Full wwPDB EM Validation Report ⓘ

Oct 12, 2026 – 03:16 PM JST

PDB ID	:	9X4O / pdb_00009x4o
EMDB ID	:	EMD-66561
Title	:	photosystem I with eight LHCI from a green alga as lichen phycobiont
Authors	:	Su, X.D.; Wei, X.L.; Li, M.
Deposited on	:	2025-10-11
Resolution	:	2.95 Å(reported)

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

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

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

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

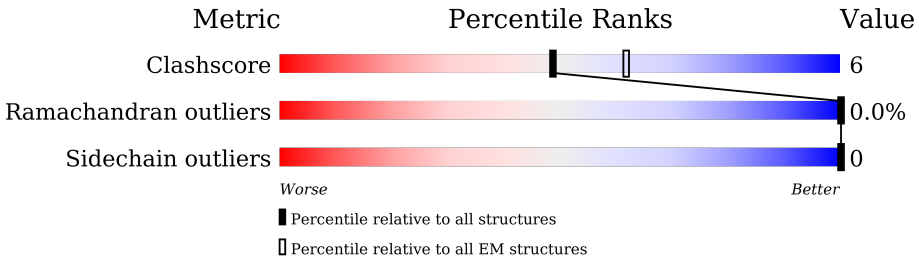
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

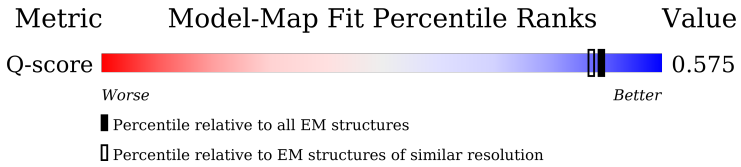
1 Overall quality at a glance

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

The reported resolution of this entry is 2.95 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.





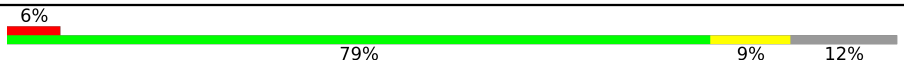
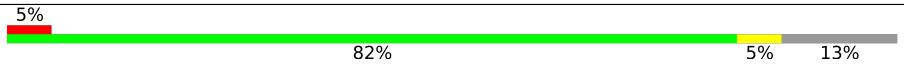
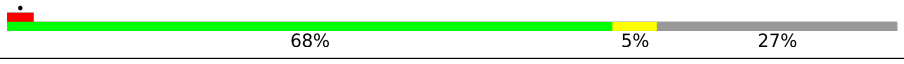
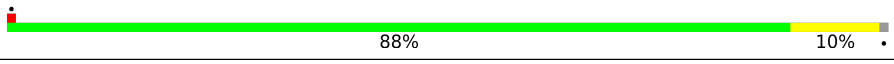
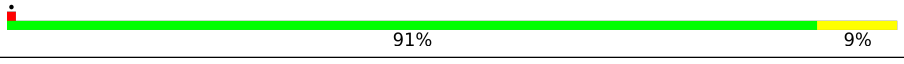
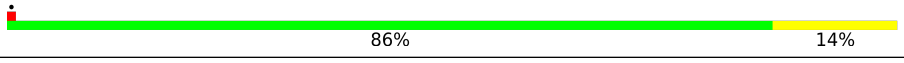
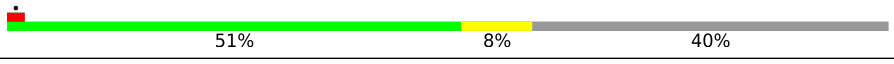
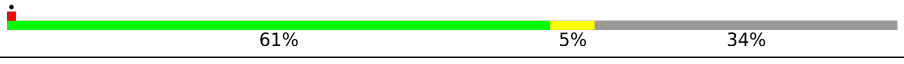
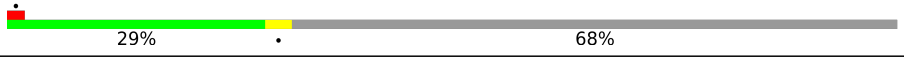
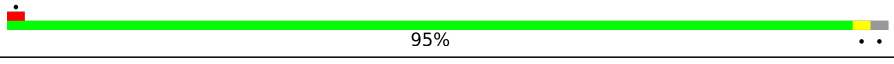
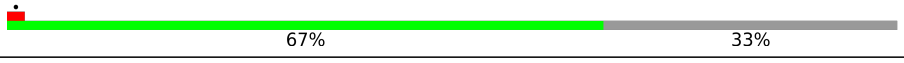
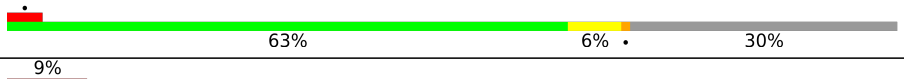
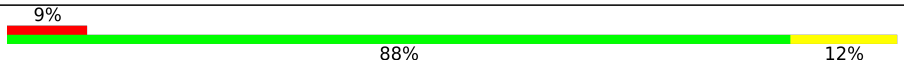
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13114 (2.45 - 3.45)

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	1	248	16% 69% 8% 23%
2	2	270	22% 71% 7% 22%
3	3	308	65% 8% 28%
4	5	271	77% 8% 15%

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Mol	Chain	Length	Quality of chain
5	6	266	
6	7	279	
7	8	263	
8	9	249	
9	A	751	
10	B	734	
11	C	81	
12	D	239	
13	E	111	
14	F	250	
15	G	163	
16	H	126	
17	I	106	
18	J	41	
19	K	126	
20	L	176	
21	M	32	

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 46832 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 Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	192	Total	C	N	O	S	0	0
			1435	928	236	267	4		

- Molecule 2 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	210	Total	C	N	O	S	0	0
			1590	1027	262	294	7		

- Molecule 3 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	223	Total	C	N	O	S	0	0
			1756	1147	286	321	2		

- Molecule 4 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	230	Total	C	N	O	S	0	0
			1791	1158	304	323	6		

- Molecule 5 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	234	Total	C	N	O	S	0	0
			1794	1170	300	318	6		

- Molecule 6 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	221	Total	C	N	O	S	0	0
			1732	1126	291	312	3		

- Molecule 7 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	230	Total	C	N	O	S	0	0
			1758	1142	293	320	3		

- Molecule 8 is a protein called Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	182	Total	C	N	O	S	0	0
			1427	925	240	258	4		

- Molecule 9 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	741	Total	C	N	O	S	0	0
			5834	3819	995	1002	18		

- Molecule 10 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	734	Total	C	N	O	S	0	0
			5822	3823	984	1003	12		

- Molecule 11 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	81	Total	C	N	O	S	0	0
			608	374	104	117	13		

- Molecule 12 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	143	Total	C	N	O	S	0	0
			1120	717	198	200	5		

- Molecule 13 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	E	62	Total	C	N	O	0	0
			484	309	86	89		

- Molecule 14 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	165	Total	C	N	O	S	0	0
			1269	813	224	229	3		

- Molecule 15 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	G	92	Total	C	N	O	0	0
			681	431	120	130		

- Molecule 16 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	H	56	Total	C	N	O	0	0
			427	275	80	72		

- Molecule 17 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	34	Total	C	N	O	S	0	0
			256	176	36	43	1		

- Molecule 18 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	40	Total	C	N	O	S	0	0
			326	222	46	57	1		

- Molecule 19 is a protein called PsaK.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	K	84	Total	C	N	O	0	0
			595	380	100	115		

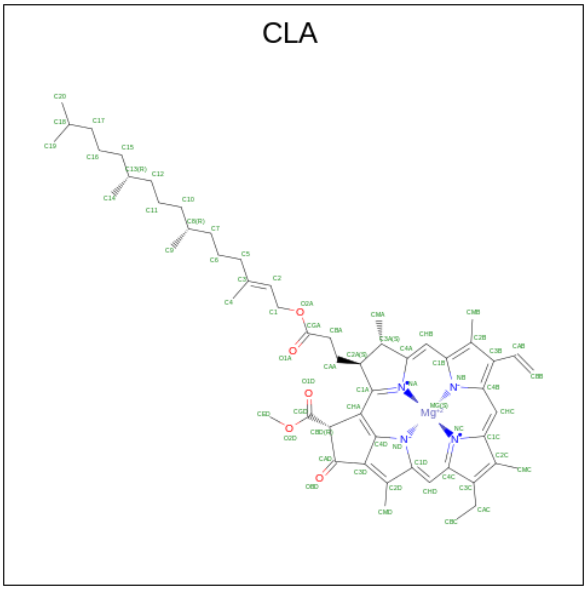
- Molecule 20 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	123	Total	C	N	O	S	0	0
			897	586	147	162	2		

- Molecule 21 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	32	Total	C	N	O	S	0	0
			246	163	38	44	1		

- 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	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
22	2	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
22	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
22	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			59	50	1	4	4	
22	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
22	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	6	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
22	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
22	7	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
22	8	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
22	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
22	9	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
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	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			52	42	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
			64	54	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
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			64	54	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
			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
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			56	46	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
			46	36	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
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	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
22	A	1	Total	C	Mg	N	O	0
			50	40	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
			50	40	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	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			60	50	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
			45	35	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
			55	45	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
			42	34	1	4	3	
22	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
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	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			56	46	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
			41	33	1	4	3	
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
			59	49	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
			63	53	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			57	48	1	4	4	
22	B	1	Total	C	Mg	N	O	0
			53	43	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
			55	45	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
			54	45	1	4	4	
22	B	1	Total	C	Mg	N	O	0
			59	49	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
			45	35	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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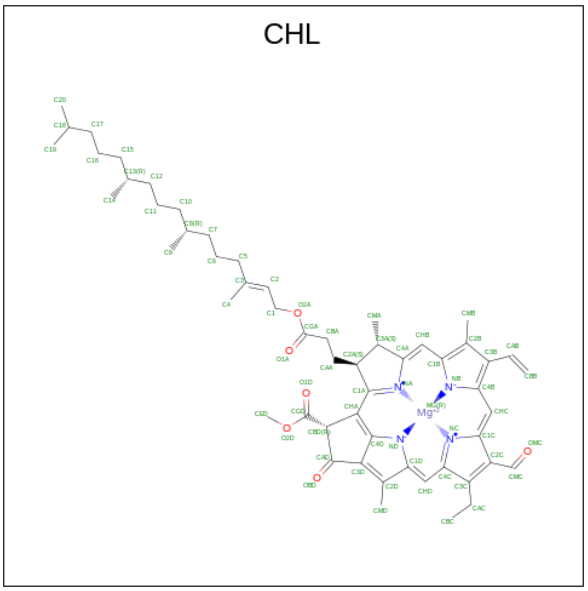
Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
22	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			55	45	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
			50	40	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
			47	37	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	F	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	F	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	G	1	Total	C	Mg	N	O	0
			55	45	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
			35	29	1	4	1	
22	H	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
22	H	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	K	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
22	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	L	1	Total	C	Mg	N	O	0
			50	40	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
			37	31	1	4	1	

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



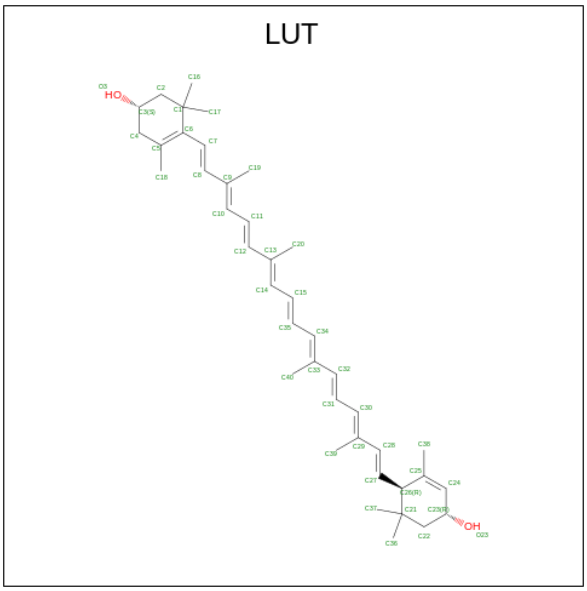
Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			54	43	1	4	6	

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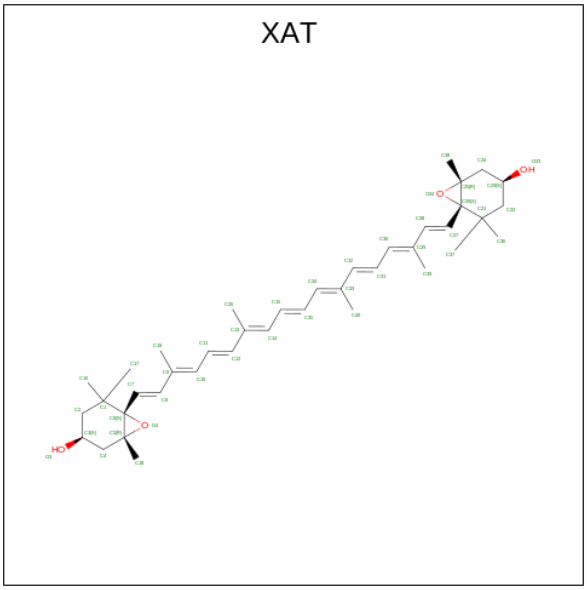
Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	8	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 24 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
24	1	1	Total C O 42 40 2	0
24	2	1	Total C O 42 40 2	0
24	3	1	Total C O 42 40 2	0
24	3	1	Total C O 42 40 2	0
24	5	1	Total C O 42 40 2	0
24	6	1	Total C O 42 40 2	0
24	7	1	Total C O 42 40 2	0
24	8	1	Total C O 42 40 2	0
24	9	1	Total C O 42 40 2	0

- Molecule 25 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



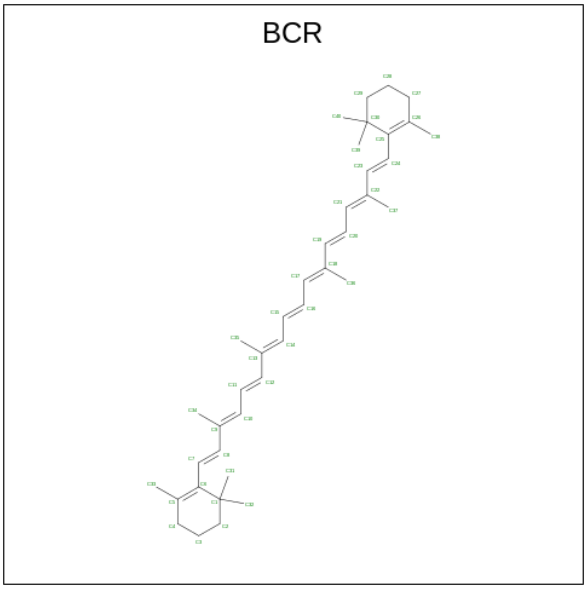
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C O 44 40 4	0
25	2	1	Total C O 44 40 4	0

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Mol	Chain	Residues	Atoms	AltConf
25	3	1	Total C O 44 40 4	0
25	5	1	Total C O 44 40 4	0
25	6	1	Total C O 44 40 4	0
25	7	1	Total C O 44 40 4	0
25	8	1	Total C O 44 40 4	0
25	9	1	Total C O 44 40 4	0

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
26	1	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	5	1	Total C 40 40	0
26	7	1	Total C 40 40	0

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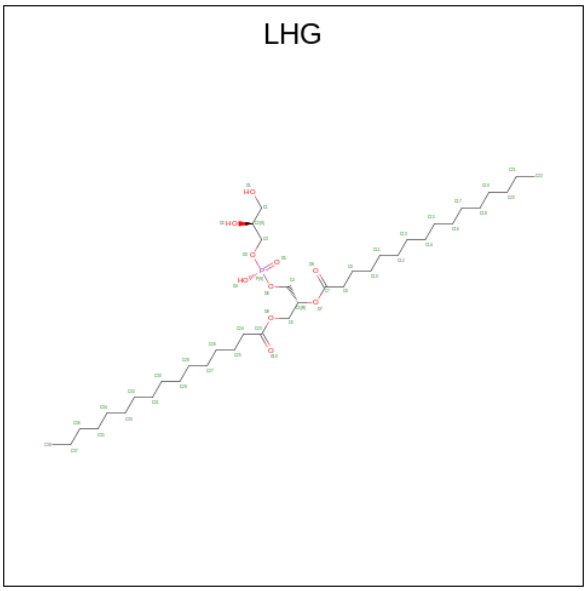
Mol	Chain	Residues	Atoms	AltConf
26	8	1	Total C 40 40	0
26	9	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	I	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	M	1	Total C 40 40	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



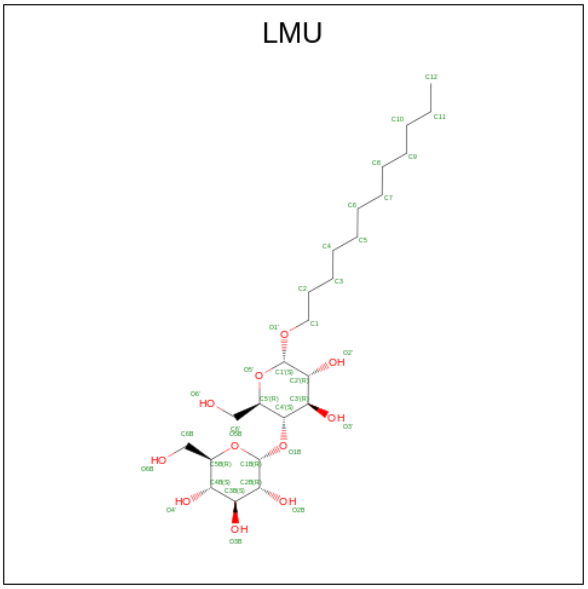
Mol	Chain	Residues	Atoms	AltConf
27	1	1	Total C O P 49 38 10 1	0
27	1	1	Total C O P 26 15 10 1	0
27	2	1	Total C O P 40 29 10 1	0
27	5	1	Total C O P 36 25 10 1	0
27	5	1	Total C O P 36 25 10 1	0
27	6	1	Total C O P 48 37 10 1	0
27	7	1	Total C O P 49 38 10 1	0
27	8	1	Total C O P 49 38 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
27	9	1	Total	C	O	P	0
			45	34	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			45	34	10	1	
27	B	1	Total	C	O	P	0
			37	26	10	1	
27	M	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 28 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



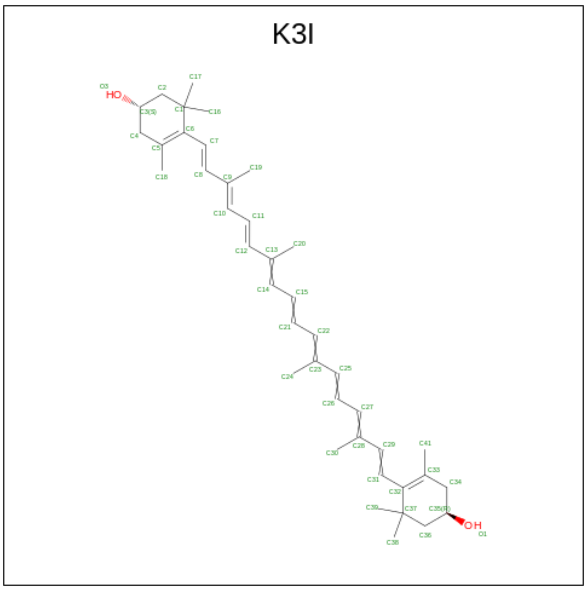
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			35	24	11	
28	3	1	Total	C	O	0
			28	17	11	
28	3	1	Total	C	O	0
			35	24	11	
28	3	1	Total	C	O	0
			35	24	11	
28	6	1	Total	C	O	0
			35	24	11	
28	6	1	Total	C	O	0
			33	22	11	

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Mol	Chain	Residues	Atoms	AltConf
28	6	1	Total C O 32 21 11	0
28	7	1	Total C O 35 24 11	0
28	9	1	Total C O 35 24 11	0
28	A	1	Total C O 30 19 11	0
28	A	1	Total C O 34 24 10	0
28	F	1	Total C O 29 18 11	0
28	G	1	Total C O 35 24 11	0
28	H	1	Total C O 35 24 11	0
28	J	1	Total C O 35 24 11	0
28	K	1	Total C O 35 24 11	0

- Molecule 29 is Zeaxanthin (CCD ID: K3I) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



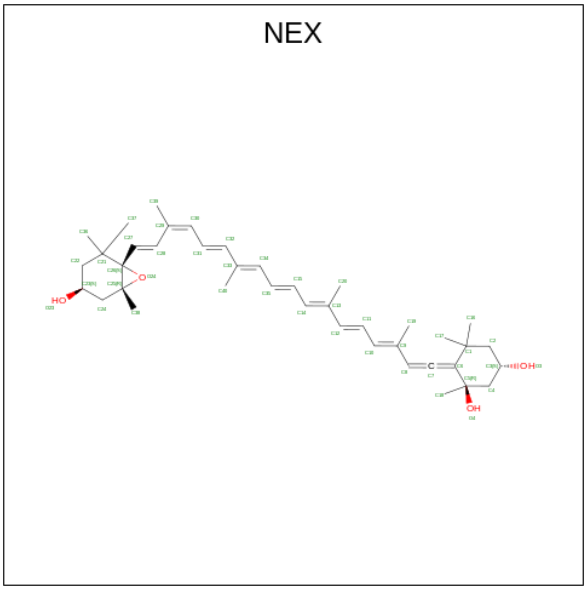
Mol	Chain	Residues	Atoms	AltConf
29	2	1	Total C O 42 40 2	0

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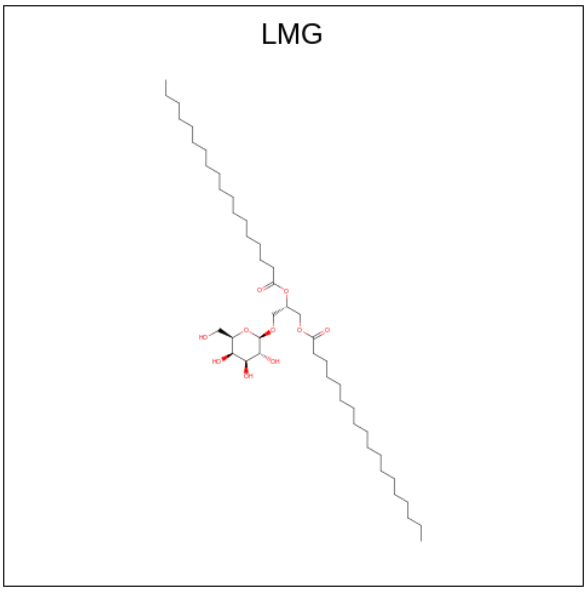
Mol	Chain	Residues	Atoms			AltConf
29	5	1	Total	C	O	0
			42	40	2	

- Molecule 30 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



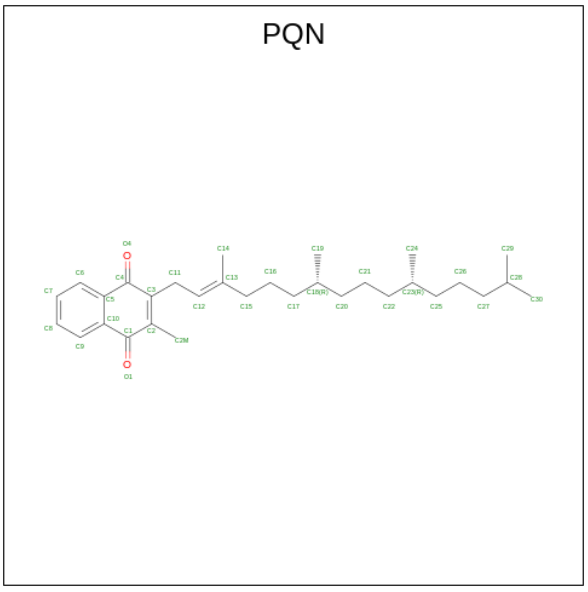
Mol	Chain	Residues	Atoms			AltConf
30	5	1	Total	C	O	0
			44	40	4	
30	6	1	Total	C	O	0
			44	40	4	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



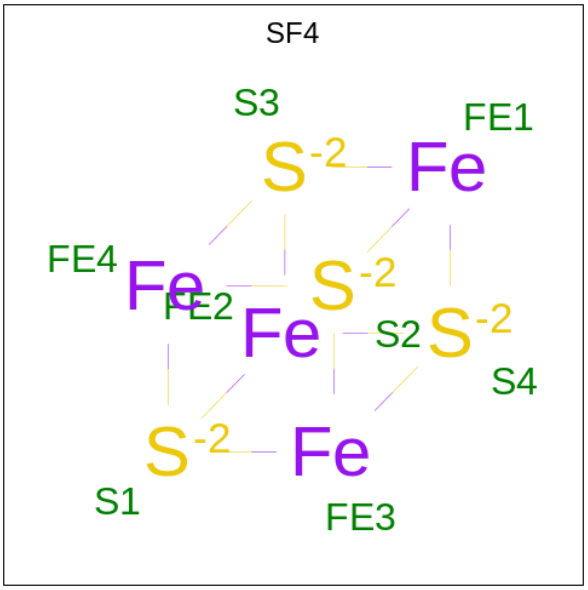
Mol	Chain	Residues	Atoms	AltConf
31	8	1	Total C O 25 17 8	0
31	9	1	Total C O 46 36 10	0
31	J	1	Total C O 42 32 10	0
31	J	1	Total C O 41 31 10	0

- Molecule 32 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



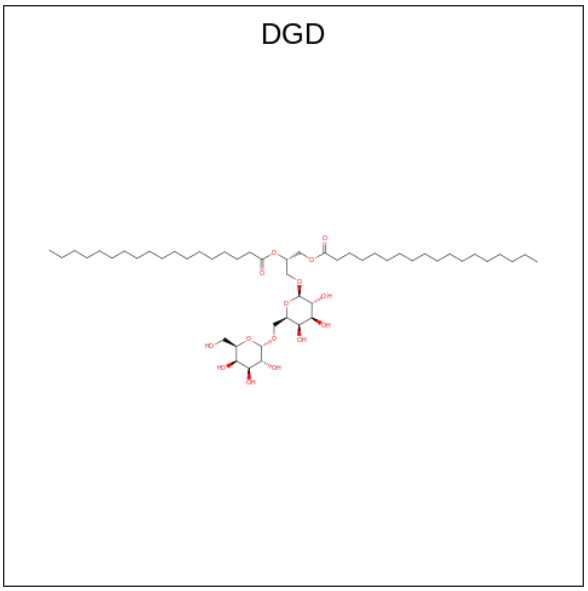
Mol	Chain	Residues	Atoms	AltConf
32	A	1	Total C O 33 31 2	0
32	B	1	Total C O 33 31 2	0

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total Fe S 8 4 4	0
33	C	1	Total Fe S 8 4 4	0
33	C	1	Total Fe S 8 4 4	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	B	1	58	43	15	0

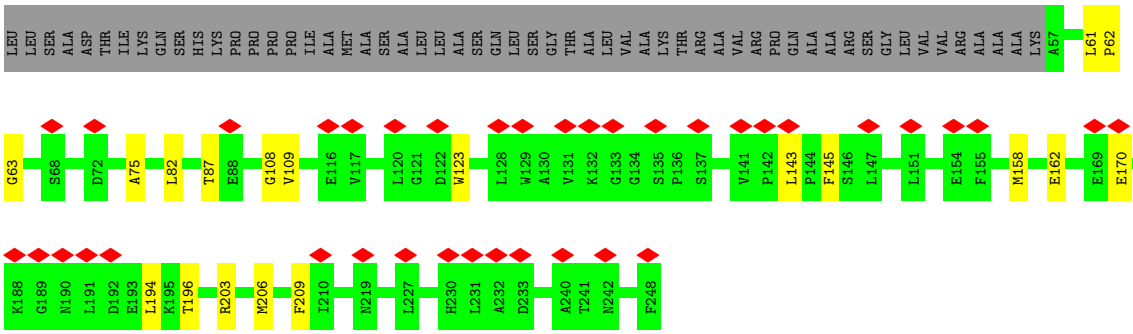
3 Residue-property plots (i)

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

• Molecule 1: Lhca1

Chain 1:

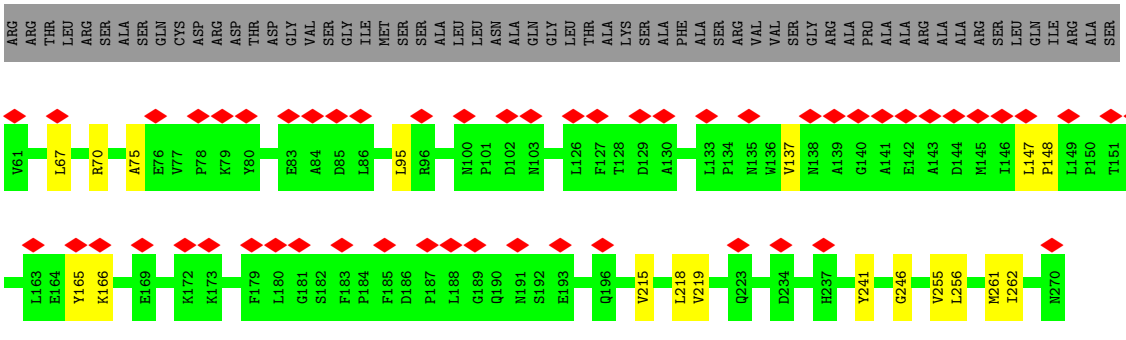




• Molecule 2: Lhca2

Chain 2:

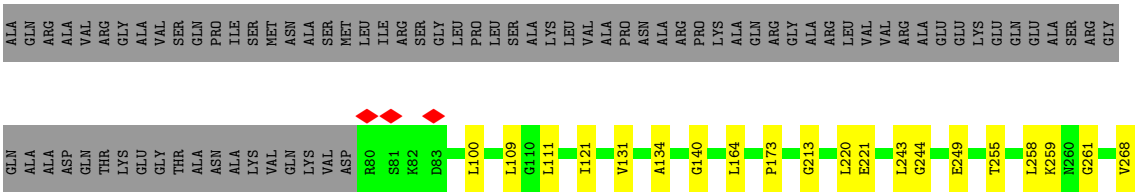


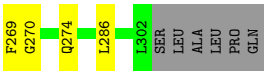


• Molecule 3: Lhca3

Chain 3:



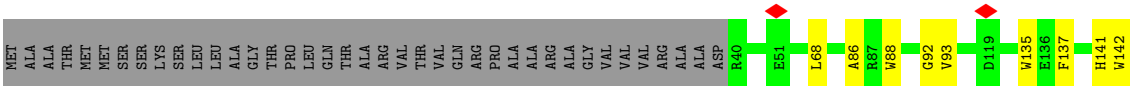


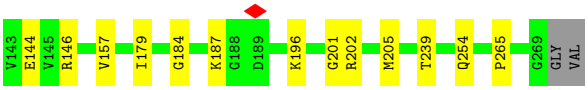


• Molecule 4: Lhca5

Chain 5:



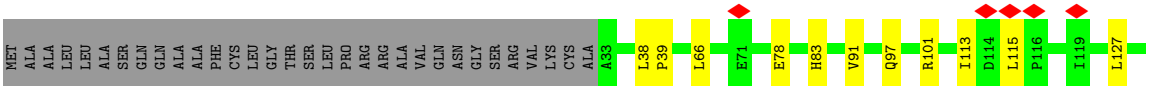


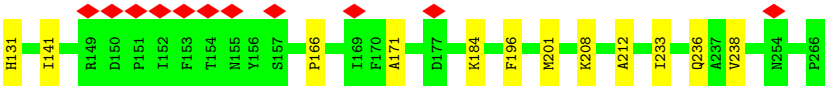


• Molecule 5: Lhca6

Chain 6:



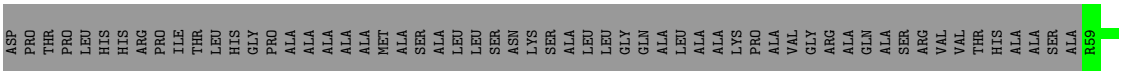


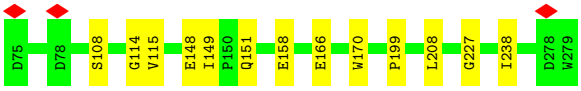


• Molecule 6: Lhca7

Chain 7:



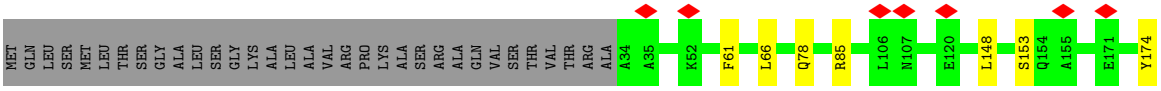


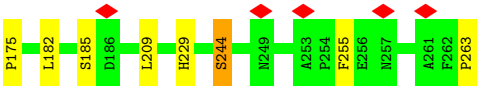


• Molecule 7: Lhca8

Chain 8:



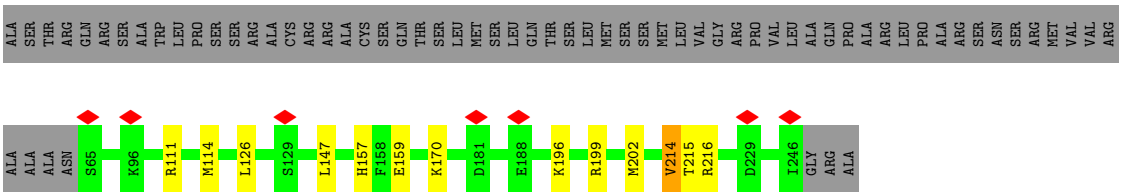




• Molecule 8: Lhca9

Chain 9:

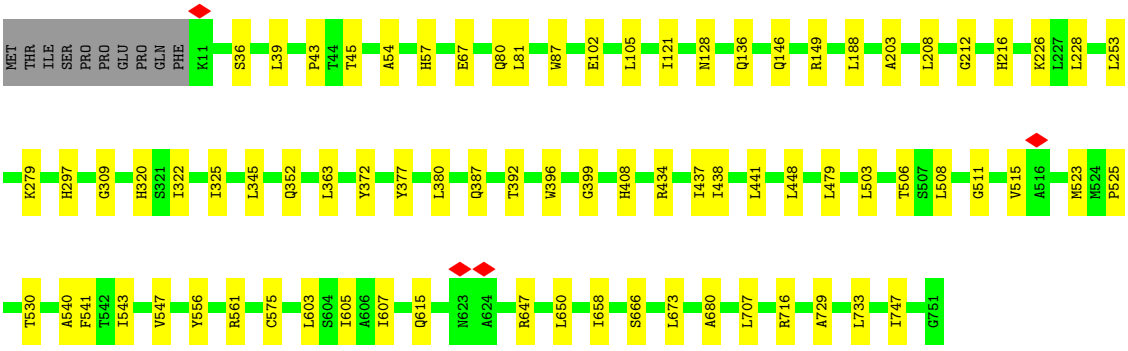




• Molecule 9: PsaA

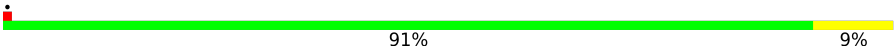
Chain A:

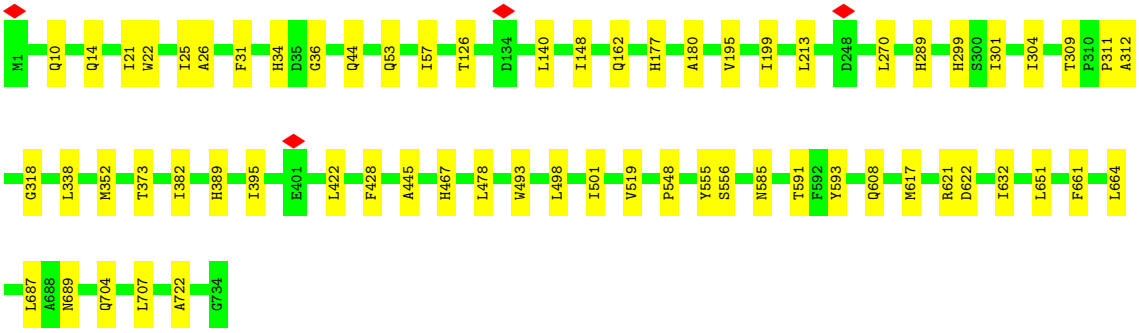




• Molecule 10: PsaB

Chain B:

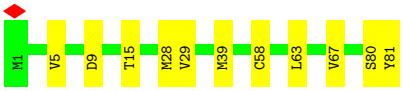




• Molecule 11: Photosystem I iron-sulfur center

Chain C:



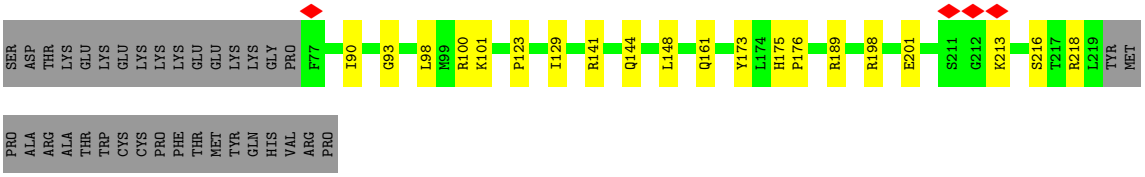


• Molecule 12: PsaD

Chain D:







• Molecule 13: PsaE

Chain E:

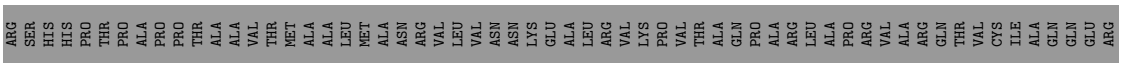


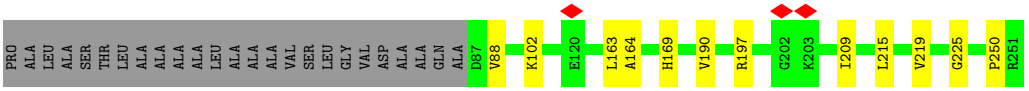


• Molecule 14: PsaF

Chain F:





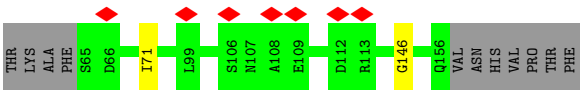


• Molecule 15: PsaG

Chain G:



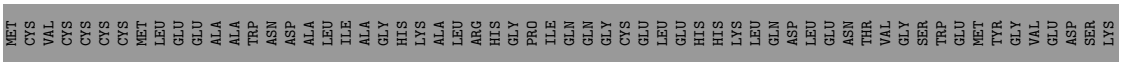


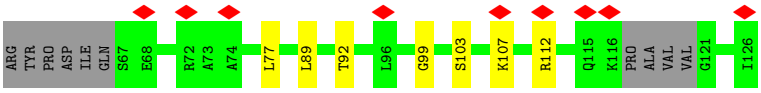


• Molecule 16: PsaH

Chain H:





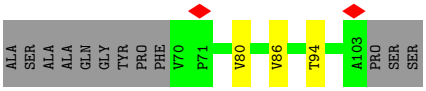


• Molecule 17: Photosystem I reaction center subunit VIII

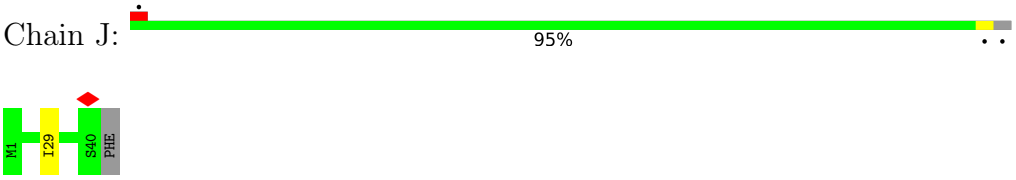
Chain I:



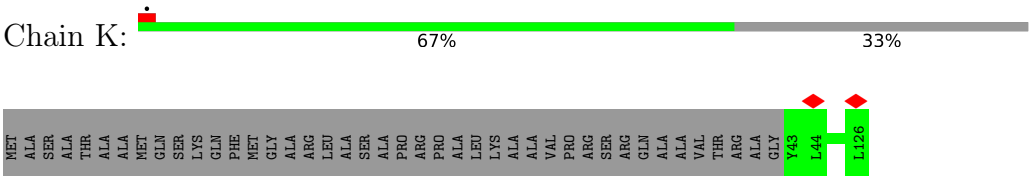




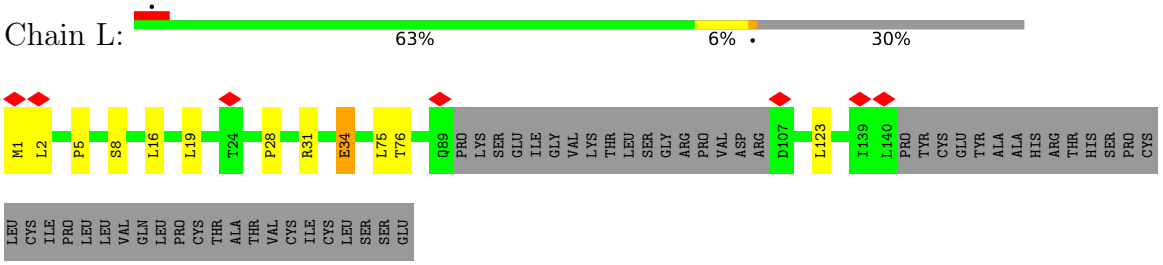
• Molecule 18: Photosystem I reaction center subunit IX



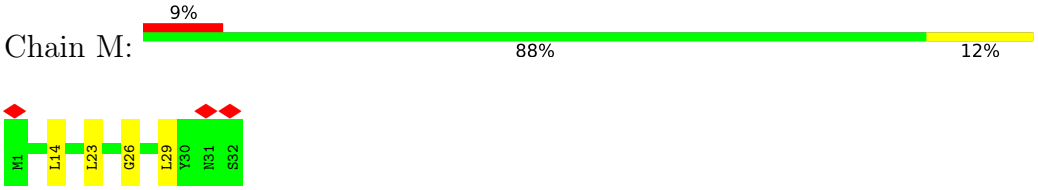
• Molecule 19: PsaK



• Molecule 20: PsaL



• Molecule 21: Photosystem I reaction center subunit XII



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69264	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	1.875	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	408.0, 408.0, 408.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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, SF4, PQN, LMU, CLA, XAT, CHL, BCR, LHG, NEX, LMG, LUT, K3I

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	1	0.28	0/1475	0.64	0/2008
2	2	0.26	0/1630	0.58	0/2225
3	3	0.24	0/1810	0.56	1/2462 (0.0%)
4	5	0.24	0/1849	0.47	0/2521
5	6	0.22	0/1851	0.48	0/2536
6	7	0.21	0/1792	0.46	0/2443
7	8	0.22	0/1812	0.51	0/2467
8	9	0.26	0/1468	0.57	2/1997 (0.1%)
9	A	0.21	0/6030	0.46	0/8224
10	B	0.21	0/6037	0.45	0/8252
11	C	0.20	0/618	0.56	0/836
12	D	0.19	0/1146	0.45	0/1545
13	E	0.14	0/495	0.34	0/674
14	F	0.24	0/1295	0.48	0/1746
15	G	0.23	0/693	0.51	0/943
16	H	0.21	0/436	0.57	0/582
17	I	0.35	0/265	0.63	0/367
18	J	0.24	0/337	0.49	0/462
19	K	0.22	0/605	0.45	0/823
20	L	0.23	0/916	0.57	1/1250 (0.1%)
21	M	0.15	0/249	0.38	0/335
All	All	0.23	0/32809	0.50	4/44698 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	5	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	121	ILE	N-CA-C	-7.12	105.60	112.29
8	9	214	VAL	CA-C-N	5.76	132.54	121.54
8	9	214	VAL	C-N-CA	5.76	132.54	121.54
20	L	34	GLU	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	5	146	ARG	Sidechain

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	1	1435	0	1409	15	0
2	2	1590	0	1588	11	0
3	3	1756	0	1708	17	0
4	5	1791	0	1729	18	0
5	6	1794	0	1785	18	0
6	7	1732	0	1657	11	0
7	8	1758	0	1720	14	0
8	9	1427	0	1398	11	0
9	A	5834	0	5700	60	0
10	B	5822	0	5577	50	0
11	C	608	0	593	7	0
12	D	1120	0	1137	13	0
13	E	484	0	481	0	0
14	F	1269	0	1302	8	0
15	G	681	0	678	1	0
16	H	427	0	440	5	0
17	I	256	0	268	3	0
18	J	326	0	327	1	0
19	K	595	0	605	0	0
20	L	897	0	930	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	M	246	0	260	4	0
22	1	493	0	418	9	0
22	2	584	0	454	11	0
22	3	612	0	588	13	0
22	5	556	0	472	10	0
22	6	716	0	648	23	0
22	7	618	0	529	10	0
22	8	544	0	449	12	0
22	9	507	0	441	14	0
22	A	2360	0	2241	60	0
22	B	2433	0	2334	66	0
22	F	153	0	132	6	0
22	G	100	0	82	1	0
22	H	112	0	65	1	0
22	J	42	0	31	0	0
22	K	179	0	138	0	0
22	L	147	0	123	3	0
23	1	144	0	101	0	0
23	3	245	0	237	8	0
23	5	388	0	339	11	0
23	6	112	0	101	5	0
23	7	113	0	101	3	0
23	8	293	0	278	12	0
23	9	90	0	60	1	0
24	1	42	0	56	4	0
24	2	42	0	56	3	0
24	3	84	0	112	11	0
24	5	42	0	56	4	0
24	6	42	0	56	2	0
24	7	42	0	56	2	0
24	8	42	0	56	3	0
24	9	42	0	56	4	0
25	1	44	0	56	4	0
25	2	44	0	56	3	0
25	3	44	0	56	4	0
25	5	44	0	56	1	0
25	6	44	0	56	5	0
25	7	44	0	56	4	0
25	8	44	0	56	4	0
25	9	44	0	56	4	0
26	1	40	0	56	3	0
26	3	80	0	112	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	5	40	0	56	5	0
26	7	40	0	56	3	0
26	8	40	0	56	2	0
26	9	40	0	56	3	0
26	A	200	0	280	18	0
26	B	240	0	336	18	0
26	F	80	0	112	11	0
26	G	40	0	56	4	0
26	I	40	0	56	3	0
26	J	80	0	112	5	0
26	K	80	0	112	3	0
26	L	80	0	112	6	0
26	M	40	0	56	4	0
27	1	75	0	96	2	0
27	2	40	0	53	3	0
27	5	72	0	84	5	0
27	6	48	0	69	6	0
27	7	49	0	74	1	0
27	8	49	0	74	3	0
27	9	45	0	63	1	0
27	A	94	0	137	6	0
27	B	37	0	44	3	0
27	M	34	0	38	3	0
28	1	35	0	46	2	0
28	3	98	0	121	3	0
28	6	100	0	122	1	0
28	7	35	0	46	1	0
28	9	35	0	46	2	0
28	A	64	0	77	0	0
28	F	29	0	31	0	0
28	G	35	0	46	2	0
28	H	35	0	46	2	0
28	J	35	0	46	1	0
28	K	35	0	46	0	0
29	2	42	0	0	0	0
29	5	42	0	0	0	0
30	5	44	0	56	5	0
30	6	44	0	56	2	0
31	8	25	0	26	0	0
31	9	46	0	62	6	0
31	J	83	0	109	1	0
32	A	33	0	46	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B	33	0	46	2	0
33	A	8	0	0	1	0
33	C	16	0	0	0	0
34	B	58	0	74	3	0
All	All	46832	0	46110	543	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 6.

All (543) 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)
22:3:408:CLA:HAB	24:3:415:LUT:H32	1.65	0.79
22:B:835:CLA:HBB1	26:F:801:BCR:H23C	1.68	0.74
23:3:406:CHL:H61	26:3:419:BCR:H19C	1.71	0.72
6:7:115:VAL:HG11	24:7:315:LUT:H12	1.72	0.70
24:3:418:LUT:H28	22:A:814:CLA:H52	1.74	0.70
22:A:818:CLA:HAB	22:A:818:CLA:H8	1.76	0.67
23:3:406:CHL:H201	26:3:417:BCR:H16C	1.77	0.67
22:A:832:CLA:HBB1	22:A:833:CLA:H2	1.78	0.65
26:B:849:BCR:H321	26:B:850:BCR:HC8	1.77	0.65
10:B:608:GLN:HE21	10:B:622:ASP:HB3	1.62	0.65
1:1:109:VAL:HG11	24:1:314:LUT:H10	1.79	0.65
4:5:93:VAL:HG11	24:5:320:LUT:H12	1.79	0.65
22:1:308:CLA:H51	22:1:308:CLA:HBB1	1.78	0.65
22:B:836:CLA:H43	18:J:29:ILE:HG21	1.79	0.65
22:3:404:CLA:H12	26:3:417:BCR:H10C	1.79	0.64
9:A:67:GLU:HG2	9:A:188:LEU:HB2	1.80	0.63
22:B:836:CLA:H52	26:F:801:BCR:H403	1.81	0.63
22:F:804:CLA:HAB	26:F:805:BCR:H382	1.79	0.63
1:1:158:MET:O	1:1:162:GLU:HB2	1.99	0.62
9:A:399:GLY:HA3	9:A:603:LEU:HD11	1.82	0.62
20:L:16:LEU:HA	20:L:19:LEU:HD12	1.81	0.62
3:3:286:LEU:HD13	24:3:415:LUT:H22	1.82	0.62
9:A:128:ASN:HB3	9:A:136:GLN:HB3	1.82	0.61
9:A:650:LEU:HD11	22:A:801:CLA:H71	1.81	0.61
5:6:38:LEU:HD21	23:6:303:CHL:HMA3	1.82	0.61
22:6:311:CLA:HAB	24:6:319:LUT:H32	1.83	0.61
10:B:301:ILE:HG21	22:B:827:CLA:HAC1	1.83	0.61
22:9:606:CLA:HBD	27:B:801:LHG:HC62	1.83	0.60
4:5:254:GLN:HB2	30:5:323:NEX:H8	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:268:VAL:HG11	25:3:416:XAT:H32	1.82	0.60
23:6:303:CHL:HBB1	27:6:322:LHG:H262	1.83	0.60
23:5:307:CHL:H2	26:5:322:BCR:H15C	1.84	0.60
27:6:322:LHG:HC91	27:6:322:LHG:H282	1.83	0.60
22:B:808:CLA:H71	22:B:816:CLA:H52	1.84	0.60
22:2:602:CLA:H61	25:2:615:XAT:H8	1.83	0.59
9:A:322:ILE:HG21	22:A:824:CLA:HAC1	1.83	0.59
8:9:170:LYS:HE2	31:9:617:LMG:HC61	1.83	0.59
23:5:302:CHL:HMA3	27:5:325:LHG:H121	1.84	0.59
22:B:806:CLA:H141	22:B:813:CLA:HBC1	1.84	0.58
22:6:316:CLA:HBB2	22:7:309:CLA:H121	1.85	0.58
22:B:816:CLA:H172	26:B:847:BCR:H312	1.84	0.58
32:A:842:PQN:H171	22:F:802:CLA:HAB	1.86	0.58
22:B:810:CLA:HAA1	17:I:80:VAL:HG22	1.86	0.58
22:A:820:CLA:H102	26:A:849:BCR:H21C	1.86	0.58
22:9:608:CLA:H62	24:9:613:LUT:H10	1.86	0.57
5:6:171:ALA:HB2	22:6:311:CLA:HBD	1.86	0.57
9:A:673:LEU:HD11	10:B:617:MET:HB2	1.87	0.57
22:5:311:CLA:H52	24:5:320:LUT:H30	1.86	0.57
22:9:602:CLA:H72	25:9:614:XAT:H8	1.87	0.57
22:6:314:CLA:H72	27:6:322:LHG:H171	1.87	0.57
22:B:815:CLA:HBB2	22:B:823:CLA:H92	1.84	0.57
11:C:58:CYS:HB3	11:C:63:LEU:HD22	1.86	0.57
9:A:80:GLN:HE21	22:A:804:CLA:HMB3	1.69	0.56
10:B:373:THR:HG23	10:B:591:THR:HG21	1.88	0.56
22:B:809:CLA:H151	22:B:831:CLA:HBB2	1.87	0.56
23:8:603:CHL:HAB	25:8:618:XAT:H32	1.88	0.56
10:B:36:GLY:H	12:D:213:LYS:HE2	1.70	0.56
26:K:203:BCR:H362	26:K:207:BCR:H403	1.85	0.56
5:6:66:LEU:HD23	6:7:208:LEU:HD21	1.88	0.56
23:7:304:CHL:HBB2	23:7:305:CHL:HAB	1.88	0.56
1:1:82:LEU:HD22	27:1:318:LHG:H262	1.88	0.56
9:A:438:ILE:HG13	9:A:556:TYR:HE2	1.71	0.56
22:B:811:CLA:HAB	22:B:812:CLA:HBA1	1.88	0.56
2:2:95:LEU:HD13	25:2:615:XAT:H21	1.88	0.55
7:8:182:LEU:HD12	24:8:617:LUT:H222	1.89	0.55
4:5:196:LYS:HD2	22:5:313:CLA:HBD	1.88	0.55
20:L:34:GLU:HG2	22:L:303:CLA:HED2	1.89	0.55
4:5:179:ILE:HD12	23:5:307:CHL:H151	1.89	0.55
22:3:404:CLA:H11	23:3:406:CHL:H13	1.89	0.55
22:9:609:CLA:H61	22:9:610:CLA:HBC1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:208:LYS:HE2	5:6:212:ALA:HB1	1.88	0.55
27:8:620:LHG:H152	27:8:620:LHG:H272	1.88	0.55
22:9:612:CLA:HBC2	27:9:616:LHG:H352	1.87	0.55
10:B:10:GLN:HE21	10:B:14:GLN:HE21	1.55	0.55
10:B:556:SER:HB3	34:B:852:DGD:HD2	1.88	0.55
10:B:722:ALA:HB2	22:B:830:CLA:HBB1	1.89	0.55
27:2:617:LHG:HC32	31:9:617:LMG:H372	1.88	0.54
8:9:216:ARG:HH22	10:B:213:LEU:HB3	1.71	0.54
9:A:543:ILE:HD11	22:A:836:CLA:HBB1	1.89	0.54
9:A:396:TRP:CD1	22:A:827:CLA:HAB	2.42	0.54
22:2:613:CLA:H3A	26:M:102:BCR:H281	1.88	0.54
22:B:806:CLA:HED2	22:B:806:CLA:HBA2	1.89	0.54
22:A:836:CLA:HED2	22:A:836:CLA:H2A	1.88	0.54
22:3:403:CLA:H43	22:5:316:CLA:HED3	1.90	0.54
22:B:803:CLA:H152	22:B:806:CLA:H192	1.89	0.54
5:6:101:ARG:HD2	28:6:323:LMU:H61	1.88	0.54
22:6:305:CLA:HBC3	25:6:320:XAT:H31	1.90	0.54
7:8:185:SER:HB3	22:8:610:CLA:HAA2	1.88	0.54
4:5:265:PRO:HB3	27:5:301:LHG:HC42	1.90	0.54
8:9:214:VAL:HG12	8:9:215:THR:HG23	1.90	0.54
3:3:140:GLY:HA2	25:3:416:XAT:H381	1.90	0.53
22:5:311:CLA:H2	24:5:320:LUT:H28	1.91	0.53
22:8:610:CLA:HBB1	22:8:612:CLA:H3A	1.91	0.53
22:9:606:CLA:HED1	27:B:801:LHG:HC92	1.91	0.53
10:B:26:ALA:HB2	34:B:852:DGD:HA32	1.91	0.53
23:8:602:CHL:HBB1	27:8:620:LHG:H121	1.90	0.53
22:B:828:CLA:HMA1	26:B:850:BCR:H17C	1.90	0.53
16:H:107:LYS:HG3	16:H:112:ARG:HH21	1.74	0.53
23:8:602:CHL:H202	23:8:602:CHL:H141	1.91	0.52
10:B:180:ALA:HB1	22:B:823:CLA:HAC2	1.90	0.52
2:2:215:VAL:HA	2:2:219:VAL:HB	1.91	0.52
30:5:323:NEX:H162	5:6:238:VAL:HG11	1.91	0.52
7:8:66:LEU:HD21	14:F:225:GLY:HA3	1.91	0.52
8:9:196:LYS:HB2	22:9:609:CLA:HAC2	1.91	0.52
9:A:479:LEU:H	9:A:530:THR:HG22	1.74	0.52
23:8:602:CHL:H91	22:8:613:CLA:H91	1.92	0.52
9:A:87:TRP:HA	22:A:806:CLA:HBB2	1.92	0.52
10:B:309:THR:HG22	10:B:318:GLY:HA3	1.90	0.52
22:B:829:CLA:H13	26:B:850:BCR:H16C	1.90	0.52
32:A:842:PQN:H141	22:F:802:CLA:HBB2	1.91	0.52
22:B:810:CLA:H3A	22:B:811:CLA:HMB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:3:406:CHL:HMB2	26:3:419:BCR:H24C	1.92	0.51
22:6:314:CLA:H71	27:6:322:LHG:H342	1.91	0.51
9:A:441:LEU:HD22	22:A:838:CLA:HBB1	1.91	0.51
22:A:841:CLA:H13	20:L:75:LEU:HD21	1.92	0.51
32:A:842:PQN:H151	22:F:802:CLA:HBB2	1.93	0.51
27:1:318:LHG:HC12	10:B:312:ALA:HB2	1.91	0.51
22:A:832:CLA:H191	10:B:21:ILE:HG21	1.92	0.51
23:3:413:CHL:HBC1	4:5:239:THR:HG22	1.92	0.51
11:C:29:VAL:HG12	12:D:189:ARG:HB3	1.92	0.51
10:B:689:ASN:HB2	12:D:100:ARG:HH22	1.76	0.50
23:6:303:CHL:H92	27:6:322:LHG:H152	1.94	0.50
9:A:320:HIS:NE2	22:A:821:CLA:C4D	2.73	0.50
10:B:338:LEU:HD22	10:B:382:ILE:HG23	1.92	0.50
22:6:318:CLA:H2A	22:6:318:CLA:HED3	1.93	0.50
22:7:308:CLA:H71	22:7:310:CLA:HMA3	1.91	0.50
9:A:658:ILE:HD12	10:B:621:ARG:HG3	1.92	0.50
6:7:108:SER:HB3	6:7:227:GLY:HA3	1.93	0.50
12:D:216:SER:HB3	12:D:218:ARG:HG2	1.94	0.50
23:5:309:CHL:HMA1	26:5:322:BCR:H353	1.92	0.50
3:3:134:ALA:HB1	3:3:261:GLY:HA3	1.94	0.50
1:1:143:LEU:HB3	1:1:145:PHE:HD2	1.77	0.50
6:7:199:PRO:HB3	22:7:306:CLA:HBC2	1.94	0.50
9:A:43:PRO:HG3	14:F:209:ILE:HD13	1.94	0.50
10:B:25:ILE:HD11	26:L:305:BCR:H383	1.93	0.50
20:L:76:THR:HG21	20:L:123:LEU:HD22	1.93	0.50
22:2:608:CLA:HBB1	22:2:610:CLA:H3A	1.94	0.49
22:7:301:CLA:H101	25:7:316:XAT:H161	1.93	0.49
9:A:320:HIS:HB3	9:A:325:ILE:HD11	1.93	0.49
22:A:804:CLA:H121	26:A:846:BCR:H272	1.94	0.49
22:A:819:CLA:HBB1	26:K:207:BCR:H373	1.95	0.49
22:B:810:CLA:H111	26:I:201:BCR:HC21	1.95	0.49
10:B:395:ILE:HD13	10:B:555:TYR:HA	1.95	0.49
5:6:201:MET:HG3	22:6:314:CLA:HAC2	1.94	0.49
4:5:68:LEU:HD13	22:5:303:CLA:H42	1.93	0.49
22:B:811:CLA:H12	22:B:830:CLA:H92	1.94	0.49
22:B:811:CLA:H43	22:B:830:CLA:H71	1.95	0.49
12:D:93:GLY:HA3	20:L:2:LEU:HD22	1.94	0.49
6:7:238:ILE:HG23	7:8:263:PRO:HB2	1.94	0.49
23:5:302:CHL:H61	23:5:302:CHL:H41	1.57	0.49
3:3:244:GLY:HA2	3:3:249:GLU:HG2	1.95	0.49
16:H:92:THR:HG23	17:I:86:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:826:CLA:HED3	22:B:826:CLA:H2A	1.94	0.48
6:7:170:TRP:HE1	22:7:314:CLA:HMA3	1.78	0.48
12:D:123:PRO:HD3	12:D:148:LEU:HD13	1.95	0.48
9:A:540:ALA:HB2	22:A:837:CLA:HMA1	1.96	0.48
22:B:820:CLA:HBA2	22:B:829:CLA:HBB2	1.95	0.48
21:M:26:GLY:HA3	27:M:101:LHG:H102	1.96	0.48
23:8:602:CHL:H41	22:8:614:CLA:H42	1.95	0.48
9:A:226:LYS:HD3	9:A:253:LEU:HB3	1.95	0.48
9:A:279:LYS:HG2	9:A:503:LEU:HD12	1.95	0.48
3:3:270:GLY:O	3:3:274:GLN:HG3	2.13	0.48
22:A:804:CLA:H41	26:A:847:BCR:H23C	1.95	0.48
2:2:137:VAL:HG21	2:2:218:LEU:HG	1.95	0.48
22:8:614:CLA:HBC1	24:8:617:LUT:H172	1.95	0.48
31:9:617:LMG:H232	31:9:617:LMG:H352	1.96	0.48
4:5:135:TRP:CE2	22:6:315:CLA:H3A	2.48	0.48
9:A:666:SER:HB2	10:B:445:ALA:HB1	1.96	0.48
22:2:601:CLA:HAB	22:2:602:CLA:HMD1	1.95	0.48
10:B:53:GLN:HG2	22:B:808:CLA:H3A	1.95	0.48
5:6:184:LYS:HD3	22:6:313:CLA:HBD	1.96	0.47
22:A:805:CLA:H151	22:A:828:CLA:HBB2	1.96	0.47
2:2:67:LEU:HB3	22:2:601:CLA:HAC1	1.97	0.47
22:A:826:CLA:H2A	22:A:826:CLA:HED3	1.96	0.47
7:8:61:PHE:CE2	23:8:602:CHL:HAB	2.49	0.47
1:1:87:THR:HG21	10:B:311:PRO:HB2	1.96	0.47
22:2:601:CLA:HED3	8:9:157:HIS:HA	1.96	0.47
22:3:402:CLA:HED2	22:3:402:CLA:H61	1.97	0.47
9:A:707:LEU:HD13	26:F:805:BCR:H311	1.95	0.47
22:B:806:CLA:H71	22:B:843:CLA:HBB2	1.96	0.47
2:2:262:ILE:HG21	27:2:617:LHG:H242	1.96	0.47
22:B:802:CLA:HBA1	22:B:802:CLA:H11	1.65	0.47
22:B:831:CLA:H3A	22:B:831:CLA:HBA2	1.56	0.47
24:3:418:LUT:H383	26:A:846:BCR:HC41	1.97	0.47
23:5:307:CHL:HBB2	23:5:308:CHL:CBB	2.45	0.47
26:5:322:BCR:H20C	26:5:322:BCR:H361	1.73	0.47
22:A:839:CLA:H51	26:F:801:BCR:H12C	1.96	0.47
1:1:75:ALA:H	1:1:196:THR:HG22	1.80	0.47
26:5:322:BCR:H11C	26:5:322:BCR:H341	1.79	0.47
9:A:216:HIS:HE1	22:A:813:CLA:ND	2.03	0.47
22:B:810:CLA:HMB3	22:B:811:CLA:HHB	1.95	0.47
3:3:213:GLY:HA2	3:3:221:GLU:HB2	1.97	0.47
4:5:137:PHE:O	4:5:141:HIS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:233:ILE:HG13	5:6:236:GLN:H	1.79	0.47
7:8:209:LEU:HD21	23:8:603:CHL:H203	1.96	0.47
26:L:305:BCR:H15C	26:L:305:BCR:H351	1.81	0.47
23:3:406:CHL:H162	23:5:302:CHL:H112	1.97	0.47
22:6:304:CLA:H61	25:6:320:XAT:H8	1.97	0.47
22:6:311:CLA:H43	22:6:311:CLA:HMB2	1.97	0.47
22:7:301:CLA:H72	25:7:316:XAT:H8	1.96	0.47
22:8:610:CLA:H92	22:8:612:CLA:HMA1	1.97	0.47
9:A:372:TYR:HA	9:A:387:GLN:HE22	1.80	0.47
10:B:44:GLN:NE2	10:B:162:GLN:HB3	2.30	0.47
10:B:177:HIS:CE1	22:B:815:CLA:NA	2.83	0.47
22:3:402:CLA:H143	22:3:407:CLA:H42	1.96	0.46
24:3:418:LUT:H30	22:A:814:CLA:H71	1.97	0.46
4:5:92:GLY:HA2	25:5:321:XAT:H381	1.96	0.46
26:A:849:BCR:H11C	26:A:849:BCR:H341	1.80	0.46
22:F:804:CLA:HMA3	22:F:804:CLA:H42	1.97	0.46
26:K:207:BCR:H351	26:K:207:BCR:H15C	1.78	0.46
4:5:86:ALA:HB1	4:5:201:GLY:HA3	1.97	0.46
4:5:135:TRP:NE1	22:6:315:CLA:H3A	2.28	0.46
22:6:318:CLA:HBA1	22:6:318:CLA:H3A	1.61	0.46
6:7:114:GLY:HA2	25:7:316:XAT:H381	1.97	0.46
7:8:78:GLN:HG3	7:8:148:LEU:HD21	1.97	0.46
22:A:823:CLA:H171	27:A:845:LHG:H142	1.97	0.46
10:B:22:TRP:CG	10:B:704:GLN:HE22	2.32	0.46
22:B:831:CLA:H72	26:B:848:BCR:H343	1.98	0.46
27:5:325:LHG:HC81	27:5:325:LHG:H272	1.96	0.46
5:6:113:ILE:HG23	5:6:115:LEU:HG	1.98	0.46
23:8:606:CHL:H62	23:8:606:CHL:H41	1.61	0.46
24:9:613:LUT:H15	24:9:613:LUT:H201	1.79	0.46
25:9:614:XAT:H15	25:9:614:XAT:H201	1.79	0.46
22:B:833:CLA:H3A	22:B:833:CLA:HBA2	1.54	0.46
22:B:835:CLA:H61	26:F:805:BCR:HC32	1.97	0.46
28:1:319:LMU:H52	28:1:319:LMU:H21	1.71	0.46
28:3:421:LMU:H1B	28:3:421:LMU:H3'	1.75	0.46
23:5:308:CHL:H171	22:6:318:CLA:H203	1.97	0.46
22:A:819:CLA:H3A	22:A:819:CLA:HBA2	1.59	0.46
26:J:101:BCR:H351	26:J:101:BCR:H15C	1.68	0.46
22:2:613:CLA:H3A	22:2:613:CLA:HBA2	1.60	0.46
24:3:418:LUT:H11	24:3:418:LUT:H191	1.78	0.46
9:A:377:TYR:HB2	9:A:380:LEU:HD22	1.97	0.46
10:B:548:PRO:HB3	14:F:250:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:198:ARG:HG2	12:D:201:GLU:HG3	1.96	0.46
22:2:611:CLA:HBB1	24:2:614:LUT:H27	1.96	0.46
4:5:144:GLU:HG3	22:5:310:CLA:C4B	2.45	0.46
30:5:323:NEX:H35	30:5:323:NEX:H401	1.79	0.46
22:9:602:CLA:CAB	25:9:614:XAT:H12	2.46	0.46
22:9:608:CLA:H122	24:9:613:LUT:H203	1.98	0.46
9:A:392:THR:HG23	9:A:607:ILE:HG21	1.96	0.46
22:A:841:CLA:HHD	26:B:851:BCR:H332	1.98	0.46
26:A:851:BCR:H24C	26:A:851:BCR:H371	1.76	0.46
26:B:846:BCR:H11C	26:B:846:BCR:H341	1.80	0.46
1:1:209:PHE:CZ	25:1:315:XAT:H28	2.50	0.46
10:B:195:VAL:HA	10:B:199:ILE:HD12	1.98	0.46
3:3:243:LEU:HB2	22:3:408:CLA:HBA1	1.98	0.46
25:8:618:XAT:H35	25:8:618:XAT:H401	1.79	0.46
22:A:834:CLA:HBA2	26:A:849:BCR:HC42	1.97	0.46
7:8:244:SER:HB3	22:8:615:CLA:C4A	2.46	0.46
23:8:603:CHL:CAB	25:8:618:XAT:H32	2.46	0.46
31:9:617:LMG:H231	10:B:148:ILE:HA	1.98	0.45
9:A:36:SER:HB3	9:A:39:LEU:HB2	1.97	0.45
9:A:434:ARG:HA	9:A:437:ILE:HD12	1.96	0.45
22:B:816:CLA:H3A	22:B:816:CLA:HBA1	1.37	0.45
12:D:175:HIS:HB3	12:D:176:PRO:HD3	1.98	0.45
22:6:316:CLA:H61	22:6:316:CLA:H41	1.64	0.45
22:A:816:CLA:H62	22:A:816:CLA:H41	1.62	0.45
20:L:5:PRO:HD2	20:L:8:SER:HB2	1.99	0.45
26:7:317:BCR:H11C	26:7:317:BCR:H341	1.76	0.45
26:8:619:BCR:H11C	26:8:619:BCR:H341	1.70	0.45
3:3:109:LEU:HD13	25:3:416:XAT:H21	1.97	0.45
3:3:173:PRO:HG3	28:3:423:LMU:H5'	1.99	0.45
32:A:842:PQN:H2M1	32:A:842:PQN:H111	1.79	0.45
10:B:299:HIS:HB3	10:B:304:ILE:HD11	1.98	0.45
24:5:320:LUT:H35	24:5:320:LUT:H401	1.76	0.45
1:1:108:GLY:HA2	25:1:315:XAT:H381	1.98	0.45
22:3:408:CLA:H41	22:3:408:CLA:H62	1.75	0.45
5:6:91:VAL:HG11	24:6:319:LUT:H12	1.98	0.45
9:A:575:CYS:HB3	33:A:850:SF4:S1	2.57	0.45
6:7:148:GLU:HG2	6:7:149:ILE:HG13	1.99	0.45
22:7:309:CLA:HBC1	27:7:318:LHG:H192	1.99	0.45
22:A:818:CLA:HBA2	22:A:818:CLA:H3A	1.62	0.45
22:1:308:CLA:H3A	22:1:308:CLA:HBA2	1.70	0.45
5:6:196:PHE:CZ	25:6:320:XAT:H30	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:7:317:BCR:H382	22:8:614:CLA:H122	1.99	0.45
8:9:126:LEU:HB3	26:9:615:BCR:H382	1.98	0.45
9:A:448:LEU:HD13	9:A:541:PHE:HA	1.99	0.45
26:A:846:BCR:H351	26:A:846:BCR:H15C	1.72	0.45
10:B:428:PHE:CD2	22:B:840:CLA:HAB	2.52	0.45
26:M:102:BCR:H20C	26:M:102:BCR:H361	1.70	0.45
22:3:408:CLA:H43	24:3:415:LUT:H30	1.99	0.45
26:8:619:BCR:H351	26:8:619:BCR:H15C	1.79	0.45
22:9:608:CLA:H3A	22:9:608:CLA:HBA2	1.65	0.45
3:3:111:LEU:HD11	22:A:811:CLA:H43	1.99	0.44
9:A:508:LEU:HD21	9:A:515:VAL:HG23	1.98	0.44
22:B:804:CLA:HHB	22:B:805:CLA:H192	1.99	0.44
4:5:184:GLY:HA3	4:5:187:LYS:HE2	1.99	0.44
22:6:311:CLA:H3A	22:6:311:CLA:HBA2	1.70	0.44
22:7:314:CLA:H3A	28:7:319:LMU:H6E	1.99	0.44
23:8:608:CHL:HBD	23:8:608:CHL:HBA1	1.99	0.44
8:9:114:MET:SD	22:9:608:CLA:HAB	2.57	0.44
9:A:57:HIS:CD2	22:A:804:CLA:HBB2	2.52	0.44
22:A:829:CLA:H152	27:A:844:LHG:H362	2.00	0.44
32:A:842:PQN:H111	26:F:801:BCR:H322	1.99	0.44
10:B:467:HIS:HA	10:B:478:LEU:HD12	1.99	0.44
10:B:519:VAL:HG21	10:B:593:TYR:HB2	1.99	0.44
10:B:585:ASN:HB2	22:B:804:CLA:HBC2	2.00	0.44
22:B:807:CLA:H3A	21:M:29:LEU:HB3	1.99	0.44
26:B:849:BCR:H24C	26:B:849:BCR:H371	1.79	0.44
26:I:201:BCR:H11C	26:I:201:BCR:H341	1.80	0.44
22:1:301:CLA:CAB	25:1:315:XAT:H12	2.47	0.44
4:5:157:VAL:HG12	5:6:39:PRO:HB2	2.00	0.44
26:9:615:BCR:H341	26:9:615:BCR:H11C	1.72	0.44
9:A:508:LEU:HD22	9:A:523:MET:HB3	1.99	0.44
22:B:844:CLA:H52	22:B:844:CLA:H11	1.79	0.44
11:C:81:TYR:HA	12:D:101:LYS:HB2	1.99	0.44
2:2:147:LEU:HD12	2:2:148:PRO:HD2	1.98	0.44
22:A:812:CLA:H122	22:A:812:CLA:H162	1.81	0.44
12:D:98:LEU:H	20:L:1:MET:HB3	1.82	0.44
22:1:311:CLA:HBC2	22:1:313:CLA:HMD2	1.99	0.44
26:1:316:BCR:H15C	26:1:316:BCR:H351	1.74	0.44
22:3:407:CLA:HBA2	22:3:407:CLA:H3A	1.53	0.44
27:5:301:LHG:HC81	27:5:301:LHG:H112	1.82	0.44
22:5:310:CLA:HBA2	22:5:310:CLA:H3A	1.59	0.44
22:A:805:CLA:H101	22:A:805:CLA:H13	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:99:GLY:H	16:H:103:SER:H	1.64	0.44
1:1:63:GLY:HA3	7:8:153:SER:HB2	1.99	0.44
22:1:301:CLA:H62	22:1:301:CLA:H41	1.67	0.44
7:8:174:TYR:HB3	22:8:610:CLA:HED2	1.99	0.44
9:A:615:GLN:HE21	9:A:747:ILE:HD13	1.82	0.44
22:A:839:CLA:HBC2	26:F:801:BCR:H10C	2.00	0.44
12:D:90:ILE:HB	12:D:129:ILE:HB	2.00	0.44
22:2:603:CLA:HBC1	22:2:606:CLA:HAC2	1.99	0.44
25:2:615:XAT:H35	25:2:615:XAT:H401	1.84	0.44
23:3:422:CHL:H151	23:3:422:CHL:H112	1.77	0.44
26:7:317:BCR:H15C	26:7:317:BCR:H351	1.78	0.44
9:A:506:THR:HG22	22:A:817:CLA:H11	2.00	0.44
26:A:847:BCR:H11C	26:A:847:BCR:H341	1.81	0.44
28:H:204:LMU:H61	27:M:101:LHG:HC5	1.99	0.44
24:2:614:LUT:H35	24:2:614:LUT:H401	1.82	0.44
22:6:318:CLA:H62	22:6:318:CLA:H102	1.82	0.44
9:A:146:GLN:HB3	9:A:377:TYR:HB3	1.99	0.44
9:A:208:LEU:HD22	26:A:846:BCR:H353	1.99	0.44
9:A:396:TRP:HA	9:A:603:LEU:HD13	1.99	0.44
22:B:811:CLA:H141	22:B:811:CLA:H162	1.85	0.44
3:3:269:PHE:HD1	22:A:814:CLA:H121	1.82	0.44
27:8:620:LHG:H112	27:8:620:LHG:HC81	1.76	0.44
22:B:827:CLA:H61	22:B:827:CLA:H41	1.66	0.44
26:G:204:BCR:H341	26:G:204:BCR:H11C	1.75	0.44
24:3:418:LUT:H15	24:3:418:LUT:H201	1.74	0.43
10:B:140:LEU:HD11	21:M:14:LEU:HD12	2.00	0.43
10:B:422:LEU:HG	22:B:841:CLA:HBB1	1.99	0.43
8:9:159:GLU:HG3	22:9:607:CLA:C4B	2.48	0.43
10:B:53:GLN:HE21	10:B:57:ILE:HD11	1.83	0.43
10:B:301:ILE:HG23	22:B:822:CLA:HED3	1.99	0.43
14:F:102:LYS:HA	14:F:102:LYS:HD3	1.80	0.43
26:1:316:BCR:H11C	26:1:316:BCR:H341	1.92	0.43
26:3:419:BCR:H24C	26:3:419:BCR:H371	1.71	0.43
9:A:216:HIS:HE1	22:A:813:CLA:C4D	2.31	0.43
26:G:204:BCR:H24C	26:G:204:BCR:H371	1.75	0.43
1:1:170:GLU:HB2	1:1:173:LYS:HB2	2.00	0.43
22:1:301:CLA:H62	22:1:301:CLA:H102	1.83	0.43
26:1:316:BCR:H361	26:1:316:BCR:H20C	1.71	0.43
2:2:261:MET:HE3	22:9:607:CLA:HHB	1.99	0.43
25:3:416:XAT:H35	25:3:416:XAT:H401	1.88	0.43
4:5:202:ARG:HA	4:5:205:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:605:ILE:HD12	22:A:801:CLA:H122	2.00	0.43
14:F:88:VAL:HG13	14:F:163:LEU:HD22	2.00	0.43
31:9:617:LMG:H221	10:B:148:ILE:HG12	2.01	0.43
22:A:808:CLA:HAB	22:B:836:CLA:HMD2	2.00	0.43
21:M:23:LEU:HD23	27:M:101:LHG:H101	1.99	0.43
3:3:131:VAL:HG22	3:3:258:LEU:HD21	2.00	0.43
30:5:323:NEX:H11	30:5:323:NEX:H191	1.88	0.43
9:A:511:GLY:HA2	9:A:525:PRO:HB3	2.01	0.43
9:A:647:ARG:HA	10:B:632:ILE:HD12	2.01	0.43
22:B:825:CLA:H43	28:G:201:LMU:H1'	1.99	0.43
12:D:161:GLN:HG3	12:D:173:TYR:HE1	1.82	0.43
30:5:323:NEX:H15	30:5:323:NEX:H201	1.82	0.43
23:6:303:CHL:H61	23:6:303:CHL:H2	1.72	0.43
26:A:848:BCR:H24C	26:A:848:BCR:H371	1.84	0.43
10:B:289:HIS:CE1	22:B:823:CLA:NC	2.86	0.43
14:F:197:ARG:HD3	14:F:215:LEU:HD11	2.00	0.43
26:F:805:BCR:H361	26:F:805:BCR:H20C	1.80	0.43
20:L:28:PRO:HG3	20:L:31:ARG:HH21	1.81	0.43
1:1:203:ARG:HA	1:1:206:MET:HE3	2.01	0.43
24:2:614:LUT:H15	24:2:614:LUT:H201	1.83	0.43
25:8:618:XAT:H363	25:8:618:XAT:H23	1.84	0.43
22:A:826:CLA:H152	22:A:834:CLA:H112	2.01	0.43
28:1:319:LMU:H102	26:B:849:BCR:H282	2.01	0.43
27:2:617:LHG:H282	27:2:617:LHG:H251	1.91	0.43
22:3:407:CLA:H111	24:3:418:LUT:H12	2.01	0.43
22:A:801:CLA:HED3	22:A:801:CLA:HBD	1.90	0.43
23:5:302:CHL:HAC2	27:5:325:LHG:HC41	2.00	0.42
5:6:97:GLN:OE1	22:6:306:CLA:ND	2.52	0.42
23:8:606:CHL:H92	23:8:606:CHL:H61	1.90	0.42
22:A:802:CLA:H143	26:A:851:BCR:HC31	2.01	0.42
26:A:848:BCR:H20C	26:A:848:BCR:H361	1.86	0.42
14:F:190:VAL:HG13	14:F:219:VAL:HG23	2.01	0.42
26:G:204:BCR:H351	26:G:204:BCR:H15C	1.72	0.42
23:5:309:CHL:HBA2	22:5:311:CLA:HMD2	2.00	0.42
22:7:309:CLA:H2	22:7:310:CLA:HMD2	2.02	0.42
9:A:212:GLY:HA2	22:A:814:CLA:HBB2	2.01	0.42
26:L:301:BCR:H15C	26:L:301:BCR:H351	1.86	0.42
9:A:54:ALA:HB2	27:A:844:LHG:HC82	2.00	0.42
9:A:149:ARG:HE	9:A:228:LEU:HD13	1.84	0.42
22:A:824:CLA:H202	22:A:824:CLA:H161	1.86	0.42
22:L:303:CLA:H62	22:L:303:CLA:H41	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:164:LEU:HD23	3:3:164:LEU:HA	1.90	0.42
23:5:319:CHL:H41	23:5:319:CHL:H61	1.56	0.42
30:6:321:NEX:H11	30:6:321:NEX:H191	1.85	0.42
9:A:203:ALA:HB2	9:A:309:GLY:HA3	2.01	0.42
10:B:498:LEU:HA	10:B:501:ILE:HG22	2.01	0.42
28:H:204:LMU:H51	17:I:94:THR:HG22	2.01	0.42
22:L:303:CLA:H51	22:L:303:CLA:H8	1.68	0.42
22:3:408:CLA:HBA2	22:3:408:CLA:H3A	1.67	0.42
26:5:322:BCR:H271	27:6:322:LHG:HC92	2.01	0.42
10:B:126:THR:HG22	10:B:270:LEU:HD21	2.01	0.42
32:B:845:PQN:H111	32:B:845:PQN:H2M1	1.83	0.42
26:F:805:BCR:H371	26:F:805:BCR:H24C	1.78	0.42
1:1:194:LEU:HD13	22:1:308:CLA:HBA2	2.00	0.42
30:6:321:NEX:H35	30:6:321:NEX:H401	1.77	0.42
32:B:845:PQN:H142	26:B:851:BCR:HC42	2.02	0.42
26:B:848:BCR:H20C	26:B:848:BCR:H361	1.85	0.42
11:C:9:ASP:HA	11:C:39:MET:HE1	2.02	0.42
22:F:802:CLA:H141	31:J:105:LMG:H312	2.02	0.42
28:J:106:LMU:H1B	28:J:106:LMU:H5'	1.81	0.42
4:5:88:TRP:CD1	22:5:310:CLA:HMD3	2.55	0.42
24:7:315:LUT:H35	24:7:315:LUT:H401	1.81	0.42
9:A:297:HIS:HE2	22:A:818:CLA:C2B	2.33	0.42
9:A:345:LEU:HB3	9:A:352:GLN:HE21	1.85	0.42
22:A:826:CLA:CGA	26:A:849:BCR:H14C	2.50	0.42
26:A:848:BCR:H15C	26:A:848:BCR:H351	1.79	0.42
10:B:661:PHE:HD1	10:B:664:LEU:HD12	1.84	0.42
22:B:804:CLA:H41	22:B:804:CLA:H62	1.57	0.42
22:B:808:CLA:HBD	22:B:808:CLA:H122	2.01	0.42
14:F:164:ALA:HA	14:F:169:HIS:HB2	2.02	0.42
22:G:202:CLA:HBA1	22:G:202:CLA:H3A	1.69	0.42
26:J:103:BCR:H11C	26:J:103:BCR:H341	1.87	0.42
2:2:255:VAL:HG23	2:2:256:LEU:HD12	2.02	0.42
24:3:415:LUT:H35	24:3:415:LUT:H401	1.78	0.42
6:7:158:GLU:HG3	23:7:304:CHL:HHB	2.02	0.42
26:A:846:BCR:H24C	26:A:846:BCR:H371	1.83	0.42
26:A:849:BCR:H24C	26:A:849:BCR:H371	1.78	0.42
10:B:352:MET:HE2	10:B:352:MET:HB3	1.95	0.42
26:B:851:BCR:H351	26:B:851:BCR:H15C	1.79	0.42
26:L:301:BCR:H371	26:L:301:BCR:H24C	1.76	0.42
8:9:147:LEU:HD13	23:9:605:CHL:HHB	2.02	0.42
10:B:31:PHE:HA	10:B:34:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:5:VAL:HG22	11:C:67:VAL:HG22	2.02	0.42
1:1:123:TRP:HB2	25:1:315:XAT:H23	2.02	0.41
3:3:255:THR:O	3:3:259:LYS:HG2	2.20	0.41
26:3:417:BCR:H292	23:3:422:CHL:HMD2	2.02	0.41
22:A:805:CLA:HBA2	22:A:805:CLA:H12	1.86	0.41
26:F:801:BCR:H24C	26:F:801:BCR:H371	1.88	0.41
26:G:204:BCR:H20C	26:G:204:BCR:H361	1.93	0.41
7:8:85:ARG:HB3	22:8:610:CLA:HBC2	2.02	0.41
22:A:801:CLA:HAB	22:B:805:CLA:C1A	2.50	0.41
22:B:809:CLA:HBA1	22:B:809:CLA:H3A	1.64	0.41
28:G:201:LMU:H22	28:G:201:LMU:H51	1.88	0.41
2:2:70:ARG:HB3	2:2:75:ALA:HB3	2.00	0.41
6:7:166:GLU:O	6:7:170:TRP:HB2	2.20	0.41
22:B:803:CLA:H142	22:B:803:CLA:H111	1.91	0.41
12:D:141:ARG:HB2	12:D:144:GLN:HG3	2.01	0.41
25:6:320:XAT:H35	25:6:320:XAT:H401	1.87	0.41
22:8:609:CLA:HBA2	22:8:609:CLA:H3A	1.53	0.41
26:9:615:BCR:H20C	26:9:615:BCR:H361	1.80	0.41
22:A:817:CLA:HBA2	22:A:817:CLA:H3A	1.58	0.41
22:B:817:CLA:H3A	26:B:848:BCR:HC41	2.02	0.41
26:L:305:BCR:H11C	26:L:305:BCR:H341	1.84	0.41
24:1:314:LUT:H31	24:1:314:LUT:H391	1.94	0.41
22:2:607:CLA:HMA1	22:H:203:CLA:H3A	2.02	0.41
28:3:421:LMU:H81	28:3:421:LMU:H51	1.74	0.41
5:6:78:GLU:HG2	5:6:141:ILE:HG13	2.02	0.41
24:9:613:LUT:H35	24:9:613:LUT:H401	1.93	0.41
28:9:618:LMU:H101	28:9:618:LMU:H72	1.85	0.41
10:B:687:LEU:HB2	26:L:301:BCR:H281	2.01	0.41
22:B:840:CLA:H3A	22:B:841:CLA:OBD	2.20	0.41
26:M:102:BCR:H24C	26:M:102:BCR:H371	1.75	0.41
22:1:308:CLA:H52	24:1:314:LUT:H30	2.01	0.41
26:3:419:BCR:H11C	26:3:419:BCR:H341	1.82	0.41
6:7:151:GLN:HG3	7:8:255:PHE:HE2	1.85	0.41
7:8:229:HIS:CG	22:8:613:CLA:HAA2	2.55	0.41
8:9:199:ARG:HA	8:9:202:MET:HE3	2.02	0.41
2:2:165:TYR:HD1	2:2:166:LYS:HD2	1.86	0.41
3:3:220:LEU:HD13	26:3:419:BCR:H282	2.02	0.41
5:6:127:LEU:O	5:6:131:HIS:HB2	2.21	0.41
9:A:81:LEU:HD11	22:A:812:CLA:HBA2	2.02	0.41
9:A:408:HIS:CE1	22:A:829:CLA:NA	2.88	0.41
9:A:547:VAL:HG21	22:A:838:CLA:HMA1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:389:HIS:CE1	22:B:832:CLA:NA	2.88	0.41
22:B:806:CLA:HED3	22:B:806:CLA:HBD	1.79	0.41
26:B:850:BCR:H20C	26:B:850:BCR:H361	1.84	0.41
16:H:89:LEU:HD23	16:H:89:LEU:HA	1.91	0.41
24:3:415:LUT:H15	24:3:415:LUT:H201	1.86	0.41
23:7:305:CHL:H192	22:7:307:CLA:H12	2.03	0.41
24:8:617:LUT:H401	24:8:617:LUT:H35	1.79	0.41
9:A:363:LEU:HD11	22:A:818:CLA:H52	2.02	0.41
22:B:802:CLA:HBA1	22:B:802:CLA:H3A	1.89	0.41
22:B:815:CLA:H91	22:B:815:CLA:H111	1.81	0.41
26:B:847:BCR:H11C	26:B:847:BCR:H341	1.85	0.41
22:2:602:CLA:H71	22:2:603:CLA:HMA1	2.02	0.41
22:6:304:CLA:CBB	25:6:320:XAT:H12	2.51	0.41
25:7:316:XAT:H31	25:7:316:XAT:H391	1.84	0.41
8:9:111:ARG:HA	8:9:114:MET:HE3	2.03	0.41
25:9:614:XAT:H173	22:B:815:CLA:H112	2.01	0.41
9:A:45:THR:HB	9:A:716:ARG:HG3	2.02	0.41
9:A:561:ARG:HD3	11:C:80:SER:HB2	2.01	0.41
22:A:809:CLA:HBA2	22:A:809:CLA:H3A	1.64	0.41
22:A:823:CLA:H122	22:A:823:CLA:H161	1.87	0.41
10:B:707:LEU:HD23	34:B:852:DGD:HA21	2.02	0.41
22:B:806:CLA:H143	22:B:806:CLA:H161	1.88	0.41
22:B:823:CLA:HBA2	22:B:823:CLA:H3A	1.54	0.41
26:J:101:BCR:H20C	26:J:101:BCR:H361	1.89	0.41
3:3:100:LEU:HD23	22:3:401:CLA:HED3	2.02	0.41
10:B:493:TRP:HE1	22:B:837:CLA:HED1	1.85	0.41
24:1:314:LUT:H15	24:1:314:LUT:H201	1.90	0.40
9:A:102:GLU:HA	9:A:105:LEU:HD12	2.02	0.40
27:A:845:LHG:H272	27:A:845:LHG:H151	2.02	0.40
10:B:651:LEU:HD23	22:B:803:CLA:H11	2.02	0.40
22:B:816:CLA:H152	22:B:816:CLA:H111	1.83	0.40
26:J:103:BCR:H20C	26:J:103:BCR:H361	1.87	0.40
4:5:142:TRP:HB2	23:6:303:CHL:H11	2.03	0.40
22:9:606:CLA:H72	22:9:606:CLA:H111	1.92	0.40
9:A:729:ALA:HA	27:A:844:LHG:H322	2.03	0.40
9:A:733:LEU:HD21	22:A:829:CLA:H193	2.03	0.40
22:A:812:CLA:H2	22:A:812:CLA:H61	1.75	0.40
22:B:808:CLA:H91	22:B:808:CLA:H112	1.91	0.40
22:B:811:CLA:H72	26:B:851:BCR:H382	2.03	0.40
15:G:71:ILE:HD13	15:G:146:GLY:HA3	2.02	0.40
26:I:201:BCR:H15C	26:I:201:BCR:H351	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:61:LEU:HD12	1:1:62:PRO:HD2	2.02	0.40
1:1:182:ASP:HB2	22:1:308:CLA:HBD	2.03	0.40
26:3:417:BCR:H20C	26:3:417:BCR:H361	1.81	0.40
5:6:83:HIS:NE2	22:6:305:CLA:NB	2.69	0.40
31:9:617:LMG:H142	31:9:617:LMG:H171	1.89	0.40
9:A:680:ALA:HB3	22:B:802:CLA:HBB2	2.02	0.40
16:H:77:LEU:HD13	20:L:123:LEU:HD23	2.03	0.40
2:2:241:TYR:HA	2:2:246:GLY:HA2	2.03	0.40
22:5:303:CLA:H203	22:5:314:CLA:H143	2.04	0.40
22:6:307:CLA:H62	22:6:307:CLA:H102	1.92	0.40
9:A:121:ILE:HD13	26:J:101:BCR:H402	2.04	0.40
9:A:448:LEU:HB3	9:A:541:PHE:HB2	2.04	0.40
26:A:849:BCR:H15C	26:A:849:BCR:H351	1.77	0.40
22:B:811:CLA:H62	22:B:811:CLA:H102	1.76	0.40
11:C:15:THR:HG22	11:C:28:MET:HE2	2.03	0.40
5:6:166:PRO:HG3	22:6:309:CLA:HBC2	2.04	0.40
7:8:175:PRO:HB3	23:8:608:CHL:HBC2	2.03	0.40
28:9:618:LMU:H22	27:B:801:LHG:H281	2.04	0.40
22:A:805:CLA:H52	27:A:844:LHG:H261	2.03	0.40
26:B:849:BCR:H11C	26:B:849:BCR:H341	1.94	0.40
26:B:850:BCR:H11C	26:B:850:BCR:H341	1.96	0.40
26:M:102:BCR:H15C	26:M:102:BCR:H351	1.90	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	1	190/248 (77%)	173 (91%)	17 (9%)	0	100	100
2	2	208/270 (77%)	193 (93%)	15 (7%)	0	100	100
3	3	221/308 (72%)	214 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	5	228/271 (84%)	220 (96%)	8 (4%)	0	100	100
5	6	232/266 (87%)	220 (95%)	12 (5%)	0	100	100
6	7	219/279 (78%)	215 (98%)	4 (2%)	0	100	100
7	8	228/263 (87%)	215 (94%)	12 (5%)	1 (0%)	30	53
8	9	180/249 (72%)	163 (91%)	17 (9%)	0	100	100
9	A	739/751 (98%)	716 (97%)	23 (3%)	0	100	100
10	B	732/734 (100%)	711 (97%)	21 (3%)	0	100	100
11	C	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
12	D	141/239 (59%)	135 (96%)	6 (4%)	0	100	100
13	E	60/111 (54%)	59 (98%)	1 (2%)	0	100	100
14	F	163/250 (65%)	161 (99%)	2 (1%)	0	100	100
15	G	90/163 (55%)	88 (98%)	2 (2%)	0	100	100
16	H	52/126 (41%)	48 (92%)	4 (8%)	0	100	100
17	I	32/106 (30%)	30 (94%)	2 (6%)	0	100	100
18	J	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
19	K	82/126 (65%)	79 (96%)	3 (4%)	0	100	100
20	L	119/176 (68%)	113 (95%)	6 (5%)	0	100	100
21	M	30/32 (94%)	30 (100%)	0	0	100	100
All	All	4063/5090 (80%)	3895 (96%)	167 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	8	244	SER

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	1	143/184 (78%)	143 (100%)	0	100	100
2	2	163/207 (79%)	163 (100%)	0	100	100
3	3	181/245 (74%)	181 (100%)	0	100	100
4	5	184/213 (86%)	184 (100%)	0	100	100
5	6	189/212 (89%)	189 (100%)	0	100	100
6	7	175/213 (82%)	175 (100%)	0	100	100
7	8	177/202 (88%)	177 (100%)	0	100	100
8	9	147/201 (73%)	147 (100%)	0	100	100
9	A	604/614 (98%)	604 (100%)	0	100	100
10	B	595/595 (100%)	595 (100%)	0	100	100
11	C	70/70 (100%)	70 (100%)	0	100	100
12	D	119/194 (61%)	119 (100%)	0	100	100
13	E	53/89 (60%)	53 (100%)	0	100	100
14	F	130/190 (68%)	130 (100%)	0	100	100
15	G	69/129 (54%)	69 (100%)	0	100	100
16	H	42/101 (42%)	42 (100%)	0	100	100
17	I	28/76 (37%)	28 (100%)	0	100	100
18	J	36/37 (97%)	36 (100%)	0	100	100
19	K	60/87 (69%)	60 (100%)	0	100	100
20	L	92/140 (66%)	92 (100%)	0	100	100
21	M	27/27 (100%)	27 (100%)	0	100	100
All	All	3284/4026 (82%)	3284 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	229	GLN
2	2	196	GLN
4	5	170	ASN
4	5	225	ASN
4	5	236	ASN
5	6	69	ASN
5	6	147	GLN

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Mol	Chain	Res	Type
6	7	101	GLN
6	7	276	ASN
7	8	227	GLN
8	9	77	GLN
8	9	123	GLN
8	9	157	HIS
8	9	191	GLN
8	9	197	ASN
8	9	234	ASN
9	A	20	ASN
9	A	216	HIS
9	A	296	HIS
9	A	615	GLN
9	A	722	GLN
10	B	10	GLN
10	B	53	GLN
10	B	156	HIS
10	B	299	HIS
10	B	368	GLN
10	B	520	HIS
10	B	585	ASN
10	B	605	ASN
10	B	608	GLN
10	B	630	GLN
10	B	704	GLN
12	D	144	GLN
12	D	195	ASN
13	E	79	GLN
14	F	236	ASN
21	M	7	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

307 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	$\#\|Z\| > 2$
22	CLA	B	827	-	60,64,73	1.36	7 (11%)	72,102,113	1.29	7 (9%)
23	CHL	9	601	8	47,51,74	1.01	3 (6%)	52,86,114	1.78	8 (15%)
31	LMG	J	105	-	41,41,55	1.03	2 (4%)	49,49,63	1.06	4 (8%)
23	CHL	6	303	5	70,74,74	0.83	5 (7%)	80,114,114	1.30	8 (10%)
31	LMG	J	104	-	42,42,55	1.04	2 (4%)	50,50,63	1.08	3 (6%)
22	CLA	7	306	-	54,58,73	1.43	6 (11%)	65,95,113	1.29	7 (10%)
23	CHL	5	302	4	67,71,74	0.83	2 (2%)	76,110,114	1.46	10 (13%)
24	LUT	6	319	-	42,43,43	0.71	0	51,60,60	1.61	13 (25%)
33	SF4	C	101	11	0,12,12	-	-	-		
22	CLA	B	816	10	69,73,73	1.26	6 (8%)	83,113,113	1.29	8 (9%)
26	BCR	A	846	-	41,41,41	0.67	0	56,56,56	2.04	16 (28%)
22	CLA	5	304	4	53,57,73	1.47	8 (15%)	67,94,113	1.59	10 (14%)
22	CLA	5	305	4	53,57,73	1.50	8 (15%)	67,94,113	1.32	6 (8%)
22	CLA	A	815	-	49,53,73	1.49	6 (12%)	59,89,113	1.40	8 (13%)
22	CLA	B	819	10	58,62,73	1.36	6 (10%)	69,99,113	1.21	5 (7%)
22	CLA	3	407	3	69,73,73	1.27	6 (8%)	83,113,113	1.21	8 (9%)
25	XAT	6	320	-	39,47,47	0.86	0	54,74,74	2.56	20 (37%)
22	CLA	B	826	10	47,51,73	1.49	6 (12%)	56,86,113	1.25	4 (7%)
22	CLA	B	834	10	47,51,73	1.48	6 (12%)	56,86,113	1.34	7 (12%)
23	CHL	5	318	4	50,54,74	1.04	4 (8%)	56,90,114	1.53	9 (16%)
33	SF4	C	102	11	0,12,12	-	-	-		
28	LMU	1	319	-	36,36,36	1.19	3 (8%)	47,47,47	1.27	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	1	312	1	69,73,73	1.26	6 (8%)	83,113,113	1.11	6 (7%)
26	BCR	K	203	-	41,41,41	0.70	0	56,56,56	2.03	15 (26%)
26	BCR	L	301	-	41,41,41	0.69	0	56,56,56	1.96	14 (25%)
22	CLA	B	830	10	64,68,73	1.29	6 (9%)	77,107,113	1.15	6 (7%)
28	LMU	6	323	-	33,33,36	1.21	2 (6%)	44,44,47	1.23	4 (9%)
26	BCR	B	850	-	41,41,41	0.70	0	56,56,56	1.98	16 (28%)
22	CLA	A	834	9	61,65,73	1.34	7 (11%)	73,103,113	1.17	4 (5%)
30	NEX	6	321	-	38,46,46	0.89	1 (2%)	50,70,70	2.28	14 (28%)
22	CLA	B	823	10	59,63,73	1.38	6 (10%)	71,101,113	1.27	4 (5%)
22	CLA	B	825	10	62,66,73	1.33	7 (11%)	74,104,113	1.25	6 (8%)
22	CLA	B	815	10	69,73,73	1.26	7 (10%)	83,113,113	1.32	7 (8%)
22	CLA	A	804	9	65,69,73	1.29	7 (10%)	78,108,113	1.30	6 (7%)
23	CHL	5	306	4	49,53,74	1.14	5 (10%)	53,88,114	1.67	9 (16%)
22	CLA	A	802	9	69,73,73	1.25	6 (8%)	83,113,113	1.31	6 (7%)
28	LMU	G	201	-	36,36,36	1.19	3 (8%)	47,47,47	1.13	3 (6%)
22	CLA	B	835	10	64,68,73	1.31	6 (9%)	77,107,113	1.33	6 (7%)
22	CLA	A	824	-	68,72,73	1.26	6 (8%)	81,111,113	1.30	7 (8%)
29	K3I	2	616	-	43,43,43	0.17	0	58,60,60	0.41	0
22	CLA	L	304	-	42,45,73	1.56	7 (16%)	50,78,113	1.30	4 (8%)
28	LMU	F	806	-	30,30,36	1.30	2 (6%)	41,41,47	0.85	0
30	NEX	5	323	-	38,46,46	0.87	1 (2%)	50,70,70	2.17	12 (24%)
22	CLA	7	310	6	48,52,73	1.54	7 (14%)	58,88,113	1.37	6 (10%)
22	CLA	1	310	1	45,50,73	1.53	7 (15%)	53,85,113	1.29	5 (9%)
28	LMU	9	618	-	36,36,36	1.18	2 (5%)	47,47,47	1.11	3 (6%)
22	CLA	G	202	15	59,63,73	1.37	6 (10%)	71,101,113	1.27	4 (5%)
28	LMU	J	106	-	36,36,36	1.20	3 (8%)	47,47,47	1.13	2 (4%)
22	CLA	6	314	-	69,73,73	1.27	5 (7%)	83,113,113	1.19	6 (7%)
22	CLA	B	814	10	56,61,73	1.45	6 (10%)	70,99,113	1.26	8 (11%)
28	LMU	3	423	-	36,36,36	1.18	2 (5%)	47,47,47	1.05	2 (4%)
26	BCR	A	847	-	41,41,41	0.69	0	56,56,56	1.90	13 (23%)
31	LMG	8	621	23	25,25,55	1.08	2 (8%)	32,32,63	1.32	2 (6%)
26	BCR	A	848	-	41,41,41	0.69	0	56,56,56	1.95	17 (30%)
22	CLA	2	612	2	69,73,73	1.28	7 (10%)	83,113,113	1.16	5 (6%)
26	BCR	B	848	-	41,41,41	0.68	0	56,56,56	1.93	14 (25%)
22	CLA	A	828	9	69,73,73	1.27	8 (11%)	83,113,113	1.20	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	2	611	2	45,49,73	1.54	6 (13%)	54,84,113	1.42	7 (12%)
27	LHG	2	617	-	39,39,48	1.04	2 (5%)	42,45,54	1.13	3 (7%)
22	CLA	5	314	4	63,67,73	1.32	5 (7%)	75,105,113	1.23	6 (8%)
23	CHL	3	406	-	70,74,74	0.88	4 (5%)	80,114,114	1.32	11 (13%)
22	CLA	9	606	-	61,65,73	1.34	6 (9%)	73,103,113	1.24	6 (8%)
22	CLA	K	205	19	46,50,73	1.51	6 (13%)	55,85,113	1.41	4 (7%)
22	CLA	A	805	9	68,72,73	1.27	7 (10%)	81,111,113	1.16	5 (6%)
26	BCR	J	101	-	41,41,41	0.69	0	56,56,56	2.15	15 (26%)
25	XAT	3	416	-	39,47,47	0.87	0	54,74,74	2.65	22 (40%)
27	LHG	9	616	-	44,44,48	1.00	2 (4%)	47,50,54	1.06	2 (4%)
26	BCR	B	851	-	41,41,41	0.71	0	56,56,56	1.68	12 (21%)
28	LMU	6	301	-	36,36,36	1.17	2 (5%)	47,47,47	1.13	4 (8%)
22	CLA	6	310	5	47,51,73	1.49	6 (12%)	56,86,113	1.29	6 (10%)
22	CLA	A	817	9	60,64,73	1.35	7 (11%)	72,102,113	1.20	5 (6%)
22	CLA	8	611	27	47,51,73	1.48	7 (14%)	56,86,113	1.39	8 (14%)
22	CLA	A	803	9	56,60,73	1.39	6 (10%)	67,97,113	1.28	9 (13%)
22	CLA	K	204	-	59,63,73	1.37	6 (10%)	71,101,113	1.19	5 (7%)
26	BCR	J	103	-	41,41,41	0.69	0	56,56,56	1.82	16 (28%)
22	CLA	2	602	2	69,73,73	1.25	6 (8%)	83,113,113	1.24	8 (9%)
22	CLA	B	811	10	69,73,73	1.25	6 (8%)	83,113,113	1.16	7 (8%)
28	LMU	K	201	-	36,36,36	1.19	3 (8%)	47,47,47	1.16	4 (8%)
22	CLA	9	609	-	60,64,73	1.35	7 (11%)	72,102,113	1.42	8 (11%)
22	CLA	6	311	5	57,61,73	1.40	6 (10%)	68,98,113	1.36	10 (14%)
27	LHG	M	101	-	33,33,48	1.13	2 (6%)	36,39,54	1.09	2 (5%)
22	CLA	1	302	1	46,50,73	1.53	8 (17%)	55,85,113	2.06	14 (25%)
22	CLA	3	404	-	65,69,73	1.31	6 (9%)	78,108,113	1.26	8 (10%)
27	LHG	1	317	22	48,48,48	0.94	2 (4%)	51,54,54	1.00	3 (5%)
28	LMU	3	421	-	36,36,36	1.12	2 (5%)	47,47,47	1.43	7 (14%)
22	CLA	A	806	9	54,58,73	1.40	5 (9%)	65,95,113	1.33	8 (12%)
26	BCR	7	317	-	41,41,41	0.69	0	56,56,56	2.18	16 (28%)
22	CLA	A	809	9	64,68,73	1.31	5 (7%)	77,107,113	1.16	3 (3%)
22	CLA	A	837	9	59,63,73	1.36	6 (10%)	71,101,113	1.24	8 (11%)
22	CLA	3	411	3	56,61,73	1.41	8 (14%)	66,98,113	1.19	4 (6%)
22	CLA	B	843	10	69,73,73	1.27	7 (10%)	83,113,113	1.14	6 (7%)
22	CLA	B	828	-	54,58,73	1.42	7 (12%)	65,95,113	1.24	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	6	309	-	46,50,73	1.53	5 (10%)	55,85,113	1.32	6 (10%)
23	CHL	3	413	-	64,68,74	0.92	5 (7%)	72,106,114	1.31	10 (13%)
22	CLA	8	604	7	48,52,73	1.59	6 (12%)	61,88,113	1.47	10 (16%)
22	CLA	B	813	10	61,65,73	1.33	5 (8%)	72,102,113	1.25	4 (5%)
22	CLA	7	302	6	47,52,73	1.55	6 (12%)	56,88,113	1.41	8 (14%)
22	CLA	B	836	10	59,63,73	1.37	8 (13%)	71,101,113	1.20	4 (5%)
22	CLA	B	808	10	69,73,73	1.25	6 (8%)	83,113,113	1.22	9 (10%)
22	CLA	B	821	10	64,68,73	1.30	6 (9%)	77,107,113	1.25	8 (10%)
24	LUT	1	314	-	42,43,43	0.72	0	51,60,60	1.62	9 (17%)
22	CLA	H	202	16	37,43,73	1.73	7 (18%)	49,76,113	1.38	7 (14%)
22	CLA	7	307	6	69,73,73	1.25	5 (7%)	83,113,113	1.15	6 (7%)
23	CHL	1	304	1	56,60,74	1.01	4 (7%)	63,97,114	1.43	10 (15%)
23	CHL	1	305	-	50,54,74	0.89	2 (4%)	56,90,114	2.32	11 (19%)
23	CHL	6	308	-	50,54,74	1.12	5 (10%)	56,90,114	1.54	12 (21%)
22	CLA	A	816	9	64,68,73	1.28	8 (12%)	77,107,113	1.22	6 (7%)
26	BCR	3	419	-	41,41,41	0.69	0	56,56,56	2.04	15 (26%)
25	XAT	2	615	-	39,47,47	0.86	0	54,74,74	2.60	18 (33%)
22	CLA	B	842	-	69,73,73	1.26	8 (11%)	83,113,113	1.15	6 (7%)
22	CLA	5	303	4	69,73,73	1.28	8 (11%)	83,113,113	1.20	8 (9%)
26	BCR	5	322	-	41,41,41	0.68	0	56,56,56	2.12	19 (33%)
24	LUT	2	614	-	42,43,43	0.71	0	51,60,60	1.81	12 (23%)
22	CLA	B	833	10	47,51,73	1.49	8 (17%)	56,86,113	1.26	4 (7%)
23	CHL	7	304	-	51,55,74	1.09	5 (9%)	57,91,114	1.43	9 (15%)
27	LHG	A	845	22	44,44,48	0.97	2 (4%)	47,50,54	0.99	3 (6%)
22	CLA	6	316	-	69,73,73	1.25	6 (8%)	83,113,113	1.17	5 (6%)
22	CLA	6	317	5	43,47,73	1.55	6 (13%)	49,81,113	1.30	4 (8%)
24	LUT	8	617	-	42,43,43	0.73	0	51,60,60	1.64	13 (25%)
22	CLA	A	813	9	54,58,73	1.42	6 (11%)	65,95,113	1.37	8 (12%)
22	CLA	A	821	9	46,50,73	1.51	6 (13%)	55,85,113	1.27	4 (7%)
22	CLA	B	820	10	63,67,73	1.33	7 (11%)	75,105,113	1.18	5 (6%)
22	CLA	7	313	6	44,48,73	1.61	7 (15%)	56,83,113	1.37	7 (12%)
26	BCR	1	316	-	41,41,41	0.68	0	56,56,56	2.00	10 (17%)
22	CLA	1	313	-	43,47,73	1.63	7 (16%)	55,82,113	1.53	6 (10%)
22	CLA	B	812	10	67,71,73	1.28	6 (8%)	80,110,113	1.20	6 (7%)
22	CLA	B	824	10	44,48,73	1.66	7 (15%)	51,82,113	1.35	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	A	820	-	64,68,73	1.32	7 (10%)	77,107,113	1.13	6 (7%)
26	BCR	M	102	-	41,41,41	0.69	0	56,56,56	1.90	10 (17%)
22	CLA	A	819	9	50,54,73	1.46	6 (12%)	60,90,113	1.25	4 (6%)
22	CLA	2	608	2	45,49,73	1.53	7 (15%)	54,84,113	1.36	6 (11%)
25	XAT	9	614	-	39,47,47	0.88	0	54,74,74	2.54	17 (31%)
22	CLA	8	615	7	47,51,73	1.64	9 (19%)	60,87,113	1.60	11 (18%)
22	CLA	7	308	6	67,71,73	1.27	6 (8%)	80,110,113	1.16	8 (10%)
22	CLA	8	610	7	65,69,73	1.30	7 (10%)	78,108,113	1.10	5 (6%)
22	CLA	2	603	2	43,48,73	1.56	6 (13%)	51,83,113	1.58	9 (17%)
22	CLA	8	613	7	69,73,73	1.28	7 (10%)	83,113,113	1.21	5 (6%)
26	BCR	9	615	-	41,41,41	0.68	0	56,56,56	2.12	20 (35%)
34	DGD	B	852	-	59,59,67	0.94	3 (5%)	73,73,81	0.94	3 (4%)
22	CLA	1	308	1	64,68,73	1.28	6 (9%)	77,107,113	1.20	8 (10%)
26	BCR	G	204	-	41,41,41	0.68	0	56,56,56	1.97	15 (26%)
22	CLA	A	808	9	54,58,73	1.42	7 (12%)	65,95,113	1.20	5 (7%)
32	PQN	A	842	-	34,34,34	0.41	0	42,45,45	1.01	3 (7%)
22	CLA	L	302	20	54,58,73	1.42	7 (12%)	65,95,113	1.32	9 (13%)
22	CLA	B	840	10	62,66,73	1.33	6 (9%)	74,104,113	1.23	7 (9%)
22	CLA	B	841	10	51,55,73	1.45	6 (11%)	61,91,113	1.31	7 (11%)
22	CLA	6	312	27	46,50,73	1.54	7 (15%)	55,85,113	1.40	6 (10%)
22	CLA	A	825	-	54,58,73	1.42	7 (12%)	65,95,113	1.28	7 (10%)
22	CLA	H	201	-	40,43,73	1.67	7 (17%)	51,76,113	1.55	6 (11%)
22	CLA	6	307	-	69,73,73	1.26	6 (8%)	83,113,113	1.15	6 (7%)
22	CLA	A	843	27	43,48,73	1.56	6 (13%)	51,83,113	1.32	5 (9%)
22	CLA	B	805	10	69,73,73	1.24	6 (8%)	83,113,113	1.12	7 (8%)
26	BCR	B	847	-	41,41,41	0.65	0	56,56,56	2.86	18 (32%)
23	CHL	5	309	-	52,56,74	1.04	3 (5%)	58,92,114	1.54	9 (15%)
22	CLA	1	303	-	44,48,73	1.61	7 (15%)	56,83,113	1.49	9 (16%)
22	CLA	K	202	19	45,49,73	1.54	7 (15%)	54,84,113	1.34	4 (7%)
22	CLA	B	829	10	69,73,73	1.26	8 (11%)	83,113,113	1.26	5 (6%)
22	CLA	3	401	3	64,68,73	1.30	6 (9%)	77,107,113	1.17	6 (7%)
25	XAT	7	316	-	39,47,47	0.86	0	54,74,74	2.62	21 (38%)
22	CLA	6	305	5	48,52,73	1.57	8 (16%)	61,88,113	1.42	7 (11%)
22	CLA	8	601	1	52,57,73	1.44	6 (11%)	62,94,113	1.26	7 (11%)
22	CLA	A	814	9	69,73,73	1.26	7 (10%)	83,113,113	1.21	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	3	408	3	69,73,73	1.25	7 (10%)	83,113,113	1.16	8 (9%)
24	LUT	7	315	-	42,43,43	0.75	0	51,60,60	1.72	12 (23%)
25	XAT	5	321	-	39,47,47	0.85	0	54,74,74	2.64	21 (38%)
22	CLA	2	609	2	45,49,73	1.58	8 (17%)	57,84,113	1.38	7 (12%)
22	CLA	A	831	9	49,53,73	1.48	6 (12%)	59,89,113	1.38	8 (13%)
22	CLA	H	203	-	46,50,73	1.50	7 (15%)	55,85,113	1.34	4 (7%)
22	CLA	B	831	10	69,73,73	1.27	7 (10%)	83,113,113	1.16	4 (4%)
27	LHG	8	620	22	48,48,48	0.95	2 (4%)	51,54,54	1.16	4 (7%)
22	CLA	3	414	3	43,48,73	1.56	6 (13%)	51,83,113	1.30	5 (9%)
22	CLA	6	315	5	49,53,73	1.50	7 (14%)	59,89,113	1.27	7 (11%)
23	CHL	5	307	-	70,74,74	1.00	5 (7%)	80,114,114	1.38	9 (11%)
23	CHL	9	605	-	51,55,74	1.12	4 (7%)	57,91,114	1.89	10 (17%)
22	CLA	9	607	8	49,53,73	1.49	5 (10%)	59,89,113	1.29	4 (6%)
24	LUT	3	418	-	42,43,43	0.77	0	51,60,60	1.83	13 (25%)
28	LMU	H	204	-	36,36,36	1.18	2 (5%)	47,47,47	1.30	5 (10%)
26	BCR	K	207	-	41,41,41	0.69	0	56,56,56	1.82	14 (25%)
22	CLA	8	609	7	49,53,73	1.50	6 (12%)	59,89,113	1.30	3 (5%)
22	CLA	A	833	9	64,68,73	1.31	5 (7%)	77,107,113	1.20	6 (7%)
28	LMU	A	853	-	34,35,36	1.28	3 (8%)	42,45,47	1.09	4 (9%)
22	CLA	A	827	9	54,58,73	1.40	7 (12%)	65,95,113	1.28	9 (13%)
22	CLA	5	311	4	63,67,73	1.30	9 (14%)	75,105,113	1.17	8 (10%)
22	CLA	8	616	7	54,58,73	1.42	6 (11%)	65,95,113	1.22	4 (6%)
22	CLA	7	309	27	63,67,73	1.31	6 (9%)	75,105,113	1.17	6 (8%)
26	BCR	I	201	-	41,41,41	0.71	0	56,56,56	2.04	17 (30%)
22	CLA	G	203	15	49,53,73	1.49	5 (10%)	59,89,113	1.47	7 (11%)
22	CLA	B	806	-	69,73,73	1.26	7 (10%)	83,113,113	1.20	8 (9%)
22	CLA	B	837	10	60,64,73	1.34	6 (10%)	72,102,113	1.23	5 (6%)
22	CLA	A	841	-	68,72,73	1.28	7 (10%)	81,111,113	1.18	7 (8%)
22	CLA	8	612	7	44,49,73	1.55	6 (13%)	52,84,113	1.46	6 (11%)
22	CLA	5	315	4	44,48,73	1.57	7 (15%)	52,82,113	1.41	9 (17%)
22	CLA	A	801	9	69,73,73	1.25	7 (10%)	83,113,113	1.13	8 (9%)
27	LHG	5	301	-	35,35,48	1.08	2 (5%)	38,41,54	1.15	3 (7%)
23	CHL	3	422	6	70,74,74	0.92	5 (7%)	80,114,114	1.47	9 (11%)
23	CHL	8	608	-	56,60,74	0.93	5 (8%)	63,97,114	1.42	13 (20%)
27	LHG	7	318	22	48,48,48	0.95	2 (4%)	51,54,54	0.97	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	2	606	-	42,45,73	1.57	7 (16%)	50,78,113	1.28	4 (8%)
22	CLA	6	318	5	69,73,73	1.25	6 (8%)	83,113,113	1.15	7 (8%)
24	LUT	3	415	-	42,43,43	0.71	0	51,60,60	1.58	7 (13%)
22	CLA	7	314	-	39,44,73	1.68	7 (17%)	52,78,113	1.49	6 (11%)
22	CLA	A	818	9	69,73,73	1.26	7 (10%)	83,113,113	1.20	8 (9%)
22	CLA	A	822	9	69,73,73	1.27	7 (10%)	83,113,113	1.15	6 (7%)
22	CLA	A	832	9	69,73,73	1.27	7 (10%)	83,113,113	1.15	6 (7%)
26	BCR	A	849	-	41,41,41	0.71	0	56,56,56	1.84	12 (21%)
22	CLA	A	836	9	54,58,73	1.40	5 (9%)	65,95,113	1.41	8 (12%)
27	LHG	B	801	-	36,36,48	1.08	2 (5%)	39,42,54	1.15	3 (7%)
22	CLA	3	403	-	69,73,73	1.26	6 (8%)	83,113,113	1.17	6 (7%)
22	CLA	8	605	-	47,51,73	1.50	6 (12%)	56,86,113	1.29	5 (8%)
22	CLA	K	206	19	45,49,73	1.53	6 (13%)	54,84,113	1.32	6 (11%)
27	LHG	1	318	22	25,25,48	1.29	2 (8%)	28,31,54	1.22	2 (7%)
23	CHL	8	606	-	70,74,74	1.00	5 (7%)	80,114,114	1.35	9 (11%)
22	CLA	L	303	20	64,68,73	1.32	6 (9%)	77,107,113	1.25	5 (6%)
22	CLA	5	310	4	69,73,73	1.27	5 (7%)	83,113,113	1.14	7 (8%)
22	CLA	9	608	8	69,73,73	1.26	7 (10%)	83,113,113	1.12	7 (8%)
28	LMU	7	319	-	36,36,36	1.21	3 (8%)	47,47,47	1.32	6 (12%)
22	CLA	9	612	8	45,49,73	1.53	6 (13%)	54,84,113	1.31	7 (12%)
24	LUT	5	320	-	42,43,43	0.73	0	51,60,60	1.67	13 (25%)
22	CLA	7	311	6	64,68,73	1.32	8 (12%)	77,107,113	1.17	4 (5%)
22	CLA	A	807	9	55,59,73	1.39	5 (9%)	66,96,113	1.25	5 (7%)
22	CLA	7	312	6	46,50,73	1.51	6 (13%)	55,85,113	1.31	7 (12%)
22	CLA	B	803	-	69,73,73	1.25	5 (7%)	83,113,113	1.22	6 (7%)
24	LUT	9	613	-	42,43,43	0.73	0	51,60,60	1.58	10 (19%)
22	CLA	7	301	6	69,73,73	1.26	6 (8%)	83,113,113	1.13	6 (7%)
22	CLA	9	603	8	59,63,73	1.38	5 (8%)	71,101,113	1.32	10 (14%)
22	CLA	B	807	10	45,49,73	1.53	7 (15%)	54,84,113	1.31	8 (14%)
22	CLA	1	301	1	65,69,73	1.31	7 (10%)	78,108,113	1.23	7 (8%)
32	PQN	B	845	-	34,34,34	0.49	0	42,45,45	0.97	2 (4%)
23	CHL	1	306	-	50,54,74	1.07	4 (8%)	56,90,114	1.44	10 (17%)
22	CLA	J	102	18	46,50,73	1.51	7 (15%)	55,85,113	1.33	3 (5%)
22	CLA	B	809	10	69,73,73	1.27	5 (7%)	83,113,113	1.21	6 (7%)
23	CHL	8	607	31	47,51,74	1.06	5 (10%)	52,86,114	1.57	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	5	312	27	46,50,73	1.51	6 (13%)	55,85,113	1.31	5 (9%)
28	LMU	6	302	-	34,34,36	1.20	2 (5%)	45,45,47	1.04	2 (4%)
22	CLA	2	605	2	41,44,73	1.58	8 (19%)	49,77,113	1.35	3 (6%)
26	BCR	A	851	-	41,41,41	0.73	0	56,56,56	2.40	20 (35%)
33	SF4	A	850	10,9	0,12,12	-	-	-		
22	CLA	B	804	-	60,64,73	1.34	7 (11%)	72,102,113	1.28	6 (8%)
28	LMU	3	420	-	29,29,36	1.31	2 (6%)	40,40,47	1.16	2 (5%)
22	CLA	2	607	2	45,49,73	1.51	7 (15%)	54,84,113	1.32	7 (12%)
22	CLA	5	316	4	45,50,73	1.60	7 (15%)	56,85,113	1.34	6 (10%)
22	CLA	9	611	8	46,50,73	1.51	7 (15%)	55,85,113	1.32	4 (7%)
28	LMU	A	852	-	31,31,36	1.25	2 (6%)	42,42,47	1.07	2 (4%)
26	BCR	F	805	-	41,41,41	0.69	0	56,56,56	2.01	18 (32%)
22	CLA	9	602	8	64,68,73	1.33	7 (10%)	77,107,113	1.17	5 (6%)
22	CLA	B	818	10	56,60,73	1.40	6 (10%)	67,97,113	1.24	5 (7%)
27	LHG	A	844	-	48,48,48	0.94	2 (4%)	51,54,54	0.94	2 (3%)
27	LHG	5	325	22	35,35,48	1.10	2 (5%)	38,41,54	1.13	3 (7%)
26	BCR	3	417	-	41,41,41	0.71	0	56,56,56	1.90	16 (28%)
22	CLA	1	311	-	69,73,73	1.27	6 (8%)	83,113,113	1.24	4 (4%)
25	XAT	1	315	-	39,47,47	0.83	0	54,74,74	2.55	19 (35%)
22	CLA	A	835	9	49,53,73	1.50	7 (14%)	59,89,113	1.32	6 (10%)
22	CLA	A	826	9	66,70,73	1.28	7 (10%)	79,109,113	1.29	7 (8%)
26	BCR	8	619	-	41,41,41	0.69	0	56,56,56	1.98	15 (26%)
26	BCR	L	305	-	41,41,41	0.68	0	56,56,56	1.92	11 (19%)
22	CLA	F	803	-	46,50,73	1.53	7 (15%)	55,85,113	1.48	8 (14%)
22	CLA	3	410	3	47,51,73	1.51	6 (12%)	56,86,113	1.43	10 (17%)
22	CLA	3	412	3	43,48,73	1.56	6 (13%)	51,83,113	1.31	8 (15%)
22	CLA	9	604	8	48,52,73	1.47	7 (14%)	56,87,113	1.36	5 (8%)
22	CLA	A	823	9	69,73,73	1.26	6 (8%)	83,113,113	1.19	6 (7%)
22	CLA	5	317	4	49,53,73	1.50	7 (14%)	59,89,113	1.33	3 (5%)
22	CLA	2	604	-	43,48,73	1.59	8 (18%)	51,83,113	1.42	4 (7%)
26	BCR	B	846	-	41,41,41	0.70	0	56,56,56	1.76	12 (21%)
23	CHL	8	603	7	70,74,74	0.93	4 (5%)	80,114,114	1.24	13 (16%)
22	CLA	2	610	2	43,47,73	1.56	7 (16%)	49,81,113	1.43	7 (14%)
22	CLA	B	802	-	64,68,73	1.29	7 (10%)	77,107,113	1.34	12 (15%)
27	LHG	6	322	22	47,47,48	0.95	2 (4%)	50,53,54	1.01	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	2	613	-	49,53,73	1.49	7 (14%)	59,89,113	1.37	6 (10%)
23	CHL	5	319	-	58,62,74	1.12	5 (8%)	65,99,114	1.17	7 (10%)
22	CLA	F	804	14	56,60,73	1.41	6 (10%)	67,97,113	1.30	7 (10%)
25	XAT	8	618	-	39,47,47	0.90	0	54,74,74	2.76	19 (35%)
22	CLA	B	810	10	63,67,73	1.31	6 (9%)	75,105,113	1.23	5 (6%)
22	CLA	7	303	-	54,58,73	1.43	6 (11%)	65,95,113	1.29	5 (7%)
22	CLA	B	817	10	59,63,73	1.35	7 (11%)	71,101,113	1.23	7 (9%)
22	CLA	6	313	5	44,49,73	1.55	6 (13%)	52,84,113	1.44	7 (13%)
22	CLA	A	812	9	68,72,73	1.26	6 (8%)	81,111,113	1.26	6 (7%)
22	CLA	3	409	3	59,63,73	1.36	6 (10%)	71,101,113	1.16	4 (5%)
23	CHL	8	602	7	70,74,74	0.96	5 (7%)	80,114,114	1.37	9 (11%)
22	CLA	B	844	27	69,73,73	1.27	8 (11%)	83,113,113	1.18	4 (4%)
22	CLA	8	614	7	64,68,73	1.29	6 (9%)	77,107,113	1.30	7 (9%)
26	BCR	F	801	-	41,41,41	0.66	0	56,56,56	1.84	17 (30%)
22	CLA	A	810	9	63,67,73	1.31	6 (9%)	75,105,113	1.12	6 (8%)
22	CLA	A	838	9	61,65,73	1.34	6 (9%)	73,103,113	1.19	9 (12%)
22	CLA	B	822	-	49,53,73	1.49	7 (14%)	59,89,113	1.34	7 (11%)
31	LMG	9	617	-	46,46,55	1.02	2 (4%)	54,54,63	0.92	3 (5%)
22	CLA	B	838	-	49,53,73	1.50	7 (14%)	59,89,113	1.32	7 (11%)
22	CLA	A	839	9	69,73,73	1.26	6 (8%)	83,113,113	1.16	5 (6%)
22	CLA	3	402	3	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
22	CLA	6	306	5	46,50,73	1.51	5 (10%)	55,85,113	1.30	4 (7%)
22	CLA	B	839	10	54,58,73	1.43	7 (12%)	65,95,113	1.28	6 (9%)
22	CLA	1	307	1	41,46,73	1.67	8 (19%)	52,81,113	1.32	6 (11%)
22	CLA	A	829	9	69,73,73	1.27	6 (8%)	83,113,113	1.12	3 (3%)
22	CLA	F	802	-	63,67,73	1.33	7 (11%)	75,105,113	1.17	5 (6%)
22	CLA	A	830	9	49,53,73	1.49	7 (14%)	59,89,113	1.31	7 (11%)
29	K3I	5	324	-	43,43,43	0.19	0	58,60,60	0.41	0
22	CLA	9	610	8	46,50,73	1.52	6 (13%)	55,85,113	1.49	9 (16%)
22	CLA	1	309	27	44,49,73	1.53	6 (13%)	52,84,113	1.33	6 (11%)
26	BCR	B	849	-	41,41,41	0.68	0	56,56,56	1.95	17 (30%)
22	CLA	B	832	10	59,63,73	1.37	7 (11%)	71,101,113	1.25	8 (11%)
22	CLA	A	811	9	58,62,73	1.37	7 (12%)	69,99,113	1.23	4 (5%)
23	CHL	3	405	3	57,61,74	0.90	5 (8%)	64,98,114	1.16	8 (12%)
22	CLA	2	601	2	57,61,73	1.37	7 (12%)	68,98,113	1.37	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CHL	5	308	-	70,74,74	0.90	5 (7%)	80,114,114	1.34	9 (11%)
22	CLA	5	313	4	44,49,73	1.55	6 (13%)	52,84,113	1.40	7 (13%)
22	CLA	6	304	5	69,73,73	1.26	6 (8%)	83,113,113	1.17	7 (8%)
22	CLA	A	840	9	46,50,73	1.52	7 (15%)	55,85,113	1.27	4 (7%)
23	CHL	7	305	-	70,74,74	0.78	4 (5%)	80,114,114	1.29	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	818	10	-	10/24/100/115	-
22	CLA	B	827	-	-	13/29/105/115	-
22	CLA	A	809	9	-	17/33/109/115	-
26	BCR	7	317	-	-	4/29/63/63	0/2/2/2
22	CLA	A	837	9	-	6/27/103/115	-
22	CLA	3	411	3	-	13/23/99/115	-
27	LHG	A	844	-	-	9/53/53/53	-
23	CHL	9	601	8	-	2/14/90/117	-
22	CLA	B	831	10	-	8/39/115/115	-
27	LHG	8	620	22	-	17/53/53/53	-
22	CLA	3	414	3	-	4/8/84/115	-
31	LMG	J	105	-	-	8/36/56/70	0/1/1/1
22	CLA	B	843	10	-	14/39/115/115	-
27	LHG	5	325	22	-	12/40/40/53	-
23	CHL	6	303	5	-	24/41/117/117	-
22	CLA	6	315	5	-	6/15/91/115	-
22	CLA	B	828	-	-	1/21/97/115	-
26	BCR	3	417	-	-	2/29/63/63	0/2/2/2
23	CHL	5	307	-	-	21/41/117/117	-
31	LMG	J	104	-	-	9/37/57/70	0/1/1/1
22	CLA	7	306	-	-	7/21/97/115	-
23	CHL	5	302	4	-	13/38/114/117	-
23	CHL	9	605	-	-	5/19/95/117	-
22	CLA	6	309	-	-	7/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	311	-	-	13/39/115/115	-
24	LUT	6	319	-	-	5/29/67/67	0/2/2/2
25	XAT	1	315	-	-	3/31/93/93	0/4/4/4
22	CLA	A	835	9	-	9/15/91/115	-
22	CLA	B	816	10	-	13/39/115/115	-
33	SF4	C	101	11	-	-	0/6/5/5
23	CHL	3	413	-	-	10/34/110/117	-
22	CLA	A	826	9	-	14/36/112/115	-
22	CLA	8	604	7	-	5/13/89/115	-
26	BCR	8	619	-	-	2/29/63/63	0/2/2/2
22	CLA	B	813	10	-	10/29/105/115	-
26	BCR	A	846	-	-	2/29/63/63	0/2/2/2
22	CLA	9	607	8	-	3/15/91/115	-
22	CLA	5	304	4	-	8/19/95/115	-
22	CLA	5	305	4	-	5/19/95/115	-
22	CLA	A	815	-	-	7/15/91/115	-
24	LUT	3	418	-	-	0/29/67/67	0/2/2/2
26	BCR	L	305	-	-	6/29/63/63	0/2/2/2
28	LMU	H	204	-	-	16/21/61/61	0/2/2/2
22	CLA	B	819	10	-	10/25/101/115	-
22	CLA	7	302	6	-	6/13/89/115	-
22	CLA	F	803	-	-	8/12/88/115	-
22	CLA	B	836	10	-	12/27/103/115	-
26	BCR	K	207	-	-	2/29/63/63	0/2/2/2
22	CLA	B	808	10	-	13/39/115/115	-
22	CLA	3	407	3	-	17/39/115/115	-
22	CLA	B	821	10	-	9/33/109/115	-
22	CLA	3	410	3	-	5/13/89/115	-
22	CLA	3	412	3	-	2/8/84/115	-
22	CLA	8	609	7	-	8/15/91/115	-
24	LUT	1	314	-	-	2/29/67/67	0/2/2/2
25	XAT	6	320	-	-	6/31/93/93	0/4/4/4
22	CLA	B	826	10	-	6/13/89/115	-
22	CLA	B	834	10	-	1/13/89/115	-
22	CLA	A	833	9	-	16/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	5	318	4	-	4/17/93/117	-
33	SF4	C	102	11	-	-	0/6/5/5
22	CLA	7	307	6	-	13/39/115/115	-
28	LMU	A	853	-	-	13/21/57/61	0/2/2/2
22	CLA	9	604	8	-	5/13/90/115	-
22	CLA	A	823	9	-	23/39/115/115	-
28	LMU	1	319	-	-	13/21/61/61	0/2/2/2
22	CLA	A	827	9	-	6/21/97/115	-
22	CLA	5	317	4	-	7/15/91/115	-
22	CLA	2	604	-	-	4/8/84/115	-
23	CHL	1	304	1	-	9/25/101/117	-
22	CLA	5	311	4	-	6/32/108/115	-
22	CLA	8	616	7	-	8/21/97/115	-
22	CLA	7	309	27	-	7/31/107/115	-
22	CLA	A	816	9	-	11/33/109/115	-
23	CHL	1	305	-	-	5/17/93/117	-
23	CHL	6	308	-	-	3/17/93/117	-
22	CLA	1	312	1	-	14/39/115/115	-
26	BCR	K	203	-	-	3/29/63/63	0/2/2/2
26	BCR	B	846	-	-	9/29/63/63	0/2/2/2
26	BCR	L	301	-	-	4/29/63/63	0/2/2/2
22	CLA	B	830	10	-	18/33/109/115	-
26	BCR	I	201	-	-	4/29/63/63	0/2/2/2
23	CHL	8	603	7	-	17/41/117/117	-
22	CLA	G	203	15	-	6/15/91/115	-
26	BCR	3	419	-	-	4/29/63/63	0/2/2/2
22	CLA	B	806	-	-	18/39/115/115	-
22	CLA	2	610	2	-	4/4/82/115	-
25	XAT	2	615	-	-	1/31/93/93	0/4/4/4
28	LMU	6	323	-	-	5/18/58/61	0/2/2/2
22	CLA	B	842	-	-	16/39/115/115	-
26	BCR	B	850	-	-	2/29/63/63	0/2/2/2
22	CLA	B	802	-	-	10/33/109/115	-
22	CLA	5	303	4	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	834	9	-	8/30/106/115	-
22	CLA	A	841	-	-	9/37/113/115	-
22	CLA	B	823	10	-	12/27/103/115	-
22	CLA	2	613	-	-	10/15/91/115	-
22	CLA	B	837	10	-	12/29/105/115	-
27	LHG	6	322	22	-	18/52/52/53	-
22	CLA	8	612	7	-	4/10/86/115	-
23	CHL	5	319	-	-	8/27/103/117	-
30	NEX	6	321	-	-	4/27/83/83	0/3/3/3
22	CLA	B	825	10	-	10/31/107/115	-
22	CLA	F	804	14	-	13/24/100/115	-
26	BCR	5	322	-	-	4/29/63/63	0/2/2/2
24	LUT	2	614	-	-	8/29/67/67	0/2/2/2
22	CLA	5	315	4	-	5/10/82/115	-
22	CLA	A	804	9	-	12/35/111/115	-
22	CLA	B	815	10	-	15/39/115/115	-
22	CLA	B	833	10	-	9/13/89/115	-
23	CHL	5	306	4	-	3/15/92/117	-
23	CHL	7	304	-	-	4/19/95/117	-
25	XAT	8	618	-	-	2/31/93/93	0/4/4/4
22	CLA	6	316	-	-	12/39/115/115	-
22	CLA	6	317	5	-	2/4/82/115	-
22	CLA	A	801	9	-	13/39/115/115	-
27	LHG	5	301	-	-	10/40/40/53	-
27	LHG	A	845	22	-	20/49/49/53	-
23	CHL	3	422	6	-	16/41/117/117	-
22	CLA	A	802	9	-	14/39/115/115	-
22	CLA	B	810	10	-	12/32/108/115	-
28	LMU	G	201	-	-	10/21/61/61	0/2/2/2
22	CLA	B	835	10	-	10/33/109/115	-
23	CHL	8	608	-	-	9/25/101/117	-
22	CLA	7	303	-	-	7/21/97/115	-
24	LUT	8	617	-	-	3/29/67/67	0/2/2/2
22	CLA	B	817	10	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	813	9	-	9/21/97/115	-
27	LHG	7	318	22	-	12/53/53/53	-
22	CLA	A	824	-	-	7/37/113/115	-
22	CLA	2	606	-	-	2/4/76/115	-
29	K3I	2	616	-	-	2/29/67/67	0/2/2/2
22	CLA	6	313	5	-	5/10/86/115	-
22	CLA	L	304	-	-	2/4/76/115	-
28	LMU	F	806	-	-	6/15/55/61	0/2/2/2
22	CLA	6	318	5	-	19/39/115/115	-
24	LUT	3	415	-	-	3/29/67/67	0/2/2/2
22	CLA	A	821	9	-	6/12/88/115	-
30	NEX	5	323	-	-	2/27/83/83	0/3/3/3
22	CLA	A	812	9	-	17/37/113/115	-
22	CLA	B	820	10	-	8/32/108/115	-
22	CLA	3	409	3	-	12/27/103/115	-
22	CLA	7	310	6	-	7/13/89/115	-
22	CLA	7	313	6	-	6/8/84/115	-
22	CLA	A	818	9	-	12/39/115/115	-
22	CLA	A	822	9	-	20/39/115/115	-
22	CLA	1	310	1	-	5/11/87/115	-
22	CLA	A	832	9	-	15/39/115/115	-
22	CLA	1	313	-	-	4/6/82/115	-
22	CLA	A	836	9	-	7/21/97/115	-
26	BCR	1	316	-	-	2/29/63/63	0/2/2/2
26	BCR	A	849	-	-	4/29/63/63	0/2/2/2
22	CLA	G	202	15	-	11/27/103/115	-
27	LHG	B	801	-	-	11/41/41/53	-
28	LMU	9	618	-	-	11/21/61/61	0/2/2/2
22	CLA	3	403	-	-	12/39/115/115	-
22	CLA	8	605	-	-	3/13/89/115	-
22	CLA	B	812	10	-	16/37/113/115	-
22	CLA	B	824	10	-	4/9/85/115	-
23	CHL	8	602	7	-	21/41/117/117	-
28	LMU	J	106	-	-	15/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	314	-	-	11/39/115/115	-
22	CLA	B	814	10	-	8/23/99/115	-
22	CLA	B	844	27	-	13/39/115/115	-
28	LMU	3	423	-	-	8/21/61/61	0/2/2/2
22	CLA	A	820	-	-	13/33/109/115	-
22	CLA	8	614	7	-	7/33/109/115	-
26	BCR	M	102	-	-	2/29/63/63	0/2/2/2
26	BCR	F	801	-	-	3/29/63/63	0/2/2/2
26	BCR	A	847	-	-	2/29/63/63	0/2/2/2
22	CLA	K	206	19	-	5/10/86/115	-
22	CLA	A	810	9	-	10/32/108/115	-
22	CLA	A	838	9	-	13/30/106/115	-
31	LMG	8	621	23	-	7/18/38/70	0/1/1/1
22	CLA	A	819	9	-	10/17/93/115	-
26	BCR	A	848	-	-	2/29/63/63	0/2/2/2
27	LHG	1	318	22	-	7/30/30/53	-
22	CLA	B	822	-	-	7/15/91/115	-
31	LMG	9	617	-	-	14/41/61/70	0/1/1/1
22	CLA	2	612	2	-	19/39/115/115	-
22	CLA	B	838	-	-	7/15/91/115	-
22	CLA	2	608	2	-	7/10/86/115	-
25	XAT	9	614	-	-	5/31/93/93	0/4/4/4
26	BCR	B	848	-	-	4/29/63/63	0/2/2/2
22	CLA	A	828	9	-	10/39/115/115	-
22	CLA	8	615	7	-	8/11/87/115	-
22	CLA	A	839	9	-	14/39/115/115	-
22	CLA	7	308	6	-	9/37/113/115	-
22	CLA	2	611	2	-	6/10/86/115	-
23	CHL	8	606	-	-	19/41/117/117	-
22	CLA	3	402	3	-	10/39/115/115	-
22	CLA	L	303	20	-	15/33/109/115	-
22	CLA	5	310	4	-	9/39/115/115	-
22	CLA	8	610	7	-	12/35/111/115	-
22	CLA	6	306	5	-	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	608	8	-	15/39/115/115	-
22	CLA	B	839	10	-	7/21/97/115	-
22	CLA	2	603	2	-	0/8/84/115	-
22	CLA	1	307	1	-	1/4/80/115	-
28	LMU	7	319	-	-	8/21/61/61	0/2/2/2
22	CLA	9	612	8	-	3/10/86/115	-
24	LUT	5	320	-	-	3/29/67/67	0/2/2/2
22	CLA	8	613	7	-	21/39/115/115	-
22	CLA	7	311	6	-	9/33/109/115	-
26	BCR	9	615	-	-	6/29/63/63	0/2/2/2
34	DGD	B	852	-	-	8/47/87/95	0/2/2/2
22	CLA	A	807	9	-	8/23/99/115	-
22	CLA	7	312	6	-	6/12/88/115	-
27	LHG	2	617	-	-	16/44/44/53	-
22	CLA	5	314	4	-	16/31/107/115	-
22	CLA	1	308	1	-	15/33/109/115	-
22	CLA	A	829	9	-	9/39/115/115	-
22	CLA	B	803	-	-	9/39/115/115	-
22	CLA	A	808	9	-	8/21/97/115	-
22	CLA	F	802	-	-	10/32/108/115	-
23	CHL	3	406	-	-	17/41/117/117	-
22	CLA	9	606	-	-	10/30/106/115	-
22	CLA	K	205	19	-	9/12/88/115	-
22	CLA	B	840	10	-	7/31/107/115	-
22	CLA	L	302	20	-	10/21/97/115	-
24	LUT	9	613	-	-	3/29/67/67	0/2/2/2
22	CLA	B	841	10	-	5/18/94/115	-
22	CLA	6	312	27	-	7/12/88/115	-
22	CLA	7	301	6	-	14/39/115/115	-
22	CLA	9	603	8	-	15/27/103/115	-
22	CLA	A	805	9	-	15/37/113/115	-
22	CLA	B	807	10	-	2/10/86/115	-
22	CLA	A	830	9	-	9/15/91/115	-
29	K3I	5	324	-	-	0/29/67/67	0/2/2/2
22	CLA	1	301	1	-	12/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PQN	B	845	-	-	2/23/43/43	0/2/2/2
22	CLA	A	825	-	-	6/21/97/115	-
23	CHL	1	306	-	-	7/17/93/117	-
22	CLA	9	610	8	-	5/12/88/115	-
22	CLA	1	309	27	-	1/10/86/115	-
26	BCR	J	101	-	-	9/29/63/63	0/2/2/2
25	XAT	3	416	-	-	1/31/93/93	0/4/4/4
26	BCR	B	849	-	-	0/29/63/63	0/2/2/2
22	CLA	B	832	10	-	7/27/103/115	-
26	BCR	B	851	-	-	0/29/63/63	0/2/2/2
22	CLA	6	310	5	-	8/13/89/115	-
27	LHG	9	616	-	-	9/49/49/53	-
22	CLA	6	307	-	-	19/39/115/115	-
22	CLA	A	811	9	-	9/26/102/115	-
28	LMU	6	301	-	-	13/21/61/61	0/2/2/2
22	CLA	A	843	27	-	4/8/84/115	-
22	CLA	J	102	18	-	7/12/88/115	-
22	CLA	A	817	9	-	9/29/105/115	-
22	CLA	B	809	10	-	16/39/115/115	-
23	CHL	8	607	31	-	2/14/90/117	-
22	CLA	5	312	27	-	3/12/88/115	-
23	CHL	3	405	3	-	6/26/102/117	-
22	CLA	2	601	2	-	13/25/101/115	-
22	CLA	B	805	10	-	17/39/115/115	-
22	CLA	8	611	27	-	4/13/89/115	-
22	CLA	A	803	9	-	5/24/100/115	-
22	CLA	K	204	-	-	7/27/103/115	-
26	BCR	B	847	-	-	8/29/63/63	0/2/2/2
23	CHL	5	309	-	-	4/20/96/117	-
22	CLA	1	303	-	-	3/8/84/115	-
23	CHL	5	308	-	-	13/41/117/117	-
26	BCR	G	204	-	-	0/29/63/63	0/2/2/2
26	BCR	J	103	-	-	6/29/63/63	0/2/2/2
22	CLA	2	602	2	-	12/39/115/115	-
22	CLA	K	202	19	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMU	6	302	-	-	9/19/59/61	0/2/2/2
22	CLA	2	605	2	-	2/2/74/115	-
22	CLA	B	829	10	-	11/39/115/115	-
26	BCR	A	851	-	-	9/29/63/63	0/2/2/2
22	CLA	B	811	10	-	13/39/115/115	-
28	LMU	K	201	-	-	11/21/61/61	0/2/2/2
32	PQN	A	842	-	-	7/23/43/43	0/2/2/2
22	CLA	9	609	-	-	16/29/105/115	-
22	CLA	3	401	3	-	10/33/109/115	-
33	SF4	A	850	10,9	-	-	0/6/5/5
22	CLA	B	804	-	-	9/29/105/115	-
28	LMU	3	420	-	-	9/14/54/61	0/2/2/2
25	XAT	7	316	-	-	4/31/93/93	0/4/4/4
22	CLA	5	313	4	-	2/10/86/115	-
22	CLA	6	304	5	-	15/39/115/115	-
22	CLA	6	305	5	-	4/13/89/115	-
22	CLA	2	607	2	-	4/10/86/115	-
22	CLA	8	601	1	-	8/19/95/115	-
22	CLA	A	814	9	-	14/39/115/115	-
22	CLA	6	311	5	-	9/25/101/115	-
22	CLA	3	408	3	-	13/39/115/115	-
22	CLA	A	840	9	-	5/12/88/115	-
27	LHG	M	101	-	-	9/38/38/53	-
22	CLA	1	302	1	-	8/12/88/115	-
22	CLA	5	316	4	-	4/8/84/115	-
22	CLA	9	611	8	-	9/12/88/115	-
22	CLA	3	404	-	-	11/35/111/115	-
24	LUT	7	315	-	-	3/29/67/67	0/2/2/2
25	XAT	5	321	-	-	2/31/93/93	0/4/4/4
27	LHG	1	317	22	-	17/53/53/53	-
28	LMU	3	421	-	-	7/21/61/61	0/2/2/2
22	CLA	2	609	2	-	3/10/86/115	-
22	CLA	A	831	9	-	4/15/91/115	-
22	CLA	H	203	-	-	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMU	A	852	-	-	5/16/56/61	0/2/2/2
26	BCR	F	805	-	-	2/29/63/63	0/2/2/2
23	CHL	7	305	-	-	22/41/117/117	-
22	CLA	A	806	9	-	4/21/97/115	-
22	CLA	9	602	8	-	9/33/109/115	-

