBA
22	B	859	CLA	C3A-C2A-CAA-CBA
22	F	404	CLA	C3A-C2A-CAA-CBA
22	H	318	CLA	C3A-C2A-CAA-CBA
22	I	601	CLA	C3A-C2A-CAA-CBA
22	K	617	CLA	C3A-C2A-CAA-CBA
22	L	410	CLA	C3A-C2A-CAA-CBA
22	N	610	CLA	C3A-C2A-CAA-CBA
22	P	609	CLA	C3A-C2A-CAA-CBA
22	Q	613	CLA	C3A-C2A-CAA-CBA
22	S	606	CLA	C3A-C2A-CAA-CBA
22	S	607	CLA	C3A-C2A-CAA-CBA
22	S	609	CLA	C3A-C2A-CAA-CBA
22	U	405	CLA	C3A-C2A-CAA-CBA
22	V	603	CLA	C3A-C2A-CAA-CBA
22	X	404	CLA	C3A-C2A-CAA-CBA
22	A	807	CLA	C3A-C2A-CAA-CBA
22	A	818	CLA	C3A-C2A-CAA-CBA
22	A	838	CLA	C3A-C2A-CAA-CBA
22	A	844	CLA	C3A-C2A-CAA-CBA
22	A	852	CLA	C3A-C2A-CAA-CBA
22	Q	610	CLA	C13-C15-C16-C17
22	A	827	CLA	C8-C10-C11-C12
27	O	301	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
26	B	851	LHG	C12-C13-C14-C15
26	L	416	LHG	C14-C15-C16-C17
26	A	846	LHG	C31-C32-C33-C34
27	F	402	LMU	C2-C3-C4-C5
27	M	102	LMU	O1'-C1-C2-C3
28	F	408	LMG	C16-C17-C18-C19
26	T	614	LHG	C23-C24-C25-C26
22	X	408	CLA	O1A-CGA-O2A-C1
22	G	608	CLA	C11-C12-C13-C15
22	O	312	CLA	C11-C12-C13-C15
22	S	605	CLA	C11-C12-C13-C14
22	T	602	CLA	C16-C17-C18-C20
22	A	808	CLA	C16-C17-C18-C20
22	A	852	CLA	C16-C17-C18-C19
25	O	304	DGD	C3B-C4B-C5B-C6B
28	J	101	LMG	C33-C34-C35-C36
28	W	401	LMG	C30-C31-C32-C33
22	G	606	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	CBD-CGD-O2D-CED
26	A	845	LHG	C15-C16-C17-C18
22	Q	612	CLA	O1D-CGD-O2D-CED
22	B	817	CLA	C4-C3-C5-C6
22	H	307	CLA	C4-C3-C5-C6
22	H	311	CLA	C4-C3-C5-C6
22	I	603	CLA	C4-C3-C5-C6
22	V	609	CLA	C4-C3-C5-C6
22	B	835	CLA	CBA-CGA-O2A-C1
22	I	603	CLA	C2-C3-C5-C6
22	A	838	CLA	C2-C3-C5-C6
28	H	317	LMG	C11-C10-O7-C8
22	W	404	CLA	O1D-CGD-O2D-CED
26	O	321	LHG	C15-C16-C17-C18
26	B	848	LHG	O1-C1-C2-O2
26	O	324	LHG	O1-C1-C2-O2
26	P	601	LHG	O1-C1-C2-O2
26	S	613	LHG	O1-C1-C2-O2
26	T	614	LHG	O1-C1-C2-O2
22	A	836	CLA	C15-C16-C17-C18
26	K	616	LHG	C29-C30-C31-C32
26	K	616	LHG	C30-C31-C32-C33
28	H	322	LMG	C11-C12-C13-C14
28	K	618	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
28	N	615	LMG	C19-C20-C21-C22
22	A	830	CLA	O1D-CGD-O2D-CED
26	O	318	LHG	O10-C23-O8-C6
26	A	846	LHG	O10-C23-O8-C6
22	A	821	CLA	C16-C17-C18-C20
22	F	405	CLA	C2B-C3B-CAB-CBB
22	H	302	CLA	C2B-C3B-CAB-CBB
22	H	306	CLA	C2B-C3B-CAB-CBB
22	H	313	CLA	C2B-C3B-CAB-CBB
22	I	606	CLA	C2B-C3B-CAB-CBB
22	L	409	CLA	C2B-C3B-CAB-CBB
22	P	610	CLA	C2B-C3B-CAB-CBB
22	Q	601	CLA	C2B-C3B-CAB-CBB
22	S	606	CLA	C2B-C3B-CAB-CBB
22	S	610	CLA	C2B-C3B-CAB-CBB
22	U	420	CLA	C2B-C3B-CAB-CBB
22	V	608	CLA	C2B-C3B-CAB-CBB
22	V	611	CLA	C2B-C3B-CAB-CBB
22	V	612	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C2B-C3B-CAB-CBB
22	A	841	CLA	C2B-C3B-CAB-CBB
22	K	602	CLA	C10-C11-C12-C13
22	N	603	CLA	C10-C11-C12-C13
22	X	412	CLA	C5-C6-C7-C8
22	A	803	CLA	C5-C6-C7-C8
27	M	102	LMU	C5-C6-C7-C8
28	J	101	LMG	C30-C31-C32-C33
28	N	615	LMG	C15-C16-C17-C18
22	A	841	CLA	C3-C5-C6-C7
26	T	614	LHG	C28-C29-C30-C31
25	B	847	DGD	C1A-C2A-C3A-C4A
28	L	401	LMG	C28-C29-C30-C31
22	Q	613	CLA	CBD-CGD-O2D-CED
26	O	321	LHG	C1-C2-C3-O3
28	L	401	LMG	C34-C35-C36-C37
28	U	423	LMG	C18-C19-C20-C21
28	B	856	LMG	O9-C10-O7-C8
26	K	619	LHG	C10-C11-C12-C13
26	N	616	LHG	C26-C27-C28-C29
26	O	323	LHG	C10-C11-C12-C13
22	U	411	CLA	C5-C6-C7-C8
22	W	409	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	844	CLA	C5-C6-C7-C8
22	B	810	CLA	O1A-CGA-O2A-C1
25	O	304	DGD	CDA-CEA-CFA-CGA
28	H	319	LMG	C29-C30-C31-C32
28	I	615	LMG	C22-C23-C24-C25
28	K	618	LMG	C39-C40-C41-C42
28	N	615	LMG	C13-C14-C15-C16
26	O	318	LHG	C23-C24-C25-C26
21	B	846	BCR	C5-C6-C7-C8
21	B	846	BCR	C23-C24-C25-C26
21	B	846	BCR	C23-C24-C25-C30
21	J	103	BCR	C1-C6-C7-C8
21	J	103	BCR	C5-C6-C7-C8
21	M	101	BCR	C23-C24-C25-C30
21	A	850	BCR	C23-C24-C25-C26
21	A	850	BCR	C23-C24-C25-C30
22	K	603	CLA	C3-C5-C6-C7
22	K	610	CLA	C3-C5-C6-C7
22	N	607	CLA	C3-C5-C6-C7
22	U	406	CLA	C3-C5-C6-C7
22	V	612	CLA	C3-C5-C6-C7
22	A	811	CLA	C3-C5-C6-C7
27	M	102	LMU	O5'-C5'-C6'-O6'
28	H	317	LMG	C30-C31-C32-C33
22	B	803	CLA	CBA-CGA-O2A-C1
22	B	804	CLA	CBA-CGA-O2A-C1
22	H	309	CLA	CBA-CGA-O2A-C1
22	K	607	CLA	CBA-CGA-O2A-C1
22	B	828	CLA	C13-C15-C16-C17
22	B	833	CLA	C15-C16-C17-C18
22	Q	610	CLA	C5-C6-C7-C8
22	W	405	CLA	C5-C6-C7-C8
22	W	411	CLA	C8-C10-C11-C12
28	K	618	LMG	C11-C10-O7-C8
28	I	614	LMG	C31-C32-C33-C34
22	H	311	CLA	O1A-CGA-O2A-C1
26	G	614	LHG	O10-C23-O8-C6
22	I	603	CLA	C11-C10-C8-C9
26	O	323	LHG	C28-C29-C30-C31
28	K	601	LMG	C29-C30-C31-C32
22	B	805	CLA	C15-C16-C17-C18
22	B	832	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	A	835	CLA	C4-C3-C5-C6
22	B	812	CLA	C2-C3-C5-C6
22	B	816	CLA	C12-C13-C15-C16
22	B	822	CLA	C11-C12-C13-C15
22	B	826	CLA	C6-C7-C8-C10
22	B	832	CLA	C6-C7-C8-C10
22	H	311	CLA	C2-C3-C5-C6
22	I	606	CLA	C2-C3-C5-C6
22	K	605	CLA	C6-C7-C8-C10
22	K	609	CLA	C11-C10-C8-C7
22	K	611	CLA	C6-C7-C8-C10
22	K	611	CLA	C12-C13-C15-C16
22	K	617	CLA	C11-C10-C8-C7
22	L	411	CLA	C11-C12-C13-C15
22	N	603	CLA	C6-C7-C8-C10
22	O	311	CLA	C2-C3-C5-C6
22	Q	604	CLA	C12-C13-C15-C16
22	Q	609	CLA	C11-C10-C8-C7
22	Q	612	CLA	C11-C12-C13-C15
22	R	601	CLA	C11-C10-C8-C7
22	T	603	CLA	C11-C10-C8-C7
22	T	607	CLA	C6-C7-C8-C10
22	V	602	CLA	C11-C12-C13-C15
22	V	603	CLA	C6-C7-C8-C10
22	W	414	CLA	C11-C12-C13-C15
22	A	806	CLA	C6-C7-C8-C10
22	A	811	CLA	C6-C7-C8-C10
22	A	816	CLA	C11-C12-C13-C15
22	A	819	CLA	C11-C10-C8-C7
22	A	820	CLA	C2-C3-C5-C6
22	A	825	CLA	C11-C10-C8-C7
22	A	828	CLA	C2-C3-C5-C6
22	A	830	CLA	C2-C3-C5-C6
22	A	830	CLA	C11-C12-C13-C15
22	A	831	CLA	C11-C10-C8-C7
22	A	840	CLA	C11-C12-C13-C15
22	B	859	CLA	C3-C5-C6-C7
22	B	804	CLA	O1A-CGA-O2A-C1
22	B	835	CLA	O1A-CGA-O2A-C1
22	K	607	CLA	O1A-CGA-O2A-C1
28	U	402	LMG	C16-C17-C18-C19
22	B	817	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	Q	612	CLA	C8-C10-C11-C12
22	W	414	CLA	C10-C11-C12-C13
22	H	303	CLA	C11-C12-C13-C14
22	N	610	CLA	C6-C7-C8-C10
22	H	309	CLA	O1D-CGD-O2D-CED
22	U	406	CLA	O1D-CGD-O2D-CED
22	O	305	CLA	CBA-CGA-O2A-C1
22	R	603	CLA	CBA-CGA-O2A-C1
22	T	604	CLA	CBA-CGA-O2A-C1
22	T	605	CLA	CBA-CGA-O2A-C1
26	O	324	LHG	C24-C23-O8-C6
28	K	601	LMG	C29-C28-O8-C9
28	I	614	LMG	C12-C13-C14-C15
28	U	423	LMG	C31-C32-C33-C34
22	B	826	CLA	C2A-CAA-CBA-CGA
22	N	610	CLA	C2A-CAA-CBA-CGA
22	S	610	CLA	C2A-CAA-CBA-CGA
22	U	414	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	C2A-CAA-CBA-CGA
22	A	814	CLA	C2A-CAA-CBA-CGA
22	A	820	CLA	C2A-CAA-CBA-CGA
22	T	604	CLA	C10-C11-C12-C13
22	A	814	CLA	C15-C16-C17-C18
26	B	851	LHG	C14-C15-C16-C17
28	F	408	LMG	C18-C19-C20-C21
28	K	601	LMG	C16-C17-C18-C19
22	O	308	CLA	C12-C13-C15-C16
22	R	603	CLA	C11-C10-C8-C7
22	U	414	CLA	C12-C13-C15-C16
22	A	825	CLA	C12-C13-C15-C16
28	U	423	LMG	C10-C11-C12-C13
22	X	410	CLA	O1D-CGD-O2D-CED
28	K	622	LMG	C29-C30-C31-C32
26	X	420	LHG	C26-C27-C28-C29
28	H	319	LMG	C14-C15-C16-C17
28	J	101	LMG	C14-C15-C16-C17
27	B	855	LMU	O5'-C5'-C6'-O6'
22	K	604	CLA	CBD-CGD-O2D-CED
22	B	832	CLA	CBA-CGA-O2A-C1
22	A	820	CLA	C16-C17-C18-C20
28	I	615	LMG	O6-C1-O1-C7
22	B	816	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	B	817	CLA	C15-C16-C17-C18
22	V	603	CLA	O1D-CGD-O2D-CED
26	O	321	LHG	C9-C10-C11-C12
26	P	601	LHG	C10-C11-C12-C13
28	B	852	LMG	C21-C22-C23-C24
28	H	317	LMG	C39-C40-C41-C42
26	X	420	LHG	C8-C7-O7-C5
28	I	614	LMG	C11-C10-O7-C8
28	U	423	LMG	C11-C10-O7-C8
28	L	401	LMG	O6-C5-C6-O5
27	L	419	LMU	C7-C8-C9-C10
28	G	616	LMG	C36-C37-C38-C39
28	U	402	LMG	C17-C18-C19-C20
22	A	812	CLA	C5-C6-C7-C8
22	L	405	CLA	CBD-CGD-O2D-CED
22	X	402	CLA	CBD-CGD-O2D-CED
26	G	614	LHG	C12-C13-C14-C15
28	H	319	LMG	O9-C10-O7-C8
25	B	847	DGD	CCB-CDB-CEB-CFB
25	F	401	DGD	O2G-C2G-C3G-O3G
26	O	321	LHG	O7-C5-C6-O8
28	B	852	LMG	O7-C8-C9-O8
28	B	856	LMG	O1-C7-C8-O7
28	G	616	LMG	O7-C8-C9-O8
28	Q	602	LMG	O1-C7-C8-O7
27	U	421	LMU	O5'-C5'-C6'-O6'
22	B	812	CLA	C16-C17-C18-C19
25	F	401	DGD	CCA-CDA-CEA-CFA
27	H	320	LMU	O5'-C5'-C6'-O6'
22	I	606	CLA	C4-C3-C5-C6
22	L	404	CLA	C4-C3-C5-C6
22	O	311	CLA	C4-C3-C5-C6
22	Q	604	CLA	C4-C3-C5-C6
22	A	820	CLA	C4-C3-C5-C6
22	A	828	CLA	C4-C3-C5-C6
28	A	855	LMG	C4-C5-C6-O5
22	G	603	CLA	C2-C3-C5-C6
22	H	307	CLA	C2-C3-C5-C6
24	J	105	DD6	C27-C29-C30-C31
24	L	413	DD6	C27-C29-C30-C31
24	L	414	DD6	C27-C29-C30-C31
24	L	415	DD6	C27-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	P	612	DD6	C27-C29-C30-C31
24	R	612	DD6	C27-C29-C30-C31
24	S	612	DD6	C27-C29-C30-C31
24	U	416	DD6	C27-C29-C30-C31
24	U	417	DD6	C27-C29-C30-C31
24	W	416	DD6	C27-C29-C30-C31
24	A	859	DD6	C27-C29-C30-C31
28	W	401	LMG	C31-C32-C33-C34
22	B	812	CLA	C14-C13-C15-C16
22	B	822	CLA	C11-C12-C13-C14
22	I	606	CLA	C6-C7-C8-C9
22	K	609	CLA	C11-C10-C8-C9
22	K	611	CLA	C14-C13-C15-C16
22	L	408	CLA	C11-C10-C8-C9
22	N	603	CLA	C6-C7-C8-C9
22	O	308	CLA	C11-C12-C13-C14
22	Q	604	CLA	C11-C10-C8-C9
22	Q	612	CLA	C11-C12-C13-C14
22	R	615	CLA	C14-C13-C15-C16
22	T	604	CLA	C14-C13-C15-C16
22	T	607	CLA	C6-C7-C8-C9
22	V	602	CLA	C11-C12-C13-C14
22	W	414	CLA	C11-C12-C13-C14
22	A	803	CLA	C14-C13-C15-C16
22	A	806	CLA	C6-C7-C8-C9
22	A	813	CLA	C11-C10-C8-C9
22	A	819	CLA	C11-C10-C8-C9
22	A	824	CLA	C6-C7-C8-C9
22	A	825	CLA	C11-C10-C8-C9
22	A	831	CLA	C11-C10-C8-C9
22	B	820	CLA	CBD-CGD-O2D-CED
26	N	616	LHG	C15-C16-C17-C18
26	S	613	LHG	C10-C11-C12-C13
26	A	846	LHG	C34-C35-C36-C37
27	B	854	LMU	C6-C7-C8-C9
28	U	402	LMG	C34-C35-C36-C37
28	U	423	LMG	C19-C20-C21-C22
22	A	803	CLA	C8-C10-C11-C12
22	B	807	CLA	C3-C5-C6-C7
22	F	404	CLA	C3-C5-C6-C7
22	B	811	CLA	C2A-CAA-CBA-CGA
22	A	819	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	F	401	DGD	CBA-CCA-CDA-CEA
26	P	601	LHG	C9-C10-C11-C12
26	T	614	LHG	C11-C12-C13-C14
28	G	616	LMG	C31-C32-C33-C34
28	A	855	LMG	C33-C34-C35-C36
22	H	313	CLA	CBA-CGA-O2A-C1
22	N	607	CLA	CBA-CGA-O2A-C1
24	J	105	DD6	C12-C11-C13-C14
22	R	605	CLA	O1D-CGD-O2D-CED
22	S	607	CLA	C8-C10-C11-C12
22	X	407	CLA	C15-C16-C17-C18
22	P	611	CLA	C4C-C3C-CAC-CBC
26	T	614	LHG	C12-C13-C14-C15
26	A	846	LHG	C14-C15-C16-C17
28	L	401	LMG	C32-C33-C34-C35
24	J	105	DD6	C10-C11-C13-C14
22	H	309	CLA	O1A-CGA-O2A-C1
22	B	804	CLA	C1A-C2A-CAA-CBA
22	B	816	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	824	CLA	C1A-C2A-CAA-CBA
22	B	827	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	859	CLA	C1A-C2A-CAA-CBA
22	F	404	CLA	C1A-C2A-CAA-CBA
22	G	611	CLA	C1A-C2A-CAA-CBA
22	H	318	CLA	C1A-C2A-CAA-CBA
22	K	617	CLA	C1A-C2A-CAA-CBA
22	L	412	CLA	C1A-C2A-CAA-CBA
22	N	610	CLA	C1A-C2A-CAA-CBA
22	O	308	CLA	C1A-C2A-CAA-CBA
22	P	602	CLA	C1A-C2A-CAA-CBA
22	P	608	CLA	C1A-C2A-CAA-CBA
22	P	609	CLA	C1A-C2A-CAA-CBA
22	Q	618	CLA	C1A-C2A-CAA-CBA
22	R	602	CLA	C1A-C2A-CAA-CBA
22	R	607	CLA	C1A-C2A-CAA-CBA
22	S	609	CLA	C1A-C2A-CAA-CBA
22	T	611	CLA	C1A-C2A-CAA-CBA
22	U	405	CLA	C1A-C2A-CAA-CBA
22	V	603	CLA	C1A-C2A-CAA-CBA
22	V	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	W	410	CLA	C1A-C2A-CAA-CBA
22	X	404	CLA	C1A-C2A-CAA-CBA
22	X	405	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	C1A-C2A-CAA-CBA
22	A	827	CLA	C1A-C2A-CAA-CBA
22	A	842	CLA	C1A-C2A-CAA-CBA
22	A	844	CLA	C1A-C2A-CAA-CBA
28	Q	602	LMG	O6-C5-C6-O5
22	X	408	CLA	C16-C17-C18-C19
22	A	810	CLA	C16-C17-C18-C20
22	A	820	CLA	C16-C17-C18-C19
26	X	420	LHG	O9-C7-O7-C5
28	Q	602	LMG	O9-C10-O7-C8
26	A	845	LHG	C8-C7-O7-C5
22	G	608	CLA	C8-C10-C11-C12
22	L	402	CLA	C8-C10-C11-C12
22	A	829	CLA	C10-C11-C12-C13
26	L	416	LHG	C3-O3-P-O6
26	O	321	LHG	C3-O3-P-O6
26	O	323	LHG	C4-O6-P-O3
26	A	845	LHG	C4-O6-P-O3
28	B	856	LMG	C34-C35-C36-C37
28	F	408	LMG	C31-C32-C33-C34
25	F	401	DGD	C1A-C2A-C3A-C4A
22	G	601	CLA	O1D-CGD-O2D-CED
22	B	803	CLA	O1A-CGA-O2A-C1
27	B	849	LMU	C1-C2-C3-C4
22	U	404	CLA	C10-C11-C12-C13
22	A	821	CLA	C15-C16-C17-C18
22	A	819	CLA	CBA-CGA-O2A-C1
26	K	619	LHG	O6-C4-C5-C6
26	X	420	LHG	O6-C4-C5-C6
25	B	847	DGD	CDA-CEA-CFA-CGA
26	Q	616	LHG	C29-C30-C31-C32
27	B	850	LMU	C3-C4-C5-C6
28	Q	602	LMG	C29-C30-C31-C32
28	Q	602	LMG	C4-C5-C6-O5
27	A	854	LMU	C5-C6-C7-C8
28	J	101	LMG	C39-C40-C41-C42
22	O	310	CLA	O1D-CGD-O2D-CED
26	K	616	LHG	C25-C26-C27-C28
22	K	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	W	411	CLA	C10-C11-C12-C13
28	A	855	LMG	C10-C11-C12-C13
26	X	420	LHG	C10-C11-C12-C13
28	G	616	LMG	C29-C30-C31-C32
22	A	806	CLA	CBA-CGA-O2A-C1
26	O	324	LHG	O10-C23-O8-C6
26	A	846	LHG	C1-C2-C3-O3
27	O	322	LMU	O5'-C5'-C6'-O6'
22	B	812	CLA	C4-C3-C5-C6
22	W	402	CLA	C4-C3-C5-C6
22	B	817	CLA	C2-C3-C5-C6
26	A	846	LHG	C28-C29-C30-C31
22	A	819	CLA	O1D-CGD-O2D-CED
27	T	617	LMU	C2-C3-C4-C5
28	W	401	LMG	C29-C30-C31-C32
28	K	601	LMG	C10-C11-C12-C13
22	T	604	CLA	O1A-CGA-O2A-C1
26	B	851	LHG	C28-C29-C30-C31
28	I	614	LMG	C29-C30-C31-C32
28	K	618	LMG	C31-C32-C33-C34
28	K	622	LMG	C32-C33-C34-C35
28	N	615	LMG	C12-C13-C14-C15
22	B	817	CLA	C16-C17-C18-C20
22	A	822	CLA	C16-C17-C18-C20
22	T	601	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	C6A-C7A-C8A-C9A
25	O	304	DGD	O1G-C1G-C2G-C3G
26	B	851	LHG	C4-C5-C6-O8
26	K	616	LHG	C4-C5-C6-O8
26	L	416	LHG	C4-C5-C6-O8
26	N	614	LHG	C4-C5-C6-O8
26	R	614	LHG	C4-C5-C6-O8
28	B	852	LMG	C7-C8-C9-O8
28	B	856	LMG	O1-C7-C8-C9
28	G	616	LMG	O1-C7-C8-C9
28	H	319	LMG	O1-C7-C8-C9
28	H	322	LMG	C7-C8-C9-O8
28	N	615	LMG	O1-C7-C8-C9
28	U	402	LMG	C7-C8-C9-O8
30	K	621	SQD	C44-C45-C46-O48
30	O	302	SQD	C44-C45-C46-O48
22	B	828	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	N	616	LHG	C7-C8-C9-C10
22	R	603	CLA	O1A-CGA-O2A-C1
25	B	847	DGD	C5D-C6D-O5D-C1E
25	O	304	DGD	C2G-C3G-O3G-C1D
28	H	322	LMG	C8-C7-O1-C1
26	O	318	LHG	C11-C10-C9-C8
26	O	321	LHG	C33-C34-C35-C36
26	R	614	LHG	C28-C29-C30-C31
28	B	856	LMG	C37-C38-C39-C40
28	U	402	LMG	C40-C41-C42-C43
22	B	859	CLA	CBD-CGD-O2D-CED
22	A	820	CLA	C15-C16-C17-C18
22	R	603	CLA	C11-C10-C8-C9
28	K	618	LMG	C18-C19-C20-C21
27	F	409	LMU	O5'-C5'-C6'-O6'
28	H	319	LMG	C10-C11-C12-C13
22	T	605	CLA	O1A-CGA-O2A-C1
22	L	410	CLA	C3-C5-C6-C7
28	T	616	LMG	C4-C5-C6-O5
27	T	617	LMU	O5'-C1'-O1'-C1
28	F	408	LMG	O6-C1-O1-C7
28	N	615	LMG	O6-C1-O1-C7
22	Q	604	CLA	C10-C11-C12-C13
22	A	831	CLA	C5-C6-C7-C8
26	P	601	LHG	C11-C10-C9-C8
26	X	420	LHG	C12-C13-C14-C15
27	K	620	LMU	O5B-C5B-C6B-O6B
27	U	422	LMU	O5B-C5B-C6B-O6B
27	W	421	LMU	O5'-C5'-C6'-O6'
28	H	319	LMG	O6-C5-C6-O5
26	O	323	LHG	O1-C1-C2-O2
26	Q	616	LHG	O1-C1-C2-O2
26	L	416	LHG	C12-C13-C14-C15
26	A	846	LHG	C25-C26-C27-C28
22	B	832	CLA	O1A-CGA-O2A-C1
22	O	305	CLA	O1A-CGA-O2A-C1
27	O	322	LMU	C2B-C1B-O1B-C4'
26	A	845	LHG	C17-C18-C19-C20
28	B	856	LMG	C38-C39-C40-C41
22	T	607	CLA	O1D-CGD-O2D-CED
22	X	409	CLA	C5-C6-C7-C8
27	O	303	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
27	O	303	LMU	O5'-C5'-C6'-O6'
28	B	856	LMG	O6-C5-C6-O5
28	K	618	LMG	O6-C5-C6-O5
22	G	603	CLA	C4-C3-C5-C6
22	N	610	CLA	C4-C3-C5-C6
22	Q	617	CLA	C4-C3-C5-C6
22	A	822	CLA	C4-C3-C5-C6
28	F	408	LMG	C29-C30-C31-C32
22	W	413	CLA	O1D-CGD-O2D-CED
28	H	319	LMG	C28-C29-C30-C31
22	Q	604	CLA	C16-C17-C18-C19
22	S	605	CLA	C11-C12-C13-C15
22	B	816	CLA	CBA-CGA-O2A-C1
22	B	827	CLA	CBA-CGA-O2A-C1
27	L	419	LMU	O5'-C5'-C6'-O6'
27	U	424	LMU	O5'-C5'-C6'-O6'
26	R	614	LHG	C9-C10-C11-C12
22	B	812	CLA	C15-C16-C17-C18
22	A	805	CLA	C5-C6-C7-C8
25	O	304	DGD	C6B-C7B-C8B-C9B
27	M	102	LMU	C4-C5-C6-C7
28	F	408	LMG	C32-C33-C34-C35
28	I	615	LMG	C38-C39-C40-C41
26	W	420	LHG	C6-C5-O7-C7
28	K	601	LMG	C9-C8-O7-C10
22	A	833	CLA	C2A-CAA-CBA-CGA
22	N	607	CLA	O1A-CGA-O2A-C1
22	R	615	CLA	C13-C15-C16-C17
22	A	835	CLA	O1D-CGD-O2D-CED
28	K	601	LMG	O6-C5-C6-O5
26	O	321	LHG	C10-C11-C12-C13
28	N	615	LMG	C16-C17-C18-C19
22	K	612	CLA	O1D-CGD-O2D-CED
22	L	410	CLA	O1D-CGD-O2D-CED
22	Q	601	CLA	O1D-CGD-O2D-CED
27	B	858	LMU	O1'-C1-C2-C3
28	B	856	LMG	C17-C18-C19-C20
28	G	616	LMG	C42-C43-C44-C45
22	V	612	CLA	CBA-CGA-O2A-C1
22	A	816	CLA	CBA-CGA-O2A-C1
22	P	609	CLA	O1D-CGD-O2D-CED
26	A	846	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	N	615	LMG	C31-C32-C33-C34
25	O	304	DGD	CCA-CDA-CEA-CFA
22	H	313	CLA	O1A-CGA-O2A-C1
25	B	847	DGD	CEA-CFA-CGA-CHA
22	L	417	CLA	C8-C10-C11-C12
27	K	620	LMU	C2'-C1'-O1'-C1
28	K	622	LMG	C2-C1-O1-C7
26	T	614	LHG	C35-C36-C37-C38
26	B	848	LHG	O8-C23-C24-C25
25	O	304	DGD	O1G-C1G-C2G-O2G
26	K	619	LHG	O7-C5-C6-O8
28	F	408	LMG	O7-C8-C9-O8
30	O	302	SQD	O47-C45-C46-O48
26	U	419	LHG	C3-O3-P-O5
28	H	319	LMG	C17-C18-C19-C20
22	A	806	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	O1A-CGA-O2A-C1
22	A	826	CLA	C16-C17-C18-C19
33	A	802	CL0	CHA-CBD-CGD-O1D
33	A	802	CL0	CHA-CBD-CGD-O2D
25	B	847	DGD	CFA-CGA-CHA-CIA
26	K	616	LHG	C28-C29-C30-C31
28	B	856	LMG	C16-C17-C18-C19
28	J	101	LMG	C34-C35-C36-C37
28	K	618	LMG	C38-C39-C40-C41
28	U	423	LMG	C34-C35-C36-C37
22	U	401	CLA	C4-C3-C5-C6
22	A	836	CLA	C4-C3-C5-C6
33	A	802	CL0	C4-C3-C5-C6
28	I	614	LMG	C30-C31-C32-C33
22	B	813	CLA	C6-C7-C8-C10
22	B	821	CLA	C6-C7-C8-C10
22	B	823	CLA	C12-C13-C15-C16
22	B	824	CLA	C12-C13-C15-C16
22	B	830	CLA	C11-C12-C13-C15
22	B	832	CLA	C11-C10-C8-C7
22	B	835	CLA	C12-C13-C15-C16
22	G	606	CLA	C11-C12-C13-C15
22	G	608	CLA	C11-C10-C8-C7
22	I	606	CLA	C6-C7-C8-C10
22	L	402	CLA	C11-C10-C8-C7
22	L	402	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	L	408	CLA	C6-C7-C8-C10
22	L	417	CLA	C6-C7-C8-C10
22	Q	612	CLA	C12-C13-C15-C16
22	R	601	CLA	C6-C7-C8-C10
22	R	605	CLA	C6-C7-C8-C10
22	R	606	CLA	C6-C7-C8-C10
22	T	604	CLA	C12-C13-C15-C16
22	U	414	CLA	C11-C12-C13-C15
22	W	410	CLA	C11-C10-C8-C7
22	X	408	CLA	C6-C7-C8-C10
22	X	412	CLA	C11-C12-C13-C15
22	A	803	CLA	C12-C13-C15-C16
22	A	804	CLA	C11-C10-C8-C7
22	A	808	CLA	C12-C13-C15-C16
22	A	815	CLA	C11-C10-C8-C7
22	A	825	CLA	C11-C12-C13-C15
22	A	835	CLA	C2-C3-C5-C6
22	A	835	CLA	C11-C12-C13-C15
22	A	836	CLA	C11-C12-C13-C15
22	A	839	CLA	C12-C13-C15-C16
22	A	840	CLA	C11-C10-C8-C7
22	A	852	CLA	C11-C12-C13-C15
23	A	843	PQN	C17-C18-C20-C21
27	X	421	LMU	C1-C2-C3-C4
28	I	615	LMG	C37-C38-C39-C40
28	N	615	LMG	C30-C31-C32-C33
22	B	824	CLA	C14-C13-C15-C16
22	B	825	CLA	C11-C12-C13-C14
22	B	828	CLA	C11-C10-C8-C9
22	B	831	CLA	C6-C7-C8-C9
22	B	831	CLA	C11-C10-C8-C9
22	B	832	CLA	C11-C10-C8-C9
22	B	835	CLA	C11-C10-C8-C9
22	B	835	CLA	C14-C13-C15-C16
22	B	859	CLA	C14-C13-C15-C16
22	G	608	CLA	C6-C7-C8-C9
22	G	608	CLA	C11-C10-C8-C9
22	H	303	CLA	C6-C7-C8-C9
22	H	303	CLA	C11-C10-C8-C9
22	H	308	CLA	C11-C10-C8-C9
22	H	311	CLA	C6-C7-C8-C9
22	K	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	L	402	CLA	C14-C13-C15-C16
22	L	408	CLA	C6-C7-C8-C9
22	L	410	CLA	C11-C10-C8-C9
22	L	411	CLA	C11-C12-C13-C14
22	L	417	CLA	C6-C7-C8-C9
22	N	607	CLA	C6-C7-C8-C9
22	Q	609	CLA	C11-C10-C8-C9
22	R	601	CLA	C6-C7-C8-C9
22	R	605	CLA	C6-C7-C8-C9
22	T	604	CLA	C6-C7-C8-C9
22	U	404	CLA	C11-C10-C8-C9
22	V	612	CLA	C14-C13-C15-C16
22	W	404	CLA	C14-C13-C15-C16
22	X	407	CLA	C11-C12-C13-C14
22	X	408	CLA	C6-C7-C8-C9
22	A	801	CLA	C11-C10-C8-C9
22	A	803	CLA	C6-C7-C8-C9
22	A	810	CLA	C11-C12-C13-C14
22	A	811	CLA	C6-C7-C8-C9
22	A	815	CLA	C11-C10-C8-C9
22	A	829	CLA	C11-C12-C13-C14
22	A	852	CLA	C6-C7-C8-C9
23	A	843	PQN	C19-C18-C20-C21
22	O	313	CLA	CBD-CGD-O2D-CED
30	F	407	SQD	C7-C8-C9-C10
27	U	421	LMU	C2-C3-C4-C5
22	B	809	CLA	CBA-CGA-O2A-C1
22	Q	612	CLA	CBA-CGA-O2A-C1
22	A	840	CLA	C8-C10-C11-C12
22	B	815	CLA	C2A-CAA-CBA-CGA
26	A	846	LHG	C11-C10-C9-C8
27	W	421	LMU	C4-C5-C6-C7
22	P	604	CLA	O1D-CGD-O2D-CED
22	S	601	CLA	CBD-CGD-O2D-CED
24	N	613	DD6	C12-C11-C13-C14
24	A	858	DD6	C12-C11-C13-C14
22	B	817	CLA	C16-C17-C18-C19
22	O	306	CLA	C11-C12-C13-C15
22	Q	604	CLA	C16-C17-C18-C20
24	F	406	DD6	C10-C11-C13-C14
24	N	613	DD6	C10-C11-C13-C14
24	A	858	DD6	C10-C11-C13-C14

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Mol	Chain	Res	Type	Atoms
22	O	313	CLA	C3-C5-C6-C7
22	N	608	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	C13-C15-C16-C17
28	H	317	LMG	C36-C37-C38-C39
28	Q	602	LMG	C32-C33-C34-C35
22	L	402	CLA	CBA-CGA-O2A-C1
22	S	604	CLA	CBA-CGA-O2A-C1
22	W	412	CLA	CBA-CGA-O2A-C1
22	A	836	CLA	CBA-CGA-O2A-C1
27	B	858	LMU	C2'-C1'-O1'-C1
28	B	852	LMG	C19-C20-C21-C22
28	W	401	LMG	C33-C34-C35-C36
22	O	313	CLA	C13-C15-C16-C17
22	R	615	CLA	C8-C10-C11-C12
22	W	411	CLA	C5-C6-C7-C8
28	K	622	LMG	C14-C15-C16-C17
26	L	416	LHG	C27-C28-C29-C30
30	K	621	SQD	C11-C10-C9-C8
22	B	837	CLA	C4B-C3B-CAB-CBB
22	H	302	CLA	C4B-C3B-CAB-CBB
22	K	605	CLA	C4B-C3B-CAB-CBB
22	P	603	CLA	C4B-C3B-CAB-CBB
22	P	610	CLA	C4B-C3B-CAB-CBB
22	Q	607	CLA	C4B-C3B-CAB-CBB
22	Q	613	CLA	C4B-C3B-CAB-CBB
22	R	607	CLA	C4B-C3B-CAB-CBB
22	S	606	CLA	C4B-C3B-CAB-CBB
22	S	609	CLA	C4B-C3B-CAB-CBB
22	T	610	CLA	C4B-C3B-CAB-CBB
22	U	415	CLA	C4B-C3B-CAB-CBB
22	V	601	CLA	C4B-C3B-CAB-CBB
22	V	610	CLA	C4B-C3B-CAB-CBB
22	V	611	CLA	C4B-C3B-CAB-CBB
22	A	824	CLA	C4B-C3B-CAB-CBB
22	A	834	CLA	C4B-C3B-CAB-CBB
22	A	837	CLA	C4B-C3B-CAB-CBB
22	B	817	CLA	C13-C15-C16-C17
26	P	601	LHG	O6-C4-C5-C6
22	B	832	CLA	C3-C5-C6-C7
22	N	610	CLA	C3-C5-C6-C7
22	O	312	CLA	C3-C5-C6-C7
28	J	101	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
27	J	104	LMU	C7-C8-C9-C10
22	A	816	CLA	C8-C10-C11-C12
28	H	322	LMG	C31-C32-C33-C34
28	J	101	LMG	C37-C38-C39-C40
22	A	832	CLA	C4-C3-C5-C6
22	L	404	CLA	C2-C3-C5-C6
22	Q	617	CLA	C2-C3-C5-C6
22	V	609	CLA	C2-C3-C5-C6
22	A	836	CLA	C2-C3-C5-C6
33	A	802	CL0	C2-C3-C5-C6
26	X	420	LHG	C9-C10-C11-C12
28	G	616	LMG	C40-C41-C42-C43
22	V	604	CLA	C11-C10-C8-C9
22	A	816	CLA	C14-C13-C15-C16
22	A	825	CLA	C14-C13-C15-C16
22	B	827	CLA	O1A-CGA-O2A-C1
22	K	608	CLA	O1D-CGD-O2D-CED
22	W	403	CLA	O1D-CGD-O2D-CED
22	X	412	CLA	C16-C17-C18-C19
25	B	847	DGD	C4A-C5A-C6A-C7A
26	N	616	LHG	C28-C29-C30-C31
28	H	322	LMG	C32-C33-C34-C35
28	K	618	LMG	C16-C17-C18-C19
28	L	401	LMG	C15-C16-C17-C18
31	W	408	CHL	C8-C10-C11-C12
26	P	601	LHG	O8-C23-C24-C25
26	K	616	LHG	C9-C10-C11-C12
22	J	102	CLA	C3A-C2A-CAA-CBA
22	K	609	CLA	C3A-C2A-CAA-CBA
22	L	412	CLA	C3A-C2A-CAA-CBA
22	P	605	CLA	C3A-C2A-CAA-CBA
22	V	608	CLA	C3A-C2A-CAA-CBA
22	V	617	CLA	C3A-C2A-CAA-CBA
22	W	410	CLA	C3A-C2A-CAA-CBA
28	J	101	LMG	C29-C30-C31-C32
27	B	857	LMU	C2-C1-O1'-C1'
25	B	847	DGD	CFB-CGB-CHB-CIB
28	G	616	LMG	C30-C31-C32-C33
28	G	616	LMG	C4-C5-C6-O5
22	B	834	CLA	C13-C15-C16-C17
22	V	612	CLA	O1A-CGA-O2A-C1
28	B	852	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
22	H	305	CLA	CBA-CGA-O2A-C1
28	I	615	LMG	C34-C35-C36-C37
22	K	604	CLA	C2A-CAA-CBA-CGA
25	F	401	DGD	C1G-C2G-C3G-O3G
25	O	304	DGD	C1G-C2G-C3G-O3G
26	O	321	LHG	C4-C5-C6-O8
26	P	601	LHG	C4-C5-C6-O8
26	W	420	LHG	C4-C5-C6-O8
28	B	852	LMG	O1-C7-C8-C9
28	F	408	LMG	C7-C8-C9-O8
28	H	319	LMG	C7-C8-C9-O8
28	K	601	LMG	O1-C7-C8-C9
28	K	601	LMG	C7-C8-C9-O8
28	Q	602	LMG	O1-C7-C8-C9
28	G	616	LMG	C32-C33-C34-C35
26	A	846	LHG	C29-C30-C31-C32
26	O	324	LHG	C27-C28-C29-C30
22	W	411	CLA	C4-C3-C5-C6
25	F	401	DGD	C3A-C4A-C5A-C6A
26	G	614	LHG	C3-O3-P-O6
26	P	601	LHG	C4-O6-P-O3
28	B	856	LMG	C28-C29-C30-C31
22	B	816	CLA	O1A-CGA-O2A-C1
22	A	816	CLA	O1A-CGA-O2A-C1
28	K	601	LMG	C32-C33-C34-C35
22	G	608	CLA	C2A-CAA-CBA-CGA
26	K	619	LHG	O1-C1-C2-O2
26	N	616	LHG	O1-C1-C2-O2
22	O	313	CLA	C5-C6-C7-C8
22	A	808	CLA	C10-C11-C12-C13
28	N	615	LMG	C21-C22-C23-C24
26	O	324	LHG	O6-C4-C5-O7
26	Q	616	LHG	O6-C4-C5-O7
26	T	614	LHG	O6-C4-C5-O7
26	X	420	LHG	O6-C4-C5-O7
26	A	846	LHG	O6-C4-C5-O7
22	U	414	CLA	CBA-CGA-O2A-C1
22	B	809	CLA	O1A-CGA-O2A-C1
22	K	602	CLA	C11-C12-C13-C14
22	G	606	CLA	O1D-CGD-O2D-CED
22	N	601	CLA	CBD-CGD-O2D-CED
22	B	837	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	K	605	CLA	C2B-C3B-CAB-CBB
22	Q	607	CLA	C2B-C3B-CAB-CBB
22	Q	613	CLA	C2B-C3B-CAB-CBB
22	R	607	CLA	C2B-C3B-CAB-CBB
22	T	610	CLA	C2B-C3B-CAB-CBB
22	U	415	CLA	C2B-C3B-CAB-CBB
22	A	824	CLA	C2B-C3B-CAB-CBB
26	X	420	LHG	C27-C28-C29-C30
28	I	615	LMG	C24-C25-C26-C27
28	L	401	LMG	C30-C31-C32-C33
25	O	304	DGD	C9B-CAB-CBB-CCB
26	O	318	LHG	C26-C27-C28-C29
26	N	614	LHG	O7-C5-C6-O8
26	T	614	LHG	O7-C5-C6-O8
26	U	419	LHG	O7-C5-C6-O8
28	H	319	LMG	O7-C8-C9-O8
28	H	322	LMG	O7-C8-C9-O8
28	K	618	LMG	O7-C8-C9-O8
28	U	402	LMG	O7-C8-C9-O8
28	U	423	LMG	O1-C7-C8-O7
22	N	603	CLA	C13-C15-C16-C17
22	A	803	CLA	O1D-CGD-O2D-CED
27	U	422	LMU	C5-C6-C7-C8
28	Q	602	LMG	C34-C35-C36-C37
22	B	823	CLA	C16-C17-C18-C19
22	X	412	CLA	C16-C17-C18-C20
22	A	822	CLA	C16-C17-C18-C19
22	I	601	CLA	C15-C16-C17-C18
22	T	609	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	C5-C6-C7-C8
26	O	318	LHG	C11-C12-C13-C14
26	A	845	LHG	O9-C7-O7-C5
22	K	609	CLA	C2-C1-O2A-CGA
22	R	606	CLA	C2-C1-O2A-CGA
22	Q	613	CLA	O1D-CGD-O2D-CED
25	O	304	DGD	C1A-C2A-C3A-C4A
22	B	806	CLA	C6-C7-C8-C9
22	B	807	CLA	C6-C7-C8-C9
22	B	830	CLA	C14-C13-C15-C16
22	B	859	CLA	C6-C7-C8-C9
22	H	311	CLA	C11-C12-C13-C14
22	K	608	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	L	402	CLA	C11-C12-C13-C14
22	L	406	CLA	C6-C7-C8-C9
22	L	406	CLA	C14-C13-C15-C16
22	U	404	CLA	C6-C7-C8-C9
22	U	414	CLA	C11-C12-C13-C14
22	V	604	CLA	C6-C7-C8-C9
22	A	801	CLA	C11-C12-C13-C14
22	A	803	CLA	C11-C10-C8-C9
22	A	821	CLA	C11-C12-C13-C14
22	A	824	CLA	C11-C10-C8-C9
22	A	829	CLA	C11-C10-C8-C9
22	A	839	CLA	C14-C13-C15-C16
22	A	840	CLA	C14-C13-C15-C16
22	A	852	CLA	C11-C12-C13-C14
26	U	419	LHG	C26-C27-C28-C29
28	K	618	LMG	C34-C35-C36-C37
22	A	833	CLA	CBD-CGD-O2D-CED
25	B	847	DGD	C7A-C8A-C9A-CAA
26	O	324	LHG	C25-C26-C27-C28
28	B	852	LMG	C17-C18-C19-C20
22	T	604	CLA	C15-C16-C17-C18
26	P	601	LHG	C5-C4-O6-P
22	Q	612	CLA	O1A-CGA-O2A-C1
28	J	101	LMG	C38-C39-C40-C41
28	T	616	LMG	C30-C31-C32-C33
22	I	610	CLA	C2A-CAA-CBA-CGA
22	Q	612	CLA	C2A-CAA-CBA-CGA
22	R	608	CLA	C2A-CAA-CBA-CGA
22	O	306	CLA	C11-C12-C13-C14
22	S	604	CLA	C11-C12-C13-C14
22	A	810	CLA	C16-C17-C18-C19
22	O	310	CLA	C10-C11-C12-C13
26	G	614	LHG	C11-C10-C9-C8
26	O	324	LHG	C12-C13-C14-C15
26	A	846	LHG	C27-C28-C29-C30
27	U	421	LMU	C3'-C4'-O1B-C1B
28	A	855	LMG	C15-C16-C17-C18
21	B	801	BCR	C11-C12-C13-C14
22	A	833	CLA	C8-C10-C11-C12
28	K	601	LMG	C11-C12-C13-C14
26	O	324	LHG	C26-C27-C28-C29
22	A	816	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	U	414	CLA	C14-C13-C15-C16
27	U	421	LMU	C6-C7-C8-C9
22	B	813	CLA	C8-C10-C11-C12
28	K	622	LMG	C17-C18-C19-C20
22	K	604	CLA	O1D-CGD-O2D-CED
25	F	401	DGD	C4A-C5A-C6A-C7A
27	H	301	LMU	O1'-C1-C2-C3
28	U	423	LMG	C16-C17-C18-C19
28	U	423	LMG	C23-C24-C25-C26
22	O	313	CLA	C8-C10-C11-C12
22	B	806	CLA	C6-C7-C8-C10
22	B	806	CLA	C12-C13-C15-C16
22	B	817	CLA	C11-C10-C8-C7
22	B	818	CLA	C11-C10-C8-C7
22	B	830	CLA	C12-C13-C15-C16
22	B	831	CLA	C6-C7-C8-C10
22	B	831	CLA	C11-C10-C8-C7
22	B	835	CLA	C11-C10-C8-C7
22	B	859	CLA	C12-C13-C15-C16
22	G	606	CLA	C6-C7-C8-C10
22	G	606	CLA	C11-C10-C8-C7
22	H	303	CLA	C6-C7-C8-C10
22	H	303	CLA	C11-C10-C8-C7
22	H	305	CLA	C6-C7-C8-C10
22	H	308	CLA	C11-C10-C8-C7
22	H	313	CLA	C11-C10-C8-C7
22	K	603	CLA	C6-C7-C8-C10
22	K	603	CLA	C11-C10-C8-C7
22	K	604	CLA	C6-C7-C8-C10
22	K	609	CLA	C6-C7-C8-C10
22	L	403	CLA	C6-C7-C8-C10
22	L	406	CLA	C6-C7-C8-C10
22	L	410	CLA	C11-C10-C8-C7
22	L	411	CLA	C12-C13-C15-C16
22	N	607	CLA	C6-C7-C8-C10
22	N	610	CLA	C2-C3-C5-C6
22	O	310	CLA	C11-C10-C8-C7
22	Q	610	CLA	C12-C13-C15-C16
22	R	605	CLA	C12-C13-C15-C16
22	R	615	CLA	C11-C10-C8-C7
22	T	603	CLA	C6-C7-C8-C10
22	T	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	T	604	CLA	C11-C12-C13-C15
22	T	607	CLA	C11-C10-C8-C7
22	U	404	CLA	C11-C10-C8-C7
22	X	403	CLA	C11-C12-C13-C15
22	X	407	CLA	C11-C12-C13-C15
22	A	801	CLA	C11-C12-C13-C15
22	A	801	CLA	C12-C13-C15-C16
22	A	803	CLA	C6-C7-C8-C10
22	A	810	CLA	C11-C12-C13-C15
22	A	829	CLA	C11-C10-C8-C7
22	A	829	CLA	C11-C12-C13-C15
22	A	840	CLA	C12-C13-C15-C16
22	A	841	CLA	C11-C10-C8-C7
22	A	842	CLA	C6-C7-C8-C10
22	A	852	CLA	C6-C7-C8-C10
25	F	401	DGD	CDA-CEA-CFA-CGA
28	B	856	LMG	C30-C31-C32-C33
32	U	418	NEX	C9-C10-C11-C12
32	V	616	NEX	C9-C10-C11-C12
25	F	401	DGD	C2G-C3G-O3G-C1D
22	X	403	CLA	C8-C10-C11-C12
22	R	602	CLA	C2A-CAA-CBA-CGA
22	S	605	CLA	C2A-CAA-CBA-CGA
22	X	408	CLA	C2A-CAA-CBA-CGA
26	X	420	LHG	C23-C24-C25-C26
26	O	323	LHG	C30-C31-C32-C33
22	H	306	CLA	C6-C7-C8-C10
22	R	601	CLA	C5-C6-C7-C8
22	Q	611	CLA	CBA-CGA-O2A-C1
22	B	802	CLA	CAA-CBA-CGA-O2A
27	U	421	LMU	C5'-C4'-O1B-C1B
28	W	401	LMG	C41-C42-C43-C44
22	X	402	CLA	O1D-CGD-O2D-CED
31	W	422	CHL	C8-C10-C11-C12
22	S	604	CLA	O1A-CGA-O2A-C1
22	B	802	CLA	CAD-CBD-CGD-O2D
22	B	803	CLA	CAD-CBD-CGD-O2D
22	B	816	CLA	CAD-CBD-CGD-O2D
22	B	828	CLA	CAD-CBD-CGD-O2D
22	B	831	CLA	CAD-CBD-CGD-O2D
22	B	838	CLA	CAD-CBD-CGD-O2D
22	B	839	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	G	605	CLA	CAD-CBD-CGD-O2D
22	G	607	CLA	CAD-CBD-CGD-O2D
22	H	303	CLA	CAD-CBD-CGD-O2D
22	I	603	CLA	CAD-CBD-CGD-O2D
22	I	604	CLA	CAD-CBD-CGD-O2D
22	I	607	CLA	CAD-CBD-CGD-O2D
22	K	613	CLA	CAD-CBD-CGD-O2D
22	K	617	CLA	CAD-CBD-CGD-O2D
22	L	408	CLA	CAD-CBD-CGD-O2D
22	N	602	CLA	CAD-CBD-CGD-O2D
22	N	604	CLA	CAD-CBD-CGD-O2D
22	N	608	CLA	CAD-CBD-CGD-O2D
22	O	310	CLA	CAD-CBD-CGD-O2D
22	O	311	CLA	CAD-CBD-CGD-O2D
22	O	312	CLA	CAD-CBD-CGD-O2D
22	P	610	CLA	CAD-CBD-CGD-O2D
22	Q	601	CLA	CAD-CBD-CGD-O2D
22	Q	610	CLA	CAD-CBD-CGD-O2D
22	R	605	CLA	CAD-CBD-CGD-O2D
22	S	610	CLA	CAD-CBD-CGD-O2D
22	U	403	CLA	CAD-CBD-CGD-O2D
22	U	409	CLA	CAD-CBD-CGD-O2D
22	U	410	CLA	CAD-CBD-CGD-O2D
22	V	603	CLA	CAD-CBD-CGD-O2D
22	V	604	CLA	CAD-CBD-CGD-O2D
22	V	609	CLA	CAD-CBD-CGD-O2D
22	V	613	CLA	CAD-CBD-CGD-O2D
22	W	404	CLA	CAD-CBD-CGD-O2D
22	W	410	CLA	CAD-CBD-CGD-O2D
22	W	413	CLA	CAD-CBD-CGD-O2D
22	X	402	CLA	CAD-CBD-CGD-O2D
22	X	403	CLA	CAD-CBD-CGD-O2D
22	X	409	CLA	CAD-CBD-CGD-O2D
22	X	419	CLA	CAD-CBD-CGD-O2D
22	A	809	CLA	CAD-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	818	CLA	CAD-CBD-CGD-O2D
22	A	827	CLA	CAD-CBD-CGD-O2D
22	A	834	CLA	CAD-CBD-CGD-O2D
22	A	838	CLA	CAD-CBD-CGD-O2D
26	O	324	LHG	C6-C5-O7-C7
31	U	408	CHL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	V	606	CHL	CAD-CBD-CGD-O2D
22	W	412	CLA	O1A-CGA-O2A-C1
22	K	608	CLA	CBA-CGA-O2A-C1
22	A	840	CLA	CBA-CGA-O2A-C1
22	L	405	CLA	O1D-CGD-O2D-CED
22	F	404	CLA	C4-C3-C5-C6
22	A	801	CLA	C4-C3-C5-C6
22	B	823	CLA	C16-C17-C18-C20
22	A	844	CLA	C2-C3-C5-C6
25	B	847	DGD	C1G-C2G-C3G-O3G
26	K	619	LHG	C4-C5-C6-O8
26	P	601	LHG	C2-C3-O3-P
26	X	420	LHG	C4-C5-C6-O8
28	G	616	LMG	C7-C8-C9-O8
28	I	615	LMG	O1-C7-C8-C9
28	K	618	LMG	C7-C8-C9-O8
22	B	830	CLA	C2C-C3C-CAC-CBC
26	P	601	LHG	O6-C4-C5-O7
22	T	611	CLA	C13-C15-C16-C17
22	A	807	CLA	C10-C11-C12-C13
22	B	808	CLA	C3-C5-C6-C7
22	R	604	CLA	C2A-CAA-CBA-CGA
22	W	414	CLA	C2A-CAA-CBA-CGA
22	K	602	CLA	C11-C12-C13-C15
22	T	607	CLA	C11-C12-C13-C15
26	O	324	LHG	C1-C2-C3-O3
22	F	405	CLA	CHA-CBD-CGD-O1D
22	F	405	CLA	CHA-CBD-CGD-O2D
22	G	601	CLA	CHA-CBD-CGD-O1D
22	G	601	CLA	CHA-CBD-CGD-O2D
22	G	603	CLA	CHA-CBD-CGD-O1D
22	I	609	CLA	CHA-CBD-CGD-O1D
22	I	609	CLA	CHA-CBD-CGD-O2D
22	L	404	CLA	CHA-CBD-CGD-O1D
22	L	404	CLA	CHA-CBD-CGD-O2D
22	N	602	CLA	CHA-CBD-CGD-O1D
22	O	305	CLA	CHA-CBD-CGD-O2D
22	P	602	CLA	CHA-CBD-CGD-O1D
22	P	602	CLA	CHA-CBD-CGD-O2D
22	P	608	CLA	CHA-CBD-CGD-O1D
22	P	608	CLA	CHA-CBD-CGD-O2D
22	Q	618	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	Q	618	CLA	CHA-CBD-CGD-O2D
22	R	607	CLA	CHA-CBD-CGD-O1D
22	S	601	CLA	CHA-CBD-CGD-O1D
22	S	601	CLA	CHA-CBD-CGD-O2D
22	T	610	CLA	CHA-CBD-CGD-O1D
22	T	610	CLA	CHA-CBD-CGD-O2D
22	U	404	CLA	CHA-CBD-CGD-O1D
22	V	617	CLA	CHA-CBD-CGD-O1D
22	X	410	CLA	CHA-CBD-CGD-O2D
22	A	810	CLA	CHA-CBD-CGD-O1D
22	A	810	CLA	CHA-CBD-CGD-O2D
22	A	824	CLA	CHA-CBD-CGD-O1D
22	A	825	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	840	CLA	CHA-CBD-CGD-O1D
22	A	840	CLA	CHA-CBD-CGD-O2D
22	A	844	CLA	CHA-CBD-CGD-O1D
22	A	844	CLA	CHA-CBD-CGD-O2D
22	L	402	CLA	O1A-CGA-O2A-C1
22	A	836	CLA	O1A-CGA-O2A-C1
25	O	304	DGD	O2G-C2G-C3G-O3G
26	L	416	LHG	O7-C5-C6-O8
26	R	614	LHG	O7-C5-C6-O8
26	W	420	LHG	O7-C5-C6-O8
28	F	408	LMG	O1-C7-C8-O7
28	I	615	LMG	O1-C7-C8-O7
28	K	601	LMG	O1-C7-C8-O7
28	K	601	LMG	O7-C8-C9-O8
28	K	618	LMG	O1-C7-C8-O7
28	G	616	LMG	O6-C5-C6-O5
27	B	854	LMU	C1-C2-C3-C4
25	B	847	DGD	C5A-C6A-C7A-C8A
26	X	420	LHG	C31-C32-C33-C34
26	A	845	LHG	C13-C14-C15-C16
28	H	319	LMG	C33-C34-C35-C36
22	H	305	CLA	O1A-CGA-O2A-C1
26	W	420	LHG	C9-C10-C11-C12
28	B	852	LMG	C14-C15-C16-C17
28	K	618	LMG	C35-C36-C37-C38
30	F	407	SQD	C25-C26-C27-C28
22	B	821	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
26	O	323	LHG	C12-C13-C14-C15
22	K	604	CLA	C3-C5-C6-C7
22	L	402	CLA	C13-C15-C16-C17
22	A	812	CLA	C4-C3-C5-C6
22	A	844	CLA	C4-C3-C5-C6
22	U	414	CLA	O1A-CGA-O2A-C1
28	I	614	LMG	C4-C5-C6-O5
22	A	822	CLA	C2-C3-C5-C6
22	B	859	CLA	O1D-CGD-O2D-CED
24	B	841	DD6	C27-C29-C30-C31
24	G	613	DD6	C27-C29-C30-C31
24	H	314	DD6	C27-C29-C30-C31
24	H	315	DD6	C27-C29-C30-C31
24	O	316	DD6	C27-C29-C30-C31
24	T	612	DD6	C27-C29-C30-C31
24	V	614	DD6	C27-C29-C30-C31
24	V	615	DD6	C27-C29-C30-C31
24	W	417	DD6	C27-C29-C30-C31
24	X	414	DD6	C27-C29-C30-C31
24	X	415	DD6	C27-C29-C30-C31
24	A	847	DD6	C27-C29-C30-C31
24	A	858	DD6	C27-C29-C30-C31
22	O	315	CLA	CBA-CGA-O2A-C1
26	L	416	LHG	C28-C29-C30-C31
28	H	317	LMG	O9-C10-O7-C8
22	B	817	CLA	C11-C10-C8-C9
22	B	828	CLA	C6-C7-C8-C9
22	K	603	CLA	C11-C10-C8-C9
22	K	604	CLA	C6-C7-C8-C9
22	O	313	CLA	C11-C10-C8-C9
22	Q	610	CLA	C14-C13-C15-C16
22	T	605	CLA	C11-C12-C13-C14
22	A	817	CLA	C11-C10-C8-C9
31	W	422	CHL	C11-C12-C13-C14
33	A	802	CL0	C6-C7-C8-C9
22	B	820	CLA	O1D-CGD-O2D-CED
26	K	619	LHG	C12-C13-C14-C15
28	I	615	LMG	C14-C15-C16-C17
22	F	404	CLA	CBD-CGD-O2D-CED
28	W	401	LMG	O6-C5-C6-O5
22	O	313	CLA	O1D-CGD-O2D-CED
27	U	424	LMU	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
28	F	408	LMG	C33-C34-C35-C36
26	K	619	LHG	C25-C26-C27-C28
22	B	804	CLA	C2A-CAA-CBA-CGA
22	K	611	CLA	C2A-CAA-CBA-CGA
22	L	411	CLA	C2A-CAA-CBA-CGA
22	A	804	CLA	C2A-CAA-CBA-CGA
22	A	842	CLA	C2A-CAA-CBA-CGA
26	H	316	LHG	O8-C23-C24-C25
22	W	410	CLA	C5-C6-C7-C8
22	Q	611	CLA	O1A-CGA-O2A-C1
24	F	406	DD6	C12-C11-C13-C14
24	X	416	DD6	C7-C6-C8-C9
24	X	416	DD6	C5-C6-C8-C9
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	826	CLA	C1A-C2A-CAA-CBA
22	H	306	CLA	C1A-C2A-CAA-CBA
22	I	607	CLA	C1A-C2A-CAA-CBA
22	O	310	CLA	C1A-C2A-CAA-CBA
22	P	605	CLA	C1A-C2A-CAA-CBA
22	U	411	CLA	C1A-C2A-CAA-CBA
22	V	608	CLA	C1A-C2A-CAA-CBA
22	X	409	CLA	C1A-C2A-CAA-CBA
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	823	CLA	C1A-C2A-CAA-CBA
22	K	603	CLA	C11-C12-C13-C15
22	W	411	CLA	C11-C12-C13-C14
22	A	821	CLA	CBD-CGD-O2D-CED
28	J	101	LMG	C36-C37-C38-C39
22	A	814	CLA	C5-C6-C7-C8
26	O	321	LHG	C4-O6-P-O3
25	B	847	DGD	CEB-CFB-CGB-CHB
26	A	845	LHG	C10-C11-C12-C13
22	S	601	CLA	O1D-CGD-O2D-CED
28	J	101	LMG	C12-C13-C14-C15
22	B	823	CLA	C13-C15-C16-C17
22	L	406	CLA	C13-C15-C16-C17
22	X	404	CLA	C3-C5-C6-C7
26	O	321	LHG	C2-C3-O3-P
26	U	419	LHG	C5-C4-O6-P
22	Q	604	CLA	C2-C3-C5-C6
27	B	857	LMU	C6-C7-C8-C9
22	B	819	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	838	CLA	C4B-C3B-CAB-CBB
22	F	403	CLA	C4B-C3B-CAB-CBB
22	I	601	CLA	C4B-C3B-CAB-CBB
22	I	608	CLA	C4B-C3B-CAB-CBB
22	K	613	CLA	C4B-C3B-CAB-CBB
22	N	608	CLA	C4B-C3B-CAB-CBB
22	N	611	CLA	C4B-C3B-CAB-CBB
22	O	315	CLA	C4B-C3B-CAB-CBB
22	P	608	CLA	C4B-C3B-CAB-CBB
22	Q	610	CLA	C4B-C3B-CAB-CBB
22	Q	618	CLA	C4B-C3B-CAB-CBB
22	R	608	CLA	C4B-C3B-CAB-CBB
22	R	610	CLA	C4B-C3B-CAB-CBB
22	S	608	CLA	C4B-C3B-CAB-CBB
22	S	615	CLA	C4B-C3B-CAB-CBB
22	V	613	CLA	C4B-C3B-CAB-CBB
22	V	617	CLA	C4B-C3B-CAB-CBB
22	W	403	CLA	C4B-C3B-CAB-CBB
22	W	414	CLA	C4B-C3B-CAB-CBB
22	X	419	CLA	C4B-C3B-CAB-CBB
22	A	836	CLA	C4B-C3B-CAB-CBB
26	B	848	LHG	C4-O6-P-O5
26	B	851	LHG	C3-O3-P-O4
26	K	616	LHG	C3-O3-P-O5
26	K	619	LHG	C3-O3-P-O5
26	K	619	LHG	C4-O6-P-O5
26	L	416	LHG	C3-O3-P-O4
26	N	616	LHG	C3-O3-P-O4
26	O	318	LHG	C4-O6-P-O5
26	O	323	LHG	C3-O3-P-O4
26	O	323	LHG	C4-O6-P-O4
26	U	419	LHG	C3-O3-P-O6
26	W	420	LHG	C3-O3-P-O4
26	A	845	LHG	C3-O3-P-O4
26	A	845	LHG	C4-O6-P-O4
22	O	313	CLA	C16-C17-C18-C20
22	X	409	CLA	C15-C16-C17-C18
22	A	852	CLA	C13-C15-C16-C17
26	O	324	LHG	O6-C4-C5-C6
26	T	614	LHG	O6-C4-C5-C6
26	T	614	LHG	C29-C30-C31-C32
22	T	609	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	842	CLA	CAA-CBA-CGA-O2A
22	G	610	CLA	C2A-CAA-CBA-CGA
22	A	807	CLA	C2A-CAA-CBA-CGA
22	A	841	CLA	C2A-CAA-CBA-CGA
22	A	840	CLA	O1A-CGA-O2A-C1
22	S	604	CLA	C11-C12-C13-C15
22	T	607	CLA	C11-C12-C13-C14
28	L	401	LMG	C37-C38-C39-C40
22	F	405	CLA	CAD-CBD-CGD-O1D
22	L	404	CLA	CAD-CBD-CGD-O1D
22	N	605	CLA	CAD-CBD-CGD-O1D
22	P	602	CLA	CAD-CBD-CGD-O1D
22	Q	606	CLA	CAD-CBD-CGD-O1D
22	T	610	CLA	CAD-CBD-CGD-O1D
22	T	611	CLA	CAD-CBD-CGD-O1D
22	W	419	CLA	CAD-CBD-CGD-O1D
22	A	844	CLA	CAD-CBD-CGD-O1D
26	O	323	LHG	O8-C23-C24-C25
26	X	420	LHG	C34-C35-C36-C37
22	O	306	CLA	C3-C5-C6-C7
26	T	614	LHG	C26-C27-C28-C29
22	A	833	CLA	O1D-CGD-O2D-CED
22	L	417	CLA	CBA-CGA-O2A-C1
28	U	402	LMG	C39-C40-C41-C42
22	B	807	CLA	C16-C17-C18-C20
22	B	833	CLA	C16-C17-C18-C19
22	H	308	CLA	C11-C12-C13-C14
22	S	602	CLA	C11-C12-C13-C15
22	H	313	CLA	C4-C3-C5-C6
22	S	602	CLA	C4-C3-C5-C6
22	B	805	CLA	C12-C13-C15-C16
22	B	806	CLA	C11-C10-C8-C7
22	B	807	CLA	C12-C13-C15-C16
22	B	814	CLA	C3A-C2A-CAA-CBA
22	B	828	CLA	C6-C7-C8-C10
22	B	832	CLA	C11-C12-C13-C15
22	B	834	CLA	C12-C13-C15-C16
22	H	313	CLA	C6-C7-C8-C10
22	I	601	CLA	C6-C7-C8-C10
22	K	608	CLA	C11-C10-C8-C7
22	L	409	CLA	C11-C10-C8-C7
22	N	606	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	N	606	CLA	C12-C13-C15-C16
22	R	605	CLA	C11-C12-C13-C15
22	R	610	CLA	C11-C10-C8-C7
22	T	611	CLA	C12-C13-C15-C16
22	A	816	CLA	C11-C10-C8-C7
22	A	817	CLA	C11-C12-C13-C15
22	A	817	CLA	C12-C13-C15-C16
22	A	820	CLA	C12-C13-C15-C16
22	A	841	CLA	C11-C12-C13-C15
33	A	802	CL0	C6-C7-C8-C10
28	I	615	LMG	C13-C14-C15-C16
28	U	402	LMG	C19-C20-C21-C22
22	W	409	CLA	C3-C5-C6-C7
22	K	617	CLA	C5-C6-C7-C8
22	A	808	CLA	C5-C6-C7-C8
28	H	319	LMG	C32-C33-C34-C35
22	O	315	CLA	O1A-CGA-O2A-C1
22	H	303	CLA	C2A-CAA-CBA-CGA
22	Q	604	CLA	C2A-CAA-CBA-CGA
22	T	604	CLA	C16-C17-C18-C20
22	U	404	CLA	C16-C17-C18-C20
27	U	422	LMU	C4'-C5'-C6'-O6'
28	B	856	LMG	C40-C41-C42-C43
26	S	613	LHG	O8-C23-C24-C25
26	U	419	LHG	C4-C5-C6-O8
28	F	408	LMG	O1-C7-C8-C9
28	H	317	LMG	O1-C7-C8-C9
28	K	618	LMG	O1-C7-C8-C9
28	T	616	LMG	O1-C7-C8-C9
28	A	855	LMG	C7-C8-C9-O8
22	J	102	CLA	CBD-CGD-O2D-CED
28	G	616	LMG	O1-C7-C8-O7
28	U	402	LMG	O1-C7-C8-O7
28	A	855	LMG	O7-C8-C9-O8
30	K	621	SQD	O47-C45-C46-O48
28	Q	602	LMG	C31-C32-C33-C34
22	B	859	CLA	C10-C11-C12-C13
25	O	304	DGD	C7B-C8B-C9B-CAB
26	A	845	LHG	C27-C28-C29-C30
27	K	620	LMU	C2-C3-C4-C5
27	J	104	LMU	C9-C10-C11-C12
28	W	401	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
22	X	410	CLA	C8-C10-C11-C12
22	A	824	CLA	C5-C6-C7-C8
22	T	605	CLA	C3-C5-C6-C7
28	K	622	LMG	C31-C32-C33-C34
22	K	608	CLA	O1A-CGA-O2A-C1
22	N	601	CLA	O1D-CGD-O2D-CED
22	B	828	CLA	C4-C3-C5-C6
28	W	401	LMG	C29-C28-O8-C9
27	L	420	LMU	C3-C4-C5-C6
22	W	402	CLA	C2-C3-C5-C6
22	A	812	CLA	C2-C3-C5-C6
22	V	609	CLA	C5-C6-C7-C8
22	B	816	CLA	C11-C10-C8-C9
22	B	818	CLA	C11-C10-C8-C9
22	B	821	CLA	C6-C7-C8-C9
22	G	606	CLA	C6-C7-C8-C9
22	I	601	CLA	C11-C10-C8-C9
22	L	403	CLA	C6-C7-C8-C9
22	O	310	CLA	C11-C10-C8-C9
22	O	313	CLA	C6-C7-C8-C9
22	O	313	CLA	C14-C13-C15-C16
22	R	603	CLA	C6-C7-C8-C9
22	R	615	CLA	C11-C10-C8-C9
22	U	414	CLA	C6-C7-C8-C9
22	W	414	CLA	C14-C13-C15-C16
22	X	412	CLA	C11-C12-C13-C14
22	A	804	CLA	C11-C10-C8-C9
22	A	807	CLA	C11-C10-C8-C9
22	A	828	CLA	C6-C7-C8-C9
22	A	841	CLA	C11-C10-C8-C9
25	B	847	DGD	CAA-CBA-CCA-CDA
22	H	306	CLA	C6-C7-C8-C9
27	L	419	LMU	O5B-C1B-O1B-C4'
22	K	604	CLA	CAA-CBA-CGA-O2A
22	B	825	CLA	C2A-CAA-CBA-CGA
22	S	604	CLA	CAA-CBA-CGA-O2A
22	R	610	CLA	C13-C15-C16-C17
24	A	858	DD6	C1-C24-C25-C26
22	U	404	CLA	C8-C10-C11-C12
27	L	420	LMU	C2'-C1'-O1'-C1
26	A	845	LHG	C16-C17-C18-C19
22	A	819	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	B	803	CLA	C2B-C3B-CAB-CBB
22	I	608	CLA	C2B-C3B-CAB-CBB
22	N	601	CLA	C2B-C3B-CAB-CBB
22	N	608	CLA	C2B-C3B-CAB-CBB
22	N	610	CLA	C2B-C3B-CAB-CBB
22	N	611	CLA	C2B-C3B-CAB-CBB
22	O	315	CLA	C2B-C3B-CAB-CBB
22	P	603	CLA	C2B-C3B-CAB-CBB
22	Q	610	CLA	C2B-C3B-CAB-CBB
22	Q	618	CLA	C2B-C3B-CAB-CBB
22	R	608	CLA	C2B-C3B-CAB-CBB
22	R	610	CLA	C2B-C3B-CAB-CBB
22	S	608	CLA	C2B-C3B-CAB-CBB
22	S	609	CLA	C2B-C3B-CAB-CBB
22	V	601	CLA	C2B-C3B-CAB-CBB
22	V	610	CLA	C2B-C3B-CAB-CBB
22	V	613	CLA	C2B-C3B-CAB-CBB
22	W	403	CLA	C2B-C3B-CAB-CBB
22	X	403	CLA	C2B-C3B-CAB-CBB
22	A	836	CLA	C2B-C3B-CAB-CBB
22	A	837	CLA	C2B-C3B-CAB-CBB
27	U	422	LMU	C1-C2-C3-C4
28	K	618	LMG	C13-C14-C15-C16
22	O	313	CLA	C10-C11-C12-C13
28	I	615	LMG	C19-C20-C21-C22
22	L	411	CLA	C4-C3-C5-C6
22	K	607	CLA	C2C-C3C-CAC-CBC
22	B	827	CLA	C5-C6-C7-C8
28	L	401	LMG	C12-C13-C14-C15
28	L	401	LMG	C14-C15-C16-C17
27	A	854	LMU	C7-C8-C9-C10
28	T	616	LMG	C17-C18-C19-C20
22	F	403	CLA	C13-C15-C16-C17
22	A	811	CLA	C5-C6-C7-C8
26	Q	616	LHG	O6-C4-C5-C6
26	R	614	LHG	C1-C2-C3-O3
22	B	812	CLA	C2A-CAA-CBA-CGA
22	H	311	CLA	C2A-CAA-CBA-CGA
22	V	612	CLA	C2A-CAA-CBA-CGA
22	A	801	CLA	C2A-CAA-CBA-CGA
22	A	844	CLA	C2A-CAA-CBA-CGA
22	G	606	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	I	606	CLA	C2-C1-O2A-CGA
22	L	406	CLA	C2-C1-O2A-CGA
22	N	606	CLA	C2-C1-O2A-CGA
22	X	405	CLA	C2-C1-O2A-CGA
22	A	822	CLA	C2-C1-O2A-CGA
26	A	846	LHG	C13-C14-C15-C16
22	L	417	CLA	O1A-CGA-O2A-C1
28	W	401	LMG	C16-C17-C18-C19
28	A	855	LMG	C31-C32-C33-C34
22	F	404	CLA	CBA-CGA-O2A-C1
22	U	401	CLA	C2-C3-C5-C6
25	O	304	DGD	CEA-CFA-CGA-CHA
26	B	851	LHG	C16-C17-C18-C19
22	S	615	CLA	O1A-CGA-O2A-C1
26	P	601	LHG	C26-C27-C28-C29
27	K	620	LMU	O5'-C1'-O1'-C1
22	B	820	CLA	C2A-CAA-CBA-CGA
22	T	605	CLA	C10-C11-C12-C13
26	X	420	LHG	C3-O3-P-O6
28	B	856	LMG	C11-C12-C13-C14
28	H	319	LMG	C11-C12-C13-C14
25	F	401	DGD	C4B-C5B-C6B-C7B
26	Q	616	LHG	C9-C10-C11-C12
27	A	857	LMU	C4'-C5'-C6'-O6'
22	F	404	CLA	O1D-CGD-O2D-CED
22	Q	609	CLA	C8-C10-C11-C12
26	N	616	LHG	C27-C28-C29-C30
26	R	614	LHG	C24-C23-O8-C6
28	U	423	LMG	O1-C7-C8-C9
22	B	826	CLA	C4-C3-C5-C6
22	K	611	CLA	C4-C3-C5-C6
22	B	816	CLA	C11-C10-C8-C7
22	B	825	CLA	C11-C12-C13-C15
22	B	828	CLA	C11-C10-C8-C7
22	B	859	CLA	C6-C7-C8-C10
22	H	305	CLA	C11-C10-C8-C7
22	K	602	CLA	C6-C7-C8-C10
22	K	605	CLA	C11-C12-C13-C15
22	V	612	CLA	C12-C13-C15-C16
22	W	404	CLA	C6-C7-C8-C10
22	A	807	CLA	C11-C10-C8-C7
22	A	832	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	842	CLA	C12-C13-C15-C16
22	A	844	CLA	C3-C5-C6-C7
22	B	805	CLA	C14-C13-C15-C16
22	B	813	CLA	C6-C7-C8-C9
22	B	816	CLA	C14-C13-C15-C16
22	B	832	CLA	C11-C12-C13-C14
22	H	313	CLA	C6-C7-C8-C9
22	K	608	CLA	C11-C10-C8-C9
22	R	601	CLA	C14-C13-C15-C16
22	R	605	CLA	C14-C13-C15-C16
22	T	603	CLA	C6-C7-C8-C9
22	W	404	CLA	C6-C7-C8-C9
22	A	801	CLA	C14-C13-C15-C16
22	A	810	CLA	C11-C10-C8-C9
22	A	816	CLA	C11-C10-C8-C9
22	A	820	CLA	C14-C13-C15-C16
22	R	607	CLA	C10-C11-C12-C13
22	J	102	CLA	O1D-CGD-O2D-CED
24	P	612	DD6	C11-C10-C9-C8
22	S	607	CLA	C11-C12-C13-C15
28	J	101	LMG	C10-C11-C12-C13
28	I	614	LMG	C15-C16-C17-C18
22	A	821	CLA	O1D-CGD-O2D-CED
28	F	408	LMG	C19-C20-C21-C22
22	F	404	CLA	O1A-CGA-O2A-C1
26	R	614	LHG	O10-C23-O8-C6
24	V	615	DD6	C7-C6-C8-C9
22	B	807	CLA	C16-C17-C18-C19
26	G	614	LHG	O1-C1-C2-C3
26	N	614	LHG	O1-C1-C2-C3
26	B	851	LHG	C2-C3-O3-P
26	K	619	LHG	C2-C3-O3-P
26	Q	616	LHG	C2-C3-O3-P
25	B	847	DGD	CBB-CCB-CDB-CEB
28	B	856	LMG	C29-C30-C31-C32
26	A	845	LHG	C23-C24-C25-C26
22	K	605	CLA	C10-C11-C12-C13
22	U	414	CLA	C5-C6-C7-C8
22	X	409	CLA	C10-C11-C12-C13
28	U	402	LMG	C37-C38-C39-C40
22	G	603	CLA	C11-C10-C8-C7
22	I	603	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	V	604	CLA	C11-C10-C8-C7
22	A	816	CLA	C12-C13-C15-C16
22	K	604	CLA	C4-C3-C5-C6
22	L	411	CLA	C2-C3-C5-C6
28	G	616	LMG	C13-C14-C15-C16
22	S	615	CLA	CBA-CGA-O2A-C1
25	F	401	DGD	C9A-CAA-CBA-CCA
27	F	409	LMU	C2-C3-C4-C5
22	A	829	CLA	CBD-CGD-O2D-CED
22	A	801	CLA	C2C-C3C-CAC-CBC
25	O	304	DGD	C7A-C8A-C9A-CAA
22	B	803	CLA	C4B-C3B-CAB-CBB
22	K	609	CLA	C4B-C3B-CAB-CBB
22	N	601	CLA	C4B-C3B-CAB-CBB
22	N	610	CLA	C4B-C3B-CAB-CBB
22	Q	604	CLA	C4B-C3B-CAB-CBB
22	R	615	CLA	C4B-C3B-CAB-CBB
22	T	605	CLA	C4B-C3B-CAB-CBB
22	U	406	CLA	C4B-C3B-CAB-CBB
22	U	412	CLA	C4B-C3B-CAB-CBB
22	X	403	CLA	C4B-C3B-CAB-CBB
22	X	412	CLA	C4B-C3B-CAB-CBB
22	A	810	CLA	C4B-C3B-CAB-CBB
22	A	813	CLA	C4B-C3B-CAB-CBB
22	L	403	CLA	C2A-CAA-CBA-CGA
22	A	829	CLA	C2A-CAA-CBA-CGA
22	A	839	CLA	C2A-CAA-CBA-CGA
28	K	622	LMG	C28-C29-C30-C31
28	A	855	LMG	C28-C29-C30-C31
22	A	826	CLA	C10-C11-C12-C13
22	K	607	CLA	C4C-C3C-CAC-CBC
28	G	616	LMG	C15-C16-C17-C18
22	H	310	CLA	CAA-CBA-CGA-O2A
22	A	820	CLA	C2C-C3C-CAC-CBC
31	W	408	CHL	C3-C5-C6-C7
22	B	804	CLA	C4-C3-C5-C6
22	X	409	CLA	C4-C3-C5-C6
22	A	829	CLA	C4-C3-C5-C6
22	P	611	CLA	CAA-CBA-CGA-O1A
22	B	804	CLA	C2-C3-C5-C6
22	K	604	CLA	C2-C3-C5-C6
22	W	409	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	F	401	DGD	C2A-C3A-C4A-C5A
28	B	852	LMG	C23-C24-C25-C26
22	P	605	CLA	CAA-CBA-CGA-O1A
22	B	836	CLA	C2-C1-O2A-CGA
22	G	603	CLA	C2-C1-O2A-CGA
22	N	603	CLA	C2-C1-O2A-CGA
22	N	607	CLA	C2-C1-O2A-CGA
22	R	602	CLA	C2-C1-O2A-CGA
22	Q	610	CLA	C10-C11-C12-C13
28	I	615	LMG	C2-C1-O1-C7
26	A	846	LHG	C30-C31-C32-C33
22	B	803	CLA	C2A-CAA-CBA-CGA
22	H	304	CLA	C2A-CAA-CBA-CGA
22	K	610	CLA	C2A-CAA-CBA-CGA
22	L	412	CLA	C2A-CAA-CBA-CGA
22	N	602	CLA	C2A-CAA-CBA-CGA
22	R	610	CLA	C2A-CAA-CBA-CGA
22	S	602	CLA	C2A-CAA-CBA-CGA
22	U	415	CLA	C2A-CAA-CBA-CGA
22	W	404	CLA	C2A-CAA-CBA-CGA
22	A	815	CLA	C2A-CAA-CBA-CGA
28	T	616	LMG	O1-C7-C8-O7
26	X	420	LHG	C2-C3-O3-P
22	H	309	CLA	C3A-C2A-CAA-CBA
22	P	611	CLA	CAA-CBA-CGA-O2A
22	S	602	CLA	C11-C12-C13-C14
28	F	408	LMG	C34-C35-C36-C37
22	B	822	CLA	C4-C3-C5-C6
22	W	409	CLA	C4-C3-C5-C6
22	B	809	CLA	C11-C10-C8-C9
22	B	810	CLA	C6-C7-C8-C9
22	K	604	CLA	C14-C13-C15-C16
22	K	605	CLA	C14-C13-C15-C16
22	K	608	CLA	C11-C12-C13-C14
22	O	308	CLA	C11-C10-C8-C9
22	T	611	CLA	C14-C13-C15-C16
22	U	405	CLA	C11-C10-C8-C9
22	U	411	CLA	C6-C7-C8-C9
22	W	410	CLA	C6-C7-C8-C9
22	X	408	CLA	C11-C10-C8-C9
22	A	808	CLA	C11-C12-C13-C14
22	A	828	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	A	831	CLA	C6-C7-C8-C9
22	A	839	CLA	C11-C12-C13-C14
22	W	413	CLA	CAA-CBA-CGA-O2A
22	V	608	CLA	CBA-CGA-O2A-C1
26	B	851	LHG	C17-C18-C19-C20
22	S	608	CLA	O1D-CGD-O2D-CED
26	L	416	LHG	C26-C27-C28-C29
28	A	855	LMG	C34-C35-C36-C37
21	B	843	BCR	C11-C10-C9-C34
21	B	843	BCR	C20-C21-C22-C37
21	A	851	BCR	C11-C10-C9-C34
21	A	851	BCR	C16-C17-C18-C36
24	F	406	DD6	C-C1-C2-C3
24	P	612	DD6	C-C1-C2-C3
28	B	856	LMG	C7-C8-C9-O8
32	U	418	NEX	C39-C29-C30-C31
32	V	616	NEX	C39-C29-C30-C31
26	N	614	LHG	C25-C26-C27-C28
22	P	604	CLA	CAA-CBA-CGA-O2A
22	B	819	CLA	C2A-CAA-CBA-CGA
28	J	101	LMG	C21-C22-C23-C24
28	Q	602	LMG	C33-C34-C35-C36
22	T	604	CLA	C16-C17-C18-C19
22	B	823	CLA	O2A-C1-C2-C3
31	W	422	CHL	O2A-C1-C2-C3
26	L	416	LHG	C24-C23-O8-C6
22	A	829	CLA	O1D-CGD-O2D-CED
28	G	616	LMG	O6-C1-O1-C7
22	W	404	CLA	C10-C11-C12-C13
22	P	604	CLA	CAA-CBA-CGA-O1A
26	O	321	LHG	C30-C31-C32-C33
28	W	401	LMG	C37-C38-C39-C40
22	B	838	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	821	CLA	C1A-C2A-CAA-CBA
22	H	303	CLA	C1A-C2A-CAA-CBA
22	R	605	CLA	C1A-C2A-CAA-CBA
22	S	602	CLA	C1A-C2A-CAA-CBA
22	V	617	CLA	C1A-C2A-CAA-CBA
22	W	415	CLA	C1A-C2A-CAA-CBA
22	A	804	CLA	C1A-C2A-CAA-CBA
22	A	840	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	813	CLA	C11-C10-C8-C7
22	B	817	CLA	C11-C12-C13-C15
22	B	833	CLA	C6-C7-C8-C10
22	B	833	CLA	C12-C13-C15-C16
22	F	403	CLA	C6-C7-C8-C10
22	F	403	CLA	C12-C13-C15-C16
22	K	604	CLA	C11-C10-C8-C7
22	R	607	CLA	C6-C7-C8-C10
22	X	403	CLA	C12-C13-C15-C16
22	A	813	CLA	C11-C12-C13-C15
22	A	817	CLA	C11-C10-C8-C7
22	A	821	CLA	C11-C12-C13-C15
22	A	822	CLA	C6-C7-C8-C10
22	A	826	CLA	C12-C13-C15-C16
31	W	422	CHL	C11-C12-C13-C15
22	B	817	CLA	C10-C11-C12-C13
22	P	603	CLA	CAA-CBA-CGA-O1A
22	G	601	CLA	CAA-CBA-CGA-O2A
22	N	608	CLA	CAA-CBA-CGA-O2A
25	F	401	DGD	CFA-CGA-CHA-CIA
27	X	418	LMU	C1-C2-C3-C4
22	B	824	CLA	C16-C17-C18-C19
28	K	622	LMG	C33-C34-C35-C36
28	L	401	LMG	C18-C19-C20-C21
22	B	824	CLA	C3-C5-C6-C7
22	B	835	CLA	C2A-CAA-CBA-CGA
22	G	602	CLA	C2A-CAA-CBA-CGA
22	O	307	CLA	C2A-CAA-CBA-CGA
22	O	313	CLA	C2A-CAA-CBA-CGA
22	W	404	CLA	C8-C10-C11-C12
22	A	829	CLA	C8-C10-C11-C12
22	N	610	CLA	C2C-C3C-CAC-CBC
22	A	837	CLA	CBA-CGA-O2A-C1
26	O	324	LHG	C33-C34-C35-C36
22	K	609	CLA	C11-C12-C13-C15
22	H	304	CLA	CAA-CBA-CGA-O1A
22	H	304	CLA	CAA-CBA-CGA-O2A
22	W	413	CLA	CAA-CBA-CGA-O1A
22	B	806	CLA	C4-C3-C5-C6
22	U	414	CLA	C4-C3-C5-C6
22	X	402	CLA	C4-C3-C5-C6
22	A	842	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	825	CLA	C10-C11-C12-C13
26	A	846	LHG	C7-C8-C9-C10
22	K	611	CLA	CBD-CGD-O2D-CED
22	B	806	CLA	C2-C3-C5-C6
22	Q	610	CLA	C2-C3-C5-C6
22	W	411	CLA	C2-C3-C5-C6
22	K	611	CLA	O1D-CGD-O2D-CED
22	B	819	CLA	C2B-C3B-CAB-CBB
22	B	838	CLA	C2B-C3B-CAB-CBB
22	F	403	CLA	C2B-C3B-CAB-CBB
22	I	601	CLA	C2B-C3B-CAB-CBB
22	K	613	CLA	C2B-C3B-CAB-CBB
22	P	608	CLA	C2B-C3B-CAB-CBB
22	Q	604	CLA	C2B-C3B-CAB-CBB
22	R	601	CLA	C2B-C3B-CAB-CBB
22	S	615	CLA	C2B-C3B-CAB-CBB
22	T	605	CLA	C2B-C3B-CAB-CBB
22	U	406	CLA	C2B-C3B-CAB-CBB
22	V	617	CLA	C2B-C3B-CAB-CBB
22	W	412	CLA	C2B-C3B-CAB-CBB
22	W	414	CLA	C2B-C3B-CAB-CBB
22	X	419	CLA	C2B-C3B-CAB-CBB
22	A	813	CLA	C2B-C3B-CAB-CBB
22	B	819	CLA	C5-C6-C7-C8
26	B	848	LHG	O10-C23-C24-C25
22	N	608	CLA	CAA-CBA-CGA-O1A
22	P	603	CLA	CAA-CBA-CGA-O2A
22	V	613	CLA	CAA-CBA-CGA-O2A
26	R	614	LHG	C12-C13-C14-C15
21	B	843	BCR	C11-C10-C9-C8
21	B	843	BCR	C20-C21-C22-C23
21	A	851	BCR	C11-C10-C9-C8
21	A	851	BCR	C16-C17-C18-C19
24	F	406	DD6	C24-C1-C2-C3
24	P	612	DD6	C24-C1-C2-C3
27	L	420	LMU	O5'-C1'-O1'-C1
22	T	609	CLA	CAA-CBA-CGA-O1A
25	B	847	DGD	O2G-C2G-C3G-O3G
26	X	420	LHG	O7-C5-C6-O8
28	B	852	LMG	O1-C7-C8-O7
22	B	828	CLA	CBA-CGA-O2A-C1
23	A	843	PQN	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
22	B	838	CLA	O1D-CGD-O2D-CED
22	G	601	CLA	CAA-CBA-CGA-O1A
22	P	605	CLA	CAA-CBA-CGA-O2A
22	S	601	CLA	CAA-CBA-CGA-O2A
22	S	608	CLA	CAA-CBA-CGA-O2A
26	L	416	LHG	C19-C20-C21-C22
27	T	618	LMU	C3-C4-C5-C6
22	B	818	CLA	C16-C17-C18-C19
22	A	828	CLA	C16-C17-C18-C20
28	H	322	LMG	O6-C1-O1-C7
22	A	817	CLA	C5-C6-C7-C8
26	K	616	LHG	C12-C13-C14-C15
26	O	321	LHG	C17-C18-C19-C20
26	L	416	LHG	O10-C23-O8-C6
22	H	310	CLA	CAA-CBA-CGA-O1A
22	T	609	CLA	CAA-CBA-CGA-O2A
22	A	801	CLA	C3-C5-C6-C7
22	I	603	CLA	C2-C1-O2A-CGA
22	U	414	CLA	C2-C1-O2A-CGA
22	B	822	CLA	C2-C3-C5-C6
22	B	826	CLA	C2-C3-C5-C6
22	B	828	CLA	O1A-CGA-O2A-C1
22	S	601	CLA	CAA-CBA-CGA-O1A
25	O	304	DGD	CFA-CGA-CHA-CIA
22	I	602	CLA	C11-C10-C8-C9
22	R	615	CLA	C6-C7-C8-C9
22	A	812	CLA	C6-C7-C8-C9
22	A	824	CLA	C11-C12-C13-C14
22	A	836	CLA	C6-C7-C8-C9
22	H	303	CLA	C5-C6-C7-C8
22	S	608	CLA	CBD-CGD-O2D-CED
22	V	608	CLA	O1A-CGA-O2A-C1
26	K	616	LHG	C10-C11-C12-C13
22	R	605	CLA	O1A-CGA-O2A-C1
22	A	808	CLA	C15-C16-C17-C18
22	H	309	CLA	C2A-CAA-CBA-CGA
22	I	602	CLA	C2A-CAA-CBA-CGA
22	O	310	CLA	C2A-CAA-CBA-CGA
22	X	403	CLA	C2A-CAA-CBA-CGA
22	H	305	CLA	C11-C12-C13-C14
22	A	840	CLA	C16-C17-C18-C20
22	B	838	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	P	609	CLA	CAA-CBA-CGA-O2A
22	A	837	CLA	O1A-CGA-O2A-C1
28	K	601	LMG	O10-C28-O8-C9
21	B	844	BCR	C23-C24-C25-C30
22	B	804	CLA	CAA-CBA-CGA-O2A
22	B	838	CLA	CAA-CBA-CGA-O2A
22	V	613	CLA	CAA-CBA-CGA-O1A
22	H	311	CLA	C15-C16-C17-C18
27	H	320	LMU	C4-C5-C6-C7
32	U	418	NEX	C33-C34-C35-C15
32	V	616	NEX	C33-C34-C35-C15
22	B	823	CLA	C4-C3-C5-C6
22	Q	610	CLA	C4-C3-C5-C6
22	T	604	CLA	C4-C3-C5-C6
22	B	804	CLA	C16-C17-C18-C20
22	S	607	CLA	C11-C12-C13-C14
26	Q	616	LHG	C28-C29-C30-C31
22	B	828	CLA	C2-C3-C5-C6
22	I	601	CLA	C2-C3-C5-C6
22	K	611	CLA	C2-C3-C5-C6
22	N	606	CLA	C2-C3-C5-C6
22	S	603	CLA	CAA-CBA-CGA-O2A
28	G	616	LMG	C8-C7-O1-C1
28	U	402	LMG	C8-C7-O1-C1
22	G	606	CLA	C15-C16-C17-C18
22	W	419	CLA	CAA-CBA-CGA-O2A
27	B	854	LMU	C4-C5-C6-C7
25	B	847	DGD	C3A-C4A-C5A-C6A
28	B	856	LMG	C33-C34-C35-C36
22	W	412	CLA	C8-C10-C11-C12
22	A	852	CLA	C8-C10-C11-C12
22	G	603	CLA	C11-C10-C8-C9
28	B	856	LMG	C14-C15-C16-C17
22	W	419	CLA	CAA-CBA-CGA-O1A
22	A	834	CLA	CAA-CBA-CGA-O2A
22	O	306	CLA	C2A-CAA-CBA-CGA
26	N	616	LHG	C30-C31-C32-C33
28	T	616	LMG	C35-C36-C37-C38
22	K	607	CLA	CBD-CGD-O2D-CED
22	R	605	CLA	CBA-CGA-O2A-C1
28	J	101	LMG	C42-C43-C44-C45
22	A	824	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	G	605	CLA	CAA-CBA-CGA-O2A
22	Q	618	CLA	CAA-CBA-CGA-O2A
22	S	608	CLA	CAA-CBA-CGA-O1A
22	R	601	CLA	C4B-C3B-CAB-CBB
22	T	611	CLA	C4B-C3B-CAB-CBB
22	W	412	CLA	C4B-C3B-CAB-CBB
28	I	614	LMG	C33-C34-C35-C36
22	X	404	CLA	C10-C11-C12-C13
22	N	606	CLA	C4-C3-C5-C6
22	O	306	CLA	C4-C3-C5-C6
22	Q	612	CLA	C4-C3-C5-C6
22	A	803	CLA	C4-C3-C5-C6
22	I	606	CLA	O1D-CGD-O2D-CED
22	F	404	CLA	C2-C3-C5-C6
22	H	311	CLA	C11-C12-C13-C15
22	I	606	CLA	C11-C10-C8-C7
22	L	407	CLA	C2-C3-C5-C6
22	U	405	CLA	C11-C10-C8-C7
22	X	404	CLA	C11-C10-C8-C7
22	A	801	CLA	C2-C3-C5-C6
22	A	824	CLA	C12-C13-C15-C16
22	A	829	CLA	C12-C13-C15-C16
22	X	407	CLA	C10-C11-C12-C13
22	N	610	CLA	C4C-C3C-CAC-CBC
27	L	420	LMU	C4-C5-C6-C7
27	O	322	LMU	C2'-C1'-O1'-C1
22	X	404	CLA	C11-C12-C13-C15
28	H	322	LMG	C12-C13-C14-C15
28	B	856	LMG	O7-C8-C9-O8
26	W	420	LHG	C24-C23-O8-C6
26	P	601	LHG	O10-C23-C24-C25
22	B	830	CLA	C13-C15-C16-C17
22	T	602	CLA	C5-C6-C7-C8
22	G	609	CLA	CAA-CBA-CGA-O2A
22	L	412	CLA	CAA-CBA-CGA-O2A
22	O	307	CLA	CAA-CBA-CGA-O2A
22	U	403	CLA	CAA-CBA-CGA-O2A
22	X	411	CLA	CAA-CBA-CGA-O2A
22	S	609	CLA	CAA-CBA-CGA-O2A
22	A	829	CLA	CAA-CBA-CGA-O2A
22	B	829	CLA	CAA-CBA-CGA-O2A
22	G	611	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	N	601	CLA	CAA-CBA-CGA-O2A
22	A	834	CLA	CAA-CBA-CGA-O1A
22	G	602	CLA	CBA-CGA-O2A-C1
25	B	847	DGD	C6B-C7B-C8B-C9B
26	T	614	LHG	C7-C8-C9-C10
22	A	808	CLA	CAA-CBA-CGA-O2A
22	O	312	CLA	C4-C3-C5-C6
22	U	404	CLA	C4-C3-C5-C6
22	W	406	CLA	C4-C3-C5-C6
22	B	816	CLA	C10-C11-C12-C13
22	T	602	CLA	C8-C10-C11-C12
22	P	607	CLA	CAA-CBA-CGA-O2A
22	V	611	CLA	CAA-CBA-CGA-O2A
22	H	313	CLA	C2-C3-C5-C6
22	T	604	CLA	C2-C3-C5-C6
27	F	409	LMU	C4-C5-C6-C7
28	U	423	LMG	C14-C15-C16-C17
22	T	611	CLA	C16-C17-C18-C20
26	B	851	LHG	O7-C7-C8-C9
26	X	420	LHG	O7-C7-C8-C9
22	B	813	CLA	C11-C10-C8-C9
22	B	828	CLA	C11-C12-C13-C14
22	G	602	CLA	C6-C7-C8-C9
22	H	308	CLA	C6-C7-C8-C9
22	K	602	CLA	C6-C7-C8-C9
22	N	606	CLA	C14-C13-C15-C16
22	R	605	CLA	C11-C12-C13-C14
22	R	610	CLA	C11-C10-C8-C9
22	U	404	CLA	C11-C12-C13-C14
22	X	403	CLA	C11-C12-C13-C14
22	A	813	CLA	C11-C12-C13-C14
22	A	816	CLA	C11-C12-C13-C14
22	A	817	CLA	C11-C12-C13-C14
22	A	826	CLA	C14-C13-C15-C16
26	W	420	LHG	O10-C23-O8-C6
22	H	318	CLA	CAA-CBA-CGA-O2A
22	L	411	CLA	C8-C10-C11-C12
22	H	305	CLA	C3A-C2A-CAA-CBA
22	N	607	CLA	C3A-C2A-CAA-CBA
22	P	607	CLA	C3A-C2A-CAA-CBA
22	Q	610	CLA	C3A-C2A-CAA-CBA
22	A	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	839	CLA	C8-C10-C11-C12
22	L	404	CLA	CAA-CBA-CGA-O2A
22	A	821	CLA	CAA-CBA-CGA-O2A
26	L	416	LHG	O8-C23-C24-C25
31	W	422	CHL	CAA-CBA-CGA-O2A
27	T	617	LMU	C3-C4-C5-C6
22	N	604	CLA	CAA-CBA-CGA-O2A
22	N	609	CLA	CAA-CBA-CGA-O2A
22	Q	607	CLA	CAA-CBA-CGA-O2A
22	B	811	CLA	CAD-CBD-CGD-O2D
22	B	813	CLA	CAD-CBD-CGD-O2D
22	B	834	CLA	CAD-CBD-CGD-O2D
22	B	836	CLA	CAD-CBD-CGD-O2D
22	B	837	CLA	CAD-CBD-CGD-O2D
22	G	603	CLA	CAD-CBD-CGD-O2D
22	H	305	CLA	CAD-CBD-CGD-O2D
22	H	306	CLA	CAD-CBD-CGD-O2D
22	H	308	CLA	CAD-CBD-CGD-O2D
22	I	608	CLA	CAD-CBD-CGD-O2D
22	K	606	CLA	CAD-CBD-CGD-O2D
22	K	607	CLA	CAD-CBD-CGD-O2D
22	K	608	CLA	CAD-CBD-CGD-O2D
22	K	609	CLA	CAD-CBD-CGD-O2D
22	L	405	CLA	CAD-CBD-CGD-O2D
22	L	406	CLA	CAD-CBD-CGD-O2D
22	L	409	CLA	CAD-CBD-CGD-O2D
22	N	606	CLA	CAD-CBD-CGD-O2D
22	N	607	CLA	CAD-CBD-CGD-O2D
22	O	314	CLA	CAD-CBD-CGD-O2D
22	O	319	CLA	CAD-CBD-CGD-O2D
22	P	604	CLA	CAD-CBD-CGD-O2D
22	Q	604	CLA	CAD-CBD-CGD-O2D
22	Q	607	CLA	CAD-CBD-CGD-O2D
22	Q	612	CLA	CAD-CBD-CGD-O2D
22	Q	617	CLA	CAD-CBD-CGD-O2D
22	R	602	CLA	CAD-CBD-CGD-O2D
22	R	608	CLA	CAD-CBD-CGD-O2D
22	S	602	CLA	CAD-CBD-CGD-O2D
22	S	603	CLA	CAD-CBD-CGD-O2D
22	S	608	CLA	CAD-CBD-CGD-O2D
22	T	602	CLA	CAD-CBD-CGD-O2D
22	T	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	U	405	CLA	CAD-CBD-CGD-O2D
22	U	413	CLA	CAD-CBD-CGD-O2D
22	V	602	CLA	CAD-CBD-CGD-O2D
22	W	403	CLA	CAD-CBD-CGD-O2D
22	W	411	CLA	CAD-CBD-CGD-O2D
22	X	408	CLA	CAD-CBD-CGD-O2D
22	X	411	CLA	CAD-CBD-CGD-O2D
22	A	807	CLA	CAD-CBD-CGD-O2D
22	A	808	CLA	CAD-CBD-CGD-O2D
22	A	812	CLA	CAD-CBD-CGD-O2D
22	A	815	CLA	CAD-CBD-CGD-O2D
22	A	821	CLA	CAD-CBD-CGD-O2D
22	A	828	CLA	CAD-CBD-CGD-O2D
28	K	622	LMG	C4-C5-C6-O5
28	B	856	LMG	C42-C43-C44-C45
28	K	601	LMG	C15-C16-C17-C18
22	A	822	CLA	C13-C15-C16-C17
28	U	423	LMG	O9-C10-O7-C8
22	B	814	CLA	CAA-CBA-CGA-O2A
22	P	609	CLA	CAA-CBA-CGA-O1A
22	R	611	CLA	CAA-CBA-CGA-O2A
22	V	617	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	CAA-CBA-CGA-O2A
26	O	318	LHG	O7-C7-C8-C9
33	A	802	CL0	CAA-CBA-CGA-O2A
22	A	817	CLA	C10-C11-C12-C13
22	I	601	CLA	C4-C3-C5-C6
22	R	607	CLA	C4-C3-C5-C6
22	A	805	CLA	C4-C3-C5-C6
22	A	801	CLA	C16-C17-C18-C20
27	K	620	LMU	C2B-C1B-O1B-C4'
22	G	605	CLA	CAA-CBA-CGA-O1A
26	X	420	LHG	C25-C26-C27-C28
26	A	845	LHG	C32-C33-C34-C35
22	A	836	CLA	C5-C6-C7-C8
22	U	414	CLA	C2-C3-C5-C6
22	X	402	CLA	C2-C3-C5-C6
22	K	605	CLA	CAA-CBA-CGA-O2A
27	H	321	LMU	C2-C3-C4-C5
28	K	618	LMG	C33-C34-C35-C36
22	X	410	CLA	O1A-CGA-O2A-C1
24	V	615	DD6	C5-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
28	N	615	LMG	C14-C15-C16-C17
24	L	414	DD6	C13-C14-C15-O1
24	N	613	DD6	C13-C14-C15-O1
24	P	612	DD6	C13-C14-C15-O1
24	W	418	DD6	C13-C14-C15-O1
26	T	614	LHG	C4-C5-C6-O8
22	Q	618	CLA	CAA-CBA-CGA-O1A
22	V	601	CLA	CAA-CBA-CGA-O2A
22	W	415	CLA	CAA-CBA-CGA-O1A
22	X	419	CLA	CAA-CBA-CGA-O2A
22	R	601	CLA	C13-C15-C16-C17
22	R	602	CLA	C5-C6-C7-C8
22	B	822	CLA	CAA-CBA-CGA-O2A
22	K	610	CLA	CAA-CBA-CGA-O2A
22	Q	605	CLA	CAA-CBA-CGA-O2A
22	B	829	CLA	CAA-CBA-CGA-O1A
22	G	609	CLA	CAA-CBA-CGA-O1A
22	U	403	CLA	CAA-CBA-CGA-O1A
22	W	415	CLA	CAA-CBA-CGA-O2A
28	U	423	LMG	C35-C36-C37-C38
22	B	821	CLA	O2A-C1-C2-C3
22	X	405	CLA	O2A-C1-C2-C3
26	R	614	LHG	C17-C18-C19-C20
22	X	410	CLA	CBA-CGA-O2A-C1
22	B	807	CLA	C2A-CAA-CBA-CGA
22	F	404	CLA	C2A-CAA-CBA-CGA
22	X	412	CLA	C2A-CAA-CBA-CGA
22	V	612	CLA	C8-C10-C11-C12
28	T	616	LMG	C16-C17-C18-C19
22	R	603	CLA	CAA-CBA-CGA-O2A
22	R	605	CLA	CAA-CBA-CGA-O2A
26	R	614	LHG	O8-C23-C24-C25
22	G	602	CLA	O1A-CGA-O2A-C1
22	H	318	CLA	CAA-CBA-CGA-O1A
22	I	605	CLA	CAA-CBA-CGA-O2A
22	I	608	CLA	CAA-CBA-CGA-O2A
22	L	412	CLA	CAA-CBA-CGA-O1A
22	N	601	CLA	CAA-CBA-CGA-O1A
22	N	604	CLA	CAA-CBA-CGA-O1A
22	P	608	CLA	CAA-CBA-CGA-O2A
22	Q	607	CLA	CAA-CBA-CGA-O1A
22	S	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	V	601	CLA	CAA-CBA-CGA-O1A
22	X	411	CLA	CAA-CBA-CGA-O1A
22	X	419	CLA	CAA-CBA-CGA-O1A
27	W	421	LMU	C1-C2-C3-C4
22	B	808	CLA	C5-C6-C7-C8
22	B	824	CLA	C16-C17-C18-C20
22	B	807	CLA	CHA-CBD-CGD-O1D
22	B	807	CLA	CHA-CBD-CGD-O2D
22	B	814	CLA	CHA-CBD-CGD-O2D
22	B	819	CLA	CHA-CBD-CGD-O2D
22	B	820	CLA	CHA-CBD-CGD-O2D
22	B	821	CLA	CHA-CBD-CGD-O1D
22	B	821	CLA	CHA-CBD-CGD-O2D
22	B	823	CLA	CHA-CBD-CGD-O2D
22	G	609	CLA	CHA-CBD-CGD-O1D
22	G	609	CLA	CHA-CBD-CGD-O2D
22	H	304	CLA	CHA-CBD-CGD-O1D
22	H	307	CLA	CHA-CBD-CGD-O1D
22	H	307	CLA	CHA-CBD-CGD-O2D
22	H	310	CLA	CHA-CBD-CGD-O2D
22	I	603	CLA	CHA-CBD-CGD-O2D
22	K	604	CLA	CHA-CBD-CGD-O2D
22	K	610	CLA	CHA-CBD-CGD-O1D
22	K	610	CLA	CHA-CBD-CGD-O2D
22	L	403	CLA	CHA-CBD-CGD-O1D
22	L	407	CLA	CHA-CBD-CGD-O1D
22	L	407	CLA	CHA-CBD-CGD-O2D
22	L	410	CLA	CHA-CBD-CGD-O2D
22	N	603	CLA	CHA-CBD-CGD-O1D
22	N	604	CLA	CHA-CBD-CGD-O1D
22	N	609	CLA	CHA-CBD-CGD-O1D
22	N	609	CLA	CHA-CBD-CGD-O2D
22	O	306	CLA	CHA-CBD-CGD-O1D
22	O	306	CLA	CHA-CBD-CGD-O2D
22	O	308	CLA	CHA-CBD-CGD-O1D
22	O	308	CLA	CHA-CBD-CGD-O2D
22	P	603	CLA	CHA-CBD-CGD-O1D
22	P	605	CLA	CHA-CBD-CGD-O1D
22	P	605	CLA	CHA-CBD-CGD-O2D
22	P	609	CLA	CHA-CBD-CGD-O2D
22	R	603	CLA	CHA-CBD-CGD-O1D
22	R	603	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	R	607	CLA	CHA-CBD-CGD-O2D
22	R	609	CLA	CHA-CBD-CGD-O1D
22	T	603	CLA	CHA-CBD-CGD-O1D
22	T	603	CLA	CHA-CBD-CGD-O2D
22	T	604	CLA	CHA-CBD-CGD-O2D
22	T	606	CLA	CHA-CBD-CGD-O2D
22	V	611	CLA	CHA-CBD-CGD-O1D
22	V	617	CLA	CHA-CBD-CGD-O2D
22	W	413	CLA	CHA-CBD-CGD-O2D
22	X	402	CLA	CHA-CBD-CGD-O2D
22	X	412	CLA	CHA-CBD-CGD-O1D
22	X	412	CLA	CHA-CBD-CGD-O2D
22	A	817	CLA	CHA-CBD-CGD-O1D
22	A	824	CLA	CHA-CBD-CGD-O2D
22	A	825	CLA	CHA-CBD-CGD-O2D
22	A	826	CLA	CHA-CBD-CGD-O1D
22	A	838	CLA	CHA-CBD-CGD-O2D
22	O	307	CLA	CAA-CBA-CGA-O1A
22	P	608	CLA	CAA-CBA-CGA-O1A
22	R	611	CLA	CAA-CBA-CGA-O1A
22	V	611	CLA	CAA-CBA-CGA-O1A
22	L	407	CLA	C4-C3-C5-C6
22	H	306	CLA	CAA-CBA-CGA-O2A
22	I	601	CLA	CAA-CBA-CGA-O2A
27	B	850	LMU	C4-C5-C6-C7
22	W	406	CLA	C2-C3-C5-C6
22	A	803	CLA	C2-C3-C5-C6
22	A	805	CLA	C2-C3-C5-C6
22	B	821	CLA	C5-C6-C7-C8
28	L	401	LMG	C16-C17-C18-C19
26	A	846	LHG	O6-C4-C5-C6
32	U	418	NEX	C28-C29-C30-C31
32	V	616	NEX	C28-C29-C30-C31
22	N	609	CLA	CAA-CBA-CGA-O1A
22	V	617	CLA	CAA-CBA-CGA-O1A
22	N	606	CLA	C15-C16-C17-C18
22	B	805	CLA	CAA-CBA-CGA-O2A
22	N	603	CLA	CAA-CBA-CGA-O2A
26	O	324	LHG	O7-C7-C8-C9
28	K	601	LMG	O8-C28-C29-C30
26	N	616	LHG	C25-C26-C27-C28
26	A	845	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
28	K	622	LMG	O7-C8-C9-O8
22	T	611	CLA	C10-C11-C12-C13
22	B	814	CLA	CAA-CBA-CGA-O1A
22	U	401	CLA	O1A-CGA-O2A-C1
22	Q	612	CLA	CAA-CBA-CGA-O2A
22	R	606	CLA	CAA-CBA-CGA-O2A
22	R	608	CLA	CAA-CBA-CGA-O2A
28	N	615	LMG	O7-C10-C11-C12
28	K	622	LMG	O6-C5-C6-O5
22	T	602	CLA	C2A-CAA-CBA-CGA
31	W	408	CHL	C2A-CAA-CBA-CGA
31	W	407	CHL	CAA-CBA-CGA-O2A
27	L	419	LMU	O1B-C1B-O5B-C5B
22	K	613	CLA	C5-C6-C7-C8
28	N	615	LMG	C10-C11-C12-C13
28	N	615	LMG	C28-C29-C30-C31
28	K	622	LMG	C11-C10-O7-C8
26	G	614	LHG	O8-C23-C24-C25
22	A	844	CLA	O1D-CGD-O2D-CED
22	B	818	CLA	C6-C7-C8-C10
22	G	606	CLA	C12-C13-C15-C16
22	K	617	CLA	C2-C3-C5-C6
22	N	606	CLA	C6-C7-C8-C10
22	R	615	CLA	C6-C7-C8-C10
22	S	602	CLA	C2-C3-C5-C6
22	V	604	CLA	C6-C7-C8-C10
22	A	812	CLA	C6-C7-C8-C10
22	A	816	CLA	C6-C7-C8-C10
22	A	825	CLA	C6-C7-C8-C10
22	A	836	CLA	C6-C7-C8-C10
22	B	818	CLA	C16-C17-C18-C20
22	A	801	CLA	C16-C17-C18-C19
28	K	618	LMG	O9-C10-O7-C8
26	N	614	LHG	O8-C23-C24-C25
22	G	610	CLA	CAA-CBA-CGA-O1A
22	B	817	CLA	C11-C12-C13-C14
22	B	818	CLA	C6-C7-C8-C9
22	B	833	CLA	C14-C13-C15-C16
22	F	403	CLA	C6-C7-C8-C9
22	F	403	CLA	C11-C10-C8-C9
22	K	611	CLA	C6-C7-C8-C9
22	A	822	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	840	CLA	C11-C10-C8-C9
22	K	609	CLA	C2B-C3B-CAB-CBB
25	O	304	DGD	C4A-C5A-C6A-C7A
27	W	421	LMU	C7-C8-C9-C10
22	Q	610	CLA	O1A-CGA-O2A-C1
22	Q	603	CLA	CAA-CBA-CGA-O2A
22	T	610	CLA	CAA-CBA-CGA-O2A
22	U	401	CLA	CBA-CGA-O2A-C1
22	B	816	CLA	CAA-CBA-CGA-O2A
26	X	420	LHG	O8-C23-C24-C25
30	V	618	SQD	C4-C5-C6-S
22	A	828	CLA	C16-C17-C18-C19
26	O	321	LHG	C28-C29-C30-C31
28	H	319	LMG	C34-C35-C36-C37
22	G	611	CLA	CAA-CBA-CGA-O1A
22	P	607	CLA	CAA-CBA-CGA-O1A
22	B	830	CLA	C4C-C3C-CAC-CBC
26	K	619	LHG	O7-C7-C8-C9
22	B	835	CLA	C8-C10-C11-C12
26	N	616	LHG	C9-C10-C11-C12
22	K	605	CLA	CAA-CBA-CGA-O1A
28	N	615	LMG	O9-C10-C11-C12
22	T	604	CLA	C5-C6-C7-C8
22	K	609	CLA	C11-C12-C13-C14
22	U	410	CLA	C4-C3-C5-C6
26	K	619	LHG	O1-C1-C2-C3
22	A	808	CLA	CAA-CBA-CGA-O1A
31	W	422	CHL	CAA-CBA-CGA-O1A
27	U	421	LMU	C5-C6-C7-C8
28	K	622	LMG	C29-C28-O8-C9
27	L	419	LMU	C3-C4-C5-C6
22	H	305	CLA	C1A-C2A-CAA-CBA
22	H	309	CLA	C1A-C2A-CAA-CBA
22	K	602	CLA	C1A-C2A-CAA-CBA
22	N	606	CLA	C1A-C2A-CAA-CBA
22	Q	610	CLA	C1A-C2A-CAA-CBA
22	V	609	CLA	C1A-C2A-CAA-CBA
22	W	411	CLA	C1A-C2A-CAA-CBA
22	A	829	CLA	C1A-C2A-CAA-CBA
22	A	840	CLA	C16-C17-C18-C19
22	S	609	CLA	CAA-CBA-CGA-O1A
22	A	821	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	I	608	CLA	CAA-CBA-CGA-O1A
22	P	606	CLA	CAA-CBA-CGA-O2A
22	K	607	CLA	O1D-CGD-O2D-CED
22	V	603	CLA	C2-C1-O2A-CGA
22	Q	610	CLA	CBA-CGA-O2A-C1
22	I	601	CLA	CAA-CBA-CGA-O1A
22	L	404	CLA	CAA-CBA-CGA-O1A
26	B	851	LHG	O9-C7-C8-C9
26	O	318	LHG	O9-C7-C8-C9
22	Q	606	CLA	CAA-CBA-CGA-O2A
22	U	412	CLA	CAA-CBA-CGA-O2A
26	H	316	LHG	C4-C5-C6-O8
22	A	826	CLA	C15-C16-C17-C18
22	P	602	CLA	C2A-CAA-CBA-CGA
22	P	605	CLA	C2A-CAA-CBA-CGA
22	P	609	CLA	C2A-CAA-CBA-CGA
22	U	404	CLA	C2A-CAA-CBA-CGA
22	V	602	CLA	C2A-CAA-CBA-CGA
22	V	609	CLA	C2A-CAA-CBA-CGA
28	B	856	LMG	C15-C16-C17-C18
22	T	605	CLA	C16-C17-C18-C19
22	U	410	CLA	C6-C7-C8-C10
22	N	603	CLA	CAA-CBA-CGA-O1A
22	A	823	CLA	CAA-CBA-CGA-O2A
22	A	830	CLA	C15-C16-C17-C18
28	I	614	LMG	O9-C10-O7-C8
22	R	607	CLA	C3-C5-C6-C7
28	L	401	LMG	C19-C20-C21-C22
22	R	605	CLA	CAA-CBA-CGA-O1A
26	O	324	LHG	O9-C7-C8-C9
26	R	614	LHG	O10-C23-C24-C25
26	X	420	LHG	O9-C7-C8-C9
27	B	850	LMU	C6-C7-C8-C9
22	I	605	CLA	CAA-CBA-CGA-O1A
22	A	852	CLA	C15-C16-C17-C18
26	Q	616	LHG	C12-C13-C14-C15
22	H	311	CLA	C4B-C3B-CAB-CBB
22	I	610	CLA	C4B-C3B-CAB-CBB
26	A	846	LHG	C3-O3-P-O5
28	H	322	LMG	O1-C7-C8-O7
22	B	822	CLA	CAA-CBA-CGA-O1A
22	Q	605	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	K	619	LHG	O9-C7-C8-C9
26	L	416	LHG	O10-C23-C24-C25
26	N	614	LHG	O10-C23-C24-C25
25	O	304	DGD	O2G-C1B-C2B-C3B
22	I	610	CLA	CAA-CBA-CGA-O2A
22	R	604	CLA	CAA-CBA-CGA-O2A
22	A	827	CLA	C3-C5-C6-C7
26	R	614	LHG	C14-C15-C16-C17
31	W	422	CHL	C5-C6-C7-C8
24	X	416	DD6	C11-C13-C14-C15
22	B	805	CLA	CAA-CBA-CGA-O1A
22	R	603	CLA	CAA-CBA-CGA-O1A
22	A	830	CLA	CAA-CBA-CGA-O1A
22	R	610	CLA	CAA-CBA-CGA-O2A
22	X	412	CLA	CAA-CBA-CGA-O2A
31	W	407	CHL	CAA-CBA-CGA-O1A
22	B	802	CLA	C16-C17-C18-C20
22	H	305	CLA	C11-C12-C13-C15
22	A	833	CLA	C16-C17-C18-C19
22	I	611	CLA	C2A-CAA-CBA-CGA
22	K	603	CLA	C2A-CAA-CBA-CGA
22	B	802	CLA	CAA-CBA-CGA-O1A
22	H	306	CLA	CAA-CBA-CGA-O1A
22	Q	612	CLA	CAA-CBA-CGA-O1A
22	L	406	CLA	C15-C16-C17-C18
22	I	610	CLA	CAA-CBA-CGA-O1A
22	N	607	CLA	C5-C6-C7-C8
22	K	617	CLA	CBD-CGD-O2D-CED
28	H	322	LMG	O6-C5-C6-O5
22	K	610	CLA	CAA-CBA-CGA-O1A
22	B	803	CLA	C4-C3-C5-C6
22	X	410	CLA	C4-C3-C5-C6
22	A	852	CLA	C4-C3-C5-C6
28	K	622	LMG	C37-C38-C39-C40
22	G	610	CLA	CAA-CBA-CGA-O2A
22	T	610	CLA	CAA-CBA-CGA-O1A
22	B	829	CLA	CAD-CBD-CGD-O1D
22	H	307	CLA	CAD-CBD-CGD-O1D
22	L	406	CLA	CAD-CBD-CGD-O1D
22	N	603	CLA	CAD-CBD-CGD-O1D
22	P	605	CLA	CAD-CBD-CGD-O1D
22	S	605	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	U	403	CLA	CAD-CBD-CGD-O1D
22	U	404	CLA	CAD-CBD-CGD-O1D
22	A	817	CLA	CAD-CBD-CGD-O1D
22	A	824	CLA	CAD-CBD-CGD-O1D
22	A	839	CLA	CAD-CBD-CGD-O1D
26	N	616	LHG	C4-C5-O7-C7
26	N	616	LHG	C6-C5-O7-C7
30	V	618	SQD	O5-C5-C6-S
22	R	608	CLA	CAA-CBA-CGA-O1A
26	G	614	LHG	O10-C23-C24-C25
28	I	615	LMG	O9-C10-C11-C12
28	I	615	LMG	C21-C22-C23-C24
22	I	603	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	C5-C6-C7-C8
22	B	835	CLA	C13-C15-C16-C17
22	B	818	CLA	C11-C12-C13-C14
22	B	825	CLA	C6-C7-C8-C9
22	B	825	CLA	C14-C13-C15-C16
22	B	827	CLA	C11-C12-C13-C14
22	B	832	CLA	C6-C7-C8-C9
22	L	402	CLA	C11-C10-C8-C9
22	R	601	CLA	C11-C10-C8-C9
22	R	601	CLA	C11-C12-C13-C14
22	T	602	CLA	C11-C10-C8-C9
22	V	612	CLA	C11-C12-C13-C14
22	A	814	CLA	C11-C12-C13-C14
22	A	824	CLA	C14-C13-C15-C16
22	A	825	CLA	C6-C7-C8-C9
22	I	611	CLA	CBD-CGD-O2D-CED
22	A	844	CLA	CBD-CGD-O2D-CED
28	G	616	LMG	C11-C12-C13-C14
22	P	602	CLA	CAA-CBA-CGA-O2A
22	R	604	CLA	CAA-CBA-CGA-O1A
22	Q	609	CLA	O1A-CGA-O2A-C1
26	K	619	LHG	C23-C24-C25-C26
22	Q	611	CLA	CAA-CBA-CGA-O2A
22	S	605	CLA	CAA-CBA-CGA-O2A
22	W	409	CLA	CAA-CBA-CGA-O2A
26	A	845	LHG	O8-C23-C24-C25
22	Q	603	CLA	CAA-CBA-CGA-O1A
28	A	855	LMG	C12-C13-C14-C15
22	W	410	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	U	423	LMG	C32-C33-C34-C35
22	B	839	CLA	CAA-CBA-CGA-O2A
22	L	411	CLA	CAA-CBA-CGA-O2A
22	S	602	CLA	CAA-CBA-CGA-O2A
22	A	826	CLA	CAA-CBA-CGA-O2A
28	U	423	LMG	O7-C10-C11-C12
26	K	616	LHG	C1-C2-C3-O3
26	O	318	LHG	C1-C2-C3-O3
23	A	843	PQN	C25-C26-C27-C28
28	J	101	LMG	C15-C16-C17-C18
28	K	601	LMG	C12-C13-C14-C15
28	A	855	LMG	C13-C14-C15-C16
22	R	606	CLA	CAA-CBA-CGA-O1A
26	R	614	LHG	O9-C7-O7-C5
26	T	614	LHG	C25-C26-C27-C28
22	N	607	CLA	C4-C3-C5-C6
26	B	851	LHG	C18-C19-C20-C21
26	O	323	LHG	C35-C36-C37-C38
22	B	804	CLA	C11-C12-C13-C15
22	B	825	CLA	C6-C7-C8-C10
22	B	825	CLA	C12-C13-C15-C16
22	F	403	CLA	C11-C10-C8-C7
22	I	602	CLA	C11-C10-C8-C7
22	K	604	CLA	C12-C13-C15-C16
22	O	313	CLA	C11-C12-C13-C15
22	R	601	CLA	C12-C13-C15-C16
22	R	603	CLA	C6-C7-C8-C10
22	T	602	CLA	C11-C10-C8-C7
22	T	605	CLA	C6-C7-C8-C10
22	V	612	CLA	C11-C12-C13-C15
22	W	409	CLA	C11-C10-C8-C7
22	W	414	CLA	C12-C13-C15-C16
22	X	409	CLA	C2-C3-C5-C6
22	A	811	CLA	C3A-C2A-CAA-CBA
22	A	829	CLA	C2-C3-C5-C6
22	A	830	CLA	C3A-C2A-CAA-CBA
22	A	842	CLA	C2-C3-C5-C6
30	V	618	SQD	C45-C44-O6-C1
22	W	409	CLA	CAA-CBA-CGA-O1A
26	X	420	LHG	O10-C23-C24-C25
22	H	312	CLA	CAA-CBA-CGA-O2A
22	P	606	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	X	413	CLA	CAA-CBA-CGA-O2A
22	B	808	CLA	CAA-CBA-CGA-O2A
22	H	309	CLA	CAA-CBA-CGA-O2A
22	L	407	CLA	CAA-CBA-CGA-O2A
22	O	308	CLA	CAA-CBA-CGA-O2A
22	W	405	CLA	CAA-CBA-CGA-O2A
22	A	807	CLA	CAA-CBA-CGA-O2A
26	K	616	LHG	O8-C23-C24-C25
28	J	101	LMG	O7-C10-C11-C12
30	K	621	SQD	O47-C7-C8-C9
30	O	302	SQD	O47-C7-C8-C9
26	G	614	LHG	C25-C26-C27-C28
28	I	615	LMG	C23-C24-C25-C26
30	K	621	SQD	C7-C8-C9-C10
24	Q	614	DD6	C2-C1-C24-C25
22	B	816	CLA	CAA-CBA-CGA-O1A
22	L	407	CLA	CAA-CBA-CGA-O1A
26	K	616	LHG	O10-C23-C24-C25
22	P	602	CLA	CAA-CBA-CGA-O1A
22	Q	601	CLA	CAA-CBA-CGA-O2A
22	Q	606	CLA	CAA-CBA-CGA-O1A
24	P	613	DD6	C1-C2-C3-C4
22	T	611	CLA	C16-C17-C18-C19
27	B	849	LMU	C2-C1-O1'-C1'
27	H	301	LMU	C2-C1-O1'-C1'
27	X	421	LMU	C2-C1-O1'-C1'
22	O	312	CLA	CAA-CBA-CGA-O2A
22	R	607	CLA	CAA-CBA-CGA-O2A
22	K	617	CLA	O1D-CGD-O2D-CED
22	W	409	CLA	O1A-CGA-O2A-C1
22	B	808	CLA	CAA-CBA-CGA-O1A
22	G	603	CLA	CAA-CBA-CGA-O1A
22	Q	609	CLA	CBA-CGA-O2A-C1
22	I	606	CLA	CBD-CGD-O2D-CED
22	T	601	CLA	CAA-CBA-CGA-O2A
22	U	412	CLA	CAA-CBA-CGA-O1A
26	H	316	LHG	C25-C26-C27-C28
27	A	854	LMU	C9-C10-C11-C12
22	G	603	CLA	CAA-CBA-CGA-O2A
26	W	420	LHG	O8-C23-C24-C25
22	Q	611	CLA	CAA-CBA-CGA-O1A
22	W	405	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
28	L	401	LMG	O10-C28-C29-C30
22	R	606	CLA	C2A-CAA-CBA-CGA
22	Q	612	CLA	C16-C17-C18-C19
27	O	320	LMU	C1-C2-C3-C4
22	A	810	CLA	C13-C15-C16-C17
22	K	617	CLA	C4-C3-C5-C6
22	Q	608	CLA	CAA-CBA-CGA-O2A
22	Q	610	CLA	CAA-CBA-CGA-O2A
22	A	832	CLA	CAA-CBA-CGA-O2A

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	L	420	LMU	C1'-C2'-C3'-C4'-C5'-O5'
27	L	419	LMU	C1'-C2'-C3'-C4'-C5'-O5'

291 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	315	CLA	2	0
22	B	838	CLA	3	0
22	O	314	CLA	1	0
27	T	618	LMU	2	0
22	A	828	CLA	4	0
22	L	411	CLA	1	0
22	G	602	CLA	1	0
26	L	416	LHG	3	0
22	W	402	CLA	2	0
28	U	423	LMG	2	0
22	S	602	CLA	1	0
28	H	319	LMG	1	0
22	B	830	CLA	4	0
22	B	812	CLA	1	0
30	K	621	SQD	1	0
22	B	835	CLA	2	0
24	B	841	DD6	1	0
22	L	404	CLA	6	0
22	S	606	CLA	1	0
32	V	616	NEX	9	0
22	A	841	CLA	3	0
21	A	849	BCR	3	0
22	V	602	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	810	CLA	1	0
27	M	102	LMU	1	0
22	B	809	CLA	4	0
22	B	821	CLA	2	0
22	B	831	CLA	2	0
22	U	412	CLA	1	0
22	B	823	CLA	3	0
22	P	610	CLA	1	0
22	W	414	CLA	1	0
21	B	844	BCR	5	0
22	O	308	CLA	4	0
28	J	101	LMG	1	0
22	V	612	CLA	7	0
22	I	607	CLA	3	0
22	A	807	CLA	1	0
22	H	310	CLA	1	0
22	S	601	CLA	1	0
27	A	857	LMU	1	0
22	K	608	CLA	4	0
21	B	843	BCR	3	0
22	F	403	CLA	2	0
22	N	602	CLA	1	0
22	K	613	CLA	4	0
22	N	601	CLA	1	0
28	F	408	LMG	3	0
28	K	601	LMG	3	0
22	T	608	CLA	2	0
22	A	822	CLA	3	0
24	Q	614	DD6	1	0
26	S	613	LHG	2	0
22	I	601	CLA	2	0
22	P	603	CLA	1	0
22	R	601	CLA	6	0
22	U	405	CLA	3	0
22	G	608	CLA	4	0
22	A	830	CLA	1	0
22	L	408	CLA	12	0
22	A	811	CLA	1	0
31	U	408	CHL	4	0
22	Q	603	CLA	1	0
22	A	815	CLA	2	0
22	W	411	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	G	610	CLA	1	0
28	N	615	LMG	1	0
27	L	420	LMU	2	0
28	B	856	LMG	4	0
22	A	808	CLA	1	0
22	W	413	CLA	2	0
22	X	413	CLA	1	0
22	A	803	CLA	1	0
28	W	401	LMG	3	0
22	B	811	CLA	1	0
22	T	605	CLA	4	0
22	B	828	CLA	2	0
22	G	609	CLA	3	0
22	Q	609	CLA	1	0
22	P	605	CLA	1	0
22	V	609	CLA	2	0
22	J	102	CLA	1	0
26	O	318	LHG	1	0
21	B	845	BCR	2	0
22	O	307	CLA	1	0
22	R	615	CLA	2	0
32	U	418	NEX	4	0
22	B	827	CLA	1	0
22	A	814	CLA	4	0
22	X	403	CLA	1	0
22	I	608	CLA	2	0
22	V	617	CLA	1	0
22	B	802	CLA	2	0
22	A	819	CLA	1	0
22	A	827	CLA	2	0
22	A	813	CLA	2	0
22	K	617	CLA	2	0
22	O	313	CLA	3	0
22	R	607	CLA	3	0
22	F	404	CLA	4	0
22	B	819	CLA	1	0
26	O	321	LHG	3	0
22	H	311	CLA	2	0
22	U	420	CLA	1	0
22	X	419	CLA	2	0
22	G	603	CLA	2	0
22	H	312	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	V	606	CHL	14	0
31	W	407	CHL	6	0
28	U	402	LMG	2	0
31	U	407	CHL	3	0
27	F	409	LMU	1	0
22	I	611	CLA	4	0
22	V	604	CLA	7	0
22	A	829	CLA	1	0
22	W	410	CLA	3	0
22	A	821	CLA	1	0
22	V	603	CLA	2	0
22	T	606	CLA	1	0
22	K	604	CLA	6	0
22	V	601	CLA	4	0
22	G	611	CLA	1	0
22	U	409	CLA	1	0
22	B	820	CLA	1	0
22	B	818	CLA	1	0
22	W	404	CLA	2	0
22	N	606	CLA	4	0
22	L	406	CLA	1	0
22	K	607	CLA	9	0
22	Q	612	CLA	1	0
22	S	605	CLA	4	0
22	A	816	CLA	2	0
22	B	824	CLA	3	0
22	T	604	CLA	1	0
22	A	812	CLA	3	0
26	W	420	LHG	2	0
22	I	606	CLA	2	0
26	P	601	LHG	1	0
22	Q	610	CLA	2	0
22	L	417	CLA	7	0
22	W	415	CLA	1	0
22	B	836	CLA	2	0
22	U	406	CLA	1	0
22	A	809	CLA	1	0
22	B	859	CLA	2	0
22	Q	601	CLA	1	0
22	R	605	CLA	5	0
22	K	609	CLA	2	0
25	F	401	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	814	CLA	1	0
22	B	834	CLA	5	0
26	N	614	LHG	1	0
22	W	409	CLA	4	0
22	A	838	CLA	3	0
22	X	404	CLA	1	0
22	W	406	CLA	3	0
22	A	842	CLA	4	0
22	B	804	CLA	2	0
31	W	408	CHL	8	0
27	H	301	LMU	1	0
31	V	605	CHL	12	0
22	X	411	CLA	1	0
22	Q	611	CLA	1	0
22	B	817	CLA	1	0
22	A	834	CLA	1	0
21	M	101	BCR	3	0
24	S	611	DD6	1	0
22	A	836	CLA	2	0
22	A	805	CLA	2	0
22	A	801	CLA	1	0
22	O	311	CLA	3	0
21	B	842	BCR	2	0
22	V	607	CLA	2	0
22	R	604	CLA	5	0
22	H	305	CLA	1	0
26	B	851	LHG	7	0
22	A	824	CLA	4	0
22	S	604	CLA	1	0
22	P	608	CLA	2	0
22	A	852	CLA	4	0
22	B	829	CLA	3	0
22	G	601	CLA	1	0
22	L	409	CLA	2	0
22	Q	608	CLA	3	0
22	A	831	CLA	2	0
22	I	602	CLA	1	0
22	N	604	CLA	1	0
22	B	816	CLA	2	0
22	B	825	CLA	3	0
22	B	839	CLA	2	0
28	I	615	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	S	607	CLA	1	0
22	T	607	CLA	1	0
27	U	424	LMU	1	0
26	N	616	LHG	1	0
22	X	409	CLA	1	0
28	Q	602	LMG	2	0
22	A	817	CLA	2	0
27	A	854	LMU	1	0
22	K	611	CLA	3	0
27	L	419	LMU	4	0
22	L	410	CLA	3	0
26	B	848	LHG	1	0
28	H	322	LMG	1	0
23	B	840	PQN	1	0
26	A	845	LHG	1	0
22	L	402	CLA	2	0
22	R	602	CLA	4	0
22	Q	613	CLA	2	0
22	B	805	CLA	1	0
22	H	313	CLA	1	0
22	S	609	CLA	1	0
22	R	606	CLA	3	0
22	P	606	CLA	3	0
22	A	820	CLA	1	0
22	A	825	CLA	2	0
22	O	312	CLA	1	0
21	A	851	BCR	3	0
22	A	839	CLA	1	0
22	P	607	CLA	1	0
22	V	608	CLA	1	0
22	A	844	CLA	4	0
25	O	304	DGD	3	0
22	B	806	CLA	4	0
22	Q	605	CLA	1	0
22	A	840	CLA	3	0
22	A	833	CLA	1	0
22	K	606	CLA	2	0
22	N	610	CLA	3	0
27	B	858	LMU	1	0
25	B	847	DGD	6	0
22	X	408	CLA	1	0
22	R	610	CLA	3	0

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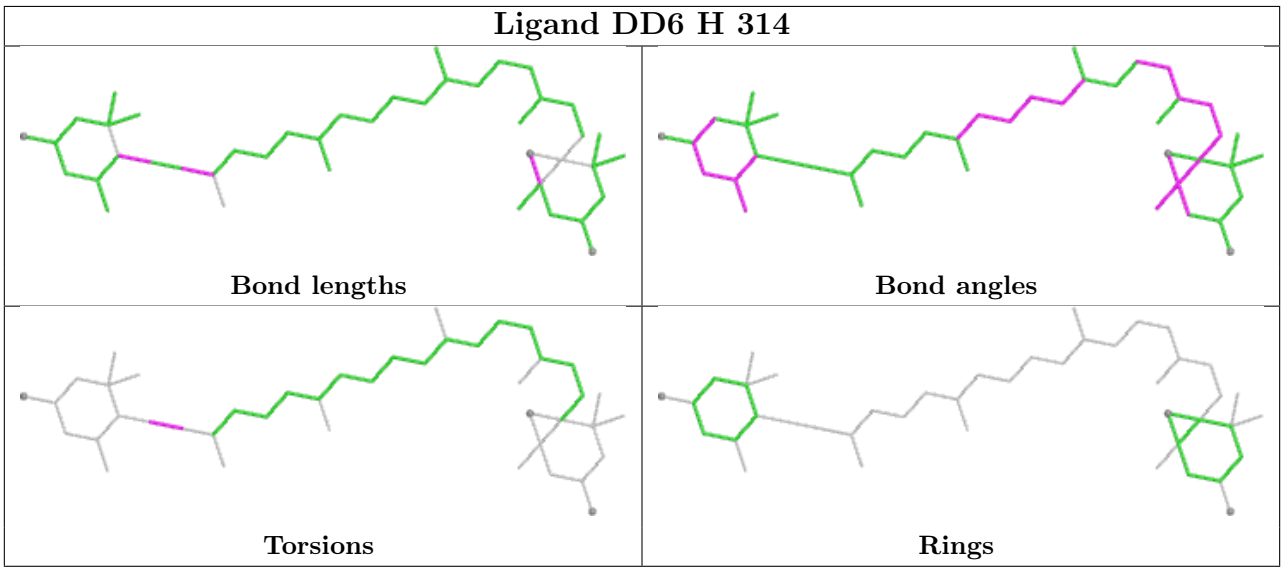
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	607	CLA	7	0
22	R	611	CLA	2	0
22	B	803	CLA	2	0
22	S	610	CLA	2	0
22	A	832	CLA	3	0
28	T	616	LMG	2	0
27	B	855	LMU	1	0
22	T	611	CLA	1	0
22	H	307	CLA	1	0
22	P	602	CLA	2	0
22	N	603	CLA	2	0
22	U	415	CLA	2	0
22	B	822	CLA	3	0
22	V	613	CLA	1	0
21	J	103	BCR	1	0
26	Q	616	LHG	1	0
22	I	603	CLA	3	0
27	H	321	LMU	1	0
22	K	603	CLA	2	0
30	O	302	SQD	8	0
22	B	813	CLA	3	0
22	U	411	CLA	1	0
22	L	412	CLA	3	0
22	H	308	CLA	2	0
26	K	616	LHG	3	0
22	S	608	CLA	2	0
30	V	618	SQD	1	0
21	B	846	BCR	1	0
22	U	401	CLA	2	0
22	A	806	CLA	4	0
22	A	804	CLA	3	0
22	P	609	CLA	1	0
22	A	823	CLA	1	0
27	K	620	LMU	2	0
21	A	848	BCR	2	0
22	K	605	CLA	3	0
22	O	309	CLA	3	0
26	A	846	LHG	2	0
22	U	404	CLA	2	0
27	O	301	LMU	4	0
21	B	801	BCR	8	0
27	U	421	LMU	1	0

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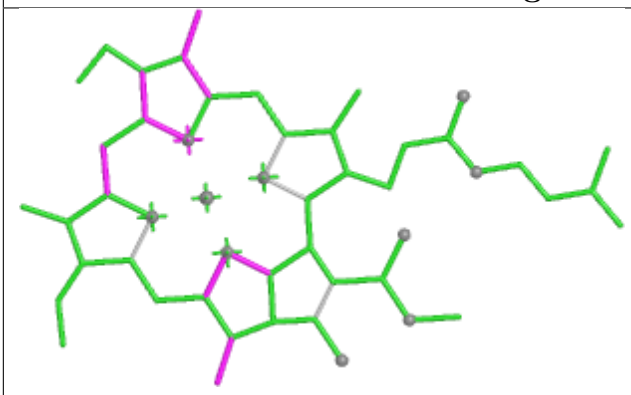
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	802	CL0	6	0
26	T	614	LHG	1	0
22	Q	604	CLA	5	0
22	Q	607	CLA	2	0
31	W	422	CHL	2	0
22	B	815	CLA	3	0
22	O	310	CLA	1	0
30	F	407	SQD	2	0
23	A	843	PQN	2	0
26	R	614	LHG	3	0
22	B	807	CLA	2	0
27	B	854	LMU	8	0
22	O	305	CLA	1	0
22	B	832	CLA	3	0
22	B	833	CLA	4	0
22	W	412	CLA	2	0

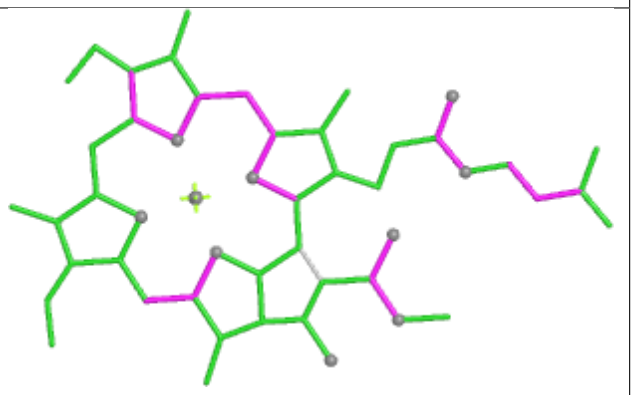
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



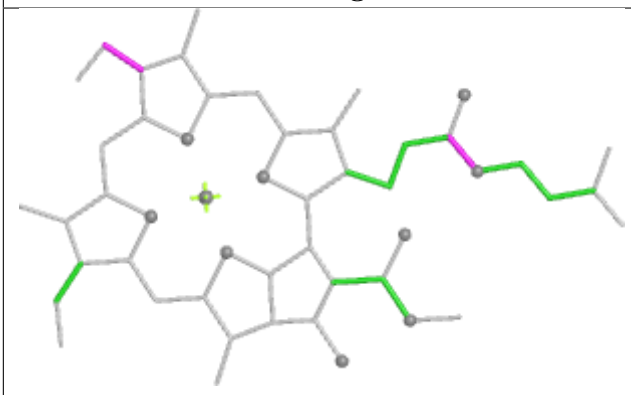
Ligand CLA O 315



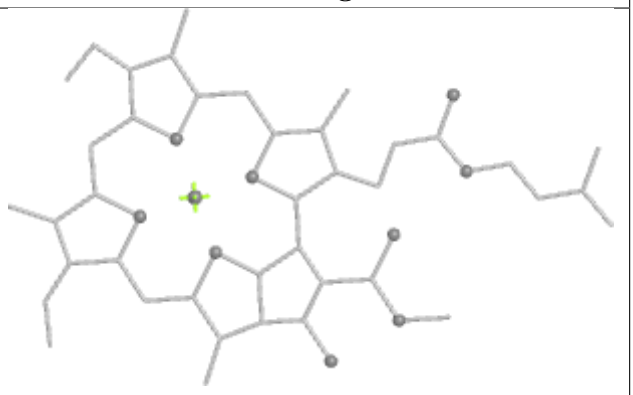
Bond lengths



Bond angles

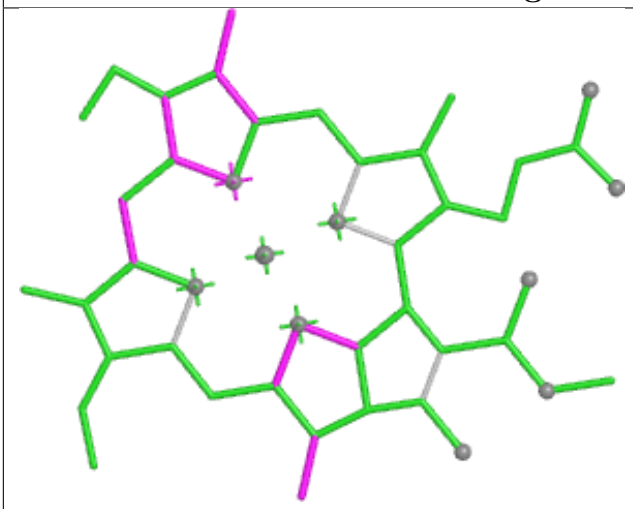


Torsions

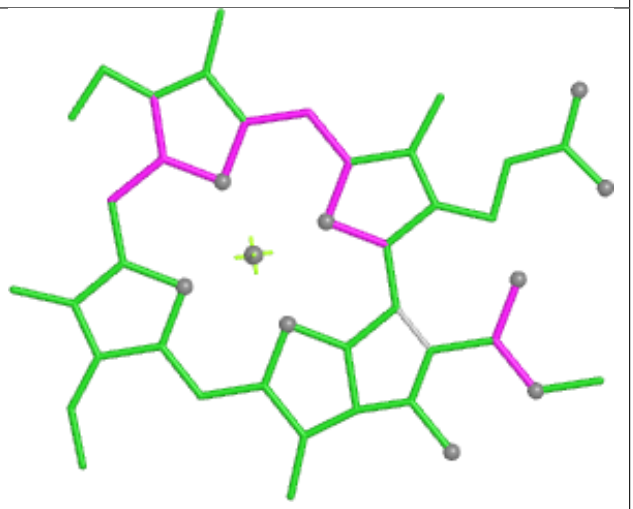


Rings

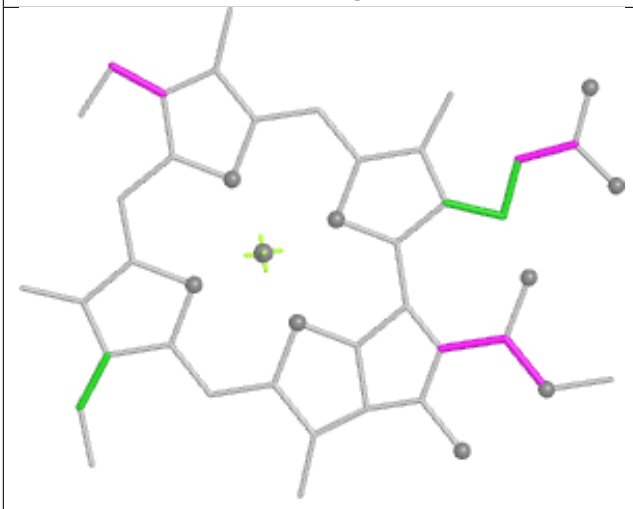
Ligand CLA B 838



Bond lengths



Bond angles

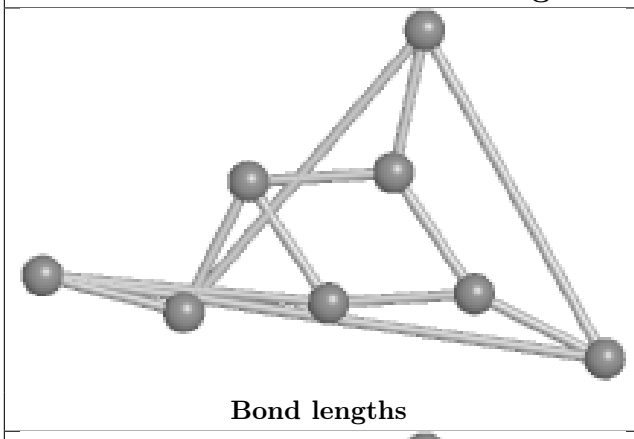


Torsions

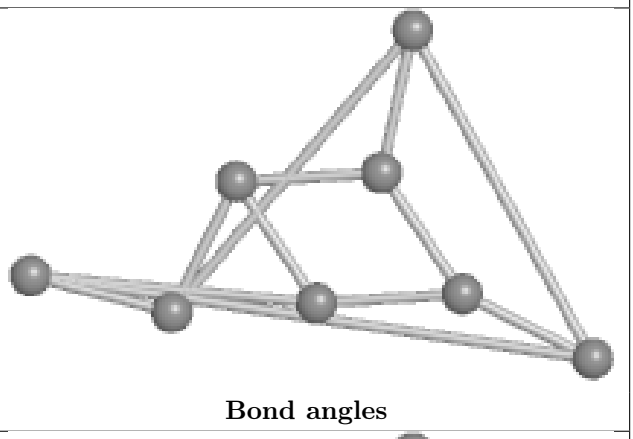


Rings

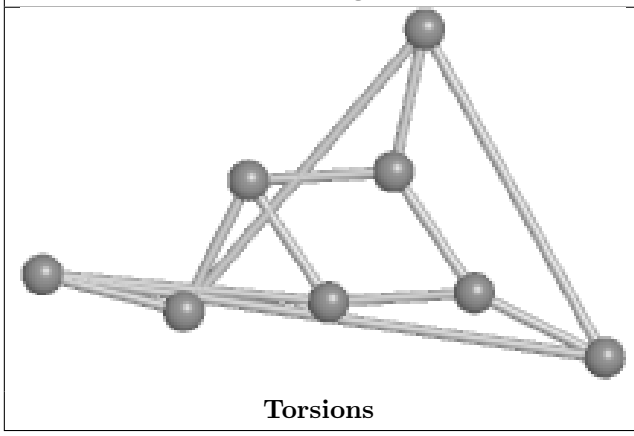
Ligand SF4 C 101



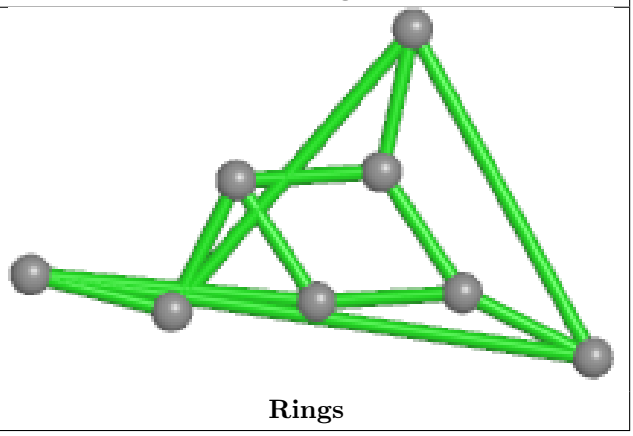
Bond lengths



Bond angles

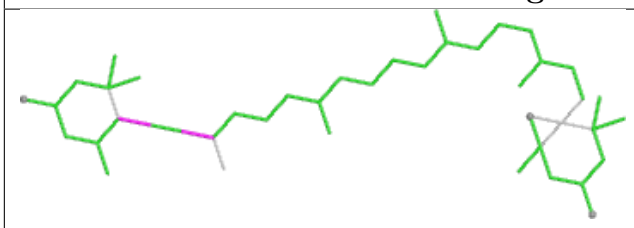


Torsions

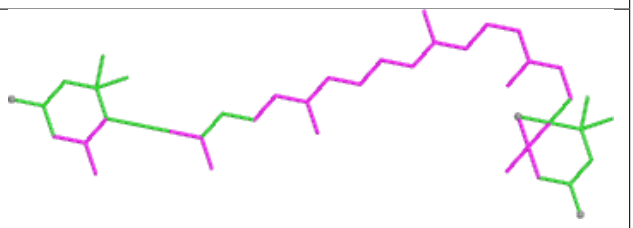


Rings

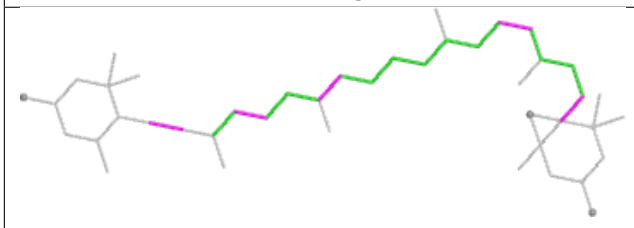
Ligand DD6 P 612



Bond lengths



Bond angles

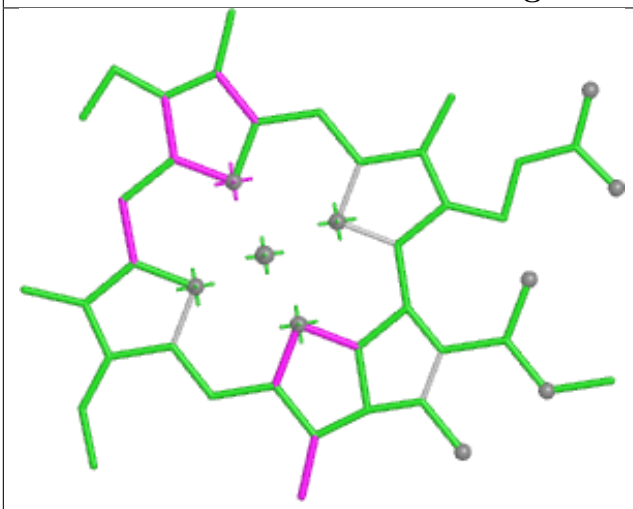


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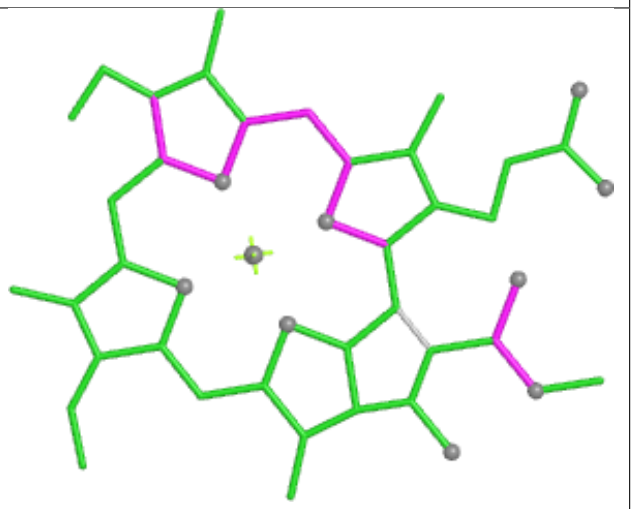


Rings

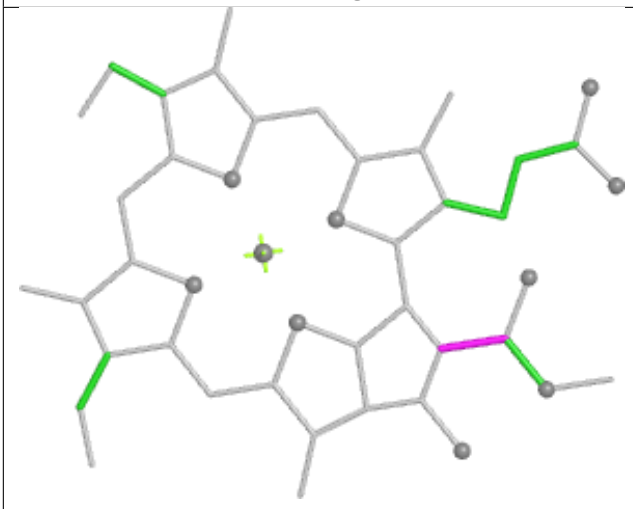
Ligand CLA O 314



Bond lengths



Bond angles

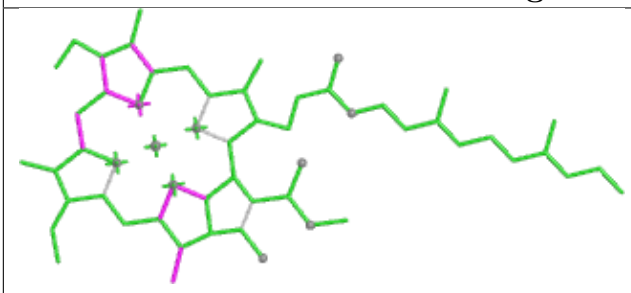


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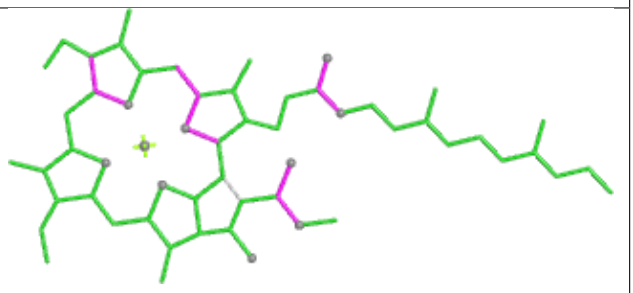


Rings

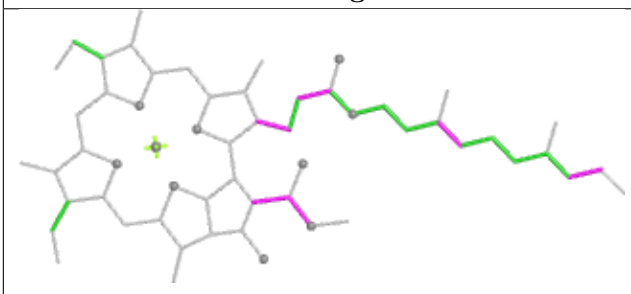
Ligand CLA L 407



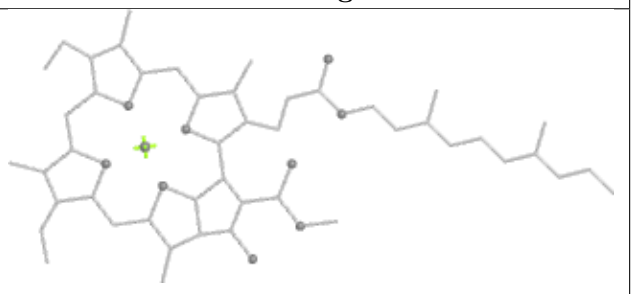
Bond lengths



Bond angles

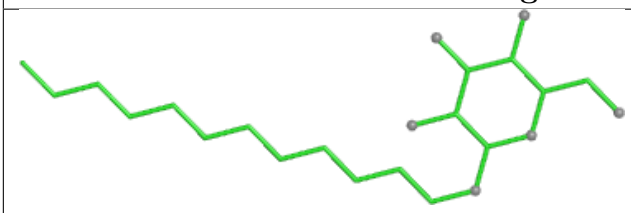


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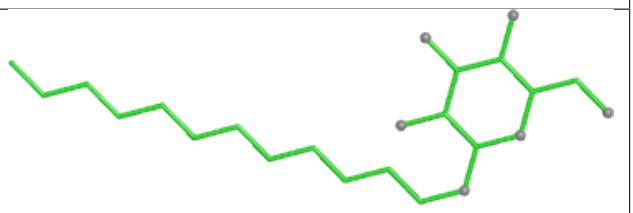


