Full wwPDB EM Validation Report ⓘ

Nov 2, 2026 – 07:17 PM JST

PDB ID	:	9XLV / pdb_00009xlv
EMDB ID	:	EMD-67007
Title	:	Cryo-EM structure of a PSI supercomplex in the leaves of Hevea brasiliensis
Authors	:	Wang, M.; Yang, Y.; Li, Z.H.; Wang, W.D.; Wang, X.C.
Deposited on	:	2025-11-08
Resolution	:	2.70 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:

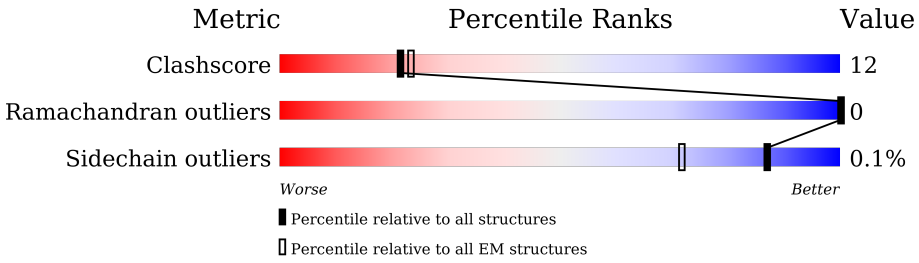
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

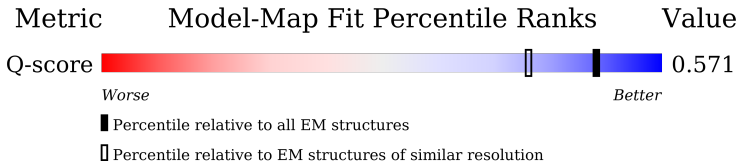
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	L	162	81% 17% ••
2	1	195	83% 17%
3	2	203	84% 16%
4	3	216	81% 19%

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Mol	Chain	Length	Quality of chain
5	4	195	77% 23%
6	A	742	78% 22%
7	B	733	81% 19%
8	C	80	70% 30%
9	D	139	81% 19%
10	E	64	89% 11%
11	F	152	67% 33%
12	G	94	80% 20%
13	H	93	86% 14%
14	I	32	84% 16%
15	J	39	77% 23%
16	K	81	90% 10%
17	O	88	81% 19%

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 37231 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 PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	162	1210	798	191	219	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	61	ASP	GLU	conflict	UNP A0ABQ9LPG4
L	73	ASP	GLU	conflict	UNP A0ABQ9LPG4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	195	1530	996	256	273	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	203	1591	1043	259	284	5	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	216	1662	1086	266	304	6	0	0

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	195	1546	1013	252	278	3	0	0

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	742	Total	C	N	O	S	0	0
			5839	3825	993	1003	18		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	733	Total	C	N	O	S	0	0
			5851	3841	998	999	13		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	80	Total	C	N	O	S	0	0
			617	381	107	118	11		

- Molecule 9 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	139	Total	C	N	O	S	0	0
			1111	713	199	195	4		

- Molecule 10 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	64	Total	C	N	O	0	0
			518	330	91	97		

- Molecule 11 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	152	Total	C	N	O	S	0	0
			1206	782	209	212	3		

- Molecule 12 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	94	Total	C	N	O	S	0	0
			724	474	118	130	2		

- Molecule 13 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	H	93	Total 710	C 466	N 112	O 132	0	0

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	32	Total 244	C 165	N 38	O 40	S 1	0	0

- Molecule 15 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	39	Total 313	C 210	N 48	O 54	S 1	0	0

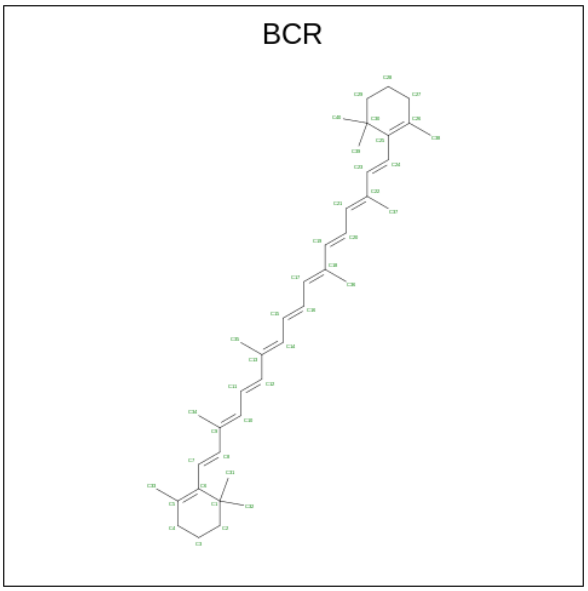
- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	81	Total 569	C 360	N 99	O 107	S 3	0	0

- Molecule 17 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	88	Total 713	C 478	N 113	O 121	S 1	0	0

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



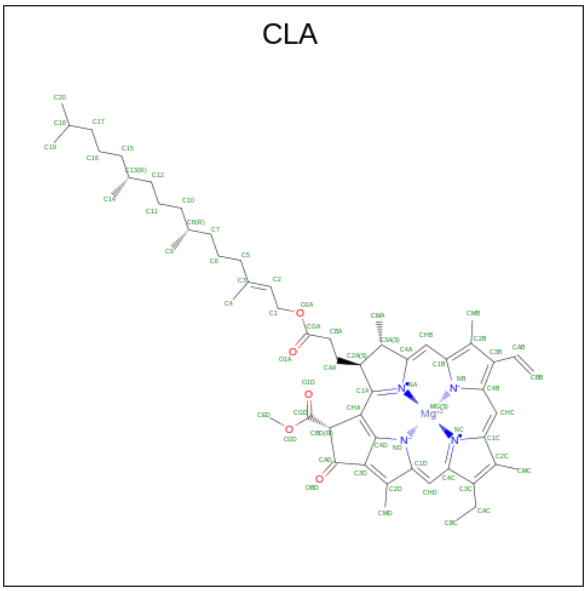
Mol	Chain	Residues	Atoms	AltConf
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	1	1	Total C 40 40	0
18	2	1	Total C 40 40	0
18	3	1	Total C 40 40	0
18	4	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	A	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	F	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 40 40	0
18	K	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0

- Molecule 19 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
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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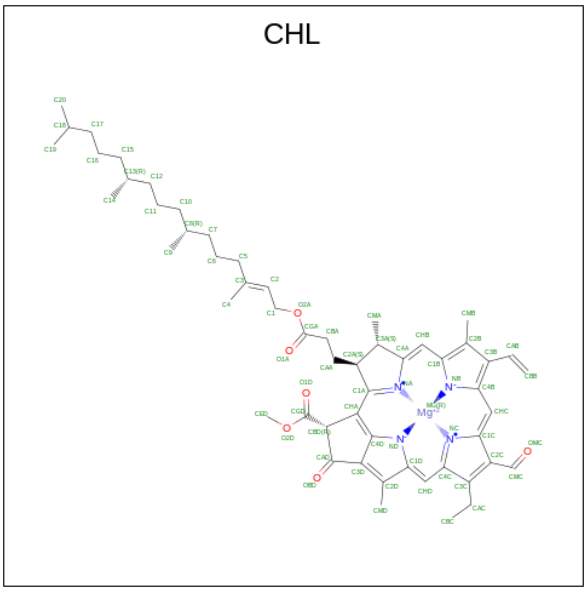
Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



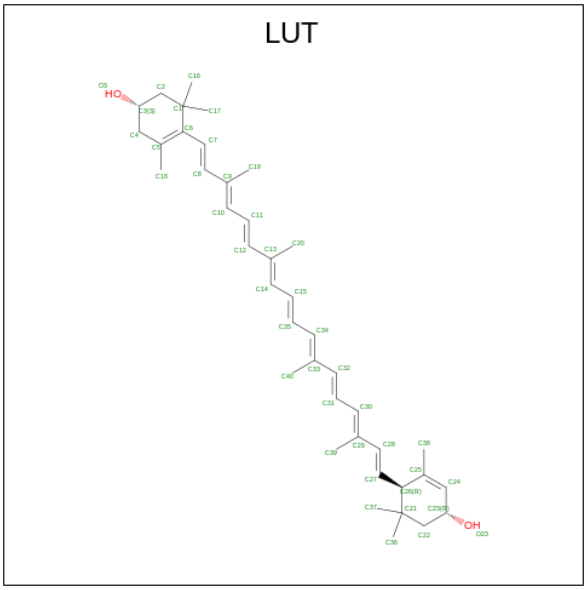
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	2	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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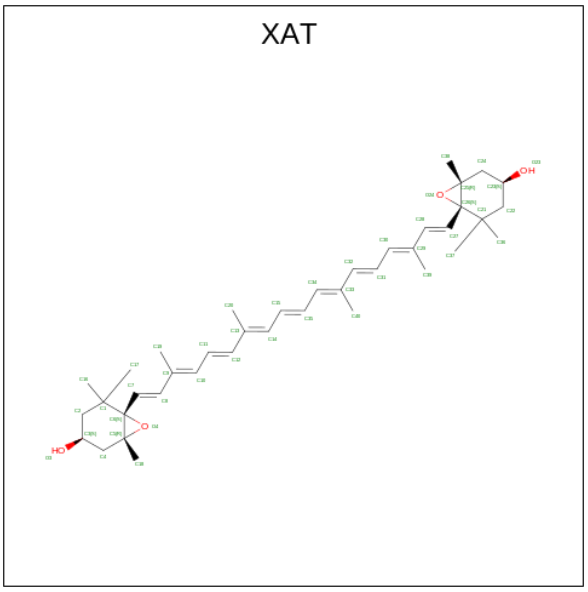
Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



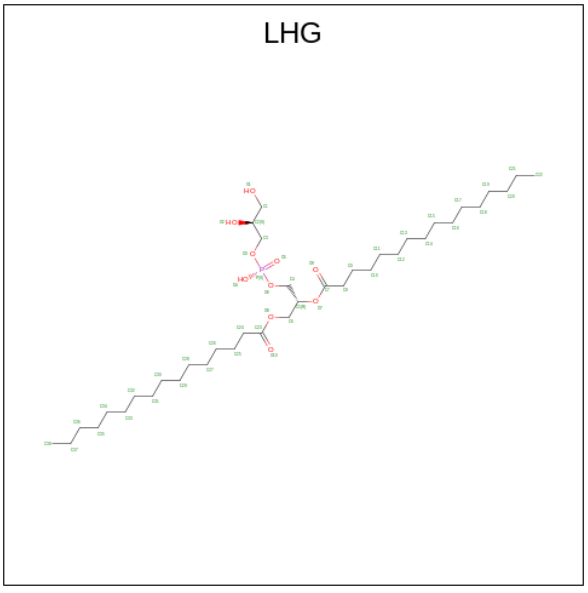
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	

- Molecule 22 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: $C_{40}H_{56}O_4$).



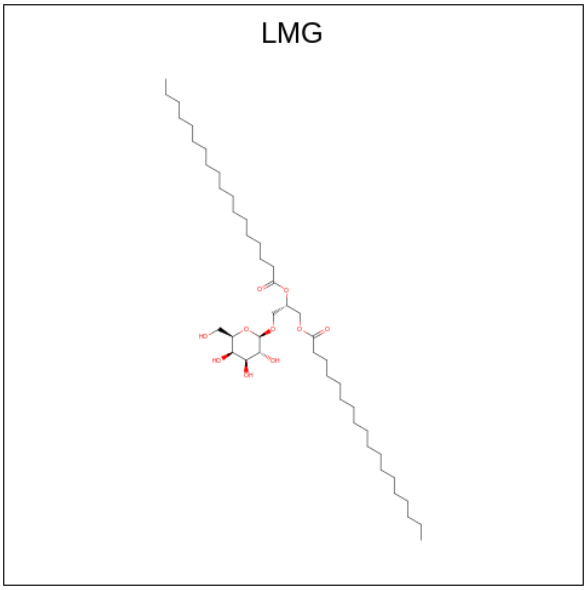
Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			23	12	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			37	26	10	1	
23	2	1	Total	C	O	P	0
			49	38	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	
23	4	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



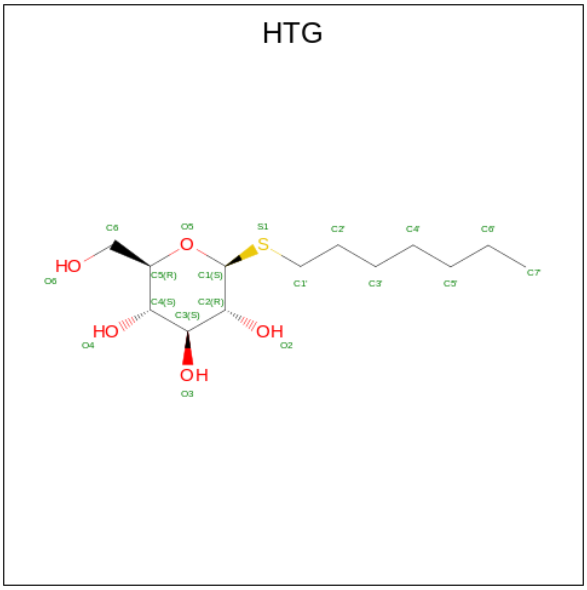
Mol	Chain	Residues	Atoms			AltConf
24	4	1	Total	C	O	0
			50	40	10	
24	B	1	Total	C	O	0
			44	34	10	

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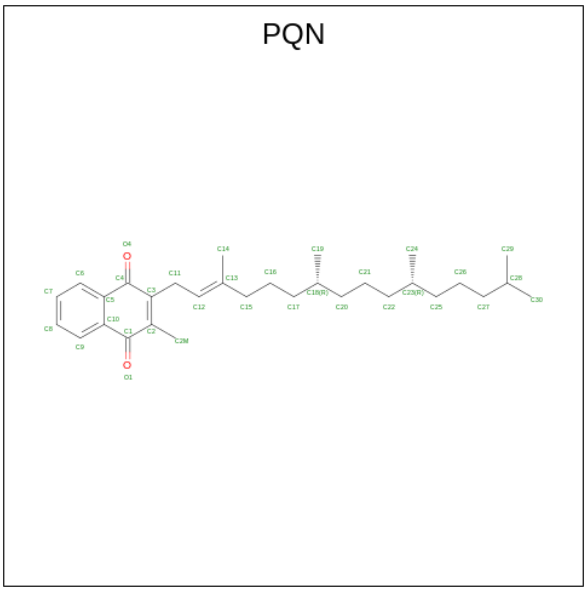
Mol	Chain	Residues	Atoms	AltConf
24	F	1	Total C O 40 30 10	0
24	G	1	Total C O 40 30 10	0
24	J	1	Total C O 51 41 10	0

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



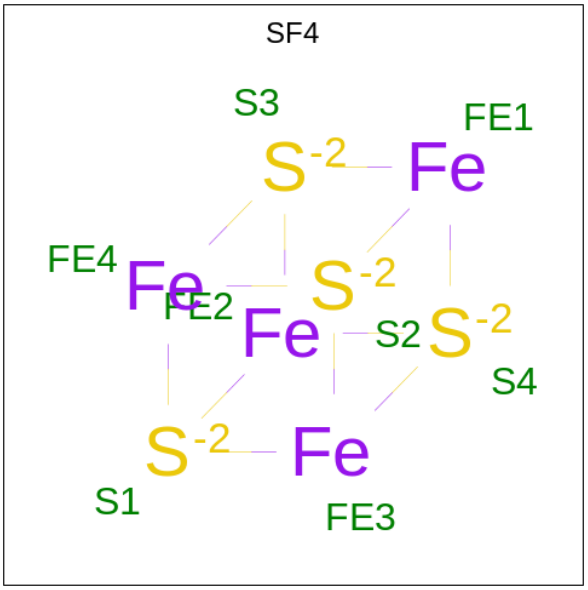
Mol	Chain	Residues	Atoms	AltConf
25	4	1	Total C O S 19 13 5 1	0
25	B	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0
25	F	1	Total C O S 19 13 5 1	0

- Molecule 26 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



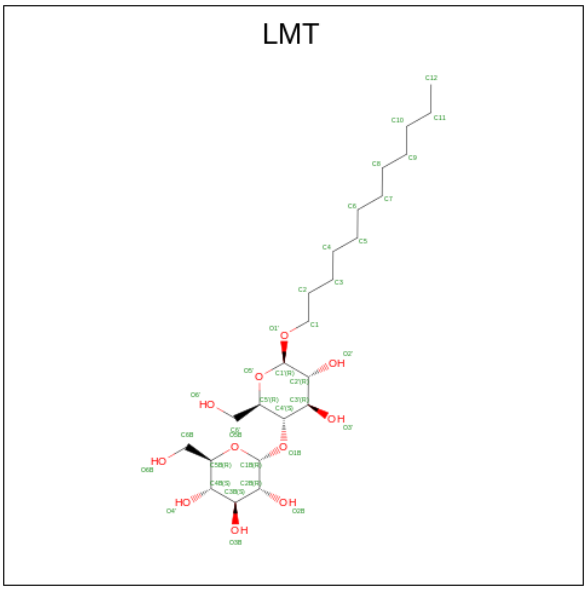
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0

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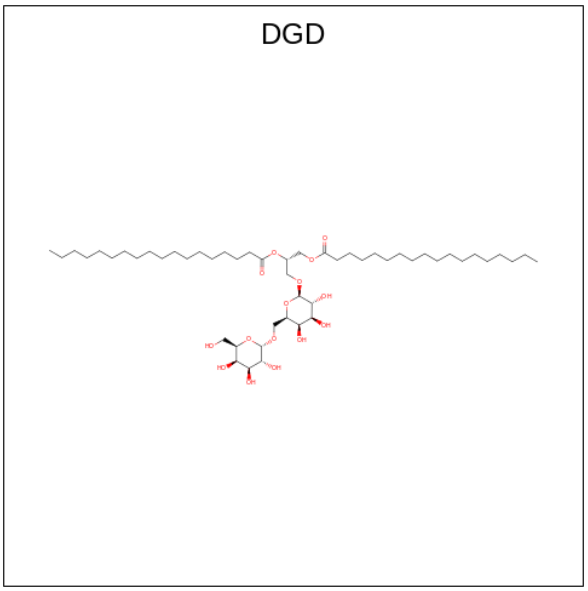
Mol	Chain	Residues	Atoms			AltConf
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	B	1	66	51	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: PsaL

Chain L:

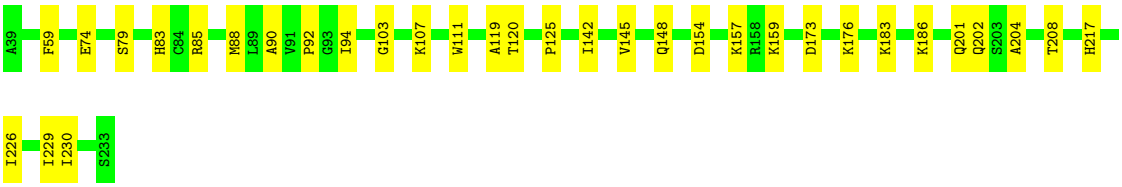




• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

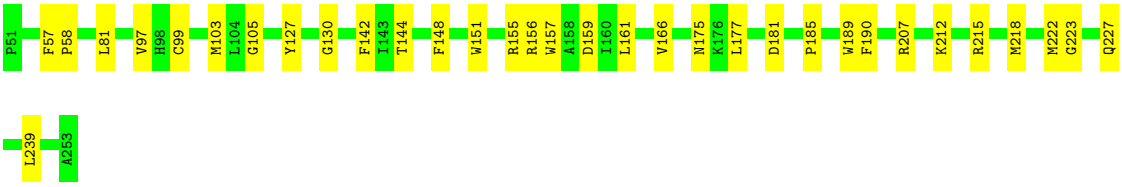




• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

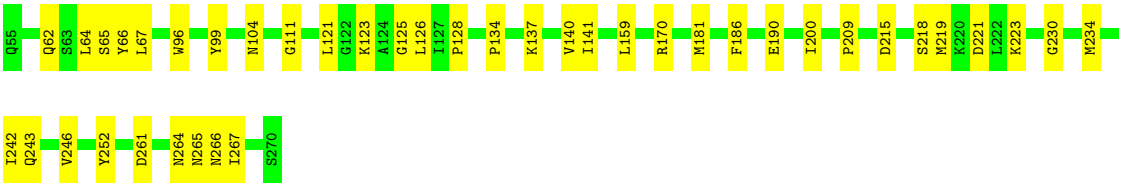




• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

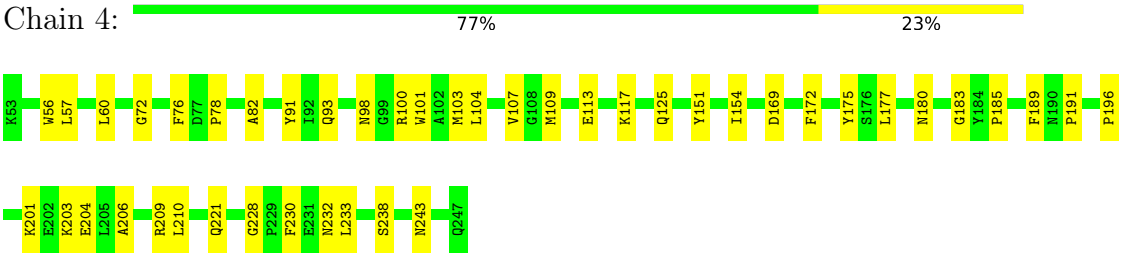
Chain 3:





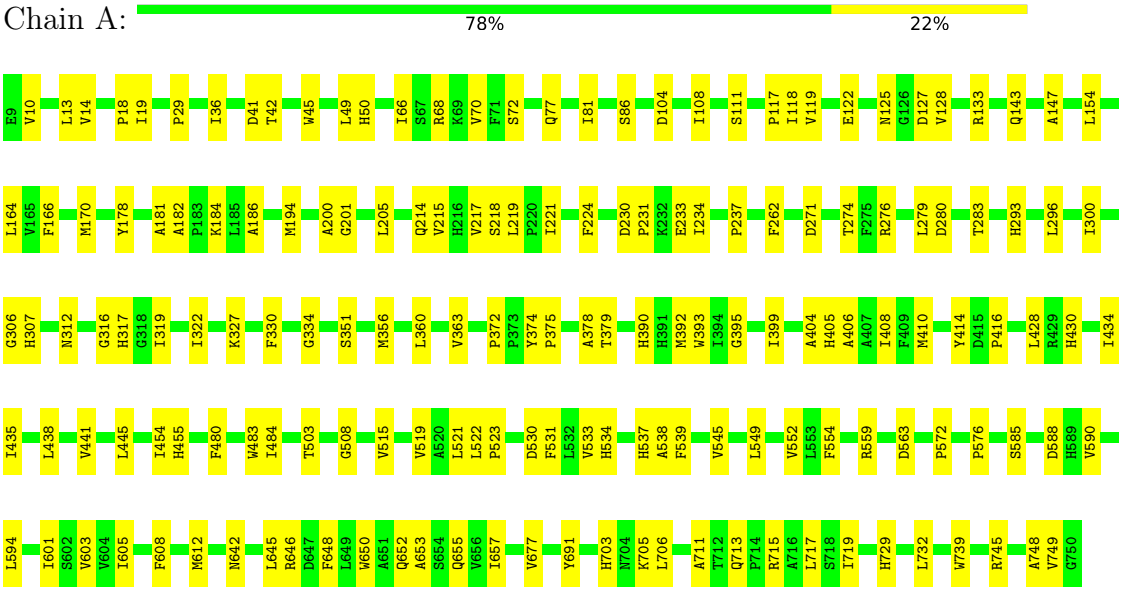
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



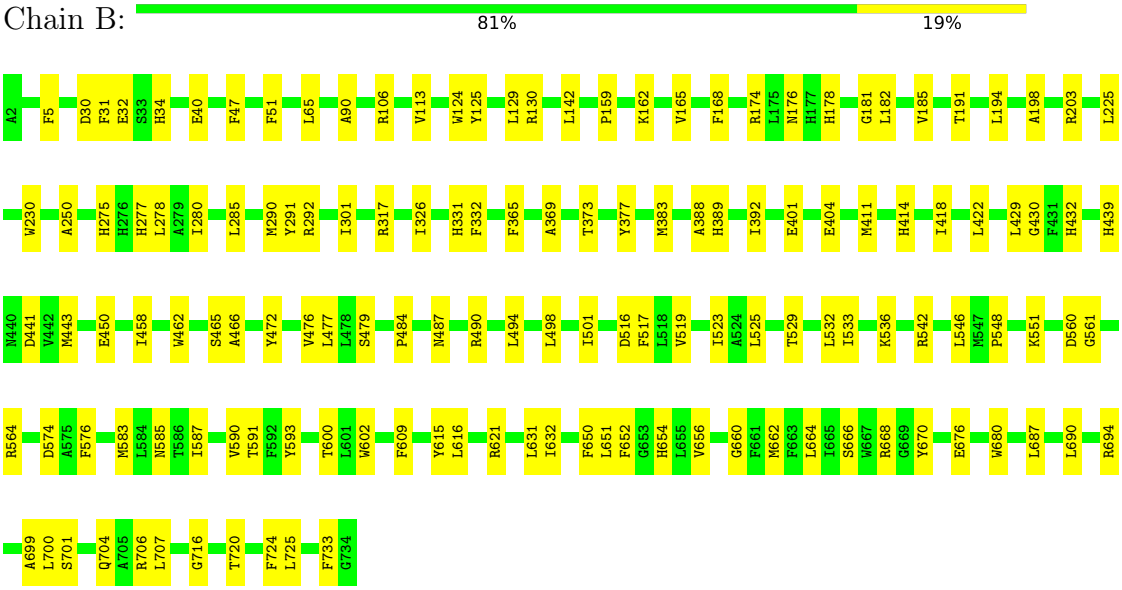
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



• Molecule 7: Photosystem I P700 chlorophyll a apoprotein A2

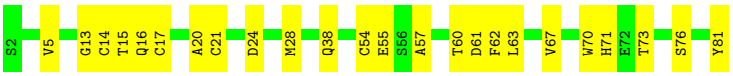
Chain B:



• Molecule 8: Photosystem I iron-sulfur center

Chain C:





• Molecule 9: PsaD

Chain D:

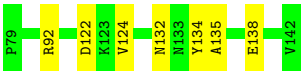




• Molecule 10: PsaE

Chain E:

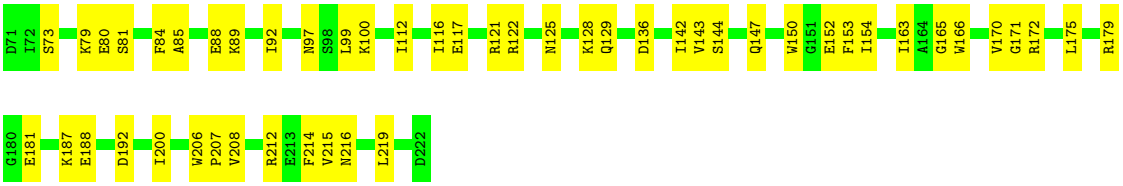




• Molecule 11: Photosystem I reaction center subunit III

Chain F:

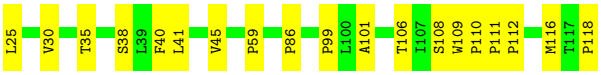




• Molecule 12: PsaG

Chain G:





• Molecule 13: PsaH

Chain H:





• Molecule 14: Photosystem I reaction center subunit VIII

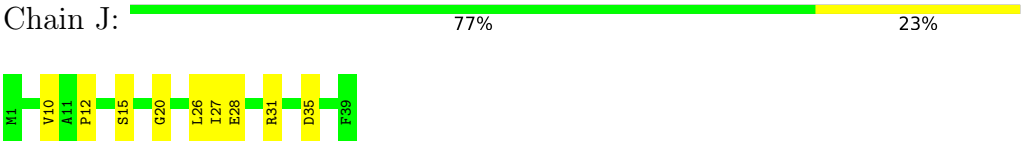
Chain I:





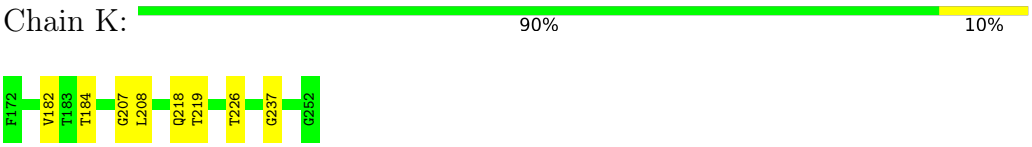
• Molecule 15: Photosystem I reaction center subunit IX

Chain J:



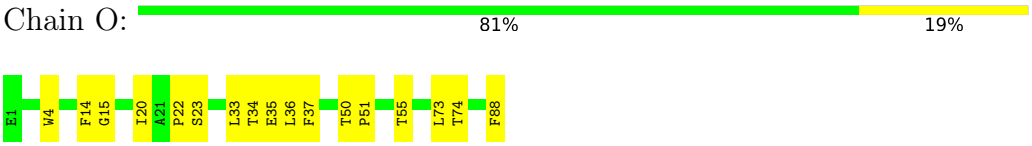
• Molecule 16: PSI-K

Chain K:



• Molecule 17: PsaO

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	618810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.724	Depositor
Minimum map value	-0.427	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.0418	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, DGD, PQN, LMT, HTG, LUT, CLA, XAT, BCR, LMG, SF4, CHL

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	L	0.36	1/1244 (0.1%)	0.54	3/1700 (0.2%)
2	1	0.13	0/1582	0.27	0/2156
3	2	0.14	0/1650	0.31	0/2257
4	3	0.13	0/1712	0.30	0/2327
5	4	0.13	0/1597	0.27	0/2180
6	A	0.15	0/6037	0.27	0/8236
7	B	0.15	0/6063	0.28	0/8280
8	C	0.18	0/630	0.44	0/853
9	D	0.15	0/1140	0.34	0/1538
10	E	0.11	0/529	0.21	0/716
11	F	0.15	0/1235	0.30	0/1665
12	G	0.18	0/744	0.38	0/1018
13	H	0.17	0/731	0.28	0/993
14	I	0.20	0/249	0.32	0/339
15	J	0.12	0/321	0.26	0/435
16	K	0.10	0/576	0.28	0/777
17	O	0.13	0/741	0.36	0/1012
All	All	0.16	1/26781 (0.0%)	0.31	3/36482 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	209	VAL	C-O	-9.51	1.12	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	209	VAL	O-C-N	-11.85	107.76	122.57
1	L	73	ASP	CA-C-N	5.41	136.33	120.97
1	L	73	ASP	C-N-CA	5.41	136.33	120.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	209	VAL	Mainchain

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	L	1210	0	1219	27	0
2	1	1530	0	1501	25	0
3	2	1591	0	1537	35	0
4	3	1662	0	1633	33	0
5	4	1546	0	1504	45	0
6	A	5839	0	5691	128	0
7	B	5851	0	5636	111	0
8	C	617	0	593	21	0
9	D	1111	0	1129	19	0
10	E	518	0	519	6	0
11	F	1206	0	1235	40	0
12	G	724	0	730	23	0
13	H	710	0	710	12	0
14	I	244	0	267	4	0
15	J	313	0	324	8	0
16	K	569	0	592	6	0
17	O	713	0	697	15	0
18	1	40	0	56	5	0
18	2	40	0	56	6	0
18	3	40	0	56	5	0
18	4	40	0	56	5	0
18	A	200	0	280	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	200	0	280	14	0
18	F	120	0	168	12	0
18	G	80	0	112	3	0
18	I	40	0	56	3	0
18	J	80	0	112	4	0
18	K	80	0	112	7	0
18	L	120	0	168	6	0
18	O	80	0	112	7	0
19	1	672	0	636	45	0
19	2	487	0	447	18	0
19	3	587	0	466	22	0
19	4	586	0	509	44	0
19	A	2690	0	2803	129	0
19	B	2493	0	2570	111	0
19	F	100	0	82	4	0
19	G	137	0	101	4	0
19	J	42	0	31	0	0
19	K	105	0	92	6	0
19	L	180	0	183	10	0
19	O	194	0	152	9	0
20	1	109	0	90	8	0
20	2	241	0	169	24	0
20	3	47	0	31	3	0
20	4	201	0	150	16	0
21	1	42	0	56	4	0
21	2	42	0	56	4	0
21	3	42	0	56	5	0
21	4	42	0	56	3	0
22	1	44	0	56	2	0
22	2	44	0	56	2	0
22	3	44	0	56	2	0
22	4	44	0	56	5	0
23	1	121	0	164	15	0
23	2	86	0	118	10	0
23	4	89	0	127	9	0
23	A	76	0	98	3	0
24	4	50	0	73	8	0
24	B	44	0	58	3	0
24	F	40	0	50	1	0
24	G	40	0	53	1	0
24	J	51	0	72	2	0
25	4	19	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	19	0	26	1	0
25	F	76	0	104	9	0
26	A	33	0	46	4	0
26	B	33	0	46	1	0
27	A	8	0	0	0	0
27	C	16	0	0	1	0
28	A	35	0	46	2	0
29	B	66	0	96	7	0
All	All	37231	0	37304	871	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 12.

All (871) 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)
19:3:303:CLA:HBB1	18:3:315:BCR:H24C	1.41	1.01
4:3:128:PRO:HD3	19:3:316:CLA:HAA1	1.46	0.97
6:A:531:PHE:HA	19:A:835:CLA:HED1	1.51	0.91
19:4:309:CLA:H11	19:4:311:CLA:HAB	1.57	0.86
17:O:14:PHE:HB3	19:O:103:CLA:HBC1	1.58	0.86
19:B:838:CLA:H13	18:I:101:BCR:H21C	1.62	0.82
8:C:17:CYS:O	8:C:21:CYS:N	2.13	0.82
3:2:144:THR:HG22	19:4:313:CLA:HAA2	1.60	0.82
7:B:411:MET:HE2	18:B:844:BCR:H402	1.62	0.81
19:A:804:CLA:H152	19:A:827:CLA:HBB2	1.63	0.80
4:3:140:VAL:HG13	4:3:141:ILE:HD12	1.61	0.80
1:L:144:LEU:HD13	18:L:305:BCR:H401	1.66	0.78
3:2:212:LYS:HE3	23:2:317:LHG:HC42	1.64	0.78
3:2:218:MET:HG2	22:2:315:XAT:H14	1.65	0.78
5:4:233:LEU:HD13	21:4:316:LUT:H163	1.65	0.77
1:L:153:ILE:HA	13:H:118:ARG:HH21	1.49	0.77
6:A:393:TRP:CD1	19:A:826:CLA:HAB	2.20	0.77
7:B:517:PHE:HA	19:B:836:CLA:HED1	1.65	0.77
19:A:822:CLA:HBB2	23:A:843:LHG:HC82	1.67	0.76
19:2:308:CLA:H52	21:2:314:LUT:H30	1.66	0.76
20:2:306:CHL:HMA1	18:2:316:BCR:H401	1.67	0.75
7:B:230:TRP:HB2	12:G:109:TRP:HH2	1.52	0.75
19:3:308:CLA:HHC	21:3:313:LUT:H31	1.69	0.74
8:C:15:THR:HA	8:C:28:MET:HE3	1.70	0.74
14:I:35:LYS:HD3	14:I:36:ILE:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:221:GLN:NE2	19:4:312:CLA:MG	1.46	0.73
19:B:816:CLA:HBA2	12:G:109:TRP:CZ2	2.23	0.72
11:F:172:ARG:HH12	11:F:219:LEU:HD12	1.54	0.72
2:1:201:GLN:NE2	19:1:311:CLA:MG	1.47	0.71
7:B:487:ASN:OD1	7:B:490:ARG:NH2	2.21	0.71
18:1:316:BCR:HC41	12:G:40:PHE:HZ	1.56	0.71
18:A:848:BCR:H362	19:A:850:CLA:H42	1.71	0.70
8:C:17:CYS:O	8:C:20:ALA:N	2.24	0.70
3:2:215:ARG:HA	3:2:218:MET:HE3	1.74	0.69
20:1:318:CHL:HMA2	5:4:154:ILE:HD13	1.75	0.69
4:3:261:ASP:HB3	4:3:264:ASN:HB2	1.75	0.69
19:A:819:CLA:H72	19:A:822:CLA:H51	1.74	0.69
3:2:185:PRO:HB3	20:2:306:CHL:HBC2	1.74	0.68
6:A:18:PRO:HB2	6:A:19:ILE:HD12	1.74	0.68
6:A:118:ILE:HG12	15:J:27:ILE:HG23	1.76	0.68
18:K:301:BCR:H353	18:K:304:BCR:H323	1.75	0.68
1:L:57:PHE:O	1:L:58:GLN:NE2	2.27	0.67
7:B:191:THR:HG21	7:B:278:LEU:HB2	1.75	0.67
4:3:186:PHE:N	4:3:190:GLU:OE2	2.24	0.67
7:B:733:PHE:HB3	13:H:160:ARG:HH11	1.57	0.67
3:2:157:TRP:HZ2	23:2:318:LHG:HC61	1.59	0.67
19:4:309:CLA:HHC	19:4:309:CLA:HBB1	1.76	0.67
12:G:116:MET:HG2	12:G:118:PRO:HD2	1.77	0.67
6:A:77:GLN:HE21	6:A:81:ILE:HG13	1.60	0.67
25:F:303:HTG:H4'2	18:F:308:BCR:H14C	1.76	0.66
19:4:303:CLA:H2	11:F:208:VAL:HG13	1.78	0.66
16:K:219:THR:HG21	16:K:226:THR:HA	1.78	0.66
19:A:815:CLA:H91	18:K:304:BCR:HC31	1.77	0.66
26:B:841:PQN:H28	29:B:847:DGD:HA82	1.78	0.66
23:1:317:LHG:H282	23:1:317:LHG:HC82	1.78	0.65
19:2:308:CLA:H2	21:2:314:LUT:H28	1.78	0.65
19:B:818:CLA:HAB	19:B:818:CLA:H8	1.78	0.65
1:L:123:LEU:HD11	13:H:144:ILE:HG23	1.78	0.65
5:4:57:LEU:HD13	19:4:301:CLA:HMA3	1.78	0.64
13:H:105:SER:O	13:H:109:GLU:HG2	1.98	0.64
20:2:304:CHL:HHC	20:2:304:CHL:HBB1	1.80	0.64
4:3:267:ILE:HD11	19:3:310:CLA:H12	1.79	0.64
9:D:166:HIS:HB3	9:D:167:PRO:HD3	1.80	0.64
6:A:72:SER:OG	6:A:178:TYR:HB2	1.98	0.64
6:A:127:ASP:OD1	6:A:133:ARG:NH1	2.31	0.64
19:3:304:CLA:HAA1	18:3:315:BCR:H23C	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:480:PHE:HB3	19:A:834:CLA:H11	1.81	0.63
7:B:560:ASP:OD2	7:B:564:ARG:NH2	2.30	0.63
6:A:13:LEU:HB3	6:A:184:LYS:HD2	1.81	0.63
6:A:316:GLY:HA2	19:A:820:CLA:HMD2	1.81	0.63
23:1:320:LHG:H381	18:B:844:BCR:HC8	1.80	0.63
6:A:317:HIS:HB3	6:A:322:ILE:HD11	1.81	0.63
3:2:148:PHE:HD2	20:2:304:CHL:HMA2	1.64	0.63
5:4:169:ASP:OD1	5:4:172:PHE:N	2.32	0.63
19:B:817:CLA:HBA2	19:B:826:CLA:HBB2	1.81	0.63
19:1:312:CLA:HBC1	21:1:314:LUT:H162	1.79	0.63
16:K:207:GLY:HA2	19:O:103:CLA:HED1	1.81	0.63
6:A:166:PHE:O	6:A:170:MET:HG2	1.99	0.62
11:F:163:ILE:HG23	19:F:306:CLA:HAA1	1.81	0.62
2:1:183:LYS:HD3	19:1:310:CLA:HBA2	1.80	0.62
23:1:320:LHG:H251	19:B:822:CLA:HBA1	1.82	0.62
4:3:170:ARG:CG	20:3:306:CHL:HHC	2.30	0.62
19:F:307:CLA:HMA2	19:F:307:CLA:H2	1.82	0.62
3:2:222:MET:HE2	19:2:302:CLA:HBB2	1.82	0.62
5:4:238:SER:O	5:4:243:ASN:ND2	2.33	0.62
19:A:818:CLA:HBB1	18:K:301:BCR:H14C	1.80	0.62
7:B:465:SER:O	7:B:479:SER:OG	2.16	0.61
19:A:839:CLA:H42	19:A:852:CLA:H193	1.82	0.61
6:A:262:PHE:HA	19:K:302:CLA:HAC2	1.80	0.61
7:B:668:ARG:NH1	7:B:699:ALA:O	2.33	0.61
5:4:221:GLN:NE2	19:4:312:CLA:ND	2.48	0.61
6:A:405:HIS:HA	6:A:408:ILE:HD12	1.83	0.61
6:A:445:LEU:HB3	6:A:539:PHE:HB2	1.83	0.61
8:C:73:THR:H	8:C:76:SER:HB3	1.65	0.61
20:4:307:CHL:HMC	20:4:315:CHL:HMC	1.82	0.60
7:B:546:LEU:O	7:B:564:ARG:NH1	2.34	0.60
20:2:306:CHL:HHC	20:2:306:CHL:HBB1	1.83	0.60
7:B:529:THR:O	7:B:533:ILE:HD12	2.01	0.60
11:F:125:ASN:O	11:F:129:GLN:HG3	2.01	0.60
19:1:311:CLA:H112	20:1:318:CHL:H8	1.83	0.60
1:L:74:THR:HG21	19:A:853:CLA:OBD	2.02	0.60
5:4:210:LEU:HB2	19:4:310:CLA:HAB	1.84	0.60
2:1:79:SER:HB2	19:1:307:CLA:HED2	1.84	0.60
19:4:303:CLA:H51	11:F:208:VAL:HA	1.82	0.60
20:2:306:CHL:HMB1	18:2:316:BCR:H393	1.84	0.60
24:4:319:LMG:H252	24:4:319:LMG:H152	1.83	0.60
3:2:161:LEU:HD12	23:2:318:LHG:H152	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:838:CLA:H42	15:J:15:SER:HA	1.85	0.59
20:4:305:CHL:HMC	20:4:306:CHL:C4C	2.33	0.59
18:F:304:BCR:HC21	25:F:305:HTG:H62	1.83	0.59
25:B:848:HTG:H61	24:F:309:LMG:HC72	1.85	0.59
19:A:810:CLA:HHC	19:A:810:CLA:HBB1	1.83	0.59
7:B:733:PHE:O	13:H:160:ARG:NH1	2.36	0.59
6:A:360:LEU:HD11	19:A:817:CLA:H71	1.83	0.59
19:B:818:CLA:HBB2	19:B:824:CLA:H203	1.85	0.59
7:B:278:LEU:HG	19:B:816:CLA:HAB	1.84	0.59
5:4:191:PRO:HD2	21:4:316:LUT:H23	1.84	0.59
19:A:804:CLA:H71	19:A:828:CLA:HBC3	1.85	0.59
8:C:17:CYS:HB3	8:C:54:CYS:HA	1.85	0.58
23:4:322:LHG:H152	25:F:301:HTG:H4'2	1.86	0.58
19:4:314:CLA:HBC1	18:F:302:BCR:H311	1.84	0.58
11:F:79:LYS:HG3	11:F:80:GLU:OE1	2.04	0.58
11:F:85:ALA:O	11:F:88:GLU:HB2	2.04	0.58
6:A:214:GLN:HA	6:A:218:SER:HB3	1.84	0.58
7:B:31:PHE:HA	7:B:34:HIS:CD2	2.39	0.58
2:1:83:HIS:HD2	22:1:315:XAT:H15	1.68	0.58
7:B:369:ALA:HB1	7:B:725:LEU:HD11	1.86	0.58
19:B:807:CLA:HHB	19:B:808:CLA:HMB3	1.86	0.58
2:1:103:GLY:HA2	2:1:107:LYS:HD2	1.86	0.57
6:A:379:THR:HG21	6:A:515:VAL:HB	1.86	0.57
6:A:519:VAL:HG11	6:A:522:LEU:HD23	1.86	0.57
5:4:206:ALA:HB3	19:4:310:CLA:HMC2	1.87	0.57
6:A:117:PRO:HA	6:A:122:GLU:HG3	1.87	0.57
6:A:118:ILE:HG13	6:A:119:VAL:HG13	1.86	0.57
6:A:231:PRO:HA	6:A:234:ILE:HD12	1.85	0.57
19:4:314:CLA:HBC3	18:F:302:BCR:HC7	1.87	0.57
7:B:230:TRP:HB2	12:G:109:TRP:CH2	2.36	0.57
19:B:838:CLA:H2	19:B:839:CLA:H143	1.87	0.57
19:A:817:CLA:H92	19:A:827:CLA:H91	1.87	0.57
5:4:203:LYS:HA	19:4:310:CLA:CMC	2.35	0.57
6:A:279:LEU:HD11	6:A:521:LEU:HD12	1.86	0.57
19:A:839:CLA:H121	19:A:854:CLA:H43	1.86	0.57
11:F:170:VAL:HG11	11:F:200:ILE:HD12	1.87	0.57
3:2:159:ASP:OD2	20:2:306:CHL:HAC2	2.04	0.56
19:2:301:CLA:H62	19:2:302:CLA:H3A	1.86	0.56
24:B:849:LMG:H362	24:B:849:LMG:H121	1.87	0.56
18:1:316:BCR:HC41	12:G:40:PHE:CZ	2.38	0.56
1:L:89:LEU:HD23	7:B:687:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:70:GLY:O	7:B:680:TRP:NE1	2.38	0.56
19:1:304:CLA:HAA1	18:1:316:BCR:H23C	1.86	0.56
17:O:33:LEU:HD12	17:O:37:PHE:HB3	1.88	0.56
6:A:280:ASP:HB3	6:A:283:THR:HG22	1.87	0.56
6:A:508:GLY:HA2	6:A:523:PRO:HB3	1.86	0.56
7:B:159:PRO:HA	7:B:162:LYS:HD3	1.88	0.56
2:1:92:PRO:HB2	19:1:303:CLA:HMC2	1.88	0.55
19:B:825:CLA:H142	19:B:840:CLA:H203	1.88	0.55
11:F:181:GLU:OE2	11:F:187:LYS:NZ	2.38	0.55
1:L:215:PHE:HB2	19:L:304:CLA:H11	1.87	0.55
2:1:202:GLN:NE2	2:1:208:THR:O	2.36	0.55
19:A:837:CLA:H192	11:F:170:VAL:HG12	1.87	0.55
11:F:175:LEU:O	11:F:179:ARG:HG3	2.05	0.55
19:A:806:CLA:H202	19:A:839:CLA:HBA1	1.88	0.55
19:B:801:CLA:HBB1	19:B:801:CLA:HMB3	1.88	0.55
6:A:739:TRP:HB2	19:A:826:CLA:HBB1	1.88	0.55
7:B:472:TYR:HB3	11:F:73:SER:HA	1.88	0.55
5:4:175:TYR:HE2	20:4:315:CHL:C4D	2.19	0.55
6:A:390:HIS:HE1	19:A:826:CLA:ND	2.04	0.55
6:A:534:HIS:HB2	19:A:835:CLA:HED2	1.88	0.55
19:B:831:CLA:H143	19:B:850:CLA:H192	1.89	0.55
11:F:214:PHE:HB2	11:F:219:LEU:HD22	1.87	0.55
2:1:201:GLN:NE2	19:1:311:CLA:ND	2.55	0.55
9:D:112:GLU:O	9:D:142:ARG:NH1	2.40	0.55
19:A:836:CLA:HHC	19:A:836:CLA:HBB1	1.89	0.55
1:L:183:ASP:OD1	1:L:184:GLY:N	2.41	0.54
2:1:204:ALA:HB1	2:1:229:ILE:HG12	1.89	0.54
6:A:657:ILE:HD12	7:B:621:ARG:HG3	1.89	0.54
19:B:823:CLA:H42	19:B:824:CLA:H112	1.88	0.54
19:B:850:CLA:H18	18:F:308:BCR:H17C	1.88	0.54
7:B:694:ARG:HG3	19:B:838:CLA:HED2	1.88	0.54
1:L:74:THR:HG22	1:L:76:VAL:H	1.73	0.54
7:B:285:LEU:HB3	18:G:201:BCR:H16C	1.88	0.54
8:C:62:PHE:HD2	9:D:190:ILE:HG21	1.73	0.54
2:1:201:GLN:NE2	19:1:311:CLA:NA	2.54	0.54
4:3:170:ARG:HG2	20:3:306:CHL:HHC	1.89	0.54
6:A:29:PRO:HB2	6:A:45:TRP:HH2	1.73	0.54
8:C:16:GLN:HB3	8:C:57:ALA:HB1	1.90	0.54
12:G:25:LEU:HD12	12:G:108:SER:HA	1.90	0.54
5:4:56:TRP:HE1	19:4:301:CLA:C1B	2.20	0.54
5:4:98:ASN:ND2	19:4:308:CLA:OBD	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:552:VAL:HG21	18:A:847:BCR:HC31	1.89	0.54
11:F:212:ARG:O	11:F:216:ASN:ND2	2.40	0.54
4:3:170:ARG:HG3	20:3:306:CHL:HHC	1.90	0.54
6:A:50:HIS:HE1	19:A:854:CLA:ND	2.06	0.54
19:A:839:CLA:H62	26:A:841:PQN:H192	1.88	0.54
5:4:101:TRP:CE2	20:4:307:CHL:HED2	2.43	0.54
6:A:404:ALA:HB2	6:A:590:VAL:HG11	1.90	0.54
6:A:68:ARG:HG2	6:A:182:ALA:HB1	1.88	0.53
6:A:279:LEU:HD21	6:A:372:PRO:HD2	1.90	0.53
9:D:153:PHE:CZ	9:D:166:HIS:HB2	2.43	0.53
19:1:307:CLA:HBA1	23:1:320:LHG:HC92	1.90	0.53
5:4:82:ALA:HB2	19:4:302:CLA:HBA1	1.88	0.53
6:A:42:THR:HG22	6:A:713:GLN:HB2	1.89	0.53
6:A:576:PRO:HD3	7:B:561:GLY:HA2	1.89	0.53
7:B:90:ALA:HA	7:B:113:VAL:HG12	1.89	0.53
15:J:10:VAL:HG22	15:J:12:PRO:HD2	1.90	0.53
23:1:317:LHG:H101	18:4:318:BCR:H333	1.91	0.53
19:B:834:CLA:HBB1	19:B:834:CLA:HMB3	1.90	0.53
6:A:307:HIS:HB3	18:K:301:BCR:H373	1.90	0.53
1:L:216:VAL:HG12	1:L:216:VAL:O	2.08	0.53
6:A:201:GLY:O	6:A:205:LEU:HB2	2.08	0.53
19:A:820:CLA:HMD1	18:K:301:BCR:H23C	1.89	0.53
19:A:838:CLA:HAB	26:A:841:PQN:H202	1.89	0.53
19:B:805:CLA:H93	19:B:813:CLA:H2	1.91	0.53
3:2:189:TRP:CE3	20:2:313:CHL:HMA3	2.43	0.53
4:3:123:LYS:HG3	4:3:252:TYR:CE2	2.43	0.53
19:B:814:CLA:H91	19:B:828:CLA:H192	1.89	0.53
19:A:850:CLA:H11	7:B:616:LEU:HD12	1.90	0.53
19:1:302:CLA:HED1	18:B:844:BCR:H313	1.91	0.52
12:G:38:SER:HB2	12:G:101:ALA:HB2	1.90	0.52
19:B:807:CLA:H72	18:I:101:BCR:HC41	1.90	0.52
10:E:135:ALA:HB3	10:E:138:GLU:HG3	1.92	0.52
18:2:316:BCR:H17C	24:4:319:LMG:H182	1.92	0.52
19:4:303:CLA:HED2	19:4:303:CLA:H43	1.92	0.52
20:4:307:CHL:HAA1	19:4:309:CLA:HMC3	1.91	0.52
23:4:322:LHG:H172	23:4:322:LHG:H281	1.92	0.52
7:B:388:ALA:HB2	7:B:576:PHE:CD1	2.45	0.52
20:1:318:CHL:H2A	20:1:318:CHL:HED2	1.91	0.52
8:C:14:CYS:SG	8:C:16:GLN:HG2	2.50	0.52
4:3:219:MET:HG3	4:3:223:LYS:HE2	1.91	0.52
19:A:822:CLA:H12	19:A:836:CLA:H121	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:187:LYS:HD2	11:F:192:ASP:HB2	1.91	0.52
12:G:99:PRO:HD3	18:G:206:BCR:H353	1.91	0.52
17:O:20:ILE:HG23	17:O:36:LEU:HD22	1.92	0.52
5:4:201:LYS:HA	19:4:309:CLA:HED3	1.92	0.52
11:F:97:ASN:HA	11:F:100:LYS:HE3	1.92	0.52
6:A:118:ILE:HG23	6:A:119:VAL:HG22	1.91	0.52
3:2:155:ARG:HE	20:2:306:CHL:CMC	2.23	0.52
4:3:62:GLN:O	4:3:65:SER:OG	2.25	0.52
6:A:454:ILE:HG22	19:A:831:CLA:HBC2	1.92	0.52
19:A:806:CLA:HAB	19:A:826:CLA:H13	1.92	0.52
19:A:808:CLA:HBB2	19:A:811:CLA:HMA3	1.92	0.52
19:A:819:CLA:H71	18:A:847:BCR:H12C	1.92	0.52
7:B:523:ILE:HG12	7:B:590:VAL:HG12	1.92	0.52
17:O:88:PHE:CE1	19:O:103:CLA:HBA2	2.45	0.52
2:1:111:TRP:CE2	2:1:119:ALA:HB2	2.45	0.51
19:1:302:CLA:H43	19:1:302:CLA:HED3	1.90	0.51
19:B:821:CLA:HBB1	19:B:822:CLA:CHD	2.40	0.51
6:A:356:MET:HG3	19:A:823:CLA:HHB	1.92	0.51
18:G:201:BCR:H362	18:G:206:BCR:H312	1.92	0.51
3:2:223:GLY:O	3:2:227:GLN:HG3	2.10	0.51
4:3:99:TYR:HD1	4:3:200:ILE:HG12	1.74	0.51
4:3:111:GLY:HA2	22:3:314:XAT:H181	1.91	0.51
12:G:30:VAL:HG11	12:G:108:SER:HB3	1.92	0.51
8:C:17:CYS:C	8:C:20:ALA:H	2.18	0.51
8:C:55:GLU:HG2	8:C:63:LEU:HD13	1.91	0.51
6:A:642:ASN:O	6:A:646:ARG:HG2	2.11	0.51
6:A:405:HIS:HE1	19:A:828:CLA:NA	2.08	0.51
19:A:818:CLA:HAB	19:A:818:CLA:H151	1.92	0.51
11:F:125:ASN:HA	11:F:128:LYS:HG2	1.92	0.51
2:1:120:THR:HA	2:1:125:PRO:HA	1.92	0.51
7:B:631:LEU:HD22	7:B:724:PHE:HA	1.93	0.51
8:C:24:ASP:OD2	9:D:166:HIS:ND1	2.42	0.51
1:L:75:PRO:HA	1:L:78:SER:OG	2.11	0.51
2:1:186:LYS:HD3	19:1:309:CLA:O1D	2.11	0.51
4:3:123:LYS:HG3	4:3:252:TYR:HE2	1.75	0.51
20:4:305:CHL:HBB2	20:4:306:CHL:CBB	2.41	0.51
8:C:61:ASP:OD2	10:E:134:TYR:OH	2.27	0.51
11:F:166:TRP:O	11:F:170:VAL:HG23	2.11	0.51
4:3:266:ASN:HD22	19:3:311:CLA:HED2	1.75	0.50
6:A:572:PRO:HB3	6:A:719:ILE:HB	1.93	0.50
7:B:40:GLU:HG3	7:B:165:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:ILE:HD11	13:H:91:LEU:HD21	1.94	0.50
19:B:823:CLA:H3A	19:B:840:CLA:HED3	1.93	0.50
1:L:207:LEU:O	1:L:217:LYS:NZ	2.43	0.50
4:3:134:PRO:HG2	4:3:137:LYS:HG3	1.94	0.50
6:A:327:LYS:HA	6:A:334:GLY:HA3	1.93	0.50
7:B:422:LEU:HD13	7:B:532:LEU:HA	1.93	0.50
19:O:103:CLA:HBC3	18:O:106:BCR:C20	2.41	0.50
19:B:816:CLA:C1	12:G:109:TRP:HE1	2.25	0.50
19:3:308:CLA:CHC	21:3:313:LUT:H31	2.39	0.50
7:B:429:LEU:HD11	19:B:836:CLA:HMB1	1.94	0.50
19:L:303:CLA:H112	19:A:853:CLA:NC	2.26	0.50
6:A:147:ALA:HB2	6:A:375:PRO:HD2	1.94	0.50
6:A:201:GLY:HA3	19:A:811:CLA:HBB1	1.94	0.50
6:A:549:LEU:HA	6:A:552:VAL:HG22	1.93	0.50
7:B:225:LEU:HA	7:B:230:TRP:CD1	2.46	0.50
12:G:116:MET:HE2	12:G:118:PRO:HG2	1.92	0.50
5:4:203:LYS:HA	19:4:310:CLA:HMC3	1.94	0.50
19:A:852:CLA:HMD3	7:B:533:ILE:HG12	1.94	0.50
12:G:86:PRO:HG2	19:G:205:CLA:HBC2	1.94	0.50
6:A:530:ASP:HA	6:A:533:VAL:HG12	1.94	0.49
17:O:34:THR:H	17:O:37:PHE:HB2	1.77	0.49
1:L:74:THR:HG23	19:A:829:CLA:HAA2	1.93	0.49
6:A:732:LEU:HD22	19:A:839:CLA:HMA1	1.93	0.49
19:A:818:CLA:H152	18:A:844:BCR:H312	1.93	0.49
7:B:275:HIS:HE1	19:B:816:CLA:ND	2.10	0.49
5:4:177:LEU:HD11	20:4:315:CHL:HBC1	1.94	0.49
6:A:646:ARG:HA	6:A:650:TRP:HB3	1.94	0.49
3:2:148:PHE:HB3	18:2:316:BCR:H23C	1.93	0.49
19:B:817:CLA:HAC2	19:B:824:CLA:H202	1.94	0.49
18:L:305:BCR:HC31	19:B:804:CLA:HMD1	1.95	0.49
19:2:303:CLA:H43	20:2:304:CHL:HBD	1.94	0.49
6:A:13:LEU:HD12	6:A:186:ALA:HB3	1.94	0.49
7:B:181:GLY:HA2	7:B:185:VAL:HB	1.95	0.49
7:B:383:MET:HE1	18:B:845:BCR:H361	1.95	0.49
11:F:85:ALA:HA	11:F:88:GLU:CG	2.42	0.49
20:4:305:CHL:CGA	18:4:318:BCR:H19C	2.42	0.49
7:B:516:ASP:OD2	7:B:593:TYR:OH	2.27	0.49
19:B:810:CLA:H202	13:H:129:GLY:HA3	1.93	0.49
1:L:109:HIS:HE1	19:L:303:CLA:C4D	2.25	0.49
19:4:310:CLA:C4B	19:4:311:CLA:HBD	2.42	0.49
6:A:10:VAL:N	6:A:312:ASN:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:821:CLA:H11	16:K:208:LEU:HD21	1.94	0.49
12:G:111:PRO:HB2	12:G:112:PRO:HD3	1.95	0.49
6:A:330:PHE:CD1	23:A:843:LHG:HC42	2.48	0.49
7:B:203:ARG:HG2	7:B:250:ALA:HB1	1.95	0.49
3:2:151:TRP:CH2	18:2:316:BCR:H12C	2.48	0.49
19:A:816:CLA:H142	19:A:816:CLA:HBC3	1.95	0.49
7:B:124:TRP:HB3	7:B:129:LEU:HD12	1.95	0.49
19:1:312:CLA:H51	20:1:318:CHL:H111	1.93	0.49
20:2:319:CHL:OBD	4:3:170:ARG:NH2	2.41	0.49
4:3:215:ASP:OD1	4:3:218:SER:OG	2.29	0.49
6:A:104:ASP:HB3	6:A:108:ILE:HD12	1.95	0.49
7:B:441:ASP:OD1	7:B:615:TYR:HB2	2.13	0.49
19:F:307:CLA:HMB2	18:F:308:BCR:H24C	1.94	0.49
18:O:106:BCR:H403	18:O:106:BCR:H371	1.95	0.49
4:3:242:ILE:O	4:3:246:VAL:HG22	2.13	0.48
19:A:832:CLA:H43	19:K:303:CLA:H122	1.94	0.48
7:B:332:PHE:CE2	18:B:845:BCR:H292	2.47	0.48
6:A:296:LEU:O	6:A:300:ILE:HG12	2.13	0.48
6:A:319:ILE:HG21	19:A:823:CLA:HAC1	1.94	0.48
6:A:559:ARG:NH2	9:D:86:THR:O	2.46	0.48
19:A:850:CLA:HBC2	7:B:585:ASN:HB2	1.94	0.48
19:A:836:CLA:H122	18:A:846:BCR:H10C	1.95	0.48
19:L:303:CLA:H3A	18:L:306:BCR:H373	1.94	0.48
6:A:351:SER:OG	6:A:406:ALA:HB2	2.14	0.48
19:1:307:CLA:H142	19:1:307:CLA:H111	1.65	0.48
19:A:806:CLA:H3A	19:A:806:CLA:HBA2	1.59	0.48
7:B:125:TYR:O	7:B:130:ARG:NH1	2.47	0.48
17:O:23:SER:HA	18:O:106:BCR:HC21	1.96	0.48
2:1:173:ASP:HB3	2:1:176:LYS:HB3	1.95	0.48
23:1:320:LHG:H282	23:1:320:LHG:H312	1.58	0.48
19:3:310:CLA:C4D	19:3:310:CLA:H11	2.43	0.48
6:A:360:LEU:HD21	19:A:817:CLA:H93	1.95	0.48
19:A:835:CLA:H62	19:A:835:CLA:H41	1.66	0.48
19:1:309:CLA:H171	19:1:309:CLA:H13	1.47	0.48
4:3:104:ASN:ND2	19:3:307:CLA:OBD	2.46	0.48
19:4:302:CLA:HBB1	22:4:317:XAT:H30	1.95	0.48
7:B:429:LEU:HB3	7:B:525:LEU:HB2	1.94	0.48
15:J:28:GLU:OE1	15:J:31:ARG:NH2	2.39	0.48
4:3:243:GLN:HE22	21:3:313:LUT:H42	1.77	0.48
5:4:189:PHE:HZ	20:4:307:CHL:NB	2.12	0.48
19:B:812:CLA:HHC	19:B:812:CLA:HBB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:819:CLA:CMB	19:B:824:CLA:HMA3	2.43	0.48
12:G:106:THR:O	12:G:110:PRO:HD3	2.13	0.48
6:A:111:SER:HB2	6:A:128:VAL:HG11	1.96	0.48
6:A:392:MET:HG3	6:A:601:ILE:HG23	1.95	0.48
6:A:713:GLN:NE2	10:E:124:VAL:O	2.46	0.48
19:B:831:CLA:H93	19:B:831:CLA:H112	1.78	0.48
3:2:105:GLY:HA2	22:2:315:XAT:H181	1.96	0.48
19:A:809:CLA:H41	19:A:809:CLA:H62	1.44	0.48
7:B:600:THR:HG21	7:B:609:PHE:HB2	1.95	0.48
7:B:662:MET:HB2	19:B:803:CLA:C1C	2.44	0.48
2:1:217:HIS:CG	19:1:311:CLA:HAA2	2.49	0.47
19:B:822:CLA:HHC	19:B:840:CLA:HED1	1.96	0.47
8:C:60:THR:OG1	8:C:62:PHE:O	2.27	0.47
8:C:61:ASP:HB2	10:E:132:ASN:CG	2.39	0.47
10:E:122:ASP:OD1	10:E:122:ASP:N	2.44	0.47
19:1:304:CLA:HBD	19:1:304:CLA:HED2	1.67	0.47
3:2:130:GLY:HA3	20:2:305:CHL:C2D	2.44	0.47
18:2:316:BCR:HC8	19:4:301:CLA:HAC1	1.95	0.47
5:4:91:TYR:OH	11:F:212:ARG:HG3	2.14	0.47
19:1:302:CLA:H151	19:1:302:CLA:H18	1.44	0.47
19:2:311:CLA:HAB	19:2:311:CLA:H121	1.96	0.47
4:3:64:LEU:HD11	16:K:218:GLN:HE22	1.79	0.47
19:A:816:CLA:HBA2	19:A:816:CLA:H3A	1.53	0.47
9:D:75:PRO:HG2	9:D:77:THR:HG23	1.96	0.47
19:1:302:CLA:H12	19:B:840:CLA:HMC3	1.96	0.47
20:2:305:CHL:HED2	20:2:305:CHL:HBD	1.60	0.47
7:B:168:PHE:O	7:B:174:ARG:NH2	2.47	0.47
19:B:819:CLA:HMB1	19:B:824:CLA:HMA3	1.96	0.47
11:F:81:SER:HB3	11:F:84:PHE:HB2	1.97	0.47
2:1:59:PHE:CD2	20:1:318:CHL:HMC	2.49	0.47
19:4:302:CLA:O1A	22:4:317:XAT:H241	2.14	0.47
19:A:824:CLA:HBB1	19:A:836:CLA:HHB	1.95	0.47
19:B:824:CLA:H71	19:B:826:CLA:H42	1.95	0.47
19:3:302:CLA:HHC	19:3:302:CLA:HBB1	1.95	0.47
6:A:200:ALA:HB2	6:A:306:GLY:HA3	1.96	0.47
19:A:819:CLA:HBC3	19:A:825:CLA:H172	1.96	0.47
19:B:816:CLA:C3	12:G:109:TRP:HE1	2.28	0.47
19:B:835:CLA:HMB1	19:B:835:CLA:HBB1	1.97	0.47
1:L:210:LEU:O	1:L:211:ASN:C	2.58	0.47
19:1:306:CLA:HMB1	18:1:316:BCR:H14C	1.96	0.47
5:4:93:GLN:HE22	5:4:183:GLY:HA2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:4:319:LMG:H292	24:4:319:LMG:HC92	1.39	0.47
6:A:545:VAL:HG21	19:A:836:CLA:HMA1	1.95	0.47
6:A:585:SER:OG	6:A:588:ASP:OD2	2.27	0.47
19:A:808:CLA:H2	19:A:811:CLA:H193	1.97	0.47
19:A:826:CLA:H162	19:A:826:CLA:H192	1.73	0.47
19:B:819:CLA:H91	19:B:819:CLA:H111	1.66	0.47
8:C:13:GLY:O	8:C:38:GLN:NE2	2.40	0.47
11:F:99:LEU:HB2	11:F:112:ILE:HG21	1.97	0.47
2:1:226:ILE:HG12	2:1:230:ILE:HG12	1.96	0.47
20:4:307:CHL:HBD	19:4:309:CLA:HAC1	1.97	0.47
19:A:831:CLA:H91	19:A:831:CLA:H111	1.65	0.47
19:A:854:CLA:C4D	15:J:12:PRO:HD3	2.45	0.47
7:B:292:ARG:HD3	12:G:59:PRO:HD3	1.95	0.47
19:B:804:CLA:HMC1	19:B:807:CLA:H201	1.96	0.47
3:2:239:LEU:HB2	21:2:314:LUT:H22	1.96	0.47
5:4:151:TYR:CD2	18:4:318:BCR:H12C	2.49	0.47
20:4:306:CHL:HBC2	23:4:320:LHG:H151	1.97	0.47
7:B:458:ILE:HG21	11:F:144:SER:HB3	1.96	0.47
7:B:519:VAL:HG21	7:B:593:TYR:HB2	1.96	0.47
19:B:806:CLA:H111	19:B:806:CLA:H71	1.44	0.47
2:1:74:GLU:OE2	2:1:159:LYS:NZ	2.32	0.47
2:1:90:ALA:O	2:1:94:ILE:HG12	2.14	0.47
2:1:148:GLN:HB3	19:1:306:CLA:HMC2	1.96	0.47
23:1:317:LHG:O5	20:1:318:CHL:HAC1	2.15	0.47
6:A:274:THR:HB	6:A:276:ARG:HG3	1.96	0.47
19:A:828:CLA:H41	19:A:828:CLA:H62	1.59	0.47
7:B:652:PHE:O	7:B:656:VAL:HG23	2.15	0.47
3:2:81:LEU:HD13	19:2:301:CLA:H42	1.97	0.46
17:O:50:THR:OG1	17:O:51:PRO:HD3	2.16	0.46
19:1:309:CLA:H61	19:1:309:CLA:H41	1.51	0.46
20:2:304:CHL:HBB2	20:2:305:CHL:CBB	2.45	0.46
19:A:801:CLA:HBB1	19:A:850:CLA:HED1	1.97	0.46
19:B:826:CLA:H152	18:B:845:BCR:H17C	1.97	0.46
5:4:117:LYS:HG3	5:4:230:PHE:HD2	1.79	0.46
6:A:217:VAL:HG13	6:A:237:PRO:HB3	1.96	0.46
19:B:826:CLA:H52	18:B:845:BCR:H14C	1.96	0.46
6:A:194:MET:HB2	19:A:811:CLA:HBC2	1.98	0.46
19:1:307:CLA:H42	23:1:320:LHG:H321	1.96	0.46
20:4:305:CHL:HAA1	20:4:305:CHL:HBD	1.97	0.46
6:A:483:TRP:HD1	17:O:55:THR:HG23	1.79	0.46
7:B:106:ARG:NH2	7:B:113:VAL:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:808:CLA:H91	19:B:809:CLA:H52	1.98	0.46
19:B:813:CLA:H171	18:B:842:BCR:H271	1.96	0.46
19:4:302:CLA:HHB	19:4:302:CLA:H2	1.97	0.46
6:A:66:ILE:O	6:A:70:VAL:HG13	2.16	0.46
19:A:801:CLA:HMB3	19:B:802:CLA:HAA1	1.98	0.46
19:A:805:CLA:H93	15:J:20:GLY:HA3	1.97	0.46
7:B:662:MET:O	7:B:666:SER:OG	2.30	0.46
23:1:320:LHG:HC61	23:1:320:LHG:H241	1.54	0.46
19:3:310:CLA:HAA1	19:3:310:CLA:HBD	1.98	0.46
23:4:322:LHG:H252	25:F:301:HTG:H5'1	1.98	0.46
6:A:224:PHE:HB3	6:A:234:ILE:HG12	1.98	0.46
6:A:503:THR:HG23	19:A:832:CLA:HED3	1.97	0.46
6:A:608:PHE:O	6:A:612:MET:HG2	2.16	0.46
19:A:852:CLA:O1A	7:B:430:GLY:HA3	2.16	0.46
7:B:365:PHE:HB3	7:B:602:TRP:CZ3	2.50	0.46
9:D:122:ARG:NH2	13:H:74:SER:OG	2.48	0.46
24:J:101:LMG:H371	24:J:101:LMG:H401	1.68	0.46
19:1:307:CLA:H141	19:1:307:CLA:H161	1.69	0.46
23:2:318:LHG:H271	25:F:301:HTG:H7'2	1.97	0.46
20:2:319:CHL:HMD2	18:3:315:BCR:HC21	1.98	0.46
4:3:125:GLY:O	4:3:126:LEU:HD22	2.16	0.46
20:4:305:CHL:H61	20:4:305:CHL:H41	1.58	0.46
6:A:646:ARG:HB2	7:B:632:ILE:HD12	1.98	0.46
6:A:703:HIS:HE1	19:A:837:CLA:C4D	2.29	0.46
19:A:838:CLA:H143	19:A:838:CLA:H112	1.79	0.46
7:B:660:GLY:O	7:B:664:LEU:HG	2.16	0.46
19:B:802:CLA:H102	19:B:802:CLA:H62	1.67	0.46
19:B:829:CLA:H91	19:B:829:CLA:H112	1.68	0.46
9:D:153:PHE:CE2	9:D:166:HIS:HB2	2.50	0.46
4:3:230:GLY:O	4:3:234:MET:HG3	2.16	0.46
19:A:820:CLA:CMD	18:K:301:BCR:H23C	2.46	0.46
11:F:122:ARG:HB2	15:J:35:ASP:OD2	2.16	0.46
19:L:302:CLA:H52	19:L:302:CLA:H8	1.64	0.45
3:2:190:PHE:HZ	20:2:306:CHL:NB	2.14	0.45
19:A:837:CLA:HAA2	19:B:831:CLA:HMB1	1.97	0.45
11:F:85:ALA:O	11:F:89:LYS:HG2	2.16	0.45
6:A:594:LEU:HD21	19:A:828:CLA:HBC1	1.99	0.45
19:A:838:CLA:H202	19:A:838:CLA:H161	1.76	0.45
19:B:803:CLA:H203	19:B:803:CLA:H162	1.70	0.45
5:4:113:GLU:OE2	5:4:125:GLN:NE2	2.23	0.45
19:4:310:CLA:HAA2	19:4:311:CLA:HED3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:154:LEU:HD23	19:A:814:CLA:HED1	1.97	0.45
19:A:838:CLA:H121	19:A:838:CLA:H8	1.67	0.45
19:B:819:CLA:H111	19:B:819:CLA:H143	1.74	0.45
19:1:309:CLA:H101	19:1:310:CLA:NC	2.32	0.45
24:4:319:LMG:H231	24:4:319:LMG:H261	1.54	0.45
6:A:86:SER:OG	6:A:164:LEU:HG	2.15	0.45
19:A:825:CLA:H162	19:A:825:CLA:H122	1.49	0.45
7:B:5:PHE:HB2	14:I:31:ILE:HA	1.97	0.45
7:B:194:LEU:HA	7:B:198:ALA:HB3	1.98	0.45
7:B:290:MET:HE1	19:B:819:CLA:C1D	2.47	0.45
7:B:587:ILE:HA	7:B:590:VAL:HG22	1.97	0.45
19:B:807:CLA:H72	18:I:101:BCR:HC31	1.98	0.45
19:B:809:CLA:H143	19:B:809:CLA:H162	1.74	0.45
19:B:810:CLA:H161	19:B:810:CLA:H141	1.73	0.45
18:F:302:BCR:H24C	18:F:302:BCR:H371	1.84	0.45
17:O:15:GLY:HA3	17:O:73:LEU:HD23	1.98	0.45
19:1:302:CLA:H91	19:1:302:CLA:H112	1.58	0.45
23:2:317:LHG:HC62	23:2:317:LHG:H242	1.43	0.45
19:4:301:CLA:HBD	19:4:301:CLA:HED2	1.60	0.45
19:B:826:CLA:H101	19:B:826:CLA:H61	1.79	0.45
19:B:838:CLA:H102	19:B:839:CLA:H142	1.97	0.45
8:C:17:CYS:HB2	8:C:21:CYS:HB3	1.44	0.45
9:D:114:PRO:HG3	9:D:139:LEU:HB2	1.97	0.45
15:J:26:LEU:HD13	18:J:103:BCR:H402	1.98	0.45
7:B:277:HIS:HA	7:B:280:ILE:HG12	1.98	0.45
19:B:802:CLA:H122	19:B:802:CLA:H161	1.55	0.45
19:B:822:CLA:CHC	19:B:840:CLA:HED1	2.47	0.45
19:B:833:CLA:H151	19:B:833:CLA:H111	1.36	0.45
9:D:143:LEU:HA	9:D:147:TYR:HD2	1.81	0.45
5:4:204:GLU:HG3	19:4:309:CLA:CHB	2.46	0.45
6:A:221:ILE:HD11	6:A:237:PRO:HG3	1.99	0.45
6:A:483:TRP:CD1	17:O:55:THR:HG23	2.52	0.45
7:B:707:LEU:HD23	29:B:847:DGD:HA21	1.97	0.45
19:B:807:CLA:H112	19:B:807:CLA:HBB1	1.99	0.45
1:L:210:LEU:HD23	1:L:210:LEU:HA	1.77	0.45
4:3:66:TYR:CD2	4:3:67:LEU:HG	2.52	0.45
6:A:745:ARG:O	6:A:749:VAL:HG22	2.16	0.45
7:B:484:PRO:HA	7:B:487:ASN:HD22	1.82	0.45
7:B:676:GLU:HG2	8:C:81:TYR:HE1	1.82	0.45
19:B:813:CLA:H143	19:B:813:CLA:H162	1.79	0.45
19:B:835:CLA:H61	19:B:835:CLA:H41	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:850:CLA:H161	19:B:850:CLA:H193	1.83	0.45
11:F:206:TRP:CD1	11:F:207:PRO:HD3	2.52	0.45
19:1:303:CLA:H42	18:1:316:BCR:H272	1.98	0.45
5:4:78:PRO:O	23:4:322:LHG:H161	2.17	0.45
5:4:109:MET:HE3	22:4:317:XAT:O4	2.17	0.45
6:A:717:LEU:HD21	26:A:841:PQN:H151	1.98	0.45
19:B:835:CLA:H41	19:F:307:CLA:HBB2	1.98	0.45
16:K:184:THR:HG22	16:K:237:GLY:HA2	1.98	0.45
19:1:302:CLA:H142	19:1:302:CLA:H111	1.74	0.45
19:1:309:CLA:H112	19:1:309:CLA:H72	1.73	0.45
19:1:311:CLA:HHB	19:1:312:CLA:HBC3	1.97	0.45
19:2:309:CLA:C1D	19:2:310:CLA:HMA3	2.47	0.45
19:A:853:CLA:H122	19:A:853:CLA:H161	1.54	0.45
7:B:411:MET:HE3	7:B:411:MET:HB3	1.87	0.45
7:B:414:HIS:CE1	7:B:418:ILE:HD11	2.52	0.45
2:1:85:ARG:HA	2:1:88:MET:HE3	1.98	0.44
23:2:318:LHG:H121	23:2:318:LHG:HC91	1.58	0.44
19:4:310:CLA:H41	19:4:310:CLA:H13	1.99	0.44
6:A:293:HIS:HE1	19:A:815:CLA:NB	2.15	0.44
12:G:35:THR:HB	19:G:204:CLA:O1A	2.17	0.44
21:4:316:LUT:H15	21:4:316:LUT:H201	1.85	0.44
6:A:230:ASP:HB3	6:A:233:GLU:HG2	2.00	0.44
6:A:705:LYS:O	6:A:706:LEU:HB2	2.17	0.44
6:A:711:ALA:N	11:F:188:GLU:OE1	2.50	0.44
19:A:802:CLA:HAB	19:A:809:CLA:H142	1.98	0.44
19:A:817:CLA:H122	19:A:817:CLA:H162	1.76	0.44
19:B:808:CLA:H141	19:B:808:CLA:H162	1.73	0.44
9:D:164:TYR:O	9:D:168:LYS:NZ	2.41	0.44
4:3:265:ASN:HB3	19:3:310:CLA:HED1	1.98	0.44
23:4:322:LHG:H111	23:4:322:LHG:HC82	1.80	0.44
7:B:326:ILE:HG12	7:B:332:PHE:CE1	2.52	0.44
7:B:716:GLY:O	7:B:720:THR:OG1	2.28	0.44
11:F:92:ILE:HD12	11:F:116:ILE:HG23	1.99	0.44
2:1:142:ILE:HA	2:1:145:VAL:HG22	1.98	0.44
20:1:318:CHL:H112	20:1:318:CHL:H71	1.72	0.44
3:2:175:ASN:HB3	20:2:313:CHL:C1B	2.48	0.44
19:4:310:CLA:H41	19:4:310:CLA:H62	1.35	0.44
6:A:645:LEU:HD22	7:B:651:LEU:HD21	1.99	0.44
7:B:388:ALA:O	7:B:392:ILE:HG13	2.15	0.44
8:C:16:GLN:HB2	27:C:102:SF4:S4	2.57	0.44
20:2:319:CHL:HAC1	18:3:315:BCR:HC31	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:72:GLY:HA2	24:4:319:LMG:HC62	2.00	0.44
6:A:390:HIS:HE1	19:A:826:CLA:C1D	2.30	0.44
19:B:814:CLA:H61	19:B:814:CLA:H2	1.76	0.44
23:1:320:LHG:H342	23:1:320:LHG:H372	1.70	0.44
3:2:97:VAL:HG11	3:2:156:ARG:CZ	2.47	0.44
23:4:320:LHG:H132	23:4:320:LHG:H162	1.58	0.44
6:A:50:HIS:HE1	19:A:854:CLA:C4D	2.30	0.44
6:A:648:PHE:O	6:A:652:GLN:HB2	2.18	0.44
19:A:837:CLA:H52	18:F:304:BCR:H19C	2.00	0.44
19:1:302:CLA:H61	19:1:302:CLA:H41	1.65	0.44
3:2:227:GLN:HG2	19:2:311:CLA:C1D	2.47	0.44
7:B:466:ALA:HB1	7:B:477:LEU:HD12	2.00	0.44
19:B:808:CLA:O1A	19:B:827:CLA:HBD	2.18	0.44
20:1:305:CHL:HBD	20:1:305:CHL:HED2	1.64	0.44
21:1:314:LUT:H15	21:1:314:LUT:H201	1.85	0.44
5:4:210:LEU:HD13	19:4:310:CLA:CMB	2.48	0.44
6:A:653:ALA:O	6:A:657:ILE:HG12	2.18	0.44
11:F:165:GLY:HA3	11:F:206:TRP:CE2	2.52	0.44
2:1:226:ILE:HD12	19:1:311:CLA:H43	1.98	0.44
19:A:819:CLA:H121	18:A:847:BCR:HC8	1.99	0.44
18:A:846:BCR:H322	17:O:74:THR:HG21	1.98	0.44
19:B:801:CLA:C1B	19:B:803:CLA:HBB1	2.48	0.44
29:B:847:DGD:HAH2	29:B:847:DGD:HAT1	1.27	0.44
1:L:88:ASN:HB3	19:L:302:CLA:HAC1	2.00	0.43
19:3:301:CLA:H92	19:3:301:CLA:H61	1.75	0.43
5:4:100:ARG:HA	5:4:103:MET:HE3	2.00	0.43
7:B:650:PHE:CZ	7:B:654:HIS:HE1	2.36	0.43
19:B:818:CLA:H41	19:B:818:CLA:H62	1.55	0.43
19:4:303:CLA:O1D	19:4:303:CLA:H12	2.18	0.43
19:4:312:CLA:H101	19:4:312:CLA:HAB	2.00	0.43
22:4:317:XAT:H11	22:4:317:XAT:H191	1.87	0.43
6:A:430:HIS:CE1	6:A:434:ILE:HD11	2.54	0.43
19:A:806:CLA:H111	19:A:806:CLA:H151	1.81	0.43
19:A:808:CLA:H61	19:A:808:CLA:H41	1.73	0.43
19:A:817:CLA:HAB	19:A:817:CLA:H8	1.99	0.43
19:A:838:CLA:HMC2	18:F:304:BCR:H381	2.00	0.43
7:B:176:ASN:ND2	7:B:291:TYR:O	2.51	0.43
7:B:583:MET:O	7:B:587:ILE:HG12	2.18	0.43
19:B:825:CLA:H143	19:B:825:CLA:H161	1.72	0.43
29:B:847:DGD:HA21	29:B:847:DGD:HA51	1.76	0.43
17:O:35:GLU:HG2	18:O:106:BCR:HC22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:102:CLA:NA	18:O:105:BCR:H14C	2.33	0.43
6:A:455:HIS:HE1	19:A:831:CLA:C1A	2.31	0.43
7:B:47:PHE:CE2	7:B:51:PHE:HE2	2.36	0.43
10:E:92:ARG:NH2	10:E:138:GLU:OE1	2.48	0.43
11:F:212:ARG:HA	11:F:215:VAL:HG22	2.01	0.43
19:2:312:CLA:HAA2	4:3:159:LEU:HD12	1.99	0.43
5:4:203:LYS:NZ	19:4:311:CLA:H3A	2.34	0.43
5:4:221:GLN:NE2	19:4:312:CLA:NA	2.66	0.43
6:A:691:TYR:OH	7:B:533:ILE:HG13	2.17	0.43
7:B:701:SER:HB3	7:B:704:GLN:HB3	2.01	0.43
9:D:203:LYS:HE2	9:D:207:LEU:HB2	2.00	0.43
23:2:318:LHG:H122	5:4:60:LEU:HA	1.99	0.43
4:3:96:TRP:CZ2	19:3:307:CLA:HED2	2.53	0.43
6:A:691:TYR:CE1	7:B:536:LYS:HD2	2.53	0.43
7:B:462:TRP:HE1	7:B:476:VAL:HG11	1.83	0.43
7:B:548:PRO:HD2	8:C:62:PHE:CE1	2.53	0.43
19:B:806:CLA:HHB	19:B:829:CLA:HAB	1.99	0.43
19:B:821:CLA:H41	19:B:821:CLA:H61	1.48	0.43
19:B:828:CLA:H161	19:B:828:CLA:H141	1.66	0.43
19:1:301:CLA:H41	19:B:840:CLA:HBB2	1.99	0.43
3:2:166:VAL:HG13	3:2:166:VAL:O	2.17	0.43
20:4:305:CHL:NA	18:4:318:BCR:H383	2.34	0.43
6:A:438:LEU:HB2	19:A:836:CLA:CBB	2.48	0.43
7:B:458:ILE:HD11	11:F:142:ILE:HD12	2.01	0.43
7:B:700:LEU:HD22	7:B:704:GLN:NE2	2.34	0.43
17:O:22:PRO:HB2	18:O:106:BCR:HC8	1.99	0.43
19:2:310:CLA:HBA2	19:2:310:CLA:H3A	1.48	0.43
5:4:196:PRO:HA	19:4:309:CLA:O1D	2.19	0.43
6:A:538:ALA:HB2	19:A:835:CLA:HMA1	2.00	0.43
19:A:804:CLA:H161	19:A:804:CLA:H122	1.66	0.43
19:A:806:CLA:H93	19:A:806:CLA:H61	1.84	0.43
19:B:811:CLA:H12	19:B:812:CLA:C4D	2.49	0.43
19:B:821:CLA:H143	19:B:821:CLA:H112	1.90	0.43
18:B:846:BCR:H20C	18:B:846:BCR:H361	1.89	0.43
6:A:147:ALA:O	6:A:218:SER:OG	2.21	0.43
18:A:844:BCR:H10C	18:A:845:BCR:H281	2.01	0.43
12:G:109:TRP:O	12:G:112:PRO:HD2	2.19	0.43
3:2:99:CYS:O	3:2:103:MET:HG3	2.19	0.43
19:3:303:CLA:CHA	19:3:316:CLA:HBC2	2.49	0.43
19:3:308:CLA:H11	21:3:313:LUT:H373	2.01	0.43
19:3:310:CLA:H3A	19:3:310:CLA:HBA2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:103:MET:O	5:4:107:VAL:HG22	2.18	0.43
6:A:729:HIS:HE1	19:A:839:CLA:C4D	2.32	0.43
26:A:841:PQN:H222	26:A:841:PQN:H18	1.92	0.43
12:G:41:LEU:HA	12:G:45:VAL:HG22	1.99	0.43
19:4:301:CLA:HMB3	23:4:322:LHG:HC11	2.01	0.43
19:4:309:CLA:C1	19:4:311:CLA:HAB	2.40	0.43
19:4:313:CLA:H3A	19:4:313:CLA:HBA2	1.82	0.43
6:A:537:HIS:HE1	6:A:603:VAL:HG12	1.84	0.43
6:A:646:ARG:HB3	7:B:632:ILE:HB	2.00	0.43
23:A:842:LHG:H131	23:A:842:LHG:H102	1.59	0.43
24:B:849:LMG:H421	24:B:849:LMG:H391	1.79	0.43
19:L:302:CLA:HMB2	19:L:303:CLA:HMA2	2.01	0.42
23:1:317:LHG:H152	23:1:317:LHG:H122	1.75	0.42
19:3:301:CLA:HBA2	22:3:314:XAT:H241	2.01	0.42
5:4:210:LEU:HD13	19:4:310:CLA:HMB3	2.00	0.42
7:B:401:GLU:OE1	9:D:195:GLN:NE2	2.52	0.42
19:B:808:CLA:H62	19:B:808:CLA:H102	1.66	0.42
8:C:5:VAL:HG22	8:C:67:VAL:HG22	2.00	0.42
9:D:69:THR:HB	9:D:70:PRO:HD3	2.01	0.42
19:1:311:CLA:H41	23:1:317:LHG:H361	2.00	0.42
19:2:308:CLA:H91	19:2:308:CLA:H111	1.75	0.42
6:A:125:ASN:HB3	6:A:133:ARG:HB3	2.01	0.42
6:A:205:LEU:HB3	18:A:845:BCR:H20C	2.01	0.42
6:A:537:HIS:CE1	6:A:603:VAL:HG12	2.54	0.42
28:A:851:LMT:H3B	18:J:104:BCR:HC31	2.01	0.42
19:B:824:CLA:H112	19:B:824:CLA:H142	1.84	0.42
13:H:133:LEU:HD21	14:I:17:LEU:HD12	2.02	0.42
19:1:301:CLA:H152	19:1:301:CLA:H18	1.89	0.42
23:2:317:LHG:H142	23:2:317:LHG:H112	1.44	0.42
24:4:319:LMG:H111	24:4:319:LMG:H321	2.02	0.42
19:B:818:CLA:H3A	19:B:818:CLA:HBA2	1.75	0.42
19:B:836:CLA:HBC2	25:F:305:HTG:H4'1	2.01	0.42
19:K:303:CLA:H91	19:K:303:CLA:H112	1.73	0.42
19:L:303:CLA:H91	19:L:303:CLA:H111	1.70	0.42
4:3:209:PRO:HD2	21:3:313:LUT:H23	2.01	0.42
4:3:267:ILE:HD12	4:3:267:ILE:H	1.84	0.42
5:4:209:ARG:HG2	19:4:302:CLA:C4C	2.49	0.42
6:A:42:THR:HB	6:A:715:ARG:HG3	2.01	0.42
19:A:836:CLA:H111	19:A:836:CLA:H152	1.71	0.42
19:B:807:CLA:H12	14:I:15:VAL:HG21	2.02	0.42
8:C:70:TRP:CG	8:C:71:HIS:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:189:SER:HB3	9:D:192:LYS:HG2	2.02	0.42
19:L:302:CLA:H203	19:L:302:CLA:H162	1.74	0.42
23:1:317:LHG:H381	18:F:302:BCR:H20C	2.02	0.42
19:4:311:CLA:H41	19:4:311:CLA:H61	1.54	0.42
6:A:363:VAL:HA	19:A:824:CLA:HED2	2.01	0.42
7:B:178:HIS:O	7:B:182:LEU:HB3	2.19	0.42
7:B:516:ASP:HA	7:B:519:VAL:HG12	2.02	0.42
1:L:109:HIS:HD2	19:A:840:CLA:H201	1.84	0.42
19:L:302:CLA:H162	19:L:302:CLA:H141	1.74	0.42
5:4:104:LEU:HD23	5:4:104:LEU:HA	1.88	0.42
6:A:41:ASP:OD1	6:A:41:ASP:N	2.49	0.42
11:F:147:GLN:HB3	25:F:310:HTG:H2	2.00	0.42
13:H:160:ARG:O	13:H:161:LEU:HD23	2.19	0.42
19:1:308:CLA:C4D	21:1:314:LUT:H382	2.50	0.42
23:2:317:LHG:O4	18:3:315:BCR:HC32	2.20	0.42
19:A:822:CLA:HHB	19:O:101:CLA:HAB	2.01	0.42
19:A:835:CLA:H11	19:A:835:CLA:H51	1.91	0.42
19:A:836:CLA:H111	19:A:836:CLA:H93	1.90	0.42
7:B:574:ASP:OD1	7:B:706:ARG:NH1	2.52	0.42
19:B:802:CLA:H62	19:B:802:CLA:H41	1.77	0.42
19:B:826:CLA:H161	19:B:826:CLA:H141	1.59	0.42
19:B:833:CLA:H2	19:B:834:CLA:HBA1	2.02	0.42
9:D:105:SER:OG	9:D:107:LYS:O	2.36	0.42
12:G:110:PRO:HG2	24:G:202:LMG:O7	2.20	0.42
19:1:308:CLA:H52	21:1:314:LUT:H30	2.01	0.42
23:1:320:LHG:H382	23:1:320:LHG:H301	2.02	0.42
6:A:410:MET:HE1	6:A:428:LEU:HD11	2.01	0.42
7:B:498:LEU:HA	7:B:501:ILE:HG22	2.00	0.42
29:B:847:DGD:HA42	29:B:847:DGD:HA71	1.54	0.42
11:F:150:TRP:CD1	11:F:154:ILE:HG13	2.55	0.42
3:2:58:PRO:C	4:3:181:MET:HE1	2.45	0.42
3:2:177:LEU:HD12	20:2:306:CHL:HBC3	2.01	0.42
23:2:318:LHG:H261	23:2:318:LHG:H292	1.83	0.42
5:4:151:TYR:HE2	20:4:307:CHL:HAB	1.83	0.42
18:4:318:BCR:H15C	18:4:318:BCR:H351	1.89	0.42
23:4:322:LHG:HC82	23:4:322:LHG:HC5	1.73	0.42
18:A:847:BCR:H11C	18:A:847:BCR:H341	1.92	0.42
7:B:432:HIS:HD2	25:F:305:HTG:H2'2	1.84	0.42
7:B:439:HIS:O	7:B:443:MET:HG2	2.20	0.42
19:B:810:CLA:H202	19:B:810:CLA:H161	1.92	0.42
19:O:101:CLA:H43	18:O:105:BCR:H403	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:142:PHE:HB2	20:2:305:CHL:HBC1	2.02	0.41
24:4:319:LMG:H192	24:4:319:LMG:H222	1.52	0.41
19:A:818:CLA:H122	19:A:818:CLA:H162	1.33	0.41
19:A:831:CLA:H52	19:A:831:CLA:H8	1.86	0.41
18:F:302:BCR:H11C	18:F:302:BCR:H341	1.87	0.41
19:O:103:CLA:HAA1	19:O:103:CLA:HED3	2.02	0.41
1:L:79:SER:O	1:L:81:LEU:N	2.53	0.41
18:L:301:BCR:H15C	19:A:840:CLA:H152	2.01	0.41
2:1:201:GLN:HG2	19:1:311:CLA:C1D	2.49	0.41
5:4:180:ASN:ND2	5:4:185:PRO:HA	2.35	0.41
19:A:801:CLA:HAB	19:B:802:CLA:NA	2.36	0.41
19:B:816:CLA:C2D	19:B:816:CLA:H2	2.50	0.41
12:G:38:SER:CB	12:G:101:ALA:HB2	2.50	0.41
1:L:79:SER:HB2	17:O:4:TRP:NE1	2.34	0.41
1:L:118:VAL:HG23	1:L:130:GLY:H	1.85	0.41
19:1:308:CLA:H92	19:1:308:CLA:H61	1.70	0.41
19:A:813:CLA:H3A	19:A:813:CLA:HBA2	1.77	0.41
19:B:831:CLA:H142	19:B:831:CLA:H111	1.73	0.41
11:F:136:ASP:OD1	11:F:136:ASP:N	2.53	0.41
1:L:114:VAL:O	1:L:118:VAL:HG12	2.20	0.41
2:1:154:ASP:OD2	2:1:157:LYS:HG2	2.20	0.41
20:4:305:CHL:HBA1	20:4:305:CHL:H3A	1.43	0.41
6:A:29:PRO:HB3	19:A:854:CLA:HAC1	2.02	0.41
19:A:809:CLA:H143	19:A:809:CLA:H161	1.94	0.41
19:A:840:CLA:H62	19:A:840:CLA:H41	1.82	0.41
19:A:850:CLA:C1D	19:B:802:CLA:H2	2.49	0.41
19:A:850:CLA:HMA3	19:B:802:CLA:H8	2.03	0.41
19:A:854:CLA:H162	19:A:854:CLA:H122	1.83	0.41
7:B:317:ARG:HD3	7:B:404:GLU:O	2.20	0.41
7:B:389:HIS:HE1	19:B:829:CLA:NA	2.17	0.41
13:H:81:ASP:CG	13:H:84:ASN:HD22	2.29	0.41
1:L:91:ALA:HB1	7:B:690:LEU:HD11	2.02	0.41
19:1:302:CLA:H101	19:1:302:CLA:H62	1.46	0.41
6:A:372:PRO:HG2	6:A:378:ALA:HB2	2.01	0.41
19:A:808:CLA:H13	18:A:845:BCR:H372	2.02	0.41
19:A:830:CLA:H203	19:A:830:CLA:H162	1.81	0.41
19:A:839:CLA:H93	19:A:839:CLA:H112	1.87	0.41
7:B:65:LEU:HD12	7:B:142:LEU:HD12	2.03	0.41
7:B:301:ILE:H	7:B:301:ILE:HG13	1.73	0.41
7:B:583:MET:HE3	7:B:583:MET:HB3	1.84	0.41
19:B:801:CLA:H172	18:B:846:BCR:H343	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:843:BCR:H20C	18:B:843:BCR:H361	1.93	0.41
18:L:305:BCR:H11C	18:L:305:BCR:H341	1.92	0.41
3:2:177:LEU:HD23	20:2:313:CHL:HMB2	2.03	0.41
19:A:809:CLA:H142	19:A:809:CLA:H112	1.71	0.41
19:B:822:CLA:H62	19:B:822:CLA:H41	1.99	0.41
19:B:827:CLA:H192	19:B:827:CLA:H161	1.76	0.41
19:B:834:CLA:HMD3	19:G:203:CLA:HBB1	2.02	0.41
11:F:172:ARG:NH1	11:F:219:LEU:HD12	2.31	0.41
19:K:303:CLA:H61	19:K:303:CLA:H41	1.64	0.41
17:O:73:LEU:HD12	19:O:101:CLA:H42	2.03	0.41
1:L:142:VAL:HG13	13:H:125:LEU:HD22	2.03	0.41
3:2:181:ASP:OD2	3:2:207:ARG:NH2	2.42	0.41
19:2:301:CLA:H41	19:2:301:CLA:H61	1.64	0.41
4:3:218:SER:HA	4:3:221:ASP:OD2	2.21	0.41
5:4:180:ASN:HD22	5:4:185:PRO:HA	1.86	0.41
6:A:438:LEU:HA	6:A:441:VAL:HG12	2.03	0.41
6:A:703:HIS:HE1	19:A:837:CLA:ND	2.19	0.41
19:A:811:CLA:H93	19:A:811:CLA:H111	1.75	0.41
19:A:819:CLA:H91	19:A:819:CLA:H112	1.84	0.41
19:B:803:CLA:H142	19:B:803:CLA:H111	1.76	0.41
19:B:809:CLA:H142	19:B:809:CLA:H111	1.84	0.41
19:B:835:CLA:O1A	19:B:836:CLA:HBD	2.20	0.41
12:G:109:TRP:HB3	12:G:110:PRO:HD3	2.03	0.41
16:K:182:VAL:HA	19:K:302:CLA:HBA1	2.02	0.41
19:2:310:CLA:HAA1	19:2:310:CLA:HBD	2.01	0.41
5:4:221:GLN:HB3	5:4:232:ASN:ND2	2.35	0.41
6:A:143:GLN:HB3	6:A:374:TYR:HB3	2.03	0.41
7:B:30:ASP:HB2	19:B:829:CLA:HBA2	2.03	0.41
7:B:576:PHE:CZ	19:B:829:CLA:HAC2	2.56	0.41
19:B:806:CLA:HAB	19:B:828:CLA:HMC1	2.02	0.41
19:1:309:CLA:H122	19:1:310:CLA:CHC	2.51	0.41
19:1:311:CLA:H142	19:1:311:CLA:H111	1.71	0.41
3:2:57:PHE:CD1	20:2:319:CHL:HMA3	2.55	0.41
3:2:151:TRP:NE1	3:2:155:ARG:HD2	2.36	0.41
3:2:190:PHE:HE1	20:2:306:CHL:HBA1	1.86	0.41
19:2:311:CLA:H93	19:2:311:CLA:H111	1.78	0.41
21:2:314:LUT:H31	21:2:314:LUT:H391	1.91	0.41
19:3:308:CLA:HMB3	19:3:309:CLA:HAA1	2.02	0.41
6:A:395:GLY:O	6:A:399:ILE:HG13	2.21	0.41
6:A:414:TYR:CE2	6:A:416:PRO:HD3	2.55	0.41
6:A:601:ILE:O	6:A:605:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:32:GLU:OE1	7:B:331:HIS:NE2	2.43	0.41
7:B:450:GLU:OE2	11:F:122:ARG:NE	2.54	0.41
7:B:494:LEU:HD23	7:B:494:LEU:HA	1.93	0.41
19:B:812:CLA:HBB1	19:B:812:CLA:H93	2.03	0.41
19:B:814:CLA:CHC	18:B:843:BCR:H15C	2.51	0.41
19:B:829:CLA:H13	29:B:847:DGD:HAF1	2.03	0.41
29:B:847:DGD:HAV2	29:B:847:DGD:HAF2	1.68	0.41
19:G:204:CLA:HBD	19:G:204:CLA:HED3	1.81	0.41
19:K:302:CLA:HBC3	18:K:304:BCR:C31	2.51	0.41
18:L:305:BCR:H15C	18:L:305:BCR:H351	1.92	0.41
19:1:307:CLA:CMC	23:1:320:LHG:H212	2.51	0.41
19:3:316:CLA:HBA2	19:3:316:CLA:H3A	1.75	0.41
19:A:802:CLA:H92	19:A:805:CLA:H192	2.03	0.41
7:B:377:TYR:CD2	19:B:827:CLA:HAB	2.56	0.41
19:B:821:CLA:H111	19:B:821:CLA:H91	1.76	0.41
11:F:143:VAL:HG12	11:F:153:PHE:HB2	2.03	0.41
18:F:304:BCR:H20C	18:F:304:BCR:H361	1.89	0.41
1:L:63:ILE:HA	1:L:73:ASP:HB2	2.02	0.40
22:1:315:XAT:H15	22:1:315:XAT:H201	1.86	0.40
19:2:307:CLA:H2	24:J:101:LMG:H232	2.02	0.40
6:A:36:ILE:HD13	6:A:49:LEU:HA	2.03	0.40
6:A:118:ILE:HD12	6:A:118:ILE:HA	1.89	0.40
6:A:655:GLN:HG2	6:A:748:ALA:HB3	2.03	0.40
19:A:801:CLA:H203	19:A:801:CLA:H162	1.89	0.40
19:A:806:CLA:H143	19:A:806:CLA:H162	1.83	0.40
19:A:817:CLA:HBA2	19:A:817:CLA:H3A	1.75	0.40
19:A:820:CLA:H3A	19:A:820:CLA:HBA2	1.70	0.40
7:B:430:GLY:HA2	7:B:525:LEU:HD22	2.03	0.40
18:B:844:BCR:H391	18:B:845:BCR:H282	2.03	0.40
4:3:121:LEU:O	4:3:126:LEU:N	2.55	0.40
19:3:309:CLA:H12	19:3:309:CLA:H51	1.88	0.40
19:4:304:CLA:C3B	22:4:317:XAT:H183	2.52	0.40
19:A:811:CLA:H61	19:A:811:CLA:H41	1.40	0.40
28:A:851:LMT:H122	18:J:103:BCR:H333	2.03	0.40
7:B:290:MET:HE1	19:B:819:CLA:C2D	2.51	0.40
7:B:441:ASP:OD1	7:B:616:LEU:N	2.54	0.40
9:D:164:TYR:CZ	9:D:167:PRO:HD2	2.57	0.40
11:F:117:GLU:HG3	11:F:121:ARG:NE	2.36	0.40
18:J:103:BCR:H15C	18:J:103:BCR:H351	1.92	0.40
19:2:301:CLA:H61	19:2:301:CLA:H92	1.73	0.40
19:3:305:CLA:H3A	19:3:305:CLA:HBA2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:837:CLA:H171	11:F:171:GLY:HA2	2.04	0.40
7:B:670:TYR:OH	19:B:803:CLA:OBD	2.39	0.40
24:B:849:LMG:H171	24:B:849:LMG:H141	1.85	0.40
9:D:90:LEU:HD23	9:D:90:LEU:HA	1.92	0.40
3:2:103:MET:HE1	19:2:308:CLA:CAB	2.51	0.40
3:2:127:TYR:CD2	20:2:305:CHL:HMA2	2.57	0.40
5:4:113:GLU:OE2	5:4:228:GLY:HA3	2.21	0.40
24:4:319:LMG:H273	24:4:319:LMG:H161	2.04	0.40
6:A:14:VAL:HG11	6:A:181:ALA:HB1	2.03	0.40
6:A:435:ILE:HG13	6:A:554:PHE:HE2	1.87	0.40
6:A:484:ILE:CD1	19:A:834:CLA:H12	2.51	0.40
6:A:563:ASP:OD1	6:A:563:ASP:N	2.54	0.40
19:A:835:CLA:H161	19:A:835:CLA:H141	1.79	0.40
7:B:326:ILE:HG12	7:B:332:PHE:CD1	2.56	0.40
7:B:373:THR:HG23	7:B:591:THR:HG21	2.04	0.40
19:B:819:CLA:HBA2	19:B:823:CLA:H43	2.03	0.40
11:F:152:GLU:O	25:F:305:HTG:H3	2.21	0.40
19:1:309:CLA:H192	19:1:309:CLA:H162	1.91	0.40
5:4:56:TRP:CD2	5:4:76:PHE:HD1	2.40	0.40
6:A:215:VAL:HA	6:A:219:LEU:HD12	2.03	0.40
6:A:271:ASP:OD1	6:A:271:ASP:N	2.53	0.40
6:A:677:VAL:HG11	6:A:732:LEU:HD23	2.03	0.40
19:A:801:CLA:H62	19:A:801:CLA:H102	1.88	0.40
7:B:542:ARG:HE	7:B:551:LYS:HD3	1.86	0.40
19:B:818:CLA:H143	19:B:818:CLA:H112	1.90	0.40
18:B:842:BCR:H24C	18:B:842:BCR:H371	1.89	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	L	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
2	1	193/195 (99%)	181 (94%)	12 (6%)	0	100	100
3	2	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
4	3	214/216 (99%)	206 (96%)	8 (4%)	0	100	100
5	4	193/195 (99%)	177 (92%)	16 (8%)	0	100	100
6	A	740/742 (100%)	721 (97%)	19 (3%)	0	100	100
7	B	731/733 (100%)	710 (97%)	21 (3%)	0	100	100
8	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
9	D	137/139 (99%)	124 (90%)	13 (10%)	0	100	100
10	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
11	F	150/152 (99%)	147 (98%)	3 (2%)	0	100	100
12	G	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
13	H	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
14	I	30/32 (94%)	30 (100%)	0	0	100	100
15	J	37/39 (95%)	37 (100%)	0	0	100	100
16	K	79/81 (98%)	79 (100%)	0	0	100	100
17	O	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
All	All	3274/3308 (99%)	3147 (96%)	127 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	L	126/126 (100%)	124 (98%)	2 (2%)	55	80
2	1	159/159 (100%)	159 (100%)	0	100	100
3	2	165/165 (100%)	165 (100%)	0	100	100
4	3	169/169 (100%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	4	164/164 (100%)	164 (100%)	0	100 100
6	A	601/601 (100%)	601 (100%)	0	100 100
7	B	596/596 (100%)	596 (100%)	0	100 100
8	C	71/71 (100%)	71 (100%)	0	100 100
9	D	119/119 (100%)	118 (99%)	1 (1%)	73 88
10	E	57/57 (100%)	57 (100%)	0	100 100
11	F	126/126 (100%)	126 (100%)	0	100 100
12	G	80/80 (100%)	80 (100%)	0	100 100
13	H	75/75 (100%)	75 (100%)	0	100 100
14	I	28/28 (100%)	28 (100%)	0	100 100
15	J	34/34 (100%)	34 (100%)	0	100 100
16	K	58/58 (100%)	58 (100%)	0	100 100
17	O	75/75 (100%)	75 (100%)	0	100 100
All	All	2703/2703 (100%)	2700 (100%)	3 (0%)	87 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	209	VAL
1	L	210	LEU
9	D	152	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	72	ASN
3	2	213	ASN
3	2	228	HIS
4	3	129	GLN
4	3	243	GLN
4	3	253	GLN
4	3	254	ASN
4	3	266	ASN
5	4	168	GLN
5	4	222	HIS
5	4	232	ASN

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Mol	Chain	Res	Type
5	4	243	ASN
6	A	91	HIS
6	A	293	HIS
6	A	485	GLN
7	B	34	HIS
7	B	64	ASN
7	B	98	GLN
7	B	196	HIS
7	B	627	ASN
7	B	630	GLN
7	B	704	GLN
9	D	135	GLN
11	F	90	GLN
11	F	149	HIS
11	F	216	ASN
12	G	84	ASN
16	K	178	ASN
16	K	250	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