All (1442) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	5	319	CHL	MG-NA	4.80	2.17	2.06
23	9	605	CHL	MG-NA	4.65	2.17	2.06
23	5	307	CHL	MG-NA	4.48	2.16	2.06
31	9	617	LMG	O7-C10	4.40	1.46	1.34
22	8	615	CLA	C1D-ND	4.36	1.43	1.37
27	9	616	LHG	O8-C23	4.34	1.46	1.33
27	5	325	LHG	O8-C23	4.32	1.46	1.33
31	9	617	LMG	O8-C28	4.32	1.46	1.33
27	2	617	LHG	O8-C23	4.31	1.45	1.33
27	A	845	LHG	O8-C23	4.29	1.45	1.33
27	7	318	LHG	O8-C23	4.28	1.45	1.33
34	B	852	DGD	O1G-C1A	4.27	1.45	1.33
27	M	101	LHG	O8-C23	4.27	1.45	1.33
23	6	308	CHL	MG-NA	4.26	2.16	2.06
27	8	620	LHG	O7-C7	4.26	1.46	1.34
27	B	801	LHG	O8-C23	4.26	1.45	1.33
31	J	104	LMG	O8-C28	4.25	1.45	1.33
27	1	318	LHG	O8-C23	4.25	1.45	1.33
27	8	620	LHG	O8-C23	4.25	1.45	1.33
22	9	607	CLA	C1D-ND	4.25	1.43	1.37
27	A	844	LHG	O8-C23	4.24	1.45	1.33
27	5	301	LHG	O8-C23	4.24	1.45	1.33
27	1	317	LHG	O8-C23	4.24	1.45	1.33
22	5	310	CLA	C1D-ND	4.23	1.43	1.37
27	9	616	LHG	O7-C7	4.21	1.46	1.34
23	3	406	CHL	C4D-ND	-4.21	1.31	1.37
27	7	318	LHG	O7-C7	4.20	1.46	1.34
27	6	322	LHG	O8-C23	4.20	1.45	1.33
27	B	801	LHG	O7-C7	4.18	1.46	1.34
27	M	101	LHG	O7-C7	4.17	1.46	1.34
27	1	318	LHG	O7-C7	4.17	1.46	1.34
22	8	604	CLA	C1D-ND	4.17	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	6	322	LHG	O7-C7	4.17	1.46	1.34
31	J	105	LMG	O8-C28	4.17	1.45	1.33
22	F	803	CLA	C1D-ND	4.16	1.42	1.37
27	1	317	LHG	O7-C7	4.16	1.46	1.34
23	5	319	CHL	MG-NC	4.15	2.16	2.06
22	2	612	CLA	C1D-ND	4.15	1.42	1.37
31	8	621	LMG	O7-C10	4.15	1.46	1.34
22	6	309	CLA	C1D-ND	4.15	1.42	1.37
31	J	104	LMG	O7-C10	4.14	1.46	1.34
22	G	202	CLA	C1D-ND	4.14	1.42	1.37
34	B	852	DGD	O2G-C1B	4.13	1.46	1.34
22	3	407	CLA	C1D-ND	4.13	1.42	1.37
23	5	302	CHL	C4D-ND	-4.13	1.32	1.37
27	5	325	LHG	O7-C7	4.12	1.45	1.34
27	2	617	LHG	O7-C7	4.12	1.45	1.34
27	A	844	LHG	O7-C7	4.12	1.45	1.34
22	B	823	CLA	C1D-ND	4.11	1.42	1.37
22	1	311	CLA	C1D-ND	4.11	1.42	1.37
22	A	812	CLA	C1D-ND	4.10	1.42	1.37
22	2	604	CLA	C1D-ND	4.09	1.42	1.37
22	7	302	CLA	C1D-ND	4.09	1.42	1.37
22	9	603	CLA	C1D-ND	4.09	1.42	1.37
22	B	809	CLA	C1D-ND	4.09	1.42	1.37
22	3	402	CLA	C1D-ND	4.08	1.42	1.37
22	A	805	CLA	C1D-ND	4.08	1.42	1.37
23	1	305	CHL	C1C-NC	4.08	1.43	1.37
22	9	610	CLA	C1D-ND	4.08	1.42	1.37
22	G	203	CLA	C1D-ND	4.07	1.42	1.37
22	B	815	CLA	C1D-ND	4.07	1.42	1.37
23	8	606	CHL	MG-NA	4.06	2.15	2.06
22	2	603	CLA	C1D-ND	4.06	1.42	1.37
22	3	404	CLA	C1D-ND	4.06	1.42	1.37
22	B	829	CLA	C1D-ND	4.05	1.42	1.37
31	J	105	LMG	O7-C10	4.05	1.45	1.34
22	A	822	CLA	C1D-ND	4.05	1.42	1.37
23	8	603	CHL	C4D-ND	-4.04	1.32	1.37
22	8	613	CLA	C1D-ND	4.04	1.42	1.37
22	B	816	CLA	C1D-ND	4.04	1.42	1.37
22	3	410	CLA	C1D-ND	4.04	1.42	1.37
22	7	306	CLA	C1D-ND	4.03	1.42	1.37
22	A	832	CLA	C1D-ND	4.03	1.42	1.37
22	B	831	CLA	C1D-ND	4.03	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	616	CLA	C1D-ND	4.03	1.42	1.37
22	A	801	CLA	C1D-ND	4.03	1.42	1.37
22	6	313	CLA	C1D-ND	4.03	1.42	1.37
23	9	605	CHL	C4D-ND	-4.03	1.32	1.37
22	6	315	CLA	C1D-ND	4.02	1.42	1.37
22	A	802	CLA	C1D-ND	4.02	1.42	1.37
22	A	833	CLA	C1D-ND	4.02	1.42	1.37
22	A	841	CLA	C1D-ND	4.02	1.42	1.37
22	9	606	CLA	C1D-ND	4.01	1.42	1.37
22	B	839	CLA	C1D-ND	4.01	1.42	1.37
22	8	609	CLA	C1D-ND	4.01	1.42	1.37
27	A	845	LHG	O7-C7	4.01	1.45	1.34
23	8	602	CHL	MG-NA	4.00	2.15	2.06
22	H	201	CLA	C1D-ND	4.00	1.42	1.37
22	6	310	CLA	C1D-ND	4.00	1.42	1.37
22	2	613	CLA	C1D-ND	4.00	1.42	1.37
22	5	313	CLA	C1D-ND	4.00	1.42	1.37
22	5	317	CLA	C1D-ND	4.00	1.42	1.37
22	7	312	CLA	C1D-ND	4.00	1.42	1.37
22	A	826	CLA	C1D-ND	4.00	1.42	1.37
22	7	311	CLA	C1D-ND	3.99	1.42	1.37
22	9	602	CLA	C1D-ND	3.99	1.42	1.37
22	3	401	CLA	C1D-ND	3.99	1.42	1.37
22	5	310	CLA	C4B-NB	3.99	1.42	1.37
22	8	612	CLA	C1D-ND	3.99	1.42	1.37
22	3	409	CLA	C1D-ND	3.99	1.42	1.37
22	2	610	CLA	C1D-ND	3.99	1.42	1.37
22	A	824	CLA	C1D-ND	3.98	1.42	1.37
27	5	301	LHG	O7-C7	3.98	1.45	1.34
22	A	836	CLA	C1D-ND	3.98	1.42	1.37
22	B	825	CLA	C1D-ND	3.98	1.42	1.37
22	5	315	CLA	C1D-ND	3.98	1.42	1.37
22	5	316	CLA	C1D-ND	3.98	1.42	1.37
22	A	843	CLA	C1D-ND	3.98	1.42	1.37
22	5	303	CLA	C1D-ND	3.97	1.42	1.37
22	5	314	CLA	C1D-ND	3.97	1.42	1.37
22	9	612	CLA	C1D-ND	3.97	1.42	1.37
22	6	312	CLA	C1D-ND	3.97	1.42	1.37
22	8	610	CLA	C1D-ND	3.97	1.42	1.37
22	3	412	CLA	C1D-ND	3.97	1.42	1.37
22	K	206	CLA	C1D-ND	3.97	1.42	1.37
22	B	841	CLA	C1D-ND	3.97	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	303	CLA	C1D-ND	3.97	1.42	1.37
22	A	823	CLA	C1D-ND	3.96	1.42	1.37
22	A	804	CLA	C1D-ND	3.96	1.42	1.37
22	7	310	CLA	C1D-ND	3.96	1.42	1.37
22	A	838	CLA	C1D-ND	3.96	1.42	1.37
22	B	838	CLA	C1D-ND	3.96	1.42	1.37
22	A	839	CLA	C1D-ND	3.96	1.42	1.37
22	9	604	CLA	C1D-ND	3.96	1.42	1.37
22	K	204	CLA	C1D-ND	3.96	1.42	1.37
22	8	614	CLA	C1D-ND	3.96	1.42	1.37
22	2	606	CLA	C1D-ND	3.95	1.42	1.37
22	B	813	CLA	C1D-ND	3.95	1.42	1.37
23	8	608	CHL	C4D-ND	-3.95	1.32	1.37
22	2	611	CLA	C1D-ND	3.95	1.42	1.37
22	6	317	CLA	C1D-ND	3.95	1.42	1.37
22	1	310	CLA	C1D-ND	3.95	1.42	1.37
22	A	835	CLA	C1D-ND	3.95	1.42	1.37
22	A	806	CLA	C1D-ND	3.94	1.42	1.37
22	A	818	CLA	C1D-ND	3.94	1.42	1.37
22	B	835	CLA	C1D-ND	3.94	1.42	1.37
22	A	809	CLA	C1D-ND	3.94	1.42	1.37
22	B	803	CLA	C1D-ND	3.94	1.42	1.37
22	A	827	CLA	C1D-ND	3.94	1.42	1.37
22	A	814	CLA	C1D-ND	3.94	1.42	1.37
23	5	308	CHL	MG-NA	3.94	2.15	2.06
22	9	607	CLA	C4B-NB	3.94	1.42	1.37
23	3	422	CHL	MG-NA	3.94	2.15	2.06
22	A	815	CLA	C1D-ND	3.94	1.42	1.37
22	2	605	CLA	C1D-ND	3.93	1.42	1.37
22	7	309	CLA	C1D-ND	3.93	1.42	1.37
22	2	601	CLA	C1D-ND	3.93	1.42	1.37
22	B	818	CLA	C1D-ND	3.93	1.42	1.37
22	B	840	CLA	C1D-ND	3.93	1.42	1.37
22	3	403	CLA	C1D-ND	3.93	1.42	1.37
22	J	102	CLA	C1D-ND	3.93	1.42	1.37
22	B	824	CLA	C1D-ND	3.93	1.42	1.37
22	B	843	CLA	C1D-ND	3.93	1.42	1.37
22	A	821	CLA	C1D-ND	3.93	1.42	1.37
22	L	304	CLA	C1D-ND	3.92	1.42	1.37
22	A	825	CLA	C1D-ND	3.92	1.42	1.37
22	B	819	CLA	C1D-ND	3.92	1.42	1.37
22	A	837	CLA	C1D-ND	3.92	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	605	CLA	C1D-ND	3.92	1.42	1.37
22	3	414	CLA	C1D-ND	3.92	1.42	1.37
22	9	611	CLA	C1D-ND	3.91	1.42	1.37
22	B	824	CLA	C3C-C4C	3.91	1.46	1.40
22	6	314	CLA	C1D-ND	3.91	1.42	1.37
22	7	308	CLA	C1D-ND	3.91	1.42	1.37
22	B	811	CLA	C1D-ND	3.91	1.42	1.37
22	1	309	CLA	C1D-ND	3.91	1.42	1.37
22	6	307	CLA	C1D-ND	3.91	1.42	1.37
22	B	842	CLA	C1D-ND	3.91	1.42	1.37
22	L	302	CLA	C1D-ND	3.91	1.42	1.37
22	B	814	CLA	C1D-ND	3.91	1.42	1.37
22	H	202	CLA	C1D-ND	3.91	1.42	1.37
22	A	829	CLA	C1D-ND	3.90	1.42	1.37
22	A	817	CLA	C1D-ND	3.90	1.42	1.37
22	A	810	CLA	C1D-ND	3.90	1.42	1.37
23	8	606	CHL	C1C-NC	3.90	1.43	1.37
22	2	609	CLA	C1D-ND	3.90	1.42	1.37
22	6	318	CLA	C1D-ND	3.90	1.42	1.37
22	6	305	CLA	C1D-ND	3.90	1.42	1.37
22	A	803	CLA	C1D-ND	3.90	1.42	1.37
22	A	831	CLA	C1D-ND	3.90	1.42	1.37
22	B	820	CLA	C1D-ND	3.90	1.42	1.37
22	A	807	CLA	C1D-ND	3.89	1.42	1.37
22	B	826	CLA	C1D-ND	3.89	1.42	1.37
22	2	608	CLA	C1D-ND	3.89	1.42	1.37
22	3	411	CLA	C1D-ND	3.89	1.42	1.37
22	7	310	CLA	C4B-NB	3.89	1.42	1.37
22	7	307	CLA	C1D-ND	3.89	1.42	1.37
22	A	811	CLA	C1D-ND	3.89	1.42	1.37
22	B	821	CLA	C1D-ND	3.89	1.42	1.37
22	5	312	CLA	C1D-ND	3.89	1.42	1.37
22	7	303	CLA	C1D-ND	3.88	1.42	1.37
22	B	844	CLA	C1D-ND	3.88	1.42	1.37
22	1	313	CLA	C1D-ND	3.88	1.42	1.37
23	7	304	CHL	MG-NA	3.88	2.15	2.06
22	1	307	CLA	C4B-NB	3.88	1.42	1.37
22	5	305	CLA	C1D-ND	3.88	1.42	1.37
22	B	812	CLA	C1D-ND	3.88	1.42	1.37
22	F	804	CLA	C4B-NB	3.88	1.42	1.37
22	6	306	CLA	C1D-ND	3.87	1.42	1.37
22	6	312	CLA	C4B-NB	3.87	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	313	CLA	C1D-ND	3.87	1.42	1.37
22	8	601	CLA	C1D-ND	3.87	1.42	1.37
22	2	602	CLA	C1D-ND	3.87	1.42	1.37
22	A	819	CLA	C1D-ND	3.86	1.42	1.37
22	B	817	CLA	C1D-ND	3.86	1.42	1.37
22	B	827	CLA	C1D-ND	3.86	1.42	1.37
22	L	303	CLA	C1D-ND	3.86	1.42	1.37
22	6	304	CLA	C1D-ND	3.86	1.42	1.37
22	1	301	CLA	C1D-ND	3.85	1.42	1.37
22	1	307	CLA	C1D-ND	3.85	1.42	1.37
22	A	840	CLA	C1D-ND	3.85	1.42	1.37
22	A	820	CLA	C1D-ND	3.85	1.42	1.37
22	B	837	CLA	C1D-ND	3.85	1.42	1.37
22	A	834	CLA	C1D-ND	3.85	1.42	1.37
22	K	202	CLA	C1D-ND	3.85	1.42	1.37
22	B	808	CLA	C1D-ND	3.84	1.42	1.37
22	1	308	CLA	C1D-ND	3.84	1.42	1.37
22	5	304	CLA	C1D-ND	3.84	1.42	1.37
22	6	311	CLA	C1D-ND	3.84	1.42	1.37
22	H	203	CLA	C1D-ND	3.84	1.42	1.37
22	B	834	CLA	C1D-ND	3.84	1.42	1.37
22	A	813	CLA	C1D-ND	3.84	1.42	1.37
22	A	816	CLA	C1D-ND	3.84	1.42	1.37
22	B	836	CLA	C1D-ND	3.83	1.42	1.37
22	7	301	CLA	C1D-ND	3.83	1.42	1.37
22	7	314	CLA	C1D-ND	3.83	1.42	1.37
22	A	828	CLA	C1D-ND	3.83	1.42	1.37
22	B	823	CLA	C4B-NB	3.83	1.42	1.37
23	5	307	CHL	C4D-ND	-3.83	1.32	1.37
22	A	813	CLA	C4B-NB	3.83	1.42	1.37
22	B	807	CLA	C1D-ND	3.83	1.42	1.37
22	1	312	CLA	C1D-ND	3.82	1.42	1.37
23	3	413	CHL	C4D-ND	-3.82	1.32	1.37
22	8	615	CLA	C4B-NB	3.82	1.42	1.37
22	B	839	CLA	C4B-NB	3.81	1.42	1.37
28	3	420	LMU	O5'-C1'	3.81	1.51	1.41
22	2	607	CLA	C4B-NB	3.81	1.42	1.37
22	A	830	CLA	C1D-ND	3.80	1.42	1.37
23	5	306	CHL	C4D-ND	-3.80	1.32	1.37
22	5	311	CLA	C1D-ND	3.80	1.42	1.37
22	B	804	CLA	C1D-ND	3.80	1.42	1.37
28	7	319	LMU	O5'-C1'	3.80	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	205	CLA	C1D-ND	3.79	1.42	1.37
22	3	411	CLA	C4B-NB	3.79	1.42	1.37
23	1	304	CHL	MG-NA	3.78	2.15	2.06
22	3	408	CLA	C1D-ND	3.78	1.42	1.37
22	B	822	CLA	C1D-ND	3.78	1.42	1.37
22	F	804	CLA	C1D-ND	3.78	1.42	1.37
22	A	808	CLA	C1D-ND	3.78	1.42	1.37
22	B	810	CLA	C1D-ND	3.77	1.42	1.37
22	F	802	CLA	C1D-ND	3.77	1.42	1.37
22	B	844	CLA	C4B-NB	3.75	1.42	1.37
22	B	828	CLA	C1D-ND	3.75	1.42	1.37
22	8	609	CLA	C4B-NB	3.75	1.42	1.37
22	F	802	CLA	C4B-NB	3.75	1.42	1.37
22	B	833	CLA	C1D-ND	3.75	1.42	1.37
22	9	603	CLA	C4B-NB	3.74	1.42	1.37
22	B	806	CLA	C1D-ND	3.74	1.42	1.37
28	F	806	LMU	O5B-C1B	3.73	1.51	1.41
22	B	805	CLA	C1D-ND	3.73	1.42	1.37
22	2	604	CLA	C4B-NB	3.73	1.42	1.37
22	2	607	CLA	C1D-ND	3.73	1.42	1.37
22	9	608	CLA	C1D-ND	3.73	1.42	1.37
22	1	311	CLA	C4B-NB	3.72	1.42	1.37
22	8	604	CLA	C4B-NB	3.72	1.42	1.37
22	B	832	CLA	C1D-ND	3.72	1.42	1.37
23	5	309	CHL	C4D-ND	-3.71	1.32	1.37
22	L	304	CLA	C4B-NB	3.71	1.42	1.37
22	7	307	CLA	C4B-NB	3.71	1.42	1.37
23	5	306	CHL	C1C-NC	3.71	1.43	1.37
22	6	314	CLA	C4B-NB	3.71	1.42	1.37
22	3	404	CLA	C4B-NB	3.71	1.42	1.37
22	6	317	CLA	C4B-NB	3.70	1.42	1.37
22	B	807	CLA	C4B-NB	3.69	1.42	1.37
22	B	830	CLA	C1D-ND	3.69	1.42	1.37
22	3	409	CLA	C4B-NB	3.68	1.42	1.37
28	6	323	LMU	O5'-C1'	3.68	1.51	1.41
22	A	808	CLA	C4B-NB	3.68	1.42	1.37
22	H	202	CLA	C4B-NB	3.68	1.42	1.37
22	1	313	CLA	C4B-NB	3.68	1.42	1.37
22	A	834	CLA	C4B-NB	3.68	1.42	1.37
22	A	820	CLA	C4B-NB	3.68	1.42	1.37
23	5	318	CHL	C4D-ND	-3.68	1.32	1.37
22	A	840	CLA	C4B-NB	3.67	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	310	CLA	C4B-NB	3.67	1.42	1.37
22	7	302	CLA	C4B-NB	3.67	1.42	1.37
22	8	610	CLA	C4B-NB	3.67	1.42	1.37
22	A	810	CLA	C4B-NB	3.67	1.42	1.37
22	B	843	CLA	C4B-NB	3.67	1.42	1.37
22	B	804	CLA	C4B-NB	3.67	1.42	1.37
22	2	606	CLA	C4B-NB	3.66	1.42	1.37
22	H	201	CLA	C4B-NB	3.66	1.42	1.37
22	B	824	CLA	C4B-NB	3.66	1.42	1.37
22	7	303	CLA	C4B-NB	3.66	1.42	1.37
28	A	853	LMU	O5B-C1B	3.66	1.51	1.41
22	5	313	CLA	C4B-NB	3.65	1.42	1.37
22	7	314	CLA	C4B-NB	3.65	1.42	1.37
22	8	613	CLA	C4B-NB	3.65	1.42	1.37
22	A	829	CLA	C4B-NB	3.65	1.42	1.37
23	5	318	CHL	MG-NA	3.65	2.14	2.06
22	9	609	CLA	C1D-ND	3.65	1.42	1.37
22	A	821	CLA	C4B-NB	3.65	1.42	1.37
22	B	832	CLA	C4B-NB	3.65	1.42	1.37
22	K	206	CLA	C4B-NB	3.64	1.42	1.37
28	H	204	LMU	O5B-C1B	3.64	1.51	1.41
23	8	607	CHL	MG-NA	3.64	2.14	2.06
22	3	414	CLA	C4B-NB	3.64	1.42	1.37
22	8	612	CLA	C4B-NB	3.64	1.42	1.37
22	5	314	CLA	C4B-NB	3.64	1.42	1.37
22	7	313	CLA	C4B-NB	3.64	1.42	1.37
22	B	842	CLA	C4B-NB	3.64	1.42	1.37
22	K	204	CLA	C4B-NB	3.64	1.42	1.37
23	9	601	CHL	C4D-ND	-3.64	1.32	1.37
22	5	316	CLA	C4B-NB	3.63	1.42	1.37
22	6	306	CLA	C4B-NB	3.63	1.42	1.37
22	1	312	CLA	C4B-NB	3.63	1.42	1.37
22	7	306	CLA	C4B-NB	3.63	1.42	1.37
22	7	311	CLA	C4B-NB	3.63	1.42	1.37
22	B	820	CLA	C4B-NB	3.63	1.42	1.37
22	9	609	CLA	C4B-NB	3.63	1.42	1.37
22	B	826	CLA	C4B-NB	3.63	1.42	1.37
22	2	612	CLA	C4B-NB	3.63	1.42	1.37
22	K	202	CLA	C4B-NB	3.63	1.42	1.37
22	2	610	CLA	C4B-NB	3.63	1.42	1.37
22	5	305	CLA	C4B-NB	3.63	1.42	1.37
22	8	611	CLA	C1D-ND	3.63	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	607	CHL	C4D-ND	-3.62	1.32	1.37
22	9	610	CLA	C4B-NB	3.62	1.42	1.37
22	6	311	CLA	C4B-NB	3.62	1.42	1.37
22	G	202	CLA	C4B-NB	3.62	1.42	1.37
28	1	319	LMU	O5'-C1'	3.62	1.51	1.41
22	L	302	CLA	C4B-NB	3.62	1.42	1.37
22	A	835	CLA	C4B-NB	3.62	1.42	1.37
22	B	814	CLA	C4B-NB	3.61	1.42	1.37
22	B	833	CLA	C4B-NB	3.61	1.42	1.37
22	B	836	CLA	C4B-NB	3.61	1.42	1.37
22	B	841	CLA	C4B-NB	3.61	1.42	1.37
22	9	611	CLA	C4B-NB	3.61	1.42	1.37
22	A	819	CLA	C4B-NB	3.61	1.42	1.37
22	B	838	CLA	C4B-NB	3.61	1.42	1.37
22	A	837	CLA	C4B-NB	3.61	1.42	1.37
22	A	843	CLA	C4B-NB	3.61	1.42	1.37
22	A	833	CLA	C4B-NB	3.61	1.42	1.37
22	B	821	CLA	C4B-NB	3.61	1.42	1.37
22	1	301	CLA	C4B-NB	3.61	1.42	1.37
22	6	313	CLA	C4B-NB	3.61	1.42	1.37
23	8	606	CHL	C4D-ND	-3.61	1.32	1.37
22	2	611	CLA	C4B-NB	3.61	1.42	1.37
22	K	205	CLA	C4B-NB	3.61	1.42	1.37
23	1	306	CHL	C4D-ND	-3.61	1.32	1.37
22	8	605	CLA	C4B-NB	3.60	1.42	1.37
22	B	840	CLA	C4B-NB	3.60	1.42	1.37
22	2	609	CLA	C4B-NB	3.60	1.42	1.37
22	3	410	CLA	C4B-NB	3.60	1.42	1.37
28	G	201	LMU	O5'-C1'	3.60	1.51	1.41
22	5	303	CLA	C4B-NB	3.60	1.42	1.37
22	6	316	CLA	C1D-ND	3.60	1.42	1.37
22	7	309	CLA	C4B-NB	3.60	1.42	1.37
22	3	401	CLA	C4B-NB	3.59	1.42	1.37
22	2	605	CLA	C4B-NB	3.59	1.42	1.37
22	9	612	CLA	C4B-NB	3.59	1.42	1.37
22	A	832	CLA	C4B-NB	3.59	1.42	1.37
22	B	822	CLA	C4B-NB	3.59	1.42	1.37
22	6	305	CLA	C4B-NB	3.59	1.42	1.37
22	A	811	CLA	C4B-NB	3.59	1.42	1.37
22	6	315	CLA	C4B-NB	3.59	1.42	1.37
22	A	809	CLA	C4B-NB	3.59	1.42	1.37
22	6	307	CLA	C4B-NB	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	203	CLA	C4B-NB	3.59	1.42	1.37
22	3	412	CLA	C4B-NB	3.58	1.42	1.37
22	J	102	CLA	C4B-NB	3.58	1.42	1.37
22	6	309	CLA	C4B-NB	3.58	1.42	1.37
22	9	608	CLA	C4B-NB	3.57	1.42	1.37
28	K	201	LMU	O5'-C1'	3.57	1.50	1.41
22	3	408	CLA	C4B-NB	3.57	1.42	1.37
22	A	841	CLA	C4B-NB	3.57	1.42	1.37
22	2	613	CLA	C4B-NB	3.57	1.42	1.37
22	A	818	CLA	C4B-NB	3.57	1.42	1.37
22	B	815	CLA	C4B-NB	3.57	1.42	1.37
28	3	423	LMU	O5'-C1'	3.57	1.50	1.41
22	6	310	CLA	C4B-NB	3.57	1.42	1.37
22	B	818	CLA	C4B-NB	3.57	1.42	1.37
22	B	819	CLA	C4B-NB	3.56	1.42	1.37
28	A	852	LMU	O5'-C1'	3.56	1.50	1.41
22	5	315	CLA	C4B-NB	3.56	1.42	1.37
22	L	303	CLA	C4B-NB	3.56	1.42	1.37
22	A	805	CLA	C4B-NB	3.56	1.42	1.37
22	B	827	CLA	C4B-NB	3.56	1.42	1.37
22	8	611	CLA	C4B-NB	3.56	1.42	1.37
22	A	822	CLA	C4B-NB	3.56	1.42	1.37
22	6	304	CLA	C4B-NB	3.55	1.42	1.37
22	5	311	CLA	C4B-NB	3.55	1.42	1.37
22	A	803	CLA	C4B-NB	3.55	1.42	1.37
22	5	304	CLA	C4B-NB	3.55	1.42	1.37
22	8	616	CLA	C4B-NB	3.55	1.42	1.37
22	F	803	CLA	C4B-NB	3.55	1.42	1.37
22	6	316	CLA	C4B-NB	3.55	1.42	1.37
22	B	825	CLA	C4B-NB	3.55	1.42	1.37
22	B	831	CLA	C4B-NB	3.54	1.42	1.37
22	B	837	CLA	C4B-NB	3.54	1.42	1.37
22	8	601	CLA	C4B-NB	3.54	1.42	1.37
22	2	603	CLA	C4B-NB	3.54	1.42	1.37
22	A	839	CLA	C4B-NB	3.54	1.42	1.37
28	6	301	LMU	O5'-C1'	3.54	1.50	1.41
28	F	806	LMU	O5'-C1'	3.53	1.50	1.41
22	B	811	CLA	C4B-NB	3.53	1.42	1.37
28	9	618	LMU	O5'-C1'	3.53	1.50	1.41
22	5	312	CLA	C4B-NB	3.53	1.42	1.37
22	A	823	CLA	C4B-NB	3.53	1.42	1.37
22	A	814	CLA	C4B-NB	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	301	CLA	C4B-NB	3.52	1.42	1.37
22	A	807	CLA	C4B-NB	3.52	1.42	1.37
22	B	809	CLA	C4B-NB	3.52	1.42	1.37
22	B	810	CLA	C4B-NB	3.52	1.42	1.37
22	B	835	CLA	C4B-NB	3.52	1.42	1.37
22	3	403	CLA	C4B-NB	3.51	1.42	1.37
23	1	304	CHL	C4D-ND	-3.51	1.32	1.37
28	A	853	LMU	O5'-C1'	3.51	1.50	1.41
22	B	829	CLA	C4B-NB	3.51	1.42	1.37
22	7	312	CLA	C4B-NB	3.51	1.42	1.37
22	B	828	CLA	C4B-NB	3.50	1.42	1.37
28	G	201	LMU	O5B-C1B	3.50	1.50	1.41
22	B	805	CLA	C4B-NB	3.50	1.42	1.37
28	6	301	LMU	O5B-C1B	3.50	1.50	1.41
22	9	602	CLA	C4B-NB	3.50	1.42	1.37
28	3	420	LMU	O5B-C1B	3.50	1.50	1.41
22	7	308	CLA	C4B-NB	3.50	1.42	1.37
22	1	303	CLA	C4B-NB	3.49	1.42	1.37
22	8	614	CLA	C4B-NB	3.49	1.42	1.37
22	A	817	CLA	C4B-NB	3.49	1.42	1.37
22	A	816	CLA	C4B-NB	3.49	1.42	1.37
22	B	812	CLA	C4B-NB	3.48	1.42	1.37
22	A	838	CLA	C4B-NB	3.48	1.42	1.37
28	J	106	LMU	O5B-C1B	3.48	1.50	1.41
22	2	602	CLA	C4B-NB	3.48	1.42	1.37
22	5	317	CLA	C4B-NB	3.48	1.42	1.37
23	8	602	CHL	C1C-NC	3.47	1.43	1.37
23	6	308	CHL	C4D-ND	-3.47	1.32	1.37
23	7	305	CHL	MG-NA	3.47	2.14	2.06
22	B	834	CLA	C4B-NB	3.47	1.42	1.37
28	9	618	LMU	O5B-C1B	3.47	1.50	1.41
28	K	201	LMU	O5B-C1B	3.47	1.50	1.41
22	B	817	CLA	C4B-NB	3.47	1.42	1.37
22	6	311	CLA	C3B-C4B	3.47	1.50	1.42
22	B	802	CLA	C1D-ND	3.47	1.42	1.37
23	5	308	CHL	C4D-ND	-3.47	1.32	1.37
22	A	801	CLA	C4B-NB	3.46	1.42	1.37
22	B	802	CLA	C4B-NB	3.46	1.42	1.37
28	6	323	LMU	O5B-C1B	3.46	1.50	1.41
22	A	830	CLA	C4B-NB	3.46	1.42	1.37
22	1	309	CLA	C4B-NB	3.45	1.42	1.37
22	B	806	CLA	C4B-NB	3.45	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	302	CLA	C4B-NB	3.45	1.42	1.37
23	3	422	CHL	C1C-NC	3.45	1.43	1.37
22	A	824	CLA	C4B-NB	3.45	1.42	1.37
28	3	423	LMU	O5B-C1B	3.45	1.50	1.41
23	5	307	CHL	C1C-NC	3.45	1.43	1.37
22	6	318	CLA	C4B-NB	3.44	1.42	1.37
22	A	828	CLA	C4B-NB	3.44	1.42	1.37
22	1	308	CLA	C4B-NB	3.44	1.42	1.37
22	A	815	CLA	C4B-NB	3.44	1.42	1.37
28	6	302	LMU	O5'-C1'	3.43	1.50	1.41
28	J	106	LMU	O5'-C1'	3.43	1.50	1.41
23	5	309	CHL	MG-NA	3.43	2.14	2.06
23	8	602	CHL	C4D-ND	-3.43	1.33	1.37
23	1	306	CHL	C1C-NC	3.43	1.42	1.37
23	5	309	CHL	C1C-NC	3.43	1.42	1.37
22	B	813	CLA	C4B-NB	3.42	1.42	1.37
22	B	803	CLA	C4B-NB	3.42	1.42	1.37
22	G	203	CLA	C4B-NB	3.42	1.42	1.37
22	A	802	CLA	C4B-NB	3.42	1.42	1.37
22	2	601	CLA	C4B-NB	3.41	1.42	1.37
22	A	825	CLA	C4B-NB	3.40	1.42	1.37
22	A	826	CLA	C4B-NB	3.39	1.41	1.37
28	H	204	LMU	O5'-C1'	3.37	1.50	1.41
22	9	604	CLA	C4B-NB	3.37	1.41	1.37
22	3	402	CLA	C4B-NB	3.37	1.41	1.37
22	9	606	CLA	C4B-NB	3.36	1.41	1.37
22	A	804	CLA	C4B-NB	3.36	1.41	1.37
22	2	608	CLA	C4B-NB	3.36	1.41	1.37
23	7	304	CHL	C1C-NC	3.35	1.42	1.37
23	6	303	CHL	C4D-ND	-3.35	1.33	1.37
22	B	808	CLA	C4B-NB	3.34	1.41	1.37
23	8	603	CHL	MG-NA	3.34	2.14	2.06
28	1	319	LMU	O5B-C1B	3.34	1.50	1.41
28	7	319	LMU	O5B-C1B	3.34	1.50	1.41
23	5	306	CHL	MG-NA	3.33	2.14	2.06
22	1	302	CLA	C1D-ND	3.33	1.41	1.37
28	6	302	LMU	O5B-C1B	3.33	1.50	1.41
28	A	852	LMU	O5B-C1B	3.32	1.50	1.41
23	3	422	CHL	C4D-ND	-3.32	1.33	1.37
22	A	812	CLA	C4B-NB	3.31	1.41	1.37
22	B	830	CLA	C4B-NB	3.31	1.41	1.37
22	A	827	CLA	C4B-NB	3.31	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	831	CLA	C4B-NB	3.31	1.41	1.37
23	3	413	CHL	MG-NA	3.30	2.14	2.06
23	1	306	CHL	MG-NC	3.29	2.14	2.06
22	A	836	CLA	C4B-NB	3.28	1.41	1.37
22	A	806	CLA	C4B-NB	3.27	1.41	1.37
23	7	304	CHL	C4D-ND	-3.25	1.33	1.37
22	1	302	CLA	C4D-ND	-3.24	1.33	1.37
22	6	312	CLA	C3B-C4B	3.22	1.50	1.42
22	3	407	CLA	C4B-NB	3.22	1.41	1.37
22	8	611	CLA	C3B-C4B	3.22	1.50	1.42
28	3	421	LMU	O5B-C1B	3.21	1.50	1.41
28	3	421	LMU	O5'-C1'	3.20	1.50	1.41
22	B	816	CLA	C4B-NB	3.20	1.41	1.37
22	B	802	CLA	C3B-C4B	3.19	1.50	1.42
22	B	806	CLA	C4D-ND	-3.19	1.33	1.37
23	9	601	CHL	C1C-NC	3.18	1.42	1.37
22	7	310	CLA	C3B-C4B	3.16	1.50	1.42
22	B	807	CLA	C3B-C4B	3.13	1.50	1.42
23	8	608	CHL	C1C-NC	3.12	1.42	1.37
22	1	301	CLA	C3B-C4B	3.12	1.50	1.42
22	9	602	CLA	C3B-C4B	3.11	1.50	1.42
22	9	608	CLA	C3B-C4B	3.10	1.50	1.42
22	1	308	CLA	C3B-C4B	3.10	1.50	1.42
22	1	303	CLA	CAB-C3B	-3.10	1.44	1.50
22	F	802	CLA	C3B-C4B	3.08	1.50	1.42
22	H	202	CLA	CAB-C3B	-3.08	1.44	1.50
22	6	309	CLA	C3B-C4B	3.08	1.50	1.42
22	6	305	CLA	CAB-C3B	-3.07	1.44	1.50
22	3	411	CLA	C4D-ND	-3.07	1.33	1.37
23	8	603	CHL	C1C-NC	3.06	1.42	1.37
22	1	313	CLA	CAB-C3B	-3.06	1.44	1.50
22	B	814	CLA	CAB-C3B	-3.06	1.44	1.50
22	B	804	CLA	C3B-C4B	3.06	1.49	1.42
22	7	314	CLA	CAB-C3B	-3.05	1.44	1.50
22	A	803	CLA	C3B-C4B	3.05	1.49	1.42
22	5	304	CLA	CAB-C3B	-3.05	1.44	1.50
22	1	302	CLA	C3B-C4B	3.05	1.49	1.42
22	2	609	CLA	CAB-C3B	-3.04	1.44	1.50
22	1	307	CLA	CAB-C3B	-3.04	1.44	1.50
22	3	408	CLA	C3B-C4B	3.04	1.49	1.42
22	5	316	CLA	CAB-C3B	-3.04	1.44	1.50
22	8	604	CLA	CAB-C3B	-3.04	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	305	CLA	CAB-C3B	-3.03	1.44	1.50
22	7	313	CLA	CAB-C3B	-3.03	1.44	1.50
22	1	312	CLA	C4D-ND	-3.03	1.33	1.37
23	1	304	CHL	MG-NC	3.03	2.13	2.06
22	6	316	CLA	C4D-ND	-3.03	1.33	1.37
22	H	201	CLA	CAB-C3B	-3.03	1.44	1.50
22	1	301	CLA	C4D-ND	-3.03	1.33	1.37
22	7	301	CLA	C3B-C4B	3.02	1.49	1.42
22	B	822	CLA	C3B-C4B	3.02	1.49	1.42
22	B	803	CLA	C4D-ND	-3.02	1.33	1.37
23	3	405	CHL	MG-NC	3.02	2.13	2.06
22	8	610	CLA	C3B-C4B	3.01	1.49	1.42
22	2	608	CLA	C4D-ND	-3.00	1.33	1.37
22	B	833	CLA	C4D-ND	-3.00	1.33	1.37
22	5	311	CLA	C4D-ND	-3.00	1.33	1.37
22	6	314	CLA	C4D-ND	-2.99	1.33	1.37
22	B	840	CLA	C3B-C4B	2.99	1.49	1.42
22	B	834	CLA	C3B-C4B	2.99	1.49	1.42
22	A	828	CLA	C4D-ND	-2.99	1.33	1.37
23	5	319	CHL	C4D-ND	-2.98	1.33	1.37
22	8	601	CLA	C3B-C4B	2.98	1.49	1.42
22	7	301	CLA	C4D-ND	-2.98	1.33	1.37
22	B	827	CLA	C3B-C4B	2.98	1.49	1.42
22	B	828	CLA	C4D-ND	-2.98	1.33	1.37
22	2	601	CLA	C3B-C4B	2.98	1.49	1.42
22	8	614	CLA	C3B-C4B	2.98	1.49	1.42
22	A	817	CLA	C4D-ND	-2.97	1.33	1.37
22	B	828	CLA	C3B-C4B	2.97	1.49	1.42
22	6	304	CLA	C3B-C4B	2.97	1.49	1.42
23	8	602	CHL	MG-NC	2.97	2.13	2.06
22	8	601	CLA	C4D-ND	-2.97	1.33	1.37
22	9	612	CLA	C3B-C4B	2.97	1.49	1.42
22	7	308	CLA	C3B-C4B	2.97	1.49	1.42
22	9	602	CLA	C4D-ND	-2.97	1.33	1.37
22	5	317	CLA	C4D-ND	-2.97	1.33	1.37
22	B	810	CLA	C4D-ND	-2.96	1.33	1.37
22	8	615	CLA	C4D-ND	-2.96	1.33	1.37
22	A	820	CLA	C3B-C4B	2.96	1.49	1.42
22	8	615	CLA	CAB-C3B	-2.96	1.44	1.50
22	6	309	CLA	C4D-ND	-2.95	1.33	1.37
22	A	827	CLA	C4D-ND	-2.95	1.33	1.37
22	A	832	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	835	CLA	C3B-C4B	2.95	1.49	1.42
22	6	311	CLA	C4D-ND	-2.95	1.33	1.37
22	B	839	CLA	C3B-C4B	2.95	1.49	1.42
22	5	313	CLA	C3B-C4B	2.95	1.49	1.42
22	A	813	CLA	C3B-C4B	2.95	1.49	1.42
22	6	304	CLA	C4D-ND	-2.95	1.33	1.37
22	A	825	CLA	C4D-ND	-2.95	1.33	1.37
22	5	312	CLA	C4D-ND	-2.95	1.33	1.37
22	A	812	CLA	C4D-ND	-2.95	1.33	1.37
22	B	843	CLA	C4D-ND	-2.95	1.33	1.37
22	9	610	CLA	C3B-C4B	2.95	1.49	1.42
22	1	309	CLA	C3B-C4B	2.95	1.49	1.42
22	B	809	CLA	C4D-ND	-2.94	1.33	1.37
22	9	604	CLA	C3B-C4B	2.94	1.49	1.42
22	A	814	CLA	C3B-C4B	2.94	1.49	1.42
22	2	602	CLA	C4D-ND	-2.94	1.33	1.37
22	2	612	CLA	C3B-C4B	2.94	1.49	1.42
22	8	613	CLA	C1B-C2B	2.94	1.50	1.43
22	3	401	CLA	C4D-ND	-2.94	1.33	1.37
22	L	303	CLA	C4D-ND	-2.94	1.33	1.37
23	6	308	CHL	C1C-NC	2.94	1.42	1.37
22	A	808	CLA	C4D-ND	-2.94	1.33	1.37
22	A	838	CLA	C4D-ND	-2.94	1.33	1.37
22	5	303	CLA	C3B-C4B	2.93	1.49	1.42
22	B	842	CLA	C3B-C4B	2.93	1.49	1.42
22	7	303	CLA	C4D-ND	-2.93	1.33	1.37
22	B	830	CLA	C4D-ND	-2.93	1.33	1.37
22	2	606	CLA	C4D-ND	-2.93	1.33	1.37
22	1	310	CLA	C3B-C4B	2.93	1.49	1.42
22	A	810	CLA	C3B-C4B	2.93	1.49	1.42
22	B	819	CLA	C4D-ND	-2.93	1.33	1.37
22	3	404	CLA	C3B-C4B	2.93	1.49	1.42
22	A	816	CLA	C4D-ND	-2.92	1.33	1.37
22	A	827	CLA	C3B-C4B	2.92	1.49	1.42
22	B	821	CLA	C4D-ND	-2.92	1.33	1.37
22	A	840	CLA	C3B-C4B	2.92	1.49	1.42
22	F	802	CLA	C4D-ND	-2.92	1.33	1.37
22	B	840	CLA	C4D-ND	-2.92	1.33	1.37
22	6	313	CLA	C3B-C4B	2.92	1.49	1.42
22	8	616	CLA	C3B-C4B	2.91	1.49	1.42
22	K	204	CLA	C3B-C4B	2.91	1.49	1.42
22	A	819	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	815	CLA	C3B-C4B	2.91	1.49	1.42
22	3	403	CLA	C3B-C4B	2.91	1.49	1.42
22	B	823	CLA	C3B-C4B	2.91	1.49	1.42
22	H	203	CLA	C3B-C4B	2.91	1.49	1.42
22	H	202	CLA	C4D-ND	-2.91	1.33	1.37
22	3	403	CLA	C4D-ND	-2.91	1.33	1.37
22	A	810	CLA	C4D-ND	-2.91	1.33	1.37
22	6	314	CLA	C3B-C4B	2.91	1.49	1.42
22	9	611	CLA	C4D-ND	-2.91	1.33	1.37
22	6	307	CLA	C4D-ND	-2.91	1.33	1.37
22	A	820	CLA	C4D-ND	-2.91	1.33	1.37
22	G	203	CLA	C3B-C4B	2.90	1.49	1.42
22	6	310	CLA	C3B-C4B	2.90	1.49	1.42
22	A	829	CLA	C4D-ND	-2.90	1.33	1.37
22	B	831	CLA	C4D-ND	-2.90	1.33	1.37
22	A	802	CLA	C3B-C4B	2.90	1.49	1.42
22	8	605	CLA	C3B-C4B	2.90	1.49	1.42
22	B	818	CLA	C3B-C4B	2.90	1.49	1.42
22	A	809	CLA	C4D-ND	-2.90	1.33	1.37
22	B	822	CLA	C4D-ND	-2.90	1.33	1.37
22	A	816	CLA	C3B-C4B	2.90	1.49	1.42
22	7	306	CLA	C4D-ND	-2.90	1.33	1.37
22	B	802	CLA	C4D-ND	-2.90	1.33	1.37
22	B	834	CLA	C4D-ND	-2.90	1.33	1.37
22	9	608	CLA	C4D-ND	-2.90	1.33	1.37
23	6	303	CHL	C1C-NC	2.90	1.42	1.37
22	9	609	CLA	C4D-ND	-2.90	1.33	1.37
22	B	819	CLA	C3B-C4B	2.89	1.49	1.42
22	2	607	CLA	C3B-C4B	2.89	1.49	1.42
22	5	317	CLA	C1B-C2B	2.89	1.50	1.43
22	A	831	CLA	C3B-C4B	2.89	1.49	1.42
23	8	606	CHL	MG-NC	2.89	2.13	2.06
22	A	837	CLA	C3B-C4B	2.89	1.49	1.42
22	7	309	CLA	C4D-ND	-2.89	1.33	1.37
22	A	821	CLA	C4D-ND	-2.89	1.33	1.37
22	L	302	CLA	C3B-C4B	2.89	1.49	1.42
23	5	308	CHL	C1C-NC	2.89	1.42	1.37
22	3	407	CLA	C4D-ND	-2.89	1.33	1.37
22	7	308	CLA	C4D-ND	-2.89	1.33	1.37
22	A	825	CLA	C3B-C4B	2.89	1.49	1.42
22	B	806	CLA	C3B-C4B	2.89	1.49	1.42
22	9	609	CLA	C3B-C4B	2.89	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	610	CLA	C4D-ND	-2.89	1.33	1.37
22	7	303	CLA	C3B-C4B	2.89	1.49	1.42
22	B	817	CLA	C3B-C4B	2.89	1.49	1.42
22	5	303	CLA	C4D-ND	-2.89	1.33	1.37
22	K	202	CLA	C3B-C4B	2.89	1.49	1.42
22	K	206	CLA	C4D-ND	-2.89	1.33	1.37
22	K	206	CLA	C3B-C4B	2.89	1.49	1.42
22	A	822	CLA	C3B-C4B	2.89	1.49	1.42
22	B	820	CLA	C4D-ND	-2.89	1.33	1.37
22	A	821	CLA	C3B-C4B	2.89	1.49	1.42
22	8	612	CLA	C3B-C4B	2.88	1.49	1.42
22	3	409	CLA	C3B-C4B	2.88	1.49	1.42
22	B	837	CLA	C3B-C4B	2.88	1.49	1.42
22	B	805	CLA	C1B-C2B	2.88	1.50	1.43
22	5	315	CLA	C3B-C4B	2.88	1.49	1.42
22	A	833	CLA	C3B-C4B	2.88	1.49	1.42
22	A	826	CLA	C3B-C4B	2.88	1.49	1.42
22	L	303	CLA	C3B-C4B	2.88	1.49	1.42
22	6	318	CLA	C3B-C4B	2.88	1.49	1.42
22	1	308	CLA	C4D-ND	-2.88	1.33	1.37
22	A	834	CLA	C3B-C4B	2.88	1.49	1.42
22	5	314	CLA	C4D-ND	-2.88	1.33	1.37
22	6	306	CLA	C4D-ND	-2.88	1.33	1.37
22	7	312	CLA	C4D-ND	-2.88	1.33	1.37
22	A	806	CLA	C4D-ND	-2.88	1.33	1.37
22	B	836	CLA	C3B-C4B	2.88	1.49	1.42
22	B	826	CLA	C3B-C4B	2.88	1.49	1.42
22	9	606	CLA	C4D-ND	-2.88	1.33	1.37
22	A	831	CLA	C4D-ND	-2.88	1.33	1.37
22	3	408	CLA	C4D-ND	-2.88	1.33	1.37
22	B	804	CLA	C4D-ND	-2.88	1.33	1.37
22	B	818	CLA	C4D-ND	-2.88	1.33	1.37
22	3	414	CLA	C3B-C4B	2.88	1.49	1.42
22	A	824	CLA	C3B-C4B	2.88	1.49	1.42
23	6	303	CHL	MG-NA	2.87	2.13	2.06
22	6	317	CLA	C3B-C4B	2.87	1.49	1.42
22	B	826	CLA	C4D-ND	-2.87	1.33	1.37
22	2	603	CLA	C3B-C4B	2.87	1.49	1.42
22	3	401	CLA	C3B-C4B	2.87	1.49	1.42
22	A	811	CLA	C3B-C4B	2.87	1.49	1.42
22	A	839	CLA	C3B-C4B	2.87	1.49	1.42
22	B	816	CLA	C3B-C4B	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	311	CLA	C4D-ND	-2.87	1.33	1.37
22	5	314	CLA	C3B-C4B	2.87	1.49	1.42
22	B	824	CLA	C3B-C4B	2.87	1.49	1.42
22	B	817	CLA	C4D-ND	-2.87	1.33	1.37
22	B	842	CLA	C4D-ND	-2.87	1.33	1.37
22	3	409	CLA	C4D-ND	-2.87	1.33	1.37
23	1	305	CHL	C4D-ND	-2.87	1.33	1.37
22	A	835	CLA	C3B-C4B	2.87	1.49	1.42
22	2	611	CLA	C3B-C4B	2.87	1.49	1.42
22	2	610	CLA	C3B-C4B	2.87	1.49	1.42
22	3	410	CLA	C3B-C4B	2.87	1.49	1.42
22	6	307	CLA	C3B-C4B	2.87	1.49	1.42
22	6	315	CLA	C3B-C4B	2.87	1.49	1.42
22	2	613	CLA	C4D-ND	-2.86	1.33	1.37
22	F	803	CLA	C3B-C4B	2.86	1.49	1.42
22	B	844	CLA	C3B-C4B	2.86	1.49	1.42
22	A	823	CLA	C4D-ND	-2.86	1.33	1.37
22	5	312	CLA	C3B-C4B	2.86	1.49	1.42
22	A	835	CLA	C4D-ND	-2.86	1.33	1.37
22	1	303	CLA	C4D-ND	-2.86	1.33	1.37
22	B	831	CLA	C3B-C4B	2.86	1.49	1.42
22	8	611	CLA	C4D-ND	-2.86	1.33	1.37
22	B	844	CLA	C4D-ND	-2.86	1.33	1.37
22	B	809	CLA	C3B-C4B	2.86	1.49	1.42
22	B	829	CLA	C3B-C4B	2.86	1.49	1.42
22	A	840	CLA	C4D-ND	-2.86	1.33	1.37
22	A	838	CLA	C3B-C4B	2.86	1.49	1.42
22	2	613	CLA	C3B-C4B	2.85	1.49	1.42
22	B	836	CLA	C4D-ND	-2.85	1.33	1.37
22	A	807	CLA	C4D-ND	-2.85	1.33	1.37
22	K	205	CLA	C3B-C4B	2.85	1.49	1.42
22	L	304	CLA	C4D-ND	-2.85	1.33	1.37
22	2	608	CLA	C3B-C4B	2.85	1.49	1.42
22	8	616	CLA	C4D-ND	-2.85	1.33	1.37
22	A	809	CLA	C3B-C4B	2.85	1.49	1.42
22	B	838	CLA	C3B-C4B	2.85	1.49	1.42
22	2	602	CLA	C3B-C4B	2.85	1.49	1.42
22	3	412	CLA	C3B-C4B	2.85	1.49	1.42
22	6	310	CLA	C4D-ND	-2.85	1.33	1.37
22	7	311	CLA	C3B-C4B	2.85	1.49	1.42
22	B	810	CLA	C3B-C4B	2.85	1.49	1.42
22	B	841	CLA	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	808	CLA	C3B-C4B	2.85	1.49	1.42
22	1	312	CLA	C3B-C4B	2.85	1.49	1.42
22	6	317	CLA	C4D-ND	-2.85	1.33	1.37
22	2	604	CLA	C3B-C4B	2.85	1.49	1.42
22	B	838	CLA	C4D-ND	-2.84	1.33	1.37
22	2	606	CLA	C3B-C4B	2.84	1.49	1.42
22	A	818	CLA	C3B-C4B	2.84	1.49	1.42
22	B	837	CLA	C4D-ND	-2.84	1.33	1.37
22	2	601	CLA	C4D-ND	-2.84	1.33	1.37
22	5	305	CLA	C4D-ND	-2.84	1.33	1.37
22	A	822	CLA	C4D-ND	-2.84	1.33	1.37
22	A	804	CLA	C3B-C4B	2.84	1.49	1.42
22	B	825	CLA	C3B-C4B	2.84	1.49	1.42
22	6	318	CLA	C4D-ND	-2.84	1.33	1.37
22	A	826	CLA	C4D-ND	-2.84	1.33	1.37
22	A	834	CLA	C4D-ND	-2.84	1.33	1.37
22	A	843	CLA	C4D-ND	-2.84	1.33	1.37
22	K	204	CLA	C4D-ND	-2.84	1.33	1.37
22	1	311	CLA	C3B-C4B	2.84	1.49	1.42
22	A	804	CLA	C1B-C2B	2.84	1.49	1.43
22	6	306	CLA	C3B-C4B	2.84	1.49	1.42
22	3	407	CLA	C3B-C4B	2.84	1.49	1.42
22	2	612	CLA	C4D-ND	-2.84	1.33	1.37
22	A	832	CLA	C3B-C4B	2.84	1.49	1.42
22	A	819	CLA	C3B-C4B	2.84	1.49	1.42
22	6	305	CLA	C4D-ND	-2.83	1.33	1.37
22	A	833	CLA	C4D-ND	-2.83	1.33	1.37
22	3	411	CLA	C3B-C4B	2.83	1.49	1.42
22	A	814	CLA	C4D-ND	-2.83	1.33	1.37
23	9	601	CHL	MG-NA	2.83	2.13	2.06
22	B	816	CLA	C4D-ND	-2.83	1.33	1.37
22	B	832	CLA	C4D-ND	-2.83	1.33	1.37
22	6	316	CLA	C3B-C4B	2.83	1.49	1.42
22	7	302	CLA	C3B-C4B	2.83	1.49	1.42
22	7	306	CLA	C3B-C4B	2.83	1.49	1.42
22	B	823	CLA	C4D-ND	-2.83	1.33	1.37
22	B	833	CLA	C3B-C4B	2.83	1.49	1.42
22	6	315	CLA	C4D-ND	-2.83	1.33	1.37
22	F	803	CLA	C4D-ND	-2.83	1.33	1.37
22	8	604	CLA	C4D-ND	-2.83	1.33	1.37
22	A	805	CLA	C3B-C4B	2.83	1.49	1.42
22	9	611	CLA	C3B-C4B	2.83	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	843	CLA	C3B-C4B	2.83	1.49	1.42
22	6	312	CLA	C4D-ND	-2.83	1.33	1.37
22	A	808	CLA	C3B-C4B	2.83	1.49	1.42
22	A	817	CLA	C3B-C4B	2.83	1.49	1.42
22	2	604	CLA	C4D-ND	-2.83	1.33	1.37
22	A	830	CLA	C3B-C4B	2.83	1.49	1.42
23	5	306	CHL	MG-NC	2.83	2.13	2.06
22	B	808	CLA	C4D-ND	-2.83	1.33	1.37
22	9	603	CLA	C3B-C4B	2.82	1.49	1.42
22	5	311	CLA	C3B-C4B	2.82	1.49	1.42
22	9	607	CLA	C1B-C2B	2.82	1.49	1.43
22	7	309	CLA	C3B-C4B	2.82	1.49	1.42
22	7	313	CLA	C4D-ND	-2.82	1.33	1.37
22	B	839	CLA	C4D-ND	-2.82	1.33	1.37
22	7	307	CLA	C3B-C4B	2.82	1.49	1.42
22	7	312	CLA	C3B-C4B	2.82	1.49	1.42
22	F	804	CLA	C3B-C4B	2.82	1.49	1.42
22	A	811	CLA	C4D-ND	-2.82	1.33	1.37
22	G	202	CLA	C3B-C4B	2.82	1.49	1.42
22	3	414	CLA	C4D-ND	-2.82	1.33	1.37
22	2	605	CLA	C3B-C4B	2.81	1.49	1.42
22	J	102	CLA	C3B-C4B	2.81	1.49	1.42
22	5	316	CLA	C4D-ND	-2.81	1.33	1.37
22	8	605	CLA	C4D-ND	-2.81	1.33	1.37
22	B	824	CLA	C4D-ND	-2.81	1.33	1.37
22	8	614	CLA	C4D-ND	-2.81	1.33	1.37
22	L	304	CLA	C3B-C4B	2.81	1.49	1.42
22	3	404	CLA	C4D-ND	-2.81	1.33	1.37
22	B	807	CLA	C4D-ND	-2.81	1.33	1.37
22	A	815	CLA	C3B-C4B	2.81	1.49	1.42
22	A	830	CLA	C4D-ND	-2.81	1.33	1.37
22	B	825	CLA	C4D-ND	-2.80	1.33	1.37
22	2	605	CLA	C4D-ND	-2.80	1.33	1.37
22	1	307	CLA	C4D-ND	-2.80	1.33	1.37
22	B	814	CLA	C4D-ND	-2.80	1.33	1.37
22	B	820	CLA	C3B-C4B	2.80	1.49	1.42
22	2	609	CLA	C4D-ND	-2.80	1.33	1.37
22	A	841	CLA	C4D-ND	-2.80	1.33	1.37
22	7	314	CLA	C1B-C2B	2.80	1.49	1.43
22	A	813	CLA	MG-NC	2.80	2.12	2.06
22	A	807	CLA	C3B-C4B	2.80	1.49	1.42
22	1	309	CLA	C4D-ND	-2.80	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	837	CLA	C4D-ND	-2.80	1.33	1.37
22	F	804	CLA	C4D-ND	-2.80	1.33	1.37
22	B	829	CLA	C4D-ND	-2.80	1.33	1.37
22	3	412	CLA	C4D-ND	-2.79	1.33	1.37
22	K	202	CLA	C4D-ND	-2.79	1.33	1.37
22	B	832	CLA	C3B-C4B	2.79	1.49	1.42
22	A	805	CLA	C4D-ND	-2.79	1.33	1.37
22	B	821	CLA	C3B-C4B	2.79	1.49	1.42
22	3	410	CLA	C4D-ND	-2.79	1.33	1.37
22	1	313	CLA	C4D-ND	-2.79	1.33	1.37
22	B	803	CLA	C3B-C4B	2.79	1.49	1.42
22	A	836	CLA	C4D-ND	-2.78	1.33	1.37
22	7	314	CLA	C4D-ND	-2.78	1.33	1.37
22	B	811	CLA	C3B-C4B	2.78	1.49	1.42
22	8	609	CLA	C3B-C4B	2.78	1.49	1.42
22	B	812	CLA	C4D-ND	-2.78	1.33	1.37
22	9	604	CLA	C4D-ND	-2.78	1.33	1.37
22	H	203	CLA	C4D-ND	-2.78	1.33	1.37
22	A	801	CLA	C1B-C2B	2.78	1.49	1.43
22	9	606	CLA	C3B-C4B	2.77	1.49	1.42
22	A	806	CLA	C3B-C4B	2.77	1.49	1.42
22	J	102	CLA	C4D-ND	-2.77	1.33	1.37
22	A	803	CLA	C4D-ND	-2.77	1.33	1.37
22	A	836	CLA	C1B-C2B	2.77	1.49	1.43
22	5	313	CLA	C4D-ND	-2.77	1.33	1.37
23	6	308	CHL	MG-NC	2.77	2.12	2.06
22	A	812	CLA	C3B-C4B	2.77	1.49	1.42
22	B	813	CLA	C4D-ND	-2.76	1.33	1.37
22	B	843	CLA	C1B-C2B	2.76	1.49	1.43
22	9	612	CLA	C4D-ND	-2.76	1.33	1.37
22	A	815	CLA	C4D-ND	-2.76	1.33	1.37
22	9	603	CLA	C4D-ND	-2.76	1.33	1.37
22	A	828	CLA	C3B-C4B	2.76	1.49	1.42
22	7	302	CLA	C4D-ND	-2.76	1.33	1.37
22	A	815	CLA	C1B-C2B	2.76	1.49	1.43
22	5	315	CLA	C4D-ND	-2.75	1.33	1.37
22	7	307	CLA	C4D-ND	-2.75	1.33	1.37
22	B	841	CLA	C3B-C4B	2.75	1.49	1.42
22	A	841	CLA	C3B-C4B	2.75	1.49	1.42
22	2	611	CLA	C4D-ND	-2.75	1.33	1.37
22	B	813	CLA	C3B-C4B	2.75	1.49	1.42
22	A	818	CLA	C4D-ND	-2.75	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	839	CLA	C4D-ND	-2.75	1.33	1.37
22	B	830	CLA	C3B-C4B	2.74	1.49	1.42
22	2	607	CLA	C4D-ND	-2.74	1.33	1.37
22	8	615	CLA	C1B-C2B	2.74	1.49	1.43
23	3	405	CHL	C1C-NC	2.74	1.41	1.37
22	2	611	CLA	C1B-C2B	2.73	1.49	1.43
23	7	305	CHL	C4D-ND	-2.73	1.33	1.37
22	9	606	CLA	C1B-C2B	2.73	1.49	1.43
22	G	202	CLA	C4D-ND	-2.73	1.33	1.37
22	B	827	CLA	C4D-ND	-2.73	1.33	1.37
22	A	824	CLA	C1B-C2B	2.72	1.49	1.43
22	3	402	CLA	C4D-ND	-2.72	1.33	1.37
22	A	843	CLA	C1B-C2B	2.72	1.49	1.43
23	5	318	CHL	C1C-NC	2.72	1.41	1.37
22	A	802	CLA	C4D-ND	-2.72	1.34	1.37
22	5	304	CLA	C4D-ND	-2.71	1.34	1.37
22	2	607	CLA	C1B-C2B	2.71	1.49	1.43
22	G	202	CLA	C1B-C2B	2.71	1.49	1.43
22	B	811	CLA	C1B-C2B	2.71	1.49	1.43
22	B	814	CLA	C1B-C2B	2.71	1.49	1.43
22	L	303	CLA	C1B-C2B	2.71	1.49	1.43
22	B	813	CLA	C1B-C2B	2.71	1.49	1.43
22	K	205	CLA	C1B-C2B	2.71	1.49	1.43
22	A	823	CLA	C3B-C4B	2.71	1.49	1.42
22	7	311	CLA	C1B-C2B	2.71	1.49	1.43
22	K	205	CLA	C4D-ND	-2.70	1.34	1.37
22	B	836	CLA	C1B-C2B	2.70	1.49	1.43
23	3	405	CHL	C1D-C2D	-2.70	1.40	1.45
22	5	305	CLA	C1B-C2B	2.70	1.49	1.43
22	8	613	CLA	C4D-ND	-2.70	1.34	1.37
22	1	307	CLA	C1B-C2B	2.70	1.49	1.43
22	7	303	CLA	C1B-C2B	2.70	1.49	1.43
22	H	201	CLA	C4D-ND	-2.70	1.34	1.37
22	8	609	CLA	C4D-ND	-2.70	1.34	1.37
22	5	310	CLA	C3B-C4B	2.70	1.49	1.42
22	A	823	CLA	C1B-C2B	2.70	1.49	1.43
22	6	307	CLA	C1B-C2B	2.69	1.49	1.43
22	A	826	CLA	C1B-C2B	2.69	1.49	1.43
22	A	816	CLA	C1B-C2B	2.69	1.49	1.43
22	B	831	CLA	C1B-C2B	2.69	1.49	1.43
22	A	805	CLA	C1B-C2B	2.69	1.49	1.43
22	2	612	CLA	C1B-C2B	2.69	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	412	CLA	C1B-C2B	2.69	1.49	1.43
22	B	805	CLA	C3B-C4B	2.69	1.49	1.42
22	A	840	CLA	C1B-C2B	2.69	1.49	1.43
22	A	801	CLA	C3B-C4B	2.69	1.49	1.42
22	B	809	CLA	C1B-C2B	2.69	1.49	1.43
22	5	314	CLA	C1B-C2B	2.69	1.49	1.43
22	8	615	CLA	MG-NA	2.69	2.12	2.06
22	2	613	CLA	C1B-C2B	2.69	1.49	1.43
22	B	823	CLA	C1B-C2B	2.68	1.49	1.43
22	2	603	CLA	C4D-ND	-2.68	1.34	1.37
22	B	812	CLA	C3B-C4B	2.68	1.49	1.42
22	3	402	CLA	C1B-C2B	2.68	1.49	1.43
22	7	306	CLA	C1B-C2B	2.68	1.49	1.43
22	L	304	CLA	C1B-C2B	2.68	1.49	1.43
22	B	835	CLA	C4D-ND	-2.68	1.34	1.37
22	1	312	CLA	C1B-C2B	2.68	1.49	1.43
22	A	807	CLA	C1B-C2B	2.68	1.49	1.43
22	A	832	CLA	C1B-C2B	2.68	1.49	1.43
22	5	316	CLA	C1B-C2B	2.68	1.49	1.43
22	6	309	CLA	C1B-C2B	2.68	1.49	1.43
22	2	606	CLA	C1B-C2B	2.68	1.49	1.43
22	A	821	CLA	C1B-C2B	2.68	1.49	1.43
22	6	318	CLA	C1B-C2B	2.68	1.49	1.43
22	B	830	CLA	C1B-C2B	2.68	1.49	1.43
22	3	410	CLA	C1B-C2B	2.68	1.49	1.43
22	B	841	CLA	C1B-C2B	2.68	1.49	1.43
22	9	609	CLA	C1B-C2B	2.68	1.49	1.43
22	8	612	CLA	C1B-C2B	2.68	1.49	1.43
22	3	402	CLA	C3B-C4B	2.68	1.49	1.42
22	1	311	CLA	C1B-C2B	2.68	1.49	1.43
22	B	824	CLA	C1B-C2B	2.68	1.49	1.43
22	6	315	CLA	C1B-C2B	2.68	1.49	1.43
22	A	822	CLA	C1B-C2B	2.68	1.49	1.43
22	5	315	CLA	C1B-C2B	2.67	1.49	1.43
22	A	819	CLA	C1B-C2B	2.67	1.49	1.43
22	G	203	CLA	C4D-ND	-2.67	1.34	1.37
22	A	829	CLA	C3B-C4B	2.67	1.49	1.42
22	A	841	CLA	C1B-C2B	2.67	1.49	1.43
22	A	814	CLA	C1B-C2B	2.67	1.49	1.43
22	B	837	CLA	C1B-C2B	2.67	1.49	1.43
22	8	613	CLA	C3B-C4B	2.67	1.49	1.42
22	6	306	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	317	CLA	C1B-C2B	2.67	1.49	1.43
22	A	812	CLA	C1B-C2B	2.67	1.49	1.43
22	G	203	CLA	C1B-C2B	2.67	1.49	1.43
22	A	839	CLA	C1B-C2B	2.67	1.49	1.43
22	5	310	CLA	C1B-C2B	2.67	1.49	1.43
22	B	810	CLA	C1B-C2B	2.67	1.49	1.43
22	B	825	CLA	C1B-C2B	2.67	1.49	1.43
22	B	811	CLA	C4D-ND	-2.67	1.34	1.37
22	A	802	CLA	C1B-C2B	2.67	1.49	1.43
22	3	411	CLA	C1B-C2B	2.66	1.49	1.43
22	5	317	CLA	C3B-C4B	2.66	1.49	1.42
22	7	313	CLA	C1B-C2B	2.66	1.49	1.43
22	8	616	CLA	C1B-C2B	2.66	1.49	1.43
22	K	202	CLA	C1B-C2B	2.66	1.49	1.43
22	1	310	CLA	C4D-ND	-2.66	1.34	1.37
22	2	605	CLA	C1B-C2B	2.66	1.49	1.43
22	B	829	CLA	C1B-C2B	2.66	1.49	1.43
22	7	310	CLA	C4D-ND	-2.66	1.34	1.37
22	6	314	CLA	C1B-C2B	2.66	1.49	1.43
22	7	307	CLA	C1B-C2B	2.66	1.49	1.43
22	A	809	CLA	C1B-C2B	2.66	1.49	1.43
23	8	603	CHL	C1D-C2D	-2.66	1.40	1.45
22	5	304	CLA	C4B-C3B	2.66	1.49	1.43
22	5	312	CLA	C1B-C2B	2.66	1.49	1.43
22	A	824	CLA	C4D-ND	-2.66	1.34	1.37
22	H	202	CLA	C4B-C3B	2.66	1.49	1.43
22	K	204	CLA	C1B-C2B	2.66	1.49	1.43
23	7	305	CHL	C1C-NC	2.66	1.41	1.37
22	B	816	CLA	C1B-C2B	2.66	1.49	1.43
22	8	612	CLA	C4D-ND	-2.66	1.34	1.37
22	2	608	CLA	C1B-C2B	2.65	1.49	1.43
22	2	610	CLA	C4D-ND	-2.65	1.34	1.37
22	A	808	CLA	C1B-C2B	2.65	1.49	1.43
22	K	206	CLA	C1B-C2B	2.65	1.49	1.43
22	6	316	CLA	C1B-C2B	2.65	1.49	1.43
22	2	609	CLA	C4B-C3B	2.65	1.49	1.43
22	B	817	CLA	C1B-C2B	2.65	1.49	1.43
22	H	201	CLA	C4B-C3B	2.65	1.49	1.43
22	3	414	CLA	C1B-C2B	2.65	1.49	1.43
22	A	801	CLA	C4D-ND	-2.65	1.34	1.37
22	5	313	CLA	C1B-C2B	2.65	1.49	1.43
23	3	406	CHL	C1C-NC	2.65	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	805	CLA	C4D-ND	-2.65	1.34	1.37
30	6	321	NEX	C7-C8	-2.65	1.27	1.32
22	A	810	CLA	C1B-C2B	2.65	1.49	1.43
22	1	309	CLA	C1B-C2B	2.64	1.49	1.43
30	5	323	NEX	C7-C8	-2.64	1.27	1.32
22	9	611	CLA	C1B-C2B	2.64	1.49	1.43
22	1	303	CLA	C4B-C3B	2.64	1.49	1.43
22	2	603	CLA	C1B-C2B	2.64	1.49	1.43
22	9	610	CLA	C1B-C2B	2.64	1.49	1.43
22	B	843	CLA	C3B-C4B	2.64	1.48	1.42
22	8	605	CLA	C1B-C2B	2.64	1.49	1.43
22	5	310	CLA	C4D-ND	-2.64	1.34	1.37
22	6	313	CLA	C4D-ND	-2.64	1.34	1.37
22	A	806	CLA	C1B-C2B	2.64	1.49	1.43
22	7	313	CLA	C4B-C3B	2.64	1.49	1.43
22	A	833	CLA	C1B-C2B	2.64	1.49	1.43
22	A	811	CLA	C1B-C2B	2.64	1.49	1.43
22	9	607	CLA	C3B-C4B	2.63	1.48	1.42
22	9	604	CLA	C1B-C2B	2.63	1.49	1.43
22	B	818	CLA	C1B-C2B	2.63	1.49	1.43
22	B	826	CLA	C1B-C2B	2.63	1.49	1.43
22	J	102	CLA	C1B-C2B	2.63	1.49	1.43
22	L	302	CLA	C1B-C2B	2.63	1.49	1.43
22	7	309	CLA	C1B-C2B	2.63	1.49	1.43
22	H	201	CLA	C1B-C2B	2.63	1.49	1.43
22	9	607	CLA	C4D-ND	-2.63	1.34	1.37
22	9	612	CLA	C1B-C2B	2.63	1.49	1.43
22	1	313	CLA	C1B-C2B	2.62	1.49	1.43
22	1	311	CLA	C4D-ND	-2.62	1.34	1.37
22	A	825	CLA	C1B-C2B	2.62	1.49	1.43
22	7	312	CLA	C1B-C2B	2.62	1.49	1.43
22	8	604	CLA	C1B-C2B	2.62	1.49	1.43
22	A	829	CLA	C1B-C2B	2.62	1.49	1.43
22	6	305	CLA	C4B-C3B	2.62	1.49	1.43
22	B	808	CLA	C1B-C2B	2.62	1.49	1.43
22	5	304	CLA	C1B-C2B	2.62	1.49	1.43
22	9	610	CLA	C4D-ND	-2.61	1.34	1.37
22	A	836	CLA	C3B-C4B	2.61	1.48	1.42
22	3	409	CLA	C1B-C2B	2.61	1.49	1.43
22	A	835	CLA	C1B-C2B	2.61	1.49	1.43
22	A	804	CLA	C4D-ND	-2.61	1.34	1.37
22	A	834	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	305	CLA	C1B-C2B	2.61	1.49	1.43
22	B	814	CLA	C4B-C3B	2.61	1.49	1.43
22	B	835	CLA	C1B-C2B	2.61	1.49	1.43
22	5	316	CLA	C4B-C3B	2.61	1.49	1.43
22	F	804	CLA	C1B-C2B	2.61	1.49	1.43
22	B	833	CLA	C1B-C2B	2.61	1.49	1.43
22	H	202	CLA	C1B-C2B	2.61	1.49	1.43
22	3	403	CLA	C1B-C2B	2.61	1.49	1.43
22	9	603	CLA	C1B-C2B	2.61	1.49	1.43
22	B	815	CLA	C1B-C2B	2.60	1.49	1.43
22	1	310	CLA	C1B-C2B	2.60	1.49	1.43
22	B	840	CLA	C1B-C2B	2.60	1.49	1.43
22	B	812	CLA	C1B-C2B	2.60	1.49	1.43
22	H	203	CLA	C1B-C2B	2.60	1.49	1.43
22	1	303	CLA	C1B-C2B	2.60	1.49	1.43
22	1	307	CLA	C4B-C3B	2.59	1.49	1.43
22	7	301	CLA	C1B-C2B	2.59	1.49	1.43
22	3	401	CLA	C1B-C2B	2.59	1.49	1.43
22	8	609	CLA	C1B-C2B	2.59	1.49	1.43
22	5	305	CLA	C4B-C3B	2.59	1.49	1.43
22	B	803	CLA	C1B-C2B	2.59	1.49	1.43
22	8	604	CLA	C4B-C3B	2.59	1.49	1.43
22	6	313	CLA	C1B-C2B	2.59	1.49	1.43
22	B	827	CLA	C1B-C2B	2.59	1.49	1.43
22	B	819	CLA	C1B-C2B	2.58	1.49	1.43
22	A	838	CLA	C1B-C2B	2.58	1.49	1.43
22	6	311	CLA	CHC-C1C	2.58	1.43	1.38
22	B	838	CLA	C1B-C2B	2.58	1.49	1.43
22	7	308	CLA	C1B-C2B	2.58	1.49	1.43
22	2	602	CLA	C1B-C2B	2.58	1.49	1.43
22	3	404	CLA	C1B-C2B	2.58	1.49	1.43
22	2	604	CLA	C1B-C2B	2.57	1.49	1.43
22	7	302	CLA	C1B-C2B	2.57	1.49	1.43
22	B	844	CLA	C1B-C2B	2.57	1.49	1.43
23	7	304	CHL	MG-NC	2.57	2.12	2.06
22	B	834	CLA	C1B-C2B	2.57	1.49	1.43
22	2	609	CLA	C1B-C2B	2.56	1.49	1.43
22	2	610	CLA	C1B-C2B	2.56	1.49	1.43
23	1	304	CHL	C1C-NC	2.56	1.41	1.37
22	A	827	CLA	C1B-C2B	2.56	1.49	1.43
22	A	828	CLA	C1B-C2B	2.56	1.49	1.43
22	7	310	CLA	C1B-C2B	2.56	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	615	CLA	C4B-C3B	2.56	1.49	1.43
22	6	310	CLA	C1B-C2B	2.56	1.49	1.43
22	A	813	CLA	C1B-C2B	2.56	1.49	1.43
22	8	601	CLA	C1B-C2B	2.56	1.49	1.43
22	5	303	CLA	C1B-C2B	2.55	1.49	1.43
22	8	610	CLA	C1B-C2B	2.55	1.49	1.43
22	A	830	CLA	C1B-C2B	2.55	1.49	1.43
22	B	820	CLA	C1B-C2B	2.54	1.49	1.43
23	3	413	CHL	MG-NC	2.54	2.12	2.06
22	3	408	CLA	C1B-C2B	2.54	1.49	1.43
22	1	313	CLA	C4B-C3B	2.54	1.49	1.43
22	8	614	CLA	C1B-C2B	2.54	1.49	1.43
22	F	803	CLA	C1B-C2B	2.54	1.49	1.43
22	6	304	CLA	C1B-C2B	2.53	1.49	1.43
22	B	806	CLA	C1B-C2B	2.52	1.49	1.43
22	A	818	CLA	C1B-C2B	2.52	1.49	1.43
22	5	311	CLA	C1B-C2B	2.52	1.49	1.43
22	B	821	CLA	C1B-C2B	2.52	1.49	1.43
22	A	837	CLA	C1B-C2B	2.51	1.49	1.43
22	B	832	CLA	C1B-C2B	2.51	1.49	1.43
22	A	803	CLA	C1B-C2B	2.51	1.49	1.43
22	A	820	CLA	C1B-C2B	2.51	1.49	1.43
23	5	319	CHL	C1C-NC	2.50	1.41	1.37
23	3	406	CHL	MG-NA	2.50	2.12	2.06
22	A	831	CLA	C1B-C2B	2.50	1.49	1.43
22	B	839	CLA	C1B-C2B	2.50	1.49	1.43
22	L	302	CLA	MG-NA	2.49	2.12	2.06
22	B	804	CLA	C1B-C2B	2.49	1.49	1.43
22	9	608	CLA	C1B-C2B	2.48	1.49	1.43
22	B	842	CLA	C1B-C2B	2.48	1.49	1.43
22	B	828	CLA	C1B-C2B	2.48	1.49	1.43
22	L	302	CLA	C4D-ND	-2.47	1.34	1.37
22	B	815	CLA	C4D-ND	-2.47	1.34	1.37
22	1	302	CLA	C1B-C2B	2.47	1.49	1.43
22	3	407	CLA	C1B-C2B	2.47	1.49	1.43
23	5	302	CHL	C1C-NC	2.46	1.41	1.37
22	A	813	CLA	C4D-ND	-2.45	1.34	1.37
22	7	314	CLA	C4B-C3B	2.45	1.49	1.43
22	A	817	CLA	C1B-C2B	2.45	1.49	1.43
22	A	829	CLA	CMB-C2B	-2.45	1.45	1.50
23	3	405	CHL	C4D-ND	-2.44	1.34	1.37
22	B	807	CLA	C1B-C2B	2.44	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	301	CLA	CHC-C1C	2.42	1.43	1.38
23	5	306	CHL	C1D-C2D	-2.42	1.40	1.45
22	2	601	CLA	C1B-C2B	2.42	1.48	1.43
22	F	802	CLA	C1B-C2B	2.41	1.48	1.43
22	B	807	CLA	CHC-C1C	2.41	1.43	1.38
23	8	607	CHL	MG-NC	2.40	2.12	2.06
22	6	312	CLA	C1B-C2B	2.40	1.48	1.43
22	3	411	CLA	MG-NC	2.40	2.12	2.06
22	9	602	CLA	CHC-C1C	2.39	1.43	1.38
22	B	802	CLA	CHC-C1C	2.38	1.43	1.38
23	7	305	CHL	C1D-C2D	-2.38	1.40	1.45
22	B	832	CLA	CMD-C2D	-2.37	1.45	1.50
23	5	307	CHL	MG-NC	2.35	2.11	2.06
23	5	307	CHL	C1D-C2D	-2.35	1.40	1.45
22	8	611	CLA	C1B-C2B	2.35	1.48	1.43
22	5	317	CLA	CMC-C2C	-2.34	1.45	1.50
22	K	202	CLA	CMD-C2D	-2.34	1.45	1.50
22	8	611	CLA	CHC-C1C	2.34	1.43	1.38
22	A	828	CLA	CMC-C2C	-2.33	1.45	1.50
22	B	822	CLA	C1B-C2B	2.32	1.48	1.43
28	A	853	LMU	C3B-C2B	-2.32	1.48	1.52
22	1	308	CLA	C1B-C2B	2.31	1.48	1.43
22	9	602	CLA	C1B-C2B	2.31	1.48	1.43
22	B	839	CLA	CMC-C2C	-2.31	1.45	1.50
22	9	608	CLA	CHC-C1C	2.30	1.43	1.38
23	5	308	CHL	MG-NC	2.29	2.11	2.06
22	B	806	CLA	CMC-C2C	-2.29	1.45	1.50
22	A	803	CLA	CHC-C1C	2.29	1.43	1.38
23	9	605	CHL	C1D-C2D	-2.29	1.40	1.45
22	K	205	CLA	CMD-C2D	-2.28	1.46	1.50
22	B	832	CLA	CMB-C2B	-2.28	1.46	1.50
23	3	405	CHL	MG-NA	2.28	2.11	2.06
22	B	828	CLA	CMD-C2D	-2.27	1.46	1.50
22	B	805	CLA	CMD-C2D	-2.27	1.46	1.50
23	1	306	CHL	MG-NA	2.26	2.11	2.06
23	3	422	CHL	MG-NC	2.26	2.11	2.06
22	7	301	CLA	CHC-C1C	2.26	1.43	1.38
22	1	308	CLA	CHC-C1C	2.25	1.43	1.38
22	1	301	CLA	C1B-C2B	2.25	1.48	1.43
22	B	812	CLA	CMB-C2B	-2.24	1.46	1.50
22	B	804	CLA	CHC-C1C	2.24	1.43	1.38
22	2	601	CLA	CHC-C1C	2.23	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	319	LMU	O5'-C5'	2.23	1.49	1.44
31	8	621	LMG	O7-C8	-2.23	1.43	1.47
22	B	802	CLA	CMD-C2D	-2.22	1.46	1.50
22	1	302	CLA	CHC-C1C	2.22	1.43	1.38
22	B	827	CLA	CMD-C2D	-2.21	1.46	1.50
23	5	318	CHL	C1D-C2D	-2.21	1.41	1.45
22	B	808	CLA	CHC-C1C	2.21	1.43	1.38
22	B	843	CLA	CMB-C2B	-2.20	1.46	1.50
23	3	406	CHL	MG-NC	2.20	2.11	2.06
22	B	840	CLA	CHC-C1C	2.20	1.43	1.38
22	A	827	CLA	CHC-C1C	2.20	1.43	1.38
22	H	203	CLA	CMD-C2D	-2.19	1.46	1.50
22	8	613	CLA	CMD-C2D	-2.19	1.46	1.50
22	6	304	CLA	CHC-C1C	2.19	1.43	1.38
22	F	804	CLA	CMD-C2D	-2.18	1.46	1.50
22	8	610	CLA	CHC-C1C	2.18	1.43	1.38
23	6	308	CHL	C1D-C2D	-2.18	1.41	1.45
22	B	839	CLA	CHC-C1C	2.18	1.43	1.38
22	3	408	CLA	CHC-C1C	2.18	1.42	1.38
22	2	601	CLA	CMC-C2C	-2.18	1.46	1.50
22	A	841	CLA	CMB-C2B	-2.18	1.46	1.50
22	B	828	CLA	CHC-C1C	2.18	1.42	1.38
22	8	615	CLA	MG-NC	2.18	2.11	2.06
22	A	815	CLA	CMD-C2D	-2.17	1.46	1.50
22	B	822	CLA	CHC-C1C	2.17	1.42	1.38
22	F	802	CLA	CMD-C2D	-2.17	1.46	1.50
22	B	820	CLA	CMB-C2B	-2.17	1.46	1.50
22	B	835	CLA	CHC-C1C	2.17	1.42	1.38
22	B	827	CLA	CHC-C1C	2.17	1.42	1.38
22	9	608	CLA	CMD-C2D	-2.17	1.46	1.50
22	9	602	CLA	MG-NC	2.17	2.11	2.06
22	F	802	CLA	CMB-C2B	-2.17	1.46	1.50
23	8	602	CHL	C1D-C2D	-2.17	1.41	1.45
22	8	609	CLA	CMB-C2B	-2.16	1.46	1.50
22	A	831	CLA	CHC-C1C	2.16	1.42	1.38
23	6	303	CHL	MG-NC	2.16	2.11	2.06
23	3	413	CHL	C1C-NC	2.16	1.41	1.37
22	1	302	CLA	CMD-C2D	-2.16	1.46	1.50
22	B	836	CLA	CMD-C2D	-2.16	1.46	1.50
22	1	312	CLA	CMD-C2D	-2.16	1.46	1.50
22	8	613	CLA	CMB-C2B	-2.15	1.46	1.50
22	A	830	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	612	CLA	CMD-C2D	-2.15	1.46	1.50
22	6	312	CLA	CHC-C1C	2.14	1.42	1.38
23	8	607	CHL	C1D-C2D	-2.14	1.41	1.45
22	3	401	CLA	CHC-C1C	2.14	1.42	1.38
22	A	820	CLA	CHC-C1C	2.14	1.42	1.38
22	B	834	CLA	CHC-C1C	2.14	1.42	1.38
23	5	308	CHL	C1D-C2D	-2.14	1.41	1.45
22	2	607	CLA	CMD-C2D	-2.14	1.46	1.50
23	7	304	CHL	C1D-C2D	-2.14	1.41	1.45
23	8	608	CHL	C1D-C2D	-2.14	1.41	1.45
22	7	308	CLA	CHC-C1C	2.14	1.42	1.38
22	7	314	CLA	CMB-C2B	-2.13	1.46	1.50
22	A	820	CLA	CMB-C2B	-2.13	1.46	1.50
28	7	319	LMU	O5'-C5'	2.13	1.49	1.44
34	B	852	DGD	O3G-C1D	2.13	1.43	1.40
22	A	828	CLA	CMD-C2D	-2.13	1.46	1.50
22	B	815	CLA	CHC-C1C	2.13	1.42	1.38
22	H	203	CLA	CHC-C1C	2.13	1.42	1.38
22	B	842	CLA	CMD-C2D	-2.13	1.46	1.50
28	K	201	LMU	O5'-C5'	2.12	1.49	1.44
22	A	826	CLA	CMC-C2C	-2.12	1.46	1.50
22	1	313	CLA	CMB-C2B	-2.12	1.46	1.50
22	B	802	CLA	C1B-C2B	2.12	1.48	1.43
22	A	841	CLA	CMD-C2D	-2.12	1.46	1.50
22	8	605	CLA	CHC-C1C	2.12	1.42	1.38
22	8	601	CLA	CHC-C1C	2.12	1.42	1.38
22	2	604	CLA	CMB-C2B	-2.12	1.46	1.50
22	5	305	CLA	CMD-C2D	-2.12	1.46	1.50
22	A	818	CLA	CMB-C2B	-2.12	1.46	1.50
22	B	822	CLA	CMB-C2B	-2.12	1.46	1.50
22	A	840	CLA	CMD-C2D	-2.11	1.46	1.50
22	9	612	CLA	CHC-C1C	2.11	1.42	1.38
22	8	611	CLA	CMD-C2D	-2.11	1.46	1.50
22	5	303	CLA	CHC-C1C	2.11	1.42	1.38
23	8	606	CHL	C1D-C2D	-2.11	1.41	1.45
22	3	411	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	838	CLA	CMB-C2B	-2.11	1.46	1.50
22	6	305	CLA	CHC-C1C	2.11	1.42	1.38
22	1	303	CLA	CHC-C1C	2.11	1.42	1.38
22	5	317	CLA	CMB-C2B	-2.11	1.46	1.50
22	A	830	CLA	CMD-C2D	-2.11	1.46	1.50
22	B	817	CLA	CHC-C1C	2.10	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	307	CLA	CHC-C1C	2.10	1.42	1.38
22	9	606	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	836	CLA	CHC-C1C	2.10	1.42	1.38
22	A	817	CLA	CHC-C1C	2.10	1.42	1.38
22	5	311	CLA	CHC-C1C	2.10	1.42	1.38
23	8	608	CHL	MG-NA	2.10	2.11	2.06
22	A	828	CLA	CMB-C2B	-2.10	1.46	1.50
22	B	826	CLA	CHC-C1C	2.10	1.42	1.38
22	9	610	CLA	C3D-C4D	2.10	1.48	1.44
22	7	302	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	830	CLA	CMD-C2D	-2.09	1.46	1.50
22	6	310	CLA	CHC-C1C	2.09	1.42	1.38
22	6	311	CLA	C1B-C2B	2.09	1.48	1.43
22	K	204	CLA	CHC-C1C	2.09	1.42	1.38
22	B	829	CLA	CMC-C2C	-2.09	1.46	1.50
22	B	831	CLA	CMD-C2D	-2.09	1.46	1.50
22	1	309	CLA	CHC-C1C	2.09	1.42	1.38
22	5	315	CLA	CHC-C1C	2.09	1.42	1.38
22	7	306	CLA	CHC-C1C	2.09	1.42	1.38
22	A	837	CLA	CHC-C1C	2.09	1.42	1.38
22	B	831	CLA	CHC-C1C	2.09	1.42	1.38
22	A	822	CLA	CMD-C2D	-2.08	1.46	1.50
22	B	821	CLA	CMB-C2B	-2.08	1.46	1.50
22	6	315	CLA	CHC-C1C	2.08	1.42	1.38
22	K	206	CLA	CHC-C1C	2.08	1.42	1.38
22	2	607	CLA	CHC-C1C	2.08	1.42	1.38
22	2	606	CLA	CBD-CAD	2.08	1.56	1.51
22	A	826	CLA	CHC-C1C	2.08	1.42	1.38
22	B	819	CLA	CHC-C1C	2.08	1.42	1.38
22	2	612	CLA	CHC-C1C	2.08	1.42	1.38
22	3	402	CLA	CMB-C2B	-2.08	1.46	1.50
22	B	844	CLA	CHC-C1C	2.08	1.42	1.38
22	B	844	CLA	CMD-C2D	-2.08	1.46	1.50
22	H	202	CLA	CHC-C1C	2.07	1.42	1.38
22	2	613	CLA	CMC-C2C	-2.07	1.46	1.50
22	A	812	CLA	CMC-C2C	-2.07	1.46	1.50
22	L	303	CLA	CHC-C1C	2.07	1.42	1.38
22	6	312	CLA	CMD-C2D	-2.07	1.46	1.50
22	3	412	CLA	CHC-C1C	2.07	1.42	1.38
22	K	202	CLA	CHC-C1C	2.07	1.42	1.38
22	6	315	CLA	CMD-C2D	-2.07	1.46	1.50
22	7	313	CLA	CHC-C1C	2.07	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	811	CLA	CHC-C1C	2.07	1.42	1.38
22	A	825	CLA	CMD-C2D	-2.07	1.46	1.50
22	A	810	CLA	CMD-C2D	-2.07	1.46	1.50
22	B	837	CLA	CHC-C1C	2.07	1.42	1.38
22	F	803	CLA	CHC-C1C	2.07	1.42	1.38
22	3	411	CLA	CMB-C2B	-2.07	1.46	1.50
22	A	801	CLA	CMB-C2B	-2.07	1.46	1.50
22	A	801	CLA	CMD-C2D	-2.07	1.46	1.50
22	5	303	CLA	CMB-C2B	-2.06	1.46	1.50
28	G	201	LMU	O5'-C5'	2.06	1.49	1.44
22	B	825	CLA	CMD-C2D	-2.06	1.46	1.50
22	A	804	CLA	CMC-C2C	-2.06	1.46	1.50
22	7	309	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	842	CLA	CMB-C2B	-2.06	1.46	1.50
22	6	307	CLA	CHC-C1C	2.06	1.42	1.38
22	L	304	CLA	CBD-CAD	2.06	1.56	1.51
22	B	815	CLA	CMB-C2B	-2.06	1.46	1.50
22	A	814	CLA	CHC-C1C	2.06	1.42	1.38
22	2	613	CLA	CHC-C1C	2.06	1.42	1.38
22	B	811	CLA	CMD-C2D	-2.06	1.46	1.50
28	J	106	LMU	O5'-C5'	2.06	1.49	1.44
22	6	313	CLA	CMD-C2D	-2.06	1.46	1.50
22	B	836	CLA	CMC-C2C	-2.06	1.46	1.50
22	9	609	CLA	CHC-C1C	2.06	1.42	1.38
22	3	404	CLA	CHC-C1C	2.06	1.42	1.38
22	B	842	CLA	CHC-C1C	2.06	1.42	1.38
22	3	402	CLA	CMD-C2D	-2.06	1.46	1.50
22	5	304	CLA	CHC-C1C	2.05	1.42	1.38
22	9	604	CLA	CHC-C1C	2.05	1.42	1.38
22	5	312	CLA	CHC-C1C	2.05	1.42	1.38
22	2	608	CLA	CHC-C1C	2.05	1.42	1.38
22	A	821	CLA	CHC-C1C	2.05	1.42	1.38
22	5	311	CLA	CMB-C2B	-2.05	1.46	1.50
23	3	422	CHL	C1D-C2D	-2.05	1.41	1.45
22	2	611	CLA	CHC-C1C	2.05	1.42	1.38
23	5	319	CHL	C1D-C2D	-2.05	1.41	1.45
23	8	607	CHL	C1C-NC	2.05	1.40	1.37
22	1	307	CLA	CMD-C2D	-2.05	1.46	1.50
22	5	315	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	806	CLA	CHC-C1C	2.05	1.42	1.38
22	8	615	CLA	C3D-C4D	2.05	1.48	1.44
22	7	312	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	808	CLA	CMD-C2D	-2.05	1.46	1.50
22	F	803	CLA	CMB-C2B	-2.05	1.46	1.50
22	6	318	CLA	CHC-C1C	2.05	1.42	1.38
22	J	102	CLA	CMD-C2D	-2.05	1.46	1.50
22	B	818	CLA	CHC-C1C	2.05	1.42	1.38
22	5	304	CLA	CMB-C2B	-2.05	1.46	1.50
23	6	303	CHL	C1D-C2D	-2.05	1.41	1.45
22	B	807	CLA	CMD-C2D	-2.04	1.46	1.50
22	1	311	CLA	CMD-C2D	-2.04	1.46	1.50
22	B	820	CLA	CHC-C1C	2.04	1.42	1.38
22	L	302	CLA	CHC-C1C	2.04	1.42	1.38
22	B	810	CLA	CHC-C1C	2.04	1.42	1.38
22	1	302	CLA	C3D-C4D	2.04	1.48	1.44
22	2	606	CLA	CHC-C1C	2.04	1.42	1.38
22	A	834	CLA	CHC-C1C	2.04	1.42	1.38
22	J	102	CLA	CHC-C1C	2.04	1.42	1.38
22	6	316	CLA	CHC-C1C	2.04	1.42	1.38
22	2	605	CLA	CBD-CAD	2.04	1.56	1.51
22	A	843	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	833	CLA	CHC-C1C	2.04	1.42	1.38
22	1	310	CLA	CMD-C2D	-2.04	1.46	1.50
22	H	201	CLA	CHC-C1C	2.04	1.42	1.38
22	7	311	CLA	CMD-C2D	-2.04	1.46	1.50
22	A	838	CLA	CHC-C1C	2.04	1.42	1.38
22	2	603	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	841	CLA	CHC-C1C	2.03	1.42	1.38
22	A	822	CLA	CHC-C1C	2.03	1.42	1.38
22	A	832	CLA	CHC-C1C	2.03	1.42	1.38
22	A	814	CLA	CMD-C2D	-2.03	1.46	1.50
22	9	604	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	816	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	827	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	834	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	838	CLA	CHC-C1C	2.03	1.42	1.38
22	2	605	CLA	CMD-C2D	-2.03	1.46	1.50
22	7	310	CLA	CMD-C2D	-2.03	1.46	1.50
22	3	408	CLA	CMD-C2D	-2.03	1.46	1.50
22	8	616	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	817	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	816	CLA	CMC-C2C	-2.03	1.46	1.50
22	7	311	CLA	CHC-C1C	2.03	1.42	1.38
22	8	610	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	825	CLA	CHC-C1C	2.03	1.42	1.38
22	2	609	CLA	CHC-C1C	2.03	1.42	1.38
22	A	804	CLA	CHC-C1C	2.03	1.42	1.38
22	G	202	CLA	CMD-C2D	-2.03	1.46	1.50
22	A	835	CLA	CMB-C2B	-2.03	1.46	1.50
22	B	804	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	609	CLA	CMB-C2B	-2.02	1.46	1.50
22	B	829	CLA	CHC-C1C	2.02	1.42	1.38
22	A	802	CLA	CHC-C1C	2.02	1.42	1.38
22	A	835	CLA	CHC-C1C	2.02	1.42	1.38
23	9	605	CHL	MG-NC	2.02	2.11	2.06
22	B	829	CLA	CMD-C2D	-2.02	1.46	1.50
22	2	602	CLA	CHC-C1C	2.02	1.42	1.38
22	A	819	CLA	CHC-C1C	2.02	1.42	1.38
22	2	610	CLA	C3D-C4D	2.02	1.48	1.44
22	A	805	CLA	CHC-C1C	2.02	1.42	1.38
22	6	305	CLA	CMB-C2B	-2.02	1.46	1.50
22	6	317	CLA	CHC-C1C	2.02	1.42	1.38
22	5	316	CLA	CHC-C1C	2.02	1.42	1.38
22	2	608	CLA	CMB-C2B	-2.02	1.46	1.50
22	A	818	CLA	CHC-C1C	2.02	1.42	1.38
22	A	840	CLA	CHC-C1C	2.02	1.42	1.38
22	B	833	CLA	CMB-C2B	-2.02	1.46	1.50
22	2	605	CLA	CHC-C1C	2.02	1.42	1.38
22	7	303	CLA	CHC-C1C	2.02	1.42	1.38
22	5	311	CLA	CMC-C2C	-2.02	1.46	1.50
22	9	611	CLA	CHC-C1C	2.02	1.42	1.38
22	7	311	CLA	CMB-C2B	-2.02	1.46	1.50
22	9	611	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	832	CLA	CMB-C2B	-2.01	1.46	1.50
22	3	407	CLA	CMB-C2B	-2.01	1.46	1.50
22	A	823	CLA	CMB-C2B	-2.01	1.46	1.50
22	B	843	CLA	CMD-C2D	-2.01	1.46	1.50
23	8	608	CHL	MG-NC	2.01	2.11	2.06
22	5	305	CLA	CHC-C1C	2.01	1.42	1.38
22	B	844	CLA	CMC-C2C	-2.01	1.46	1.50
22	3	403	CLA	CHC-C1C	2.01	1.42	1.38
22	B	824	CLA	CHC-C1C	2.01	1.42	1.38
22	8	614	CLA	CHC-C1C	2.01	1.42	1.38
22	7	310	CLA	CHC-C1C	2.01	1.42	1.38
22	2	604	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	808	CLA	CHC-C1C	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	9	609	CLA	CMC-C2C	-2.01	1.46	1.50
22	1	310	CLA	MG-NA	2.01	2.11	2.06
22	2	610	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	825	CLA	CMB-C2B	-2.01	1.46	1.50
22	1	301	CLA	CMB-C2B	-2.01	1.46	1.50
22	3	410	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	824	CLA	C3D-C4D	2.01	1.48	1.44
22	A	811	CLA	CMD-C2D	-2.01	1.46	1.50
22	5	311	CLA	CMD-C2D	-2.01	1.46	1.50
22	8	612	CLA	CHC-C1C	2.01	1.42	1.38
22	B	833	CLA	CMD-C2D	-2.01	1.46	1.50
22	A	816	CLA	CHC-C1C	2.00	1.42	1.38
22	A	805	CLA	CMD-C2D	-2.00	1.46	1.50
22	A	816	CLA	CMC-C2C	-2.00	1.46	1.50
22	5	313	CLA	CMD-C2D	-2.00	1.46	1.50
23	3	413	CHL	C1D-C2D	-2.00	1.41	1.45
22	2	604	CLA	CHC-C1C	2.00	1.42	1.38
22	A	817	CLA	CMB-C2B	-2.00	1.46	1.50
22	3	414	CLA	CHC-C1C	2.00	1.42	1.38
22	A	839	CLA	CHC-C1C	2.00	1.42	1.38
22	5	303	CLA	CMD-C2D	-2.00	1.46	1.50
22	B	823	CLA	CMB-C2B	-2.00	1.46	1.50
22	3	409	CLA	CHC-C1C	2.00	1.42	1.38
22	L	304	CLA	CMD-C2D	-2.00	1.46	1.50

All (2298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	618	XAT	O24-C25-C24	11.97	122.37	113.38
23	1	305	CHL	C1D-ND-C4D	-11.87	97.90	106.33
26	B	847	BCR	C39-C30-C25	-11.11	92.28	110.30
23	9	605	CHL	C4A-NA-C1A	9.62	111.03	106.71
30	6	321	NEX	O24-C25-C24	8.92	120.08	113.38
26	B	847	BCR	C40-C30-C39	-8.82	81.46	108.53
23	3	422	CHL	C4A-NA-C1A	8.26	110.42	106.71
23	9	601	CHL	C4A-NA-C1A	8.11	110.35	106.71
23	1	305	CHL	C4A-NA-C1A	8.09	110.34	106.71
25	2	615	XAT	O24-C25-C24	7.81	119.25	113.38
26	A	851	BCR	C7-C8-C9	-7.60	114.75	126.23
25	3	416	XAT	O24-C25-C24	7.45	118.98	113.38
25	1	315	XAT	O24-C25-C24	7.41	118.95	113.38
25	6	320	XAT	O4-C5-C4	7.33	118.89	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	2	615	XAT	O4-C5-C4	7.25	118.83	113.38
26	B	847	BCR	C40-C30-C25	7.23	122.02	110.30
25	5	321	XAT	O4-C5-C4	7.14	118.75	113.38
23	8	606	CHL	C4A-NA-C1A	6.93	109.82	106.71
22	B	815	CLA	C4A-NA-C1A	6.86	109.79	106.71
23	8	602	CHL	C4A-NA-C1A	6.81	109.77	106.71
23	5	307	CHL	C4A-NA-C1A	6.81	109.77	106.71
25	9	614	XAT	O24-C25-C24	6.77	118.47	113.38
25	8	618	XAT	O4-C5-C4	6.76	118.46	113.38
23	5	306	CHL	C4A-NA-C1A	6.76	109.74	106.71
26	7	317	BCR	C7-C8-C9	-6.67	116.15	126.23
23	5	302	CHL	C4A-NA-C1A	6.65	109.69	106.71
22	B	835	CLA	C4A-NA-C1A	6.58	109.67	106.71
23	5	308	CHL	C4A-NA-C1A	6.57	109.66	106.71
30	5	323	NEX	O24-C25-C24	6.56	118.31	113.38
25	3	416	XAT	O4-C5-C4	6.50	118.27	113.38
25	5	321	XAT	O24-C25-C24	6.44	118.22	113.38
23	6	303	CHL	C4A-NA-C1A	6.40	109.58	106.71
25	6	320	XAT	O24-C25-C24	6.34	118.14	113.38
25	9	614	XAT	O4-C5-C4	6.29	118.10	113.38
23	7	305	CHL	C4A-NA-C1A	6.27	109.53	106.71
25	3	416	XAT	C26-C27-C28	-6.27	112.73	125.99
23	5	318	CHL	C4A-NA-C1A	6.26	109.52	106.71
22	B	823	CLA	C4A-NA-C1A	6.16	109.47	106.71
22	1	302	CLA	C1D-ND-C4D	-6.14	101.98	106.33
23	3	406	CHL	C1D-ND-C4D	-6.12	101.98	106.33
26	L	305	BCR	C7-C8-C9	-6.07	117.07	126.23
22	2	613	CLA	C4A-NA-C1A	6.03	109.42	106.71
22	L	303	CLA	C4A-NA-C1A	5.98	109.40	106.71
25	7	316	XAT	O24-C25-C38	5.98	122.22	115.06
26	J	101	BCR	C11-C10-C9	-5.98	118.78	127.31
26	J	101	BCR	C15-C14-C13	-5.97	118.78	127.31
23	6	308	CHL	C4A-NA-C1A	5.96	109.39	106.71
22	A	804	CLA	C4A-NA-C1A	5.93	109.37	106.71
26	3	419	BCR	C7-C8-C9	-5.92	117.29	126.23
22	A	826	CLA	C4A-NA-C1A	5.92	109.37	106.71
22	A	836	CLA	C4A-NA-C1A	5.91	109.36	106.71
23	8	607	CHL	C4A-NA-C1A	5.91	109.36	106.71
23	1	304	CHL	C4A-NA-C1A	5.90	109.36	106.71
26	1	316	BCR	C20-C21-C22	-5.89	118.90	127.31
22	A	824	CLA	C4A-NA-C1A	5.89	109.35	106.71
23	7	304	CHL	C4A-NA-C1A	5.88	109.35	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	316	XAT	C38-C25-C26	-5.87	112.43	122.26
22	B	816	CLA	C4A-NA-C1A	5.87	109.34	106.71
22	A	812	CLA	C4A-NA-C1A	5.86	109.34	106.71
26	F	805	BCR	C16-C17-C18	-5.85	118.97	127.31
22	5	304	CLA	CAA-C2A-C3A	-5.84	96.79	112.78
22	G	203	CLA	C4A-NA-C1A	5.80	109.31	106.71
22	8	613	CLA	C4A-NA-C1A	5.78	109.31	106.71
22	7	314	CLA	C4A-NA-C1A	5.78	109.30	106.71
22	B	829	CLA	C4A-NA-C1A	5.77	109.30	106.71
22	1	313	CLA	C4A-NA-C1A	5.77	109.30	106.71
25	9	614	XAT	C18-C5-C6	-5.77	112.60	122.26
22	H	203	CLA	C4A-NA-C1A	5.77	109.30	106.71
26	M	102	BCR	C16-C17-C18	-5.74	119.12	127.31
22	A	802	CLA	C4A-NA-C1A	5.74	109.28	106.71
22	5	304	CLA	C4A-NA-C1A	5.72	109.28	106.71
22	B	813	CLA	C4A-NA-C1A	5.72	109.28	106.71
22	1	311	CLA	C4A-NA-C1A	5.69	109.27	106.71
25	5	321	XAT	C26-C27-C28	-5.69	113.96	125.99
22	9	604	CLA	C4A-NA-C1A	5.69	109.26	106.71
22	6	305	CLA	C4A-NA-C1A	5.67	109.26	106.71
23	5	309	CHL	C4A-NA-C1A	5.67	109.26	106.71
22	3	402	CLA	C4A-NA-C1A	5.65	109.25	106.71
22	K	205	CLA	C4A-NA-C1A	5.64	109.24	106.71
25	1	315	XAT	C26-C27-C28	-5.62	114.11	125.99
22	H	201	CLA	C4A-NA-C1A	5.59	109.22	106.71
23	5	302	CHL	C1D-ND-C4D	-5.58	102.37	106.33
26	J	101	BCR	C7-C8-C9	-5.58	117.81	126.23
26	B	847	BCR	C39-C30-C29	-5.54	86.76	108.91
26	9	615	BCR	C11-C10-C9	-5.53	119.42	127.31
25	1	315	XAT	C18-C5-C6	-5.52	113.00	122.26
22	A	814	CLA	C4A-NA-C1A	5.52	109.19	106.71
26	B	850	BCR	C7-C8-C9	-5.51	117.92	126.23
22	B	827	CLA	C4A-NA-C1A	5.50	109.18	106.71
25	3	416	XAT	C18-C5-C6	-5.49	113.06	122.26
25	5	321	XAT	C38-C25-C26	-5.47	113.09	122.26
25	7	316	XAT	C15-C14-C13	-5.45	119.54	127.31
26	1	316	BCR	C24-C23-C22	-5.44	118.01	126.23
25	6	320	XAT	C38-C25-C26	-5.43	113.15	122.26
23	5	309	CHL	C1D-ND-C4D	-5.43	102.47	106.33
25	1	315	XAT	O4-C5-C4	5.41	117.44	113.38
22	J	102	CLA	C4A-NA-C1A	5.40	109.13	106.71
22	5	317	CLA	C4A-NA-C1A	5.39	109.13	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	604	CLA	C4A-NA-C1A	5.34	109.11	106.71
22	1	302	CLA	C2A-C3A-C4A	-5.33	93.25	101.87
22	B	844	CLA	C4A-NA-C1A	5.32	109.10	106.71
25	7	316	XAT	C18-C5-C6	-5.32	113.34	122.26
22	2	605	CLA	C4A-NA-C1A	5.31	109.09	106.71
26	9	615	BCR	C7-C8-C9	-5.31	118.21	126.23
25	8	618	XAT	C18-C5-C6	-5.31	113.36	122.26
22	5	305	CLA	C4A-NA-C1A	5.31	109.09	106.71
22	G	202	CLA	C4A-NA-C1A	5.30	109.09	106.71
22	3	404	CLA	C4A-NA-C1A	5.30	109.09	106.71
26	B	846	BCR	C11-C10-C9	-5.30	119.75	127.31
22	A	823	CLA	C4A-NA-C1A	5.29	109.08	106.71
22	B	808	CLA	C4A-NA-C1A	5.27	109.08	106.71
22	8	612	CLA	C4A-NA-C1A	5.27	109.07	106.71
26	A	851	BCR	C24-C23-C22	-5.27	118.28	126.23
25	9	614	XAT	C38-C25-C26	-5.25	113.46	122.26
25	2	615	XAT	C18-C5-C6	-5.25	113.47	122.26
22	9	609	CLA	CAC-C3C-C4C	5.24	131.61	124.81
22	A	815	CLA	C4A-NA-C1A	5.24	109.06	106.71
26	8	619	BCR	C11-C10-C9	-5.24	119.84	127.31
22	B	825	CLA	C4A-NA-C1A	5.23	109.06	106.71
22	3	411	CLA	C4A-NA-C1A	5.22	109.06	106.71
26	I	201	BCR	C24-C23-C22	-5.22	118.35	126.23
22	A	831	CLA	C4A-NA-C1A	5.21	109.05	106.71
30	5	323	NEX	C38-C25-C26	-5.20	113.54	122.26
25	1	315	XAT	C38-C25-C26	-5.20	113.54	122.26
22	2	601	CLA	C4A-NA-C1A	5.20	109.04	106.71
22	1	302	CLA	C2A-C1A-CHA	5.20	132.95	123.86
25	5	321	XAT	C18-C5-C6	-5.19	113.56	122.26
25	7	316	XAT	O4-C5-C18	5.19	121.27	115.06
22	B	841	CLA	C4A-NA-C1A	5.18	109.04	106.71
22	B	810	CLA	C4A-NA-C1A	5.18	109.03	106.71
25	6	320	XAT	C26-C27-C28	-5.17	115.07	125.99
25	6	320	XAT	C18-C5-C6	-5.16	113.61	122.26
22	B	824	CLA	C4A-NA-C1A	5.16	109.03	106.71
22	A	811	CLA	C4A-NA-C1A	5.16	109.03	106.71
22	B	821	CLA	C4A-NA-C1A	5.15	109.02	106.71
26	8	619	BCR	C7-C8-C9	-5.15	118.45	126.23
22	7	313	CLA	C4A-NA-C1A	5.14	109.02	106.71
22	6	309	CLA	C4A-NA-C1A	5.14	109.02	106.71
22	A	835	CLA	C4A-NA-C1A	5.13	109.01	106.71
25	3	416	XAT	C38-C25-C26	-5.12	113.67	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	7	316	XAT	O24-C25-C24	5.12	117.23	113.38
26	G	204	BCR	C15-C14-C13	-5.11	120.02	127.31
22	5	303	CLA	C4A-NA-C1A	5.10	109.00	106.71
22	5	316	CLA	C4A-NA-C1A	5.10	109.00	106.71
25	3	416	XAT	C6-C7-C8	-5.10	115.22	125.99
26	5	322	BCR	C16-C17-C18	-5.09	120.04	127.31
22	9	606	CLA	C4A-NA-C1A	5.09	109.00	106.71
22	F	803	CLA	C4A-NA-C1A	5.08	108.99	106.71
26	M	102	BCR	C20-C21-C22	-5.08	120.06	127.31
26	1	316	BCR	C16-C17-C18	-5.08	120.06	127.31
22	B	820	CLA	C4A-NA-C1A	5.07	108.99	106.71
22	6	312	CLA	C4A-NA-C1A	5.07	108.98	106.71
22	7	311	CLA	C4A-NA-C1A	5.07	108.98	106.71
25	5	321	XAT	C6-C7-C8	-5.07	115.28	125.99
22	A	819	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	7	316	XAT	O4-C5-C4	5.05	117.18	113.38
22	7	306	CLA	C4A-NA-C1A	5.05	108.98	106.71
26	A	851	BCR	C33-C5-C6	-5.04	118.86	124.53
22	3	403	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	2	615	XAT	C26-C27-C28	-5.04	115.33	125.99
25	5	321	XAT	O24-C25-C38	5.03	121.09	115.06
22	8	614	CLA	C4A-NA-C1A	5.03	108.97	106.71
25	8	618	XAT	C6-C7-C8	-5.03	115.36	125.99
22	2	602	CLA	C4A-NA-C1A	5.02	108.97	106.71
26	A	846	BCR	C15-C14-C13	-5.02	120.14	127.31
22	8	609	CLA	C4A-NA-C1A	5.02	108.96	106.71
22	9	611	CLA	C4A-NA-C1A	5.01	108.96	106.71
22	A	807	CLA	C4A-NA-C1A	5.01	108.96	106.71
23	8	607	CHL	C1D-ND-C4D	-5.00	102.78	106.33
22	6	316	CLA	C4A-NA-C1A	5.00	108.95	106.71
22	B	838	CLA	C4A-NA-C1A	5.00	108.95	106.71
26	9	615	BCR	C16-C17-C18	-4.98	120.20	127.31
24	3	418	LUT	C15-C14-C13	-4.98	120.20	127.31
22	B	836	CLA	C4A-NA-C1A	4.98	108.94	106.71
22	B	831	CLA	C4A-NA-C1A	4.96	108.94	106.71
22	2	603	CLA	C4A-NA-C1A	4.96	108.94	106.71
22	F	804	CLA	C4A-NA-C1A	4.96	108.94	106.71
22	K	202	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	1	316	BCR	C15-C14-C13	-4.96	120.24	127.31
22	A	816	CLA	C4A-NA-C1A	4.95	108.93	106.71
22	B	817	CLA	C4A-NA-C1A	4.95	108.93	106.71
22	A	806	CLA	C4A-NA-C1A	4.93	108.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	304	CLA	C4A-NA-C1A	4.93	108.92	106.71
22	6	306	CLA	C4A-NA-C1A	4.93	108.92	106.71
26	7	317	BCR	C11-C10-C9	-4.93	120.28	127.31
25	1	315	XAT	O4-C5-C18	4.93	120.96	115.06
22	B	803	CLA	C4A-NA-C1A	4.92	108.92	106.71
22	B	840	CLA	C4A-NA-C1A	4.92	108.92	106.71
22	B	818	CLA	C4A-NA-C1A	4.91	108.92	106.71
22	B	804	CLA	C4A-NA-C1A	4.91	108.91	106.71
26	7	317	BCR	C16-C17-C18	-4.91	120.31	127.31
22	8	605	CLA	C4A-NA-C1A	4.90	108.91	106.71
25	6	320	XAT	O24-C25-C38	4.90	120.93	115.06
22	6	317	CLA	C4A-NA-C1A	4.90	108.91	106.71
26	5	322	BCR	C20-C21-C22	-4.89	120.33	127.31
22	B	837	CLA	C4A-NA-C1A	4.89	108.91	106.71
26	A	849	BCR	C7-C8-C9	-4.88	118.86	126.23
22	B	809	CLA	C4A-NA-C1A	4.88	108.90	106.71
23	3	422	CHL	C1D-ND-C4D	-4.88	102.87	106.33
24	5	320	LUT	C35-C34-C33	-4.87	120.36	127.31
25	2	615	XAT	C38-C25-C26	-4.86	114.12	122.26
22	8	615	CLA	CAA-C2A-C3A	-4.86	99.48	112.78
22	A	832	CLA	C4A-NA-C1A	4.85	108.89	106.71
22	2	608	CLA	C4A-NA-C1A	4.84	108.88	106.71
22	9	609	CLA	C4A-NA-C1A	4.84	108.88	106.71
26	F	805	BCR	C20-C21-C22	-4.83	120.41	127.31
22	A	809	CLA	C4A-NA-C1A	4.83	108.88	106.71
22	1	309	CLA	C4A-NA-C1A	4.82	108.87	106.71
22	3	401	CLA	C4A-NA-C1A	4.82	108.87	106.71
26	B	849	BCR	C16-C17-C18	-4.81	120.44	127.31
22	1	303	CLA	C4A-NA-C1A	4.81	108.87	106.71
26	K	203	BCR	C3-C4-C5	-4.81	105.49	114.08
26	5	322	BCR	C11-C10-C9	-4.81	120.45	127.31
22	A	843	CLA	C4A-NA-C1A	4.80	108.86	106.71
23	9	601	CHL	C1D-ND-C4D	-4.80	102.93	106.33
26	B	848	BCR	C7-C8-C9	-4.79	118.99	126.23
22	7	309	CLA	C4A-NA-C1A	4.79	108.86	106.71
22	2	603	CLA	CAA-C2A-C3A	-4.78	104.95	116.10
22	A	834	CLA	C4A-NA-C1A	4.76	108.85	106.71
22	B	811	CLA	C4A-NA-C1A	4.76	108.84	106.71
26	A	849	BCR	C11-C10-C9	-4.75	120.53	127.31
22	2	606	CLA	C4A-NA-C1A	4.75	108.84	106.71
22	A	839	CLA	C4A-NA-C1A	4.74	108.84	106.71
30	6	321	NEX	C38-C25-C26	-4.74	114.31	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1	304	CHL	C1D-ND-C4D	-4.74	102.97	106.33
22	A	833	CLA	C4A-NA-C1A	4.74	108.83	106.71
26	L	301	BCR	C28-C27-C26	-4.73	105.64	114.08
22	6	304	CLA	C4A-NA-C1A	4.73	108.83	106.71
30	6	321	NEX	C31-C30-C29	-4.72	120.57	127.31
26	L	301	BCR	C20-C21-C22	-4.72	120.58	127.31
26	G	204	BCR	C11-C10-C9	-4.72	120.58	127.31
22	B	842	CLA	C4A-NA-C1A	4.72	108.83	106.71
25	1	315	XAT	C6-C7-C8	-4.71	116.03	125.99
22	9	607	CLA	C4A-NA-C1A	4.71	108.82	106.71
22	A	837	CLA	C4A-NA-C1A	4.70	108.82	106.71
22	B	833	CLA	C4A-NA-C1A	4.70	108.82	106.71
23	8	602	CHL	C1D-ND-C4D	-4.69	103.00	106.33
22	L	302	CLA	C4A-NA-C1A	4.69	108.81	106.71
22	A	813	CLA	C4A-NA-C1A	4.68	108.81	106.71
22	B	819	CLA	C4A-NA-C1A	4.68	108.81	106.71
24	1	314	LUT	C35-C34-C33	-4.68	120.63	127.31
22	2	611	CLA	C4A-NA-C1A	4.68	108.81	106.71
26	A	851	BCR	C8-C9-C10	4.67	126.11	118.94
25	6	320	XAT	C6-C7-C8	-4.67	116.13	125.99
22	6	318	CLA	C4A-NA-C1A	4.66	108.80	106.71
22	K	204	CLA	C4A-NA-C1A	4.66	108.80	106.71
22	B	834	CLA	C4A-NA-C1A	4.65	108.80	106.71
26	B	851	BCR	C15-C14-C13	-4.64	120.68	127.31
25	8	618	XAT	O4-C5-C18	4.64	120.62	115.06
22	A	805	CLA	C4A-NA-C1A	4.64	108.79	106.71
30	5	323	NEX	O24-C25-C38	4.63	120.61	115.06
23	8	606	CHL	C1D-ND-C4D	-4.63	103.04	106.33
22	7	310	CLA	C4A-NA-C1A	4.63	108.79	106.71
26	B	848	BCR	C24-C23-C22	-4.63	119.24	126.23
22	7	301	CLA	C4A-NA-C1A	4.63	108.79	106.71
26	3	419	BCR	C24-C23-C22	-4.62	119.25	126.23
22	A	829	CLA	C4A-NA-C1A	4.62	108.78	106.71
22	A	818	CLA	C4A-NA-C1A	4.61	108.78	106.71
22	8	601	CLA	C4A-NA-C1A	4.60	108.77	106.71
25	9	614	XAT	C26-C27-C28	-4.60	116.27	125.99
24	2	614	LUT	C31-C30-C29	-4.60	120.75	127.31
26	7	317	BCR	C15-C14-C13	-4.59	120.75	127.31
26	A	851	BCR	C34-C9-C10	-4.59	116.49	122.92
22	A	840	CLA	C4A-NA-C1A	4.59	108.77	106.71
24	3	415	LUT	C35-C34-C33	-4.58	120.77	127.31
22	K	206	CLA	C4A-NA-C1A	4.58	108.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	9	614	XAT	C6-C7-C8	-4.57	116.32	125.99
22	B	830	CLA	C4A-NA-C1A	4.57	108.76	106.71
25	9	614	XAT	O24-C25-C38	4.57	120.53	115.06
22	7	312	CLA	C4A-NA-C1A	4.56	108.75	106.71
25	9	614	XAT	O4-C5-C18	4.56	120.52	115.06
22	3	410	CLA	C4A-NA-C1A	4.55	108.75	106.71
22	B	806	CLA	C4A-NA-C1A	4.54	108.75	106.71
26	K	203	BCR	C16-C17-C18	-4.54	120.83	127.31
31	8	621	LMG	C8-O7-C10	-4.54	112.04	117.88
22	A	803	CLA	C4A-NA-C1A	4.53	108.74	106.71
22	6	307	CLA	C4A-NA-C1A	4.52	108.74	106.71
26	A	848	BCR	C16-C17-C18	-4.52	120.86	127.31
26	K	203	BCR	C20-C21-C22	-4.50	120.88	127.31
26	J	103	BCR	C16-C17-C18	-4.50	120.89	127.31
22	5	312	CLA	C4A-NA-C1A	4.50	108.73	106.71
26	A	851	BCR	C20-C21-C22	-4.50	120.89	127.31
22	B	826	CLA	C4A-NA-C1A	4.50	108.73	106.71
22	A	825	CLA	C4A-NA-C1A	4.49	108.73	106.71
22	2	609	CLA	C4A-NA-C1A	4.49	108.72	106.71
27	8	620	LHG	O7-C7-C8	4.49	121.17	111.50
24	8	617	LUT	C35-C34-C33	-4.48	120.91	127.31
26	8	619	BCR	C16-C17-C18	-4.48	120.92	127.31
25	2	615	XAT	C6-C7-C8	-4.47	116.53	125.99
26	F	805	BCR	C24-C23-C22	-4.47	119.47	126.23
22	A	808	CLA	C4A-NA-C1A	4.47	108.72	106.71
22	B	812	CLA	C4A-NA-C1A	4.47	108.72	106.71
26	J	103	BCR	C15-C14-C13	-4.47	120.93	127.31
22	7	308	CLA	C4A-NA-C1A	4.46	108.71	106.71
22	3	409	CLA	C4A-NA-C1A	4.46	108.71	106.71
26	3	417	BCR	C20-C21-C22	-4.45	120.97	127.31
23	5	306	CHL	C1D-ND-C4D	-4.44	103.18	106.33
22	6	310	CLA	C4A-NA-C1A	4.43	108.70	106.71
22	A	821	CLA	C4A-NA-C1A	4.42	108.69	106.71
23	1	306	CHL	C1D-ND-C4D	-4.42	103.20	106.33
26	5	322	BCR	C15-C14-C13	-4.41	121.01	127.31
26	B	850	BCR	C16-C17-C18	-4.40	121.03	127.31
24	7	315	LUT	C35-C34-C33	-4.40	121.04	127.31
22	9	610	CLA	C4A-NA-C1A	4.40	108.68	106.71
26	A	848	BCR	C15-C14-C13	-4.39	121.05	127.31
26	A	849	BCR	C15-C14-C13	-4.38	121.05	127.31
26	F	801	BCR	C11-C10-C9	-4.38	121.05	127.31
22	6	313	CLA	C4A-NA-C1A	4.38	108.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	847	BCR	C16-C17-C18	-4.38	121.06	127.31
22	8	604	CLA	C4A-NA-C1A	4.36	108.67	106.71
26	A	846	BCR	C24-C23-C22	-4.36	119.65	126.23
26	A	848	BCR	C7-C8-C9	-4.36	119.65	126.23
22	7	302	CLA	C4A-NA-C1A	4.35	108.66	106.71
22	A	830	CLA	C4A-NA-C1A	4.35	108.66	106.71
30	6	321	NEX	C35-C34-C33	-4.35	121.11	127.31
22	2	610	CLA	C4A-NA-C1A	4.35	108.66	106.71
22	1	307	CLA	C4A-NA-C1A	4.34	108.66	106.71
26	L	301	BCR	C24-C23-C22	-4.34	119.68	126.23
23	3	413	CHL	C1D-ND-C4D	-4.34	103.25	106.33
22	3	414	CLA	C4A-NA-C1A	4.33	108.65	106.71
25	7	316	XAT	C35-C34-C33	-4.31	121.16	127.31
24	7	315	LUT	C35-C15-C14	-4.31	114.65	123.47
26	7	317	BCR	C38-C26-C25	-4.30	119.70	124.53
23	5	318	CHL	C1D-ND-C4D	-4.29	103.28	106.33
26	8	619	BCR	C15-C14-C13	-4.29	121.19	127.31
25	3	416	XAT	O4-C5-C18	4.28	120.19	115.06
26	3	417	BCR	C15-C14-C13	-4.28	121.20	127.31
24	9	613	LUT	C15-C14-C13	-4.27	121.21	127.31
26	B	846	BCR	C16-C17-C18	-4.27	121.22	127.31
25	2	615	XAT	O4-C5-C18	4.27	120.17	115.06
26	I	201	BCR	C16-C17-C18	-4.26	121.23	127.31
22	3	412	CLA	C4A-NA-C1A	4.26	108.62	106.71
22	A	827	CLA	C4A-NA-C1A	4.26	108.62	106.71
22	7	307	CLA	C4A-NA-C1A	4.25	108.62	106.71
22	2	607	CLA	C4A-NA-C1A	4.25	108.62	106.71
26	I	201	BCR	C11-C10-C9	-4.24	121.26	127.31
26	L	305	BCR	C15-C14-C13	-4.24	121.27	127.31
24	3	418	LUT	C11-C10-C9	-4.23	121.27	127.31
22	H	201	CLA	CAA-C2A-C3A	-4.23	106.22	116.10
22	F	802	CLA	C4A-NA-C1A	4.23	108.61	106.71
26	K	207	BCR	C15-C14-C13	-4.23	121.28	127.31
25	9	614	XAT	C15-C14-C13	-4.23	121.28	127.31
26	A	846	BCR	C11-C10-C9	-4.22	121.28	127.31
22	5	311	CLA	C4A-NA-C1A	4.22	108.60	106.71
26	G	204	BCR	C7-C8-C9	-4.21	119.87	126.23
26	L	305	BCR	C11-C10-C9	-4.21	121.31	127.31
26	K	203	BCR	C11-C10-C9	-4.20	121.31	127.31
23	6	303	CHL	C1D-ND-C4D	-4.19	103.36	106.33
22	B	843	CLA	C4A-NA-C1A	4.19	108.59	106.71
27	B	801	LHG	O7-C7-C8	4.19	120.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	302	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
27	2	617	LHG	O7-C7-C8	4.18	120.50	111.50
22	7	303	CLA	C4A-NA-C1A	4.18	108.58	106.71
26	A	847	BCR	C16-C17-C18	-4.17	121.36	127.31
22	A	822	CLA	C4A-NA-C1A	4.16	108.58	106.71
27	9	616	LHG	O7-C7-C8	4.15	120.45	111.50
22	1	301	CLA	C4A-NA-C1A	4.15	108.57	106.71
26	M	102	BCR	C7-C8-C9	-4.15	119.97	126.23
26	B	849	BCR	C20-C21-C22	-4.14	121.40	127.31
26	M	102	BCR	C24-C23-C22	-4.14	119.98	126.23
26	G	204	BCR	C24-C23-C22	-4.13	119.99	126.23
26	A	848	BCR	C11-C10-C9	-4.13	121.42	127.31
31	8	621	LMG	O7-C10-C11	4.13	120.39	111.50
26	A	851	BCR	C16-C17-C18	-4.12	121.42	127.31
26	F	801	BCR	C28-C27-C26	-4.12	106.73	114.08
22	6	315	CLA	C4A-NA-C1A	4.11	108.56	106.71
24	2	614	LUT	C35-C34-C33	-4.11	121.44	127.31
27	5	301	LHG	O7-C7-C8	4.11	120.36	111.50
26	I	201	BCR	C20-C21-C22	-4.11	121.45	127.31
22	B	822	CLA	C4A-NA-C1A	4.10	108.55	106.71
26	L	305	BCR	C16-C17-C18	-4.10	121.45	127.31
26	3	417	BCR	C16-C17-C18	-4.10	121.46	127.31
24	2	614	LUT	C15-C14-C13	-4.09	121.47	127.31
22	A	820	CLA	C4A-NA-C1A	4.09	108.54	106.71
26	A	847	BCR	C15-C14-C13	-4.08	121.48	127.31
25	1	315	XAT	O24-C25-C38	4.08	119.95	115.06
22	1	313	CLA	CAA-C2A-C3A	-4.06	106.63	116.10
26	I	201	BCR	C7-C8-C9	-4.06	120.10	126.23
30	5	323	NEX	C35-C34-C33	-4.05	121.54	127.31
27	1	318	LHG	O7-C7-C8	4.03	120.19	111.50
25	8	618	XAT	C35-C34-C33	-4.03	121.56	127.31
23	5	307	CHL	C1D-ND-C4D	-4.02	103.48	106.33
22	B	805	CLA	C4A-NA-C1A	4.02	108.51	106.71
26	A	846	BCR	C7-C8-C9	-4.02	120.17	126.23
26	F	805	BCR	C28-C27-C26	-4.01	106.91	114.08
22	5	315	CLA	C4A-NA-C1A	4.01	108.51	106.71
26	5	322	BCR	C24-C23-C22	-4.01	120.17	126.23
25	2	615	XAT	O24-C25-C38	4.01	119.86	115.06
22	2	612	CLA	C4A-NA-C1A	4.01	108.51	106.71
22	3	408	CLA	C4A-NA-C1A	4.01	108.51	106.71
23	3	406	CHL	C4A-NA-C1A	4.01	108.51	106.71
23	7	304	CHL	C1D-ND-C4D	-4.01	103.49	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	L	301	BCR	C16-C17-C18	-4.00	121.59	127.31
22	6	314	CLA	CAA-C2A-C3A	-4.00	101.84	112.78
22	A	817	CLA	C4A-NA-C1A	3.98	108.50	106.71
27	M	101	LHG	O7-C7-C8	3.97	120.07	111.50
26	B	848	BCR	C16-C17-C18	-3.97	121.64	127.31
25	5	321	XAT	O4-C5-C18	3.97	119.81	115.06
26	3	419	BCR	C15-C14-C13	-3.96	121.66	127.31
22	1	302	CLA	CHB-C1B-NB	3.96	128.45	124.26
26	A	849	BCR	C24-C23-C22	-3.95	120.26	126.23
23	5	308	CHL	C1D-ND-C4D	-3.95	103.53	106.33
26	7	317	BCR	C20-C21-C22	-3.94	121.68	127.31
26	3	417	BCR	C24-C23-C22	-3.93	120.29	126.23
27	1	317	LHG	O7-C7-C8	3.93	119.97	111.50
22	B	832	CLA	C4A-NA-C1A	3.93	108.47	106.71
26	K	207	BCR	C11-C10-C9	-3.93	121.70	127.31
31	J	104	LMG	O7-C10-C11	3.92	119.95	111.50
25	6	320	XAT	O4-C5-C18	3.92	119.75	115.06
22	H	202	CLA	C4A-NA-C1A	3.91	108.47	106.71
22	8	611	CLA	CMB-C2B-C1B	-3.91	119.41	125.37
26	A	847	BCR	C11-C10-C9	-3.91	121.73	127.31
26	3	419	BCR	C20-C21-C22	-3.91	121.73	127.31
26	L	305	BCR	C24-C23-C22	-3.91	120.33	126.23
26	A	846	BCR	C20-C21-C22	-3.90	121.74	127.31
22	9	612	CLA	C4A-NA-C1A	3.90	108.46	106.71
22	9	610	CLA	CAA-C2A-C3A	-3.89	104.54	114.26
26	J	101	BCR	C38-C26-C25	-3.89	120.16	124.53
26	F	801	BCR	C3-C4-C5	-3.89	107.13	114.08
22	B	802	CLA	C4A-NA-C1A	3.89	108.45	106.71
23	1	306	CHL	C4A-NA-C1A	3.89	108.45	106.71
25	7	316	XAT	C26-C27-C28	-3.88	117.78	125.99
27	7	318	LHG	O7-C7-C8	3.88	119.87	111.50
22	5	314	CLA	C4A-NA-C1A	3.88	108.45	106.71
22	2	604	CLA	CAA-C2A-C3A	-3.88	104.57	114.26
25	2	615	XAT	C35-C34-C33	-3.87	121.78	127.31
22	5	313	CLA	C4A-NA-C1A	3.87	108.45	106.71
30	5	323	NEX	C27-C28-C29	-3.87	119.52	125.53
26	3	419	BCR	C11-C10-C9	-3.87	121.78	127.31
24	9	613	LUT	C7-C8-C9	-3.87	120.39	126.23
22	A	828	CLA	C4A-NA-C1A	3.87	108.44	106.71
25	7	316	XAT	C6-C7-C8	-3.87	117.81	125.99
26	A	848	BCR	C20-C21-C22	-3.86	121.79	127.31
26	K	207	BCR	C24-C23-C22	-3.86	120.40	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	314	CLA	CAA-C2A-C3A	-3.85	107.12	116.10
22	B	815	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
27	5	325	LHG	O7-C7-C8	3.84	119.77	111.50
22	3	407	CLA	C4A-NA-C1A	3.83	108.43	106.71
22	8	611	CLA	C4A-NA-C1A	3.83	108.43	106.71
22	B	814	CLA	C4A-NA-C1A	3.83	108.43	106.71
26	K	203	BCR	C15-C14-C13	-3.83	121.85	127.31
22	1	312	CLA	C4A-NA-C1A	3.82	108.42	106.71
22	B	839	CLA	C4A-NA-C1A	3.82	108.42	106.71
24	3	418	LUT	C7-C8-C9	-3.82	120.47	126.23
25	7	316	XAT	C11-C10-C9	-3.81	121.87	127.31
25	8	618	XAT	C27-C28-C29	-3.80	119.64	125.53
26	8	619	BCR	C20-C21-C22	-3.80	121.89	127.31
26	5	322	BCR	C33-C5-C6	-3.79	120.27	124.53
26	3	417	BCR	C7-C8-C9	-3.79	120.51	126.23
26	A	847	BCR	C24-C23-C22	-3.79	120.52	126.23
31	J	105	LMG	O7-C10-C11	3.79	119.66	111.50
22	6	314	CLA	C4A-NA-C1A	3.78	108.41	106.71
26	B	849	BCR	C24-C23-C22	-3.78	120.53	126.23
26	9	615	BCR	C20-C21-C22	-3.78	121.92	127.31
22	6	312	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
23	8	608	CHL	C1D-ND-C4D	-3.76	103.66	106.33
26	I	201	BCR	C15-C14-C13	-3.76	121.95	127.31
22	F	803	CLA	CAA-C2A-C3A	-3.76	104.87	114.26
23	9	605	CHL	C1D-ND-C4D	-3.76	103.67	106.33
26	B	849	BCR	C38-C26-C25	-3.75	120.31	124.53
28	J	106	LMU	O5'-C5'-C4'	3.75	117.66	109.75
26	A	847	BCR	C38-C26-C25	-3.75	120.32	124.53
26	I	201	BCR	C30-C25-C26	-3.74	117.34	122.61
22	5	313	CLA	CAA-C2A-C3A	-3.74	104.91	114.26
22	2	610	CLA	CAA-C2A-C3A	-3.74	104.92	114.26
22	8	612	CLA	CAA-C2A-C3A	-3.74	104.92	114.26
27	A	845	LHG	O7-C7-C8	3.74	119.56	111.50
26	7	317	BCR	C3-C4-C5	-3.74	107.40	114.08
34	B	852	DGD	O2G-C1B-C2B	3.73	119.55	111.50
26	J	103	BCR	C7-C8-C9	-3.73	120.60	126.23
23	1	305	CHL	C1C-C2C-C3C	-3.73	104.15	107.11
24	5	320	LUT	C35-C15-C14	-3.73	115.84	123.47
22	6	313	CLA	CAA-C2A-C3A	-3.72	104.96	114.26
22	A	810	CLA	C4A-NA-C1A	3.72	108.38	106.71
26	A	847	BCR	C20-C21-C22	-3.71	122.01	127.31
26	I	201	BCR	C27-C26-C25	-3.71	117.34	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	847	BCR	C7-C8-C9	-3.70	120.64	126.23
26	M	102	BCR	C11-C10-C9	-3.69	122.05	127.31
23	1	305	CHL	CHB-C1B-NB	-3.69	120.36	124.26
27	6	322	LHG	O7-C7-C8	3.68	119.44	111.50
22	5	315	CLA	C2A-C3A-C4A	-3.68	102.21	106.26
28	H	204	LMU	C4B-C3B-C2B	3.67	117.23	110.82
26	A	846	BCR	C16-C17-C18	-3.66	122.09	127.31
23	3	413	CHL	C4A-NA-C1A	3.65	108.35	106.71
26	K	203	BCR	C1-C6-C5	-3.65	117.47	122.61
26	L	301	BCR	C33-C5-C6	-3.65	120.43	124.53
26	3	419	BCR	C16-C17-C18	-3.65	122.11	127.31
26	K	203	BCR	C33-C5-C4	3.64	120.62	113.62
26	B	846	BCR	C7-C8-C9	-3.63	120.74	126.23
26	K	207	BCR	C20-C21-C22	-3.63	122.14	127.31
28	6	323	LMU	C2'-C3'-C4'	3.61	117.93	109.68
26	G	204	BCR	C28-C27-C26	-3.61	107.62	114.08
26	A	848	BCR	C38-C26-C25	-3.61	120.47	124.53
25	7	316	XAT	C4-C3-C2	-3.61	103.80	110.77
26	K	207	BCR	C16-C17-C18	-3.61	122.16	127.31
26	9	615	BCR	C30-C25-C26	-3.61	117.53	122.61
30	5	323	NEX	C15-C14-C13	-3.61	122.16	127.31
22	A	841	CLA	C4A-NA-C1A	3.60	108.32	106.71
26	L	305	BCR	C20-C21-C22	-3.60	122.18	127.31
30	6	321	NEX	C15-C14-C13	-3.60	122.18	127.31
22	B	802	CLA	CMB-C2B-C1B	-3.59	119.90	125.37
25	1	315	XAT	C11-C10-C9	-3.59	122.19	127.31
25	9	614	XAT	C35-C34-C33	-3.58	122.19	127.31
26	B	848	BCR	C15-C14-C13	-3.58	122.20	127.31
22	9	602	CLA	C4A-NA-C1A	3.58	108.31	106.71
26	J	101	BCR	C15-C16-C17	-3.57	116.16	123.47
25	3	416	XAT	C15-C14-C13	-3.57	122.21	127.31
25	5	321	XAT	C35-C34-C33	-3.57	122.22	127.31
26	K	203	BCR	C4-C5-C6	-3.56	117.57	122.73
22	L	302	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
22	9	608	CLA	C4A-NA-C1A	3.55	108.30	106.71
26	A	849	BCR	C16-C17-C18	-3.55	122.24	127.31
26	K	207	BCR	C7-C8-C9	-3.55	120.87	126.23
22	6	311	CLA	C4A-NA-C1A	3.55	108.30	106.71
26	A	849	BCR	C20-C21-C22	-3.54	122.25	127.31
22	A	838	CLA	C4A-NA-C1A	3.54	108.30	106.71
26	M	102	BCR	C16-C15-C14	-3.54	116.22	123.47
26	A	846	BCR	C28-C27-C26	-3.54	107.76	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	8	619	BCR	C38-C26-C25	-3.54	120.56	124.53
26	B	851	BCR	C38-C26-C25	-3.53	120.56	124.53
26	J	101	BCR	C11-C12-C13	-3.53	116.49	126.42
26	A	846	BCR	C33-C5-C6	-3.53	120.57	124.53
26	L	301	BCR	C7-C8-C9	-3.52	120.92	126.23
26	F	801	BCR	C15-C16-C17	-3.51	116.28	123.47
22	B	807	CLA	C4A-NA-C1A	3.51	108.28	106.71
28	3	421	LMU	O1B-C4'-C3'	3.51	116.62	107.28
22	1	302	CLA	C2D-C1D-ND	3.51	112.69	110.10
28	3	421	LMU	C2'-C3'-C4'	3.51	117.69	109.68
26	B	850	BCR	C20-C21-C22	-3.50	122.32	127.31
27	8	620	LHG	O8-C23-C24	3.49	122.86	111.91
27	A	844	LHG	O7-C7-C8	3.49	119.03	111.50
26	L	301	BCR	C11-C10-C9	-3.49	122.33	127.31
23	8	603	CHL	C4A-NA-C1A	3.49	108.27	106.71
23	8	608	CHL	C2A-C3A-C4A	-3.49	96.24	101.87
26	J	101	BCR	C24-C23-C22	-3.48	120.97	126.23
22	B	815	CLA	O2D-CGD-CBD	3.48	117.44	111.27
26	K	203	BCR	C7-C8-C9	-3.48	120.98	126.23
22	2	613	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
25	5	321	XAT	C15-C14-C13	-3.47	122.36	127.31
26	B	848	BCR	C20-C21-C22	-3.47	122.36	127.31
22	7	314	CLA	CBD-CHA-C1A	3.47	132.99	127.43
26	G	204	BCR	C33-C5-C6	-3.47	120.63	124.53
26	5	322	BCR	C7-C8-C9	-3.47	121.00	126.23
26	B	849	BCR	C3-C4-C5	-3.45	107.92	114.08
24	3	418	LUT	C18-C5-C6	-3.45	120.66	124.53
22	8	616	CLA	C4A-NA-C1A	3.44	108.25	106.71
26	K	203	BCR	C24-C23-C22	-3.44	121.04	126.23
26	B	851	BCR	C15-C16-C17	-3.43	116.44	123.47
26	A	851	BCR	C30-C25-C26	-3.43	117.78	122.61
25	3	416	XAT	O24-C25-C38	3.43	119.17	115.06
22	5	314	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
30	6	321	NEX	O24-C25-C38	3.42	119.16	115.06
23	5	319	CHL	C4A-NA-C1A	3.42	108.24	106.71
28	7	319	LMU	C1'-O5'-C5'	3.41	120.38	113.69
28	6	301	LMU	C2'-C3'-C4'	3.41	117.46	109.68
24	3	415	LUT	C11-C10-C9	-3.41	122.45	127.31
22	B	805	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
30	5	323	NEX	C31-C30-C29	-3.40	122.46	127.31
22	8	615	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
30	6	321	NEX	C11-C10-C9	-3.39	122.47	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	5	321	XAT	C30-C31-C32	-3.39	112.63	123.22
26	A	846	BCR	C3-C4-C5	-3.39	108.03	114.08
26	3	417	BCR	C28-C27-C26	-3.39	108.03	114.08
22	6	311	CLA	CMB-C2B-C1B	-3.38	120.21	125.37
26	L	301	BCR	C15-C14-C13	-3.38	122.49	127.31
26	J	103	BCR	C11-C10-C9	-3.38	122.49	127.31
24	2	614	LUT	C37-C21-C26	3.37	114.65	109.55
24	2	614	LUT	C11-C10-C9	-3.37	122.50	127.31
26	B	847	BCR	C15-C14-C13	-3.37	122.50	127.31
26	F	801	BCR	C7-C8-C9	-3.37	121.15	126.23
22	B	828	CLA	C4A-NA-C1A	3.36	108.22	106.71
23	8	603	CHL	C1D-ND-C4D	-3.36	103.95	106.33
25	2	615	XAT	C15-C14-C13	-3.35	122.52	127.31
26	F	801	BCR	C20-C21-C22	-3.35	122.53	127.31
26	A	851	BCR	C10-C11-C12	-3.35	112.78	123.22
22	9	603	CLA	C4A-NA-C1A	3.34	108.21	106.71
28	A	852	LMU	C1B-O1B-C4'	-3.34	109.71	117.96
26	G	204	BCR	C20-C21-C22	-3.33	122.55	127.31
23	9	605	CHL	C1D-CHD-C4C	-3.33	118.87	126.06
22	9	609	CLA	CBC-CAC-C3C	3.33	121.61	112.43
22	K	205	CLA	CAA-C2A-C3A	-3.32	105.95	114.26
22	A	833	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
25	1	315	XAT	C35-C34-C33	-3.32	122.57	127.31
25	1	315	XAT	C4-C3-C2	-3.32	104.37	110.77
26	B	847	BCR	C40-C30-C29	3.31	122.16	108.91
26	F	805	BCR	C16-C15-C14	-3.31	116.69	123.47
22	B	822	CLA	CMB-C2B-C1B	-3.31	120.32	125.37
24	3	415	LUT	C15-C14-C13	-3.31	122.59	127.31
26	B	847	BCR	C11-C10-C9	-3.30	122.61	127.31
23	6	308	CHL	C1D-ND-C4D	-3.29	104.00	106.33
24	3	415	LUT	C7-C8-C9	-3.29	121.27	126.23
26	B	850	BCR	C28-C27-C26	-3.29	108.21	114.08
26	B	848	BCR	C28-C27-C26	-3.29	108.21	114.08
22	1	302	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
26	J	101	BCR	C28-C27-C26	-3.28	108.22	114.08
31	9	617	LMG	O7-C10-C11	3.27	118.54	111.50
22	B	832	CLA	CMB-C2B-C1B	-3.27	120.39	125.37
26	K	207	BCR	C3-C4-C5	-3.27	108.24	114.08
26	G	204	BCR	C16-C17-C18	-3.27	122.65	127.31
26	A	848	BCR	C24-C23-C22	-3.27	121.30	126.23
22	6	311	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
28	3	423	LMU	C1B-O1B-C4'	-3.26	109.91	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	3	421	LMU	O1'-C1'-C2'	3.25	113.38	108.30
26	5	322	BCR	C38-C26-C25	-3.25	120.88	124.53
26	9	615	BCR	C33-C5-C6	-3.25	120.88	124.53
26	J	103	BCR	C28-C27-C26	-3.25	108.27	114.08
22	A	801	CLA	C4A-NA-C1A	3.25	108.17	106.71
30	6	321	NEX	C27-C28-C29	-3.24	120.50	125.53
22	1	308	CLA	C4A-NA-C1A	3.23	108.16	106.71
22	H	202	CLA	CBD-CHA-C1A	3.23	131.48	128.06
25	8	618	XAT	C37-C21-C36	-3.23	102.60	107.37
25	8	618	XAT	C31-C30-C29	-3.23	122.70	127.31
22	9	602	CLA	C3B-C4B-NB	-3.23	107.52	110.52
26	3	419	BCR	C33-C5-C6	-3.23	120.91	124.53
22	F	803	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
23	8	603	CHL	C3B-C4B-NB	-3.22	107.53	110.52
22	2	607	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
28	G	201	LMU	C1B-O1B-C4'	-3.22	109.99	117.96
23	3	405	CHL	CHA-C4D-ND	-3.22	125.76	132.50
22	3	402	CLA	CAA-C2A-C3A	-3.22	103.97	112.78
28	H	204	LMU	C3B-C4B-C5B	3.21	115.97	110.24
25	7	316	XAT	C31-C30-C29	-3.21	122.72	127.31
26	3	419	BCR	C30-C25-C26	-3.21	118.09	122.61
22	A	818	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
22	5	312	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
25	6	320	XAT	C35-C34-C33	-3.21	122.73	127.31
22	8	610	CLA	C4A-NA-C1A	3.21	108.15	106.71
24	6	319	LUT	C10-C11-C12	-3.21	113.21	123.22
26	B	846	BCR	C20-C19-C18	-3.21	117.41	126.42
26	J	101	BCR	C20-C21-C22	-3.20	122.74	127.31
22	2	608	CLA	CAA-C2A-C3A	-3.20	108.62	116.10
30	6	321	NEX	C26-C27-C28	-3.20	119.22	125.99
22	A	815	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
25	7	316	XAT	C24-C23-C22	-3.20	104.60	110.77
22	1	301	CLA	C3B-C4B-NB	-3.19	107.55	110.52
28	6	302	LMU	C1B-O1B-C4'	-3.19	110.06	117.96
26	3	419	BCR	C28-C27-C26	-3.19	108.38	114.08
26	B	846	BCR	C28-C27-C26	-3.19	108.38	114.08
23	5	307	CHL	C2C-C3C-C4C	3.19	108.76	106.49
26	9	615	BCR	C15-C14-C13	-3.18	122.77	127.31
22	5	310	CLA	C4A-NA-C1A	3.18	108.14	106.71
28	3	420	LMU	C2'-C3'-C4'	3.18	116.94	109.68
22	7	307	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
26	B	850	BCR	C16-C15-C14	-3.17	116.97	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1	314	LUT	C35-C15-C14	-3.17	116.98	123.47
24	6	319	LUT	C15-C14-C13	-3.17	122.79	127.31
23	5	307	CHL	CHD-C4C-C3C	-3.17	120.19	124.84
26	A	851	BCR	C33-C5-C4	3.16	119.69	113.62
23	7	305	CHL	CHA-C4D-ND	-3.16	125.89	132.50
23	8	602	CHL	C1C-C2C-C3C	-3.16	104.61	107.11
24	7	315	LUT	C10-C11-C12	-3.15	113.37	123.22
24	3	418	LUT	C2-C3-C4	3.15	114.62	110.30
22	2	611	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
28	1	319	LMU	C2'-C3'-C4'	3.15	116.87	109.68
28	K	201	LMU	C2'-C3'-C4'	3.14	116.86	109.68
25	3	416	XAT	C35-C34-C33	-3.14	122.82	127.31
26	B	850	BCR	C38-C26-C27	3.14	119.64	113.62
24	9	613	LUT	C15-C35-C34	-3.14	117.05	123.47
26	3	417	BCR	C38-C26-C25	-3.13	121.02	124.53
22	2	607	CLA	O2D-CGD-CBD	3.13	116.83	111.27
24	6	319	LUT	C31-C30-C29	-3.13	122.85	127.31
26	J	101	BCR	C16-C17-C18	-3.13	122.85	127.31
22	8	611	CLA	CMB-C2B-C3B	3.12	134.14	126.59
22	6	311	CLA	CHB-C1B-NB	3.12	127.56	124.26
26	A	851	BCR	C15-C14-C13	-3.12	122.86	127.31
22	1	311	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
26	1	316	BCR	C20-C19-C18	-3.11	117.68	126.42
24	8	617	LUT	C35-C15-C14	-3.11	117.11	123.47
25	9	614	XAT	C15-C35-C34	-3.11	117.11	123.47
22	2	609	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	8	604	CLA	CHC-C4B-NB	3.10	127.54	124.26
26	9	615	BCR	C11-C12-C13	-3.10	117.71	126.42
24	7	315	LUT	C30-C31-C32	-3.10	113.56	123.22
26	B	849	BCR	C7-C8-C9	-3.10	121.56	126.23
26	B	850	BCR	C15-C14-C13	-3.09	122.90	127.31
22	B	811	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	B	821	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
26	J	103	BCR	C20-C21-C22	-3.08	122.91	127.31
25	6	320	XAT	C15-C14-C13	-3.08	122.91	127.31
26	B	846	BCR	C20-C21-C22	-3.08	122.92	127.31
28	J	106	LMU	C1'-O5'-C5'	3.08	119.73	113.69
25	3	416	XAT	C4-C3-C2	-3.08	104.83	110.77
26	A	846	BCR	C33-C5-C4	3.08	119.53	113.62
22	1	301	CLA	CHB-C1B-NB	3.08	127.51	124.26
22	5	310	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	8	603	CHL	CHD-C4C-C3C	-3.06	120.33	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	9	615	BCR	C33-C5-C4	3.06	119.50	113.62
26	B	850	BCR	C11-C10-C9	-3.06	122.94	127.31
22	1	310	CLA	C4A-NA-C1A	3.06	108.08	106.71
26	7	317	BCR	C2-C1-C6	3.06	115.19	110.48
28	7	319	LMU	O5'-C5'-C4'	3.06	116.20	109.75
24	6	319	LUT	C35-C34-C33	-3.06	122.94	127.31
26	1	316	BCR	C38-C26-C25	-3.06	121.10	124.53
23	1	305	CHL	CHC-C4B-NB	-3.05	121.02	124.26
22	2	601	CLA	CHB-C4A-NA	3.05	128.73	124.51
22	B	802	CLA	CMB-C2B-C3B	3.05	133.97	126.59
22	B	802	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
22	8	615	CLA	CHB-C4A-NA	3.04	128.72	124.51
26	9	615	BCR	C16-C15-C14	-3.04	117.24	123.47
22	8	611	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
26	B	849	BCR	C33-C5-C6	-3.04	121.12	124.53
22	B	834	CLA	CMB-C2B-C1B	-3.03	120.75	125.37
26	B	850	BCR	C38-C26-C25	-3.03	121.12	124.53
22	L	304	CLA	CAA-C2A-C3A	-3.03	109.03	116.10
25	9	614	XAT	C4-C3-C2	-3.03	104.92	110.77
22	A	813	CLA	CHD-C1D-ND	-3.03	121.67	124.45
25	6	320	XAT	C11-C10-C9	-3.03	122.99	127.31
25	6	320	XAT	C4-C3-C2	-3.03	104.93	110.77
22	1	303	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
22	B	832	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	3	422	CHL	C1C-C2C-C3C	-3.02	104.72	107.11
25	6	320	XAT	C24-C23-C22	-3.02	104.94	110.77
26	J	101	BCR	C38-C26-C27	3.02	119.41	113.62
26	K	203	BCR	C38-C26-C25	-3.02	121.14	124.53
26	B	849	BCR	C11-C10-C9	-3.01	123.01	127.31
22	A	802	CLA	CMB-C2B-C1B	-3.01	120.78	125.37
22	8	609	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	2	614	LUT	C37-C21-C36	-3.01	103.45	107.89
22	K	202	CLA	CAA-C2A-C3A	-3.01	109.07	116.10
30	5	323	NEX	C24-C23-C22	-3.01	104.96	110.77
25	2	615	XAT	C30-C31-C32	-3.01	113.83	123.22
26	9	615	BCR	C3-C4-C5	-3.01	108.70	114.08
26	7	317	BCR	C30-C25-C26	-3.01	118.38	122.61
22	B	836	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	A	801	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	B	842	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
22	B	802	CLA	CHB-C4A-NA	3.00	128.66	124.51
26	I	201	BCR	C1-C6-C5	-3.00	118.38	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	J	102	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
22	A	824	CLA	CAA-C2A-C3A	-3.00	104.56	112.78
22	A	806	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
26	3	419	BCR	C30-C25-C24	3.00	124.26	115.78
26	B	849	BCR	C15-C14-C13	-3.00	123.03	127.31
22	G	203	CLA	CMB-C2B-C1B	-3.00	120.80	125.37
32	A	842	PQN	C11-C12-C13	-3.00	121.80	126.79
26	F	805	BCR	C33-C5-C6	-3.00	121.16	124.53
22	A	840	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
22	H	201	CLA	CHB-C4A-NA	2.99	128.65	124.51
26	B	851	BCR	C24-C23-C22	-2.99	121.71	126.23
26	3	417	BCR	C11-C10-C9	-2.99	123.04	127.31
26	B	850	BCR	C23-C24-C25	-2.99	118.80	127.20
26	L	305	BCR	C38-C26-C25	-2.99	121.17	124.53
24	3	418	LUT	C18-C5-C4	2.99	119.90	114.36
22	9	603	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
26	K	207	BCR	C38-C26-C25	-2.99	121.18	124.53
23	9	601	CHL	CHB-C1B-NB	-2.98	121.10	124.26
26	A	848	BCR	C38-C26-C27	2.98	119.34	113.62
22	8	615	CLA	CHC-C4B-NB	2.98	127.41	124.26
26	A	849	BCR	C38-C26-C25	-2.97	121.19	124.53
26	A	851	BCR	C38-C26-C27	2.97	119.33	113.62
26	7	317	BCR	C38-C26-C27	2.97	119.33	113.62
25	3	416	XAT	C30-C31-C32	-2.97	113.94	123.22
22	B	816	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	A	816	CLA	CMB-C2B-C1B	-2.97	120.85	125.37
22	1	310	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
22	1	301	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	B	848	BCR	C38-C26-C25	-2.97	121.19	124.53
22	9	611	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
25	8	618	XAT	C4-C3-C2	-2.96	105.06	110.77
22	9	609	CLA	CAC-C3C-C2C	-2.96	122.47	127.53
22	G	203	CLA	CHB-C4A-NA	2.96	128.60	124.51
24	3	418	LUT	C15-C35-C34	-2.96	117.42	123.47
22	8	615	CLA	C1D-ND-C4D	-2.96	104.23	106.33
22	7	313	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	6	310	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
26	5	322	BCR	C38-C26-C27	2.95	119.29	113.62
22	A	824	CLA	CMB-C2B-C1B	-2.95	120.87	125.37
26	3	417	BCR	C10-C11-C12	-2.95	114.00	123.22
22	7	309	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	A	802	CLA	CAA-C2A-C3A	-2.95	104.70	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	839	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
22	6	304	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
23	5	307	CHL	C3B-C4B-NB	-2.95	107.78	110.52
23	1	306	CHL	CHC-C4B-NB	-2.94	121.14	124.26
22	9	608	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
26	5	322	BCR	C28-C27-C26	-2.94	108.83	114.08
26	B	848	BCR	C34-C9-C10	-2.93	118.81	122.92
22	A	810	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
24	1	314	LUT	C15-C14-C13	-2.93	123.12	127.31
22	8	613	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	2	615	XAT	C4-C3-C2	-2.93	105.11	110.77
22	3	410	CLA	CHB-C4A-NA	2.93	128.56	124.51
22	B	827	CLA	CHB-C4A-NA	2.93	128.56	124.51
22	1	308	CLA	CHB-C4A-NA	2.93	128.56	124.51
27	2	617	LHG	O8-C23-C24	2.93	121.10	111.91
22	A	829	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
22	B	806	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
26	B	850	BCR	C24-C23-C22	-2.92	121.82	126.23
26	5	322	BCR	C35-C13-C14	-2.92	118.83	122.92
22	A	832	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	8	618	XAT	C38-C25-C26	-2.92	117.37	122.26
22	B	837	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	2	602	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	5	309	CHL	C3B-C4B-NB	-2.91	107.82	110.52
22	1	302	CLA	CHA-C1A-NA	-2.91	119.74	126.40
22	B	835	CLA	CHB-C4A-NA	2.91	128.53	124.51
22	A	822	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	B	850	BCR	C3-C4-C5	-2.90	108.89	114.08
22	9	603	CLA	CHC-C4B-NB	2.90	127.33	124.26
26	B	847	BCR	C33-C5-C6	-2.90	121.27	124.53
22	5	315	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	7	310	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
28	9	618	LMU	O1B-C4'-C3'	2.90	115.00	107.28
22	9	607	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	1	314	LUT	C22-C23-C24	2.90	115.04	111.74
22	9	606	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	1	308	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
26	L	305	BCR	C33-C5-C6	-2.90	121.28	124.53
22	5	304	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	A	847	BCR	C1-C6-C5	-2.89	118.54	122.61
22	A	811	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	2	605	CLA	CAA-C2A-C3A	-2.89	109.35	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	1	305	CHL	C3B-C4B-NB	-2.89	107.83	110.52
22	1	308	CLA	O2D-CGD-CBD	2.89	116.41	111.27
22	A	827	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
31	J	105	LMG	C8-O7-C10	-2.89	110.68	117.79
24	5	320	LUT	C7-C8-C9	-2.89	121.87	126.23
26	5	322	BCR	C11-C12-C13	-2.89	118.30	126.42
22	A	815	CLA	CMB-C2B-C1B	-2.89	120.97	125.37
22	A	824	CLA	CHB-C4A-NA	2.89	128.50	124.51
26	J	103	BCR	C24-C23-C22	-2.89	121.88	126.23
22	F	804	CLA	CHB-C4A-NA	2.89	128.50	124.51
22	B	841	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	7	305	CHL	CHB-C1B-NB	-2.88	121.20	124.26
26	K	207	BCR	C33-C5-C6	-2.88	121.29	124.53
26	I	201	BCR	C4-C5-C6	-2.88	118.55	122.73
22	2	610	CLA	CHB-C4A-NA	2.88	128.50	124.51
22	3	409	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	7	312	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	B	848	BCR	C11-C10-C9	-2.88	123.20	127.31
22	8	612	CLA	CHB-C4A-NA	2.88	128.49	124.51
26	9	615	BCR	C38-C26-C27	2.88	119.15	113.62
22	6	317	CLA	CAA-C2A-C3A	-2.88	109.38	116.10
22	5	317	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	G	204	BCR	C15-C16-C17	-2.88	117.58	123.47
26	9	615	BCR	C38-C26-C25	-2.88	121.30	124.53
22	A	826	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	B	810	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	1	303	CLA	CAA-C2A-C3A	-2.88	109.39	116.10
26	B	849	BCR	C16-C15-C14	-2.88	117.58	123.47
26	B	851	BCR	C16-C17-C18	-2.87	123.21	127.31
22	B	833	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	5	321	XAT	C4-C3-C2	-2.87	105.22	110.77
26	9	615	BCR	C23-C24-C25	-2.87	119.13	127.20
27	9	616	LHG	O8-C23-C24	2.87	120.92	111.91
22	G	202	CLA	CHB-C4A-NA	2.87	128.48	124.51
22	B	843	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	9	610	CLA	CHB-C4A-NA	2.87	128.48	124.51
28	A	853	LMU	C6B-C5B-C4B	-2.87	109.54	113.54
26	B	848	BCR	C3-C4-C5	-2.87	108.96	114.08
26	A	851	BCR	C27-C26-C25	-2.87	118.57	122.73
22	2	601	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	B	812	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
22	B	808	CLA	CAA-C2A-C3A	-2.87	104.93	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	601	CLA	CMB-C2B-C1B	-2.86	121.01	125.37
24	1	314	LUT	C31-C30-C29	-2.86	123.23	127.31
24	7	315	LUT	C15-C14-C13	-2.86	123.23	127.31
22	8	614	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	3	401	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	3	416	XAT	C24-C23-C22	-2.86	105.25	110.77
26	B	851	BCR	C10-C11-C12	-2.86	114.30	123.22
22	A	823	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	1	310	CLA	CHB-C4A-NA	2.86	128.46	124.51
26	K	207	BCR	C33-C5-C4	2.86	119.11	113.62
22	9	609	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	B	819	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
22	7	302	CLA	CHB-C4A-NA	2.85	128.46	124.51
22	7	306	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	3	408	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	A	821	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	6	314	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	9	604	CLA	CHB-C4A-NA	2.85	128.45	124.51
24	9	613	LUT	C30-C31-C32	-2.85	114.33	123.22
25	1	315	XAT	C39-C29-C28	2.85	122.56	118.08
22	A	802	CLA	CHB-C4A-NA	2.85	128.45	124.51
22	G	202	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	5	321	XAT	C39-C29-C28	2.85	122.56	118.08
25	6	320	XAT	C39-C29-C28	2.85	122.56	118.08
22	2	608	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	8	616	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	A	836	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	B	840	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	5	305	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	6	315	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	B	835	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	2	611	CLA	CAC-C3C-C4C	2.84	128.49	124.81
22	A	807	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	F	802	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	B	826	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	8	619	BCR	C24-C23-C22	-2.84	121.95	126.23
22	A	816	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	1	313	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	A	817	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
22	2	606	CLA	CAA-C2A-C3A	-2.83	109.48	116.10
22	3	402	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	6	313	CLA	CHB-C4A-NA	2.83	128.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	K	205	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	B	818	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	9	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	8	617	LUT	C7-C8-C9	-2.83	121.96	126.23
28	1	319	LMU	C4B-C3B-C2B	2.83	115.76	110.82
22	B	813	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	B	844	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	5	313	CLA	CHB-C4A-NA	2.83	128.42	124.51
22	G	203	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	B	847	BCR	C29-C30-C25	2.83	114.83	110.48
28	H	204	LMU	O5B-C1B-C2B	2.82	116.33	110.35
22	B	807	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	I	201	BCR	C33-C5-C4	2.82	119.04	113.62
22	A	825	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	9	614	XAT	C24-C23-C22	-2.82	105.32	110.77
24	3	418	LUT	C35-C34-C33	-2.82	123.28	127.31
22	B	804	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
22	6	305	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
26	B	850	BCR	C10-C11-C12	-2.82	114.42	123.22
22	B	829	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
22	8	604	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	5	310	CLA	C1D-ND-C4D	-2.82	104.33	106.33
22	A	830	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	B	830	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	M	102	BCR	C20-C19-C18	-2.81	118.51	126.42
26	B	849	BCR	C33-C5-C4	2.81	119.02	113.62
22	6	309	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	B	847	BCR	C30-C25-C26	-2.81	118.65	122.61
22	3	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	6	311	CLA	CMB-C2B-C3B	2.81	133.40	126.59
22	B	816	CLA	CHB-C4A-NA	2.81	128.40	124.51
22	B	825	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	K	206	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	9	602	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	B	848	BCR	C38-C26-C27	2.81	119.01	113.62
22	9	602	CLA	CHB-C1B-NB	2.81	127.23	124.26
22	3	402	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	7	310	CLA	CHB-C4A-NA	2.81	128.39	124.51
22	J	102	CLA	CHB-C4A-NA	2.80	128.39	124.51
22	8	605	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
22	6	318	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	A	848	BCR	C30-C25-C26	-2.80	118.67	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	834	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	B	809	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	B	839	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
22	K	205	CLA	CHB-C4A-NA	2.80	128.38	124.51
22	B	838	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	7	310	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
22	5	311	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	A	808	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	A	812	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	A	835	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	B	822	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	2	603	CLA	CHB-C4A-NA	2.79	128.37	124.51
22	1	312	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	3	404	CLA	CHB-C4A-NA	2.79	128.37	124.51
24	8	617	LUT	C15-C14-C13	-2.79	123.33	127.31
23	9	605	CHL	CHB-C1B-NB	-2.79	121.31	124.26
22	A	841	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	A	802	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	G	204	BCR	C33-C5-C4	2.78	118.96	113.62
22	A	814	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
22	B	834	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	B	829	CLA	CHB-C4A-NA	2.77	128.35	124.51
22	B	802	CLA	CHB-C1B-NB	2.77	127.19	124.26
22	3	410	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	A	812	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	K	202	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
26	3	417	BCR	C38-C26-C27	2.77	118.94	113.62
26	B	849	BCR	C38-C26-C27	2.77	118.94	113.62
23	8	608	CHL	CHC-C4B-NB	-2.77	121.33	124.26
22	A	831	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
22	B	815	CLA	CHB-C4A-NA	2.77	128.34	124.51
22	8	614	CLA	CHD-C1D-ND	-2.77	121.91	124.45
22	A	838	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	A	813	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
24	5	320	LUT	C30-C31-C32	-2.76	114.60	123.22
26	M	102	BCR	C15-C14-C13	-2.76	123.37	127.31
22	3	407	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	8	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	B	803	CLA	CMB-C2B-C1B	-2.76	121.17	125.37
22	B	828	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	A	820	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	B	839	CLA	CHB-C4A-NA	2.76	128.32	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	8	617	LUT	C10-C11-C12	-2.76	114.61	123.22
26	F	805	BCR	C15-C14-C13	-2.75	123.38	127.31
22	B	827	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
28	7	319	LMU	C4B-C3B-C2B	2.75	115.63	110.82
22	5	314	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	1	308	CLA	C3B-C4B-NB	-2.75	107.96	110.52
23	5	302	CHL	C2C-C3C-C4C	2.75	108.45	106.49
22	9	603	CLA	CHB-C4A-NA	2.75	128.31	124.51
22	9	603	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	6	303	CHL	C3B-C4B-NB	-2.75	107.97	110.52
22	7	308	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
22	1	309	CLA	CMB-C2B-C1B	-2.75	121.19	125.37
22	A	837	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	8	602	CHL	C3B-C4B-NB	-2.74	107.97	110.52
22	F	804	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
22	B	805	CLA	CHC-C4B-NB	2.74	127.16	124.26
22	A	836	CLA	CHB-C4A-NA	2.74	128.31	124.51
22	H	203	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	B	823	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	8	614	CLA	CMB-C2B-C1B	-2.74	121.20	125.37
22	A	807	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	B	820	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	1	303	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	8	618	XAT	C37-C21-C26	2.73	117.43	110.05
22	5	303	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
22	3	408	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	2	614	LUT	C10-C11-C12	-2.73	114.69	123.22
22	B	809	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
22	3	403	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
22	7	307	CLA	CHB-C4A-NA	2.73	128.29	124.51
22	A	804	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
25	5	321	XAT	C28-C29-C30	-2.73	114.75	118.94
22	1	309	CLA	O2D-CGD-O1D	-2.73	117.89	124.09
22	3	410	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
22	A	806	CLA	CMB-C2B-C1B	-2.73	121.21	125.37
26	B	851	BCR	C11-C10-C9	-2.73	123.42	127.31
22	A	803	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	5	322	BCR	C20-C19-C18	-2.73	118.75	126.42
27	B	801	LHG	O8-C23-C24	2.73	120.47	111.91
22	1	303	CLA	C3B-C4B-NB	-2.73	108.40	110.23
27	5	325	LHG	O8-C23-C24	2.72	120.46	111.91
25	5	321	XAT	C24-C23-C22	-2.72	105.51	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	612	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	B	808	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	J	105	LMG	O8-C28-C29	2.72	120.44	111.91
22	6	316	CLA	CHD-C1D-ND	-2.72	121.95	124.45
22	B	804	CLA	CMB-C2B-C1B	-2.72	121.23	125.37
22	F	802	CLA	CHB-C1B-NB	2.72	127.13	124.26
28	7	319	LMU	C3B-C4B-C5B	2.71	115.08	110.24
22	B	817	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
25	9	614	XAT	C39-C29-C28	2.71	122.35	118.08
22	9	602	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	B	848	BCR	C37-C22-C21	-2.71	119.13	122.92
22	1	302	CLA	O2D-CGD-CBD	2.71	116.08	111.27
24	1	314	LUT	C10-C11-C12	-2.71	114.77	123.22
22	A	826	CLA	CHB-C4A-NA	2.71	128.26	124.51
22	A	804	CLA	CHB-C4A-NA	2.71	128.25	124.51
22	A	839	CLA	CHB-C4A-NA	2.71	128.25	124.51
22	6	307	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	A	839	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
28	K	201	LMU	C1B-O1B-C4'	-2.70	111.28	117.96
22	B	811	CLA	CHB-C4A-NA	2.70	128.24	124.51
28	3	420	LMU	C1B-O1B-C4'	-2.70	111.29	117.96
22	6	306	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
22	5	304	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	6	312	CLA	CHB-C4A-NA	2.69	128.24	124.51
22	A	813	CLA	CHB-C4A-NA	2.69	128.24	124.51
26	F	805	BCR	C8-C7-C6	-2.69	119.64	127.20
25	2	615	XAT	C11-C10-C9	-2.69	123.47	127.31
23	9	605	CHL	C2C-C3C-C4C	2.69	108.41	106.49
22	1	311	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	A	819	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
22	A	805	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
30	5	323	NEX	C26-C27-C28	-2.68	120.32	125.99
24	6	319	LUT	C20-C13-C12	2.68	122.30	118.08
26	A	848	BCR	C23-C24-C25	-2.68	119.67	127.20
22	B	813	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	3	406	CHL	C3B-C4B-NB	-2.68	108.03	110.52
22	7	303	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	8	606	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
26	B	846	BCR	C15-C14-C13	-2.68	123.48	127.31
22	2	612	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	9	604	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
22	3	403	CLA	CHB-C4A-NA	2.68	128.21	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	837	CLA	CHB-C4A-NA	2.68	128.21	124.51
27	5	301	LHG	C5-O7-C7	-2.68	111.20	117.79
22	3	407	CLA	CHB-C4A-NA	2.68	128.21	124.51
22	5	304	CLA	CBA-CAA-C2A	2.68	121.76	113.86
26	8	619	BCR	C2-C1-C6	2.67	114.60	110.48
26	M	102	BCR	C28-C27-C26	-2.67	109.30	114.08
26	1	316	BCR	C11-C10-C9	-2.67	123.49	127.31
22	8	601	CLA	O2D-CGD-O1D	-2.67	118.02	124.09
23	9	605	CHL	C2A-C1A-CHA	2.67	128.53	123.86
24	2	614	LUT	C15-C35-C34	-2.67	118.00	123.47
22	L	303	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
22	F	803	CLA	CHB-C4A-NA	2.67	128.20	124.51
26	A	847	BCR	C33-C5-C4	2.67	118.74	113.62
23	3	413	CHL	C3B-C4B-NB	-2.67	108.04	110.52
23	6	303	CHL	C1C-C2C-C3C	-2.67	105.00	107.11
24	7	315	LUT	C39-C29-C28	2.67	122.28	118.08
25	1	315	XAT	C28-C29-C30	-2.67	114.85	118.94
22	B	814	CLA	O2D-CGD-O1D	-2.66	118.04	124.09
26	F	805	BCR	C33-C5-C4	2.66	118.73	113.62
22	8	614	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	5	323	NEX	C11-C10-C9	-2.66	123.52	127.31
22	6	306	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	B	824	CLA	CHC-C1C-C2C	-2.66	123.45	129.77
22	7	301	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	B	803	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	2	604	CLA	O2D-CGD-O1D	-2.66	118.06	124.09
22	6	311	CLA	C3B-C4B-NB	-2.66	108.05	110.52
26	B	847	BCR	C24-C23-C22	-2.66	122.22	126.23
22	B	806	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	F	805	BCR	C11-C10-C9	-2.65	123.53	127.31
22	A	823	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	7	303	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	5	320	LUT	C39-C29-C28	2.65	122.25	118.08
22	F	804	CLA	C2A-C1A-CHA	2.65	128.49	123.86
24	8	617	LUT	C39-C29-C28	2.65	122.25	118.08
26	B	846	BCR	C16-C15-C14	-2.65	118.05	123.47
28	6	323	LMU	O5'-C1'-C2'	2.65	115.95	110.35
22	B	829	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
22	2	613	CLA	O2D-CGD-CBD	2.65	115.97	111.27
22	7	311	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	A	828	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	A	847	BCR	C38-C26-C27	2.64	118.69	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	819	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	A	843	CLA	O2D-CGD-O1D	-2.64	118.09	124.09
22	8	611	CLA	CHB-C1B-NB	2.64	127.05	124.26
26	3	419	BCR	C38-C26-C25	-2.64	121.57	124.53
26	B	846	BCR	C11-C12-C13	-2.63	119.02	126.42
26	A	846	BCR	C38-C26-C25	-2.63	121.57	124.53
22	3	412	CLA	O2D-CGD-O1D	-2.63	118.11	124.09
23	8	603	CHL	C3D-C4D-ND	-2.63	105.99	110.24
22	6	311	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	A	805	CLA	CHB-C4A-NA	2.63	128.14	124.51
22	B	840	CLA	CHD-C1D-ND	-2.63	122.04	124.45
26	3	419	BCR	C38-C26-C27	2.62	118.66	113.62
22	K	204	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
26	F	801	BCR	C24-C23-C22	-2.62	122.28	126.23
22	A	801	CLA	CHC-C4B-NB	2.62	127.03	124.26
26	B	851	BCR	C20-C21-C22	-2.62	123.57	127.31
25	2	615	XAT	C15-C35-C34	-2.62	118.11	123.47
22	6	313	CLA	O2D-CGD-O1D	-2.62	118.14	124.09
22	A	833	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	5	302	CHL	C3B-C4B-NB	-2.61	108.09	110.52
22	A	826	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
28	K	201	LMU	O5'-C5'-C4'	2.61	115.26	109.75
22	5	314	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	B	831	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	2	609	CLA	CMB-C2B-C3B	2.61	130.36	123.59
24	8	617	LUT	C30-C31-C32	-2.61	115.07	123.22
22	B	827	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
22	A	819	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	9	617	LMG	O8-C28-C29	2.61	120.10	111.91
24	9	613	LUT	C38-C25-C24	-2.61	117.97	123.56
26	F	805	BCR	C7-C8-C9	-2.61	122.29	126.23
22	B	841	CLA	CHC-C4B-NB	2.61	127.02	124.26
22	2	612	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	L	301	BCR	C37-C22-C21	-2.60	119.28	122.92
22	K	206	CLA	CAA-C2A-C3A	-2.60	110.02	116.10
22	A	824	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	5	308	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
25	2	615	XAT	C39-C29-C28	2.60	122.17	118.08
22	A	836	CLA	CMB-C2B-C1B	-2.60	121.41	125.37
23	6	303	CHL	C2C-C3C-C4C	2.60	108.34	106.49
22	A	803	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	3	413	CHL	C2C-C3C-C4C	2.60	108.34	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	5	323	NEX	C39-C29-C30	-2.60	119.29	122.92
26	A	851	BCR	C16-C15-C14	-2.60	118.16	123.47
22	9	611	CLA	CHD-C1D-ND	-2.59	122.07	124.45
22	5	316	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	B	847	BCR	C38-C26-C25	-2.59	121.62	124.53
23	5	306	CHL	CHD-C4C-C3C	-2.59	121.03	124.84
26	B	847	BCR	C20-C21-C22	-2.59	123.61	127.31
22	8	610	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
22	7	307	CLA	O2D-CGD-CBD	2.59	115.87	111.27
22	3	414	CLA	O2D-CGD-O1D	-2.59	118.21	124.09
22	8	604	CLA	CAB-C3B-C2B	2.59	130.29	123.59
22	3	411	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	7	302	CLA	O2D-CGD-O1D	-2.58	118.23	124.09
23	5	319	CHL	C3B-C4B-NB	-2.58	108.12	110.52
22	A	838	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	1	313	CLA	CAB-C3B-C2B	2.58	130.27	123.59
22	A	835	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	1	307	CLA	O2D-CGD-O1D	-2.58	118.24	124.09
22	1	313	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	A	834	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	A	837	CLA	CHD-C1D-ND	-2.58	122.09	124.45
23	3	406	CHL	C2C-C3C-C4C	2.58	108.33	106.49
22	A	802	CLA	CMB-C2B-C3B	2.58	132.82	126.59
23	8	607	CHL	C2C-C3C-C4C	2.57	108.32	106.49
22	1	310	CLA	O2D-CGD-O1D	-2.57	118.25	124.09
32	B	845	PQN	C11-C12-C13	-2.57	122.51	126.79
22	B	821	CLA	CHB-C1B-NB	2.57	126.98	124.26
22	2	611	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	8	601	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	9	606	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	5	306	CHL	C2C-C3C-C4C	2.57	108.32	106.49
22	3	411	CLA	O2D-CGD-O1D	-2.57	118.26	124.09
23	5	318	CHL	C3B-C4B-NB	-2.57	108.13	110.52
22	B	822	CLA	CMB-C2B-C3B	2.57	132.80	126.59
25	8	618	XAT	C10-C11-C12	-2.56	115.21	123.22
26	A	847	BCR	C4-C5-C6	-2.56	119.01	122.73
22	1	308	CLA	CHB-C1B-NB	2.56	126.97	124.26
25	1	315	XAT	C15-C14-C13	-2.56	123.65	127.31
22	B	817	CLA	CMB-C2B-C1B	-2.56	121.47	125.37
22	2	602	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	I	201	BCR	C38-C26-C27	2.56	118.53	113.62
22	8	609	CLA	CHB-C4A-NA	2.56	128.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	824	CLA	O2D-CGD-O1D	-2.56	118.28	124.09
22	A	841	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	2	609	CLA	C3B-C4B-NB	-2.56	108.52	110.23
22	B	804	CLA	C2B-C1B-NB	2.56	111.95	110.23
23	3	405	CHL	C2C-C3C-C4C	2.56	108.31	106.49
23	3	422	CHL	C3B-C4B-NB	-2.56	108.14	110.52
22	A	809	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	6	316	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	8	604	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
22	H	203	CLA	CAA-C2A-C3A	-2.55	107.88	114.26
22	B	814	CLA	CAA-C2A-C3A	-2.55	105.78	112.78
22	B	824	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	2	614	LUT	C38-C25-C24	-2.55	118.10	123.56
22	2	612	CLA	CHD-C1D-ND	-2.55	122.11	124.45
26	3	419	BCR	C33-C5-C4	2.55	118.52	113.62
22	A	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	817	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	840	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	8	612	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
22	A	822	CLA	CHD-C1D-ND	-2.55	122.11	124.45
23	3	405	CHL	C3B-C4B-NB	-2.55	108.15	110.52
27	1	317	LHG	O8-C23-C24	2.55	119.90	111.91
22	5	313	CLA	O2D-CGD-O1D	-2.55	118.31	124.09
22	6	309	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	A	816	CLA	CMB-C2B-C3B	2.55	132.75	126.59
22	A	814	CLA	CMB-C2B-C1B	-2.55	121.49	125.37
22	B	814	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	5	302	CHL	CHB-C1B-NB	-2.54	121.56	124.26
27	8	620	LHG	C5-O7-C7	-2.54	111.53	117.79
22	2	611	CLA	CAA-C2A-C3A	-2.54	110.16	116.10
22	B	834	CLA	CMB-C2B-C3B	2.54	132.75	126.59
22	A	816	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	A	831	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	2	609	CLA	CAB-C3B-C2B	2.54	130.18	123.59
22	5	316	CLA	CAB-C3B-C2B	2.54	130.18	123.59
23	8	608	CHL	C3B-C4B-NB	-2.54	108.16	110.52
22	6	305	CLA	CMB-C2B-C3B	2.54	130.18	123.59
22	H	201	CLA	CAB-C3B-C2B	2.54	130.18	123.59
26	F	801	BCR	C35-C13-C12	2.54	122.08	118.08
26	8	619	BCR	C38-C26-C27	2.54	118.50	113.62
23	5	319	CHL	C1-C2-C3	-2.54	121.65	126.04
22	3	401	CLA	CHB-C4A-NA	2.54	128.03	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	847	BCR	C3-C4-C5	-2.54	109.54	114.08
24	7	315	LUT	C20-C13-C12	2.54	122.08	118.08
28	6	323	LMU	C4B-C3B-C2B	2.54	115.26	110.82
22	B	821	CLA	CHC-C4B-NB	2.54	126.94	124.26
22	A	809	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
22	7	314	CLA	CAB-C3B-C2B	2.54	130.16	123.59
22	B	825	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	5	309	CHL	C2C-C3C-C4C	2.53	108.30	106.49
22	7	303	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
22	9	608	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	A	811	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	5	305	CLA	CAB-C3B-C2B	2.53	130.16	123.59
22	6	305	CLA	CAB-C3B-C2B	2.53	130.16	123.59
24	3	415	LUT	C35-C15-C14	-2.53	118.28	123.47
22	B	831	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	2	603	CLA	O2D-CGD-O1D	-2.53	118.34	124.09
22	9	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	9	601	CHL	C3B-C4B-NB	-2.53	108.17	110.52
22	A	843	CLA	CAA-C2A-C3A	-2.53	110.19	116.10
22	B	837	CLA	CHD-C1D-ND	-2.53	122.13	124.45
22	3	414	CLA	CAA-C2A-C3A	-2.53	110.20	116.10
25	3	416	XAT	C39-C29-C28	2.53	122.06	118.08
22	9	610	CLA	CMB-C2B-C1B	-2.53	121.52	125.37
22	B	818	CLA	CHB-C4A-NA	2.53	128.00	124.51
22	B	843	CLA	CHC-C4B-NB	2.53	126.93	124.26
22	7	313	CLA	CAB-C3B-C2B	2.53	130.13	123.59
22	B	814	CLA	CAB-C3B-C2B	2.53	130.13	123.59
23	9	601	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
22	5	317	CLA	CHB-C4A-NA	2.52	128.00	124.51
30	5	323	NEX	C16-C1-C6	-2.52	108.22	110.47
22	6	312	CLA	C3B-C4B-NB	-2.52	108.18	110.52
23	5	309	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
24	2	614	LUT	C18-C5-C6	-2.52	121.70	124.53
22	7	313	CLA	CHB-C4A-NA	2.52	128.00	124.51
27	5	301	LHG	O8-C23-C24	2.52	119.81	111.91
34	B	852	DGD	O1G-C1A-C2A	2.52	119.81	111.91
22	9	603	CLA	C2A-C1A-CHA	2.52	128.26	123.86
26	8	619	BCR	C3-C4-C5	-2.52	109.58	114.08
22	6	318	CLA	CHB-C4A-NA	2.52	127.99	124.51
24	3	418	LUT	C30-C31-C32	-2.52	115.36	123.22
22	5	305	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	7	308	CLA	CHB-C4A-NA	2.52	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	6	319	LUT	C35-C15-C14	-2.52	118.32	123.47
22	1	307	CLA	CAB-C3B-C2B	2.51	130.11	123.59
23	5	302	CHL	C1D-CHD-C4C	-2.51	120.63	126.06
24	3	415	LUT	C38-C25-C24	-2.51	118.18	123.56
22	A	833	CLA	O2D-CGD-CBD	2.51	115.73	111.27
22	6	310	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	1	306	CHL	C2C-C3C-C4C	2.51	108.28	106.49
22	A	815	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	8	616	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	8	607	CHL	C3B-C4B-NB	-2.51	108.19	110.52
22	A	825	CLA	CHD-C1D-ND	-2.51	122.15	124.45
26	F	801	BCR	C27-C26-C25	-2.51	119.09	122.73
22	B	803	CLA	CMB-C2B-C3B	2.51	132.66	126.59
23	8	608	CHL	C2C-C3C-C4C	2.51	108.28	106.49
26	3	419	BCR	C15-C16-C17	-2.50	118.34	123.47
22	B	844	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	H	201	CLA	CMB-C2B-C3B	2.50	130.08	123.59
22	L	303	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	K	203	BCR	C33-C5-C6	-2.50	121.72	124.53
22	3	409	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	A	822	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	2	602	CLA	O1D-CGD-CBD	2.50	129.60	124.48
23	9	605	CHL	C3B-C4B-NB	-2.50	108.19	110.52
22	1	309	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	6	313	CLA	CHC-C4B-NB	2.50	126.90	124.26
22	B	833	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	8	608	CHL	C2A-C1A-CHA	2.50	128.23	123.86
22	A	841	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
22	2	609	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	G	203	CLA	CMB-C2B-C3B	2.50	132.64	126.59
22	8	613	CLA	CHB-C4A-NA	2.50	127.96	124.51
22	B	810	CLA	CHB-C4A-NA	2.50	127.96	124.51
26	A	849	BCR	C3-C4-C5	-2.49	109.62	114.08
27	M	101	LHG	O8-C23-C24	2.49	119.74	111.91
22	8	615	CLA	CAB-C3B-C2B	2.49	130.05	123.59
24	9	613	LUT	C18-C5-C6	-2.49	121.73	124.53
26	7	317	BCR	C23-C24-C25	-2.49	120.20	127.20
22	7	306	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	A	814	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	B	834	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	2	601	CLA	CMB-C2B-C3B	2.49	132.63	126.59
23	5	308	CHL	C3B-C4B-NB	-2.49	108.20	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	8	618	XAT	C35-C15-C14	-2.49	118.37	123.47
27	1	318	LHG	O8-C23-C24	2.49	119.73	111.91
22	6	304	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	9	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
27	8	620	LHG	O8-C23-O10	-2.49	117.30	123.59
22	1	312	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	3	406	CHL	C3D-C4D-ND	-2.49	106.21	110.24
22	A	824	CLA	C2A-C1A-CHA	2.49	128.21	123.86
22	A	843	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	A	810	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	1	303	CLA	CMB-C2B-C3B	2.49	130.04	123.59
26	8	619	BCR	C11-C12-C13	-2.49	119.43	126.42
22	2	602	CLA	CHD-C1D-ND	-2.49	122.17	124.45
22	6	316	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	2	604	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	5	310	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
22	9	603	CLA	CHB-C1B-NB	2.48	126.89	124.26
27	A	844	LHG	O8-C23-C24	2.48	119.70	111.91
22	7	301	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	8	618	XAT	C26-C27-C28	2.48	131.24	125.99
22	1	311	CLA	O2D-CGD-CBD	2.48	115.68	111.27
22	1	301	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	8	605	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	B	840	CLA	C3B-C4B-NB	-2.48	108.21	110.52
23	3	422	CHL	C2C-C3C-C4C	2.48	108.26	106.49
22	7	313	CLA	CMB-C2B-C3B	2.48	130.01	123.59
22	B	820	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	6	308	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
24	5	320	LUT	C10-C11-C12	-2.48	115.49	123.22
31	J	104	LMG	C8-O7-C10	-2.48	111.70	117.79
22	5	304	CLA	CAB-C3B-C2B	2.48	130.00	123.59
23	7	304	CHL	C2C-C3C-C4C	2.47	108.25	106.49
24	5	320	LUT	C11-C10-C9	-2.47	123.78	127.31
22	7	309	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	A	817	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	8	608	CHL	CHD-C4C-C3C	-2.47	121.21	124.84
22	B	812	CLA	CHC-C4B-NB	2.47	126.87	124.26
22	5	304	CLA	C3B-C4B-NB	-2.47	108.58	110.23
22	B	838	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	A	803	CLA	CMB-C2B-C1B	-2.47	121.61	125.37
22	B	834	CLA	CHD-C1D-ND	-2.47	122.19	124.45
22	B	833	CLA	CHD-C1D-ND	-2.46	122.19	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	5	304	CLA	CMB-C2B-C3B	2.46	129.98	123.59
22	7	302	CLA	CAA-C2A-C3A	-2.46	106.03	112.78
22	H	203	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	A	830	CLA	C3B-C4B-NB	-2.46	108.23	110.52
22	B	816	CLA	CMB-C2B-C1B	-2.46	121.62	125.37
26	G	204	BCR	C11-C12-C13	-2.46	119.50	126.42
26	A	849	BCR	C15-C16-C17	-2.46	118.43	123.47
22	1	307	CLA	CAA-C2A-C3A	-2.46	110.36	116.10
22	3	414	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	K	206	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	B	804	CLA	CMB-C2B-C3B	2.46	132.55	126.59
22	K	202	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	L	302	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
22	H	202	CLA	CMB-C2B-C3B	2.46	129.96	123.59
22	5	316	CLA	CMB-C2B-C3B	2.46	129.96	123.59
22	2	605	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	B	826	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	A	805	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
23	6	308	CHL	C3B-C4B-NB	-2.46	108.24	110.52
22	H	202	CLA	C3B-C4B-NB	-2.46	108.59	110.23
22	6	311	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	6	314	CLA	CHD-C1D-ND	-2.45	122.20	124.45
22	6	307	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	J	101	BCR	C3-C4-C5	-2.45	109.70	114.08
26	A	846	BCR	C15-C16-C17	-2.45	118.45	123.47
22	A	824	CLA	CMB-C2B-C3B	2.45	132.52	126.59
23	7	305	CHL	C2A-C1A-CHA	2.45	128.14	123.86
26	L	301	BCR	C16-C15-C14	-2.45	118.46	123.47
22	8	604	CLA	CMB-C2B-C3B	2.45	129.93	123.59
22	B	823	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	8	610	CLA	CHB-C4A-NA	2.45	127.89	124.51
26	J	103	BCR	C33-C5-C6	-2.45	121.78	124.53
22	7	311	CLA	CHD-C1D-ND	-2.45	122.21	124.45
22	8	615	CLA	CHB-C1B-NB	2.44	126.84	124.26
22	B	807	CLA	C3B-C4B-NB	-2.44	108.25	110.52
26	B	849	BCR	C8-C7-C6	-2.44	120.34	127.20
23	5	306	CHL	CHD-C1D-ND	2.44	126.70	124.45
22	B	825	CLA	CMB-C2B-C1B	-2.44	121.65	125.37
26	B	846	BCR	C29-C30-C25	2.44	114.24	110.48
22	A	825	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	A	820	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	5	306	CHL	CHB-C1B-NB	-2.44	121.68	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	8	601	CLA	C3B-C4B-NB	-2.44	108.25	110.52
22	2	610	CLA	C2A-C1A-CHA	2.44	128.12	123.86
27	6	322	LHG	O8-C23-C24	2.44	119.55	111.91
24	7	315	LUT	C38-C25-C24	-2.43	118.35	123.56
22	9	612	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	5	319	CHL	C3D-C4D-ND	-2.43	106.30	110.24
22	1	301	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	A	846	BCR	C1-C6-C5	-2.43	119.19	122.61
22	A	827	CLA	CHB-C4A-NA	2.43	127.88	124.51
34	B	852	DGD	C2G-O2G-C1B	-2.43	111.80	117.79
22	A	804	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
25	7	316	XAT	C40-C33-C34	-2.43	119.52	122.92
26	A	851	BCR	C28-C27-C26	-2.43	109.74	114.08
23	6	308	CHL	C2C-C3C-C4C	2.43	108.22	106.49
28	1	319	LMU	C1B-O1B-C4'	-2.43	111.95	117.96
22	9	608	CLA	C3B-C4B-NB	-2.43	108.26	110.52
22	B	806	CLA	CHD-C1D-ND	-2.43	122.22	124.45
23	5	319	CHL	C2C-C3C-C4C	2.43	108.22	106.49
22	A	837	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	A	840	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	8	606	CHL	C3D-C4D-ND	-2.43	106.31	110.24
28	3	421	LMU	C4B-C3B-C2B	2.43	115.06	110.82
22	A	821	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	A	818	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	B	814	CLA	CHD-C1D-ND	-2.43	122.22	124.45
22	6	310	CLA	O2D-CGD-CBD	2.42	115.58	111.27
22	B	811	CLA	O2D-CGD-CBD	2.42	115.58	111.27
22	K	204	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	7	302	CLA	C2A-C1A-CHA	2.42	128.10	123.86
22	2	611	CLA	O2D-CGD-CBD	2.42	115.58	111.27
25	6	320	XAT	C15-C35-C34	-2.42	118.51	123.47
22	5	312	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	3	406	CHL	CHD-C4C-C3C	-2.42	121.28	124.84
26	B	850	BCR	C27-C26-C25	-2.42	119.22	122.73
26	F	805	BCR	C10-C11-C12	-2.42	115.66	123.22
22	B	807	CLA	CMB-C2B-C1B	-2.42	121.68	125.37
24	5	320	LUT	C38-C25-C24	-2.42	118.38	123.56
22	6	317	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	9	610	CLA	C2A-C1A-CHA	2.42	128.09	123.86
22	L	302	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	8	613	CLA	C1-C2-C3	-2.42	121.86	126.04
22	B	802	CLA	C3B-C4B-NB	-2.42	108.27	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	9	613	LUT	C35-C34-C33	-2.42	123.86	127.31
26	J	103	BCR	C1-C6-C5	-2.42	119.21	122.61
22	3	410	CLA	C2A-C1A-CHA	2.42	128.09	123.86
22	7	306	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	6	322	LHG	C5-O7-C7	-2.42	111.84	117.79
22	F	803	CLA	O2D-CGD-CBD	2.42	115.56	111.27
26	B	847	BCR	C7-C8-C9	-2.42	122.58	126.23
26	9	615	BCR	C20-C19-C18	-2.42	119.63	126.42
22	7	312	CLA	CHB-C4A-NA	2.42	127.85	124.51
24	2	614	LUT	C7-C8-C9	-2.41	122.59	126.23
22	7	312	CLA	CHD-C1D-ND	-2.41	122.23	124.45
22	1	313	CLA	CMB-C2B-C3B	2.41	129.85	123.59
22	A	832	CLA	CHC-C4B-NB	2.41	126.81	124.26
22	5	311	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	1	304	CHL	C2C-C3C-C4C	2.41	108.21	106.49
23	1	304	CHL	C1C-C2C-C3C	-2.41	105.20	107.11
24	8	617	LUT	C38-C25-C24	-2.41	118.40	123.56
30	6	321	NEX	C24-C23-C22	-2.41	106.12	110.77
22	2	607	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	6	305	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	5	318	CHL	CHB-C1B-NB	-2.41	121.71	124.26
22	B	808	CLA	CMB-C2B-C1B	-2.41	121.70	125.37
27	A	845	LHG	O8-C23-C24	2.41	119.46	111.91
23	7	304	CHL	C3D-C4D-ND	-2.41	106.34	110.24
22	B	842	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	807	CLA	CHB-C1B-NB	2.40	126.80	124.26
23	1	304	CHL	C3B-C4B-NB	-2.40	108.28	110.52
22	A	841	CLA	CHC-C4B-NB	2.40	126.80	124.26
22	5	305	CLA	CMB-C2B-C3B	2.40	129.82	123.59
22	8	601	CLA	CHD-C1D-ND	-2.40	122.25	124.45
22	B	822	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	A	806	CLA	CMB-C2B-C3B	2.40	132.40	126.59
22	6	313	CLA	C2A-C1A-CHA	2.40	128.05	123.86
22	6	314	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	5	322	BCR	C12-C13-C14	2.40	122.62	118.94
22	2	603	CLA	CHC-C4B-NB	2.40	126.79	124.26
22	3	412	CLA	CHB-C4A-NA	2.40	127.82	124.51
22	2	606	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	6	315	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	F	805	BCR	C29-C30-C25	2.39	114.17	110.48
22	B	843	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	1	303	CLA	CAB-C3B-C2B	2.39	129.79	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	312	CLA	CHB-C1B-NB	2.39	126.79	124.26
22	G	203	CLA	C2A-C1A-CHA	2.39	128.04	123.86
22	A	837	CLA	CHB-C1B-NB	2.39	126.79	124.26
22	1	307	CLA	CMB-C2B-C3B	2.39	129.78	123.59
23	5	308	CHL	C2C-C3C-C4C	2.39	108.19	106.49
26	F	801	BCR	C12-C13-C14	-2.39	115.28	118.94
23	3	413	CHL	C1D-CHD-C4C	-2.39	120.91	126.06
23	7	304	CHL	CHB-C1B-NB	-2.39	121.73	124.26
25	3	416	XAT	O24-C25-C26	-2.39	56.98	58.96
23	7	305	CHL	C3B-C4B-NB	-2.39	108.30	110.52
25	1	315	XAT	C18-C5-C4	2.38	116.96	114.28
22	A	828	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	1	302	CLA	C3B-C4B-NB	-2.38	108.31	110.52
23	9	605	CHL	C3D-C4D-ND	-2.38	106.38	110.24
23	5	302	CHL	C3D-C4D-ND	-2.38	106.39	110.24
22	2	603	CLA	CMB-C2B-C1B	-2.38	121.75	125.37
22	A	827	CLA	C3B-C4B-NB	-2.38	108.31	110.52
25	2	615	XAT	C24-C23-C22	-2.38	106.18	110.77
22	B	838	CLA	CHB-C1B-NB	2.38	126.77	124.26
24	6	319	LUT	C15-C35-C34	-2.37	118.61	123.47
23	6	308	CHL	CHB-C1B-NB	-2.37	121.74	124.26
23	7	304	CHL	C3B-C4B-NB	-2.37	108.31	110.52
24	3	415	LUT	C31-C30-C29	-2.37	123.92	127.31
22	8	615	CLA	O1D-CGD-CBD	2.37	129.34	124.48
26	8	619	BCR	C23-C24-C25	-2.37	120.54	127.20
31	J	104	LMG	O8-C28-C29	2.37	119.35	111.91
23	1	305	CHL	CHA-C1A-NA	-2.37	120.97	126.40
22	B	807	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	1	316	BCR	C3-C4-C5	-2.37	109.84	114.08
23	8	602	CHL	CHD-C1D-ND	2.37	126.63	124.45
26	5	322	BCR	C33-C5-C4	2.37	118.17	113.62
22	B	803	CLA	C2B-C1B-NB	2.37	111.82	110.23
25	5	321	XAT	C18-C5-C4	2.37	116.94	114.28
22	L	302	CLA	CHD-C1D-ND	-2.37	122.28	124.45
22	A	831	CLA	C3B-C4B-NB	-2.37	108.32	110.52
22	H	202	CLA	CAB-C3B-C2B	2.37	129.72	123.59
26	7	317	BCR	C24-C23-C22	-2.37	122.66	126.23
26	5	322	BCR	C30-C25-C26	-2.36	119.28	122.61
22	B	805	CLA	O1D-CGD-CBD	2.36	129.32	124.48
22	A	818	CLA	CHB-C1B-NB	2.36	126.76	124.26
24	3	418	LUT	C39-C29-C28	2.36	121.80	118.08
26	B	851	BCR	C21-C20-C19	-2.36	115.84	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	315	CLA	CHC-C4B-NB	2.36	126.76	124.26
22	5	303	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	L	304	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	A	836	CLA	CMB-C2B-C3B	2.36	132.31	126.59
24	6	319	LUT	C31-C32-C33	-2.36	119.79	126.42
22	2	613	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	B	828	CLA	CHB-C1B-NB	2.36	126.75	124.26
26	1	316	BCR	C38-C26-C27	2.36	118.15	113.62
26	K	207	BCR	C1-C6-C5	-2.36	119.29	122.61
26	A	848	BCR	C3-C4-C5	-2.36	109.87	114.08
22	A	836	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
26	B	846	BCR	C33-C5-C6	-2.35	121.88	124.53
23	1	306	CHL	C3D-C4D-ND	-2.35	106.43	110.24
22	3	410	CLA	CHC-C4B-NB	2.35	126.75	124.26
22	3	412	CLA	CHD-C1D-ND	-2.35	122.29	124.45
24	9	613	LUT	C10-C11-C12	-2.35	115.88	123.22
22	B	830	CLA	CHB-C4A-NA	2.35	127.77	124.51
26	A	846	BCR	C38-C26-C27	2.35	118.13	113.62
22	L	303	CLA	CHD-C1D-ND	-2.35	122.29	124.45
22	A	812	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
24	8	617	LUT	C21-C26-C27	-2.35	109.73	112.70
22	A	806	CLA	CHD-C1D-ND	-2.35	122.30	124.45
22	8	611	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	B	814	CLA	CMB-C2B-C3B	2.35	129.67	123.59
22	A	818	CLA	CMB-C2B-C1B	-2.35	121.80	125.37
22	1	309	CLA	CMB-C2B-C3B	2.35	132.27	126.59
22	A	803	CLA	CHB-C1B-NB	2.34	126.74	124.26
22	A	817	CLA	CHB-C1B-NB	2.34	126.74	124.26
22	5	310	CLA	O2D-CGD-CBD	2.34	115.43	111.27
22	A	830	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	B	821	CLA	CHD-C1D-ND	-2.34	122.30	124.45
22	B	830	CLA	CHC-C4B-NB	2.34	126.73	124.26
22	9	603	CLA	C2B-C1B-NB	2.34	111.80	110.23
23	5	306	CHL	C3B-C4B-NB	-2.34	108.34	110.52
22	7	311	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	B	821	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	A	815	CLA	CMB-C2B-C3B	2.34	132.25	126.59
22	6	312	CLA	O1D-CGD-CBD	2.34	129.27	124.48
23	7	305	CHL	C1C-C2C-C3C	-2.34	105.26	107.11
22	5	314	CLA	CHD-C1D-ND	-2.34	122.31	124.45
22	5	303	CLA	CHB-C1B-NB	2.34	126.73	124.26
22	1	307	CLA	CHB-C4A-NA	2.34	127.74	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	847	BCR	C16-C15-C14	-2.33	118.69	123.47
22	A	803	CLA	C3B-C4B-NB	-2.33	108.35	110.52
25	6	320	XAT	C28-C29-C30	-2.33	115.36	118.94
28	1	319	LMU	O5B-C5B-C4B	2.33	113.93	109.69
26	F	801	BCR	C36-C18-C19	2.33	121.75	118.08
22	6	315	CLA	CHD-C1D-ND	-2.33	122.31	124.45
23	3	405	CHL	C1D-CHD-C4C	-2.33	121.03	126.06
22	3	408	CLA	CMB-C2B-C1B	-2.33	121.82	125.37
22	B	832	CLA	CMB-C2B-C3B	2.33	132.23	126.59
25	3	416	XAT	C11-C10-C9	-2.33	123.99	127.31
22	2	603	CLA	C2A-C1A-CHA	2.33	127.91	123.85
22	B	822	CLA	CHD-C1D-ND	-2.33	122.32	124.45
24	6	319	LUT	C19-C9-C8	2.32	121.74	118.08
23	6	303	CHL	C3D-C4D-ND	-2.32	106.48	110.24
24	5	320	LUT	C21-C26-C27	-2.32	109.76	112.70
22	B	838	CLA	CHD-C1D-ND	-2.32	122.32	124.45
22	B	828	CLA	CMB-C2B-C1B	-2.32	121.83	125.37
26	K	203	BCR	C1-C6-C7	2.32	122.35	115.78
23	9	605	CHL	CHA-C1A-NA	-2.32	121.08	126.40
22	A	830	CLA	CHB-C1B-NB	2.32	126.71	124.26
26	A	849	BCR	C11-C12-C13	-2.32	119.90	126.42
28	H	204	LMU	C2'-C3'-C4'	2.32	114.98	109.68
23	1	305	CHL	C2C-C3C-C4C	2.32	108.14	106.49
22	9	608	CLA	CHB-C1B-NB	2.32	126.71	124.26
24	3	418	LUT	C38-C25-C24	-2.32	118.61	123.56
22	8	601	CLA	CHB-C1B-NB	2.32	126.71	124.26
23	8	608	CHL	CHB-C1B-NB	-2.31	121.81	124.26
23	8	606	CHL	CHC-C1C-C2C	-2.31	117.72	126.11
23	5	318	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
26	3	417	BCR	C15-C16-C17	-2.31	118.74	123.47
24	8	617	LUT	C11-C10-C9	-2.31	124.01	127.31
22	F	802	CLA	C3B-C4B-NB	-2.31	108.37	110.52
28	K	201	LMU	C1'-C2'-C3'	2.31	114.80	110.00
22	B	828	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	5	320	LUT	C15-C14-C13	-2.31	124.02	127.31
22	A	830	CLA	CHC-C4B-NB	2.31	126.70	124.26
22	1	312	CLA	O2D-CGD-CBD	2.31	115.36	111.27
23	3	405	CHL	C2A-C3A-C4A	-2.30	98.15	101.87
22	B	805	CLA	CHB-C4A-NA	2.30	127.70	124.51
28	H	204	LMU	C1B-O1B-C4'	-2.30	112.26	117.96
22	3	410	CLA	CMB-C2B-C1B	-2.30	121.86	125.37
22	A	827	CLA	CHB-C1B-NB	2.30	126.69	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	813	CLA	CAA-CBA-CGA	-2.30	106.53	113.25
22	B	822	CLA	CHB-C1B-NB	2.30	126.69	124.26
22	B	828	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	2	608	CLA	CMA-C3A-C2A	-2.30	110.73	116.10
22	8	615	CLA	CMB-C2B-C3B	2.30	129.55	123.59
24	6	319	LUT	C38-C25-C24	-2.30	118.64	123.56
22	8	614	CLA	CMB-C2B-C3B	2.30	132.15	126.59
28	3	421	LMU	O5'-C5'-C4'	2.30	114.60	109.75
22	8	605	CLA	CHD-C1D-ND	-2.30	122.34	124.45
22	2	608	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	1	305	CHL	C2A-C1A-CHA	2.30	127.87	123.86
22	8	615	CLA	C4A-NA-C1A	2.30	107.74	106.71
22	3	402	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
22	5	303	CLA	CHD-C1D-ND	-2.29	122.35	124.45
32	A	842	PQN	C2M-C2-C3	-2.29	120.66	124.40
22	2	602	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
22	A	826	CLA	CMB-C2B-C1B	-2.29	121.88	125.37
28	9	618	LMU	O5B-C5B-C4B	2.29	113.85	109.69
23	3	406	CHL	C1D-CHD-C4C	-2.29	121.12	126.06
22	A	832	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	7	302	CLA	CHC-C4B-NB	2.29	126.68	124.26
22	B	814	CLA	C3B-C4B-NB	-2.29	108.70	110.23
22	A	817	CLA	C3B-C4B-NB	-2.29	108.39	110.52
22	A	813	CLA	CMB-C2B-C1B	-2.29	121.89	125.37
25	3	416	XAT	C18-C5-C4	2.28	116.85	114.28
23	6	308	CHL	CHD-C1D-ND	2.28	126.55	124.45
25	1	315	XAT	C15-C35-C34	-2.28	118.80	123.47
22	1	302	CLA	CAA-C2A-C1A	2.28	117.19	112.14
26	A	851	BCR	C35-C13-C12	2.28	121.67	118.08
22	8	614	CLA	CHB-C1B-NB	2.28	126.67	124.26
22	5	315	CLA	CHB-C4A-NA	2.28	127.83	124.34
22	H	202	CLA	CHD-C1D-ND	-2.28	122.36	124.45
24	5	320	LUT	C28-C29-C30	-2.28	115.44	118.94
22	B	807	CLA	CAA-C2A-C3A	-2.28	110.78	116.10
22	7	306	CLA	CHC-C4B-NB	2.28	126.67	124.26
27	B	801	LHG	C5-O7-C7	-2.28	112.18	117.79
24	7	315	LUT	C19-C9-C8	2.28	121.67	118.08
25	8	618	XAT	C19-C9-C8	2.28	121.67	118.08
26	J	103	BCR	C16-C15-C14	-2.28	118.80	123.47
22	5	311	CLA	CHB-C1B-NB	2.28	126.67	124.26
26	A	846	BCR	C11-C12-C13	-2.28	120.01	126.42
26	J	101	BCR	C23-C24-C25	-2.28	120.81	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	3	416	XAT	C38-C25-C24	2.28	116.84	114.28
25	7	316	XAT	C20-C13-C14	-2.28	119.73	122.92
22	5	315	CLA	CHD-C1D-ND	-2.28	122.36	124.45
26	B	849	BCR	C1-C6-C5	-2.28	119.41	122.61
27	7	318	LHG	O8-C23-C24	2.27	119.04	111.91
22	9	612	CLA	CAA-C2A-C3A	-2.27	110.80	116.10
22	A	815	CLA	O2D-CGD-CBD	2.27	115.31	111.27
28	3	421	LMU	C1-O1'-C1'	-2.27	110.07	113.84
25	9	614	XAT	C18-C5-C4	2.27	116.83	114.28
24	7	315	LUT	C28-C29-C30	-2.27	115.46	118.94
22	3	408	CLA	CHD-C1D-ND	-2.27	122.37	124.45
25	7	316	XAT	C11-C12-C13	-2.27	120.04	126.42
22	B	841	CLA	CHB-C1B-NB	2.27	126.66	124.26
22	B	841	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	8	602	CHL	C2C-C3C-C4C	2.27	108.11	106.49
22	1	302	CLA	C2C-C1C-NC	2.27	112.10	109.97
22	B	816	CLA	C2A-C1A-CHA	2.27	127.83	123.86
22	A	818	CLA	CHC-C4B-NB	2.27	126.66	124.26
22	A	831	CLA	CMB-C2B-C1B	-2.27	121.92	125.37
23	5	308	CHL	C3D-C4D-ND	-2.27	106.57	110.24
23	8	602	CHL	C3D-C4D-ND	-2.27	106.57	110.24
22	3	412	CLA	CAA-C2A-C3A	-2.27	110.81	116.10
22	6	311	CLA	CHB-C1B-C2B	-2.26	120.84	127.24
22	9	608	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
22	A	804	CLA	CMB-C2B-C1B	-2.26	121.92	125.37
22	B	836	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	1	302	CLA	CHB-C1B-C2B	-2.26	120.84	127.24
22	3	404	CLA	C2A-C1A-CHA	2.26	127.82	123.86
22	8	611	CLA	C3B-C4B-NB	-2.26	108.42	110.52
22	8	604	CLA	CHB-C1B-NB	2.26	126.65	124.26
25	6	320	XAT	C30-C31-C32	-2.26	116.16	123.22
22	A	820	CLA	CHB-C1B-NB	2.26	126.65	124.26
22	9	612	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	A	815	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	A	813	CLA	O2D-CGD-CBD	2.26	115.28	111.27
22	B	812	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	F	802	CLA	CHB-C4A-NA	2.26	127.64	124.51
22	2	608	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	3	407	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	B	810	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	7	301	CLA	C3B-C4B-NB	-2.26	108.42	110.52
26	F	801	BCR	C38-C26-C27	2.26	117.95	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	7	303	CLA	CHD-C1D-ND	-2.26	122.38	124.45
22	B	817	CLA	CMB-C2B-C3B	2.25	132.05	126.59
26	J	101	BCR	C30-C25-C26	-2.25	119.44	122.61
22	B	835	CLA	C2A-C1A-CHA	2.25	127.80	123.86
22	B	842	CLA	CHD-C1D-ND	-2.25	122.38	124.45
23	1	304	CHL	CHC-C1C-NC	-2.25	120.79	124.20
22	A	833	CLA	CHD-C1D-ND	-2.25	122.39	124.45
24	3	418	LUT	C11-C12-C13	-2.25	120.09	126.42
22	B	808	CLA	CHB-C4A-NA	2.25	127.62	124.51
22	7	310	CLA	CHB-C1B-NB	2.25	126.64	124.26
22	8	615	CLA	O2A-CGA-O1A	-2.25	117.70	123.30
22	A	801	CLA	CHB-C4A-NA	2.25	127.62	124.51
26	K	207	BCR	C15-C16-C17	-2.25	118.87	123.47
22	B	828	CLA	C3B-C4B-NB	-2.25	108.43	110.52
22	7	308	CLA	CHD-C1D-ND	-2.25	122.39	124.45
22	A	808	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	9	601	CHL	C2C-C3C-C4C	2.25	108.09	106.49
26	L	305	BCR	C3-C4-C5	-2.24	110.07	114.08
22	B	821	CLA	O2D-CGD-CBD	2.24	115.25	111.27
28	A	852	LMU	C4B-C3B-C2B	2.24	114.74	110.82
24	8	617	LUT	C28-C29-C30	-2.24	115.50	118.94
22	B	816	CLA	CMB-C2B-C3B	2.24	132.02	126.59
23	5	302	CHL	CHC-C1C-NC	-2.24	120.80	124.20
23	8	608	CHL	C4A-NA-C1A	2.24	107.71	106.71
28	7	319	LMU	O1B-C1B-C2B	2.24	113.90	108.10
23	6	308	CHL	C3D-C4D-ND	-2.24	106.61	110.24
22	B	826	CLA	CHD-C1D-ND	-2.24	122.40	124.45
23	8	602	CHL	CHD-C4C-C3C	-2.24	121.55	124.84
23	9	601	CHL	C3D-C4D-ND	-2.24	106.62	110.24
25	5	321	XAT	O24-C25-C26	-2.24	57.11	58.96
26	L	301	BCR	C33-C5-C4	2.24	117.91	113.62
22	2	607	CLA	CAA-C2A-C3A	-2.24	110.88	116.10
26	A	851	BCR	C32-C1-C6	-2.24	106.67	110.30
23	7	304	CHL	C2B-C1B-NB	-2.24	108.73	110.23
22	2	607	CLA	C3B-C4B-NB	-2.24	108.44	110.52
26	9	615	BCR	C24-C23-C22	-2.24	122.86	126.23
23	8	608	CHL	CHA-C1A-NA	-2.24	121.28	126.40
22	7	306	CLA	CHB-C1B-NB	2.23	126.62	124.26
22	3	407	CLA	C2D-C1D-ND	-2.23	108.46	110.10
26	J	103	BCR	C15-C16-C17	-2.23	118.90	123.47
22	6	314	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
22	3	412	CLA	CHC-C4B-NB	2.23	126.62	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	806	CLA	C1-C2-C3	-2.23	123.14	126.75
22	9	610	CLA	CMB-C2B-C3B	2.23	132.00	126.59
22	2	612	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
23	3	422	CHL	CHB-C1B-NB	-2.23	121.89	124.26
22	7	309	CLA	CHB-C1B-NB	2.23	126.62	124.26
22	5	315	CLA	C3A-C4A-CHB	-2.23	120.22	124.24
22	A	835	CLA	CHD-C1D-ND	-2.23	122.40	124.45
22	5	305	CLA	C3B-C4B-NB	-2.23	108.74	110.23
22	6	304	CLA	CHD-C1D-ND	-2.23	122.41	124.45
23	3	405	CHL	C1C-C2C-C3C	-2.23	105.35	107.11
23	8	603	CHL	CGD-CBD-CAD	2.23	117.95	110.73
26	A	851	BCR	C1-C6-C7	2.23	122.08	115.78
23	8	603	CHL	CMD-C2D-C1D	2.23	128.64	124.71
22	B	806	CLA	C3B-C4B-NB	-2.22	108.45	110.52
24	9	613	LUT	C40-C33-C32	2.22	121.58	118.08
22	B	803	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	A	803	CLA	CMB-C2B-C3B	2.22	131.97	126.59
22	B	834	CLA	CHB-C1B-NB	2.22	126.61	124.26
22	H	202	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	B	842	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
25	3	416	XAT	C15-C35-C34	-2.22	118.92	123.47
22	1	308	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	6	307	CLA	CHD-C1D-ND	-2.22	122.41	124.45
22	L	302	CLA	CHB-C1B-NB	2.22	126.61	124.26
26	B	849	BCR	C10-C11-C12	-2.22	116.29	123.22
22	5	313	CLA	CMB-C2B-C1B	-2.22	121.99	125.37
22	1	308	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
26	I	201	BCR	C20-C19-C18	-2.22	120.18	126.42
22	8	604	CLA	C2A-C1A-CHA	2.22	127.74	123.86
22	9	607	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	9	605	CHL	CHC-C1C-NC	-2.22	120.84	124.20
22	2	610	CLA	CHC-C4B-NB	2.22	126.60	124.26
26	K	207	BCR	C8-C7-C6	-2.22	120.98	127.20
22	7	313	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	7	302	CLA	CHB-C1B-NB	2.22	126.60	124.26
26	B	851	BCR	C36-C18-C19	2.22	121.57	118.08
23	8	606	CHL	C2B-C1B-NB	-2.22	108.75	110.23
25	1	315	XAT	C30-C31-C32	-2.21	116.31	123.22
22	B	815	CLA	C3A-C2A-C1A	2.21	104.66	101.34
23	5	302	CHL	C3A-C2A-C1A	2.21	104.66	101.34
22	6	306	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	9	614	XAT	C30-C31-C32	-2.21	116.31	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	850	BCR	C30-C25-C26	-2.21	119.50	122.61
22	3	407	CLA	CHB-C1B-NB	2.21	126.60	124.26
22	B	802	CLA	CHD-C1D-ND	-2.21	122.42	124.45
27	5	325	LHG	C5-O7-C7	-2.21	112.35	117.79
23	3	405	CHL	C4A-NA-C1A	2.21	107.70	106.71
23	7	305	CHL	CHA-C1A-NA	-2.21	121.33	126.40
26	F	801	BCR	C23-C24-C25	-2.21	120.99	127.20
25	1	315	XAT	C24-C23-C22	-2.21	106.50	110.77
22	A	819	CLA	CHD-C1D-ND	-2.21	122.42	124.45
22	5	312	CLA	C3B-C4B-NB	-2.21	108.47	110.52
22	1	303	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	5	307	CHL	CHD-C1D-ND	2.21	126.48	124.45
22	9	609	CLA	CHD-C1D-ND	-2.21	122.42	124.45
22	2	609	CLA	CHB-C1B-NB	2.21	126.59	124.26
26	A	848	BCR	C16-C15-C14	-2.21	118.95	123.47
22	B	839	CLA	C1-C2-C3	-2.21	123.18	126.75
23	5	306	CHL	C3D-C4D-ND	-2.21	106.67	110.24
22	A	818	CLA	CHD-C1D-ND	-2.21	122.43	124.45
24	7	315	LUT	C21-C26-C27	-2.21	109.91	112.70
22	6	304	CLA	C3B-C4B-NB	-2.21	108.47	110.52
26	G	204	BCR	C1-C6-C5	-2.20	119.51	122.61
23	3	413	CHL	C2A-C3A-C4A	-2.20	98.31	101.87
22	B	812	CLA	CHD-C1D-ND	-2.20	122.43	124.45
23	1	306	CHL	C3B-C4B-NB	-2.20	108.47	110.52
22	A	804	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	K	203	BCR	C16-C15-C14	-2.20	118.97	123.47
26	1	316	BCR	C34-C9-C8	2.20	121.54	118.08
22	B	811	CLA	CHC-C4B-NB	2.20	126.59	124.26
26	9	615	BCR	C27-C26-C25	-2.20	119.54	122.73
22	B	813	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
26	7	317	BCR	C11-C12-C13	-2.20	120.24	126.42
22	A	838	CLA	CMB-C2B-C1B	-2.20	122.02	125.37
26	7	317	BCR	C20-C19-C18	-2.20	120.24	126.42
28	7	319	LMU	O1B-C4'-C3'	2.20	113.12	107.28
25	7	316	XAT	O4-C5-C6	-2.20	57.14	58.96
22	6	315	CLA	CHB-C1B-NB	2.20	126.58	124.26
22	8	612	CLA	C2A-C1A-CHA	2.19	127.70	123.86
23	3	413	CHL	CHC-C1C-NC	-2.19	120.88	124.20
22	B	819	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	B	841	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	B	805	CLA	C3B-C4B-NB	-2.19	108.48	110.52
25	5	321	XAT	C35-C15-C14	-2.19	118.98	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	831	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	6	313	CLA	CHB-C1B-NB	2.19	126.58	124.26
22	9	603	CLA	CHA-C1A-NA	-2.19	121.38	126.40
22	B	842	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
22	6	309	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	9	604	CLA	CHD-C1D-ND	-2.19	122.44	124.45
28	6	301	LMU	C1B-O1B-C4'	-2.19	112.55	117.96
22	B	824	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	6	316	CLA	C3B-C4B-NB	-2.19	108.49	110.52
22	A	816	CLA	C4-C3-C5	2.19	118.95	115.27
22	3	403	CLA	CHD-C1D-ND	-2.19	122.44	124.45
22	7	309	CLA	CHC-C4B-NB	2.18	126.57	124.26
22	7	307	CLA	CHD-C1D-ND	-2.18	122.45	124.45
22	A	810	CLA	CHD-C1D-ND	-2.18	122.45	124.45
24	5	320	LUT	C17-C1-C6	-2.18	106.76	110.30
22	B	809	CLA	CMB-C2B-C1B	-2.18	122.05	125.37
24	7	315	LUT	C3-C4-C5	-2.18	107.51	111.85
26	B	851	BCR	C34-C9-C8	2.18	121.51	118.08
22	A	803	CLA	CHD-C1D-ND	-2.18	122.45	124.45
22	3	414	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	3	406	CHL	CMD-C2D-C1D	2.18	128.55	124.71
25	5	321	XAT	C11-C10-C9	-2.18	124.20	127.31
23	5	319	CHL	CHC-C1C-NC	-2.18	120.90	124.20
22	6	307	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
26	A	851	BCR	C38-C26-C25	-2.18	122.08	124.53
22	B	840	CLA	CHB-C1B-NB	2.18	126.56	124.26
23	8	607	CHL	CHC-C1C-NC	-2.18	120.90	124.20
22	A	828	CLA	CHC-C4B-NB	2.18	126.56	124.26
26	F	805	BCR	C1-C6-C5	-2.18	119.55	122.61
22	A	832	CLA	CHB-C1B-NB	2.17	126.56	124.26
22	1	301	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
28	9	618	LMU	C1'-C2'-C3'	2.17	114.52	110.00
22	B	807	CLA	CMB-C2B-C3B	2.17	131.85	126.59
23	5	309	CHL	C3D-C4D-ND	-2.17	106.72	110.24
26	8	619	BCR	C16-C15-C14	-2.17	119.02	123.47
22	2	611	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	A	801	CLA	O1D-CGD-CBD	2.17	128.93	124.48
26	F	801	BCR	C2-C1-C6	2.17	113.82	110.48
22	B	829	CLA	CMB-C2B-C1B	-2.17	122.06	125.37
24	1	314	LUT	C7-C8-C9	-2.17	122.96	126.23
22	6	311	CLA	O2D-CGD-CBD	2.17	115.12	111.27
22	A	827	CLA	CHD-C1D-ND	-2.17	122.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	1	317	LHG	C5-O7-C7	-2.17	112.45	117.79
22	5	304	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
26	B	849	BCR	C20-C19-C18	-2.17	120.32	126.42
22	2	610	CLA	CHB-C1B-NB	2.17	126.55	124.26
24	9	613	LUT	C11-C10-C9	-2.17	124.22	127.31
22	A	823	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	K	206	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	K	207	BCR	C4-C5-C6	-2.17	119.59	122.73
28	1	319	LMU	O5'-C5'-C4'	2.17	114.32	109.75
22	A	831	CLA	CMB-C2B-C3B	2.16	131.83	126.59
26	F	805	BCR	C20-C19-C18	-2.16	120.34	126.42
23	5	318	CHL	CHC-C1C-NC	-2.16	120.92	124.20
23	7	304	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
23	6	308	CHL	C2B-C1B-NB	-2.16	108.78	110.23
22	B	802	CLA	C1-O2A-CGA	2.16	122.12	116.44
23	8	603	CHL	C2C-C3C-C4C	2.16	108.03	106.49
31	9	617	LMG	O6-C5-C6	2.16	111.81	106.44
26	M	102	BCR	C33-C5-C6	-2.16	122.10	124.53
22	A	831	CLA	CHB-C1B-NB	2.16	126.55	124.26
24	8	617	LUT	C20-C13-C12	2.16	121.48	118.08
22	A	837	CLA	CMB-C2B-C1B	-2.16	122.08	125.37
26	J	103	BCR	C21-C20-C19	-2.16	116.48	123.22
23	1	306	CHL	CHB-C1B-NB	-2.16	121.97	124.26
22	2	607	CLA	CMA-C3A-C2A	-2.16	111.06	116.10
23	3	406	CHL	CHC-C1C-NC	-2.16	120.93	124.20
22	3	408	CLA	CHB-C1B-NB	2.16	126.54	124.26
22	B	827	CLA	C2A-C1A-CHA	2.16	127.63	123.86
22	5	316	CLA	C3B-C4B-NB	-2.16	108.79	110.23
26	L	305	BCR	C38-C26-C27	2.16	117.76	113.62
22	A	801	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	3	407	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
26	A	849	BCR	C38-C26-C27	2.15	117.75	113.62
26	3	417	BCR	C20-C19-C18	-2.15	120.36	126.42
22	B	832	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	K	203	BCR	C8-C7-C6	-2.15	121.16	127.20
23	7	305	CHL	C2C-C3C-C4C	2.15	108.02	106.49
26	7	317	BCR	C28-C27-C26	-2.15	110.24	114.08
22	A	839	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	7	306	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	9	606	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	A	811	CLA	CHD-C1D-ND	-2.15	122.48	124.45
22	B	840	CLA	O2A-CGA-O1A	-2.15	118.17	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	815	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	B	830	CLA	C3B-C4B-NB	-2.15	108.52	110.52
22	8	610	CLA	CHB-C1B-NB	2.15	126.53	124.26
25	8	618	XAT	C15-C14-C13	-2.15	124.25	127.31
26	9	615	BCR	C4-C5-C6	-2.15	119.62	122.73
24	5	320	LUT	C20-C13-C12	2.15	121.46	118.08
26	8	619	BCR	C34-C9-C10	-2.15	119.92	122.92
22	6	304	CLA	CHB-C1B-NB	2.15	126.53	124.26
22	5	314	CLA	CBA-CAA-C2A	2.14	118.14	114.28
22	3	408	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
22	B	832	CLA	CHB-C4A-NA	2.14	127.47	124.51
26	A	846	BCR	C8-C7-C6	-2.14	121.19	127.20
26	B	848	BCR	C30-C25-C26	-2.14	119.60	122.61
22	B	838	CLA	CHC-C4B-NB	2.14	126.53	124.26
26	A	851	BCR	C20-C19-C18	-2.14	120.40	126.42
26	A	847	BCR	C30-C25-C26	-2.14	119.60	122.61
22	A	828	CLA	C1-C2-C3	-2.14	122.34	126.04
22	K	204	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	8	603	CHL	C1D-CHD-C4C	-2.14	121.44	126.06
22	5	303	CLA	C3B-C4B-NB	-2.14	108.53	110.52
22	5	303	CLA	CMB-C2B-C1B	-2.14	122.11	125.37
23	1	306	CHL	CMD-C2D-C1D	2.14	128.48	124.71
28	A	853	LMU	O5B-C5B-C4B	2.14	113.01	110.06
25	9	614	XAT	C28-C29-C30	-2.14	115.66	118.94
22	1	303	CLA	CHB-C1B-NB	2.14	126.52	124.26
22	B	802	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
22	A	829	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	A	815	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
28	6	323	LMU	C1'-C2'-C3'	2.14	114.45	110.00
22	A	814	CLA	CMB-C2B-C3B	2.14	131.76	126.59
22	9	610	CLA	CHC-C4B-NB	2.13	126.52	124.26
22	7	314	CLA	CHB-C4A-NA	2.13	127.46	124.51
26	I	201	BCR	C28-C27-C26	-2.13	110.27	114.08
22	6	305	CLA	C3B-C4B-NB	-2.13	108.80	110.23
23	5	308	CHL	CHD-C4C-C3C	-2.13	121.70	124.84
22	6	309	CLA	C3B-C4B-NB	-2.13	108.54	110.52
22	2	601	CLA	CHB-C1B-NB	2.13	126.51	124.26
22	A	820	CLA	C3B-C4B-NB	-2.13	108.54	110.52
22	B	802	CLA	CHB-C1B-C2B	-2.13	121.22	127.24
22	A	837	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	5	309	CHL	CHD-C4C-C3C	-2.13	121.71	124.84
22	7	312	CLA	C3B-C4B-NB	-2.13	108.54	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G	201	LMU	C4B-C3B-C2B	2.13	114.53	110.82
26	B	846	BCR	C35-C13-C12	2.13	121.43	118.08
22	F	803	CLA	CMB-C2B-C1B	-2.13	122.13	125.37
22	B	808	CLA	CHD-C1D-ND	-2.13	122.50	124.45
26	A	848	BCR	C28-C27-C26	-2.12	110.28	114.08
22	3	411	CLA	C4-C3-C5	2.12	118.84	115.27
24	2	614	LUT	C31-C32-C33	-2.12	120.45	126.42
23	3	422	CHL	CHA-C1A-NA	-2.12	121.54	126.40
22	7	301	CLA	CHB-C1B-NB	2.12	126.50	124.26
23	8	603	CHL	C1C-C2C-C3C	-2.12	105.43	107.11
22	3	407	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
22	2	603	CLA	CMB-C2B-C3B	2.12	131.72	126.59
28	6	302	LMU	C2'-C3'-C4'	2.12	114.52	109.68
27	A	845	LHG	C5-O7-C7	-2.12	112.57	117.79
22	B	827	CLA	CMB-C2B-C1B	-2.12	122.14	125.37
22	A	833	CLA	CHB-C1B-NB	2.12	126.50	124.26
22	B	835	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	9	603	CLA	CHB-C1B-C2B	-2.12	121.25	127.24
22	5	315	CLA	C3B-C4B-NB	-2.12	108.55	110.52
23	5	309	CHL	CMD-C2D-C1D	2.12	128.44	124.71
22	9	608	CLA	CHD-C1D-ND	-2.12	122.51	124.45
22	B	825	CLA	CHD-C1D-ND	-2.12	122.51	124.45
22	3	404	CLA	CMB-C2B-C1B	-2.12	122.15	125.37
23	3	422	CHL	C3D-C4D-ND	-2.12	106.81	110.24
28	1	319	LMU	O1B-C1B-C2B	2.12	113.58	108.10
22	A	823	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	3	403	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
22	6	318	CLA	CHD-C1D-ND	-2.11	122.51	124.45
26	F	801	BCR	C4-C5-C6	-2.11	119.66	122.73
22	F	804	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	5	310	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	6	304	CLA	CMB-C2B-C1B	-2.11	122.16	125.37
22	B	804	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	B	817	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	5	307	CHL	CHA-C1A-NA	-2.11	121.57	126.40
22	7	312	CLA	CHC-C4B-NB	2.11	126.49	124.26
23	1	304	CHL	C2B-C1B-NB	-2.11	108.82	110.23
25	6	320	XAT	C40-C33-C32	2.11	121.40	118.08
26	F	805	BCR	C35-C13-C12	2.11	121.40	118.08
23	8	607	CHL	CHD-C4C-C3C	-2.11	121.74	124.84
24	3	418	LUT	C8-C7-C6	-2.11	121.28	127.20
22	A	805	CLA	CHD-C1D-ND	-2.11	122.52	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	2	602	CLA	CMB-C2B-C3B	2.11	131.69	126.59
22	A	837	CLA	C3B-C4B-NB	-2.11	108.56	110.52
24	1	314	LUT	C19-C9-C8	2.11	121.40	118.08
30	6	321	NEX	C39-C29-C30	-2.11	119.97	122.92
22	A	810	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
23	1	306	CHL	C2B-C1B-NB	-2.11	108.82	110.23
23	1	304	CHL	C3D-C4D-ND	-2.11	106.83	110.24
22	6	305	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	1	305	CHL	CHD-C1D-ND	2.11	126.39	124.45
22	8	601	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
22	8	612	CLA	CHC-C4B-NB	2.11	126.49	124.26
26	L	301	BCR	C38-C26-C27	2.11	117.66	113.62
22	A	838	CLA	CHB-C1B-NB	2.10	126.48	124.26
23	5	306	CHL	C2B-C1B-NB	-2.10	108.82	110.23
22	7	301	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	6	310	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	9	612	CLA	CHB-C1B-NB	2.10	126.48	124.26
24	8	617	LUT	C18-C5-C6	-2.10	122.17	124.53
22	B	837	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
22	6	317	CLA	CHD-C1D-ND	-2.10	122.52	124.45
22	8	613	CLA	CHD-C1D-ND	-2.10	122.52	124.45
25	2	615	XAT	C28-C29-C30	-2.10	115.72	118.94
26	J	101	BCR	C2-C1-C6	2.10	113.72	110.48
23	6	308	CHL	CHC-C1C-NC	-2.10	121.02	124.20
22	7	302	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	G	202	CLA	C2A-C1A-CHA	2.10	127.53	123.86
22	5	312	CLA	CHB-C1B-NB	2.10	126.48	124.26
30	6	321	NEX	C35-C15-C14	-2.10	119.17	123.47
22	6	318	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
23	1	305	CHL	C2B-C1B-NB	-2.10	108.82	110.23
23	7	304	CHL	CHD-C1D-ND	2.10	126.38	124.45
26	A	848	BCR	C15-C16-C17	-2.10	119.17	123.47
22	G	203	CLA	CHA-C1A-NA	-2.10	121.59	126.40
22	L	302	CLA	C1-C2-C3	-2.10	123.36	126.75
22	A	825	CLA	CHB-C1B-NB	2.10	126.48	124.26
22	L	302	CLA	C3B-C4B-NB	-2.10	108.57	110.52
22	5	316	CLA	CHD-C1D-ND	-2.10	122.53	124.45
26	3	417	BCR	C34-C9-C8	2.10	121.38	118.08
22	A	826	CLA	CMB-C2B-C3B	2.10	131.66	126.59
26	I	201	BCR	C15-C16-C17	-2.10	119.18	123.47
25	5	321	XAT	C19-C9-C8	2.10	121.38	118.08
22	B	819	CLA	CMB-C2B-C1B	-2.09	122.18	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3	413	CHL	C3D-C4D-ND	-2.09	106.85	110.24
26	G	204	BCR	C21-C20-C19	-2.09	116.68	123.22
26	A	849	BCR	C2-C1-C6	2.09	113.70	110.48
23	8	603	CHL	C1-O2A-CGA	2.09	121.94	116.44
22	B	806	CLA	CHB-C1B-NB	2.09	126.47	124.26
24	6	319	LUT	C39-C29-C28	2.09	121.37	118.08
22	A	832	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
22	3	412	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	3	403	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	A	813	CLA	CMB-C2B-C3B	2.09	131.65	126.59
26	J	103	BCR	C33-C5-C4	2.09	117.63	113.62
22	3	410	CLA	CMB-C2B-C3B	2.09	131.65	126.59
22	7	308	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	A	801	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
22	F	804	CLA	C2B-C1B-NB	2.09	111.63	110.23
26	L	301	BCR	C38-C26-C25	-2.09	122.18	124.53
22	1	309	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	A	835	CLA	CHB-C1B-NB	2.09	126.47	124.26
22	B	828	CLA	CMB-C2B-C3B	2.09	131.64	126.59
26	A	847	BCR	C33-C5-C6	-2.09	122.18	124.53
23	5	308	CHL	CHD-C1D-ND	2.09	126.37	124.45
22	A	807	CLA	CHD-C1D-ND	-2.09	122.54	124.45
22	A	838	CLA	CHD-C1D-ND	-2.09	122.54	124.45
22	B	839	CLA	C3B-C4B-NB	-2.09	108.58	110.52
22	6	315	CLA	O2A-CGA-O1A	-2.09	118.10	123.30
22	B	818	CLA	CHD-C1D-ND	-2.09	122.54	124.45
23	5	302	CHL	CMD-C2D-C1D	2.09	128.39	124.71
26	7	317	BCR	C4-C5-C6	-2.09	119.70	122.73
26	5	322	BCR	C8-C7-C6	-2.09	121.34	127.20
24	6	319	LUT	C30-C31-C32	-2.09	116.71	123.22
23	8	607	CHL	C2B-C1B-NB	-2.09	108.83	110.23
22	2	601	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	1	306	CHL	CHC-C1C-NC	-2.08	121.04	124.20
25	7	316	XAT	C18-C5-C4	2.08	116.62	114.28
24	1	314	LUT	C21-C26-C27	-2.08	110.07	112.70
22	7	309	CLA	C3B-C4B-NB	-2.08	108.58	110.52
23	8	606	CHL	CHB-C1B-NB	-2.08	122.05	124.26
22	A	818	CLA	O2D-CGD-CBD	2.08	114.97	111.27
22	A	820	CLA	CHD-C1D-ND	-2.08	122.54	124.45
30	6	321	NEX	O24-C25-C26	-2.08	57.23	58.96
22	A	825	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	B	849	BCR	C30-C25-C26	-2.08	119.68	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	3	406	CHL	C2A-C3A-C4A	-2.08	98.51	101.87
26	I	201	BCR	C16-C15-C14	-2.08	119.21	123.47
26	3	417	BCR	C23-C24-C25	-2.08	121.36	127.20
25	3	416	XAT	C28-C29-C30	-2.08	115.75	118.94
28	6	301	LMU	C4B-C3B-C2B	2.08	114.46	110.82
23	6	303	CHL	CHB-C1B-NB	-2.08	122.05	124.26
22	6	318	CLA	CHC-C4B-NB	2.08	126.46	124.26
26	8	619	BCR	C20-C19-C18	-2.08	120.57	126.42
26	9	615	BCR	C1-C6-C5	-2.08	119.68	122.61
26	J	103	BCR	C11-C12-C13	-2.08	120.58	126.42
22	B	808	CLA	C3B-C4B-NB	-2.08	108.59	110.52
22	B	831	CLA	CHB-C1B-NB	2.08	126.46	124.26
26	F	805	BCR	C36-C18-C17	-2.08	120.01	122.92
22	B	808	CLA	CMB-C2B-C3B	2.08	131.62	126.59
25	8	618	XAT	O24-C25-C26	-2.07	57.24	58.96
23	8	606	CHL	CHD-C1D-ND	2.07	126.36	124.45
25	7	316	XAT	O24-C25-C26	-2.07	57.24	58.96
22	B	815	CLA	C2A-C1A-CHA	2.07	127.48	123.86
22	7	308	CLA	CHB-C1B-NB	2.07	126.45	124.26
22	3	408	CLA	CMB-C2B-C3B	2.07	131.60	126.59
22	B	806	CLA	C2A-C1A-CHA	2.07	127.48	123.86
22	2	606	CLA	CHD-C1D-ND	-2.07	122.55	124.45
22	L	304	CLA	CHD-C1D-ND	-2.07	122.55	124.45
26	5	322	BCR	C23-C24-C25	-2.07	121.39	127.20
31	J	105	LMG	O7-C10-O9	-2.07	118.70	123.70
23	8	603	CHL	C3D-C2D-C1D	-2.07	103.01	105.83
22	9	606	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	A	853	LMU	C2'-C3'-C4'	2.07	114.41	109.68
26	B	847	BCR	C20-C19-C18	-2.07	120.61	126.42
22	B	812	CLA	CHB-C1B-NB	2.07	126.45	124.26
25	8	618	XAT	C24-C23-C22	-2.07	106.78	110.77
22	A	839	CLA	C3B-C4B-NB	-2.07	108.60	110.52
25	3	416	XAT	C19-C9-C8	2.07	121.33	118.08
22	6	318	CLA	CHB-C1B-NB	2.07	126.44	124.26
22	A	821	CLA	CHD-C1D-ND	-2.07	122.56	124.45
22	B	811	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
22	A	827	CLA	CMB-C2B-C3B	2.06	131.59	126.59
22	A	822	CLA	C3B-C4B-NB	-2.06	108.60	110.52
23	7	305	CHL	CHC-C1C-NC	-2.06	121.07	124.20
22	A	807	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	6	310	CLA	C3B-C4B-NB	-2.06	108.60	110.52
22	9	610	CLA	CHB-C1B-NB	2.06	126.44	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	832	CLA	C2D-C1D-ND	-2.06	108.58	110.10
22	9	607	CLA	C1D-ND-C4D	-2.06	104.87	106.33
22	A	830	CLA	CHD-C1D-ND	-2.06	122.56	124.45
25	5	321	XAT	C15-C35-C34	-2.06	119.25	123.47
22	5	315	CLA	CHC-C4B-NB	2.06	126.44	124.26
22	A	812	CLA	C3B-C4B-NB	-2.06	108.60	110.52
22	B	827	CLA	C3B-C4B-NB	-2.06	108.60	110.52
23	3	406	CHL	C2B-C1B-NB	-2.06	108.85	110.23
23	8	606	CHL	C3B-C4B-NB	-2.06	108.60	110.52
22	8	610	CLA	CMB-C2B-C1B	-2.06	122.23	125.37
22	B	805	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	5	313	CLA	C2A-C1A-CHA	2.06	127.46	123.86
23	3	413	CHL	CHA-C1A-NA	-2.06	121.68	126.40
22	A	841	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	A	825	CLA	C1-C2-C3	-2.06	123.42	126.75
22	F	803	CLA	CHB-C1B-NB	2.06	126.44	124.26
22	5	311	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
26	I	201	BCR	C3-C4-C5	-2.06	110.40	114.08
22	3	404	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
22	B	817	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
23	8	607	CHL	C3D-C4D-ND	-2.06	106.91	110.24
22	B	843	CLA	CHD-C1D-ND	-2.06	122.56	124.45
26	F	801	BCR	C10-C11-C12	-2.06	116.80	123.22
22	7	312	CLA	CHB-C1B-NB	2.06	126.43	124.26
23	1	304	CHL	CHB-C1B-NB	-2.05	122.08	124.26
22	A	827	CLA	CHC-C4B-NB	2.05	126.43	124.26
22	F	804	CLA	CHA-C1A-NA	-2.05	121.69	126.40
22	7	307	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
22	B	832	CLA	CHB-C1B-NB	2.05	126.43	124.26
22	A	838	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
23	3	422	CHL	CHD-C1D-ND	2.05	126.34	124.45
22	A	827	CLA	CMB-C2B-C1B	-2.05	122.24	125.37
26	F	801	BCR	C21-C20-C19	-2.05	116.81	123.22
22	5	315	CLA	CHB-C1B-NB	2.05	126.43	124.26
28	3	423	LMU	O5B-C5B-C4B	2.05	113.42	109.69
22	5	311	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
22	1	312	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	2	613	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	1	312	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	818	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	830	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
22	1	310	CLA	C2B-C1B-NB	2.05	111.61	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	409	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	A	826	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	B	811	CLA	C3B-C4B-NB	-2.05	108.61	110.52
22	B	843	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
28	G	201	LMU	C3B-C4B-C5B	2.05	113.89	110.24
22	7	308	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
28	6	301	LMU	O5'-C1'-C2'	2.05	114.68	110.35
22	H	201	CLA	CAD-CBD-CHA	2.05	107.44	105.14
22	B	835	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
22	A	812	CLA	C2A-C1A-CHA	2.05	127.44	123.86
26	B	850	BCR	C35-C13-C12	2.05	121.30	118.08
24	6	319	LUT	C8-C7-C6	-2.05	121.46	127.20
22	7	313	CLA	C3B-C4B-NB	-2.05	108.86	110.23
22	5	311	CLA	C1-C2-C3	-2.05	122.51	126.04
28	3	421	LMU	C6'-C5'-C4'	-2.04	107.37	113.33
23	1	304	CHL	CMD-C2D-C1D	2.04	128.31	124.71
22	B	838	CLA	C3B-C4B-NB	-2.04	108.62	110.52
22	7	314	CLA	CMA-C3A-C2A	-2.04	111.33	116.10
22	A	838	CLA	CMB-C2B-C3B	2.04	131.53	126.59
26	A	848	BCR	C11-C12-C13	-2.04	120.68	126.42
26	B	848	BCR	C27-C26-C25	-2.04	119.77	122.73
23	8	608	CHL	C3D-C4D-ND	-2.04	106.93	110.24
25	7	316	XAT	C12-C13-C14	2.04	122.07	118.94
22	F	803	CLA	C2A-C1A-CHA	2.04	127.43	123.86
22	7	310	CLA	C2A-C1A-CHA	2.04	127.43	123.86
23	6	308	CHL	CHA-C1A-NA	-2.04	121.73	126.40
23	8	608	CHL	CHD-C1D-ND	2.04	126.33	124.45
22	A	828	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
23	3	405	CHL	CHA-C1A-NA	-2.04	121.73	126.40
22	5	310	CLA	C1-C2-C3	-2.04	122.52	126.04
26	3	419	BCR	C27-C26-C25	-2.04	119.77	122.73
26	3	417	BCR	C30-C25-C24	2.04	121.54	115.78
23	5	309	CHL	C2B-C1B-NB	-2.04	108.87	110.23
26	9	615	BCR	C28-C27-C26	-2.04	110.44	114.08
23	5	308	CHL	CHC-C1C-NC	-2.04	121.11	124.20
22	K	204	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	B	841	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
22	A	836	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
22	5	313	CLA	CMB-C2B-C3B	2.03	131.51	126.59
22	3	401	CLA	CHD-C1D-ND	-2.03	122.58	124.45
22	8	611	CLA	CHD-C1D-ND	-2.03	122.58	124.45
22	B	824	CLA	C4C-C3C-C2C	-2.03	106.64	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	9	612	CLA	CMB-C2B-C1B	-2.03	122.27	125.37
22	A	838	CLA	CAA-CBA-CGA	-2.03	107.31	113.25
22	2	603	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	3	402	CLA	CHC-C4B-NB	2.03	126.41	124.26
25	1	315	XAT	O4-C5-C6	-2.03	57.28	58.96
28	1	319	LMU	C1B-C2B-C3B	2.03	114.23	110.00
22	2	602	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	3	404	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	J	103	BCR	C37-C22-C23	2.03	121.28	118.08
26	J	103	BCR	C3-C4-C5	-2.03	110.45	114.08
26	L	301	BCR	C29-C30-C25	2.03	113.61	110.48
22	A	810	CLA	CHB-C1B-NB	2.03	126.41	124.26
22	3	412	CLA	C3B-C4B-NB	-2.03	108.63	110.52
25	3	416	XAT	O4-C5-C6	-2.03	57.28	58.96
22	A	801	CLA	CBA-CAA-C2A	-2.03	107.87	113.86
23	9	601	CHL	CHC-C1C-NC	-2.03	121.13	124.20
22	3	410	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	B	816	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	L	303	CLA	C3B-C4B-NB	-2.03	108.64	110.52
22	5	303	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	6	309	CLA	CHB-C1B-NB	2.03	126.40	124.26
22	A	840	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	B	844	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	B	809	CLA	CMB-C2B-C3B	2.02	131.49	126.59
22	3	401	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
22	A	806	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
23	5	319	CHL	CHA-C4D-ND	-2.02	128.26	132.50
22	A	822	CLA	CHB-C1B-NB	2.02	126.40	124.26
22	2	613	CLA	O2A-CGA-O1A	-2.02	118.25	123.30
26	G	204	BCR	C29-C30-C25	2.02	113.60	110.48
23	6	308	CHL	CHD-C4C-C3C	-2.02	121.87	124.84
22	K	206	CLA	C3B-C4B-NB	-2.02	108.64	110.52
22	8	605	CLA	CMB-C2B-C1B	-2.02	122.29	125.37
23	5	307	CHL	C2B-C1B-NB	-2.02	108.88	110.23
23	8	607	CHL	C1D-CHD-C4C	-2.02	121.69	126.06
22	8	604	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	9	606	CLA	O2D-CGD-CBD	2.02	114.86	111.27
30	6	321	NEX	C31-C32-C33	-2.02	120.74	126.42
26	B	851	BCR	C38-C26-C27	2.02	117.50	113.62
22	A	834	CLA	CHD-C1D-ND	-2.02	122.60	124.45
22	A	841	CLA	CAC-C3C-C4C	2.02	127.43	124.81
22	B	808	CLA	O2A-CGA-O1A	-2.02	118.49	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	3	417	BCR	C30-C25-C26	-2.02	119.77	122.61
22	7	308	CLA	C3B-C4B-NB	-2.02	108.64	110.52
22	9	609	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
22	B	828	CLA	C1-C2-C3	-2.02	123.48	126.75
22	B	810	CLA	O2D-CGD-CBD	2.02	114.86	111.27
22	B	820	CLA	CHD-C1D-ND	-2.02	122.60	124.45
28	A	853	LMU	O5'-C5'-C4'	2.02	114.01	109.75
22	A	808	CLA	C1-C2-C3	-2.02	123.48	126.75
22	2	601	CLA	C3B-C4B-NB	-2.02	108.64	110.52
22	A	836	CLA	C1-C2-C3	-2.02	123.49	126.75
22	B	816	CLA	CHA-C1A-NA	-2.02	121.78	126.40
22	B	836	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	L	302	CLA	O1D-CGD-CBD	2.02	128.61	124.48
22	B	821	CLA	CMB-C2B-C1B	-2.02	122.30	125.37
22	1	302	CLA	CHC-C4B-NB	2.02	126.39	124.26
22	A	835	CLA	C3B-C4B-NB	-2.02	108.64	110.52
23	8	602	CHL	C2B-C1B-NB	-2.02	108.88	110.23
28	1	319	LMU	C1'-C2'-C3'	2.01	114.19	110.00
22	B	820	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	6	320	XAT	O24-C25-C26	-2.01	57.29	58.96
23	3	413	CHL	C2B-C1B-NB	-2.01	108.88	110.23
23	6	303	CHL	C2B-C1B-NB	-2.01	108.88	110.23
26	L	305	BCR	C15-C16-C17	-2.01	119.35	123.47
23	5	318	CHL	C2B-C1B-NB	-2.01	108.88	110.23
23	8	608	CHL	C2B-C1B-NB	-2.01	108.88	110.23
22	A	803	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
23	5	318	CHL	CHD-C1D-ND	2.01	126.30	124.45
22	2	610	CLA	CHA-C1A-NA	-2.01	121.79	126.40
22	B	806	CLA	O2D-CGD-CBD	2.01	114.84	111.27
26	F	805	BCR	C3-C4-C5	-2.01	110.49	114.08
22	A	814	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	A	808	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	5	311	CLA	C3B-C4B-NB	-2.01	108.65	110.52
22	B	809	CLA	C1-C2-C3	-2.01	122.57	126.04
22	9	604	CLA	CMB-C2B-C1B	-2.01	122.31	125.37
22	B	802	CLA	C2B-C1B-NB	2.01	111.58	110.23
23	8	603	CHL	C2A-C3A-C4A	-2.01	98.63	101.87
26	A	848	BCR	C2-C1-C6	2.01	113.57	110.48
22	B	825	CLA	CMB-C2B-C3B	2.01	131.45	126.59
26	5	322	BCR	C27-C26-C25	-2.01	119.82	122.73
26	G	204	BCR	C38-C26-C25	-2.01	122.28	124.53
22	A	823	CLA	CHC-C4B-NB	2.01	126.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	6	307	CLA	C3B-C4B-NB	-2.00	108.66	110.52
23	5	318	CHL	C2C-C3C-C4C	2.00	107.92	106.49
22	3	401	CLA	CMB-C2B-C1B	-2.00	122.32	125.37
22	3	410	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	B	823	CLA	C2A-C1A-CHA	2.00	127.36	123.86
22	8	616	CLA	CHD-C1D-ND	-2.00	122.61	124.45
22	A	843	CLA	CHD-C1D-ND	-2.00	122.61	124.45
32	A	842	PQN	C21-C22-C23	-2.00	109.44	115.92
22	3	404	CLA	CMB-C2B-C3B	2.00	131.44	126.59
26	A	848	BCR	C20-C19-C18	-2.00	120.79	126.42
23	5	307	CHL	C3D-C4D-ND	-2.00	107.00	110.24
27	2	617	LHG	C5-O7-C7	-2.00	112.86	117.79
32	B	845	PQN	C16-C17-C18	-2.00	109.45	115.92
22	5	304	CLA	C2A-C1A-CHA	2.00	127.36	123.86
25	6	320	XAT	C18-C5-C4	2.00	116.53	114.28
25	2	615	XAT	O4-C5-C6	-2.00	57.30	58.96