Rings

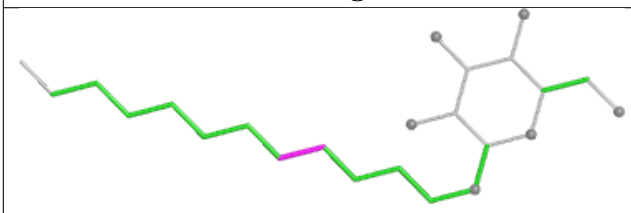
Ligand LMU T 618



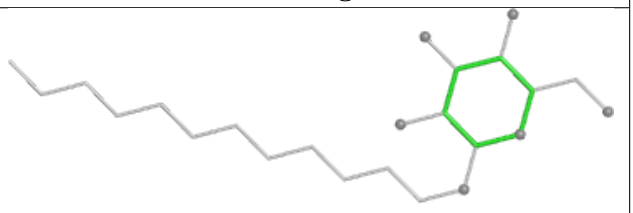
Bond lengths



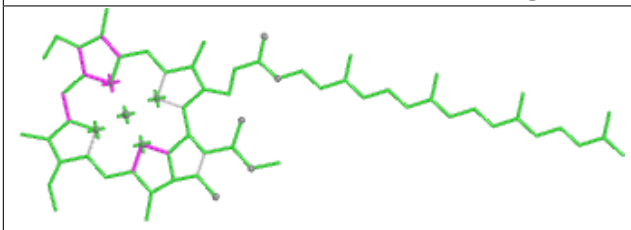
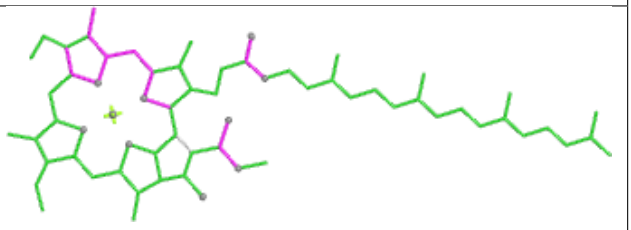
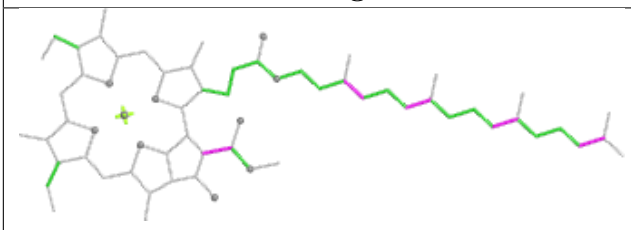
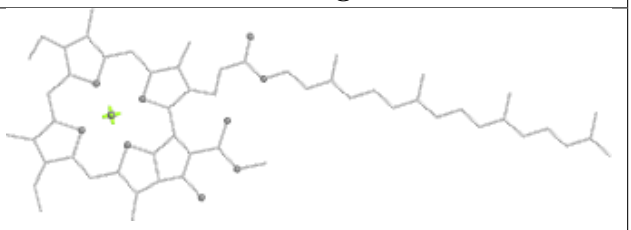
Bond angles

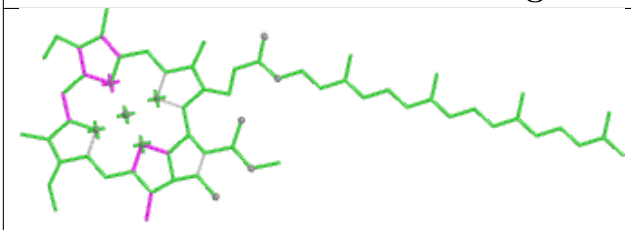
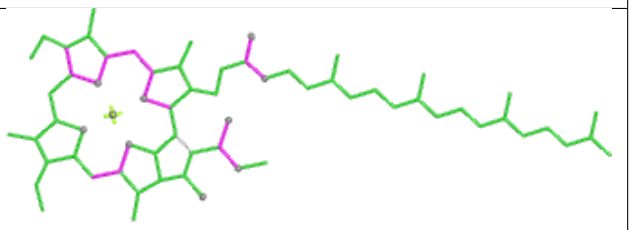
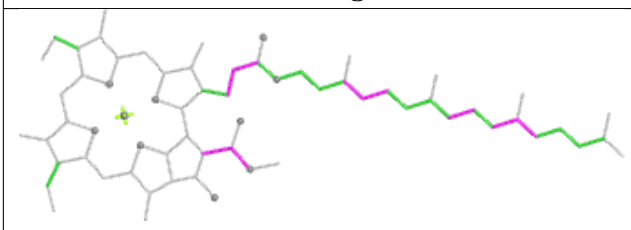
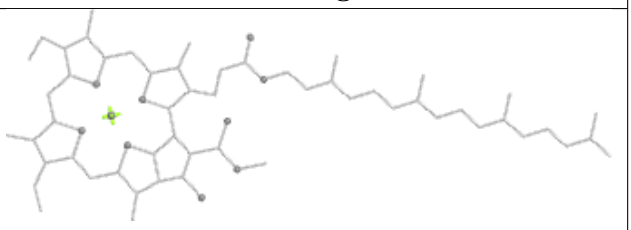


Torsions

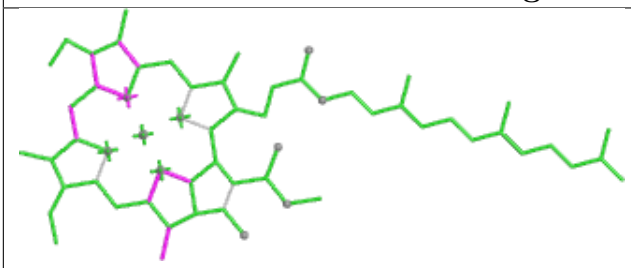


Rings

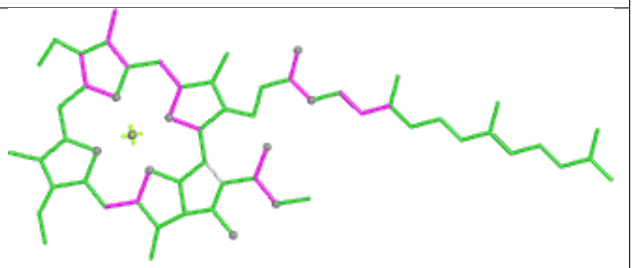
Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

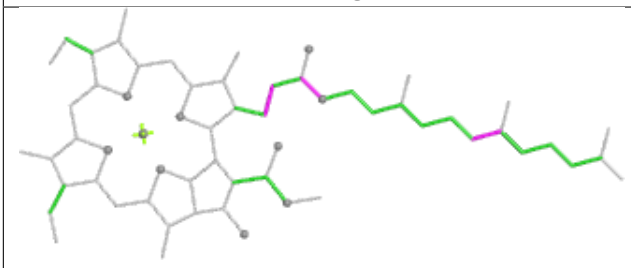
Ligand CLA G 602



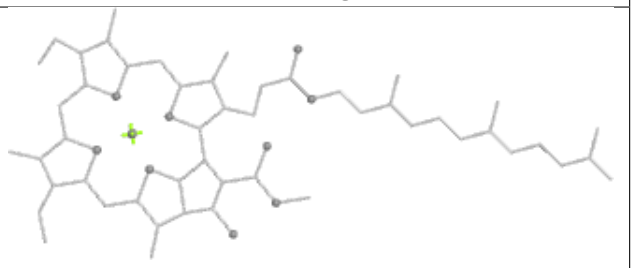
Bond lengths



Bond angles

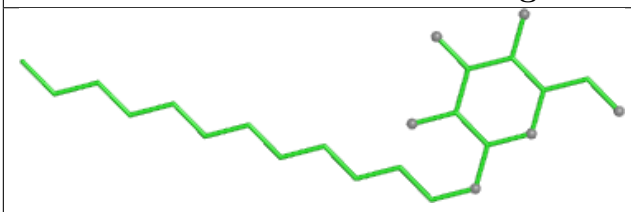


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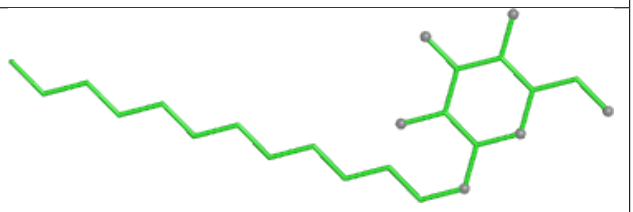


Rings

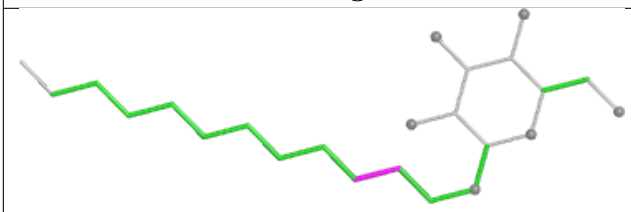
Ligand LMU X 418



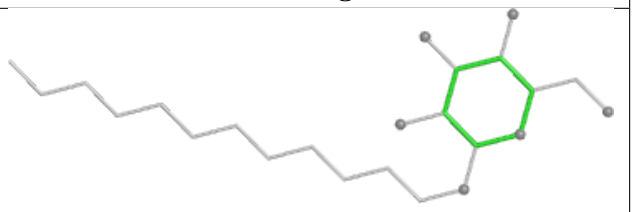
Bond lengths



Bond angles

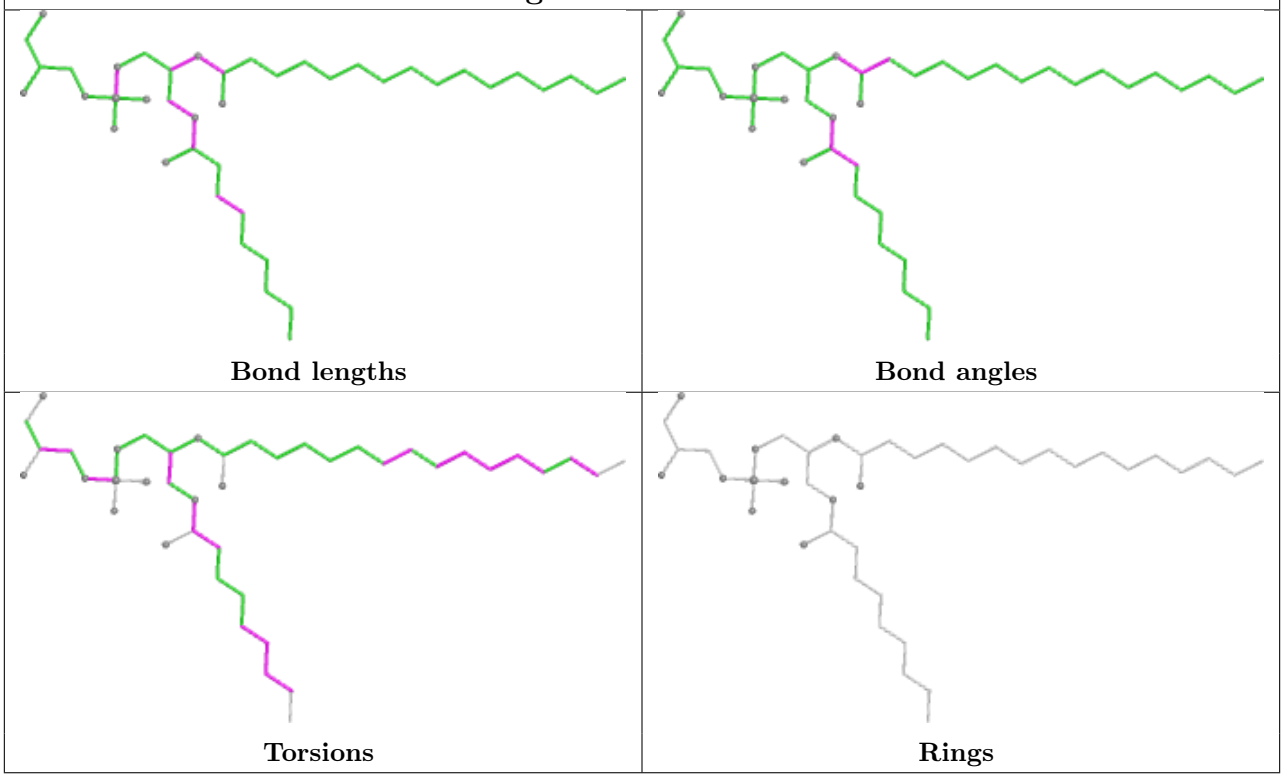


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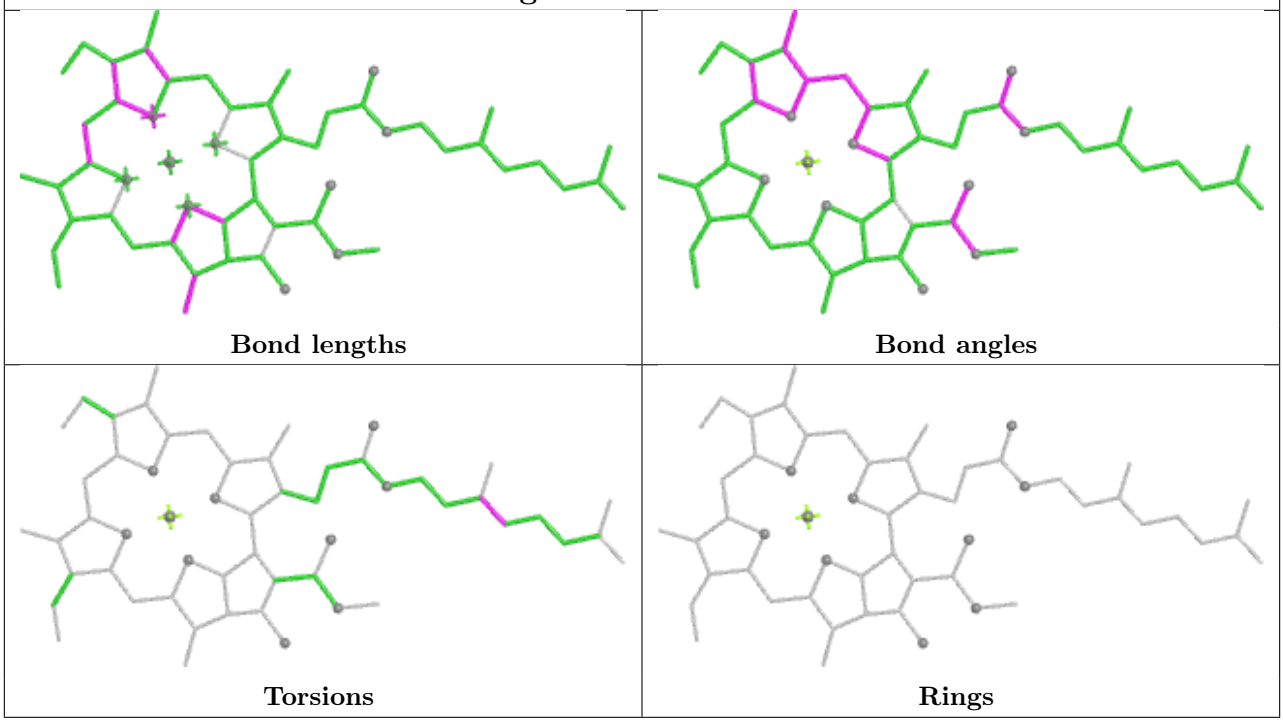


Rings

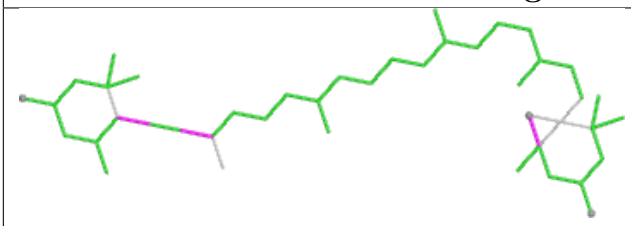
Ligand LHG L 416



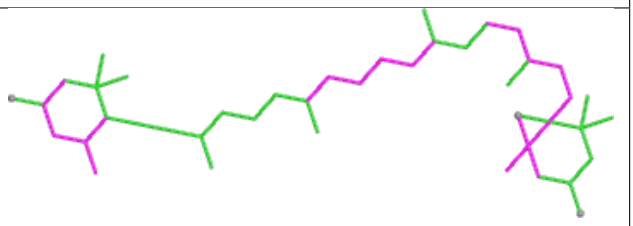
Ligand CLA W 402



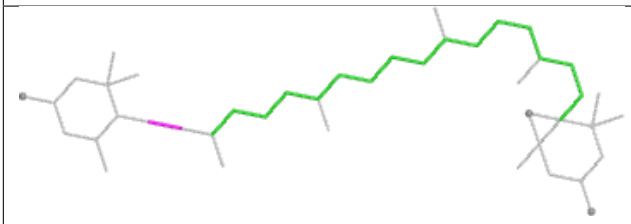
Ligand DD6 V 614



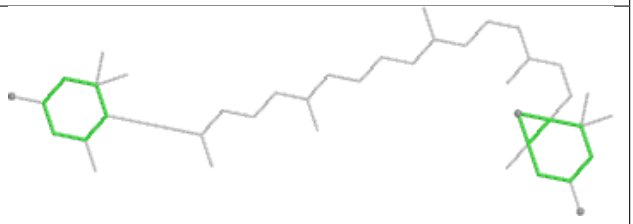
Bond lengths



Bond angles

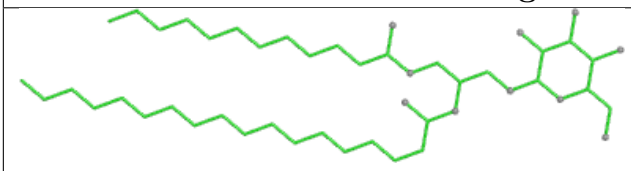


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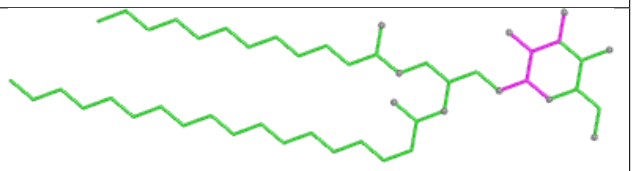


Rings

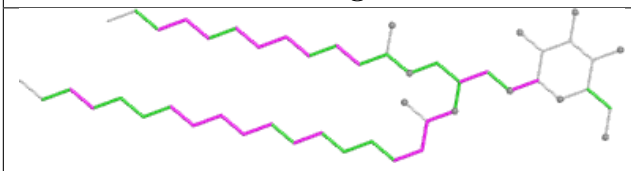
Ligand LMG U 423



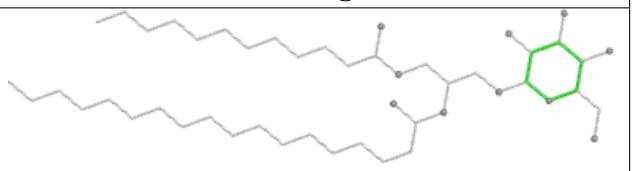
Bond lengths



Bond angles

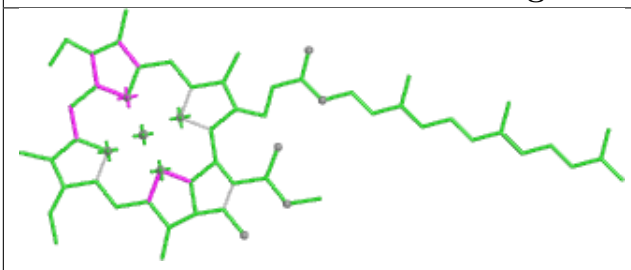


Torsions

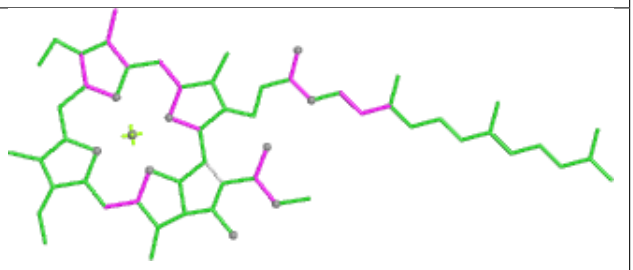


Rings

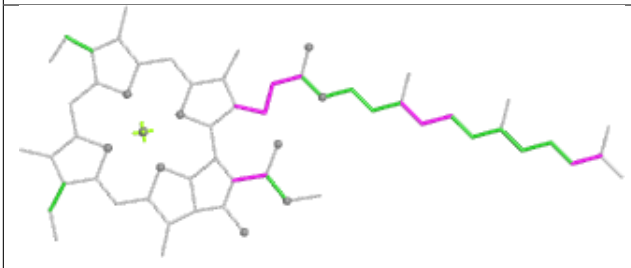
Ligand CLA S 602



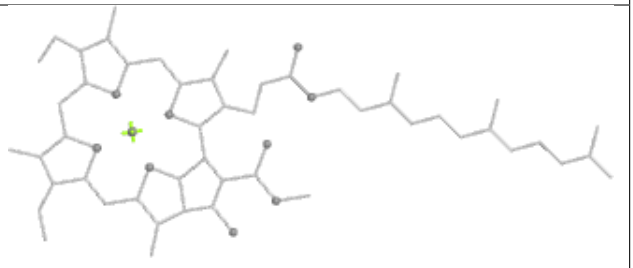
Bond lengths



Bond angles

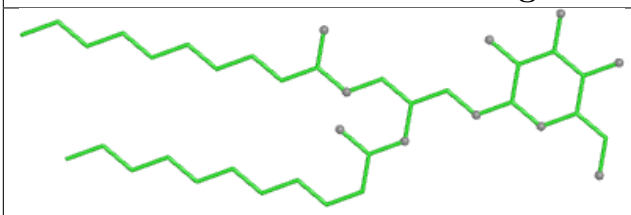


Torsions

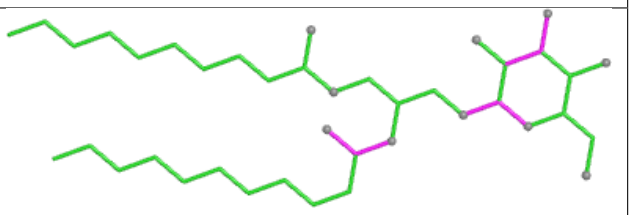


Rings

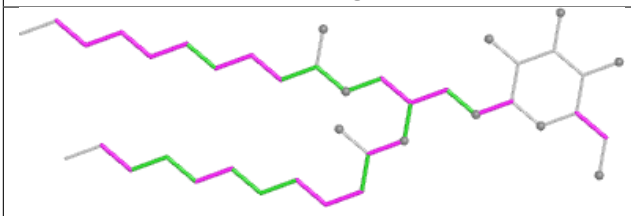
Ligand LMG H 319



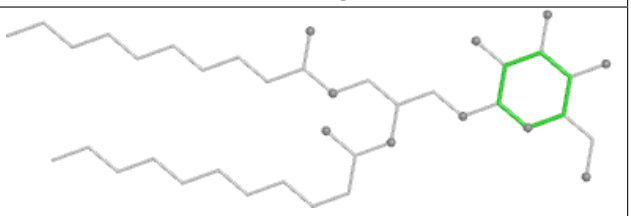
Bond lengths



Bond angles

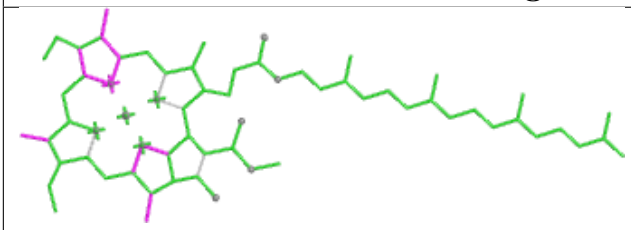


Torsions

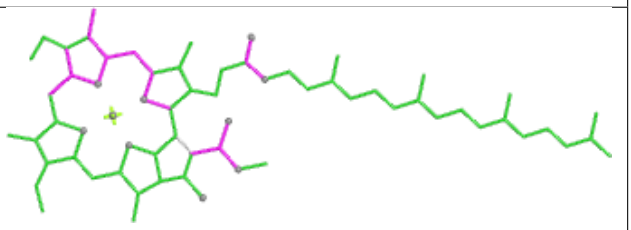


Rings

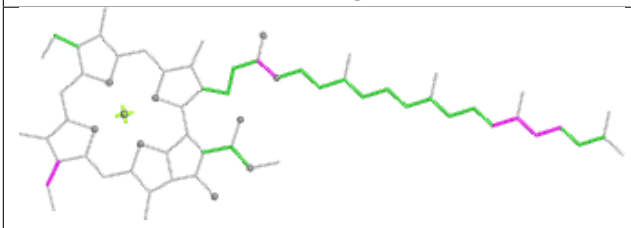
Ligand CLA B 830



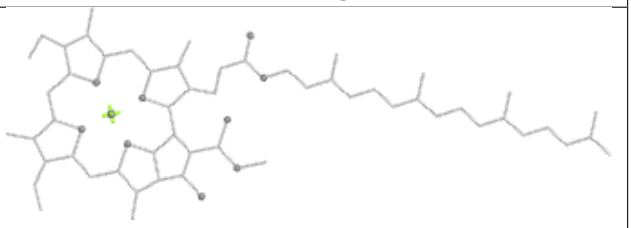
Bond lengths



Bond angles

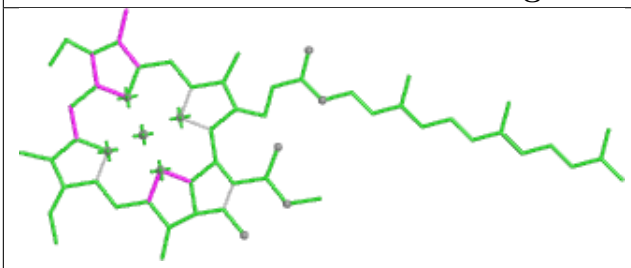


Torsions

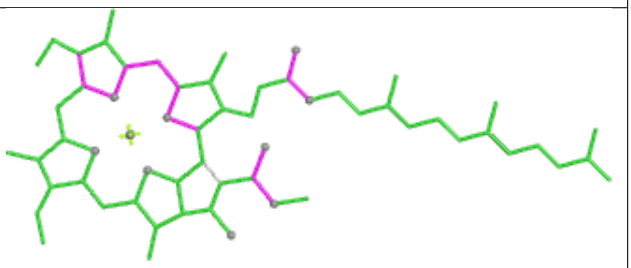


Rings

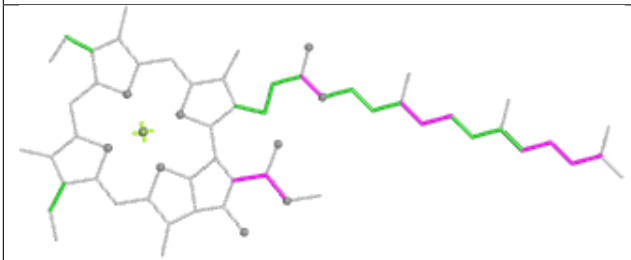
Ligand CLA X 410



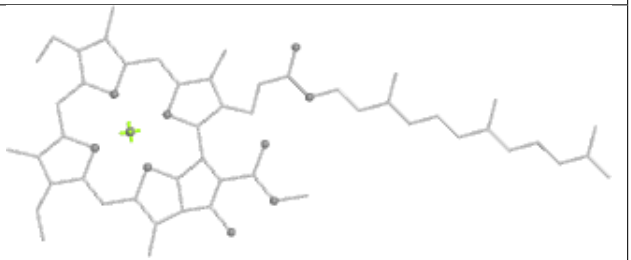
Bond lengths



Bond angles

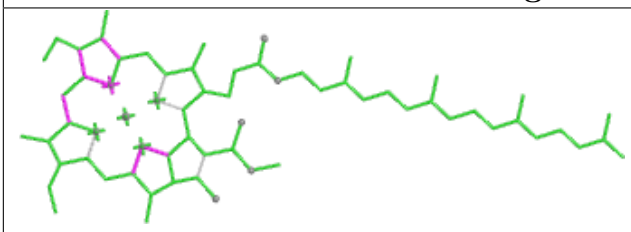


Torsions

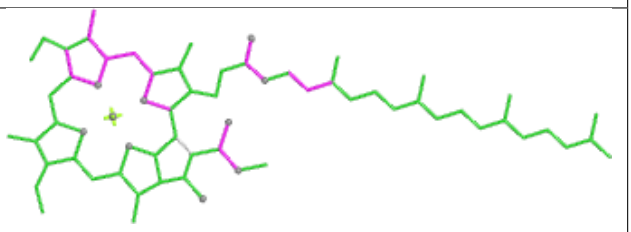


Rings

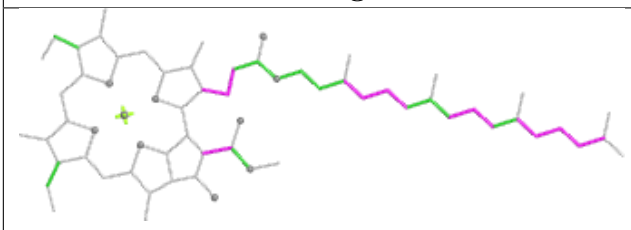
Ligand CLA B 812



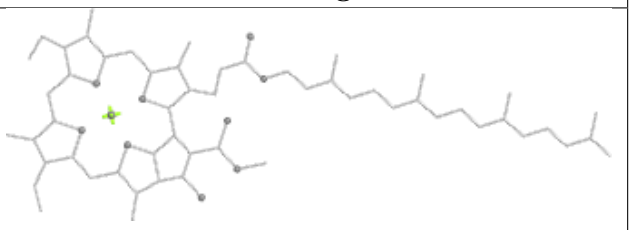
Bond lengths



Bond angles

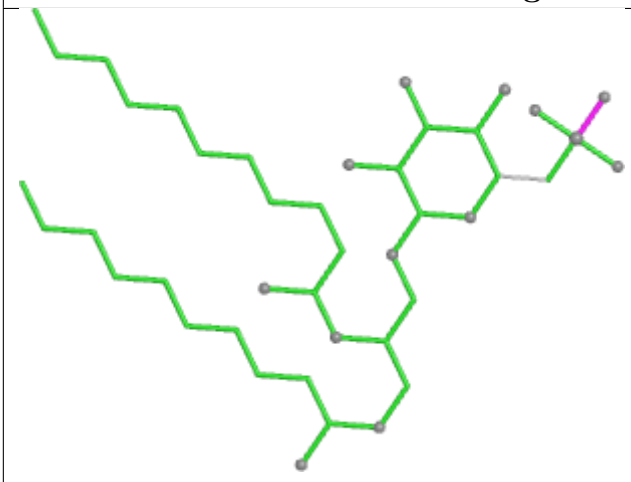


Torsions

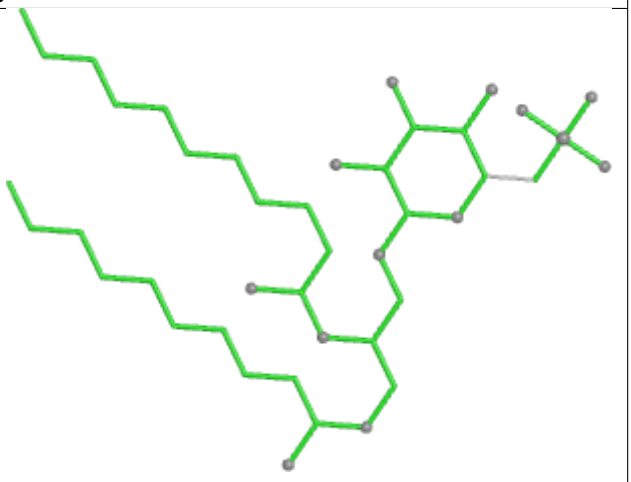


Rings

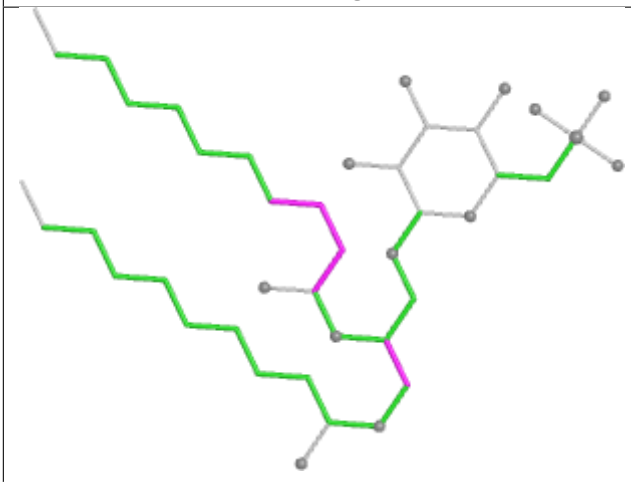
Ligand SQD K 621



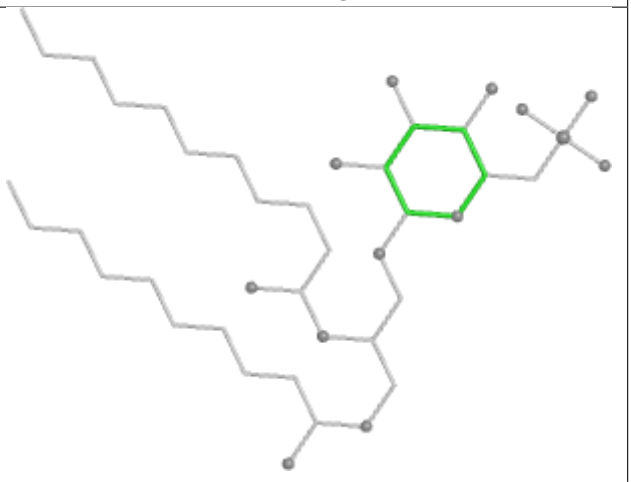
Bond lengths



Bond angles

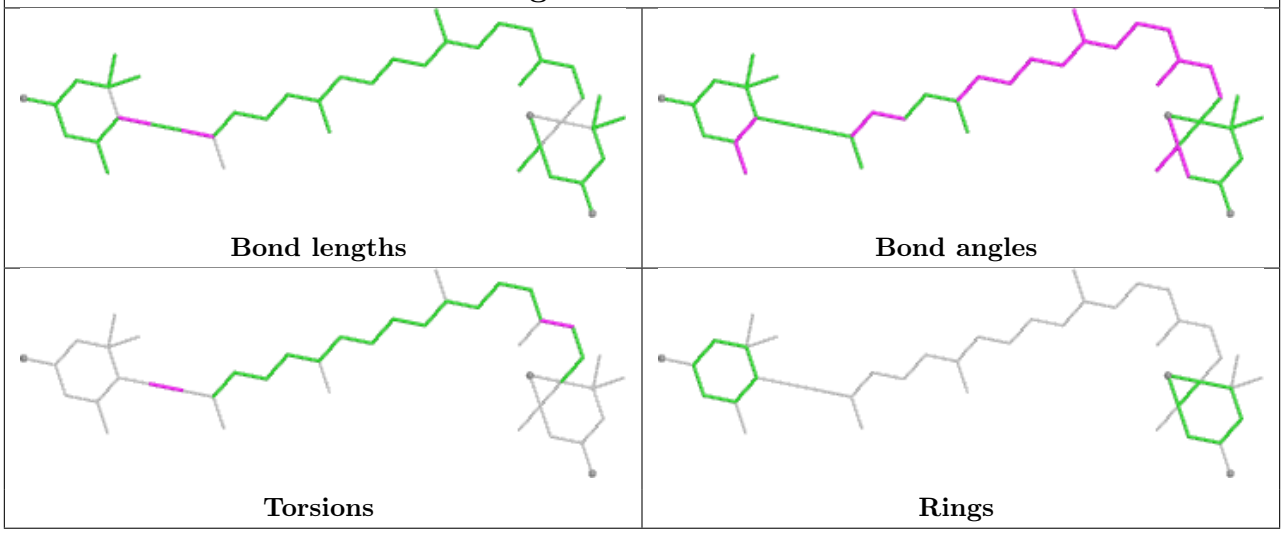


Torsions

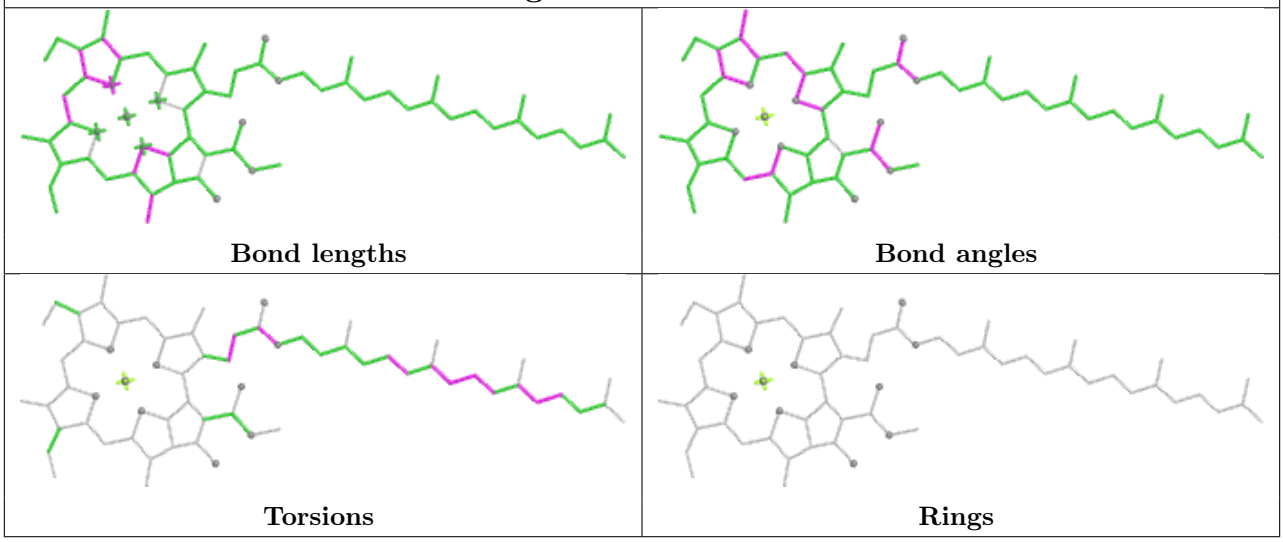


Rings

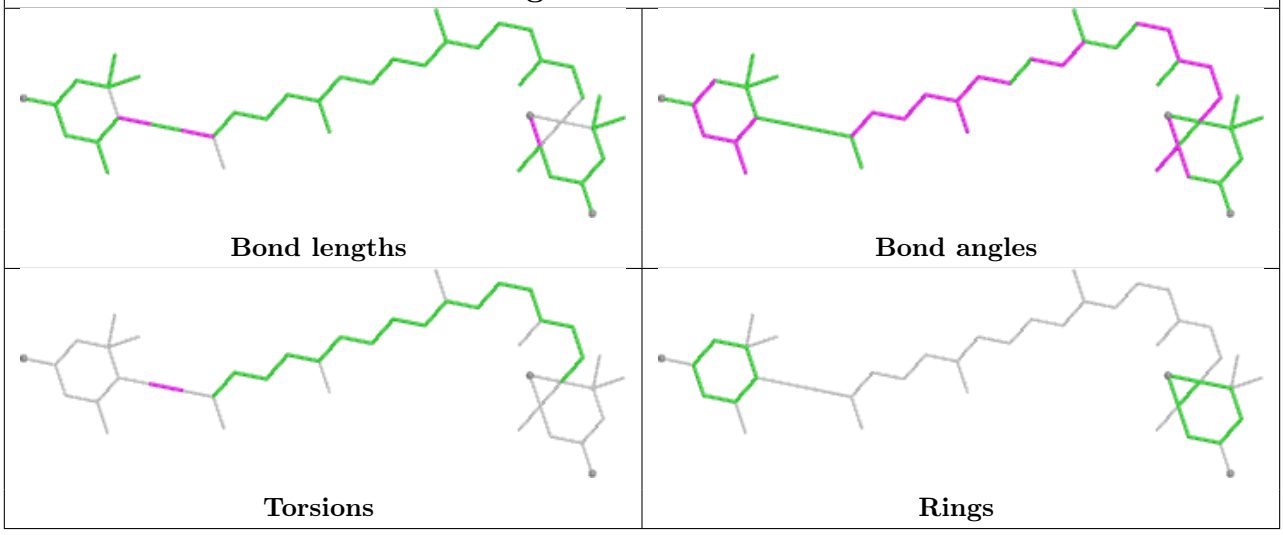
Ligand DD6 J 105

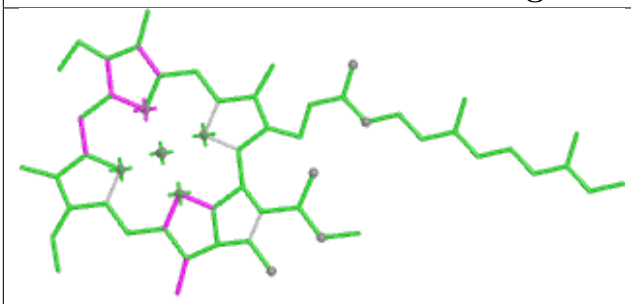
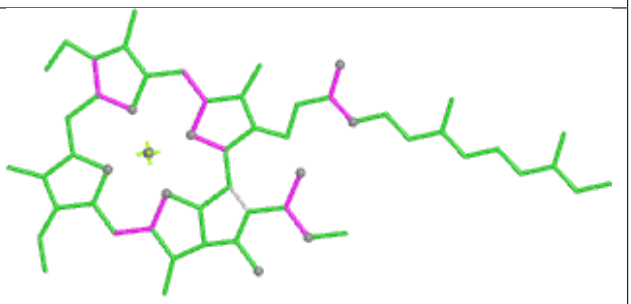
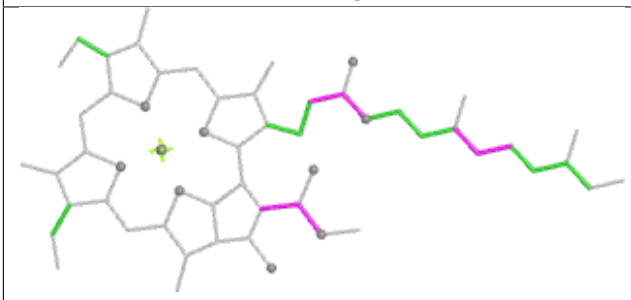
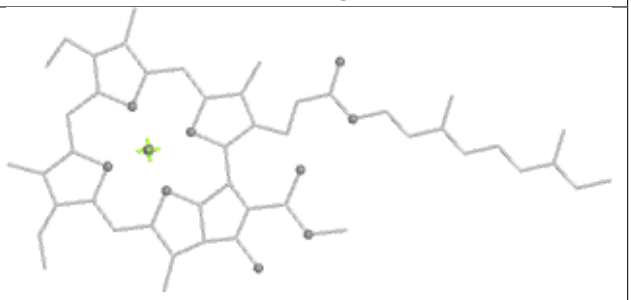


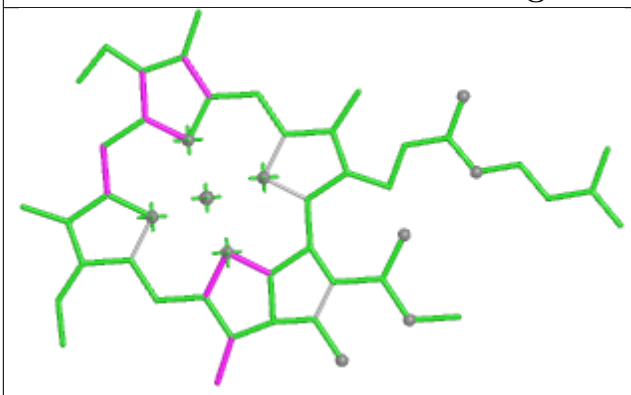
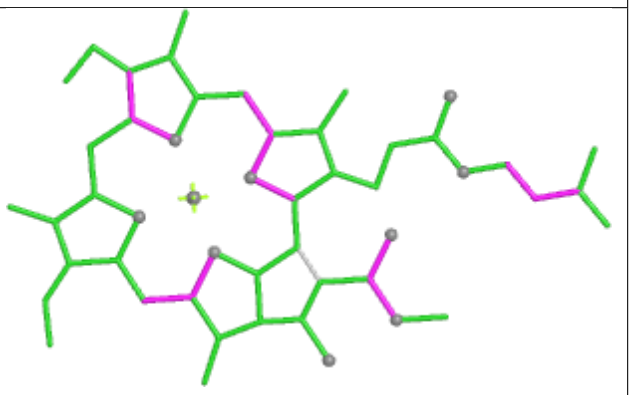
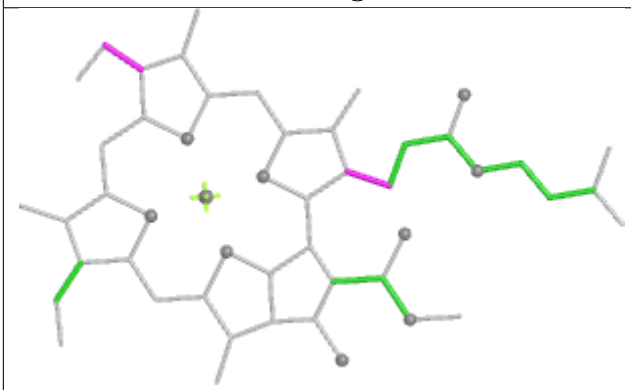
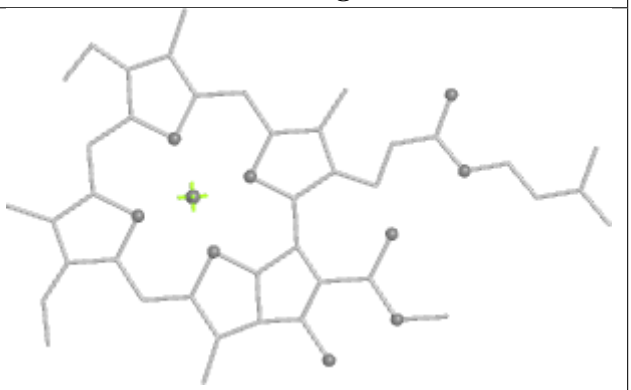
Ligand CLA B 835



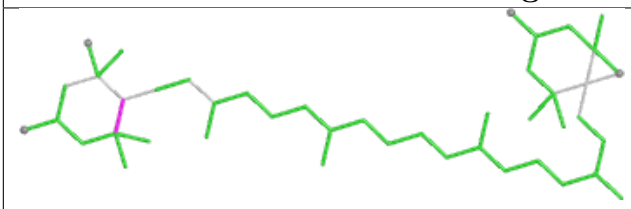
Ligand DD6 B 841



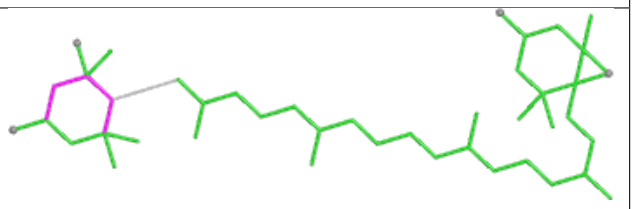
Ligand CLA L 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA S 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX V 616



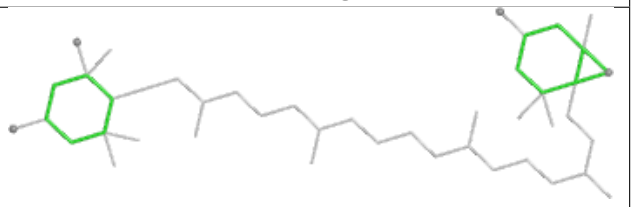
Bond lengths



Bond angles

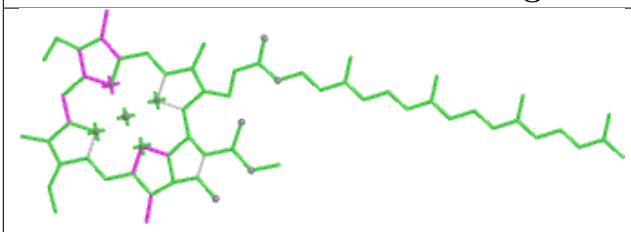


Torsions

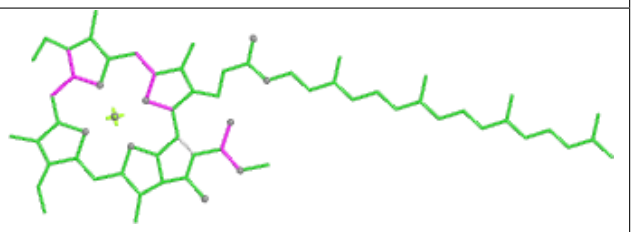


Rings

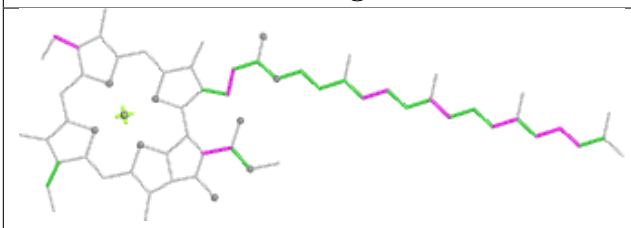
Ligand CLA A 841



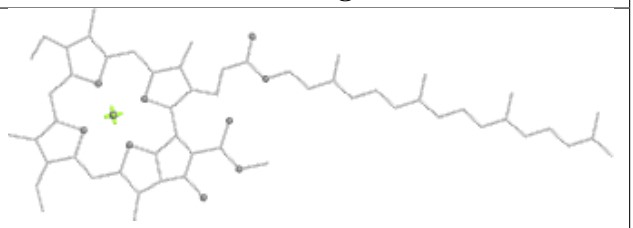
Bond lengths



Bond angles

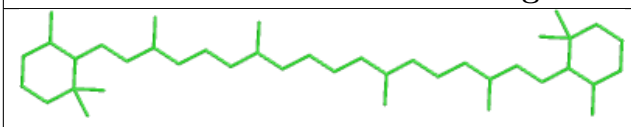


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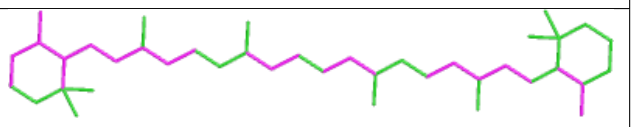


Rings

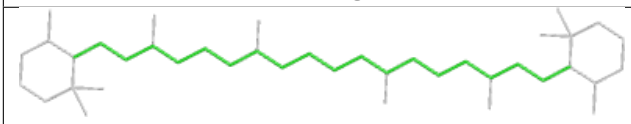
Ligand BCR A 849



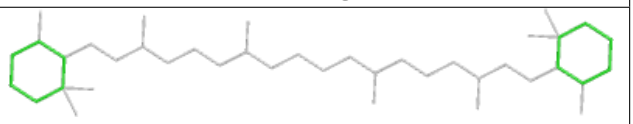
Bond lengths



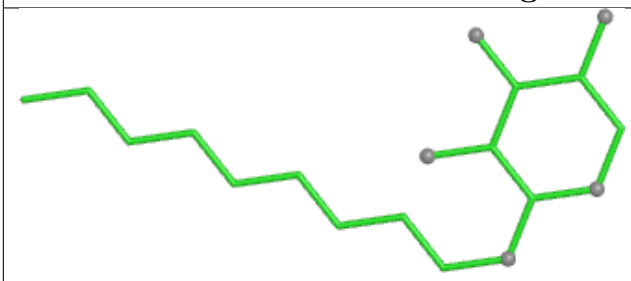
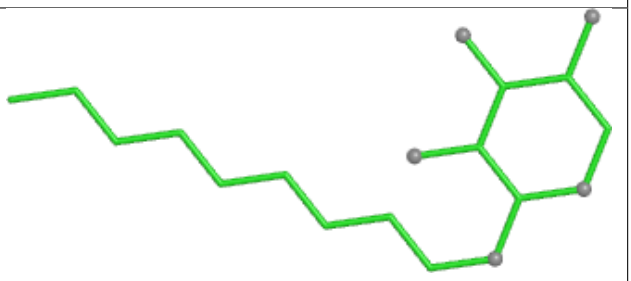
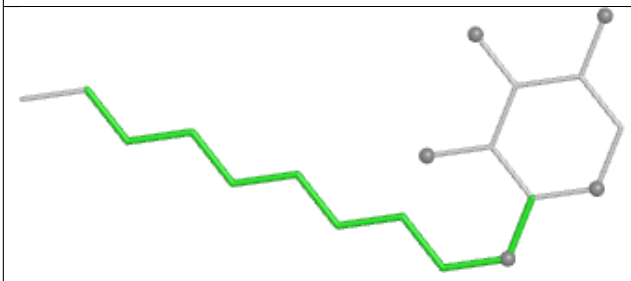
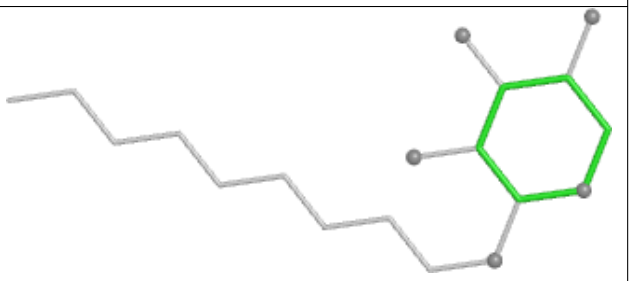
Bond angles

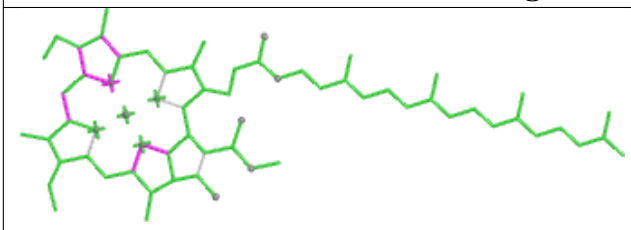
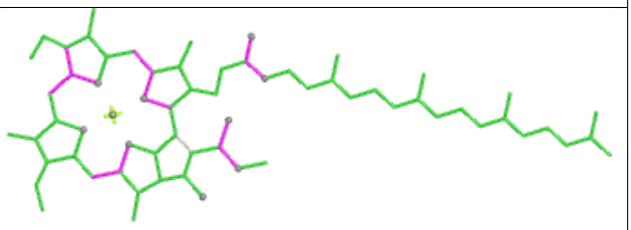
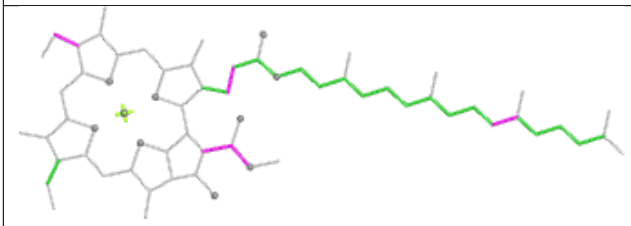
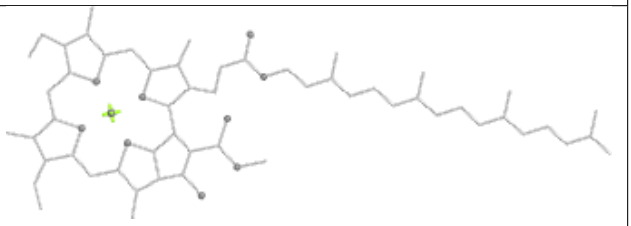


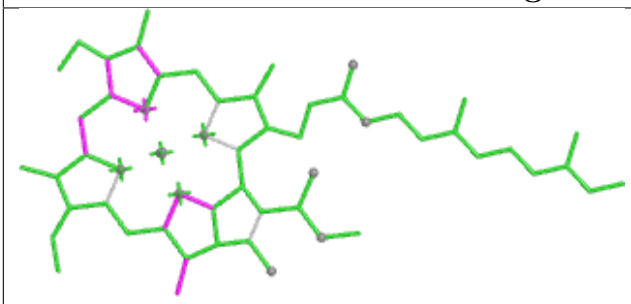
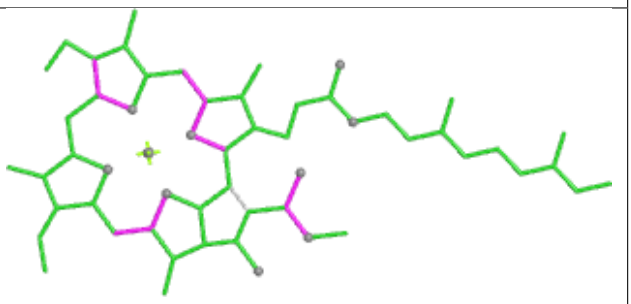
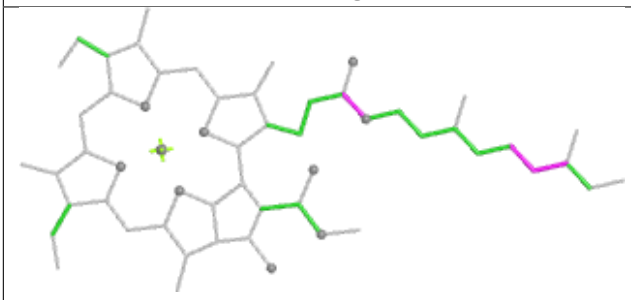
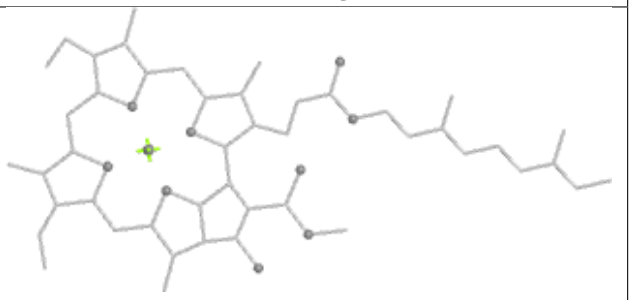
Torsions

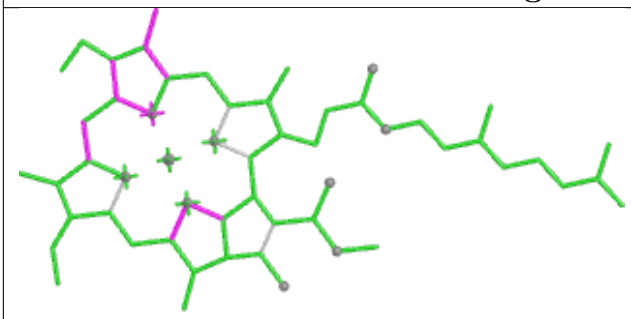
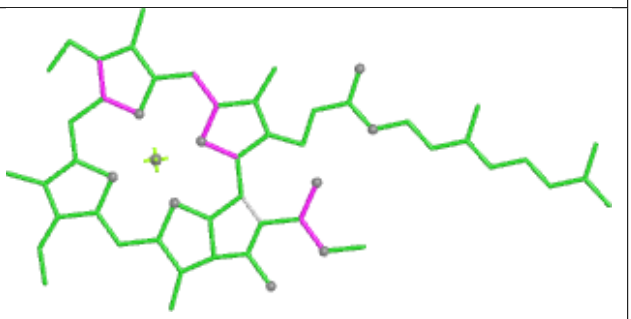
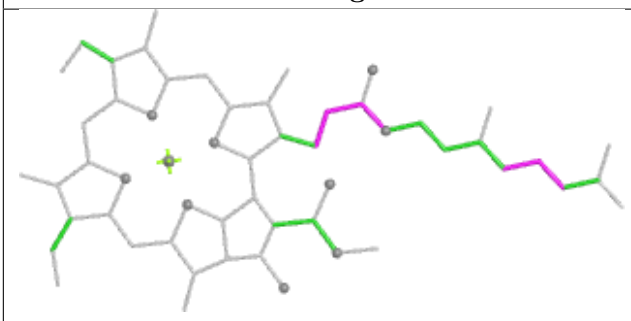
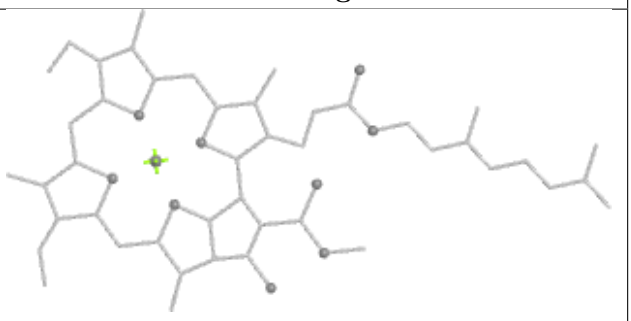


Rings

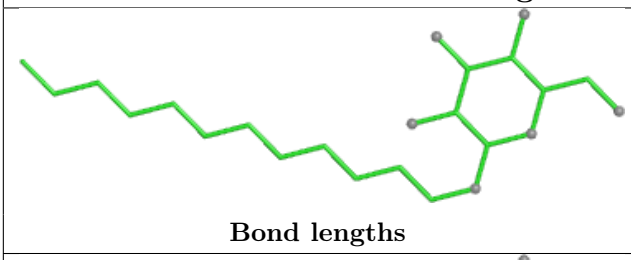
Ligand LMU B 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

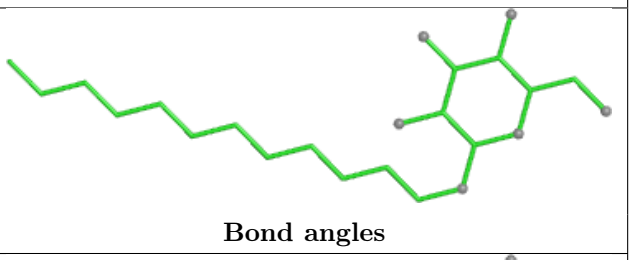
Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

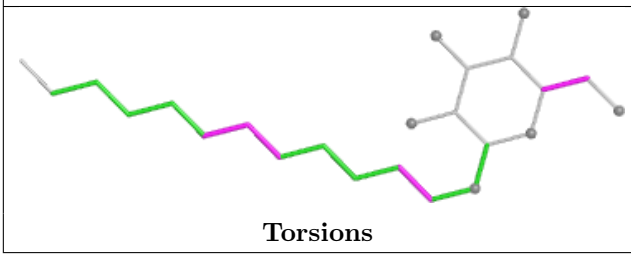
Ligand LMU M 102



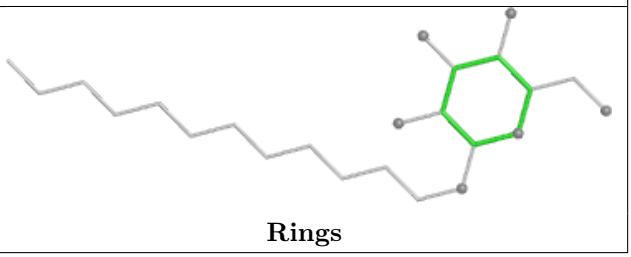
Bond lengths



Bond angles

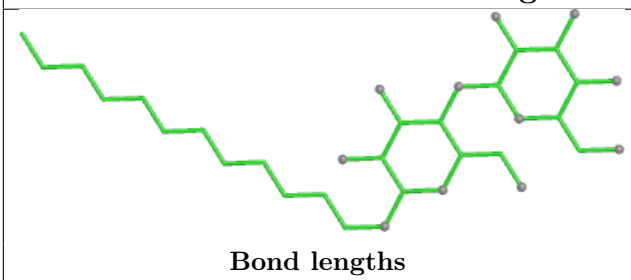


Torsions

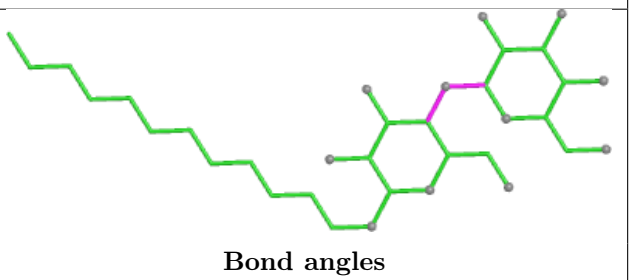


Rings

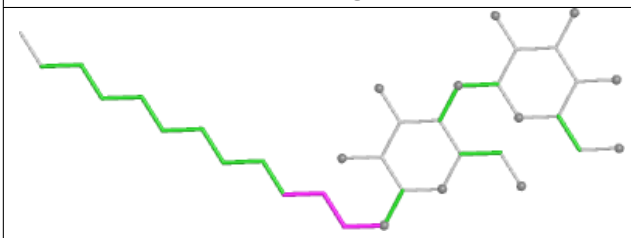
Ligand LMU X 421



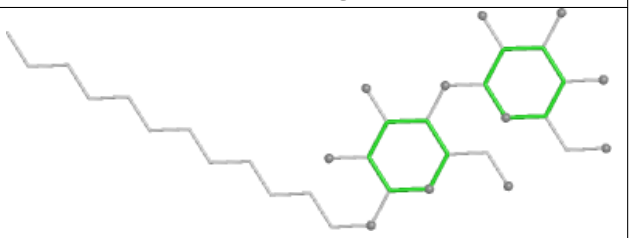
Bond lengths



Bond angles

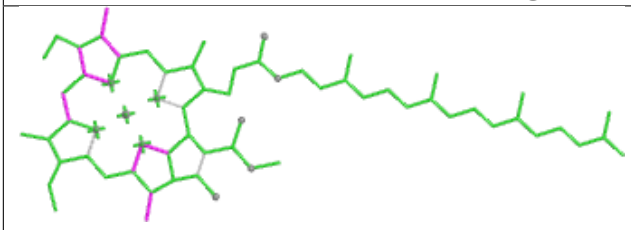


Torsions

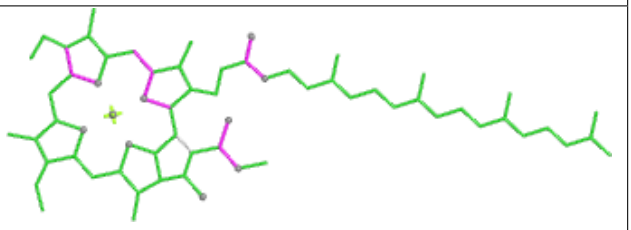


Rings

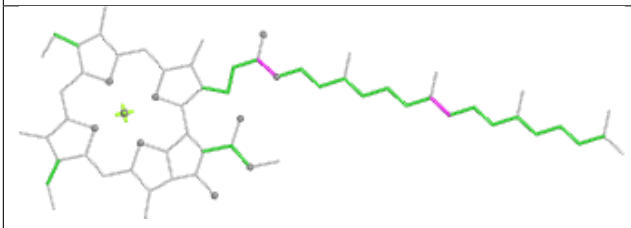
Ligand CLA B 809



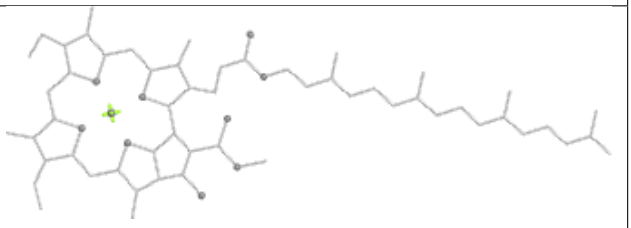
Bond lengths



Bond angles

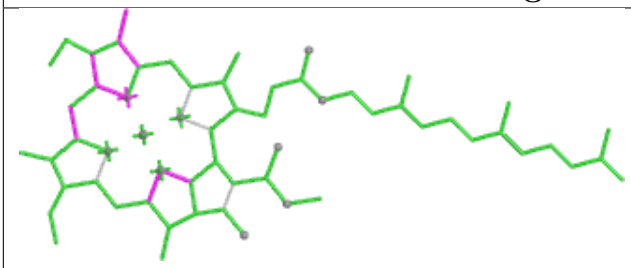


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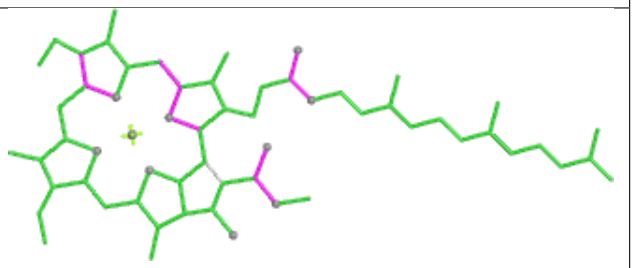


Rings

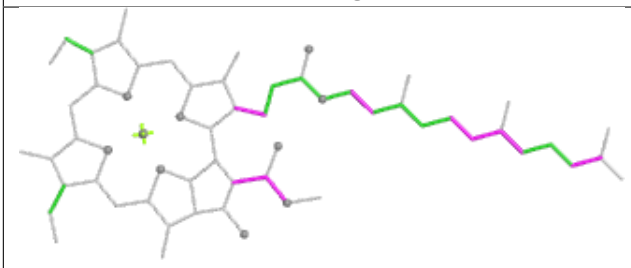
Ligand CLA B 821



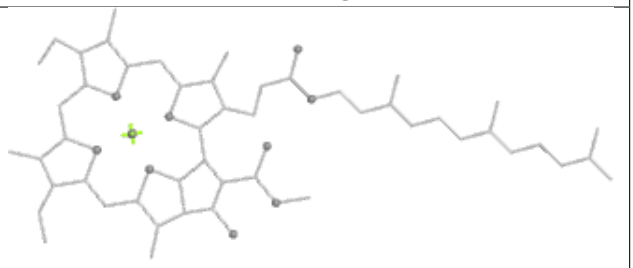
Bond lengths



Bond angles

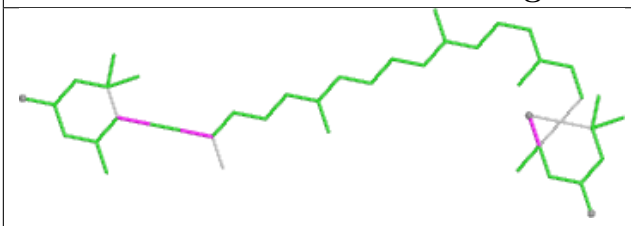


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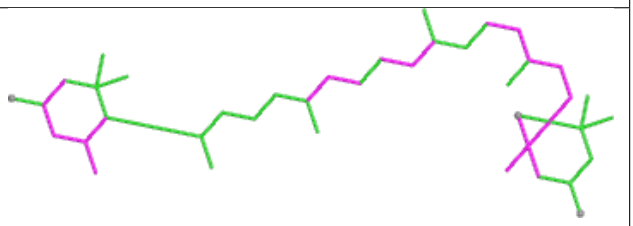


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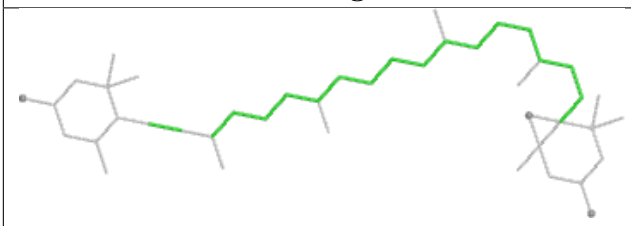
Ligand DD6 G 612



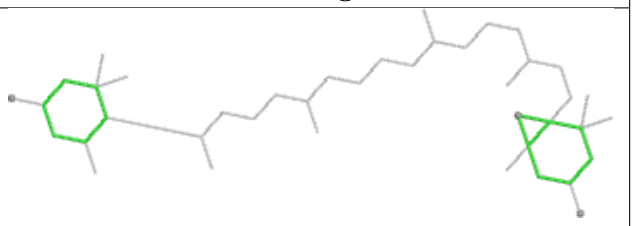
Bond lengths



Bond angles

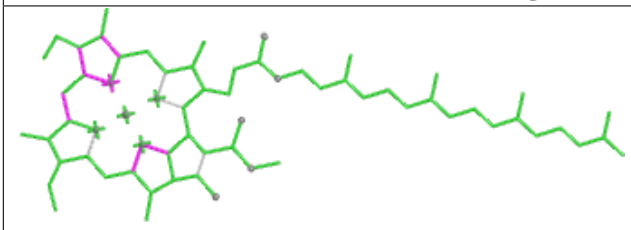


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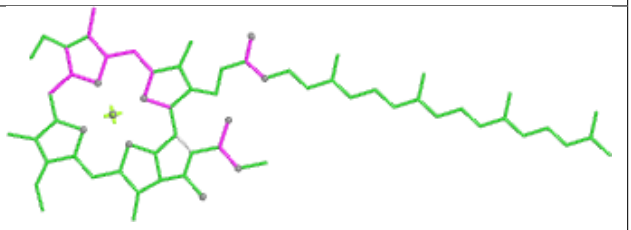


Rings

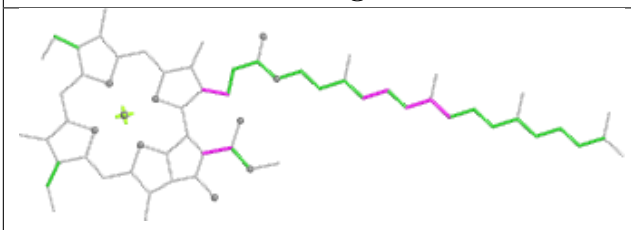
Ligand CLA B 831



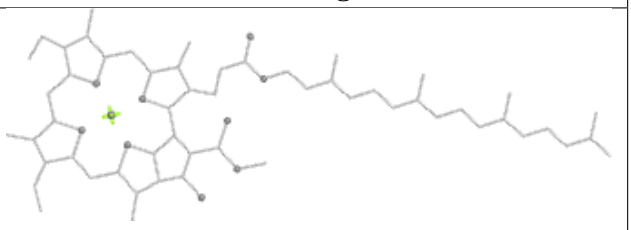
Bond lengths



Bond angles

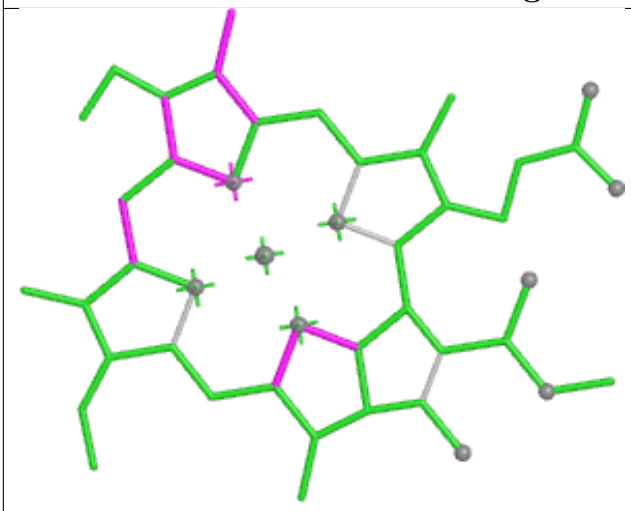


Torsions

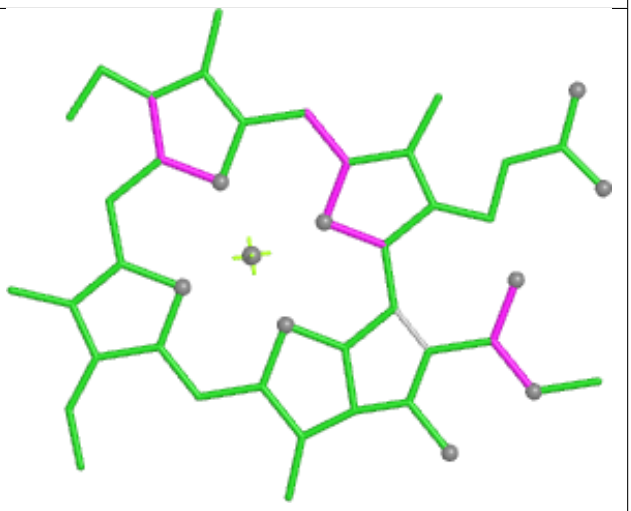


Rings

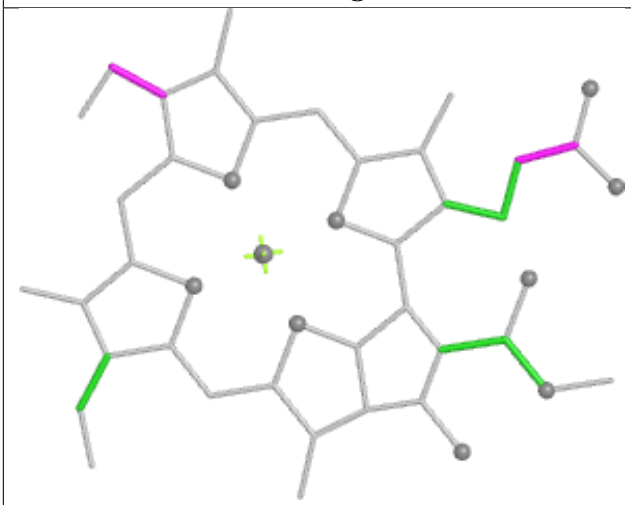
Ligand CLA U 412



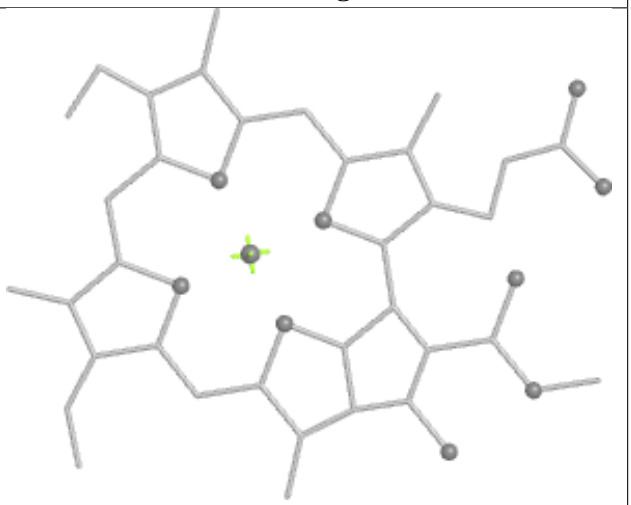
Bond lengths



Bond angles

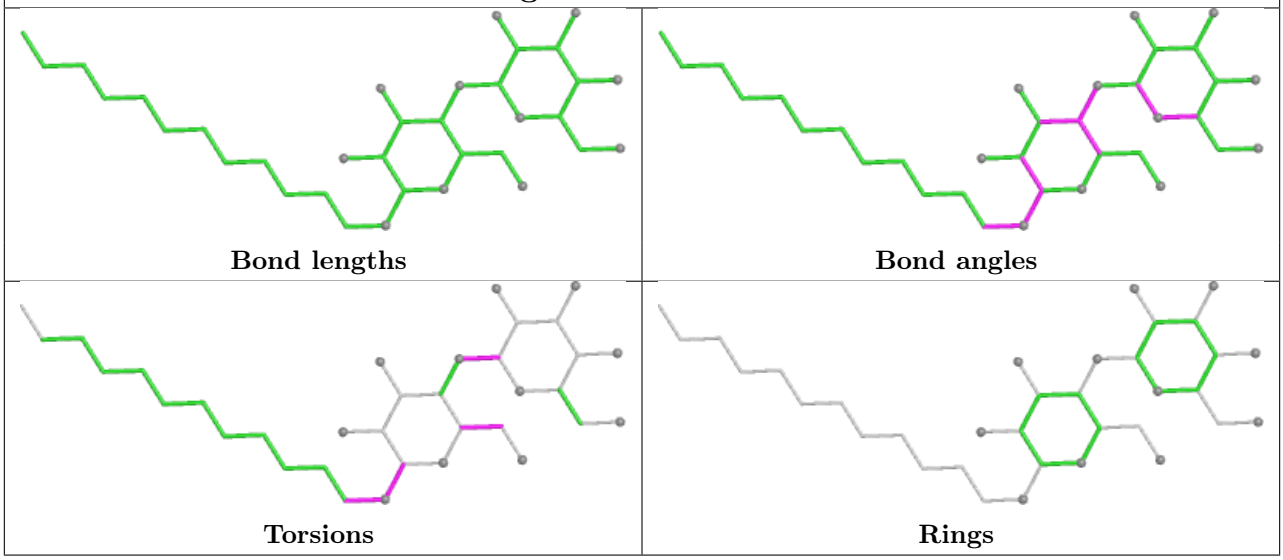


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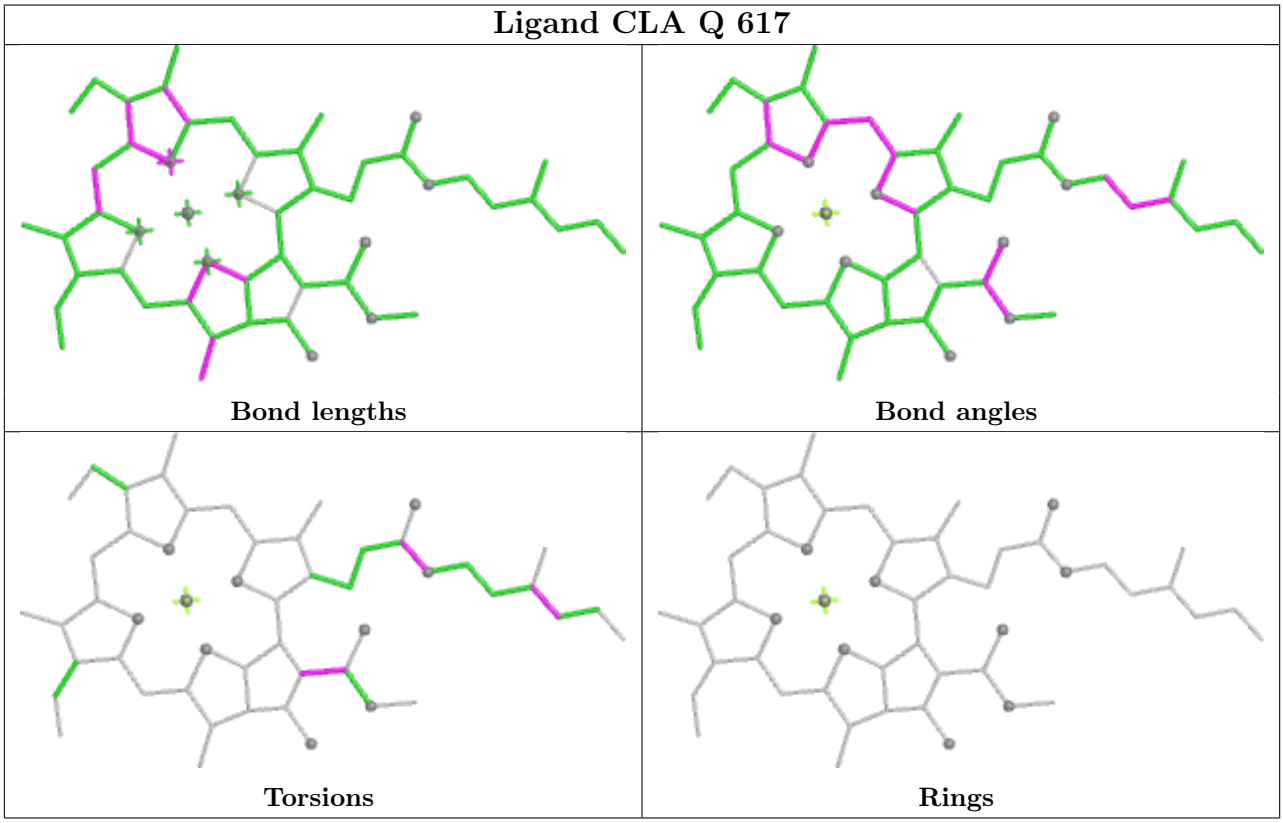


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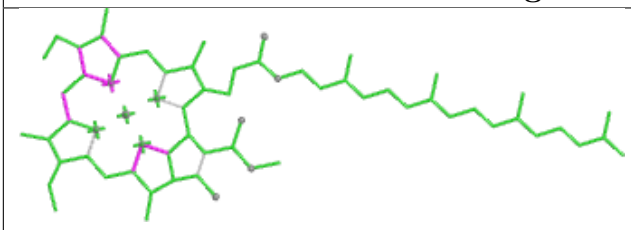
Ligand LMU O 322



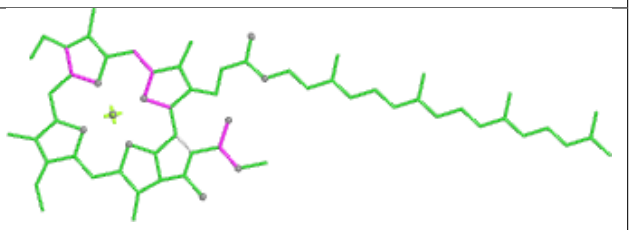
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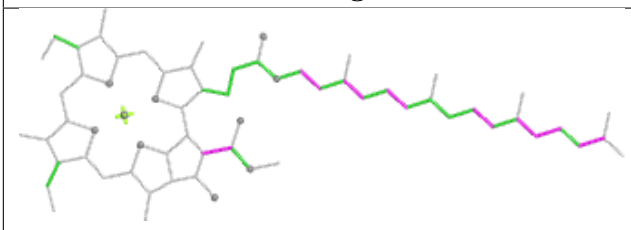
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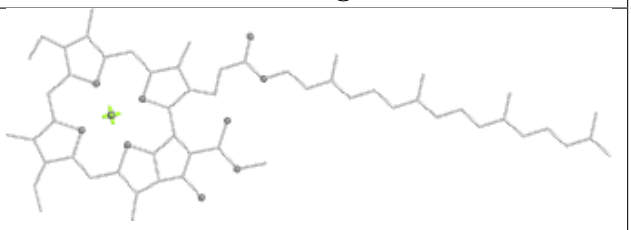
Bond lengths



Bond angles

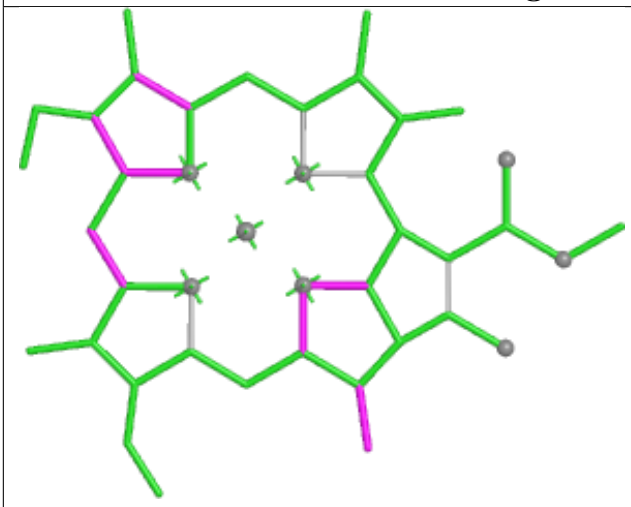


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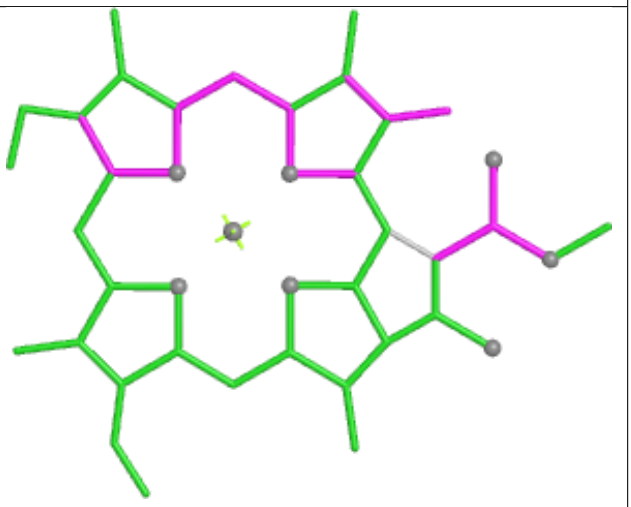


Rings

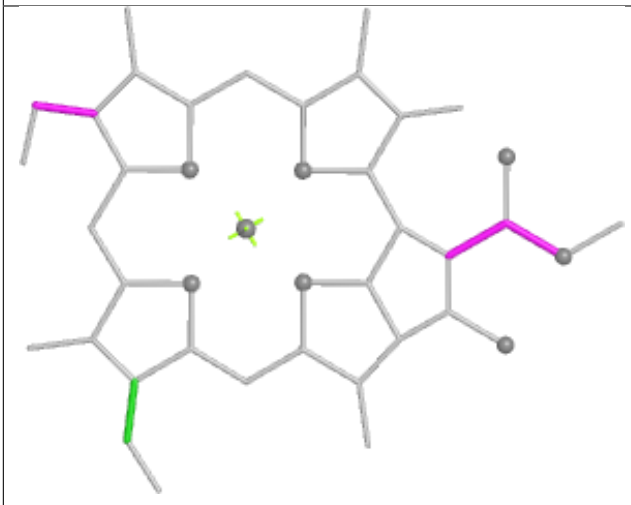
Ligand CLA P 610



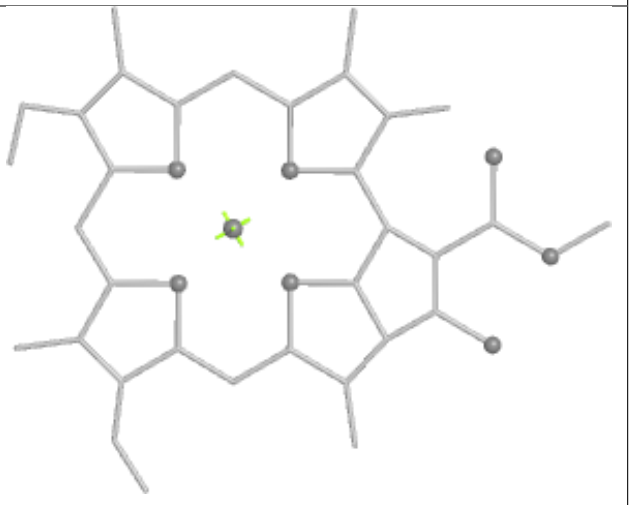
Bond lengths



Bond angles

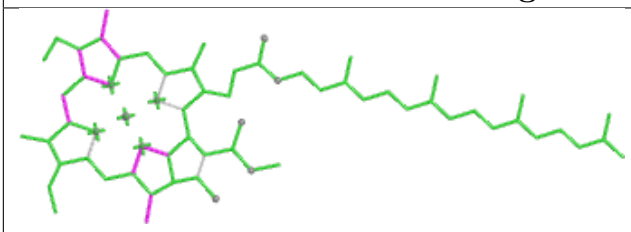


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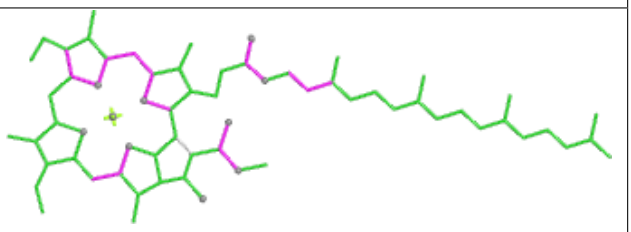


Rings

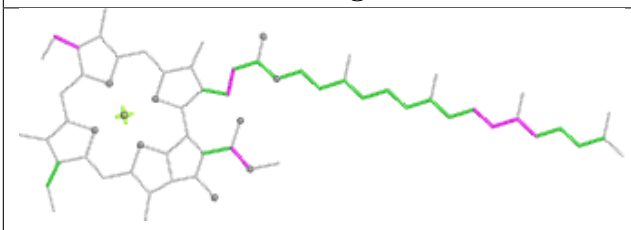
Ligand CLA W 414



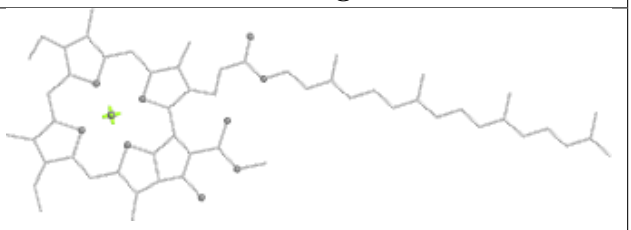
Bond lengths



Bond angles



Torsions

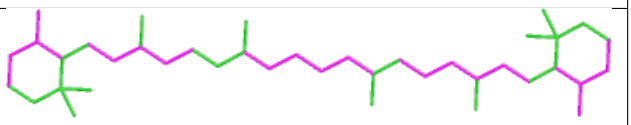


Rings

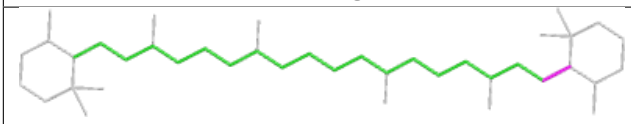
Ligand BCR B 844



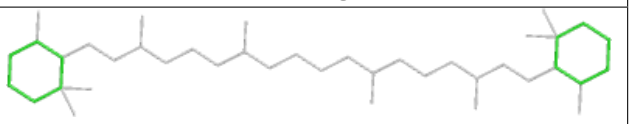
Bond lengths



Bond angles

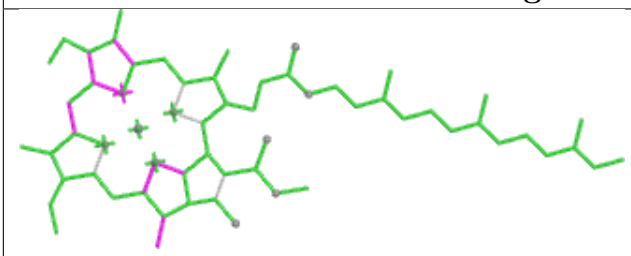


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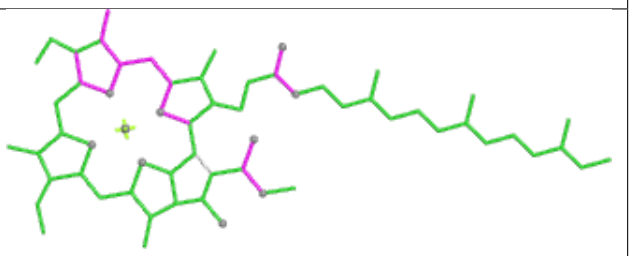


Rings

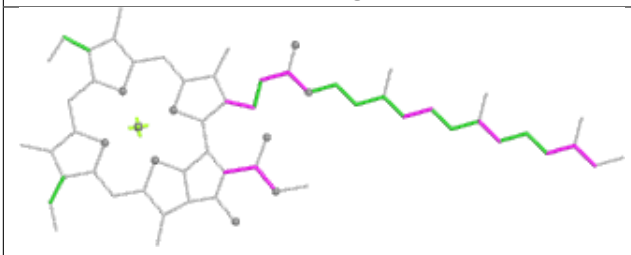
Ligand CLA O 308



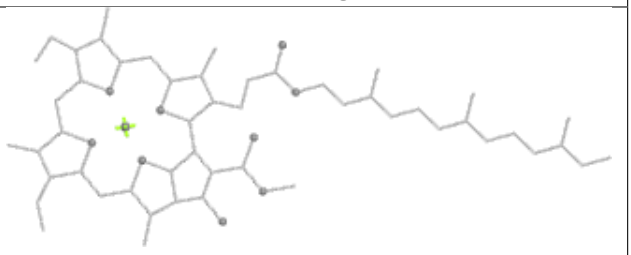
Bond lengths



Bond angles

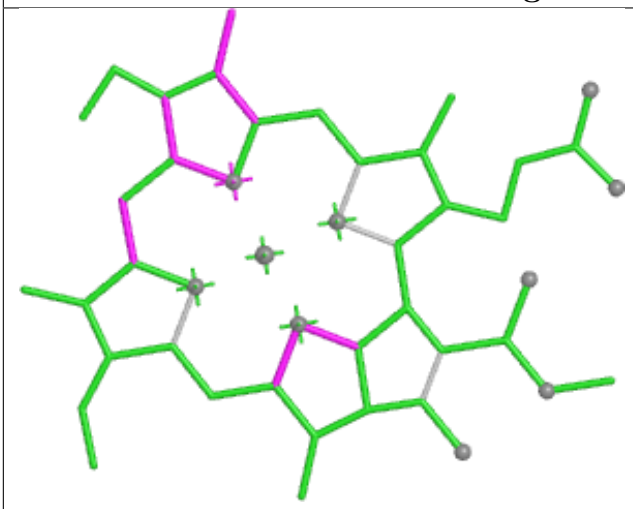


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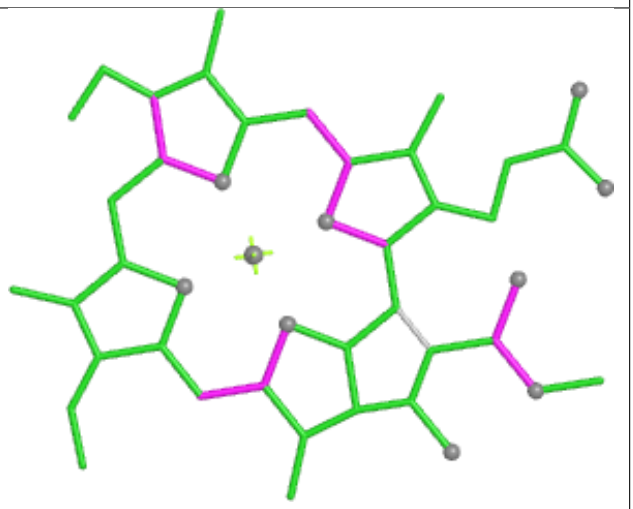


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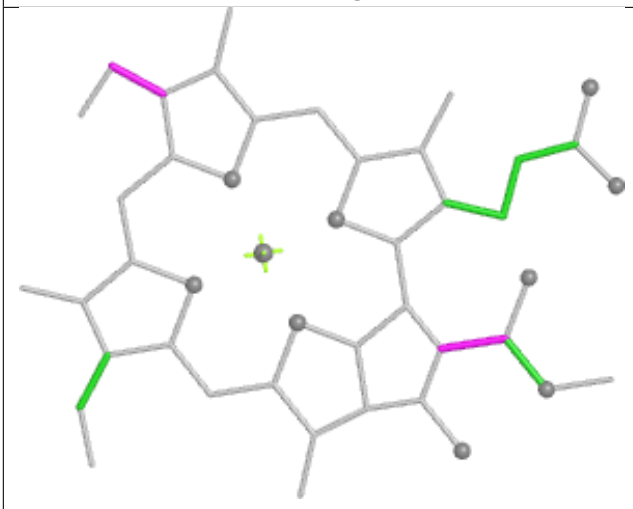
Ligand CLA H 302



Bond lengths



Bond angles

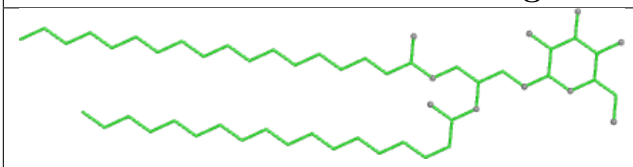


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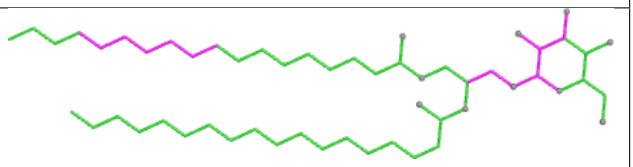


Rings

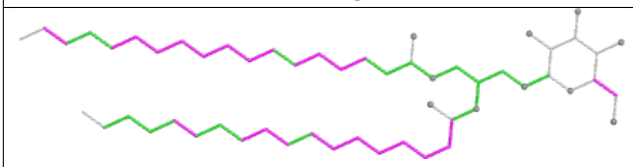
Ligand LMG J 101



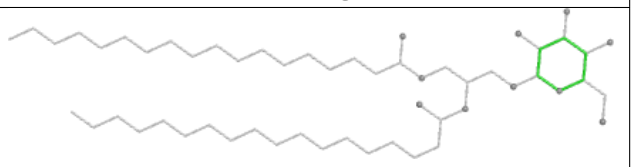
Bond lengths



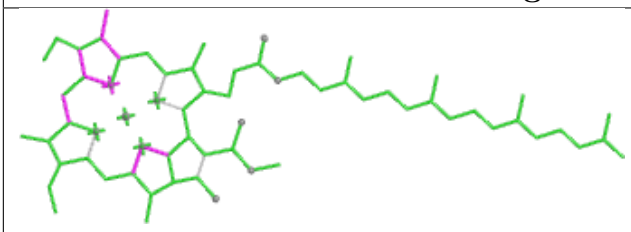
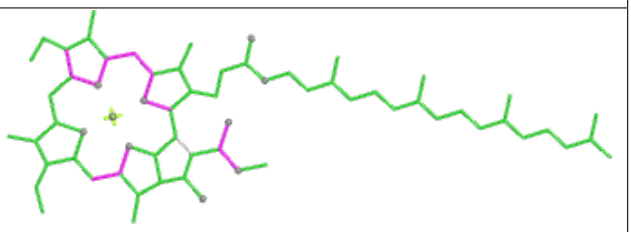
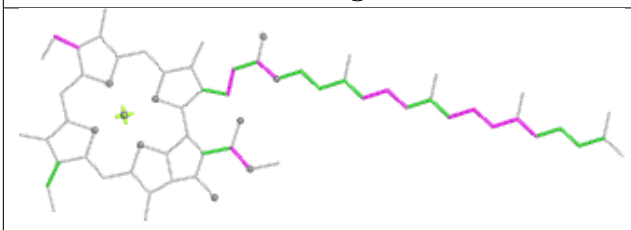
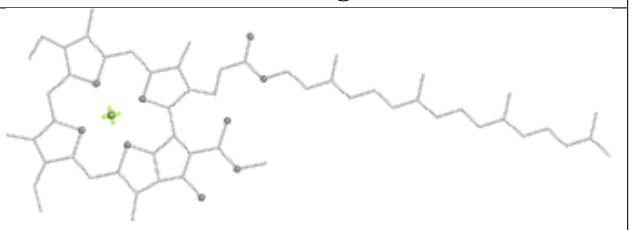
Bond angles

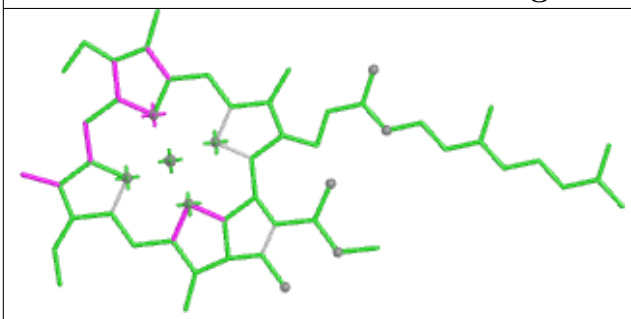
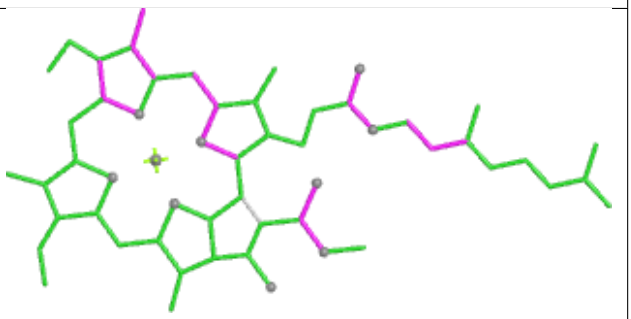
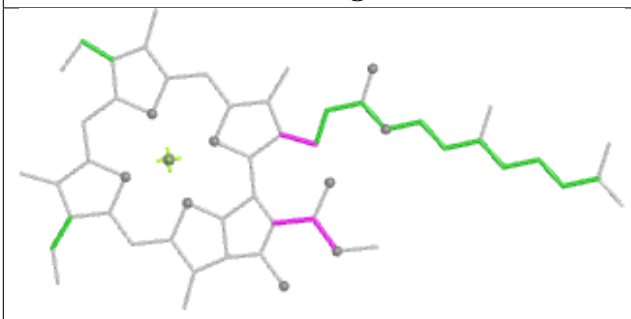
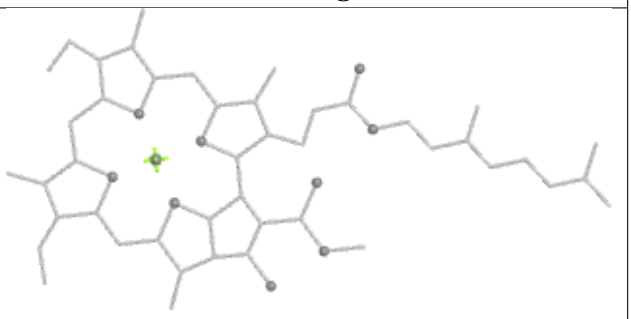


Torsions

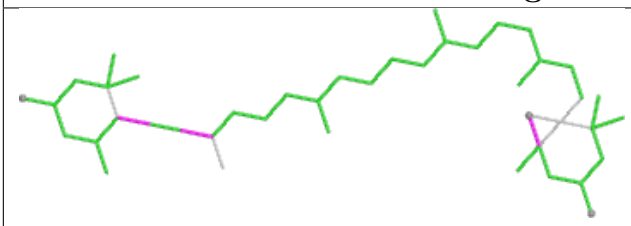


Rings

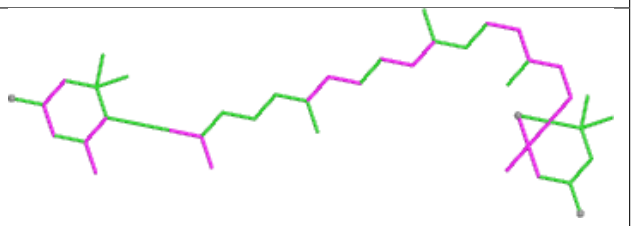
Ligand CLA V 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA I 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

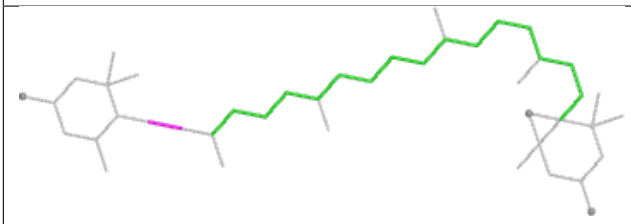
Ligand DD6 U 416



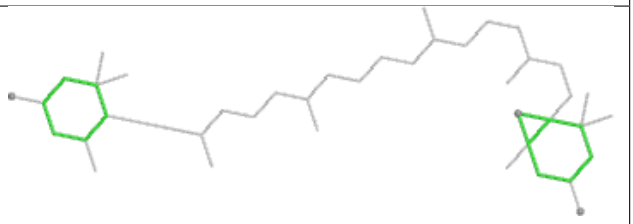
Bond lengths



Bond angles

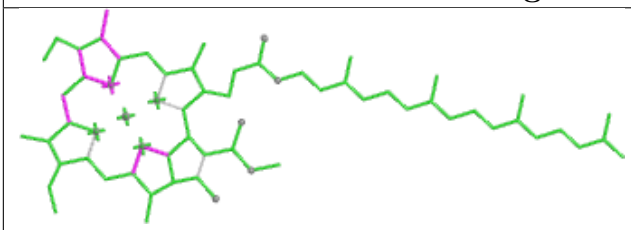


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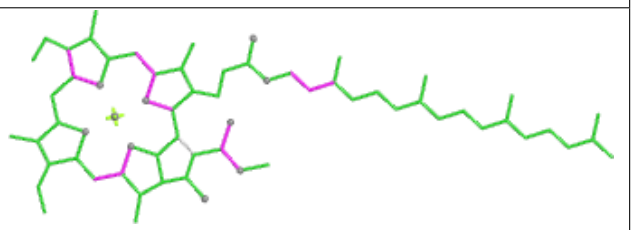


Rings

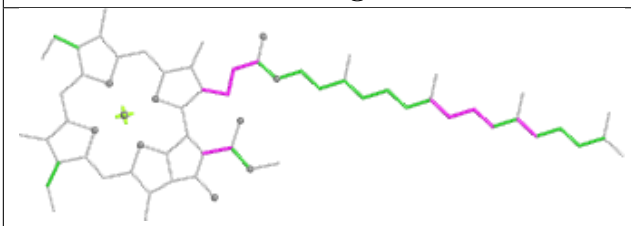
Ligand CLA A 807



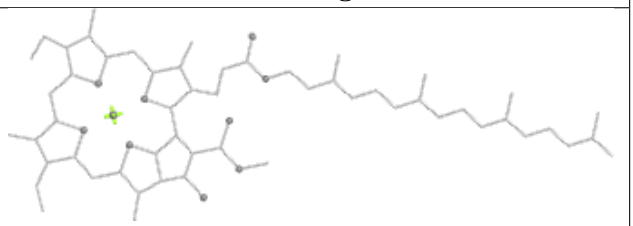
Bond lengths



Bond angles

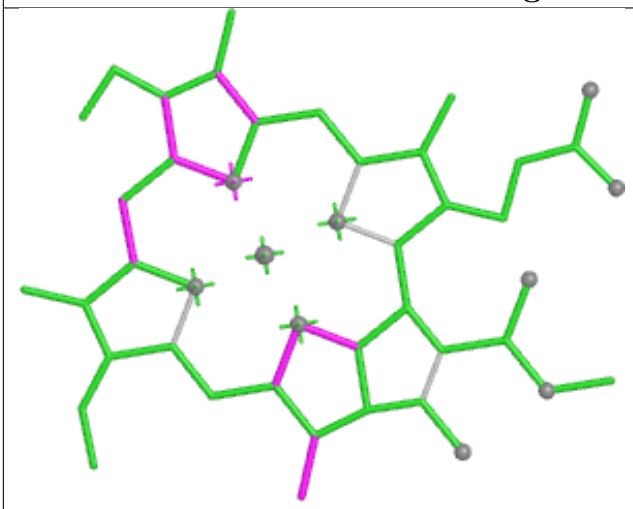


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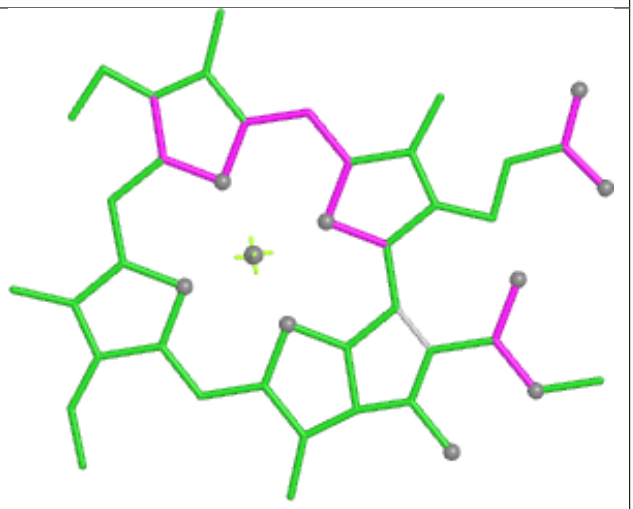


Rings

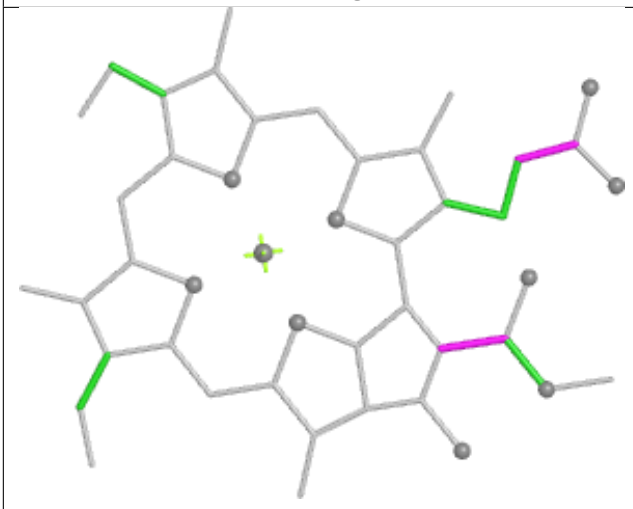
Ligand CLA H 310



Bond lengths



Bond angles

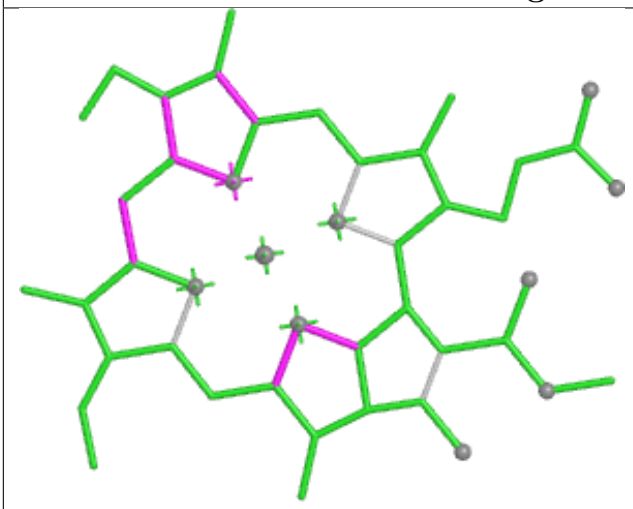


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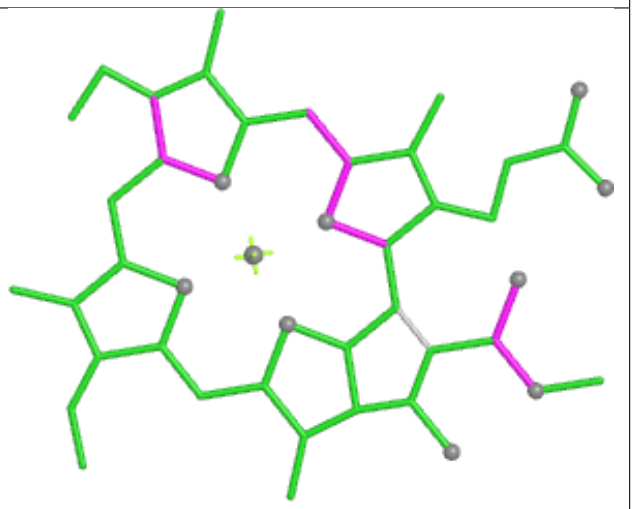


Rings

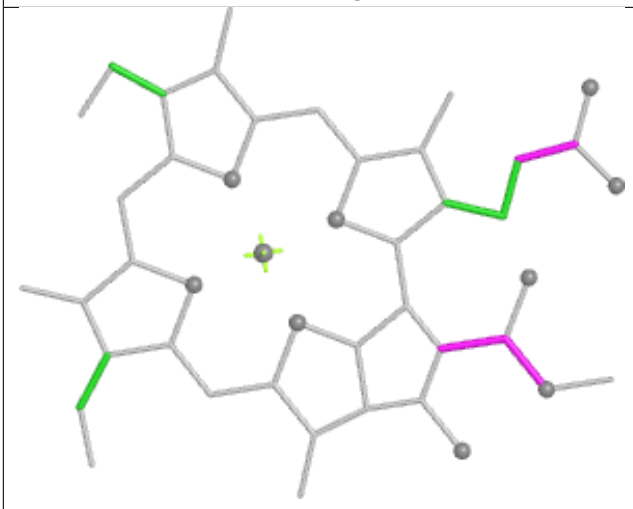
Ligand CLA S 601



Bond lengths



Bond angles

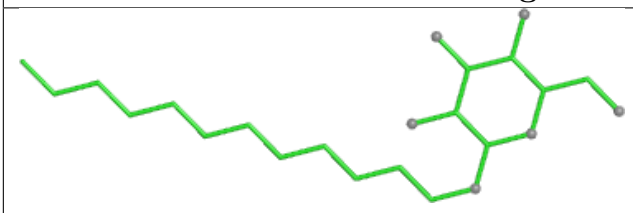


Torsions

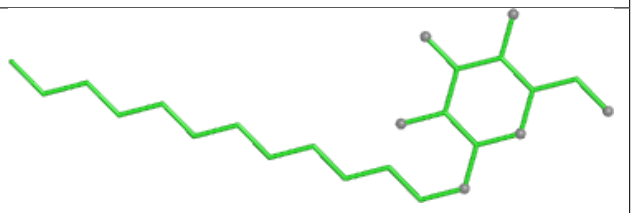


Rings

Ligand LMU A 857



Bond lengths



Bond angles

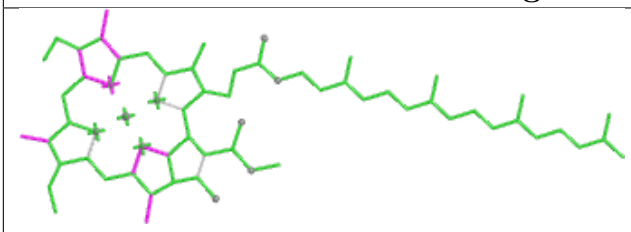


Torsions

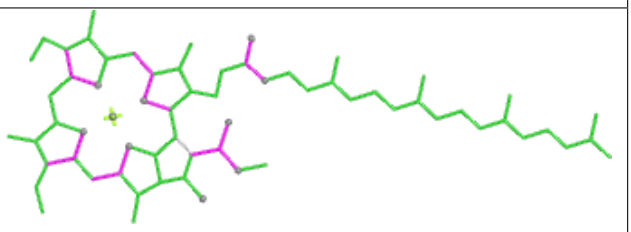


Rings

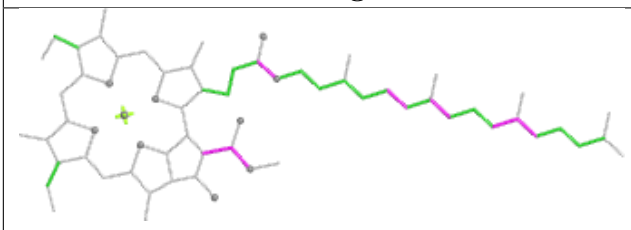
Ligand CLA K 608



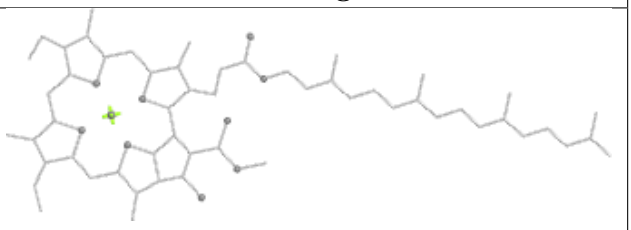
Bond lengths



Bond angles



Torsions

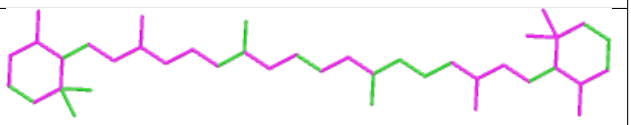


Rings

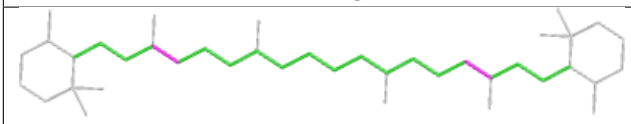
Ligand BCR B 843



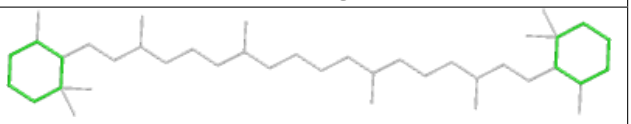
Bond lengths



Bond angles

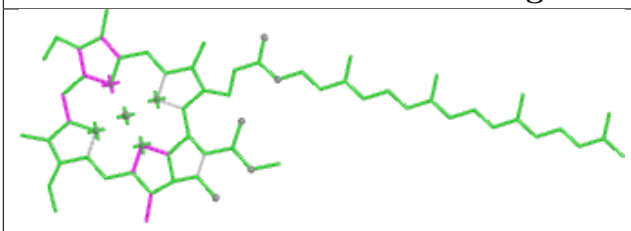


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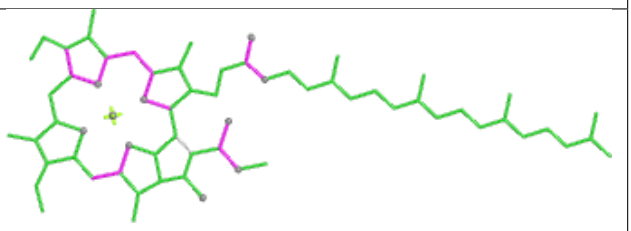


Rings

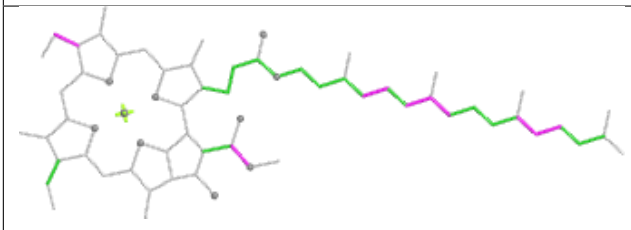
Ligand CLA F 403



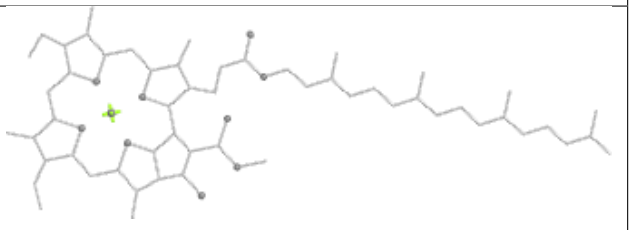
Bond lengths



Bond angles

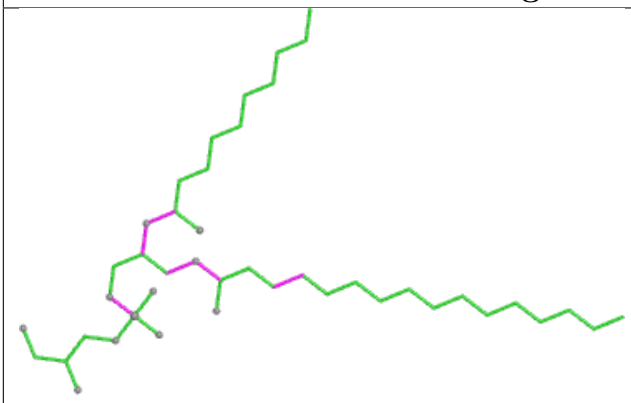


Torsions

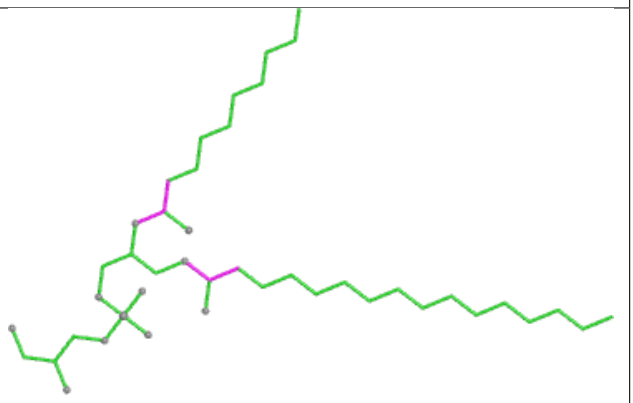


Rings

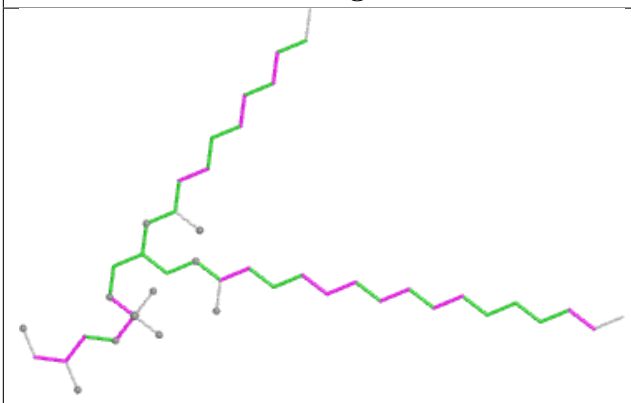
Ligand LHG O 323



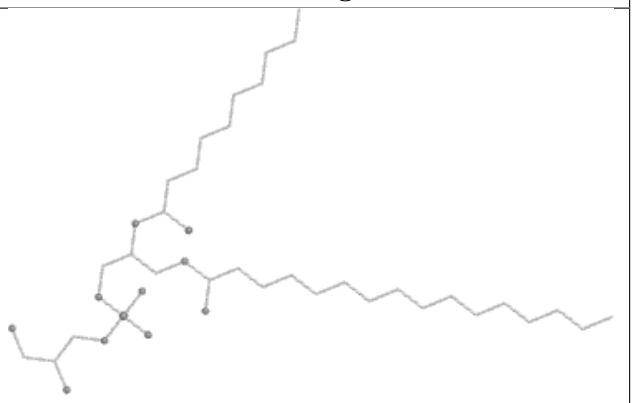
Bond lengths



Bond angles

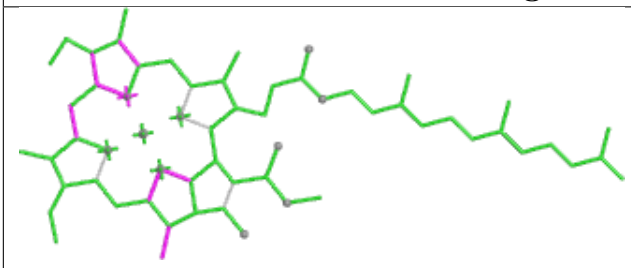


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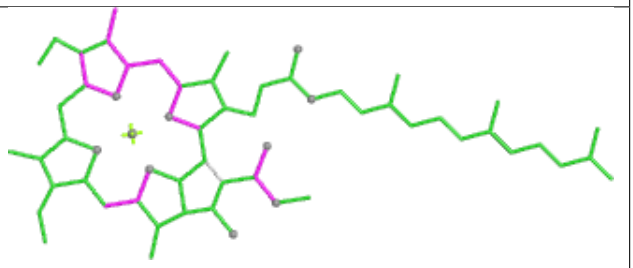


Rings

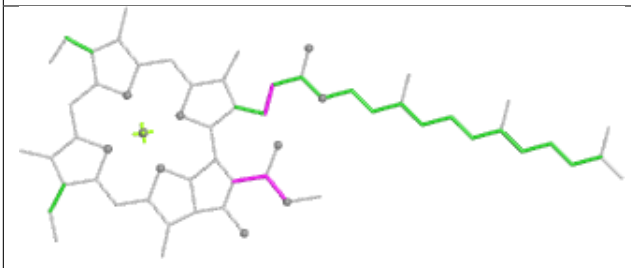
Ligand CLA N 602



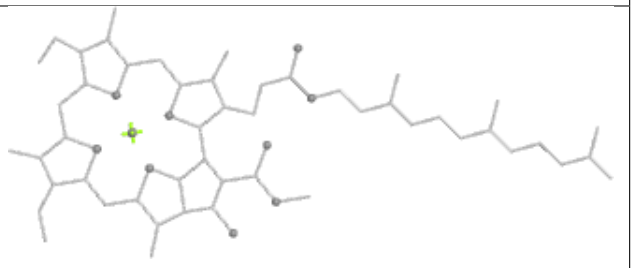
Bond lengths



Bond angles

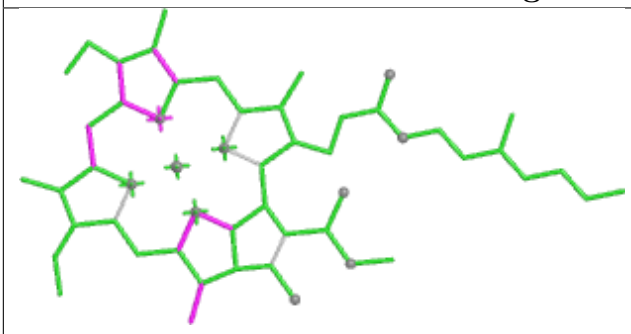


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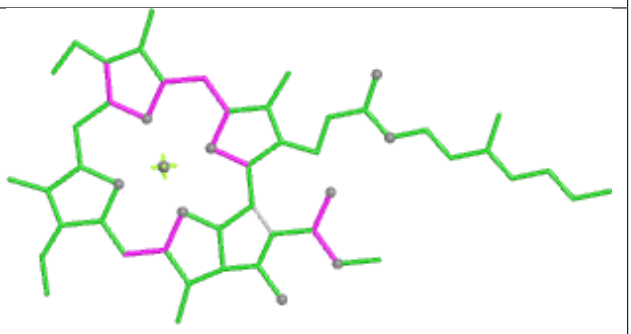


Rings

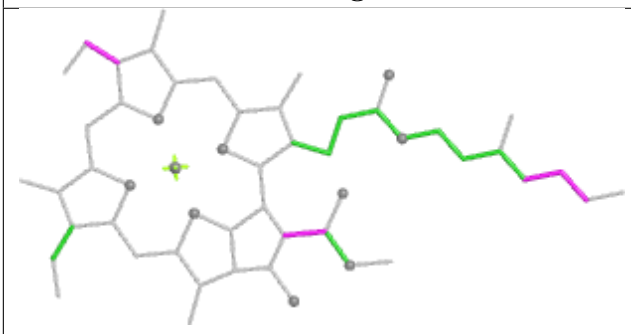
Ligand CLA K 613



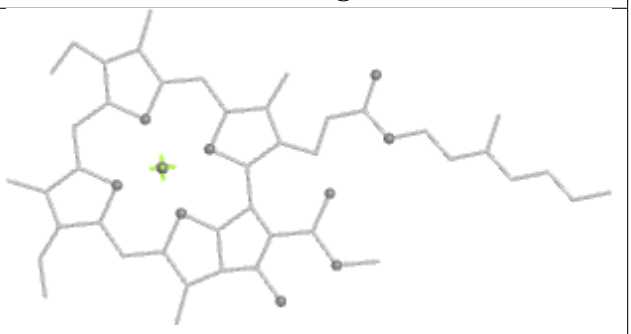
Bond lengths



Bond angles

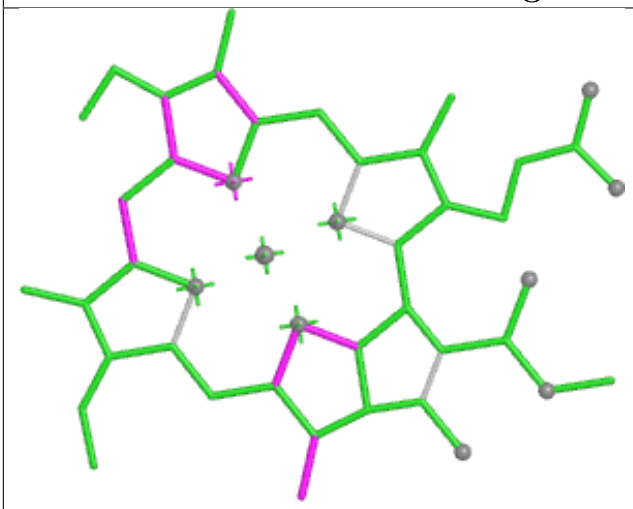


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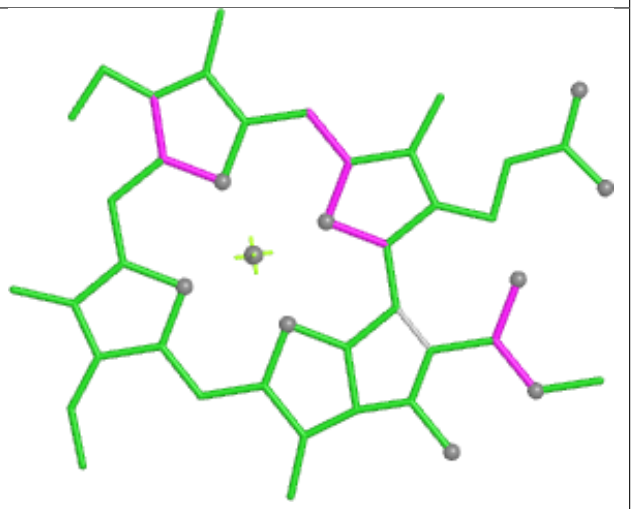


Rings

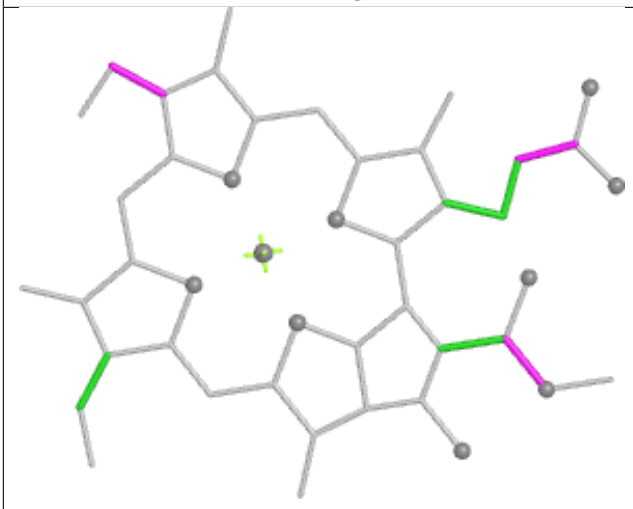
Ligand CLA N 601



Bond lengths



Bond angles

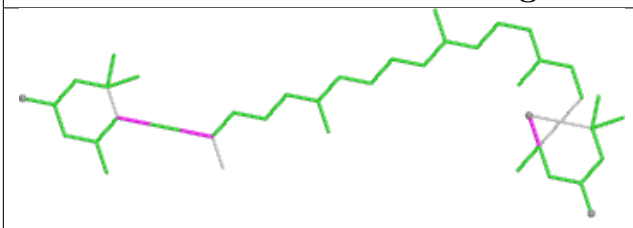


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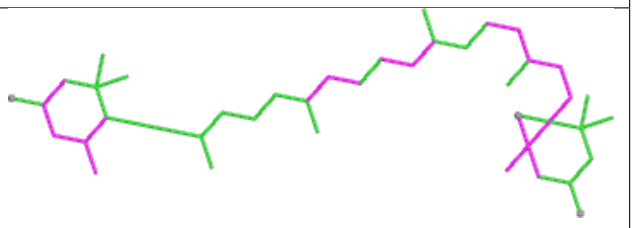


Rings

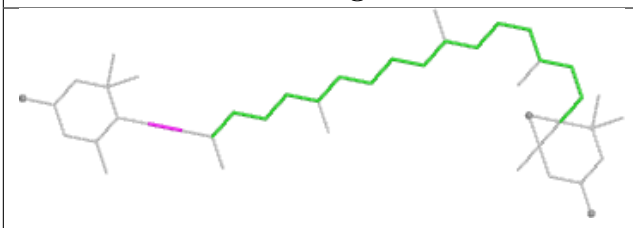
Ligand DD6 W 417



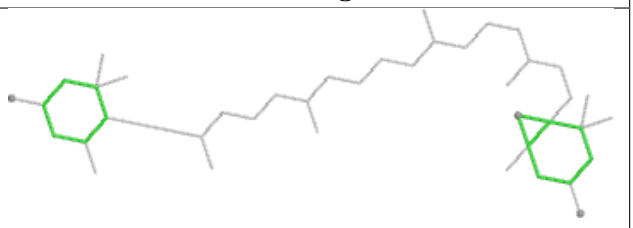
Bond lengths



Bond angles

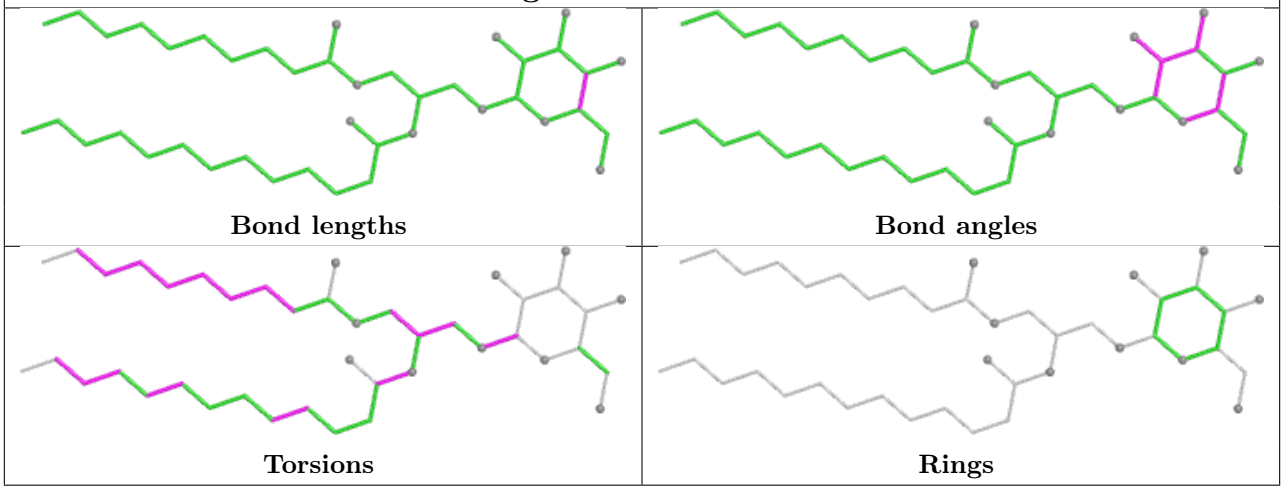


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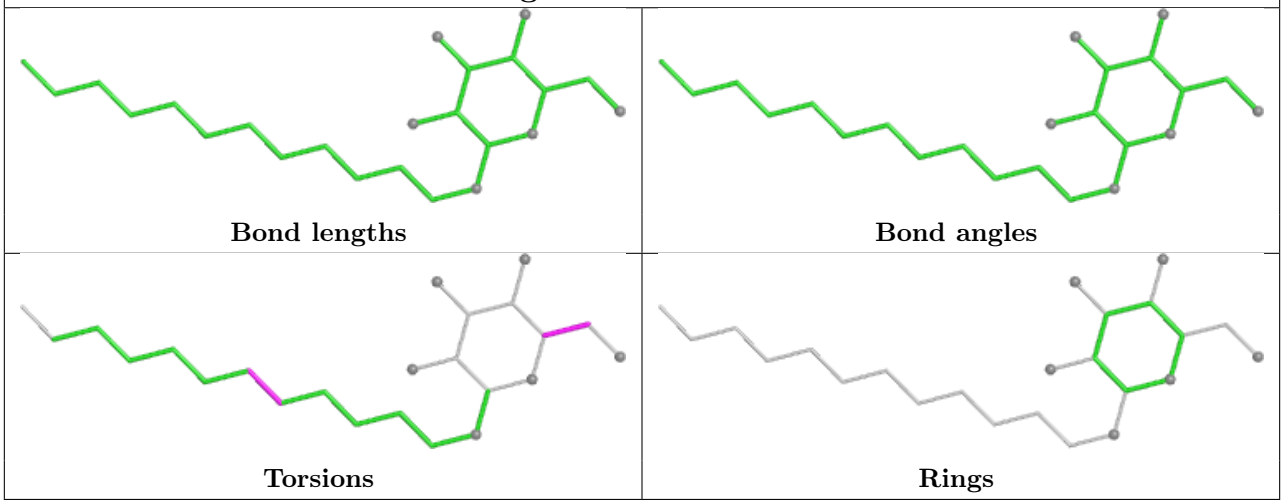


Rings

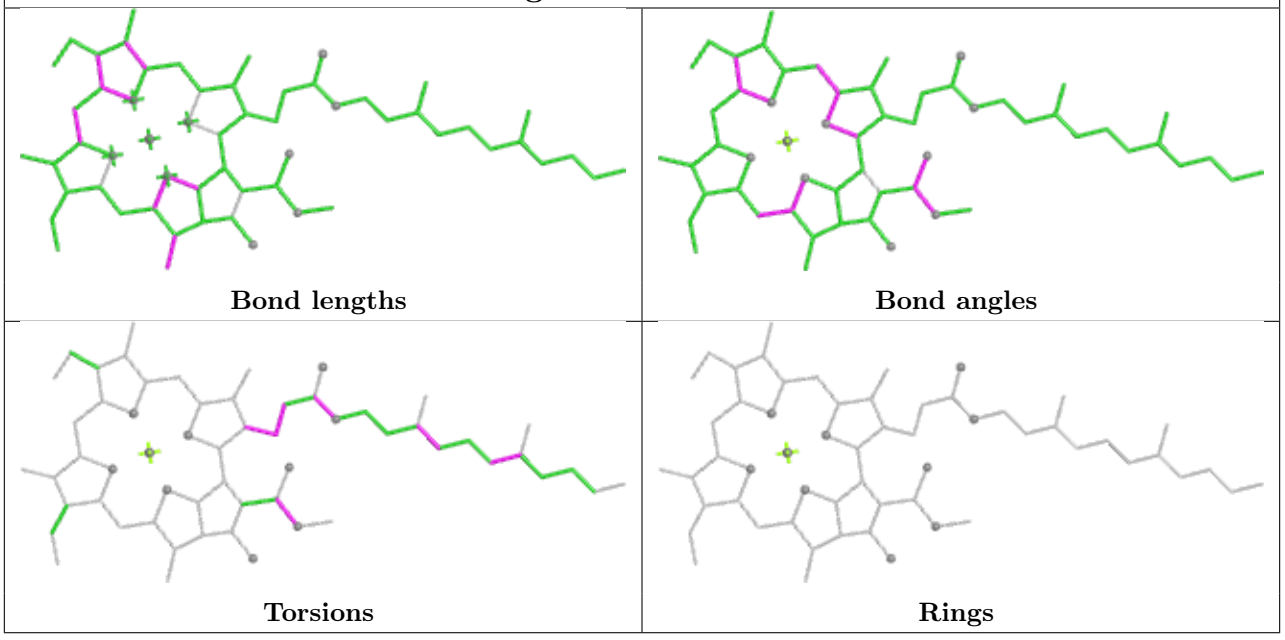
Ligand LMG F 408



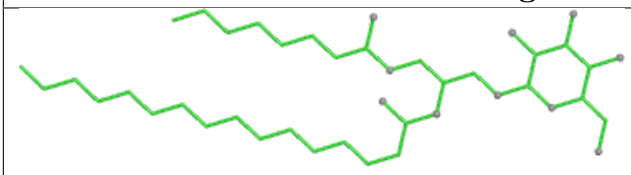
Ligand LMU H 320



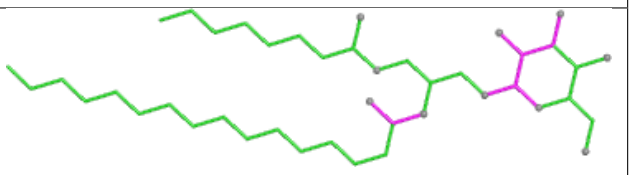
Ligand CLA B 826



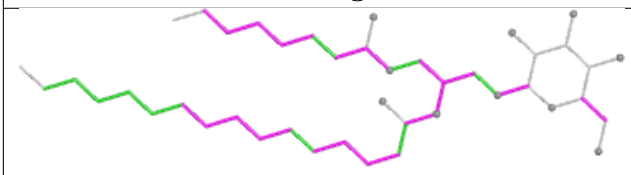
Ligand LMG K 601



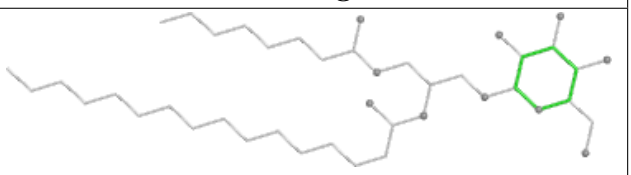
Bond lengths



Bond angles

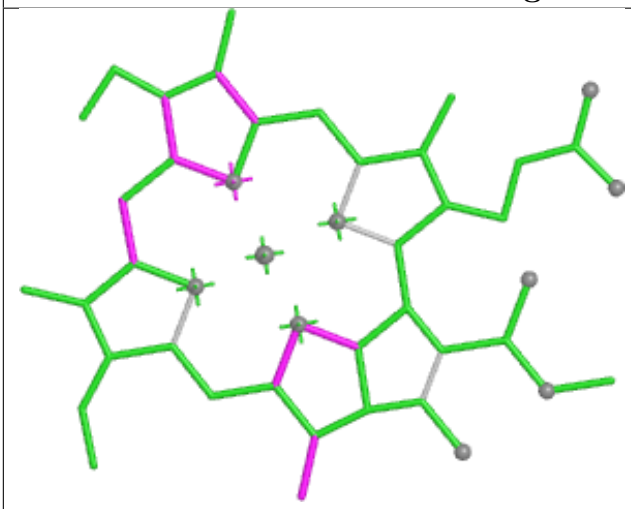


Torsions

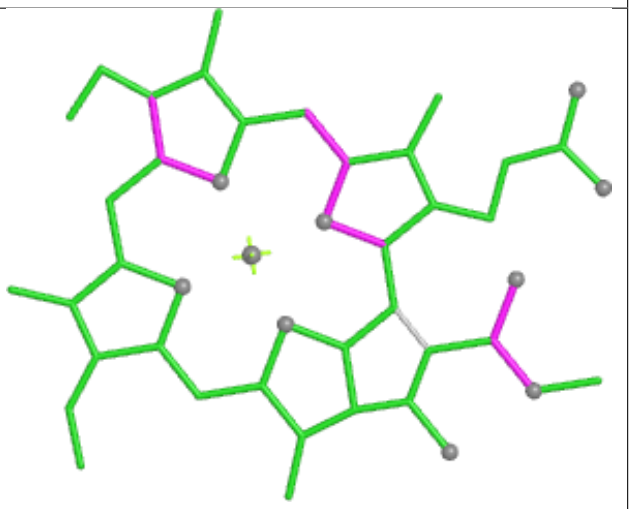


Rings

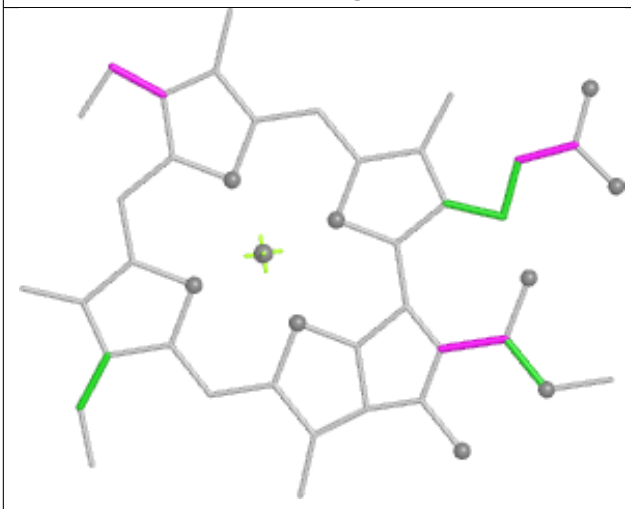
Ligand CLA V 611



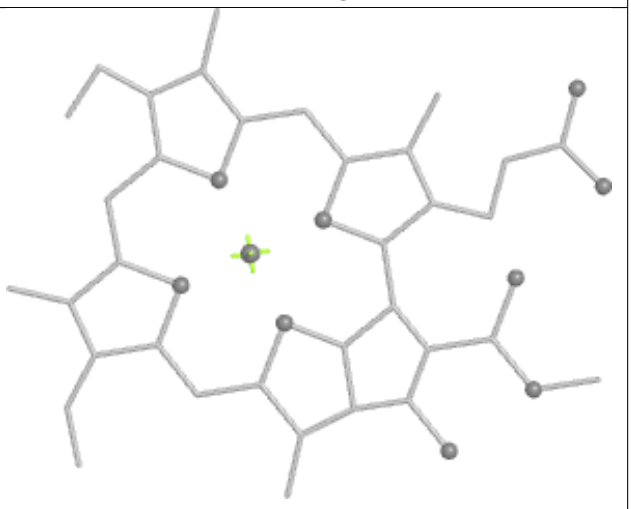
Bond lengths



Bond angles

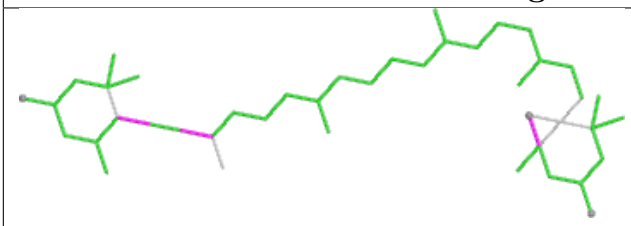


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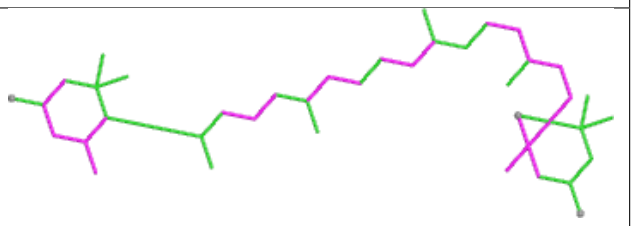


Rings

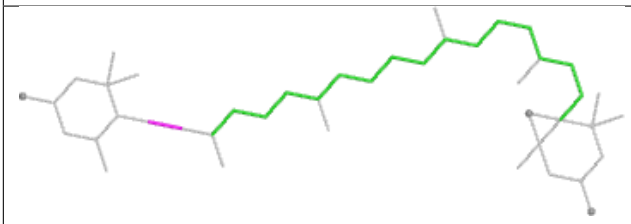
Ligand DD6 S 612



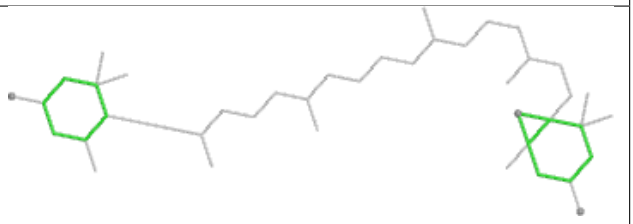
Bond lengths



Bond angles

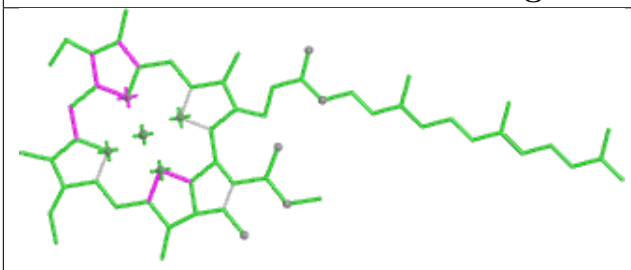


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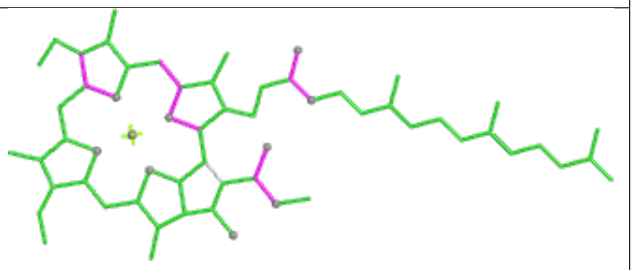


Rings

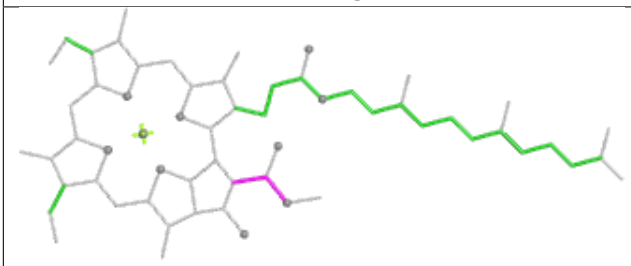
Ligand CLA T 608



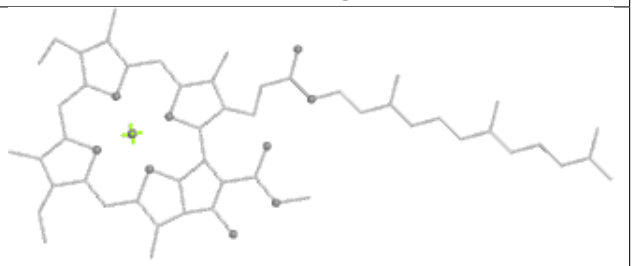
Bond lengths



Bond angles

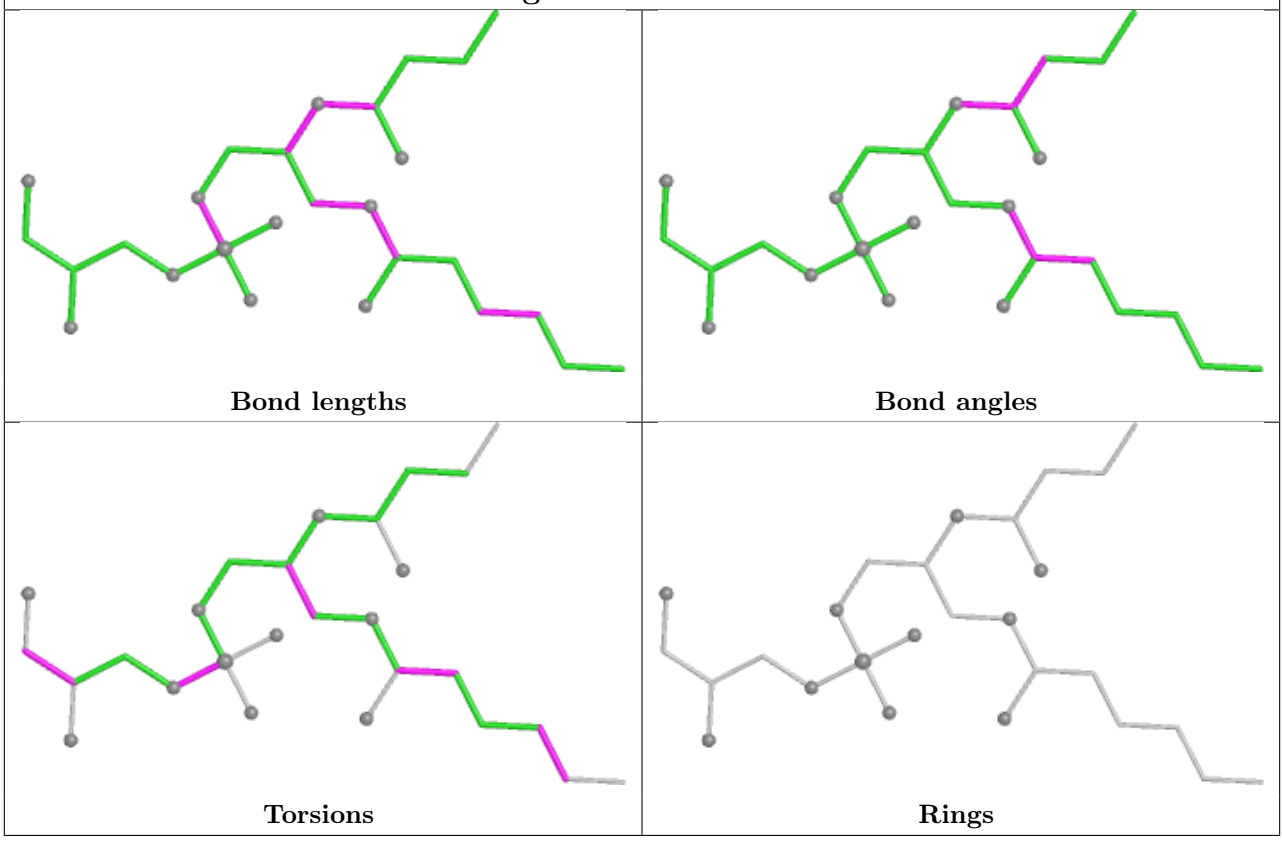


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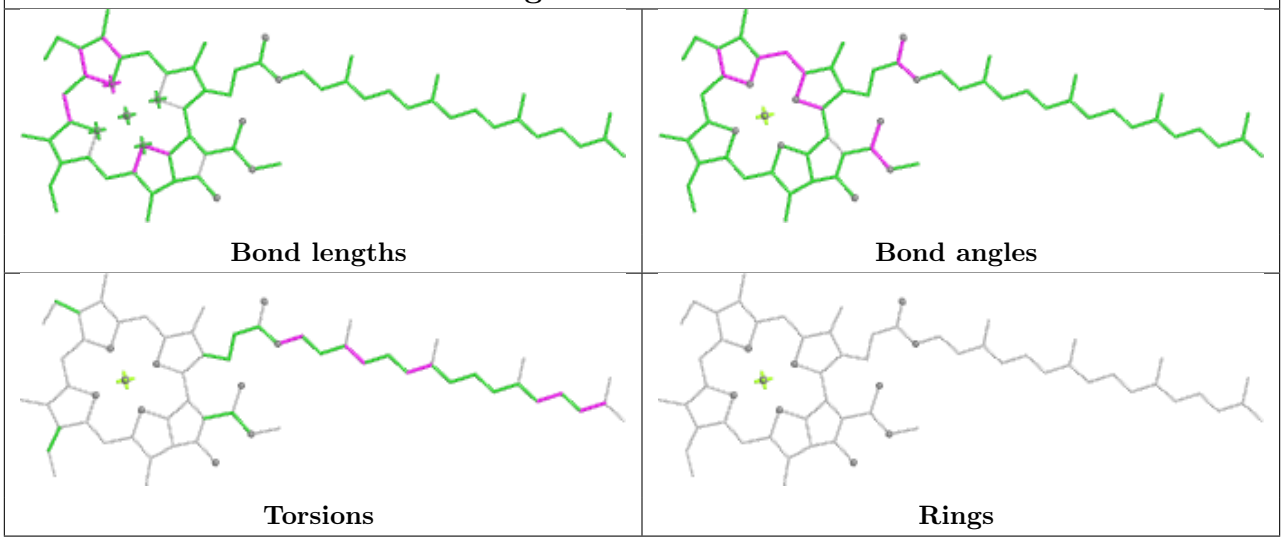