220 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	$\#\|Z\| > 2$
19	CLA	B	831	7	64,68,73	1.24	7 (10%)	77,107,113	0.91	3 (3%)
19	CLA	A	853	6	69,73,73	1.21	7 (10%)	83,113,113	0.93	3 (3%)
19	CLA	A	822	6	59,63,73	1.25	7 (11%)	71,101,113	1.03	4 (5%)
19	CLA	3	311	4	49,53,73	1.40	6 (12%)	59,89,113	1.12	5 (8%)
19	CLA	A	811	-	69,73,73	1.19	7 (10%)	83,113,113	0.98	4 (4%)
19	CLA	4	312	-	60,64,73	1.26	7 (11%)	72,102,113	1.06	5 (6%)
19	CLA	B	810	7	69,73,73	1.19	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	B	825	-	69,73,73	1.17	7 (10%)	83,113,113	0.94	4 (4%)
20	CHL	4	305	5	60,64,74	1.24	8 (13%)	68,102,114	1.12	5 (7%)
19	CLA	1	309	23	69,73,73	1.18	6 (8%)	83,113,113	0.83	3 (3%)
21	LUT	2	314	-	42,43,43	1.62	8 (19%)	51,60,60	1.61	10 (19%)
19	CLA	B	814	7	69,73,73	1.25	8 (11%)	83,113,113	0.98	4 (4%)
19	CLA	B	820	7	54,58,73	1.37	7 (12%)	65,95,113	1.04	3 (4%)
19	CLA	A	828	6	69,73,73	1.30	8 (11%)	83,113,113	0.95	3 (3%)
23	LHG	4	322	-	39,39,48	0.33	0	42,45,54	0.35	0
19	CLA	3	304	-	46,50,73	1.43	6 (13%)	55,85,113	1.14	4 (7%)
23	LHG	2	318	-	48,48,48	0.28	0	51,54,54	0.34	0
20	CHL	3	306	-	51,55,74	1.27	6 (11%)	57,91,114	1.18	6 (10%)
19	CLA	B	816	7	59,63,73	1.28	7 (11%)	71,101,113	1.07	5 (7%)
19	CLA	4	308	5	54,58,73	1.35	6 (11%)	65,95,113	1.01	4 (6%)
26	PQN	A	841	-	34,34,34	0.34	0	42,45,45	0.56	1 (2%)
19	CLA	A	837	6	69,73,73	1.19	6 (8%)	83,113,113	0.91	3 (3%)
19	CLA	B	828	-	69,73,73	1.22	7 (10%)	83,113,113	0.89	3 (3%)
19	CLA	B	822	7	59,63,73	1.25	7 (11%)	71,101,113	1.05	4 (5%)
20	CHL	2	306	-	55,59,74	1.23	7 (12%)	62,96,114	1.13	5 (8%)
19	CLA	A	803	6	69,73,73	1.19	7 (10%)	83,113,113	0.98	4 (4%)
19	CLA	B	819	-	69,73,73	1.19	7 (10%)	83,113,113	0.93	4 (4%)
19	CLA	A	835	6	69,73,73	1.19	7 (10%)	83,113,113	1.02	5 (6%)
19	CLA	1	312	2	59,63,73	1.29	6 (10%)	71,101,113	0.97	3 (4%)
18	BCR	2	316	-	41,41,41	1.68	8 (19%)	56,56,56	1.67	12 (21%)
21	LUT	1	314	-	42,43,43	1.59	8 (19%)	51,60,60	1.56	10 (19%)
19	CLA	A	814	-	49,53,73	1.42	7 (14%)	59,89,113	1.09	3 (5%)
19	CLA	A	817	6	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	3	303	-	49,53,73	1.41	6 (12%)	59,89,113	1.09	4 (6%)
18	BCR	G	201	-	41,41,41	1.71	8 (19%)	56,56,56	1.63	11 (19%)
22	XAT	2	315	-	39,47,47	1.69	8 (20%)	54,74,74	1.72	10 (18%)
18	BCR	A	846	-	41,41,41	1.69	8 (19%)	56,56,56	1.52	10 (17%)
19	CLA	B	823	7	64,68,73	1.23	6 (9%)	77,107,113	0.97	3 (3%)
18	BCR	A	848	-	41,41,41	1.71	8 (19%)	56,56,56	1.53	10 (17%)
23	LHG	A	843	19	26,26,48	0.37	0	29,32,54	0.43	0
19	CLA	B	802	7	69,73,73	1.17	7 (10%)	83,113,113	0.89	3 (3%)
20	CHL	4	306	-	55,59,74	1.26	7 (12%)	62,96,114	1.12	5 (8%)
18	BCR	J	104	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	B	808	7	69,73,73	1.20	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	B	813	7	69,73,73	1.20	7 (10%)	83,113,113	0.96	3 (3%)
19	CLA	A	821	6	55,59,73	1.31	7 (12%)	66,96,113	1.14	5 (7%)
19	CLA	2	310	3	56,60,73	1.32	8 (14%)	67,97,113	1.12	7 (10%)
19	CLA	4	303	5	64,68,73	1.28	8 (12%)	77,107,113	1.02	5 (6%)
20	CHL	4	315	5	47,51,74	1.41	8 (17%)	52,86,114	1.15	4 (7%)
25	HTG	F	310	-	19,19,19	0.19	0	23,24,24	0.40	0
18	BCR	O	105	-	41,41,41	1.70	8 (19%)	56,56,56	1.57	10 (17%)
19	CLA	1	308	2	64,68,73	1.19	7 (10%)	77,107,113	1.03	4 (5%)
18	BCR	B	844	-	41,41,41	1.69	8 (19%)	56,56,56	1.63	12 (21%)
18	BCR	3	315	-	41,41,41	1.69	8 (19%)	56,56,56	1.60	11 (19%)
19	CLA	K	302	-	49,53,73	1.41	7 (14%)	59,89,113	1.14	5 (8%)
23	LHG	1	319	19	22,22,48	0.33	0	25,28,54	0.46	0
23	LHG	1	320	-	48,48,48	0.29	0	51,54,54	0.32	0
18	BCR	B	842	-	41,41,41	1.70	8 (19%)	56,56,56	1.56	11 (19%)
18	BCR	F	304	-	41,41,41	1.67	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	B	801	-	69,73,73	1.19	7 (10%)	83,113,113	0.93	4 (4%)
20	CHL	4	307	-	55,59,74	1.24	7 (12%)	62,96,114	1.13	6 (9%)
28	LMT	A	851	-	36,36,36	0.18	0	47,47,47	0.31	0
19	CLA	1	313	2	50,54,73	1.33	6 (12%)	60,90,113	1.06	3 (5%)
19	CLA	B	812	7	59,63,73	1.28	7 (11%)	71,101,113	1.05	5 (7%)
19	CLA	A	829	6	54,58,73	1.34	7 (12%)	65,95,113	1.02	3 (4%)
19	CLA	F	306	-	49,53,73	1.39	6 (12%)	59,89,113	1.11	4 (6%)
19	CLA	4	304	-	54,58,73	1.29	6 (11%)	65,95,113	1.05	4 (6%)
19	CLA	B	826	7	69,73,73	1.22	8 (11%)	83,113,113	0.89	4 (4%)
19	CLA	O	101	23	56,60,73	1.34	6 (10%)	67,97,113	0.95	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	G	204	-	54,58,73	1.35	7 (12%)	65,95,113	0.94	3 (4%)
19	CLA	A	809	6	69,73,73	1.19	7 (10%)	83,113,113	1.04	4 (4%)
19	CLA	B	850	7	69,73,73	1.21	7 (10%)	83,113,113	1.08	5 (6%)
19	CLA	A	816	6	69,73,73	1.17	7 (10%)	83,113,113	0.99	5 (6%)
18	BCR	K	301	-	41,41,41	1.71	8 (19%)	56,56,56	1.66	11 (19%)
19	CLA	4	311	19,5	56,60,73	1.32	7 (12%)	67,97,113	1.17	7 (10%)
19	CLA	F	307	11	59,63,73	1.27	7 (11%)	71,101,113	0.98	3 (4%)
19	CLA	1	301	2	69,73,73	1.16	6 (8%)	83,113,113	1.02	5 (6%)
18	BCR	A	844	-	41,41,41	1.66	8 (19%)	56,56,56	1.64	12 (21%)
19	CLA	3	307	4	54,58,73	1.39	7 (12%)	65,95,113	0.99	3 (4%)
19	CLA	B	832	7	62,66,73	1.31	8 (12%)	74,104,113	1.10	6 (8%)
19	CLA	4	301	-	50,54,73	1.41	7 (14%)	60,90,113	1.05	3 (5%)
19	CLA	A	818	6	69,73,73	1.22	7 (10%)	83,113,113	0.96	4 (4%)
20	CHL	2	304	-	47,51,74	1.34	6 (12%)	52,86,114	1.19	6 (11%)
20	CHL	2	319	3	57,61,74	1.23	6 (10%)	64,98,114	1.10	5 (7%)
19	CLA	B	838	-	69,73,73	1.18	7 (10%)	83,113,113	0.98	5 (6%)
18	BCR	4	318	-	41,41,41	1.70	8 (19%)	56,56,56	1.71	12 (21%)
19	CLA	O	104	-	49,53,73	1.36	6 (12%)	59,89,113	1.23	5 (8%)
19	CLA	2	307	3	54,58,73	1.37	7 (12%)	65,95,113	1.22	6 (9%)
21	LUT	4	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.68	10 (19%)
20	CHL	2	313	-	47,51,74	1.34	7 (14%)	52,86,114	1.30	8 (15%)
19	CLA	G	203	-	45,49,73	1.45	6 (13%)	54,84,113	1.22	4 (7%)
19	CLA	1	306	-	50,54,73	1.38	7 (14%)	60,90,113	1.10	4 (6%)
19	CLA	B	804	7	49,53,73	1.44	8 (16%)	59,89,113	1.10	4 (6%)
19	CLA	4	310	19	64,68,73	1.31	8 (12%)	77,107,113	1.06	9 (11%)
19	CLA	A	820	6	53,57,73	1.37	8 (15%)	62,93,113	1.09	3 (4%)
20	CHL	1	305	2	52,56,74	1.25	6 (11%)	58,92,114	1.23	5 (8%)
19	CLA	A	838	-	69,73,73	1.20	6 (8%)	83,113,113	0.93	3 (3%)
18	BCR	F	302	-	41,41,41	1.72	8 (19%)	56,56,56	1.68	11 (19%)
19	CLA	3	305	4	51,55,73	1.36	7 (13%)	61,91,113	1.03	3 (4%)
19	CLA	B	835	7	64,68,73	1.29	8 (12%)	77,107,113	0.93	3 (3%)
19	CLA	2	309	23	45,49,73	1.50	6 (13%)	54,84,113	1.08	3 (5%)
19	CLA	A	850	-	69,73,73	1.20	7 (10%)	83,113,113	0.92	4 (4%)
19	CLA	2	311	-	69,73,73	1.19	6 (8%)	83,113,113	1.03	6 (7%)
23	LHG	2	317	19	36,36,48	0.33	0	39,42,54	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	O	102	17	49,53,73	1.35	6 (12%)	59,89,113	1.19	5 (8%)
19	CLA	B	836	7	69,73,73	1.16	7 (10%)	83,113,113	1.01	4 (4%)
19	CLA	3	308	4	54,58,73	1.29	7 (12%)	65,95,113	1.10	5 (7%)
19	CLA	A	839	6	69,73,73	1.20	7 (10%)	83,113,113	0.97	3 (3%)
22	XAT	3	314	-	39,47,47	1.70	8 (20%)	54,74,74	1.75	10 (18%)
24	LMG	J	101	-	51,51,55	0.24	0	59,59,63	0.31	0
25	HTG	F	301	-	19,19,19	0.25	0	23,24,24	0.55	0
25	HTG	4	321	-	19,19,19	0.23	0	23,24,24	0.36	0
19	CLA	A	819	-	69,73,73	1.19	7 (10%)	83,113,113	0.91	4 (4%)
19	CLA	B	805	7	69,73,73	1.19	7 (10%)	83,113,113	0.92	3 (3%)
19	CLA	A	804	6	69,73,73	1.20	8 (11%)	83,113,113	0.89	3 (3%)
18	BCR	L	301	-	41,41,41	1.66	8 (19%)	56,56,56	1.47	9 (16%)
19	CLA	B	821	7	69,73,73	1.24	8 (11%)	83,113,113	0.96	4 (4%)
18	BCR	A	845	-	41,41,41	1.63	8 (19%)	56,56,56	1.51	10 (17%)
19	CLA	3	309	4	56,60,73	1.33	7 (12%)	67,97,113	1.01	4 (5%)
19	CLA	A	823	-	69,73,73	1.21	8 (11%)	83,113,113	0.88	3 (3%)
19	CLA	A	802	6	59,63,73	1.28	7 (11%)	71,101,113	1.01	4 (5%)
25	HTG	B	848	-	19,19,19	0.27	0	23,24,24	0.60	0
19	CLA	A	826	6	69,73,73	1.16	6 (8%)	83,113,113	0.97	5 (6%)
19	CLA	A	808	6	69,73,73	1.16	7 (10%)	83,113,113	1.01	4 (4%)
19	CLA	A	801	6	69,73,73	1.19	7 (10%)	83,113,113	0.93	4 (4%)
19	CLA	K	303	-	64,68,73	1.23	7 (10%)	77,107,113	0.96	4 (5%)
19	CLA	B	818	7	64,68,73	1.26	7 (10%)	77,107,113	1.00	4 (5%)
19	CLA	1	311	-	64,68,73	1.24	6 (9%)	77,107,113	1.02	5 (6%)
19	CLA	1	303	-	55,59,73	1.32	7 (12%)	66,96,113	1.03	4 (6%)
19	CLA	2	302	3	55,59,73	1.32	7 (12%)	66,96,113	1.05	4 (6%)
19	CLA	4	309	5	64,68,73	1.24	7 (10%)	77,107,113	1.15	6 (7%)
19	CLA	A	830	6	69,73,73	1.20	7 (10%)	83,113,113	0.97	4 (4%)
19	CLA	B	809	7	69,73,73	1.25	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	3	312	4	50,54,73	1.38	7 (14%)	60,90,113	1.08	4 (6%)
19	CLA	A	832	6	54,58,73	1.32	6 (11%)	65,95,113	1.00	3 (4%)
19	CLA	B	806	7	69,73,73	1.22	6 (8%)	83,113,113	0.89	3 (3%)
18	BCR	F	308	-	41,41,41	1.64	8 (19%)	56,56,56	1.49	10 (17%)
19	CLA	B	840	23	69,73,73	1.18	6 (8%)	83,113,113	0.90	3 (3%)
19	CLA	A	810	6	58,62,73	1.31	7 (12%)	69,99,113	1.02	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	B	845	-	41,41,41	1.67	8 (19%)	56,56,56	1.52	10 (17%)
19	CLA	L	304	-	54,58,73	1.38	7 (12%)	65,95,113	1.00	3 (4%)
19	CLA	A	825	6	69,73,73	1.22	8 (11%)	83,113,113	0.91	4 (4%)
19	CLA	G	205	12	50,54,73	1.36	7 (14%)	60,90,113	1.17	5 (8%)
19	CLA	B	817	7	63,67,73	1.21	6 (9%)	75,105,113	1.06	5 (6%)
19	CLA	A	833	6	49,53,73	1.40	7 (14%)	59,89,113	1.18	5 (8%)
19	CLA	A	805	-	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
20	CHL	1	318	2	65,69,74	1.08	6 (9%)	74,108,114	0.98	5 (6%)
19	CLA	3	310	4	59,63,73	1.29	7 (11%)	71,101,113	1.03	5 (7%)
18	BCR	1	316	-	41,41,41	1.73	8 (19%)	56,56,56	1.79	14 (25%)
19	CLA	1	304	2	46,50,73	1.48	8 (17%)	55,85,113	1.11	3 (5%)
19	CLA	B	837	7	51,55,73	1.35	7 (13%)	61,91,113	1.09	4 (6%)
29	DGD	B	847	-	67,67,67	0.80	2 (2%)	81,81,81	1.09	5 (6%)
27	SF4	C	102	8	0,12,12	-	-	-		
25	HTG	F	303	-	19,19,19	0.22	0	23,24,24	0.50	0
27	SF4	A	849	7,6	0,12,12	-	-	-		
19	CLA	A	836	6	69,73,73	1.15	7 (10%)	83,113,113	1.09	7 (8%)
23	LHG	A	842	-	48,48,48	0.30	0	51,54,54	0.36	0
19	CLA	B	807	7	69,73,73	1.20	7 (10%)	83,113,113	0.91	3 (3%)
19	CLA	A	812	6	59,63,73	1.34	8 (13%)	71,101,113	1.12	6 (8%)
19	CLA	A	827	6	69,73,73	1.21	7 (10%)	83,113,113	0.90	3 (3%)
22	XAT	4	317	-	39,47,47	1.76	8 (20%)	54,74,74	1.89	13 (24%)
22	XAT	1	315	-	39,47,47	1.64	8 (20%)	54,74,74	1.66	10 (18%)
18	BCR	O	106	-	41,41,41	1.70	8 (19%)	56,56,56	1.70	12 (21%)
19	CLA	B	830	7	54,58,73	1.31	7 (12%)	65,95,113	1.02	4 (6%)
24	LMG	F	309	-	40,40,55	0.27	0	48,48,63	0.33	0
19	CLA	B	833	7	69,73,73	1.14	6 (8%)	83,113,113	1.03	4 (4%)
19	CLA	3	301	4	64,68,73	1.21	7 (10%)	77,107,113	1.01	5 (6%)
19	CLA	1	302	2	69,73,73	1.18	7 (10%)	83,113,113	0.91	4 (4%)
19	CLA	B	824	-	69,73,73	1.19	7 (10%)	83,113,113	0.96	4 (4%)
19	CLA	A	813	-	54,58,73	1.33	7 (12%)	65,95,113	1.11	5 (7%)
19	CLA	B	815	-	59,63,73	1.28	7 (11%)	71,101,113	1.06	5 (7%)
18	BCR	G	206	-	41,41,41	1.67	8 (19%)	56,56,56	1.62	11 (19%)
19	CLA	3	316	-	49,53,73	1.39	7 (14%)	59,89,113	1.05	4 (6%)
18	BCR	A	847	-	41,41,41	1.66	8 (19%)	56,56,56	1.50	9 (16%)
19	CLA	L	302	1	69,73,73	1.21	7 (10%)	83,113,113	1.00	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	1	307	2	69,73,73	1.20	7 (10%)	83,113,113	0.94	5 (6%)
27	SF4	C	101	8	0,12,12	-	-	-		
19	CLA	3	302	4	54,58,73	1.36	8 (14%)	65,95,113	1.02	4 (6%)
18	BCR	J	103	-	41,41,41	1.67	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	L	303	1	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	2	308	3	64,68,73	1.21	8 (12%)	77,107,113	1.11	7 (9%)
19	CLA	B	834	-	49,53,73	1.37	7 (14%)	59,89,113	1.14	5 (8%)
19	CLA	B	803	-	69,73,73	1.19	7 (10%)	83,113,113	1.01	5 (6%)
24	LMG	G	202	-	40,40,55	0.22	0	48,48,63	0.23	0
18	BCR	L	306	-	41,41,41	1.65	8 (19%)	56,56,56	1.45	9 (16%)
19	CLA	A	806	6	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	A	831	6	69,73,73	1.23	8 (11%)	83,113,113	1.01	4 (4%)
19	CLA	2	303	-	64,68,73	1.25	7 (10%)	77,107,113	0.97	4 (5%)
24	LMG	4	319	-	50,50,55	0.25	0	58,58,63	0.32	0
19	CLA	J	102	15	46,50,73	1.44	7 (15%)	55,85,113	1.19	5 (9%)
18	BCR	I	101	-	41,41,41	1.69	8 (19%)	56,56,56	1.65	12 (21%)
23	LHG	4	320	-	48,48,48	0.28	0	51,54,54	0.33	0
18	BCR	K	304	-	41,41,41	1.69	8 (19%)	56,56,56	1.73	12 (21%)
23	LHG	1	317	19	48,48,48	0.29	0	51,54,54	0.41	0
19	CLA	4	302	5	64,68,73	1.22	8 (12%)	77,107,113	1.03	5 (6%)
25	HTG	F	305	-	19,19,19	0.33	0	23,24,24	0.48	0
19	CLA	O	103	-	56,60,73	1.26	6 (10%)	67,97,113	1.05	4 (5%)
18	BCR	B	843	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	11 (19%)
19	CLA	4	313	5	49,53,73	1.39	6 (12%)	59,89,113	1.13	4 (6%)
20	CHL	2	305	-	52,56,74	1.26	6 (11%)	58,92,114	1.05	3 (5%)
24	LMG	B	849	-	44,44,55	0.23	0	52,52,63	0.31	0
18	BCR	L	305	-	41,41,41	1.69	8 (19%)	56,56,56	1.65	11 (19%)
19	CLA	A	807	6	69,73,73	1.19	7 (10%)	83,113,113	0.95	3 (3%)
19	CLA	A	852	-	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
19	CLA	A	854	6	69,73,73	1.17	7 (10%)	83,113,113	0.99	5 (6%)
19	CLA	B	811	7	58,62,73	1.33	8 (13%)	73,100,113	1.09	4 (5%)
19	CLA	1	310	2	56,60,73	1.31	6 (10%)	67,97,113	1.03	4 (5%)
19	CLA	A	824	-	69,73,73	1.18	6 (8%)	83,113,113	0.89	3 (3%)
19	CLA	2	301	3	69,73,73	1.16	6 (8%)	83,113,113	0.94	4 (4%)
19	CLA	4	314	5	51,55,73	1.36	6 (11%)	61,91,113	1.08	4 (6%)
21	LUT	3	313	-	42,43,43	1.64	8 (19%)	51,60,60	1.63	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	2	312	3	47,51,73	1.45	7 (14%)	56,86,113	1.18	5 (8%)
19	CLA	B	827	7	69,73,73	1.18	7 (10%)	83,113,113	1.05	5 (6%)
19	CLA	A	815	6	69,73,73	1.20	7 (10%)	83,113,113	0.89	3 (3%)
19	CLA	B	829	7	69,73,73	1.21	7 (10%)	83,113,113	1.03	4 (4%)
19	CLA	B	839	7	69,73,73	1.19	6 (8%)	83,113,113	0.97	4 (4%)
19	CLA	A	840	-	69,73,73	1.21	8 (11%)	83,113,113	0.89	3 (3%)
26	PQN	B	841	-	34,34,34	0.37	0	42,45,45	0.61	1 (2%)
18	BCR	B	846	-	41,41,41	1.66	8 (19%)	56,56,56	1.48	10 (17%)
19	CLA	A	834	6	55,59,73	1.39	8 (14%)	66,96,113	0.98	3 (4%)

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
19	CLA	B	831	7	-	14/33/109/115	-
19	CLA	A	853	6	-	14/39/115/115	-
19	CLA	A	822	6	-	11/27/103/115	-
19	CLA	3	311	4	-	9/15/91/115	-
19	CLA	A	811	-	-	24/39/115/115	-
19	CLA	4	312	-	-	9/29/105/115	-
19	CLA	B	810	7	-	16/39/115/115	-
19	CLA	B	825	-	-	21/39/115/115	-
20	CHL	4	305	5	-	16/29/105/117	-
19	CLA	1	309	23	-	23/39/115/115	-
21	LUT	2	314	-	-	11/29/67/67	0/2/2/2
19	CLA	B	814	7	-	19/39/115/115	-
19	CLA	B	820	7	-	13/21/97/115	-
19	CLA	A	828	6	-	19/39/115/115	-
23	LHG	4	322	-	-	28/44/44/53	-
19	CLA	3	304	-	-	6/12/88/115	-
23	LHG	2	318	-	-	30/53/53/53	-
20	CHL	3	306	-	-	11/19/95/117	-
19	CLA	B	816	7	-	14/27/103/115	-
19	CLA	4	308	5	-	10/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PQN	A	841	-	-	3/23/43/43	0/2/2/2
19	CLA	A	837	6	-	21/39/115/115	-
19	CLA	B	828	-	-	20/39/115/115	-
19	CLA	B	822	7	-	13/27/103/115	-
20	CHL	2	306	-	-	11/23/99/117	-
19	CLA	A	803	6	-	11/39/115/115	-
19	CLA	B	819	-	-	17/39/115/115	-
19	CLA	A	835	6	-	14/39/115/115	-
19	CLA	1	312	2	-	19/27/103/115	-
18	BCR	2	316	-	-	24/29/63/63	0/2/2/2
21	LUT	1	314	-	-	13/29/67/67	0/2/2/2
19	CLA	A	814	-	-	8/15/91/115	-
19	CLA	A	817	6	-	14/39/115/115	-
19	CLA	3	303	-	-	5/15/91/115	-
18	BCR	G	201	-	-	15/29/63/63	0/2/2/2
22	XAT	2	315	-	-	10/31/93/93	0/4/4/4
18	BCR	A	846	-	-	8/29/63/63	0/2/2/2
19	CLA	B	823	7	-	20/33/109/115	-
18	BCR	A	848	-	-	21/29/63/63	0/2/2/2
23	LHG	A	843	19	-	15/31/31/53	-
19	CLA	B	802	7	-	16/39/115/115	-
20	CHL	4	306	-	-	12/23/99/117	-
18	BCR	J	104	-	-	20/29/63/63	0/2/2/2
19	CLA	B	808	7	-	12/39/115/115	-
19	CLA	B	813	7	-	18/39/115/115	-
19	CLA	A	821	6	-	13/23/99/115	-
19	CLA	2	310	3	-	13/24/100/115	-
19	CLA	4	303	5	-	17/33/109/115	-
20	CHL	4	315	5	-	10/14/90/117	-
25	HTG	F	310	-	-	4/10/30/30	0/1/1/1
18	BCR	O	105	-	-	22/29/63/63	0/2/2/2
19	CLA	1	308	2	-	13/33/109/115	-
18	BCR	B	844	-	-	13/29/63/63	0/2/2/2
18	BCR	3	315	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	K	302	-	-	10/15/91/115	-
23	LHG	1	319	19	-	8/26/26/53	-
23	LHG	1	320	-	-	36/53/53/53	-
18	BCR	B	842	-	-	14/29/63/63	0/2/2/2
18	BCR	F	304	-	-	18/29/63/63	0/2/2/2
19	CLA	B	801	-	-	9/39/115/115	-
20	CHL	4	307	-	-	11/23/99/117	-
28	LMT	A	851	-	-	13/21/61/61	0/2/2/2
19	CLA	1	313	2	-	8/17/93/115	-
19	CLA	B	812	7	-	9/27/103/115	-
19	CLA	A	829	6	-	13/21/97/115	-
19	CLA	F	306	-	-	3/15/91/115	-
19	CLA	4	304	-	-	12/21/97/115	-
19	CLA	B	826	7	-	10/39/115/115	-
19	CLA	O	101	23	-	12/24/100/115	-
19	CLA	G	204	-	-	6/21/97/115	-
19	CLA	A	809	6	-	14/39/115/115	-
19	CLA	B	850	7	-	12/39/115/115	-
19	CLA	A	816	6	-	22/39/115/115	-
18	BCR	K	301	-	-	17/29/63/63	0/2/2/2
19	CLA	4	311	19,5	-	13/24/100/115	-
19	CLA	F	307	11	-	10/27/103/115	-
19	CLA	1	301	2	-	15/39/115/115	-
18	BCR	A	844	-	-	19/29/63/63	0/2/2/2
19	CLA	3	307	4	-	10/21/97/115	-
19	CLA	B	832	7	-	14/31/107/115	-
19	CLA	4	301	-	-	4/17/93/115	-
19	CLA	A	818	6	-	20/39/115/115	-
20	CHL	2	304	-	-	5/14/90/117	-
20	CHL	2	319	3	-	15/26/102/117	-
19	CLA	B	838	-	-	14/39/115/115	-
18	BCR	4	318	-	-	16/29/63/63	0/2/2/2
19	CLA	O	104	-	-	10/15/91/115	-
19	CLA	2	307	3	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LUT	4	316	-	-	15/29/67/67	0/2/2/2
20	CHL	2	313	-	-	8/14/90/117	-
19	CLA	G	203	-	-	6/10/86/115	-
19	CLA	1	306	-	-	10/17/93/115	-
19	CLA	B	804	7	-	5/15/91/115	-
19	CLA	4	310	19	-	19/33/109/115	-
19	CLA	A	820	6	-	12/20/96/115	-
20	CHL	1	305	2	-	16/20/96/117	-
19	CLA	A	838	-	-	24/39/115/115	-
18	BCR	F	302	-	-	18/29/63/63	0/2/2/2
19	CLA	3	305	4	-	7/18/94/115	-
19	CLA	B	835	7	-	14/33/109/115	-
19	CLA	2	309	23	-	4/10/86/115	-
19	CLA	A	850	-	-	17/39/115/115	-
19	CLA	2	311	-	-	15/39/115/115	-
23	LHG	2	317	19	-	22/41/41/53	-
19	CLA	O	102	17	-	9/15/91/115	-
19	CLA	B	836	7	-	12/39/115/115	-
19	CLA	3	308	4	-	11/21/97/115	-
19	CLA	A	839	6	-	20/39/115/115	-
22	XAT	3	314	-	-	6/31/93/93	0/4/4/4
24	LMG	J	101	-	-	26/46/66/70	0/1/1/1
25	HTG	F	301	-	-	8/10/30/30	0/1/1/1
25	HTG	4	321	-	-	7/10/30/30	0/1/1/1
19	CLA	A	819	-	-	9/39/115/115	-
19	CLA	B	805	7	-	12/39/115/115	-
19	CLA	A	804	6	-	15/39/115/115	-
18	BCR	L	301	-	-	16/29/63/63	0/2/2/2
19	CLA	B	821	7	-	19/39/115/115	-
18	BCR	A	845	-	-	20/29/63/63	0/2/2/2
19	CLA	3	309	4	-	3/24/100/115	-
19	CLA	A	823	-	-	9/39/115/115	-
19	CLA	A	802	6	-	7/27/103/115	-
25	HTG	B	848	-	-	5/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	826	6	-	15/39/115/115	-
19	CLA	A	808	6	-	22/39/115/115	-
19	CLA	A	801	6	-	12/39/115/115	-
19	CLA	K	303	-	-	17/33/109/115	-
19	CLA	B	818	7	-	17/33/109/115	-
19	CLA	1	311	-	-	14/33/109/115	-
19	CLA	1	303	-	-	7/23/99/115	-
19	CLA	2	302	3	-	8/23/99/115	-
19	CLA	4	309	5	-	14/33/109/115	-
19	CLA	A	830	6	-	19/39/115/115	-
19	CLA	B	809	7	-	18/39/115/115	-
19	CLA	3	312	4	-	2/17/93/115	-
19	CLA	A	832	6	-	8/21/97/115	-
19	CLA	B	806	7	-	22/39/115/115	-
18	BCR	F	308	-	-	13/29/63/63	0/2/2/2
19	CLA	B	840	23	-	11/39/115/115	-
19	CLA	A	810	6	-	4/26/102/115	-
18	BCR	B	845	-	-	13/29/63/63	0/2/2/2
19	CLA	L	304	-	-	8/21/97/115	-
19	CLA	A	825	6	-	12/39/115/115	-
19	CLA	G	205	12	-	4/17/93/115	-
19	CLA	B	817	7	-	11/32/108/115	-
19	CLA	A	833	6	-	7/15/91/115	-
19	CLA	A	805	-	-	17/39/115/115	-
20	CHL	1	318	2	-	15/35/111/117	-
19	CLA	3	310	4	-	13/27/103/115	-
18	BCR	1	316	-	-	22/29/63/63	0/2/2/2
19	CLA	1	304	2	-	5/12/88/115	-
19	CLA	B	837	7	-	5/18/94/115	-
29	DGD	B	847	-	-	26/55/95/95	0/2/2/2
27	SF4	C	102	8	-	-	0/6/5/5
25	HTG	F	303	-	-	6/10/30/30	0/1/1/1
27	SF4	A	849	7,6	-	-	0/6/5/5
19	CLA	A	836	6	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	A	842	-	-	27/53/53/53	-
19	CLA	B	807	7	-	12/39/115/115	-
19	CLA	A	812	6	-	10/27/103/115	-
19	CLA	A	827	6	-	18/39/115/115	-
22	XAT	4	317	-	-	8/31/93/93	0/4/4/4
22	XAT	1	315	-	-	12/31/93/93	0/4/4/4
18	BCR	O	106	-	-	20/29/63/63	0/2/2/2
19	CLA	B	830	7	-	10/21/97/115	-
24	LMG	F	309	-	-	11/35/55/70	0/1/1/1
19	CLA	B	833	7	-	22/39/115/115	-
19	CLA	3	301	4	-	16/33/109/115	-
19	CLA	1	302	2	-	27/39/115/115	-
19	CLA	B	824	-	-	11/39/115/115	-
19	CLA	A	813	-	-	11/21/97/115	-
19	CLA	B	815	-	-	12/27/103/115	-
18	BCR	G	206	-	-	21/29/63/63	0/2/2/2
19	CLA	3	316	-	-	6/15/91/115	-
18	BCR	A	847	-	-	16/29/63/63	0/2/2/2
19	CLA	L	302	1	-	20/39/115/115	-
19	CLA	1	307	2	-	23/39/115/115	-
27	SF4	C	101	8	-	-	0/6/5/5
19	CLA	3	302	4	-	6/21/97/115	-
18	BCR	J	103	-	-	19/29/63/63	0/2/2/2
19	CLA	L	303	1	-	17/39/115/115	-
19	CLA	2	308	3	-	7/33/109/115	-
19	CLA	B	834	-	-	2/15/91/115	-
19	CLA	B	803	-	-	11/39/115/115	-
24	LMG	G	202	-	-	17/35/55/70	0/1/1/1
18	BCR	L	306	-	-	12/29/63/63	0/2/2/2
19	CLA	A	806	6	-	19/39/115/115	-
19	CLA	A	831	6	-	18/39/115/115	-
19	CLA	2	303	-	-	22/33/109/115	-
24	LMG	4	319	-	-	27/45/65/70	0/1/1/1
19	CLA	J	102	15	-	6/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	I	101	-	-	14/29/63/63	0/2/2/2
23	LHG	4	320	-	-	35/53/53/53	-
18	BCR	K	304	-	-	22/29/63/63	0/2/2/2
23	LHG	1	317	19	-	30/53/53/53	-
19	CLA	4	302	5	-	14/33/109/115	-
25	HTG	F	305	-	-	5/10/30/30	0/1/1/1
19	CLA	O	103	-	-	11/24/100/115	-
18	BCR	B	843	-	-	17/29/63/63	0/2/2/2
19	CLA	4	313	5	-	10/15/91/115	-
20	CHL	2	305	-	-	12/20/96/117	-
24	LMG	B	849	-	-	20/39/59/70	0/1/1/1
18	BCR	L	305	-	-	14/29/63/63	0/2/2/2
19	CLA	A	807	6	-	18/39/115/115	-
19	CLA	A	852	-	-	8/39/115/115	-
19	CLA	A	854	6	-	18/39/115/115	-
19	CLA	B	811	7	-	14/25/101/115	-
19	CLA	1	310	2	-	15/24/100/115	-
19	CLA	A	824	-	-	17/39/115/115	-
19	CLA	2	301	3	-	18/39/115/115	-
19	CLA	4	314	5	-	6/18/94/115	-
21	LUT	3	313	-	-	20/29/67/67	0/2/2/2
19	CLA	2	312	3	-	2/13/89/115	-
19	CLA	B	827	7	-	22/39/115/115	-
19	CLA	A	815	6	-	19/39/115/115	-
19	CLA	B	829	7	-	16/39/115/115	-
19	CLA	B	839	7	-	20/39/115/115	-
19	CLA	A	840	-	-	22/39/115/115	-
26	PQN	B	841	-	-	2/23/43/43	0/2/2/2
18	BCR	B	846	-	-	16/29/63/63	0/2/2/2
19	CLA	A	834	6	-	10/23/99/115	-

All (1376) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	310	CLA	C1C-C2C	-4.95	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	817	CLA	C1C-C2C	-4.77	1.35	1.44
19	4	309	CLA	C4C-C3C	-4.76	1.36	1.45
19	A	814	CLA	C4C-C3C	-4.76	1.36	1.45
19	3	312	CLA	C4C-C3C	-4.76	1.36	1.45
19	3	308	CLA	C4C-C3C	-4.75	1.36	1.45
19	4	303	CLA	C4C-C3C	-4.74	1.36	1.45
19	A	830	CLA	C4C-C3C	-4.74	1.36	1.45
19	A	853	CLA	C4C-C3C	-4.72	1.36	1.45
19	2	309	CLA	C4C-C3C	-4.71	1.36	1.45
19	B	809	CLA	C1C-C2C	-4.71	1.35	1.44
19	B	840	CLA	C4C-C3C	-4.71	1.36	1.45
19	A	825	CLA	C4C-C3C	-4.70	1.36	1.45
19	B	804	CLA	C4C-C3C	-4.70	1.36	1.45
19	B	803	CLA	C4C-C3C	-4.70	1.36	1.45
19	B	807	CLA	C4C-C3C	-4.69	1.37	1.45
19	B	828	CLA	C4C-C3C	-4.68	1.37	1.45
19	A	831	CLA	C1C-C2C	-4.68	1.35	1.44
19	3	307	CLA	C4C-C3C	-4.67	1.37	1.45
19	F	306	CLA	C4C-C3C	-4.67	1.37	1.45
19	B	816	CLA	C4C-C3C	-4.66	1.37	1.45
19	A	813	CLA	C4C-C3C	-4.66	1.37	1.45
19	1	312	CLA	C4C-C3C	-4.66	1.37	1.45
19	B	808	CLA	C4C-C3C	-4.66	1.37	1.45
19	A	838	CLA	C4C-C3C	-4.65	1.37	1.45
19	A	828	CLA	MG-NA	4.65	2.17	2.06
19	4	302	CLA	C4C-C3C	-4.65	1.37	1.45
19	B	832	CLA	C1C-C2C	-4.65	1.35	1.44
19	4	301	CLA	C1C-C2C	-4.65	1.35	1.44
19	A	835	CLA	C4C-C3C	-4.64	1.37	1.45
19	4	309	CLA	C1C-C2C	-4.64	1.35	1.44
19	2	308	CLA	C4C-C3C	-4.64	1.37	1.45
19	A	827	CLA	C4C-C3C	-4.63	1.37	1.45
19	B	801	CLA	C4C-C3C	-4.63	1.37	1.45
19	A	823	CLA	C4C-C3C	-4.63	1.37	1.45
19	A	824	CLA	C4C-C3C	-4.63	1.37	1.45
19	2	302	CLA	C4C-C3C	-4.63	1.37	1.45
19	1	310	CLA	C4C-C3C	-4.63	1.37	1.45
19	A	802	CLA	C4C-C3C	-4.63	1.37	1.45
19	B	806	CLA	C4C-C3C	-4.63	1.37	1.45
19	B	829	CLA	C1C-C2C	-4.63	1.35	1.44
19	A	852	CLA	C4C-C3C	-4.62	1.37	1.45
19	A	822	CLA	C1C-C2C	-4.62	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	826	CLA	C4C-C3C	-4.62	1.37	1.45
19	A	804	CLA	C4C-C3C	-4.62	1.37	1.45
19	3	301	CLA	C4C-C3C	-4.62	1.37	1.45
19	A	801	CLA	C4C-C3C	-4.62	1.37	1.45
19	B	824	CLA	C4C-C3C	-4.62	1.37	1.45
19	L	303	CLA	C4C-C3C	-4.61	1.37	1.45
19	A	803	CLA	C1C-C2C	-4.61	1.35	1.44
19	A	839	CLA	C4C-C3C	-4.61	1.37	1.45
19	A	818	CLA	C4C-C3C	-4.61	1.37	1.45
19	B	814	CLA	C4C-C3C	-4.61	1.37	1.45
19	B	818	CLA	C4C-C3C	-4.61	1.37	1.45
19	A	806	CLA	C4C-C3C	-4.60	1.37	1.45
19	A	830	CLA	C1C-C2C	-4.60	1.35	1.44
19	A	805	CLA	C4C-C3C	-4.60	1.37	1.45
19	A	817	CLA	C4C-C3C	-4.60	1.37	1.45
19	B	839	CLA	C1C-C2C	-4.60	1.35	1.44
19	B	833	CLA	C4C-C3C	-4.60	1.37	1.45
19	A	807	CLA	C4C-C3C	-4.60	1.37	1.45
19	B	850	CLA	C4C-C3C	-4.59	1.37	1.45
19	B	802	CLA	C4C-C3C	-4.59	1.37	1.45
19	B	815	CLA	C4C-C3C	-4.59	1.37	1.45
19	A	812	CLA	C4C-C3C	-4.59	1.37	1.45
19	1	301	CLA	C4C-C3C	-4.59	1.37	1.45
19	B	839	CLA	C4C-C3C	-4.59	1.37	1.45
19	B	815	CLA	C1C-C2C	-4.59	1.35	1.44
19	A	809	CLA	C4C-C3C	-4.59	1.37	1.45
19	A	815	CLA	C4C-C3C	-4.59	1.37	1.45
19	A	810	CLA	C4C-C3C	-4.59	1.37	1.45
19	B	808	CLA	C1C-C2C	-4.59	1.35	1.44
19	3	311	CLA	C4C-C3C	-4.58	1.37	1.45
19	B	810	CLA	C4C-C3C	-4.58	1.37	1.45
19	1	302	CLA	C4C-C3C	-4.58	1.37	1.45
19	1	308	CLA	C4C-C3C	-4.58	1.37	1.45
19	4	313	CLA	C4C-C3C	-4.58	1.37	1.45
19	A	837	CLA	C4C-C3C	-4.58	1.37	1.45
19	B	831	CLA	C4C-C3C	-4.58	1.37	1.45
19	3	303	CLA	C1C-C2C	-4.58	1.35	1.44
19	2	301	CLA	C4C-C3C	-4.58	1.37	1.45
19	O	102	CLA	C4C-C3C	-4.58	1.37	1.45
19	1	306	CLA	C4C-C3C	-4.58	1.37	1.45
19	A	819	CLA	C4C-C3C	-4.58	1.37	1.45
19	3	316	CLA	C4C-C3C	-4.57	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	828	CLA	C1C-C2C	-4.57	1.35	1.44
19	B	832	CLA	C4C-C3C	-4.57	1.37	1.45
19	B	819	CLA	C4C-C3C	-4.57	1.37	1.45
19	1	309	CLA	C4C-C3C	-4.57	1.37	1.45
19	A	835	CLA	C1C-C2C	-4.56	1.35	1.44
19	B	825	CLA	C4C-C3C	-4.56	1.37	1.45
19	B	835	CLA	C4C-C3C	-4.56	1.37	1.45
19	1	303	CLA	C4C-C3C	-4.56	1.37	1.45
19	B	837	CLA	C1C-C2C	-4.56	1.35	1.44
19	A	840	CLA	C4C-C3C	-4.56	1.37	1.45
19	G	205	CLA	C1C-C2C	-4.55	1.35	1.44
19	A	803	CLA	C4C-C3C	-4.55	1.37	1.45
19	B	818	CLA	C1C-C2C	-4.55	1.35	1.44
19	3	310	CLA	C4C-C3C	-4.55	1.37	1.45
19	B	812	CLA	C4C-C3C	-4.55	1.37	1.45
19	A	833	CLA	C4C-C3C	-4.55	1.37	1.45
19	G	204	CLA	C4C-C3C	-4.55	1.37	1.45
19	A	827	CLA	C1C-C2C	-4.55	1.35	1.44
19	A	854	CLA	C1C-C2C	-4.55	1.35	1.44
19	A	816	CLA	C4C-C3C	-4.55	1.37	1.45
19	B	823	CLA	C1C-C2C	-4.55	1.35	1.44
19	B	821	CLA	C4C-C3C	-4.55	1.37	1.45
19	B	835	CLA	C1C-C2C	-4.55	1.35	1.44
19	3	310	CLA	C1C-C2C	-4.54	1.35	1.44
19	B	836	CLA	C4C-C3C	-4.54	1.37	1.45
19	A	816	CLA	C1C-C2C	-4.54	1.35	1.44
19	B	838	CLA	C4C-C3C	-4.54	1.37	1.45
19	B	809	CLA	C4C-C3C	-4.54	1.37	1.45
19	A	815	CLA	C1C-C2C	-4.54	1.35	1.44
19	A	808	CLA	C4C-C3C	-4.54	1.37	1.45
19	A	840	CLA	C1C-C2C	-4.54	1.35	1.44
19	O	103	CLA	C1C-C2C	-4.54	1.35	1.44
19	B	819	CLA	C1C-C2C	-4.54	1.35	1.44
19	4	303	CLA	C1C-C2C	-4.54	1.35	1.44
19	A	854	CLA	C4C-C3C	-4.54	1.37	1.45
19	A	832	CLA	C4C-C3C	-4.53	1.37	1.45
19	B	822	CLA	C4C-C3C	-4.53	1.37	1.45
19	L	302	CLA	C4C-C3C	-4.53	1.37	1.45
19	1	304	CLA	C4C-C3C	-4.53	1.37	1.45
19	1	307	CLA	C4C-C3C	-4.53	1.37	1.45
19	G	203	CLA	C4C-C3C	-4.53	1.37	1.45
19	B	801	CLA	C1C-C2C	-4.53	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	814	CLA	C1C-C2C	-4.53	1.35	1.44
19	B	806	CLA	C1C-C2C	-4.53	1.35	1.44
19	B	831	CLA	C1C-C2C	-4.53	1.35	1.44
19	F	307	CLA	C1C-C2C	-4.53	1.35	1.44
19	2	303	CLA	C4C-C3C	-4.53	1.37	1.45
19	B	814	CLA	C1C-C2C	-4.52	1.35	1.44
19	O	101	CLA	C4C-C3C	-4.52	1.37	1.45
19	A	812	CLA	C1C-C2C	-4.52	1.35	1.44
19	A	839	CLA	C1C-C2C	-4.52	1.35	1.44
19	2	312	CLA	C4C-C3C	-4.52	1.37	1.45
19	1	302	CLA	C1C-C2C	-4.52	1.35	1.44
19	2	312	CLA	C1C-C2C	-4.52	1.35	1.44
19	A	850	CLA	C4C-C3C	-4.52	1.37	1.45
19	B	826	CLA	C1C-C2C	-4.52	1.35	1.44
19	4	308	CLA	C4C-C3C	-4.52	1.37	1.45
19	G	205	CLA	C4C-C3C	-4.51	1.37	1.45
19	1	310	CLA	C1C-C2C	-4.51	1.35	1.44
19	A	834	CLA	C4C-C3C	-4.51	1.37	1.45
19	A	817	CLA	C1C-C2C	-4.51	1.35	1.44
19	4	312	CLA	C1C-C2C	-4.51	1.35	1.44
19	B	803	CLA	C1C-C2C	-4.51	1.35	1.44
19	3	309	CLA	C4C-C3C	-4.51	1.37	1.45
19	A	806	CLA	C1C-C2C	-4.51	1.35	1.44
19	K	302	CLA	C1C-C2C	-4.51	1.35	1.44
19	1	313	CLA	C4C-C3C	-4.51	1.37	1.45
19	B	840	CLA	C1C-C2C	-4.51	1.35	1.44
19	3	305	CLA	C4C-C3C	-4.51	1.37	1.45
19	A	818	CLA	C1C-C2C	-4.50	1.35	1.44
19	A	807	CLA	C1C-C2C	-4.50	1.35	1.44
19	B	828	CLA	C1C-C2C	-4.50	1.35	1.44
19	4	314	CLA	C1C-C2C	-4.50	1.35	1.44
19	B	816	CLA	C1C-C2C	-4.50	1.35	1.44
19	A	811	CLA	C1C-C2C	-4.50	1.35	1.44
19	2	310	CLA	C1C-C2C	-4.50	1.35	1.44
19	B	820	CLA	C1C-C2C	-4.50	1.35	1.44
19	2	311	CLA	C4C-C3C	-4.50	1.37	1.45
19	A	834	CLA	C1C-C2C	-4.50	1.35	1.44
19	2	303	CLA	C1C-C2C	-4.50	1.35	1.44
19	L	303	CLA	C1C-C2C	-4.50	1.35	1.44
19	B	834	CLA	C1C-C2C	-4.50	1.35	1.44
20	4	307	CHL	C4C-C3C	-4.50	1.37	1.45
19	A	829	CLA	C1C-C2C	-4.49	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	811	CLA	C4C-C3C	-4.49	1.37	1.45
19	1	311	CLA	C4C-C3C	-4.49	1.37	1.45
19	1	311	CLA	C1C-C2C	-4.49	1.35	1.44
19	A	820	CLA	C4C-C3C	-4.49	1.37	1.45
19	A	823	CLA	C1C-C2C	-4.49	1.35	1.44
19	B	830	CLA	C4C-C3C	-4.49	1.37	1.45
19	B	813	CLA	C1C-C2C	-4.49	1.35	1.44
19	A	832	CLA	C1C-C2C	-4.48	1.35	1.44
19	B	830	CLA	C1C-C2C	-4.48	1.35	1.44
19	2	311	CLA	C1C-C2C	-4.48	1.35	1.44
19	B	827	CLA	C4C-C3C	-4.48	1.37	1.45
19	K	303	CLA	C4C-C3C	-4.48	1.37	1.45
19	4	314	CLA	C4C-C3C	-4.48	1.37	1.45
19	B	824	CLA	C1C-C2C	-4.48	1.35	1.44
19	B	813	CLA	C4C-C3C	-4.48	1.37	1.45
19	3	304	CLA	C1C-C2C	-4.48	1.35	1.44
19	O	101	CLA	C1C-C2C	-4.48	1.35	1.44
19	L	304	CLA	C4C-C3C	-4.48	1.37	1.45
19	3	316	CLA	C1C-C2C	-4.48	1.35	1.44
19	4	304	CLA	C4C-C3C	-4.48	1.37	1.45
19	L	302	CLA	C1C-C2C	-4.48	1.35	1.44
19	B	837	CLA	C4C-C3C	-4.47	1.37	1.45
19	L	304	CLA	C1C-C2C	-4.47	1.35	1.44
19	B	834	CLA	C4C-C3C	-4.47	1.37	1.45
19	3	304	CLA	C4C-C3C	-4.47	1.37	1.45
19	B	805	CLA	C1C-C2C	-4.47	1.35	1.44
19	B	802	CLA	C1C-C2C	-4.47	1.35	1.44
19	B	805	CLA	C4C-C3C	-4.47	1.37	1.45
19	1	303	CLA	C1C-C2C	-4.47	1.35	1.44
19	1	304	CLA	C1C-C2C	-4.47	1.35	1.44
19	B	827	CLA	C1C-C2C	-4.47	1.35	1.44
22	4	317	XAT	C10-C9	4.47	1.41	1.35
19	2	307	CLA	C1C-C2C	-4.47	1.35	1.44
19	A	813	CLA	C1C-C2C	-4.47	1.35	1.44
19	A	831	CLA	C4C-C3C	-4.47	1.37	1.45
19	B	825	CLA	C1C-C2C	-4.46	1.35	1.44
19	A	821	CLA	C1C-C2C	-4.46	1.35	1.44
19	2	307	CLA	C4C-C3C	-4.46	1.37	1.45
19	B	807	CLA	C1C-C2C	-4.46	1.35	1.44
19	A	829	CLA	C4C-C3C	-4.46	1.37	1.45
19	A	826	CLA	C1C-C2C	-4.46	1.35	1.44
19	A	805	CLA	C1C-C2C	-4.46	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	850	CLA	C1C-C2C	-4.46	1.35	1.44
19	3	312	CLA	C1C-C2C	-4.46	1.35	1.44
19	A	852	CLA	C1C-C2C	-4.45	1.35	1.44
19	A	808	CLA	C1C-C2C	-4.45	1.35	1.44
19	3	303	CLA	C4C-C3C	-4.45	1.37	1.45
19	4	301	CLA	C4C-C3C	-4.45	1.37	1.45
19	1	312	CLA	C1C-C2C	-4.45	1.36	1.44
19	B	838	CLA	C1C-C2C	-4.45	1.36	1.44
19	4	312	CLA	C4C-C3C	-4.45	1.37	1.45
19	A	809	CLA	C1C-C2C	-4.45	1.36	1.44
19	3	311	CLA	C1C-C2C	-4.44	1.36	1.44
19	G	204	CLA	C1C-C2C	-4.44	1.36	1.44
19	A	801	CLA	C1C-C2C	-4.44	1.36	1.44
19	A	810	CLA	C1C-C2C	-4.44	1.36	1.44
19	B	811	CLA	C4C-C3C	-4.44	1.37	1.45
19	B	811	CLA	C1C-C2C	-4.44	1.36	1.44
19	2	310	CLA	C4C-C3C	-4.44	1.37	1.45
19	A	837	CLA	C1C-C2C	-4.44	1.36	1.44
19	A	828	CLA	C4C-C3C	-4.44	1.37	1.45
19	3	309	CLA	C1C-C2C	-4.43	1.36	1.44
19	3	302	CLA	C1C-C2C	-4.43	1.36	1.44
19	4	304	CLA	C1C-C2C	-4.43	1.36	1.44
19	A	804	CLA	C1C-C2C	-4.43	1.36	1.44
19	A	822	CLA	C4C-C3C	-4.43	1.37	1.45
19	A	836	CLA	C4C-C3C	-4.43	1.37	1.45
19	O	102	CLA	C1C-C2C	-4.43	1.36	1.44
19	B	850	CLA	C1C-C2C	-4.43	1.36	1.44
19	B	823	CLA	C4C-C3C	-4.43	1.37	1.45
19	B	836	CLA	C1C-C2C	-4.42	1.36	1.44
19	A	821	CLA	C4C-C3C	-4.42	1.37	1.45
19	3	307	CLA	C1C-C2C	-4.42	1.36	1.44
19	1	307	CLA	C1C-C2C	-4.42	1.36	1.44
19	3	302	CLA	C4C-C3C	-4.42	1.37	1.45
19	4	308	CLA	C1C-C2C	-4.42	1.36	1.44
19	2	302	CLA	C1C-C2C	-4.41	1.36	1.44
19	3	305	CLA	C1C-C2C	-4.41	1.36	1.44
19	4	313	CLA	C1C-C2C	-4.41	1.36	1.44
19	A	826	CLA	C4C-C3C	-4.41	1.37	1.45
19	B	820	CLA	C4C-C3C	-4.41	1.37	1.45
19	1	309	CLA	C1C-C2C	-4.41	1.36	1.44
19	4	311	CLA	C4C-C3C	-4.41	1.37	1.45
20	3	306	CHL	C4C-C3C	-4.41	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	819	CLA	C1C-C2C	-4.40	1.36	1.44
19	2	309	CLA	C1C-C2C	-4.40	1.36	1.44
19	O	104	CLA	C4C-C3C	-4.39	1.37	1.45
19	A	838	CLA	C1C-C2C	-4.39	1.36	1.44
19	O	103	CLA	C4C-C3C	-4.39	1.37	1.45
19	K	303	CLA	C1C-C2C	-4.39	1.36	1.44
19	J	102	CLA	C4C-C3C	-4.39	1.37	1.45
19	A	836	CLA	C1C-C2C	-4.39	1.36	1.44
19	A	825	CLA	C1C-C2C	-4.38	1.36	1.44
19	A	853	CLA	C1C-C2C	-4.38	1.36	1.44
19	B	817	CLA	C4C-C3C	-4.38	1.37	1.45
19	B	821	CLA	C1C-C2C	-4.37	1.36	1.44
19	B	833	CLA	C1C-C2C	-4.37	1.36	1.44
19	B	829	CLA	C4C-C3C	-4.37	1.37	1.45
20	4	315	CHL	C4C-C3C	-4.37	1.37	1.45
19	A	833	CLA	C1C-C2C	-4.37	1.36	1.44
19	4	311	CLA	C1C-C2C	-4.37	1.36	1.44
19	G	203	CLA	C1C-C2C	-4.36	1.36	1.44
19	F	306	CLA	C1C-C2C	-4.36	1.36	1.44
19	1	313	CLA	C1C-C2C	-4.36	1.36	1.44
20	2	319	CHL	C4C-C3C	-4.36	1.37	1.45
20	4	305	CHL	C4C-C3C	-4.36	1.37	1.45
19	1	301	CLA	C1C-C2C	-4.36	1.36	1.44
20	4	306	CHL	C4C-C3C	-4.35	1.37	1.45
19	B	812	CLA	C1C-C2C	-4.35	1.36	1.44
19	4	310	CLA	C4C-C3C	-4.35	1.37	1.45
19	A	824	CLA	C1C-C2C	-4.35	1.36	1.44
20	2	313	CHL	C4C-C3C	-4.35	1.37	1.45
20	2	304	CHL	C4C-C3C	-4.34	1.37	1.45
19	B	822	CLA	C1C-C2C	-4.34	1.36	1.44
19	A	820	CLA	C1C-C2C	-4.34	1.36	1.44
19	F	307	CLA	C4C-C3C	-4.34	1.37	1.45
19	K	302	CLA	C4C-C3C	-4.34	1.37	1.45
19	1	306	CLA	C1C-C2C	-4.34	1.36	1.44
19	J	102	CLA	C1C-C2C	-4.32	1.36	1.44
19	1	308	CLA	C1C-C2C	-4.32	1.36	1.44
19	2	301	CLA	C1C-C2C	-4.31	1.36	1.44
19	O	104	CLA	C1C-C2C	-4.30	1.36	1.44
20	1	305	CHL	C4C-C3C	-4.29	1.37	1.45
19	B	810	CLA	C1C-C2C	-4.29	1.36	1.44
19	B	804	CLA	C1C-C2C	-4.26	1.36	1.44
19	4	302	CLA	C1C-C2C	-4.26	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	305	CHL	C4C-C3C	-4.26	1.37	1.45
19	A	802	CLA	C1C-C2C	-4.26	1.36	1.44
19	3	308	CLA	C1C-C2C	-4.25	1.36	1.44
19	3	301	CLA	C1C-C2C	-4.24	1.36	1.44
19	A	834	CLA	MG-NA	4.22	2.16	2.06
20	2	306	CHL	C4C-C3C	-4.22	1.37	1.45
20	1	318	CHL	C4C-C3C	-4.22	1.37	1.45
20	4	315	CHL	MG-NA	4.21	2.16	2.06
18	K	301	BCR	C10-C9	4.17	1.41	1.35
18	1	316	BCR	C21-C22	4.16	1.41	1.35
22	4	317	XAT	C34-C33	4.14	1.41	1.35
22	4	317	XAT	C14-C13	4.13	1.41	1.35
19	B	821	CLA	MG-NA	4.12	2.16	2.06
19	2	308	CLA	C1C-C2C	-4.11	1.36	1.44
19	A	812	CLA	MG-NA	4.10	2.16	2.06
22	3	314	XAT	C10-C9	4.10	1.41	1.35
22	2	315	XAT	C34-C33	4.09	1.41	1.35
18	F	302	BCR	C21-C22	4.06	1.41	1.35
19	B	814	CLA	MG-NA	4.05	2.15	2.06
18	4	318	BCR	C21-C22	4.04	1.41	1.35
21	3	313	LUT	C30-C29	4.04	1.41	1.35
21	4	316	LUT	C10-C9	4.03	1.41	1.35
19	B	835	CLA	MG-NA	4.02	2.15	2.06
20	4	305	CHL	MG-NA	4.02	2.15	2.06
18	1	316	BCR	C14-C13	4.01	1.41	1.35
18	1	316	BCR	C17-C18	4.00	1.41	1.35
29	B	847	DGD	O2G-C1B	3.99	1.45	1.34
29	B	847	DGD	O1G-C1A	3.99	1.45	1.33
18	1	316	BCR	C10-C9	3.97	1.41	1.35
21	3	313	LUT	C10-C9	3.96	1.41	1.35
22	2	315	XAT	C10-C9	3.96	1.41	1.35
18	K	304	BCR	C21-C22	3.95	1.41	1.35
18	F	302	BCR	C10-C9	3.95	1.41	1.35
18	F	302	BCR	C17-C18	3.94	1.41	1.35
18	O	106	BCR	C10-C9	3.94	1.41	1.35
18	O	105	BCR	C17-C18	3.93	1.41	1.35
18	F	302	BCR	C14-C13	3.93	1.41	1.35
19	3	302	CLA	MG-NA	3.93	2.15	2.06
19	L	304	CLA	MG-NA	3.92	2.15	2.06
19	L	302	CLA	MG-NA	3.91	2.15	2.06
19	4	303	CLA	MG-NA	3.89	2.15	2.06
18	A	848	BCR	C14-C13	3.89	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	312	CLA	MG-NA	3.89	2.15	2.06
18	2	316	BCR	C21-C22	3.88	1.40	1.35
19	B	832	CLA	MG-NA	3.88	2.15	2.06
18	J	104	BCR	C17-C18	3.87	1.40	1.35
18	B	844	BCR	C10-C9	3.86	1.40	1.35
18	O	106	BCR	C14-C13	3.86	1.40	1.35
18	G	201	BCR	C21-C22	3.85	1.40	1.35
18	O	106	BCR	C17-C18	3.84	1.40	1.35
21	3	313	LUT	C34-C33	3.84	1.40	1.35
18	K	304	BCR	C10-C9	3.83	1.40	1.35
18	J	104	BCR	C14-C13	3.83	1.40	1.35
21	2	314	LUT	C34-C33	3.83	1.40	1.35
19	B	850	CLA	MG-NA	3.82	2.15	2.06
21	4	316	LUT	C34-C33	3.81	1.40	1.35
19	A	831	CLA	MG-NA	3.81	2.15	2.06
22	4	317	XAT	C30-C29	3.81	1.40	1.35
18	B	843	BCR	C17-C18	3.80	1.40	1.35
19	4	311	CLA	MG-NA	3.80	2.15	2.06
18	A	846	BCR	C10-C9	3.80	1.40	1.35
21	3	313	LUT	C14-C13	3.80	1.40	1.35
18	O	105	BCR	C21-C22	3.79	1.40	1.35
22	3	314	XAT	C34-C33	3.79	1.40	1.35
18	K	301	BCR	C14-C13	3.78	1.40	1.35
18	B	843	BCR	C21-C22	3.78	1.40	1.35
19	O	101	CLA	MG-NA	3.78	2.15	2.06
21	2	314	LUT	C14-C13	3.78	1.40	1.35
18	I	101	BCR	C14-C13	3.78	1.40	1.35
18	4	318	BCR	C14-C13	3.76	1.40	1.35
18	O	105	BCR	C10-C9	3.76	1.40	1.35
18	K	304	BCR	C17-C18	3.76	1.40	1.35
18	I	101	BCR	C10-C9	3.75	1.40	1.35
19	3	309	CLA	MG-NA	3.74	2.15	2.06
18	2	316	BCR	C17-C18	3.73	1.40	1.35
19	J	102	CLA	MG-NA	3.73	2.15	2.06
18	3	315	BCR	C10-C9	3.72	1.40	1.35
18	K	301	BCR	C21-C22	3.72	1.40	1.35
18	2	316	BCR	C14-C13	3.72	1.40	1.35
18	G	201	BCR	C10-C9	3.71	1.40	1.35
21	2	314	LUT	C10-C9	3.71	1.40	1.35
18	J	103	BCR	C21-C22	3.71	1.40	1.35
21	4	316	LUT	C14-C13	3.71	1.40	1.35
22	3	314	XAT	C14-C13	3.71	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	315	XAT	C30-C29	3.70	1.40	1.35
22	2	315	XAT	C14-C13	3.70	1.40	1.35
19	K	303	CLA	MG-NA	3.69	2.15	2.06
19	A	818	CLA	MG-NA	3.69	2.15	2.06
19	1	304	CLA	MG-NA	3.69	2.15	2.06
19	A	820	CLA	MG-NA	3.69	2.15	2.06
18	K	301	BCR	C17-C18	3.69	1.40	1.35
18	G	201	BCR	C17-C18	3.68	1.40	1.35
18	B	844	BCR	C14-C13	3.68	1.40	1.35
18	3	315	BCR	C14-C13	3.68	1.40	1.35
22	3	314	XAT	C30-C29	3.67	1.40	1.35
18	J	104	BCR	C21-C22	3.67	1.40	1.35
18	O	105	BCR	C14-C13	3.66	1.40	1.35
18	A	848	BCR	C17-C18	3.66	1.40	1.35
18	A	844	BCR	C10-C9	3.65	1.40	1.35
18	B	842	BCR	C10-C9	3.65	1.40	1.35
19	2	310	CLA	MG-NA	3.65	2.14	2.06
22	1	315	XAT	C10-C9	3.65	1.40	1.35
18	A	848	BCR	C10-C9	3.65	1.40	1.35
18	B	842	BCR	C21-C22	3.63	1.40	1.35
19	3	310	CLA	MG-NA	3.63	2.14	2.06
18	I	101	BCR	C17-C18	3.63	1.40	1.35
18	G	206	BCR	C10-C9	3.63	1.40	1.35
18	O	106	BCR	C21-C22	3.63	1.40	1.35
18	B	842	BCR	C17-C18	3.62	1.40	1.35
19	4	301	CLA	MG-NA	3.62	2.14	2.06
21	2	314	LUT	C30-C29	3.62	1.40	1.35
18	L	305	BCR	C14-C13	3.62	1.40	1.35
18	B	842	BCR	C14-C13	3.61	1.40	1.35
18	B	843	BCR	C10-C9	3.61	1.40	1.35
21	1	314	LUT	C34-C33	3.60	1.40	1.35
19	B	829	CLA	MG-NA	3.60	2.14	2.06
19	2	307	CLA	MG-NA	3.60	2.14	2.06
21	1	314	LUT	C10-C9	3.59	1.40	1.35
18	2	316	BCR	C10-C9	3.59	1.40	1.35
18	K	304	BCR	C14-C13	3.59	1.40	1.35
18	B	844	BCR	C17-C18	3.59	1.40	1.35
18	4	318	BCR	C17-C18	3.58	1.40	1.35
18	J	103	BCR	C17-C18	3.58	1.40	1.35
19	1	312	CLA	MG-NA	3.58	2.14	2.06
19	B	806	CLA	MG-NA	3.58	2.14	2.06
20	4	306	CHL	MG-NA	3.56	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	845	BCR	C10-C9	3.56	1.40	1.35
19	K	302	CLA	MG-NA	3.56	2.14	2.06
18	L	305	BCR	C10-C9	3.56	1.40	1.35
18	J	103	BCR	C10-C9	3.55	1.40	1.35
21	1	314	LUT	C14-C13	3.55	1.40	1.35
18	A	846	BCR	C14-C13	3.55	1.40	1.35
18	J	104	BCR	C10-C9	3.55	1.40	1.35
18	3	315	BCR	C21-C22	3.55	1.40	1.35
19	G	203	CLA	MG-NA	3.55	2.14	2.06
19	B	820	CLA	MG-NA	3.54	2.14	2.06
18	F	304	BCR	C17-C18	3.54	1.40	1.35
21	4	316	LUT	C30-C29	3.54	1.40	1.35
19	2	311	CLA	MG-NA	3.53	2.14	2.06
19	B	826	CLA	MG-NA	3.53	2.14	2.06
18	A	847	BCR	C21-C22	3.52	1.40	1.35
19	A	825	CLA	MG-NA	3.52	2.14	2.06
19	2	309	CLA	MG-NA	3.52	2.14	2.06
19	A	810	CLA	MG-NA	3.51	2.14	2.06
18	L	305	BCR	C17-C18	3.51	1.40	1.35
18	G	201	BCR	C14-C13	3.51	1.40	1.35
18	J	103	BCR	C14-C13	3.49	1.40	1.35
19	3	307	CLA	MG-NA	3.49	2.14	2.06
19	1	311	CLA	MG-NA	3.49	2.14	2.06
18	3	315	BCR	C17-C18	3.48	1.40	1.35
19	B	831	CLA	MG-NA	3.47	2.14	2.06
19	G	204	CLA	MG-NA	3.47	2.14	2.06
19	4	312	CLA	MG-NA	3.46	2.14	2.06
18	A	844	BCR	C17-C18	3.46	1.40	1.35
19	B	818	CLA	MG-NA	3.46	2.14	2.06
18	L	301	BCR	C14-C13	3.45	1.40	1.35
19	B	809	CLA	MG-NA	3.45	2.14	2.06
18	4	318	BCR	C10-C9	3.45	1.40	1.35
19	1	307	CLA	MG-NA	3.45	2.14	2.06
22	1	315	XAT	C14-C13	3.44	1.40	1.35
20	2	319	CHL	MG-NA	3.44	2.14	2.06
19	B	813	CLA	MG-NA	3.44	2.14	2.06
18	G	206	BCR	C17-C18	3.43	1.40	1.35
19	3	304	CLA	MG-NA	3.42	2.14	2.06
19	B	824	CLA	MG-NA	3.42	2.14	2.06
20	2	313	CHL	MG-NA	3.42	2.14	2.06
18	F	304	BCR	C10-C9	3.42	1.40	1.35
18	A	846	BCR	C23-C22	-3.41	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	804	CLA	MG-NA	3.41	2.14	2.06
18	I	101	BCR	C21-C22	3.41	1.40	1.35
19	A	838	CLA	MG-NA	3.41	2.14	2.06
22	1	315	XAT	C34-C33	3.40	1.40	1.35
19	A	823	CLA	MG-NA	3.40	2.14	2.06
18	G	206	BCR	C21-C22	3.40	1.40	1.35
18	F	304	BCR	C21-C22	3.40	1.40	1.35
19	B	828	CLA	MG-NA	3.40	2.14	2.06
18	B	844	BCR	C21-C22	3.40	1.40	1.35
19	3	303	CLA	MG-NA	3.39	2.14	2.06
18	A	844	BCR	C14-C13	3.39	1.40	1.35
18	B	846	BCR	C10-C9	3.39	1.40	1.35
19	B	812	CLA	MG-NA	3.39	2.14	2.06
18	B	845	BCR	C21-C22	3.38	1.40	1.35
18	B	845	BCR	C14-C13	3.38	1.40	1.35
19	2	303	CLA	MG-NA	3.37	2.14	2.06
19	3	316	CLA	MG-NA	3.37	2.14	2.06
19	B	811	CLA	MG-NA	3.37	2.14	2.06
19	3	311	CLA	MG-NA	3.36	2.14	2.06
19	A	837	CLA	MG-NA	3.36	2.14	2.06
18	L	301	BCR	C17-C18	3.36	1.40	1.35
18	L	301	BCR	C21-C22	3.36	1.40	1.35
19	A	804	CLA	MG-NA	3.36	2.14	2.06
18	F	308	BCR	C23-C22	-3.36	1.38	1.45
19	A	835	CLA	MG-NA	3.36	2.14	2.06
19	A	805	CLA	MG-NA	3.35	2.14	2.06
21	1	314	LUT	C30-C29	3.35	1.40	1.35
19	A	833	CLA	MG-NA	3.35	2.14	2.06
18	A	847	BCR	C17-C18	3.34	1.40	1.35
19	A	811	CLA	MG-NA	3.34	2.14	2.06
19	A	809	CLA	MG-NA	3.34	2.14	2.06
19	A	817	CLA	MG-NA	3.34	2.14	2.06
18	B	845	BCR	C23-C22	-3.33	1.38	1.45
22	1	315	XAT	C30-C29	3.32	1.40	1.35
18	A	848	BCR	C21-C22	3.32	1.40	1.35
18	B	843	BCR	C14-C13	3.32	1.40	1.35
18	F	304	BCR	C14-C13	3.31	1.40	1.35
18	L	305	BCR	C21-C22	3.31	1.40	1.35
19	3	305	CLA	MG-NA	3.31	2.14	2.06
19	A	821	CLA	MG-NA	3.31	2.14	2.06
18	F	308	BCR	C17-C18	3.30	1.40	1.35
19	A	839	CLA	MG-NA	3.30	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	310	CLA	MG-NA	3.30	2.14	2.06
19	A	853	CLA	MG-NA	3.30	2.14	2.06
18	L	306	BCR	C23-C22	-3.30	1.38	1.45
18	L	306	BCR	C8-C9	-3.29	1.38	1.45
20	2	305	CHL	MG-NA	3.29	2.14	2.06
19	1	303	CLA	MG-NA	3.29	2.14	2.06
19	A	815	CLA	MG-NA	3.29	2.14	2.06
18	B	846	BCR	C23-C22	-3.28	1.38	1.45
19	F	307	CLA	MG-NA	3.28	2.14	2.06
18	A	845	BCR	C21-C22	3.28	1.40	1.35
19	B	805	CLA	MG-NA	3.27	2.14	2.06
18	F	308	BCR	C10-C9	3.27	1.40	1.35
18	A	848	BCR	C23-C22	-3.27	1.38	1.45
19	B	815	CLA	MG-NA	3.27	2.14	2.06
19	3	301	CLA	MG-NA	3.26	2.14	2.06
19	B	819	CLA	MG-NA	3.26	2.14	2.06
19	B	816	CLA	MG-NA	3.26	2.14	2.06
19	A	827	CLA	MG-NA	3.26	2.14	2.06
19	4	313	CLA	MG-NA	3.26	2.14	2.06
19	4	308	CLA	MG-NA	3.25	2.14	2.06
18	3	315	BCR	C23-C22	-3.25	1.39	1.45
18	L	306	BCR	C17-C18	3.25	1.40	1.35
18	G	206	BCR	C8-C9	-3.25	1.39	1.45
18	A	845	BCR	C8-C9	-3.24	1.39	1.45
18	F	308	BCR	C21-C22	3.24	1.40	1.35
20	2	304	CHL	MG-NA	3.24	2.14	2.06
18	A	847	BCR	C8-C9	-3.23	1.39	1.45
18	A	846	BCR	C8-C9	-3.23	1.39	1.45
18	B	845	BCR	C17-C18	3.23	1.40	1.35
18	A	844	BCR	C23-C22	-3.23	1.39	1.45
18	G	206	BCR	C14-C13	3.23	1.40	1.35
18	L	301	BCR	C10-C9	3.22	1.40	1.35
18	B	846	BCR	C14-C13	3.22	1.40	1.35
18	L	305	BCR	C23-C22	-3.21	1.39	1.45
19	4	314	CLA	MG-NA	3.20	2.13	2.06
19	1	309	CLA	MG-NA	3.20	2.13	2.06
19	A	840	CLA	MG-NA	3.20	2.13	2.06
19	A	850	CLA	MG-NA	3.20	2.13	2.06
18	B	846	BCR	C21-C22	3.19	1.40	1.35
19	A	814	CLA	MG-NA	3.19	2.13	2.06
18	L	306	BCR	C21-C22	3.19	1.40	1.35
18	A	845	BCR	C10-C9	3.19	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	846	BCR	C17-C18	3.19	1.40	1.35
18	B	843	BCR	C23-C22	-3.18	1.39	1.45
18	J	104	BCR	C8-C9	-3.18	1.39	1.45
18	L	306	BCR	C14-C13	3.18	1.40	1.35
18	L	305	BCR	C8-C9	-3.18	1.39	1.45
19	B	808	CLA	MG-NA	3.18	2.13	2.06
19	1	306	CLA	MG-NA	3.17	2.13	2.06
19	F	306	CLA	MG-NA	3.17	2.13	2.06
18	L	306	BCR	C10-C9	3.17	1.40	1.35
19	4	310	CLA	MG-ND	-3.17	1.99	2.05
18	A	844	BCR	C21-C22	3.16	1.40	1.35
18	B	846	BCR	C17-C18	3.16	1.40	1.35
18	B	846	BCR	C8-C9	-3.16	1.39	1.45
20	2	306	CHL	C2C-C1C	-3.15	1.38	1.44
19	A	819	CLA	MG-NA	3.15	2.13	2.06
18	A	845	BCR	C14-C13	3.15	1.40	1.35
19	3	312	CLA	MG-NA	3.14	2.13	2.06
18	L	301	BCR	C8-C9	-3.14	1.39	1.45
18	A	844	BCR	C8-C9	-3.14	1.39	1.45
18	4	318	BCR	C8-C9	-3.13	1.39	1.45
19	1	302	CLA	MG-NA	3.13	2.13	2.06
18	F	304	BCR	C8-C9	-3.13	1.39	1.45
18	L	301	BCR	C23-C22	-3.13	1.39	1.45
18	B	842	BCR	C23-C22	-3.12	1.39	1.45
18	A	845	BCR	C23-C22	-3.12	1.39	1.45
19	A	803	CLA	MG-NA	3.12	2.13	2.06
18	A	847	BCR	C23-C22	-3.12	1.39	1.45
18	B	844	BCR	C23-C22	-3.12	1.39	1.45
19	B	839	CLA	MG-NA	3.12	2.13	2.06
19	A	802	CLA	MG-NA	3.11	2.13	2.06
18	I	101	BCR	C23-C22	-3.11	1.39	1.45
19	2	302	CLA	MG-NA	3.11	2.13	2.06
18	3	315	BCR	C8-C9	-3.11	1.39	1.45
18	F	304	BCR	C23-C22	-3.10	1.39	1.45
19	1	301	CLA	MG-NA	3.10	2.13	2.06
18	A	847	BCR	C14-C13	3.10	1.39	1.35
18	G	206	BCR	C23-C22	-3.09	1.39	1.45
20	1	318	CHL	C2C-C1C	-3.08	1.38	1.44
18	J	103	BCR	C23-C22	-3.08	1.39	1.45
18	A	848	BCR	C8-C9	-3.08	1.39	1.45
20	4	315	CHL	C2C-C1C	-3.07	1.38	1.44
18	2	316	BCR	C8-C9	-3.07	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	306	CHL	C2C-C1C	-3.07	1.38	1.44
18	G	201	BCR	C8-C9	-3.07	1.39	1.45
19	A	806	CLA	MG-NA	3.06	2.13	2.06
19	B	801	CLA	MG-NA	3.06	2.13	2.06
19	G	205	CLA	MG-NA	3.06	2.13	2.06
19	A	801	CLA	MG-NA	3.06	2.13	2.06
18	B	843	BCR	C8-C9	-3.05	1.39	1.45
18	F	308	BCR	C8-C9	-3.04	1.39	1.45
19	2	301	CLA	MG-NA	3.04	2.13	2.06
20	4	305	CHL	C2C-C1C	-3.03	1.38	1.44
19	A	824	CLA	MG-NA	3.03	2.13	2.06
20	2	319	CHL	C2C-C1C	-3.02	1.38	1.44
18	A	847	BCR	C10-C9	3.02	1.39	1.35
18	O	105	BCR	C23-C22	-3.02	1.39	1.45
18	K	304	BCR	C8-C9	-3.01	1.39	1.45
20	2	305	CHL	C2C-C1C	-3.00	1.38	1.44
20	2	313	CHL	C2C-C1C	-3.00	1.38	1.44
20	2	306	CHL	MG-NA	3.00	2.13	2.06
18	G	201	BCR	C23-C22	-3.00	1.39	1.45
18	F	308	BCR	C14-C13	3.00	1.39	1.35
19	B	810	CLA	MG-NA	3.00	2.13	2.06
18	J	103	BCR	C8-C9	-2.99	1.39	1.45
18	B	845	BCR	C8-C9	-2.99	1.39	1.45
20	3	306	CHL	C2C-C1C	-2.98	1.38	1.44
18	K	301	BCR	C23-C22	-2.98	1.39	1.45
19	B	823	CLA	MG-NA	2.98	2.13	2.06
19	B	822	CLA	MG-NA	2.98	2.13	2.06
19	A	830	CLA	MG-NA	2.98	2.13	2.06
21	1	314	LUT	C8-C9	-2.97	1.39	1.45
19	A	807	CLA	MG-NA	2.97	2.13	2.06
18	O	105	BCR	C8-C9	-2.97	1.39	1.45
19	B	807	CLA	MG-NA	2.97	2.13	2.06
18	B	844	BCR	C8-C9	-2.97	1.39	1.45
18	A	845	BCR	C17-C18	2.97	1.39	1.35
18	A	846	BCR	C21-C22	2.96	1.39	1.35
20	4	307	CHL	C2C-C1C	-2.96	1.38	1.44
18	B	842	BCR	C8-C9	-2.96	1.39	1.45
19	4	309	CLA	MG-NA	2.95	2.13	2.06
18	A	846	BCR	C19-C18	-2.95	1.39	1.45
19	O	102	CLA	MG-NA	2.94	2.13	2.06
20	2	304	CHL	C2C-C1C	-2.94	1.39	1.44
19	4	304	CLA	MG-NA	2.93	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	I	101	BCR	C8-C9	-2.93	1.39	1.45
18	2	316	BCR	C23-C22	-2.93	1.39	1.45
18	1	316	BCR	C23-C22	-2.93	1.39	1.45
19	L	303	CLA	MG-NA	2.93	2.13	2.06
20	1	305	CHL	C2C-C1C	-2.92	1.39	1.44
18	O	106	BCR	C23-C22	-2.91	1.39	1.45
21	2	314	LUT	C8-C9	-2.91	1.39	1.45
19	B	828	CLA	C1D-C2D	-2.90	1.39	1.45
21	4	316	LUT	C8-C9	-2.89	1.39	1.45
19	A	832	CLA	MG-NA	2.89	2.13	2.06
18	O	106	BCR	C8-C9	-2.89	1.39	1.45
18	A	845	BCR	C19-C18	-2.88	1.39	1.45
18	F	302	BCR	C8-C9	-2.88	1.39	1.45
19	B	807	CLA	C3D-C4D	-2.88	1.37	1.44
19	B	810	CLA	C3D-C4D	-2.88	1.37	1.44
19	2	309	CLA	C1D-C2D	-2.87	1.39	1.45
19	4	308	CLA	C1D-C2D	-2.87	1.39	1.45
18	J	104	BCR	C23-C22	-2.86	1.39	1.45
18	L	306	BCR	C12-C13	-2.86	1.39	1.45
19	O	103	CLA	MG-NA	2.86	2.13	2.06
19	A	854	CLA	MG-NA	2.86	2.13	2.06
19	O	104	CLA	MG-NA	2.85	2.13	2.06
19	B	825	CLA	MG-NA	2.85	2.13	2.06
19	B	807	CLA	C1D-C2D	-2.84	1.39	1.45
21	3	313	LUT	C8-C9	-2.84	1.39	1.45
19	A	822	CLA	MG-NA	2.84	2.13	2.06
18	A	848	BCR	C19-C18	-2.83	1.39	1.45
19	4	310	CLA	C1D-C2D	-2.83	1.39	1.45
18	A	847	BCR	C12-C13	-2.83	1.39	1.45
19	A	813	CLA	MG-NA	2.82	2.13	2.06
19	B	837	CLA	MG-NA	2.82	2.13	2.06
19	1	307	CLA	C1D-C2D	-2.82	1.39	1.45
19	A	829	CLA	C3D-C4D	-2.81	1.37	1.44
19	A	805	CLA	C3D-C4D	-2.81	1.37	1.44
19	A	816	CLA	C3D-C4D	-2.81	1.37	1.44
18	K	301	BCR	C8-C9	-2.80	1.39	1.45
19	B	836	CLA	C3D-C4D	-2.80	1.37	1.44
18	B	846	BCR	C19-C18	-2.80	1.39	1.45
19	2	302	CLA	C3D-C4D	-2.80	1.37	1.44
19	A	808	CLA	MG-NA	2.80	2.12	2.06
19	A	827	CLA	C1D-C2D	-2.80	1.39	1.45
19	A	836	CLA	MG-NA	2.80	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	817	CLA	C3D-C4D	-2.79	1.37	1.44
19	K	302	CLA	C3D-C4D	-2.79	1.37	1.44
19	B	828	CLA	C3D-C4D	-2.78	1.37	1.44
19	A	853	CLA	C3D-C4D	-2.78	1.37	1.44
19	B	840	CLA	MG-NA	2.78	2.12	2.06
18	F	302	BCR	C23-C22	-2.78	1.40	1.45
18	K	304	BCR	C23-C22	-2.78	1.40	1.45
22	1	315	XAT	C32-C33	-2.78	1.40	1.45
19	B	805	CLA	C3D-C4D	-2.78	1.37	1.44
19	B	814	CLA	C3D-C4D	-2.77	1.37	1.44
19	A	803	CLA	C3D-C4D	-2.77	1.37	1.44
19	3	307	CLA	C1D-C2D	-2.77	1.39	1.45
19	4	309	CLA	C1B-C2B	-2.76	1.36	1.43
19	1	302	CLA	C3D-C4D	-2.76	1.37	1.44
19	L	303	CLA	C3D-C4D	-2.76	1.37	1.44
19	4	310	CLA	C3D-C4D	-2.76	1.37	1.44
19	B	806	CLA	C3D-C4D	-2.76	1.37	1.44
19	B	827	CLA	MG-NA	2.76	2.12	2.06
20	3	306	CHL	C3D-C4D	-2.76	1.37	1.44
19	B	823	CLA	C3D-C4D	-2.76	1.37	1.44
19	1	309	CLA	C1D-C2D	-2.76	1.39	1.45
19	4	302	CLA	MG-NA	2.75	2.12	2.06
19	B	825	CLA	C3D-C4D	-2.75	1.38	1.44
19	B	827	CLA	C3D-C4D	-2.75	1.38	1.44
20	3	306	CHL	MG-NA	2.75	2.12	2.06
20	1	318	CHL	C3D-C4D	-2.75	1.38	1.44
22	1	315	XAT	C28-C29	-2.75	1.40	1.45
19	B	838	CLA	C3D-C4D	-2.75	1.38	1.44
19	A	852	CLA	C1D-C2D	-2.75	1.39	1.45
19	B	838	CLA	MG-NA	2.75	2.12	2.06
19	A	854	CLA	C3D-C4D	-2.75	1.38	1.44
19	B	850	CLA	C3D-C4D	-2.75	1.38	1.44
19	B	840	CLA	C3D-C4D	-2.74	1.38	1.44
19	B	830	CLA	MG-NA	2.74	2.12	2.06
19	B	821	CLA	C1D-C2D	-2.74	1.39	1.45
18	F	308	BCR	C12-C13	-2.74	1.40	1.45
19	A	829	CLA	C1D-C2D	-2.74	1.39	1.45
18	B	843	BCR	C12-C13	-2.74	1.40	1.45
19	A	809	CLA	C3D-C4D	-2.74	1.38	1.44
19	A	804	CLA	C3D-C4D	-2.73	1.38	1.44
18	4	318	BCR	C23-C22	-2.73	1.40	1.45
19	A	826	CLA	C1D-C2D	-2.73	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	835	CLA	C3D-C4D	-2.73	1.38	1.44
19	A	824	CLA	C3D-C4D	-2.73	1.38	1.44
19	B	816	CLA	C3D-C4D	-2.73	1.38	1.44
22	3	314	XAT	C28-C29	-2.73	1.40	1.45
19	A	822	CLA	C3D-C4D	-2.73	1.38	1.44
18	1	316	BCR	C8-C9	-2.73	1.40	1.45
20	4	307	CHL	MG-NA	2.72	2.12	2.06
19	A	831	CLA	C3D-C4D	-2.72	1.38	1.44
19	B	817	CLA	C3D-C4D	-2.72	1.38	1.44
19	1	311	CLA	C3D-C4D	-2.72	1.38	1.44
19	1	313	CLA	MG-NA	2.71	2.12	2.06
19	A	821	CLA	C3D-C4D	-2.71	1.38	1.44
19	1	306	CLA	C3D-C4D	-2.71	1.38	1.44
19	4	310	CLA	C1B-C2B	-2.71	1.36	1.43
19	A	828	CLA	C1D-C2D	-2.71	1.40	1.45
18	F	308	BCR	C19-C18	-2.71	1.40	1.45
19	A	807	CLA	C1D-C2D	-2.71	1.40	1.45
19	B	802	CLA	C3D-C4D	-2.70	1.38	1.44
18	A	847	BCR	C19-C18	-2.70	1.40	1.45
19	B	811	CLA	C3D-C4D	-2.70	1.38	1.44
19	A	808	CLA	C3D-C4D	-2.70	1.38	1.44
19	B	836	CLA	MG-NA	2.70	2.12	2.06
18	L	306	BCR	C19-C18	-2.70	1.40	1.45
19	A	839	CLA	C3D-C4D	-2.70	1.38	1.44
19	A	804	CLA	C1D-C2D	-2.70	1.40	1.45
19	B	809	CLA	C1D-C2D	-2.70	1.40	1.45
19	A	818	CLA	C3D-C4D	-2.70	1.38	1.44
19	A	837	CLA	C3D-C4D	-2.70	1.38	1.44
19	B	820	CLA	C3D-C4D	-2.70	1.38	1.44
19	B	829	CLA	C3D-C4D	-2.70	1.38	1.44
19	A	819	CLA	C3D-C4D	-2.70	1.38	1.44
19	B	803	CLA	C3D-C4D	-2.69	1.38	1.44
19	B	839	CLA	C3D-C4D	-2.69	1.38	1.44
19	A	815	CLA	C3D-C4D	-2.69	1.38	1.44
19	B	830	CLA	C3D-C4D	-2.69	1.38	1.44
19	A	838	CLA	C1D-C2D	-2.69	1.40	1.45
19	A	840	CLA	C3D-C4D	-2.69	1.38	1.44
19	A	823	CLA	C1D-C2D	-2.69	1.40	1.45
19	A	827	CLA	C3D-C4D	-2.69	1.38	1.44
19	B	819	CLA	C3D-C4D	-2.69	1.38	1.44
19	B	808	CLA	C3D-C4D	-2.69	1.38	1.44
19	A	852	CLA	MG-NA	2.69	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	830	CLA	C3D-C4D	-2.69	1.38	1.44
19	B	840	CLA	C1D-C2D	-2.68	1.40	1.45
19	A	818	CLA	C1D-C2D	-2.68	1.40	1.45
19	B	818	CLA	C3D-C4D	-2.68	1.38	1.44
18	A	845	BCR	C12-C13	-2.68	1.40	1.45
19	G	204	CLA	C3D-C4D	-2.68	1.38	1.44
18	B	845	BCR	C19-C18	-2.67	1.40	1.45
21	1	314	LUT	C32-C33	-2.67	1.40	1.45
19	A	820	CLA	C1D-C2D	-2.67	1.40	1.45
19	B	823	CLA	C1D-C2D	-2.67	1.40	1.45
19	L	302	CLA	C3D-C4D	-2.67	1.38	1.44
19	B	831	CLA	C3D-C4D	-2.67	1.38	1.44
19	B	820	CLA	C1D-C2D	-2.67	1.40	1.45
19	B	837	CLA	C3D-C4D	-2.67	1.38	1.44
19	A	811	CLA	C3D-C4D	-2.67	1.38	1.44
20	1	305	CHL	C3D-C4D	-2.67	1.38	1.44
19	B	809	CLA	C3D-C4D	-2.67	1.38	1.44
19	A	802	CLA	C3D-C4D	-2.66	1.38	1.44
19	4	303	CLA	C3D-C4D	-2.66	1.38	1.44
19	B	804	CLA	C3D-C4D	-2.66	1.38	1.44
19	A	814	CLA	C3D-C4D	-2.66	1.38	1.44
19	G	205	CLA	C3D-C4D	-2.66	1.38	1.44
19	A	816	CLA	MG-NA	2.66	2.12	2.06
19	A	812	CLA	C3D-C4D	-2.66	1.38	1.44
19	A	839	CLA	C1D-C2D	-2.66	1.40	1.45
19	B	832	CLA	C1D-C2D	-2.66	1.40	1.45
19	B	833	CLA	C3D-C4D	-2.66	1.38	1.44
19	A	807	CLA	C3D-C4D	-2.66	1.38	1.44
19	L	303	CLA	C1D-C2D	-2.66	1.40	1.45
18	F	304	BCR	C12-C13	-2.66	1.40	1.45
19	B	824	CLA	C3D-C4D	-2.65	1.38	1.44
19	A	806	CLA	C3D-C4D	-2.65	1.38	1.44
19	A	852	CLA	C3D-C4D	-2.65	1.38	1.44
19	1	307	CLA	C3D-C4D	-2.65	1.38	1.44
19	3	304	CLA	C3D-C4D	-2.65	1.38	1.44
19	4	314	CLA	C3D-C4D	-2.65	1.38	1.44
19	F	307	CLA	C3D-C4D	-2.65	1.38	1.44
19	A	840	CLA	C1D-C2D	-2.65	1.40	1.45
19	A	826	CLA	MG-NA	2.65	2.12	2.06
20	4	307	CHL	C3D-C4D	-2.65	1.38	1.44
21	4	316	LUT	C28-C29	-2.65	1.40	1.45
18	B	846	BCR	C12-C13	-2.65	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	810	CLA	C3D-C4D	-2.64	1.38	1.44
19	A	836	CLA	C3D-C4D	-2.64	1.38	1.44
20	1	305	CHL	MG-NA	2.64	2.12	2.06
18	A	844	BCR	C19-C18	-2.64	1.40	1.45
19	B	808	CLA	C1D-C2D	-2.64	1.40	1.45
19	A	837	CLA	C1D-C2D	-2.64	1.40	1.45
19	A	815	CLA	C1D-C2D	-2.64	1.40	1.45
19	4	313	CLA	C3D-C4D	-2.64	1.38	1.44
19	A	829	CLA	MG-NA	2.64	2.12	2.06
19	B	826	CLA	C1D-C2D	-2.64	1.40	1.45
19	B	826	CLA	C3D-C4D	-2.64	1.38	1.44
20	2	304	CHL	C3D-C4D	-2.64	1.38	1.44
18	B	844	BCR	C19-C18	-2.64	1.40	1.45
19	B	835	CLA	C1D-C2D	-2.63	1.40	1.45
19	B	813	CLA	C3D-C4D	-2.63	1.38	1.44
19	B	832	CLA	C3D-C4D	-2.63	1.38	1.44
19	1	313	CLA	C3D-C4D	-2.63	1.38	1.44
18	L	305	BCR	C19-C18	-2.63	1.40	1.45
22	4	317	XAT	C28-C29	-2.63	1.40	1.45
19	A	813	CLA	C3D-C4D	-2.63	1.38	1.44
19	A	834	CLA	C3D-C4D	-2.63	1.38	1.44
19	A	826	CLA	C3D-C4D	-2.63	1.38	1.44
19	B	806	CLA	C1D-C2D	-2.63	1.40	1.45
19	A	828	CLA	C3D-C4D	-2.63	1.38	1.44
19	A	850	CLA	C1D-C2D	-2.63	1.40	1.45
19	A	833	CLA	C3D-C4D	-2.63	1.38	1.44
19	1	301	CLA	C3D-C4D	-2.63	1.38	1.44
19	A	801	CLA	C1D-C2D	-2.63	1.40	1.45
22	1	315	XAT	C8-C9	-2.62	1.40	1.45
19	2	309	CLA	C3D-C4D	-2.62	1.38	1.44
19	A	824	CLA	C1D-C2D	-2.62	1.40	1.45
19	B	802	CLA	C1D-C2D	-2.62	1.40	1.45
19	B	801	CLA	C3D-C4D	-2.62	1.38	1.44
18	L	301	BCR	C12-C13	-2.61	1.40	1.45
19	B	822	CLA	C3D-C4D	-2.61	1.38	1.44
18	F	304	BCR	C19-C18	-2.61	1.40	1.45
19	A	825	CLA	C1D-C2D	-2.61	1.40	1.45
19	3	301	CLA	C3D-C4D	-2.61	1.38	1.44
20	2	319	CHL	C3D-C4D	-2.61	1.38	1.44
19	A	825	CLA	C3D-C4D	-2.61	1.38	1.44
19	B	839	CLA	C1D-C2D	-2.61	1.40	1.45
19	1	304	CLA	C3D-C4D	-2.61	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	835	CLA	C3D-C4D	-2.61	1.38	1.44
19	G	204	CLA	C1D-C2D	-2.61	1.40	1.45
19	L	304	CLA	C3D-C4D	-2.61	1.38	1.44
20	4	315	CHL	MG-NC	2.61	2.12	2.06
18	G	206	BCR	C19-C18	-2.60	1.40	1.45
19	4	312	CLA	C3D-C4D	-2.60	1.38	1.44
19	B	812	CLA	C3D-C4D	-2.60	1.38	1.44
19	B	809	CLA	C1B-C2B	-2.60	1.37	1.43
19	3	312	CLA	C3D-C4D	-2.60	1.38	1.44
19	B	834	CLA	C3D-C4D	-2.60	1.38	1.44
19	1	309	CLA	C3D-C4D	-2.60	1.38	1.44
19	1	312	CLA	C3D-C4D	-2.60	1.38	1.44
19	A	832	CLA	C3D-C4D	-2.60	1.38	1.44
19	B	821	CLA	C3D-C4D	-2.60	1.38	1.44
19	3	305	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	852	CLA	C1B-C2B	-2.59	1.37	1.43
19	2	303	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	802	CLA	C1B-C2B	-2.59	1.37	1.43
19	2	301	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	850	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	810	CLA	C1D-C2D	-2.59	1.40	1.45
19	B	803	CLA	C1D-C2D	-2.59	1.40	1.45
22	3	314	XAT	C32-C33	-2.59	1.40	1.45
22	2	315	XAT	C32-C33	-2.59	1.40	1.45
19	1	308	CLA	C3D-C4D	-2.59	1.38	1.44
20	4	306	CHL	C3D-C4D	-2.59	1.38	1.44
19	2	307	CLA	C1D-C2D	-2.59	1.40	1.45
19	A	823	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	802	CLA	C1D-C2D	-2.59	1.40	1.45
20	2	313	CHL	C3D-C4D	-2.59	1.38	1.44
19	3	308	CLA	C3D-C4D	-2.58	1.38	1.44
19	A	830	CLA	C1D-C2D	-2.58	1.40	1.45
19	2	311	CLA	C3D-C4D	-2.58	1.38	1.44
19	4	302	CLA	C3D-C4D	-2.58	1.38	1.44
19	B	805	CLA	C1D-C2D	-2.58	1.40	1.45
19	B	802	CLA	MG-NA	2.58	2.12	2.06
19	4	304	CLA	C3D-C4D	-2.57	1.38	1.44
19	G	203	CLA	C3D-C4D	-2.57	1.38	1.44
19	B	814	CLA	C1D-C2D	-2.57	1.40	1.45
19	A	832	CLA	C1D-C2D	-2.57	1.40	1.45
18	3	315	BCR	C19-C18	-2.57	1.40	1.45
19	A	828	CLA	MG-NC	2.57	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	O	101	CLA	C3D-C4D	-2.57	1.38	1.44
19	F	306	CLA	C3D-C4D	-2.57	1.38	1.44
19	O	102	CLA	C3D-C4D	-2.57	1.38	1.44
19	L	304	CLA	C1D-C2D	-2.57	1.40	1.45
19	A	838	CLA	C3D-C4D	-2.57	1.38	1.44
19	B	804	CLA	C1D-C2D	-2.57	1.40	1.45
19	3	309	CLA	C3D-C4D	-2.57	1.38	1.44
18	K	304	BCR	C12-C13	-2.57	1.40	1.45
19	3	305	CLA	C1D-C2D	-2.57	1.40	1.45
19	1	310	CLA	C3D-C4D	-2.57	1.38	1.44
19	2	312	CLA	C3D-C4D	-2.57	1.38	1.44
19	1	308	CLA	MG-NA	2.56	2.12	2.06
19	2	307	CLA	C3D-C4D	-2.56	1.38	1.44
19	4	303	CLA	C1D-C2D	-2.56	1.40	1.45
19	2	308	CLA	C1B-C2B	-2.56	1.37	1.43
19	3	302	CLA	C3D-C4D	-2.56	1.38	1.44
19	1	308	CLA	C1B-C2B	-2.56	1.37	1.43
18	G	206	BCR	C12-C13	-2.56	1.40	1.45
19	B	819	CLA	C1B-C2B	-2.56	1.37	1.43
19	J	102	CLA	C3D-C4D	-2.56	1.38	1.44
19	B	827	CLA	C1D-C2D	-2.56	1.40	1.45
19	2	310	CLA	C1D-C2D	-2.55	1.40	1.45
20	2	306	CHL	C3D-C4D	-2.55	1.38	1.44
19	A	817	CLA	C1B-C2B	-2.55	1.37	1.43
18	A	846	BCR	C12-C13	-2.55	1.40	1.45
18	L	305	BCR	C12-C13	-2.55	1.40	1.45
19	2	308	CLA	MG-NA	2.55	2.12	2.06
19	1	311	CLA	C1D-C2D	-2.55	1.40	1.45
19	B	815	CLA	C3D-C4D	-2.55	1.38	1.44
19	A	853	CLA	C1B-C2B	-2.55	1.37	1.43
19	A	853	CLA	C1D-C2D	-2.55	1.40	1.45
19	2	302	CLA	C1B-C2B	-2.55	1.37	1.43
19	K	303	CLA	C3D-C4D	-2.55	1.38	1.44
19	2	308	CLA	C1B-NB	-2.55	1.34	1.37
19	F	307	CLA	C1D-C2D	-2.54	1.40	1.45
22	1	315	XAT	C12-C13	-2.54	1.40	1.45
19	L	302	CLA	C1D-C2D	-2.54	1.40	1.45
19	A	854	CLA	C1D-C2D	-2.54	1.40	1.45
18	4	318	BCR	C12-C13	-2.54	1.40	1.45
19	1	304	CLA	C1D-C2D	-2.54	1.40	1.45
19	3	310	CLA	C3D-C4D	-2.54	1.38	1.44
19	2	311	CLA	C1D-C2D	-2.54	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	845	BCR	C12-C13	-2.54	1.40	1.45
19	2	303	CLA	C1B-C2B	-2.53	1.37	1.43
21	1	314	LUT	C28-C29	-2.53	1.40	1.45
19	B	838	CLA	C1D-C2D	-2.53	1.40	1.45
19	3	307	CLA	C3D-C4D	-2.53	1.38	1.44
19	A	833	CLA	C1B-C2B	-2.53	1.37	1.43
19	3	303	CLA	C3D-C4D	-2.53	1.38	1.44
19	A	820	CLA	C3D-C4D	-2.53	1.38	1.44
19	O	101	CLA	C1D-C2D	-2.53	1.40	1.45
19	O	104	CLA	C3D-C4D	-2.53	1.38	1.44
19	4	311	CLA	C3D-C4D	-2.53	1.38	1.44
19	1	306	CLA	C1D-C2D	-2.53	1.40	1.45
19	B	818	CLA	C1B-C2B	-2.52	1.37	1.43
19	B	810	CLA	C1D-C2D	-2.52	1.40	1.45
19	B	833	CLA	MG-NA	2.52	2.12	2.06
18	A	844	BCR	C12-C13	-2.52	1.40	1.45
19	B	816	CLA	C1D-C2D	-2.52	1.40	1.45
19	B	815	CLA	C1D-C2D	-2.52	1.40	1.45
19	1	303	CLA	C3D-C4D	-2.52	1.38	1.44
19	A	819	CLA	C1D-C2D	-2.52	1.40	1.45
19	1	312	CLA	C1D-C2D	-2.52	1.40	1.45
19	A	816	CLA	C1D-C2D	-2.52	1.40	1.45
19	B	818	CLA	C1D-C2D	-2.52	1.40	1.45
19	A	809	CLA	C1D-C2D	-2.52	1.40	1.45
19	B	812	CLA	C1B-C2B	-2.51	1.37	1.43
19	4	301	CLA	C3D-C4D	-2.51	1.38	1.44
18	B	842	BCR	C19-C18	-2.51	1.40	1.45
22	2	315	XAT	C28-C29	-2.51	1.40	1.45
19	A	833	CLA	C1D-C2D	-2.51	1.40	1.45
19	B	837	CLA	C1D-C2D	-2.51	1.40	1.45
20	2	305	CHL	C3D-C4D	-2.51	1.38	1.44
20	4	305	CHL	C3D-C4D	-2.51	1.38	1.44
19	A	836	CLA	C1B-C2B	-2.51	1.37	1.43
19	A	834	CLA	C1D-C2D	-2.51	1.40	1.45
19	4	308	CLA	C3D-C4D	-2.51	1.38	1.44
19	3	304	CLA	C1B-C2B	-2.51	1.37	1.43
19	3	311	CLA	C3D-C4D	-2.51	1.38	1.44
19	A	850	CLA	C1B-C2B	-2.51	1.37	1.43
19	B	830	CLA	C1D-C2D	-2.50	1.40	1.45
19	B	834	CLA	C1B-C2B	-2.50	1.37	1.43
21	2	314	LUT	C28-C29	-2.50	1.40	1.45
18	B	842	BCR	C12-C13	-2.50	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	816	CLA	C1B-C2B	-2.50	1.37	1.43
21	4	316	LUT	C32-C33	-2.50	1.40	1.45
20	2	304	CHL	C1B-C2B	-2.50	1.37	1.43
18	3	315	BCR	C12-C13	-2.49	1.40	1.45
18	A	848	BCR	C12-C13	-2.49	1.40	1.45
20	4	315	CHL	C3D-C4D	-2.49	1.38	1.44
20	3	306	CHL	C1D-C2D	-2.49	1.40	1.45
19	4	311	CLA	C1B-C2B	-2.49	1.37	1.43
19	B	813	CLA	C1D-C2D	-2.49	1.40	1.45
19	B	804	CLA	C1B-C2B	-2.49	1.37	1.43
19	A	826	CLA	C1B-C2B	-2.49	1.37	1.43
19	B	835	CLA	C1B-C2B	-2.49	1.37	1.43
19	O	103	CLA	C3D-C4D	-2.48	1.38	1.44
18	L	301	BCR	C19-C18	-2.48	1.40	1.45
19	2	308	CLA	C3D-C4D	-2.48	1.38	1.44
19	A	813	CLA	C1D-C2D	-2.48	1.40	1.45
21	2	314	LUT	C12-C13	-2.48	1.40	1.45
19	A	806	CLA	C1D-C2D	-2.48	1.40	1.45
18	J	103	BCR	C19-C18	-2.48	1.40	1.45
19	A	810	CLA	C1B-C2B	-2.48	1.37	1.43
19	A	814	CLA	C1D-C2D	-2.48	1.40	1.45
20	4	315	CHL	C1D-C2D	-2.48	1.40	1.45
19	4	310	CLA	MG-NB	-2.48	2.00	2.05
19	B	828	CLA	C1B-C2B	-2.47	1.37	1.43
19	B	833	CLA	C1D-C2D	-2.47	1.40	1.45
19	3	308	CLA	C1B-C2B	-2.47	1.37	1.43
21	1	314	LUT	C12-C13	-2.47	1.40	1.45
19	2	310	CLA	C3D-C4D	-2.47	1.38	1.44
19	B	825	CLA	C1B-C2B	-2.47	1.37	1.43
19	B	825	CLA	C1D-C2D	-2.47	1.40	1.45
19	B	830	CLA	C1B-C2B	-2.46	1.37	1.43
19	A	809	CLA	C1B-C2B	-2.46	1.37	1.43
19	A	829	CLA	C1B-C2B	-2.46	1.37	1.43
19	4	312	CLA	C1D-C2D	-2.46	1.40	1.45
19	A	812	CLA	C1B-C2B	-2.46	1.37	1.43
19	A	801	CLA	C3D-C4D	-2.46	1.38	1.44
19	A	811	CLA	C1B-C2B	-2.46	1.37	1.43
19	1	313	CLA	C1D-C2D	-2.46	1.40	1.45
19	A	822	CLA	C1D-C2D	-2.46	1.40	1.45
19	A	828	CLA	C1B-C2B	-2.46	1.37	1.43
19	B	831	CLA	C1D-C2D	-2.46	1.40	1.45
19	A	834	CLA	C1B-C2B	-2.45	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	310	CLA	C1D-C2D	-2.45	1.40	1.45
19	1	302	CLA	C1D-C2D	-2.45	1.40	1.45
19	B	834	CLA	C1B-NB	-2.45	1.34	1.37
19	B	834	CLA	MG-NA	2.45	2.12	2.06
19	2	302	CLA	C1D-C2D	-2.45	1.40	1.45
19	3	304	CLA	C1D-C2D	-2.45	1.40	1.45
19	3	312	CLA	C1D-C2D	-2.45	1.40	1.45
19	A	817	CLA	C1D-C2D	-2.45	1.40	1.45
18	I	101	BCR	C12-C13	-2.45	1.40	1.45
19	B	812	CLA	C1D-C2D	-2.45	1.40	1.45
18	J	104	BCR	C12-C13	-2.45	1.40	1.45
19	1	302	CLA	C1B-C2B	-2.45	1.37	1.43
22	4	317	XAT	C32-C33	-2.45	1.40	1.45
19	A	834	CLA	MG-NC	2.45	2.12	2.06
19	A	840	CLA	C1B-C2B	-2.45	1.37	1.43
18	2	316	BCR	C12-C13	-2.44	1.40	1.45
18	I	101	BCR	C19-C18	-2.44	1.40	1.45
19	A	814	CLA	C1B-C2B	-2.44	1.37	1.43
19	4	309	CLA	C3D-C4D	-2.44	1.38	1.44
19	B	831	CLA	C1B-C2B	-2.44	1.37	1.43
18	G	201	BCR	C12-C13	-2.44	1.40	1.45
19	A	805	CLA	C1B-C2B	-2.44	1.37	1.43
19	B	824	CLA	C1B-C2B	-2.44	1.37	1.43
20	2	313	CHL	C1D-C2D	-2.43	1.40	1.45
19	A	803	CLA	C1D-C2D	-2.43	1.40	1.45
19	A	828	CLA	C1B-NB	-2.43	1.34	1.37
19	2	307	CLA	C1B-C2B	-2.43	1.37	1.43
19	4	302	CLA	C1B-C2B	-2.43	1.37	1.43
18	G	201	BCR	C19-C18	-2.43	1.40	1.45
19	3	308	CLA	C1D-C2D	-2.43	1.40	1.45
18	O	105	BCR	C12-C13	-2.43	1.40	1.45
19	B	806	CLA	C1B-C2B	-2.43	1.37	1.43
19	B	838	CLA	C1B-C2B	-2.43	1.37	1.43
18	K	301	BCR	C19-C18	-2.42	1.40	1.45
19	2	303	CLA	C1D-C2D	-2.42	1.40	1.45
18	B	843	BCR	C19-C18	-2.42	1.40	1.45
19	A	803	CLA	C1B-C2B	-2.42	1.37	1.43
19	A	812	CLA	C1B-NB	-2.42	1.34	1.37
19	1	310	CLA	C1D-C2D	-2.42	1.40	1.45
19	A	808	CLA	C1D-C2D	-2.42	1.40	1.45
19	A	821	CLA	C1B-C2B	-2.42	1.37	1.43
19	B	822	CLA	C1B-C2B	-2.42	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	805	CLA	C1D-C2D	-2.42	1.40	1.45
19	A	824	CLA	C1B-C2B	-2.41	1.37	1.43
19	A	835	CLA	C1D-C2D	-2.41	1.40	1.45
19	3	316	CLA	C3D-C4D	-2.41	1.38	1.44
19	G	203	CLA	C1B-C2B	-2.41	1.37	1.43
19	3	301	CLA	C1B-C2B	-2.41	1.37	1.43
19	A	813	CLA	C1B-NB	-2.41	1.34	1.37
19	B	811	CLA	C1D-C2D	-2.41	1.40	1.45
19	B	803	CLA	C1B-C2B	-2.41	1.37	1.43
19	3	309	CLA	MG-NC	2.41	2.12	2.06
19	B	803	CLA	MG-NA	2.41	2.12	2.06
19	B	850	CLA	C1D-C2D	-2.41	1.40	1.45
19	A	831	CLA	C1D-C2D	-2.41	1.40	1.45
19	L	303	CLA	C1B-C2B	-2.41	1.37	1.43
19	A	837	CLA	C1B-C2B	-2.41	1.37	1.43
19	G	204	CLA	C1B-C2B	-2.40	1.37	1.43
19	A	819	CLA	C1B-C2B	-2.40	1.37	1.43
19	L	302	CLA	C1B-C2B	-2.40	1.37	1.43
19	A	827	CLA	C1B-C2B	-2.40	1.37	1.43
19	B	810	CLA	C1B-C2B	-2.40	1.37	1.43
19	4	314	CLA	C1D-C2D	-2.40	1.40	1.45
18	B	844	BCR	C12-C13	-2.40	1.40	1.45
19	A	838	CLA	C1B-C2B	-2.40	1.37	1.43
19	A	808	CLA	C1B-C2B	-2.39	1.37	1.43
19	B	801	CLA	C1D-C2D	-2.39	1.40	1.45
19	B	801	CLA	C1B-C2B	-2.39	1.37	1.43
19	B	824	CLA	C1D-C2D	-2.39	1.40	1.45
19	A	832	CLA	C1B-C2B	-2.39	1.37	1.43
21	2	314	LUT	C32-C33	-2.39	1.40	1.45
19	A	813	CLA	C1B-C2B	-2.39	1.37	1.43
20	4	306	CHL	C1D-C2D	-2.39	1.40	1.45
19	B	807	CLA	C1B-C2B	-2.39	1.37	1.43
19	3	303	CLA	C1B-C2B	-2.39	1.37	1.43
19	4	301	CLA	C1B-C2B	-2.39	1.37	1.43
19	B	815	CLA	C1B-C2B	-2.38	1.37	1.43
19	4	311	CLA	C1D-C2D	-2.38	1.40	1.45
19	1	303	CLA	C1B-C2B	-2.38	1.37	1.43
19	B	840	CLA	C1B-C2B	-2.38	1.37	1.43
19	B	827	CLA	C1B-C2B	-2.38	1.37	1.43
19	A	839	CLA	C1B-C2B	-2.38	1.37	1.43
19	B	850	CLA	C1B-C2B	-2.38	1.37	1.43
19	K	303	CLA	C1D-C2D	-2.38	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	804	CLA	C1B-C2B	-2.38	1.37	1.43
19	F	306	CLA	C1D-C2D	-2.38	1.40	1.45
19	B	819	CLA	C1D-C2D	-2.38	1.40	1.45
19	4	313	CLA	C1B-C2B	-2.38	1.37	1.43
20	4	307	CHL	C1D-C2D	-2.38	1.40	1.45
19	B	817	CLA	C1D-C2D	-2.37	1.40	1.45
19	B	821	CLA	C1B-C2B	-2.37	1.37	1.43
18	J	104	BCR	C19-C18	-2.37	1.40	1.45
21	3	313	LUT	C28-C29	-2.37	1.40	1.45
19	B	836	CLA	C1D-C2D	-2.37	1.40	1.45
19	4	303	CLA	C1B-C2B	-2.37	1.37	1.43
22	3	314	XAT	C12-C13	-2.37	1.40	1.45
19	B	809	CLA	C1B-NB	-2.37	1.34	1.37
19	F	306	CLA	C1B-C2B	-2.37	1.37	1.43
19	3	303	CLA	C1D-C2D	-2.37	1.40	1.45
21	3	313	LUT	C12-C13	-2.37	1.40	1.45
20	1	318	CHL	C1B-C2B	-2.37	1.37	1.43
19	B	829	CLA	C1B-C2B	-2.36	1.37	1.43
19	B	829	CLA	C1D-C2D	-2.36	1.40	1.45
20	2	319	CHL	C1B-C2B	-2.36	1.37	1.43
19	B	834	CLA	C1D-C2D	-2.36	1.40	1.45
20	4	305	CHL	C1D-C2D	-2.36	1.40	1.45
19	B	826	CLA	C1B-C2B	-2.36	1.37	1.43
19	B	833	CLA	C1B-C2B	-2.36	1.37	1.43
19	4	304	CLA	C1D-C2D	-2.36	1.40	1.45
18	O	106	BCR	C19-C18	-2.36	1.40	1.45
19	B	822	CLA	C1D-C2D	-2.36	1.40	1.45
19	4	301	CLA	C1D-C2D	-2.36	1.40	1.45
19	2	312	CLA	C1B-C2B	-2.36	1.37	1.43
19	1	303	CLA	C1D-C2D	-2.36	1.40	1.45
19	A	825	CLA	C1B-C2B	-2.36	1.37	1.43
19	B	811	CLA	CAB-C3B	-2.36	1.45	1.50
19	B	836	CLA	C1B-C2B	-2.36	1.37	1.43
18	K	304	BCR	C19-C18	-2.35	1.40	1.45
19	B	823	CLA	C1B-C2B	-2.35	1.37	1.43
19	A	812	CLA	C1D-C2D	-2.35	1.40	1.45
20	3	306	CHL	C1B-C2B	-2.35	1.37	1.43
19	G	205	CLA	C1D-C2D	-2.35	1.40	1.45
19	B	808	CLA	C1B-C2B	-2.35	1.37	1.43
19	G	205	CLA	C1B-C2B	-2.35	1.37	1.43
19	A	811	CLA	C1D-C2D	-2.35	1.40	1.45
19	2	310	CLA	C1B-C2B	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	319	CHL	C1D-C2D	-2.35	1.40	1.45
19	K	302	CLA	C1B-C2B	-2.35	1.37	1.43
19	A	807	CLA	C1B-C2B	-2.35	1.37	1.43
19	3	311	CLA	C1D-C2D	-2.35	1.40	1.45
20	4	306	CHL	C1B-C2B	-2.34	1.37	1.43
21	3	313	LUT	C32-C33	-2.34	1.40	1.45
19	A	835	CLA	C1B-C2B	-2.34	1.37	1.43
19	A	836	CLA	C1D-C2D	-2.34	1.40	1.45
19	1	304	CLA	C1B-C2B	-2.34	1.37	1.43
19	1	309	CLA	C1B-C2B	-2.34	1.37	1.43
20	4	315	CHL	C1B-C2B	-2.34	1.37	1.43
21	4	316	LUT	C12-C13	-2.34	1.40	1.45
19	B	814	CLA	C1B-NB	-2.34	1.34	1.37
19	1	308	CLA	C1D-C2D	-2.34	1.40	1.45
19	3	309	CLA	C1D-C2D	-2.33	1.40	1.45
19	L	304	CLA	C1B-C2B	-2.33	1.37	1.43
19	2	301	CLA	C1D-C2D	-2.33	1.40	1.45
19	4	304	CLA	C1B-C2B	-2.33	1.37	1.43
19	1	301	CLA	C1B-C2B	-2.33	1.37	1.43
20	2	305	CHL	C1D-C2D	-2.33	1.40	1.45
19	2	308	CLA	C1D-C2D	-2.33	1.40	1.45
19	A	831	CLA	C1B-C2B	-2.33	1.37	1.43
19	1	313	CLA	C1B-C2B	-2.33	1.37	1.43
19	A	820	CLA	C1B-C2B	-2.33	1.37	1.43
19	B	813	CLA	C1B-C2B	-2.33	1.37	1.43
19	2	301	CLA	C1B-C2B	-2.33	1.37	1.43
19	B	816	CLA	C1B-C2B	-2.33	1.37	1.43
19	L	304	CLA	MG-NC	2.33	2.11	2.06
19	A	818	CLA	C1B-C2B	-2.33	1.37	1.43
19	4	314	CLA	C1B-C2B	-2.33	1.37	1.43
19	B	803	CLA	C1B-NB	-2.32	1.34	1.37
19	B	820	CLA	C1B-C2B	-2.32	1.37	1.43
19	F	307	CLA	C1B-C2B	-2.32	1.37	1.43
19	A	806	CLA	C1B-C2B	-2.32	1.37	1.43
19	A	854	CLA	C1B-C2B	-2.32	1.37	1.43
19	J	102	CLA	C1D-C2D	-2.32	1.40	1.45
19	B	811	CLA	C1B-C2B	-2.32	1.37	1.43
20	2	306	CHL	C1D-C2D	-2.32	1.40	1.45
19	2	303	CLA	C1B-NB	-2.32	1.34	1.37
19	4	312	CLA	C1B-C2B	-2.32	1.37	1.43
19	3	316	CLA	C1B-C2B	-2.32	1.37	1.43
19	1	310	CLA	C1B-C2B	-2.31	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	318	CHL	C1D-C2D	-2.31	1.40	1.45
19	4	310	CLA	C1B-NB	-2.31	1.34	1.37
19	1	311	CLA	C1B-C2B	-2.31	1.37	1.43
19	1	312	CLA	C1B-C2B	-2.31	1.37	1.43
19	2	309	CLA	C1B-C2B	-2.31	1.37	1.43
19	K	303	CLA	C1B-C2B	-2.31	1.37	1.43
18	O	106	BCR	C12-C13	-2.31	1.41	1.45
20	4	307	CHL	C1B-C2B	-2.30	1.37	1.43
19	A	822	CLA	C1B-C2B	-2.30	1.37	1.43
20	2	304	CHL	C1D-C2D	-2.30	1.40	1.45
19	A	815	CLA	C1B-C2B	-2.30	1.37	1.43
18	F	302	BCR	C12-C13	-2.30	1.41	1.45
18	J	103	BCR	C12-C13	-2.30	1.41	1.45
19	B	826	CLA	C1B-NB	-2.30	1.35	1.37
19	O	102	CLA	C1D-C2D	-2.30	1.40	1.45
19	B	821	CLA	MG-NC	2.30	2.11	2.06
19	3	311	CLA	C1B-C2B	-2.30	1.37	1.43
19	B	832	CLA	C1B-C2B	-2.30	1.37	1.43
20	2	313	CHL	C1B-C2B	-2.30	1.37	1.43
19	1	306	CLA	C1B-C2B	-2.29	1.37	1.43
18	4	318	BCR	C19-C18	-2.29	1.41	1.45
20	1	305	CHL	C1B-C2B	-2.29	1.37	1.43
19	3	302	CLA	C1D-C2D	-2.29	1.40	1.45
19	3	302	CLA	MG-NC	2.29	2.11	2.06
19	3	302	CLA	C1B-C2B	-2.29	1.37	1.43
19	4	309	CLA	C1D-C2D	-2.29	1.40	1.45
19	O	104	CLA	C1B-C2B	-2.28	1.37	1.43
22	2	315	XAT	C12-C13	-2.28	1.41	1.45
19	B	839	CLA	C1B-C2B	-2.28	1.37	1.43
19	A	802	CLA	C1B-NB	-2.28	1.35	1.37
18	F	302	BCR	C19-C18	-2.28	1.41	1.45
20	2	306	CHL	C1B-C2B	-2.28	1.37	1.43
19	A	823	CLA	C1B-C2B	-2.28	1.37	1.43
19	B	817	CLA	C1B-C2B	-2.28	1.37	1.43
19	B	805	CLA	C1B-C2B	-2.28	1.37	1.43
19	A	830	CLA	C1B-C2B	-2.28	1.37	1.43
19	3	301	CLA	C1D-C2D	-2.28	1.40	1.45
18	O	105	BCR	C19-C18	-2.27	1.41	1.45
19	B	814	CLA	C1B-C2B	-2.27	1.37	1.43
19	3	312	CLA	C1B-C2B	-2.27	1.37	1.43
19	3	307	CLA	C1B-C2B	-2.27	1.37	1.43
22	3	314	XAT	C8-C9	-2.27	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	302	CLA	C1D-C2D	-2.27	1.40	1.45
20	4	305	CHL	C1B-C2B	-2.27	1.37	1.43
19	4	309	CLA	C1B-NB	-2.27	1.35	1.37
19	O	103	CLA	C1B-C2B	-2.26	1.37	1.43
19	O	102	CLA	C1B-C2B	-2.26	1.37	1.43
20	2	305	CHL	C1B-C2B	-2.26	1.37	1.43
19	4	313	CLA	C1D-C2D	-2.26	1.40	1.45
19	K	302	CLA	C1D-C2D	-2.26	1.40	1.45
19	B	837	CLA	C1B-C2B	-2.26	1.37	1.43
19	G	203	CLA	C1D-C2D	-2.25	1.40	1.45
19	O	103	CLA	C1D-C2D	-2.25	1.40	1.45
18	2	316	BCR	C19-C18	-2.25	1.41	1.45
19	A	821	CLA	C1D-C2D	-2.25	1.40	1.45
19	B	822	CLA	C1B-NB	-2.25	1.35	1.37
19	3	316	CLA	C1D-C2D	-2.25	1.40	1.45
19	4	308	CLA	C1B-C2B	-2.25	1.38	1.43
19	B	829	CLA	C1B-NB	-2.25	1.35	1.37
19	O	101	CLA	C1B-C2B	-2.24	1.38	1.43
19	1	308	CLA	C1B-NB	-2.24	1.35	1.37
19	A	852	CLA	C1B-NB	-2.24	1.35	1.37
19	A	803	CLA	C1B-NB	-2.24	1.35	1.37
19	B	804	CLA	C1B-NB	-2.24	1.35	1.37
19	B	832	CLA	C1B-NB	-2.24	1.35	1.37
19	1	304	CLA	MG-NC	2.24	2.11	2.06
19	A	805	CLA	C1B-NB	-2.24	1.35	1.37
19	A	853	CLA	C1B-NB	-2.24	1.35	1.37
19	4	301	CLA	C1B-NB	-2.24	1.35	1.37
18	1	316	BCR	C12-C13	-2.24	1.41	1.45
19	3	309	CLA	C1B-C2B	-2.24	1.38	1.43
19	J	102	CLA	C1B-C2B	-2.24	1.38	1.43
19	B	828	CLA	C1B-NB	-2.23	1.35	1.37
19	1	307	CLA	C1B-C2B	-2.23	1.38	1.43
20	1	305	CHL	C1D-C2D	-2.23	1.40	1.45
19	2	311	CLA	C1B-C2B	-2.23	1.38	1.43
19	3	310	CLA	C1B-C2B	-2.23	1.38	1.43
19	A	801	CLA	C1B-C2B	-2.23	1.38	1.43
19	A	831	CLA	C1B-NB	-2.23	1.35	1.37
19	4	303	CLA	MG-NC	2.22	2.11	2.06
19	B	835	CLA	C1B-NB	-2.22	1.35	1.37
19	2	310	CLA	MG-NC	2.22	2.11	2.06
19	A	854	CLA	C1B-NB	-2.22	1.35	1.37
19	B	814	CLA	MG-NC	2.21	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	2	315	XAT	C8-C9	-2.21	1.41	1.45
19	B	835	CLA	MG-NC	2.21	2.11	2.06
19	A	811	CLA	C1B-NB	-2.21	1.35	1.37
18	K	301	BCR	C12-C13	-2.20	1.41	1.45
19	B	824	CLA	C1B-NB	-2.20	1.35	1.37
19	2	307	CLA	C1B-NB	-2.20	1.35	1.37
19	A	810	CLA	C1B-NB	-2.20	1.35	1.37
19	3	308	CLA	MG-NA	2.20	2.11	2.06
19	3	305	CLA	C1B-C2B	-2.19	1.38	1.43
18	1	316	BCR	C19-C18	-2.19	1.41	1.45
19	1	304	CLA	C1B-NB	-2.19	1.35	1.37
19	B	805	CLA	C1B-NB	-2.19	1.35	1.37
19	A	836	CLA	C1B-NB	-2.19	1.35	1.37
20	4	315	CHL	C1B-NB	-2.18	1.35	1.37
19	1	301	CLA	C1D-C2D	-2.18	1.41	1.45
19	B	850	CLA	C1B-NB	-2.18	1.35	1.37
20	1	318	CHL	MG-NA	2.18	2.11	2.06
19	O	104	CLA	C1D-C2D	-2.18	1.41	1.45
20	4	305	CHL	MG-NC	2.18	2.11	2.06
19	4	311	CLA	MG-NC	2.18	2.11	2.06
19	A	834	CLA	C1B-NB	-2.17	1.35	1.37
19	B	812	CLA	C1B-NB	-2.17	1.35	1.37
19	B	815	CLA	C1B-NB	-2.17	1.35	1.37
19	A	808	CLA	C1B-NB	-2.17	1.35	1.37
19	1	302	CLA	C1B-NB	-2.17	1.35	1.37
19	A	827	CLA	C1B-NB	-2.17	1.35	1.37
19	2	312	CLA	MG-NC	2.17	2.11	2.06
19	A	823	CLA	C1B-NB	-2.17	1.35	1.37
20	2	306	CHL	C1B-NB	-2.16	1.35	1.37
19	B	813	CLA	C1B-NB	-2.15	1.35	1.37
19	4	312	CLA	C1B-NB	-2.15	1.35	1.37
19	4	303	CLA	C1B-NB	-2.15	1.35	1.37
19	A	850	CLA	C1B-NB	-2.15	1.35	1.37
19	A	825	CLA	MG-NC	2.15	2.11	2.06
19	2	312	CLA	C1D-C2D	-2.15	1.41	1.45
19	A	815	CLA	C1B-NB	-2.15	1.35	1.37
19	B	821	CLA	C1B-NB	-2.14	1.35	1.37
19	B	817	CLA	MG-NA	2.14	2.11	2.06
19	A	817	CLA	C1B-NB	-2.14	1.35	1.37
19	B	802	CLA	C1B-C2B	-2.13	1.38	1.43
19	G	205	CLA	C1B-NB	-2.12	1.35	1.37
19	B	804	CLA	MG-NC	2.12	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	825	CLA	C1B-NB	-2.12	1.35	1.37
22	4	317	XAT	C12-C13	-2.12	1.41	1.45
20	4	307	CHL	C1B-NB	-2.12	1.35	1.37
19	3	308	CLA	C1B-NB	-2.11	1.35	1.37
19	A	814	CLA	C1B-NB	-2.11	1.35	1.37
19	A	820	CLA	MG-NC	2.11	2.11	2.06
19	A	819	CLA	C1B-NB	-2.11	1.35	1.37
19	B	802	CLA	CHB-C1B	2.11	1.44	1.39
19	B	801	CLA	C1B-NB	-2.10	1.35	1.37
19	A	812	CLA	MG-NC	2.10	2.11	2.06
19	A	829	CLA	C1B-NB	-2.10	1.35	1.37
19	B	818	CLA	MG-NC	2.10	2.11	2.06
19	2	310	CLA	C1B-NB	-2.10	1.35	1.37
19	A	821	CLA	C1B-NB	-2.10	1.35	1.37
19	B	808	CLA	C1B-NB	-2.10	1.35	1.37
19	A	840	CLA	MG-NC	2.10	2.11	2.06
19	A	835	CLA	C1B-NB	-2.09	1.35	1.37
19	B	831	CLA	C1B-NB	-2.09	1.35	1.37
19	3	310	CLA	C1B-NB	-2.09	1.35	1.37
19	L	302	CLA	C1B-NB	-2.09	1.35	1.37
22	4	317	XAT	C8-C9	-2.09	1.41	1.45
19	A	818	CLA	C1B-NB	-2.09	1.35	1.37
19	A	806	CLA	C1B-NB	-2.09	1.35	1.37
19	B	811	CLA	C1B-NB	-2.08	1.35	1.37
19	A	816	CLA	C1B-NB	-2.08	1.35	1.37
19	G	204	CLA	C1B-NB	-2.08	1.35	1.37
19	B	810	CLA	C1B-NB	-2.08	1.35	1.37
19	B	807	CLA	C1B-NB	-2.08	1.35	1.37
19	K	303	CLA	C1B-NB	-2.08	1.35	1.37
19	A	840	CLA	C1B-NB	-2.07	1.35	1.37
19	B	838	CLA	C1B-NB	-2.07	1.35	1.37
19	K	302	CLA	MG-NC	2.07	2.11	2.06
19	L	303	CLA	C1B-NB	-2.07	1.35	1.37
19	4	302	CLA	MG-NB	2.07	2.09	2.05
19	4	302	CLA	C1B-NB	-2.07	1.35	1.37
19	2	308	CLA	MG-NB	2.06	2.09	2.05
19	A	833	CLA	C1B-NB	-2.06	1.35	1.37
19	A	839	CLA	C1B-NB	-2.06	1.35	1.37
19	1	306	CLA	C1B-NB	-2.06	1.35	1.37
20	4	306	CHL	MG-NC	2.06	2.11	2.06
19	B	837	CLA	C1B-NB	-2.06	1.35	1.37
19	J	102	CLA	C1B-NB	-2.06	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	804	CLA	C1B-NB	-2.05	1.35	1.37
19	A	801	CLA	CHB-C1B	2.05	1.44	1.39
19	1	303	CLA	C1B-NB	-2.05	1.35	1.37
20	4	305	CHL	CHB-C1B	2.05	1.44	1.39
19	A	823	CLA	MG-NC	2.05	2.11	2.06
19	3	312	CLA	C1B-NB	-2.05	1.35	1.37
19	A	822	CLA	C1B-NB	-2.04	1.35	1.37
19	3	316	CLA	C1B-NB	-2.04	1.35	1.37
19	B	832	CLA	MG-NC	2.04	2.11	2.06
19	3	301	CLA	C1B-NB	-2.04	1.35	1.37
19	3	307	CLA	C1B-NB	-2.04	1.35	1.37
19	A	809	CLA	C1B-NB	-2.03	1.35	1.37
19	A	820	CLA	C1B-NB	-2.03	1.35	1.37
19	A	830	CLA	C1B-NB	-2.03	1.35	1.37
19	B	819	CLA	C1B-NB	-2.03	1.35	1.37
19	F	307	CLA	C1B-NB	-2.03	1.35	1.37
19	A	804	CLA	MG-NC	2.03	2.11	2.06
19	3	305	CLA	C1B-NB	-2.02	1.35	1.37
19	B	827	CLA	C1B-NB	-2.02	1.35	1.37
19	3	302	CLA	C1B-NB	-2.02	1.35	1.37
19	B	820	CLA	MG-NC	2.02	2.11	2.06
19	B	825	CLA	C1B-NB	-2.02	1.35	1.37
19	A	807	CLA	C1B-NB	-2.02	1.35	1.37
19	B	826	CLA	MG-NC	2.02	2.11	2.06
19	1	307	CLA	C1B-NB	-2.01	1.35	1.37
19	B	816	CLA	C1B-NB	-2.01	1.35	1.37
19	B	830	CLA	C1B-NB	-2.01	1.35	1.37
19	2	302	CLA	C1B-NB	-2.01	1.35	1.37
20	2	313	CHL	C1B-NB	-2.01	1.35	1.37
19	A	831	CLA	MG-NC	2.01	2.11	2.06
19	B	836	CLA	C1B-NB	-2.01	1.35	1.37