There are no chirality outliers.

All (2544) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	1	301	CLA	C2B-C3B-CAB-CBB
22	1	301	CLA	C4B-C3B-CAB-CBB
22	1	301	CLA	C2-C3-C5-C6
22	1	301	CLA	C4-C3-C5-C6
22	1	302	CLA	C3A-C2A-CAA-CBA
22	1	302	CLA	C4B-C3B-CAB-CBB
22	1	302	CLA	CBD-CGD-O2D-CED
22	1	307	CLA	CAD-CBD-CGD-O2D
22	1	308	CLA	C3A-C2A-CAA-CBA
22	1	308	CLA	CHA-CBD-CGD-O1D
22	1	308	CLA	CHA-CBD-CGD-O2D
22	1	309	CLA	C1A-C2A-CAA-CBA
22	1	310	CLA	C2B-C3B-CAB-CBB
22	1	310	CLA	C4B-C3B-CAB-CBB
22	1	313	CLA	CHA-CBD-CGD-O1D
22	2	601	CLA	C1A-C2A-CAA-CBA
22	2	601	CLA	C3A-C2A-CAA-CBA
22	2	602	CLA	C1A-C2A-CAA-CBA
22	2	602	CLA	C3A-C2A-CAA-CBA
22	2	604	CLA	C1A-C2A-CAA-CBA
22	2	605	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	2	605	CLA	C4B-C3B-CAB-CBB
22	2	607	CLA	C2B-C3B-CAB-CBB
22	2	607	CLA	C4B-C3B-CAB-CBB
22	2	609	CLA	C1A-C2A-CAA-CBA
22	2	610	CLA	C1A-C2A-CAA-CBA
22	2	610	CLA	C3A-C2A-CAA-CBA
22	2	612	CLA	C1A-C2A-CAA-CBA
22	2	612	CLA	C6-C7-C8-C9
22	2	613	CLA	C1A-C2A-CAA-CBA
22	2	613	CLA	C2B-C3B-CAB-CBB
22	2	613	CLA	C4B-C3B-CAB-CBB
22	3	402	CLA	C1A-C2A-CAA-CBA
22	3	407	CLA	C2B-C3B-CAB-CBB
22	3	407	CLA	C4B-C3B-CAB-CBB
22	3	408	CLA	C1A-C2A-CAA-CBA
22	3	408	CLA	C3A-C2A-CAA-CBA
22	3	409	CLA	C2B-C3B-CAB-CBB
22	3	409	CLA	C4B-C3B-CAB-CBB
22	3	410	CLA	C1A-C2A-CAA-CBA
22	3	410	CLA	C3A-C2A-CAA-CBA
22	3	411	CLA	C2B-C3B-CAB-CBB
22	3	411	CLA	C4B-C3B-CAB-CBB
22	3	411	CLA	C4-C3-C5-C6
22	3	414	CLA	C2B-C3B-CAB-CBB
22	3	414	CLA	C4B-C3B-CAB-CBB
22	5	305	CLA	C3A-C2A-CAA-CBA
22	5	310	CLA	C3A-C2A-CAA-CBA
22	5	312	CLA	C2B-C3B-CAB-CBB
22	5	312	CLA	C4B-C3B-CAB-CBB
22	5	313	CLA	C1A-C2A-CAA-CBA
22	5	313	CLA	C3A-C2A-CAA-CBA
22	5	314	CLA	C4B-C3B-CAB-CBB
22	6	306	CLA	C1A-C2A-CAA-CBA
22	6	306	CLA	C3A-C2A-CAA-CBA
22	6	307	CLA	CBD-CGD-O2D-CED
22	6	310	CLA	C3A-C2A-CAA-CBA
22	6	310	CLA	CHA-CBD-CGD-O1D
22	6	310	CLA	CHA-CBD-CGD-O2D
22	6	311	CLA	C1A-C2A-CAA-CBA
22	6	311	CLA	C3A-C2A-CAA-CBA
22	6	312	CLA	C1A-C2A-CAA-CBA
22	6	313	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	6	313	CLA	C2B-C3B-CAB-CBB
22	6	313	CLA	C4B-C3B-CAB-CBB
22	6	314	CLA	C4B-C3B-CAB-CBB
22	6	316	CLA	C2-C3-C5-C6
22	6	316	CLA	C4-C3-C5-C6
22	6	318	CLA	C1A-C2A-CAA-CBA
22	6	318	CLA	C3A-C2A-CAA-CBA
22	6	318	CLA	CHA-CBD-CGD-O1D
22	6	318	CLA	CHA-CBD-CGD-O2D
22	7	307	CLA	C1A-C2A-CAA-CBA
22	7	309	CLA	C2B-C3B-CAB-CBB
22	7	309	CLA	C4B-C3B-CAB-CBB
22	7	311	CLA	C2B-C3B-CAB-CBB
22	7	311	CLA	C4B-C3B-CAB-CBB
22	7	312	CLA	C3A-C2A-CAA-CBA
22	7	312	CLA	C2B-C3B-CAB-CBB
22	7	312	CLA	C4B-C3B-CAB-CBB
22	7	313	CLA	C1A-C2A-CAA-CBA
22	7	313	CLA	C3A-C2A-CAA-CBA
22	8	601	CLA	C2A-CAA-CBA-CGA
22	8	601	CLA	C4B-C3B-CAB-CBB
22	8	609	CLA	C1A-C2A-CAA-CBA
22	8	609	CLA	C3A-C2A-CAA-CBA
22	8	609	CLA	C2A-CAA-CBA-CGA
22	8	610	CLA	C3A-C2A-CAA-CBA
22	8	612	CLA	C1A-C2A-CAA-CBA
22	8	612	CLA	C3A-C2A-CAA-CBA
22	8	613	CLA	C4B-C3B-CAB-CBB
22	8	613	CLA	C14-C13-C15-C16
22	8	614	CLA	CHA-CBD-CGD-O1D
22	8	614	CLA	CHA-CBD-CGD-O2D
22	8	616	CLA	C1A-C2A-CAA-CBA
22	9	602	CLA	C2B-C3B-CAB-CBB
22	9	602	CLA	C4B-C3B-CAB-CBB
22	9	604	CLA	C2A-CAA-CBA-CGA
22	9	608	CLA	C1A-C2A-CAA-CBA
22	9	608	CLA	C3A-C2A-CAA-CBA
22	9	609	CLA	C2B-C3B-CAB-CBB
22	9	609	CLA	C4B-C3B-CAB-CBB
22	9	609	CLA	CHA-CBD-CGD-O1D
22	9	609	CLA	CHA-CBD-CGD-O2D
22	9	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	9	610	CLA	C3A-C2A-CAA-CBA
22	9	610	CLA	CBD-CGD-O2D-CED
22	9	611	CLA	C1A-C2A-CAA-CBA
22	9	611	CLA	C2B-C3B-CAB-CBB
22	9	611	CLA	C4B-C3B-CAB-CBB
22	9	611	CLA	CHA-CBD-CGD-O1D
22	9	611	CLA	CHA-CBD-CGD-O2D
22	9	611	CLA	CAD-CBD-CGD-O1D
22	A	801	CLA	C2B-C3B-CAB-CBB
22	A	801	CLA	C4B-C3B-CAB-CBB
22	A	801	CLA	CBD-CGD-O2D-CED
22	A	802	CLA	C1A-C2A-CAA-CBA
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	808	CLA	C2B-C3B-CAB-CBB
22	A	808	CLA	C4B-C3B-CAB-CBB
22	A	809	CLA	C1A-C2A-CAA-CBA
22	A	809	CLA	C3A-C2A-CAA-CBA
22	A	809	CLA	CHA-CBD-CGD-O1D
22	A	809	CLA	CHA-CBD-CGD-O2D
22	A	810	CLA	C4B-C3B-CAB-CBB
22	A	813	CLA	CHA-CBD-CGD-O1D
22	A	813	CLA	CHA-CBD-CGD-O2D
22	A	813	CLA	CBD-CGD-O2D-CED
22	A	817	CLA	C1A-C2A-CAA-CBA
22	A	817	CLA	C3A-C2A-CAA-CBA
22	A	817	CLA	C2B-C3B-CAB-CBB
22	A	817	CLA	C4B-C3B-CAB-CBB
22	A	818	CLA	C1A-C2A-CAA-CBA
22	A	818	CLA	C3A-C2A-CAA-CBA
22	A	819	CLA	C3A-C2A-CAA-CBA
22	A	819	CLA	CBA-CGA-O2A-C1
22	A	821	CLA	CBD-CGD-O2D-CED
22	A	822	CLA	C1A-C2A-CAA-CBA
22	A	822	CLA	C2B-C3B-CAB-CBB
22	A	822	CLA	C4B-C3B-CAB-CBB
22	A	822	CLA	CHA-CBD-CGD-O1D
22	A	822	CLA	CHA-CBD-CGD-O2D
22	A	822	CLA	CAD-CBD-CGD-O1D
22	A	822	CLA	CBD-CGD-O2D-CED
22	A	823	CLA	C2B-C3B-CAB-CBB
22	A	823	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	823	CLA	C4-C3-C5-C6
22	A	824	CLA	C1A-C2A-CAA-CBA
22	A	824	CLA	C3A-C2A-CAA-CBA
22	A	826	CLA	CHA-CBD-CGD-O1D
22	A	826	CLA	CHA-CBD-CGD-O2D
22	A	828	CLA	C1A-C2A-CAA-CBA
22	A	830	CLA	C1A-C2A-CAA-CBA
22	A	830	CLA	C3A-C2A-CAA-CBA
22	A	832	CLA	CBD-CGD-O2D-CED
22	A	834	CLA	C2B-C3B-CAB-CBB
22	A	834	CLA	C4B-C3B-CAB-CBB
22	A	835	CLA	C1A-C2A-CAA-CBA
22	A	835	CLA	C3A-C2A-CAA-CBA
22	A	835	CLA	CHA-CBD-CGD-O1D
22	A	835	CLA	CHA-CBD-CGD-O2D
22	A	836	CLA	CBD-CGD-O2D-CED
22	A	838	CLA	C1A-C2A-CAA-CBA
22	A	838	CLA	CHA-CBD-CGD-O1D
22	A	838	CLA	CHA-CBD-CGD-O2D
22	A	838	CLA	C11-C10-C8-C9
22	A	839	CLA	C1A-C2A-CAA-CBA
22	A	839	CLA	C3A-C2A-CAA-CBA
22	A	839	CLA	CHA-CBD-CGD-O1D
22	A	839	CLA	CHA-CBD-CGD-O2D
22	A	840	CLA	C4B-C3B-CAB-CBB
22	A	841	CLA	C1A-C2A-CAA-CBA
22	A	841	CLA	C2B-C3B-CAB-CBB
22	A	841	CLA	C4B-C3B-CAB-CBB
22	B	802	CLA	CBA-CGA-O2A-C1
22	B	802	CLA	O1A-CGA-O2A-C1
22	B	802	CLA	CBD-CGD-O2D-CED
22	B	804	CLA	CHA-CBD-CGD-O1D
22	B	804	CLA	CBD-CGD-O2D-CED
22	B	804	CLA	C4-C3-C5-C6
22	B	805	CLA	C2B-C3B-CAB-CBB
22	B	805	CLA	C4B-C3B-CAB-CBB
22	B	805	CLA	CBD-CGD-O2D-CED
22	B	806	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C1A-C2A-CAA-CBA
22	B	810	CLA	C1A-C2A-CAA-CBA
22	B	811	CLA	C1A-C2A-CAA-CBA
22	B	811	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	811	CLA	C2B-C3B-CAB-CBB
22	B	811	CLA	C4B-C3B-CAB-CBB
22	B	812	CLA	C1A-C2A-CAA-CBA
22	B	812	CLA	C2A-CAA-CBA-CGA
22	B	812	CLA	CBD-CGD-O2D-CED
22	B	814	CLA	CHA-CBD-CGD-O2D
22	B	815	CLA	C2B-C3B-CAB-CBB
22	B	815	CLA	C4B-C3B-CAB-CBB
22	B	815	CLA	CHA-CBD-CGD-O1D
22	B	815	CLA	CHA-CBD-CGD-O2D
22	B	816	CLA	C1A-C2A-CAA-CBA
22	B	816	CLA	C3A-C2A-CAA-CBA
22	B	816	CLA	CBD-CGD-O2D-CED
22	B	818	CLA	CHA-CBD-CGD-O1D
22	B	818	CLA	CHA-CBD-CGD-O2D
22	B	818	CLA	CBD-CGD-O2D-CED
22	B	823	CLA	C1A-C2A-CAA-CBA
22	B	823	CLA	C3A-C2A-CAA-CBA
22	B	827	CLA	C2-C3-C5-C6
22	B	827	CLA	C4-C3-C5-C6
22	B	830	CLA	C1A-C2A-CAA-CBA
22	B	830	CLA	C3A-C2A-CAA-CBA
22	B	830	CLA	CHA-CBD-CGD-O1D
22	B	830	CLA	CHA-CBD-CGD-O2D
22	B	831	CLA	C1A-C2A-CAA-CBA
22	B	831	CLA	C3A-C2A-CAA-CBA
22	B	833	CLA	C1A-C2A-CAA-CBA
22	B	833	CLA	C3A-C2A-CAA-CBA
22	B	833	CLA	C2B-C3B-CAB-CBB
22	B	833	CLA	C4B-C3B-CAB-CBB
22	B	833	CLA	CHA-CBD-CGD-O1D
22	B	833	CLA	CHA-CBD-CGD-O2D
22	B	838	CLA	CBD-CGD-O2D-CED
22	B	841	CLA	C2B-C3B-CAB-CBB
22	B	841	CLA	C4B-C3B-CAB-CBB
22	B	843	CLA	C2B-C3B-CAB-CBB
22	B	843	CLA	C4B-C3B-CAB-CBB
22	B	843	CLA	CHA-CBD-CGD-O1D
22	B	843	CLA	CHA-CBD-CGD-O2D
22	B	843	CLA	CBD-CGD-O2D-CED
22	B	844	CLA	CHA-CBD-CGD-O1D
22	B	844	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	F	802	CLA	C11-C10-C8-C9
22	F	803	CLA	C1A-C2A-CAA-CBA
22	F	804	CLA	C2B-C3B-CAB-CBB
22	F	804	CLA	C4B-C3B-CAB-CBB
22	G	203	CLA	CBD-CGD-O2D-CED
22	H	203	CLA	C1A-C2A-CAA-CBA
22	K	202	CLA	C2B-C3B-CAB-CBB
22	K	202	CLA	C4B-C3B-CAB-CBB
22	K	202	CLA	CBD-CGD-O2D-CED
22	K	205	CLA	C4B-C3B-CAB-CBB
22	K	205	CLA	CHA-CBD-CGD-O1D
22	K	205	CLA	CHA-CBD-CGD-O2D
22	K	205	CLA	CAD-CBD-CGD-O1D
22	K	205	CLA	CAD-CBD-CGD-O2D
22	L	302	CLA	C2B-C3B-CAB-CBB
22	L	302	CLA	C4B-C3B-CAB-CBB
22	L	302	CLA	CBD-CGD-O2D-CED
22	L	303	CLA	C1A-C2A-CAA-CBA
22	L	303	CLA	CHA-CBD-CGD-O1D
22	L	303	CLA	CHA-CBD-CGD-O2D
23	1	304	CHL	C1A-C2A-CAA-CBA
23	1	304	CHL	C3A-C2A-CAA-CBA
23	1	304	CHL	C2B-C3B-CAB-CBB
23	1	304	CHL	C4B-C3B-CAB-CBB
23	1	306	CHL	C1A-C2A-CAA-CBA
23	1	306	CHL	C2B-C3B-CAB-CBB
23	1	306	CHL	C4B-C3B-CAB-CBB
23	3	405	CHL	C1A-C2A-CAA-CBA
23	3	405	CHL	C3A-C2A-CAA-CBA
23	3	405	CHL	C2B-C3B-CAB-CBB
23	3	405	CHL	C4B-C3B-CAB-CBB
23	3	406	CHL	C1-C2-C3-C4
23	3	413	CHL	C2B-C3B-CAB-CBB
23	3	413	CHL	C4B-C3B-CAB-CBB
23	3	413	CHL	CBD-CGD-O2D-CED
23	3	413	CHL	O1D-CGD-O2D-CED
23	3	422	CHL	C3A-C2A-CAA-CBA
23	3	422	CHL	C2B-C3B-CAB-CBB
23	3	422	CHL	C4B-C3B-CAB-CBB
23	5	302	CHL	C11-C10-C8-C9
23	5	306	CHL	C2B-C3B-CAB-CBB
23	5	306	CHL	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	5	307	CHL	C2B-C3B-CAB-CBB
23	5	307	CHL	C4B-C3B-CAB-CBB
23	5	307	CHL	C1-C2-C3-C4
23	5	307	CHL	C1-C2-C3-C5
23	5	318	CHL	C2B-C3B-CAB-CBB
23	5	318	CHL	C4B-C3B-CAB-CBB
23	5	319	CHL	C1A-C2A-CAA-CBA
23	5	319	CHL	C3A-C2A-CAA-CBA
23	5	319	CHL	C1-C2-C3-C4
23	5	319	CHL	C4-C3-C5-C6
23	6	303	CHL	C1A-C2A-CAA-CBA
23	6	303	CHL	C3A-C2A-CAA-CBA
23	6	303	CHL	C2B-C3B-CAB-CBB
23	6	303	CHL	C4B-C3B-CAB-CBB
23	6	308	CHL	C4B-C3B-CAB-CBB
23	7	304	CHL	C2B-C3B-CAB-CBB
23	7	305	CHL	C1A-C2A-CAA-CBA
23	7	305	CHL	C2B-C3B-CAB-CBB
23	7	305	CHL	C4B-C3B-CAB-CBB
23	7	305	CHL	CAD-CBD-CGD-O1D
23	7	305	CHL	CAD-CBD-CGD-O2D
23	8	602	CHL	C1-C2-C3-C4
23	8	603	CHL	C3A-C2A-CAA-CBA
23	8	603	CHL	CBA-CGA-O2A-C1
23	8	603	CHL	O1A-CGA-O2A-C1
23	8	603	CHL	C2B-C3B-CAB-CBB
23	8	603	CHL	C4B-C3B-CAB-CBB
23	8	606	CHL	CHA-CBD-CGD-O1D
23	8	606	CHL	CHA-CBD-CGD-O2D
23	8	606	CHL	C2-C3-C5-C6
23	8	606	CHL	C4-C3-C5-C6
23	8	607	CHL	C2B-C3B-CAB-CBB
23	8	607	CHL	C4B-C3B-CAB-CBB
23	8	608	CHL	C2B-C3B-CAB-CBB
23	8	608	CHL	C4B-C3B-CAB-CBB
23	9	605	CHL	C2B-C3B-CAB-CBB
23	9	605	CHL	C4B-C3B-CAB-CBB
24	1	314	LUT	C1-C6-C7-C8
24	2	614	LUT	C5-C6-C7-C8
24	2	614	LUT	C7-C8-C9-C10
24	2	614	LUT	C7-C8-C9-C19
24	6	319	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	1	315	XAT	C7-C8-C9-C19
25	6	320	XAT	C7-C8-C9-C19
25	9	614	XAT	C7-C8-C9-C19
26	3	419	BCR	C7-C8-C9-C10
26	3	419	BCR	C7-C8-C9-C34
26	3	419	BCR	C23-C24-C25-C26
26	7	317	BCR	C7-C8-C9-C10
26	7	317	BCR	C7-C8-C9-C34
26	9	615	BCR	C7-C8-C9-C10
26	9	615	BCR	C7-C8-C9-C34
26	9	615	BCR	C21-C22-C23-C24
26	9	615	BCR	C37-C22-C23-C24
26	A	846	BCR	C7-C8-C9-C34
26	A	849	BCR	C7-C8-C9-C10
26	A	849	BCR	C7-C8-C9-C34
26	A	851	BCR	C7-C8-C9-C10
26	A	851	BCR	C7-C8-C9-C34
26	A	851	BCR	C19-C20-C21-C22
26	B	846	BCR	C7-C8-C9-C10
26	B	846	BCR	C7-C8-C9-C34
26	B	846	BCR	C11-C12-C13-C14
26	B	846	BCR	C11-C12-C13-C35
26	B	846	BCR	C37-C22-C23-C24
26	B	847	BCR	C5-C6-C7-C8
26	B	847	BCR	C7-C8-C9-C10
26	B	847	BCR	C7-C8-C9-C34
26	B	850	BCR	C7-C8-C9-C10
26	B	850	BCR	C7-C8-C9-C34
26	I	201	BCR	C21-C22-C23-C24
26	I	201	BCR	C37-C22-C23-C24
26	I	201	BCR	C23-C24-C25-C26
26	J	101	BCR	C7-C8-C9-C10
26	J	101	BCR	C7-C8-C9-C34
26	J	101	BCR	C11-C12-C13-C14
26	J	101	BCR	C11-C12-C13-C35
26	J	101	BCR	C21-C22-C23-C24
26	J	101	BCR	C37-C22-C23-C24
26	J	103	BCR	C7-C8-C9-C10
26	J	103	BCR	C7-C8-C9-C34
26	J	103	BCR	C37-C22-C23-C24
26	K	203	BCR	C21-C22-C23-C24
26	K	203	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	L	301	BCR	C23-C24-C25-C30
26	L	305	BCR	C7-C8-C9-C10
26	L	305	BCR	C7-C8-C9-C34
27	1	317	LHG	O2-C2-C3-O3
27	1	317	LHG	C3-O3-P-O4
27	1	318	LHG	C3-O3-P-O5
27	2	617	LHG	C4-O6-P-O4
27	5	301	LHG	C3-O3-P-O5
27	5	301	LHG	C4-O6-P-O5
27	5	325	LHG	C3-O3-P-O5
27	5	325	LHG	C4-O6-P-O3
27	5	325	LHG	C4-O6-P-O4
27	5	325	LHG	C4-O6-P-O5
27	6	322	LHG	C4-O6-P-O3
27	6	322	LHG	C4-O6-P-O5
27	8	620	LHG	C3-O3-P-O4
27	8	620	LHG	C3-O3-P-O5
27	8	620	LHG	O9-C7-O7-C5
27	8	620	LHG	C8-C7-O7-C5
27	A	844	LHG	C3-O3-P-O5
27	A	844	LHG	C4-O6-P-O5
27	A	845	LHG	O1-C1-C2-C3
27	A	845	LHG	C4-O6-P-O4
27	M	101	LHG	C4-O6-P-O3
28	1	319	LMU	O5'-C1'-O1'-C1
28	3	420	LMU	C2'-C1'-O1'-C1
28	3	420	LMU	O5'-C1'-O1'-C1
28	3	421	LMU	C2-C1-O1'-C1'
28	3	423	LMU	C2'-C1'-O1'-C1
28	3	423	LMU	O5'-C1'-O1'-C1
28	6	301	LMU	C2'-C1'-O1'-C1
28	6	301	LMU	O5'-C1'-O1'-C1
28	6	301	LMU	C2-C1-O1'-C1'
28	9	618	LMU	C2'-C1'-O1'-C1
28	A	853	LMU	C2'-C1'-O1'-C1
28	A	853	LMU	O5'-C1'-O1'-C1
28	F	806	LMU	O5B-C1B-O1B-C4'
28	G	201	LMU	C2'-C1'-O1'-C1
28	G	201	LMU	O5'-C1'-O1'-C1
28	G	201	LMU	C2-C1-O1'-C1'
28	H	204	LMU	C2'-C1'-O1'-C1
28	H	204	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
28	J	106	LMU	O5'-C1'-O1'-C1
31	8	621	LMG	O1-C7-C8-C9
31	9	617	LMG	O1-C7-C8-O7
34	B	852	DGD	O6D-C1D-O3G-C3G
28	3	421	LMU	C3'-C4'-O1B-C1B
22	5	317	CLA	O1D-CGD-O2D-CED
22	A	801	CLA	O1D-CGD-O2D-CED
22	A	815	CLA	O1D-CGD-O2D-CED
22	B	838	CLA	O1D-CGD-O2D-CED
22	G	203	CLA	O1D-CGD-O2D-CED
22	L	302	CLA	O1D-CGD-O2D-CED
22	1	313	CLA	O1D-CGD-O2D-CED
22	2	613	CLA	O1D-CGD-O2D-CED
22	6	307	CLA	O1D-CGD-O2D-CED
22	9	609	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	O1D-CGD-O2D-CED
22	B	805	CLA	O1D-CGD-O2D-CED
22	F	802	CLA	O1D-CGD-O2D-CED
22	1	303	CLA	CBD-CGD-O2D-CED
22	1	313	CLA	CBD-CGD-O2D-CED
22	2	602	CLA	CBD-CGD-O2D-CED
22	2	608	CLA	CBD-CGD-O2D-CED
22	2	613	CLA	CBD-CGD-O2D-CED
22	3	402	CLA	CBD-CGD-O2D-CED
22	3	404	CLA	CBD-CGD-O2D-CED
22	3	408	CLA	CBD-CGD-O2D-CED
22	5	317	CLA	CBD-CGD-O2D-CED
22	6	304	CLA	CBD-CGD-O2D-CED
22	6	311	CLA	CBD-CGD-O2D-CED
22	6	312	CLA	CBD-CGD-O2D-CED
22	6	315	CLA	CBD-CGD-O2D-CED
22	7	306	CLA	CBD-CGD-O2D-CED
22	8	604	CLA	CBD-CGD-O2D-CED
22	8	615	CLA	CBD-CGD-O2D-CED
22	8	616	CLA	CBD-CGD-O2D-CED
22	9	609	CLA	CBD-CGD-O2D-CED
22	9	611	CLA	CBD-CGD-O2D-CED
22	A	810	CLA	CBD-CGD-O2D-CED
22	A	815	CLA	CBD-CGD-O2D-CED
22	A	816	CLA	CBD-CGD-O2D-CED
22	A	823	CLA	CBD-CGD-O2D-CED
22	A	827	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	833	CLA	CBD-CGD-O2D-CED
22	B	813	CLA	CBD-CGD-O2D-CED
22	B	819	CLA	CBD-CGD-O2D-CED
22	B	830	CLA	CBD-CGD-O2D-CED
22	B	832	CLA	CBD-CGD-O2D-CED
22	B	842	CLA	CBD-CGD-O2D-CED
22	B	844	CLA	CBD-CGD-O2D-CED
22	F	802	CLA	CBD-CGD-O2D-CED
22	F	803	CLA	CBD-CGD-O2D-CED
22	J	102	CLA	CBD-CGD-O2D-CED
22	K	205	CLA	CBD-CGD-O2D-CED
22	1	312	CLA	O1A-CGA-O2A-C1
28	6	323	LMU	O5B-C1B-O1B-C4'
22	3	402	CLA	O1D-CGD-O2D-CED
22	3	404	CLA	O1D-CGD-O2D-CED
22	7	306	CLA	O1D-CGD-O2D-CED
22	A	821	CLA	O1D-CGD-O2D-CED
22	A	823	CLA	O1D-CGD-O2D-CED
22	A	827	CLA	O1D-CGD-O2D-CED
28	7	319	LMU	O5B-C1B-O1B-C4'
28	A	853	LMU	O5B-C1B-O1B-C4'
22	8	615	CLA	O1D-CGD-O2D-CED
22	8	616	CLA	O1D-CGD-O2D-CED
22	A	813	CLA	O1D-CGD-O2D-CED
22	A	822	CLA	O1D-CGD-O2D-CED
22	B	802	CLA	O1D-CGD-O2D-CED
22	B	804	CLA	O1D-CGD-O2D-CED
22	B	806	CLA	O1D-CGD-O2D-CED
22	B	843	CLA	O1D-CGD-O2D-CED
22	1	312	CLA	CBA-CGA-O2A-C1
22	2	601	CLA	CBD-CGD-O2D-CED
22	2	609	CLA	CBD-CGD-O2D-CED
22	3	401	CLA	CBD-CGD-O2D-CED
22	3	410	CLA	CBD-CGD-O2D-CED
22	5	305	CLA	CBD-CGD-O2D-CED
22	5	315	CLA	CBD-CGD-O2D-CED
22	6	305	CLA	CBD-CGD-O2D-CED
22	6	318	CLA	CBD-CGD-O2D-CED
22	7	310	CLA	CBD-CGD-O2D-CED
22	9	608	CLA	CBD-CGD-O2D-CED
22	A	808	CLA	CBD-CGD-O2D-CED
22	A	826	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	815	CLA	CBD-CGD-O2D-CED
22	B	817	CLA	CBD-CGD-O2D-CED
22	B	826	CLA	CBD-CGD-O2D-CED
22	G	202	CLA	CBD-CGD-O2D-CED
22	7	307	CLA	O1A-CGA-O2A-C1
22	8	601	CLA	O1A-CGA-O2A-C1
22	A	805	CLA	O1A-CGA-O2A-C1
22	A	807	CLA	O1A-CGA-O2A-C1
22	A	814	CLA	O1A-CGA-O2A-C1
22	A	837	CLA	O1A-CGA-O2A-C1
22	B	810	CLA	O1A-CGA-O2A-C1
22	B	844	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	O1A-CGA-O2A-C1
22	9	610	CLA	O1D-CGD-O2D-CED
22	B	818	CLA	O1D-CGD-O2D-CED
22	K	202	CLA	O1D-CGD-O2D-CED
22	1	302	CLA	O1D-CGD-O2D-CED
22	A	832	CLA	O1D-CGD-O2D-CED
22	A	836	CLA	O1D-CGD-O2D-CED
22	B	812	CLA	O1D-CGD-O2D-CED
22	B	816	CLA	O1D-CGD-O2D-CED
22	1	301	CLA	CBD-CGD-O2D-CED
22	6	309	CLA	CBD-CGD-O2D-CED
22	7	313	CLA	CBD-CGD-O2D-CED
22	8	605	CLA	CBD-CGD-O2D-CED
22	A	829	CLA	CBD-CGD-O2D-CED
22	2	608	CLA	O1D-CGD-O2D-CED
22	1	301	CLA	C3-C5-C6-C7
22	3	409	CLA	C3-C5-C6-C7
22	7	307	CLA	C3-C5-C6-C7
22	A	834	CLA	C3-C5-C6-C7
22	B	812	CLA	C3-C5-C6-C7
22	B	823	CLA	C3-C5-C6-C7
23	3	422	CHL	C3-C5-C6-C7
23	7	305	CHL	C3-C5-C6-C7
23	8	603	CHL	C3-C5-C6-C7
22	7	307	CLA	CBA-CGA-O2A-C1
22	8	601	CLA	CBA-CGA-O2A-C1
22	A	805	CLA	CBA-CGA-O2A-C1
22	A	807	CLA	CBA-CGA-O2A-C1
22	A	809	CLA	CBA-CGA-O2A-C1
22	A	837	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	810	CLA	CBA-CGA-O2A-C1
22	3	408	CLA	O1D-CGD-O2D-CED
22	9	606	CLA	CBD-CGD-O2D-CED
22	A	830	CLA	CBD-CGD-O2D-CED
22	F	804	CLA	CBD-CGD-O2D-CED
22	9	609	CLA	C2C-C3C-CAC-CBC
22	8	616	CLA	O1A-CGA-O2A-C1
28	9	618	LMU	C3'-C4'-O1B-C1B
28	3	420	LMU	O5'-C5'-C6'-O6'
28	6	302	LMU	O5'-C5'-C6'-O6'
22	3	411	CLA	C2-C3-C5-C6
23	5	319	CHL	C2-C3-C5-C6
22	A	834	CLA	CBD-CGD-O2D-CED
22	2	602	CLA	C2A-CAA-CBA-CGA
22	5	305	CLA	C2A-CAA-CBA-CGA
22	8	615	CLA	C2A-CAA-CBA-CGA
22	A	803	CLA	C2A-CAA-CBA-CGA
22	A	805	CLA	C2A-CAA-CBA-CGA
22	A	807	CLA	C2A-CAA-CBA-CGA
22	A	827	CLA	C2A-CAA-CBA-CGA
22	A	839	CLA	C2A-CAA-CBA-CGA
22	A	841	CLA	C2A-CAA-CBA-CGA
22	B	803	CLA	C2A-CAA-CBA-CGA
22	B	820	CLA	C2A-CAA-CBA-CGA
22	B	827	CLA	C2A-CAA-CBA-CGA
22	B	830	CLA	C2A-CAA-CBA-CGA
22	B	842	CLA	C2A-CAA-CBA-CGA
22	G	202	CLA	C2A-CAA-CBA-CGA
22	L	303	CLA	C2A-CAA-CBA-CGA
23	1	306	CHL	C2A-CAA-CBA-CGA
23	7	305	CHL	C2A-CAA-CBA-CGA
22	9	609	CLA	O1A-CGA-O2A-C1
22	1	312	CLA	C3-C5-C6-C7
22	5	314	CLA	C3-C5-C6-C7
22	9	609	CLA	C3-C5-C6-C7
22	A	809	CLA	C3-C5-C6-C7
22	A	838	CLA	C3-C5-C6-C7
22	B	802	CLA	C3-C5-C6-C7
22	B	804	CLA	C3-C5-C6-C7
22	B	816	CLA	C3-C5-C6-C7
22	B	836	CLA	C3-C5-C6-C7
22	2	602	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	9	603	CLA	CBA-CGA-O2A-C1
22	9	609	CLA	CBA-CGA-O2A-C1
22	A	814	CLA	CBA-CGA-O2A-C1
22	A	839	CLA	CBA-CGA-O2A-C1
22	B	816	CLA	CBA-CGA-O2A-C1
22	B	820	CLA	CBA-CGA-O2A-C1
22	B	844	CLA	CBA-CGA-O2A-C1
22	2	602	CLA	O1D-CGD-O2D-CED
22	J	102	CLA	O1D-CGD-O2D-CED
23	5	319	CHL	C1-C2-C3-C5
22	A	840	CLA	CBD-CGD-O2D-CED
22	K	206	CLA	CBD-CGD-O2D-CED
22	1	303	CLA	O1D-CGD-O2D-CED
22	8	604	CLA	O1D-CGD-O2D-CED
22	B	819	CLA	O1D-CGD-O2D-CED
22	F	803	CLA	O1D-CGD-O2D-CED
22	1	301	CLA	O1A-CGA-O2A-C1
22	9	602	CLA	O1A-CGA-O2A-C1
22	9	603	CLA	O1A-CGA-O2A-C1
22	A	809	CLA	O1A-CGA-O2A-C1
22	A	813	CLA	O1A-CGA-O2A-C1
22	A	832	CLA	O1A-CGA-O2A-C1
22	B	808	CLA	O1A-CGA-O2A-C1
22	B	816	CLA	O1A-CGA-O2A-C1
28	6	302	LMU	O5B-C5B-C6B-O6B
28	J	106	LMU	O5'-C5'-C6'-O6'
28	K	201	LMU	O5'-C5'-C6'-O6'
22	1	311	CLA	CBD-CGD-O2D-CED
22	6	310	CLA	CBD-CGD-O2D-CED
22	7	312	CLA	CBD-CGD-O2D-CED
22	8	613	CLA	CBD-CGD-O2D-CED
22	A	807	CLA	CBD-CGD-O2D-CED
22	A	814	CLA	CBD-CGD-O2D-CED
22	A	835	CLA	CBD-CGD-O2D-CED
22	B	821	CLA	CBD-CGD-O2D-CED
22	B	822	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	CBD-CGD-O2D-CED
22	B	833	CLA	CBD-CGD-O2D-CED
22	B	836	CLA	CBD-CGD-O2D-CED
22	B	840	CLA	CBD-CGD-O2D-CED
22	H	203	CLA	CBD-CGD-O2D-CED
22	A	833	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	813	CLA	O1D-CGD-O2D-CED
22	2	601	CLA	C3-C5-C6-C7
22	6	314	CLA	C3-C5-C6-C7
22	6	318	CLA	C3-C5-C6-C7
22	A	816	CLA	C3-C5-C6-C7
22	B	805	CLA	C3-C5-C6-C7
22	1	301	CLA	CBA-CGA-O2A-C1
22	8	616	CLA	CBA-CGA-O2A-C1
22	9	602	CLA	CBA-CGA-O2A-C1
22	A	810	CLA	CBA-CGA-O2A-C1
22	A	813	CLA	CBA-CGA-O2A-C1
22	A	818	CLA	CBA-CGA-O2A-C1
22	2	602	CLA	O1A-CGA-O2A-C1
28	J	106	LMU	O5B-C5B-C6B-O6B
22	B	842	CLA	O1D-CGD-O2D-CED
22	K	205	CLA	O1D-CGD-O2D-CED
22	9	602	CLA	CBD-CGD-O2D-CED
22	9	603	CLA	CBD-CGD-O2D-CED
22	A	811	CLA	CBD-CGD-O2D-CED
28	A	853	LMU	O5'-C5'-C6'-O6'
22	9	611	CLA	O1D-CGD-O2D-CED
22	A	818	CLA	O1A-CGA-O2A-C1
28	1	319	LMU	O5B-C5B-C6B-O6B
22	6	315	CLA	O1D-CGD-O2D-CED
22	A	816	CLA	O1D-CGD-O2D-CED
28	J	106	LMU	C5'-C4'-O1B-C1B
22	A	817	CLA	CBD-CGD-O2D-CED
22	8	613	CLA	C3-C5-C6-C7
22	F	802	CLA	C3-C5-C6-C7
22	A	832	CLA	CBA-CGA-O2A-C1
22	B	808	CLA	CBA-CGA-O2A-C1
22	B	832	CLA	O1D-CGD-O2D-CED
22	A	839	CLA	O1A-CGA-O2A-C1
22	B	820	CLA	O1A-CGA-O2A-C1
28	3	420	LMU	O5B-C1B-O1B-C4'
22	A	816	CLA	C4-C3-C5-C6
23	5	302	CHL	C4-C3-C5-C6
22	A	816	CLA	C2-C3-C5-C6
22	B	804	CLA	C2-C3-C5-C6
23	5	302	CHL	C2-C3-C5-C6
22	5	316	CLA	C2A-CAA-CBA-CGA
22	A	802	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	804	CLA	C2A-CAA-CBA-CGA
23	5	319	CHL	C2A-CAA-CBA-CGA
22	B	844	CLA	O1D-CGD-O2D-CED
28	9	618	LMU	O5B-C5B-C6B-O6B
28	A	852	LMU	O5B-C5B-C6B-O6B
22	9	606	CLA	CBA-CGA-O2A-C1
28	J	106	LMU	C4'-C5'-C6'-O6'
22	6	304	CLA	O1D-CGD-O2D-CED
22	6	311	CLA	O1D-CGD-O2D-CED
22	6	312	CLA	O1D-CGD-O2D-CED
22	B	815	CLA	O1D-CGD-O2D-CED
22	B	830	CLA	O1D-CGD-O2D-CED
22	A	810	CLA	O1A-CGA-O2A-C1
22	3	401	CLA	O1D-CGD-O2D-CED
22	6	305	CLA	O1D-CGD-O2D-CED
22	6	318	CLA	O1D-CGD-O2D-CED
22	7	310	CLA	O1D-CGD-O2D-CED
22	9	608	CLA	O1D-CGD-O2D-CED
22	A	826	CLA	O1D-CGD-O2D-CED
22	B	826	CLA	O1D-CGD-O2D-CED
22	3	410	CLA	O1D-CGD-O2D-CED
27	1	317	LHG	C1-C2-C3-O3
27	2	617	LHG	C1-C2-C3-O3
22	1	308	CLA	CBA-CGA-O2A-C1
22	2	612	CLA	CBA-CGA-O2A-C1
22	3	404	CLA	CBA-CGA-O2A-C1
22	6	307	CLA	CBA-CGA-O2A-C1
22	6	311	CLA	CBA-CGA-O2A-C1
22	6	314	CLA	CBA-CGA-O2A-C1
22	7	311	CLA	CBA-CGA-O2A-C1
22	9	608	CLA	CBA-CGA-O2A-C1
22	A	811	CLA	CBA-CGA-O2A-C1
22	A	827	CLA	CBA-CGA-O2A-C1
22	A	828	CLA	CBA-CGA-O2A-C1
22	B	809	CLA	CBA-CGA-O2A-C1
22	B	835	CLA	CBA-CGA-O2A-C1
22	G	202	CLA	CBA-CGA-O2A-C1
22	L	302	CLA	CBA-CGA-O2A-C1
22	L	303	CLA	CBA-CGA-O2A-C1
22	B	807	CLA	CBD-CGD-O2D-CED
22	B	835	CLA	CBD-CGD-O2D-CED
28	3	420	LMU	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
28	6	302	LMU	C4'-C5'-C6'-O6'
22	A	812	CLA	C15-C16-C17-C18
23	7	305	CHL	C10-C11-C12-C13
22	5	314	CLA	C2A-CAA-CBA-CGA
22	B	813	CLA	C2A-CAA-CBA-CGA
28	A	852	LMU	C4B-C5B-C6B-O6B
28	1	319	LMU	C4B-C5B-C6B-O6B
22	1	301	CLA	C5-C6-C7-C8
22	A	809	CLA	C5-C6-C7-C8
22	A	812	CLA	C8-C10-C11-C12
23	6	303	CHL	C10-C11-C12-C13
23	8	606	CHL	C10-C11-C12-C13
27	7	318	LHG	O2-C2-C3-O3
28	J	106	LMU	C2'-C1'-O1'-C1
22	7	311	CLA	O1A-CGA-O2A-C1
22	3	408	CLA	C4-C3-C5-C6
22	1	308	CLA	C6-C7-C8-C9
22	2	612	CLA	C11-C10-C8-C9
22	6	307	CLA	C14-C13-C15-C16
23	3	406	CHL	C14-C13-C15-C16
23	3	413	CHL	C11-C10-C8-C9
23	5	307	CHL	C6-C7-C8-C9
23	5	308	CHL	C11-C10-C8-C9
23	7	305	CHL	C6-C7-C8-C9
23	7	305	CHL	C14-C13-C15-C16
23	8	606	CHL	C11-C10-C8-C9
23	8	606	CHL	C14-C13-C15-C16
22	9	602	CLA	C2A-CAA-CBA-CGA
22	F	802	CLA	C2A-CAA-CBA-CGA
23	9	605	CHL	C2A-CAA-CBA-CGA
24	2	614	LUT	C27-C28-C29-C39
24	6	319	LUT	C11-C12-C13-C20
24	9	613	LUT	C7-C8-C9-C19
26	B	847	BCR	C37-C22-C23-C24
30	6	321	NEX	C27-C28-C29-C39
24	2	614	LUT	C27-C28-C29-C30
26	B	847	BCR	C21-C22-C23-C24
27	1	317	LHG	C23-C24-C25-C26
27	A	845	LHG	C23-C24-C25-C26
22	2	612	CLA	O1A-CGA-O2A-C1
22	6	307	CLA	O1A-CGA-O2A-C1
22	6	314	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	9	608	CLA	O1A-CGA-O2A-C1
22	A	828	CLA	O1A-CGA-O2A-C1
22	L	303	CLA	O1A-CGA-O2A-C1
22	3	404	CLA	C8-C10-C11-C12
22	8	613	CLA	C15-C16-C17-C18
22	B	830	CLA	C8-C10-C11-C12
23	3	406	CHL	C13-C15-C16-C17
23	5	307	CHL	C8-C10-C11-C12
23	8	602	CHL	C13-C15-C16-C17
22	A	808	CLA	O1D-CGD-O2D-CED
22	B	817	CLA	O1D-CGD-O2D-CED
22	2	609	CLA	O1D-CGD-O2D-CED
22	A	836	CLA	CBA-CGA-O2A-C1
31	9	617	LMG	C29-C28-O8-C9
22	1	308	CLA	C10-C11-C12-C13
22	5	314	CLA	C8-C10-C11-C12
22	6	316	CLA	C15-C16-C17-C18
22	A	804	CLA	C8-C10-C11-C12
22	B	816	CLA	C5-C6-C7-C8
22	B	821	CLA	C5-C6-C7-C8
22	B	844	CLA	C8-C10-C11-C12
28	J	106	LMU	C3'-C4'-O1B-C1B
22	3	407	CLA	C8-C10-C11-C12
22	3	408	CLA	C10-C11-C12-C13
22	5	311	CLA	C5-C6-C7-C8
22	7	301	CLA	C15-C16-C17-C18
22	9	609	CLA	C5-C6-C7-C8
22	A	822	CLA	C13-C15-C16-C17
22	B	802	CLA	C5-C6-C7-C8
22	B	816	CLA	C8-C10-C11-C12
22	B	840	CLA	C5-C6-C7-C8
23	6	303	CHL	C15-C16-C17-C18
28	9	618	LMU	C4B-C5B-C6B-O6B
22	B	835	CLA	O1A-CGA-O2A-C1
22	A	819	CLA	CBD-CGD-O2D-CED
22	5	314	CLA	C10-C11-C12-C13
22	A	805	CLA	C15-C16-C17-C18
22	A	823	CLA	C13-C15-C16-C17
22	B	816	CLA	C10-C11-C12-C13
22	B	830	CLA	C10-C11-C12-C13
22	A	802	CLA	C3-C5-C6-C7
22	A	816	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	9	609	CLA	C4C-C3C-CAC-CBC
22	6	318	CLA	C8-C10-C11-C12
22	A	823	CLA	C15-C16-C17-C18
22	B	808	CLA	C15-C16-C17-C18
22	B	809	CLA	C5-C6-C7-C8
32	A	842	PQN	C25-C26-C27-C28
22	2	601	CLA	O1D-CGD-O2D-CED
22	B	810	CLA	CBD-CGD-O2D-CED
28	H	204	LMU	O5B-C1B-O1B-C4'
22	B	833	CLA	C2A-CAA-CBA-CGA
22	8	613	CLA	C13-C15-C16-C17
22	B	806	CLA	C5-C6-C7-C8
22	F	802	CLA	C8-C10-C11-C12
22	1	312	CLA	C11-C12-C13-C15
22	8	614	CLA	C11-C10-C8-C7
22	A	804	CLA	C11-C10-C8-C7
22	A	820	CLA	C11-C10-C8-C7
22	A	826	CLA	C12-C13-C15-C16
22	A	838	CLA	C11-C10-C8-C7
22	B	805	CLA	C6-C7-C8-C10
23	8	602	CHL	C11-C10-C8-C7
22	A	827	CLA	O1A-CGA-O2A-C1
22	G	202	CLA	O1A-CGA-O2A-C1
22	L	302	CLA	O1A-CGA-O2A-C1
28	J	106	LMU	O1'-C1-C2-C3
24	2	614	LUT	C9-C10-C11-C12
22	1	308	CLA	C2A-CAA-CBA-CGA
22	6	318	CLA	C2A-CAA-CBA-CGA
22	A	835	CLA	C2A-CAA-CBA-CGA
23	1	304	CHL	C2A-CAA-CBA-CGA
23	3	406	CHL	C2A-CAA-CBA-CGA
23	3	422	CHL	C2A-CAA-CBA-CGA
22	1	301	CLA	O1D-CGD-O2D-CED
22	5	305	CLA	O1D-CGD-O2D-CED
22	5	315	CLA	O1D-CGD-O2D-CED
22	7	313	CLA	O1D-CGD-O2D-CED
22	8	605	CLA	O1D-CGD-O2D-CED
22	A	829	CLA	O1D-CGD-O2D-CED
22	G	202	CLA	O1D-CGD-O2D-CED
22	1	311	CLA	C5-C6-C7-C8
22	9	603	CLA	C5-C6-C7-C8
22	A	822	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	1	308	CLA	O1A-CGA-O2A-C1
22	3	404	CLA	O1A-CGA-O2A-C1
22	B	809	CLA	O1A-CGA-O2A-C1
22	9	607	CLA	CBD-CGD-O2D-CED
22	B	820	CLA	CBD-CGD-O2D-CED
28	9	618	LMU	O5'-C1'-O1'-C1
22	A	832	CLA	C13-C15-C16-C17
22	B	803	CLA	C13-C15-C16-C17
23	3	422	CHL	C13-C15-C16-C17
28	G	201	LMU	O1'-C1-C2-C3
31	8	621	LMG	C10-C11-C12-C13
22	6	309	CLA	O1D-CGD-O2D-CED
22	3	402	CLA	C15-C16-C17-C18
23	7	305	CHL	C15-C16-C17-C18
23	8	606	CHL	C5-C6-C7-C8
22	6	311	CLA	O1A-CGA-O2A-C1
22	9	606	CLA	O1A-CGA-O2A-C1
22	A	811	CLA	O1A-CGA-O2A-C1
31	J	104	LMG	C28-C29-C30-C31
28	6	302	LMU	C4B-C5B-C6B-O6B
22	2	612	CLA	C5-C6-C7-C8
22	A	802	CLA	C15-C16-C17-C18
22	B	805	CLA	C5-C6-C7-C8
22	B	811	CLA	C10-C11-C12-C13
23	5	302	CHL	C8-C10-C11-C12
23	8	602	CHL	C15-C16-C17-C18
28	A	853	LMU	C4'-C5'-C6'-O6'
28	J	106	LMU	C4B-C5B-C6B-O6B
22	A	836	CLA	O1A-CGA-O2A-C1
28	6	301	LMU	C2B-C1B-O1B-C4'
22	3	408	CLA	C13-C15-C16-C17
22	6	318	CLA	C10-C11-C12-C13
22	6	318	CLA	C13-C15-C16-C17
22	B	836	CLA	C5-C6-C7-C8
23	3	422	CHL	C15-C16-C17-C18
27	1	318	LHG	C4-O6-P-O3
27	2	617	LHG	C3-O3-P-O6
27	6	322	LHG	C3-O3-P-O6
27	8	620	LHG	C3-O3-P-O6
27	8	620	LHG	C4-O6-P-O3
27	B	801	LHG	C4-O6-P-O3
22	6	304	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	6	303	CHL	C3-C5-C6-C7
22	5	304	CLA	CBA-CGA-O2A-C1
22	K	204	CLA	C5-C6-C7-C8
23	3	406	CHL	C8-C10-C11-C12
22	A	816	CLA	O1A-CGA-O2A-C1
22	A	834	CLA	O1D-CGD-O2D-CED
27	A	844	LHG	C23-C24-C25-C26
22	A	830	CLA	O1D-CGD-O2D-CED
22	F	804	CLA	O1D-CGD-O2D-CED
28	A	852	LMU	O5'-C5'-C6'-O6'
31	9	617	LMG	O9-C10-O7-C8
22	B	836	CLA	C4-C3-C5-C6
22	6	316	CLA	C10-C11-C12-C13
22	A	841	CLA	C15-C16-C17-C18
22	B	844	CLA	C10-C11-C12-C13
22	9	606	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	C2A-CAA-CBA-CGA
22	A	817	CLA	C2A-CAA-CBA-CGA
22	B	809	CLA	C2A-CAA-CBA-CGA
22	B	811	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	C11-C12-C13-C15
23	5	308	CHL	C16-C17-C18-C19
22	A	839	CLA	C3-C5-C6-C7
22	B	806	CLA	C3-C5-C6-C7
22	3	403	CLA	CBA-CGA-O2A-C1
22	3	408	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	CBA-CGA-O2A-C1
22	8	610	CLA	CBA-CGA-O2A-C1
22	B	840	CLA	CBA-CGA-O2A-C1
27	8	620	LHG	C10-C11-C12-C13
27	5	301	LHG	C8-C7-O7-C5
31	9	617	LMG	C11-C10-O7-C8
23	5	307	CHL	C10-C11-C12-C13
22	3	411	CLA	C2A-CAA-CBA-CGA
22	B	819	CLA	C2A-CAA-CBA-CGA
27	6	322	LHG	C11-C12-C13-C14
22	9	603	CLA	C6-C7-C8-C10
22	A	812	CLA	C16-C17-C18-C20
22	A	832	CLA	C16-C17-C18-C19
28	6	301	LMU	C5-C6-C7-C8
27	5	301	LHG	O9-C7-O7-C5
27	8	620	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	A	845	LHG	C11-C12-C13-C14
22	B	836	CLA	O1D-CGD-O2D-CED
22	K	206	CLA	O1D-CGD-O2D-CED
28	6	302	LMU	C4-C5-C6-C7
28	6	323	LMU	C4-C5-C6-C7
28	H	204	LMU	C7-C8-C9-C10
22	A	840	CLA	O1D-CGD-O2D-CED
23	8	603	CHL	C5-C6-C7-C8
27	2	617	LHG	O2-C2-C3-O3
22	A	824	CLA	CAA-CBA-CGA-O2A
27	A	845	LHG	C16-C17-C18-C19
28	7	319	LMU	C5-C6-C7-C8
22	6	316	CLA	C3-C5-C6-C7
22	B	813	CLA	C3-C5-C6-C7
34	B	852	DGD	C2D-C1D-O3G-C3G
22	2	601	CLA	CBA-CGA-O2A-C1
22	A	822	CLA	CBA-CGA-O2A-C1
22	A	823	CLA	CBA-CGA-O2A-C1
22	B	842	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CAA-CBA-CGA-O2A
27	1	317	LHG	C32-C33-C34-C35
27	A	845	LHG	C29-C30-C31-C32
28	J	106	LMU	C4-C5-C6-C7
23	5	308	CHL	C15-C16-C17-C18
22	5	304	CLA	O1A-CGA-O2A-C1
22	3	411	CLA	C6-C7-C8-C10
22	6	314	CLA	C16-C17-C18-C20
22	A	816	CLA	C11-C12-C13-C14
22	B	836	CLA	C6-C7-C8-C9
22	7	312	CLA	O1D-CGD-O2D-CED
22	B	821	CLA	O1D-CGD-O2D-CED
22	B	840	CLA	O1D-CGD-O2D-CED
22	3	409	CLA	C4-C3-C5-C6
27	A	845	LHG	C30-C31-C32-C33
22	3	407	CLA	C14-C13-C15-C16
22	6	318	CLA	C11-C10-C8-C9
22	6	318	CLA	C14-C13-C15-C16
22	A	823	CLA	C6-C7-C8-C9
22	B	830	CLA	C6-C7-C8-C9
23	7	305	CHL	C11-C12-C13-C14
23	8	602	CHL	C11-C10-C8-C9
22	A	814	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	3	407	CLA	C5-C6-C7-C8
22	A	816	CLA	C10-C11-C12-C13
22	5	310	CLA	C2A-CAA-CBA-CGA
22	A	811	CLA	C2A-CAA-CBA-CGA
22	B	814	CLA	C2A-CAA-CBA-CGA
22	B	829	CLA	C2A-CAA-CBA-CGA
31	9	617	LMG	O10-C28-O8-C9
26	J	103	BCR	C21-C22-C23-C24
23	5	307	CHL	C3-C5-C6-C7
27	6	322	LHG	C29-C30-C31-C32
27	B	801	LHG	C11-C10-C9-C8
22	8	613	CLA	O1D-CGD-O2D-CED
22	A	807	CLA	O1D-CGD-O2D-CED
27	7	318	LHG	C11-C10-C9-C8
27	B	801	LHG	C24-C25-C26-C27
28	H	204	LMU	C3-C4-C5-C6
28	K	201	LMU	C6-C7-C8-C9
28	H	204	LMU	O5'-C5'-C6'-O6'
22	1	308	CLA	C4B-C3B-CAB-CBB
22	1	312	CLA	C4B-C3B-CAB-CBB
22	2	606	CLA	C4B-C3B-CAB-CBB
22	2	608	CLA	C4B-C3B-CAB-CBB
22	2	610	CLA	C4B-C3B-CAB-CBB
22	5	310	CLA	C4B-C3B-CAB-CBB
22	6	316	CLA	C4B-C3B-CAB-CBB
22	6	317	CLA	C4B-C3B-CAB-CBB
22	7	306	CLA	C4B-C3B-CAB-CBB
22	9	603	CLA	C4B-C3B-CAB-CBB
22	A	805	CLA	C4B-C3B-CAB-CBB
22	A	820	CLA	C4B-C3B-CAB-CBB
22	A	823	CLA	C4B-C3B-CAB-CBB
22	A	828	CLA	C4B-C3B-CAB-CBB
22	A	830	CLA	C4B-C3B-CAB-CBB
22	A	832	CLA	C4B-C3B-CAB-CBB
22	A	833	CLA	C4B-C3B-CAB-CBB
22	A	835	CLA	C4B-C3B-CAB-CBB
22	A	839	CLA	C4B-C3B-CAB-CBB
22	A	843	CLA	C4B-C3B-CAB-CBB
22	B	810	CLA	C4B-C3B-CAB-CBB
22	B	820	CLA	C4B-C3B-CAB-CBB
22	B	823	CLA	C4B-C3B-CAB-CBB
22	B	824	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	826	CLA	C4B-C3B-CAB-CBB
22	B	836	CLA	C4B-C3B-CAB-CBB
22	B	838	CLA	C4B-C3B-CAB-CBB
22	B	839	CLA	C4B-C3B-CAB-CBB
22	B	840	CLA	C4B-C3B-CAB-CBB
22	B	844	CLA	C4B-C3B-CAB-CBB
22	G	202	CLA	C4B-C3B-CAB-CBB
22	J	102	CLA	C4B-C3B-CAB-CBB
22	K	206	CLA	C4B-C3B-CAB-CBB
22	L	304	CLA	C4B-C3B-CAB-CBB
23	5	302	CHL	C4B-C3B-CAB-CBB
23	5	309	CHL	C4B-C3B-CAB-CBB
23	7	304	CHL	C4B-C3B-CAB-CBB
22	7	301	CLA	C16-C17-C18-C19
22	A	812	CLA	C16-C17-C18-C19
22	A	823	CLA	C16-C17-C18-C20
22	B	814	CLA	C6-C7-C8-C9
22	B	814	CLA	C6-C7-C8-C10
22	B	819	CLA	C6-C7-C8-C9
22	B	832	CLA	C6-C7-C8-C9
23	3	406	CHL	C16-C17-C18-C19
23	3	422	CHL	C16-C17-C18-C19
22	3	404	CLA	C10-C11-C12-C13
22	8	614	CLA	C8-C10-C11-C12
27	6	322	LHG	C12-C13-C14-C15
28	6	301	LMU	C7-C8-C9-C10
28	6	302	LMU	O1'-C1-C2-C3
28	A	853	LMU	O1'-C1-C2-C3
28	K	201	LMU	C2-C3-C4-C5
22	6	310	CLA	O1D-CGD-O2D-CED
22	A	835	CLA	O1D-CGD-O2D-CED
22	B	822	CLA	O1D-CGD-O2D-CED
27	2	617	LHG	C27-C28-C29-C30
28	6	301	LMU	C2-C3-C4-C5
22	A	802	CLA	C13-C15-C16-C17
22	1	310	CLA	C3A-C2A-CAA-CBA
22	2	613	CLA	C3A-C2A-CAA-CBA
22	3	402	CLA	C3A-C2A-CAA-CBA
22	7	303	CLA	C3A-C2A-CAA-CBA
22	7	307	CLA	C3A-C2A-CAA-CBA
22	8	615	CLA	C3A-C2A-CAA-CBA
22	A	802	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	805	CLA	C3A-C2A-CAA-CBA
22	A	808	CLA	C3A-C2A-CAA-CBA
22	A	822	CLA	C3A-C2A-CAA-CBA
22	A	831	CLA	C3A-C2A-CAA-CBA
22	A	832	CLA	C3A-C2A-CAA-CBA
22	A	836	CLA	C3A-C2A-CAA-CBA
22	A	838	CLA	C3A-C2A-CAA-CBA
22	B	808	CLA	C3A-C2A-CAA-CBA
22	B	810	CLA	C3A-C2A-CAA-CBA
22	B	812	CLA	C3A-C2A-CAA-CBA
22	B	839	CLA	C3A-C2A-CAA-CBA
22	B	843	CLA	C3A-C2A-CAA-CBA
22	F	804	CLA	C3A-C2A-CAA-CBA
23	5	307	CHL	C3A-C2A-CAA-CBA
23	7	304	CHL	C3A-C2A-CAA-CBA
22	L	303	CLA	C8-C10-C11-C12
28	6	323	LMU	C2-C1-O1'-C1'
28	J	106	LMU	C2-C1-O1'-C1'
27	7	318	LHG	C10-C11-C12-C13
28	6	301	LMU	O1'-C1-C2-C3
22	B	833	CLA	O1D-CGD-O2D-CED
22	H	203	CLA	O1D-CGD-O2D-CED
28	K	201	LMU	C4'-C5'-C6'-O6'
22	3	411	CLA	C6-C7-C8-C9
22	6	314	CLA	C16-C17-C18-C19
22	7	301	CLA	C16-C17-C18-C20
22	B	819	CLA	C6-C7-C8-C10
22	B	832	CLA	C6-C7-C8-C10
22	K	204	CLA	C6-C7-C8-C10
28	7	319	LMU	C4-C5-C6-C7
28	H	204	LMU	C4-C5-C6-C7
23	5	306	CHL	C2A-CAA-CBA-CGA
27	M	101	LHG	C4-C5-C6-O8
22	A	841	CLA	CBD-CGD-O2D-CED
22	B	837	CLA	CBD-CGD-O2D-CED
22	1	311	CLA	O1D-CGD-O2D-CED
22	A	822	CLA	C3-C5-C6-C7
28	3	420	LMU	O1'-C1-C2-C3
28	3	423	LMU	C6-C7-C8-C9
28	G	201	LMU	C4-C5-C6-C7
22	A	832	CLA	C4-C3-C5-C6
22	1	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	3	408	CLA	C2-C3-C5-C6
22	A	832	CLA	C2-C3-C5-C6
22	B	817	CLA	C2-C3-C5-C6
31	J	105	LMG	C11-C10-O7-C8
22	B	825	CLA	O1D-CGD-O2D-CED
28	1	319	LMU	O5'-C5'-C6'-O6'
22	1	301	CLA	C2A-CAA-CBA-CGA
22	A	837	CLA	C2A-CAA-CBA-CGA
22	F	804	CLA	C2A-CAA-CBA-CGA
22	3	411	CLA	CAA-CBA-CGA-O2A
28	G	201	LMU	C7-C8-C9-C10
27	7	318	LHG	C23-C24-C25-C26
22	B	836	CLA	C6-C7-C8-C10
23	3	422	CHL	C16-C17-C18-C20
22	1	302	CLA	C2B-C3B-CAB-CBB
22	1	308	CLA	C2B-C3B-CAB-CBB
22	1	312	CLA	C2B-C3B-CAB-CBB
22	2	606	CLA	C2B-C3B-CAB-CBB
22	2	608	CLA	C2B-C3B-CAB-CBB
22	3	412	CLA	C2B-C3B-CAB-CBB
22	5	310	CLA	C2B-C3B-CAB-CBB
22	5	314	CLA	C2B-C3B-CAB-CBB
22	5	315	CLA	C2B-C3B-CAB-CBB
22	6	314	CLA	C2B-C3B-CAB-CBB
22	6	316	CLA	C2B-C3B-CAB-CBB
22	7	306	CLA	C2B-C3B-CAB-CBB
22	8	601	CLA	C2B-C3B-CAB-CBB
22	8	613	CLA	C2B-C3B-CAB-CBB
22	9	606	CLA	C2B-C3B-CAB-CBB
22	A	805	CLA	C2B-C3B-CAB-CBB
22	A	810	CLA	C2B-C3B-CAB-CBB
22	A	812	CLA	C2B-C3B-CAB-CBB
22	A	819	CLA	C2B-C3B-CAB-CBB
22	A	820	CLA	C2B-C3B-CAB-CBB
22	A	828	CLA	C2B-C3B-CAB-CBB
22	A	830	CLA	C2B-C3B-CAB-CBB
22	A	832	CLA	C2B-C3B-CAB-CBB
22	A	833	CLA	C2B-C3B-CAB-CBB
22	A	835	CLA	C2B-C3B-CAB-CBB
22	A	839	CLA	C2B-C3B-CAB-CBB
22	A	840	CLA	C2B-C3B-CAB-CBB
22	A	843	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	B	810	CLA	C2B-C3B-CAB-CBB
22	B	820	CLA	C2B-C3B-CAB-CBB
22	B	823	CLA	C2B-C3B-CAB-CBB
22	B	824	CLA	C2B-C3B-CAB-CBB
22	B	826	CLA	C2B-C3B-CAB-CBB
22	B	836	CLA	C2B-C3B-CAB-CBB
22	B	838	CLA	C2B-C3B-CAB-CBB
22	B	840	CLA	C2B-C3B-CAB-CBB
22	B	844	CLA	C2B-C3B-CAB-CBB
22	G	202	CLA	C2B-C3B-CAB-CBB
22	H	203	CLA	C2B-C3B-CAB-CBB
22	J	102	CLA	C2B-C3B-CAB-CBB
22	K	205	CLA	C2B-C3B-CAB-CBB
22	K	206	CLA	C2B-C3B-CAB-CBB
22	L	304	CLA	C2B-C3B-CAB-CBB
23	5	302	CHL	C2B-C3B-CAB-CBB
23	5	309	CHL	C2B-C3B-CAB-CBB
23	6	308	CHL	C2B-C3B-CAB-CBB
28	1	319	LMU	C2B-C1B-O1B-C4'
22	3	408	CLA	O1A-CGA-O2A-C1
22	5	303	CLA	O1A-CGA-O2A-C1
22	8	610	CLA	O1A-CGA-O2A-C1
22	A	839	CLA	CBD-CGD-O2D-CED
31	J	105	LMG	O9-C10-O7-C8
22	1	312	CLA	C2-C1-O2A-CGA
34	B	852	DGD	C4E-C5E-C6E-O5E
27	9	616	LHG	C30-C31-C32-C33
28	A	853	LMU	C11-C10-C9-C8
22	A	801	CLA	C8-C10-C11-C12
22	A	838	CLA	C5-C6-C7-C8
22	2	601	CLA	O1A-CGA-O2A-C1
22	3	403	CLA	O1A-CGA-O2A-C1
22	B	840	CLA	O1A-CGA-O2A-C1
28	H	204	LMU	C4B-C5B-C6B-O6B
28	J	106	LMU	C2-C3-C4-C5
31	J	105	LMG	C13-C14-C15-C16
24	1	314	LUT	C5-C6-C7-C8
24	2	614	LUT	C1-C6-C7-C8
24	6	319	LUT	C5-C6-C7-C8
24	7	315	LUT	C1-C6-C7-C8
24	7	315	LUT	C5-C6-C7-C8
24	8	617	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	8	617	LUT	C5-C6-C7-C8
26	1	316	BCR	C1-C6-C7-C8
26	1	316	BCR	C5-C6-C7-C8
26	3	419	BCR	C23-C24-C25-C30
26	A	851	BCR	C23-C24-C25-C26
26	A	851	BCR	C23-C24-C25-C30
26	B	847	BCR	C1-C6-C7-C8
26	B	847	BCR	C23-C24-C25-C26
26	B	847	BCR	C23-C24-C25-C30
26	I	201	BCR	C23-C24-C25-C30
26	J	103	BCR	C1-C6-C7-C8
26	J	103	BCR	C5-C6-C7-C8
26	L	301	BCR	C23-C24-C25-C26
26	L	305	BCR	C1-C6-C7-C8
26	L	305	BCR	C5-C6-C7-C8
26	M	102	BCR	C23-C24-C25-C26
26	M	102	BCR	C23-C24-C25-C30
29	2	616	K3I	C1-C6-C7-C8
29	2	616	K3I	C5-C6-C7-C8
27	1	317	LHG	C25-C26-C27-C28
28	6	302	LMU	C5-C6-C7-C8
22	3	402	CLA	CBA-CGA-O2A-C1
22	A	825	CLA	CBA-CGA-O2A-C1
22	F	804	CLA	CBA-CGA-O2A-C1
22	6	316	CLA	C13-C15-C16-C17
22	B	811	CLA	C15-C16-C17-C18
27	5	325	LHG	C28-C29-C30-C31
28	1	319	LMU	C4-C5-C6-C7
22	9	602	CLA	O1D-CGD-O2D-CED
22	A	822	CLA	O1A-CGA-O2A-C1
22	A	823	CLA	O1A-CGA-O2A-C1
22	B	842	CLA	O1A-CGA-O2A-C1
28	J	106	LMU	C1-C2-C3-C4
22	A	826	CLA	C8-C10-C11-C12
22	B	811	CLA	C5-C6-C7-C8
22	A	826	CLA	C4-C3-C5-C6
22	B	809	CLA	C4-C3-C5-C6
22	B	817	CLA	C4-C3-C5-C6
22	L	303	CLA	C4-C3-C5-C6
22	2	612	CLA	C11-C12-C13-C15
22	3	403	CLA	C6-C7-C8-C10
22	3	407	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	3	407	CLA	C12-C13-C15-C16
22	3	409	CLA	C2-C3-C5-C6
22	5	314	CLA	C11-C10-C8-C7
22	6	318	CLA	C11-C10-C8-C7
22	6	318	CLA	C12-C13-C15-C16
22	A	801	CLA	C2-C3-C5-C6
22	A	802	CLA	C6-C7-C8-C10
22	A	814	CLA	C11-C12-C13-C15
22	A	823	CLA	C6-C7-C8-C10
22	A	826	CLA	C2-C3-C5-C6
22	B	805	CLA	C11-C10-C8-C7
22	B	830	CLA	C2-C3-C5-C6
22	B	830	CLA	C6-C7-C8-C10
23	7	305	CHL	C6-C7-C8-C10
22	1	311	CLA	O1A-CGA-O2A-C1
22	7	307	CLA	C8-C10-C11-C12
22	B	825	CLA	C5-C6-C7-C8
22	A	816	CLA	C11-C12-C13-C15
22	A	832	CLA	C16-C17-C18-C20
23	8	602	CHL	C16-C17-C18-C19
22	9	603	CLA	O1D-CGD-O2D-CED
22	A	811	CLA	O1D-CGD-O2D-CED
22	A	812	CLA	C3-C5-C6-C7
22	3	407	CLA	CBA-CGA-O2A-C1
22	A	804	CLA	CBA-CGA-O2A-C1
22	B	837	CLA	CBA-CGA-O2A-C1
22	5	303	CLA	C2A-CAA-CBA-CGA
22	7	311	CLA	C2A-CAA-CBA-CGA
22	8	610	CLA	C2A-CAA-CBA-CGA
22	A	809	CLA	C2A-CAA-CBA-CGA
22	B	831	CLA	C2A-CAA-CBA-CGA
23	3	413	CHL	C2A-CAA-CBA-CGA
28	9	618	LMU	O1'-C1-C2-C3
28	A	852	LMU	O1'-C1-C2-C3
22	A	817	CLA	C11-C10-C8-C7
22	B	827	CLA	C11-C10-C8-C7
22	B	837	CLA	C11-C10-C8-C7
27	M	101	LHG	C23-C24-C25-C26
22	6	307	CLA	C10-C11-C12-C13
22	B	806	CLA	C13-C15-C16-C17
34	B	852	DGD	C6B-C7B-C8B-C9B
28	6	302	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
28	A	853	LMU	C4-C5-C6-C7
22	A	824	CLA	C15-C16-C17-C18
22	B	802	CLA	C8-C10-C11-C12
22	B	825	CLA	C8-C10-C11-C12
27	1	317	LHG	C31-C32-C33-C34
27	A	845	LHG	C8-C7-O7-C5
27	6	322	LHG	O6-C4-C5-O7
27	A	844	LHG	C17-C18-C19-C20
28	A	853	LMU	C3-C4-C5-C6
27	A	845	LHG	O9-C7-O7-C5
22	3	411	CLA	C3-C5-C6-C7
28	1	319	LMU	C2'-C1'-O1'-C1
28	F	806	LMU	C2'-C1'-O1'-C1
28	K	201	LMU	C2'-C1'-O1'-C1
27	M	101	LHG	O7-C5-C6-O8
28	A	853	LMU	O5B-C5B-C6B-O6B
22	A	809	CLA	C11-C12-C13-C14
27	A	845	LHG	C27-C28-C29-C30
28	J	106	LMU	C6-C7-C8-C9
31	J	105	LMG	C14-C15-C16-C17
22	8	610	CLA	C5-C6-C7-C8
22	B	843	CLA	C13-C15-C16-C17
22	A	817	CLA	O1D-CGD-O2D-CED
22	3	407	CLA	C4-C3-C5-C6
27	9	616	LHG	C7-C8-C9-C10
31	J	105	LMG	C4-C5-C6-O5
22	B	809	CLA	C2-C3-C5-C6
22	B	810	CLA	C2-C3-C5-C6
22	B	836	CLA	C2-C3-C5-C6
28	K	201	LMU	O1'-C1-C2-C3
22	1	312	CLA	C11-C12-C13-C14
22	2	612	CLA	C11-C12-C13-C14
22	5	314	CLA	C11-C10-C8-C9
22	7	308	CLA	C6-C7-C8-C9
22	A	802	CLA	C6-C7-C8-C9
22	A	804	CLA	C11-C10-C8-C9
22	A	814	CLA	C11-C12-C13-C14
22	A	818	CLA	C11-C10-C8-C9
22	A	820	CLA	C11-C10-C8-C9
22	A	826	CLA	C14-C13-C15-C16
22	B	805	CLA	C6-C7-C8-C9
22	B	805	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	805	CLA	C14-C13-C15-C16
22	B	806	CLA	C11-C10-C8-C9
22	B	815	CLA	C11-C12-C13-C14
32	B	845	PQN	C16-C17-C18-C19
27	6	322	LHG	C28-C29-C30-C31
22	2	612	CLA	C3-C5-C6-C7
28	1	319	LMU	O5B-C1B-O1B-C4'
28	6	301	LMU	O5B-C1B-O1B-C4'
22	2	601	CLA	C2A-CAA-CBA-CGA
22	A	808	CLA	C2A-CAA-CBA-CGA
22	B	816	CLA	C2A-CAA-CBA-CGA
22	B	817	CLA	C2A-CAA-CBA-CGA
26	8	619	BCR	C7-C8-C9-C34
26	K	207	BCR	C37-C22-C23-C24
22	6	307	CLA	C13-C15-C16-C17
26	8	619	BCR	C7-C8-C9-C10
26	A	846	BCR	C7-C8-C9-C10
22	3	402	CLA	O1A-CGA-O2A-C1
22	F	804	CLA	O1A-CGA-O2A-C1
22	B	835	CLA	O1D-CGD-O2D-CED
22	1	308	CLA	C1A-C2A-CAA-CBA
22	1	310	CLA	C1A-C2A-CAA-CBA
22	1	312	CLA	C1A-C2A-CAA-CBA
22	5	305	CLA	C1A-C2A-CAA-CBA
22	5	310	CLA	C1A-C2A-CAA-CBA
22	5	311	CLA	C1A-C2A-CAA-CBA
22	6	310	CLA	C1A-C2A-CAA-CBA
22	6	315	CLA	C1A-C2A-CAA-CBA
22	7	303	CLA	C1A-C2A-CAA-CBA
22	8	610	CLA	C1A-C2A-CAA-CBA
22	8	614	CLA	C1A-C2A-CAA-CBA
22	8	615	CLA	C1A-C2A-CAA-CBA
22	9	609	CLA	C1A-C2A-CAA-CBA
22	A	805	CLA	C1A-C2A-CAA-CBA
22	A	808	CLA	C1A-C2A-CAA-CBA
22	A	810	CLA	C1A-C2A-CAA-CBA
22	A	813	CLA	C1A-C2A-CAA-CBA
22	A	819	CLA	C1A-C2A-CAA-CBA
22	A	820	CLA	C1A-C2A-CAA-CBA
22	A	823	CLA	C1A-C2A-CAA-CBA
22	A	827	CLA	C1A-C2A-CAA-CBA
22	A	829	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	831	CLA	C1A-C2A-CAA-CBA
22	A	832	CLA	C1A-C2A-CAA-CBA
22	A	836	CLA	C1A-C2A-CAA-CBA
22	B	814	CLA	C1A-C2A-CAA-CBA
22	B	817	CLA	C1A-C2A-CAA-CBA
22	B	822	CLA	C1A-C2A-CAA-CBA
22	B	825	CLA	C1A-C2A-CAA-CBA
22	B	832	CLA	C1A-C2A-CAA-CBA
22	B	839	CLA	C1A-C2A-CAA-CBA
22	B	843	CLA	C1A-C2A-CAA-CBA
22	F	804	CLA	C1A-C2A-CAA-CBA
22	G	202	CLA	C1A-C2A-CAA-CBA
23	3	422	CHL	C1A-C2A-CAA-CBA
23	5	307	CHL	C1A-C2A-CAA-CBA
23	5	309	CHL	C1A-C2A-CAA-CBA
23	7	304	CHL	C1A-C2A-CAA-CBA
23	8	603	CHL	C1A-C2A-CAA-CBA
22	3	407	CLA	C16-C17-C18-C20
22	A	823	CLA	C16-C17-C18-C19
22	K	204	CLA	C6-C7-C8-C9
22	3	410	CLA	C2A-CAA-CBA-CGA
31	J	104	LMG	C11-C10-O7-C8
26	B	846	BCR	C19-C20-C21-C22
27	2	617	LHG	C4-O6-P-O3
27	5	301	LHG	C3-O3-P-O6
27	A	845	LHG	C4-O6-P-O3
22	B	809	CLA	CBD-CGD-O2D-CED
22	8	610	CLA	C3-C5-C6-C7
22	2	612	CLA	C13-C15-C16-C17
31	9	617	LMG	C10-C11-C12-C13
22	A	829	CLA	C13-C15-C16-C17
22	A	825	CLA	O1A-CGA-O2A-C1
23	5	308	CHL	C16-C17-C18-C20
28	9	618	LMU	C1-C2-C3-C4
22	B	811	CLA	C3-C5-C6-C7
22	A	801	CLA	C4-C3-C5-C6
22	B	830	CLA	C4-C3-C5-C6
22	2	604	CLA	C3A-C2A-CAA-CBA
22	6	313	CLA	C3A-C2A-CAA-CBA
22	F	803	CLA	C3A-C2A-CAA-CBA
28	G	201	LMU	C6-C7-C8-C9
22	8	613	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	7	305	CHL	C5-C6-C7-C8
22	B	807	CLA	O1D-CGD-O2D-CED
28	9	618	LMU	C6-C7-C8-C9
28	K	201	LMU	C5-C6-C7-C8
22	3	407	CLA	O1A-CGA-O2A-C1
22	A	804	CLA	O1A-CGA-O2A-C1
22	B	837	CLA	O1A-CGA-O2A-C1
22	7	302	CLA	C2A-CAA-CBA-CGA
22	G	203	CLA	C2A-CAA-CBA-CGA
31	9	617	LMG	C7-C8-C9-O8
27	A	845	LHG	C17-C18-C19-C20
22	3	409	CLA	C5-C6-C7-C8
22	5	310	CLA	C5-C6-C7-C8
23	3	406	CHL	C15-C16-C17-C18
22	5	310	CLA	CAA-CBA-CGA-O2A
22	A	801	CLA	CAA-CBA-CGA-O2A
27	6	322	LHG	C23-C24-C25-C26
28	A	852	LMU	C4-C5-C6-C7
28	K	201	LMU	O5B-C5B-C6B-O6B
31	J	104	LMG	C37-C38-C39-C40
31	9	617	LMG	C28-C29-C30-C31
22	B	839	CLA	CBD-CGD-O2D-CED
28	F	806	LMU	O5B-C5B-C6B-O6B
22	1	312	CLA	C4-C3-C5-C6
22	3	404	CLA	C4-C3-C5-C6
22	9	603	CLA	C4-C3-C5-C6
22	9	606	CLA	C4-C3-C5-C6
22	B	810	CLA	C4-C3-C5-C6
22	A	838	CLA	C8-C10-C11-C12
22	B	823	CLA	CBA-CGA-O2A-C1
22	2	612	CLA	C15-C16-C17-C18
22	3	407	CLA	C15-C16-C17-C18
27	A	845	LHG	C28-C29-C30-C31
22	7	303	CLA	C2A-CAA-CBA-CGA
22	A	806	CLA	C2A-CAA-CBA-CGA
23	5	307	CHL	C2A-CAA-CBA-CGA
22	6	316	CLA	C2-C1-O2A-CGA
22	7	306	CLA	C2-C1-O2A-CGA
23	1	304	CHL	C2-C1-O2A-CGA
23	8	608	CHL	C2-C1-O2A-CGA
22	A	819	CLA	O1D-CGD-O2D-CED
28	F	806	LMU	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	H	204	LMU	C3'-C4'-O1B-C1B
22	3	403	CLA	C8-C10-C11-C12
22	7	308	CLA	C8-C10-C11-C12
22	3	401	CLA	CBA-CGA-O2A-C1
23	5	307	CHL	C16-C17-C18-C19
23	8	602	CHL	C16-C17-C18-C20
22	A	826	CLA	C10-C11-C12-C13
23	1	304	CHL	C1-C2-C3-C5
22	B	820	CLA	O1D-CGD-O2D-CED
28	9	618	LMU	C5-C6-C7-C8
31	9	617	LMG	C18-C19-C20-C21
22	B	823	CLA	C5-C6-C7-C8
22	B	819	CLA	C2-C1-O2A-CGA
22	5	314	CLA	C5-C6-C7-C8
22	A	812	CLA	C10-C11-C12-C13
22	1	312	CLA	C2-C3-C5-C6
22	3	404	CLA	C2-C3-C5-C6
22	5	303	CLA	C12-C13-C15-C16
22	5	311	CLA	C11-C10-C8-C7
22	6	307	CLA	C11-C10-C8-C7
22	6	318	CLA	C11-C12-C13-C15
22	7	308	CLA	C6-C7-C8-C10
22	7	308	CLA	C12-C13-C15-C16
22	9	603	CLA	C2-C3-C5-C6
22	9	606	CLA	C2-C3-C5-C6
22	9	608	CLA	C6-C7-C8-C10
22	A	801	CLA	C6-C7-C8-C10
22	A	805	CLA	C12-C13-C15-C16
22	A	818	CLA	C11-C10-C8-C7
22	A	826	CLA	C11-C12-C13-C15
22	B	805	CLA	C12-C13-C15-C16
22	B	806	CLA	C11-C10-C8-C7
22	B	809	CLA	C12-C13-C15-C16
22	B	812	CLA	C12-C13-C15-C16
22	B	815	CLA	C11-C12-C13-C15
22	B	816	CLA	C11-C10-C8-C7
22	B	842	CLA	C11-C10-C8-C7
22	B	843	CLA	C12-C13-C15-C16
22	F	802	CLA	C11-C10-C8-C7
22	L	303	CLA	C2-C3-C5-C6
23	3	406	CHL	C12-C13-C15-C16
23	3	422	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	5	307	CHL	C12-C13-C15-C16
23	6	303	CHL	C11-C10-C8-C7
23	6	303	CHL	C12-C13-C15-C16
23	7	305	CHL	C11-C10-C8-C7
23	7	305	CHL	C12-C13-C15-C16
23	8	602	CHL	C6-C7-C8-C10
23	8	603	CHL	C6-C7-C8-C10
32	A	842	PQN	C16-C17-C18-C20
32	B	845	PQN	C16-C17-C18-C20
31	8	621	LMG	C11-C12-C13-C14
22	3	403	CLA	C6-C7-C8-C9
22	5	311	CLA	C11-C10-C8-C9
22	7	301	CLA	C11-C12-C13-C14
22	8	610	CLA	C11-C12-C13-C14
22	9	608	CLA	C6-C7-C8-C9
22	A	805	CLA	C14-C13-C15-C16
22	A	812	CLA	C11-C10-C8-C9
22	A	814	CLA	C14-C13-C15-C16
22	A	818	CLA	C6-C7-C8-C9
22	A	822	CLA	C11-C10-C8-C9
22	A	826	CLA	C11-C12-C13-C14
22	B	812	CLA	C14-C13-C15-C16
22	B	842	CLA	C11-C10-C8-C9
22	B	843	CLA	C14-C13-C15-C16
23	7	305	CHL	C11-C10-C8-C9
23	8	603	CHL	C11-C10-C8-C9
23	8	603	CHL	C11-C12-C13-C14
27	B	801	LHG	C9-C10-C11-C12
22	3	407	CLA	C10-C11-C12-C13
22	L	303	CLA	C10-C11-C12-C13
23	8	606	CHL	C8-C10-C11-C12
22	3	401	CLA	C2A-CAA-CBA-CGA
22	B	821	CLA	C2A-CAA-CBA-CGA
22	9	607	CLA	O1D-CGD-O2D-CED
26	L	305	BCR	C37-C22-C23-C24
23	3	406	CHL	C16-C17-C18-C20
26	B	846	BCR	C21-C22-C23-C24
22	B	827	CLA	C3-C5-C6-C7
22	B	810	CLA	O1D-CGD-O2D-CED
22	1	311	CLA	C8-C10-C11-C12
28	1	319	LMU	C5-C6-C7-C8
28	6	323	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	1	311	CLA	C4B-C3B-CAB-CBB
22	2	604	CLA	C4B-C3B-CAB-CBB
22	2	611	CLA	C4B-C3B-CAB-CBB
22	2	612	CLA	C4B-C3B-CAB-CBB
22	3	403	CLA	C4B-C3B-CAB-CBB
22	3	412	CLA	C4B-C3B-CAB-CBB
22	5	303	CLA	C4B-C3B-CAB-CBB
22	5	315	CLA	C4B-C3B-CAB-CBB
22	6	306	CLA	C4B-C3B-CAB-CBB
22	6	307	CLA	C4B-C3B-CAB-CBB
22	6	315	CLA	C4B-C3B-CAB-CBB
22	7	302	CLA	C4B-C3B-CAB-CBB
22	7	303	CLA	C4B-C3B-CAB-CBB
22	7	307	CLA	C4B-C3B-CAB-CBB
22	8	609	CLA	C4B-C3B-CAB-CBB
22	9	606	CLA	C4B-C3B-CAB-CBB
22	9	608	CLA	C4B-C3B-CAB-CBB
22	A	807	CLA	C4B-C3B-CAB-CBB
22	A	809	CLA	C4B-C3B-CAB-CBB
22	A	811	CLA	C4B-C3B-CAB-CBB
22	A	812	CLA	C4B-C3B-CAB-CBB
22	A	819	CLA	C4B-C3B-CAB-CBB
22	A	825	CLA	C4B-C3B-CAB-CBB
22	A	837	CLA	C4B-C3B-CAB-CBB
22	B	806	CLA	C4B-C3B-CAB-CBB
22	B	812	CLA	C4B-C3B-CAB-CBB
22	B	821	CLA	C4B-C3B-CAB-CBB
22	B	831	CLA	C4B-C3B-CAB-CBB
22	B	837	CLA	C4B-C3B-CAB-CBB
22	H	203	CLA	C4B-C3B-CAB-CBB
22	L	303	CLA	C4B-C3B-CAB-CBB
23	8	602	CHL	C4B-C3B-CAB-CBB
23	8	606	CHL	C4B-C3B-CAB-CBB
23	9	601	CHL	C4B-C3B-CAB-CBB
22	A	828	CLA	C15-C16-C17-C18
27	5	325	LHG	O6-C4-C5-C6
27	6	322	LHG	O6-C4-C5-C6
27	2	617	LHG	C23-C24-C25-C26
22	A	802	CLA	CBA-CGA-O2A-C1
22	B	815	CLA	CBA-CGA-O2A-C1
27	8	620	LHG	C24-C23-O8-C6
28	H	204	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
34	B	852	DGD	O6E-C5E-C6E-O5E
22	6	311	CLA	C4-C3-C5-C6
23	8	602	CHL	C4-C3-C5-C6
23	8	602	CHL	C2-C3-C5-C6
31	J	104	LMG	C31-C32-C33-C34
31	J	104	LMG	O9-C10-O7-C8
22	B	827	CLA	C11-C10-C8-C9
22	A	832	CLA	C10-C11-C12-C13
22	B	805	CLA	C8-C10-C11-C12
22	B	817	CLA	CBA-CGA-O2A-C1
22	2	612	CLA	C3A-C2A-CAA-CBA
22	A	823	CLA	C3A-C2A-CAA-CBA
22	G	202	CLA	C3A-C2A-CAA-CBA
22	L	303	CLA	C3A-C2A-CAA-CBA
22	6	304	CLA	C8-C10-C11-C12
25	8	618	XAT	C29-C30-C31-C32
28	1	319	LMU	C2-C1-O1'-C1'
28	3	420	LMU	C2-C1-O1'-C1'
28	7	319	LMU	C2-C1-O1'-C1'
28	9	618	LMU	C2-C1-O1'-C1'
28	F	806	LMU	C2-C1-O1'-C1'
28	H	204	LMU	C2-C1-O1'-C1'
28	K	201	LMU	C2-C1-O1'-C1'
22	B	842	CLA	C8-C10-C11-C12
27	1	317	LHG	C30-C31-C32-C33
22	A	820	CLA	CBA-CGA-O2A-C1
27	1	318	LHG	C24-C23-O8-C6
22	A	823	CLA	C8-C10-C11-C12
27	1	317	LHG	C4-C5-C6-O8
31	9	617	LMG	O1-C7-C8-C9
28	3	423	LMU	C1-C2-C3-C4
22	A	829	CLA	C4-C3-C5-C6
22	B	825	CLA	C4-C3-C5-C6
22	1	308	CLA	C5-C6-C7-C8
22	B	815	CLA	C13-C15-C16-C17
23	7	305	CHL	C13-C15-C16-C17
27	7	318	LHG	C4-O6-P-O3
22	7	306	CLA	C2A-CAA-CBA-CGA
23	8	608	CHL	C2A-CAA-CBA-CGA
27	A	845	LHG	O1-C1-C2-O2
22	3	401	CLA	O1A-CGA-O2A-C1
22	B	823	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	1	311	CLA	C2B-C3B-CAB-CBB
22	2	604	CLA	C2B-C3B-CAB-CBB
22	2	610	CLA	C2B-C3B-CAB-CBB
22	2	611	CLA	C2B-C3B-CAB-CBB
22	6	306	CLA	C2B-C3B-CAB-CBB
22	6	307	CLA	C2B-C3B-CAB-CBB
22	6	315	CLA	C2B-C3B-CAB-CBB
22	6	317	CLA	C2B-C3B-CAB-CBB
22	7	307	CLA	C2B-C3B-CAB-CBB
22	8	609	CLA	C2B-C3B-CAB-CBB
22	9	603	CLA	C2B-C3B-CAB-CBB
22	A	807	CLA	C2B-C3B-CAB-CBB
22	A	811	CLA	C2B-C3B-CAB-CBB
22	A	837	CLA	C2B-C3B-CAB-CBB
22	B	821	CLA	C2B-C3B-CAB-CBB
22	B	839	CLA	C2B-C3B-CAB-CBB
22	L	303	CLA	C2B-C3B-CAB-CBB
28	3	421	LMU	C6-C7-C8-C9
22	A	839	CLA	O1D-CGD-O2D-CED
28	6	301	LMU	C6-C7-C8-C9
31	8	621	LMG	O1-C7-C8-O7
31	J	104	LMG	O7-C8-C9-O8
22	A	841	CLA	O1D-CGD-O2D-CED
23	3	413	CHL	C11-C12-C13-C14
28	H	204	LMU	C5'-C4'-O1B-C1B
23	5	307	CHL	C16-C17-C18-C20
22	2	612	CLA	C10-C11-C12-C13
22	6	307	CLA	C8-C10-C11-C12
22	B	835	CLA	C8-C10-C11-C12
22	A	810	CLA	C11-C12-C13-C14
22	9	602	CLA	C2-C1-O2A-CGA
22	A	828	CLA	C2-C1-O2A-CGA
22	B	818	CLA	C2-C1-O2A-CGA
23	3	422	CHL	C2-C1-O2A-CGA
23	8	606	CHL	C2-C1-O2A-CGA
22	B	837	CLA	O1D-CGD-O2D-CED
22	5	303	CLA	C14-C13-C15-C16
22	6	307	CLA	C11-C10-C8-C9
22	6	314	CLA	C6-C7-C8-C9
22	A	809	CLA	C6-C7-C8-C9
22	A	818	CLA	C11-C12-C13-C14
22	B	806	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	3	406	CHL	C11-C10-C8-C9
23	5	302	CHL	C14-C13-C15-C16
23	5	307	CHL	C11-C12-C13-C14
23	5	307	CHL	C14-C13-C15-C16
23	6	303	CHL	C11-C12-C13-C14
23	6	303	CHL	C14-C13-C15-C16
22	A	807	CLA	C4-C3-C5-C6
22	1	311	CLA	C2A-CAA-CBA-CGA
22	3	407	CLA	C16-C17-C18-C19
22	9	603	CLA	C6-C7-C8-C9
23	8	602	CHL	C3-C5-C6-C7
24	5	320	LUT	C5-C6-C7-C8
26	A	848	BCR	C5-C6-C7-C8
26	A	849	BCR	C1-C6-C7-C8
26	A	849	BCR	C5-C6-C7-C8
26	B	846	BCR	C23-C24-C25-C26
26	B	846	BCR	C23-C24-C25-C30
26	J	101	BCR	C5-C6-C7-C8
22	A	812	CLA	C2-C3-C5-C6
31	J	105	LMG	O6-C5-C6-O5
22	5	314	CLA	CAA-CBA-CGA-O2A
22	7	312	CLA	C1A-C2A-CAA-CBA
22	J	102	CLA	C1A-C2A-CAA-CBA
24	9	613	LUT	C7-C8-C9-C10
25	1	315	XAT	C7-C8-C9-C10
25	6	320	XAT	C7-C8-C9-C10
25	6	320	XAT	C31-C32-C33-C34
25	9	614	XAT	C7-C8-C9-C10
22	6	316	CLA	C8-C10-C11-C12
28	3	420	LMU	O5B-C5B-C6B-O6B
27	B	801	LHG	C10-C11-C12-C13
22	B	837	CLA	C11-C10-C8-C9
27	M	101	LHG	C7-C8-C9-C10
28	3	421	LMU	C11-C10-C9-C8
22	3	411	CLA	C2-C1-O2A-CGA
22	5	314	CLA	C2-C1-O2A-CGA
23	7	305	CHL	C8-C10-C11-C12
22	2	602	CLA	C11-C10-C8-C7
22	7	301	CLA	C6-C7-C8-C10
22	7	301	CLA	C11-C12-C13-C15
22	7	301	CLA	C12-C13-C15-C16
22	8	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	8	613	CLA	C12-C13-C15-C16
22	9	608	CLA	C12-C13-C15-C16
22	A	809	CLA	C6-C7-C8-C10
22	A	812	CLA	C11-C10-C8-C7
22	A	814	CLA	C12-C13-C15-C16
22	A	818	CLA	C6-C7-C8-C10
22	A	818	CLA	C11-C12-C13-C15
22	A	822	CLA	C11-C10-C8-C7
22	B	803	CLA	C11-C10-C8-C7
22	B	806	CLA	C11-C12-C13-C15
22	B	812	CLA	C11-C10-C8-C7
22	B	842	CLA	C11-C12-C13-C15
23	3	406	CHL	C11-C10-C8-C7
23	5	302	CHL	C11-C10-C8-C7
23	5	302	CHL	C12-C13-C15-C16
23	5	307	CHL	C6-C7-C8-C10
23	5	307	CHL	C11-C12-C13-C15
23	5	308	CHL	C11-C12-C13-C15
23	8	603	CHL	C11-C12-C13-C15
23	8	606	CHL	C11-C10-C8-C7
23	8	606	CHL	C11-C12-C13-C15
23	8	606	CHL	C12-C13-C15-C16
22	6	307	CLA	C3-C5-C6-C7
23	8	606	CHL	C16-C17-C18-C20
22	B	838	CLA	C2A-CAA-CBA-CGA
23	6	303	CHL	C2A-CAA-CBA-CGA
27	8	620	LHG	C26-C27-C28-C29
22	A	814	CLA	C10-C11-C12-C13
22	B	809	CLA	C3-C5-C6-C7
22	A	803	CLA	CBA-CGA-O2A-C1
22	B	818	CLA	CBA-CGA-O2A-C1
27	2	617	LHG	C24-C23-O8-C6
28	3	421	LMU	C4'-C5'-C6'-O6'
22	A	831	CLA	CBD-CGD-O2D-CED
22	2	613	CLA	CAD-CBD-CGD-O2D
22	3	408	CLA	CAD-CBD-CGD-O2D
22	5	315	CLA	CAD-CBD-CGD-O2D
22	6	315	CLA	CAD-CBD-CGD-O2D
22	8	604	CLA	CAD-CBD-CGD-O2D
22	8	609	CLA	CAD-CBD-CGD-O2D
22	8	610	CLA	CAD-CBD-CGD-O2D
22	9	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	9	610	CLA	CAD-CBD-CGD-O2D
22	9	611	CLA	CAD-CBD-CGD-O2D
22	A	810	CLA	CAD-CBD-CGD-O2D
22	A	825	CLA	CAD-CBD-CGD-O2D
22	A	829	CLA	CAD-CBD-CGD-O2D
22	A	830	CLA	CAD-CBD-CGD-O2D
22	A	836	CLA	CAD-CBD-CGD-O2D
22	B	805	CLA	CAD-CBD-CGD-O2D
22	B	812	CLA	CAD-CBD-CGD-O2D
22	B	827	CLA	CAD-CBD-CGD-O2D
22	B	832	CLA	CAD-CBD-CGD-O2D
22	B	842	CLA	CAD-CBD-CGD-O2D
22	F	802	CLA	CAD-CBD-CGD-O2D
22	F	804	CLA	CAD-CBD-CGD-O2D
22	G	203	CLA	CAD-CBD-CGD-O2D
23	8	608	CHL	CAD-CBD-CGD-O2D
28	1	319	LMU	C1-C2-C3-C4
28	A	853	LMU	C6-C7-C8-C9
22	B	823	CLA	C4-C3-C5-C6
28	K	201	LMU	O5'-C1'-O1'-C1
22	3	404	CLA	C5-C6-C7-C8
27	5	325	LHG	O6-C4-C5-O7
31	9	617	LMG	C32-C33-C34-C35
27	7	318	LHG	C1-C2-C3-O3
22	1	313	CLA	CHA-CBD-CGD-O2D
22	2	607	CLA	CHA-CBD-CGD-O1D
22	2	607	CLA	CHA-CBD-CGD-O2D
22	2	608	CLA	CHA-CBD-CGD-O1D
22	2	608	CLA	CHA-CBD-CGD-O2D
22	2	611	CLA	CHA-CBD-CGD-O1D
22	2	611	CLA	CHA-CBD-CGD-O2D
22	3	401	CLA	CHA-CBD-CGD-O1D
22	3	401	CLA	CHA-CBD-CGD-O2D
22	5	304	CLA	CHA-CBD-CGD-O1D
22	5	304	CLA	CHA-CBD-CGD-O2D
22	5	317	CLA	CHA-CBD-CGD-O1D
22	5	317	CLA	CHA-CBD-CGD-O2D
22	6	304	CLA	CHA-CBD-CGD-O1D
22	8	611	CLA	CHA-CBD-CGD-O1D
22	8	615	CLA	CHA-CBD-CGD-O1D
22	8	615	CLA	CHA-CBD-CGD-O2D
22	A	815	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	815	CLA	CHA-CBD-CGD-O2D
22	A	818	CLA	CHA-CBD-CGD-O1D
22	A	818	CLA	CHA-CBD-CGD-O2D
22	A	819	CLA	CHA-CBD-CGD-O1D
22	A	823	CLA	CHA-CBD-CGD-O1D
22	A	823	CLA	CHA-CBD-CGD-O2D
22	A	833	CLA	CHA-CBD-CGD-O1D
22	B	808	CLA	CHA-CBD-CGD-O1D
22	B	808	CLA	CHA-CBD-CGD-O2D
22	B	811	CLA	CHA-CBD-CGD-O1D
22	B	811	CLA	CHA-CBD-CGD-O2D
22	B	825	CLA	CHA-CBD-CGD-O1D
22	B	825	CLA	CHA-CBD-CGD-O2D
22	F	803	CLA	CHA-CBD-CGD-O1D
22	F	803	CLA	CHA-CBD-CGD-O2D
22	F	804	CLA	CHA-CBD-CGD-O1D
22	J	102	CLA	CHA-CBD-CGD-O1D
22	J	102	CLA	CHA-CBD-CGD-O2D
23	5	318	CHL	CHA-CBD-CGD-O1D
23	5	318	CHL	CHA-CBD-CGD-O2D
23	6	303	CHL	CHA-CBD-CGD-O1D
23	6	303	CHL	CHA-CBD-CGD-O2D
23	9	605	CHL	CHA-CBD-CGD-O1D
23	9	605	CHL	CHA-CBD-CGD-O2D
22	A	802	CLA	O1A-CGA-O2A-C1
22	A	820	CLA	O1A-CGA-O2A-C1
22	B	817	CLA	O1A-CGA-O2A-C1
27	1	318	LHG	O10-C23-O8-C6
27	8	620	LHG	O10-C23-O8-C6
27	1	317	LHG	O7-C5-C6-O8
27	5	325	LHG	O7-C5-C6-O8
22	7	301	CLA	CBA-CGA-O2A-C1
27	6	322	LHG	C24-C23-O8-C6
28	H	204	LMU	C11-C10-C9-C8
22	B	815	CLA	O1A-CGA-O2A-C1
34	B	852	DGD	C5B-C6B-C7B-C8B
22	1	311	CLA	C14-C13-C15-C16
22	7	301	CLA	C6-C7-C8-C9
22	8	614	CLA	C11-C10-C8-C9
22	B	802	CLA	C11-C10-C8-C9
22	B	803	CLA	C11-C10-C8-C9
22	B	829	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	842	CLA	C11-C12-C13-C14
22	B	809	CLA	O1D-CGD-O2D-CED
22	B	839	CLA	O1D-CGD-O2D-CED
22	A	803	CLA	O1A-CGA-O2A-C1
22	5	314	CLA	CBA-CGA-O2A-C1
22	B	813	CLA	CBA-CGA-O2A-C1
22	B	815	CLA	C8-C10-C11-C12
22	B	815	CLA	C10-C11-C12-C13
22	6	304	CLA	C2A-CAA-CBA-CGA
22	3	409	CLA	CBD-CGD-O2D-CED
28	3	420	LMU	C1-C2-C3-C4
22	B	813	CLA	C5-C6-C7-C8
22	B	817	CLA	C3-C5-C6-C7
22	3	409	CLA	C1A-C2A-CAA-CBA
22	3	414	CLA	CHA-CBD-CGD-O2D
22	7	302	CLA	C1A-C2A-CAA-CBA
22	7	309	CLA	C1A-C2A-CAA-CBA
22	B	819	CLA	C1A-C2A-CAA-CBA
22	B	824	CLA	CHA-CBD-CGD-O2D
22	B	834	CLA	C1A-C2A-CAA-CBA
22	A	801	CLA	CBA-CGA-O2A-C1
28	A	853	LMU	C1-C2-C3-C4
27	1	317	LHG	C3-O3-P-O6
27	5	325	LHG	C3-O3-P-O6
27	A	844	LHG	C3-O3-P-O6
27	A	844	LHG	C33-C34-C35-C36
22	B	808	CLA	C4-C3-C5-C6
22	B	825	CLA	C2-C3-C5-C6
22	8	613	CLA	O1A-CGA-O2A-C1
22	B	818	CLA	O1A-CGA-O2A-C1
22	6	309	CLA	C4B-C3B-CAB-CBB
22	6	312	CLA	C4B-C3B-CAB-CBB
22	7	310	CLA	C4B-C3B-CAB-CBB
22	F	802	CLA	C4B-C3B-CAB-CBB
23	1	305	CHL	C4B-C3B-CAB-CBB
27	1	318	LHG	C4-O6-P-O5
27	2	617	LHG	C3-O3-P-O5
27	2	617	LHG	C4-O6-P-O5
27	6	322	LHG	C3-O3-P-O4
27	8	620	LHG	C4-O6-P-O5
27	A	845	LHG	C4-O6-P-O5
27	B	801	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
27	M	101	LHG	C4-O6-P-O4
22	5	303	CLA	C16-C17-C18-C20
22	5	314	CLA	C11-C12-C13-C14
22	A	833	CLA	C11-C12-C13-C15
22	7	309	CLA	O2A-C1-C2-C3
22	A	805	CLA	O2A-C1-C2-C3
22	A	812	CLA	O2A-C1-C2-C3
28	F	806	LMU	O5'-C1'-O1'-C1
27	8	620	LHG	O6-C4-C5-C6
27	5	301	LHG	C9-C10-C11-C12
22	9	609	CLA	C2A-CAA-CBA-CGA
22	B	815	CLA	C2A-CAA-CBA-CGA
28	6	301	LMU	C1-C2-C3-C4
22	5	310	CLA	C15-C16-C17-C18
22	2	608	CLA	CAD-CBD-CGD-O1D
22	3	401	CLA	CAD-CBD-CGD-O1D
22	5	304	CLA	CAD-CBD-CGD-O1D
22	5	317	CLA	CAD-CBD-CGD-O1D
22	6	304	CLA	CAD-CBD-CGD-O1D
22	6	312	CLA	CAD-CBD-CGD-O1D
22	8	615	CLA	CAD-CBD-CGD-O1D
22	A	804	CLA	CAD-CBD-CGD-O1D
22	A	813	CLA	CAD-CBD-CGD-O1D
22	A	823	CLA	CAD-CBD-CGD-O1D
22	A	838	CLA	CAD-CBD-CGD-O1D
22	B	808	CLA	CAD-CBD-CGD-O1D
22	B	843	CLA	CAD-CBD-CGD-O1D
23	6	303	CHL	CAD-CBD-CGD-O1D
23	8	602	CHL	CAD-CBD-CGD-O1D
23	8	608	CHL	C2-C3-C5-C6
27	2	617	LHG	O10-C23-O8-C6
22	7	309	CLA	C3-C5-C6-C7
27	6	322	LHG	C27-C28-C29-C30
27	2	617	LHG	C24-C25-C26-C27
23	6	303	CHL	C16-C17-C18-C20
22	1	311	CLA	C12-C13-C15-C16
22	2	612	CLA	C6-C7-C8-C10
22	6	307	CLA	C12-C13-C15-C16
22	6	314	CLA	C6-C7-C8-C10
22	6	316	CLA	C11-C12-C13-C15
22	7	311	CLA	C11-C10-C8-C7
22	A	802	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	A	838	CLA	C6-C7-C8-C10
22	B	802	CLA	C11-C10-C8-C7
22	B	808	CLA	C11-C12-C13-C15
22	B	809	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	C6-C7-C8-C10
22	B	837	CLA	C6-C7-C8-C10
22	B	844	CLA	C11-C10-C8-C7
23	8	602	CHL	C12-C13-C15-C16
24	2	614	LUT	C25-C26-C27-C28
27	8	620	LHG	O6-C4-C5-O7
25	2	615	XAT	C9-C10-C11-C12
28	J	106	LMU	C3-C4-C5-C6
22	8	601	CLA	CAD-CBD-CGD-O1D
22	A	843	CLA	CAD-CBD-CGD-O1D
22	B	819	CLA	CBA-CGA-O2A-C1
31	9	617	LMG	O7-C8-C9-O8
27	6	322	LHG	C11-C10-C9-C8
22	A	801	CLA	O1A-CGA-O2A-C1
31	8	621	LMG	C4-C5-C6-O5
22	8	613	CLA	CBA-CGA-O2A-C1
22	3	407	CLA	CAA-CBA-CGA-O2A
22	1	308	CLA	C11-C10-C8-C9
22	2	602	CLA	C11-C10-C8-C9
22	6	318	CLA	C11-C12-C13-C14
22	9	608	CLA	C14-C13-C15-C16
22	A	801	CLA	C6-C7-C8-C9
22	A	838	CLA	C6-C7-C8-C9
22	B	812	CLA	C11-C10-C8-C9
23	5	308	CHL	C11-C12-C13-C14
23	8	606	CHL	C11-C12-C13-C14
32	A	842	PQN	C16-C17-C18-C19
27	6	322	LHG	O10-C23-O8-C6
22	6	314	CLA	C5-C6-C7-C8
22	7	301	CLA	O1A-CGA-O2A-C1
22	L	302	CLA	C2A-CAA-CBA-CGA
22	A	831	CLA	O1D-CGD-O2D-CED
22	B	810	CLA	C11-C12-C13-C14
25	6	320	XAT	C31-C32-C33-C40
22	A	812	CLA	C13-C15-C16-C17
22	B	804	CLA	C5-C6-C7-C8
28	7	319	LMU	C2-C3-C4-C5
31	J	105	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	6	319	LUT	C11-C12-C13-C14
26	L	305	BCR	C21-C22-C23-C24
30	6	321	NEX	C27-C28-C29-C30
22	2	612	CLA	C2B-C3B-CAB-CBB
22	3	402	CLA	C2B-C3B-CAB-CBB
22	3	403	CLA	C2B-C3B-CAB-CBB
22	5	303	CLA	C2B-C3B-CAB-CBB
22	5	311	CLA	C2B-C3B-CAB-CBB
22	6	310	CLA	C2B-C3B-CAB-CBB
22	6	312	CLA	C2B-C3B-CAB-CBB
22	7	301	CLA	C2B-C3B-CAB-CBB
22	7	302	CLA	C2B-C3B-CAB-CBB
22	7	303	CLA	C2B-C3B-CAB-CBB
22	7	308	CLA	C2B-C3B-CAB-CBB
22	8	612	CLA	C2B-C3B-CAB-CBB
22	8	616	CLA	C2B-C3B-CAB-CBB
22	9	608	CLA	C2B-C3B-CAB-CBB
22	A	809	CLA	C2B-C3B-CAB-CBB
22	A	825	CLA	C2B-C3B-CAB-CBB
22	B	806	CLA	C2B-C3B-CAB-CBB
22	B	812	CLA	C2B-C3B-CAB-CBB
22	B	813	CLA	C2B-C3B-CAB-CBB
22	B	831	CLA	C2B-C3B-CAB-CBB
22	B	835	CLA	C2B-C3B-CAB-CBB
22	B	837	CLA	C2B-C3B-CAB-CBB
22	B	842	CLA	C2B-C3B-CAB-CBB
22	F	803	CLA	C2B-C3B-CAB-CBB
22	K	204	CLA	C2B-C3B-CAB-CBB
23	1	305	CHL	C2B-C3B-CAB-CBB
23	3	406	CHL	C2B-C3B-CAB-CBB
23	5	308	CHL	C2B-C3B-CAB-CBB
23	8	602	CHL	C2B-C3B-CAB-CBB
23	8	606	CHL	C2B-C3B-CAB-CBB
23	9	601	CHL	C2B-C3B-CAB-CBB
22	B	841	CLA	O1A-CGA-O2A-C1
28	3	421	LMU	C9-C10-C11-C12
22	3	408	CLA	C3-C5-C6-C7
22	A	833	CLA	C4-C3-C5-C6
22	6	311	CLA	C2-C3-C5-C6
22	B	841	CLA	CBA-CGA-O2A-C1
23	8	606	CHL	C3-C5-C6-C7
31	9	617	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
22	1	301	CLA	C2-C1-O2A-CGA
22	1	308	CLA	C2-C1-O2A-CGA
22	2	601	CLA	C2-C1-O2A-CGA
22	A	814	CLA	C2-C1-O2A-CGA
22	A	837	CLA	C2-C1-O2A-CGA
22	A	838	CLA	C2-C1-O2A-CGA
22	5	303	CLA	C16-C17-C18-C19
28	G	201	LMU	O5'-C5'-C6'-O6'
28	1	319	LMU	C2-C3-C4-C5
22	K	204	CLA	O1A-CGA-O2A-C1
23	1	304	CHL	CAA-CBA-CGA-O2A
22	5	303	CLA	C13-C15-C16-C17
22	A	824	CLA	C4-C3-C5-C6
28	3	423	LMU	C3'-C4'-O1B-C1B
24	5	320	LUT	C1-C6-C7-C8
26	A	848	BCR	C1-C6-C7-C8
26	J	101	BCR	C1-C6-C7-C8
22	B	823	CLA	C2-C3-C5-C6
22	3	409	CLA	O1D-CGD-O2D-CED
28	A	853	LMU	C7-C8-C9-C10
22	8	613	CLA	C16-C17-C18-C20
23	3	405	CHL	C2A-CAA-CBA-CGA
23	3	406	CHL	C1-C2-C3-C5
27	1	318	LHG	C3-O3-P-O6
27	5	301	LHG	C4-O6-P-O3
27	7	318	LHG	C3-O3-P-O6
27	9	616	LHG	C3-O3-P-O6
27	9	616	LHG	C4-O6-P-O3
27	A	844	LHG	C4-O6-P-O3
27	A	845	LHG	C3-O3-P-O6
27	B	801	LHG	C3-O3-P-O6
27	M	101	LHG	C3-O3-P-O6
22	A	823	CLA	C5-C6-C7-C8
22	3	411	CLA	CBA-CGA-O2A-C1
22	B	827	CLA	CBA-CGA-O2A-C1
27	5	325	LHG	C4-C5-C6-O8
22	3	403	CLA	C4-C3-C5-C6
22	7	307	CLA	C12-C13-C15-C16
23	6	303	CHL	C11-C12-C13-C15
32	A	842	PQN	C21-C22-C23-C25
22	7	301	CLA	C14-C13-C15-C16
22	7	308	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	809	CLA	C14-C13-C15-C16
22	B	816	CLA	C11-C10-C8-C9
22	B	837	CLA	C6-C7-C8-C9
23	3	422	CHL	C6-C7-C8-C9
23	8	603	CHL	C6-C7-C8-C9
24	3	415	LUT	C29-C30-C31-C32
25	1	315	XAT	C9-C10-C11-C12
23	3	413	CHL	C10-C11-C12-C13
22	K	204	CLA	CBA-CGA-O2A-C1
28	6	323	LMU	C2-C3-C4-C5
27	A	845	LHG	C2-C3-O3-P
22	B	831	CLA	C8-C10-C11-C12
22	B	842	CLA	C15-C16-C17-C18
23	5	319	CHL	C3-C5-C6-C7
28	3	423	LMU	O5B-C5B-C6B-O6B
22	A	833	CLA	C2-C3-C5-C6
22	5	314	CLA	C11-C12-C13-C15
22	B	827	CLA	O1A-CGA-O2A-C1
22	B	803	CLA	C10-C11-C12-C13
22	B	814	CLA	CAA-CBA-CGA-O2A
34	B	852	DGD	C9B-CAB-CBB-CCB
23	3	422	CHL	C10-C11-C12-C13
22	3	402	CLA	C4B-C3B-CAB-CBB
22	5	311	CLA	C4B-C3B-CAB-CBB
22	6	304	CLA	C4B-C3B-CAB-CBB
22	6	310	CLA	C4B-C3B-CAB-CBB
22	7	301	CLA	C4B-C3B-CAB-CBB
22	7	308	CLA	C4B-C3B-CAB-CBB
22	8	612	CLA	C4B-C3B-CAB-CBB
22	8	616	CLA	C4B-C3B-CAB-CBB
22	B	813	CLA	C4B-C3B-CAB-CBB
22	B	818	CLA	C4B-C3B-CAB-CBB
22	B	819	CLA	C4B-C3B-CAB-CBB
22	B	835	CLA	C4B-C3B-CAB-CBB
22	B	842	CLA	C4B-C3B-CAB-CBB
22	F	803	CLA	C4B-C3B-CAB-CBB
22	K	204	CLA	C4B-C3B-CAB-CBB
23	3	406	CHL	C4B-C3B-CAB-CBB
23	5	308	CHL	C4B-C3B-CAB-CBB
22	A	833	CLA	C11-C12-C13-C14
25	9	614	XAT	C29-C30-C31-C32
26	9	615	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	F	801	BCR	C13-C14-C15-C16
22	5	310	CLA	CAA-CBA-CGA-O1A
22	2	611	CLA	CBD-CGD-O2D-CED
22	B	825	CLA	C10-C11-C12-C13
22	7	311	CLA	C2-C3-C5-C6
22	A	824	CLA	C2-C3-C5-C6
28	3	423	LMU	O1'-C1-C2-C3
23	3	422	CHL	C5-C6-C7-C8
22	7	310	CLA	CAA-CBA-CGA-O1A
22	B	843	CLA	CAA-CBA-CGA-O2A
22	A	811	CLA	C2-C1-O2A-CGA
27	1	317	LHG	C24-C25-C26-C27
22	A	822	CLA	C8-C10-C11-C12
22	A	803	CLA	C3-C5-C6-C7
22	5	316	CLA	CAA-CBA-CGA-O1A
22	5	304	CLA	C2A-CAA-CBA-CGA
22	7	301	CLA	C2A-CAA-CBA-CGA
22	A	801	CLA	CAA-CBA-CGA-O1A
22	6	307	CLA	C3A-C2A-CAA-CBA
22	8	616	CLA	C3A-C2A-CAA-CBA
22	A	813	CLA	C3A-C2A-CAA-CBA
22	A	828	CLA	C3A-C2A-CAA-CBA
22	B	806	CLA	C3A-C2A-CAA-CBA
23	1	306	CHL	C3A-C2A-CAA-CBA
27	B	801	LHG	O9-C7-O7-C5
28	H	204	LMU	C1-C2-C3-C4
28	H	204	LMU	C5-C6-C7-C8
22	7	311	CLA	C4-C3-C5-C6
22	B	821	CLA	C4-C3-C5-C6
27	8	620	LHG	C11-C10-C9-C8
22	5	314	CLA	CBD-CGD-O2D-CED
22	B	808	CLA	C2-C3-C5-C6
22	7	311	CLA	C11-C10-C8-C9
22	B	815	CLA	C14-C13-C15-C16
23	5	307	CHL	C11-C10-C8-C9
22	8	613	CLA	C16-C17-C18-C19
25	7	316	XAT	C40-C33-C34-C35
26	5	322	BCR	C35-C13-C14-C15
26	A	851	BCR	C11-C10-C9-C34
26	B	848	BCR	C11-C10-C9-C34
26	B	848	BCR	C20-C21-C22-C37
26	F	805	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
26	L	301	BCR	C20-C21-C22-C37
30	5	323	NEX	C39-C29-C30-C31
30	6	321	NEX	C39-C29-C30-C31
27	2	617	LHG	O9-C7-O7-C5
22	7	310	CLA	CAA-CBA-CGA-O2A
22	8	604	CLA	CAA-CBA-CGA-O2A
22	A	816	CLA	C2A-CAA-CBA-CGA
23	5	309	CHL	C2A-CAA-CBA-CGA
22	6	304	CLA	CBA-CGA-O2A-C1
31	J	104	LMG	C35-C36-C37-C38
26	7	317	BCR	C37-C22-C23-C24
22	B	811	CLA	C13-C15-C16-C17
22	B	844	CLA	C15-C16-C17-C18
23	6	303	CHL	C13-C15-C16-C17
23	3	406	CHL	C4-C3-C5-C6
22	6	307	CLA	C1A-C2A-CAA-CBA
22	8	605	CLA	C1A-C2A-CAA-CBA
22	8	611	CLA	C1A-C2A-CAA-CBA
22	9	604	CLA	C1A-C2A-CAA-CBA
22	A	833	CLA	C1A-C2A-CAA-CBA
22	B	806	CLA	C1A-C2A-CAA-CBA
22	B	809	CLA	C1A-C2A-CAA-CBA
22	B	818	CLA	C1A-C2A-CAA-CBA
22	B	841	CLA	C1A-C2A-CAA-CBA
23	5	308	CHL	C1A-C2A-CAA-CBA
23	8	608	CHL	C1A-C2A-CAA-CBA
22	3	404	CLA	C11-C10-C8-C7
22	6	304	CLA	C6-C7-C8-C10
22	A	820	CLA	C6-C7-C8-C10
22	A	829	CLA	C2-C3-C5-C6
22	B	809	CLA	C11-C10-C8-C7
22	B	812	CLA	C6-C7-C8-C10
23	5	307	CHL	C11-C10-C8-C7
22	5	314	CLA	O1D-CGD-O2D-CED
22	8	604	CLA	CAA-CBA-CGA-O1A
24	6	319	LUT	C33-C34-C35-C15
23	8	602	CHL	CAA-CBA-CGA-O2A
22	B	803	CLA	C16-C17-C18-C19
22	9	608	CLA	C3-C5-C6-C7
22	B	814	CLA	C3-C5-C6-C7
23	8	603	CHL	C2A-CAA-CBA-CGA
23	8	606	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	5	307	CHL	C15-C16-C17-C18
22	A	826	CLA	CBA-CGA-O2A-C1
22	7	309	CLA	C2-C3-C5-C6
22	3	403	CLA	C16-C17-C18-C19
22	A	828	CLA	C13-C15-C16-C17
22	3	403	CLA	C2-C3-C5-C6
23	6	303	CHL	C2-C3-C5-C6
22	3	401	CLA	C2B-C3B-CAB-CBB
22	6	309	CLA	C2B-C3B-CAB-CBB
22	6	318	CLA	C2B-C3B-CAB-CBB
22	7	310	CLA	C2B-C3B-CAB-CBB
22	8	610	CLA	C2B-C3B-CAB-CBB
22	9	604	CLA	C2B-C3B-CAB-CBB
22	9	612	CLA	C2B-C3B-CAB-CBB
22	A	821	CLA	C2B-C3B-CAB-CBB
22	A	829	CLA	C2B-C3B-CAB-CBB
22	B	818	CLA	C2B-C3B-CAB-CBB
22	B	819	CLA	C2B-C3B-CAB-CBB
22	B	827	CLA	C2B-C3B-CAB-CBB
22	F	802	CLA	C2B-C3B-CAB-CBB
22	9	608	CLA	C15-C16-C17-C18
28	3	421	LMU	O1'-C1-C2-C3
22	B	805	CLA	C16-C17-C18-C20
25	7	316	XAT	C32-C33-C34-C35
26	5	322	BCR	C12-C13-C14-C15
26	A	851	BCR	C11-C10-C9-C8
26	B	848	BCR	C11-C10-C9-C8
26	B	848	BCR	C20-C21-C22-C23
26	F	805	BCR	C16-C17-C18-C19
26	L	301	BCR	C20-C21-C22-C23
30	5	323	NEX	C28-C29-C30-C31
30	6	321	NEX	C28-C29-C30-C31
22	G	203	CLA	CAA-CBA-CGA-O1A
22	3	409	CLA	CBA-CGA-O2A-C1
22	7	308	CLA	O1D-CGD-O2D-CED
25	3	416	XAT	C9-C10-C11-C12
26	3	417	BCR	C9-C10-C11-C12
22	5	316	CLA	CAA-CBA-CGA-O2A
22	7	302	CLA	CAA-CBA-CGA-O2A
22	G	203	CLA	CAA-CBA-CGA-O2A
28	H	204	LMU	C2B-C1B-O1B-C4'
22	7	302	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	B	832	CLA	C2-C1-O2A-CGA
22	B	837	CLA	C2-C1-O2A-CGA
22	6	312	CLA	C3A-C2A-CAA-CBA
22	B	821	CLA	C2-C3-C5-C6
23	3	406	CHL	C2-C3-C5-C6
22	B	830	CLA	O1A-CGA-O2A-C1
23	6	303	CHL	C5-C6-C7-C8
22	B	805	CLA	CAA-CBA-CGA-O2A
32	A	842	PQN	C21-C22-C23-C24
22	B	830	CLA	CBA-CGA-O2A-C1
22	6	304	CLA	O1A-CGA-O2A-C1
22	A	826	CLA	O1A-CGA-O2A-C1
22	9	603	CLA	C3-C5-C6-C7
22	B	830	CLA	C3-C5-C6-C7
23	8	608	CHL	C4-C3-C5-C6
22	A	817	CLA	CAA-CBA-CGA-O2A
23	8	603	CHL	C16-C17-C18-C20
22	B	822	CLA	CAA-CBA-CGA-O2A
22	3	409	CLA	O1A-CGA-O2A-C1
24	3	415	LUT	C1-C6-C7-C8
26	5	322	BCR	C1-C6-C7-C8
26	5	322	BCR	C5-C6-C7-C8
22	5	304	CLA	CAA-CBA-CGA-O2A
22	B	811	CLA	CAA-CBA-CGA-O2A
26	A	847	BCR	C37-C22-C23-C24
27	5	301	LHG	C10-C11-C12-C13
25	5	321	XAT	C9-C10-C11-C12
26	9	615	BCR	C15-C16-C17-C18
26	A	851	BCR	C13-C14-C15-C16
32	A	842	PQN	C14-C13-C15-C16
22	1	302	CLA	C1A-C2A-CAA-CBA
22	K	205	CLA	C1A-C2A-CAA-CBA
26	F	801	BCR	C11-C12-C13-C14
26	K	207	BCR	C21-C22-C23-C24
22	B	835	CLA	C10-C11-C12-C13
22	7	308	CLA	CBD-CGD-O2D-CED
22	A	815	CLA	CAA-CBA-CGA-O2A
22	A	833	CLA	C3-C5-C6-C7
31	9	617	LMG	C36-C37-C38-C39
27	7	318	LHG	C25-C26-C27-C28
22	3	401	CLA	C4B-C3B-CAB-CBB
22	6	318	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	8	610	CLA	C4B-C3B-CAB-CBB
22	9	612	CLA	C4B-C3B-CAB-CBB
22	A	821	CLA	C4B-C3B-CAB-CBB
22	A	829	CLA	C4B-C3B-CAB-CBB
22	B	827	CLA	C4B-C3B-CAB-CBB
22	B	830	CLA	C4B-C3B-CAB-CBB
23	8	602	CHL	C1-C2-C3-C5
22	B	813	CLA	C2-C1-O2A-CGA
23	5	308	CHL	C4-C3-C5-C6
22	1	308	CLA	C11-C10-C8-C7
22	3	408	CLA	C11-C10-C8-C7
22	A	820	CLA	C2-C3-C5-C6
23	7	305	CHL	C11-C12-C13-C15
22	1	312	CLA	C8-C10-C11-C12
22	A	823	CLA	C3-C5-C6-C7
28	6	301	LMU	C4-C5-C6-C7
23	1	304	CHL	C1-C2-C3-C4
24	8	617	LUT	C29-C30-C31-C32
24	9	613	LUT	C9-C10-C11-C12
26	J	101	BCR	C9-C10-C11-C12
22	B	809	CLA	CAA-CBA-CGA-O2A
27	1	318	LHG	C7-C8-C9-C10
22	L	303	CLA	C5-C6-C7-C8
27	6	322	LHG	C10-C11-C12-C13
22	A	814	CLA	C15-C16-C17-C18
22	6	305	CLA	CAA-CBA-CGA-O1A
22	A	809	CLA	CAA-CBA-CGA-O2A
27	5	325	LHG	O8-C23-C24-C25
22	1	312	CLA	C10-C11-C12-C13
28	K	201	LMU	C1-C2-C3-C4
27	1	317	LHG	O8-C23-C24-C25
22	A	822	CLA	C4-C3-C5-C6
23	1	305	CHL	CAA-CBA-CGA-O2A
22	B	808	CLA	C11-C12-C13-C14
22	B	844	CLA	C11-C10-C8-C9
23	8	602	CHL	C6-C7-C8-C9
23	8	602	CHL	C14-C13-C15-C16
27	6	322	LHG	C13-C14-C15-C16
22	A	830	CLA	CAA-CBA-CGA-O1A
27	9	616	LHG	C31-C32-C33-C34
28	3	423	LMU	C5'-C4'-O1B-C1B
22	5	304	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	5	316	CLA	CBD-CGD-O2D-CED
22	8	611	CLA	C3A-C2A-CAA-CBA
22	9	604	CLA	C3A-C2A-CAA-CBA
22	B	829	CLA	C3A-C2A-CAA-CBA
23	5	308	CHL	C3A-C2A-CAA-CBA
22	A	834	CLA	O1A-CGA-O2A-C1
22	A	804	CLA	CAA-CBA-CGA-O2A
22	A	805	CLA	CAA-CBA-CGA-O2A
27	6	322	LHG	C15-C16-C17-C18
22	6	311	CLA	CAD-CBD-CGD-O2D
22	6	314	CLA	CAD-CBD-CGD-O2D
22	7	306	CLA	CAD-CBD-CGD-O2D
22	9	608	CLA	CAD-CBD-CGD-O2D
22	9	612	CLA	CAD-CBD-CGD-O2D
22	A	803	CLA	CAD-CBD-CGD-O2D
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	811	CLA	CAD-CBD-CGD-O2D
22	A	812	CLA	CAD-CBD-CGD-O2D
22	A	814	CLA	CAD-CBD-CGD-O2D
22	A	819	CLA	CAD-CBD-CGD-O2D
22	A	822	CLA	CAD-CBD-CGD-O2D
22	A	833	CLA	CAD-CBD-CGD-O2D
22	A	840	CLA	CAD-CBD-CGD-O2D
22	B	828	CLA	CAD-CBD-CGD-O2D
22	B	837	CLA	CAD-CBD-CGD-O2D
22	B	839	CLA	CAD-CBD-CGD-O2D
22	L	302	CLA	CAD-CBD-CGD-O2D
22	3	403	CLA	C16-C17-C18-C20
22	B	803	CLA	C16-C17-C18-C20
23	5	302	CHL	C3-C5-C6-C7
31	8	621	LMG	O9-C10-O7-C8
22	B	823	CLA	C2-C1-O2A-CGA
22	B	829	CLA	C2-C1-O2A-CGA
22	5	317	CLA	CAA-CBA-CGA-O2A
27	7	318	LHG	C17-C18-C19-C20
22	A	839	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	C4-C3-C5-C6
22	8	609	CLA	CAA-CBA-CGA-O2A
22	B	822	CLA	CAA-CBA-CGA-O1A
22	A	822	CLA	C2-C3-C5-C6
25	8	618	XAT	C11-C12-C13-C14
26	7	317	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	5	321	XAT	O4-C6-C7-C8
25	7	316	XAT	O24-C26-C27-C28
25	9	614	XAT	O4-C6-C7-C8
25	9	614	XAT	O24-C26-C27-C28
31	J	104	LMG	C7-C8-C9-O8
27	B	801	LHG	O6-C4-C5-O7
22	L	302	CLA	CAA-CBA-CGA-O2A
22	A	806	CLA	CBD-CGD-O2D-CED
22	1	312	CLA	O2A-C1-C2-C3
22	B	806	CLA	O2A-C1-C2-C3
22	B	827	CLA	O2A-C1-C2-C3
23	3	405	CHL	O2A-C1-C2-C3
23	8	608	CHL	O2A-C1-C2-C3
22	8	613	CLA	C2A-CAA-CBA-CGA
22	5	317	CLA	CAA-CBA-CGA-O1A
31	8	621	LMG	C12-C13-C14-C15
22	2	612	CLA	C16-C17-C18-C20
22	B	829	CLA	C16-C17-C18-C19
22	1	302	CLA	CHA-CBD-CGD-O1D
22	1	302	CLA	CHA-CBD-CGD-O2D
22	1	303	CLA	CHA-CBD-CGD-O1D
22	1	311	CLA	CHA-CBD-CGD-O1D
22	1	311	CLA	CHA-CBD-CGD-O2D
22	2	601	CLA	CHA-CBD-CGD-O1D
22	2	613	CLA	CHA-CBD-CGD-O2D
22	5	303	CLA	CHA-CBD-CGD-O2D
22	5	312	CLA	CHA-CBD-CGD-O2D
22	6	304	CLA	CHA-CBD-CGD-O2D
22	6	309	CLA	CHA-CBD-CGD-O1D
22	6	309	CLA	CHA-CBD-CGD-O2D
22	7	303	CLA	CHA-CBD-CGD-O1D
22	7	303	CLA	CHA-CBD-CGD-O2D
22	7	309	CLA	CHA-CBD-CGD-O2D
22	7	313	CLA	CHA-CBD-CGD-O1D
22	7	313	CLA	CHA-CBD-CGD-O2D
22	8	611	CLA	CHA-CBD-CGD-O2D
22	8	613	CLA	CHA-CBD-CGD-O1D
22	8	613	CLA	CHA-CBD-CGD-O2D
22	A	802	CLA	CHA-CBD-CGD-O1D
22	A	802	CLA	CHA-CBD-CGD-O2D
22	A	805	CLA	CHA-CBD-CGD-O1D
22	A	821	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	833	CLA	CHA-CBD-CGD-O2D
22	B	804	CLA	CHA-CBD-CGD-O2D
22	B	822	CLA	CHA-CBD-CGD-O1D
22	B	822	CLA	CHA-CBD-CGD-O2D
22	B	826	CLA	CHA-CBD-CGD-O1D
22	B	826	CLA	CHA-CBD-CGD-O2D
22	B	831	CLA	CHA-CBD-CGD-O1D
22	B	831	CLA	CHA-CBD-CGD-O2D
22	B	835	CLA	CHA-CBD-CGD-O1D
22	B	835	CLA	CHA-CBD-CGD-O2D
22	B	836	CLA	CHA-CBD-CGD-O1D
22	B	836	CLA	CHA-CBD-CGD-O2D
22	G	202	CLA	CHA-CBD-CGD-O1D
22	K	206	CLA	CHA-CBD-CGD-O2D
23	1	305	CHL	CHA-CBD-CGD-O2D
23	8	602	CHL	CHA-CBD-CGD-O1D
23	8	603	CHL	CHA-CBD-CGD-O1D
23	8	603	CHL	CHA-CBD-CGD-O2D
23	1	305	CHL	CAA-CBA-CGA-O1A
22	2	612	CLA	CAA-CBA-CGA-O2A
22	B	806	CLA	C2-C3-C5-C6
22	8	609	CLA	CAA-CBA-CGA-O1A
22	A	815	CLA	CAA-CBA-CGA-O1A
22	A	830	CLA	CAA-CBA-CGA-O2A
23	1	306	CHL	CAA-CBA-CGA-O2A
22	F	804	CLA	CAA-CBA-CGA-O2A
27	9	616	LHG	O7-C5-C6-O8
28	7	319	LMU	C2B-C1B-O1B-C4'
28	9	618	LMU	C5'-C4'-O1B-C1B
22	9	603	CLA	CAA-CBA-CGA-O2A
22	9	606	CLA	CAA-CBA-CGA-O2A
23	3	413	CHL	CAA-CBA-CGA-O2A
23	7	305	CHL	CAA-CBA-CGA-O2A
27	2	617	LHG	O7-C7-C8-C9
23	8	602	CHL	C2A-CAA-CBA-CGA
22	B	829	CLA	C13-C15-C16-C17
22	A	834	CLA	CBA-CGA-O2A-C1
27	2	617	LHG	C8-C7-O7-C5
27	B	801	LHG	C8-C7-O7-C5
22	A	804	CLA	C11-C12-C13-C15
27	8	620	LHG	C24-C25-C26-C27
22	3	404	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	6	304	CLA	C6-C7-C8-C9
22	6	316	CLA	C11-C12-C13-C14
22	7	307	CLA	C14-C13-C15-C16
22	A	802	CLA	C11-C12-C13-C14
22	A	820	CLA	C6-C7-C8-C9
22	B	809	CLA	C11-C10-C8-C9
22	B	812	CLA	C6-C7-C8-C9
25	6	320	XAT	C9-C10-C11-C12
25	6	320	XAT	C29-C30-C31-C32
22	6	304	CLA	C2B-C3B-CAB-CBB
22	A	815	CLA	C2B-C3B-CAB-CBB
28	7	319	LMU	C3-C4-C5-C6
22	G	202	CLA	C3-C5-C6-C7
28	G	201	LMU	C3-C4-C5-C6
22	B	838	CLA	CAA-CBA-CGA-O2A
22	B	829	CLA	CAA-CBA-CGA-O2A
27	M	101	LHG	C25-C26-C27-C28
22	6	305	CLA	CAA-CBA-CGA-O2A
22	8	614	CLA	C11-C12-C13-C14
22	B	823	CLA	C6-C7-C8-C10
22	B	806	CLA	CAA-CBA-CGA-O2A
26	3	417	BCR	C7-C8-C9-C10
26	A	847	BCR	C21-C22-C23-C24
26	K	203	BCR	C7-C8-C9-C10
22	B	808	CLA	C13-C15-C16-C17
28	6	301	LMU	C4'-C5'-C6'-O6'
27	5	301	LHG	C11-C10-C9-C8
22	3	407	CLA	C1A-C2A-CAA-CBA
22	3	411	CLA	CHA-CBD-CGD-O2D
22	7	310	CLA	C1A-C2A-CAA-CBA
22	9	607	CLA	C1A-C2A-CAA-CBA
22	A	834	CLA	C1A-C2A-CAA-CBA
22	B	802	CLA	C1A-C2A-CAA-CBA
22	B	803	CLA	C1A-C2A-CAA-CBA
22	B	820	CLA	C1A-C2A-CAA-CBA
22	B	829	CLA	C1A-C2A-CAA-CBA
23	5	302	CHL	C1A-C2A-CAA-CBA
22	B	805	CLA	C16-C17-C18-C19
22	L	302	CLA	CAA-CBA-CGA-O1A
22	B	830	CLA	CAA-CBA-CGA-O2A
22	A	833	CLA	C5-C6-C7-C8
22	A	825	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	B	843	CLA	C2-C1-O2A-CGA
22	A	805	CLA	CAA-CBA-CGA-O1A
22	A	809	CLA	CAA-CBA-CGA-O1A
27	2	617	LHG	O9-C7-C8-C9
31	J	105	LMG	O1-C7-C8-C9
22	9	603	CLA	C2A-CAA-CBA-CGA
27	1	317	LHG	O10-C23-C24-C25
22	A	806	CLA	O1D-CGD-O2D-CED
27	A	845	LHG	C24-C25-C26-C27
22	2	613	CLA	CAA-CBA-CGA-O2A
22	A	820	CLA	C4-C3-C5-C6
23	6	303	CHL	C4-C3-C5-C6
27	9	616	LHG	O8-C23-C24-C25
22	A	839	CLA	CAA-CBA-CGA-O1A
27	7	318	LHG	C16-C17-C18-C19
28	7	319	LMU	C2'-C1'-O1'-C1
22	9	604	CLA	C4B-C3B-CAB-CBB
27	1	317	LHG	C3-O3-P-O5
27	7	318	LHG	C3-O3-P-O5
27	7	318	LHG	C4-O6-P-O4
27	9	616	LHG	C4-O6-P-O5
27	A	845	LHG	C3-O3-P-O5
27	M	101	LHG	C3-O3-P-O5
27	B	801	LHG	C11-C12-C13-C14
22	2	612	CLA	CAA-CBA-CGA-O1A
23	3	413	CHL	CAA-CBA-CGA-O1A
27	5	325	LHG	O10-C23-C24-C25
23	1	306	CHL	CAA-CBA-CGA-O1A
24	3	415	LUT	C5-C6-C7-C8
26	A	851	BCR	C5-C6-C7-C8
22	8	613	CLA	C8-C10-C11-C12
23	5	302	CHL	C5-C6-C7-C8
22	A	804	CLA	CAA-CBA-CGA-O1A
22	F	804	CLA	CAA-CBA-CGA-O1A
27	A	844	LHG	C24-C25-C26-C27
22	A	812	CLA	CAA-CBA-CGA-O2A
22	B	812	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	C16-C17-C18-C19
22	3	402	CLA	C2A-CAA-CBA-CGA
32	A	842	PQN	C20-C21-C22-C23
28	1	319	LMU	C7-C8-C9-C10
22	A	804	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	6	304	CLA	C4-C3-C5-C6
22	2	601	CLA	CAD-CBD-CGD-O1D
22	6	309	CLA	CAD-CBD-CGD-O1D
22	7	307	CLA	CAD-CBD-CGD-O1D
22	8	613	CLA	CAD-CBD-CGD-O1D
22	A	821	CLA	CAD-CBD-CGD-O1D
22	A	841	CLA	CAD-CBD-CGD-O1D
23	3	422	CHL	CAD-CBD-CGD-O1D
23	5	302	CHL	CAD-CBD-CGD-O1D
22	9	603	CLA	CAA-CBA-CGA-O1A
22	2	602	CLA	C5-C6-C7-C8
22	A	805	CLA	C11-C12-C13-C14
22	A	810	CLA	C11-C10-C8-C9
22	A	812	CLA	C6-C7-C8-C9
22	B	842	CLA	C6-C7-C8-C9
23	7	305	CHL	CAA-CBA-CGA-O1A
22	B	821	CLA	C11-C12-C13-C15
22	A	833	CLA	CAA-CBA-CGA-O2A
27	5	301	LHG	O7-C7-C8-C9
22	2	613	CLA	CAA-CBA-CGA-O1A
22	B	838	CLA	CAA-CBA-CGA-O1A
22	9	606	CLA	CAA-CBA-CGA-O1A
22	2	601	CLA	CAA-CBA-CGA-O2A
22	3	409	CLA	CAA-CBA-CGA-O2A
22	8	601	CLA	CAA-CBA-CGA-O2A
22	8	613	CLA	CAA-CBA-CGA-O2A
22	L	303	CLA	CAA-CBA-CGA-O2A
27	1	317	LHG	O7-C7-C8-C9
22	2	611	CLA	O1D-CGD-O2D-CED
28	6	302	LMU	C7-C8-C9-C10
22	7	307	CLA	CAA-CBA-CGA-O1A
28	G	201	LMU	C4'-C5'-C6'-O6'
23	6	303	CHL	C16-C17-C18-C19
22	2	602	CLA	C4-C3-C5-C6
26	F	801	BCR	C11-C12-C13-C35
31	J	104	LMG	C29-C30-C31-C32
22	1	310	CLA	CHA-CBD-CGD-O1D
22	3	407	CLA	C11-C10-C8-C7
22	3	411	CLA	CHA-CBD-CGD-O1D
22	3	414	CLA	CHA-CBD-CGD-O1D
22	6	307	CLA	C6-C7-C8-C10
22	6	313	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	8	601	CLA	CAD-CBD-CGD-O2D
22	A	823	CLA	C12-C13-C15-C16
22	A	841	CLA	C3A-C2A-CAA-CBA
22	A	843	CLA	CAD-CBD-CGD-O2D
22	B	803	CLA	C3A-C2A-CAA-CBA
22	B	814	CLA	CHA-CBD-CGD-O1D
22	B	824	CLA	CHA-CBD-CGD-O1D
22	B	842	CLA	C6-C7-C8-C10
23	3	406	CHL	C6-C7-C8-C10
23	6	303	CHL	C6-C7-C8-C10
22	6	307	CLA	CAA-CBA-CGA-O2A
22	7	307	CLA	CAA-CBA-CGA-O2A
22	9	609	CLA	CAA-CBA-CGA-O2A
22	A	808	CLA	CAA-CBA-CGA-O2A
22	A	814	CLA	CAA-CBA-CGA-O2A
23	5	308	CHL	CAA-CBA-CGA-O2A
24	5	320	LUT	C27-C28-C29-C30
24	7	315	LUT	C27-C28-C29-C30
25	7	316	XAT	C7-C8-C9-C10
22	9	609	CLA	CAA-CBA-CGA-O1A
22	B	806	CLA	CAA-CBA-CGA-O1A
23	5	308	CHL	CAA-CBA-CGA-O1A
23	6	308	CHL	CAA-CBA-CGA-O1A
22	B	829	CLA	C16-C17-C18-C20
22	A	824	CLA	CBA-CGA-O2A-C1
22	2	602	CLA	CAA-CBA-CGA-O2A
22	B	810	CLA	CAA-CBA-CGA-O2A
22	3	403	CLA	O1D-CGD-O2D-CED
22	2	601	CLA	CAA-CBA-CGA-O1A
22	A	833	CLA	CAA-CBA-CGA-O1A
27	A	845	LHG	C15-C16-C17-C18
22	A	820	CLA	CAA-CBA-CGA-O2A
22	B	827	CLA	CAA-CBA-CGA-O2A
23	6	303	CHL	CAA-CBA-CGA-O2A
27	A	844	LHG	O8-C23-C24-C25
34	B	852	DGD	O1G-C1A-C2A-C3A
22	A	832	CLA	C15-C16-C17-C18
22	6	307	CLA	CAA-CBA-CGA-O1A
22	8	613	CLA	CAA-CBA-CGA-O1A
22	B	829	CLA	CAA-CBA-CGA-O1A
27	1	317	LHG	O9-C7-C8-C9
27	9	616	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	A	828	CLA	C2A-CAA-CBA-CGA
22	A	820	CLA	C10-C11-C12-C13
27	8	620	LHG	O7-C7-C8-C9

There are no ring outliers.