Rings

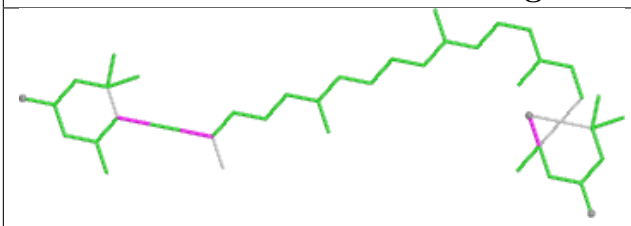
Ligand LHG H 316



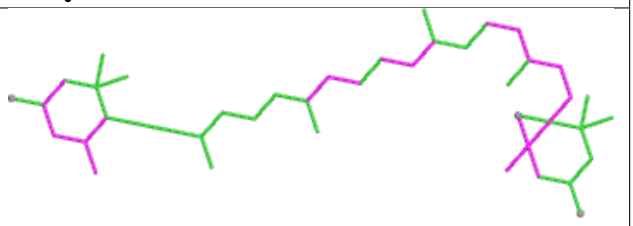
Ligand CLA A 822



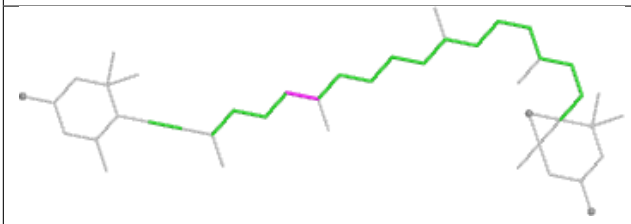
Ligand DD6 Q 614



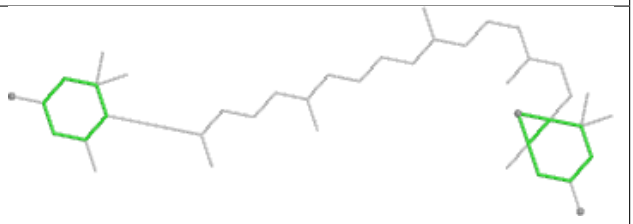
Bond lengths



Bond angles

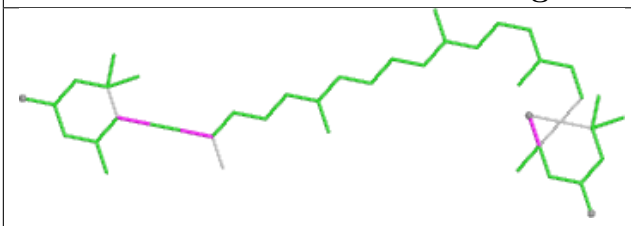


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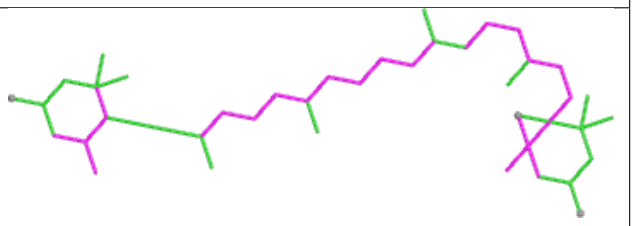


Rings

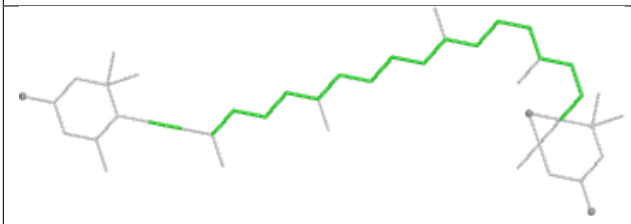
Ligand DD6 I 613



Bond lengths



Bond angles

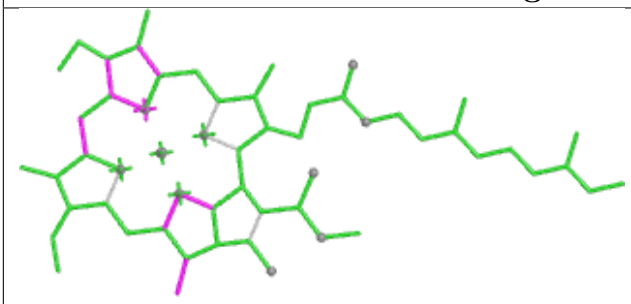


Torsions

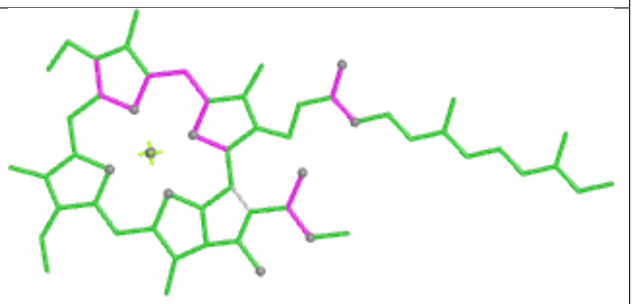


Rings

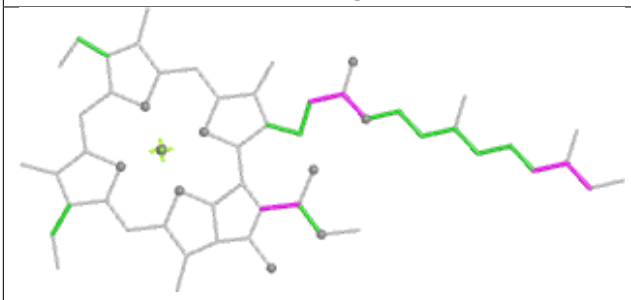
Ligand CLA R 603



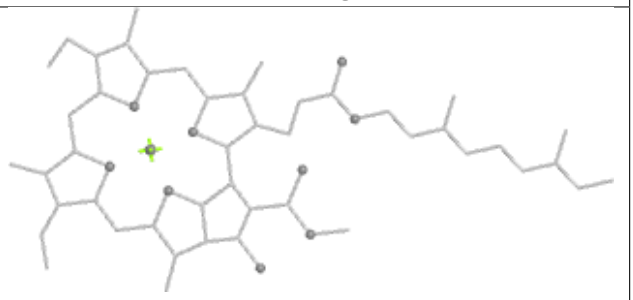
Bond lengths



Bond angles

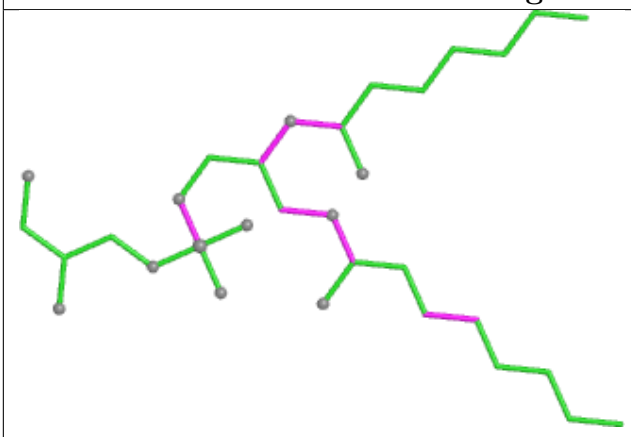


Torsions

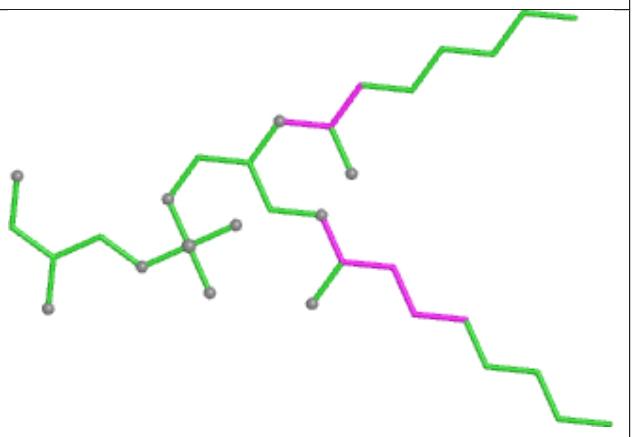


Rings

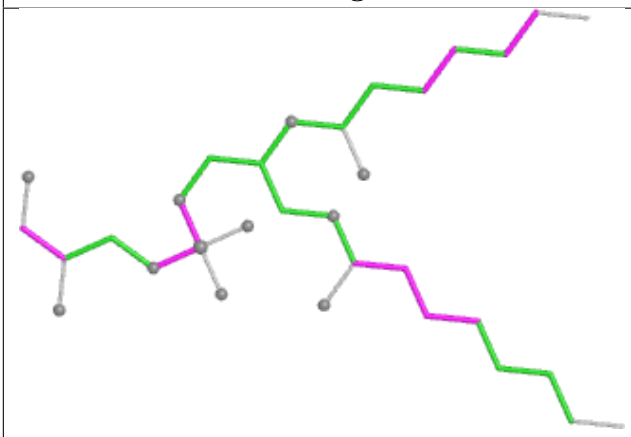
Ligand LHG S 613



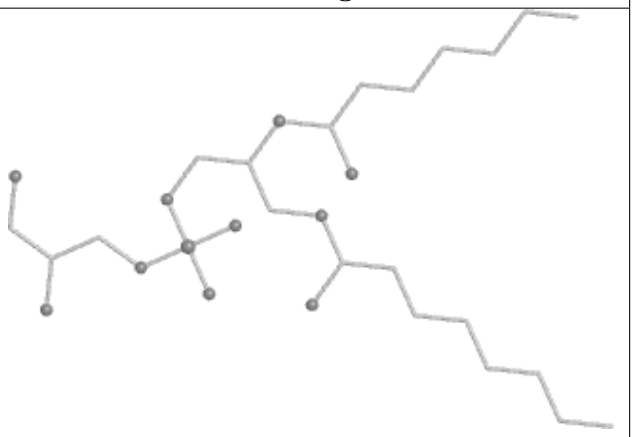
Bond lengths



Bond angles

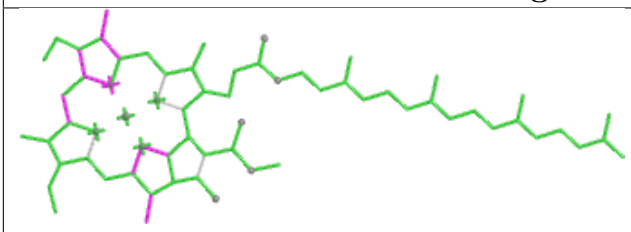


Torsions

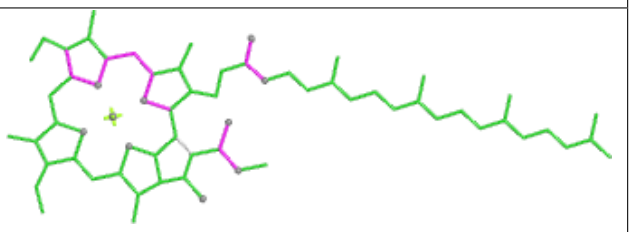


Rings

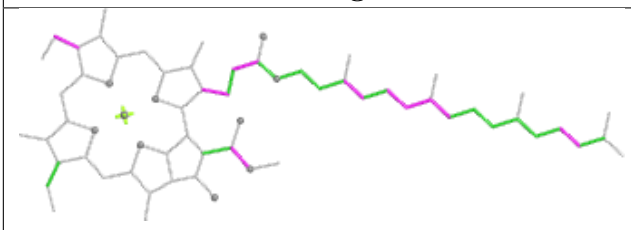
Ligand CLA I 601



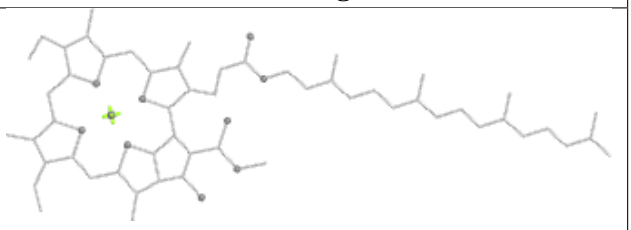
Bond lengths



Bond angles

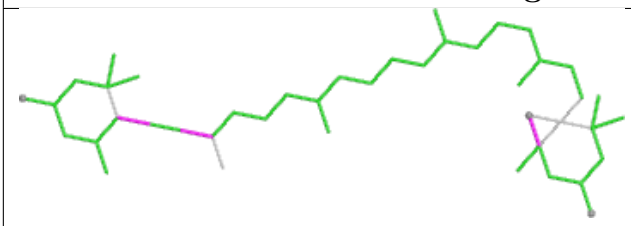


Torsions

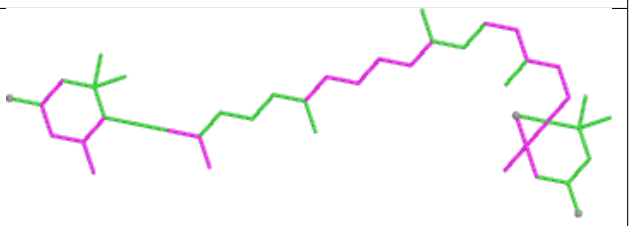


Rings

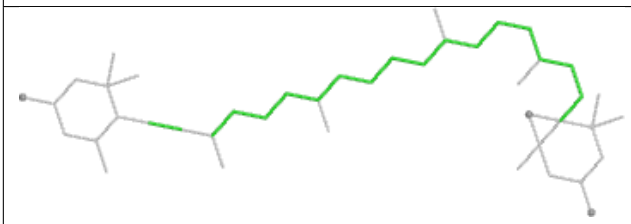
Ligand DD6 N 612



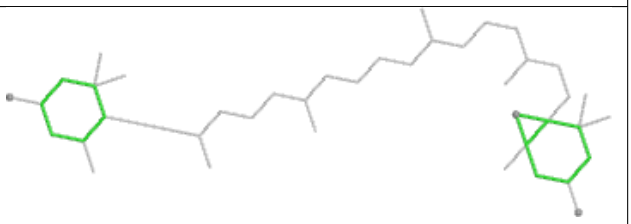
Bond lengths



Bond angles

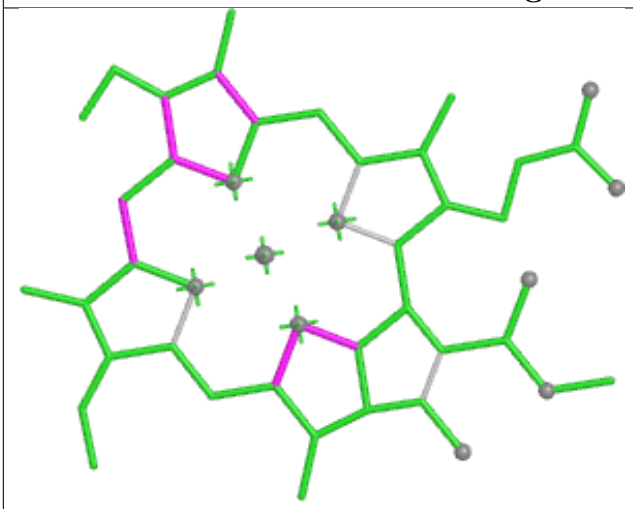


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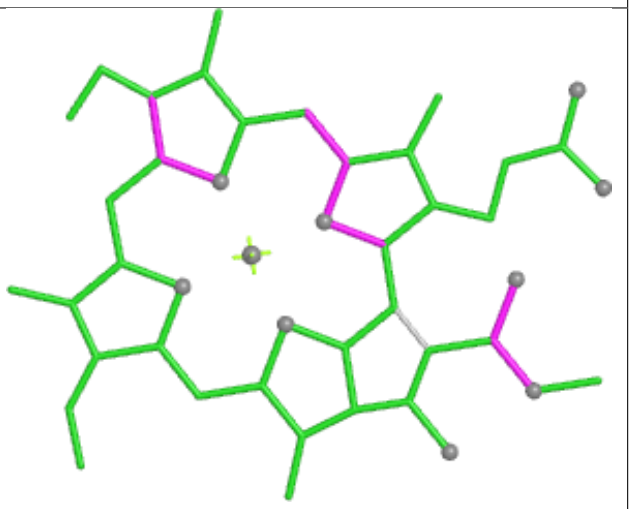


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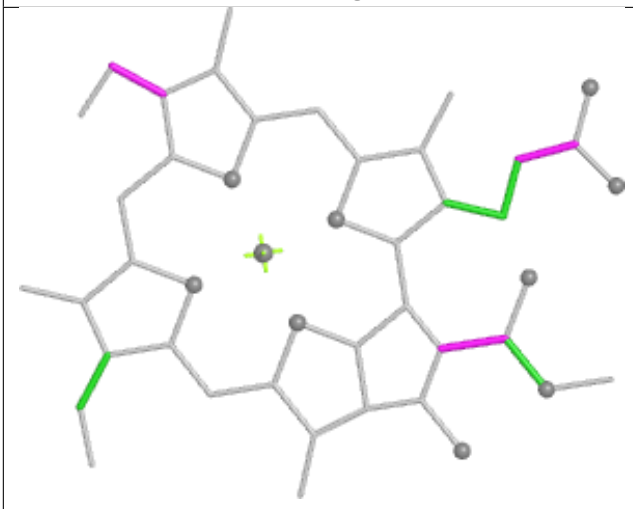
Ligand CLA P 603



Bond lengths



Bond angles

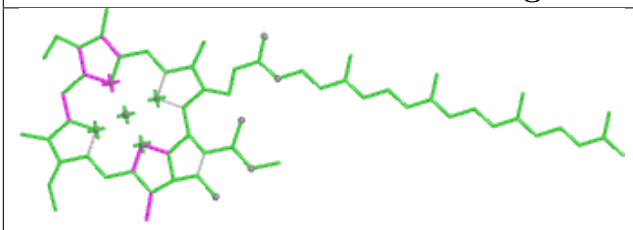


Torsions

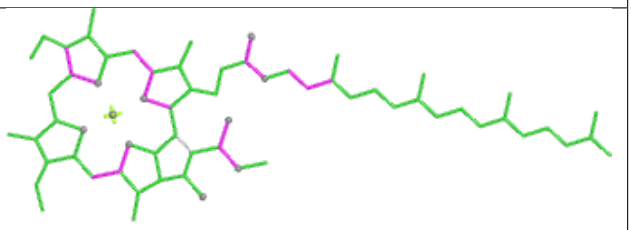


Rings

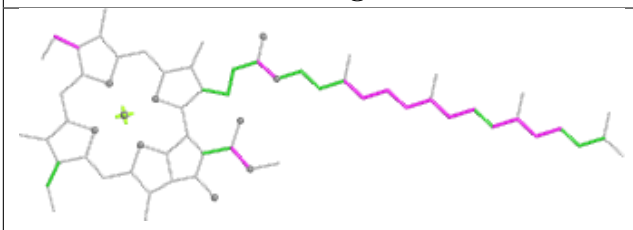
Ligand CLA R 601



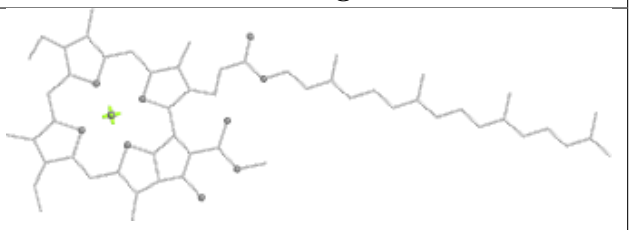
Bond lengths



Bond angles

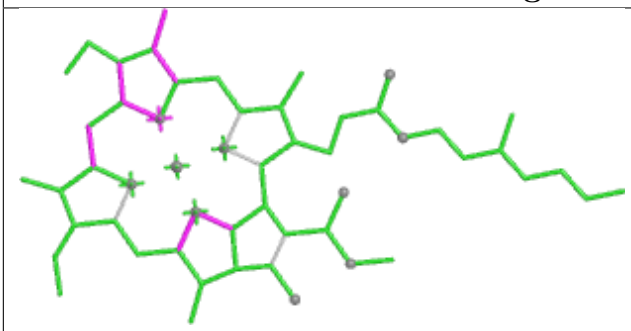


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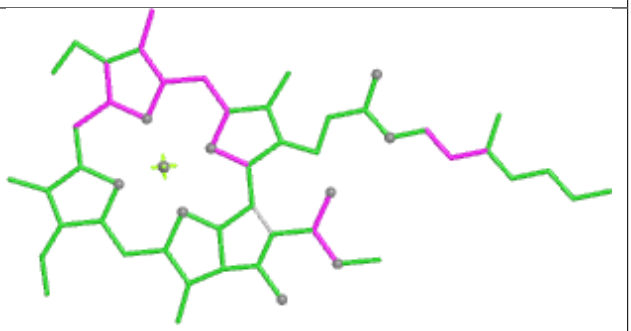


Rings

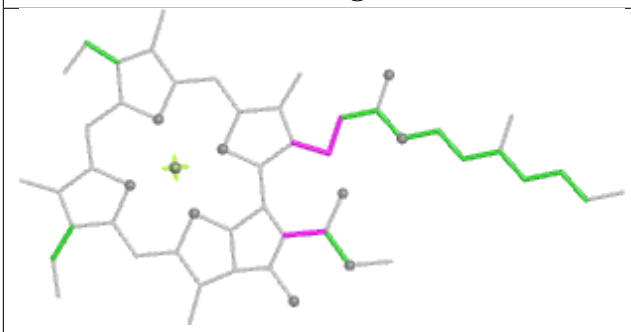
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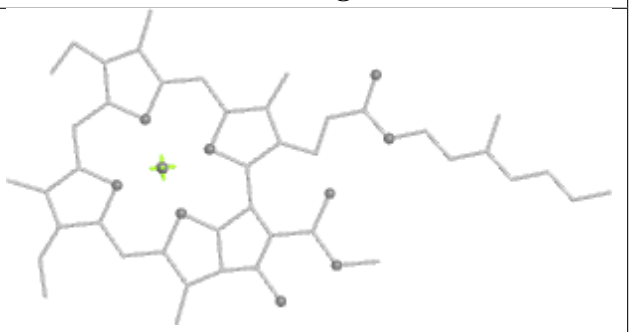
Bond lengths



Bond angles

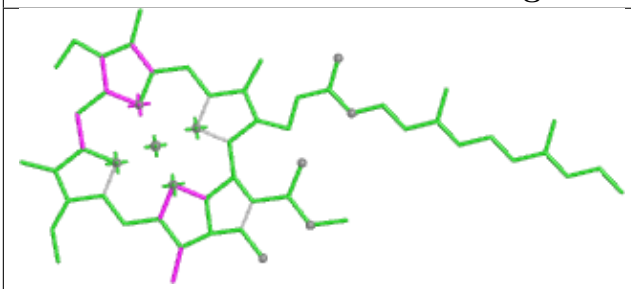


Torsions

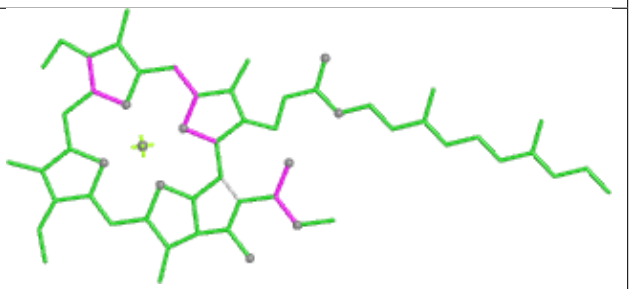


Rings

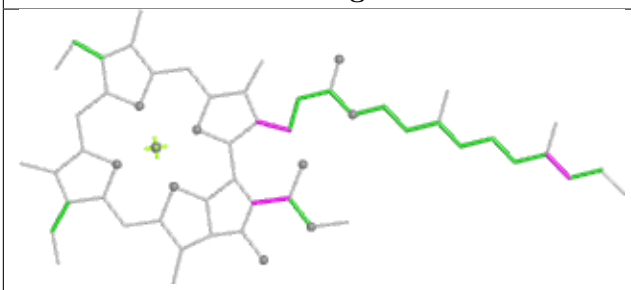
Ligand CLA U 405



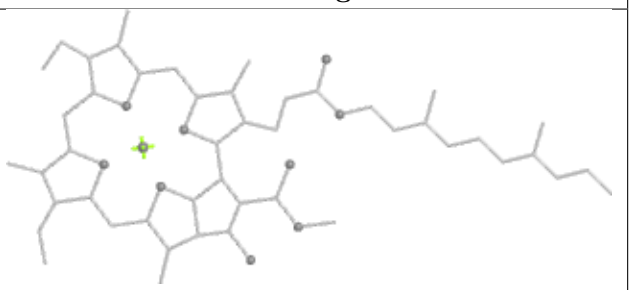
Bond lengths



Bond angles

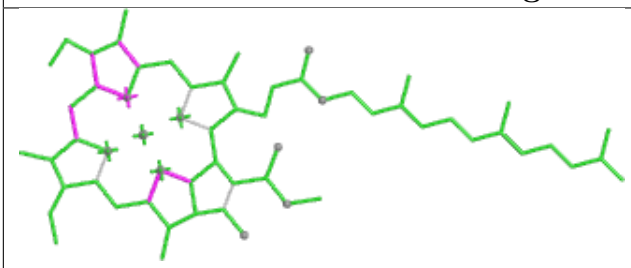


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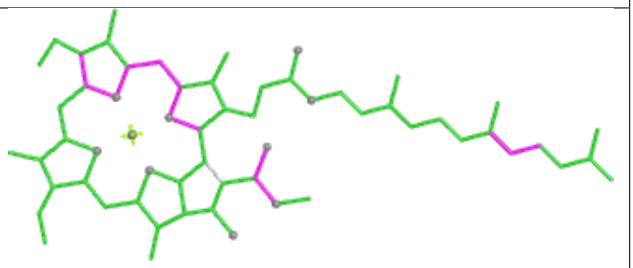


Rings

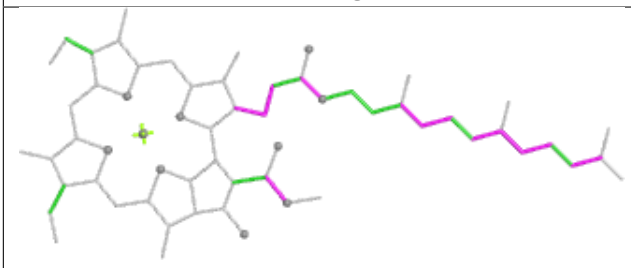
Ligand CLA G 608



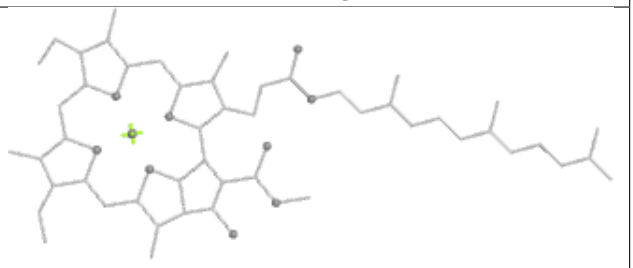
Bond lengths



Bond angles

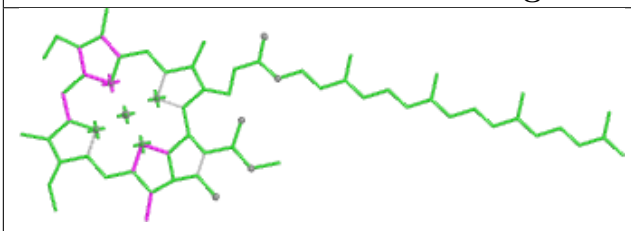


Torsions

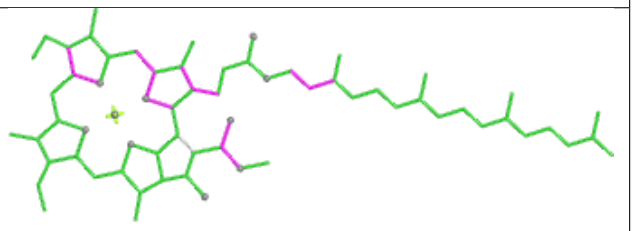


Rings

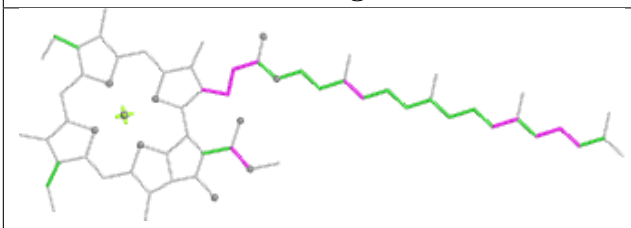
Ligand CLA A 830



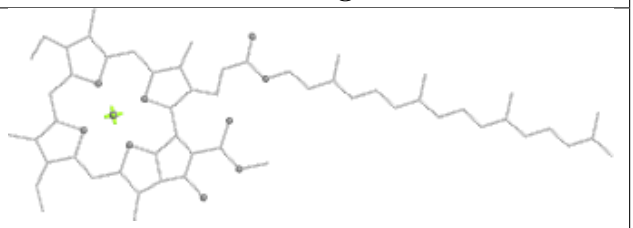
Bond lengths



Bond angles



Torsions



Rings

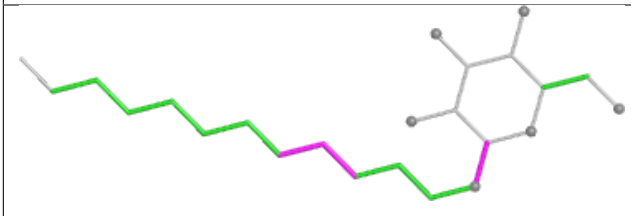
Ligand LMU T 617



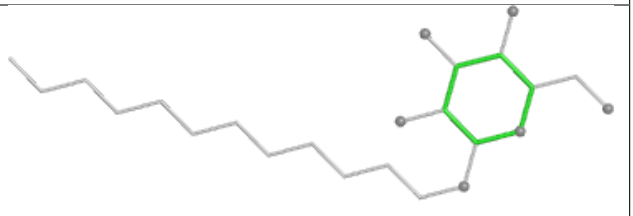
Bond lengths



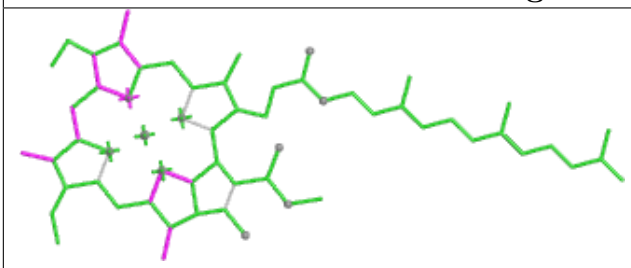
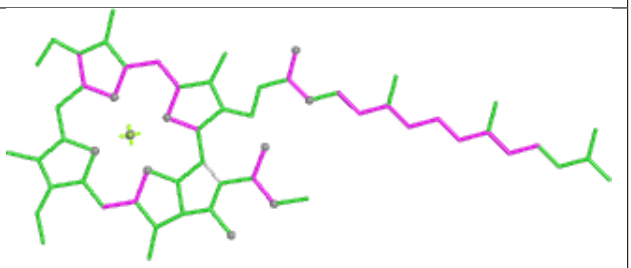
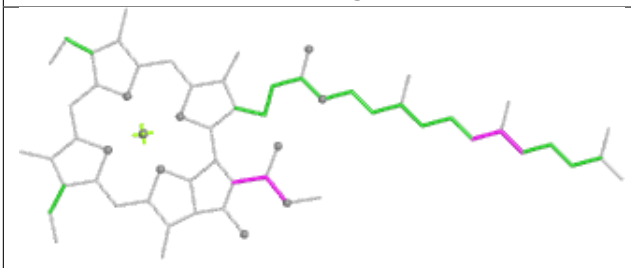
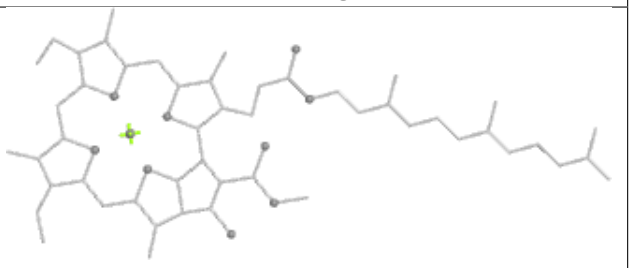
Bond angles

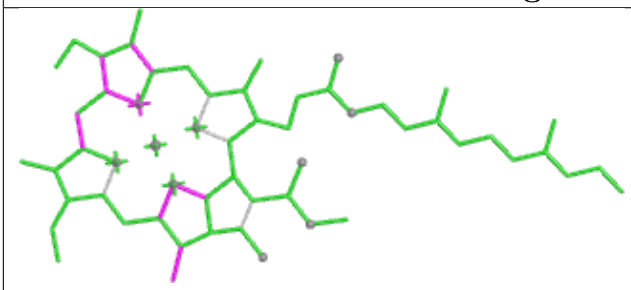
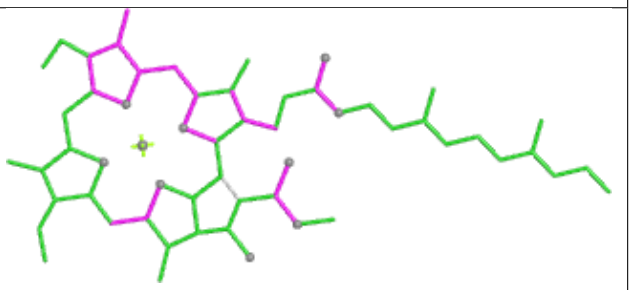
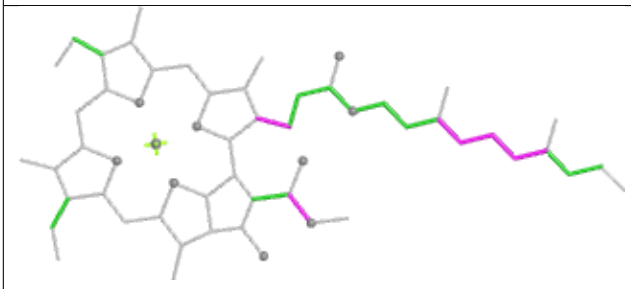
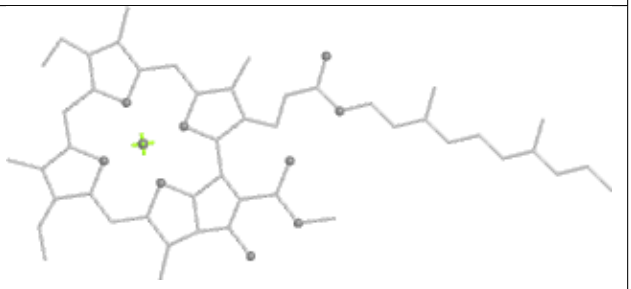


Torsions

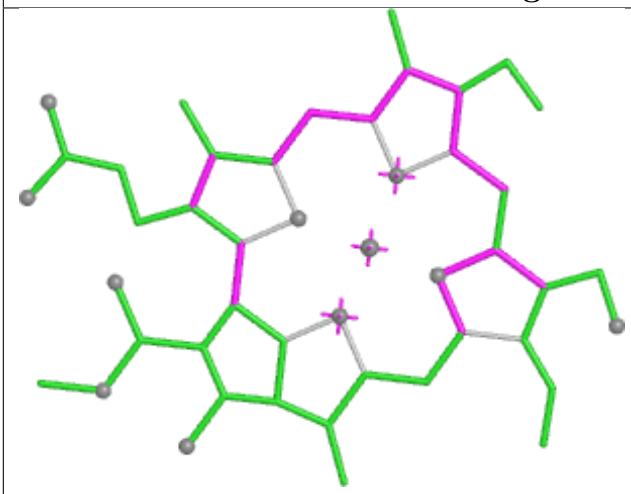


Rings

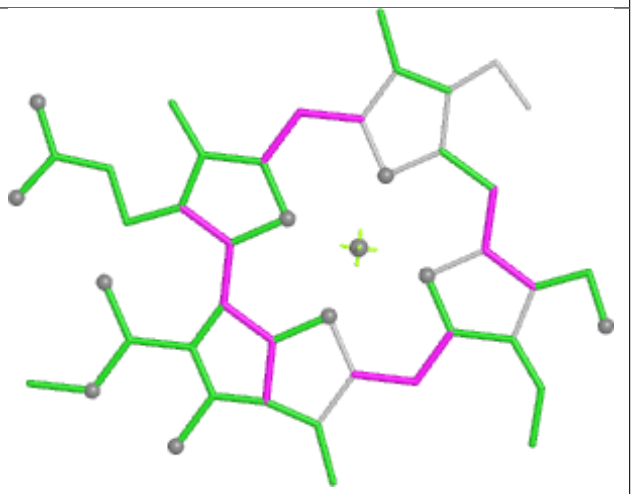
Ligand CLA L 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

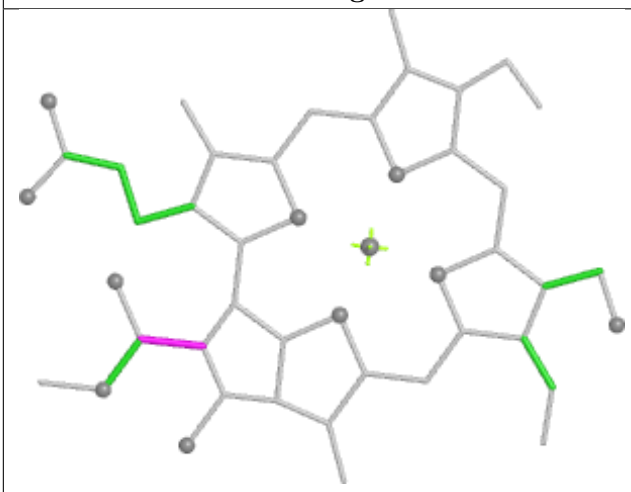
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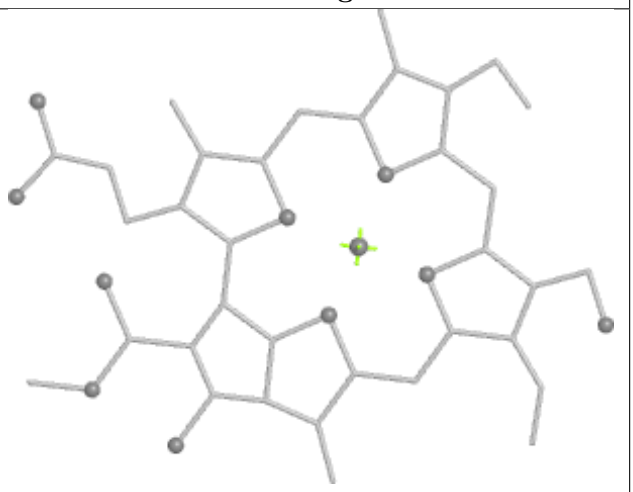
Bond lengths



Bond angles

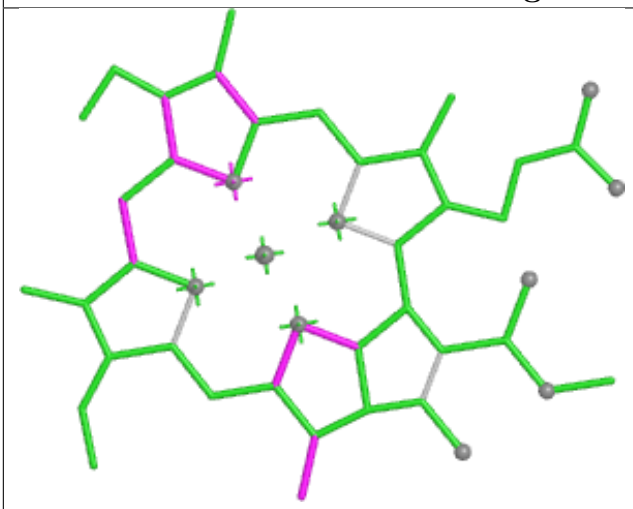


Torsions

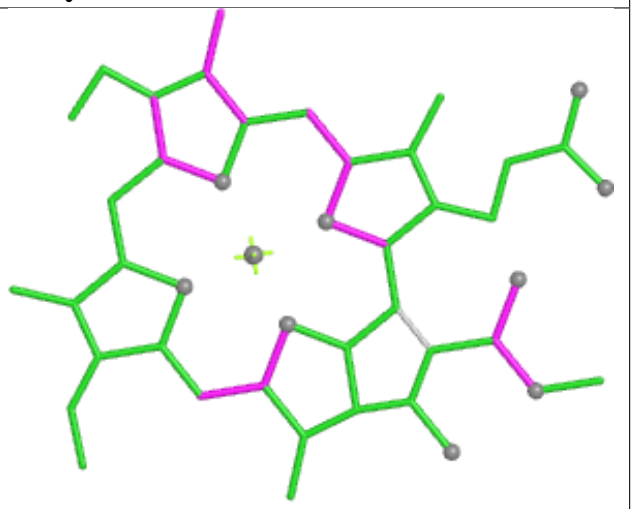


Rings

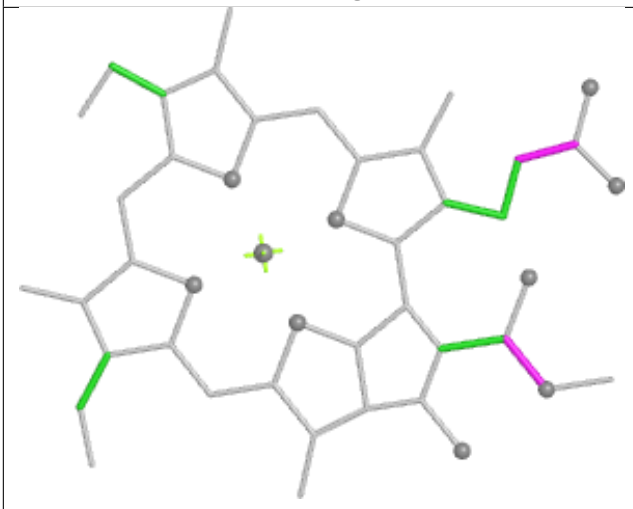
Ligand CLA Q 603



Bond lengths



Bond angles

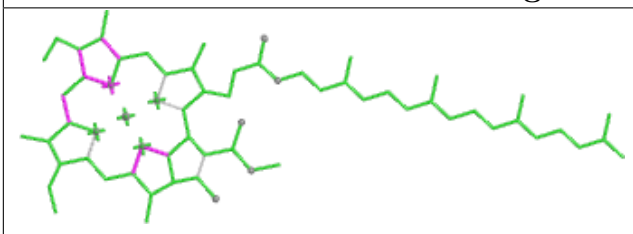


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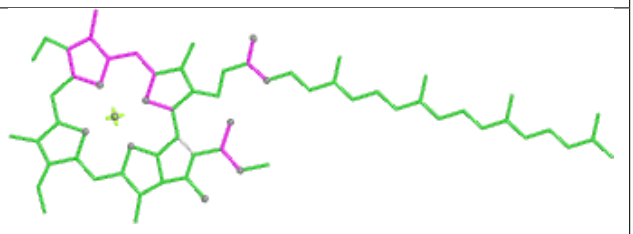


Rings

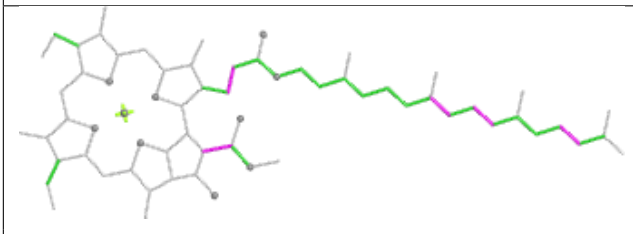
Ligand CLA A 815



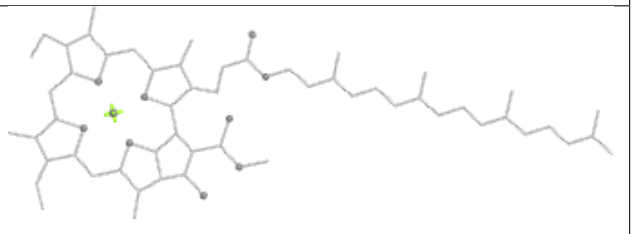
Bond lengths



Bond angles

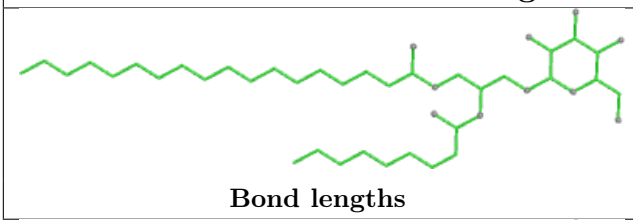


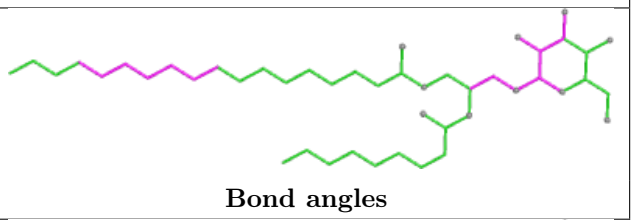
Torsions

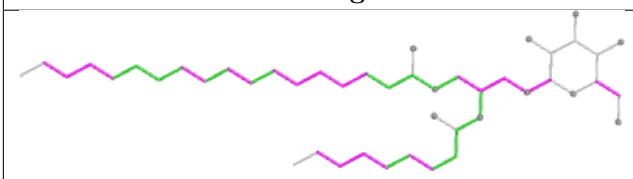


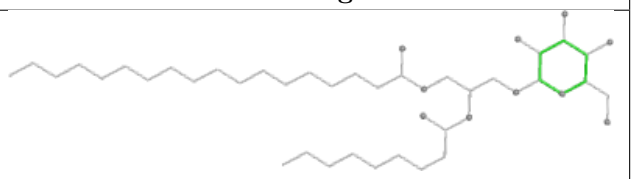
Rings

Ligand LMG G 616

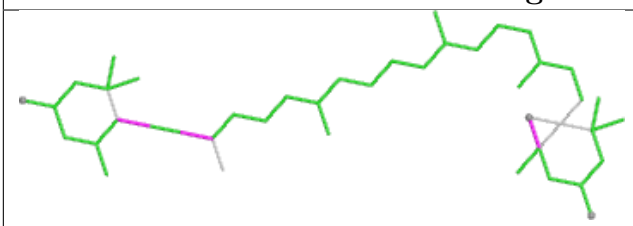

Bond lengths

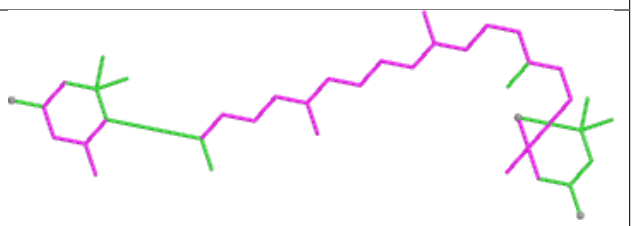

Bond angles

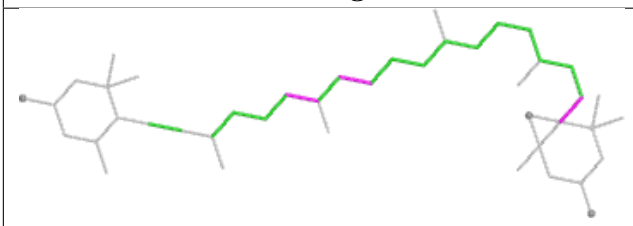

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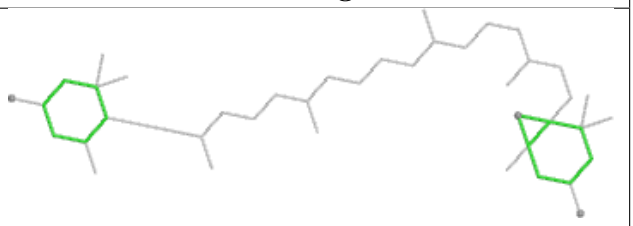

Rings

Ligand DD6 P 613

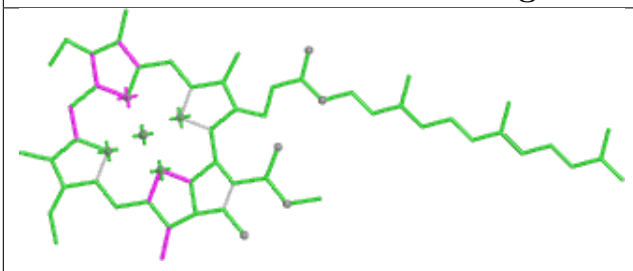

Bond lengths

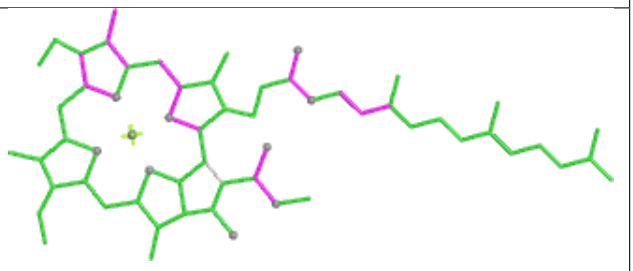

Bond angles

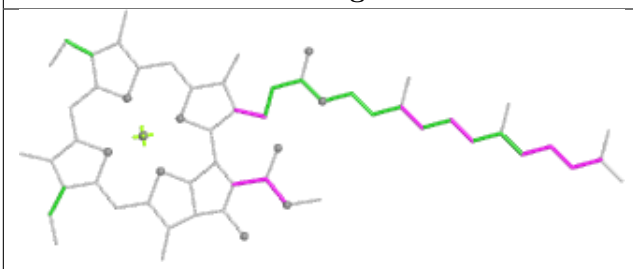

Torsions

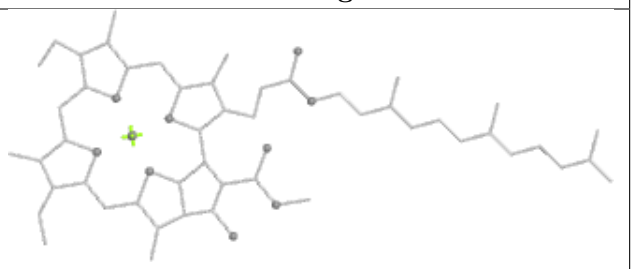

Rings

Ligand CLA W 411

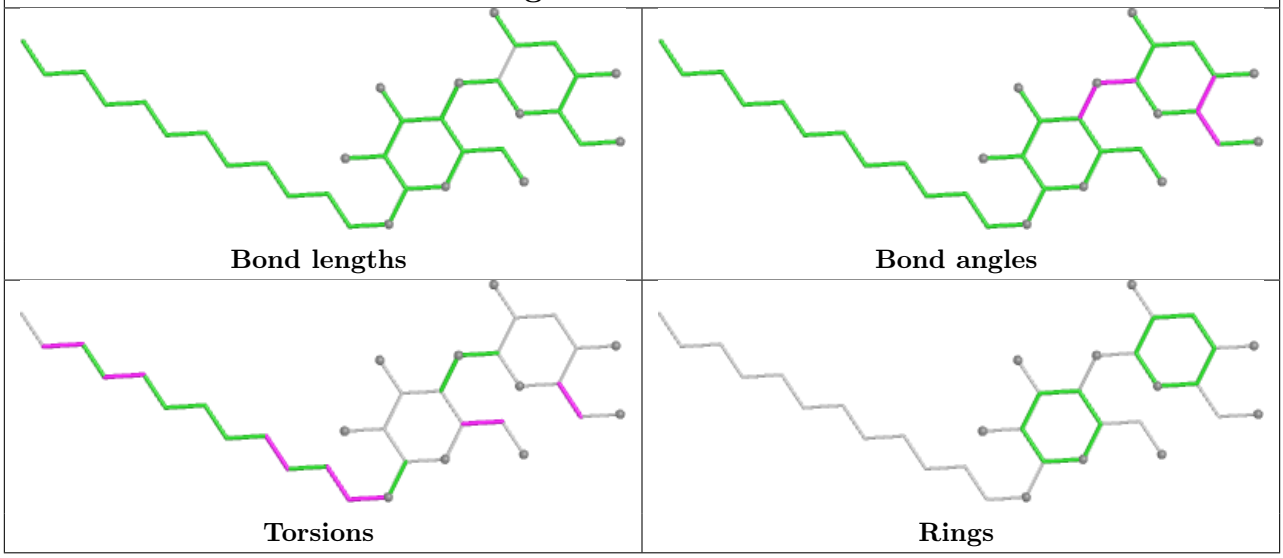

Bond lengths


Bond angles

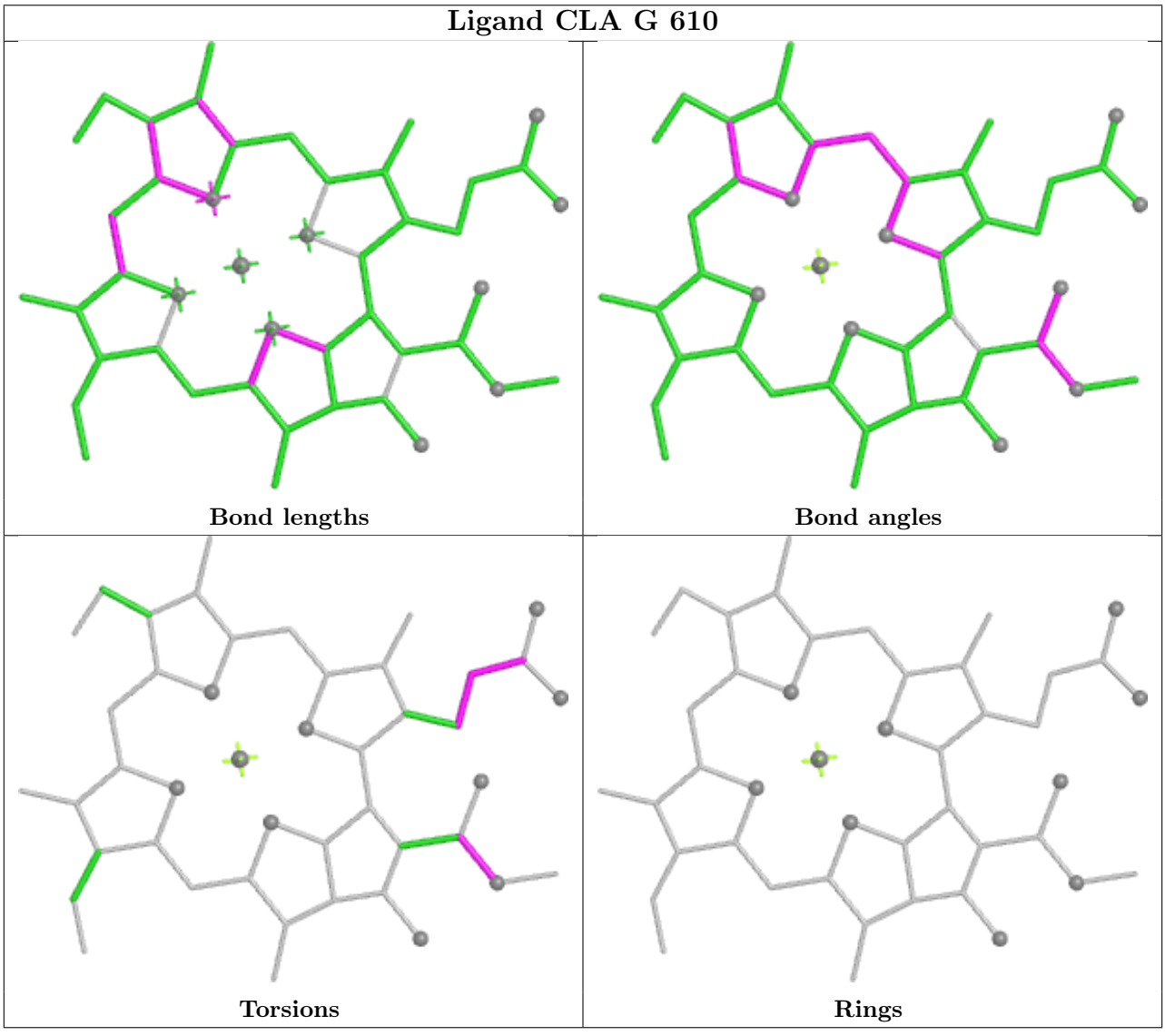

Torsions


Rings

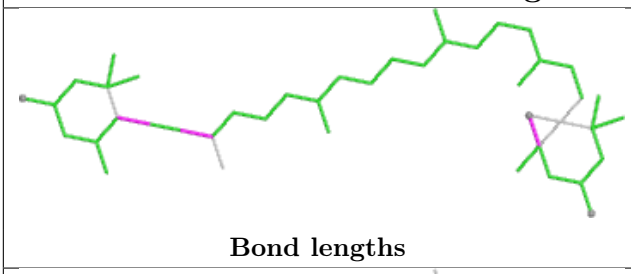
Ligand LMU J 104



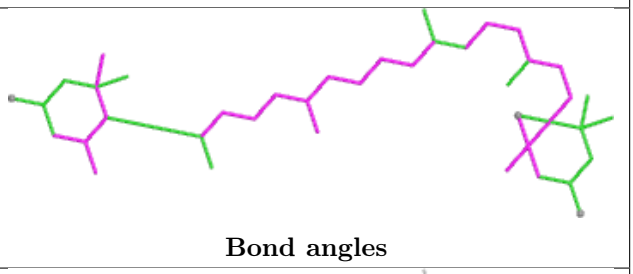
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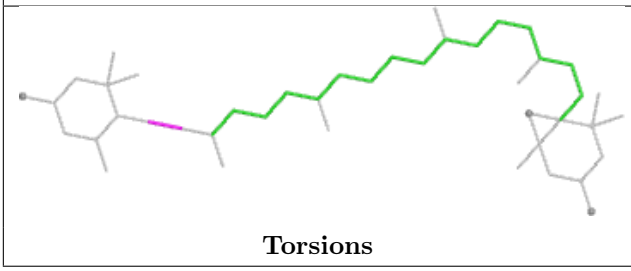
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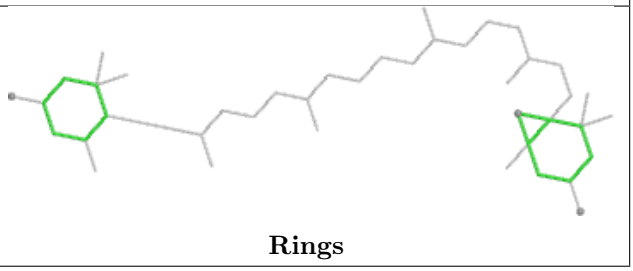
Bond lengths



Bond angles

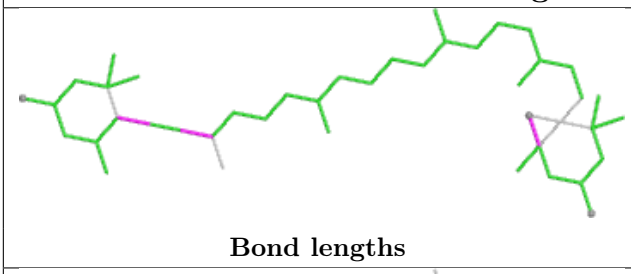


Torsions

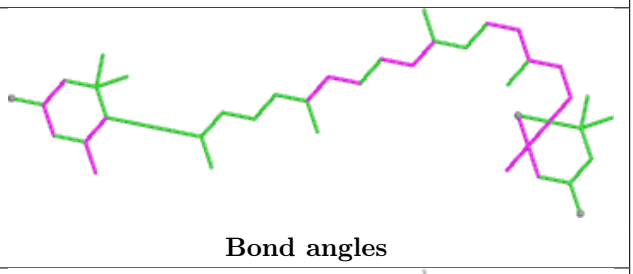


Rings

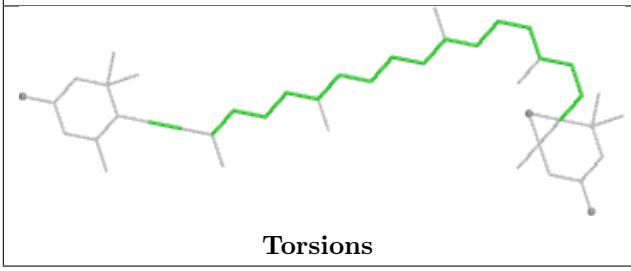
Ligand DD6 I 612



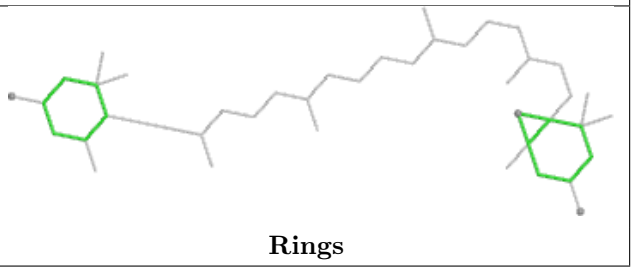
Bond lengths



Bond angles

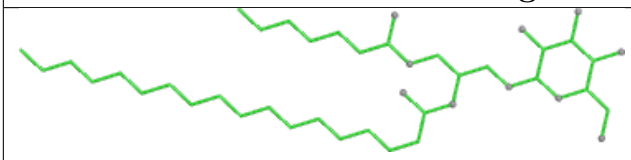


Torsions

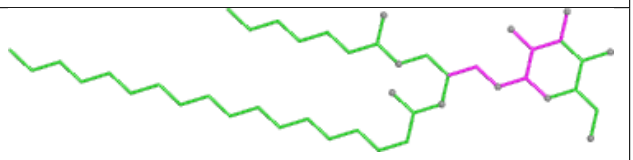


Rings

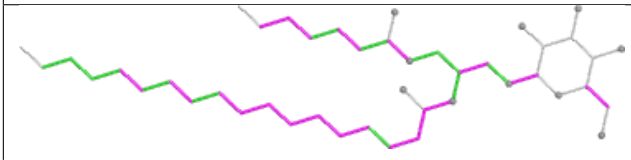
Ligand LMG N 615



Bond lengths



Bond angles

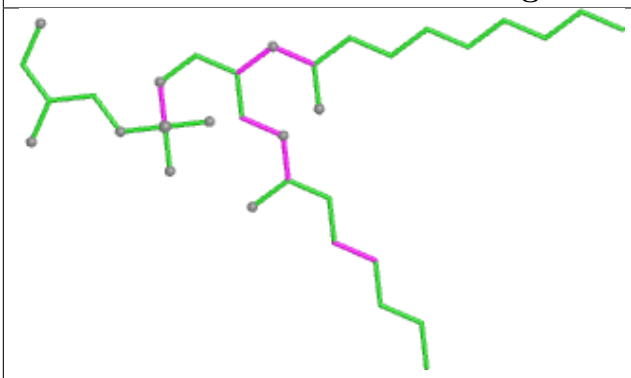


Torsions

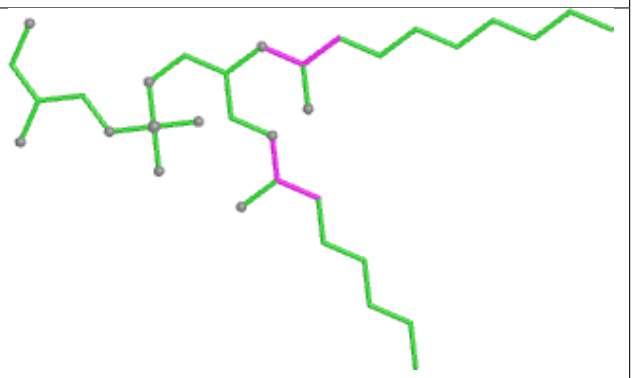


Rings

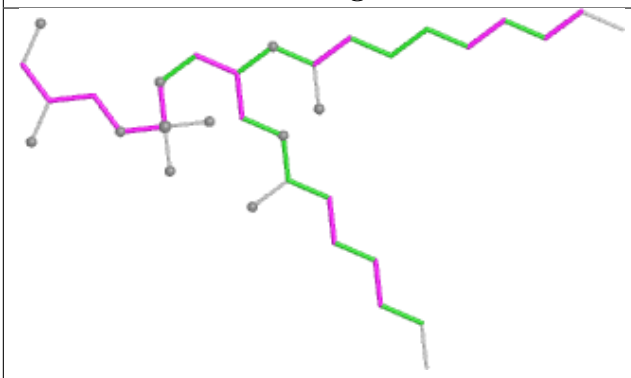
Ligand LHG K 619



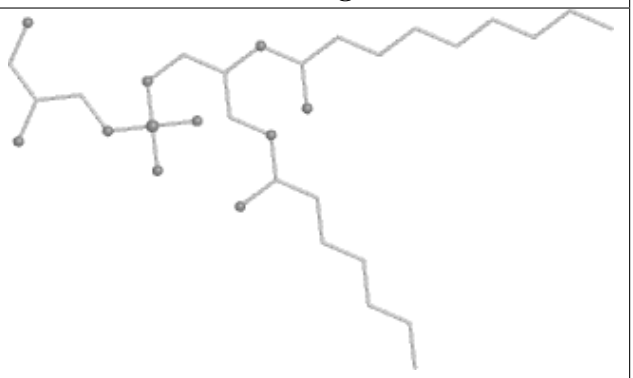
Bond lengths



Bond angles

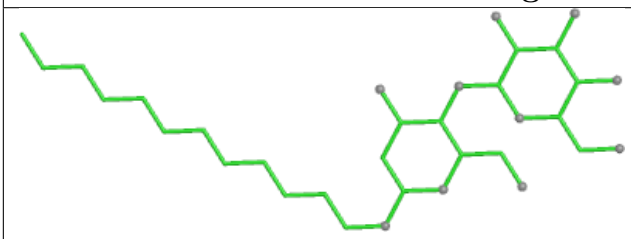


Torsions

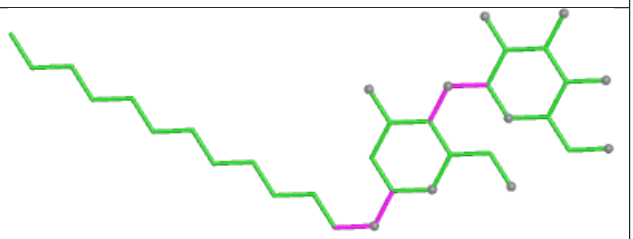


Rings

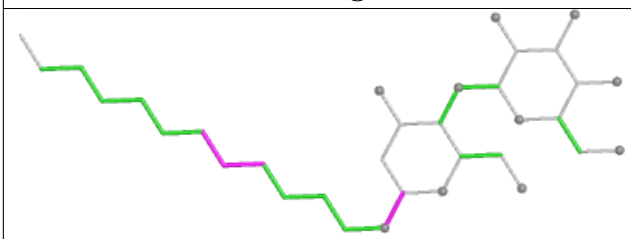
Ligand LMU L 420



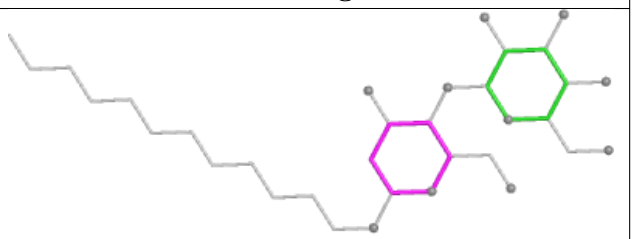
Bond lengths



Bond angles

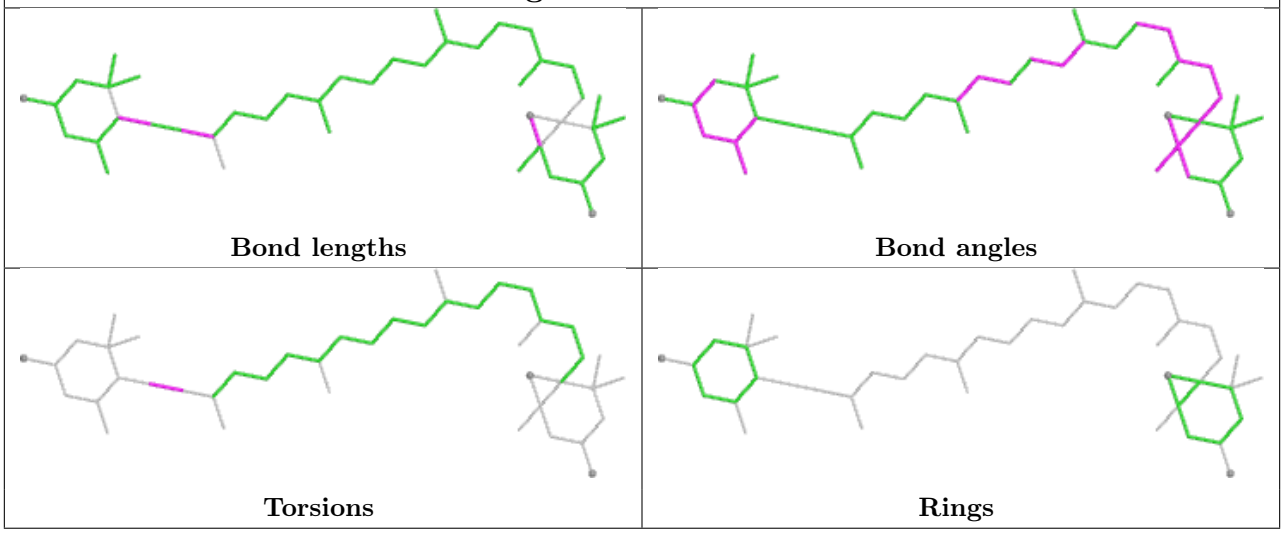


Torsions

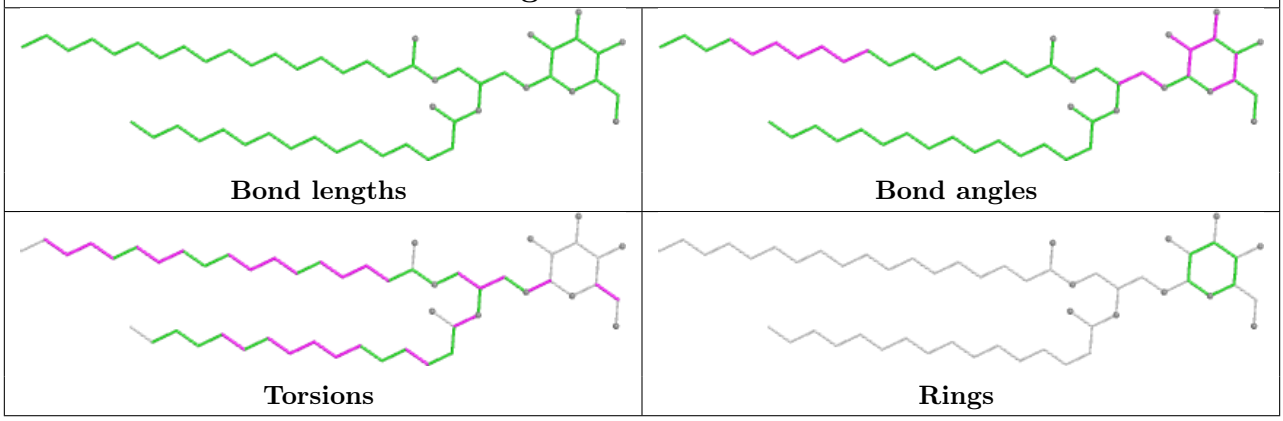


Rings

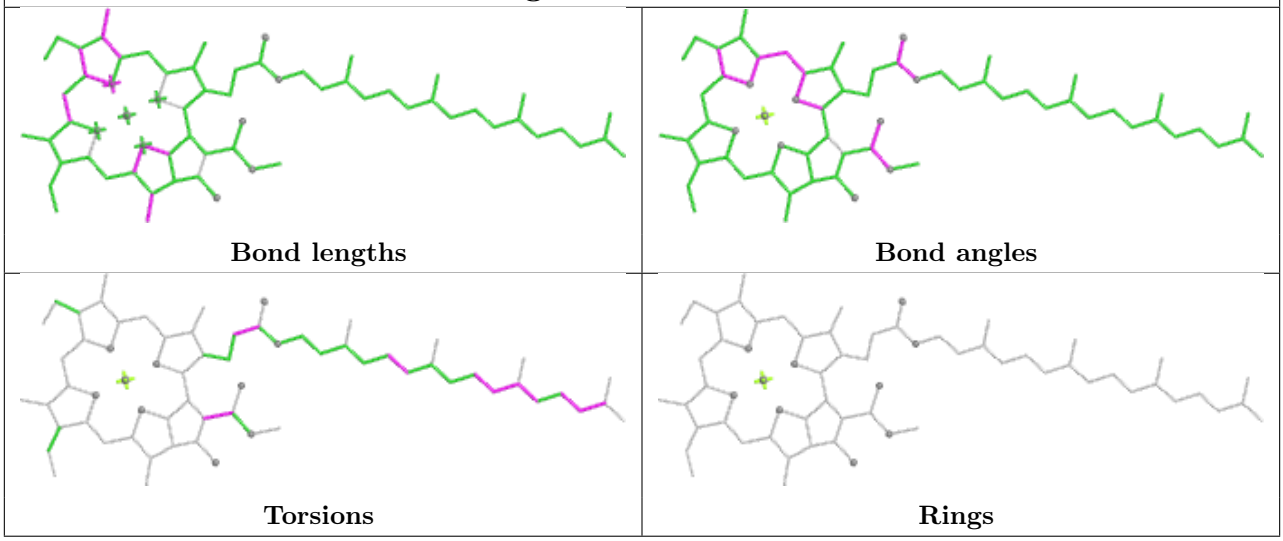
Ligand DD6 R 612



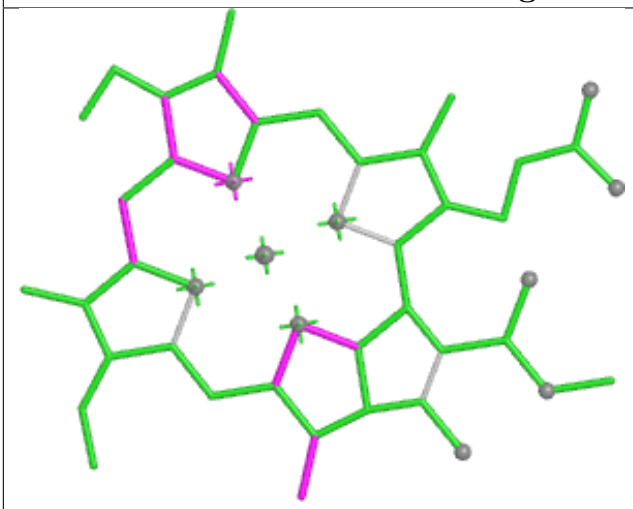
Ligand LMG B 856



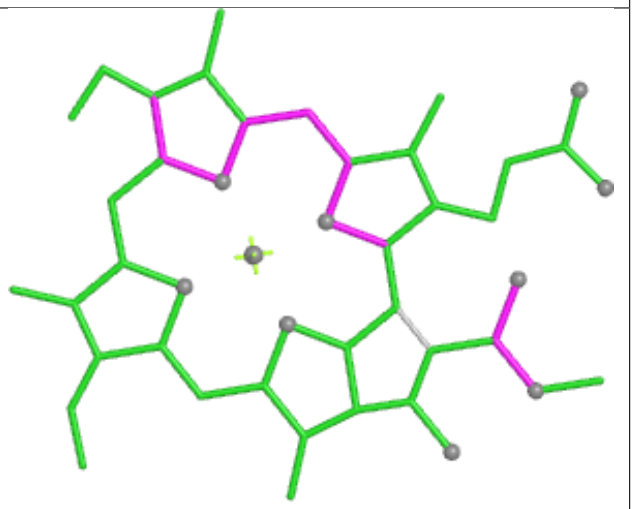
Ligand CLA A 808



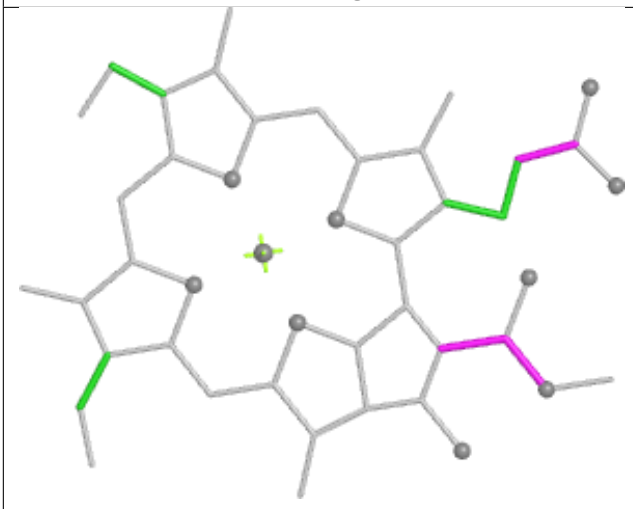
Ligand CLA W 413



Bond lengths



Bond angles

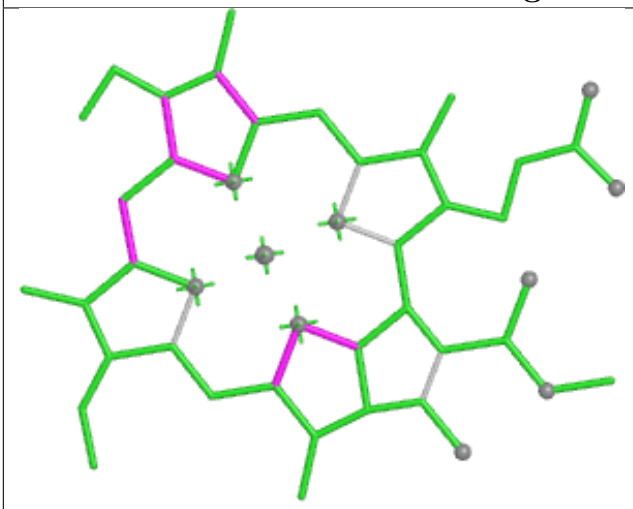


Torsions

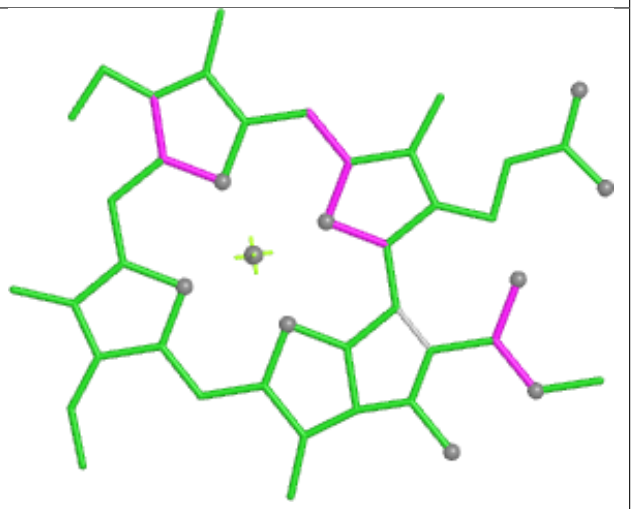


Rings

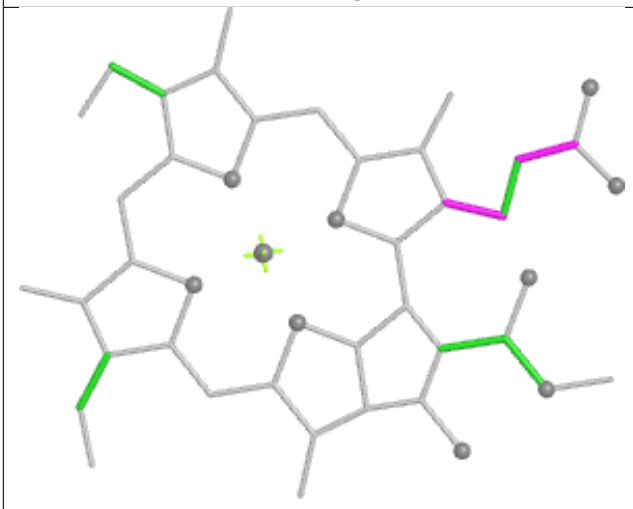
Ligand CLA X 413



Bond lengths



Bond angles

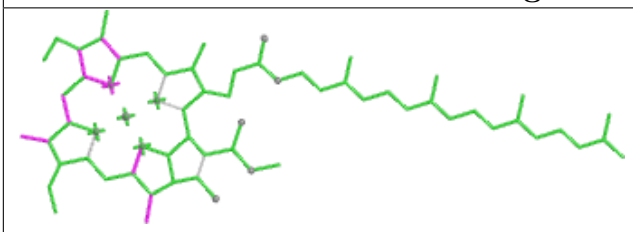


Torsions

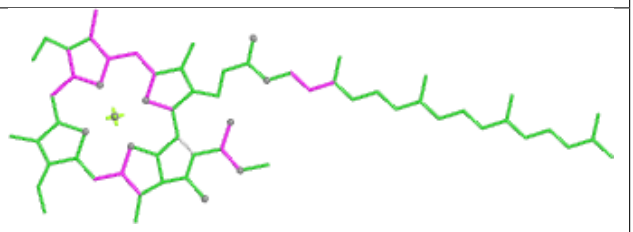


Rings

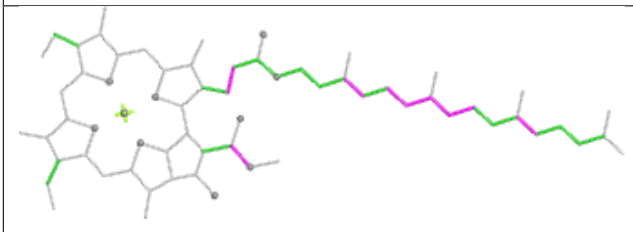
Ligand CLA A 803



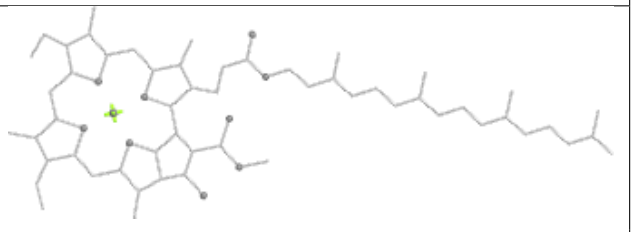
Bond lengths



Bond angles

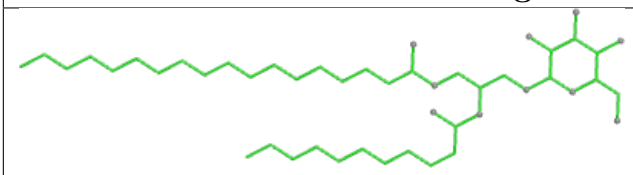


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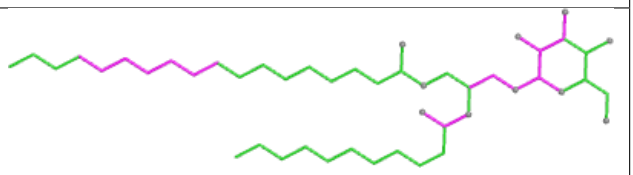


Rings

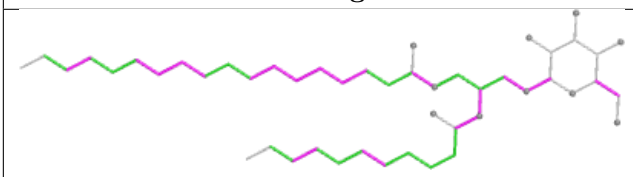
Ligand LMG W 401



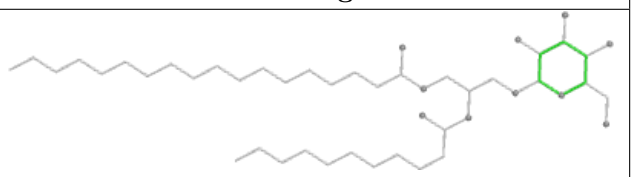
Bond lengths



Bond angles

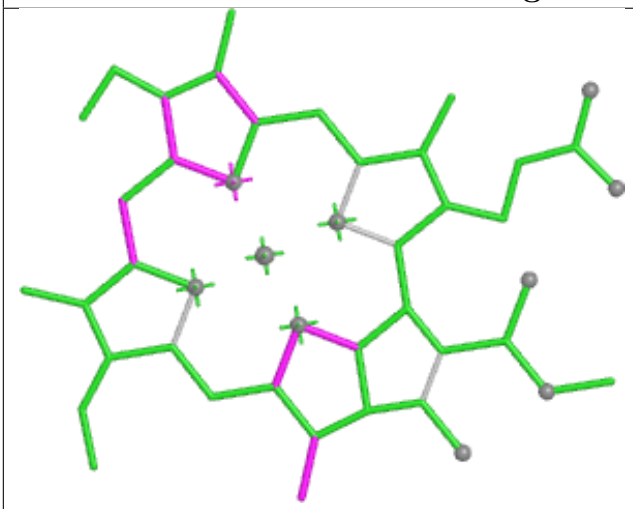


Torsions

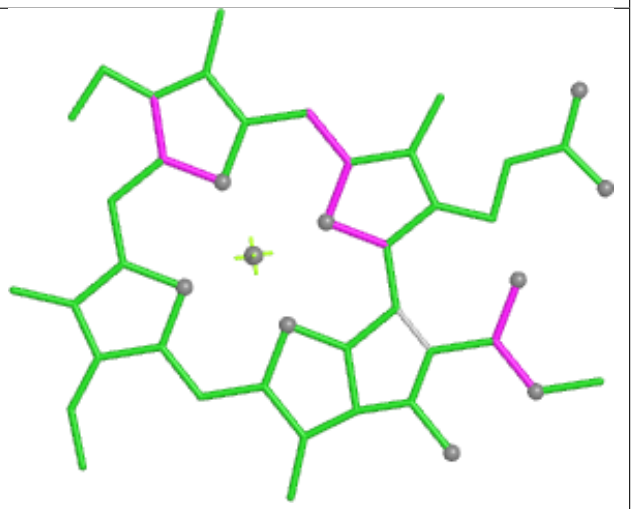


Rings

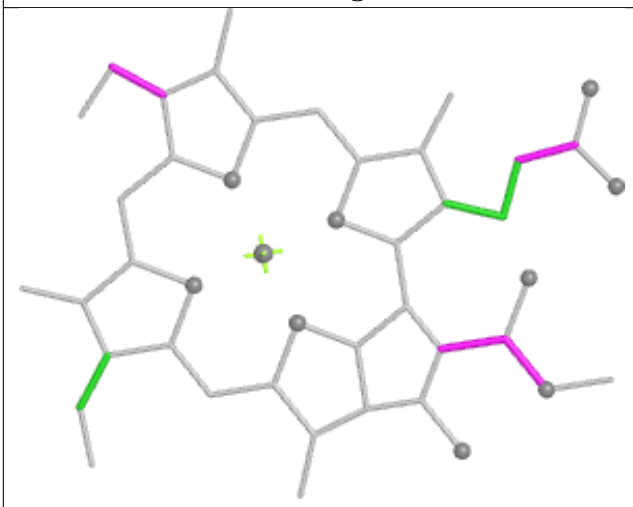
Ligand CLA N 608



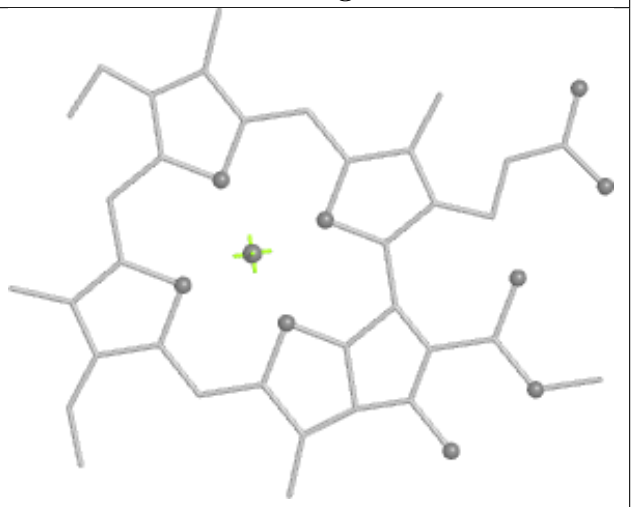
Bond lengths



Bond angles

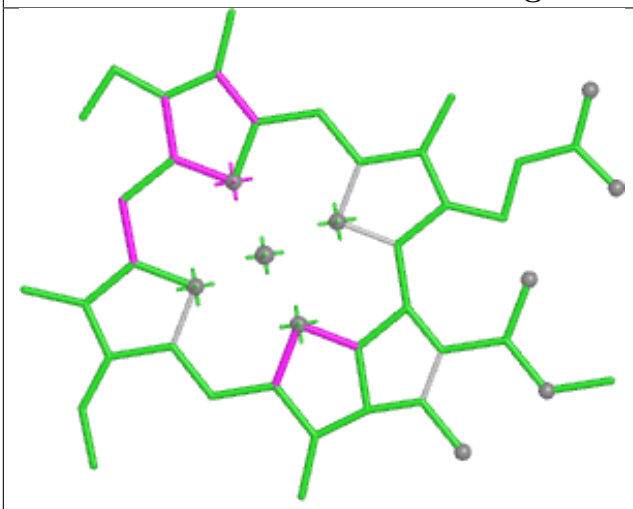


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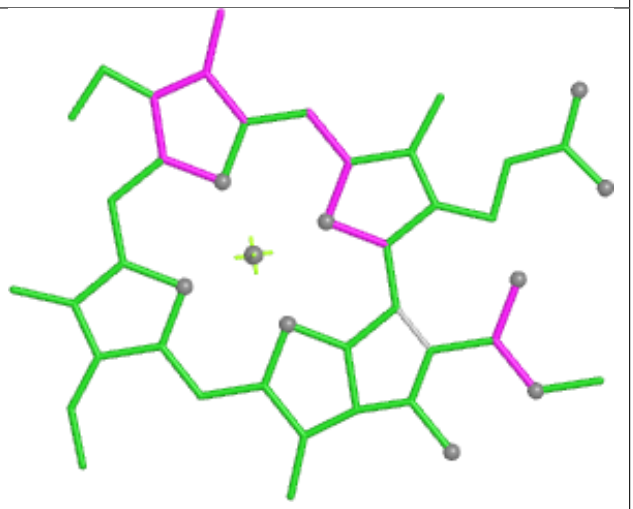


Rings

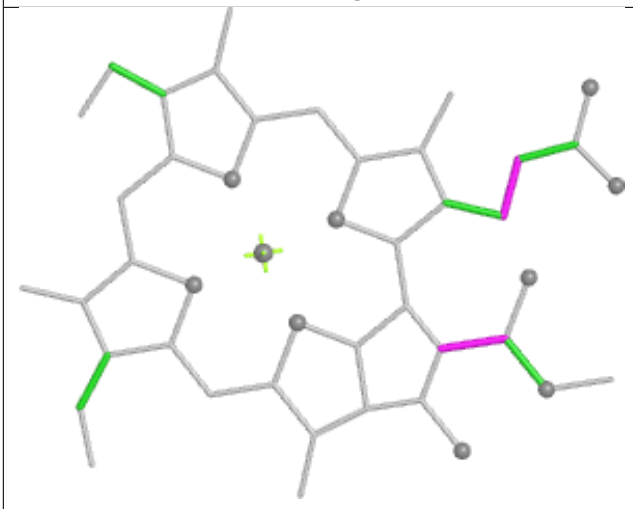
Ligand CLA B 811



Bond lengths



Bond angles

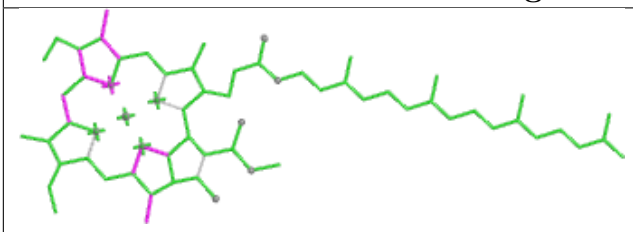


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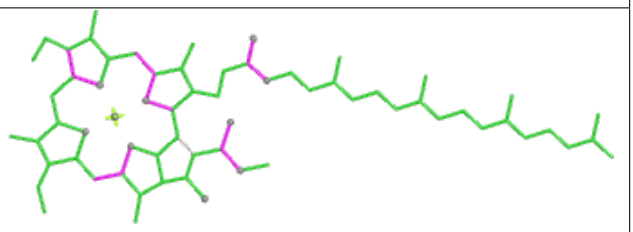


Rings

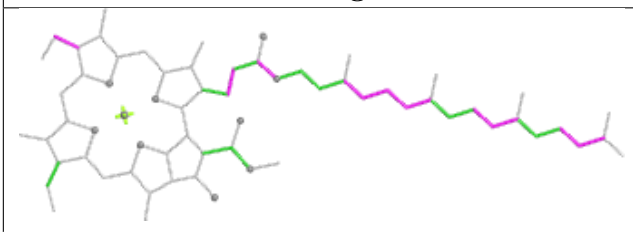
Ligand CLA T 605



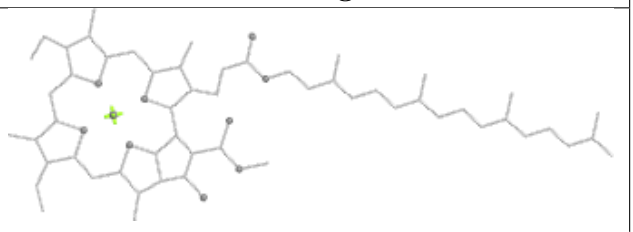
Bond lengths



Bond angles

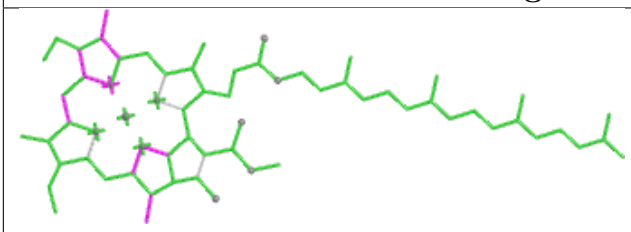


Torsions

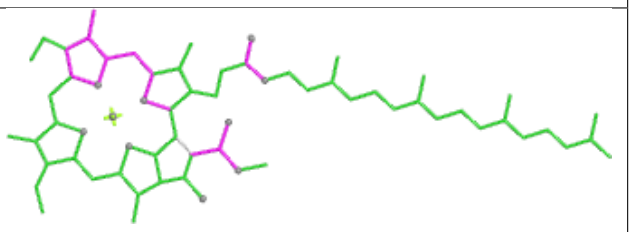


Rings

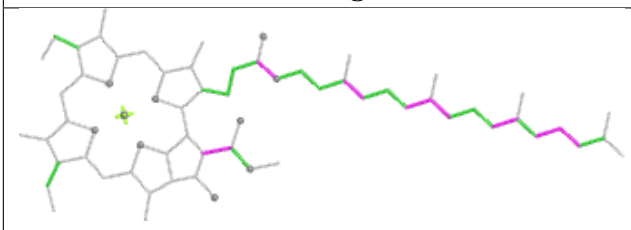
Ligand CLA B 828



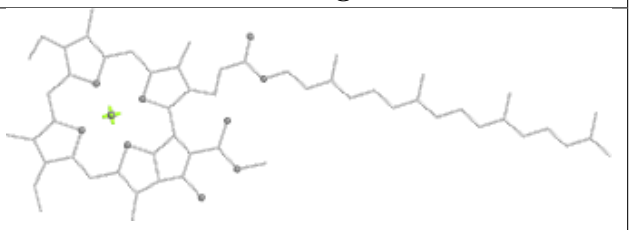
Bond lengths



Bond angles

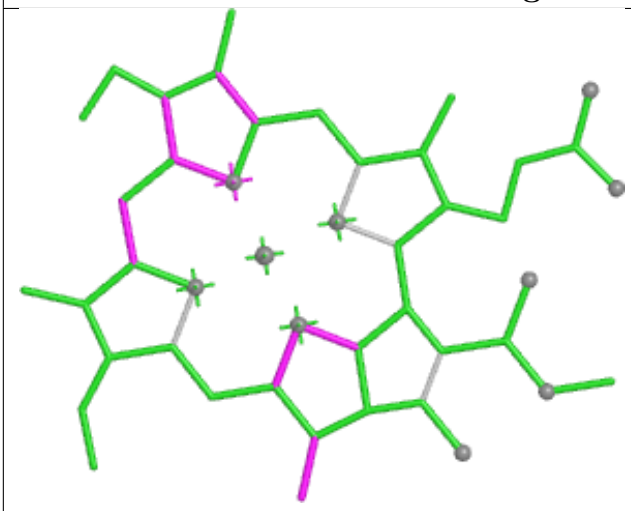


Torsions

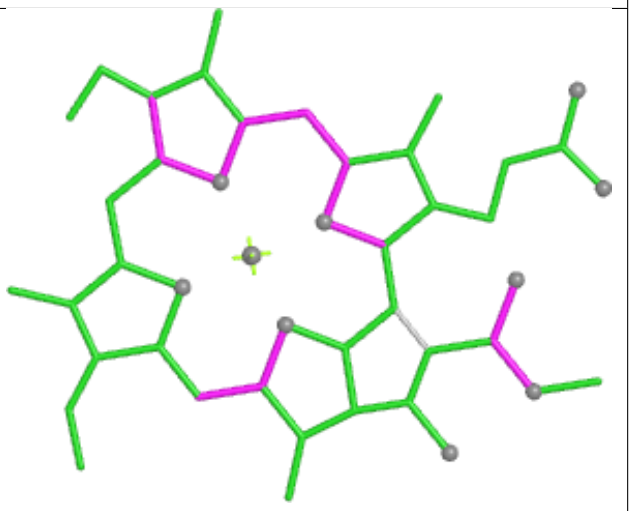


Rings

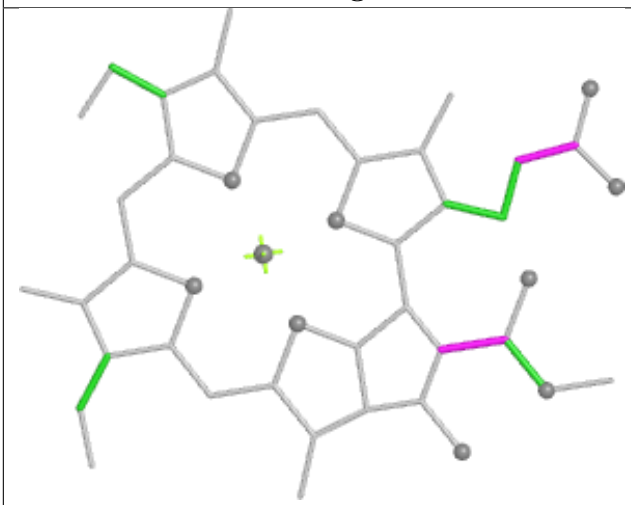
Ligand CLA G 609



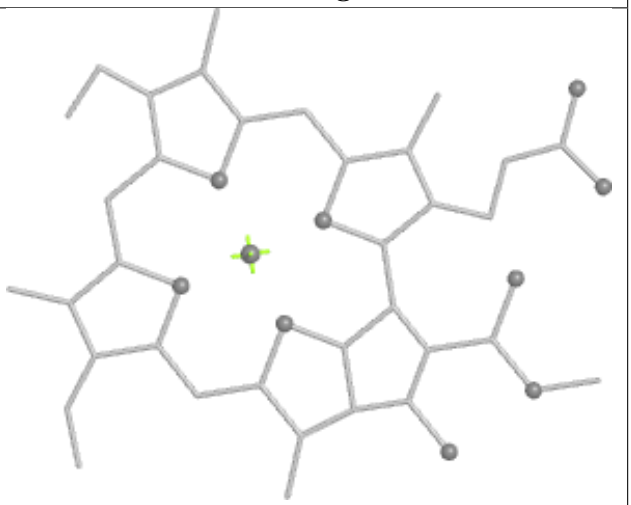
Bond lengths



Bond angles

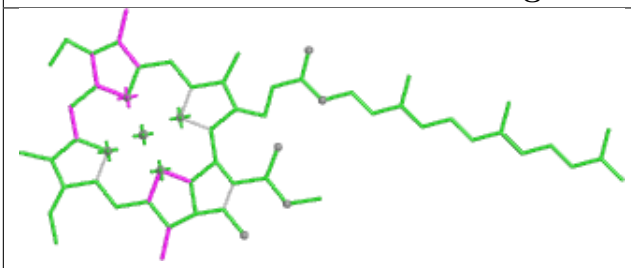


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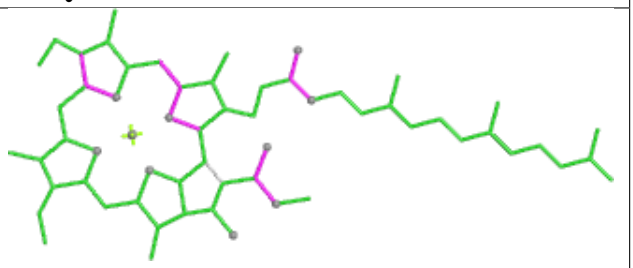


Rings

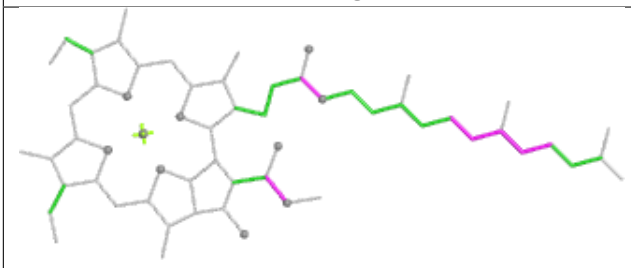
Ligand CLA Q 609



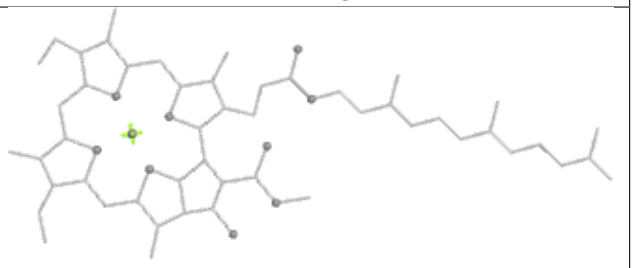
Bond lengths



Bond angles

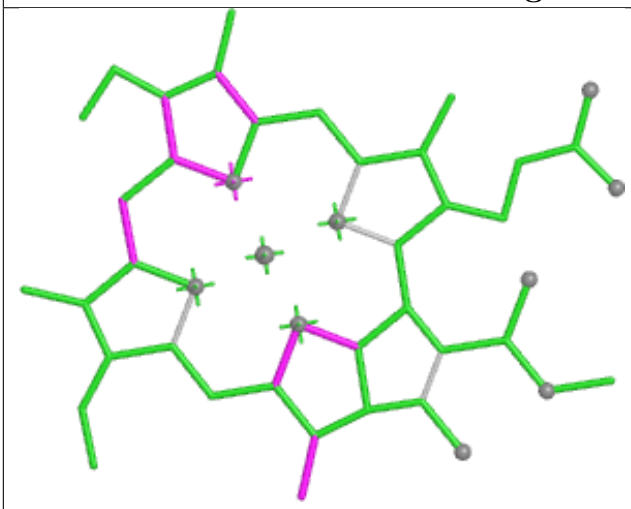


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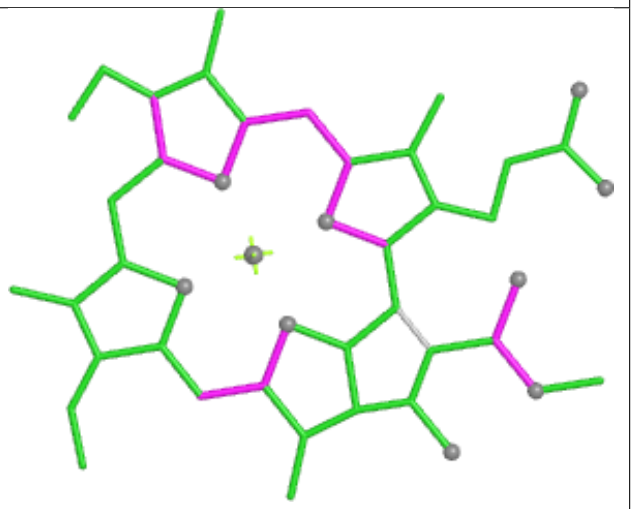


Rings

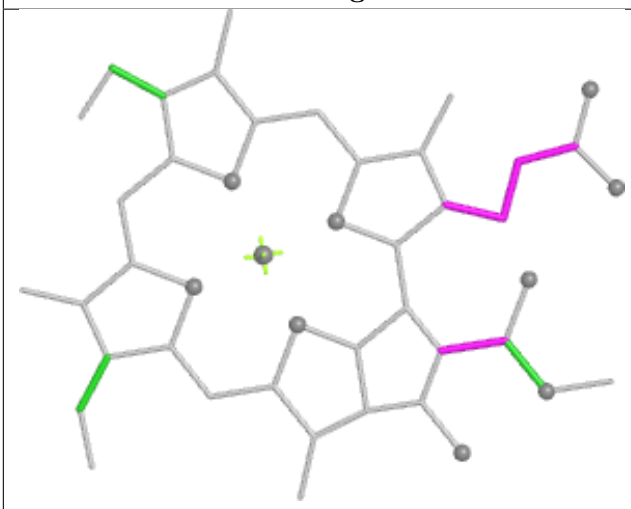
Ligand CLA P 605



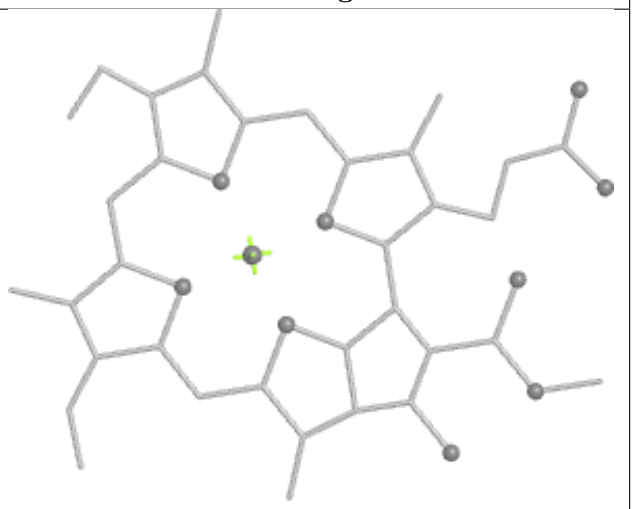
Bond lengths



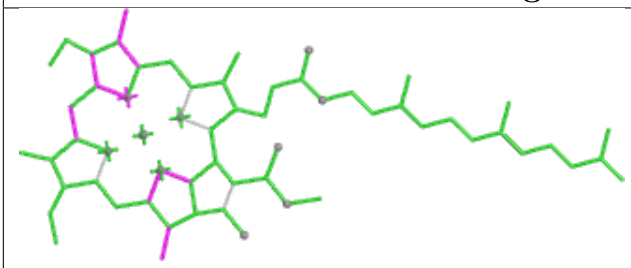
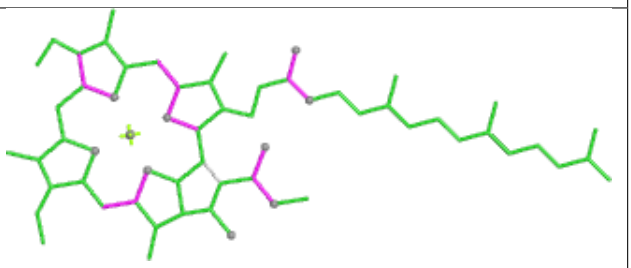
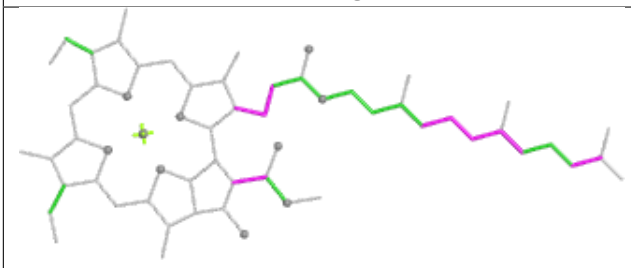
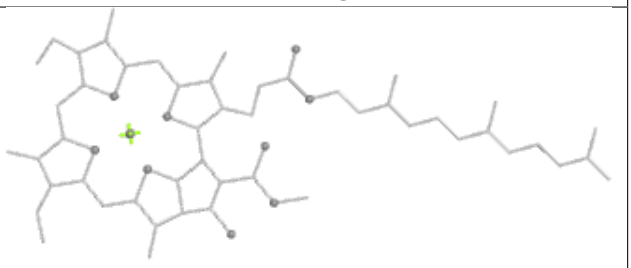
Bond angles

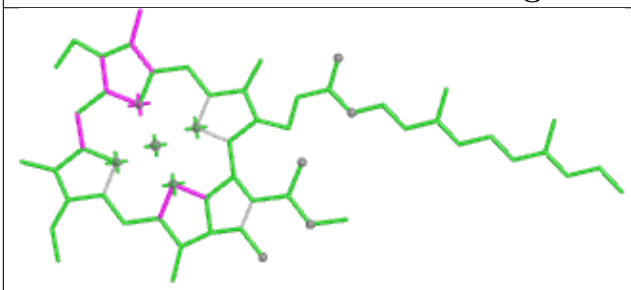
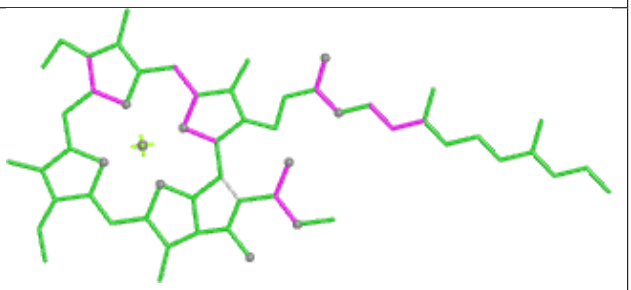
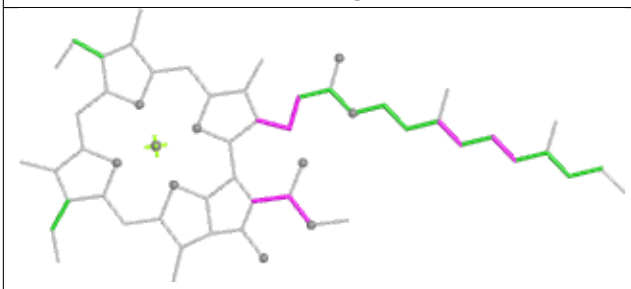
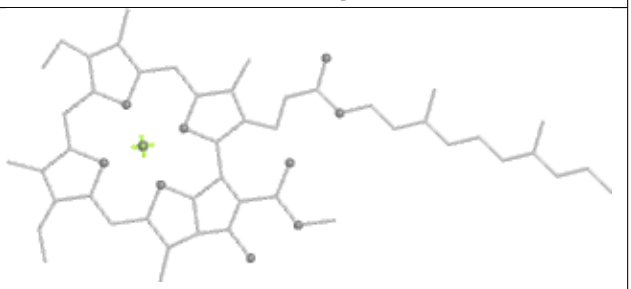


Torsions

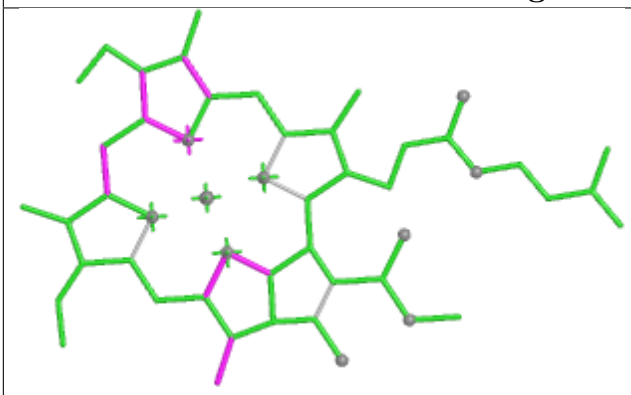


Rings

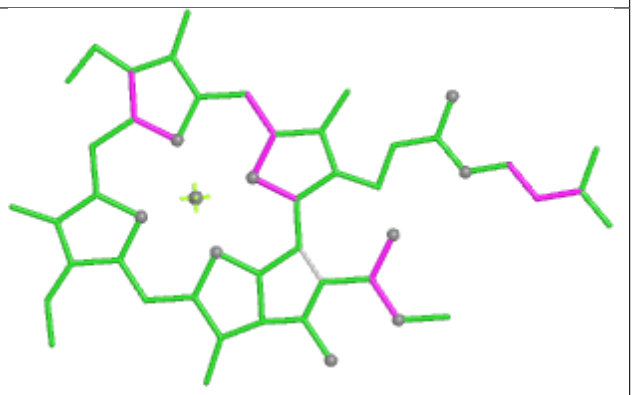
Ligand CLA H 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA V 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

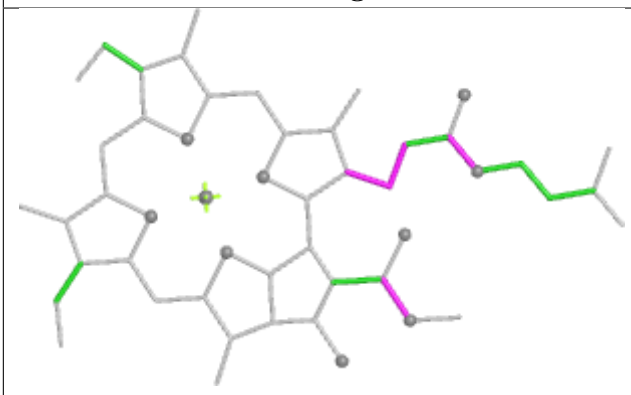
Ligand CLA J 102



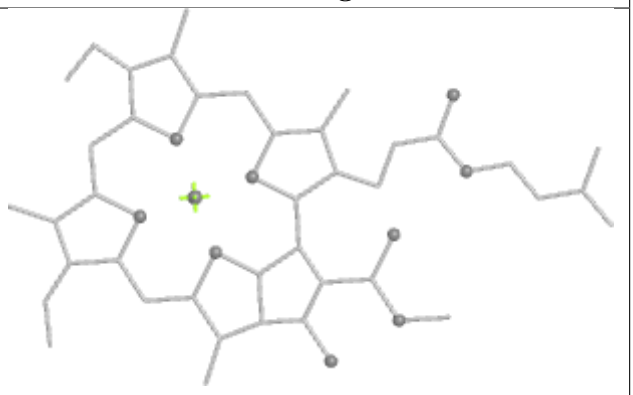
Bond lengths



Bond angles

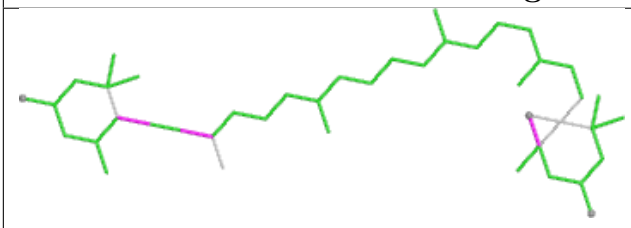


Torsions

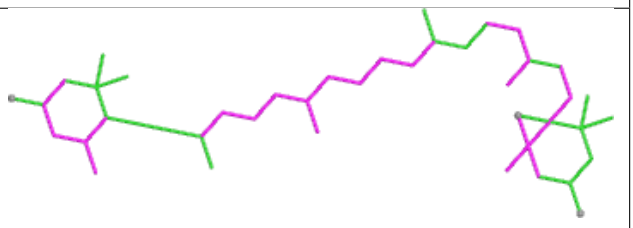


Rings

Ligand DD6 N 613



Bond lengths



Bond angles

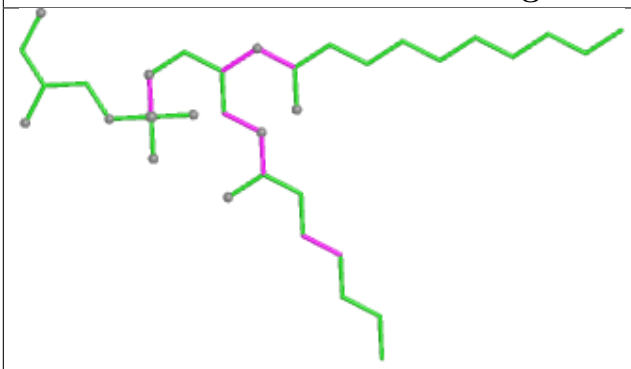


Torsions

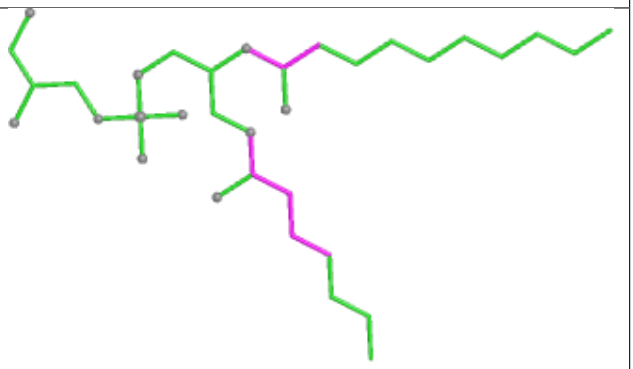


Rings

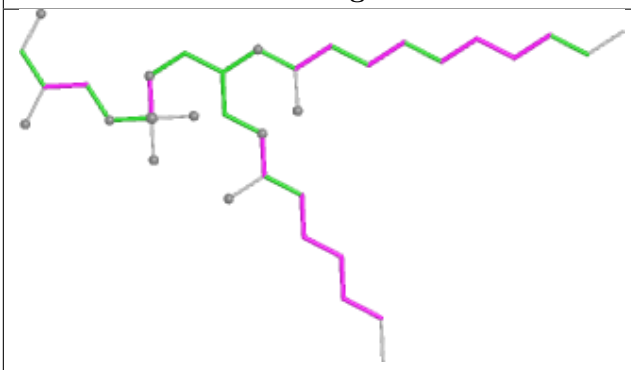
Ligand LHG O 318



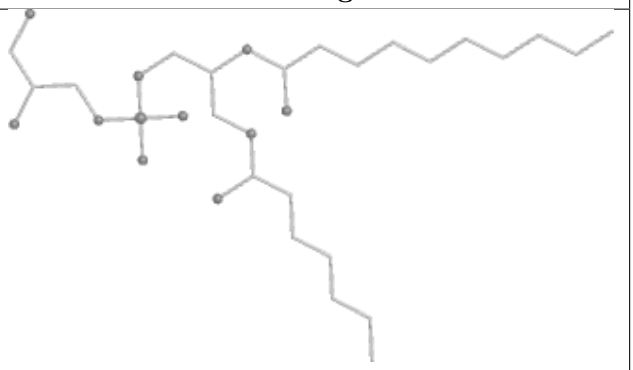
Bond lengths



Bond angles



Torsions

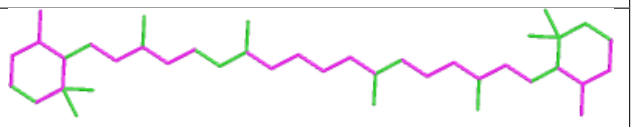


Rings

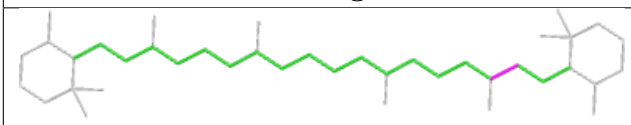
Ligand BCR B 845



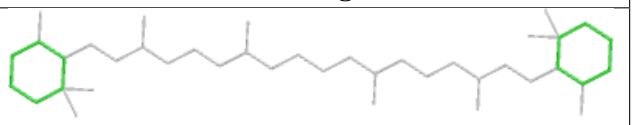
Bond lengths



Bond angles

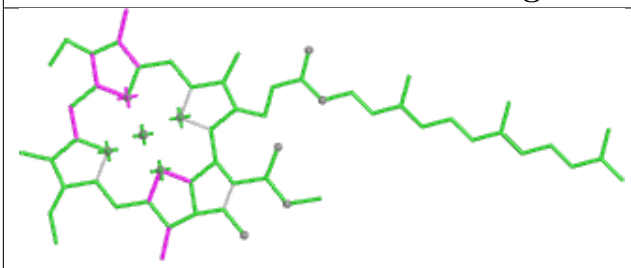


Torsions

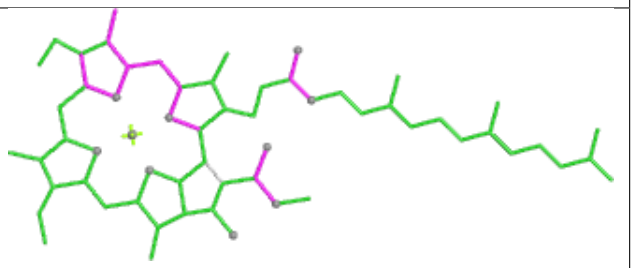


Rings

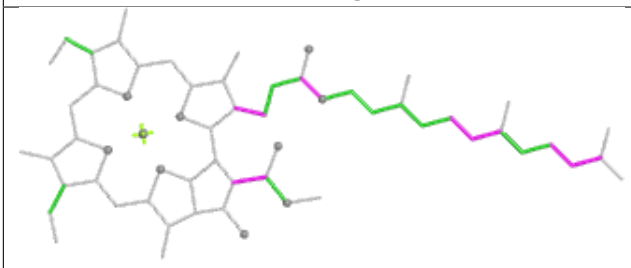
Ligand CLA K 602



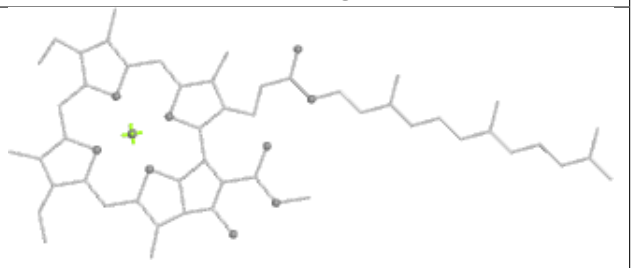
Bond lengths



Bond angles

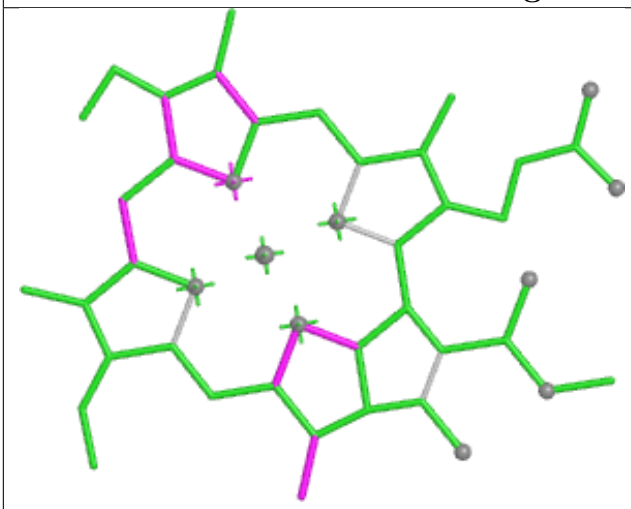


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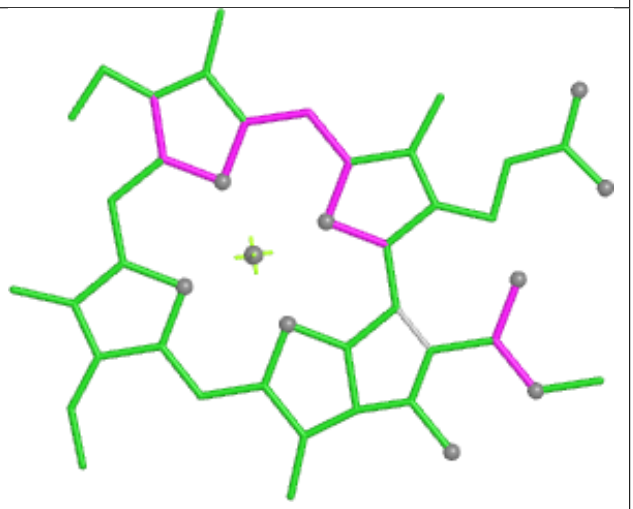


Rings

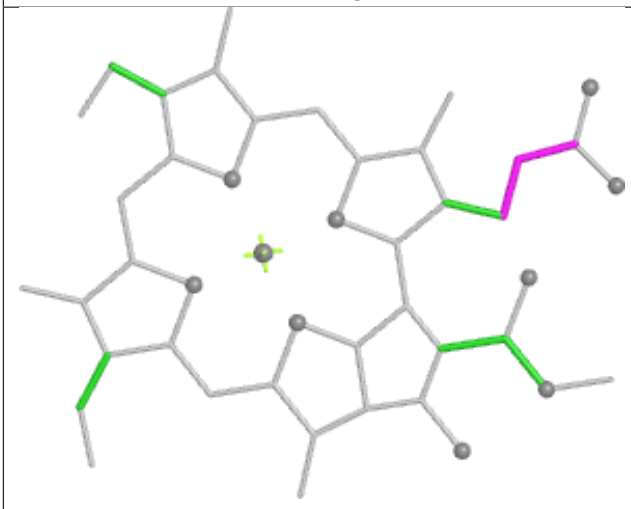
Ligand CLA O 307



Bond lengths



Bond angles

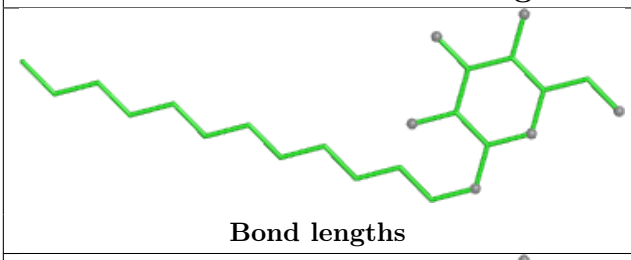


Torsions

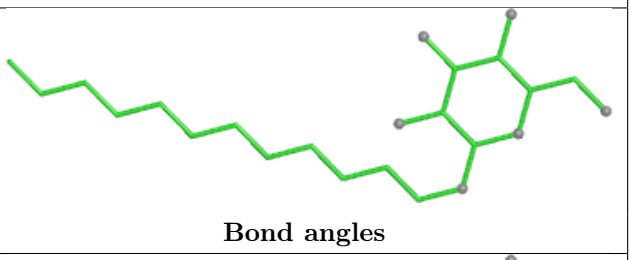


Rings

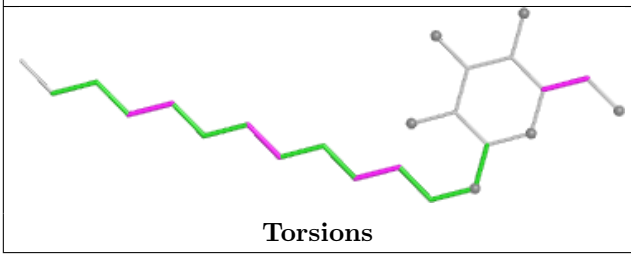
Ligand LMU W 421



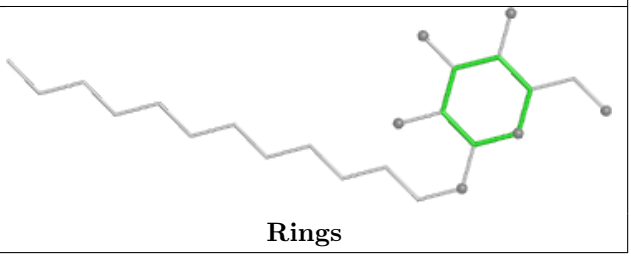
Bond lengths



Bond angles

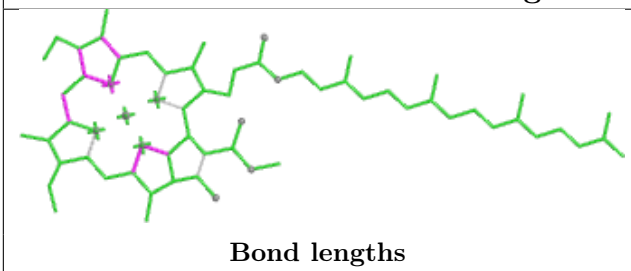


Torsions

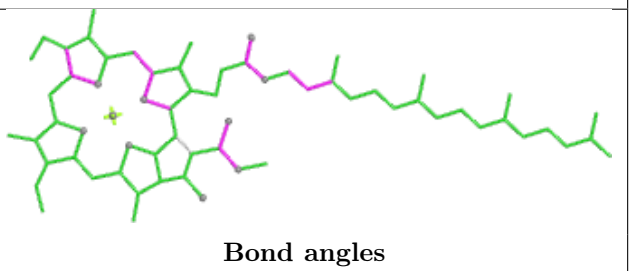


Rings

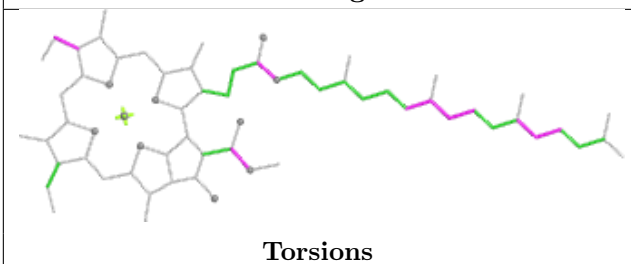
Ligand CLA R 615



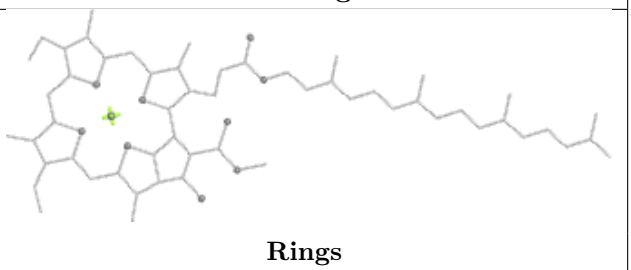
Bond lengths



Bond angles

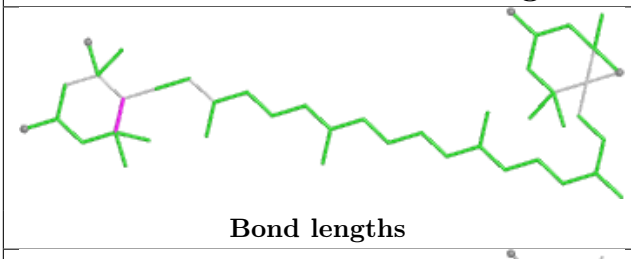


Torsions

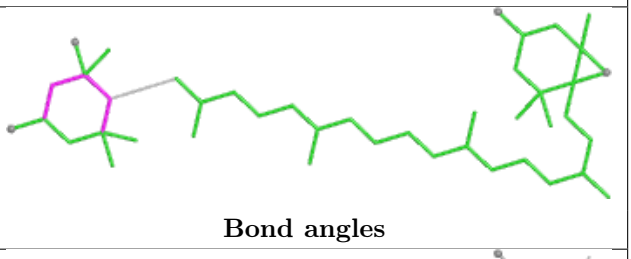


Rings

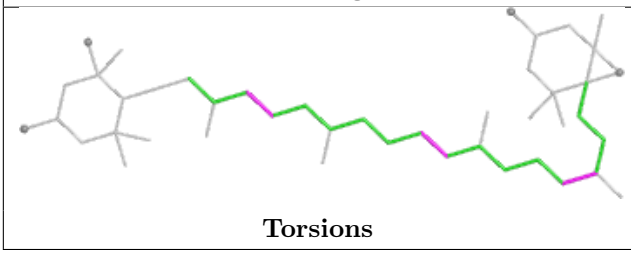
Ligand NEX U 418



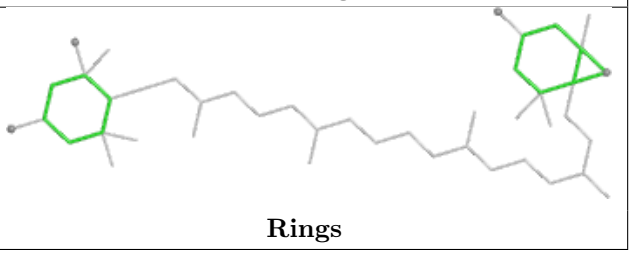
Bond lengths



Bond angles

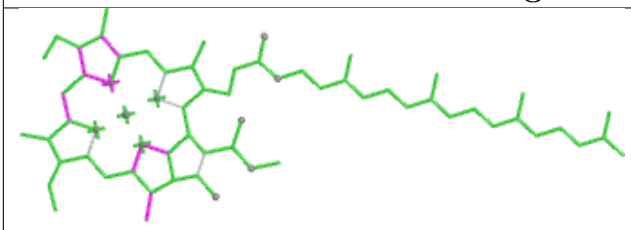


Torsions

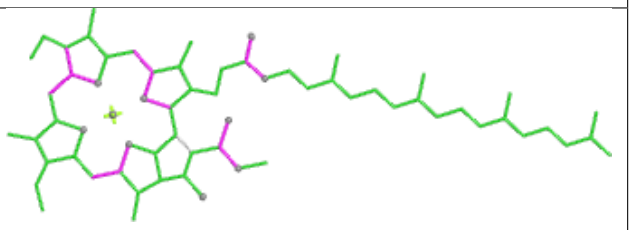


Rings

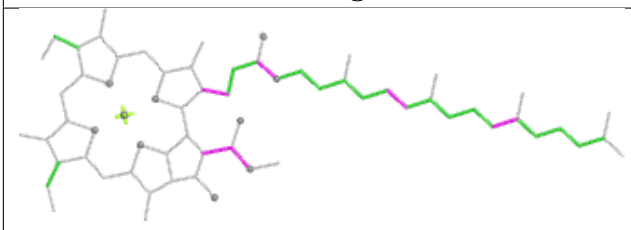
Ligand CLA B 827



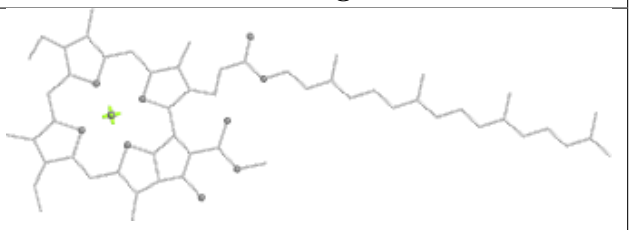
Bond lengths



Bond angles

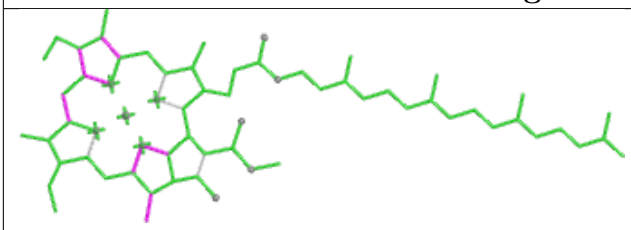


Torsions

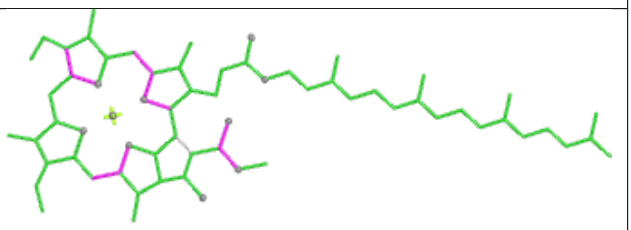


Rings

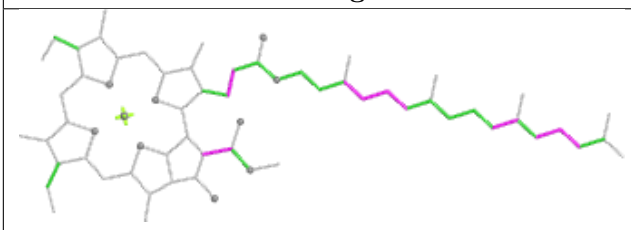
Ligand CLA A 814



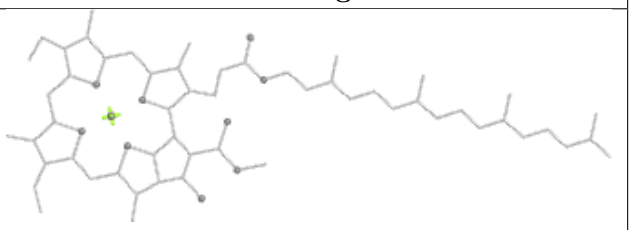
Bond lengths



Bond angles

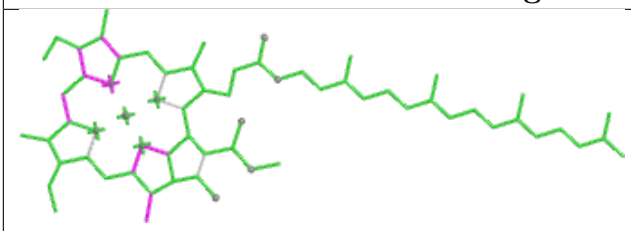


Torsions

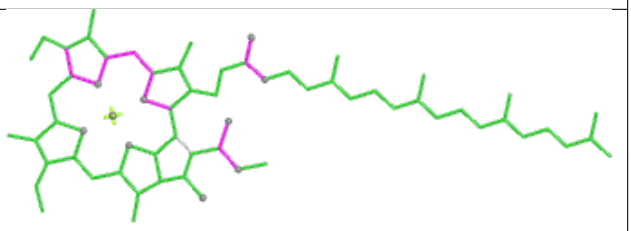


Rings

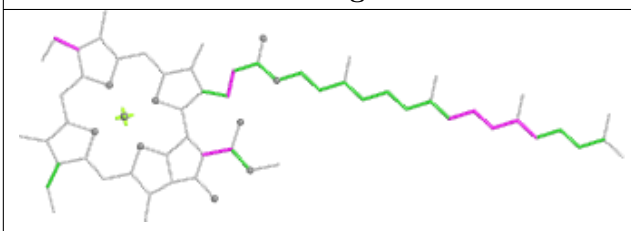
Ligand CLA X 403



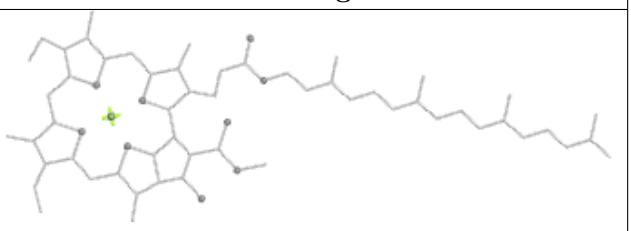
Bond lengths



Bond angles

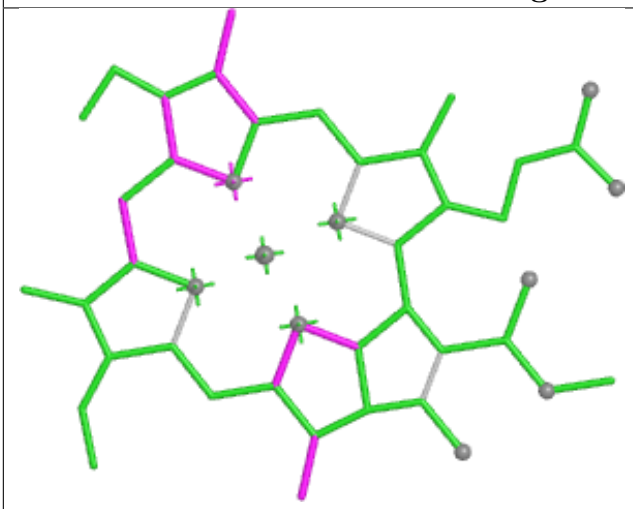


Torsions

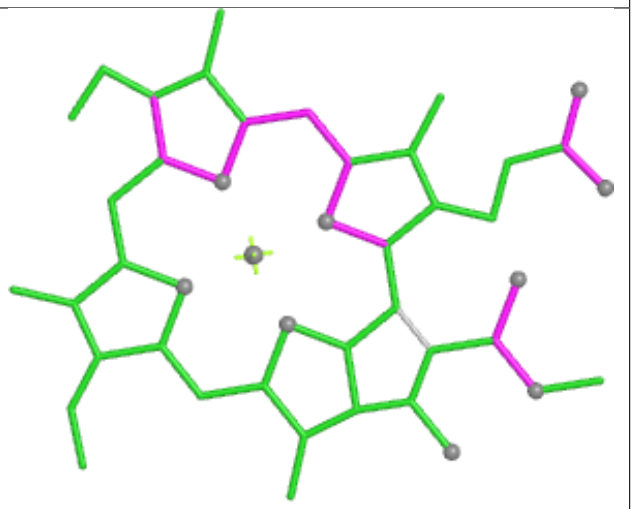


Rings

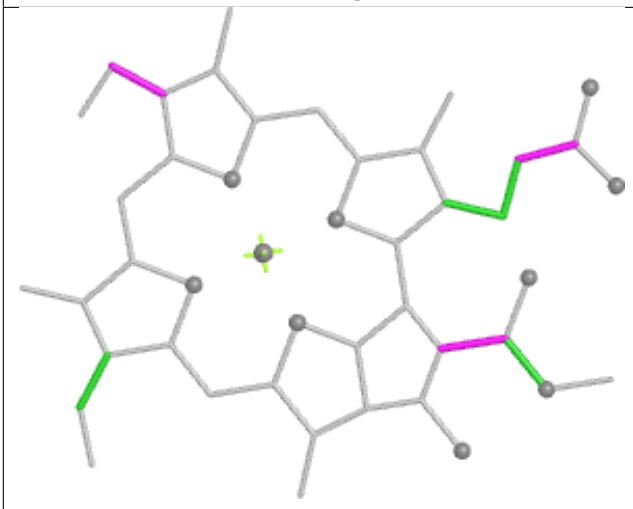
Ligand CLA I 608



Bond lengths



Bond angles

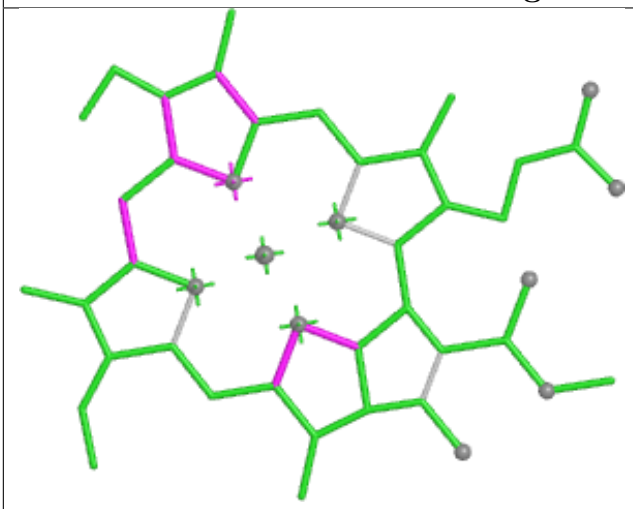


Torsions

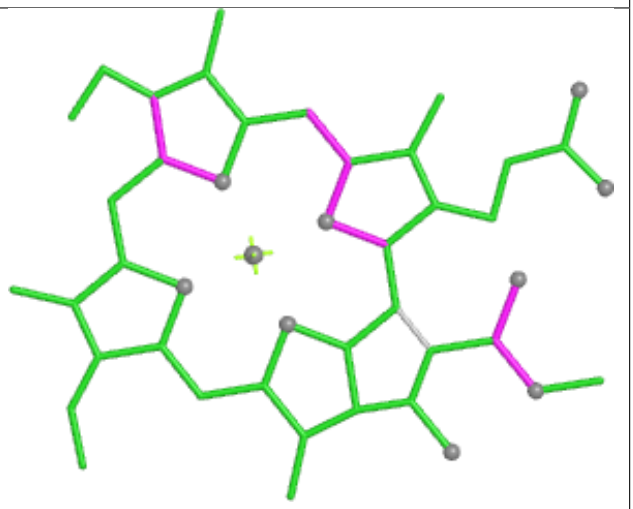


Rings

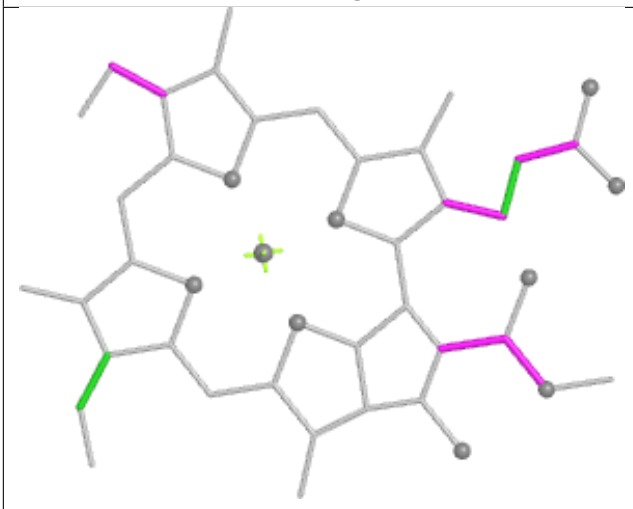
Ligand CLA V 617



Bond lengths



Bond angles

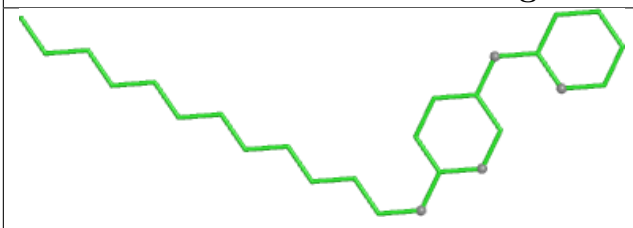


Torsions

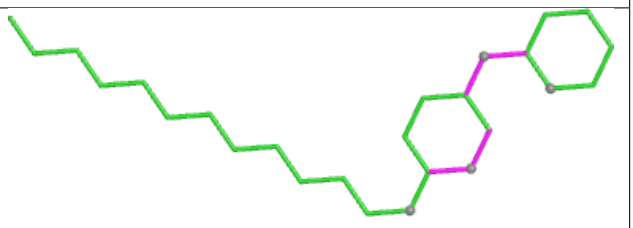


Rings

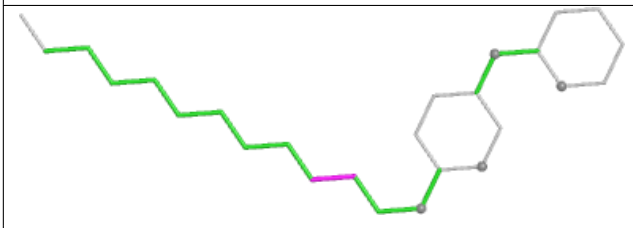
Ligand LMU O 320



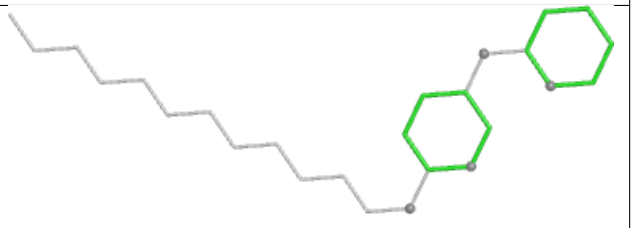
Bond lengths



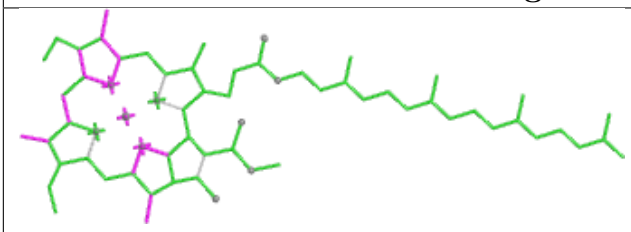
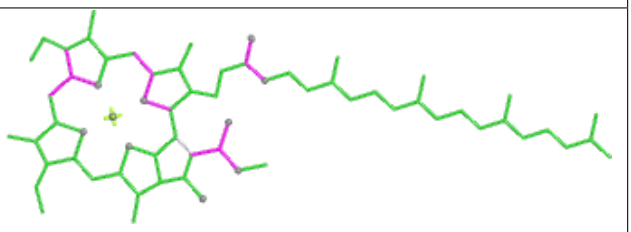
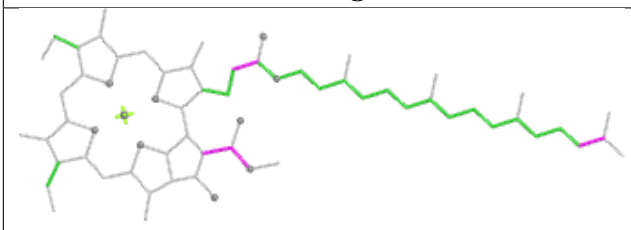
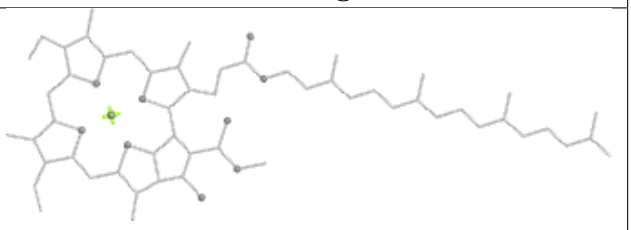
Bond angles

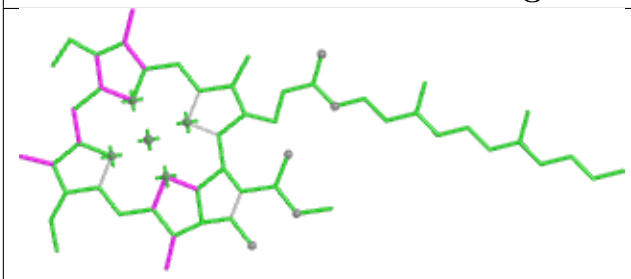
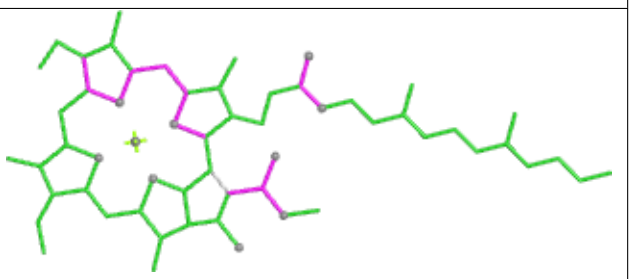
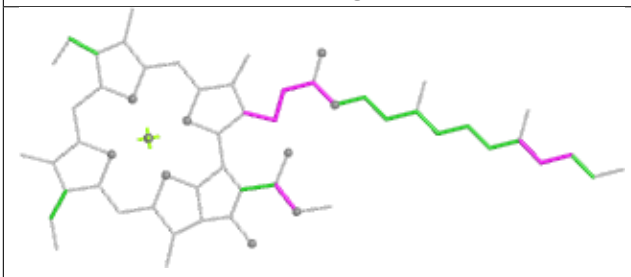
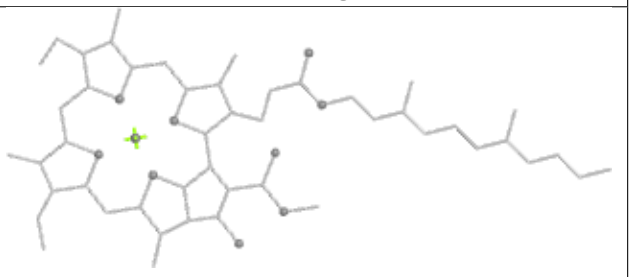


Torsions

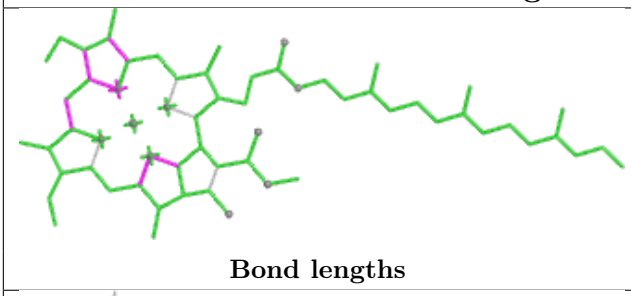


Rings

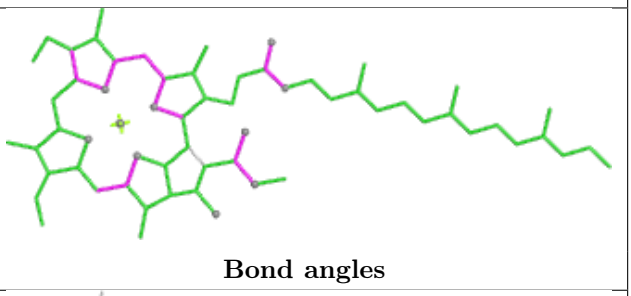
Ligand CLA B 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

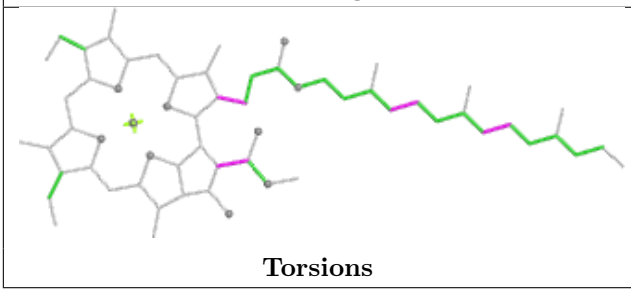
Ligand CLA A 827



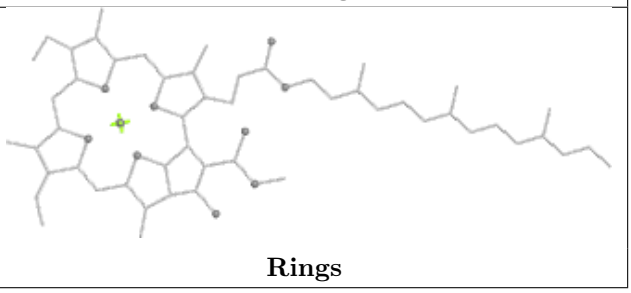
Bond lengths



Bond angles

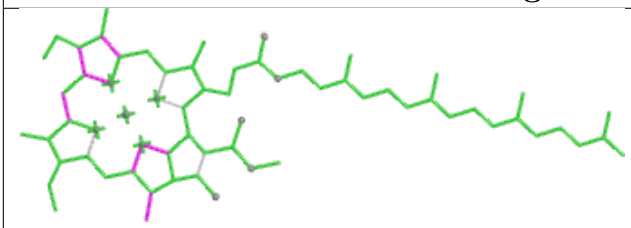


Torsions

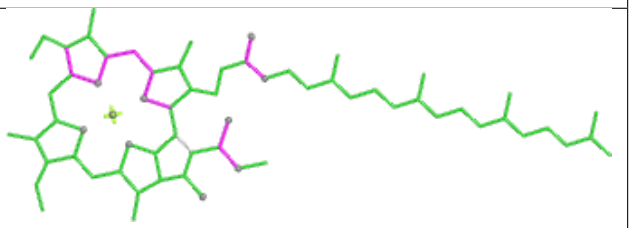


Rings

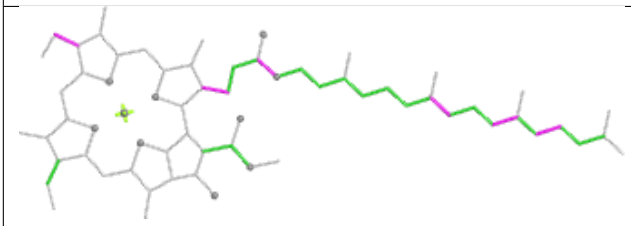
Ligand CLA A 813



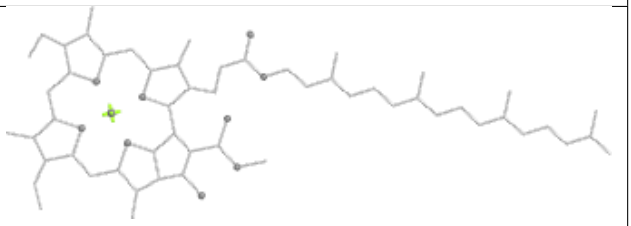
Bond lengths



Bond angles

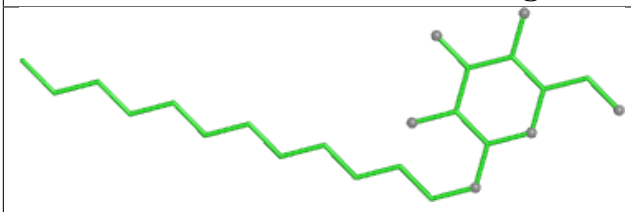


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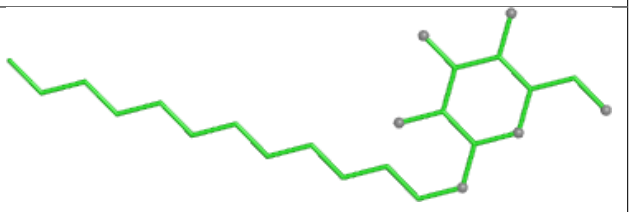