All (1066) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	309	CLA	CHD-C1D-ND	-5.25	119.63	124.45
20	1	305	CHL	CHD-C1D-ND	-5.09	119.77	124.45
29	B	847	DGD	O2G-C1B-C2B	4.97	122.20	111.50
19	O	104	CLA	CHD-C1D-ND	-4.71	120.13	124.45
19	2	307	CLA	C4D-CHA-C1A	4.62	126.87	121.25
19	B	850	CLA	CHD-C1D-ND	-4.56	120.26	124.45
19	B	836	CLA	CHD-C1D-ND	-4.54	120.28	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	809	CLA	CHD-C1D-ND	-4.53	120.29	124.45
19	G	203	CLA	CHD-C1D-ND	-4.52	120.30	124.45
18	1	316	BCR	C1-C6-C5	-4.45	116.34	122.61
18	O	106	BCR	C37-C22-C21	-4.43	116.72	122.92
18	4	318	BCR	C37-C22-C21	-4.41	116.75	122.92
18	F	308	BCR	C34-C9-C10	-4.40	116.75	122.92
19	B	829	CLA	CHD-C1D-ND	-4.40	120.41	124.45
20	4	306	CHL	CHD-C1D-ND	-4.39	120.42	124.45
18	L	305	BCR	C37-C22-C21	-4.38	116.79	122.92
18	J	104	BCR	C37-C22-C21	-4.37	116.80	122.92
22	4	317	XAT	C32-C33-C34	4.35	125.61	118.94
19	4	304	CLA	CHD-C1D-ND	-4.35	120.46	124.45
19	A	812	CLA	C4D-CHA-C1A	4.34	126.53	121.25
19	1	301	CLA	CHD-C1D-ND	-4.34	120.47	124.45
21	3	313	LUT	C15-C35-C34	4.34	132.36	123.47
19	B	832	CLA	C4D-CHA-C1A	4.33	126.52	121.25
18	A	848	BCR	C15-C16-C17	4.33	132.34	123.47
18	A	847	BCR	C34-C9-C10	-4.31	116.88	122.92
19	B	801	CLA	CHD-C1D-ND	-4.31	120.49	124.45
19	A	812	CLA	CHD-C1D-ND	-4.30	120.50	124.45
18	F	302	BCR	C37-C22-C21	-4.30	116.90	122.92
19	A	808	CLA	CHD-C1D-ND	-4.30	120.51	124.45
18	O	106	BCR	C15-C16-C17	4.27	132.22	123.47
19	B	803	CLA	CHD-C1D-ND	-4.27	120.53	124.45
18	J	103	BCR	C34-C9-C10	-4.27	116.95	122.92
22	2	315	XAT	C19-C9-C10	-4.27	116.95	122.92
19	O	102	CLA	CHD-C1D-ND	-4.26	120.54	124.45
19	B	850	CLA	C4D-CHA-C1A	4.26	126.43	121.25
18	A	844	BCR	C37-C22-C21	-4.23	117.00	122.92
18	4	318	BCR	C15-C16-C17	4.22	132.12	123.47
22	4	317	XAT	C19-C9-C10	-4.22	117.02	122.92
18	F	302	BCR	C15-C16-C17	4.22	132.11	123.47
19	G	205	CLA	CHD-C1D-ND	-4.22	120.58	124.45
18	2	316	BCR	C37-C22-C21	-4.21	117.02	122.92
18	G	206	BCR	C37-C22-C21	-4.20	117.03	122.92
18	I	101	BCR	C34-C9-C10	-4.20	117.03	122.92
18	F	304	BCR	C37-C22-C21	-4.20	117.04	122.92
18	K	304	BCR	C37-C22-C21	-4.20	117.04	122.92
21	4	316	LUT	C39-C29-C30	-4.20	117.05	122.92
18	J	103	BCR	C37-C22-C21	-4.19	117.05	122.92
18	K	301	BCR	C37-C22-C21	-4.19	117.05	122.92
19	4	313	CLA	CHD-C1D-ND	-4.19	120.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	821	CLA	CHD-C1D-ND	-4.19	120.60	124.45
21	1	314	LUT	C19-C9-C10	-4.18	117.07	122.92
18	1	316	BCR	C34-C9-C10	-4.18	117.07	122.92
22	3	314	XAT	C15-C35-C34	4.17	132.02	123.47
19	B	833	CLA	CHD-C1D-ND	-4.17	120.62	124.45
21	2	314	LUT	C19-C9-C10	-4.17	117.08	122.92
18	F	302	BCR	C34-C9-C10	-4.16	117.09	122.92
22	3	314	XAT	C19-C9-C10	-4.16	117.09	122.92
19	B	822	CLA	CHD-C1D-ND	-4.16	120.64	124.45
18	O	106	BCR	C34-C9-C10	-4.15	117.10	122.92
18	B	845	BCR	C34-C9-C10	-4.15	117.11	122.92
18	A	845	BCR	C34-C9-C10	-4.15	117.11	122.92
18	B	843	BCR	C34-C9-C10	-4.15	117.12	122.92
18	I	101	BCR	C37-C22-C21	-4.15	117.12	122.92
19	1	308	CLA	CHD-C1D-ND	-4.14	120.64	124.45
18	G	201	BCR	C34-C9-C10	-4.14	117.12	122.92
19	B	821	CLA	C4D-CHA-C1A	4.14	126.28	121.25
21	1	314	LUT	C39-C29-C30	-4.14	117.13	122.92
21	2	314	LUT	C39-C29-C30	-4.14	117.13	122.92
22	2	315	XAT	C39-C29-C30	-4.14	117.13	122.92
19	2	308	CLA	CHD-C1D-ND	-4.13	120.66	124.45
19	B	825	CLA	CHD-C1D-ND	-4.13	120.66	124.45
22	2	315	XAT	C15-C35-C34	4.13	131.93	123.47
19	A	803	CLA	CHD-C1D-ND	-4.12	120.67	124.45
18	1	316	BCR	C37-C22-C21	-4.12	117.15	122.92
18	1	316	BCR	C15-C16-C17	4.12	131.91	123.47
21	3	313	LUT	C39-C29-C30	-4.12	117.16	122.92
18	B	846	BCR	C34-C9-C10	-4.11	117.16	122.92
21	4	316	LUT	C19-C9-C10	-4.11	117.16	122.92
22	1	315	XAT	C39-C29-C30	-4.11	117.16	122.92
18	L	305	BCR	C34-C9-C10	-4.11	117.16	122.92
19	2	307	CLA	CHD-C1D-ND	-4.11	120.68	124.45
18	A	846	BCR	C37-C22-C21	-4.10	117.19	122.92
18	4	318	BCR	C34-C9-C10	-4.09	117.19	122.92
18	O	105	BCR	C34-C9-C10	-4.09	117.19	122.92
19	A	805	CLA	CHD-C1D-ND	-4.09	120.69	124.45
19	F	306	CLA	CHD-C1D-ND	-4.09	120.69	124.45
18	L	306	BCR	C37-C22-C21	-4.09	117.19	122.92
18	B	844	BCR	C34-C9-C10	-4.09	117.19	122.92
18	B	842	BCR	C37-C22-C21	-4.09	117.20	122.92
18	A	847	BCR	C37-C22-C21	-4.08	117.20	122.92
21	3	313	LUT	C19-C9-C10	-4.08	117.21	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	844	BCR	C34-C9-C10	-4.08	117.21	122.92
19	B	818	CLA	C4D-CHA-C1A	4.08	126.21	121.25
18	A	844	BCR	C16-C15-C14	4.08	131.83	123.47
18	3	315	BCR	C34-C9-C10	-4.07	117.22	122.92
19	4	309	CLA	C4D-CHA-C1A	4.07	126.20	121.25
19	3	303	CLA	CHD-C1D-ND	-4.07	120.71	124.45
18	B	842	BCR	C34-C9-C10	-4.07	117.22	122.92
18	A	848	BCR	C37-C22-C21	-4.07	117.23	122.92
18	F	304	BCR	C34-C9-C10	-4.06	117.23	122.92
18	3	315	BCR	C37-C22-C21	-4.06	117.24	122.92
18	K	304	BCR	C34-C9-C10	-4.06	117.24	122.92
19	A	836	CLA	CHD-C1D-ND	-4.05	120.73	124.45
18	L	301	BCR	C34-C9-C10	-4.05	117.25	122.92
22	1	315	XAT	C19-C9-C10	-4.04	117.26	122.92
18	L	301	BCR	C37-C22-C21	-4.04	117.26	122.92
18	A	848	BCR	C34-C9-C10	-4.04	117.27	122.92
19	A	816	CLA	CHD-C1D-ND	-4.03	120.75	124.45
18	B	845	BCR	C37-C22-C21	-4.03	117.28	122.92
22	4	317	XAT	C12-C13-C14	4.02	125.12	118.94
19	1	310	CLA	CHD-C1D-ND	-4.02	120.76	124.45
18	B	844	BCR	C15-C16-C17	4.02	131.71	123.47
19	B	816	CLA	C4D-CHA-C1A	4.02	126.14	121.25
19	A	831	CLA	CHD-C1D-ND	-4.02	120.76	124.45
18	A	845	BCR	C37-C22-C21	-4.01	117.30	122.92
21	4	316	LUT	C35-C15-C14	4.01	131.69	123.47
22	3	314	XAT	C39-C29-C30	-4.01	117.31	122.92
19	2	302	CLA	CHD-C1D-ND	-4.01	120.77	124.45
19	A	820	CLA	C4D-CHA-C1A	4.00	126.12	121.25
19	B	817	CLA	CHD-C1D-ND	-4.00	120.78	124.45
18	F	308	BCR	C37-C22-C21	-4.00	117.32	122.92
18	O	105	BCR	C37-C22-C21	-3.99	117.33	122.92
22	4	317	XAT	C20-C13-C14	-3.99	117.33	122.92
19	A	854	CLA	CHD-C1D-ND	-3.99	120.79	124.45
19	B	814	CLA	C4D-CHA-C1A	3.99	126.10	121.25
18	B	844	BCR	C37-C22-C21	-3.99	117.34	122.92
19	A	833	CLA	CHD-C1D-ND	-3.99	120.79	124.45
19	A	833	CLA	C4D-CHA-C1A	3.98	126.09	121.25
22	4	317	XAT	C39-C29-C30	-3.97	117.36	122.92
18	K	301	BCR	C16-C15-C14	3.96	131.60	123.47
19	4	314	CLA	C4D-CHA-C1A	3.96	126.06	121.25
19	A	813	CLA	C4D-CHA-C1A	3.96	126.06	121.25
19	A	818	CLA	C4D-CHA-C1A	3.95	126.06	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	K	301	BCR	C34-C9-C10	-3.94	117.40	122.92
22	4	317	XAT	C40-C33-C34	-3.94	117.40	122.92
18	L	306	BCR	C34-C9-C10	-3.94	117.40	122.92
18	G	206	BCR	C34-C9-C10	-3.94	117.41	122.92
19	3	312	CLA	CHD-C1D-ND	-3.94	120.83	124.45
18	2	316	BCR	C34-C9-C10	-3.94	117.41	122.92
18	B	843	BCR	C16-C15-C14	3.94	131.54	123.47
19	B	834	CLA	CHD-C1D-ND	-3.93	120.84	124.45
20	4	305	CHL	C4D-CHA-C1A	3.93	126.03	121.25
19	B	827	CLA	CHD-C1D-ND	-3.92	120.85	124.45
18	B	843	BCR	C37-C22-C21	-3.92	117.42	122.92
19	2	312	CLA	C4D-CHA-C1A	3.92	126.03	121.25
18	G	201	BCR	C37-C22-C21	-3.92	117.44	122.92
19	B	827	CLA	C4D-CHA-C1A	3.92	126.02	121.25
19	3	311	CLA	C4D-CHA-C1A	3.91	126.01	121.25
18	B	846	BCR	C37-C22-C21	-3.91	117.45	122.92
19	A	835	CLA	CHD-C1D-ND	-3.91	120.86	124.45
18	L	301	BCR	C16-C15-C14	3.90	131.47	123.47
18	J	104	BCR	C34-C9-C10	-3.90	117.46	122.92
19	A	836	CLA	C4D-CHA-C1A	3.88	125.97	121.25
19	4	303	CLA	CHD-C1D-ND	-3.87	120.89	124.45
18	A	846	BCR	C34-C9-C10	-3.87	117.50	122.92
19	B	815	CLA	CHD-C1D-ND	-3.87	120.90	124.45
22	3	314	XAT	C32-C33-C34	3.86	124.87	118.94
19	A	811	CLA	CHD-C1D-ND	-3.86	120.91	124.45
19	B	833	CLA	C4D-CHA-C1A	3.86	125.95	121.25
20	3	306	CHL	CHD-C1D-ND	-3.86	120.91	124.45
19	A	821	CLA	C4D-CHA-C1A	3.86	125.94	121.25
18	K	304	BCR	C16-C15-C14	3.85	131.35	123.47
19	B	824	CLA	CHD-C1D-ND	-3.84	120.93	124.45
18	J	104	BCR	C16-C15-C14	3.84	131.33	123.47
19	3	301	CLA	CHD-C1D-ND	-3.83	120.93	124.45
19	2	312	CLA	CHD-C1D-ND	-3.83	120.93	124.45
19	2	311	CLA	C4D-CHA-C1A	3.82	125.90	121.25
19	A	806	CLA	CHD-C1D-ND	-3.81	120.95	124.45
19	B	808	CLA	CHD-C1D-ND	-3.81	120.95	124.45
19	B	816	CLA	CHD-C1D-ND	-3.81	120.95	124.45
19	B	836	CLA	C4D-CHA-C1A	3.81	125.88	121.25
19	A	830	CLA	CHD-C1D-ND	-3.81	120.95	124.45
19	O	102	CLA	C4D-CHA-C1A	3.81	125.88	121.25
19	L	303	CLA	C4D-CHA-C1A	3.80	125.88	121.25
19	L	304	CLA	C4D-CHA-C1A	3.80	125.88	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	830	CLA	CHD-C1D-ND	-3.79	120.97	124.45
19	A	817	CLA	C4D-CHA-C1A	3.79	125.86	121.25
18	O	106	BCR	C16-C15-C14	3.79	131.24	123.47
19	1	310	CLA	C4D-CHA-C1A	3.79	125.86	121.25
19	3	308	CLA	CHD-C1D-ND	-3.79	120.97	124.45
19	B	819	CLA	CHD-C1D-ND	-3.78	120.98	124.45
19	J	102	CLA	CHD-C1D-ND	-3.78	120.98	124.45
20	2	304	CHL	CHD-C1D-ND	-3.78	120.98	124.45
19	B	839	CLA	C4D-CHA-C1A	3.78	125.85	121.25
19	A	835	CLA	C4D-CHA-C1A	3.78	125.85	121.25
19	B	837	CLA	CHD-C1D-ND	-3.77	120.99	124.45
19	L	302	CLA	C4D-CHA-C1A	3.77	125.84	121.25
18	K	301	BCR	C35-C13-C14	-3.77	117.64	122.92
21	2	314	LUT	C35-C15-C14	3.77	131.20	123.47
19	3	309	CLA	C4D-CHA-C1A	3.76	125.83	121.25
19	1	311	CLA	C4D-CHA-C1A	3.76	125.82	121.25
19	K	302	CLA	CHD-C1D-ND	-3.76	121.00	124.45
19	B	835	CLA	C4D-CHA-C1A	3.76	125.82	121.25
22	1	315	XAT	C35-C15-C14	3.76	131.17	123.47
22	2	315	XAT	C35-C15-C14	3.75	131.15	123.47
19	4	313	CLA	C4D-CHA-C1A	3.74	125.81	121.25
19	A	852	CLA	CHD-C1D-ND	-3.74	121.01	124.45
19	F	306	CLA	C4D-CHA-C1A	3.74	125.80	121.25
19	A	824	CLA	CHD-C1D-ND	-3.74	121.02	124.45
19	B	838	CLA	C4D-CHA-C1A	3.74	125.80	121.25
19	1	312	CLA	C4D-CHA-C1A	3.74	125.80	121.25
19	A	831	CLA	C4D-CHA-C1A	3.74	125.80	121.25
19	3	301	CLA	C4D-CHA-C1A	3.73	125.79	121.25
20	2	319	CHL	C4D-CHA-C1A	3.73	125.79	121.25
20	2	305	CHL	CHD-C1D-ND	-3.73	121.03	124.45
18	4	318	BCR	C36-C18-C17	-3.73	117.70	122.92
19	G	205	CLA	C4D-CHA-C1A	3.72	125.78	121.25
19	B	814	CLA	CHD-C1D-ND	-3.72	121.03	124.45
19	B	819	CLA	C4D-CHA-C1A	3.72	125.78	121.25
19	A	813	CLA	CHD-C1D-ND	-3.72	121.03	124.45
19	4	302	CLA	CHD-C1D-ND	-3.72	121.04	124.45
19	L	303	CLA	CHD-C1D-ND	-3.72	121.04	124.45
20	3	306	CHL	C4D-CHA-C1A	3.71	125.77	121.25
19	A	839	CLA	C4D-CHA-C1A	3.71	125.76	121.25
19	B	818	CLA	CHD-C1D-ND	-3.70	121.05	124.45
19	A	817	CLA	CHD-C1D-ND	-3.70	121.06	124.45
20	2	319	CHL	CHD-C1D-ND	-3.69	121.06	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	822	CLA	CHD-C1D-ND	-3.69	121.06	124.45
22	3	314	XAT	C40-C33-C34	-3.69	117.76	122.92
19	4	312	CLA	C4D-CHA-C1A	3.68	125.73	121.25
18	G	206	BCR	C35-C13-C14	-3.68	117.76	122.92
18	G	206	BCR	C15-C16-C17	3.68	131.02	123.47
19	3	310	CLA	CHD-C1D-ND	-3.67	121.08	124.45
19	A	819	CLA	CHD-C1D-ND	-3.67	121.08	124.45
19	A	814	CLA	CHD-C1D-ND	-3.67	121.08	124.45
19	B	838	CLA	CHD-C1D-ND	-3.67	121.08	124.45
18	O	105	BCR	C16-C15-C14	3.67	130.99	123.47
22	3	314	XAT	C35-C15-C14	3.67	130.99	123.47
19	3	309	CLA	CHD-C1D-ND	-3.67	121.08	124.45
19	1	301	CLA	C4D-CHA-C1A	3.67	125.71	121.25
19	B	837	CLA	C4D-CHA-C1A	3.66	125.71	121.25
18	L	305	BCR	C29-C30-C25	3.66	116.12	110.48
19	B	822	CLA	C4D-CHA-C1A	3.66	125.70	121.25
19	B	807	CLA	C4D-CHA-C1A	3.66	125.70	121.25
19	A	808	CLA	C4D-CHA-C1A	3.66	125.70	121.25
19	1	311	CLA	CHD-C1D-ND	-3.65	121.10	124.45
19	4	314	CLA	CHD-C1D-ND	-3.65	121.10	124.45
20	1	318	CHL	CHD-C1D-ND	-3.65	121.10	124.45
20	4	307	CHL	CHD-C1D-ND	-3.65	121.10	124.45
19	A	850	CLA	CHD-C1D-ND	-3.65	121.10	124.45
19	B	813	CLA	C4D-CHA-C1A	3.65	125.69	121.25
19	L	302	CLA	CHD-C1D-ND	-3.65	121.10	124.45
19	4	312	CLA	CHD-C1D-ND	-3.65	121.10	124.45
18	G	201	BCR	C16-C15-C14	3.64	130.93	123.47
19	B	820	CLA	C4D-CHA-C1A	3.64	125.68	121.25
19	2	301	CLA	C4D-CHA-C1A	3.64	125.67	121.25
18	1	316	BCR	C36-C18-C17	-3.63	117.83	122.92
19	A	830	CLA	C4D-CHA-C1A	3.63	125.67	121.25
18	I	101	BCR	C16-C15-C14	3.63	130.91	123.47
19	A	811	CLA	C4D-CHA-C1A	3.62	125.66	121.25
19	A	837	CLA	C4D-CHA-C1A	3.62	125.66	121.25
19	B	832	CLA	CHD-C1D-ND	-3.62	121.13	124.45
19	4	303	CLA	C4D-CHA-C1A	3.62	125.66	121.25
19	B	840	CLA	C4D-CHA-C1A	3.62	125.66	121.25
18	3	315	BCR	C16-C15-C14	3.62	130.89	123.47
18	K	304	BCR	C15-C16-C17	3.62	130.89	123.47
18	B	843	BCR	C15-C16-C17	3.62	130.89	123.47
18	F	304	BCR	C15-C16-C17	3.62	130.88	123.47
20	4	315	CHL	C4D-CHA-C1A	3.62	125.65	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	811	CLA	CHD-C1D-ND	-3.62	121.13	124.45
18	B	844	BCR	C16-C15-C14	3.61	130.88	123.47
19	3	316	CLA	CHD-C1D-ND	-3.61	121.14	124.45
18	3	315	BCR	C15-C16-C17	3.61	130.86	123.47
19	K	303	CLA	C4D-CHA-C1A	3.61	125.64	121.25
21	4	316	LUT	C20-C13-C14	-3.60	117.88	122.92
19	B	812	CLA	C4D-CHA-C1A	3.60	125.63	121.25
19	J	102	CLA	C4D-CHA-C1A	3.60	125.62	121.25
19	1	302	CLA	CHD-C1D-ND	-3.59	121.15	124.45
19	1	303	CLA	C4D-CHA-C1A	3.59	125.62	121.25
19	B	834	CLA	C4D-CHA-C1A	3.59	125.62	121.25
19	2	301	CLA	CHD-C1D-ND	-3.59	121.16	124.45
18	A	844	BCR	C35-C13-C14	-3.58	117.91	122.92
18	L	305	BCR	C16-C15-C14	3.58	130.81	123.47
18	F	302	BCR	C16-C15-C14	3.58	130.80	123.47
19	B	809	CLA	C4D-CHA-C1A	3.58	125.60	121.25
19	A	822	CLA	C4D-CHA-C1A	3.58	125.60	121.25
19	G	203	CLA	C4D-CHA-C1A	3.58	125.60	121.25
19	B	830	CLA	C4D-CHA-C1A	3.57	125.60	121.25
18	G	201	BCR	C15-C16-C17	3.57	130.79	123.47
21	1	314	LUT	C35-C15-C14	3.57	130.78	123.47
19	A	853	CLA	C4D-CHA-C1A	3.56	125.58	121.25
19	1	312	CLA	CHD-C1D-ND	-3.56	121.18	124.45
19	2	310	CLA	CHD-C1D-ND	-3.56	121.18	124.45
18	J	103	BCR	C35-C13-C14	-3.56	117.94	122.92
19	3	311	CLA	CHD-C1D-ND	-3.55	121.19	124.45
19	A	809	CLA	C4D-CHA-C1A	3.55	125.57	121.25
18	G	201	BCR	C35-C13-C14	-3.55	117.95	122.92
22	3	314	XAT	C20-C13-C14	-3.55	117.95	122.92
20	4	306	CHL	C4D-CHA-C1A	3.55	125.57	121.25
18	A	844	BCR	C1-C6-C5	-3.55	117.61	122.61
19	B	805	CLA	CHD-C1D-ND	-3.54	121.20	124.45
18	B	844	BCR	C35-C13-C14	-3.54	117.96	122.92
20	4	307	CHL	C4D-CHA-C1A	3.54	125.56	121.25
18	B	846	BCR	C35-C13-C14	-3.54	117.96	122.92
18	4	318	BCR	C23-C22-C21	3.54	124.38	118.94
18	F	304	BCR	C35-C13-C14	-3.54	117.97	122.92
19	4	311	CLA	CHD-C1D-ND	-3.54	121.20	124.45
19	3	307	CLA	C4D-CHA-C1A	3.54	125.55	121.25
19	A	801	CLA	CHD-C1D-ND	-3.53	121.21	124.45
18	B	842	BCR	C16-C15-C14	3.53	130.71	123.47
19	A	803	CLA	C4D-CHA-C1A	3.53	125.55	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1	315	XAT	C40-C33-C34	-3.53	117.97	122.92
19	2	303	CLA	CHD-C1D-ND	-3.53	121.21	124.45
19	B	815	CLA	C4D-CHA-C1A	3.53	125.55	121.25
19	O	101	CLA	C4D-CHA-C1A	3.53	125.55	121.25
19	A	819	CLA	C4D-CHA-C1A	3.53	125.55	121.25
20	4	305	CHL	CHD-C1D-ND	-3.53	121.21	124.45
18	2	316	BCR	C16-C15-C14	3.53	130.70	123.47
19	B	810	CLA	CHD-C1D-ND	-3.53	121.21	124.45
18	3	315	BCR	C36-C18-C17	-3.53	117.98	122.92
19	A	810	CLA	C4D-CHA-C1A	3.53	125.54	121.25
19	A	853	CLA	CHD-C1D-ND	-3.51	121.23	124.45
18	F	308	BCR	C16-C15-C14	3.51	130.66	123.47
19	A	814	CLA	C4D-CHA-C1A	3.51	125.52	121.25
18	F	302	BCR	C36-C18-C17	-3.51	118.01	122.92
19	1	303	CLA	CHD-C1D-ND	-3.50	121.23	124.45
19	A	838	CLA	CHD-C1D-ND	-3.50	121.23	124.45
18	B	845	BCR	C36-C18-C17	-3.50	118.02	122.92
18	O	106	BCR	C35-C13-C14	-3.50	118.02	122.92
19	2	309	CLA	C4D-CHA-C1A	3.50	125.51	121.25
20	2	313	CHL	CHD-C1D-ND	-3.50	121.24	124.45
19	B	828	CLA	C4D-CHA-C1A	3.50	125.50	121.25
21	2	314	LUT	C20-C13-C14	-3.50	118.03	122.92
18	1	316	BCR	C16-C15-C14	3.50	130.63	123.47
19	3	304	CLA	C4D-CHA-C1A	3.49	125.50	121.25
19	A	838	CLA	C4D-CHA-C1A	3.49	125.50	121.25
19	1	313	CLA	CHD-C1D-ND	-3.49	121.24	124.45
19	F	307	CLA	C4D-CHA-C1A	3.49	125.50	121.25
19	3	302	CLA	CHD-C1D-ND	-3.49	121.25	124.45
19	2	311	CLA	CHD-C1D-ND	-3.49	121.25	124.45
18	G	206	BCR	C36-C18-C17	-3.49	118.03	122.92
21	3	313	LUT	C40-C33-C34	-3.49	118.04	122.92
19	B	811	CLA	C4D-CHA-C1A	3.49	125.49	121.25
19	3	312	CLA	C4D-CHA-C1A	3.49	125.49	121.25
19	A	834	CLA	C4D-CHA-C1A	3.48	125.49	121.25
19	A	807	CLA	C4D-CHA-C1A	3.48	125.48	121.25
22	2	315	XAT	C20-C13-C14	-3.48	118.06	122.92
18	L	306	BCR	C16-C15-C14	3.47	130.59	123.47
18	K	304	BCR	C36-C18-C17	-3.47	118.06	122.92
18	I	101	BCR	C36-C18-C17	-3.47	118.06	122.92
19	A	824	CLA	C4D-CHA-C1A	3.47	125.47	121.25
18	K	301	BCR	C36-C18-C17	-3.47	118.06	122.92
18	1	316	BCR	C35-C13-C14	-3.47	118.07	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	311	CLA	CHA-C1A-NA	-3.47	118.46	126.40
20	2	305	CHL	C4D-CHA-C1A	3.47	125.47	121.25
19	B	805	CLA	C4D-CHA-C1A	3.46	125.46	121.25
19	A	828	CLA	CHD-C1D-ND	-3.46	121.27	124.45
18	4	318	BCR	C16-C15-C14	3.46	130.56	123.47
18	A	845	BCR	C35-C13-C14	-3.46	118.08	122.92
18	A	847	BCR	C35-C13-C14	-3.46	118.08	122.92
18	O	105	BCR	C15-C16-C17	3.46	130.56	123.47
18	K	304	BCR	C30-C25-C26	-3.46	117.74	122.61
18	J	103	BCR	C16-C15-C14	3.46	130.56	123.47
19	1	304	CLA	C4D-CHA-C1A	3.46	125.46	121.25
19	3	304	CLA	CHD-C1D-ND	-3.46	121.28	124.45
18	B	845	BCR	C35-C13-C14	-3.45	118.09	122.92
19	A	826	CLA	CHD-C1D-ND	-3.45	121.29	124.45
19	A	839	CLA	CHD-C1D-ND	-3.45	121.29	124.45
18	2	316	BCR	C15-C16-C17	3.45	130.53	123.47
18	F	302	BCR	C35-C13-C14	-3.45	118.10	122.92
19	A	820	CLA	CHD-C1D-ND	-3.44	121.29	124.45
19	O	103	CLA	CHD-C1D-ND	-3.44	121.29	124.45
18	F	304	BCR	C36-C18-C17	-3.44	118.11	122.92
19	A	802	CLA	C4D-CHA-C1A	3.44	125.43	121.25
18	4	318	BCR	C35-C13-C14	-3.43	118.11	122.92
21	1	314	LUT	C20-C13-C14	-3.43	118.11	122.92
18	G	201	BCR	C12-C13-C14	3.43	124.21	118.94
18	A	846	BCR	C36-C18-C17	-3.43	118.12	122.92
18	2	316	BCR	C29-C30-C25	3.43	115.76	110.48
19	1	306	CLA	C4D-CHA-C1A	3.43	125.42	121.25
18	3	315	BCR	C35-C13-C14	-3.43	118.12	122.92
19	B	825	CLA	C4D-CHA-C1A	3.43	125.42	121.25
19	3	316	CLA	C4D-CHA-C1A	3.42	125.42	121.25
18	K	304	BCR	C35-C13-C14	-3.42	118.13	122.92
18	I	101	BCR	C15-C16-C17	3.42	130.48	123.47
18	I	101	BCR	C35-C13-C14	-3.42	118.13	122.92
18	B	842	BCR	C35-C13-C14	-3.42	118.14	122.92
19	B	812	CLA	CHD-C1D-ND	-3.42	121.31	124.45
18	L	305	BCR	C15-C16-C17	3.41	130.47	123.47
19	B	813	CLA	CHD-C1D-ND	-3.41	121.32	124.45
18	J	103	BCR	C15-C16-C17	3.41	130.47	123.47
18	K	301	BCR	C12-C13-C14	3.41	124.18	118.94
18	F	302	BCR	C23-C22-C21	3.41	124.17	118.94
19	B	817	CLA	C4D-CHA-C1A	3.41	125.40	121.25
19	A	827	CLA	C4D-CHA-C1A	3.41	125.40	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	4	317	XAT	C35-C15-C14	3.41	130.46	123.47
18	O	106	BCR	C36-C18-C17	-3.41	118.15	122.92
22	1	315	XAT	C20-C13-C14	-3.40	118.16	122.92
19	A	816	CLA	C4D-CHA-C1A	3.40	125.39	121.25
18	B	846	BCR	C36-C18-C17	-3.40	118.16	122.92
18	J	104	BCR	C36-C18-C17	-3.40	118.17	122.92
18	J	103	BCR	C36-C18-C17	-3.39	118.17	122.92
18	G	201	BCR	C36-C18-C17	-3.39	118.17	122.92
18	O	105	BCR	C35-C13-C14	-3.39	118.18	122.92
19	4	310	CLA	CHD-C1D-ND	-3.39	121.34	124.45
18	B	843	BCR	C36-C18-C17	-3.38	118.18	122.92
19	2	303	CLA	C4D-CHA-C1A	3.38	125.36	121.25
22	1	315	XAT	C32-C33-C34	3.38	124.13	118.94
19	B	802	CLA	CHD-C1D-ND	-3.38	121.35	124.45
19	B	810	CLA	C4D-CHA-C1A	3.37	125.36	121.25
18	K	304	BCR	C1-C6-C5	-3.37	117.86	122.61
18	2	316	BCR	C36-C18-C17	-3.37	118.20	122.92
18	O	105	BCR	C36-C18-C17	-3.37	118.20	122.92
18	1	316	BCR	C19-C18-C17	3.37	124.12	118.94
19	1	313	CLA	C4D-CHA-C1A	3.37	125.35	121.25
19	O	103	CLA	C4D-CHA-C1A	3.36	125.34	121.25
19	B	831	CLA	C4D-CHA-C1A	3.36	125.34	121.25
18	G	206	BCR	C16-C15-C14	3.36	130.36	123.47
18	B	846	BCR	C15-C16-C17	3.36	130.35	123.47
19	3	310	CLA	C4D-CHA-C1A	3.36	125.33	121.25
18	J	104	BCR	C29-C30-C25	3.35	115.64	110.48
18	A	845	BCR	C16-C15-C14	3.35	130.34	123.47
18	L	305	BCR	C35-C13-C14	-3.35	118.23	122.92
18	B	844	BCR	C36-C18-C17	-3.35	118.23	122.92
18	L	305	BCR	C36-C18-C17	-3.35	118.23	122.92
18	J	104	BCR	C35-C13-C14	-3.35	118.23	122.92
19	B	801	CLA	C4D-CHA-C1A	3.35	125.32	121.25
19	A	832	CLA	CHD-C1D-ND	-3.34	121.38	124.45
19	B	839	CLA	CHD-C1D-ND	-3.34	121.38	124.45
18	L	301	BCR	C36-C18-C17	-3.34	118.24	122.92
19	A	825	CLA	C4D-CHA-C1A	3.34	125.32	121.25
19	B	840	CLA	CHD-C1D-ND	-3.34	121.38	124.45
21	2	314	LUT	C15-C35-C34	3.34	130.32	123.47
18	L	306	BCR	C35-C13-C14	-3.34	118.25	122.92
18	B	846	BCR	C16-C15-C14	3.34	130.31	123.47
18	2	316	BCR	C35-C13-C14	-3.34	118.25	122.92
19	A	832	CLA	C4D-CHA-C1A	3.33	125.31	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	844	BCR	C12-C13-C14	3.33	124.06	118.94
18	F	304	BCR	C16-C15-C14	3.33	130.29	123.47
18	L	301	BCR	C35-C13-C14	-3.33	118.26	122.92
20	2	304	CHL	C4D-CHA-C1A	3.33	125.30	121.25
19	3	305	CLA	C4D-CHA-C1A	3.32	125.30	121.25
19	2	302	CLA	C4D-CHA-C1A	3.32	125.29	121.25
19	3	303	CLA	C4D-CHA-C1A	3.32	125.29	121.25
19	B	806	CLA	C4D-CHA-C1A	3.32	125.29	121.25
21	3	313	LUT	C20-C13-C14	-3.32	118.27	122.92
18	A	846	BCR	C19-C18-C17	3.32	124.03	118.94
19	B	804	CLA	C4D-CHA-C1A	3.32	125.29	121.25
18	A	847	BCR	C16-C15-C14	3.32	130.27	123.47
19	1	307	CLA	C4D-CHA-C1A	3.31	125.28	121.25
18	B	845	BCR	C15-C16-C17	3.31	130.26	123.47
19	B	804	CLA	CHD-C1D-ND	-3.31	121.41	124.45
18	A	845	BCR	C36-C18-C17	-3.31	118.29	122.92
20	1	305	CHL	C4D-CHA-C1A	3.31	125.27	121.25
21	2	314	LUT	C12-C13-C14	3.30	124.01	118.94
18	A	847	BCR	C36-C18-C17	-3.30	118.30	122.92
18	K	301	BCR	C2-C1-C6	3.30	115.56	110.48
19	A	852	CLA	C4D-CHA-C1A	3.29	125.26	121.25
22	3	314	XAT	C12-C13-C14	3.29	123.99	118.94
19	A	829	CLA	C4D-CHA-C1A	3.29	125.25	121.25
19	B	831	CLA	CHD-C1D-ND	-3.29	121.43	124.45
18	B	842	BCR	C15-C16-C17	3.29	130.21	123.47
18	G	206	BCR	C19-C18-C17	3.28	123.98	118.94
22	1	315	XAT	C15-C35-C34	3.28	130.20	123.47
19	A	834	CLA	CHD-C1D-ND	-3.28	121.44	124.45
19	B	809	CLA	CHD-C1D-ND	-3.28	121.44	124.45
19	A	805	CLA	C4D-CHA-C1A	3.28	125.24	121.25
18	3	315	BCR	C19-C18-C17	3.28	123.97	118.94
18	B	842	BCR	C36-C18-C17	-3.27	118.34	122.92
19	A	837	CLA	CHD-C1D-ND	-3.27	121.45	124.45
21	4	316	LUT	C40-C33-C34	-3.27	118.35	122.92
21	2	314	LUT	C40-C33-C34	-3.27	118.35	122.92
19	1	309	CLA	C4D-CHA-C1A	3.27	125.22	121.25
18	2	316	BCR	C1-C6-C5	-3.26	118.02	122.61
19	3	302	CLA	C4D-CHA-C1A	3.26	125.21	121.25
19	F	307	CLA	CHD-C1D-ND	-3.26	121.46	124.45
19	B	824	CLA	C4D-CHA-C1A	3.25	125.20	121.25
19	A	828	CLA	C4D-CHA-C1A	3.25	125.20	121.25
18	F	302	BCR	C19-C18-C17	3.25	123.92	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	301	CLA	C4D-CHA-C1A	3.25	125.20	121.25
18	O	106	BCR	C12-C13-C14	3.25	123.92	118.94
19	A	854	CLA	C4D-CHA-C1A	3.24	125.20	121.25
19	A	840	CLA	C4D-CHA-C1A	3.24	125.19	121.25
18	K	301	BCR	C15-C16-C17	3.24	130.11	123.47
18	F	308	BCR	C36-C18-C17	-3.24	118.39	122.92
18	G	206	BCR	C12-C13-C14	3.24	123.91	118.94
19	A	826	CLA	C4D-CHA-C1A	3.24	125.19	121.25
20	2	313	CHL	CAA-C2A-C3A	-3.23	106.18	114.26
19	B	806	CLA	CHD-C1D-ND	-3.23	121.48	124.45
21	3	313	LUT	C32-C33-C34	3.23	123.90	118.94
19	A	810	CLA	CHD-C1D-ND	-3.23	121.49	124.45
18	A	846	BCR	C35-C13-C14	-3.23	118.40	122.92
21	1	314	LUT	C40-C33-C34	-3.22	118.41	122.92
19	B	820	CLA	CHD-C1D-ND	-3.22	121.49	124.45
19	B	821	CLA	CHD-C1D-ND	-3.22	121.49	124.45
18	F	304	BCR	C12-C13-C14	3.22	123.88	118.94
18	I	101	BCR	C1-C6-C5	-3.22	118.08	122.61
19	K	302	CLA	C4D-CHA-C1A	3.22	125.17	121.25
18	A	846	BCR	C15-C16-C17	3.22	130.06	123.47
18	I	101	BCR	C12-C13-C14	3.21	123.87	118.94
18	A	848	BCR	C35-C13-C14	-3.21	118.43	122.92
19	A	802	CLA	CHD-C1D-ND	-3.21	121.50	124.45
21	4	316	LUT	C12-C13-C14	3.21	123.86	118.94
19	A	806	CLA	C4D-CHA-C1A	3.21	125.15	121.25
19	B	829	CLA	C4D-CHA-C1A	3.21	125.15	121.25
22	2	315	XAT	C40-C33-C34	-3.20	118.43	122.92
18	F	302	BCR	C12-C13-C14	3.20	123.86	118.94
19	B	803	CLA	C4D-CHA-C1A	3.20	125.15	121.25
19	A	807	CLA	CHD-C1D-ND	-3.20	121.51	124.45
19	3	307	CLA	CHD-C1D-ND	-3.20	121.51	124.45
18	A	844	BCR	C12-C13-C14	3.20	123.85	118.94
18	4	318	BCR	C12-C13-C14	3.20	123.84	118.94
19	A	818	CLA	CHD-C1D-ND	-3.19	121.52	124.45
19	1	307	CLA	CHD-C1D-ND	-3.19	121.52	124.45
19	1	302	CLA	C4D-CHA-C1A	3.19	125.13	121.25
18	B	845	BCR	C16-C15-C14	3.19	130.00	123.47
19	B	807	CLA	CHD-C1D-ND	-3.19	121.53	124.45
19	B	826	CLA	C4D-CHA-C1A	3.18	125.12	121.25
18	K	304	BCR	C19-C18-C17	3.18	123.82	118.94
18	G	201	BCR	C29-C30-C25	3.18	115.37	110.48
19	A	823	CLA	CHD-C1D-ND	-3.16	121.55	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	825	CLA	CHD-C1D-ND	-3.16	121.55	124.45
20	2	306	CHL	CHD-C1D-ND	-3.16	121.55	124.45
19	K	303	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	A	847	BCR	C15-C16-C17	3.16	129.94	123.47
18	B	842	BCR	C12-C13-C14	3.16	123.78	118.94
19	G	204	CLA	CHD-C1D-ND	-3.15	121.56	124.45
18	B	843	BCR	C35-C13-C14	-3.15	118.51	122.92
18	3	315	BCR	C12-C13-C14	3.15	123.77	118.94
20	4	315	CHL	CHD-C1D-ND	-3.14	121.56	124.45
18	F	304	BCR	C2-C1-C6	3.14	115.32	110.48
19	A	804	CLA	C4D-CHA-C1A	3.14	125.07	121.25
19	L	304	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	A	815	CLA	CHD-C1D-ND	-3.14	121.57	124.45
20	1	318	CHL	C4D-CHA-C1A	3.14	125.07	121.25
18	K	304	BCR	C12-C13-C14	3.14	123.76	118.94
18	O	106	BCR	C30-C25-C26	-3.14	118.20	122.61
19	O	101	CLA	CHD-C1D-ND	-3.14	121.57	124.45
18	K	301	BCR	C19-C18-C17	3.14	123.75	118.94
18	J	104	BCR	C15-C16-C17	3.13	129.90	123.47
18	L	306	BCR	C36-C18-C17	-3.13	118.53	122.92
19	4	301	CLA	CHD-C1D-ND	-3.13	121.58	124.45
18	1	316	BCR	C12-C13-C14	3.13	123.75	118.94
18	B	845	BCR	C19-C18-C17	3.13	123.74	118.94
18	F	304	BCR	C19-C18-C17	3.13	123.74	118.94
18	G	201	BCR	C19-C18-C17	3.12	123.73	118.94
18	B	844	BCR	C19-C18-C17	3.12	123.73	118.94
20	4	305	CHL	C4A-NA-C1A	3.12	108.11	106.71
21	1	314	LUT	C15-C35-C34	3.12	129.86	123.47
18	B	843	BCR	C19-C18-C17	3.12	123.72	118.94
21	4	316	LUT	C15-C35-C34	3.11	129.84	123.47
18	F	308	BCR	C35-C13-C14	-3.11	118.57	122.92
22	4	317	XAT	C8-C9-C10	3.11	123.71	118.94
19	B	823	CLA	C4D-CHA-C1A	3.10	125.03	121.25
19	A	829	CLA	CHD-C1D-ND	-3.10	121.61	124.45
18	A	844	BCR	C36-C18-C17	-3.10	118.59	122.92
18	A	845	BCR	C12-C13-C14	3.09	123.69	118.94
19	1	306	CLA	CHD-C1D-ND	-3.09	121.61	124.45
19	4	310	CLA	CHA-C1A-NA	-3.09	119.31	126.40
22	2	315	XAT	C12-C13-C14	3.09	123.69	118.94
18	F	308	BCR	C15-C16-C17	3.09	129.80	123.47
18	O	105	BCR	C12-C13-C14	3.09	123.68	118.94
19	B	828	CLA	CHD-C1D-ND	-3.09	121.62	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	801	CLA	CHA-C1A-NA	-3.09	119.33	126.40
18	B	846	BCR	C12-C13-C14	3.09	123.67	118.94
21	4	316	LUT	C32-C33-C34	3.08	123.67	118.94
19	A	823	CLA	C4D-CHA-C1A	3.08	125.00	121.25
18	B	843	BCR	C8-C9-C10	3.08	123.67	118.94
20	2	306	CHL	C4D-CHA-C1A	3.07	124.98	121.25
18	B	845	BCR	C12-C13-C14	3.06	123.64	118.94
18	O	105	BCR	C19-C18-C17	3.06	123.64	118.94
22	2	315	XAT	C32-C33-C34	3.06	123.64	118.94
18	4	318	BCR	C19-C18-C17	3.06	123.64	118.94
18	J	103	BCR	C19-C18-C17	3.05	123.63	118.94
18	J	103	BCR	C12-C13-C14	3.05	123.62	118.94
18	A	848	BCR	C16-C15-C14	3.04	129.71	123.47
18	B	846	BCR	C19-C18-C17	3.04	123.61	118.94
18	O	106	BCR	C19-C18-C17	3.03	123.60	118.94
29	B	847	DGD	C2G-O2G-C1B	-3.03	110.33	117.79
18	A	846	BCR	C16-C15-C14	3.03	129.68	123.47
18	L	305	BCR	C12-C13-C14	3.03	123.59	118.94
19	B	823	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	L	306	BCR	C12-C13-C14	3.02	123.57	118.94
18	J	104	BCR	C19-C18-C17	3.02	123.57	118.94
19	A	804	CLA	CHD-C1D-ND	-3.01	121.69	124.45
21	3	313	LUT	C35-C15-C14	3.01	129.65	123.47
18	A	848	BCR	C36-C18-C17	-3.01	118.70	122.92
21	1	314	LUT	C12-C13-C14	3.01	123.56	118.94
18	L	301	BCR	C12-C13-C14	3.00	123.55	118.94
18	L	305	BCR	C19-C18-C17	3.00	123.54	118.94
19	1	308	CLA	C4D-CHA-C1A	3.00	124.89	121.25
18	I	101	BCR	C19-C18-C17	2.99	123.54	118.94
21	3	313	LUT	C12-C13-C14	2.99	123.53	118.94
18	J	104	BCR	C12-C13-C14	2.98	123.52	118.94
20	2	313	CHL	CHA-C1A-NA	-2.98	119.56	126.40
22	4	317	XAT	C15-C35-C34	2.98	129.57	123.47
19	A	840	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	3	305	CLA	CHD-C1D-ND	-2.97	121.72	124.45
21	1	314	LUT	C32-C33-C34	2.97	123.49	118.94
18	A	847	BCR	C12-C13-C14	2.96	123.49	118.94
19	3	308	CLA	C4D-CHA-C1A	2.96	124.85	121.25
18	A	847	BCR	C19-C18-C17	2.96	123.48	118.94
19	2	310	CLA	CHA-C1A-NA	-2.96	119.63	126.40
18	K	304	BCR	C23-C22-C21	2.96	123.48	118.94
18	A	848	BCR	C19-C18-C17	2.95	123.47	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	301	BCR	C19-C18-C17	2.95	123.47	118.94
19	G	204	CLA	C4D-CHA-C1A	2.95	124.83	121.25
18	B	842	BCR	C19-C18-C17	2.94	123.46	118.94
21	2	314	LUT	C32-C33-C34	2.94	123.46	118.94
19	2	307	CLA	C1D-ND-C4D	2.94	108.42	106.33
22	1	315	XAT	C12-C13-C14	2.93	123.44	118.94
19	B	835	CLA	CHD-C1D-ND	-2.93	121.76	124.45
18	G	206	BCR	C2-C1-C6	2.92	114.98	110.48
19	2	309	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	2	311	CLA	C4A-NA-C1A	2.91	108.02	106.71
18	A	845	BCR	C15-C16-C17	2.91	129.44	123.47
19	4	304	CLA	C4D-CHA-C1A	2.91	124.79	121.25
19	A	827	CLA	CHD-C1D-ND	-2.90	121.79	124.45
19	B	827	CLA	C1D-ND-C4D	2.90	108.39	106.33
21	4	316	LUT	C28-C29-C30	2.89	123.38	118.94
18	A	848	BCR	C12-C13-C14	2.89	123.38	118.94
19	2	310	CLA	C4D-CHA-C1A	2.89	124.77	121.25
19	B	808	CLA	C4D-CHA-C1A	2.88	124.75	121.25
18	G	206	BCR	C23-C22-C21	2.87	123.35	118.94
21	4	316	LUT	C8-C9-C10	2.87	123.34	118.94
19	A	850	CLA	CHA-C1A-NA	-2.87	119.83	126.40
19	O	103	CLA	CHA-C1A-NA	-2.87	119.84	126.40
20	2	306	CHL	CHA-C1A-NA	-2.86	119.84	126.40
18	2	316	BCR	C12-C13-C14	2.86	123.34	118.94
19	B	827	CLA	CHA-C1A-NA	-2.85	119.87	126.40
18	F	308	BCR	C19-C18-C17	2.85	123.31	118.94
18	A	846	BCR	C23-C22-C21	2.84	123.30	118.94
18	A	845	BCR	C19-C18-C17	2.84	123.29	118.94
18	A	844	BCR	C8-C9-C10	2.83	123.29	118.94
19	A	823	CLA	CHA-C1A-NA	-2.83	119.91	126.40
18	L	306	BCR	C15-C16-C17	2.83	129.26	123.47
19	2	311	CLA	CHA-C1A-NA	-2.83	119.93	126.40
19	A	853	CLA	CHA-C1A-NA	-2.83	119.93	126.40
19	B	824	CLA	CHA-C1A-NA	-2.82	119.93	126.40
19	O	104	CLA	CHA-C1A-NA	-2.82	119.93	126.40
19	1	308	CLA	CHA-C1A-NA	-2.82	119.93	126.40
19	A	807	CLA	CHA-C1A-NA	-2.82	119.94	126.40
21	3	313	LUT	C28-C29-C30	2.82	123.27	118.94
20	2	305	CHL	CHA-C1A-NA	-2.82	119.94	126.40
19	4	308	CLA	CHA-C1A-NA	-2.82	119.94	126.40
19	3	305	CLA	CHA-C1A-NA	-2.81	119.96	126.40
18	K	301	BCR	C23-C22-C21	2.81	123.25	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	302	CLA	C4D-CHA-C1A	2.81	124.67	121.25
19	B	826	CLA	CHA-C1A-NA	-2.80	119.98	126.40
19	B	837	CLA	CHA-C1A-NA	-2.80	119.98	126.40
19	B	823	CLA	CHA-C1A-NA	-2.80	119.98	126.40
20	4	306	CHL	CHA-C1A-NA	-2.80	119.99	126.40
19	L	304	CLA	CHA-C1A-NA	-2.80	120.00	126.40
19	K	303	CLA	CHA-C1A-NA	-2.79	120.00	126.40
19	B	831	CLA	CHA-C1A-NA	-2.79	120.01	126.40
19	A	818	CLA	CHA-C1A-NA	-2.79	120.01	126.40
18	2	316	BCR	C19-C18-C17	2.79	123.22	118.94
19	2	303	CLA	CHA-C1A-NA	-2.79	120.01	126.40
19	1	307	CLA	CHA-C1A-NA	-2.78	120.02	126.40
19	A	827	CLA	CHA-C1A-NA	-2.78	120.02	126.40
19	1	304	CLA	CHD-C1D-ND	-2.78	121.90	124.45
18	A	846	BCR	C8-C9-C10	2.78	123.21	118.94
18	A	848	BCR	C1-C6-C5	-2.78	118.69	122.61
19	1	304	CLA	CHA-C1A-NA	-2.78	120.04	126.40
20	4	305	CHL	CHA-C1A-NA	-2.77	120.05	126.40
19	3	310	CLA	CHA-C1A-NA	-2.77	120.06	126.40
19	A	833	CLA	CHA-C1A-NA	-2.77	120.06	126.40
19	A	802	CLA	CHA-C1A-NA	-2.77	120.06	126.40
19	B	850	CLA	CHA-C1A-NA	-2.76	120.07	126.40
19	B	838	CLA	CHA-C1A-NA	-2.76	120.07	126.40
18	A	846	BCR	C12-C13-C14	2.76	123.18	118.94
19	B	828	CLA	CHA-C1A-NA	-2.76	120.08	126.40
19	1	306	CLA	CHA-C1A-NA	-2.75	120.09	126.40
19	4	312	CLA	CHA-C1A-NA	-2.75	120.09	126.40
19	B	815	CLA	CHA-C1A-NA	-2.75	120.10	126.40
19	4	309	CLA	CHA-C1A-NA	-2.75	120.11	126.40
19	2	308	CLA	C3B-C4B-NB	-2.75	107.97	110.52
19	B	834	CLA	CHA-C1A-NA	-2.75	120.11	126.40
19	4	308	CLA	CHD-C1D-ND	-2.74	121.93	124.45
19	B	802	CLA	CHA-C1A-NA	-2.74	120.12	126.40
19	L	302	CLA	CHA-C1A-NA	-2.74	120.12	126.40
19	A	810	CLA	CHA-C1A-NA	-2.74	120.12	126.40
19	2	308	CLA	CHA-C1A-NA	-2.74	120.12	126.40
18	B	843	BCR	C12-C13-C14	2.74	123.14	118.94
19	A	826	CLA	CHA-C1A-NA	-2.74	120.12	126.40
19	A	813	CLA	CHA-C1A-NA	-2.73	120.14	126.40
20	2	304	CHL	CHA-C1A-NA	-2.73	120.14	126.40
19	3	316	CLA	CHA-C1A-NA	-2.73	120.14	126.40
19	3	302	CLA	CHA-C1A-NA	-2.73	120.14	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	304	CLA	CHA-C1A-NA	-2.73	120.15	126.40
19	4	308	CLA	C4D-CHA-C1A	2.73	124.57	121.25
19	1	309	CLA	CHA-C1A-NA	-2.73	120.15	126.40
19	O	104	CLA	C4D-CHA-C1A	2.73	124.57	121.25
20	4	307	CHL	CHA-C1A-NA	-2.73	120.16	126.40
20	1	305	CHL	CHD-C1D-C2D	2.72	131.19	125.48
19	A	804	CLA	CHA-C1A-NA	-2.72	120.17	126.40
19	A	829	CLA	CHA-C1A-NA	-2.72	120.18	126.40
19	2	312	CLA	CHA-C1A-NA	-2.71	120.18	126.40
18	O	106	BCR	C23-C22-C21	2.71	123.10	118.94
19	3	308	CLA	CHA-C1A-NA	-2.71	120.19	126.40
19	A	840	CLA	CHA-C1A-NA	-2.71	120.19	126.40
18	I	101	BCR	C8-C9-C10	2.71	123.10	118.94
19	B	822	CLA	CHA-C1A-NA	-2.71	120.19	126.40
19	A	821	CLA	CHA-C1A-NA	-2.71	120.20	126.40
19	B	807	CLA	CHA-C1A-NA	-2.71	120.20	126.40
19	A	838	CLA	CHA-C1A-NA	-2.70	120.20	126.40
19	O	102	CLA	CHA-C1A-NA	-2.70	120.21	126.40
18	F	302	BCR	C8-C9-C10	2.70	123.08	118.94
19	A	809	CLA	CHA-C1A-NA	-2.70	120.22	126.40
19	A	836	CLA	CHA-C1A-NA	-2.70	120.22	126.40
20	2	319	CHL	CHA-C1A-NA	-2.70	120.23	126.40
19	G	203	CLA	CHA-C1A-NA	-2.69	120.23	126.40
20	1	305	CHL	CHA-C1A-NA	-2.69	120.23	126.40
19	3	311	CLA	CHA-C1A-NA	-2.69	120.23	126.40
19	A	805	CLA	CHA-C1A-NA	-2.69	120.23	126.40
19	A	832	CLA	CHA-C1A-NA	-2.69	120.24	126.40
19	A	825	CLA	CHA-C1A-NA	-2.69	120.24	126.40
20	1	318	CHL	CHA-C1A-NA	-2.69	120.25	126.40
19	A	834	CLA	CHA-C1A-NA	-2.68	120.25	126.40
19	1	309	CLA	CHD-C1D-ND	-2.68	121.99	124.45
19	4	302	CLA	CHA-C1A-NA	-2.68	120.25	126.40
20	4	315	CHL	CHA-C1A-NA	-2.68	120.25	126.40
19	B	809	CLA	CHA-C1A-NA	-2.68	120.25	126.40
19	B	817	CLA	CHA-C1A-NA	-2.68	120.26	126.40
18	L	306	BCR	C19-C18-C17	2.68	123.06	118.94
19	B	840	CLA	CHA-C1A-NA	-2.68	120.26	126.40
19	B	839	CLA	C4A-NA-C1A	2.68	107.91	106.71
19	B	812	CLA	CHA-C1A-NA	-2.68	120.26	126.40
19	B	818	CLA	CHA-C1A-NA	-2.68	120.26	126.40
19	B	801	CLA	CHA-C1A-NA	-2.68	120.26	126.40
20	3	306	CHL	CHA-C1A-NA	-2.68	120.26	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	302	CLA	CHA-C1A-NA	-2.68	120.26	126.40
18	B	845	BCR	C23-C22-C21	2.68	123.05	118.94
19	2	301	CLA	CHA-C1A-NA	-2.68	120.27	126.40
19	B	811	CLA	CHA-C1A-NA	-2.67	120.28	126.40
19	A	839	CLA	CHA-C1A-NA	-2.67	120.28	126.40
19	B	803	CLA	CHA-C1A-NA	-2.67	120.28	126.40
18	A	844	BCR	C19-C18-C17	2.67	123.04	118.94
19	2	302	CLA	CHA-C1A-NA	-2.67	120.29	126.40
19	1	311	CLA	CHA-C1A-NA	-2.67	120.29	126.40
22	4	317	XAT	C28-C29-C30	2.67	123.03	118.94
19	B	806	CLA	CHA-C1A-NA	-2.66	120.30	126.40
19	B	821	CLA	CHA-C1A-NA	-2.66	120.30	126.40
19	B	832	CLA	CHA-C1A-NA	-2.66	120.30	126.40
19	B	835	CLA	CHA-C1A-NA	-2.66	120.30	126.40
19	1	303	CLA	CHA-C1A-NA	-2.66	120.30	126.40
19	4	303	CLA	CHA-C1A-NA	-2.66	120.30	126.40
19	2	309	CLA	CHA-C1A-NA	-2.66	120.31	126.40
19	4	314	CLA	CHA-C1A-NA	-2.65	120.32	126.40
19	A	815	CLA	C4D-CHA-C1A	2.65	124.48	121.25
19	4	310	CLA	C1D-ND-C4D	2.65	108.22	106.33
19	B	819	CLA	CHA-C1A-NA	-2.65	120.33	126.40
20	2	313	CHL	C4D-CHA-C1A	2.65	124.48	121.25
19	O	104	CLA	CHD-C1D-C2D	2.65	131.04	125.48
19	A	822	CLA	CHA-C1A-NA	-2.65	120.33	126.40
19	A	814	CLA	CHA-C1A-NA	-2.65	120.33	126.40
18	O	106	BCR	C8-C9-C10	2.65	123.00	118.94
19	A	816	CLA	CHA-C1A-NA	-2.65	120.34	126.40
19	4	301	CLA	CHA-C1A-NA	-2.65	120.34	126.40
20	4	307	CHL	C4A-NA-C1A	2.64	107.89	106.71
18	I	101	BCR	C23-C22-C21	2.64	123.00	118.94
19	A	837	CLA	CHA-C1A-NA	-2.64	120.34	126.40
19	J	102	CLA	CHA-C1A-NA	-2.64	120.35	126.40
19	3	307	CLA	CHA-C1A-NA	-2.64	120.36	126.40
19	B	820	CLA	CHA-C1A-NA	-2.64	120.36	126.40
19	B	816	CLA	CHA-C1A-NA	-2.63	120.36	126.40
19	3	303	CLA	CHA-C1A-NA	-2.63	120.37	126.40
19	A	852	CLA	CHA-C1A-NA	-2.63	120.37	126.40
18	J	103	BCR	C8-C9-C10	2.63	122.98	118.94
19	A	820	CLA	CHA-C1A-NA	-2.63	120.37	126.40
19	L	303	CLA	CHA-C1A-NA	-2.63	120.38	126.40
19	A	815	CLA	CHA-C1A-NA	-2.63	120.38	126.40
22	4	317	XAT	C30-C31-C32	2.63	131.42	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	813	CLA	CHA-C1A-NA	-2.63	120.38	126.40
19	1	312	CLA	CHA-C1A-NA	-2.62	120.39	126.40
18	2	316	BCR	C23-C22-C21	2.62	122.97	118.94
19	B	839	CLA	CHA-C1A-NA	-2.62	120.40	126.40
19	B	804	CLA	CHA-C1A-NA	-2.61	120.41	126.40
19	4	311	CLA	C2A-C1A-CHA	2.61	128.43	123.86
19	G	205	CLA	CHA-C1A-NA	-2.61	120.42	126.40
19	A	836	CLA	C4A-NA-C1A	2.61	107.88	106.71
19	4	313	CLA	CHA-C1A-NA	-2.61	120.42	126.40
19	A	817	CLA	CHA-C1A-NA	-2.61	120.42	126.40
19	A	819	CLA	CHA-C1A-NA	-2.60	120.44	126.40
19	F	306	CLA	CHA-C1A-NA	-2.60	120.44	126.40
19	B	826	CLA	CHD-C1D-ND	-2.60	122.06	124.45
18	B	845	BCR	C8-C9-C10	2.60	122.94	118.94
18	G	201	BCR	C8-C9-C10	2.60	122.94	118.94
19	A	828	CLA	CHA-C1A-NA	-2.60	120.44	126.40
18	L	301	BCR	C15-C16-C17	2.60	128.81	123.47
19	1	302	CLA	CHA-C1A-NA	-2.60	120.45	126.40
19	B	833	CLA	CHA-C1A-NA	-2.60	120.45	126.40
19	1	313	CLA	CHA-C1A-NA	-2.59	120.46	126.40
19	4	311	CLA	CHB-C1B-NB	-2.59	121.51	124.26
19	A	830	CLA	CHA-C1A-NA	-2.59	120.47	126.40
19	F	307	CLA	CHA-C1A-NA	-2.59	120.47	126.40
19	G	204	CLA	CHA-C1A-NA	-2.59	120.47	126.40
19	A	835	CLA	CHA-C1A-NA	-2.59	120.47	126.40
19	A	811	CLA	CHA-C1A-NA	-2.59	120.47	126.40
18	J	103	BCR	C23-C22-C21	2.59	122.91	118.94
19	B	830	CLA	CHA-C1A-NA	-2.58	120.48	126.40
18	J	104	BCR	C23-C22-C21	2.58	122.91	118.94
19	B	829	CLA	CHA-C1A-NA	-2.58	120.48	126.40
19	B	805	CLA	CHA-C1A-NA	-2.58	120.49	126.40
19	3	312	CLA	CHA-C1A-NA	-2.57	120.50	126.40
19	4	312	CLA	C4A-NA-C1A	2.57	107.86	106.71
19	4	309	CLA	CHD-C1D-C2D	2.57	130.87	125.48
19	1	311	CLA	C4A-NA-C1A	2.57	107.86	106.71
19	4	304	CLA	CHA-C1A-NA	-2.57	120.52	126.40
19	B	825	CLA	CHA-C1A-NA	-2.56	120.52	126.40
19	3	309	CLA	CHA-C1A-NA	-2.56	120.53	126.40
18	L	306	BCR	C23-C22-C21	2.56	122.87	118.94
19	A	808	CLA	CHA-C1A-NA	-2.56	120.54	126.40
19	2	308	CLA	C4D-CHA-C1A	2.56	124.36	121.25
19	A	806	CLA	CHA-C1A-NA	-2.56	120.54	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	3	313	LUT	C8-C9-C10	2.56	122.87	118.94
19	A	854	CLA	CHA-C1A-NA	-2.55	120.55	126.40
19	B	808	CLA	CHA-C1A-NA	-2.55	120.56	126.40
18	L	305	BCR	C8-C9-C10	2.55	122.85	118.94
18	B	844	BCR	C8-C9-C10	2.55	122.85	118.94
18	L	305	BCR	C23-C22-C21	2.55	122.85	118.94
19	3	301	CLA	CHA-C1A-NA	-2.54	120.58	126.40
19	A	812	CLA	CHA-C1A-NA	-2.54	120.58	126.40
19	1	301	CLA	CHA-C1A-NA	-2.53	120.60	126.40
19	B	814	CLA	CHA-C1A-NA	-2.53	120.60	126.40
18	F	308	BCR	C12-C13-C14	2.53	122.82	118.94
21	2	314	LUT	C28-C29-C30	2.52	122.81	118.94
19	O	101	CLA	CHA-C1A-NA	-2.52	120.62	126.40
18	A	844	BCR	C15-C16-C17	2.52	128.64	123.47
22	3	314	XAT	C8-C9-C10	2.52	122.81	118.94
19	B	829	CLA	CHD-C1D-C2D	2.52	130.76	125.48
18	1	316	BCR	C29-C30-C25	2.51	114.35	110.48
19	A	824	CLA	CHA-C1A-NA	-2.51	120.65	126.40
19	3	310	CLA	C4A-NA-C1A	2.51	107.83	106.71
18	1	316	BCR	C8-C9-C10	2.51	122.79	118.94
19	1	310	CLA	CHA-C1A-NA	-2.51	120.66	126.40
19	B	850	CLA	CHD-C1D-C2D	2.50	130.72	125.48
19	B	836	CLA	CHA-C1A-NA	-2.50	120.68	126.40
19	2	307	CLA	CHD-C1D-C2D	2.49	130.71	125.48
19	B	836	CLA	CHD-C1D-C2D	2.49	130.70	125.48
19	L	302	CLA	C4A-NA-C1A	2.48	107.82	106.71
19	A	803	CLA	CHA-C1A-NA	-2.48	120.71	126.40
18	1	316	BCR	C23-C22-C21	2.48	122.75	118.94
22	1	315	XAT	C28-C29-C30	2.48	122.74	118.94
18	B	843	BCR	C30-C25-C26	-2.48	119.12	122.61
18	A	844	BCR	C23-C22-C21	2.47	122.73	118.94
18	B	842	BCR	C8-C9-C10	2.47	122.73	118.94
19	A	831	CLA	CHA-C1A-NA	-2.47	120.75	126.40
18	B	842	BCR	C23-C22-C21	2.46	122.72	118.94
18	F	308	BCR	C8-C9-C10	2.46	122.72	118.94
19	G	205	CLA	CHD-C1D-C2D	2.46	130.64	125.48
22	3	314	XAT	C28-C29-C30	2.46	122.71	118.94
22	2	315	XAT	C28-C29-C30	2.46	122.71	118.94
22	2	315	XAT	C8-C9-C10	2.46	122.71	118.94
29	B	847	DGD	O1G-C1A-C2A	2.46	119.61	111.91
18	G	206	BCR	C8-C9-C10	2.45	122.70	118.94
19	4	310	CLA	C4A-NA-C1A	2.45	107.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	812	CLA	CHD-C1D-C2D	2.45	130.61	125.48
19	4	302	CLA	C3B-C4B-NB	-2.45	108.25	110.52
21	1	314	LUT	C28-C29-C30	2.44	122.69	118.94
19	2	310	CLA	C2A-C1A-CHA	2.44	128.12	123.86
19	B	810	CLA	CHA-C1A-NA	-2.44	120.82	126.40
19	2	307	CLA	CHA-C1A-NA	-2.43	120.83	126.40
19	A	801	CLA	C2A-C1A-CHA	2.43	128.11	123.86
19	A	809	CLA	CHD-C1D-C2D	2.42	130.56	125.48
20	4	306	CHL	C4A-NA-C1A	2.42	107.80	106.71
20	4	315	CHL	C2C-C3C-C4C	2.42	108.22	106.49
20	2	304	CHL	C2C-C3C-C4C	2.42	108.21	106.49
19	A	808	CLA	CHD-C1D-C2D	2.41	130.54	125.48
19	B	817	CLA	CHD-C1D-C2D	2.41	130.54	125.48
19	A	850	CLA	C4D-CHA-C1A	2.41	124.18	121.25
19	A	801	CLA	C4D-CHA-C1A	2.40	124.17	121.25
19	A	816	CLA	CHD-C1D-C2D	2.40	130.50	125.48
19	A	825	CLA	C4A-NA-C1A	2.39	107.78	106.71
19	A	826	CLA	C1D-ND-C4D	2.39	108.03	106.33
22	4	317	XAT	C5-C4-C3	-2.39	108.03	112.75
18	4	318	BCR	C1-C6-C5	-2.38	119.27	122.61
19	B	832	CLA	C1D-ND-C4D	2.37	108.02	106.33
19	A	813	CLA	C4A-NA-C1A	2.37	107.77	106.71
19	B	816	CLA	C4A-NA-C1A	2.37	107.77	106.71
19	A	835	CLA	CHD-C1D-C2D	2.37	130.45	125.48
22	4	317	XAT	C10-C11-C12	2.37	130.60	123.22
18	3	315	BCR	C8-C9-C10	2.36	122.57	118.94
19	B	827	CLA	CHD-C1D-C2D	2.36	130.43	125.48
19	K	302	CLA	CMD-C2D-C1D	2.36	128.87	124.71
18	B	843	BCR	C23-C22-C21	2.36	122.56	118.94
19	G	203	CLA	CHD-C1D-C2D	2.35	130.42	125.48
18	A	845	BCR	C30-C25-C26	-2.35	119.30	122.61
19	A	854	CLA	CHD-C1D-C2D	2.35	130.41	125.48
18	I	101	BCR	C30-C25-C26	-2.35	119.31	122.61
19	A	821	CLA	CHD-C1D-C2D	2.35	130.41	125.48
19	B	817	CLA	C1D-ND-C4D	2.35	108.00	106.33
19	4	310	CLA	C4D-CHA-C1A	2.35	124.10	121.25
19	A	818	CLA	C4A-NA-C1A	2.34	107.76	106.71
19	O	102	CLA	CHD-C1D-C2D	2.34	130.40	125.48
20	4	306	CHL	CHD-C1D-C2D	2.34	130.38	125.48
19	1	301	CLA	CHD-C1D-C2D	2.34	130.38	125.48
19	4	304	CLA	CHD-C1D-C2D	2.33	130.37	125.48
20	4	307	CHL	C2C-C3C-C4C	2.32	108.15	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	B	833	CLA	CHD-C1D-C2D	2.32	130.35	125.48
19	2	308	CLA	CHC-C4B-NB	-2.32	121.80	124.26
19	B	803	CLA	CHD-C1D-C2D	2.32	130.34	125.48
18	B	842	BCR	C1-C6-C5	-2.31	119.35	122.61
19	A	835	CLA	C1D-ND-C4D	2.31	107.98	106.33
18	A	848	BCR	C8-C9-C10	2.31	122.48	118.94
19	2	310	CLA	CAA-C2A-C1A	2.31	119.53	111.97
18	A	844	BCR	C29-C30-C25	2.30	114.03	110.48
18	4	318	BCR	C29-C30-C25	2.30	114.02	110.48
19	B	832	CLA	C4A-NA-C1A	2.30	107.74	106.71
19	4	313	CLA	CHD-C1D-C2D	2.30	130.30	125.48
19	A	836	CLA	CHD-C1D-C2D	2.30	130.30	125.48
19	B	801	CLA	CHD-C1D-C2D	2.29	130.29	125.48
19	B	825	CLA	CHD-C1D-C2D	2.28	130.27	125.48
19	2	302	CLA	CHD-C1D-C2D	2.28	130.27	125.48
19	B	850	CLA	C4A-NA-C1A	2.28	107.73	106.71
26	B	841	PQN	C11-C3-C4	-2.27	116.07	118.50
19	B	821	CLA	C4A-NA-C1A	2.27	107.73	106.71
19	A	831	CLA	CHD-C1D-C2D	2.27	130.24	125.48
20	1	305	CHL	C2C-C3C-C4C	2.27	108.11	106.49
20	2	313	CHL	C2C-C3C-C4C	2.27	108.11	106.49
19	A	803	CLA	CHD-C1D-C2D	2.26	130.23	125.48
19	B	824	CLA	CHD-C1D-C2D	2.26	130.21	125.48
18	B	846	BCR	C8-C9-C10	2.26	122.40	118.94
19	B	834	CLA	CHD-C1D-C2D	2.26	130.21	125.48
18	F	304	BCR	C23-C22-C21	2.25	122.40	118.94
18	1	316	BCR	C1-C6-C7	2.25	122.15	115.78
18	K	304	BCR	C8-C9-C10	2.25	122.39	118.94
19	B	822	CLA	CHD-C1D-C2D	2.25	130.20	125.48
18	3	315	BCR	C23-C22-C21	2.25	122.39	118.94
19	3	302	CLA	CHC-C4B-NB	-2.25	121.88	124.26
20	2	313	CHL	C4A-NA-C1A	2.24	107.72	106.71
19	A	805	CLA	CHD-C1D-C2D	2.24	130.17	125.48
20	4	305	CHL	C2C-C3C-C4C	2.23	108.08	106.49
19	A	833	CLA	C4A-NA-C1A	2.22	107.71	106.71
19	A	812	CLA	C1D-ND-C4D	2.22	107.91	106.33
19	B	814	CLA	CHD-C1D-C2D	2.22	130.14	125.48
19	4	308	CLA	C1D-ND-C4D	2.22	107.91	106.33
20	3	306	CHL	CHD-C1D-C2D	2.22	130.13	125.48
18	B	844	BCR	C29-C30-C25	2.22	113.89	110.48
18	4	318	BCR	C8-C9-C10	2.22	122.34	118.94
18	O	105	BCR	C2-C1-C6	2.21	113.88	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	319	CHL	C2C-C3C-C4C	2.21	108.06	106.49
21	2	314	LUT	C8-C9-C10	2.20	122.32	118.94
19	1	307	CLA	C4A-NA-C1A	2.20	107.70	106.71
19	A	854	CLA	C1D-ND-C4D	2.20	107.90	106.33
19	L	302	CLA	CHD-C1D-C2D	2.20	130.10	125.48
19	1	308	CLA	CHD-C1D-C2D	2.20	130.10	125.48
19	3	303	CLA	CHD-C1D-C2D	2.20	130.10	125.48
20	1	318	CHL	CHD-C1D-C2D	2.20	130.10	125.48
18	B	844	BCR	C23-C22-C21	2.20	122.32	118.94
18	B	846	BCR	C37-C22-C23	2.20	121.54	118.08
18	O	105	BCR	C8-C9-C10	2.20	122.31	118.94
18	3	315	BCR	C29-C30-C25	2.19	113.86	110.48
19	4	311	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
19	O	102	CLA	C4A-NA-C1A	2.19	107.69	106.71
19	J	102	CLA	CHD-C1D-C2D	2.19	130.07	125.48
20	3	306	CHL	C1D-ND-C4D	2.19	107.89	106.33
19	A	822	CLA	CHD-C1D-C2D	2.19	130.07	125.48
19	4	310	CLA	C2A-C1A-CHA	2.19	127.68	123.86
19	4	311	CLA	C4A-NA-C1A	2.18	107.69	106.71
19	B	815	CLA	CHD-C1D-C2D	2.18	130.05	125.48
19	2	312	CLA	CHD-C1D-C2D	2.18	130.05	125.48
19	4	310	CLA	CHD-C1D-C2D	2.18	130.04	125.48
19	3	312	CLA	CHD-C1D-C2D	2.18	130.04	125.48
19	2	312	CLA	C4A-NA-C1A	2.17	107.68	106.71
19	G	205	CLA	C1D-ND-C4D	2.17	107.88	106.33
18	O	106	BCR	C1-C6-C5	-2.17	119.56	122.61
19	B	838	CLA	C4A-NA-C1A	2.17	107.68	106.71
19	A	816	CLA	C1D-ND-C4D	2.17	107.88	106.33
19	A	802	CLA	C3B-C4B-NB	-2.17	108.51	110.52
20	2	313	CHL	CAA-C2A-C1A	2.16	116.93	112.14
19	B	832	CLA	CHD-C1D-C2D	2.16	130.02	125.48
19	1	307	CLA	C1D-ND-C4D	2.16	107.87	106.33
21	1	314	LUT	C8-C9-C10	2.16	122.26	118.94
19	K	303	CLA	C4A-NA-C1A	2.16	107.68	106.71
19	1	310	CLA	CHD-C1D-C2D	2.16	130.01	125.48
19	2	310	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
19	A	810	CLA	C4A-NA-C1A	2.16	107.68	106.71
19	B	838	CLA	CHD-C1D-C2D	2.16	130.00	125.48
19	B	815	CLA	C4A-NA-C1A	2.16	107.67	106.71
20	2	306	CHL	C4A-NA-C1A	2.15	107.67	106.71
19	4	312	CLA	CHD-C1D-C2D	2.15	130.00	125.48
18	J	103	BCR	C30-C25-C26	-2.15	119.59	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	301	CLA	C3B-C4B-NB	-2.15	108.52	110.52
29	B	847	DGD	C3G-O3G-C1D	-2.15	109.54	113.74
19	B	837	CLA	CHD-C1D-C2D	2.15	129.98	125.48
19	F	306	CLA	CHD-C1D-C2D	2.14	129.98	125.48
19	K	302	CLA	CHD-C1D-C2D	2.14	129.97	125.48
19	A	817	CLA	CHD-C1D-C2D	2.14	129.97	125.48
19	B	816	CLA	CHD-C1D-C2D	2.14	129.97	125.48
19	A	833	CLA	CHD-C1D-C2D	2.14	129.97	125.48
18	B	844	BCR	C1-C6-C5	-2.14	119.61	122.61
19	A	811	CLA	CHD-C1D-C2D	2.13	129.95	125.48
19	B	834	CLA	C4A-NA-C1A	2.13	107.66	106.71
20	2	304	CHL	CHD-C1D-C2D	2.13	129.94	125.48
18	G	201	BCR	C2-C1-C6	2.13	113.75	110.48
19	1	301	CLA	C3B-C4B-NB	-2.12	108.55	110.52
19	A	826	CLA	CHD-C1D-C2D	2.12	129.93	125.48
19	B	802	CLA	C4D-CHA-C1A	2.12	123.83	121.25
19	4	309	CLA	C3B-C4B-NB	-2.12	108.55	110.52
19	2	311	CLA	C1D-ND-C4D	2.12	107.84	106.33
19	B	811	CLA	CHD-C1D-C2D	2.11	129.91	125.48
26	A	841	PQN	C11-C3-C4	-2.11	116.24	118.50
19	B	818	CLA	CHD-C1D-C2D	2.10	129.89	125.48
18	F	304	BCR	C8-C9-C10	2.10	122.17	118.94
19	B	812	CLA	C4A-NA-C1A	2.10	107.65	106.71
18	F	302	BCR	C21-C20-C19	2.10	129.76	123.22
19	3	311	CLA	C4A-NA-C1A	2.10	107.65	106.71
19	3	308	CLA	C3B-C4B-NB	-2.10	108.57	110.52
20	2	319	CHL	CHD-C1D-C2D	2.09	129.87	125.48
19	B	819	CLA	CHD-C1D-C2D	2.09	129.87	125.48
19	B	809	CLA	C4A-NA-C1A	2.09	107.65	106.71
18	K	301	BCR	C8-C9-C10	2.09	122.15	118.94
19	A	813	CLA	CHD-C1D-C2D	2.09	129.86	125.48
20	1	318	CHL	C2C-C3C-C4C	2.09	107.98	106.49
19	B	804	CLA	C3B-C4B-NB	-2.09	108.58	110.52
19	B	830	CLA	CHD-C1D-C2D	2.09	129.85	125.48
19	A	806	CLA	CHD-C1D-C2D	2.09	129.85	125.48
19	A	830	CLA	CHD-C1D-C2D	2.08	129.85	125.48
19	B	808	CLA	CHD-C1D-C2D	2.08	129.84	125.48
19	4	310	CLA	C3B-C4B-NB	-2.08	108.59	110.52
19	B	812	CLA	CHC-C4B-NB	-2.08	122.06	124.26
20	3	306	CHL	C2C-C3C-C4C	2.07	107.97	106.49
19	B	803	CLA	C3B-C4B-NB	-2.07	108.60	110.52
19	4	309	CLA	CHC-C4B-NB	-2.07	122.07	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	304	CHL	C1C-C2C-C3C	-2.07	105.47	107.11
19	O	103	CLA	CHD-C1D-C2D	2.07	129.81	125.48
19	2	308	CLA	CHD-C1D-C2D	2.07	129.81	125.48
19	L	303	CLA	CHD-C1D-C2D	2.07	129.81	125.48
18	J	104	BCR	C8-C9-C10	2.06	122.11	118.94
19	1	302	CLA	CHD-C1D-C2D	2.06	129.80	125.48
19	A	819	CLA	CHD-C1D-C2D	2.06	129.80	125.48
19	3	316	CLA	CHD-C1D-C2D	2.06	129.79	125.48
19	1	303	CLA	C4A-NA-C1A	2.05	107.63	106.71
20	4	307	CHL	CHD-C1D-C2D	2.05	129.78	125.48
22	1	315	XAT	C8-C9-C10	2.05	122.09	118.94
19	B	810	CLA	C3B-C4B-NB	-2.05	108.61	110.52
19	3	310	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	O	104	CLA	C1D-ND-C4D	2.05	107.79	106.33
19	A	821	CLA	CMD-C2D-C1D	2.05	128.33	124.71
19	3	309	CLA	CHD-C1D-C2D	2.05	129.78	125.48
19	4	303	CLA	CGD-CBD-CAD	-2.05	104.10	110.73
19	3	311	CLA	CHD-C1D-C2D	2.04	129.77	125.48
19	3	301	CLA	CHD-C1D-C2D	2.04	129.77	125.48
19	A	852	CLA	CHD-C1D-C2D	2.04	129.76	125.48
19	2	303	CLA	CHD-C1D-C2D	2.04	129.76	125.48
19	2	311	CLA	CHD-C1D-C2D	2.04	129.76	125.48
18	2	316	BCR	C8-C9-C10	2.04	122.07	118.94
19	B	826	CLA	C4A-NA-C1A	2.04	107.62	106.71
19	1	311	CLA	CHD-C1D-C2D	2.04	129.75	125.48
19	2	301	CLA	CHD-C1D-C2D	2.04	129.75	125.48
18	A	847	BCR	C34-C9-C8	2.03	121.28	118.08
19	2	308	CLA	C2C-C1C-NC	-2.03	108.07	109.97
19	3	308	CLA	CHD-C1D-C2D	2.03	129.74	125.48
19	L	302	CLA	C1D-ND-C4D	2.03	107.78	106.33
19	2	307	CLA	C2D-C1D-ND	-2.03	108.61	110.10
19	4	310	CLA	C2D-C1D-ND	-2.03	108.61	110.10
20	2	313	CHL	C2A-C1A-CHA	2.02	127.39	123.86
18	A	845	BCR	C23-C22-C21	2.02	122.04	118.94
19	A	812	CLA	C4A-NA-C1A	2.02	107.61	106.71
29	B	847	DGD	O2G-C1B-O1B	-2.02	118.83	123.70
18	F	308	BCR	C1-C6-C5	-2.02	119.77	122.61
19	4	311	CLA	CHD-C1D-C2D	2.02	129.71	125.48
19	A	850	CLA	CHD-C1D-C2D	2.02	129.71	125.48
19	4	302	CLA	CHD-C1D-C2D	2.01	129.71	125.48
19	2	310	CLA	CHD-C1D-C2D	2.01	129.69	125.48
20	2	306	CHL	C2C-C3C-C4C	2.01	107.92	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	J	102	CLA	C4A-NA-C1A	2.01	107.61	106.71
19	3	304	CLA	CHD-C1D-C2D	2.01	129.69	125.48
19	4	314	CLA	CHD-C1D-C2D	2.01	129.69	125.48
19	A	836	CLA	CHC-C4B-NB	-2.01	122.13	124.26
19	1	306	CLA	C4A-NA-C1A	2.01	107.61	106.71
18	L	301	BCR	C23-C22-C21	2.00	122.02	118.94
19	A	836	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
18	1	316	BCR	C4-C5-C6	-2.00	119.83	122.73
19	4	303	CLA	CHD-C1D-C2D	2.00	129.68	125.48

There are no chirality outliers.