217 monomers are involved in 415 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	827	CLA	2	0
31	J	105	LMG	1	0
23	6	303	CHL	5	0
22	7	306	CLA	1	0
23	5	302	CHL	4	0
24	6	319	LUT	2	0
22	B	816	CLA	4	0
26	A	846	BCR	5	0
22	3	407	CLA	3	0
25	6	320	XAT	5	0
22	B	826	CLA	1	0
28	1	319	LMU	2	0
26	K	203	BCR	1	0
26	L	301	BCR	3	0
22	B	830	CLA	3	0
28	6	323	LMU	1	0
26	B	850	BCR	5	0
22	A	834	CLA	2	0
30	6	321	NEX	2	0
22	B	823	CLA	4	0
22	B	825	CLA	1	0
22	B	815	CLA	4	0
22	A	804	CLA	4	0
22	A	802	CLA	1	0
28	G	201	LMU	2	0
22	B	835	CLA	2	0
22	A	824	CLA	2	0
30	5	323	NEX	5	0
22	7	310	CLA	2	0
28	9	618	LMU	2	0
22	G	202	CLA	1	0
28	J	106	LMU	1	0
22	6	314	CLA	3	0
28	3	423	LMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	847	BCR	2	0
26	A	848	BCR	3	0
26	B	848	BCR	3	0
22	A	828	CLA	1	0
22	2	611	CLA	1	0
27	2	617	LHG	3	0
22	5	314	CLA	1	0
23	3	406	CHL	5	0
22	9	606	CLA	3	0
22	A	805	CLA	4	0
26	J	101	BCR	3	0
25	3	416	XAT	4	0
27	9	616	LHG	1	0
26	B	851	BCR	4	0
22	A	817	CLA	2	0
26	J	103	BCR	2	0
22	2	602	CLA	3	0
22	B	811	CLA	8	0
22	9	609	CLA	2	0
22	6	311	CLA	4	0
27	M	101	LHG	3	0
22	3	404	CLA	2	0
28	3	421	LMU	2	0
22	A	806	CLA	1	0
26	7	317	BCR	3	0
22	A	809	CLA	1	0
22	A	837	CLA	1	0
22	B	843	CLA	1	0
22	B	828	CLA	1	0
22	6	309	CLA	1	0
23	3	413	CHL	1	0
22	B	813	CLA	1	0
22	B	836	CLA	3	0
22	B	808	CLA	4	0
24	1	314	LUT	4	0
22	7	307	CLA	1	0
22	A	816	CLA	1	0
26	3	419	BCR	5	0
25	2	615	XAT	3	0
22	5	303	CLA	2	0
26	5	322	BCR	5	0
24	2	614	LUT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	833	CLA	1	0
23	7	304	CHL	2	0
27	A	845	LHG	2	0
22	6	316	CLA	2	0
24	8	617	LUT	3	0
22	A	813	CLA	2	0
22	A	821	CLA	1	0
22	B	820	CLA	1	0
26	1	316	BCR	3	0
22	1	313	CLA	1	0
22	B	812	CLA	1	0
22	A	820	CLA	1	0
26	M	102	BCR	4	0
22	A	819	CLA	2	0
22	2	608	CLA	1	0
25	9	614	XAT	4	0
22	8	615	CLA	1	0
22	7	308	CLA	1	0
22	8	610	CLA	5	0
22	2	603	CLA	2	0
22	8	613	CLA	2	0
26	9	615	BCR	3	0
34	B	852	DGD	3	0
22	1	308	CLA	5	0
26	G	204	BCR	4	0
22	A	808	CLA	1	0
32	A	842	PQN	5	0
22	B	840	CLA	2	0
22	B	841	CLA	2	0
22	6	307	CLA	1	0
22	B	805	CLA	2	0
26	B	847	BCR	2	0
23	5	309	CHL	2	0
22	B	829	CLA	2	0
22	3	401	CLA	1	0
25	7	316	XAT	4	0
22	6	305	CLA	2	0
22	A	814	CLA	4	0
22	3	408	CLA	5	0
24	7	315	LUT	2	0
25	5	321	XAT	1	0
22	H	203	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	831	CLA	3	0
27	8	620	LHG	3	0
22	6	315	CLA	2	0
23	5	307	CHL	3	0
23	9	605	CHL	1	0
22	9	607	CLA	2	0
24	3	418	LUT	6	0
28	H	204	LMU	2	0
26	K	207	BCR	3	0
22	8	609	CLA	1	0
22	A	833	CLA	1	0
22	A	827	CLA	1	0
22	5	311	CLA	3	0
22	7	309	CLA	3	0
26	I	201	BCR	3	0
22	B	806	CLA	6	0
22	B	837	CLA	1	0
22	A	841	CLA	2	0
22	8	612	CLA	2	0
22	A	801	CLA	4	0
27	5	301	LHG	2	0
23	3	422	CHL	2	0
23	8	608	CHL	2	0
27	7	318	LHG	1	0
22	2	606	CLA	1	0
22	6	318	CLA	4	0
24	3	415	LUT	5	0
22	7	314	CLA	2	0
22	A	818	CLA	4	0
22	A	832	CLA	2	0
26	A	849	BCR	6	0
22	A	836	CLA	2	0
27	B	801	LHG	3	0
22	3	403	CLA	1	0
27	1	318	LHG	2	0
23	8	606	CHL	2	0
22	L	303	CLA	3	0
22	5	310	CLA	3	0
22	9	608	CLA	4	0
28	7	319	LMU	1	0
22	9	612	CLA	1	0
24	5	320	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	803	CLA	3	0
24	9	613	LUT	4	0
22	7	301	CLA	2	0
22	B	807	CLA	1	0
22	1	301	CLA	3	0
32	B	845	PQN	2	0
22	B	809	CLA	2	0
26	A	851	BCR	2	0
33	A	850	SF4	1	0
22	B	804	CLA	3	0
22	2	607	CLA	1	0
22	5	316	CLA	1	0
26	F	805	BCR	5	0
22	9	602	CLA	2	0
27	A	844	LHG	4	0
27	5	325	LHG	3	0
26	3	417	BCR	4	0
22	1	311	CLA	1	0
25	1	315	XAT	4	0
22	A	826	CLA	3	0
26	8	619	BCR	2	0
26	L	305	BCR	3	0
22	A	823	CLA	2	0
26	B	846	BCR	1	0
23	8	603	CHL	3	0
22	2	610	CLA	1	0
22	B	802	CLA	3	0
27	6	322	LHG	6	0
22	2	613	CLA	2	0
23	5	319	CHL	1	0
22	F	804	CLA	2	0
25	8	618	XAT	4	0
22	B	810	CLA	4	0
22	B	817	CLA	1	0
22	6	313	CLA	1	0
22	A	812	CLA	3	0
23	8	602	CHL	5	0
22	B	844	CLA	1	0
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26	F	801	BCR	6	0
22	A	838	CLA	2	0
22	B	822	CLA	1	0

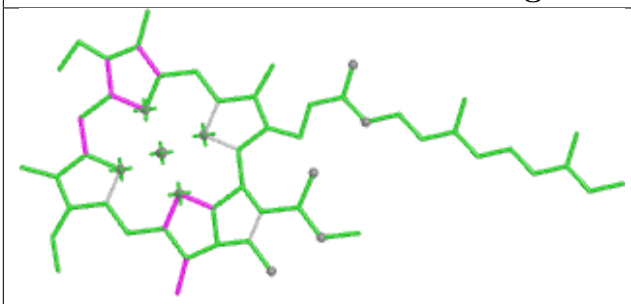
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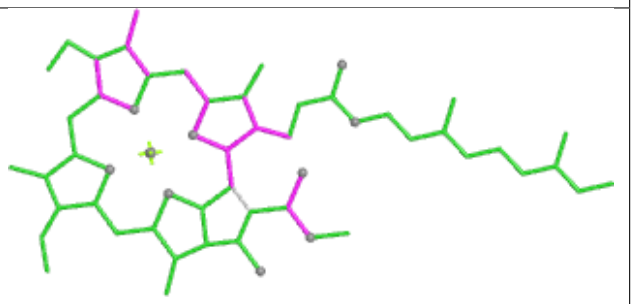
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	9	617	LMG	6	0
22	A	839	CLA	2	0
22	3	402	CLA	2	0
22	6	306	CLA	1	0
22	A	829	CLA	3	0
22	F	802	CLA	4	0
22	9	610	CLA	1	0
26	B	849	BCR	4	0
22	B	832	CLA	1	0
22	A	811	CLA	1	0
22	2	601	CLA	3	0
23	5	308	CHL	2	0
22	5	313	CLA	1	0
22	6	304	CLA	2	0
23	7	305	CHL	2	0

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.

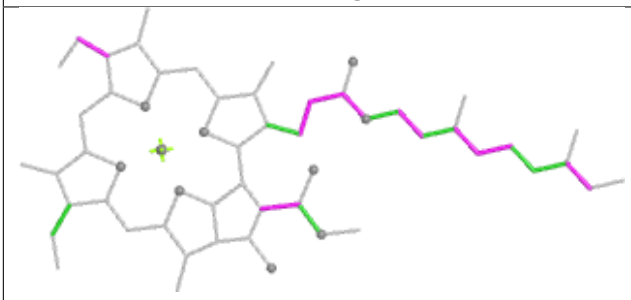
Ligand CLA B 827



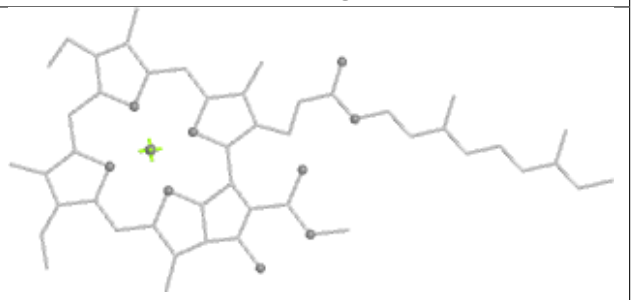
Bond lengths



Bond angles

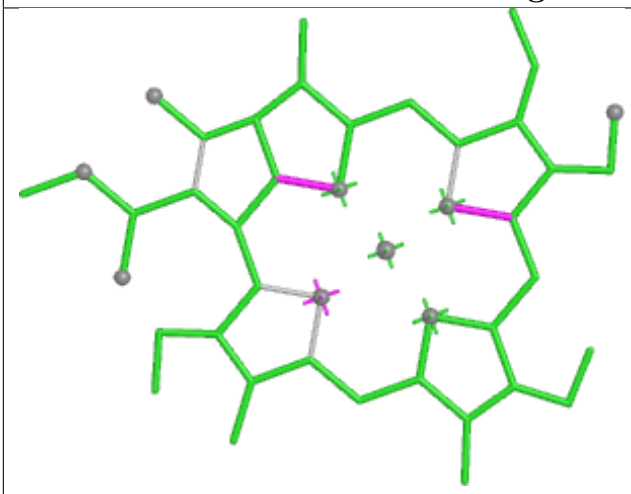


Torsions

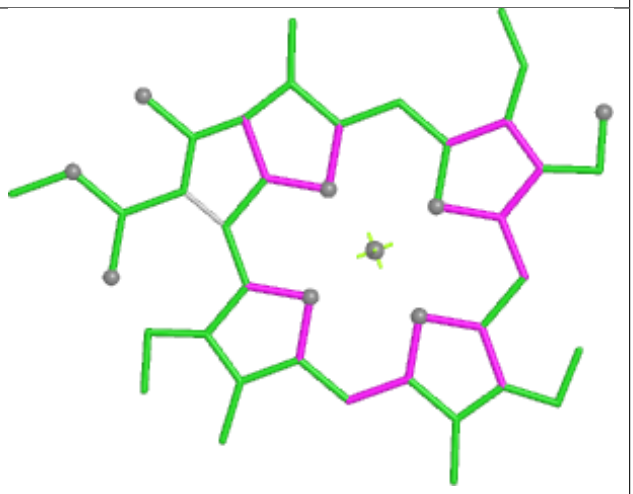


Rings

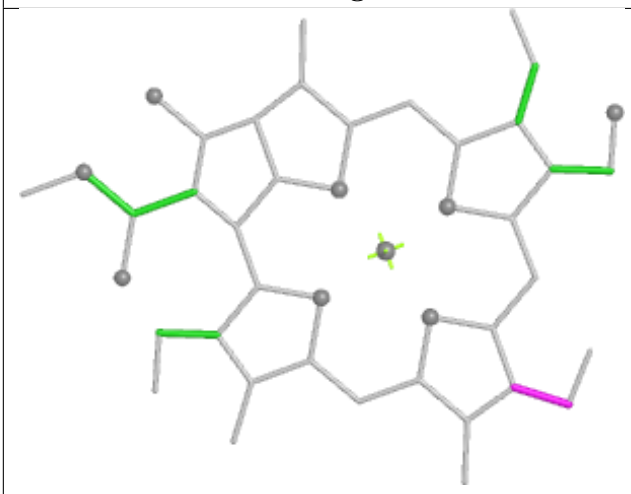
Ligand CHL 9 601



Bond lengths



Bond angles

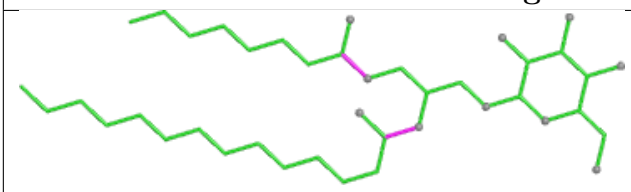


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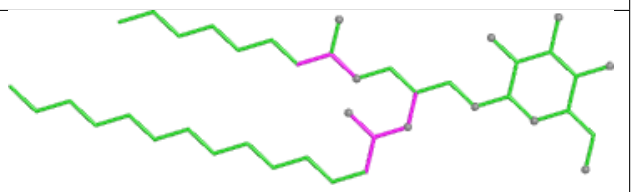


Rings

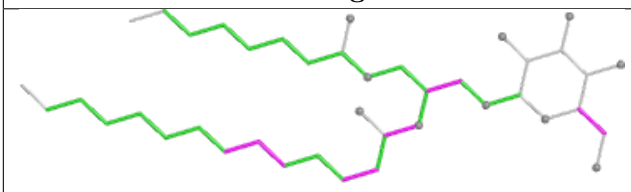
Ligand LMG J 105



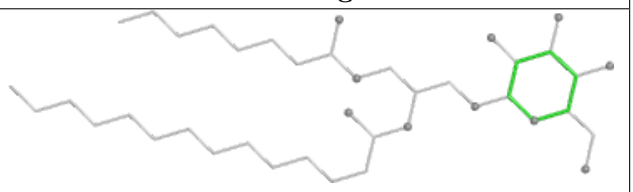
Bond lengths



Bond angles

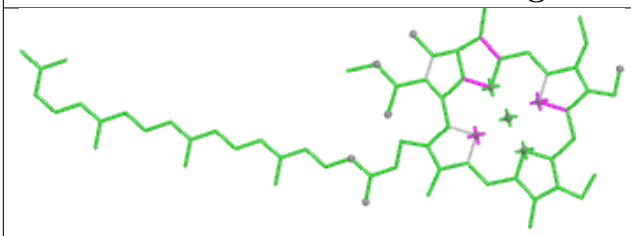


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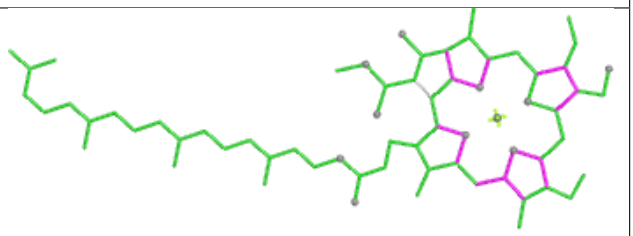


Rings

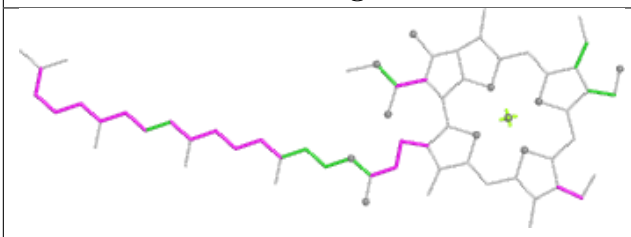
Ligand CHL 6 303



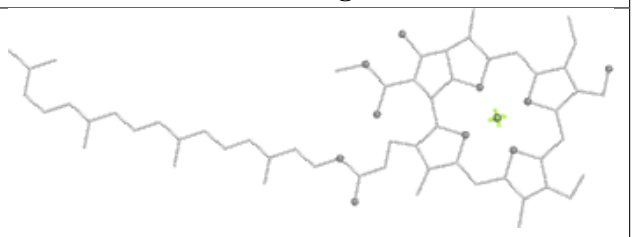
Bond lengths



Bond angles

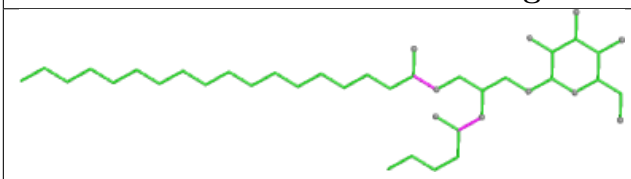


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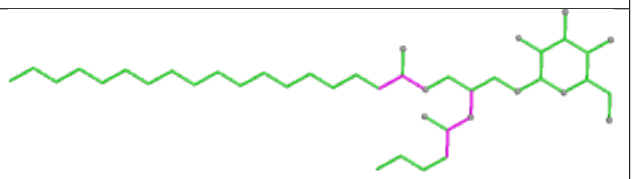


Rings

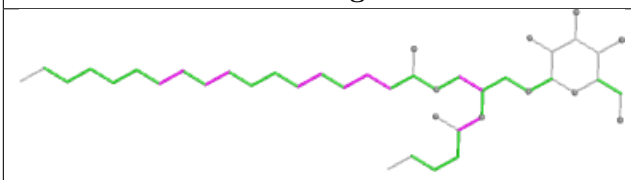
Ligand LMG J 104



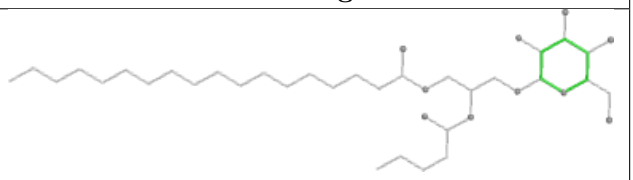
Bond lengths



Bond angles

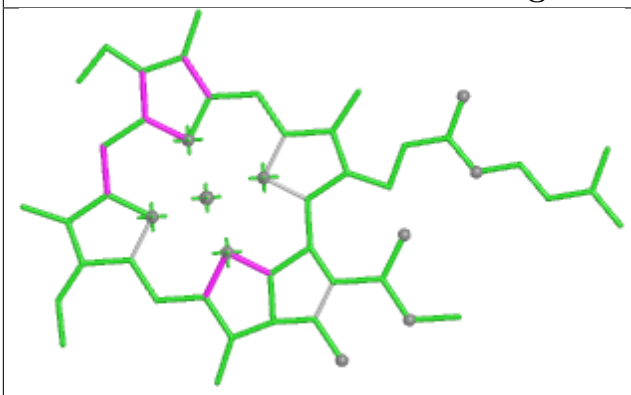


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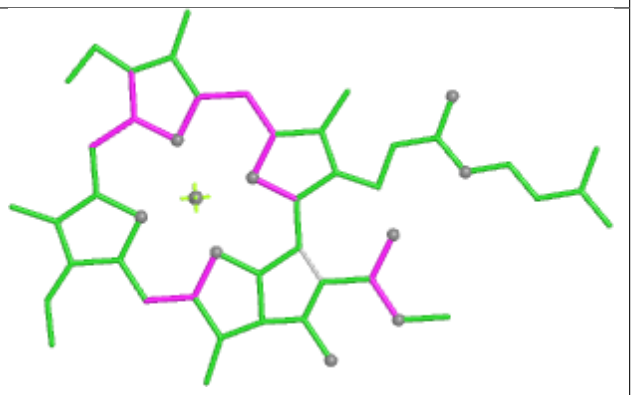


Rings

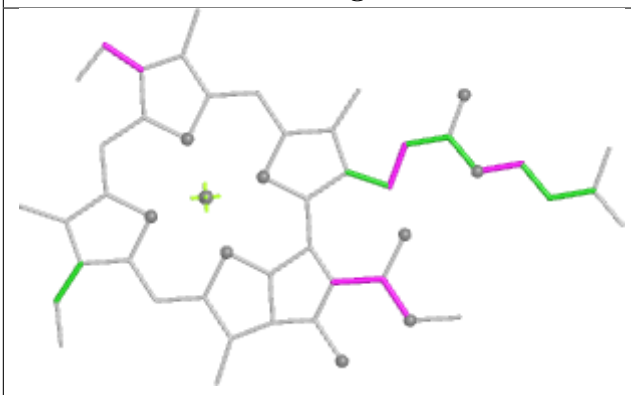
Ligand CLA 7 306



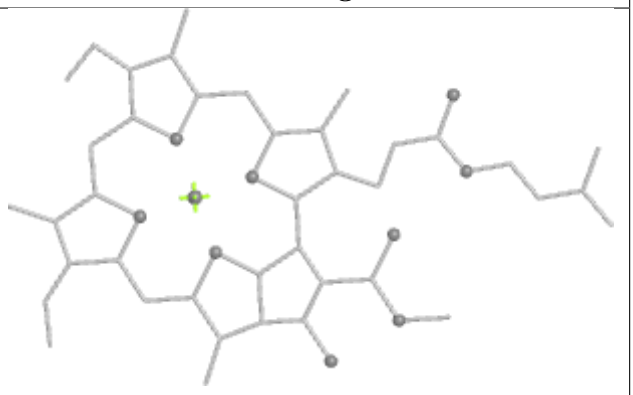
Bond lengths



Bond angles

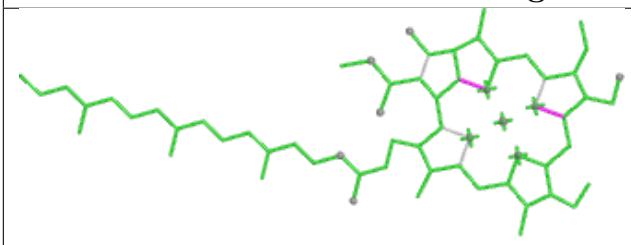


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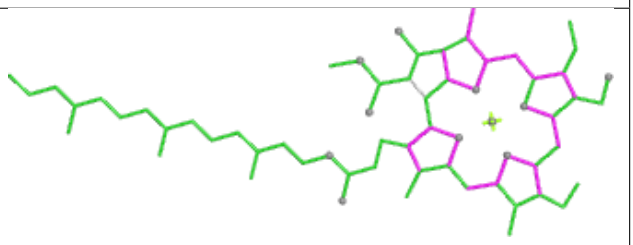


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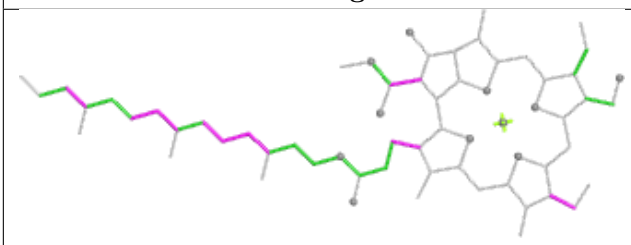
Ligand CHL 5 302



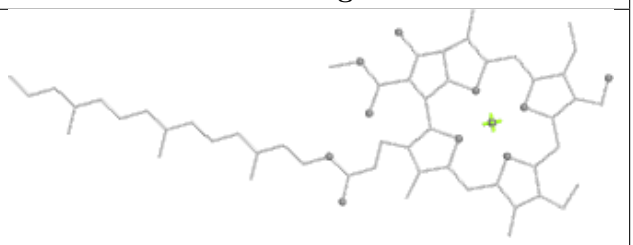
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Bond angles

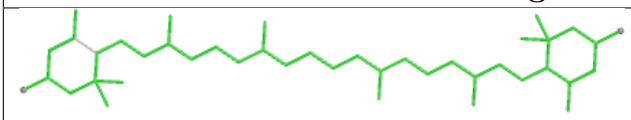


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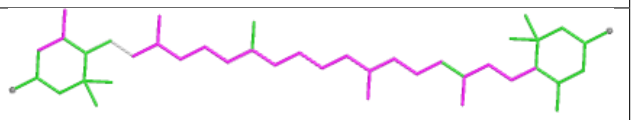


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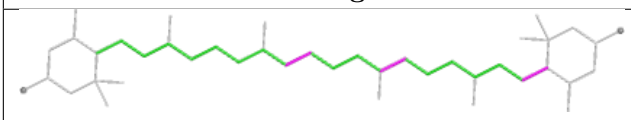
Ligand LUT 6 319



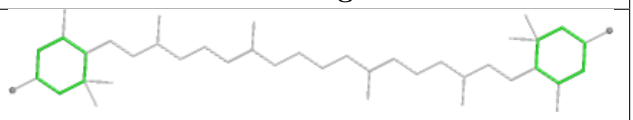
Bond lengths



Bond angles

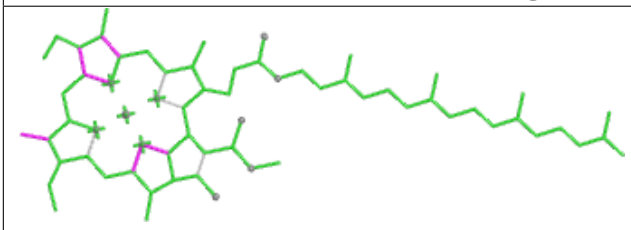


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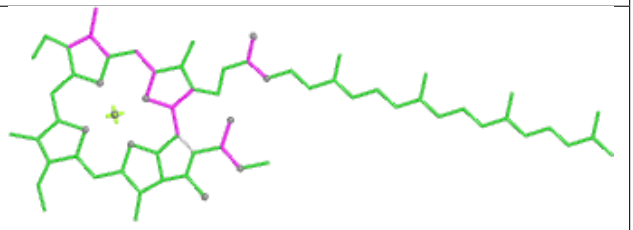


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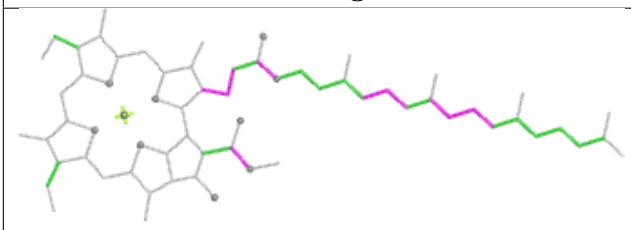
Ligand CLA B 816



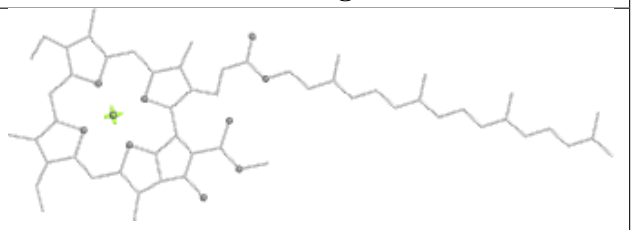
Bond lengths



Bond angles

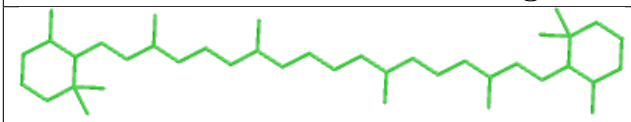


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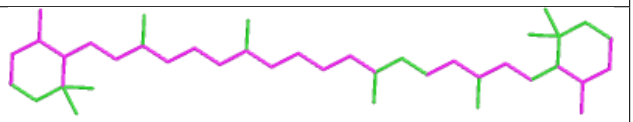


Rings

Ligand BCR A 846



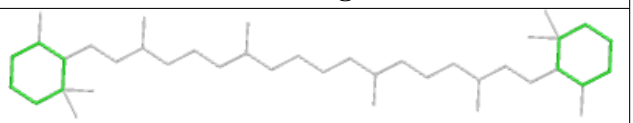
Bond lengths



Bond angles

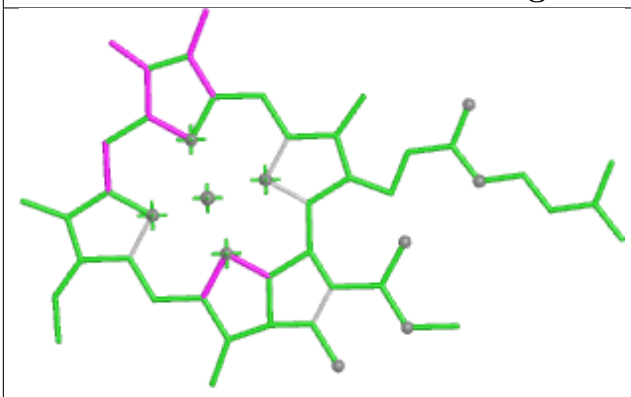


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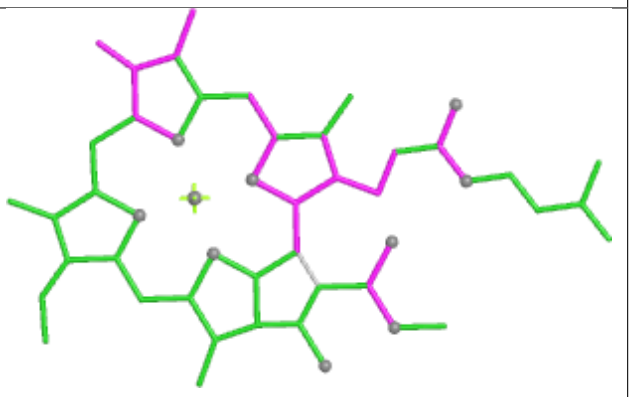


Rings

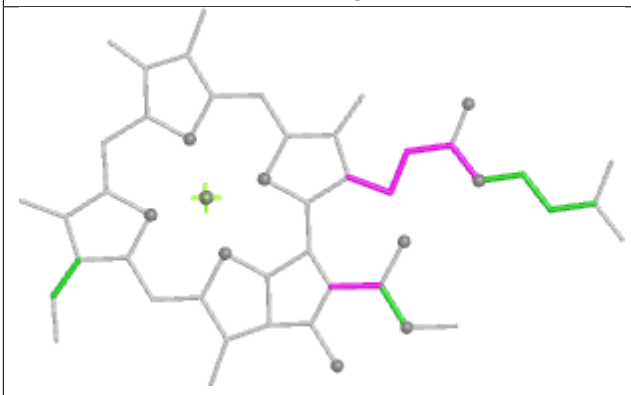
Ligand CLA 5 304



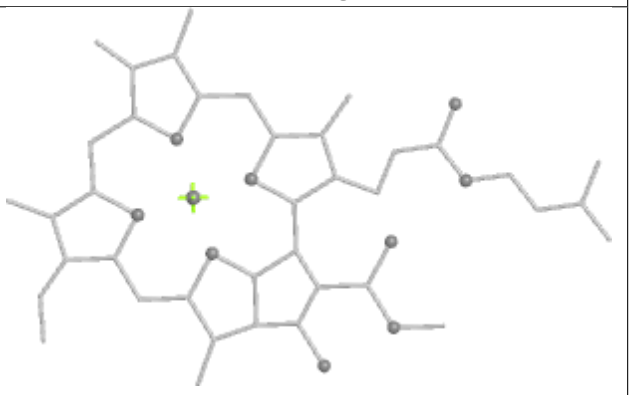
Bond lengths



Bond angles

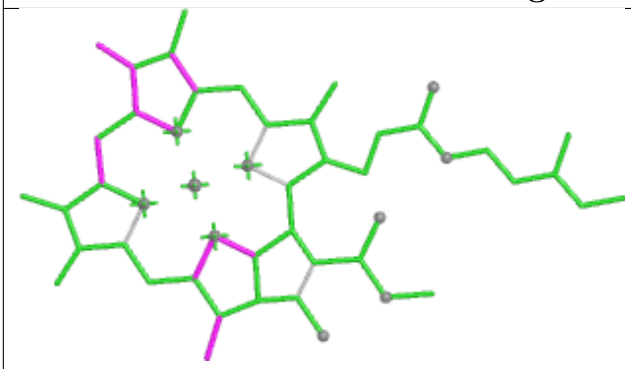


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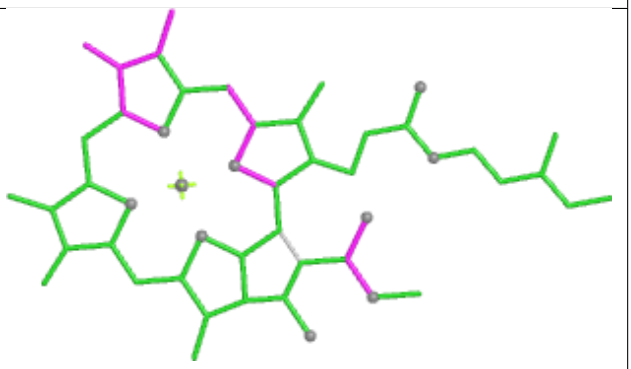


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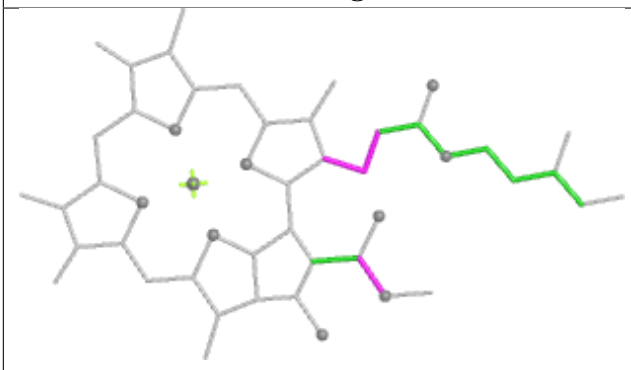
Ligand CLA 5 305



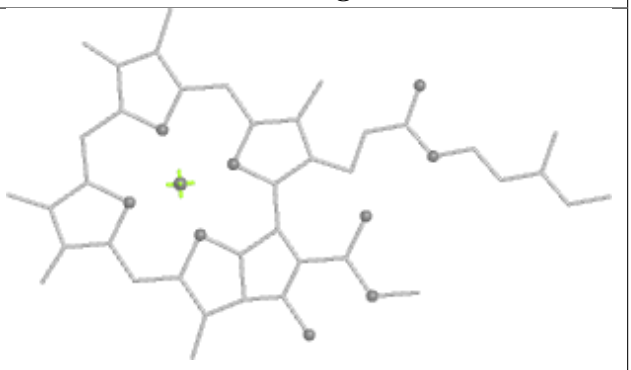
Bond lengths



Bond angles

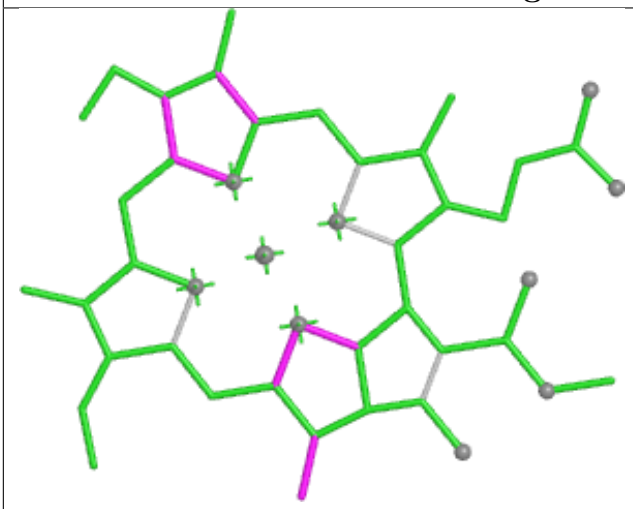


Torsions

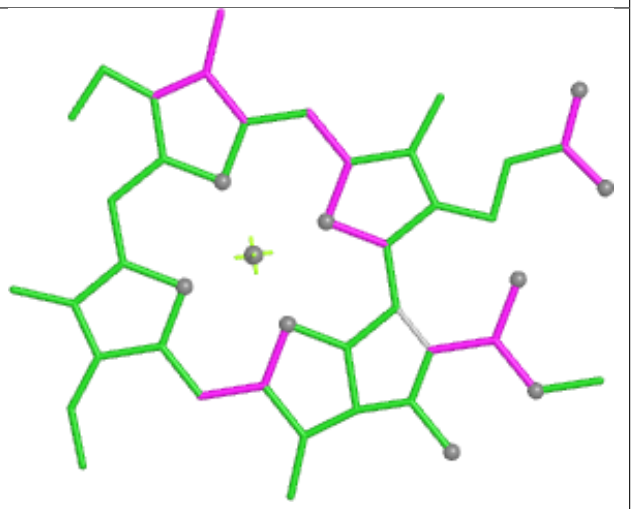


Rings

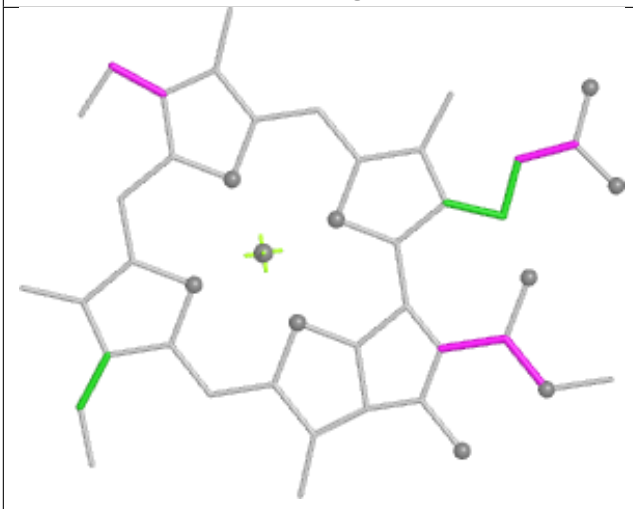
Ligand CLA A 815



Bond lengths



Bond angles

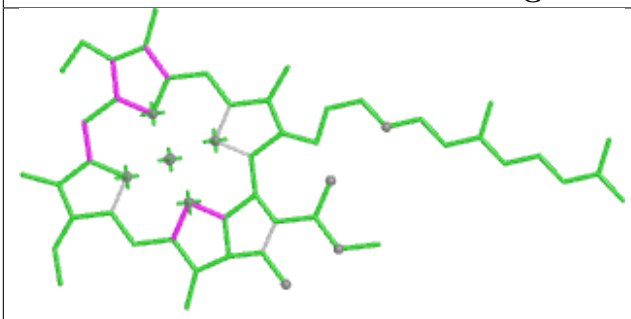


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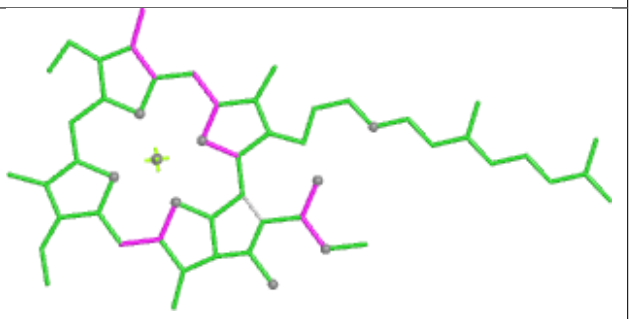


Rings

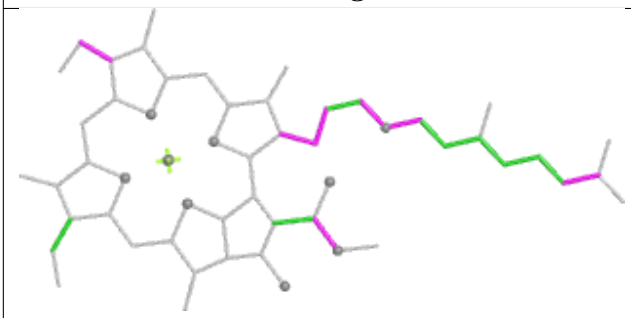
Ligand CLA B 819



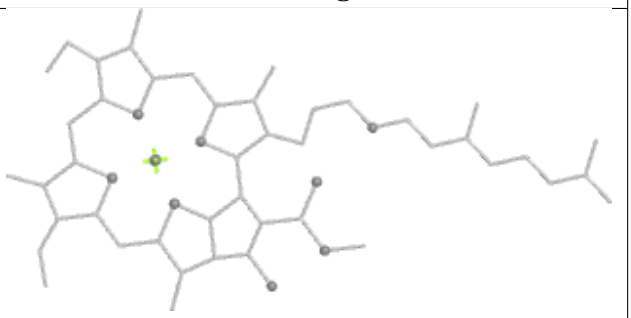
Bond lengths



Bond angles

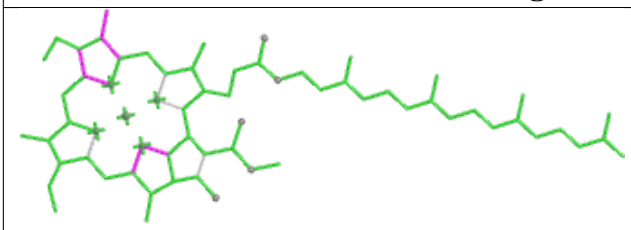


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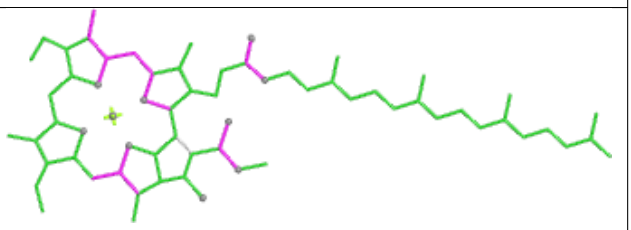


Rings

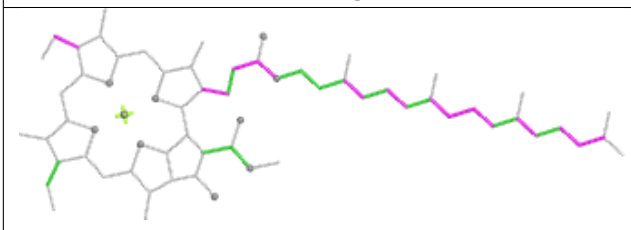
Ligand CLA 3 407



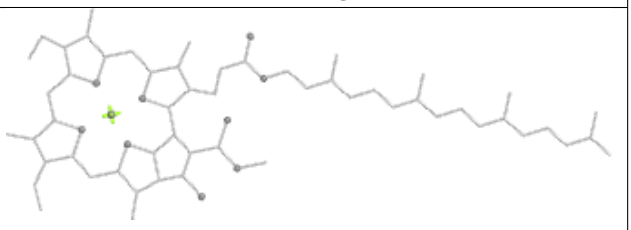
Bond lengths



Bond angles

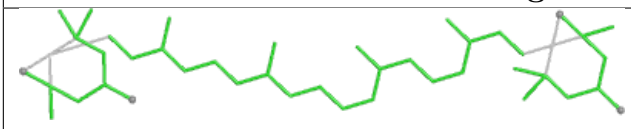


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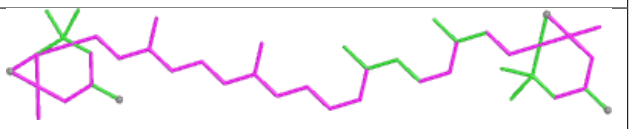


Rings

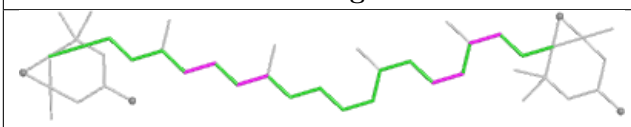
Ligand XAT 6 320



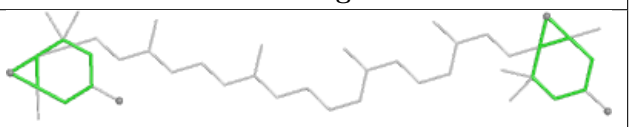
Bond lengths



Bond angles

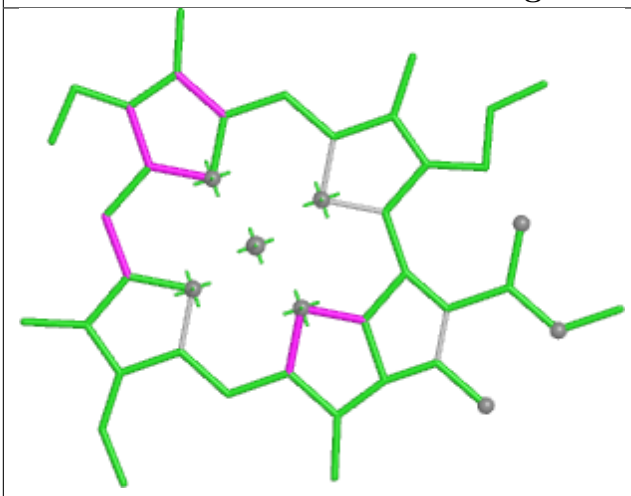


Torsions

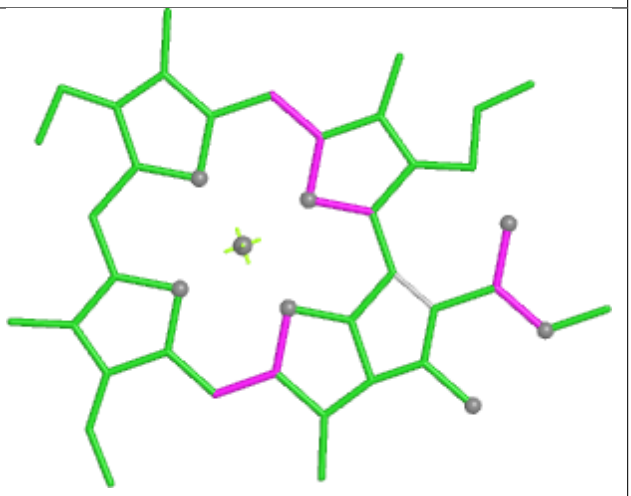


Rings

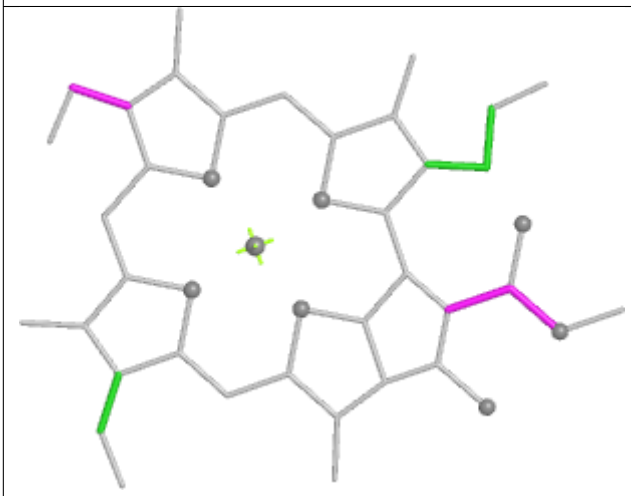
Ligand CLA B 826



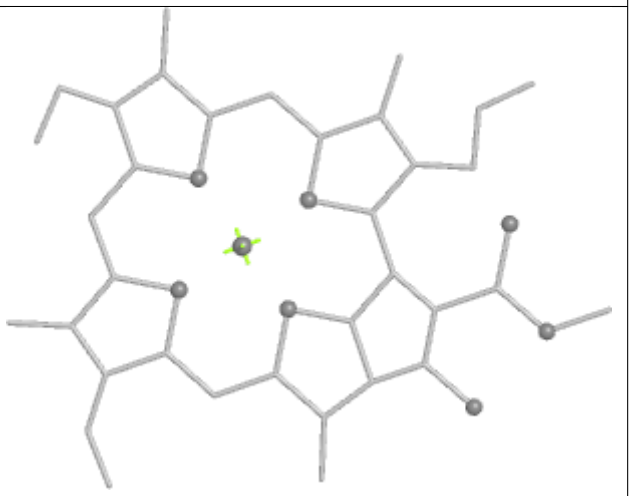
Bond lengths



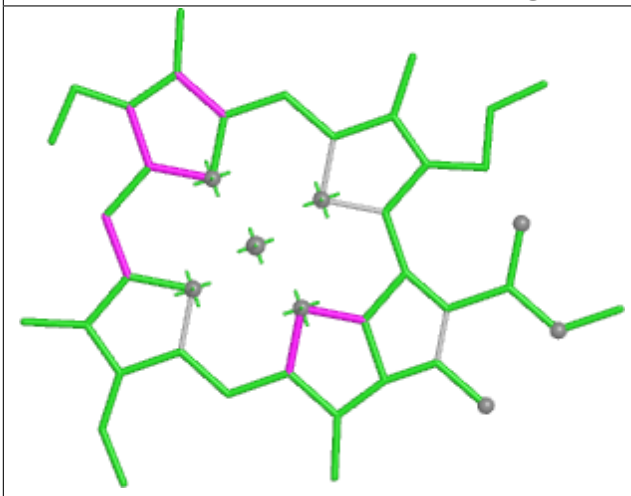
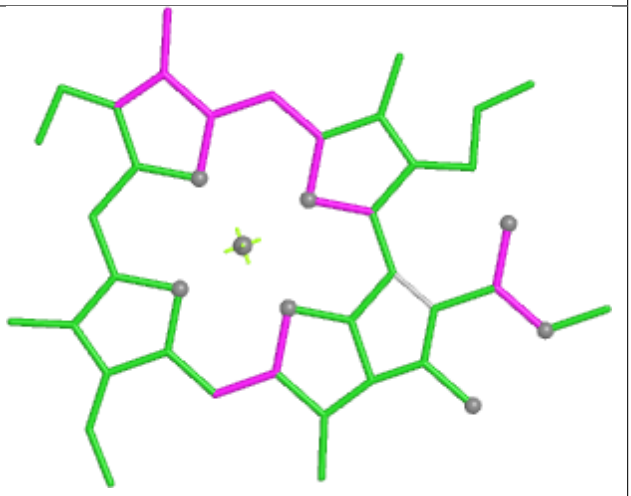
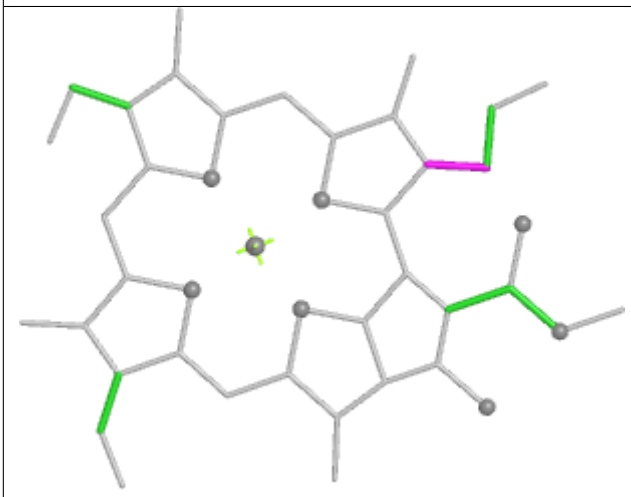
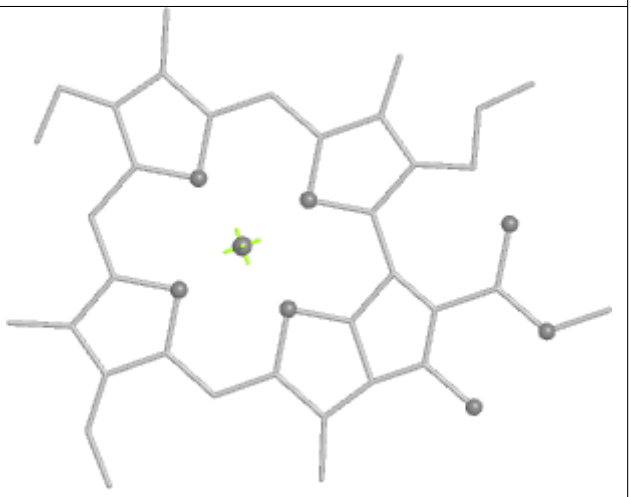
Bond angles



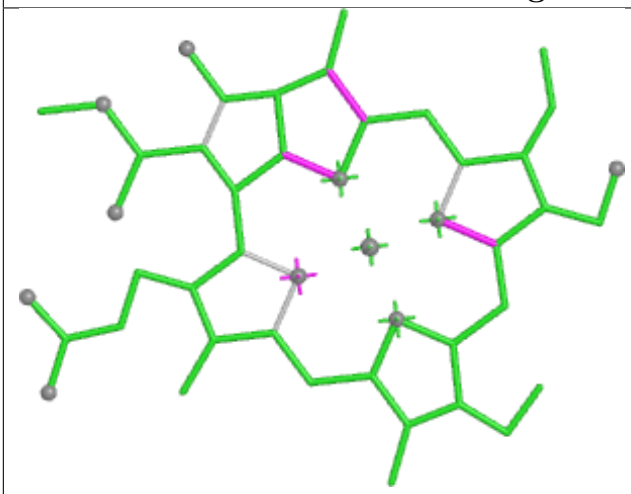
Torsions



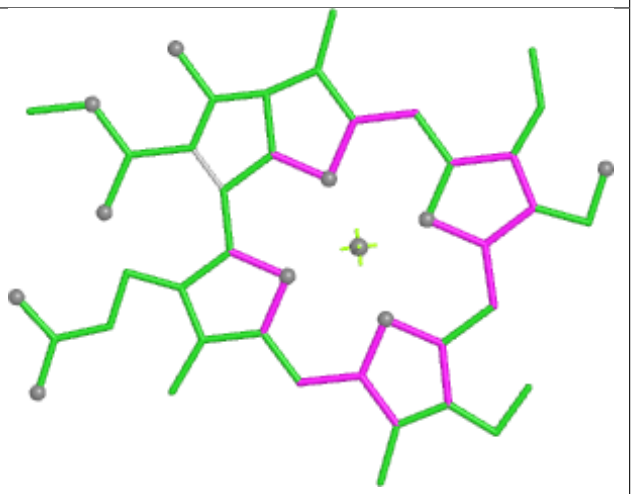
Rings

Ligand CLA B 834	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

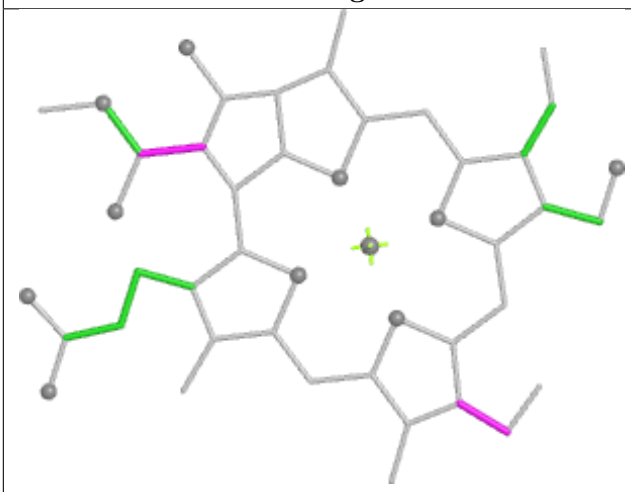
Ligand CHL 5 318



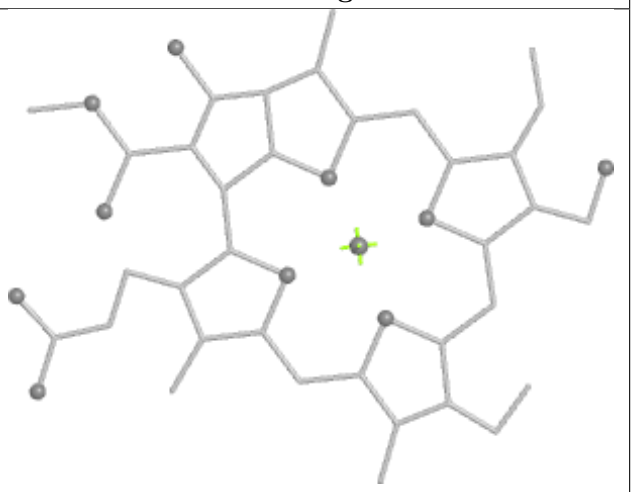
Bond lengths



Bond angles

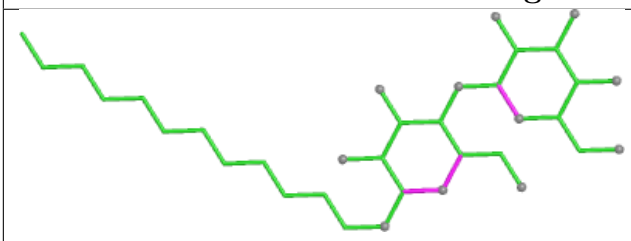


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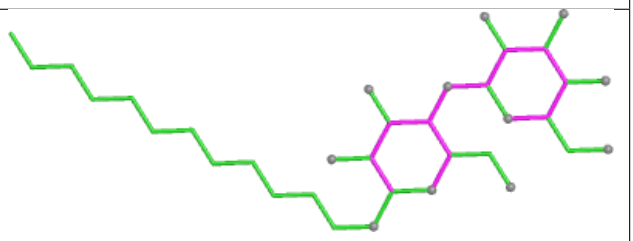


Rings

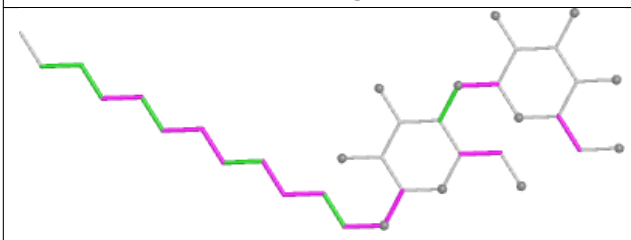
Ligand LMU 1 319



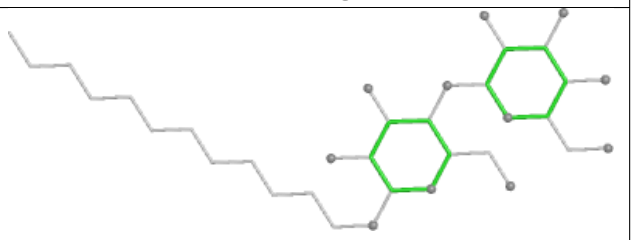
Bond lengths



Bond angles

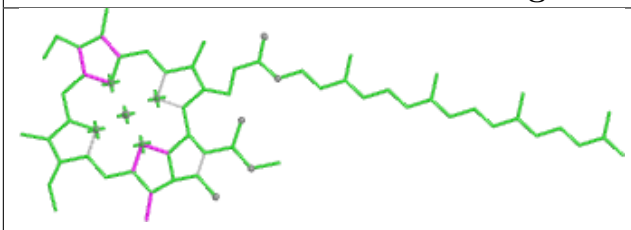


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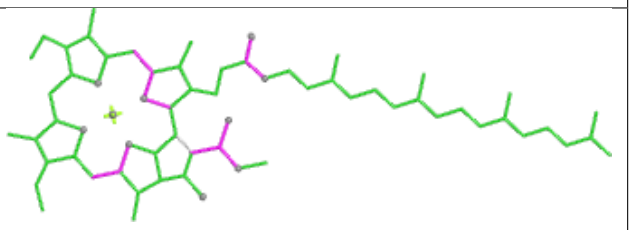


Rings

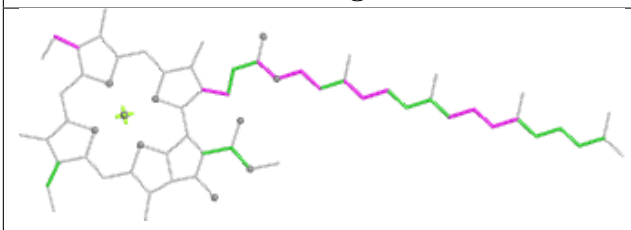
Ligand CLA 1 312



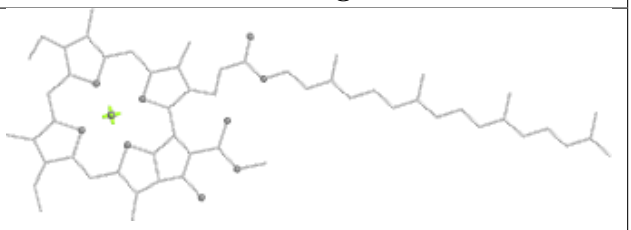
Bond lengths



Bond angles

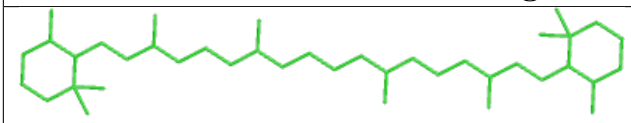


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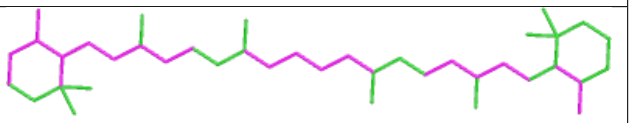


Rings

Ligand BCR K 203



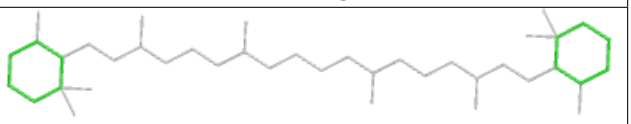
Bond lengths



Bond angles



Torsions

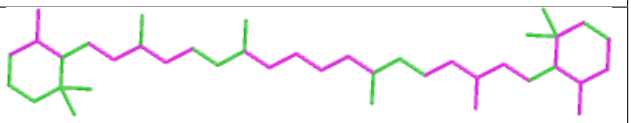


Rings

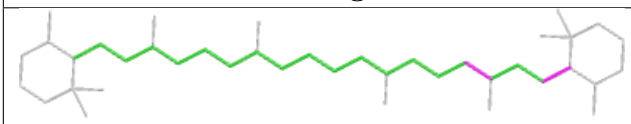
Ligand BCR L 301



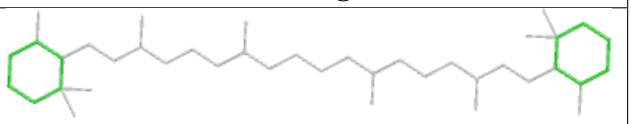
Bond lengths



Bond angles

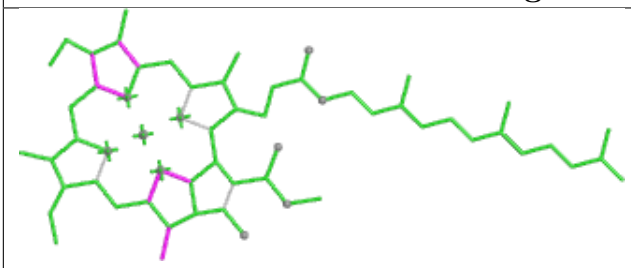


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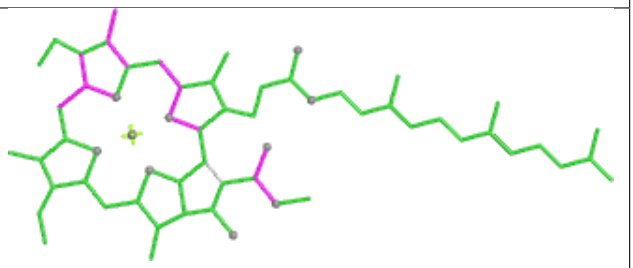


Rings

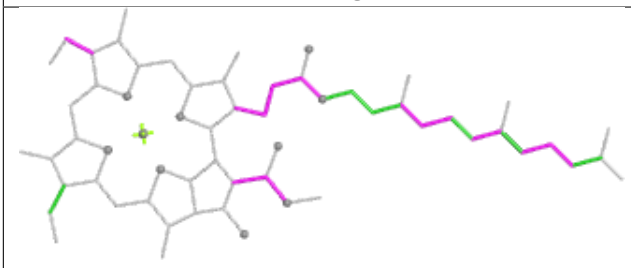
Ligand CLA B 830



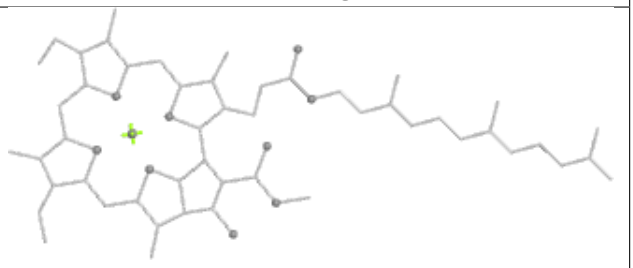
Bond lengths



Bond angles

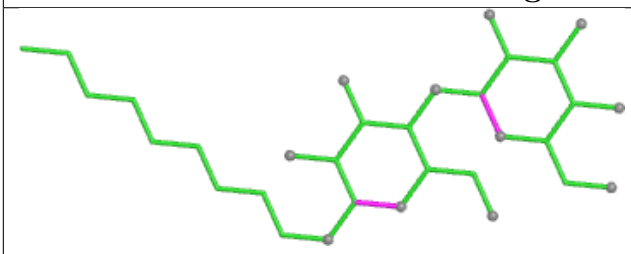


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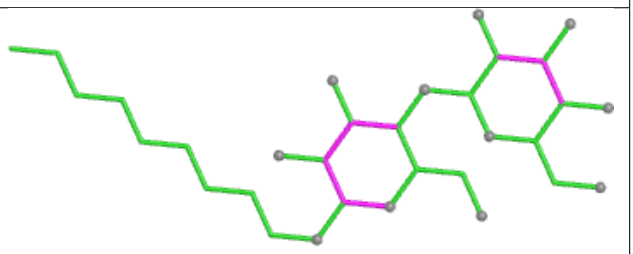


Rings

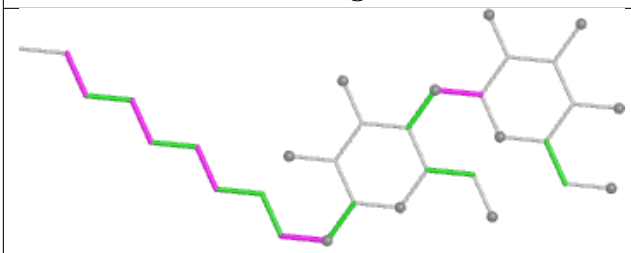
Ligand LMU 6 323



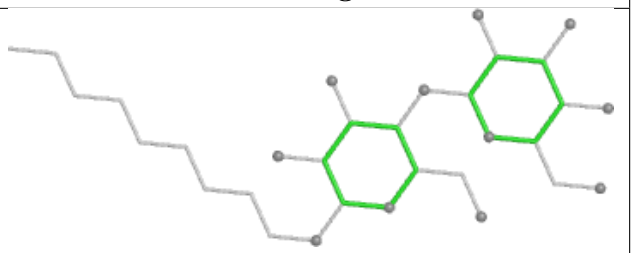
Bond lengths



Bond angles



Torsions

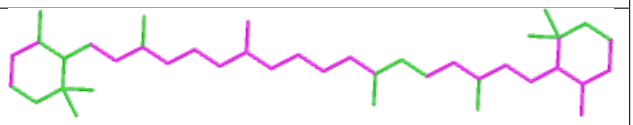


Rings

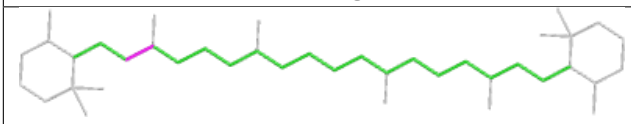
Ligand BCR B 850



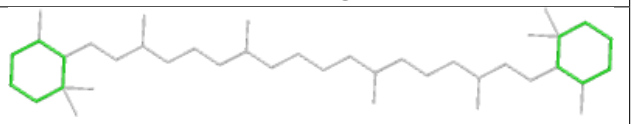
Bond lengths



Bond angles

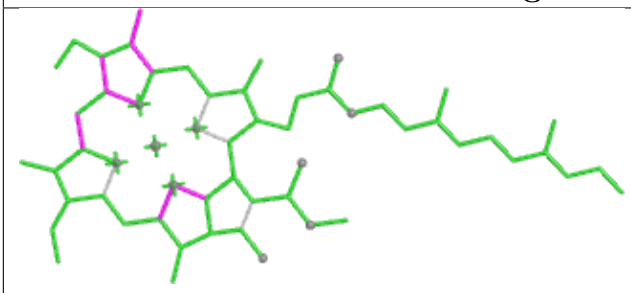


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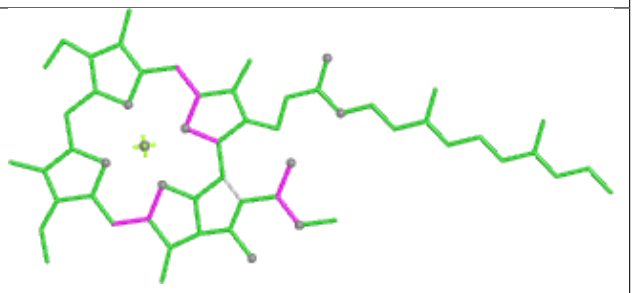


Rings

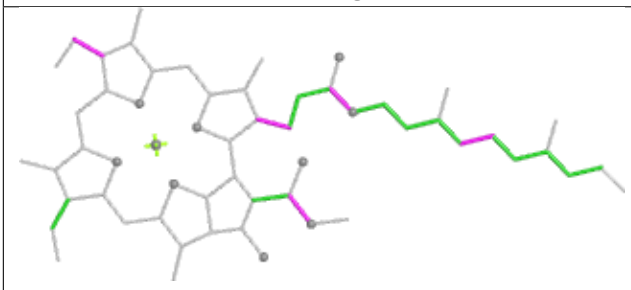
Ligand CLA A 834



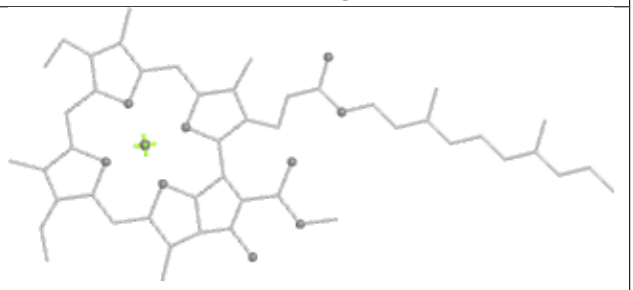
Bond lengths



Bond angles

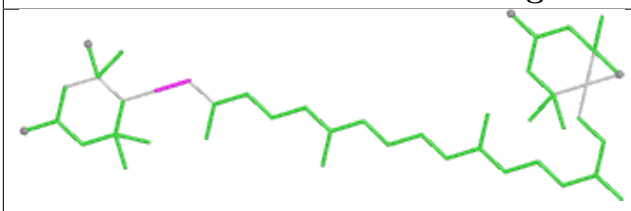


Torsions

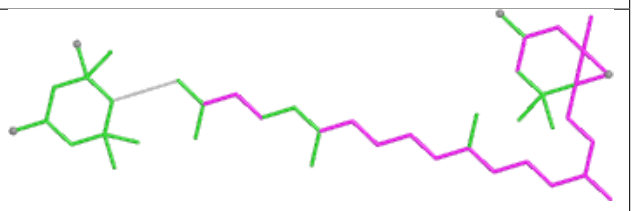


Rings

Ligand NEX 6 321



Bond lengths



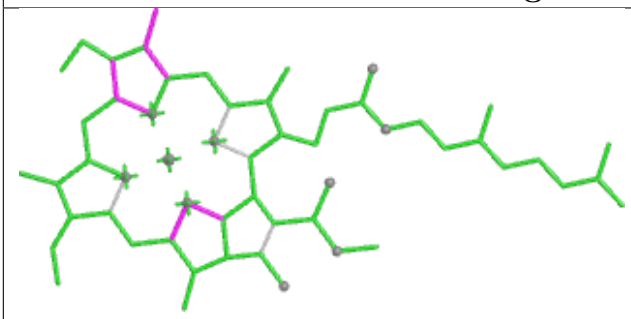
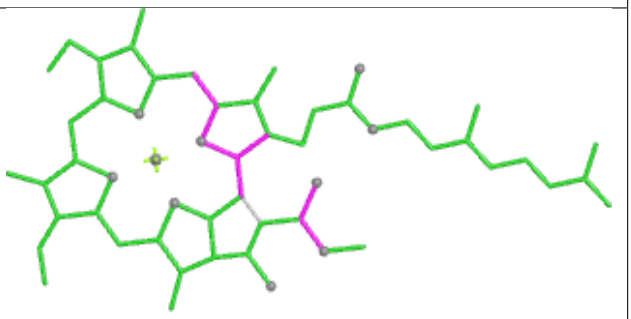
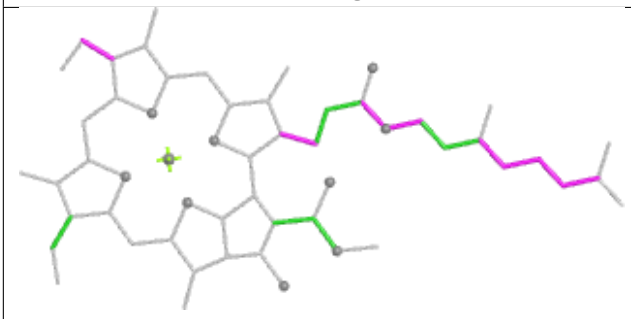
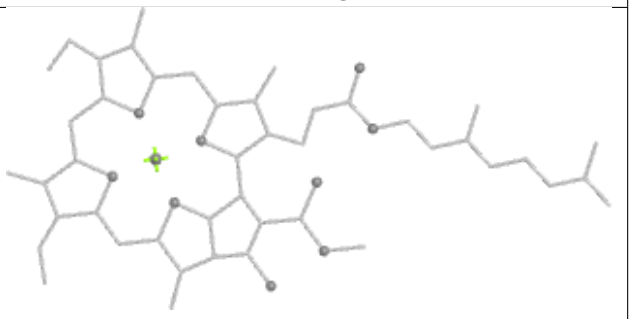
Bond angles

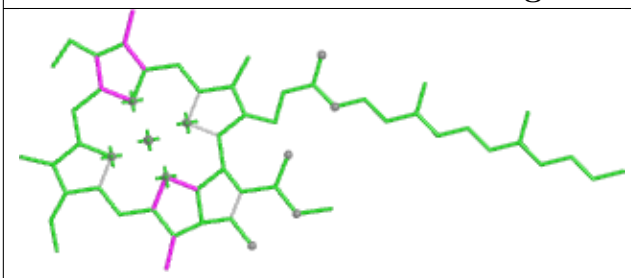
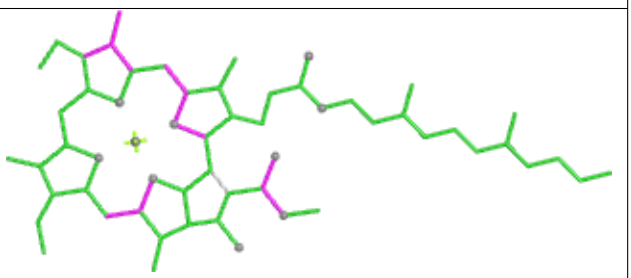
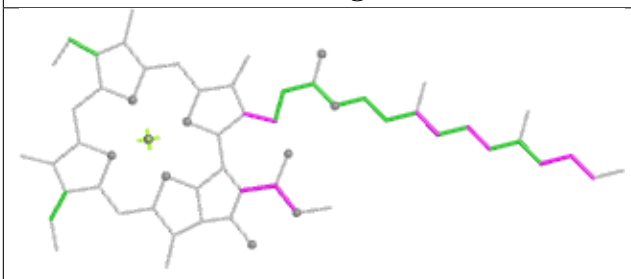
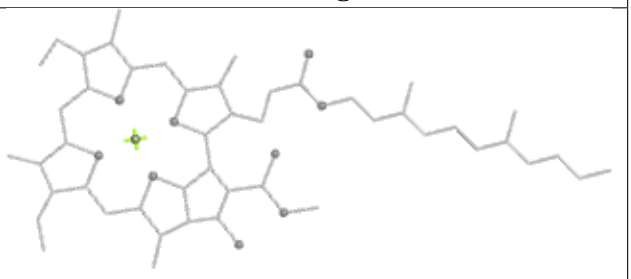


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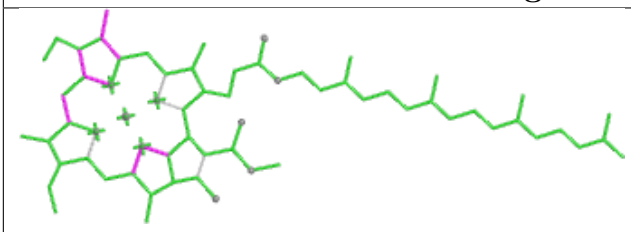


Rings

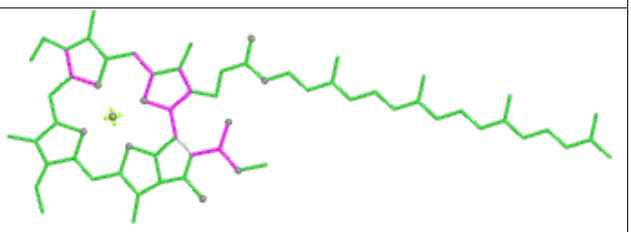
Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

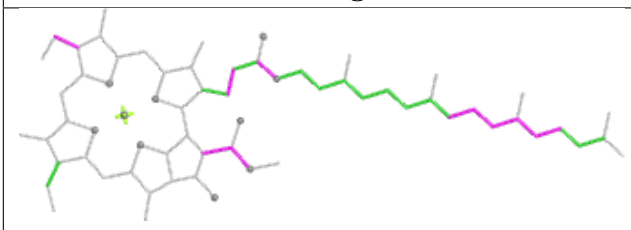
Ligand CLA B 815



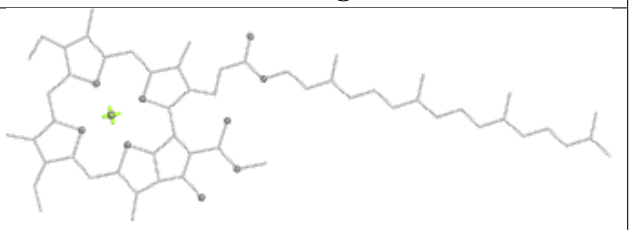
Bond lengths



Bond angles

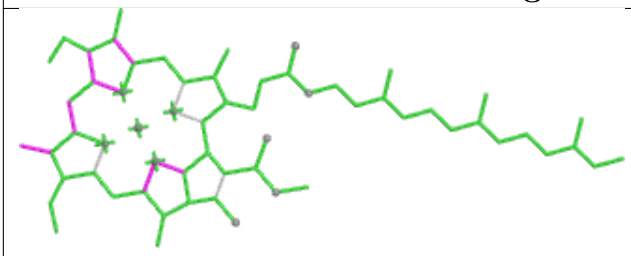


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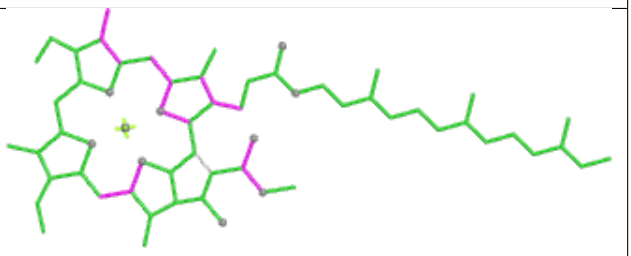


Rings

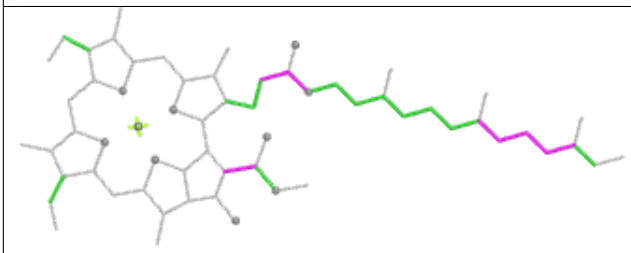
Ligand CLA A 804



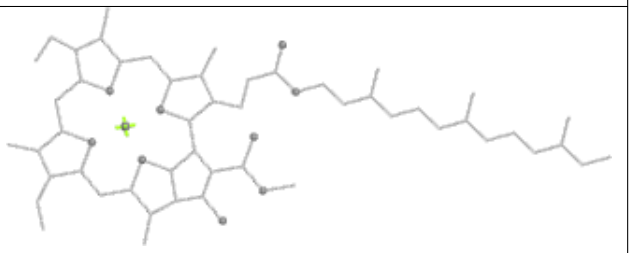
Bond lengths



Bond angles

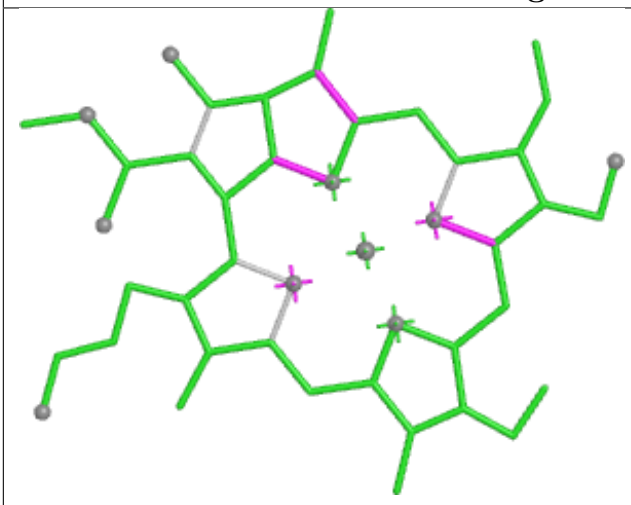


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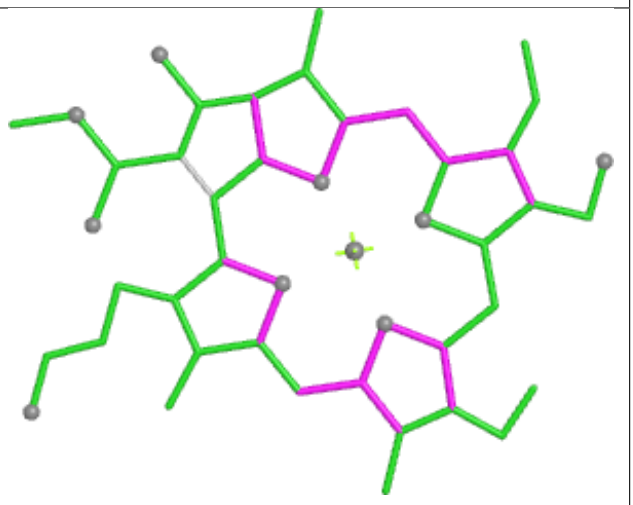


Rings

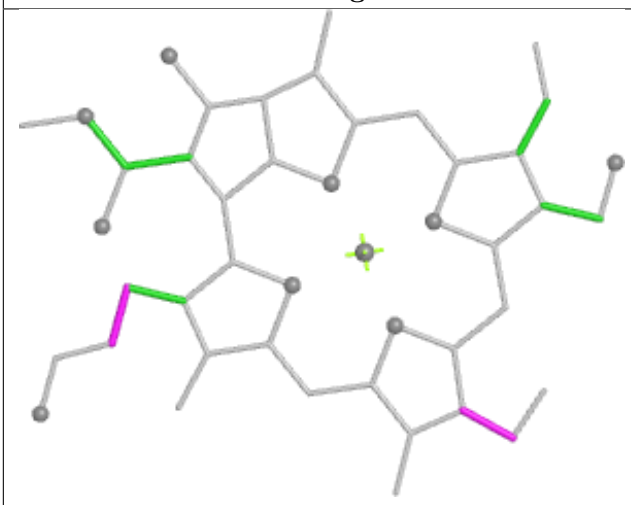
Ligand CHL 5 306



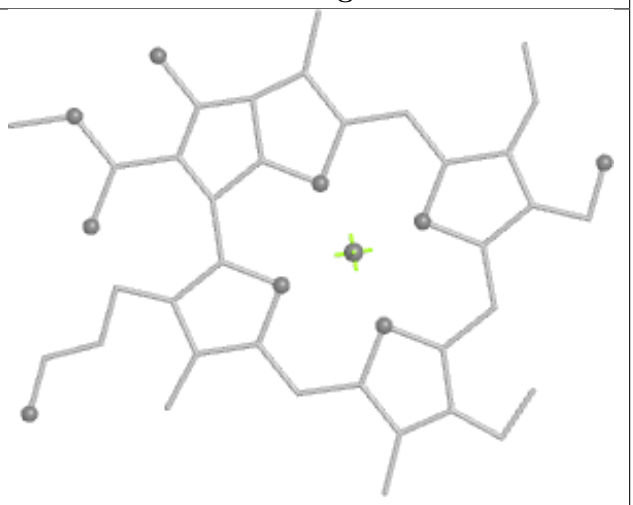
Bond lengths



Bond angles

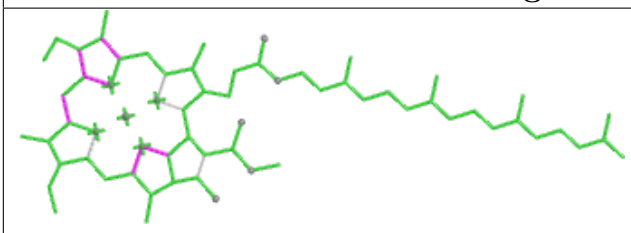


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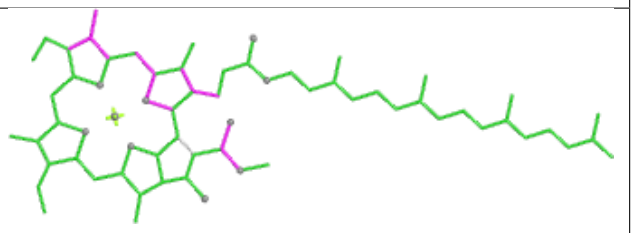


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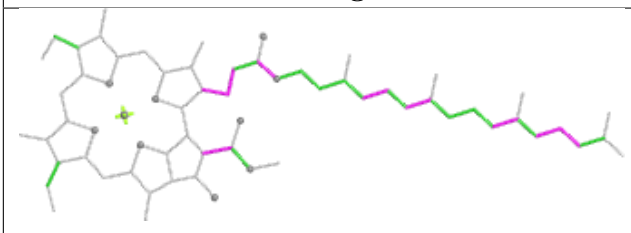
Ligand CLA A 802



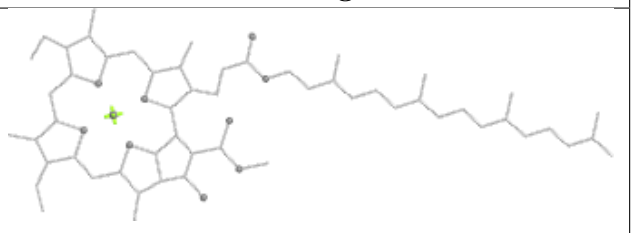
Bond lengths



Bond angles

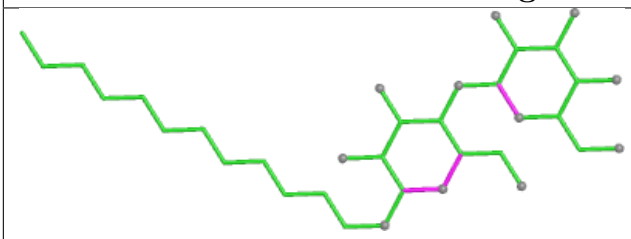


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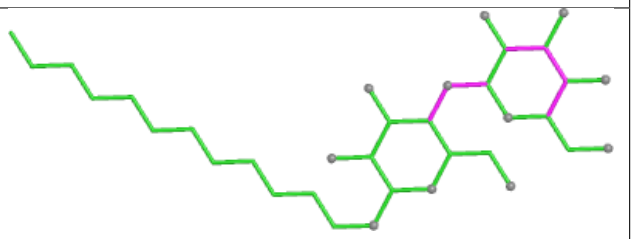


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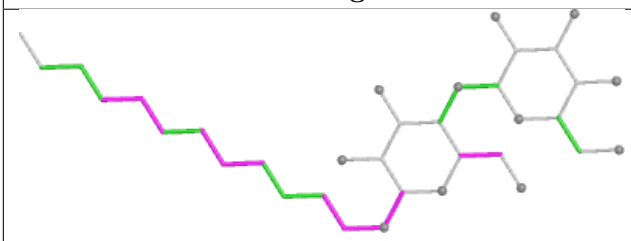
Ligand LMU G 201



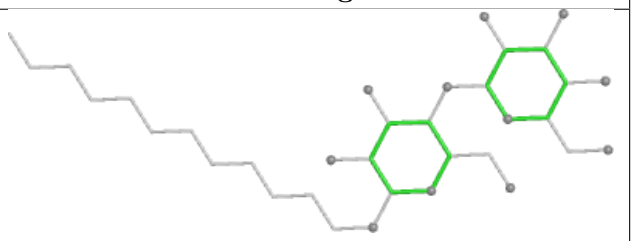
Bond lengths



Bond angles

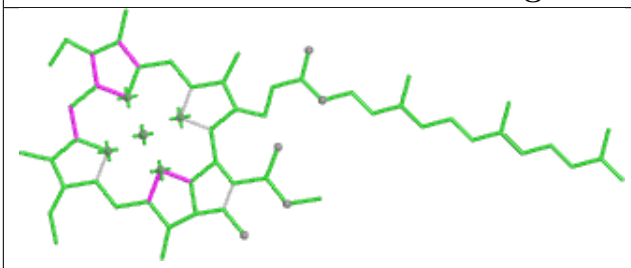


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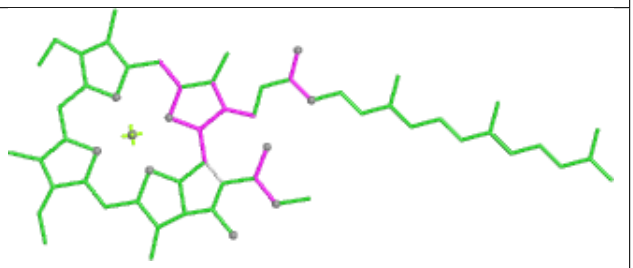


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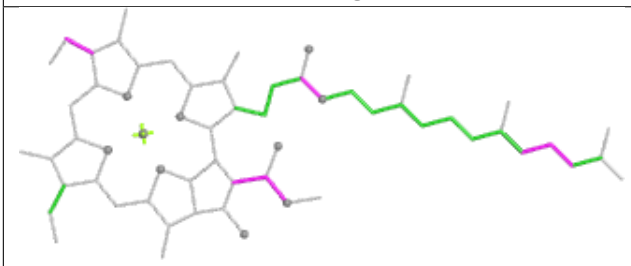
Ligand CLA B 835



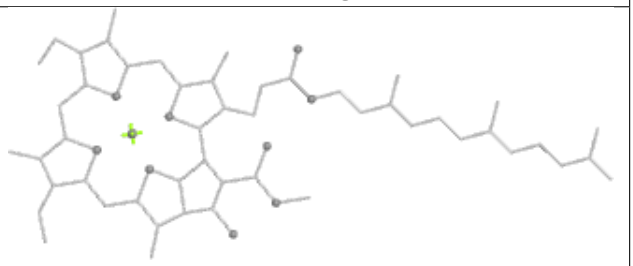
Bond lengths



Bond angles

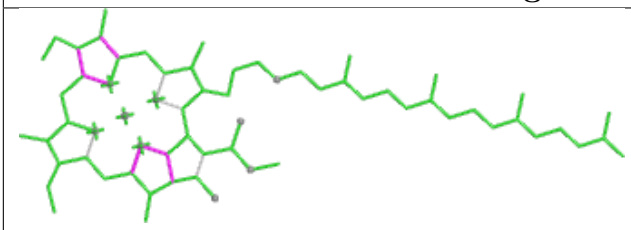


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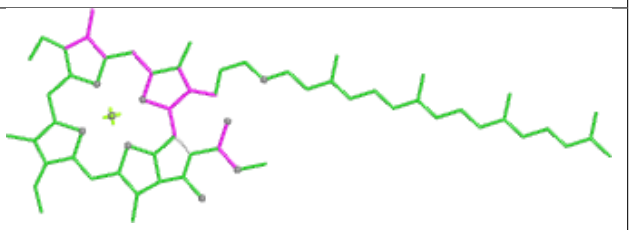


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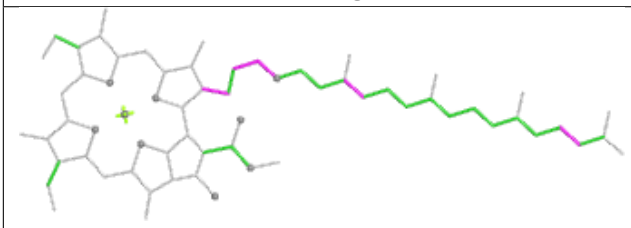
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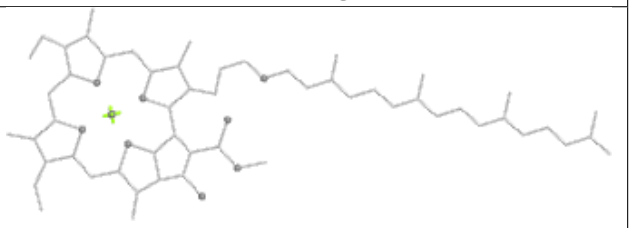
Bond lengths



Bond angles

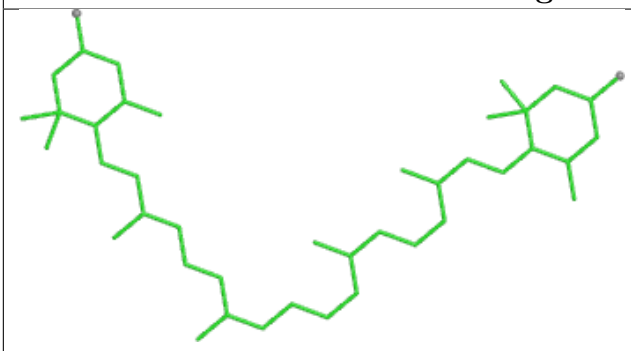


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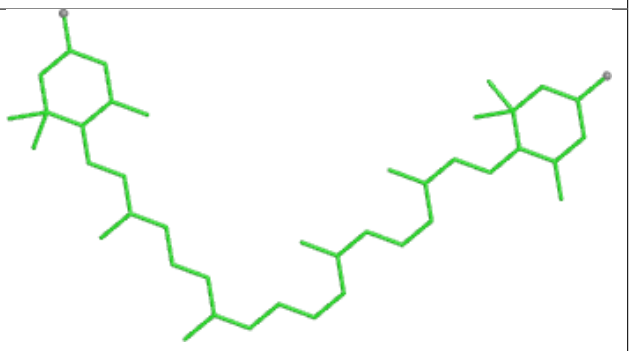


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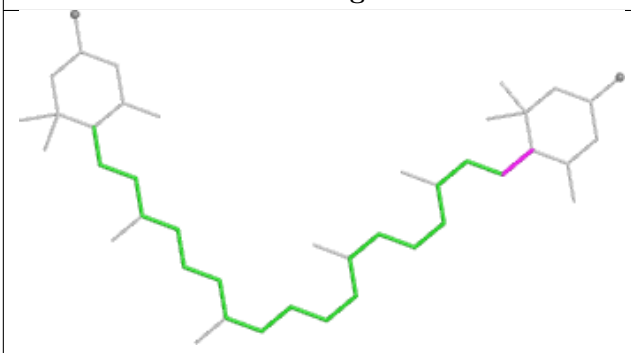
Ligand K3I 2 616



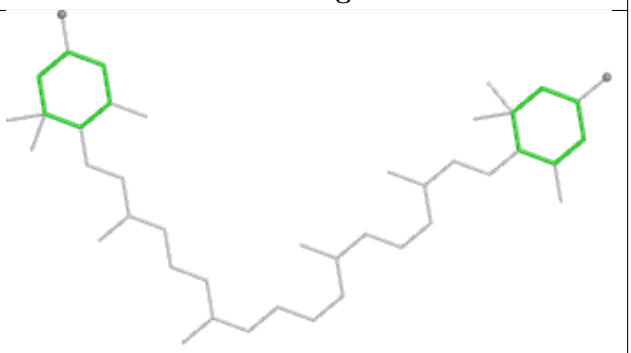
Bond lengths



Bond angles

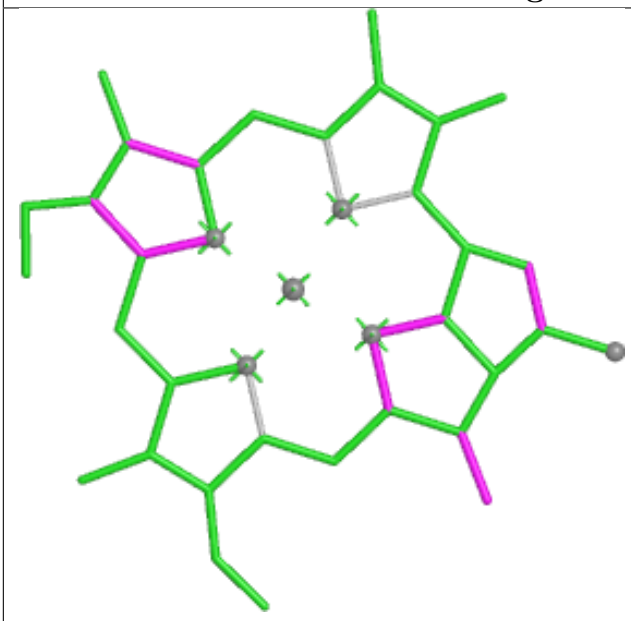


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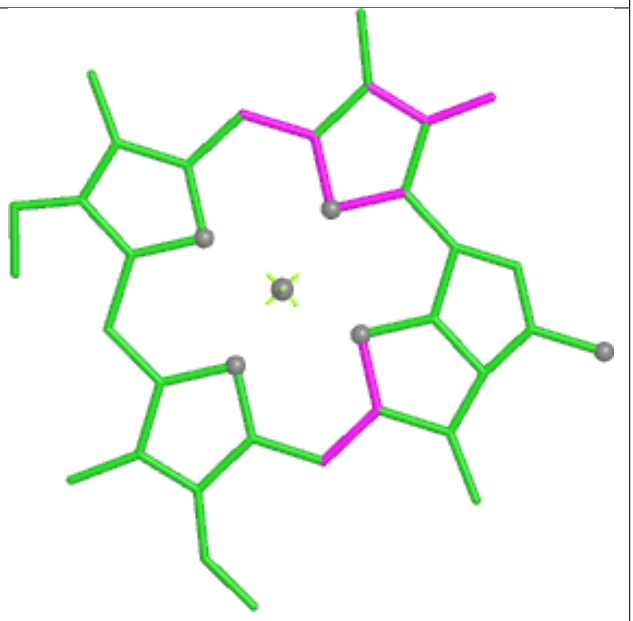


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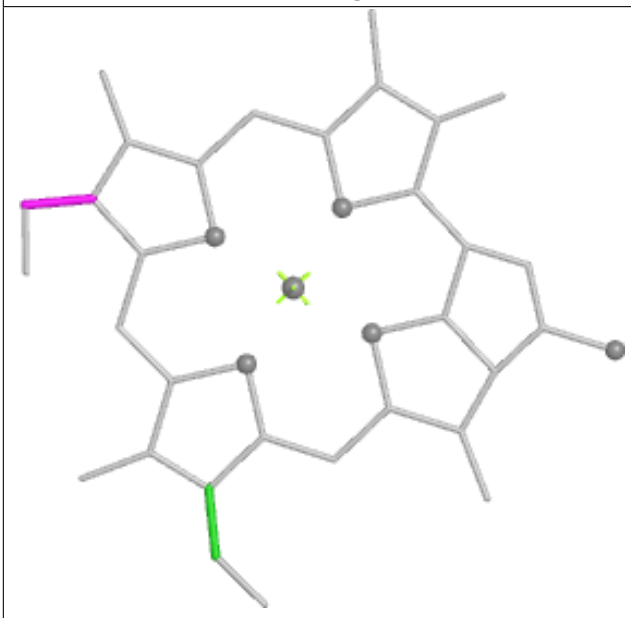
Ligand CLA L 304



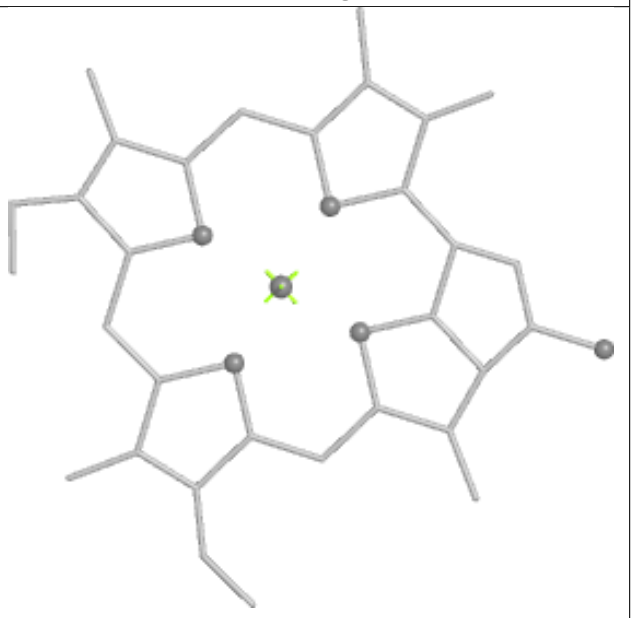
Bond lengths



Bond angles

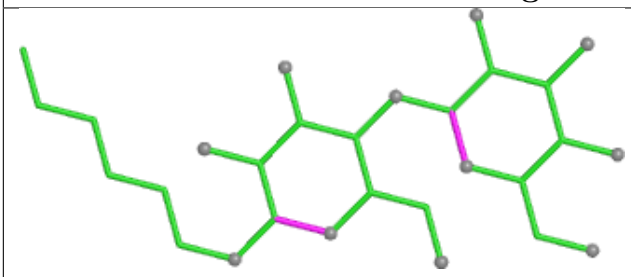


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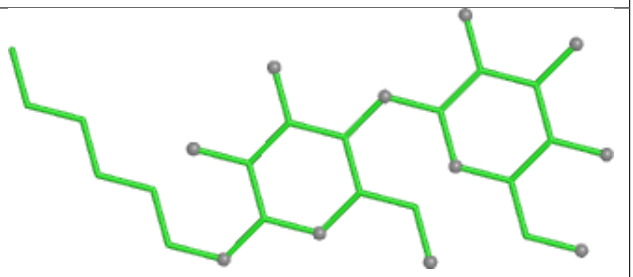


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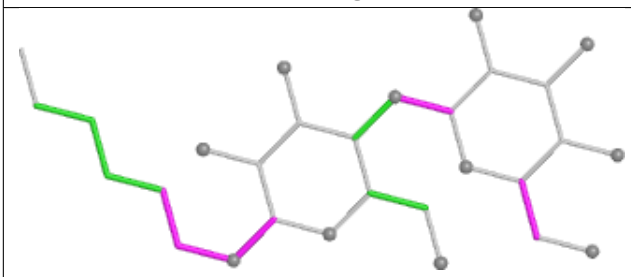
Ligand LMU F 806



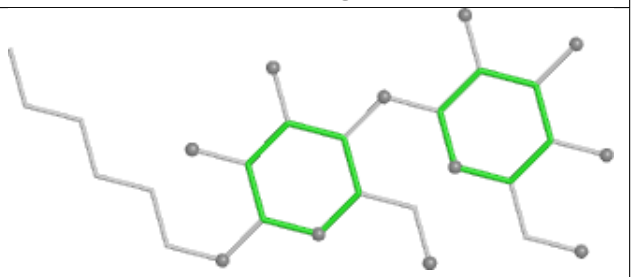
Bond lengths



Bond angles

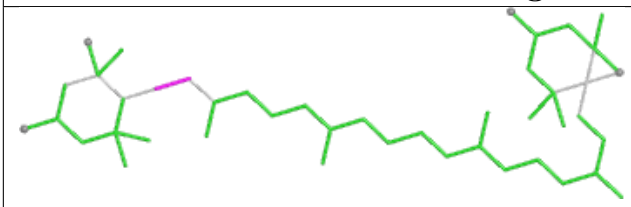


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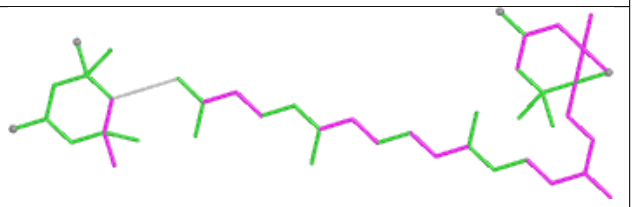


Rings

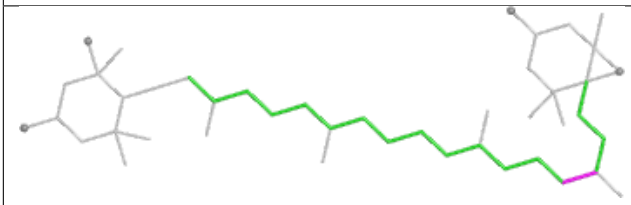
Ligand NEX 5 323



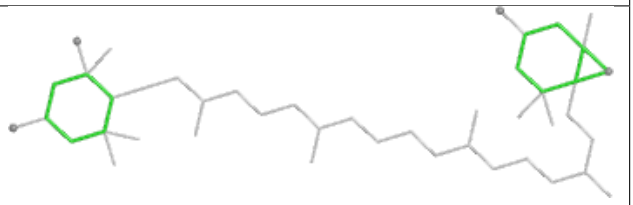
Bond lengths



Bond angles

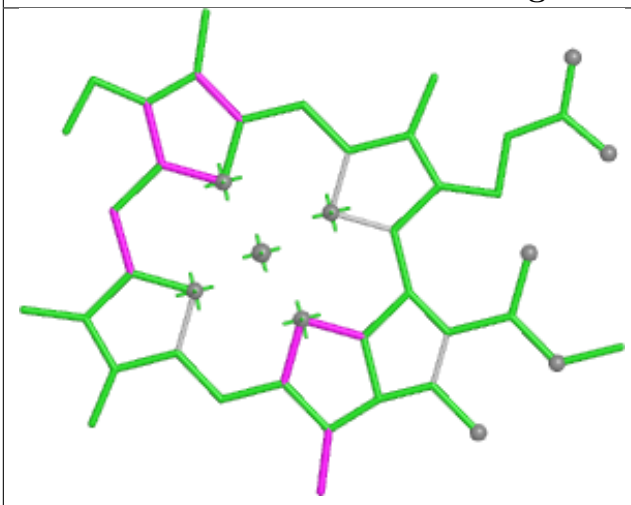


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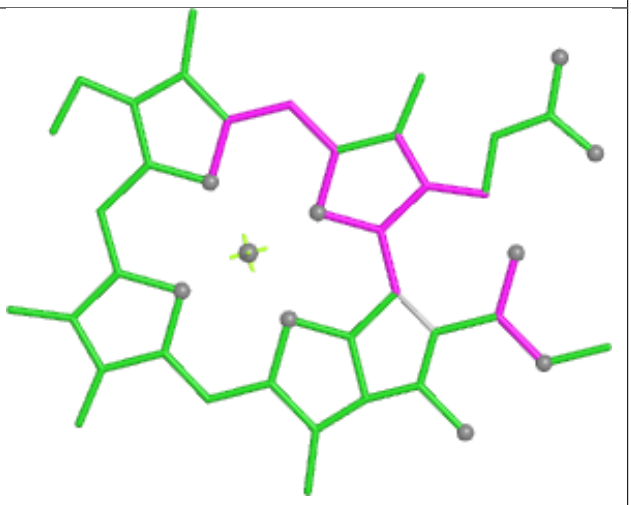


Rings

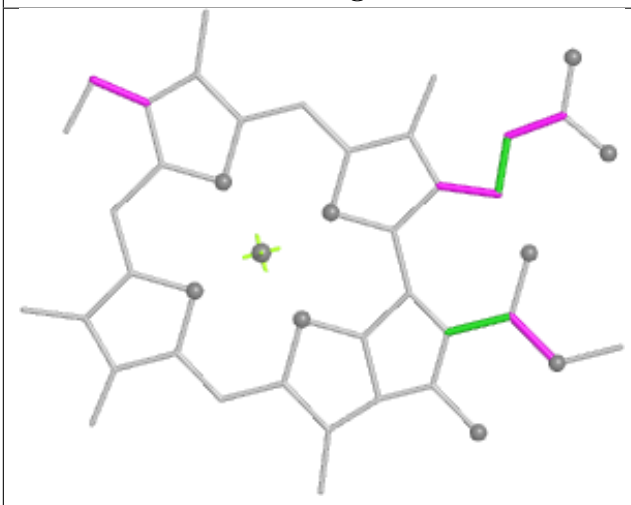
Ligand CLA 7 310



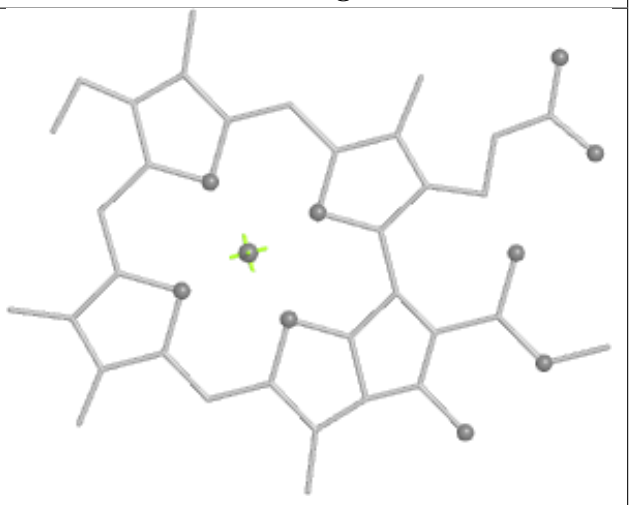
Bond lengths



Bond angles

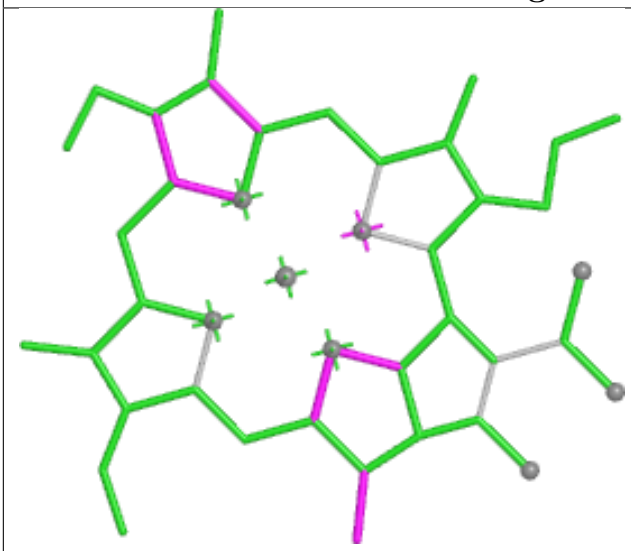


Torsions



Rings

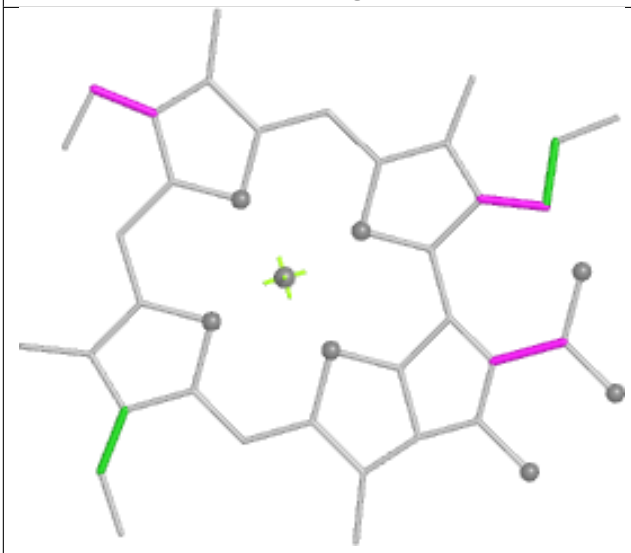
Ligand CLA 1 310



Bond lengths



Bond angles

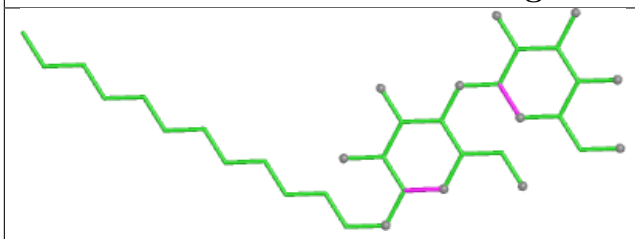


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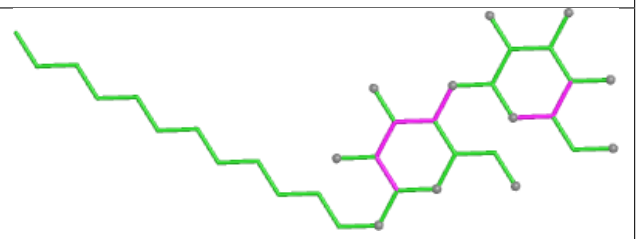


Rings

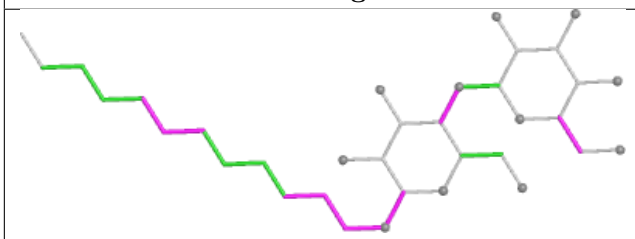
Ligand LMU 9 618



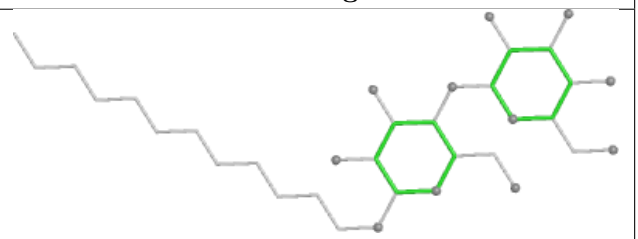
Bond lengths



Bond angles

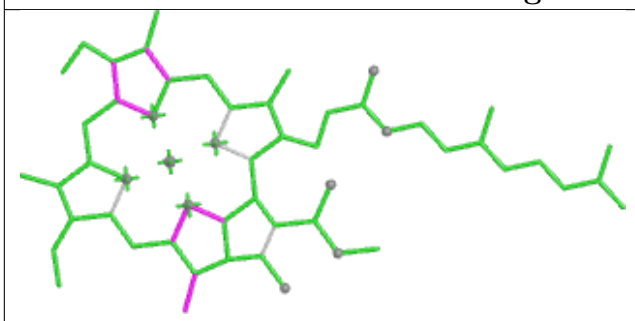


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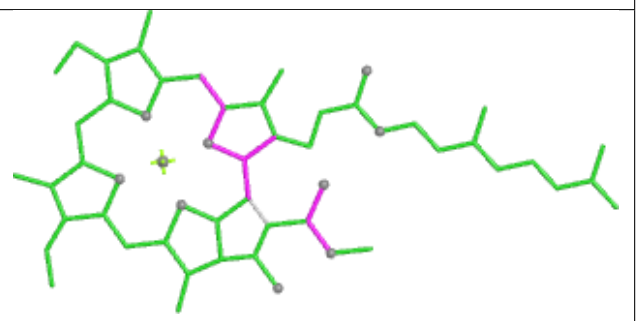


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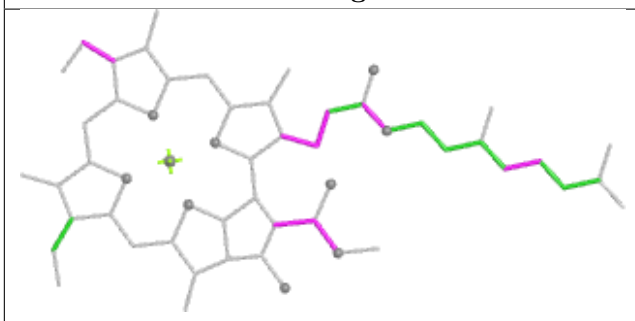
Ligand CLA G 202



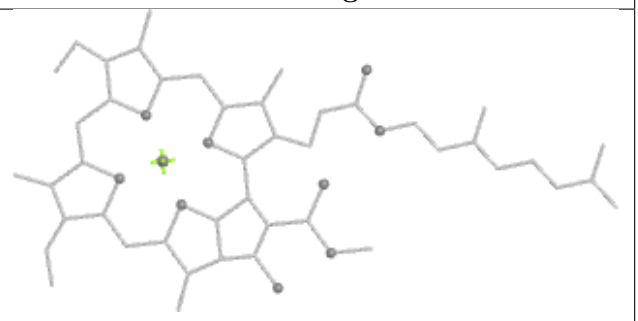
Bond lengths



Bond angles

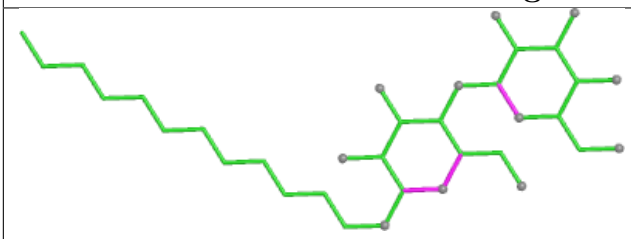


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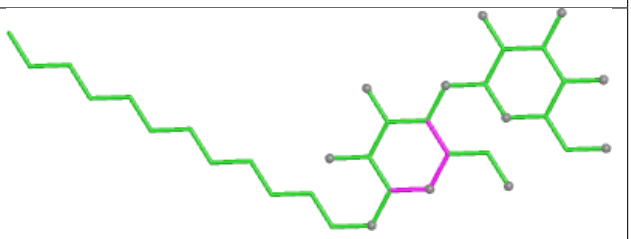


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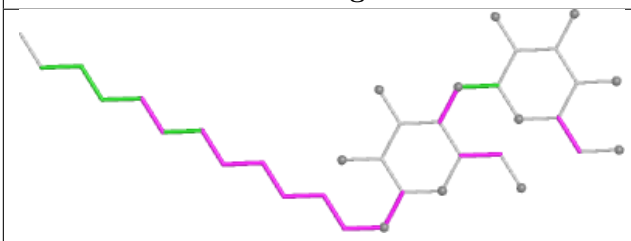
Ligand LMU J 106



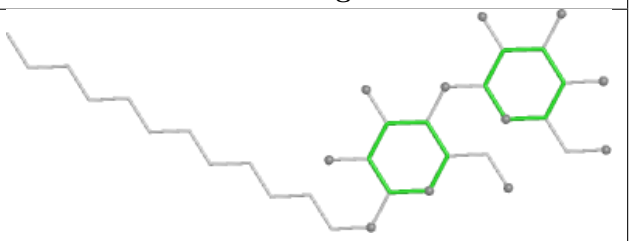
Bond lengths



Bond angles

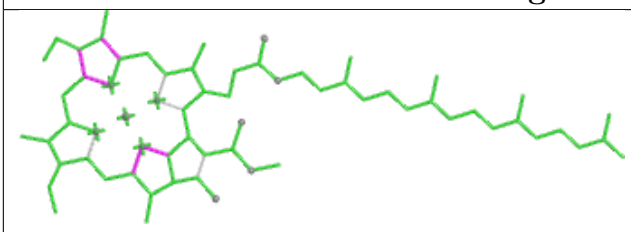


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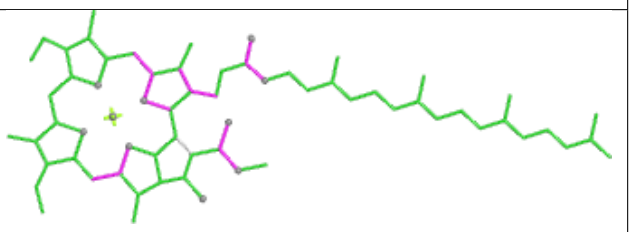


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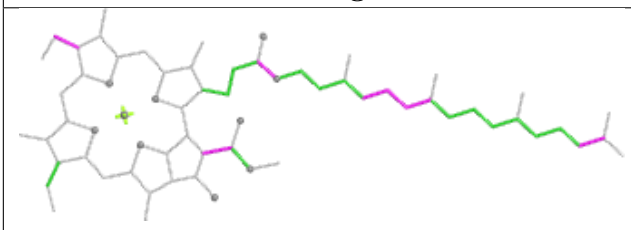
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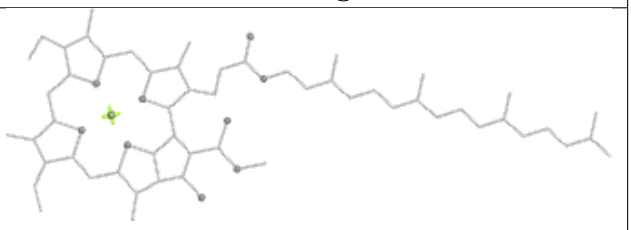
Bond lengths



Bond angles

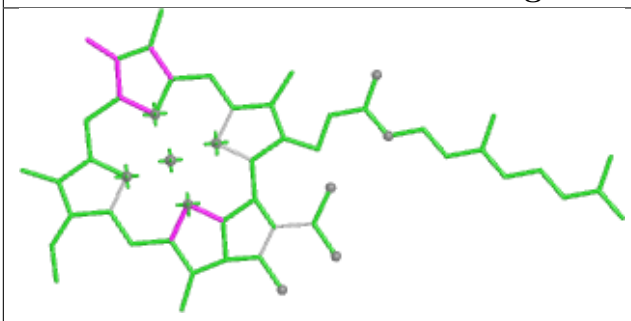


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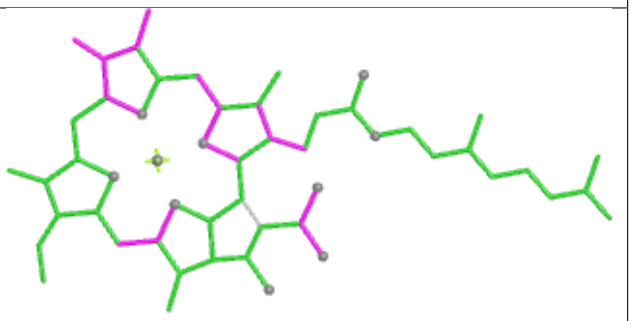


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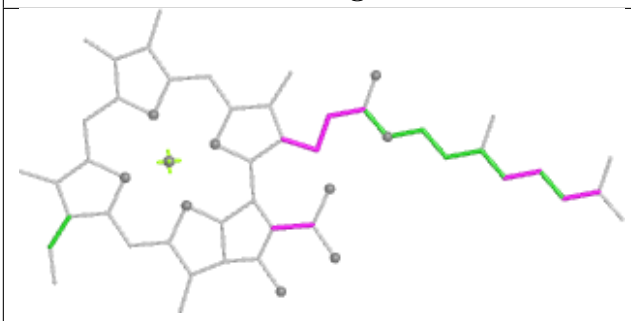
Ligand CLA B 814



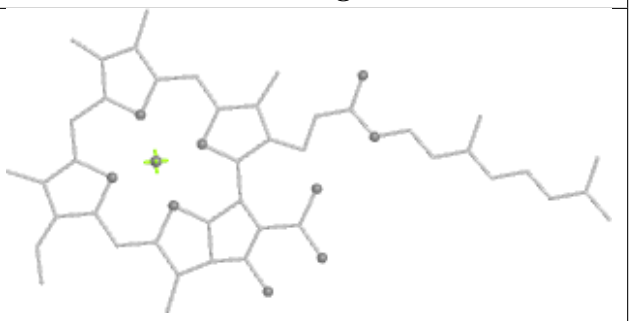
Bond lengths



Bond angles

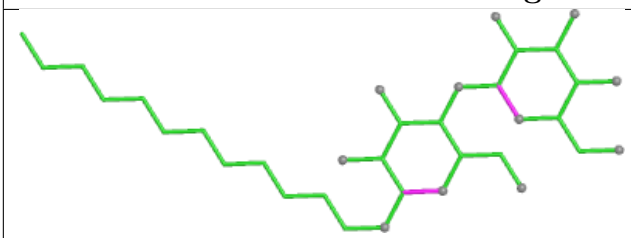


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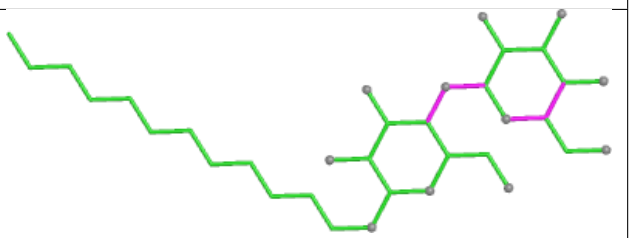


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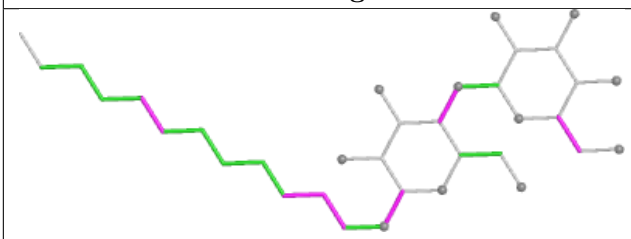
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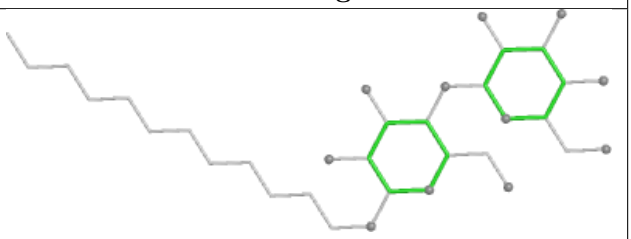
Bond lengths



Bond angles



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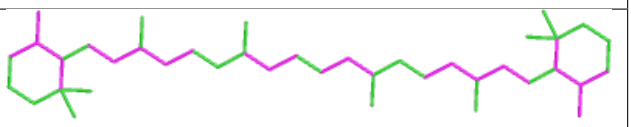


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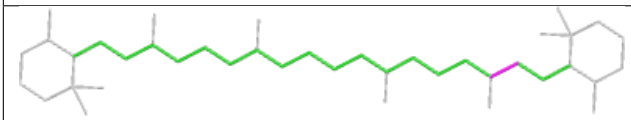
Ligand BCR A 847



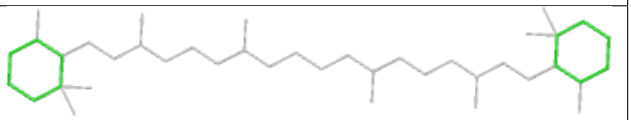
Bond lengths



Bond angles

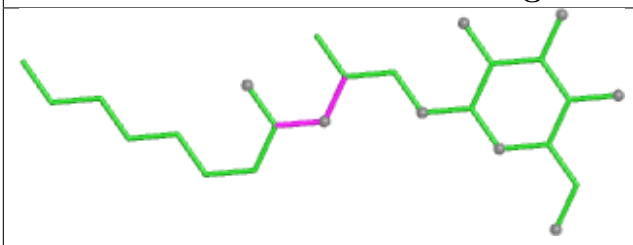


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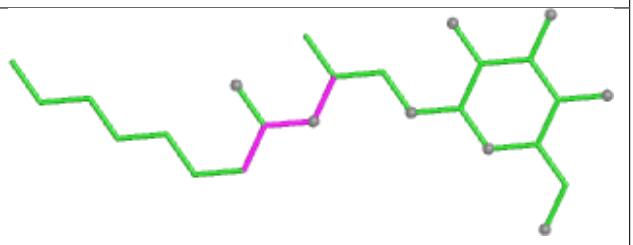


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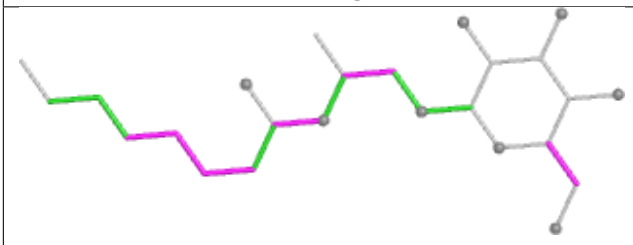
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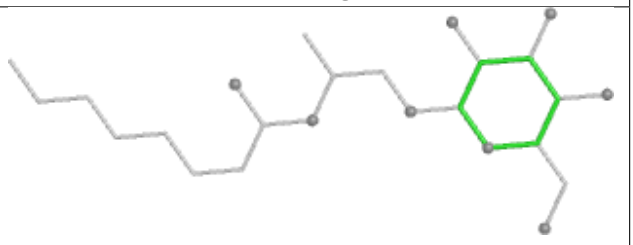
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Bond angles

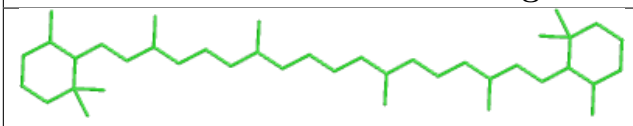


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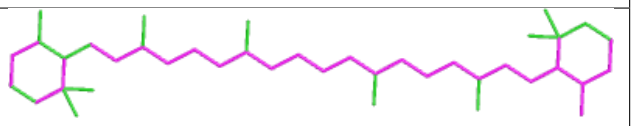


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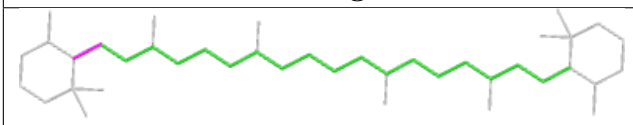
Ligand BCR A 848



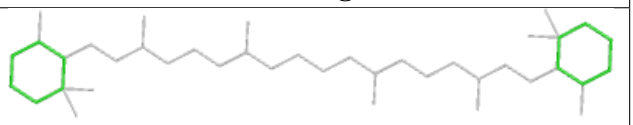
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Bond angles

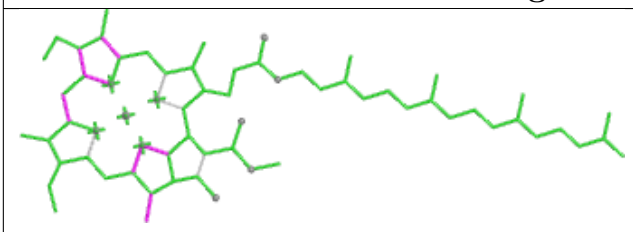


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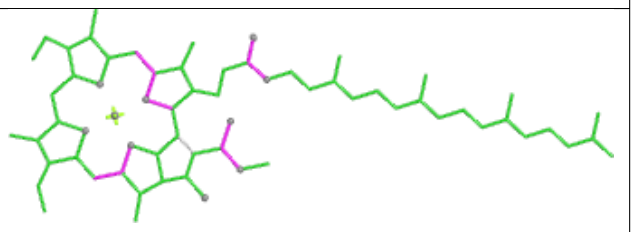


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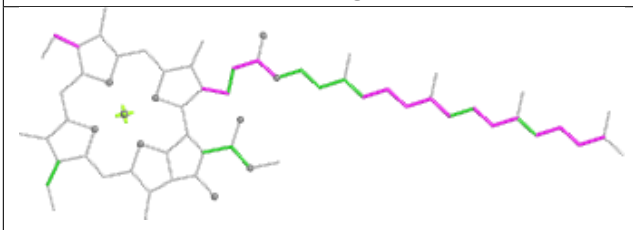
Ligand CLA 2 612



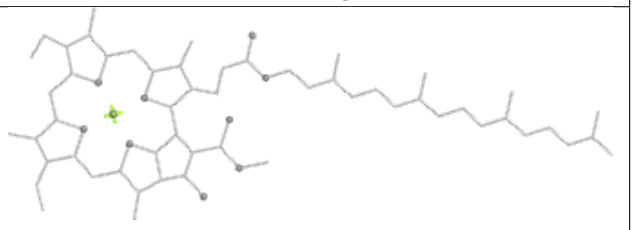
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Bond angles

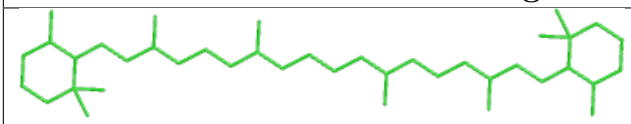


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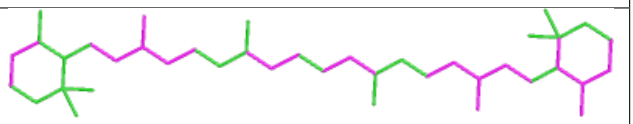


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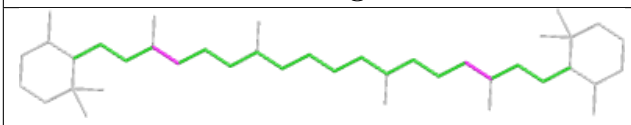
Ligand BCR B 848



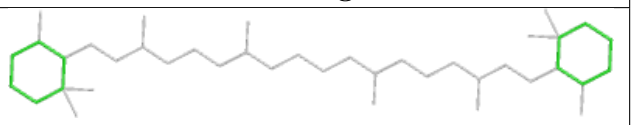
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Bond angles

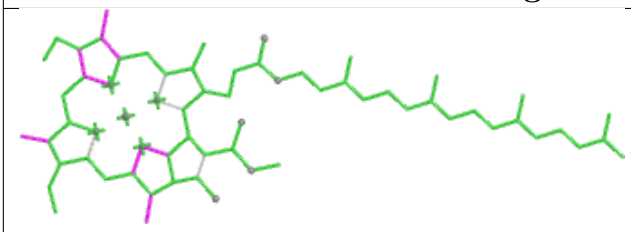


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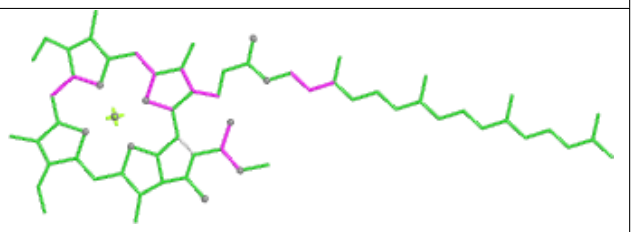


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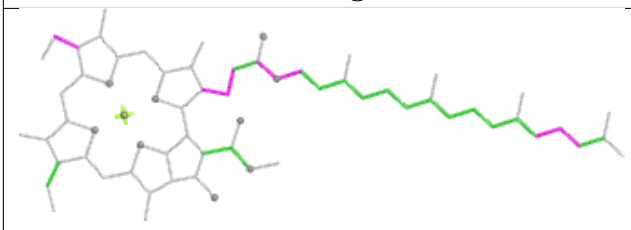
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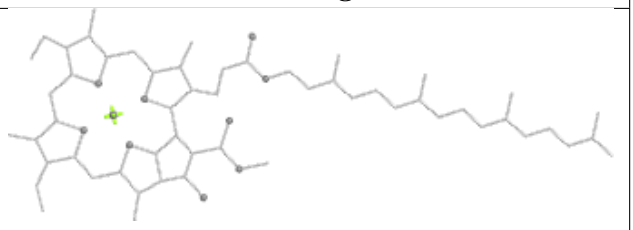
Bond lengths



Bond angles

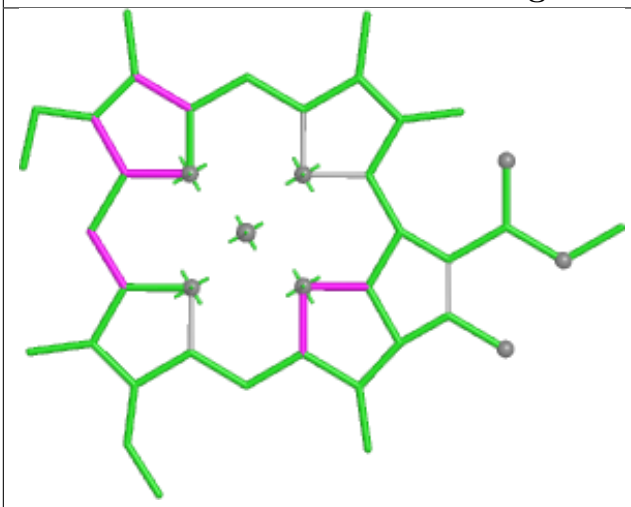


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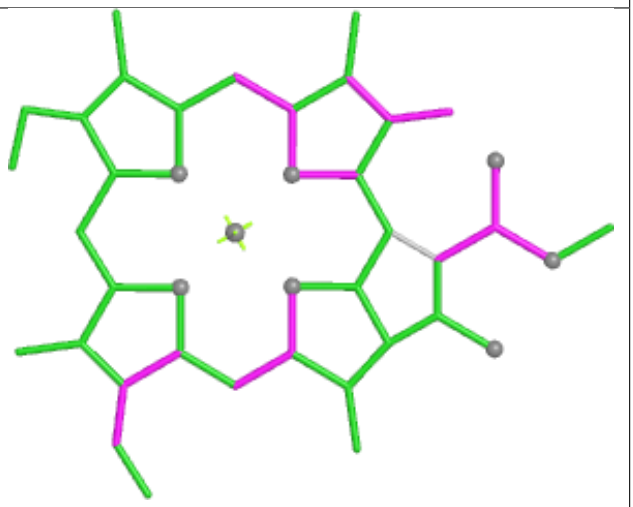


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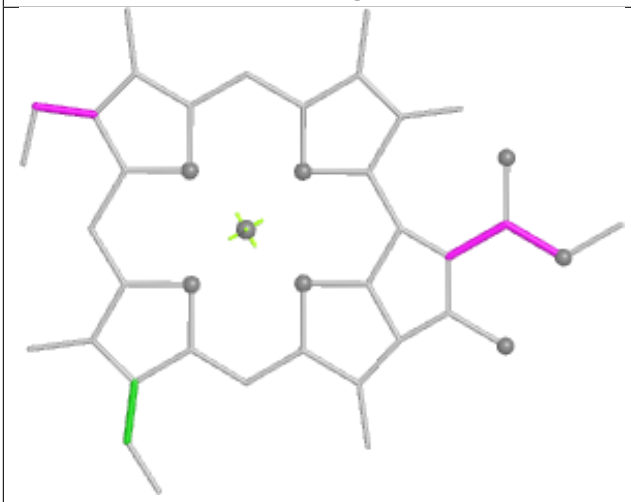
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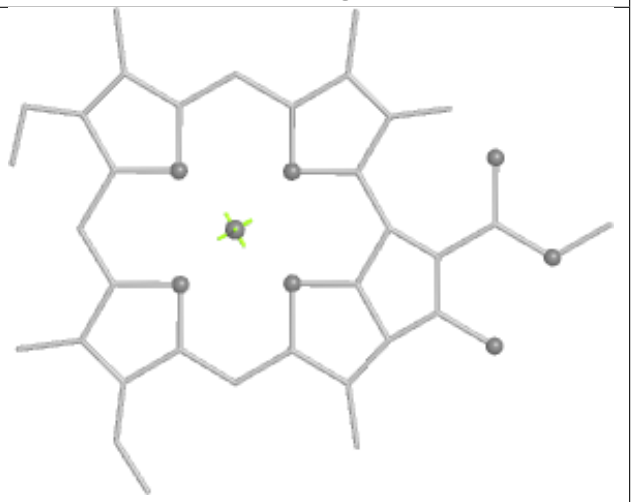
Bond lengths



Bond angles

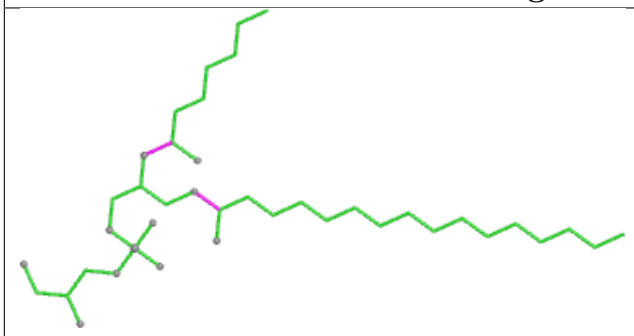


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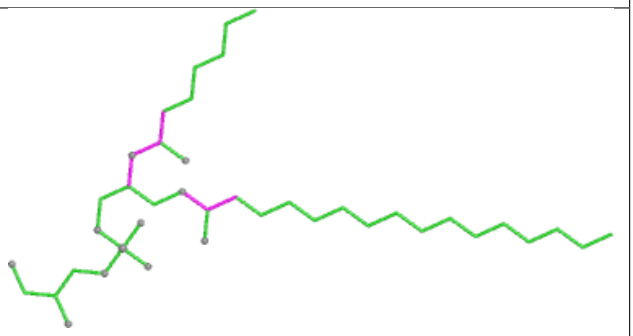


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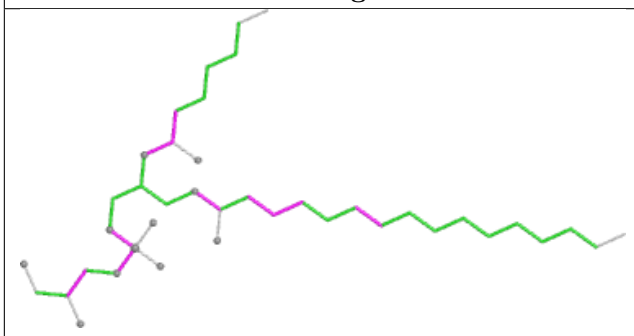
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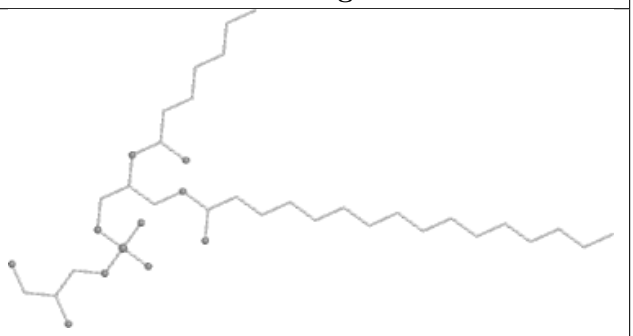
Bond lengths



Bond angles

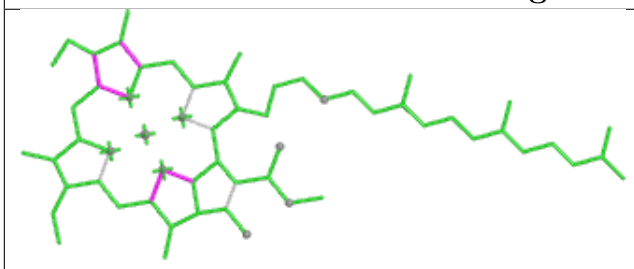


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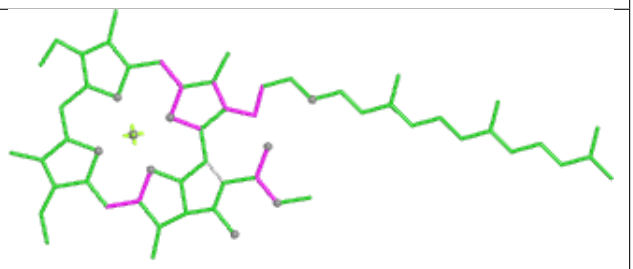


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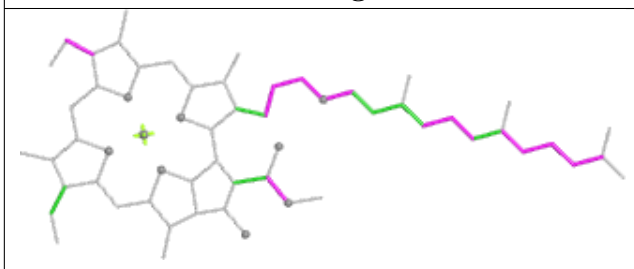
Ligand CLA 5 314



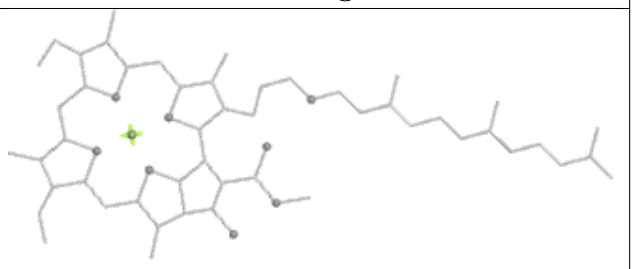
Bond lengths



Bond angles

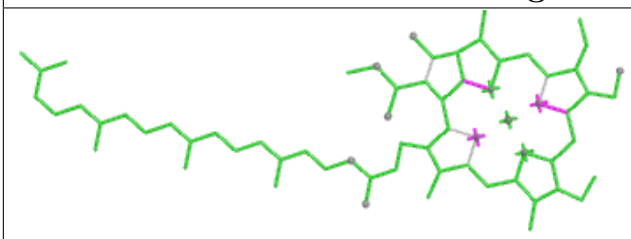


Torsions

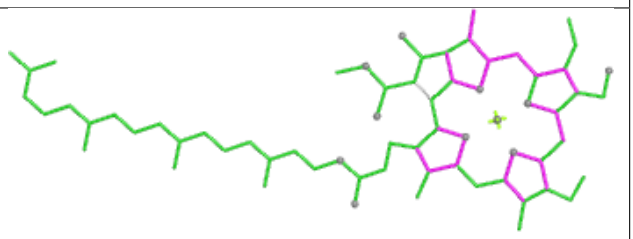


Rings

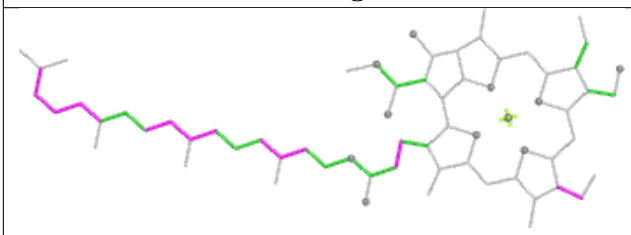
Ligand CHL 3 406



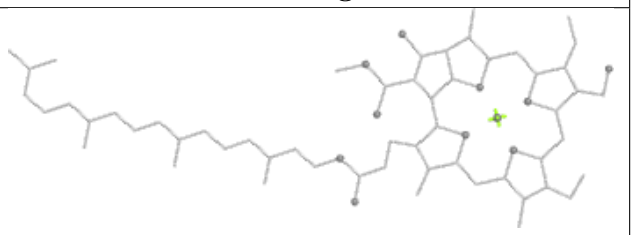
Bond lengths



Bond angles

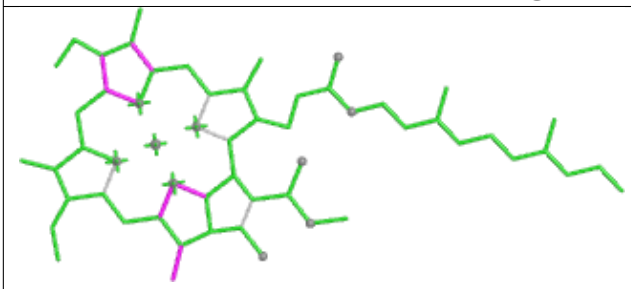


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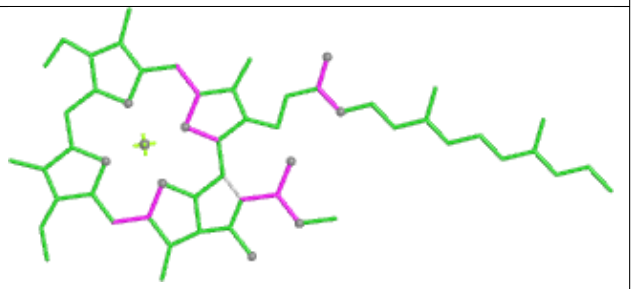


Rings

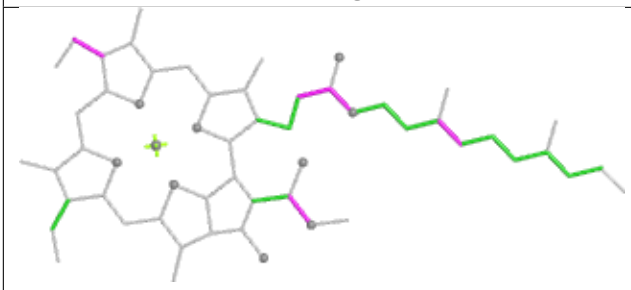
Ligand CLA 9 606



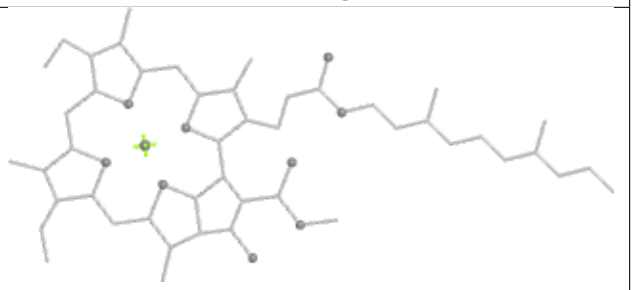
Bond lengths



Bond angles

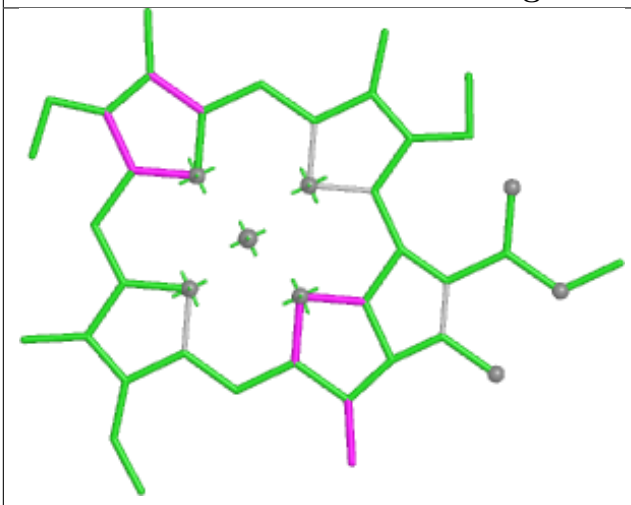


Torsions

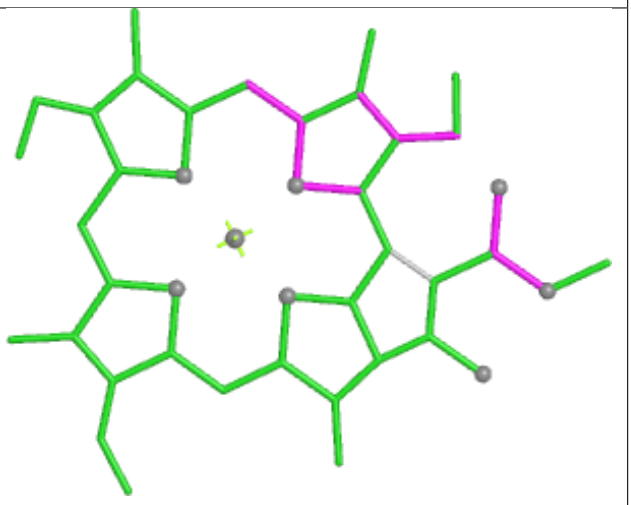


Rings

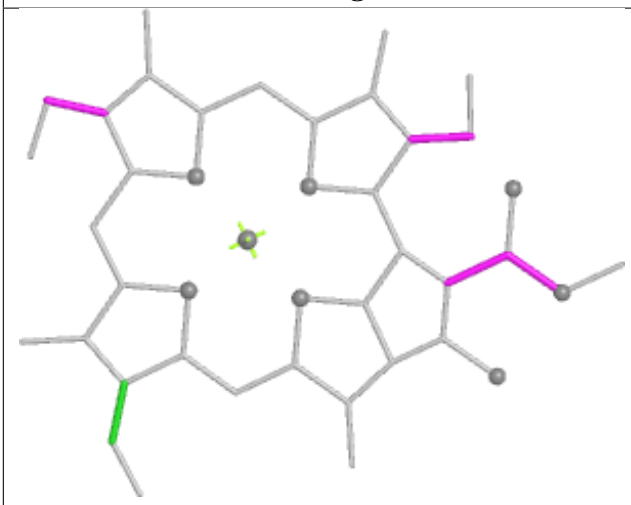
Ligand CLA K 205



Bond lengths



Bond angles

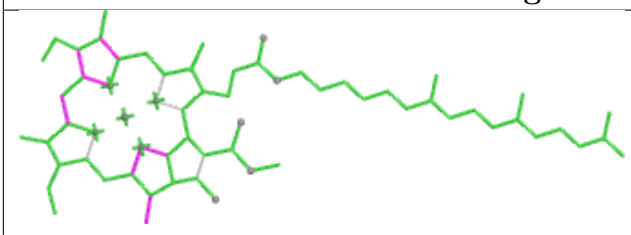


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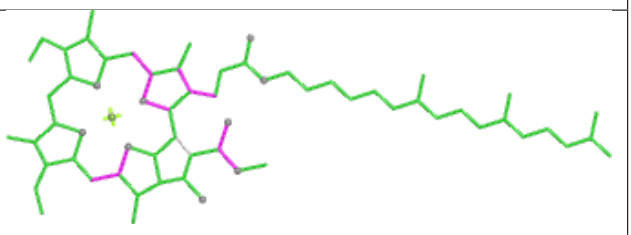