Rings

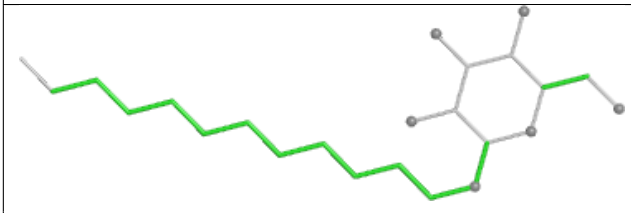
Ligand LMU L 418



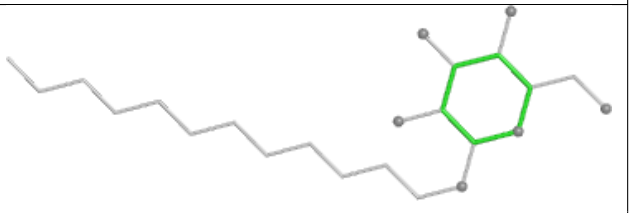
Bond lengths



Bond angles

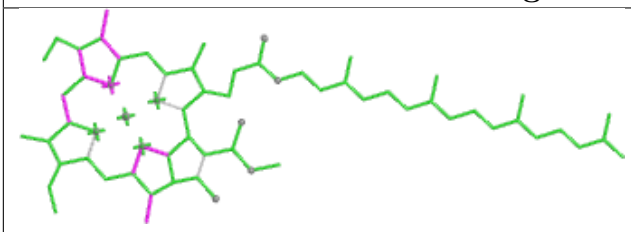


Torsions

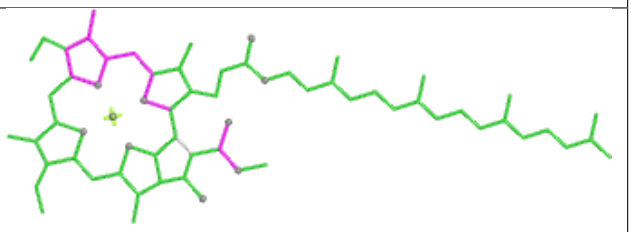


Rings

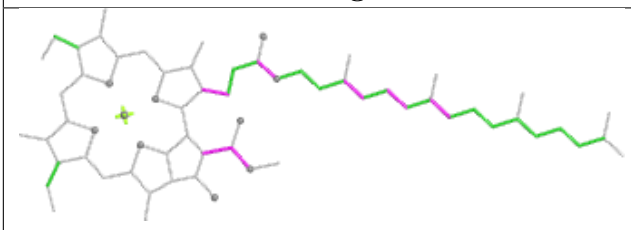
Ligand CLA K 617



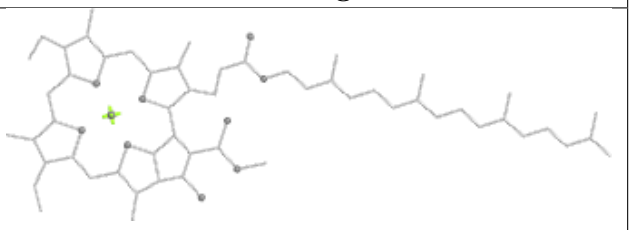
Bond lengths



Bond angles

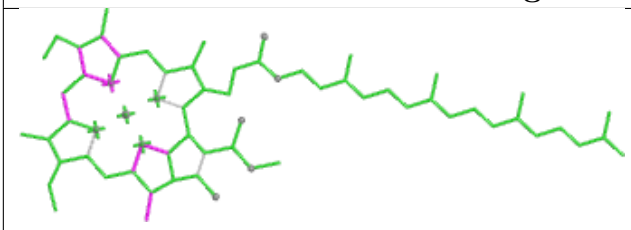


Torsions

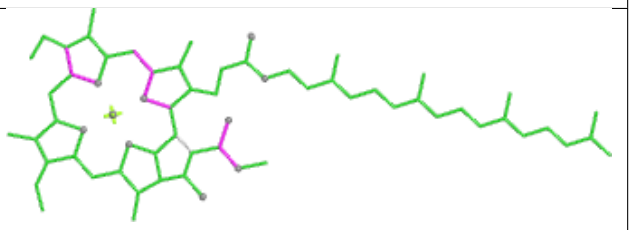


Rings

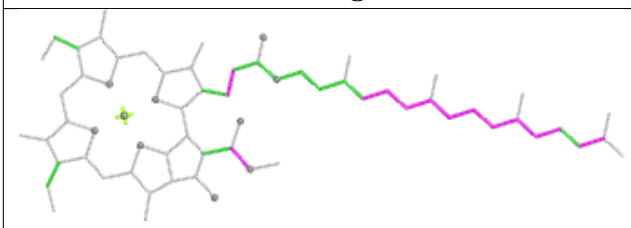
Ligand CLA O 313



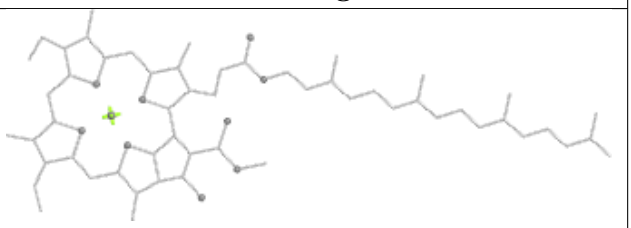
Bond lengths



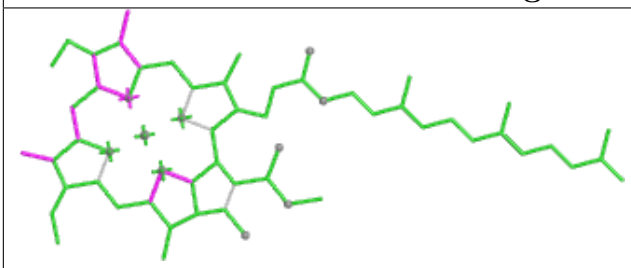
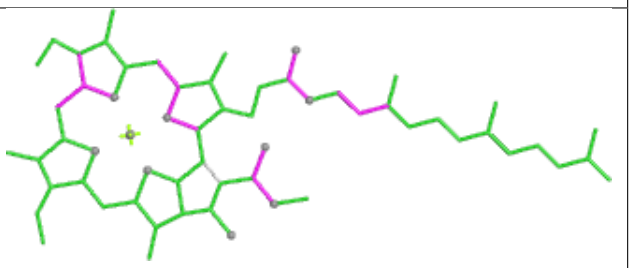
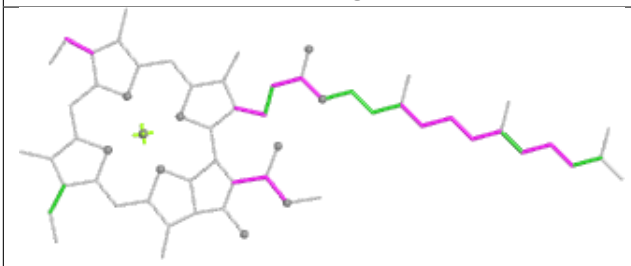
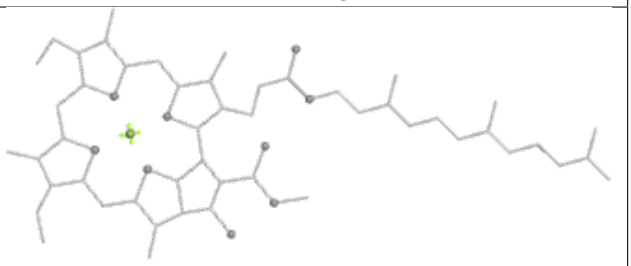
Bond angles

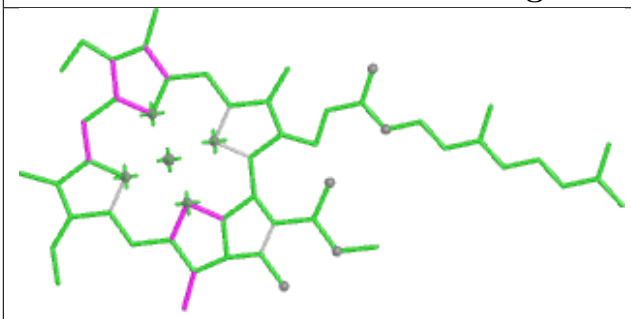
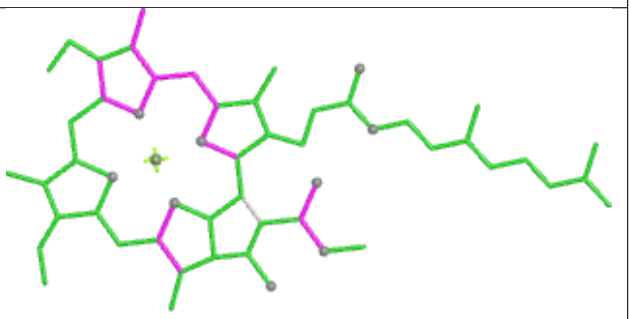
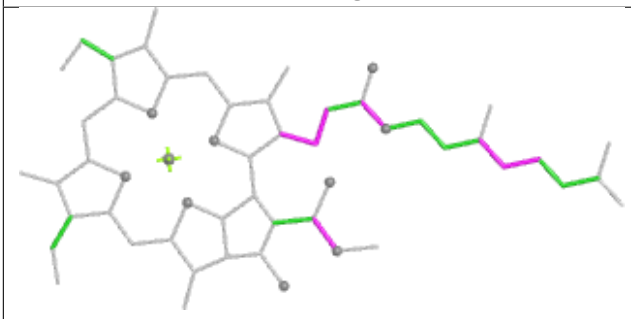
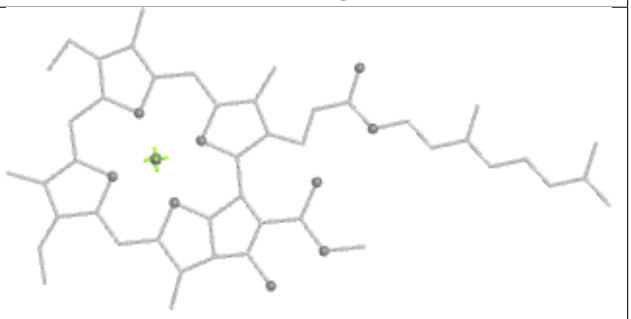


Torsions

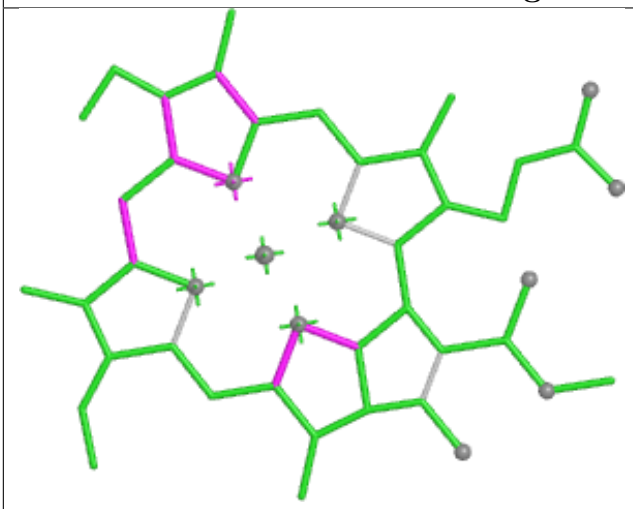


Rings

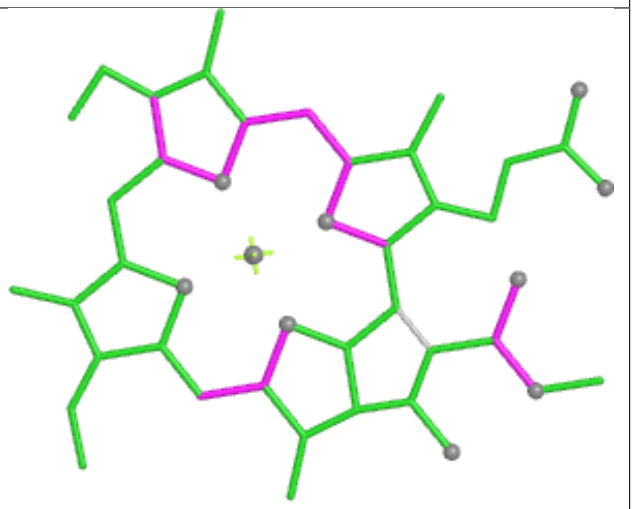
Ligand CLA R 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

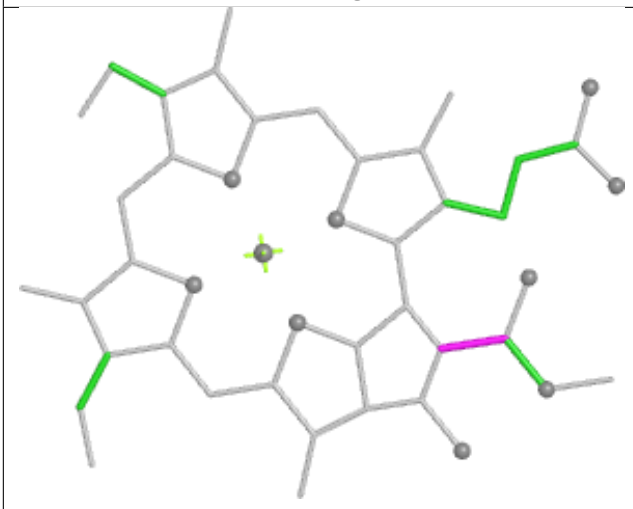
Ligand CLA O 319



Bond lengths



Bond angles

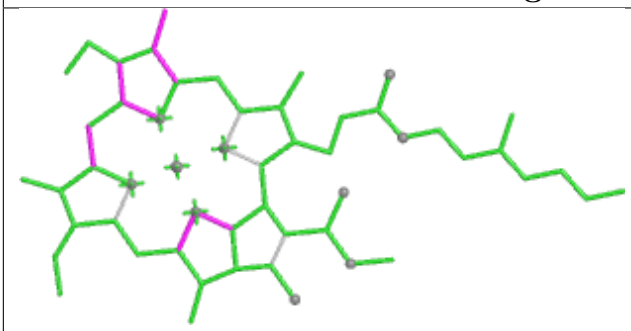


Torsions

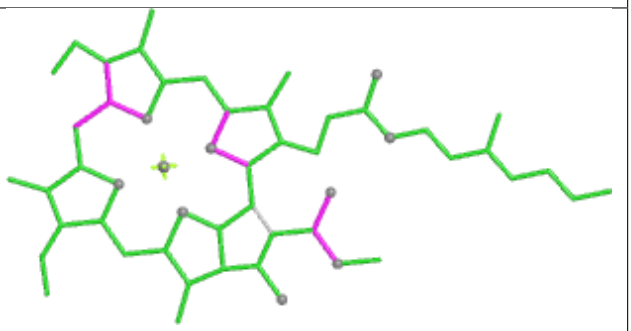


Rings

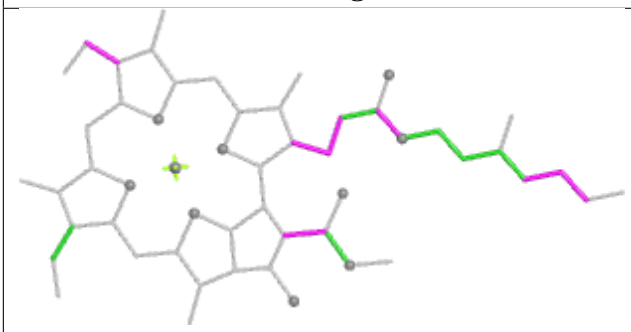
Ligand CLA B 819



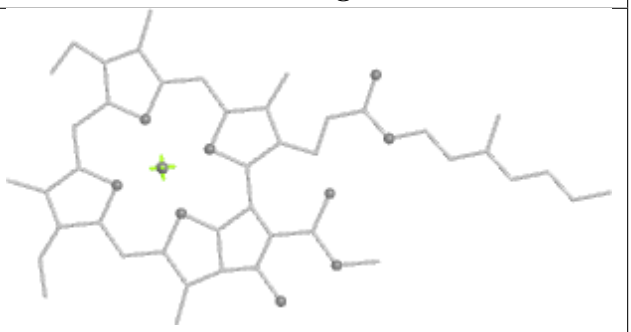
Bond lengths



Bond angles

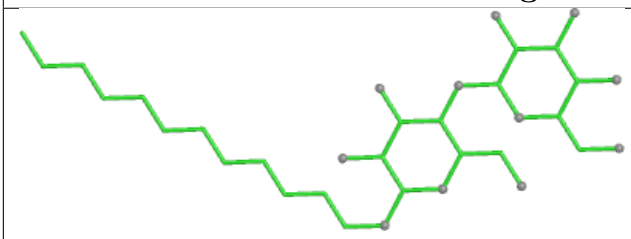


Torsions

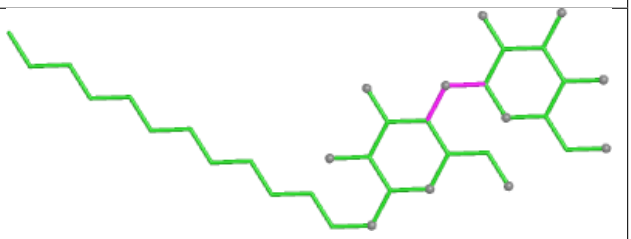


Rings

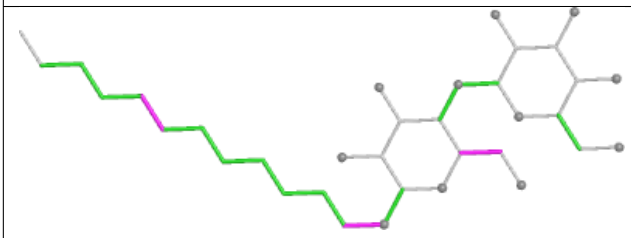
Ligand LMU B 857



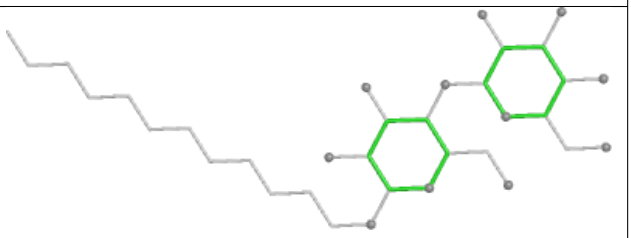
Bond lengths



Bond angles

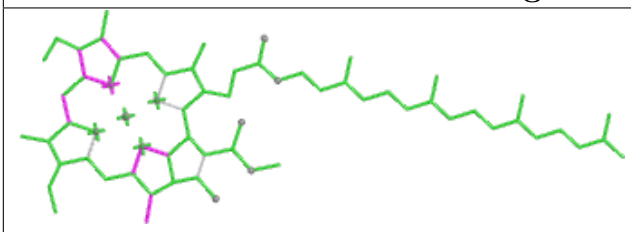


Torsions

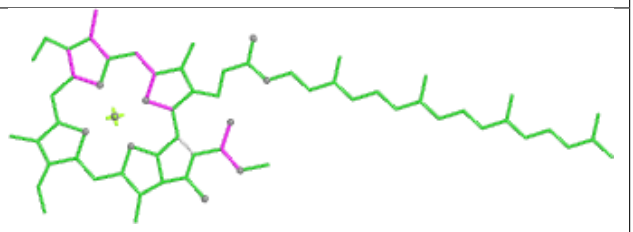


Rings

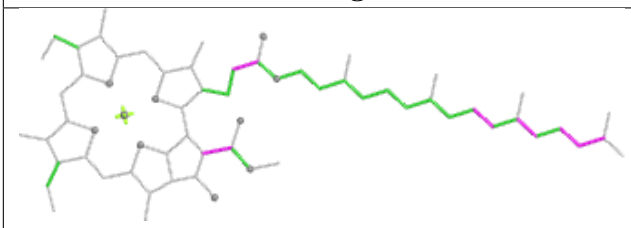
Ligand CLA A 826



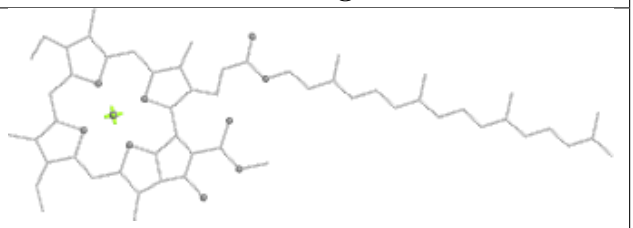
Bond lengths



Bond angles

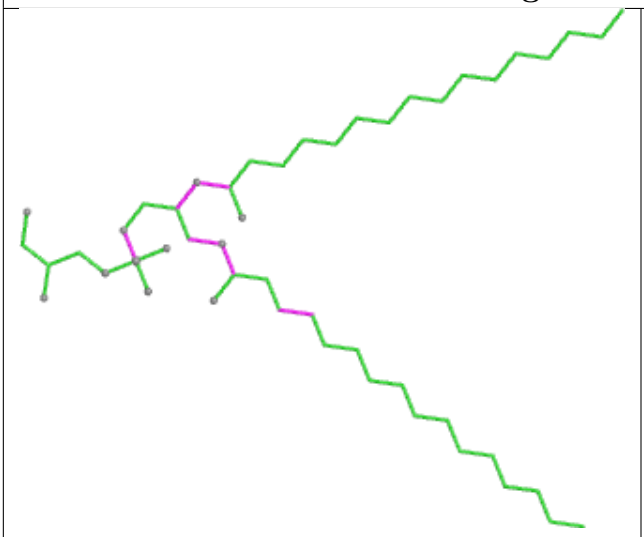


Torsions

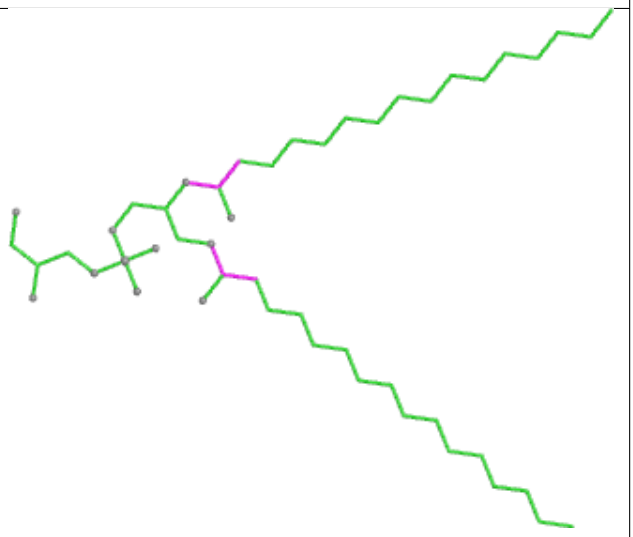


Rings

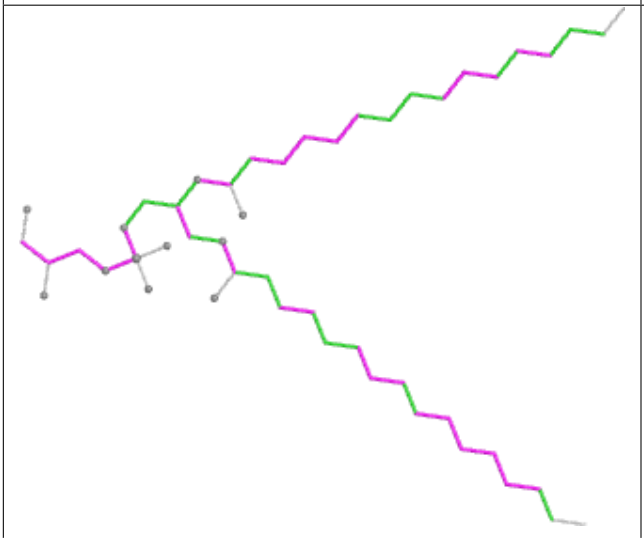
Ligand LHG O 321



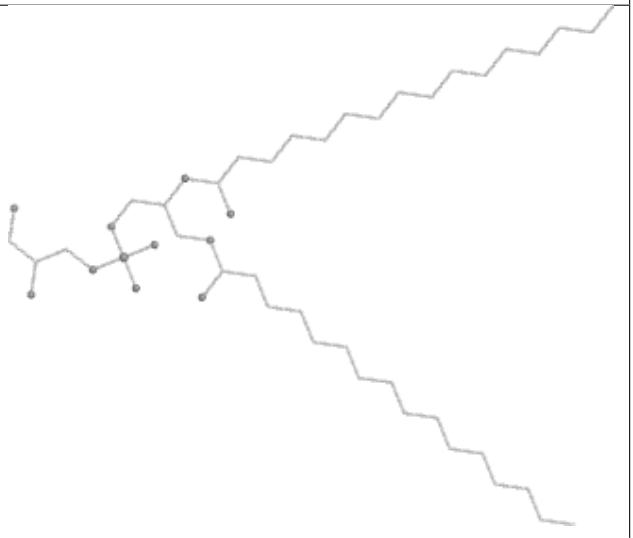
Bond lengths



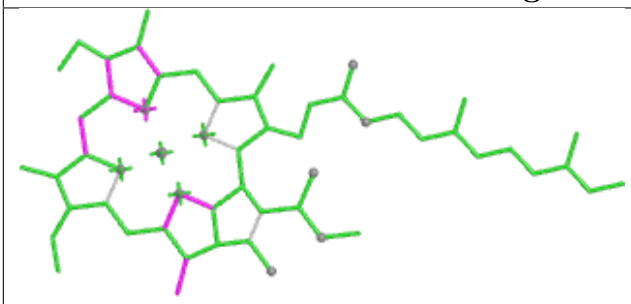
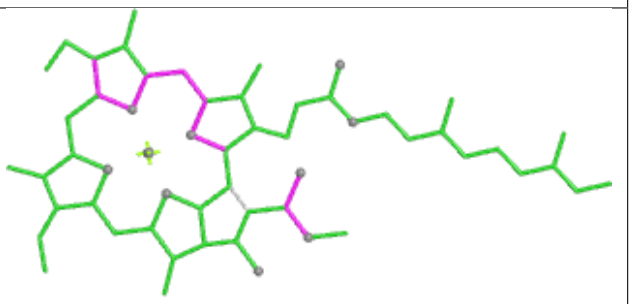
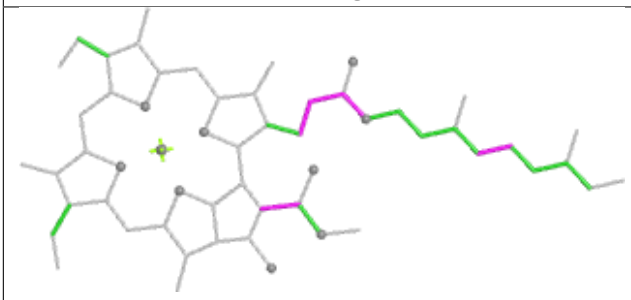
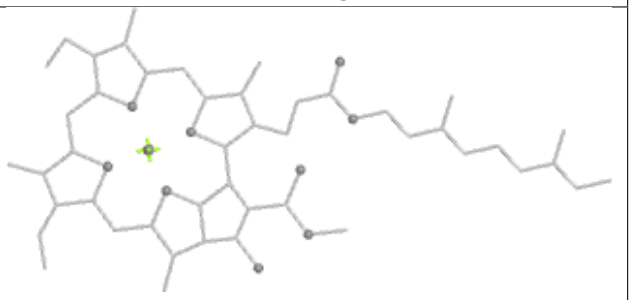
Bond angles

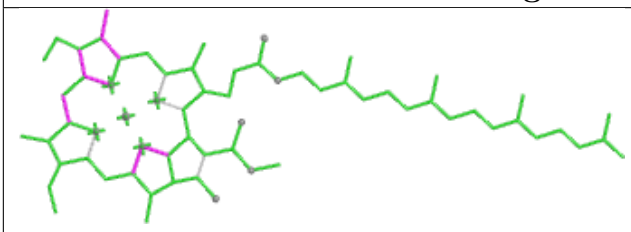
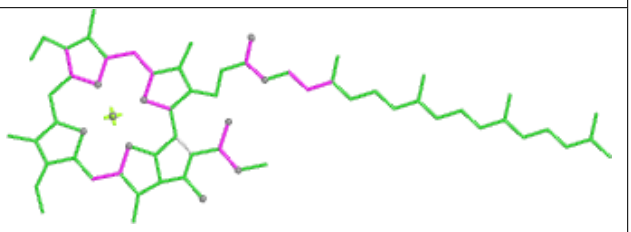
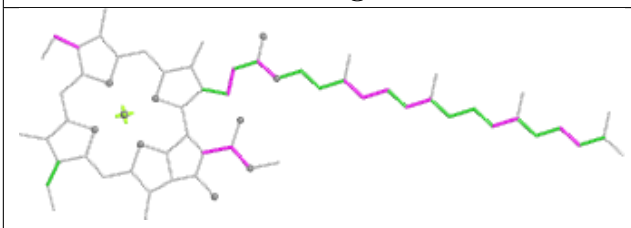
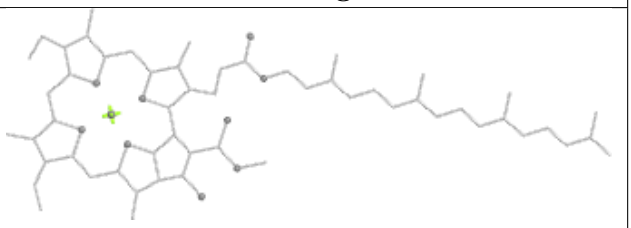


Torsions

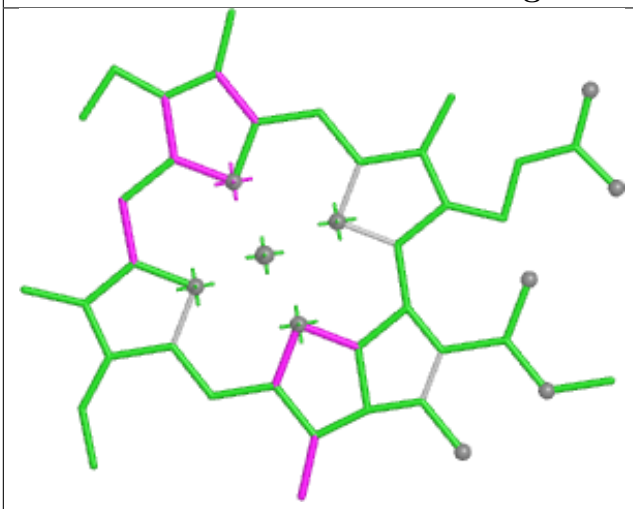


Rings

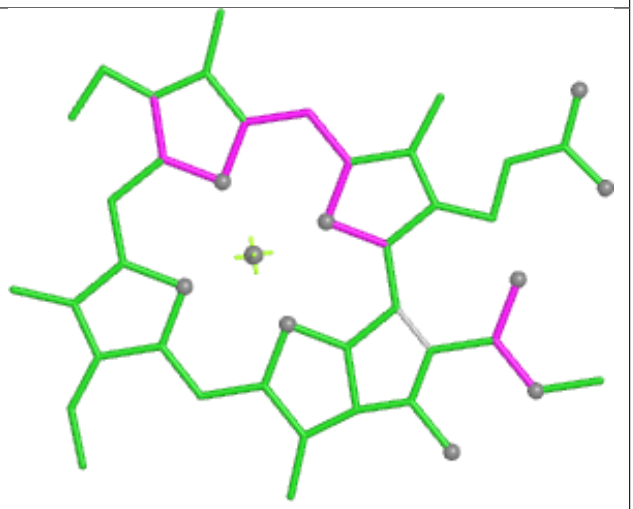
Ligand CLA K 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

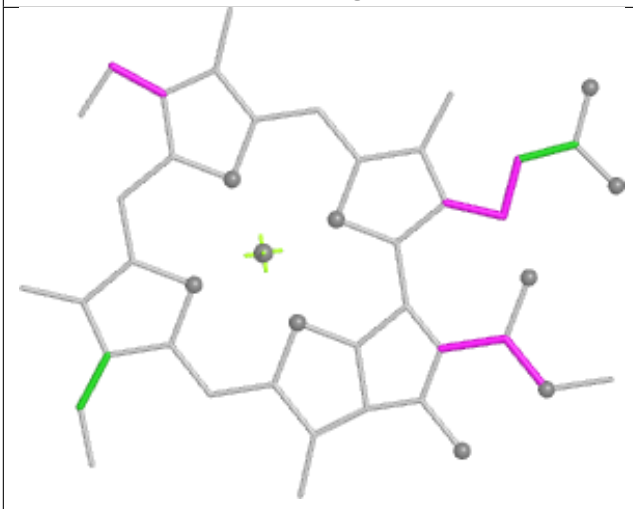
Ligand CLA U 420



Bond lengths



Bond angles

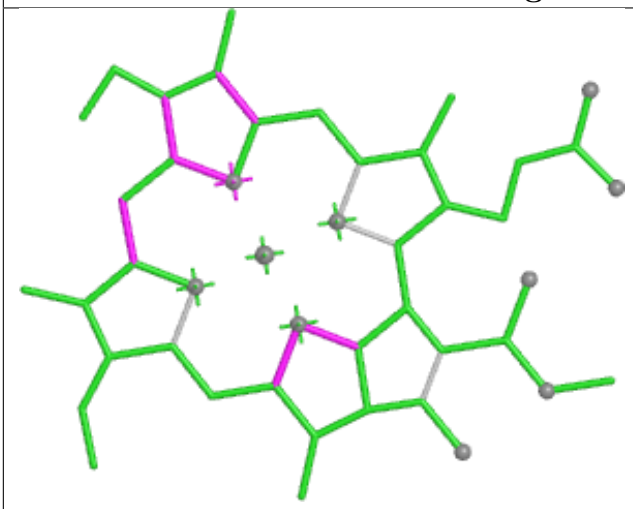


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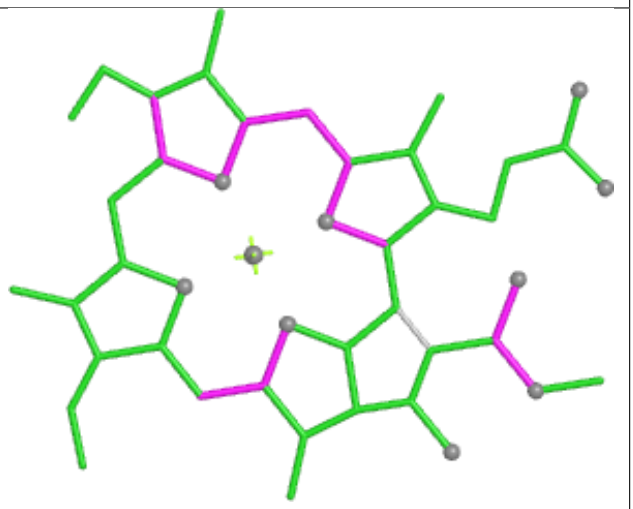


Rings

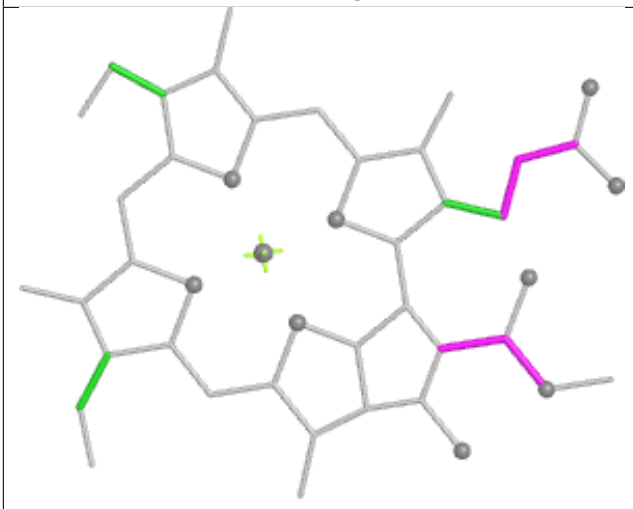
Ligand CLA P 604



Bond lengths



Bond angles

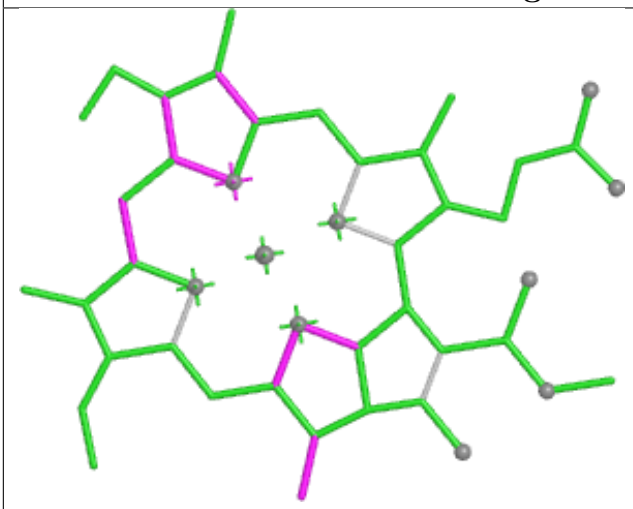


Torsions

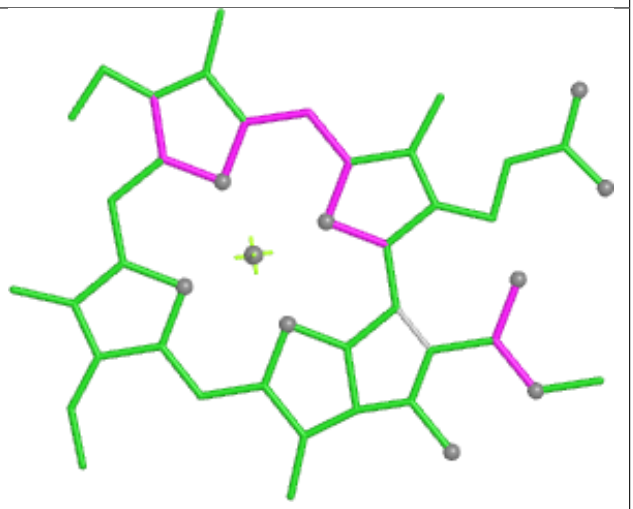


Rings

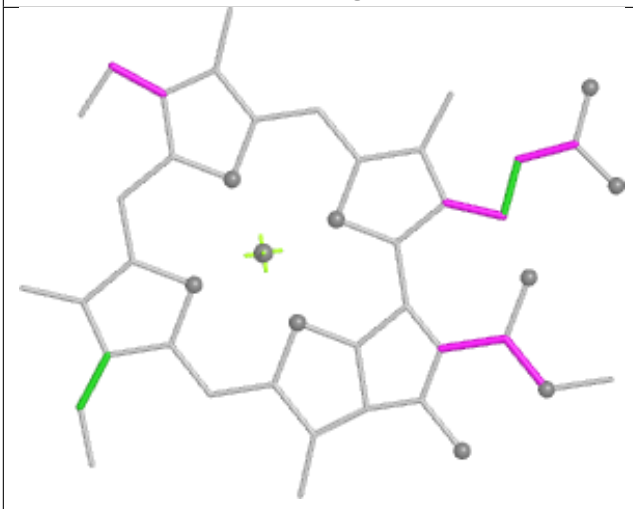
Ligand CLA X 419



Bond lengths



Bond angles

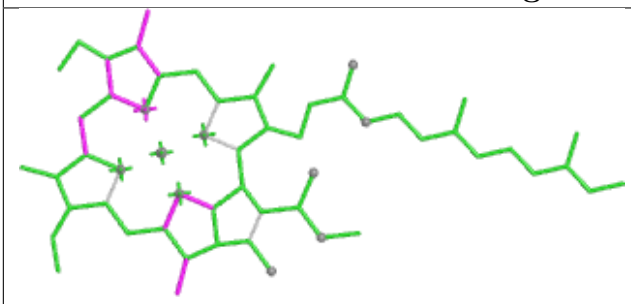


Torsions

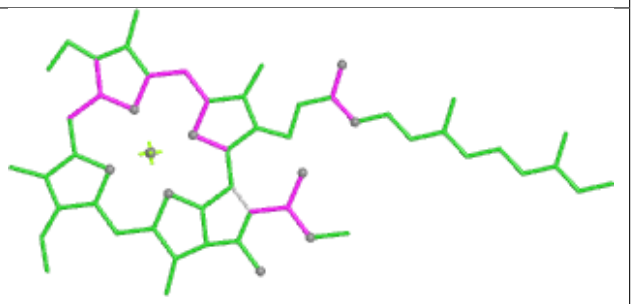


Rings

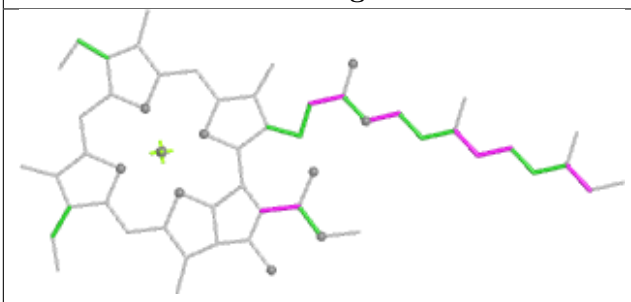
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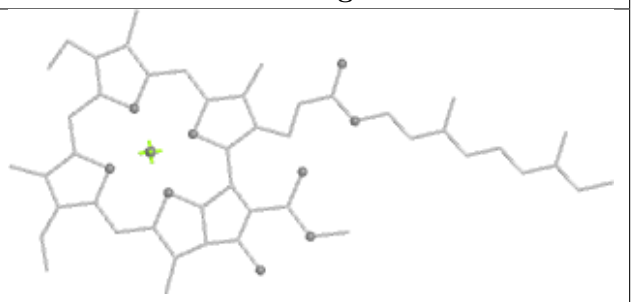
Bond lengths



Bond angles

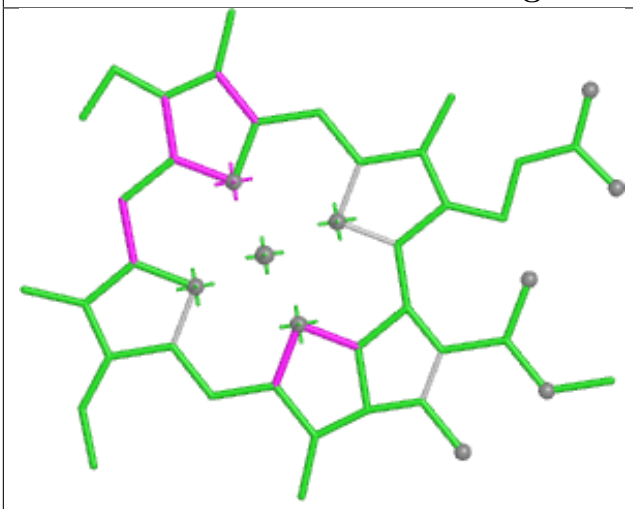


Torsions

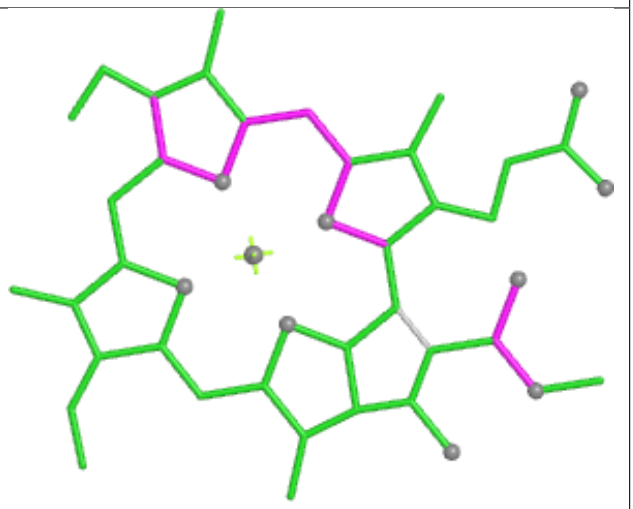


Rings

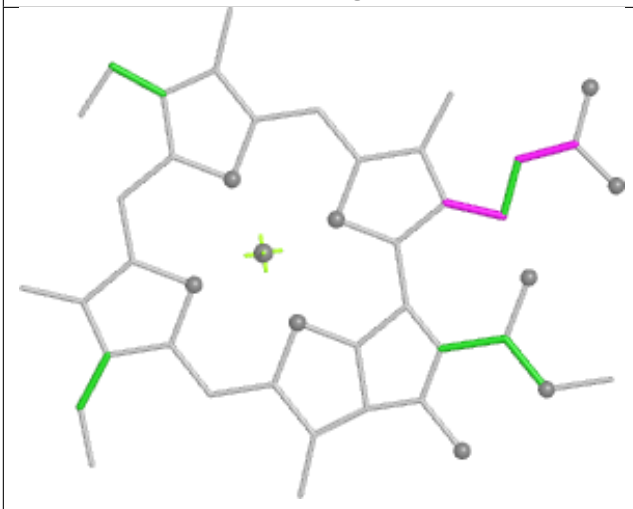
Ligand CLA H 312



Bond lengths



Bond angles

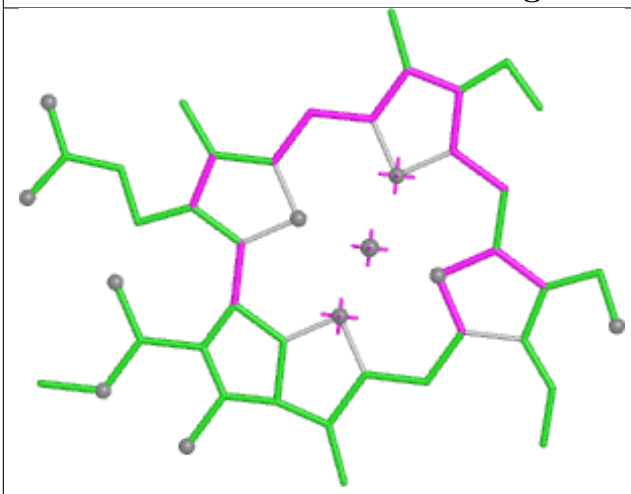


Torsions

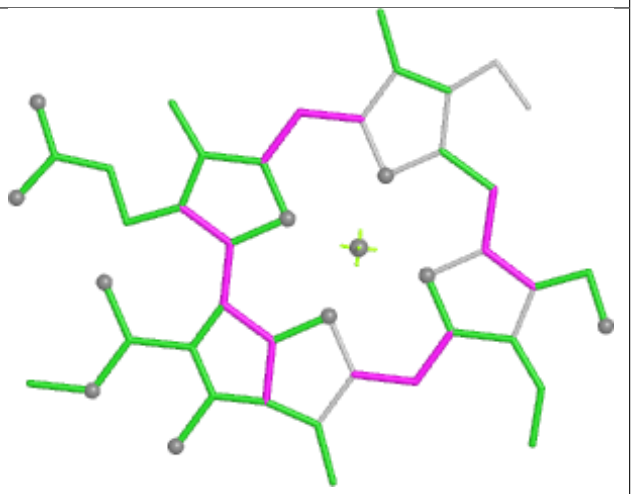


Rings

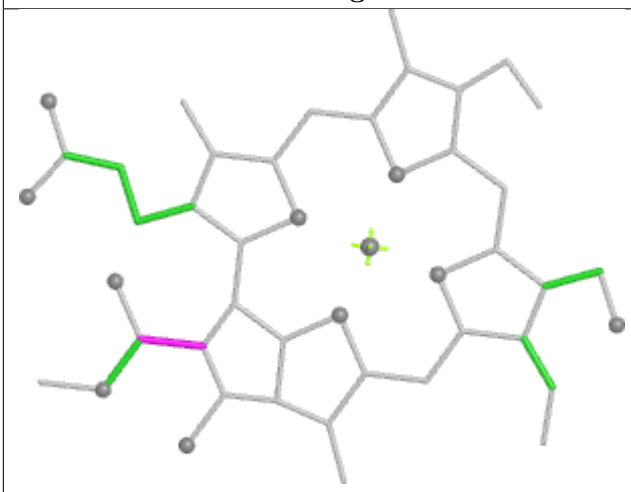
Ligand CHL V 606



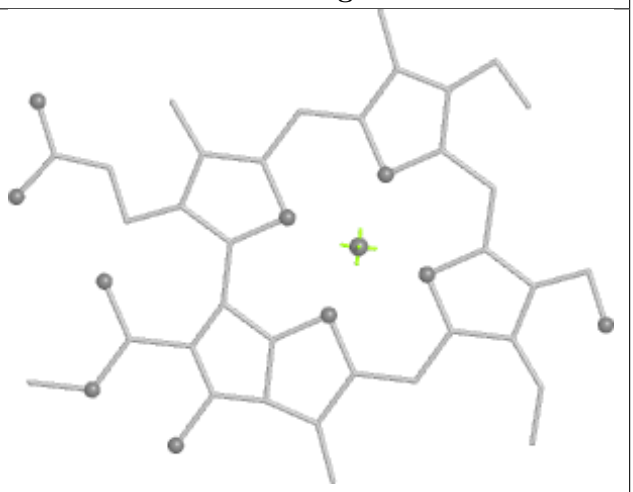
Bond lengths



Bond angles

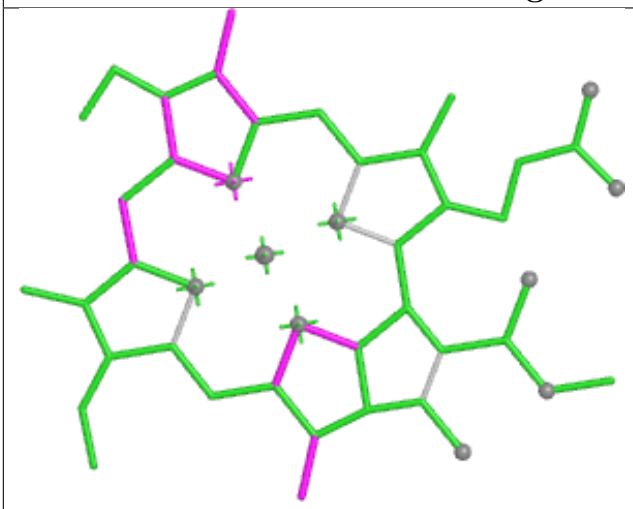


Torsions

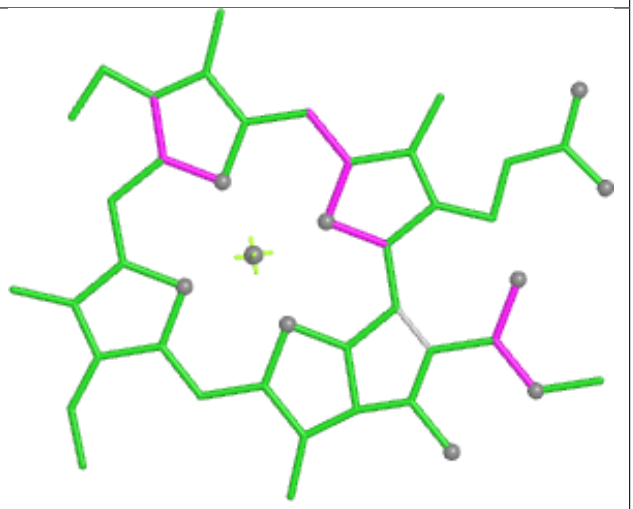


Rings

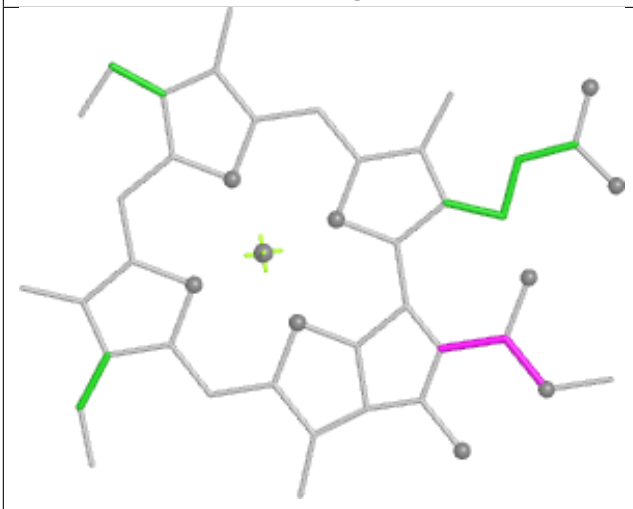
Ligand CLA L 405



Bond lengths



Bond angles

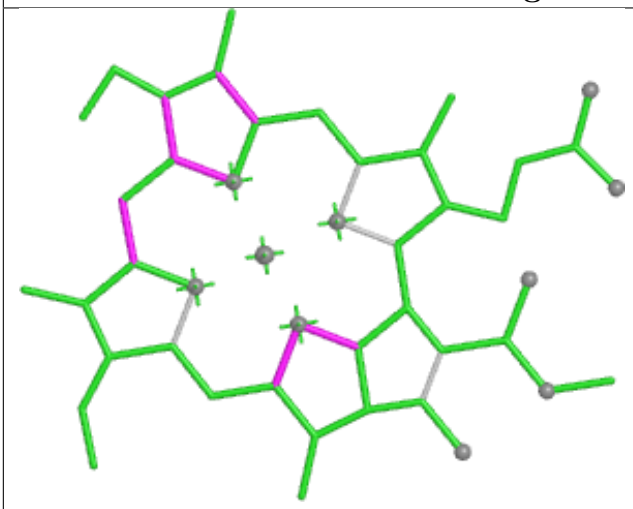


Torsions

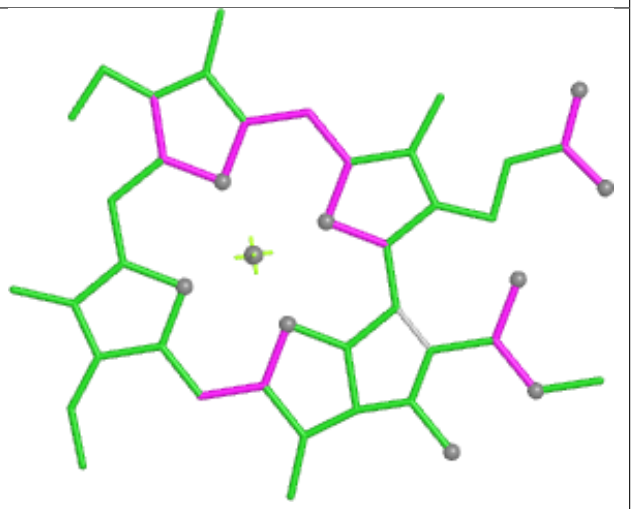


Rings

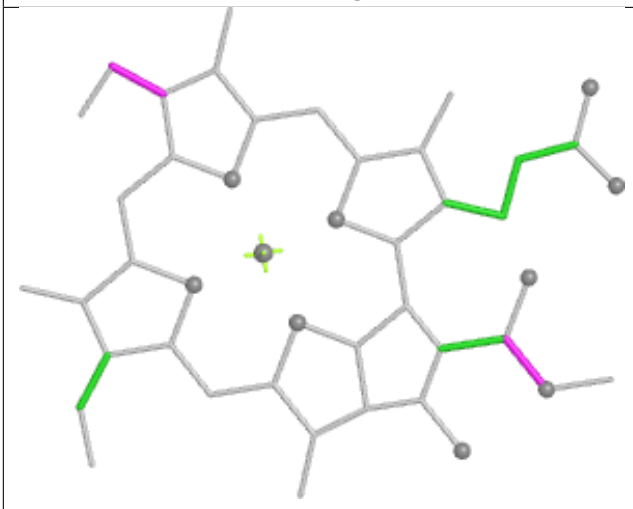
Ligand CLA V 610



Bond lengths



Bond angles

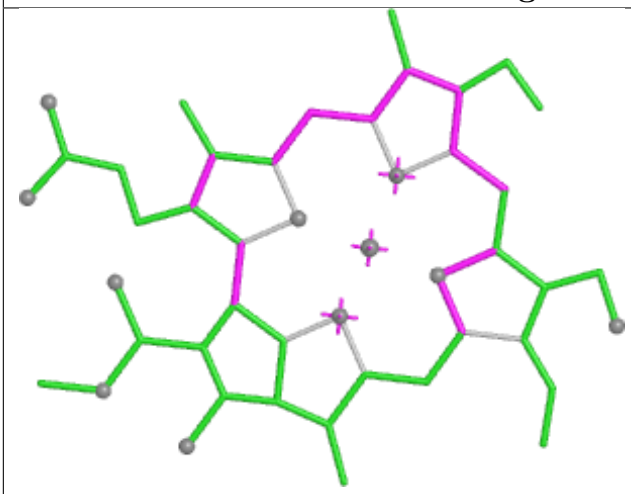


Torsions

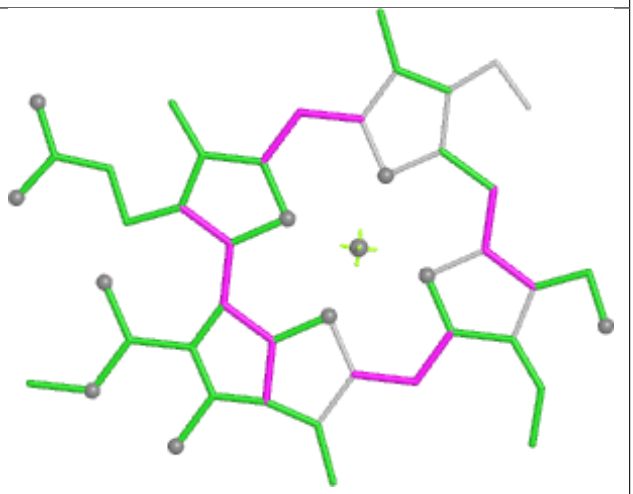


Rings

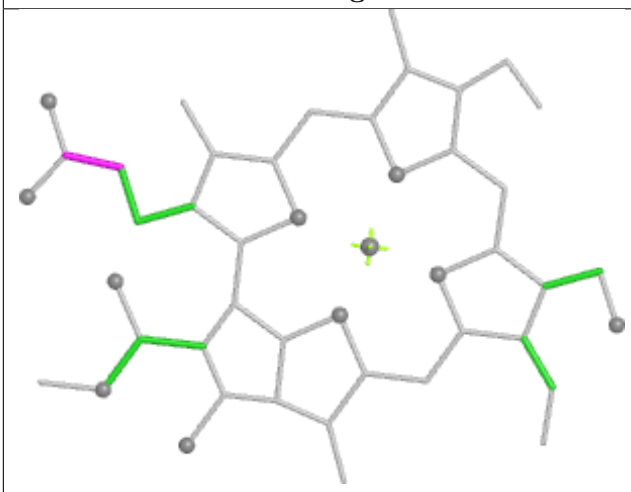
Ligand CHL W 407



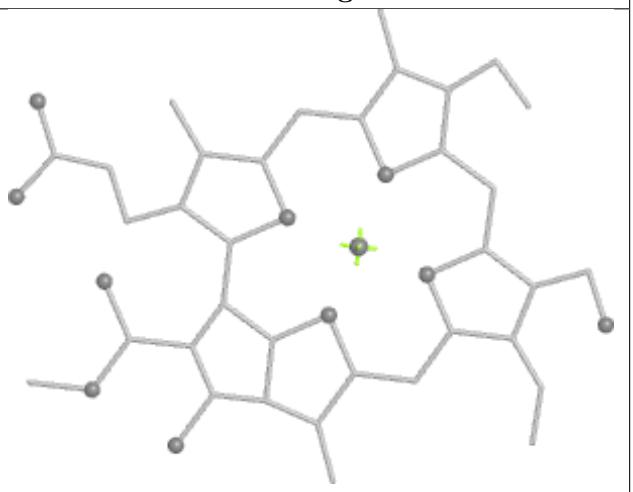
Bond lengths



Bond angles

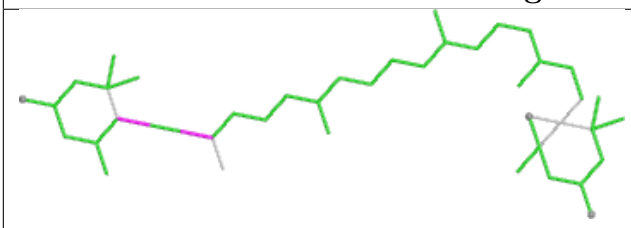


Torsions

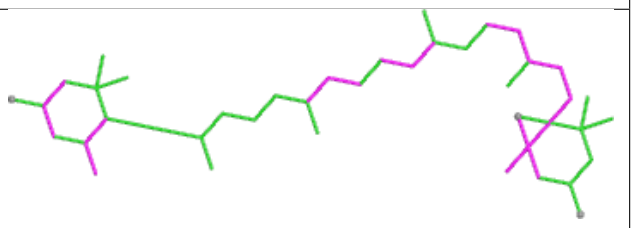


Rings

Ligand DD6 X 415



Bond lengths



Bond angles

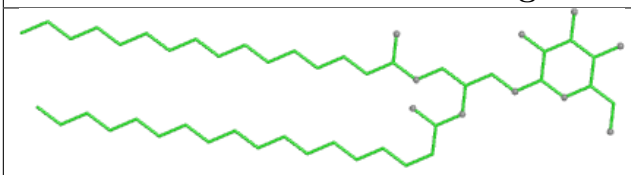


Torsions

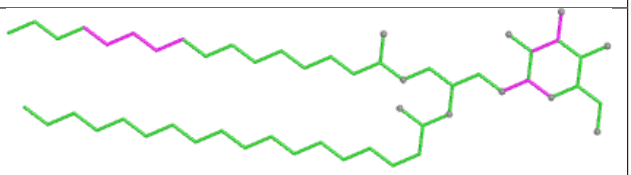


Rings

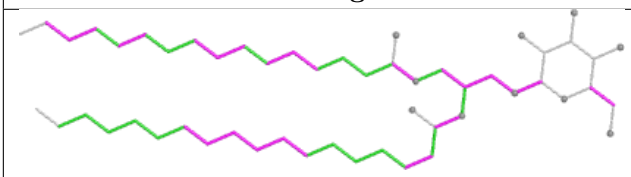
Ligand LMG U 402



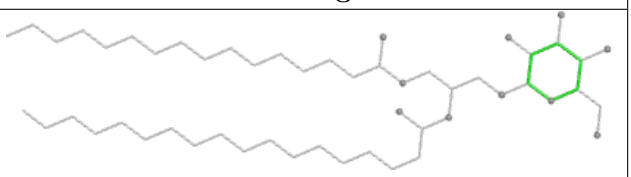
Bond lengths



Bond angles

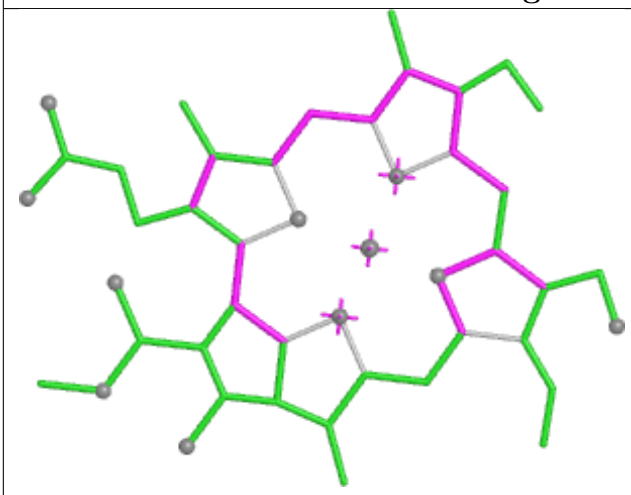


Torsions

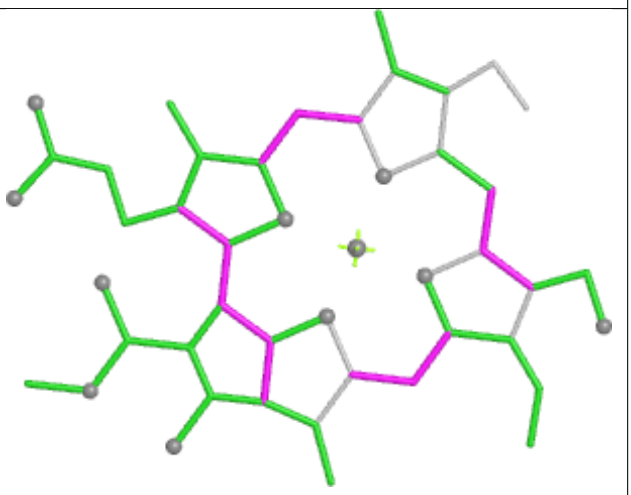


Rings

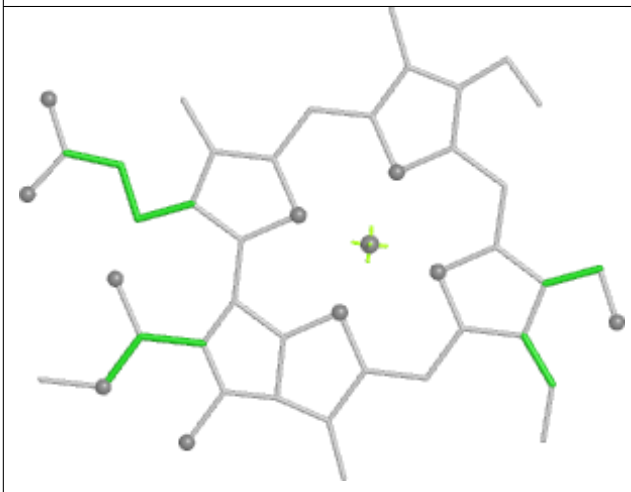
Ligand CHL U 407



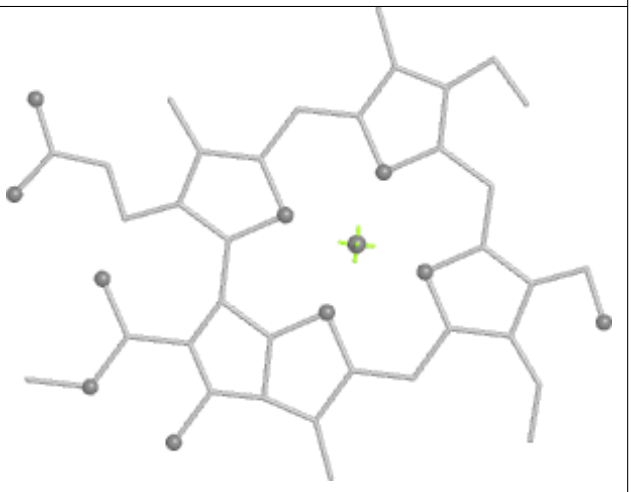
Bond lengths



Bond angles

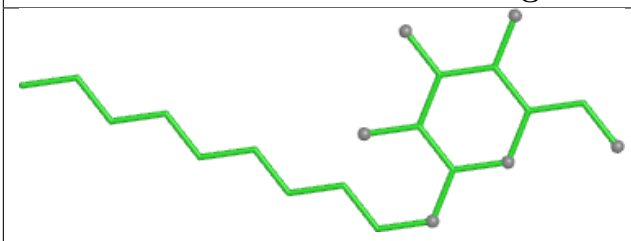


Torsions

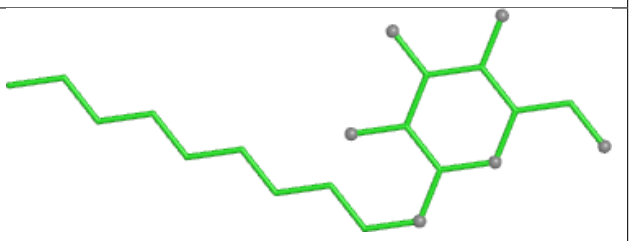


Rings

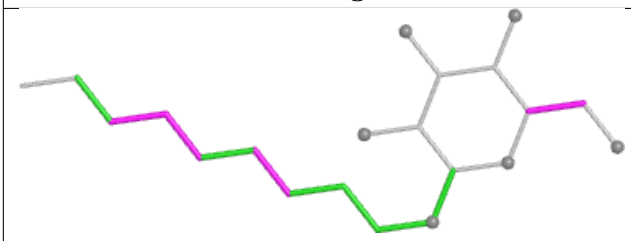
Ligand LMU F 409



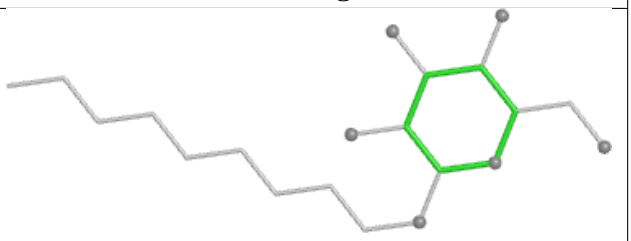
Bond lengths



Bond angles

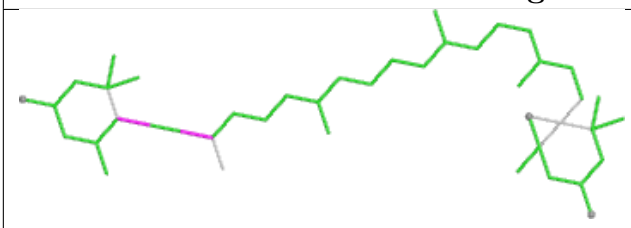


Torsions

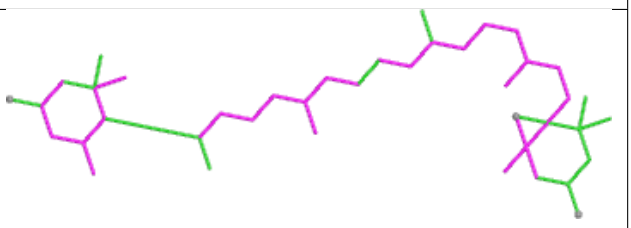


Rings

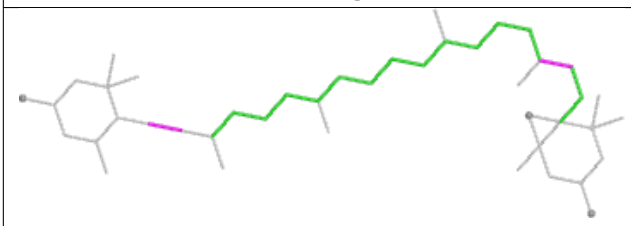
Ligand DD6 L 415



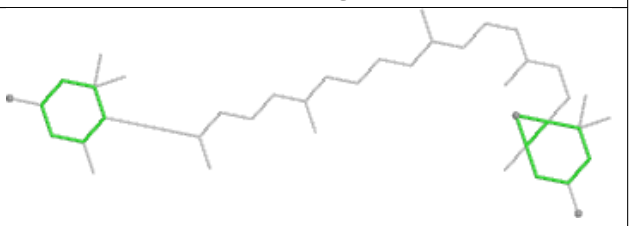
Bond lengths



Bond angles

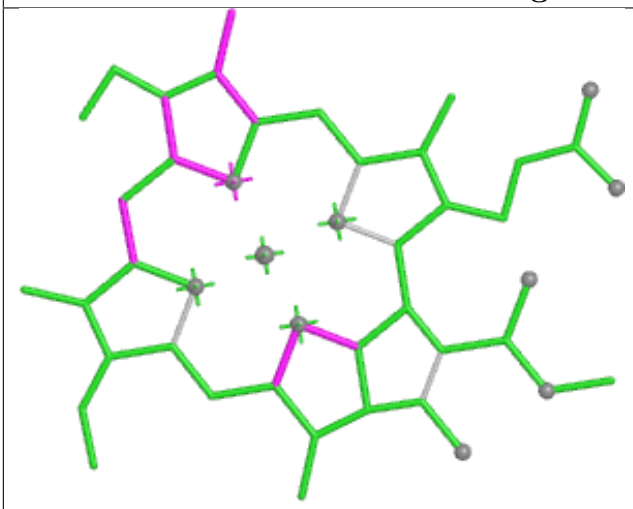


Torsions

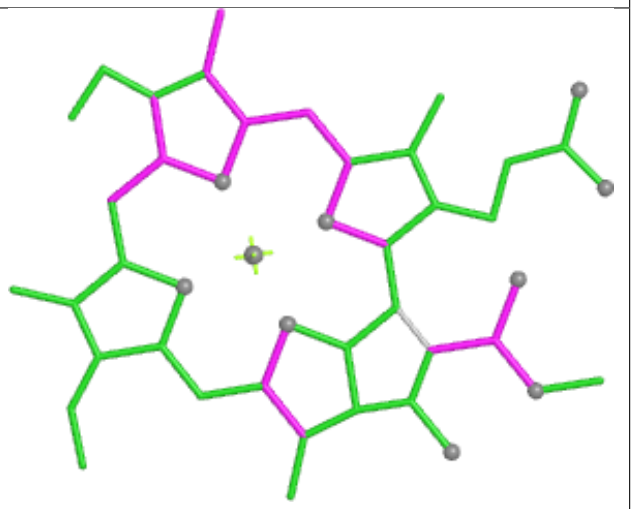


Rings

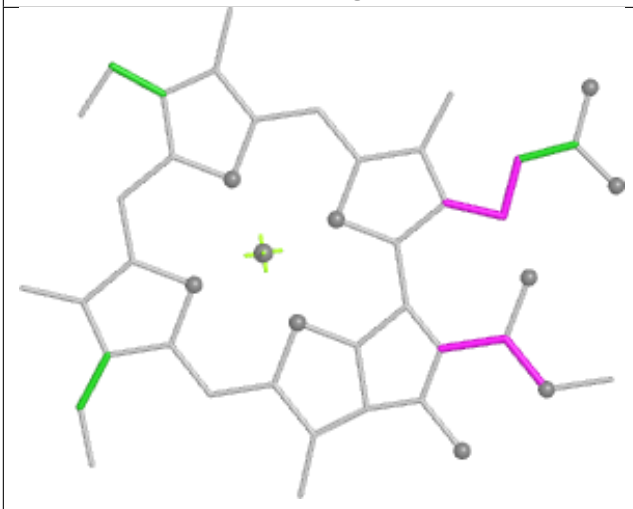
Ligand CLA I 611



Bond lengths



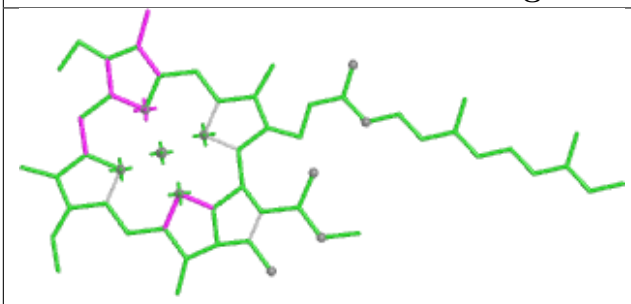
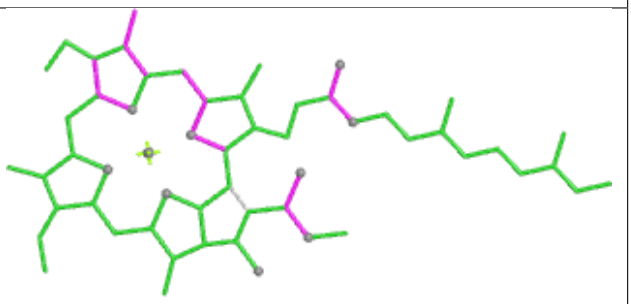
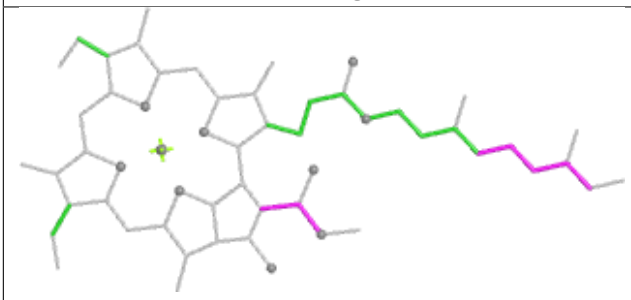
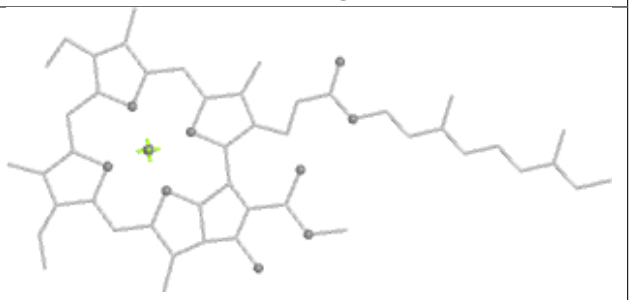
Bond angles

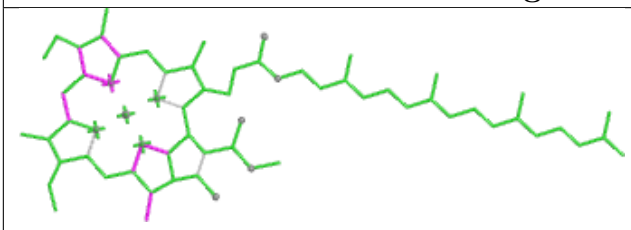
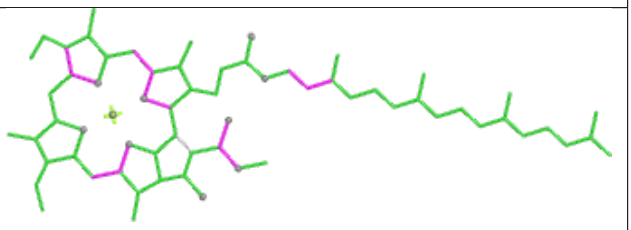
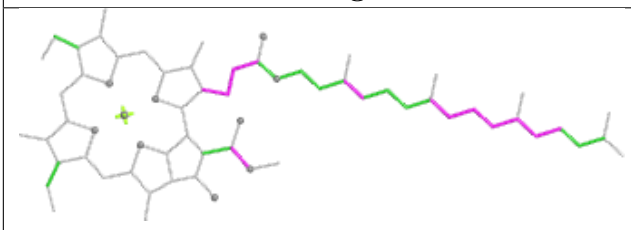
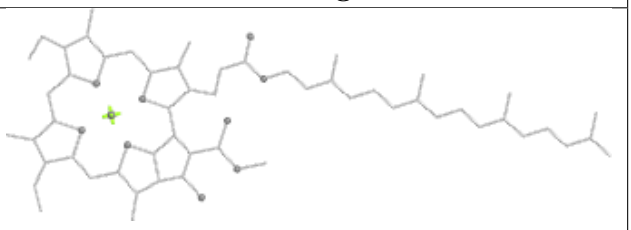


Torsions

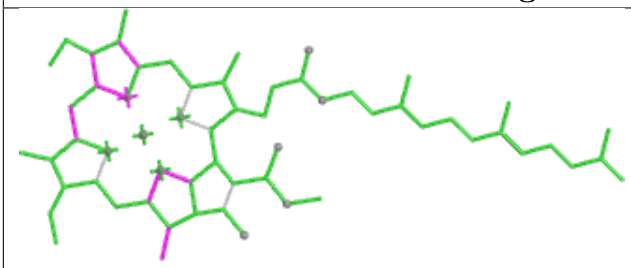


Rings

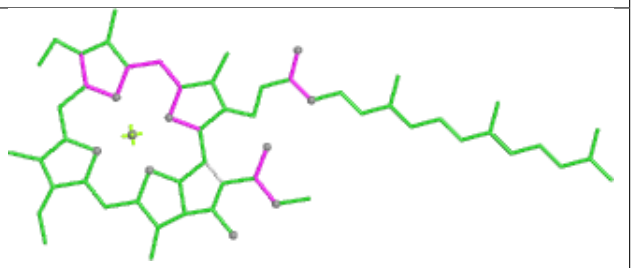
Ligand CLA V 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

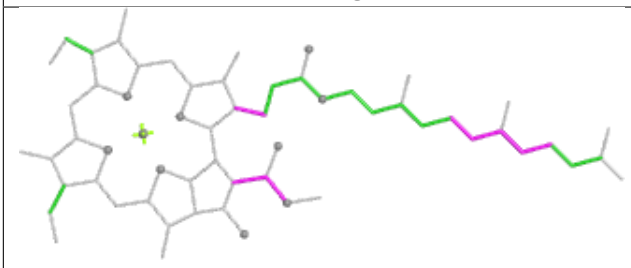
Ligand CLA W 410



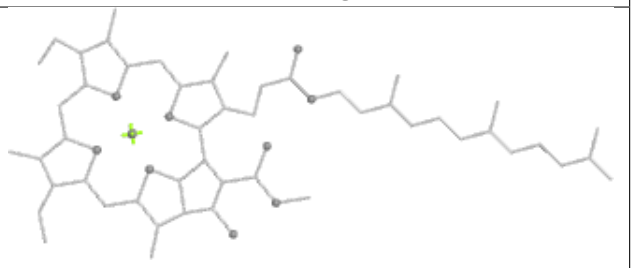
Bond lengths



Bond angles

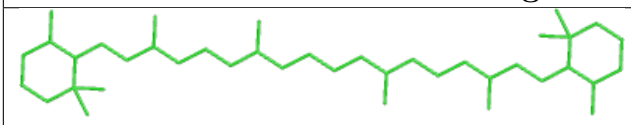


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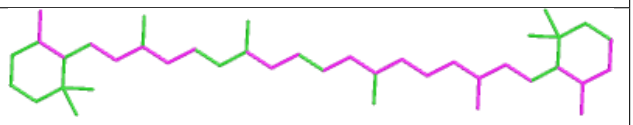


Rings

Ligand BCR A 850



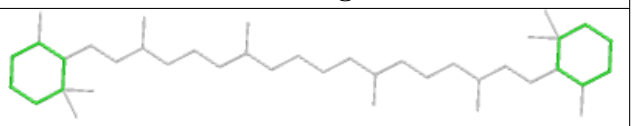
Bond lengths



Bond angles

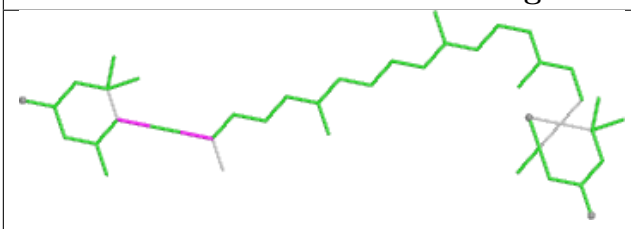


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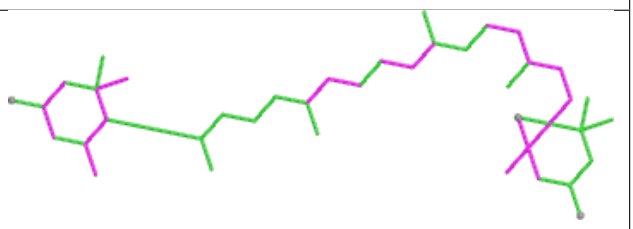


Rings

Ligand DD6 K 615



Bond lengths



Bond angles

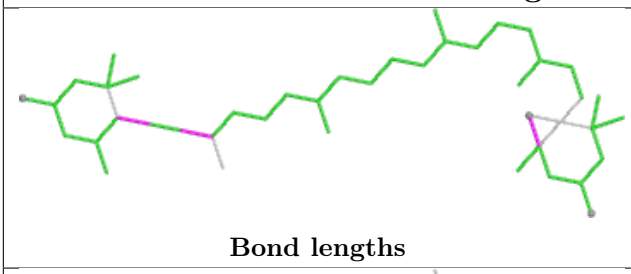


Torsions

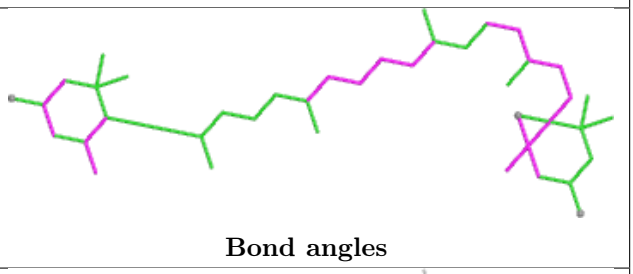


Rings

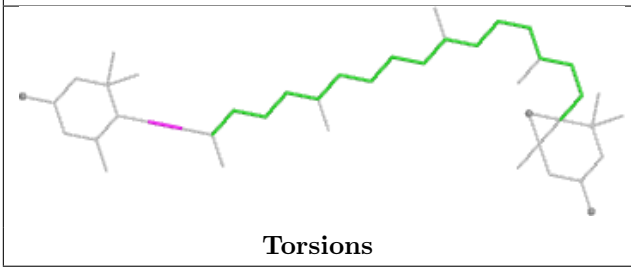
Ligand DD6 X 414



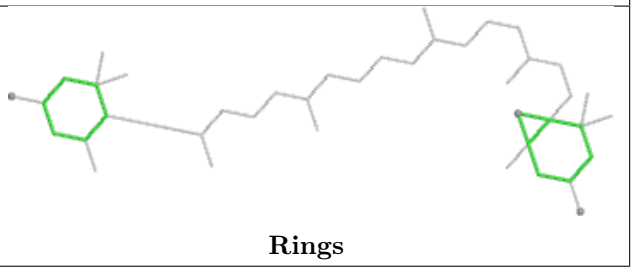
Bond lengths



Bond angles

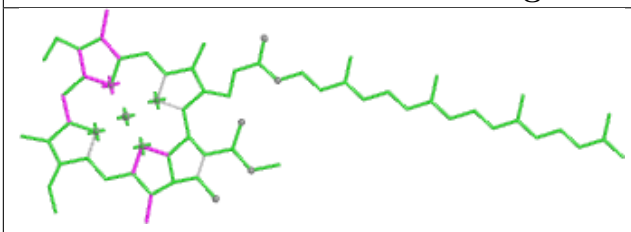


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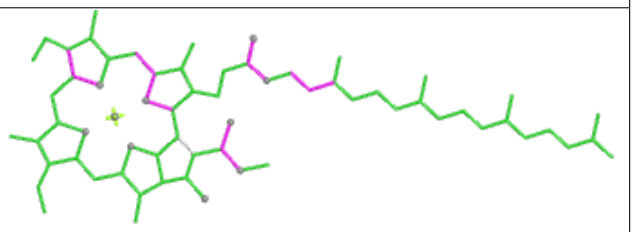


Rings

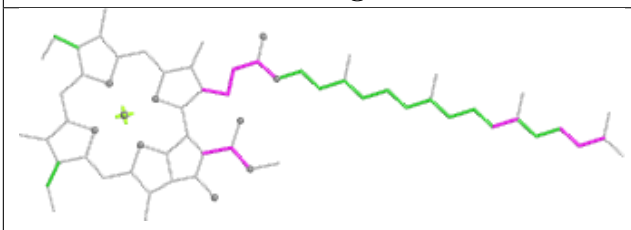
Ligand CLA A 821



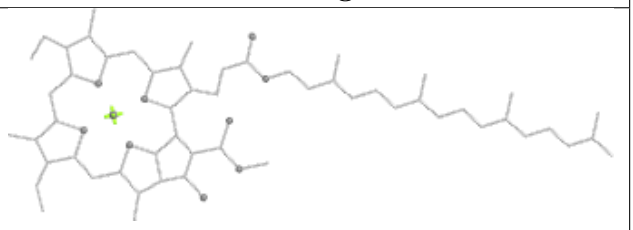
Bond lengths



Bond angles

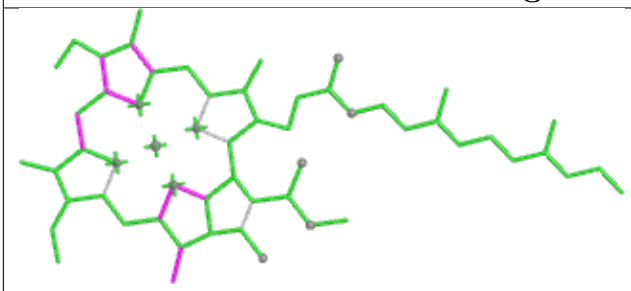


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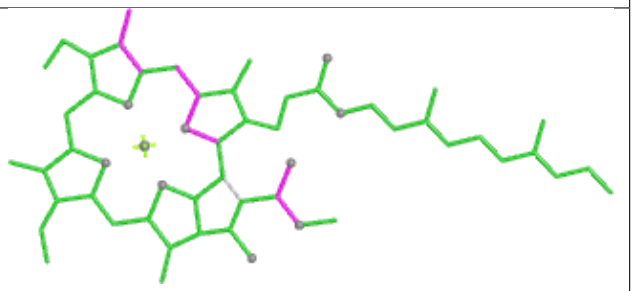


Rings

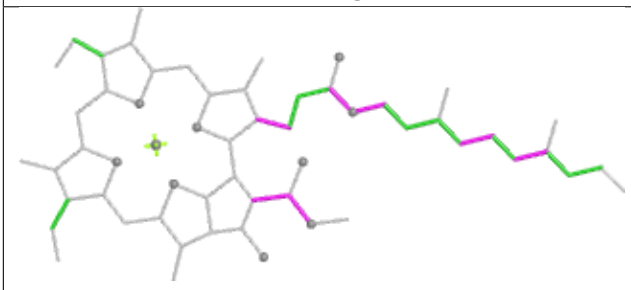
Ligand CLA V 603



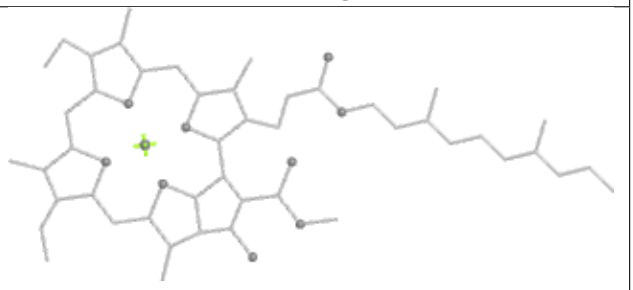
Bond lengths



Bond angles

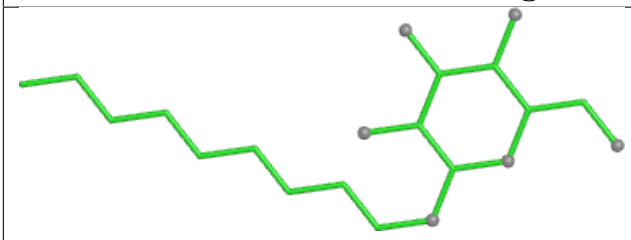


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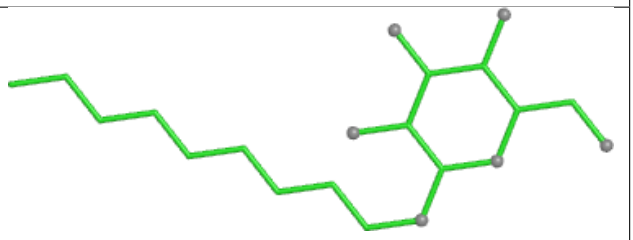


Rings

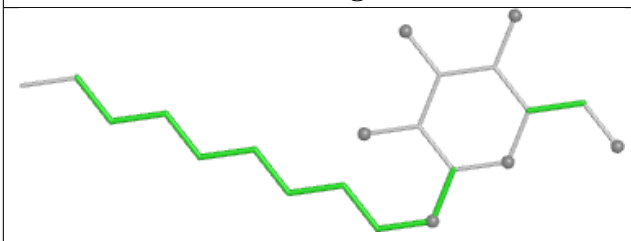
Ligand LMU T 615



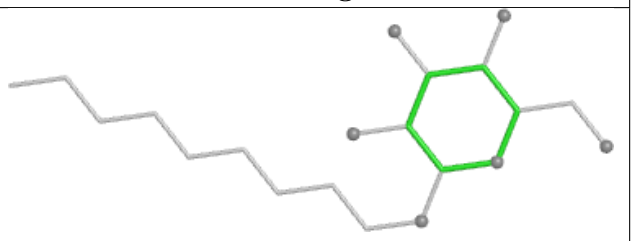
Bond lengths



Bond angles

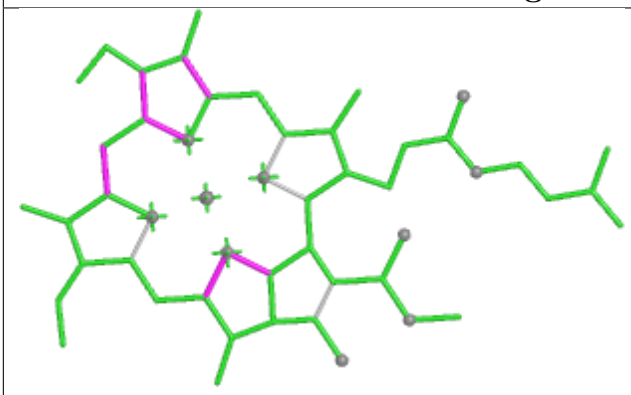


Torsions

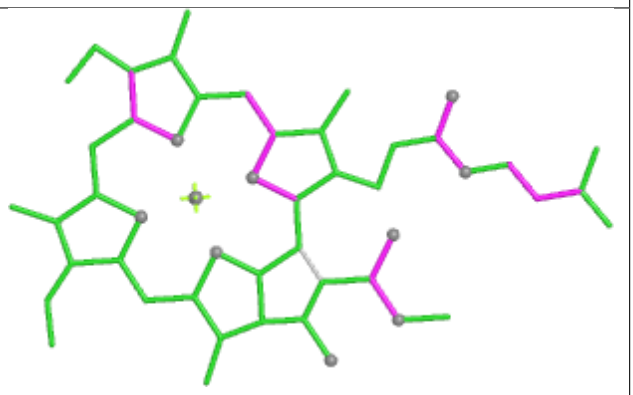


Rings

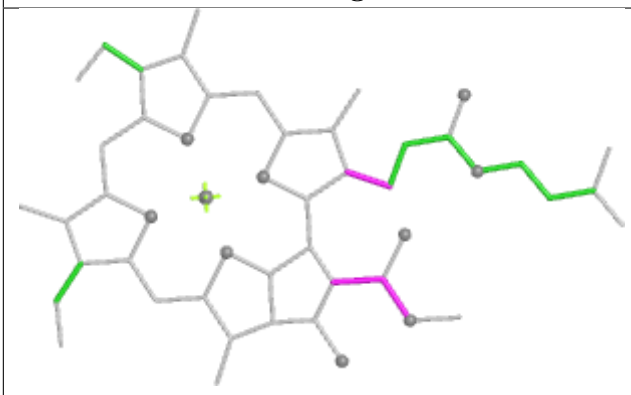
Ligand CLA T 606



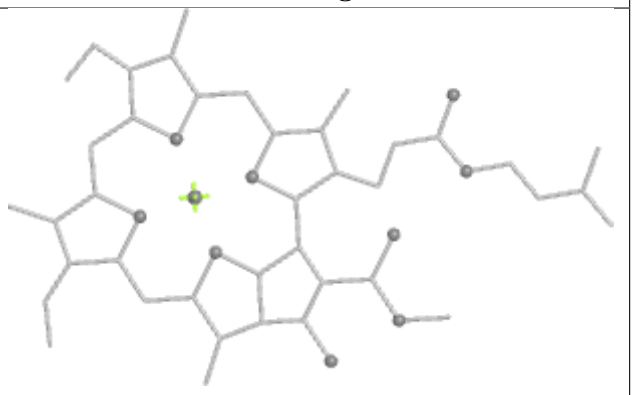
Bond lengths



Bond angles

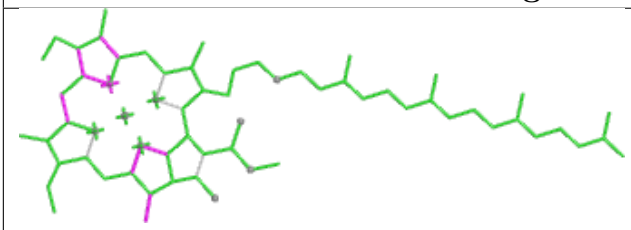


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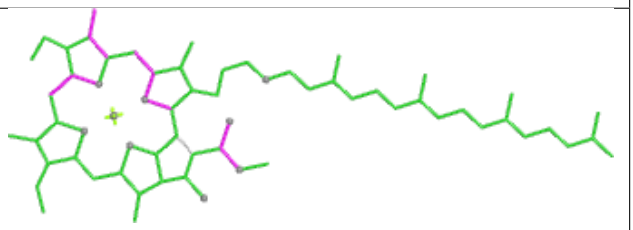


Rings

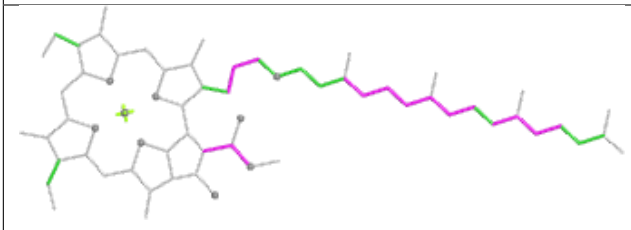
Ligand CLA K 604



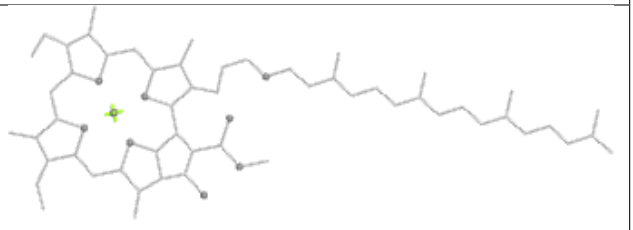
Bond lengths



Bond angles

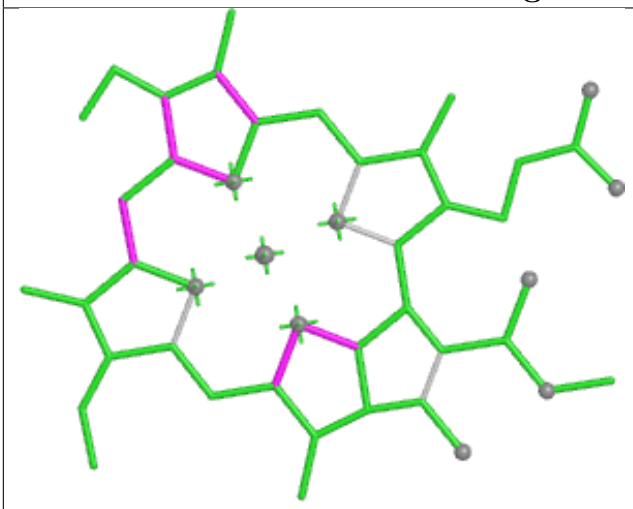


Torsions

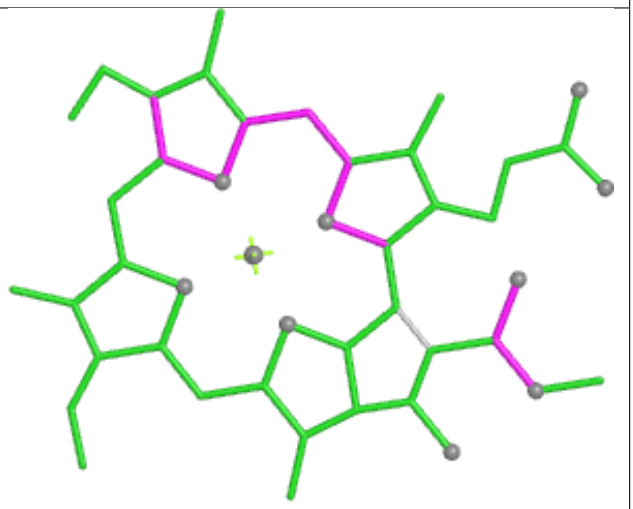


Rings

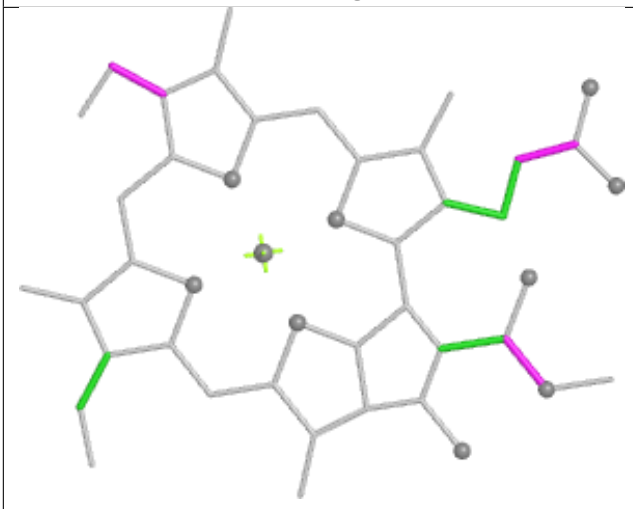
Ligand CLA V 601



Bond lengths



Bond angles

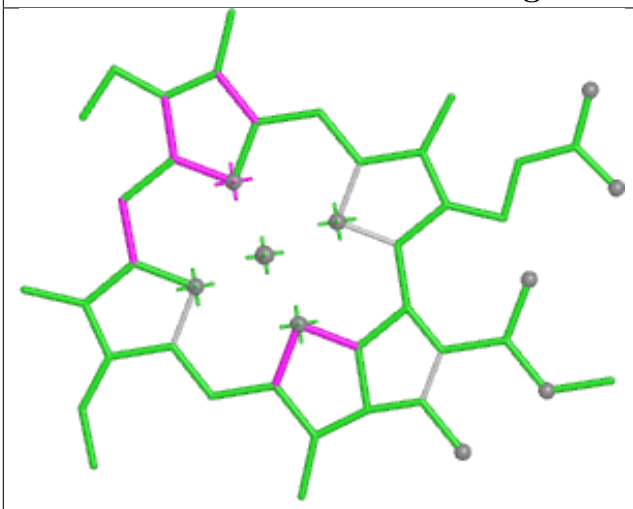


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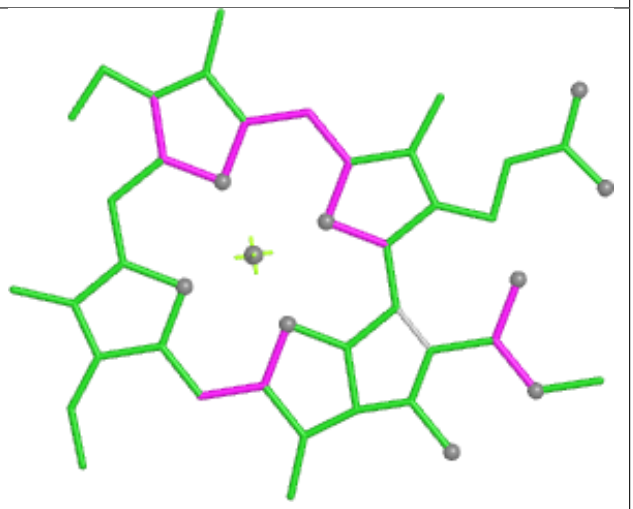


Rings

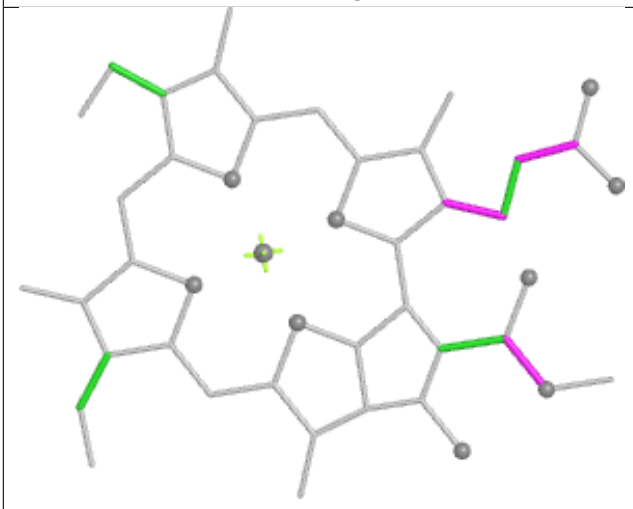
Ligand CLA G 611



Bond lengths



Bond angles

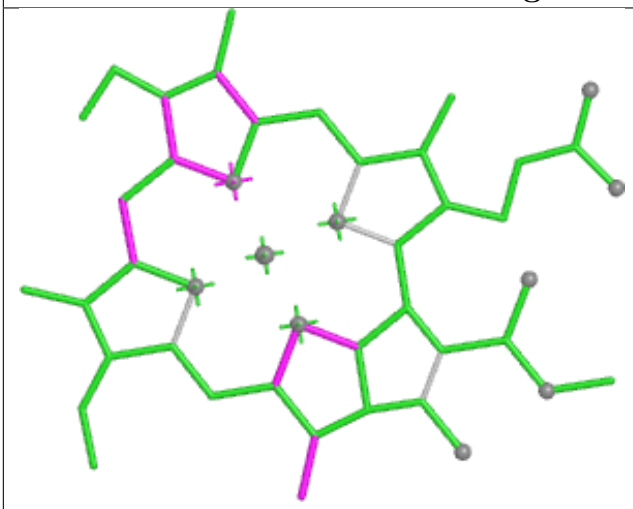


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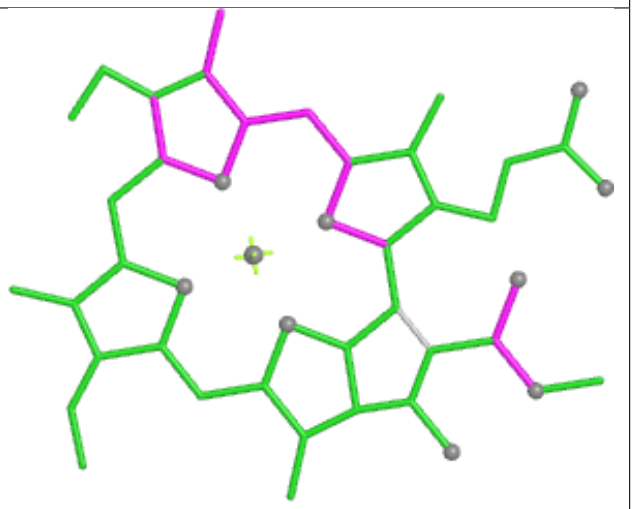


Rings

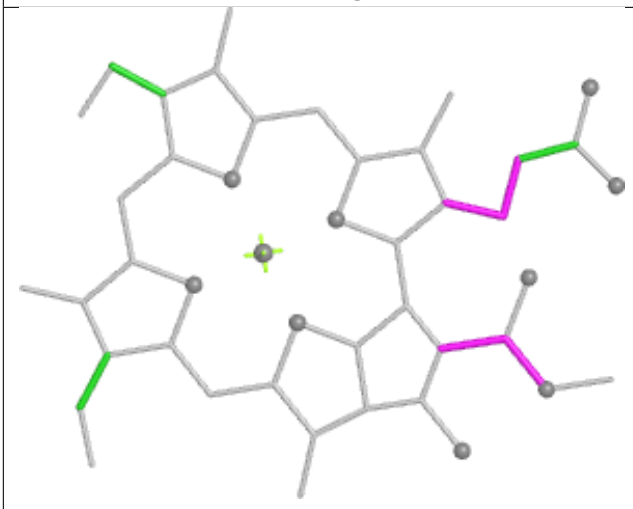
Ligand CLA U 409



Bond lengths



Bond angles

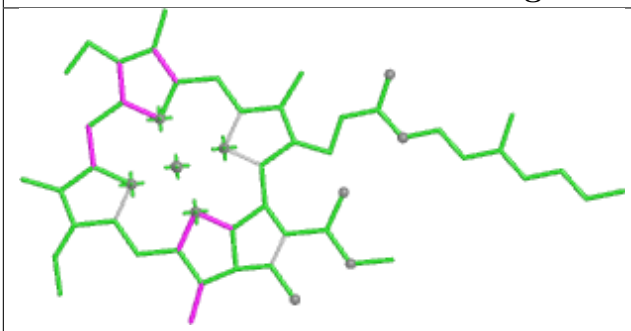


Torsions

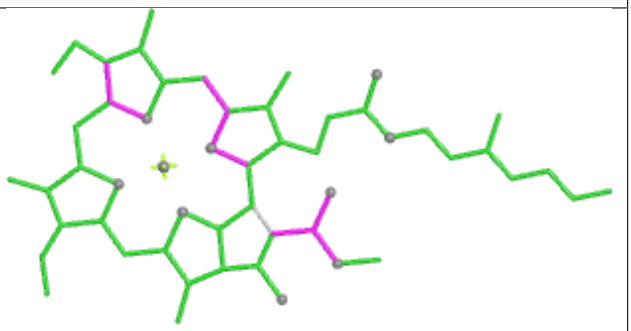


Rings

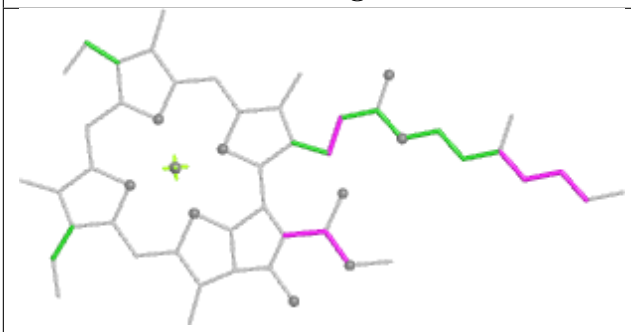
Ligand CLA B 820



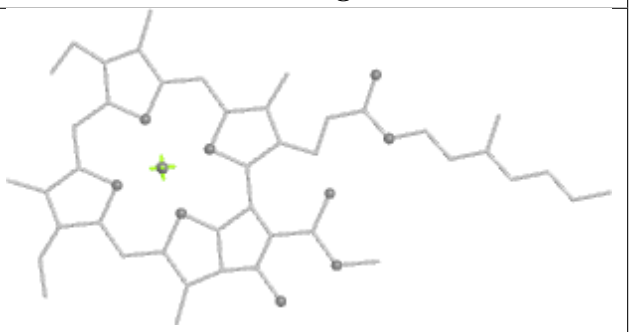
Bond lengths



Bond angles

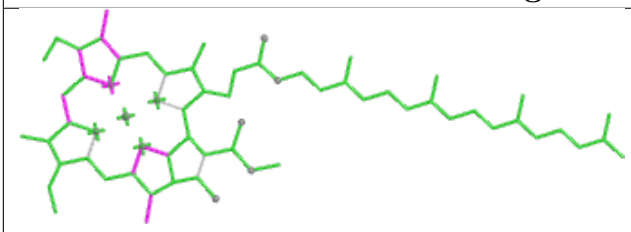


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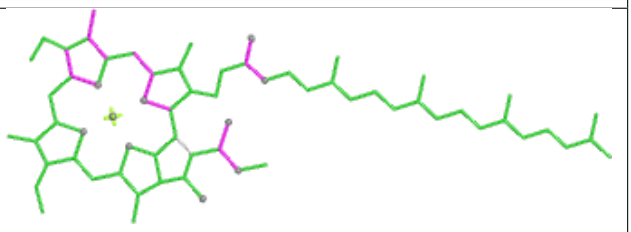


Rings

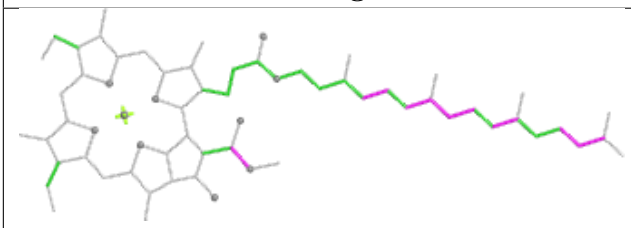
Ligand CLA B 818



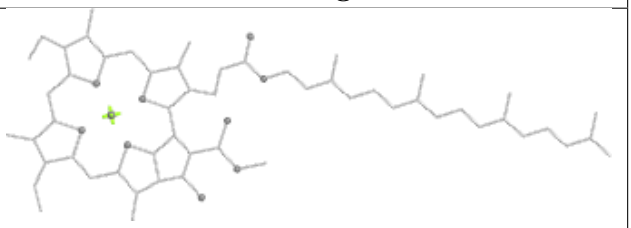
Bond lengths



Bond angles

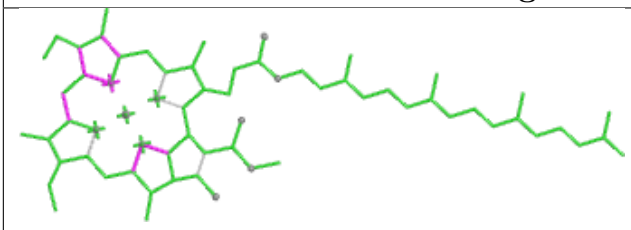


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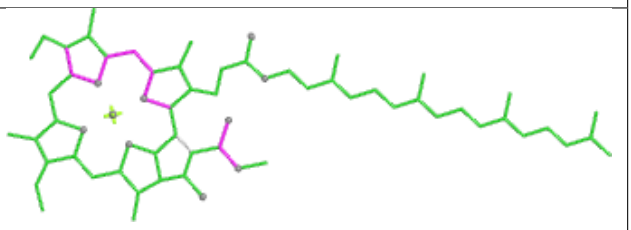


Rings

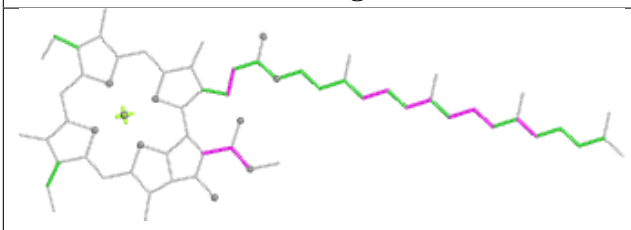
Ligand CLA W 404



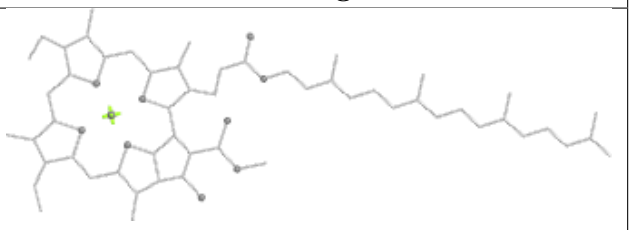
Bond lengths



Bond angles

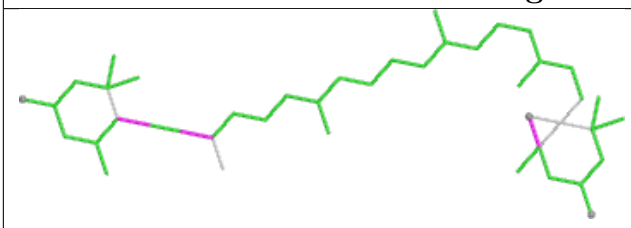


Torsions

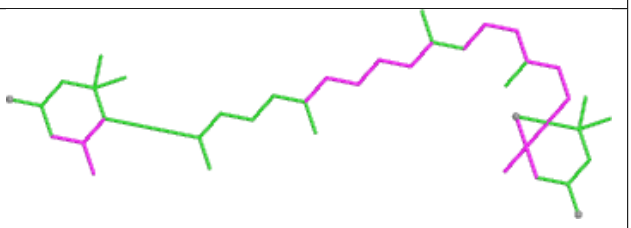


Rings

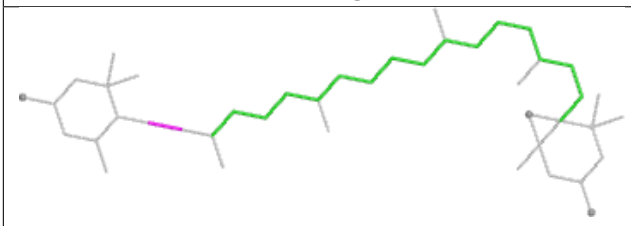
Ligand DD6 T 612



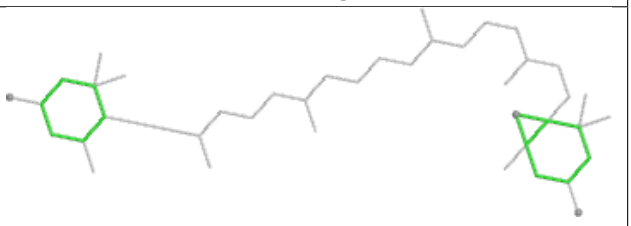
Bond lengths



Bond angles

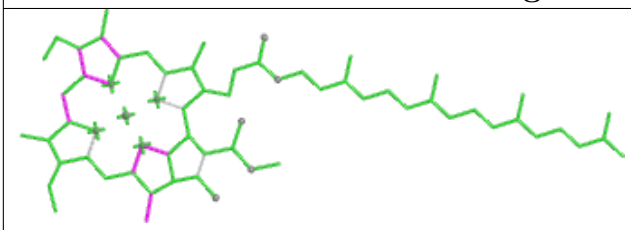


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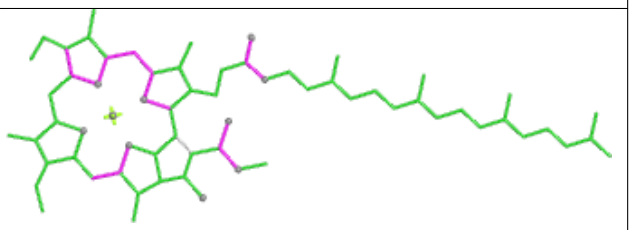


Rings

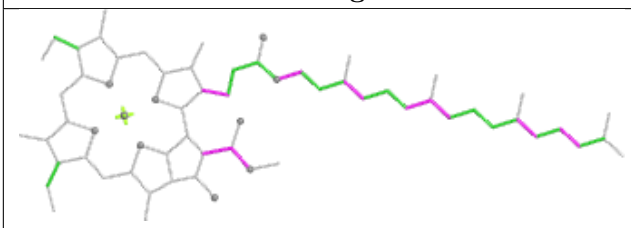
Ligand CLA N 606



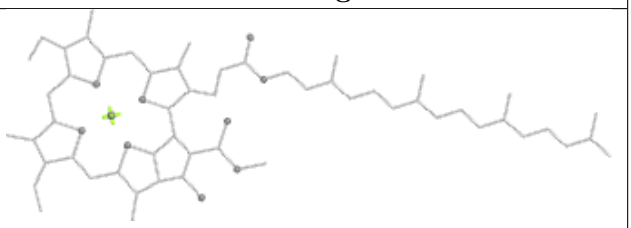
Bond lengths



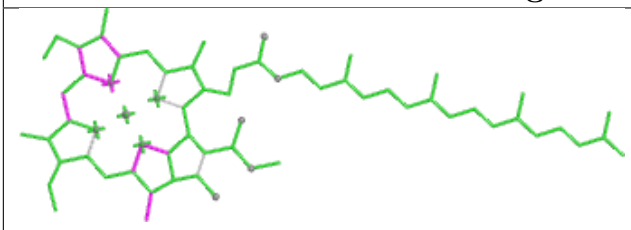
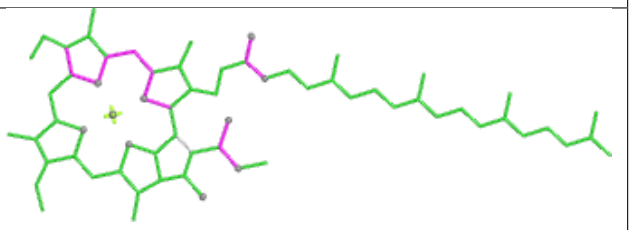
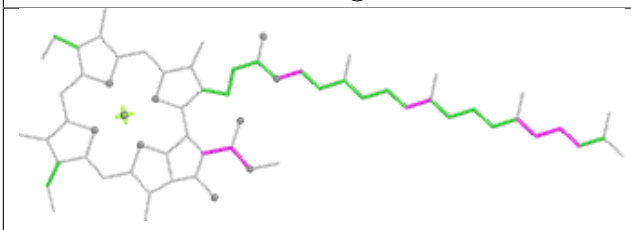
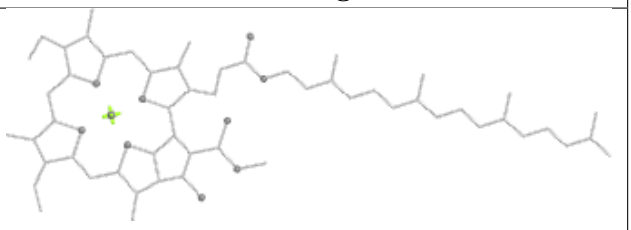
Bond angles

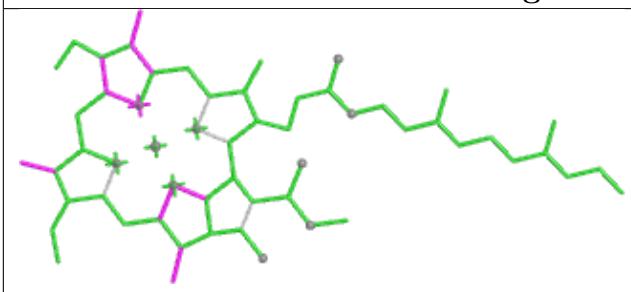
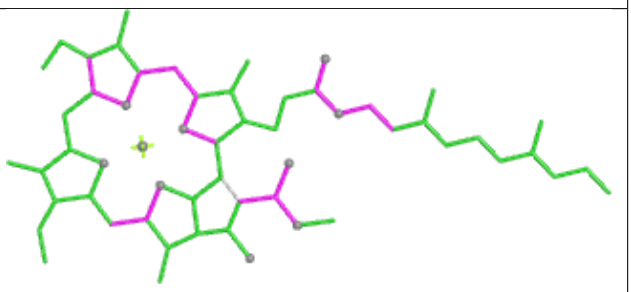
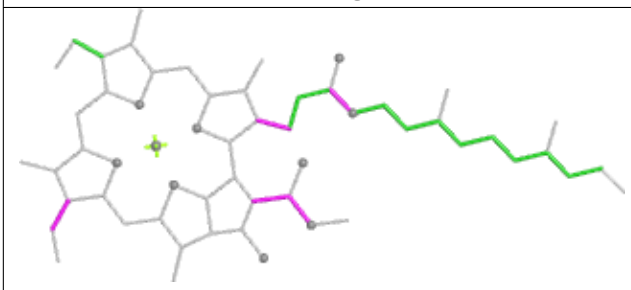
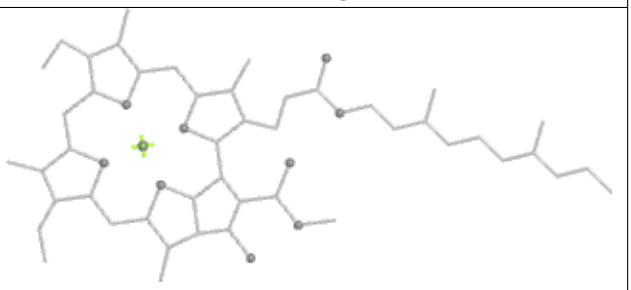


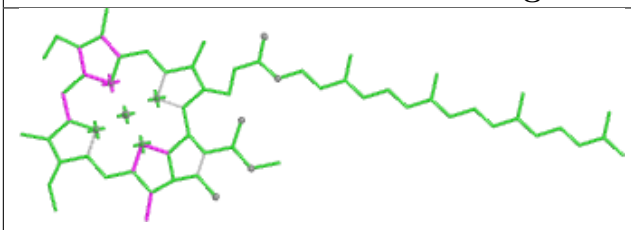
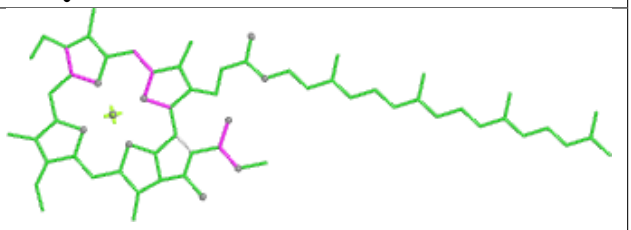
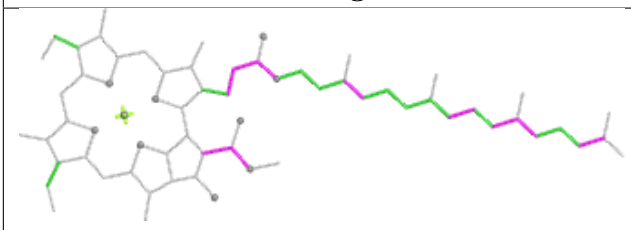
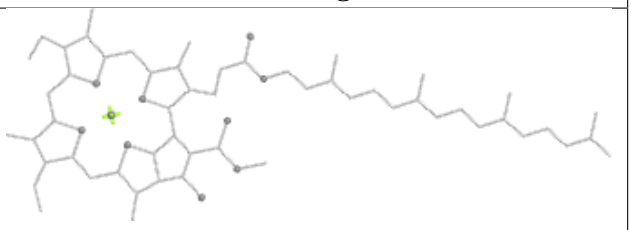
Torsions

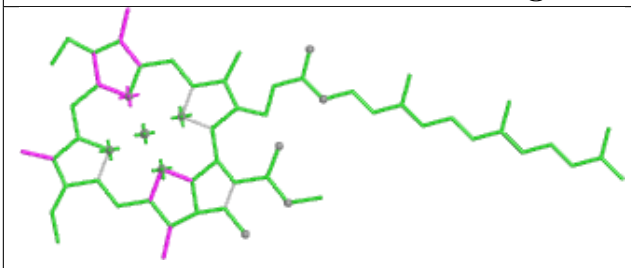
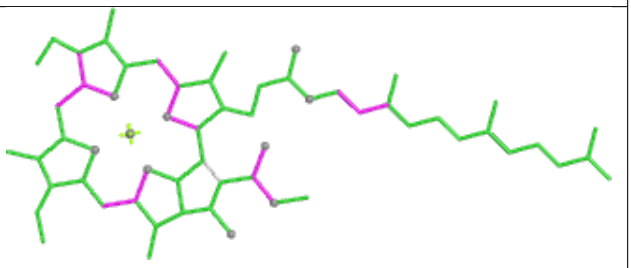
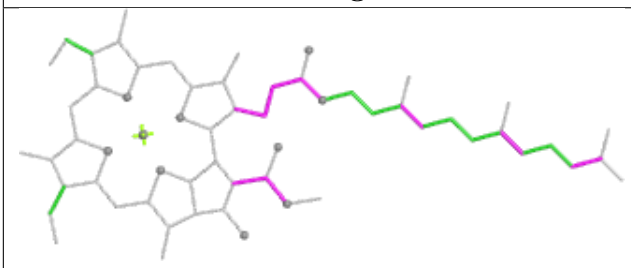
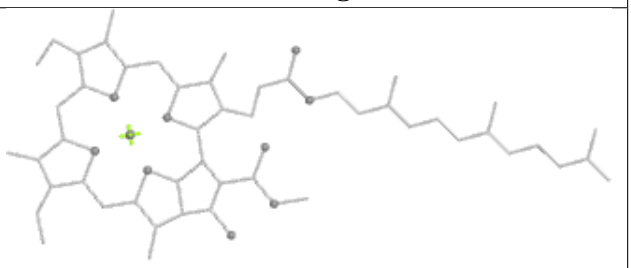


Rings

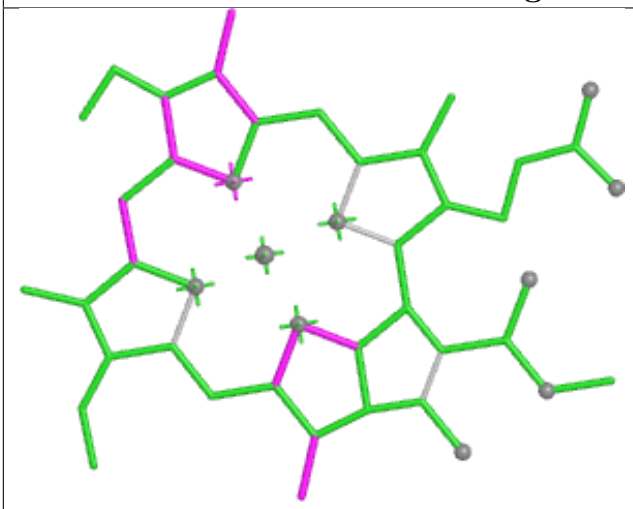
Ligand CLA L 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA K 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

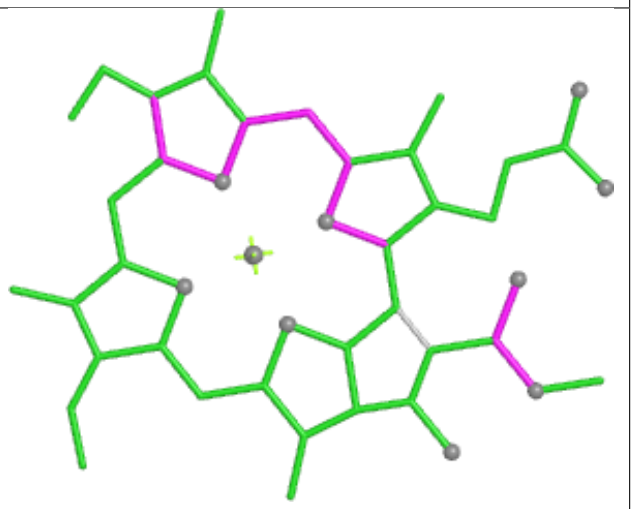
Ligand CLA Q 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA S 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

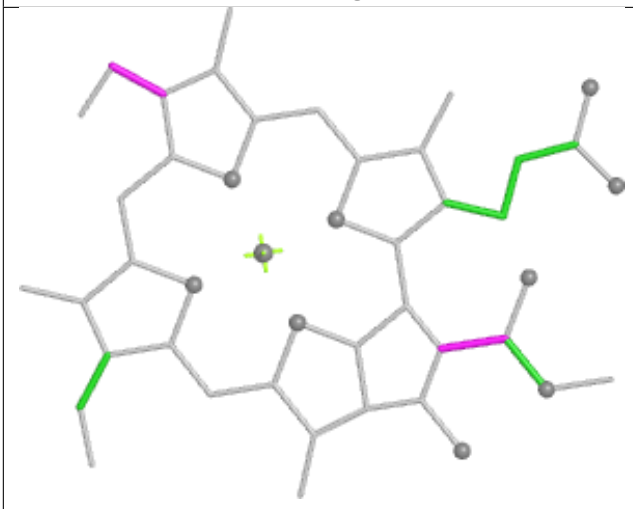
Ligand CLA B 837



Bond lengths



Bond angles

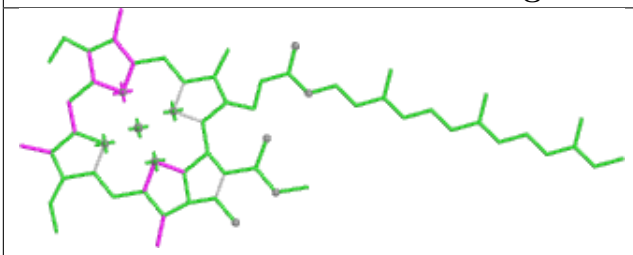


Torsions

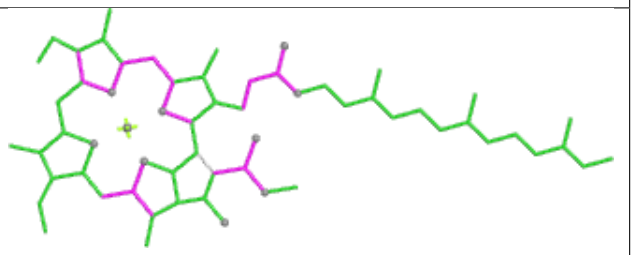


Rings

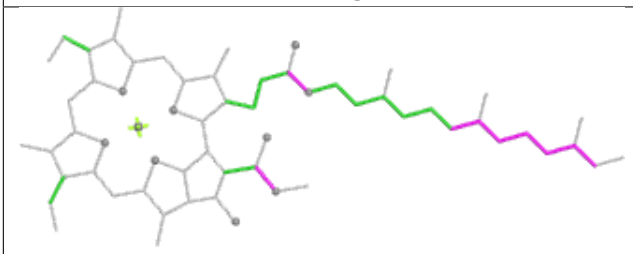
Ligand CLA A 816



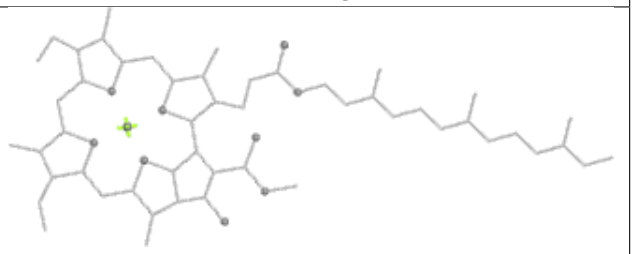
Bond lengths



Bond angles

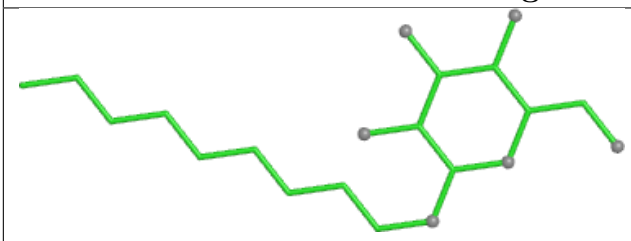


Torsions

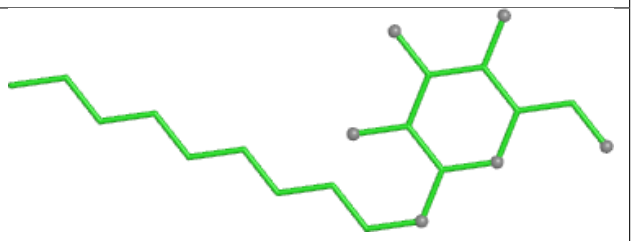


Rings

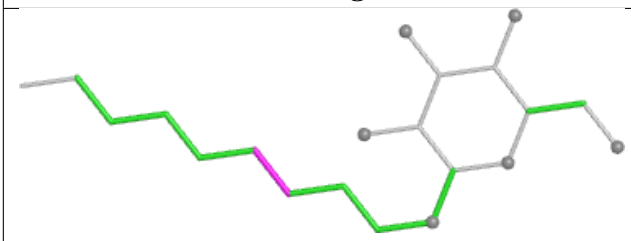
Ligand LMU F 402



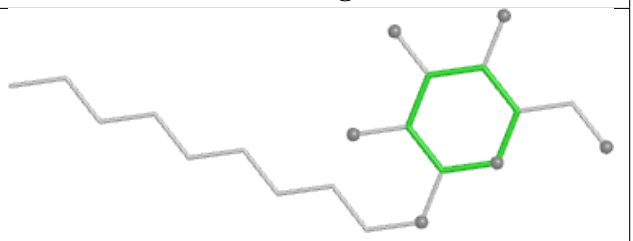
Bond lengths



Bond angles

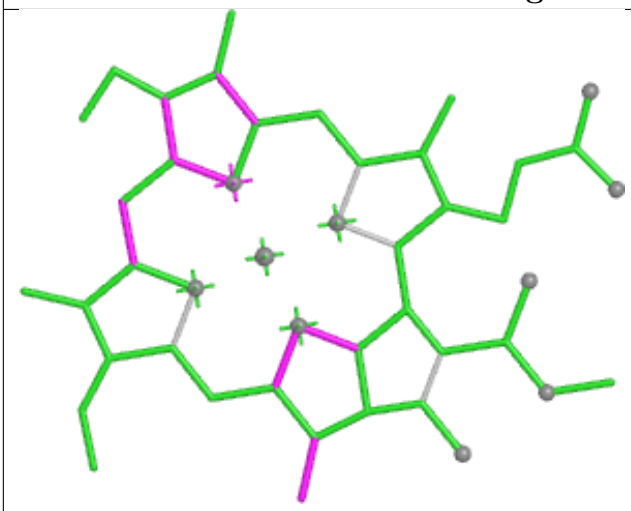


Torsions

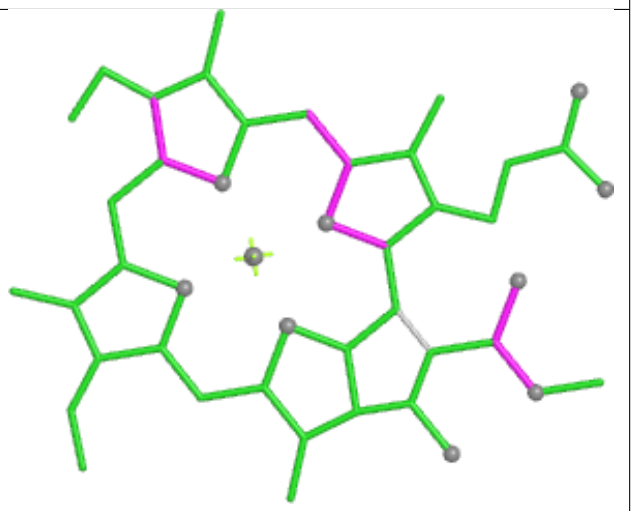


Rings

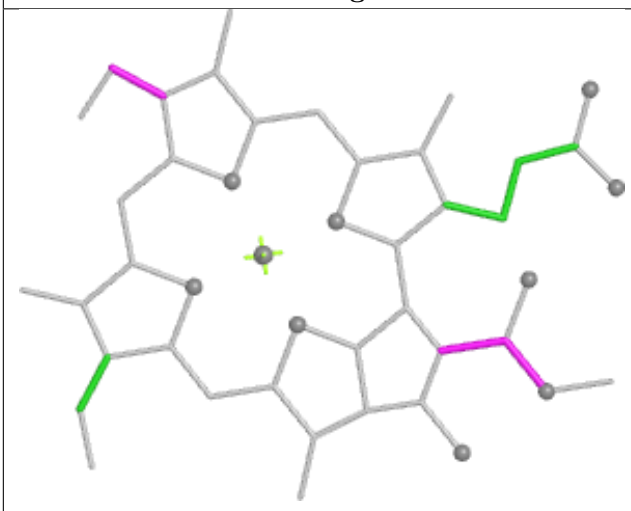
Ligand CLA F 405



Bond lengths



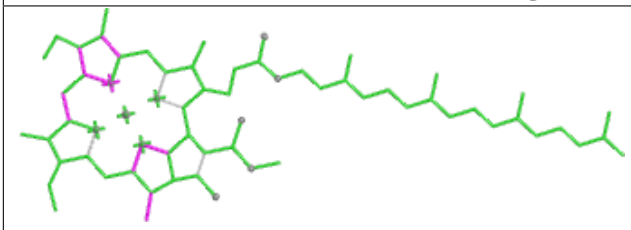
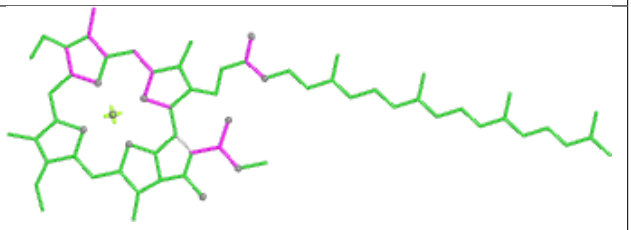
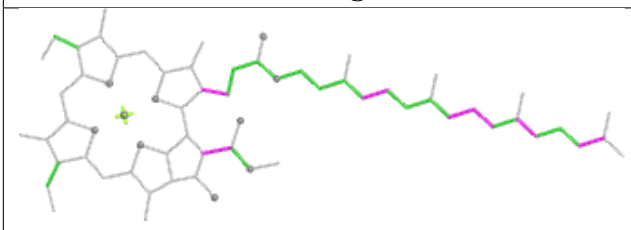
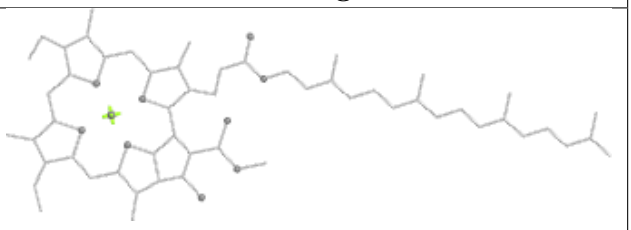
Bond angles

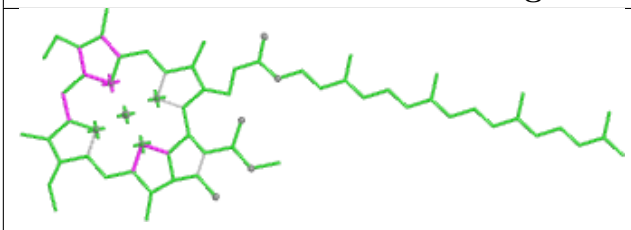
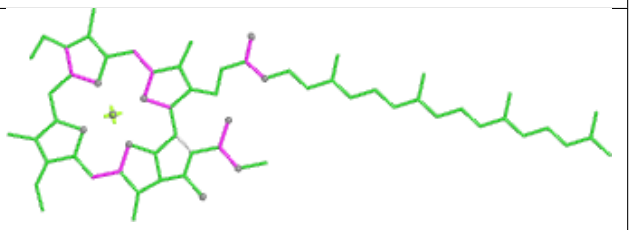
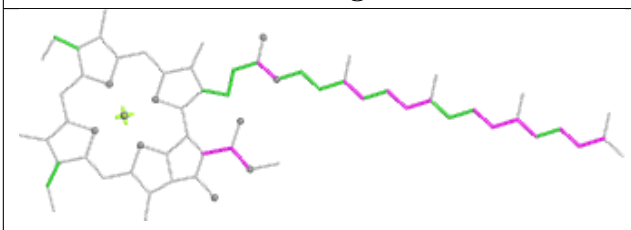
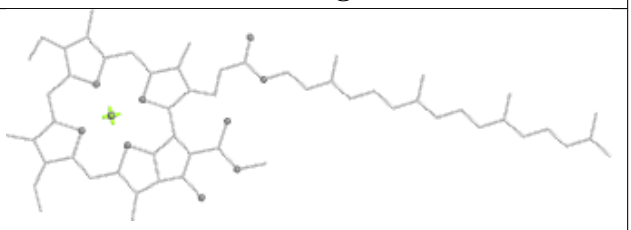


Torsions

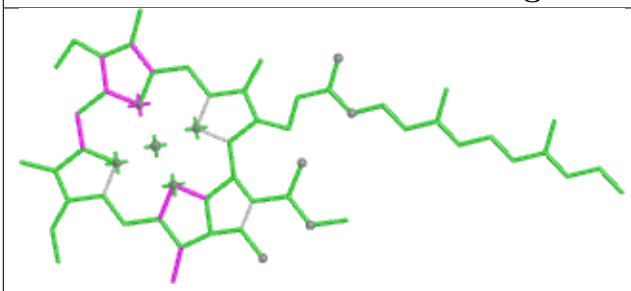


Rings

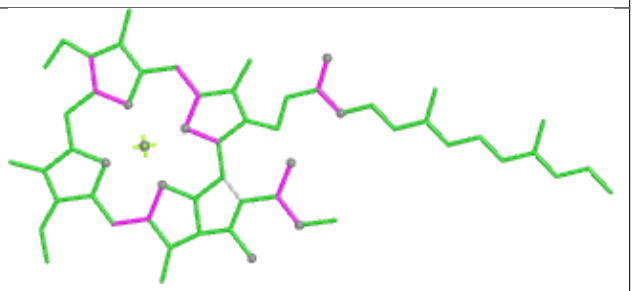
Ligand CLA B 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA T 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

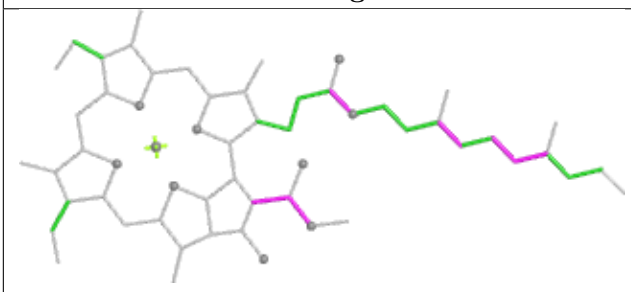
Ligand CLA A 812



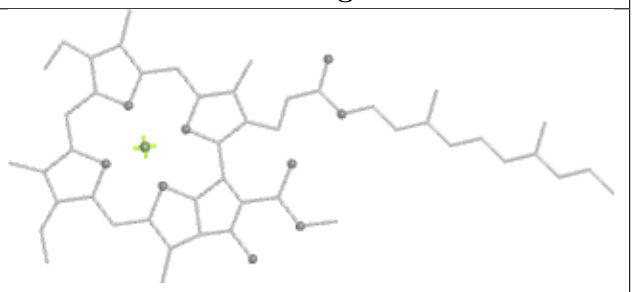
Bond lengths



Bond angles

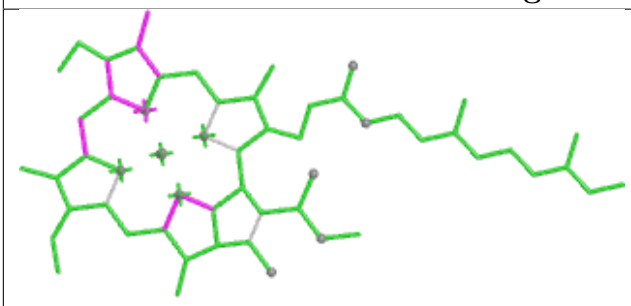


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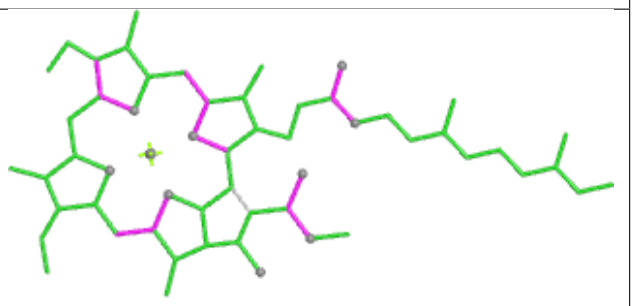


Rings

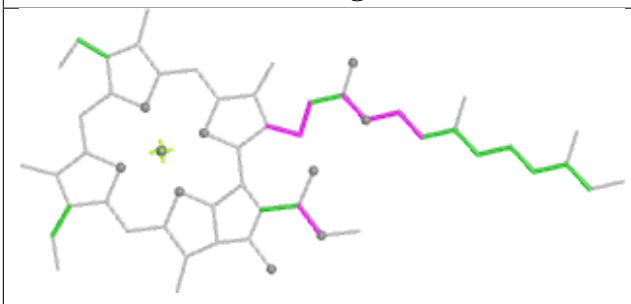
Ligand CLA X 405



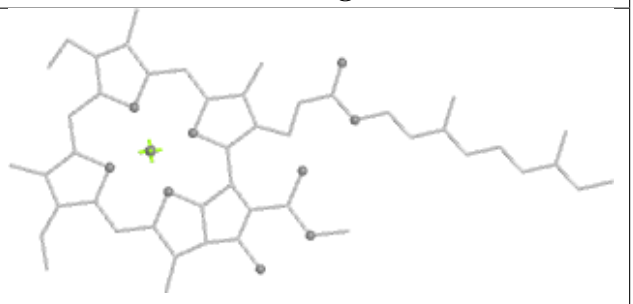
Bond lengths



Bond angles

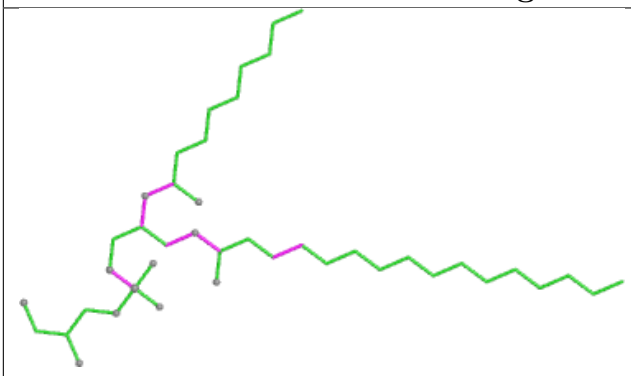


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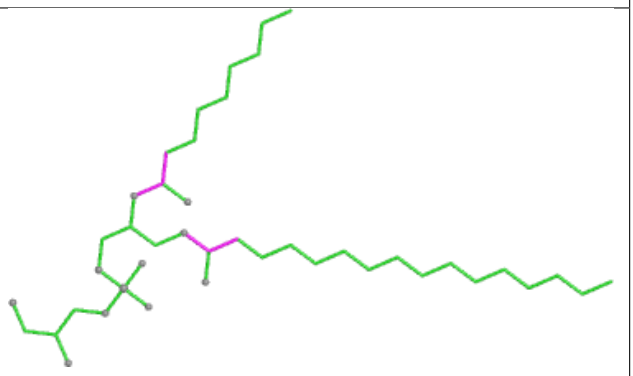


Rings

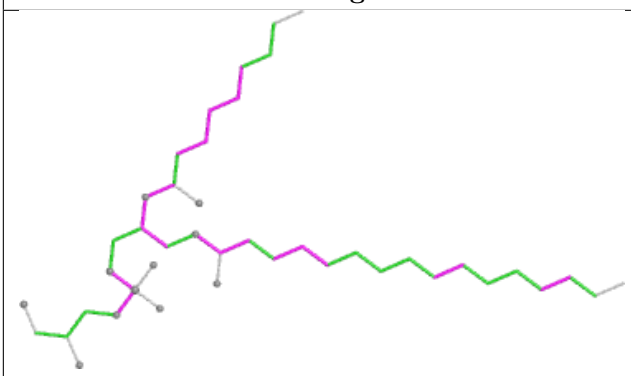
Ligand LHG W 420



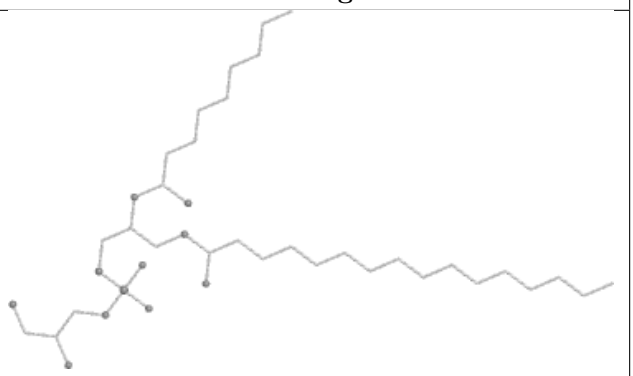
Bond lengths



Bond angles

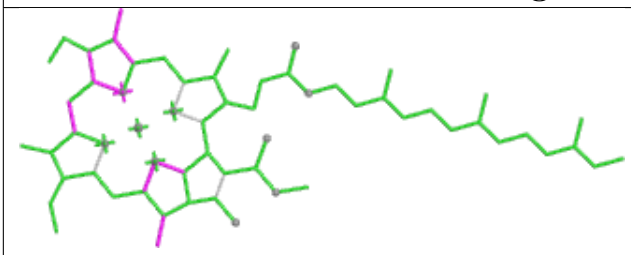


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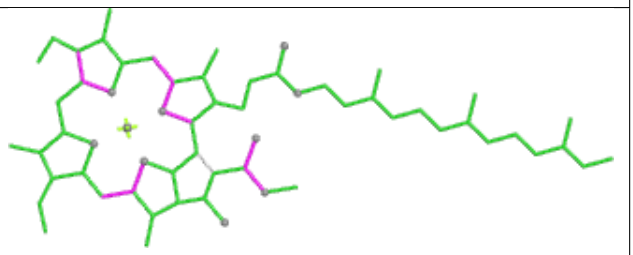


Rings

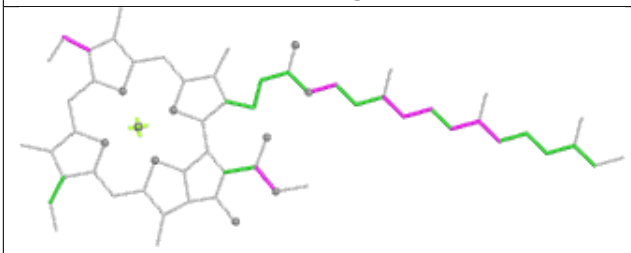
Ligand CLA I 606



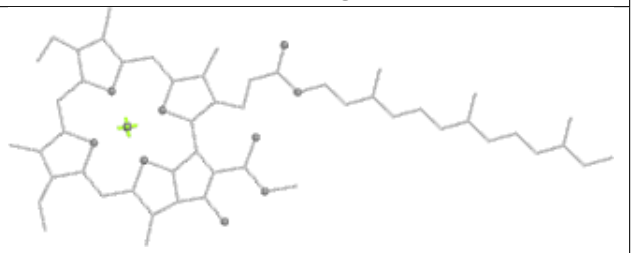
Bond lengths



Bond angles

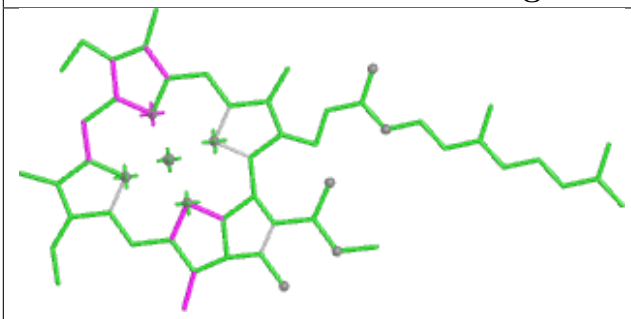


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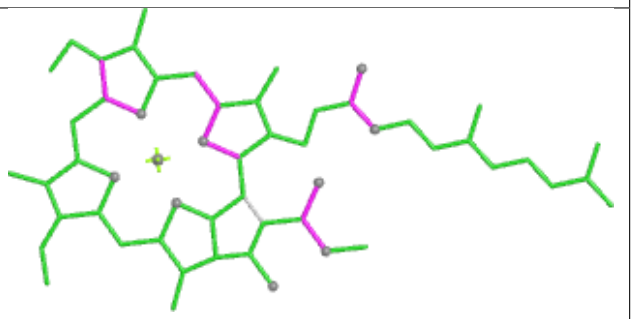


Rings

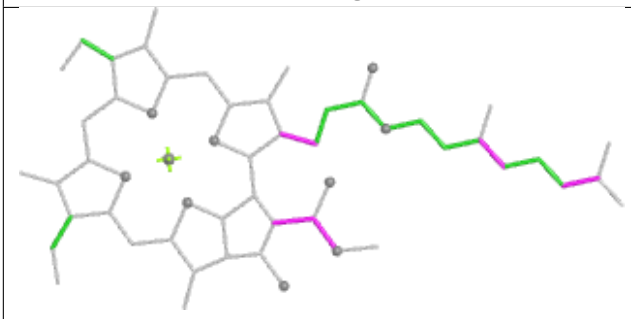
Ligand CLA U 410



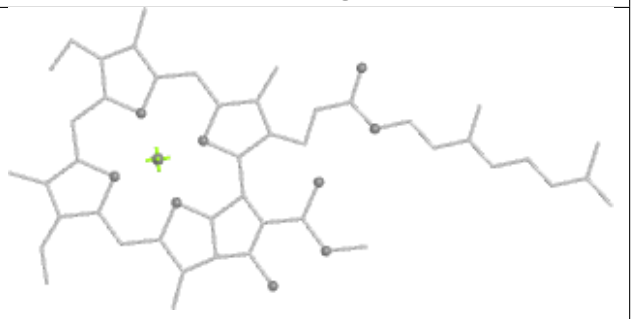
Bond lengths



Bond angles

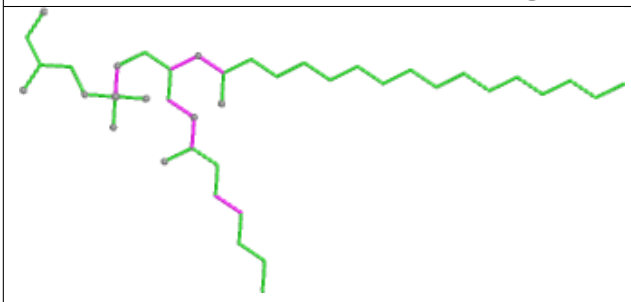


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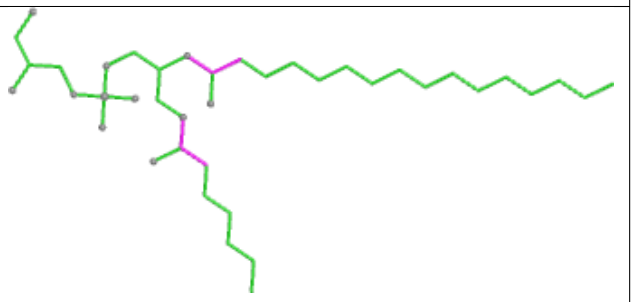


Rings

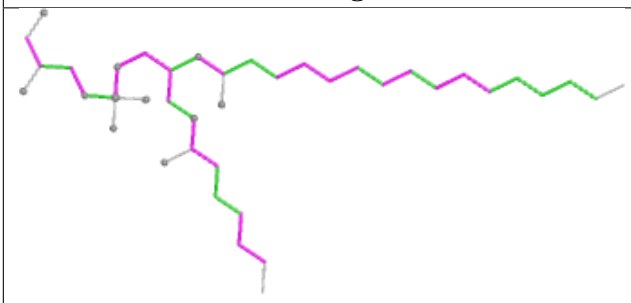
Ligand LHG P 601



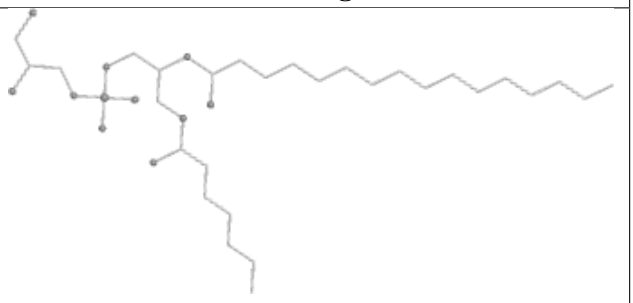
Bond lengths



Bond angles

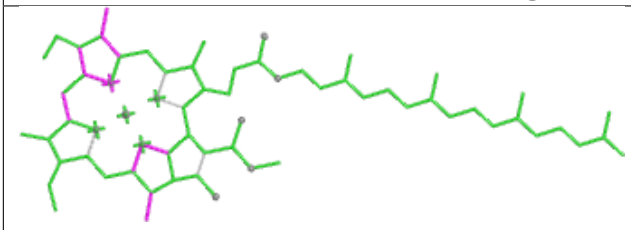


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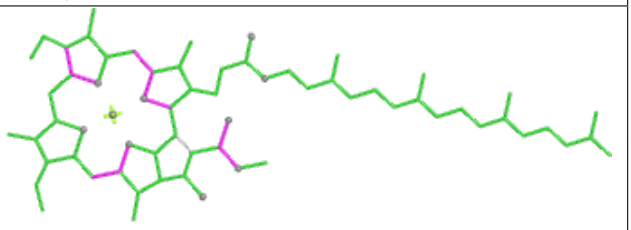