All (3018) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	L	301	BCR	C14-C15-C16-C17
18	L	301	BCR	C16-C17-C18-C19
18	L	301	BCR	C16-C17-C18-C36
18	L	301	BCR	C17-C18-C19-C20
18	L	301	BCR	C36-C18-C19-C20
18	L	301	BCR	C18-C19-C20-C21
18	L	301	BCR	C20-C21-C22-C23
18	L	301	BCR	C20-C21-C22-C37
18	L	305	BCR	C14-C15-C16-C17
18	L	305	BCR	C19-C20-C21-C22
18	L	305	BCR	C20-C21-C22-C23
18	L	305	BCR	C20-C21-C22-C37
18	L	305	BCR	C23-C24-C25-C26
18	L	306	BCR	C17-C18-C19-C20
18	L	306	BCR	C36-C18-C19-C20
18	L	306	BCR	C18-C19-C20-C21
18	1	316	BCR	C6-C7-C8-C9
18	1	316	BCR	C7-C8-C9-C10
18	1	316	BCR	C7-C8-C9-C34
18	1	316	BCR	C11-C10-C9-C34
18	1	316	BCR	C10-C11-C12-C13
18	1	316	BCR	C12-C13-C14-C15
18	1	316	BCR	C35-C13-C14-C15
18	1	316	BCR	C15-C16-C17-C18
18	1	316	BCR	C20-C21-C22-C23
18	1	316	BCR	C20-C21-C22-C37
18	1	316	BCR	C21-C22-C23-C24
18	1	316	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	1	316	BCR	C22-C23-C24-C25
18	1	316	BCR	C23-C24-C25-C30
18	2	316	BCR	C6-C7-C8-C9
18	2	316	BCR	C7-C8-C9-C10
18	2	316	BCR	C7-C8-C9-C34
18	2	316	BCR	C10-C11-C12-C13
18	2	316	BCR	C13-C14-C15-C16
18	2	316	BCR	C14-C15-C16-C17
18	2	316	BCR	C17-C18-C19-C20
18	2	316	BCR	C36-C18-C19-C20
18	2	316	BCR	C18-C19-C20-C21
18	2	316	BCR	C21-C22-C23-C24
18	2	316	BCR	C37-C22-C23-C24
18	3	315	BCR	C6-C7-C8-C9
18	3	315	BCR	C11-C10-C9-C8
18	3	315	BCR	C11-C10-C9-C34
18	3	315	BCR	C20-C21-C22-C23
18	3	315	BCR	C20-C21-C22-C37
18	3	315	BCR	C22-C23-C24-C25
18	3	315	BCR	C23-C24-C25-C30
18	4	318	BCR	C17-C18-C19-C20
18	4	318	BCR	C36-C18-C19-C20
18	4	318	BCR	C20-C21-C22-C23
18	4	318	BCR	C20-C21-C22-C37
18	4	318	BCR	C22-C23-C24-C25
18	4	318	BCR	C23-C24-C25-C26
18	A	844	BCR	C5-C6-C7-C8
18	A	844	BCR	C6-C7-C8-C9
18	A	844	BCR	C7-C8-C9-C10
18	A	844	BCR	C7-C8-C9-C34
18	A	844	BCR	C11-C10-C9-C8
18	A	844	BCR	C11-C10-C9-C34
18	A	844	BCR	C11-C12-C13-C14
18	A	844	BCR	C11-C12-C13-C35
18	A	844	BCR	C21-C22-C23-C24
18	A	844	BCR	C37-C22-C23-C24
18	A	845	BCR	C9-C10-C11-C12
18	A	845	BCR	C11-C12-C13-C14
18	A	845	BCR	C11-C12-C13-C35
18	A	845	BCR	C12-C13-C14-C15
18	A	845	BCR	C35-C13-C14-C15
18	A	845	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	A	845	BCR	C16-C17-C18-C19
18	A	845	BCR	C16-C17-C18-C36
18	A	845	BCR	C37-C22-C23-C24
18	A	845	BCR	C22-C23-C24-C25
18	A	846	BCR	C12-C13-C14-C15
18	A	846	BCR	C35-C13-C14-C15
18	A	847	BCR	C7-C8-C9-C10
18	A	847	BCR	C7-C8-C9-C34
18	A	847	BCR	C21-C22-C23-C24
18	A	847	BCR	C37-C22-C23-C24
18	A	847	BCR	C23-C24-C25-C30
18	A	848	BCR	C10-C11-C12-C13
18	A	848	BCR	C11-C12-C13-C14
18	A	848	BCR	C11-C12-C13-C35
18	A	848	BCR	C17-C18-C19-C20
18	A	848	BCR	C36-C18-C19-C20
18	B	842	BCR	C7-C8-C9-C10
18	B	842	BCR	C7-C8-C9-C34
18	B	842	BCR	C10-C11-C12-C13
18	B	842	BCR	C35-C13-C14-C15
18	B	843	BCR	C11-C10-C9-C8
18	B	843	BCR	C11-C10-C9-C34
18	B	843	BCR	C14-C15-C16-C17
18	B	843	BCR	C20-C21-C22-C23
18	B	843	BCR	C20-C21-C22-C37
18	B	844	BCR	C10-C11-C12-C13
18	B	844	BCR	C14-C15-C16-C17
18	B	844	BCR	C20-C21-C22-C23
18	B	844	BCR	C20-C21-C22-C37
18	B	844	BCR	C22-C23-C24-C25
18	B	845	BCR	C11-C10-C9-C8
18	B	845	BCR	C11-C10-C9-C34
18	B	845	BCR	C12-C13-C14-C15
18	B	845	BCR	C35-C13-C14-C15
18	B	845	BCR	C14-C15-C16-C17
18	B	845	BCR	C20-C21-C22-C23
18	B	845	BCR	C20-C21-C22-C37
18	B	845	BCR	C22-C23-C24-C25
18	B	846	BCR	C1-C6-C7-C8
18	B	846	BCR	C7-C8-C9-C10
18	B	846	BCR	C7-C8-C9-C34
18	B	846	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	B	846	BCR	C11-C10-C9-C34
18	B	846	BCR	C20-C21-C22-C23
18	B	846	BCR	C20-C21-C22-C37
18	B	846	BCR	C21-C22-C23-C24
18	B	846	BCR	C37-C22-C23-C24
18	B	846	BCR	C23-C24-C25-C30
18	F	302	BCR	C7-C8-C9-C10
18	F	302	BCR	C7-C8-C9-C34
18	F	302	BCR	C14-C15-C16-C17
18	F	302	BCR	C16-C17-C18-C19
18	F	302	BCR	C16-C17-C18-C36
18	F	302	BCR	C17-C18-C19-C20
18	F	302	BCR	C36-C18-C19-C20
18	F	302	BCR	C18-C19-C20-C21
18	F	302	BCR	C20-C21-C22-C23
18	F	302	BCR	C20-C21-C22-C37
18	F	304	BCR	C7-C8-C9-C10
18	F	304	BCR	C7-C8-C9-C34
18	F	304	BCR	C10-C11-C12-C13
18	F	304	BCR	C11-C12-C13-C14
18	F	304	BCR	C11-C12-C13-C35
18	F	304	BCR	C12-C13-C14-C15
18	F	304	BCR	C35-C13-C14-C15
18	F	304	BCR	C21-C22-C23-C24
18	F	304	BCR	C37-C22-C23-C24
18	F	308	BCR	C11-C12-C13-C14
18	F	308	BCR	C11-C12-C13-C35
18	F	308	BCR	C16-C17-C18-C19
18	F	308	BCR	C16-C17-C18-C36
18	F	308	BCR	C18-C19-C20-C21
18	G	201	BCR	C7-C8-C9-C10
18	G	201	BCR	C7-C8-C9-C34
18	G	201	BCR	C14-C15-C16-C17
18	G	201	BCR	C16-C17-C18-C19
18	G	201	BCR	C16-C17-C18-C36
18	G	201	BCR	C21-C22-C23-C24
18	G	201	BCR	C37-C22-C23-C24
18	G	206	BCR	C11-C12-C13-C14
18	G	206	BCR	C11-C12-C13-C35
18	G	206	BCR	C17-C18-C19-C20
18	G	206	BCR	C36-C18-C19-C20
18	G	206	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
18	G	206	BCR	C22-C23-C24-C25
18	G	206	BCR	C23-C24-C25-C30
18	I	101	BCR	C12-C13-C14-C15
18	I	101	BCR	C35-C13-C14-C15
18	I	101	BCR	C14-C15-C16-C17
18	I	101	BCR	C17-C18-C19-C20
18	I	101	BCR	C36-C18-C19-C20
18	I	101	BCR	C18-C19-C20-C21
18	I	101	BCR	C20-C21-C22-C23
18	I	101	BCR	C20-C21-C22-C37
18	J	103	BCR	C11-C10-C9-C8
18	J	103	BCR	C11-C10-C9-C34
18	J	103	BCR	C10-C11-C12-C13
18	J	103	BCR	C11-C12-C13-C14
18	J	103	BCR	C11-C12-C13-C35
18	J	103	BCR	C14-C15-C16-C17
18	J	103	BCR	C16-C17-C18-C19
18	J	103	BCR	C16-C17-C18-C36
18	J	103	BCR	C21-C22-C23-C24
18	J	103	BCR	C37-C22-C23-C24
18	J	104	BCR	C6-C7-C8-C9
18	J	104	BCR	C11-C10-C9-C8
18	J	104	BCR	C11-C10-C9-C34
18	K	301	BCR	C6-C7-C8-C9
18	K	301	BCR	C7-C8-C9-C10
18	K	301	BCR	C7-C8-C9-C34
18	K	301	BCR	C18-C19-C20-C21
18	K	301	BCR	C20-C21-C22-C37
18	K	304	BCR	C6-C7-C8-C9
18	K	304	BCR	C7-C8-C9-C34
18	K	304	BCR	C11-C10-C9-C34
18	K	304	BCR	C10-C11-C12-C13
18	K	304	BCR	C17-C18-C19-C20
18	K	304	BCR	C36-C18-C19-C20
18	K	304	BCR	C20-C21-C22-C23
18	K	304	BCR	C20-C21-C22-C37
18	K	304	BCR	C37-C22-C23-C24
18	K	304	BCR	C22-C23-C24-C25
18	O	105	BCR	C6-C7-C8-C9
18	O	105	BCR	C7-C8-C9-C10
18	O	105	BCR	C7-C8-C9-C34
18	O	105	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	O	105	BCR	C11-C10-C9-C34
18	O	105	BCR	C10-C11-C12-C13
18	O	105	BCR	C12-C13-C14-C15
18	O	105	BCR	C35-C13-C14-C15
18	O	105	BCR	C17-C18-C19-C20
18	O	105	BCR	C36-C18-C19-C20
18	O	105	BCR	C18-C19-C20-C21
18	O	105	BCR	C19-C20-C21-C22
18	O	105	BCR	C20-C21-C22-C23
18	O	105	BCR	C20-C21-C22-C37
18	O	105	BCR	C22-C23-C24-C25
18	O	106	BCR	C7-C8-C9-C10
18	O	106	BCR	C7-C8-C9-C34
18	O	106	BCR	C9-C10-C11-C12
18	O	106	BCR	C14-C15-C16-C17
18	O	106	BCR	C16-C17-C18-C19
18	O	106	BCR	C16-C17-C18-C36
18	O	106	BCR	C22-C23-C24-C25
19	L	302	CLA	C1-C2-C3-C4
19	L	303	CLA	C11-C10-C8-C9
19	L	304	CLA	C1-C2-C3-C4
19	L	304	CLA	C1-C2-C3-C5
19	1	301	CLA	C2B-C3B-CAB-CBB
19	1	301	CLA	C4B-C3B-CAB-CBB
19	1	302	CLA	C1-C2-C3-C4
19	1	303	CLA	C2B-C3B-CAB-CBB
19	1	303	CLA	C4B-C3B-CAB-CBB
19	1	303	CLA	C2-C3-C5-C6
19	1	304	CLA	CBD-CGD-O2D-CED
19	1	306	CLA	C1A-C2A-CAA-CBA
19	1	307	CLA	C4B-C3B-CAB-CBB
19	1	307	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	C4-C3-C5-C6
19	1	309	CLA	C2B-C3B-CAB-CBB
19	1	309	CLA	C4B-C3B-CAB-CBB
19	1	309	CLA	C1-C2-C3-C4
19	1	309	CLA	C1-C2-C3-C5
19	1	310	CLA	C2B-C3B-CAB-CBB
19	1	310	CLA	C4B-C3B-CAB-CBB
19	1	310	CLA	C1-C2-C3-C4
19	1	310	CLA	C1-C2-C3-C5
19	1	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	1	311	CLA	C1-C2-C3-C4
19	1	311	CLA	C1-C2-C3-C5
19	1	312	CLA	C1A-C2A-CAA-CBA
19	1	312	CLA	C2B-C3B-CAB-CBB
19	1	312	CLA	C4B-C3B-CAB-CBB
19	1	312	CLA	CHA-CBD-CGD-O1D
19	1	312	CLA	CHA-CBD-CGD-O2D
19	1	312	CLA	C1-C2-C3-C4
19	1	312	CLA	C1-C2-C3-C5
19	1	312	CLA	C4-C3-C5-C6
19	1	313	CLA	CBA-CGA-O2A-C1
19	1	313	CLA	CBD-CGD-O2D-CED
19	2	301	CLA	C2B-C3B-CAB-CBB
19	2	301	CLA	C4B-C3B-CAB-CBB
19	2	301	CLA	C2-C3-C5-C6
19	2	301	CLA	C4-C3-C5-C6
19	2	302	CLA	CBD-CGD-O2D-CED
19	2	302	CLA	C1-C2-C3-C4
19	2	302	CLA	C2-C3-C5-C6
19	2	302	CLA	C4-C3-C5-C6
19	2	303	CLA	C1A-C2A-CAA-CBA
19	2	303	CLA	C1-C2-C3-C4
19	2	307	CLA	C1A-C2A-CAA-CBA
19	2	309	CLA	C2B-C3B-CAB-CBB
19	2	309	CLA	C4B-C3B-CAB-CBB
19	2	309	CLA	CHA-CBD-CGD-O1D
19	2	309	CLA	CHA-CBD-CGD-O2D
19	2	310	CLA	C1A-C2A-CAA-CBA
19	2	310	CLA	CBD-CGD-O2D-CED
19	2	310	CLA	C1-C2-C3-C4
19	2	310	CLA	C1-C2-C3-C5
19	2	311	CLA	C2B-C3B-CAB-CBB
19	2	311	CLA	C4B-C3B-CAB-CBB
19	2	311	CLA	C1-C2-C3-C4
19	2	311	CLA	C1-C2-C3-C5
19	2	312	CLA	C2B-C3B-CAB-CBB
19	2	312	CLA	C4B-C3B-CAB-CBB
19	3	302	CLA	C1-C2-C3-C4
19	3	302	CLA	C1-C2-C3-C5
19	3	303	CLA	C2B-C3B-CAB-CBB
19	3	303	CLA	C4B-C3B-CAB-CBB
19	3	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	3	304	CLA	C2B-C3B-CAB-CBB
19	3	304	CLA	C4B-C3B-CAB-CBB
19	3	304	CLA	CBD-CGD-O2D-CED
19	3	305	CLA	C2B-C3B-CAB-CBB
19	3	305	CLA	C4B-C3B-CAB-CBB
19	3	307	CLA	C1A-C2A-CAA-CBA
19	3	307	CLA	C3A-C2A-CAA-CBA
19	3	307	CLA	C2B-C3B-CAB-CBB
19	3	307	CLA	C4B-C3B-CAB-CBB
19	3	307	CLA	CBD-CGD-O2D-CED
19	3	307	CLA	O1D-CGD-O2D-CED
19	3	307	CLA	C1-C2-C3-C4
19	3	307	CLA	C1-C2-C3-C5
19	3	310	CLA	CBD-CGD-O2D-CED
19	3	310	CLA	C1-C2-C3-C4
19	3	310	CLA	C1-C2-C3-C5
19	3	311	CLA	C2A-CAA-CBA-CGA
19	3	311	CLA	C2B-C3B-CAB-CBB
19	3	311	CLA	C4B-C3B-CAB-CBB
19	3	311	CLA	CBD-CGD-O2D-CED
19	3	316	CLA	C3A-C2A-CAA-CBA
19	3	316	CLA	C2B-C3B-CAB-CBB
19	3	316	CLA	C4B-C3B-CAB-CBB
19	3	316	CLA	CBD-CGD-O2D-CED
19	4	301	CLA	CHA-CBD-CGD-O1D
19	4	301	CLA	CHA-CBD-CGD-O2D
19	4	301	CLA	CBD-CGD-O2D-CED
19	4	302	CLA	C1A-C2A-CAA-CBA
19	4	302	CLA	C3A-C2A-CAA-CBA
19	4	302	CLA	C1-C2-C3-C4
19	4	302	CLA	C1-C2-C3-C5
19	4	303	CLA	C1A-C2A-CAA-CBA
19	4	304	CLA	C1A-C2A-CAA-CBA
19	4	308	CLA	C1A-C2A-CAA-CBA
19	4	308	CLA	C3A-C2A-CAA-CBA
19	4	308	CLA	C2B-C3B-CAB-CBB
19	4	308	CLA	C4B-C3B-CAB-CBB
19	4	308	CLA	C1-C2-C3-C4
19	4	308	CLA	C1-C2-C3-C5
19	4	309	CLA	C1A-C2A-CAA-CBA
19	4	309	CLA	C3A-C2A-CAA-CBA
19	4	309	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	4	309	CLA	C1-C2-C3-C5
19	4	310	CLA	C1-C2-C3-C4
19	4	310	CLA	C4-C3-C5-C6
19	4	311	CLA	C2B-C3B-CAB-CBB
19	4	311	CLA	C4B-C3B-CAB-CBB
19	4	311	CLA	C1-C2-C3-C4
19	4	311	CLA	C1-C2-C3-C5
19	4	312	CLA	C2B-C3B-CAB-CBB
19	4	312	CLA	C4B-C3B-CAB-CBB
19	4	312	CLA	C6-C7-C8-C9
19	4	313	CLA	C1A-C2A-CAA-CBA
19	4	313	CLA	C3A-C2A-CAA-CBA
19	4	313	CLA	C2B-C3B-CAB-CBB
19	4	313	CLA	C4B-C3B-CAB-CBB
19	4	314	CLA	C3A-C2A-CAA-CBA
19	4	314	CLA	C4B-C3B-CAB-CBB
19	A	801	CLA	C2B-C3B-CAB-CBB
19	A	801	CLA	C4B-C3B-CAB-CBB
19	A	801	CLA	CBD-CGD-O2D-CED
19	A	801	CLA	O1D-CGD-O2D-CED
19	A	801	CLA	C1-C2-C3-C4
19	A	802	CLA	C1-C2-C3-C4
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C2B-C3B-CAB-CBB
19	A	806	CLA	C4B-C3B-CAB-CBB
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C4B-C3B-CAB-CBB
19	A	808	CLA	C1A-C2A-CAA-CBA
19	A	808	CLA	C2B-C3B-CAB-CBB
19	A	808	CLA	C4B-C3B-CAB-CBB
19	A	808	CLA	C1-C2-C3-C4
19	A	809	CLA	C1A-C2A-CAA-CBA
19	A	809	CLA	C2B-C3B-CAB-CBB
19	A	809	CLA	C4B-C3B-CAB-CBB
19	A	809	CLA	C2-C3-C5-C6
19	A	809	CLA	C4-C3-C5-C6
19	A	811	CLA	C1-C2-C3-C4
19	A	811	CLA	C1-C2-C3-C5
19	A	811	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	813	CLA	C1A-C2A-CAA-CBA
19	A	813	CLA	C3A-C2A-CAA-CBA
19	A	813	CLA	C2B-C3B-CAB-CBB
19	A	813	CLA	C4B-C3B-CAB-CBB
19	A	813	CLA	C1-C2-C3-C4
19	A	813	CLA	C1-C2-C3-C5
19	A	815	CLA	CHA-CBD-CGD-O2D
19	A	815	CLA	C1-C2-C3-C4
19	A	815	CLA	C1-C2-C3-C5
19	A	816	CLA	C3A-C2A-CAA-CBA
19	A	816	CLA	C2B-C3B-CAB-CBB
19	A	816	CLA	C4B-C3B-CAB-CBB
19	A	816	CLA	C2-C3-C5-C6
19	A	816	CLA	C4-C3-C5-C6
19	A	816	CLA	C14-C13-C15-C16
19	A	817	CLA	C1A-C2A-CAA-CBA
19	A	817	CLA	C3A-C2A-CAA-CBA
19	A	818	CLA	O2A-C1-C2-C3
19	A	818	CLA	C1-C2-C3-C4
19	A	818	CLA	C1-C2-C3-C5
19	A	818	CLA	C11-C10-C8-C9
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C2B-C3B-CAB-CBB
19	A	822	CLA	C4B-C3B-CAB-CBB
19	A	824	CLA	C6-C7-C8-C9
19	A	825	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C12-C13-C15-C16
19	A	826	CLA	C1-C2-C3-C4
19	A	826	CLA	C14-C13-C15-C16
19	A	827	CLA	C2A-CAA-CBA-CGA
19	A	828	CLA	C1A-C2A-CAA-CBA
19	A	828	CLA	CHA-CBD-CGD-O1D
19	A	828	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	C4-C3-C5-C6
19	A	829	CLA	C2B-C3B-CAB-CBB
19	A	829	CLA	C4B-C3B-CAB-CBB
19	A	829	CLA	O2A-C1-C2-C3
19	A	829	CLA	C1-C2-C3-C4
19	A	829	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
19	A	830	CLA	C2B-C3B-CAB-CBB
19	A	830	CLA	C4B-C3B-CAB-CBB
19	A	830	CLA	C1-C2-C3-C4
19	A	830	CLA	C1-C2-C3-C5
19	A	831	CLA	C2B-C3B-CAB-CBB
19	A	831	CLA	C4B-C3B-CAB-CBB
19	A	831	CLA	CHA-CBD-CGD-O1D
19	A	831	CLA	CHA-CBD-CGD-O2D
19	A	832	CLA	C2B-C3B-CAB-CBB
19	A	832	CLA	C4B-C3B-CAB-CBB
19	A	835	CLA	C2B-C3B-CAB-CBB
19	A	835	CLA	C4B-C3B-CAB-CBB
19	A	835	CLA	C1-C2-C3-C4
19	A	836	CLA	CHA-CBD-CGD-O1D
19	A	836	CLA	CHA-CBD-CGD-O2D
19	A	837	CLA	C2B-C3B-CAB-CBB
19	A	837	CLA	C4B-C3B-CAB-CBB
19	A	837	CLA	C1-C2-C3-C4
19	A	838	CLA	C2B-C3B-CAB-CBB
19	A	838	CLA	C4B-C3B-CAB-CBB
19	A	838	CLA	CBD-CGD-O2D-CED
19	A	840	CLA	C2-C1-O2A-CGA
19	A	840	CLA	C2B-C3B-CAB-CBB
19	A	840	CLA	C4B-C3B-CAB-CBB
19	A	840	CLA	C1-C2-C3-C4
19	A	840	CLA	C1-C2-C3-C5
19	A	840	CLA	C2-C3-C5-C6
19	A	840	CLA	C4-C3-C5-C6
19	A	850	CLA	C4-C3-C5-C6
19	A	854	CLA	C1A-C2A-CAA-CBA
19	A	854	CLA	C1-C2-C3-C4
19	A	854	CLA	C2-C3-C5-C6
19	A	854	CLA	C4-C3-C5-C6
19	B	802	CLA	C2B-C3B-CAB-CBB
19	B	802	CLA	C4B-C3B-CAB-CBB
19	B	802	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	CBD-CGD-O2D-CED
19	B	802	CLA	C1-C2-C3-C4
19	B	803	CLA	CBD-CGD-O2D-CED
19	B	805	CLA	C1A-C2A-CAA-CBA
19	B	805	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	806	CLA	C2B-C3B-CAB-CBB
19	B	806	CLA	C4B-C3B-CAB-CBB
19	B	806	CLA	C1-C2-C3-C4
19	B	807	CLA	C2B-C3B-CAB-CBB
19	B	807	CLA	C4B-C3B-CAB-CBB
19	B	808	CLA	CHA-CBD-CGD-O1D
19	B	808	CLA	CHA-CBD-CGD-O2D
19	B	810	CLA	C1-C2-C3-C4
19	B	810	CLA	C1-C2-C3-C5
19	B	811	CLA	C1A-C2A-CAA-CBA
19	B	811	CLA	C4-C3-C5-C6
19	B	812	CLA	C1-C2-C3-C4
19	B	812	CLA	C1-C2-C3-C5
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	C3A-C2A-CAA-CBA
19	B	814	CLA	CBD-CGD-O2D-CED
19	B	814	CLA	C1-C2-C3-C4
19	B	815	CLA	C1A-C2A-CAA-CBA
19	B	815	CLA	C1-C2-C3-C4
19	B	815	CLA	C1-C2-C3-C5
19	B	816	CLA	C2B-C3B-CAB-CBB
19	B	816	CLA	C4B-C3B-CAB-CBB
19	B	816	CLA	C1-C2-C3-C4
19	B	816	CLA	C1-C2-C3-C5
19	B	817	CLA	C2B-C3B-CAB-CBB
19	B	817	CLA	C4B-C3B-CAB-CBB
19	B	818	CLA	C3A-C2A-CAA-CBA
19	B	818	CLA	C1-C2-C3-C4
19	B	818	CLA	C1-C2-C3-C5
19	B	820	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	C1-C2-C3-C4
19	B	820	CLA	C1-C2-C3-C5
19	B	821	CLA	CBD-CGD-O2D-CED
19	B	821	CLA	C2-C3-C5-C6
19	B	821	CLA	C4-C3-C5-C6
19	B	821	CLA	C6-C7-C8-C10
19	B	822	CLA	C1A-C2A-CAA-CBA
19	B	822	CLA	C1-C2-C3-C4
19	B	822	CLA	C1-C2-C3-C5
19	B	822	CLA	C2-C3-C5-C6
19	B	822	CLA	C4-C3-C5-C6
19	B	823	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	B	823	CLA	C4B-C3B-CAB-CBB
19	B	823	CLA	O2A-C1-C2-C3
19	B	823	CLA	C1-C2-C3-C4
19	B	823	CLA	C1-C2-C3-C5
19	B	826	CLA	C2B-C3B-CAB-CBB
19	B	827	CLA	C1-C2-C3-C4
19	B	828	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C3A-C2A-CAA-CBA
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	830	CLA	C1A-C2A-CAA-CBA
19	B	830	CLA	C3A-C2A-CAA-CBA
19	B	830	CLA	C2B-C3B-CAB-CBB
19	B	830	CLA	C4B-C3B-CAB-CBB
19	B	830	CLA	C1-C2-C3-C5
19	B	831	CLA	CBD-CGD-O2D-CED
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	C2B-C3B-CAB-CBB
19	B	832	CLA	C4B-C3B-CAB-CBB
19	B	832	CLA	C2-C3-C5-C6
19	B	832	CLA	C4-C3-C5-C6
19	B	833	CLA	C1-C2-C3-C4
19	B	833	CLA	C1-C2-C3-C5
19	B	834	CLA	CBD-CGD-O2D-CED
19	B	835	CLA	C1A-C2A-CAA-CBA
19	B	835	CLA	C3A-C2A-CAA-CBA
19	B	835	CLA	C1-C2-C3-C4
19	B	836	CLA	C2B-C3B-CAB-CBB
19	B	838	CLA	C2B-C3B-CAB-CBB
19	B	838	CLA	C4B-C3B-CAB-CBB
19	B	838	CLA	C1-C2-C3-C4
19	B	839	CLA	C1A-C2A-CAA-CBA
19	B	839	CLA	C3A-C2A-CAA-CBA
19	B	839	CLA	C2-C3-C5-C6
19	B	839	CLA	C4-C3-C5-C6
19	B	840	CLA	C2B-C3B-CAB-CBB
19	B	840	CLA	C4B-C3B-CAB-CBB
19	B	840	CLA	C11-C10-C8-C9
19	B	850	CLA	C1A-C2A-CAA-CBA
19	B	850	CLA	C1-C2-C3-C4
19	F	307	CLA	C2B-C3B-CAB-CBB
19	F	307	CLA	C4B-C3B-CAB-CBB
19	G	203	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	G	203	CLA	CAD-CBD-CGD-O1D
19	G	203	CLA	CAD-CBD-CGD-O2D
19	G	204	CLA	CBD-CGD-O2D-CED
19	G	205	CLA	CBA-CGA-O2A-C1
19	J	102	CLA	C1A-C2A-CAA-CBA
19	J	102	CLA	C2B-C3B-CAB-CBB
19	J	102	CLA	C4B-C3B-CAB-CBB
19	K	302	CLA	C1A-C2A-CAA-CBA
19	K	302	CLA	C3A-C2A-CAA-CBA
19	K	302	CLA	CBD-CGD-O2D-CED
19	K	303	CLA	C1-C2-C3-C4
19	K	303	CLA	C1-C2-C3-C5
19	K	303	CLA	C2-C3-C5-C6
19	K	303	CLA	C4-C3-C5-C6
19	O	101	CLA	C1-C2-C3-C4
19	O	101	CLA	C1-C2-C3-C5
19	O	101	CLA	C2-C3-C5-C6
19	O	101	CLA	C4-C3-C5-C6
19	O	103	CLA	C1A-C2A-CAA-CBA
19	O	103	CLA	C1-C2-C3-C4
19	O	103	CLA	C1-C2-C3-C5
19	O	103	CLA	C2-C3-C5-C6
19	O	103	CLA	C4-C3-C5-C6
19	O	104	CLA	C1A-C2A-CAA-CBA
19	O	104	CLA	C2B-C3B-CAB-CBB
19	O	104	CLA	C4B-C3B-CAB-CBB
20	1	305	CHL	C1A-C2A-CAA-CBA
20	1	305	CHL	C2B-C3B-CAB-CBB
20	1	305	CHL	C4B-C3B-CAB-CBB
20	1	305	CHL	C1C-C2C-CMC-OMC
20	1	305	CHL	C3C-C2C-CMC-OMC
20	1	305	CHL	CHA-CBD-CGD-O1D
20	1	305	CHL	CHA-CBD-CGD-O2D
20	1	305	CHL	CBD-CGD-O2D-CED
20	1	318	CHL	C2B-C3B-CAB-CBB
20	1	318	CHL	C4B-C3B-CAB-CBB
20	1	318	CHL	C1C-C2C-CMC-OMC
20	1	318	CHL	C3C-C2C-CMC-OMC
20	1	318	CHL	CBD-CGD-O2D-CED
20	1	318	CHL	C1-C2-C3-C4
20	1	318	CHL	C1-C2-C3-C5
20	2	304	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
20	2	305	CHL	C1C-C2C-CMC-OMC
20	2	305	CHL	C3C-C2C-CMC-OMC
20	2	305	CHL	CBD-CGD-O2D-CED
20	2	306	CHL	C1A-C2A-CAA-CBA
20	2	306	CHL	C1C-C2C-CMC-OMC
20	2	306	CHL	C3C-C2C-CMC-OMC
20	2	306	CHL	O2A-C1-C2-C3
20	2	306	CHL	C1-C2-C3-C4
20	2	306	CHL	C1-C2-C3-C5
20	2	313	CHL	C1A-C2A-CAA-CBA
20	2	313	CHL	C3A-C2A-CAA-CBA
20	2	313	CHL	C2B-C3B-CAB-CBB
20	2	313	CHL	C4B-C3B-CAB-CBB
20	2	313	CHL	C1C-C2C-CMC-OMC
20	2	313	CHL	C3C-C2C-CMC-OMC
20	2	313	CHL	CBD-CGD-O2D-CED
20	2	313	CHL	O1D-CGD-O2D-CED
20	2	319	CHL	C1C-C2C-CMC-OMC
20	2	319	CHL	C3C-C2C-CMC-OMC
20	3	306	CHL	C2B-C3B-CAB-CBB
20	3	306	CHL	C4B-C3B-CAB-CBB
20	3	306	CHL	C1C-C2C-CMC-OMC
20	3	306	CHL	C3C-C2C-CMC-OMC
20	4	305	CHL	C1A-C2A-CAA-CBA
20	4	305	CHL	C3A-C2A-CAA-CBA
20	4	305	CHL	C2B-C3B-CAB-CBB
20	4	305	CHL	C4B-C3B-CAB-CBB
20	4	305	CHL	C1C-C2C-CMC-OMC
20	4	305	CHL	C3C-C2C-CMC-OMC
20	4	305	CHL	CBD-CGD-O2D-CED
20	4	305	CHL	C1-C2-C3-C4
20	4	305	CHL	C2-C3-C5-C6
20	4	305	CHL	C4-C3-C5-C6
20	4	306	CHL	C1A-C2A-CAA-CBA
20	4	306	CHL	C3A-C2A-CAA-CBA
20	4	306	CHL	C2B-C3B-CAB-CBB
20	4	306	CHL	C4B-C3B-CAB-CBB
20	4	306	CHL	C1C-C2C-CMC-OMC
20	4	306	CHL	C3C-C2C-CMC-OMC
20	4	306	CHL	CBD-CGD-O2D-CED
20	4	306	CHL	C1-C2-C3-C4
20	4	306	CHL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
20	4	307	CHL	C1A-C2A-CAA-CBA
20	4	307	CHL	C3A-C2A-CAA-CBA
20	4	307	CHL	C2B-C3B-CAB-CBB
20	4	307	CHL	C4B-C3B-CAB-CBB
20	4	307	CHL	C1C-C2C-CMC-OMC
20	4	315	CHL	C1A-C2A-CAA-CBA
20	4	315	CHL	C3A-C2A-CAA-CBA
20	4	315	CHL	C3C-C2C-CMC-OMC
21	1	314	LUT	C11-C10-C9-C8
21	1	314	LUT	C11-C10-C9-C19
21	1	314	LUT	C10-C11-C12-C13
21	1	314	LUT	C11-C12-C13-C14
21	1	314	LUT	C11-C12-C13-C20
21	1	314	LUT	C31-C32-C33-C34
21	1	314	LUT	C31-C32-C33-C40
21	2	314	LUT	C1-C6-C7-C8
21	2	314	LUT	C11-C10-C9-C8
21	2	314	LUT	C11-C10-C9-C19
21	2	314	LUT	C10-C11-C12-C13
21	2	314	LUT	C11-C12-C13-C14
21	2	314	LUT	C11-C12-C13-C20
21	2	314	LUT	C14-C15-C35-C34
21	3	313	LUT	C10-C11-C12-C13
21	3	313	LUT	C11-C12-C13-C14
21	3	313	LUT	C11-C12-C13-C20
21	3	313	LUT	C27-C28-C29-C30
21	3	313	LUT	C27-C28-C29-C39
21	3	313	LUT	C28-C29-C30-C31
21	3	313	LUT	C39-C29-C30-C31
21	3	313	LUT	C29-C30-C31-C32
21	3	313	LUT	C31-C32-C33-C34
21	3	313	LUT	C31-C32-C33-C40
21	3	313	LUT	C32-C33-C34-C35
21	3	313	LUT	C40-C33-C34-C35
21	4	316	LUT	C9-C10-C11-C12
21	4	316	LUT	C10-C11-C12-C13
21	4	316	LUT	C26-C27-C28-C29
21	4	316	LUT	C27-C28-C29-C30
21	4	316	LUT	C27-C28-C29-C39
21	4	316	LUT	C30-C31-C32-C33
21	4	316	LUT	C31-C32-C33-C34
21	4	316	LUT	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
22	1	315	XAT	C7-C8-C9-C19
22	1	315	XAT	C11-C10-C9-C8
22	1	315	XAT	C11-C10-C9-C19
22	1	315	XAT	C10-C11-C12-C13
22	1	315	XAT	C29-C30-C31-C32
22	2	315	XAT	C11-C10-C9-C8
22	2	315	XAT	C11-C10-C9-C19
22	2	315	XAT	C12-C13-C14-C15
22	2	315	XAT	C20-C13-C14-C15
22	2	315	XAT	C14-C15-C35-C34
22	3	314	XAT	C14-C15-C35-C34
22	4	317	XAT	C12-C13-C14-C15
22	4	317	XAT	C20-C13-C14-C15
22	4	317	XAT	C29-C30-C31-C32
22	4	317	XAT	C31-C32-C33-C34
22	4	317	XAT	C31-C32-C33-C40
23	1	317	LHG	C3-O3-P-O5
23	1	317	LHG	C4-O6-P-O5
23	1	319	LHG	C4-O6-P-O3
23	1	319	LHG	C4-O6-P-O4
23	1	319	LHG	C4-O6-P-O5
23	1	320	LHG	O1-C1-C2-C3
23	1	320	LHG	C1-C2-C3-O3
23	1	320	LHG	C3-O3-P-O4
23	1	320	LHG	C3-O3-P-O5
23	2	317	LHG	C1-C2-C3-O3
23	2	317	LHG	C3-O3-P-O5
23	2	317	LHG	C4-O6-P-O5
23	2	318	LHG	O1-C1-C2-C3
23	2	318	LHG	C3-O3-P-O4
23	2	318	LHG	C3-O3-P-O5
23	2	318	LHG	C3-O3-P-O6
23	2	318	LHG	C4-O6-P-O5
23	2	318	LHG	C8-C7-O7-C5
23	4	320	LHG	O1-C1-C2-O2
23	4	320	LHG	O1-C1-C2-C3
23	4	320	LHG	C4-O6-P-O3
23	4	320	LHG	C4-O6-P-O5
23	4	320	LHG	O9-C7-O7-C5
23	4	320	LHG	C8-C7-O7-C5
23	4	322	LHG	C4-O6-P-O4
23	4	322	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
23	4	322	LHG	C8-C7-O7-C5
23	A	843	LHG	C3-O3-P-O5
23	A	843	LHG	C4-O6-P-O5
23	A	843	LHG	O9-C7-O7-C5
23	A	843	LHG	C8-C7-O7-C5
24	4	319	LMG	C2-C1-O1-C7
24	4	319	LMG	O6-C1-O1-C7
24	4	319	LMG	C29-C28-O8-C9
24	G	202	LMG	C2-C1-O1-C7
24	G	202	LMG	O6-C1-O1-C7
24	G	202	LMG	O9-C10-O7-C8
24	G	202	LMG	C11-C10-O7-C8
24	J	101	LMG	C11-C10-O7-C8
25	4	321	HTG	O5-C1-S1-C1'
25	B	848	HTG	C2-C1-S1-C1'
25	B	848	HTG	O5-C1-S1-C1'
25	F	303	HTG	C2-C1-S1-C1'
25	F	303	HTG	O5-C1-S1-C1'
25	F	305	HTG	O5-C1-S1-C1'
28	A	851	LMT	C2-C1-O1'-C1'
19	1	303	CLA	O1D-CGD-O2D-CED
19	2	310	CLA	O1D-CGD-O2D-CED
19	3	308	CLA	O1D-CGD-O2D-CED
19	4	301	CLA	O1D-CGD-O2D-CED
19	4	310	CLA	O1D-CGD-O2D-CED
19	B	802	CLA	O1D-CGD-O2D-CED
19	F	307	CLA	O1D-CGD-O2D-CED
19	G	204	CLA	O1D-CGD-O2D-CED
19	O	103	CLA	O1D-CGD-O2D-CED
19	1	302	CLA	C15-C16-C17-C18
19	1	304	CLA	O1D-CGD-O2D-CED
19	1	313	CLA	O1D-CGD-O2D-CED
19	B	803	CLA	O1D-CGD-O2D-CED
19	B	814	CLA	O1D-CGD-O2D-CED
19	B	820	CLA	O1D-CGD-O2D-CED
20	1	305	CHL	O1D-CGD-O2D-CED
20	2	305	CHL	O1D-CGD-O2D-CED
20	4	306	CHL	O1D-CGD-O2D-CED
20	4	307	CHL	O1D-CGD-O2D-CED
19	1	302	CLA	CBD-CGD-O2D-CED
19	1	303	CLA	CBD-CGD-O2D-CED
19	2	303	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	3	301	CLA	CBD-CGD-O2D-CED
19	3	308	CLA	CBD-CGD-O2D-CED
19	4	303	CLA	CBD-CGD-O2D-CED
19	4	309	CLA	CBD-CGD-O2D-CED
19	4	310	CLA	CBD-CGD-O2D-CED
19	4	311	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	CBD-CGD-O2D-CED
19	A	809	CLA	CBD-CGD-O2D-CED
19	A	814	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	CBD-CGD-O2D-CED
19	A	821	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	CBD-CGD-O2D-CED
19	A	830	CLA	CBD-CGD-O2D-CED
19	A	831	CLA	CBD-CGD-O2D-CED
19	A	854	CLA	CBD-CGD-O2D-CED
19	B	806	CLA	CBD-CGD-O2D-CED
19	B	810	CLA	CBD-CGD-O2D-CED
19	B	816	CLA	CBD-CGD-O2D-CED
19	B	819	CLA	CBD-CGD-O2D-CED
19	B	838	CLA	CBD-CGD-O2D-CED
19	F	307	CLA	CBD-CGD-O2D-CED
19	J	102	CLA	CBD-CGD-O2D-CED
19	O	102	CLA	CBD-CGD-O2D-CED
19	O	103	CLA	CBD-CGD-O2D-CED
20	3	306	CHL	CBD-CGD-O2D-CED
20	4	307	CHL	CBD-CGD-O2D-CED
19	L	302	CLA	O1A-CGA-O2A-C1
19	A	813	CLA	O1A-CGA-O2A-C1
23	1	320	LHG	O10-C23-O8-C6
23	2	317	LHG	O10-C23-O8-C6
23	2	318	LHG	O10-C23-O8-C6
24	4	319	LMG	O10-C28-O8-C9
19	G	205	CLA	O1A-CGA-O2A-C1
19	2	302	CLA	O1D-CGD-O2D-CED
19	3	310	CLA	O1D-CGD-O2D-CED
19	4	309	CLA	O1D-CGD-O2D-CED
19	A	821	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	O1D-CGD-O2D-CED
19	A	826	CLA	C10-C11-C12-C13
19	1	307	CLA	O1D-CGD-O2D-CED
19	1	311	CLA	O1D-CGD-O2D-CED
19	3	304	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	809	CLA	O1D-CGD-O2D-CED
19	A	826	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1D-CGD-O2D-CED
19	B	821	CLA	O1D-CGD-O2D-CED
19	B	831	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	O1D-CGD-O2D-CED
20	1	318	CHL	O1D-CGD-O2D-CED
20	4	305	CHL	O1D-CGD-O2D-CED
19	L	302	CLA	CBA-CGA-O2A-C1
19	A	813	CLA	CBA-CGA-O2A-C1
19	O	101	CLA	CBA-CGA-O2A-C1
23	1	320	LHG	C24-C23-O8-C6
23	2	317	LHG	C24-C23-O8-C6
19	1	312	CLA	CBD-CGD-O2D-CED
19	A	813	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	CBD-CGD-O2D-CED
19	A	834	CLA	CBD-CGD-O2D-CED
19	A	839	CLA	CBD-CGD-O2D-CED
19	B	809	CLA	CBD-CGD-O2D-CED
19	B	811	CLA	CBD-CGD-O2D-CED
19	B	827	CLA	CBD-CGD-O2D-CED
20	2	319	CHL	CBD-CGD-O2D-CED
20	4	315	CHL	CBD-CGD-O2D-CED
19	1	309	CLA	O1A-CGA-O2A-C1
19	2	303	CLA	O1A-CGA-O2A-C1
19	A	839	CLA	O1A-CGA-O2A-C1
19	A	840	CLA	O1A-CGA-O2A-C1
19	B	812	CLA	O1A-CGA-O2A-C1
19	B	815	CLA	O1A-CGA-O2A-C1
19	O	101	CLA	O1A-CGA-O2A-C1
19	3	303	CLA	O1D-CGD-O2D-CED
19	3	311	CLA	O1D-CGD-O2D-CED
19	3	316	CLA	O1D-CGD-O2D-CED
19	A	838	CLA	O1D-CGD-O2D-CED
19	K	302	CLA	O1D-CGD-O2D-CED
20	3	306	CHL	O1D-CGD-O2D-CED
19	L	304	CLA	CBD-CGD-O2D-CED
19	B	808	CLA	CBD-CGD-O2D-CED
19	B	839	CLA	CBD-CGD-O2D-CED
19	1	309	CLA	C13-C15-C16-C17
25	F	301	HTG	S1-C1'-C2'-C3'
25	F	303	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
19	B	838	CLA	O1D-CGD-O2D-CED
19	J	102	CLA	O1D-CGD-O2D-CED
23	2	318	LHG	O9-C7-O7-C5
24	J	101	LMG	O9-C10-O7-C8
19	4	310	CLA	C3-C5-C6-C7
19	A	822	CLA	C3-C5-C6-C7
19	A	831	CLA	C3-C5-C6-C7
19	A	850	CLA	C3-C5-C6-C7
19	A	853	CLA	C3-C5-C6-C7
19	B	806	CLA	C3-C5-C6-C7
19	B	809	CLA	C3-C5-C6-C7
19	B	811	CLA	C3-C5-C6-C7
19	B	814	CLA	C3-C5-C6-C7
19	1	309	CLA	CBA-CGA-O2A-C1
19	1	310	CLA	CBA-CGA-O2A-C1
19	1	312	CLA	CBA-CGA-O2A-C1
19	A	817	CLA	CBA-CGA-O2A-C1
19	A	829	CLA	CBA-CGA-O2A-C1
19	A	839	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	CBA-CGA-O2A-C1
20	1	305	CHL	CBA-CGA-O2A-C1
20	2	319	CHL	CBA-CGA-O2A-C1
23	2	318	LHG	C24-C23-O8-C6
24	B	849	LMG	C29-C28-O8-C9
19	B	832	CLA	CBD-CGD-O2D-CED
19	1	313	CLA	O1A-CGA-O2A-C1
19	2	310	CLA	C3-C5-C6-C7
19	1	302	CLA	C4-C3-C5-C6
19	2	303	CLA	C4-C3-C5-C6
19	A	835	CLA	C4-C3-C5-C6
19	1	308	CLA	C2-C3-C5-C6
19	1	312	CLA	C2-C3-C5-C6
19	A	811	CLA	C2-C3-C5-C6
19	A	828	CLA	C2-C3-C5-C6
19	A	850	CLA	C2-C3-C5-C6
19	B	811	CLA	C2-C3-C5-C6
19	1	301	CLA	CBD-CGD-O2D-CED
19	A	833	CLA	CBD-CGD-O2D-CED
19	B	829	CLA	CBD-CGD-O2D-CED
19	1	310	CLA	C2A-CAA-CBA-CGA
19	4	311	CLA	C2A-CAA-CBA-CGA
19	A	807	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	820	CLA	C2A-CAA-CBA-CGA
19	A	822	CLA	C2A-CAA-CBA-CGA
19	A	840	CLA	C2A-CAA-CBA-CGA
19	B	814	CLA	C2A-CAA-CBA-CGA
19	B	831	CLA	C2A-CAA-CBA-CGA
19	B	838	CLA	C2A-CAA-CBA-CGA
19	O	102	CLA	C2A-CAA-CBA-CGA
19	O	104	CLA	C2A-CAA-CBA-CGA
20	2	305	CHL	C2A-CAA-CBA-CGA
20	2	319	CHL	C2A-CAA-CBA-CGA
20	4	307	CHL	C2A-CAA-CBA-CGA
19	2	301	CLA	C3-C5-C6-C7
19	A	806	CLA	C3-C5-C6-C7
19	A	816	CLA	C3-C5-C6-C7
19	A	837	CLA	C3-C5-C6-C7
19	B	815	CLA	C3-C5-C6-C7
19	2	302	CLA	CBA-CGA-O2A-C1
19	2	303	CLA	CBA-CGA-O2A-C1
19	4	303	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	CBA-CGA-O2A-C1
19	B	812	CLA	CBA-CGA-O2A-C1
20	4	306	CHL	CBA-CGA-O2A-C1
19	4	303	CLA	O1D-CGD-O2D-CED
19	4	312	CLA	O1D-CGD-O2D-CED
19	A	814	CLA	O1D-CGD-O2D-CED
19	L	302	CLA	C1-C2-C3-C5
19	1	302	CLA	C1-C2-C3-C5
19	2	302	CLA	C1-C2-C3-C5
19	2	303	CLA	C1-C2-C3-C5
19	A	837	CLA	C1-C2-C3-C5
19	A	854	CLA	C1-C2-C3-C5
19	B	814	CLA	C1-C2-C3-C5
19	2	301	CLA	CBD-CGD-O2D-CED
19	O	101	CLA	CBD-CGD-O2D-CED
25	F	310	HTG	S1-C1'-C2'-C3'
19	3	301	CLA	O1D-CGD-O2D-CED
24	B	849	LMG	C4-C5-C6-O5
19	1	310	CLA	O1A-CGA-O2A-C1
19	1	312	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	O1A-CGA-O2A-C1
19	A	817	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	O1A-CGA-O2A-C1
20	1	305	CHL	O1A-CGA-O2A-C1
20	2	306	CHL	O1A-CGA-O2A-C1
20	2	319	CHL	O1A-CGA-O2A-C1
20	4	307	CHL	O1A-CGA-O2A-C1
23	4	320	LHG	O10-C23-O8-C6
24	B	849	LMG	O10-C28-O8-C9
24	J	101	LMG	C35-C36-C37-C38
19	2	303	CLA	O1D-CGD-O2D-CED
18	2	316	BCR	C9-C10-C11-C12
18	2	316	BCR	C19-C20-C21-C22
18	3	315	BCR	C19-C20-C21-C22
18	A	846	BCR	C9-C10-C11-C12
18	A	848	BCR	C19-C20-C21-C22
18	B	843	BCR	C9-C10-C11-C12
18	B	843	BCR	C15-C16-C17-C18
18	F	302	BCR	C15-C16-C17-C18
18	F	302	BCR	C19-C20-C21-C22
18	J	104	BCR	C19-C20-C21-C22
18	K	301	BCR	C19-C20-C21-C22
19	1	310	CLA	CBD-CGD-O2D-CED
19	4	302	CLA	CBD-CGD-O2D-CED
19	A	806	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
19	B	815	CLA	CBD-CGD-O2D-CED
19	G	205	CLA	CBD-CGD-O2D-CED
19	O	104	CLA	CBD-CGD-O2D-CED
20	2	304	CHL	CBD-CGD-O2D-CED
19	B	806	CLA	O1D-CGD-O2D-CED
19	O	102	CLA	O1D-CGD-O2D-CED
19	L	303	CLA	C3-C5-C6-C7
19	A	811	CLA	C3-C5-C6-C7
19	A	815	CLA	C3-C5-C6-C7
19	A	840	CLA	C3-C5-C6-C7
19	A	804	CLA	CBA-CGA-O2A-C1
19	A	806	CLA	CBA-CGA-O2A-C1
23	A	843	LHG	C24-C23-O8-C6
23	1	320	LHG	C9-C10-C11-C12
19	2	302	CLA	O1A-CGA-O2A-C1
19	4	303	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	O1A-CGA-O2A-C1
19	A	815	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	J	101	LMG	C4-C5-C6-O5
19	B	819	CLA	O1D-CGD-O2D-CED
19	1	306	CLA	CBD-CGD-O2D-CED
19	A	827	CLA	CBD-CGD-O2D-CED
19	A	828	CLA	CBD-CGD-O2D-CED
19	B	801	CLA	CBD-CGD-O2D-CED
19	B	804	CLA	CBD-CGD-O2D-CED
19	K	303	CLA	CBD-CGD-O2D-CED
23	2	317	LHG	C11-C12-C13-C14
20	4	306	CHL	O1A-CGA-O2A-C1
23	4	320	LHG	C13-C14-C15-C16
23	4	322	LHG	C10-C11-C12-C13
23	A	842	LHG	C10-C11-C12-C13
23	A	842	LHG	C17-C18-C19-C20
24	4	319	LMG	C23-C24-C25-C26
24	B	849	LMG	C37-C38-C39-C40
24	B	849	LMG	C39-C40-C41-C42
24	F	309	LMG	C14-C15-C16-C17
24	G	202	LMG	C14-C15-C16-C17
24	J	101	LMG	C17-C18-C19-C20
19	1	302	CLA	O1D-CGD-O2D-CED
19	4	311	CLA	O1D-CGD-O2D-CED
20	1	318	CHL	C3-C5-C6-C7
19	3	309	CLA	CBA-CGA-O2A-C1
20	2	306	CHL	CBA-CGA-O2A-C1
20	4	307	CHL	CBA-CGA-O2A-C1
23	4	320	LHG	C24-C23-O8-C6
19	A	854	CLA	O1D-CGD-O2D-CED
25	F	301	HTG	O5-C5-C6-O6
23	2	318	LHG	C9-C10-C11-C12
24	B	849	LMG	C14-C15-C16-C17
19	K	303	CLA	C10-C11-C12-C13
24	4	319	LMG	O6-C5-C6-O5
28	A	851	LMT	O5B-C5B-C6B-O6B
19	1	309	CLA	C4-C3-C5-C6
19	4	311	CLA	C4-C3-C5-C6
19	A	839	CLA	C4-C3-C5-C6
19	B	816	CLA	C4-C3-C5-C6
19	B	818	CLA	C4-C3-C5-C6
19	1	309	CLA	C2-C3-C5-C6
19	4	310	CLA	C2-C3-C5-C6
19	4	311	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A	839	CLA	C2-C3-C5-C6
19	B	816	CLA	C2-C3-C5-C6
19	B	818	CLA	C2-C3-C5-C6
19	2	303	CLA	C2A-CAA-CBA-CGA
19	A	850	CLA	C2A-CAA-CBA-CGA
19	B	809	CLA	C2A-CAA-CBA-CGA
19	B	817	CLA	C2A-CAA-CBA-CGA
19	K	302	CLA	C2A-CAA-CBA-CGA
19	A	831	CLA	O1D-CGD-O2D-CED
23	1	320	LHG	C18-C19-C20-C21
24	B	849	LMG	O6-C5-C6-O5
24	J	101	LMG	O6-C5-C6-O5
19	3	309	CLA	O1A-CGA-O2A-C1
23	A	843	LHG	O10-C23-O8-C6
29	B	847	DGD	CAA-CBA-CCA-CDA
19	4	308	CLA	CBA-CGA-O2A-C1
19	A	829	CLA	CBD-CGD-O2D-CED
19	B	833	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	O1D-CGD-O2D-CED
19	4	308	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	C1-C2-C3-C5
19	A	835	CLA	C1-C2-C3-C5
19	B	816	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	CBD-CGD-O2D-CED
19	A	813	CLA	O1D-CGD-O2D-CED
23	1	320	LHG	C16-C17-C18-C19
24	4	319	LMG	C19-C20-C21-C22
19	A	809	CLA	C3-C5-C6-C7
19	B	808	CLA	C3-C5-C6-C7
19	1	312	CLA	O1D-CGD-O2D-CED
19	1	302	CLA	CBA-CGA-O2A-C1
19	A	834	CLA	CBA-CGA-O2A-C1
19	A	838	CLA	CBA-CGA-O2A-C1
19	B	809	CLA	CBA-CGA-O2A-C1
20	2	305	CHL	CBA-CGA-O2A-C1
24	F	309	LMG	C29-C28-O8-C9
24	4	319	LMG	C4-C5-C6-O5
19	B	811	CLA	O1D-CGD-O2D-CED
18	A	845	BCR	C19-C20-C21-C22
18	G	201	BCR	C9-C10-C11-C12
18	G	206	BCR	C9-C10-C11-C12
18	K	304	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	K	304	BCR	C15-C16-C17-C18
18	O	106	BCR	C13-C14-C15-C16
23	4	322	LHG	C23-C24-C25-C26
29	B	847	DGD	C9B-CAB-CBB-CCB
19	1	307	CLA	C8-C10-C11-C12
19	B	828	CLA	C5-C6-C7-C8
25	F	301	HTG	C4-C5-C6-O6
28	A	851	LMT	C4B-C5B-C6B-O6B
19	2	311	CLA	C8-C10-C11-C12
19	4	310	CLA	C5-C6-C7-C8
19	A	827	CLA	C13-C15-C16-C17
19	B	811	CLA	C5-C6-C7-C8
19	B	826	CLA	C13-C15-C16-C17
19	B	838	CLA	C15-C16-C17-C18
23	1	320	LHG	O2-C2-C3-O3
23	2	317	LHG	O2-C2-C3-O3
20	2	319	CHL	C3-C5-C6-C7
23	4	320	LHG	C28-C29-C30-C31
19	2	303	CLA	C2-C3-C5-C6
19	L	302	CLA	C14-C13-C15-C16
19	1	302	CLA	C11-C10-C8-C9
19	1	302	CLA	C11-C12-C13-C14
19	1	307	CLA	C6-C7-C8-C9
19	1	307	CLA	C11-C12-C13-C14
19	1	307	CLA	C14-C13-C15-C16
19	1	308	CLA	C6-C7-C8-C9
19	2	311	CLA	C11-C10-C8-C9
19	3	301	CLA	C6-C7-C8-C9
19	A	807	CLA	C11-C10-C8-C9
19	A	811	CLA	C11-C10-C8-C9
19	A	818	CLA	C6-C7-C8-C9
19	A	824	CLA	C14-C13-C15-C16
19	A	825	CLA	C11-C10-C8-C9
19	A	831	CLA	C11-C10-C8-C9
19	A	837	CLA	C14-C13-C15-C16
19	A	838	CLA	C6-C7-C8-C9
19	A	839	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C12-C13-C14
19	A	853	CLA	C11-C10-C8-C9
19	B	803	CLA	C11-C12-C13-C14
19	B	806	CLA	C6-C7-C8-C9
19	B	807	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	B	808	CLA	C14-C13-C15-C16
19	B	809	CLA	C14-C13-C15-C16
19	B	813	CLA	C14-C13-C15-C16
19	B	817	CLA	C11-C10-C8-C9
19	B	818	CLA	C6-C7-C8-C9
19	B	821	CLA	C11-C12-C13-C14
19	B	821	CLA	C14-C13-C15-C16
19	B	825	CLA	C11-C10-C8-C9
19	B	825	CLA	C14-C13-C15-C16
19	B	826	CLA	C14-C13-C15-C16
19	B	827	CLA	C11-C12-C13-C14
19	B	829	CLA	C11-C10-C8-C9
19	B	831	CLA	C11-C10-C8-C9
19	B	833	CLA	C14-C13-C15-C16
19	B	836	CLA	C11-C12-C13-C14
19	K	303	CLA	C11-C10-C8-C9
19	A	820	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	O1D-CGD-O2D-CED
19	B	809	CLA	O1D-CGD-O2D-CED
19	1	302	CLA	C13-C15-C16-C17
19	A	816	CLA	C2A-CAA-CBA-CGA
18	L	305	BCR	C7-C8-C9-C34
18	L	305	BCR	C36-C18-C19-C20
18	L	305	BCR	C37-C22-C23-C24
18	L	306	BCR	C37-C22-C23-C24
18	1	316	BCR	C11-C12-C13-C35
18	3	315	BCR	C37-C22-C23-C24
18	4	318	BCR	C7-C8-C9-C34
18	A	845	BCR	C7-C8-C9-C34
18	A	847	BCR	C36-C18-C19-C20
18	A	848	BCR	C7-C8-C9-C34
18	B	843	BCR	C11-C12-C13-C35
18	B	843	BCR	C37-C22-C23-C24
18	B	846	BCR	C11-C12-C13-C35
18	G	206	BCR	C7-C8-C9-C34
18	J	103	BCR	C36-C18-C19-C20
18	J	104	BCR	C37-C22-C23-C24
18	L	305	BCR	C7-C8-C9-C10
18	L	305	BCR	C17-C18-C19-C20
18	L	305	BCR	C21-C22-C23-C24
18	3	315	BCR	C21-C22-C23-C24
18	4	318	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
18	A	848	BCR	C21-C22-C23-C24
18	B	843	BCR	C11-C12-C13-C14
18	B	846	BCR	C11-C12-C13-C14
18	J	104	BCR	C21-C22-C23-C24
18	O	105	BCR	C21-C22-C23-C24
18	O	106	BCR	C21-C22-C23-C24
23	A	842	LHG	C13-C14-C15-C16
23	A	843	LHG	C7-C8-C9-C10
19	1	302	CLA	O1A-CGA-O2A-C1
24	F	309	LMG	O10-C28-O8-C9
19	L	302	CLA	C15-C16-C17-C18
19	2	301	CLA	C5-C6-C7-C8
19	A	805	CLA	C13-C15-C16-C17
19	A	826	CLA	C15-C16-C17-C18
19	A	850	CLA	C10-C11-C12-C13
19	A	852	CLA	C10-C11-C12-C13
19	3	312	CLA	CBA-CGA-O2A-C1
19	L	302	CLA	CBD-CGD-O2D-CED
24	J	101	LMG	C37-C38-C39-C40
25	F	303	HTG	C2'-C3'-C4'-C5'
19	A	839	CLA	C3-C5-C6-C7
19	B	818	CLA	C3-C5-C6-C7
19	A	802	CLA	CBA-CGA-O2A-C1
19	A	832	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
19	2	303	CLA	C8-C10-C11-C12
19	4	303	CLA	C10-C11-C12-C13
19	A	818	CLA	C15-C16-C17-C18
19	A	837	CLA	C5-C6-C7-C8
19	A	838	CLA	C15-C16-C17-C18
19	A	853	CLA	C15-C16-C17-C18
19	B	819	CLA	C8-C10-C11-C12
19	B	819	CLA	C15-C16-C17-C18
19	B	828	CLA	C13-C15-C16-C17
19	B	836	CLA	C13-C15-C16-C17
19	B	839	CLA	C8-C10-C11-C12
24	B	849	LMG	C28-C29-C30-C31
23	1	320	LHG	C14-C15-C16-C17
25	4	321	HTG	C3'-C4'-C5'-C6'
19	L	303	CLA	C8-C10-C11-C12
19	1	307	CLA	C10-C11-C12-C13
19	1	312	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	2	301	CLA	C10-C11-C12-C13
19	2	303	CLA	C5-C6-C7-C8
19	2	308	CLA	C5-C6-C7-C8
19	A	815	CLA	C8-C10-C11-C12
19	A	816	CLA	C5-C6-C7-C8
19	A	816	CLA	C8-C10-C11-C12
19	A	816	CLA	C13-C15-C16-C17
19	A	837	CLA	C8-C10-C11-C12
19	B	802	CLA	C15-C16-C17-C18
19	B	805	CLA	C15-C16-C17-C18
19	B	809	CLA	C13-C15-C16-C17
19	B	824	CLA	C15-C16-C17-C18
19	B	838	CLA	C1-C2-C3-C5
19	A	839	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	O1D-CGD-O2D-CED
23	1	317	LHG	O1-C1-C2-O2
19	A	834	CLA	O1A-CGA-O2A-C1
19	B	809	CLA	O1A-CGA-O2A-C1
25	4	321	HTG	O5-C5-C6-O6
19	4	313	CLA	CBD-CGD-O2D-CED
20	2	319	CHL	O1D-CGD-O2D-CED
20	4	315	CHL	O1D-CGD-O2D-CED
19	L	303	CLA	C13-C15-C16-C17
19	2	311	CLA	C5-C6-C7-C8
19	2	311	CLA	C10-C11-C12-C13
19	A	805	CLA	C8-C10-C11-C12
19	A	809	CLA	C13-C15-C16-C17
19	A	811	CLA	C8-C10-C11-C12
19	A	853	CLA	C8-C10-C11-C12
19	B	809	CLA	C10-C11-C12-C13
19	B	825	CLA	C13-C15-C16-C17
19	B	839	CLA	C5-C6-C7-C8
19	A	808	CLA	C3-C5-C6-C7
19	B	836	CLA	CBA-CGA-O2A-C1
24	G	202	LMG	C29-C28-O8-C9
19	A	808	CLA	C13-C15-C16-C17
19	A	817	CLA	C8-C10-C11-C12
19	B	806	CLA	C5-C6-C7-C8
19	B	807	CLA	C5-C6-C7-C8
19	B	807	CLA	C13-C15-C16-C17
19	B	827	CLA	C8-C10-C11-C12
19	O	103	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	4	310	CLA	C8-C10-C11-C12
19	B	817	CLA	C5-C6-C7-C8
19	B	808	CLA	O1D-CGD-O2D-CED
19	1	302	CLA	C6-C7-C8-C10
19	1	309	CLA	C11-C10-C8-C7
19	2	301	CLA	C11-C10-C8-C7
19	2	308	CLA	C6-C7-C8-C10
19	A	811	CLA	C11-C10-C8-C7
19	A	818	CLA	C11-C10-C8-C7
19	A	818	CLA	C12-C13-C15-C16
19	A	819	CLA	C11-C12-C13-C15
19	A	824	CLA	C6-C7-C8-C10
19	A	824	CLA	C11-C10-C8-C7
19	A	836	CLA	C11-C12-C13-C15
19	A	837	CLA	C12-C13-C15-C16
19	A	839	CLA	C11-C10-C8-C7
19	A	853	CLA	C12-C13-C15-C16
19	A	854	CLA	C6-C7-C8-C10
19	B	806	CLA	C11-C10-C8-C7
19	B	810	CLA	C11-C12-C13-C15
19	B	814	CLA	C6-C7-C8-C10
19	B	819	CLA	C6-C7-C8-C10
19	B	827	CLA	C6-C7-C8-C10
19	B	827	CLA	C12-C13-C15-C16
19	B	833	CLA	C11-C12-C13-C15
19	B	835	CLA	C6-C7-C8-C10
19	B	807	CLA	C3-C5-C6-C7
20	2	305	CHL	O1A-CGA-O2A-C1
18	A	844	BCR	C9-C10-C11-C12
18	A	847	BCR	C19-C20-C21-C22
18	B	843	BCR	C13-C14-C15-C16
18	B	846	BCR	C13-C14-C15-C16
18	O	106	BCR	C19-C20-C21-C22
19	L	303	CLA	C2A-CAA-CBA-CGA
19	1	301	CLA	C2A-CAA-CBA-CGA
19	L	304	CLA	O1D-CGD-O2D-CED
19	B	839	CLA	O1D-CGD-O2D-CED
19	4	312	CLA	C5-C6-C7-C8
19	A	809	CLA	C10-C11-C12-C13
28	A	851	LMT	O1'-C1-C2-C3
20	3	306	CHL	CBA-CGA-O2A-C1
19	A	838	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	822	CLA	CBD-CGD-O2D-CED
19	1	308	CLA	C5-C6-C7-C8
19	A	818	CLA	C13-C15-C16-C17
19	B	803	CLA	C15-C16-C17-C18
19	B	818	CLA	C8-C10-C11-C12
20	1	318	CHL	C5-C6-C7-C8
20	4	305	CHL	C5-C6-C7-C8
18	1	316	BCR	C18-C19-C20-C21
18	4	318	BCR	C10-C11-C12-C13
18	4	318	BCR	C18-C19-C20-C21
18	A	844	BCR	C10-C11-C12-C13
18	A	848	BCR	C18-C19-C20-C21
18	B	843	BCR	C10-C11-C12-C13
18	B	845	BCR	C10-C11-C12-C13
18	G	206	BCR	C10-C11-C12-C13
18	G	206	BCR	C18-C19-C20-C21
18	I	101	BCR	C10-C11-C12-C13
18	J	104	BCR	C10-C11-C12-C13
18	J	104	BCR	C18-C19-C20-C21
18	O	106	BCR	C10-C11-C12-C13
18	O	106	BCR	C18-C19-C20-C21
22	4	317	XAT	C30-C31-C32-C33
23	4	322	LHG	O2-C2-C3-O3
19	1	312	CLA	C3-C5-C6-C7
19	1	301	CLA	C13-C15-C16-C17
19	1	302	CLA	C5-C6-C7-C8
19	3	301	CLA	C10-C11-C12-C13
19	A	806	CLA	C13-C15-C16-C17
19	A	808	CLA	C15-C16-C17-C18
19	A	809	CLA	C8-C10-C11-C12
19	B	810	CLA	C13-C15-C16-C17
19	A	835	CLA	CBA-CGA-O2A-C1
23	1	320	LHG	C28-C29-C30-C31
19	B	830	CLA	O1A-CGA-O2A-C1
19	L	302	CLA	C10-C11-C12-C13
19	1	309	CLA	C10-C11-C12-C13
19	4	309	CLA	C5-C6-C7-C8
19	A	804	CLA	C8-C10-C11-C12
19	A	838	CLA	C10-C11-C12-C13
19	B	831	CLA	C10-C11-C12-C13
23	1	320	LHG	C34-C35-C36-C37
29	B	847	DGD	CEA-CFA-CGA-CHA

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Mol	Chain	Res	Type	Atoms
19	A	832	CLA	O1A-CGA-O2A-C1
19	A	811	CLA	C15-C16-C17-C18
19	A	854	CLA	C10-C11-C12-C13
19	B	826	CLA	C15-C16-C17-C18
19	B	833	CLA	C13-C15-C16-C17
23	1	317	LHG	C4-O6-P-O3
23	1	320	LHG	C3-O3-P-O6
23	2	317	LHG	C4-O6-P-O3
23	2	318	LHG	C4-O6-P-O3
23	4	320	LHG	C3-O3-P-O6
23	4	322	LHG	C3-O3-P-O6
23	4	322	LHG	C4-O6-P-O3
23	A	842	LHG	C3-O3-P-O6
23	A	843	LHG	C3-O3-P-O6
24	J	101	LMG	C40-C41-C42-C43
19	B	820	CLA	CBA-CGA-O2A-C1
19	K	303	CLA	CBA-CGA-O2A-C1
25	4	321	HTG	C1'-C2'-C3'-C4'
25	F	305	HTG	C1'-C2'-C3'-C4'
25	F	310	HTG	C1'-C2'-C3'-C4'
19	4	304	CLA	CBD-CGD-O2D-CED
19	1	307	CLA	C13-C15-C16-C17
19	B	805	CLA	C10-C11-C12-C13
19	B	806	CLA	C10-C11-C12-C13
26	A	841	PQN	C25-C26-C27-C28
23	1	320	LHG	C7-C8-C9-C10
19	A	827	CLA	C4-C3-C5-C6
19	A	806	CLA	C5-C6-C7-C8
19	3	305	CLA	C2A-CAA-CBA-CGA
19	4	310	CLA	C2A-CAA-CBA-CGA
19	A	806	CLA	C2A-CAA-CBA-CGA
19	B	810	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	CBA-CGA-O2A-C1
19	B	831	CLA	CBA-CGA-O2A-C1
19	1	302	CLA	C8-C10-C11-C12
18	3	315	BCR	C9-C10-C11-C12
18	A	846	BCR	C13-C14-C15-C16
18	K	304	BCR	C13-C14-C15-C16
18	K	304	BCR	C19-C20-C21-C22
18	O	106	BCR	C15-C16-C17-C18
21	1	314	LUT	C9-C10-C11-C12
22	2	315	XAT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	1	317	LHG	C15-C16-C17-C18
24	4	319	LMG	C29-C30-C31-C32
28	A	851	LMT	C3-C4-C5-C6
19	A	833	CLA	O1D-CGD-O2D-CED
18	L	301	BCR	C11-C10-C9-C34
18	L	306	BCR	C16-C17-C18-C36
18	2	316	BCR	C11-C10-C9-C34
18	2	316	BCR	C35-C13-C14-C15
18	4	318	BCR	C11-C10-C9-C34
18	4	318	BCR	C16-C17-C18-C36
18	A	845	BCR	C20-C21-C22-C37
18	A	847	BCR	C11-C10-C9-C34
18	A	847	BCR	C35-C13-C14-C15
18	A	848	BCR	C11-C10-C9-C34
18	A	848	BCR	C35-C13-C14-C15
18	B	842	BCR	C11-C10-C9-C34
18	B	842	BCR	C16-C17-C18-C36
18	B	842	BCR	C20-C21-C22-C37
18	B	843	BCR	C35-C13-C14-C15
18	B	843	BCR	C16-C17-C18-C36
18	B	844	BCR	C35-C13-C14-C15
18	F	304	BCR	C11-C10-C9-C34
18	F	304	BCR	C20-C21-C22-C37
18	G	201	BCR	C20-C21-C22-C37
18	G	206	BCR	C11-C10-C9-C34
18	I	101	BCR	C11-C10-C9-C34
18	J	103	BCR	C20-C21-C22-C37
18	J	104	BCR	C16-C17-C18-C36
18	K	304	BCR	C35-C13-C14-C15
21	2	314	LUT	C20-C13-C14-C15
21	3	313	LUT	C11-C10-C9-C19
21	4	316	LUT	C40-C33-C34-C35
22	1	315	XAT	C39-C29-C30-C31
22	4	317	XAT	C40-C33-C34-C35
19	2	303	CLA	C3-C5-C6-C7
19	A	812	CLA	C3-C5-C6-C7
23	2	318	LHG	C12-C13-C14-C15
23	4	322	LHG	C17-C18-C19-C20
24	4	319	LMG	C21-C22-C23-C24
24	B	849	LMG	C36-C37-C38-C39
24	J	101	LMG	C20-C21-C22-C23
29	B	847	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
29	B	847	DGD	C3B-C4B-C5B-C6B
19	B	832	CLA	O1D-CGD-O2D-CED
19	1	302	CLA	C16-C17-C18-C20
19	3	310	CLA	C6-C7-C8-C9
19	A	801	CLA	C16-C17-C18-C19
19	B	810	CLA	C16-C17-C18-C19
19	B	811	CLA	C6-C7-C8-C9
19	B	816	CLA	C6-C7-C8-C10
19	A	831	CLA	CBA-CGA-O2A-C1
23	A	842	LHG	C24-C23-O8-C6
23	4	320	LHG	C25-C26-C27-C28
23	4	322	LHG	C25-C26-C27-C28
24	4	319	LMG	C22-C23-C24-C25
24	F	309	LMG	C17-C18-C19-C20
24	J	101	LMG	C29-C30-C31-C32
29	B	847	DGD	C3A-C4A-C5A-C6A
29	B	847	DGD	C5A-C6A-C7A-C8A
19	2	307	CLA	C1-C2-C3-C4
19	3	308	CLA	C1-C2-C3-C4
19	3	308	CLA	C1-C2-C3-C5
19	A	832	CLA	C1-C2-C3-C5
19	B	830	CLA	C1-C2-C3-C4
19	G	204	CLA	C1-C2-C3-C5
23	2	317	LHG	C28-C29-C30-C31
23	4	322	LHG	C14-C15-C16-C17
19	O	101	CLA	O1D-CGD-O2D-CED
23	4	322	LHG	C5-C4-O6-P
28	A	851	LMT	C5-C6-C7-C8
19	O	104	CLA	O1D-CGD-O2D-CED
23	1	317	LHG	C11-C12-C13-C14
24	J	101	LMG	C38-C39-C40-C41
19	3	310	CLA	C3-C5-C6-C7
19	1	301	CLA	O1D-CGD-O2D-CED
19	2	301	CLA	O1D-CGD-O2D-CED
18	L	301	BCR	C11-C10-C9-C8
18	L	306	BCR	C16-C17-C18-C19
18	1	316	BCR	C11-C10-C9-C8
18	2	316	BCR	C11-C10-C9-C8
18	2	316	BCR	C12-C13-C14-C15
18	4	318	BCR	C11-C10-C9-C8
18	4	318	BCR	C16-C17-C18-C19
18	A	845	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	A	847	BCR	C12-C13-C14-C15
18	A	848	BCR	C11-C10-C9-C8
18	A	848	BCR	C12-C13-C14-C15
18	B	842	BCR	C11-C10-C9-C8
18	B	842	BCR	C12-C13-C14-C15
18	B	842	BCR	C16-C17-C18-C19
18	B	842	BCR	C20-C21-C22-C23
18	B	843	BCR	C12-C13-C14-C15
18	B	843	BCR	C16-C17-C18-C19
18	B	844	BCR	C12-C13-C14-C15
18	F	304	BCR	C11-C10-C9-C8
18	F	304	BCR	C20-C21-C22-C23
18	G	201	BCR	C20-C21-C22-C23
18	G	206	BCR	C11-C10-C9-C8
18	J	103	BCR	C20-C21-C22-C23
18	J	104	BCR	C16-C17-C18-C19
18	K	301	BCR	C20-C21-C22-C23
18	K	304	BCR	C11-C10-C9-C8
18	K	304	BCR	C12-C13-C14-C15
21	2	314	LUT	C12-C13-C14-C15
21	3	313	LUT	C11-C10-C9-C8
21	4	316	LUT	C32-C33-C34-C35
22	1	315	XAT	C28-C29-C30-C31
22	4	317	XAT	C32-C33-C34-C35
19	B	802	CLA	C1-C2-C3-C5
19	B	827	CLA	C1-C2-C3-C5
23	1	320	LHG	C31-C32-C33-C34
24	F	309	LMG	C18-C19-C20-C21
19	A	850	CLA	C15-C16-C17-C18
19	A	835	CLA	O1A-CGA-O2A-C1
24	G	202	LMG	O10-C28-O8-C9
19	2	301	CLA	C16-C17-C18-C20
19	2	311	CLA	C16-C17-C18-C19
19	A	824	CLA	C16-C17-C18-C19
19	K	303	CLA	C11-C12-C13-C15
19	B	815	CLA	O1D-CGD-O2D-CED
19	B	829	CLA	O1D-CGD-O2D-CED
19	1	307	CLA	C4-C3-C5-C6
19	A	825	CLA	C4-C3-C5-C6
19	F	307	CLA	C4-C3-C5-C6
19	1	302	CLA	C2-C3-C5-C6
19	A	827	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	1	301	CLA	C11-C12-C13-C14
19	A	815	CLA	C11-C12-C13-C14
19	A	819	CLA	C11-C10-C8-C9
19	A	825	CLA	C14-C13-C15-C16
19	A	852	CLA	C14-C13-C15-C16
19	B	807	CLA	C11-C10-C8-C9
19	B	828	CLA	C11-C10-C8-C9
19	L	303	CLA	C5-C6-C7-C8
19	A	838	CLA	C13-C15-C16-C17
19	B	827	CLA	C15-C16-C17-C18
19	4	313	CLA	C2A-CAA-CBA-CGA
19	A	833	CLA	C2A-CAA-CBA-CGA
19	B	801	CLA	C2A-CAA-CBA-CGA
19	B	828	CLA	C2A-CAA-CBA-CGA
20	4	305	CHL	C2A-CAA-CBA-CGA
19	A	802	CLA	O1A-CGA-O2A-C1
19	B	820	CLA	O1A-CGA-O2A-C1
19	B	836	CLA	O1A-CGA-O2A-C1
18	2	316	BCR	C11-C12-C13-C35
18	3	315	BCR	C11-C12-C13-C35
18	A	845	BCR	C36-C18-C19-C20
18	A	848	BCR	C37-C22-C23-C24
18	O	105	BCR	C37-C22-C23-C24
18	O	106	BCR	C37-C22-C23-C24
21	4	316	LUT	C11-C12-C13-C20
25	B	848	HTG	C2'-C3'-C4'-C5'
23	1	317	LHG	O1-C1-C2-C3
23	4	322	LHG	O1-C1-C2-C3
18	2	316	BCR	C11-C12-C13-C14
18	3	315	BCR	C11-C12-C13-C14
18	A	845	BCR	C17-C18-C19-C20
18	A	847	BCR	C17-C18-C19-C20
18	K	304	BCR	C7-C8-C9-C10
21	4	316	LUT	C11-C12-C13-C14
22	1	315	XAT	C7-C8-C9-C10
19	A	818	CLA	C3-C5-C6-C7
19	1	311	CLA	C10-C11-C12-C13
23	1	320	LHG	C30-C31-C32-C33
24	J	101	LMG	C28-C29-C30-C31
23	1	317	LHG	C25-C26-C27-C28
23	4	320	LHG	C15-C16-C17-C18
29	B	847	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
29	B	847	DGD	C7A-C8A-C9A-CAA
19	L	302	CLA	C4B-C3B-CAB-CBB
19	L	303	CLA	C4B-C3B-CAB-CBB
19	L	304	CLA	C4B-C3B-CAB-CBB
19	1	302	CLA	C4B-C3B-CAB-CBB
19	1	306	CLA	C4B-C3B-CAB-CBB
19	1	313	CLA	C4B-C3B-CAB-CBB
19	3	301	CLA	C4B-C3B-CAB-CBB
19	3	308	CLA	C4B-C3B-CAB-CBB
19	4	302	CLA	C4B-C3B-CAB-CBB
19	4	304	CLA	C4B-C3B-CAB-CBB
19	A	804	CLA	C4B-C3B-CAB-CBB
19	A	805	CLA	C4B-C3B-CAB-CBB
19	A	818	CLA	C4B-C3B-CAB-CBB
19	B	819	CLA	C4B-C3B-CAB-CBB
19	B	826	CLA	C4B-C3B-CAB-CBB
19	B	836	CLA	C4B-C3B-CAB-CBB
19	F	306	CLA	C4B-C3B-CAB-CBB
19	K	302	CLA	C4B-C3B-CAB-CBB
19	O	101	CLA	C4B-C3B-CAB-CBB
19	O	102	CLA	C4B-C3B-CAB-CBB
20	2	305	CHL	C4B-C3B-CAB-CBB
20	4	315	CHL	C4B-C3B-CAB-CBB
19	1	302	CLA	C16-C17-C18-C19
19	4	310	CLA	C11-C12-C13-C14
19	4	310	CLA	C11-C12-C13-C15
19	A	816	CLA	C16-C17-C18-C19
19	B	811	CLA	C6-C7-C8-C10
19	B	815	CLA	C6-C7-C8-C9
19	B	815	CLA	C6-C7-C8-C10
19	B	823	CLA	C11-C12-C13-C14
19	B	823	CLA	C11-C12-C13-C15
19	B	829	CLA	C16-C17-C18-C20
19	B	835	CLA	C10-C11-C12-C13
19	G	205	CLA	O1D-CGD-O2D-CED
23	1	320	LHG	C11-C10-C9-C8
24	4	319	LMG	C33-C34-C35-C36
24	B	849	LMG	C30-C31-C32-C33
24	J	101	LMG	C21-C22-C23-C24
19	A	837	CLA	CBD-CGD-O2D-CED
19	A	806	CLA	O1D-CGD-O2D-CED
23	1	320	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
24	J	101	LMG	C11-C12-C13-C14
29	B	847	DGD	C9A-CAA-CBA-CCA
23	4	320	LHG	C7-C8-C9-C10
19	A	825	CLA	C13-C15-C16-C17
19	B	808	CLA	C10-C11-C12-C13
19	B	818	CLA	C5-C6-C7-C8
19	K	303	CLA	O1A-CGA-O2A-C1
19	A	836	CLA	O1D-CGD-O2D-CED
24	4	319	LMG	C31-C32-C33-C34
19	4	302	CLA	O1D-CGD-O2D-CED
19	1	306	CLA	C3A-C2A-CAA-CBA
19	1	310	CLA	C3A-C2A-CAA-CBA
19	1	312	CLA	C3A-C2A-CAA-CBA
19	2	303	CLA	C3A-C2A-CAA-CBA
19	2	307	CLA	C3A-C2A-CAA-CBA
19	2	310	CLA	C3A-C2A-CAA-CBA
19	3	311	CLA	C3A-C2A-CAA-CBA
19	4	303	CLA	C3A-C2A-CAA-CBA
19	4	304	CLA	C3A-C2A-CAA-CBA
19	4	310	CLA	C3A-C2A-CAA-CBA
19	4	311	CLA	C3A-C2A-CAA-CBA
19	A	804	CLA	C3A-C2A-CAA-CBA
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	C3A-C2A-CAA-CBA
19	A	809	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A	825	CLA	C3A-C2A-CAA-CBA
19	A	830	CLA	C3A-C2A-CAA-CBA
19	A	834	CLA	C3A-C2A-CAA-CBA
19	A	854	CLA	C3A-C2A-CAA-CBA
19	B	822	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	F	307	CLA	C3A-C2A-CAA-CBA
19	O	104	CLA	C3A-C2A-CAA-CBA
20	1	305	CHL	C3A-C2A-CAA-CBA
19	1	306	CLA	CBA-CGA-O2A-C1
19	A	812	CLA	C6-C7-C8-C9
19	A	816	CLA	C16-C17-C18-C20
19	A	827	CLA	C16-C17-C18-C19
23	2	317	LHG	C24-C25-C26-C27
28	A	851	LMT	C2-C3-C4-C5
29	B	847	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
20	2	304	CHL	O1D-CGD-O2D-CED
24	J	101	LMG	C22-C23-C24-C25
19	B	817	CLA	O2A-C1-C2-C3
18	A	847	BCR	C14-C15-C16-C17
18	K	301	BCR	C14-C15-C16-C17
18	K	304	BCR	C14-C15-C16-C17
18	O	105	BCR	C14-C15-C16-C17
21	3	313	LUT	C14-C15-C35-C34
22	1	315	XAT	C14-C15-C35-C34
24	B	849	LMG	C10-C11-C12-C13
24	4	319	LMG	C17-C18-C19-C20
19	A	836	CLA	C4-C3-C5-C6
19	B	823	CLA	C4-C3-C5-C6
19	A	812	CLA	C2-C3-C5-C6
19	A	835	CLA	C2-C3-C5-C6
19	A	836	CLA	C2-C3-C5-C6
19	B	814	CLA	C2-C3-C5-C6
19	B	823	CLA	C2-C3-C5-C6
23	2	317	LHG	C8-C7-O7-C5
23	1	317	LHG	C10-C11-C12-C13
25	F	310	HTG	C2'-C3'-C4'-C5'
19	A	801	CLA	C1-C2-C3-C5
23	2	318	LHG	O1-C1-C2-O2
23	2	318	LHG	C13-C14-C15-C16
29	B	847	DGD	CDB-CEB-CFB-CGB
19	B	821	CLA	O1A-CGA-O2A-C1
23	A	842	LHG	O10-C23-O8-C6
19	L	302	CLA	C2B-C3B-CAB-CBB
19	L	303	CLA	C2B-C3B-CAB-CBB
19	L	304	CLA	C2B-C3B-CAB-CBB
19	1	302	CLA	C2B-C3B-CAB-CBB
19	1	306	CLA	C2B-C3B-CAB-CBB
19	1	307	CLA	C2B-C3B-CAB-CBB
19	1	313	CLA	C2B-C3B-CAB-CBB
19	2	303	CLA	C2B-C3B-CAB-CBB
19	3	301	CLA	C2B-C3B-CAB-CBB
19	3	308	CLA	C2B-C3B-CAB-CBB
19	3	310	CLA	C2B-C3B-CAB-CBB
19	4	302	CLA	C2B-C3B-CAB-CBB
19	4	304	CLA	C2B-C3B-CAB-CBB
19	4	314	CLA	C2B-C3B-CAB-CBB
19	A	804	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	805	CLA	C2B-C3B-CAB-CBB
19	A	807	CLA	C2B-C3B-CAB-CBB
19	A	811	CLA	C2B-C3B-CAB-CBB
19	A	818	CLA	C2B-C3B-CAB-CBB
19	B	819	CLA	C2B-C3B-CAB-CBB
19	F	306	CLA	C2B-C3B-CAB-CBB
19	G	203	CLA	C2B-C3B-CAB-CBB
19	K	302	CLA	C2B-C3B-CAB-CBB
19	O	101	CLA	C2B-C3B-CAB-CBB
19	O	102	CLA	C2B-C3B-CAB-CBB
20	2	305	CHL	C2B-C3B-CAB-CBB
20	4	315	CHL	C2B-C3B-CAB-CBB
23	1	320	LHG	C33-C34-C35-C36
19	B	810	CLA	O1A-CGA-O2A-C1
19	B	831	CLA	O1A-CGA-O2A-C1
23	2	318	LHG	C7-C8-C9-C10
23	4	322	LHG	C1-C2-C3-O3
25	B	848	HTG	C3'-C4'-C5'-C6'
23	2	317	LHG	O9-C7-O7-C5
19	4	303	CLA	C2-C1-O2A-CGA
24	J	101	LMG	C34-C35-C36-C37
19	A	827	CLA	C15-C16-C17-C18
19	A	839	CLA	C10-C11-C12-C13
28	A	851	LMT	C1-C2-C3-C4
29	B	847	DGD	C4E-C5E-C6E-O5E
23	4	320	LHG	C17-C18-C19-C20
24	4	319	LMG	C30-C31-C32-C33
25	F	301	HTG	C2'-C3'-C4'-C5'
19	L	303	CLA	C16-C17-C18-C20
19	A	801	CLA	C16-C17-C18-C20
29	B	847	DGD	C1B-C2B-C3B-C4B
18	L	301	BCR	C1-C6-C7-C8
18	L	301	BCR	C5-C6-C7-C8
18	L	305	BCR	C23-C24-C25-C30
18	L	306	BCR	C23-C24-C25-C26
18	L	306	BCR	C23-C24-C25-C30
18	1	316	BCR	C23-C24-C25-C26
18	3	315	BCR	C23-C24-C25-C26
18	4	318	BCR	C23-C24-C25-C30
18	A	844	BCR	C1-C6-C7-C8
18	A	847	BCR	C1-C6-C7-C8
18	A	848	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	A	848	BCR	C23-C24-C25-C30
18	B	844	BCR	C23-C24-C25-C26
18	B	844	BCR	C23-C24-C25-C30
18	B	846	BCR	C5-C6-C7-C8
18	B	846	BCR	C23-C24-C25-C26
18	F	302	BCR	C23-C24-C25-C26
18	F	302	BCR	C23-C24-C25-C30
18	G	201	BCR	C23-C24-C25-C30
18	G	206	BCR	C23-C24-C25-C26
18	J	103	BCR	C23-C24-C25-C26
18	J	103	BCR	C23-C24-C25-C30
18	J	104	BCR	C1-C6-C7-C8
18	J	104	BCR	C5-C6-C7-C8
18	O	105	BCR	C23-C24-C25-C26
18	O	105	BCR	C23-C24-C25-C30
18	O	106	BCR	C23-C24-C25-C26
18	O	106	BCR	C23-C24-C25-C30
19	B	819	CLA	C3-C5-C6-C7
19	B	821	CLA	C3-C5-C6-C7
21	1	314	LUT	C1-C6-C7-C8
21	1	314	LUT	C5-C6-C7-C8
21	2	314	LUT	C5-C6-C7-C8
23	2	317	LHG	C11-C10-C9-C8
19	B	840	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	C13-C15-C16-C17
19	A	824	CLA	C10-C11-C12-C13
19	A	840	CLA	C8-C10-C11-C12
19	A	850	CLA	C13-C15-C16-C17
19	B	831	CLA	C8-C10-C11-C12
23	A	842	LHG	C12-C13-C14-C15
19	A	831	CLA	O1A-CGA-O2A-C1
19	4	312	CLA	C11-C10-C8-C9
23	2	318	LHG	C35-C36-C37-C38
24	4	319	LMG	C20-C21-C22-C23
19	3	312	CLA	O1A-CGA-O2A-C1
19	B	819	CLA	C10-C11-C12-C13
19	A	812	CLA	C4-C3-C5-C6
19	A	827	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	O1D-CGD-O2D-CED
19	L	303	CLA	C6-C7-C8-C10
19	1	307	CLA	C2-C3-C5-C6
19	A	803	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	A	805	CLA	C6-C7-C8-C10
19	A	815	CLA	C12-C13-C15-C16
19	A	817	CLA	C11-C12-C13-C15
19	A	818	CLA	C6-C7-C8-C10
19	A	824	CLA	C11-C12-C13-C15
19	A	824	CLA	C12-C13-C15-C16
19	A	825	CLA	C2-C3-C5-C6
19	A	827	CLA	C11-C12-C13-C15
19	A	835	CLA	C6-C7-C8-C10
19	A	838	CLA	C2-C3-C5-C6
19	B	806	CLA	C11-C12-C13-C15
19	B	809	CLA	C11-C10-C8-C7
19	B	809	CLA	C12-C13-C15-C16
19	B	813	CLA	C12-C13-C15-C16
19	B	818	CLA	C11-C10-C8-C7
19	B	825	CLA	C12-C13-C15-C16
19	B	827	CLA	C11-C12-C13-C15
19	B	833	CLA	C6-C7-C8-C10
19	F	307	CLA	C2-C3-C5-C6
23	A	842	LHG	C19-C20-C21-C22
24	G	202	LMG	C11-C12-C13-C14
18	L	305	BCR	C15-C16-C17-C18
18	4	318	BCR	C19-C20-C21-C22
18	B	842	BCR	C19-C20-C21-C22
18	F	308	BCR	C9-C10-C11-C12
18	O	105	BCR	C13-C14-C15-C16
19	A	824	CLA	C16-C17-C18-C20
19	B	825	CLA	C16-C17-C18-C19
19	1	310	CLA	O1D-CGD-O2D-CED
19	B	804	CLA	O1D-CGD-O2D-CED
24	J	101	LMG	C10-C11-C12-C13
19	3	310	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	CBA-CGA-O2A-C1
19	B	802	CLA	CBA-CGA-O2A-C1
19	B	813	CLA	CBA-CGA-O2A-C1
23	1	317	LHG	C24-C23-O8-C6
24	J	101	LMG	C32-C33-C34-C35
19	A	811	CLA	C2A-CAA-CBA-CGA
19	B	828	CLA	C15-C16-C17-C18
19	B	835	CLA	C8-C10-C11-C12
23	4	320	LHG	C9-C10-C11-C12
29	B	847	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
19	4	312	CLA	C11-C10-C8-C7
24	F	309	LMG	C28-C29-C30-C31
19	1	301	CLA	C15-C16-C17-C18
19	B	829	CLA	C15-C16-C17-C18
19	A	819	CLA	C3-C5-C6-C7
23	1	317	LHG	C12-C13-C14-C15
18	F	302	BCR	C6-C7-C8-C9
18	K	301	BCR	C22-C23-C24-C25
19	A	831	CLA	C16-C17-C18-C19
24	B	849	LMG	O6-C1-O1-C7
19	A	824	CLA	C5-C6-C7-C8
19	1	306	CLA	O1D-CGD-O2D-CED
19	B	801	CLA	O1D-CGD-O2D-CED
23	4	322	LHG	C9-C10-C11-C12
24	G	202	LMG	C16-C17-C18-C19
23	1	320	LHG	C8-C7-O7-C5
24	4	319	LMG	C11-C10-O7-C8
22	2	315	XAT	C10-C11-C12-C13
18	J	104	BCR	C14-C15-C16-C17
19	1	302	CLA	C10-C11-C12-C13
19	B	822	CLA	CBD-CGD-O2D-CED
23	1	320	LHG	O9-C7-O7-C5
24	4	319	LMG	O9-C10-O7-C8
19	4	311	CLA	C3-C5-C6-C7
24	B	849	LMG	C2-C1-O1-C7
19	L	302	CLA	C5-C6-C7-C8
19	B	836	CLA	C15-C16-C17-C18
29	B	847	DGD	O2G-C2G-C3G-O3G
25	F	303	HTG	C4'-C5'-C6'-C7'
23	2	318	LHG	C10-C11-C12-C13
19	A	819	CLA	C10-C11-C12-C13
19	B	840	CLA	C5-C6-C7-C8
19	B	814	CLA	C4-C3-C5-C6
23	1	320	LHG	C23-C24-C25-C26
23	A	842	LHG	C23-C24-C25-C26
23	A	843	LHG	C9-C10-C11-C12
19	L	303	CLA	C6-C7-C8-C9
19	1	302	CLA	C6-C7-C8-C9
19	A	805	CLA	C6-C7-C8-C9
19	A	815	CLA	C6-C7-C8-C9
19	A	815	CLA	C14-C13-C15-C16
19	A	817	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	A	818	CLA	C14-C13-C15-C16
19	A	824	CLA	C11-C10-C8-C9
19	A	824	CLA	C11-C12-C13-C14
19	A	827	CLA	C11-C12-C13-C14
19	A	828	CLA	C14-C13-C15-C16
19	A	835	CLA	C6-C7-C8-C9
19	B	806	CLA	C11-C12-C13-C14
19	B	809	CLA	C11-C10-C8-C9
19	B	814	CLA	C6-C7-C8-C9
19	B	824	CLA	C11-C10-C8-C9
19	B	827	CLA	C14-C13-C15-C16
19	B	833	CLA	C6-C7-C8-C9
19	B	835	CLA	C6-C7-C8-C9
19	B	839	CLA	C14-C13-C15-C16
19	3	301	CLA	C2A-CAA-CBA-CGA
18	K	304	BCR	C11-C12-C13-C35
18	O	106	BCR	C36-C18-C19-C20
19	B	809	CLA	C8-C10-C11-C12
24	J	101	LMG	C30-C31-C32-C33
18	K	304	BCR	C11-C12-C13-C14
18	K	304	BCR	C21-C22-C23-C24
18	O	106	BCR	C17-C18-C19-C20
19	B	840	CLA	O1A-CGA-O2A-C1
19	L	304	CLA	C1A-C2A-CAA-CBA
19	1	301	CLA	C1A-C2A-CAA-CBA
19	1	308	CLA	C1A-C2A-CAA-CBA
19	1	309	CLA	C1A-C2A-CAA-CBA
19	1	310	CLA	C1A-C2A-CAA-CBA
19	2	308	CLA	C1A-C2A-CAA-CBA
19	3	308	CLA	C1A-C2A-CAA-CBA
19	3	311	CLA	C1A-C2A-CAA-CBA
19	3	316	CLA	C1A-C2A-CAA-CBA
19	4	310	CLA	C1A-C2A-CAA-CBA
19	4	314	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C1A-C2A-CAA-CBA
19	A	830	CLA	C1A-C2A-CAA-CBA
19	A	832	CLA	C1A-C2A-CAA-CBA
19	A	834	CLA	C1A-C2A-CAA-CBA
19	A	839	CLA	C1A-C2A-CAA-CBA
19	A	853	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C1A-C2A-CAA-CBA
19	B	814	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	817	CLA	C1A-C2A-CAA-CBA
19	B	818	CLA	C1A-C2A-CAA-CBA
19	B	820	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	C1A-C2A-CAA-CBA
19	B	837	CLA	C1A-C2A-CAA-CBA
19	B	840	CLA	C1A-C2A-CAA-CBA
19	F	307	CLA	C1A-C2A-CAA-CBA
20	3	306	CHL	C1A-C2A-CAA-CBA
24	G	202	LMG	O6-C5-C6-O5
19	L	303	CLA	C16-C17-C18-C19
19	3	310	CLA	C6-C7-C8-C10
19	A	827	CLA	C16-C17-C18-C20
19	A	831	CLA	C16-C17-C18-C20
19	B	816	CLA	C6-C7-C8-C9
23	1	320	LHG	C11-C12-C13-C14
18	2	316	BCR	C15-C16-C17-C18
22	3	314	XAT	C13-C14-C15-C35
19	B	803	CLA	C8-C10-C11-C12
19	B	832	CLA	C5-C6-C7-C8
23	1	320	LHG	C29-C30-C31-C32
23	4	320	LHG	C23-C24-C25-C26
19	B	823	CLA	C3-C5-C6-C7
23	2	318	LHG	C5-C4-O6-P
19	A	838	CLA	C8-C10-C11-C12
19	B	824	CLA	C5-C6-C7-C8
19	1	301	CLA	CBA-CGA-O2A-C1
19	A	816	CLA	CBA-CGA-O2A-C1
24	G	202	LMG	C20-C21-C22-C23
20	3	306	CHL	O1A-CGA-O2A-C1
23	2	318	LHG	C27-C28-C29-C30
19	B	825	CLA	C15-C16-C17-C18
19	K	303	CLA	C11-C12-C13-C14
20	4	305	CHL	C6-C7-C8-C9
19	B	833	CLA	O1D-CGD-O2D-CED
19	A	807	CLA	C3-C5-C6-C7
19	A	803	CLA	C13-C15-C16-C17
19	B	833	CLA	C10-C11-C12-C13
23	A	842	LHG	C24-C25-C26-C27
23	4	320	LHG	C1-C2-C3-O3
19	A	808	CLA	C4-C3-C5-C6
19	A	838	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B	802	CLA	C4-C3-C5-C6
19	J	102	CLA	C3A-C2A-CAA-CBA
24	B	849	LMG	C33-C34-C35-C36
28	A	851	LMT	C4-C5-C6-C7
19	L	302	CLA	C8-C10-C11-C12
19	A	828	CLA	O1A-CGA-O2A-C1
23	2	318	LHG	C14-C15-C16-C17
28	A	851	LMT	C6-C7-C8-C9
19	A	818	CLA	C10-C11-C12-C13
19	A	854	CLA	C15-C16-C17-C18
19	B	822	CLA	C2A-CAA-CBA-CGA
19	B	827	CLA	C16-C17-C18-C20
19	4	313	CLA	O1D-CGD-O2D-CED
24	J	101	LMG	O1-C7-C8-C9
19	A	815	CLA	C13-C15-C16-C17
19	A	852	CLA	C15-C16-C17-C18
19	B	813	CLA	C13-C15-C16-C17
24	4	319	LMG	C37-C38-C39-C40
19	3	310	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	O1A-CGA-O2A-C1
23	1	317	LHG	O10-C23-O8-C6
24	G	202	LMG	C21-C22-C23-C24
19	K	303	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	C10-C11-C12-C13
25	F	303	HTG	O5-C5-C6-O6
29	B	847	DGD	CBB-CCB-CDB-CEB
19	L	302	CLA	C3-C5-C6-C7
19	A	803	CLA	C15-C16-C17-C18
19	B	828	CLA	C10-C11-C12-C13
23	2	318	LHG	C17-C18-C19-C20
23	1	320	LHG	O1-C1-C2-O2
24	4	319	LMG	C36-C37-C38-C39
19	A	805	CLA	C5-C6-C7-C8
19	A	840	CLA	C10-C11-C12-C13
23	2	317	LHG	C25-C26-C27-C28
23	2	318	LHG	C11-C10-C9-C8
23	A	842	LHG	C14-C15-C16-C17
19	L	302	CLA	O1D-CGD-O2D-CED
19	B	823	CLA	C5-C6-C7-C8
18	1	316	BCR	C16-C17-C18-C36
18	3	315	BCR	C16-C17-C18-C36
21	1	314	LUT	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	4	309	CLA	C4-C3-C5-C6
23	2	317	LHG	C12-C13-C14-C15
25	F	305	HTG	C2'-C3'-C4'-C5'
19	2	301	CLA	C16-C17-C18-C19
19	L	303	CLA	CBA-CGA-O2A-C1
19	B	828	CLA	CBA-CGA-O2A-C1
19	B	839	CLA	CBA-CGA-O2A-C1
19	B	832	CLA	C10-C11-C12-C13
24	B	849	LMG	C34-C35-C36-C37
20	2	306	CHL	CBD-CGD-O2D-CED
19	A	835	CLA	C13-C15-C16-C17
19	A	852	CLA	C8-C10-C11-C12
19	B	820	CLA	C2A-CAA-CBA-CGA
19	O	101	CLA	C2A-CAA-CBA-CGA
19	B	813	CLA	O1A-CGA-O2A-C1
19	2	307	CLA	C1-C2-C3-C5
19	3	302	CLA	C2-C1-O2A-CGA
19	A	832	CLA	C1-C2-C3-C4
19	B	839	CLA	C2-C1-O2A-CGA
19	G	204	CLA	C1-C2-C3-C4
19	A	823	CLA	O1D-CGD-O2D-CED
19	A	831	CLA	C13-C15-C16-C17
19	B	840	CLA	C15-C16-C17-C18
23	1	320	LHG	C2-C3-O3-P
23	1	320	LHG	C35-C36-C37-C38
24	G	202	LMG	C13-C14-C15-C16
19	B	811	CLA	CBA-CGA-O2A-C1
23	4	322	LHG	C24-C23-O8-C6
23	4	320	LHG	O6-C4-C5-O7
19	A	828	CLA	C16-C17-C18-C19
19	A	850	CLA	C16-C17-C18-C20
19	3	310	CLA	C5-C6-C7-C8
19	A	803	CLA	C10-C11-C12-C13
23	2	318	LHG	C31-C32-C33-C34
23	4	320	LHG	C11-C10-C9-C8
19	4	304	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	O1D-CGD-O2D-CED
23	4	322	LHG	C7-C8-C9-C10
19	1	301	CLA	C8-C10-C11-C12
19	3	301	CLA	C5-C6-C7-C8
18	3	315	BCR	C16-C17-C18-C19
18	A	847	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	I	101	BCR	C11-C10-C9-C8
21	1	314	LUT	C32-C33-C34-C35
23	1	319	LHG	O7-C5-C6-O8
19	A	816	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	C16-C17-C18-C20
25	F	301	HTG	C4'-C5'-C6'-C7'
19	1	302	CLA	C12-C13-C15-C16
19	1	307	CLA	C11-C10-C8-C7
19	1	309	CLA	C6-C7-C8-C10
19	1	309	CLA	C12-C13-C15-C16
19	2	301	CLA	C11-C12-C13-C15
19	2	311	CLA	C11-C10-C8-C7
19	2	311	CLA	C12-C13-C15-C16
19	4	309	CLA	C2-C3-C5-C6
19	4	309	CLA	C11-C10-C8-C7
19	4	312	CLA	C6-C7-C8-C10
19	A	805	CLA	C12-C13-C15-C16
19	A	808	CLA	C11-C12-C13-C15
19	A	811	CLA	C11-C12-C13-C15
19	A	816	CLA	C12-C13-C15-C16
19	A	826	CLA	C11-C10-C8-C7
19	A	826	CLA	C11-C12-C13-C15
19	A	826	CLA	C12-C13-C15-C16
19	A	827	CLA	C12-C13-C15-C16
19	A	828	CLA	C11-C10-C8-C7
19	A	828	CLA	C12-C13-C15-C16
19	A	830	CLA	C11-C10-C8-C7
19	A	830	CLA	C12-C13-C15-C16
19	A	831	CLA	C11-C10-C8-C7
19	A	835	CLA	C11-C12-C13-C15
19	A	836	CLA	C12-C13-C15-C16
19	A	839	CLA	C6-C7-C8-C10
19	A	840	CLA	C6-C7-C8-C10
19	A	840	CLA	C11-C12-C13-C15
19	A	840	CLA	C12-C13-C15-C16
19	A	850	CLA	C11-C10-C8-C7
19	B	802	CLA	C12-C13-C15-C16
19	B	807	CLA	C11-C10-C8-C7
19	B	807	CLA	C12-C13-C15-C16
19	B	824	CLA	C11-C10-C8-C7
19	B	824	CLA	C12-C13-C15-C16
19	B	825	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	B	839	CLA	C12-C13-C15-C16
19	K	303	CLA	C6-C7-C8-C10
23	1	320	LHG	C13-C14-C15-C16
19	1	302	CLA	C14-C13-C15-C16
19	1	307	CLA	C11-C10-C8-C9
19	1	309	CLA	C6-C7-C8-C9
19	1	309	CLA	C14-C13-C15-C16
19	2	301	CLA	C11-C10-C8-C9
19	2	301	CLA	C11-C12-C13-C14
19	2	308	CLA	C6-C7-C8-C9
19	2	311	CLA	C14-C13-C15-C16
19	4	309	CLA	C11-C10-C8-C9
19	A	803	CLA	C11-C12-C13-C14
19	A	805	CLA	C14-C13-C15-C16
19	A	811	CLA	C11-C12-C13-C14
19	A	816	CLA	C11-C10-C8-C9
19	A	826	CLA	C11-C12-C13-C14
19	A	827	CLA	C14-C13-C15-C16
19	A	828	CLA	C11-C10-C8-C9
19	A	836	CLA	C14-C13-C15-C16
19	A	837	CLA	C11-C12-C13-C14
19	A	839	CLA	C6-C7-C8-C9
19	A	840	CLA	C6-C7-C8-C9
19	A	840	CLA	C11-C12-C13-C14
19	A	850	CLA	C11-C10-C8-C9
19	A	853	CLA	C14-C13-C15-C16
19	B	806	CLA	C11-C10-C8-C9
19	B	810	CLA	C11-C12-C13-C14
19	B	813	CLA	C11-C12-C13-C14
19	B	819	CLA	C6-C7-C8-C9
19	B	823	CLA	C11-C10-C8-C9
19	B	829	CLA	C14-C13-C15-C16
18	F	308	BCR	C14-C15-C16-C17
23	4	322	LHG	C13-C14-C15-C16
19	4	304	CLA	CBA-CGA-O2A-C1
19	A	824	CLA	CBA-CGA-O2A-C1
19	A	830	CLA	C15-C16-C17-C18
19	B	838	CLA	C13-C15-C16-C17
18	A	846	BCR	C11-C12-C13-C35
18	F	308	BCR	C37-C22-C23-C24
18	J	104	BCR	C7-C8-C9-C34
18	K	301	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	K	301	BCR	C37-C22-C23-C24
19	A	811	CLA	C16-C17-C18-C19
19	B	839	CLA	C16-C17-C18-C19
18	A	845	BCR	C21-C22-C23-C24
18	B	843	BCR	C21-C22-C23-C24
18	G	206	BCR	C7-C8-C9-C10
25	F	310	HTG	C4'-C5'-C6'-C7'
19	A	835	CLA	C3-C5-C6-C7
19	A	837	CLA	O1D-CGD-O2D-CED
19	A	809	CLA	C15-C16-C17-C18
19	B	813	CLA	C15-C16-C17-C18
20	1	318	CHL	C8-C10-C11-C12
19	1	301	CLA	O1A-CGA-O2A-C1
19	A	808	CLA	CBA-CGA-O2A-C1
19	A	819	CLA	CBA-CGA-O2A-C1
19	A	808	CLA	C8-C10-C11-C12
19	B	814	CLA	C5-C6-C7-C8
19	B	821	CLA	C8-C10-C11-C12
19	B	817	CLA	C10-C11-C12-C13
24	4	319	LMG	C16-C17-C18-C19
19	1	308	CLA	C4B-C3B-CAB-CBB
19	2	303	CLA	C4B-C3B-CAB-CBB
19	3	310	CLA	C4B-C3B-CAB-CBB
19	A	811	CLA	C4B-C3B-CAB-CBB
19	A	824	CLA	C4B-C3B-CAB-CBB
19	A	827	CLA	C4B-C3B-CAB-CBB
19	A	853	CLA	C4B-C3B-CAB-CBB
19	A	854	CLA	C4B-C3B-CAB-CBB
19	B	803	CLA	C4B-C3B-CAB-CBB
19	B	818	CLA	C4B-C3B-CAB-CBB
19	B	821	CLA	C4B-C3B-CAB-CBB
19	B	824	CLA	C4B-C3B-CAB-CBB
19	B	825	CLA	C4B-C3B-CAB-CBB
19	B	827	CLA	C4B-C3B-CAB-CBB
19	B	825	CLA	C16-C17-C18-C20
19	A	807	CLA	C5-C6-C7-C8
23	1	320	LHG	O6-C4-C5-C6
19	B	839	CLA	C3-C5-C6-C7
19	B	802	CLA	C5-C6-C7-C8
23	A	842	LHG	C32-C33-C34-C35
19	2	310	CLA	C4-C3-C5-C6
19	A	827	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	J	101	LMG	C14-C15-C16-C17
19	A	811	CLA	CBA-CGA-O2A-C1
23	1	317	LHG	C2-C3-O3-P
23	4	320	LHG	C2-C3-O3-P
19	B	823	CLA	CBD-CGD-O2D-CED
19	3	305	CLA	C3A-C2A-CAA-CBA
19	A	822	CLA	C3A-C2A-CAA-CBA
19	O	103	CLA	C3A-C2A-CAA-CBA
20	2	306	CHL	C3A-C2A-CAA-CBA
19	B	825	CLA	C10-C11-C12-C13
23	1	317	LHG	C11-C10-C9-C8
29	B	847	DGD	O6E-C5E-C6E-O5E
18	1	316	BCR	C19-C20-C21-C22
18	A	848	BCR	C15-C16-C17-C18
18	B	844	BCR	C19-C20-C21-C22
18	B	845	BCR	C19-C20-C21-C22
23	4	320	LHG	C27-C28-C29-C30
23	A	842	LHG	C15-C16-C17-C18
19	B	812	CLA	C6-C7-C8-C10
19	B	829	CLA	C16-C17-C18-C19
19	A	821	CLA	CBA-CGA-O2A-C1
19	B	825	CLA	CBA-CGA-O2A-C1
19	A	854	CLA	C8-C10-C11-C12
19	B	829	CLA	C8-C10-C11-C12
19	B	850	CLA	C15-C16-C17-C18
23	1	317	LHG	C4-C5-C6-O8
23	1	319	LHG	C4-C5-C6-O8
19	B	811	CLA	O2A-C1-C2-C3
19	B	830	CLA	O2A-C1-C2-C3
19	B	850	CLA	O2A-C1-C2-C3
19	B	828	CLA	O1A-CGA-O2A-C1
23	4	322	LHG	O10-C23-O8-C6
24	F	309	LMG	C16-C17-C18-C19
19	4	303	CLA	C8-C10-C11-C12
20	4	307	CHL	C3C-C2C-CMC-OMC
19	L	303	CLA	O1A-CGA-O2A-C1
19	B	839	CLA	O1A-CGA-O2A-C1
19	A	822	CLA	O1D-CGD-O2D-CED
19	4	304	CLA	C2A-CAA-CBA-CGA
23	A	842	LHG	O6-C4-C5-O7
19	B	833	CLA	CBA-CGA-O2A-C1
19	B	811	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	805	CLA	C16-C17-C18-C20
19	A	828	CLA	C16-C17-C18-C20
20	1	318	CHL	C11-C12-C13-C14
23	1	317	LHG	C27-C28-C29-C30
19	B	818	CLA	C2B-C3B-CAB-CBB
19	B	821	CLA	C2B-C3B-CAB-CBB
19	B	827	CLA	C2B-C3B-CAB-CBB
23	1	317	LHG	C9-C10-C11-C12
24	G	202	LMG	C12-C13-C14-C15
19	A	808	CLA	O1A-CGA-O2A-C1
19	A	824	CLA	O1A-CGA-O2A-C1
23	1	317	LHG	O7-C5-C6-O8
19	4	302	CLA	CBA-CGA-O2A-C1
19	1	311	CLA	C11-C12-C13-C14
19	2	311	CLA	C16-C17-C18-C20
19	A	826	CLA	C16-C17-C18-C19
19	A	830	CLA	C16-C17-C18-C20
19	A	837	CLA	C16-C17-C18-C19
19	B	821	CLA	C16-C17-C18-C19
19	B	827	CLA	C16-C17-C18-C19
20	1	318	CHL	C10-C11-C12-C13
19	A	818	CLA	C2-C1-O2A-CGA
19	A	854	CLA	C2-C1-O2A-CGA
19	B	814	CLA	C2-C1-O2A-CGA
19	B	827	CLA	C2-C1-O2A-CGA
23	1	317	LHG	C28-C29-C30-C31
19	B	818	CLA	C10-C11-C12-C13
25	F	301	HTG	C1'-C2'-C3'-C4'
19	1	311	CLA	C11-C10-C8-C9
19	3	301	CLA	C11-C10-C8-C9
19	A	803	CLA	C6-C7-C8-C9
19	A	808	CLA	C11-C10-C8-C9
19	A	818	CLA	C11-C12-C13-C14
19	A	840	CLA	C14-C13-C15-C16
19	B	810	CLA	C14-C13-C15-C16
19	B	814	CLA	C14-C13-C15-C16
19	B	821	CLA	C6-C7-C8-C9
19	B	825	CLA	C6-C7-C8-C9
19	B	828	CLA	C14-C13-C15-C16
19	B	833	CLA	C11-C10-C8-C9
19	B	836	CLA	C14-C13-C15-C16
19	K	303	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	806	CLA	C15-C16-C17-C18
19	1	303	CLA	C4-C3-C5-C6
23	1	320	LHG	C5-C4-O6-P
23	2	317	LHG	C5-C4-O6-P
29	B	847	DGD	CFA-CGA-CHA-CIA
19	A	804	CLA	C2A-CAA-CBA-CGA
19	A	839	CLA	C2A-CAA-CBA-CGA
19	B	810	CLA	C2A-CAA-CBA-CGA
19	1	308	CLA	C11-C12-C13-C14
19	A	804	CLA	C16-C17-C18-C19
19	A	812	CLA	C6-C7-C8-C10
19	B	835	CLA	C11-C12-C13-C14
18	A	847	BCR	C5-C6-C7-C8
18	A	847	BCR	C23-C24-C25-C26
18	F	308	BCR	C23-C24-C25-C26
18	F	308	BCR	C23-C24-C25-C30
18	G	201	BCR	C5-C6-C7-C8
18	G	201	BCR	C23-C24-C25-C26
18	I	101	BCR	C1-C6-C7-C8
18	I	101	BCR	C5-C6-C7-C8
18	J	104	BCR	C23-C24-C25-C26
18	J	104	BCR	C23-C24-C25-C30
18	K	301	BCR	C1-C6-C7-C8
18	K	301	BCR	C5-C6-C7-C8
21	3	313	LUT	C5-C6-C7-C8
21	4	316	LUT	C1-C6-C7-C8
21	4	316	LUT	C5-C6-C7-C8
19	A	828	CLA	C5-C6-C7-C8
19	A	836	CLA	C13-C15-C16-C17
19	B	822	CLA	O1D-CGD-O2D-CED
19	4	304	CLA	O1A-CGA-O2A-C1
18	L	306	BCR	C21-C22-C23-C24
18	1	316	BCR	C11-C12-C13-C14
18	A	845	BCR	C7-C8-C9-C10
18	A	848	BCR	C7-C8-C9-C10
18	J	103	BCR	C17-C18-C19-C20
23	1	320	LHG	C32-C33-C34-C35
19	A	819	CLA	O1A-CGA-O2A-C1
19	B	839	CLA	C16-C17-C18-C20
19	1	311	CLA	C5-C6-C7-C8
23	1	319	LHG	O6-C4-C5-C6
23	4	322	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
23	A	842	LHG	O6-C4-C5-C6
19	L	303	CLA	C11-C10-C8-C7
19	L	303	CLA	C12-C13-C15-C16
19	1	308	CLA	C11-C10-C8-C7
19	1	311	CLA	C11-C10-C8-C7
19	2	303	CLA	C6-C7-C8-C10
19	3	301	CLA	C11-C10-C8-C7
19	A	808	CLA	C12-C13-C15-C16
19	A	818	CLA	C11-C12-C13-C15
19	A	830	CLA	C11-C12-C13-C15
19	A	837	CLA	C11-C12-C13-C15
19	A	838	CLA	C6-C7-C8-C10
19	A	853	CLA	C6-C7-C8-C10
19	B	813	CLA	C11-C12-C13-C15
19	B	818	CLA	C6-C7-C8-C10
19	B	821	CLA	C11-C12-C13-C15
19	B	821	CLA	C12-C13-C15-C16
19	B	823	CLA	C11-C10-C8-C7
19	B	825	CLA	C11-C10-C8-C7
19	B	831	CLA	C11-C10-C8-C7
19	B	833	CLA	C12-C13-C15-C16
19	B	836	CLA	C12-C13-C15-C16
19	B	838	CLA	C12-C13-C15-C16
19	B	839	CLA	C11-C10-C8-C7
19	B	850	CLA	C12-C13-C15-C16
19	B	801	CLA	C8-C10-C11-C12
19	B	813	CLA	C8-C10-C11-C12
18	3	315	BCR	C13-C14-C15-C16
18	B	846	BCR	C15-C16-C17-C18
18	F	302	BCR	C13-C14-C15-C16
18	J	103	BCR	C19-C20-C21-C22
18	J	104	BCR	C13-C14-C15-C16
22	1	315	XAT	C9-C10-C11-C12
22	3	314	XAT	C29-C30-C31-C32
20	4	305	CHL	C6-C7-C8-C10
19	B	808	CLA	C15-C16-C17-C18
19	1	303	CLA	C2A-CAA-CBA-CGA
18	L	301	BCR	C35-C13-C14-C15
18	L	306	BCR	C11-C10-C9-C34
18	A	844	BCR	C16-C17-C18-C36
18	J	103	BCR	C35-C13-C14-C15
18	O	106	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
22	2	315	XAT	C40-C33-C34-C35
25	B	848	HTG	C2'-C1'-S1-C1
19	A	805	CLA	C3-C5-C6-C7
29	B	847	DGD	CCA-CDA-CEA-CFA
19	A	807	CLA	CBD-CGD-O2D-CED
19	A	850	CLA	C16-C17-C18-C19
19	1	309	CLA	C15-C16-C17-C18
19	A	812	CLA	CBA-CGA-O2A-C1
19	B	819	CLA	CBA-CGA-O2A-C1
19	2	303	CLA	C10-C11-C12-C13
19	A	823	CLA	C8-C10-C11-C12
19	1	301	CLA	CAD-CBD-CGD-O2D
19	1	302	CLA	CAD-CBD-CGD-O2D
19	2	301	CLA	CAD-CBD-CGD-O2D
19	2	303	CLA	CAD-CBD-CGD-O2D
19	3	301	CLA	CAD-CBD-CGD-O2D
19	3	307	CLA	CAD-CBD-CGD-O2D
19	4	302	CLA	CAD-CBD-CGD-O2D
19	4	308	CLA	CAD-CBD-CGD-O2D
19	A	820	CLA	CAD-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O2D
19	B	824	CLA	CAD-CBD-CGD-O2D
19	B	837	CLA	CAD-CBD-CGD-O2D
19	B	838	CLA	CAD-CBD-CGD-O2D
19	F	306	CLA	CAD-CBD-CGD-O2D
20	2	319	CHL	CAD-CBD-CGD-O2D
20	3	306	CHL	CAD-CBD-CGD-O2D
23	4	322	LHG	C12-C13-C14-C15
19	B	826	CLA	C5-C6-C7-C8
18	A	846	BCR	C6-C7-C8-C9
18	G	206	BCR	C6-C7-C8-C9
18	J	104	BCR	C22-C23-C24-C25
19	3	301	CLA	CBA-CGA-O2A-C1
19	A	810	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	C4-C3-C5-C6
19	A	811	CLA	C16-C17-C18-C20
19	B	812	CLA	C6-C7-C8-C9
19	B	813	CLA	C16-C17-C18-C19
23	2	317	LHG	C4-C5-C6-O8
24	F	309	LMG	C7-C8-C9-O8
29	B	847	DGD	O1G-C1G-C2G-C3G
29	B	847	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
19	A	811	CLA	O1A-CGA-O2A-C1
19	A	821	CLA	O1A-CGA-O2A-C1
19	B	833	CLA	O1A-CGA-O2A-C1
23	1	317	LHG	O6-C4-C5-O7
23	1	319	LHG	O6-C4-C5-O7
23	1	320	LHG	O6-C4-C5-O7
23	4	322	LHG	O6-C4-C5-O7
19	B	814	CLA	C15-C16-C17-C18
19	L	302	CLA	C16-C17-C18-C20
20	1	318	CHL	C11-C12-C13-C15
19	4	303	CLA	CHA-CBD-CGD-O1D
19	4	310	CLA	CHA-CBD-CGD-O1D
19	A	803	CLA	CHA-CBD-CGD-O1D
19	A	803	CLA	CHA-CBD-CGD-O2D
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O2D
19	A	815	CLA	CHA-CBD-CGD-O1D
19	A	829	CLA	CHA-CBD-CGD-O1D
19	A	850	CLA	CHA-CBD-CGD-O1D
19	A	850	CLA	CHA-CBD-CGD-O2D
19	A	854	CLA	CHA-CBD-CGD-O1D
19	A	854	CLA	CHA-CBD-CGD-O2D
19	B	804	CLA	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O2D
19	B	811	CLA	CHA-CBD-CGD-O1D
19	B	811	CLA	CHA-CBD-CGD-O2D
19	1	302	CLA	C3-C5-C6-C7
19	B	832	CLA	C3-C5-C6-C7
19	B	825	CLA	O1A-CGA-O2A-C1
18	L	306	BCR	C11-C10-C9-C8
18	1	316	BCR	C16-C17-C18-C19
18	A	844	BCR	C16-C17-C18-C19
18	J	103	BCR	C12-C13-C14-C15
24	J	101	LMG	C13-C14-C15-C16
23	2	317	LHG	O7-C5-C6-O8
23	2	318	LHG	O7-C5-C6-O8
19	1	311	CLA	C8-C10-C11-C12
23	4	322	LHG	O1-C1-C2-O2
20	2	306	CHL	O1D-CGD-O2D-CED
24	4	319	LMG	C24-C25-C26-C27
24	B	849	LMG	C12-C13-C14-C15
19	L	303	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	1	301	CLA	C11-C10-C8-C9
19	1	308	CLA	C11-C10-C8-C9
19	2	303	CLA	C6-C7-C8-C9
19	A	808	CLA	C14-C13-C15-C16
19	A	854	CLA	C6-C7-C8-C9
19	B	838	CLA	C14-C13-C15-C16
19	B	850	CLA	C14-C13-C15-C16
19	1	306	CLA	O1A-CGA-O2A-C1
19	A	812	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C16-C17-C18-C20
19	A	802	CLA	C3-C5-C6-C7
20	3	306	CHL	C2A-CAA-CBA-CGA
19	A	817	CLA	CBD-CGD-O2D-CED
19	4	302	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	CBA-CGA-O2A-C1
18	A	846	BCR	C11-C12-C13-C14
18	K	301	BCR	C21-C22-C23-C24
23	4	320	LHG	C26-C27-C28-C29
23	A	842	LHG	C9-C10-C11-C12
19	4	311	CLA	C1A-C2A-CAA-CBA
19	A	829	CLA	C1A-C2A-CAA-CBA
19	B	823	CLA	C1A-C2A-CAA-CBA
19	B	826	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C16-C17-C18-C19
19	B	803	CLA	C16-C17-C18-C20
19	B	828	CLA	C16-C17-C18-C19
19	1	310	CLA	C2-C1-O2A-CGA
19	A	839	CLA	C2-C1-O2A-CGA
19	B	832	CLA	C2-C1-O2A-CGA
19	B	850	CLA	CBD-CGD-O2D-CED
25	F	305	HTG	C3'-C4'-C5'-C6'
29	B	847	DGD	C7B-C8B-C9B-CAB
19	B	814	CLA	C13-C15-C16-C17
23	2	317	LHG	C3-O3-P-O6
23	A	843	LHG	C4-O6-P-O3
23	2	318	LHG	O2-C2-C3-O3
19	B	828	CLA	C4-C3-C5-C6
23	2	317	LHG	C2-C3-O3-P
19	B	819	CLA	O1A-CGA-O2A-C1
19	1	311	CLA	C4B-C3B-CAB-CBB
19	2	310	CLA	C4B-C3B-CAB-CBB
19	4	303	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	A	815	CLA	C4B-C3B-CAB-CBB
19	A	821	CLA	C4B-C3B-CAB-CBB
19	B	820	CLA	C4B-C3B-CAB-CBB
19	B	833	CLA	C4B-C3B-CAB-CBB
19	G	204	CLA	C4B-C3B-CAB-CBB
20	2	319	CHL	C4B-C3B-CAB-CBB
23	1	317	LHG	C4-O6-P-O4
23	2	317	LHG	C4-O6-P-O4
23	2	318	LHG	C4-O6-P-O4
23	4	320	LHG	C3-O3-P-O4
23	4	320	LHG	C3-O3-P-O5
23	4	322	LHG	C3-O3-P-O4
23	4	322	LHG	C3-O3-P-O5
23	A	842	LHG	C3-O3-P-O5
23	A	843	LHG	C3-O3-P-O4
19	A	838	CLA	C16-C17-C18-C20
23	4	320	LHG	C35-C36-C37-C38
19	A	807	CLA	CBA-CGA-O2A-C1
19	4	309	CLA	C2A-CAA-CBA-CGA
19	A	836	CLA	C3-C5-C6-C7
19	L	302	CLA	C16-C17-C18-C19
19	A	805	CLA	C16-C17-C18-C19
19	A	803	CLA	CAD-CBD-CGD-O1D
19	A	821	CLA	C2-C3-C5-C6
19	A	850	CLA	CAD-CBD-CGD-O1D
19	B	836	CLA	CAD-CBD-CGD-O1D
24	4	319	LMG	C18-C19-C20-C21
24	4	319	LMG	C12-C13-C14-C15
19	B	806	CLA	C8-C10-C11-C12
19	A	836	CLA	C16-C17-C18-C19
19	B	818	CLA	C11-C12-C13-C14
19	1	307	CLA	C6-C7-C8-C10
19	1	307	CLA	C12-C13-C15-C16
19	4	303	CLA	C11-C10-C8-C7
19	4	310	CLA	C11-C10-C8-C7
19	A	805	CLA	C11-C10-C8-C7
19	A	807	CLA	C11-C10-C8-C7
19	A	837	CLA	C11-C10-C8-C7
19	A	838	CLA	C11-C10-C8-C7
19	A	852	CLA	C11-C10-C8-C7
19	A	853	CLA	C11-C10-C8-C7
19	B	805	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	806	CLA	C6-C7-C8-C10
19	B	817	CLA	C11-C10-C8-C7
19	B	819	CLA	C12-C13-C15-C16
19	B	823	CLA	C3A-C2A-CAA-CBA
19	B	825	CLA	C11-C12-C13-C15
25	4	321	HTG	C2-C1-S1-C1'
25	F	301	HTG	C2-C1-S1-C1'
25	F	305	HTG	C2-C1-S1-C1'
24	B	849	LMG	C13-C14-C15-C16
18	B	845	BCR	C9-C10-C11-C12
21	2	314	LUT	C9-C10-C11-C12
19	4	310	CLA	CAA-CBA-CGA-O2A
23	4	320	LHG	C19-C20-C21-C22
19	A	810	CLA	O1A-CGA-O2A-C1
19	A	836	CLA	C10-C11-C12-C13
19	4	308	CLA	C2A-CAA-CBA-CGA
19	B	803	CLA	C2A-CAA-CBA-CGA
23	A	842	LHG	C16-C17-C18-C19
25	4	321	HTG	C4-C5-C6-O6
20	2	304	CHL	C1C-C2C-CMC-OMC
20	4	315	CHL	C1C-C2C-CMC-OMC
24	4	319	LMG	O1-C7-C8-O7
24	F	309	LMG	O7-C8-C9-O8
24	J	101	LMG	O1-C7-C8-O7
19	3	301	CLA	O1A-CGA-O2A-C1
18	A	846	BCR	C14-C15-C16-C17
19	A	837	CLA	C16-C17-C18-C20
26	B	841	PQN	C13-C15-C16-C17
19	A	807	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	O1A-CGA-O2A-C1
19	2	308	CLA	C8-C10-C11-C12
25	4	321	HTG	S1-C1'-C2'-C3'
23	4	322	LHG	C18-C19-C20-C21
19	1	309	CLA	C11-C10-C8-C9
19	A	805	CLA	C11-C10-C8-C9
19	A	806	CLA	C14-C13-C15-C16
19	A	828	CLA	C11-C12-C13-C14
19	A	837	CLA	C6-C7-C8-C9
19	A	840	CLA	C11-C10-C8-C9
19	A	853	CLA	C6-C7-C8-C9
19	B	825	CLA	C11-C12-C13-C14
19	B	839	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	850	CLA	O1D-CGD-O2D-CED
18	B	844	BCR	C6-C7-C8-C9
18	B	842	BCR	C11-C12-C13-C35
19	A	838	CLA	C16-C17-C18-C19
19	B	818	CLA	C11-C12-C13-C15
19	B	821	CLA	C16-C17-C18-C20
19	1	308	CLA	C2B-C3B-CAB-CBB
19	1	311	CLA	C2B-C3B-CAB-CBB
19	A	824	CLA	C2B-C3B-CAB-CBB
19	A	825	CLA	C2B-C3B-CAB-CBB
19	A	826	CLA	C2B-C3B-CAB-CBB
19	A	827	CLA	C2B-C3B-CAB-CBB
19	A	853	CLA	C2B-C3B-CAB-CBB
19	A	854	CLA	C2B-C3B-CAB-CBB
19	B	803	CLA	C2B-C3B-CAB-CBB
19	B	820	CLA	C2B-C3B-CAB-CBB
19	B	824	CLA	C2B-C3B-CAB-CBB
19	B	825	CLA	C2B-C3B-CAB-CBB
19	B	833	CLA	C2B-C3B-CAB-CBB
19	1	309	CLA	C3-C5-C6-C7
20	2	305	CHL	CAA-CBA-CGA-O2A
23	4	320	LHG	C16-C17-C18-C19
19	A	808	CLA	C2-C3-C5-C6
19	A	807	CLA	O1D-CGD-O2D-CED
24	4	319	LMG	C28-C29-C30-C31
19	A	820	CLA	C1-C2-C3-C4
19	4	303	CLA	C5-C6-C7-C8
19	B	816	CLA	C5-C6-C7-C8
23	1	317	LHG	O6-C4-C5-C6
23	4	320	LHG	O6-C4-C5-C6
19	A	815	CLA	C2A-CAA-CBA-CGA
19	3	308	CLA	C2-C1-O2A-CGA
19	4	304	CLA	C1-C2-C3-C4
19	4	309	CLA	C2-C1-O2A-CGA
19	4	304	CLA	CAA-CBA-CGA-O2A
19	1	308	CLA	C8-C10-C11-C12
19	B	803	CLA	C10-C11-C12-C13
21	3	313	LUT	C26-C27-C28-C29
23	2	317	LHG	C10-C11-C12-C13
19	A	839	CLA	C8-C10-C11-C12
18	B	845	BCR	C23-C24-C25-C26
18	B	845	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
18	G	206	BCR	C1-C6-C7-C8
19	B	802	CLA	C2-C3-C5-C6
19	B	810	CLA	C2-C3-C5-C6
19	1	312	CLA	C6-C7-C8-C9
18	L	301	BCR	C12-C13-C14-C15
22	2	315	XAT	C32-C33-C34-C35
19	A	807	CLA	C15-C16-C17-C18
19	B	806	CLA	C1-C2-C3-C5
23	1	317	LHG	C3-O3-P-O6
19	B	823	CLA	O1D-CGD-O2D-CED
24	4	319	LMG	O1-C7-C8-C9
19	B	829	CLA	C4-C3-C5-C6
24	G	202	LMG	C17-C18-C19-C20
19	B	829	CLA	C11-C10-C8-C7
19	B	829	CLA	C12-C13-C15-C16
19	B	833	CLA	C11-C10-C8-C7
23	4	320	LHG	C12-C13-C14-C15
19	A	826	CLA	C11-C10-C8-C9
19	A	830	CLA	C11-C10-C8-C9
19	A	830	CLA	C14-C13-C15-C16
19	A	836	CLA	C11-C12-C13-C14
18	A	848	BCR	C9-C10-C11-C12
19	A	826	CLA	C16-C17-C18-C20
19	3	302	CLA	C2A-CAA-CBA-CGA
19	A	818	CLA	C2A-CAA-CBA-CGA
19	B	828	CLA	C16-C17-C18-C20
23	1	317	LHG	C16-C17-C18-C19
23	1	319	LHG	C2-C3-O3-P
18	K	301	BCR	C17-C18-C19-C20
19	B	823	CLA	O1A-CGA-O2A-C1
23	1	320	LHG	C27-C28-C29-C30
19	A	827	CLA	CBA-CGA-O2A-C1
19	B	817	CLA	CBA-CGA-O2A-C1
19	B	823	CLA	CBA-CGA-O2A-C1
19	F	307	CLA	CBA-CGA-O2A-C1
19	B	817	CLA	O1A-CGA-O2A-C1
23	4	320	LHG	C14-C15-C16-C17
19	A	825	CLA	C4B-C3B-CAB-CBB
19	A	839	CLA	C4B-C3B-CAB-CBB
19	B	828	CLA	C4B-C3B-CAB-CBB
19	B	835	CLA	C11-C12-C13-C15
19	A	814	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	A	845	BCR	C15-C16-C17-C18
18	G	206	BCR	C13-C14-C15-C16
21	3	313	LUT	C9-C10-C11-C12
21	4	316	LUT	C29-C30-C31-C32
19	B	833	CLA	C3-C5-C6-C7
19	2	308	CLA	O1A-CGA-O2A-C1
19	A	853	CLA	C5-C6-C7-C8
18	A	845	BCR	C18-C19-C20-C21
18	F	302	BCR	C10-C11-C12-C13
19	F	307	CLA	O1A-CGA-O2A-C1
19	A	801	CLA	CAA-CBA-CGA-O2A
23	1	317	LHG	C32-C33-C34-C35
20	4	305	CHL	C1-C2-C3-C5
23	4	320	LHG	C32-C33-C34-C35
19	A	830	CLA	C2-C1-O2A-CGA
19	A	850	CLA	C2-C1-O2A-CGA
19	B	801	CLA	C15-C16-C17-C18
19	1	308	CLA	C11-C12-C13-C15
19	A	830	CLA	C16-C17-C18-C19
19	A	829	CLA	C2A-CAA-CBA-CGA
19	A	834	CLA	C2A-CAA-CBA-CGA
19	A	801	CLA	CBA-CGA-O2A-C1
23	4	320	LHG	C30-C31-C32-C33
19	A	812	CLA	C3A-C2A-CAA-CBA
19	B	801	CLA	C3A-C2A-CAA-CBA
19	B	809	CLA	C3A-C2A-CAA-CBA
19	B	829	CLA	C3A-C2A-CAA-CBA
23	4	322	LHG	C11-C10-C9-C8
18	B	844	BCR	C9-C10-C11-C12
19	A	802	CLA	C4-C3-C5-C6
24	B	849	LMG	C32-C33-C34-C35
19	A	831	CLA	C2-C3-C5-C6
19	B	828	CLA	C2-C3-C5-C6
19	2	301	CLA	C6-C7-C8-C9
19	4	302	CLA	C6-C7-C8-C9
19	B	819	CLA	C11-C10-C8-C9
19	O	103	CLA	C2C-C3C-CAC-CBC
19	B	813	CLA	C10-C11-C12-C13
23	1	317	LHG	C1-C2-C3-O3
19	A	828	CLA	O2A-C1-C2-C3
20	2	319	CHL	O2A-C1-C2-C3
19	K	302	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	3	308	CLA	O1A-CGA-O2A-C1
18	F	308	BCR	C21-C22-C23-C24
19	A	814	CLA	CAA-CBA-CGA-O2A
19	O	102	CLA	CAA-CBA-CGA-O1A
19	A	831	CLA	C4-C3-C5-C6
19	1	313	CLA	C1A-C2A-CAA-CBA
19	3	305	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	838	CLA	C1A-C2A-CAA-CBA
19	B	801	CLA	C1A-C2A-CAA-CBA
19	B	809	CLA	C1A-C2A-CAA-CBA
19	B	816	CLA	C1A-C2A-CAA-CBA
19	L	302	CLA	C12-C13-C15-C16
19	A	804	CLA	C11-C10-C8-C7
19	A	839	CLA	C11-C12-C13-C15
19	A	852	CLA	C11-C12-C13-C15
19	B	803	CLA	C11-C12-C13-C15
19	B	807	CLA	C11-C12-C13-C15
19	B	808	CLA	C11-C10-C8-C7
19	B	809	CLA	C6-C7-C8-C10
19	B	814	CLA	C12-C13-C15-C16
19	B	827	CLA	C11-C10-C8-C7
19	B	828	CLA	C11-C10-C8-C7
19	B	832	CLA	C6-C7-C8-C10
19	1	309	CLA	C5-C6-C7-C8
19	A	807	CLA	C10-C11-C12-C13
19	4	304	CLA	C1-C2-C3-C5
19	3	311	CLA	CAA-CBA-CGA-O1A
18	L	301	BCR	C15-C16-C17-C18
24	F	309	LMG	C32-C33-C34-C35
19	A	814	CLA	C2A-CAA-CBA-CGA
29	B	847	DGD	O6D-C5D-C6D-O5D
19	A	840	CLA	C5-C6-C7-C8
19	B	824	CLA	C8-C10-C11-C12
19	B	850	CLA	C13-C15-C16-C17
19	3	311	CLA	CAA-CBA-CGA-O2A
24	J	101	LMG	C12-C13-C14-C15
19	A	820	CLA	O2A-C1-C2-C3
19	B	831	CLA	C11-C12-C13-C14
19	B	806	CLA	C4-C3-C5-C6
19	B	825	CLA	C4-C3-C5-C6
19	A	827	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	818	CLA	C8-C10-C11-C12
19	1	304	CLA	C2B-C3B-CAB-CBB
19	2	310	CLA	C2B-C3B-CAB-CBB
19	4	303	CLA	C2B-C3B-CAB-CBB
19	A	815	CLA	C2B-C3B-CAB-CBB
19	A	820	CLA	C2B-C3B-CAB-CBB
19	A	821	CLA	C2B-C3B-CAB-CBB
19	B	828	CLA	C2B-C3B-CAB-CBB
19	B	831	CLA	C2B-C3B-CAB-CBB
19	G	204	CLA	C2B-C3B-CAB-CBB
20	2	319	CHL	C2B-C3B-CAB-CBB
23	1	317	LHG	O2-C2-C3-O3
23	A	842	LHG	O9-C7-O7-C5
19	B	824	CLA	C2A-CAA-CBA-CGA
18	G	206	BCR	C15-C16-C17-C18
18	J	104	BCR	C9-C10-C11-C12
18	K	301	BCR	C9-C10-C11-C12
21	3	313	LUT	C33-C34-C35-C15
19	O	102	CLA	CAA-CBA-CGA-O2A
25	F	301	HTG	C3'-C4'-C5'-C6'
24	B	849	LMG	C35-C36-C37-C38
19	A	801	CLA	O1A-CGA-O2A-C1
19	B	850	CLA	C10-C11-C12-C13
19	L	304	CLA	C2-C1-O2A-CGA
19	1	307	CLA	C2-C1-O2A-CGA
19	4	302	CLA	C2-C1-O2A-CGA
19	B	820	CLA	C2-C1-O2A-CGA
19	A	802	CLA	C2-C3-C5-C6
19	A	809	CLA	C11-C12-C13-C14
19	B	819	CLA	C11-C12-C13-C14
19	B	810	CLA	C8-C10-C11-C12
19	B	837	CLA	C2-C1-O2A-CGA
19	1	308	CLA	C2A-CAA-CBA-CGA
19	B	812	CLA	C2A-CAA-CBA-CGA
23	1	317	LHG	C23-C24-C25-C26
28	A	851	LMT	C9-C10-C11-C12
18	L	305	BCR	C1-C6-C7-C8
18	2	316	BCR	C23-C24-C25-C26
18	2	316	BCR	C23-C24-C25-C30
18	A	844	BCR	C23-C24-C25-C26
18	A	844	BCR	C23-C24-C25-C30
18	F	304	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
18	G	201	BCR	C1-C6-C7-C8
18	G	206	BCR	C5-C6-C7-C8
21	3	313	LUT	C1-C6-C7-C8
19	A	816	CLA	CAA-CBA-CGA-O2A
19	B	840	CLA	CAA-CBA-CGA-O2A
23	2	318	LHG	C4-C5-C6-O8
19	4	313	CLA	CAA-CBA-CGA-O2A
19	K	302	CLA	CAA-CBA-CGA-O2A
19	3	301	CLA	C8-C10-C11-C12
20	1	305	CHL	C2-C1-O2A-CGA
18	L	306	BCR	C13-C14-C15-C16
18	F	304	BCR	C19-C20-C21-C22
19	2	308	CLA	CBA-CGA-O2A-C1
19	B	835	CLA	C4-C3-C5-C6
20	2	319	CHL	C4-C3-C5-C6
18	J	104	BCR	C7-C8-C9-C10
19	A	831	CLA	C8-C10-C11-C12
23	A	842	LHG	C28-C29-C30-C31
19	B	829	CLA	C2-C3-C5-C6
19	B	801	CLA	C13-C15-C16-C17
19	A	833	CLA	CAA-CBA-CGA-O2A
19	O	103	CLA	C4C-C3C-CAC-CBC
19	B	802	CLA	C8-C10-C11-C12
19	B	805	CLA	C8-C10-C11-C12
19	2	301	CLA	C2A-CAA-CBA-CGA
19	A	808	CLA	C2A-CAA-CBA-CGA
23	4	320	LHG	C29-C30-C31-C32
19	1	304	CLA	C4B-C3B-CAB-CBB
19	A	817	CLA	C4B-C3B-CAB-CBB
19	A	820	CLA	C4B-C3B-CAB-CBB
19	A	826	CLA	C4B-C3B-CAB-CBB
19	B	822	CLA	C4B-C3B-CAB-CBB
19	B	831	CLA	C4B-C3B-CAB-CBB
19	B	835	CLA	C1-C2-C3-C5
19	A	817	CLA	O1D-CGD-O2D-CED
20	1	305	CHL	C2C-C3C-CAC-CBC
28	A	851	LMT	C4'-C5'-C6'-O6'
19	1	301	CLA	C11-C10-C8-C7
19	2	310	CLA	C2-C3-C5-C6
19	A	806	CLA	C12-C13-C15-C16
19	A	816	CLA	C11-C10-C8-C7
19	A	823	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B	825	CLA	C2-C3-C5-C6
19	B	826	CLA	C11-C12-C13-C15
26	A	841	PQN	C16-C17-C18-C20
19	3	301	CLA	C1-C2-C3-C4
19	A	803	CLA	C1-C2-C3-C4
19	A	817	CLA	C1-C2-C3-C4
19	A	819	CLA	C1-C2-C3-C4
19	A	831	CLA	C1-C2-C3-C4
19	B	805	CLA	C1-C2-C3-C4
19	B	813	CLA	C1-C2-C3-C4
19	B	824	CLA	C1-C2-C3-C4
19	B	829	CLA	C1-C2-C3-C4
19	B	839	CLA	C1-C2-C3-C4
20	2	319	CHL	C1-C2-C3-C4
19	B	813	CLA	C16-C17-C18-C20
19	O	104	CLA	CAA-CBA-CGA-O2A
19	B	831	CLA	C5-C6-C7-C8
19	A	832	CLA	C2A-CAA-CBA-CGA
19	3	308	CLA	CBA-CGA-O2A-C1
18	2	316	BCR	C16-C17-C18-C36
18	A	848	BCR	C16-C17-C18-C36
18	B	844	BCR	C11-C10-C9-C34
18	F	308	BCR	C35-C13-C14-C15
18	I	101	BCR	C16-C17-C18-C36
22	1	315	XAT	C40-C33-C34-C35
22	3	314	XAT	C20-C13-C14-C15
24	J	101	LMG	C16-C17-C18-C19
19	A	806	CLA	CAA-CBA-CGA-O2A
23	2	318	LHG	C26-C27-C28-C29
19	3	301	CLA	C4-C3-C5-C6
19	A	802	CLA	C1-C2-C3-C5
19	B	806	CLA	C2-C3-C5-C6
19	4	303	CLA	C11-C10-C8-C9
19	4	310	CLA	C11-C10-C8-C9
19	A	803	CLA	C14-C13-C15-C16
19	A	819	CLA	C11-C12-C13-C14
19	A	837	CLA	C11-C10-C8-C9
19	A	838	CLA	C11-C10-C8-C9
19	A	852	CLA	C11-C10-C8-C9
19	B	829	CLA	C6-C7-C8-C9
19	B	831	CLA	C6-C7-C8-C9
19	L	302	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	1	307	CLA	C3A-C2A-CAA-CBA
19	1	313	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	811	CLA	C3A-C2A-CAA-CBA
19	A	838	CLA	C3A-C2A-CAA-CBA
19	B	815	CLA	C3A-C2A-CAA-CBA
19	B	826	CLA	C3A-C2A-CAA-CBA
19	B	850	CLA	C3A-C2A-CAA-CBA
19	3	303	CLA	CAD-CBD-CGD-O2D
19	3	308	CLA	CAD-CBD-CGD-O2D
19	4	309	CLA	CAD-CBD-CGD-O2D
19	4	310	CLA	CAD-CBD-CGD-O2D
19	4	313	CLA	CAD-CBD-CGD-O2D
19	A	804	CLA	CAD-CBD-CGD-O2D
19	A	805	CLA	CAD-CBD-CGD-O2D
19	A	811	CLA	CAD-CBD-CGD-O2D
19	A	812	CLA	CAD-CBD-CGD-O2D
19	A	823	CLA	CAD-CBD-CGD-O2D
19	A	830	CLA	CAD-CBD-CGD-O2D
19	B	805	CLA	CAD-CBD-CGD-O2D
19	B	813	CLA	CAD-CBD-CGD-O2D
19	B	821	CLA	CAD-CBD-CGD-O2D
19	B	822	CLA	CAD-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O2D
19	B	826	CLA	CAD-CBD-CGD-O2D
19	B	830	CLA	CAD-CBD-CGD-O2D
19	B	835	CLA	CAD-CBD-CGD-O2D
19	K	302	CLA	CAD-CBD-CGD-O2D
20	2	304	CHL	CAD-CBD-CGD-O2D
23	A	842	LHG	C29-C30-C31-C32
19	1	307	CLA	C15-C16-C17-C18
19	B	838	CLA	C5-C6-C7-C8
24	F	309	LMG	C30-C31-C32-C33
19	K	303	CLA	CAA-CBA-CGA-O2A
23	A	842	LHG	C11-C10-C9-C8
18	A	844	BCR	C22-C23-C24-C25
19	1	310	CLA	C4-C3-C5-C6
19	B	801	CLA	C4-C3-C5-C6
19	4	313	CLA	CAA-CBA-CGA-O1A
23	1	317	LHG	C17-C18-C19-C20
19	A	823	CLA	CAA-CBA-CGA-O2A
18	B	842	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B	813	CLA	CAA-CBA-CGA-O2A
19	B	837	CLA	CAA-CBA-CGA-O2A
18	L	301	BCR	C10-C11-C12-C13
19	A	833	CLA	CAA-CBA-CGA-O1A
19	1	312	CLA	O2A-C1-C2-C3
19	A	823	CLA	O2A-C1-C2-C3
19	B	816	CLA	O2A-C1-C2-C3
19	B	805	CLA	CBA-CGA-O2A-C1
19	4	302	CLA	C2A-CAA-CBA-CGA
19	B	827	CLA	C2A-CAA-CBA-CGA
19	B	840	CLA	C10-C11-C12-C13
19	3	302	CLA	CAA-CBA-CGA-O2A
19	O	104	CLA	CAA-CBA-CGA-O1A
23	4	320	LHG	O2-C2-C3-O3
29	B	847	DGD	CEB-CFB-CGB-CHB
18	F	304	BCR	C13-C14-C15-C16
19	1	306	CLA	CHA-CBD-CGD-O1D
19	1	306	CLA	CHA-CBD-CGD-O2D
19	1	307	CLA	CHA-CBD-CGD-O1D
19	1	307	CLA	CHA-CBD-CGD-O2D
19	1	309	CLA	CHA-CBD-CGD-O1D
19	1	309	CLA	CHA-CBD-CGD-O2D
19	3	304	CLA	CHA-CBD-CGD-O1D
19	3	304	CLA	CHA-CBD-CGD-O2D
19	4	303	CLA	CHA-CBD-CGD-O2D
19	A	808	CLA	CHA-CBD-CGD-O1D
19	A	808	CLA	CHA-CBD-CGD-O2D
19	A	814	CLA	CHA-CBD-CGD-O1D
19	A	814	CLA	CHA-CBD-CGD-O2D
19	A	817	CLA	CHA-CBD-CGD-O1D
19	A	817	CLA	CHA-CBD-CGD-O2D
19	A	821	CLA	CHA-CBD-CGD-O1D
19	A	821	CLA	CHA-CBD-CGD-O2D
19	A	822	CLA	CHA-CBD-CGD-O1D
19	A	822	CLA	CHA-CBD-CGD-O2D
19	A	829	CLA	CHA-CBD-CGD-O2D
19	A	833	CLA	CHA-CBD-CGD-O1D
19	A	833	CLA	CHA-CBD-CGD-O2D
19	A	834	CLA	CHA-CBD-CGD-O2D
19	A	837	CLA	CHA-CBD-CGD-O1D
19	A	837	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	838	CLA	CHA-CBD-CGD-O2D
19	B	807	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	B	815	CLA	CHA-CBD-CGD-O1D
19	B	819	CLA	CHA-CBD-CGD-O1D
19	B	819	CLA	CHA-CBD-CGD-O2D
19	B	820	CLA	CHA-CBD-CGD-O2D
19	B	828	CLA	CHA-CBD-CGD-O2D
19	B	836	CLA	CHA-CBD-CGD-O1D
19	G	203	CLA	CHA-CBD-CGD-O1D
19	G	203	CLA	CHA-CBD-CGD-O2D
19	O	102	CLA	CHA-CBD-CGD-O1D
19	O	102	CLA	CHA-CBD-CGD-O2D
19	O	104	CLA	CHA-CBD-CGD-O1D
20	2	305	CHL	CHA-CBD-CGD-O1D
20	2	305	CHL	CHA-CBD-CGD-O2D
20	4	315	CHL	CHA-CBD-CGD-O1D
20	4	315	CHL	CHA-CBD-CGD-O2D
23	1	320	LHG	O7-C7-C8-C9
18	2	316	BCR	C16-C17-C18-C19
18	A	848	BCR	C16-C17-C18-C19
18	F	308	BCR	C12-C13-C14-C15
22	3	314	XAT	C12-C13-C14-C15
19	2	310	CLA	CAA-CBA-CGA-O2A
19	B	805	CLA	CAA-CBA-CGA-O2A
19	B	835	CLA	CAA-CBA-CGA-O2A
23	A	843	LHG	O7-C5-C6-O8
19	B	814	CLA	O1A-CGA-O2A-C1
19	A	811	CLA	CAA-CBA-CGA-O2A
23	A	843	LHG	O7-C7-C8-C9
19	B	823	CLA	C8-C10-C11-C12
19	A	825	CLA	CBA-CGA-O2A-C1
19	A	838	CLA	CAA-CBA-CGA-O2A
23	A	842	LHG	O7-C7-C8-C9
19	B	808	CLA	C4-C3-C5-C6
23	1	317	LHG	C14-C15-C16-C17
19	1	307	CLA	C11-C12-C13-C15
20	1	305	CHL	CAA-CBA-CGA-O2A
28	A	851	LMT	C11-C10-C9-C8
19	A	804	CLA	C11-C10-C8-C9
19	A	811	CLA	C6-C7-C8-C9
19	A	815	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	830	CLA	C11-C12-C13-C14
19	A	835	CLA	C11-C12-C13-C14
19	B	809	CLA	C6-C7-C8-C9
19	B	827	CLA	C6-C7-C8-C9
19	B	833	CLA	C11-C12-C13-C14
19	B	839	CLA	C11-C12-C13-C14
19	A	806	CLA	CAA-CBA-CGA-O1A
18	F	304	BCR	C9-C10-C11-C12
19	A	850	CLA	C8-C10-C11-C12
19	A	839	CLA	C2B-C3B-CAB-CBB
19	B	822	CLA	C2B-C3B-CAB-CBB
18	F	304	BCR	C14-C15-C16-C17
19	A	825	CLA	O1A-CGA-O2A-C1
19	B	808	CLA	C5-C6-C7-C8
19	3	310	CLA	C2A-CAA-CBA-CGA
19	A	810	CLA	C2A-CAA-CBA-CGA
29	B	847	DGD	CCB-CDB-CEB-CFB
19	B	822	CLA	C6-C7-C8-C10
26	A	841	PQN	C26-C27-C28-C30
24	J	101	LMG	C15-C16-C17-C18
23	A	842	LHG	O1-C1-C2-C3
20	2	319	CHL	C2-C3-C5-C6
19	A	850	CLA	C5-C6-C7-C8
23	2	318	LHG	C29-C30-C31-C32
19	B	837	CLA	CAA-CBA-CGA-O1A
21	1	314	LUT	C27-C28-C29-C30
22	1	315	XAT	C31-C32-C33-C34
22	3	314	XAT	C11-C12-C13-C14
19	L	302	CLA	C1A-C2A-CAA-CBA
19	1	307	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C1A-C2A-CAA-CBA
19	K	303	CLA	C1A-C2A-CAA-CBA
19	B	805	CLA	O1A-CGA-O2A-C1
19	B	814	CLA	CBA-CGA-O2A-C1
23	A	843	LHG	C4-C5-C6-O8
24	B	849	LMG	O1-C7-C8-C9
19	A	813	CLA	C2A-CAA-CBA-CGA
19	A	817	CLA	C2A-CAA-CBA-CGA
19	A	852	CLA	C2A-CAA-CBA-CGA
19	A	819	CLA	C16-C17-C18-C19
19	A	823	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	B	835	CLA	CAA-CBA-CGA-O1A
19	A	807	CLA	C13-C15-C16-C17
19	A	816	CLA	C15-C16-C17-C18
19	B	836	CLA	C5-C6-C7-C8
19	3	305	CLA	O1A-CGA-O2A-C1
19	A	823	CLA	C4-C3-C5-C6
19	1	310	CLA	CAA-CBA-CGA-O2A
19	B	833	CLA	CAA-CBA-CGA-O2A
19	3	302	CLA	CAA-CBA-CGA-O1A
18	F	302	BCR	C22-C23-C24-C25
18	G	206	BCR	C14-C15-C16-C17
19	3	309	CLA	C4B-C3B-CAB-CBB
19	A	814	CLA	C4B-C3B-CAB-CBB
19	1	311	CLA	C11-C12-C13-C15
19	A	811	CLA	CAA-CBA-CGA-O1A
19	K	303	CLA	CAA-CBA-CGA-O1A
18	O	105	BCR	C1-C6-C7-C8
18	O	106	BCR	C1-C6-C7-C8
19	2	310	CLA	CAA-CBA-CGA-O1A
19	B	808	CLA	C8-C10-C11-C12
19	1	311	CLA	C2A-CAA-CBA-CGA
19	B	816	CLA	C2A-CAA-CBA-CGA
23	1	320	LHG	O9-C7-C8-C9
23	2	318	LHG	C33-C34-C35-C36
23	4	322	LHG	C15-C16-C17-C18
23	A	842	LHG	C8-C7-O7-C5
19	1	309	CLA	CAD-CBD-CGD-O1D
19	4	311	CLA	CAD-CBD-CGD-O1D
19	A	821	CLA	CAD-CBD-CGD-O1D
19	A	822	CLA	CAD-CBD-CGD-O1D
19	B	820	CLA	CAD-CBD-CGD-O1D
19	B	827	CLA	CAD-CBD-CGD-O1D
19	B	840	CLA	CAD-CBD-CGD-O1D
19	O	101	CLA	CAD-CBD-CGD-O1D
19	B	806	CLA	O1A-CGA-O2A-C1
19	A	838	CLA	CAA-CBA-CGA-O1A
19	B	813	CLA	CAA-CBA-CGA-O1A
26	B	841	PQN	C23-C25-C26-C27
19	2	311	CLA	C6-C7-C8-C9
19	B	805	CLA	C11-C12-C13-C14
19	B	827	CLA	C11-C10-C8-C9
19	B	832	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	838	CLA	C11-C10-C8-C9
20	1	305	CHL	CAA-CBA-CGA-O1A
19	3	305	CLA	CBA-CGA-O2A-C1
19	2	303	CLA	CAA-CBA-CGA-O2A
19	4	314	CLA	CAA-CBA-CGA-O2A
19	A	834	CLA	CAA-CBA-CGA-O2A
19	B	806	CLA	CAA-CBA-CGA-O2A
19	B	812	CLA	CAA-CBA-CGA-O2A
23	A	842	LHG	C35-C36-C37-C38
19	L	302	CLA	C2A-CAA-CBA-CGA
19	2	307	CLA	CAA-CBA-CGA-O2A
19	A	808	CLA	CAA-CBA-CGA-O2A
19	1	302	CLA	C11-C12-C13-C15
19	1	304	CLA	C3A-C2A-CAA-CBA
19	4	303	CLA	C6-C7-C8-C10
19	A	801	CLA	C12-C13-C15-C16
19	A	804	CLA	C11-C12-C13-C15
19	A	810	CLA	C2-C3-C5-C6
19	A	828	CLA	C3A-C2A-CAA-CBA
19	A	837	CLA	C6-C7-C8-C10
19	A	840	CLA	C11-C10-C8-C7
19	A	853	CLA	C11-C12-C13-C15
23	A	842	LHG	O9-C7-C8-C9
23	A	843	LHG	O9-C7-C8-C9
19	1	302	CLA	CAA-CBA-CGA-O2A
19	B	828	CLA	CAA-CBA-CGA-O2A
19	A	816	CLA	C10-C11-C12-C13
18	G	201	BCR	C17-C18-C19-C20
22	2	315	XAT	C31-C32-C33-C34
19	4	314	CLA	CAA-CBA-CGA-O1A
18	A	844	BCR	C19-C20-C21-C22
18	K	301	BCR	C13-C14-C15-C16
24	G	202	LMG	C24-C25-C26-C27
19	3	307	CLA	CAA-CBA-CGA-O2A
19	A	807	CLA	CAA-CBA-CGA-O2A
19	2	307	CLA	CAA-CBA-CGA-O1A
19	B	806	CLA	CAA-CBA-CGA-O1A
19	B	812	CLA	CAA-CBA-CGA-O1A
19	B	833	CLA	CAA-CBA-CGA-O1A
19	B	806	CLA	C15-C16-C17-C18
19	1	310	CLA	CAA-CBA-CGA-O1A
19	A	821	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	1	312	CLA	C6-C7-C8-C10
19	B	809	CLA	C15-C16-C17-C18
19	2	303	CLA	CAA-CBA-CGA-O1A
19	A	834	CLA	CAA-CBA-CGA-O1A
19	2	311	CLA	C4-C3-C5-C6
19	B	850	CLA	CAA-CBA-CGA-O2A
20	1	318	CHL	CAA-CBA-CGA-O2A
24	G	202	LMG	O7-C10-C11-C12