Rings

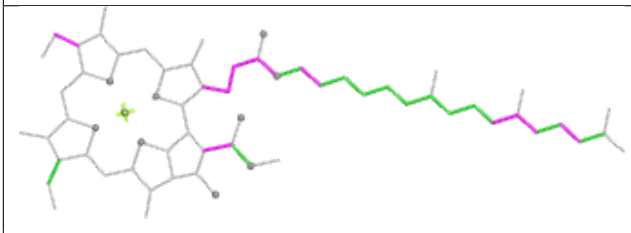
Ligand CLA A 805



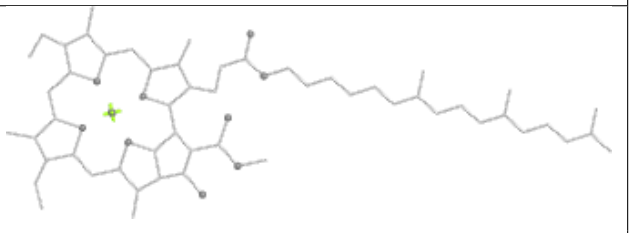
Bond lengths



Bond angles

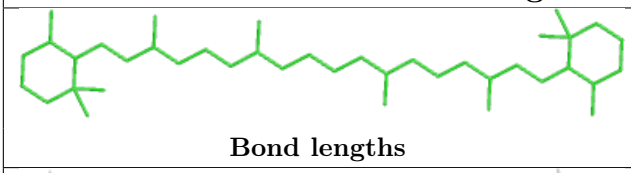


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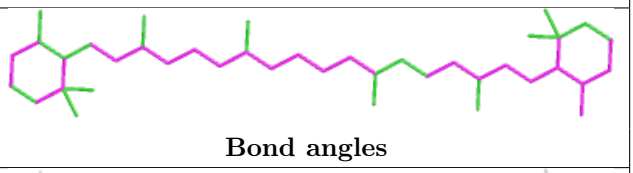


Rings

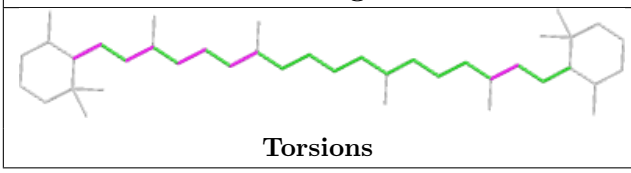
Ligand BCR J 101



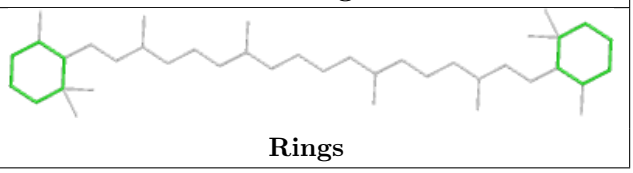
Bond lengths



Bond angles

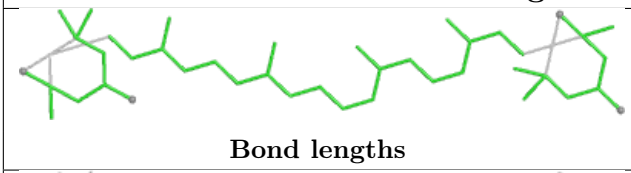


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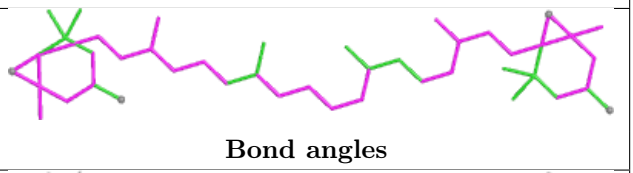


Rings

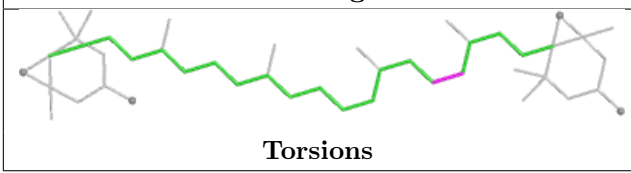
Ligand XAT 3 416



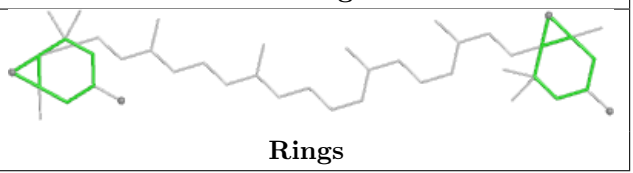
Bond lengths



Bond angles

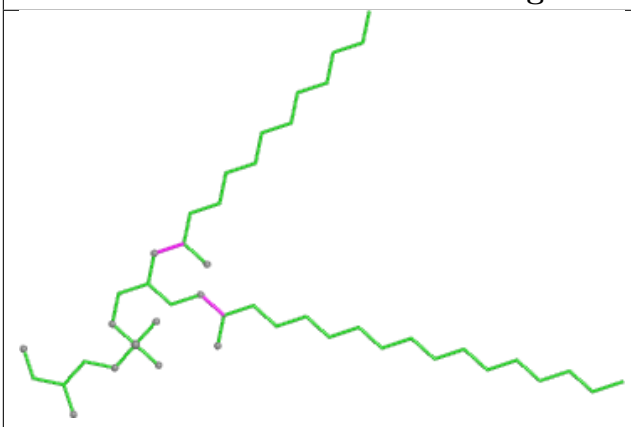


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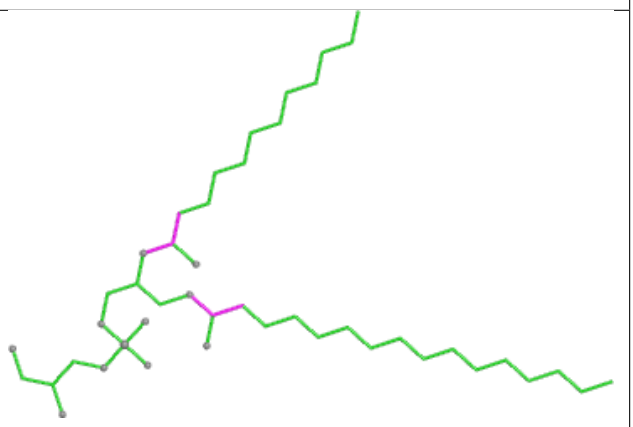


Rings

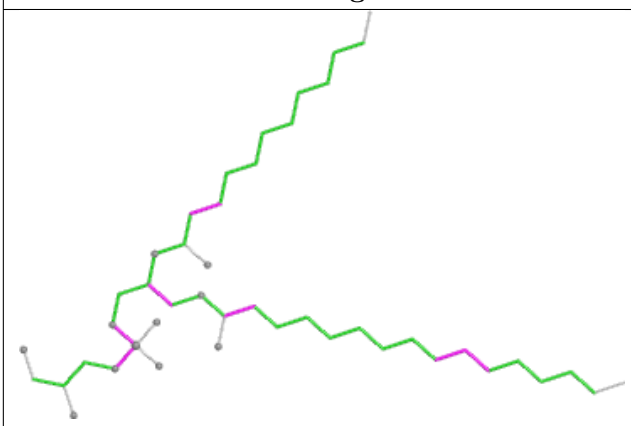
Ligand LHG 9 616



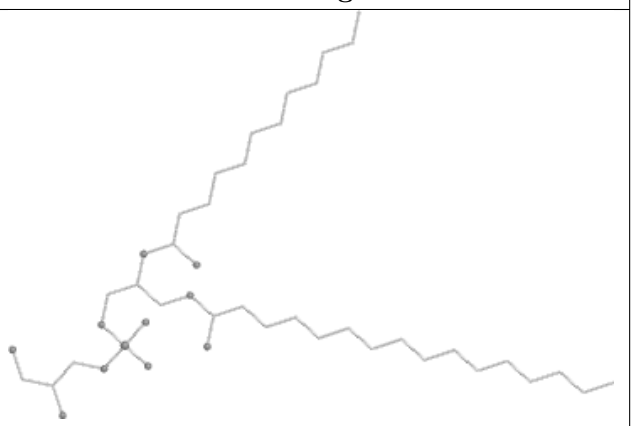
Bond lengths



Bond angles

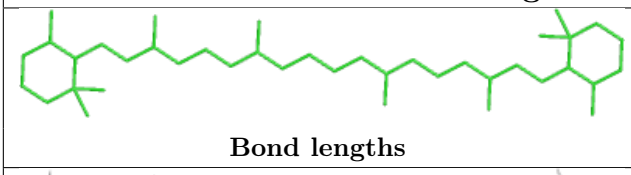


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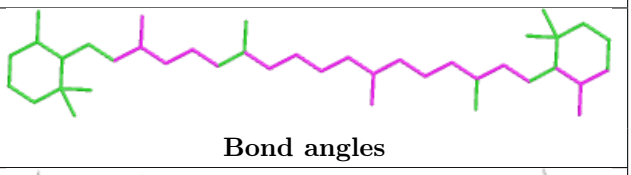


Rings

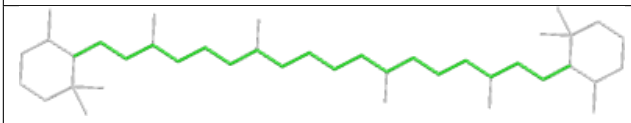
Ligand BCR B 851



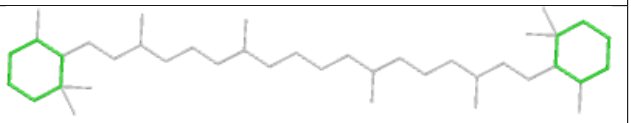
Bond lengths



Bond angles

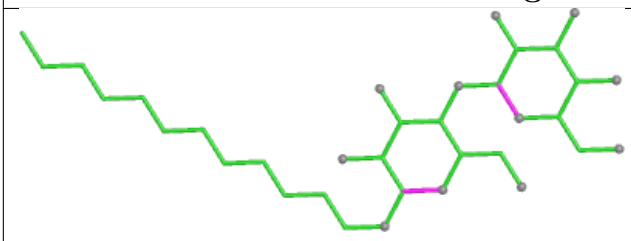


Torsions

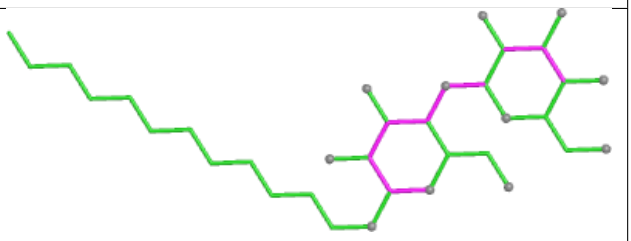


Rings

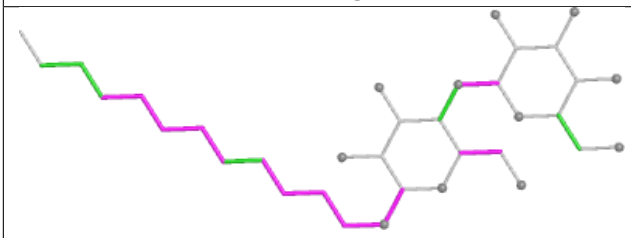
Ligand LMU 6 301



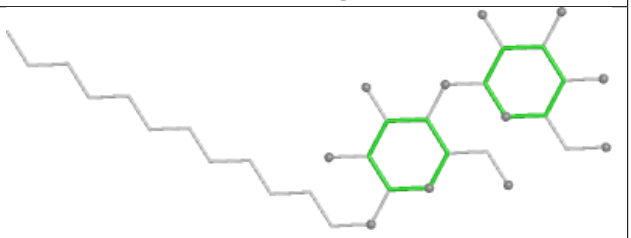
Bond lengths



Bond angles

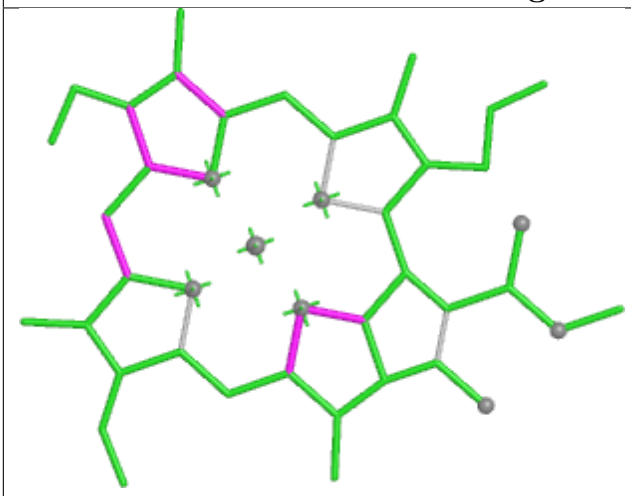


Torsions

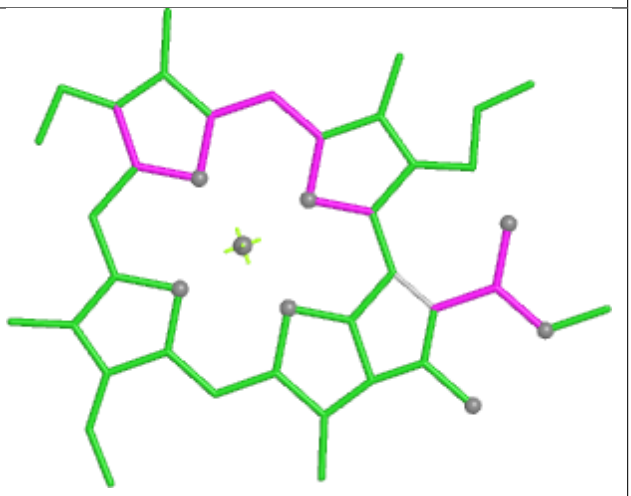


Rings

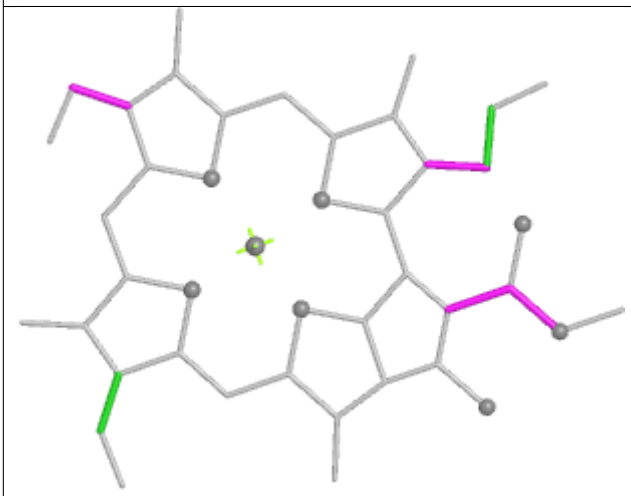
Ligand CLA 6 310



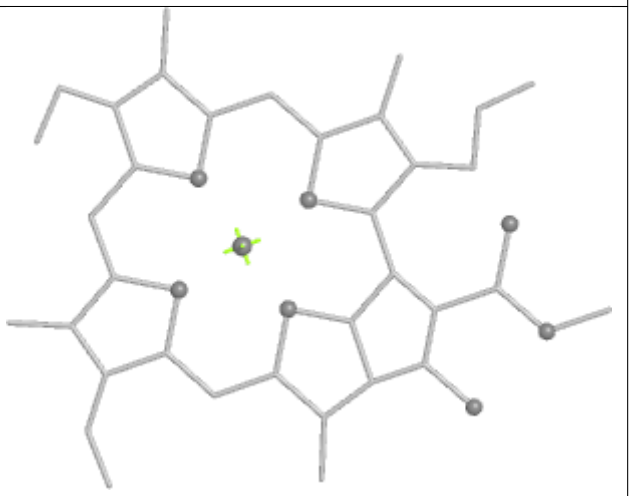
Bond lengths



Bond angles

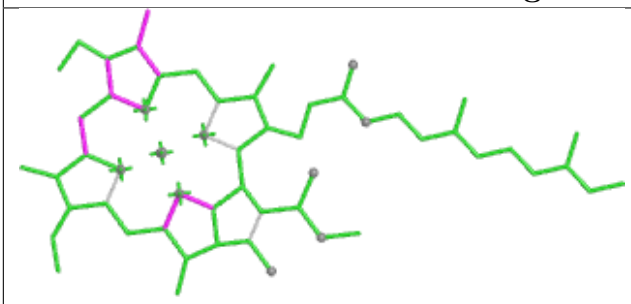


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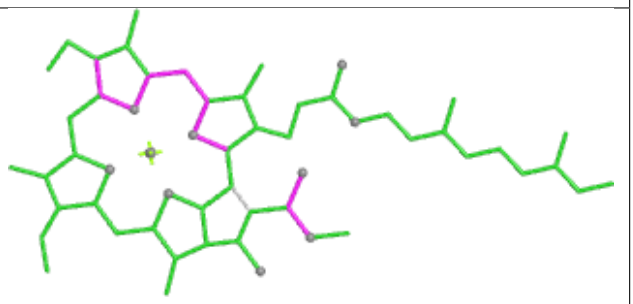


Rings

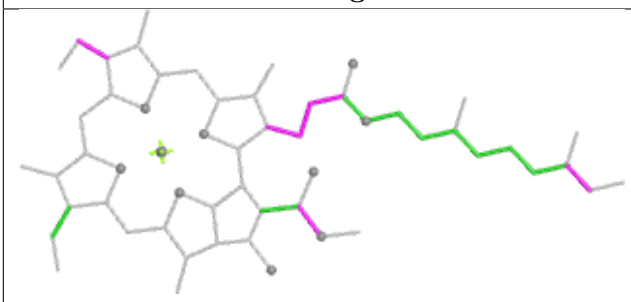
Ligand CLA A 817



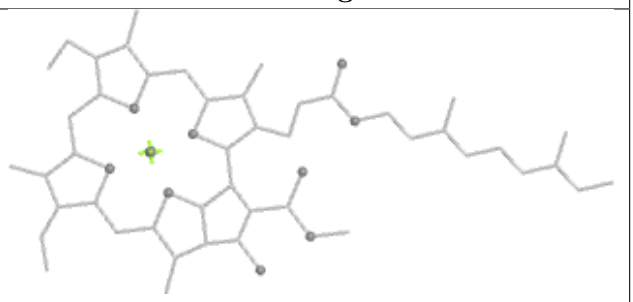
Bond lengths



Bond angles

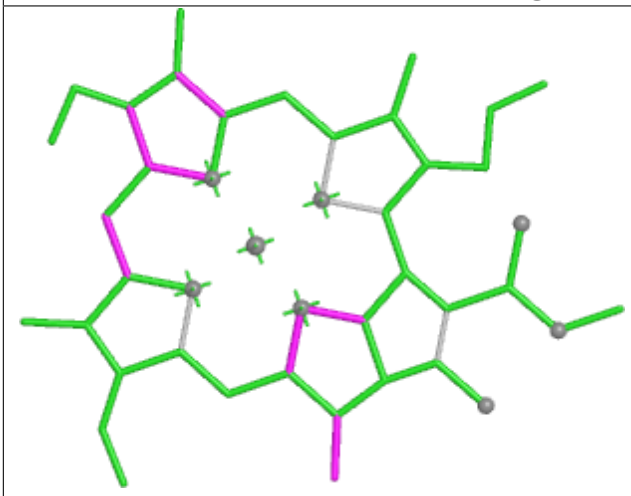


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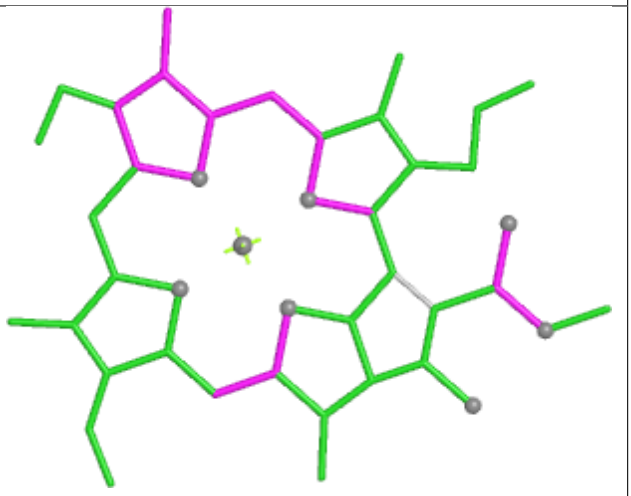


Rings

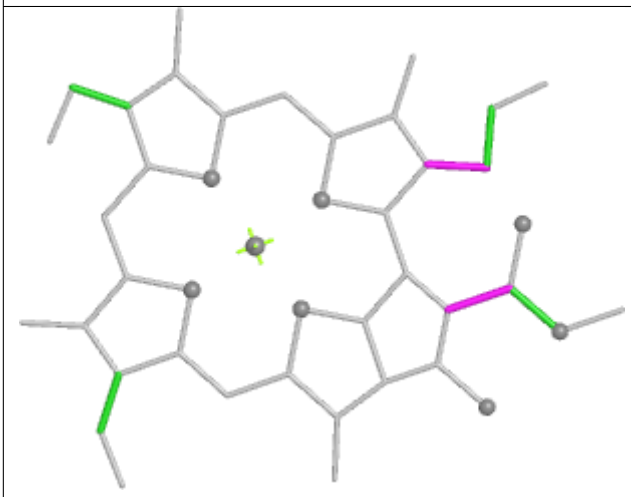
Ligand CLA 8 611



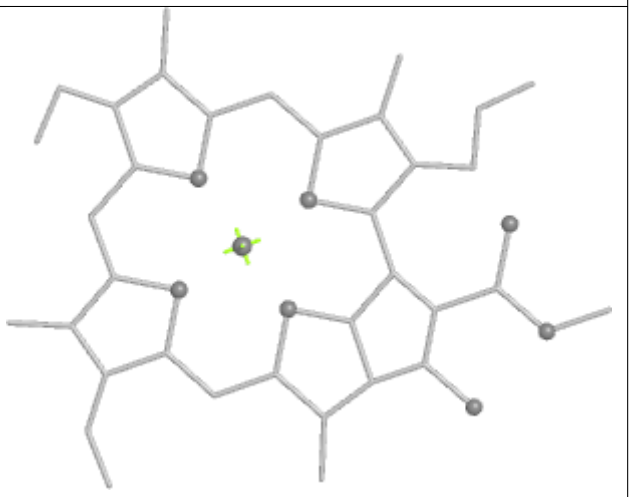
Bond lengths



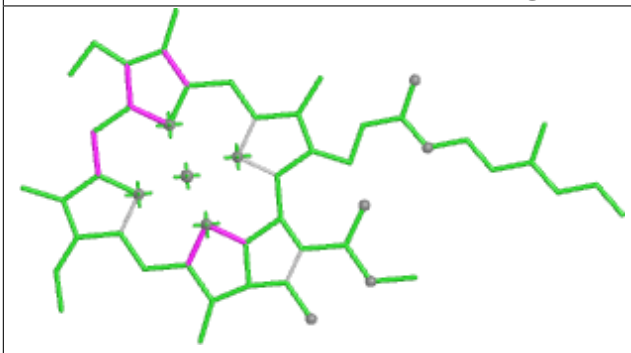
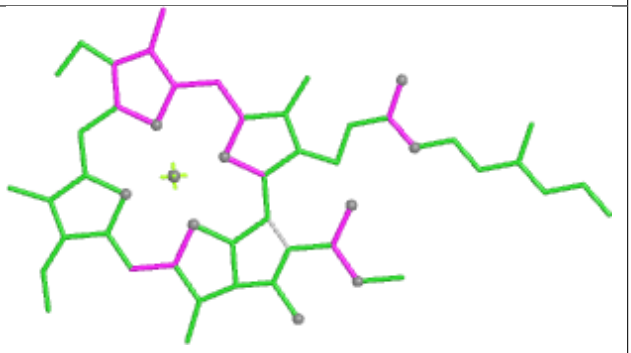
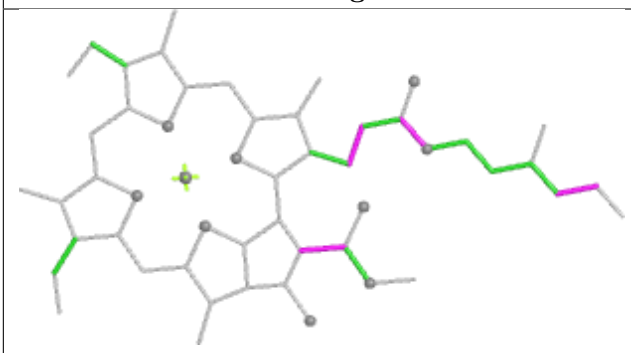
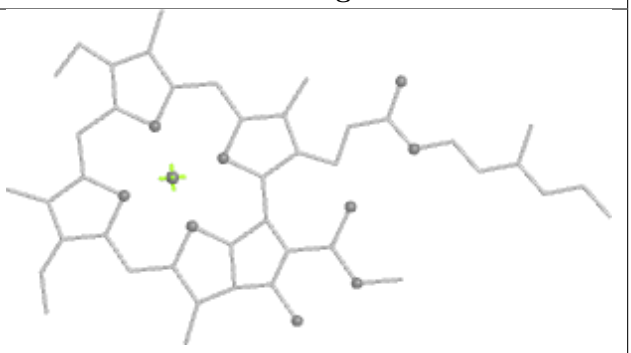
Bond angles

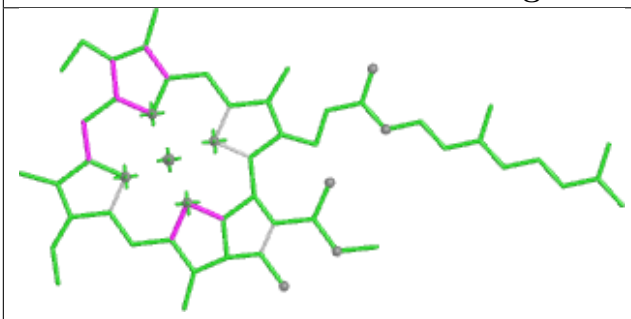
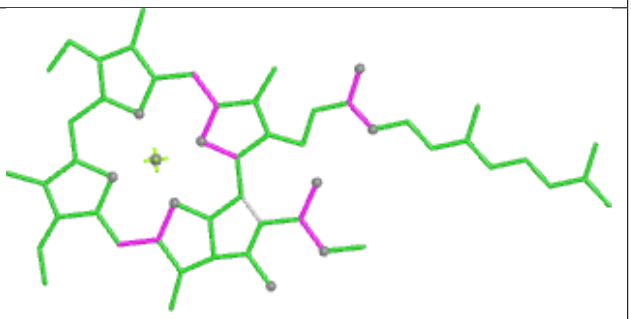
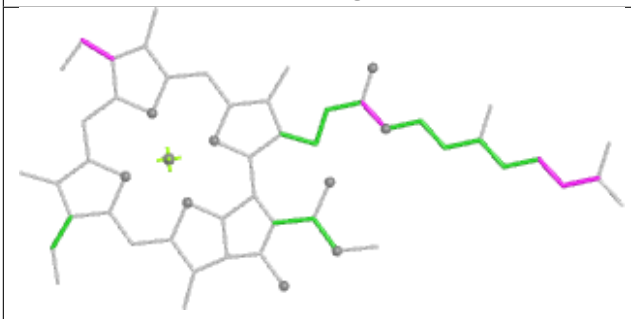
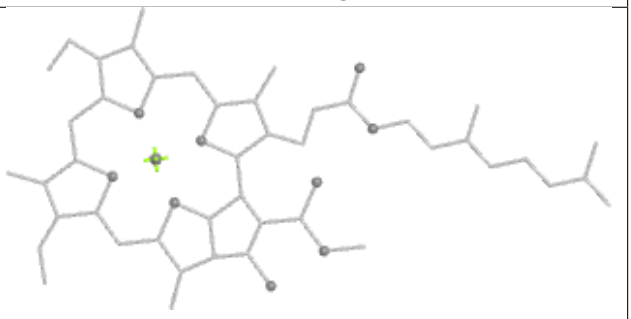


Torsions

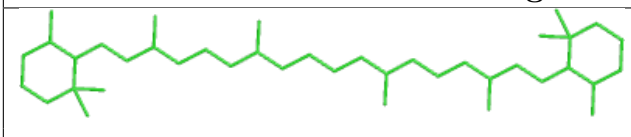


Rings

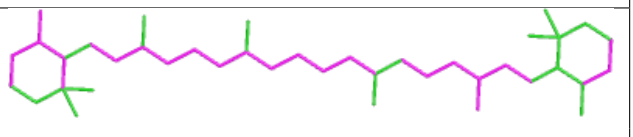
Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA K 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

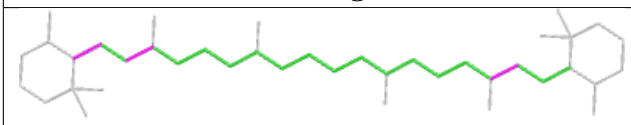
Ligand BCR J 103



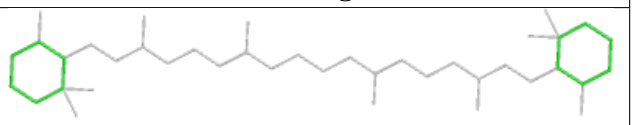
Bond lengths



Bond angles

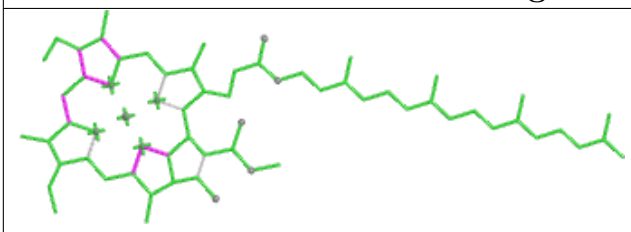


Torsions

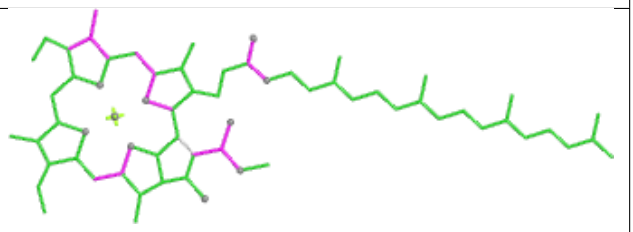


Rings

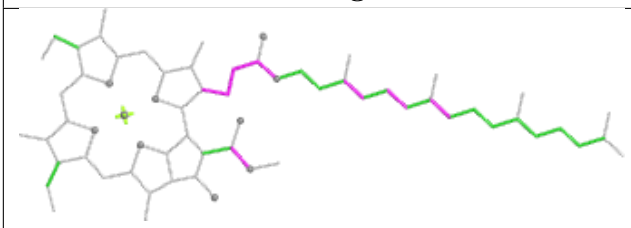
Ligand CLA 2 602



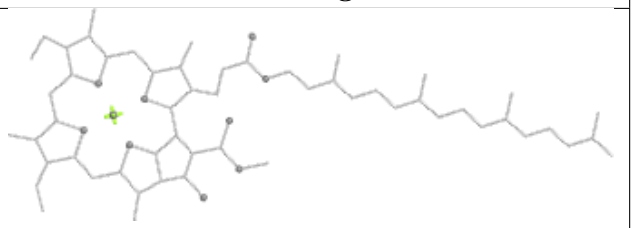
Bond lengths



Bond angles

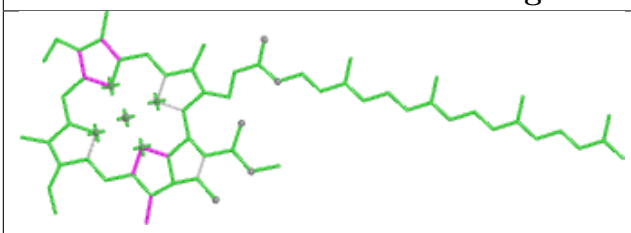


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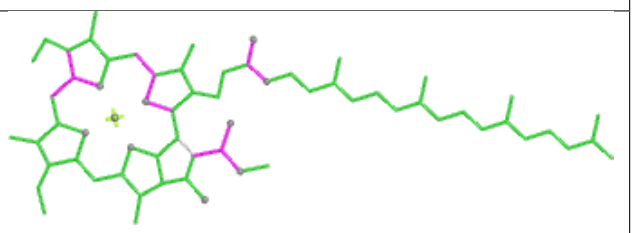


Rings

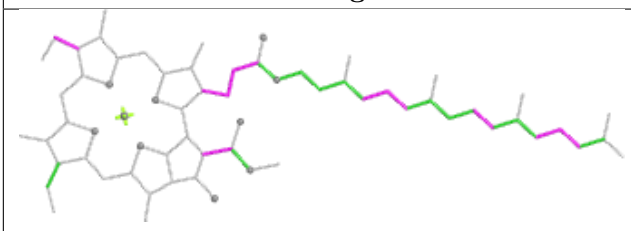
Ligand CLA B 811



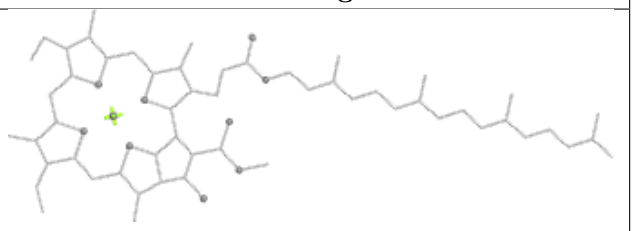
Bond lengths



Bond angles

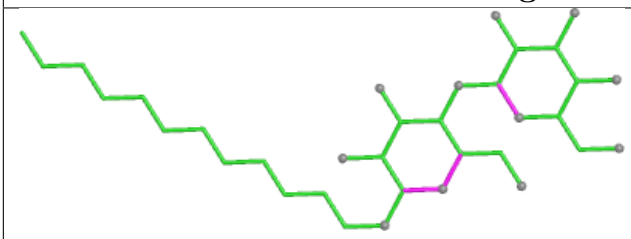


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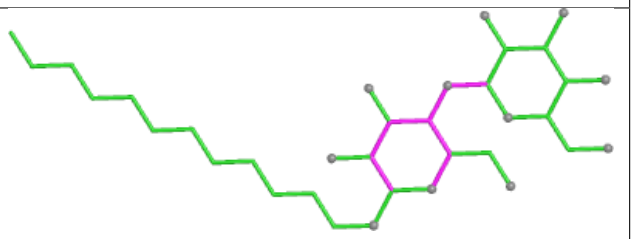


Rings

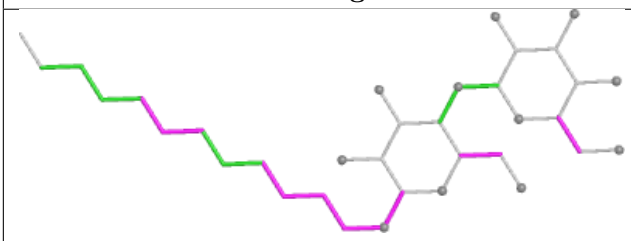
Ligand LMU K 201



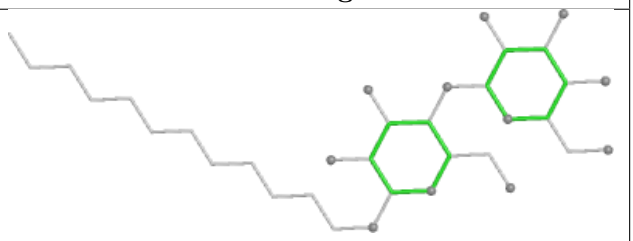
Bond lengths



Bond angles

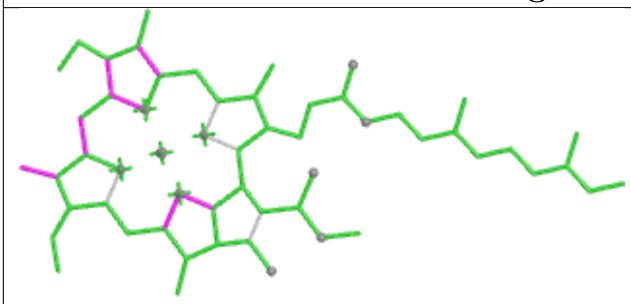


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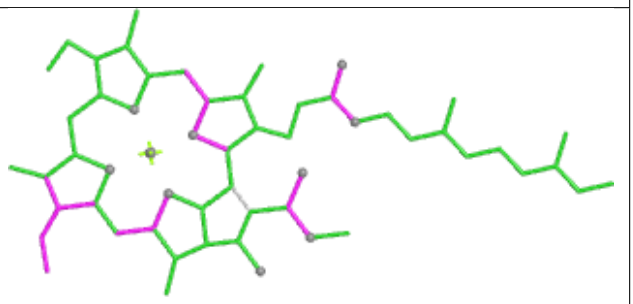


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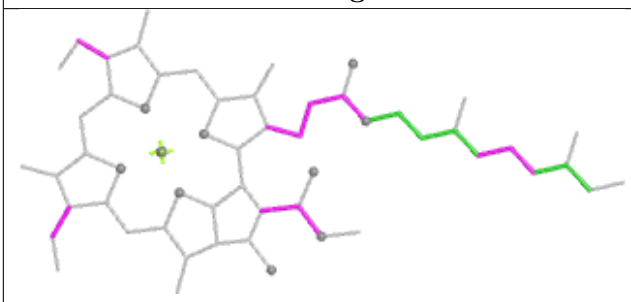
Ligand CLA 9 609



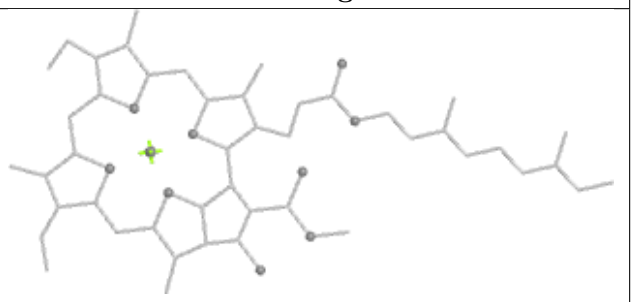
Bond lengths



Bond angles

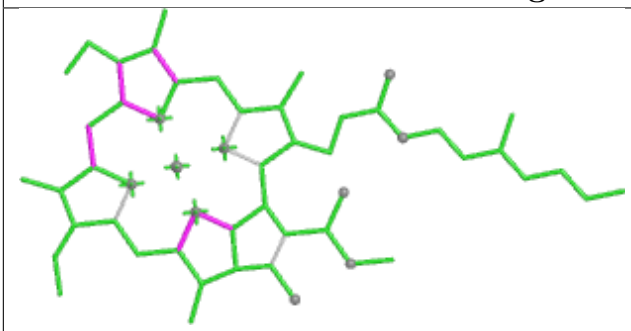


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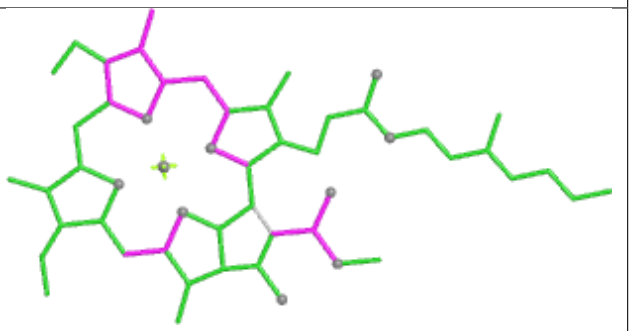


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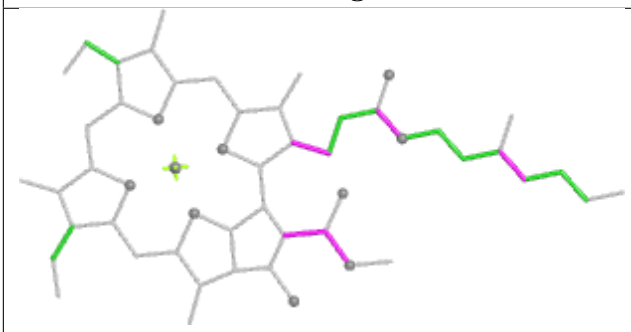
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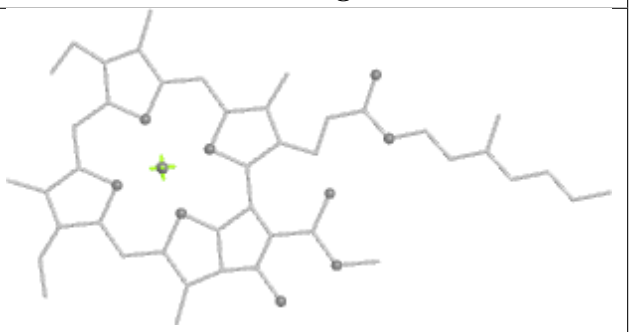
Bond lengths



Bond angles

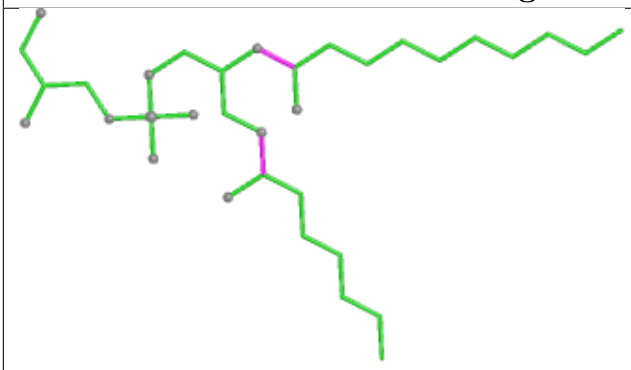


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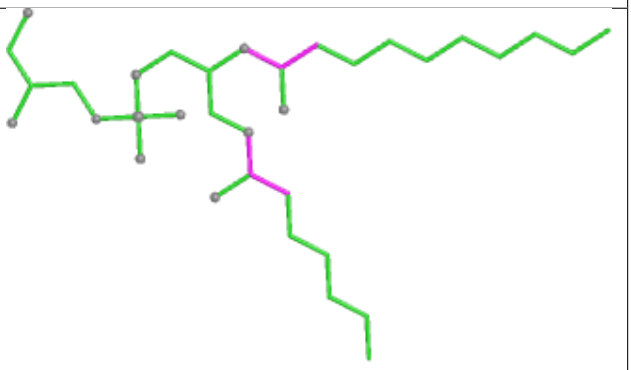


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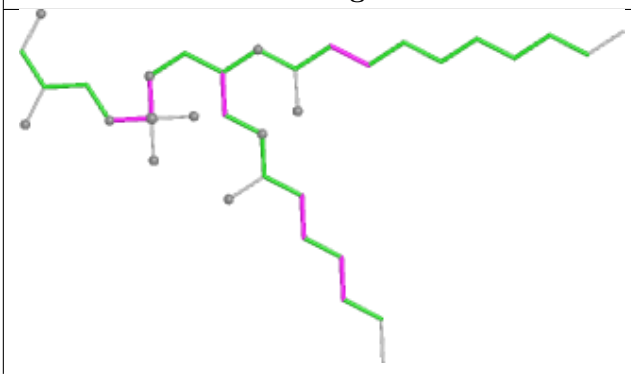
Ligand LHG M 101



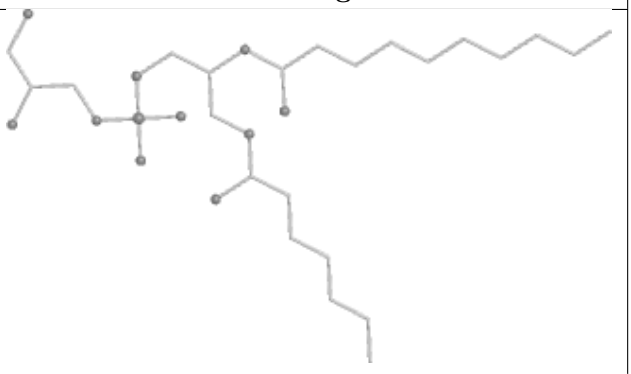
Bond lengths



Bond angles

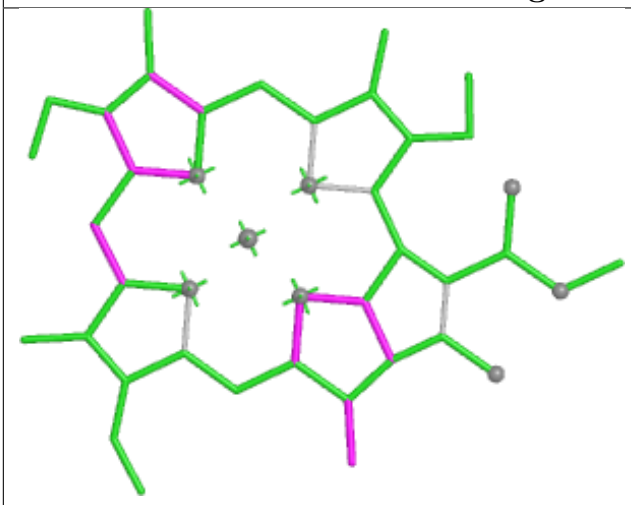


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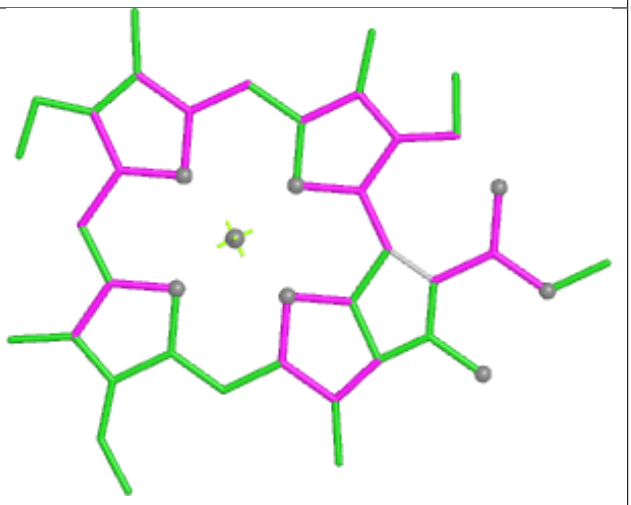


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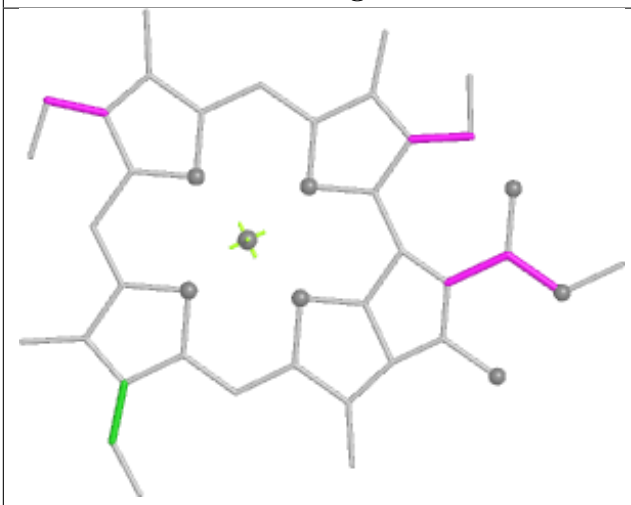
Ligand CLA 1 302



Bond lengths



Bond angles

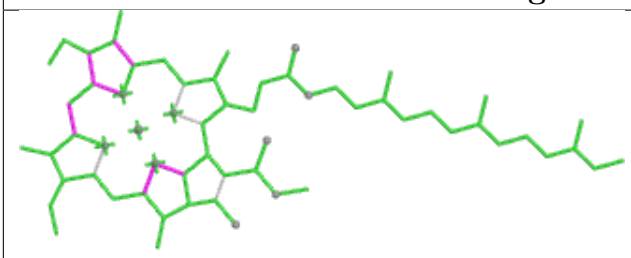


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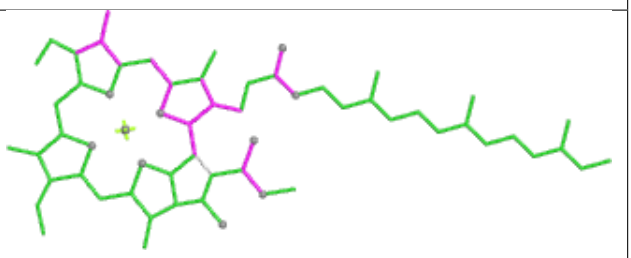


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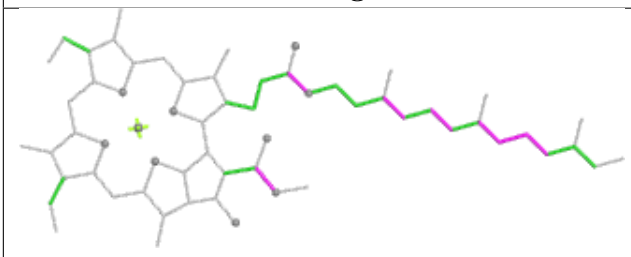
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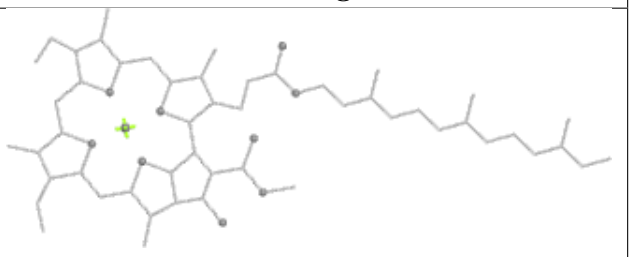
Bond lengths



Bond angles

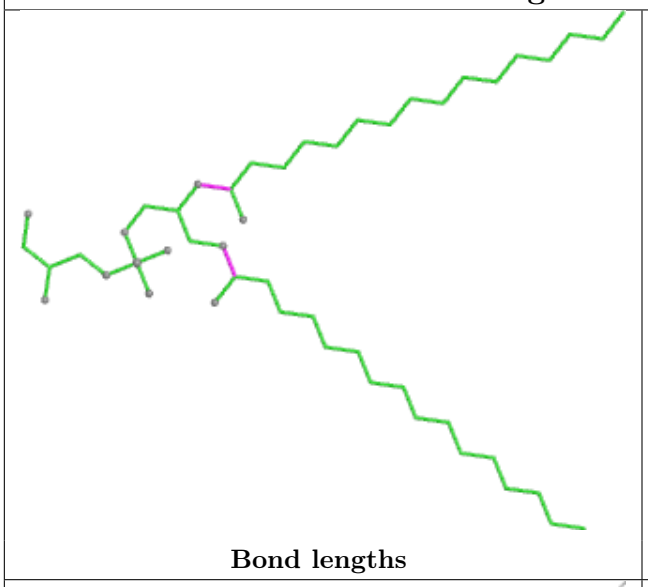


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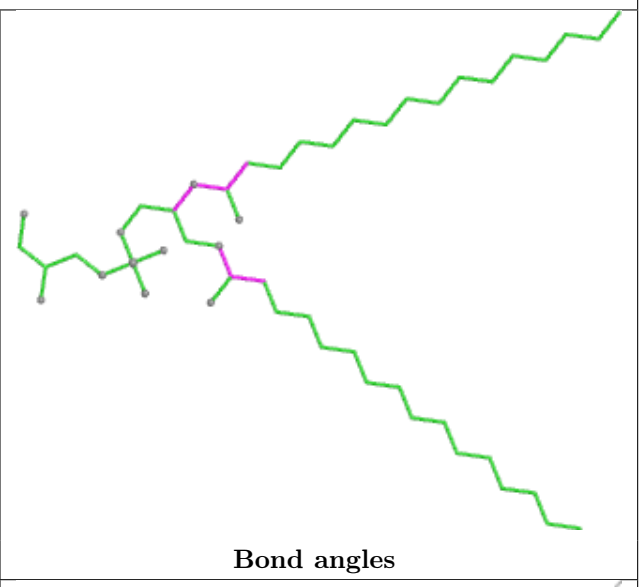


Rings

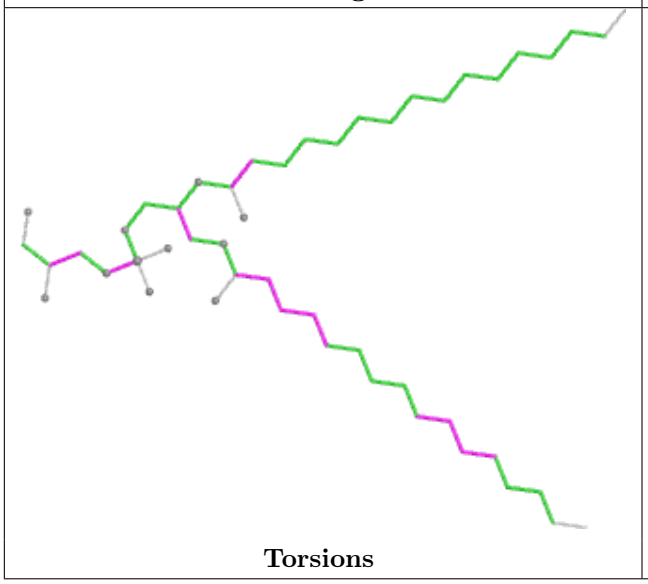
Ligand LHG 1 317



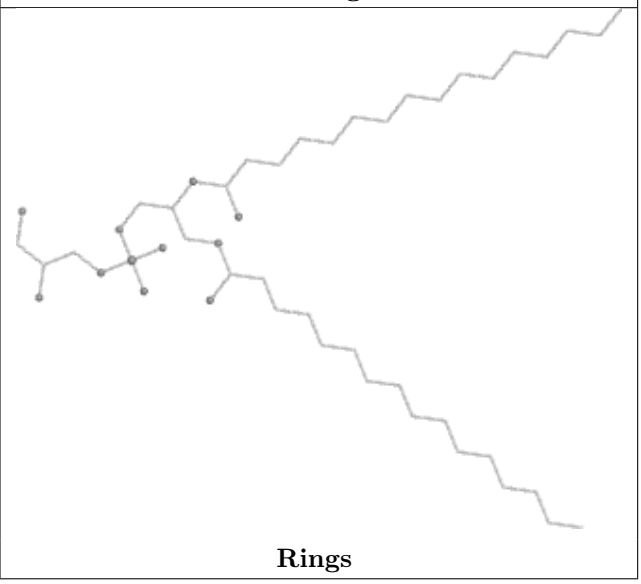
Bond lengths



Bond angles

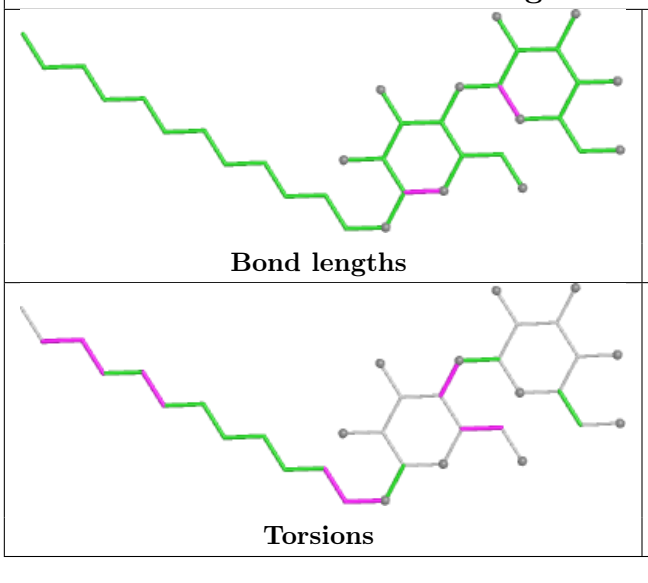


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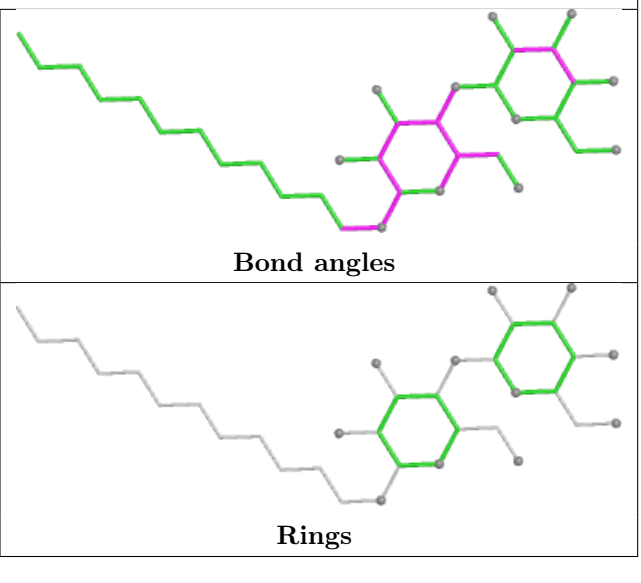


Rings

Ligand LMU 3 421



Bond lengths

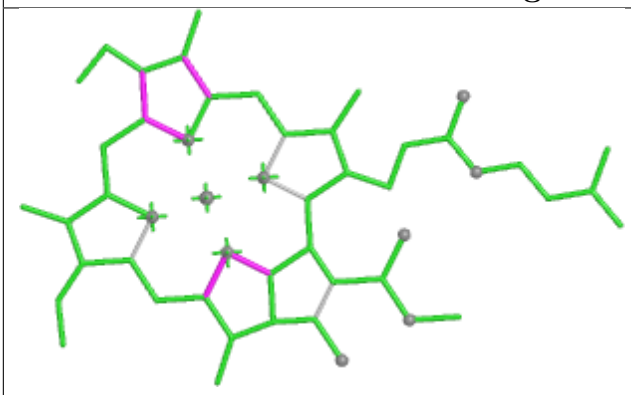


Bond angles

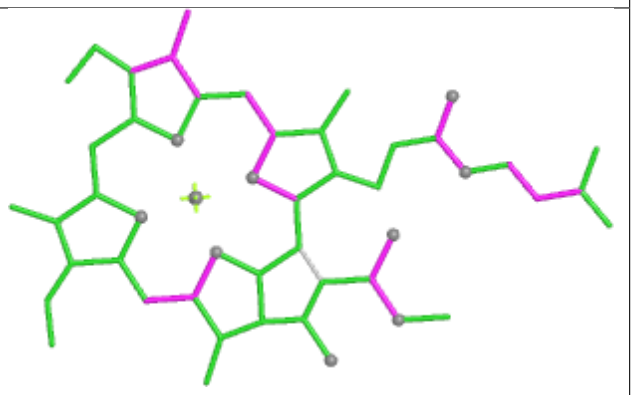
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Rings

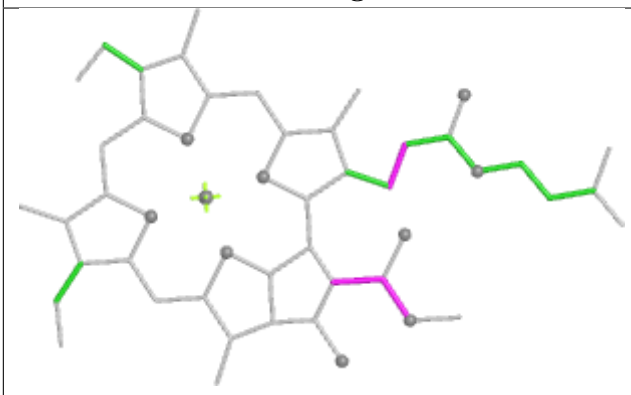
Ligand CLA A 806



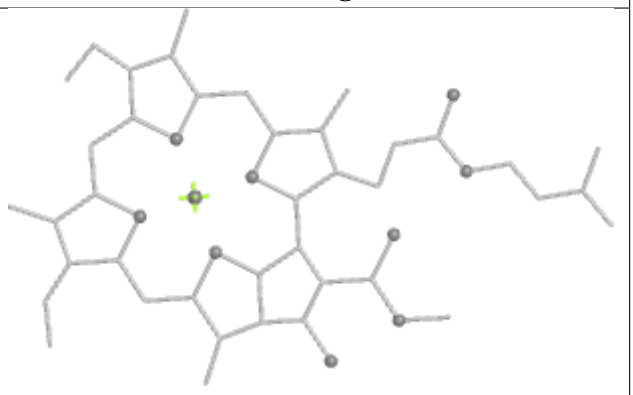
Bond lengths



Bond angles



Torsions

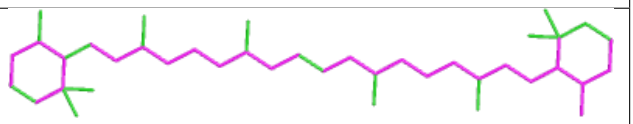


Rings

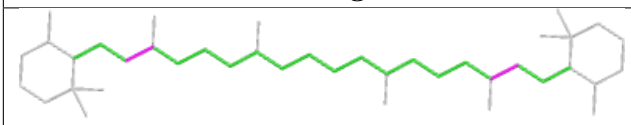
Ligand BCR 7 317



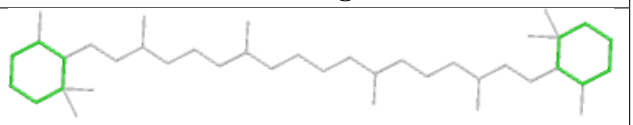
Bond lengths



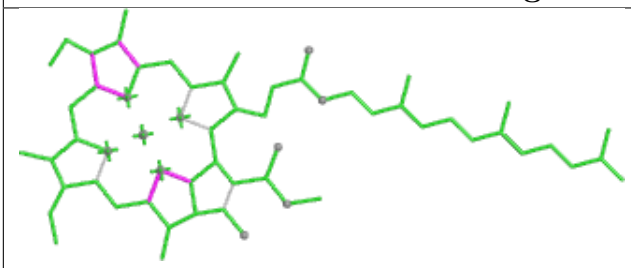
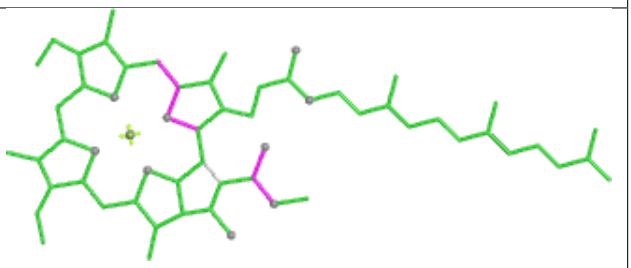
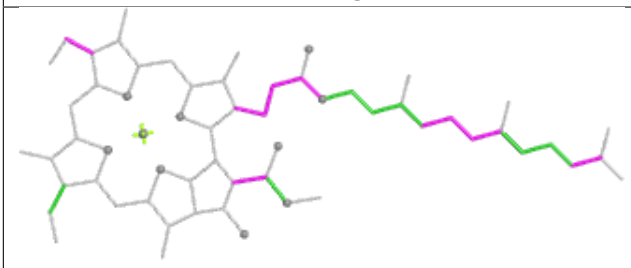
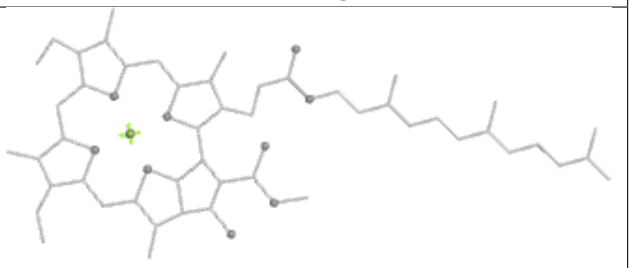
Bond angles

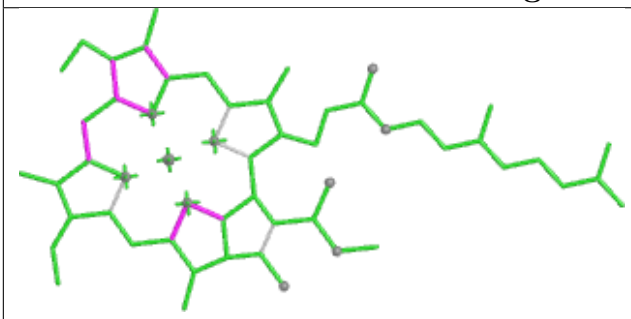
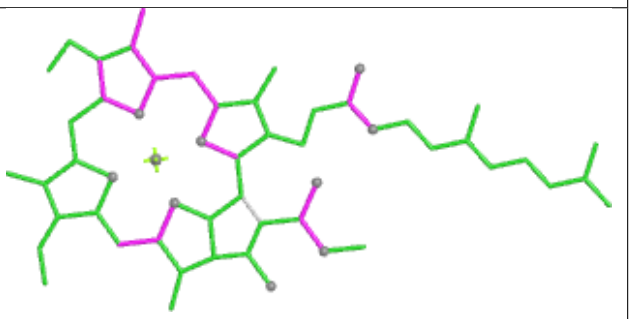
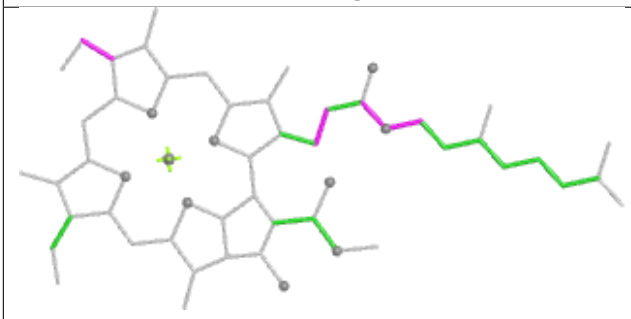
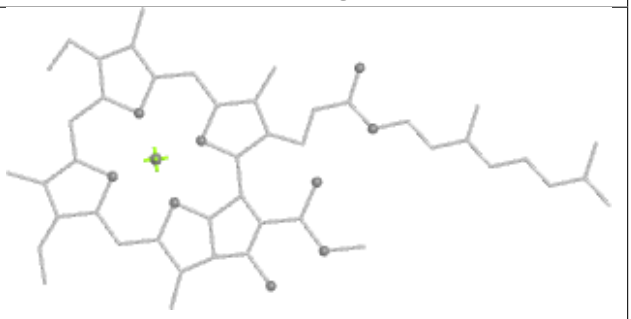


Torsions

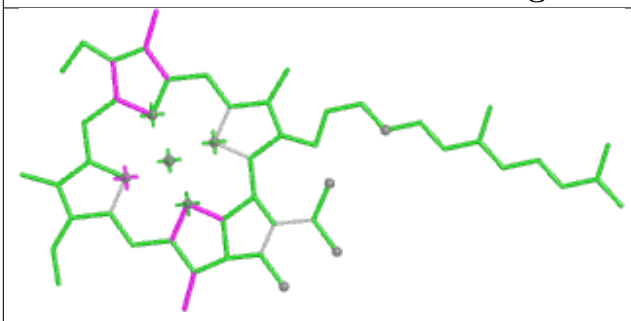


Rings

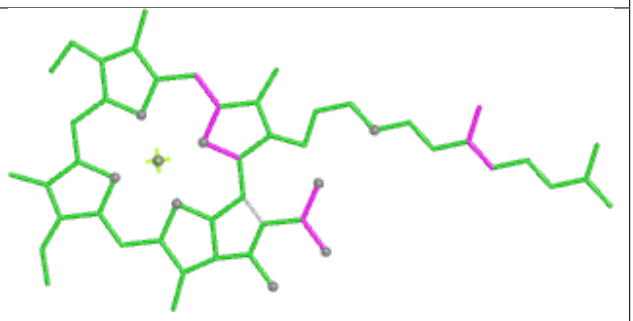
Ligand CLA A 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

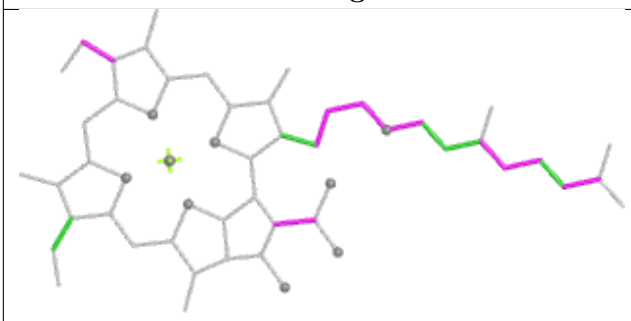
Ligand CLA 3 411



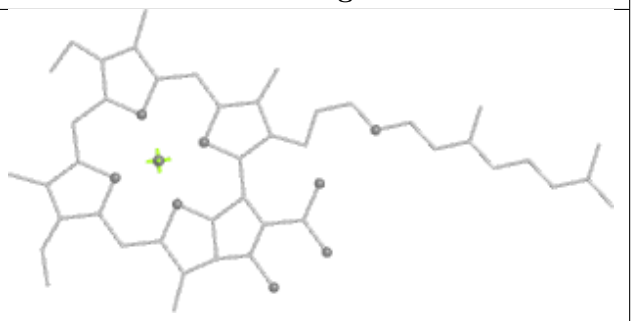
Bond lengths



Bond angles

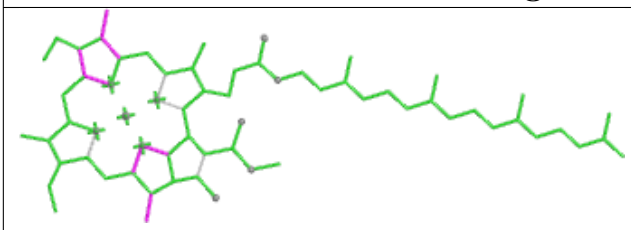


Torsions

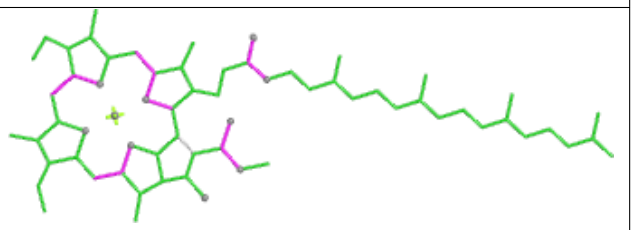


Rings

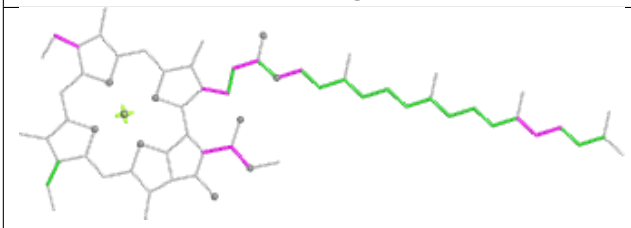
Ligand CLA B 843



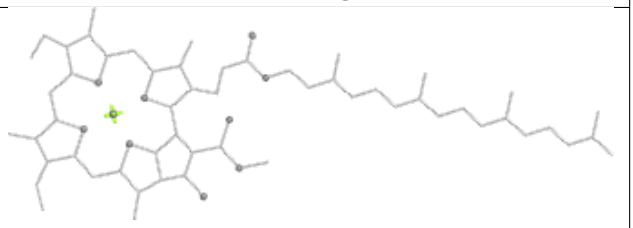
Bond lengths



Bond angles

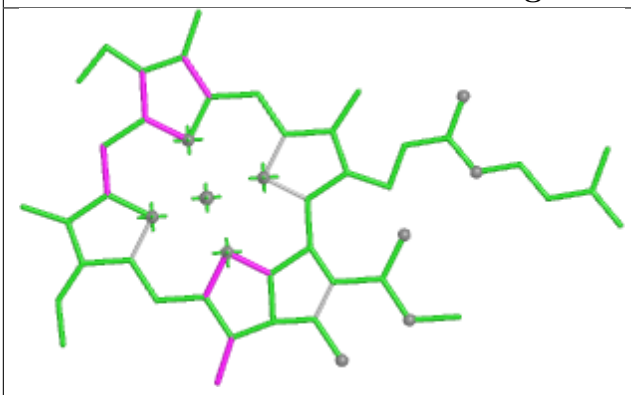


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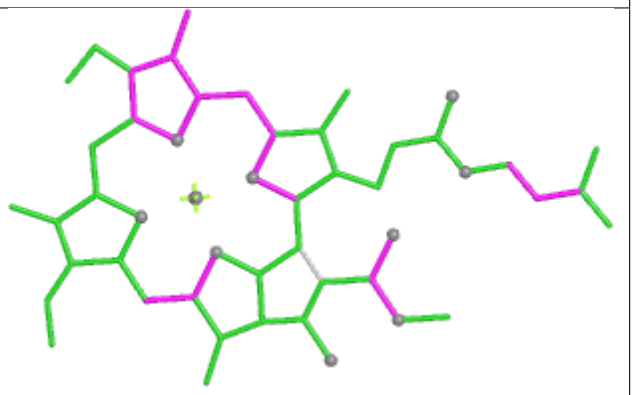


Rings

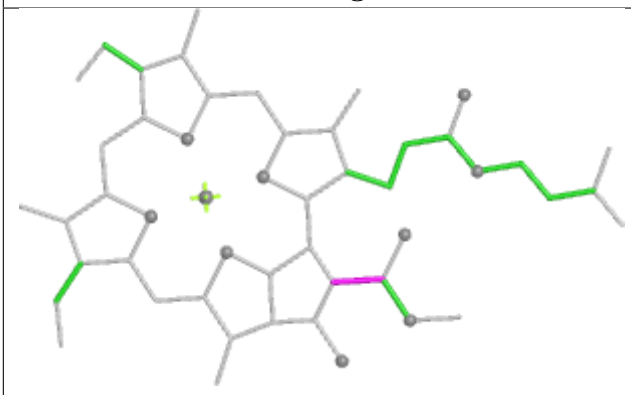
Ligand CLA B 828



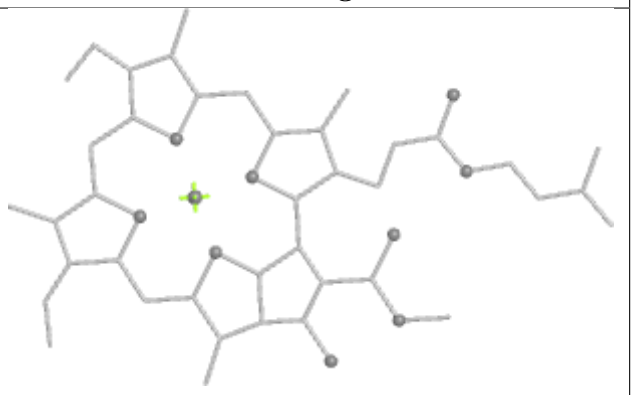
Bond lengths



Bond angles

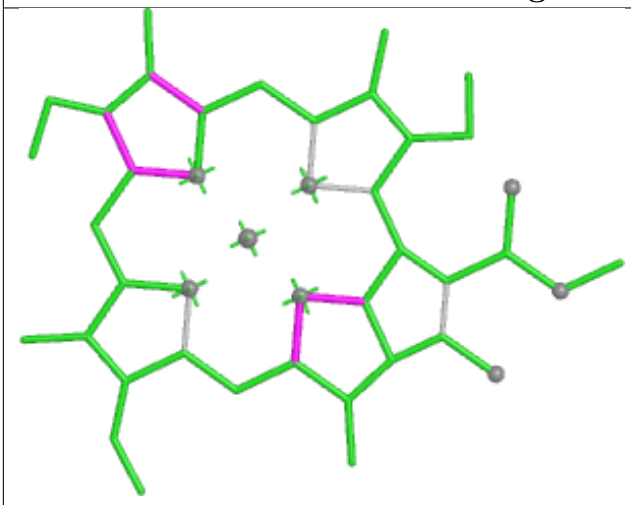


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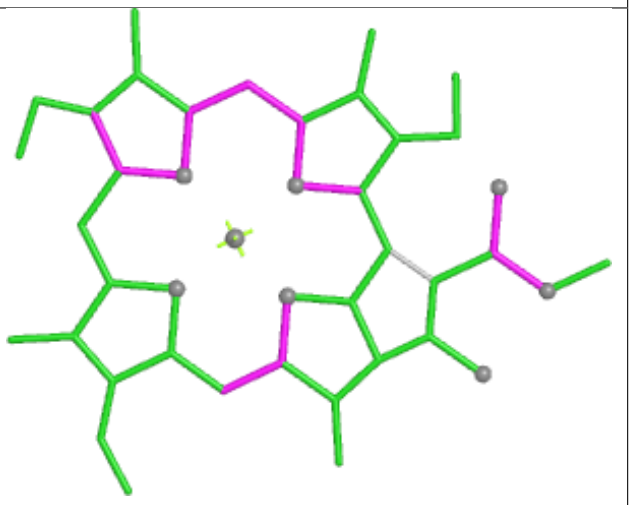


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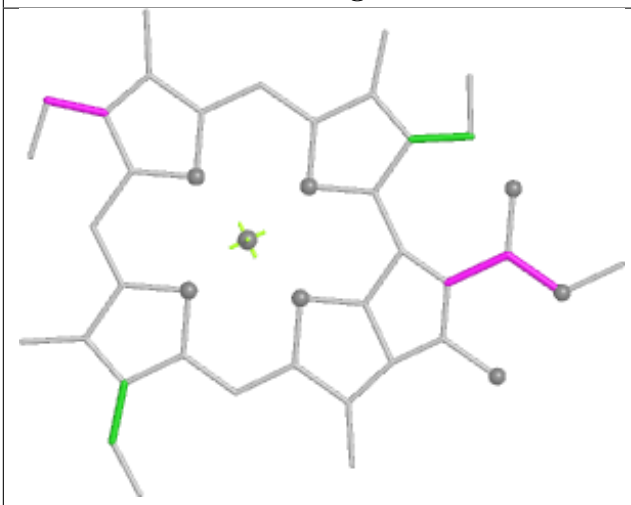
Ligand CLA 6 309



Bond lengths



Bond angles

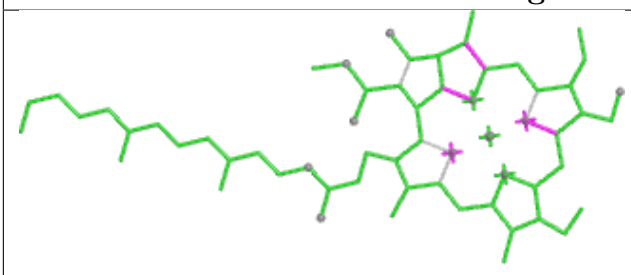


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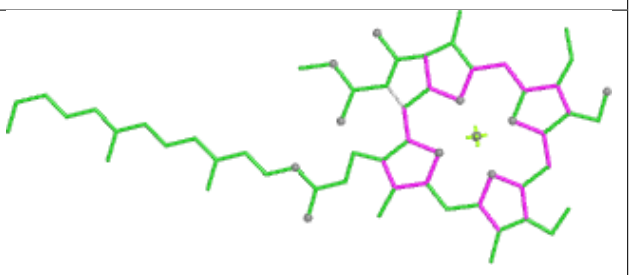


Rings

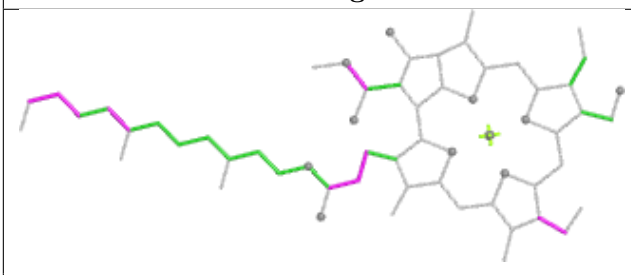
Ligand CHL 3 413



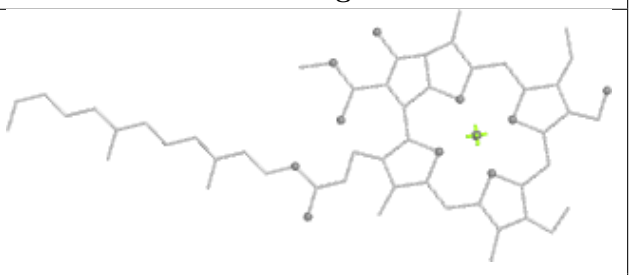
Bond lengths



Bond angles

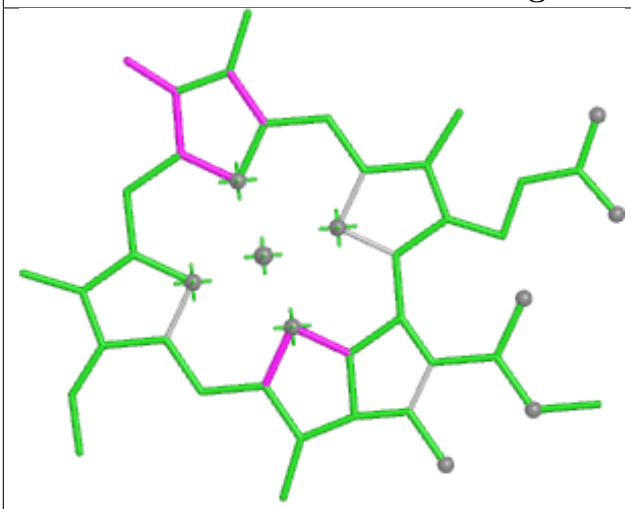


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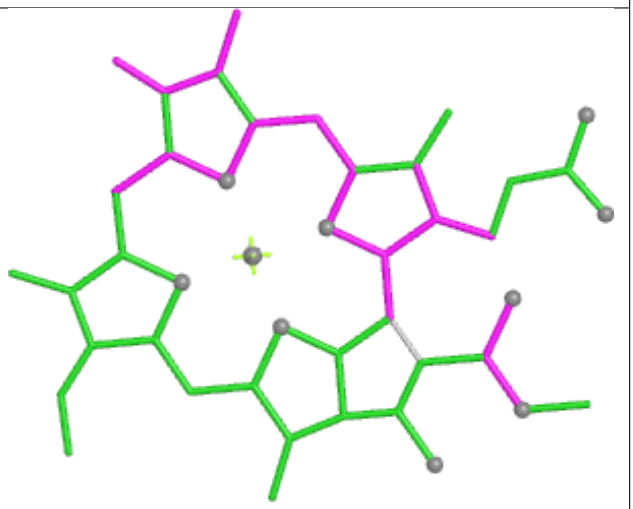


Rings

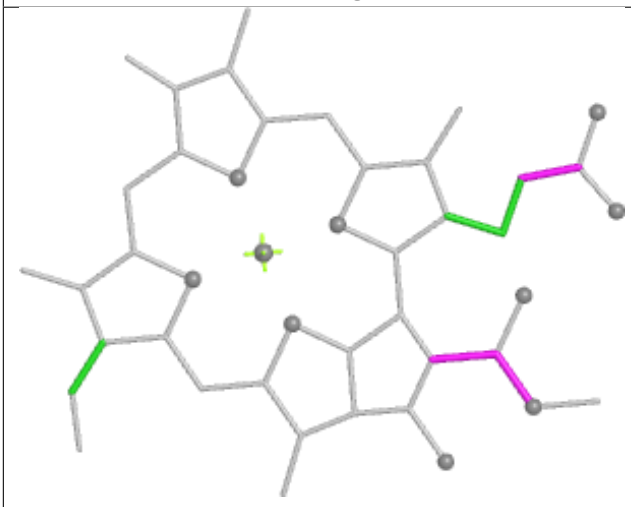
Ligand CLA 8 604



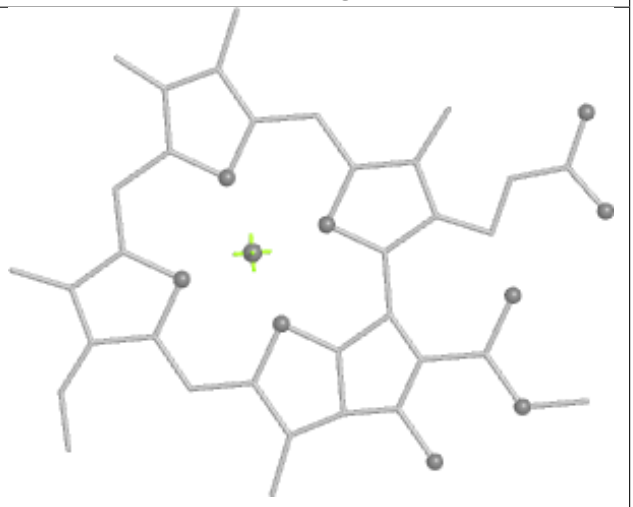
Bond lengths



Bond angles

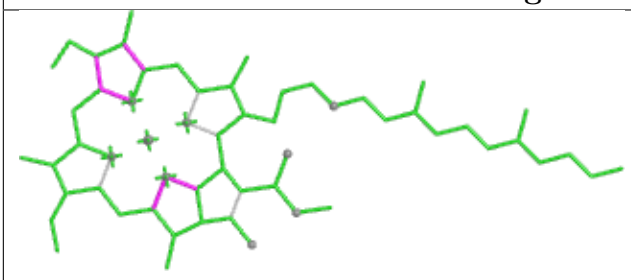


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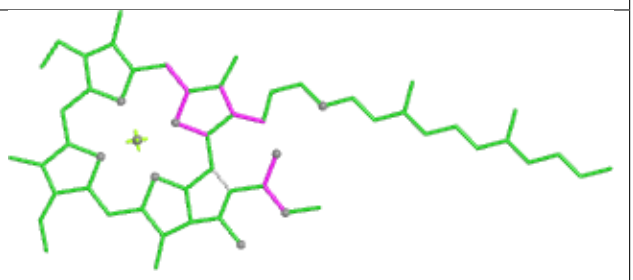


Rings

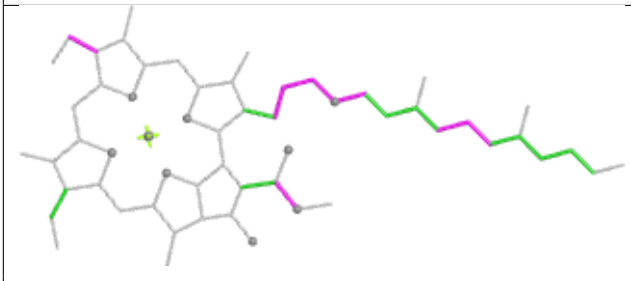
Ligand CLA B 813



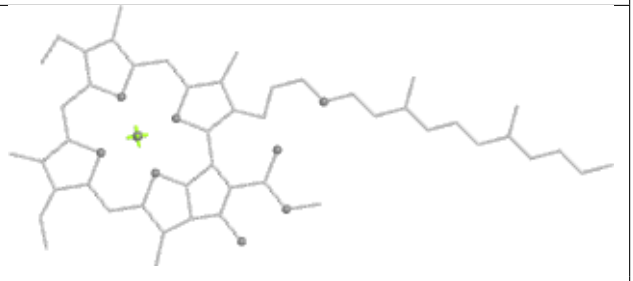
Bond lengths



Bond angles

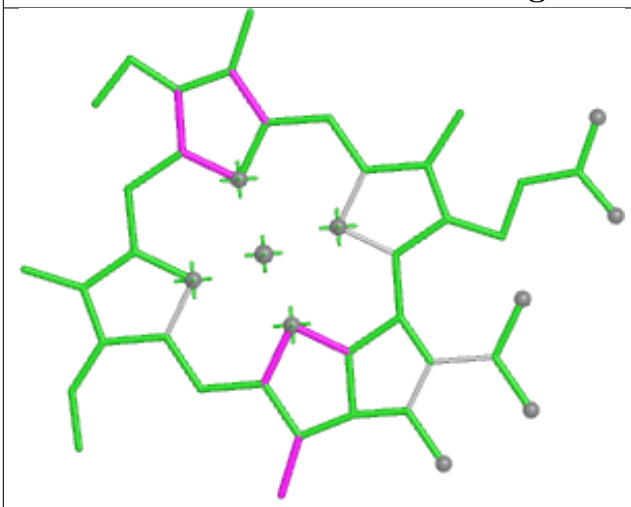


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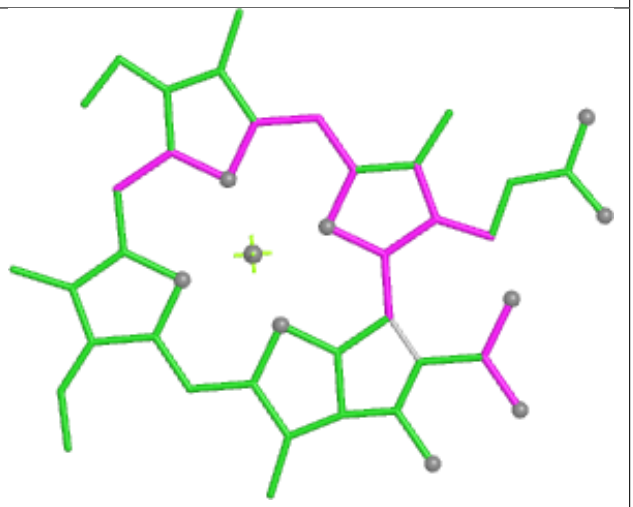


Rings

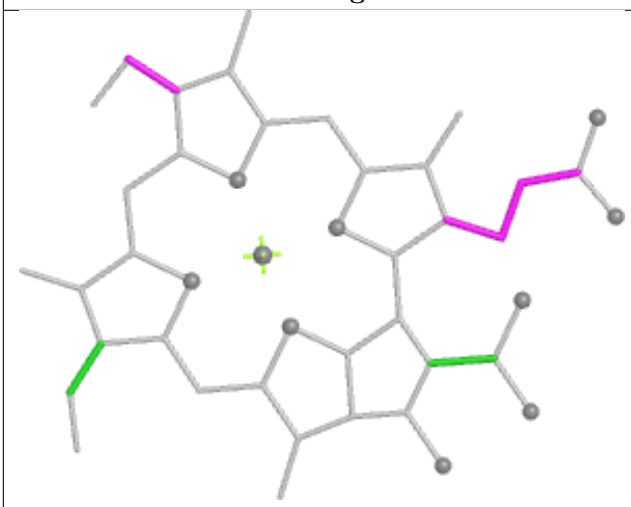
Ligand CLA 7 302



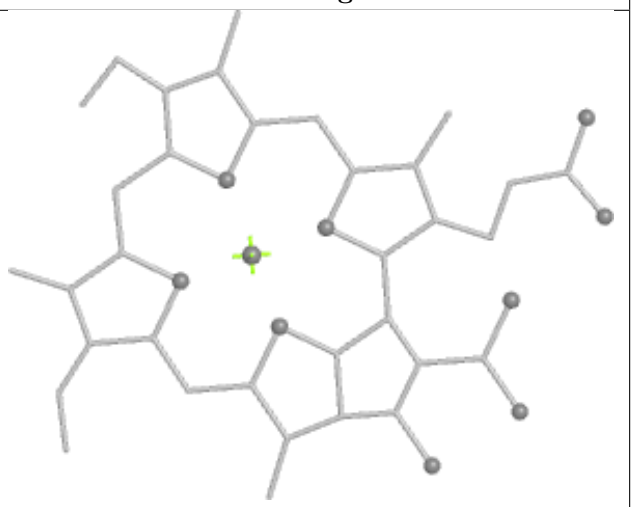
Bond lengths



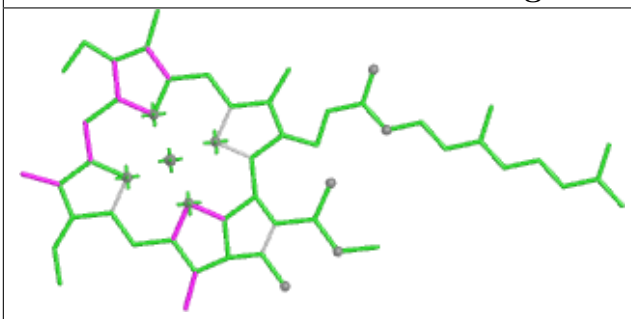
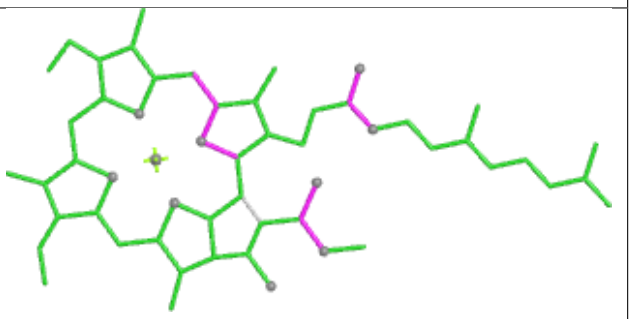
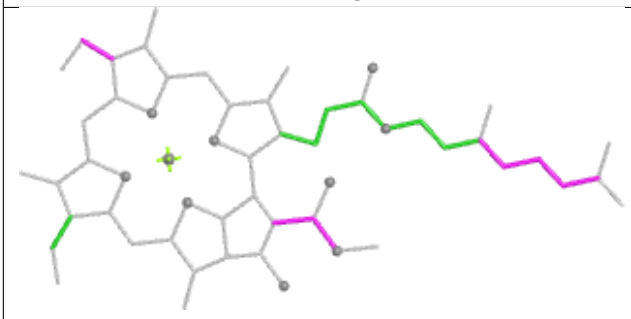
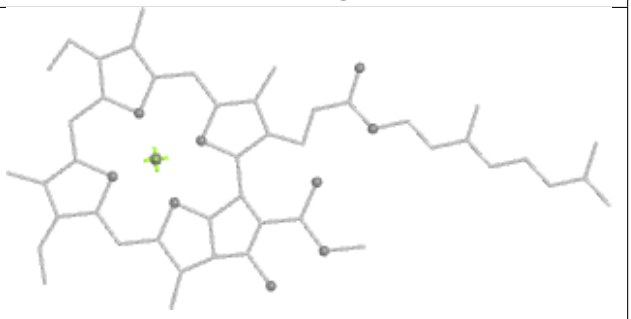
Bond angles

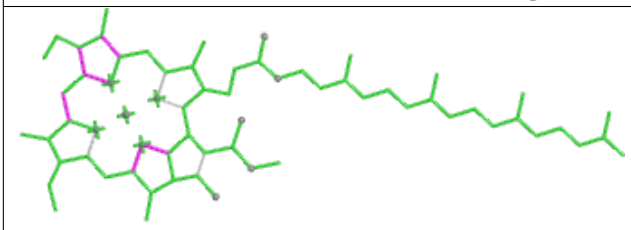
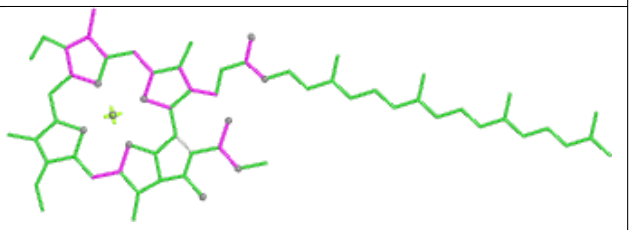
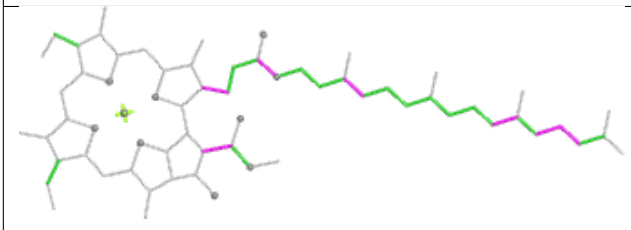
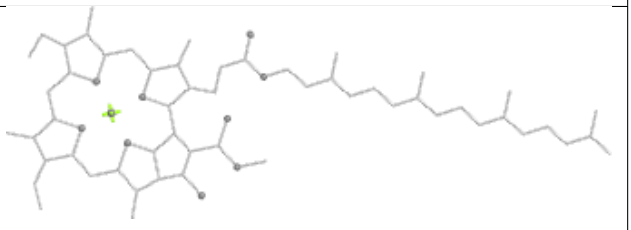


Torsions

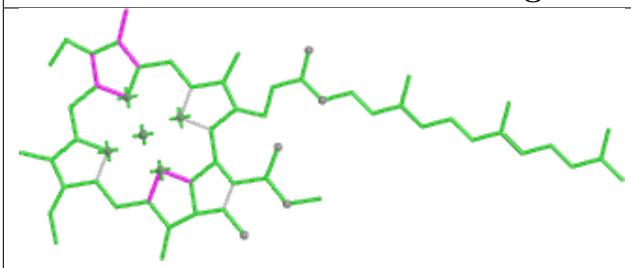


Rings

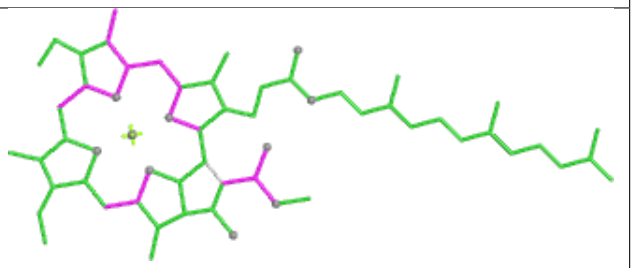
Ligand CLA B 836	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

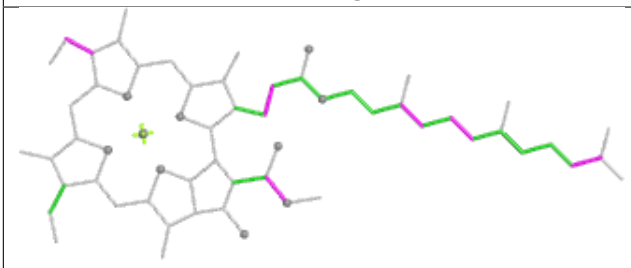
Ligand CLA B 821



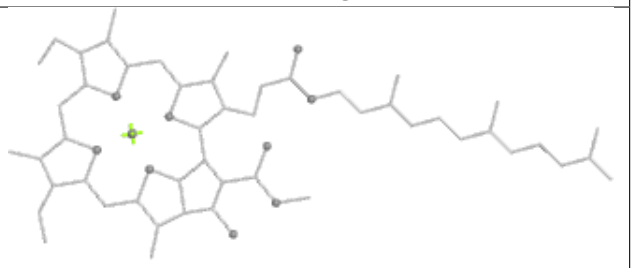
Bond lengths



Bond angles

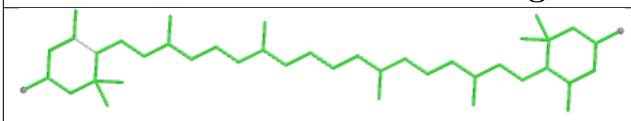


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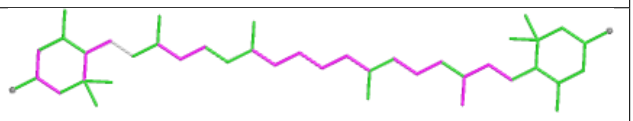


Rings

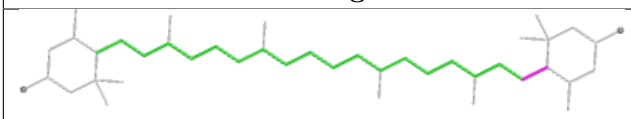
Ligand LUT 1 314



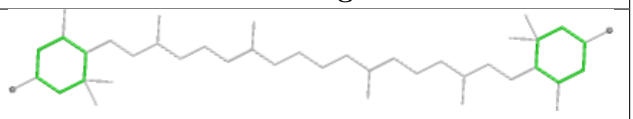
Bond lengths



Bond angles

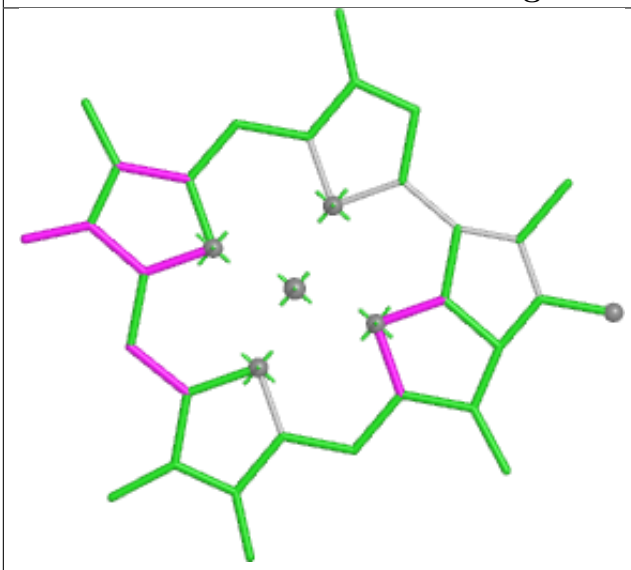


Torsions



Rings

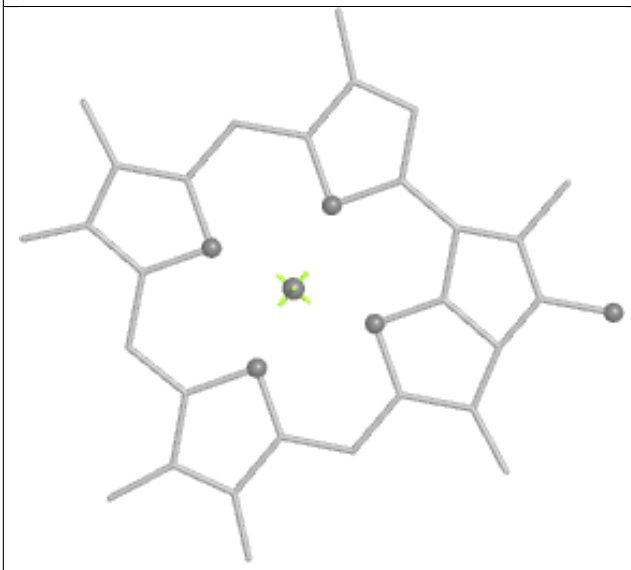
Ligand CLA H 202



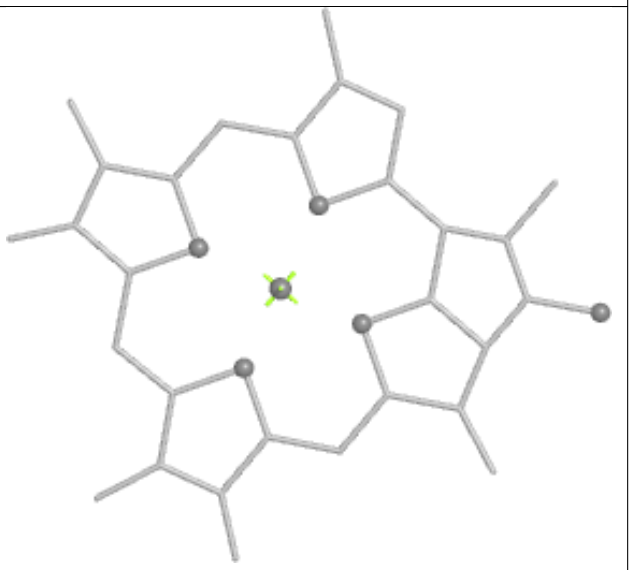
Bond lengths



Bond angles

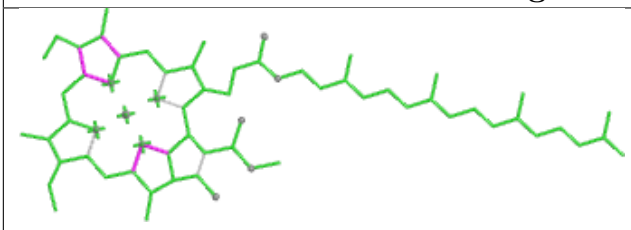


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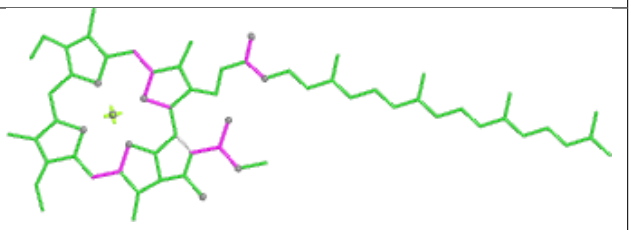


Rings

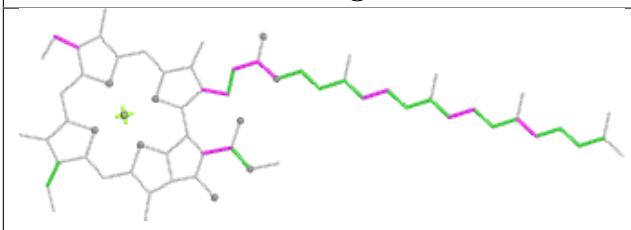
Ligand CLA 7 307



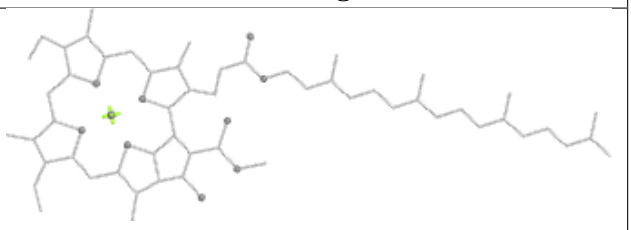
Bond lengths



Bond angles

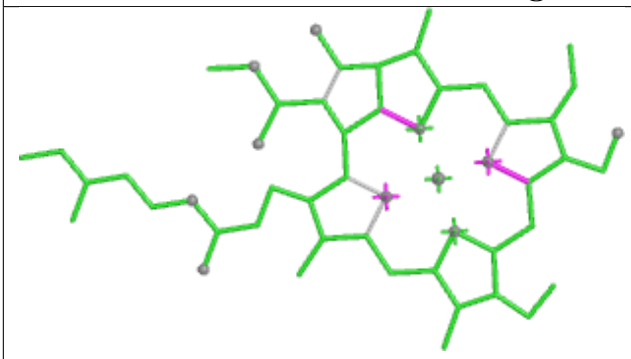


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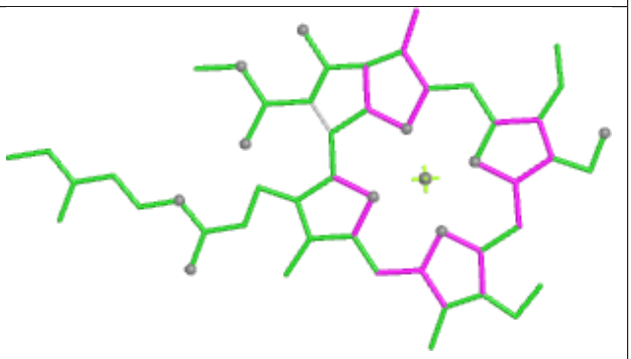


Rings

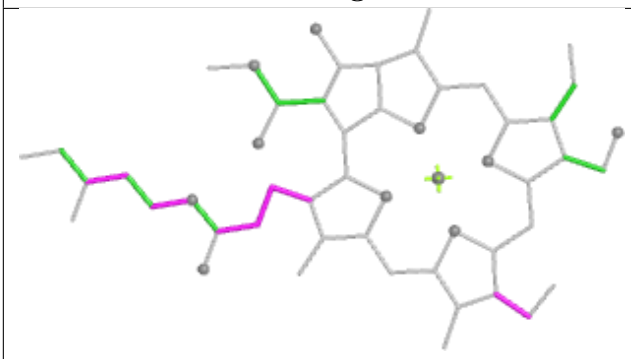
Ligand CHL 1 304



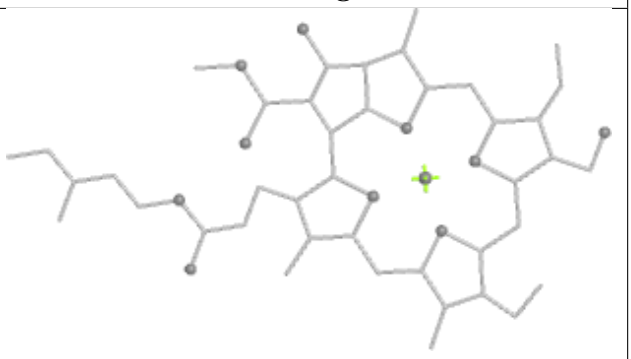
Bond lengths



Bond angles

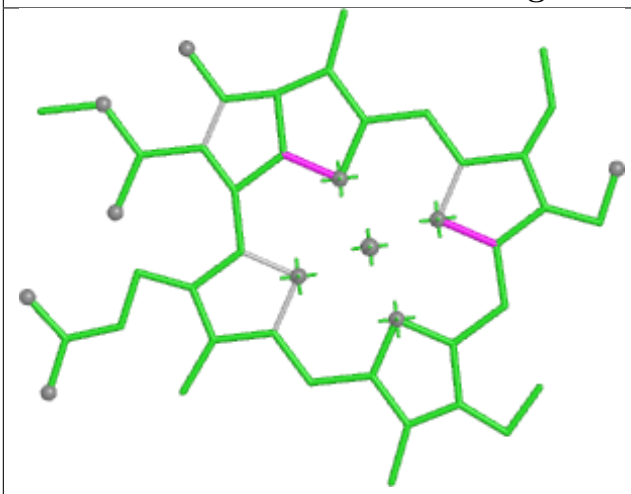


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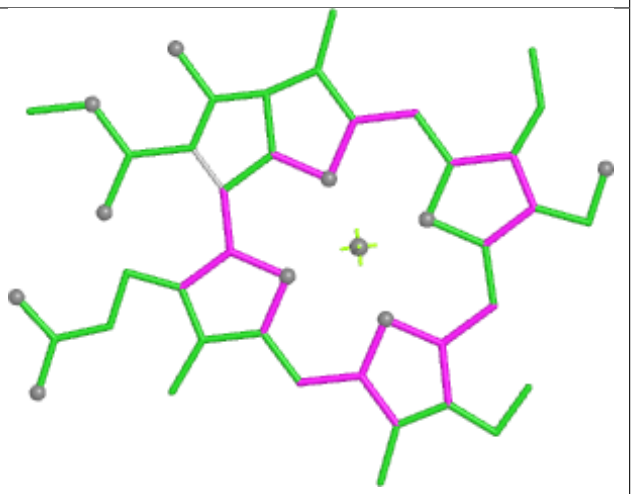


Rings

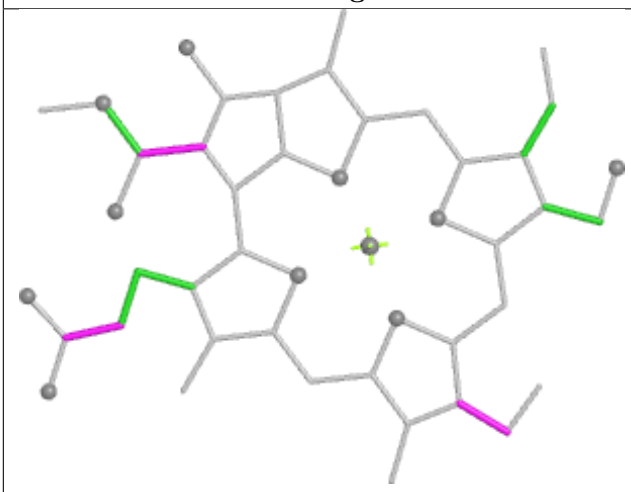
Ligand CHL 1 305



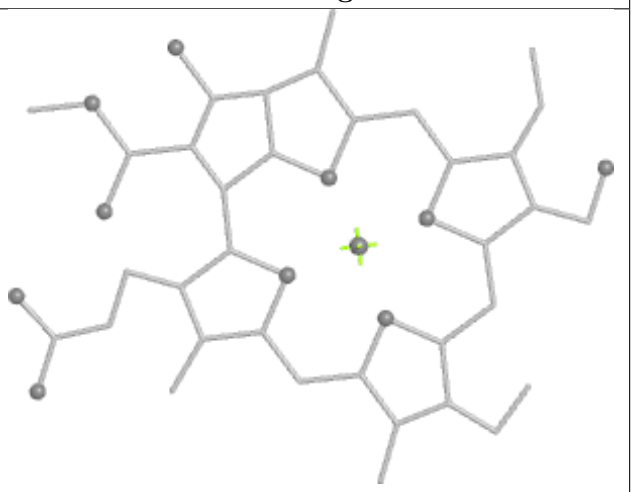
Bond lengths



Bond angles

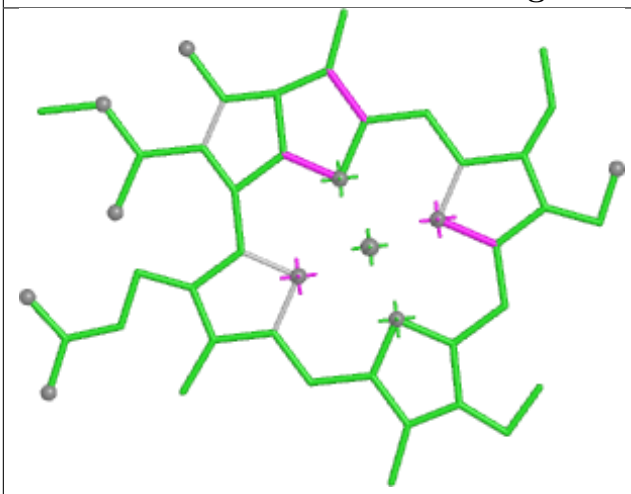


Torsions

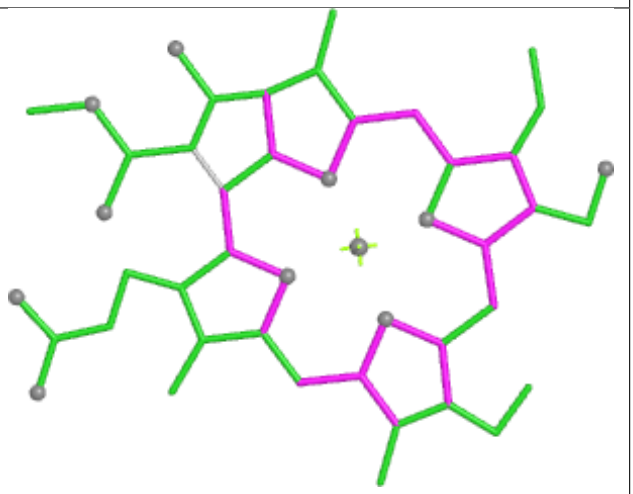


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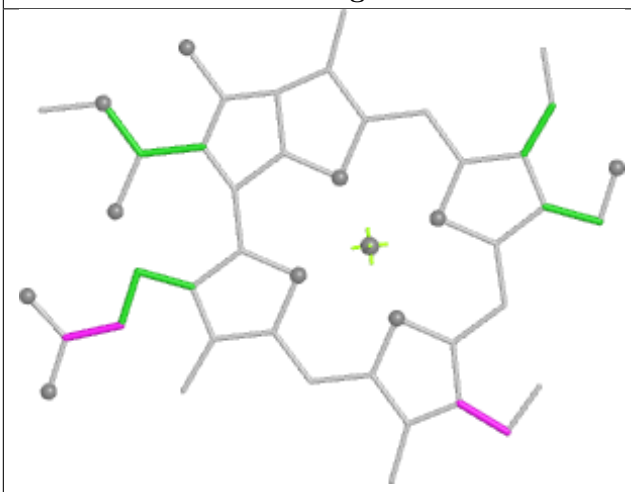
Ligand CHL 6 308



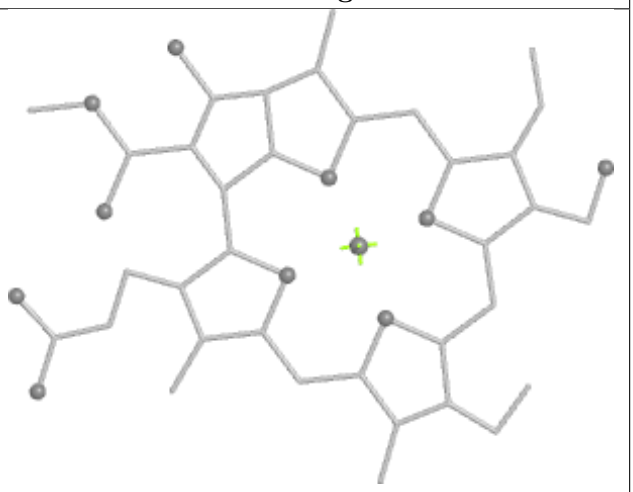
Bond lengths



Bond angles

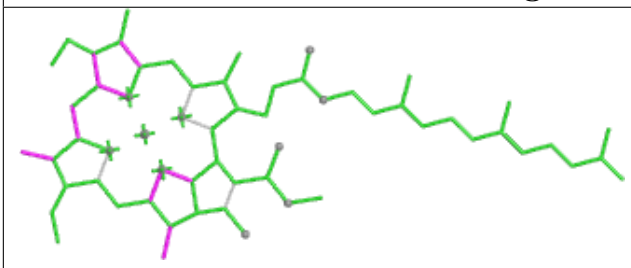


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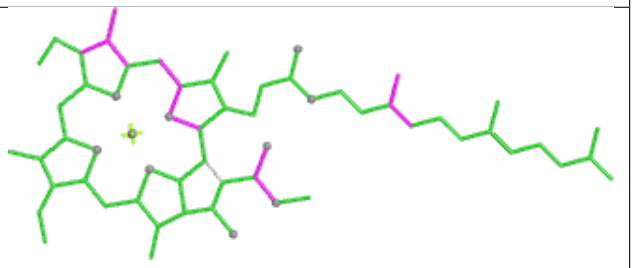


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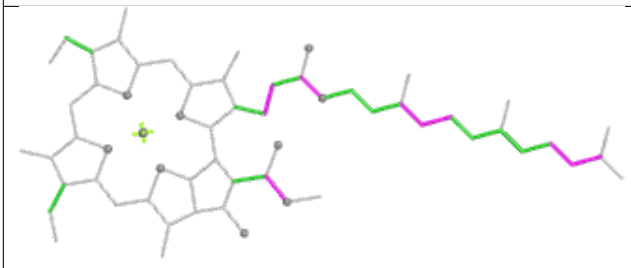
Ligand CLA A 816



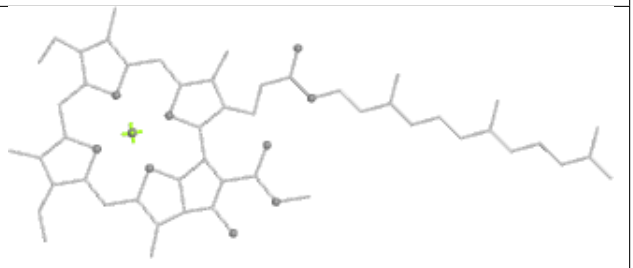
Bond lengths



Bond angles

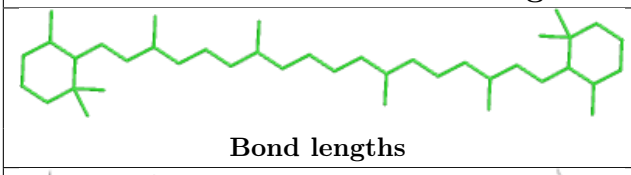


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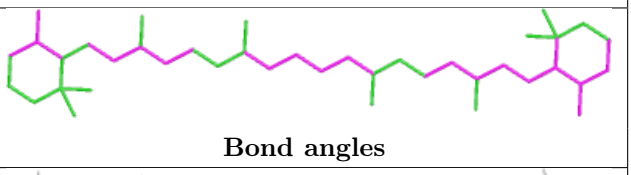


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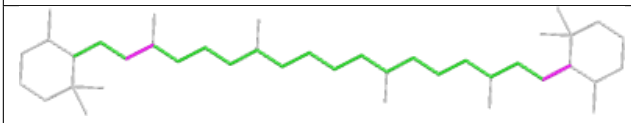
Ligand BCR 3 419



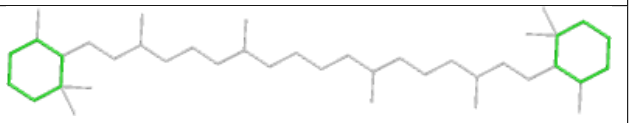
Bond lengths



Bond angles



Torsions

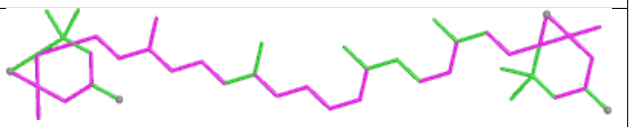


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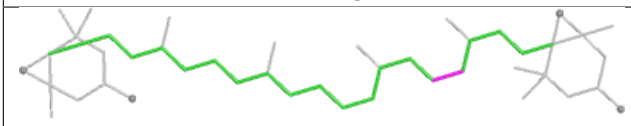
Ligand XAT 2 615



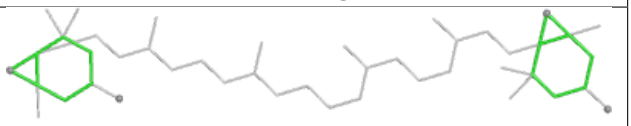
Bond lengths



Bond angles

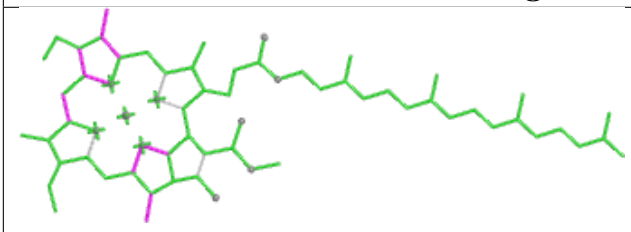


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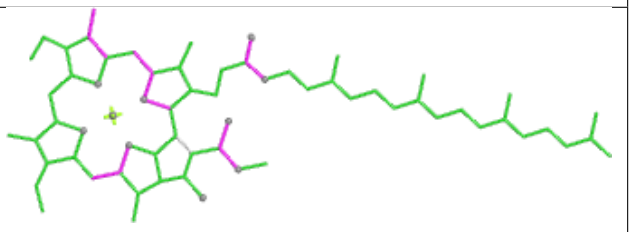


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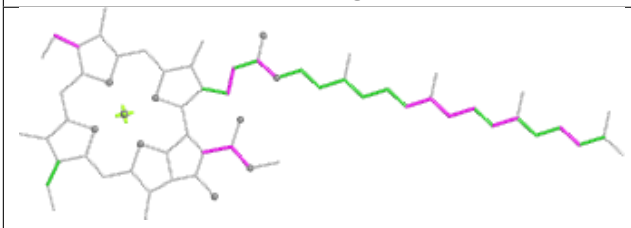
Ligand CLA B 842



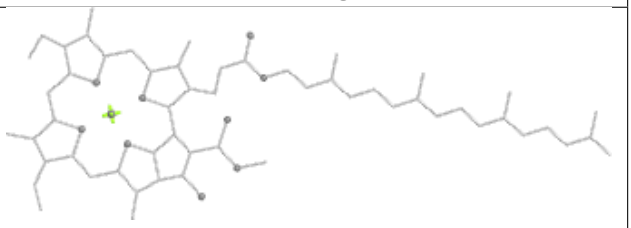
Bond lengths



Bond angles

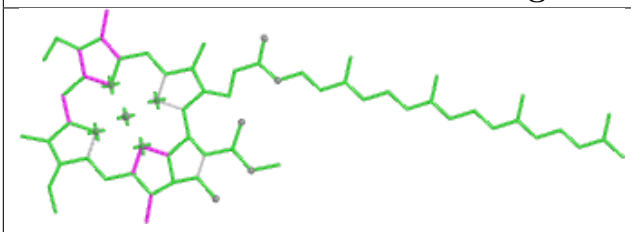


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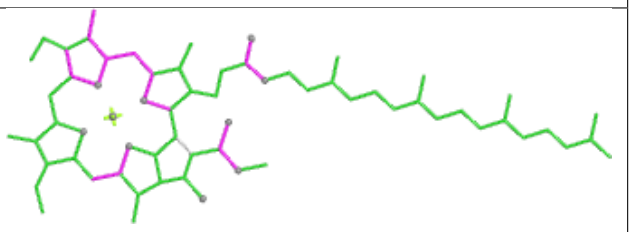


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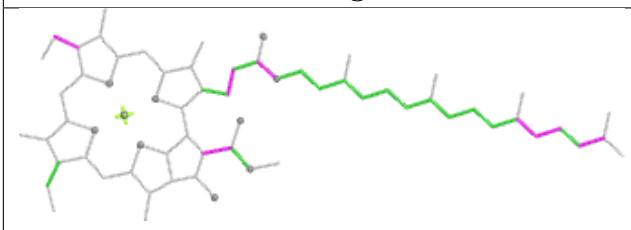
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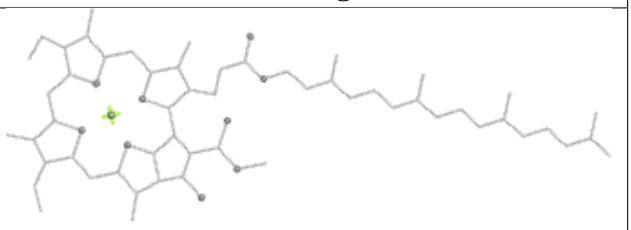
Bond lengths



Bond angles



Torsions

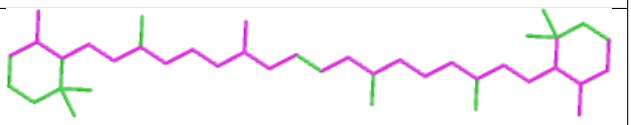


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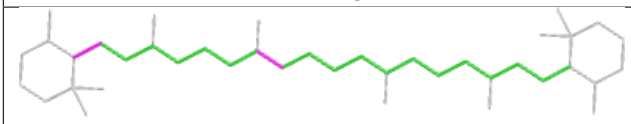
Ligand BCR 5 322



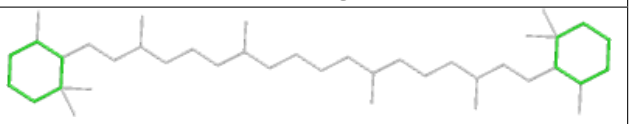
Bond lengths



Bond angles

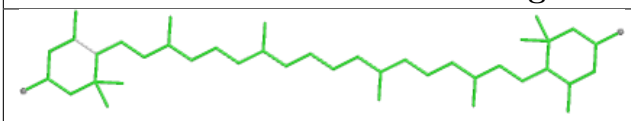


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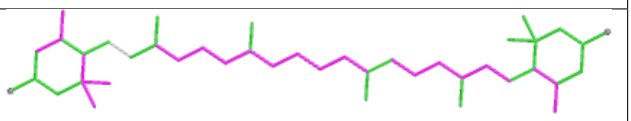


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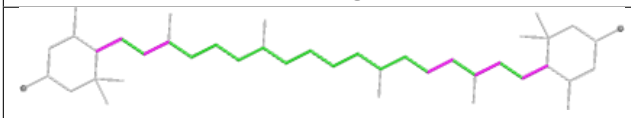
Ligand LUT 2 614



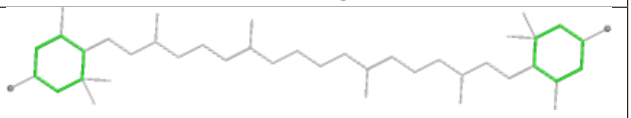
Bond lengths



Bond angles

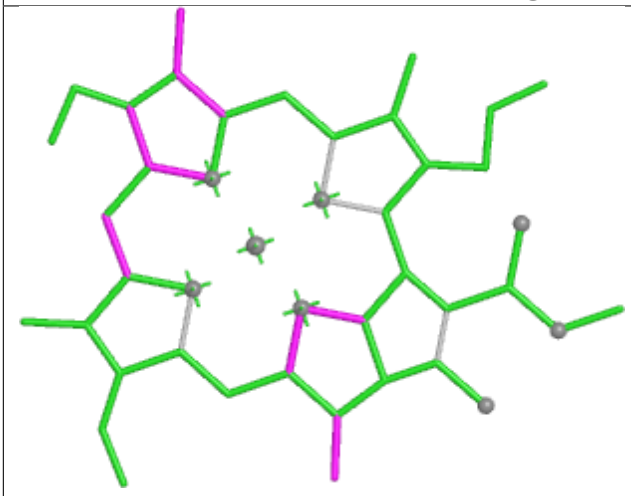


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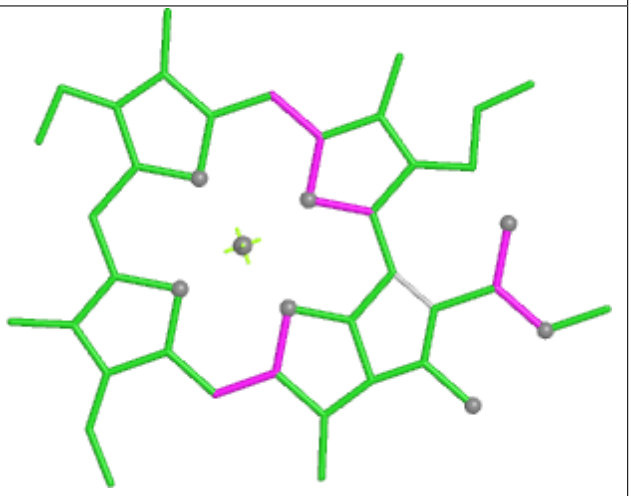


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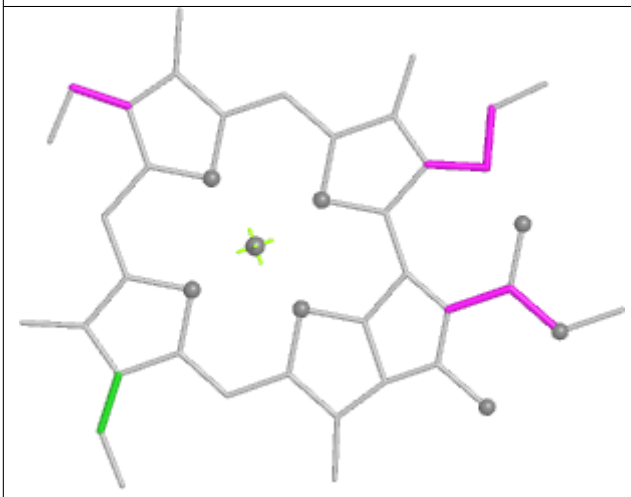
Ligand CLA B 833



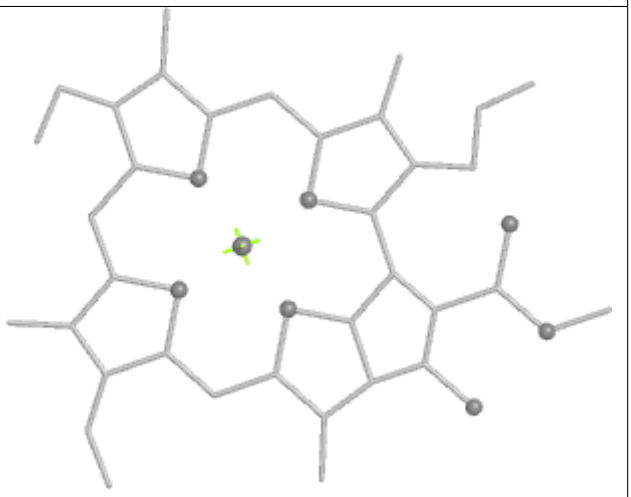
Bond lengths



Bond angles

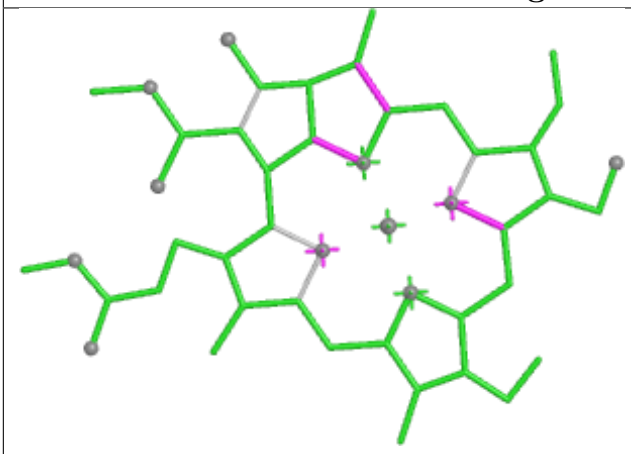


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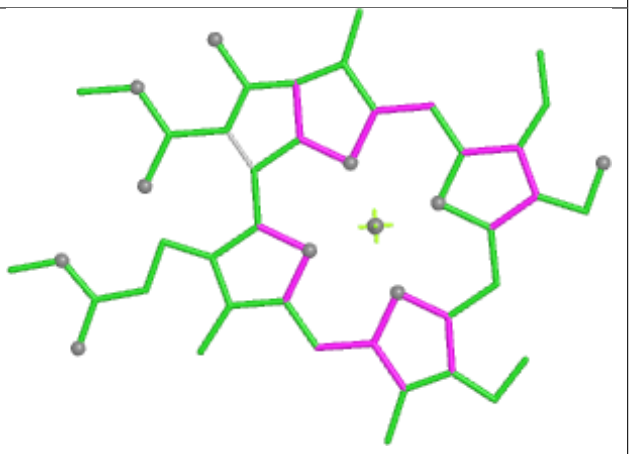


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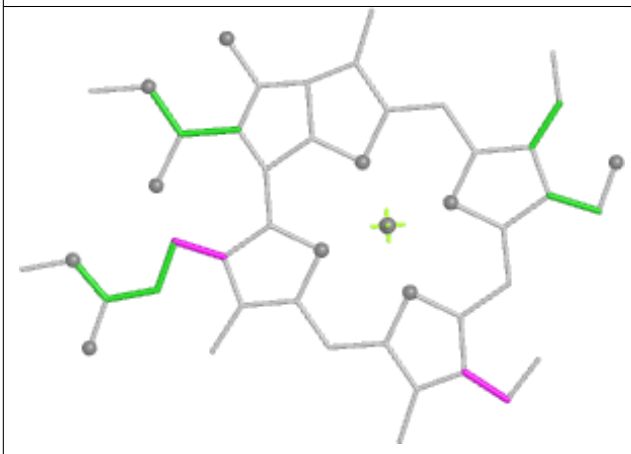
Ligand CHL 7 304



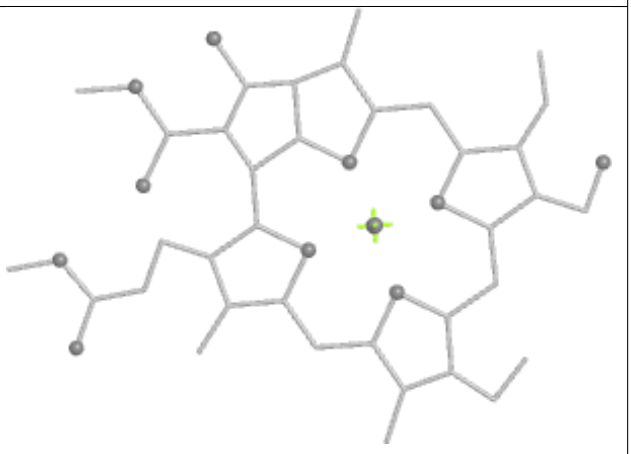
Bond lengths



Bond angles

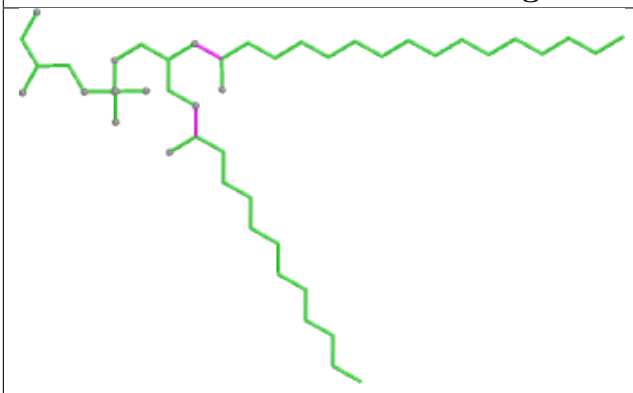


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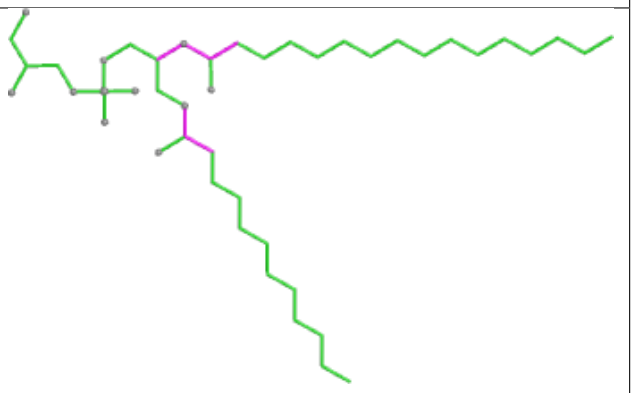


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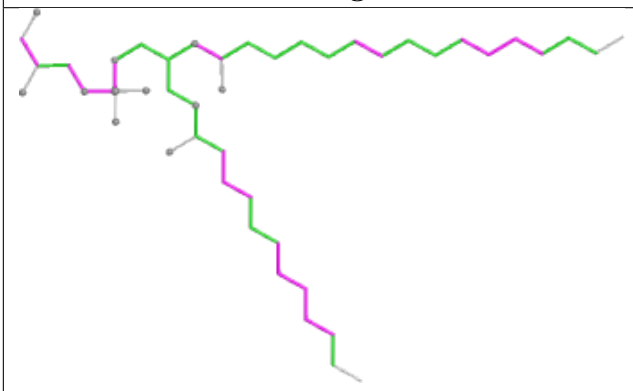
Ligand LHG A 845



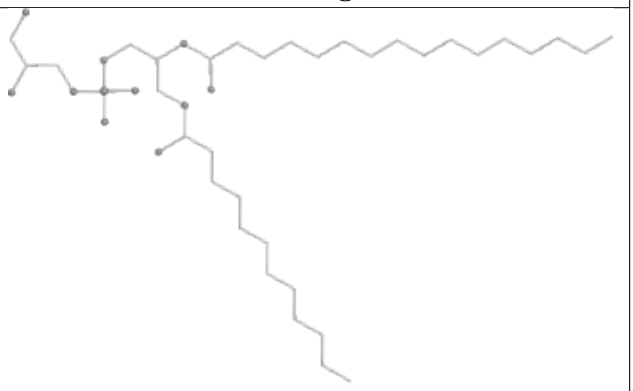
Bond lengths



Bond angles

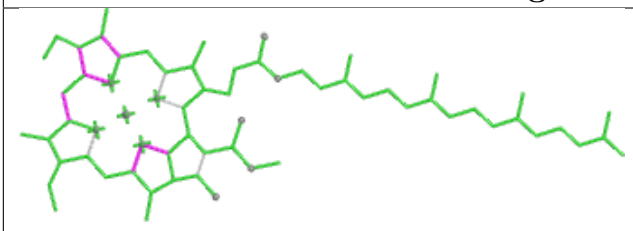


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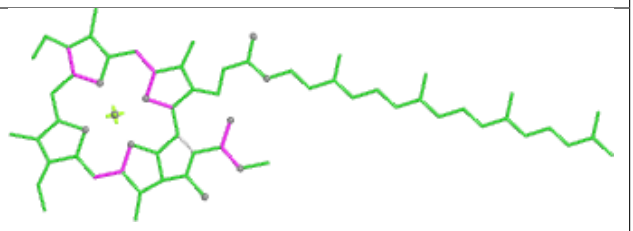


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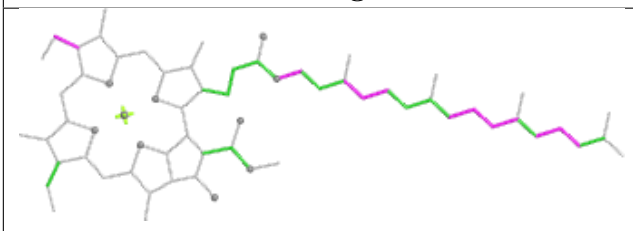
Ligand CLA 6 316



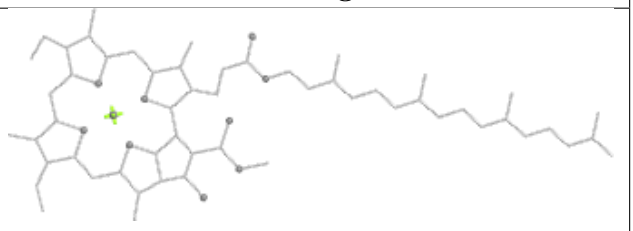
Bond lengths



Bond angles

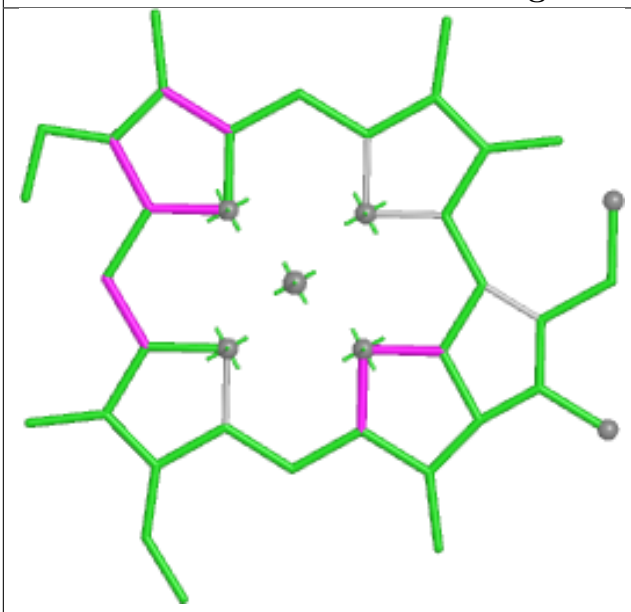


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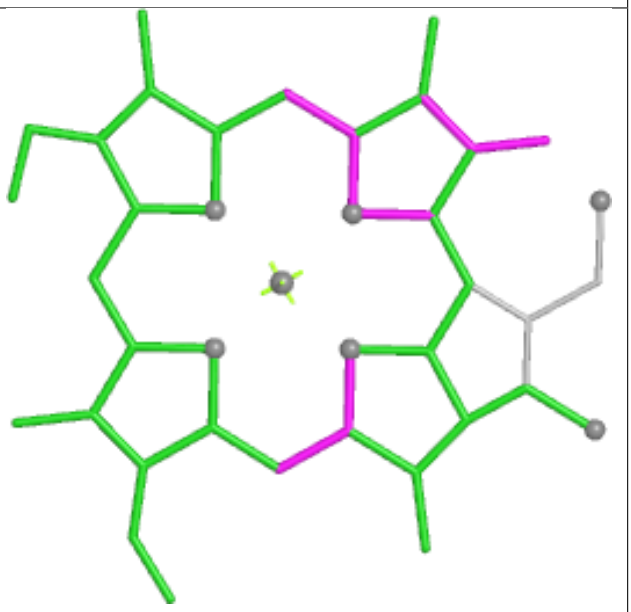


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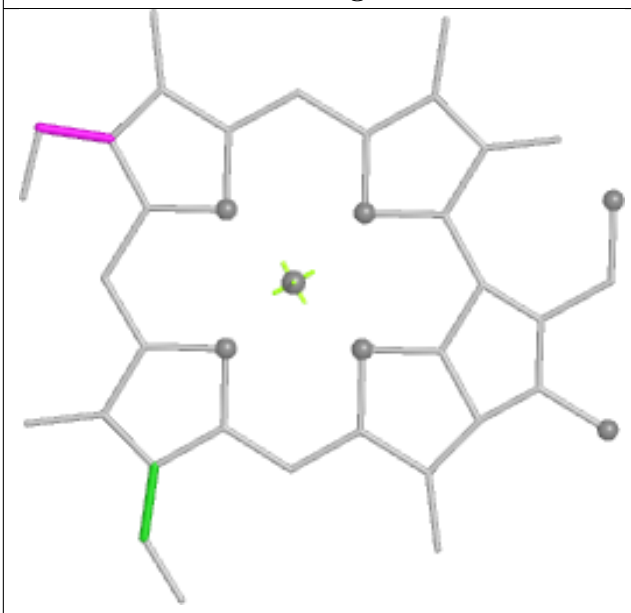
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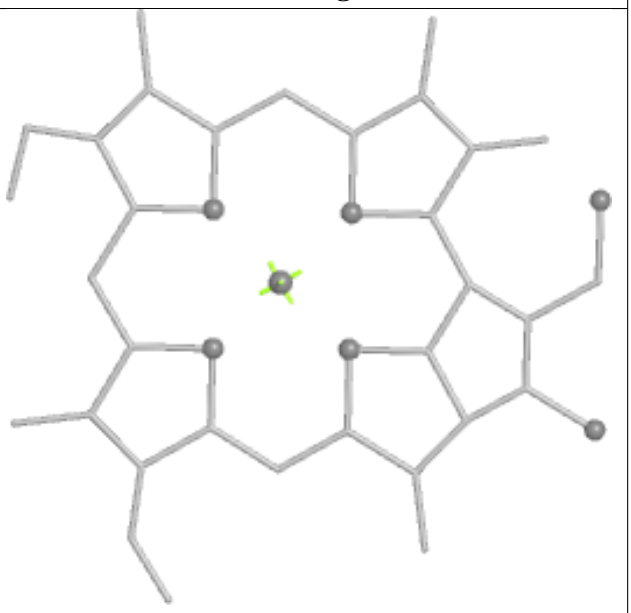
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Bond angles

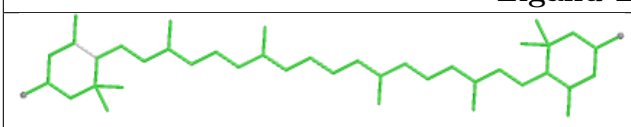


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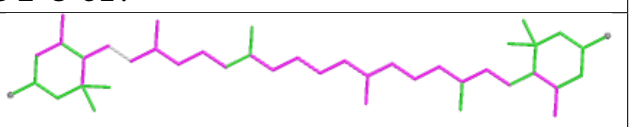


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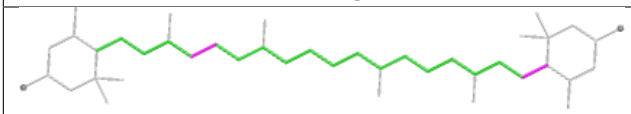
Ligand LUT 8 617



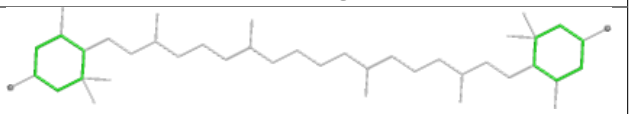
Bond lengths



Bond angles

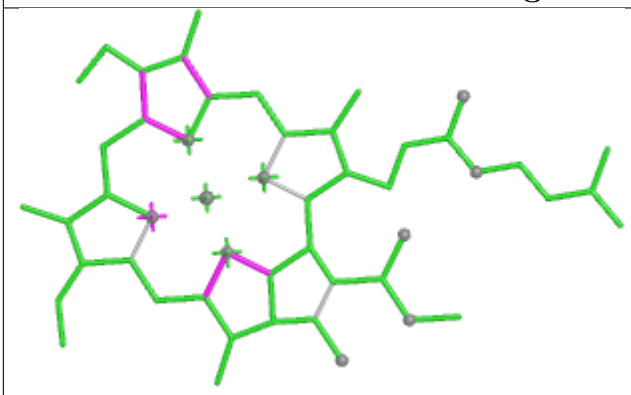


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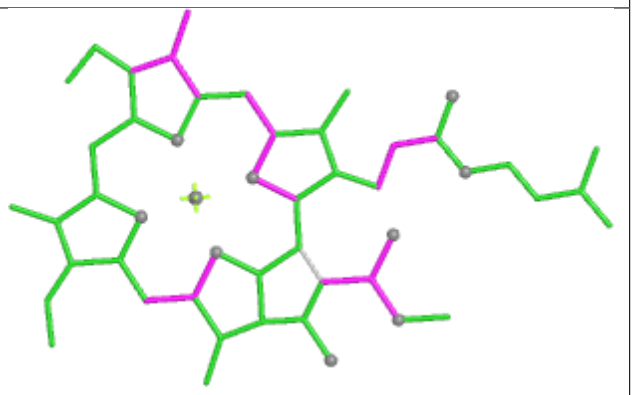


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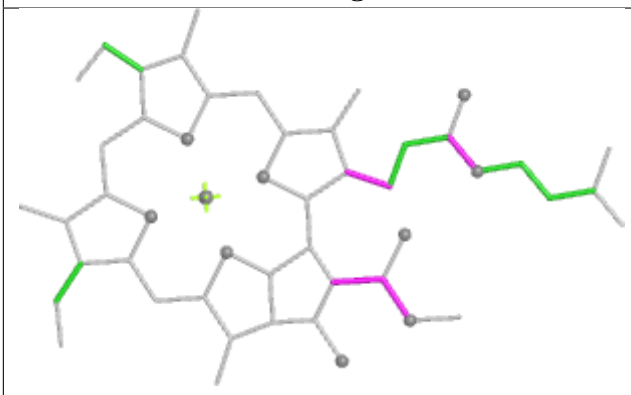
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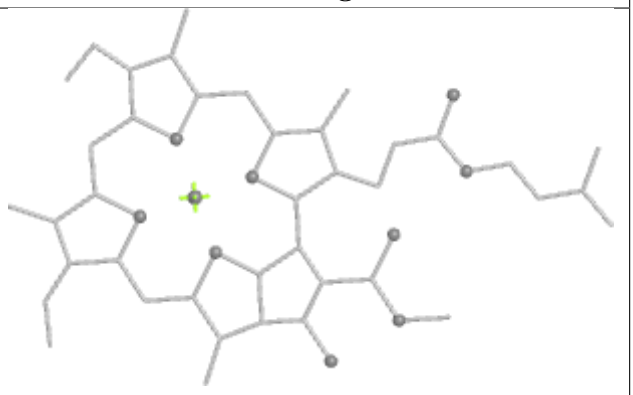
Bond lengths



Bond angles

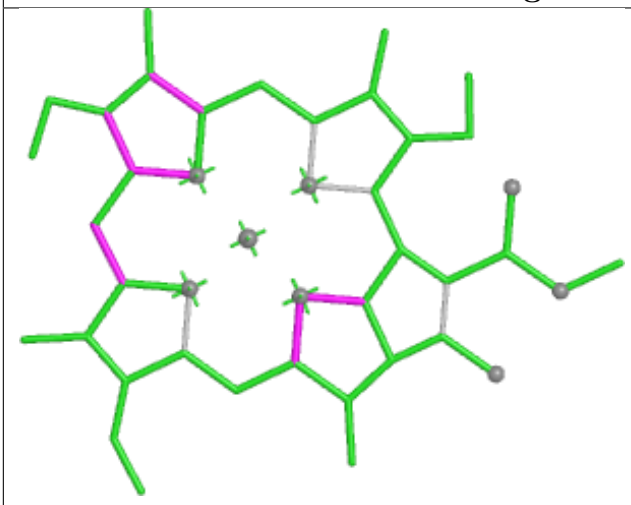


Torsions

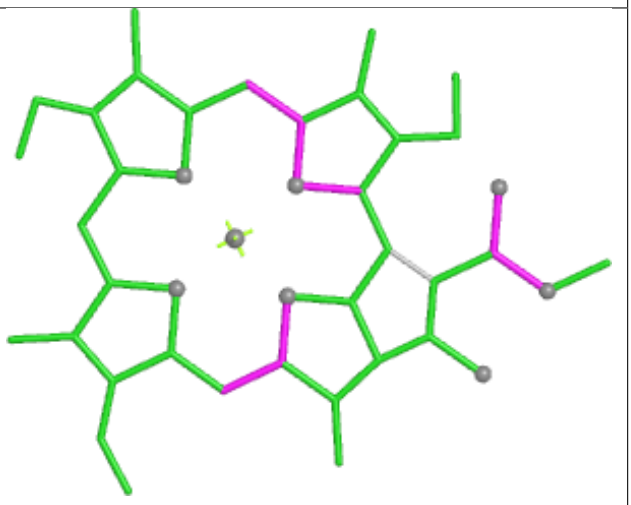


Rings

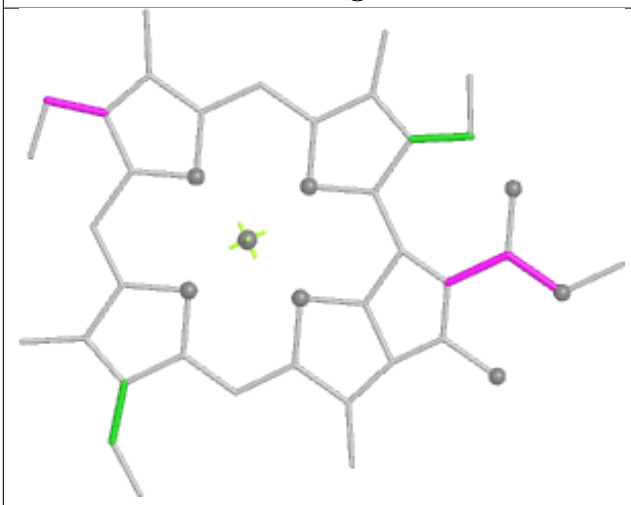
Ligand CLA A 821



Bond lengths



Bond angles

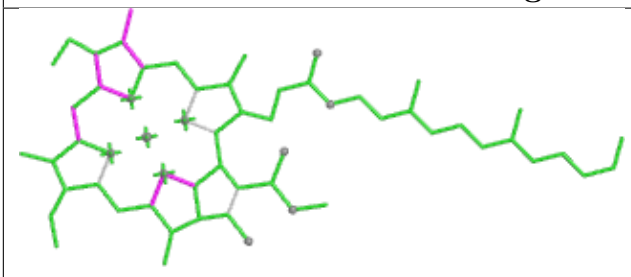


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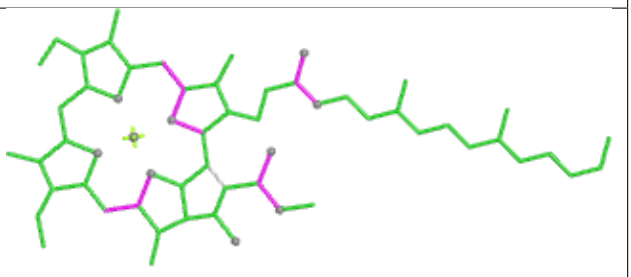


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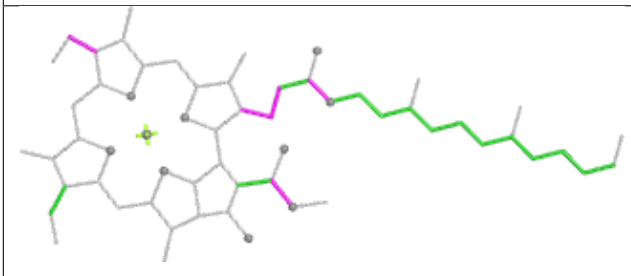
Ligand CLA B 820



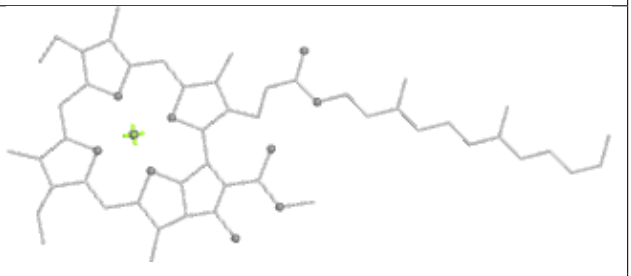
Bond lengths



Bond angles

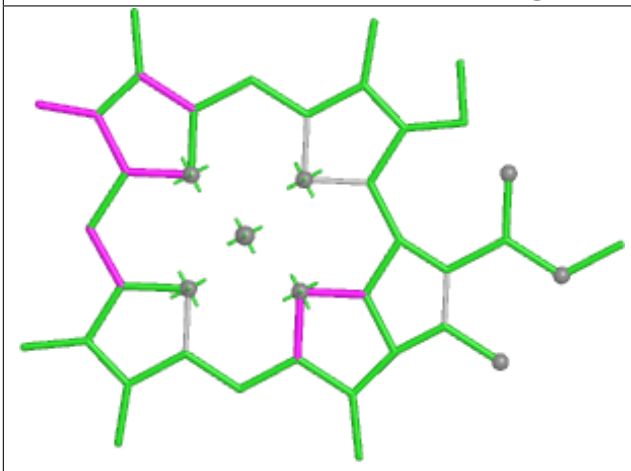


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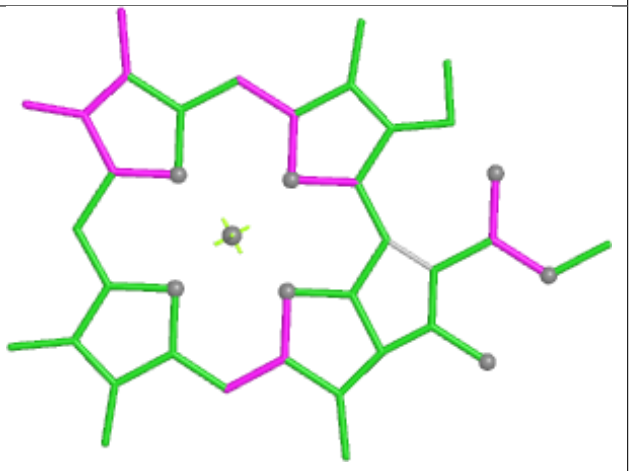


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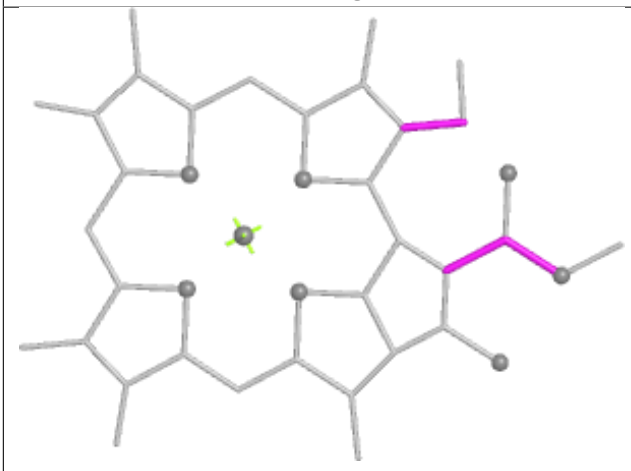
Ligand CLA 7 313



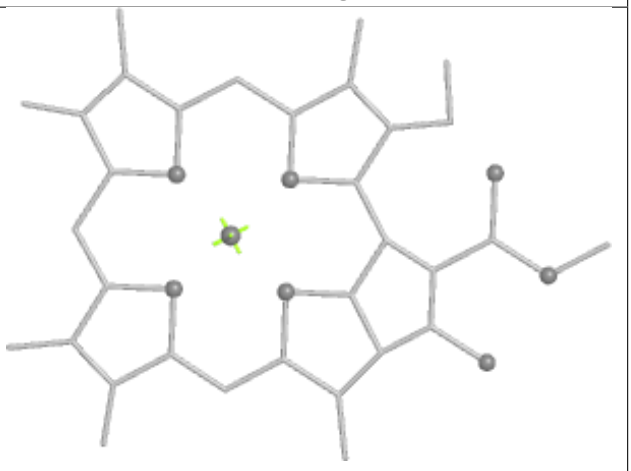
Bond lengths



Bond angles



Torsions

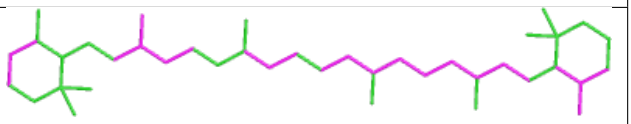


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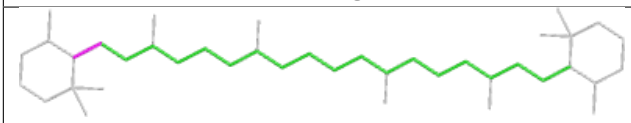
Ligand BCR 1 316



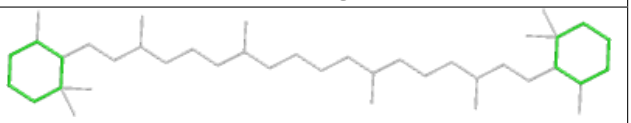
Bond lengths



Bond angles

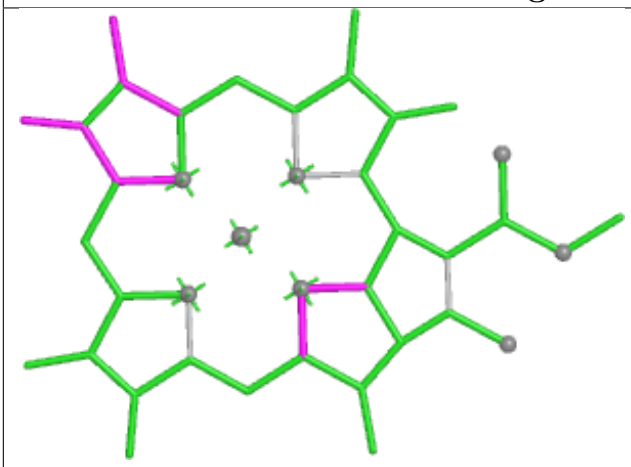


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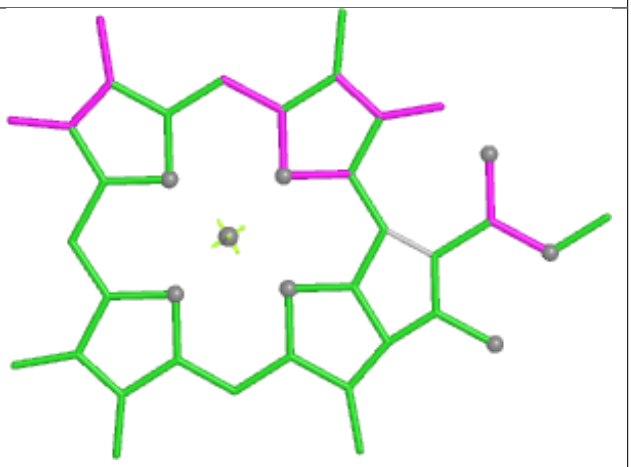


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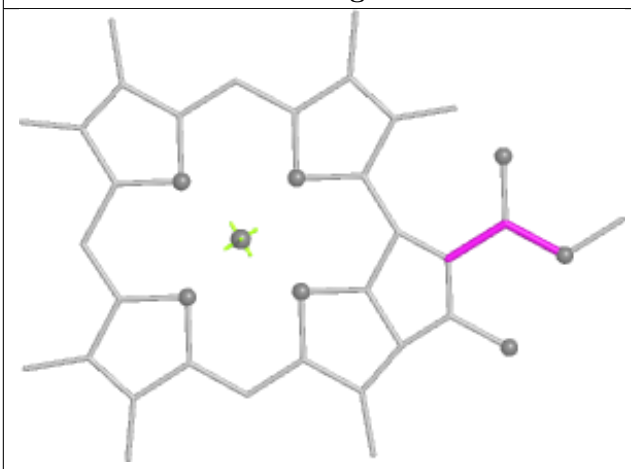
Ligand CLA 1 313



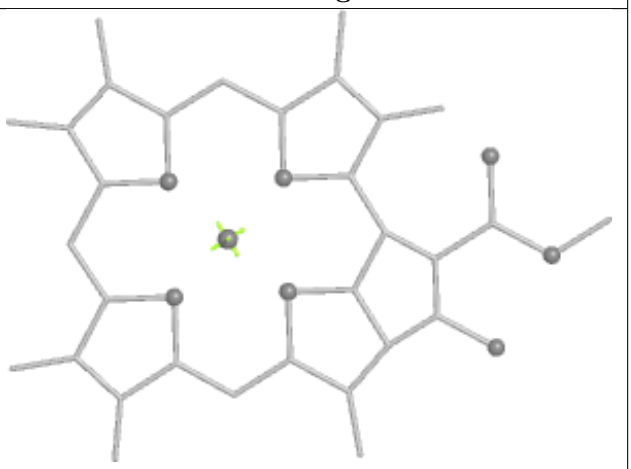
Bond lengths



Bond angles

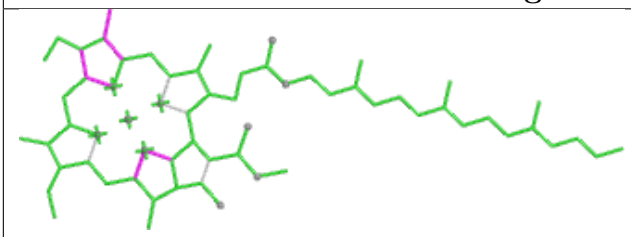


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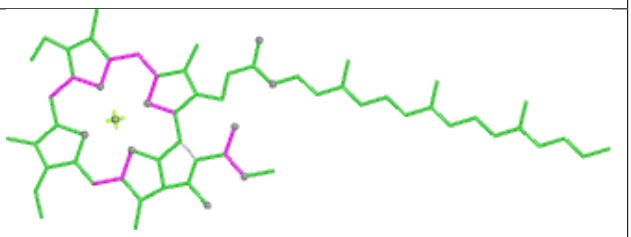


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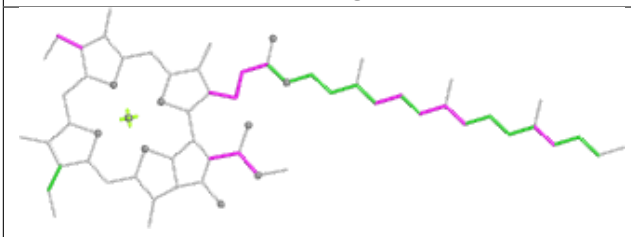
Ligand CLA B 812



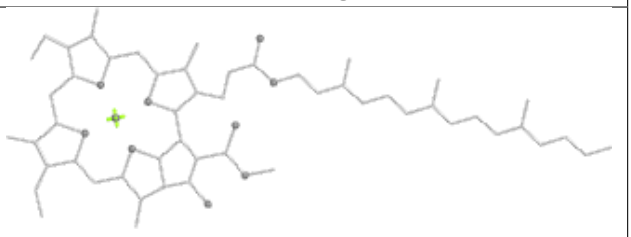
Bond lengths



Bond angles

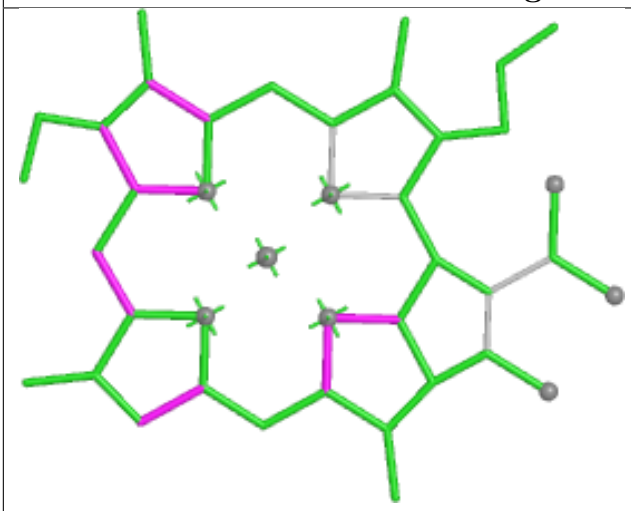


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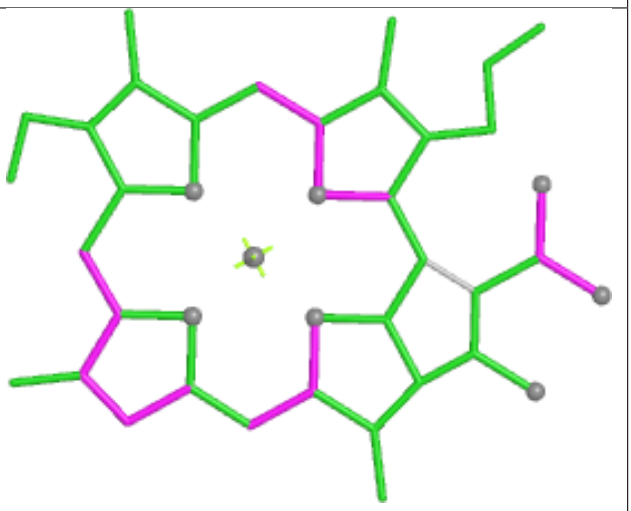


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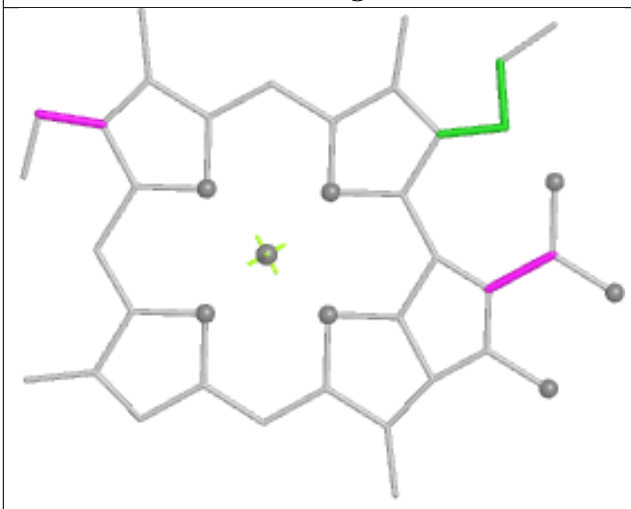
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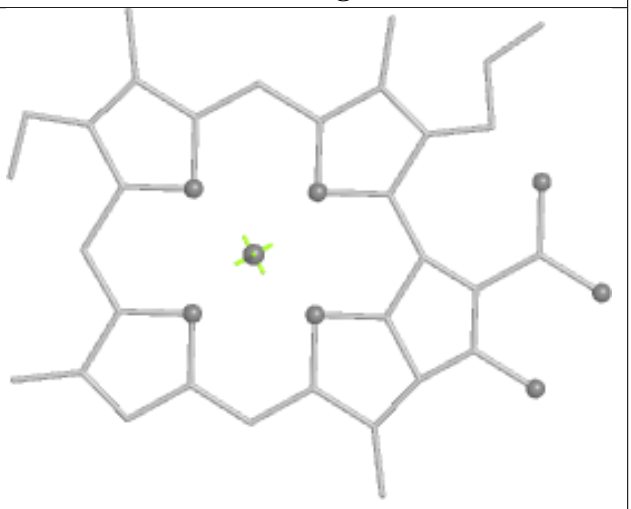
Bond lengths



Bond angles

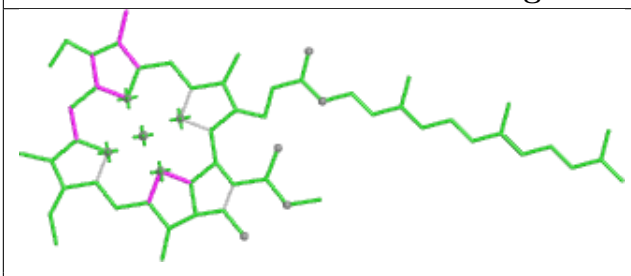


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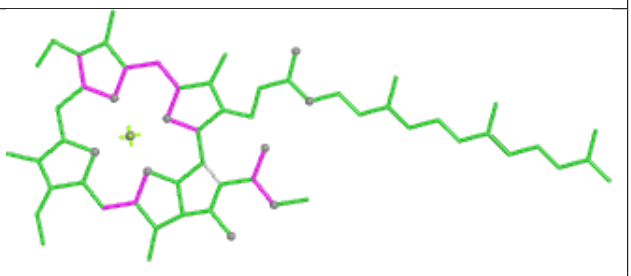


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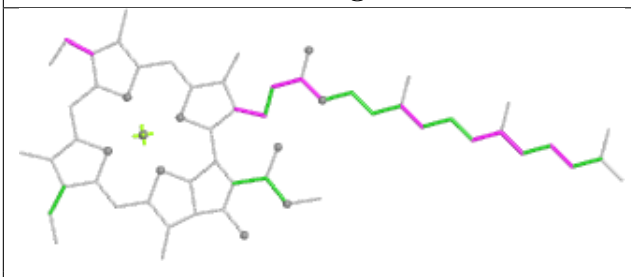
Ligand CLA A 820



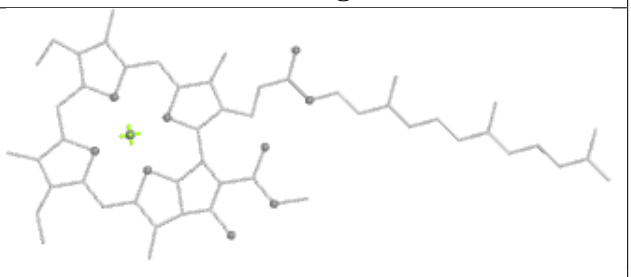
Bond lengths



Bond angles

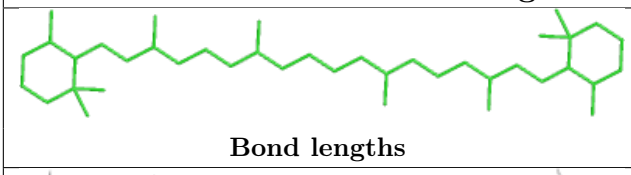


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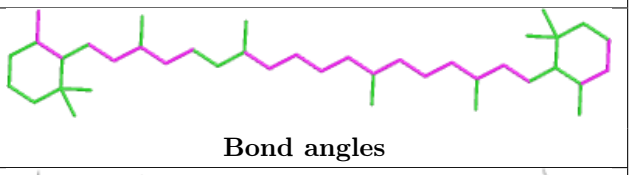


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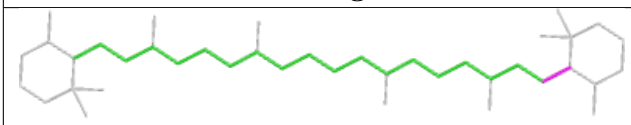
Ligand BCR M 102