Rings

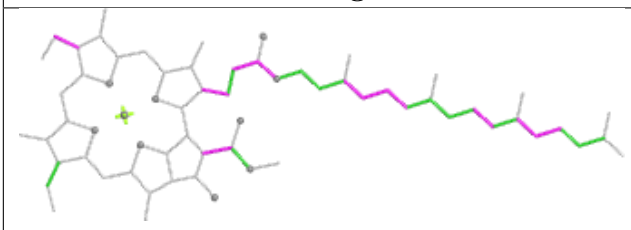
Ligand CLA Q 610



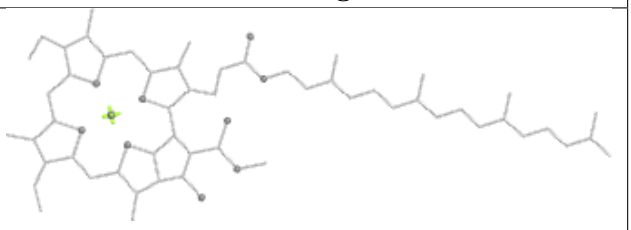
Bond lengths



Bond angles

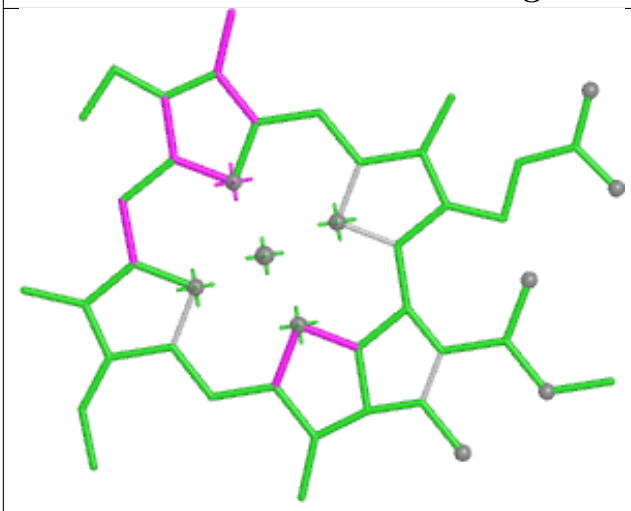


Torsions

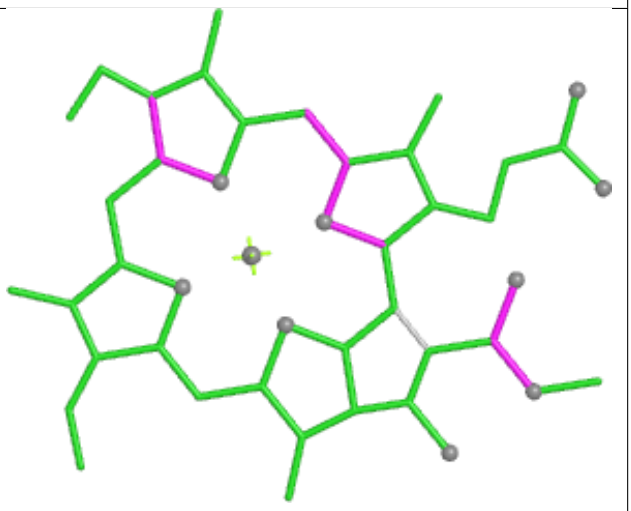


Rings

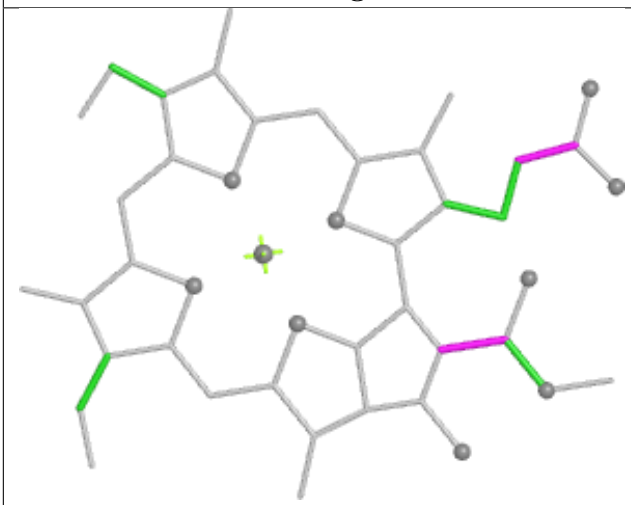
Ligand CLA G 605



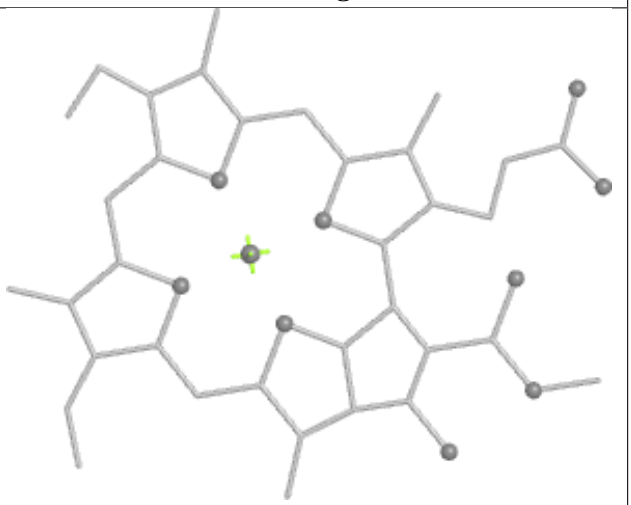
Bond lengths



Bond angles

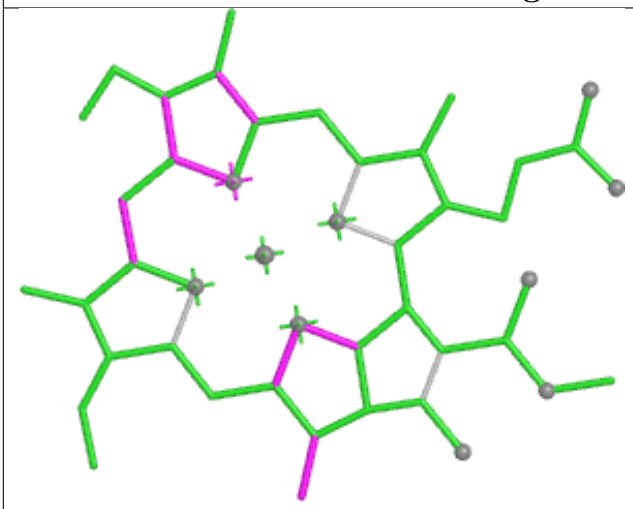


Torsions

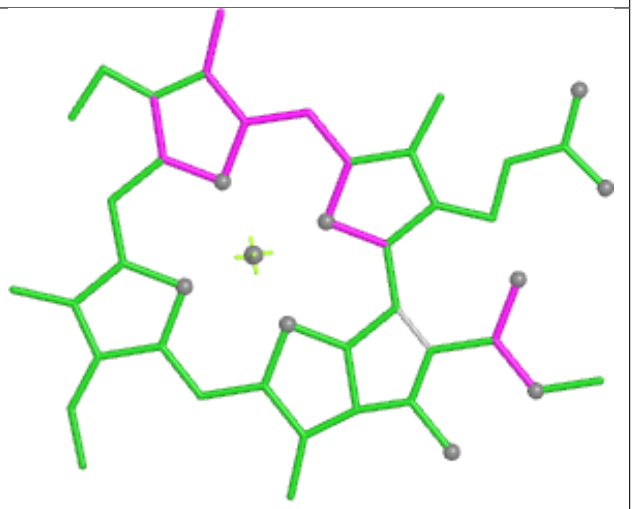


Rings

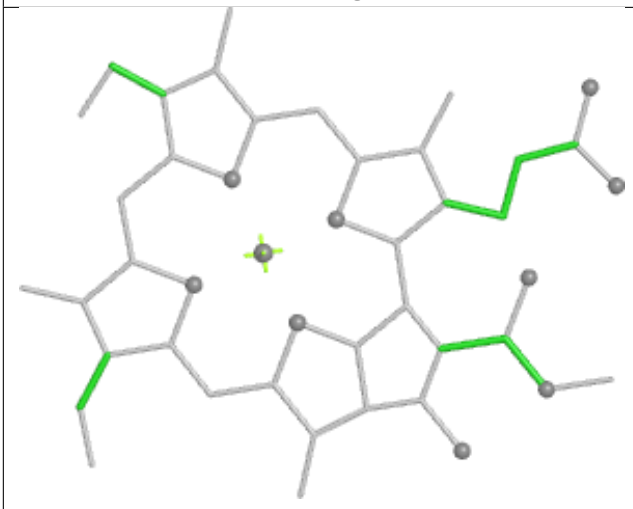
Ligand CLA G 604



Bond lengths



Bond angles

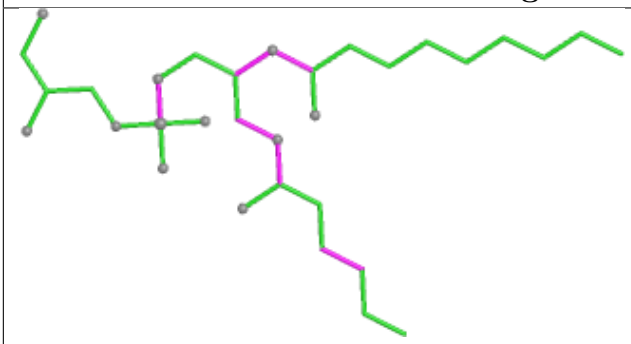


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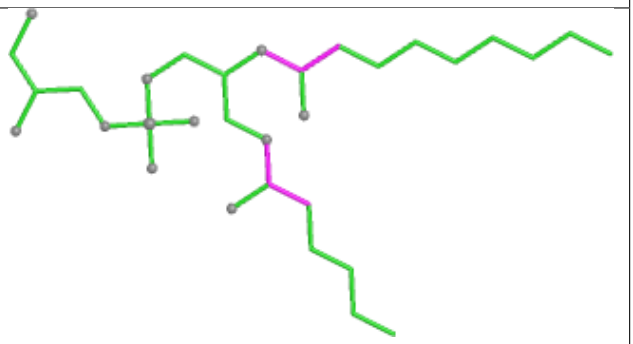


Rings

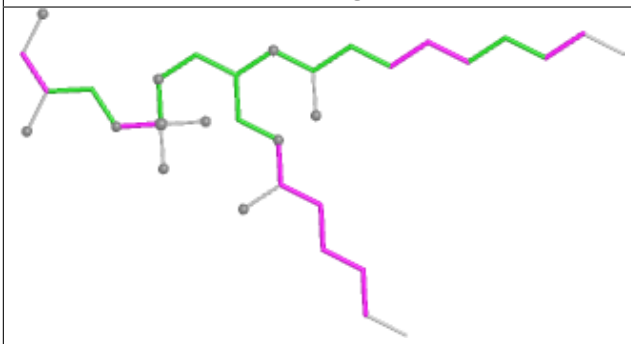
Ligand LHG G 614



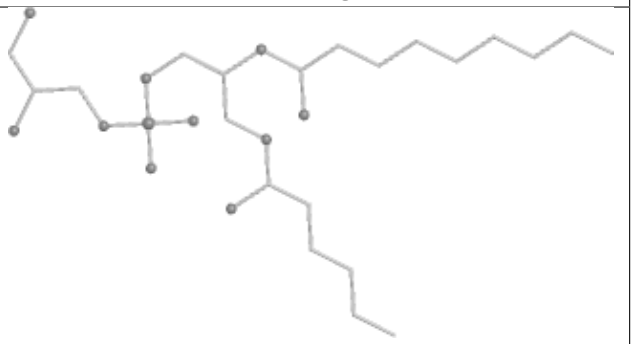
Bond lengths



Bond angles

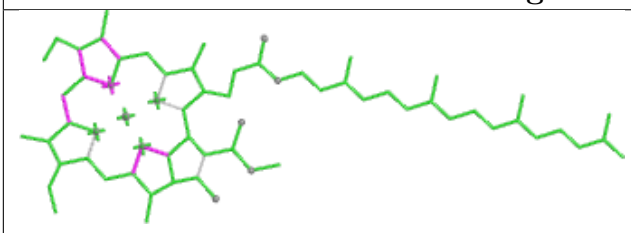


Torsions

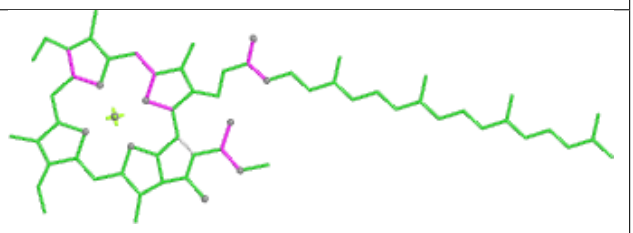


Rings

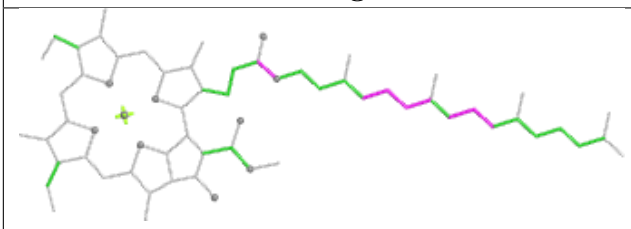
Ligand CLA L 417



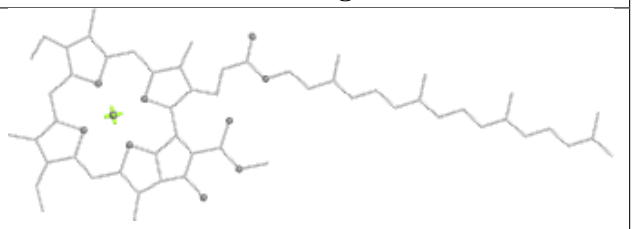
Bond lengths



Bond angles

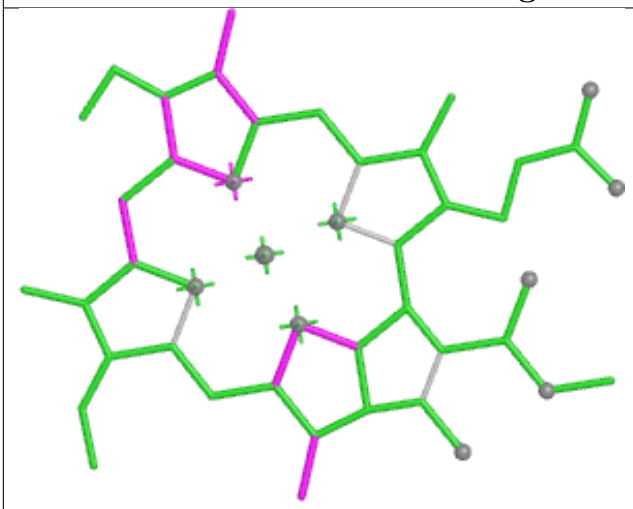


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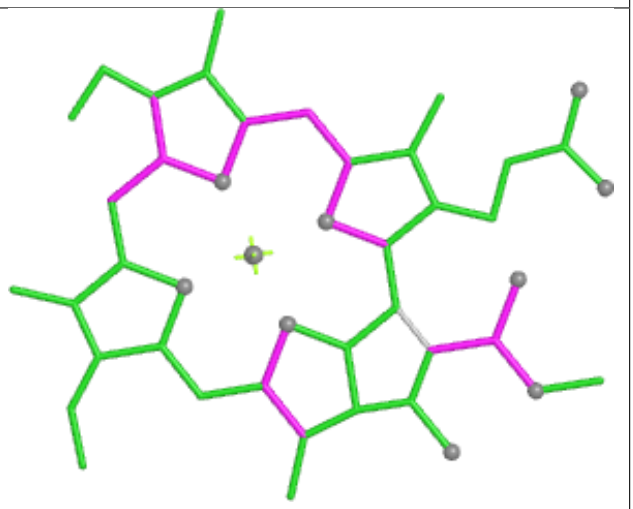


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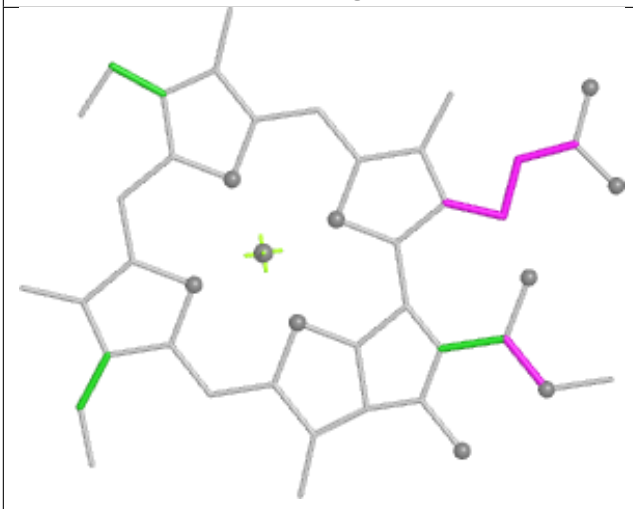
Ligand CLA W 415



Bond lengths



Bond angles

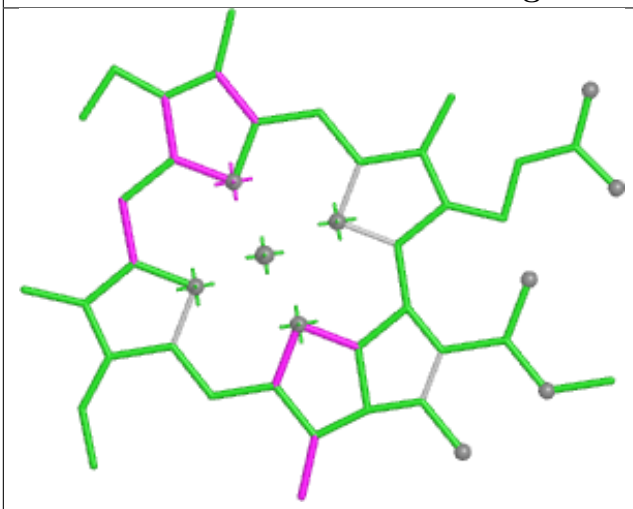


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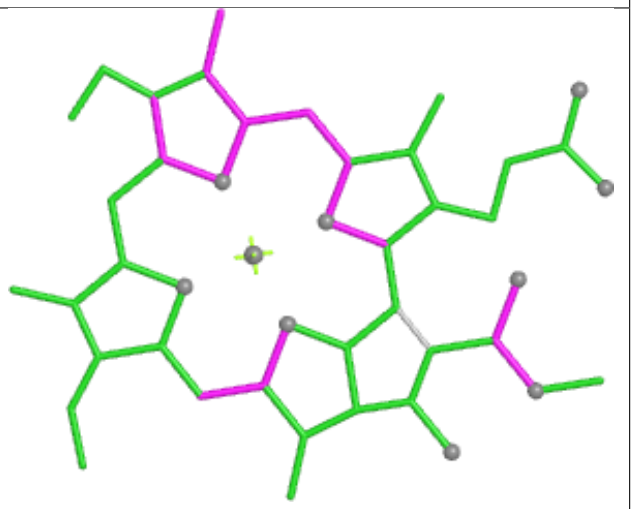


Rings

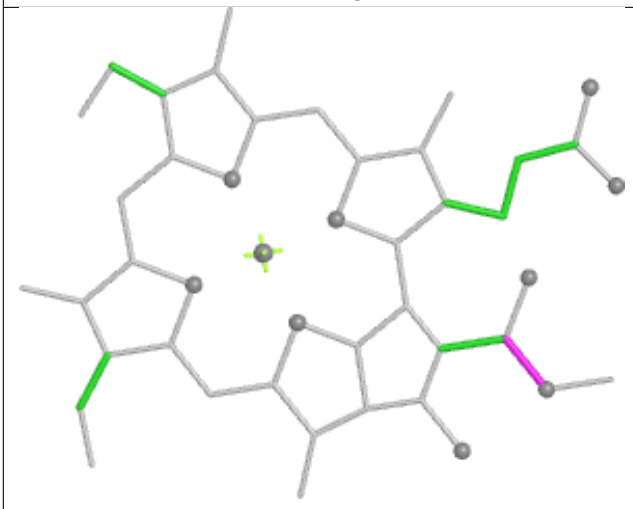
Ligand CLA K 612



Bond lengths



Bond angles

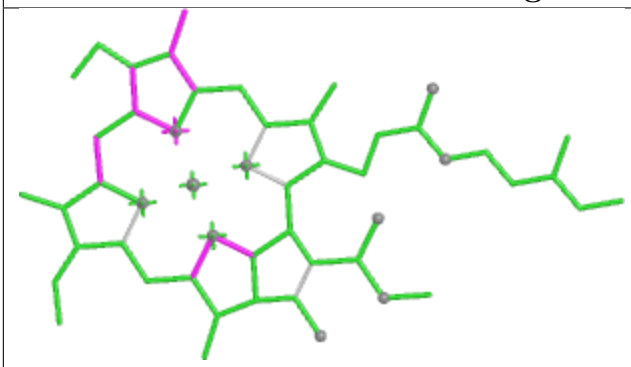


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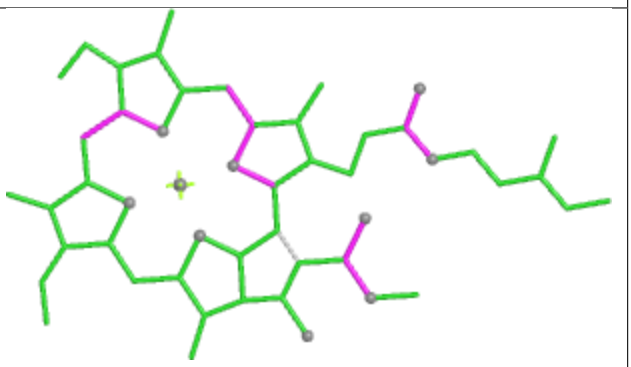


Rings

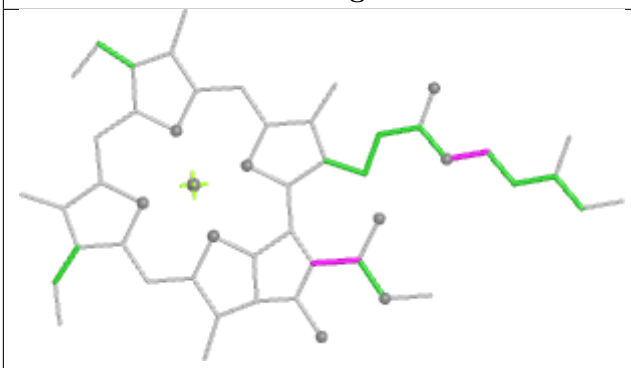
Ligand CLA B 836



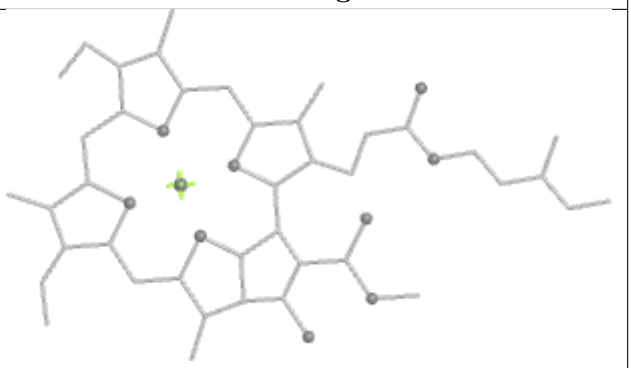
Bond lengths



Bond angles

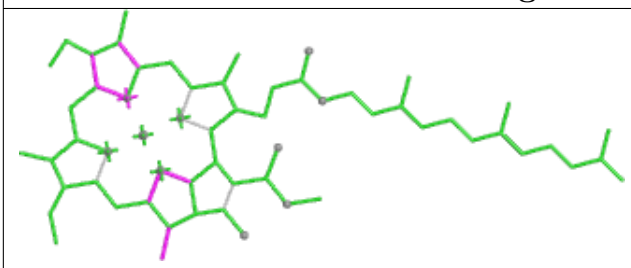


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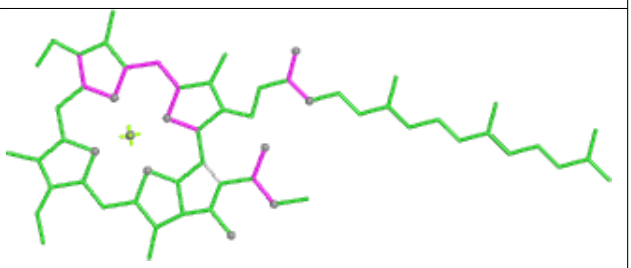


Rings

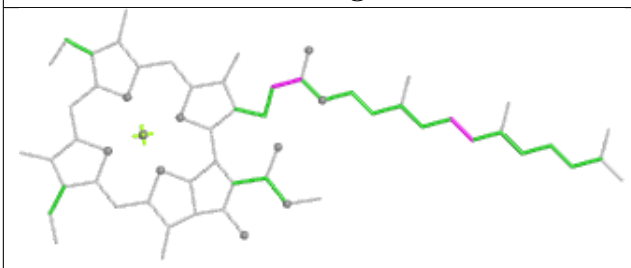
Ligand CLA W 405



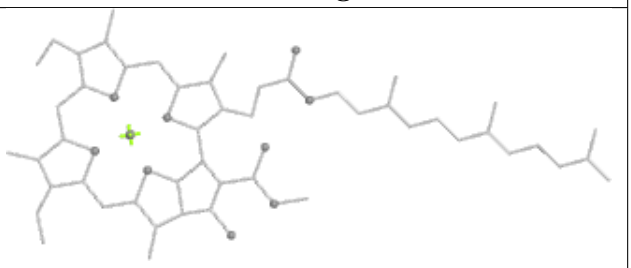
Bond lengths



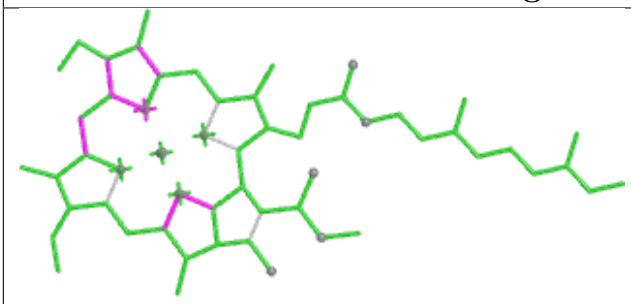
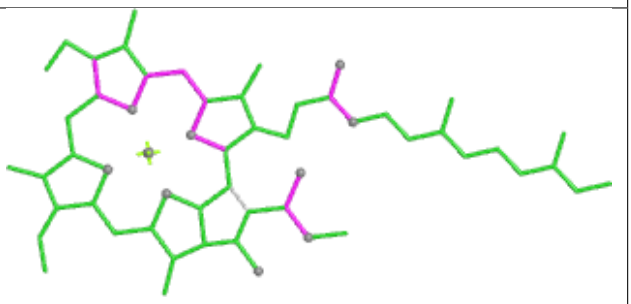
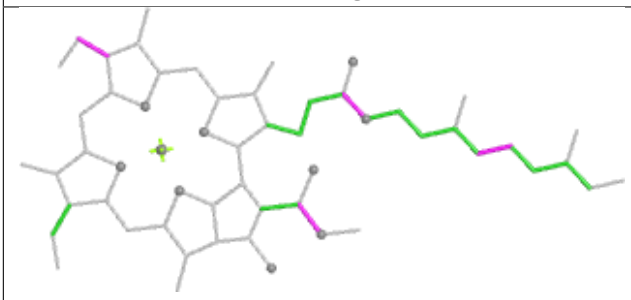
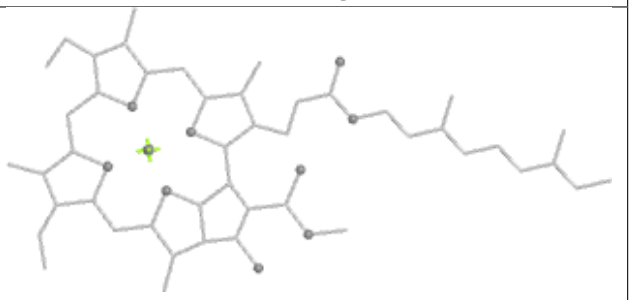
Bond angles



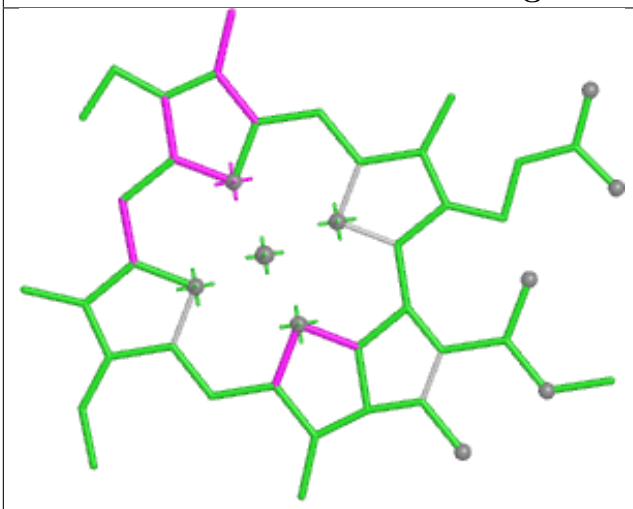
Torsions



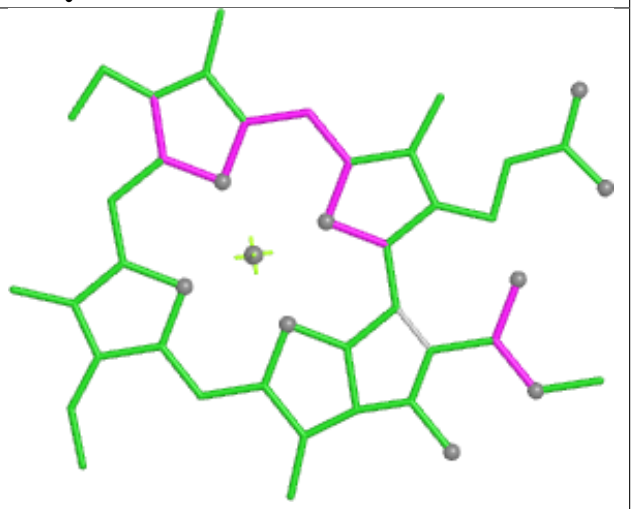
Rings

Ligand CLA U 406	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

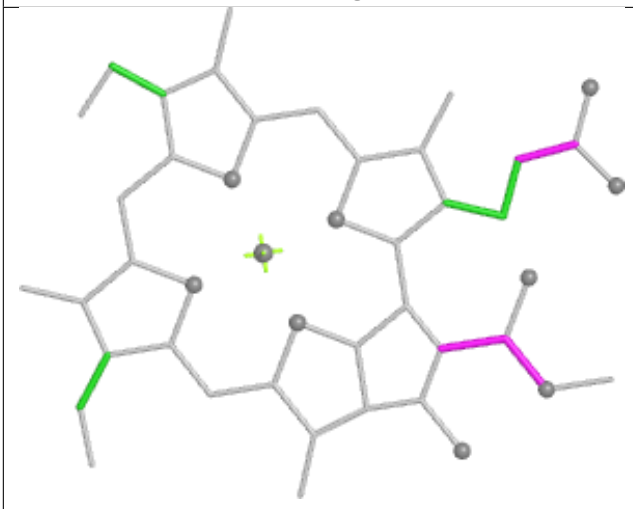
Ligand CLA Q 606



Bond lengths



Bond angles

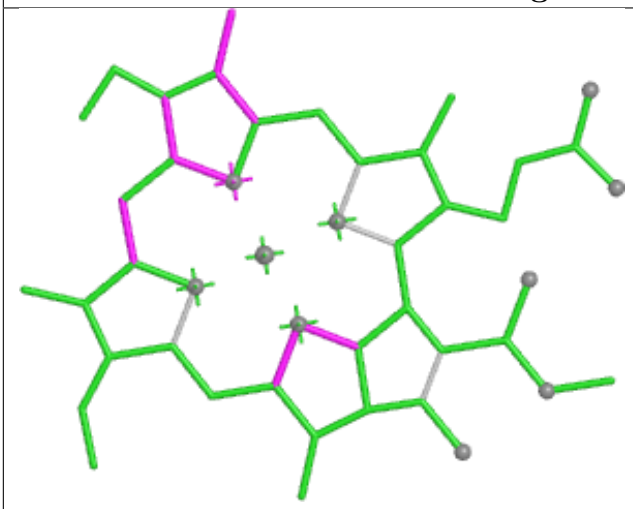


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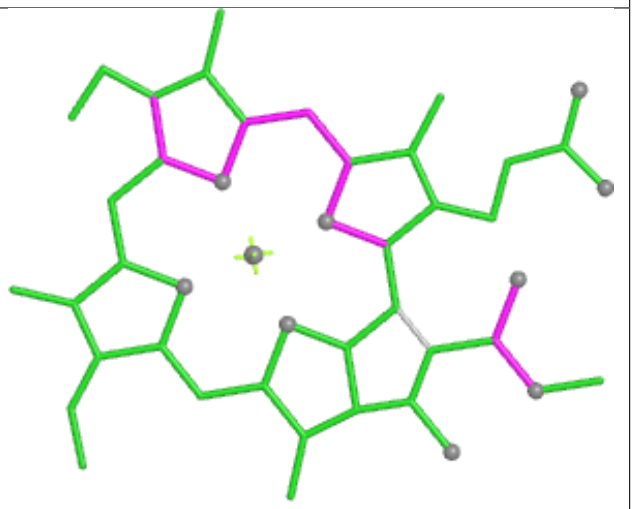


Rings

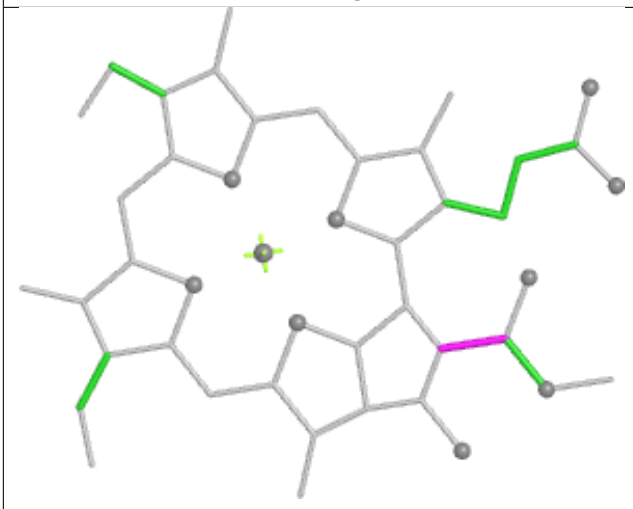
Ligand CLA I 604



Bond lengths



Bond angles

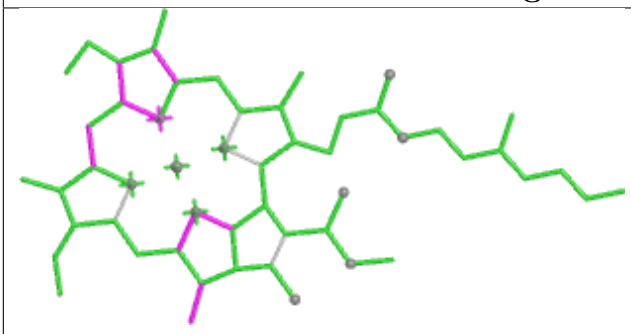


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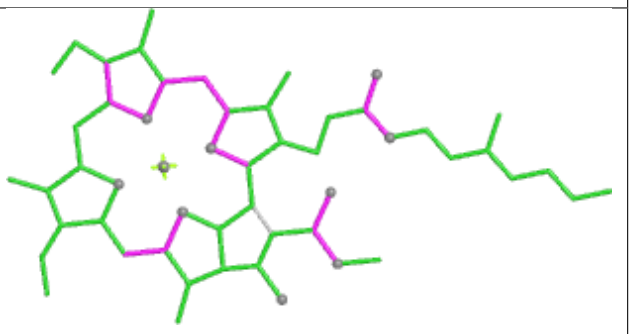


Rings

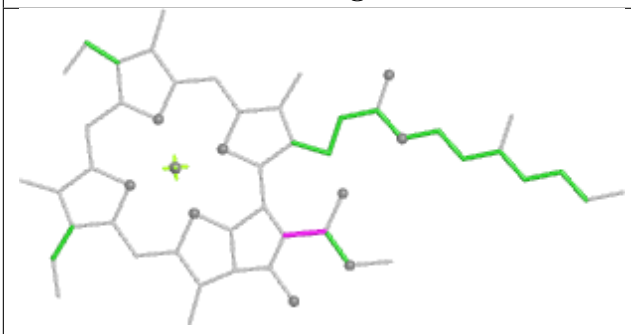
Ligand CLA A 809



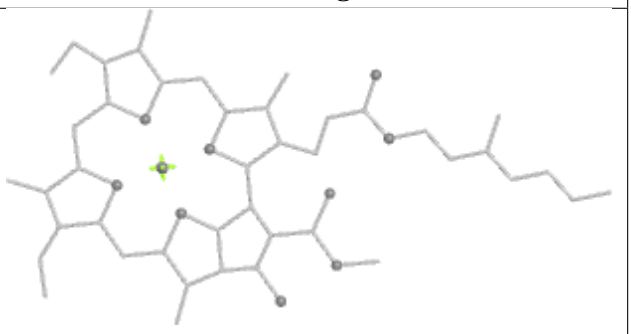
Bond lengths



Bond angles

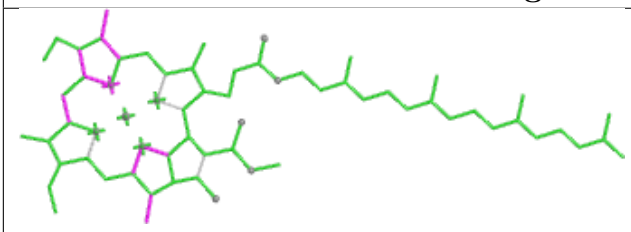


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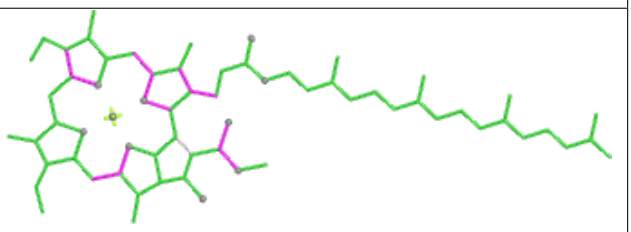


Rings

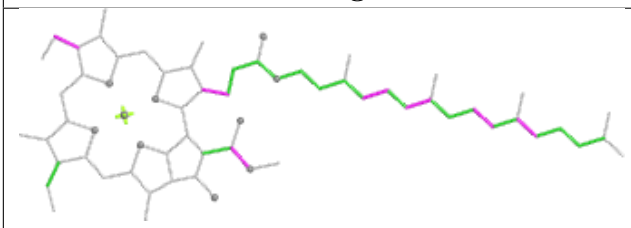
Ligand CLA B 859



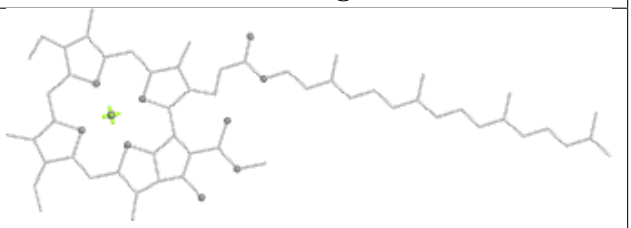
Bond lengths



Bond angles

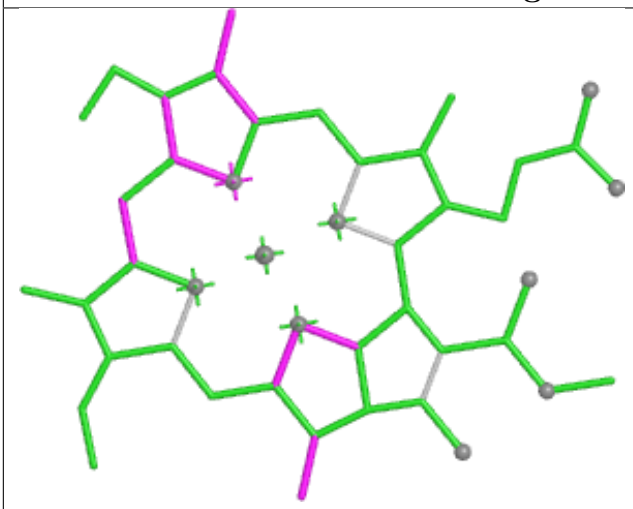


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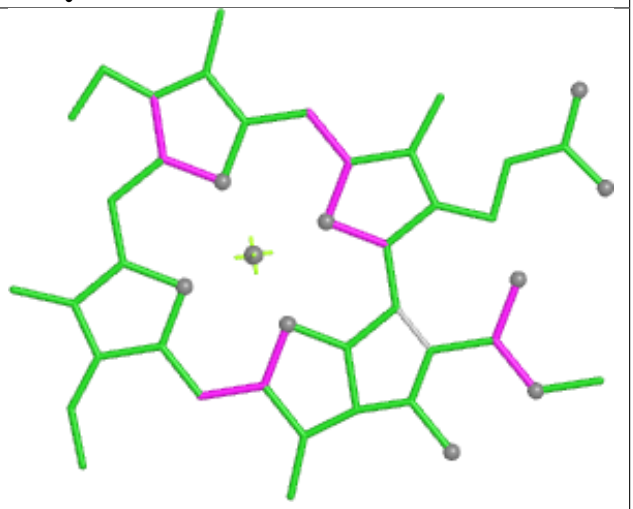


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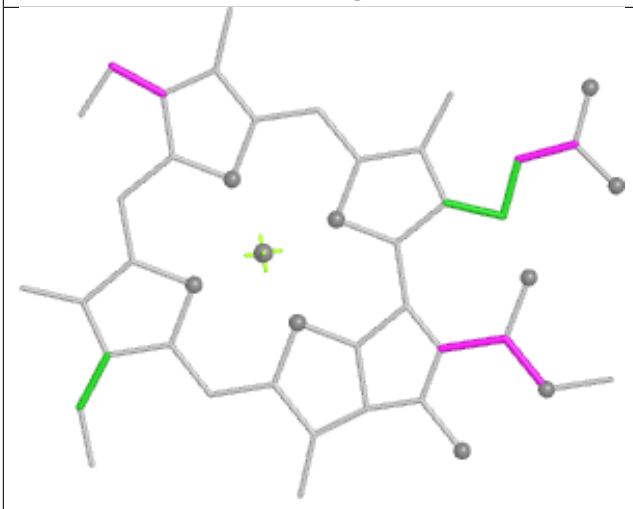
Ligand CLA Q 601



Bond lengths



Bond angles

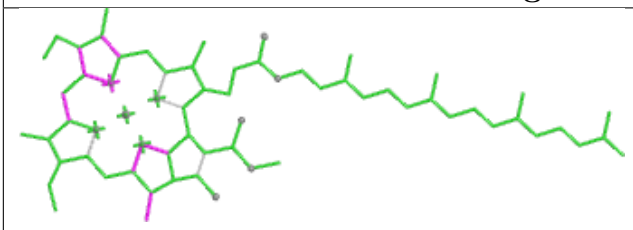


Torsions

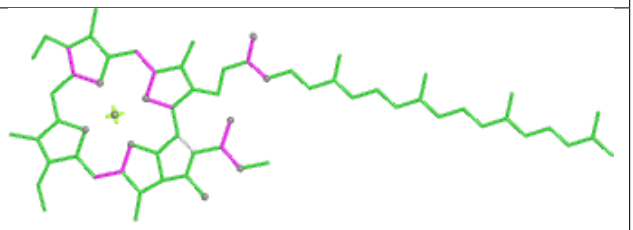


Rings

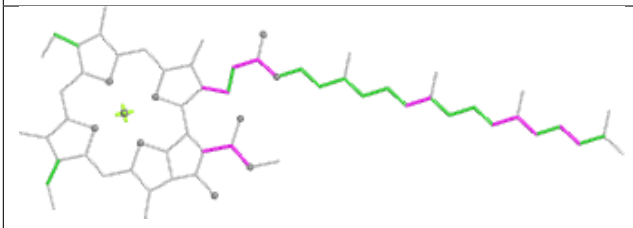
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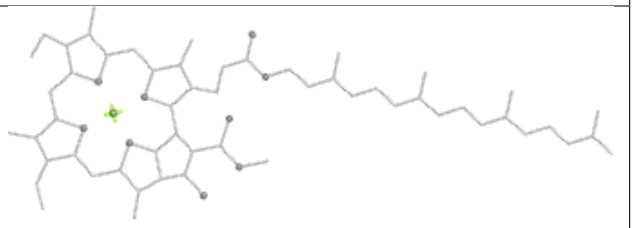
Bond lengths



Bond angles

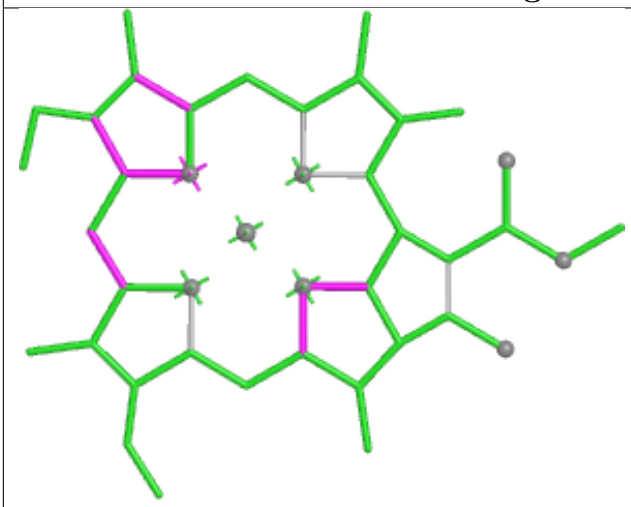


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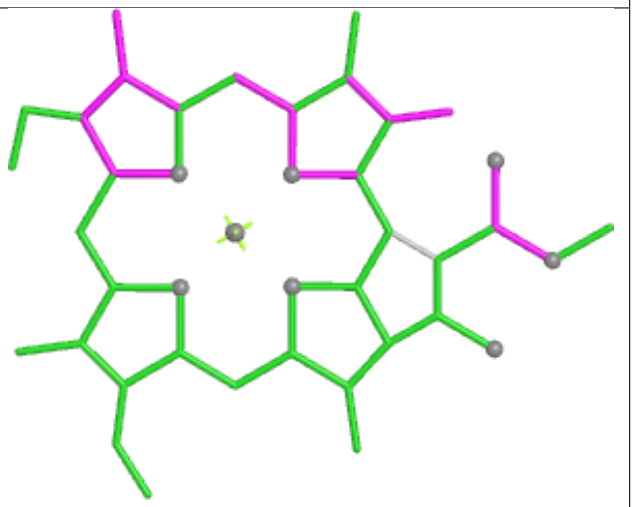


Rings

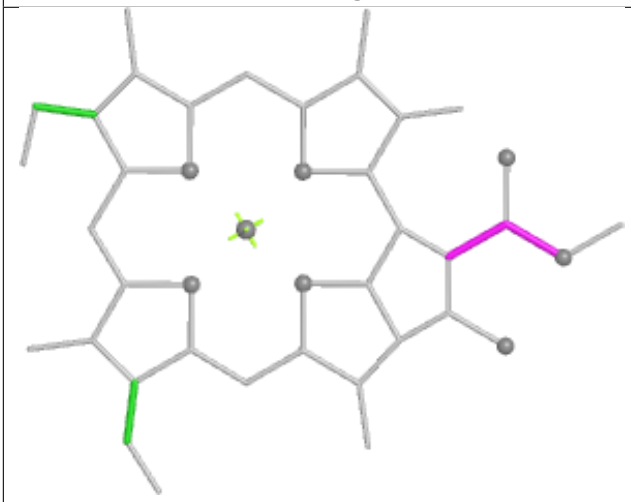
Ligand CLA R 609



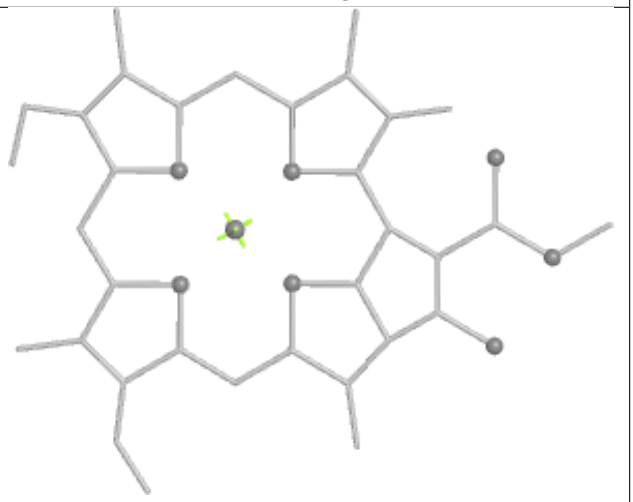
Bond lengths



Bond angles

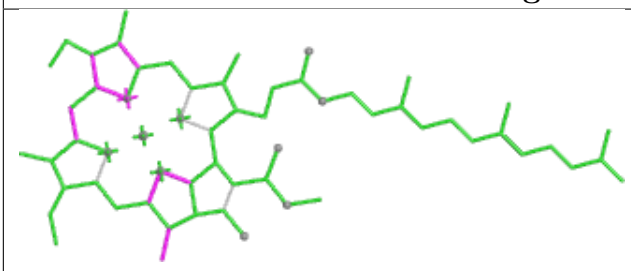


Torsions

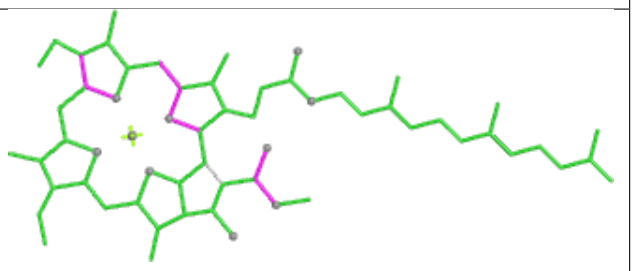


Rings

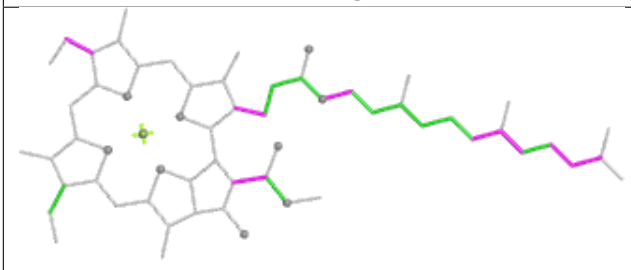
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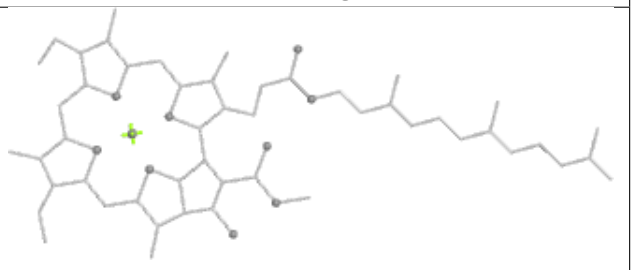
Bond lengths



Bond angles

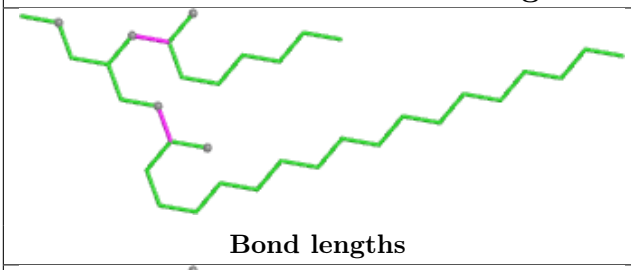


Torsions

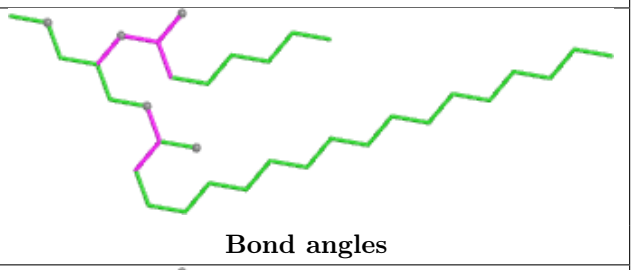


Rings

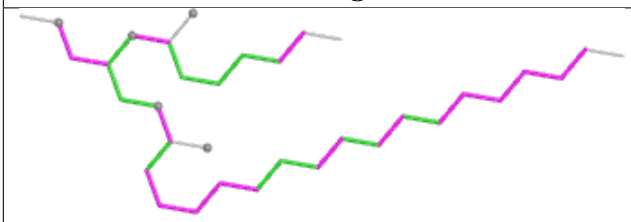
Ligand DGD F 401



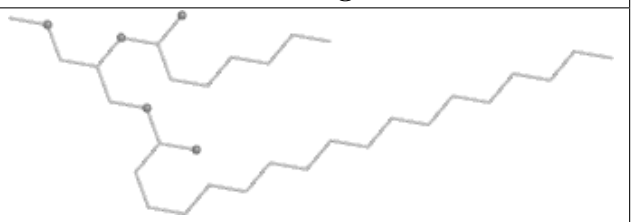
Bond lengths



Bond angles

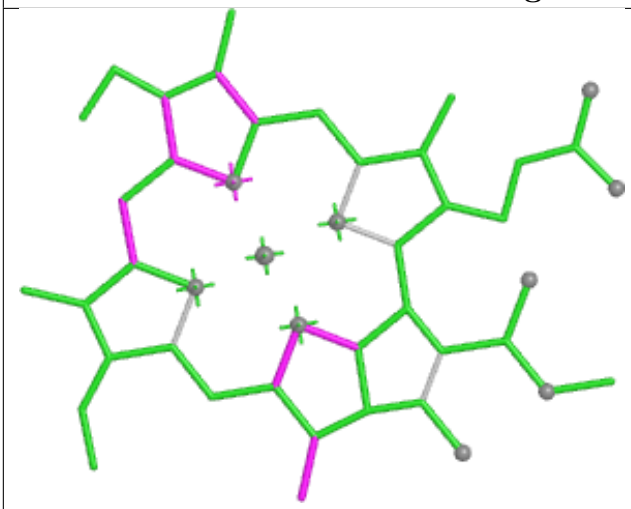


Torsions

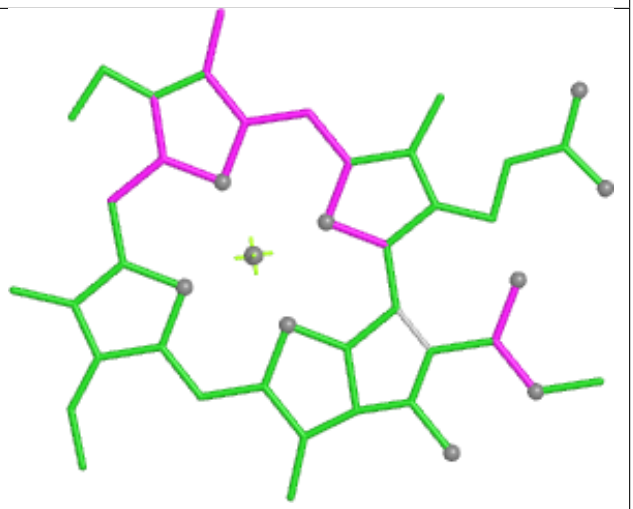


Rings

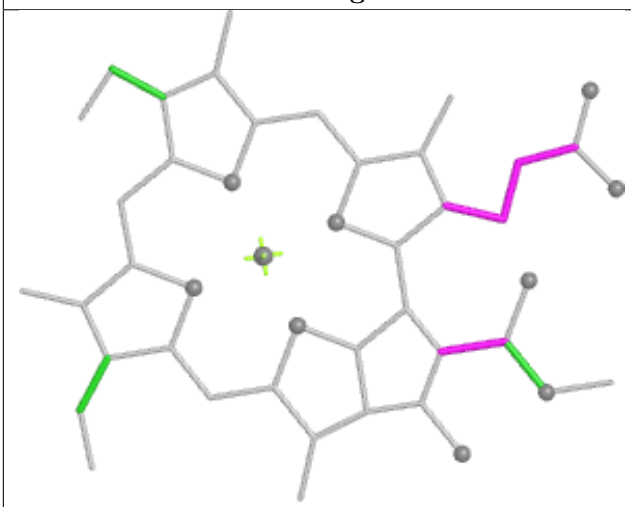
Ligand CLA B 814



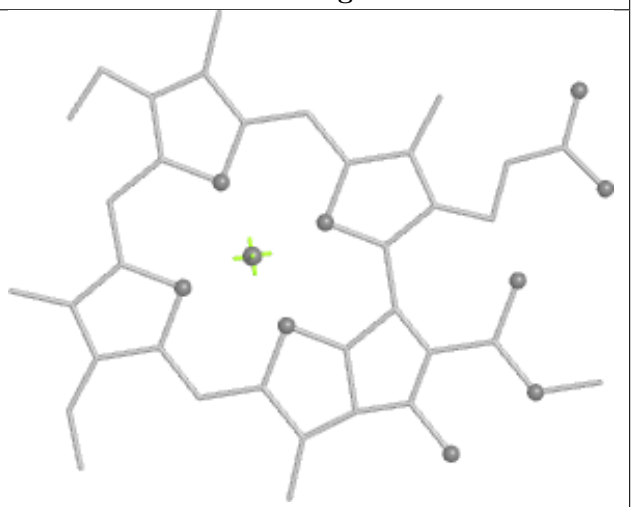
Bond lengths



Bond angles

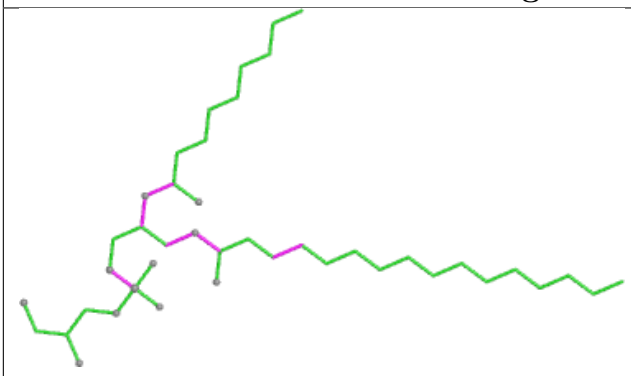


Torsions

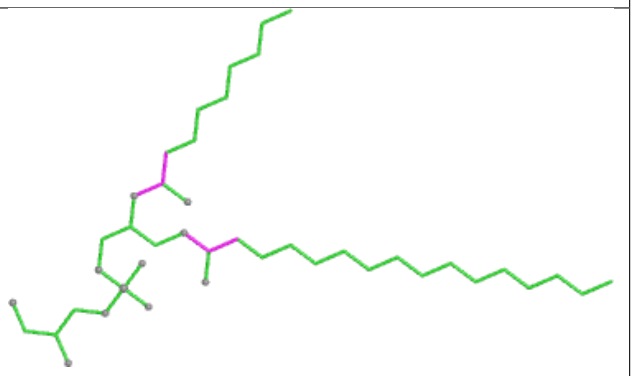


Rings

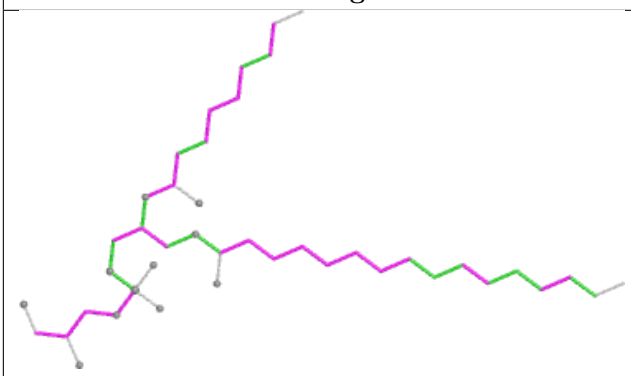
Ligand LHG X 420



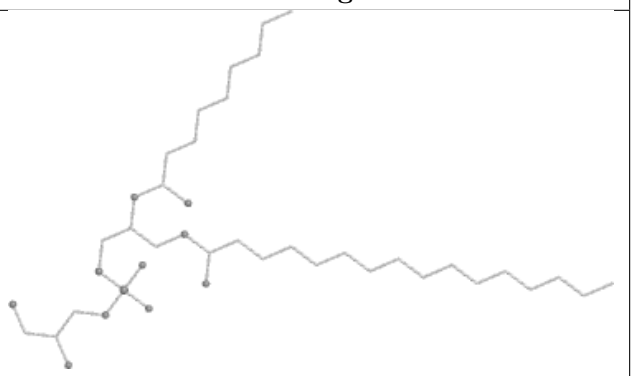
Bond lengths



Bond angles

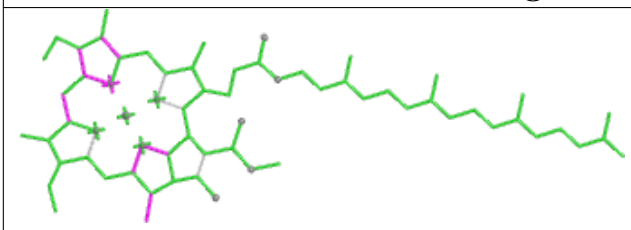


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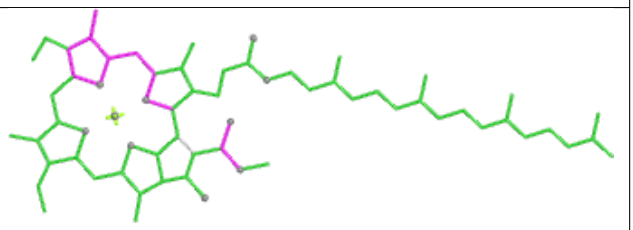


Rings

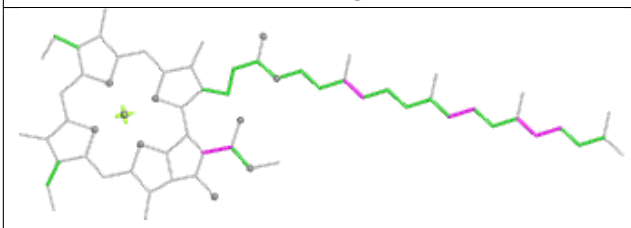
Ligand CLA B 834



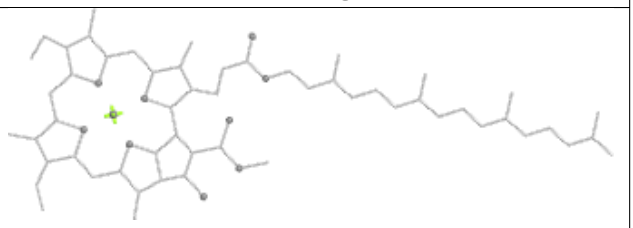
Bond lengths



Bond angles

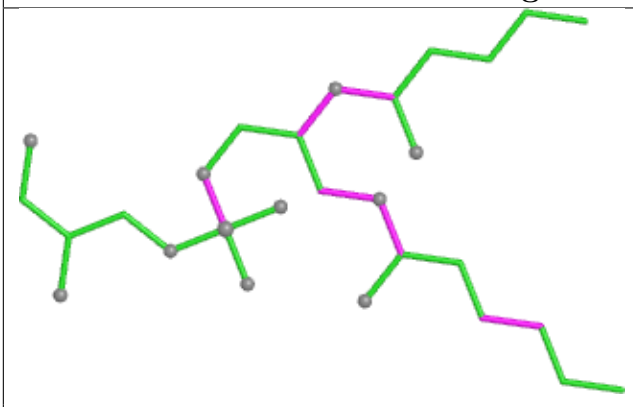


Torsions

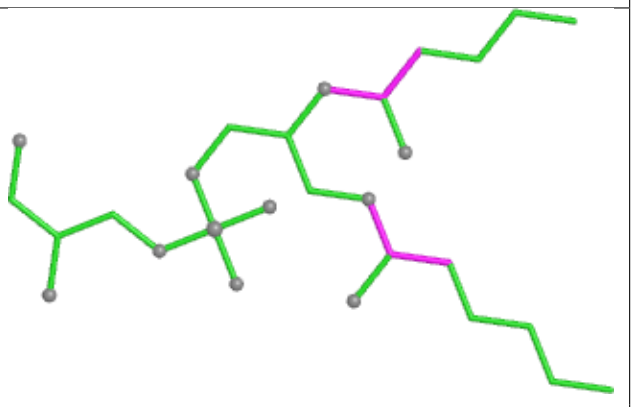


Rings

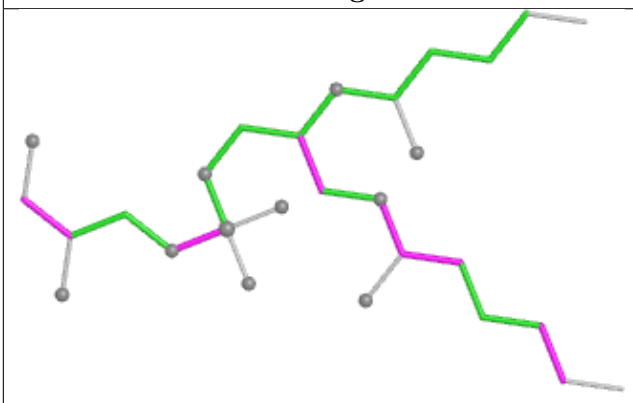
Ligand LHG N 614



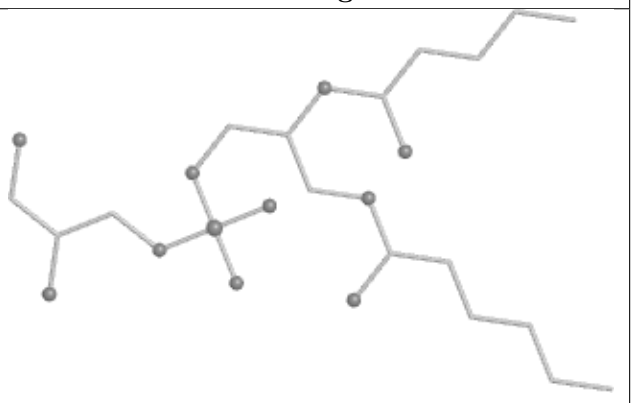
Bond lengths



Bond angles

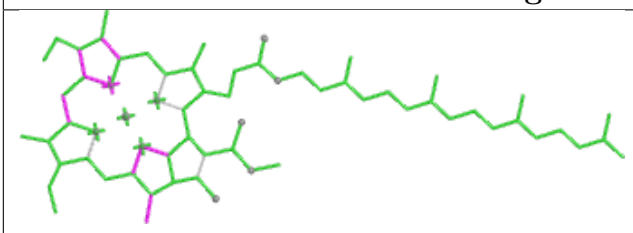


Torsions

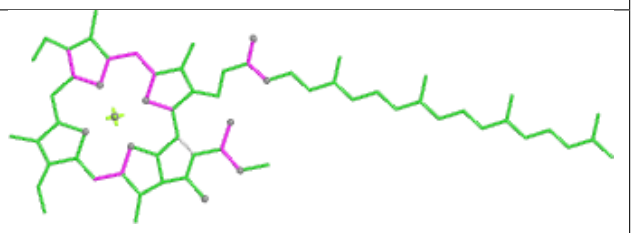


Rings

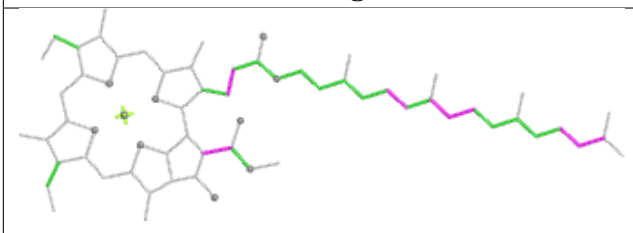
Ligand CLA T 602



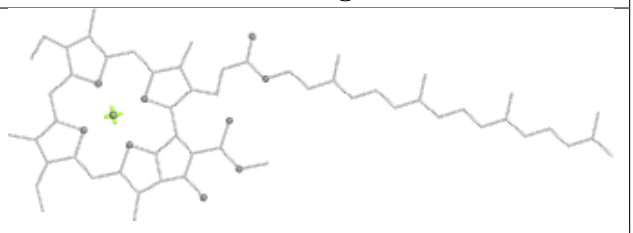
Bond lengths



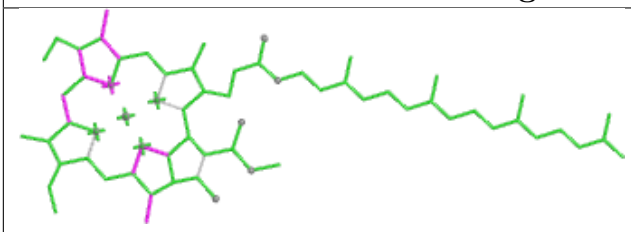
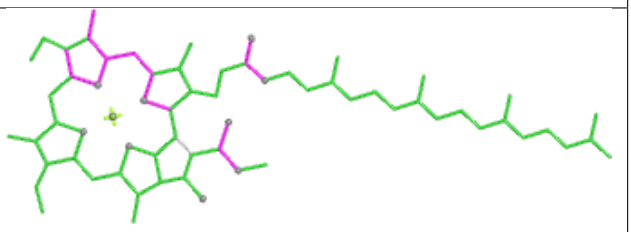
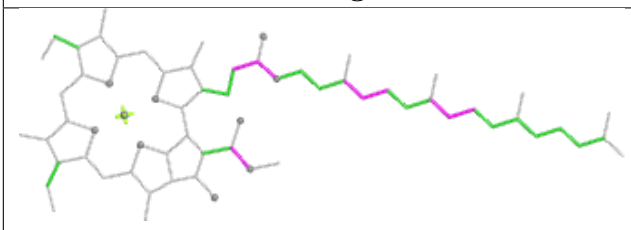
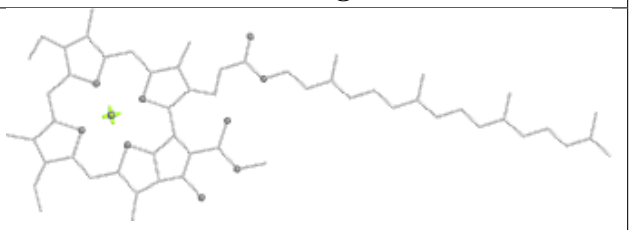
Bond angles

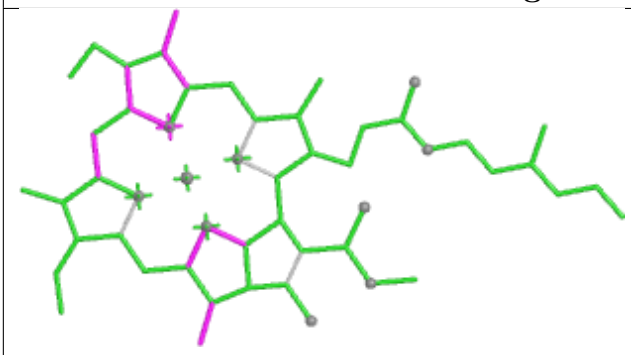
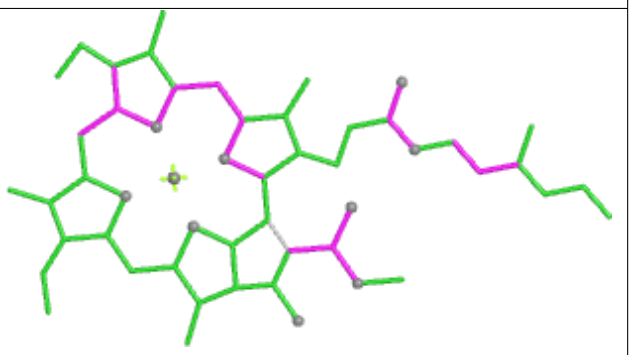
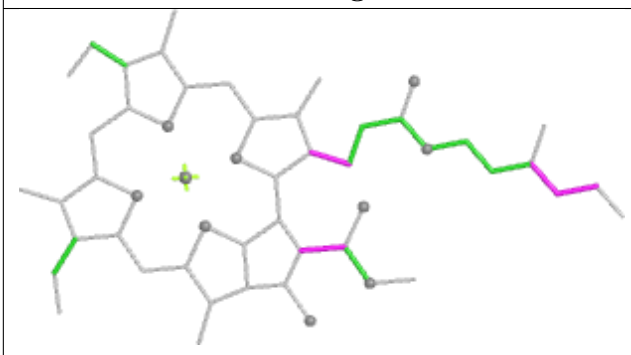
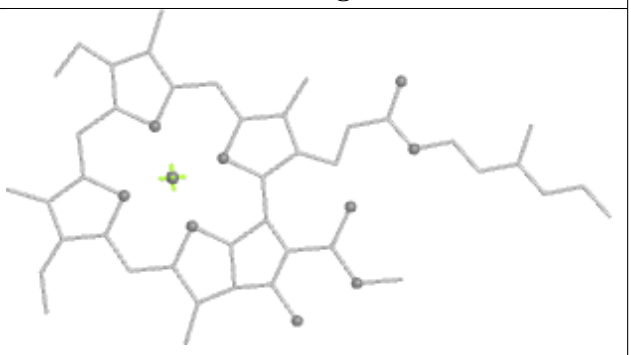


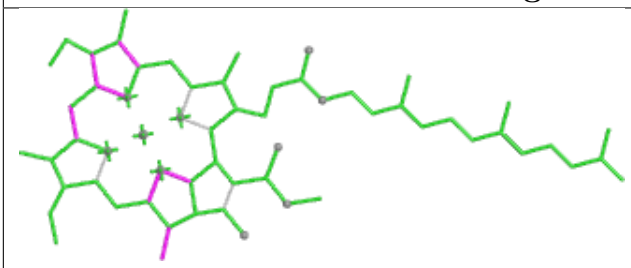
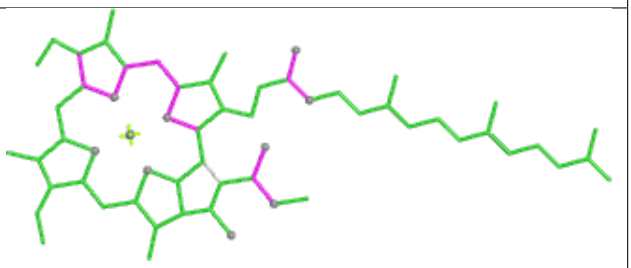
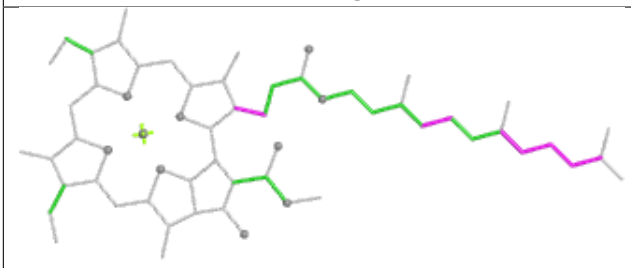
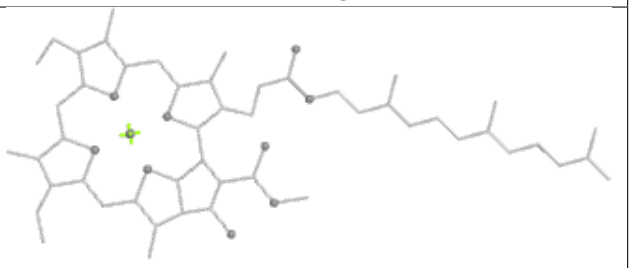
Torsions

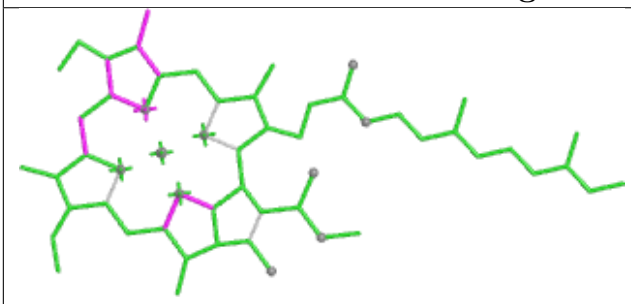
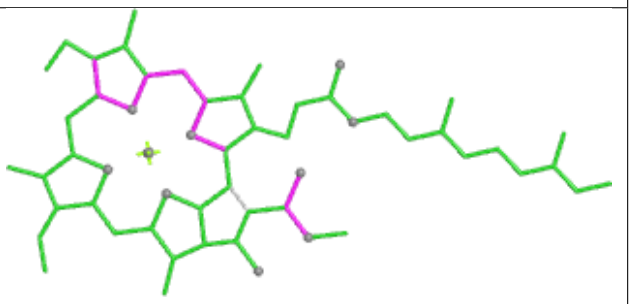
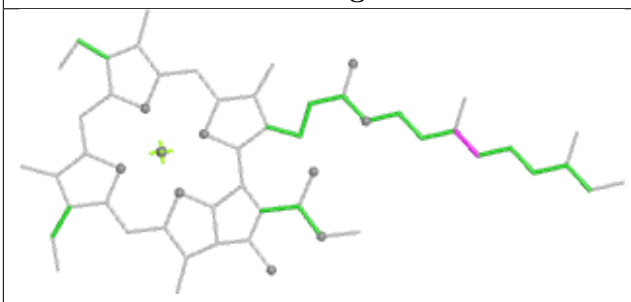
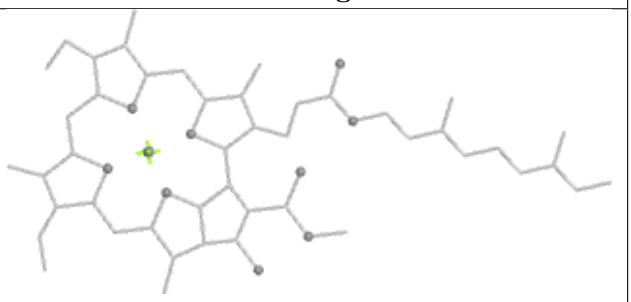


Rings

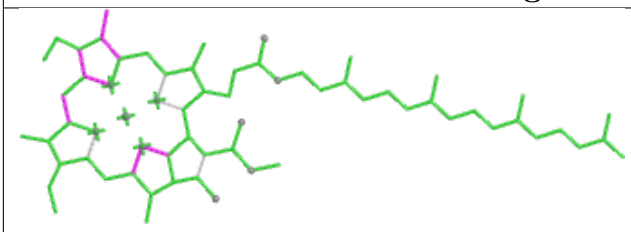
Ligand CLA W 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

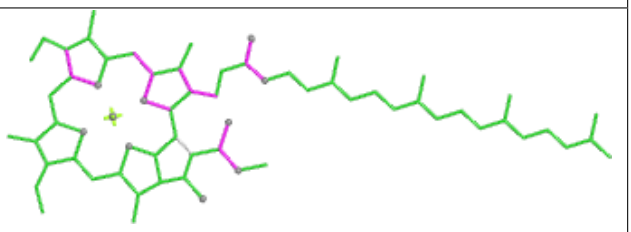
Ligand CLA X 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA W 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

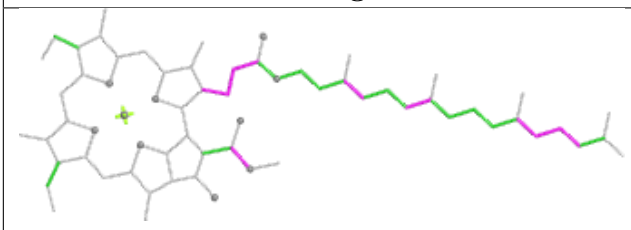
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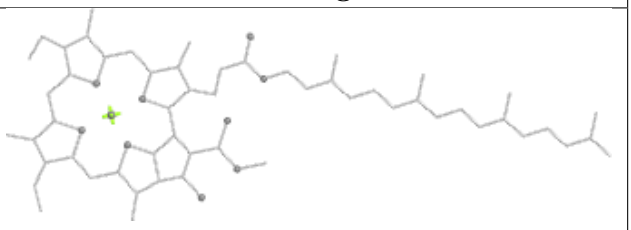
Bond lengths



Bond angles

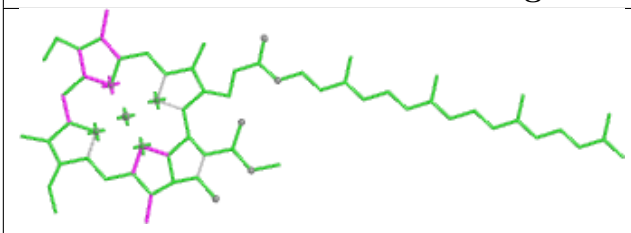


Torsions

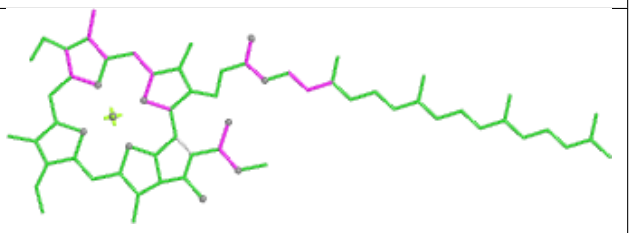


Rings

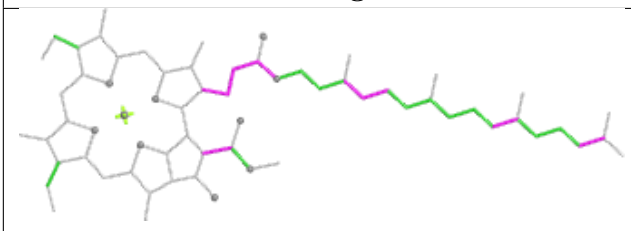
Ligand CLA B 804



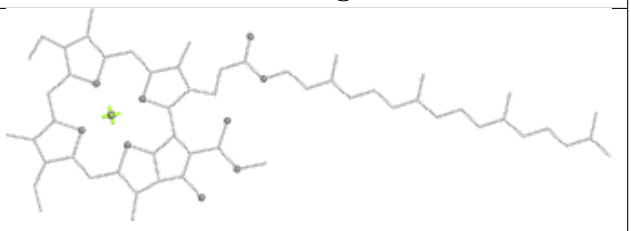
Bond lengths



Bond angles

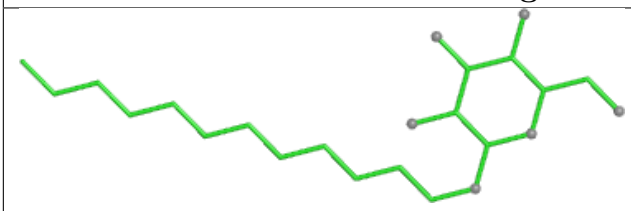


Torsions

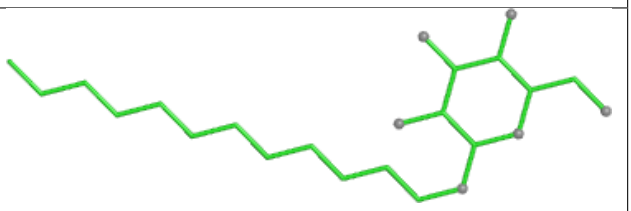


Rings

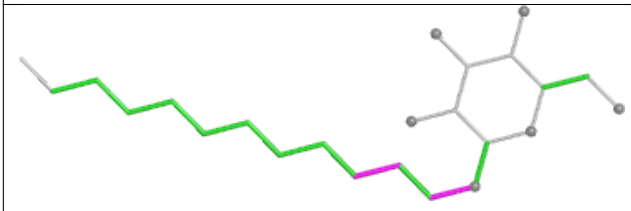
Ligand LMU B 849



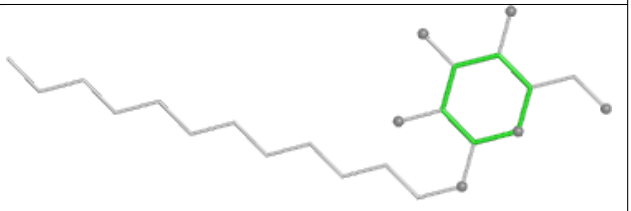
Bond lengths



Bond angles

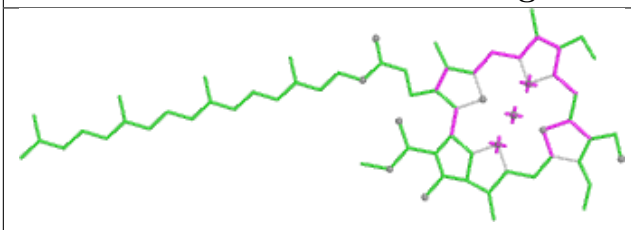


Torsions

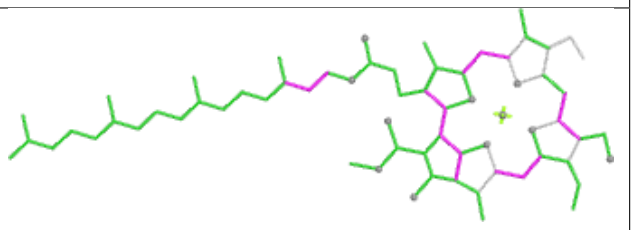


Rings

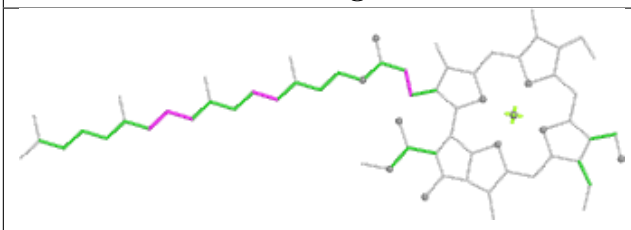
Ligand CHL W 408



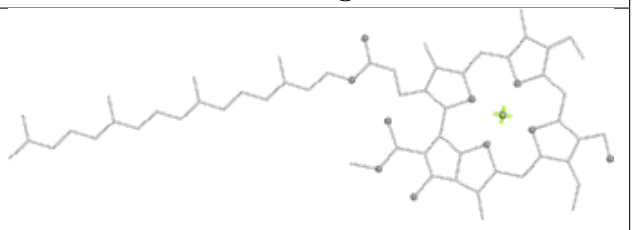
Bond lengths



Bond angles

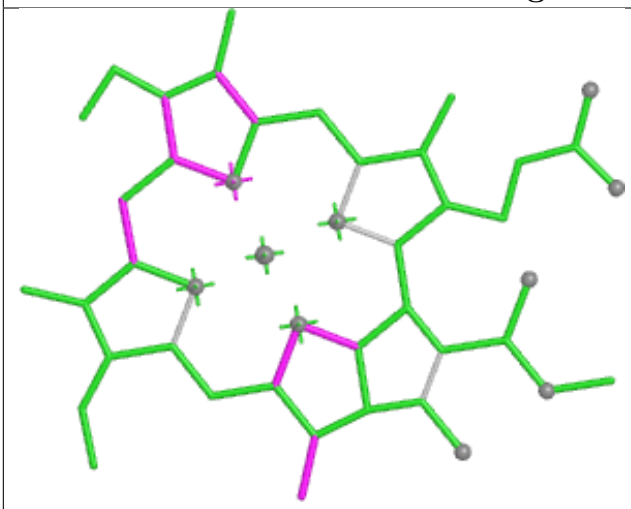


Torsions

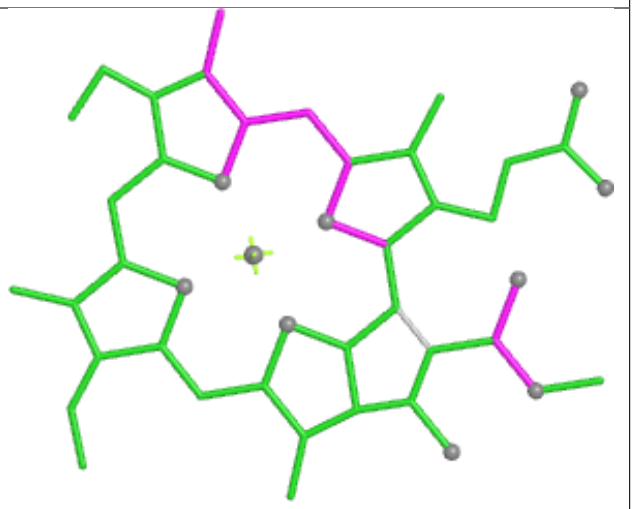


Rings

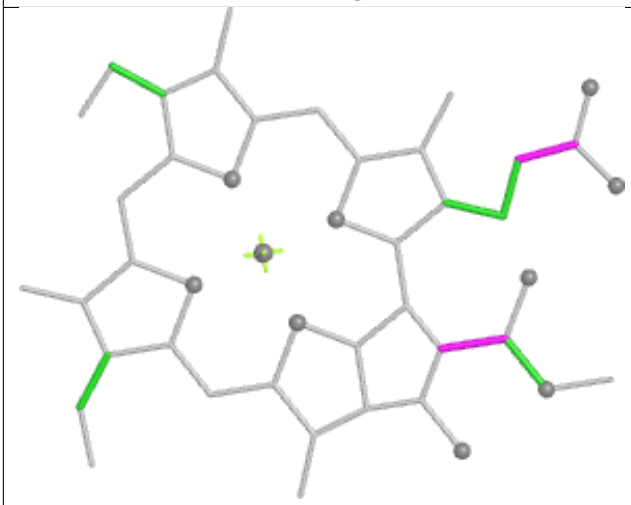
Ligand CLA S 603



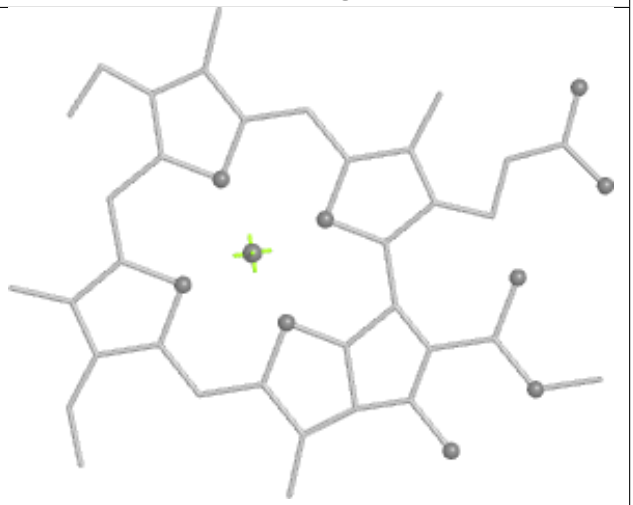
Bond lengths



Bond angles

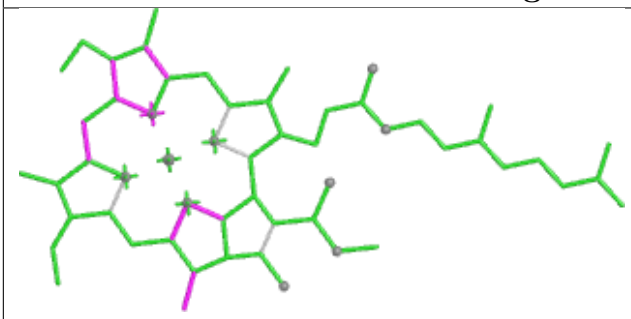


Torsions

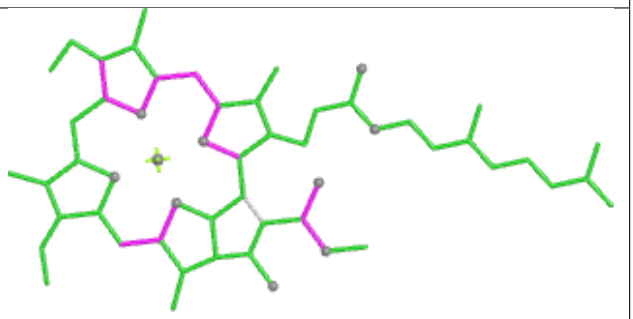


Rings

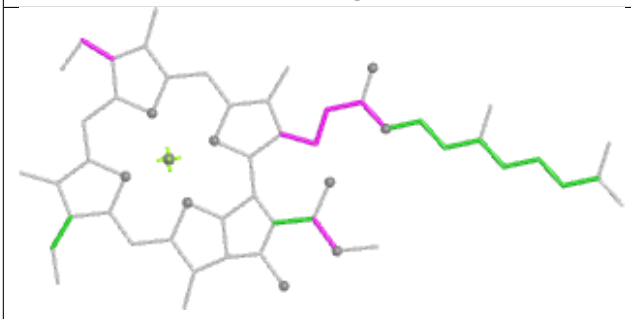
Ligand CLA H 309



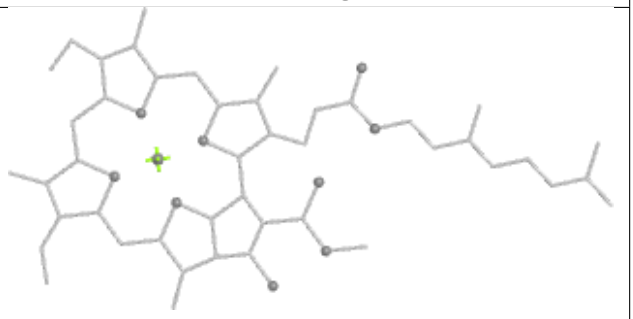
Bond lengths



Bond angles

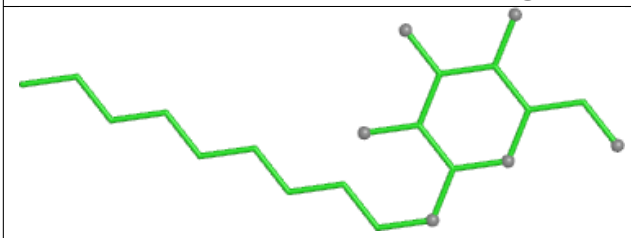


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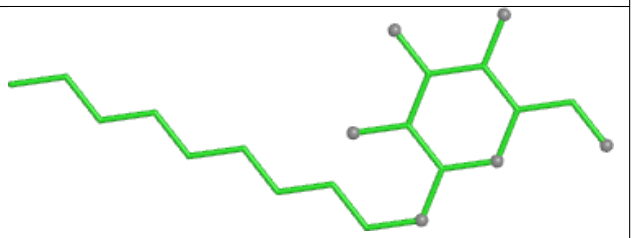


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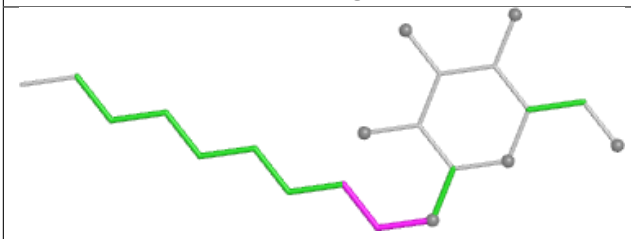
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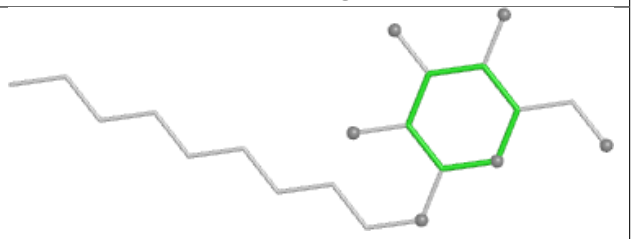
Bond lengths



Bond angles

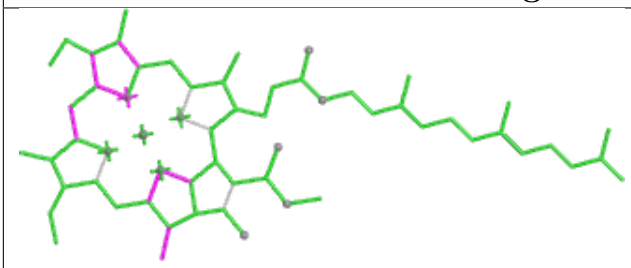


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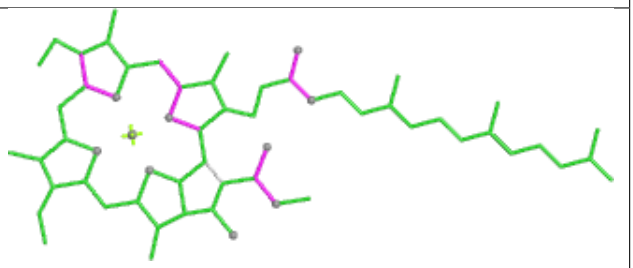


Rings

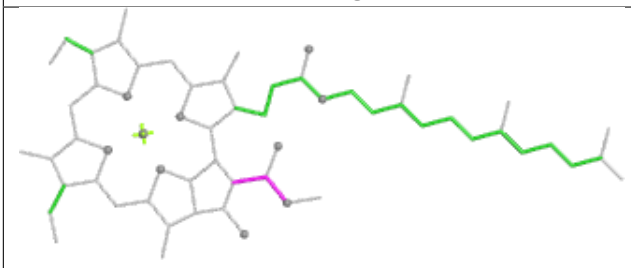
Ligand CLA G 607



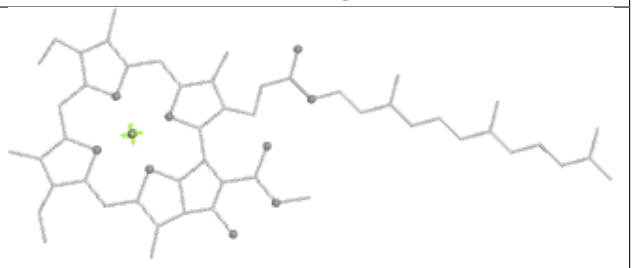
Bond lengths



Bond angles

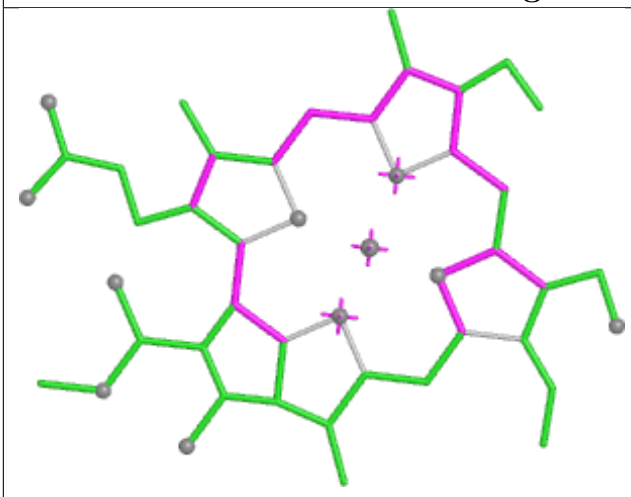


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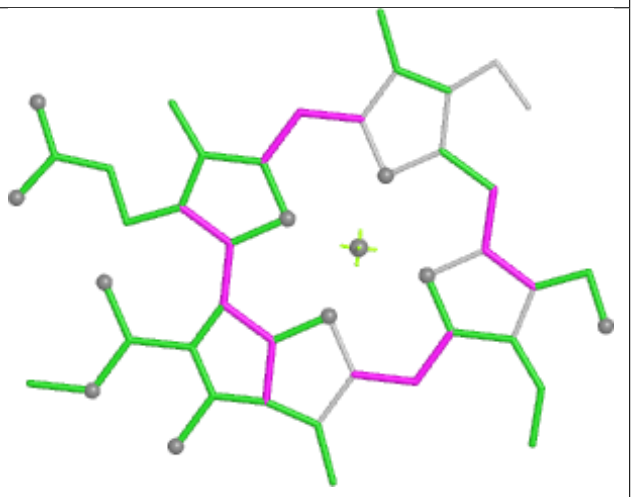


Rings

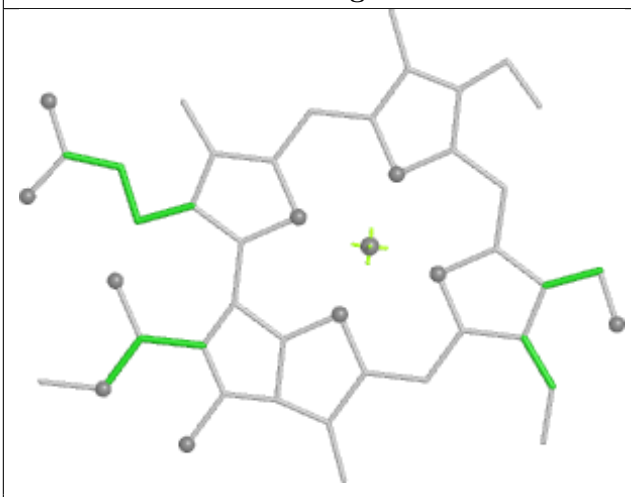
Ligand CHL V 605



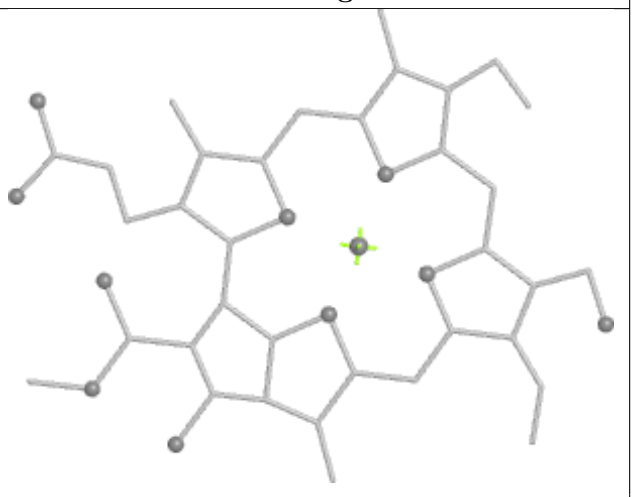
Bond lengths



Bond angles

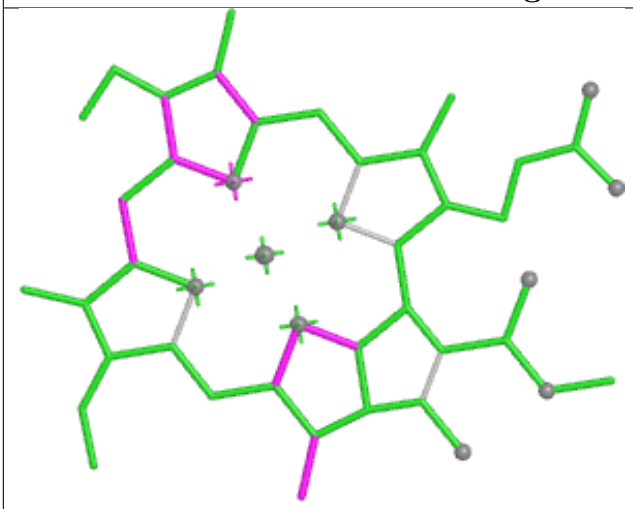


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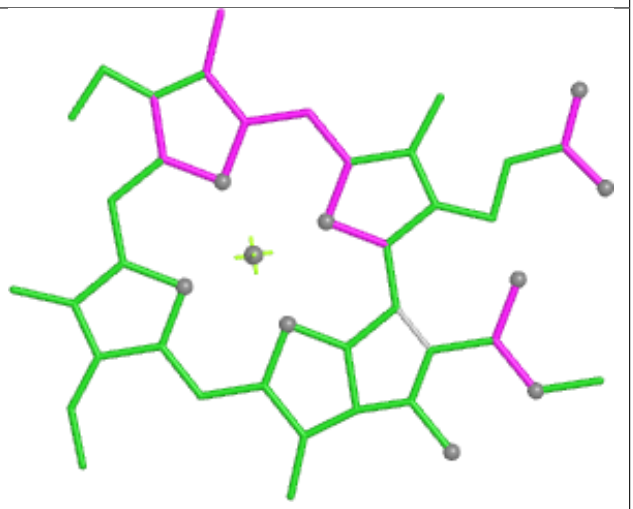


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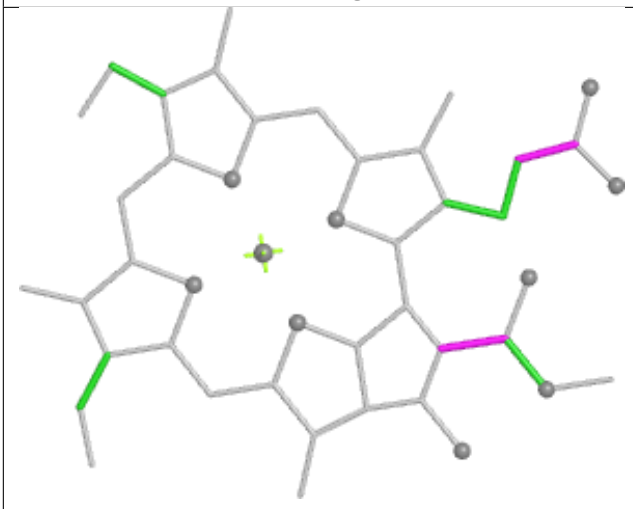
Ligand CLA X 411



Bond lengths



Bond angles

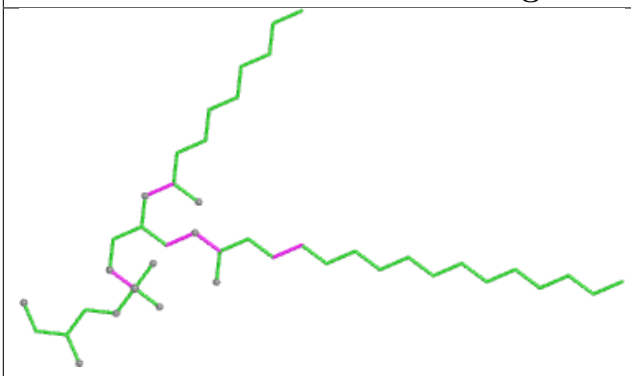


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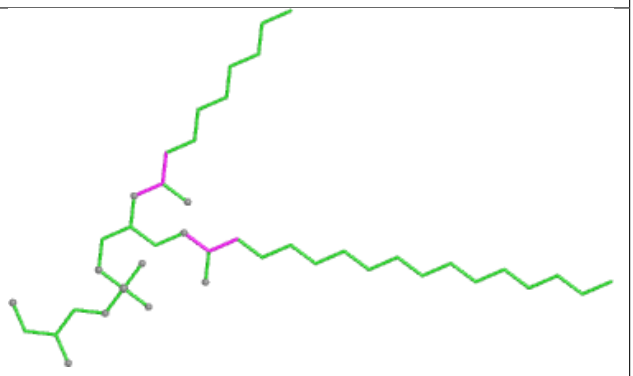


Rings

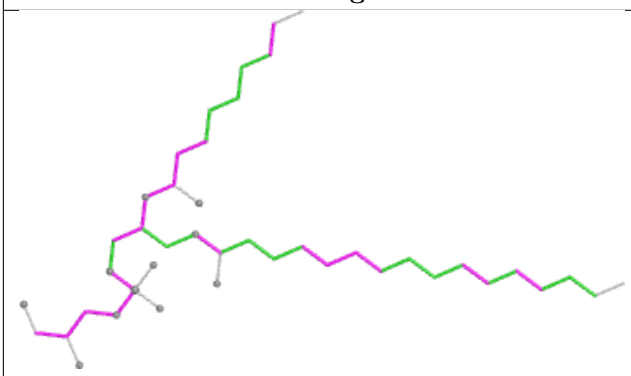
Ligand LHG O 324



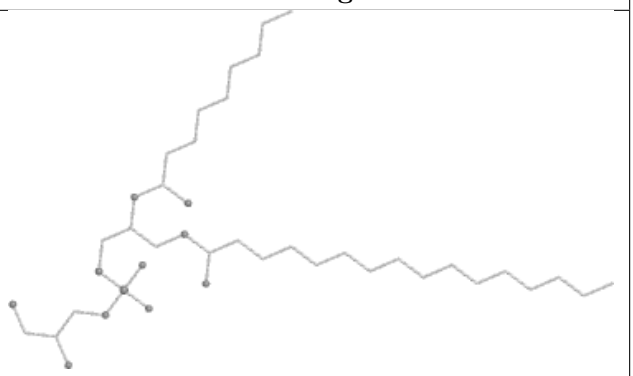
Bond lengths



Bond angles

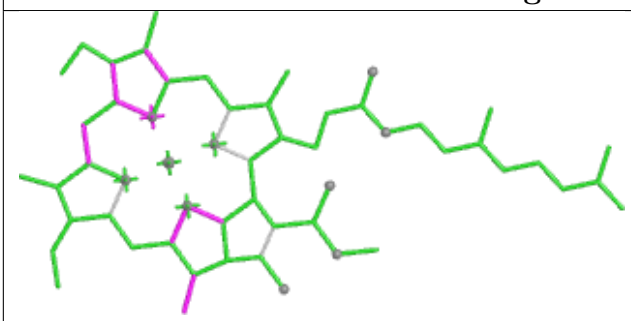


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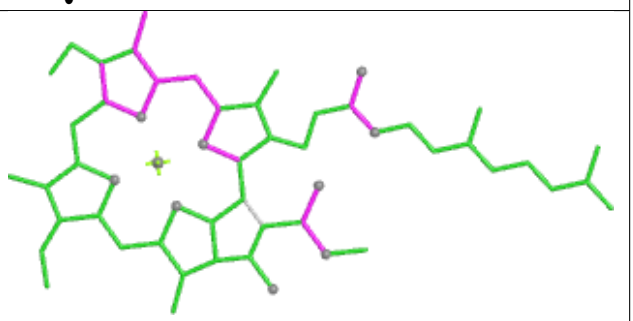


Rings

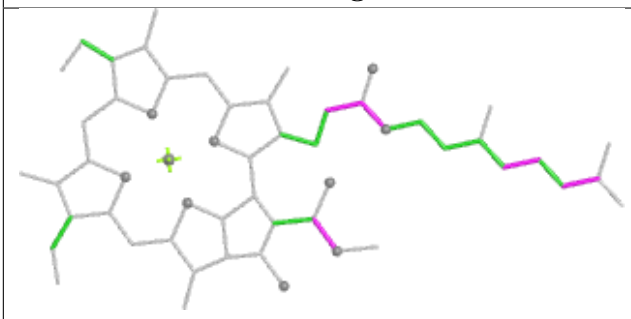
Ligand CLA Q 611



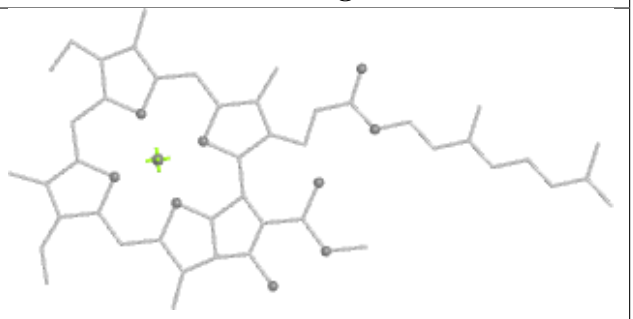
Bond lengths



Bond angles

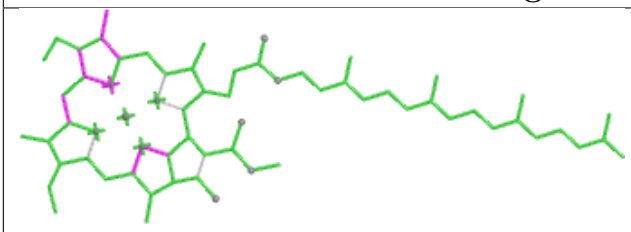


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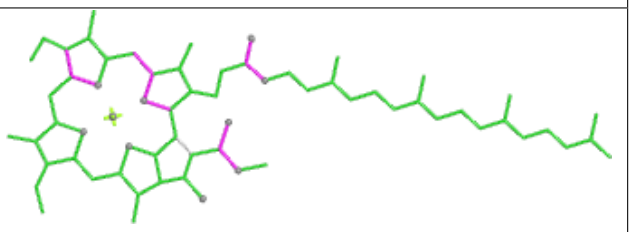


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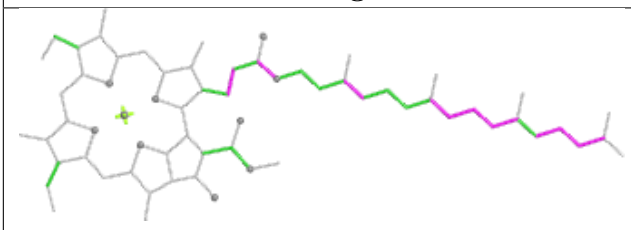
Ligand CLA B 817



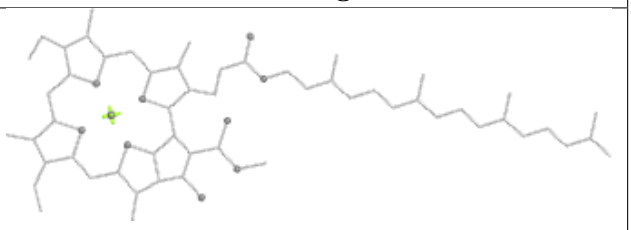
Bond lengths



Bond angles

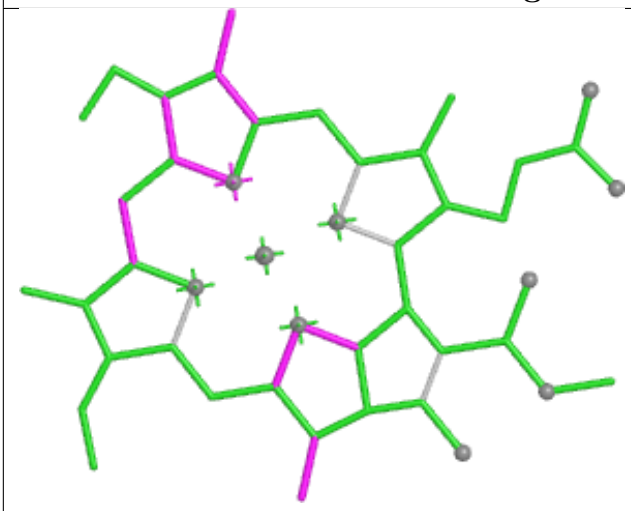


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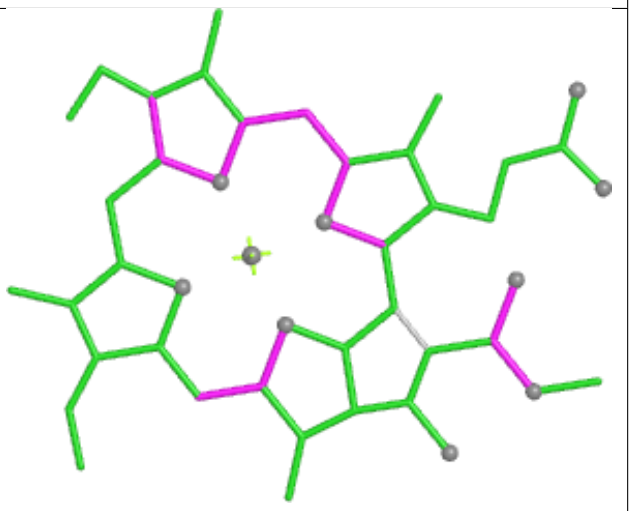


Rings

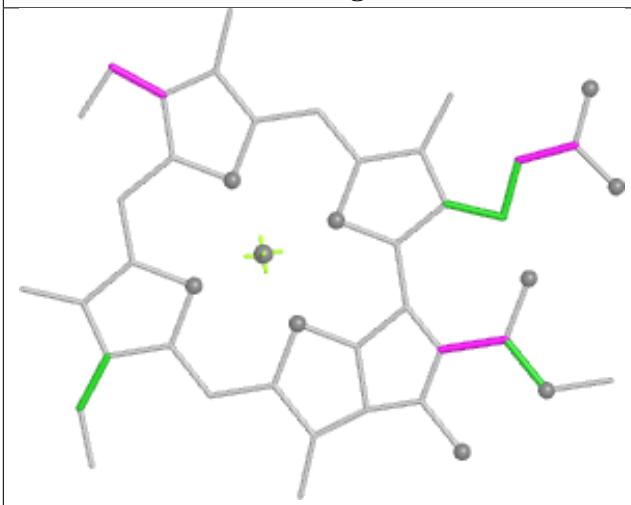
Ligand CLA A 834



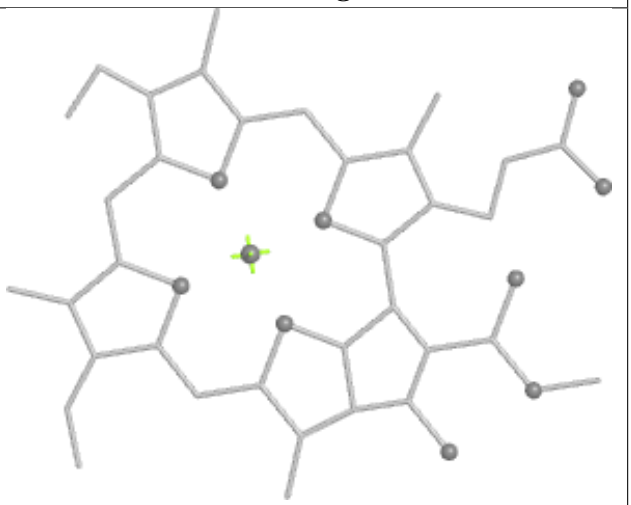
Bond lengths



Bond angles

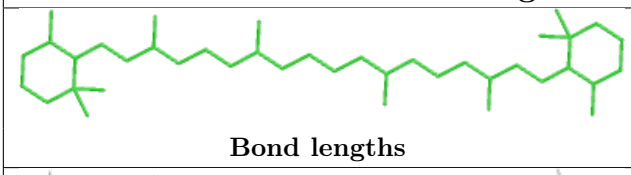


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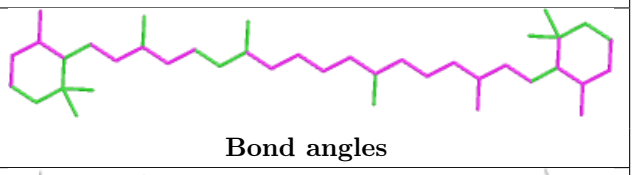


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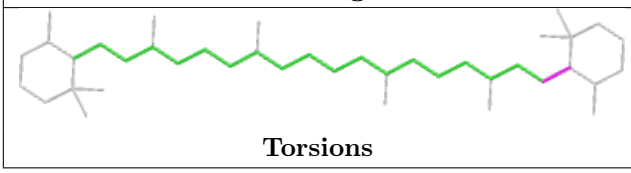
Ligand BCR M 101



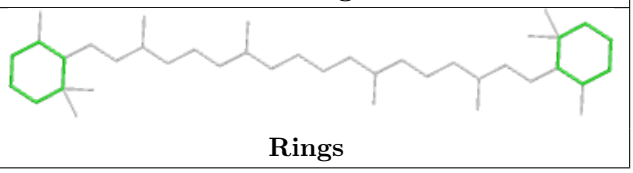
Bond lengths



Bond angles



Torsions

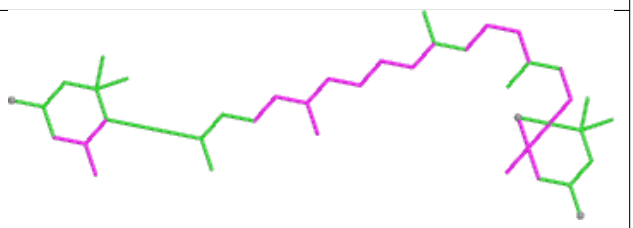


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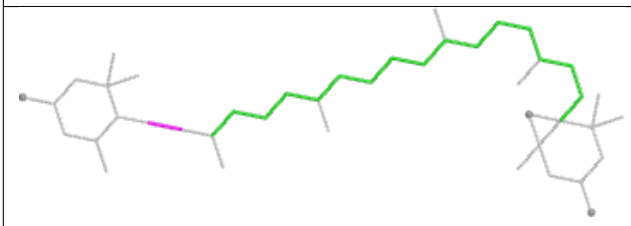
Ligand DD6 S 611



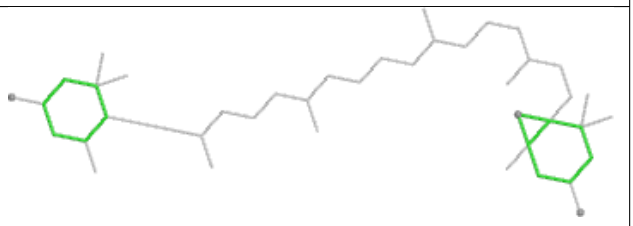
Bond lengths



Bond angles

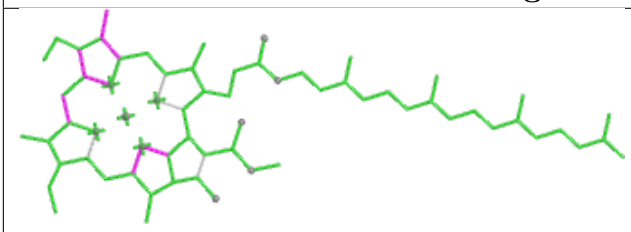


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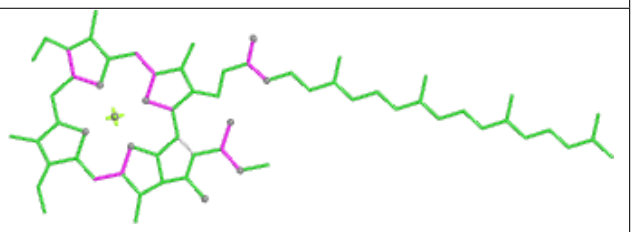


Rings

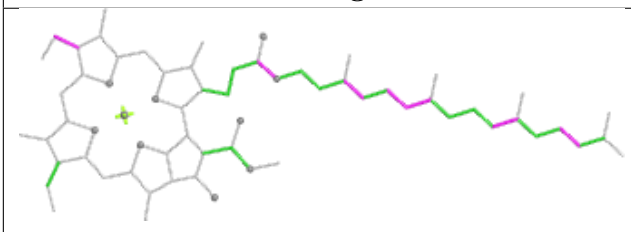
Ligand CLA A 836



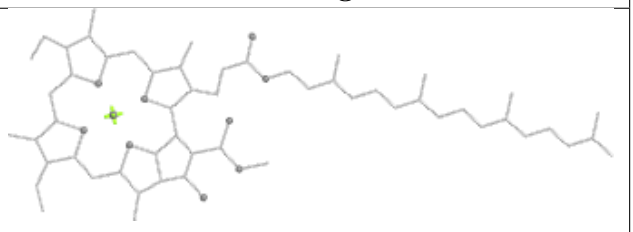
Bond lengths



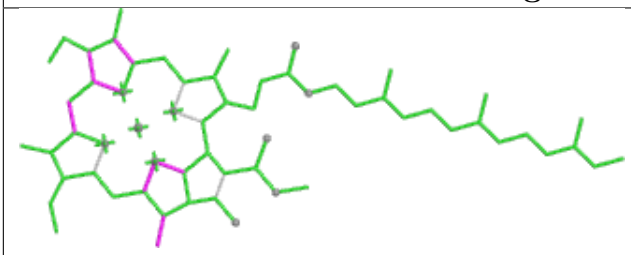
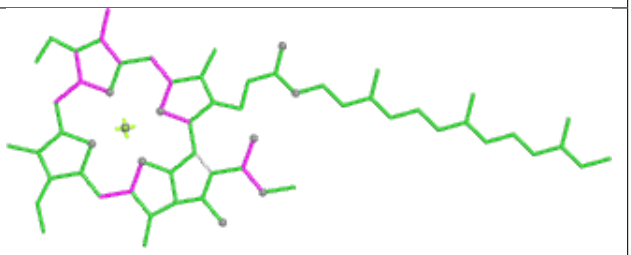
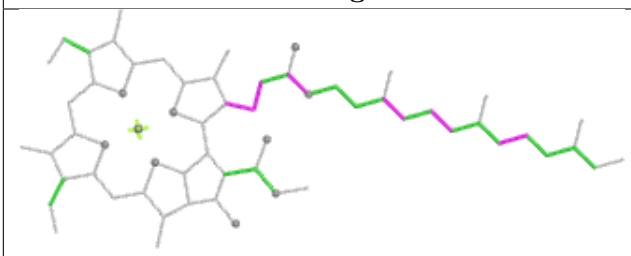
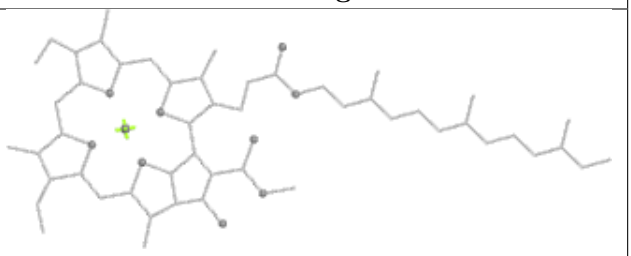
Bond angles

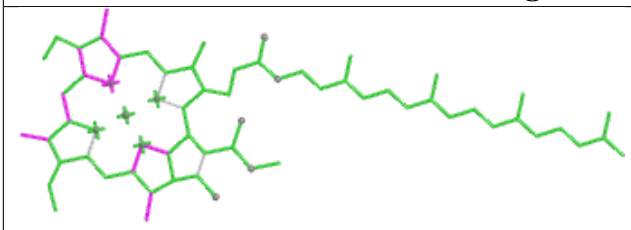
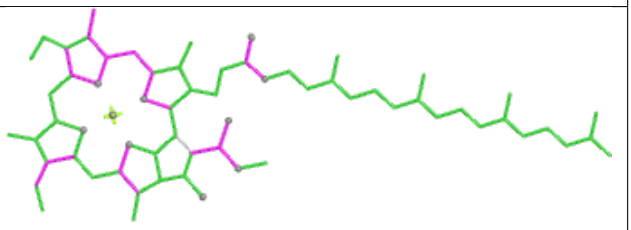
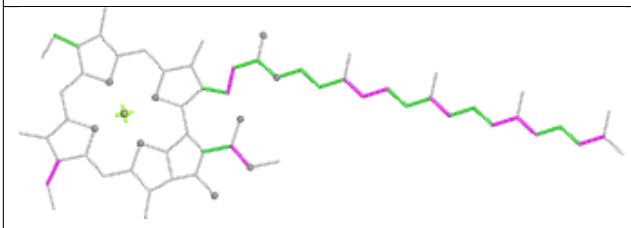
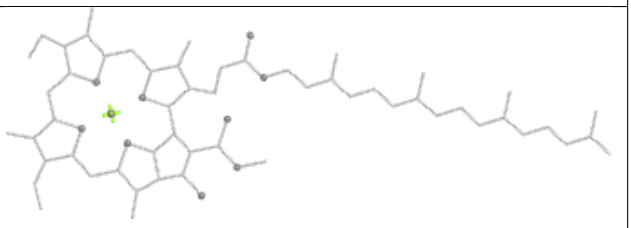


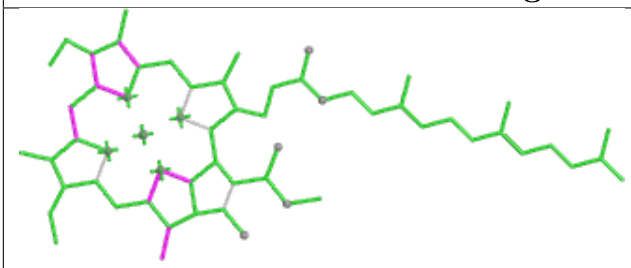
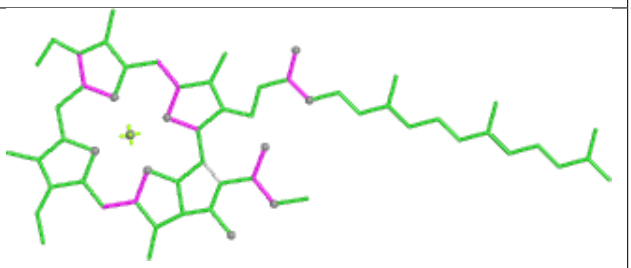
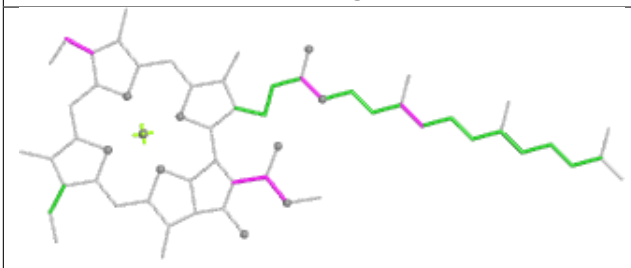
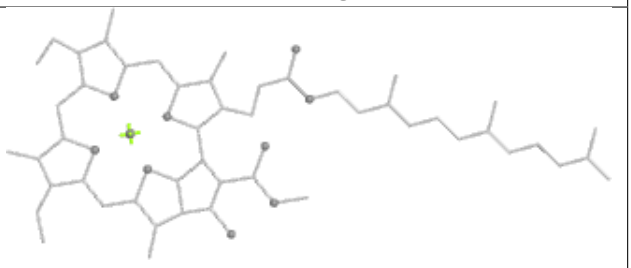
Torsions

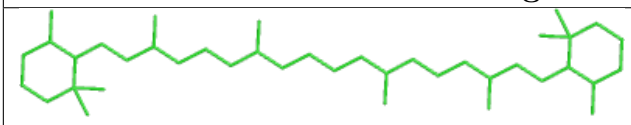
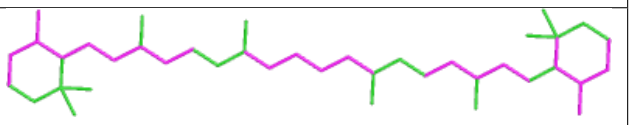
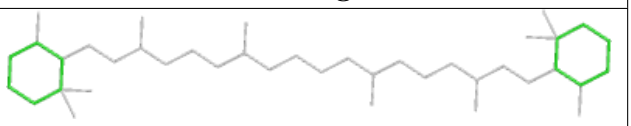


Rings

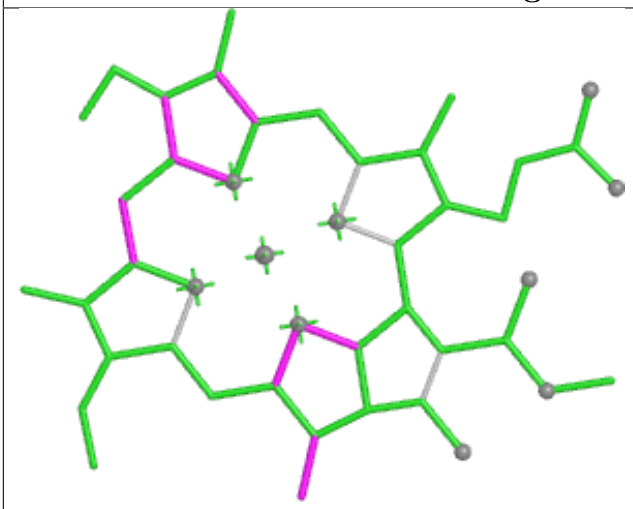
Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

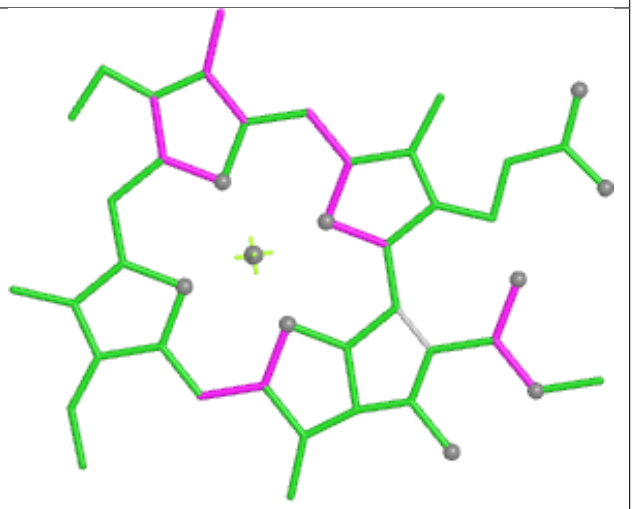
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

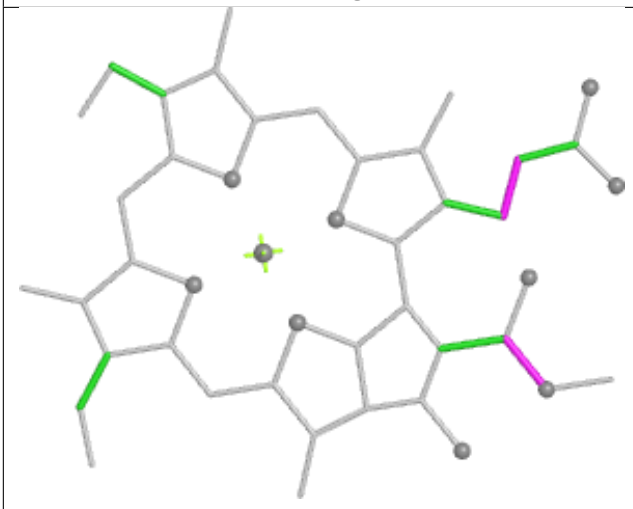
Ligand CLA V 607



Bond lengths



Bond angles

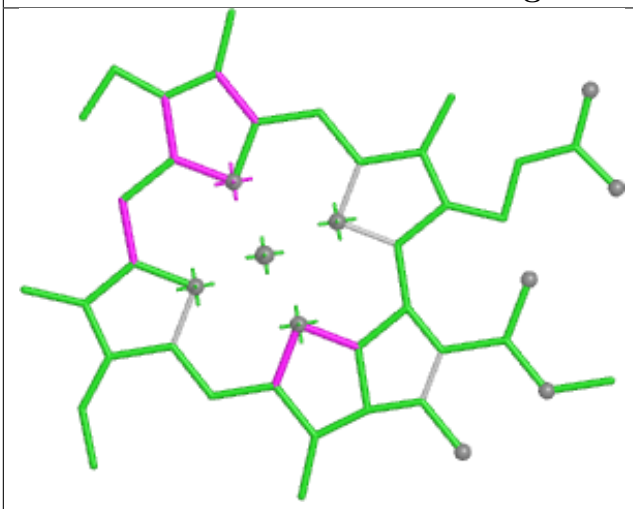


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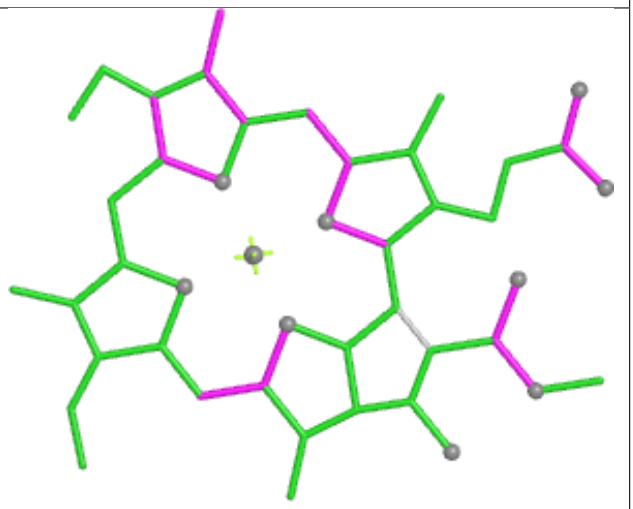


Rings

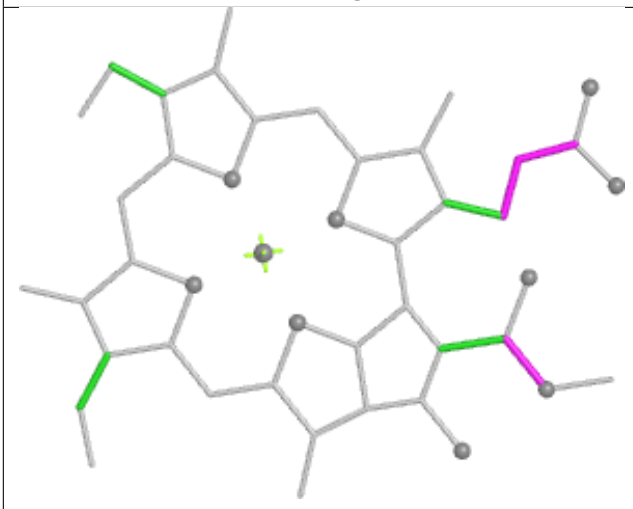
Ligand CLA R 604



Bond lengths



Bond angles

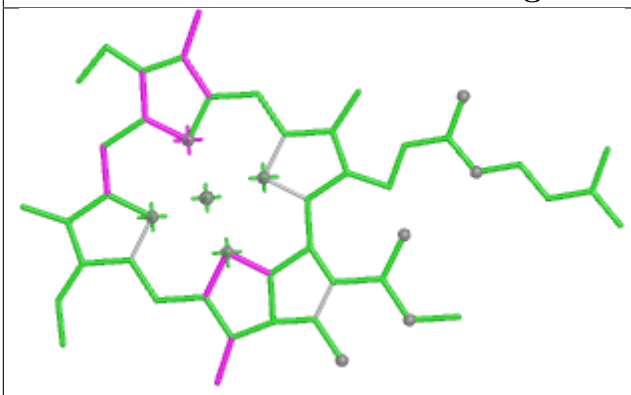


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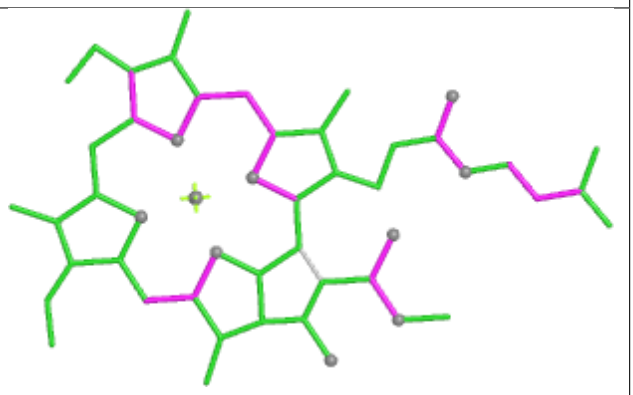


Rings

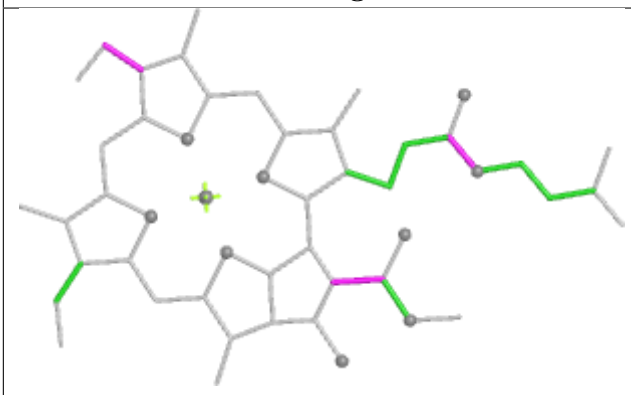
Ligand CLA A 837



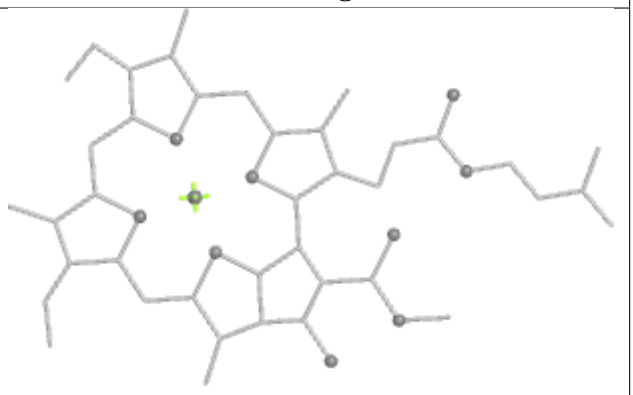
Bond lengths



Bond angles

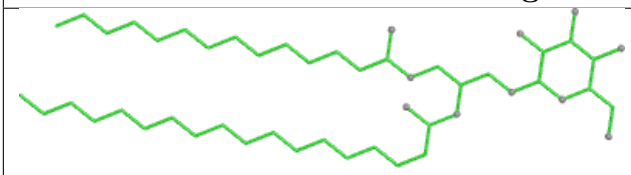


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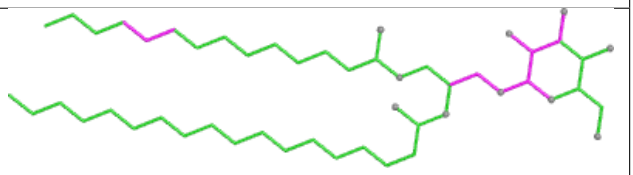


Rings

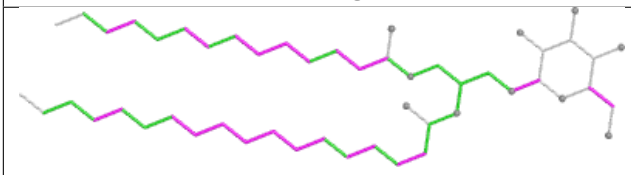
Ligand LMG L 401



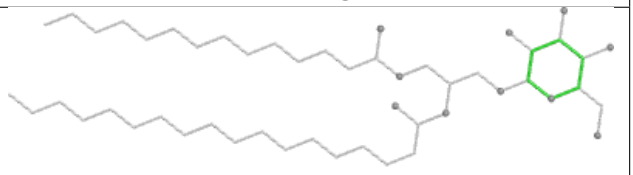
Bond lengths



Bond angles

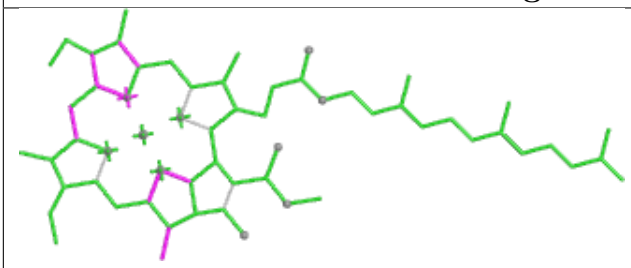


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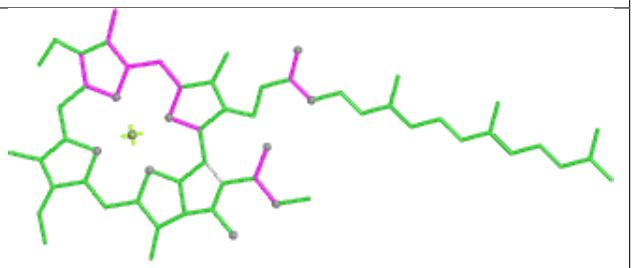


Rings

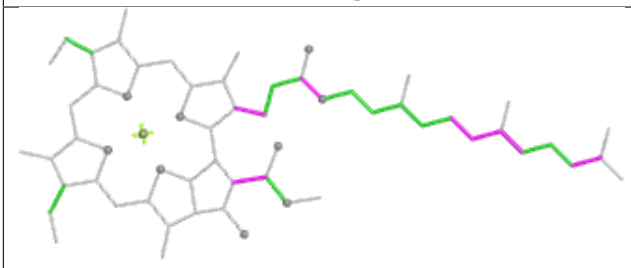
Ligand CLA H 305



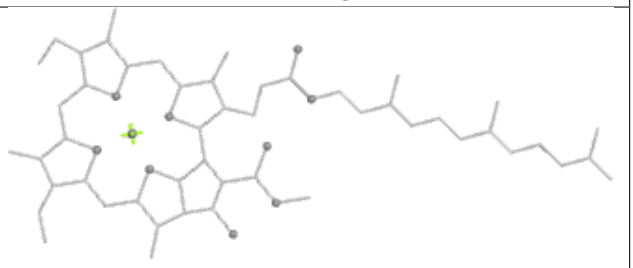
Bond lengths



Bond angles

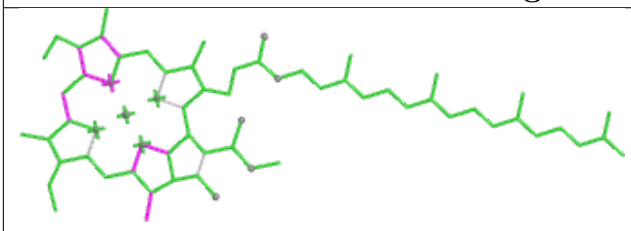


Torsions

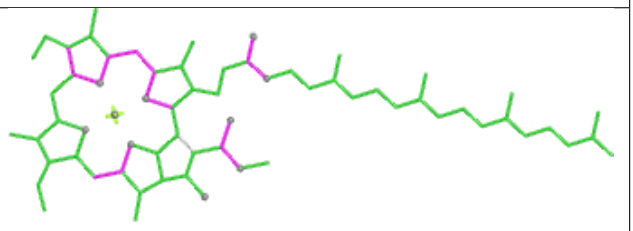


Rings

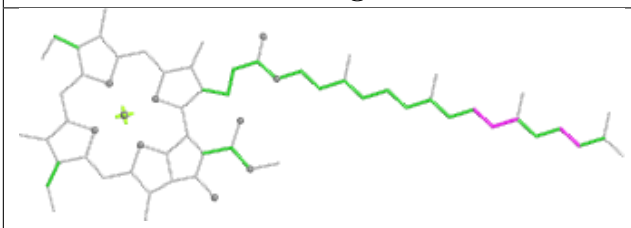
Ligand CLA X 407



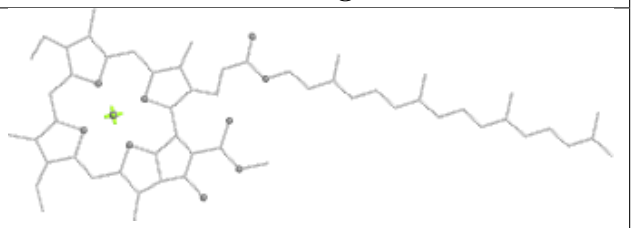
Bond lengths



Bond angles

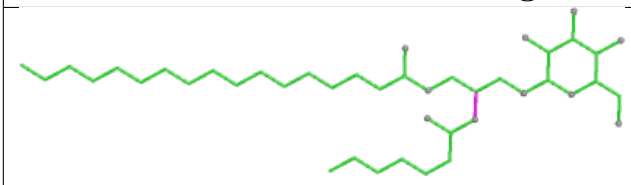


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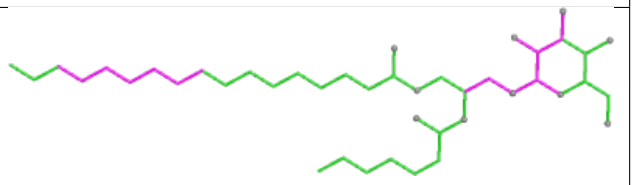


Rings

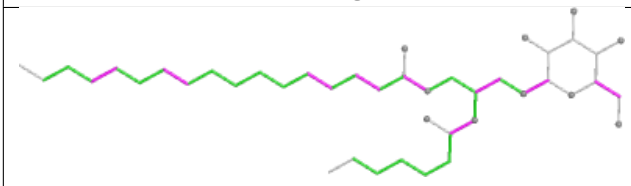
Ligand LMG H 317



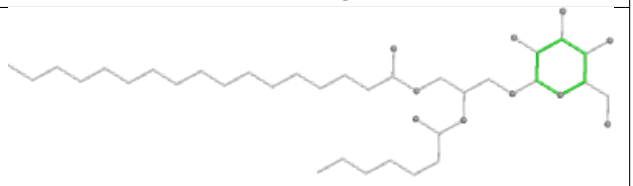
Bond lengths



Bond angles

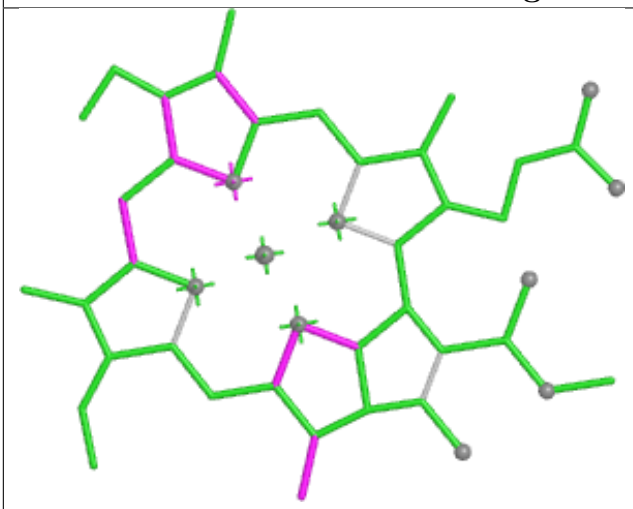


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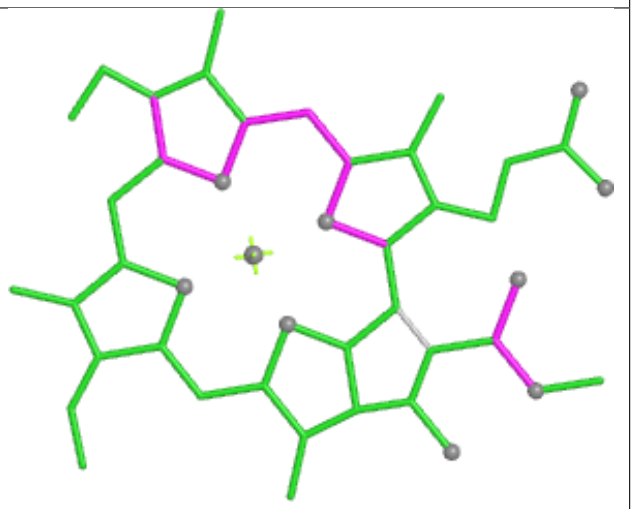


Rings

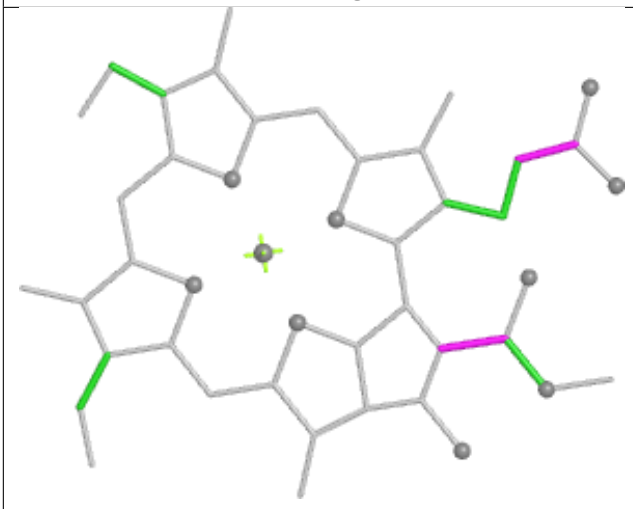
Ligand CLA N 609



Bond lengths



Bond angles

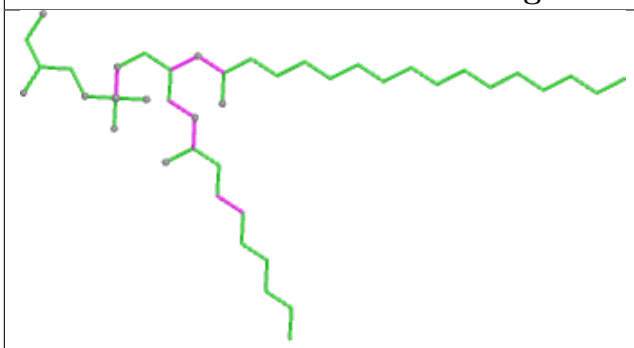


Torsions

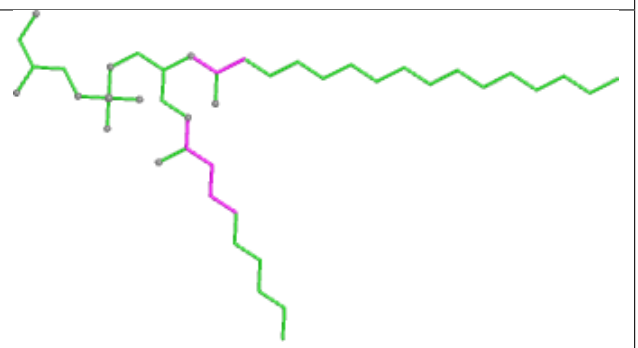


Rings

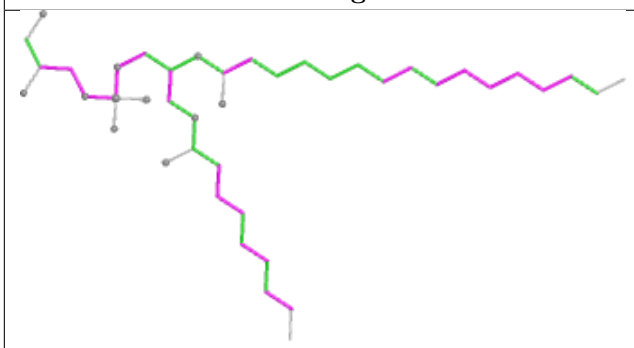
Ligand LHG B 851



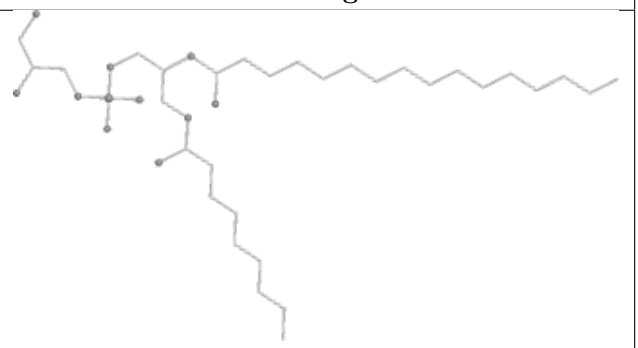
Bond lengths



Bond angles

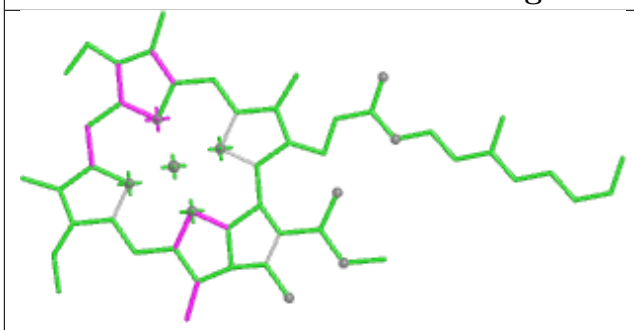


Torsions

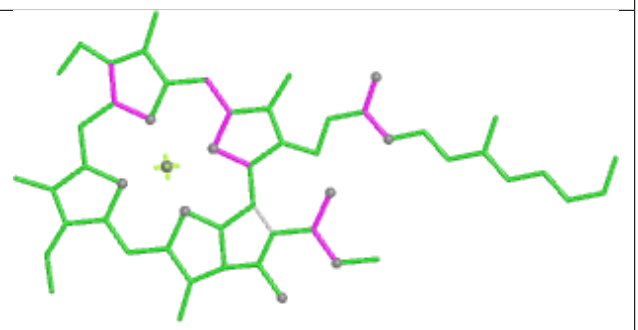


Rings

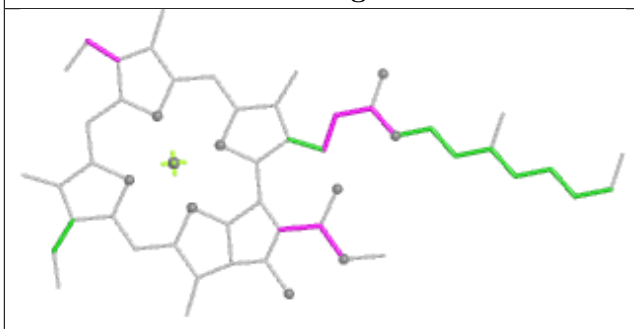
Ligand CLA R 608



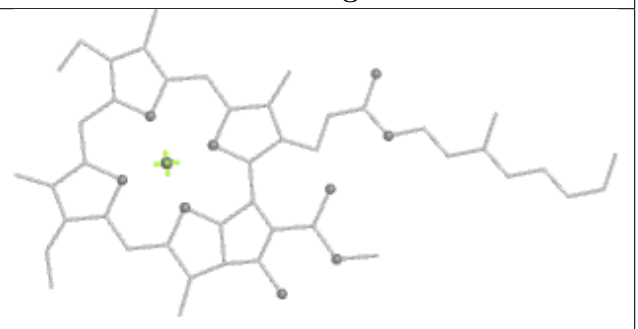
Bond lengths



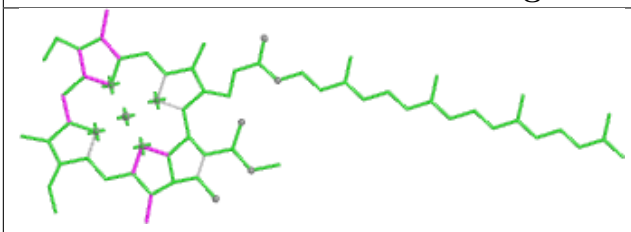
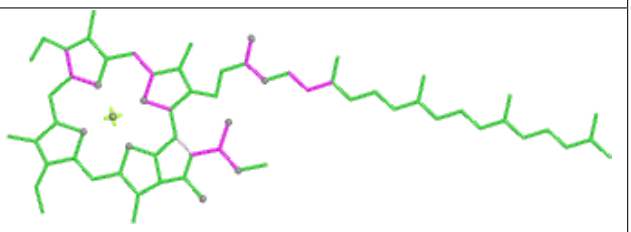
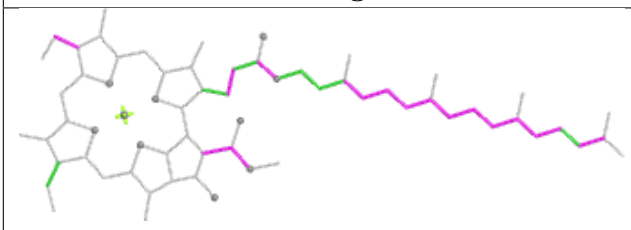
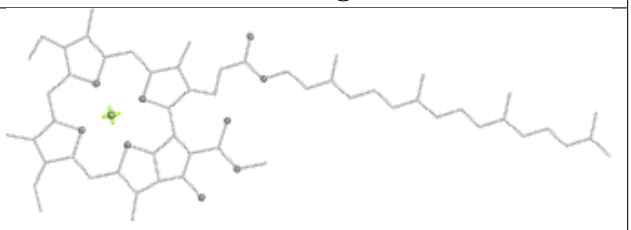
Bond angles

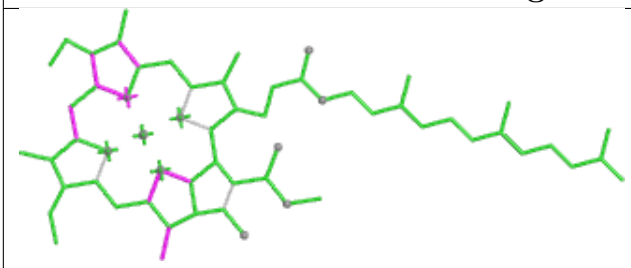
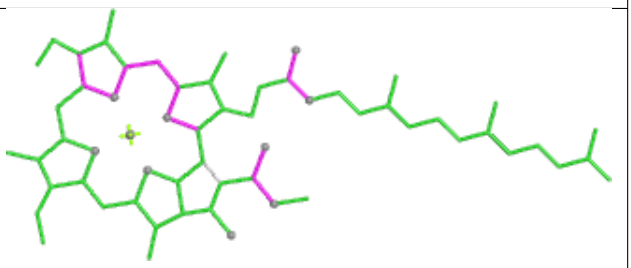
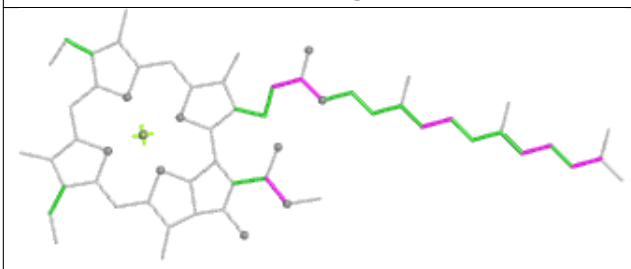
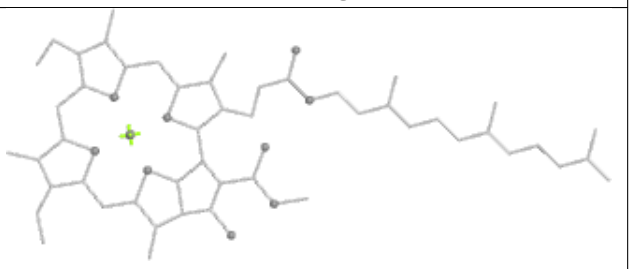