There are no ring outliers.

203 monomers are involved in 544 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	831	CLA	4	0
19	A	853	CLA	3	0
19	A	822	CLA	4	0
19	3	311	CLA	1	0
19	A	811	CLA	6	0
19	4	312	CLA	4	0
19	B	810	CLA	3	0
19	B	825	CLA	2	0
20	4	305	CHL	7	0
19	1	309	CLA	7	0
21	2	314	LUT	4	0
19	B	814	CLA	3	0
19	A	828	CLA	4	0
23	4	322	LHG	7	0
19	3	304	CLA	1	0
23	2	318	LHG	6	0
20	3	306	CHL	3	0
19	B	816	CLA	6	0
19	4	308	CLA	1	0
26	A	841	PQN	4	0
19	A	837	CLA	6	0
19	B	828	CLA	3	0
19	B	822	CLA	5	0
20	2	306	CHL	9	0
19	B	819	CLA	7	0
19	A	835	CLA	6	0
19	1	312	CLA	3	0
18	2	316	BCR	6	0
21	1	314	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	814	CLA	1	0
19	A	817	CLA	6	0
19	3	303	CLA	2	0
18	G	201	BCR	2	0
22	2	315	XAT	2	0
18	A	846	BCR	2	0
19	B	823	CLA	3	0
18	A	848	BCR	1	0
23	A	843	LHG	2	0
19	B	802	CLA	7	0
20	4	306	CHL	3	0
18	J	104	BCR	1	0
19	B	808	CLA	5	0
19	B	813	CLA	3	0
19	A	821	CLA	1	0
19	2	310	CLA	3	0
19	4	303	CLA	4	0
20	4	315	CHL	3	0
25	F	310	HTG	1	0
18	O	105	BCR	2	0
19	1	308	CLA	3	0
18	B	844	BCR	4	0
18	3	315	BCR	5	0
19	K	302	CLA	3	0
23	1	320	LHG	9	0
18	B	842	BCR	2	0
18	F	304	BCR	4	0
19	B	801	CLA	3	0
20	4	307	CHL	6	0
28	A	851	LMT	2	0
19	B	812	CLA	3	0
19	A	829	CLA	1	0
19	F	306	CLA	1	0
19	4	304	CLA	1	0
19	B	826	CLA	6	0
19	O	101	CLA	3	0
19	G	204	CLA	2	0
19	A	809	CLA	4	0
19	B	850	CLA	3	0
19	A	816	CLA	2	0
18	K	301	BCR	5	0
19	4	311	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F	307	CLA	3	0
19	1	301	CLA	2	0
18	A	844	BCR	2	0
19	3	307	CLA	2	0
19	4	301	CLA	5	0
19	A	818	CLA	4	0
20	2	304	CHL	4	0
20	2	319	CHL	4	0
19	B	838	CLA	4	0
18	4	318	BCR	5	0
19	2	307	CLA	1	0
21	4	316	LUT	3	0
20	2	313	CHL	3	0
19	G	203	CLA	1	0
19	1	306	CLA	2	0
19	B	804	CLA	2	0
19	4	310	CLA	10	0
19	A	820	CLA	4	0
20	1	305	CHL	1	0
19	A	838	CLA	6	0
18	F	302	BCR	5	0
19	3	305	CLA	1	0
19	B	835	CLA	4	0
19	2	309	CLA	1	0
19	A	850	CLA	6	0
19	2	311	CLA	3	0
23	2	317	LHG	4	0
19	O	102	CLA	1	0
19	B	836	CLA	4	0
19	3	308	CLA	4	0
19	A	839	CLA	7	0
22	3	314	XAT	2	0
24	J	101	LMG	2	0
25	F	301	HTG	3	0
19	A	819	CLA	5	0
19	B	805	CLA	1	0
19	A	804	CLA	3	0
18	L	301	BCR	1	0
19	B	821	CLA	4	0
18	A	845	BCR	3	0
19	3	309	CLA	2	0
19	A	823	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	802	CLA	2	0
25	B	848	HTG	1	0
19	A	826	CLA	6	0
19	A	808	CLA	4	0
19	A	801	CLA	5	0
19	K	303	CLA	3	0
19	B	818	CLA	5	0
19	1	311	CLA	10	0
19	1	303	CLA	2	0
19	2	302	CLA	2	0
19	4	309	CLA	8	0
19	A	830	CLA	1	0
19	B	809	CLA	3	0
19	A	832	CLA	2	0
19	B	806	CLA	3	0
18	F	308	BCR	3	0
19	B	840	CLA	6	0
19	A	810	CLA	1	0
18	B	845	BCR	5	0
19	L	304	CLA	1	0
19	A	825	CLA	2	0
19	G	205	CLA	1	0
19	B	817	CLA	2	0
19	A	805	CLA	2	0
20	1	318	CHL	7	0
19	3	310	CLA	5	0
18	1	316	BCR	5	0
19	1	304	CLA	2	0
29	B	847	DGD	7	0
27	C	102	SF4	1	0
25	F	303	HTG	1	0
19	A	836	CLA	8	0
23	A	842	LHG	1	0
19	B	807	CLA	6	0
19	A	827	CLA	2	0
22	4	317	XAT	5	0
22	1	315	XAT	2	0
18	O	106	BCR	5	0
24	F	309	LMG	1	0
19	B	833	CLA	2	0
19	3	301	CLA	2	0
19	1	302	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	824	CLA	7	0
19	A	813	CLA	1	0
18	G	206	BCR	2	0
19	3	316	CLA	3	0
18	A	847	BCR	4	0
19	L	302	CLA	5	0
19	1	307	CLA	6	0
19	3	302	CLA	1	0
18	J	103	BCR	3	0
19	L	303	CLA	5	0
19	2	308	CLA	4	0
19	B	834	CLA	3	0
19	B	803	CLA	5	0
24	G	202	LMG	1	0
18	L	306	BCR	1	0
19	A	806	CLA	6	0
19	A	831	CLA	4	0
19	2	303	CLA	1	0
24	4	319	LMG	8	0
18	I	101	BCR	3	0
23	4	320	LHG	2	0
18	K	304	BCR	3	0
23	1	317	LHG	6	0
19	4	302	CLA	5	0
25	F	305	HTG	4	0
19	O	103	CLA	5	0
18	B	843	BCR	2	0
19	4	313	CLA	2	0
20	2	305	CHL	5	0
24	B	849	LMG	3	0
18	L	305	BCR	4	0
19	A	852	CLA	3	0
19	A	854	CLA	6	0
19	B	811	CLA	1	0
19	1	310	CLA	3	0
19	A	824	CLA	2	0
19	2	301	CLA	4	0
19	4	314	CLA	2	0
21	3	313	LUT	5	0
19	2	312	CLA	1	0
19	B	827	CLA	3	0
19	A	815	CLA	2	0

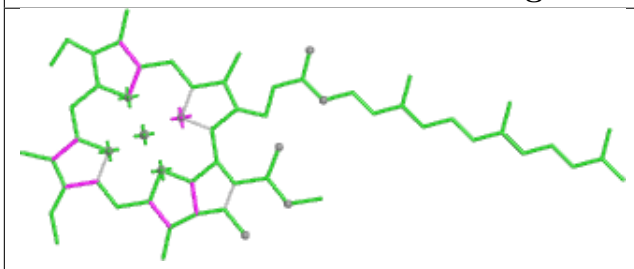
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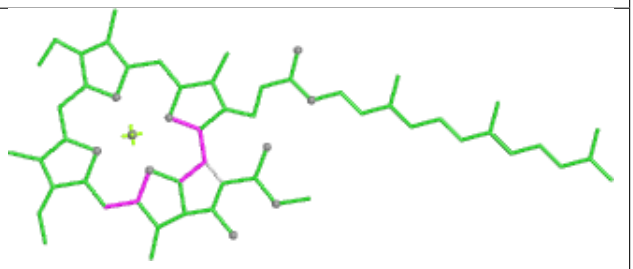
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	829	CLA	6	0
19	B	839	CLA	2	0
19	A	840	CLA	3	0
26	B	841	PQN	1	0
18	B	846	BCR	2	0
19	A	834	CLA	2	0

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

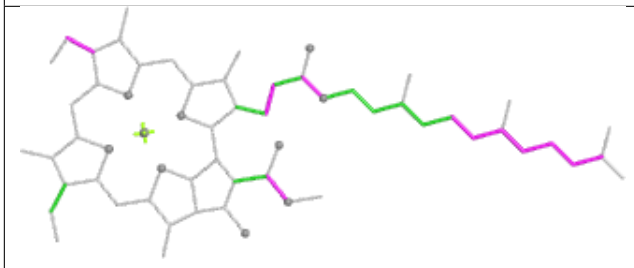
Ligand CLA B 831



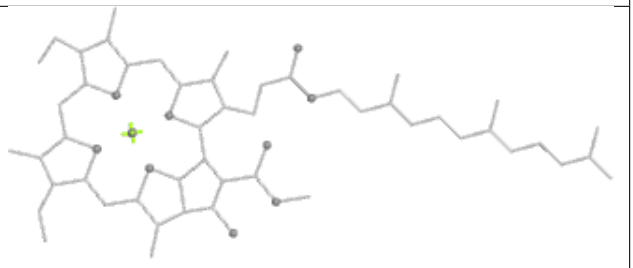
Bond lengths



Bond angles

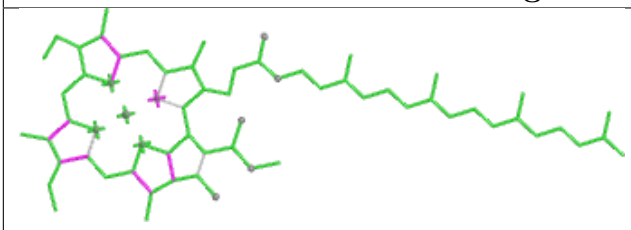


Torsions

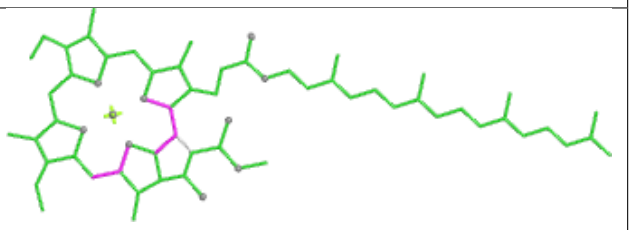


Rings

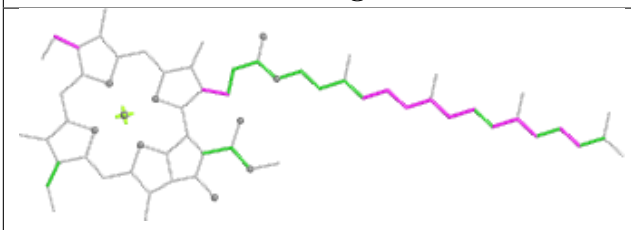
Ligand CLA A 853



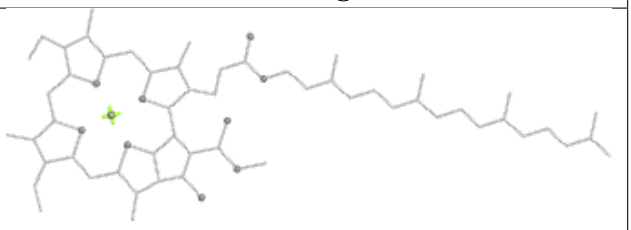
Bond lengths



Bond angles

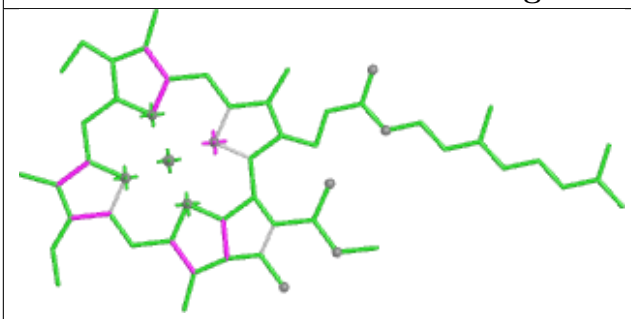


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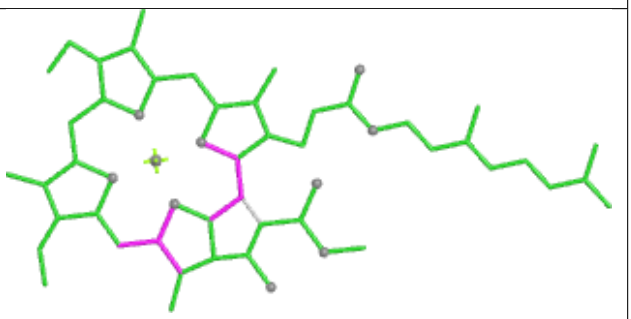


Rings

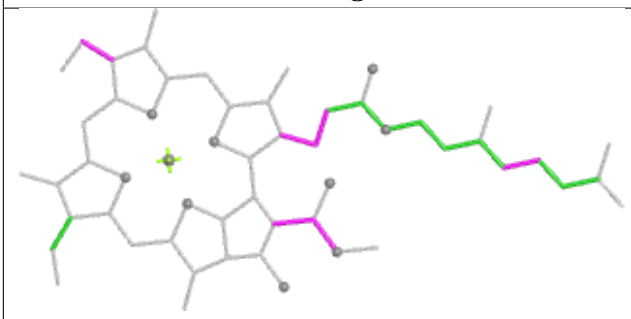
Ligand CLA A 822



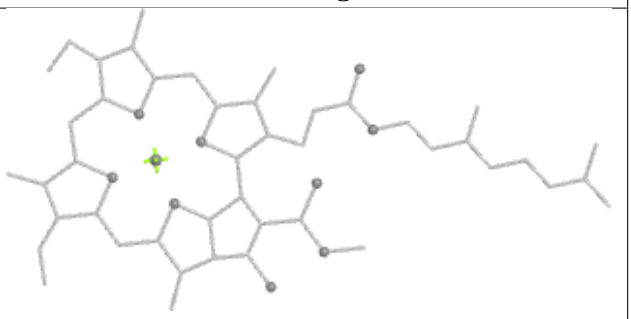
Bond lengths



Bond angles

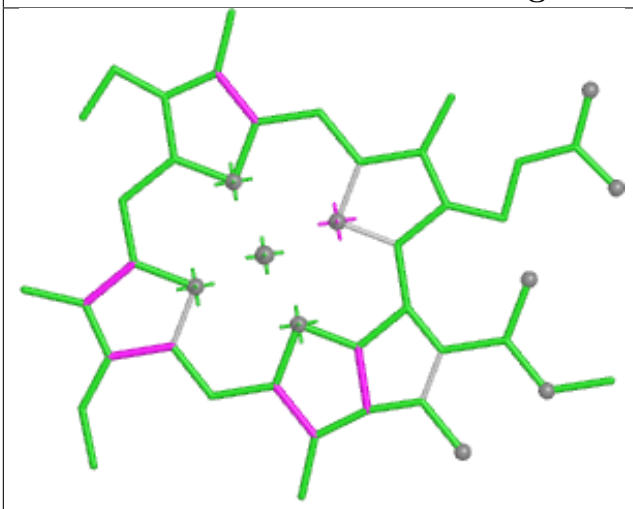


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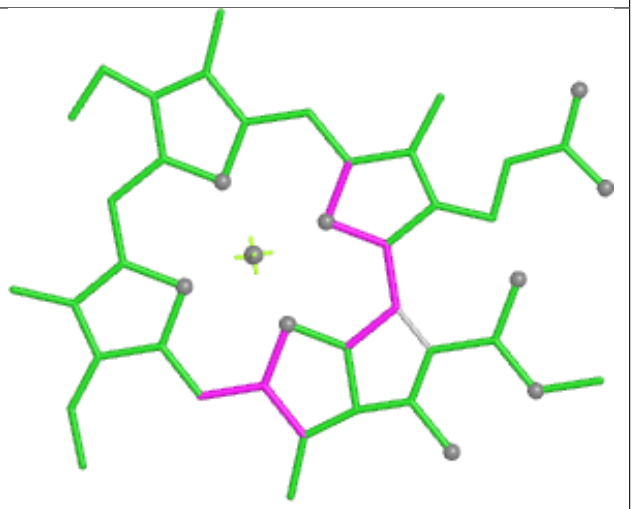


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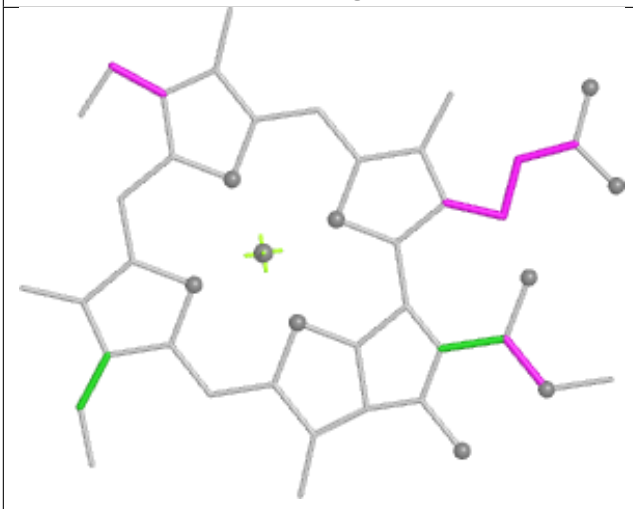
Ligand CLA 3 311



Bond lengths



Bond angles

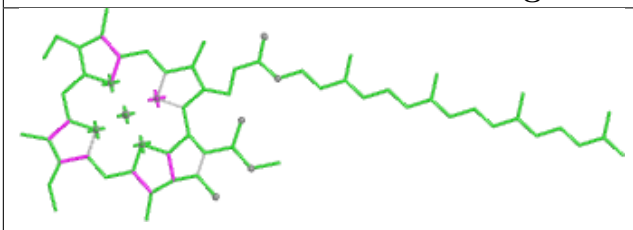


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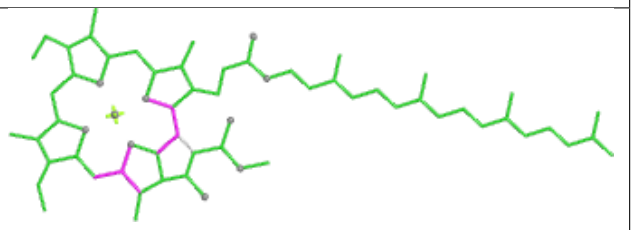


Rings

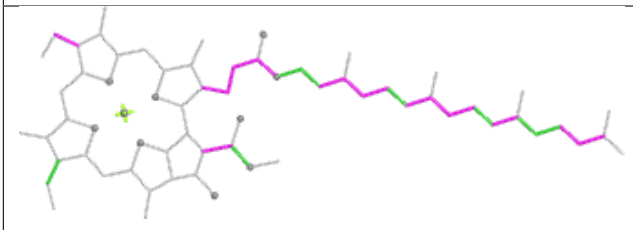
Ligand CLA A 811



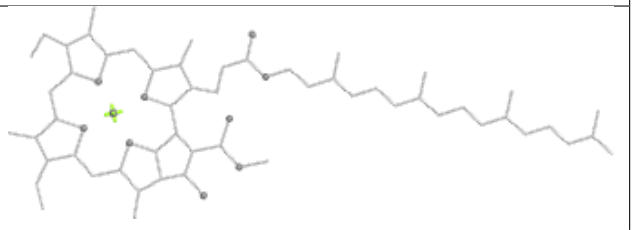
Bond lengths



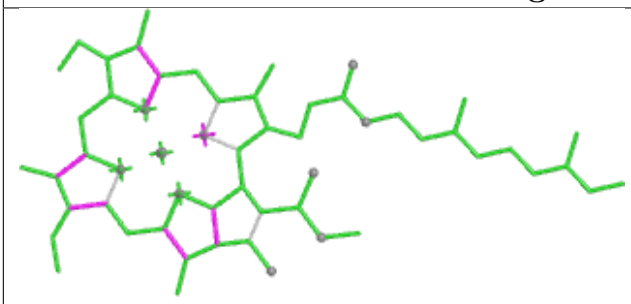
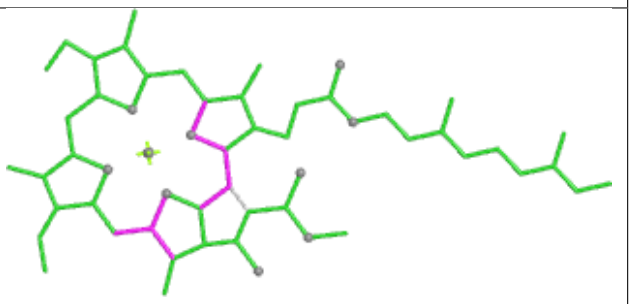
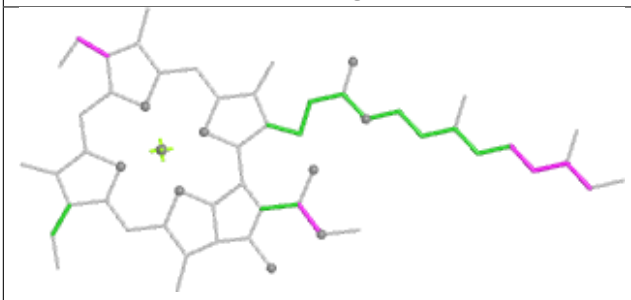
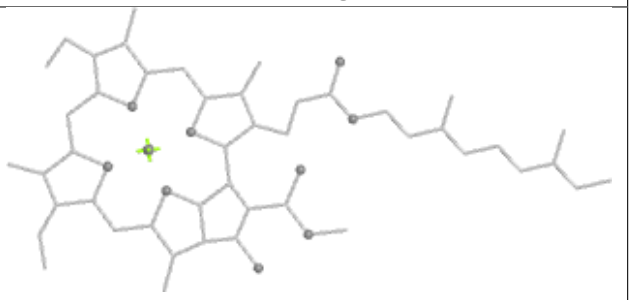
Bond angles

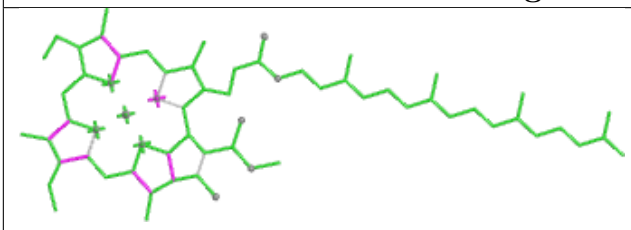
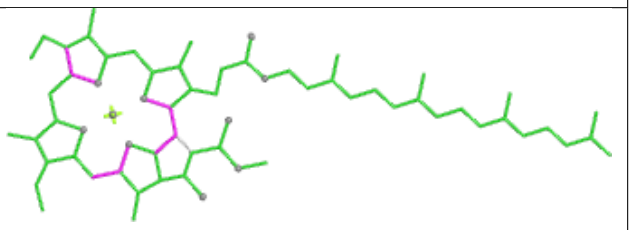
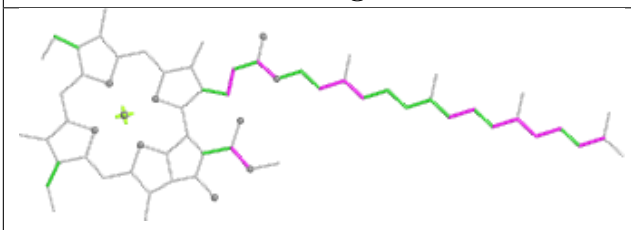
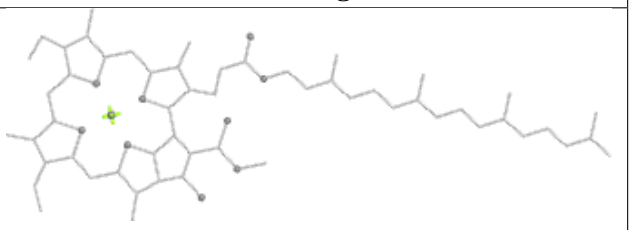


Torsions

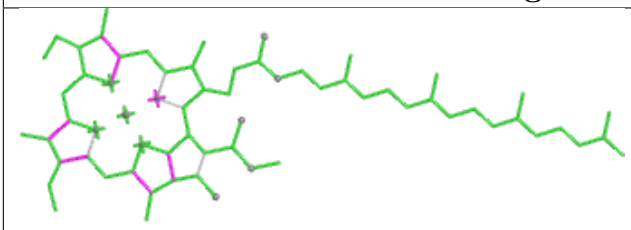


Rings

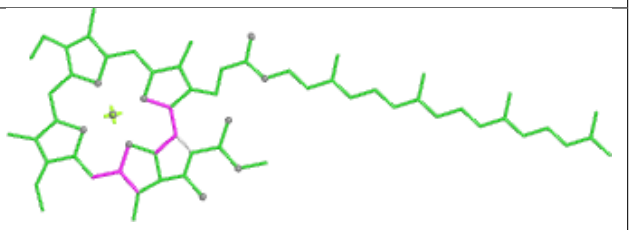
Ligand CLA 4 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

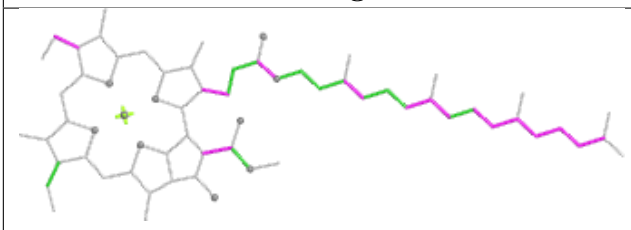
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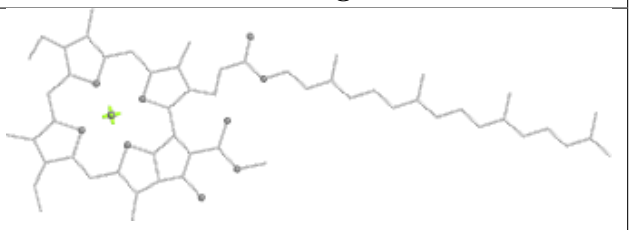
Bond lengths



Bond angles

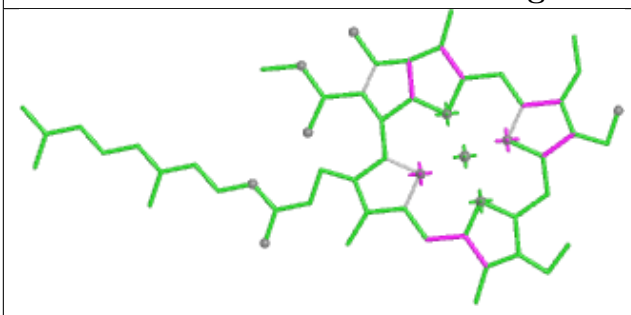


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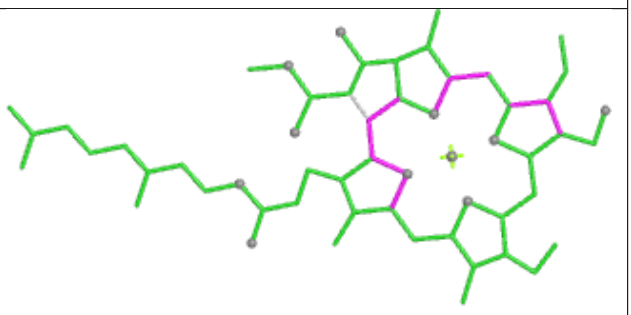


Rings

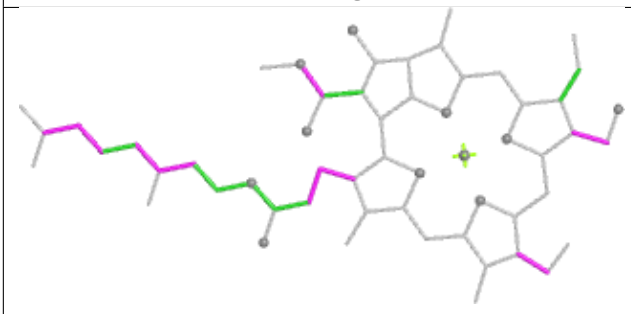
Ligand CHL 4 305



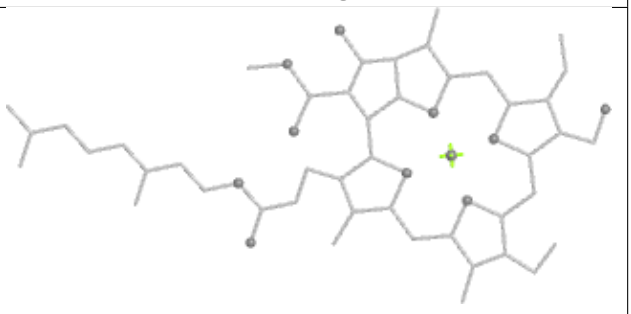
Bond lengths



Bond angles

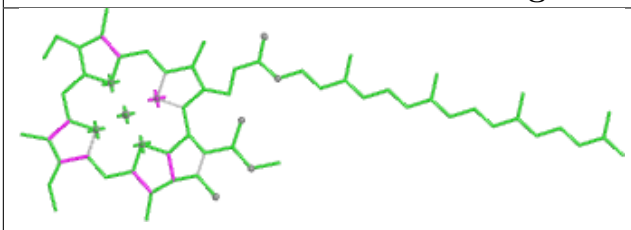


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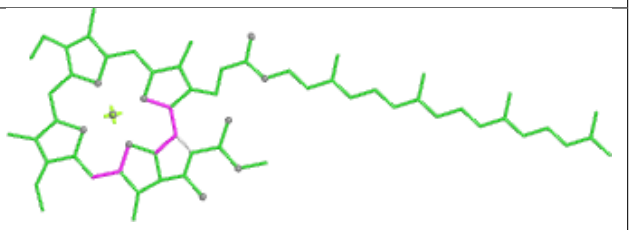


Rings

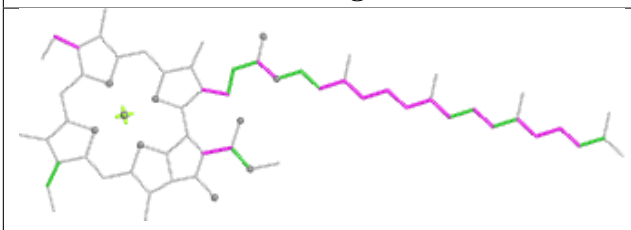
Ligand CLA 1 309



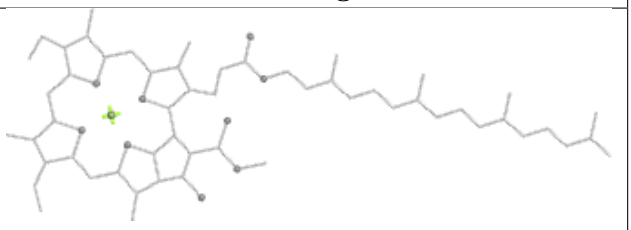
Bond lengths



Bond angles

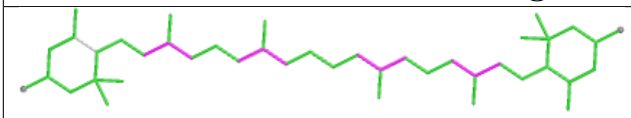


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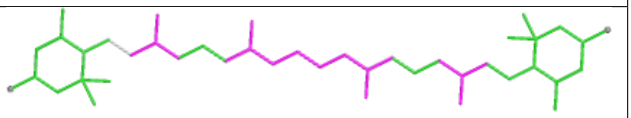


Rings

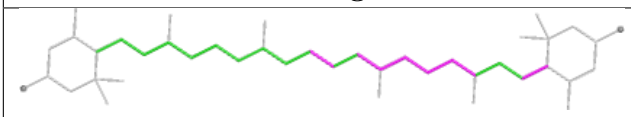
Ligand LUT 2 314



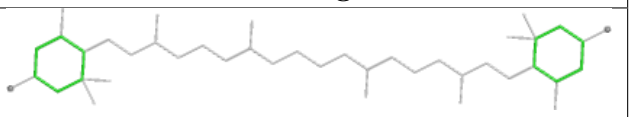
Bond lengths



Bond angles

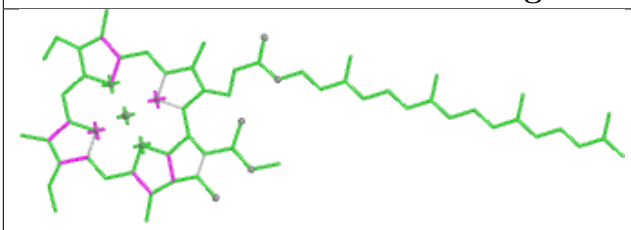


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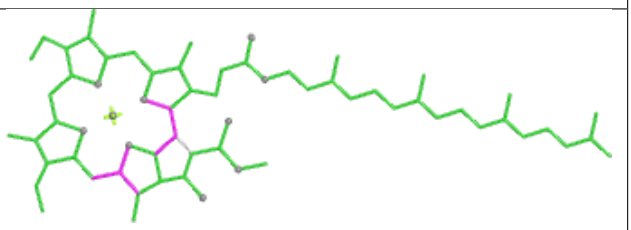


Rings

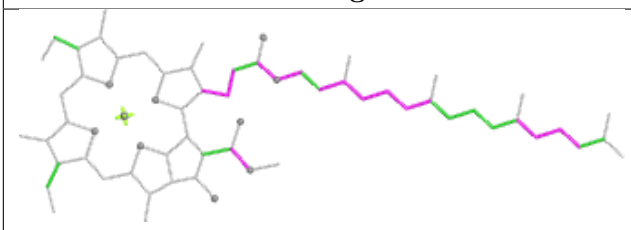
Ligand CLA B 814



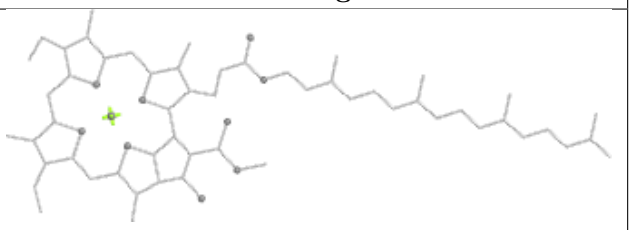
Bond lengths



Bond angles

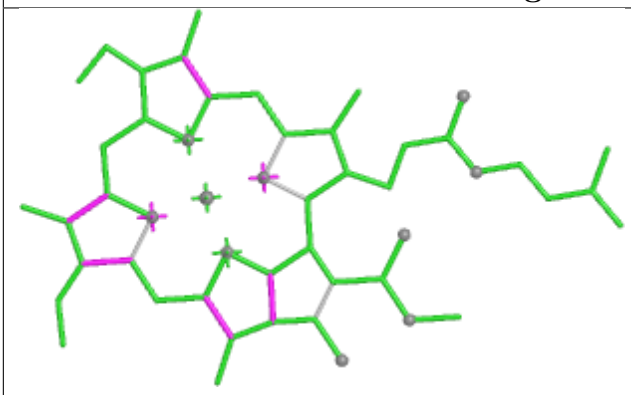


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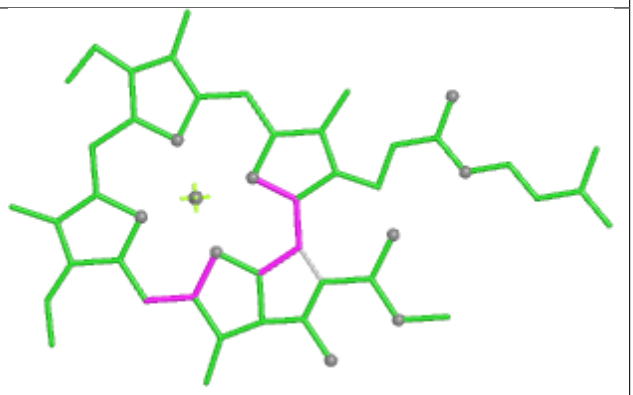


Rings

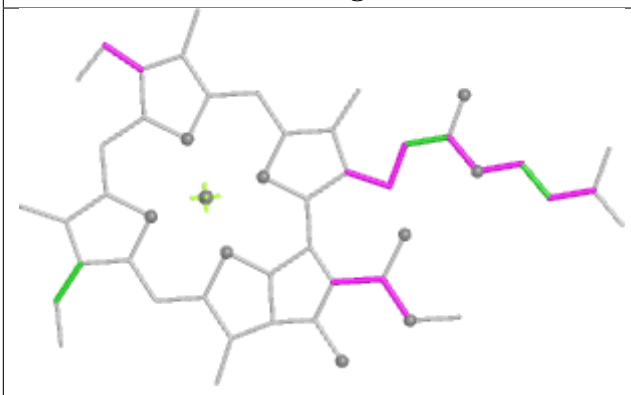
Ligand CLA B 820



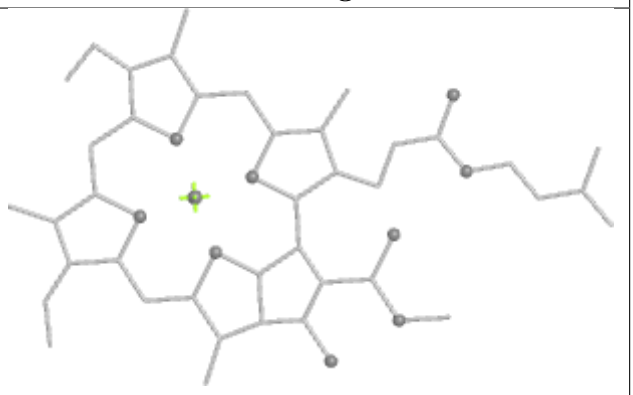
Bond lengths



Bond angles

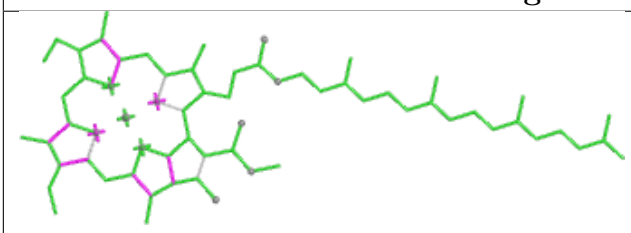


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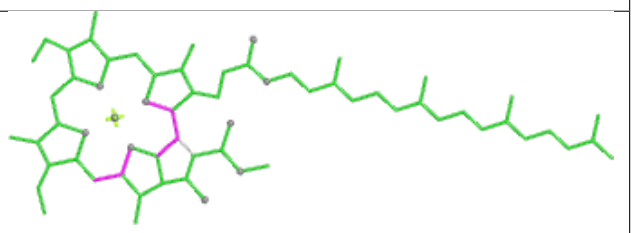


Rings

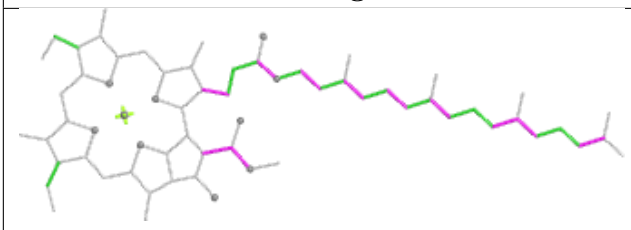
Ligand CLA A 828



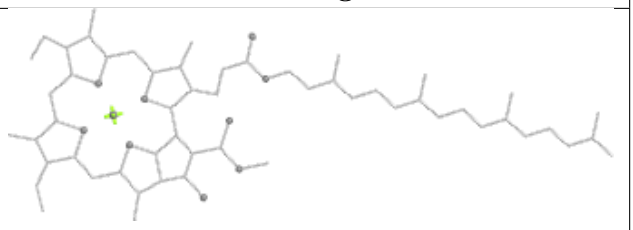
Bond lengths



Bond angles

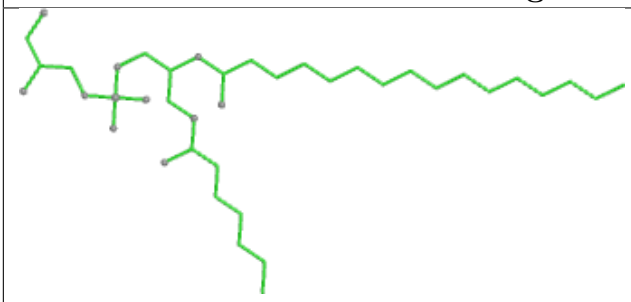


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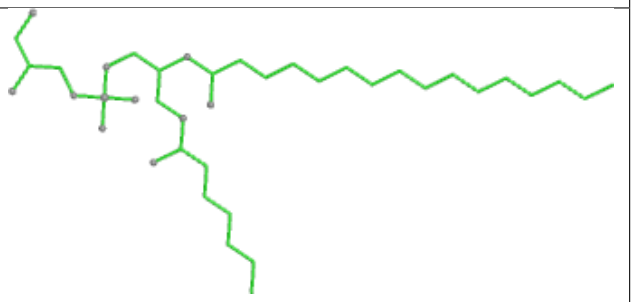


Rings

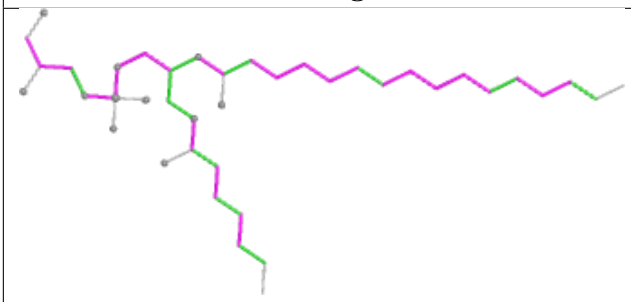
Ligand LHG 4 322



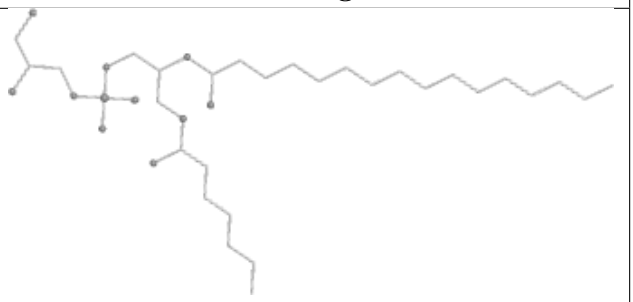
Bond lengths



Bond angles

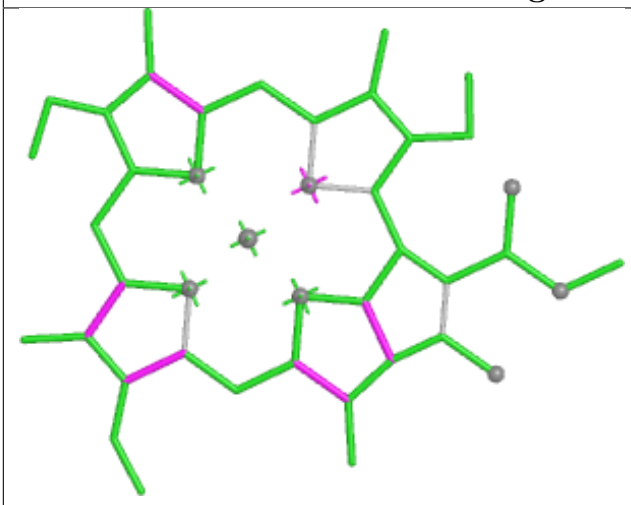


Torsions

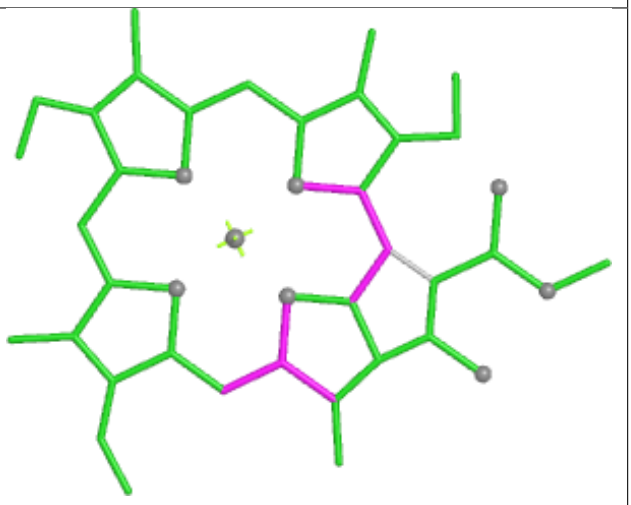


Rings

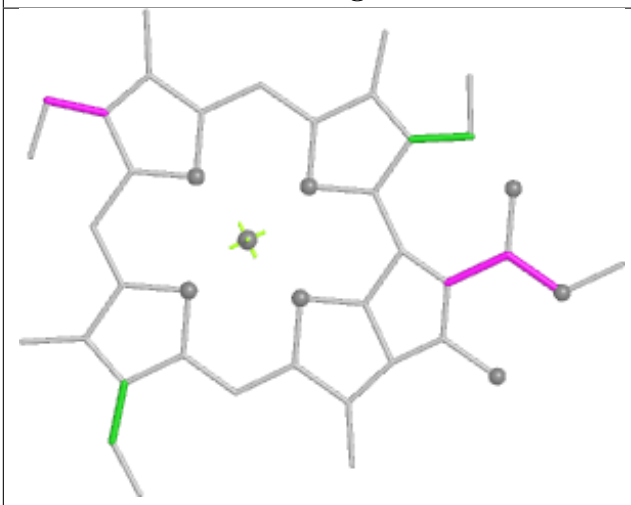
Ligand CLA 3 304



Bond lengths



Bond angles

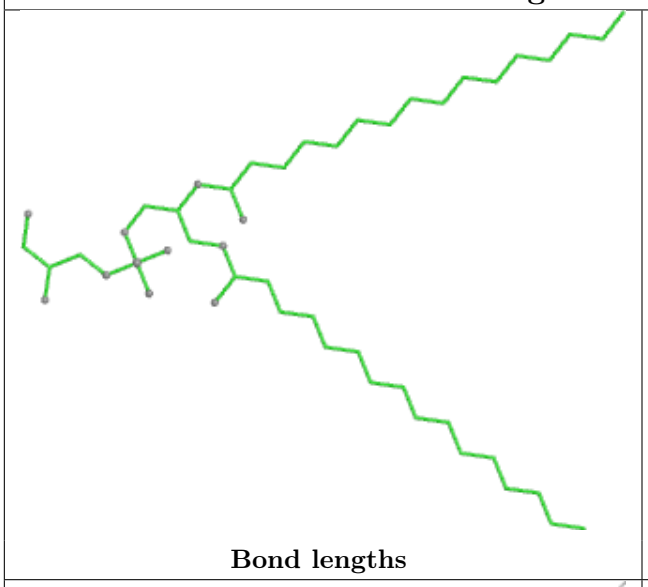


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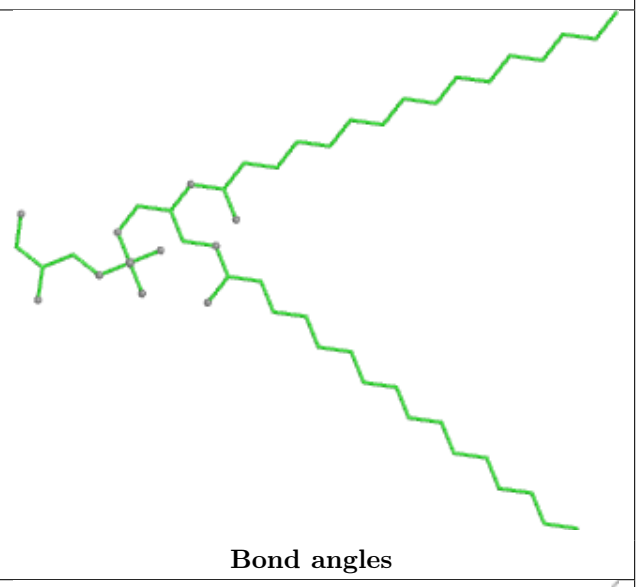


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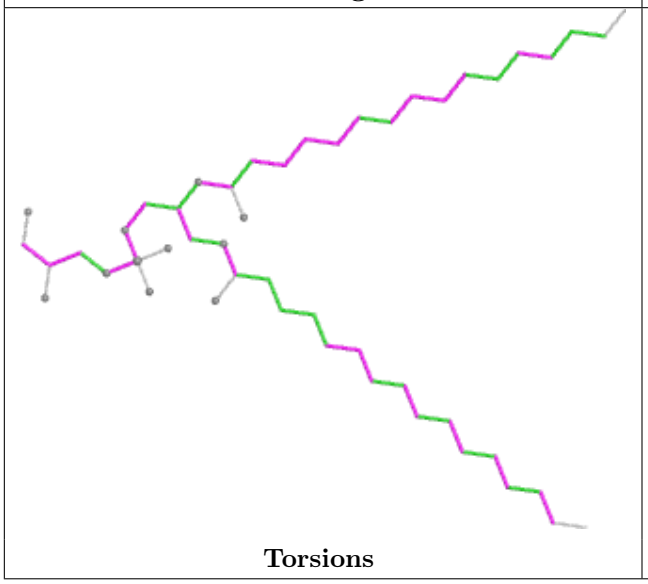
Ligand LHG 2 318



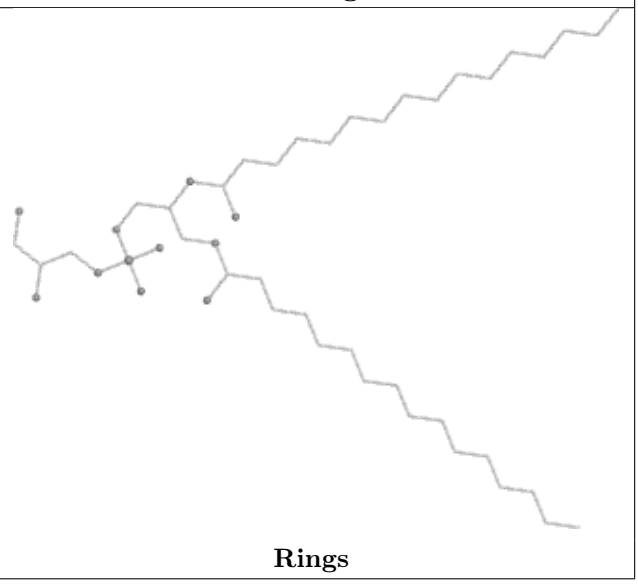
Bond lengths



Bond angles

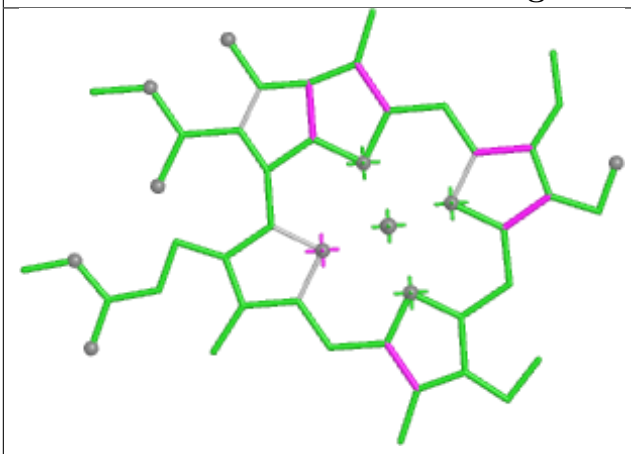


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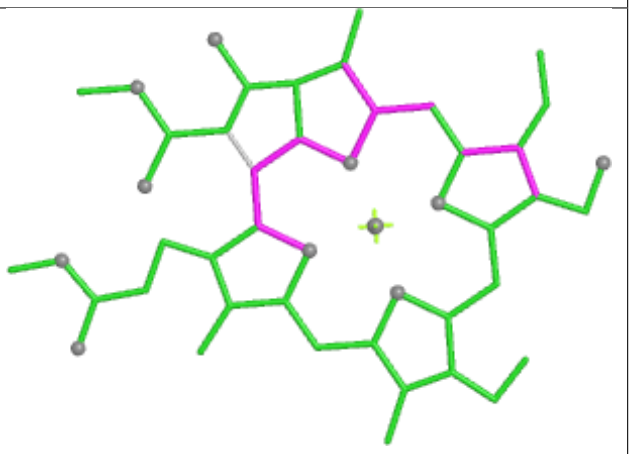


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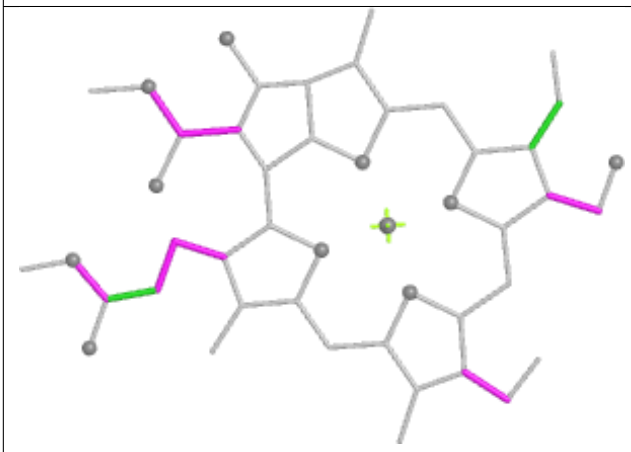
Ligand CHL 3 306



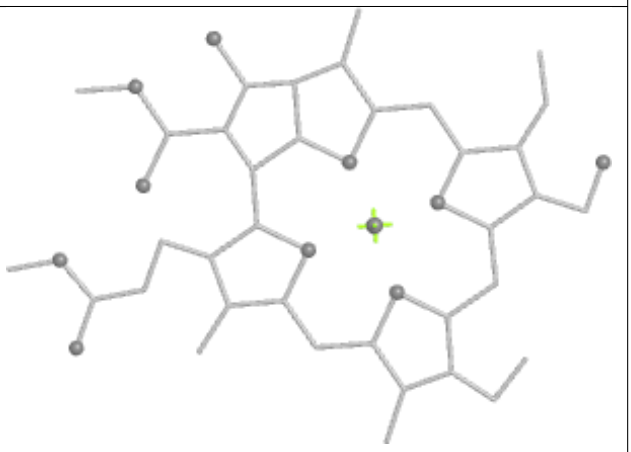
Bond lengths



Bond angles

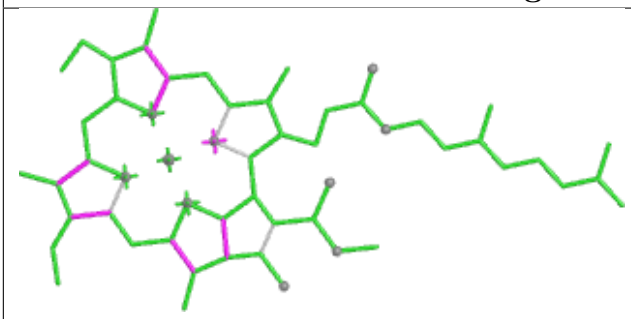


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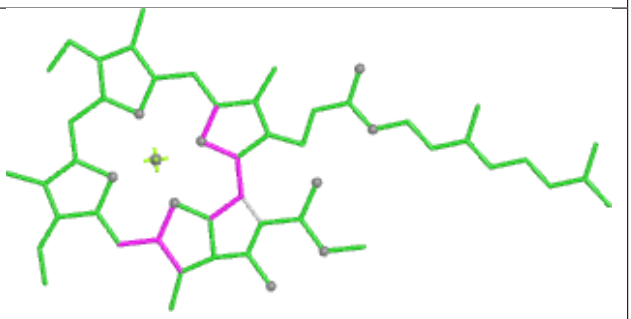


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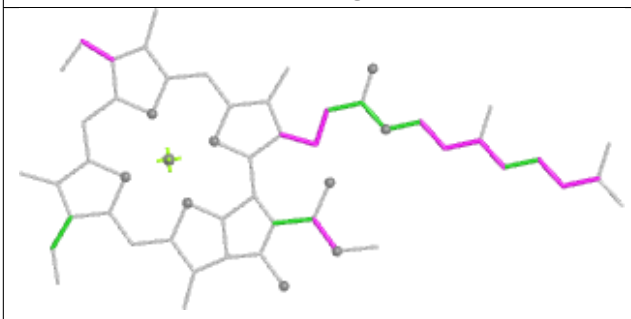
Ligand CLA B 816



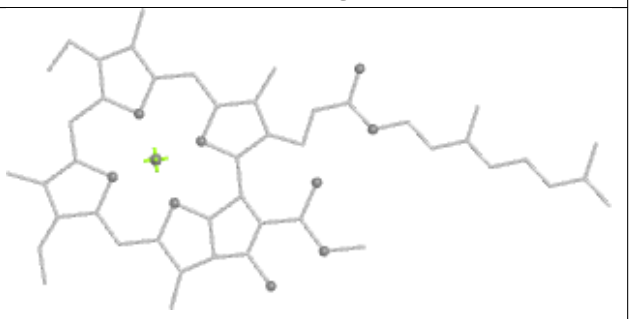
Bond lengths



Bond angles

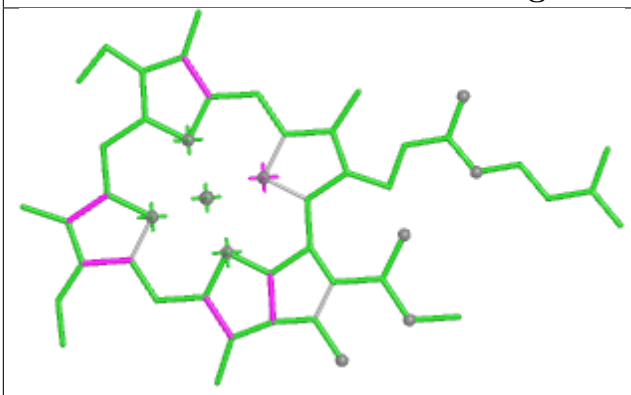


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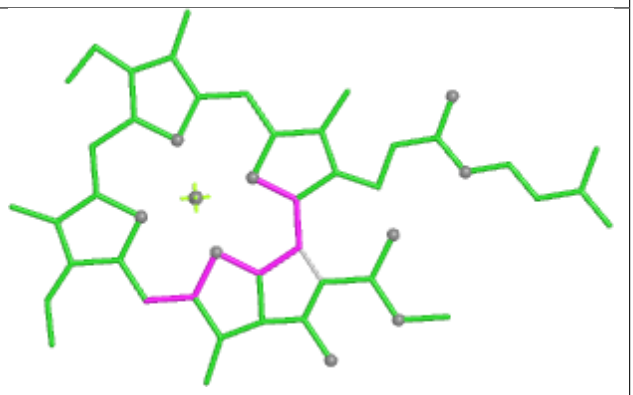


Rings

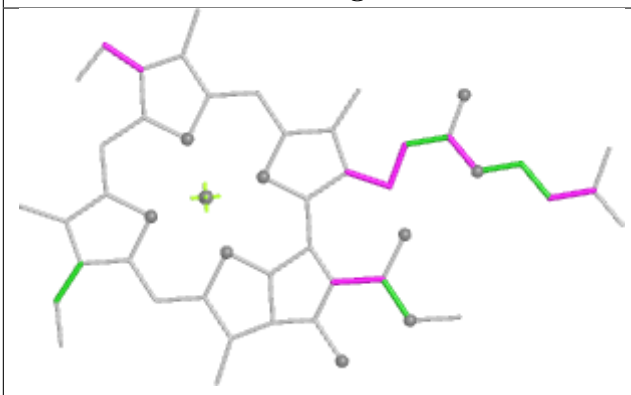
Ligand CLA 4 308



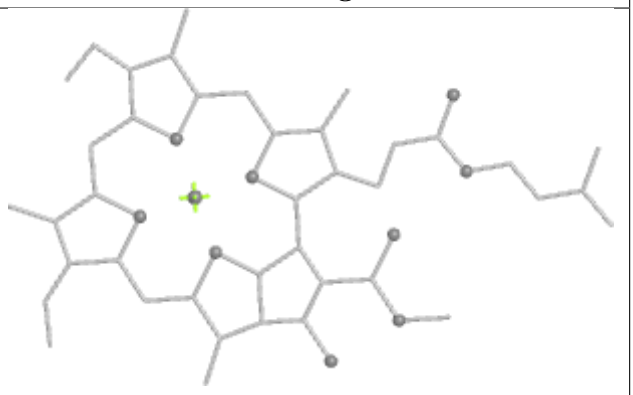
Bond lengths



Bond angles

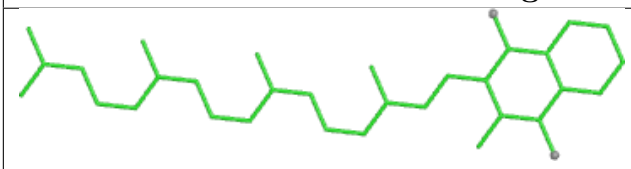


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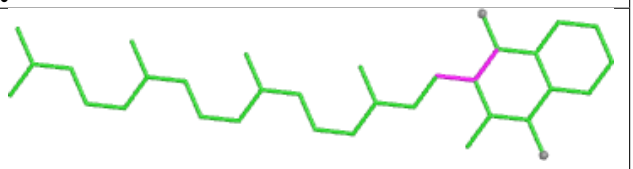


Rings

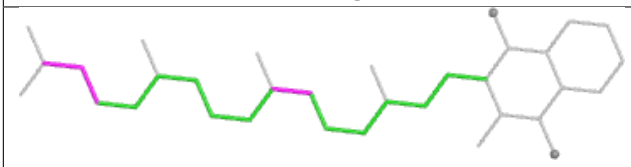
Ligand PQN A 841



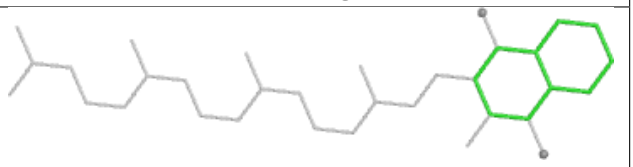
Bond lengths



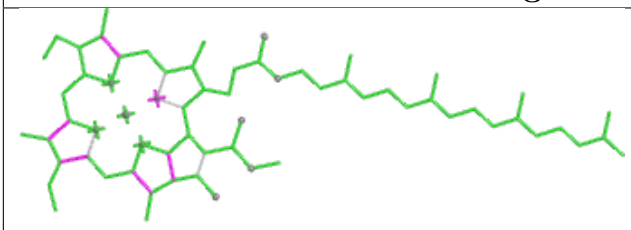
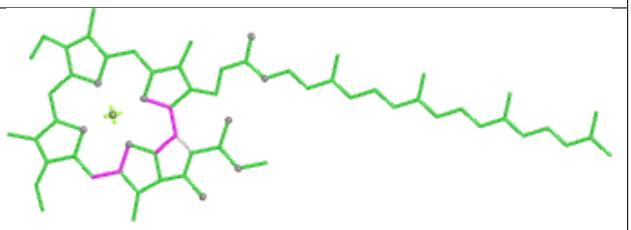
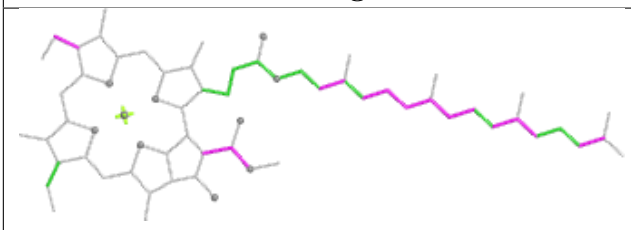
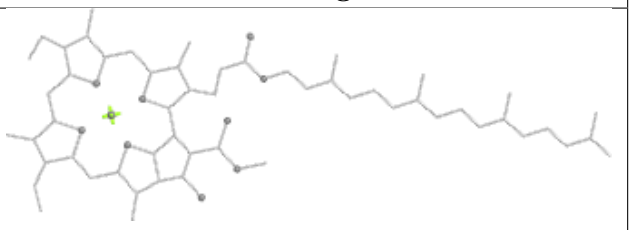
Bond angles

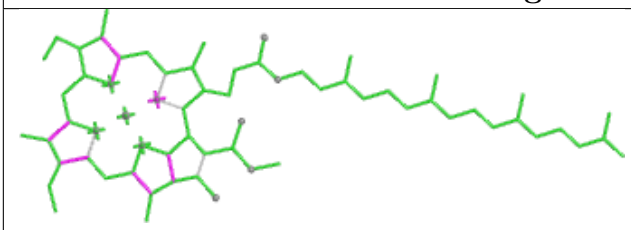
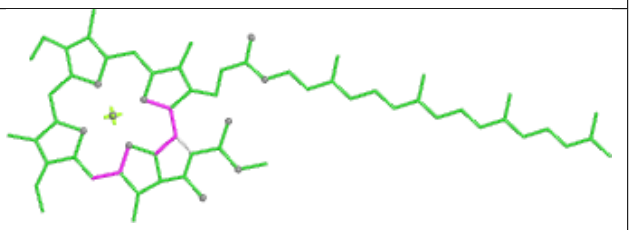
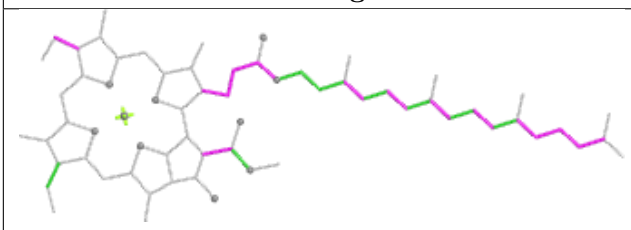
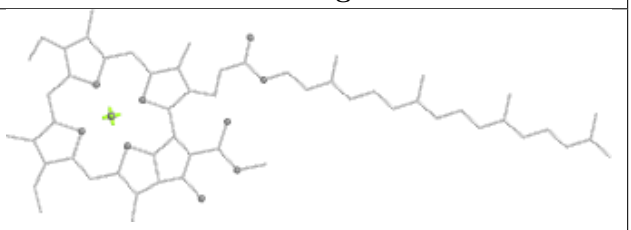