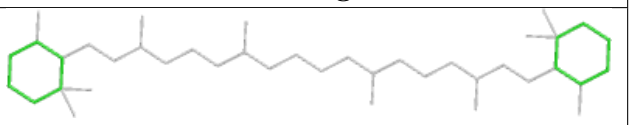
Bond lengths



Bond angles

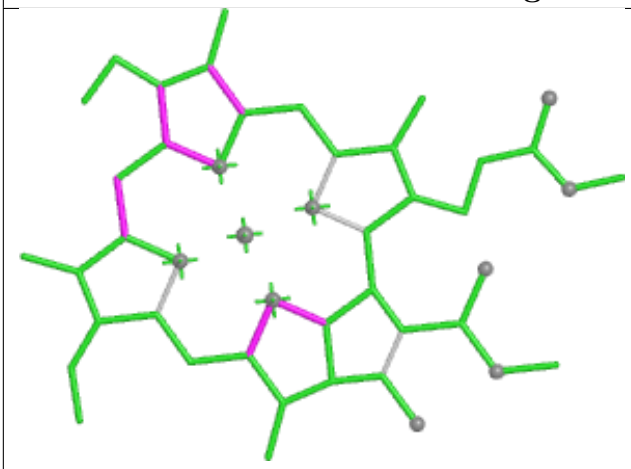


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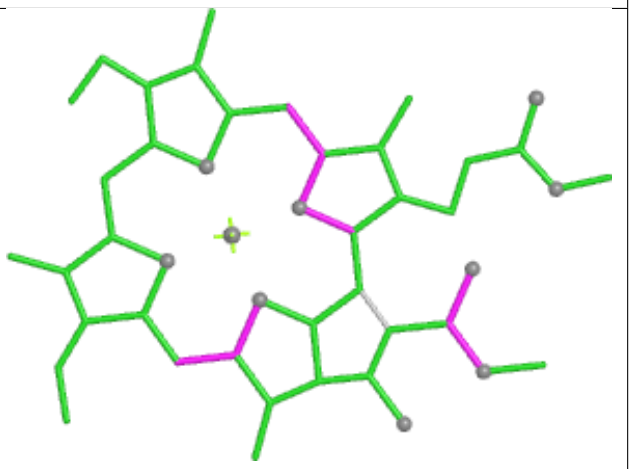


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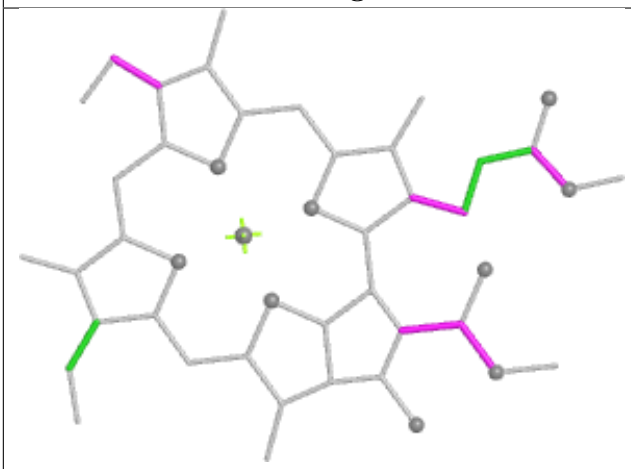
Ligand CLA A 819



Bond lengths



Bond angles

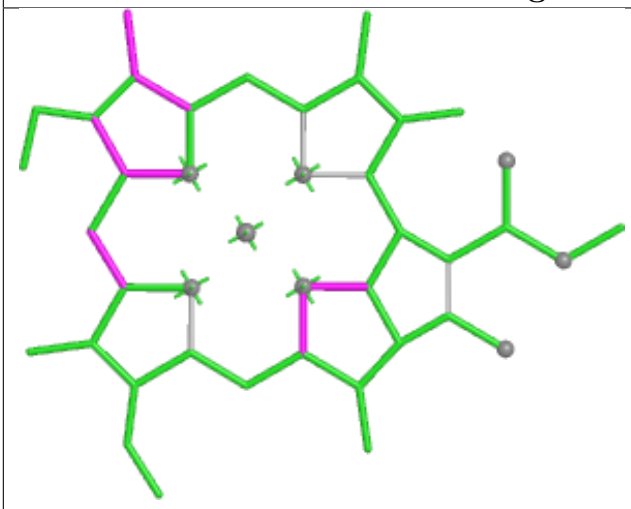


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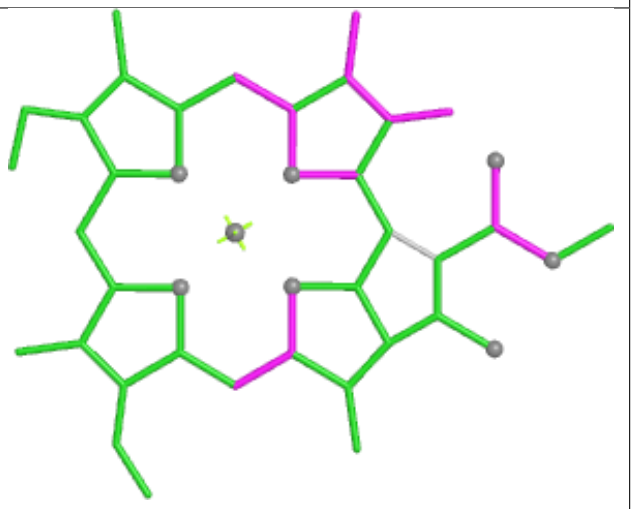


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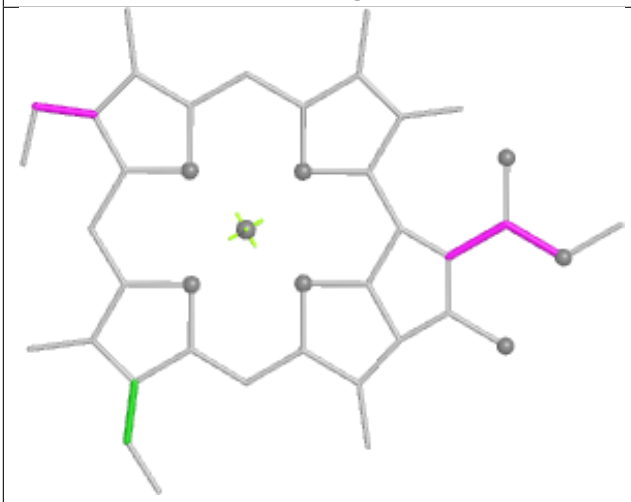
Ligand CLA 2 608



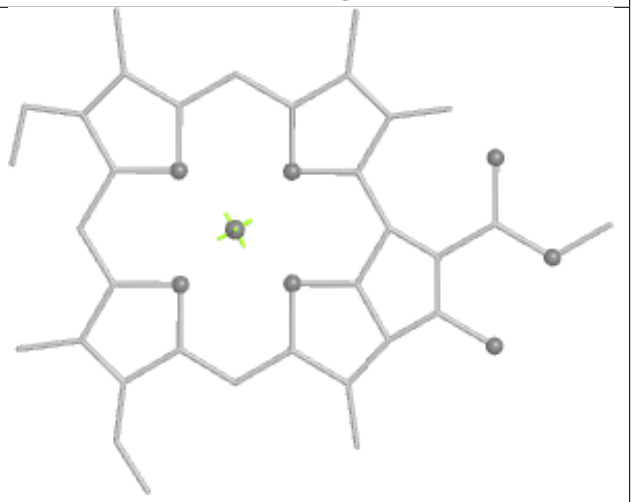
Bond lengths



Bond angles

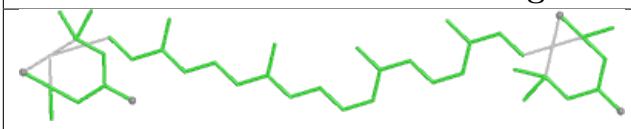


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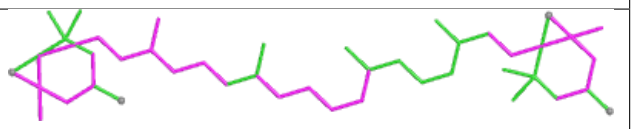


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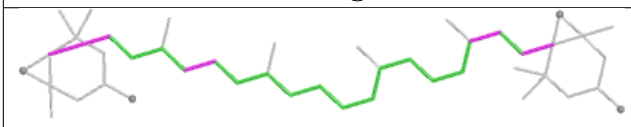
Ligand XAT 9 614



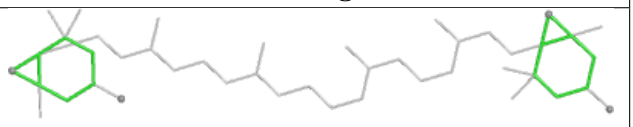
Bond lengths



Bond angles

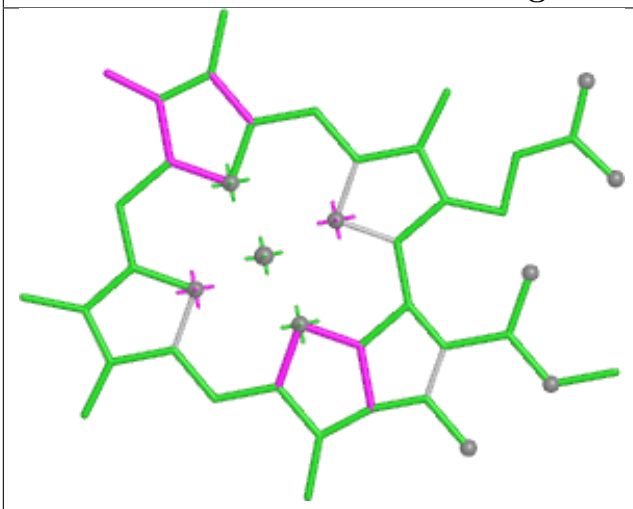


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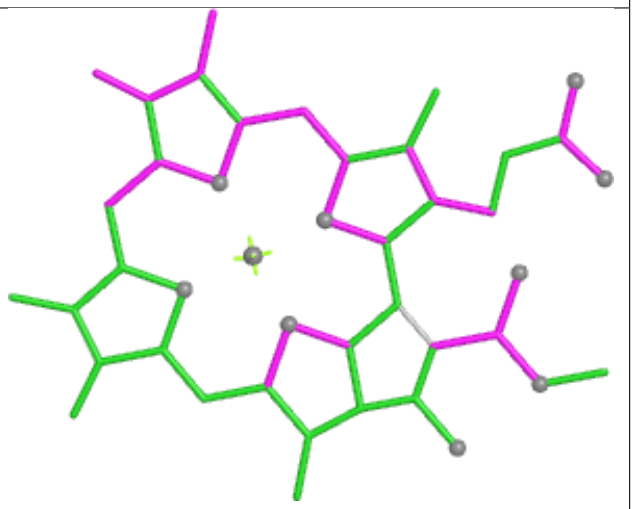


Rings

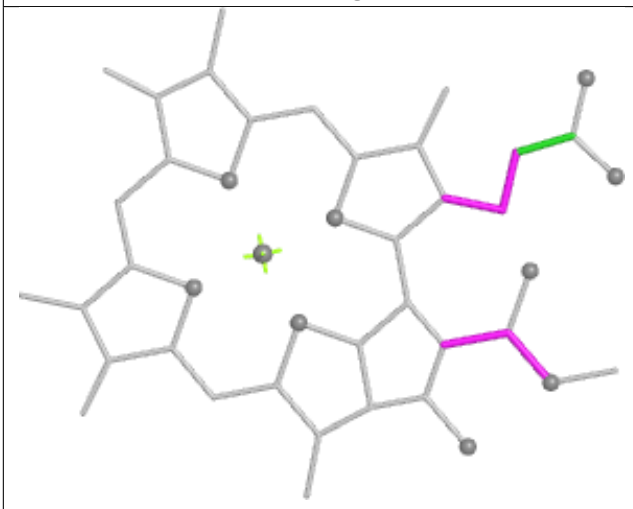
Ligand CLA 8 615



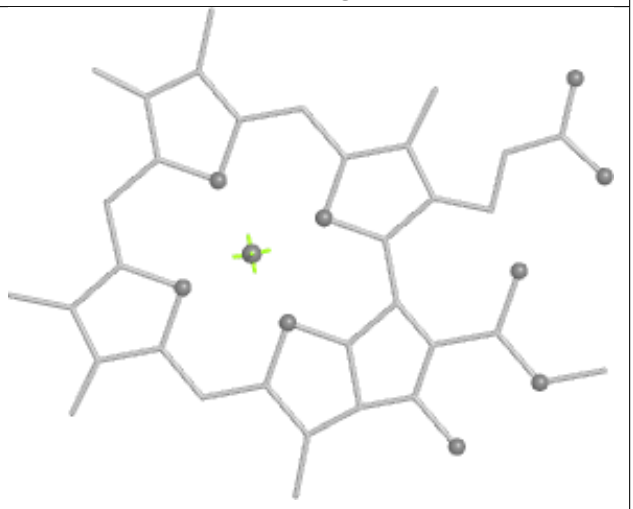
Bond lengths



Bond angles

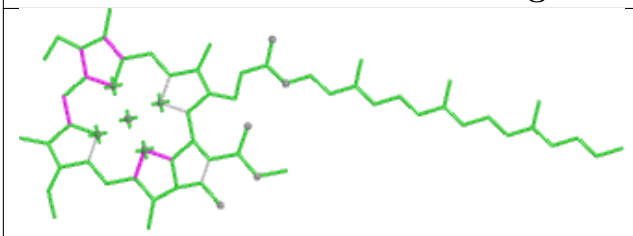


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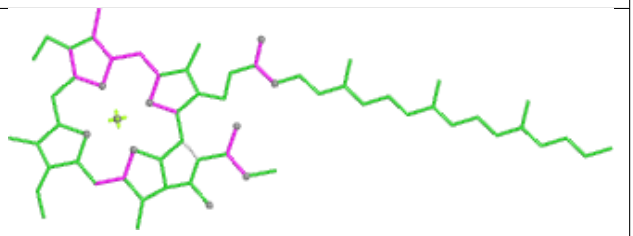


Rings

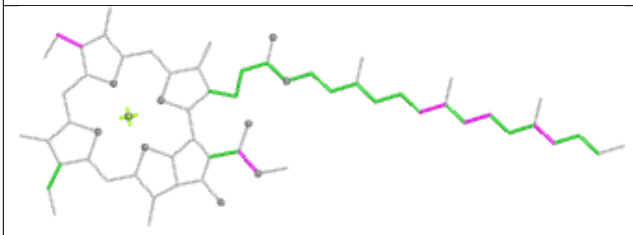
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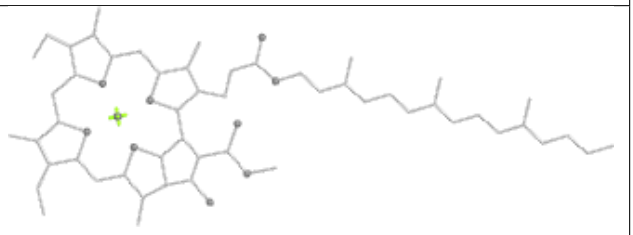
Bond lengths



Bond angles

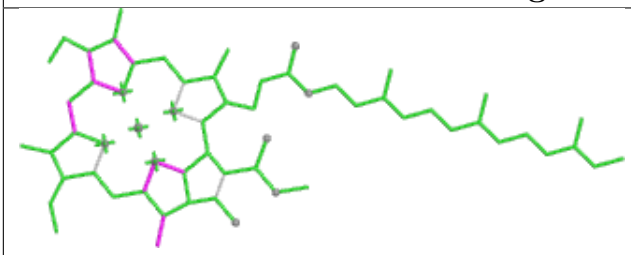


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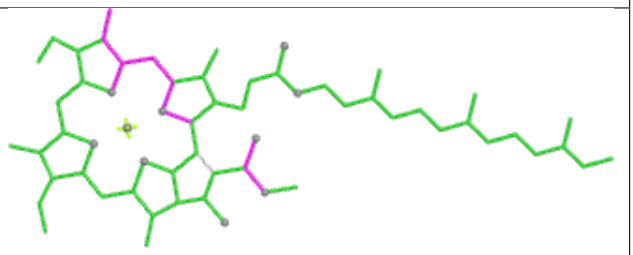


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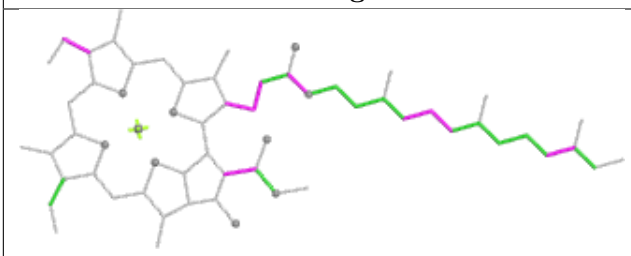
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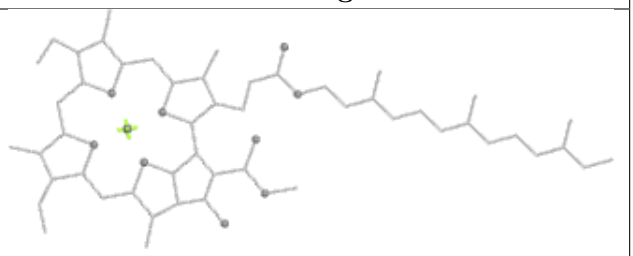
Bond lengths



Bond angles

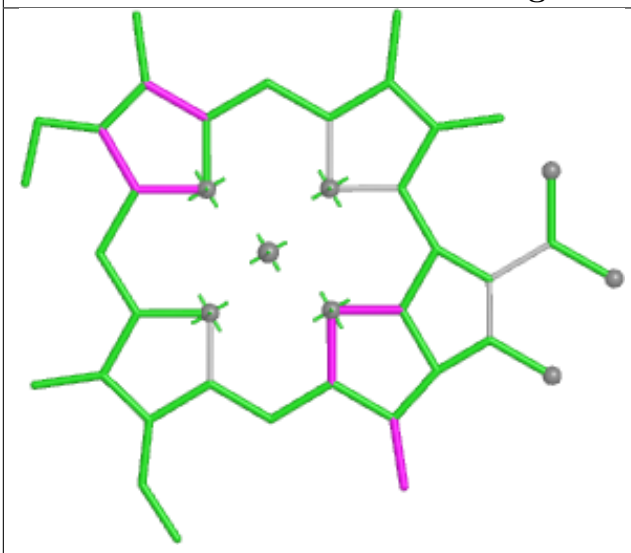


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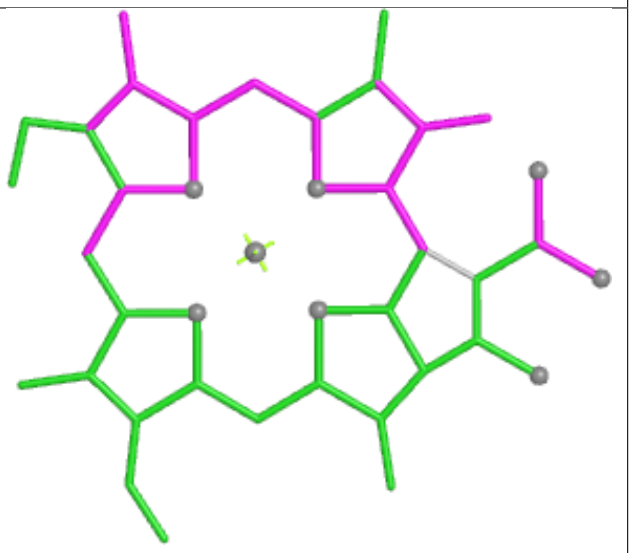


Rings

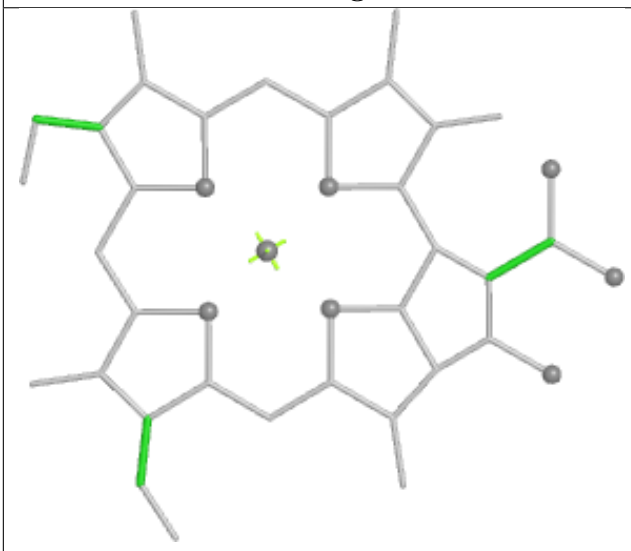
Ligand CLA 2 603



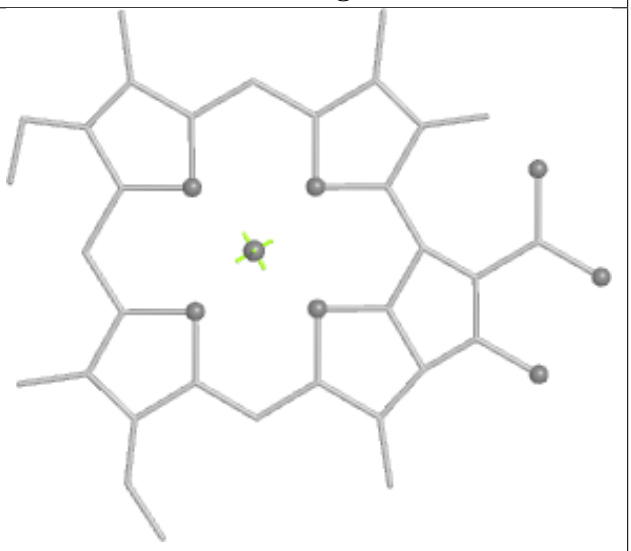
Bond lengths



Bond angles

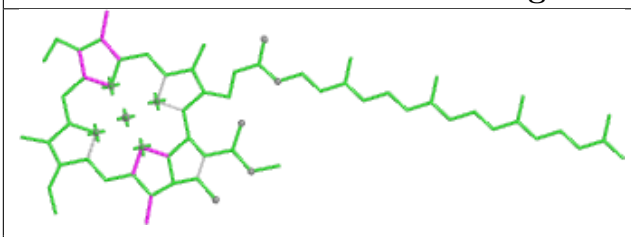


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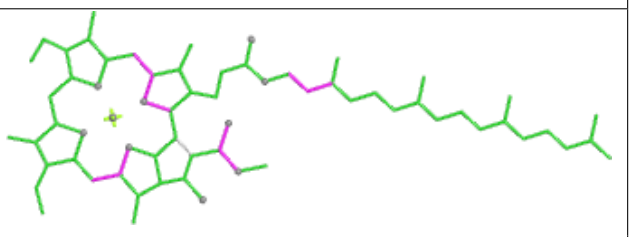


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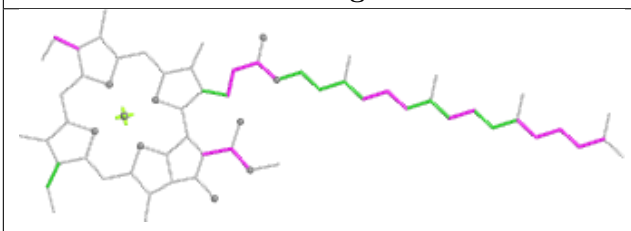
Ligand CLA 8 613



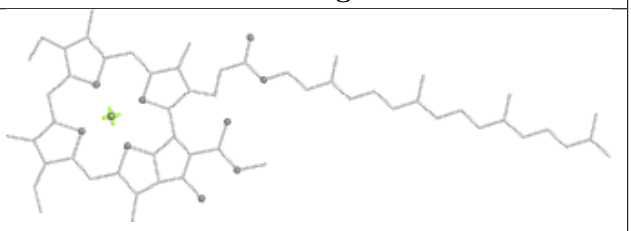
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Bond angles

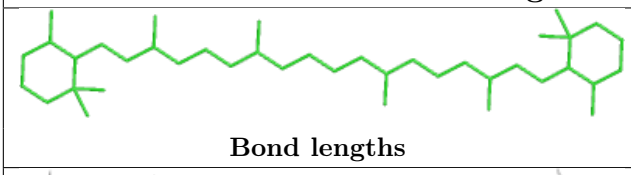


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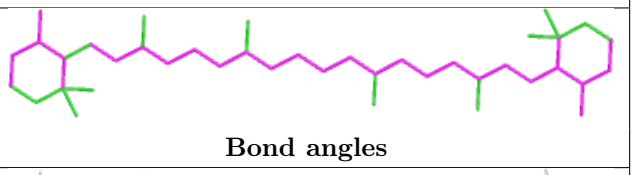


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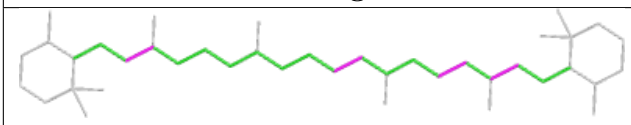
Ligand BCR 9 615



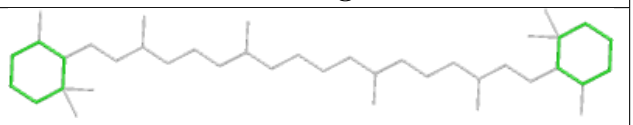
Bond lengths



Bond angles

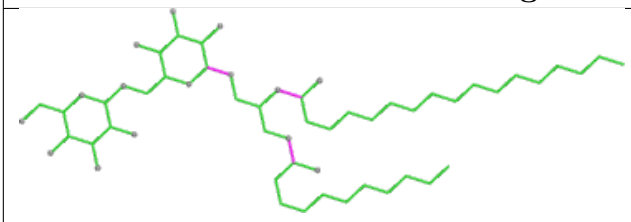


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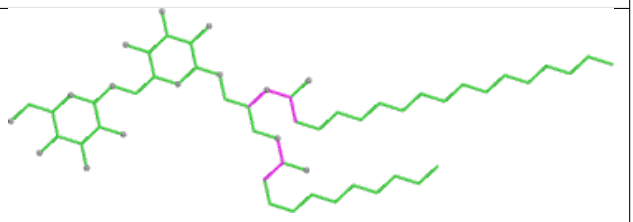


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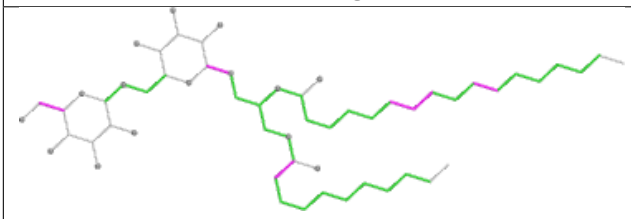
Ligand DGD B 852



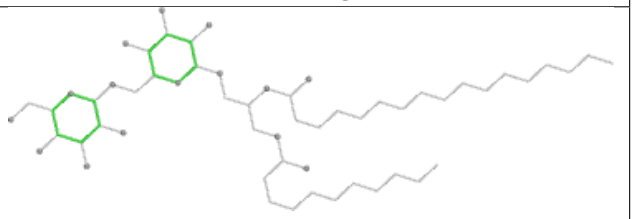
Bond lengths



Bond angles

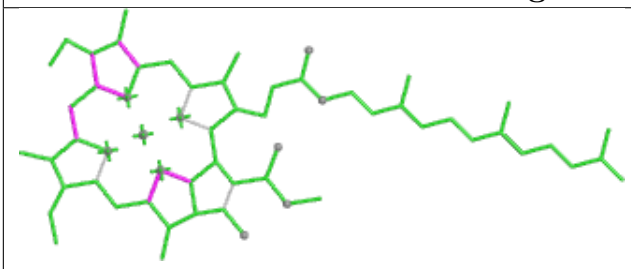


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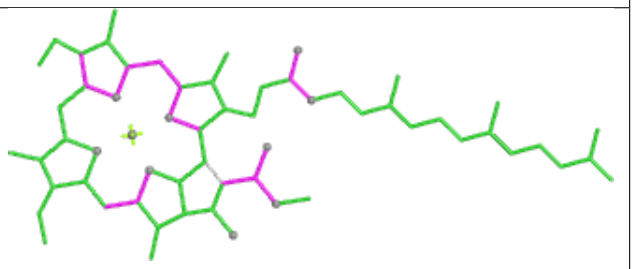


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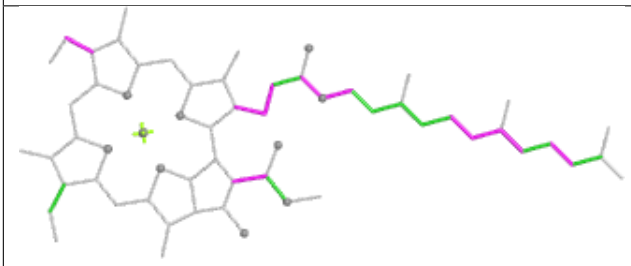
Ligand CLA 1 308



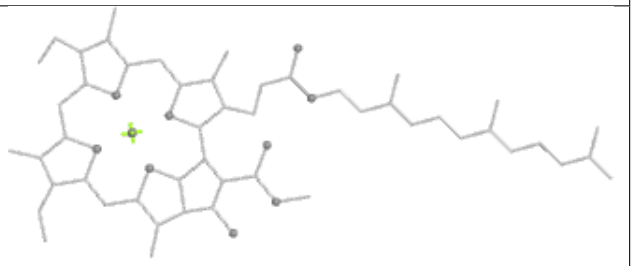
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Bond angles

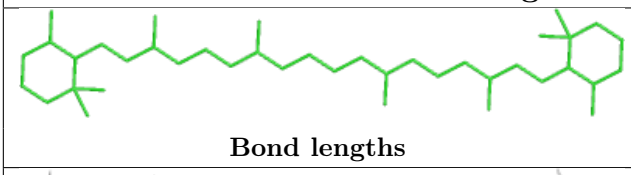


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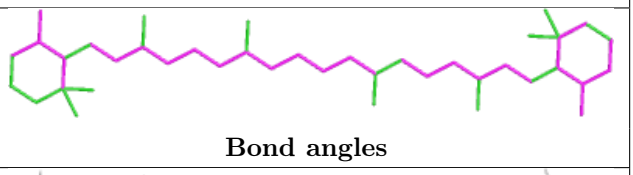


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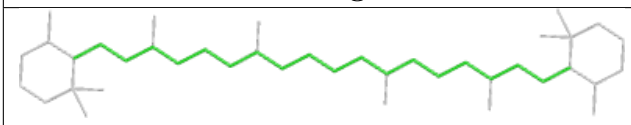
Ligand BCR G 204



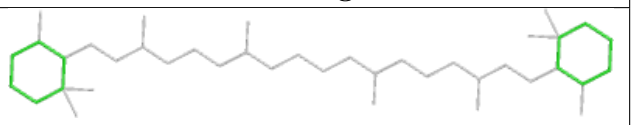
Bond lengths



Bond angles

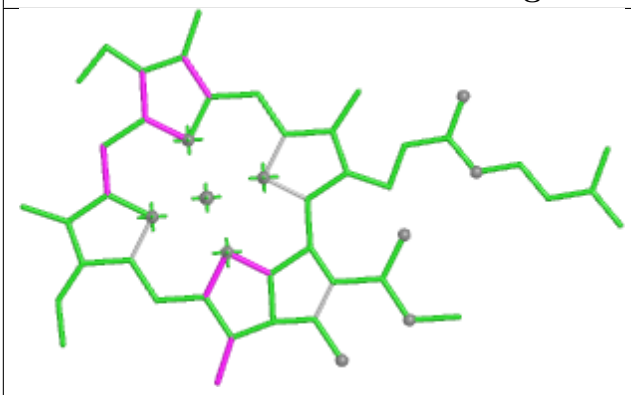


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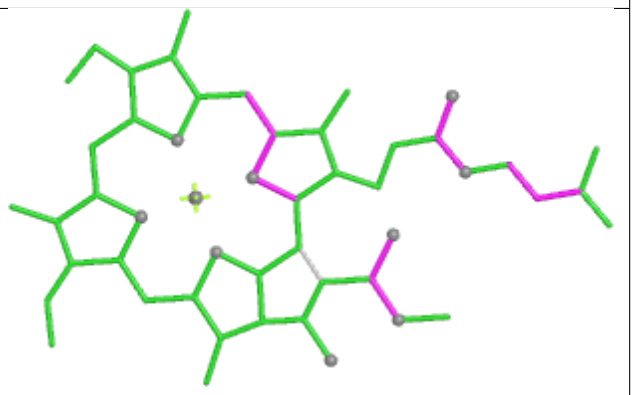


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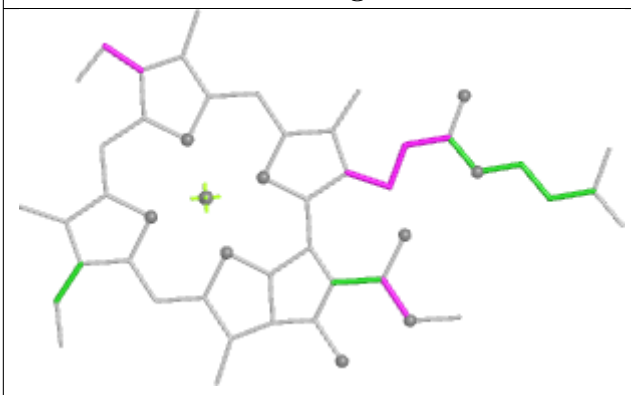
Ligand CLA A 808



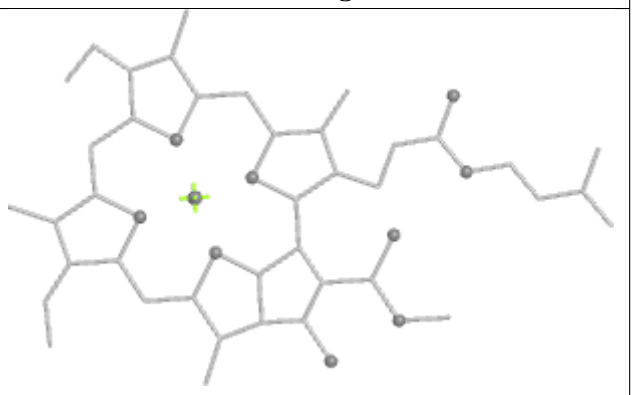
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Bond angles

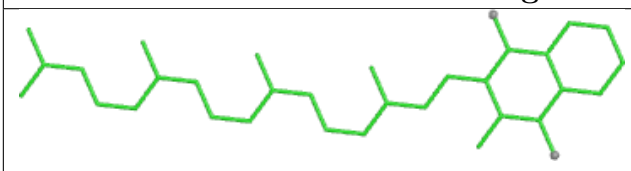


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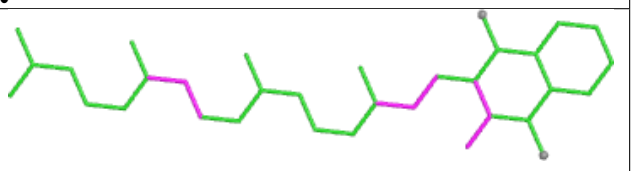


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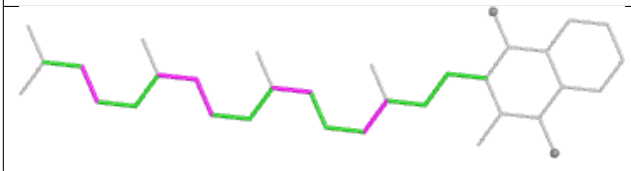
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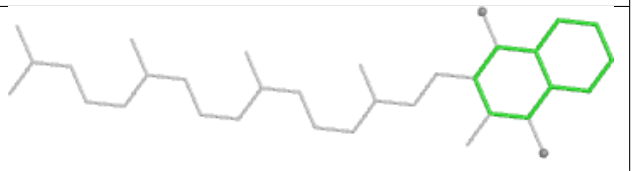
Bond lengths



Bond angles

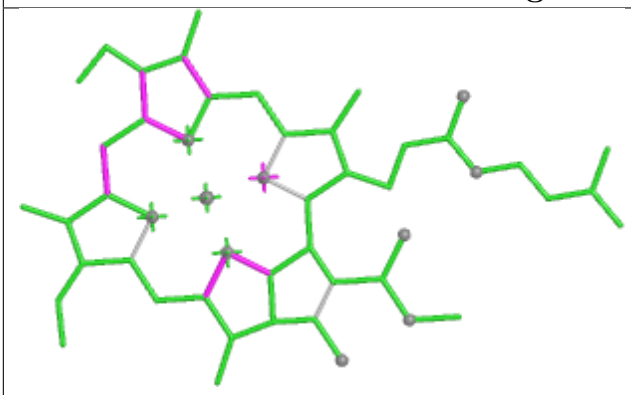


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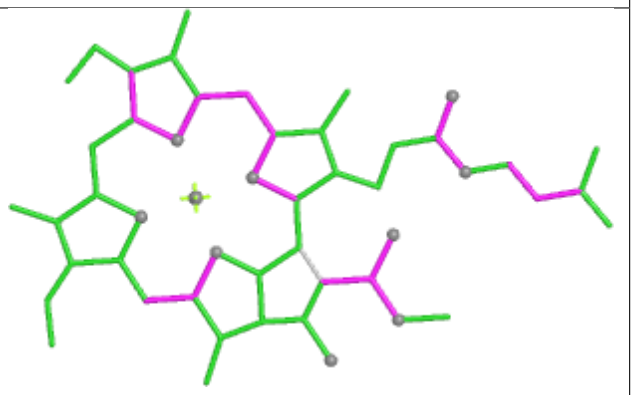


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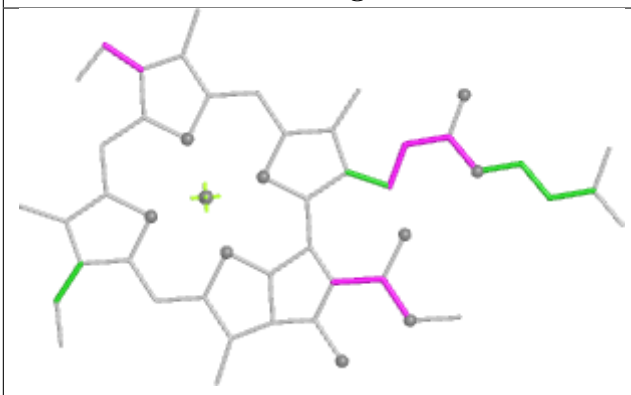
Ligand CLA L 302



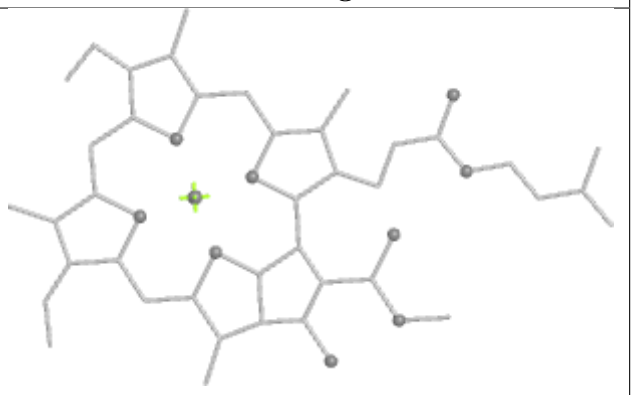
Bond lengths



Bond angles

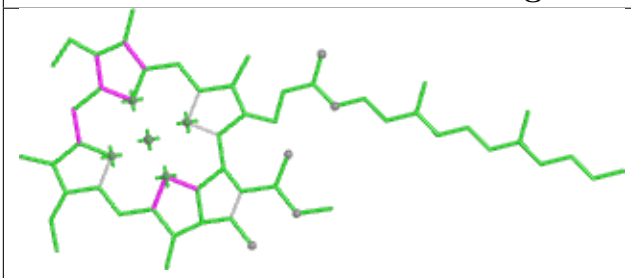


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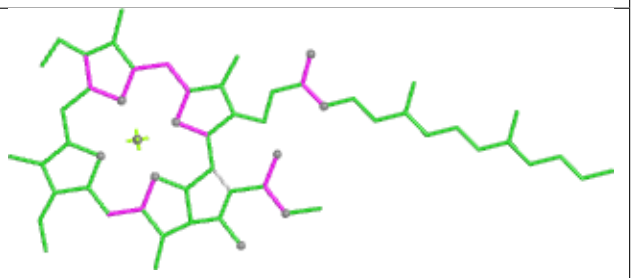


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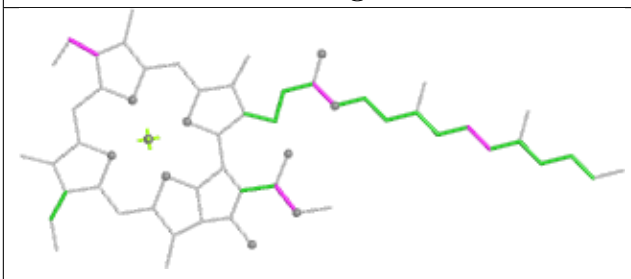
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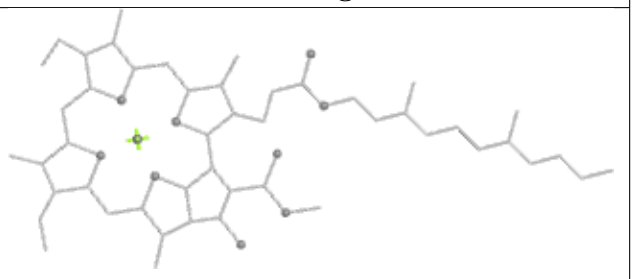
Bond lengths



Bond angles

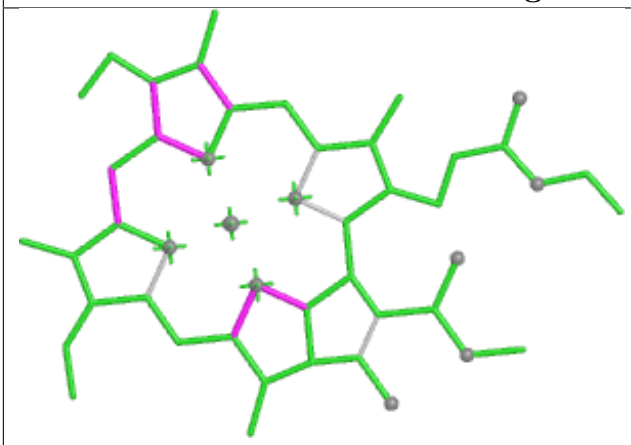


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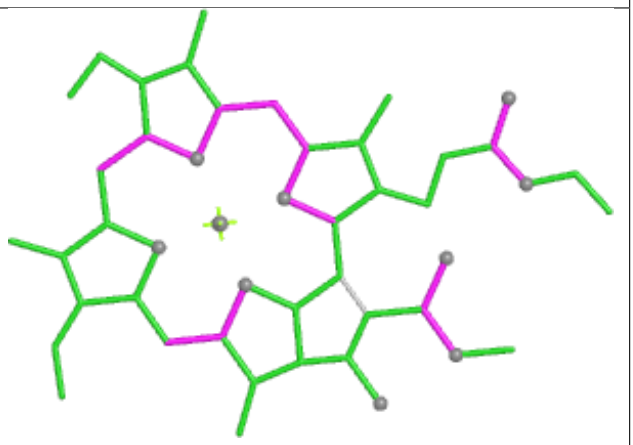


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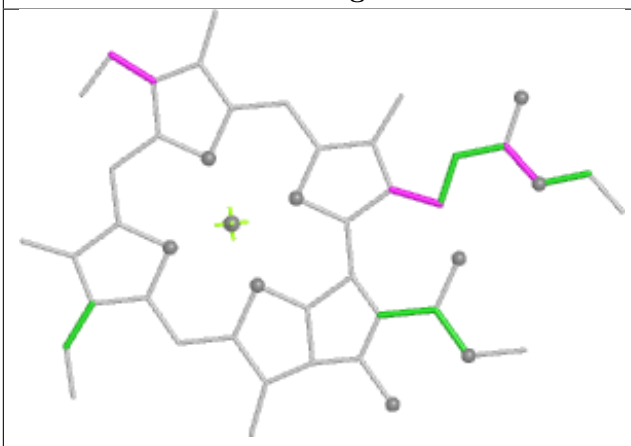
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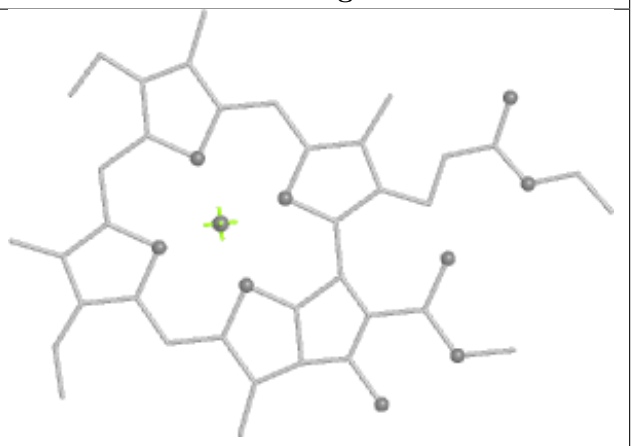
Bond lengths



Bond angles

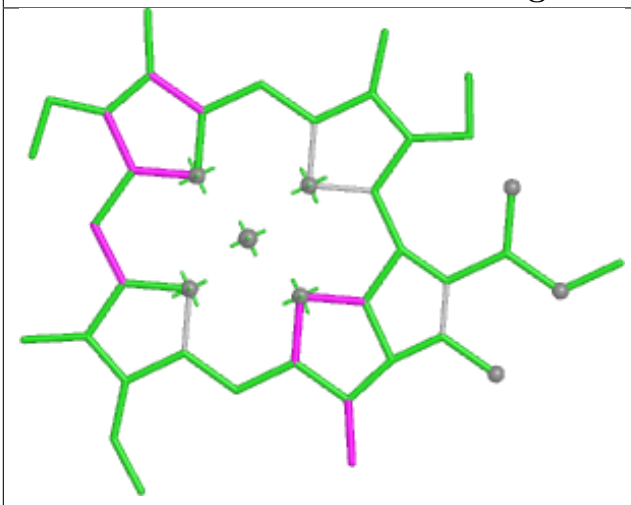


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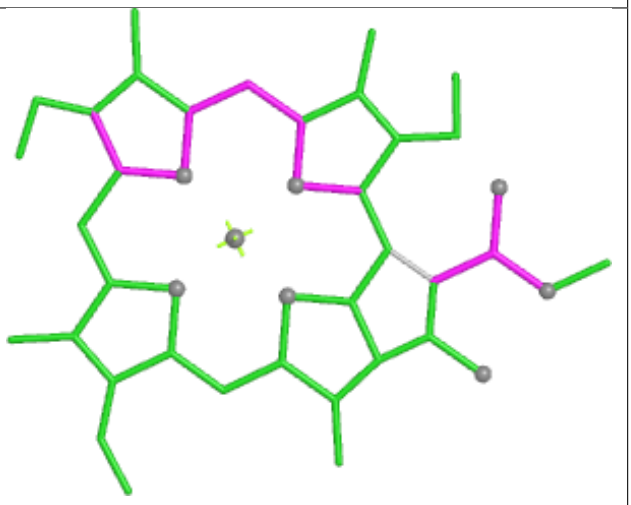


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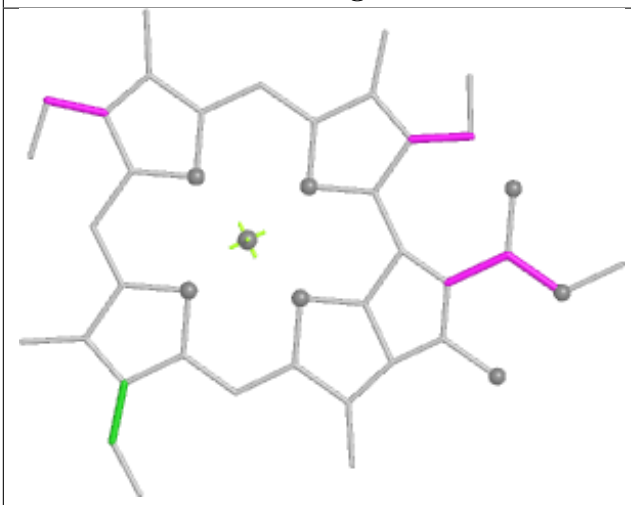
Ligand CLA 6 312



Bond lengths



Bond angles

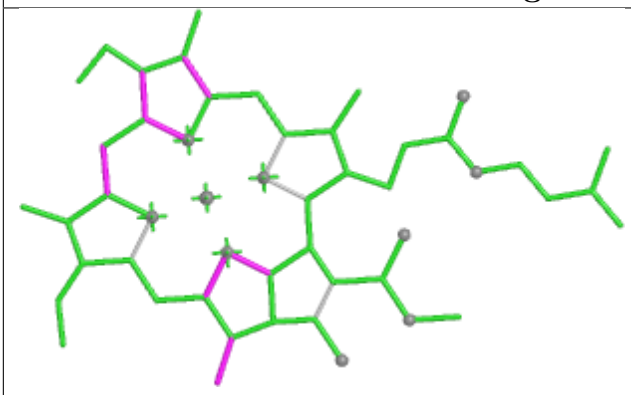


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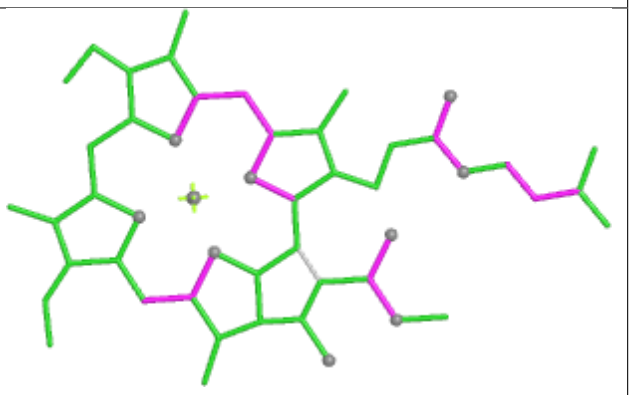


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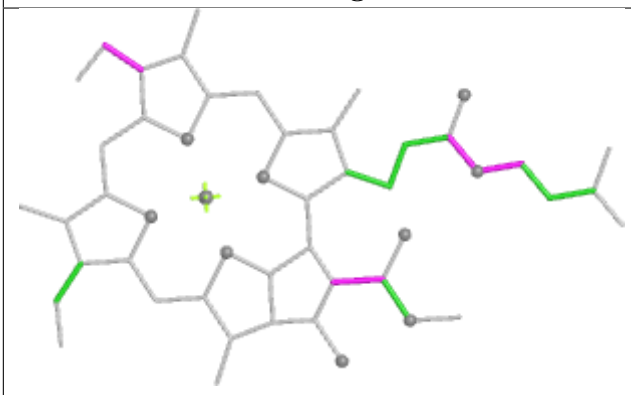
Ligand CLA A 825



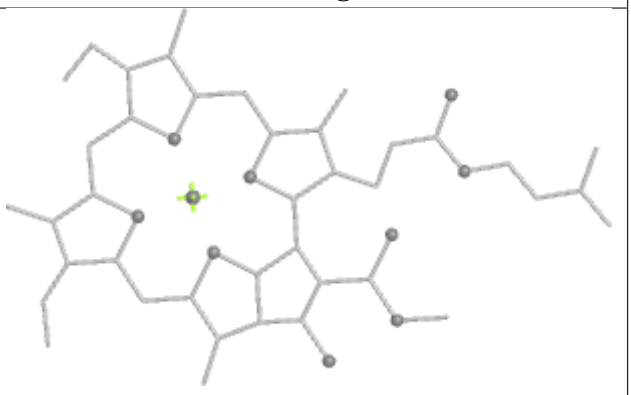
Bond lengths



Bond angles

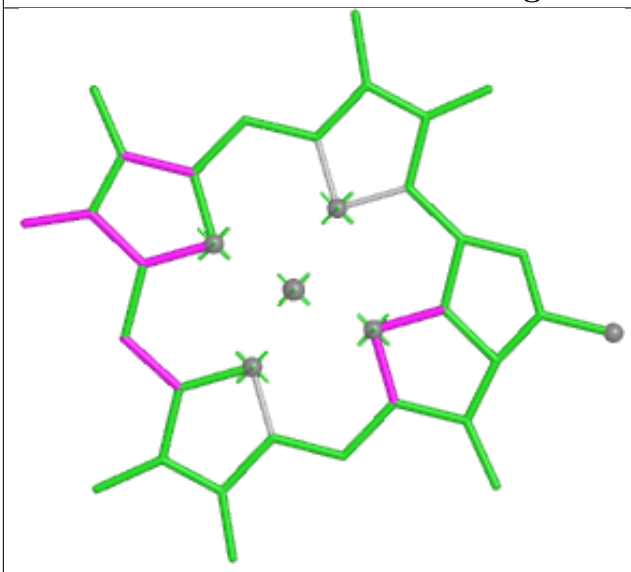


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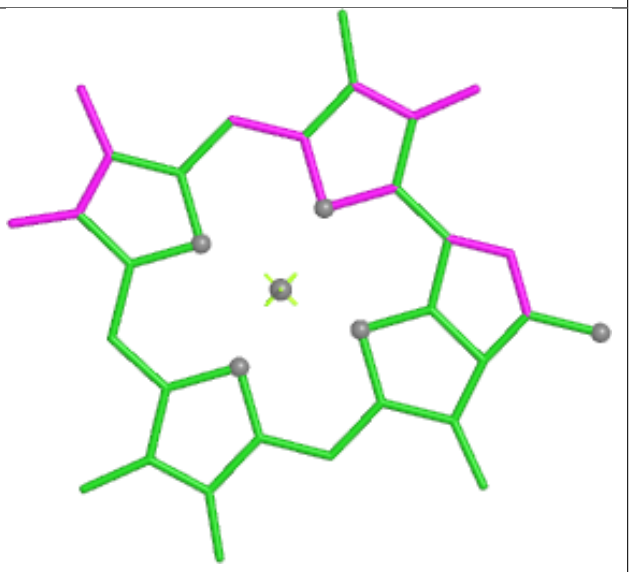


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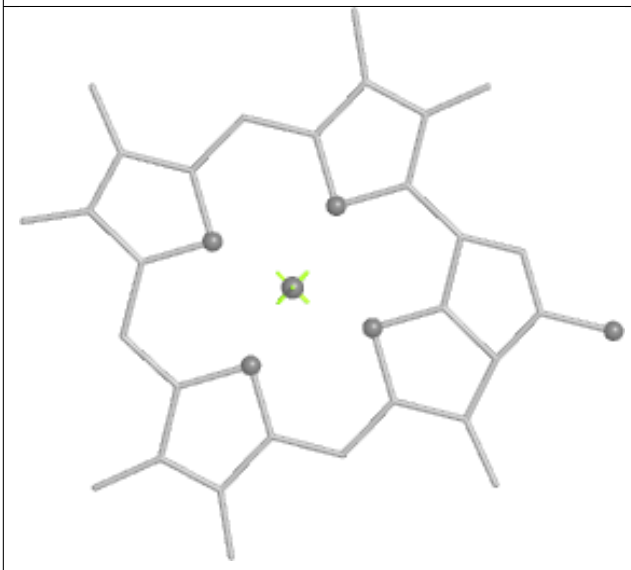
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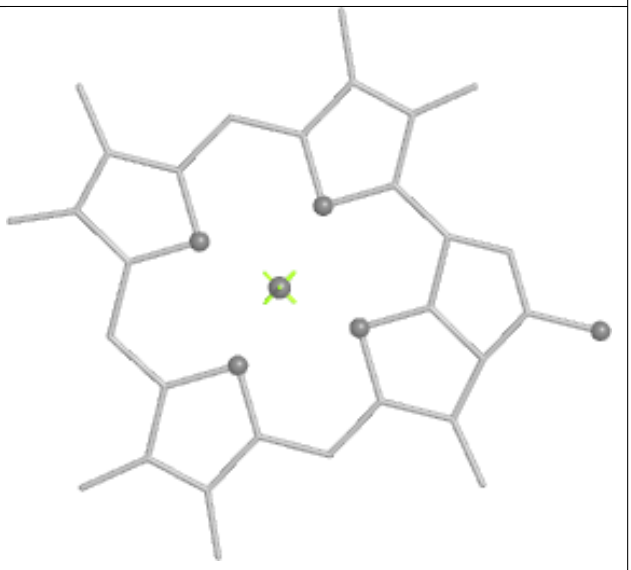
Bond lengths



Bond angles

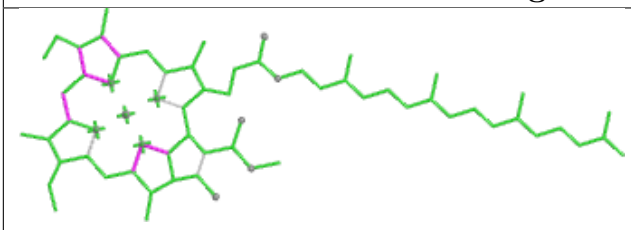


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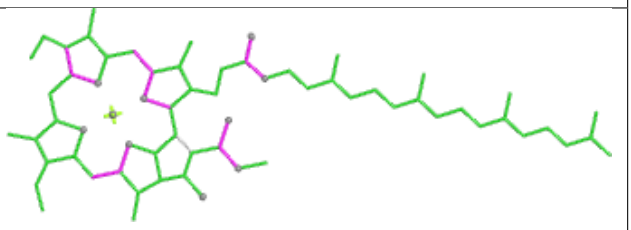


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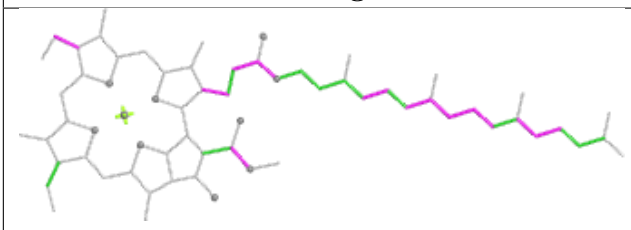
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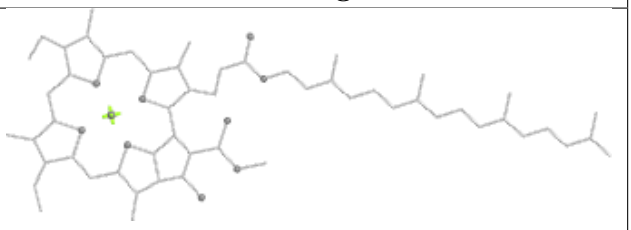
Bond lengths



Bond angles

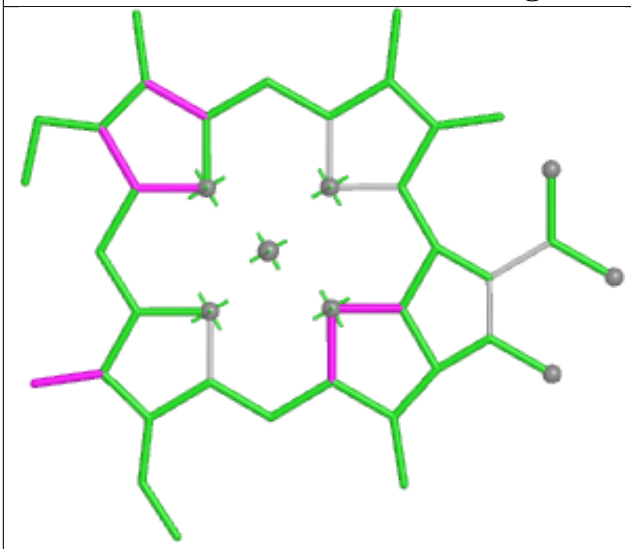


Torsions

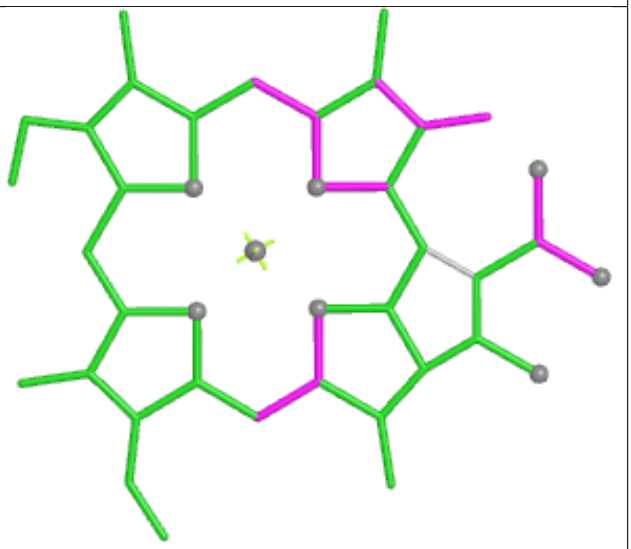


Rings

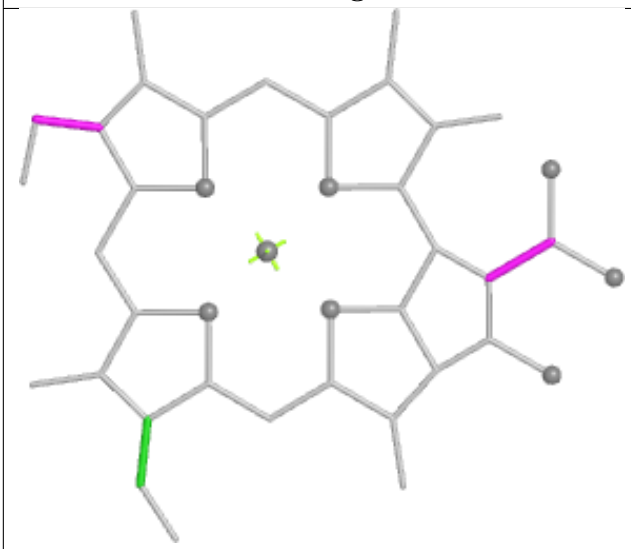
Ligand CLA A 843



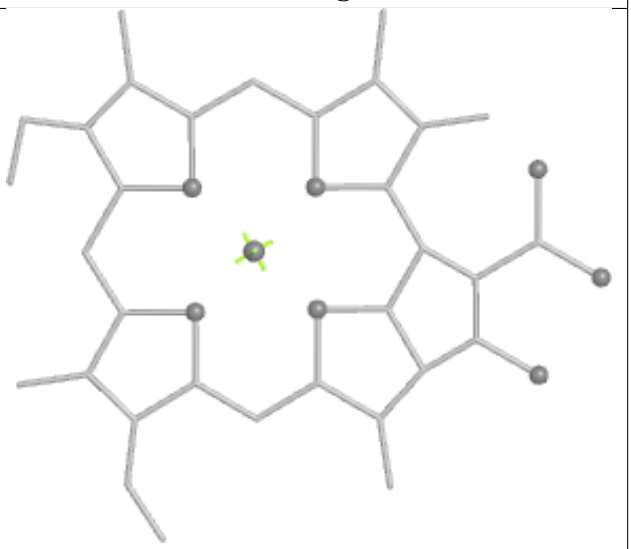
Bond lengths



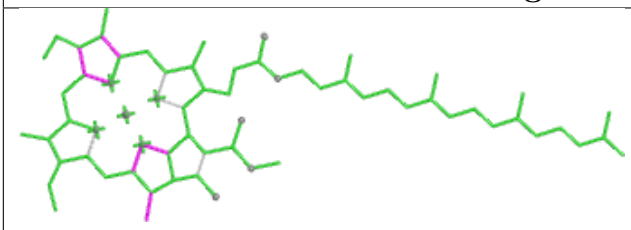
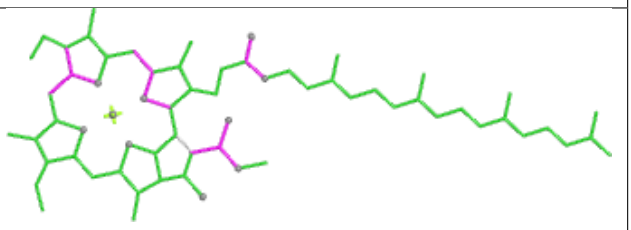
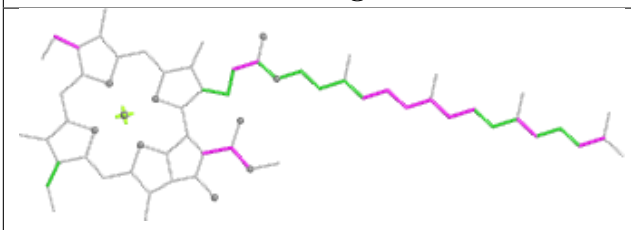
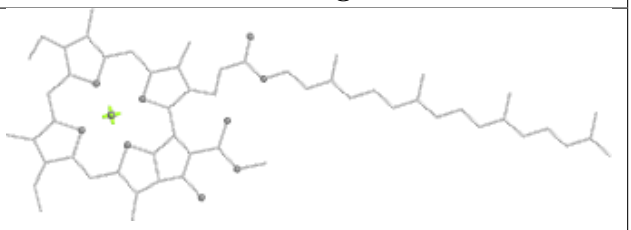
Bond angles

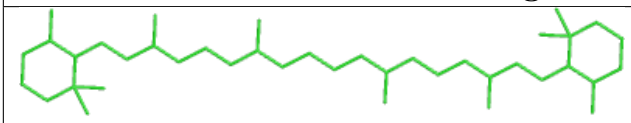
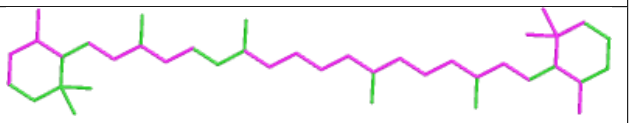
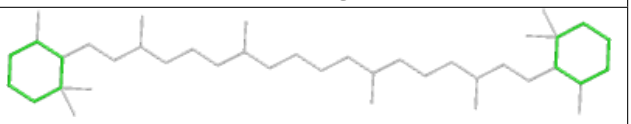


Torsions

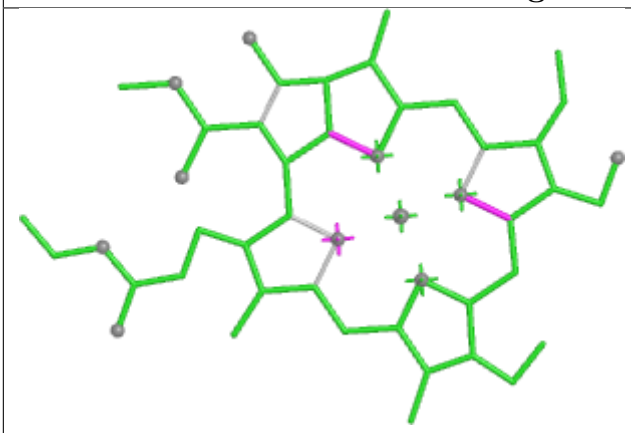


Rings

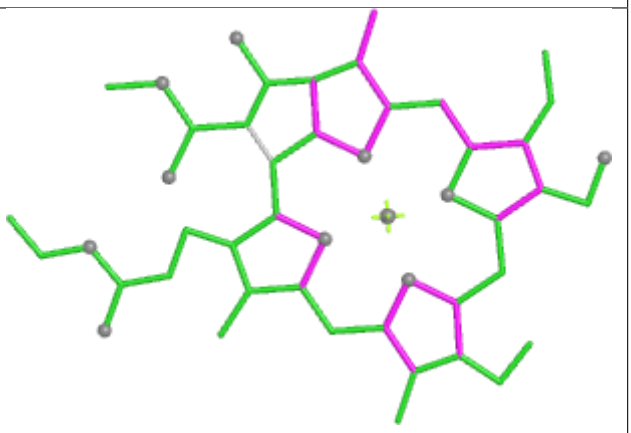
Ligand CLA B 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

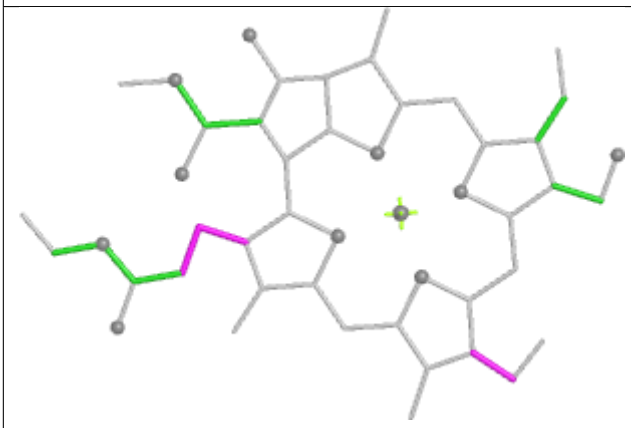
Ligand CHL 5 309



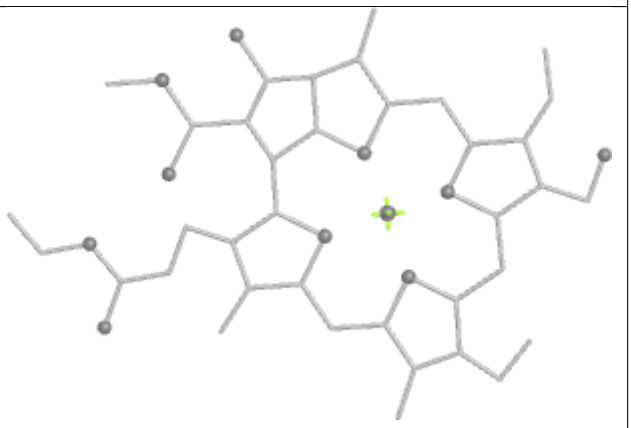
Bond lengths



Bond angles

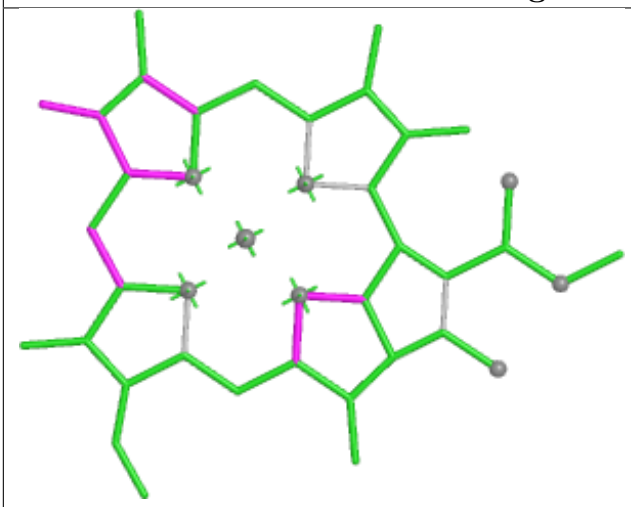


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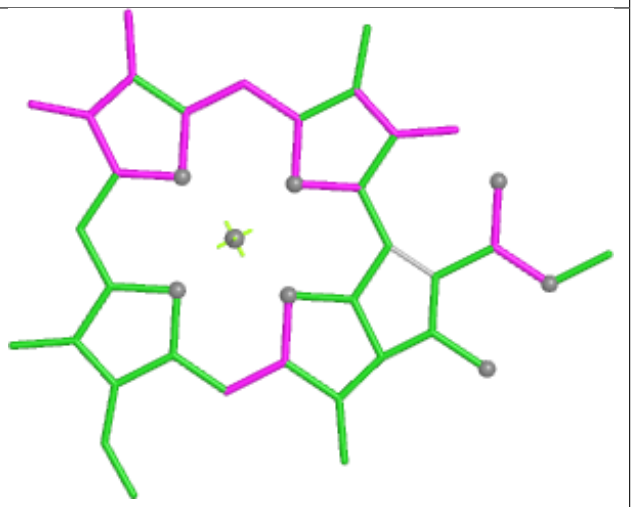


Rings

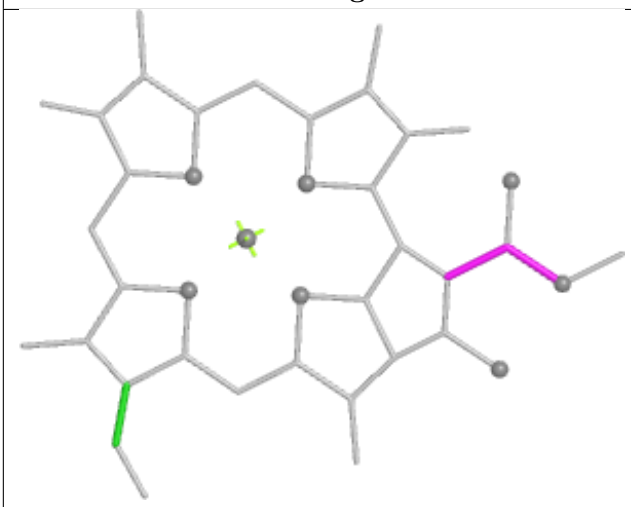
Ligand CLA 1 303



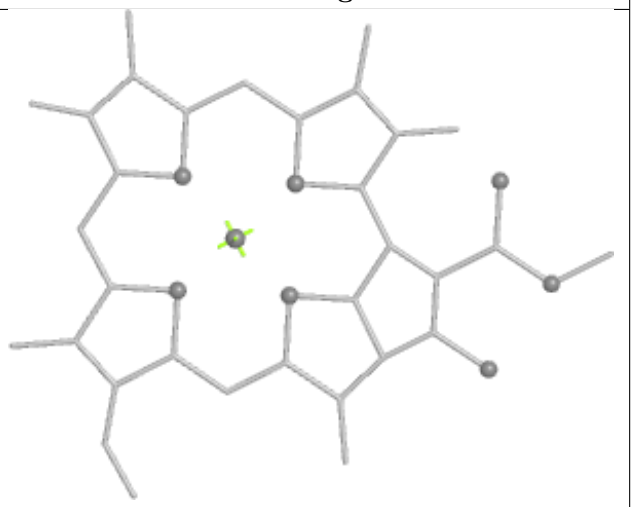
Bond lengths



Bond angles

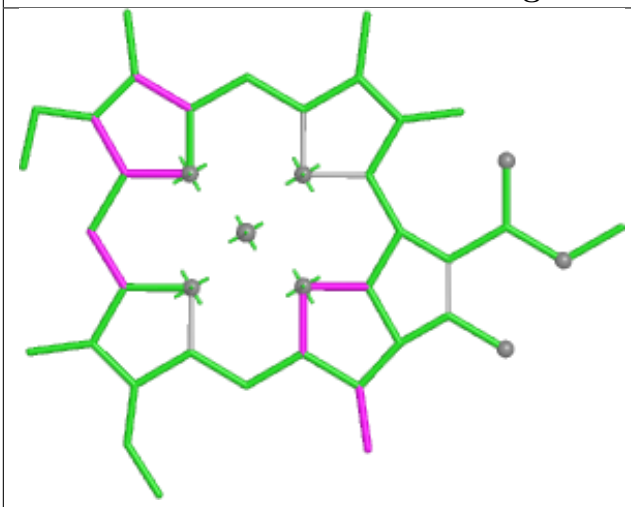


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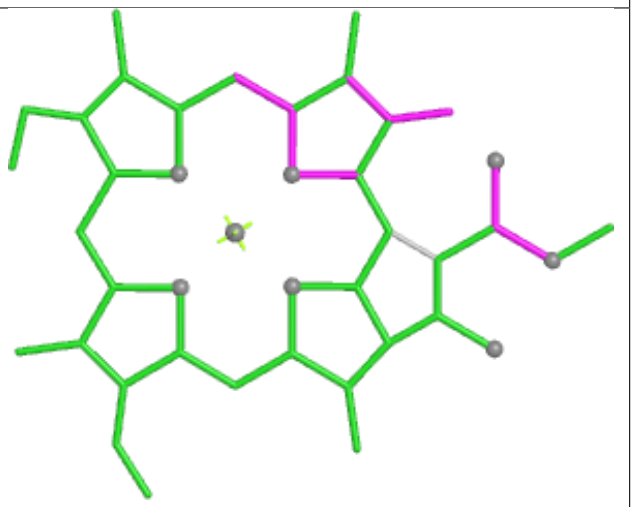


Rings

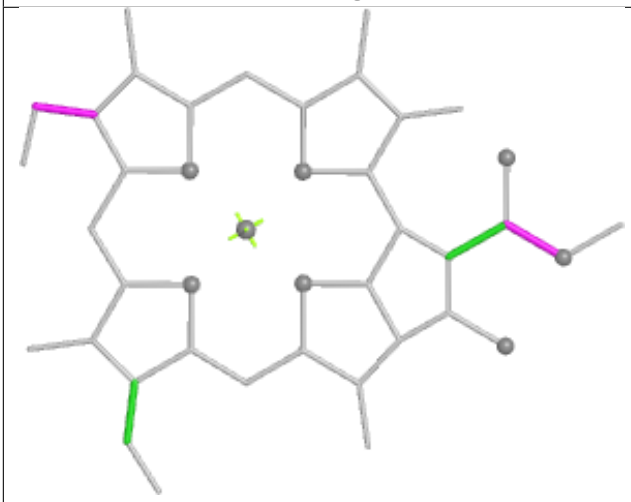
Ligand CLA K 202



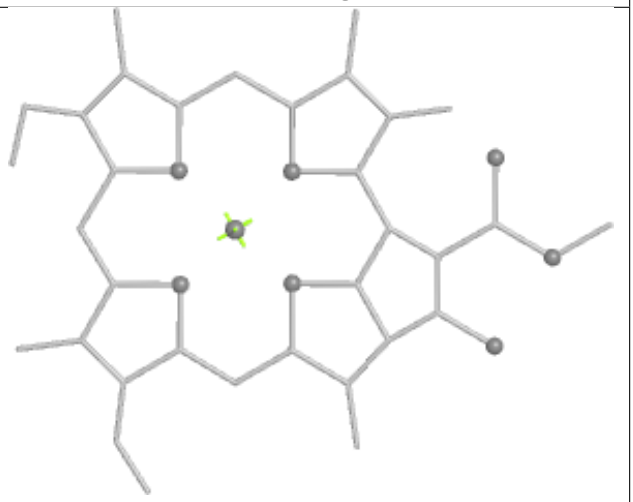
Bond lengths



Bond angles

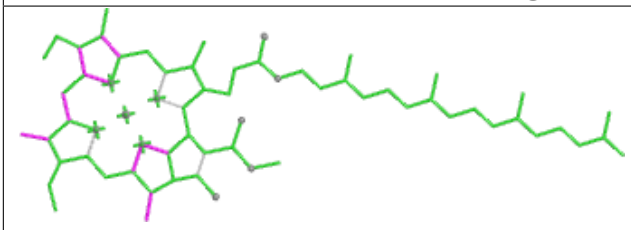


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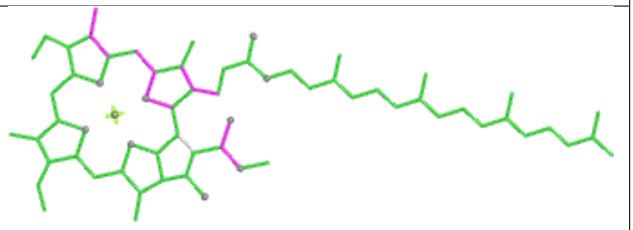


Rings

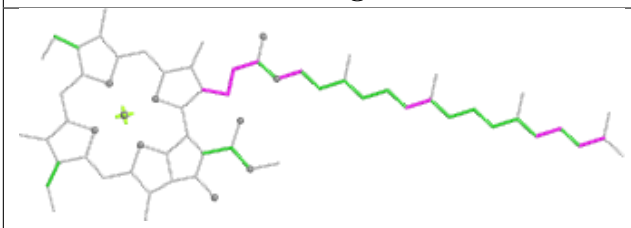
Ligand CLA B 829



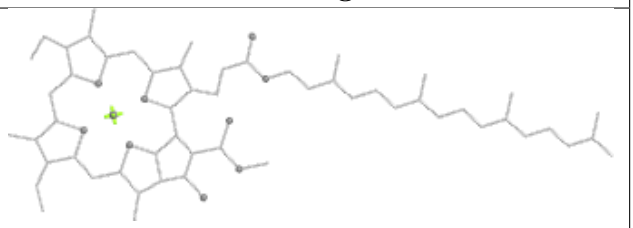
Bond lengths



Bond angles

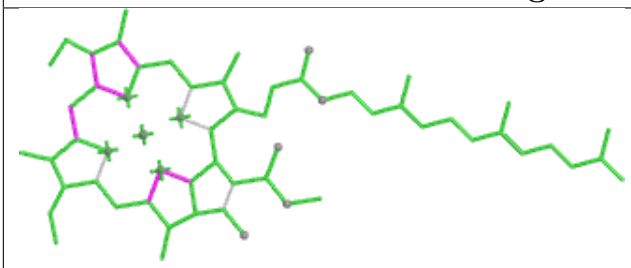


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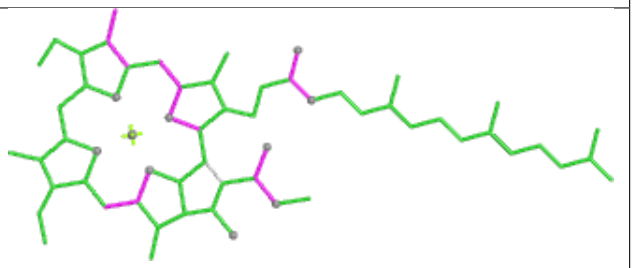


Rings

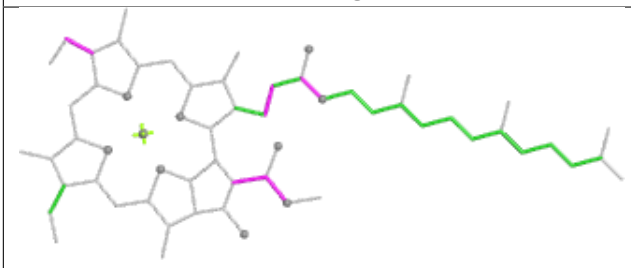
Ligand CLA 3 401



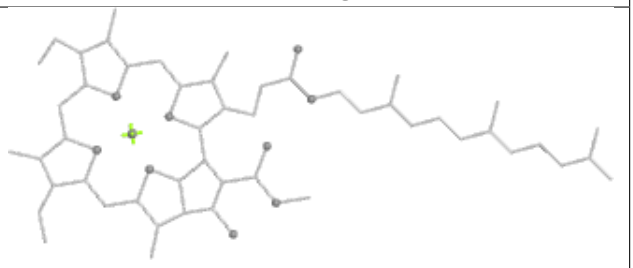
Bond lengths



Bond angles

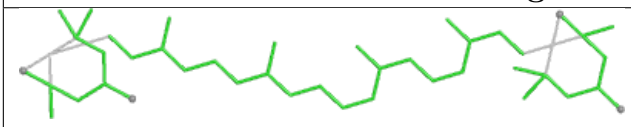


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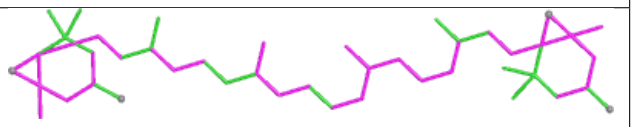


Rings

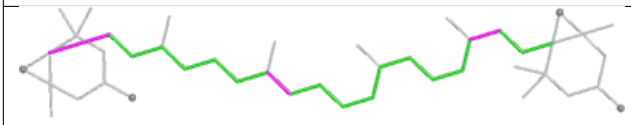
Ligand XAT 7 316



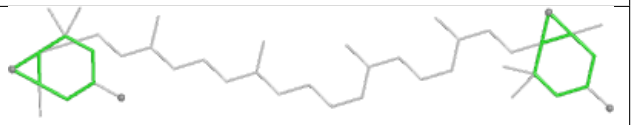
Bond lengths



Bond angles

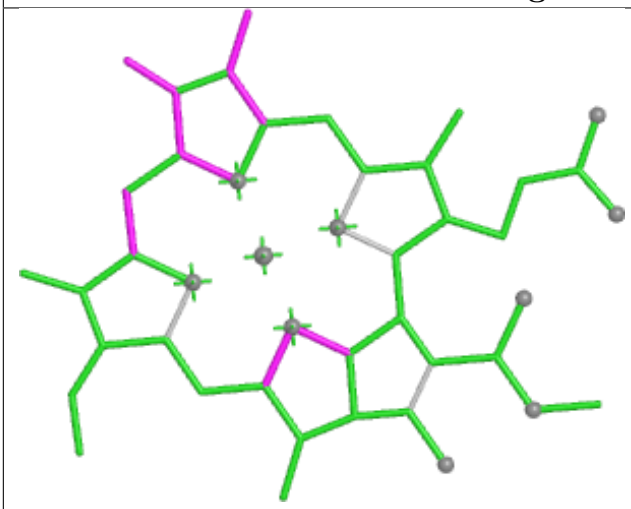


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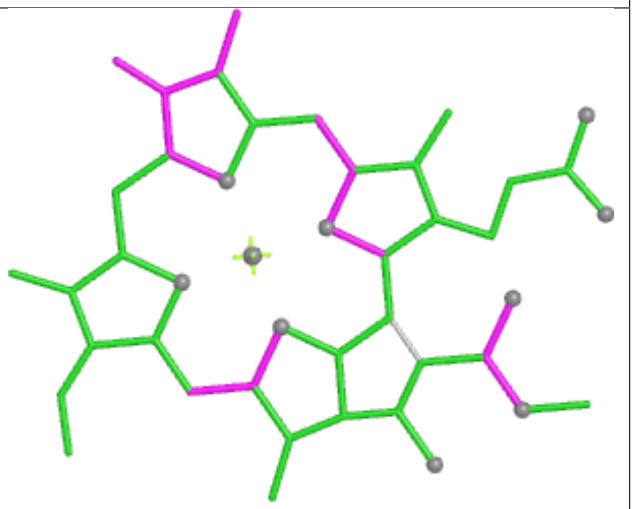


Rings

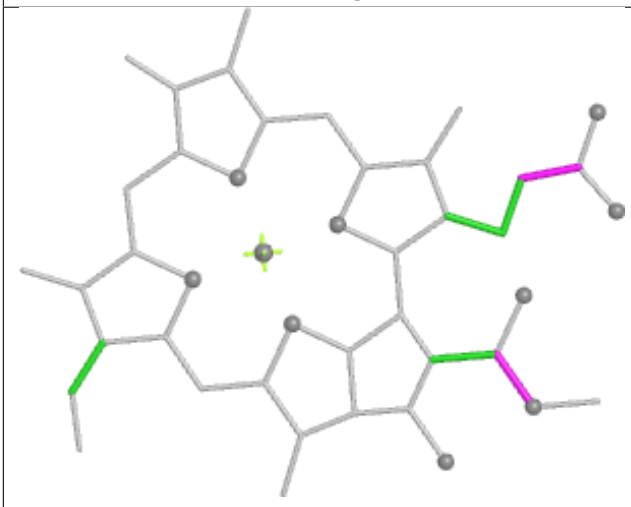
Ligand CLA 6 305



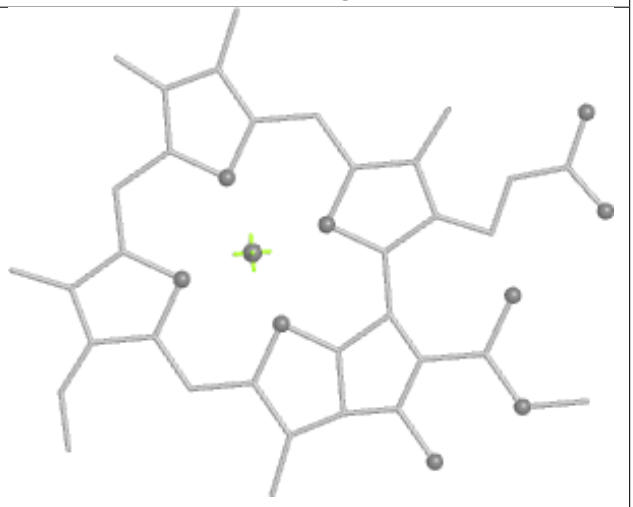
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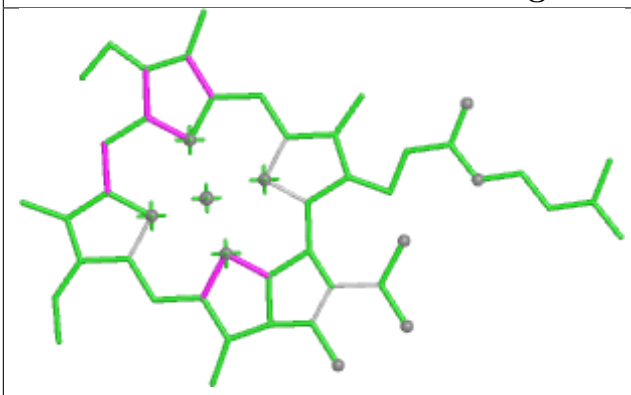


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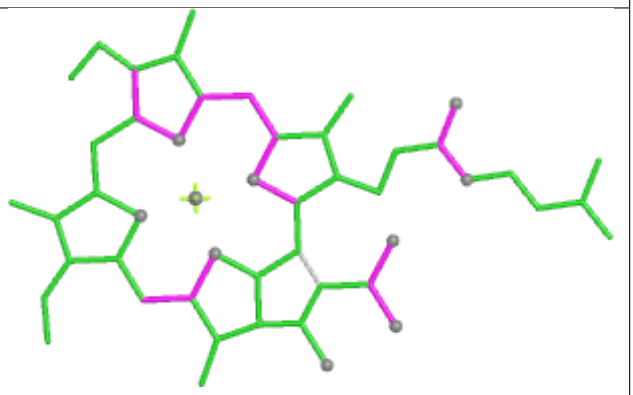


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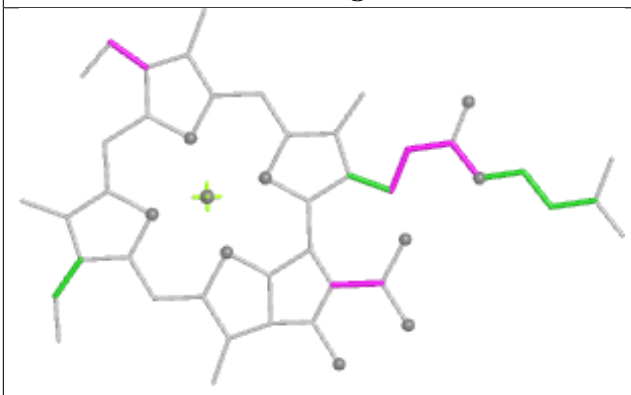
Ligand CLA 8 601



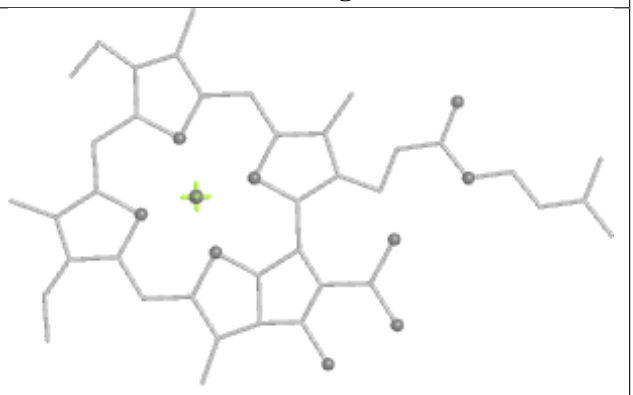
Bond lengths



Bond angles

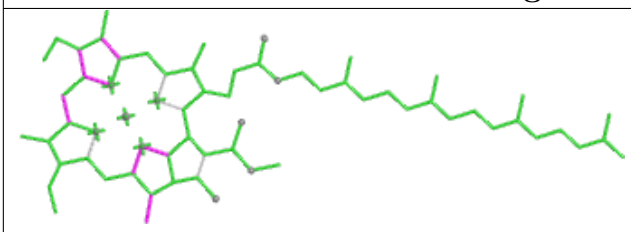


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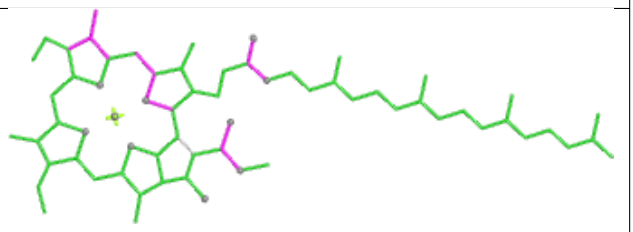


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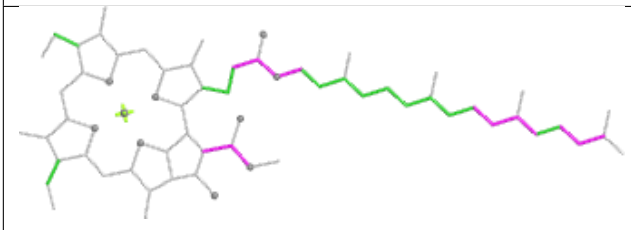
Ligand CLA A 814



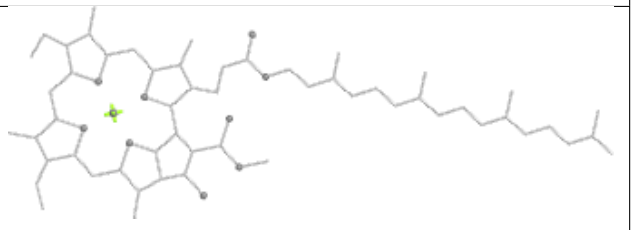
Bond lengths



Bond angles

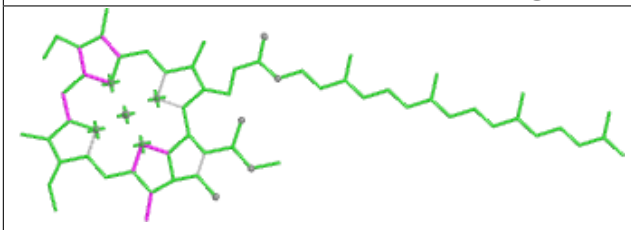


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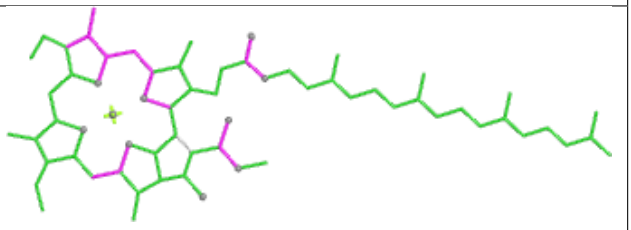


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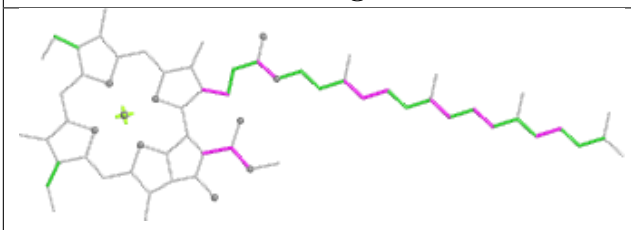
Ligand CLA 3 408



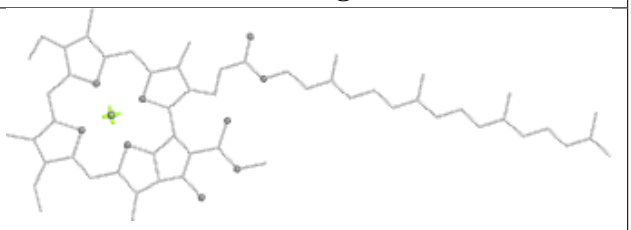
Bond lengths



Bond angles



Torsions



Rings

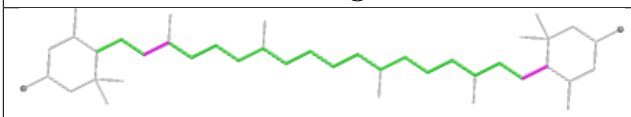
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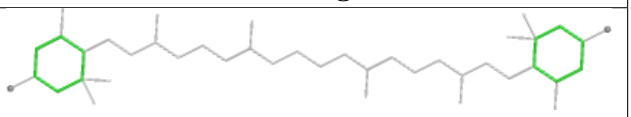
Bond lengths



Bond angles

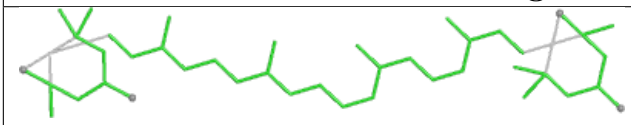


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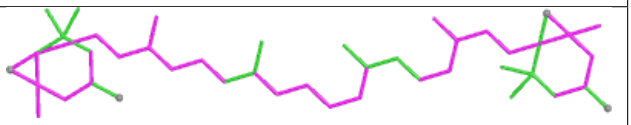


Rings

Ligand XAT 5 321



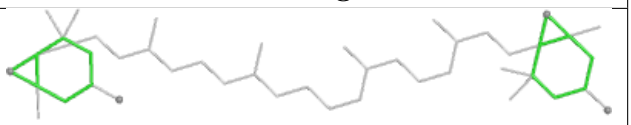
Bond lengths



Bond angles

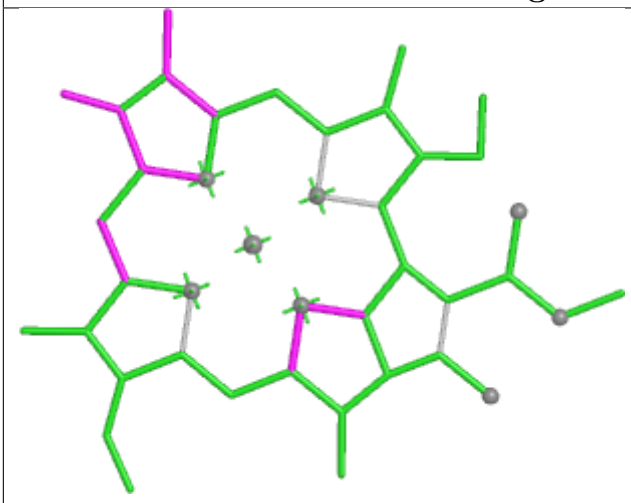


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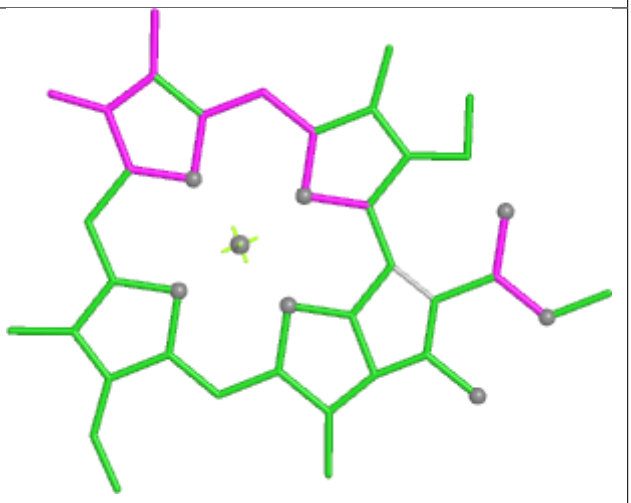


Rings

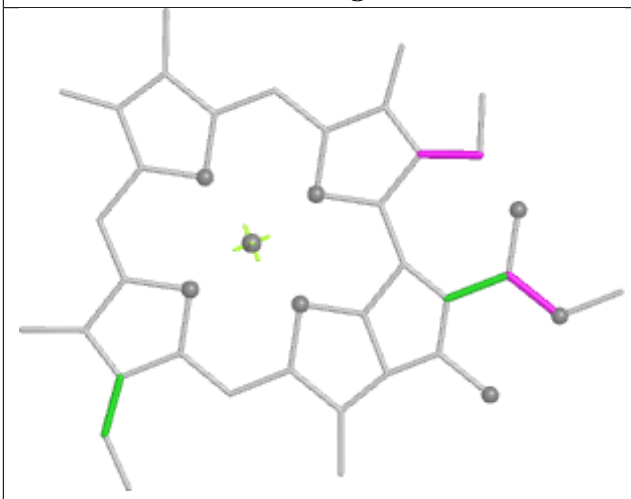
Ligand CLA 2 609



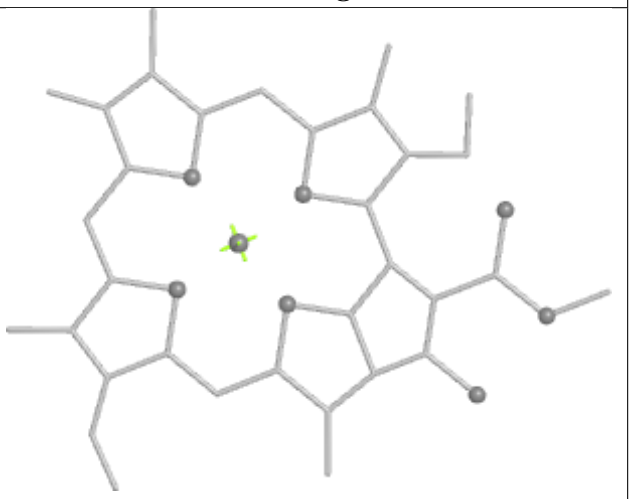
Bond lengths



Bond angles

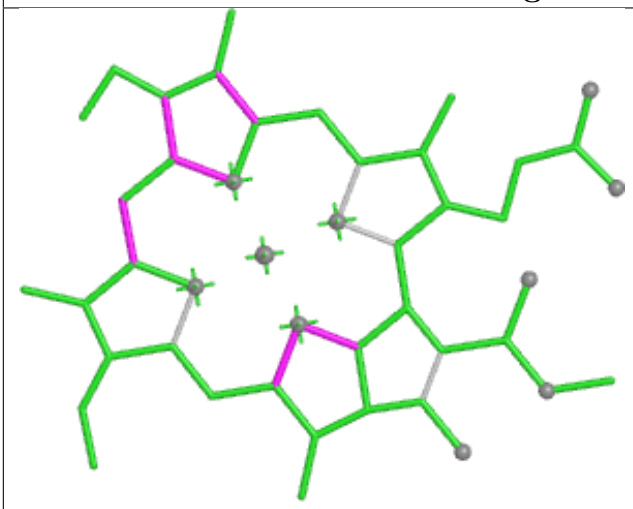


Torsions

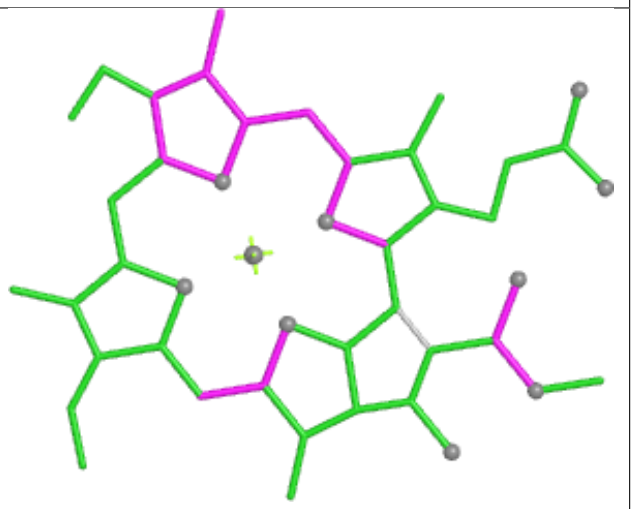


Rings

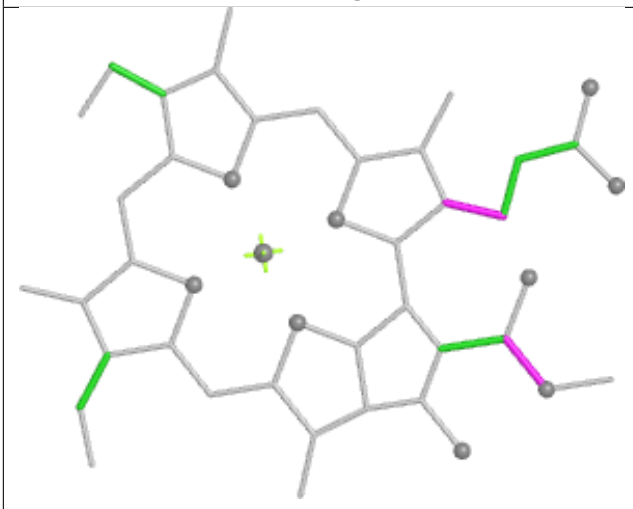
Ligand CLA A 831



Bond lengths



Bond angles

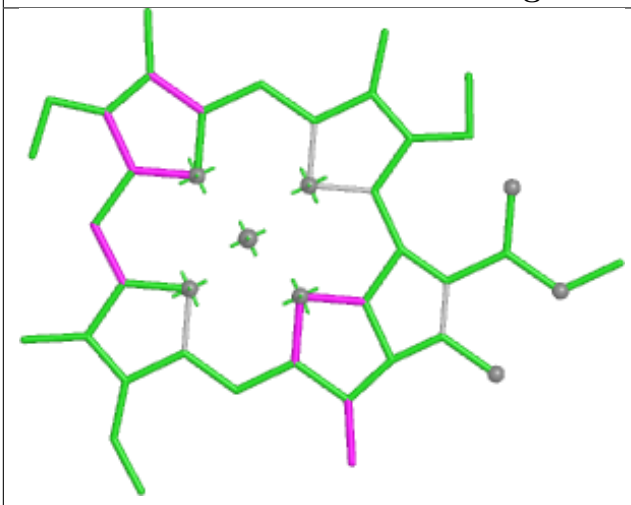


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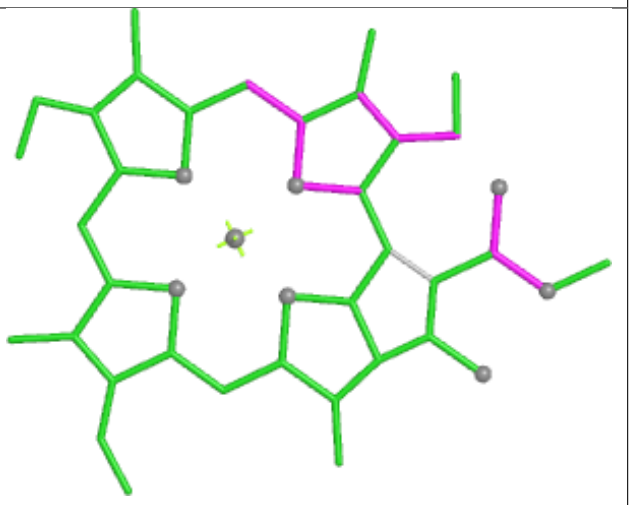


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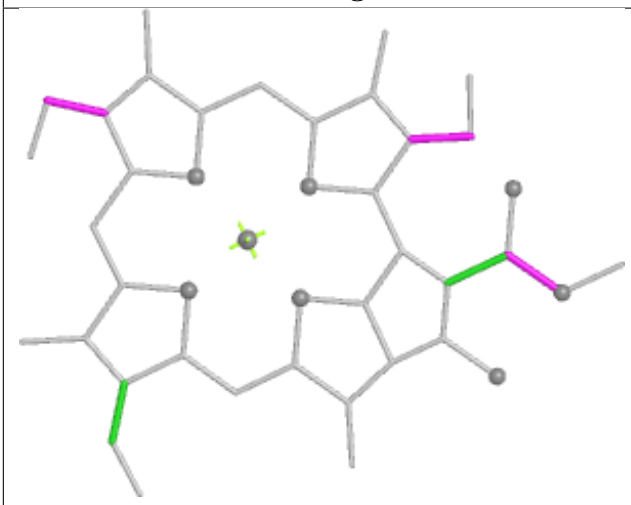
Ligand CLA H 203



Bond lengths



Bond angles

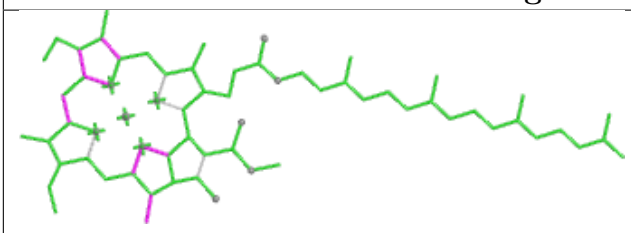


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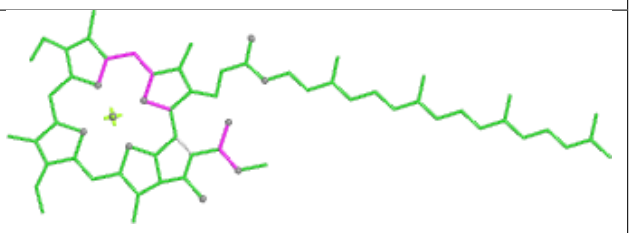


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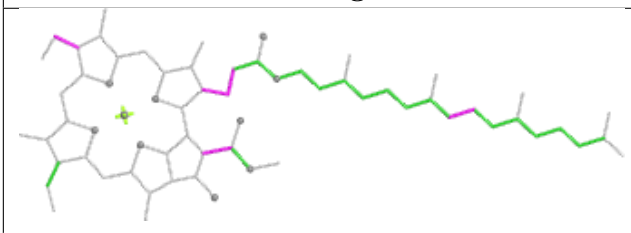
Ligand CLA B 831



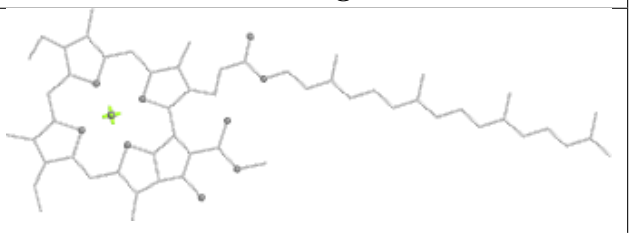
Bond lengths



Bond angles

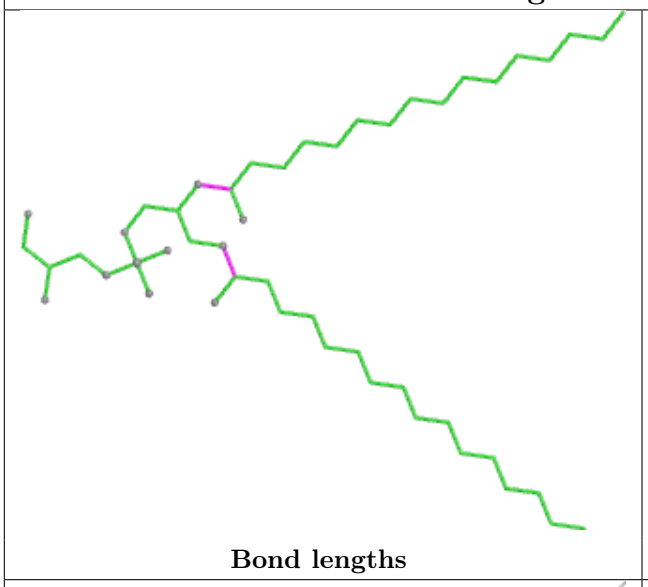


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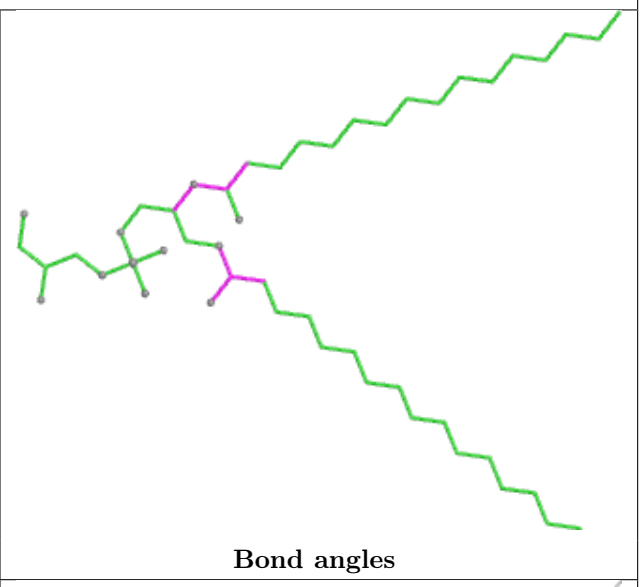


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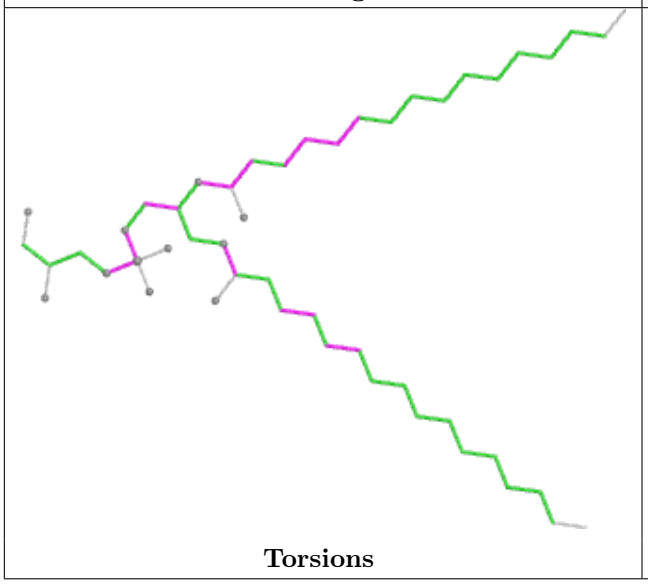
Ligand LHG 8 620



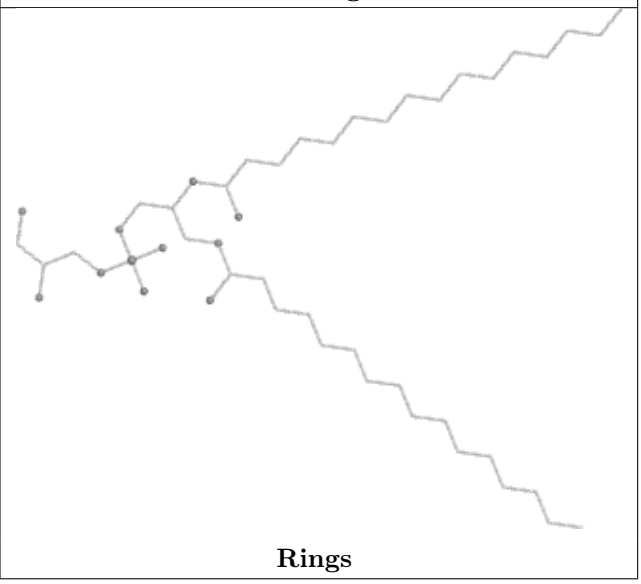
Bond lengths



Bond angles

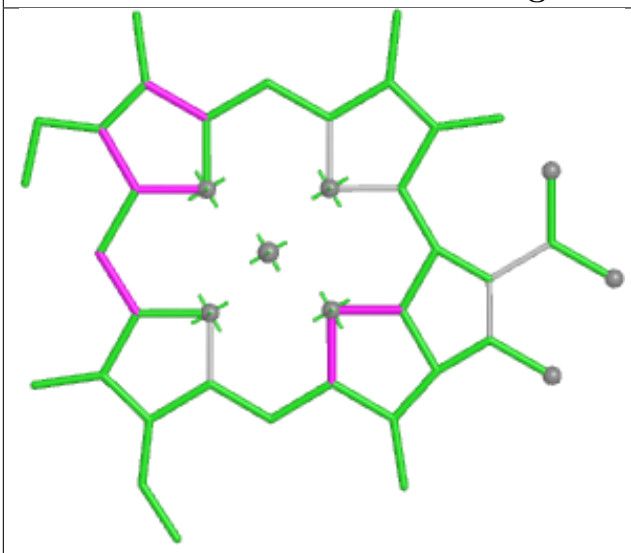


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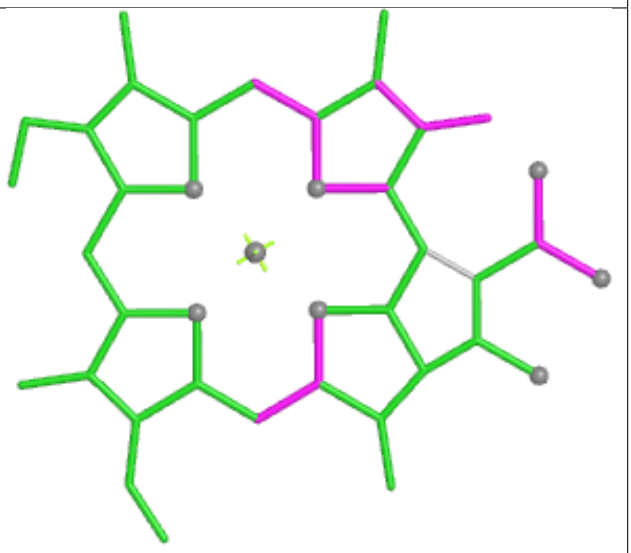


Rings

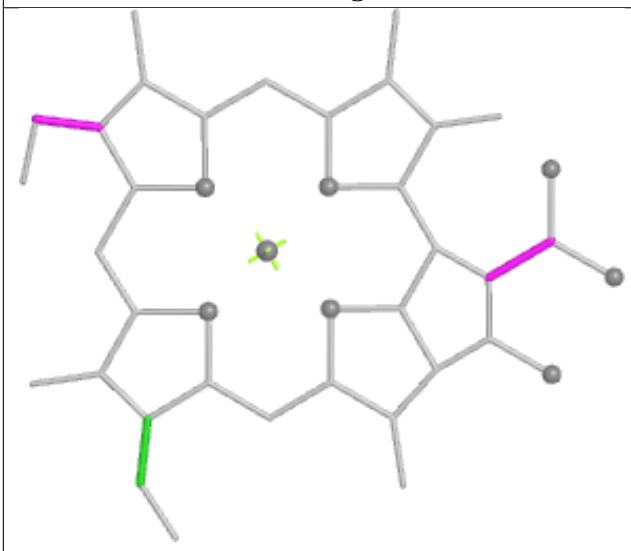
Ligand CLA 3 414



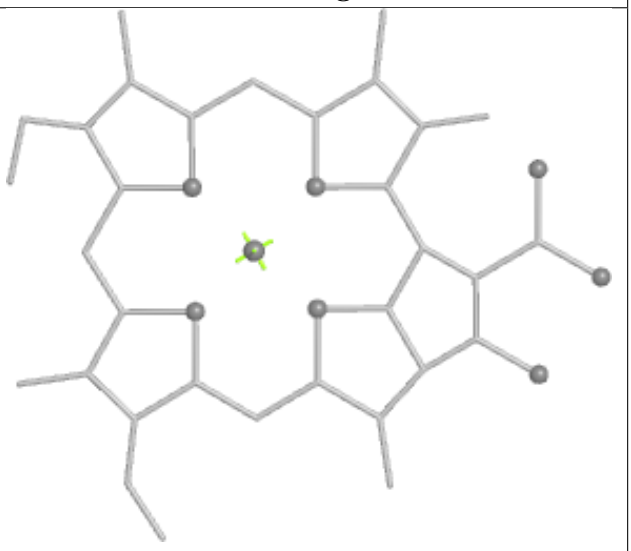
Bond lengths



Bond angles

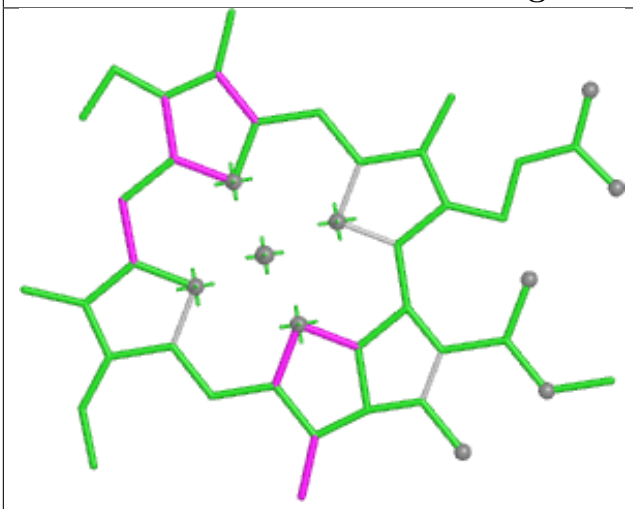


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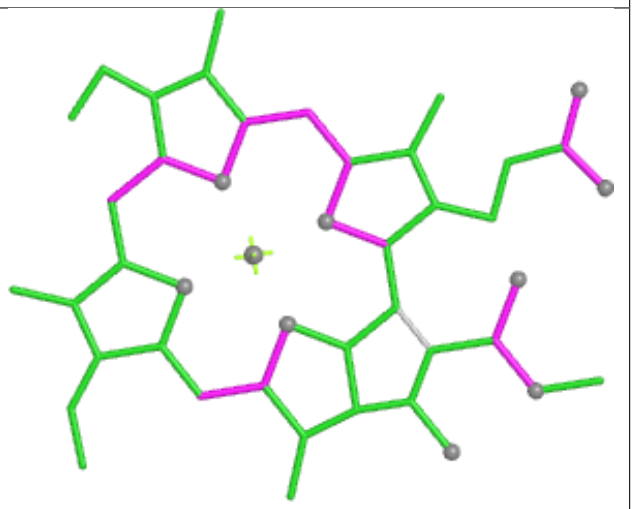


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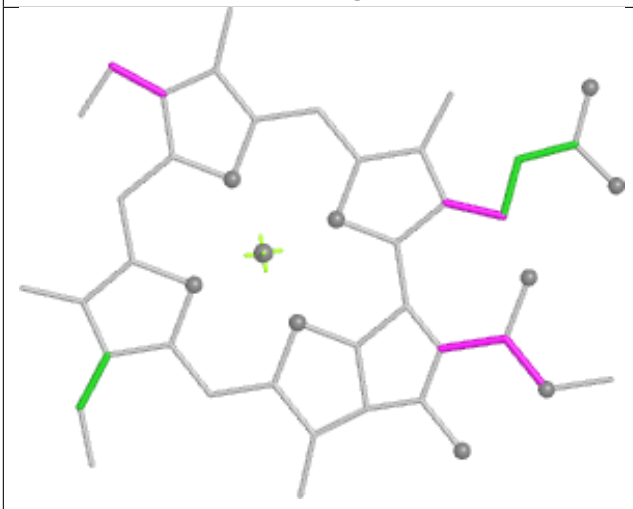
Ligand CLA 6 315



Bond lengths



Bond angles

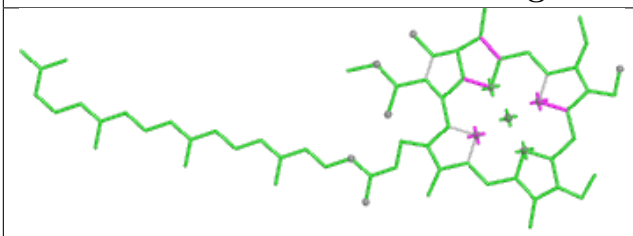


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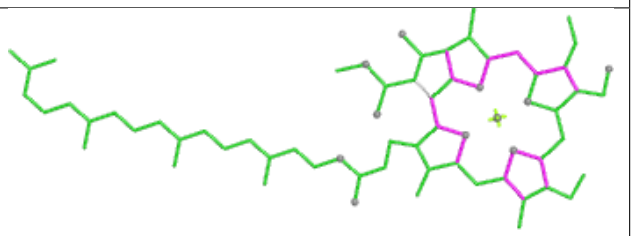


Rings

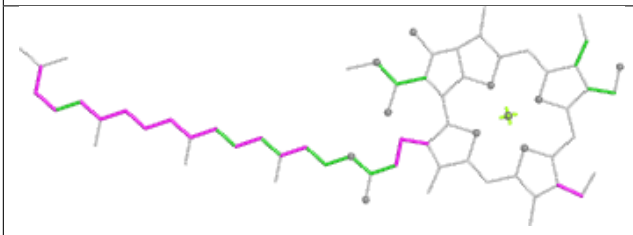
Ligand CHL 5 307



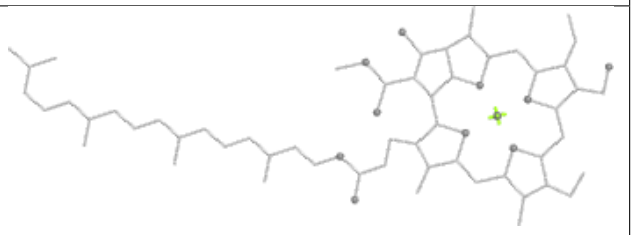
Bond lengths



Bond angles

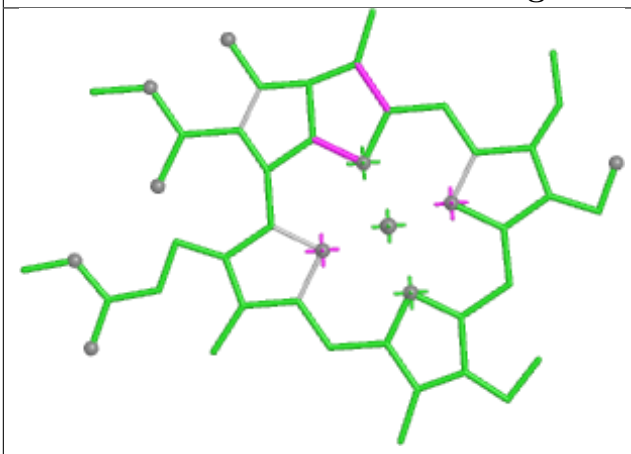


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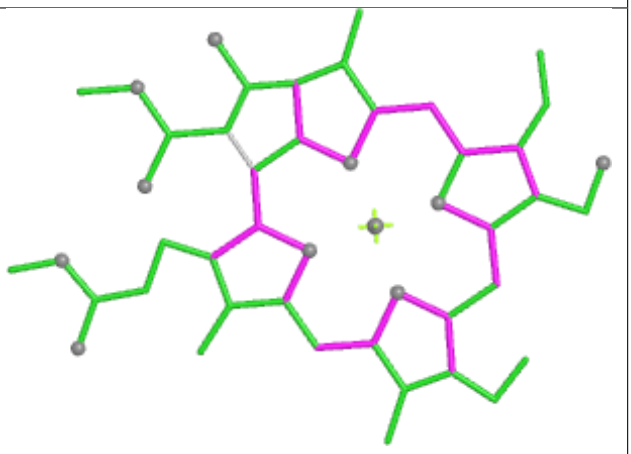


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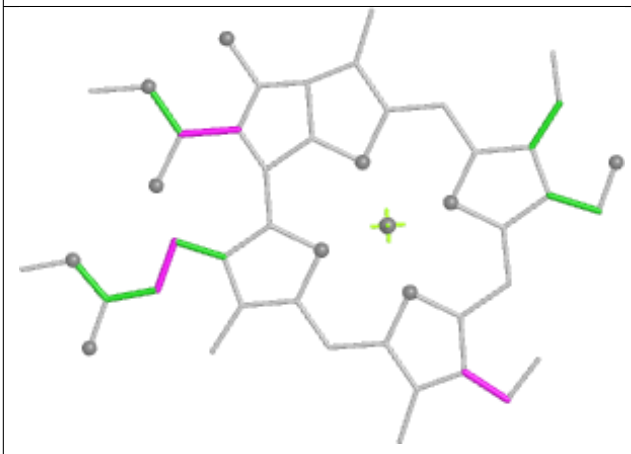
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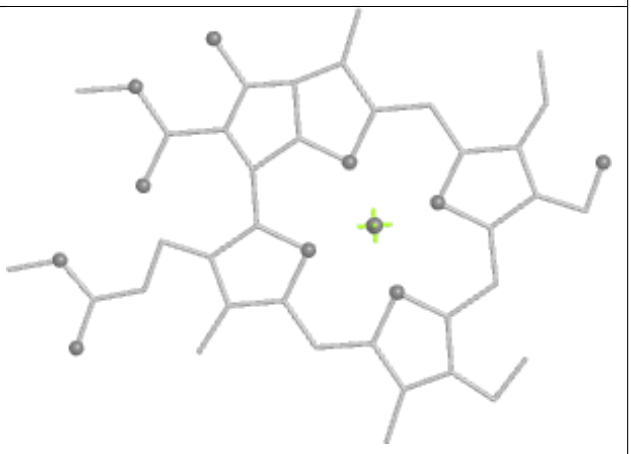
Bond lengths



Bond angles

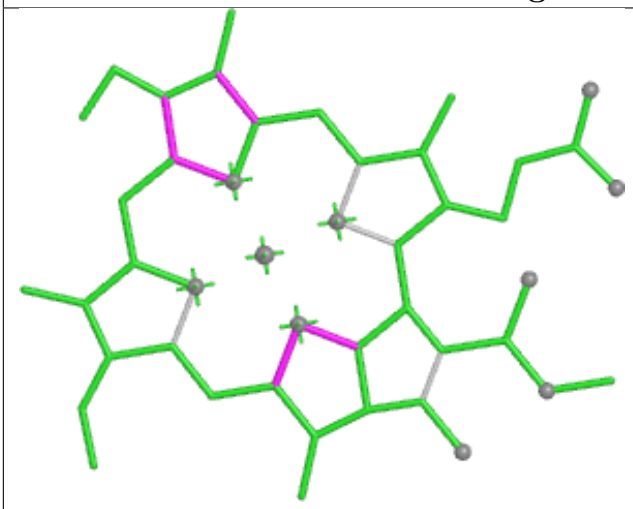


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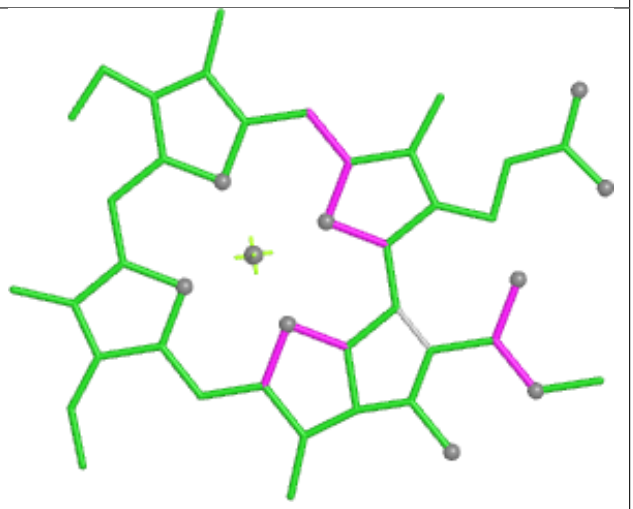


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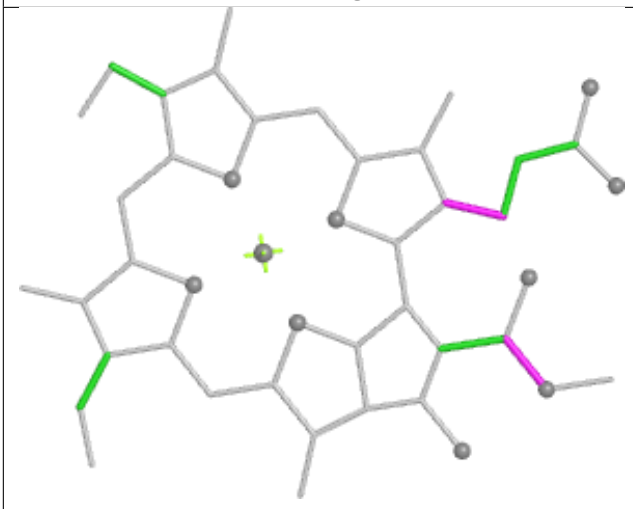
Ligand CLA 9 607



Bond lengths



Bond angles

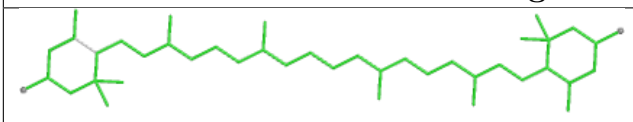


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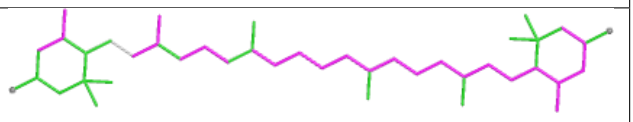


Rings

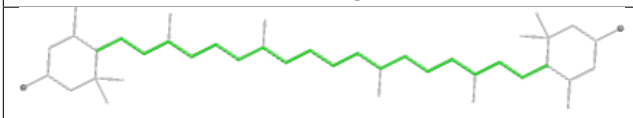
Ligand LUT 3 418



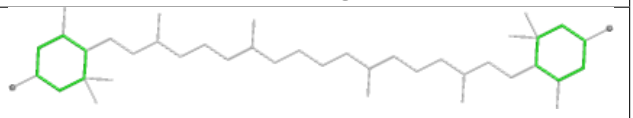
Bond lengths



Bond angles

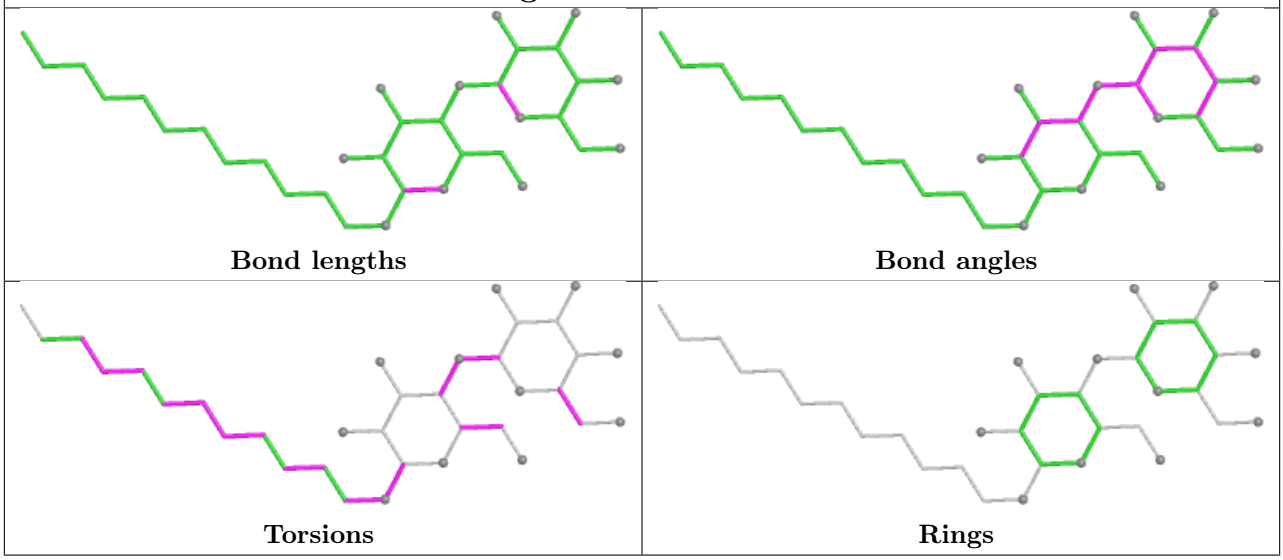


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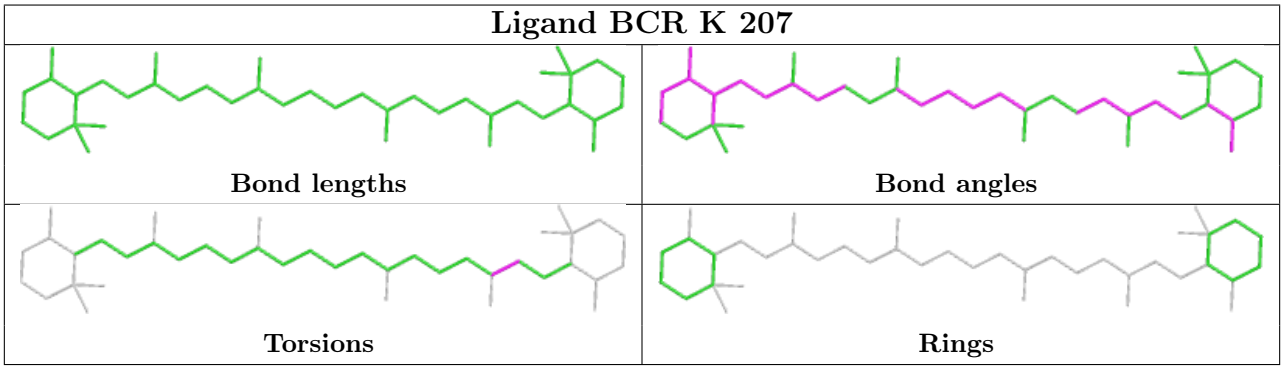


Rings

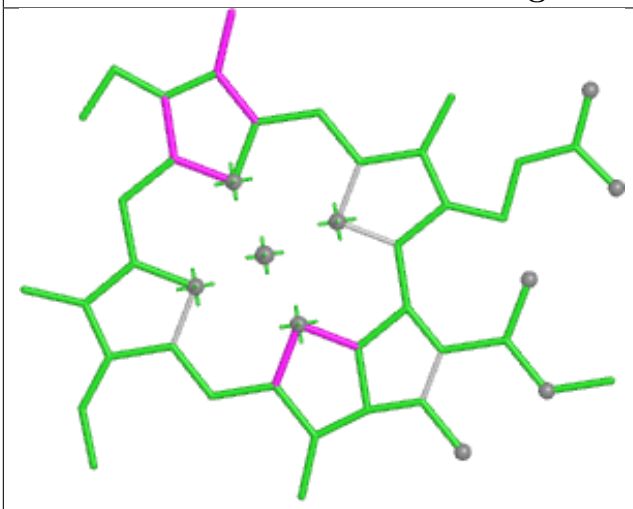
Ligand LMU H 204



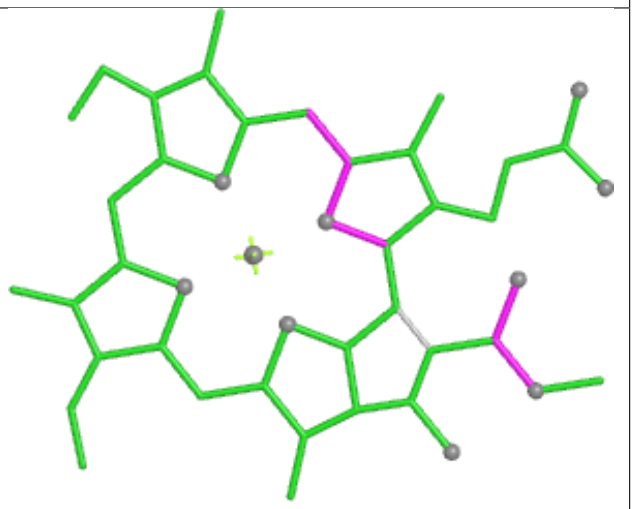
Ligand BCR K 207



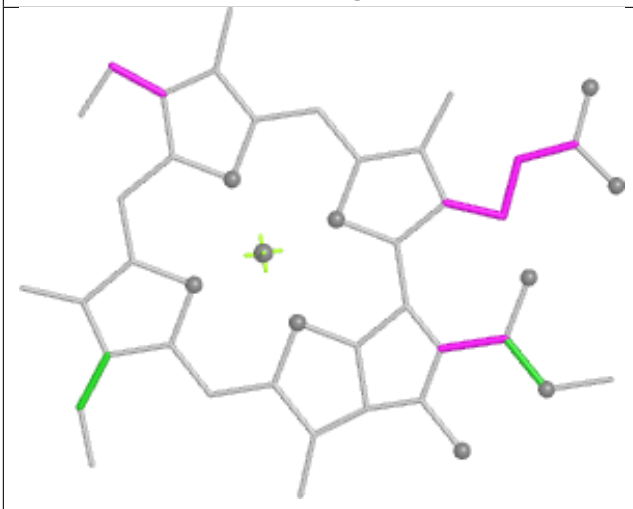
Ligand CLA 8 609



Bond lengths



Bond angles

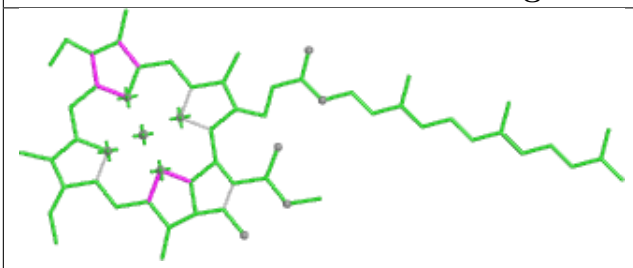


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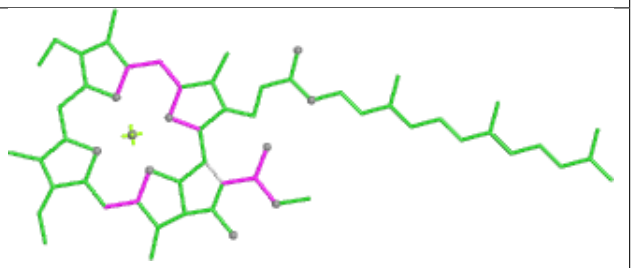


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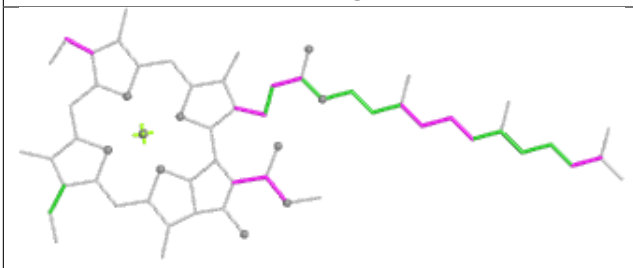
Ligand CLA A 833



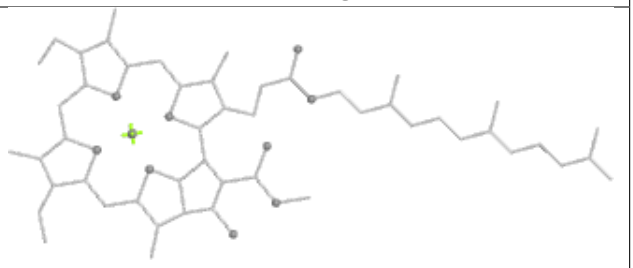
Bond lengths



Bond angles

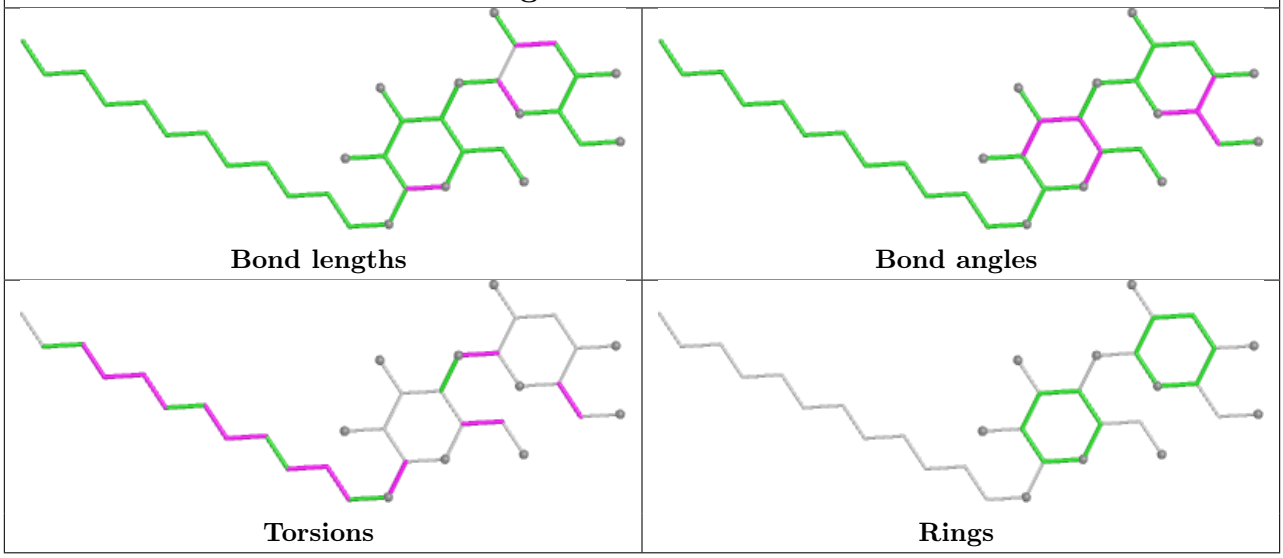


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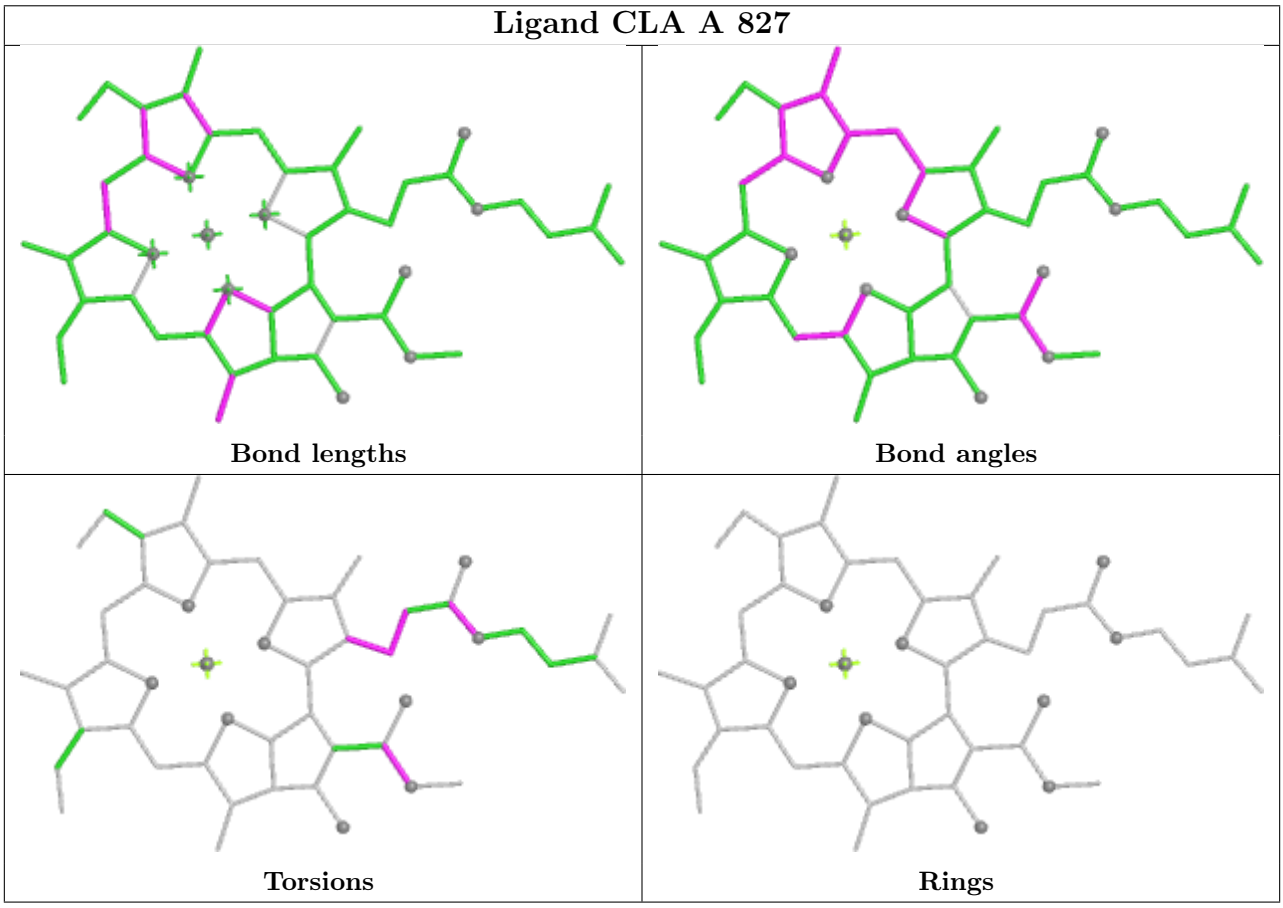


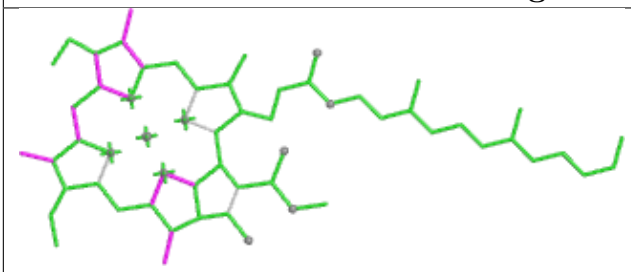
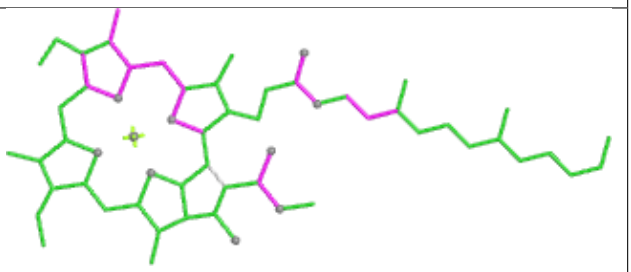
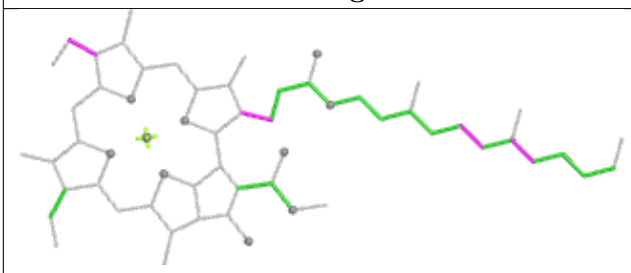
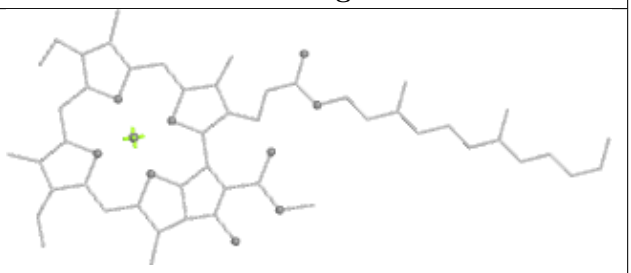
Rings

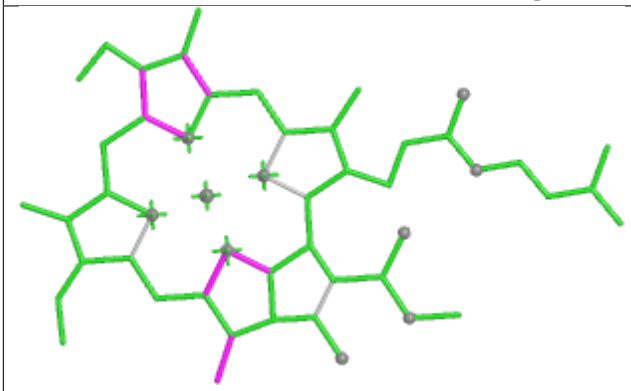
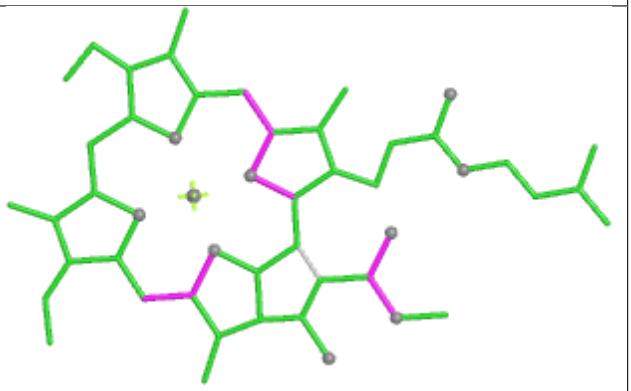
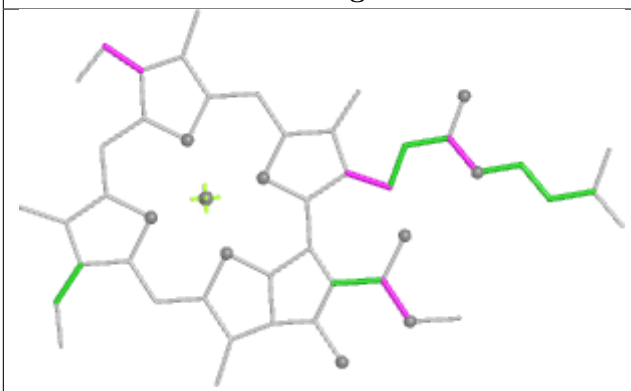
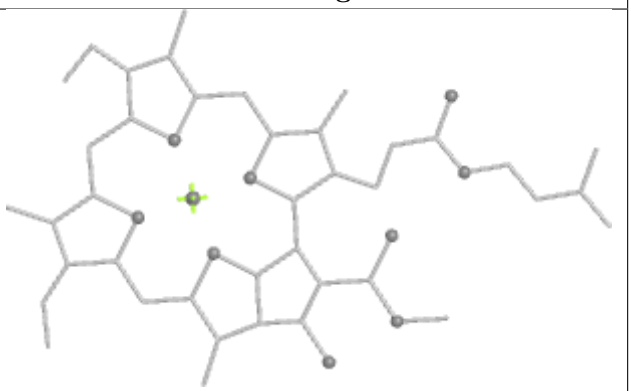
Ligand LMU A 853



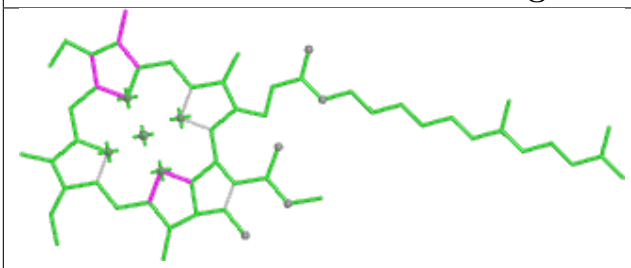
Ligand CLA A 827



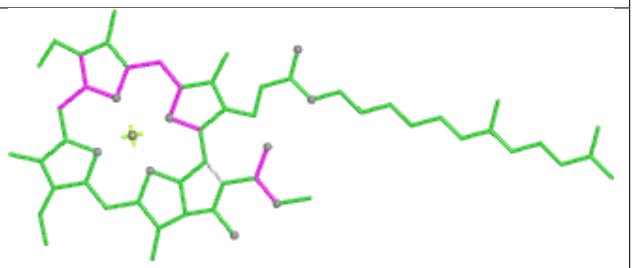
Ligand CLA 5 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 8 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

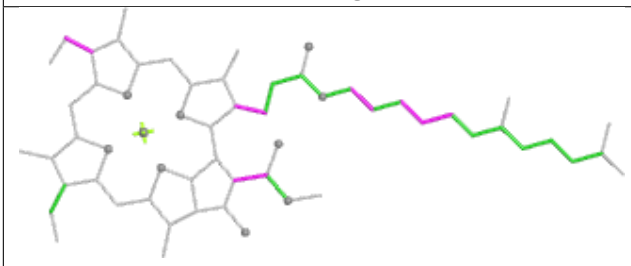
Ligand CLA 7 309



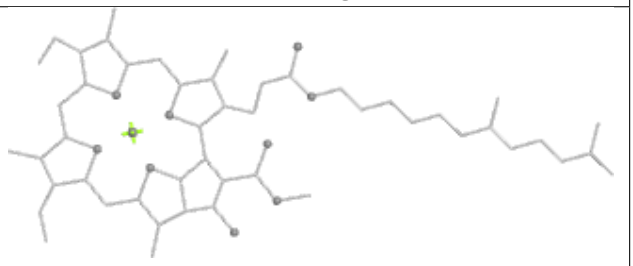
Bond lengths



Bond angles



Torsions

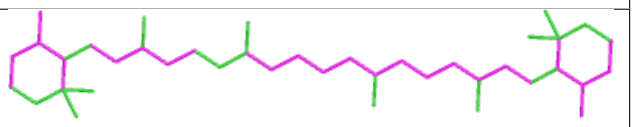


Rings

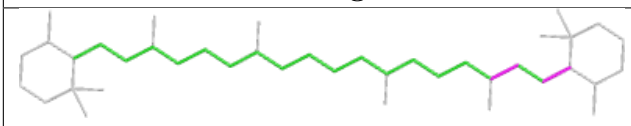
Ligand BCR I 201



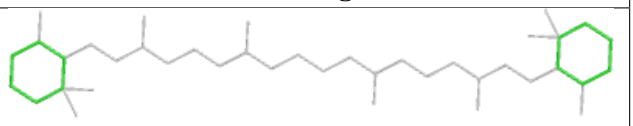
Bond lengths



Bond angles

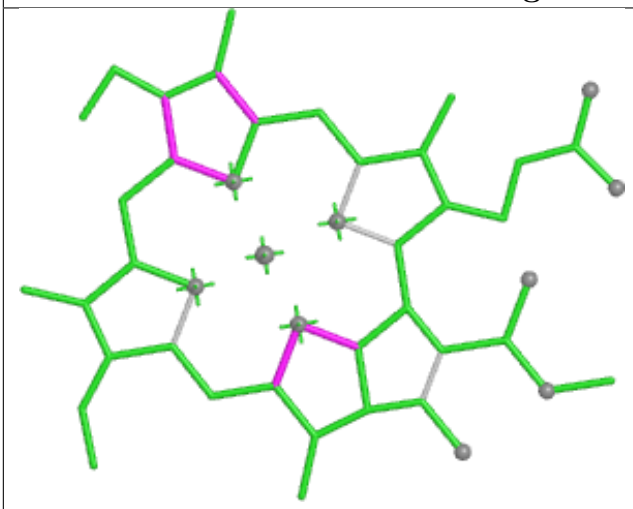


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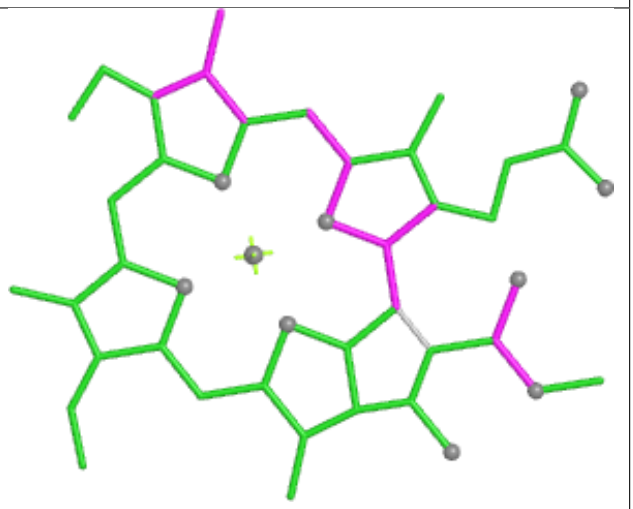


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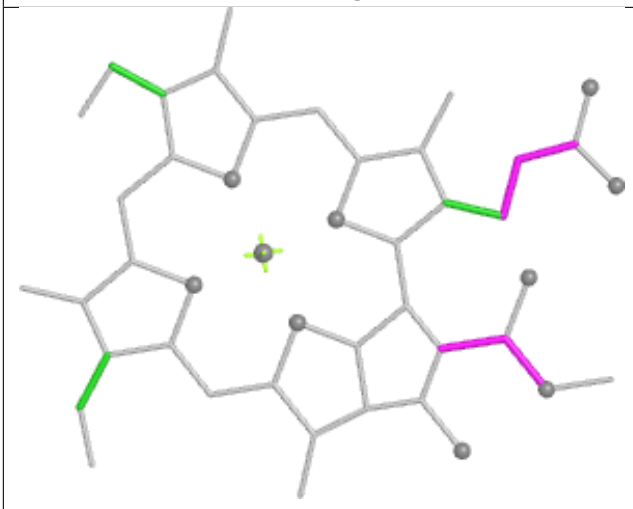
Ligand CLA G 203



Bond lengths



Bond angles

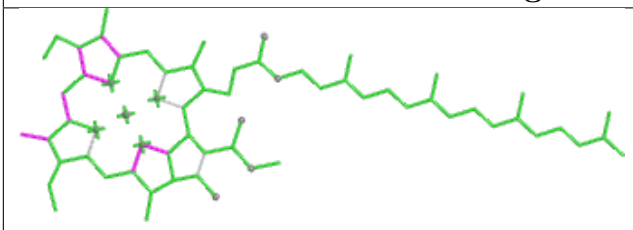


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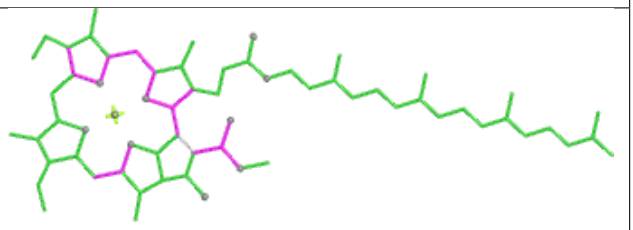


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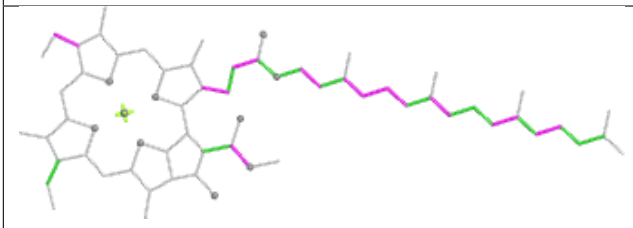
Ligand CLA B 806



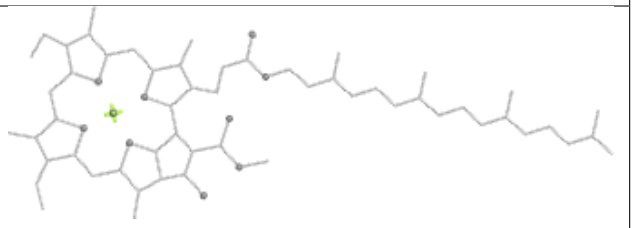
Bond lengths



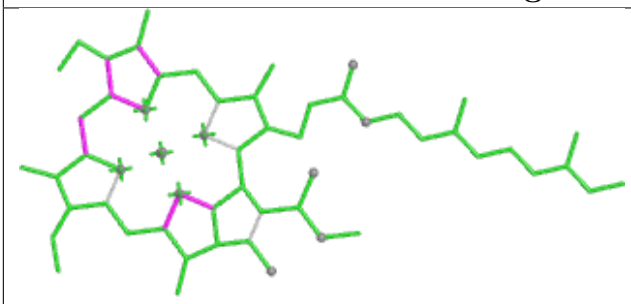
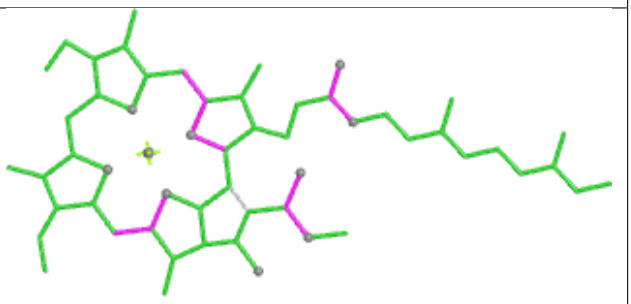
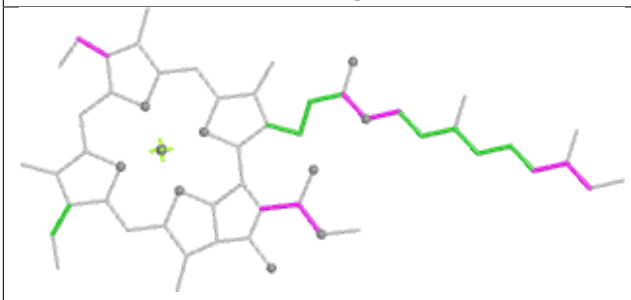
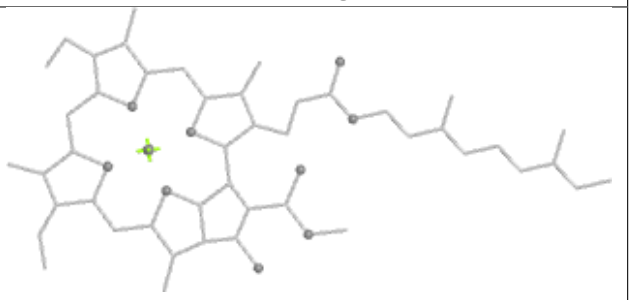
Bond angles

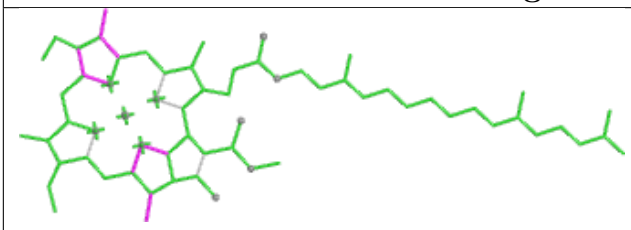
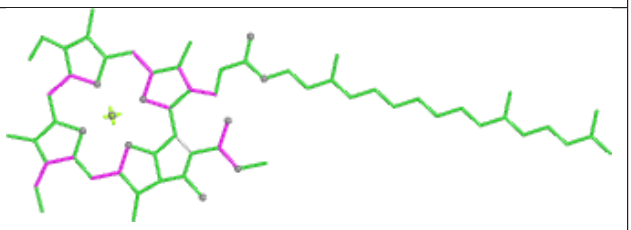
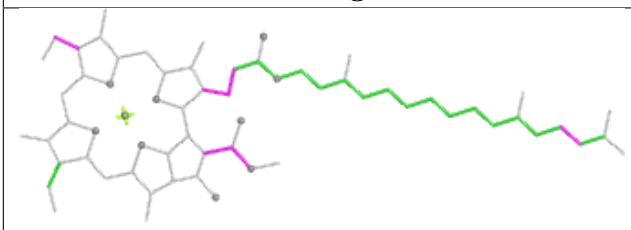
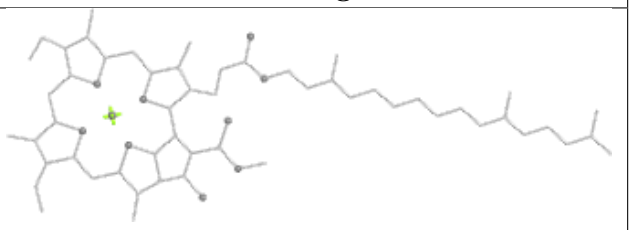


Torsions

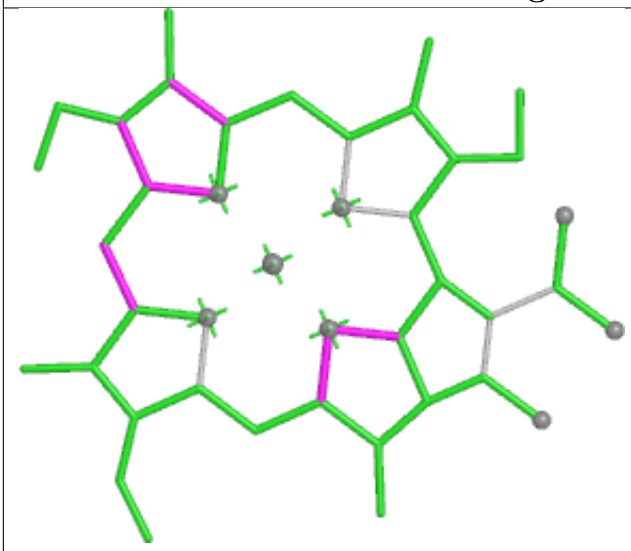


Rings

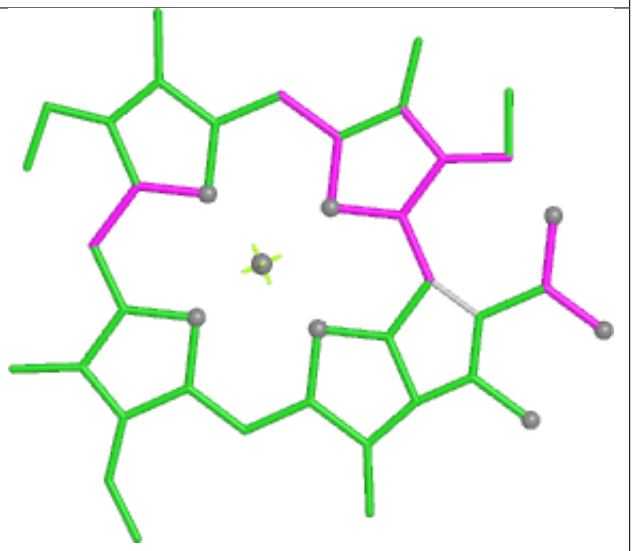
Ligand CLA B 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

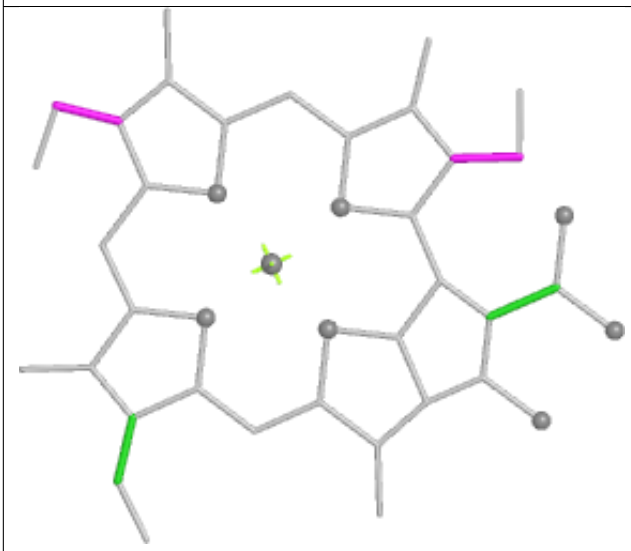
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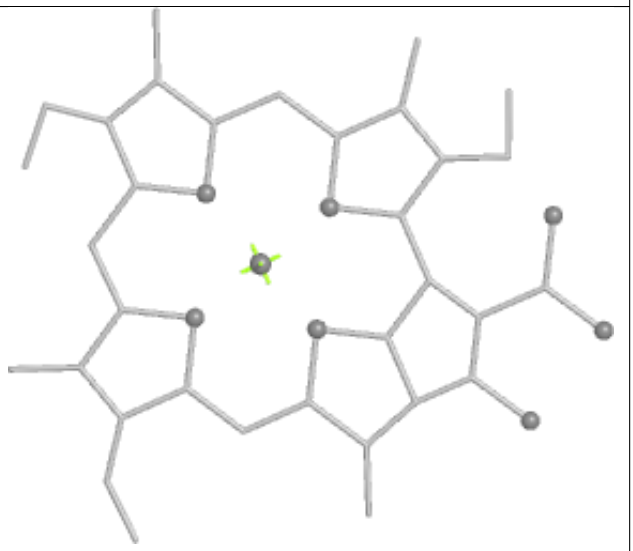
Bond lengths



Bond angles

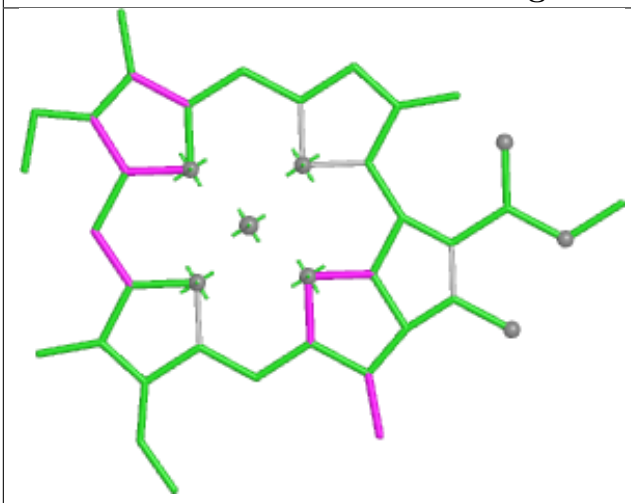


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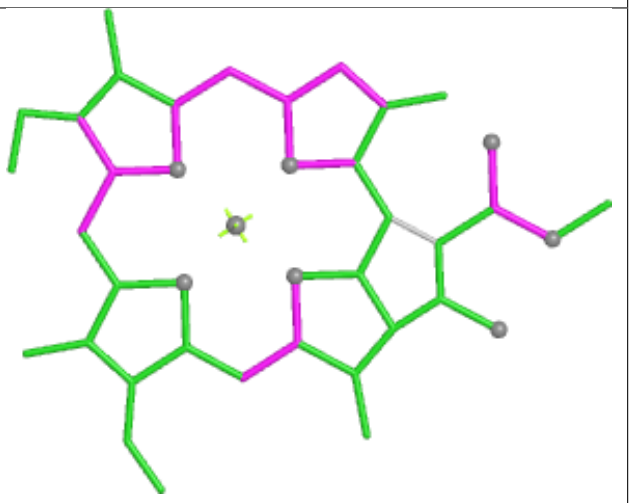


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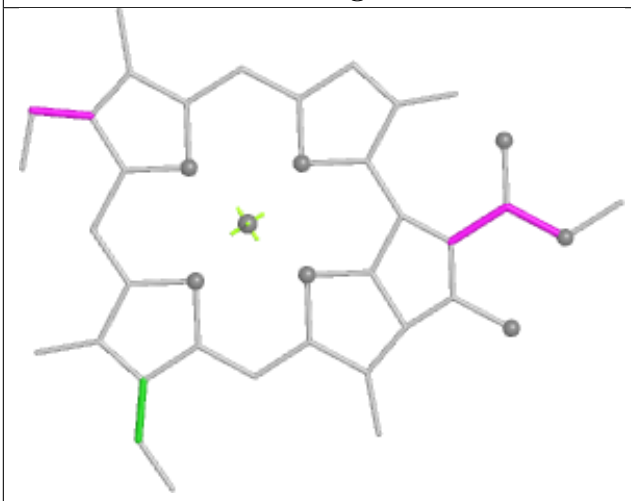
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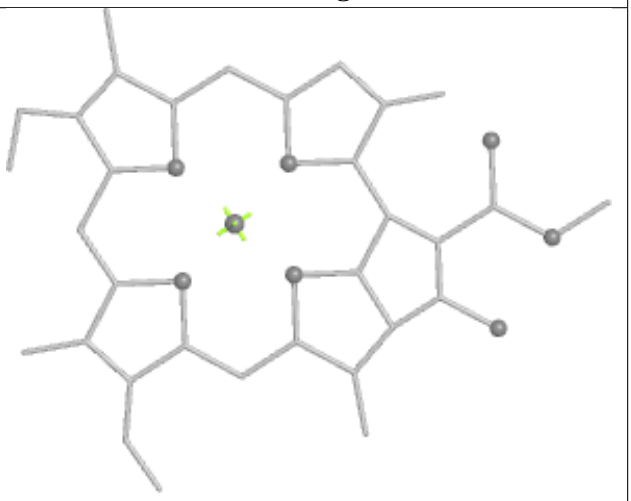
Bond lengths