Torsions

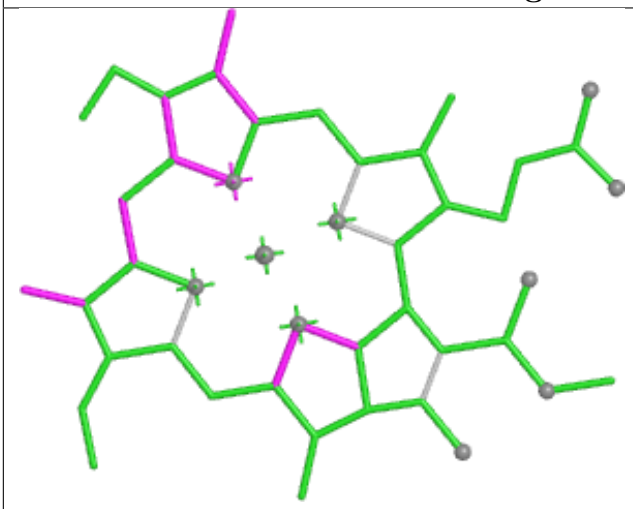


Rings

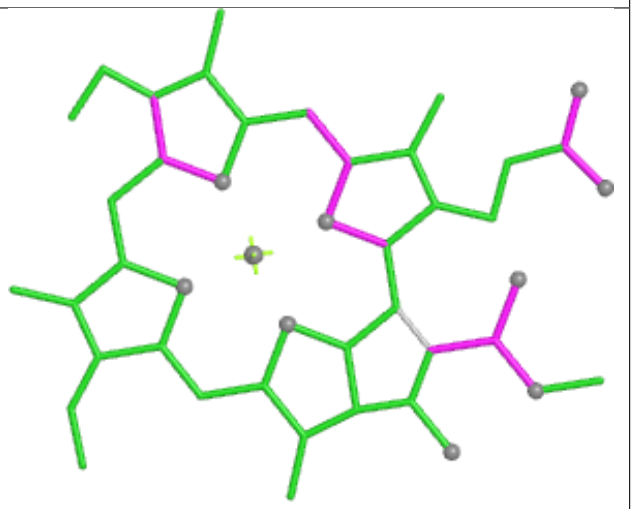
Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA S 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

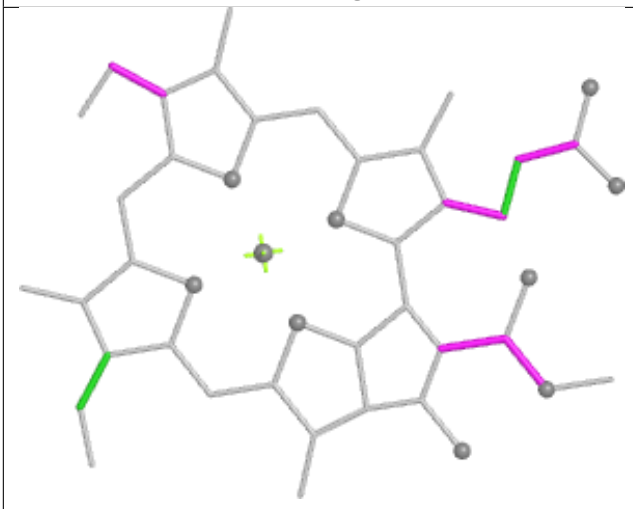
Ligand CLA P 608



Bond lengths



Bond angles

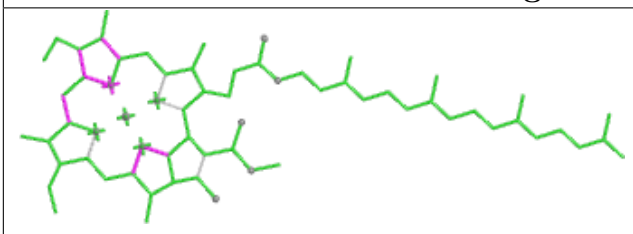


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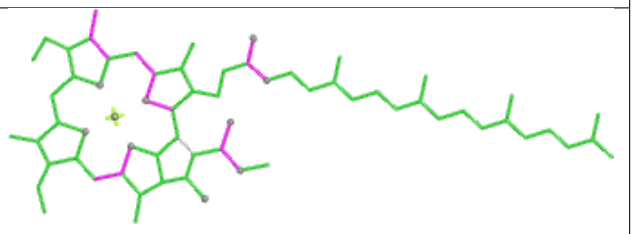


Rings

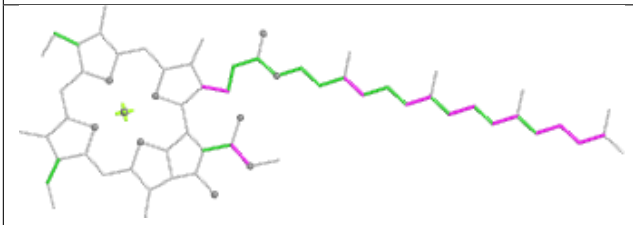
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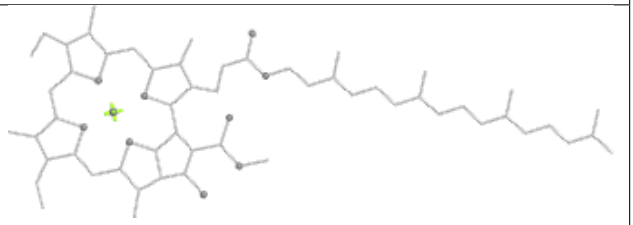
Bond lengths



Bond angles

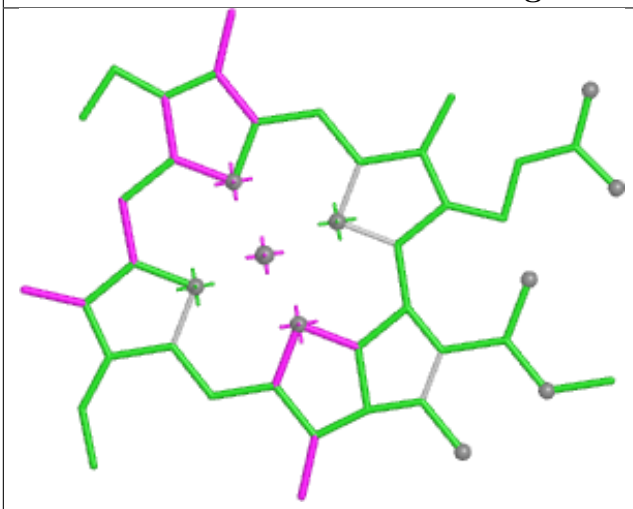


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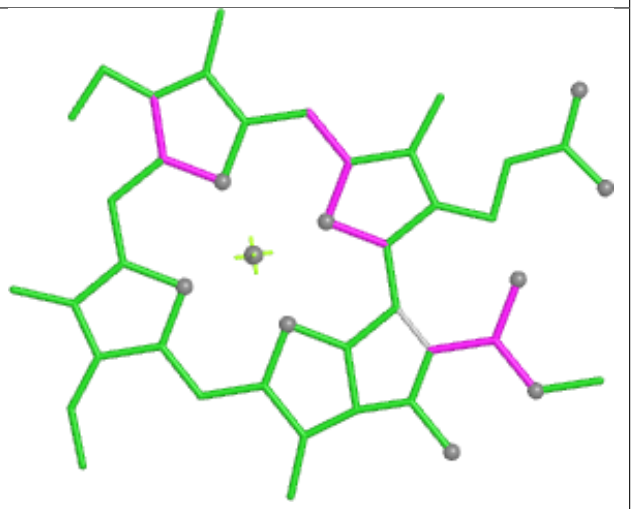


Rings

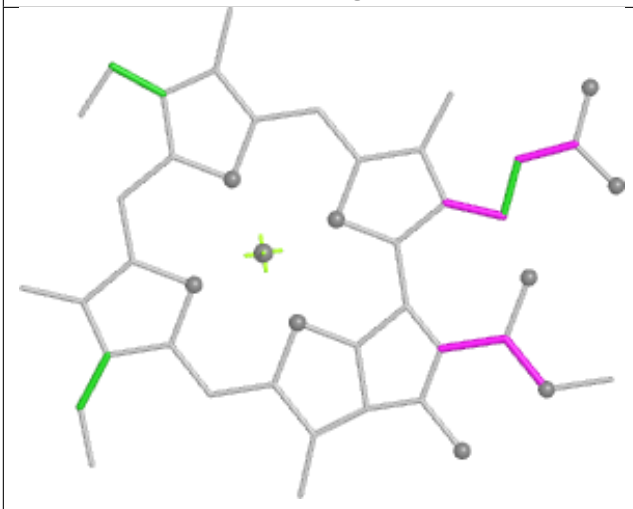
Ligand CLA B 829



Bond lengths



Bond angles

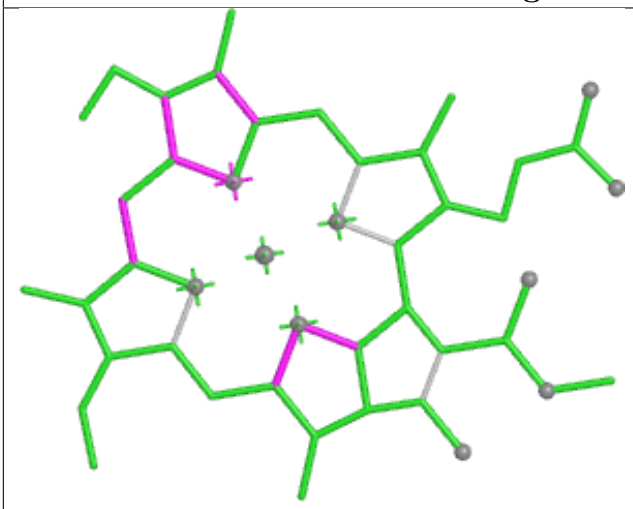


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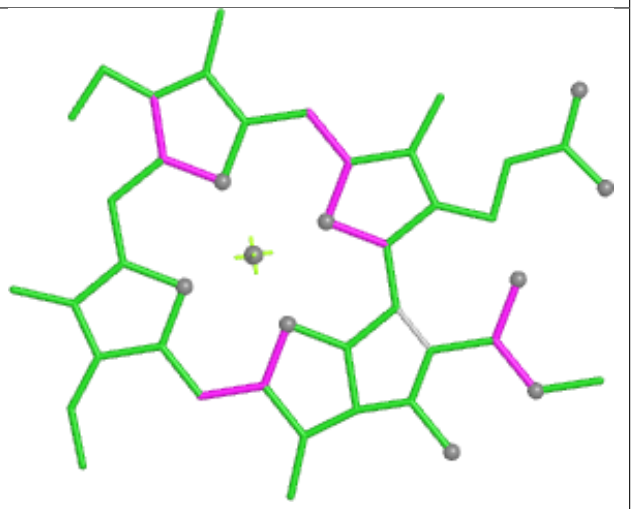


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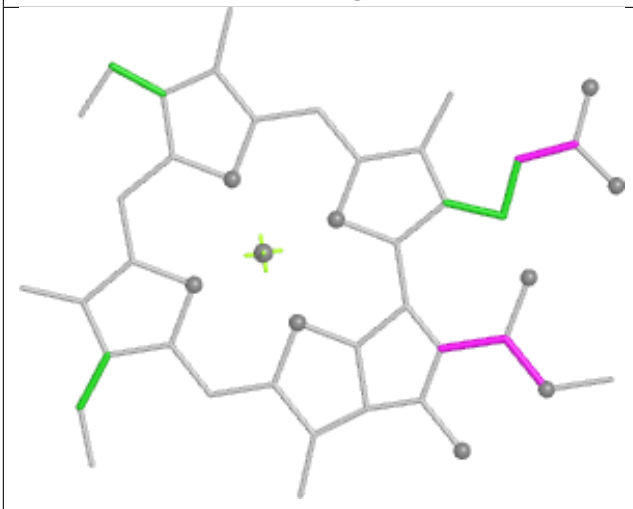
Ligand CLA G 601



Bond lengths



Bond angles

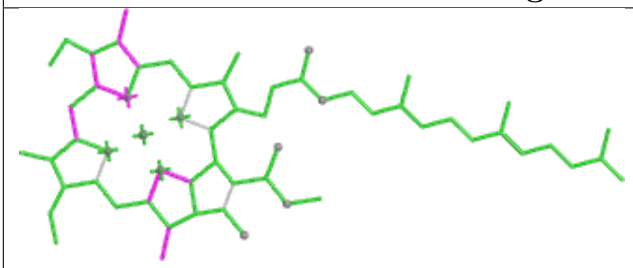


Torsions

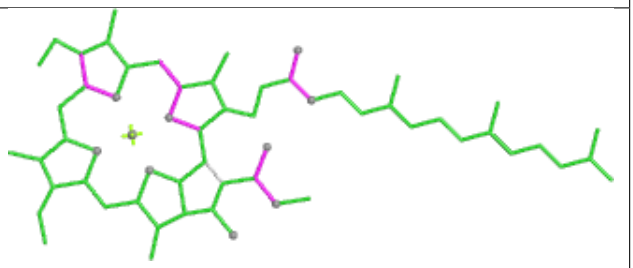


Rings

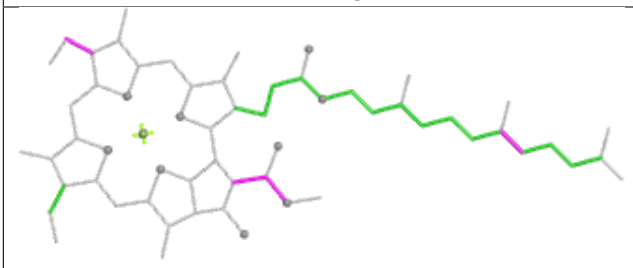
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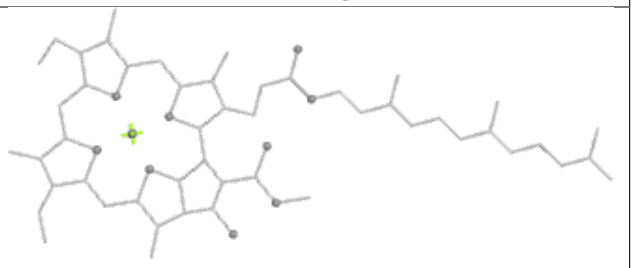
Bond lengths



Bond angles

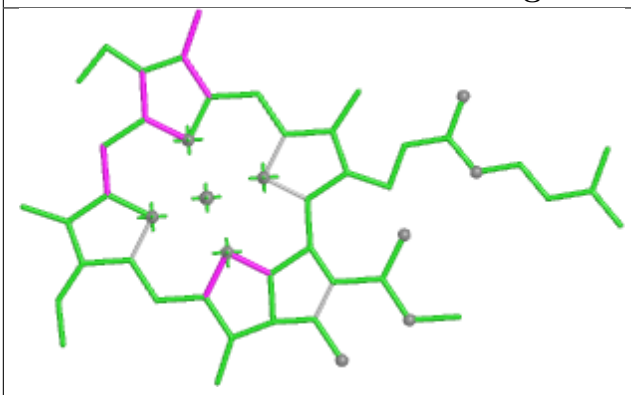


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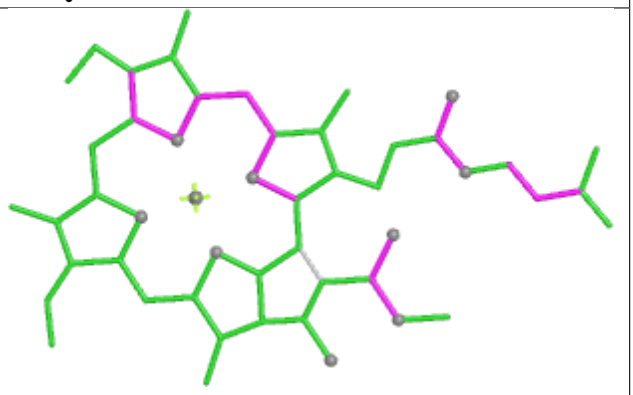


Rings

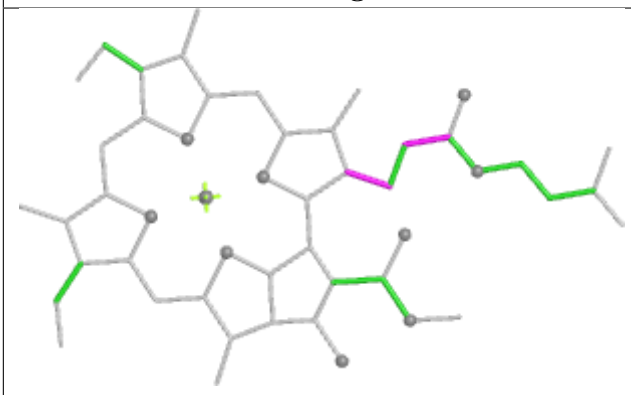
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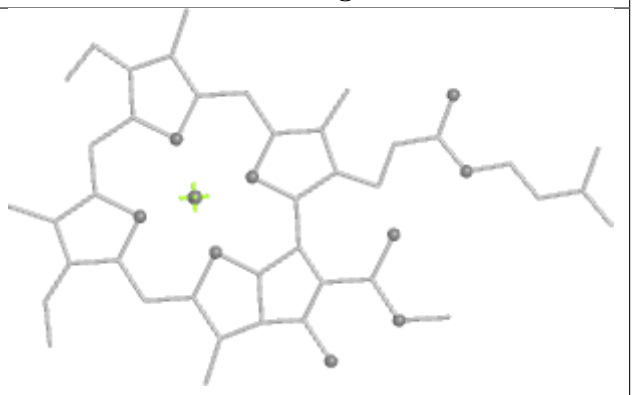
Bond lengths



Bond angles

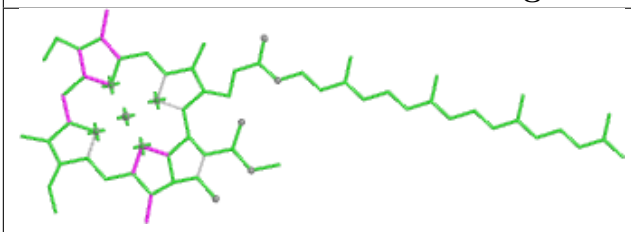


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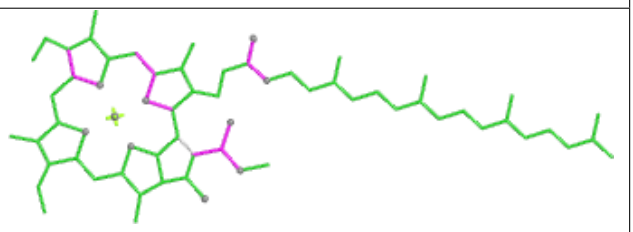


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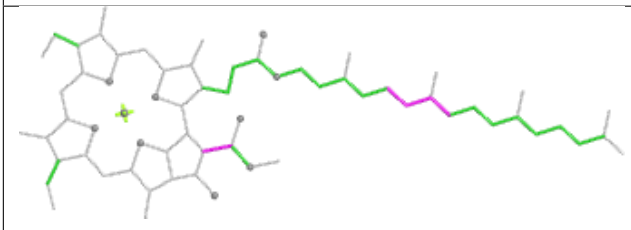
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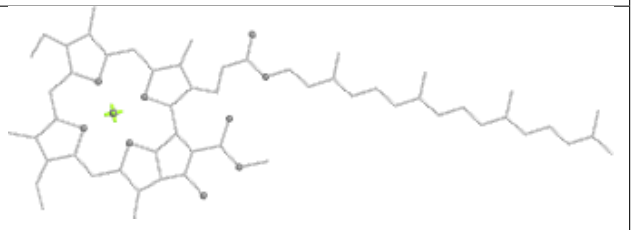
Bond lengths



Bond angles

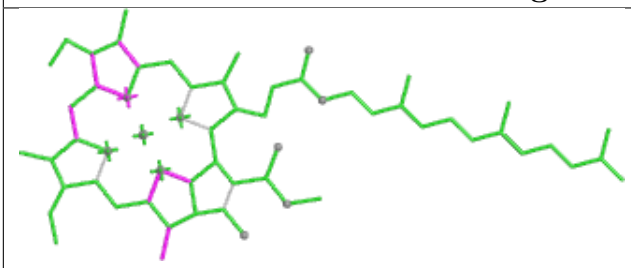


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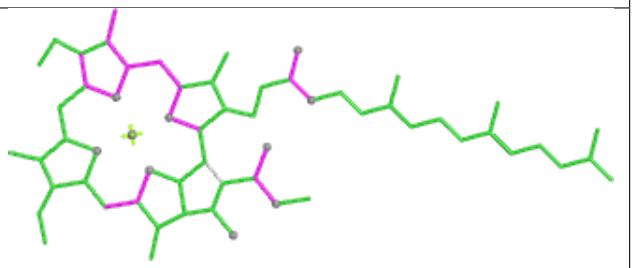


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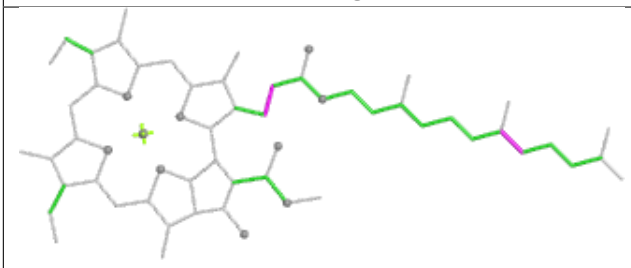
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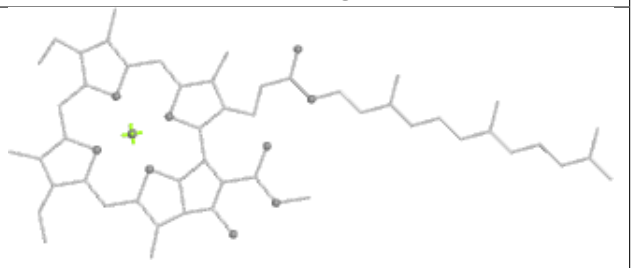
Bond lengths



Bond angles

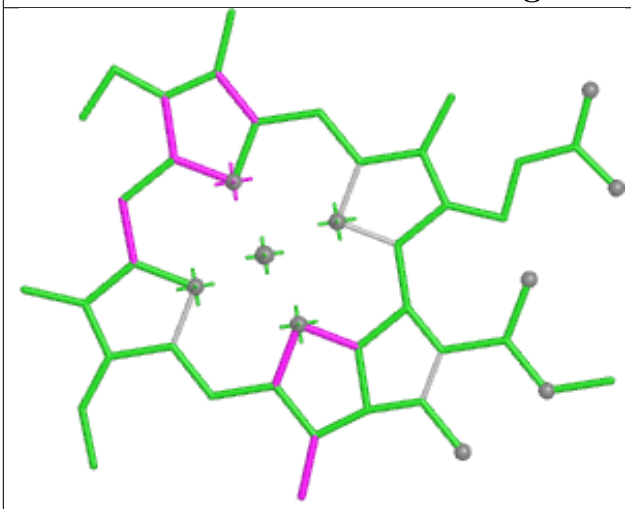


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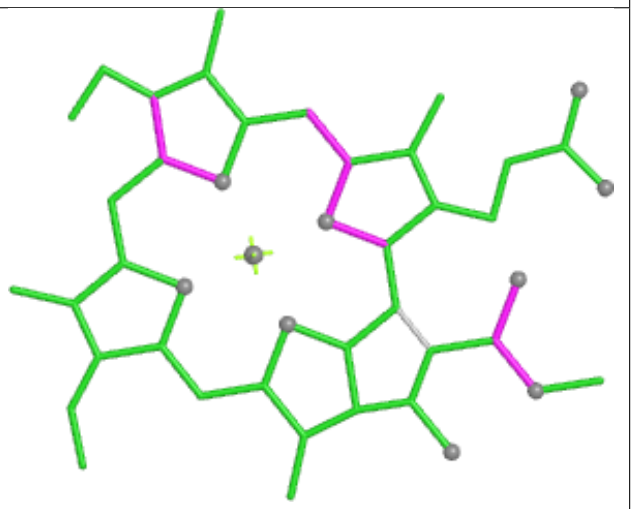


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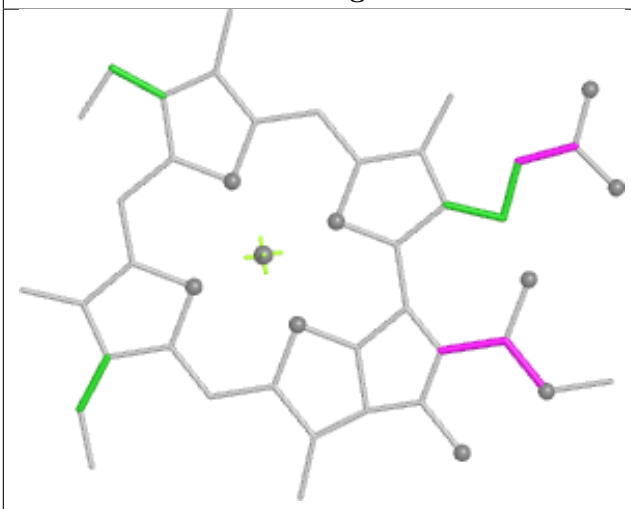
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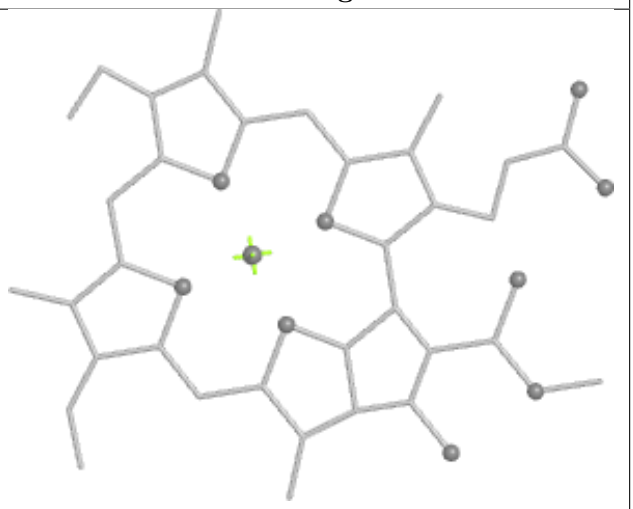
Bond lengths



Bond angles

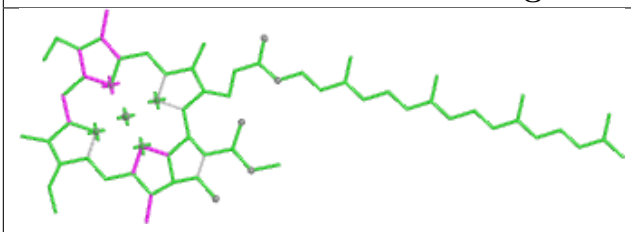


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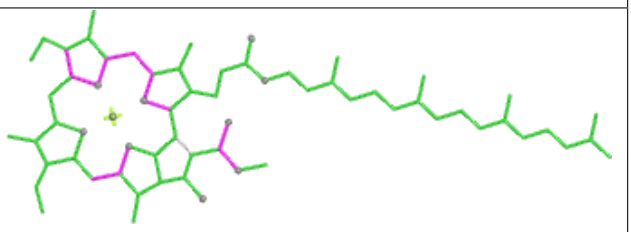


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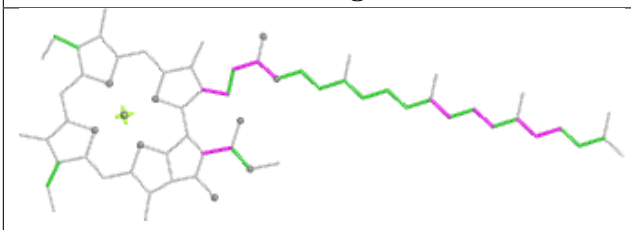
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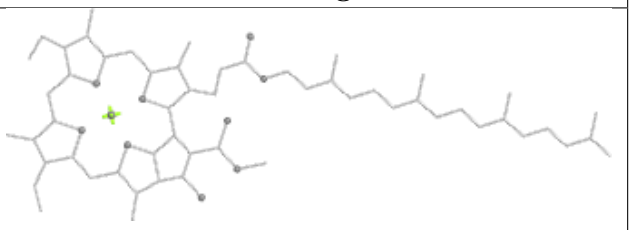
Bond lengths



Bond angles

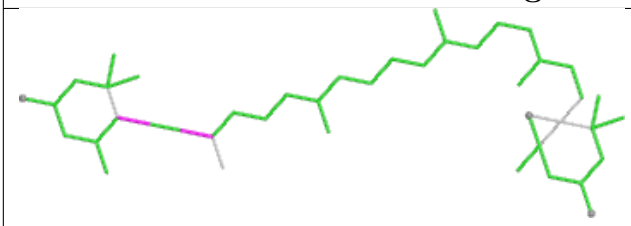


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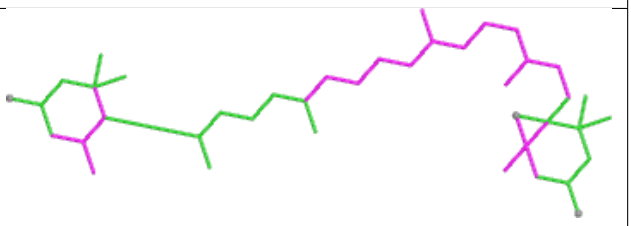


Rings

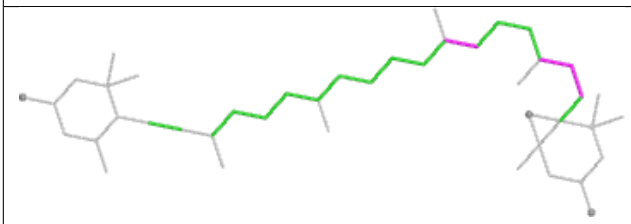
Ligand DD6 X 416



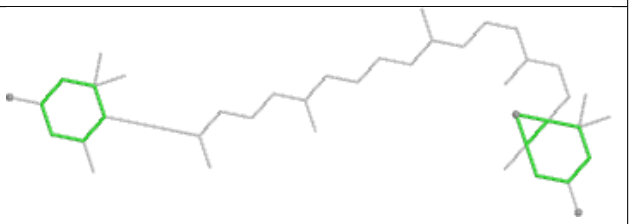
Bond lengths



Bond angles

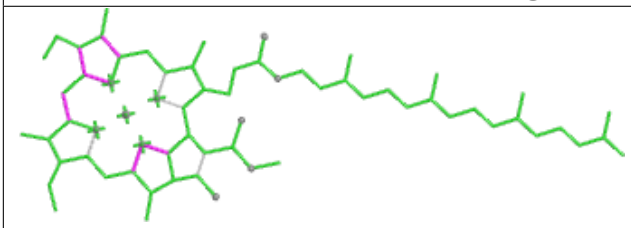


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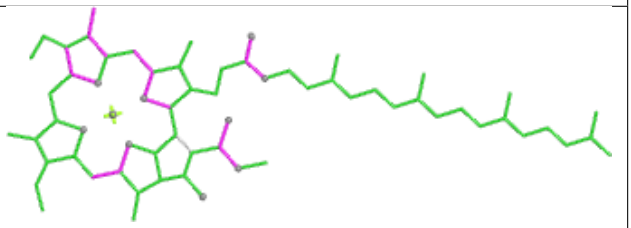


Rings

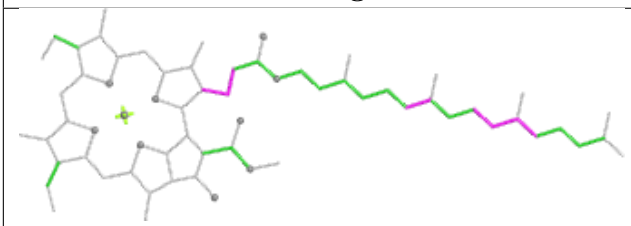
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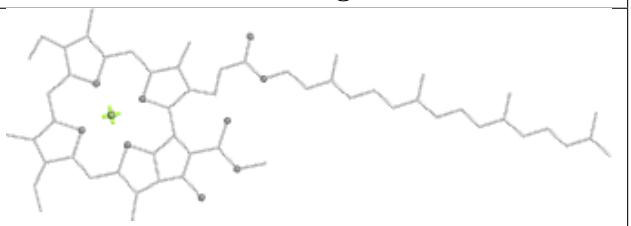
Bond lengths



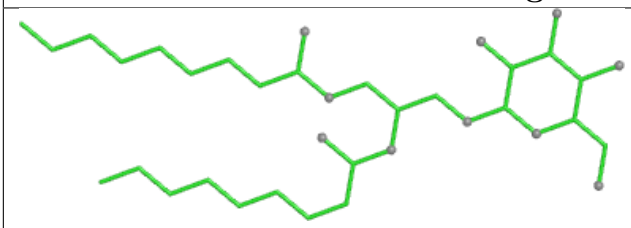
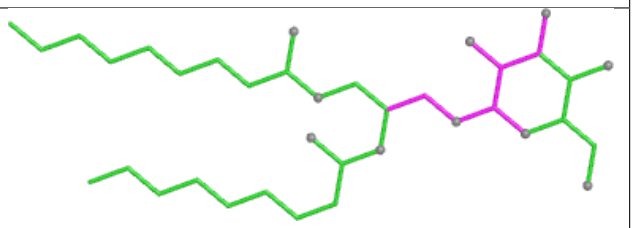
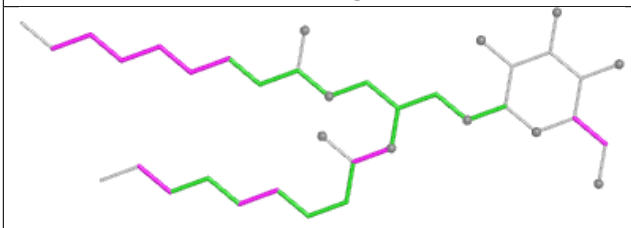
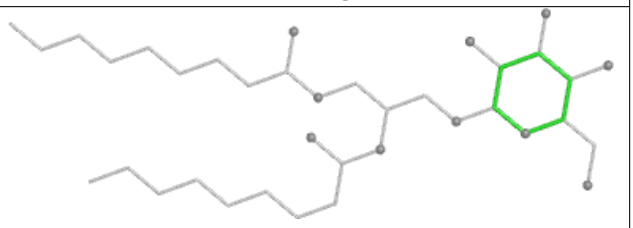
Bond angles

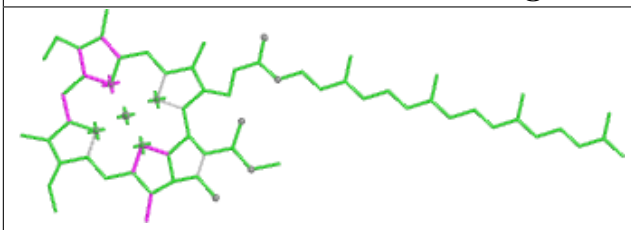
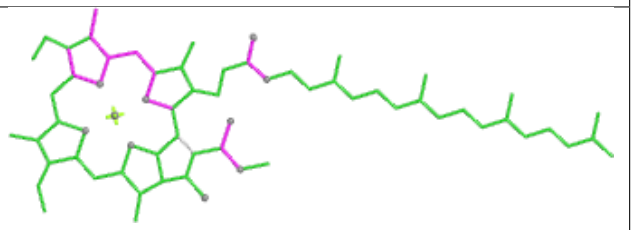
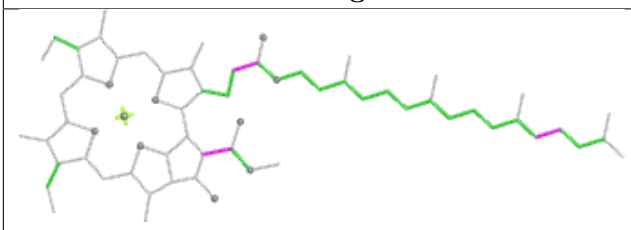
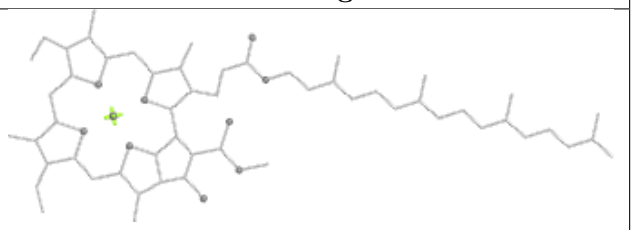


Torsions

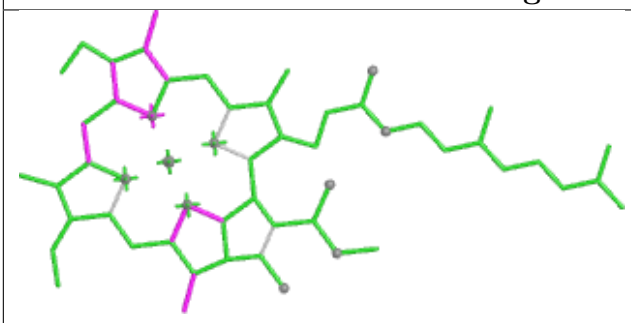


Rings

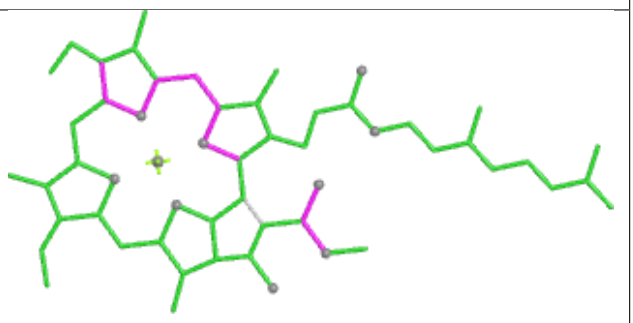
Ligand LMG I 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

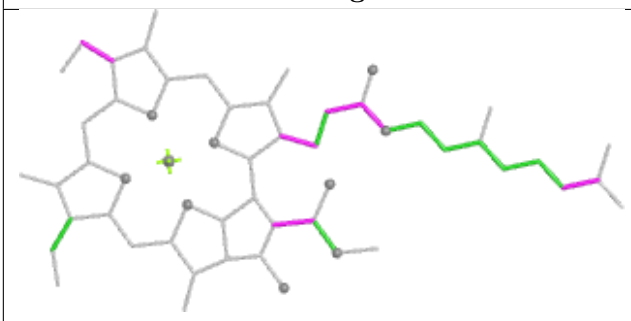
Ligand CLA H 306



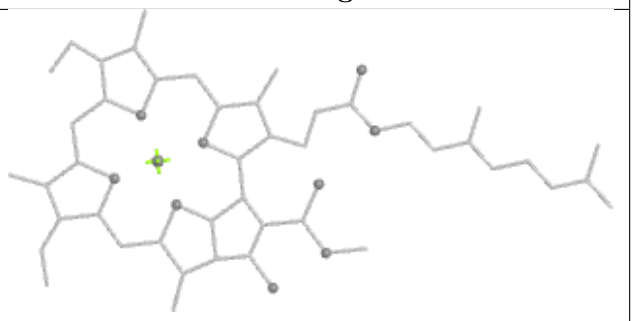
Bond lengths



Bond angles

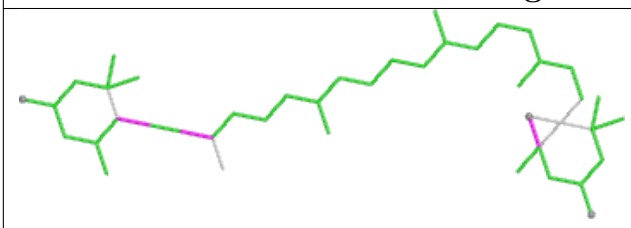


Torsions

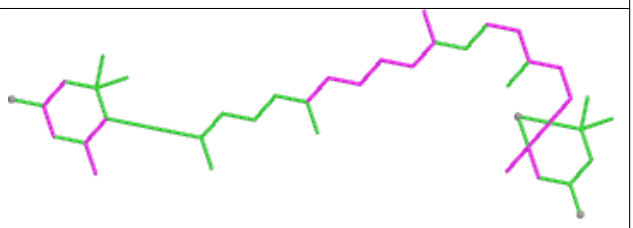


Rings

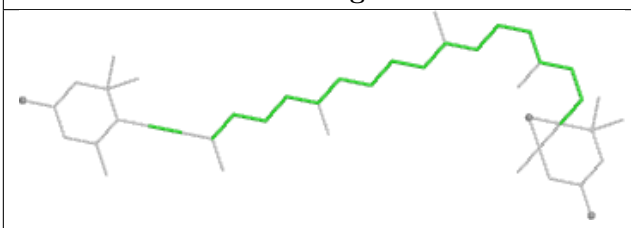
Ligand DD6 X 401



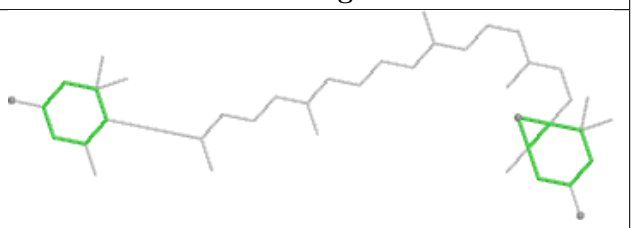
Bond lengths



Bond angles



Torsions

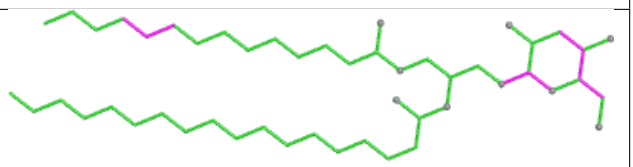


Rings

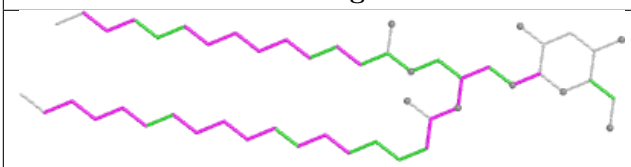
Ligand LMG I 615



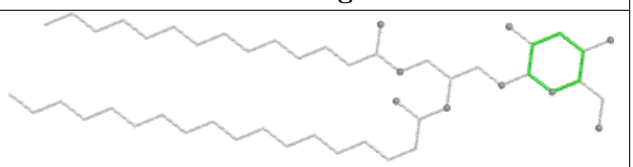
Bond lengths



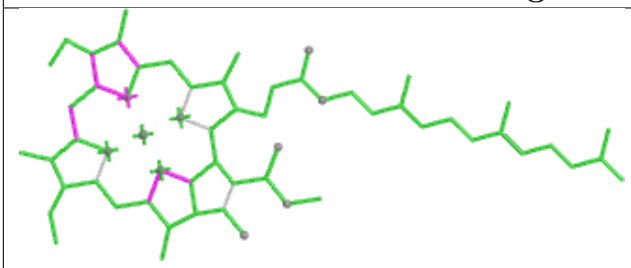
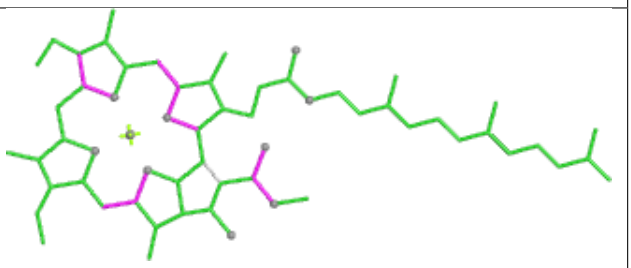
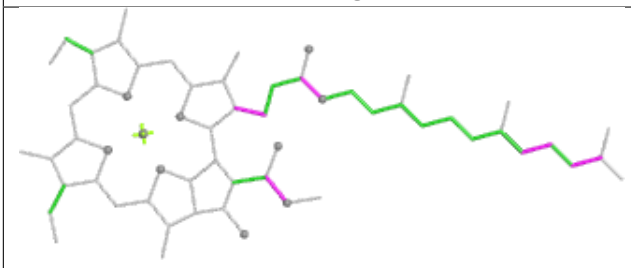
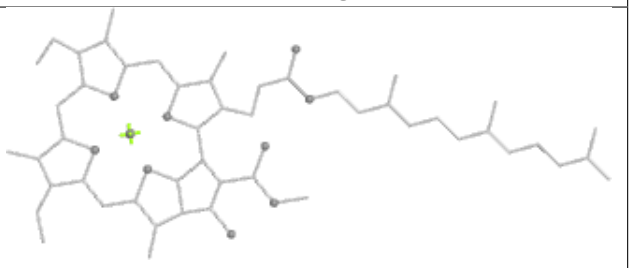
Bond angles

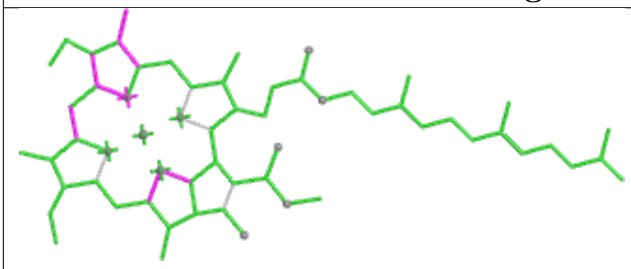
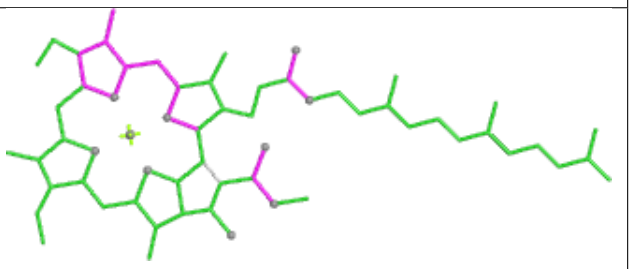
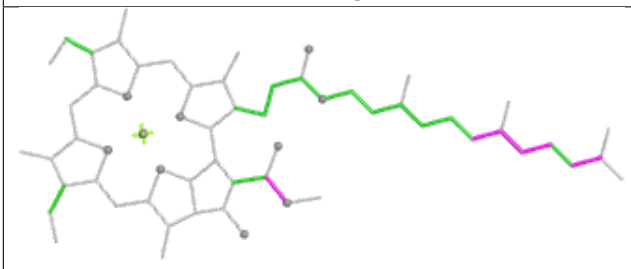
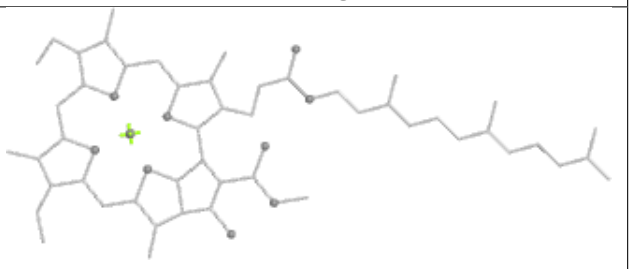


Torsions

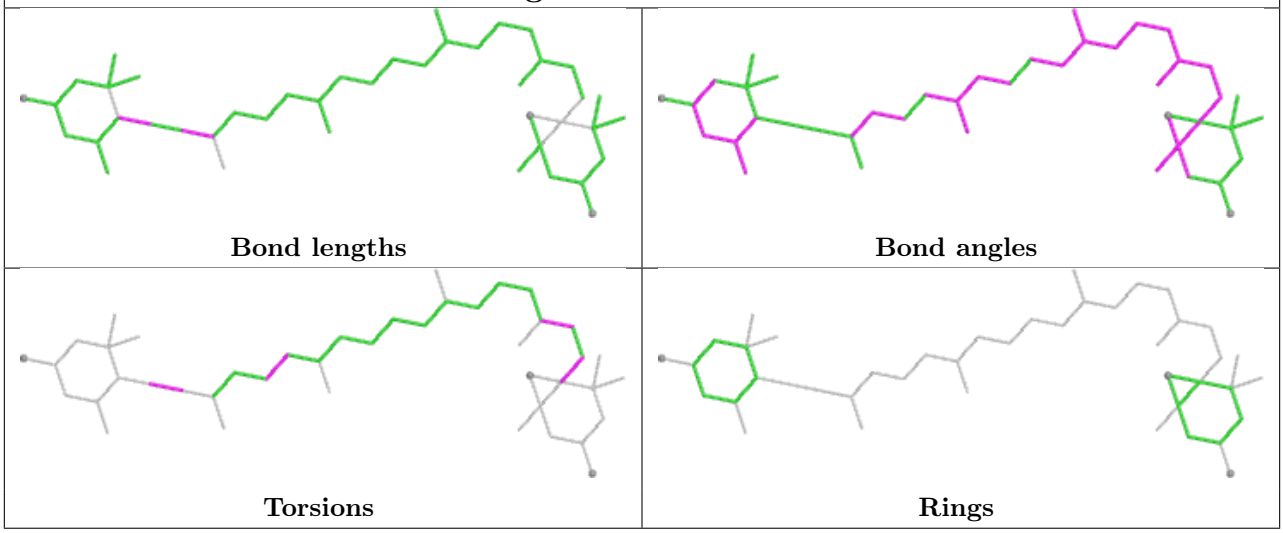


Rings

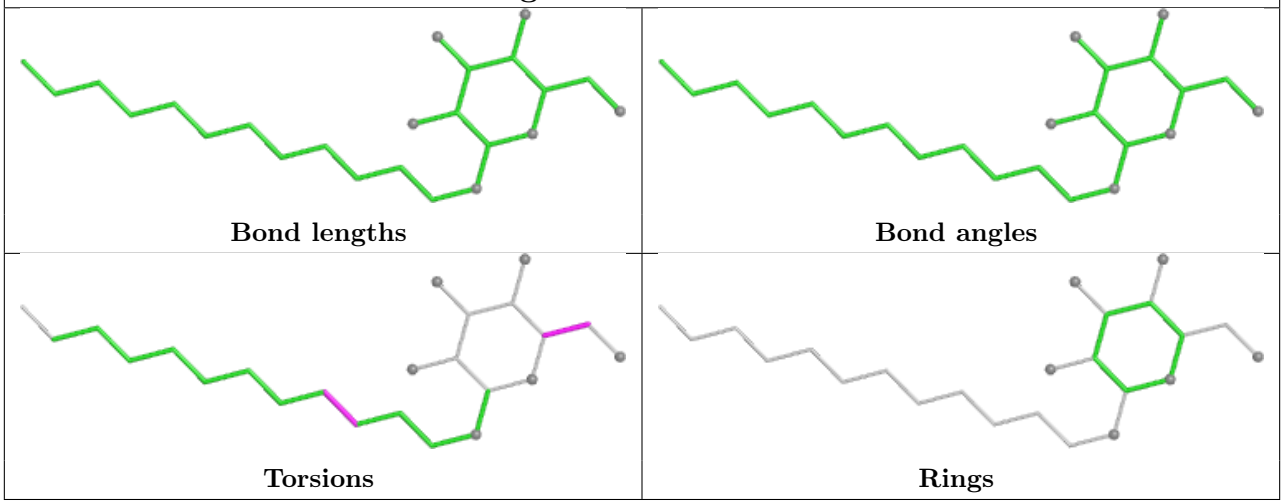
Ligand CLA S 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA T 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

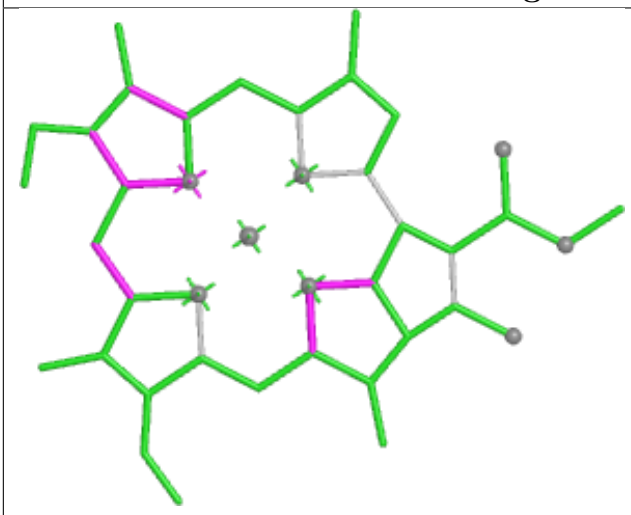
Ligand DD6 A 858



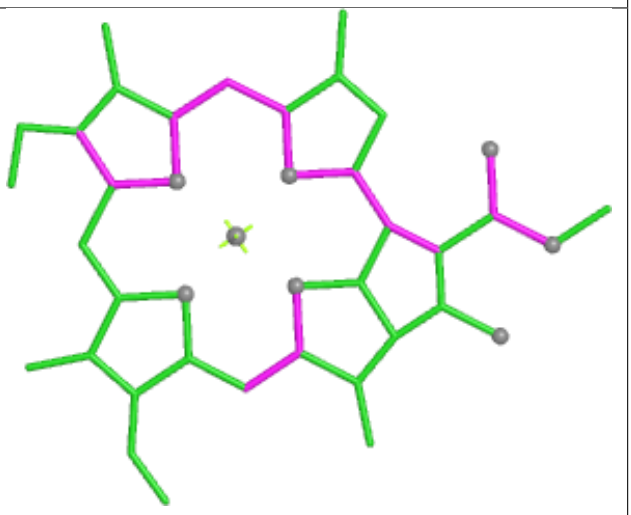
Ligand LMU U 424



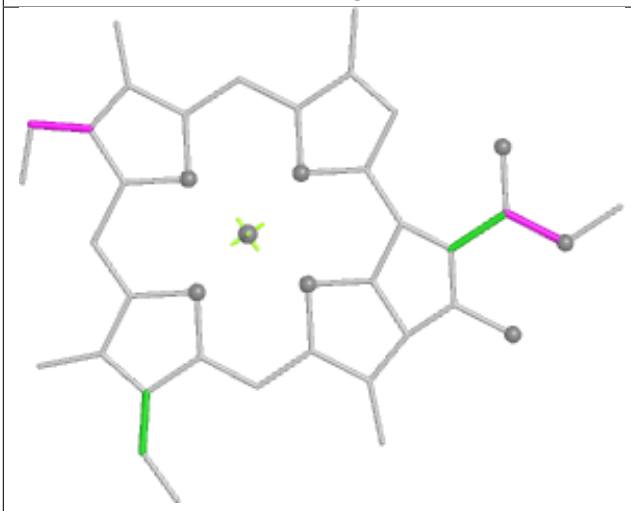
Ligand CLA N 611



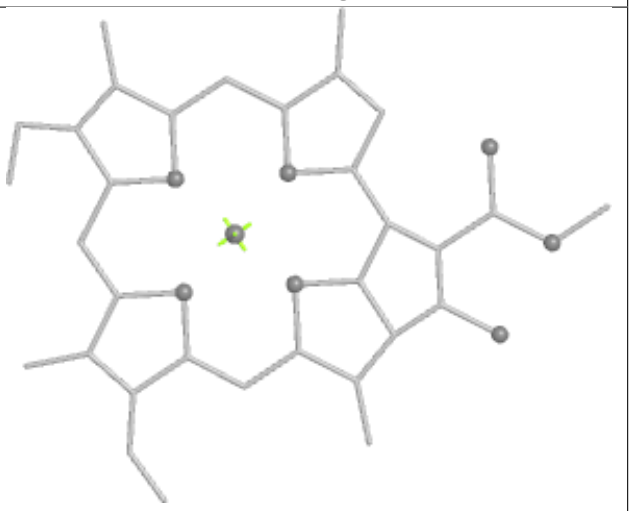
Bond lengths



Bond angles

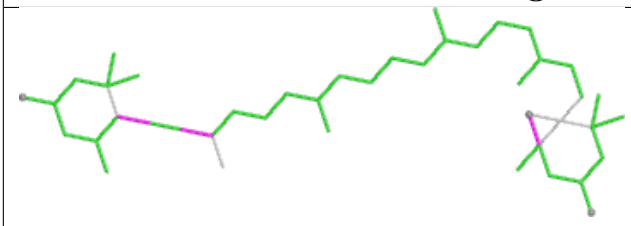


Torsions

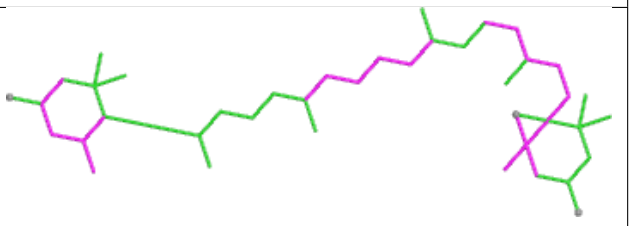


Rings

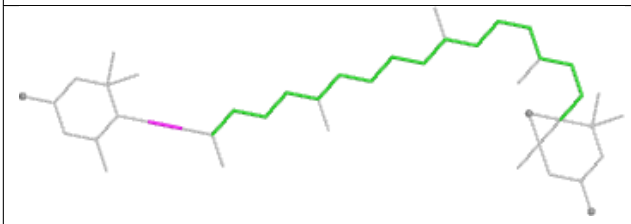
Ligand DD6 L 413



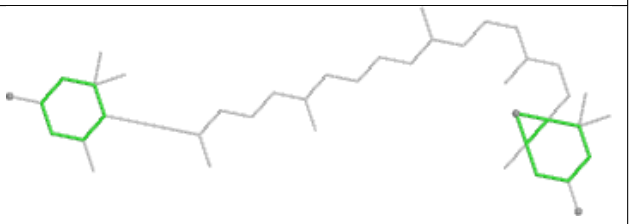
Bond lengths



Bond angles

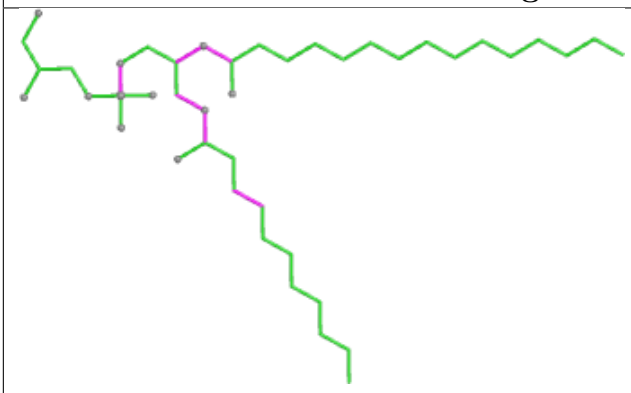


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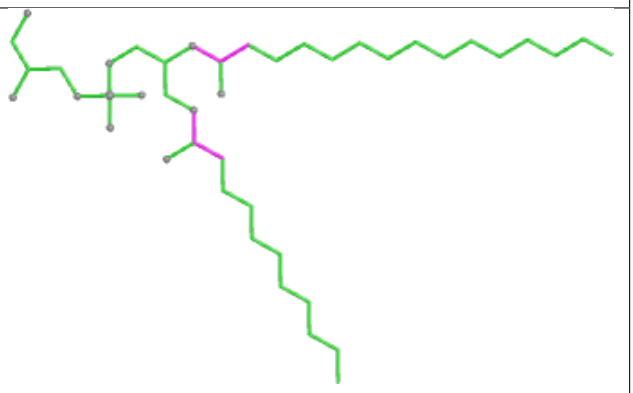


Rings

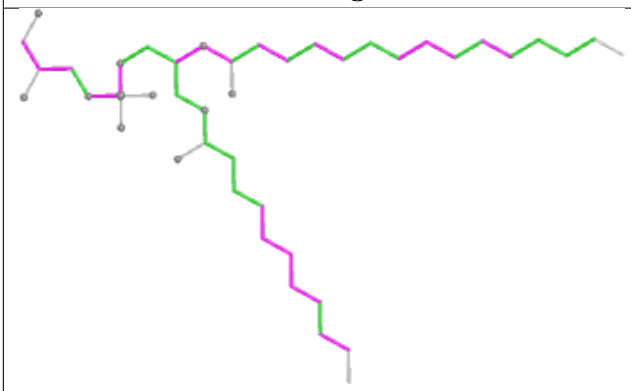
Ligand LHG N 616



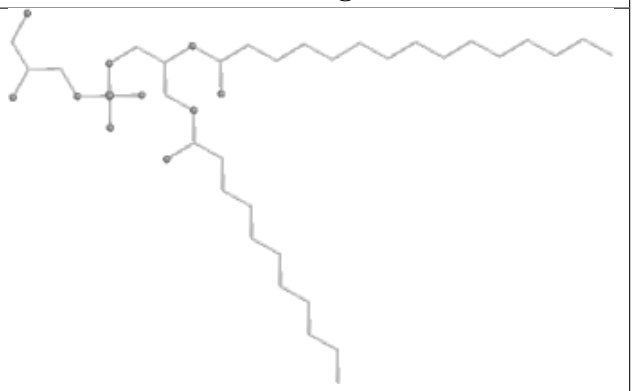
Bond lengths



Bond angles

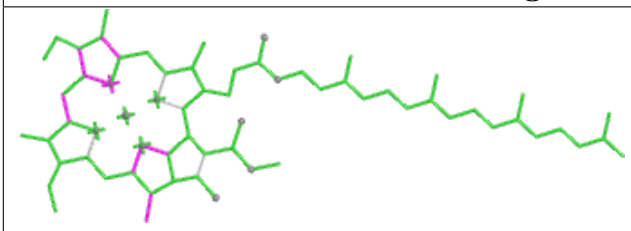


Torsions

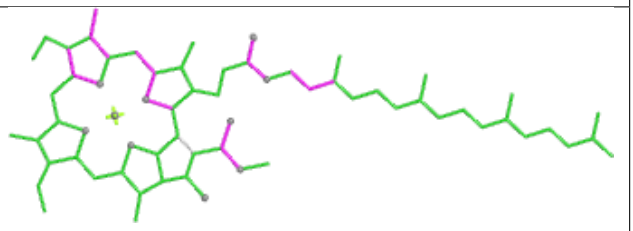


Rings

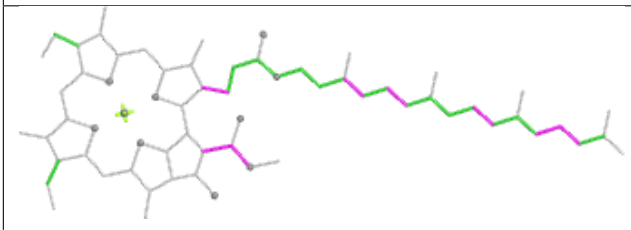
Ligand CLA X 409



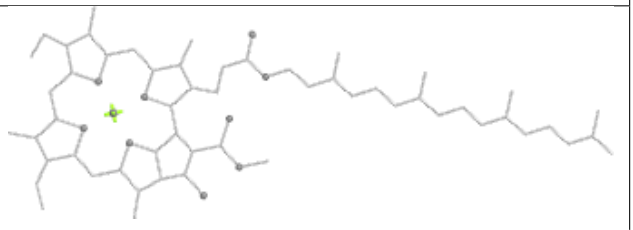
Bond lengths



Bond angles

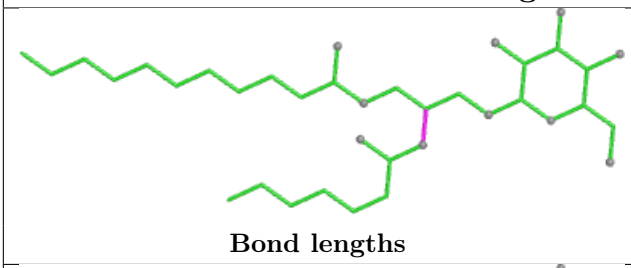


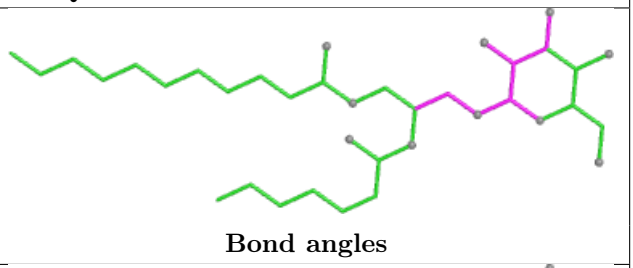
Torsions

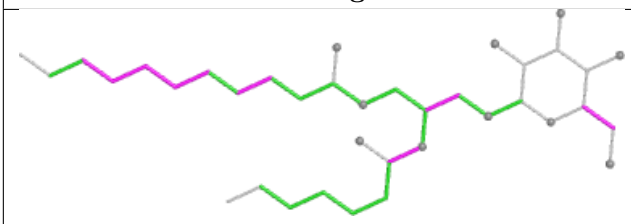


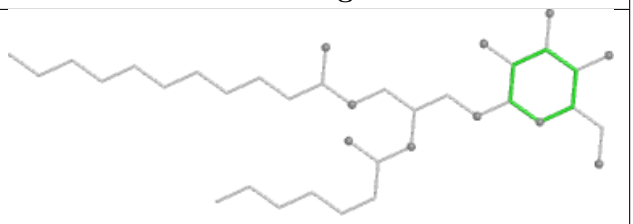
Rings

Ligand LMG Q 602

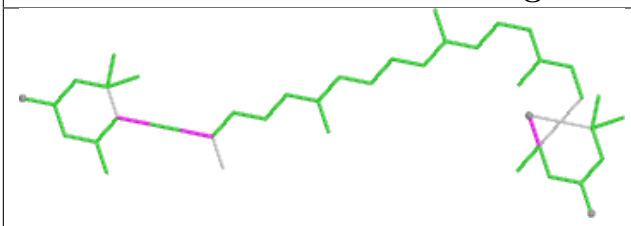

Bond lengths

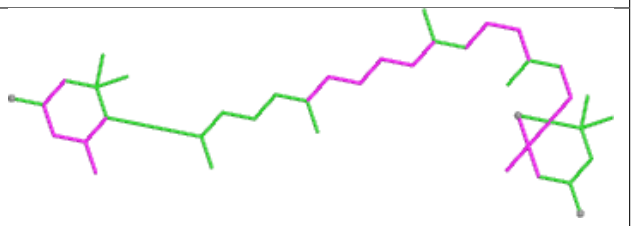

Bond angles

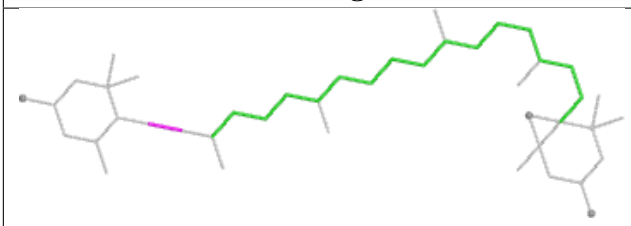

Torsions

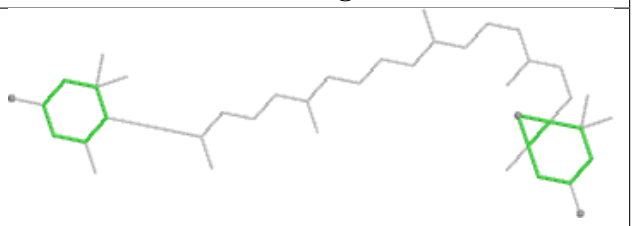

Rings

Ligand DD6 H 315

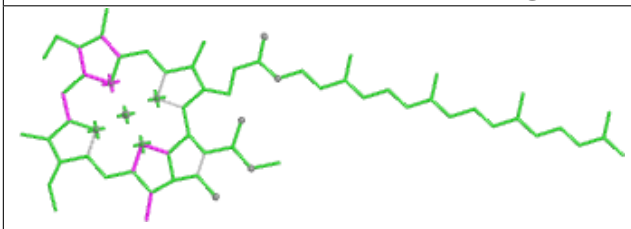

Bond lengths

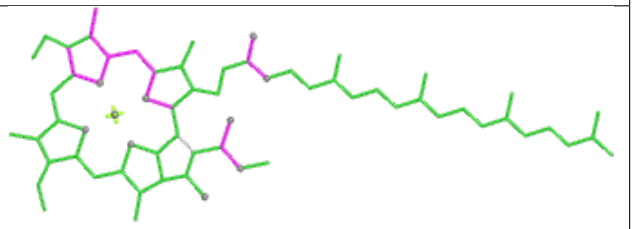

Bond angles

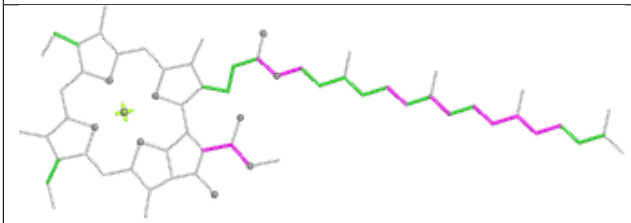

Torsions

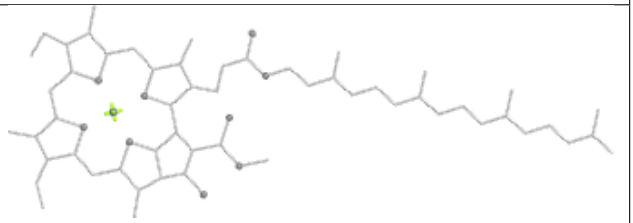

Rings

Ligand CLA A 817

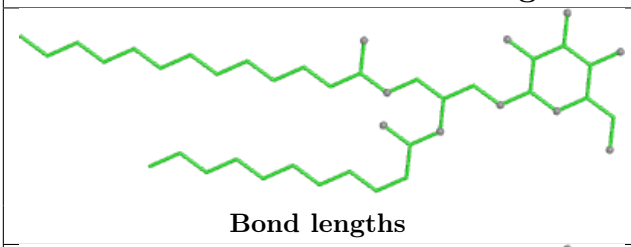

Bond lengths

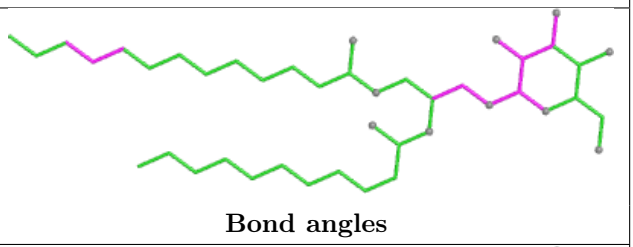

Bond angles

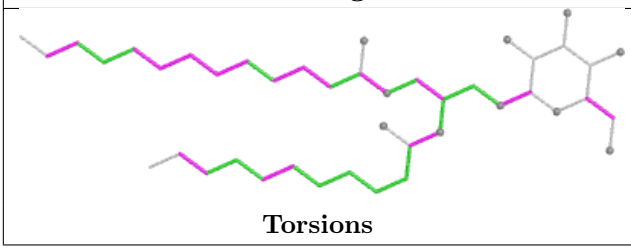

Torsions

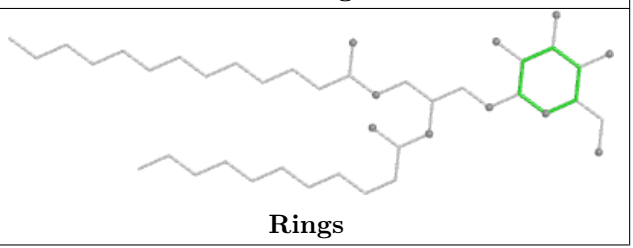

Rings

Ligand LMG K 622

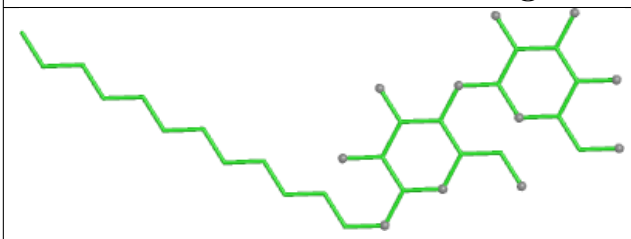

Bond lengths

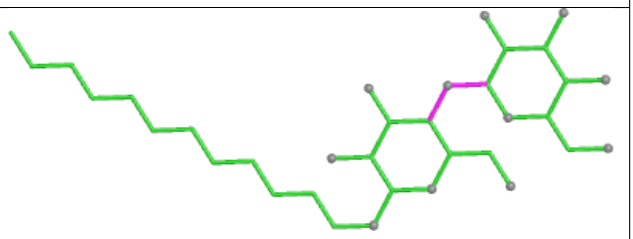

Bond angles

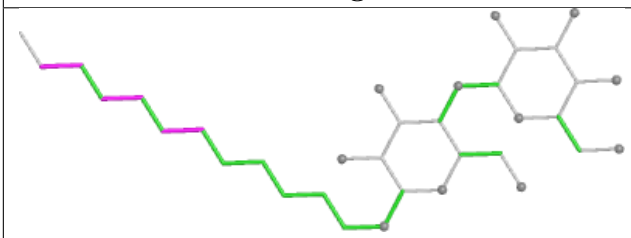

Torsions

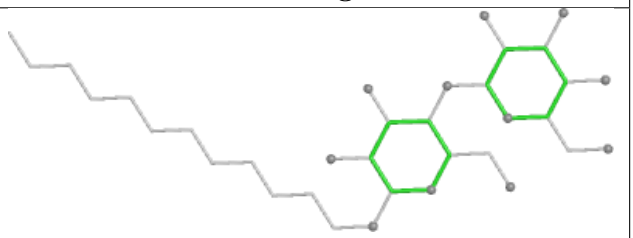

Rings

Ligand LMU A 854

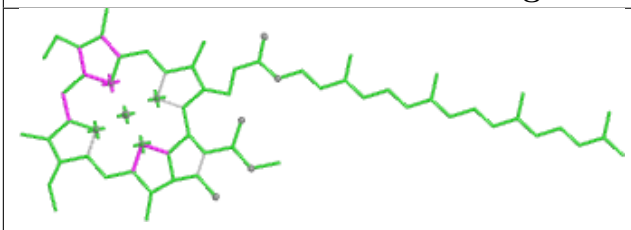

Bond lengths

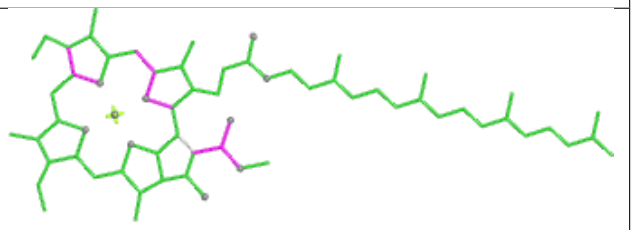

Bond angles

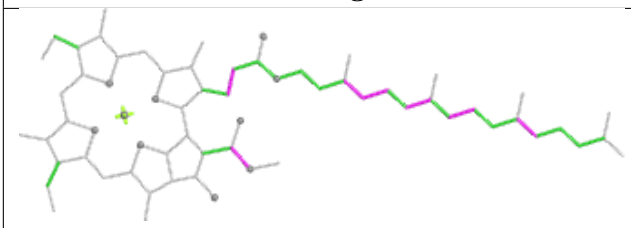

Torsions

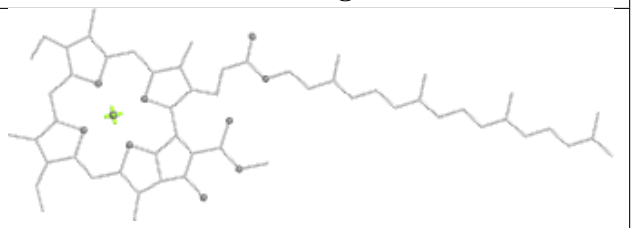

Rings

Ligand CLA K 611

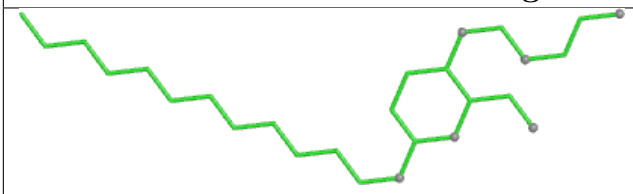

Bond lengths


Bond angles

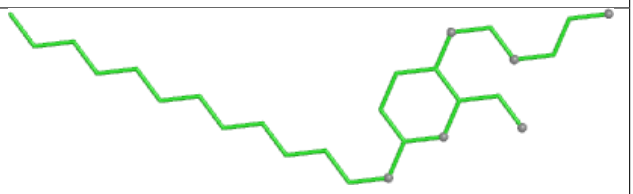

Torsions


Rings

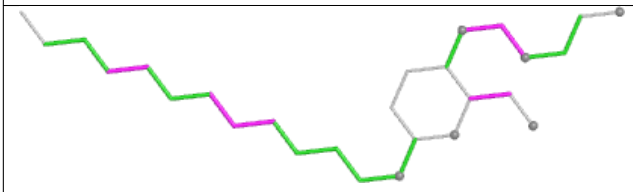
Ligand LMU L 419



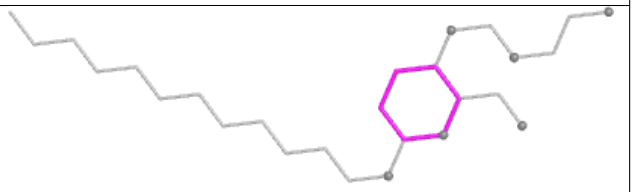
Bond lengths



Bond angles

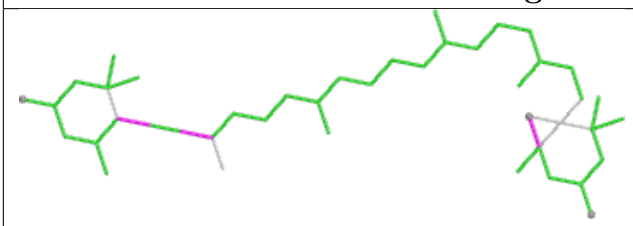


Torsions

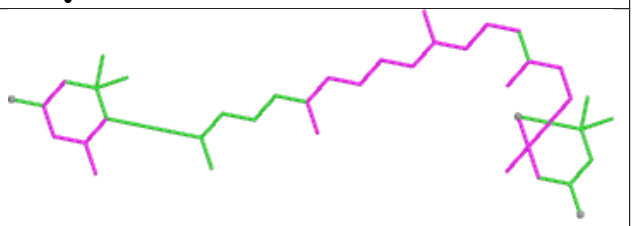


Rings

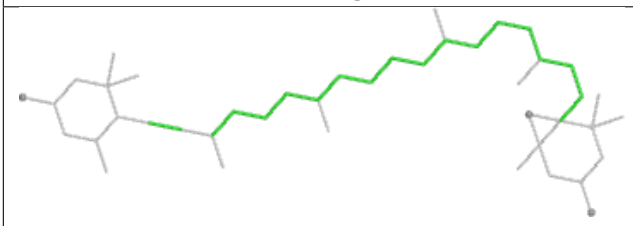
Ligand DD6 Q 615



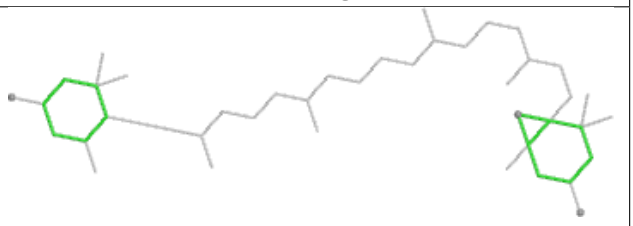
Bond lengths



Bond angles

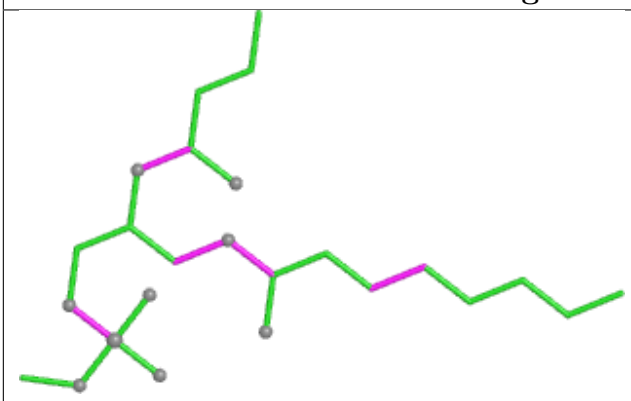


Torsions

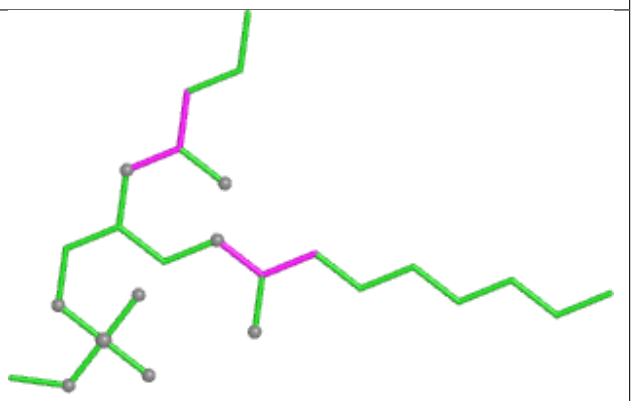


Rings

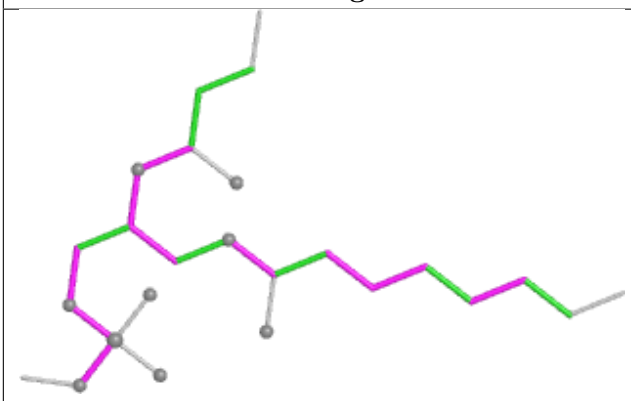
Ligand LHG U 419



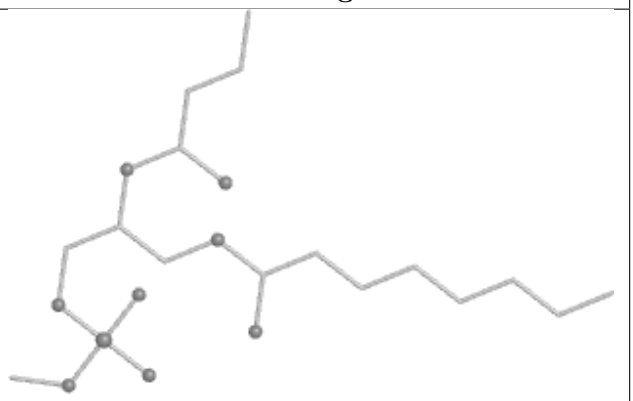
Bond lengths



Bond angles

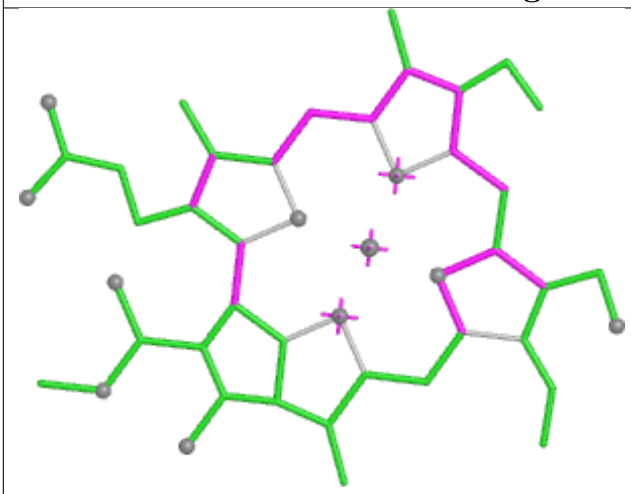


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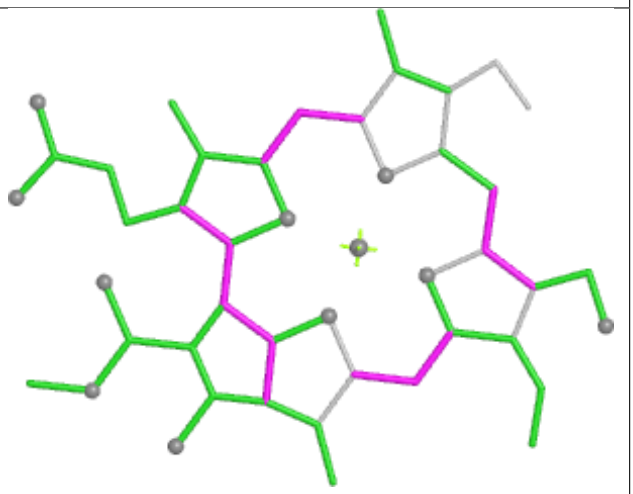


Rings

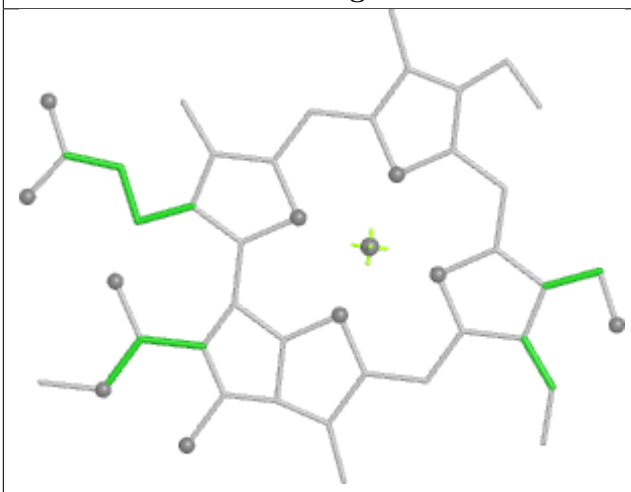
Ligand CHL X 406



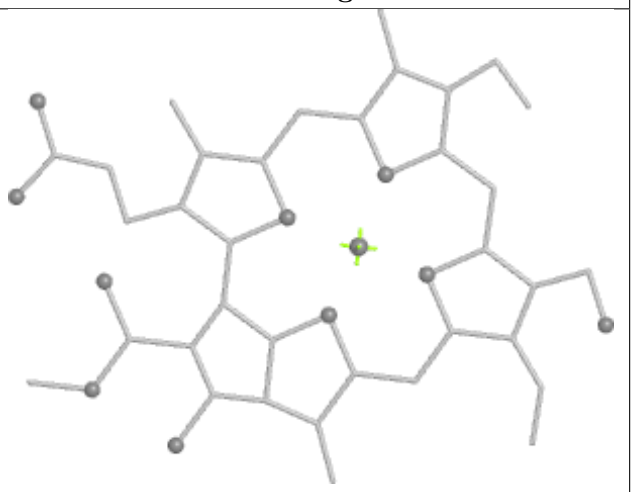
Bond lengths



Bond angles

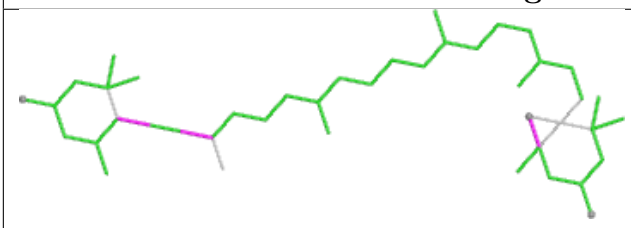


Torsions

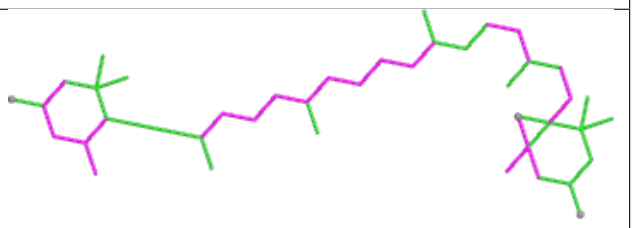


Rings

Ligand DD6 A 859



Bond lengths



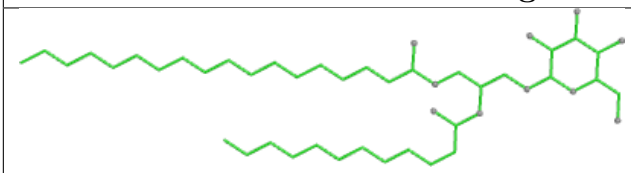
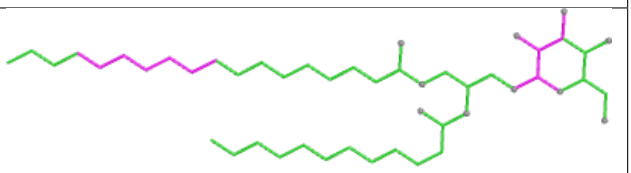
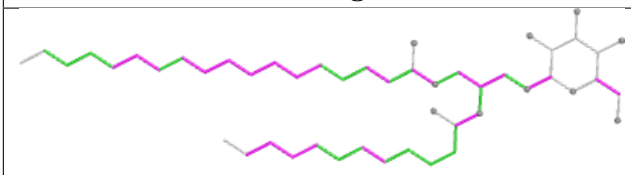
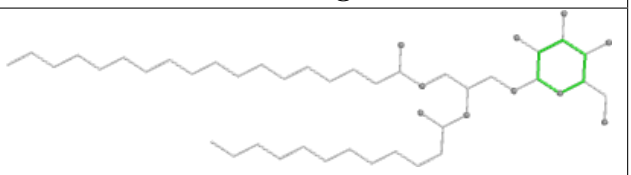
Bond angles

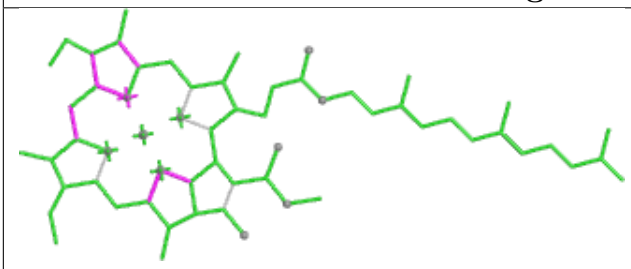
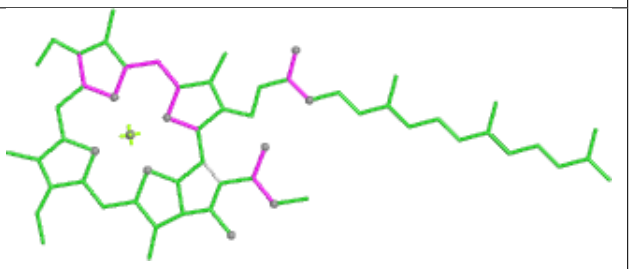
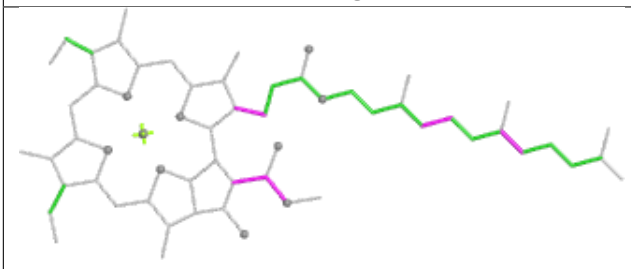
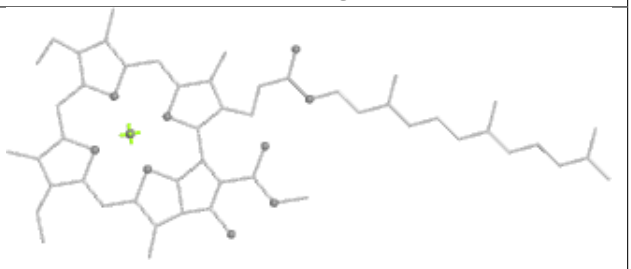


Torsions

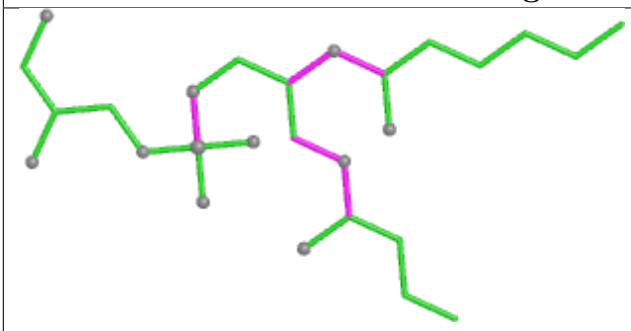


Rings

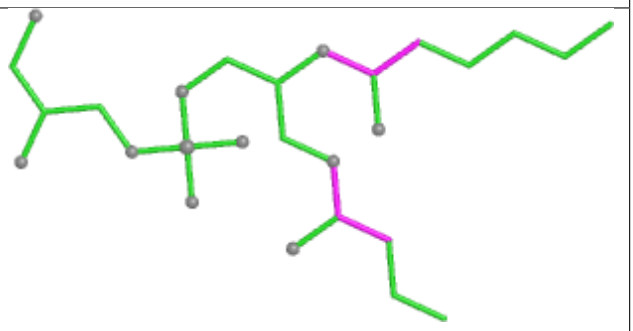
Ligand LMG K 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

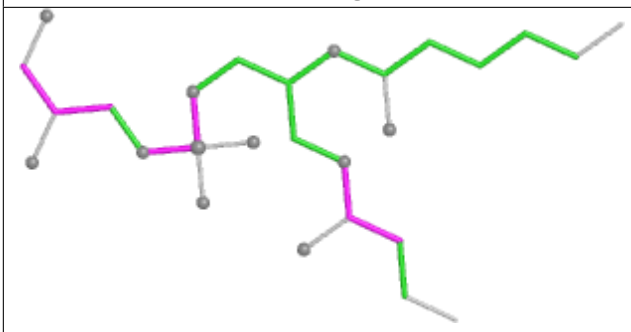
Ligand LHG B 848



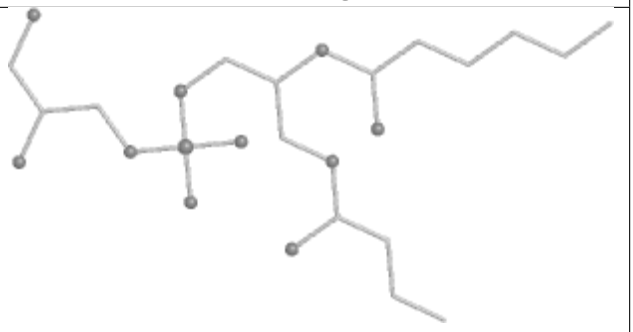
Bond lengths



Bond angles

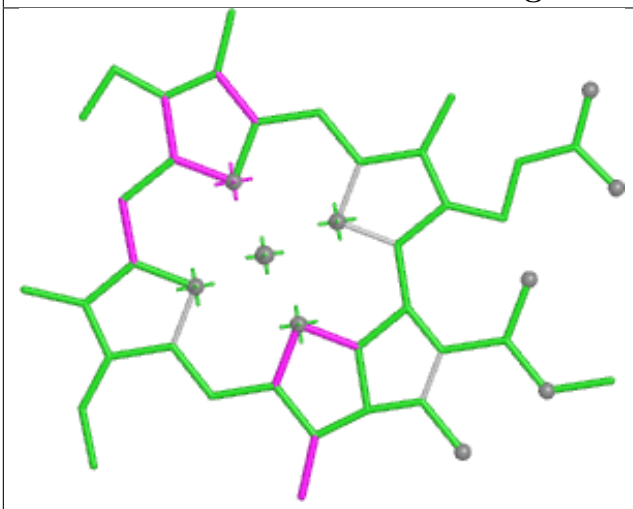


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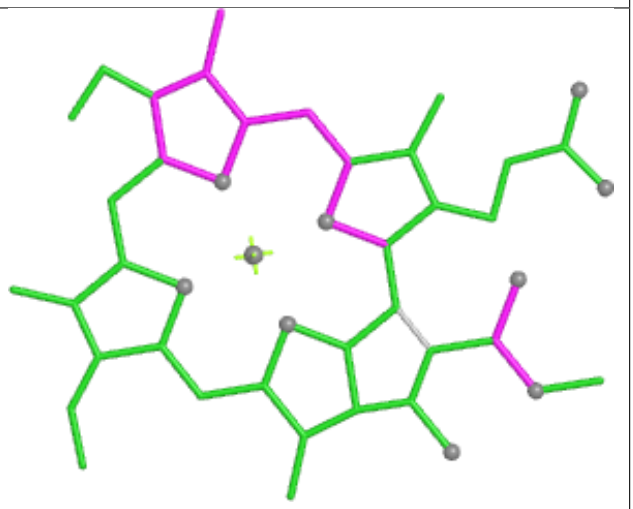


Rings

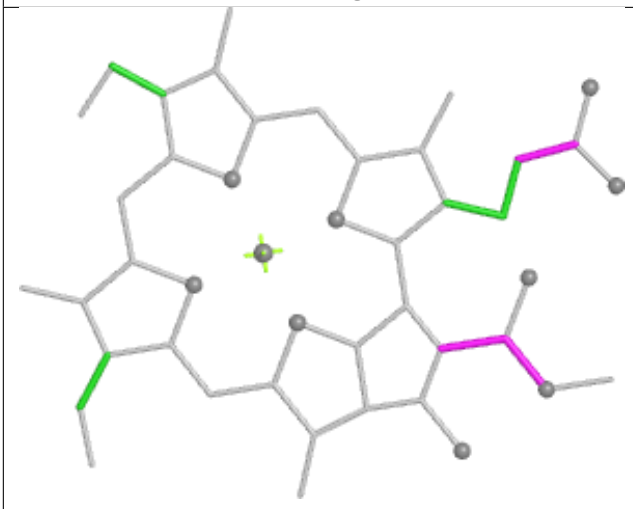
Ligand CLA T 609



Bond lengths



Bond angles

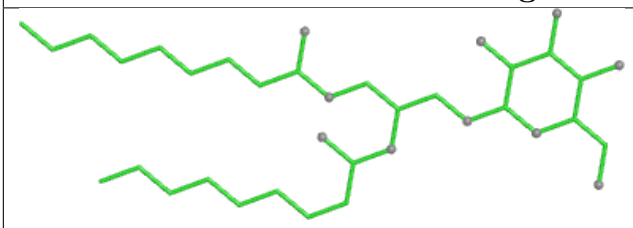


Torsions

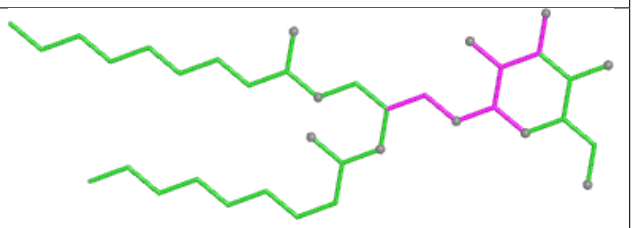


Rings

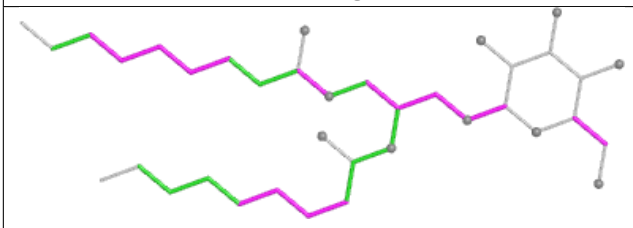
Ligand LMG H 322



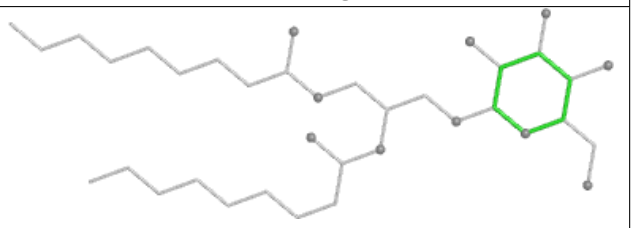
Bond lengths



Bond angles

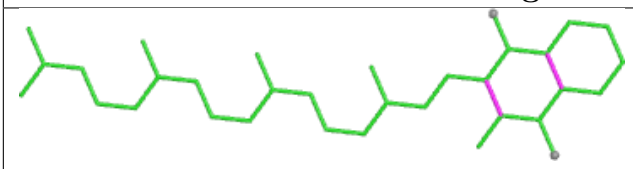


Torsions

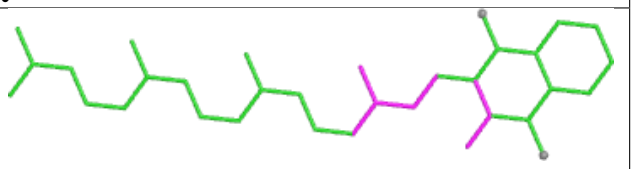


Rings

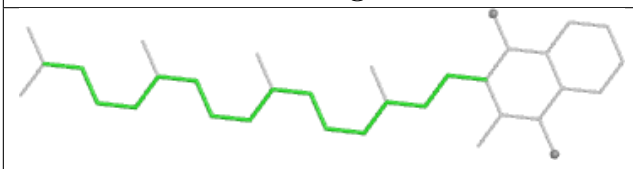
Ligand PQN B 840



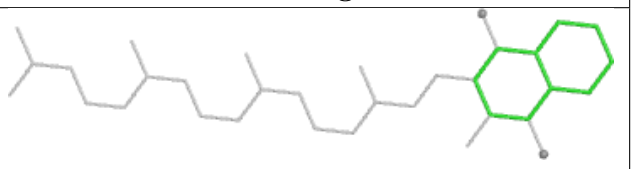
Bond lengths



Bond angles

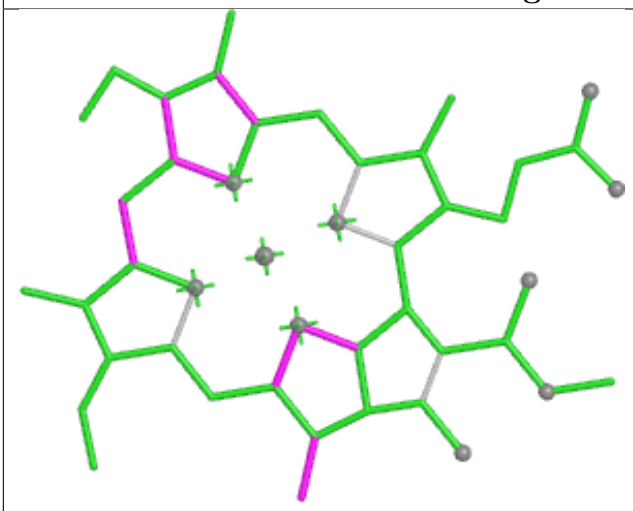


Torsions

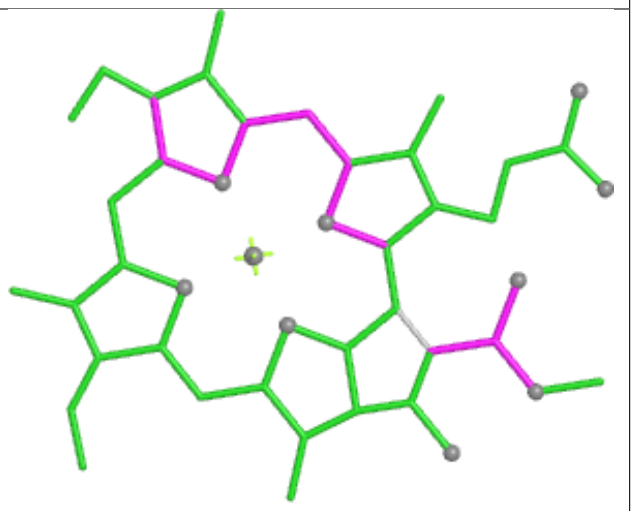


Rings

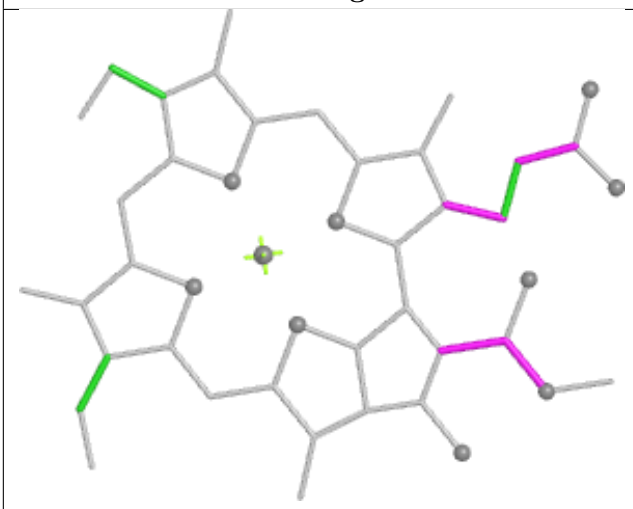
Ligand CLA U 403



Bond lengths



Bond angles

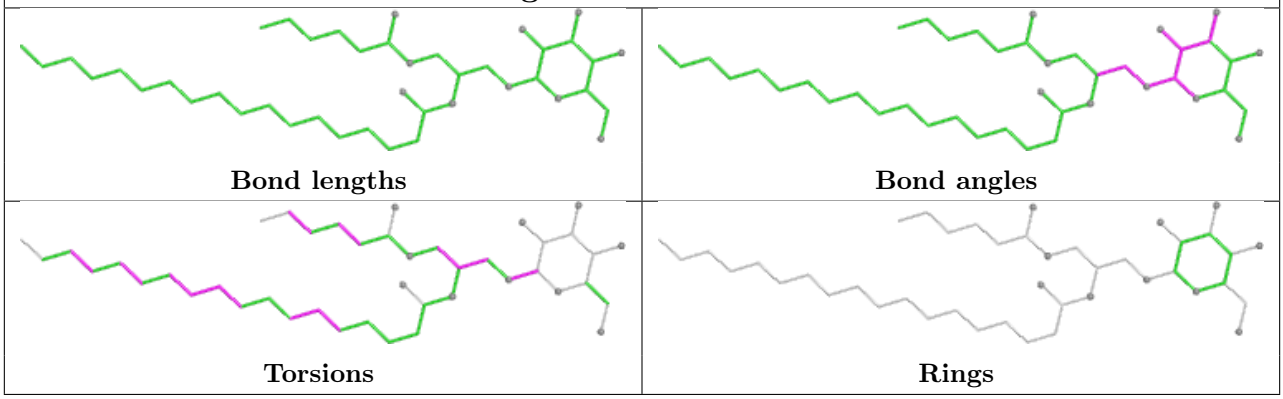


Torsions

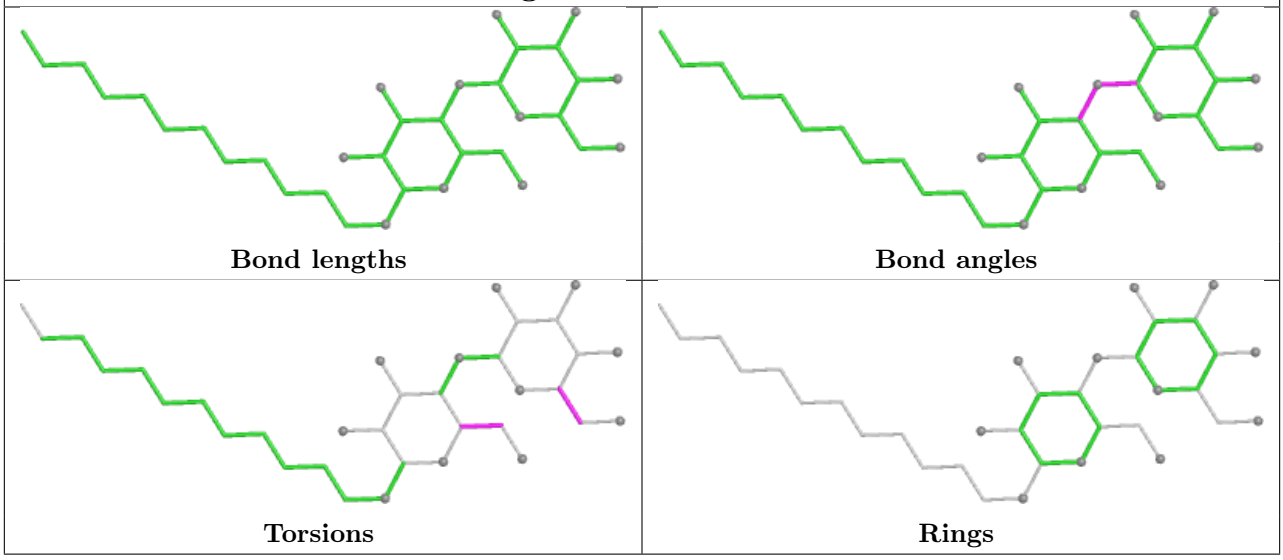


Rings

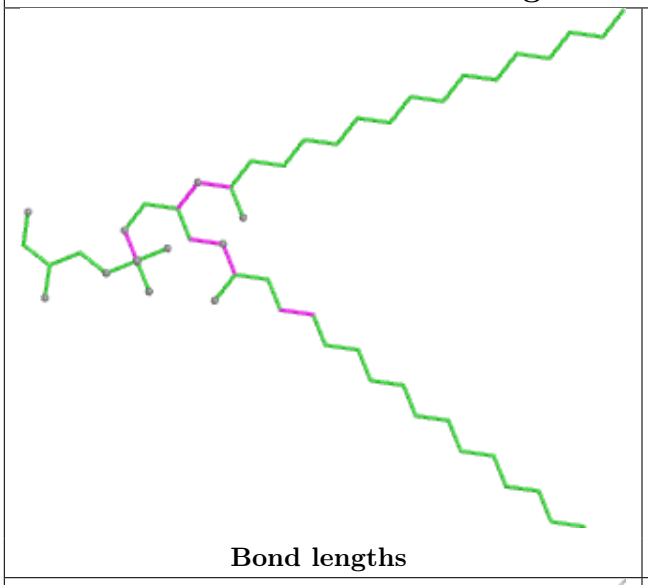
Ligand LMG B 852



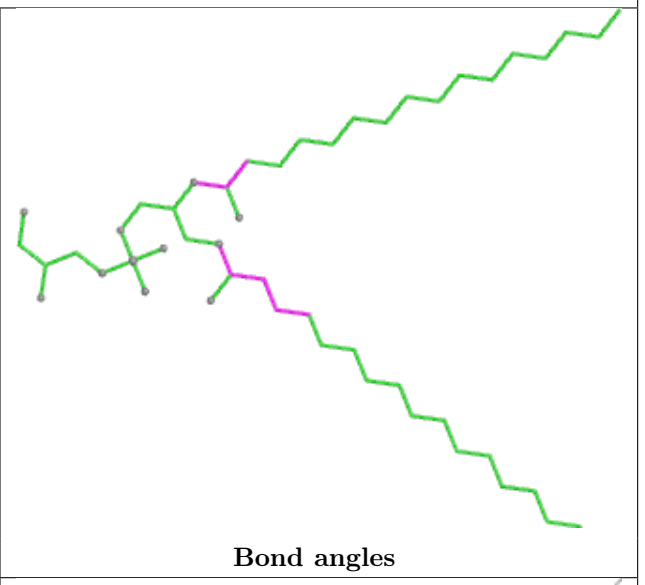
Ligand LMU O 303



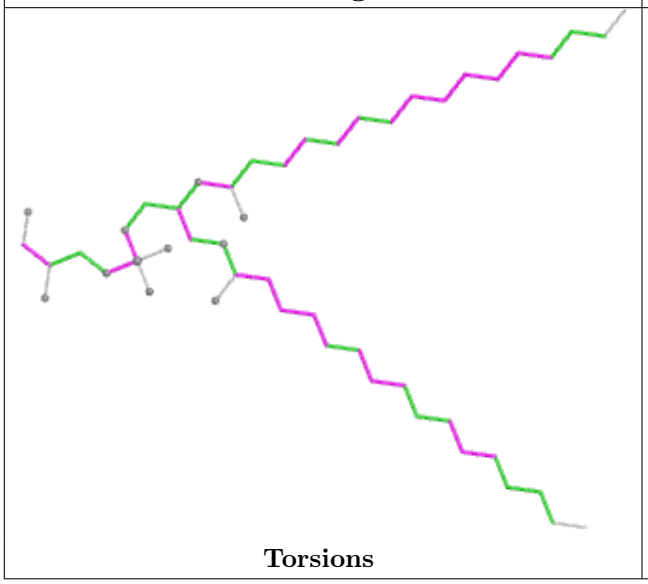
Ligand LHG A 845



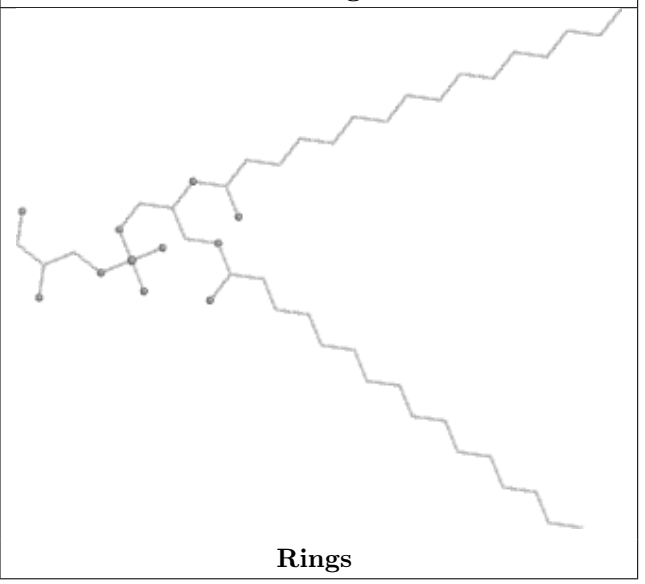
Bond lengths



Bond angles

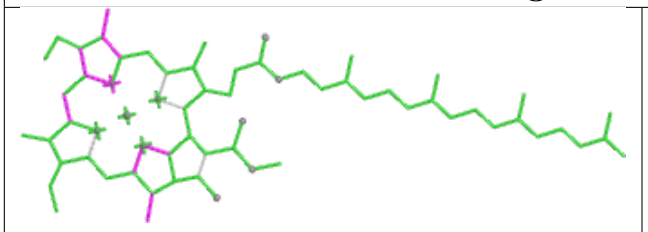


Torsions

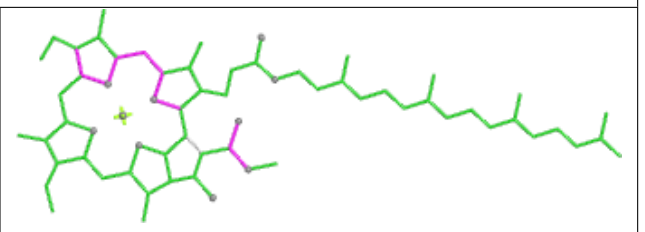


Rings

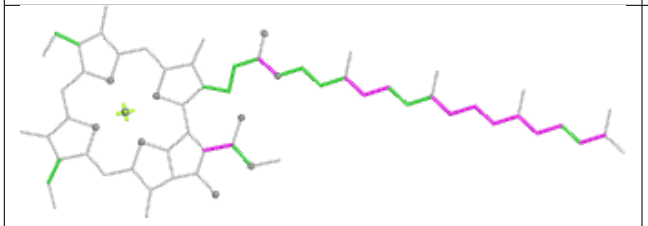
Ligand CLA L 402



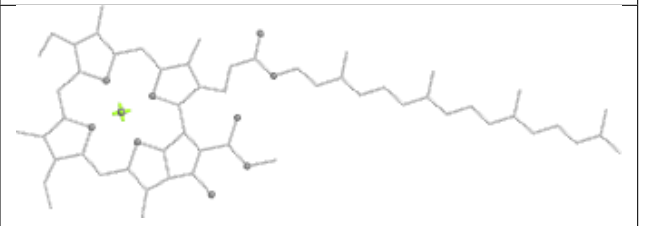
Bond lengths



Bond angles

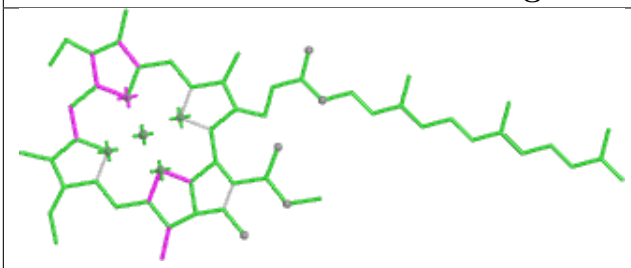


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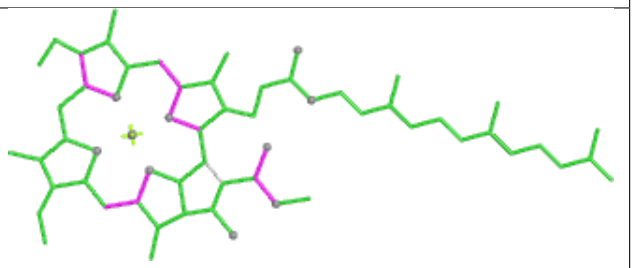


Rings

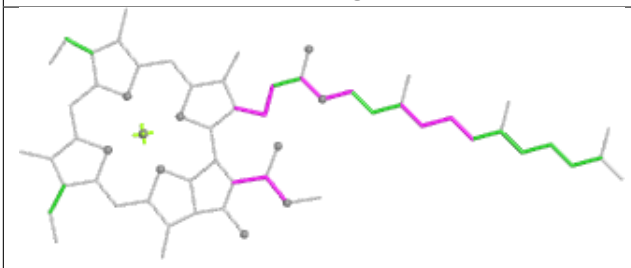
Ligand CLA R 602



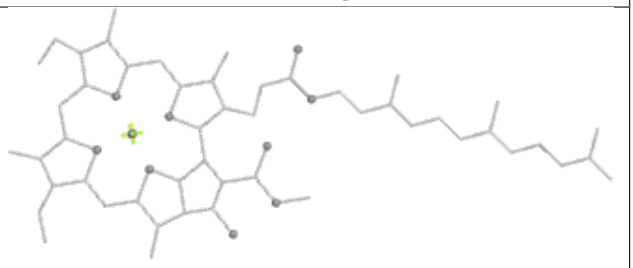
Bond lengths



Bond angles

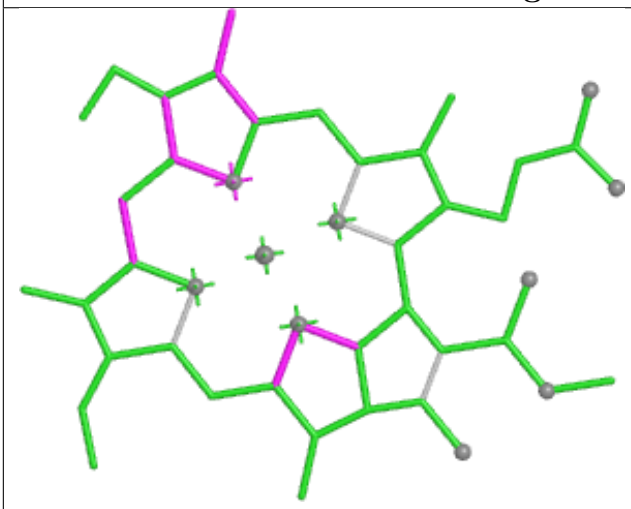


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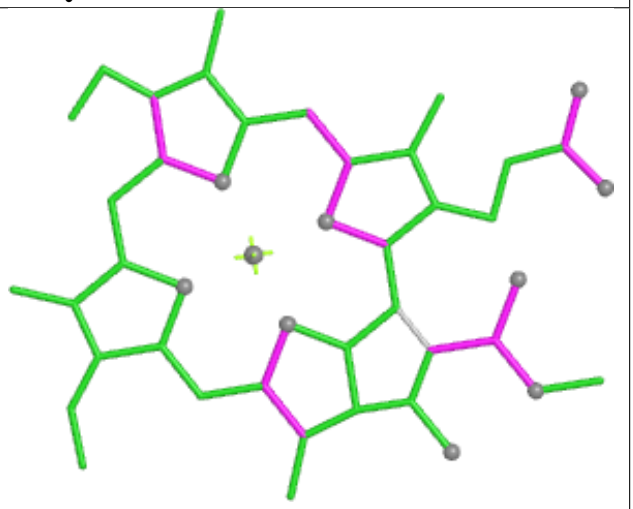


Rings

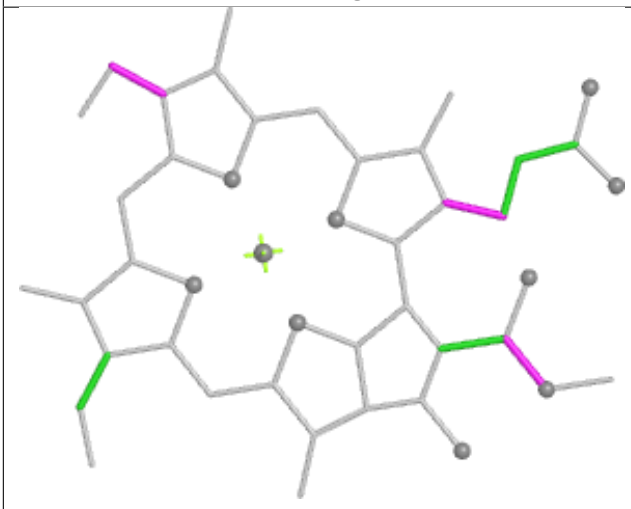
Ligand CLA Q 613



Bond lengths



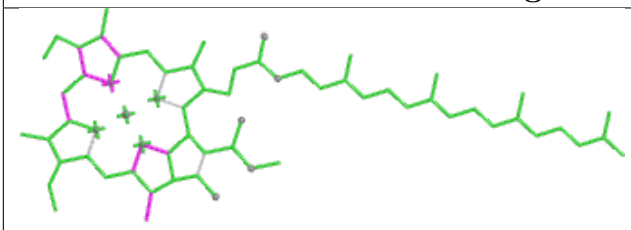
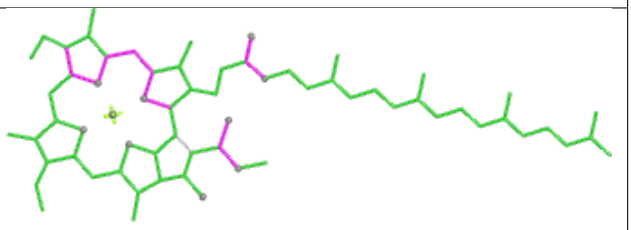
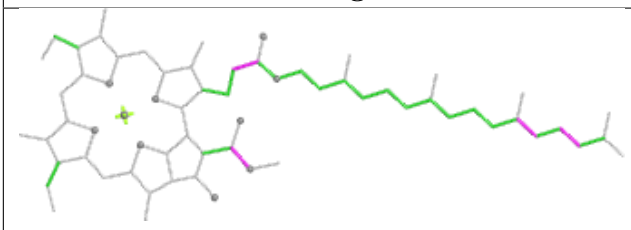
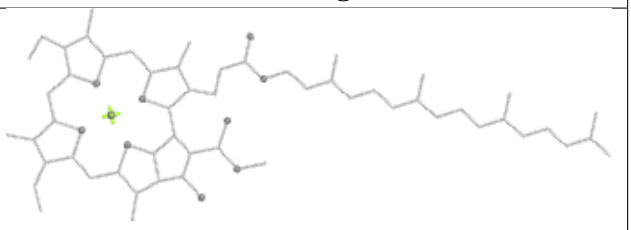
Bond angles

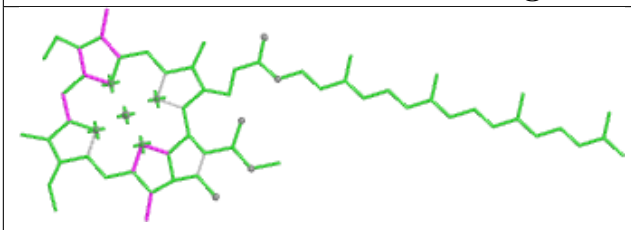
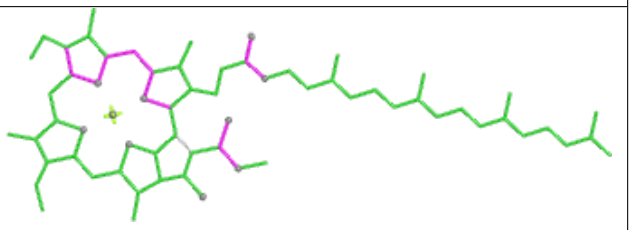
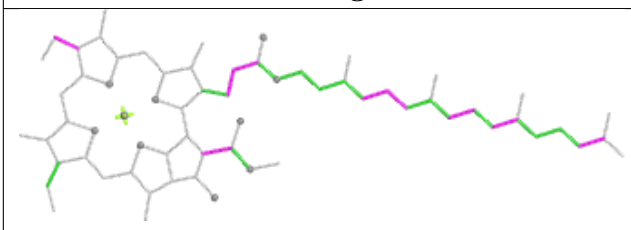
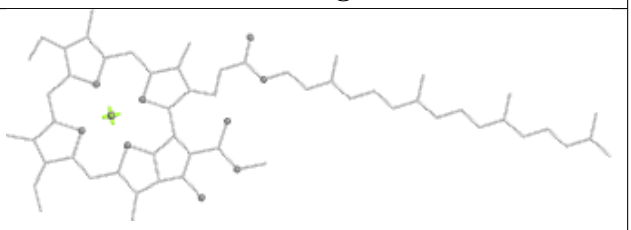


Torsions

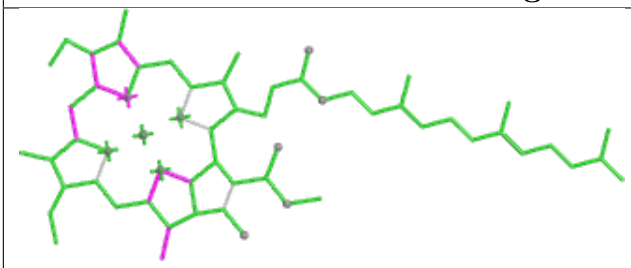


Rings

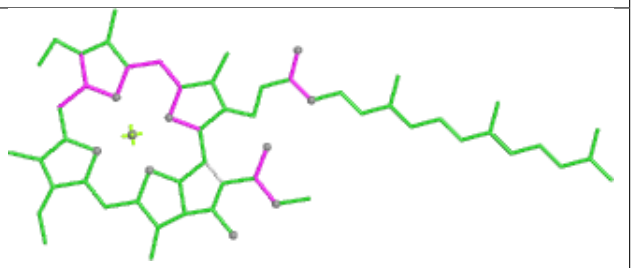
Ligand CLA B 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA X 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

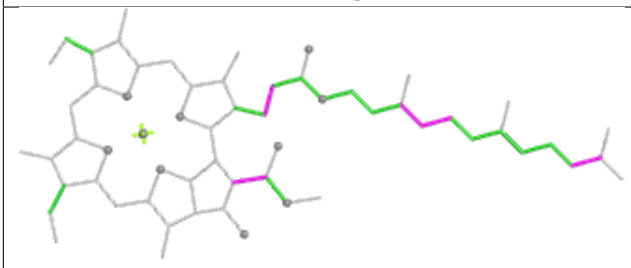
Ligand CLA O 306



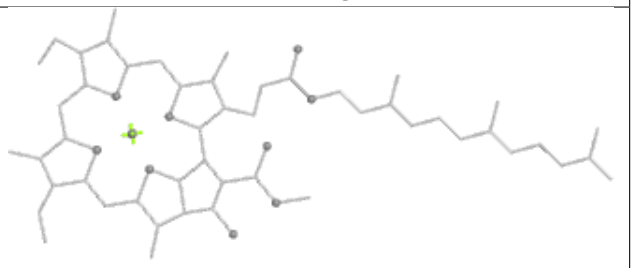
Bond lengths



Bond angles

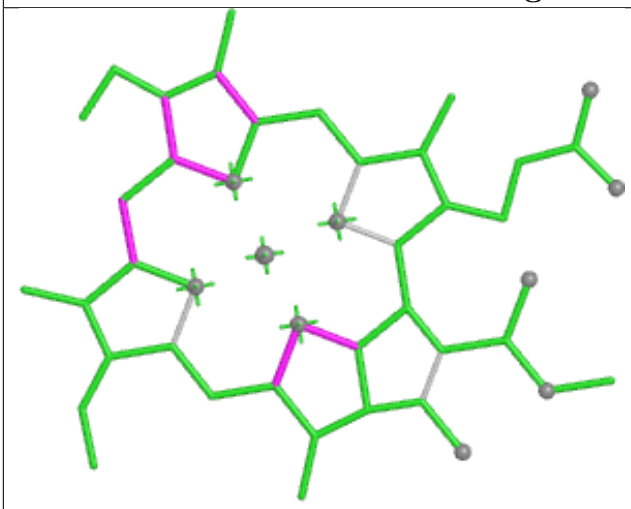


Torsions

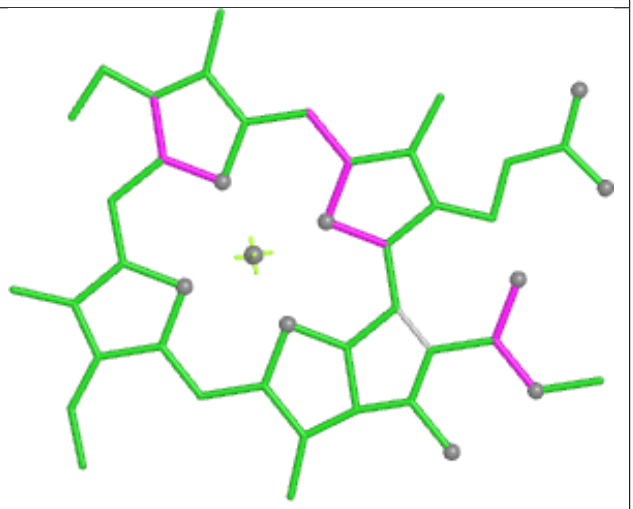


Rings

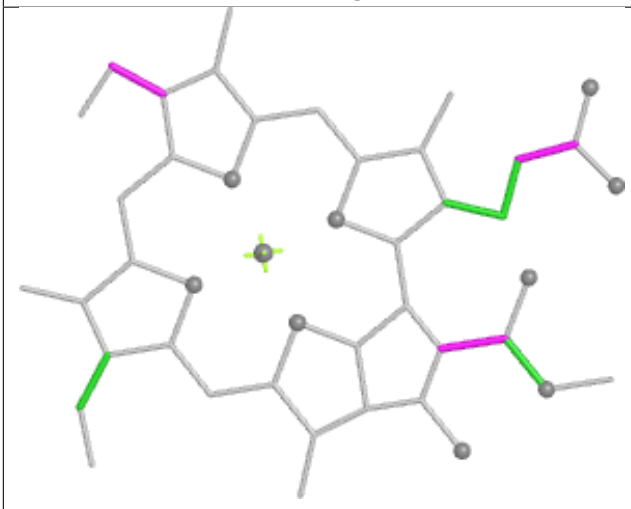
Ligand CLA T 610



Bond lengths



Bond angles

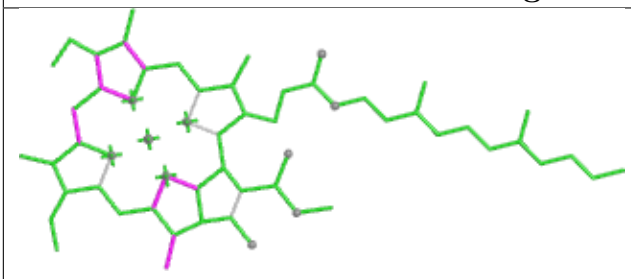


Torsions

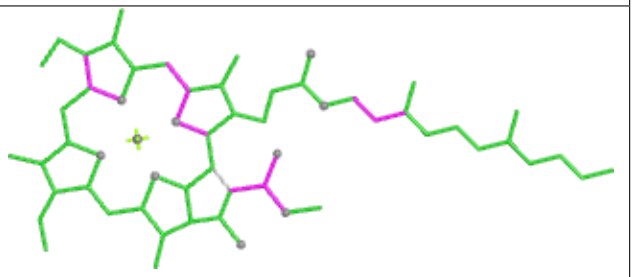


Rings

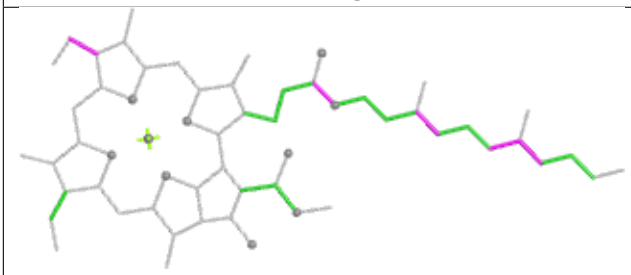
Ligand CLA H 313



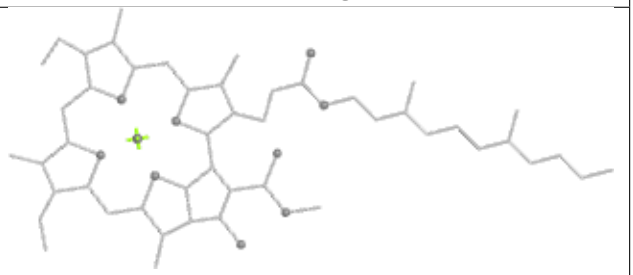
Bond lengths



Bond angles

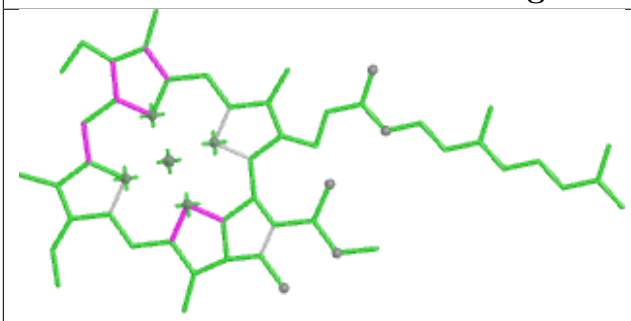


Torsions

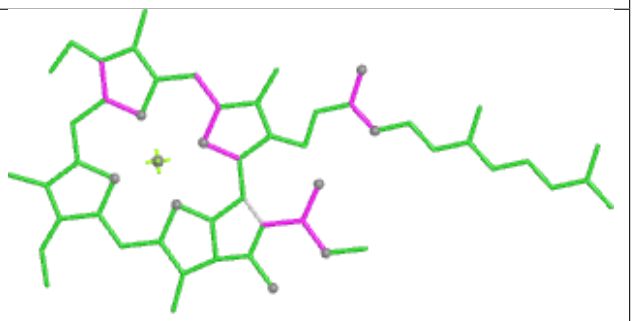


Rings

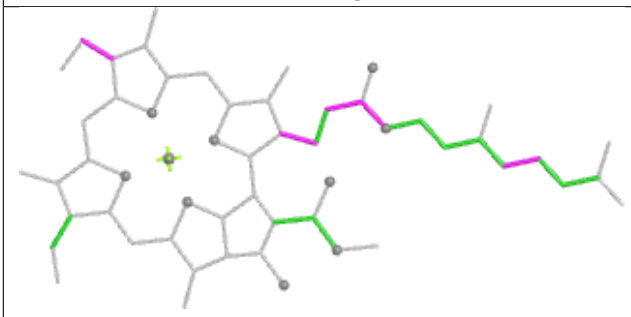
Ligand CLA S 609



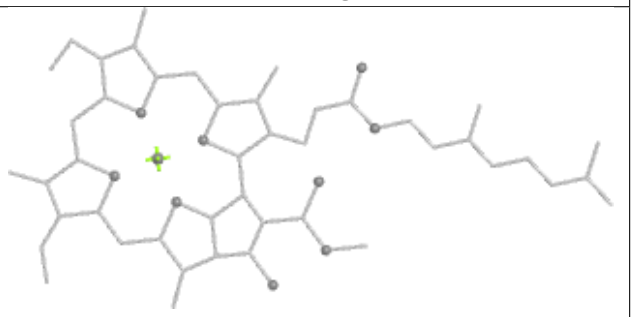
Bond lengths



Bond angles

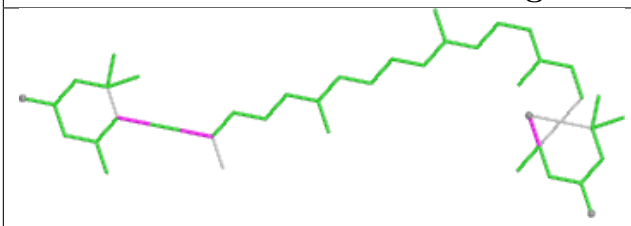


Torsions

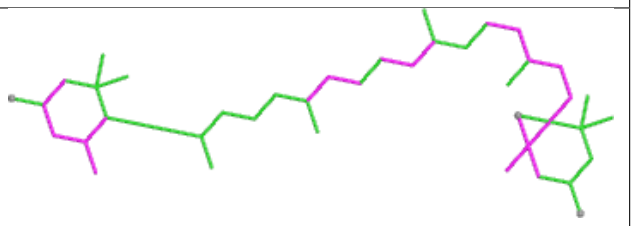


Rings

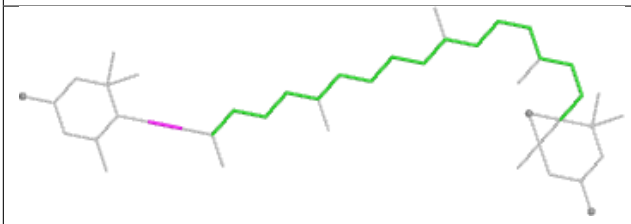
Ligand DD6 T 613



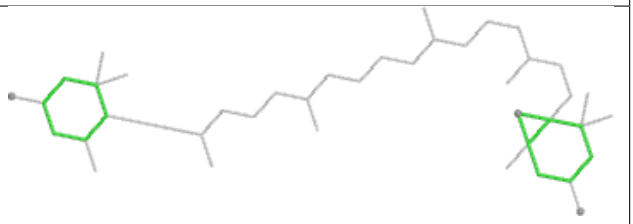
Bond lengths



Bond angles

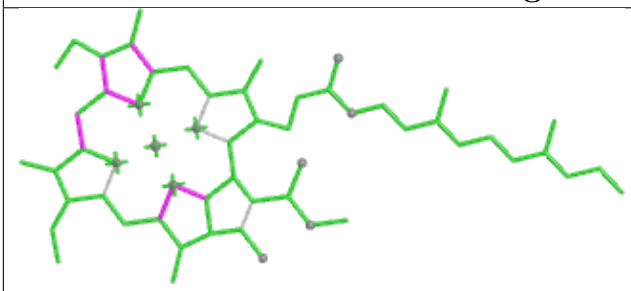


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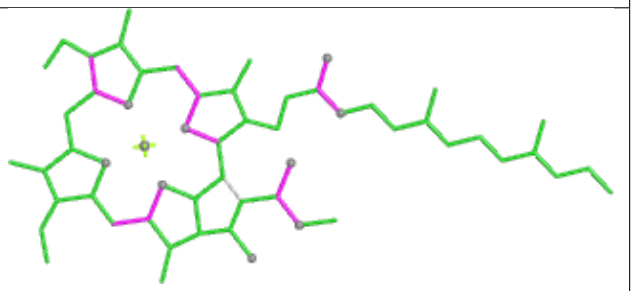


Rings

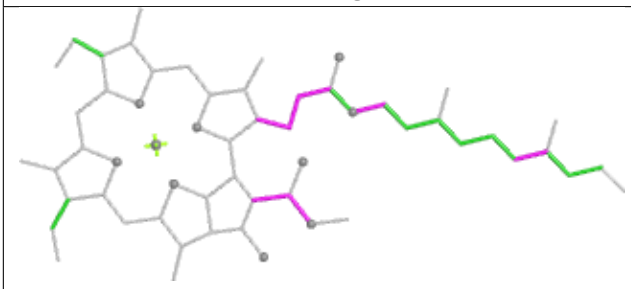
Ligand CLA R 606



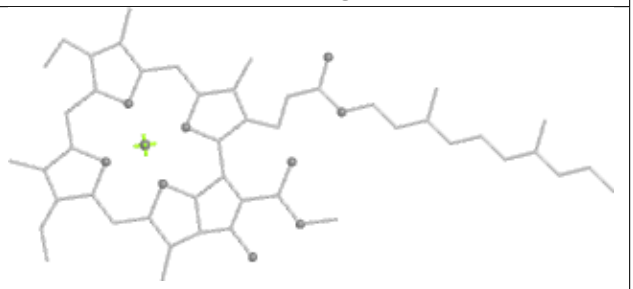
Bond lengths



Bond angles

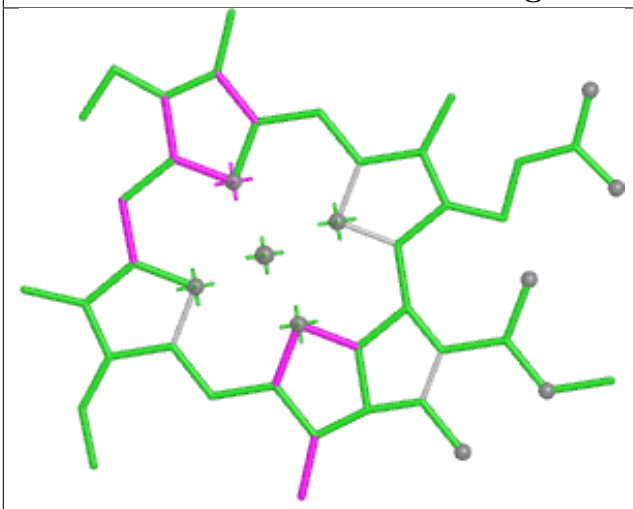


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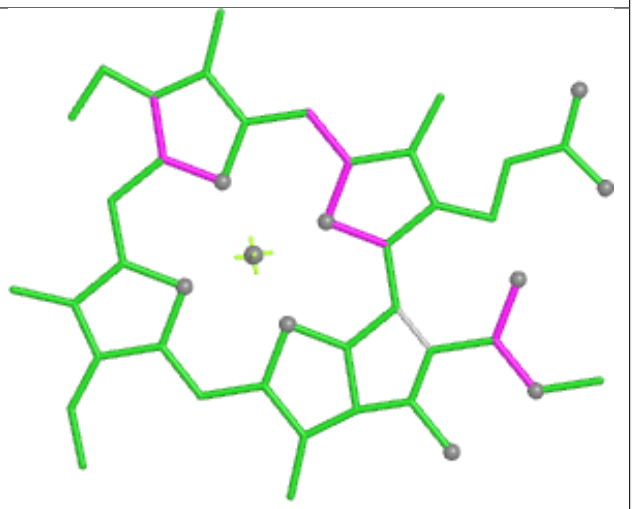


Rings

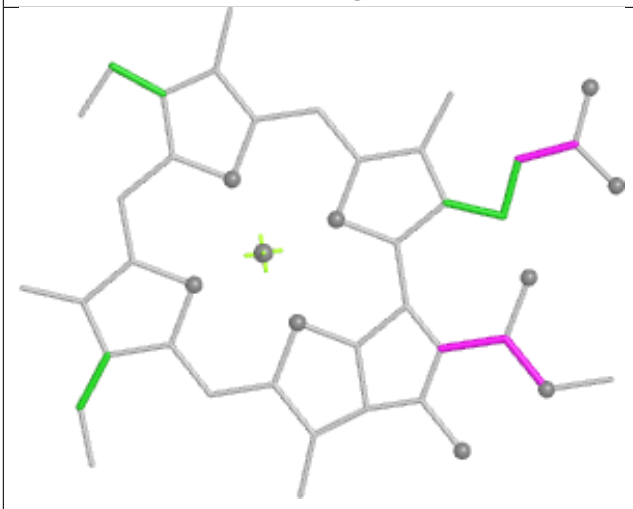
Ligand CLA T 601



Bond lengths



Bond angles

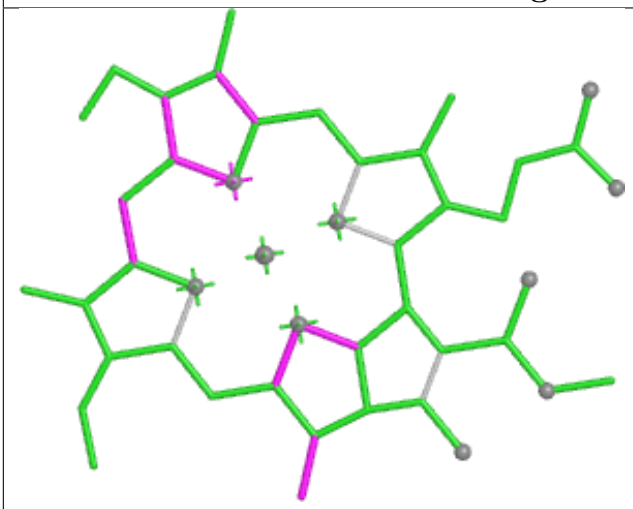


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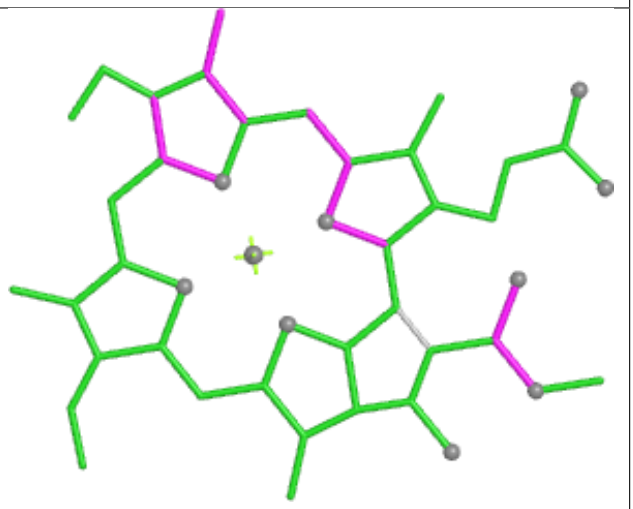


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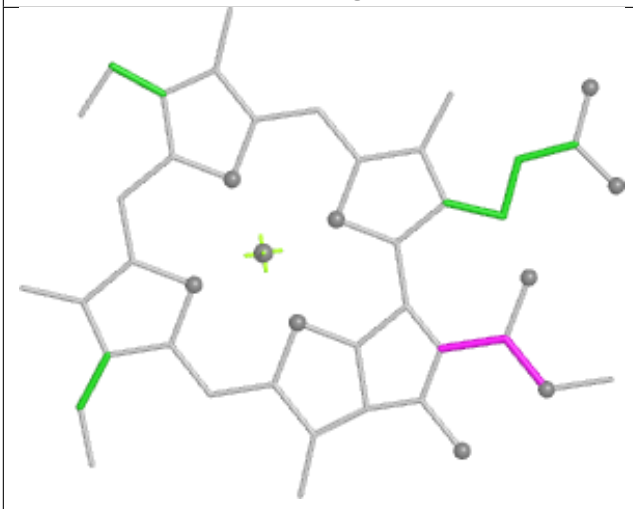
Ligand CLA I 609



Bond lengths



Bond angles

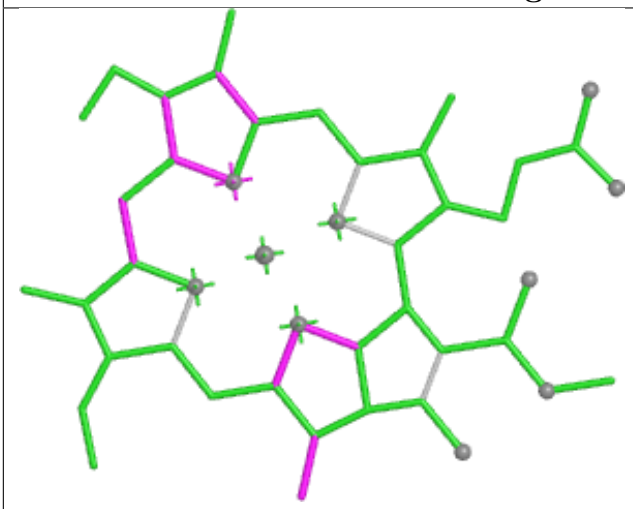


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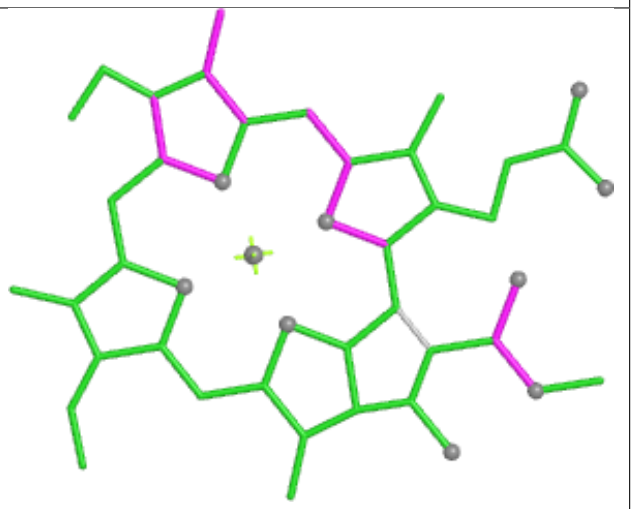


Rings

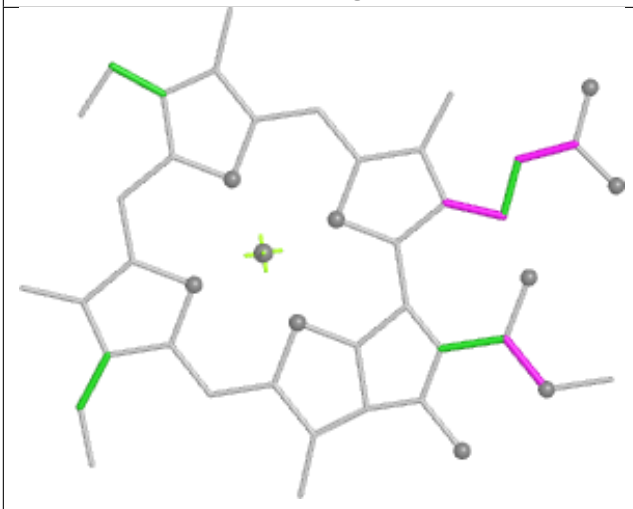
Ligand CLA P 606



Bond lengths



Bond angles

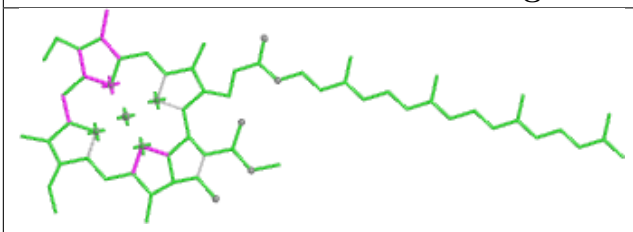


Torsions

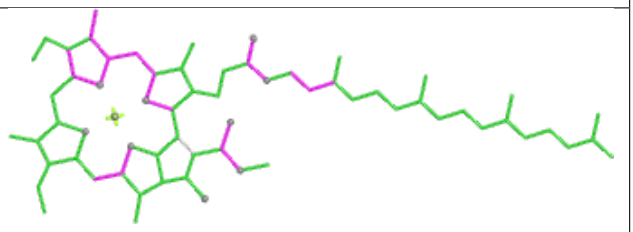


Rings

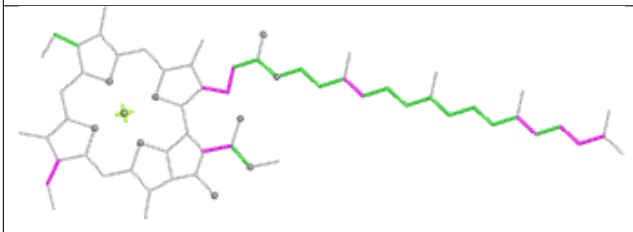
Ligand CLA A 820



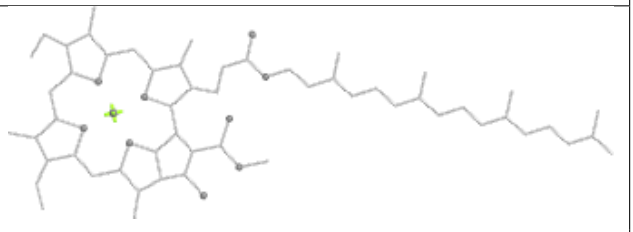
Bond lengths



Bond angles

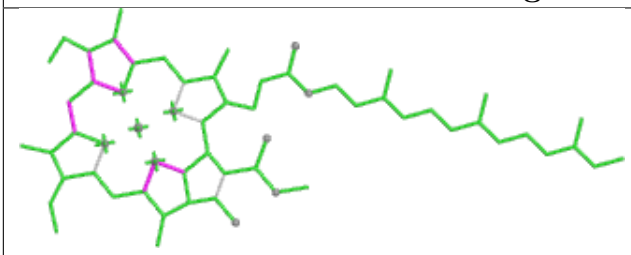


Torsions

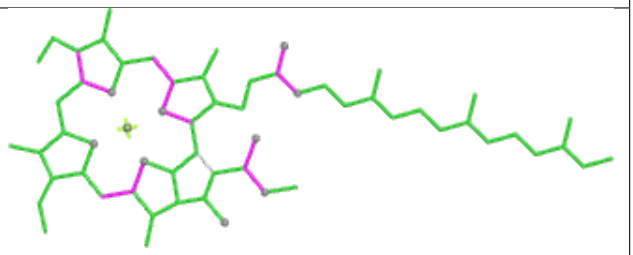


Rings

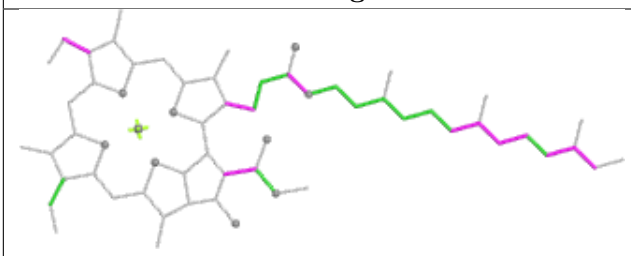
Ligand CLA A 825



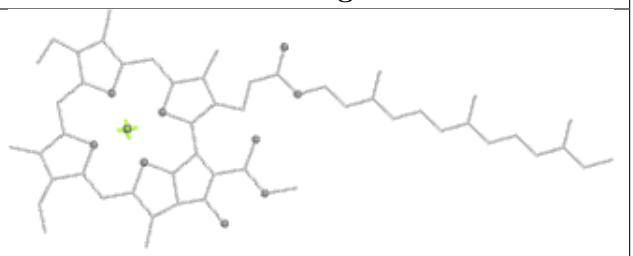
Bond lengths



Bond angles

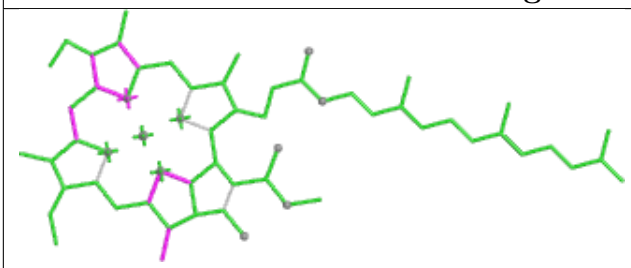


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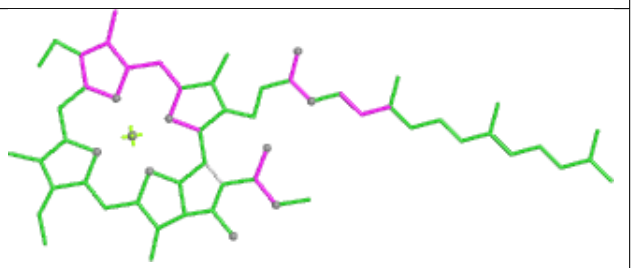