Torsions

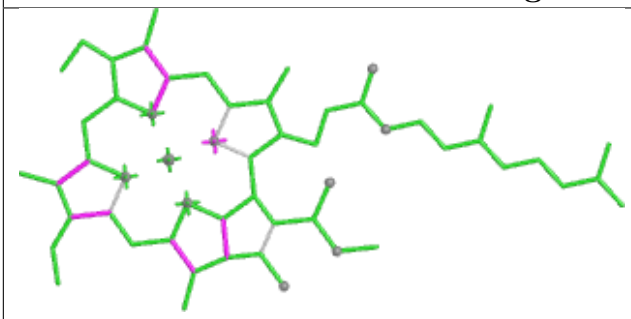


Rings

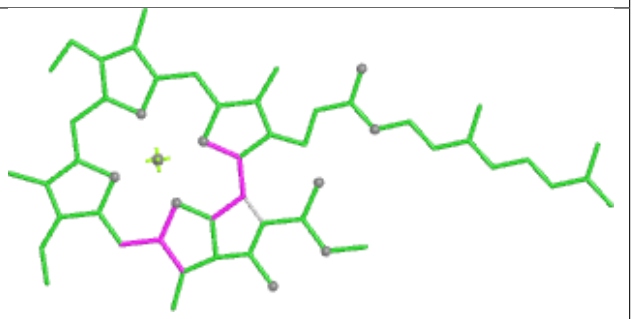
Ligand CLA A 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

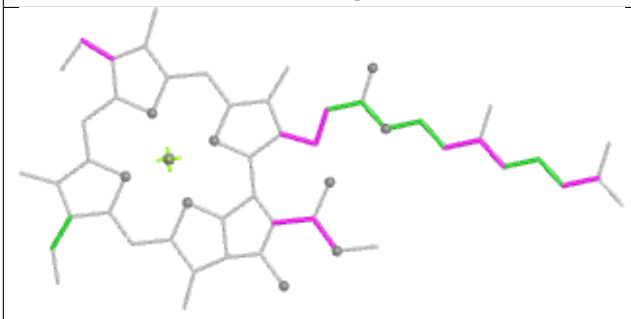
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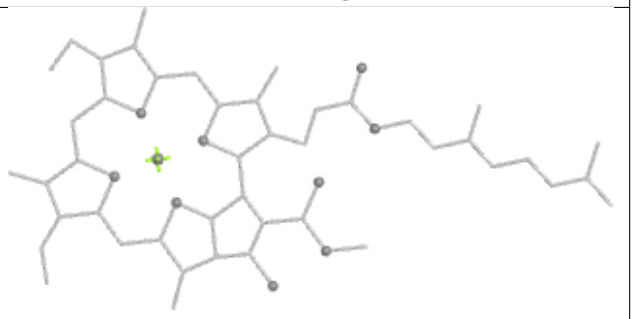
Bond lengths



Bond angles

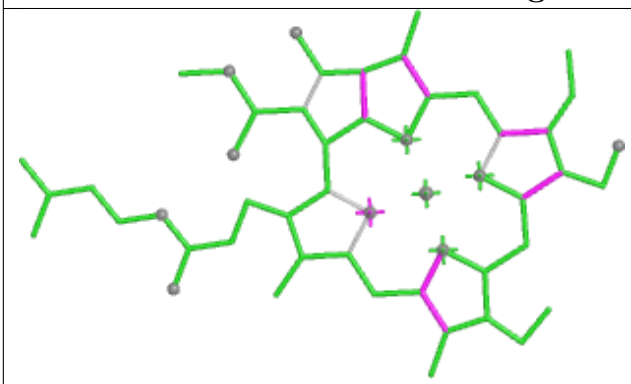


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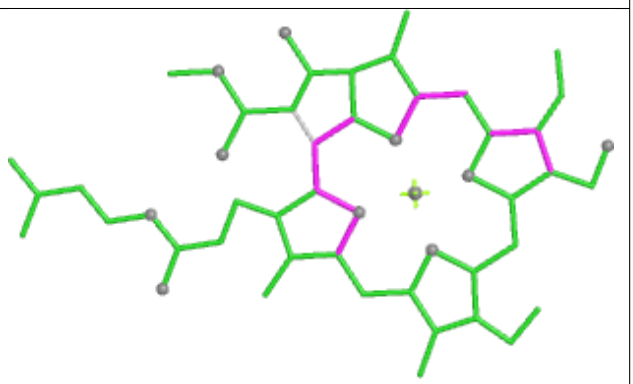


Rings

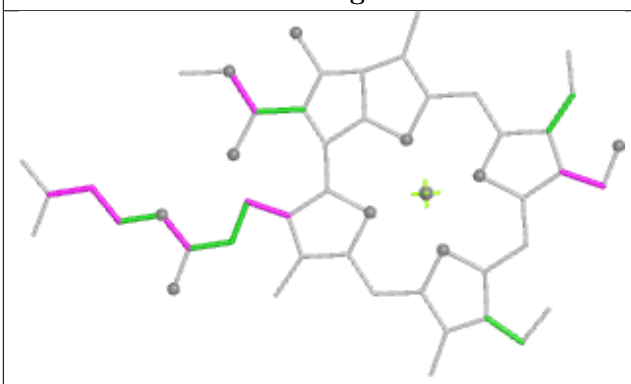
Ligand CHL 2 306



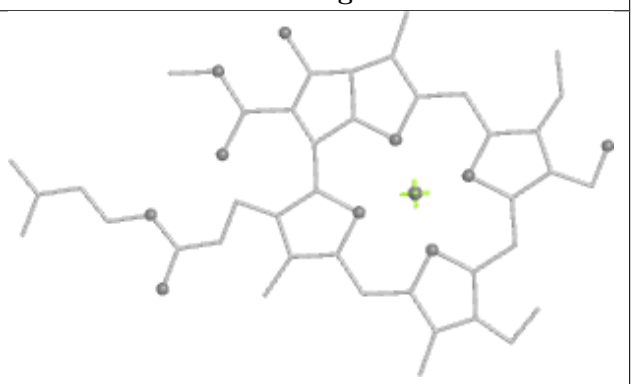
Bond lengths



Bond angles

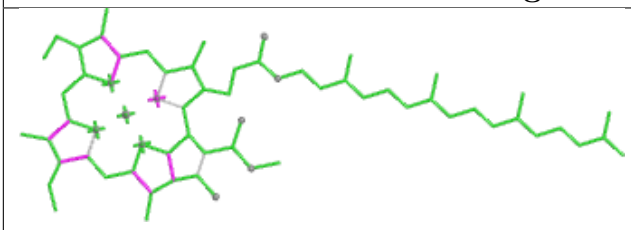


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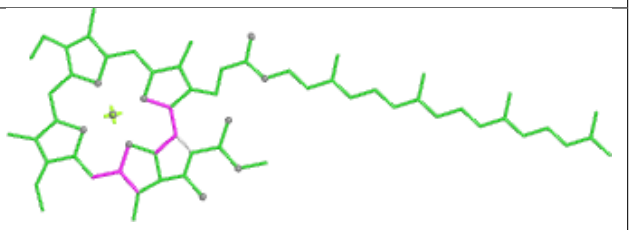


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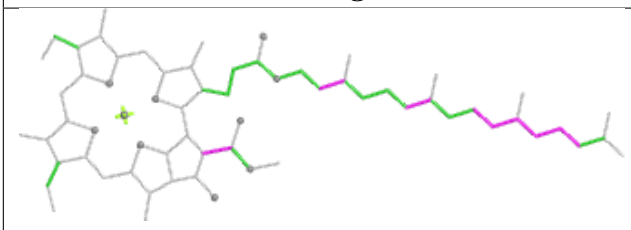
Ligand CLA A 803



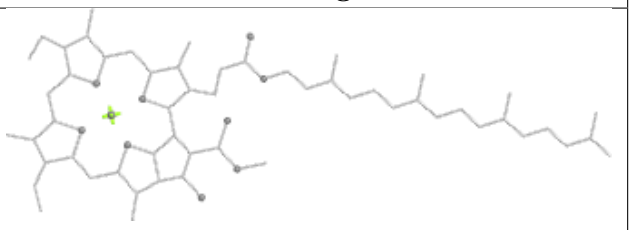
Bond lengths



Bond angles

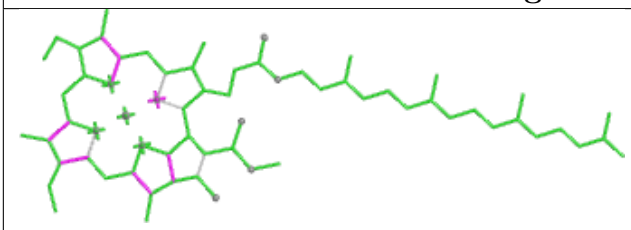


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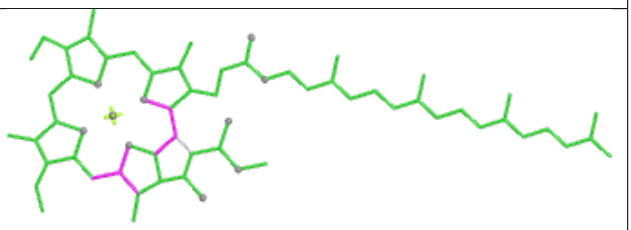


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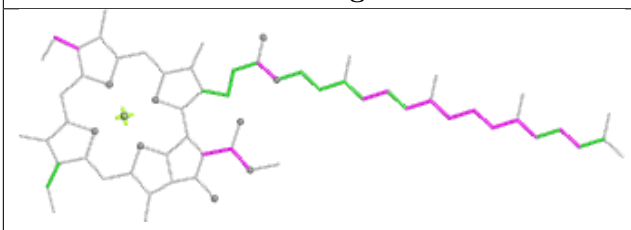
Ligand CLA B 819



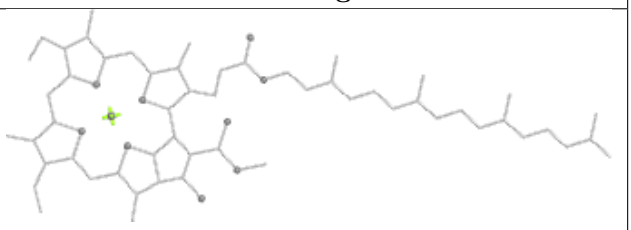
Bond lengths



Bond angles

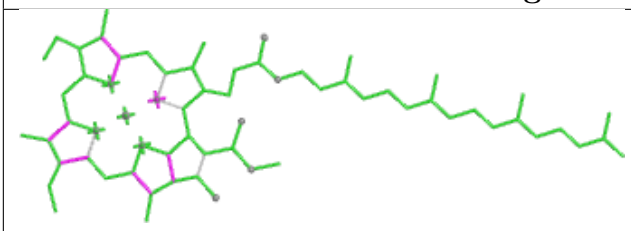


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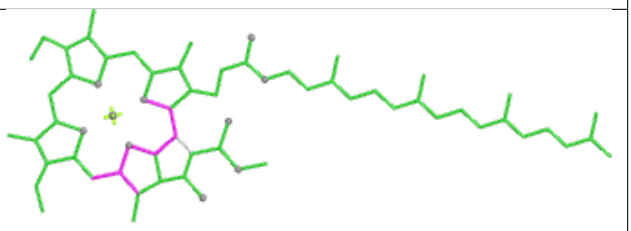


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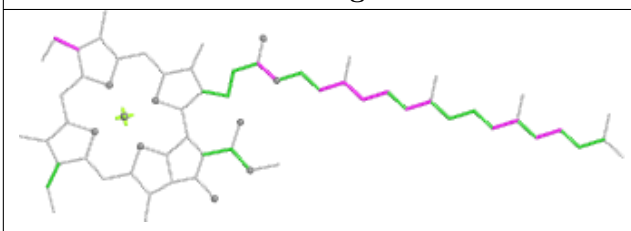
Ligand CLA A 835



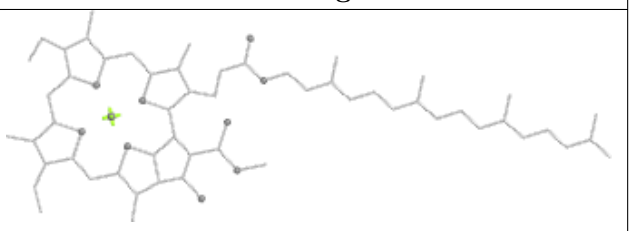
Bond lengths



Bond angles

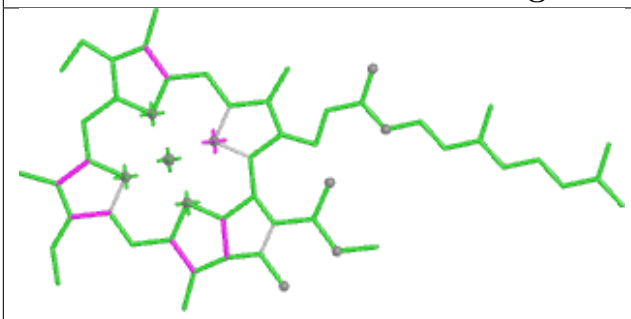


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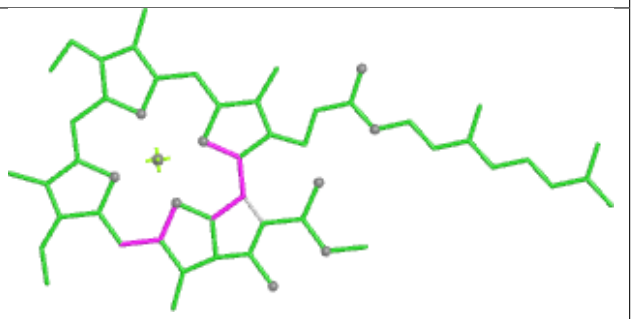


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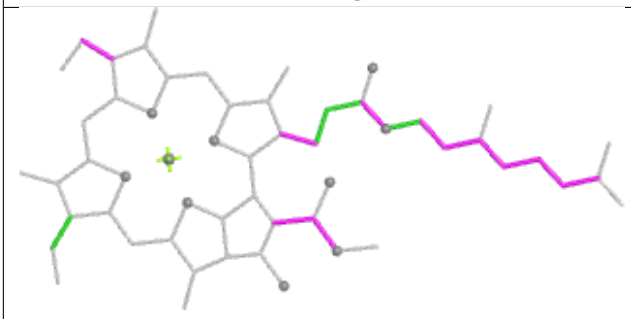
Ligand CLA 1 312



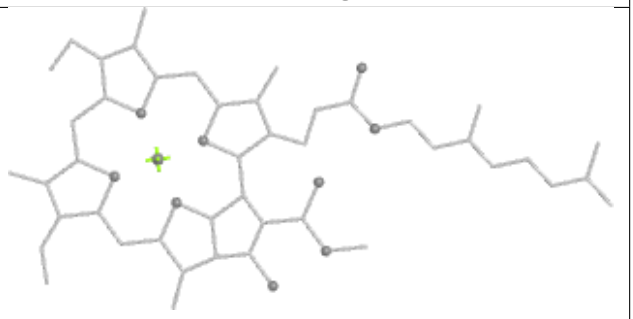
Bond lengths



Bond angles

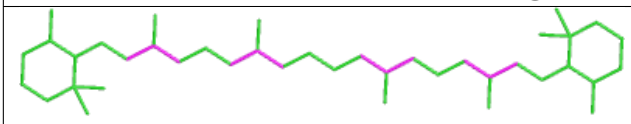


Torsions



Rings

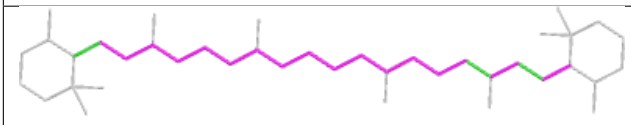
Ligand BCR 2 316



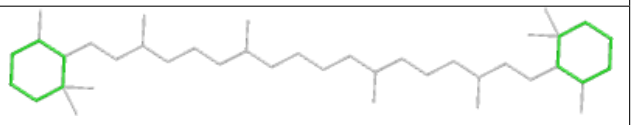
Bond lengths



Bond angles

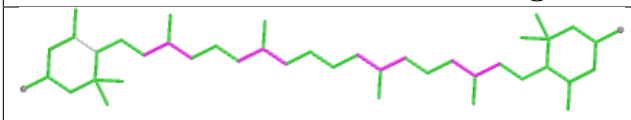


Torsions

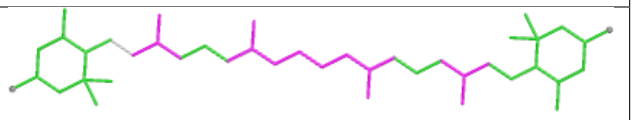


Rings

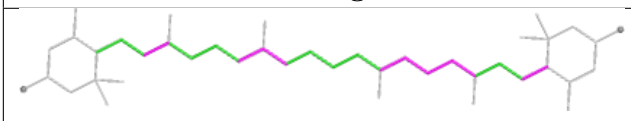
Ligand LUT 1 314



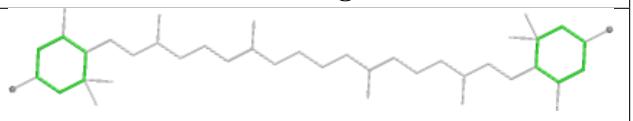
Bond lengths



Bond angles

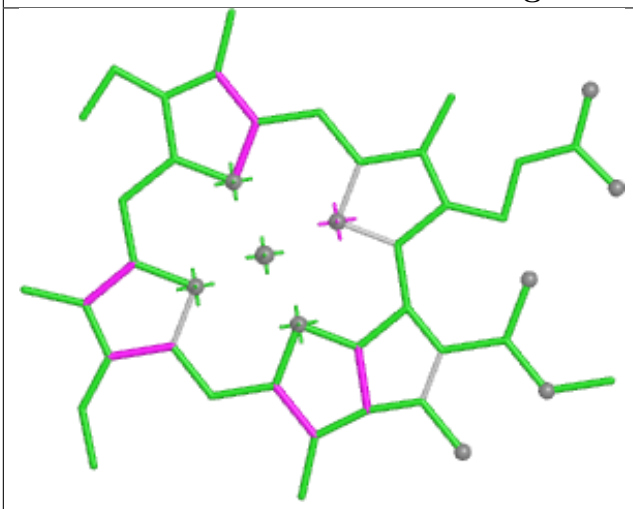


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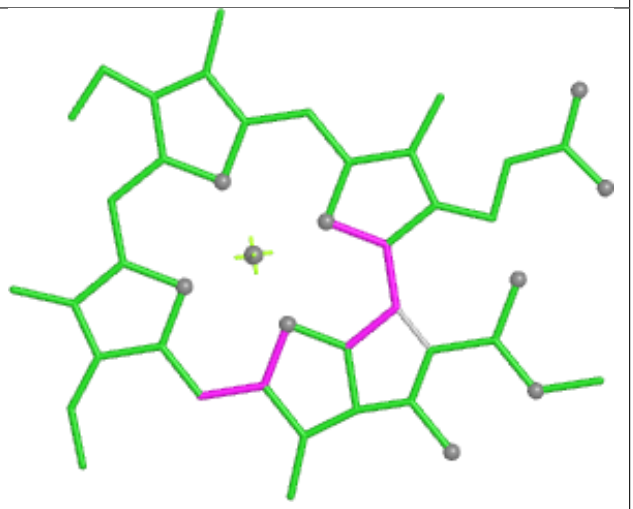


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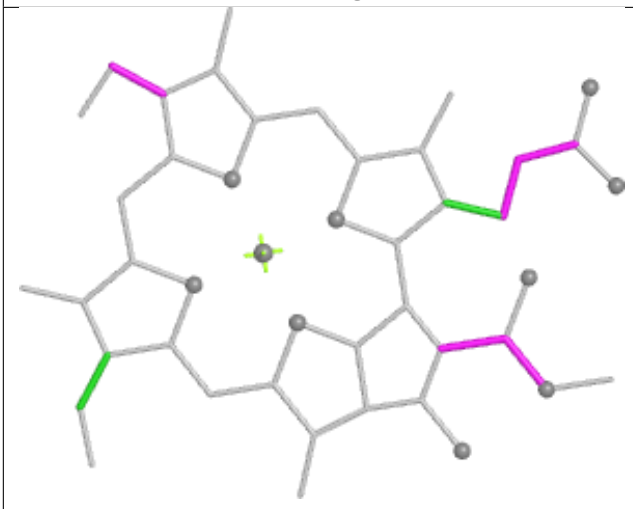
Ligand CLA A 814



Bond lengths



Bond angles

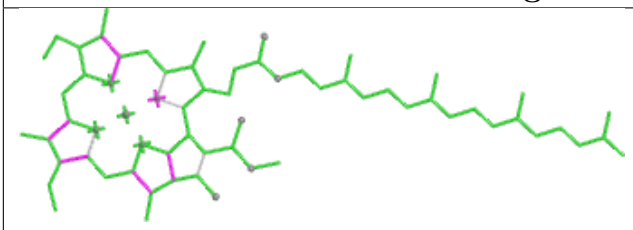


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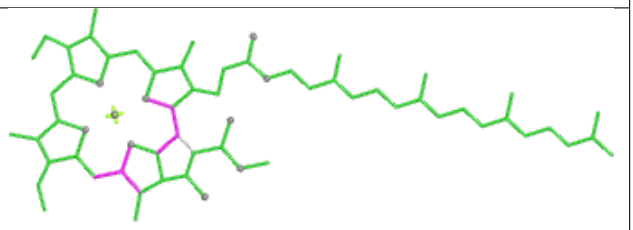


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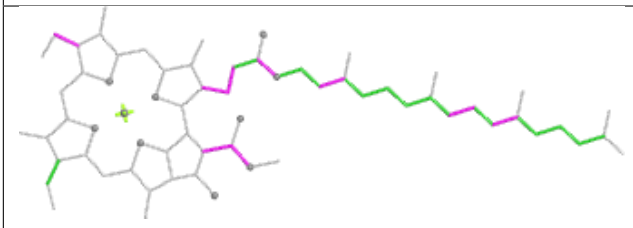
Ligand CLA A 817



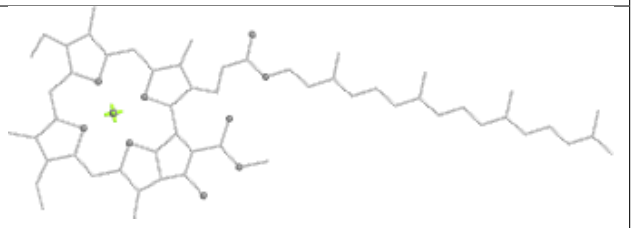
Bond lengths



Bond angles

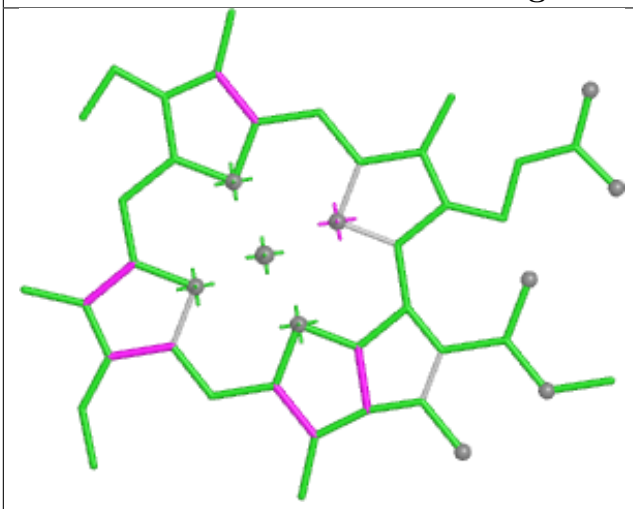


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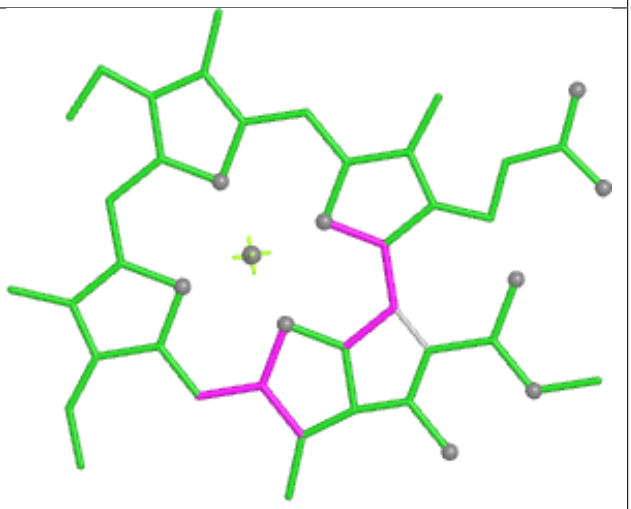


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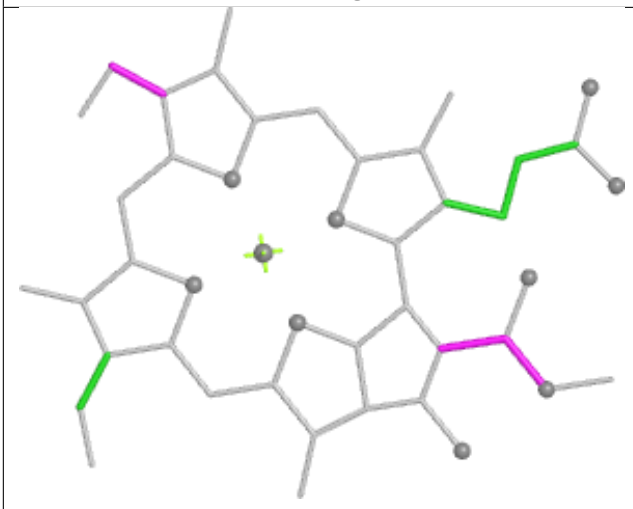
Ligand CLA 3 303



Bond lengths



Bond angles

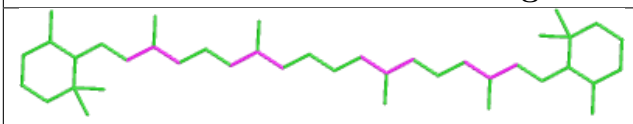


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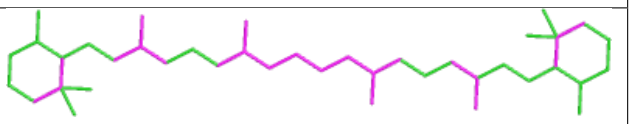


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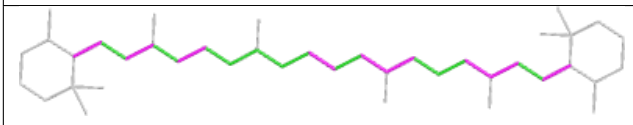
Ligand BCR G 201



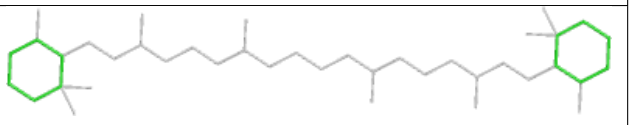
Bond lengths



Bond angles



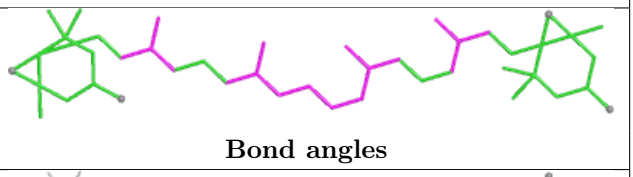
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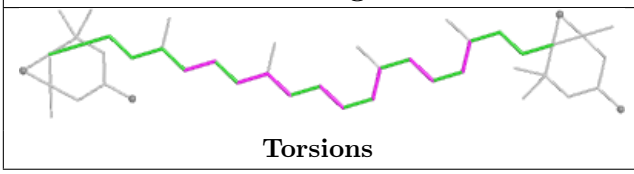


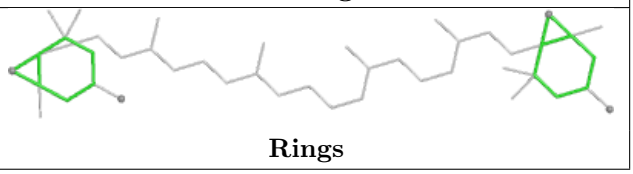
Rings

Ligand XAT 2 315

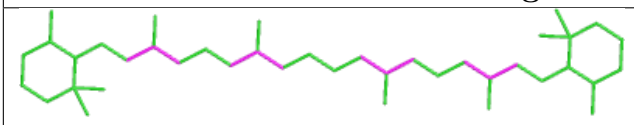

Bond lengths

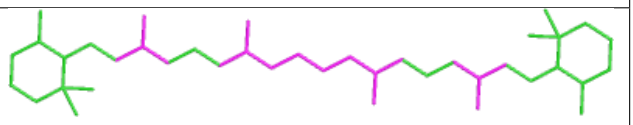

Bond angles

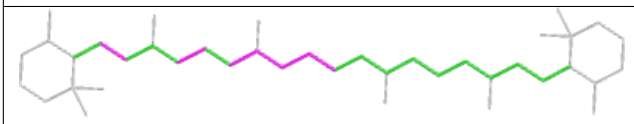

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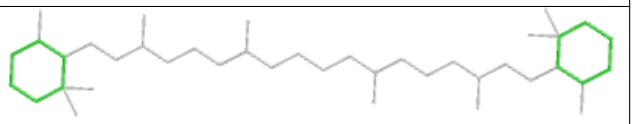

Rings

Ligand BCR A 846

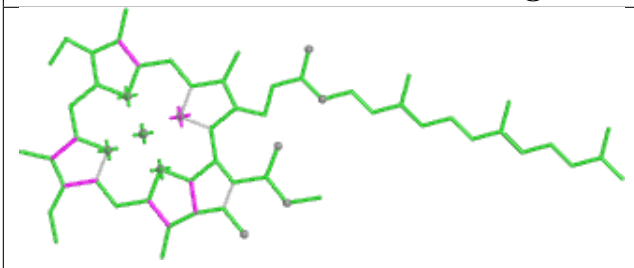

Bond lengths

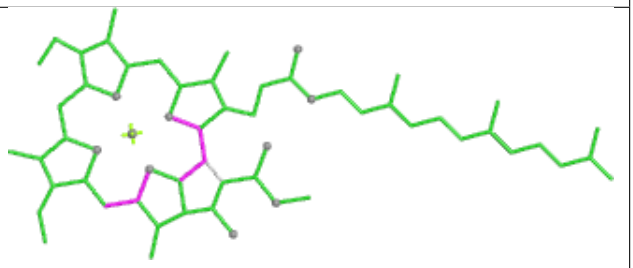

Bond angles

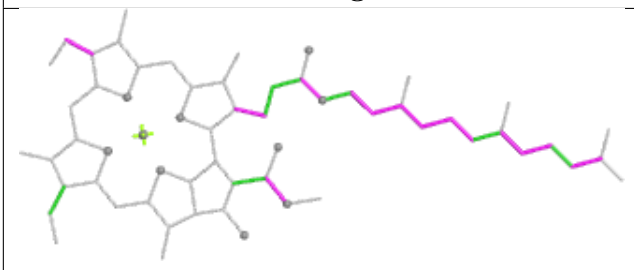

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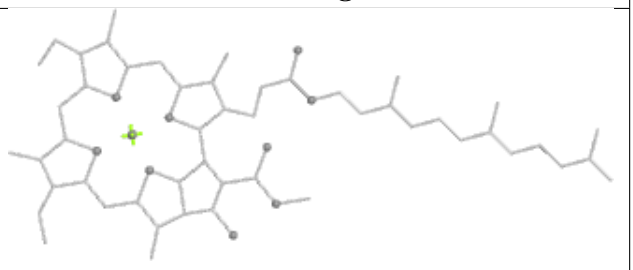

Rings

Ligand CLA B 823

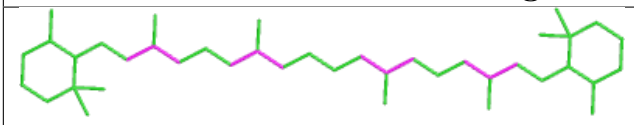

Bond lengths

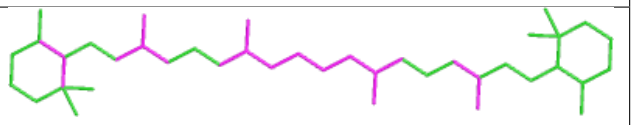

Bond angles

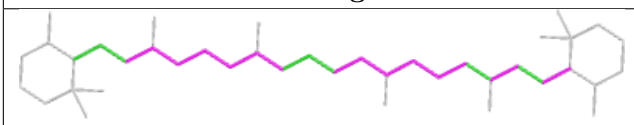

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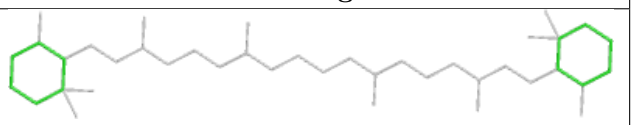

Rings

Ligand BCR A 848

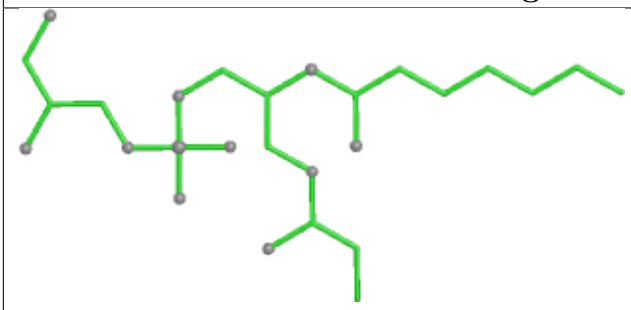

Bond lengths


Bond angles

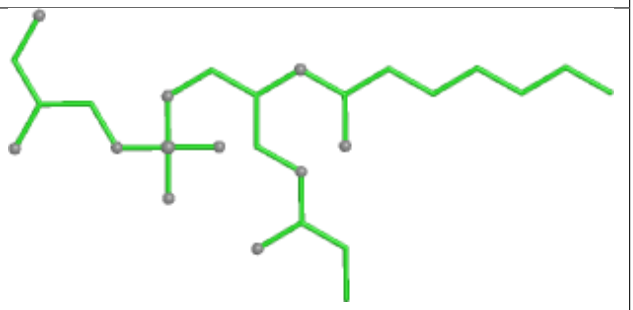

Torsions


Rings

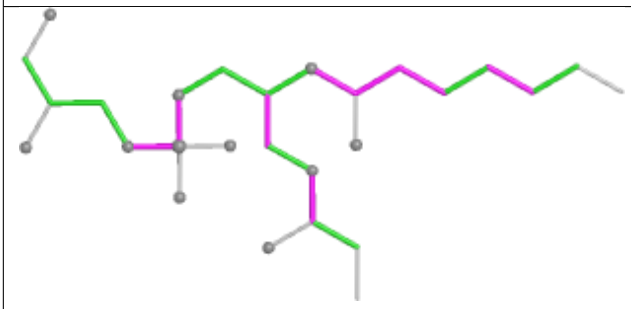
Ligand LHG A 843



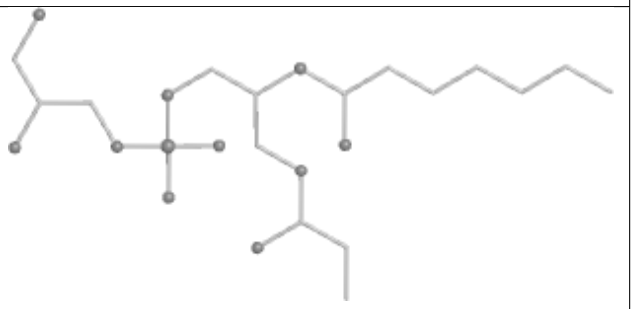
Bond lengths



Bond angles

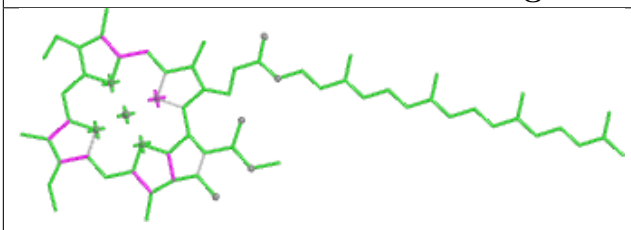


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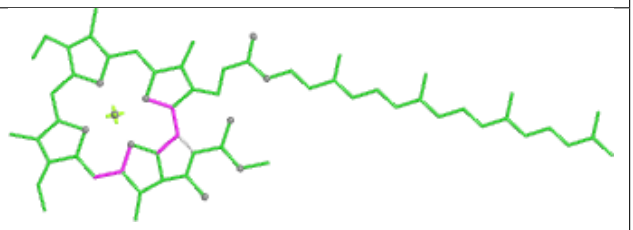


Rings

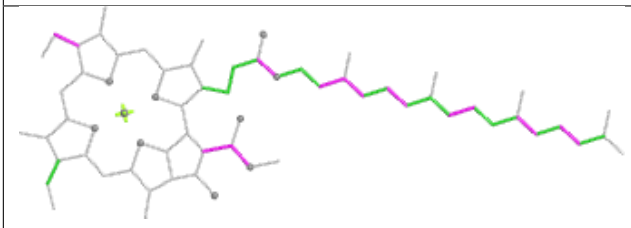
Ligand CLA B 802



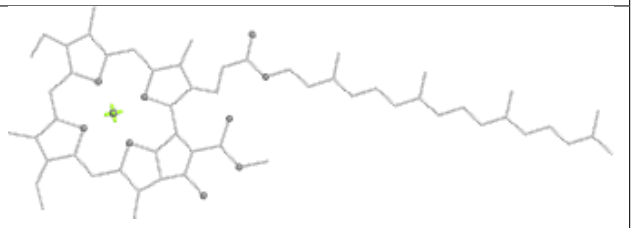
Bond lengths



Bond angles

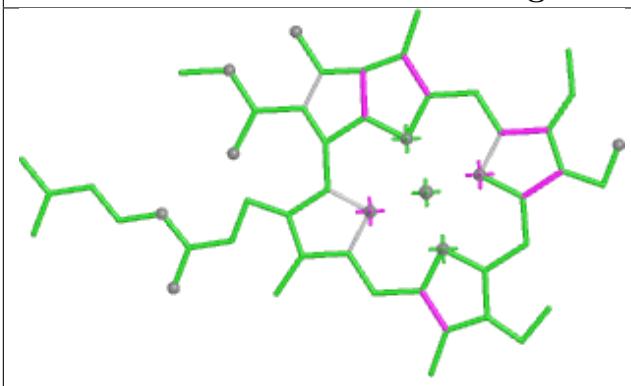


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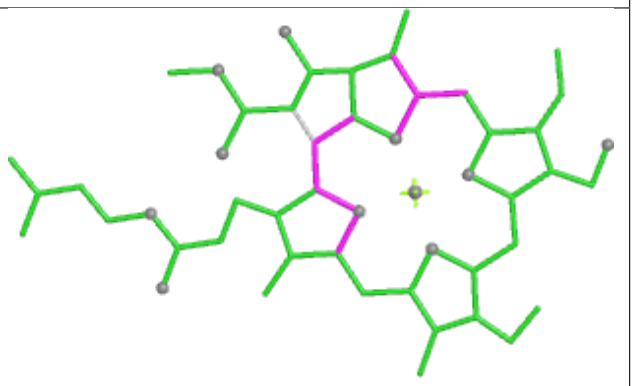


Rings

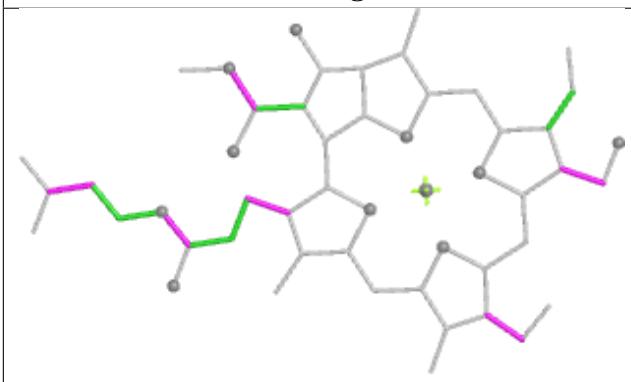
Ligand CHL 4 306



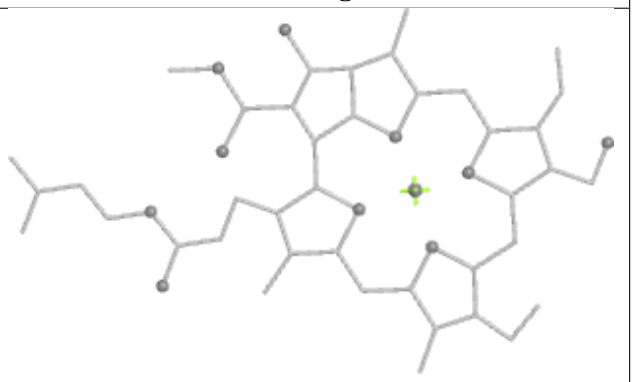
Bond lengths



Bond angles

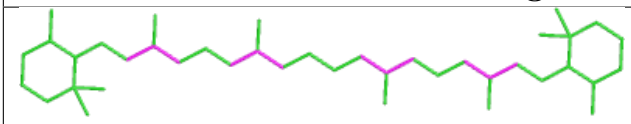


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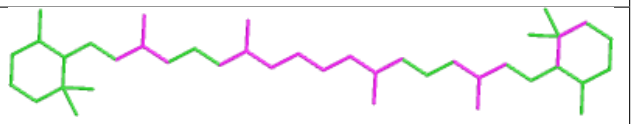


Rings

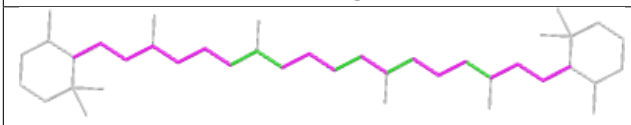
Ligand BCR J 104



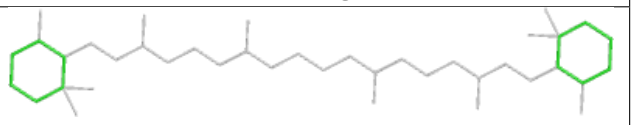
Bond lengths



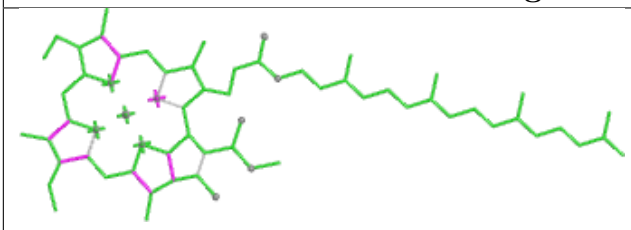
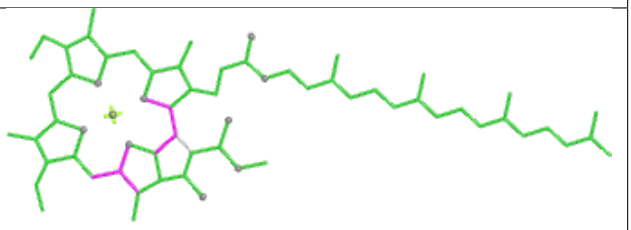
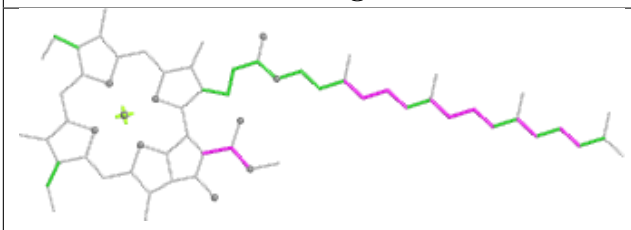
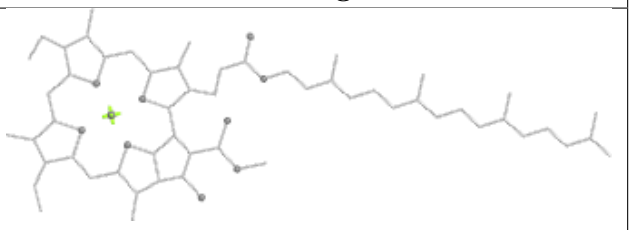
Bond angles

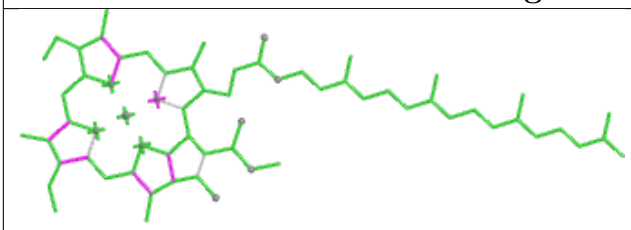
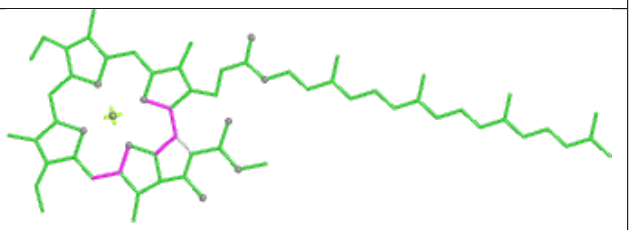
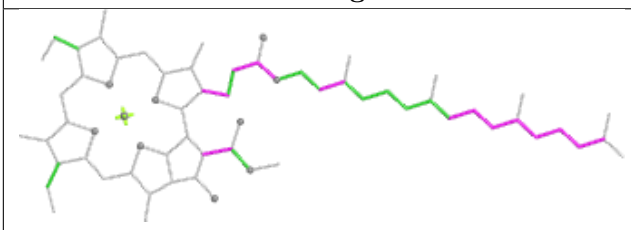
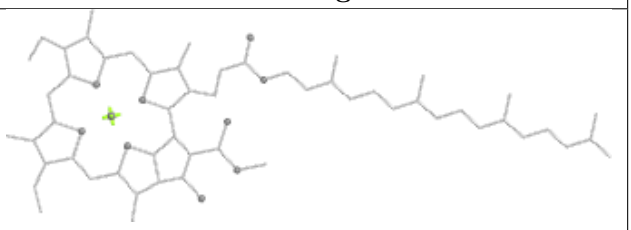


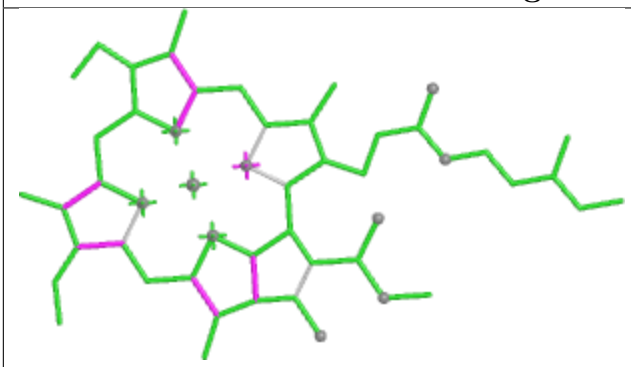
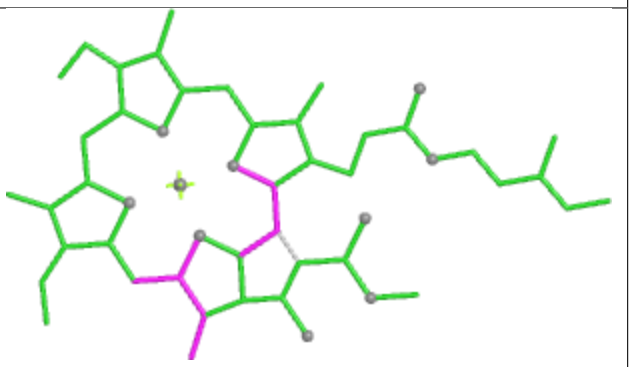
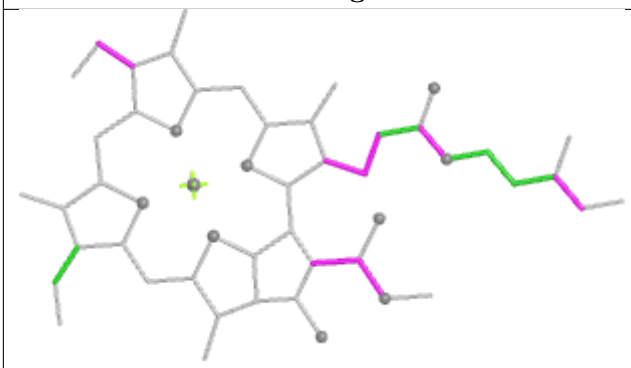
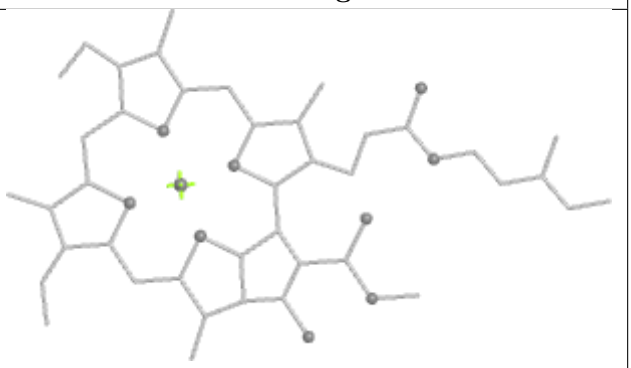
Torsions

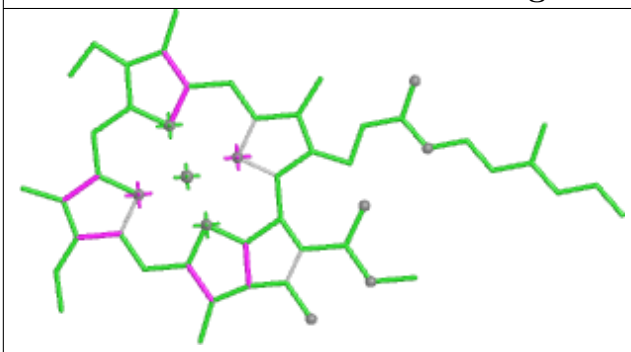
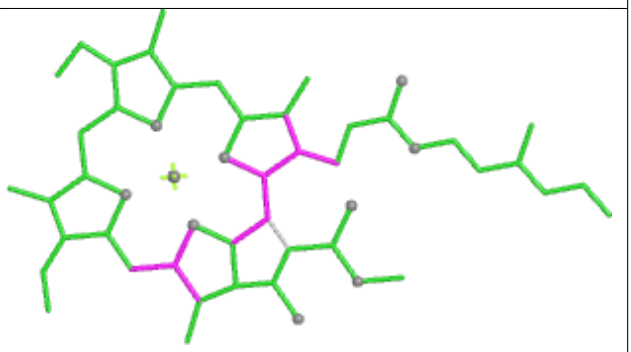
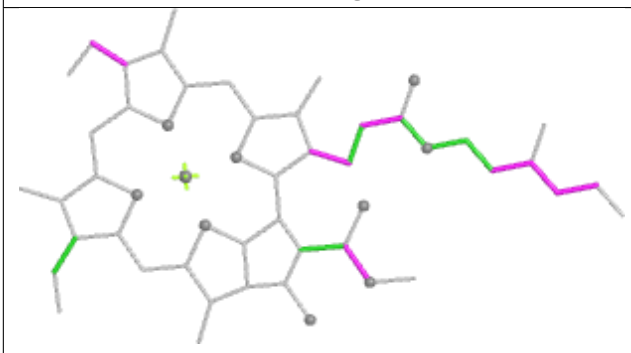
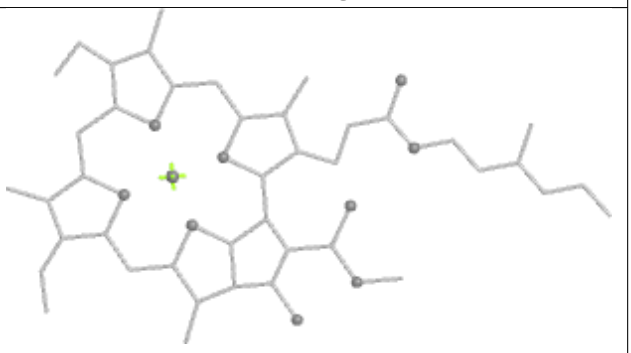


Rings

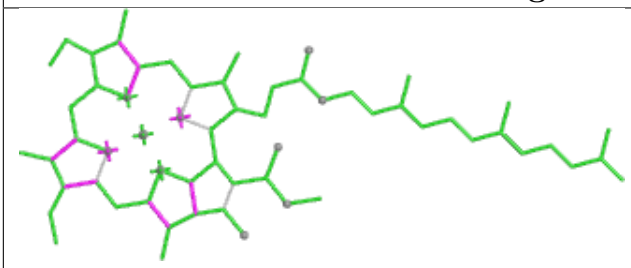
Ligand CLA B 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

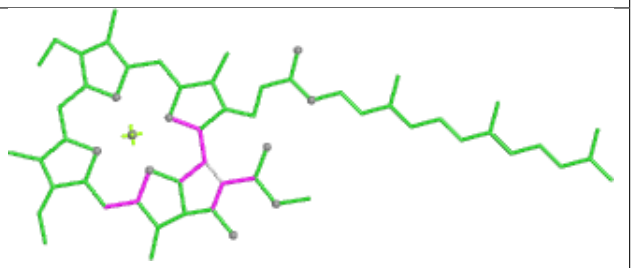
Ligand CLA A 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

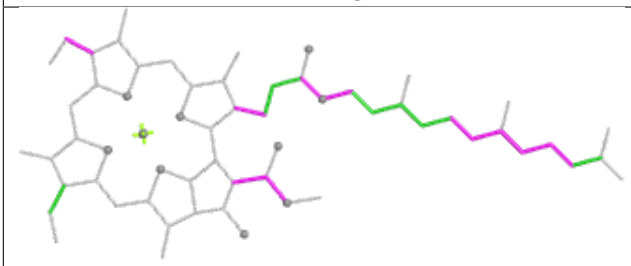
Ligand CLA 4 303



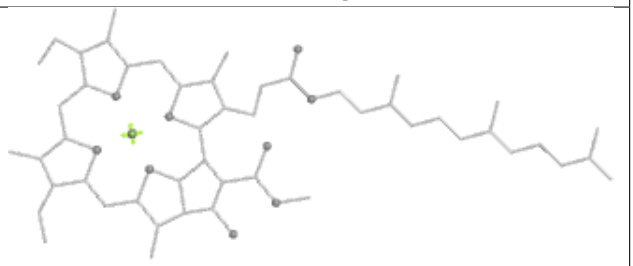
Bond lengths



Bond angles

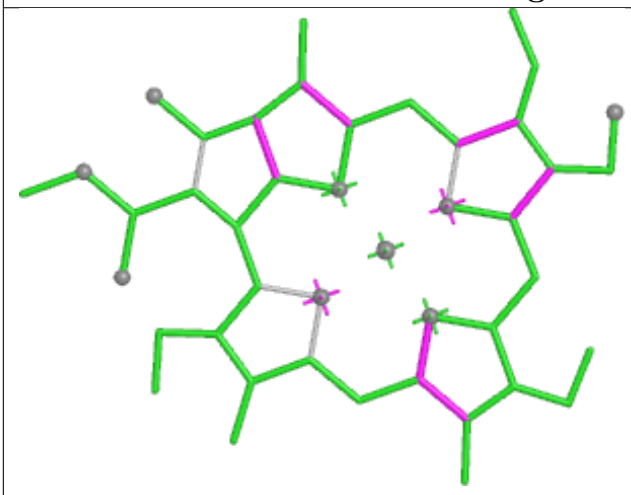


Torsions

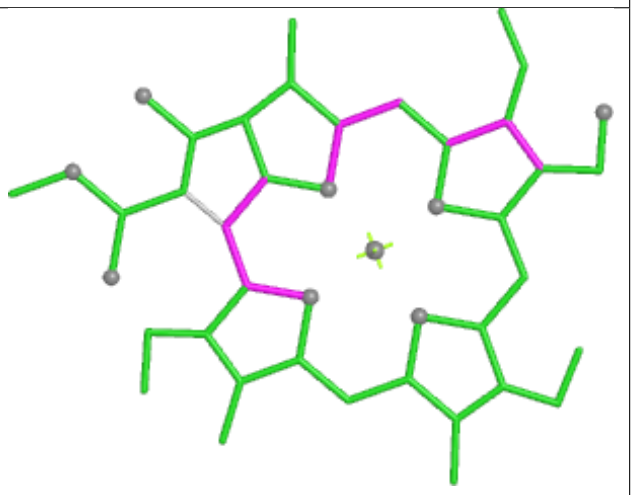


Rings

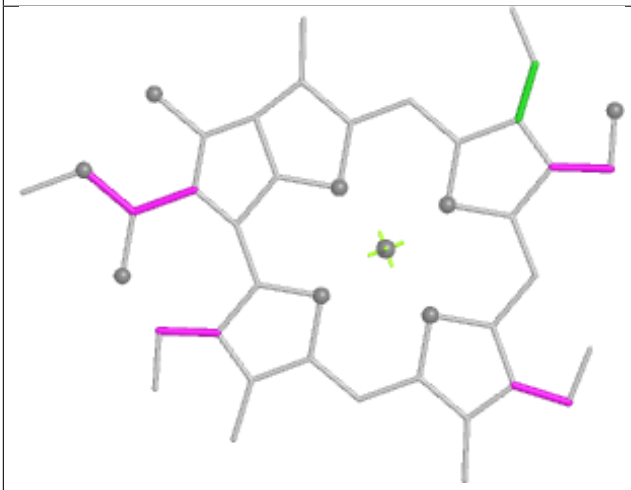
Ligand CHL 4 315



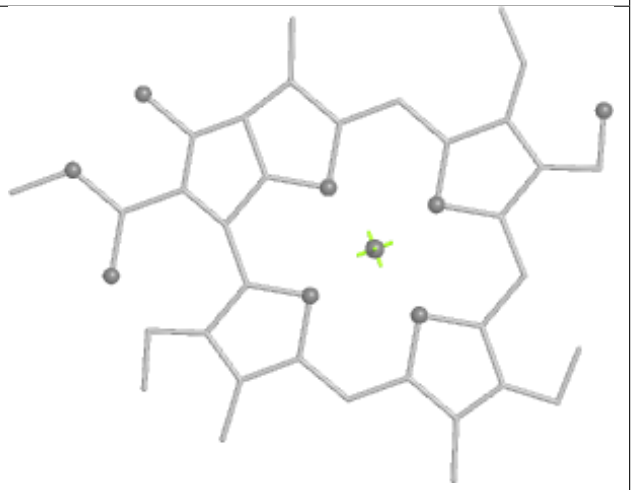
Bond lengths



Bond angles

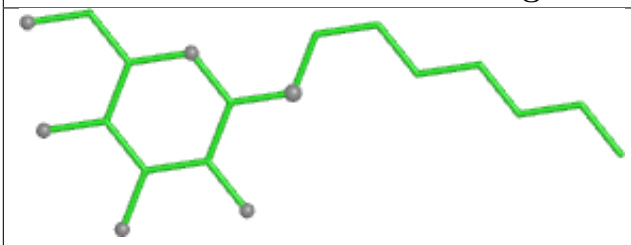


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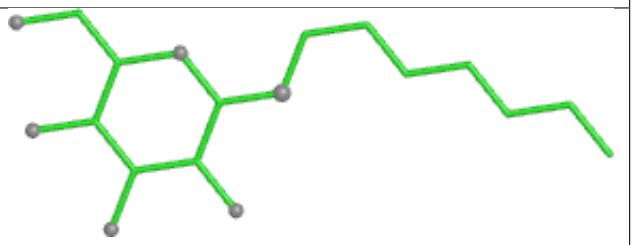


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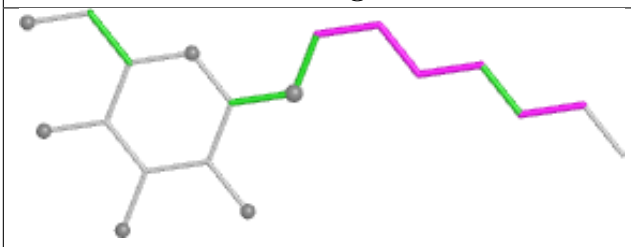
Ligand HTG F 310



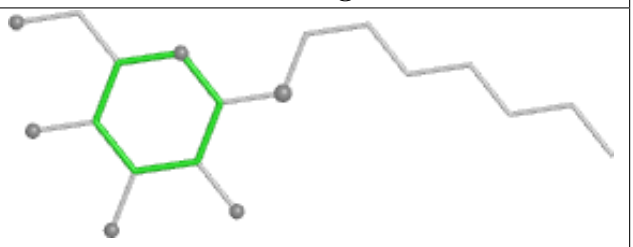
Bond lengths



Bond angles

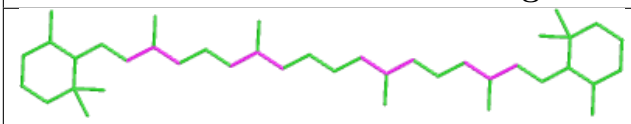


Torsions



Rings

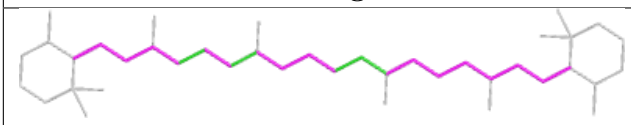
Ligand BCR O 105



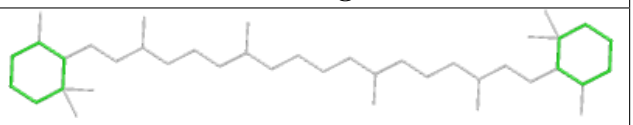
Bond lengths



Bond angles

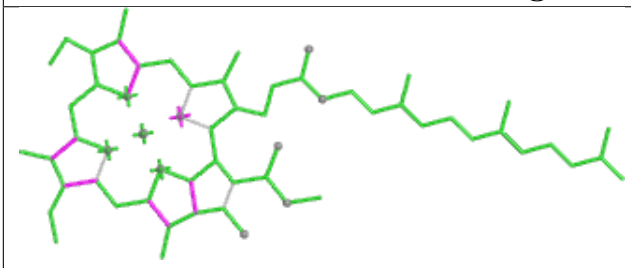


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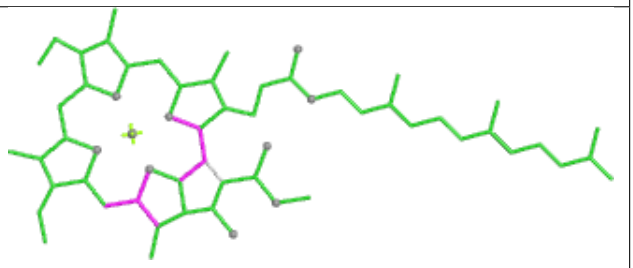


Rings

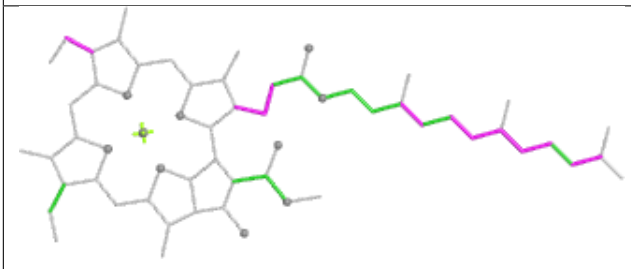
Ligand CLA 1 308



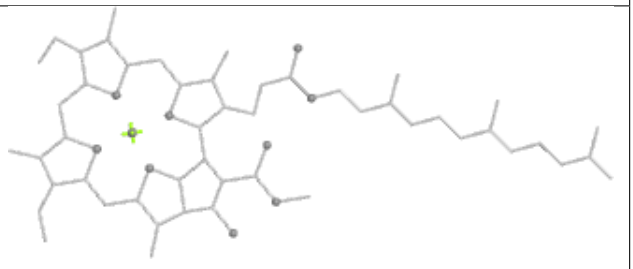
Bond lengths



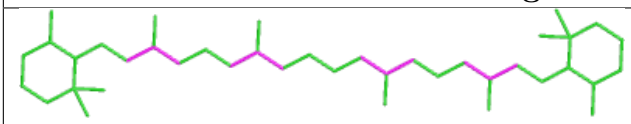
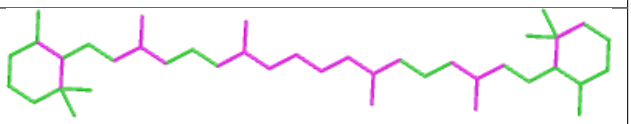
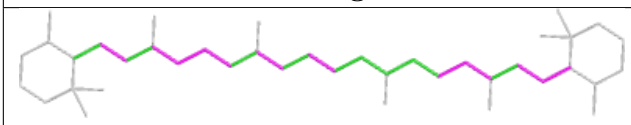
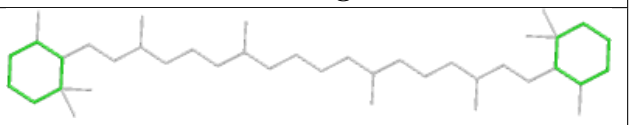
Bond angles

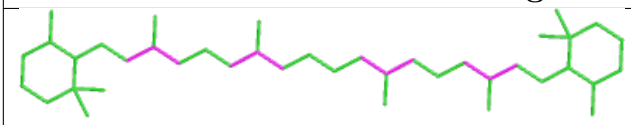
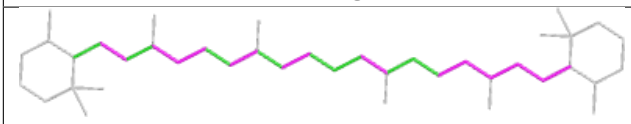
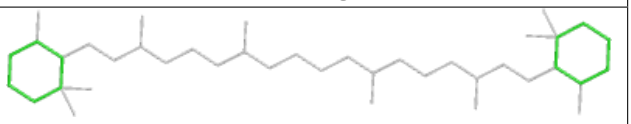


Torsions

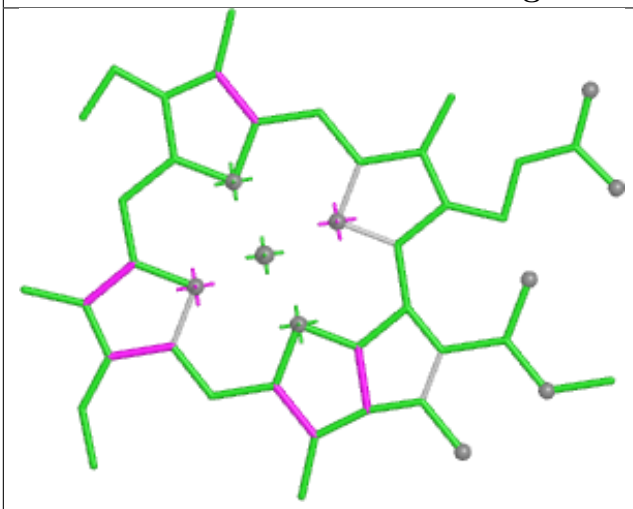


Rings

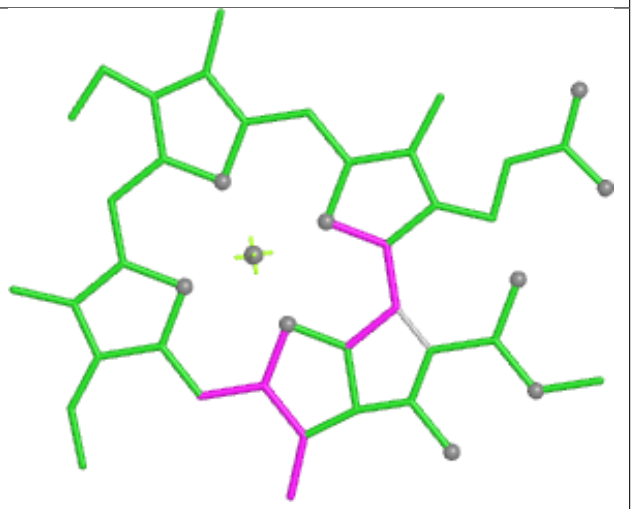
Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR 3 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

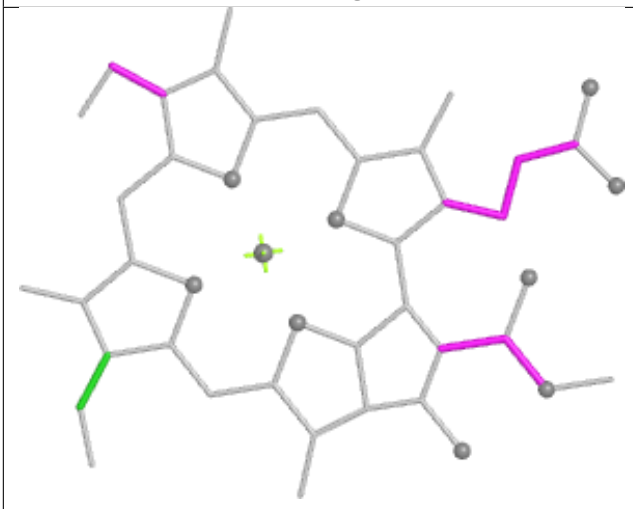
Ligand CLA K 302



Bond lengths



Bond angles

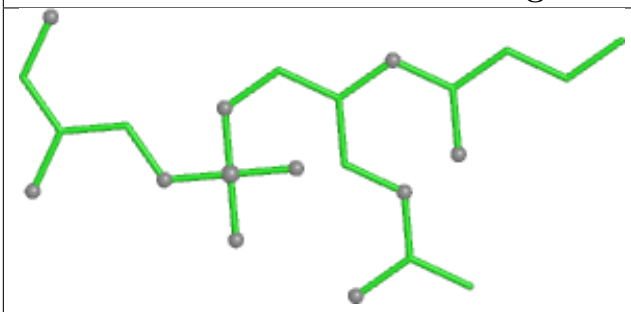


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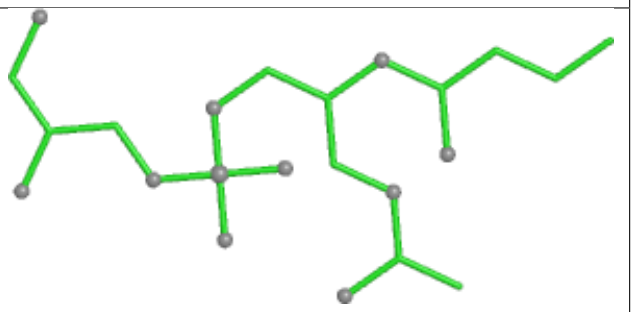


Rings

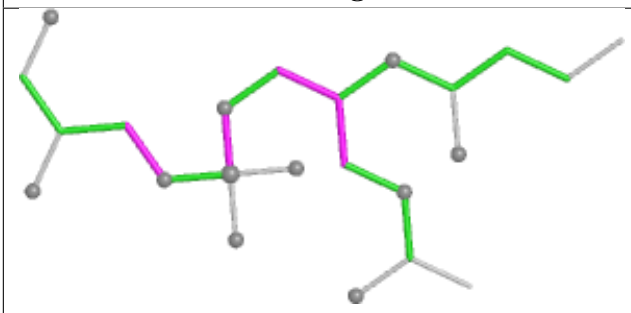
Ligand LHG 1 319



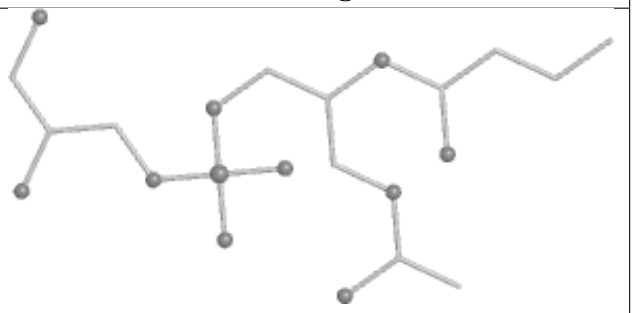
Bond lengths



Bond angles

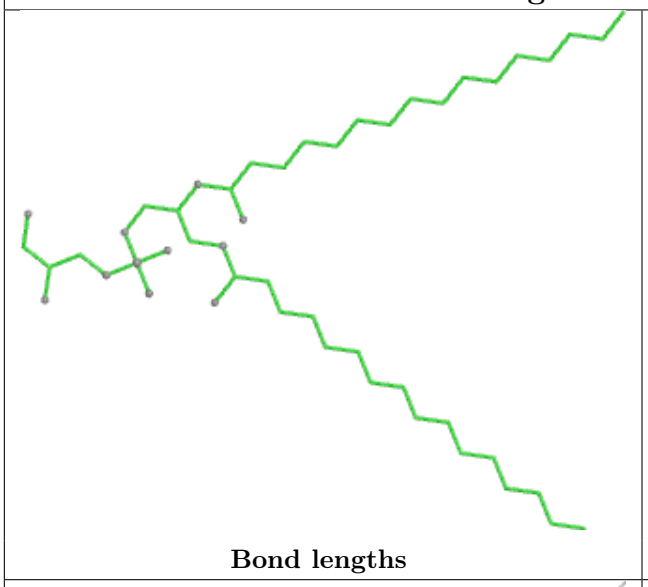


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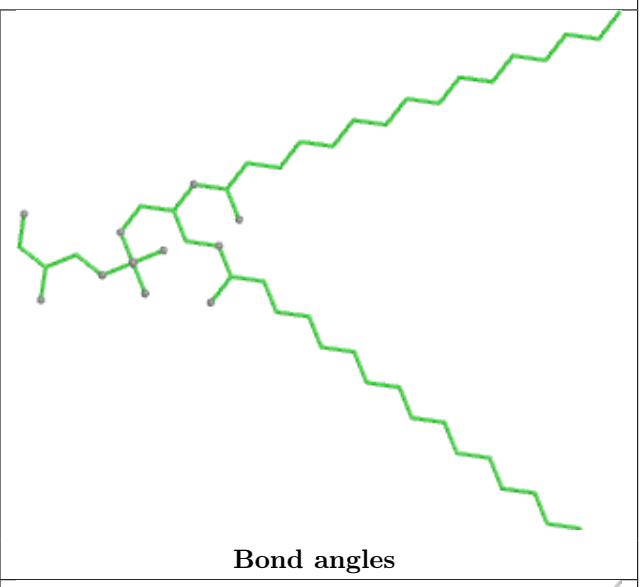


Rings

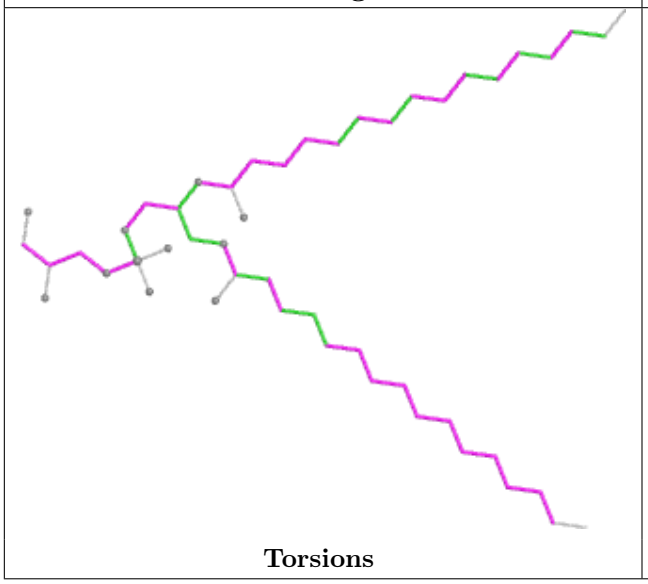
Ligand LHG 1 320



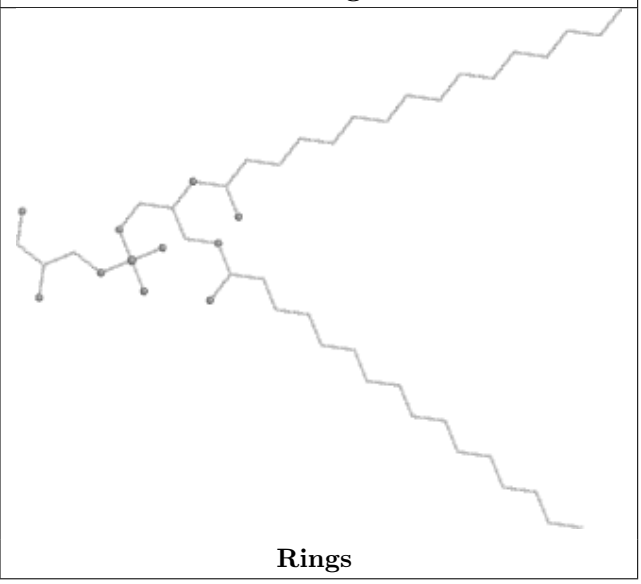
Bond lengths



Bond angles

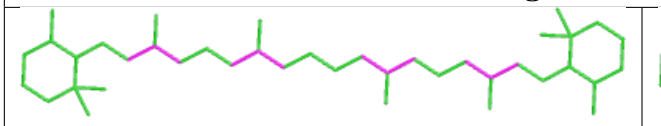


Torsions



Rings

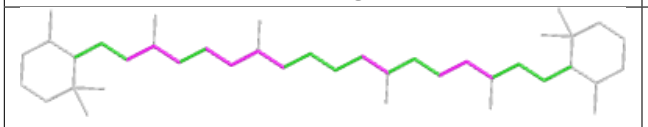
Ligand BCR B 842



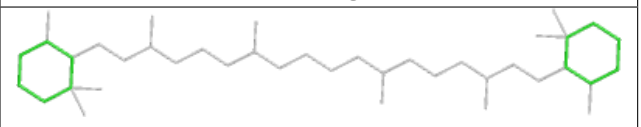
Bond lengths



Bond angles



Torsions

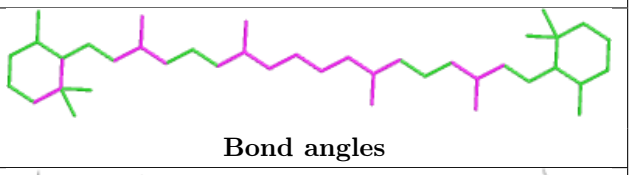


Rings

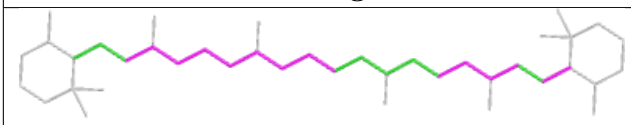
Ligand BCR F 304



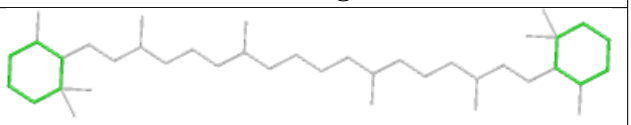
Bond lengths



Bond angles

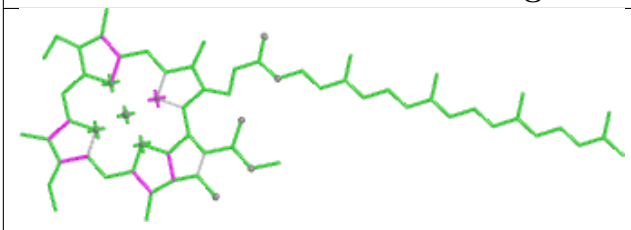


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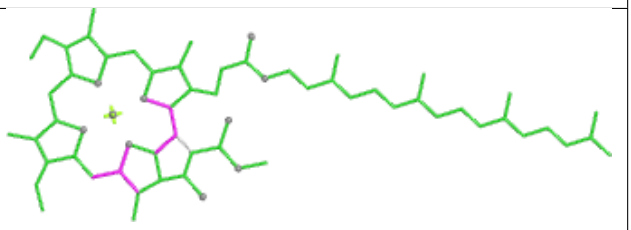


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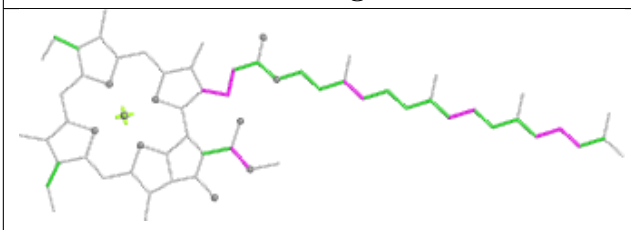
Ligand CLA B 801



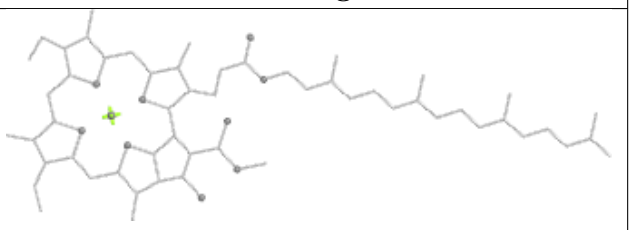
Bond lengths



Bond angles

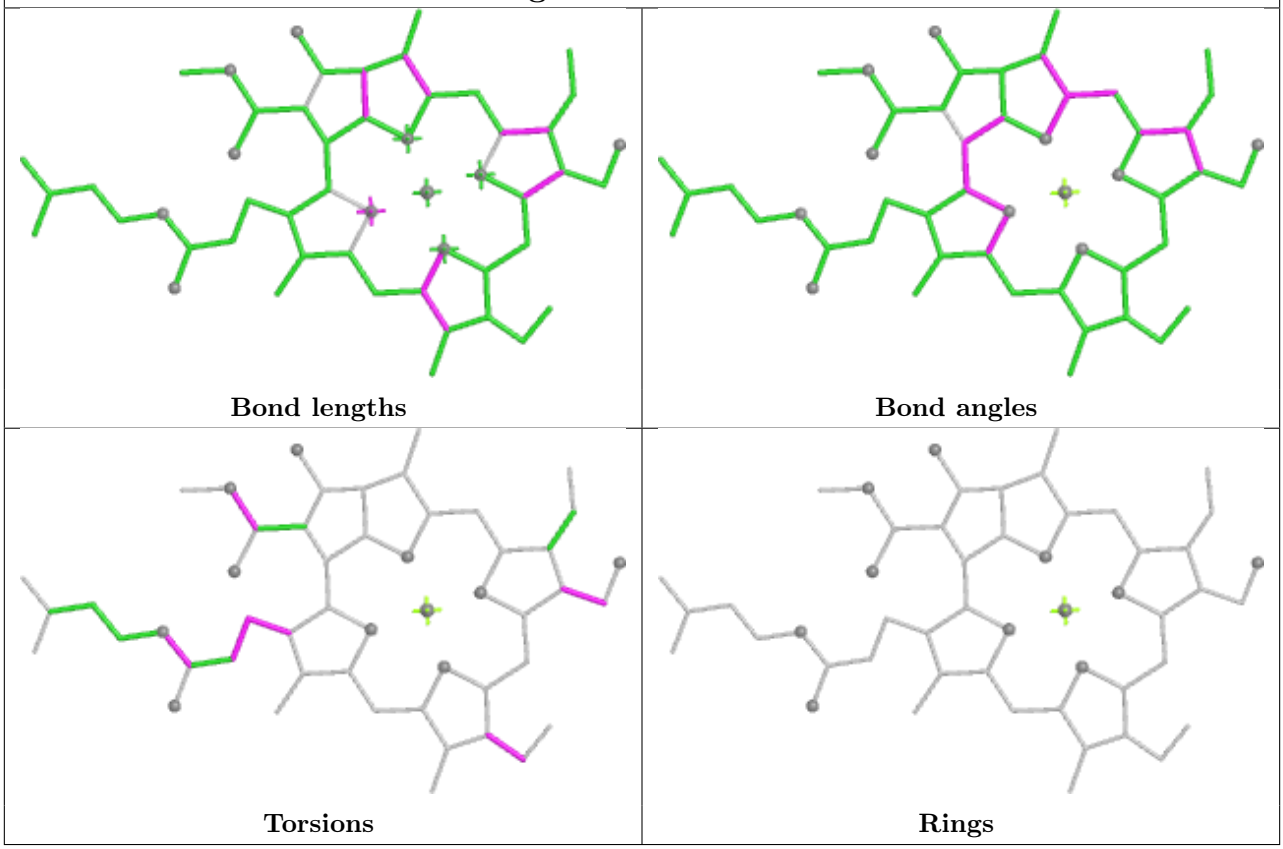


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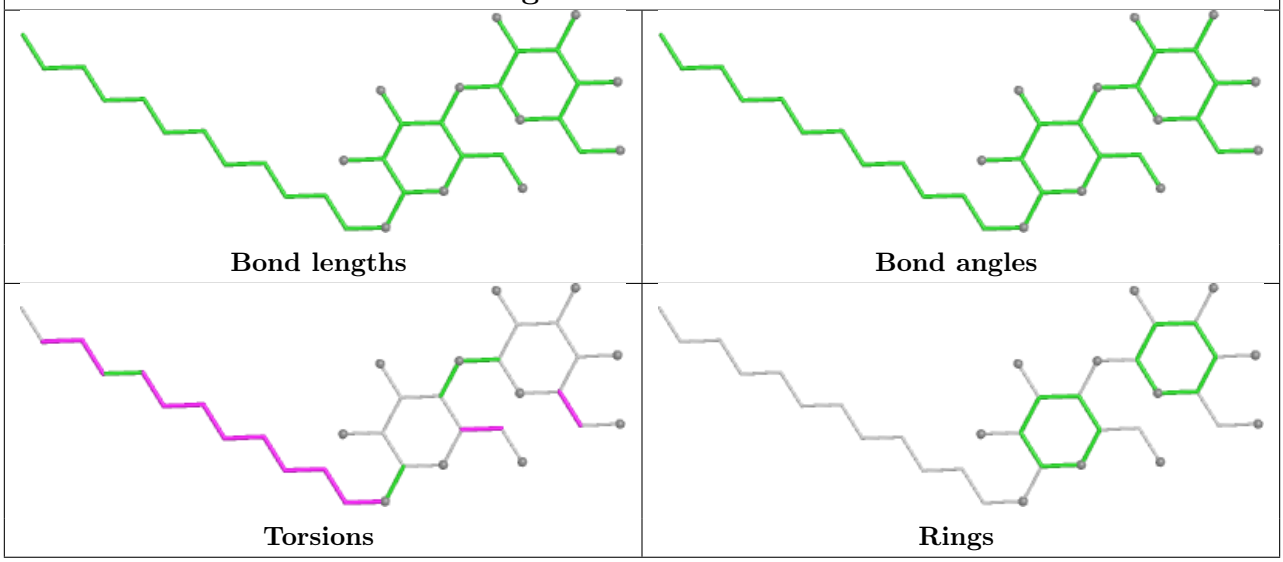


Rings

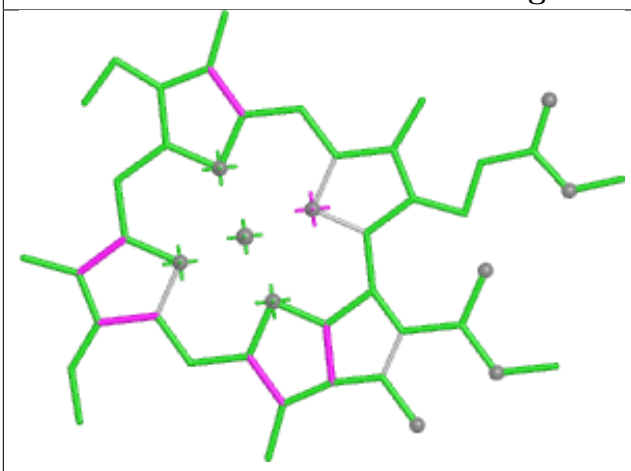
Ligand CHL 4 307



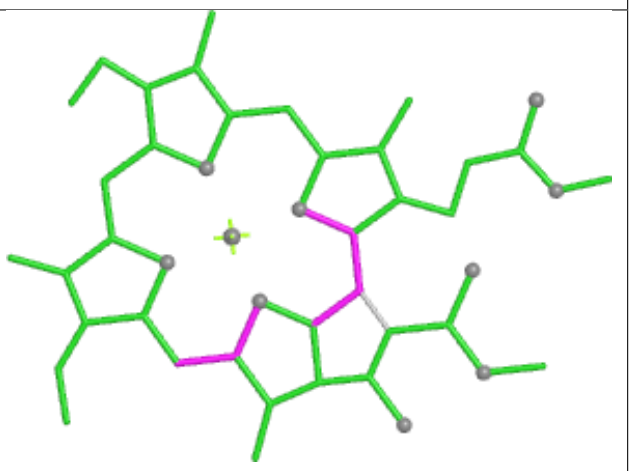
Ligand LMT A 851



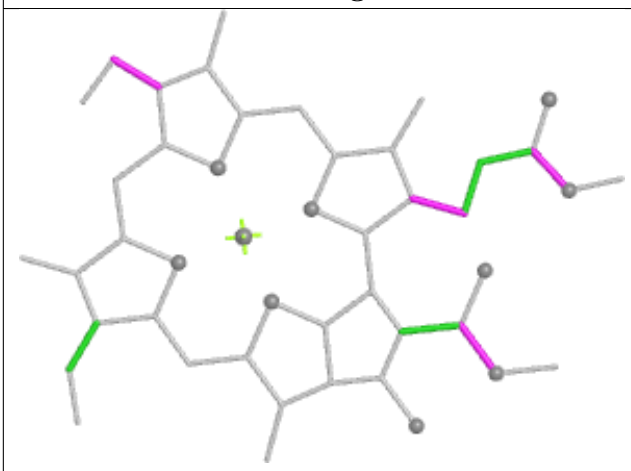
Ligand CLA 1 313



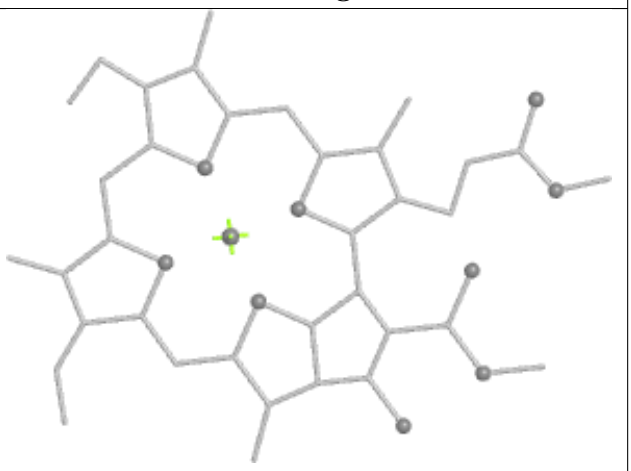
Bond lengths



Bond angles

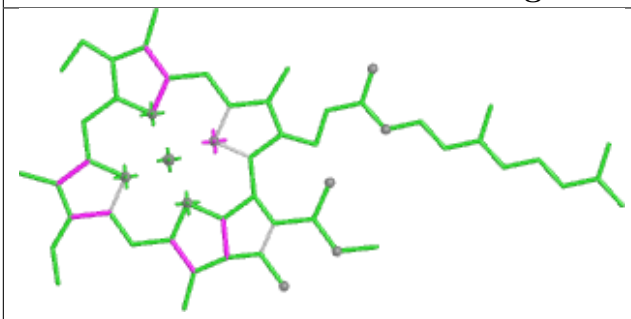


Torsions

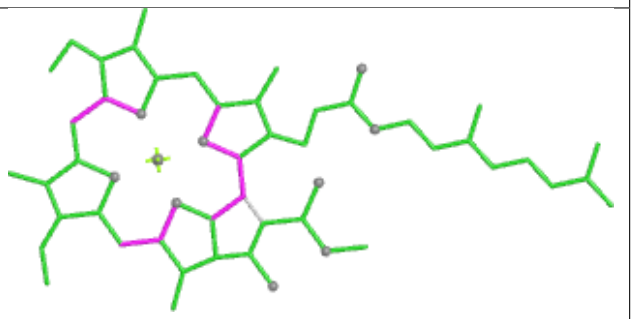


Rings

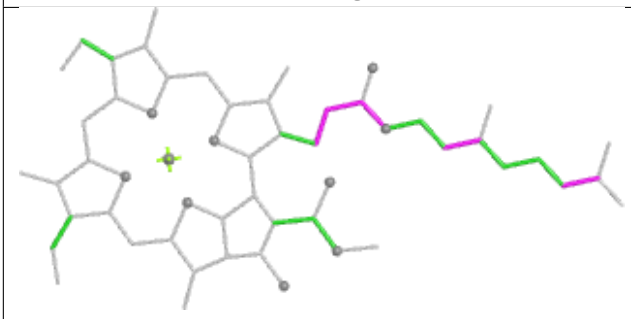
Ligand CLA B 812



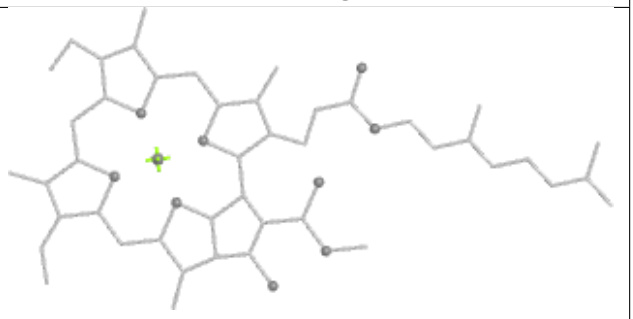
Bond lengths



Bond angles

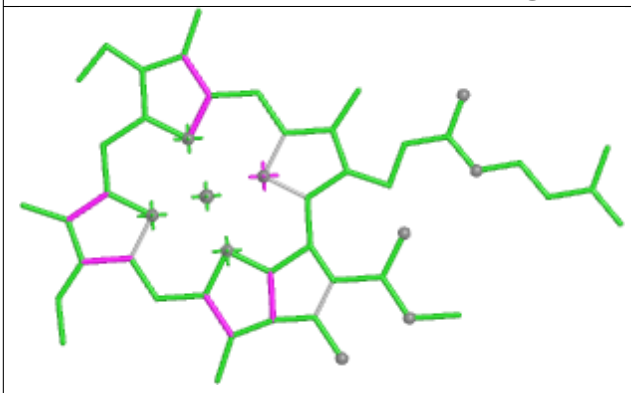


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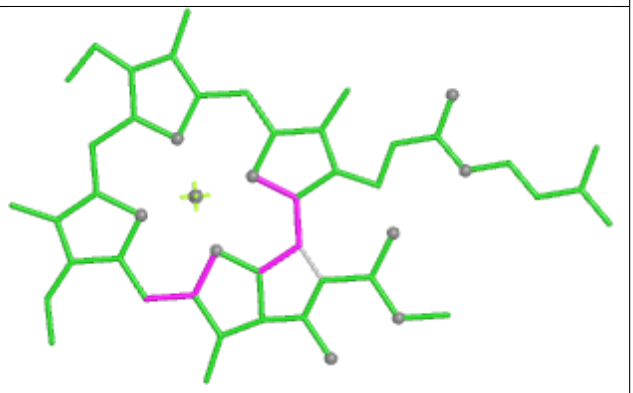


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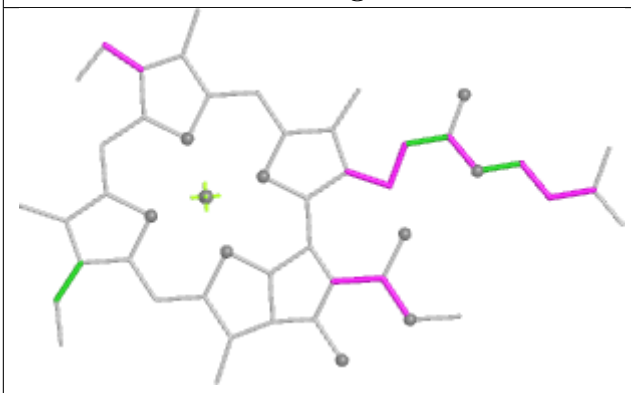
Ligand CLA A 829



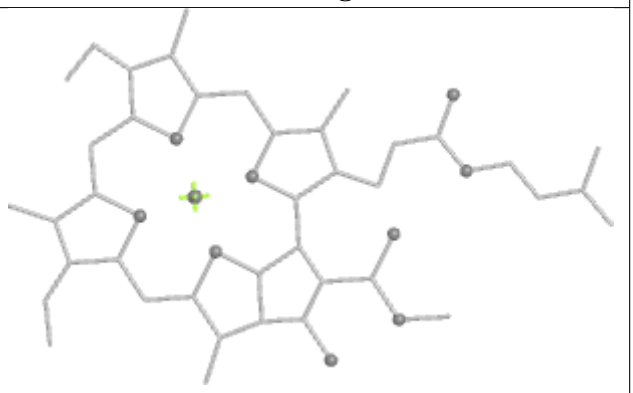
Bond lengths



Bond angles

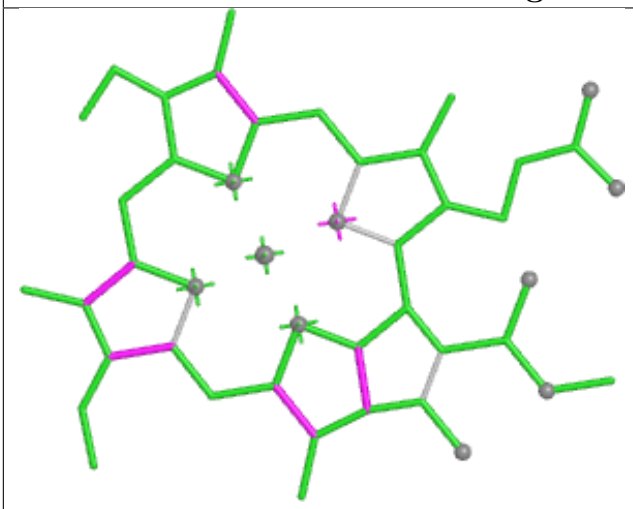


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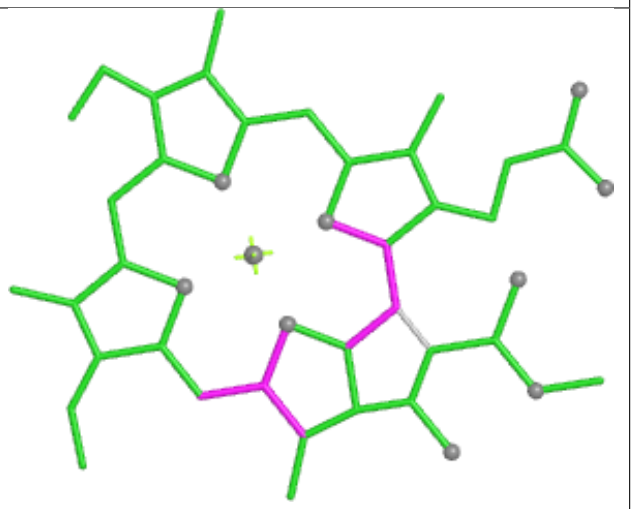


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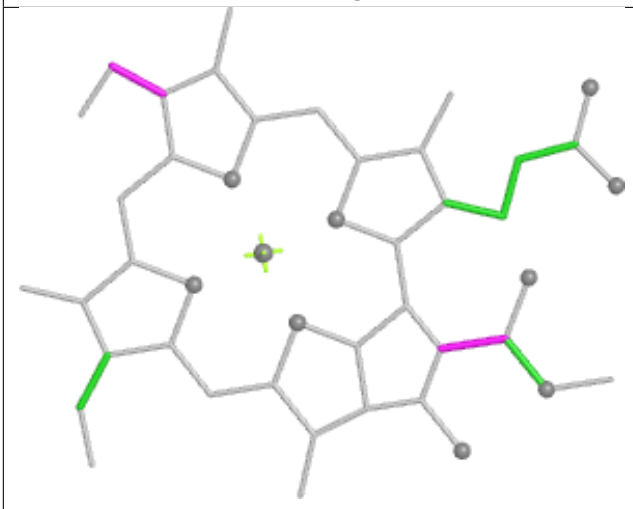
Ligand CLA F 306



Bond lengths



Bond angles

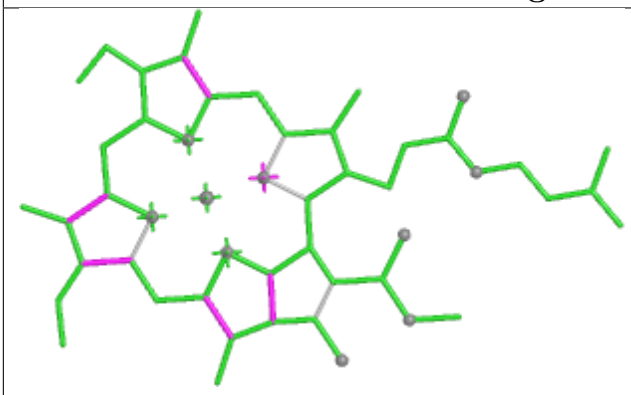


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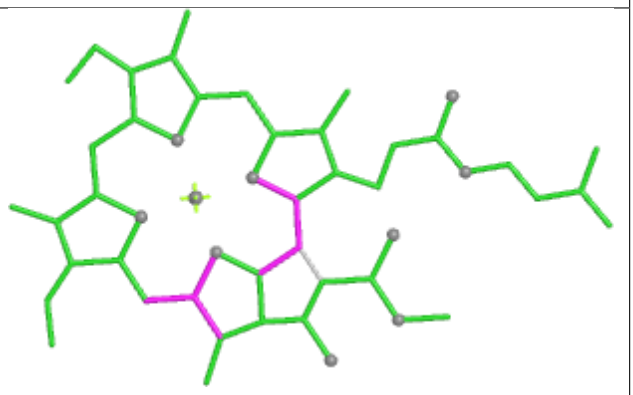


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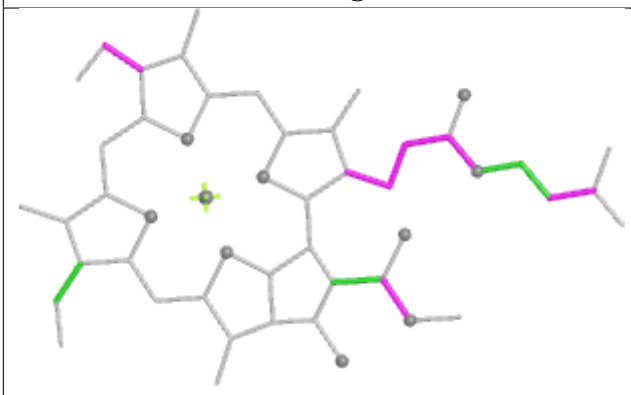
Ligand CLA 4 304



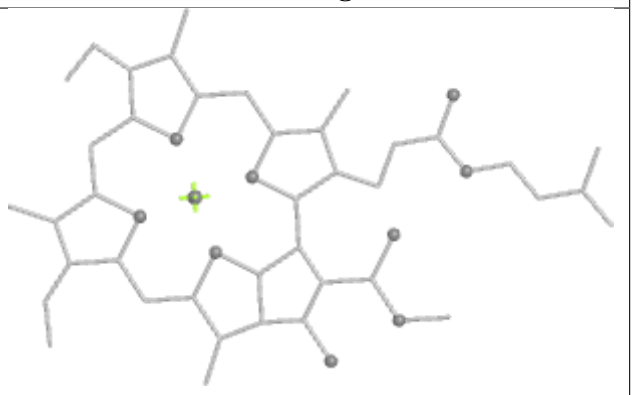
Bond lengths



Bond angles

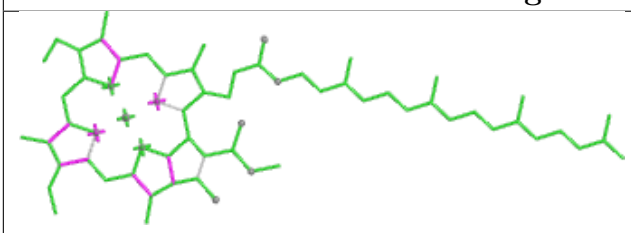


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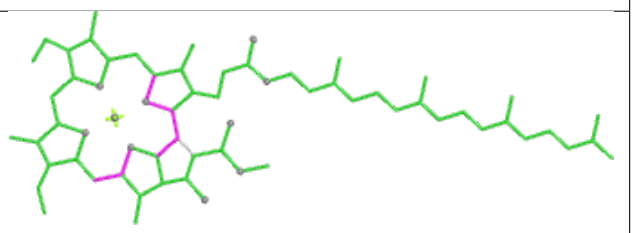


Rings

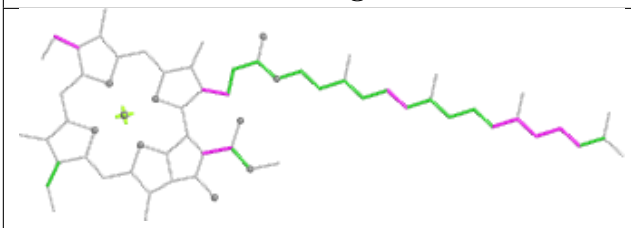
Ligand CLA B 826



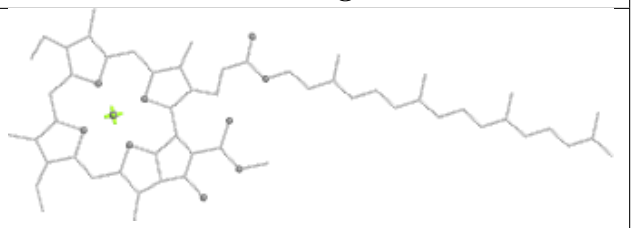
Bond lengths



Bond angles

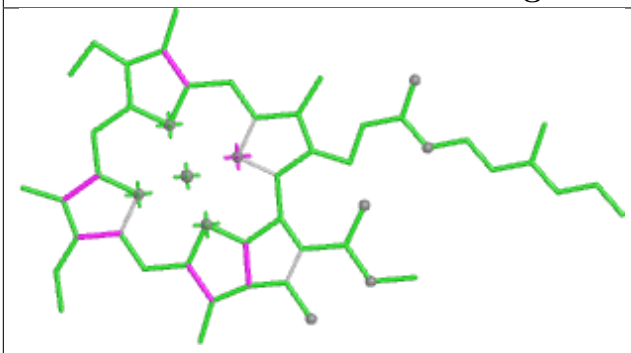


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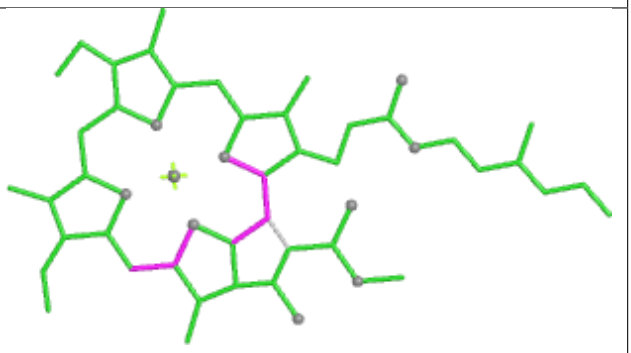


Rings

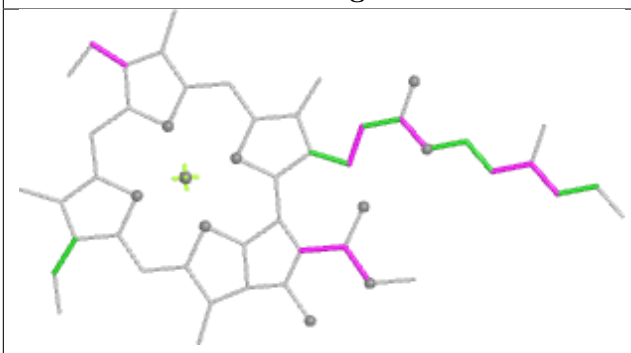
Ligand CLA O 101



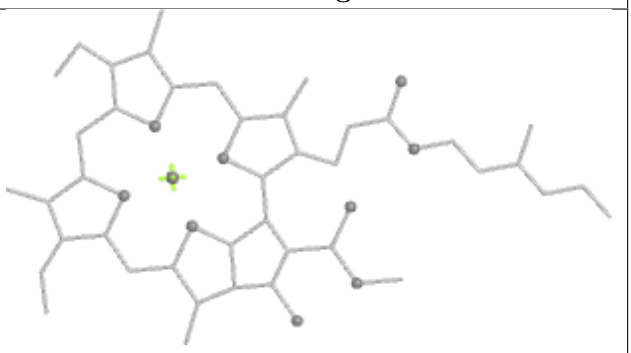
Bond lengths



Bond angles

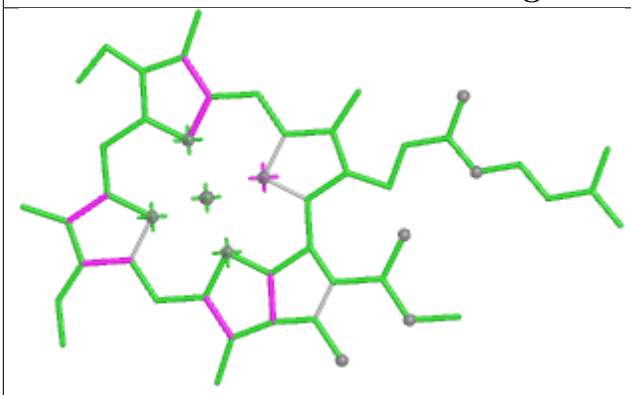


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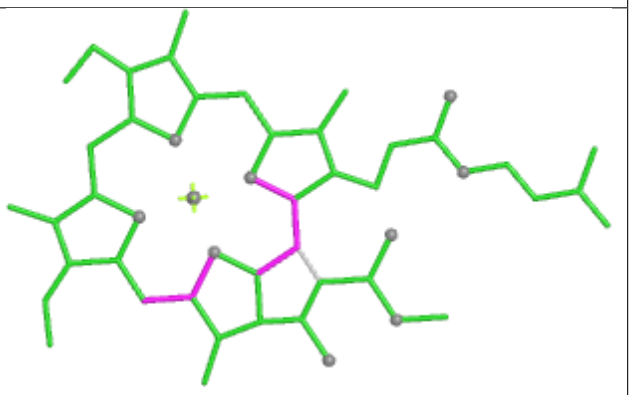