Bond angles

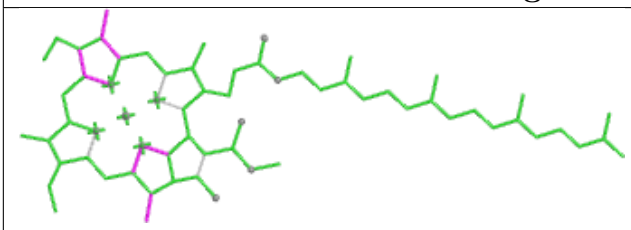


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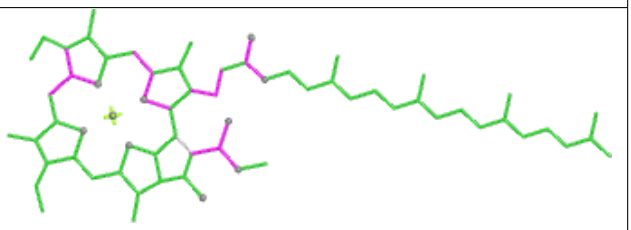


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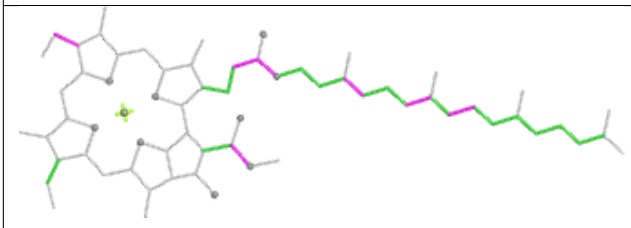
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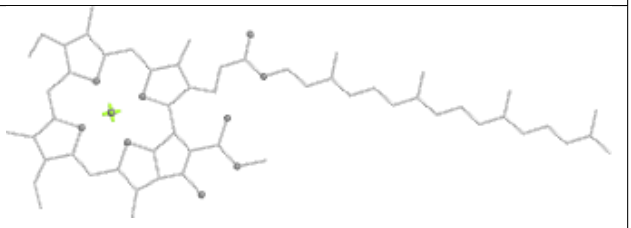
Bond lengths



Bond angles

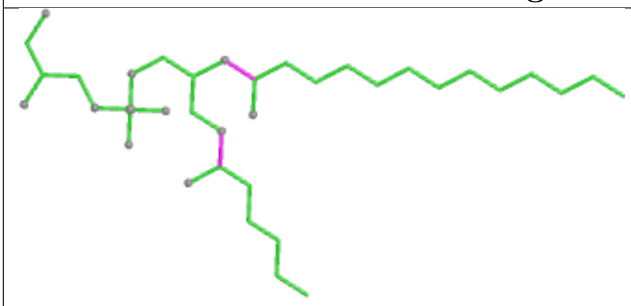


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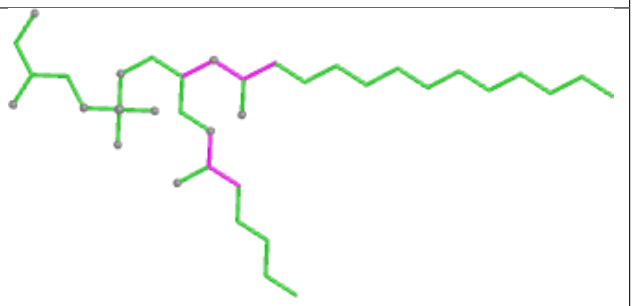


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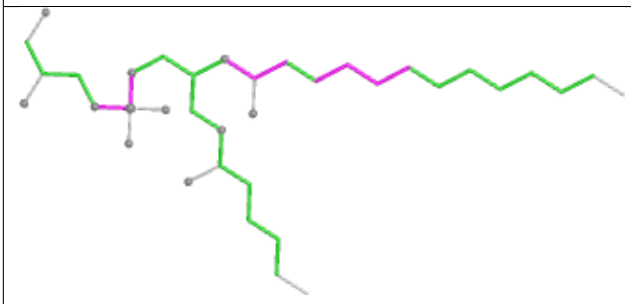
Ligand LHG 5 301



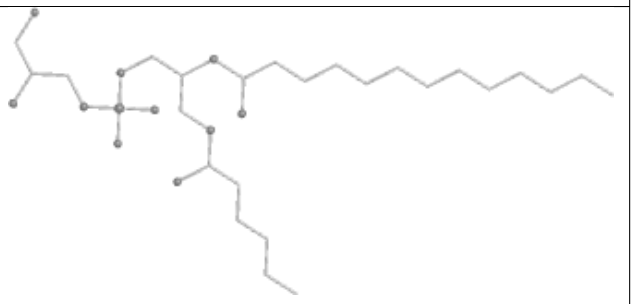
Bond lengths



Bond angles

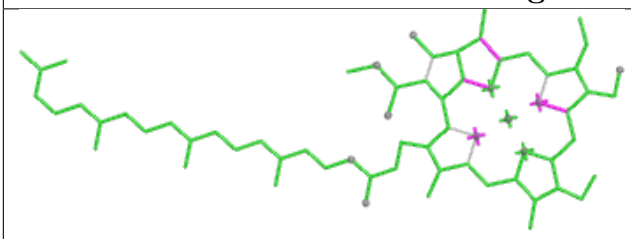


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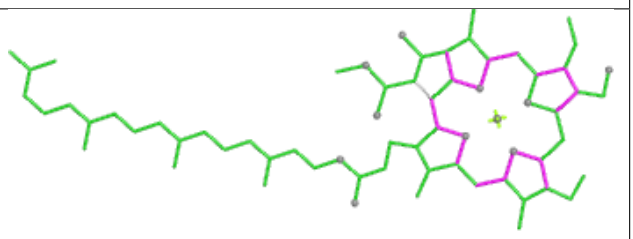


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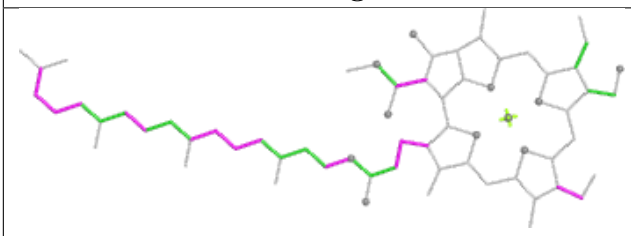
Ligand CHL 3 422



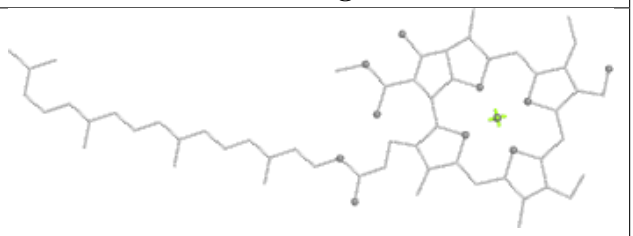
Bond lengths



Bond angles

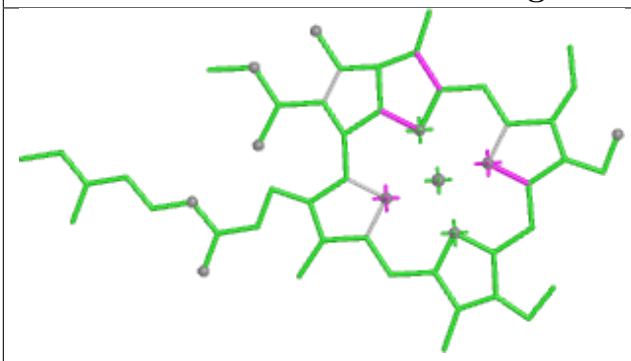


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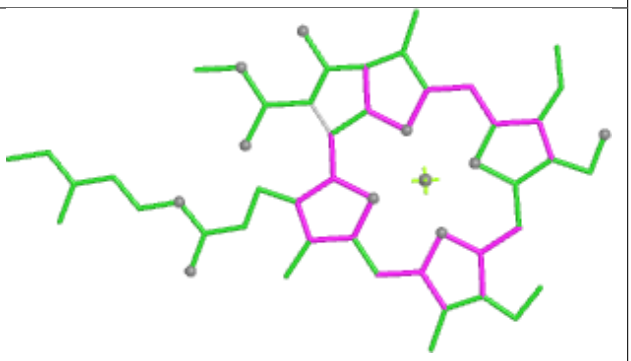


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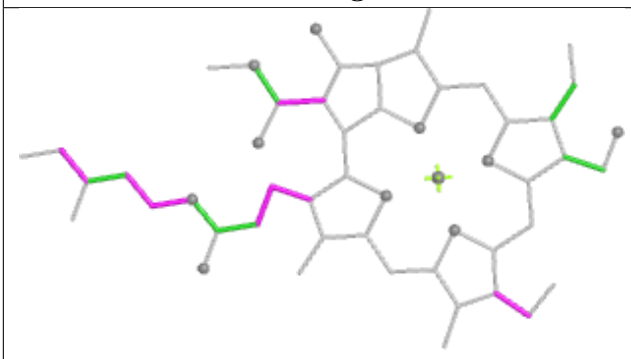
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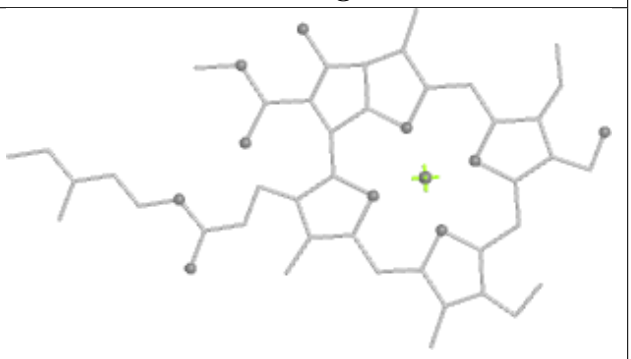
Bond lengths



Bond angles

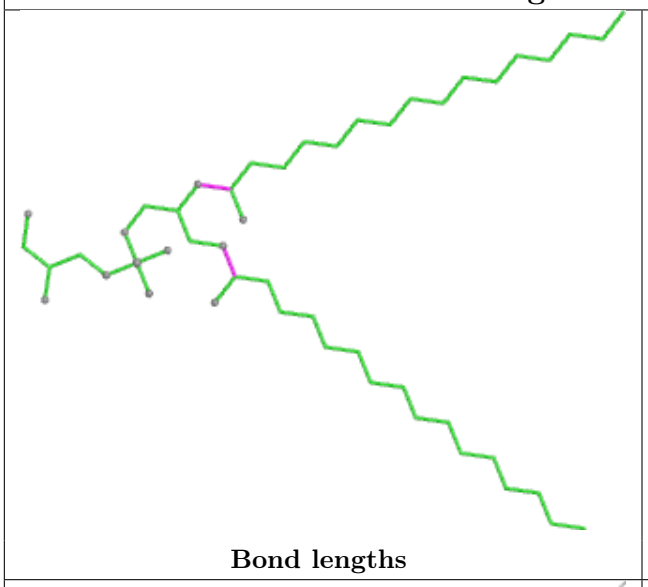


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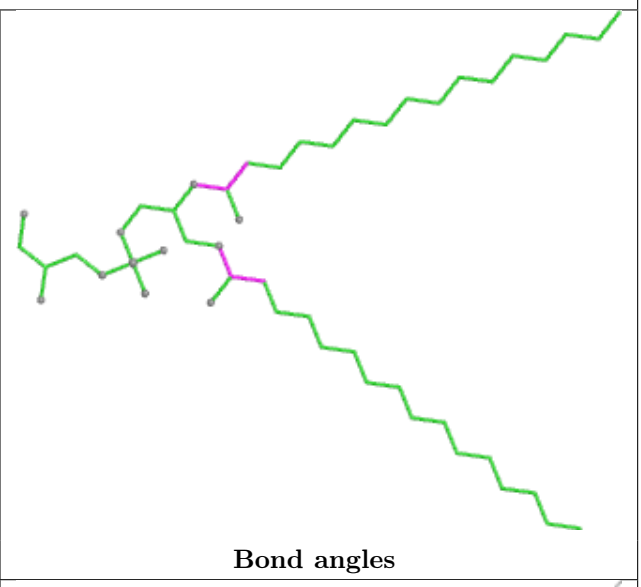


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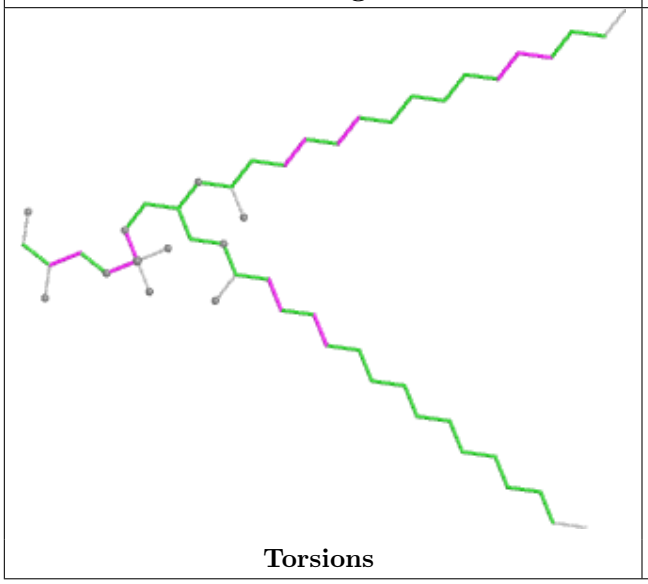
Ligand LHG 7 318



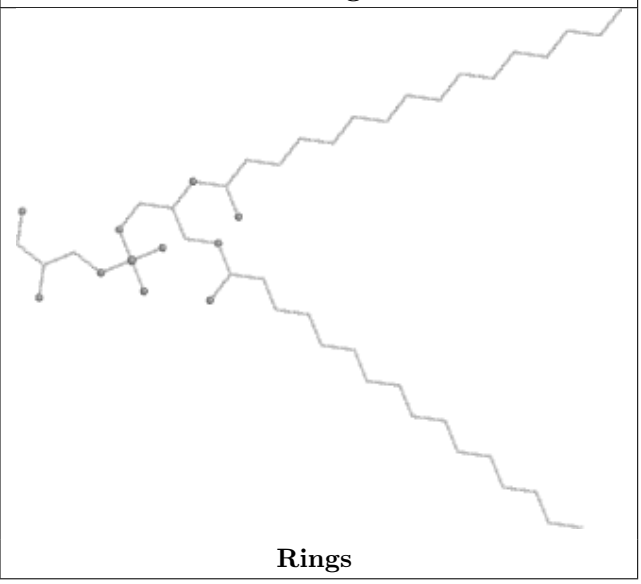
Bond lengths



Bond angles



Torsions

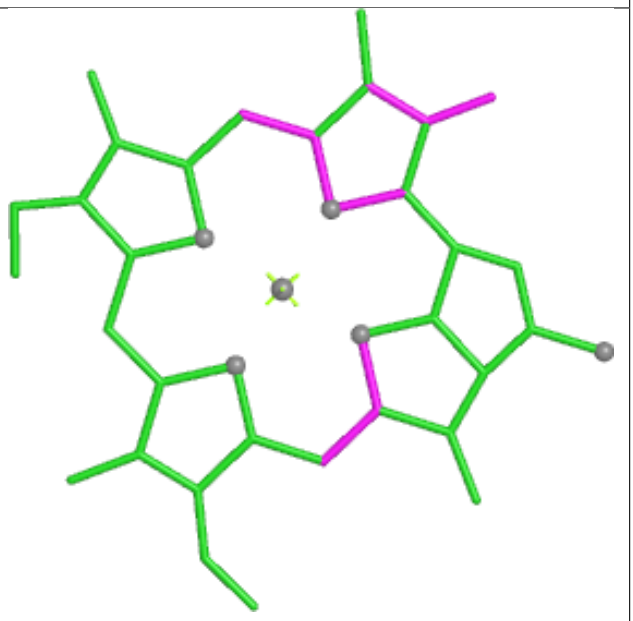


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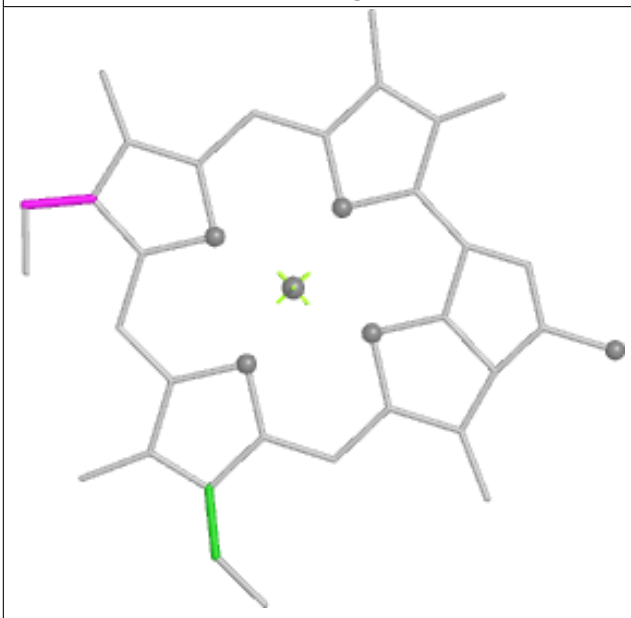
Ligand CLA 2 606



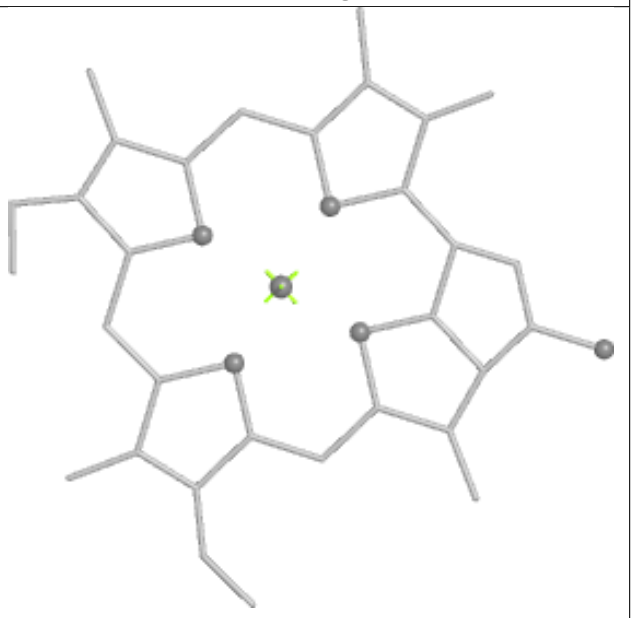
Bond lengths



Bond angles

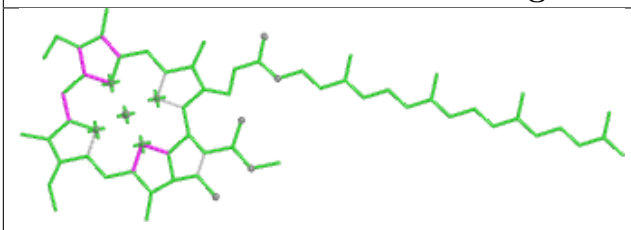


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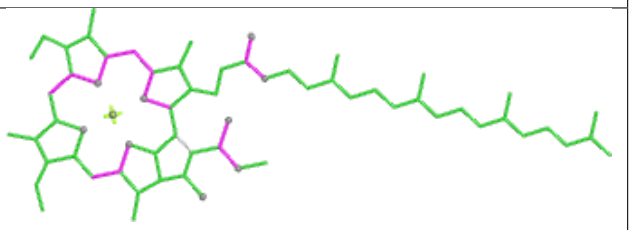


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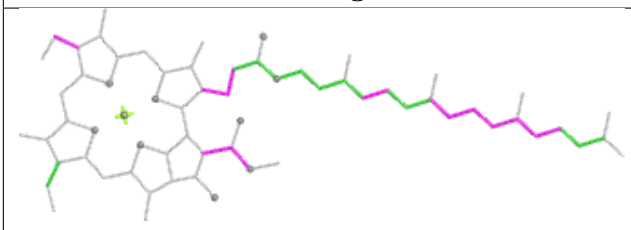
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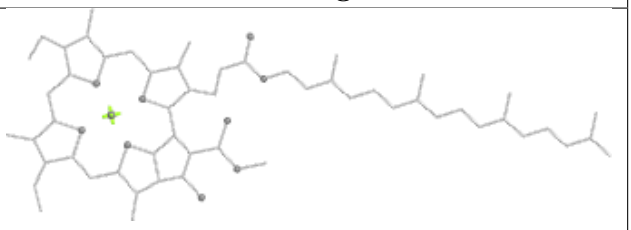
Bond lengths



Bond angles

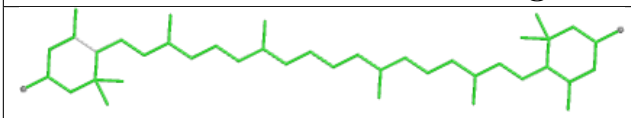


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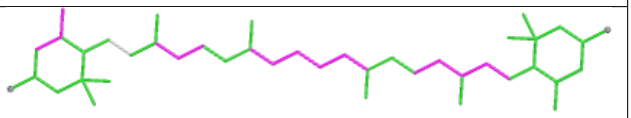


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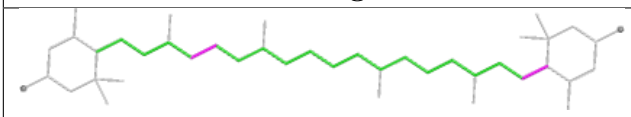
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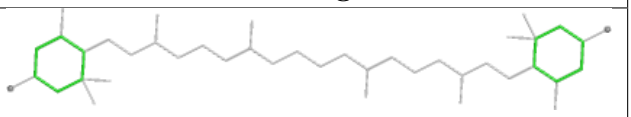
Bond lengths



Bond angles

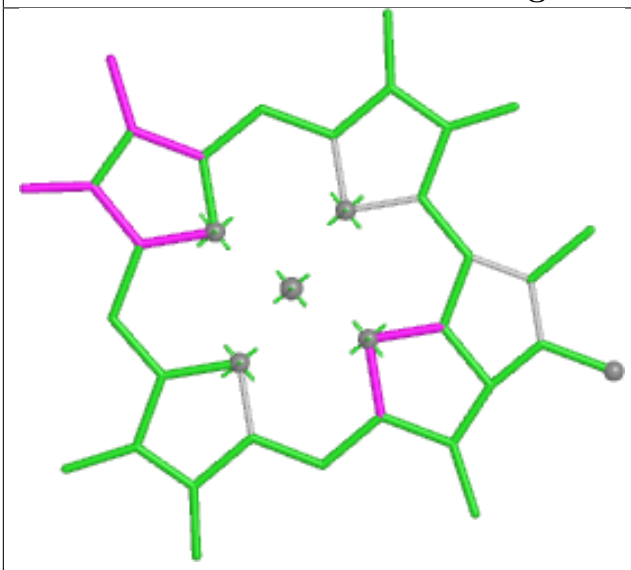


Torsions

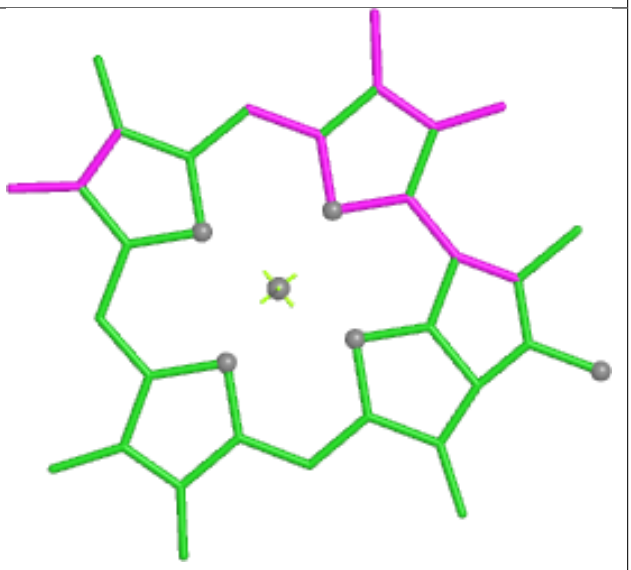


Rings

Ligand CLA 7 314



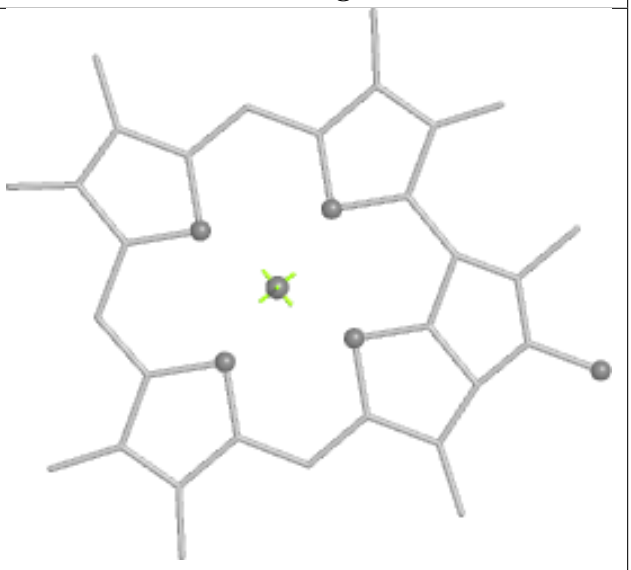
Bond lengths



Bond angles

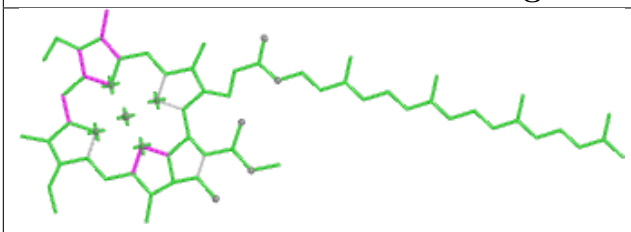


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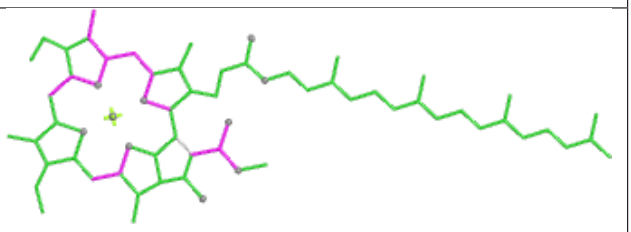


Rings

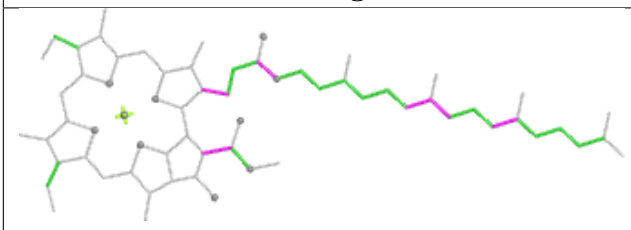
Ligand CLA A 818



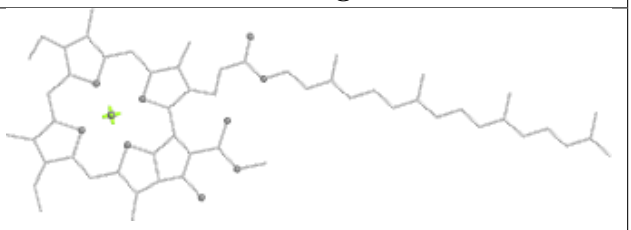
Bond lengths



Bond angles

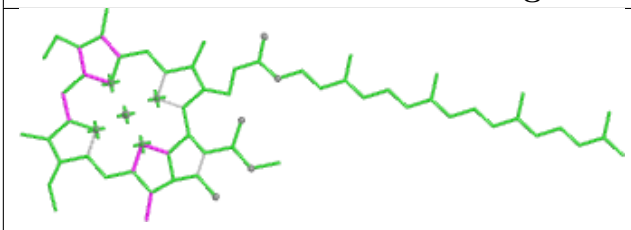


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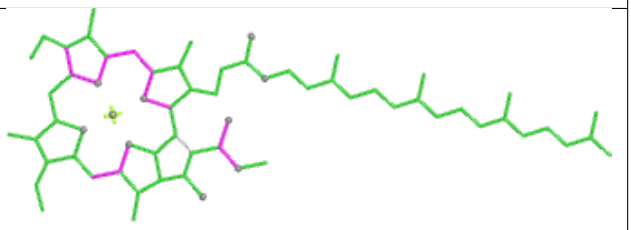


Rings

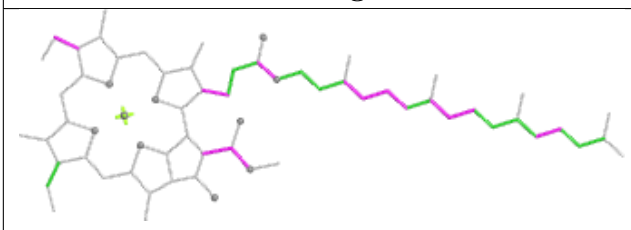
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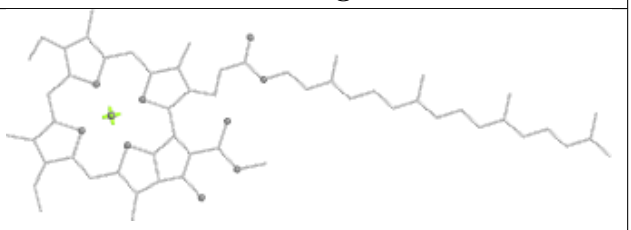
Bond lengths



Bond angles

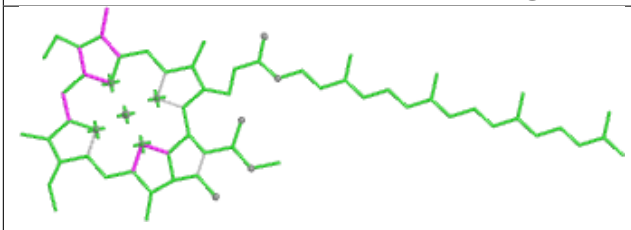


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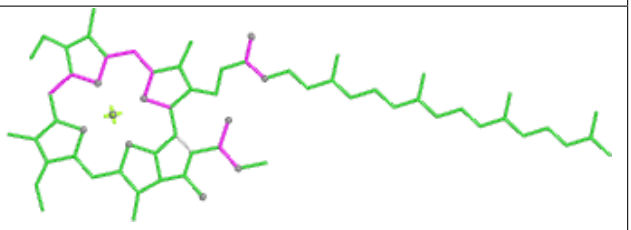


Rings

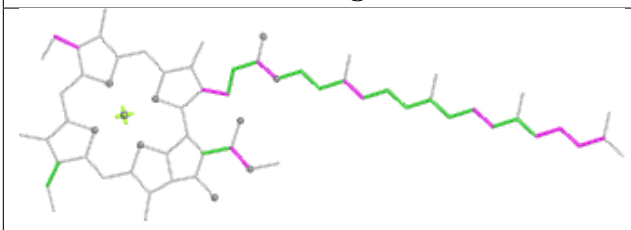
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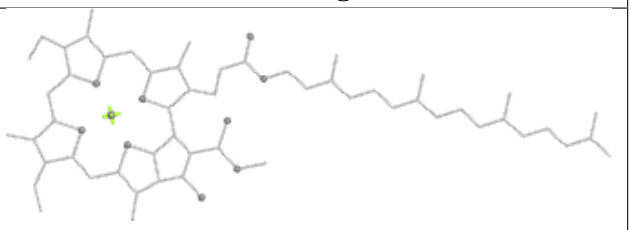
Bond lengths



Bond angles

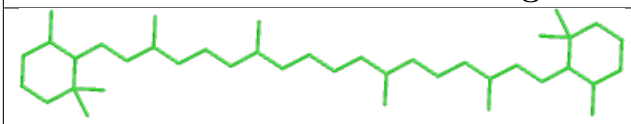


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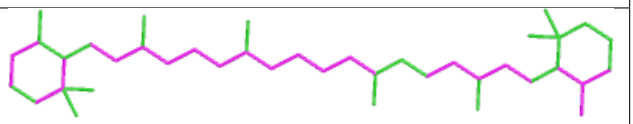


Rings

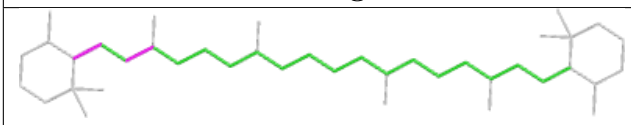
Ligand BCR A 849



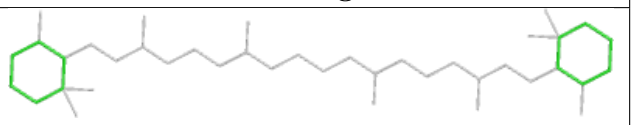
Bond lengths



Bond angles

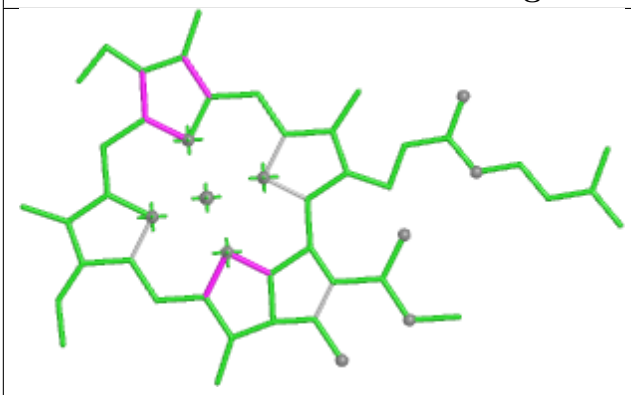


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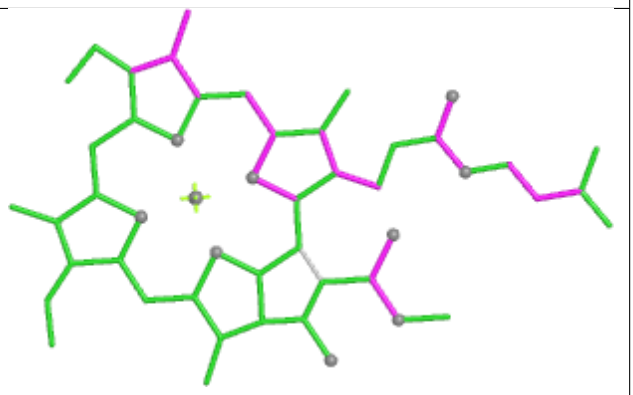


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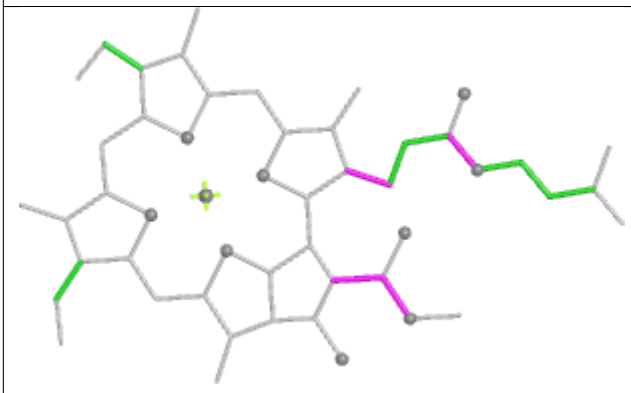
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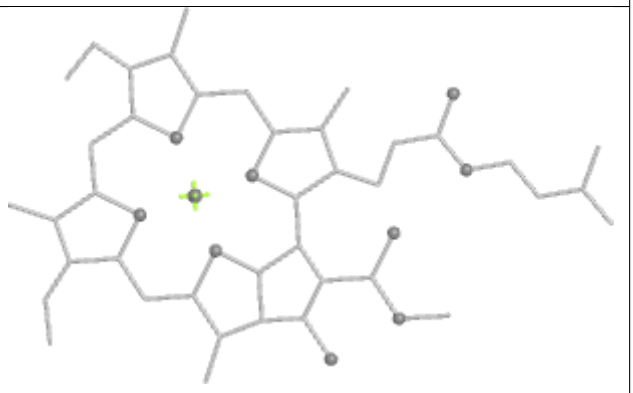
Bond lengths



Bond angles

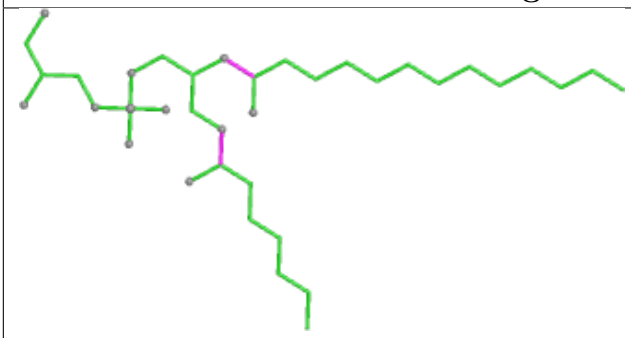


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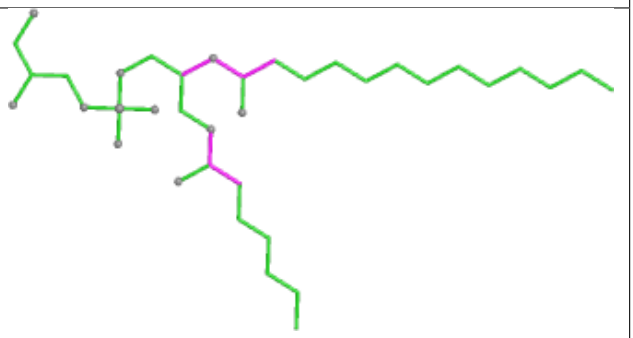


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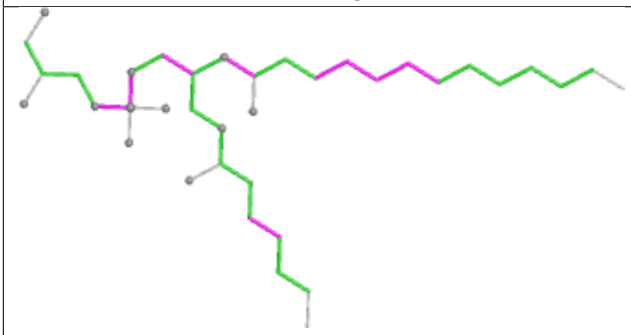
Ligand LHG B 801



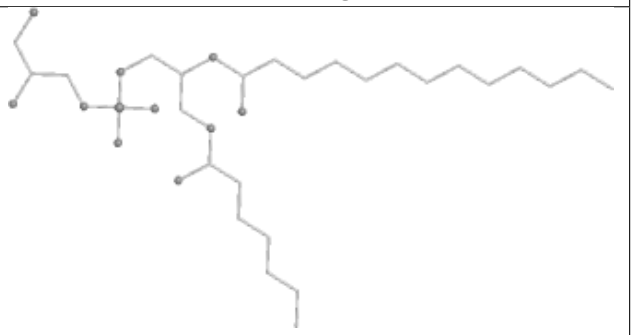
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Bond angles

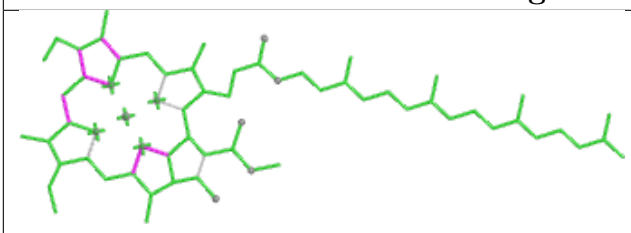


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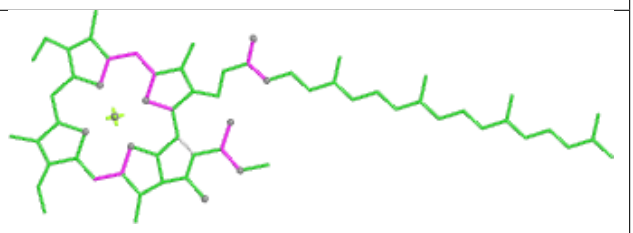


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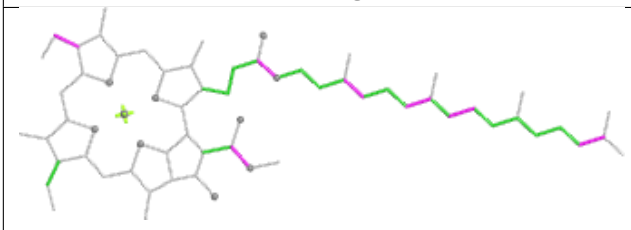
Ligand CLA 3 403



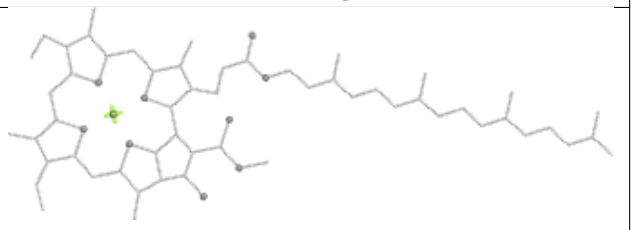
Bond lengths



Bond angles

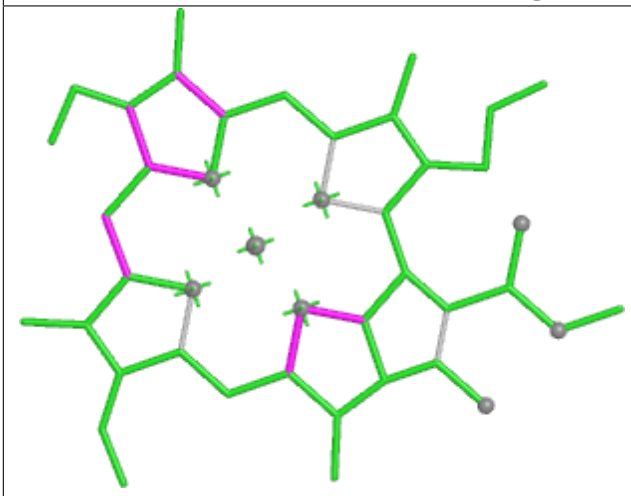


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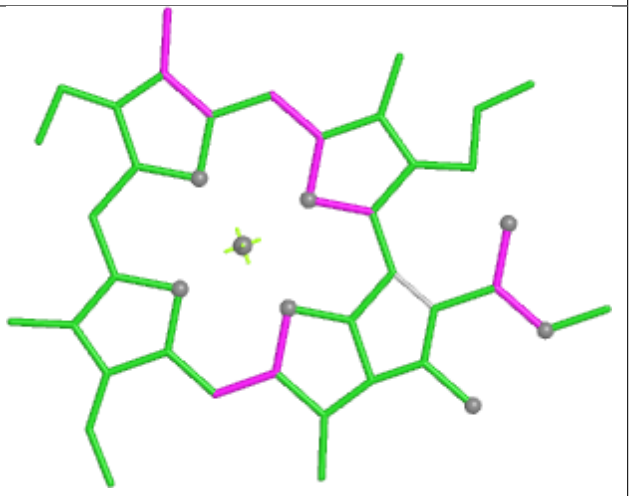


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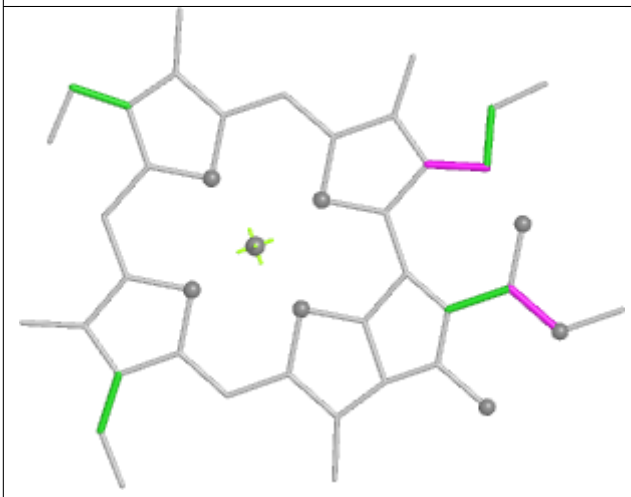
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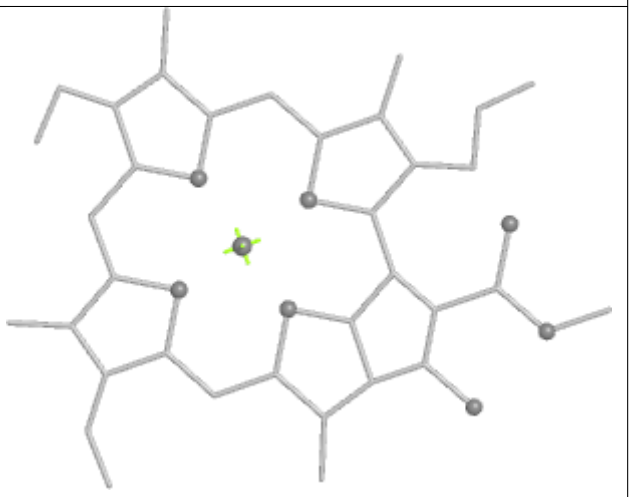
Bond lengths



Bond angles

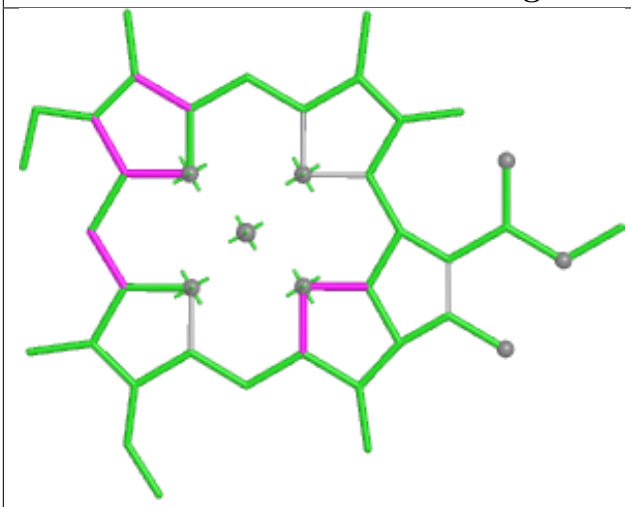


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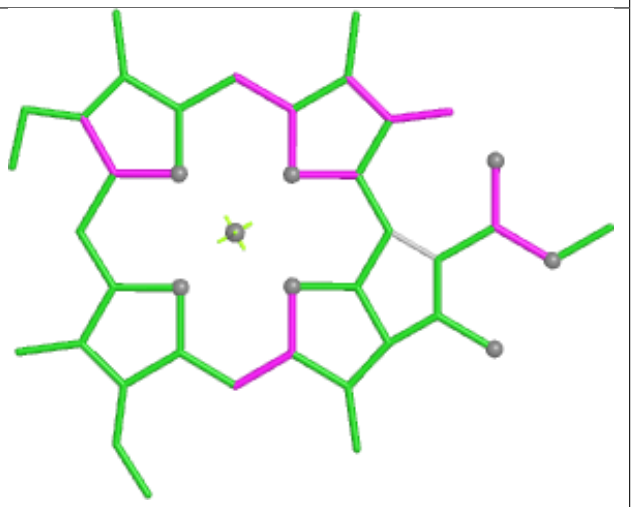


Rings

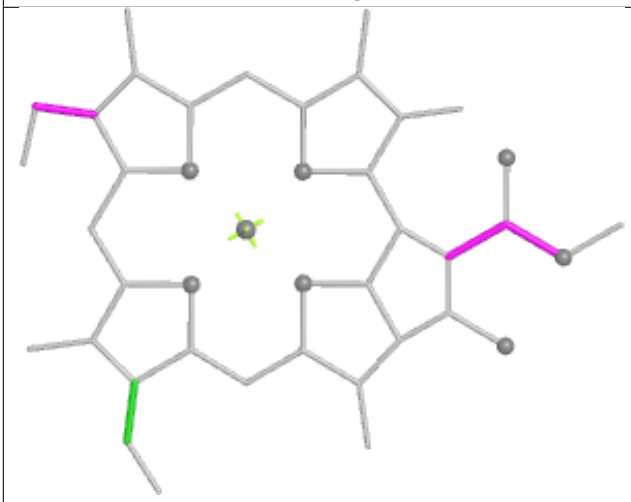
Ligand CLA K 206



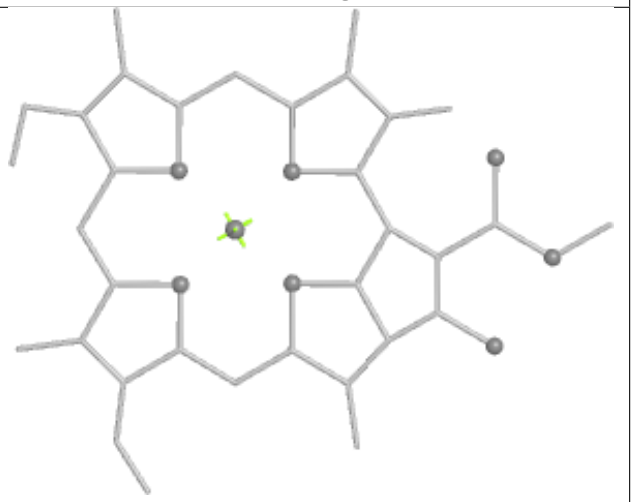
Bond lengths



Bond angles

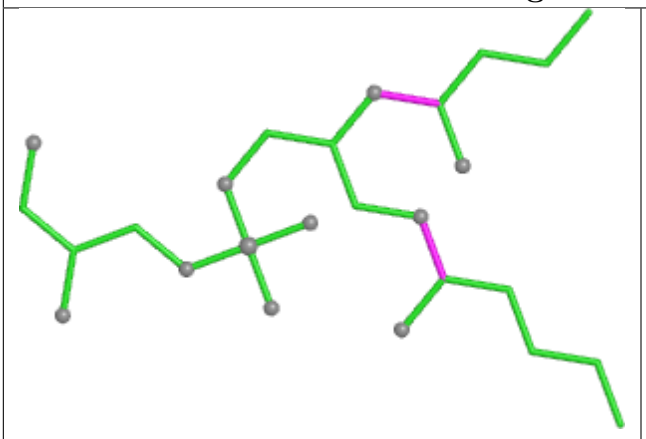


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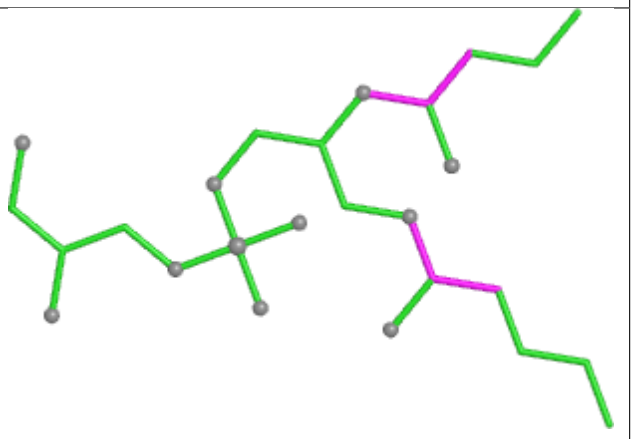


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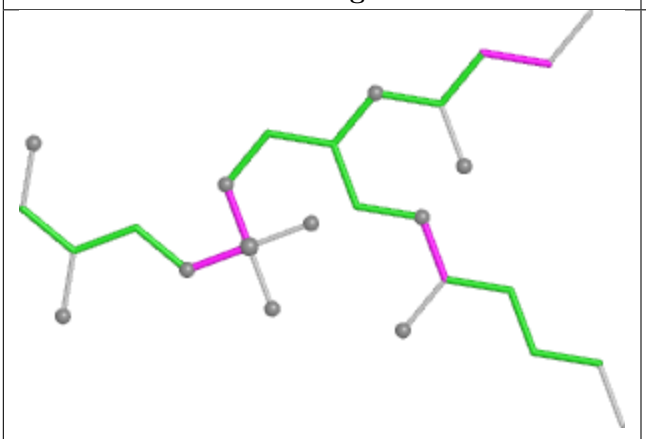
Ligand LHG 1 318



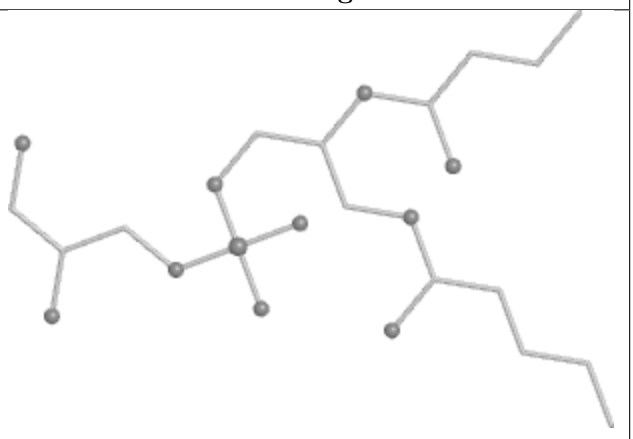
Bond lengths



Bond angles

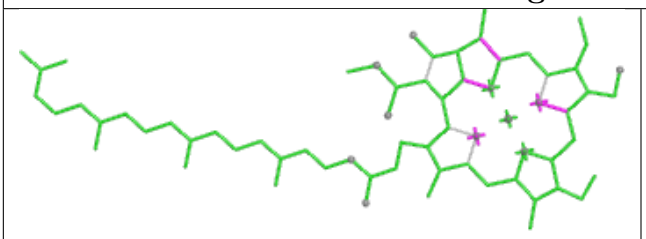


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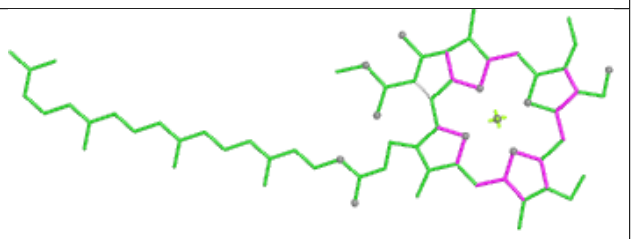


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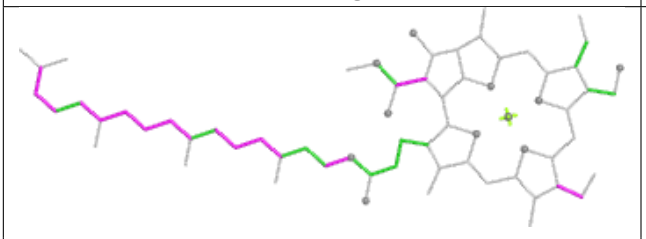
Ligand CHL 8 606



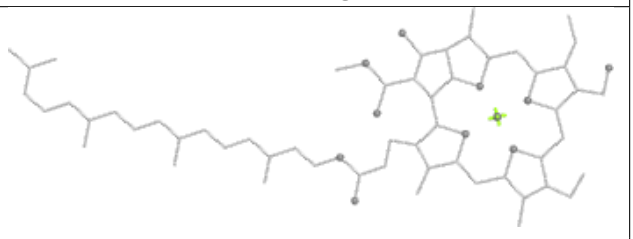
Bond lengths



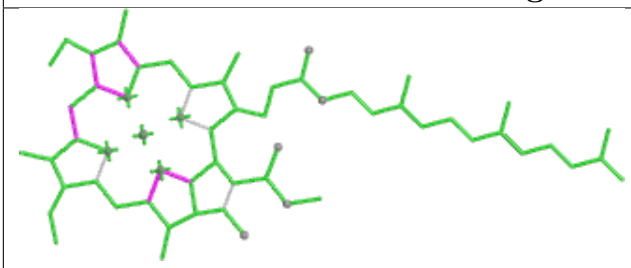
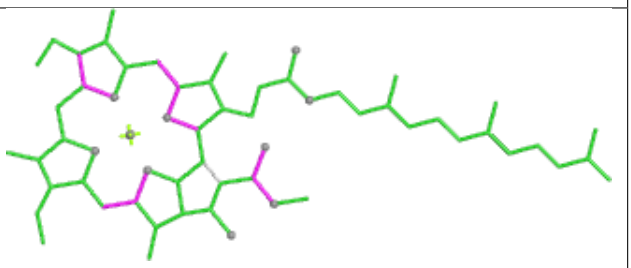
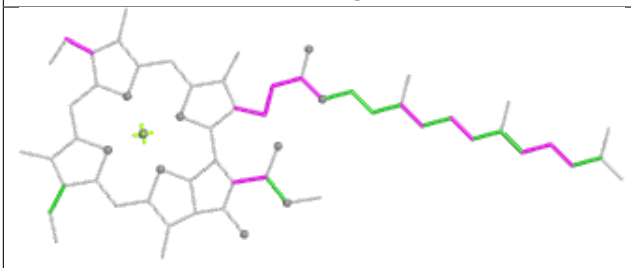
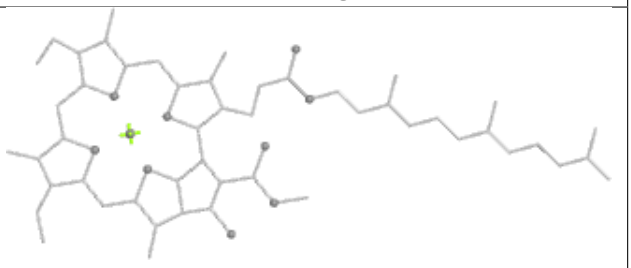
Bond angles

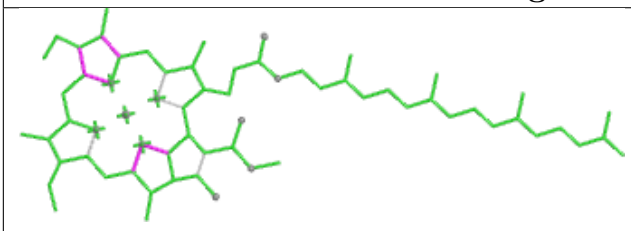
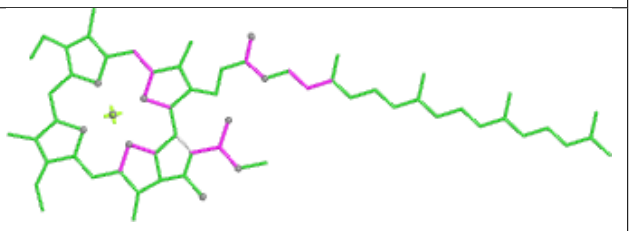
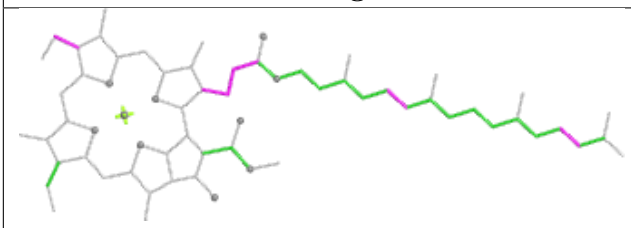
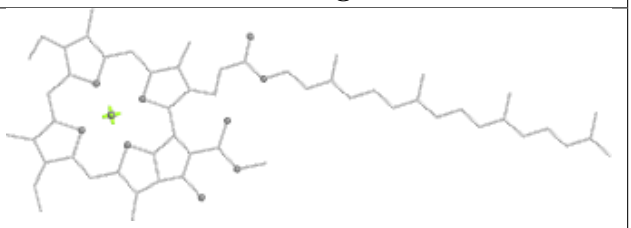


Torsions

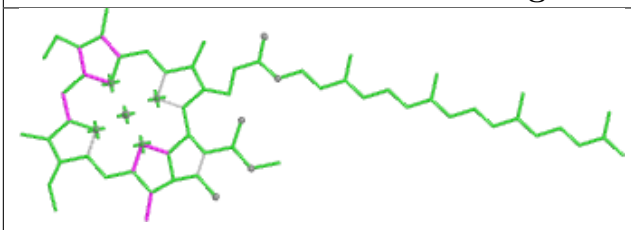


Rings

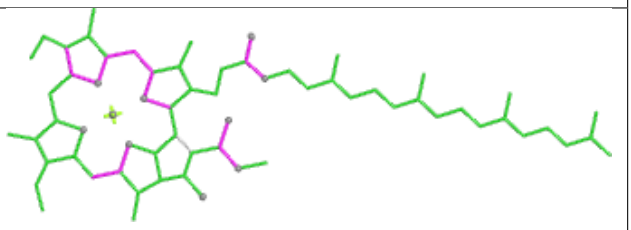
Ligand CLA L 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

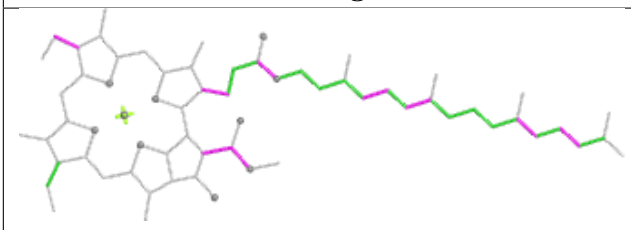
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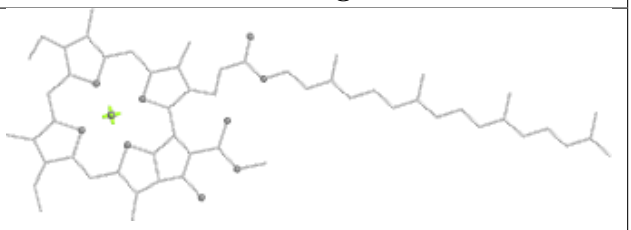
Bond lengths



Bond angles

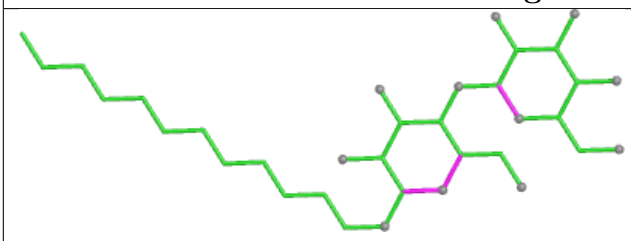


Torsions

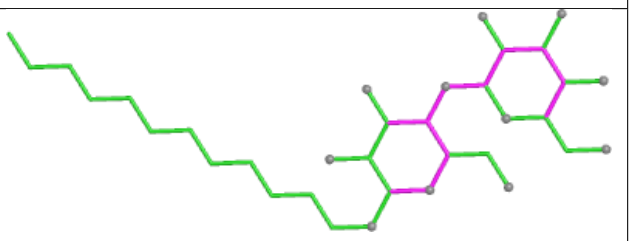


Rings

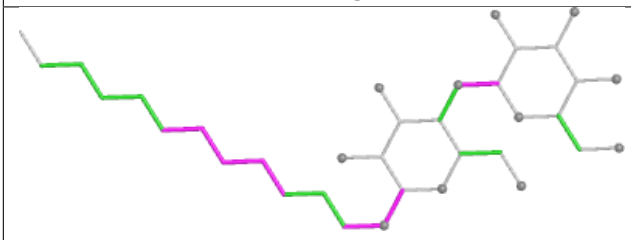
Ligand LMU 7 319



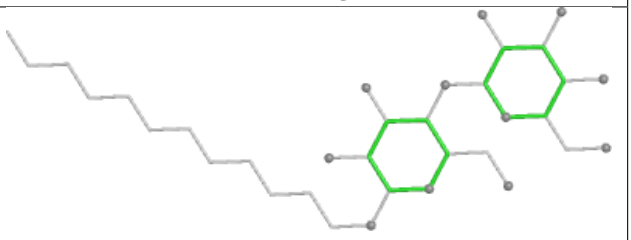
Bond lengths



Bond angles

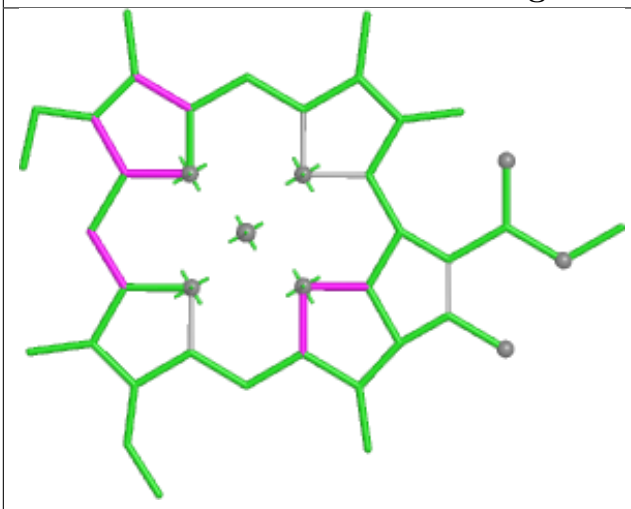


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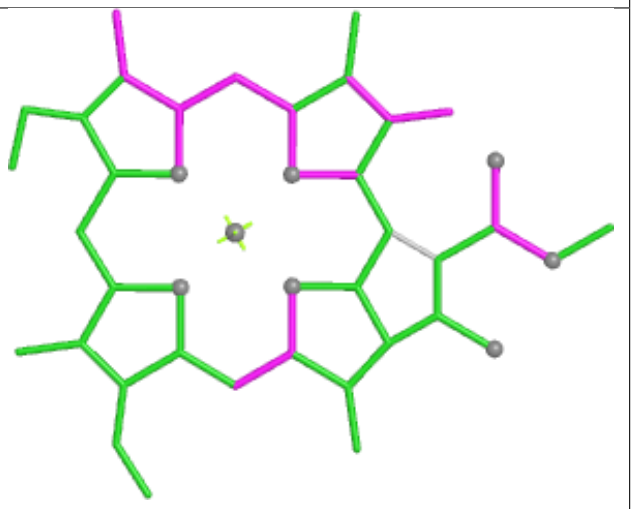


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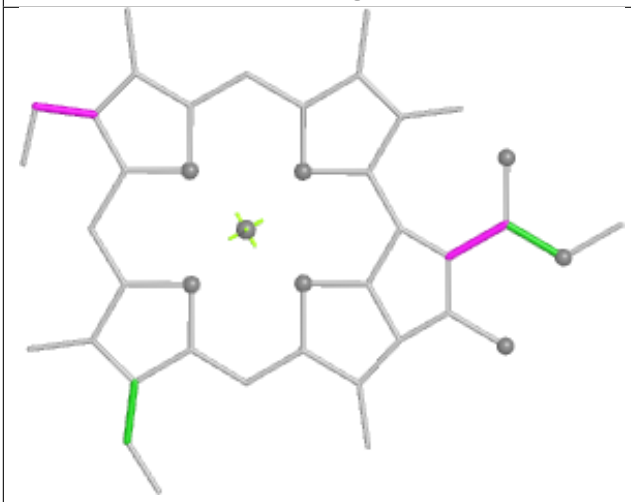
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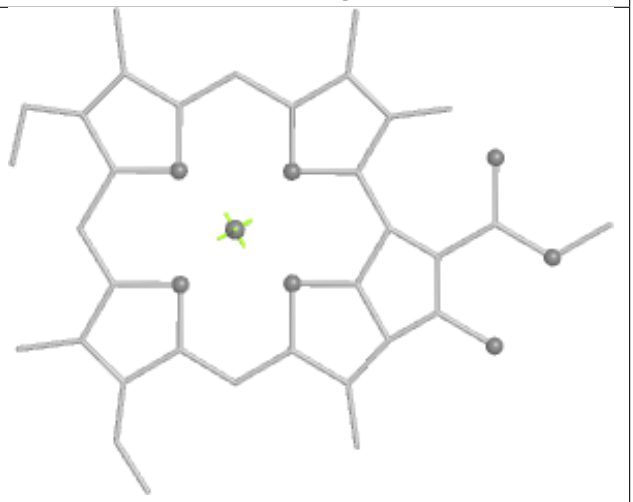
Bond lengths



Bond angles

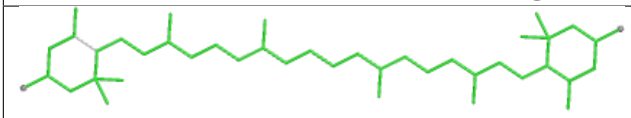


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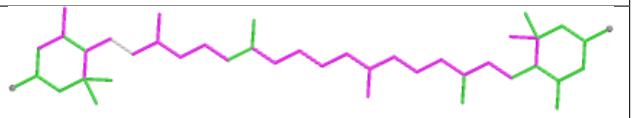


Rings

Ligand LUT 5 320



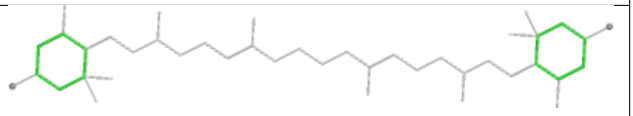
Bond lengths



Bond angles

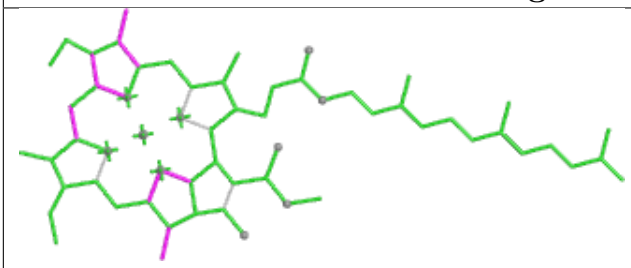


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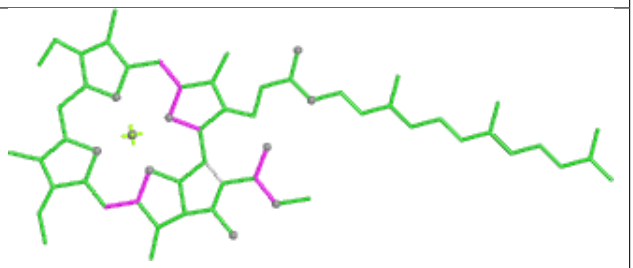


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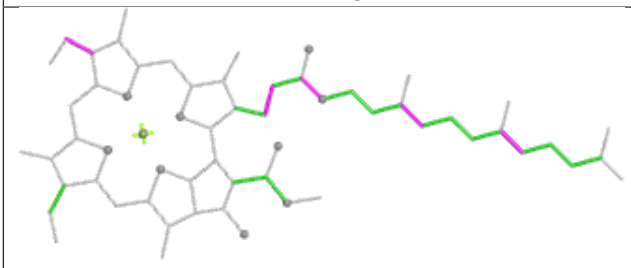
Ligand CLA 7 311



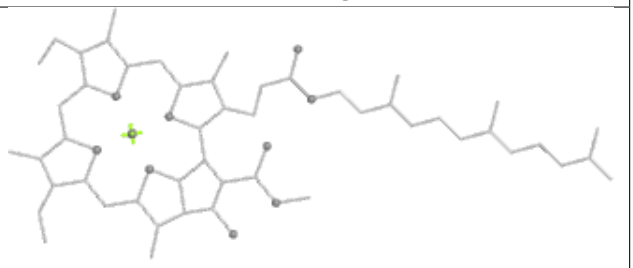
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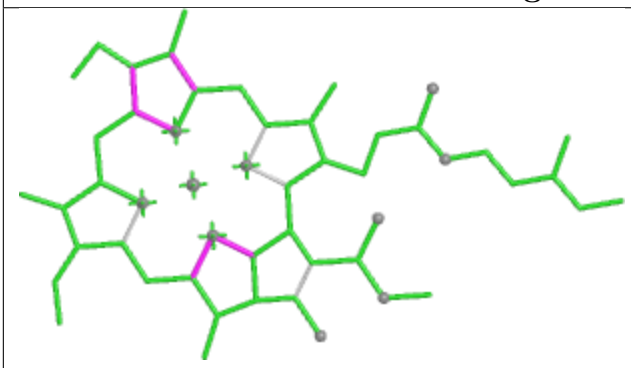


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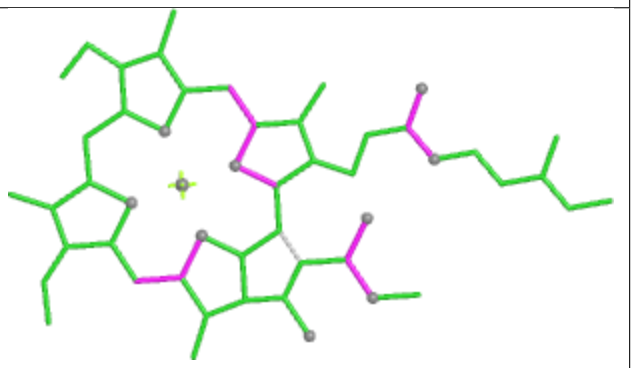


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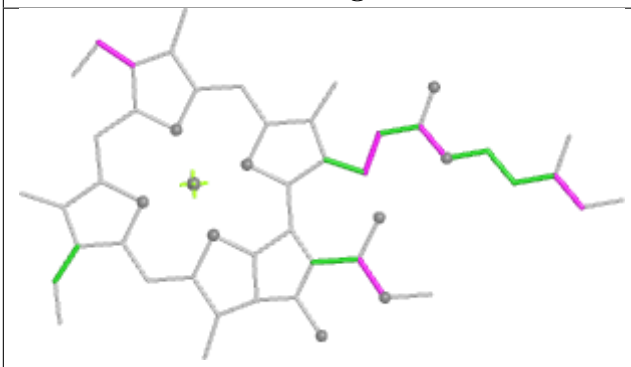
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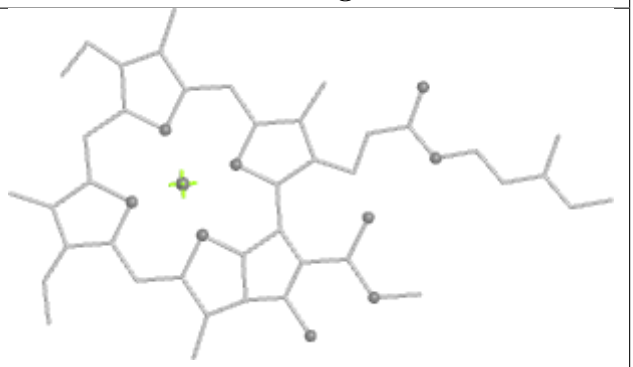
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Bond angles

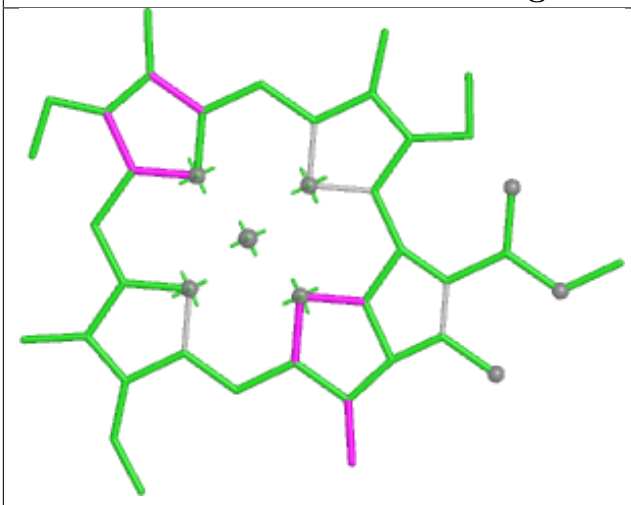


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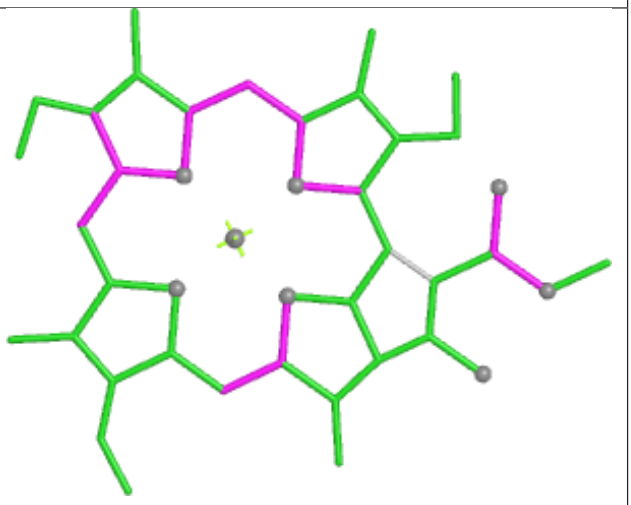


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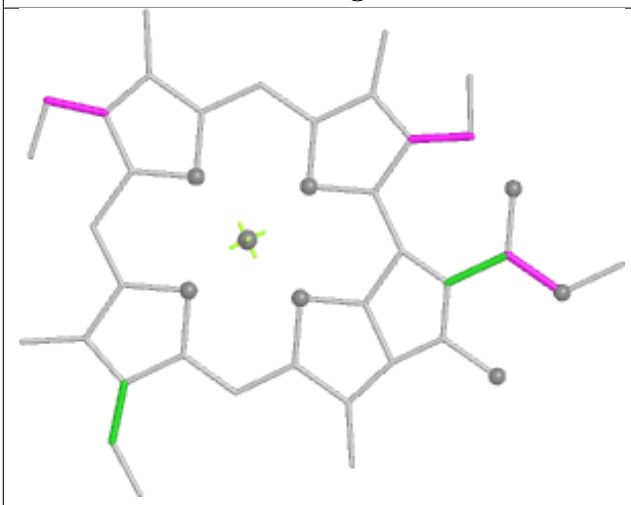
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Bond lengths



Bond angles

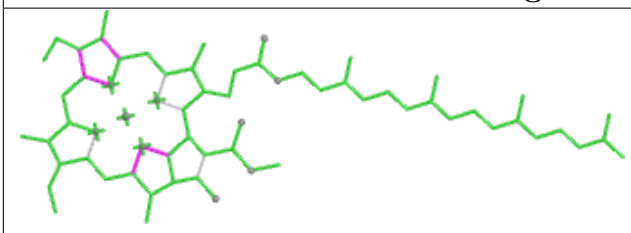


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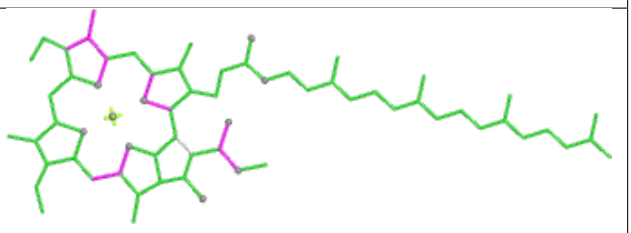


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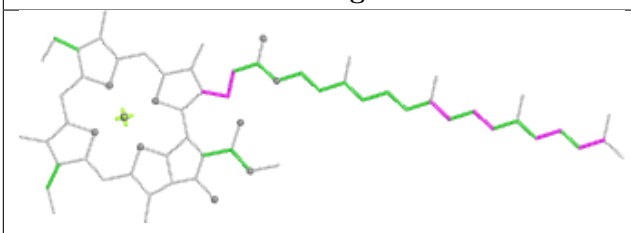
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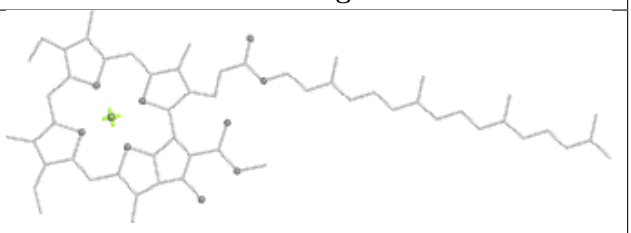
Bond lengths



Bond angles

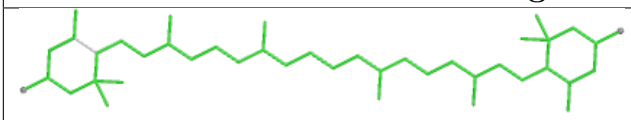


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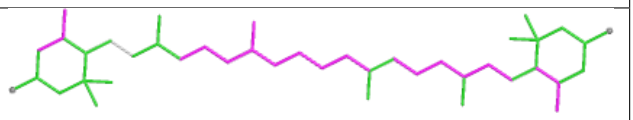


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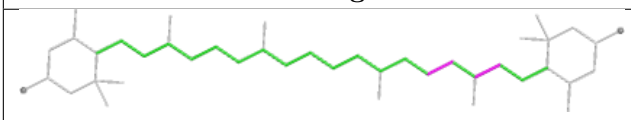
Ligand LUT 9 613



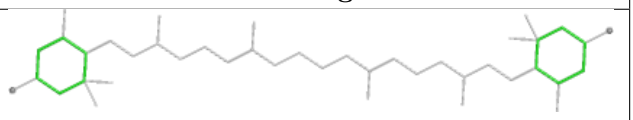
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Bond angles

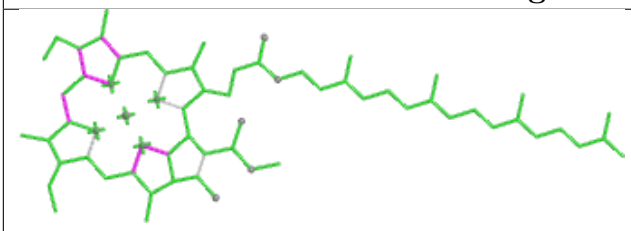


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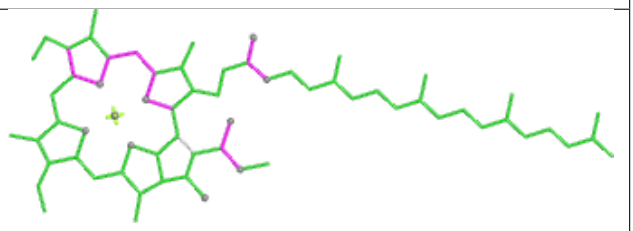


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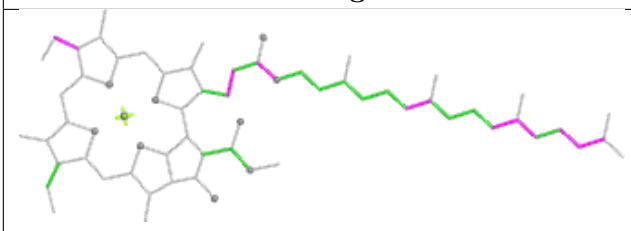
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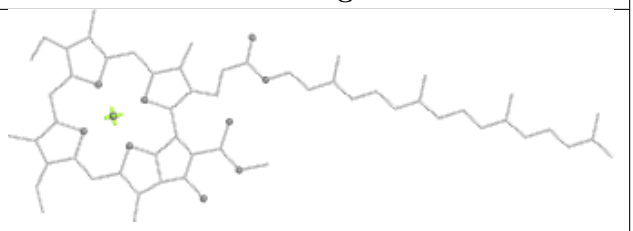
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Bond angles

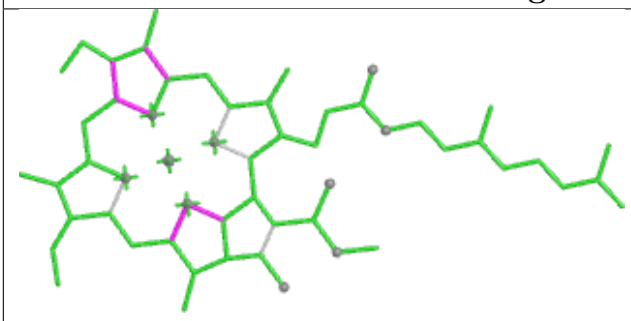


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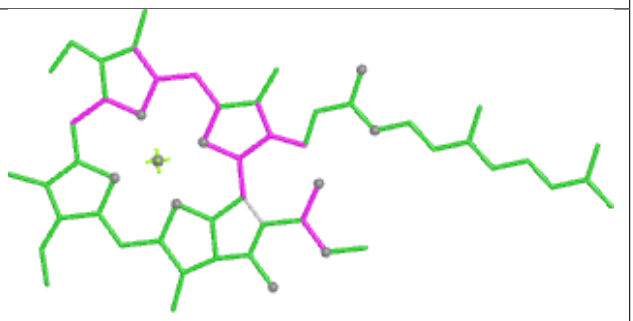


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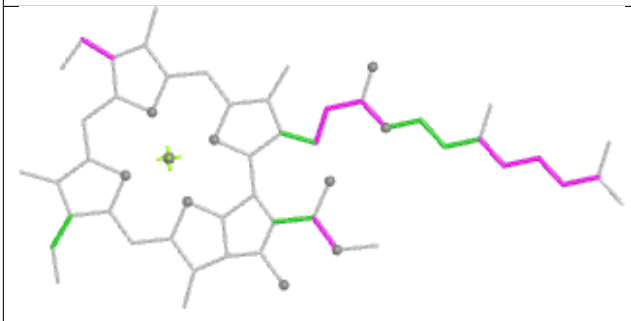
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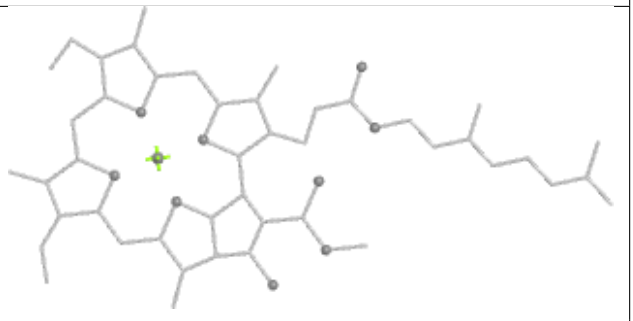
Bond lengths



Bond angles

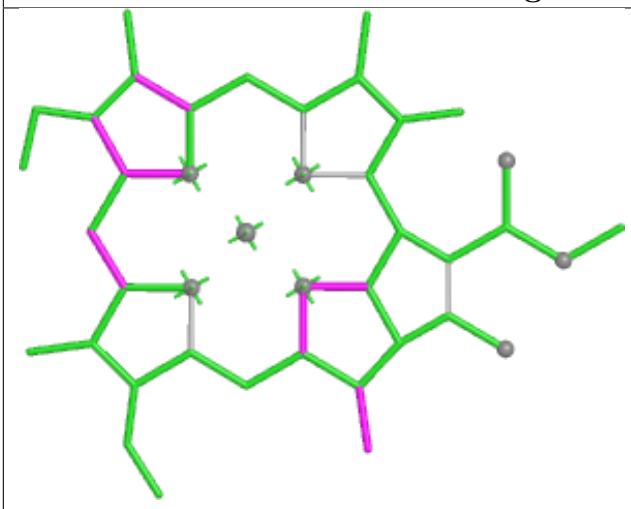


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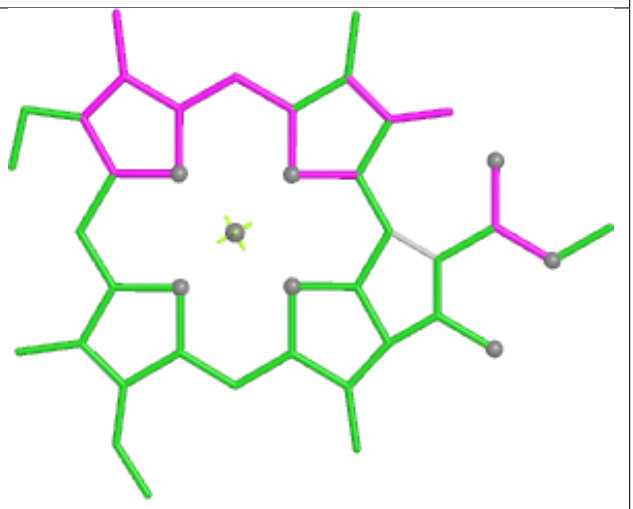


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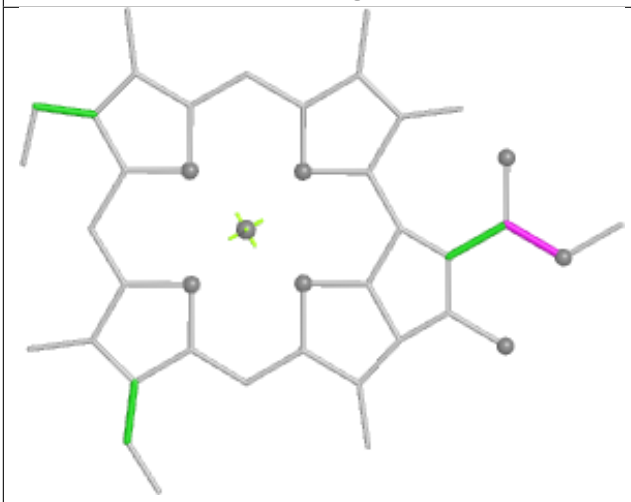
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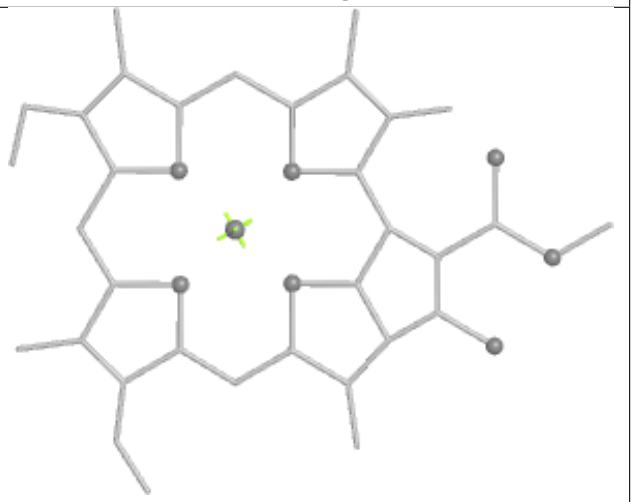
Bond lengths



Bond angles

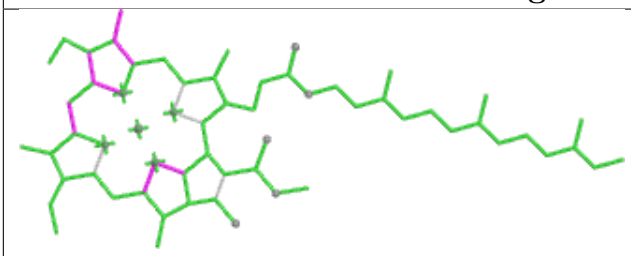


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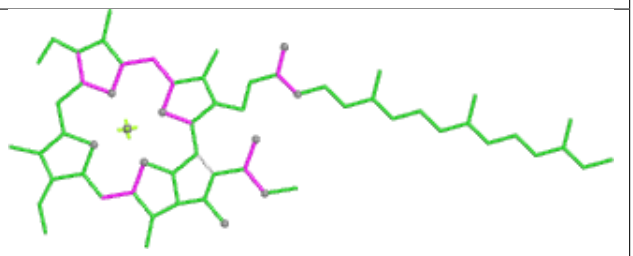


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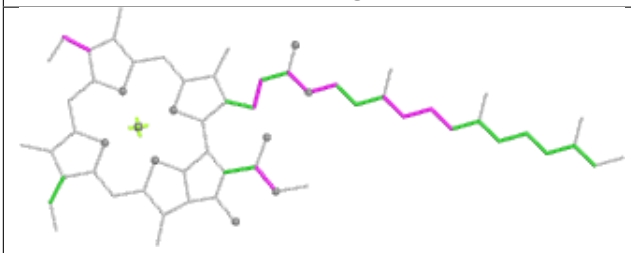
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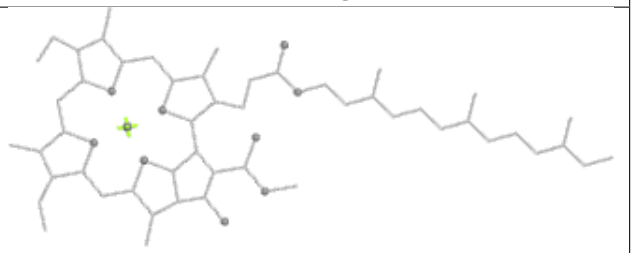
Bond lengths



Bond angles

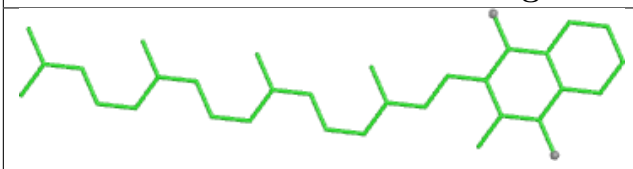


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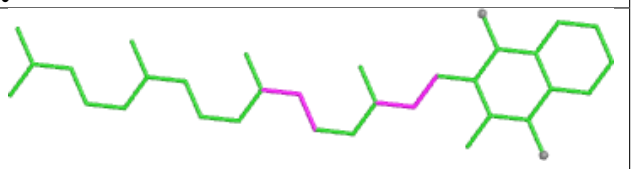


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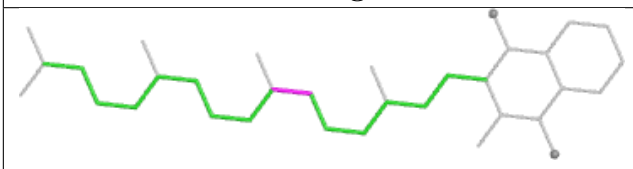
Ligand PQN B 845



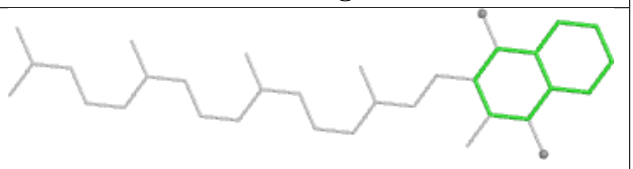
Bond lengths



Bond angles

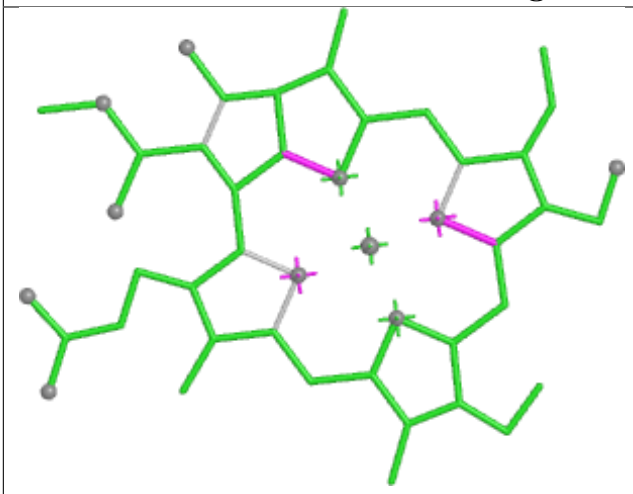


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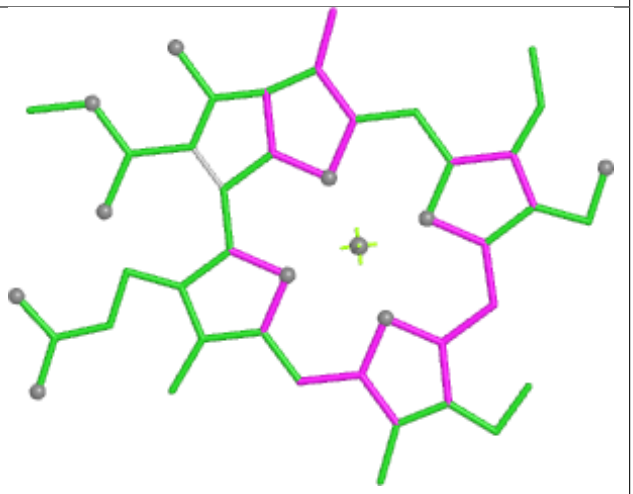


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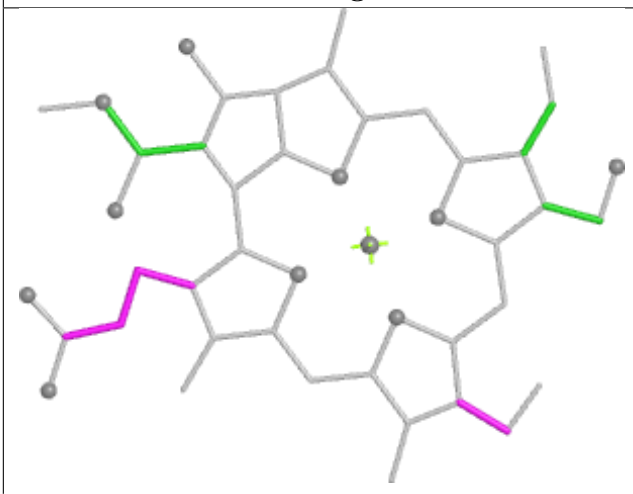
Ligand CHL 1 306



Bond lengths



Bond angles

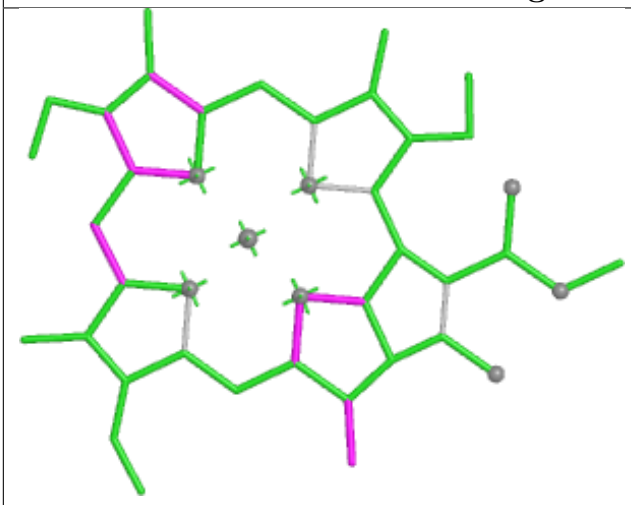


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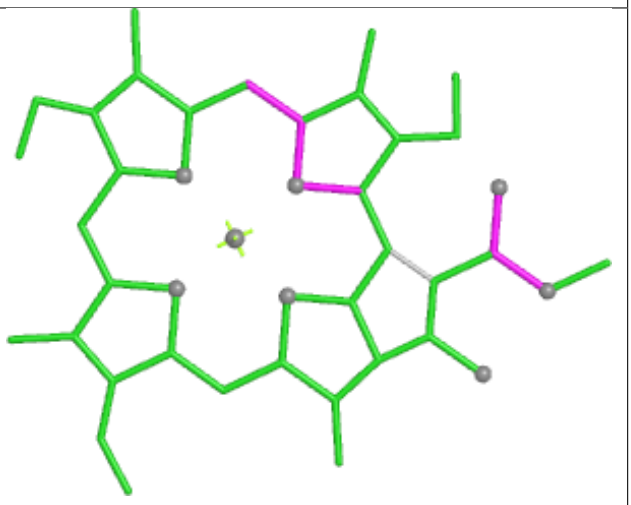


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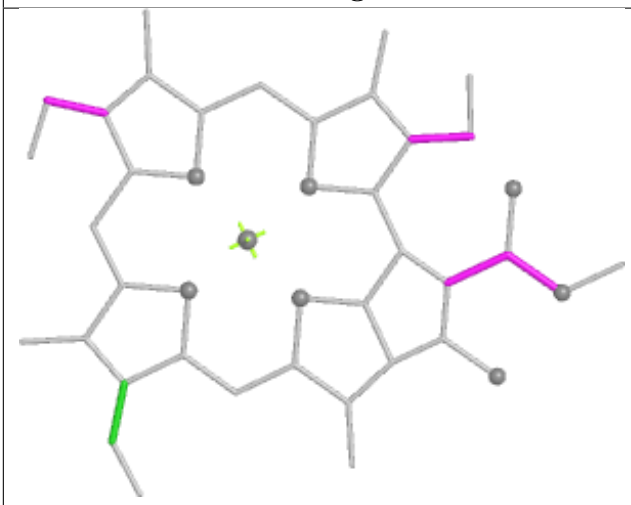
Ligand CLA J 102



Bond lengths



Bond angles

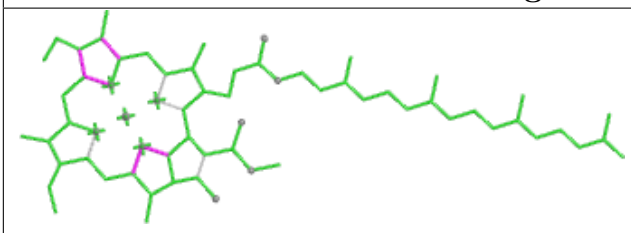


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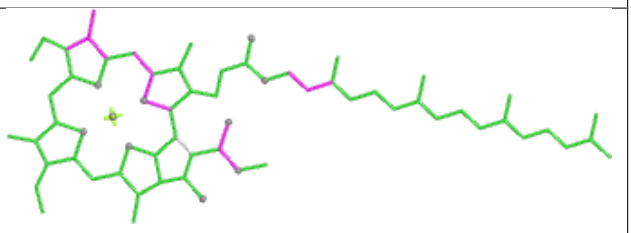


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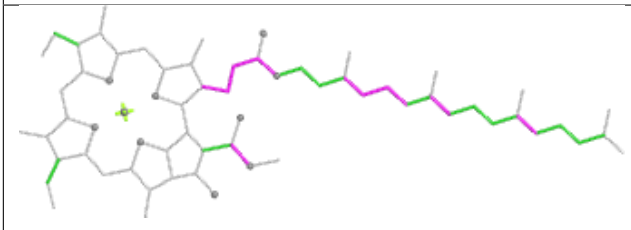
Ligand CLA B 809



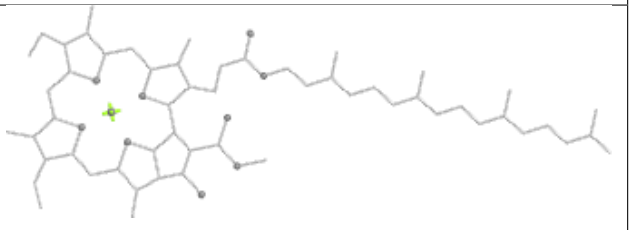
Bond lengths



Bond angles

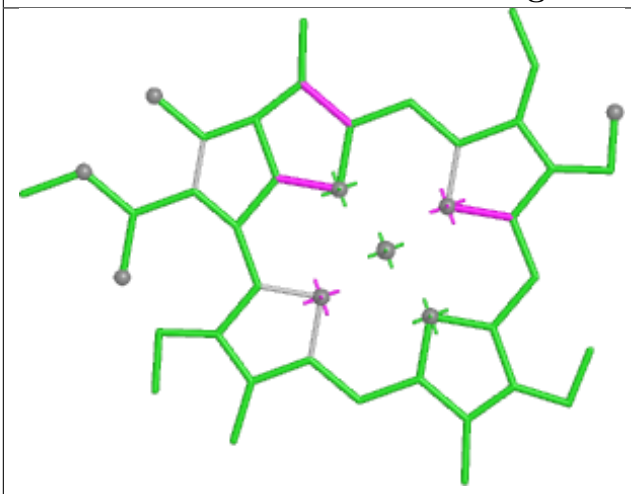


Torsions

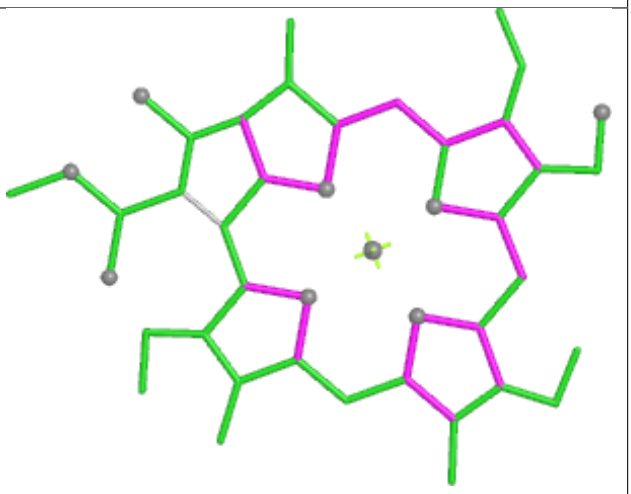


Rings

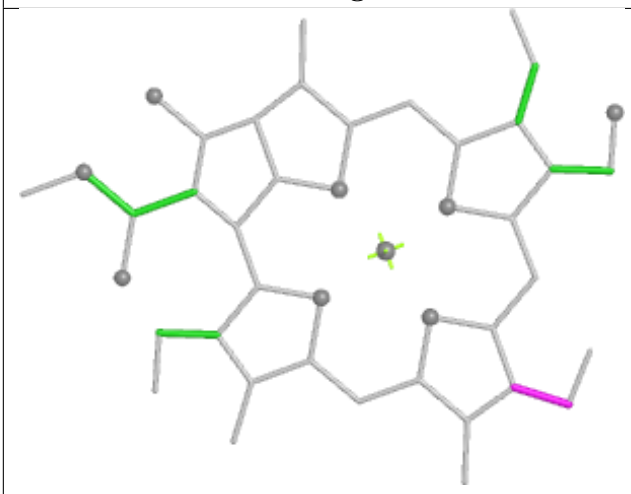
Ligand CHL 8 607



Bond lengths



Bond angles

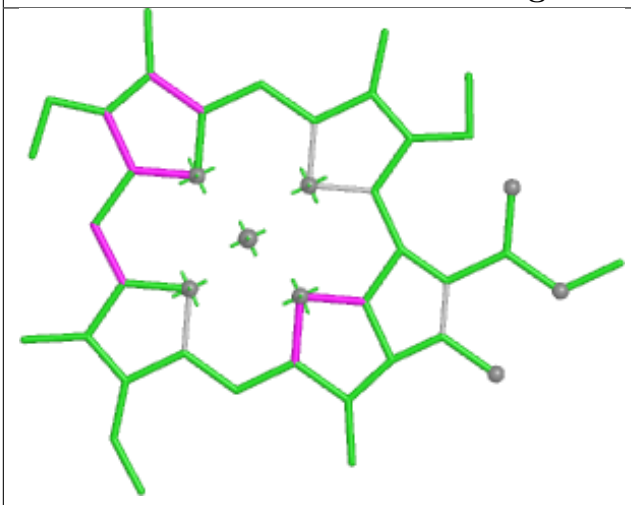


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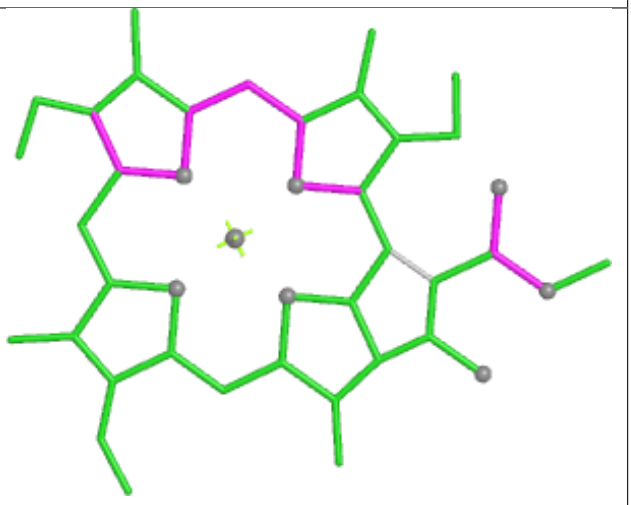


Rings

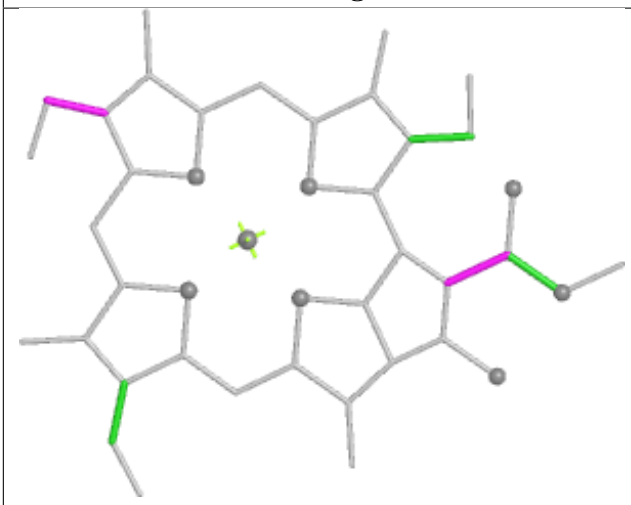
Ligand CLA 5 312



Bond lengths



Bond angles

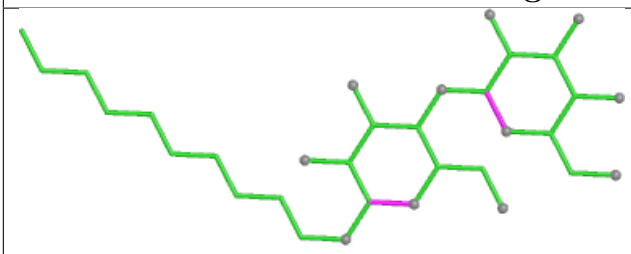


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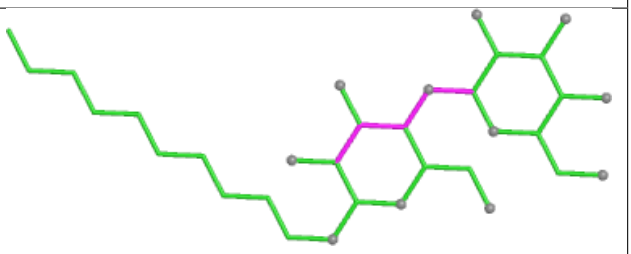


Rings

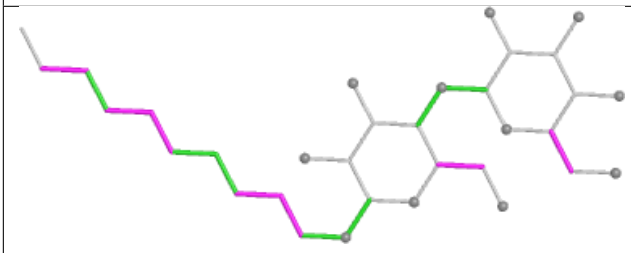
Ligand LMU 6 302



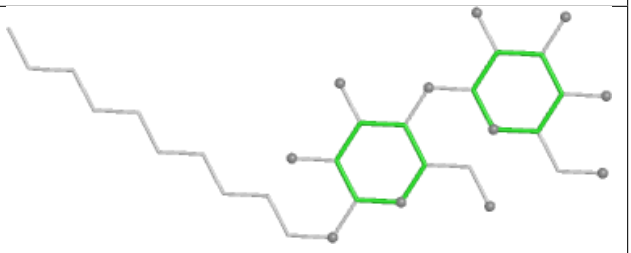
Bond lengths



Bond angles

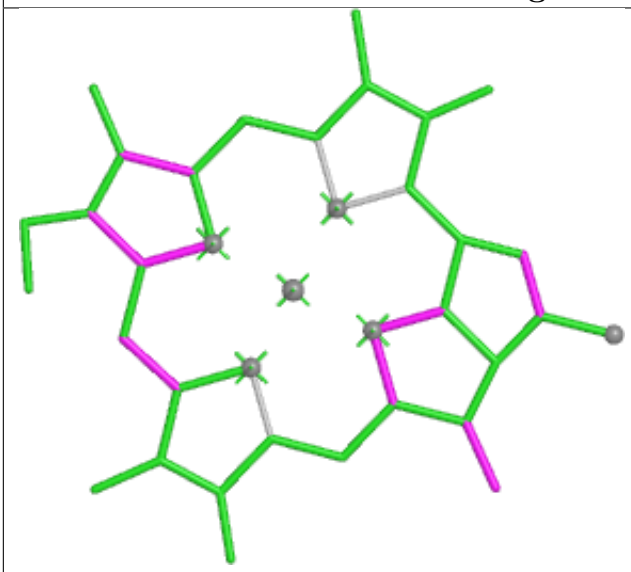


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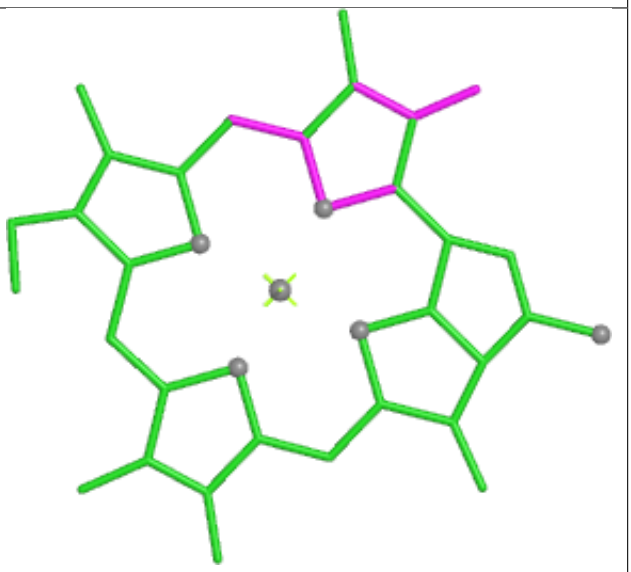


Rings

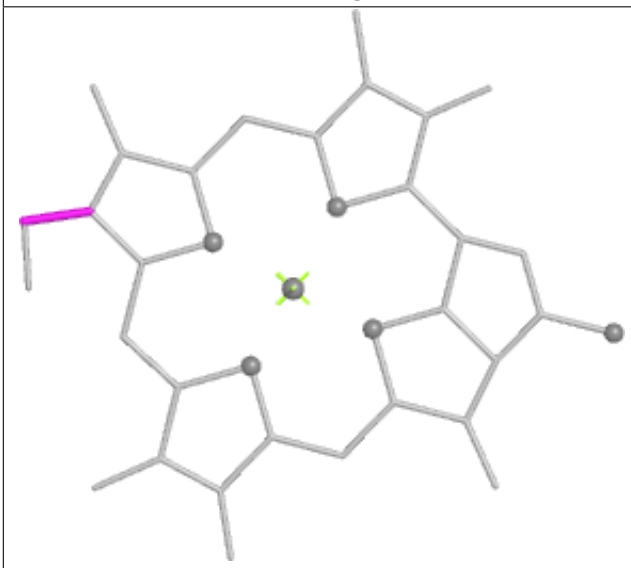
Ligand CLA 2 605



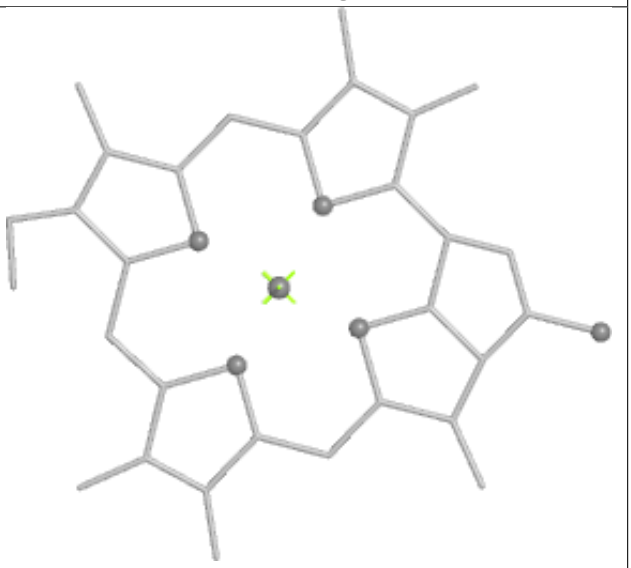
Bond lengths



Bond angles

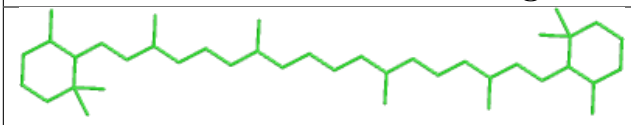


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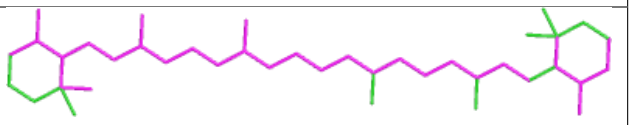


Rings

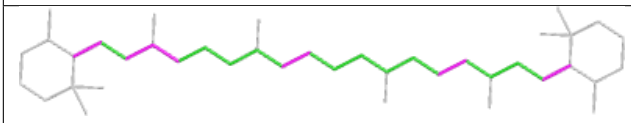
Ligand BCR A 851



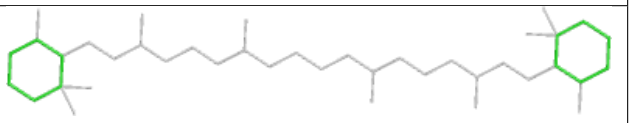
Bond lengths



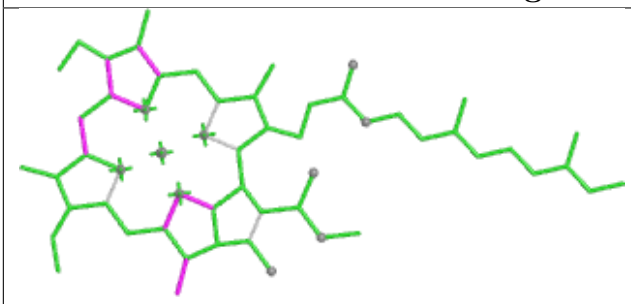
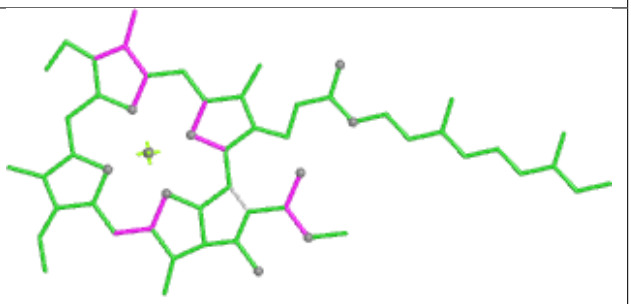
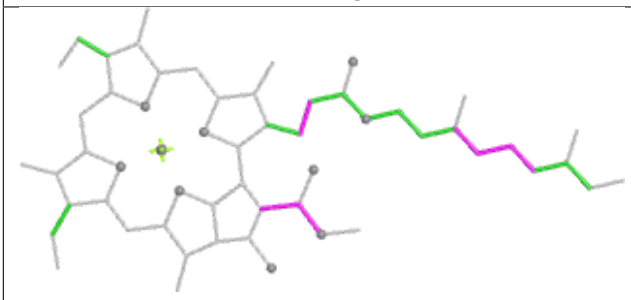
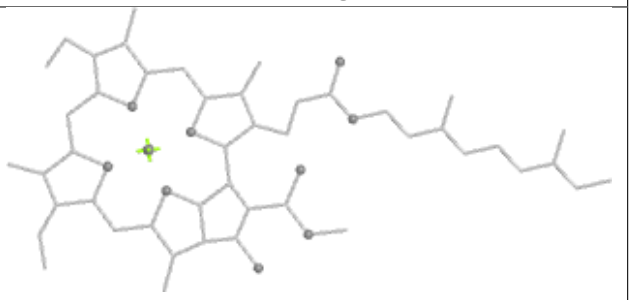
Bond angles

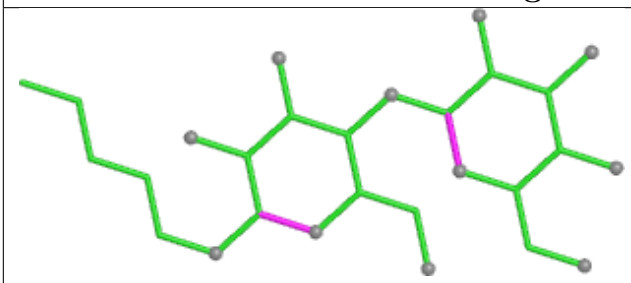
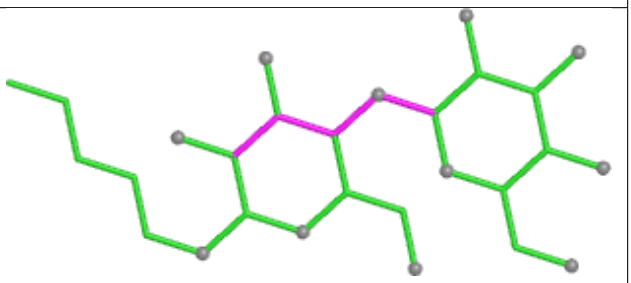
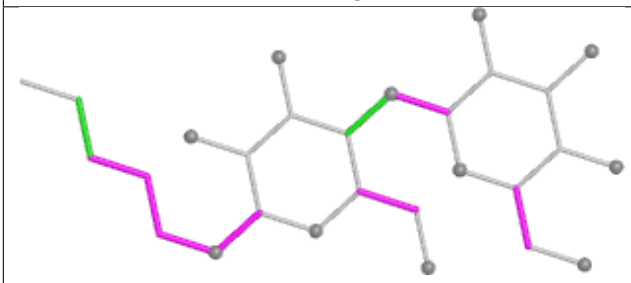
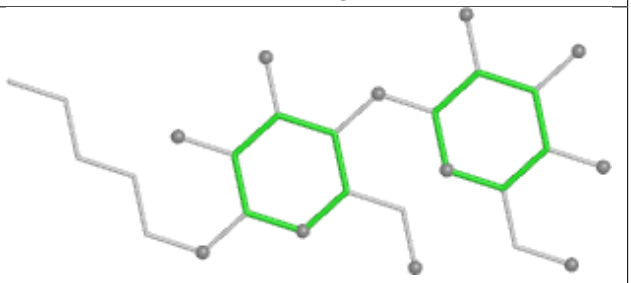


Torsions

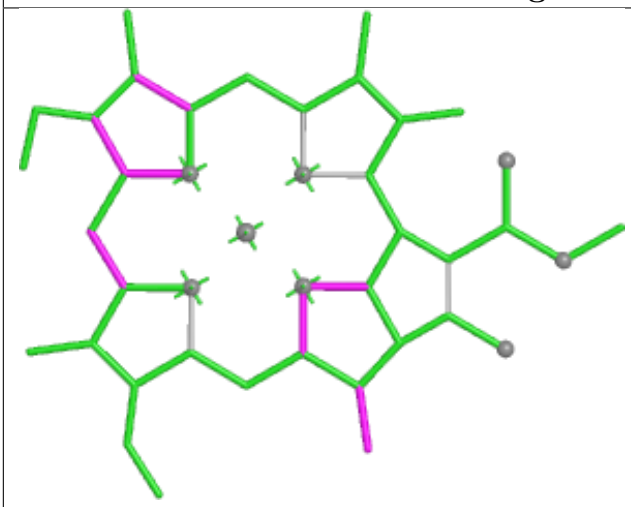


Rings

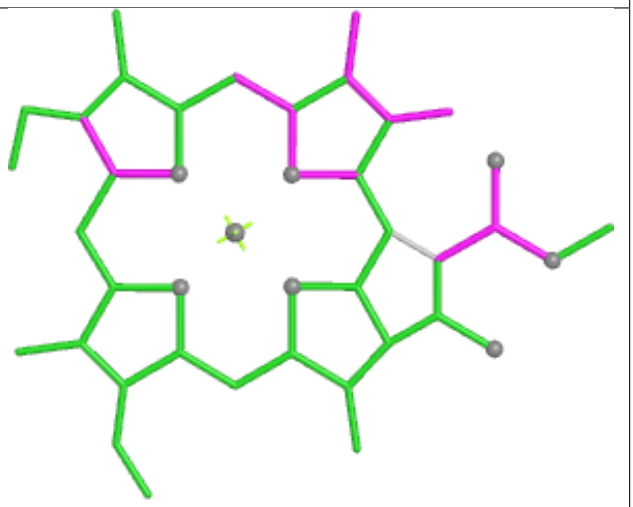
Ligand CLA B 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU 3 420	
 Bond lengths	 Bond angles
 Torsions	 Rings

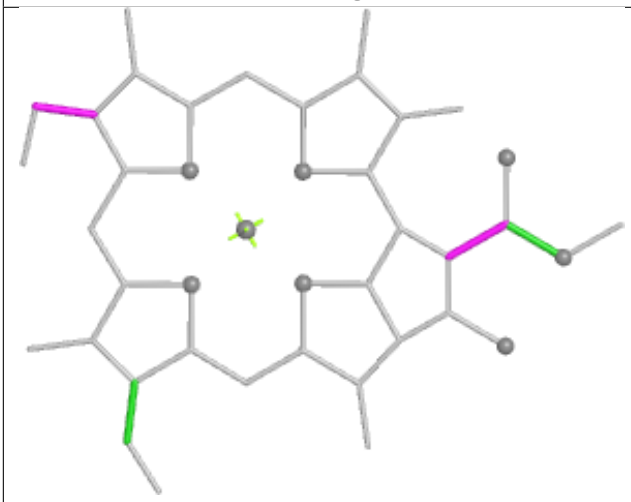
Ligand CLA 2 607



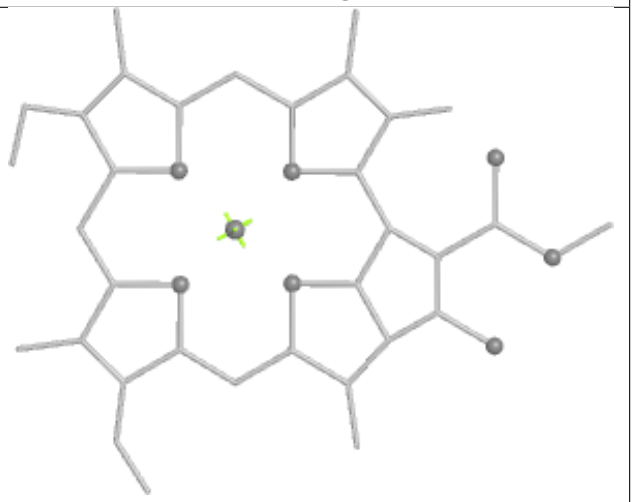
Bond lengths



Bond angles

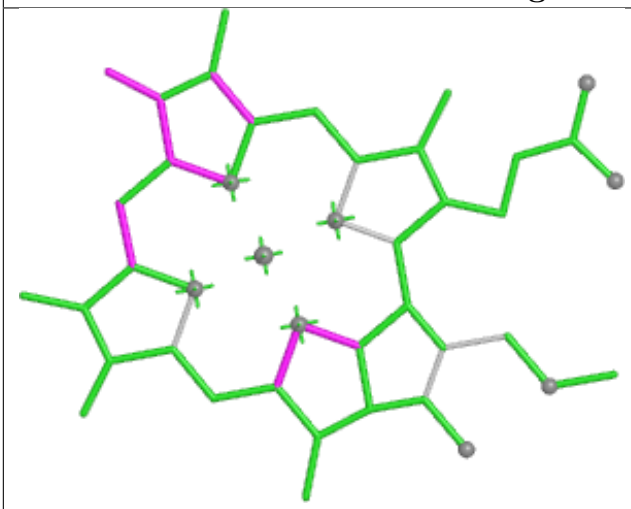


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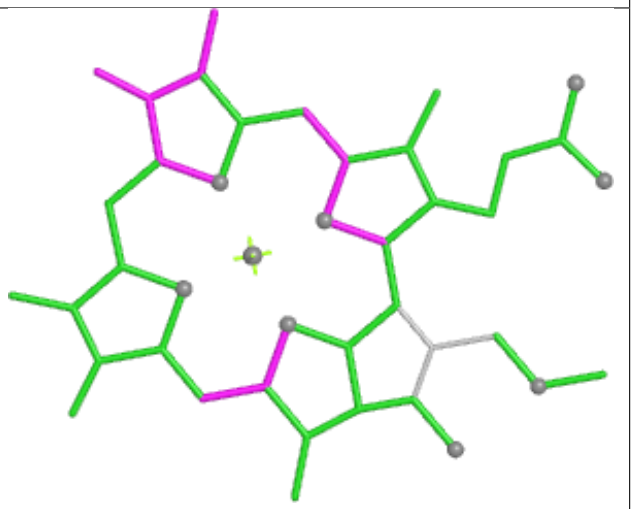


Rings

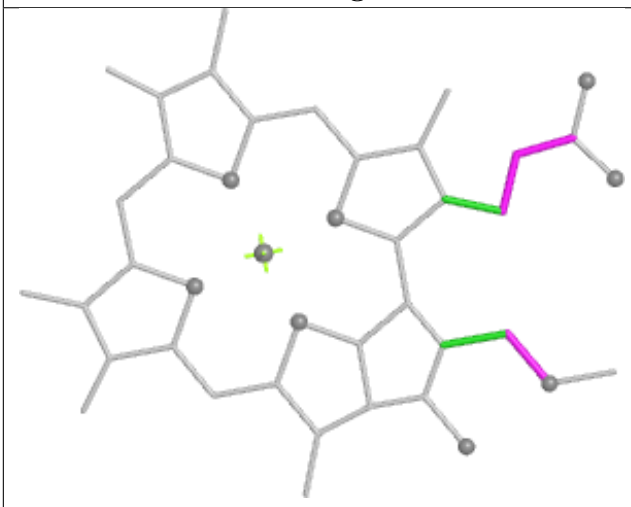
Ligand CLA 5 316



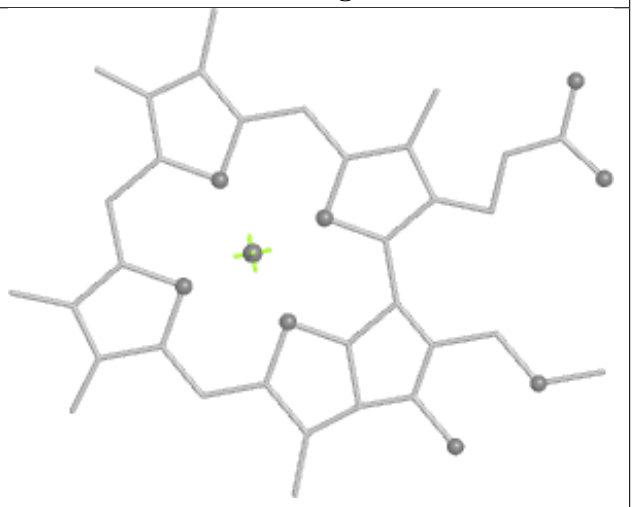
Bond lengths



Bond angles

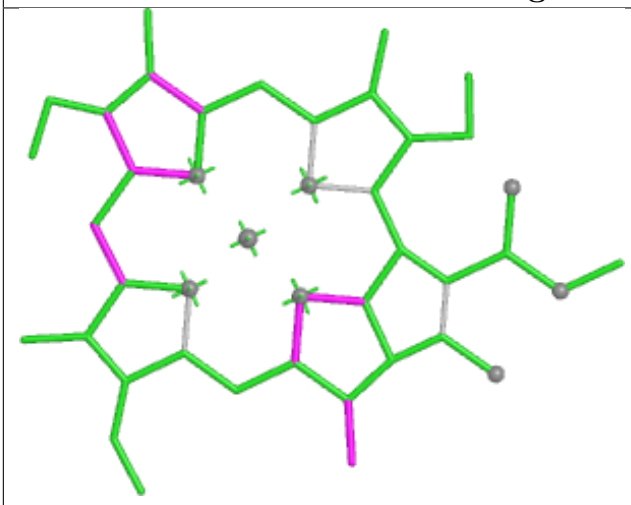


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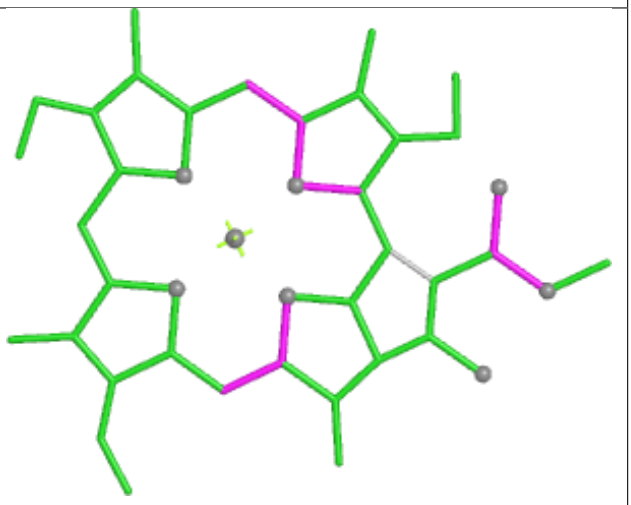


Rings

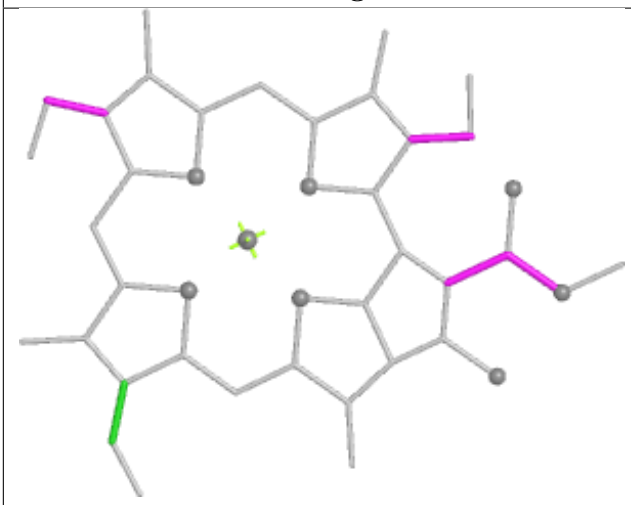
Ligand CLA 9 611



Bond lengths



Bond angles

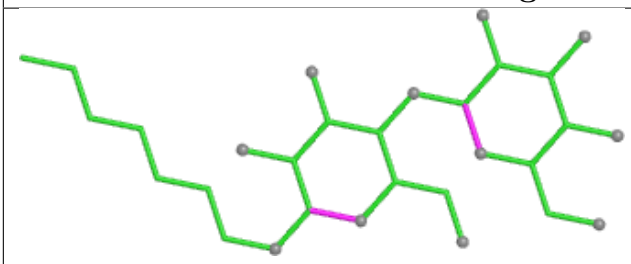


Torsions

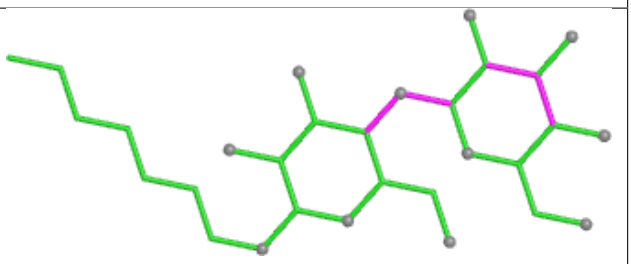


Rings

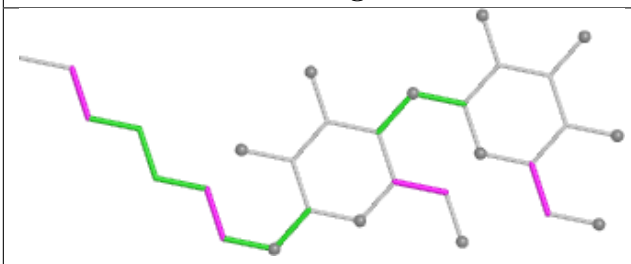
Ligand LMU A 852



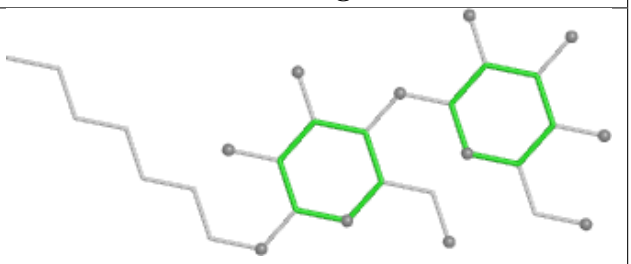
Bond lengths



Bond angles

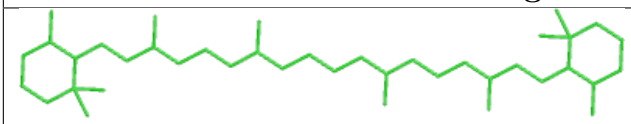


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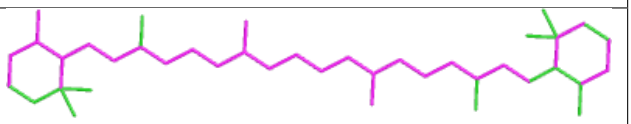


Rings

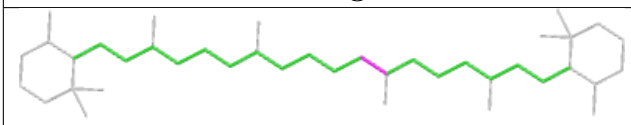
Ligand BCR F 805



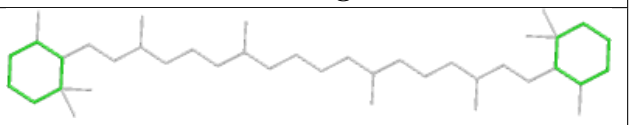
Bond lengths



Bond angles

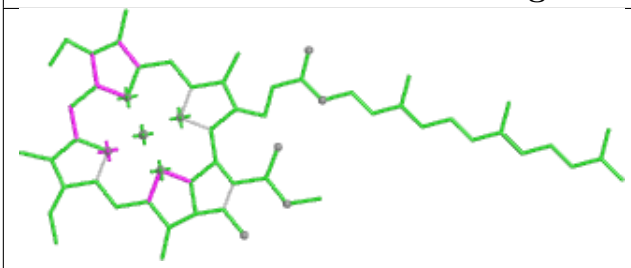


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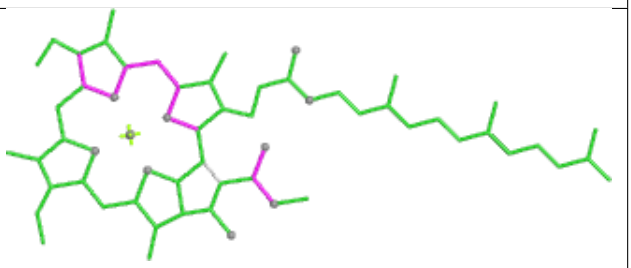


Rings

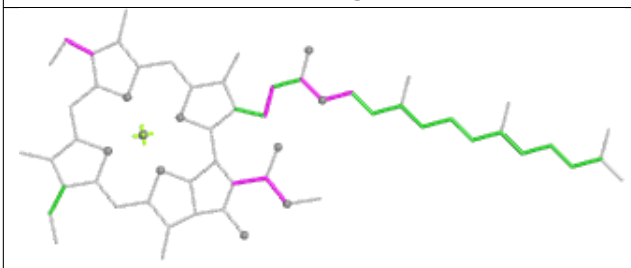
Ligand CLA 9 602



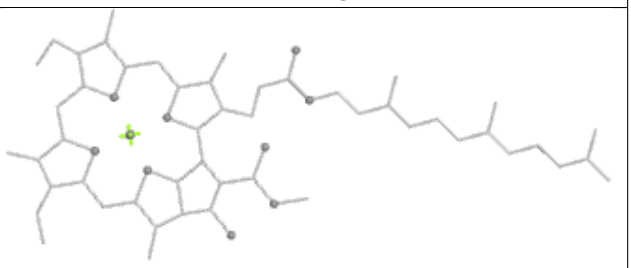
Bond lengths



Bond angles

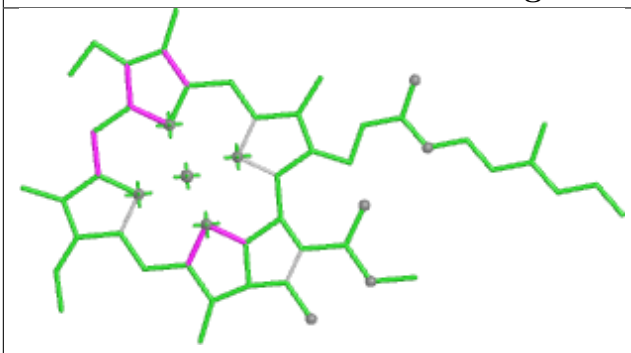


Torsions

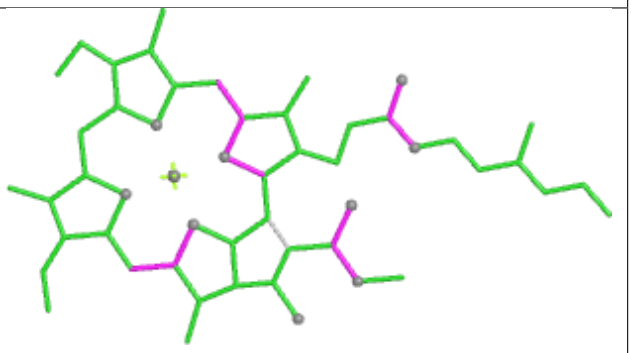


Rings

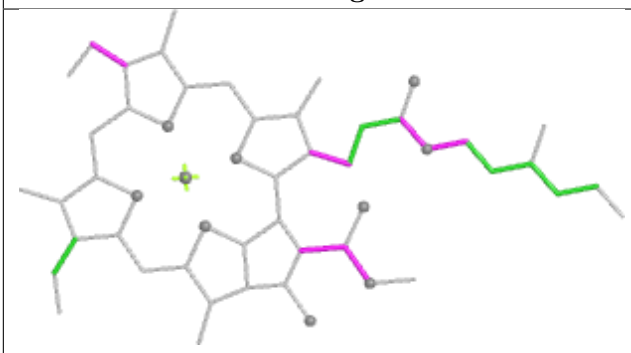
Ligand CLA B 818



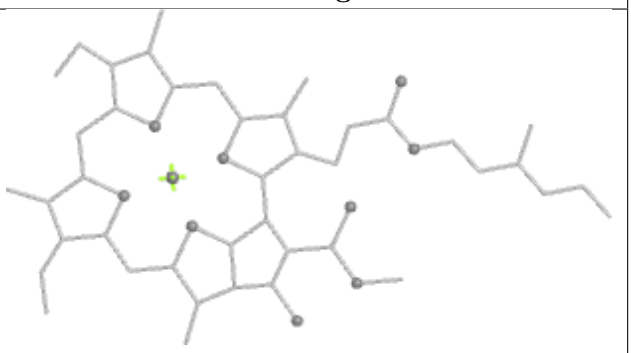
Bond lengths



Bond angles

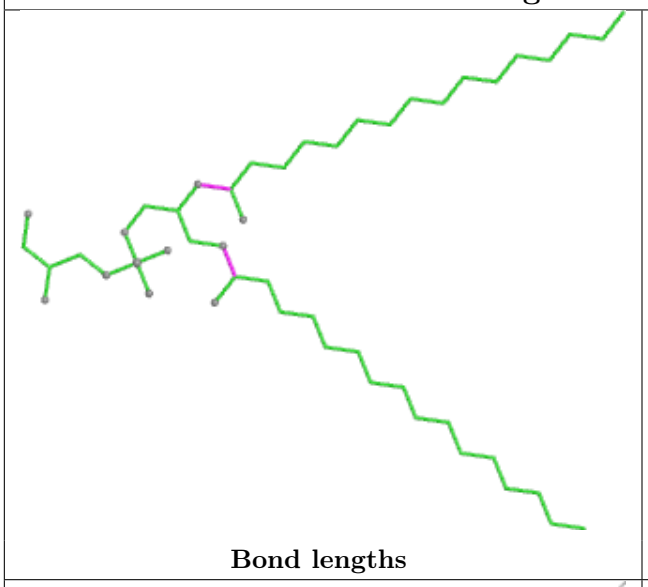


Torsions

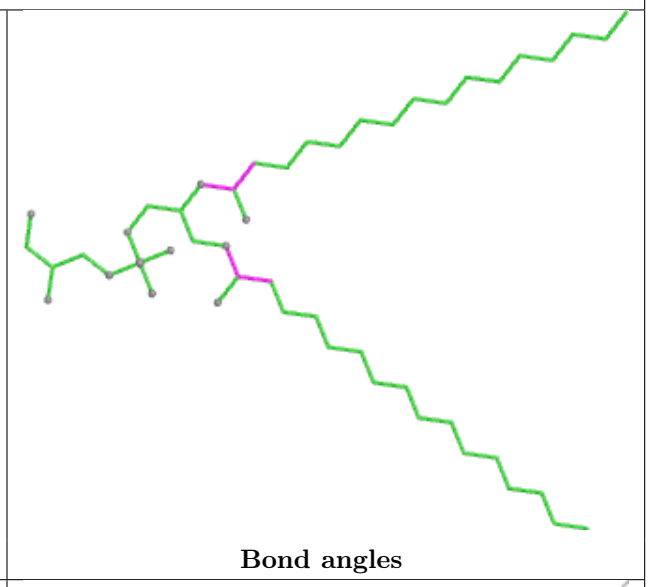


Rings

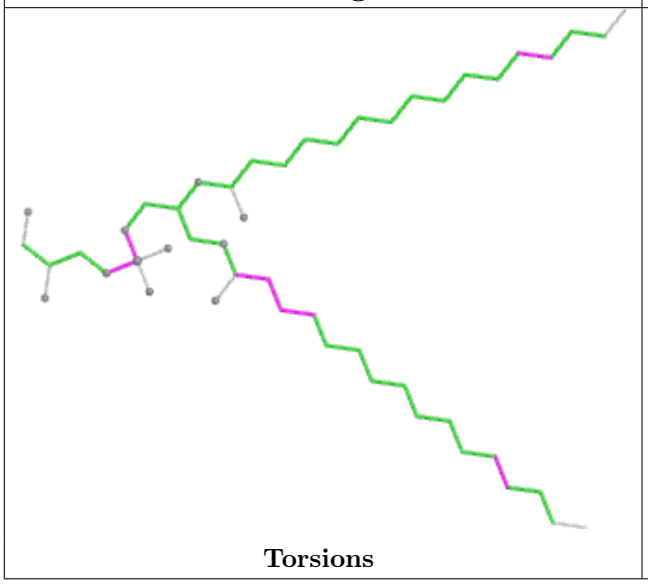
Ligand LHG A 844



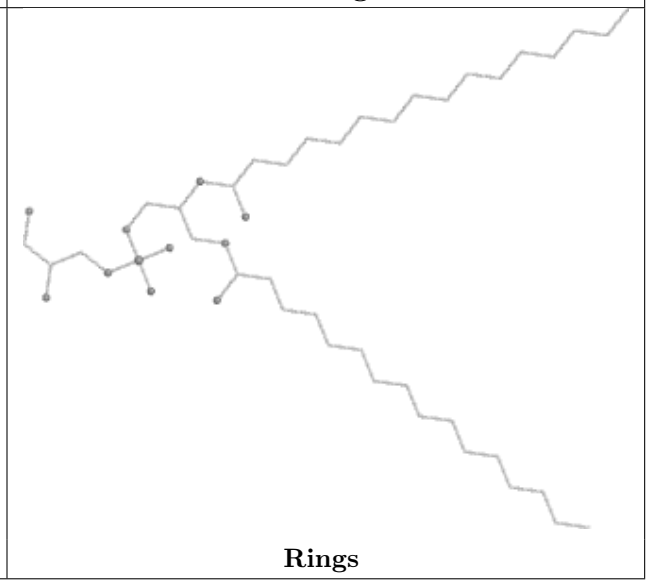
Bond lengths



Bond angles

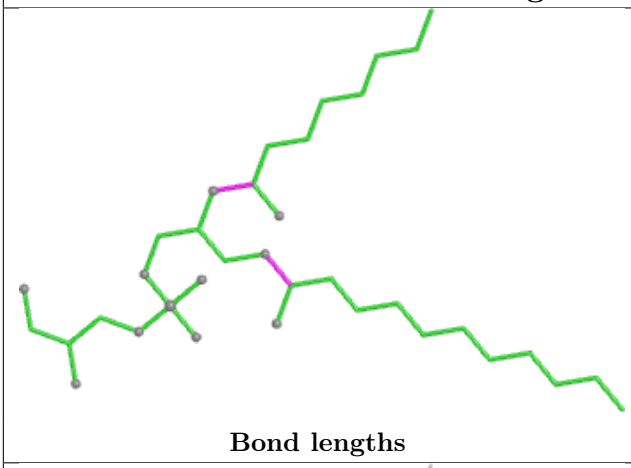


Torsions

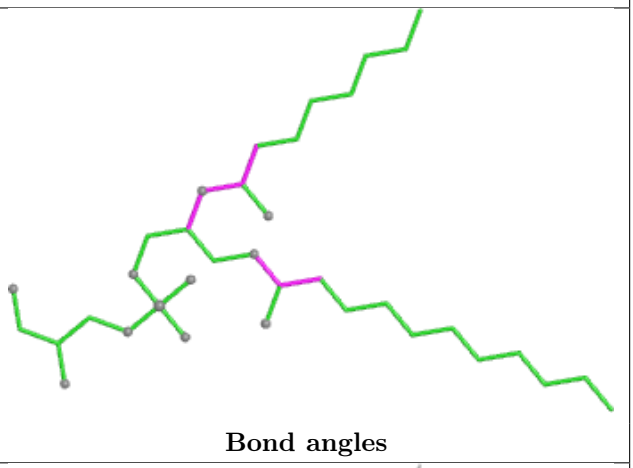


Rings

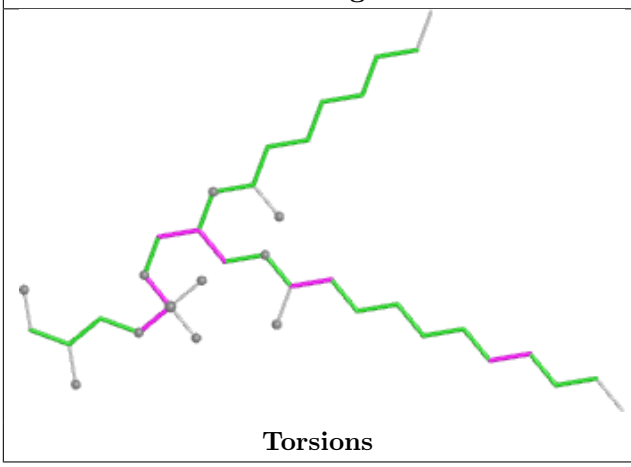
Ligand LHG 5 325



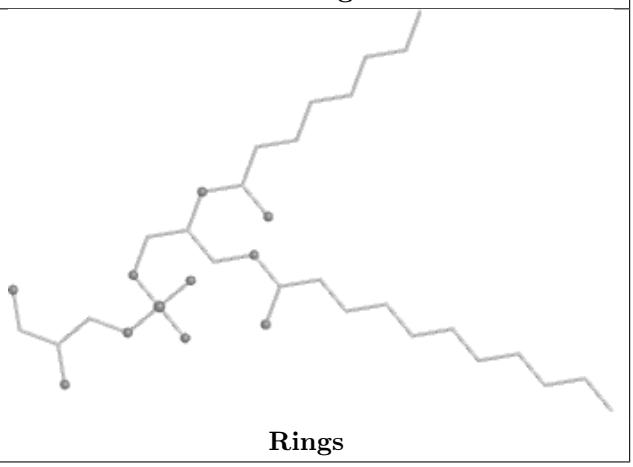
Bond lengths



Bond angles

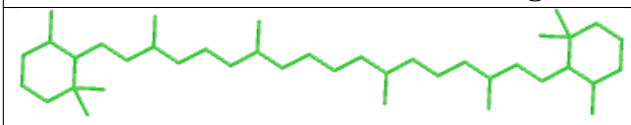


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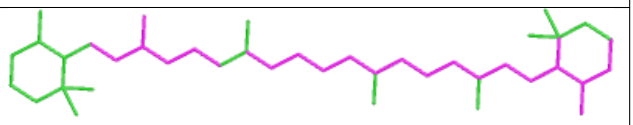


Rings

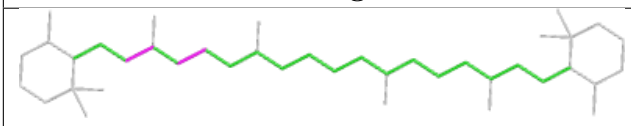
Ligand BCR 3 417



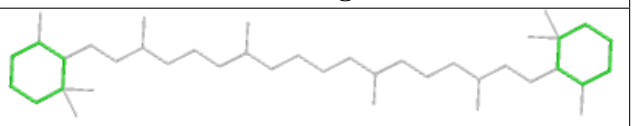
Bond lengths



Bond angles

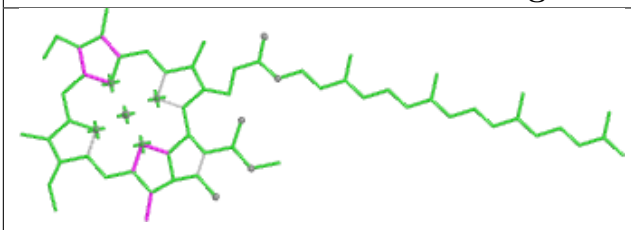


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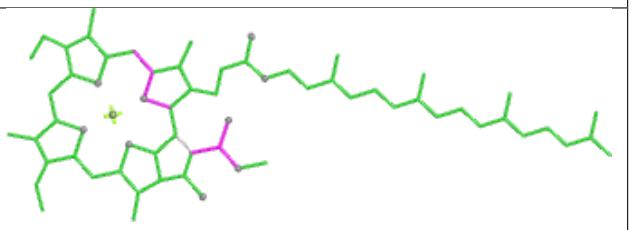


Rings

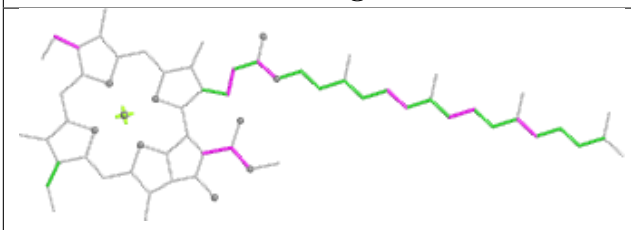
Ligand CLA 1 311



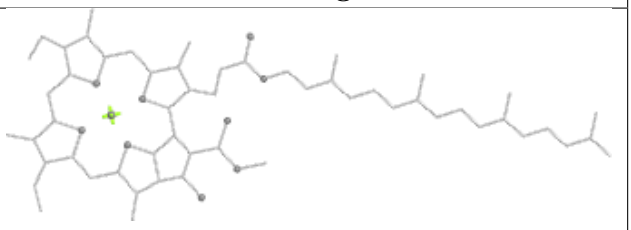
Bond lengths



Bond angles

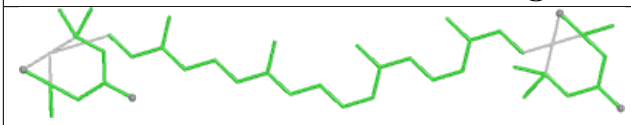


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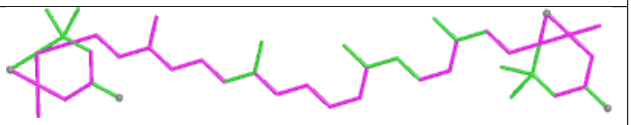


Rings

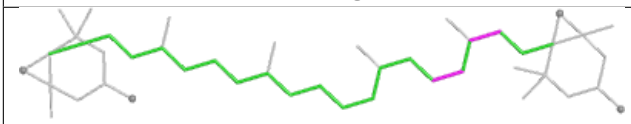
Ligand XAT 1 315



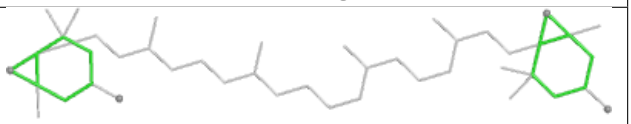
Bond lengths



Bond angles

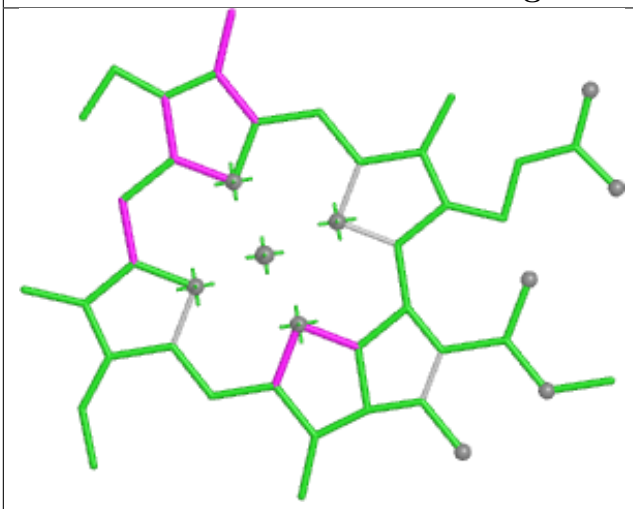


Torsions

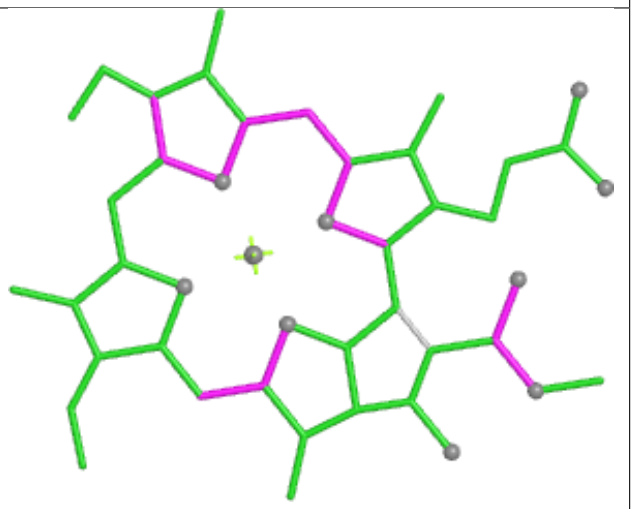


Rings

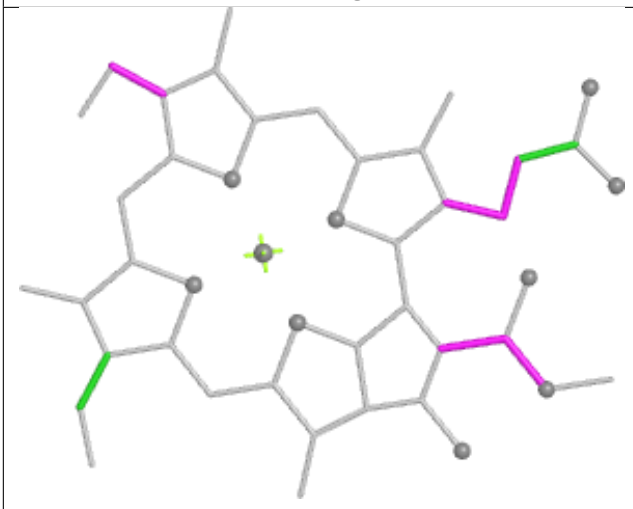
Ligand CLA A 835



Bond lengths



Bond angles

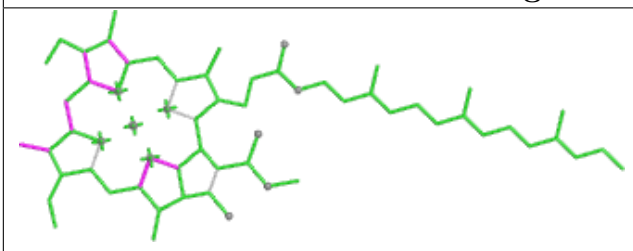


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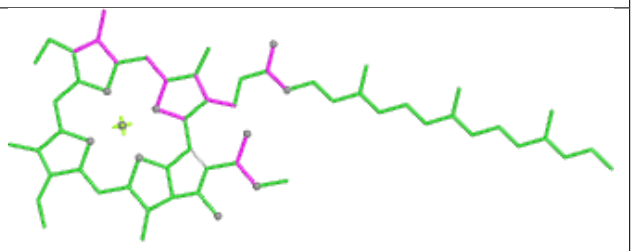


Rings

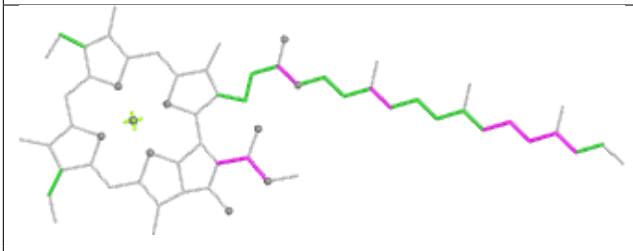
Ligand CLA A 826



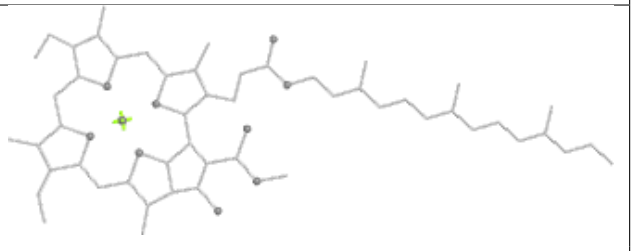
Bond lengths



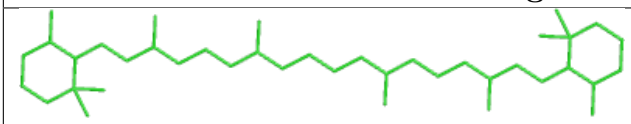
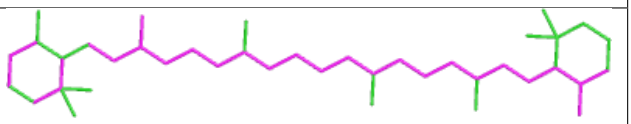
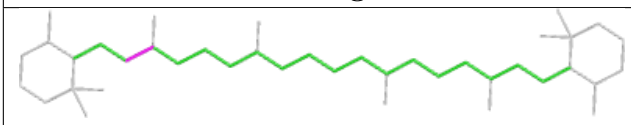
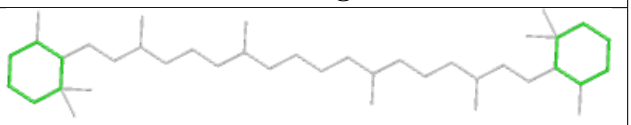
Bond angles

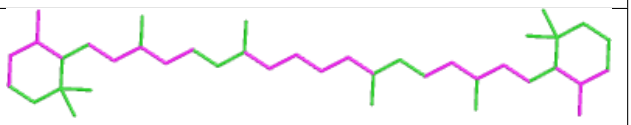
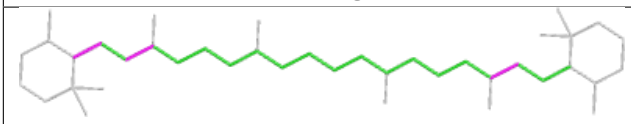
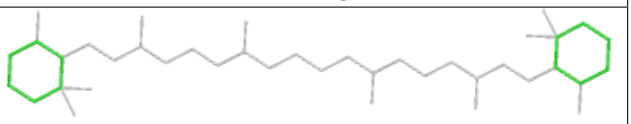


Torsions

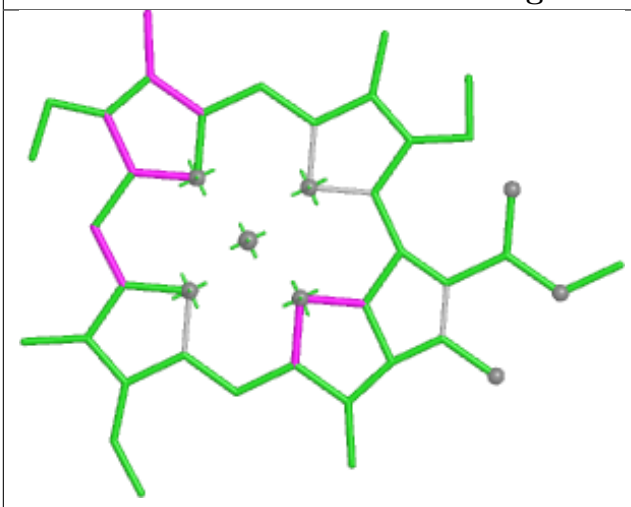


Rings

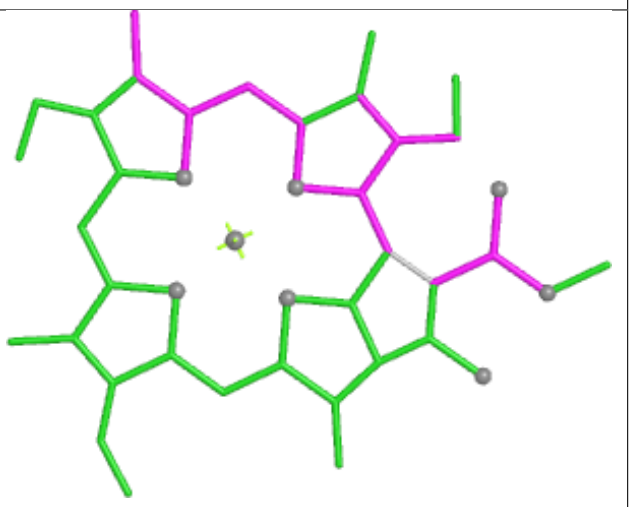
Ligand BCR 8 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR L 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

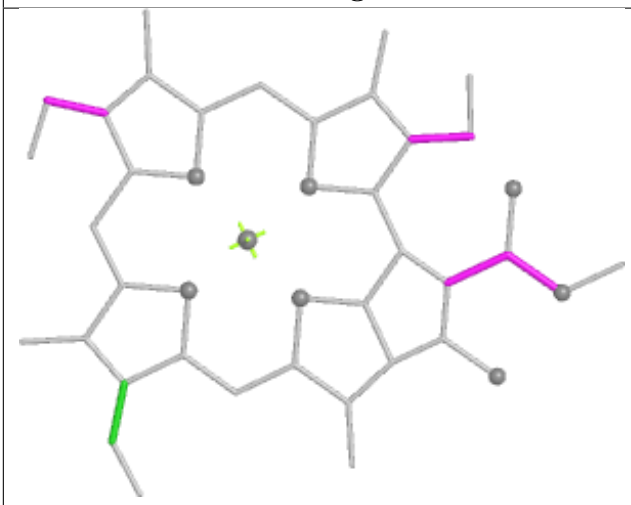
Ligand CLA F 803



Bond lengths



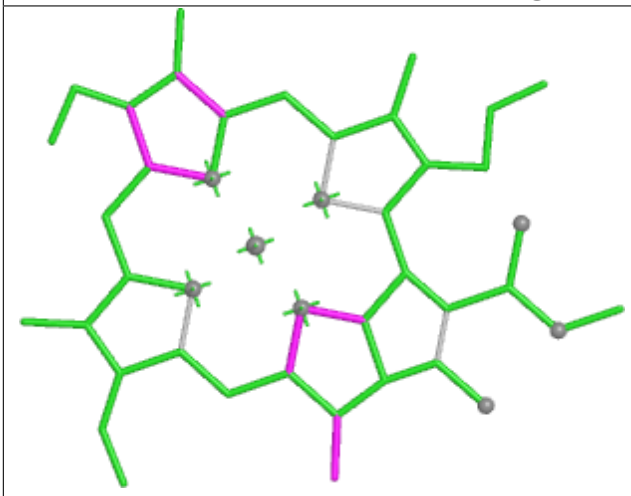
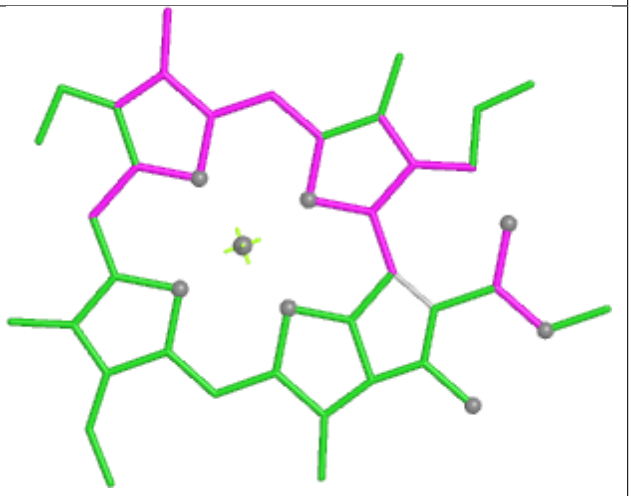
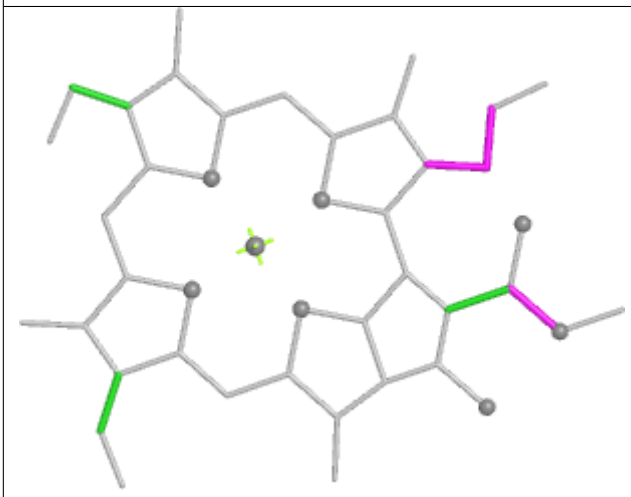
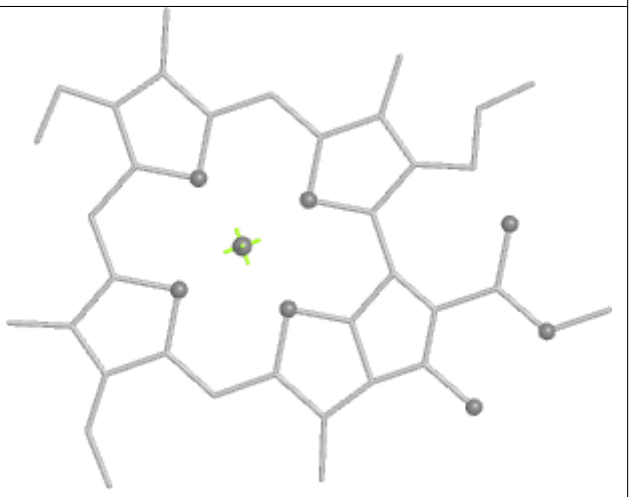
Bond angles