Rings

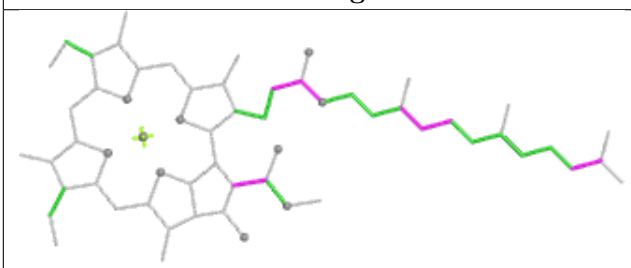
Ligand CLA O 312



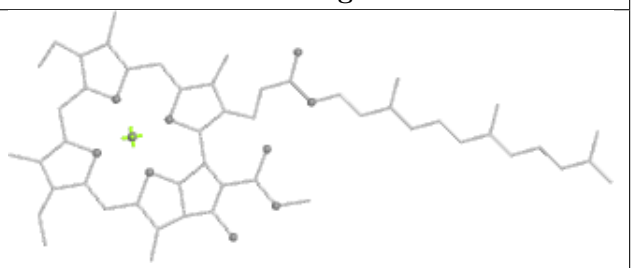
Bond lengths



Bond angles



Torsions

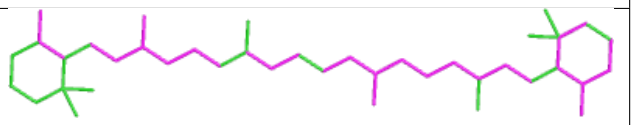


Rings

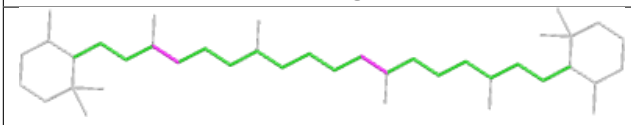
Ligand BCR A 851



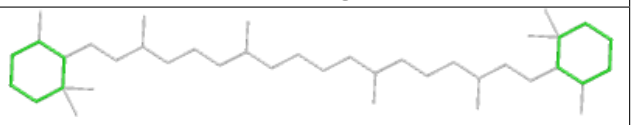
Bond lengths



Bond angles

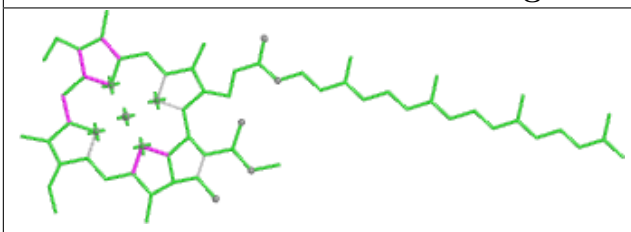


Torsions

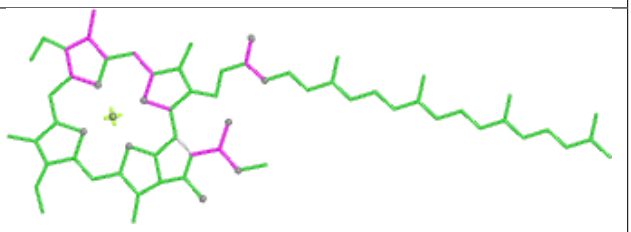


Rings

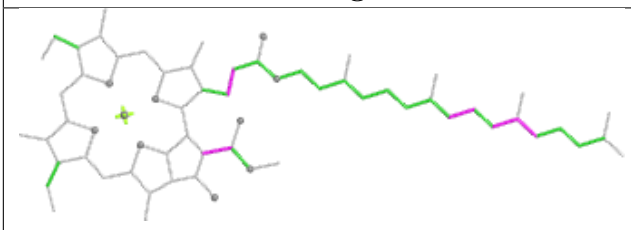
Ligand CLA A 839



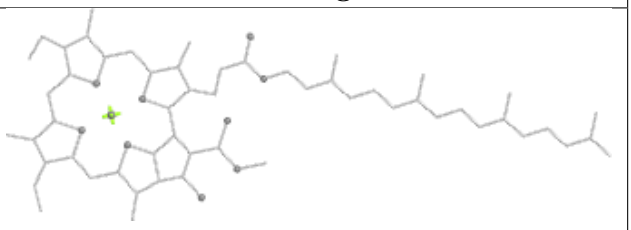
Bond lengths



Bond angles

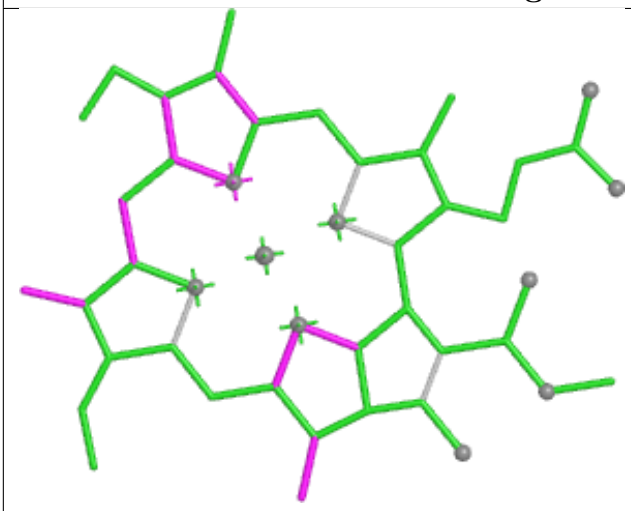


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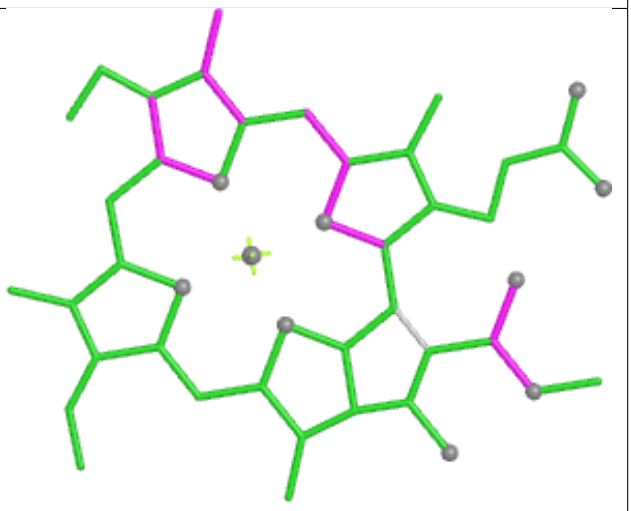


Rings

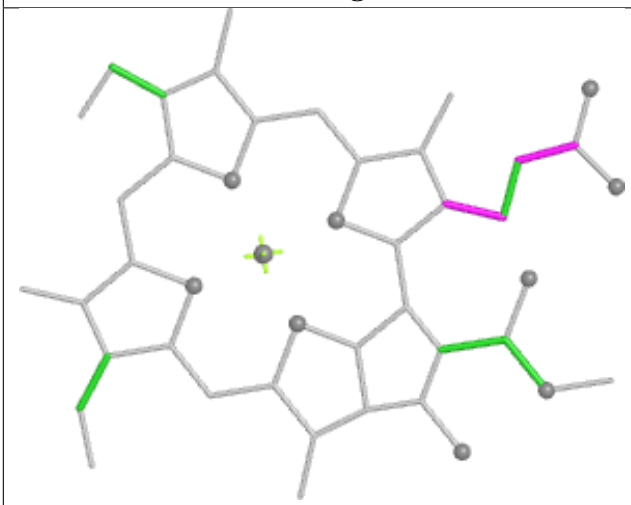
Ligand CLA P 607



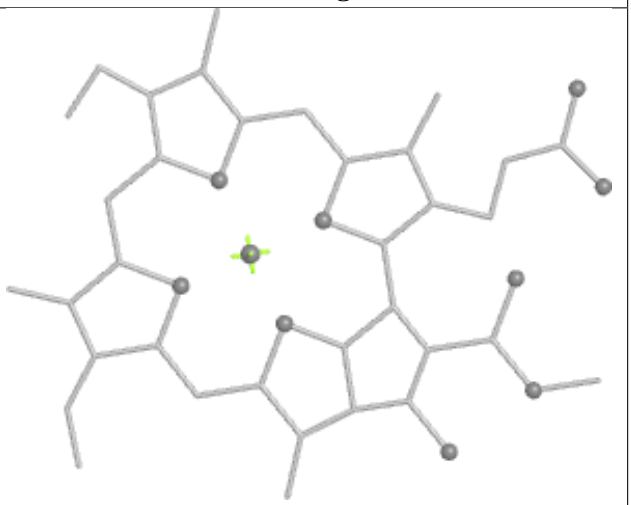
Bond lengths



Bond angles

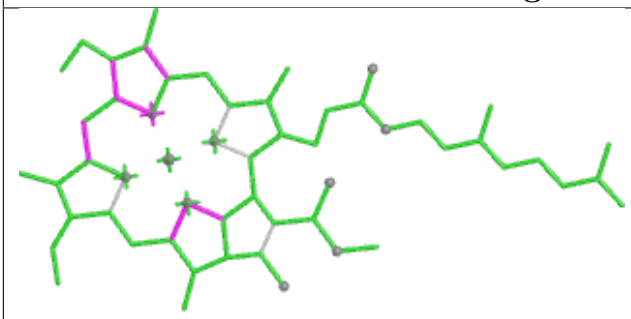


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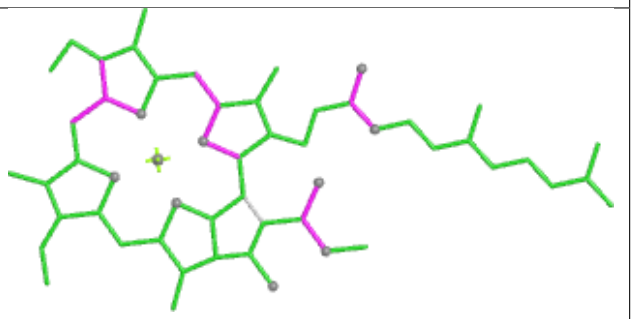


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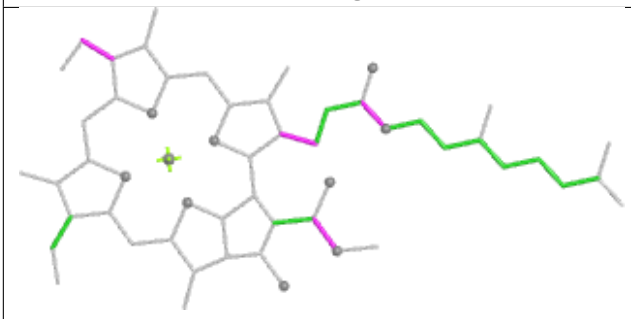
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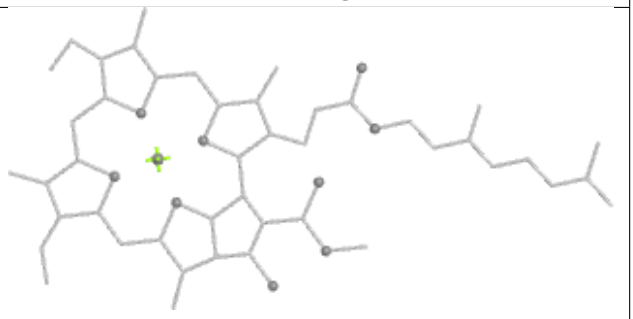
Bond lengths



Bond angles

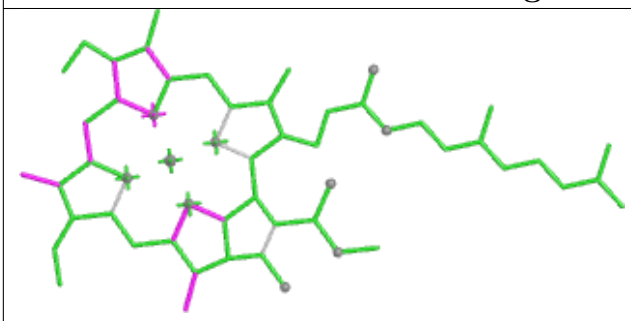


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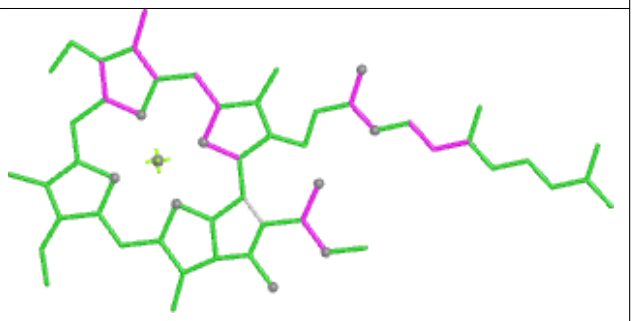


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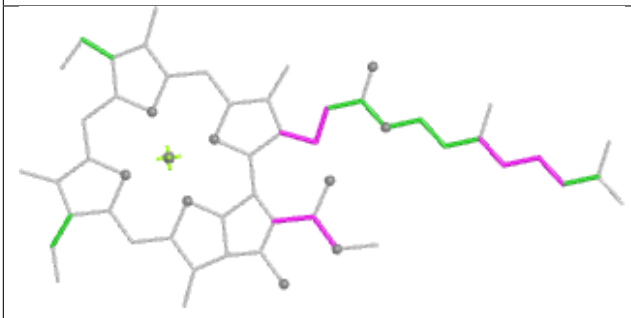
Ligand CLA A 844



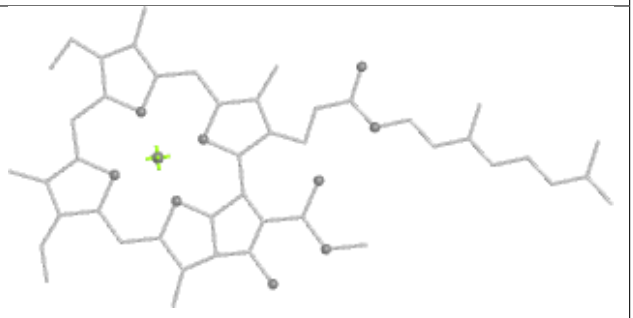
Bond lengths



Bond angles

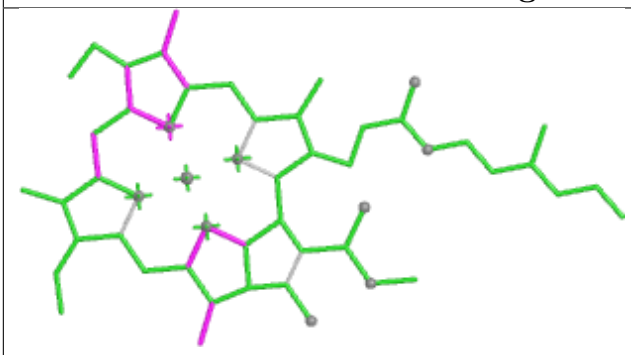


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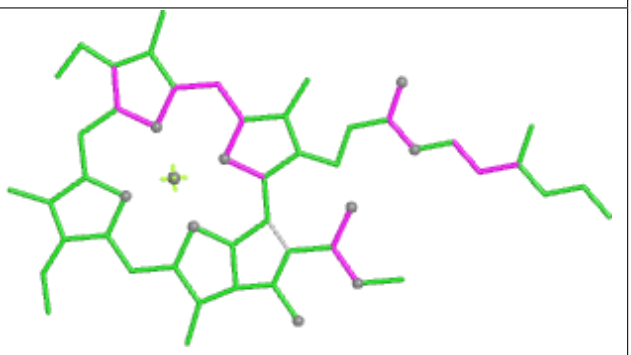


Rings

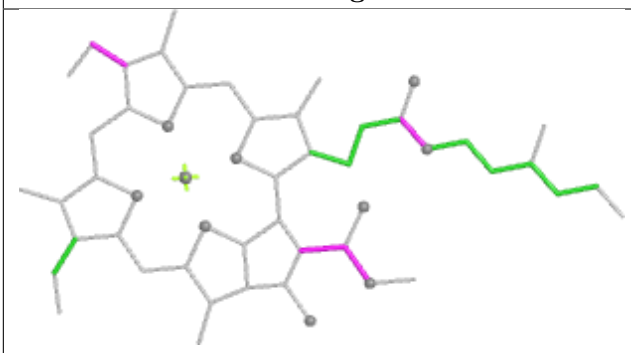
Ligand CLA W 403



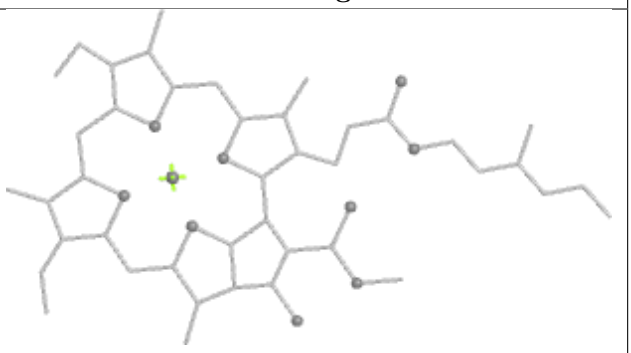
Bond lengths



Bond angles

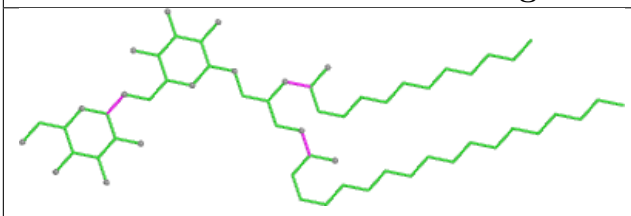


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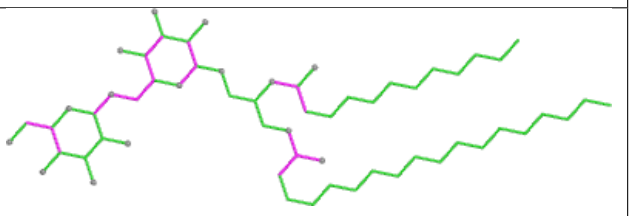


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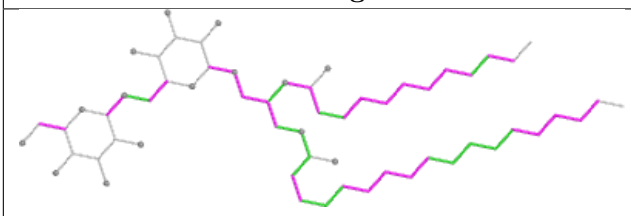
Ligand DGD O 304



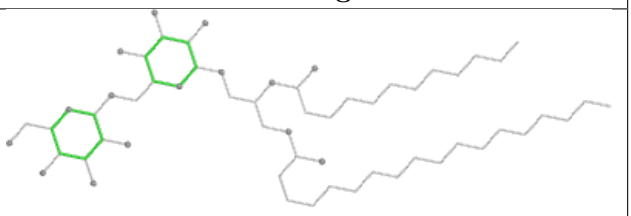
Bond lengths



Bond angles

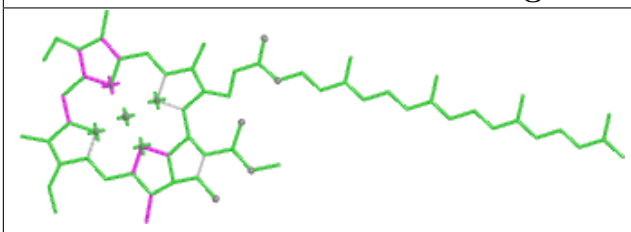


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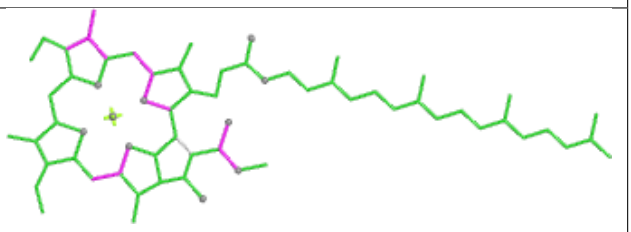


Rings

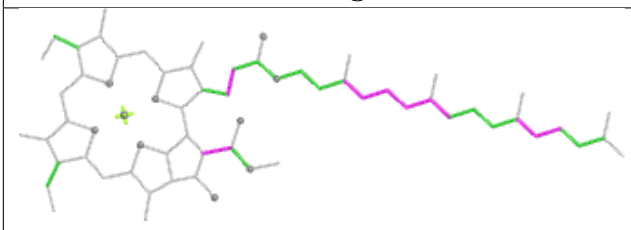
Ligand CLA B 806



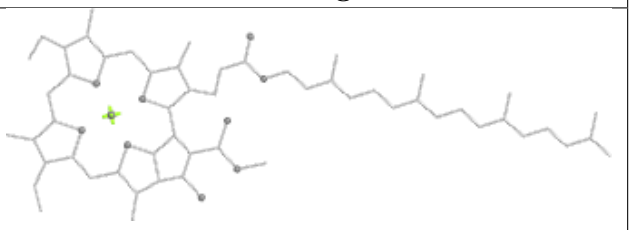
Bond lengths



Bond angles

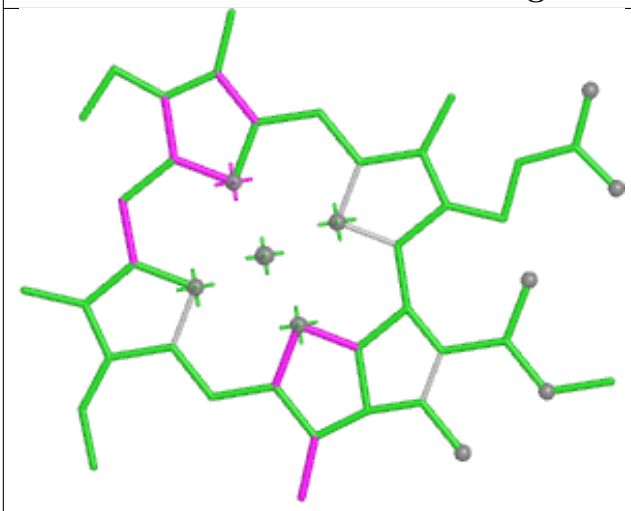


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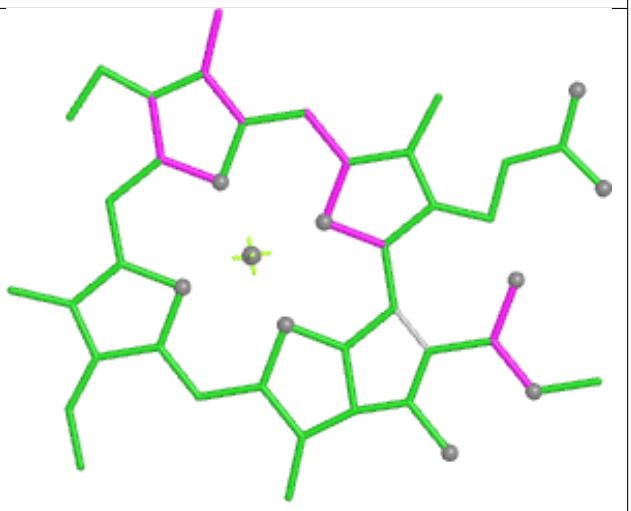


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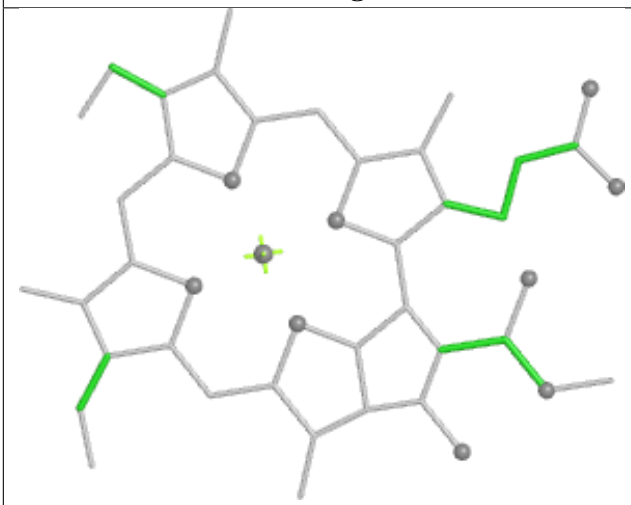
Ligand CLA S 614



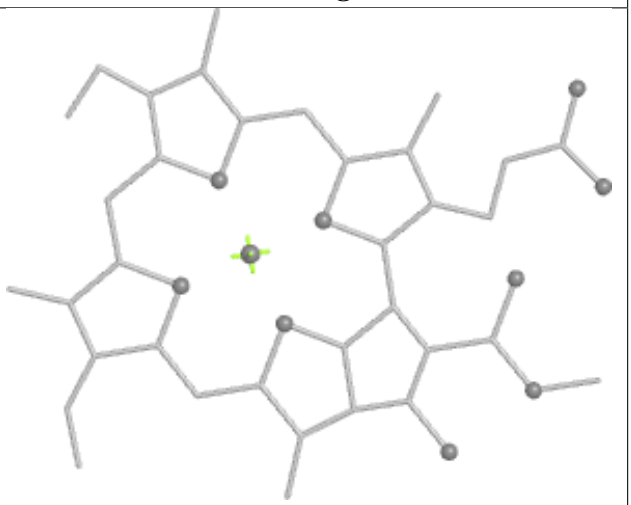
Bond lengths



Bond angles

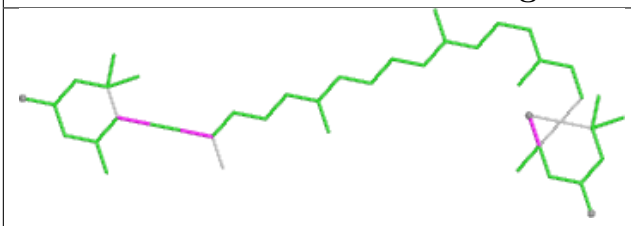


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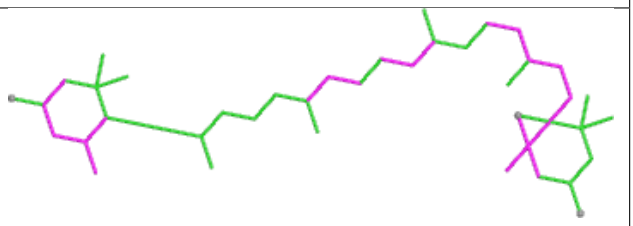


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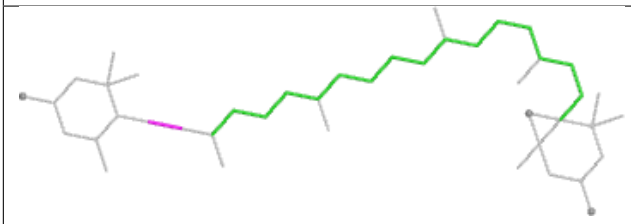
Ligand DD6 W 416



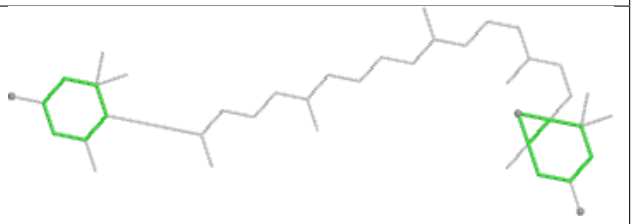
Bond lengths



Bond angles

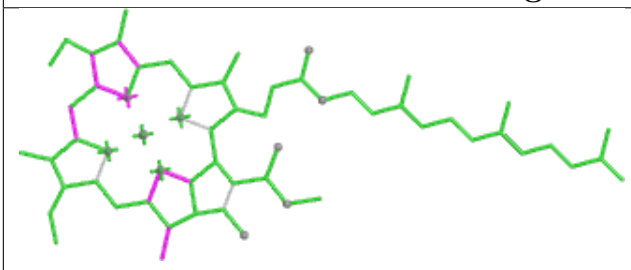


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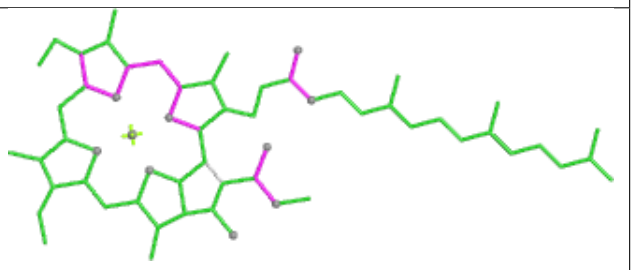


Rings

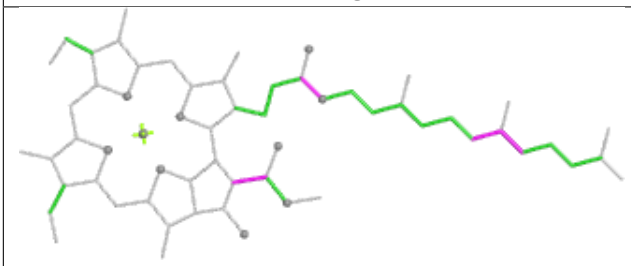
Ligand CLA T 603



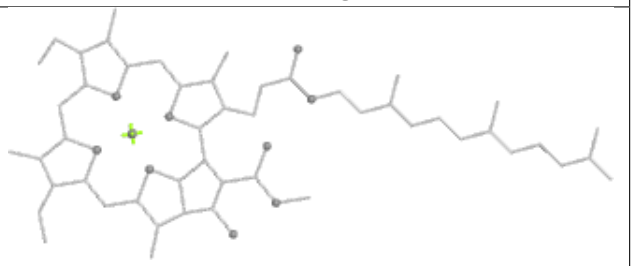
Bond lengths



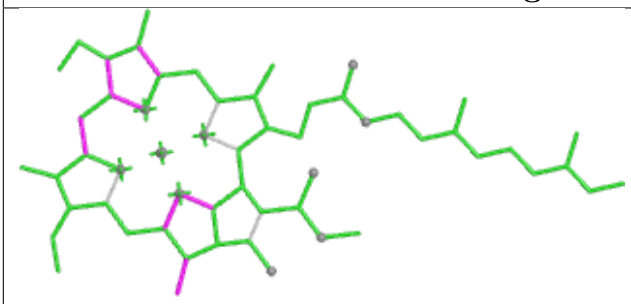
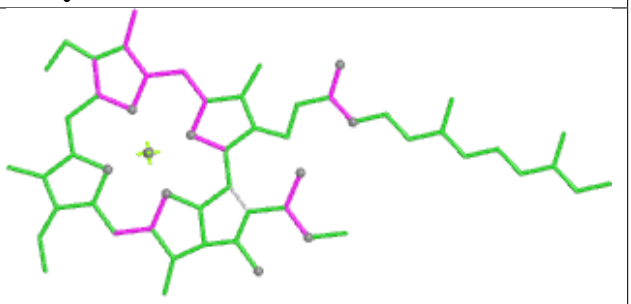
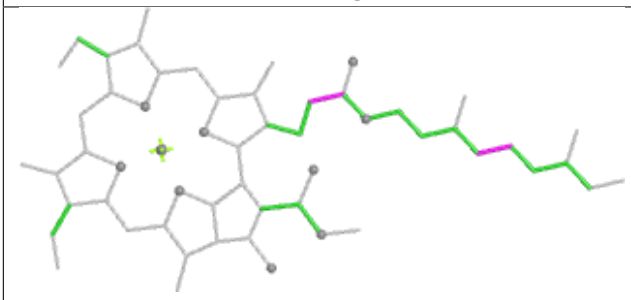
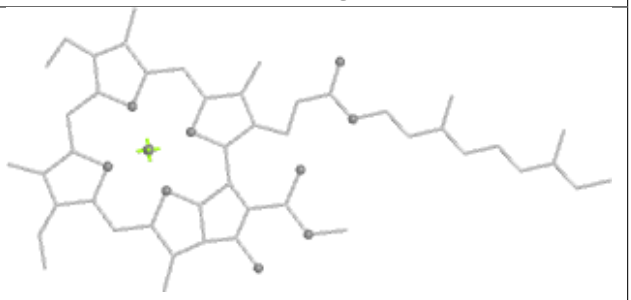
Bond angles

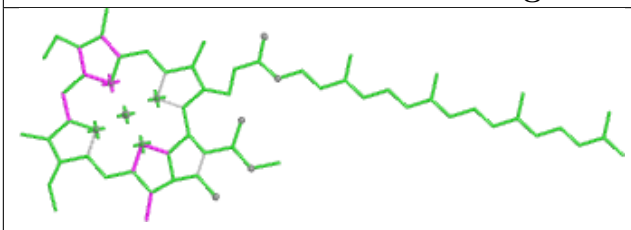
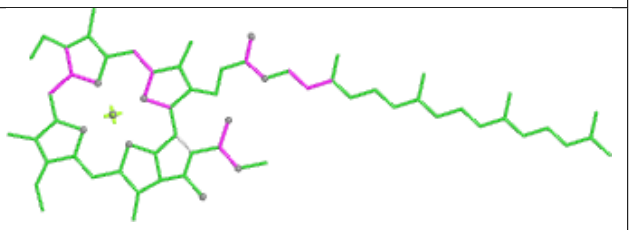
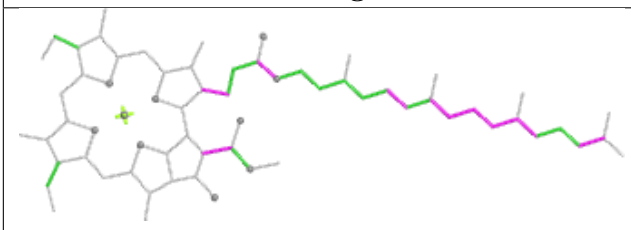
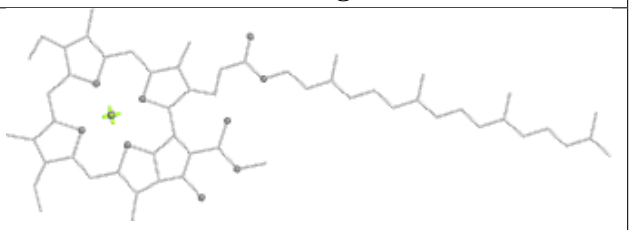


Torsions

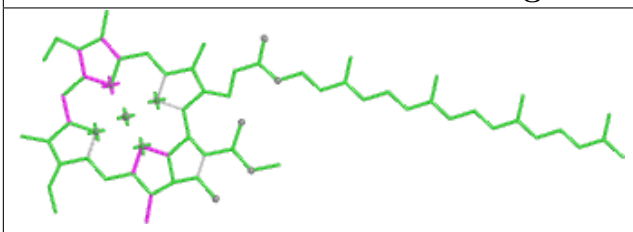


Rings

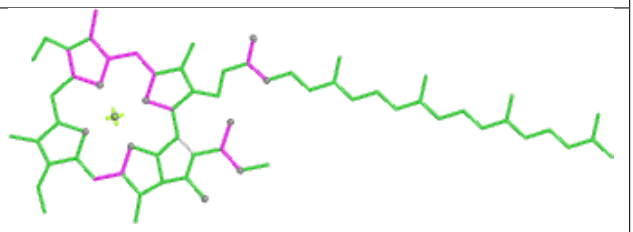
Ligand CLA Q 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

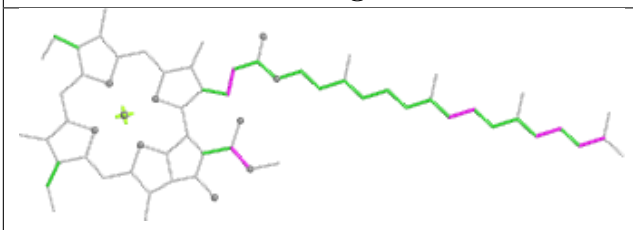
Ligand CLA A 833



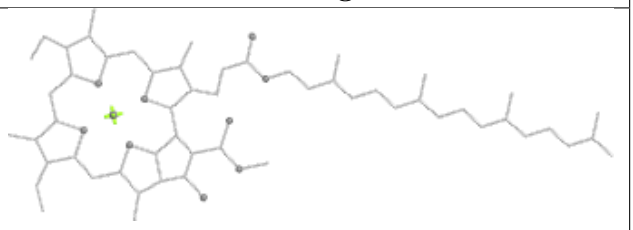
Bond lengths



Bond angles

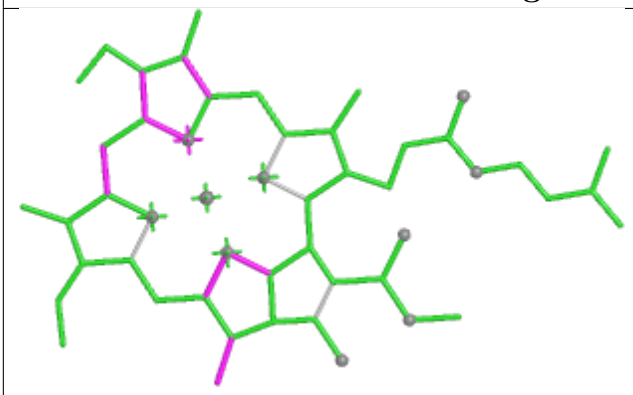


Torsions

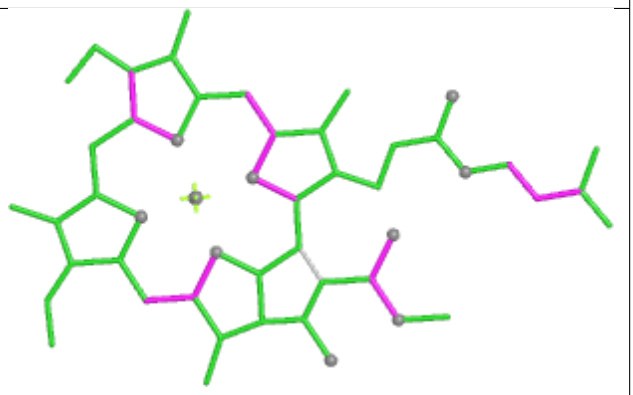


Rings

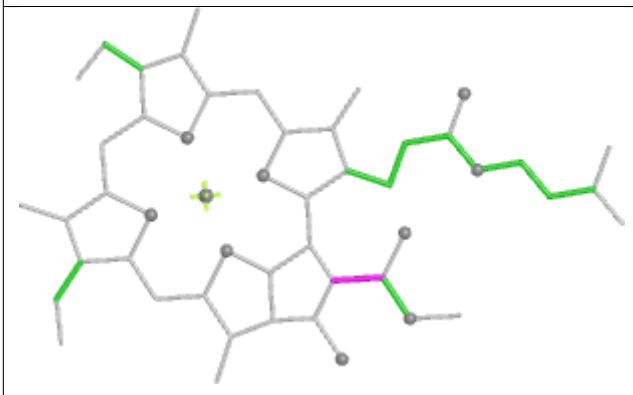
Ligand CLA K 606



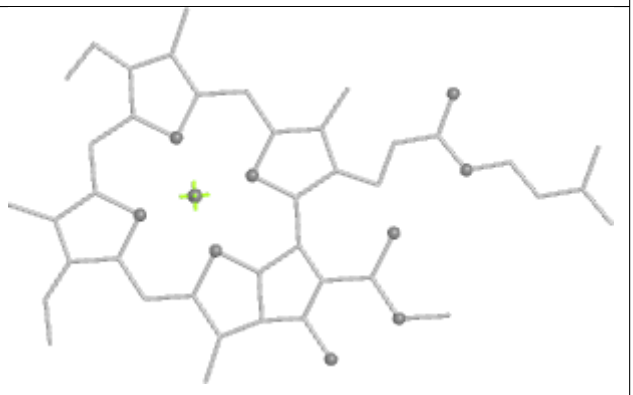
Bond lengths



Bond angles

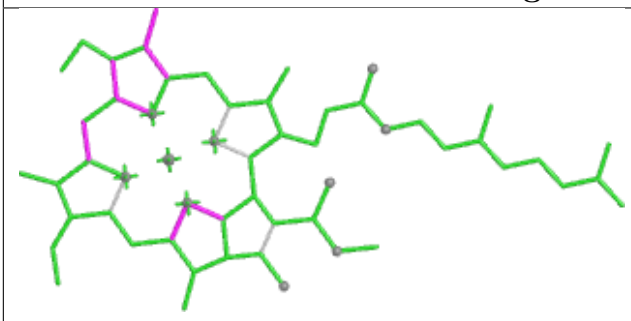


Torsions

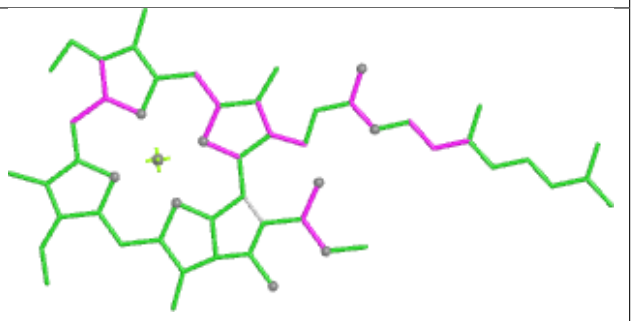


Rings

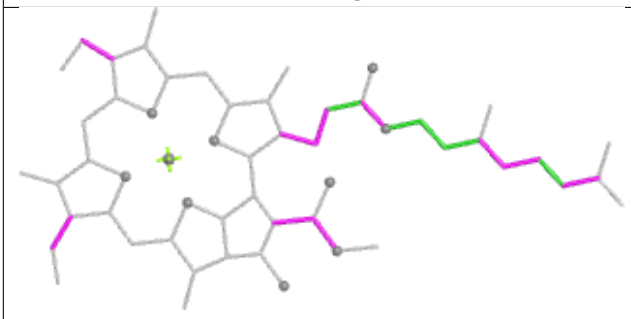
Ligand CLA N 610



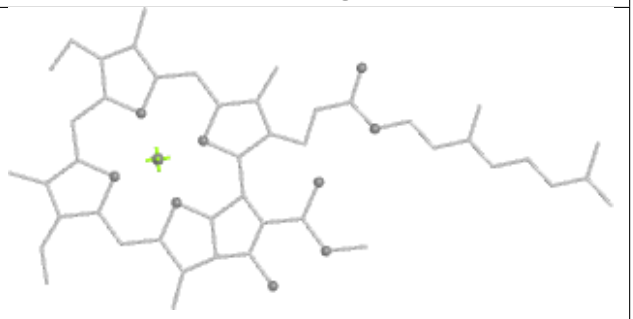
Bond lengths



Bond angles

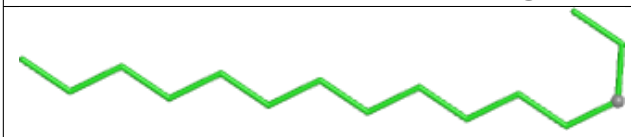


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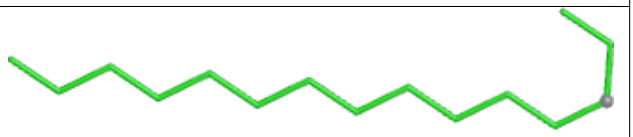


Rings

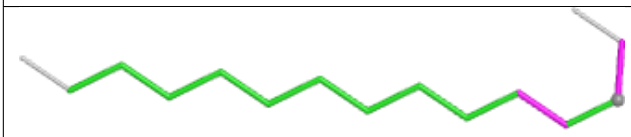
Ligand LMU B 858



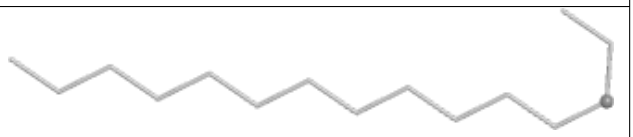
Bond lengths



Bond angles

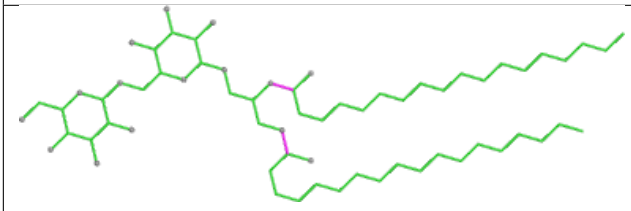


Torsions

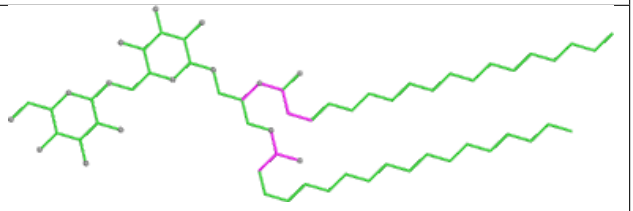


Rings

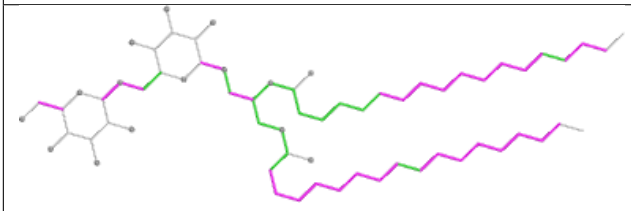
Ligand DGD B 847



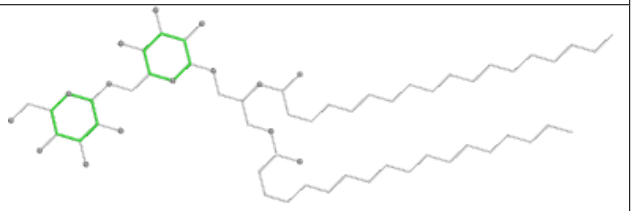
Bond lengths



Bond angles

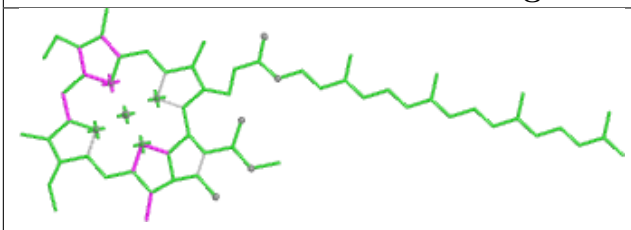


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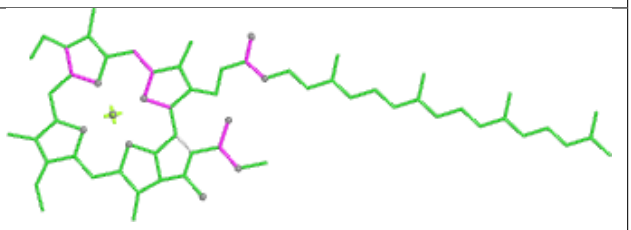


Rings

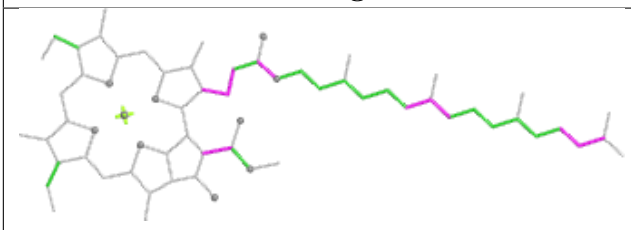
Ligand CLA X 408



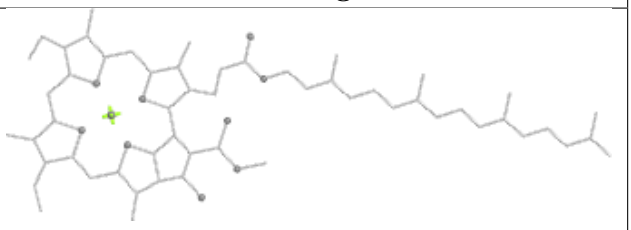
Bond lengths



Bond angles

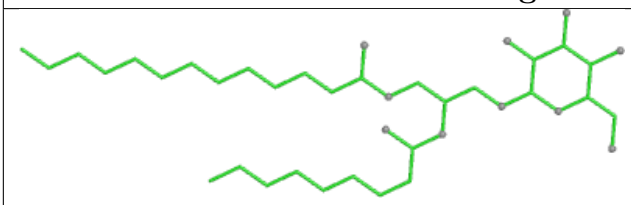


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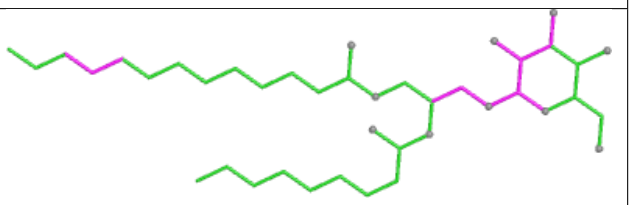


Rings

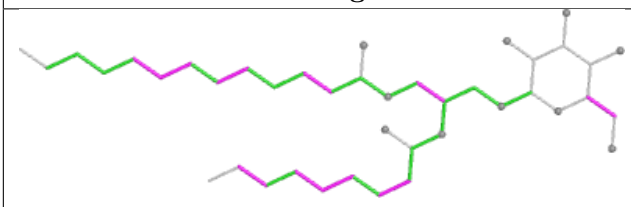
Ligand LMG A 855



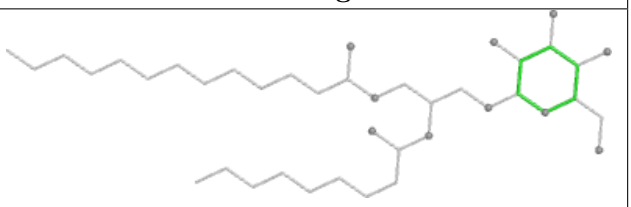
Bond lengths



Bond angles

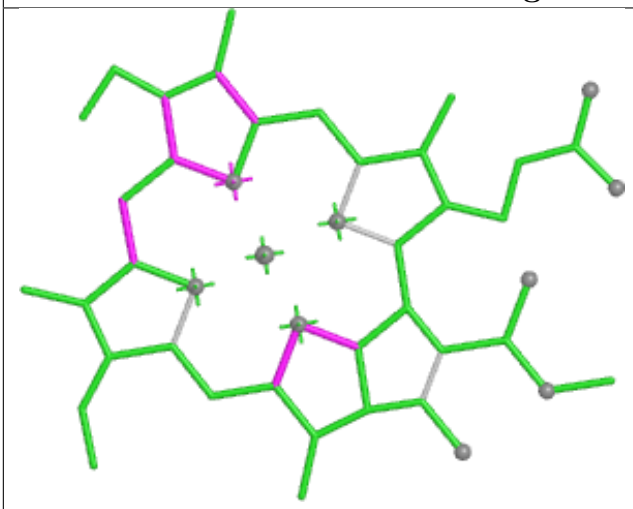


Torsions

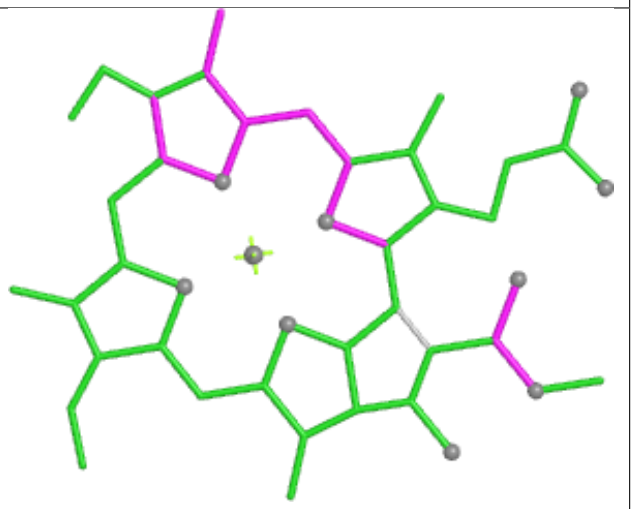


Rings

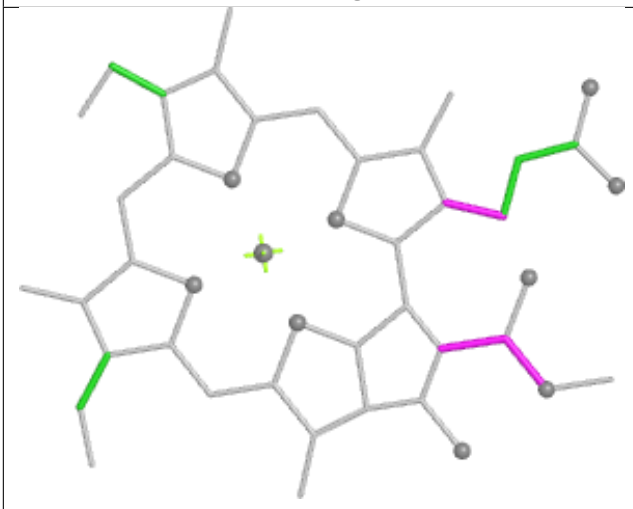
Ligand CLA U 413



Bond lengths



Bond angles

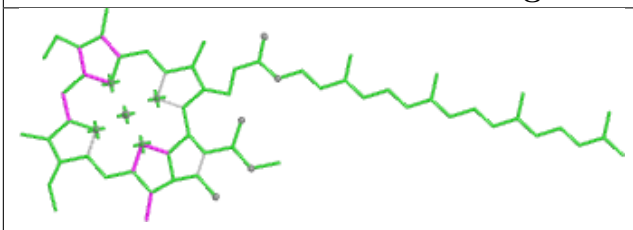


Torsions

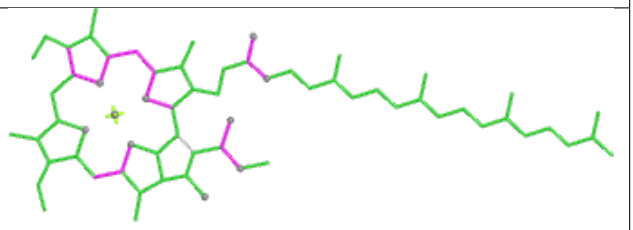


Rings

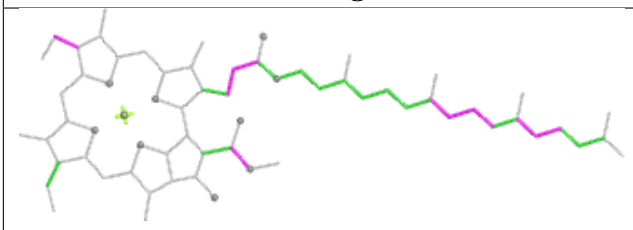
Ligand CLA R 610



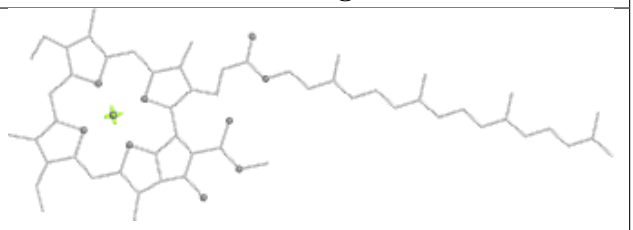
Bond lengths



Bond angles

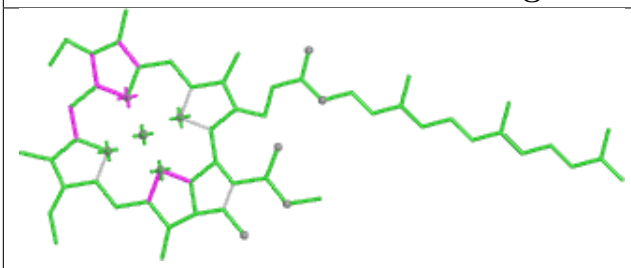


Torsions

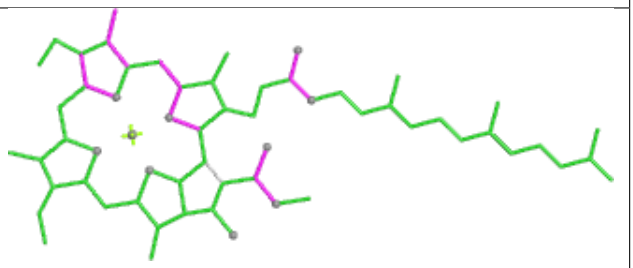


Rings

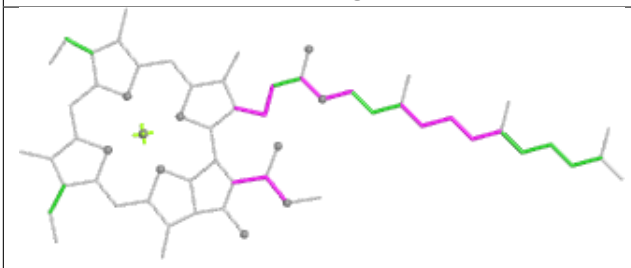
Ligand CLA N 607



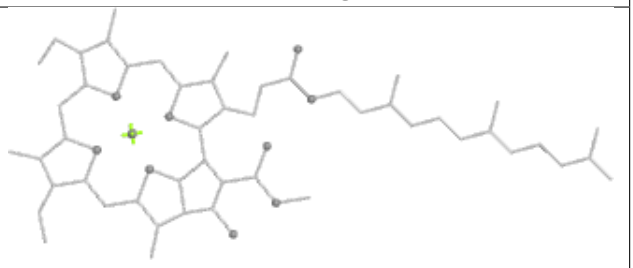
Bond lengths



Bond angles

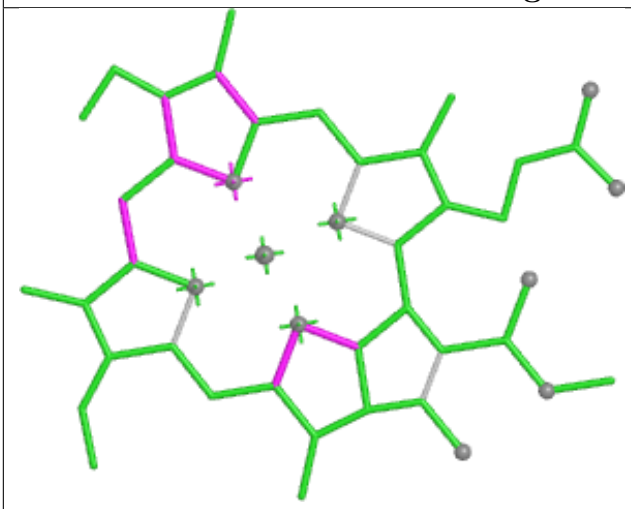


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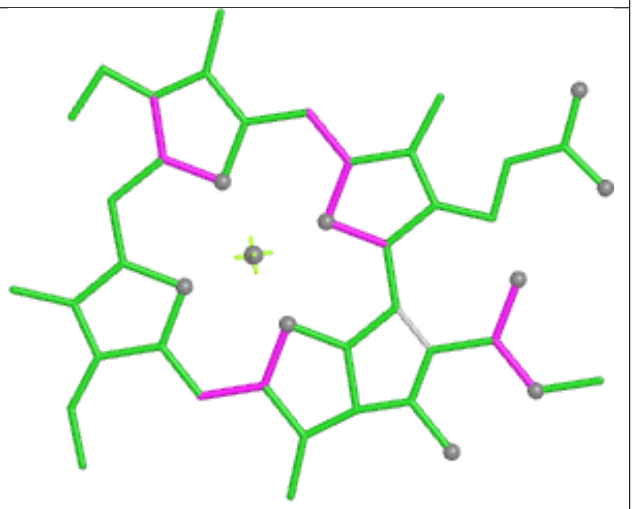


Rings

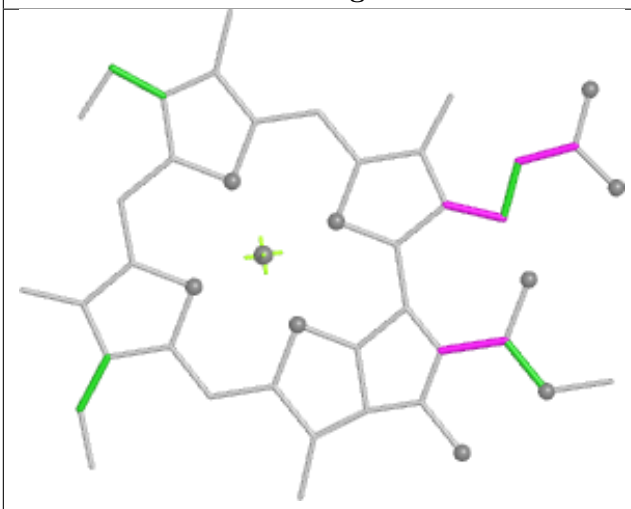
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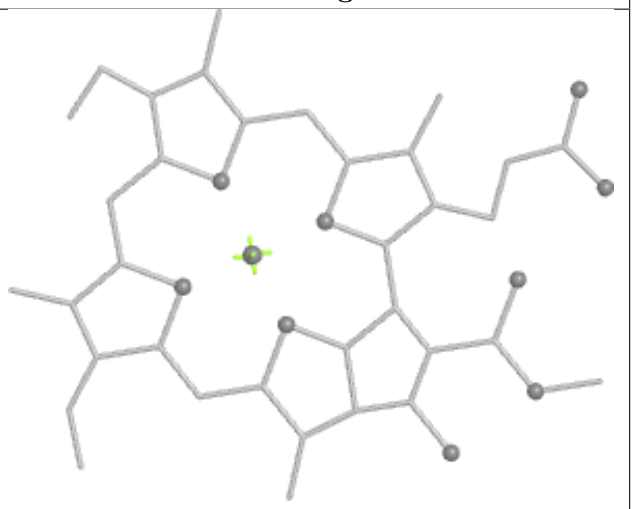
Bond lengths



Bond angles

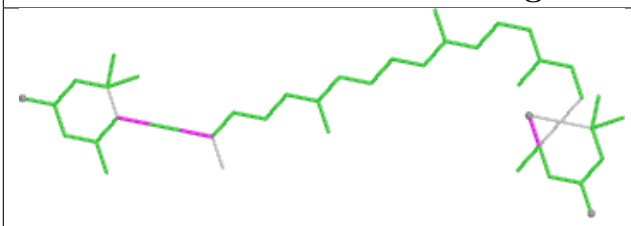


Torsions

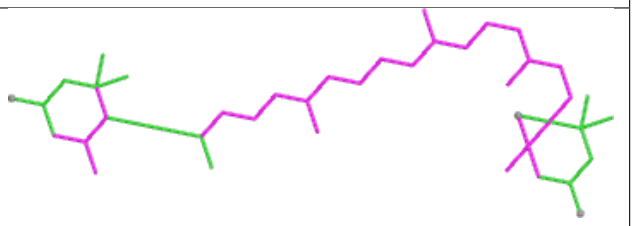


Rings

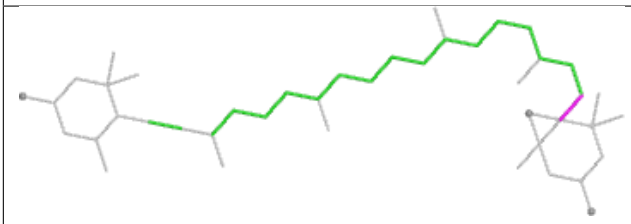
Ligand DD6 R 613



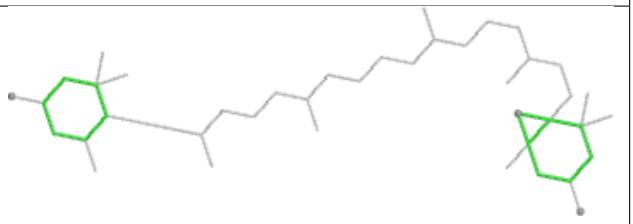
Bond lengths



Bond angles

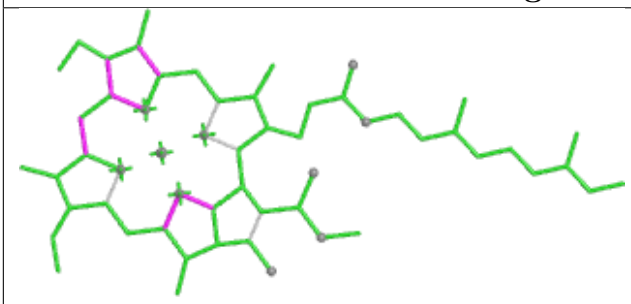


Torsions

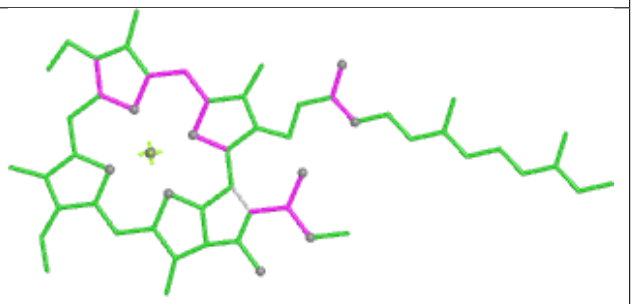


Rings

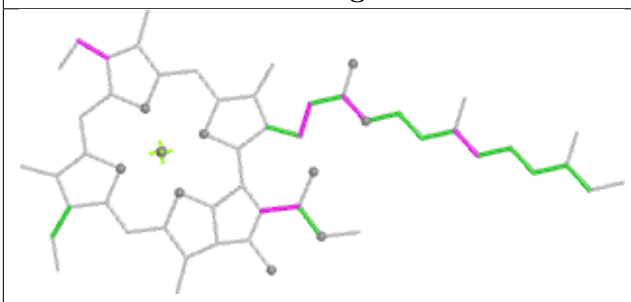
Ligand CLA B 803



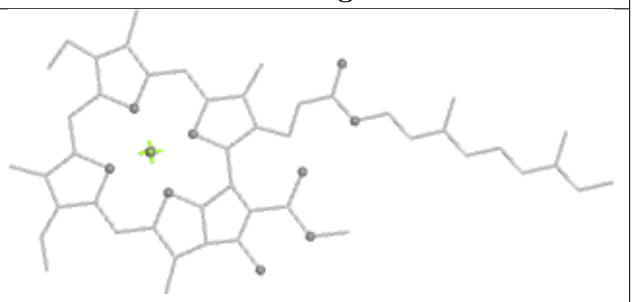
Bond lengths



Bond angles

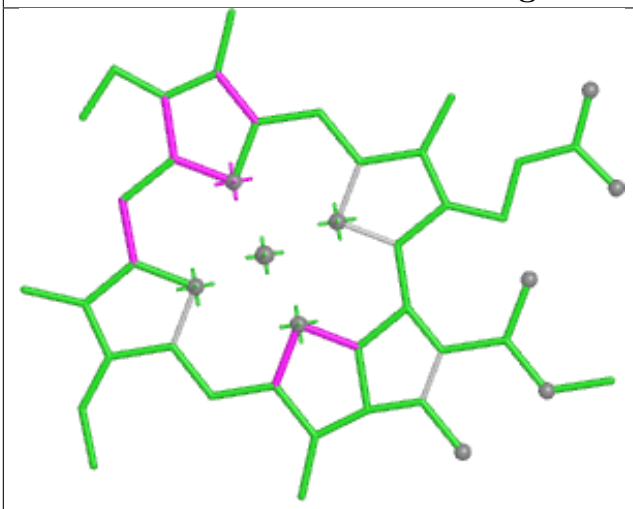


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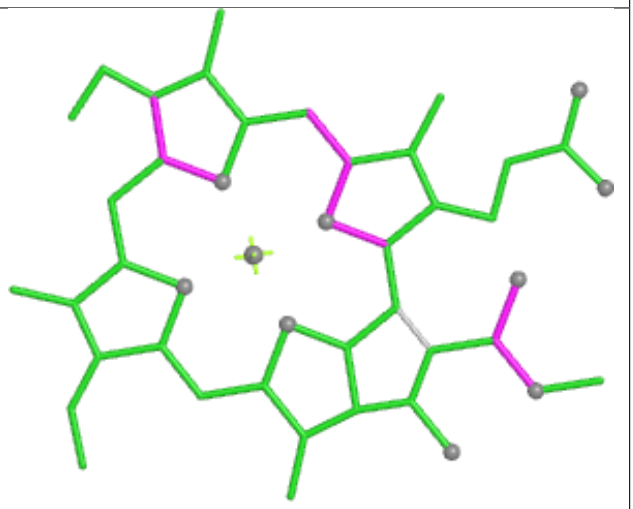


Rings

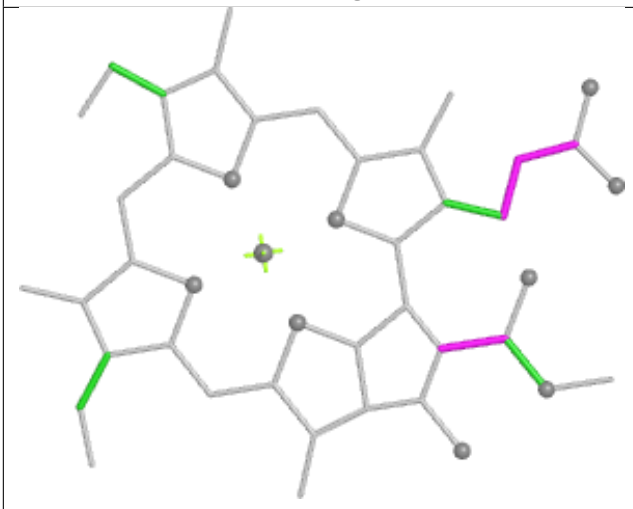
Ligand CLA W 419



Bond lengths



Bond angles

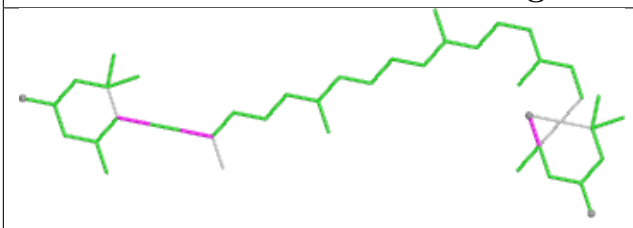


Torsions

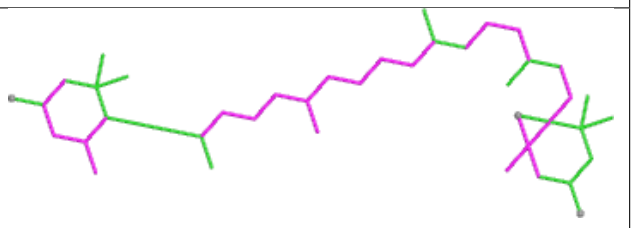


Rings

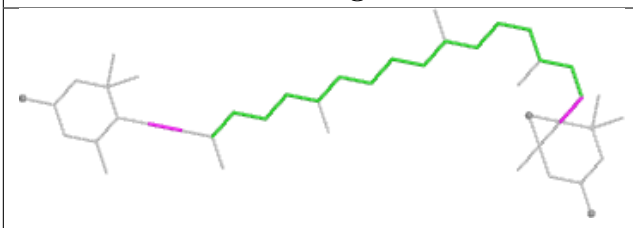
Ligand DD6 L 414



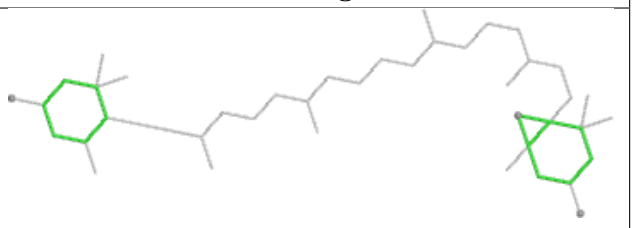
Bond lengths



Bond angles

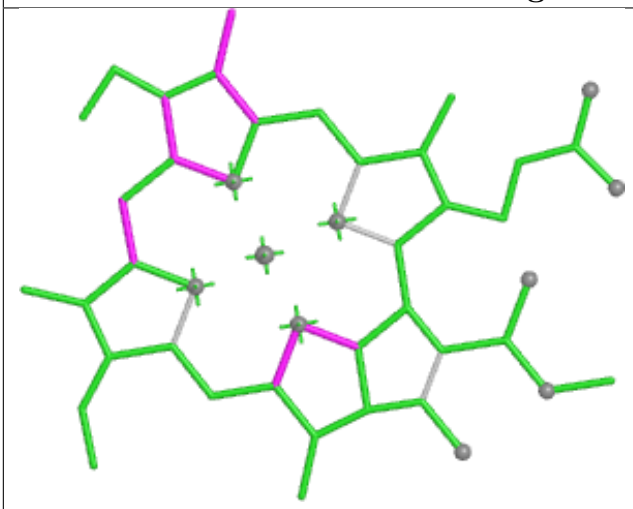


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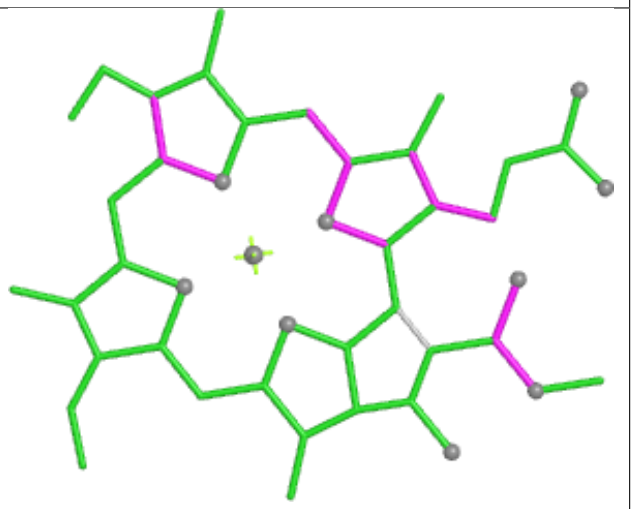


Rings

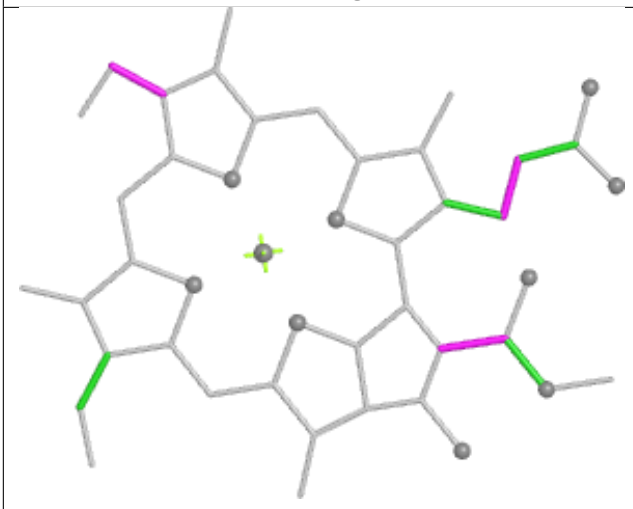
Ligand CLA S 610



Bond lengths



Bond angles

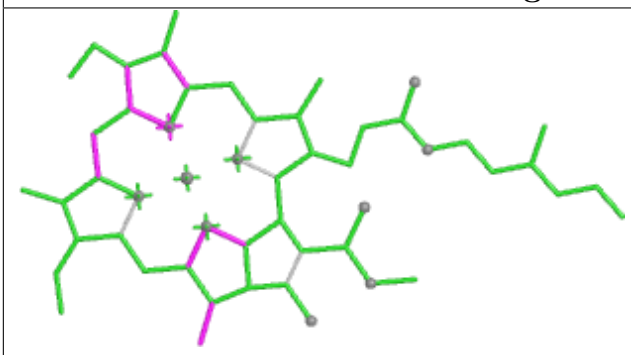


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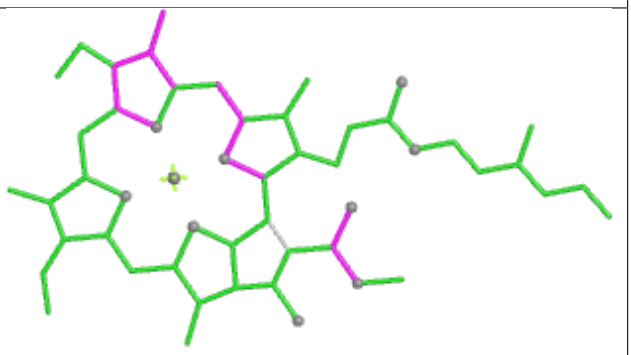


Rings

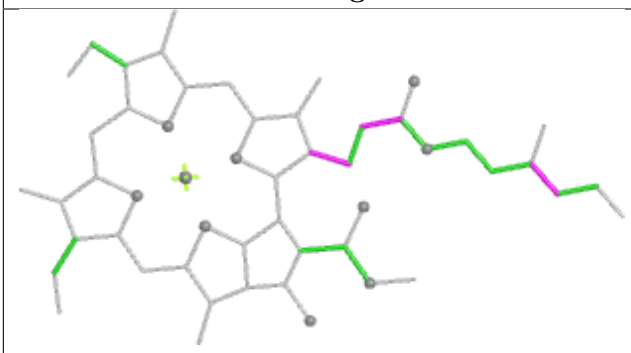
Ligand CLA A 832



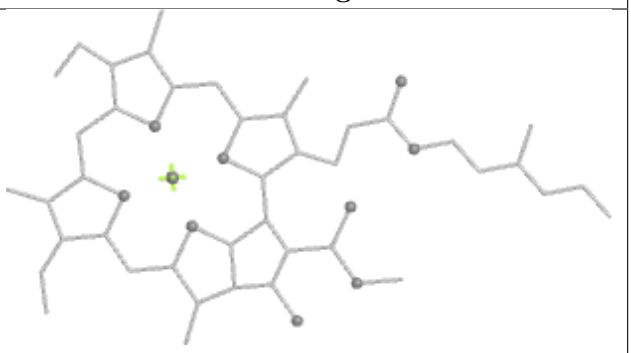
Bond lengths



Bond angles

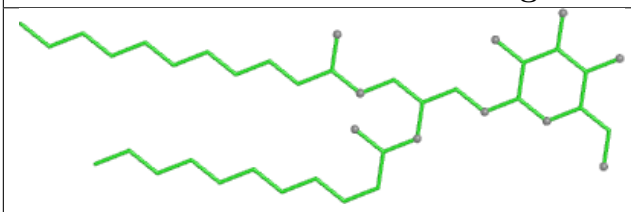


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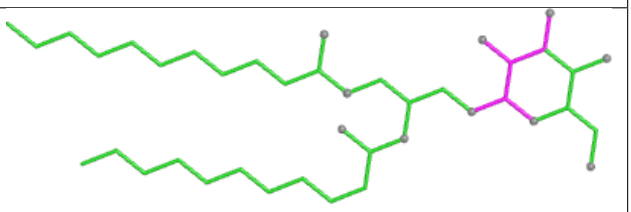


Rings

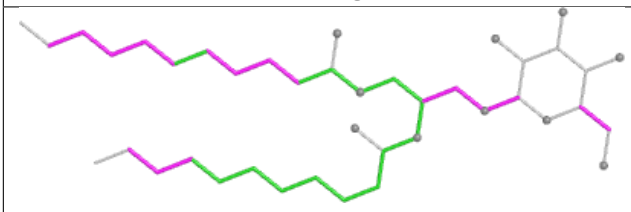
Ligand LMG T 616



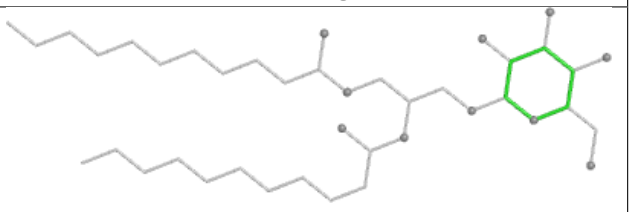
Bond lengths



Bond angles

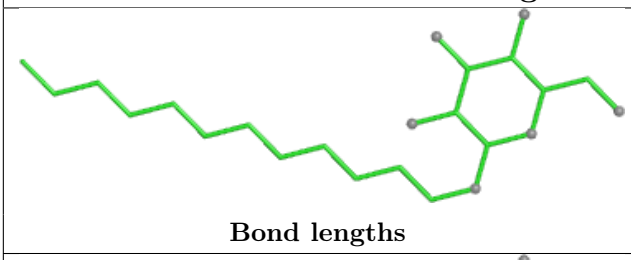


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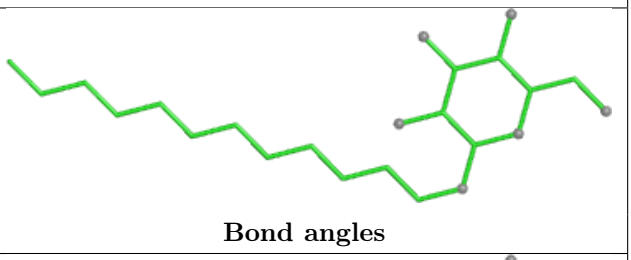


Rings

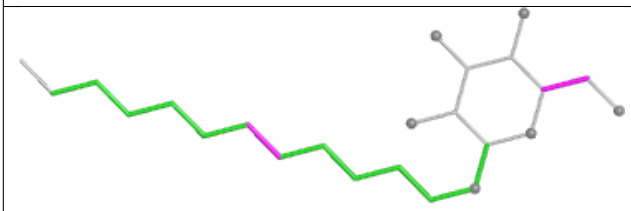
Ligand LMU B 855



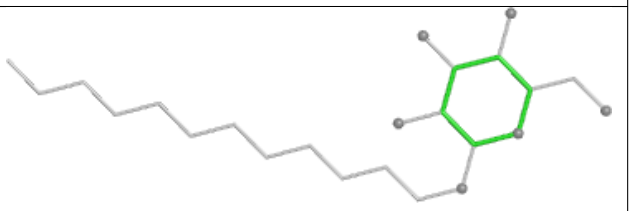
Bond lengths



Bond angles

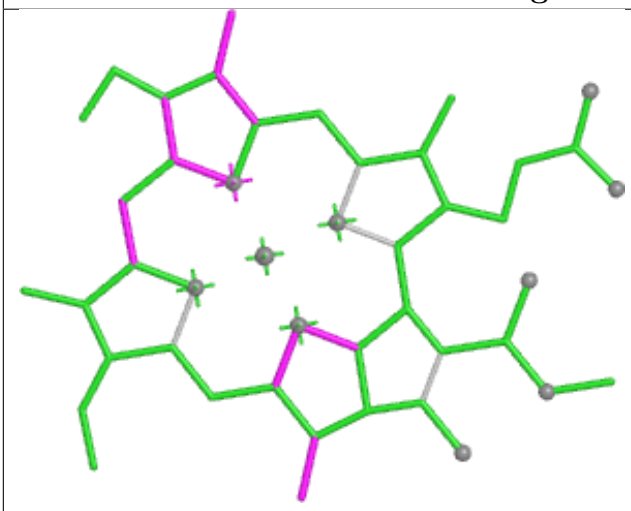


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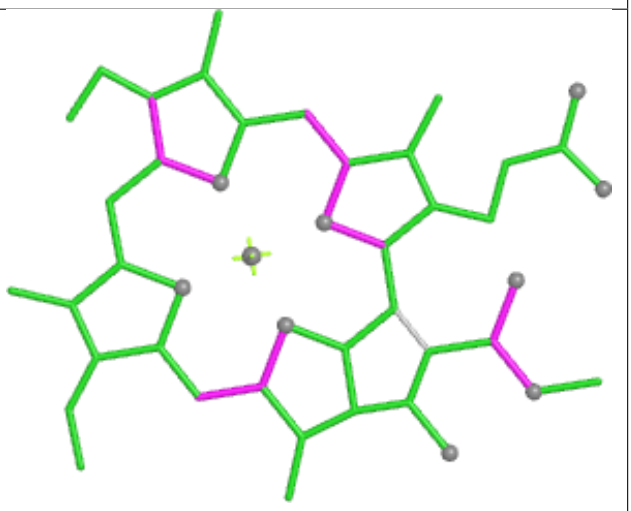


Rings

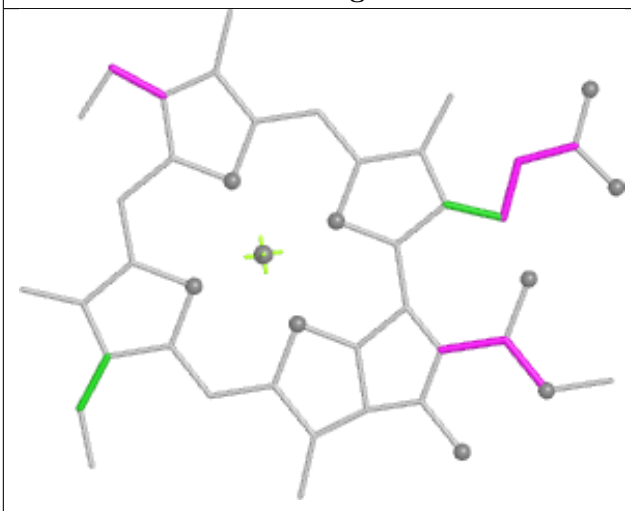
Ligand CLA I 610



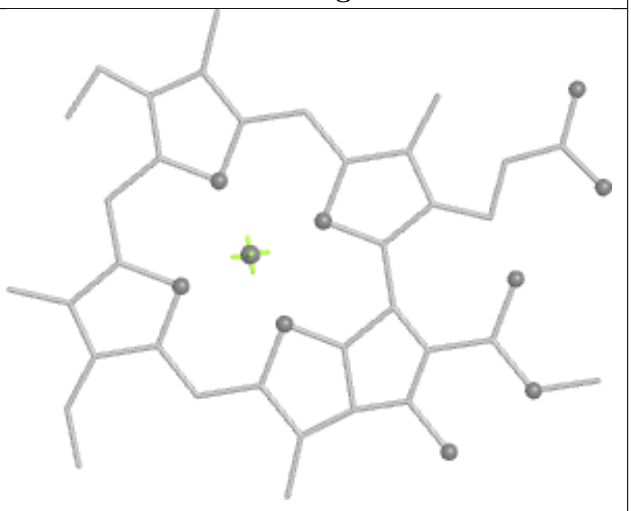
Bond lengths



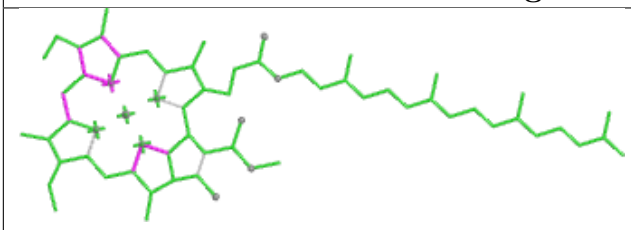
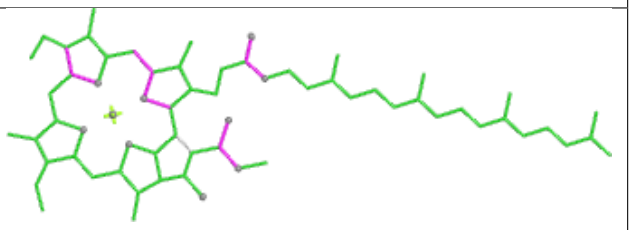
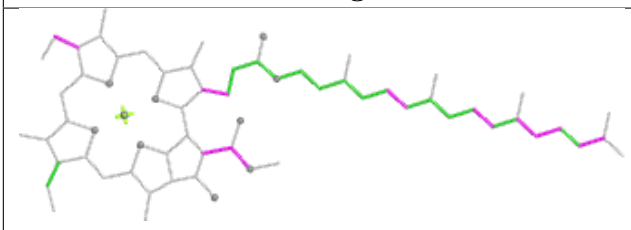
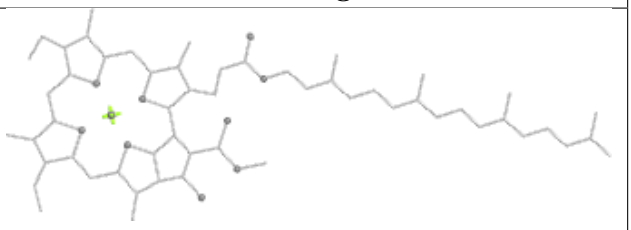
Bond angles

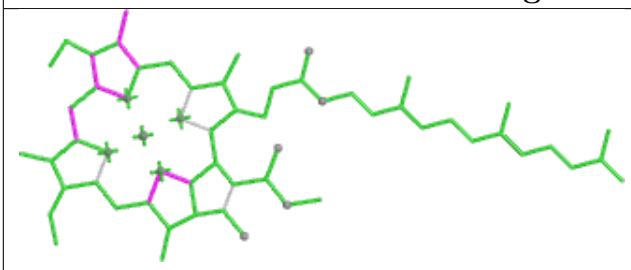
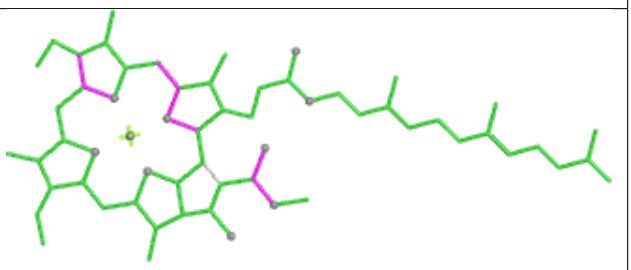
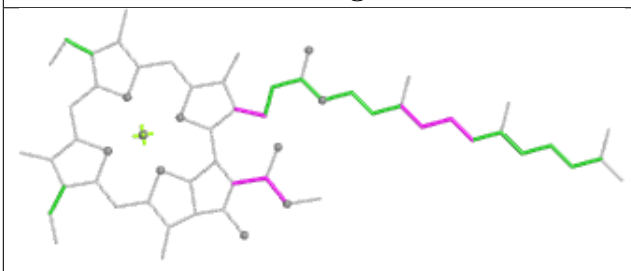
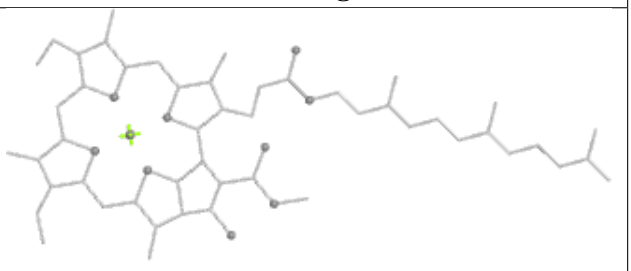


Torsions

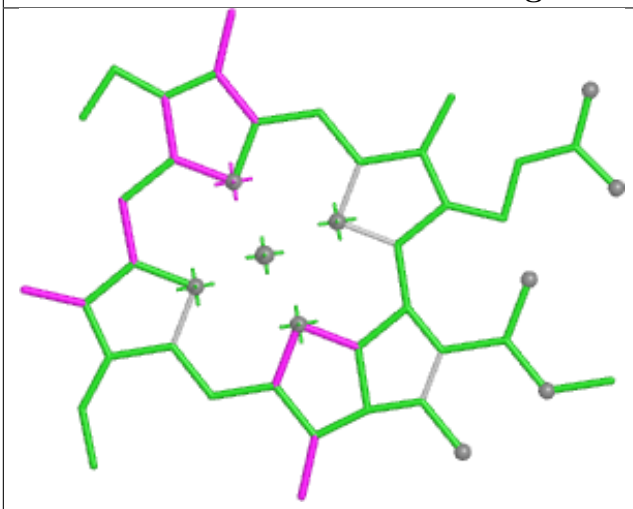


Rings

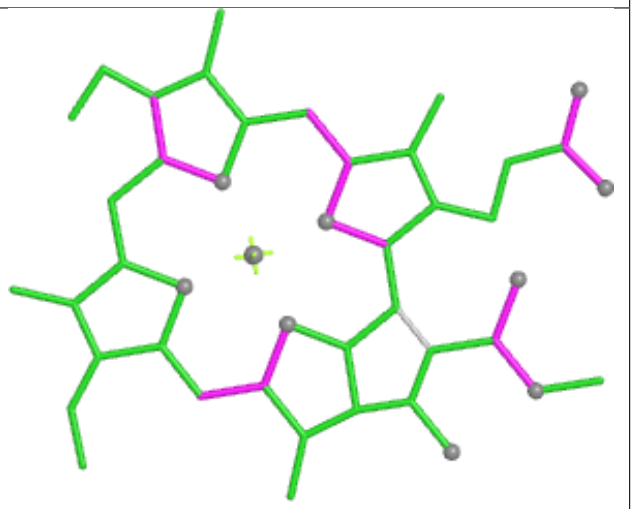
Ligand CLA T 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

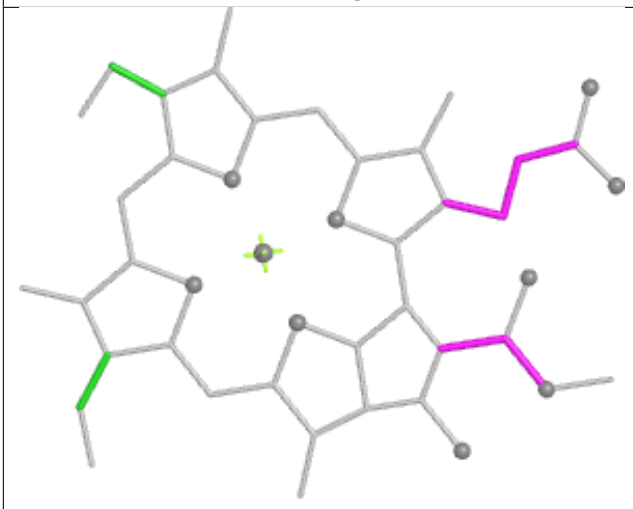
Ligand CLA P 602



Bond lengths



Bond angles

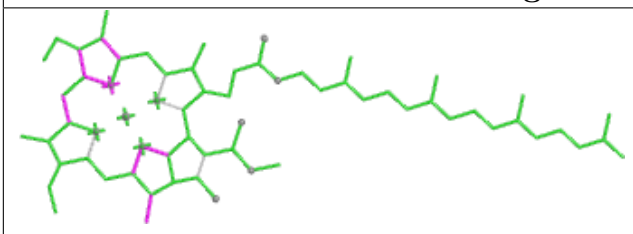


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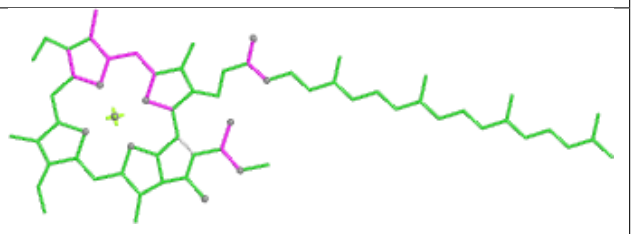


Rings

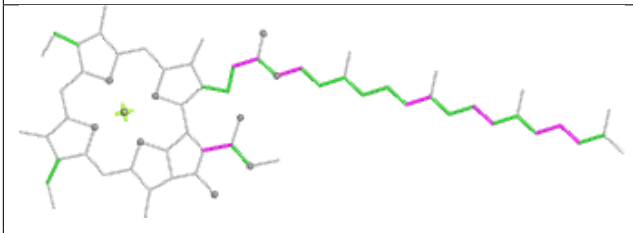
Ligand CLA N 603



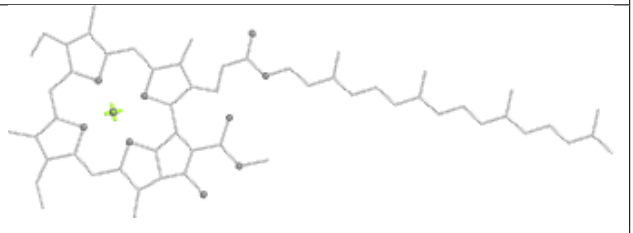
Bond lengths



Bond angles

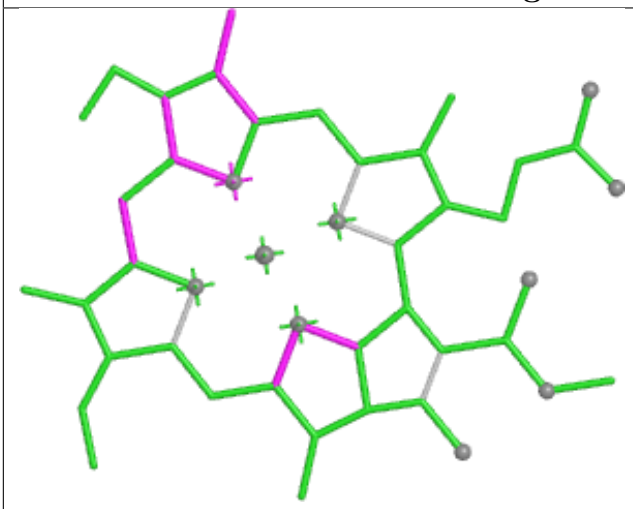


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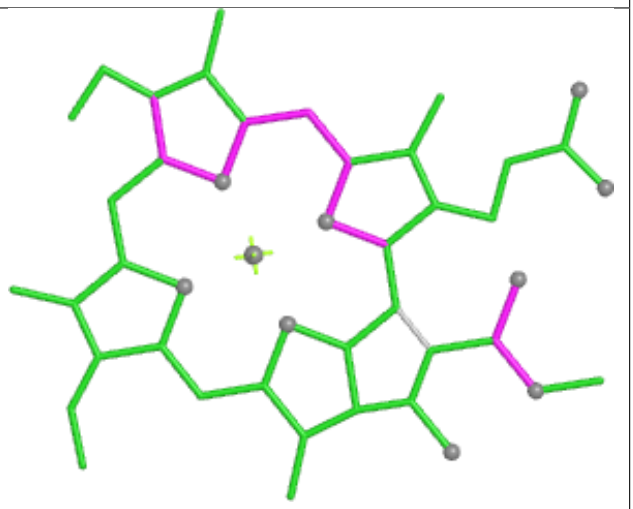


Rings

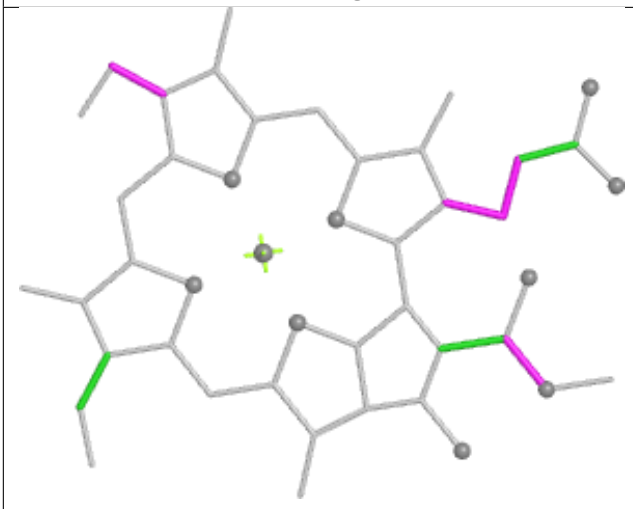
Ligand CLA U 415



Bond lengths



Bond angles

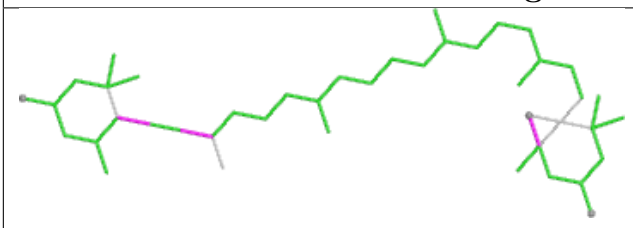


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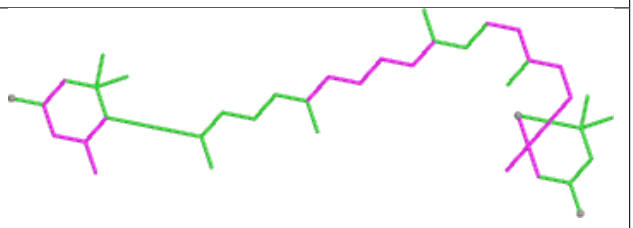


Rings

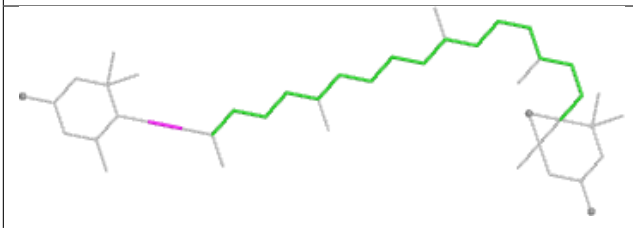
Ligand DD6 O 316



Bond lengths



Bond angles

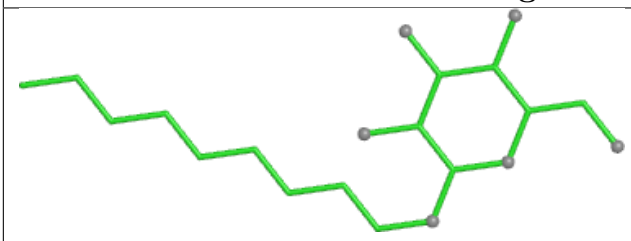


Torsions

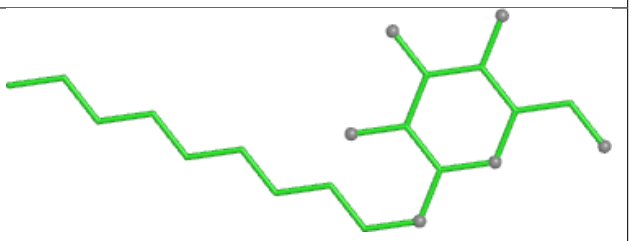


Rings

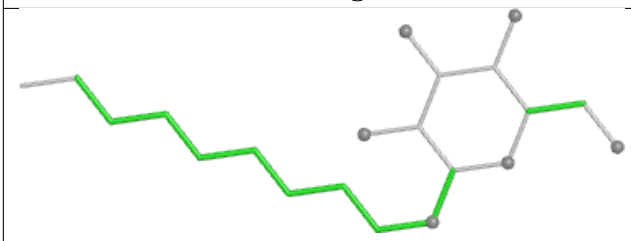
Ligand LMU G 615



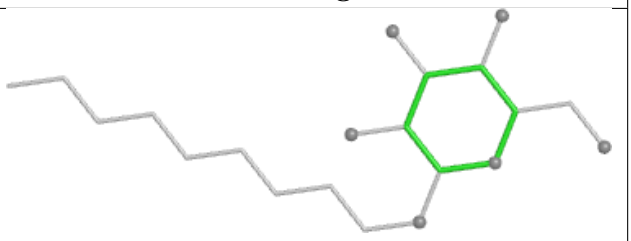
Bond lengths



Bond angles

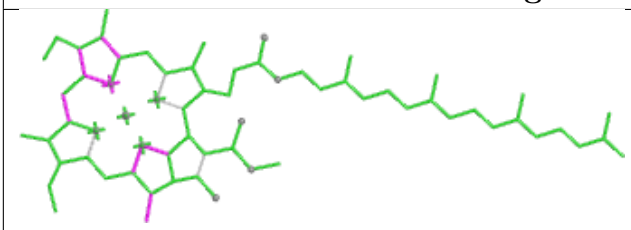


Torsions

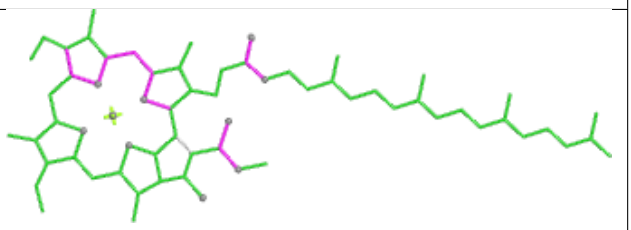


Rings

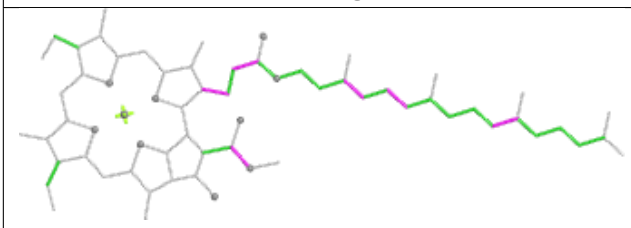
Ligand CLA B 822



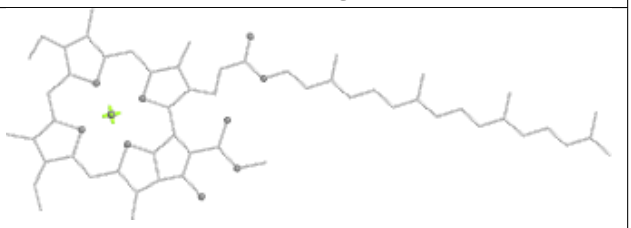
Bond lengths



Bond angles

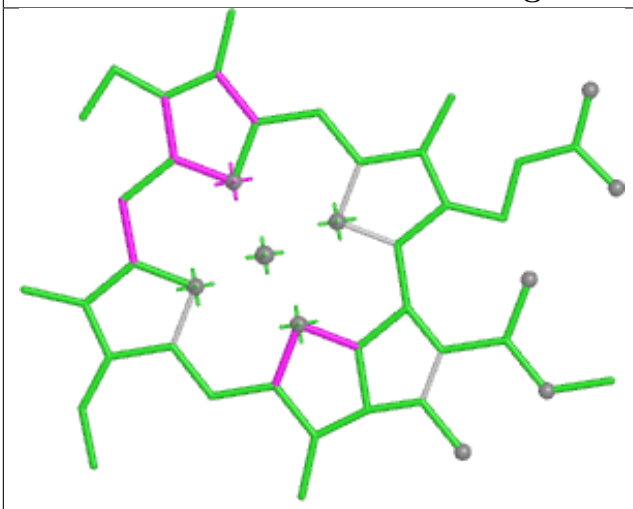


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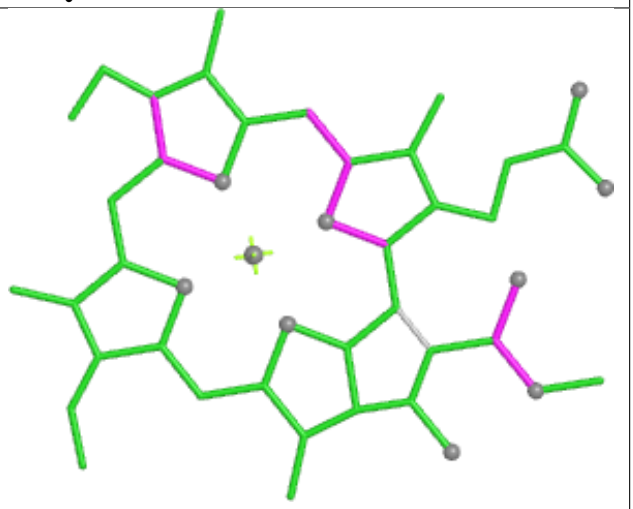


Rings

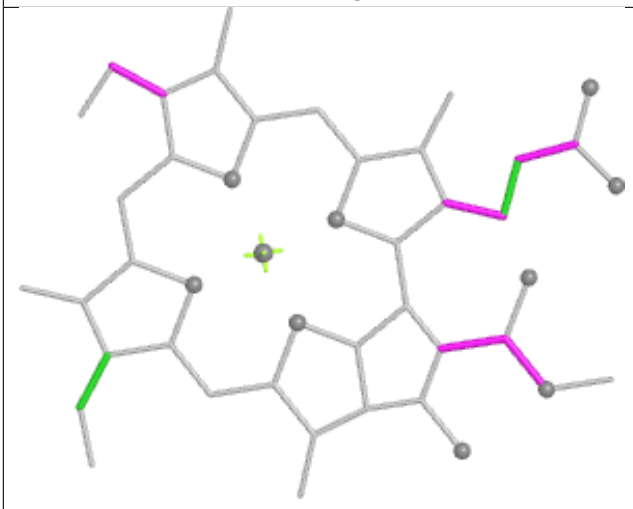
Ligand CLA Q 618



Bond lengths



Bond angles

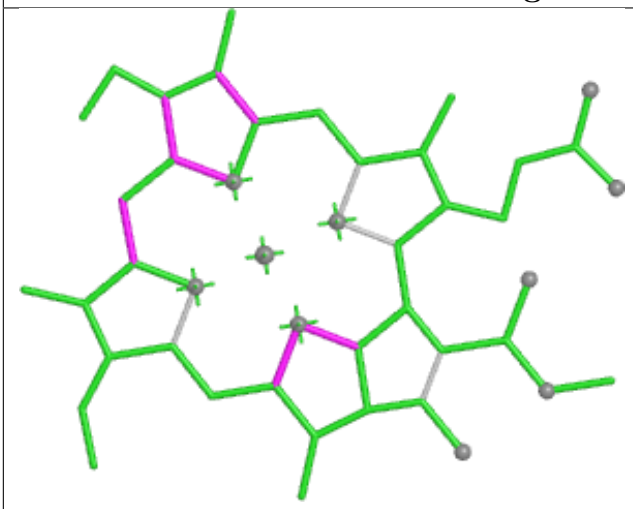


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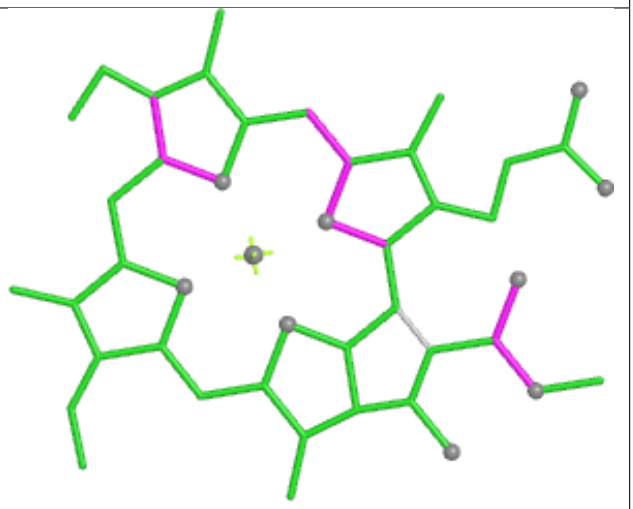


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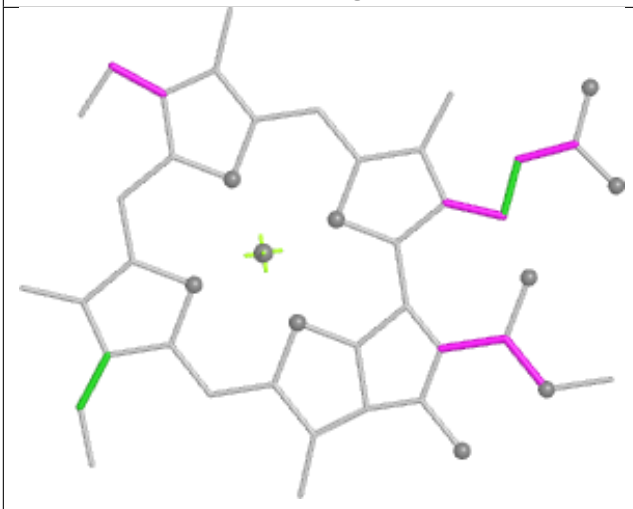
Ligand CLA V 613



Bond lengths



Bond angles

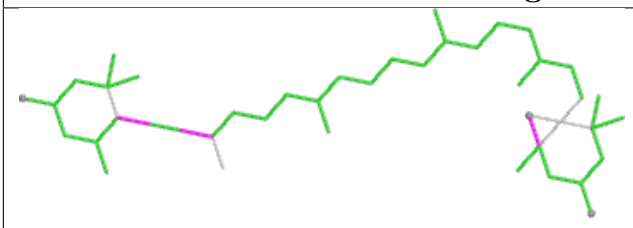


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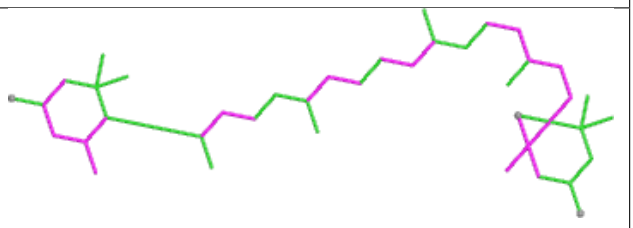


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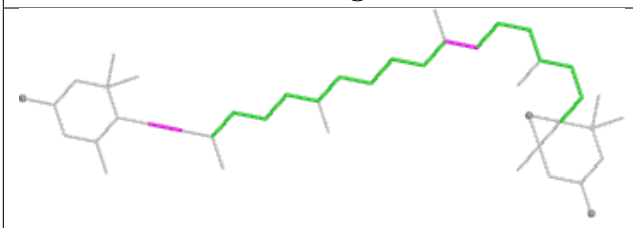
Ligand DD6 V 615



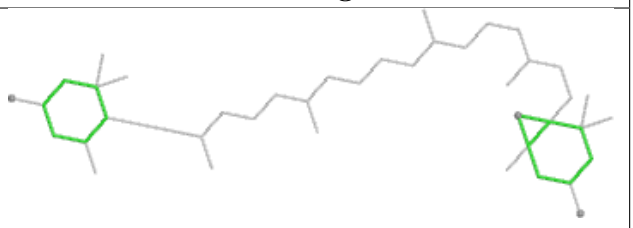
Bond lengths



Bond angles

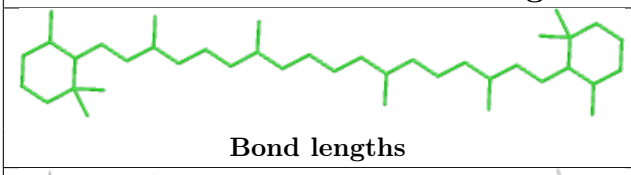


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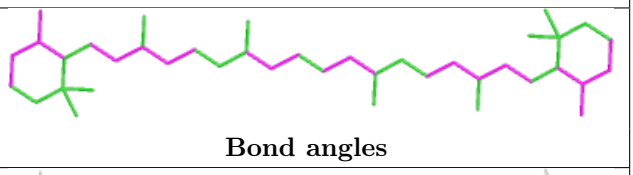


Rings

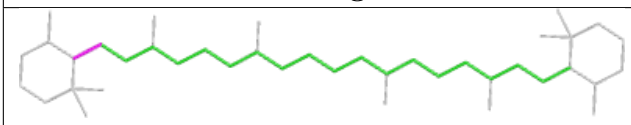
Ligand BCR J 103



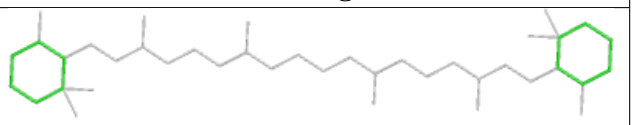
Bond lengths



Bond angles

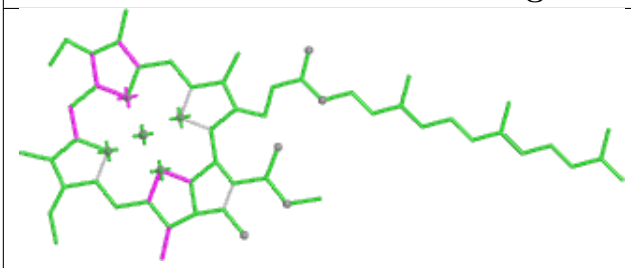


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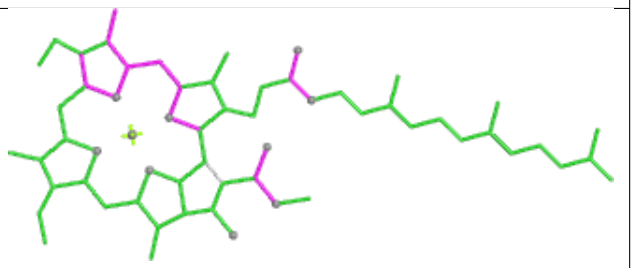


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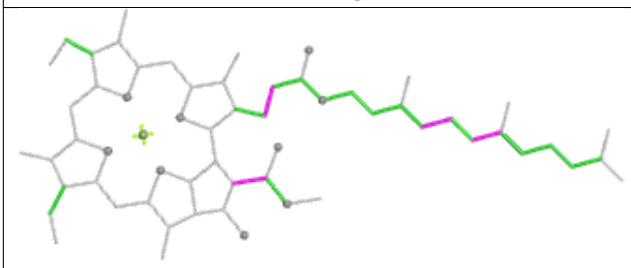
Ligand CLA L 403



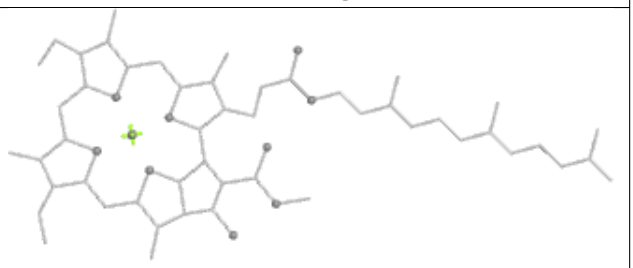
Bond lengths



Bond angles

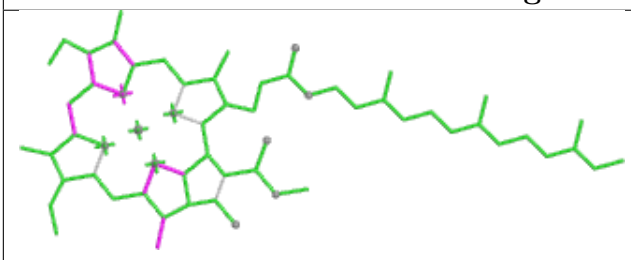


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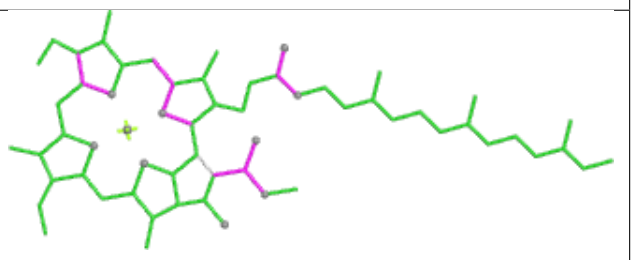


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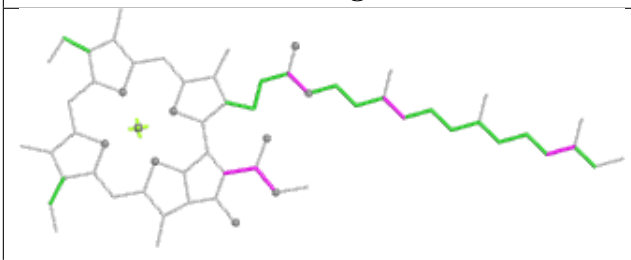
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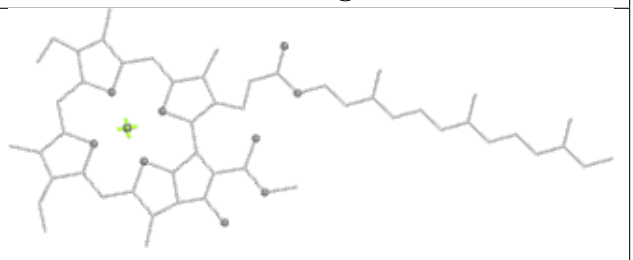
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Bond angles

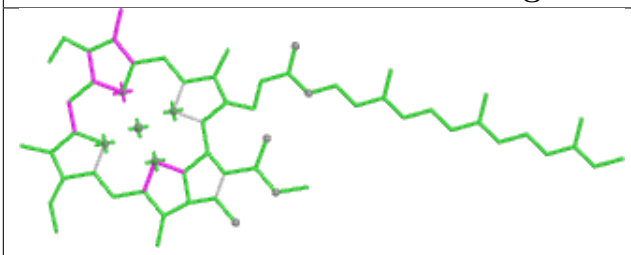


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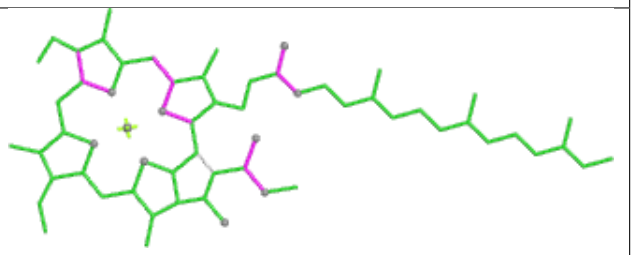


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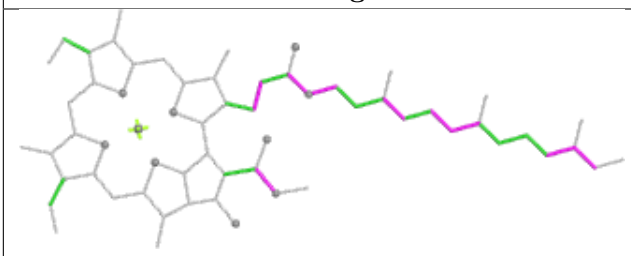
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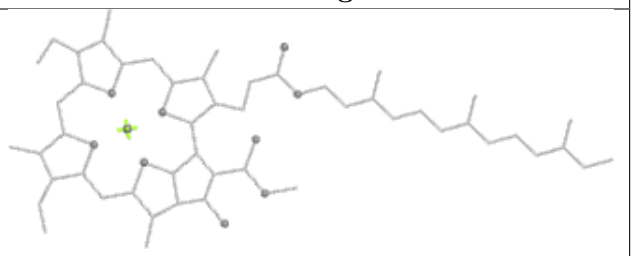
Bond lengths



Bond angles

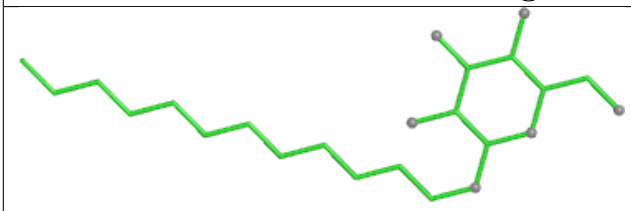


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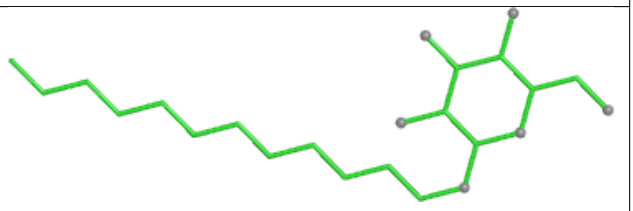


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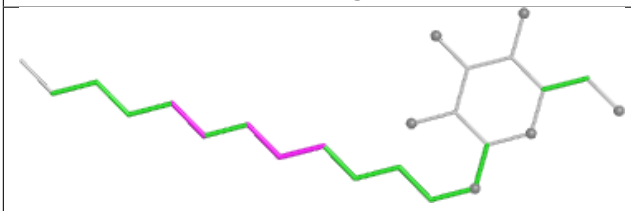
Ligand LMU B 850



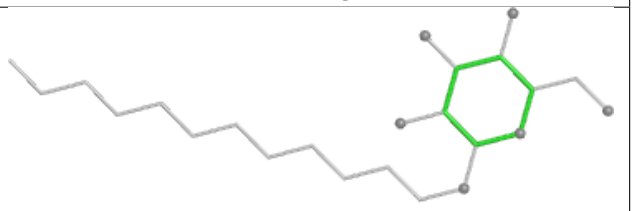
Bond lengths



Bond angles

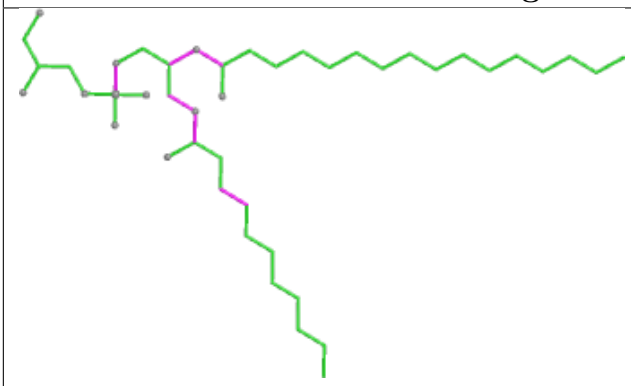


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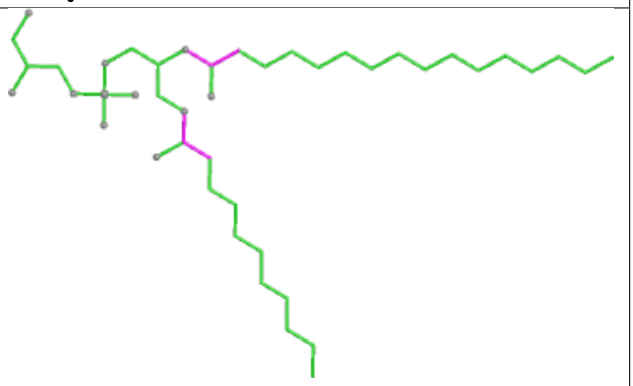


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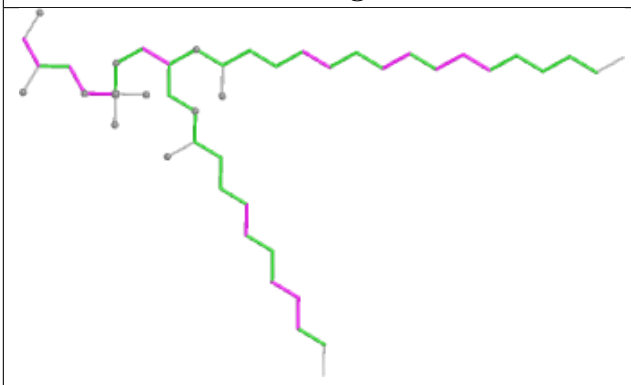
Ligand LHG Q 616



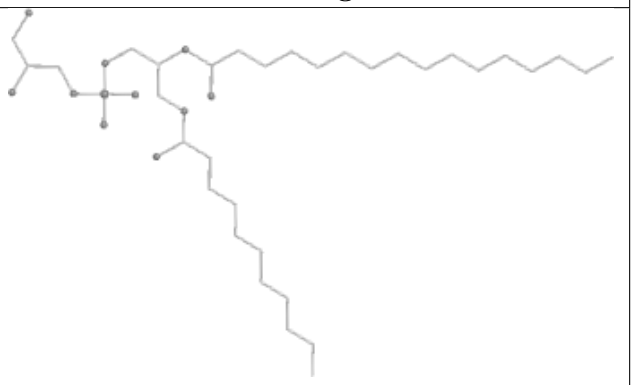
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Bond angles

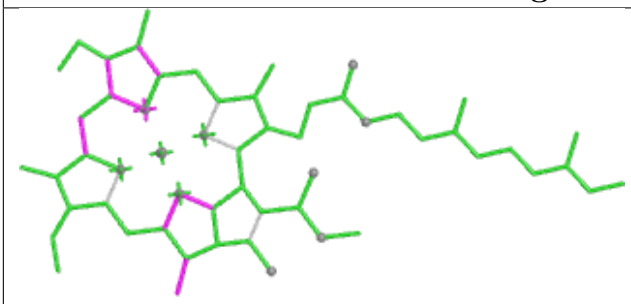


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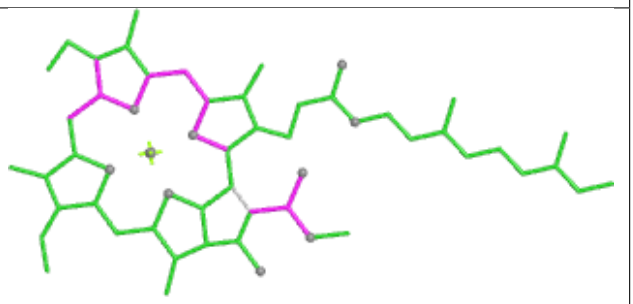


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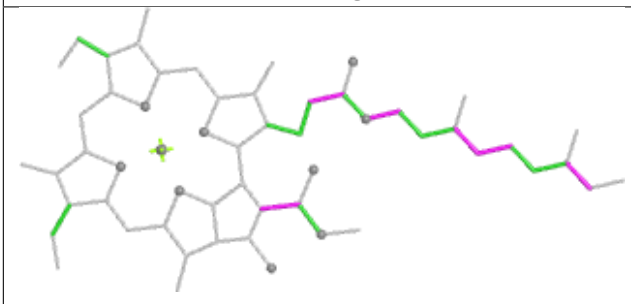
Ligand CLA I 603



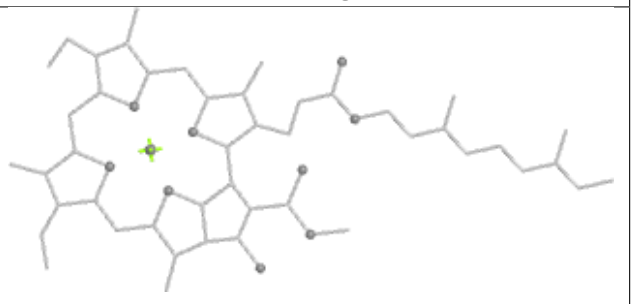
Bond lengths



Bond angles

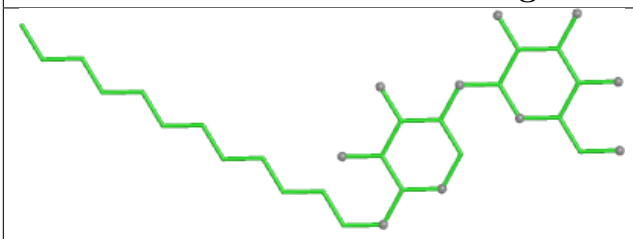


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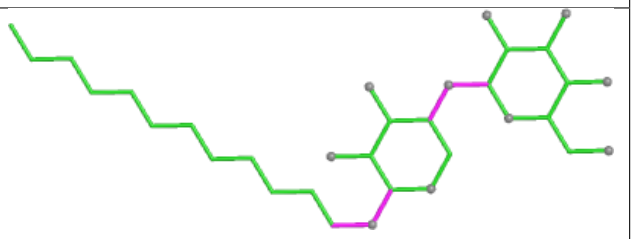


Rings

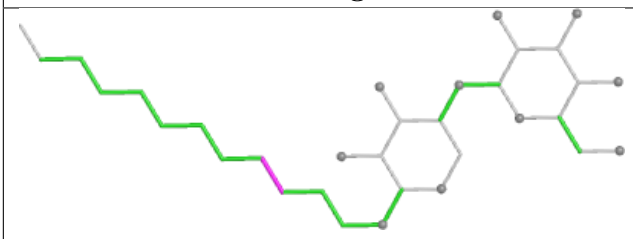
Ligand LMU H 321



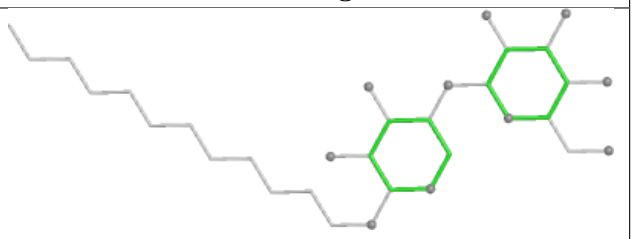
Bond lengths



Bond angles

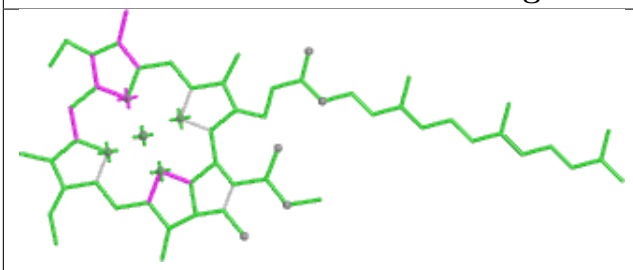


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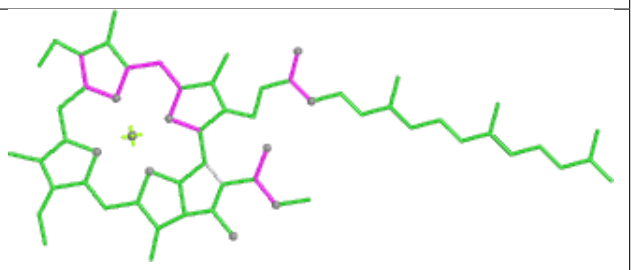


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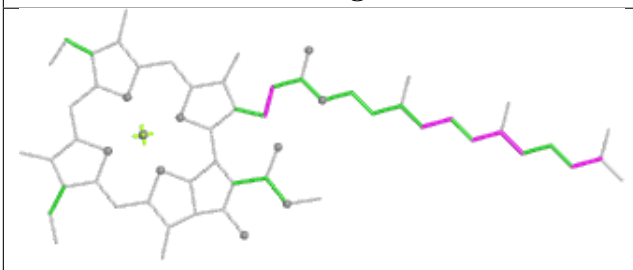
Ligand CLA K 603



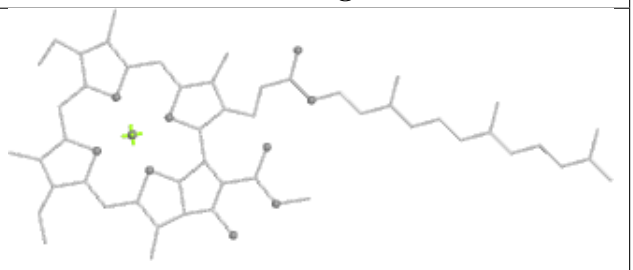
Bond lengths



Bond angles

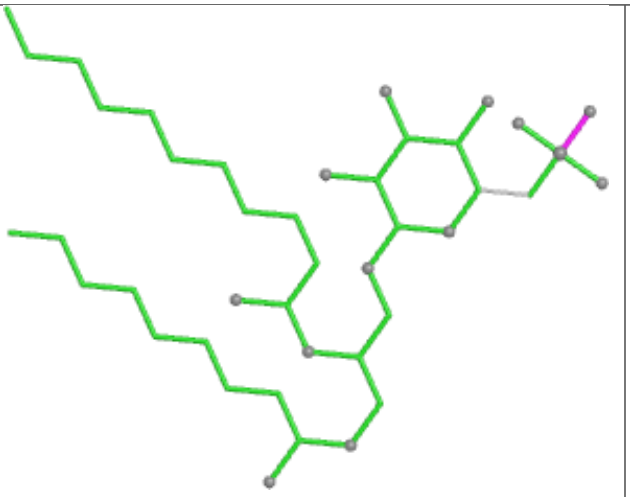


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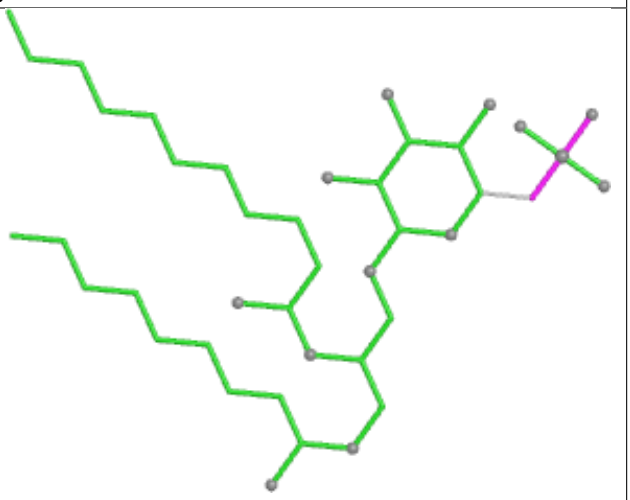


Rings

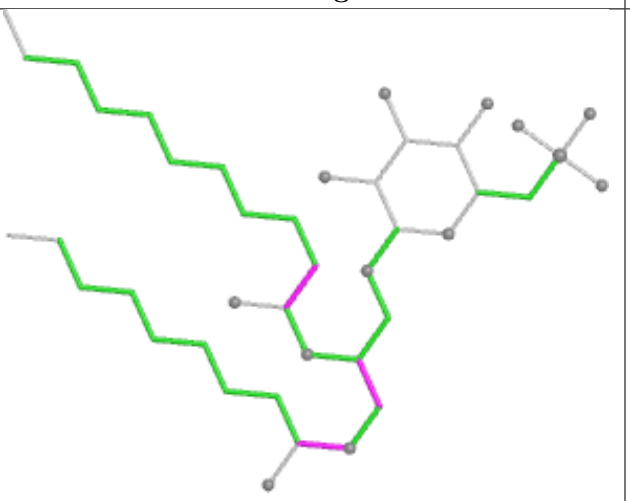
Ligand SQD O 302



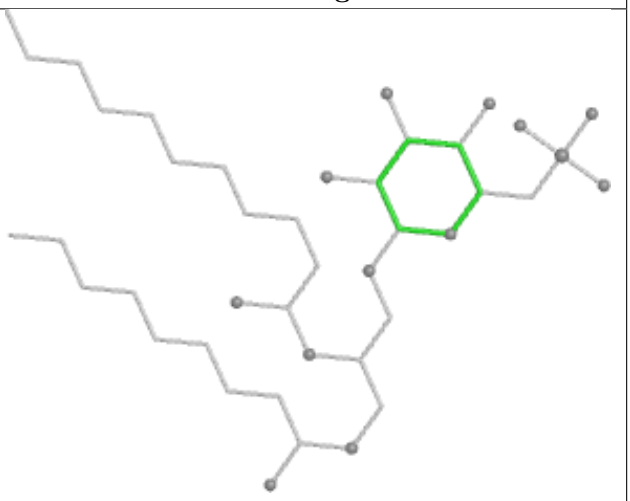
Bond lengths



Bond angles

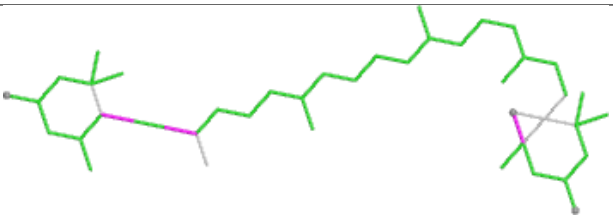


Torsions

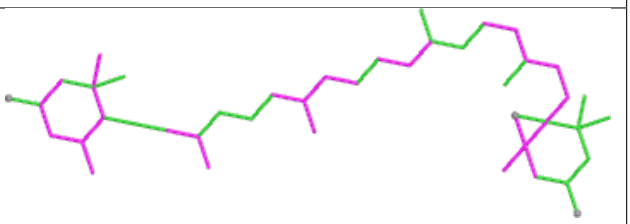


Rings

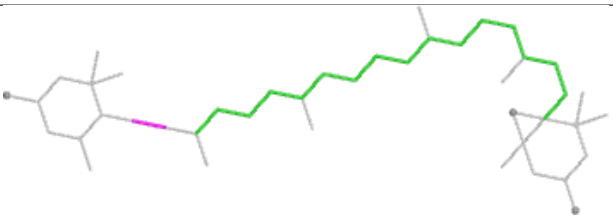
Ligand DD6 U 417



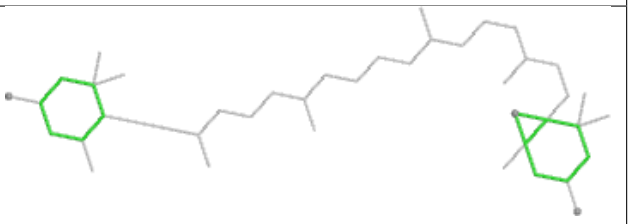
Bond lengths



Bond angles

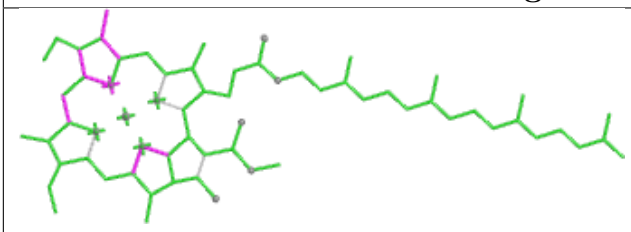


Torsions

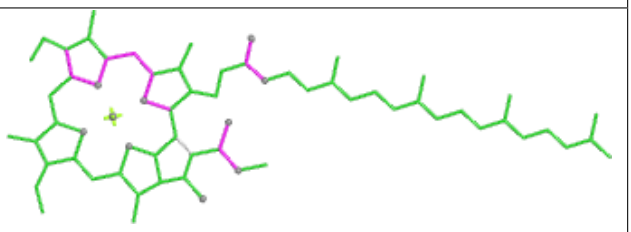


Rings

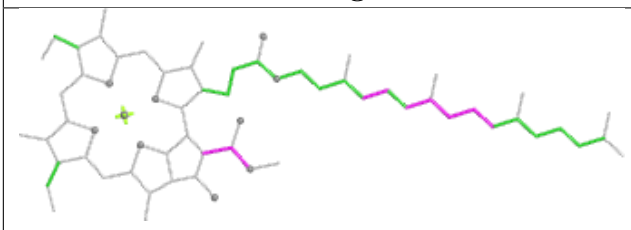
Ligand CLA B 813



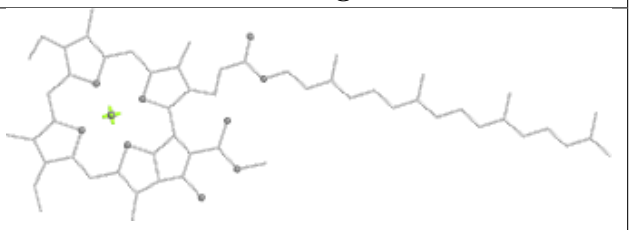
Bond lengths



Bond angles

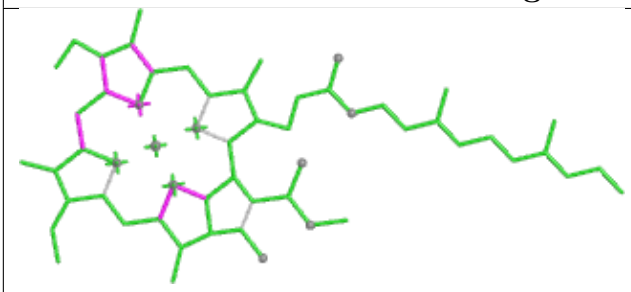


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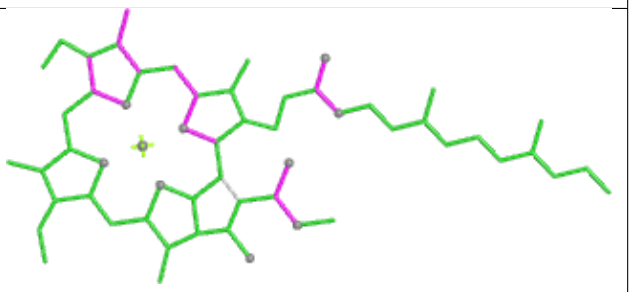


Rings

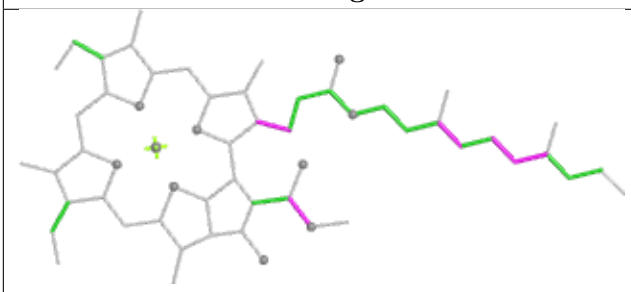
Ligand CLA U 411



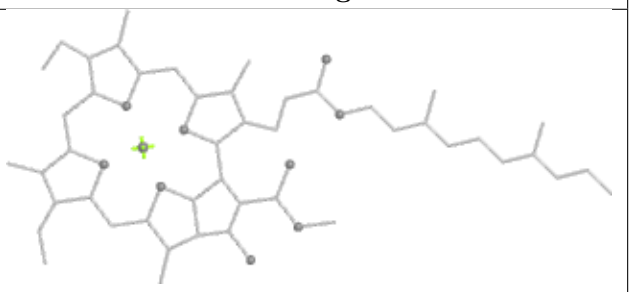
Bond lengths



Bond angles

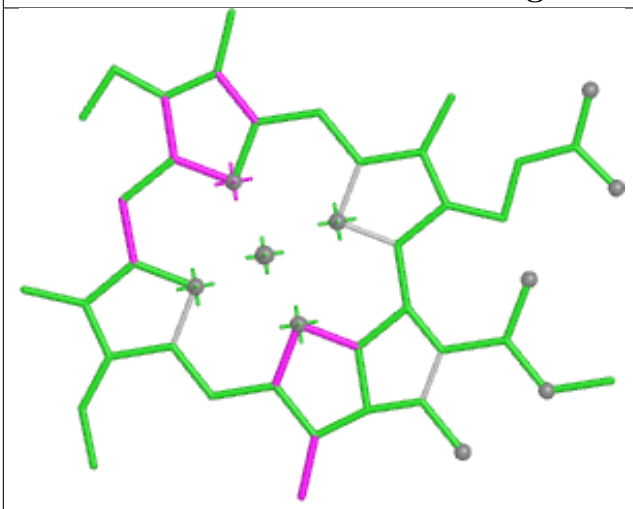


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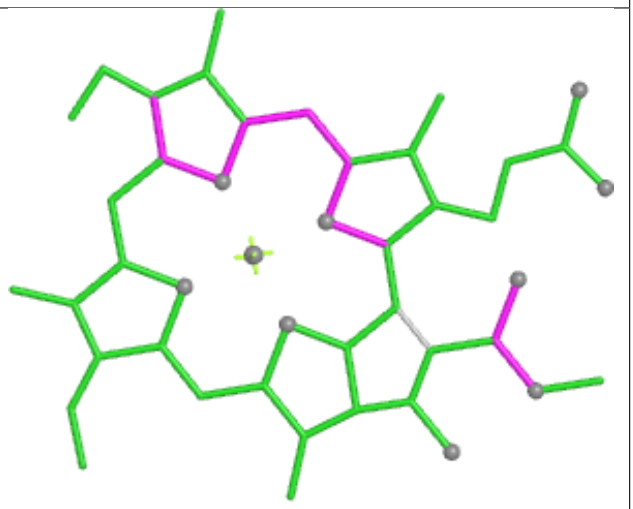


Rings

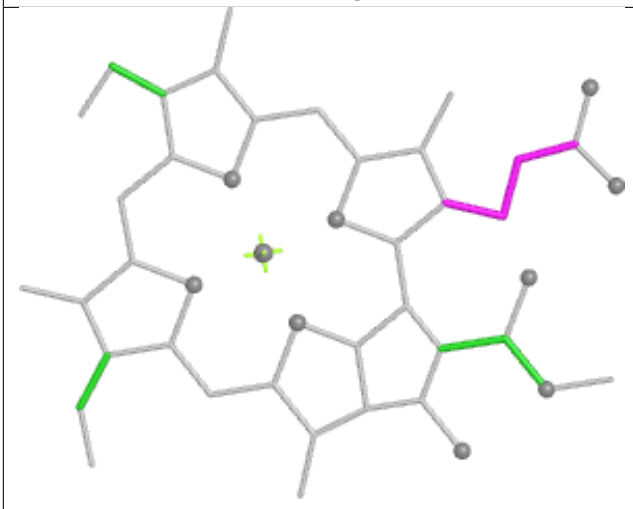
Ligand CLA L 412



Bond lengths



Bond angles

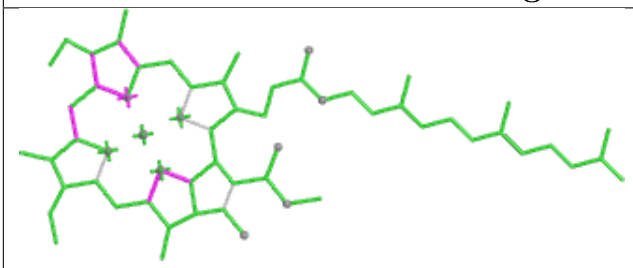


Torsions

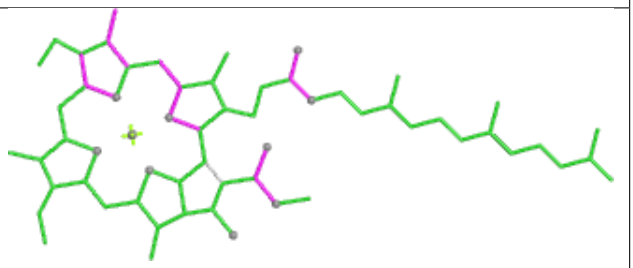


Rings

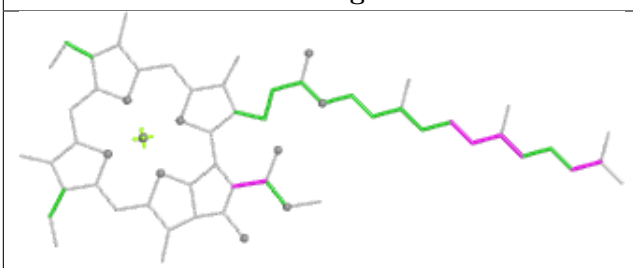
Ligand CLA H 308



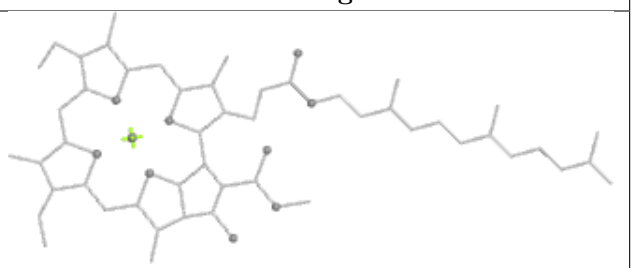
Bond lengths



Bond angles

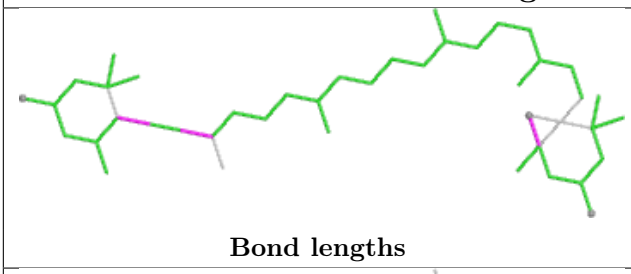


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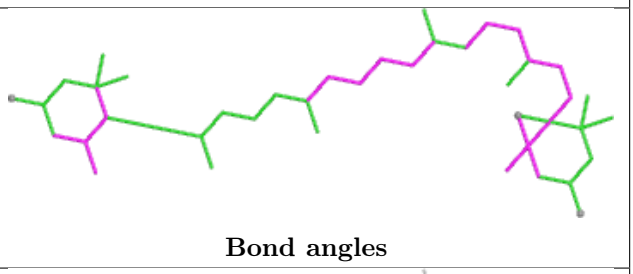


Rings

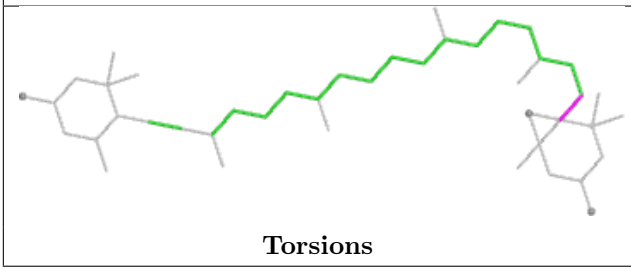
Ligand DD6 W 418



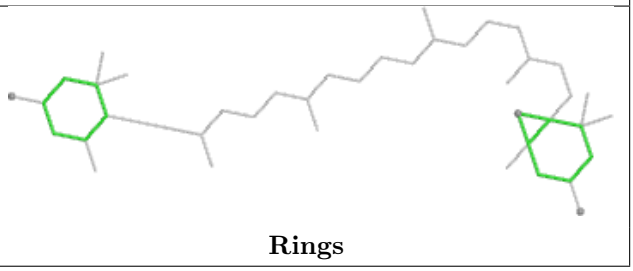
Bond lengths



Bond angles

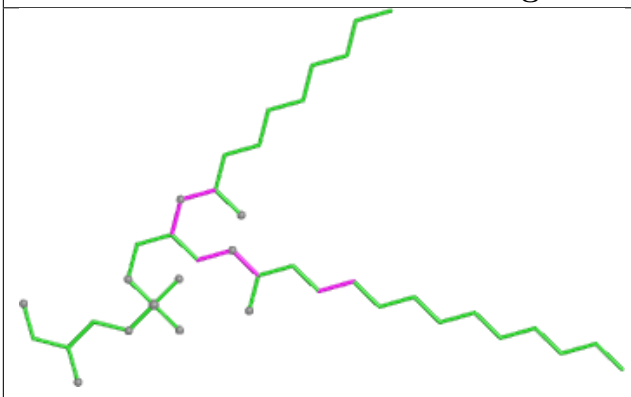


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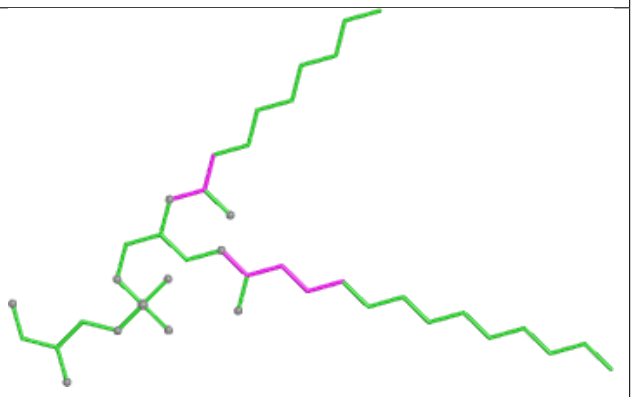


Rings

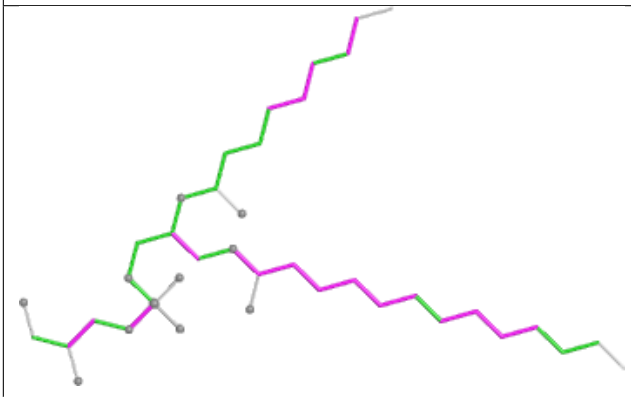
Ligand LHG K 616



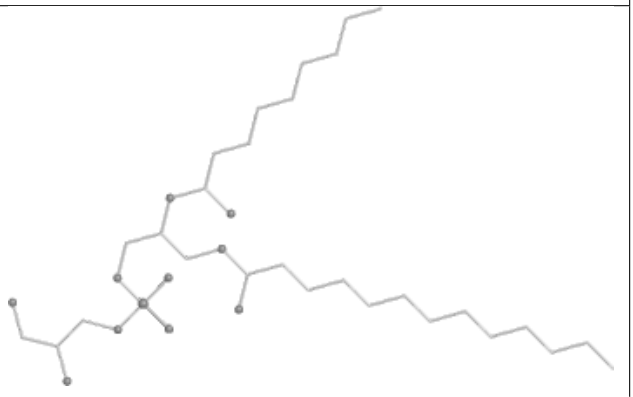
Bond lengths



Bond angles

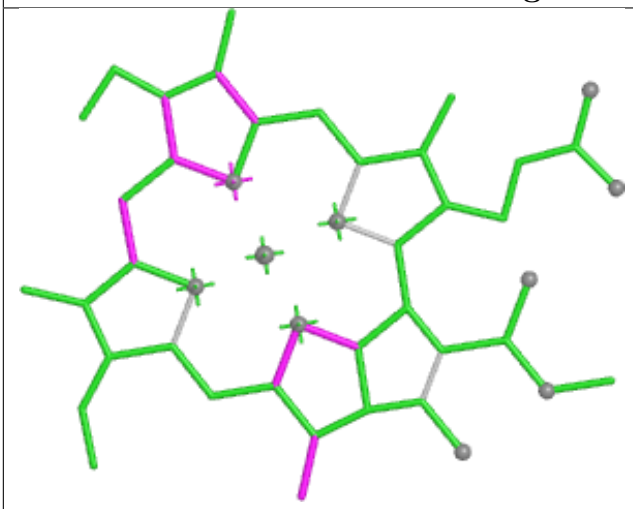


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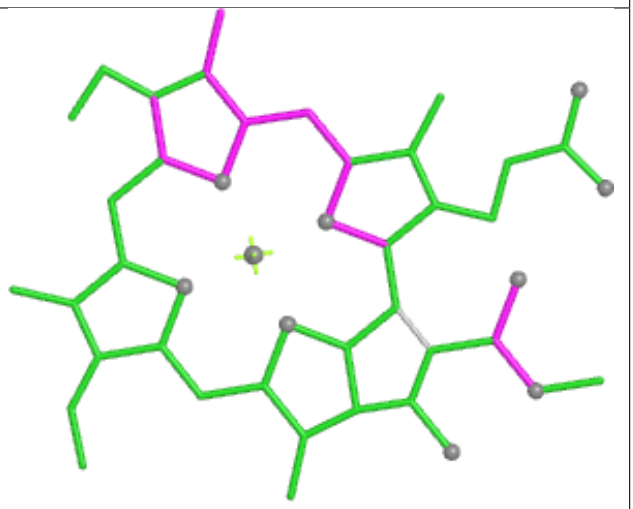


Rings

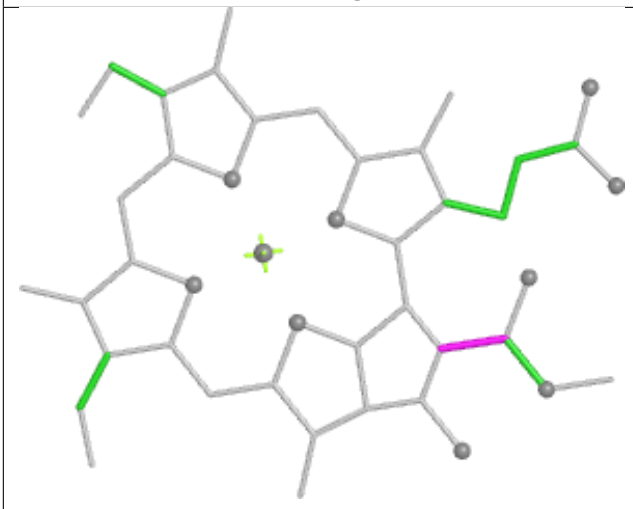
Ligand CLA N 605



Bond lengths



Bond angles

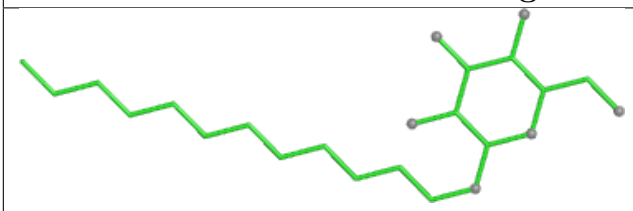


Torsions

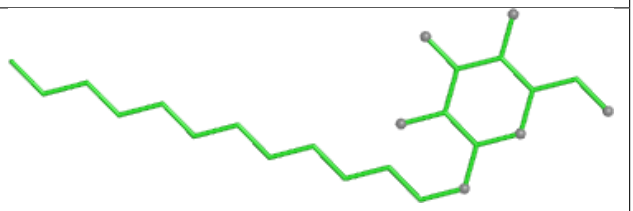


Rings

Ligand LMU A 853



Bond lengths



Bond angles

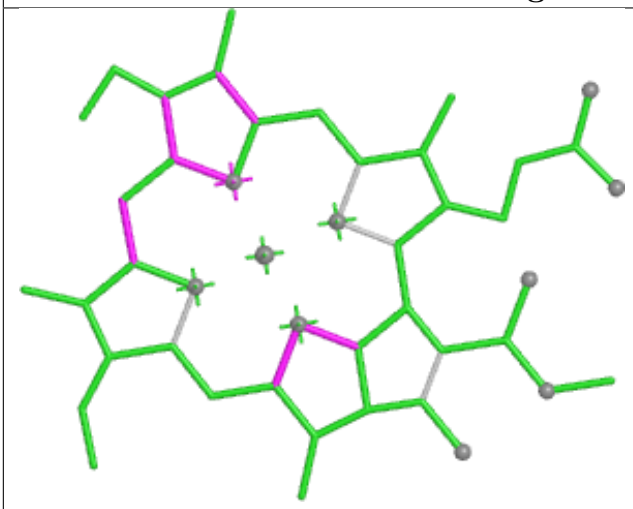


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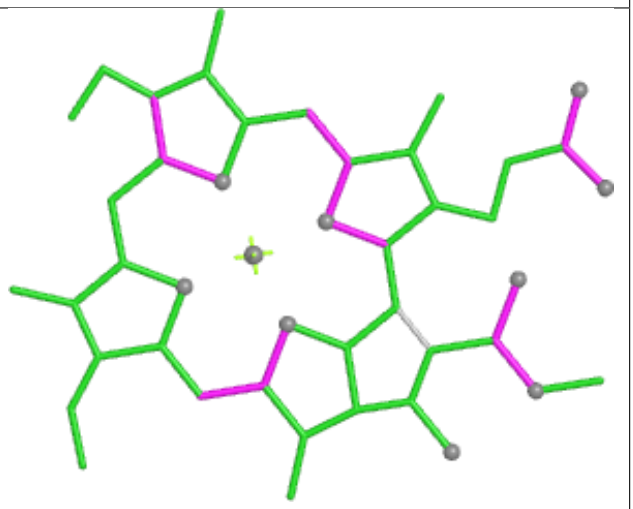