Rings

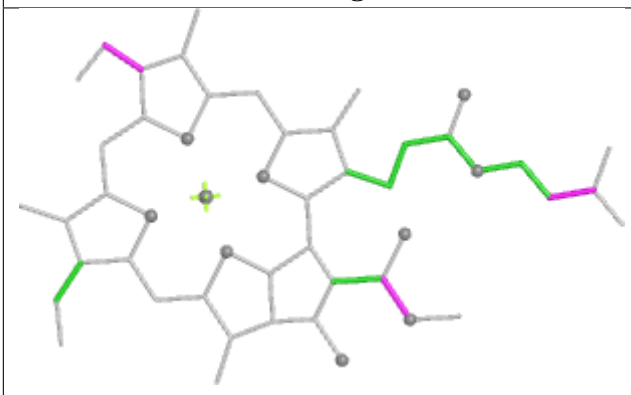
Ligand CLA G 204



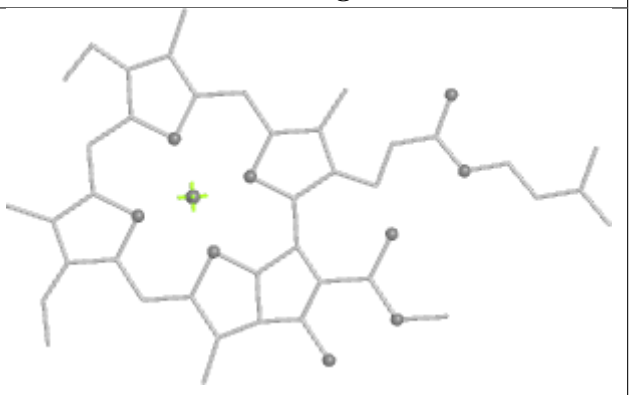
Bond lengths



Bond angles

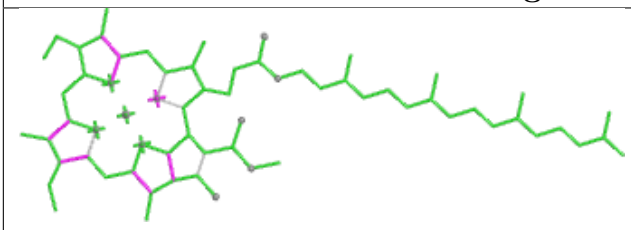


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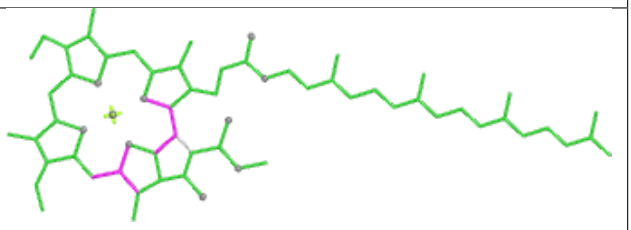


Rings

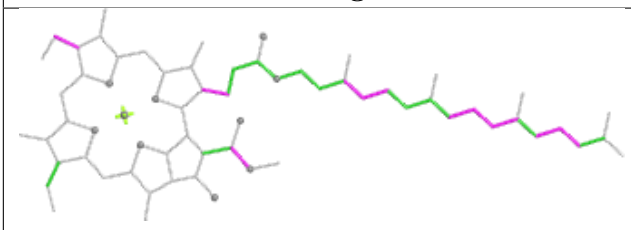
Ligand CLA A 809



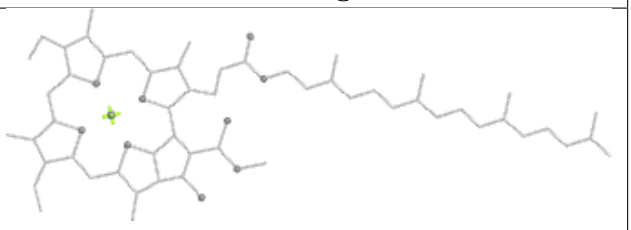
Bond lengths



Bond angles

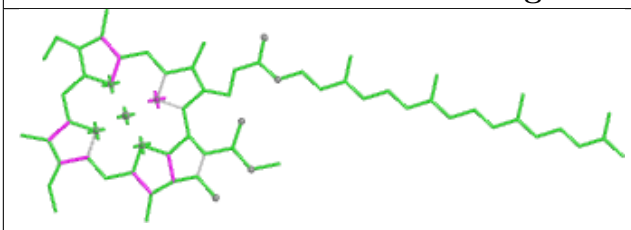


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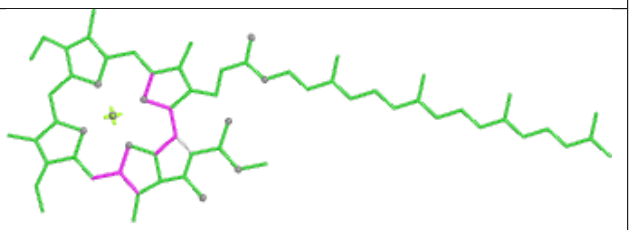


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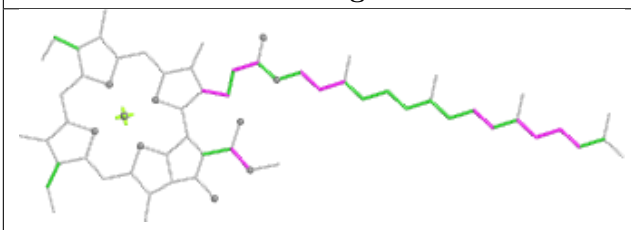
Ligand CLA B 850



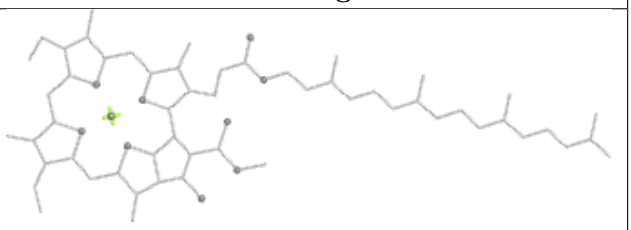
Bond lengths



Bond angles

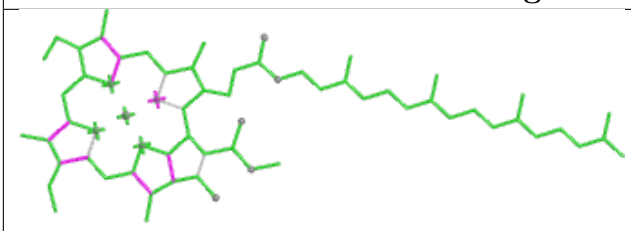


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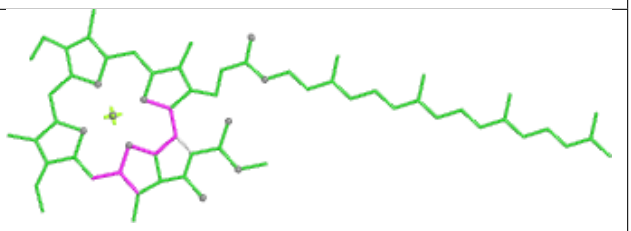


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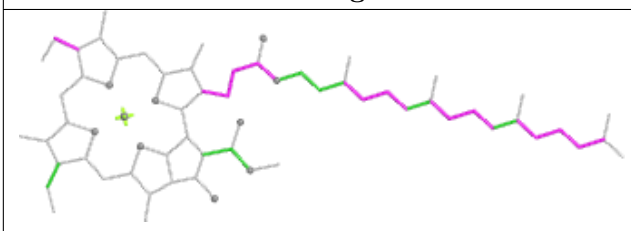
Ligand CLA A 816



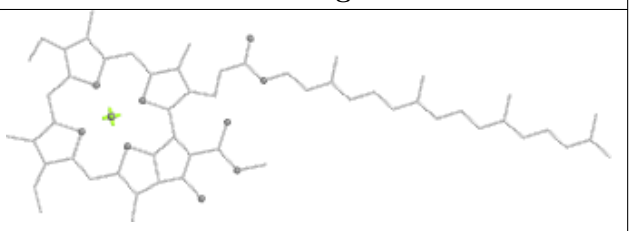
Bond lengths



Bond angles



Torsions

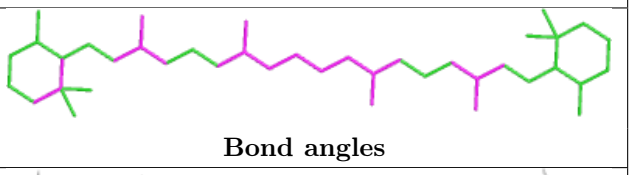


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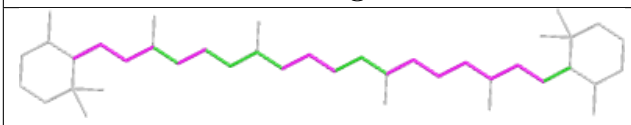
Ligand BCR K 301



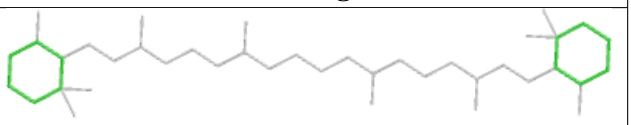
Bond lengths



Bond angles

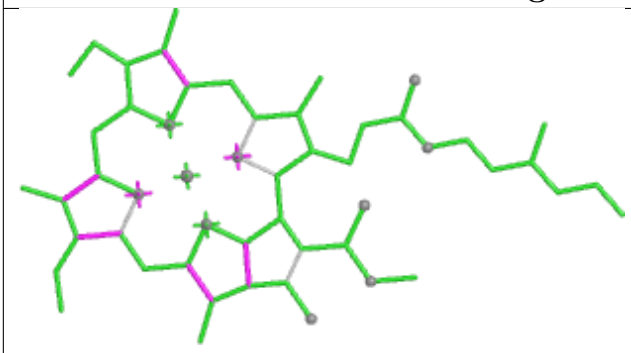


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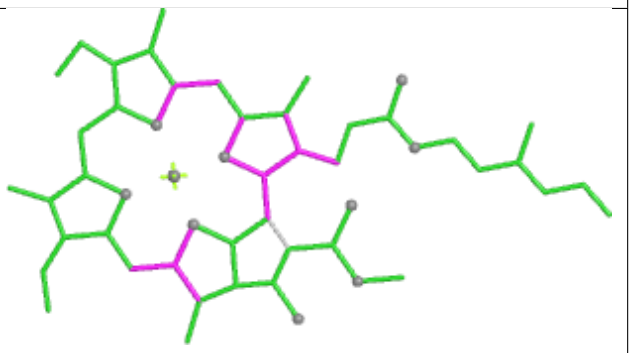


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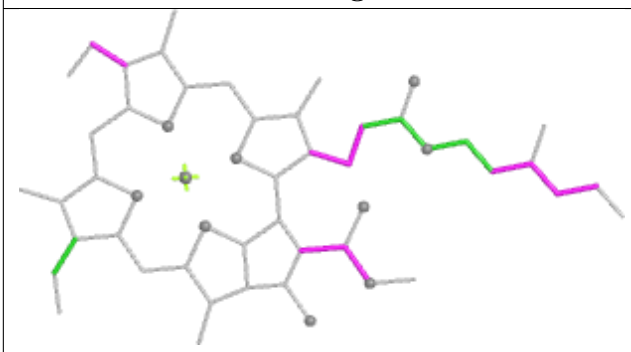
Ligand CLA 4 311



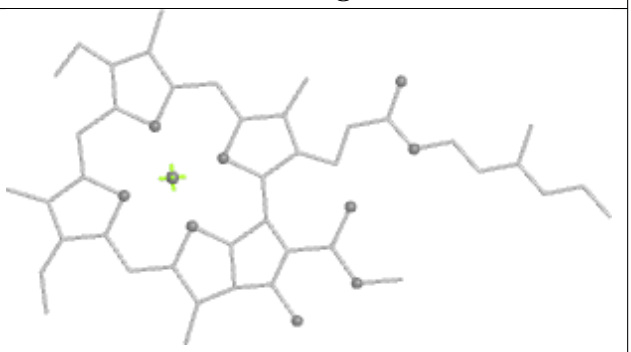
Bond lengths



Bond angles

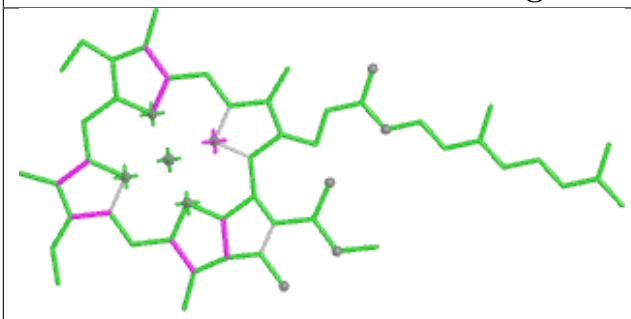


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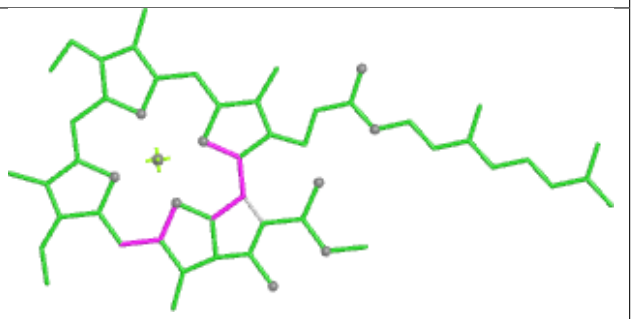


Rings

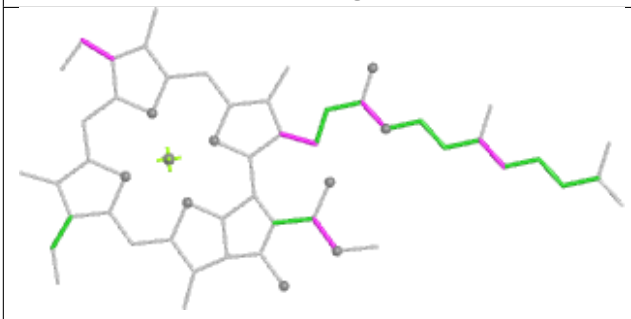
Ligand CLA F 307



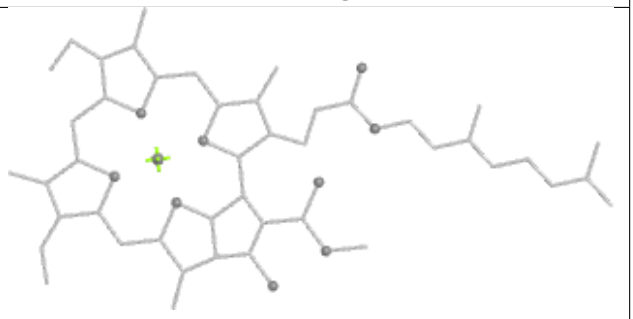
Bond lengths



Bond angles

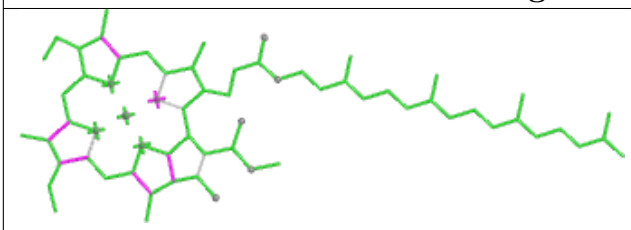


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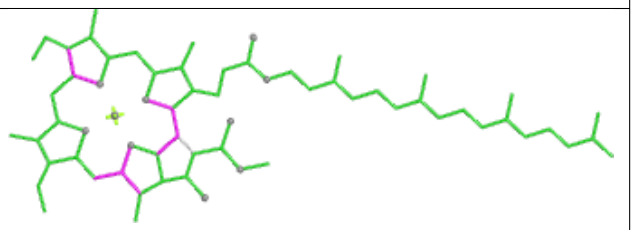


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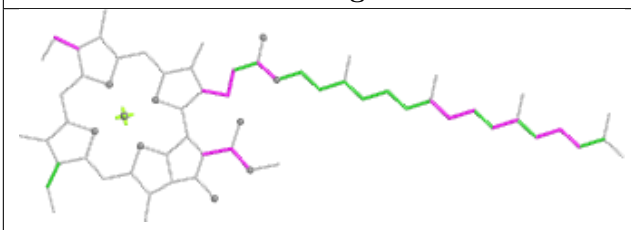
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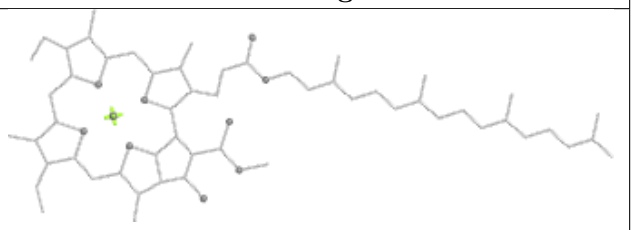
Bond lengths



Bond angles

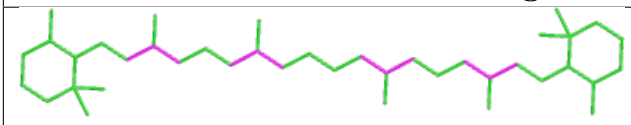


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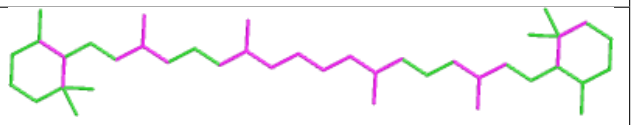


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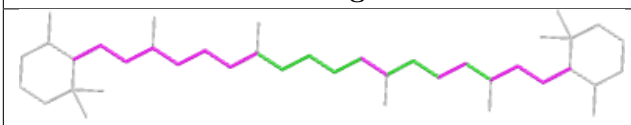
Ligand BCR A 844



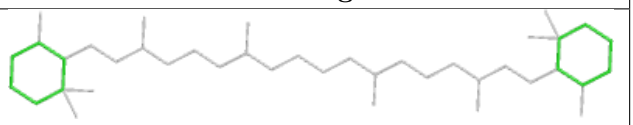
Bond lengths



Bond angles

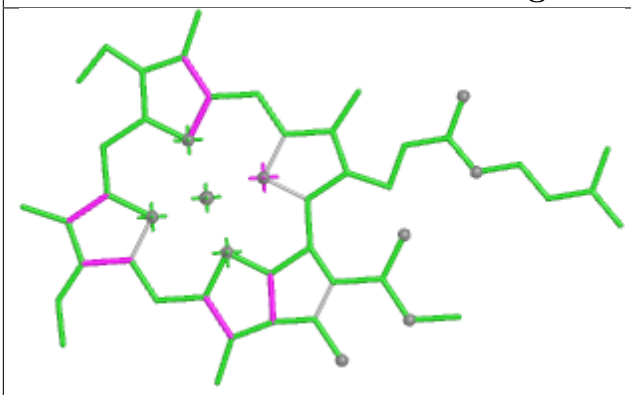


Torsions

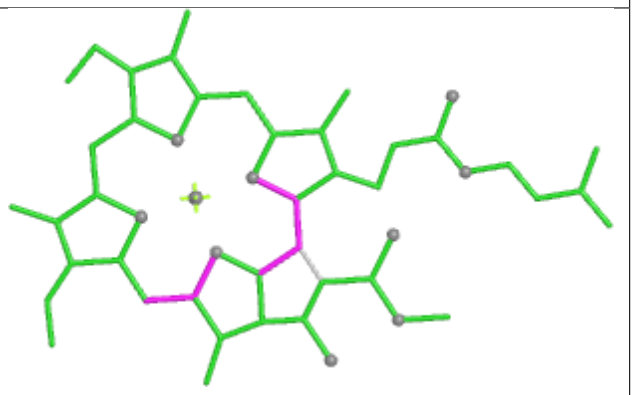


Rings

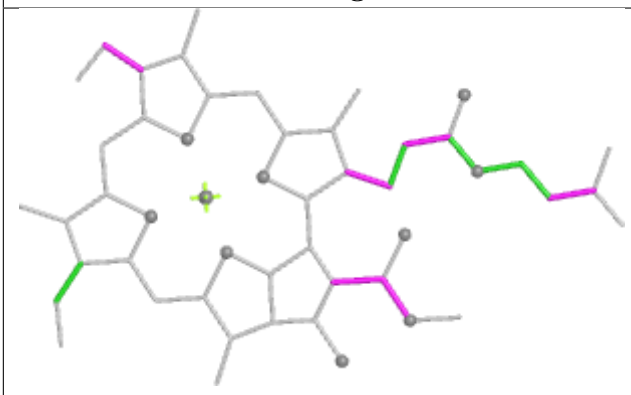
Ligand CLA 3 307



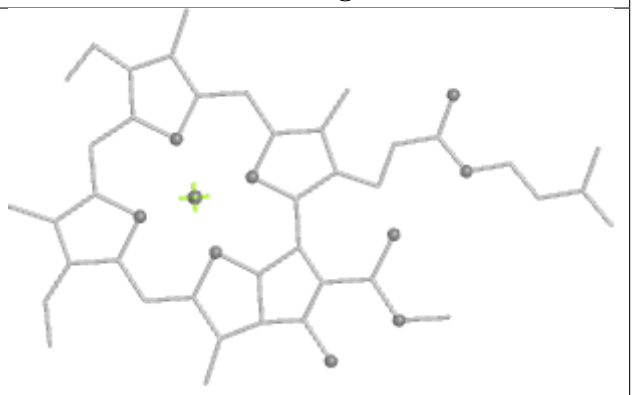
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Bond angles

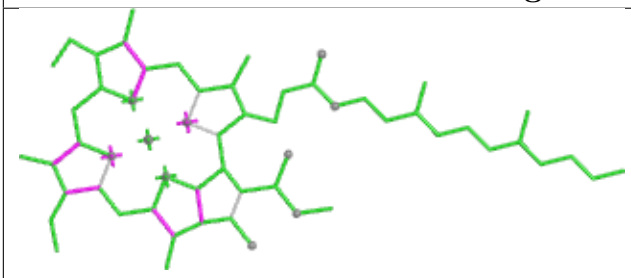


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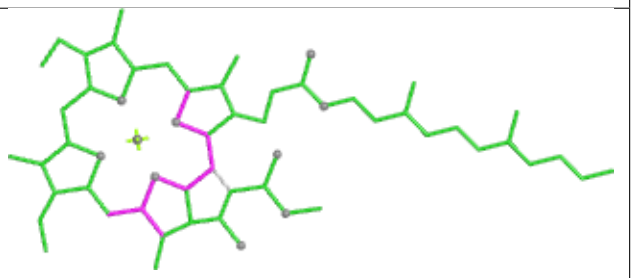


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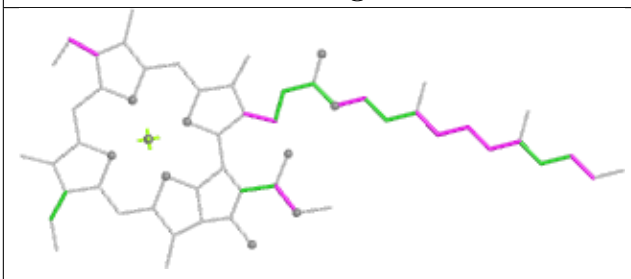
Ligand CLA B 832



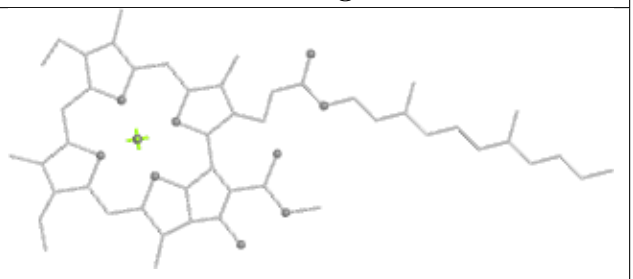
Bond lengths



Bond angles

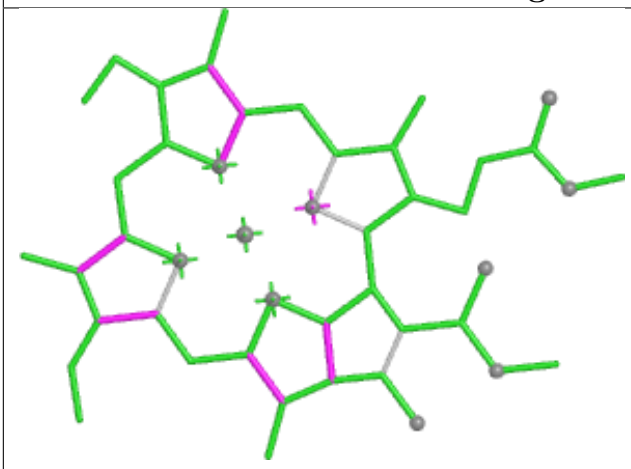


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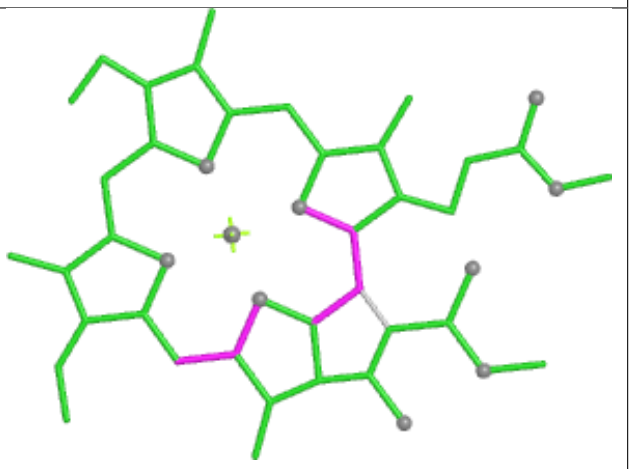


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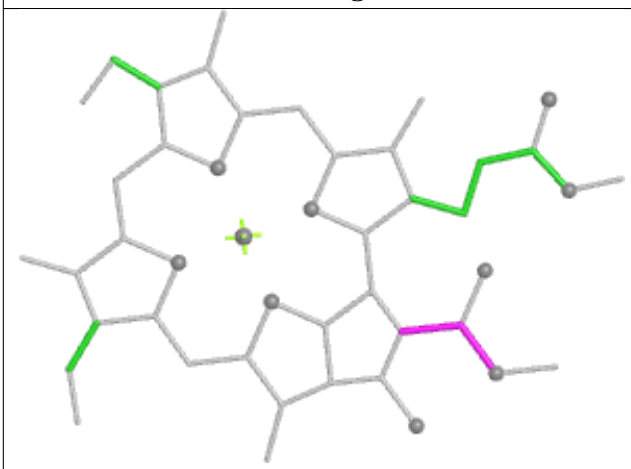
Ligand CLA 4 301



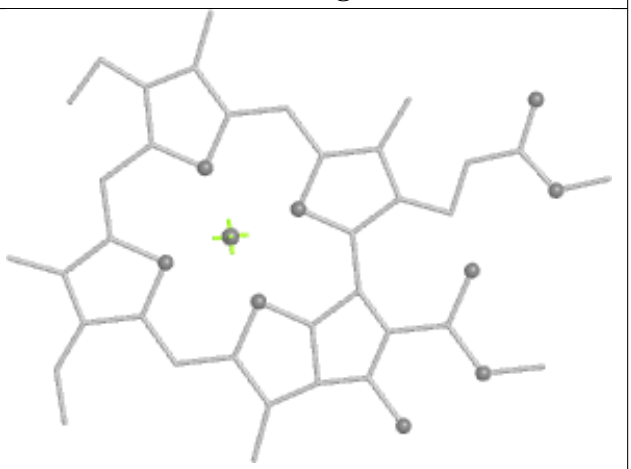
Bond lengths



Bond angles

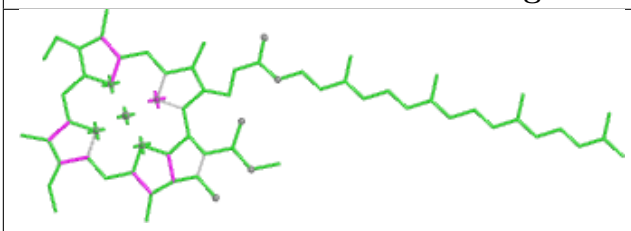


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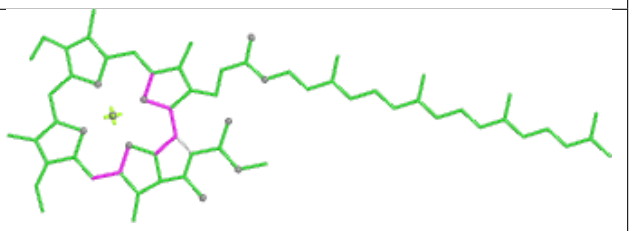


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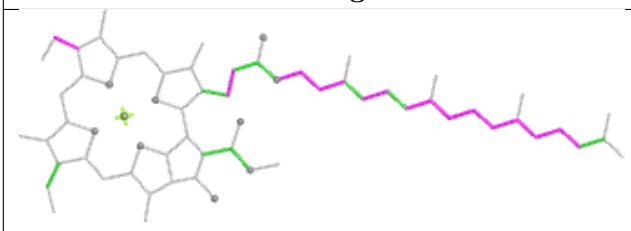
Ligand CLA A 818



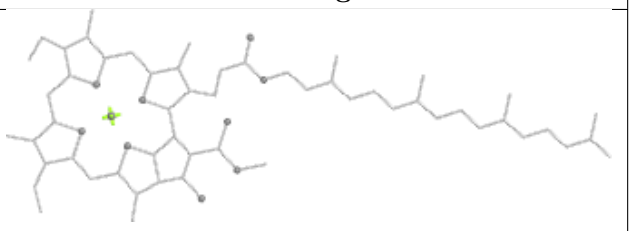
Bond lengths



Bond angles

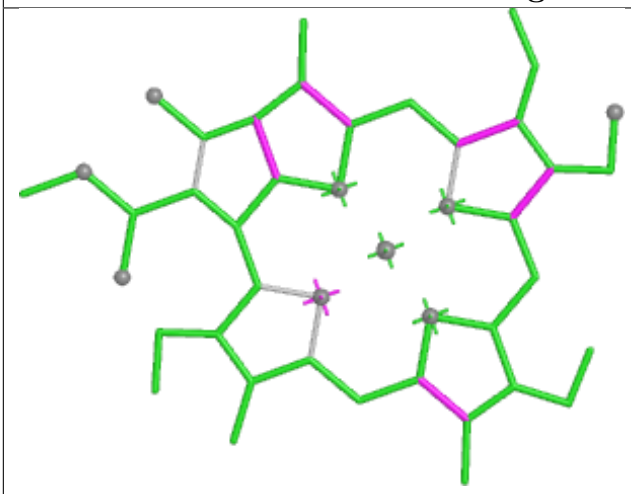


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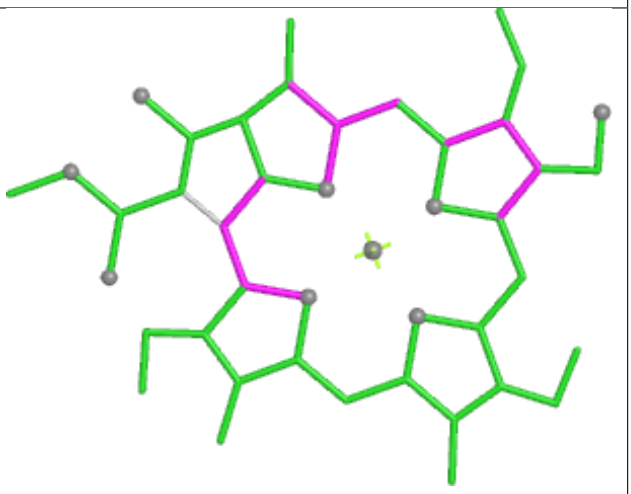


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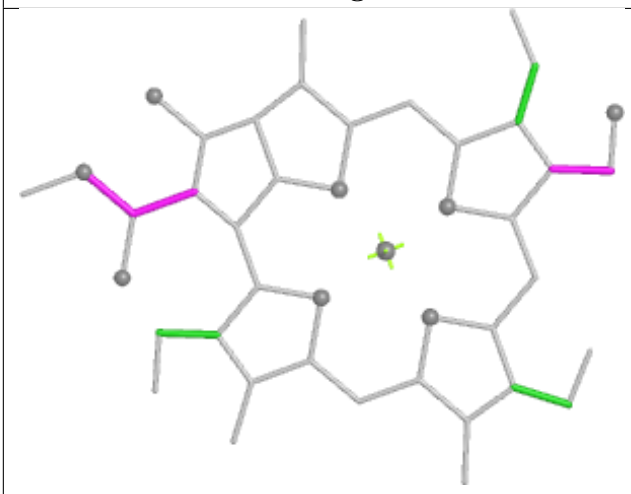
Ligand CHL 2 304



Bond lengths



Bond angles

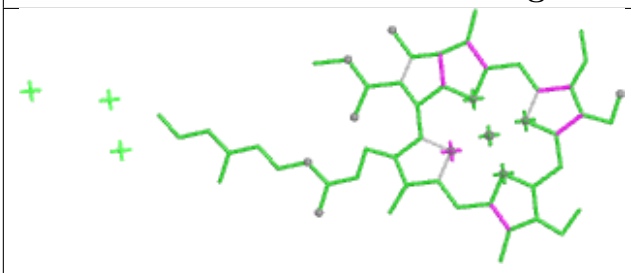


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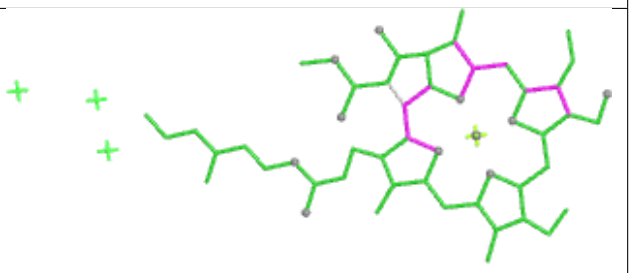


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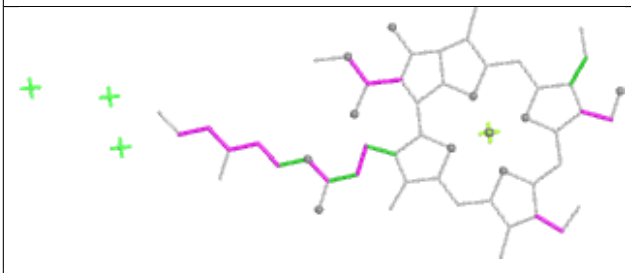
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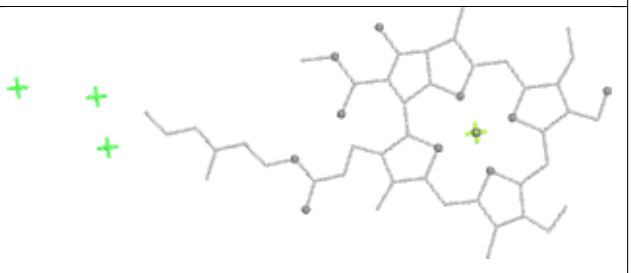
Bond lengths



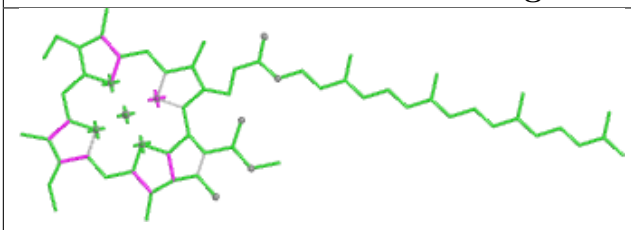
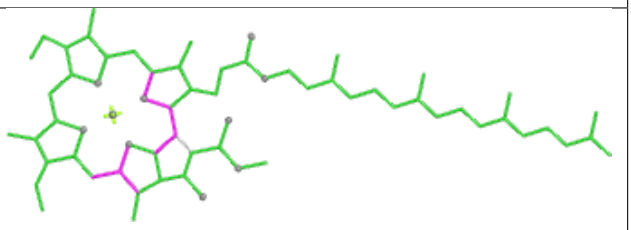
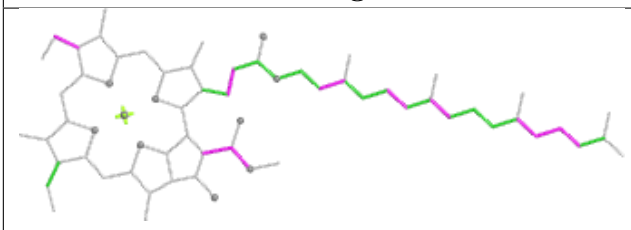
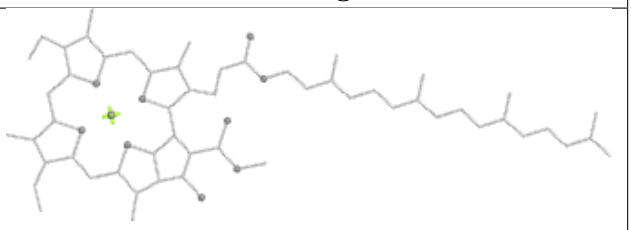
Bond angles

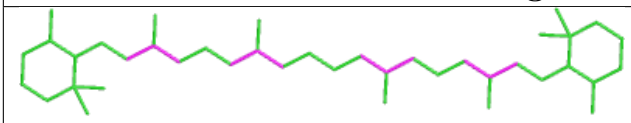
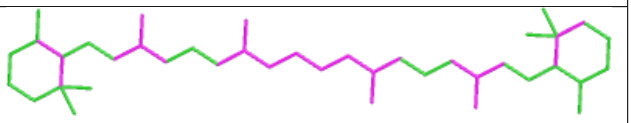
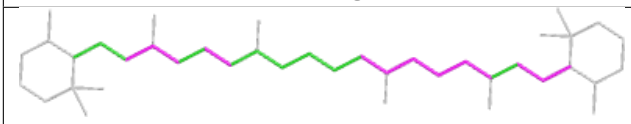
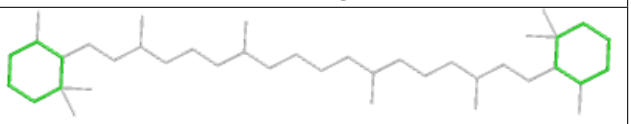


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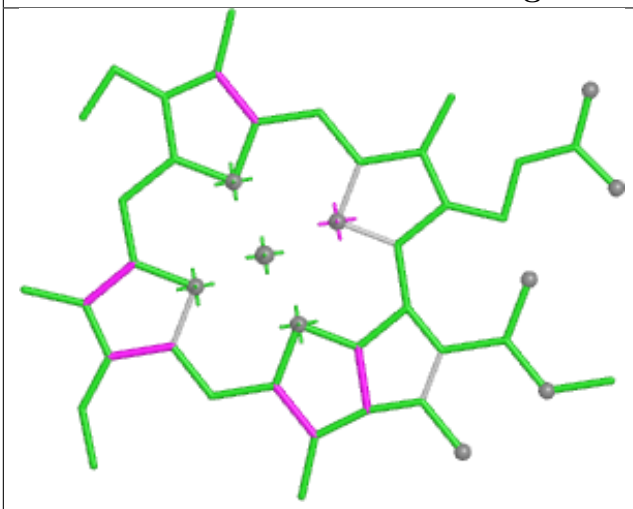


Rings

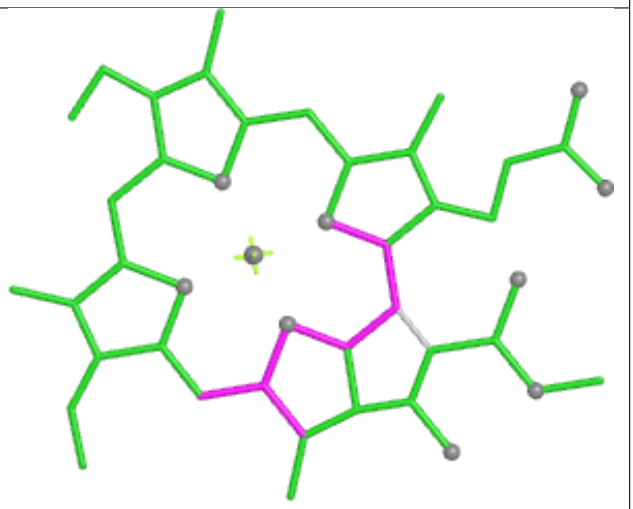
Ligand CLA B 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 4 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

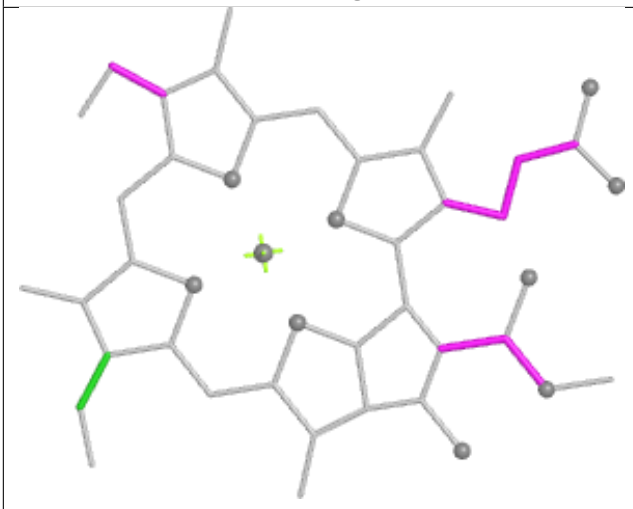
Ligand CLA O 104



Bond lengths



Bond angles

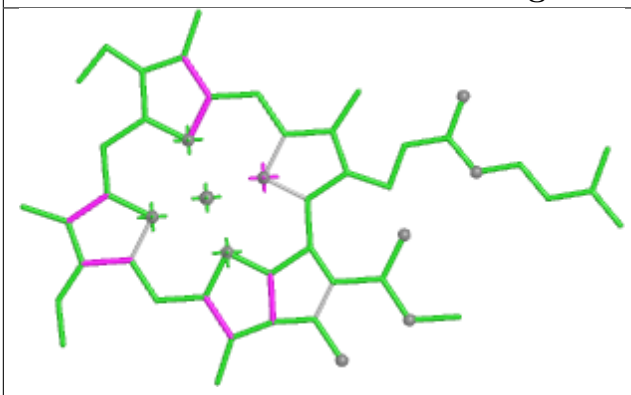


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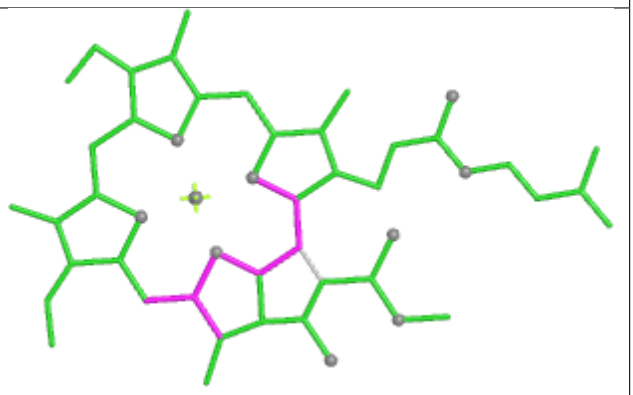


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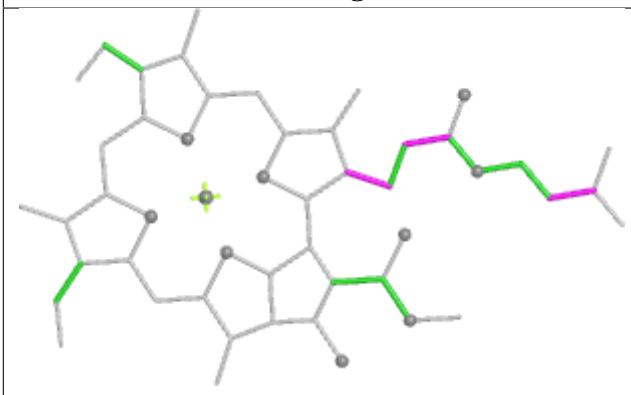
Ligand CLA 2 307



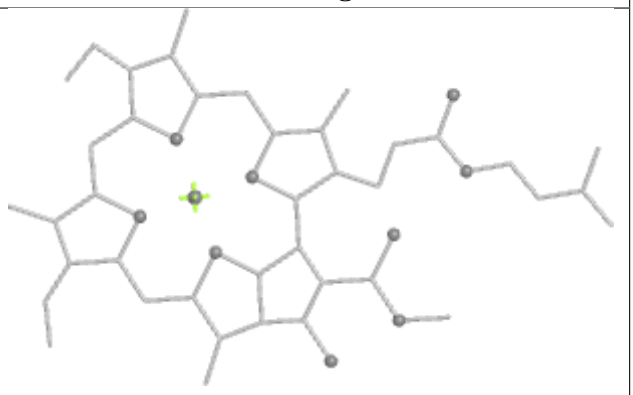
Bond lengths



Bond angles

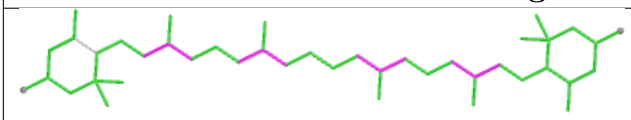


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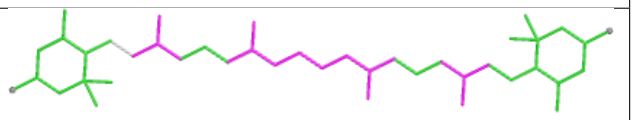


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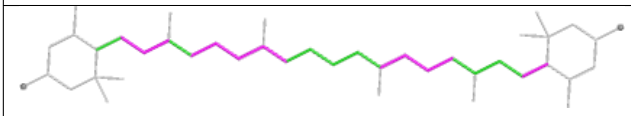
Ligand LUT 4 316



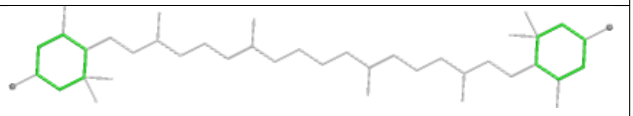
Bond lengths



Bond angles

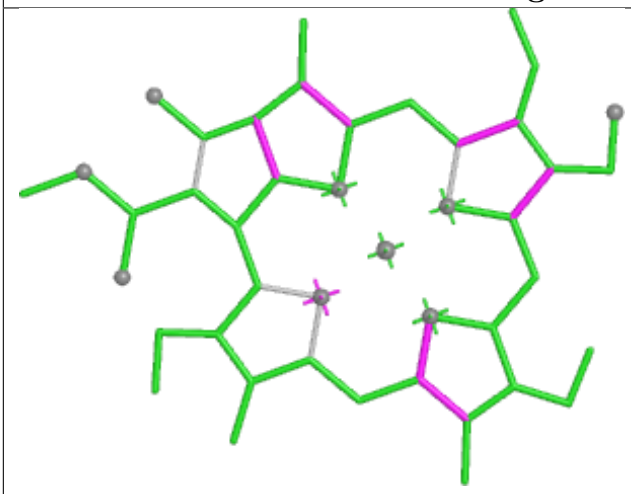


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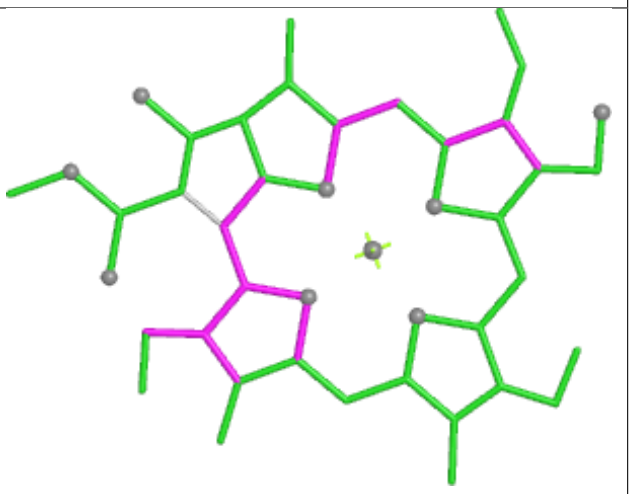


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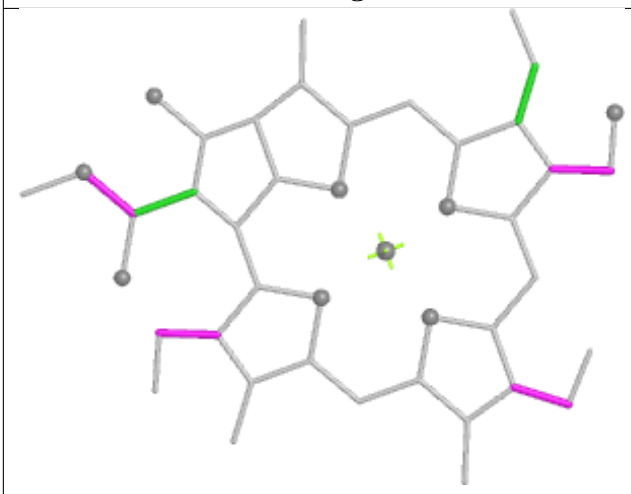
Ligand CHL 2 313



Bond lengths



Bond angles

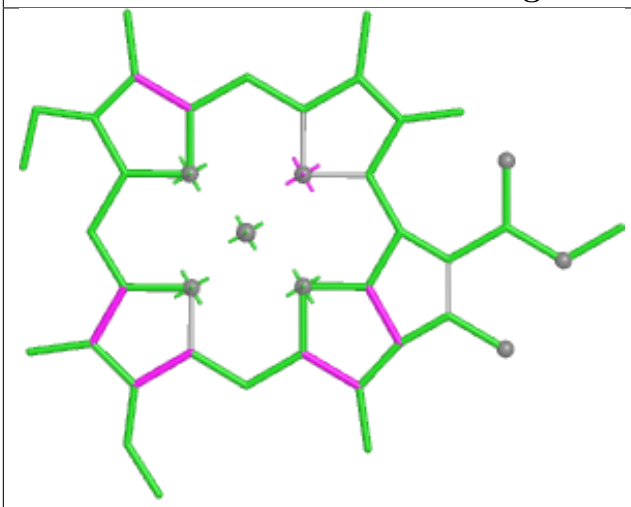


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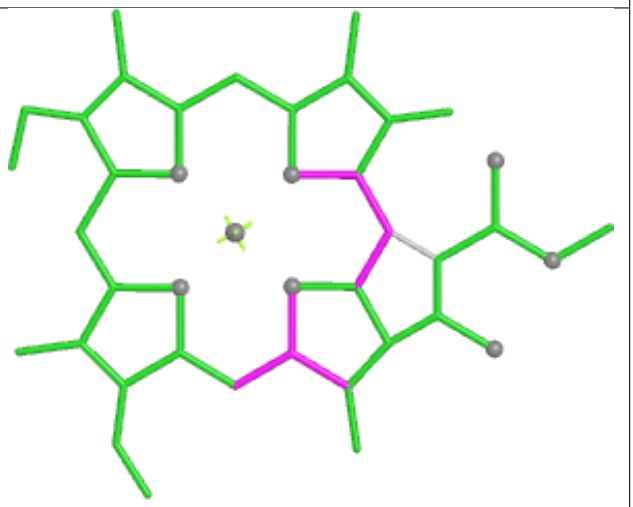


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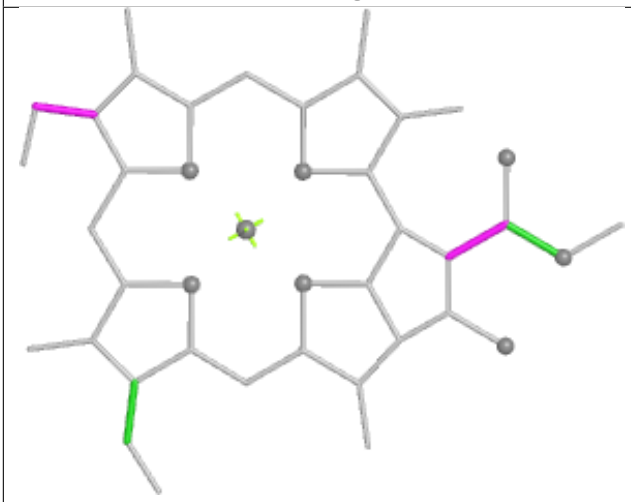
Ligand CLA G 203



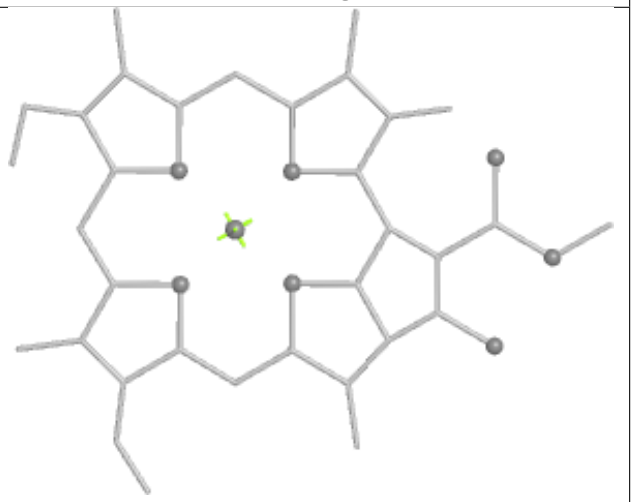
Bond lengths



Bond angles

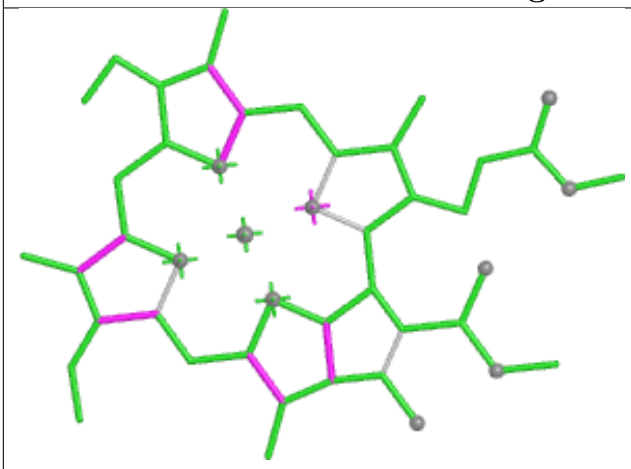


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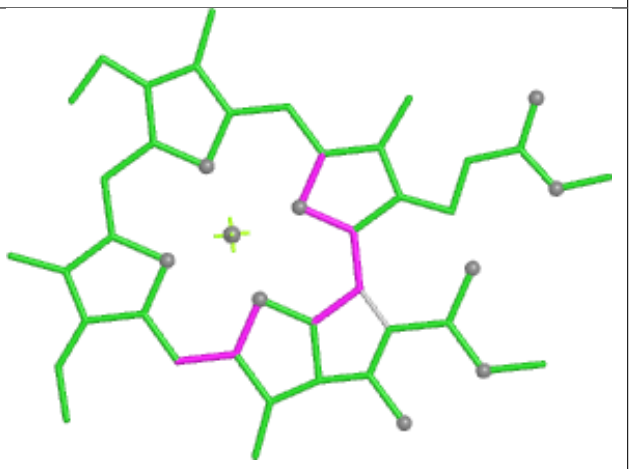


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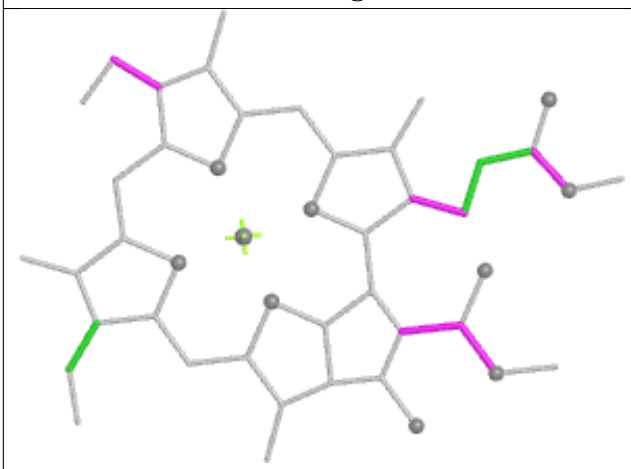
Ligand CLA 1 306



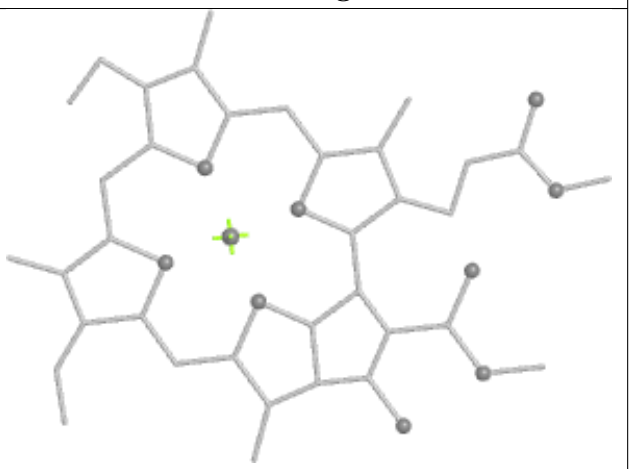
Bond lengths



Bond angles

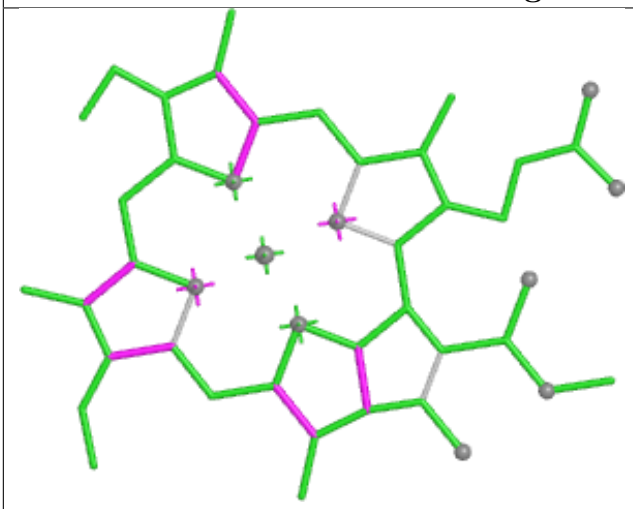


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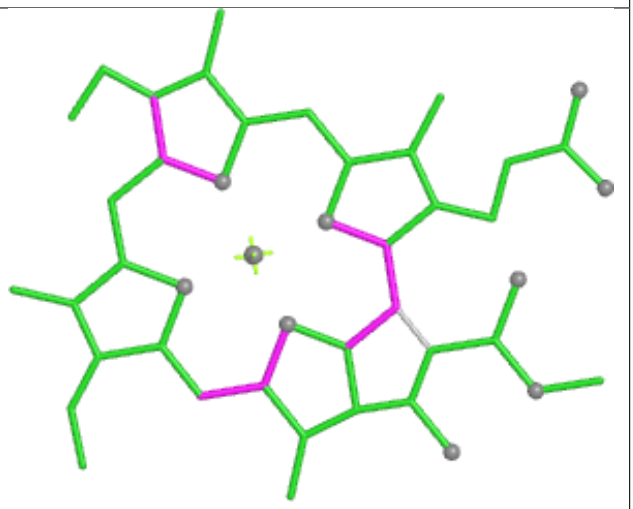


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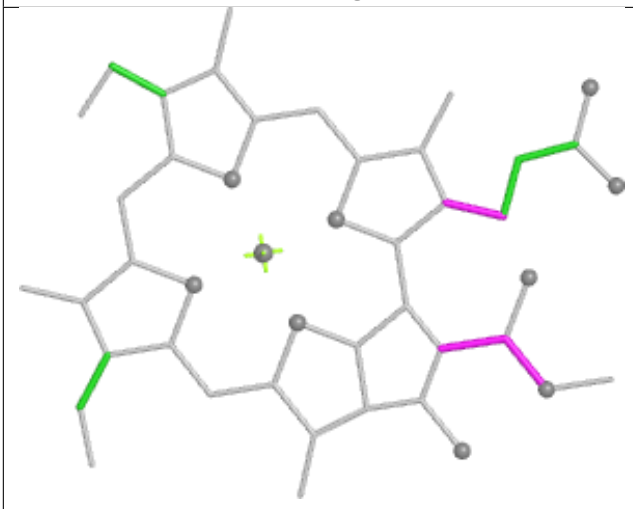
Ligand CLA B 804



Bond lengths



Bond angles

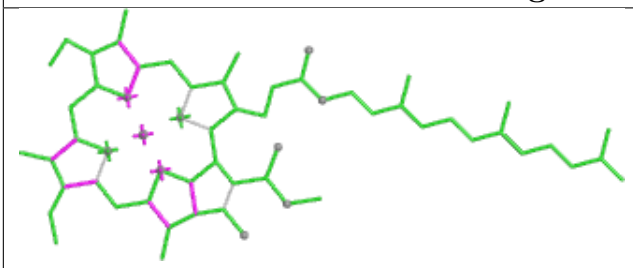


Torsions

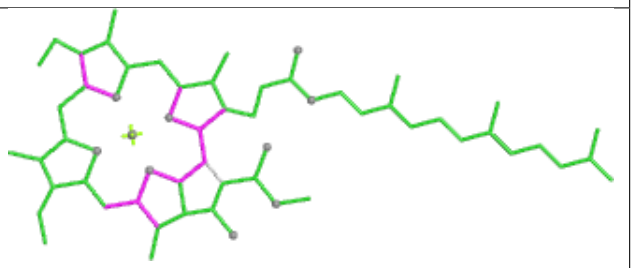


Rings

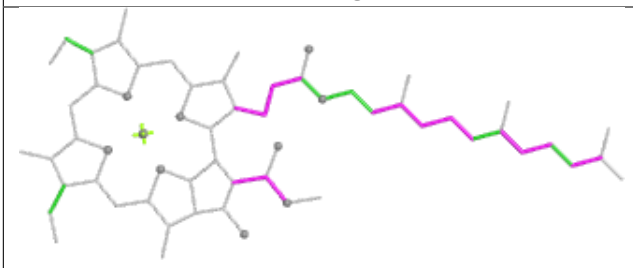
Ligand CLA 4 310



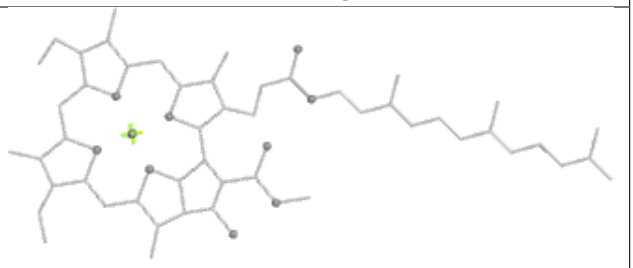
Bond lengths



Bond angles

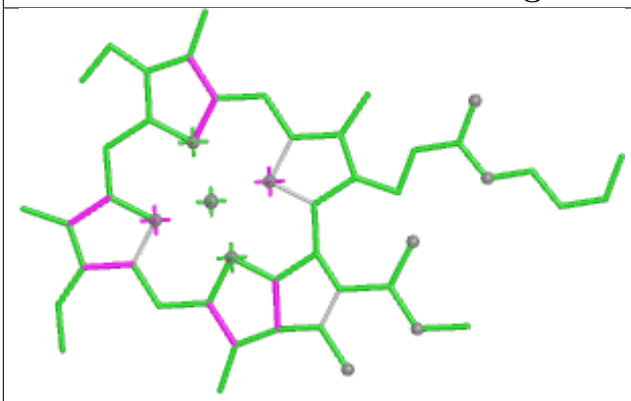


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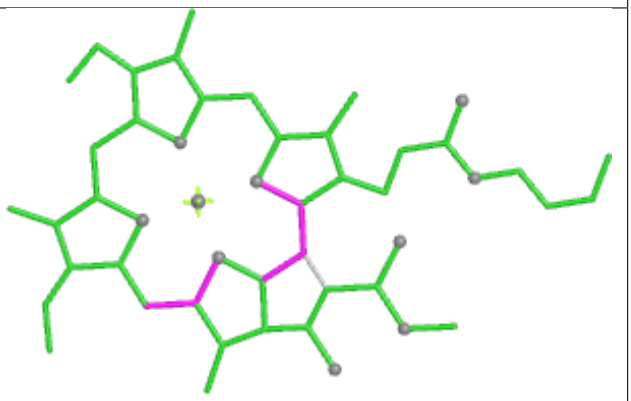


Rings

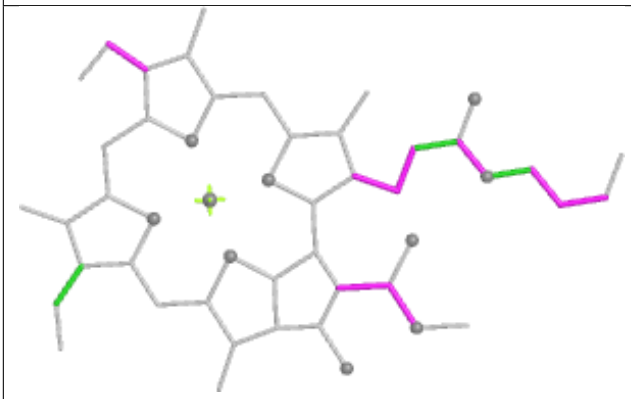
Ligand CLA A 820



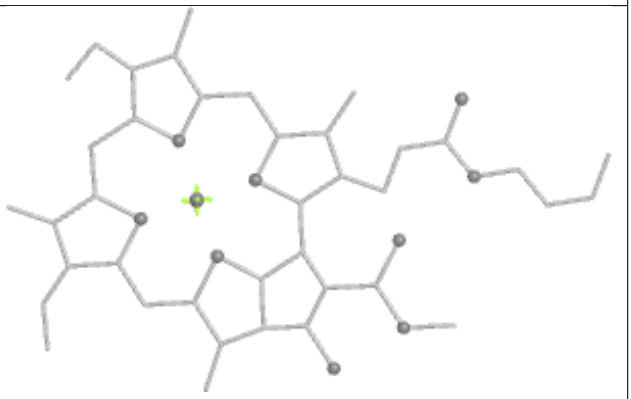
Bond lengths



Bond angles

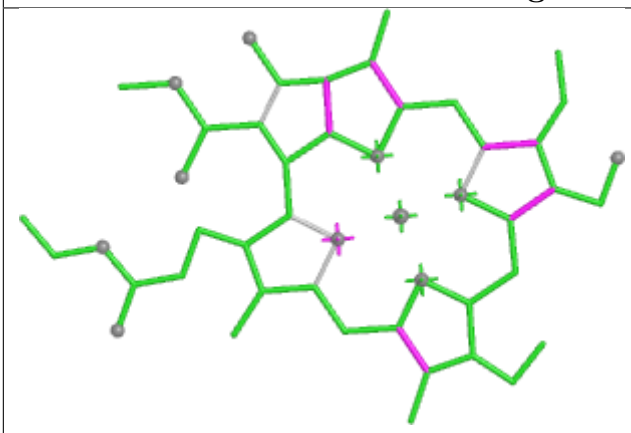


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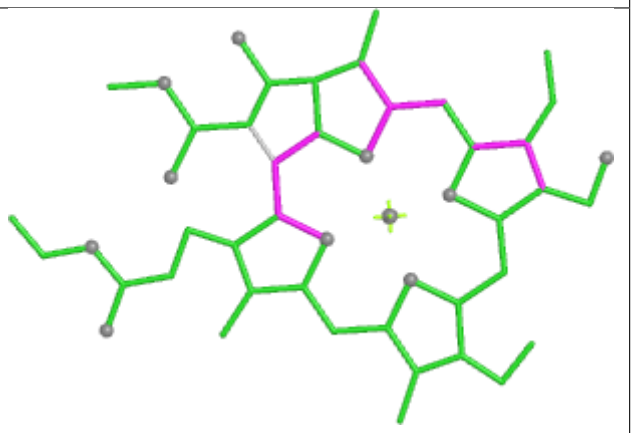


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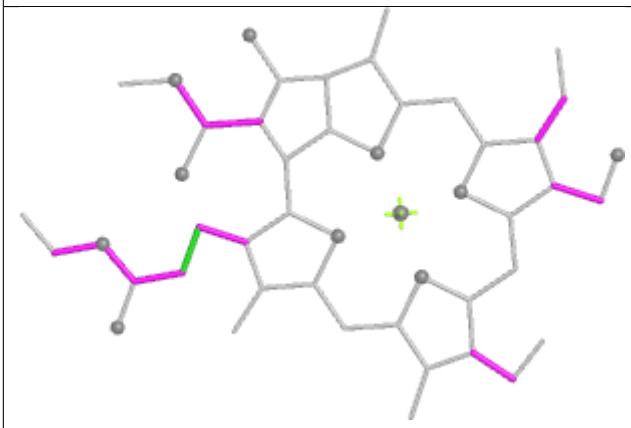
Ligand CHL 1 305



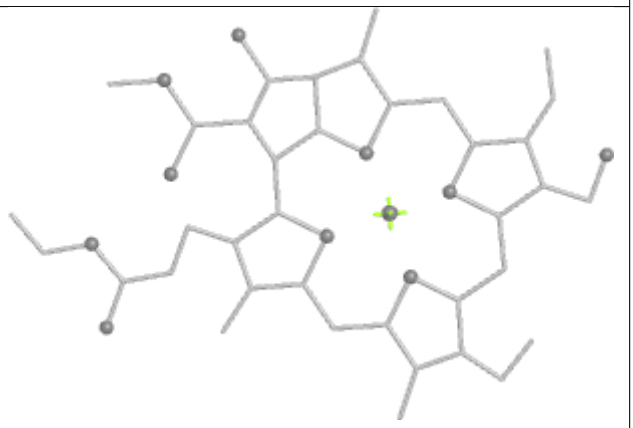
Bond lengths



Bond angles

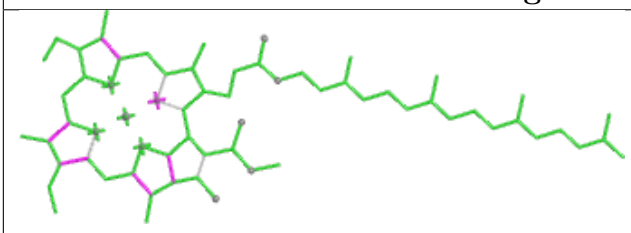


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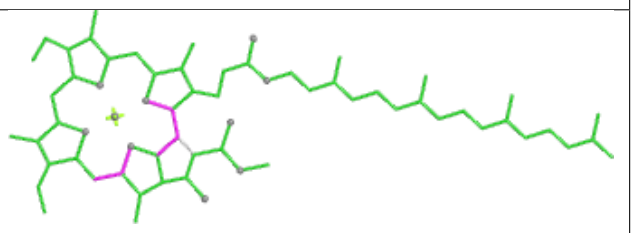


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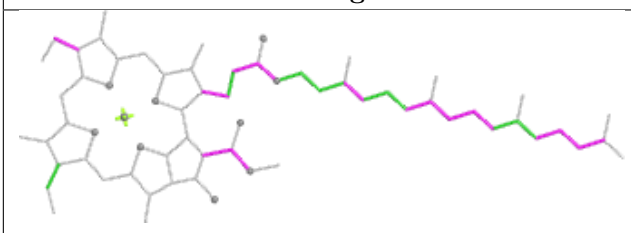
Ligand CLA A 838



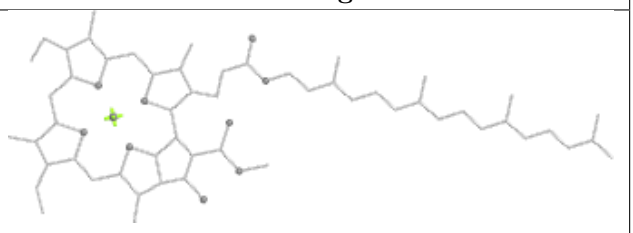
Bond lengths



Bond angles



Torsions

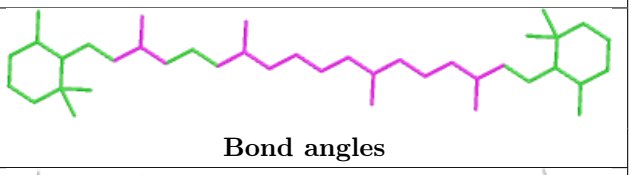


Rings

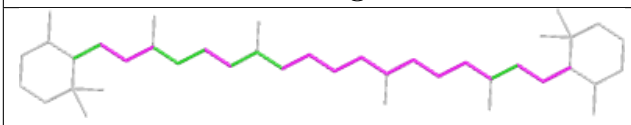
Ligand BCR F 302



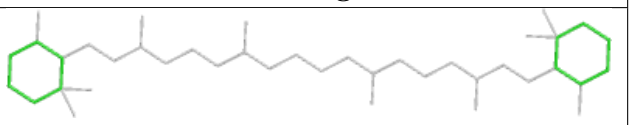
Bond lengths



Bond angles

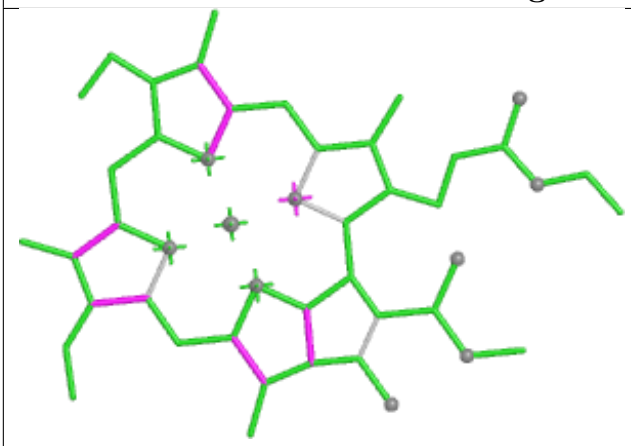


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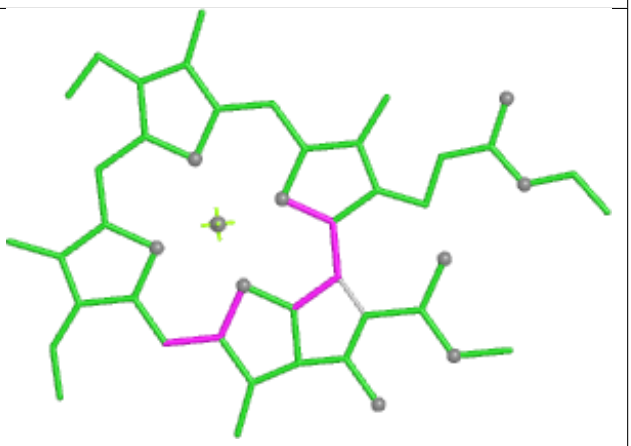


Rings

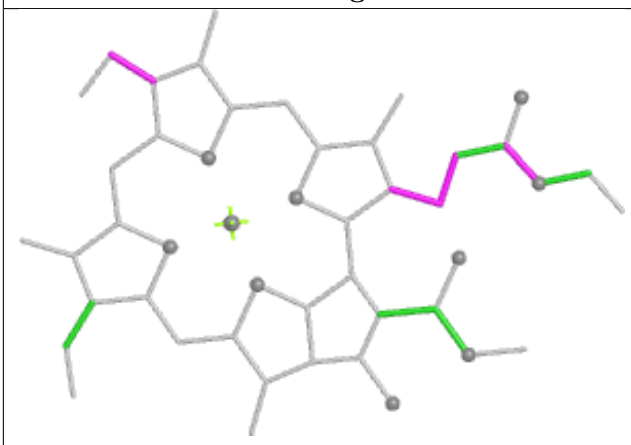
Ligand CLA 3 305



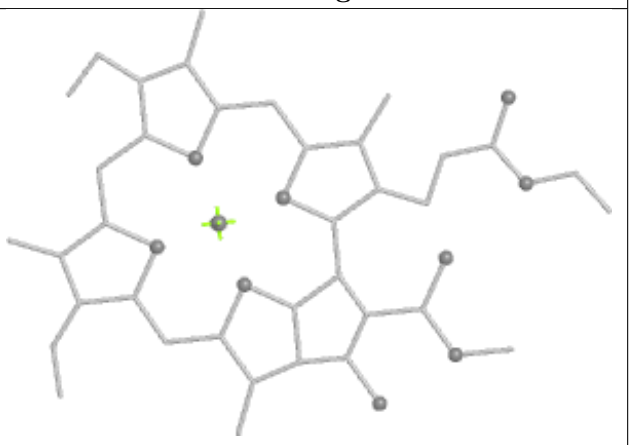
Bond lengths



Bond angles

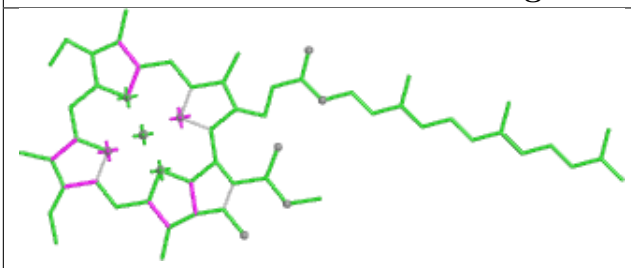


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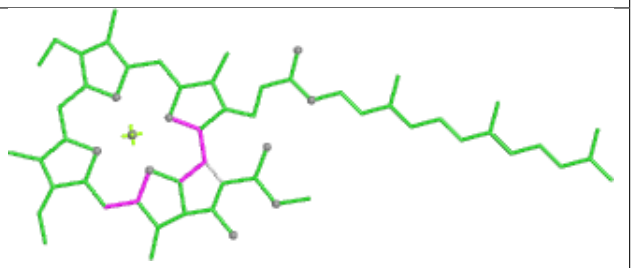


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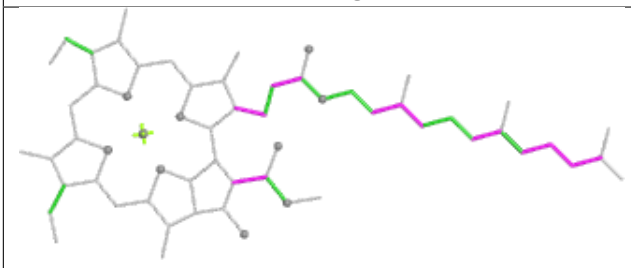
Ligand CLA B 835



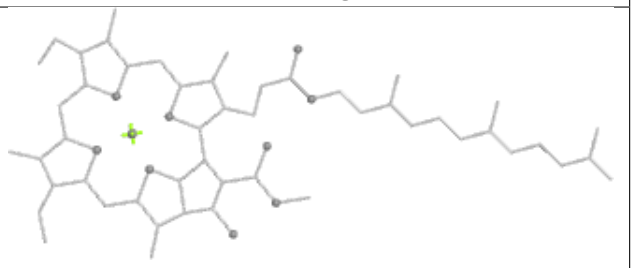
Bond lengths



Bond angles

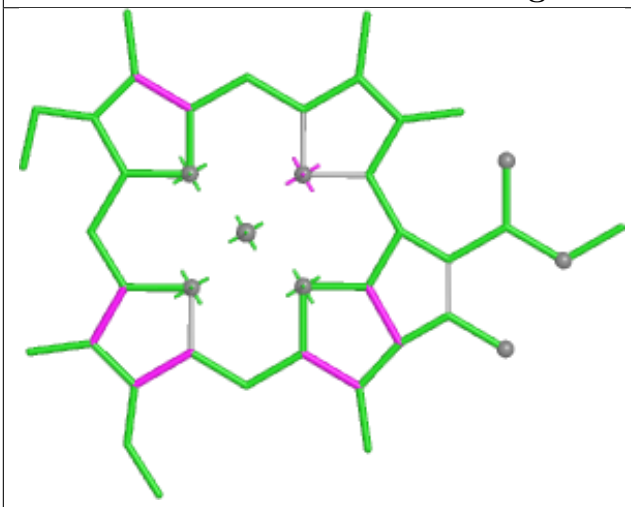


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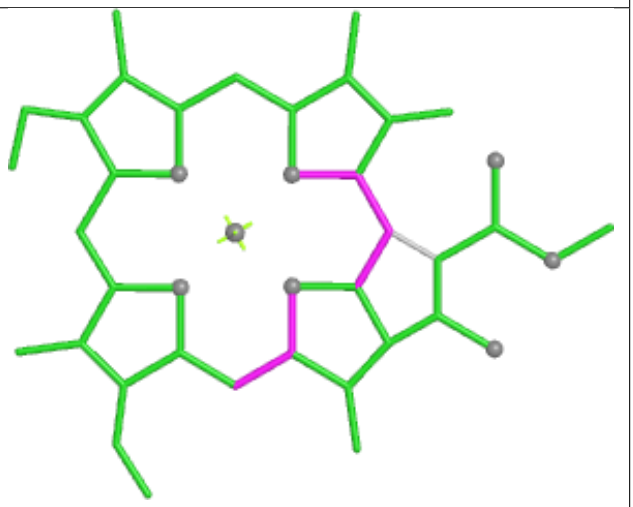


Rings

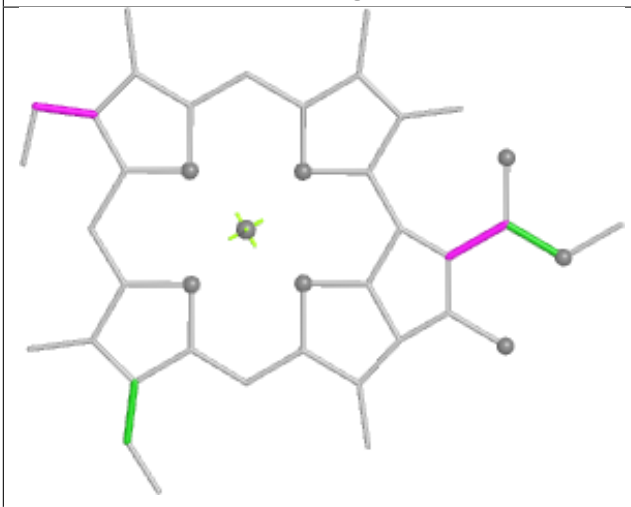
Ligand CLA 2 309



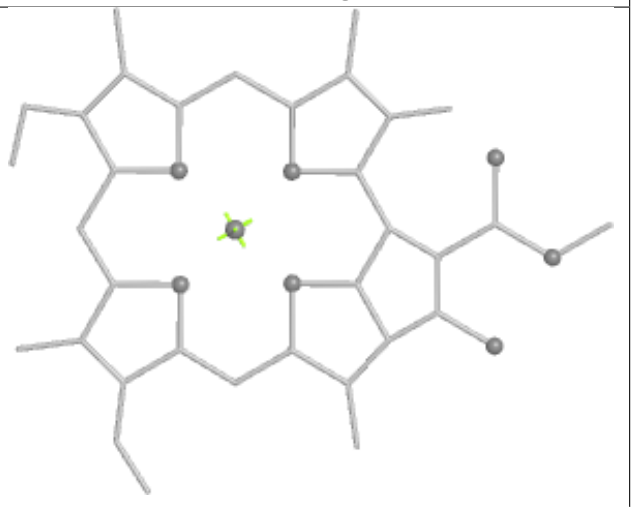
Bond lengths



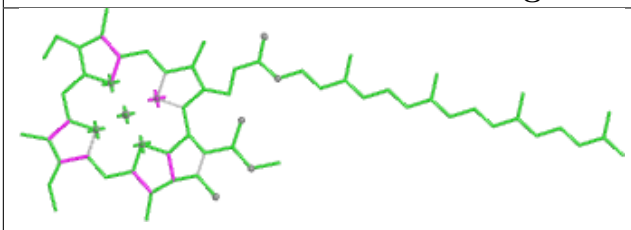
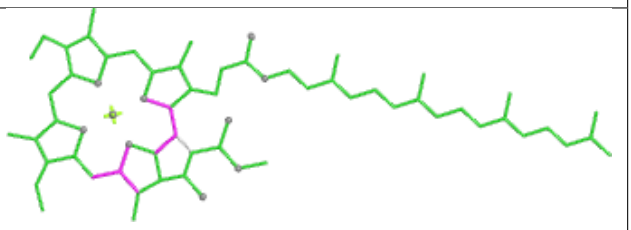
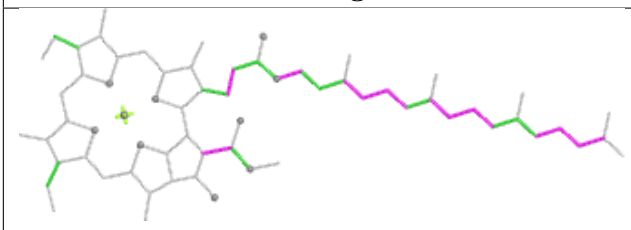
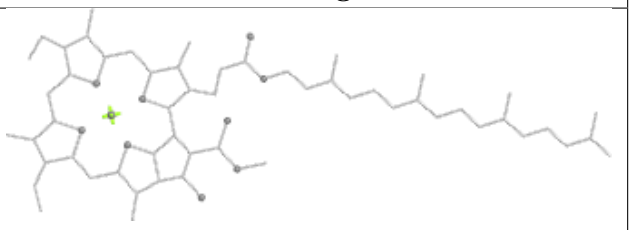
Bond angles

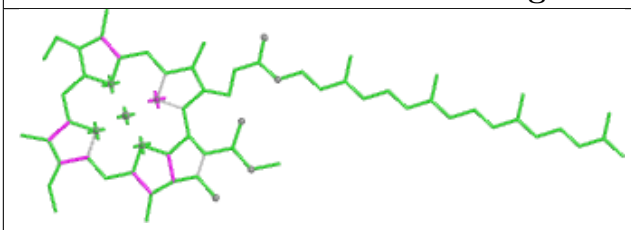
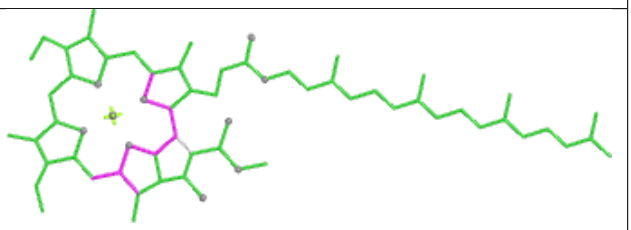
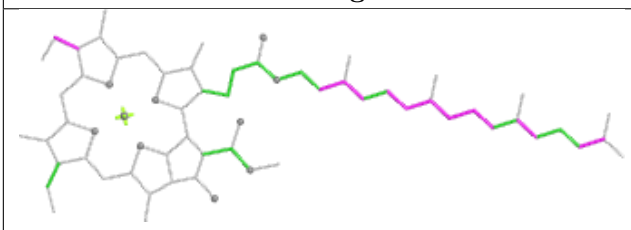
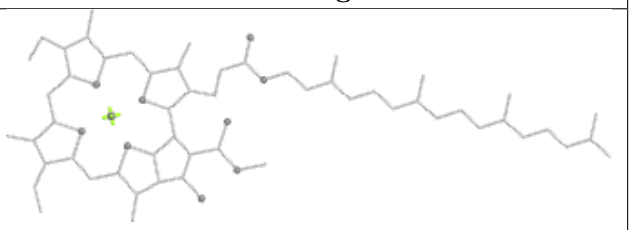


Torsions

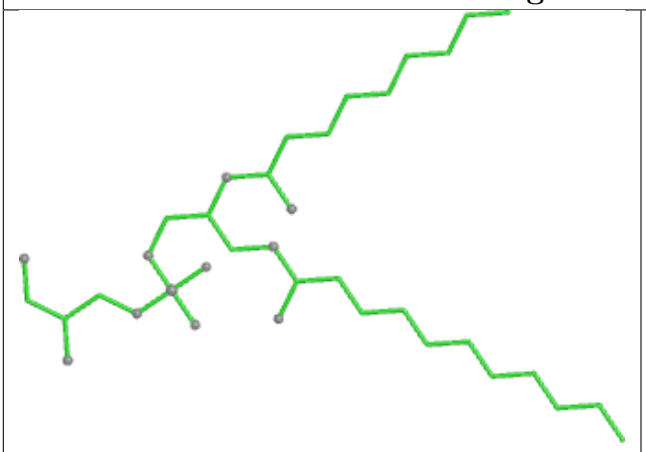


Rings

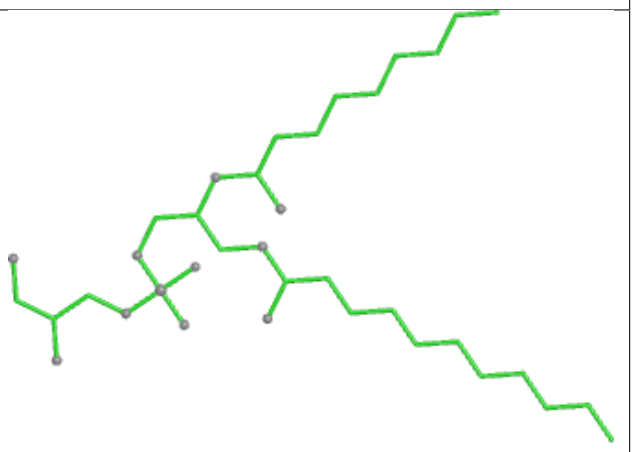
Ligand CLA A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

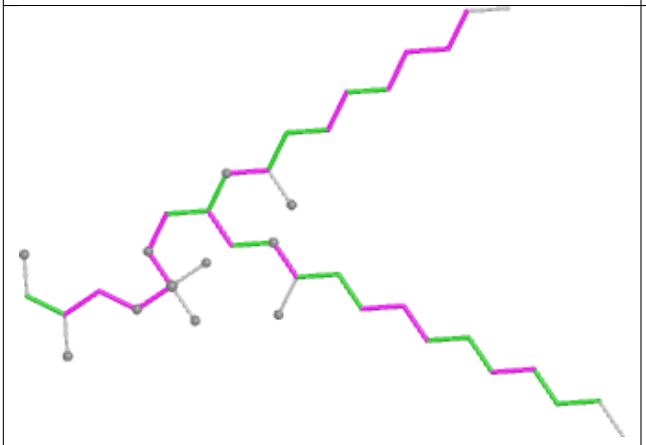
Ligand LHG 2 317



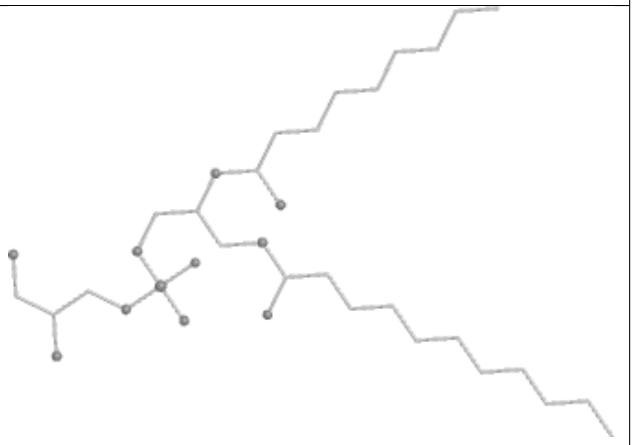
Bond lengths



Bond angles

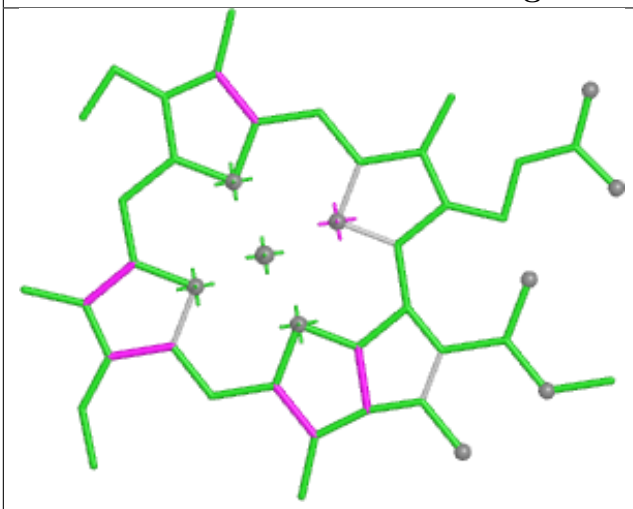


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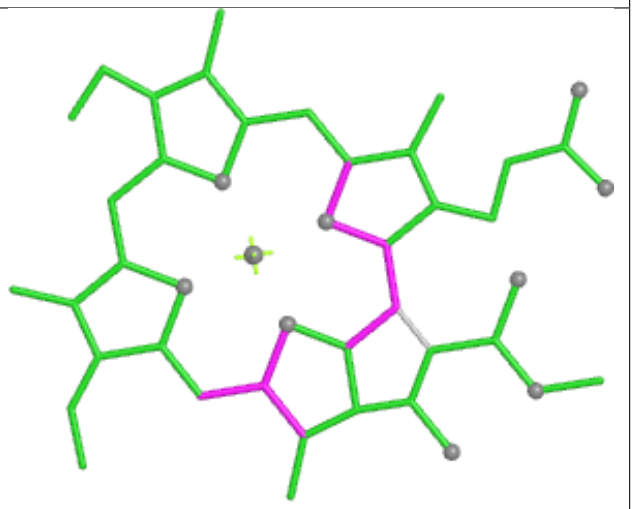


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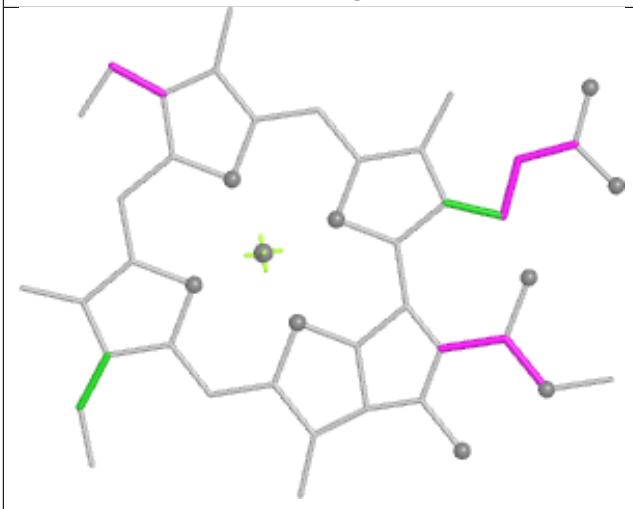
Ligand CLA O 102



Bond lengths



Bond angles

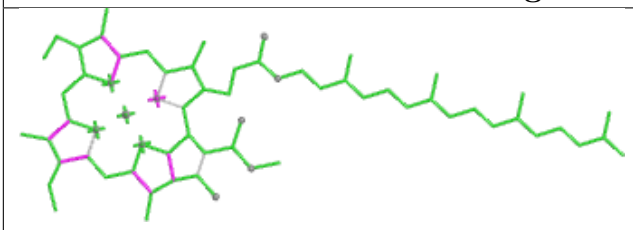


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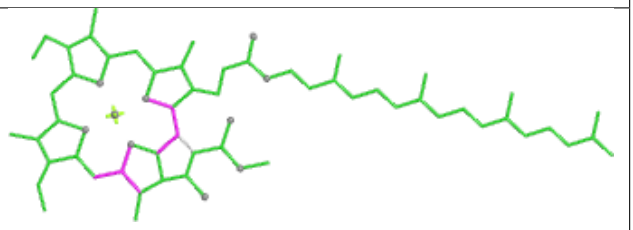


Rings

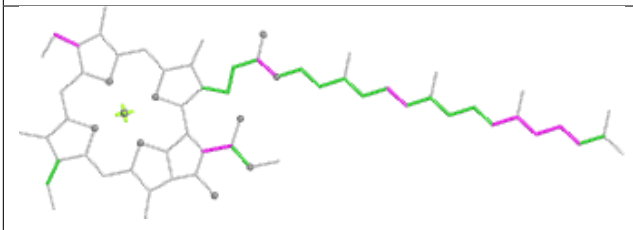
Ligand CLA B 836



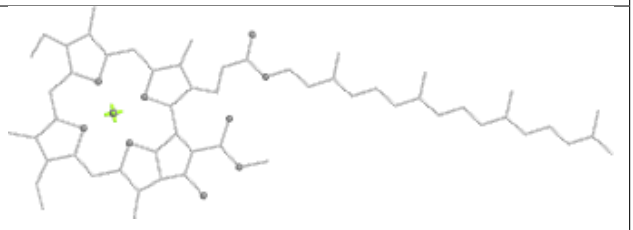
Bond lengths



Bond angles

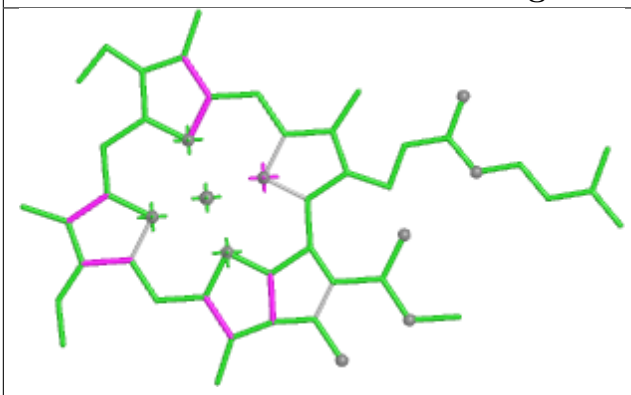


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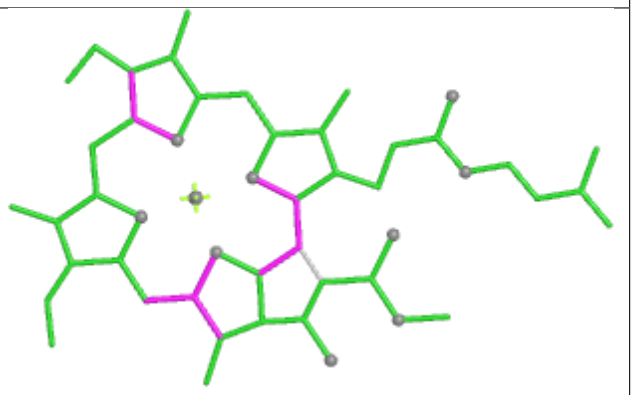


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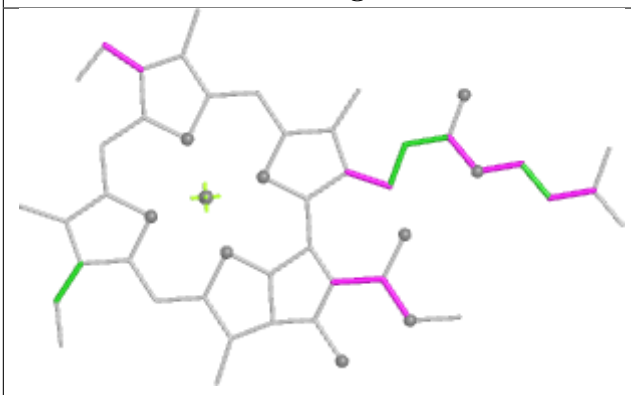
Ligand CLA 3 308



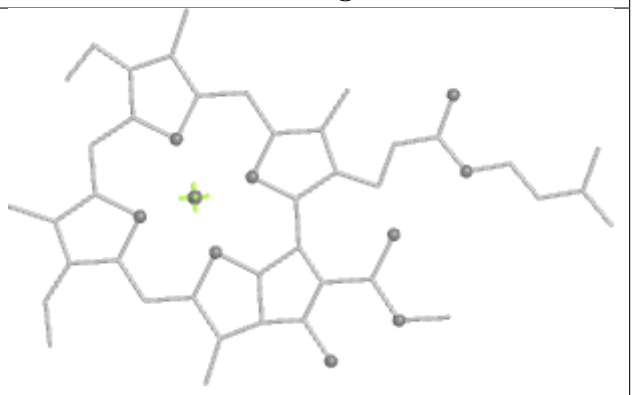
Bond lengths



Bond angles

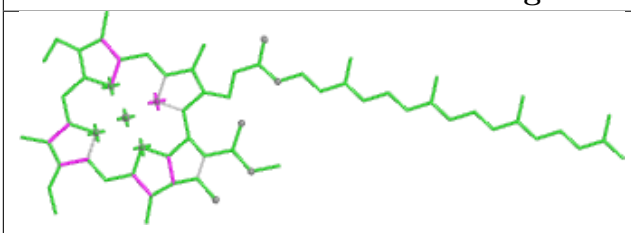


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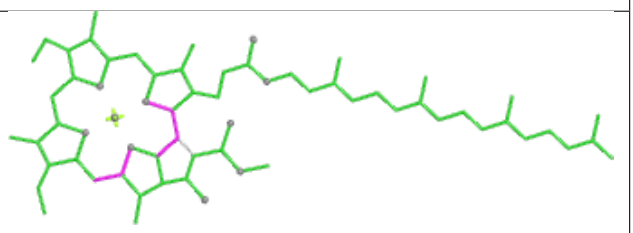


Rings

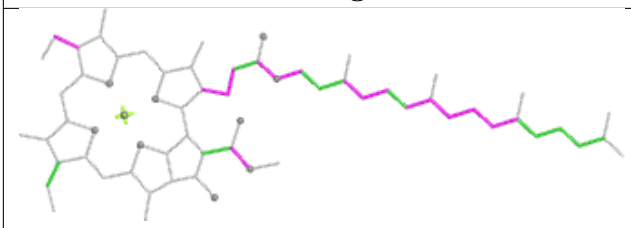
Ligand CLA A 839



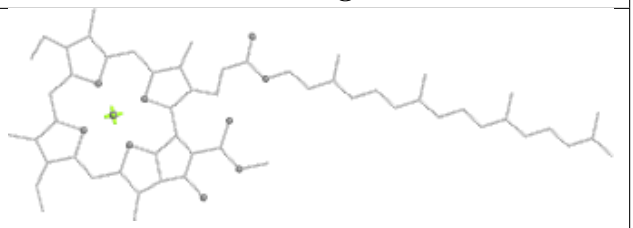
Bond lengths



Bond angles

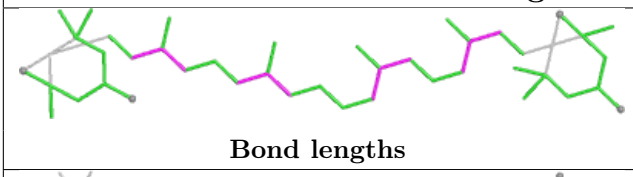


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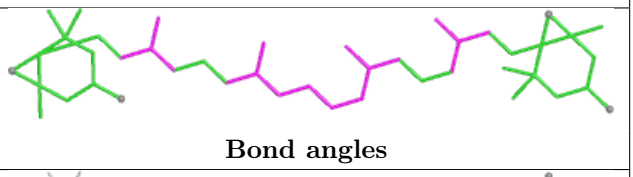


Rings

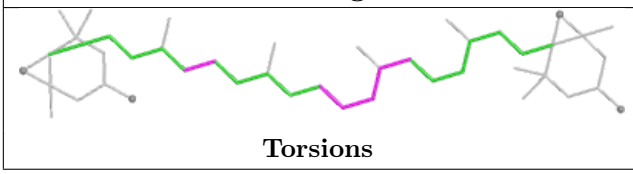
Ligand XAT 3 314



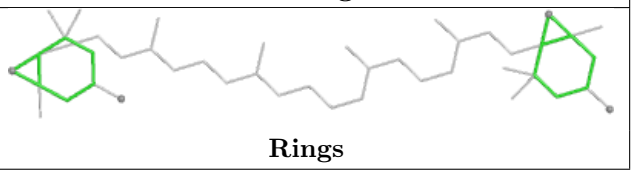
Bond lengths



Bond angles

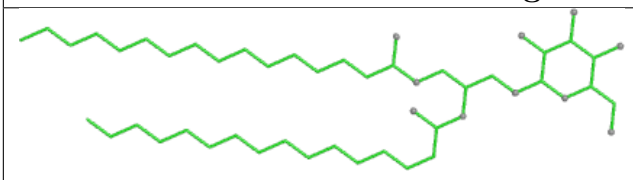


Torsions

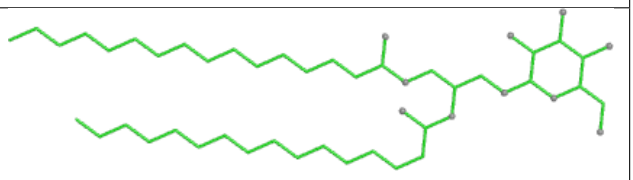


Rings

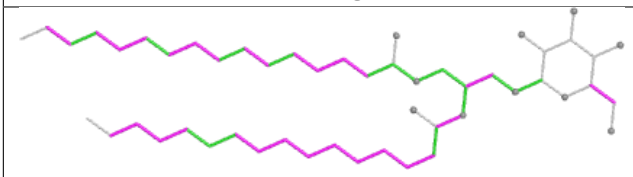
Ligand LMG J 101



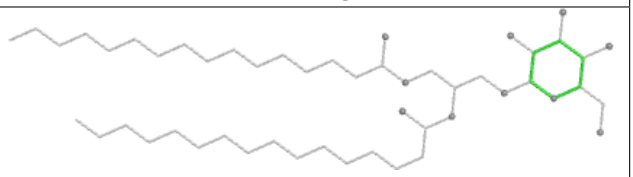
Bond lengths



Bond angles

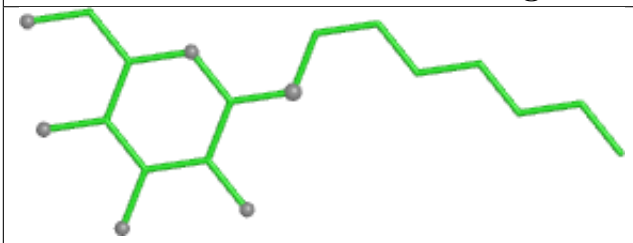


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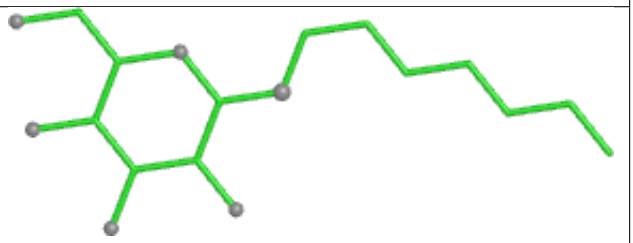


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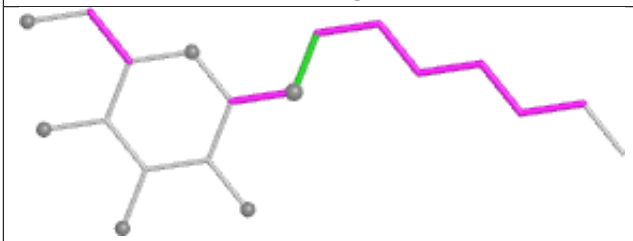
Ligand HTG F 301



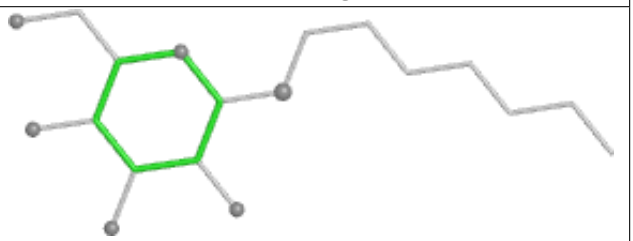
Bond lengths



Bond angles

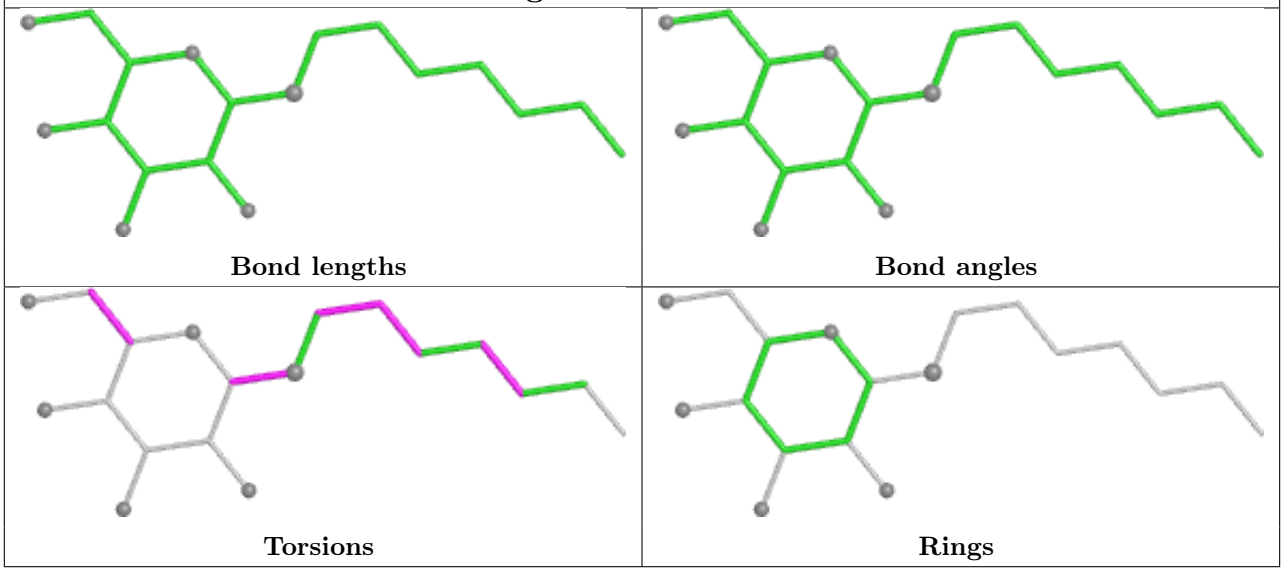


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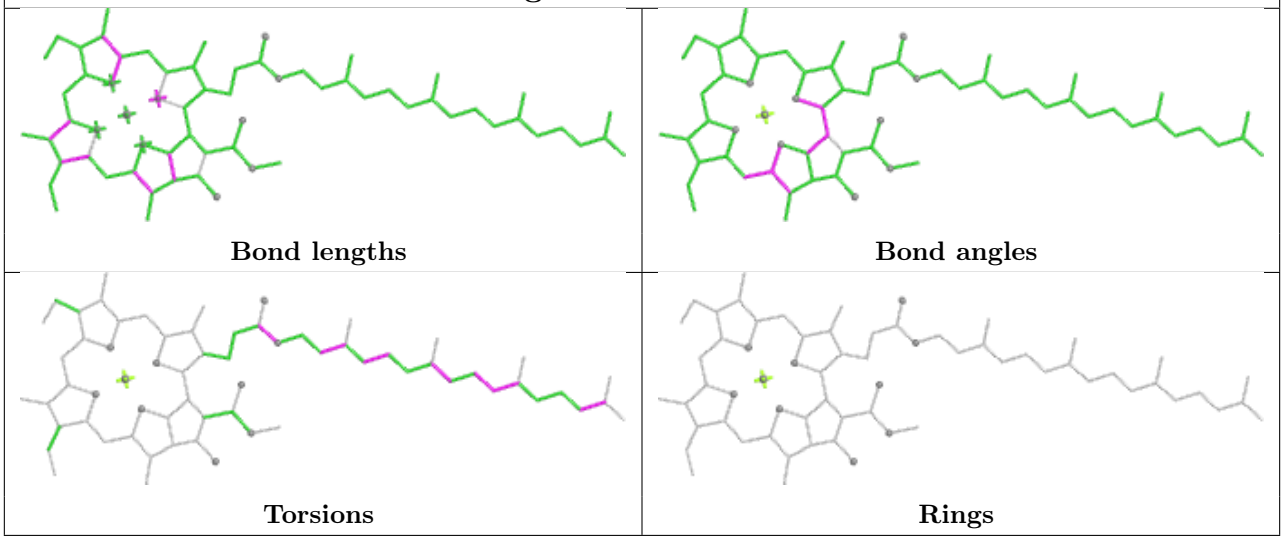