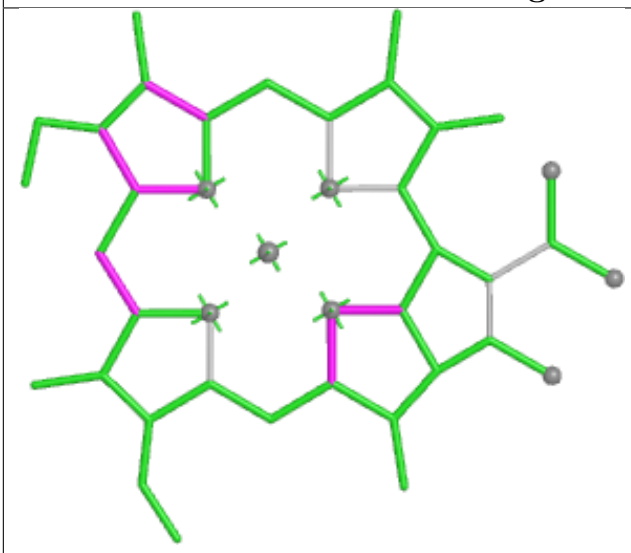
Torsions



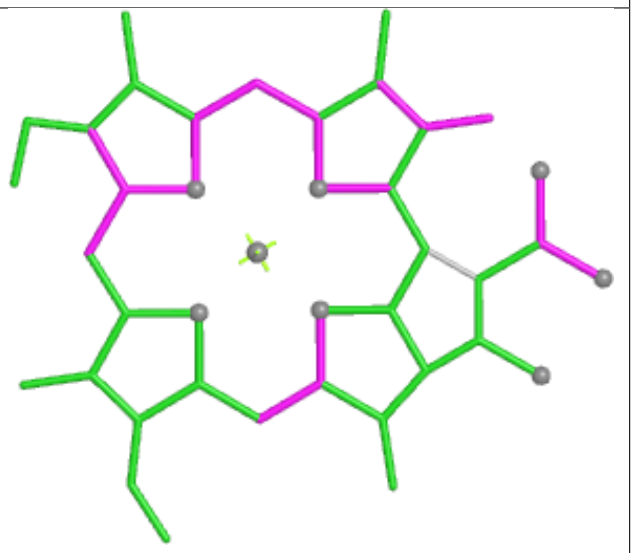
Rings

Ligand CLA 3 410	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

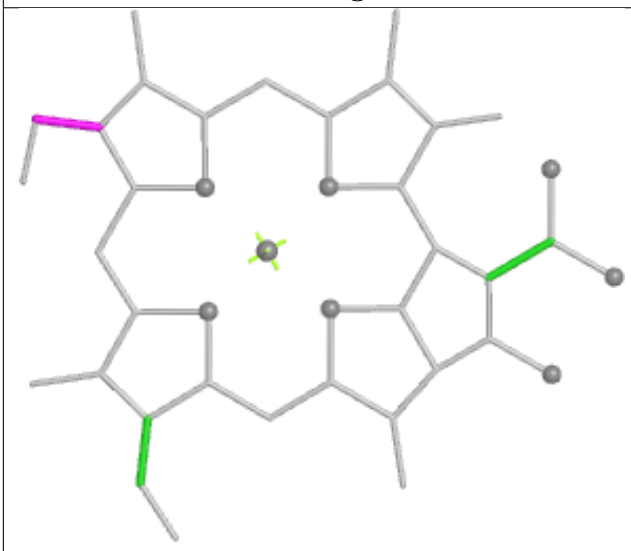
Ligand CLA 3 412



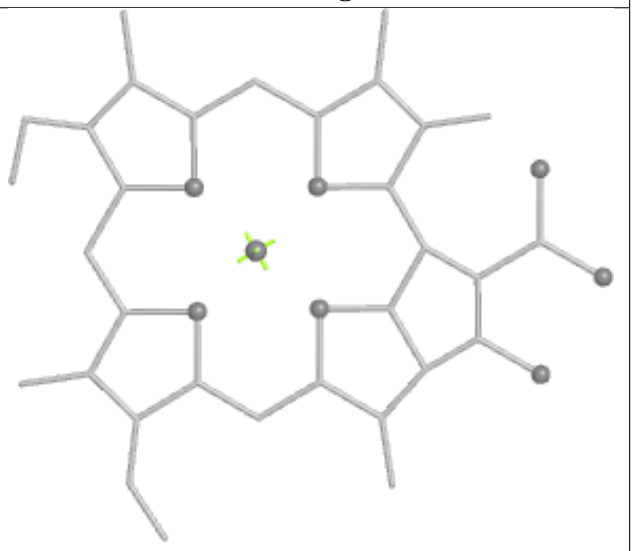
Bond lengths



Bond angles

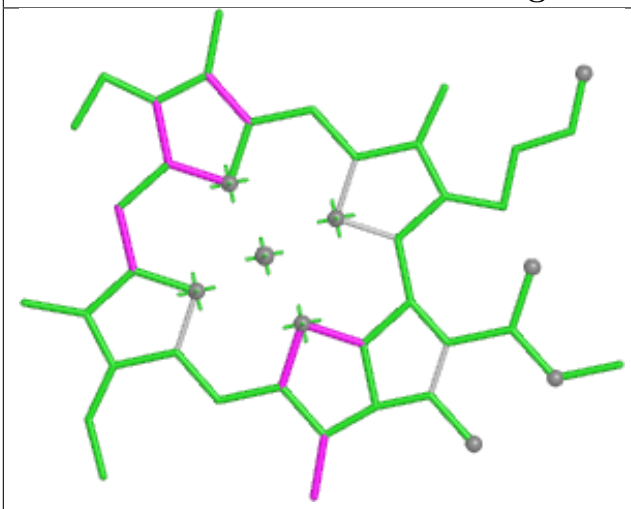


Torsions

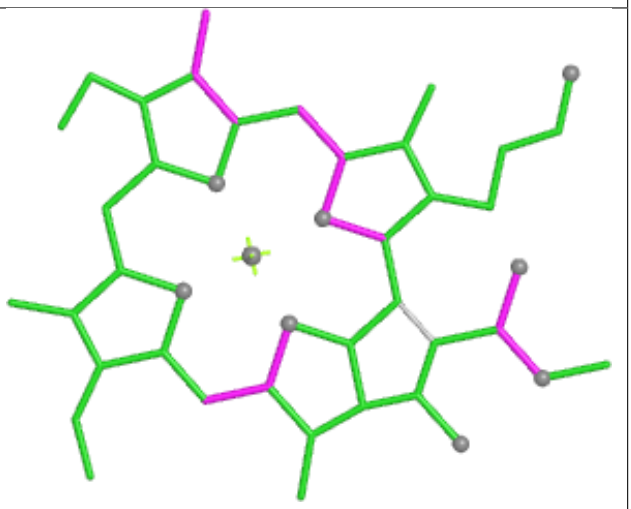


Rings

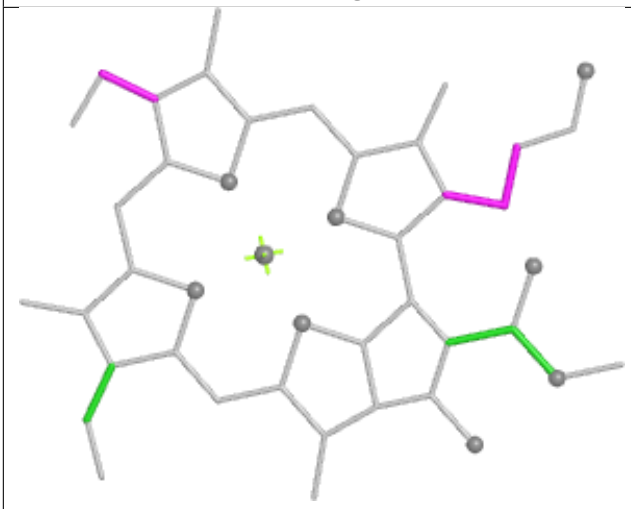
Ligand CLA 9 604



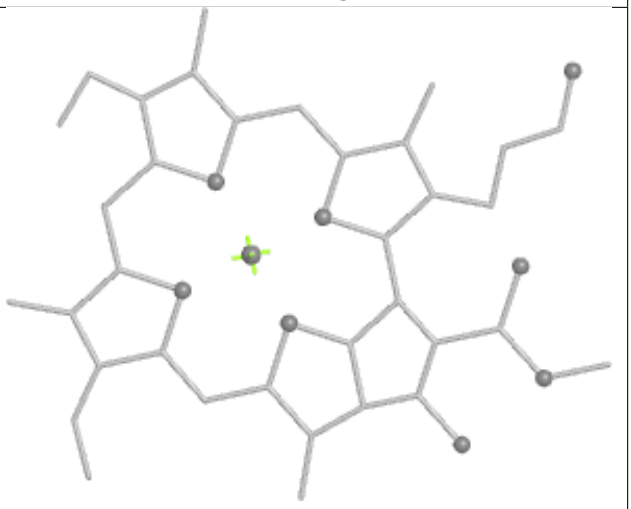
Bond lengths



Bond angles

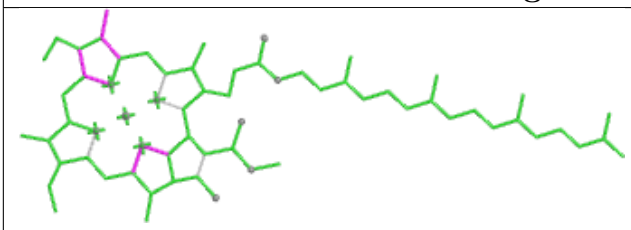


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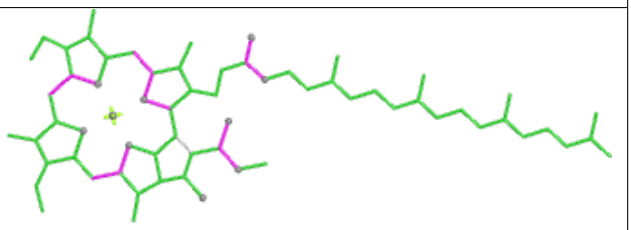


Rings

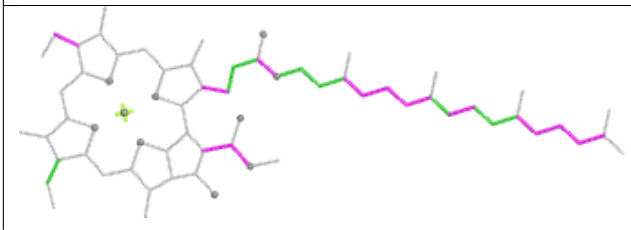
Ligand CLA A 823



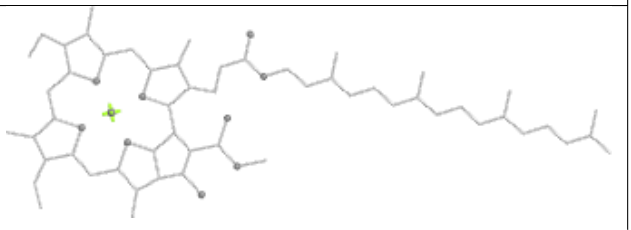
Bond lengths



Bond angles

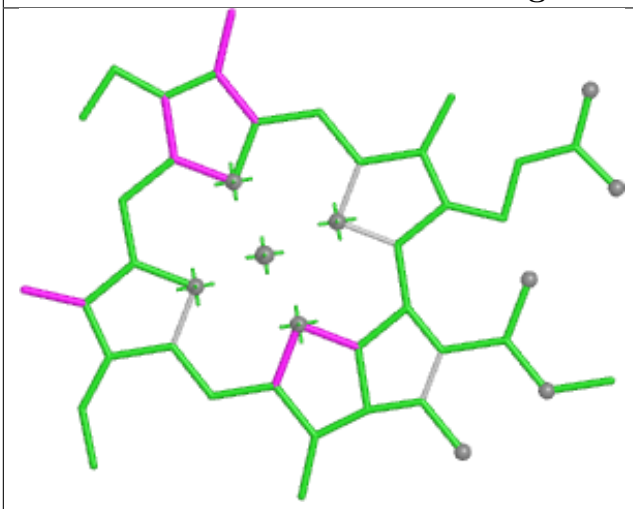


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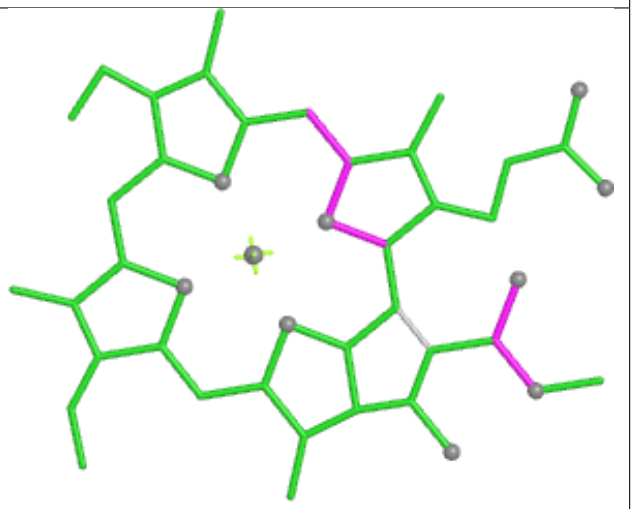


Rings

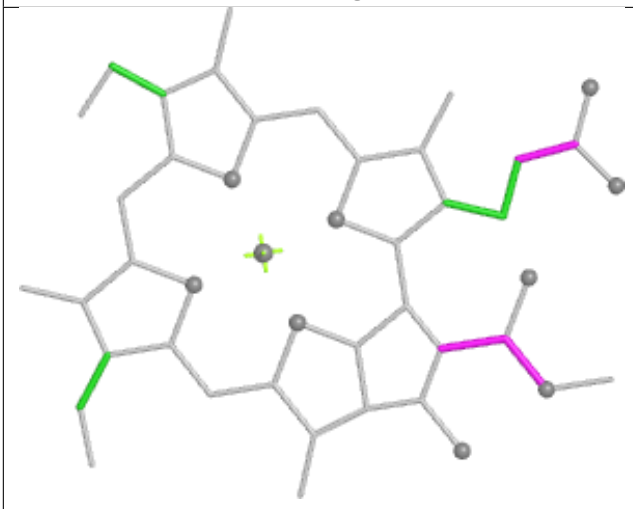
Ligand CLA 5 317



Bond lengths



Bond angles

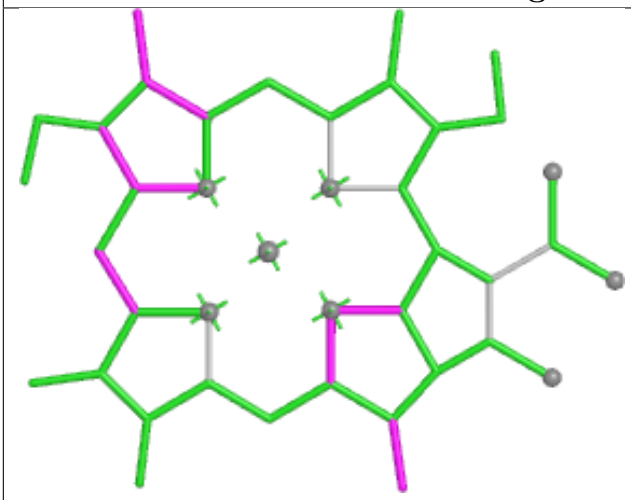


Torsions

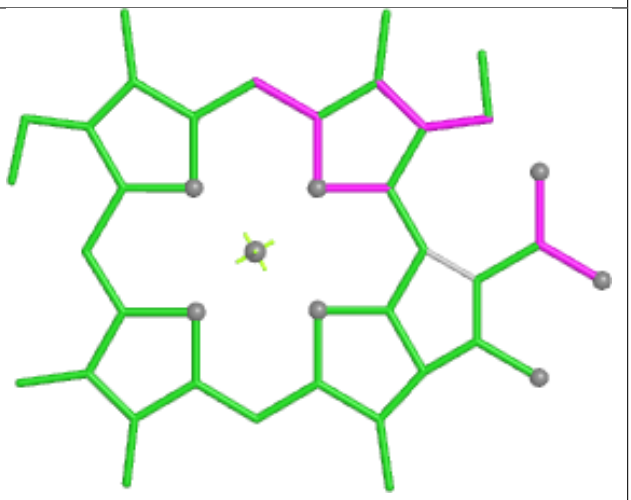


Rings

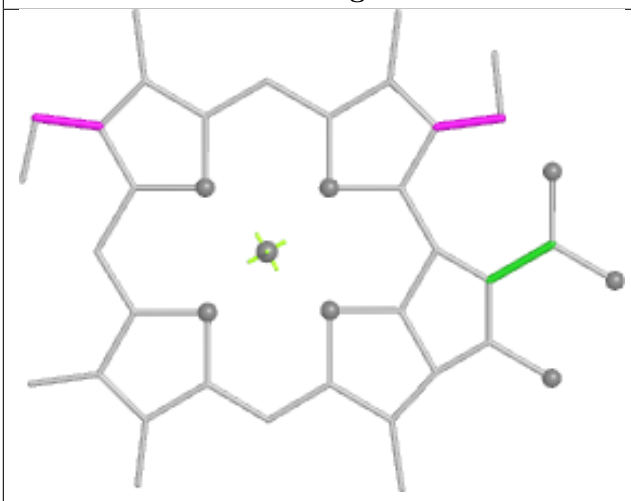
Ligand CLA 2 604



Bond lengths



Bond angles

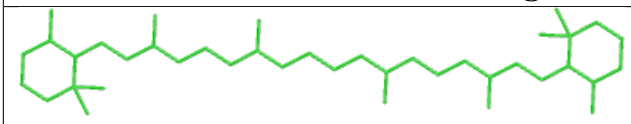


Torsions

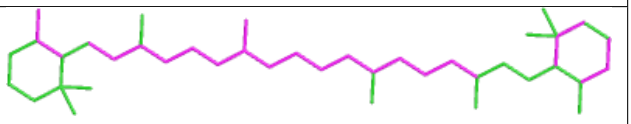


Rings

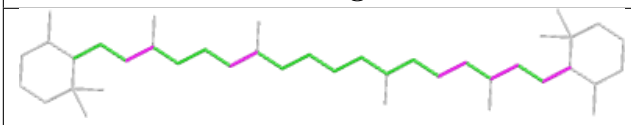
Ligand BCR B 846



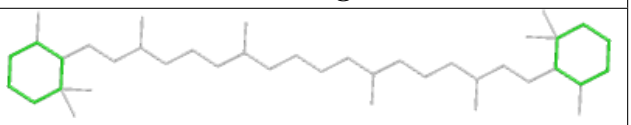
Bond lengths



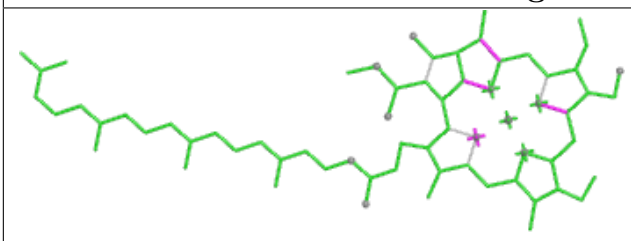
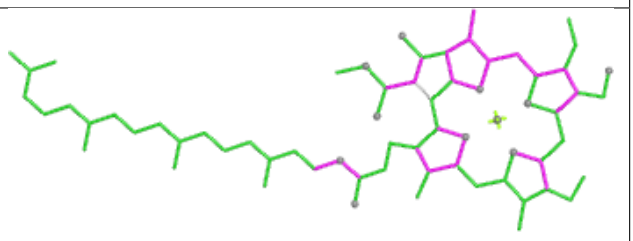
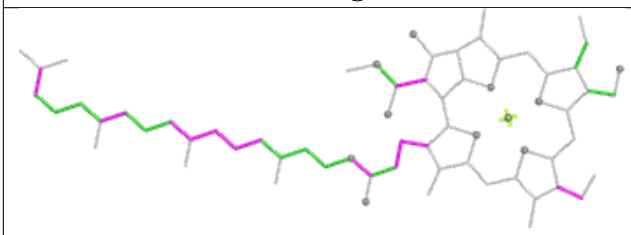
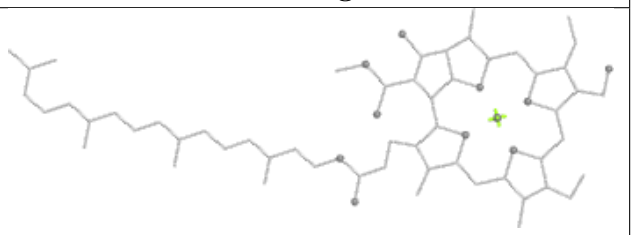
Bond angles



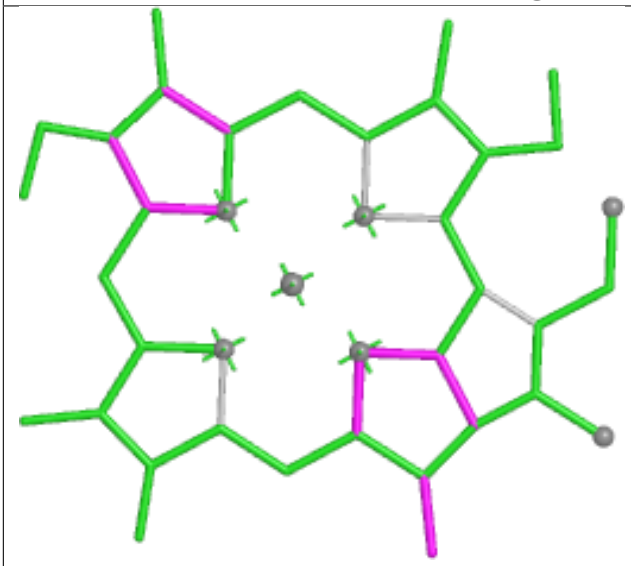
Torsions



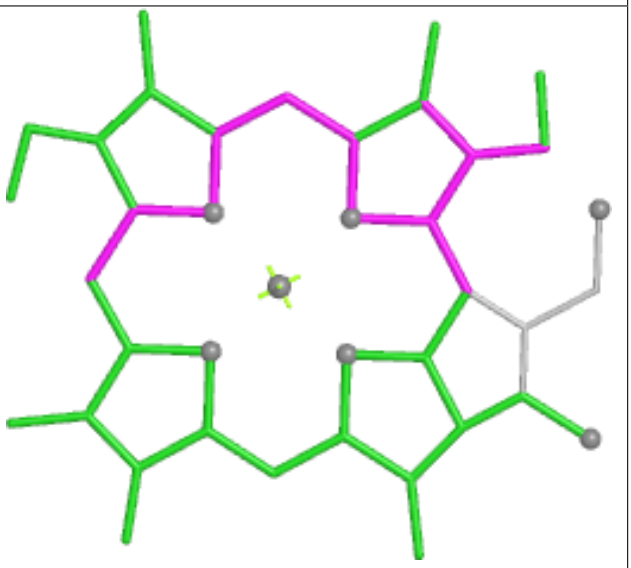
Rings

Ligand CHL 8 603	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

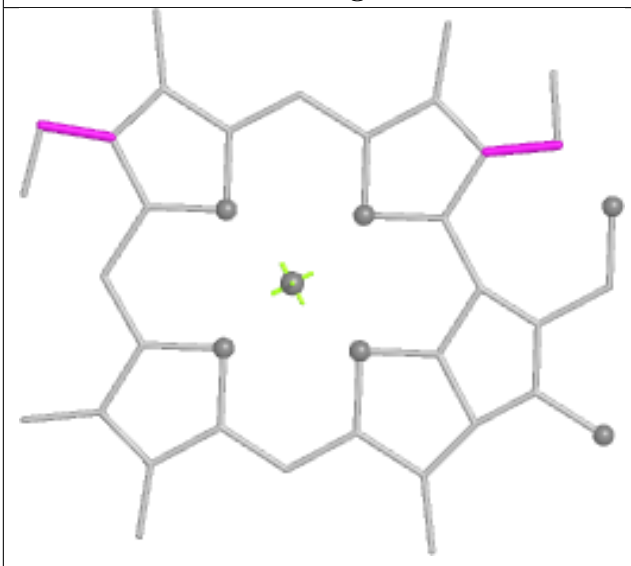
Ligand CLA 2 610



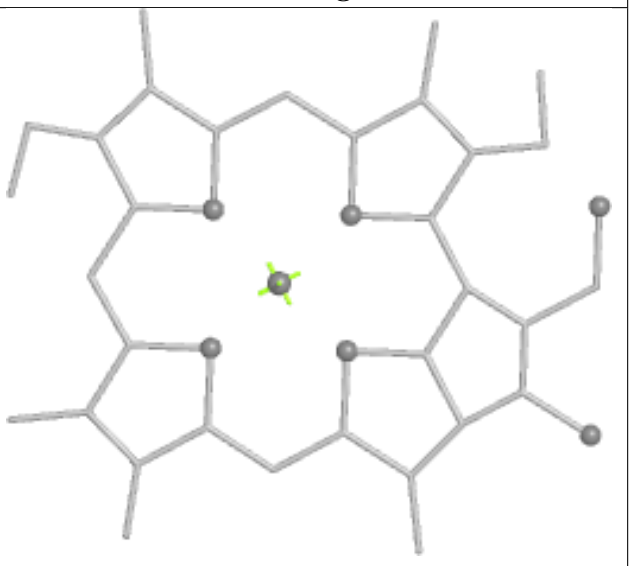
Bond lengths



Bond angles

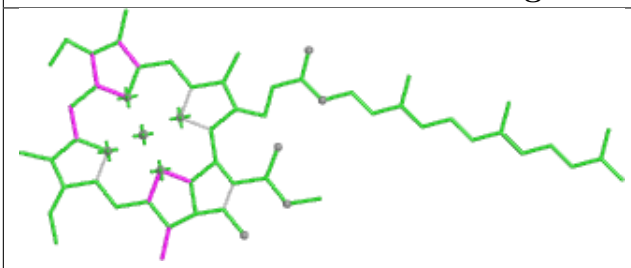


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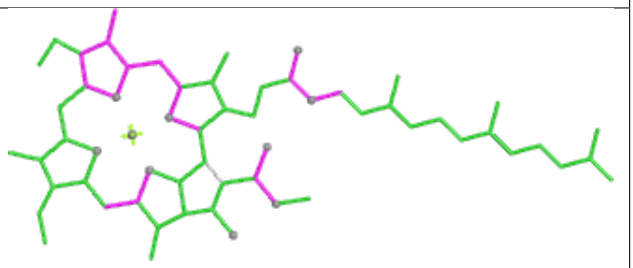


Rings

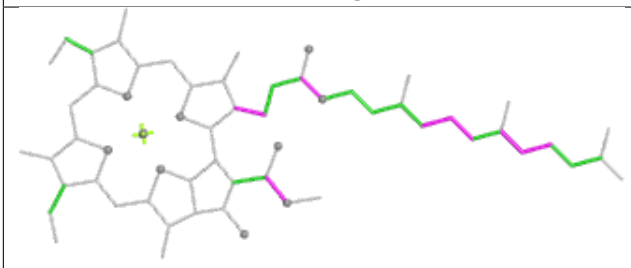
Ligand CLA B 802



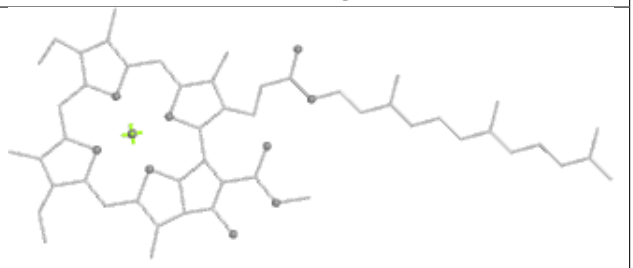
Bond lengths



Bond angles

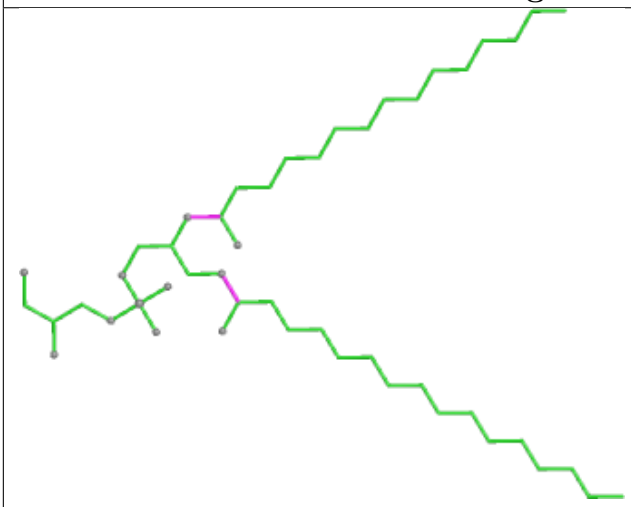


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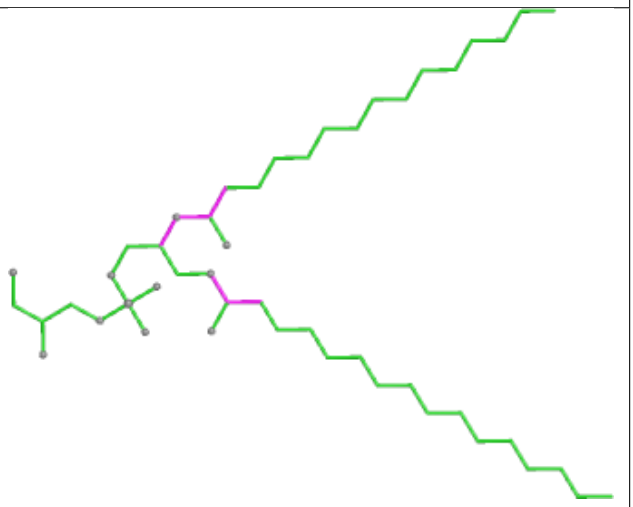


Rings

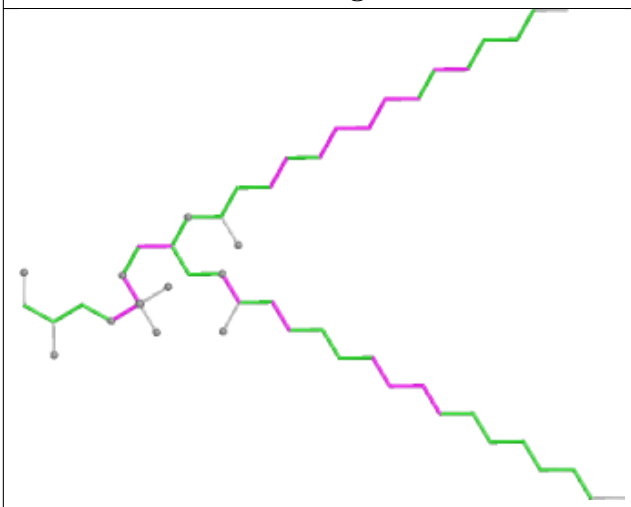
Ligand LHG 6 322



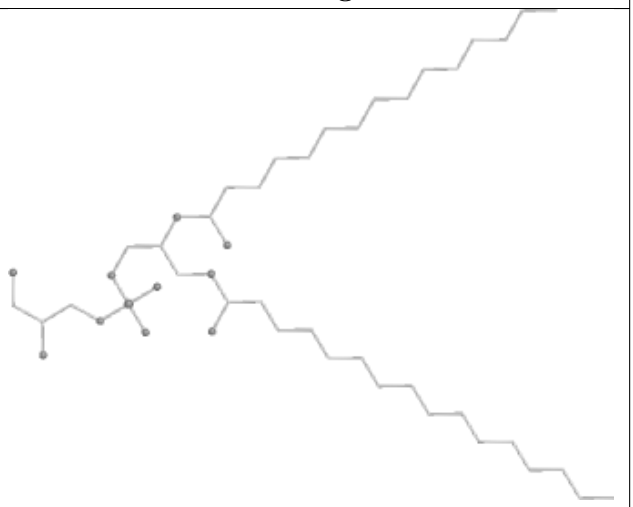
Bond lengths



Bond angles

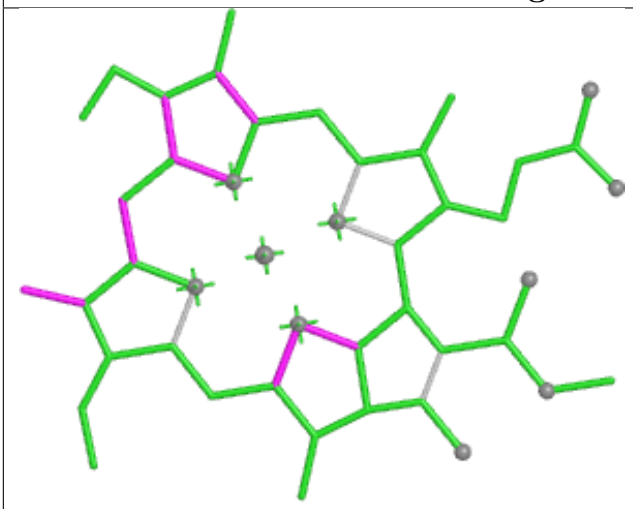


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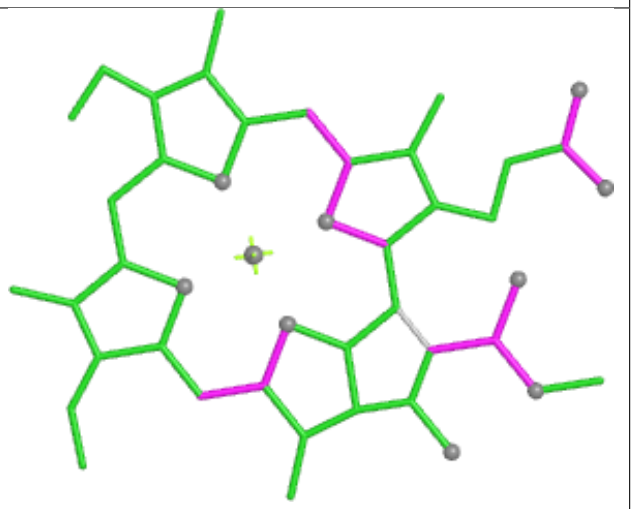


Rings

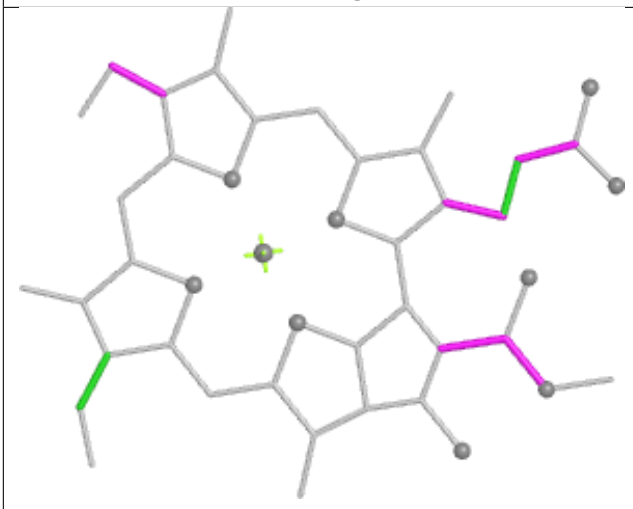
Ligand CLA 2 613



Bond lengths



Bond angles

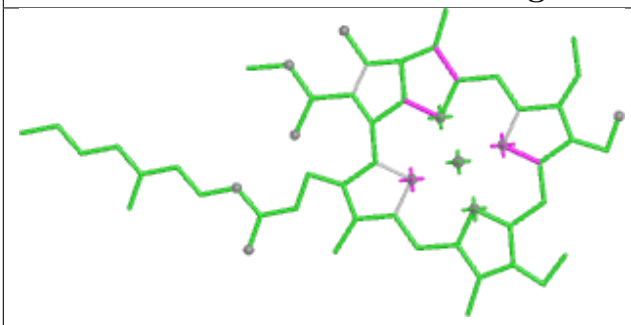


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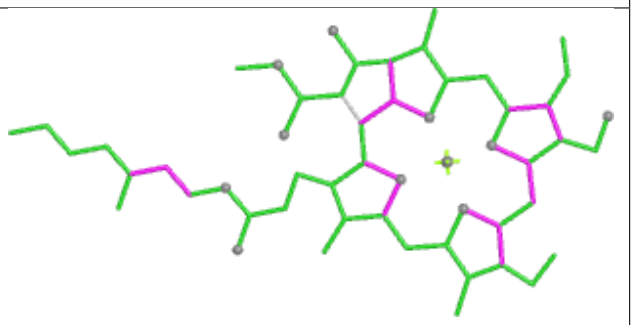


Rings

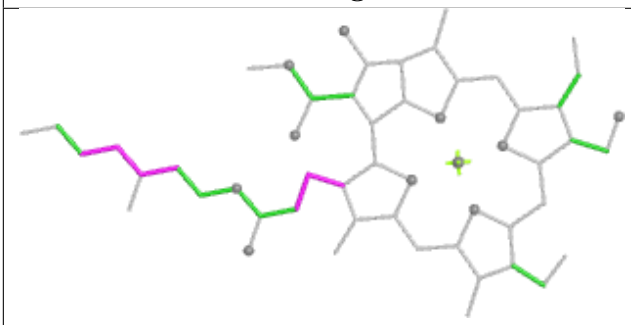
Ligand CHL 5 319



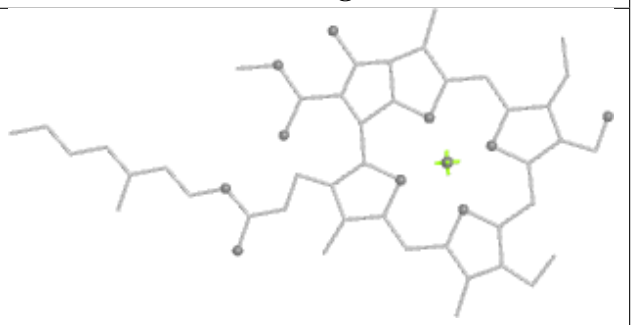
Bond lengths



Bond angles

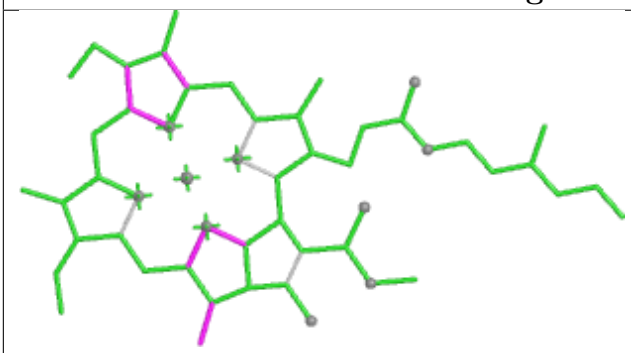


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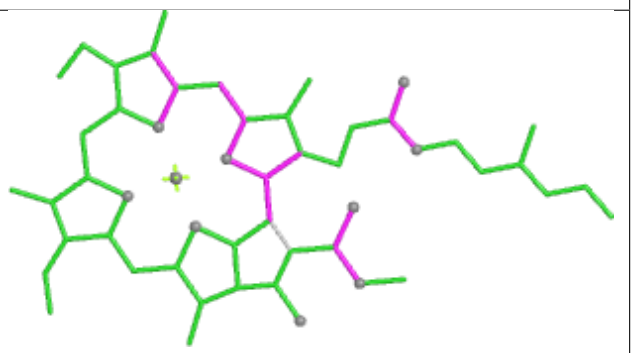


Rings

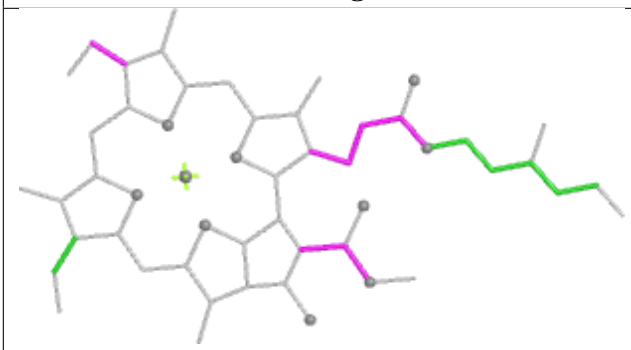
Ligand CLA F 804



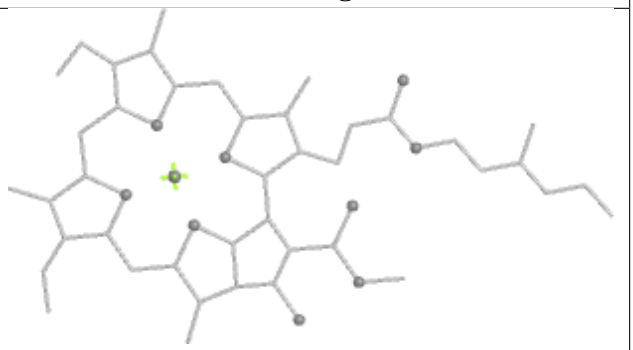
Bond lengths



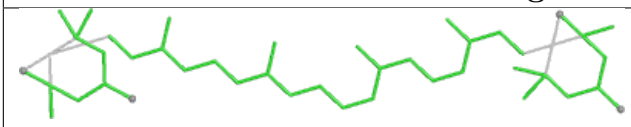
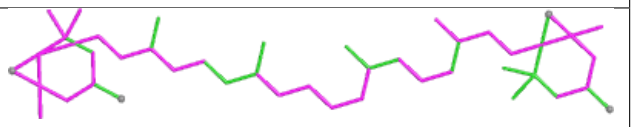
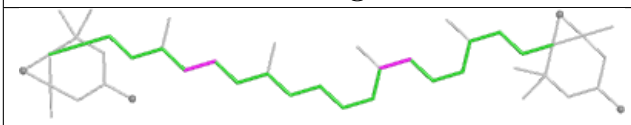
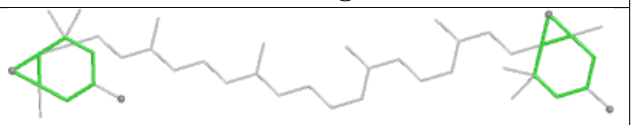
Bond angles

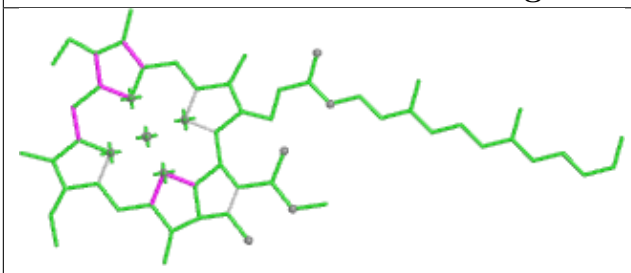
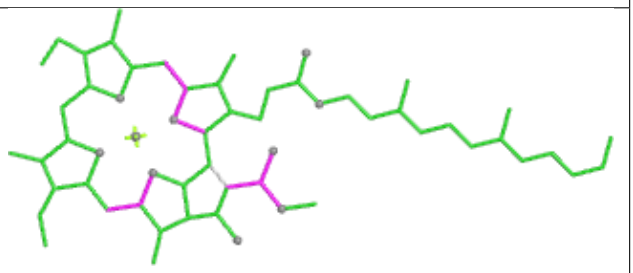
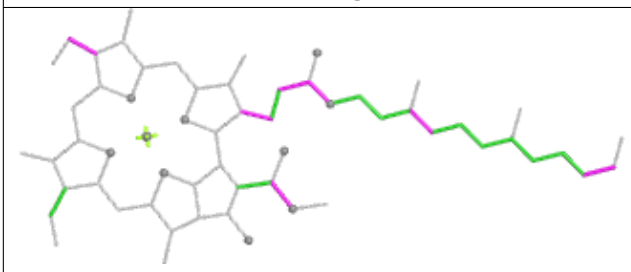
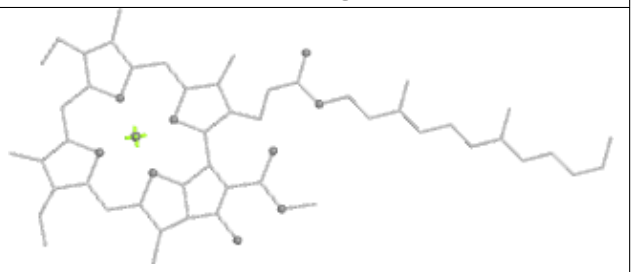


Torsions

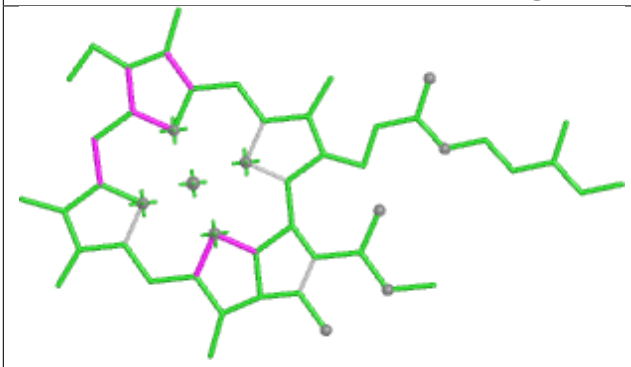


Rings

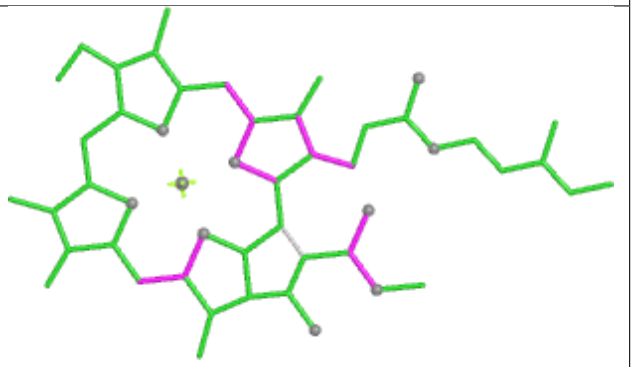
Ligand XAT 8 618	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 810	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

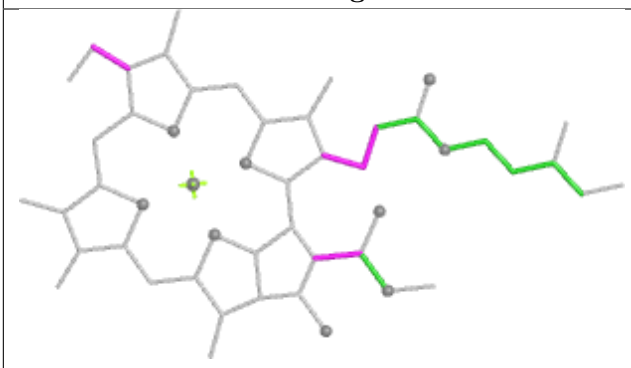
Ligand CLA 7 303



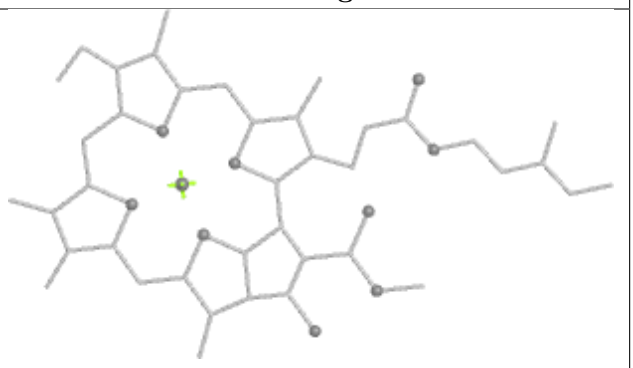
Bond lengths



Bond angles

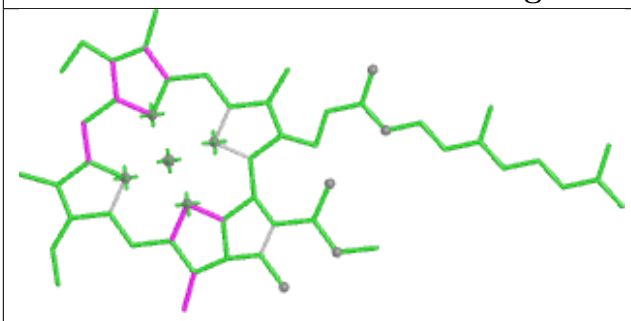


Torsions

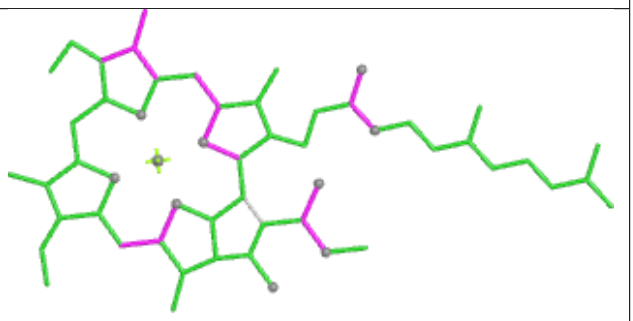


Rings

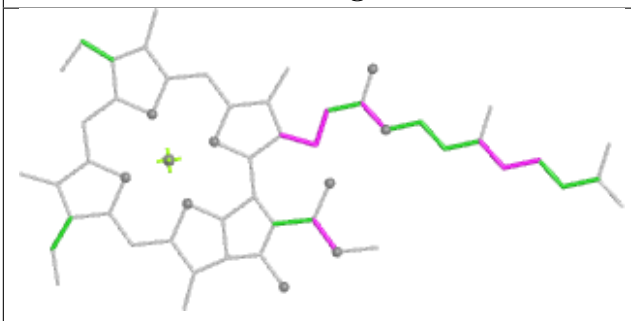
Ligand CLA B 817



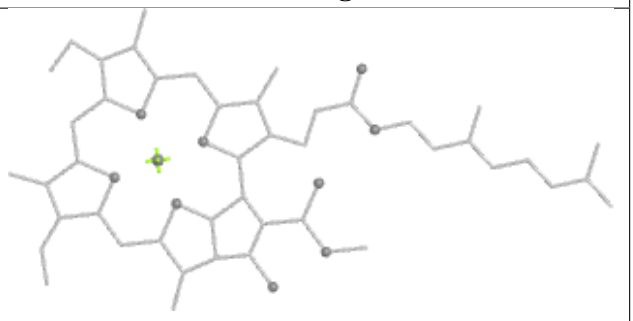
Bond lengths



Bond angles

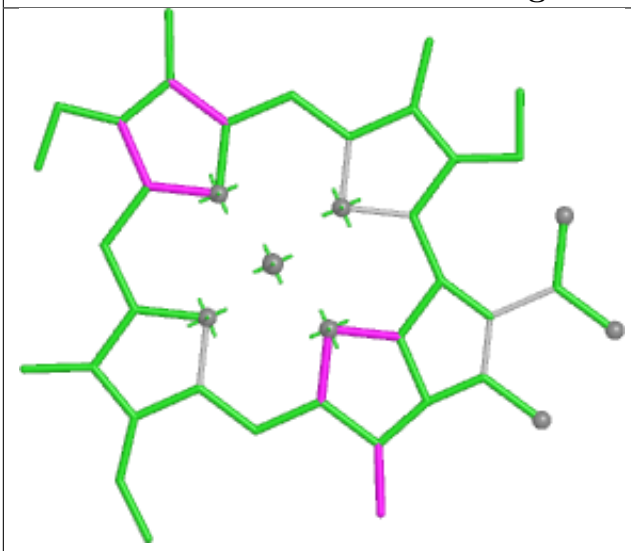


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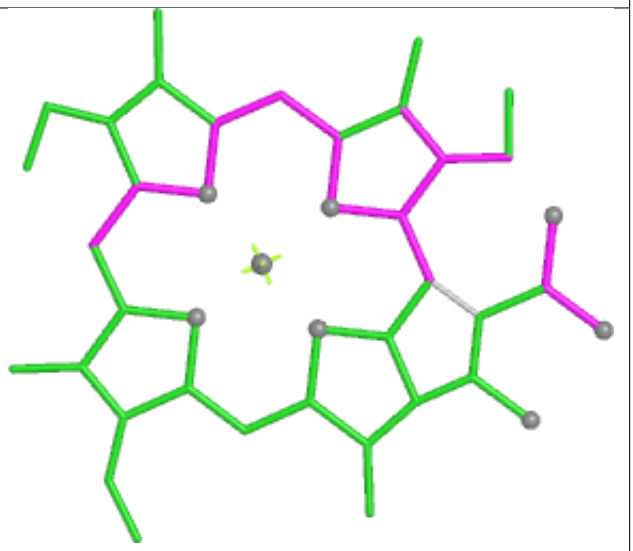


Rings

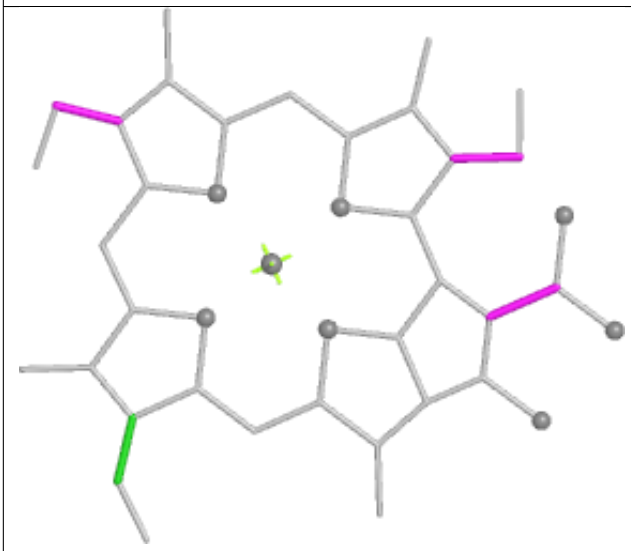
Ligand CLA 6 313



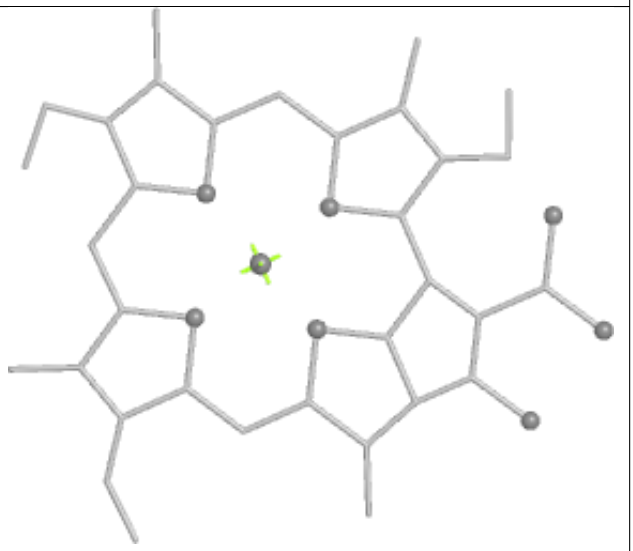
Bond lengths



Bond angles

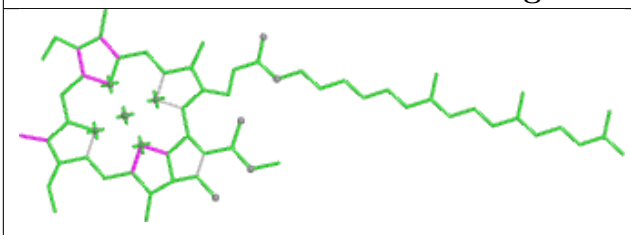


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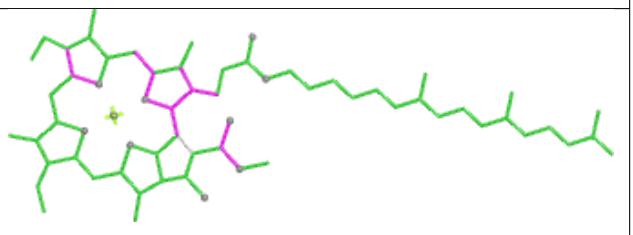


Rings

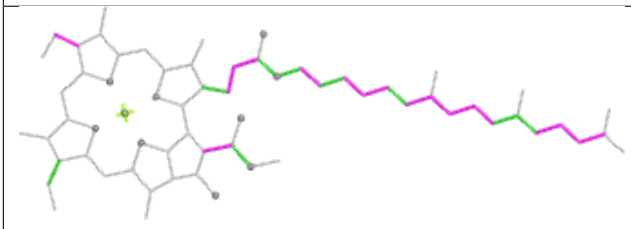
Ligand CLA A 812



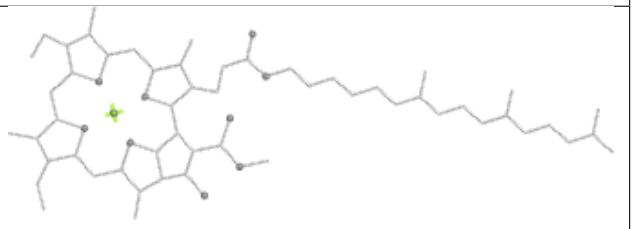
Bond lengths



Bond angles

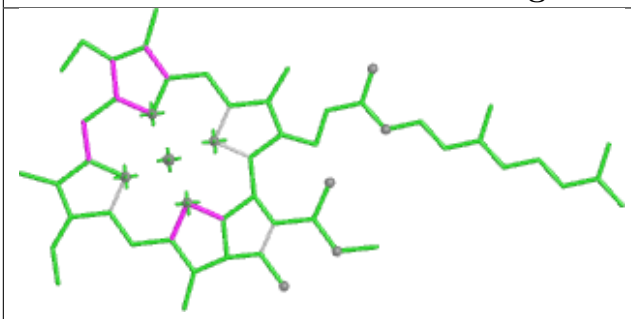


Torsions

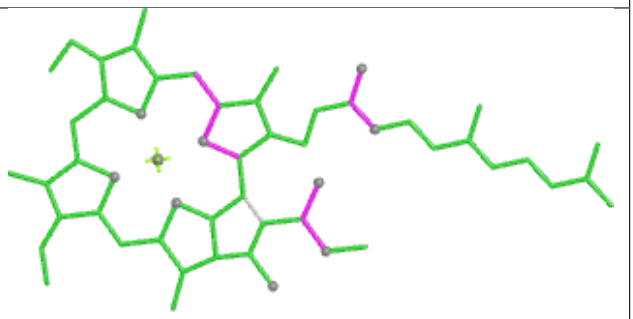


Rings

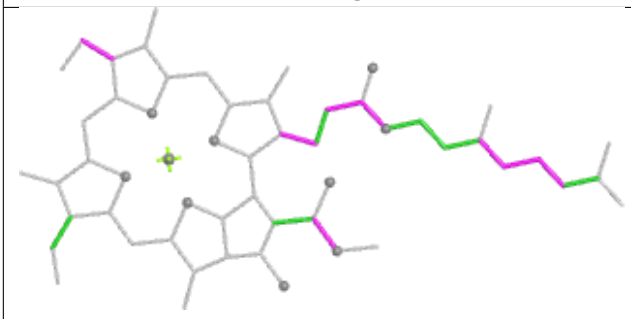
Ligand CLA 3 409



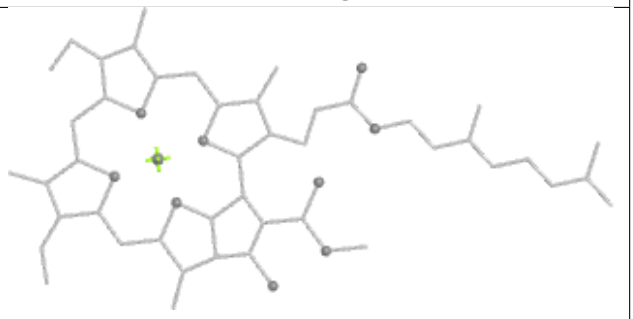
Bond lengths



Bond angles

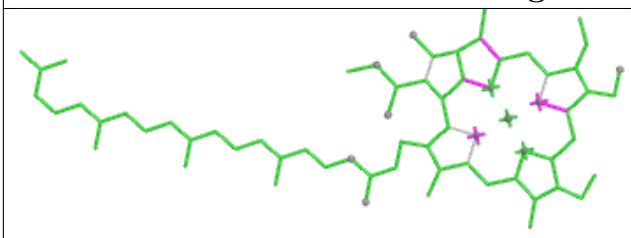


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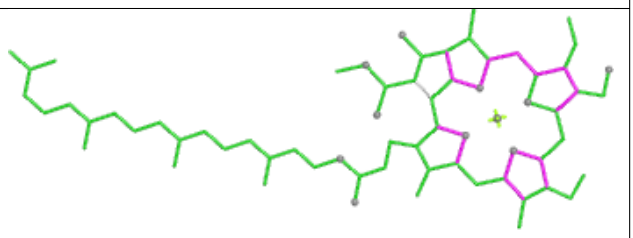


Rings

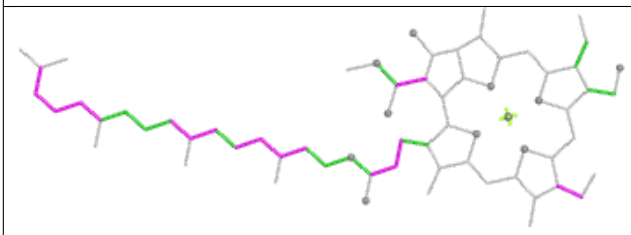
Ligand CHL 8 602



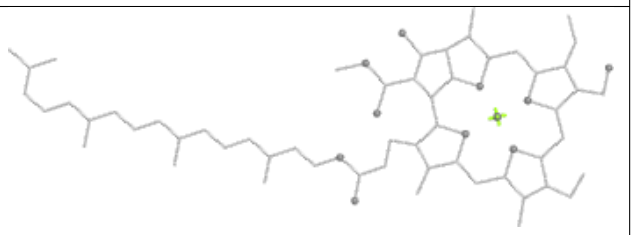
Bond lengths



Bond angles

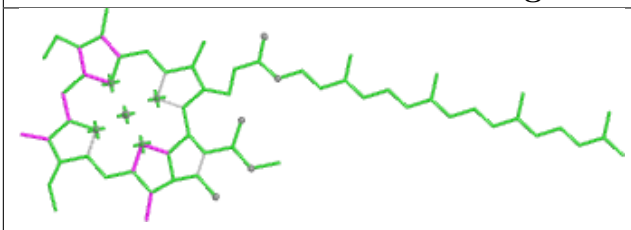


Torsions

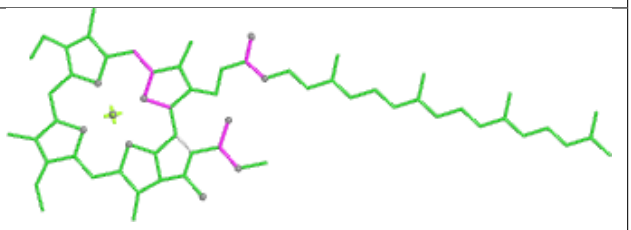


Rings

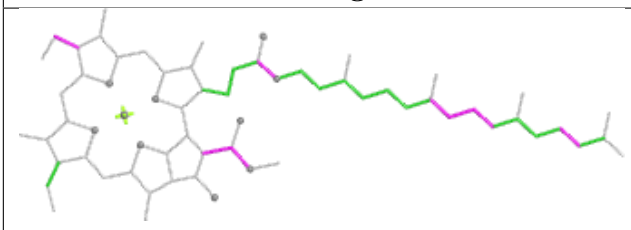
Ligand CLA B 844



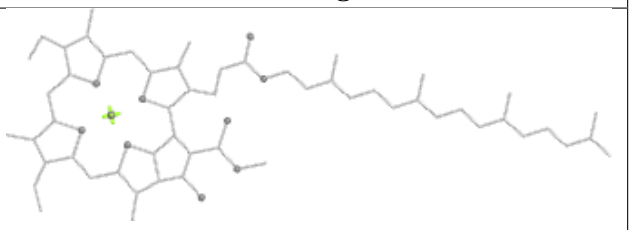
Bond lengths



Bond angles

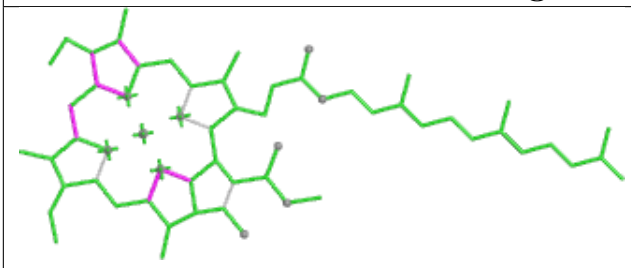


Torsions

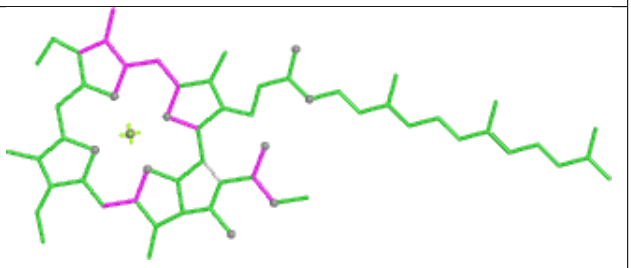


Rings

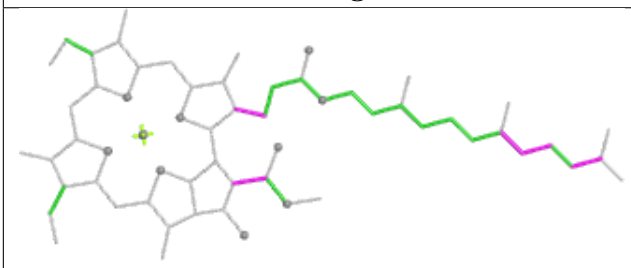
Ligand CLA 8 614



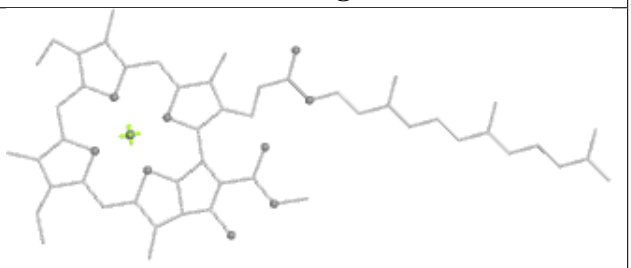
Bond lengths



Bond angles



Torsions

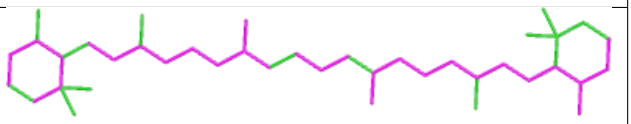


Rings

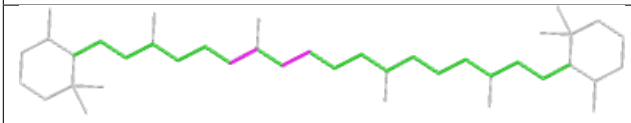
Ligand BCR F 801



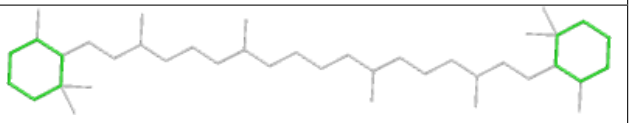
Bond lengths



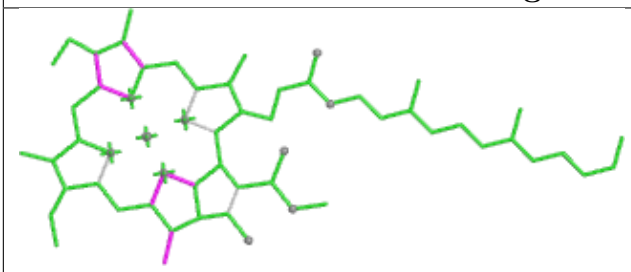
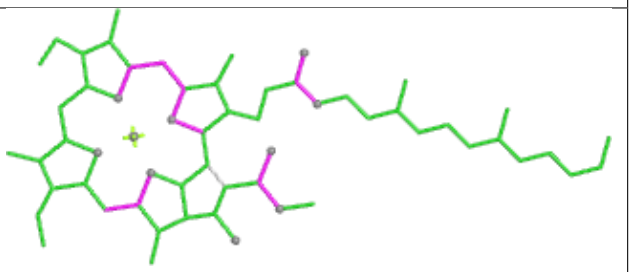
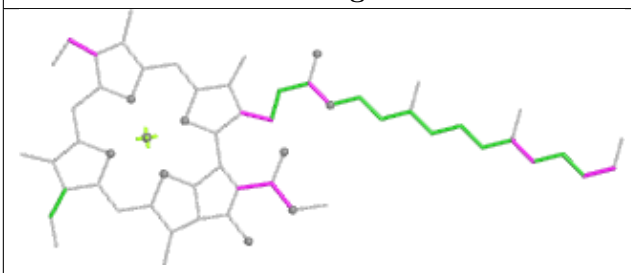
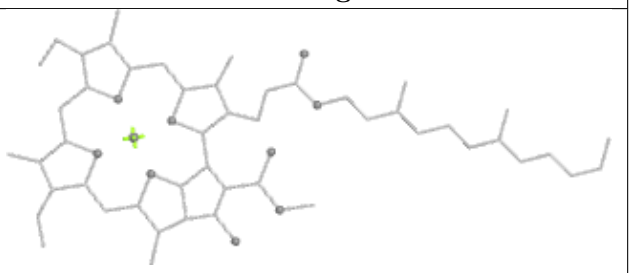
Bond angles

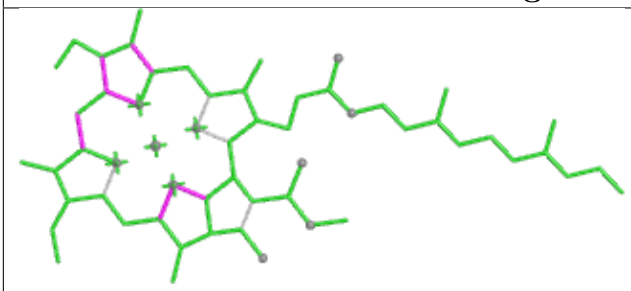
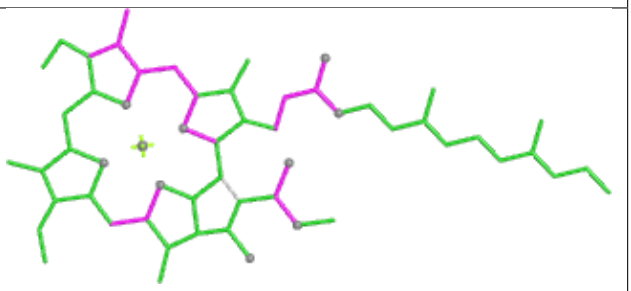
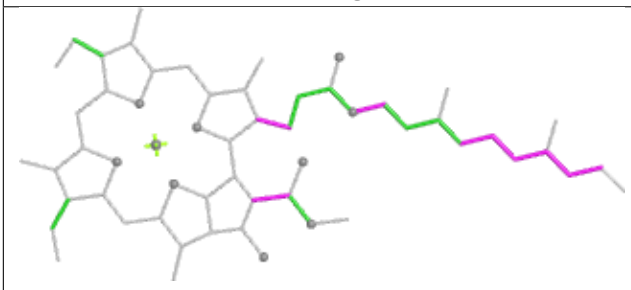
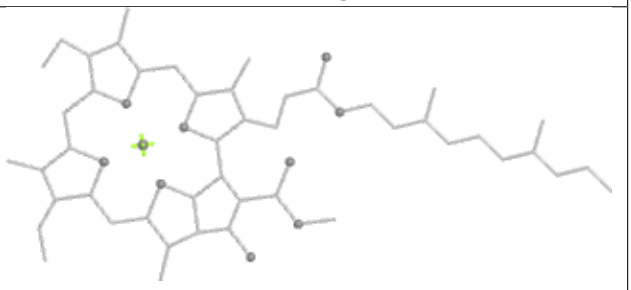


Torsions

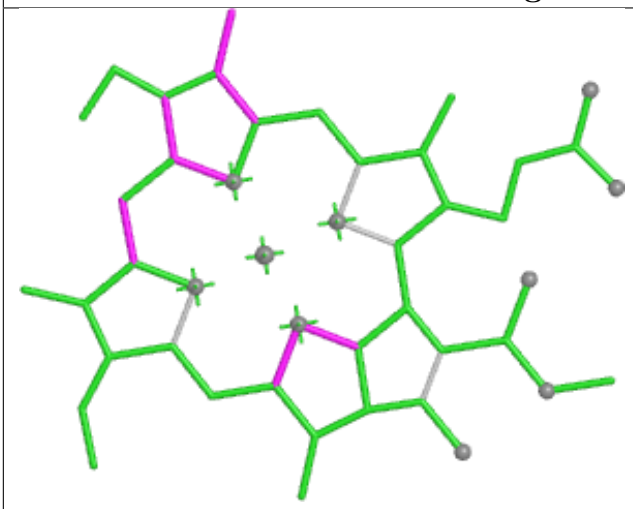


Rings

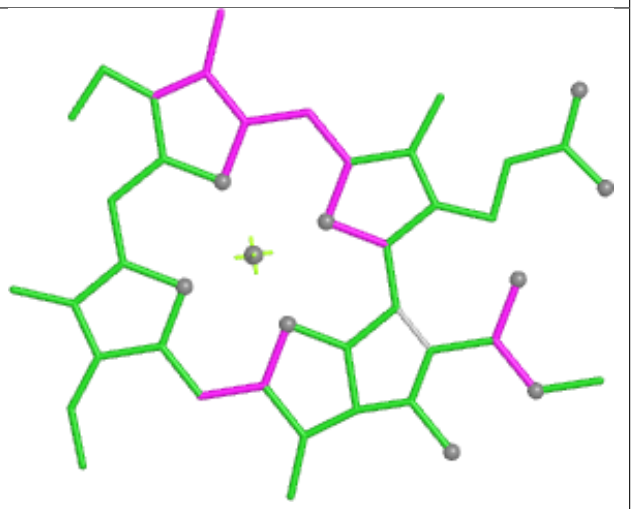
Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

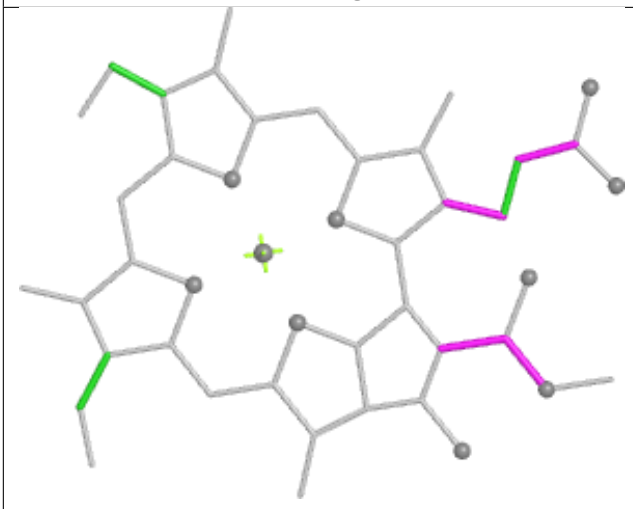
Ligand CLA B 822



Bond lengths



Bond angles

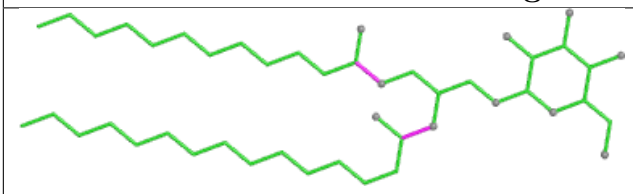


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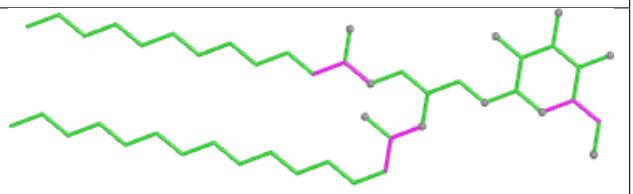


Rings

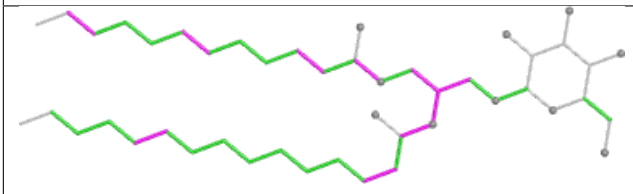
Ligand LMG 9 617



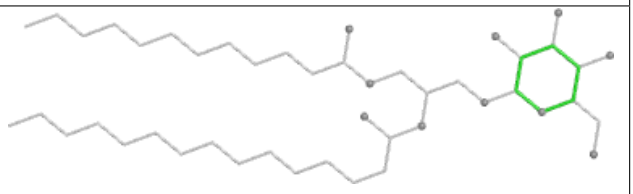
Bond lengths



Bond angles

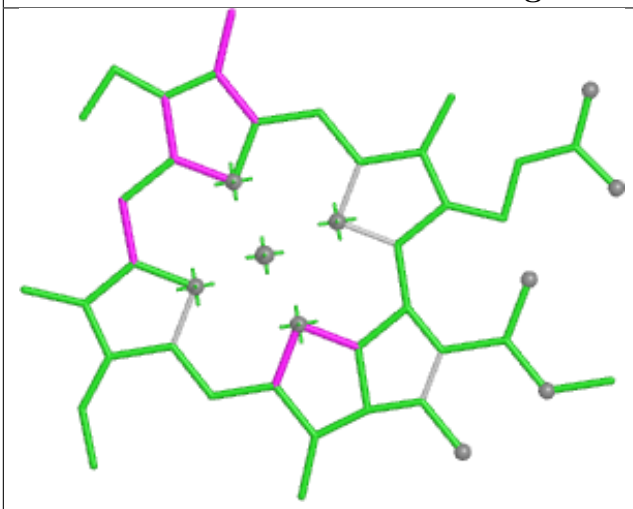


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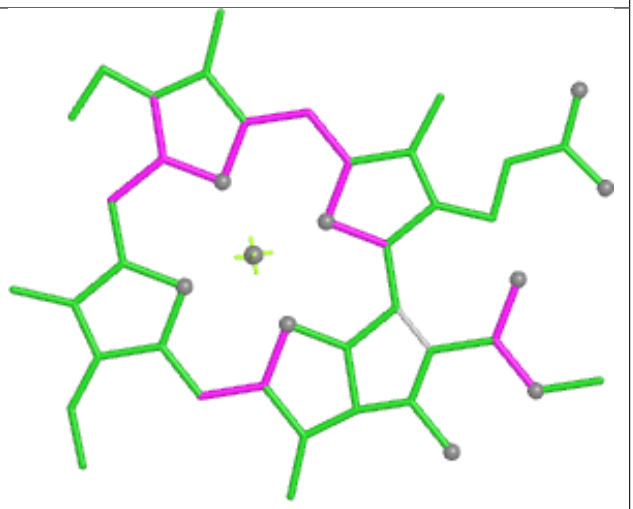


Rings

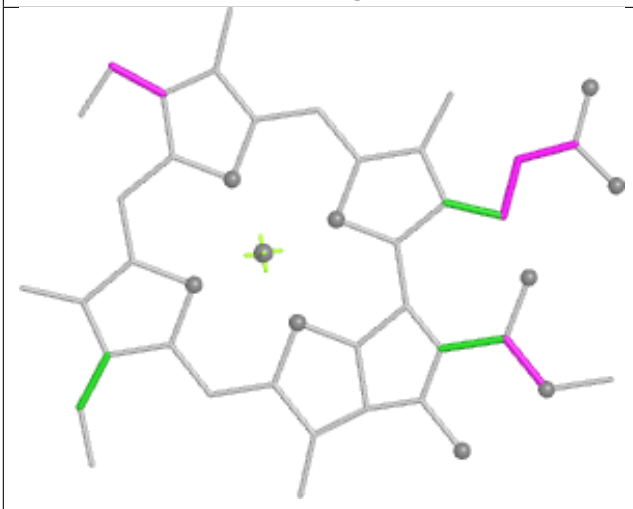
Ligand CLA B 838



Bond lengths



Bond angles

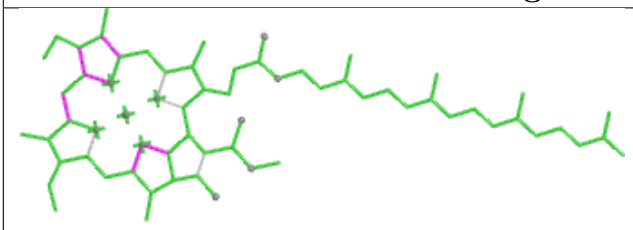


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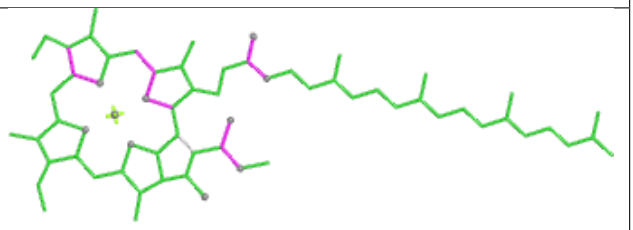


Rings

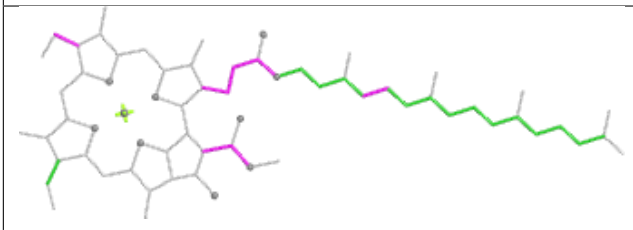
Ligand CLA A 839



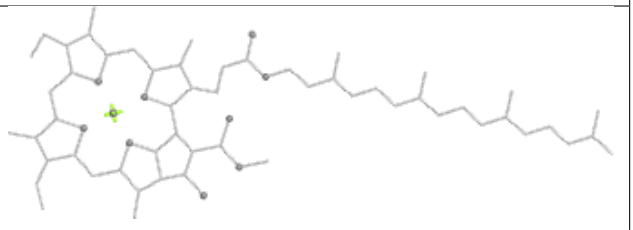
Bond lengths



Bond angles

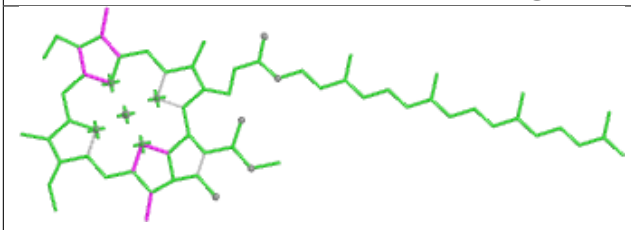


Torsions

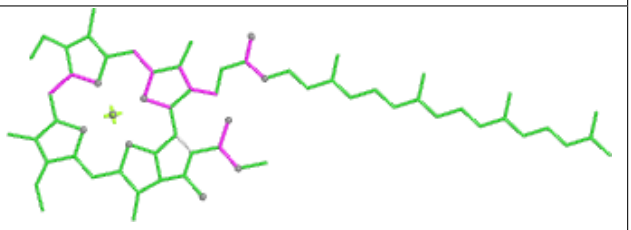


Rings

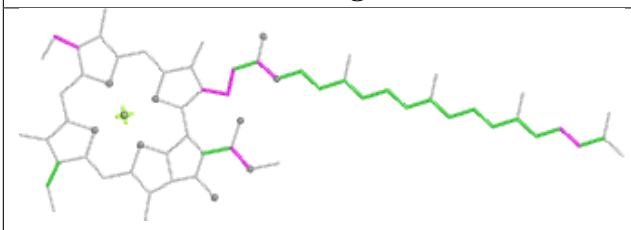
Ligand CLA 3 402



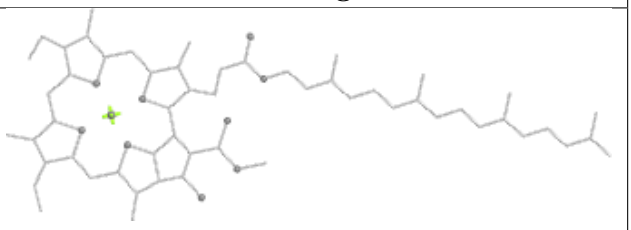
Bond lengths



Bond angles

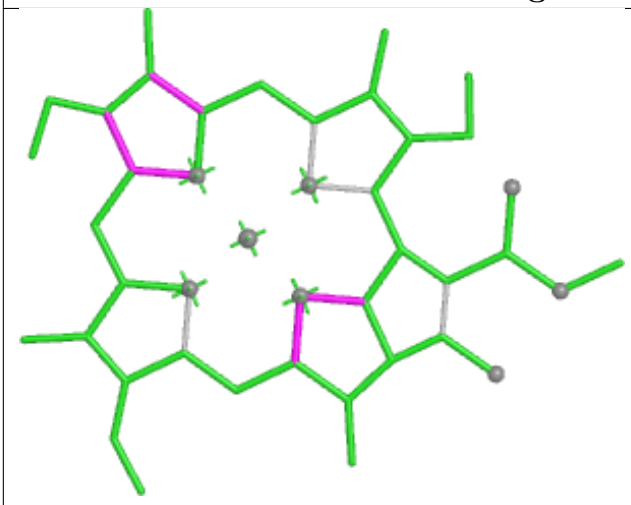


Torsions

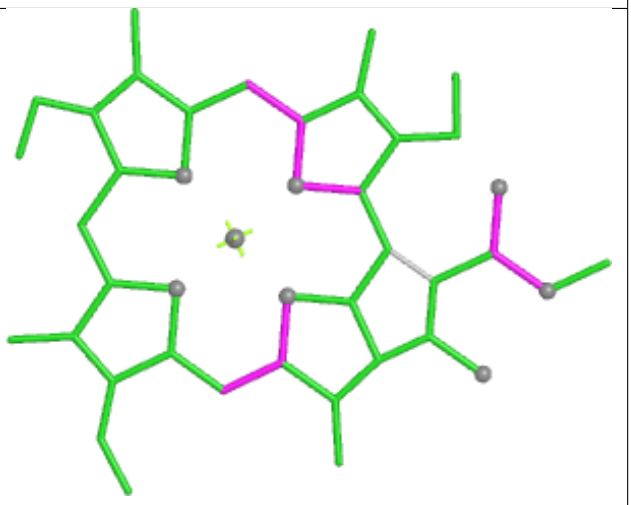


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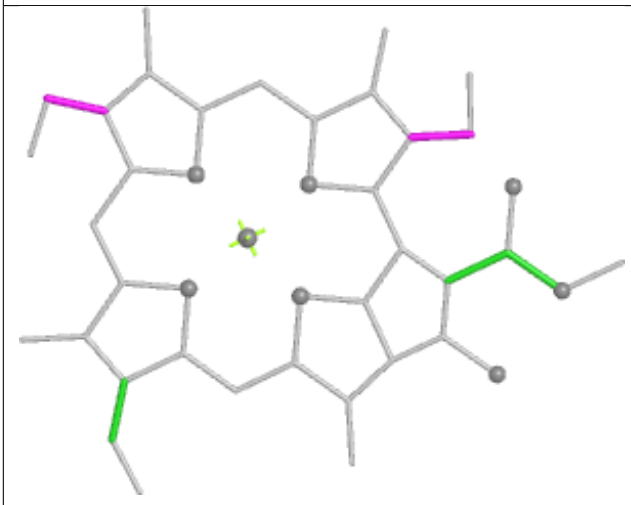
Ligand CLA 6 306



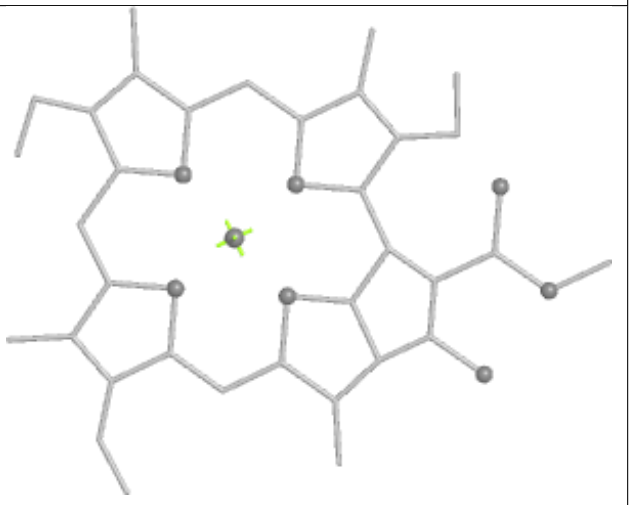
Bond lengths



Bond angles

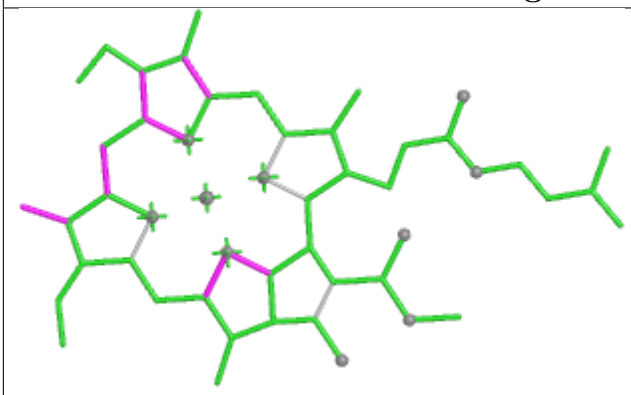


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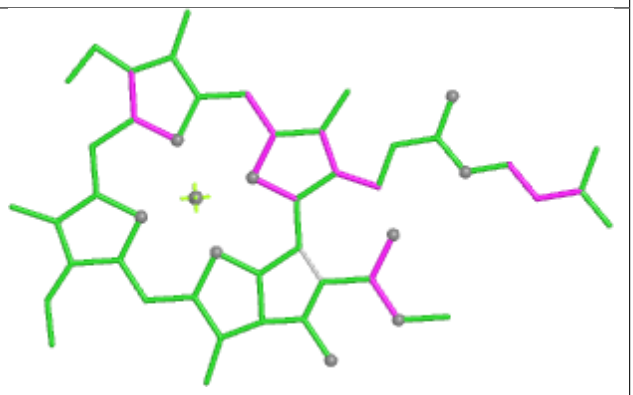


Rings

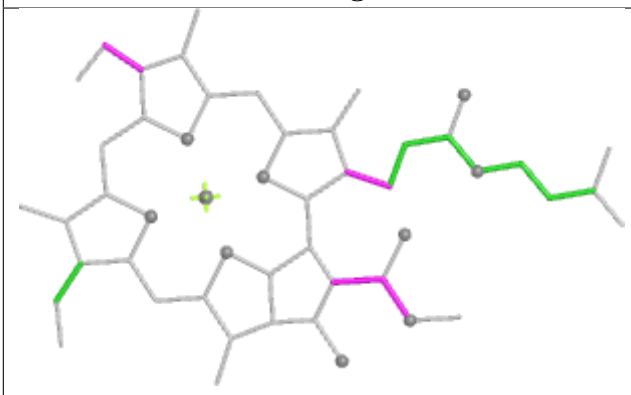
Ligand CLA B 839



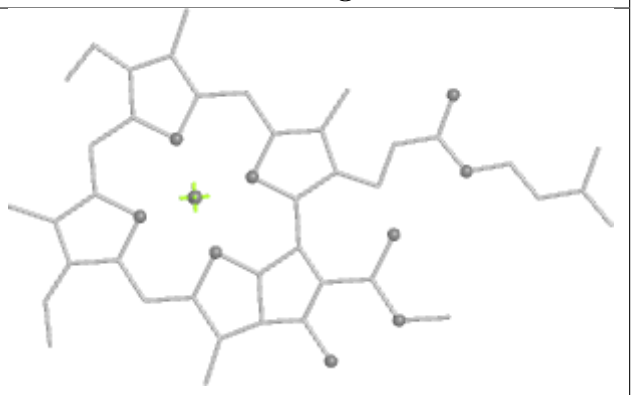
Bond lengths



Bond angles

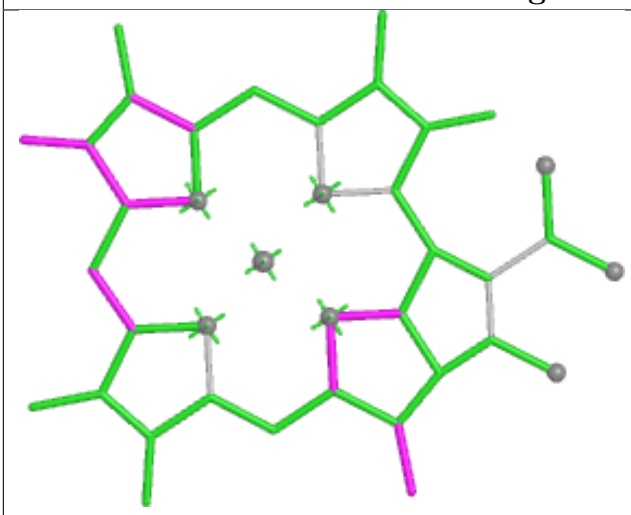


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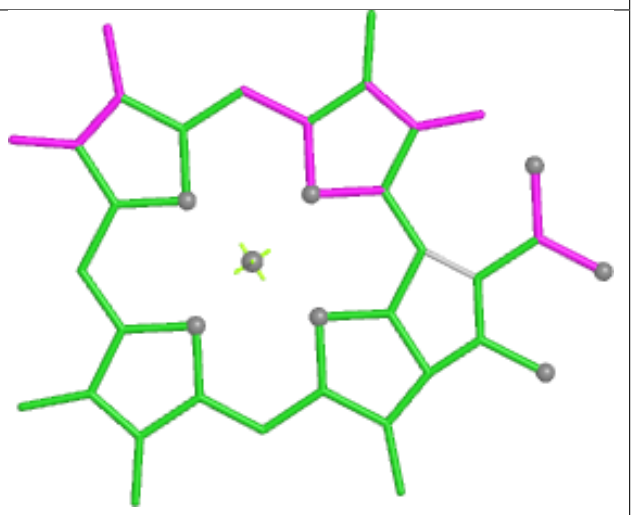


Rings

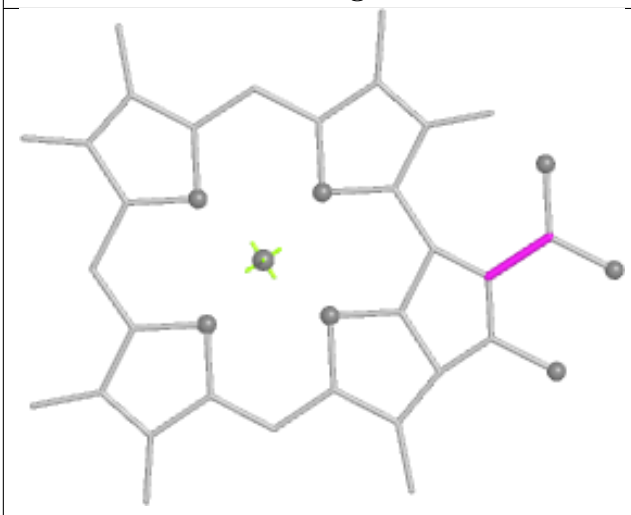
Ligand CLA 1 307



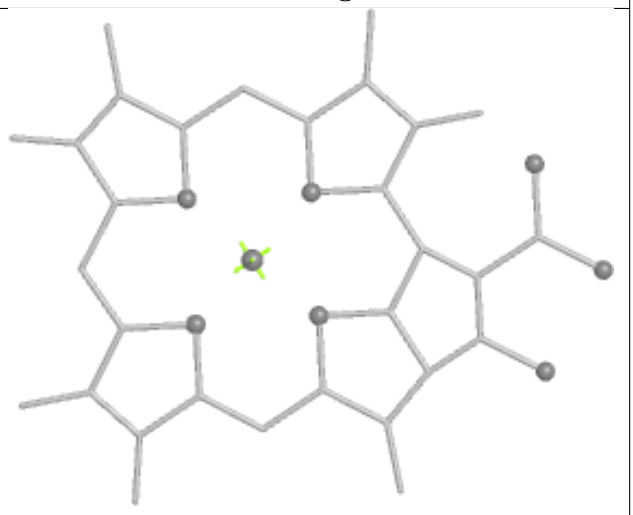
Bond lengths



Bond angles

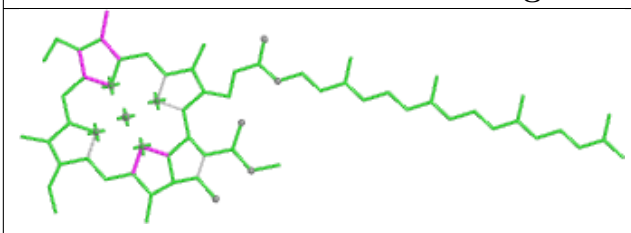


Torsions

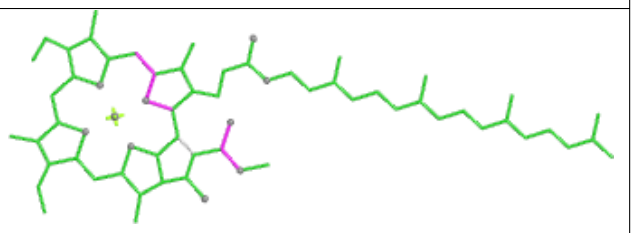


Rings

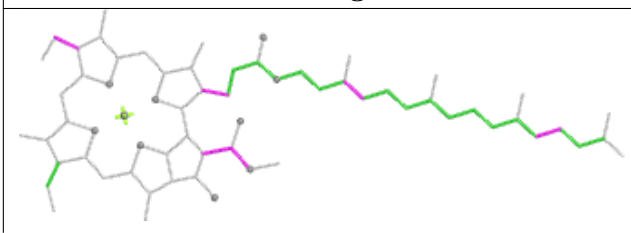
Ligand CLA A 829



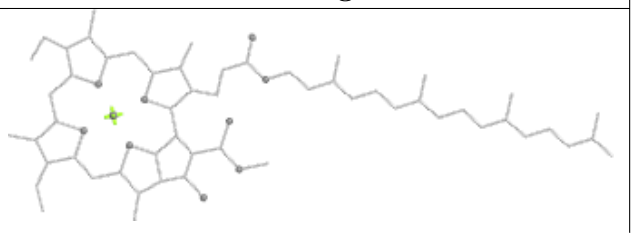
Bond lengths



Bond angles

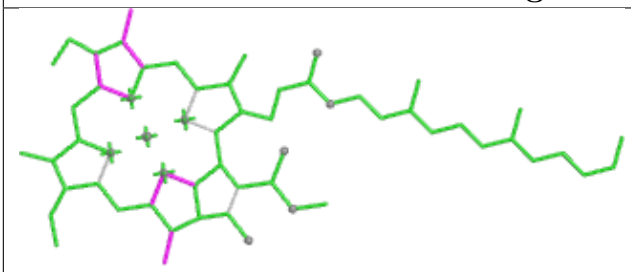


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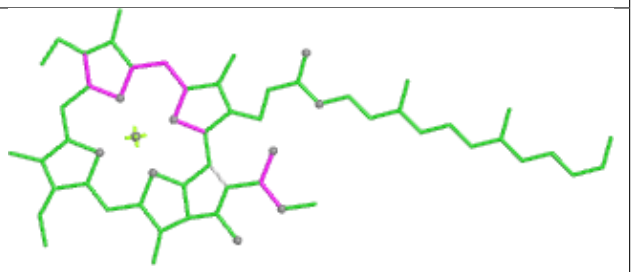


Rings

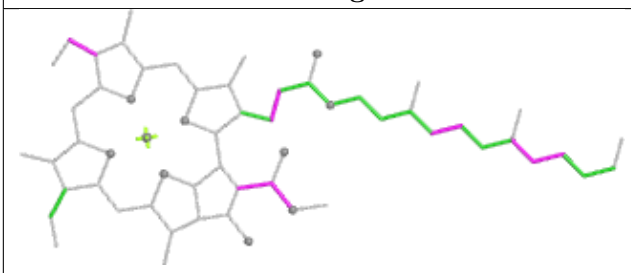
Ligand CLA F 802



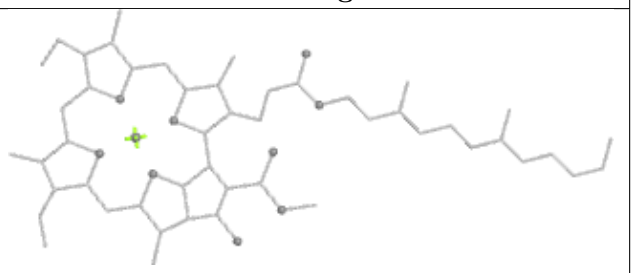
Bond lengths



Bond angles

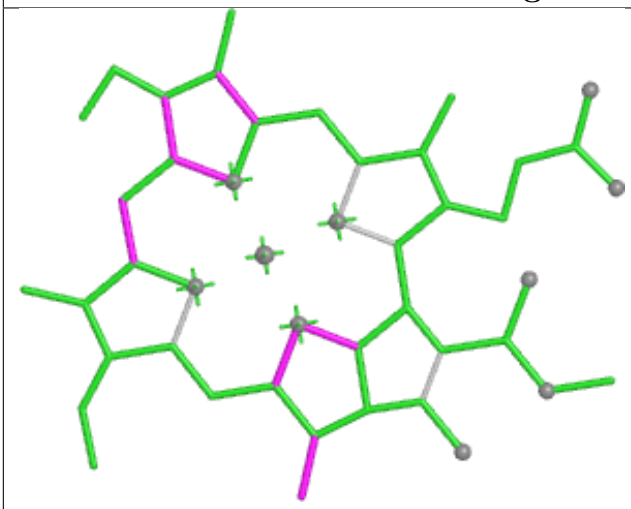


Torsions

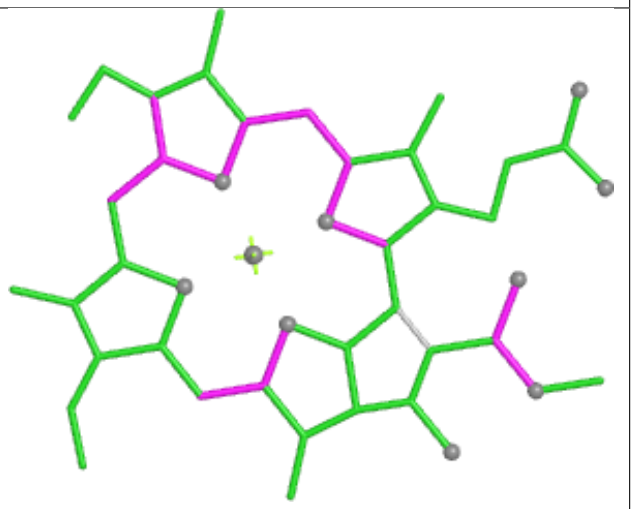


Rings

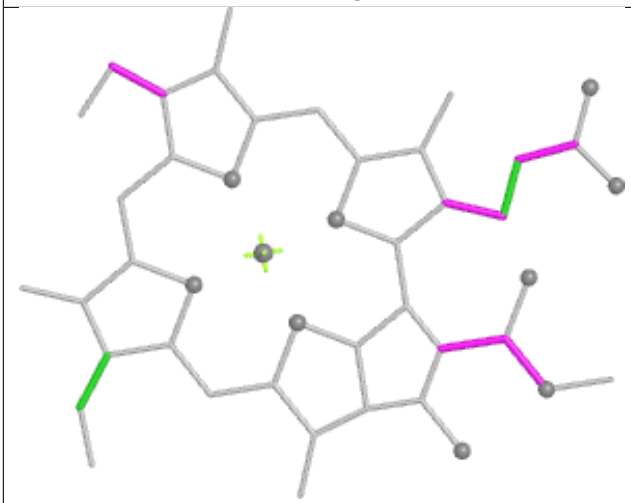
Ligand CLA A 830



Bond lengths



Bond angles

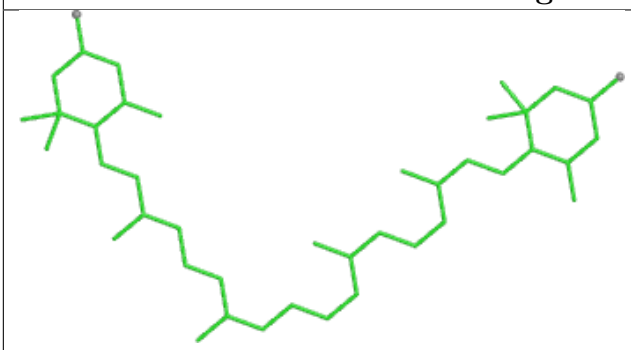


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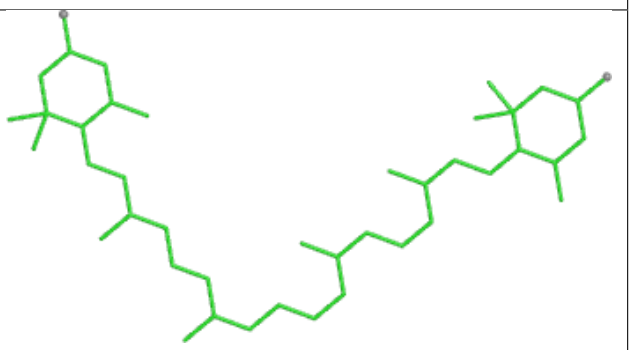


Rings

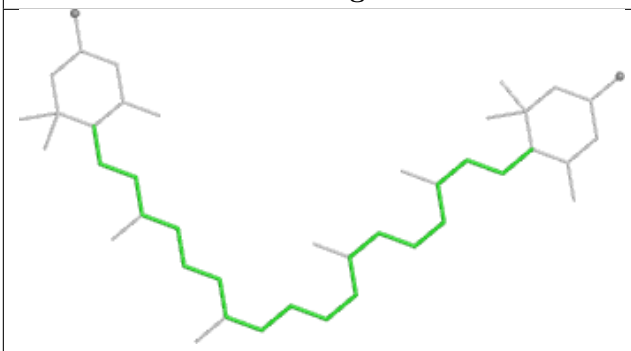
Ligand K3I 5 324



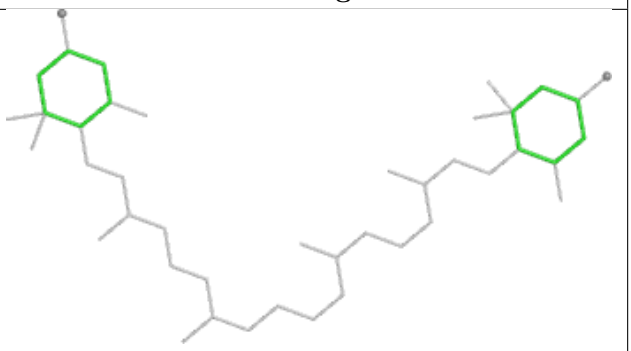
Bond lengths



Bond angles

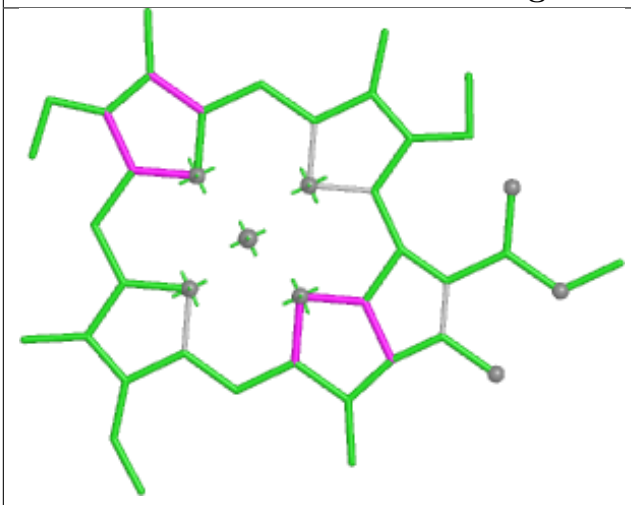


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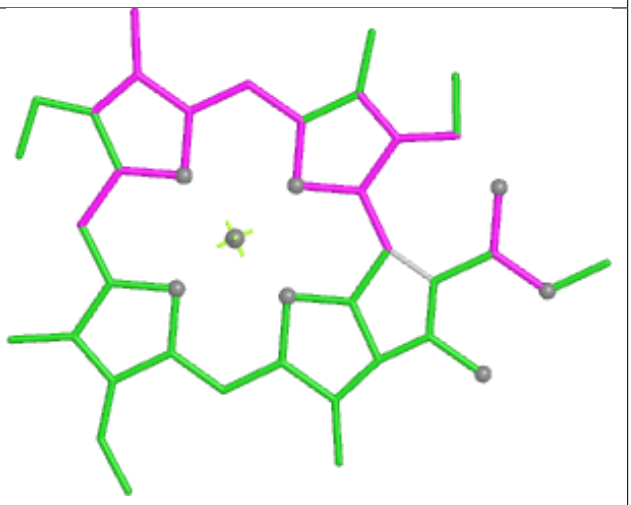


Rings

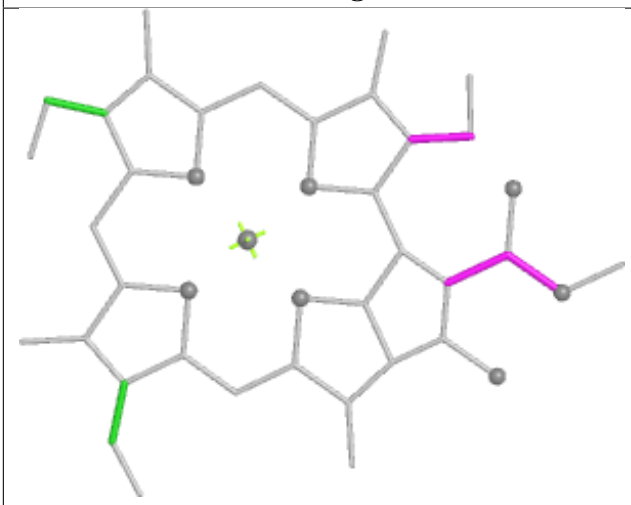
Ligand CLA 9 610



Bond lengths



Bond angles

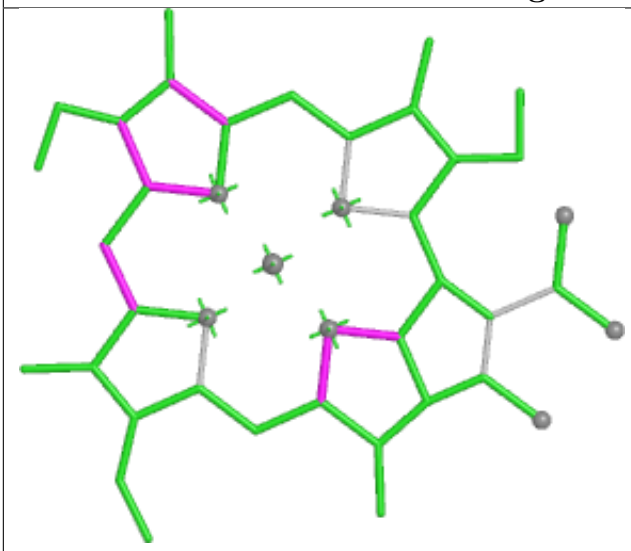


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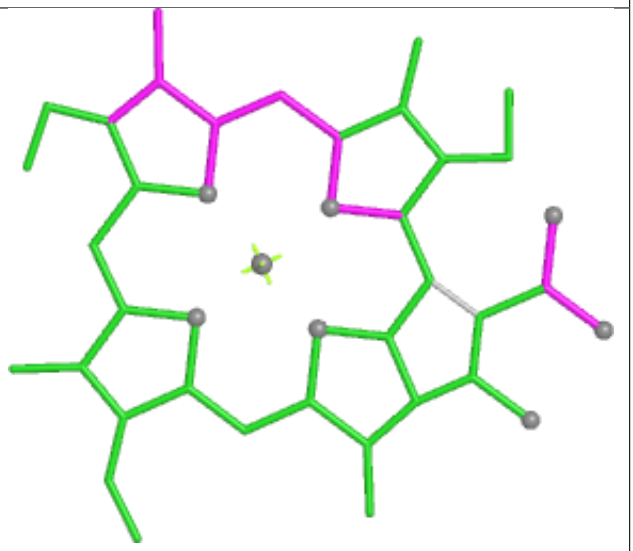


Rings

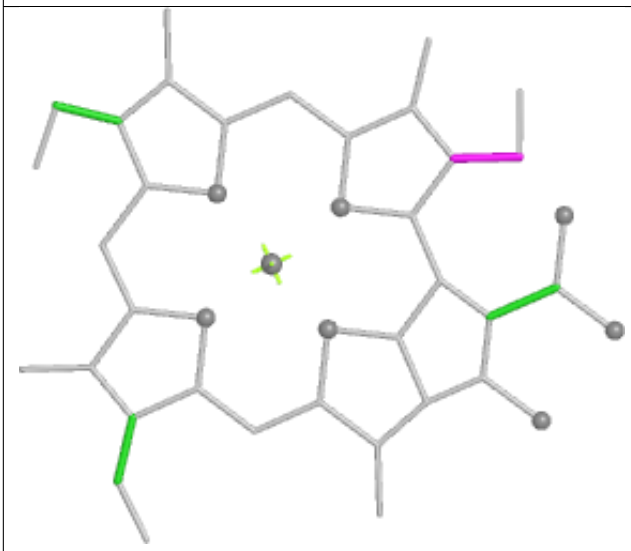
Ligand CLA 1 309



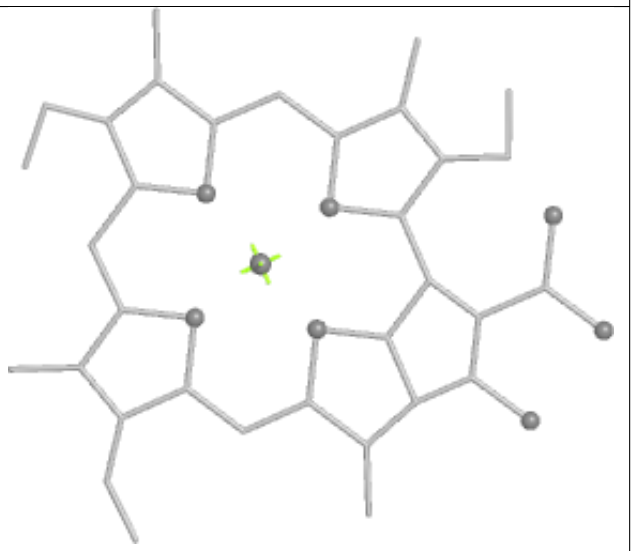
Bond lengths



Bond angles

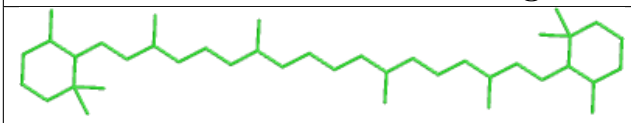


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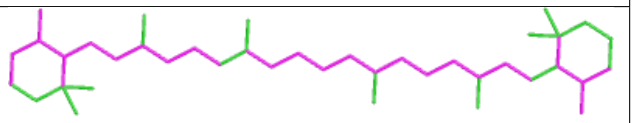


Rings

Ligand BCR B 849



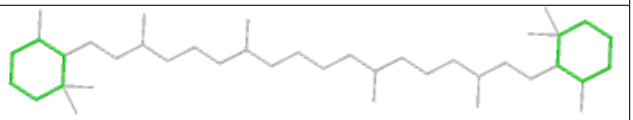
Bond lengths



Bond angles

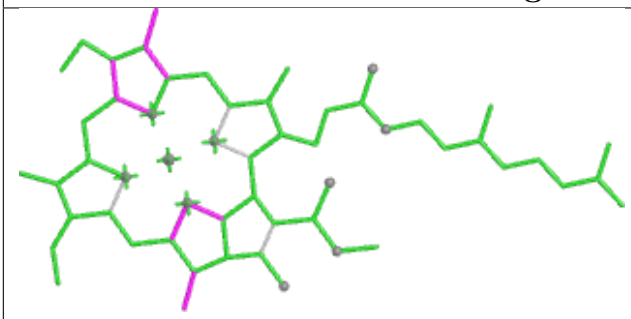


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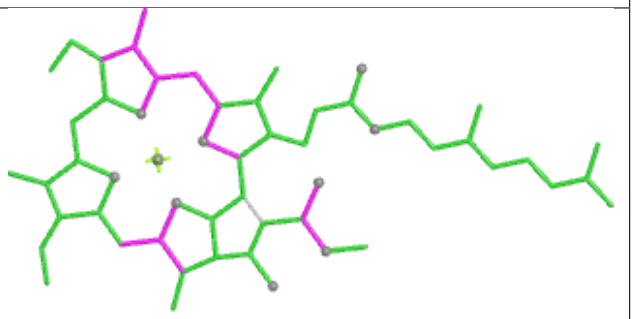


Rings

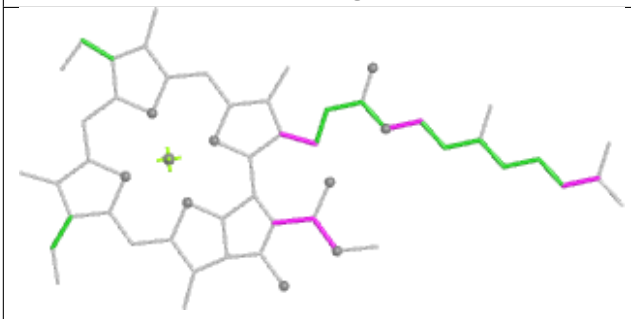
Ligand CLA B 832



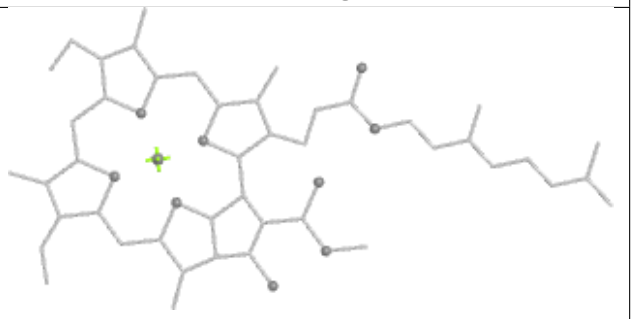
Bond lengths



Bond angles

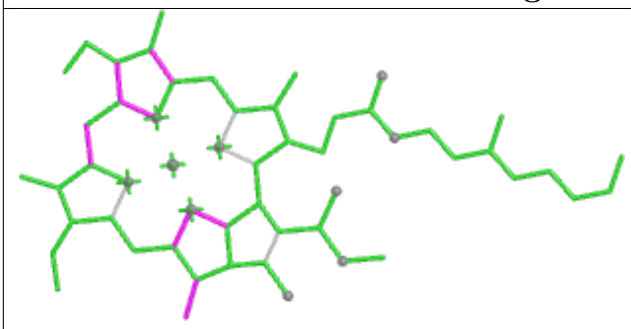


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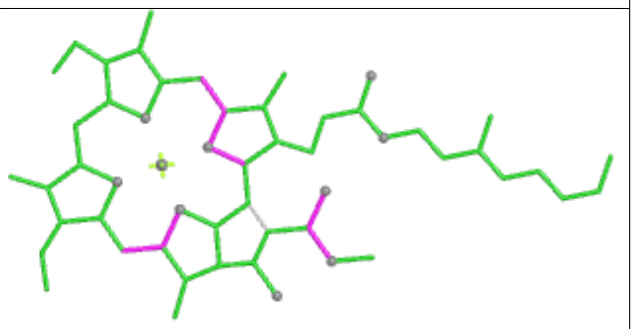


Rings

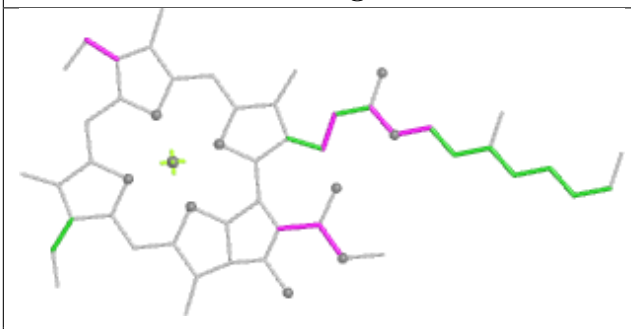
Ligand CLA A 811



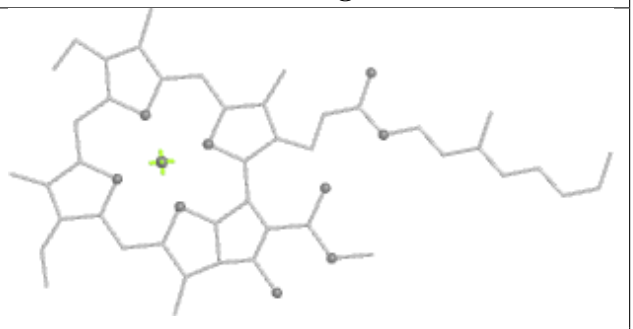
Bond lengths



Bond angles

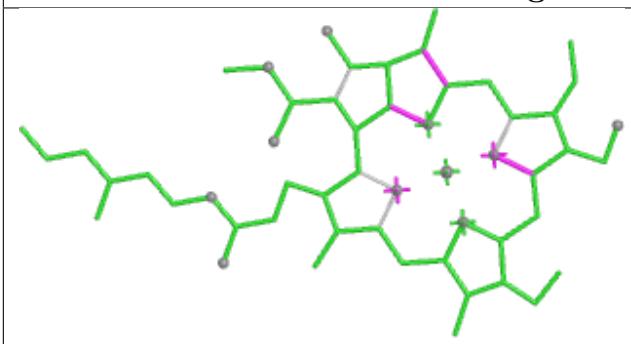


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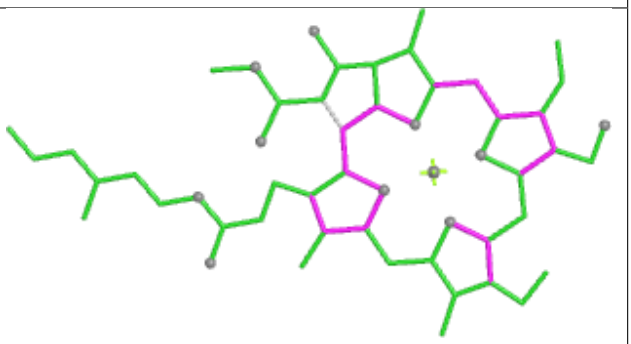


Rings

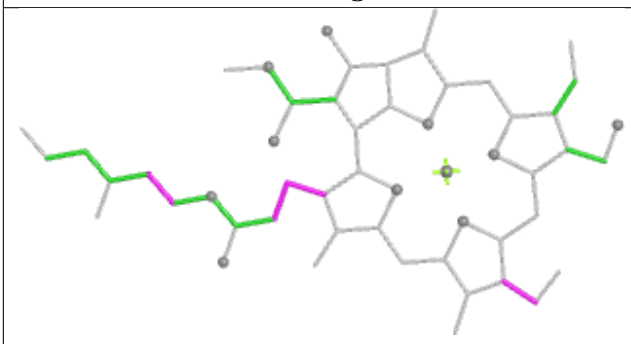
Ligand CHL 3 405



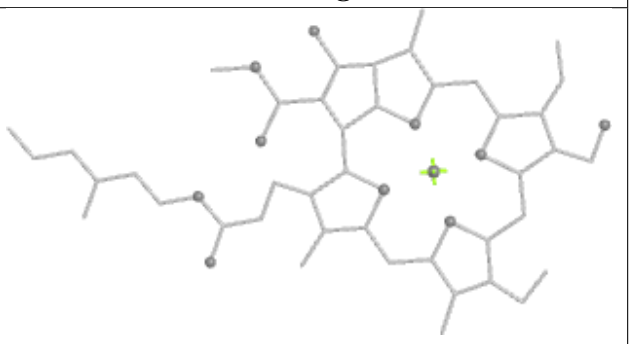
Bond lengths



Bond angles

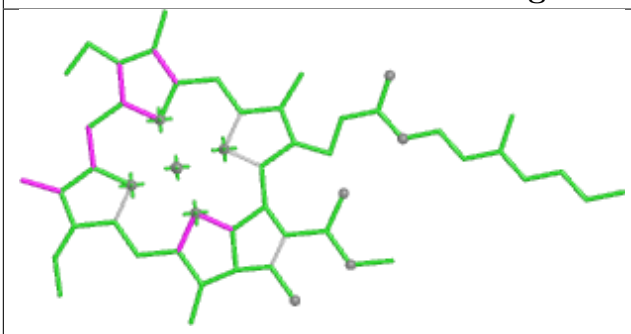


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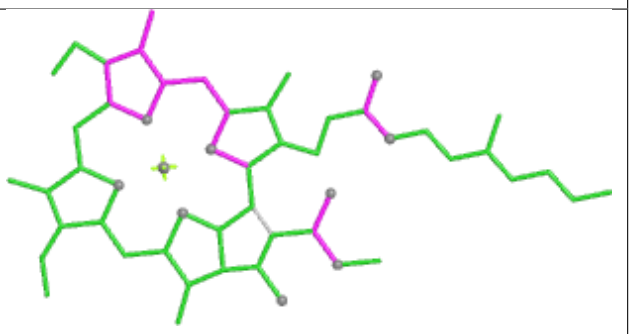


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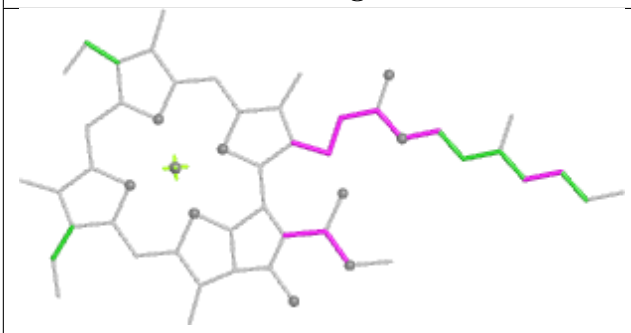
Ligand CLA 2 601



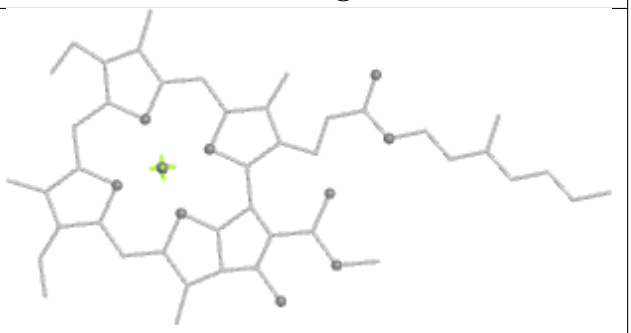
Bond lengths



Bond angles

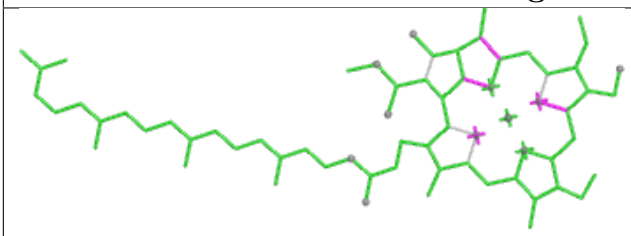


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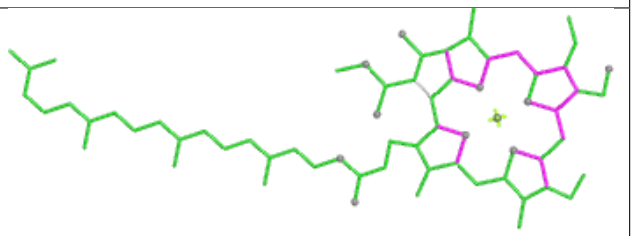


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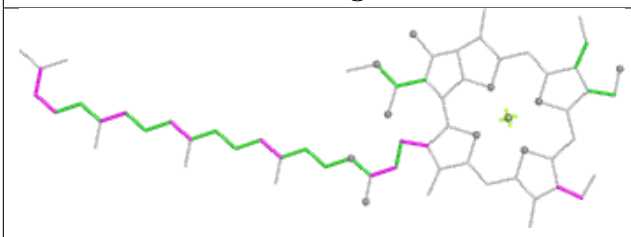
Ligand CHL 5 308



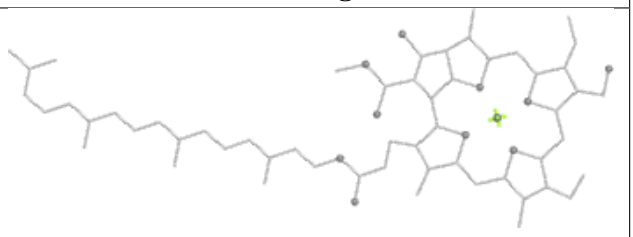
Bond lengths



Bond angles

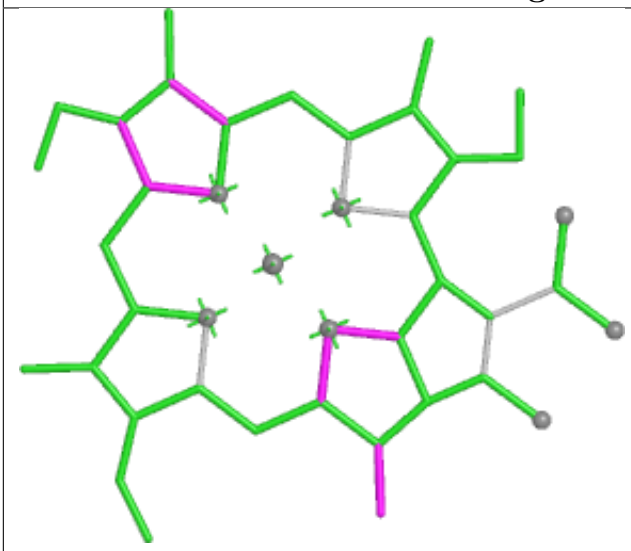


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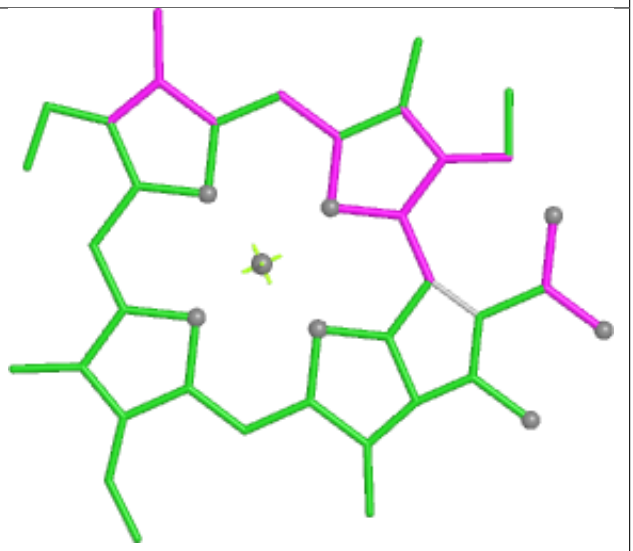


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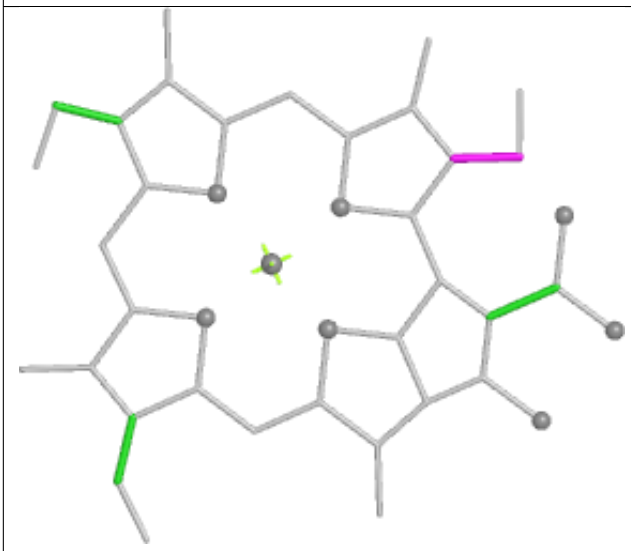
Ligand CLA 5 313



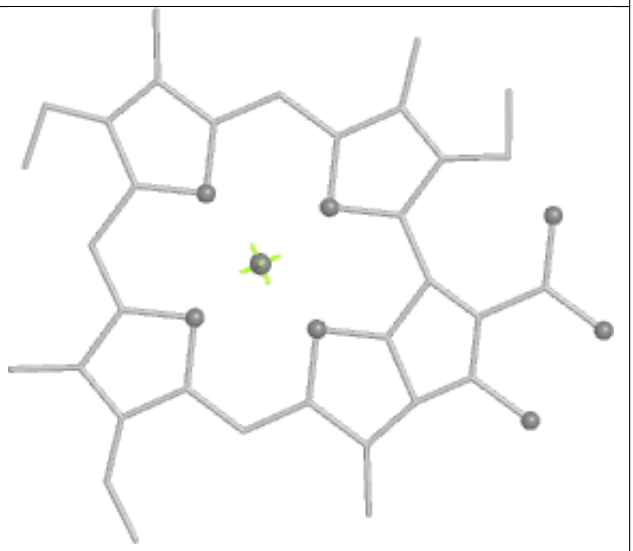
Bond lengths



Bond angles

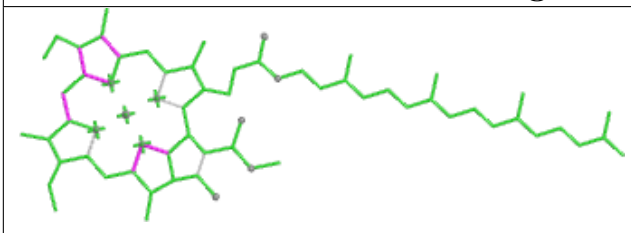


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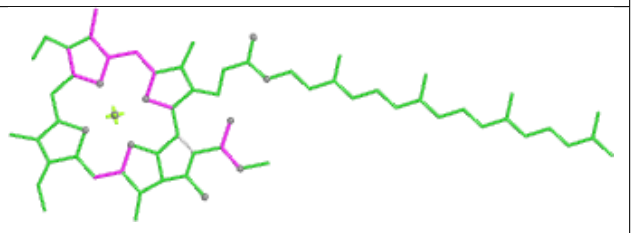


Rings

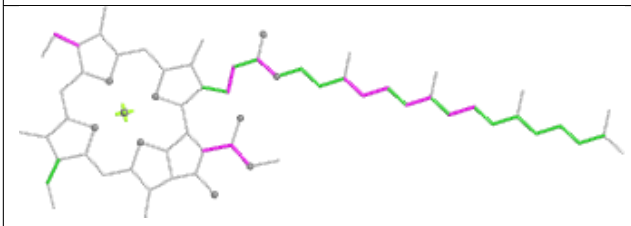
Ligand CLA 6 304



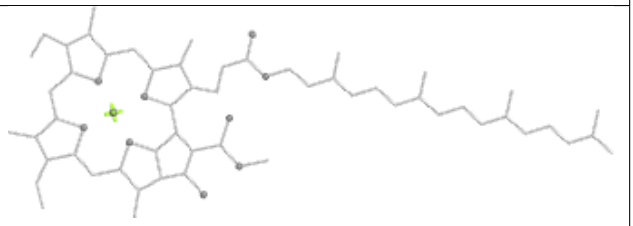
Bond lengths



Bond angles

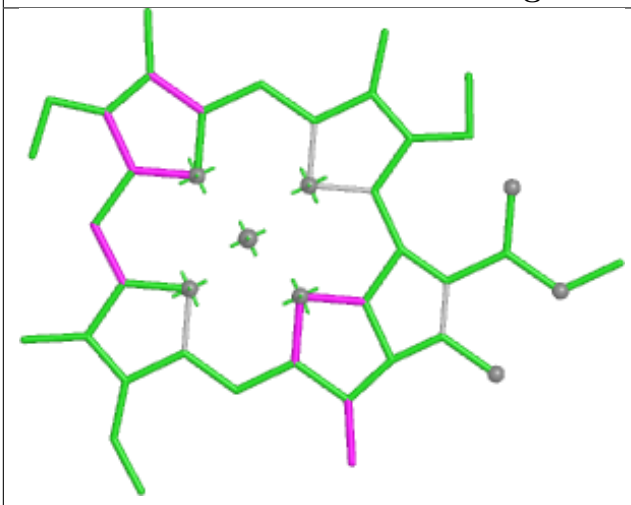


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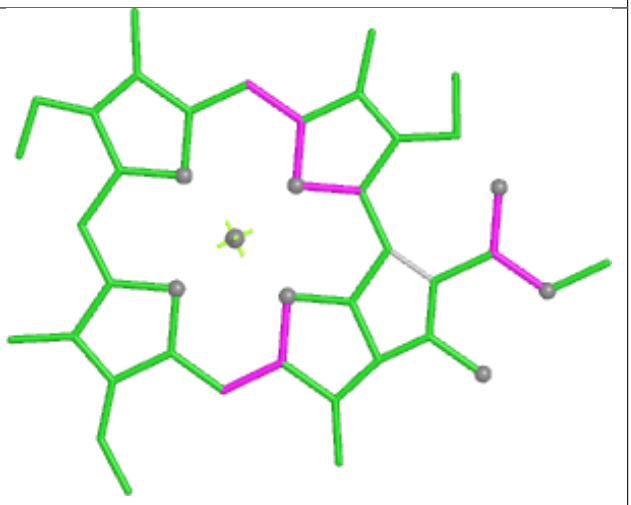


Rings

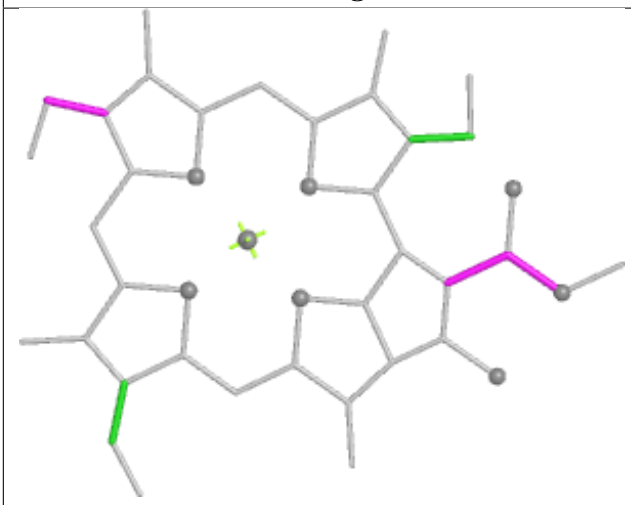
Ligand CLA A 840



Bond lengths



Bond angles

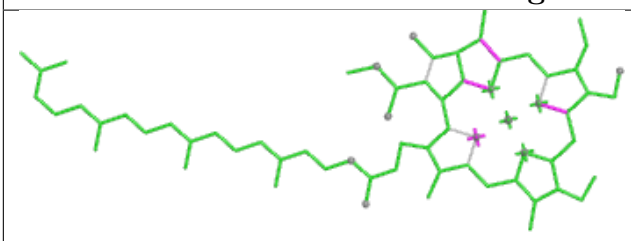


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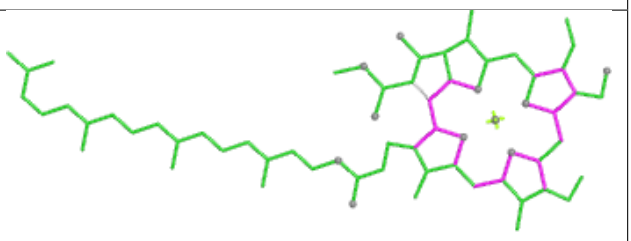


Rings

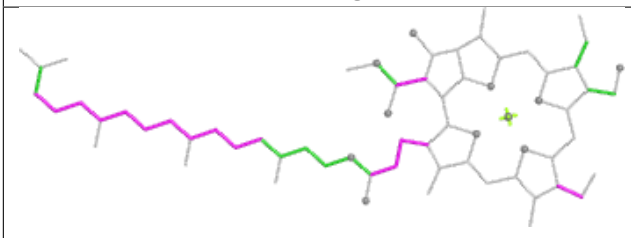
Ligand CHL 7 305



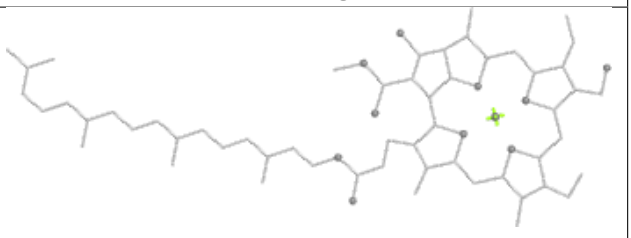
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

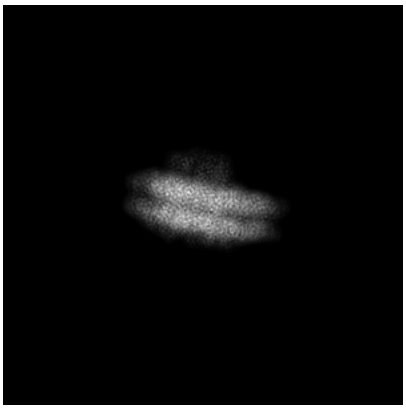
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66561. These allow visual inspection of the internal detail of the map and identification of artifacts.

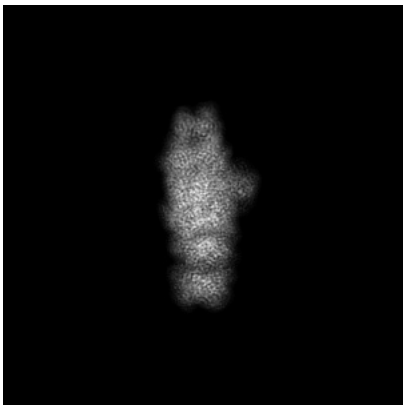
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

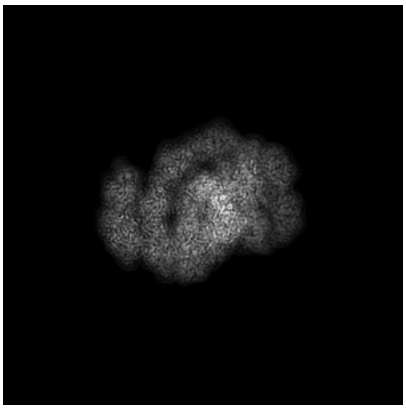
6.1.1 Primary map



X

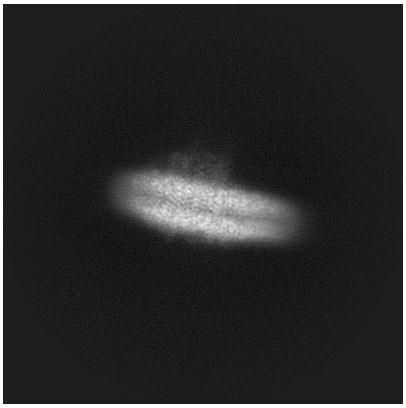


Y

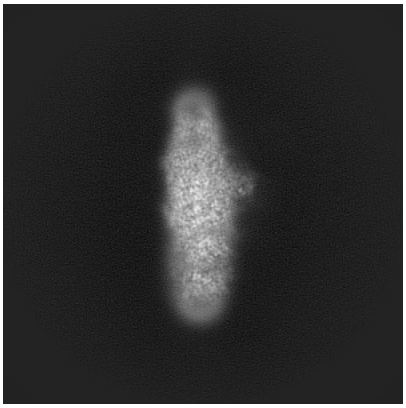


Z

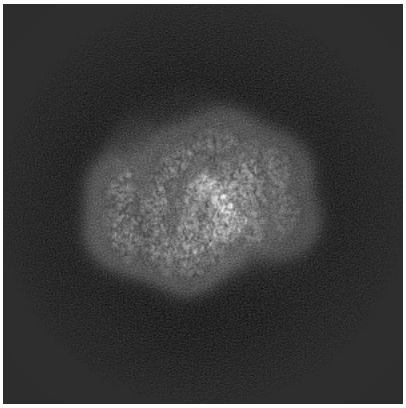
6.1.2 Raw map



X



Y

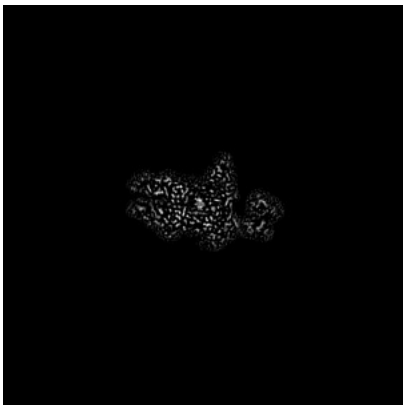


Z

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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 200

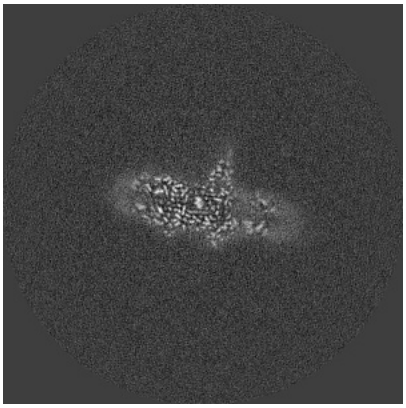


Y Index: 200

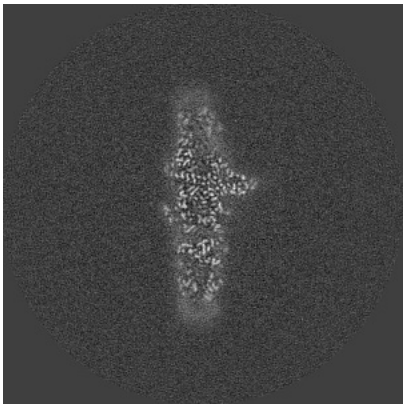


Z Index: 200

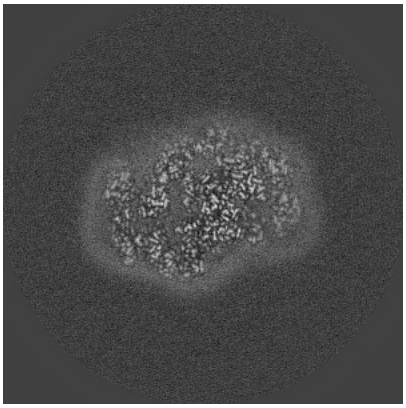
6.2.2 Raw map



X Index: 200



Y Index: 200

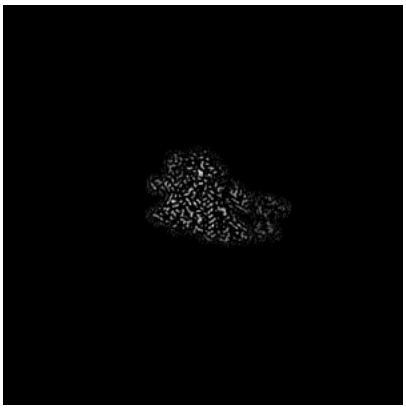


Z Index: 200

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

6.3 Largest variance slices (i)

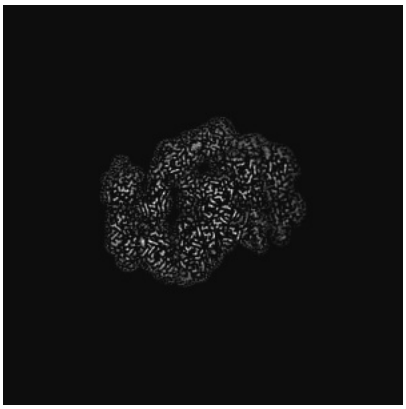
6.3.1 Primary map



X Index: 220

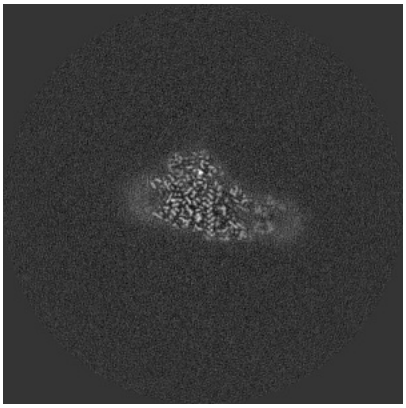


Y Index: 176

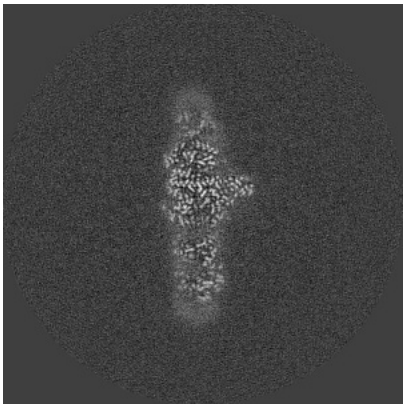


Z Index: 197

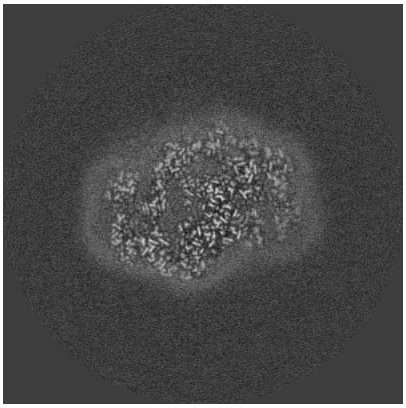
6.3.2 Raw map



X Index: 220



Y Index: 207

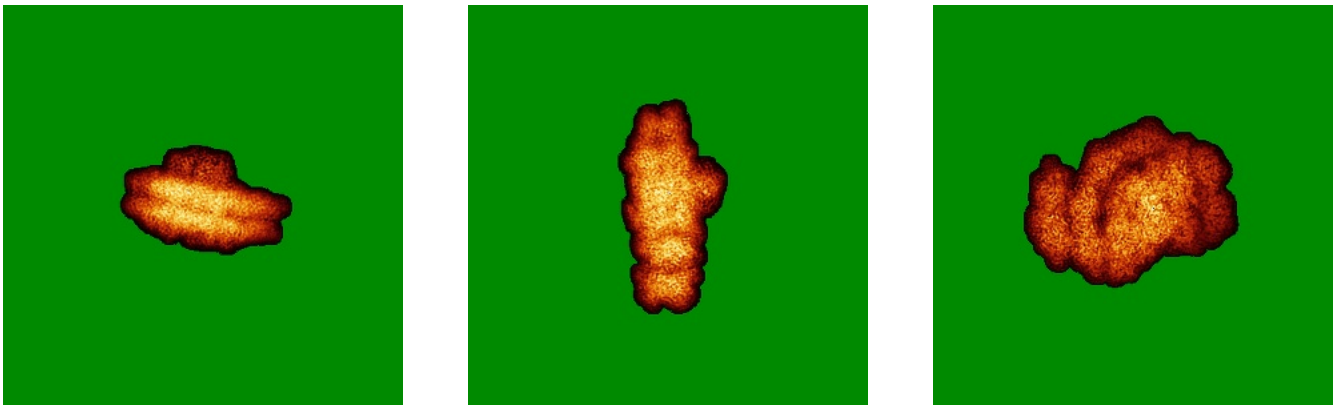


Z Index: 197

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

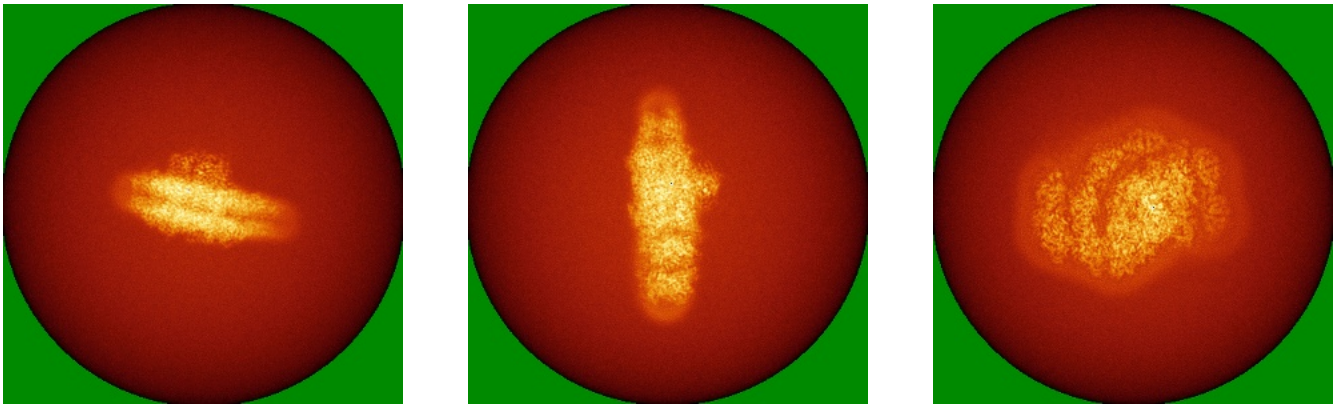
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

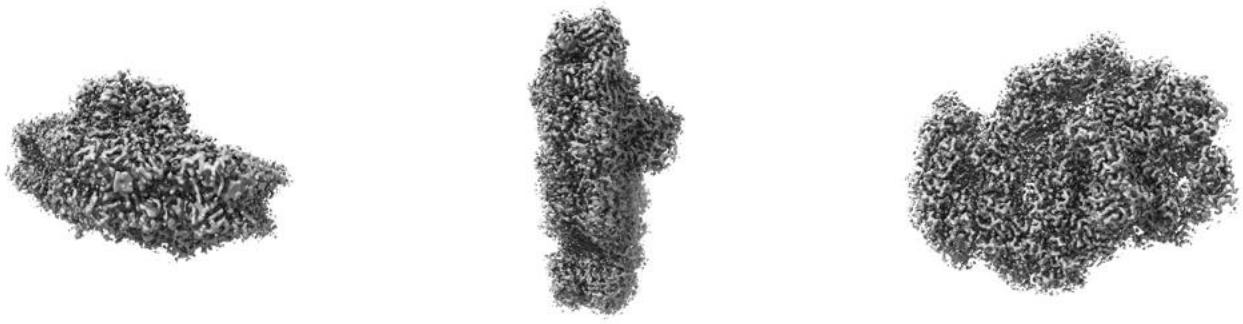


X Y Z

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)

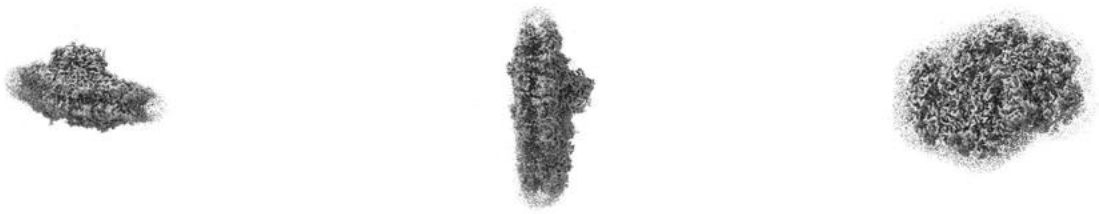
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

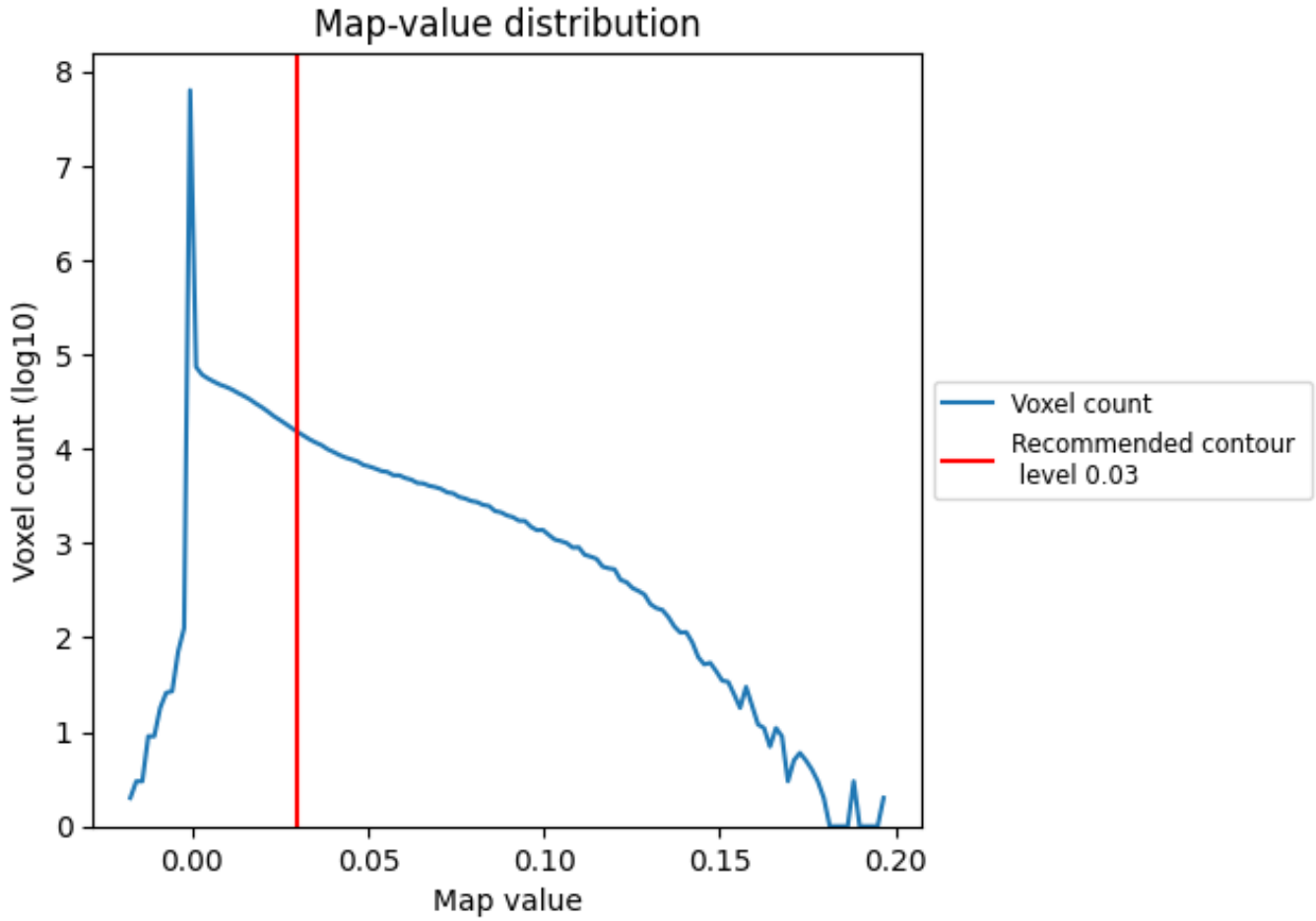
6.6 Mask visualisation (i)

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

7 Map analysis

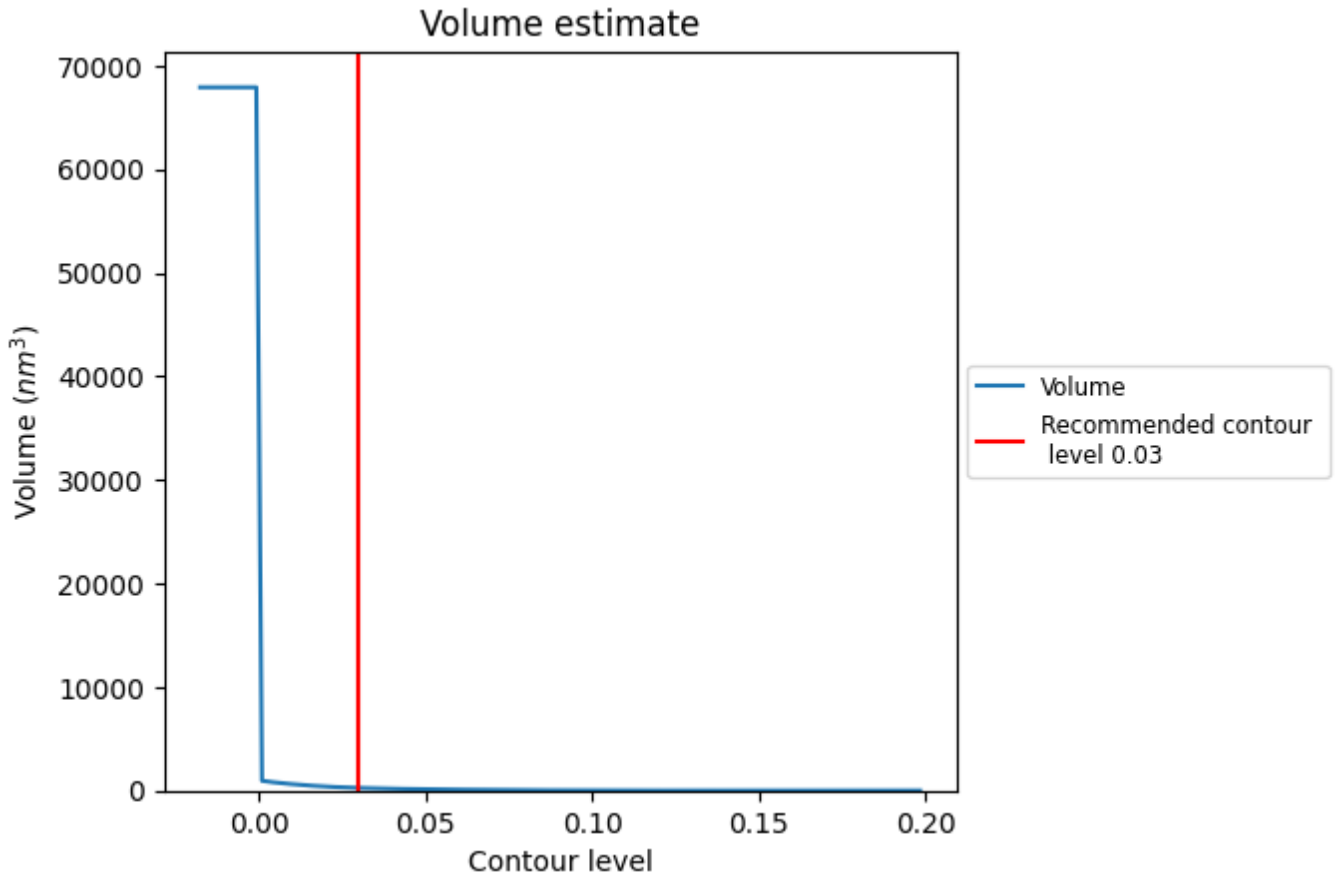
This section contains the results of statistical analysis of the map.

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.

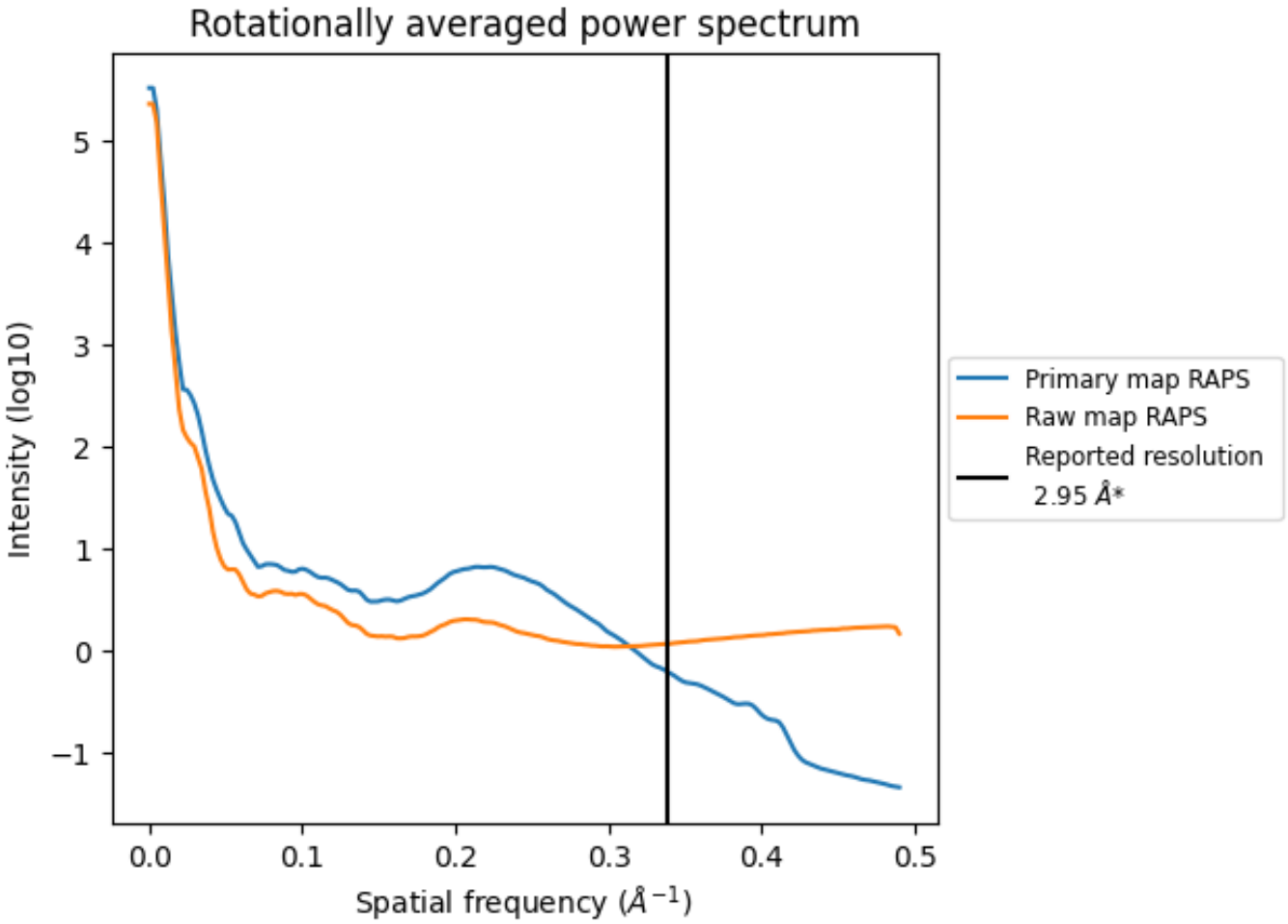
7.2 Volume estimate



The volume at the recommended contour level is 253 nm^3; this corresponds to an approximate mass of 229 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)

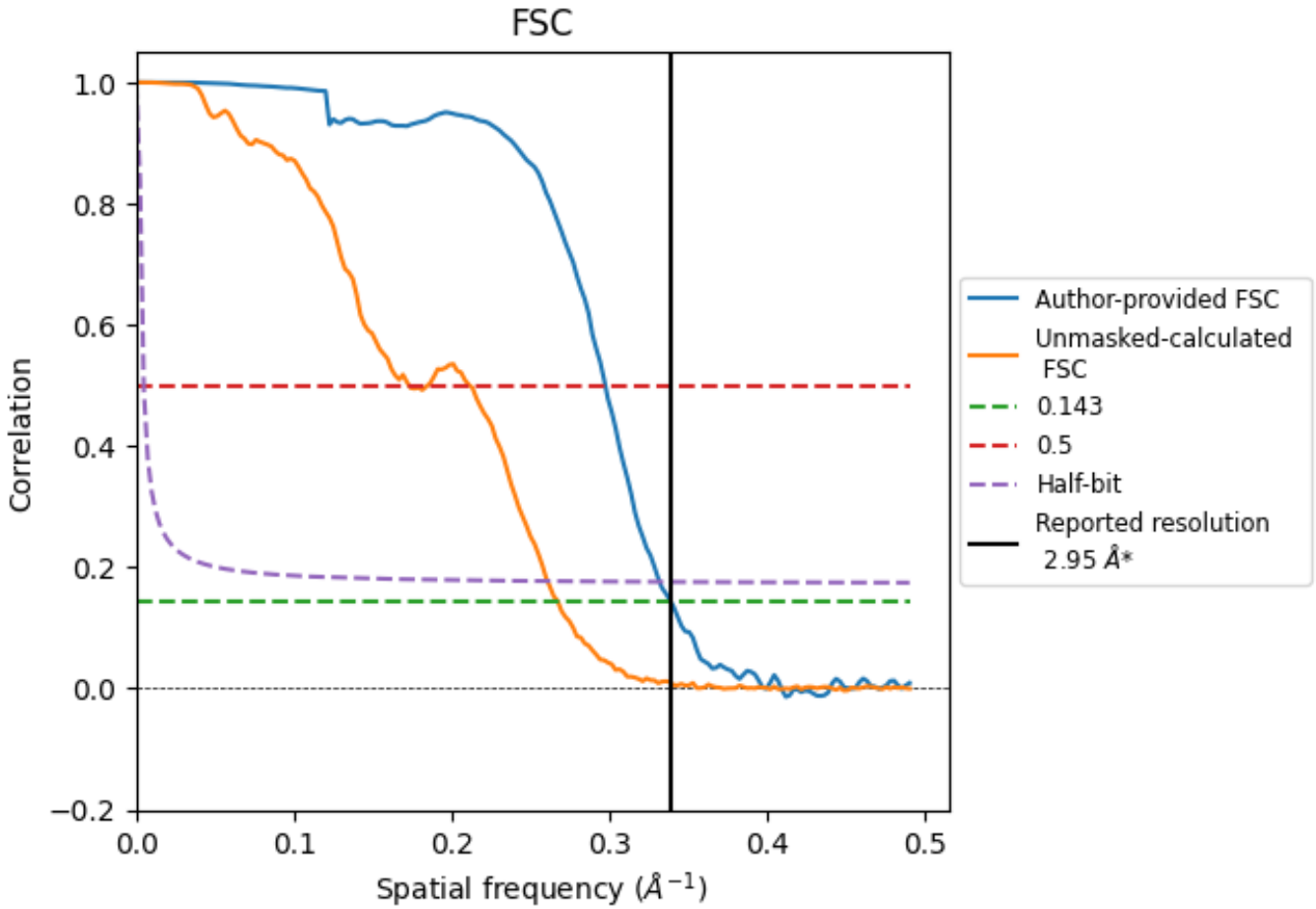


*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

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 0.339 Å^{-1}

8.2 Resolution estimates (i)

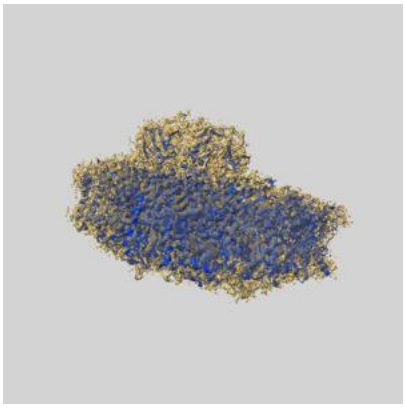
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.36	3.01
Unmasked-calculated*	3.74	5.78	3.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.95 by more than 10 %

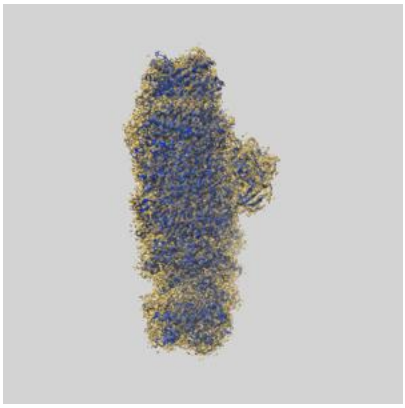
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66561 and PDB model 9X4O. Per-residue inclusion information can be found in section 3 on page 29.

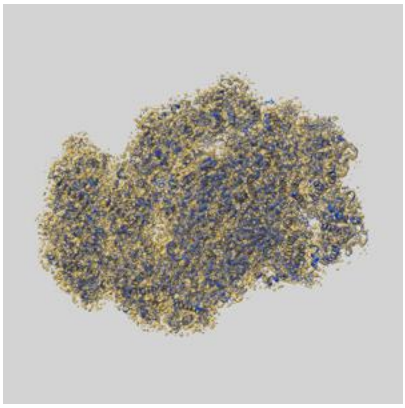
9.1 Map-model overlay



X



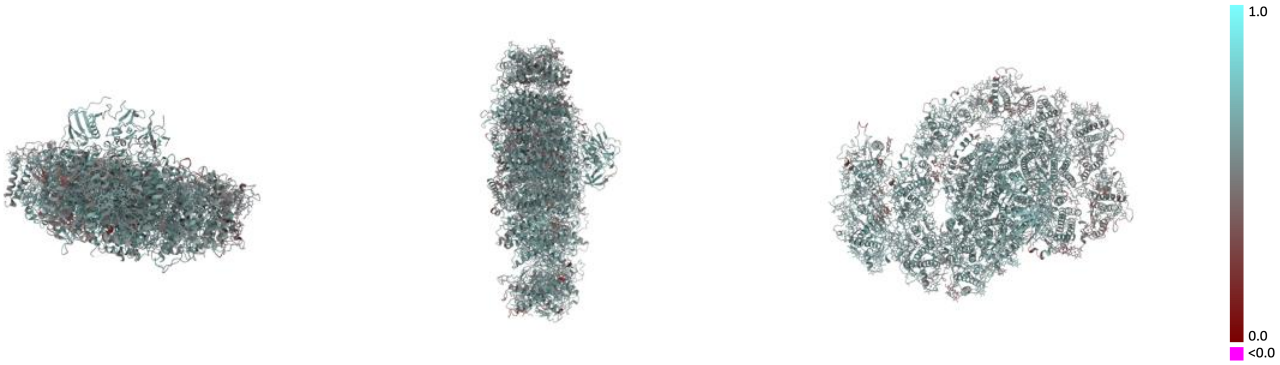
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

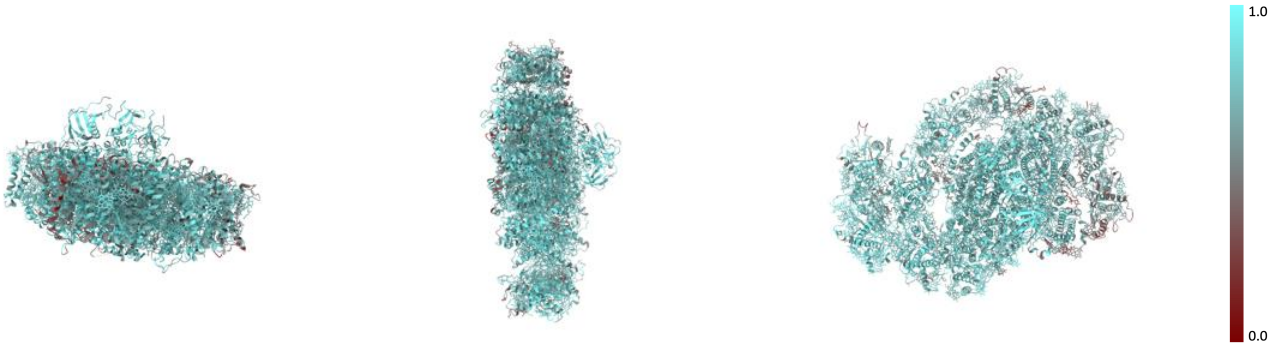
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

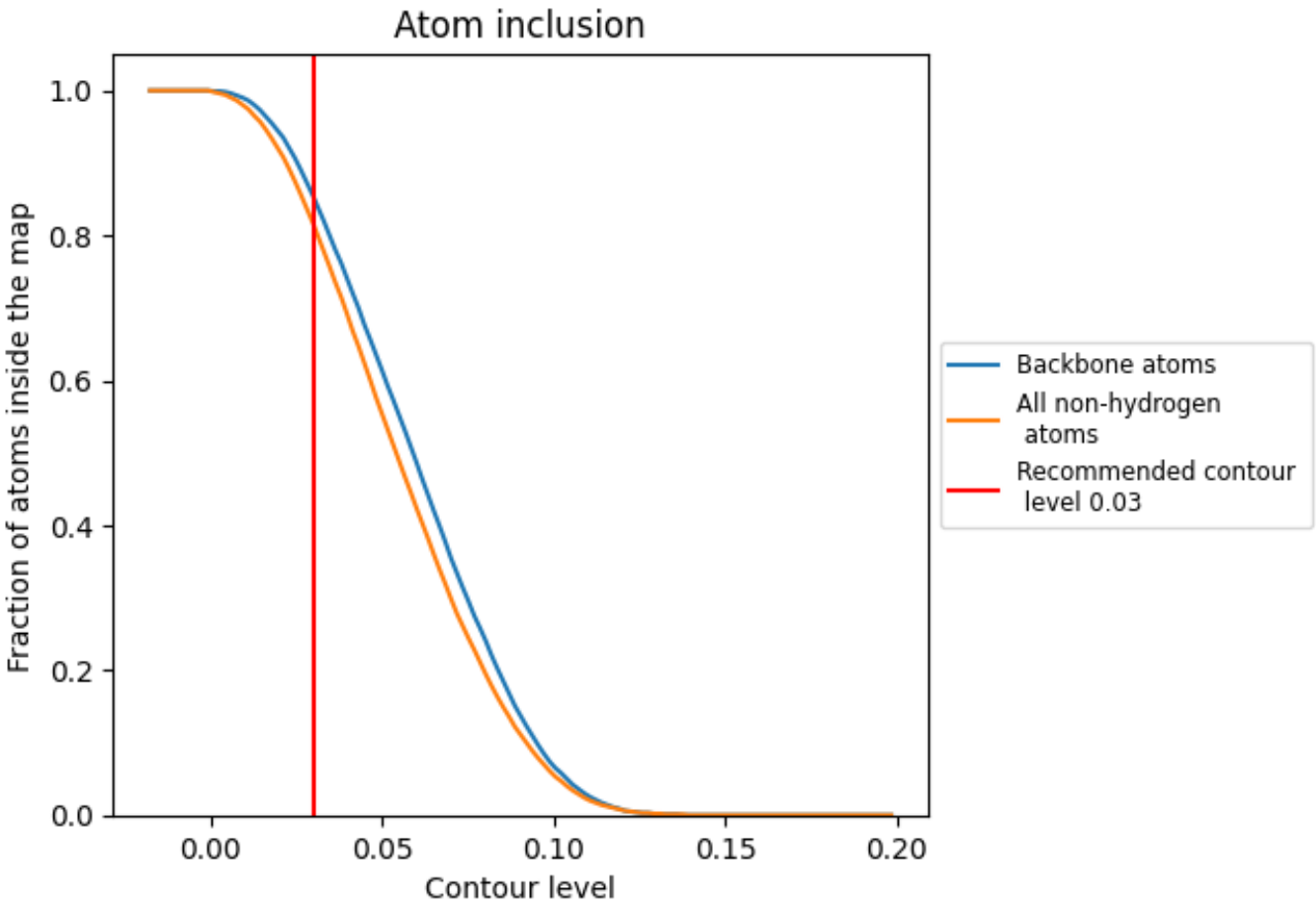
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 82% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.5750
1	0.6340	0.4850
2	0.5700	0.4780
3	0.8310	0.5730
5	0.8550	0.5930
6	0.7790	0.5450
7	0.8580	0.5890
8	0.7890	0.5540
9	0.7080	0.5230
A	0.9080	0.6270
B	0.9040	0.6230
C	0.8900	0.5980
D	0.7950	0.5700
E	0.8380	0.5890
F	0.8020	0.5620
G	0.6850	0.5070
H	0.6030	0.4750
I	0.7920	0.5640
J	0.7880	0.5610
K	0.7590	0.5350
L	0.7270	0.5320
M	0.6590	0.5230