Rings

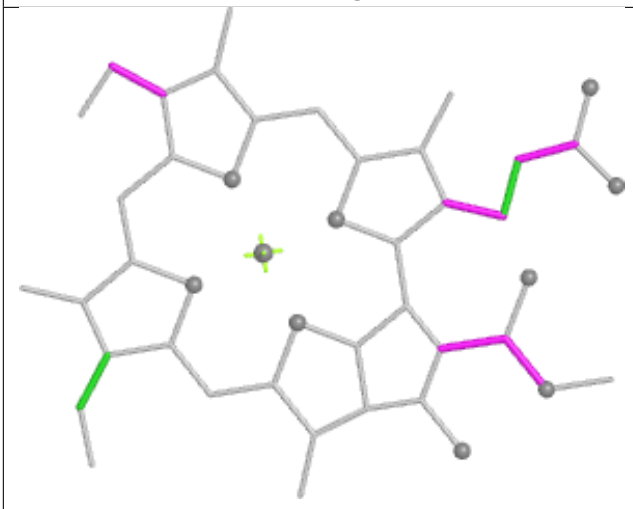
Ligand CLA S 608



Bond lengths



Bond angles

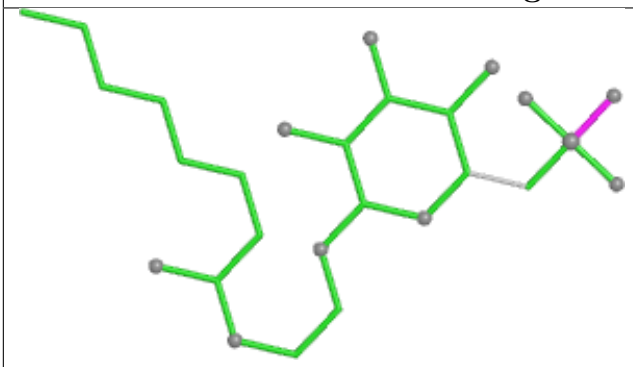


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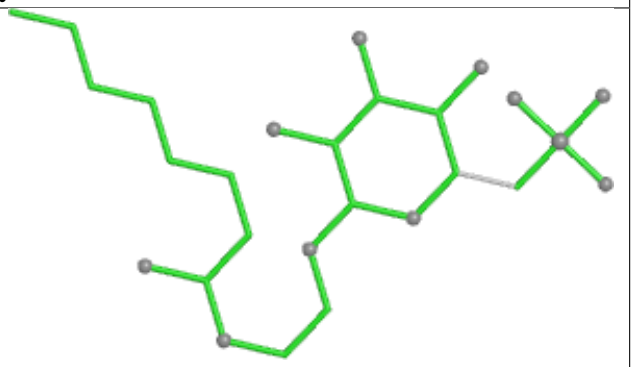


Rings

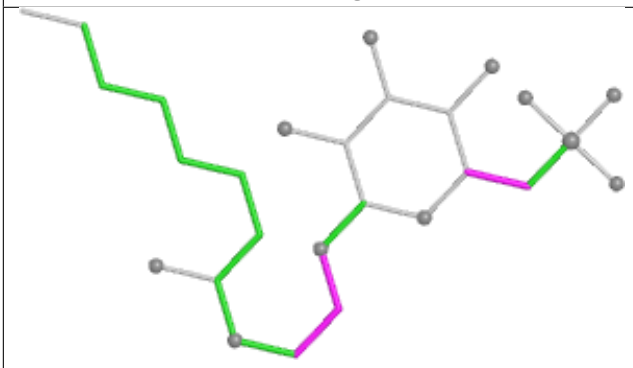
Ligand SQD V 618



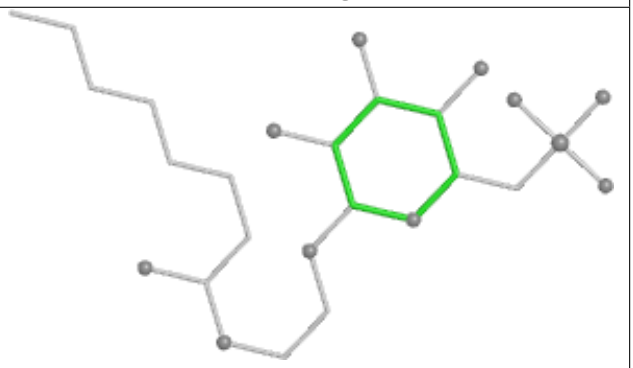
Bond lengths



Bond angles



Torsions

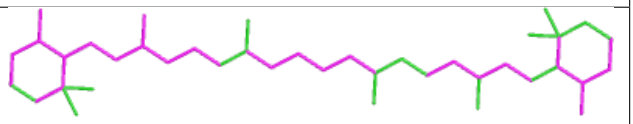


Rings

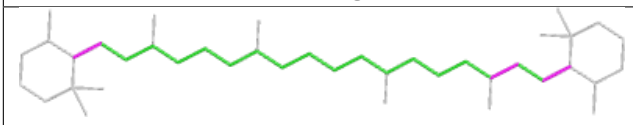
Ligand BCR B 846



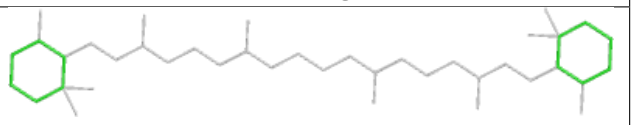
Bond lengths



Bond angles

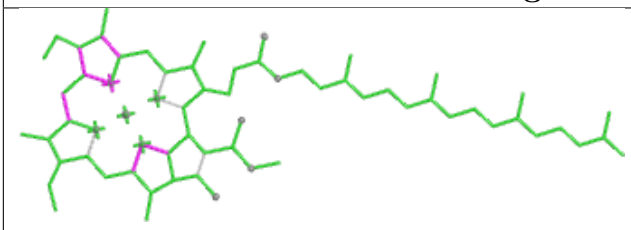


Torsions

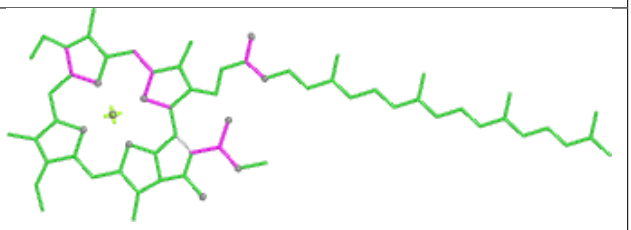


Rings

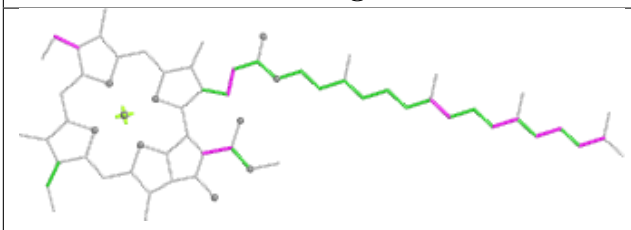
Ligand CLA A 810



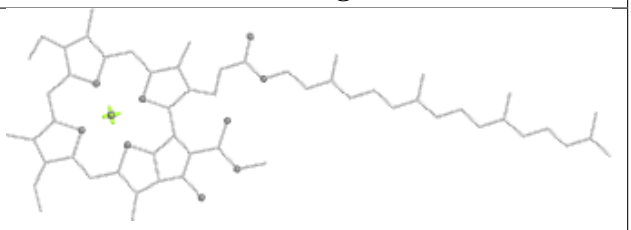
Bond lengths



Bond angles

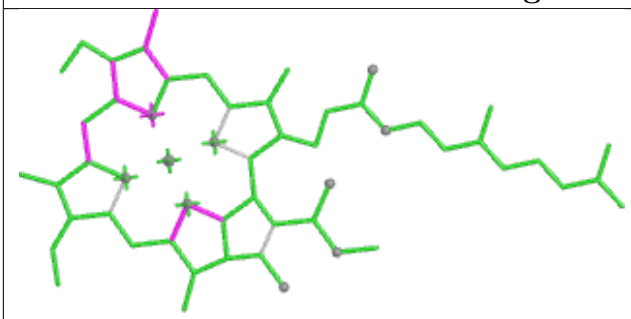


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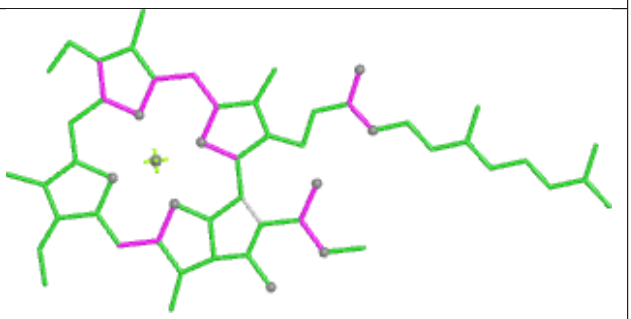


Rings

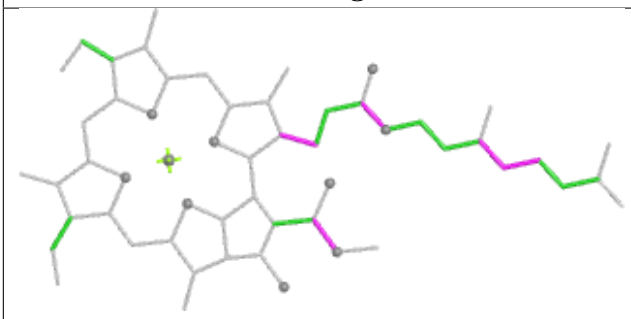
Ligand CLA U 401



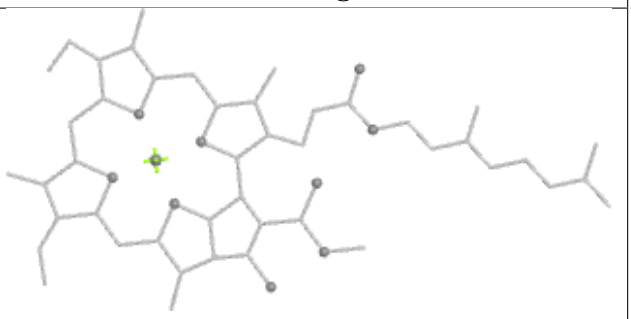
Bond lengths



Bond angles

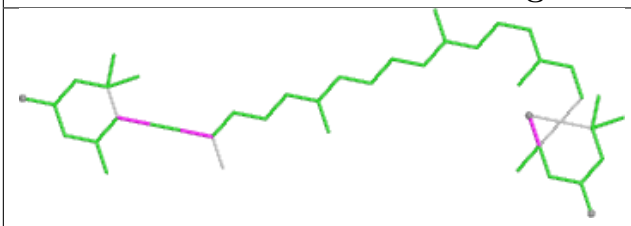


Torsions

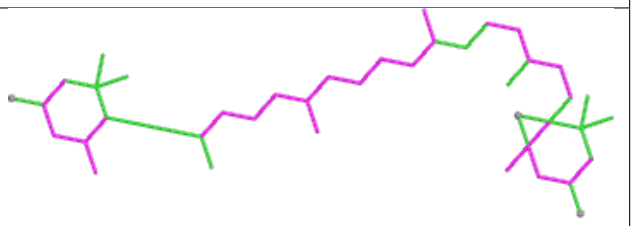


Rings

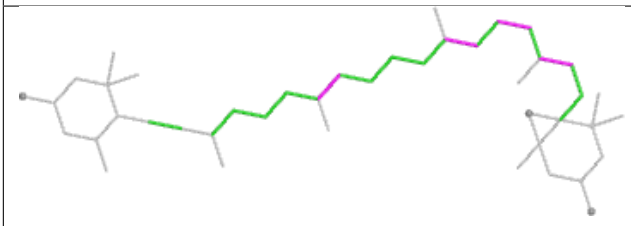
Ligand DD6 F 406



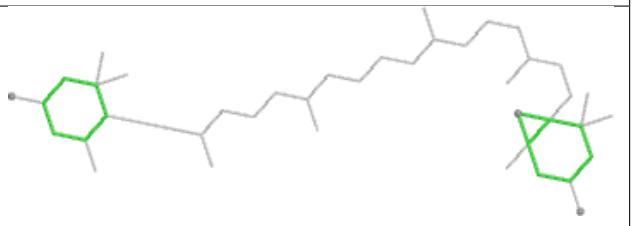
Bond lengths



Bond angles

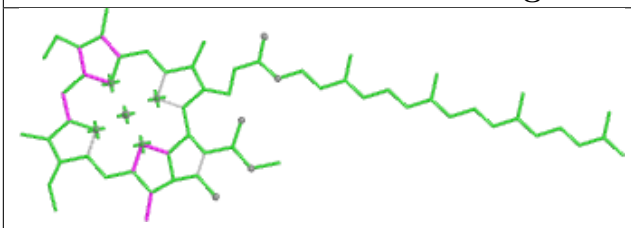


Torsions

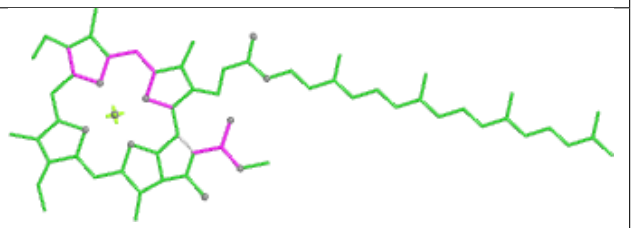


Rings

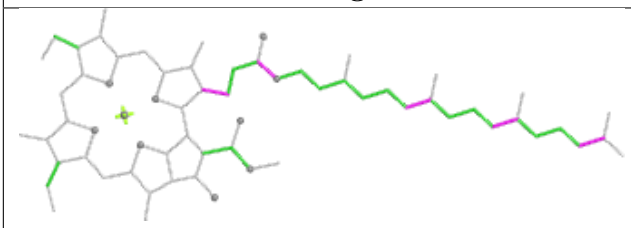
Ligand CLA A 806



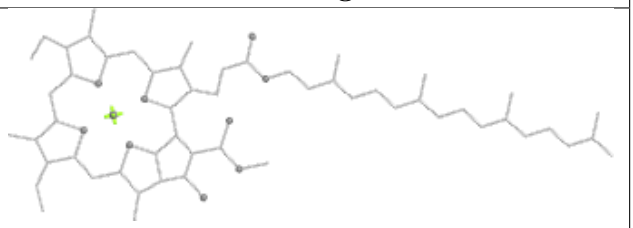
Bond lengths



Bond angles

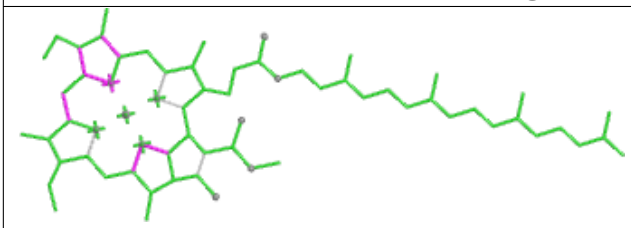


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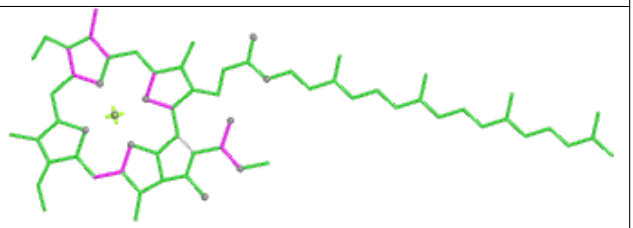


Rings

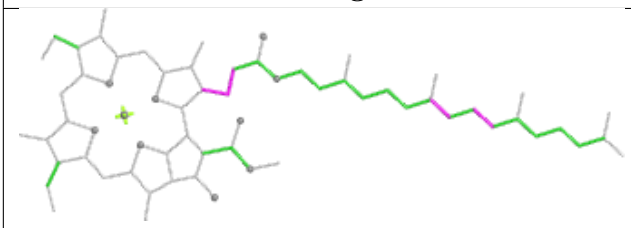
Ligand CLA A 804



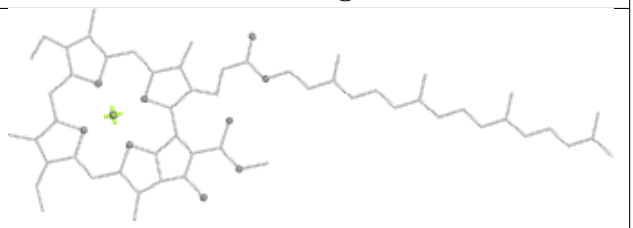
Bond lengths



Bond angles

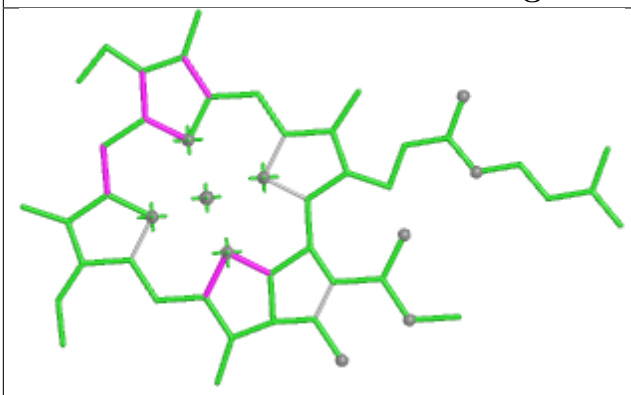


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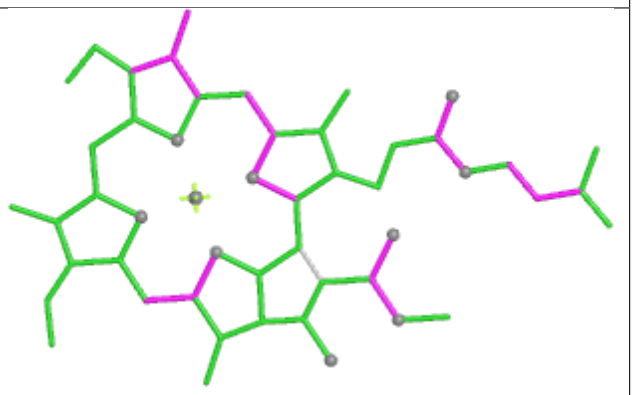


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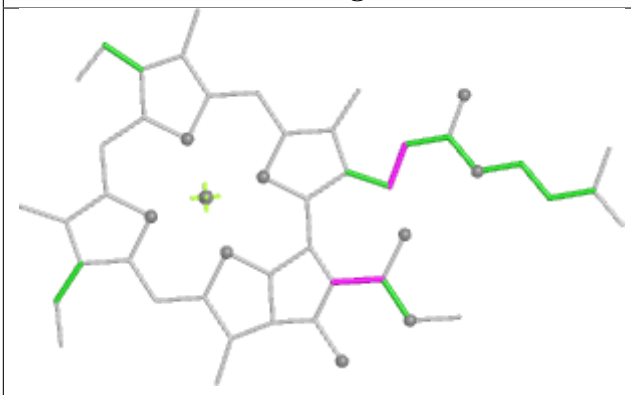
Ligand CLA X 417



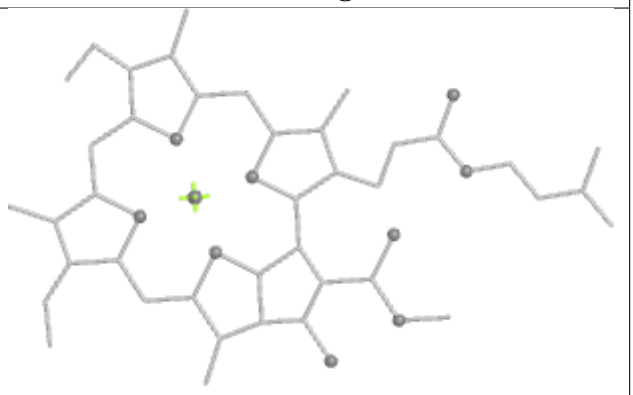
Bond lengths



Bond angles

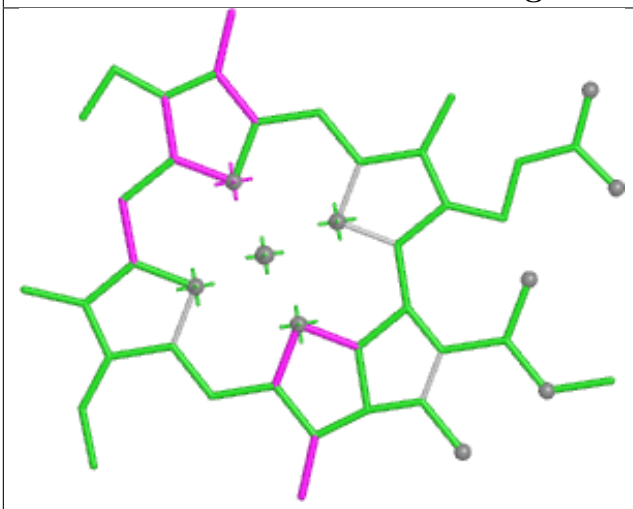


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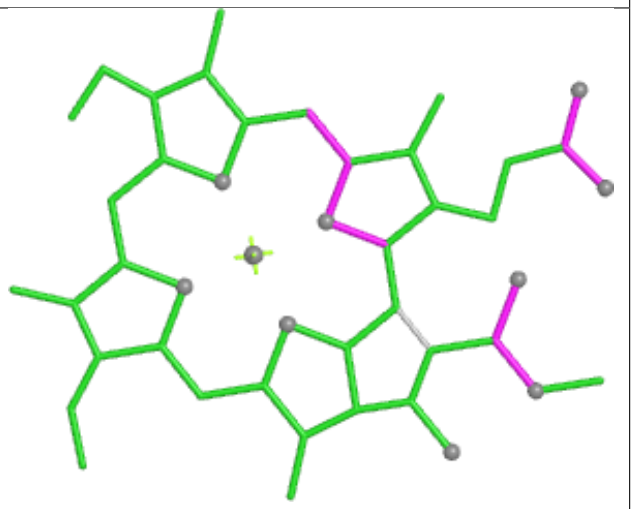


Rings

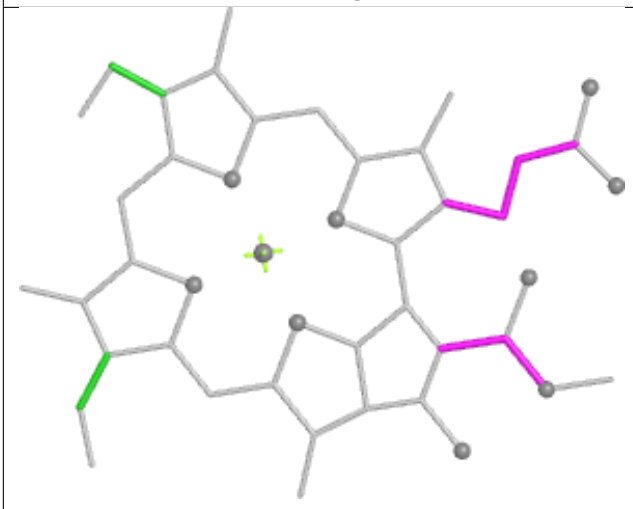
Ligand CLA P 609



Bond lengths



Bond angles

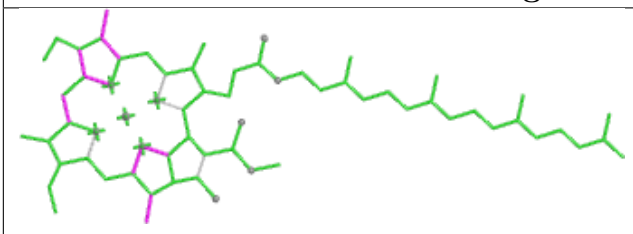


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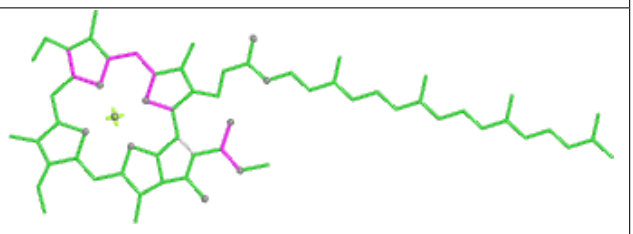


Rings

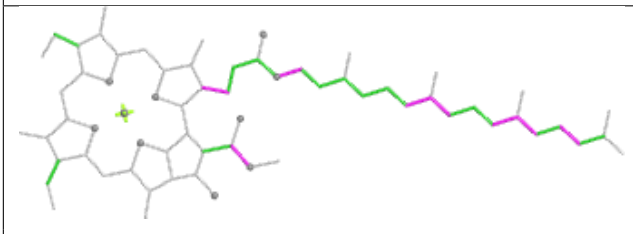
Ligand CLA G 606



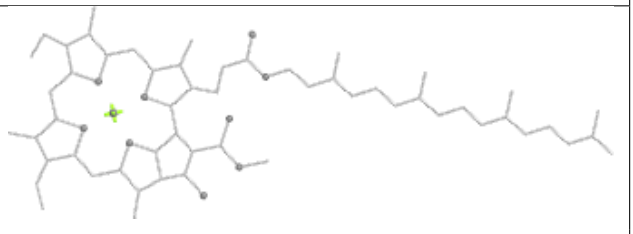
Bond lengths



Bond angles

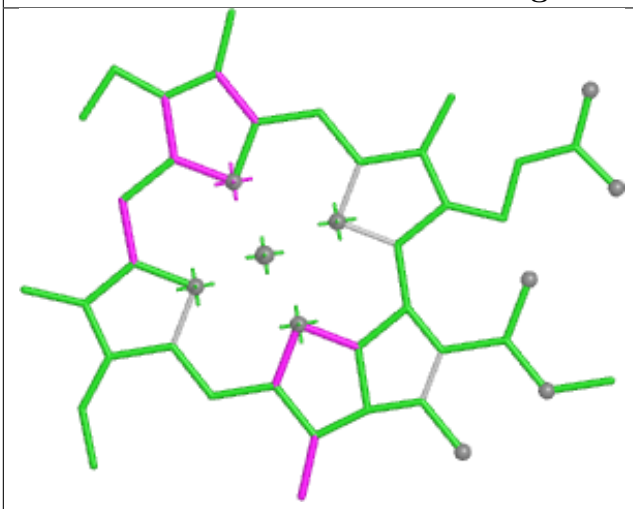


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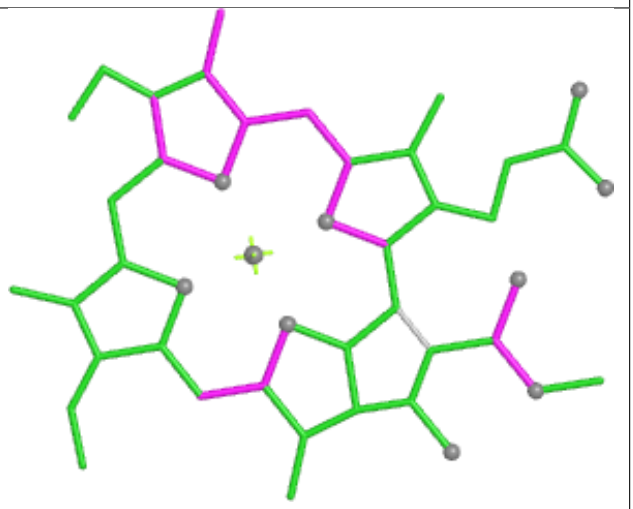


Rings

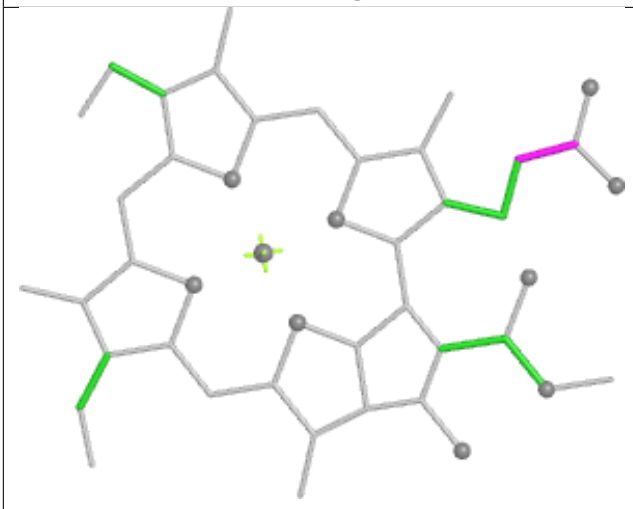
Ligand CLA I 605



Bond lengths



Bond angles

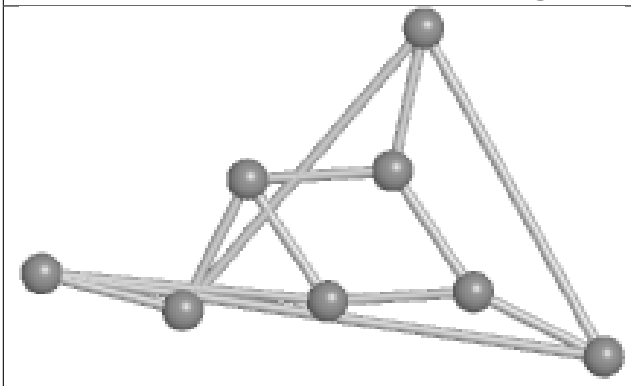


Torsions

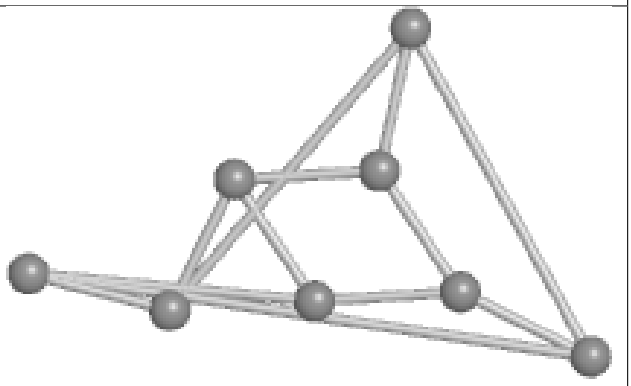


Rings

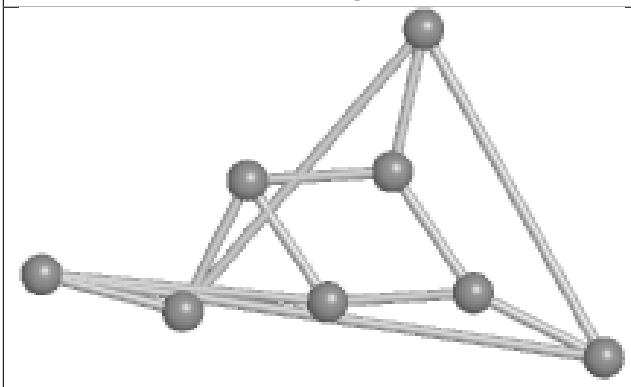
Ligand SF4 B 860



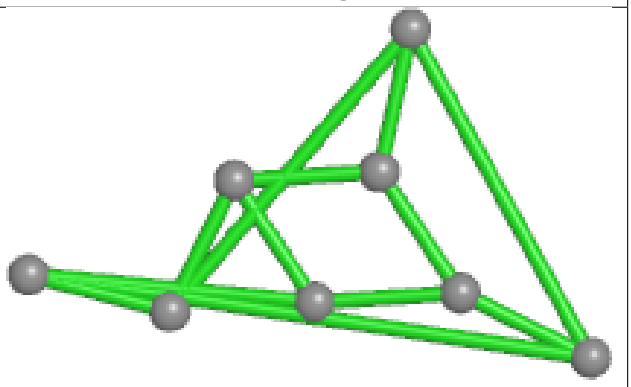
Bond lengths



Bond angles

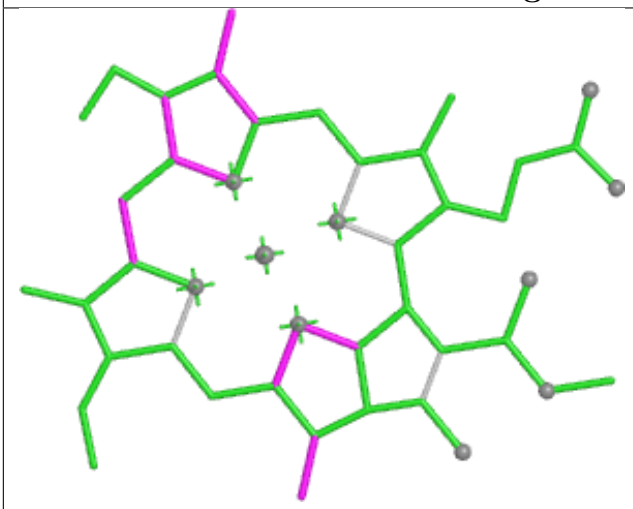


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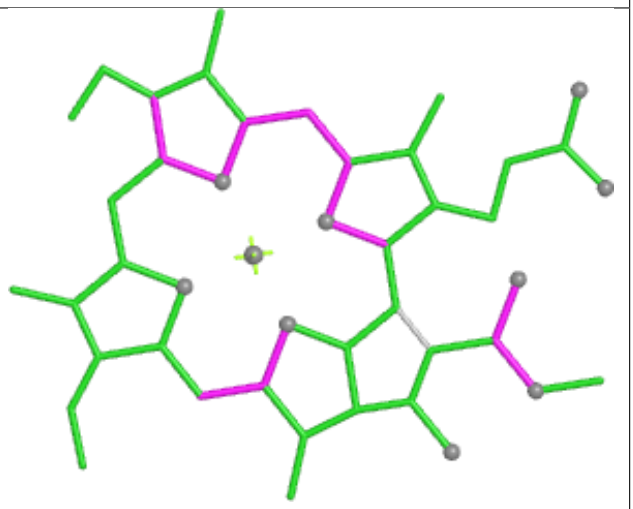


Rings

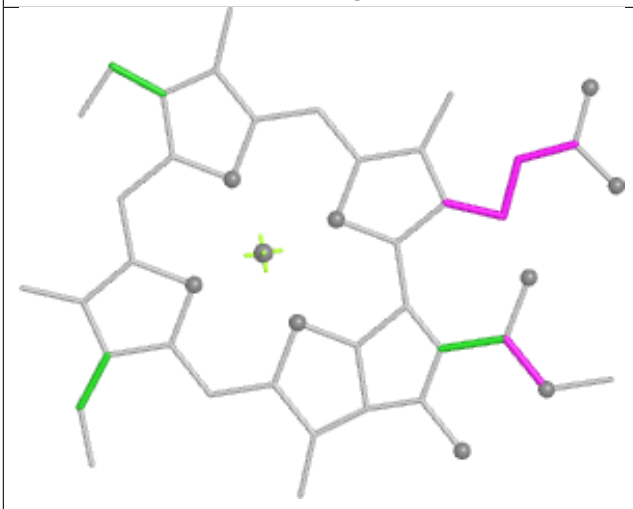
Ligand CLA A 823



Bond lengths



Bond angles

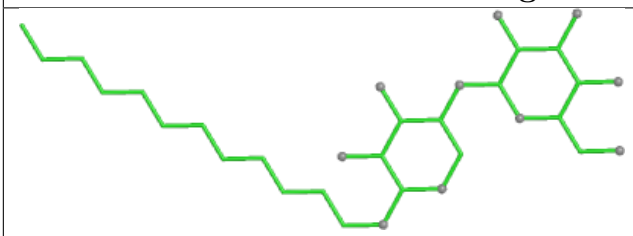


Torsions

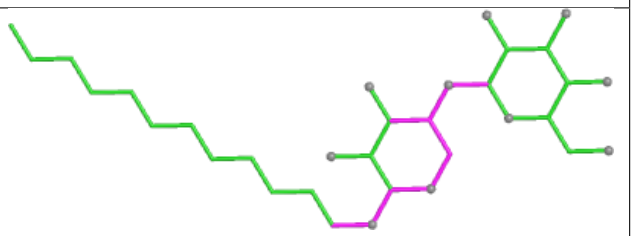


Rings

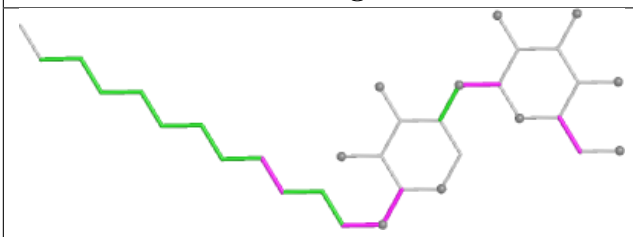
Ligand LMU K 620



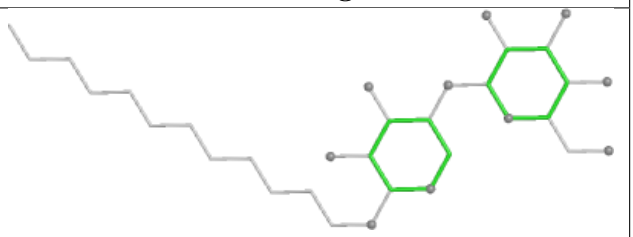
Bond lengths



Bond angles

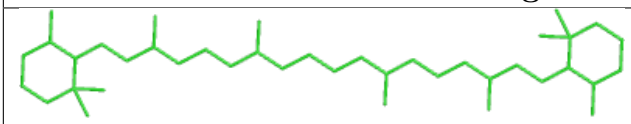


Torsions

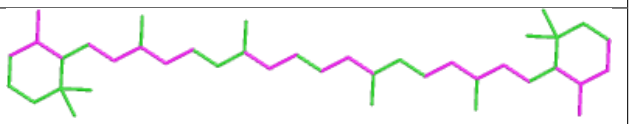


Rings

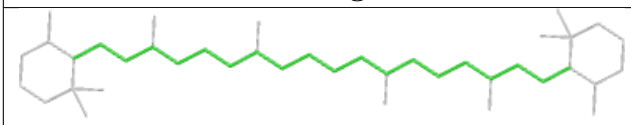
Ligand BCR A 848



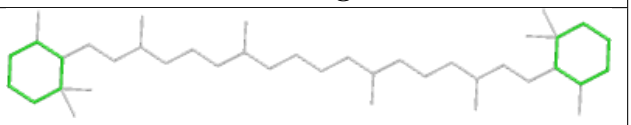
Bond lengths



Bond angles

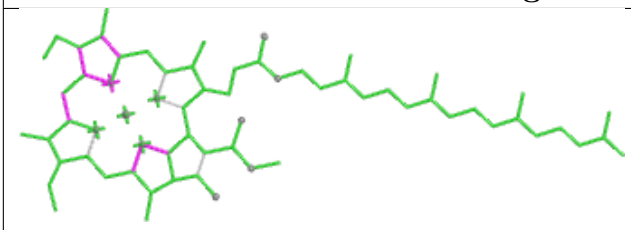


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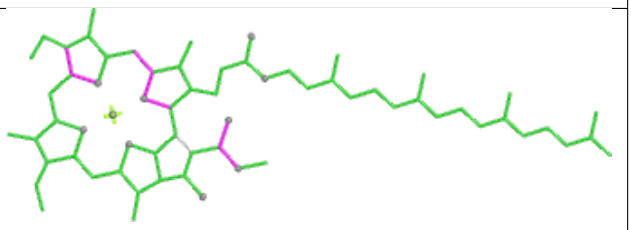


Rings

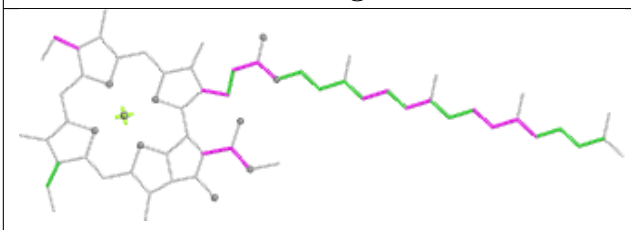
Ligand CLA K 605



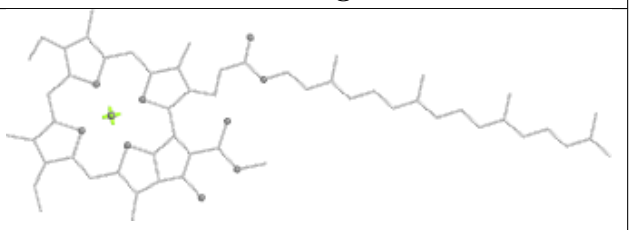
Bond lengths



Bond angles

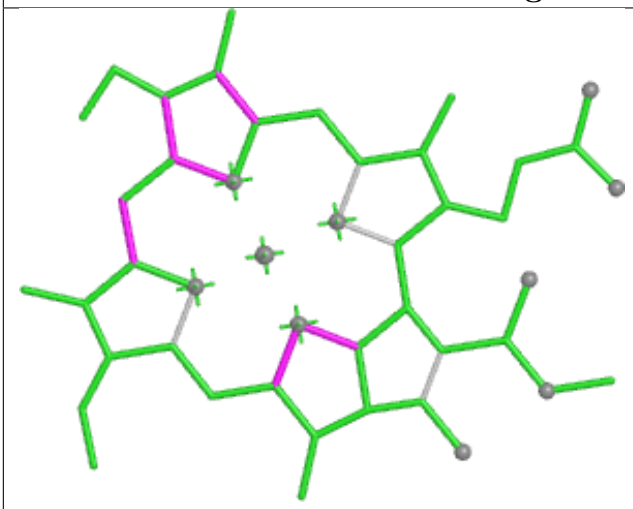


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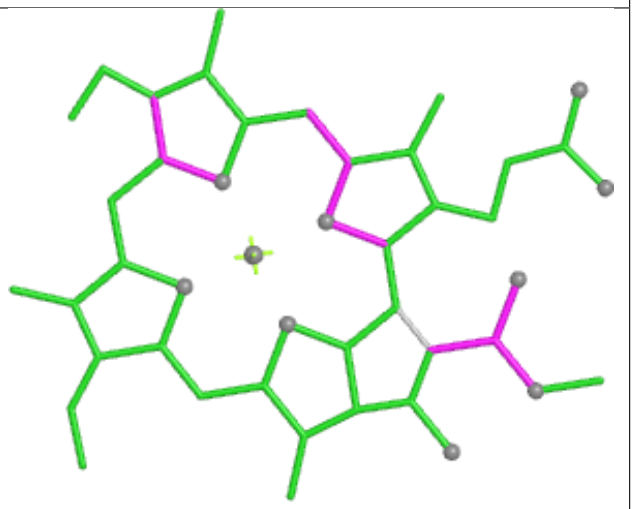


Rings

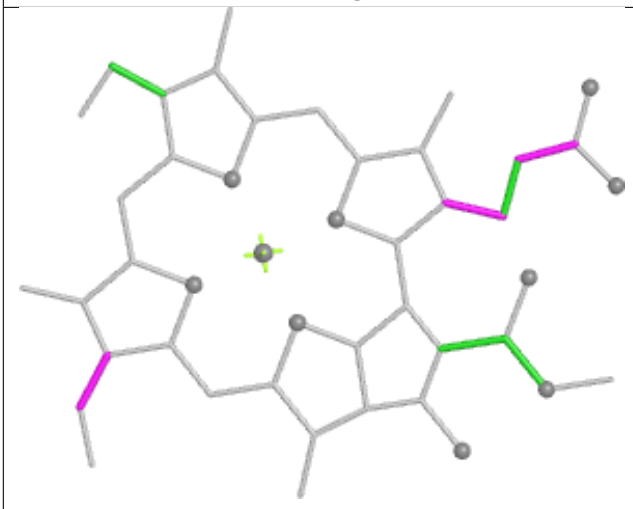
Ligand CLA P 611



Bond lengths



Bond angles

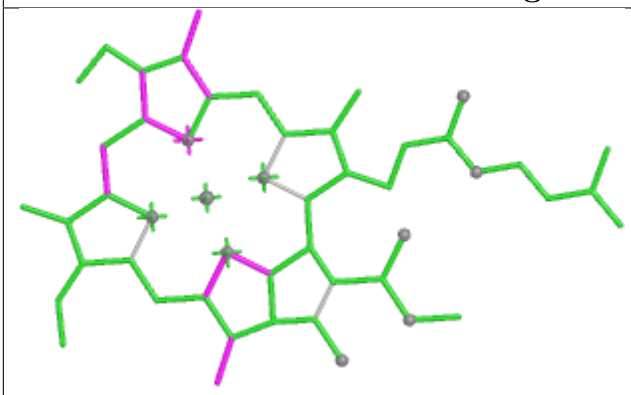


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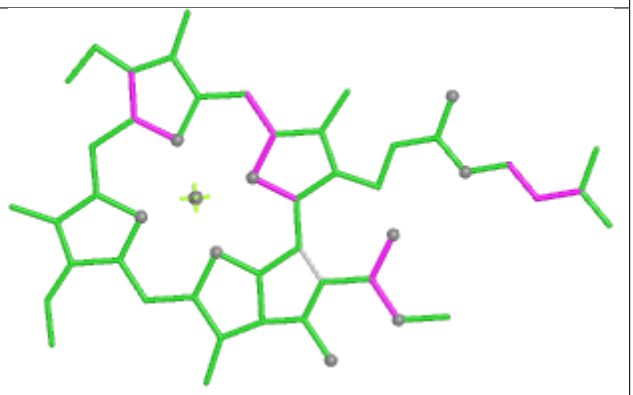


Rings

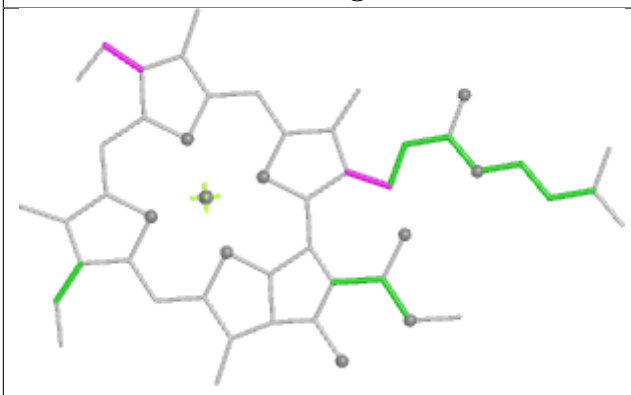
Ligand CLA O 309



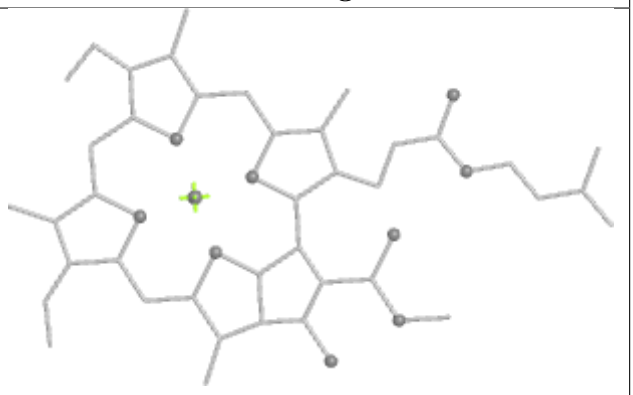
Bond lengths



Bond angles

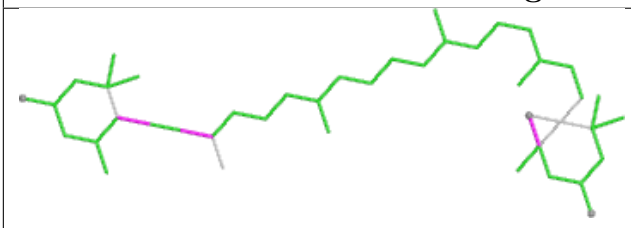


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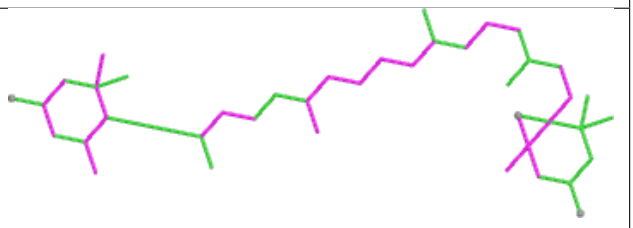


Rings

Ligand DD6 O 317



Bond lengths



Bond angles

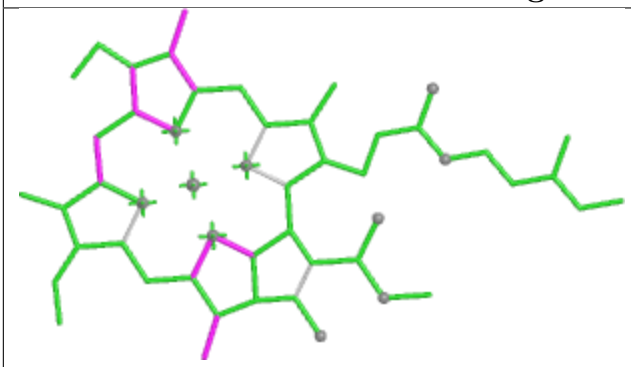


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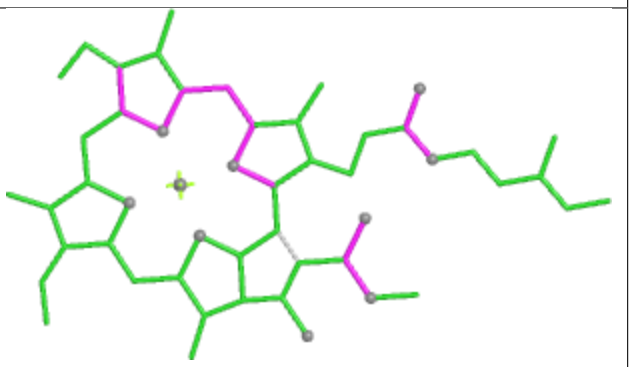


Rings

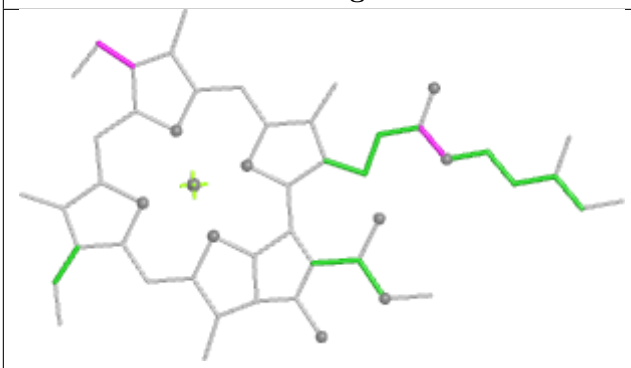
Ligand CLA S 615



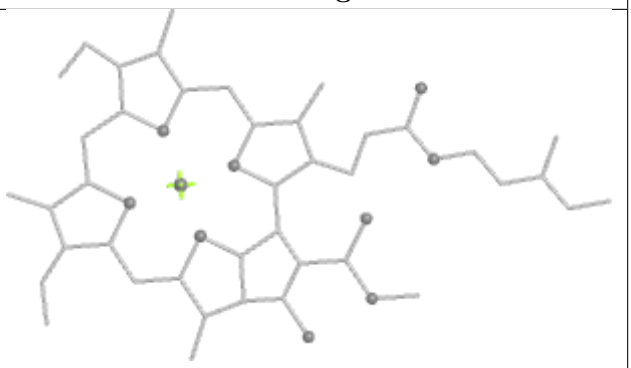
Bond lengths



Bond angles

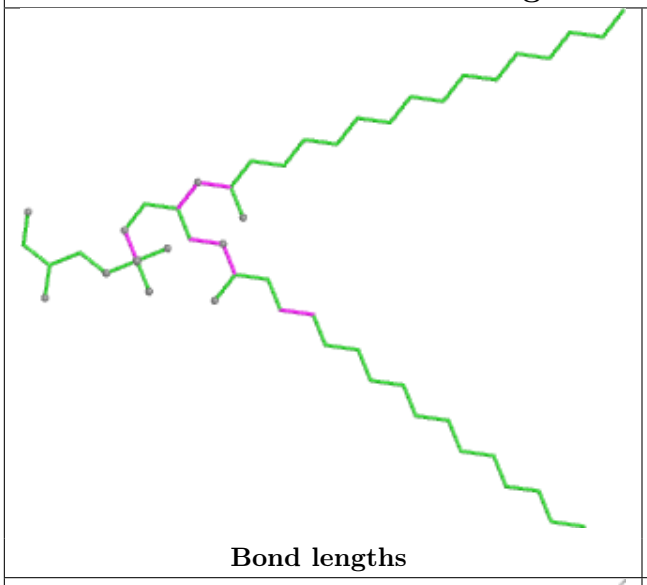


Torsions

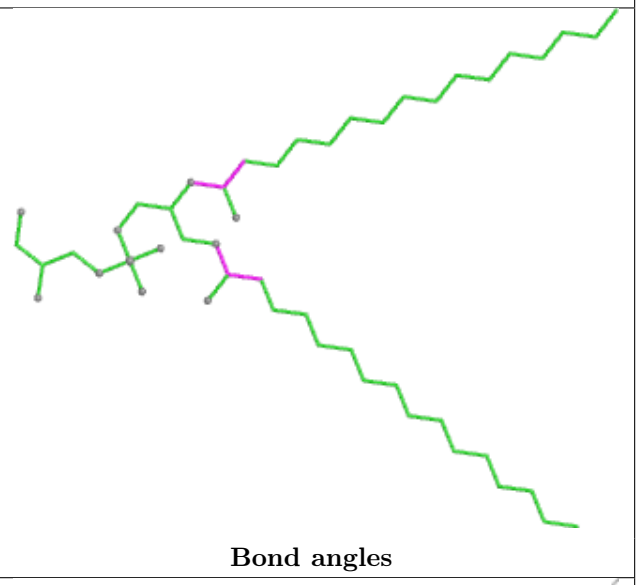


Rings

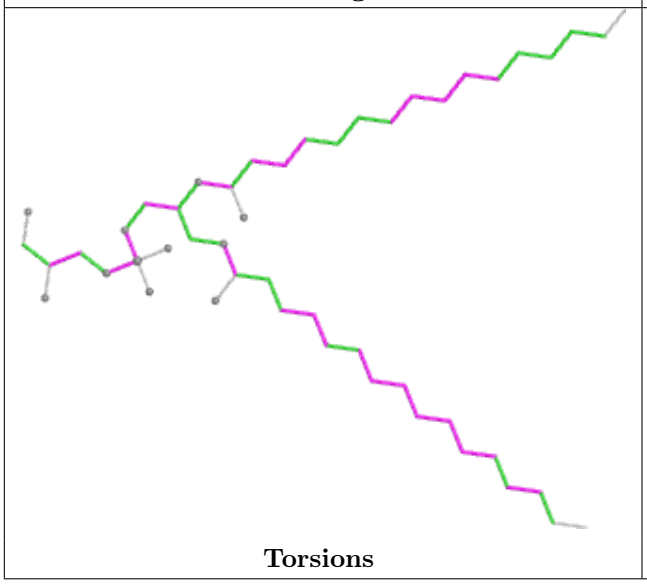
Ligand LHG A 846



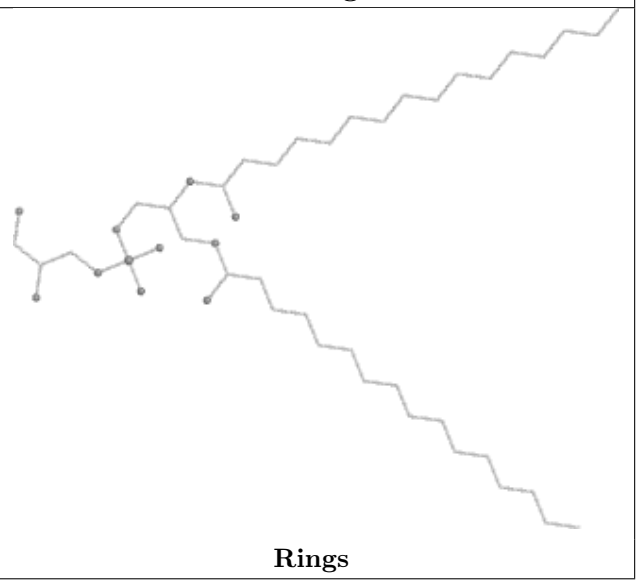
Bond lengths



Bond angles

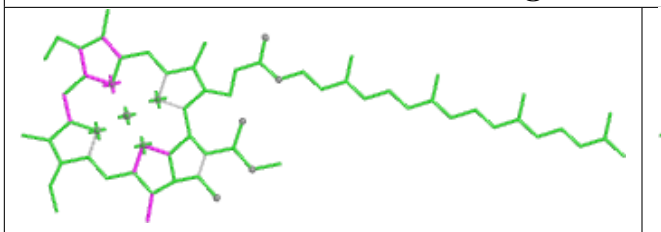


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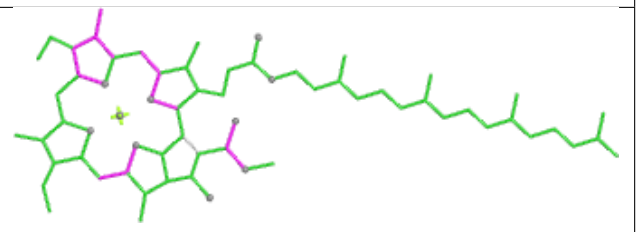


Rings

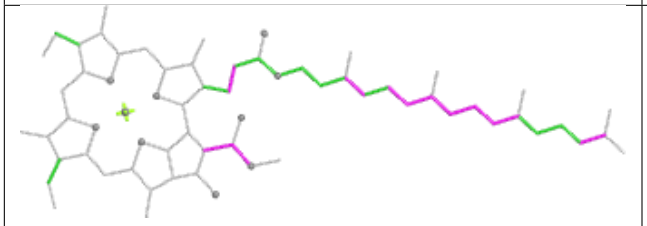
Ligand CLA U 404



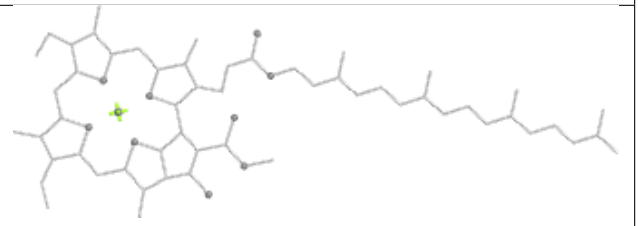
Bond lengths



Bond angles

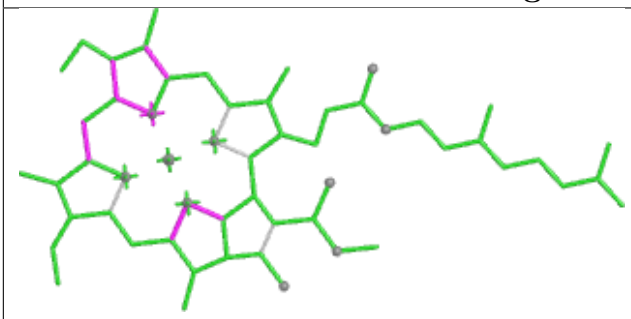


Torsions

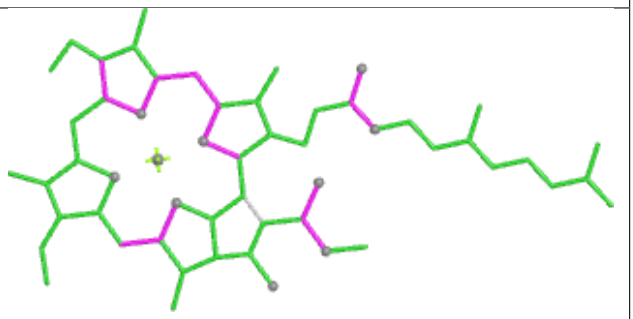


Rings

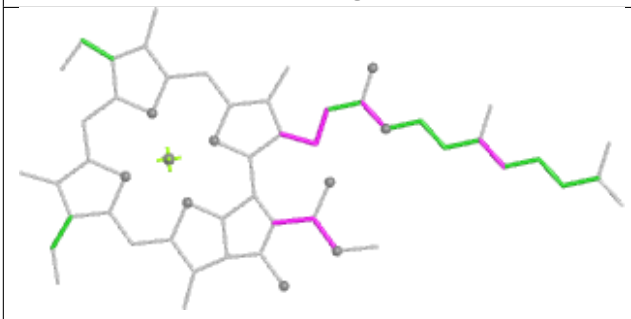
Ligand CLA X 402



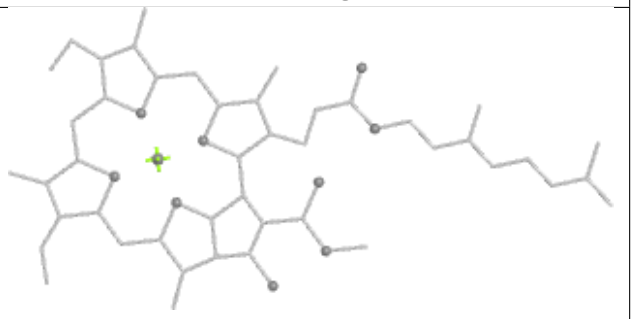
Bond lengths



Bond angles

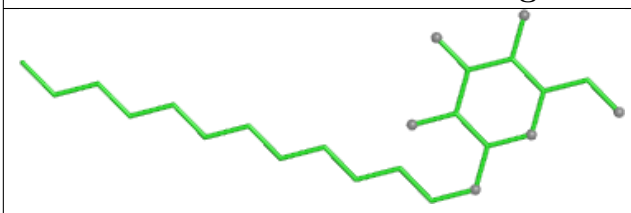


Torsions

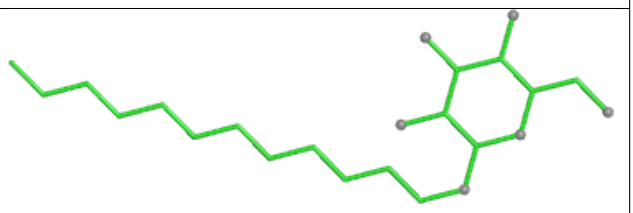


Rings

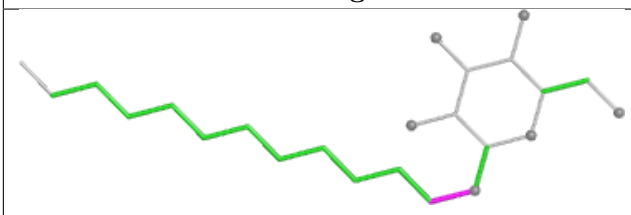
Ligand LMU O 301



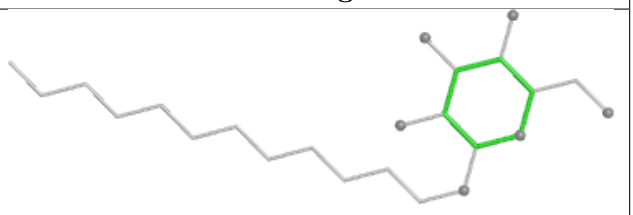
Bond lengths



Bond angles

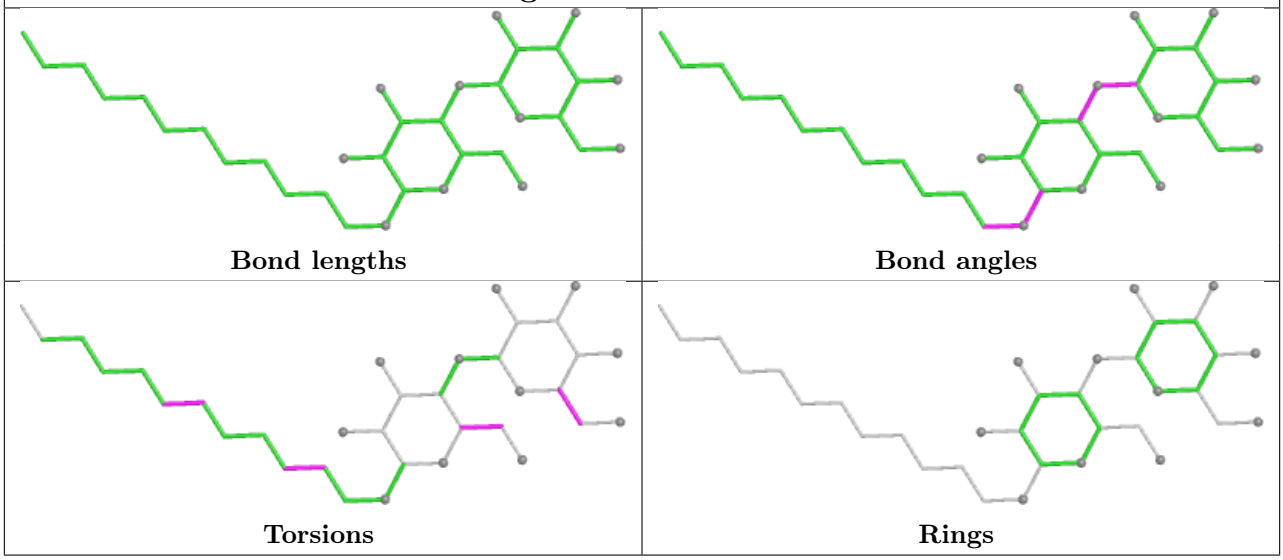


Torsions

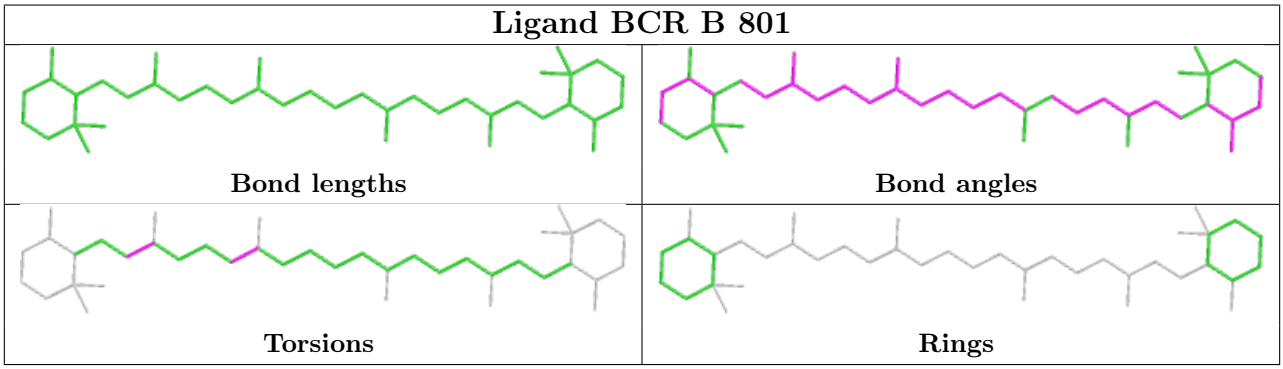


Rings

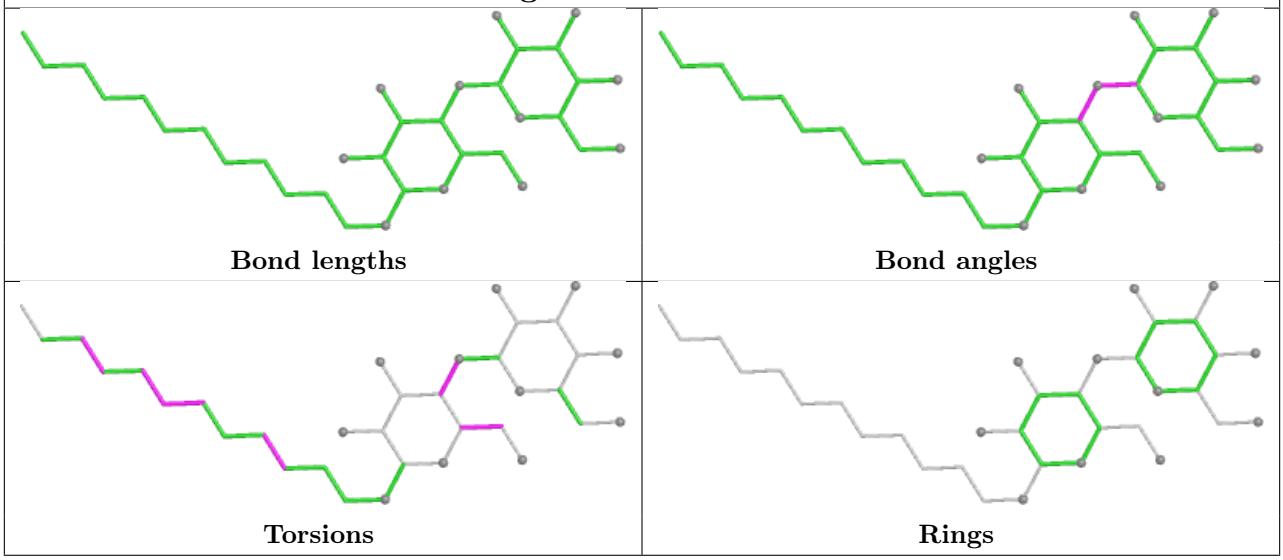
Ligand LMU U 422



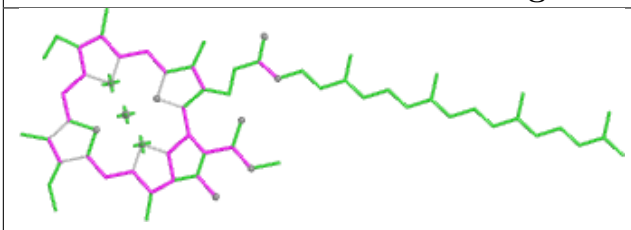
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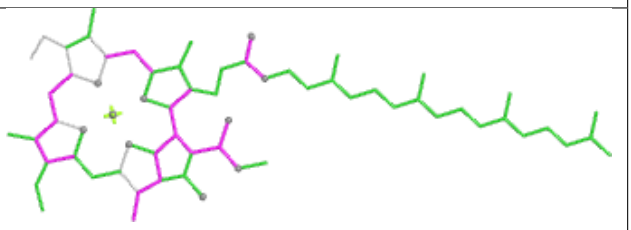
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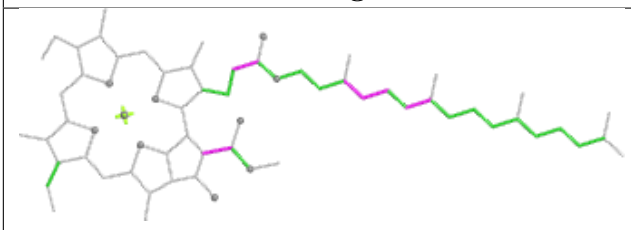
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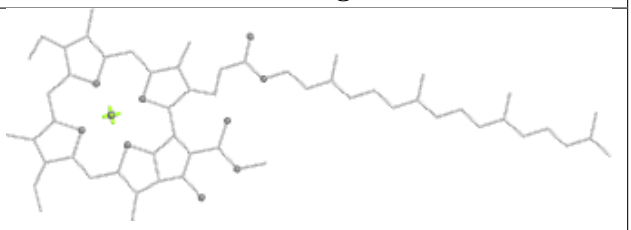
Bond lengths



Bond angles

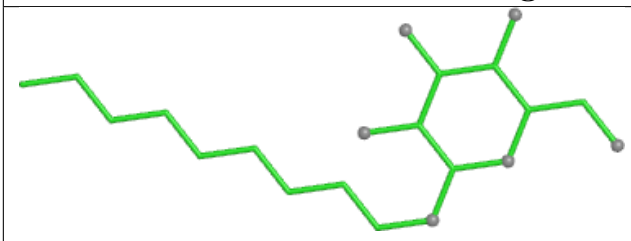


Torsions

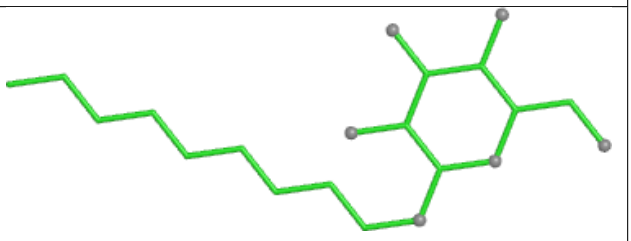


Rings

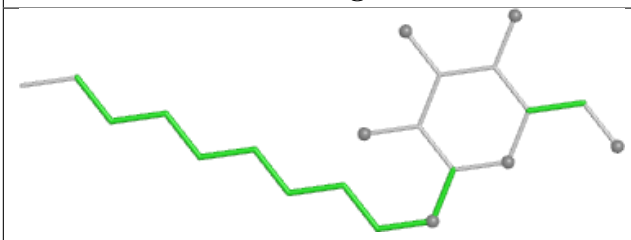
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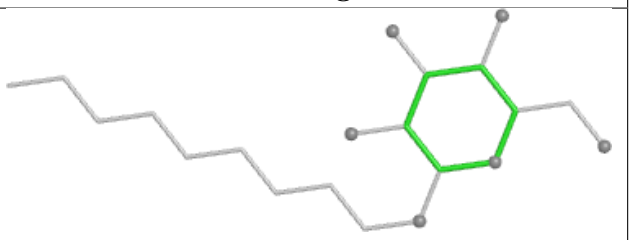
Bond lengths



Bond angles

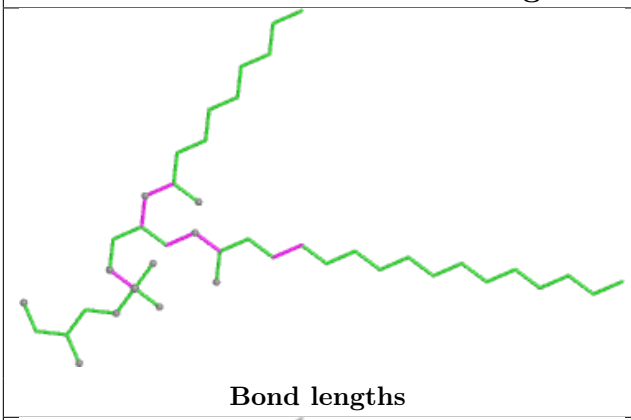


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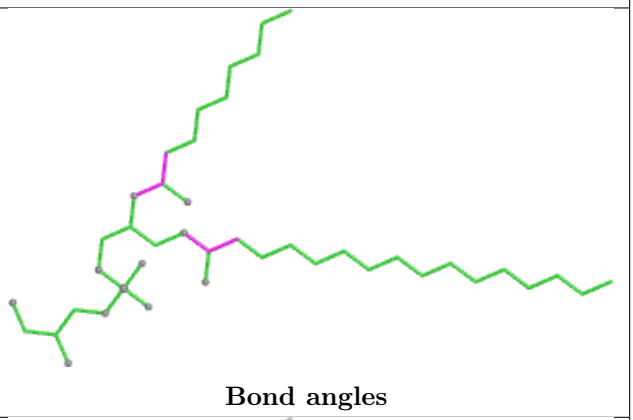


Rings

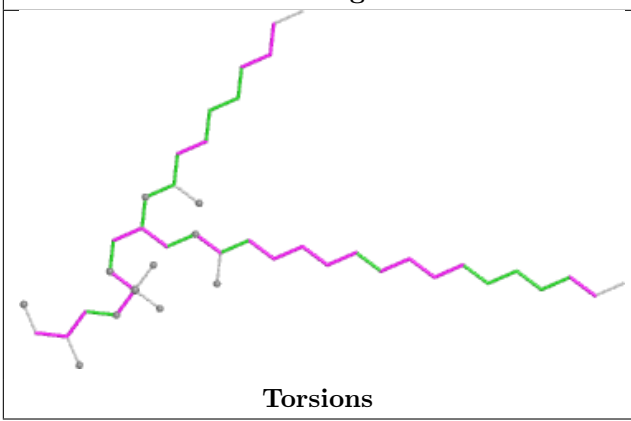
Ligand LHG T 614



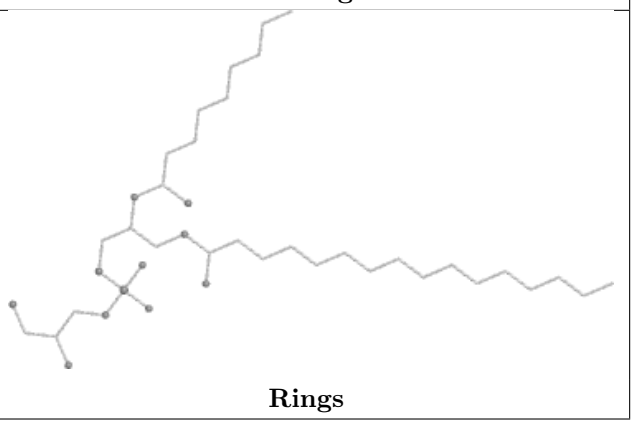
Bond lengths



Bond angles

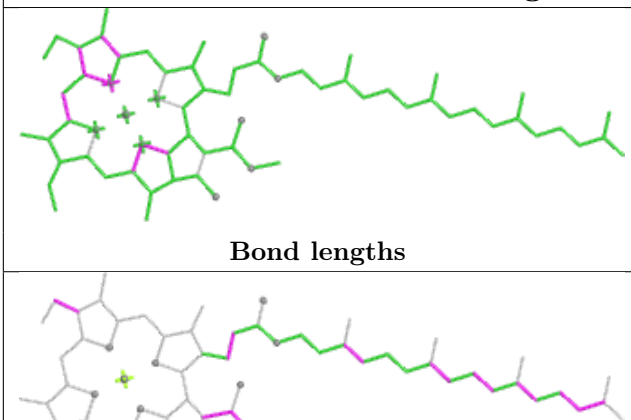


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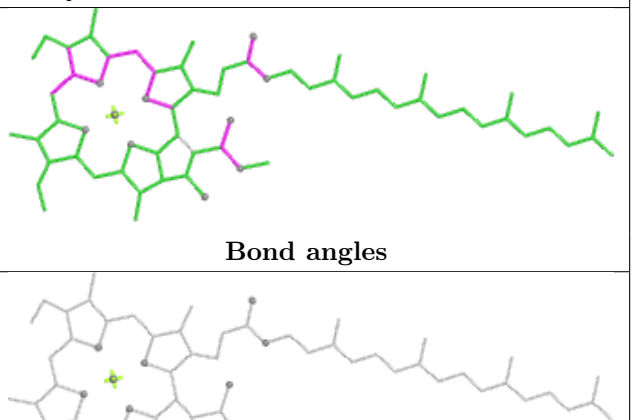


Rings

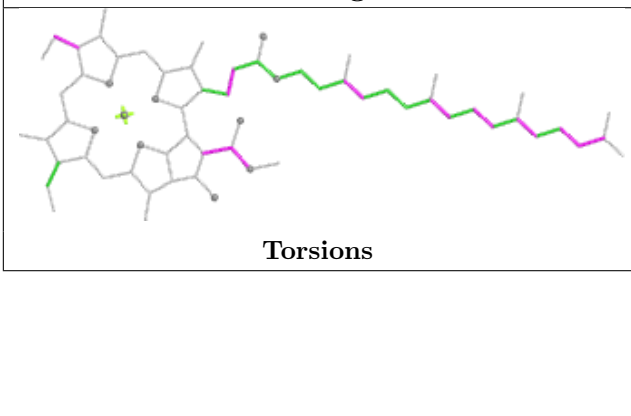
Ligand CLA Q 604



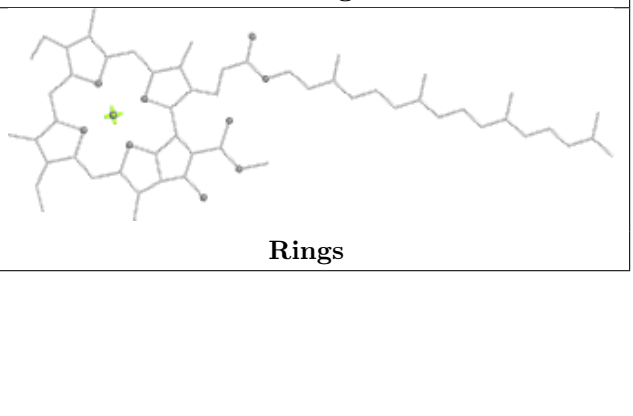
Bond lengths



Bond angles

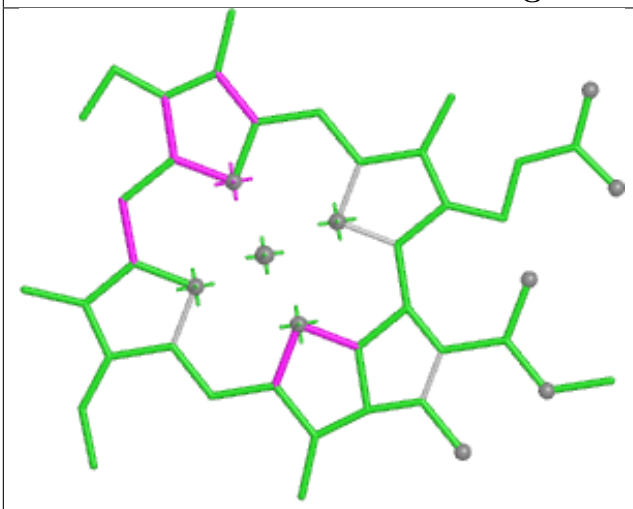


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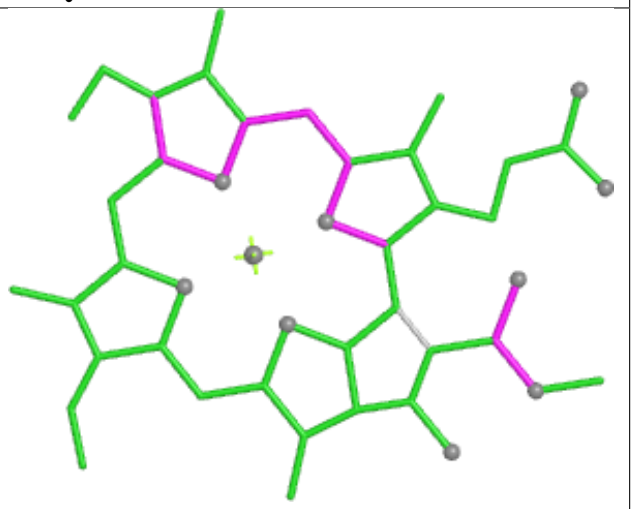


Rings

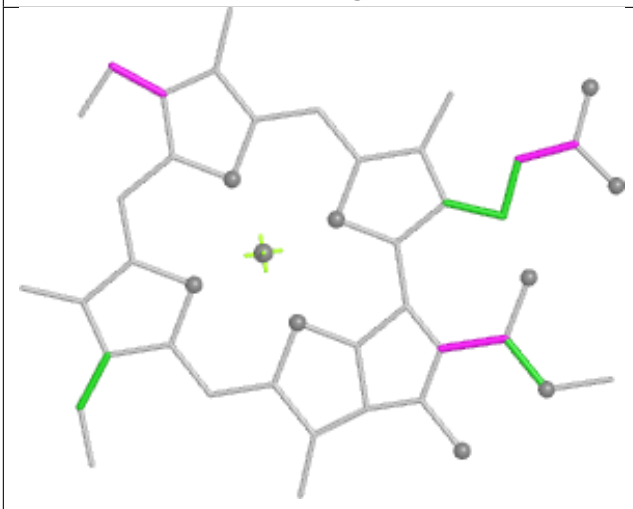
Ligand CLA Q 607



Bond lengths



Bond angles

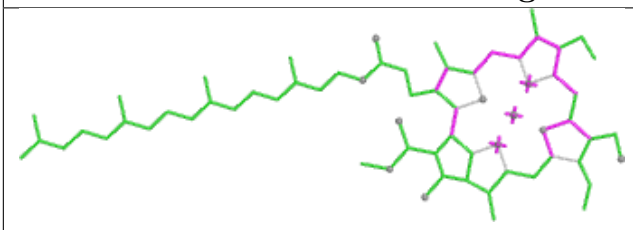


Torsions

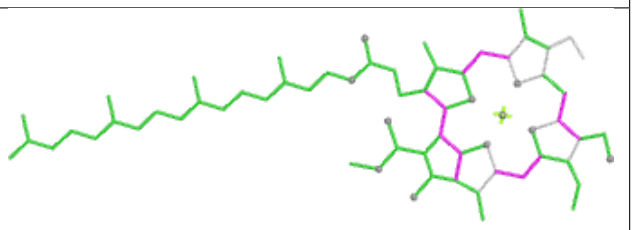


Rings

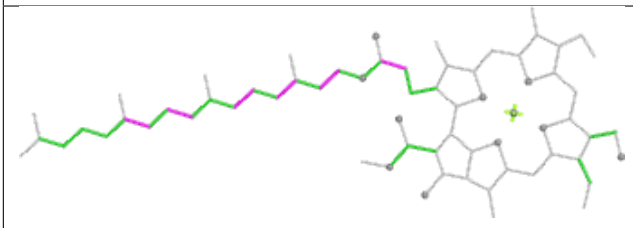
Ligand CHL W 422



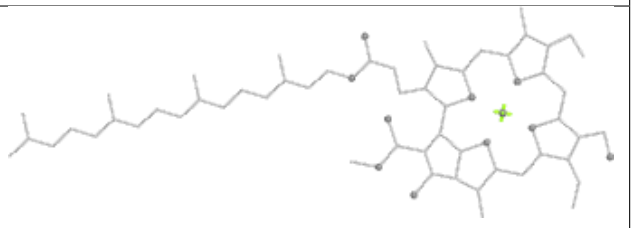
Bond lengths



Bond angles

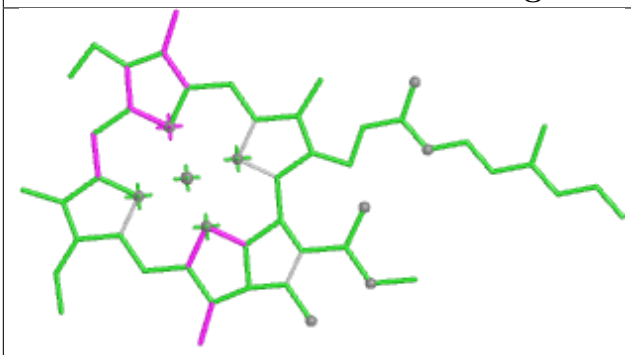


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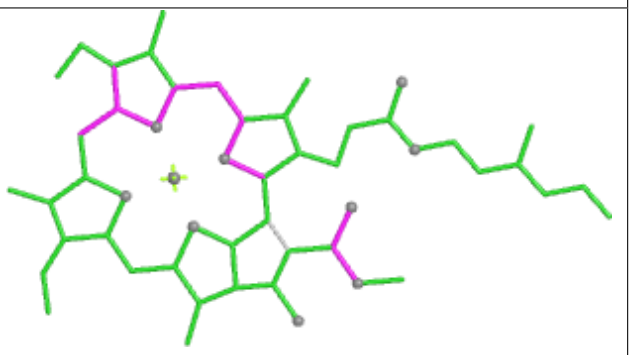


Rings

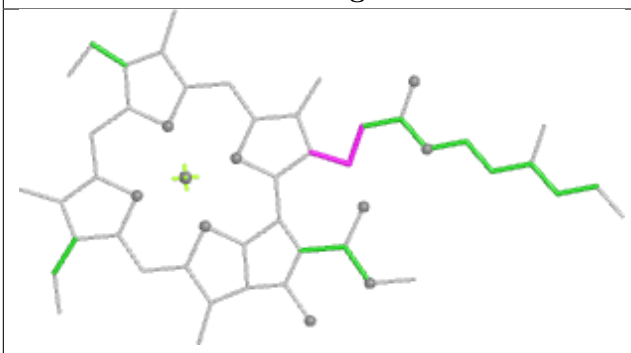
Ligand CLA B 815



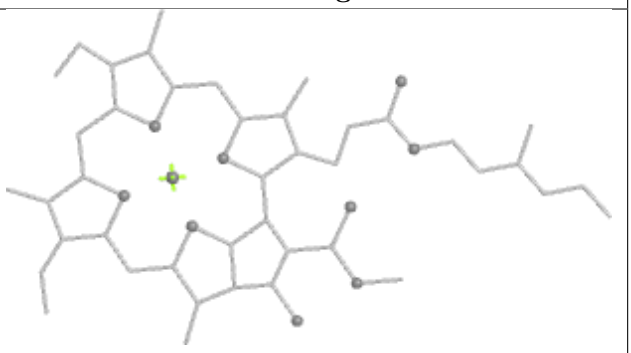
Bond lengths



Bond angles

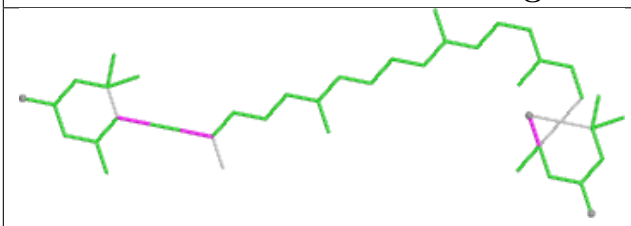


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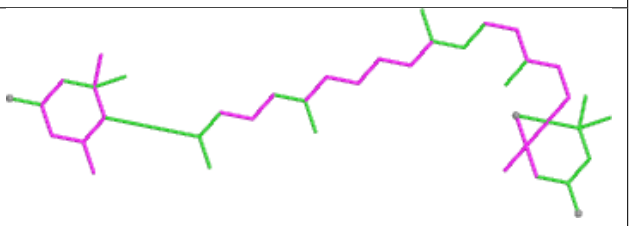


Rings

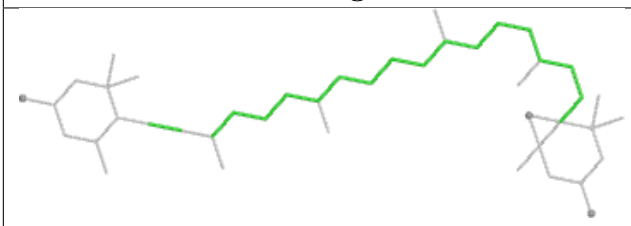
Ligand DD6 K 614



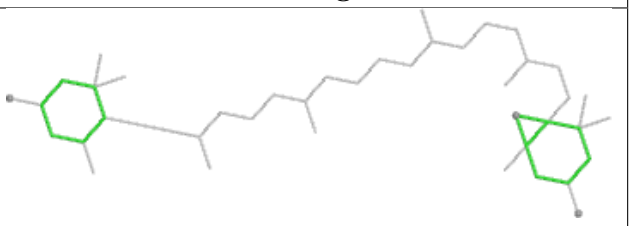
Bond lengths



Bond angles

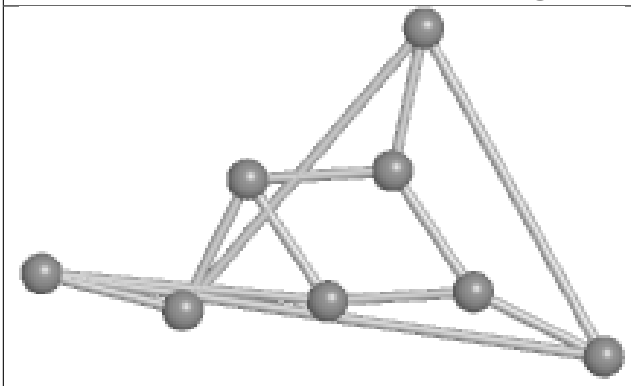


Torsions

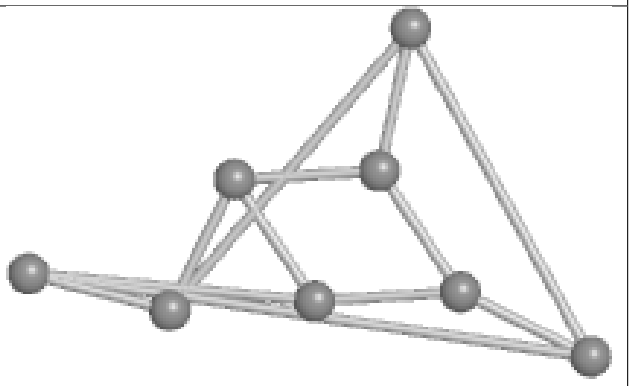


Rings

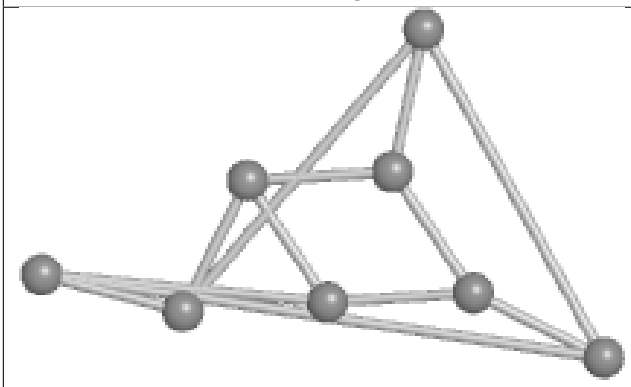
Ligand SF4 C 102



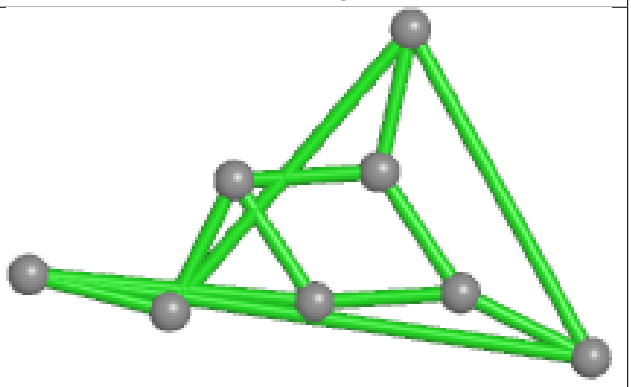
Bond lengths



Bond angles

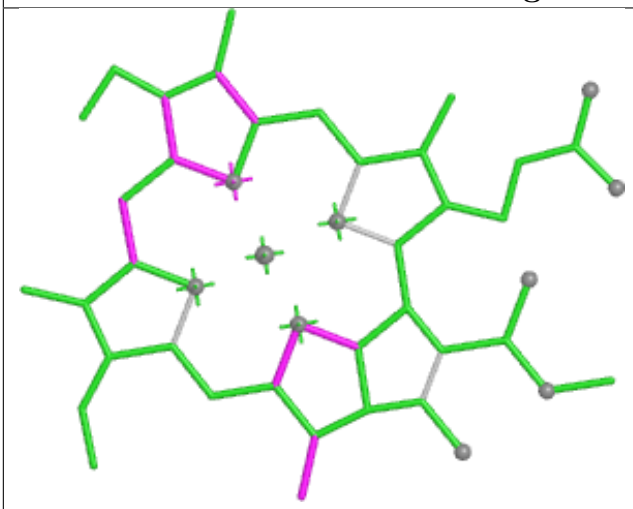


Torsions

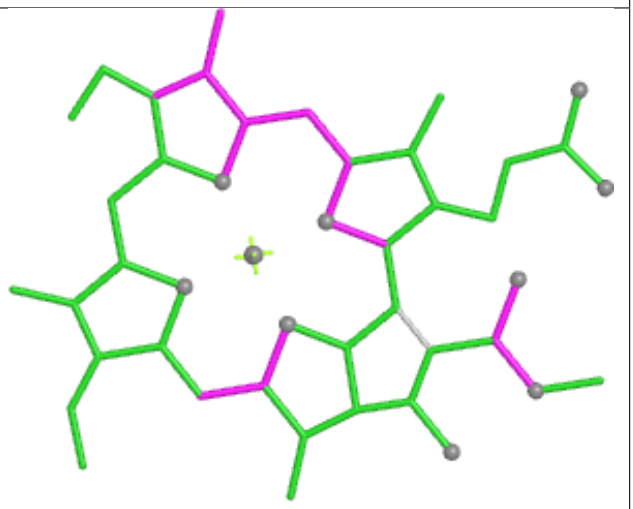


Rings

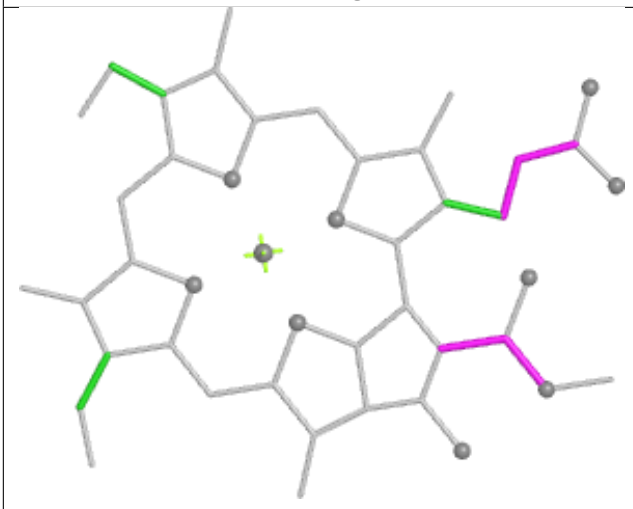
Ligand CLA H 304



Bond lengths



Bond angles

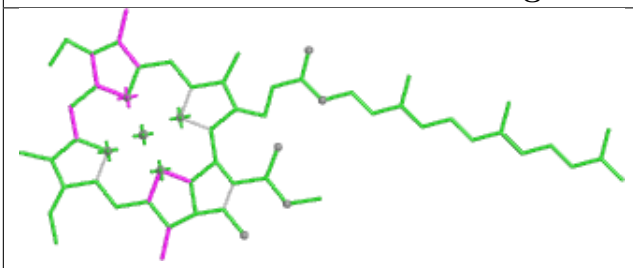


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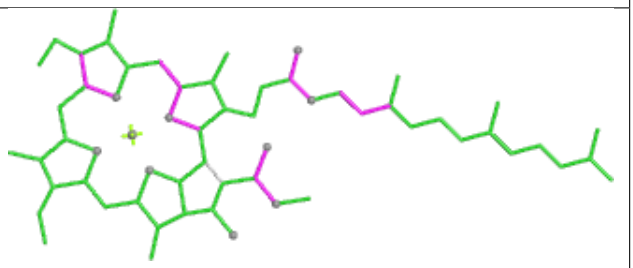


Rings

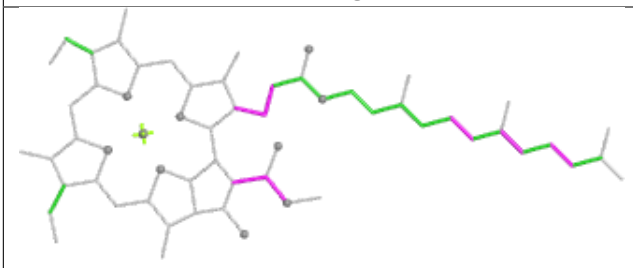
Ligand CLA O 310



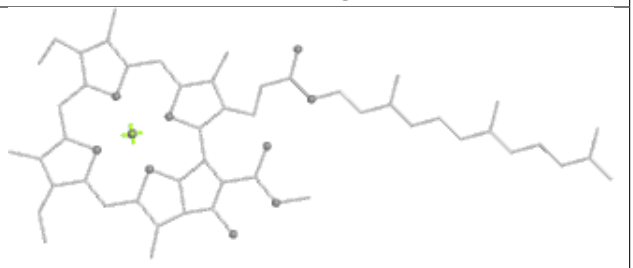
Bond lengths



Bond angles

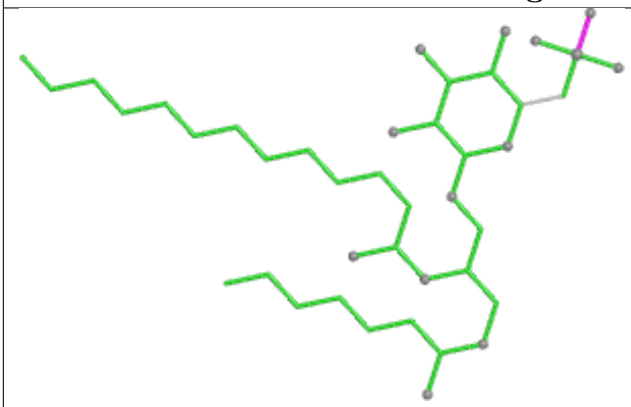


Torsions

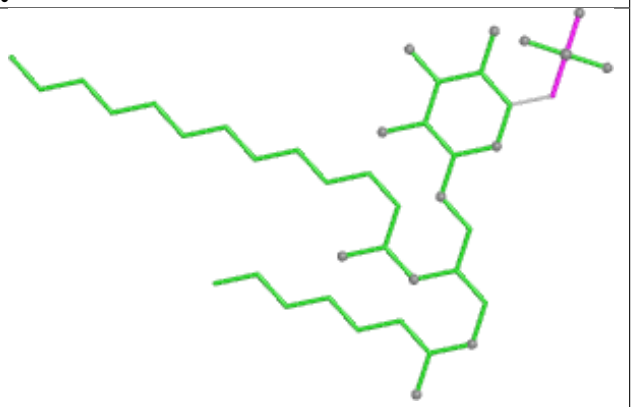


Rings

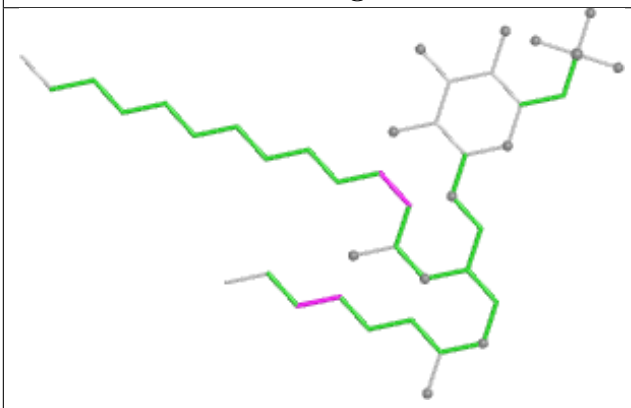
Ligand SQD F 407



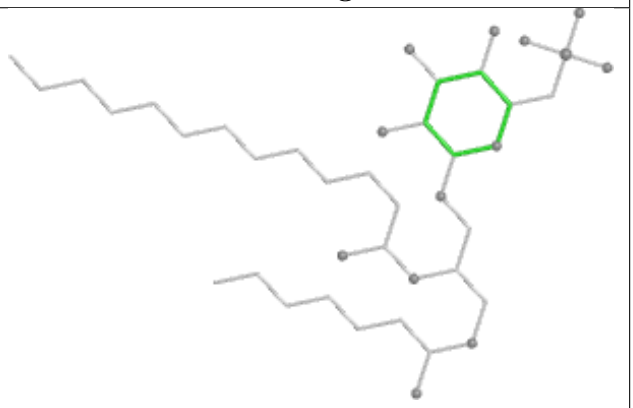
Bond lengths



Bond angles

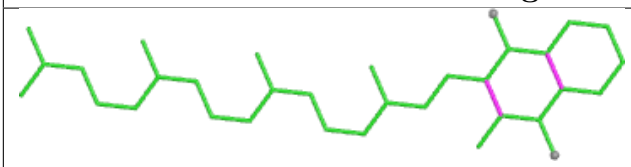


Torsions

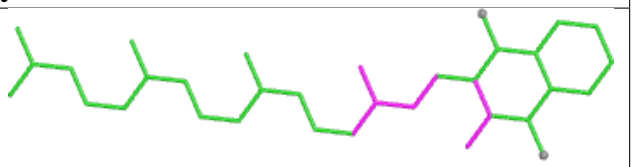


Rings

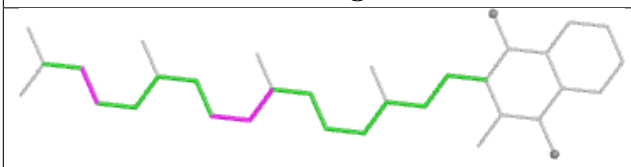
Ligand PQN A 843



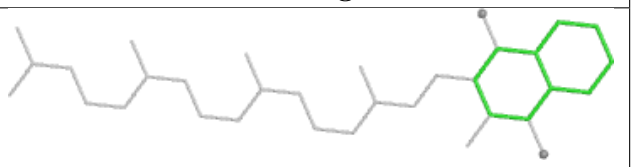
Bond lengths



Bond angles

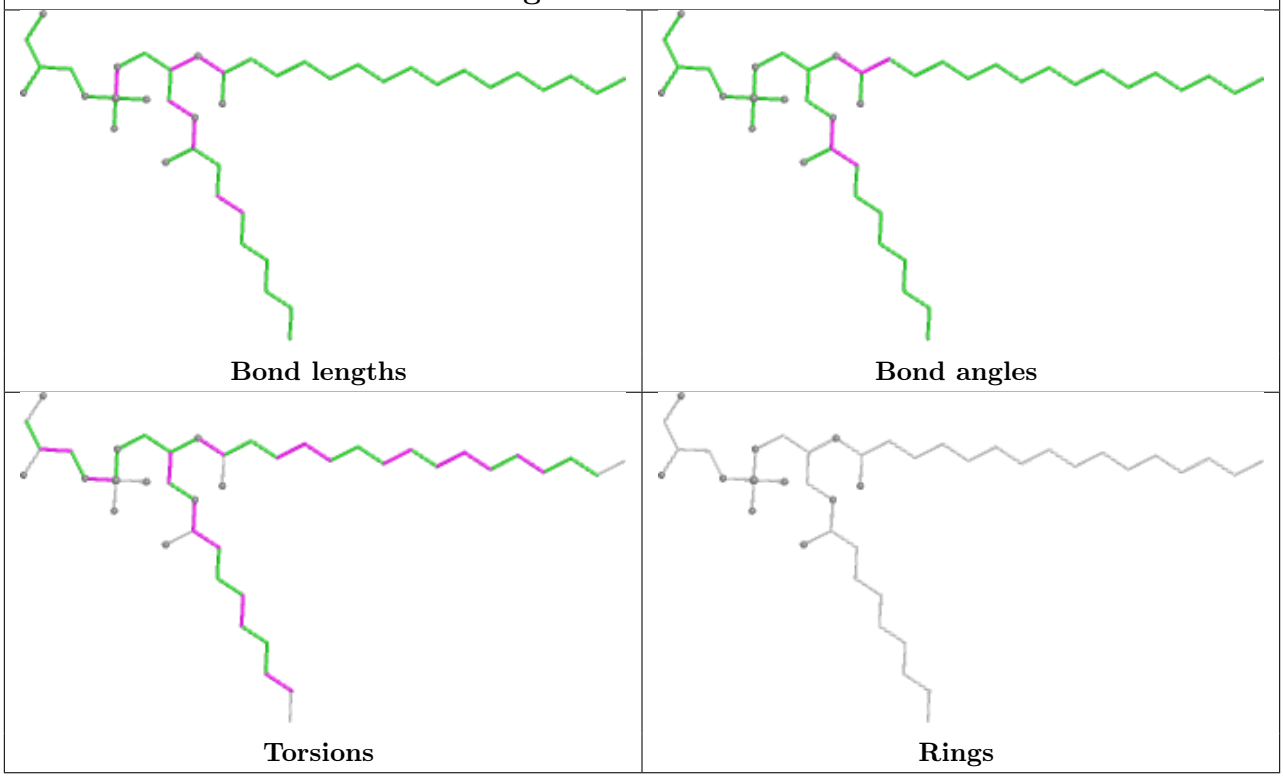


Torsions

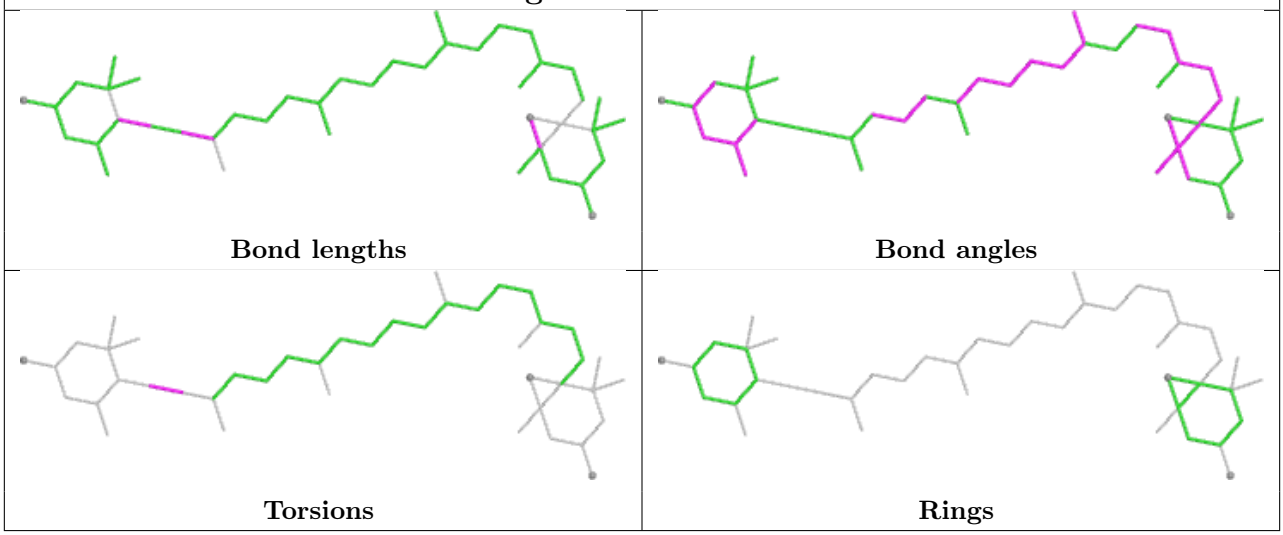


Rings

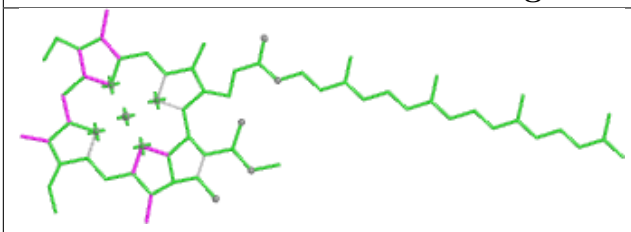
Ligand LHG R 614



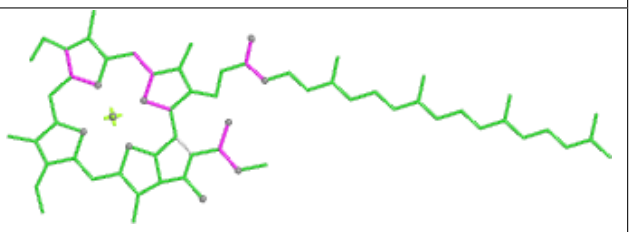
Ligand DD6 A 847



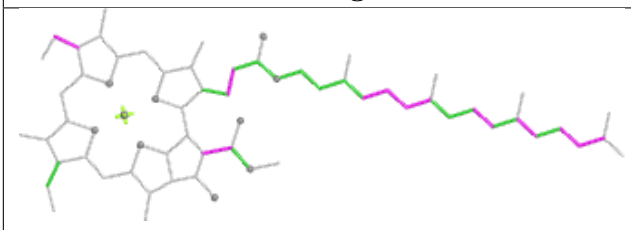
Ligand CLA B 807



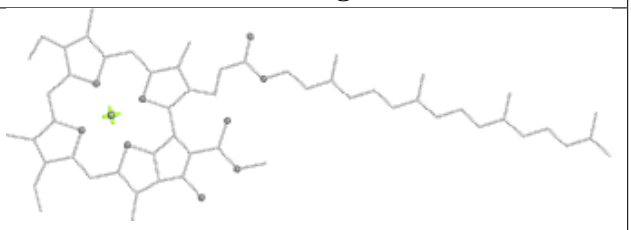
Bond lengths



Bond angles

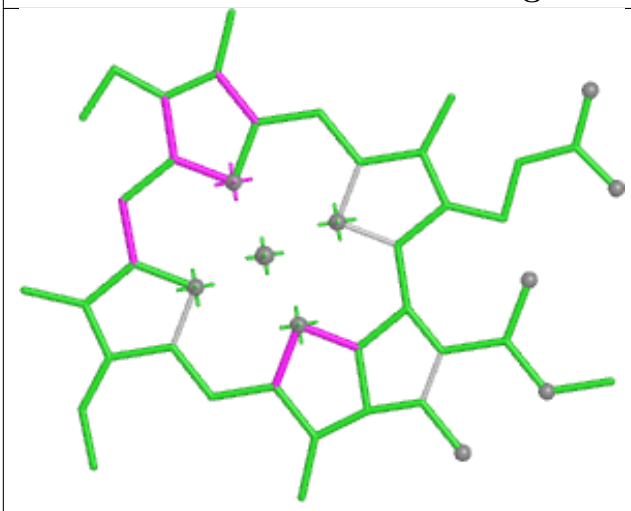


Torsions

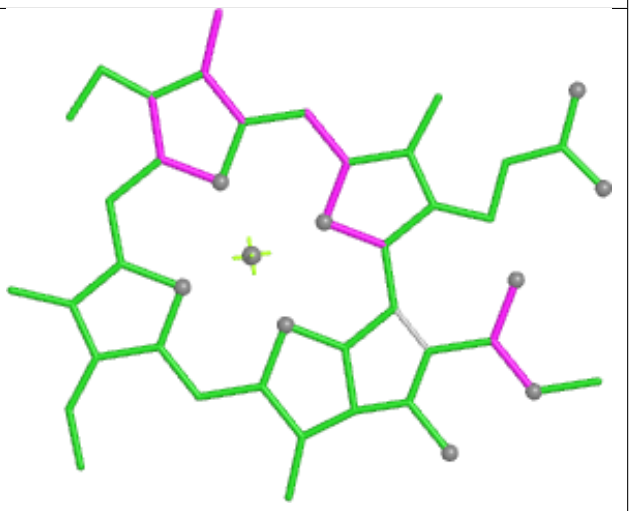


Rings

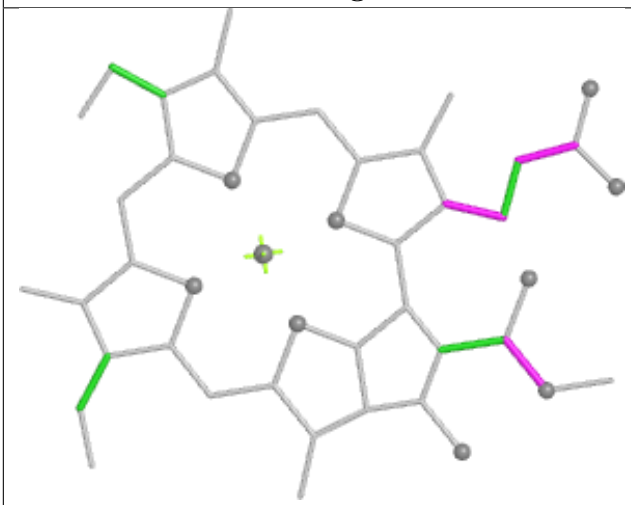
Ligand CLA H 318



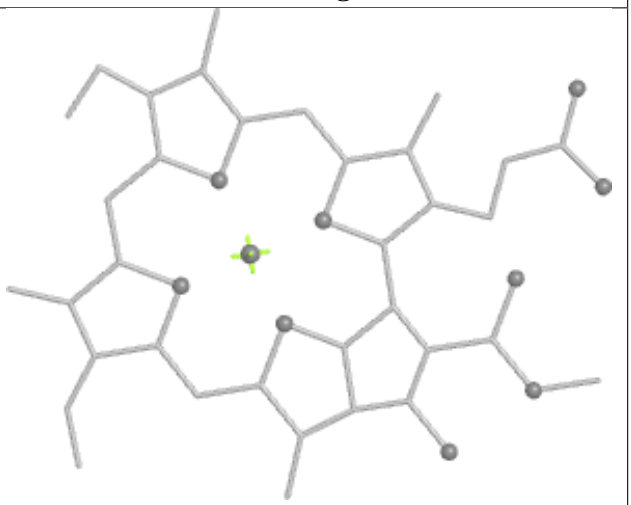
Bond lengths



Bond angles

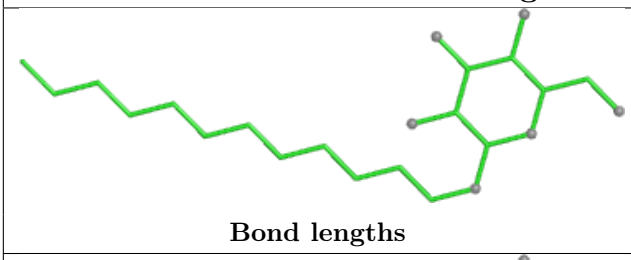


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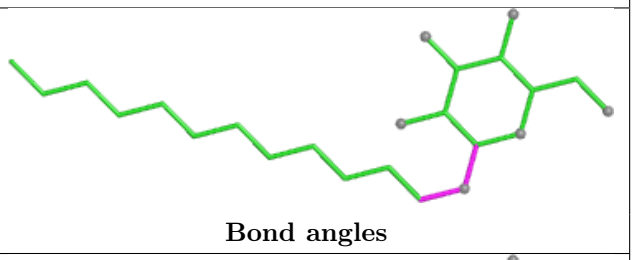


Rings

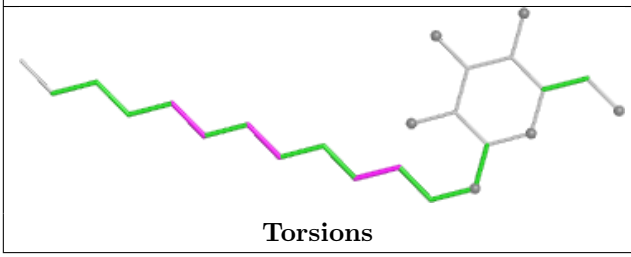
Ligand LMU B 854



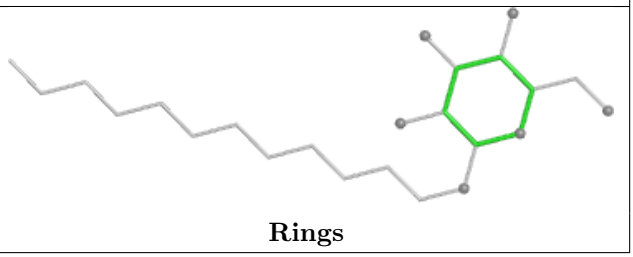
Bond lengths



Bond angles

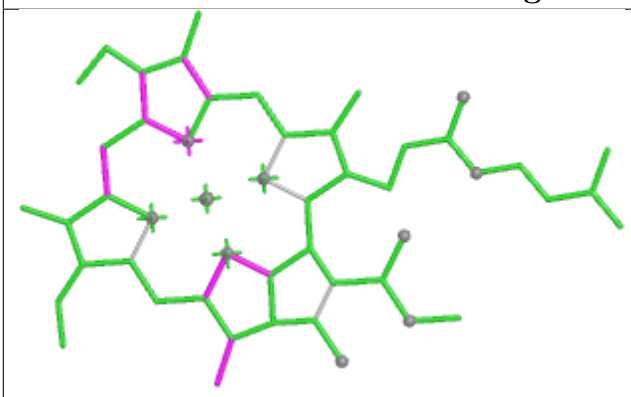


Torsions

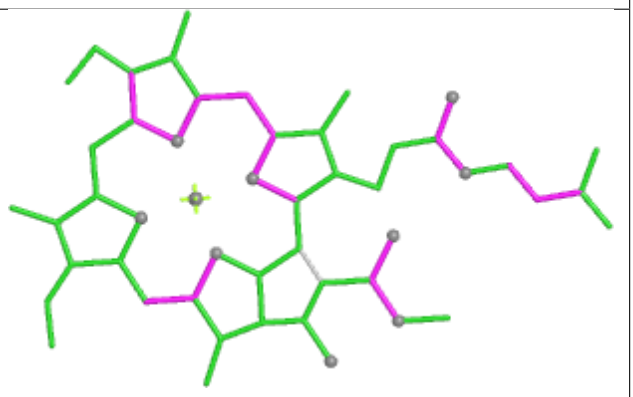


Rings

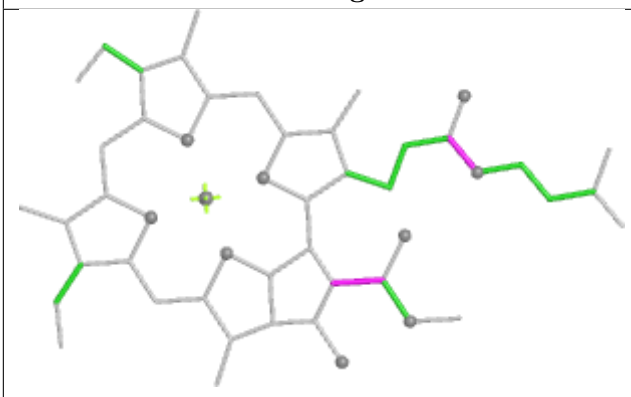
Ligand CLA O 305



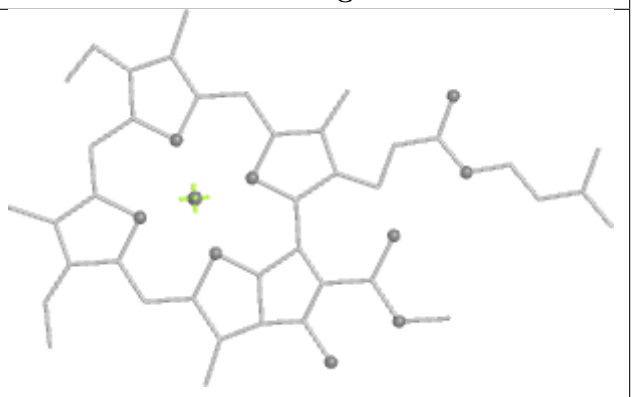
Bond lengths



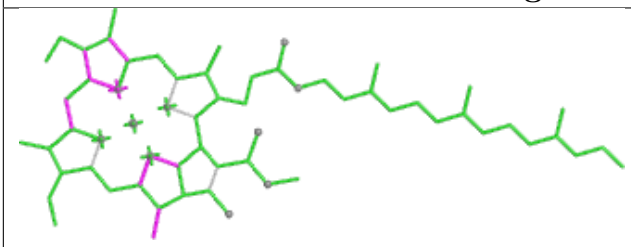
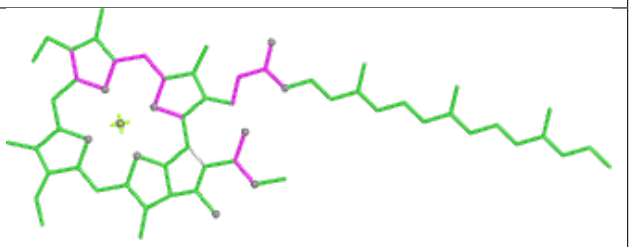
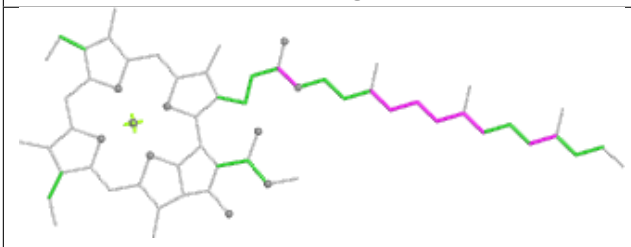
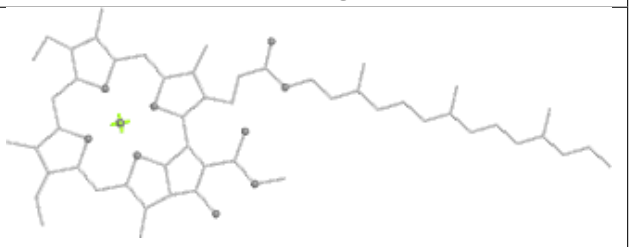
Bond angles

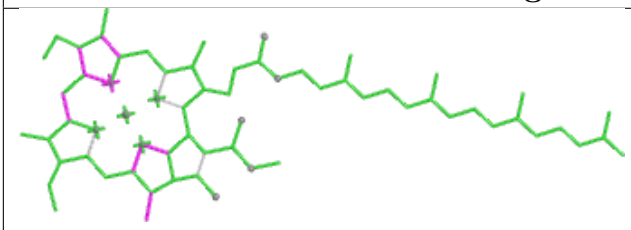
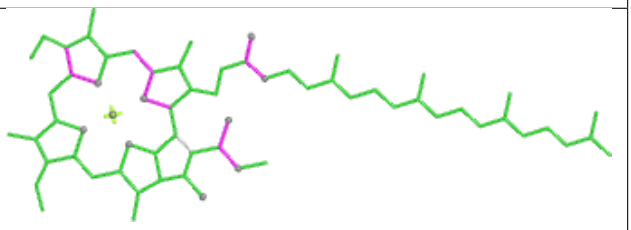
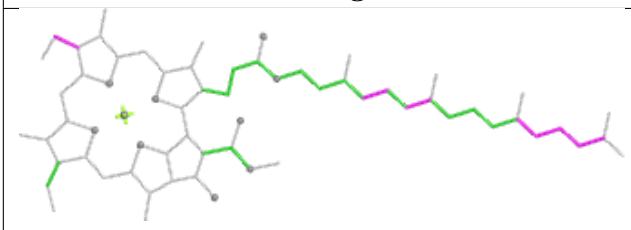
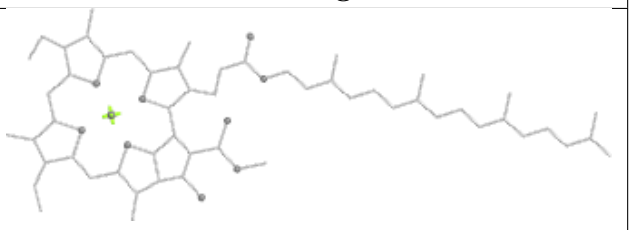


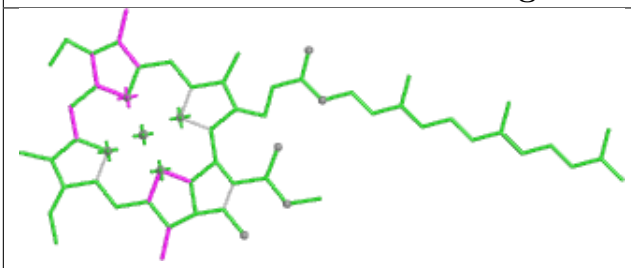
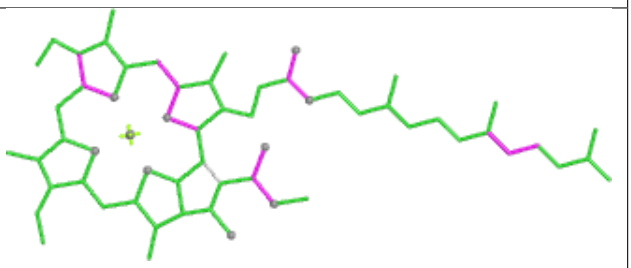
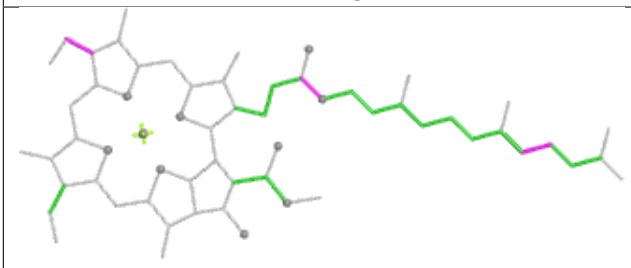
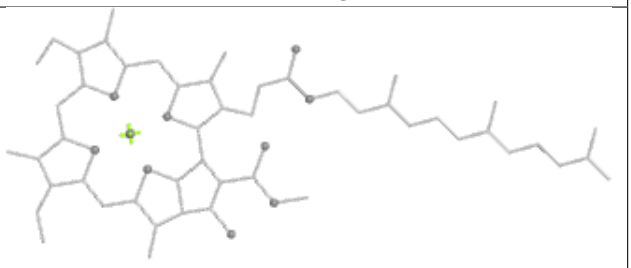
Torsions



Rings

Ligand CLA B 832	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 412	
 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.

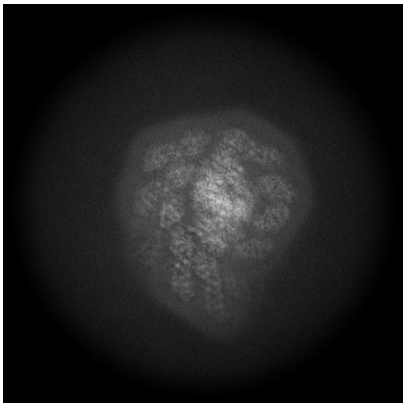
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-63994. These allow visual inspection of the internal detail of the map and identification of artifacts.

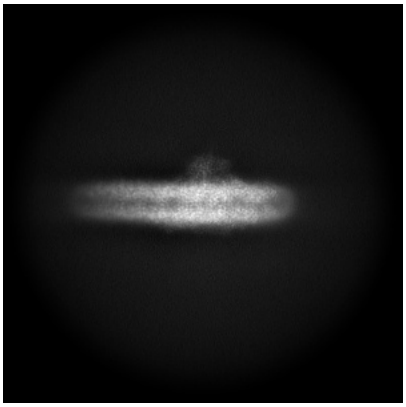
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

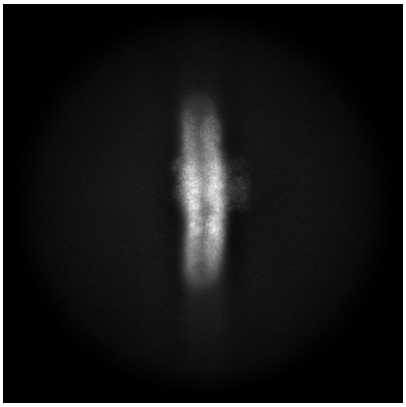
6.1.1 Primary map



X



Y

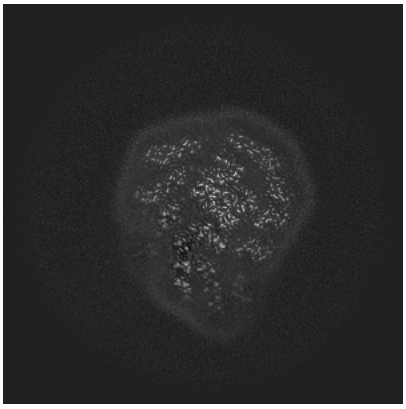


Z

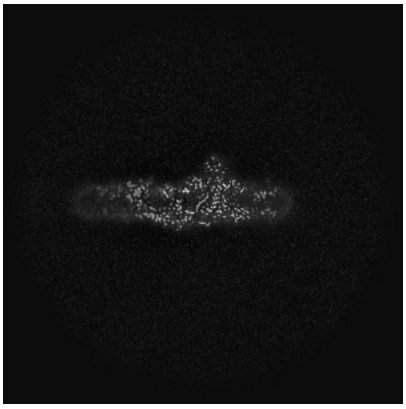
The images above show the map projected in three orthogonal directions.

6.2 Central slices

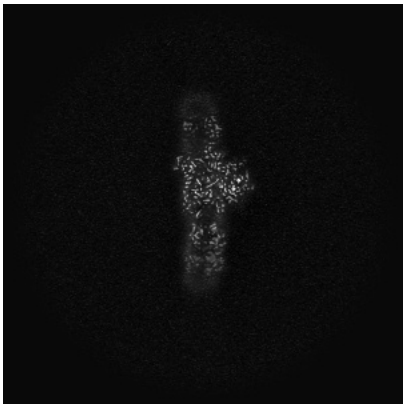
6.2.1 Primary map



X Index: 256



Y Index: 256

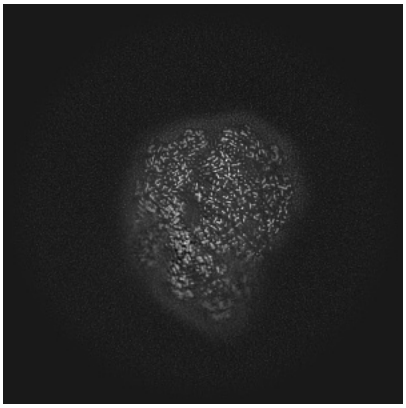


Z Index: 256

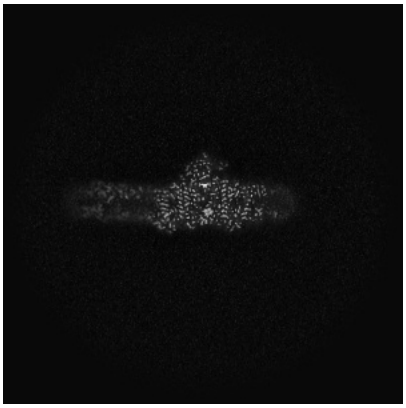
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

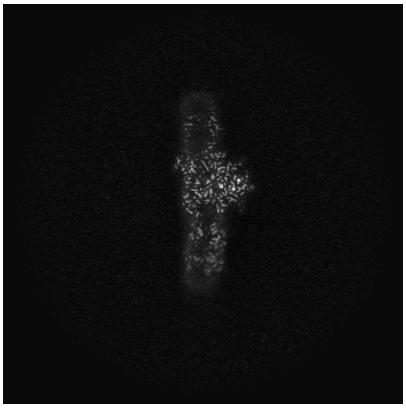
6.3.1 Primary map



X Index: 270



Y Index: 278

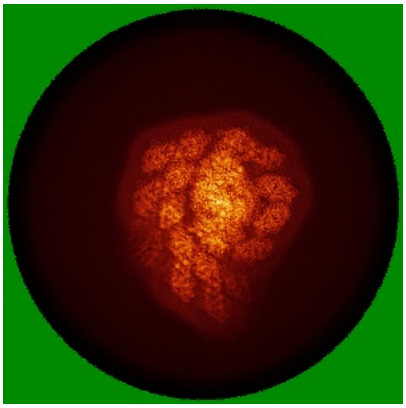


Z Index: 257

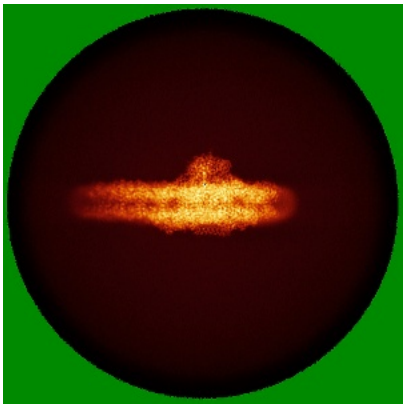
The images above show the largest variance slices of the map in three orthogonal directions.

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

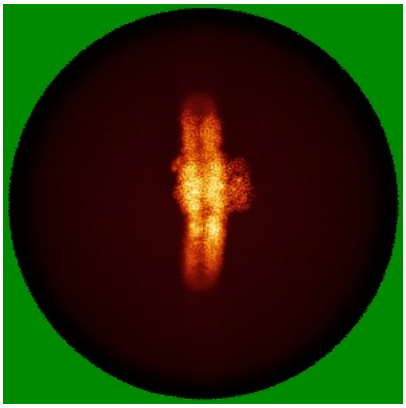
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

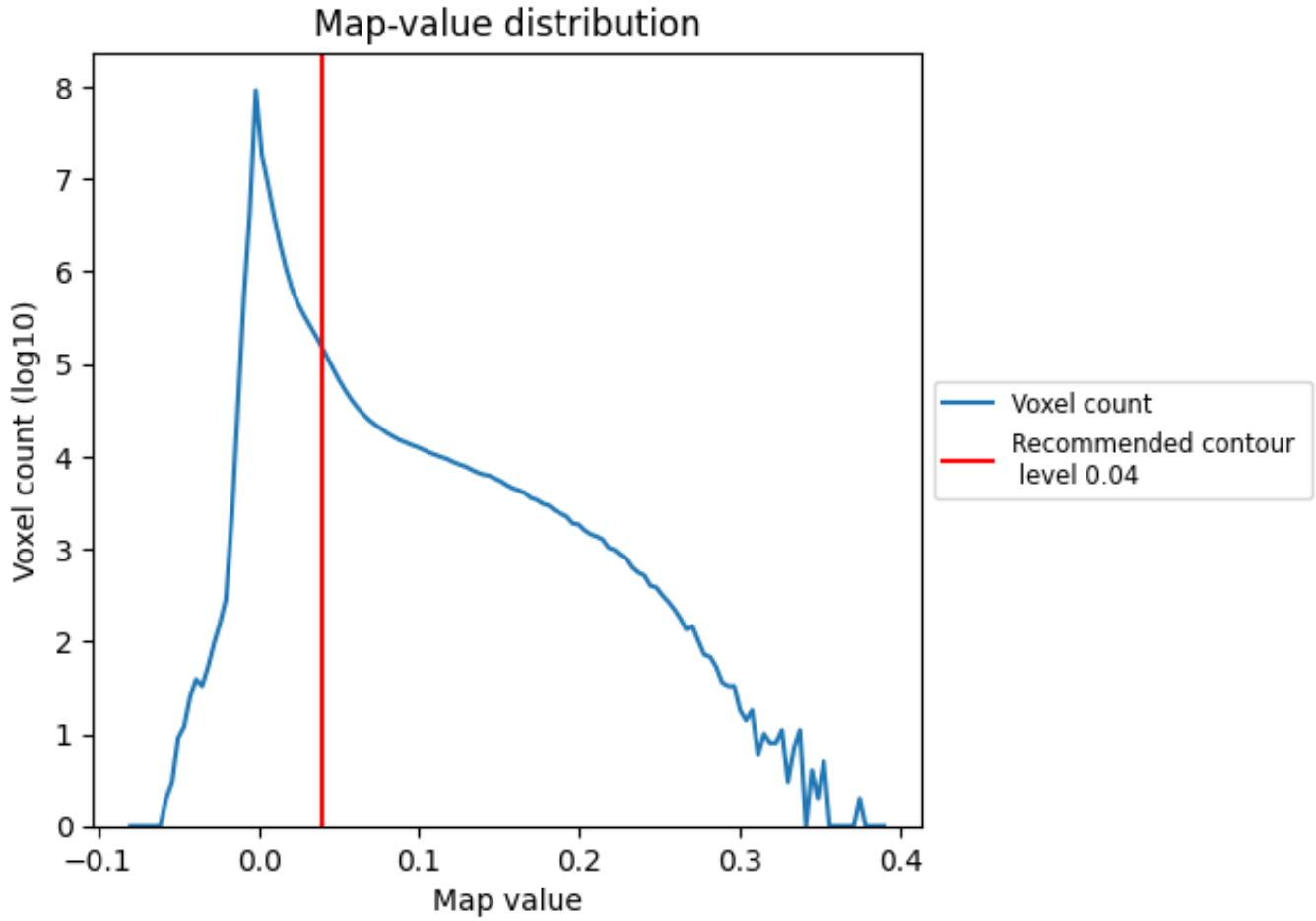
6.6 Mask visualisation (i)

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

7 Map analysis

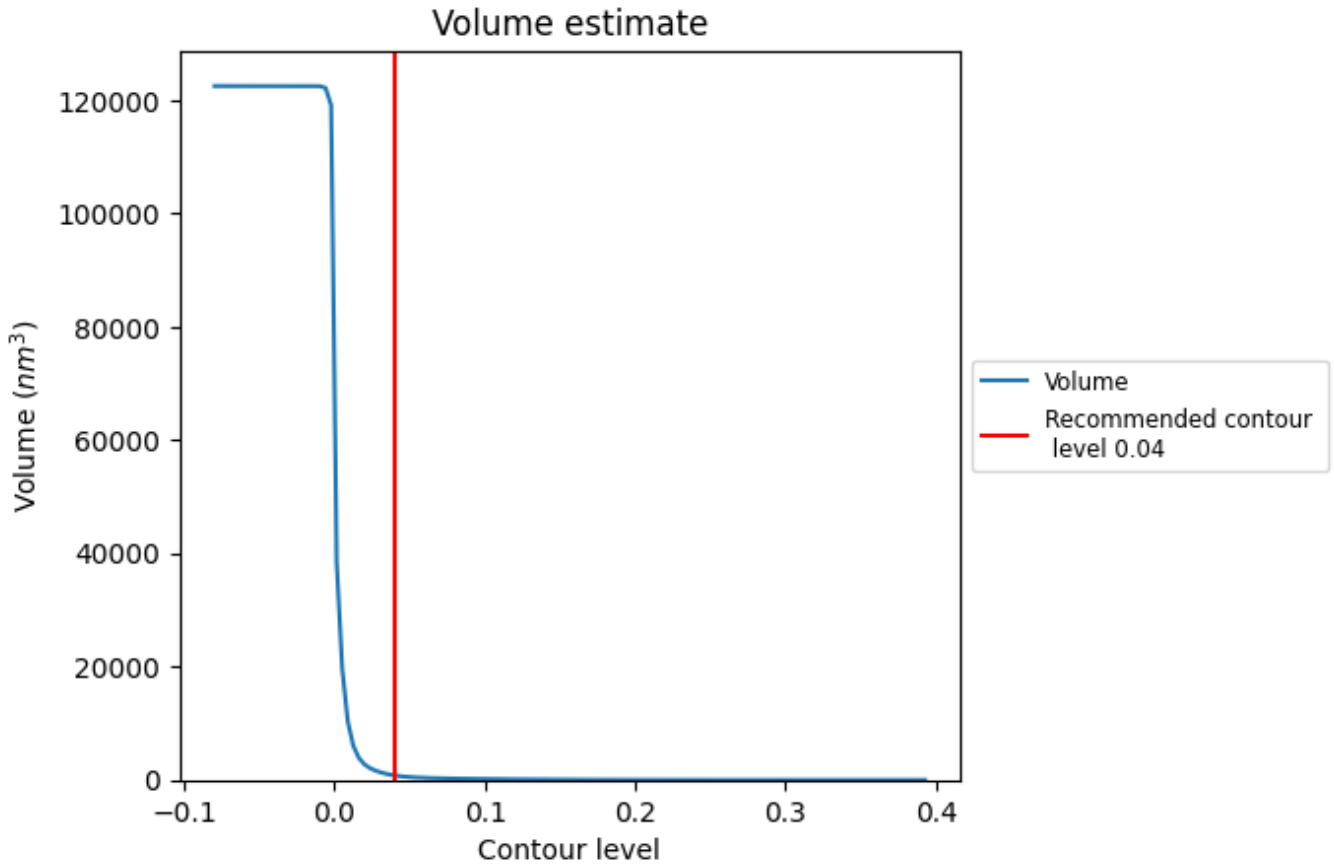
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

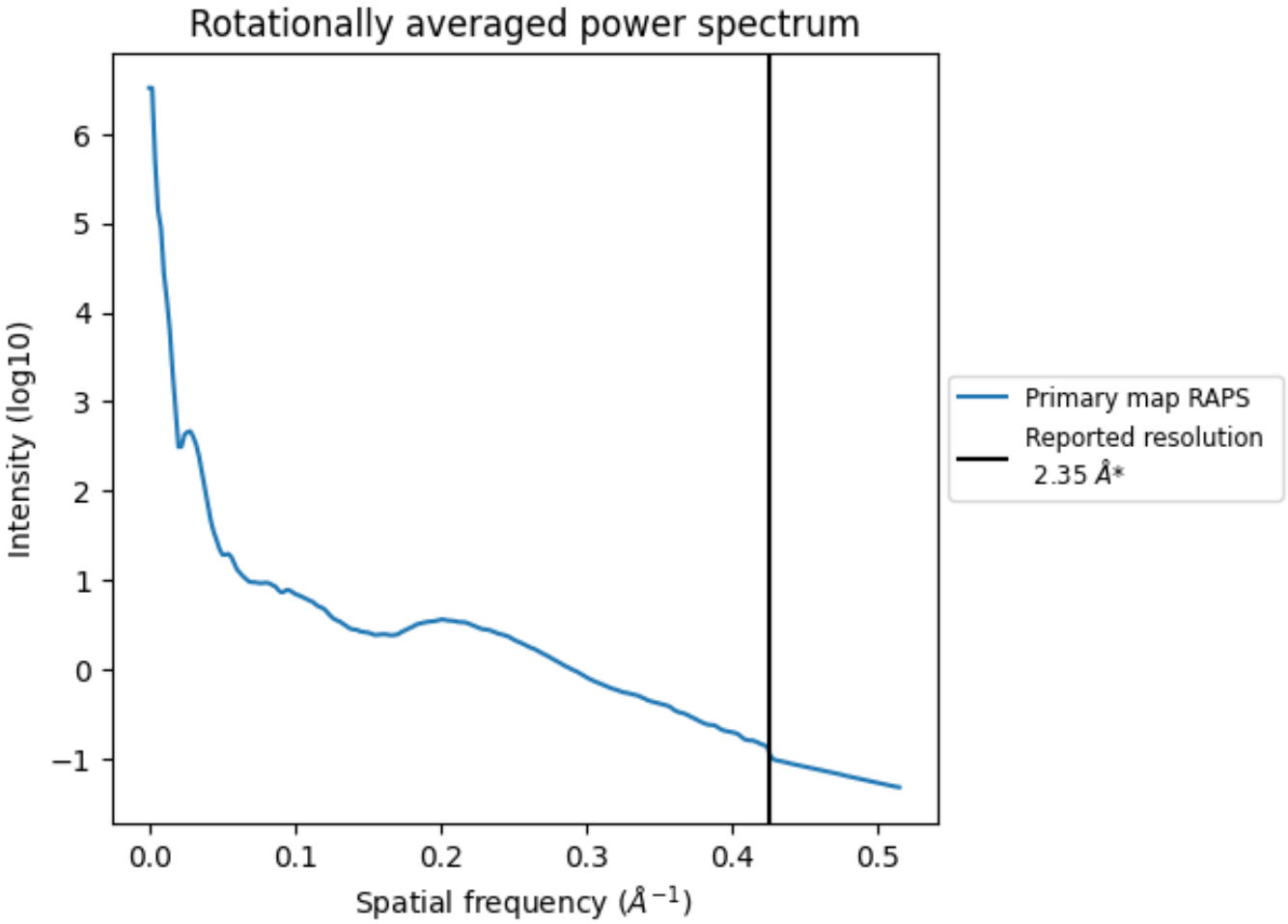
7.2 Volume estimate



The volume at the recommended contour level is 801 nm^3; this corresponds to an approximate mass of 724 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)

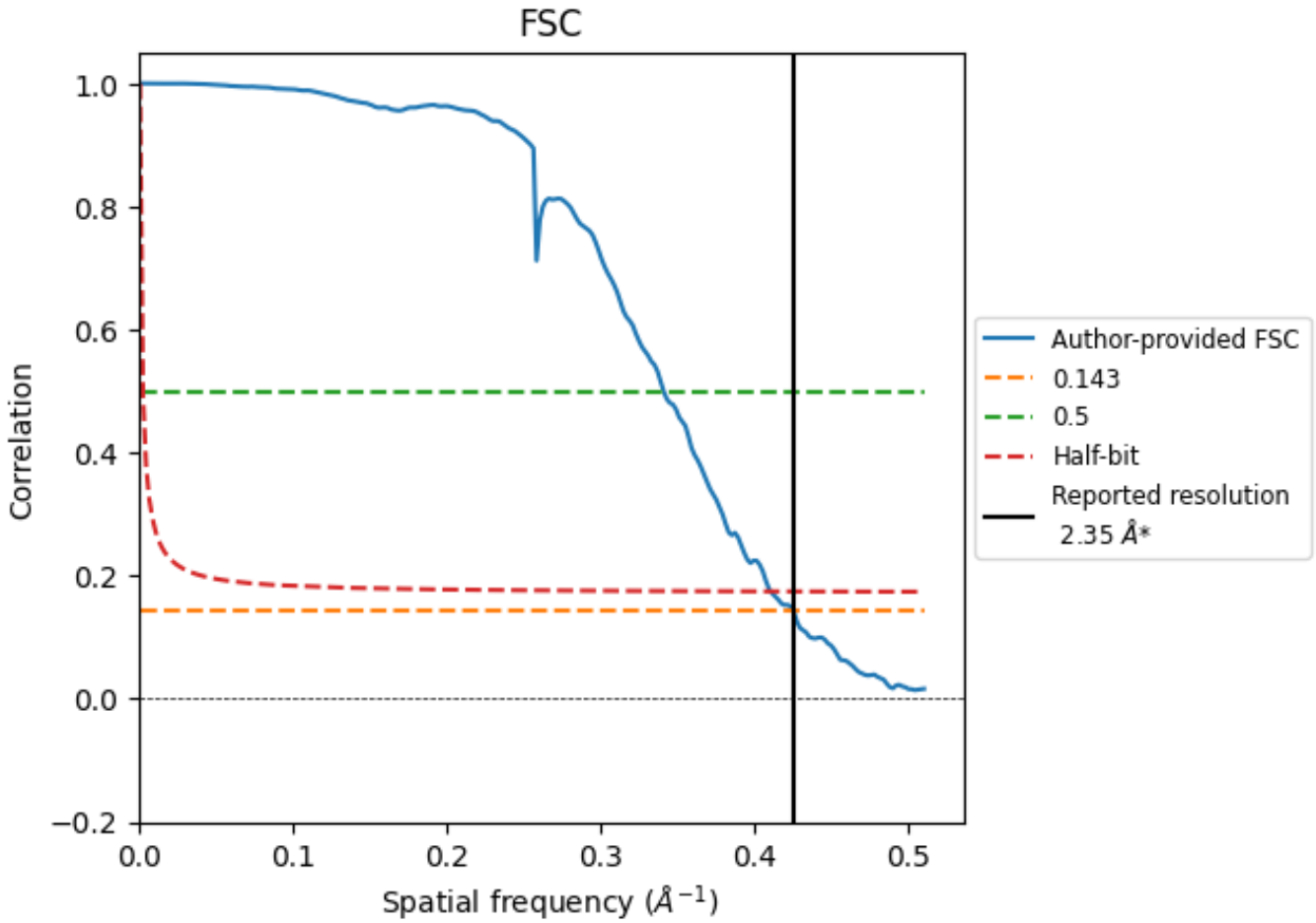


*Reported resolution corresponds to spatial frequency of 0.426 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.426 $Å^{-1}$

8.2 Resolution estimates (i)

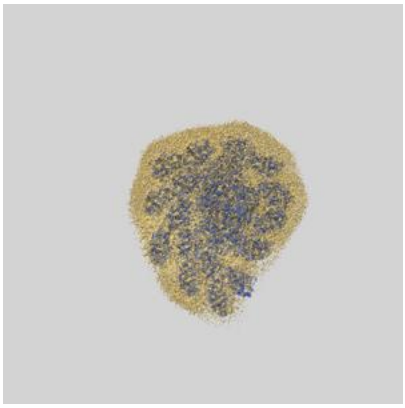
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.35	2.93	2.43
Unmasked-calculated*	-	-	-

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

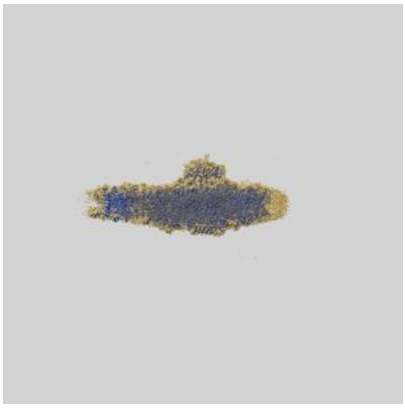
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63994 and PDB model 9UAS. Per-residue inclusion information can be found in section 3 on page 35.

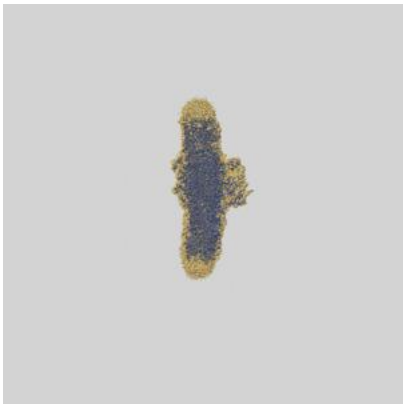
9.1 Map-model overlay



X



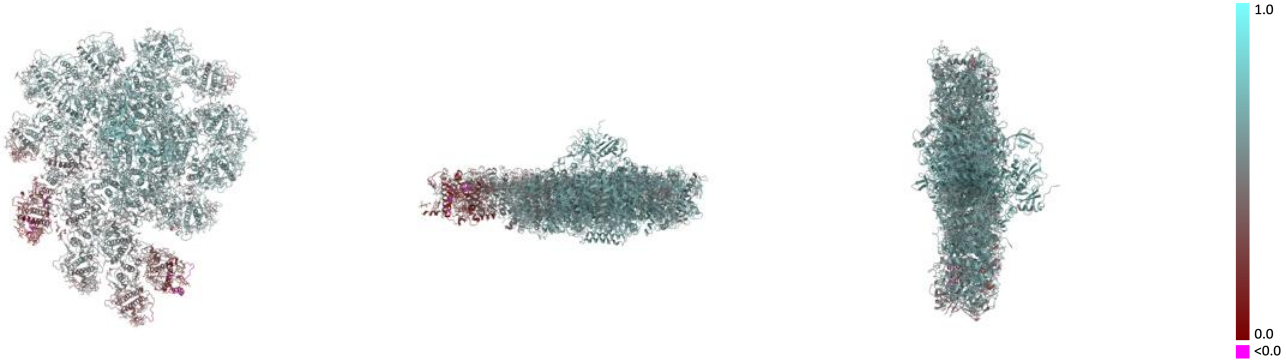
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

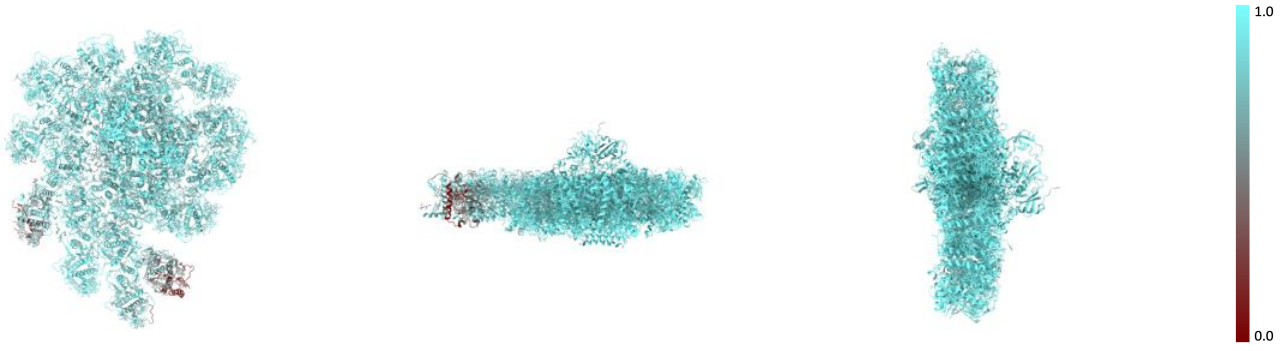
9.2 Q-score mapped to coordinate model



X Y Z

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

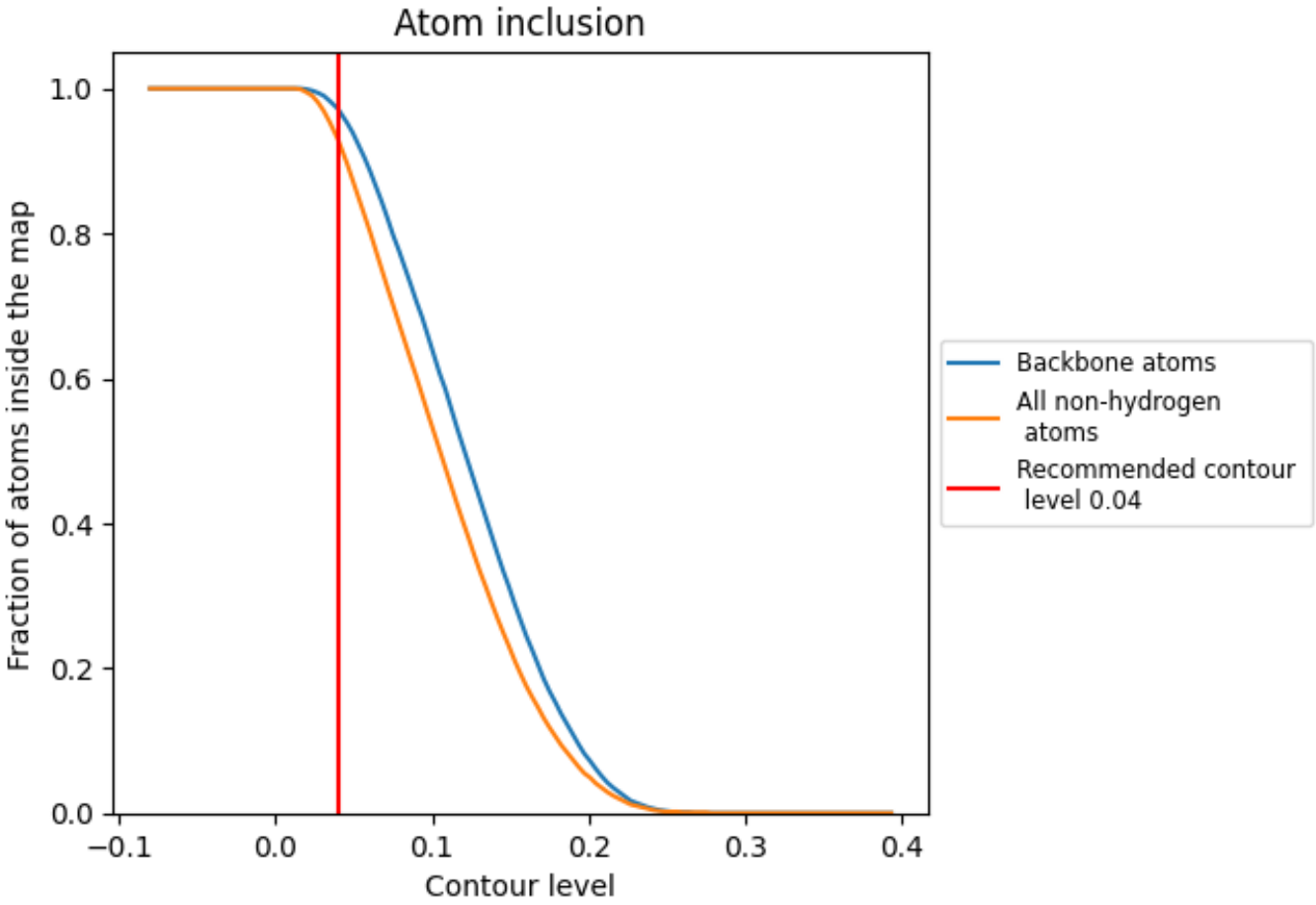
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.5550
A	0.9840	0.6580
B	0.9780	0.6190
C	0.9970	0.6770
D	0.9510	0.6400
E	0.9560	0.6350
F	0.9620	0.6150
G	0.9560	0.5620
H	0.9670	0.5870
I	0.9400	0.4830
J	0.9420	0.6280
K	0.9690	0.6110
L	0.9710	0.5060
M	0.9840	0.5760
N	0.9490	0.4660
O	0.9660	0.4920
P	0.7790	0.3540
Q	0.9570	0.5030
R	0.4970	0.2490
S	0.9380	0.5600
T	0.9500	0.6030
U	0.9200	0.5570
V	0.6770	0.2230
W	0.9550	0.6060
X	0.9420	0.6030