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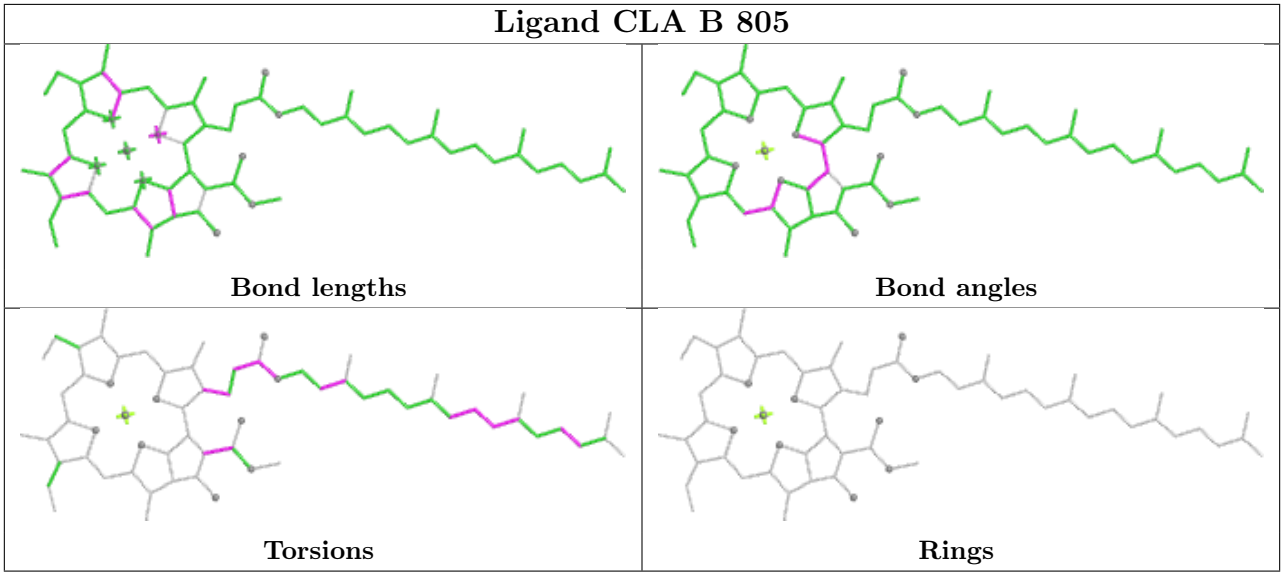
Ligand HTG 4 321



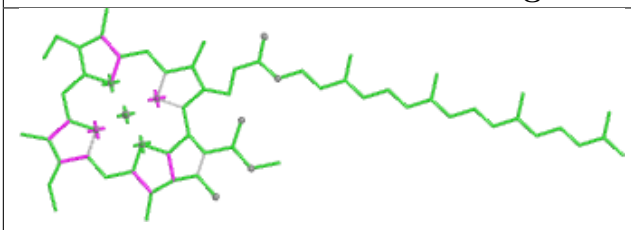
Ligand CLA A 819



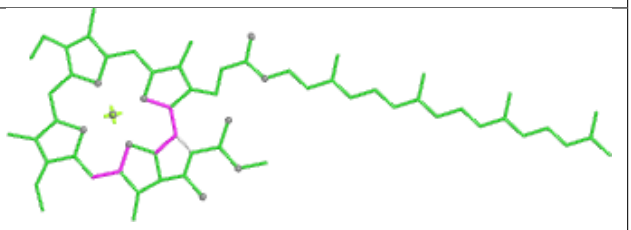
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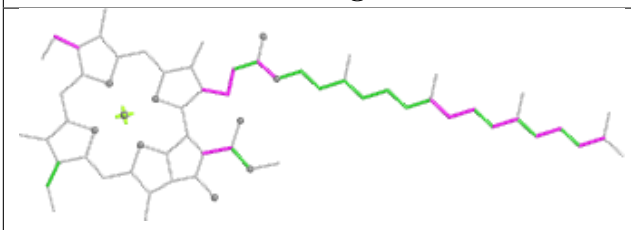
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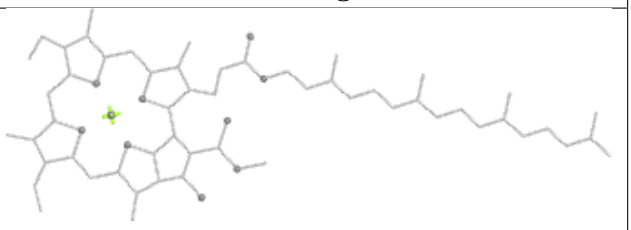
Bond lengths



Bond angles

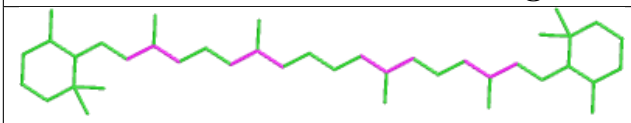


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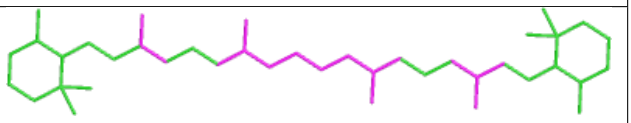


Rings

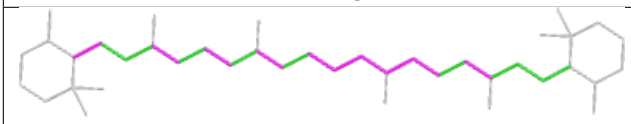
Ligand BCR L 301



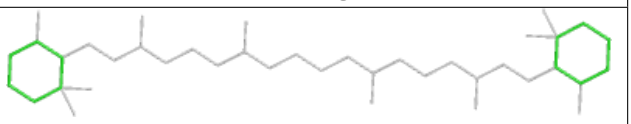
Bond lengths



Bond angles

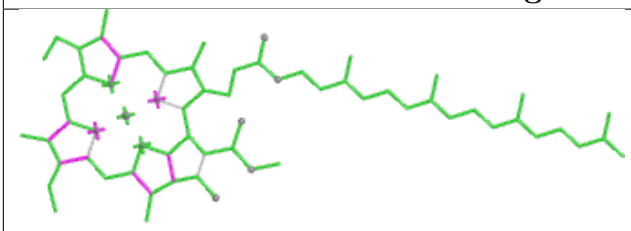


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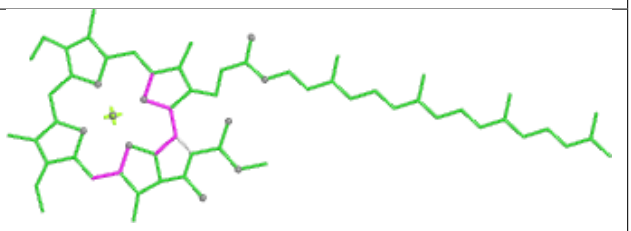


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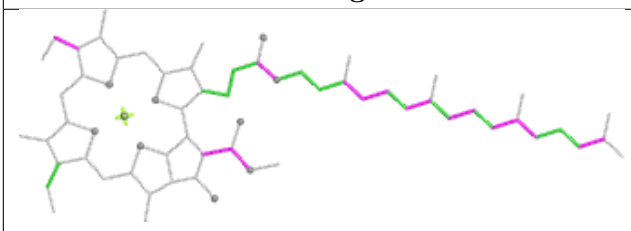
Ligand CLA B 821



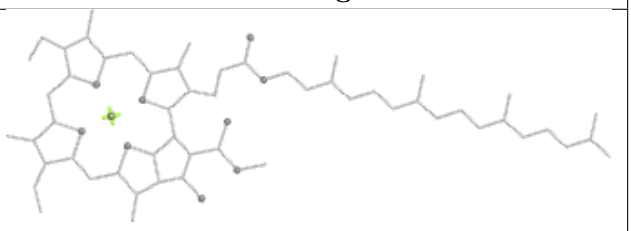
Bond lengths



Bond angles



Torsions

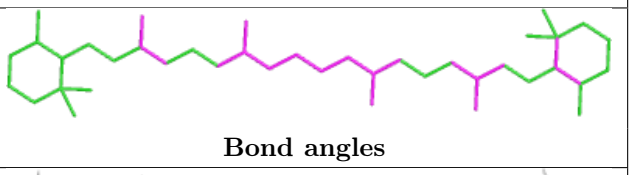


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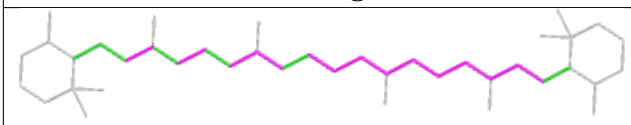
Ligand BCR A 845



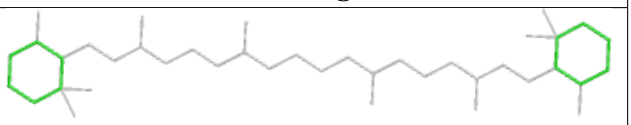
Bond lengths



Bond angles

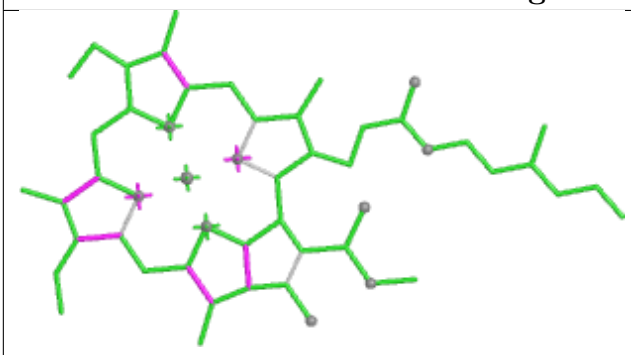


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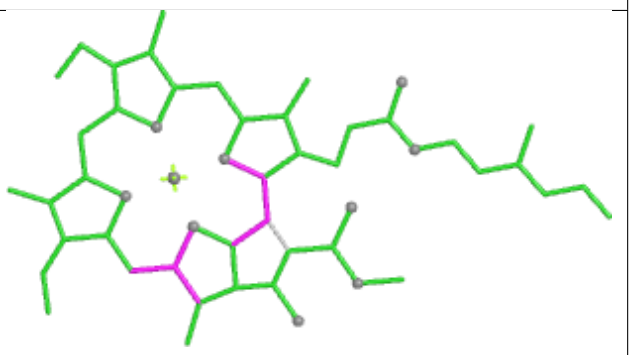


Rings

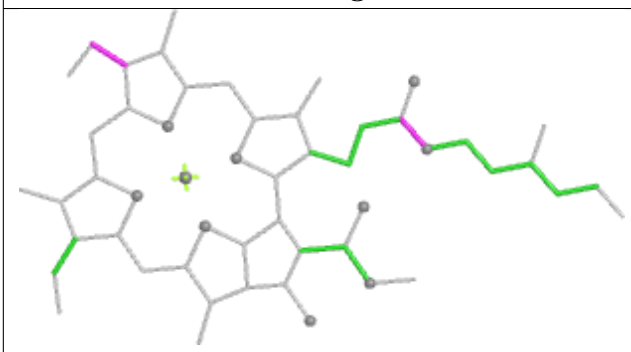
Ligand CLA 3 309



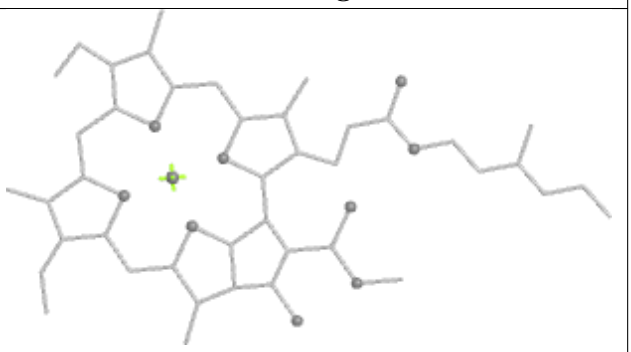
Bond lengths



Bond angles

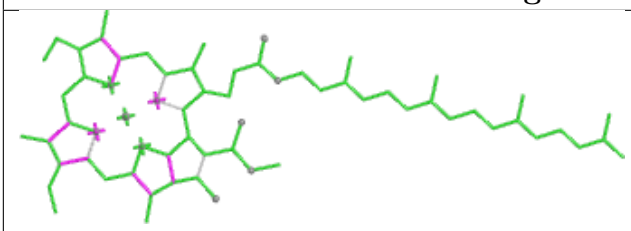


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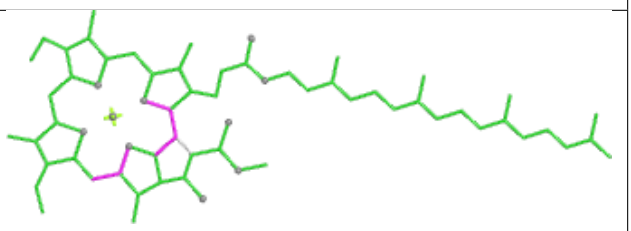


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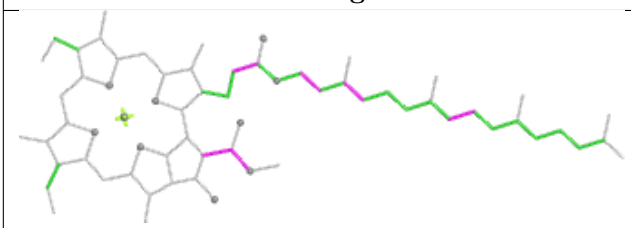
Ligand CLA A 823



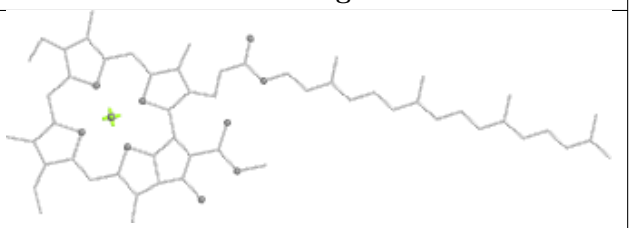
Bond lengths



Bond angles

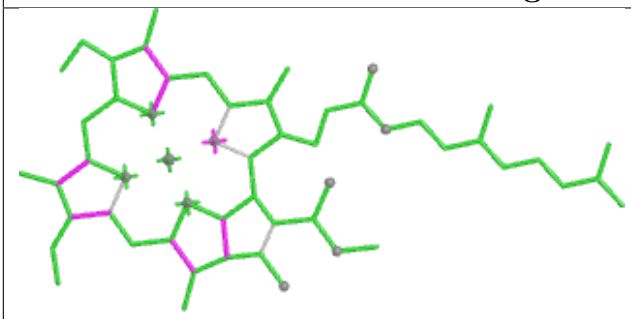


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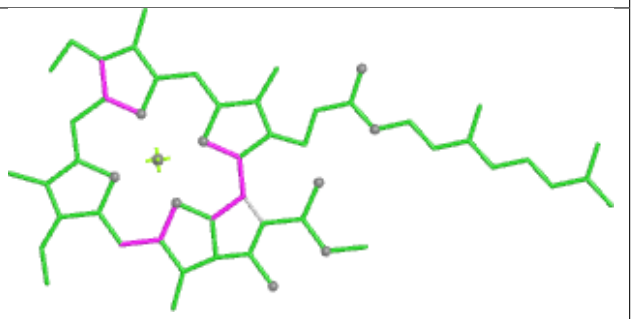


Rings

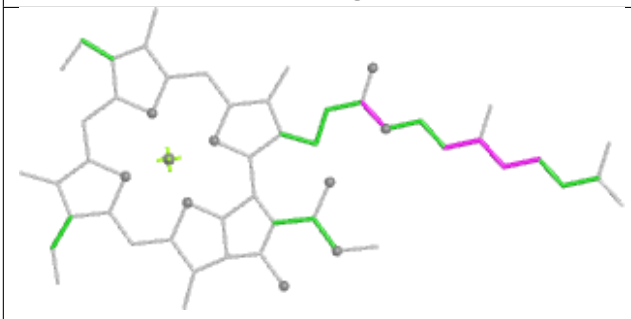
Ligand CLA A 802



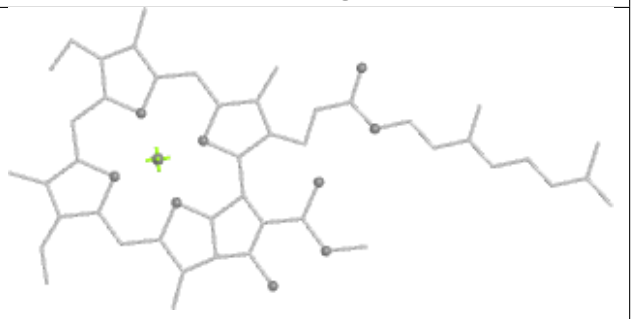
Bond lengths



Bond angles

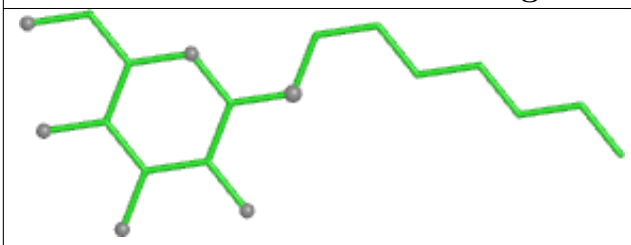


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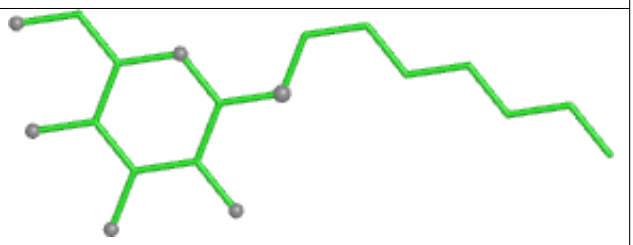


Rings

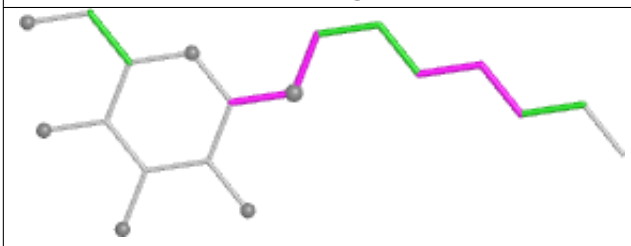
Ligand HTG B 848



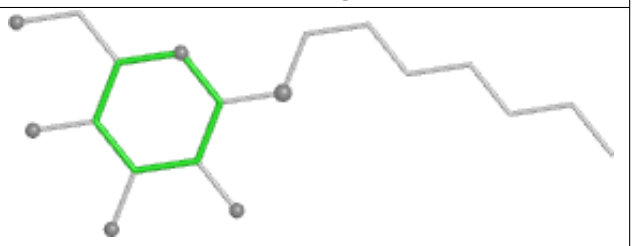
Bond lengths



Bond angles

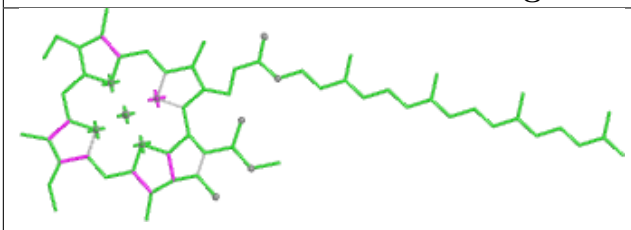


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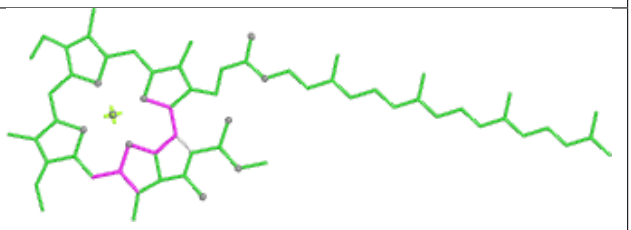


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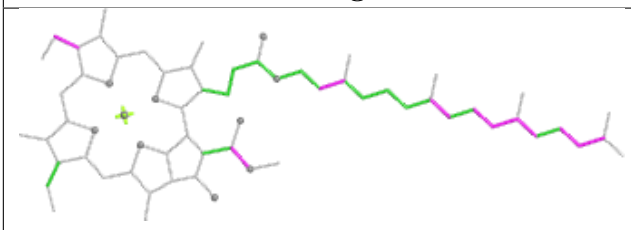
Ligand CLA A 826



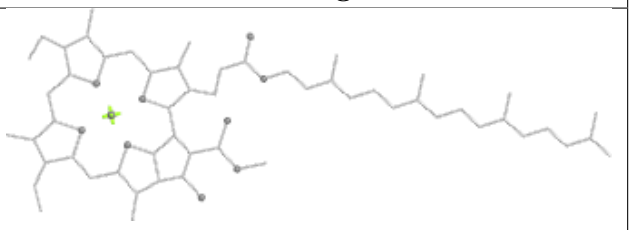
Bond lengths



Bond angles

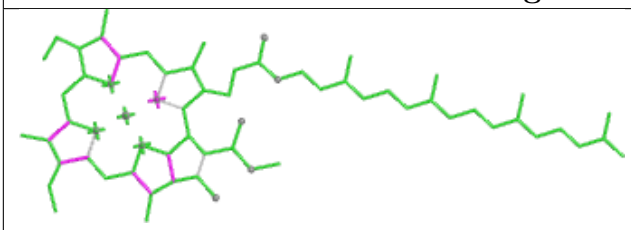


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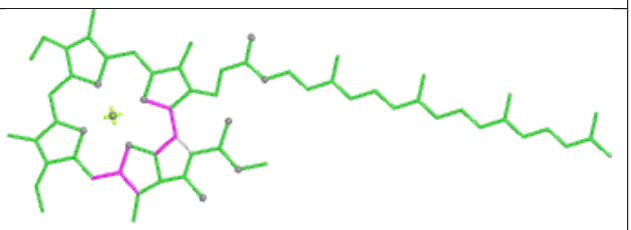


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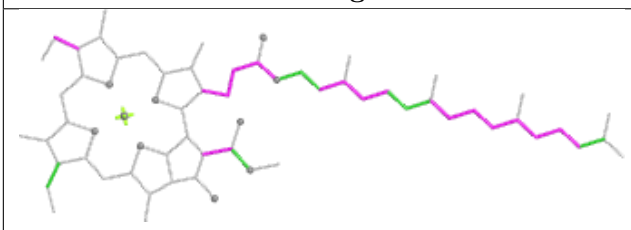
Ligand CLA A 808



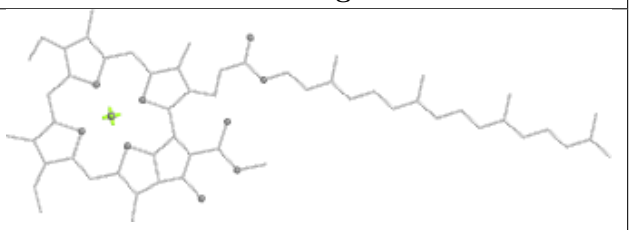
Bond lengths



Bond angles

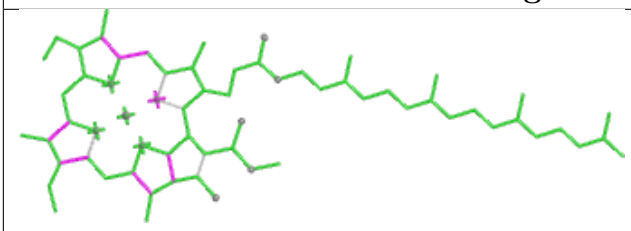


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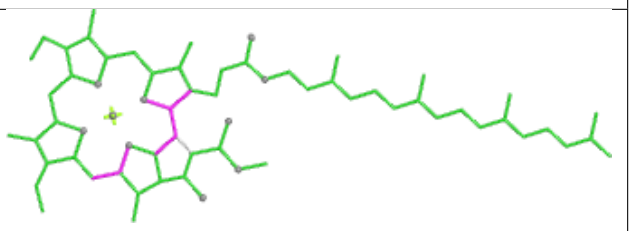


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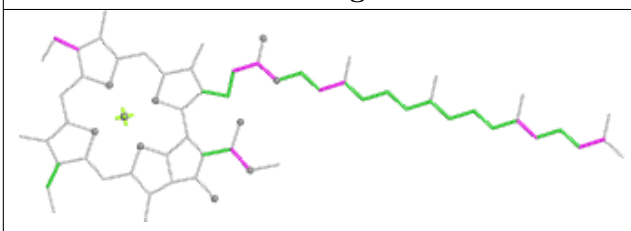
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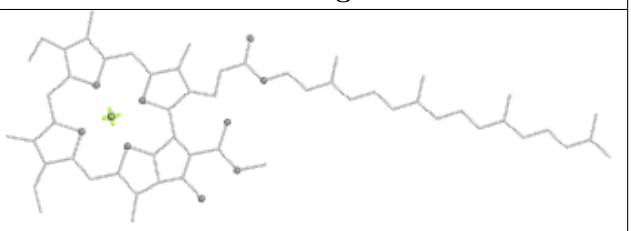
Bond lengths



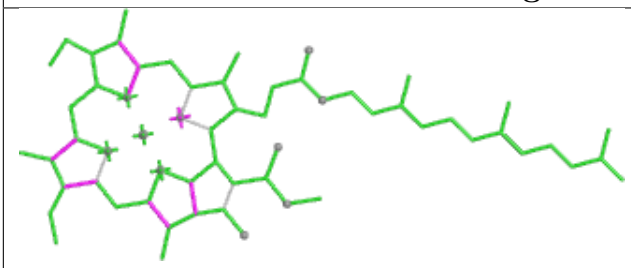
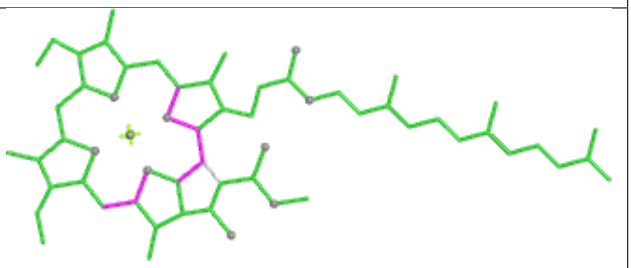
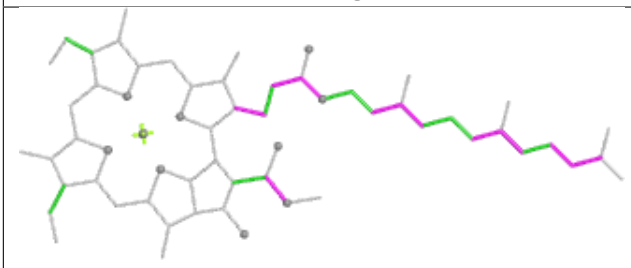
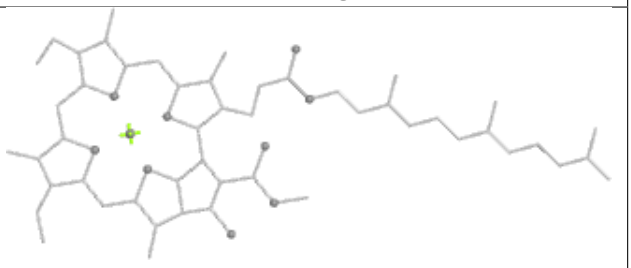
Bond angles

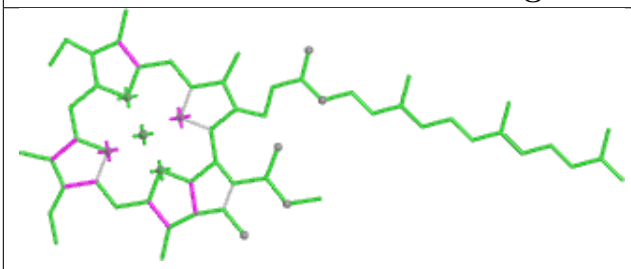
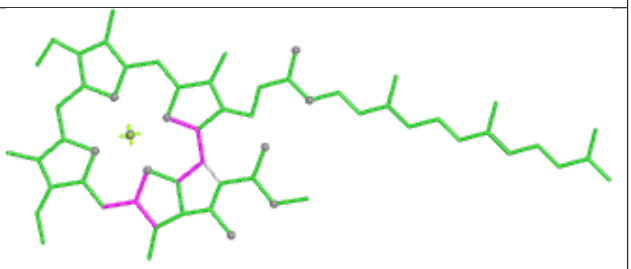
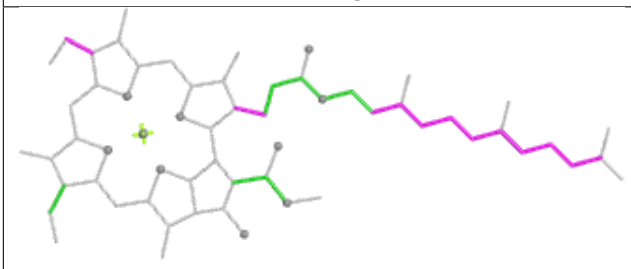
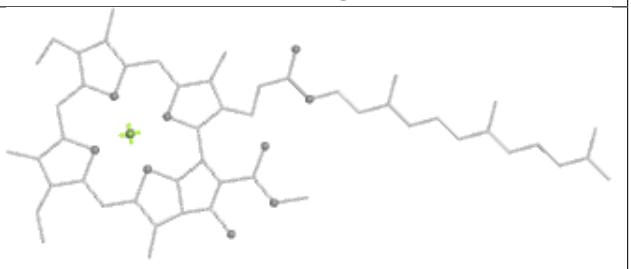


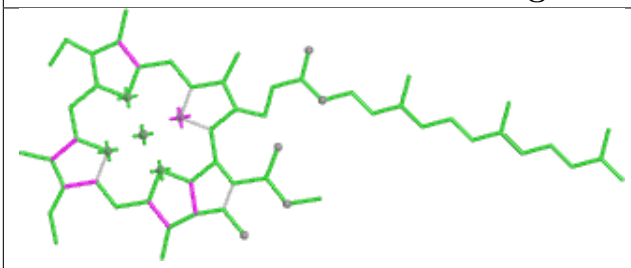
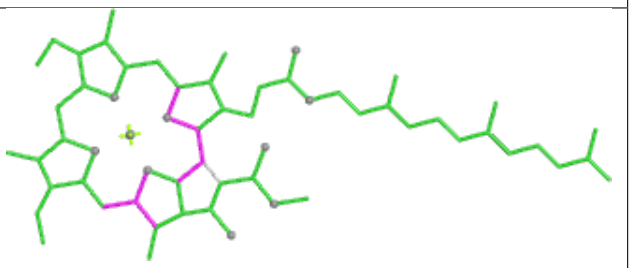
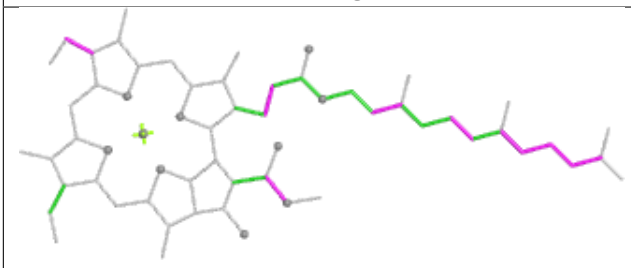
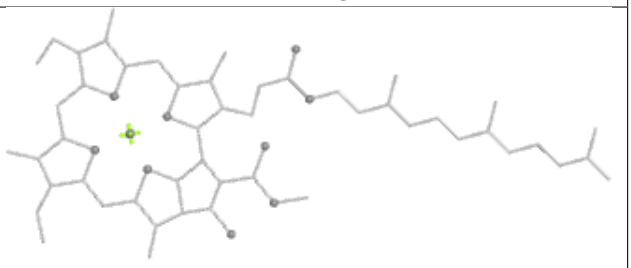
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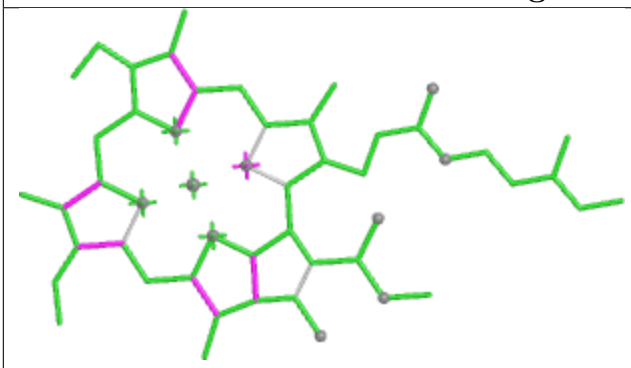
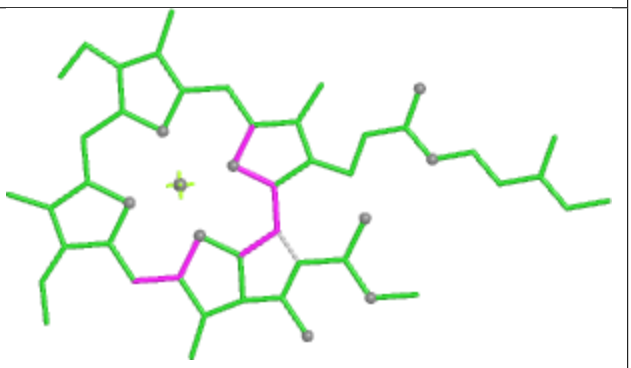
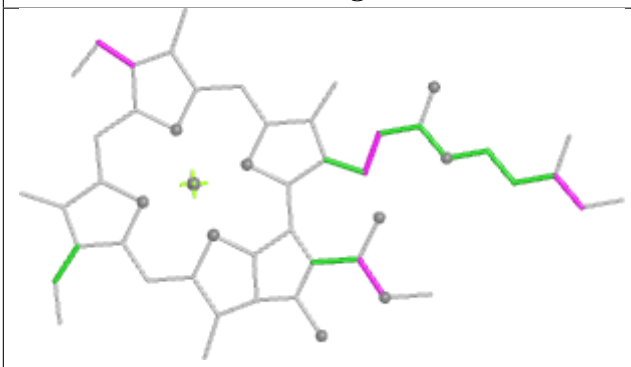
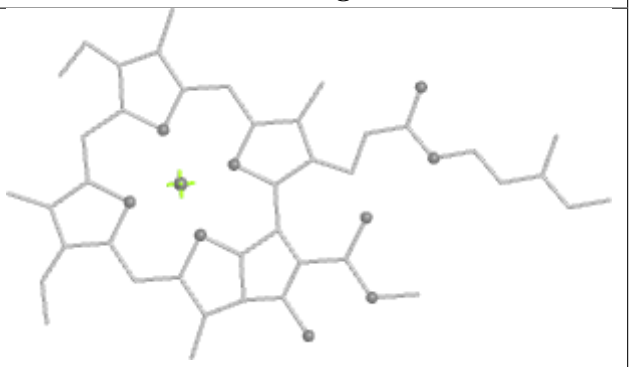


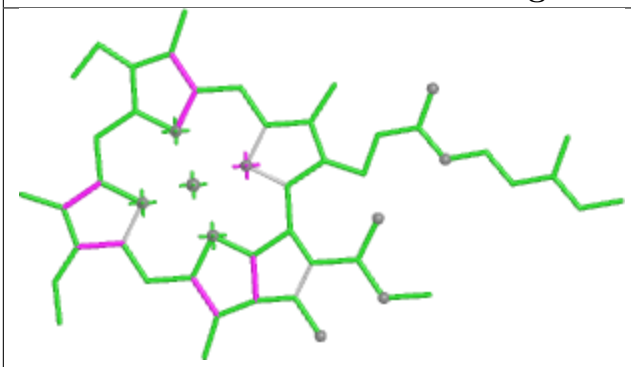
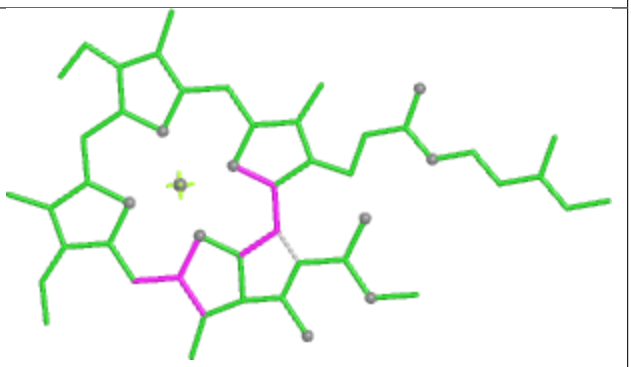
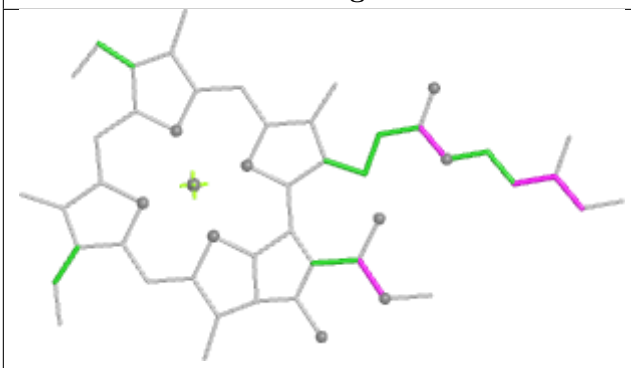
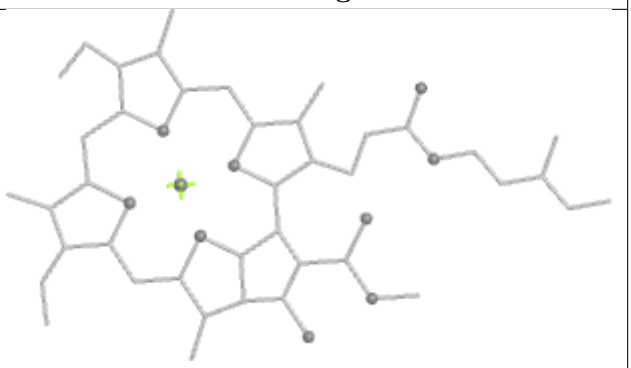
Rings

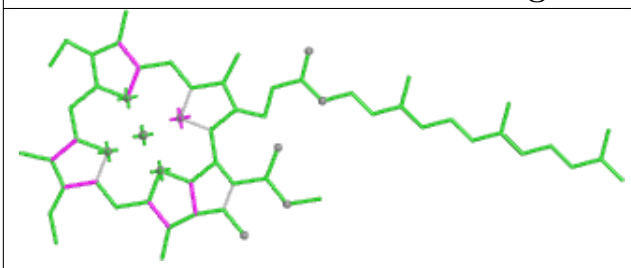
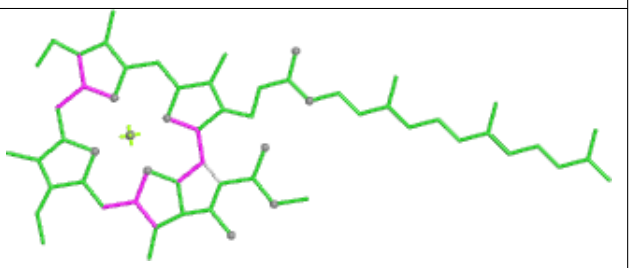
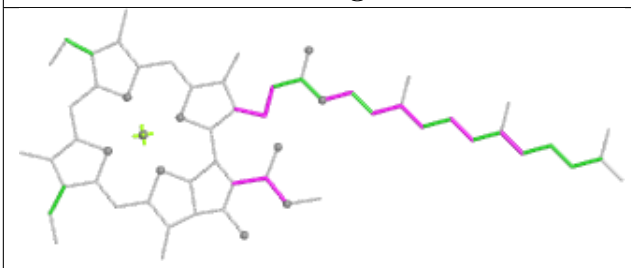
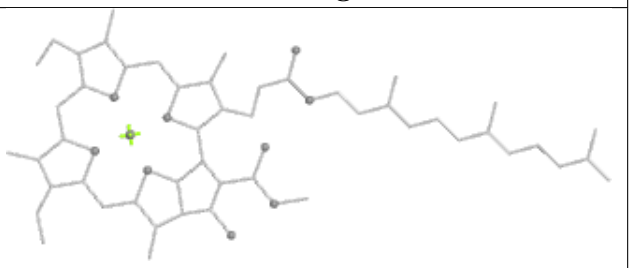
Ligand CLA K 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

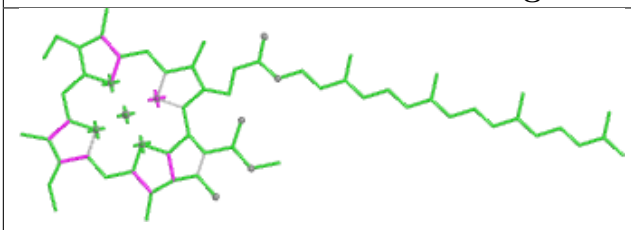
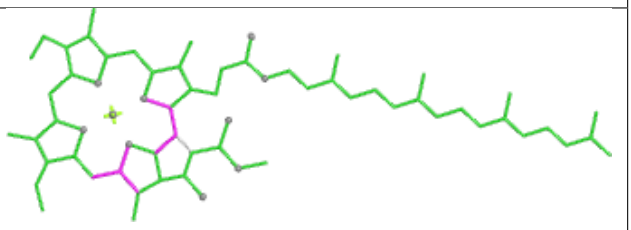
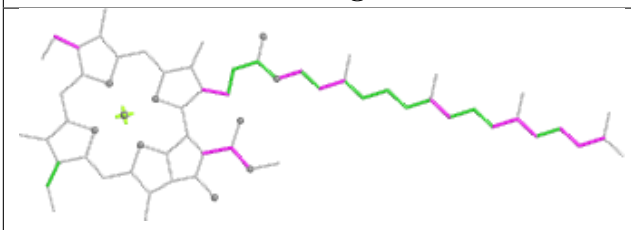
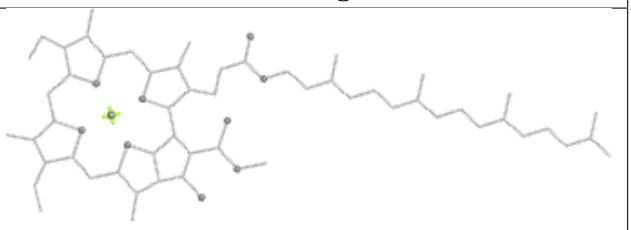
Ligand CLA B 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

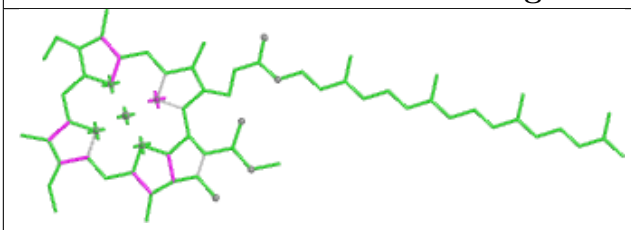
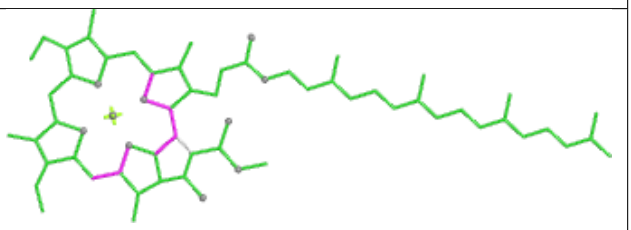
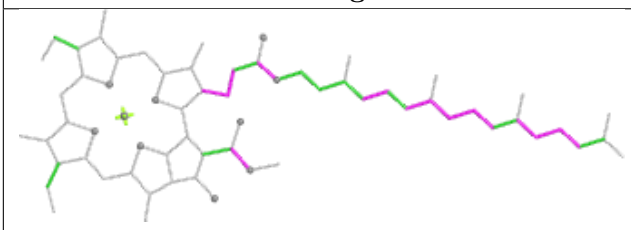
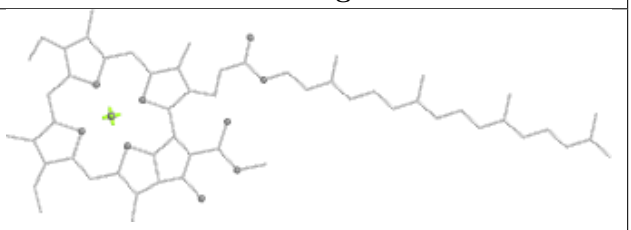
Ligand CLA 1 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

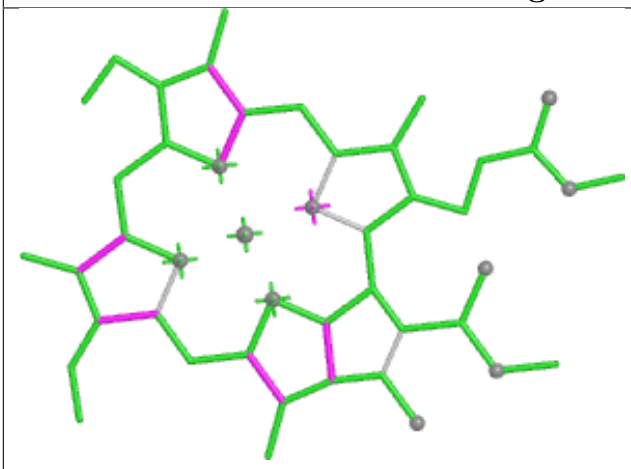
Ligand CLA 2 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

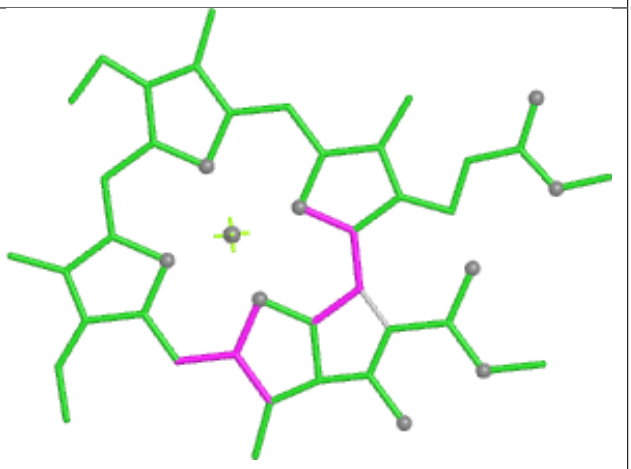
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

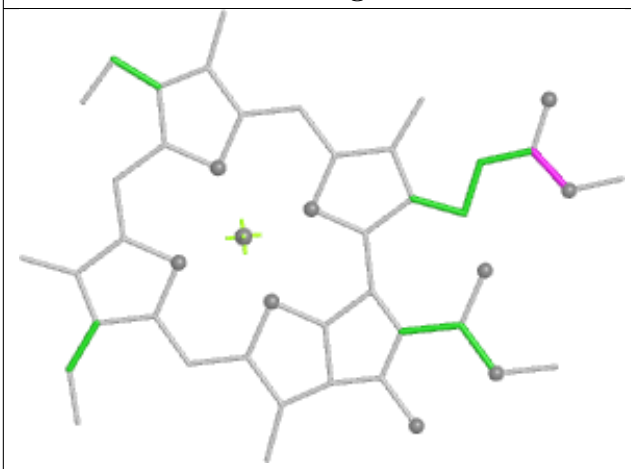
Ligand CLA 3 312



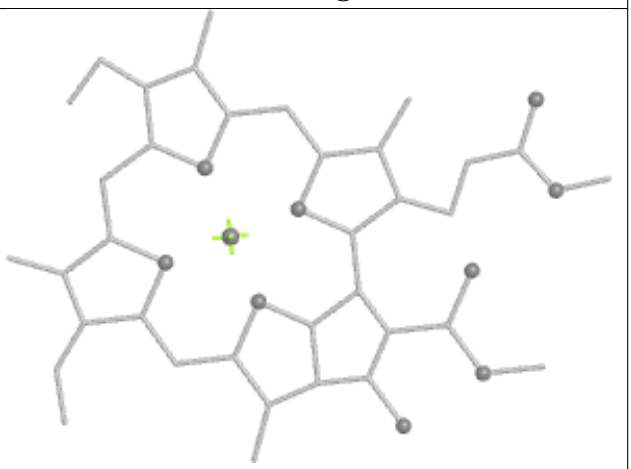
Bond lengths



Bond angles

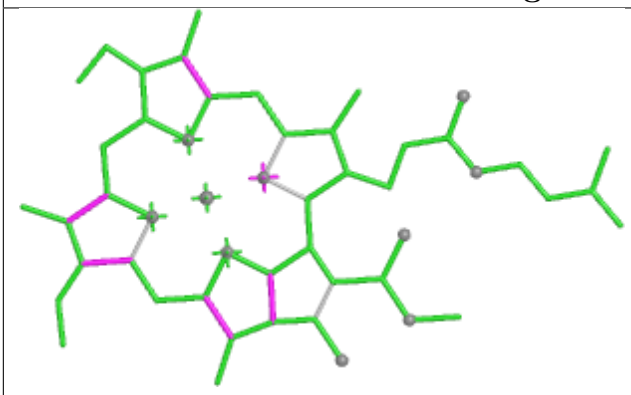


Torsions

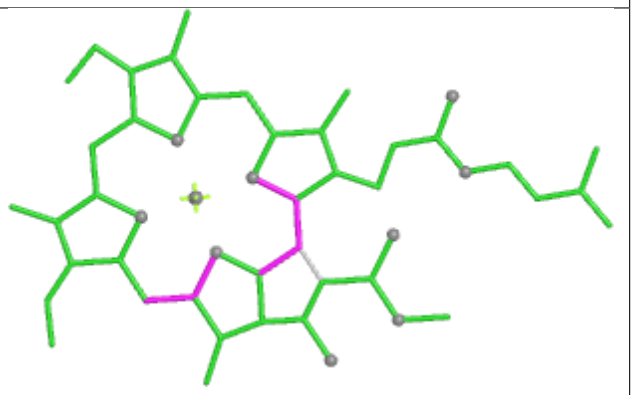


Rings

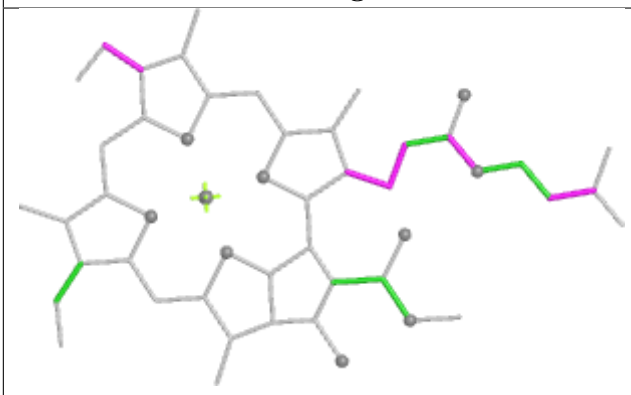
Ligand CLA A 832



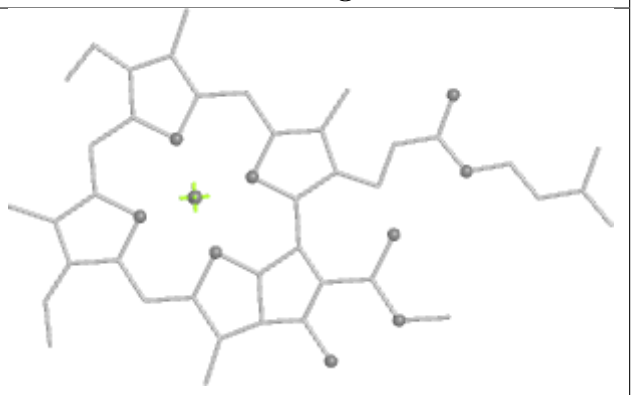
Bond lengths



Bond angles

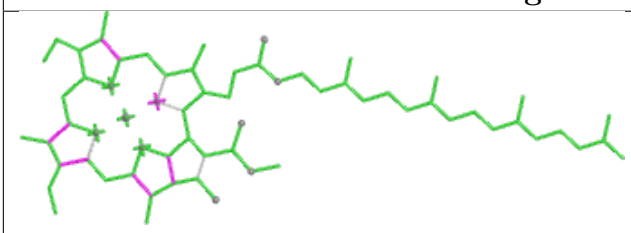


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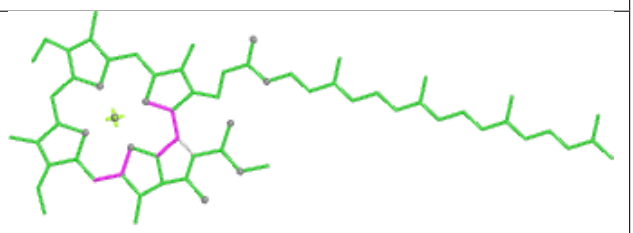


Rings

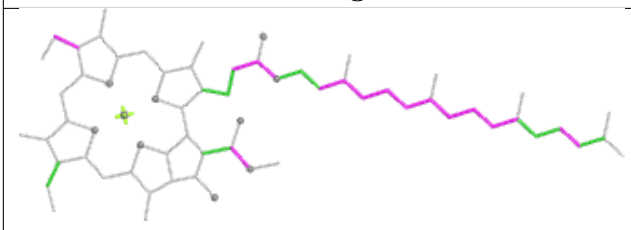
Ligand CLA B 806



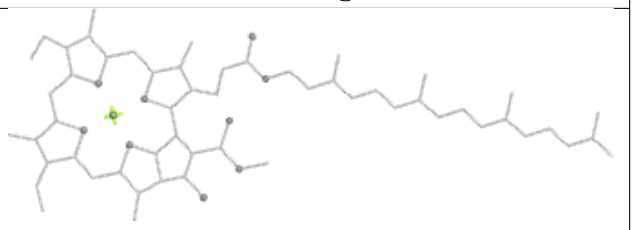
Bond lengths



Bond angles



Torsions

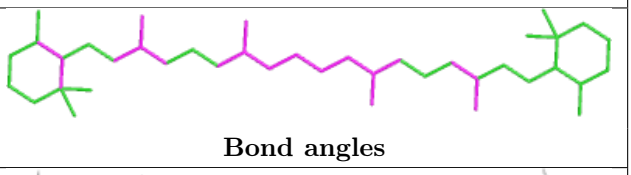


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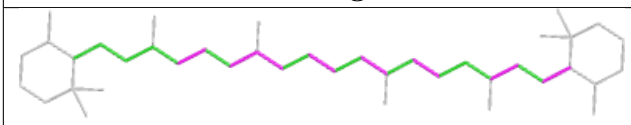
Ligand BCR F 308



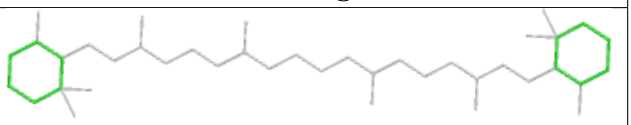
Bond lengths



Bond angles

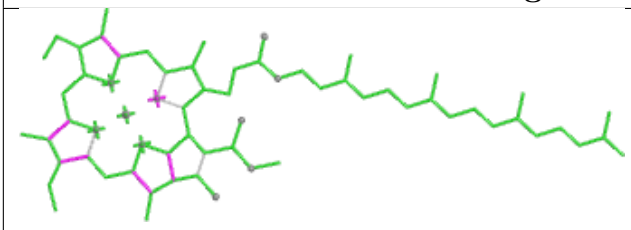


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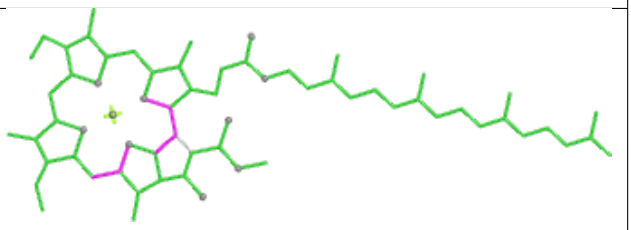


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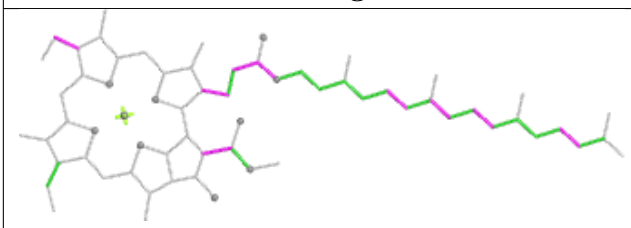
Ligand CLA B 840



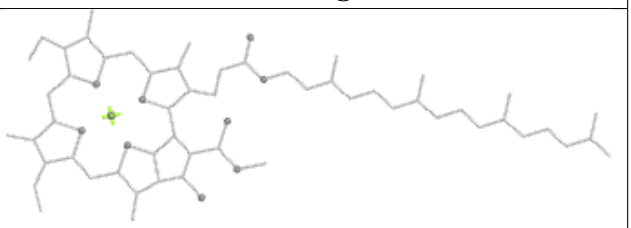
Bond lengths



Bond angles

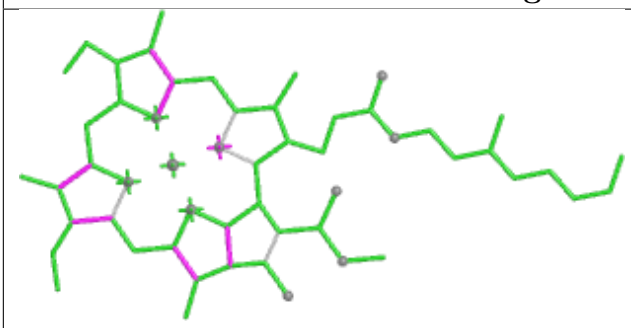


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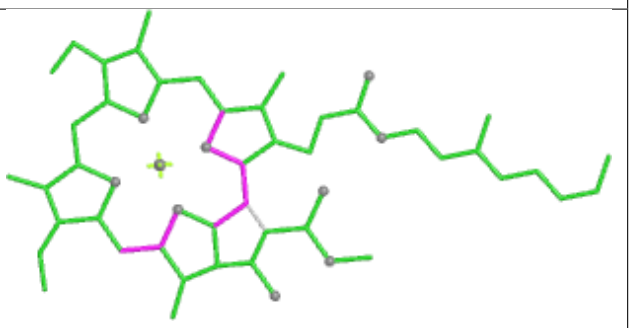


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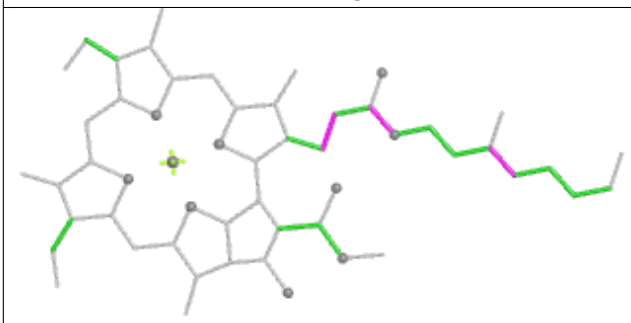
Ligand CLA A 810



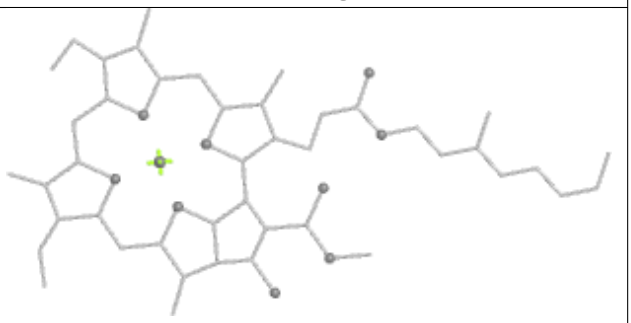
Bond lengths



Bond angles



Torsions

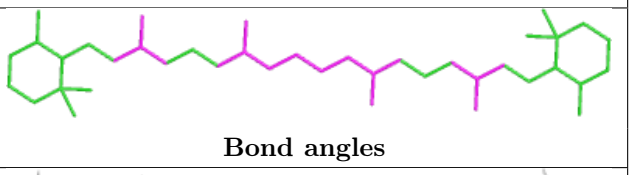


Rings

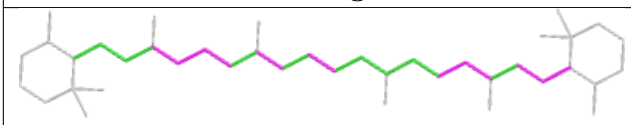
Ligand BCR B 845



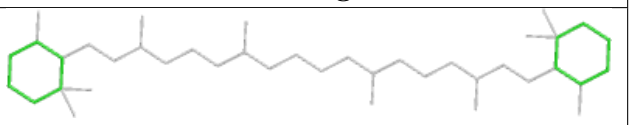
Bond lengths



Bond angles

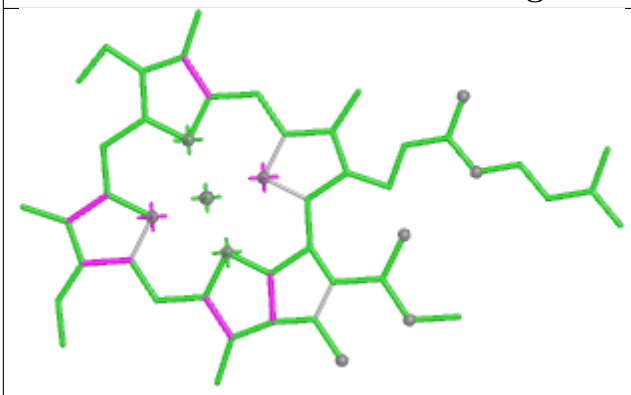


Torsions

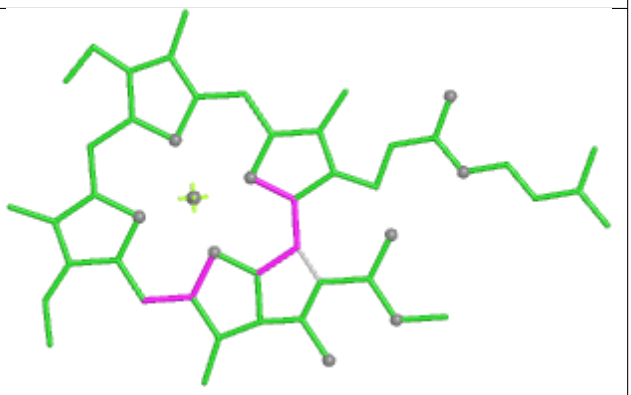


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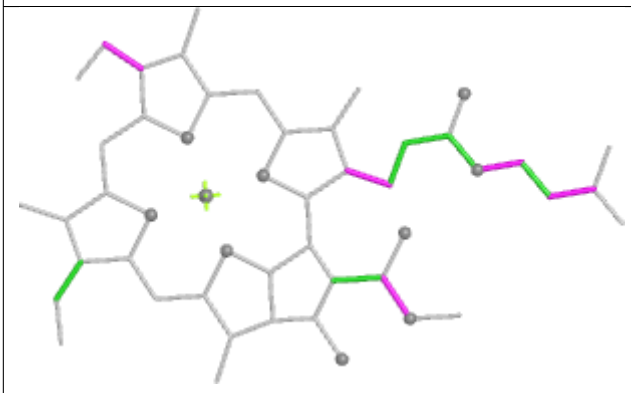
Ligand CLA L 304



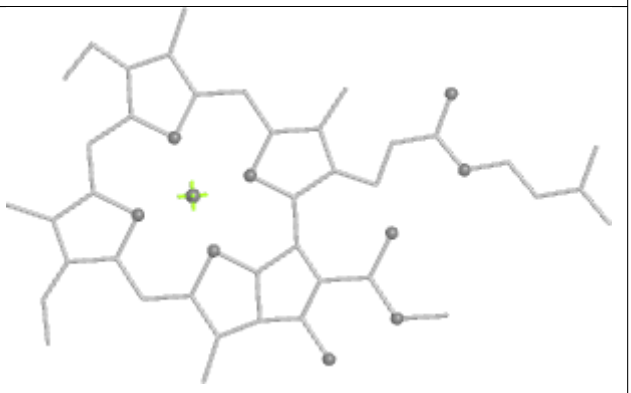
Bond lengths



Bond angles

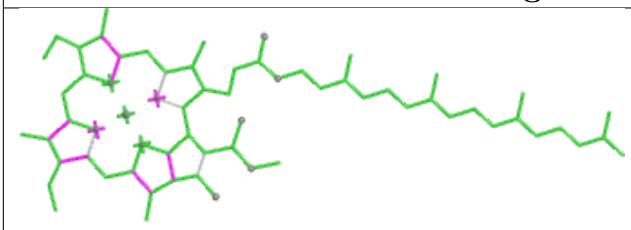


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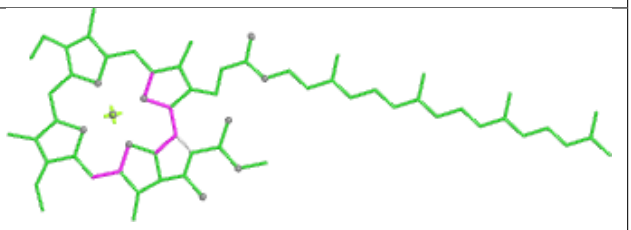


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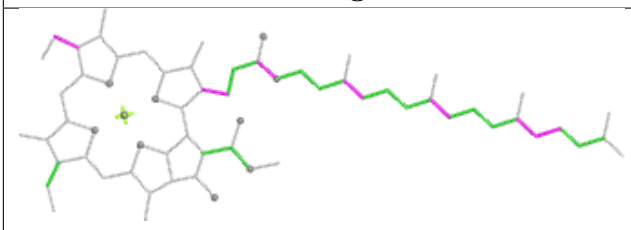
Ligand CLA A 825



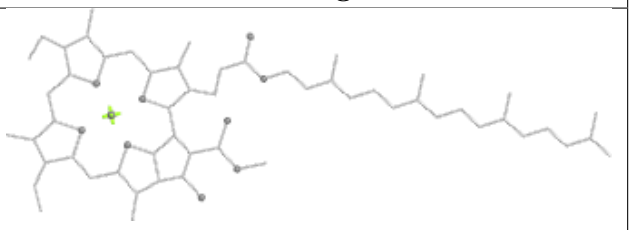
Bond lengths



Bond angles

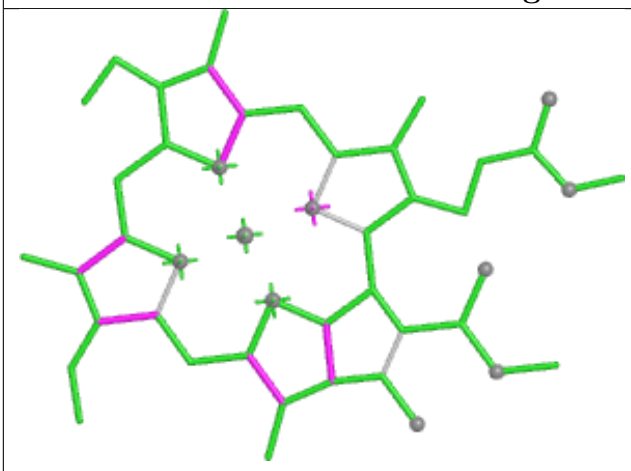


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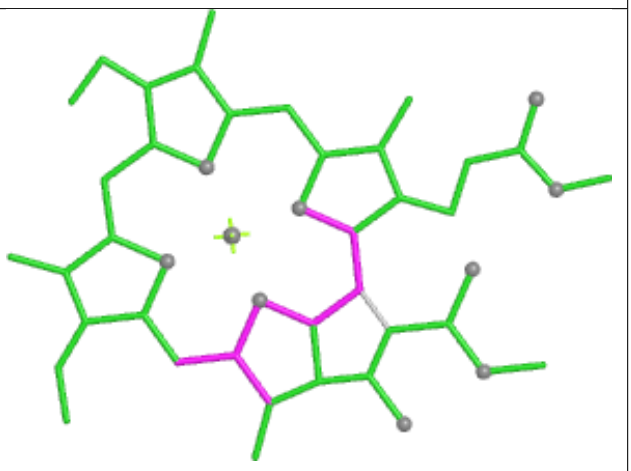


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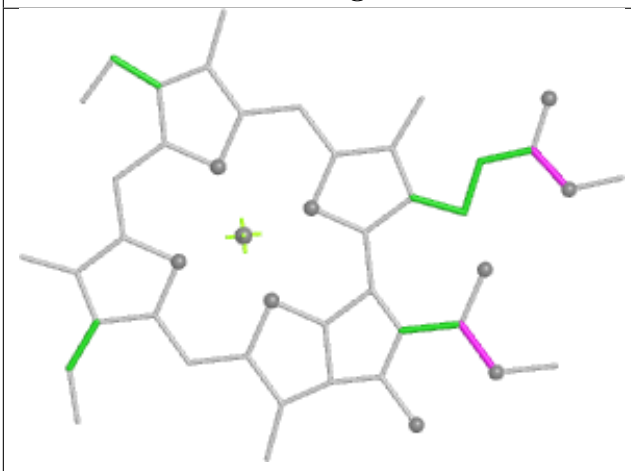
Ligand CLA G 205



Bond lengths



Bond angles

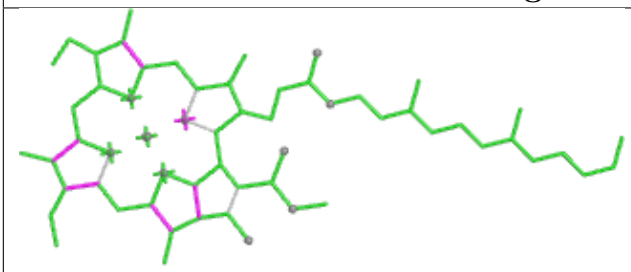


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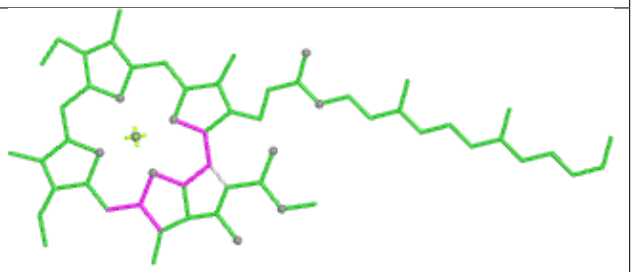


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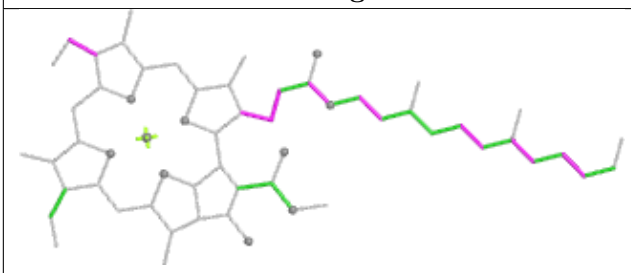
Ligand CLA B 817



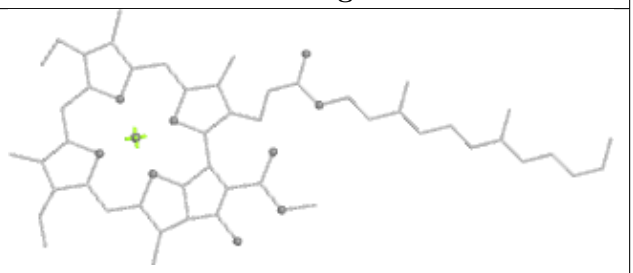
Bond lengths



Bond angles

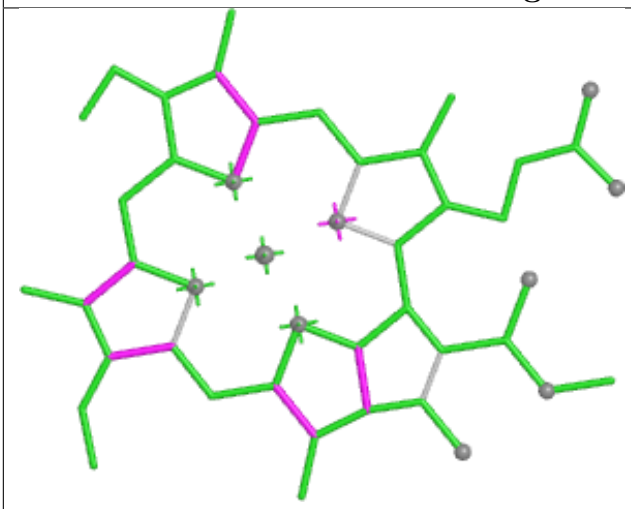


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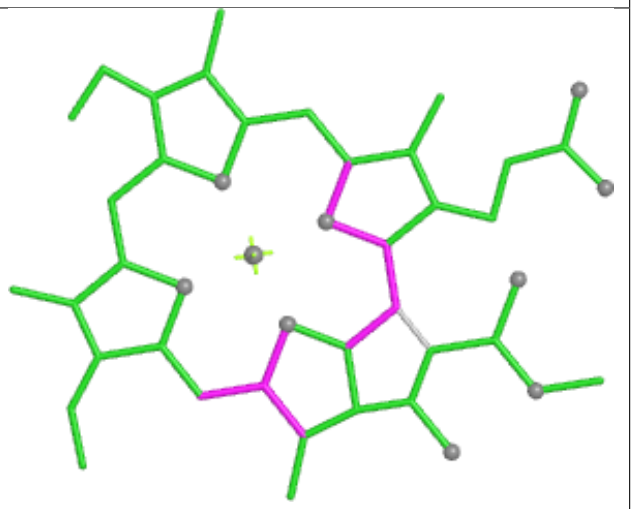


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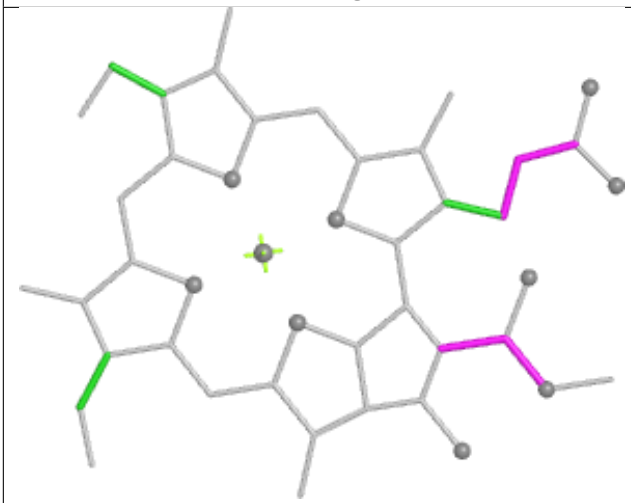
Ligand CLA A 833



Bond lengths



Bond angles

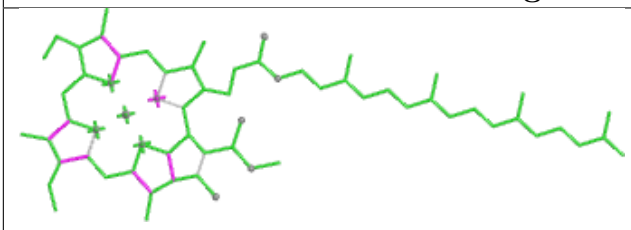


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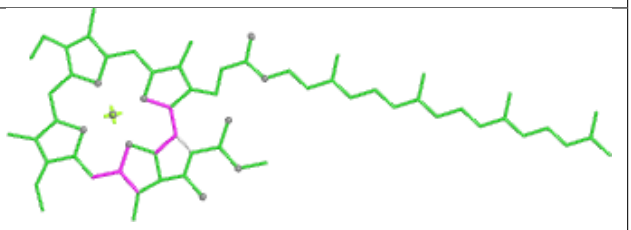


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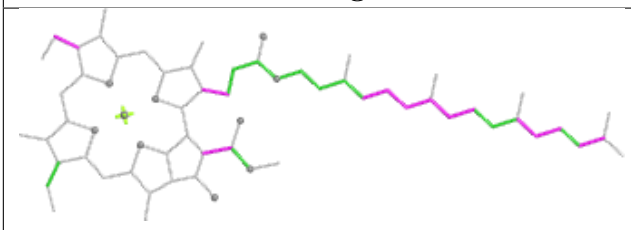
Ligand CLA A 805



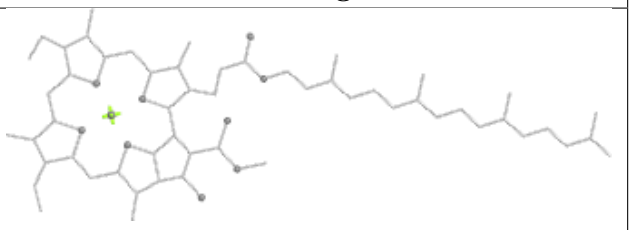
Bond lengths



Bond angles

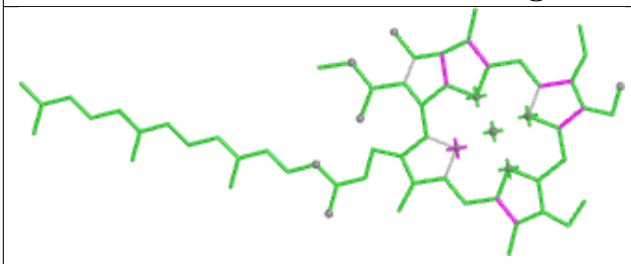


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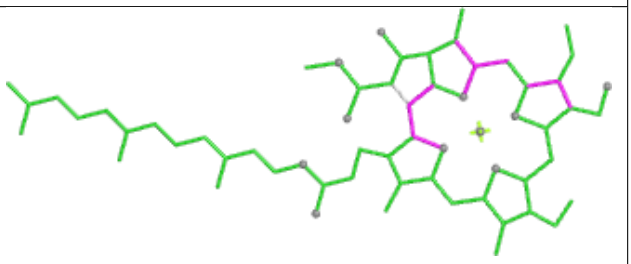


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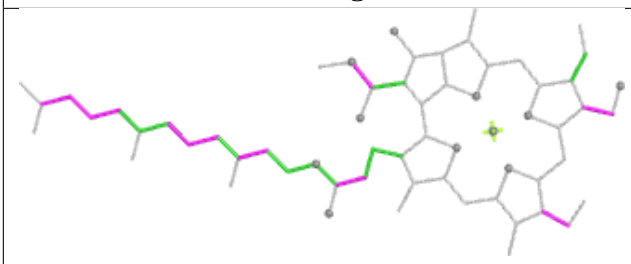
Ligand CHL 1 318



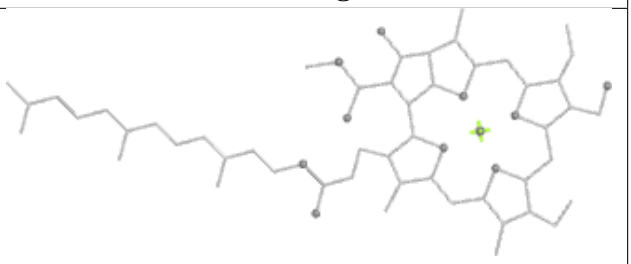
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Bond angles

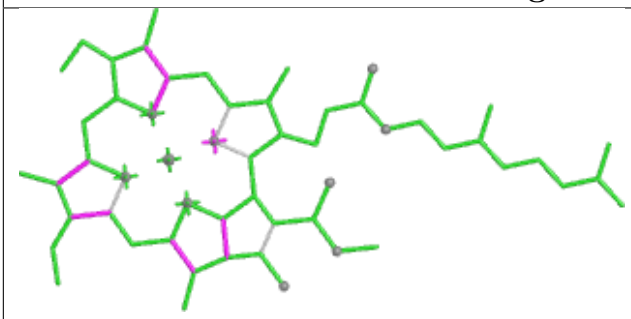


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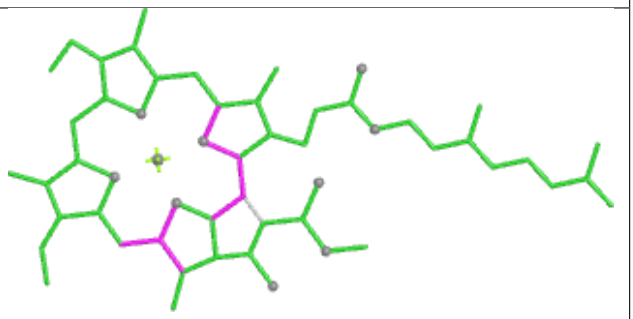


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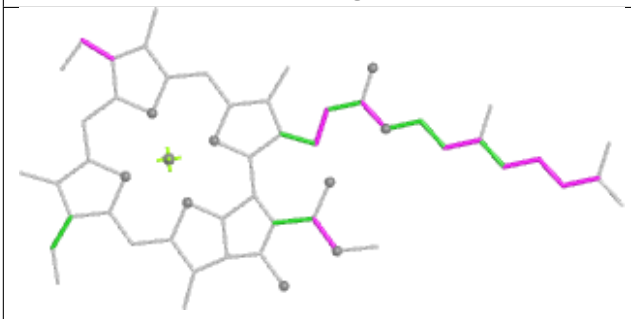
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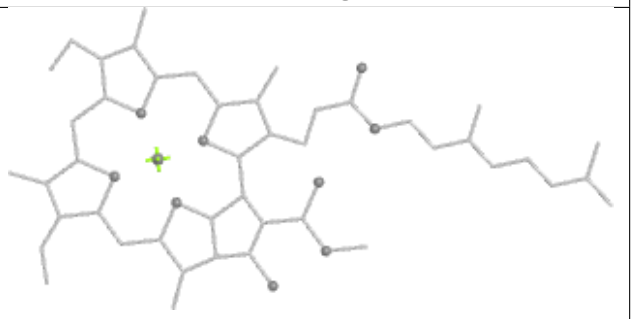
Bond lengths



Bond angles

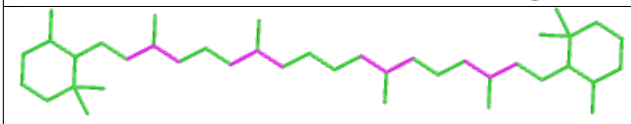


Torsions



Rings

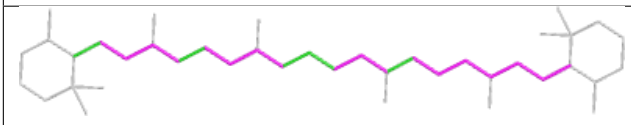
Ligand BCR 1 316



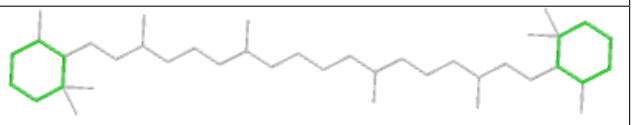
Bond lengths



Bond angles

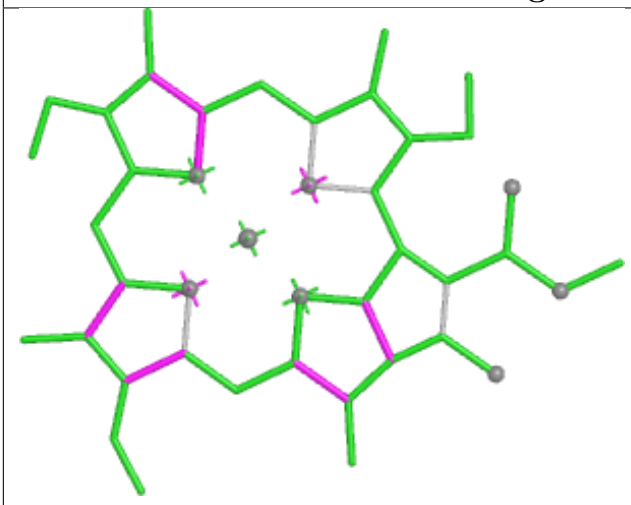


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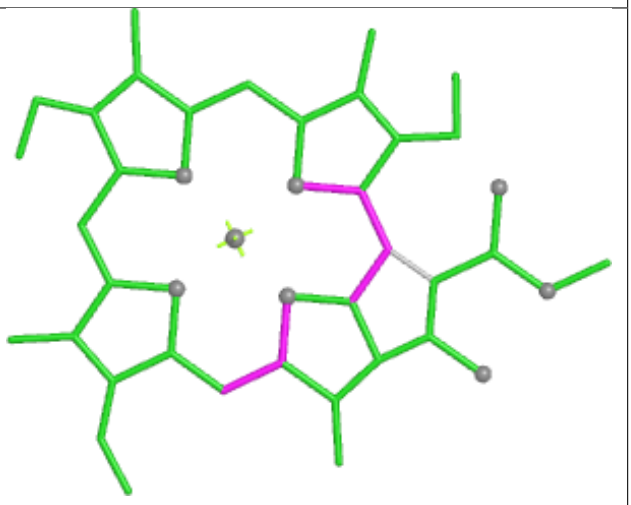


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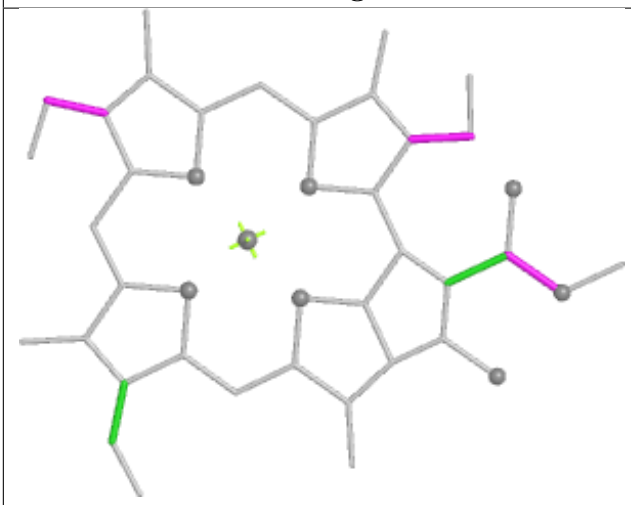
Ligand CLA 1 304



Bond lengths



Bond angles

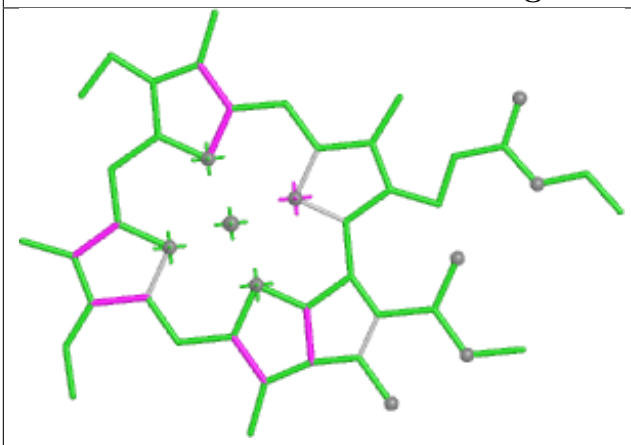


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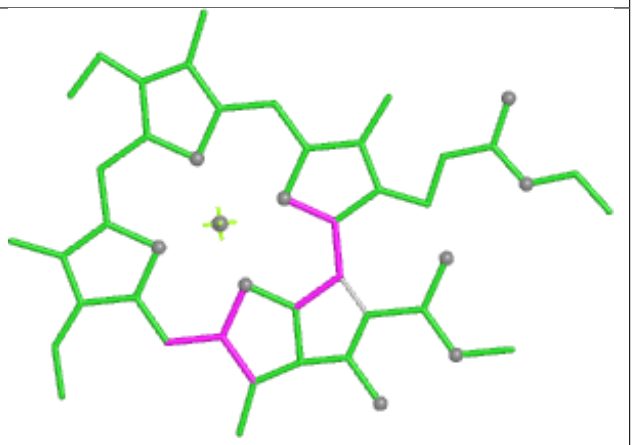


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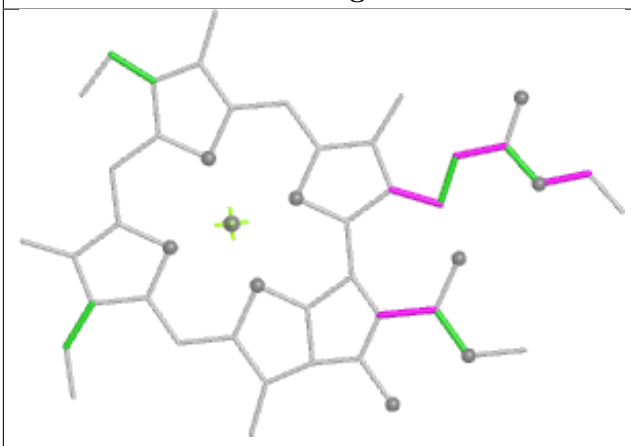
Ligand CLA B 837



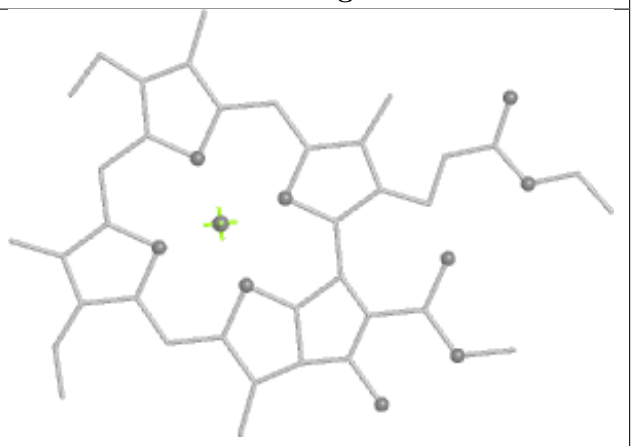
Bond lengths



Bond angles

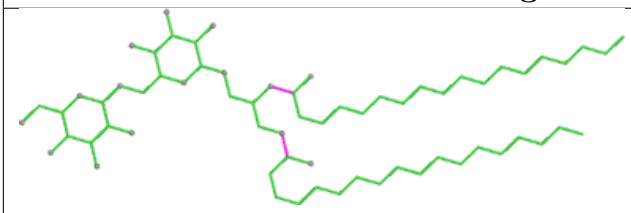


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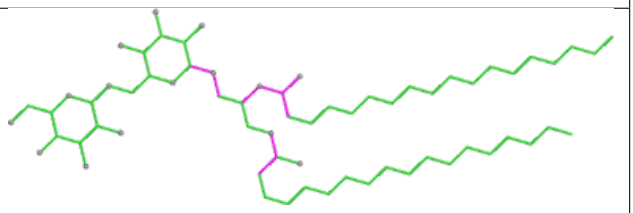


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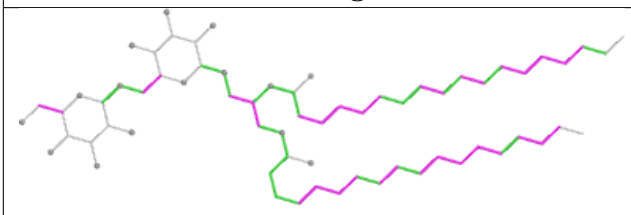
Ligand DGD B 847



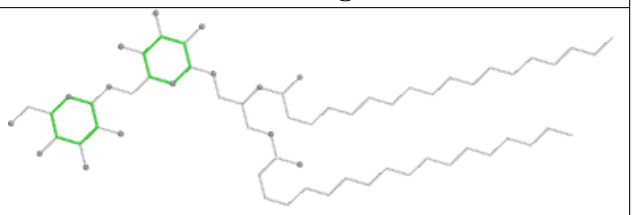
Bond lengths



Bond angles

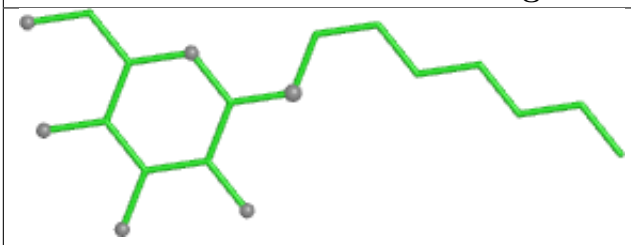


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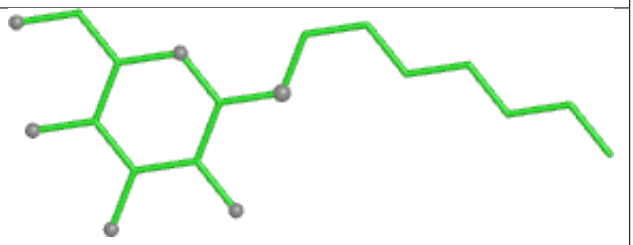


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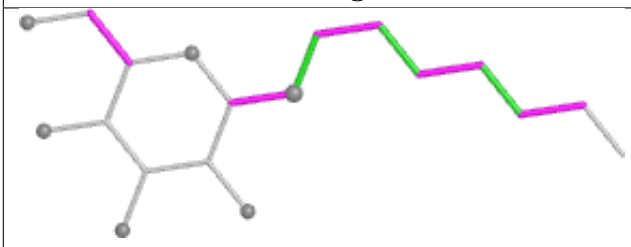
Ligand HTG F 303



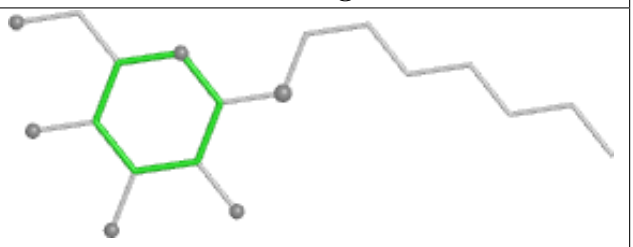
Bond lengths



Bond angles

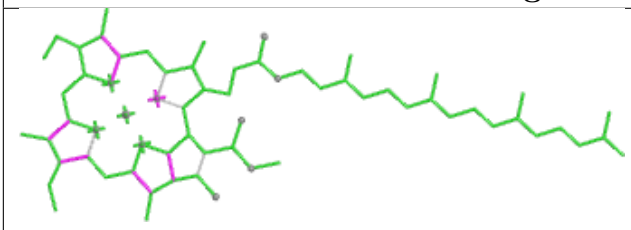


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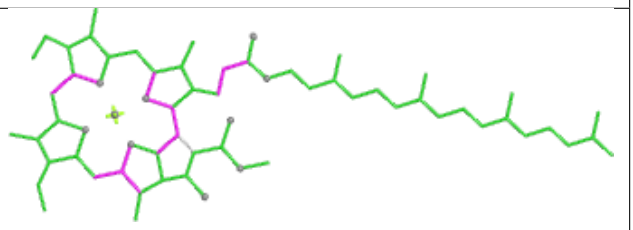


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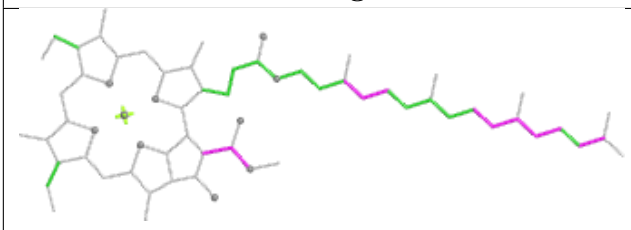
Ligand CLA A 836



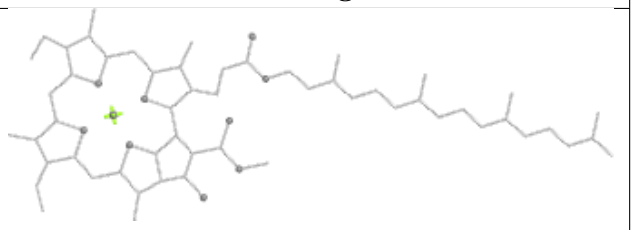
Bond lengths



Bond angles

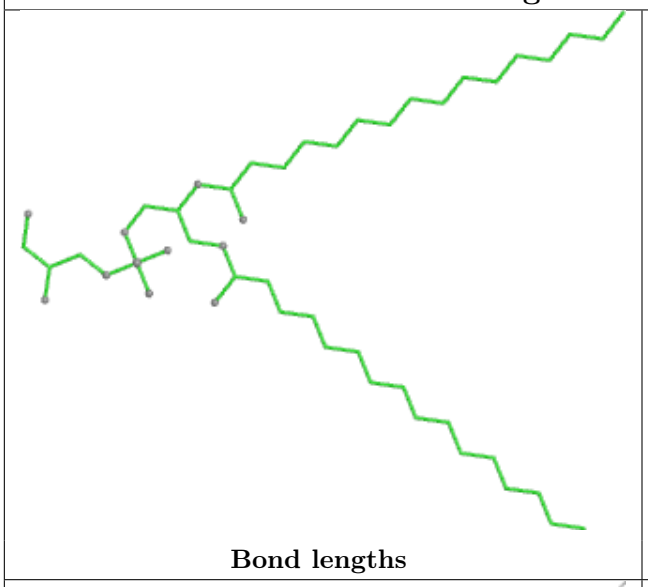


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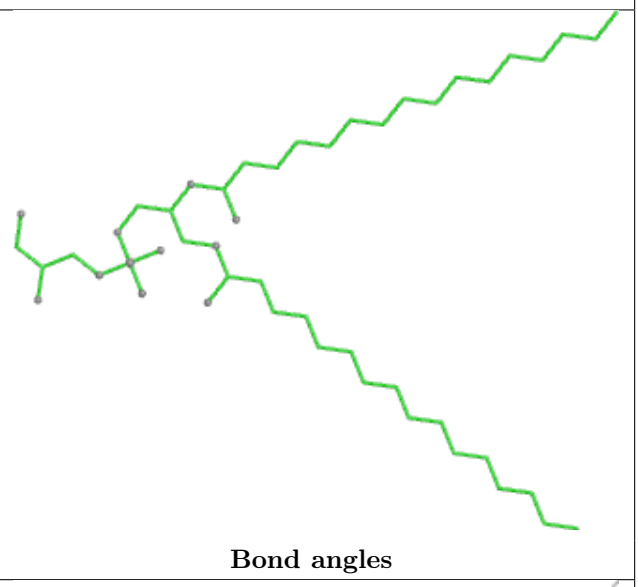


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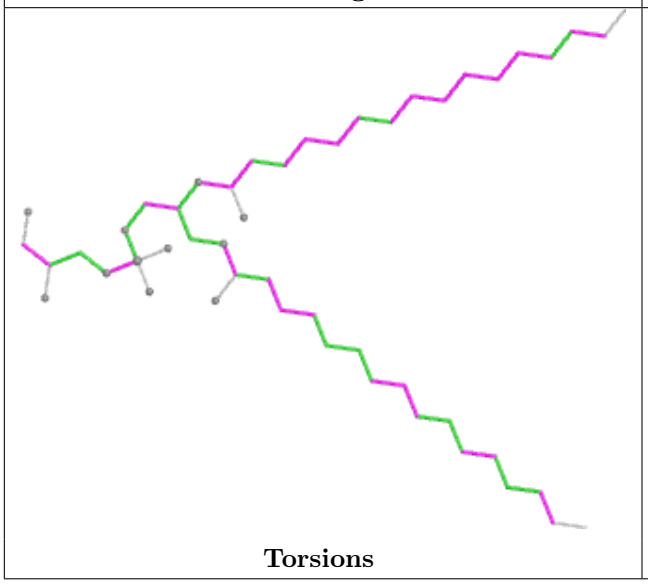
Ligand LHG A 842



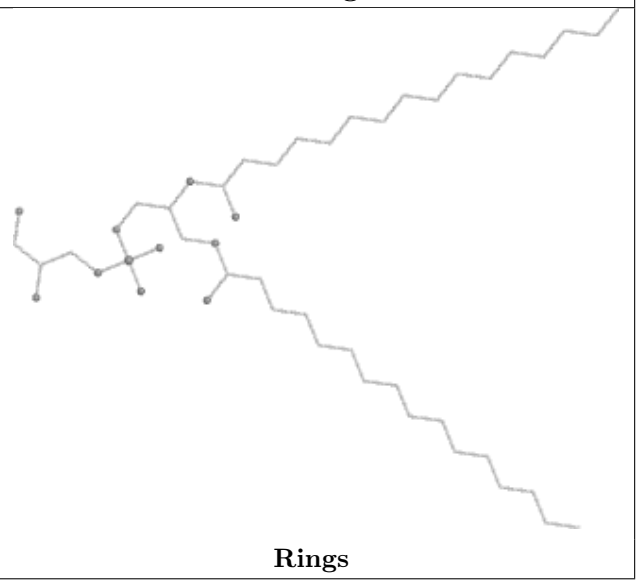
Bond lengths



Bond angles

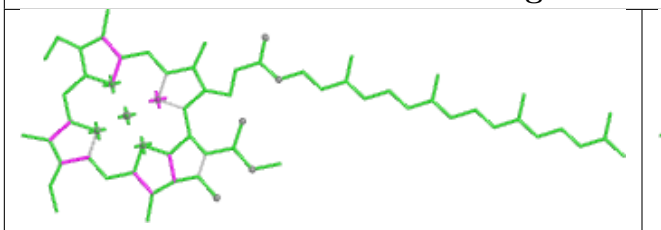


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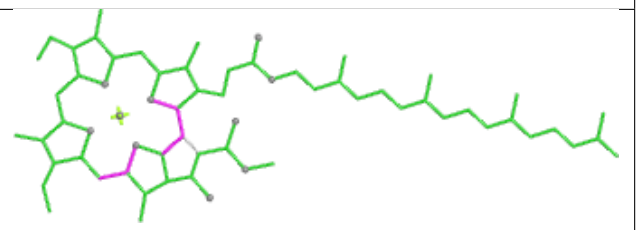


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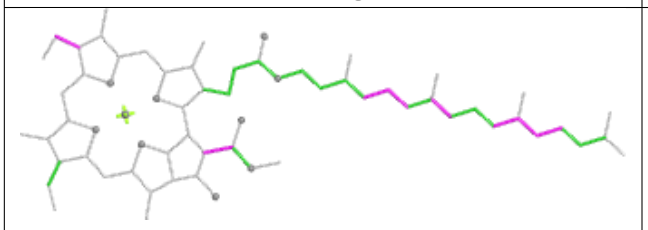
Ligand CLA B 807



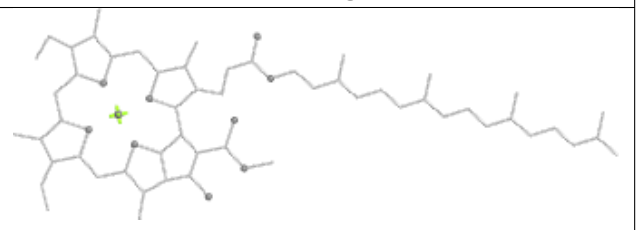
Bond lengths



Bond angles

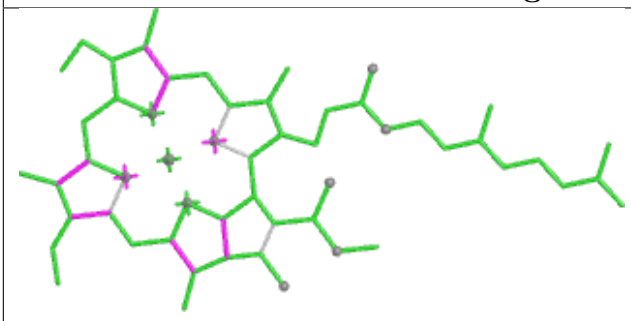


Torsions

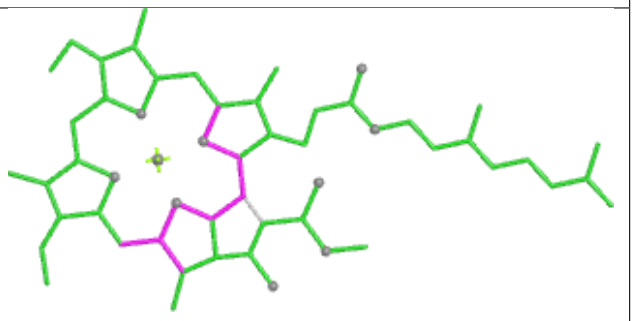


Rings

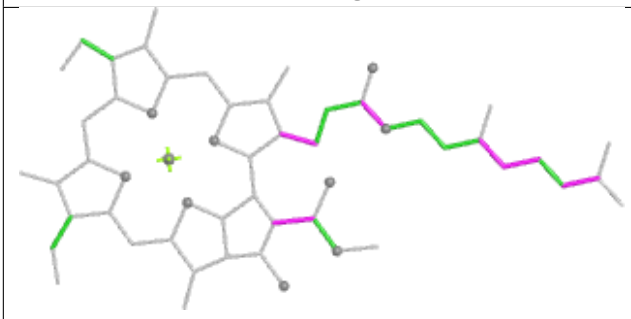
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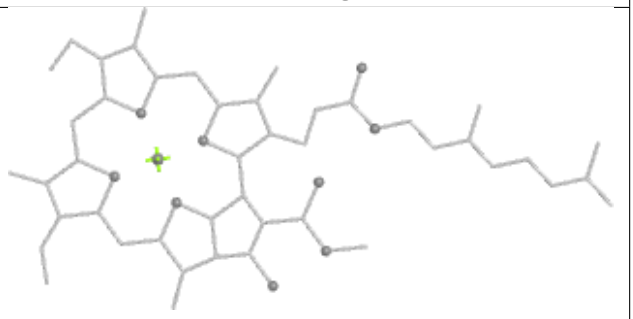
Bond lengths



Bond angles

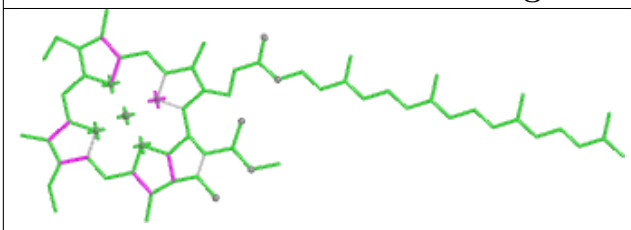


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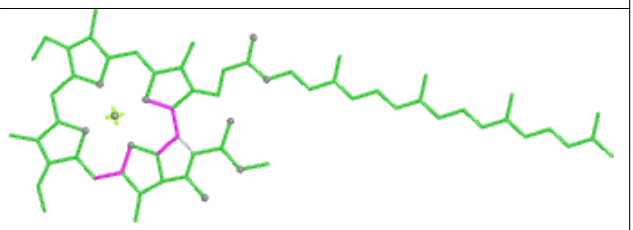


Rings

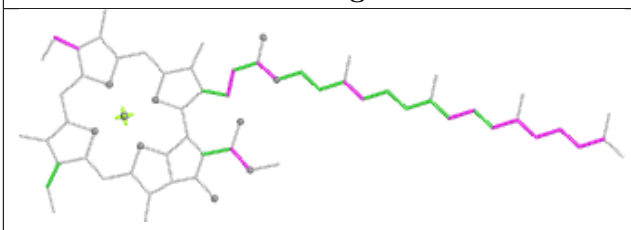
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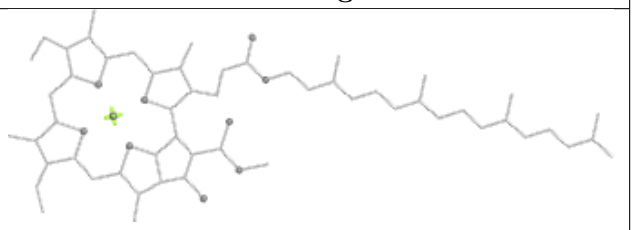
Bond lengths



Bond angles

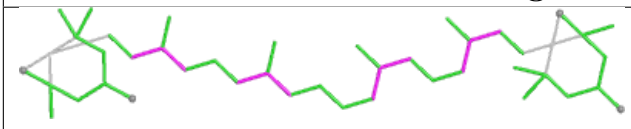


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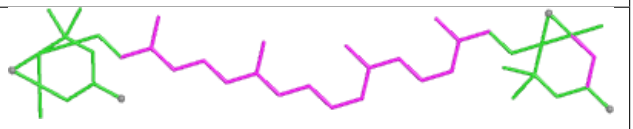


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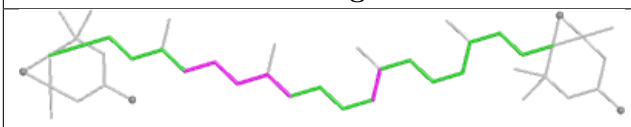
Ligand XAT 4 317



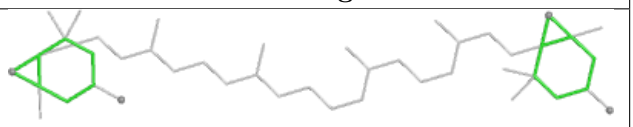
Bond lengths



Bond angles



Torsions

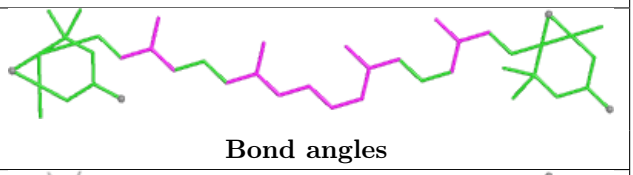


Rings

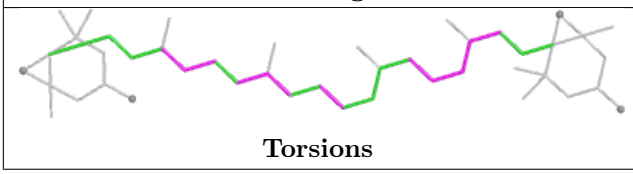
Ligand XAT 1 315



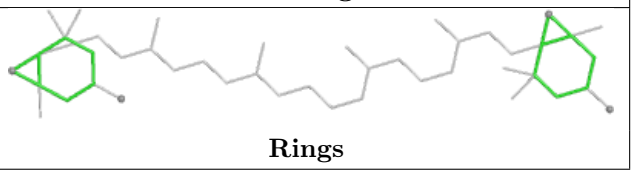
Bond lengths



Bond angles

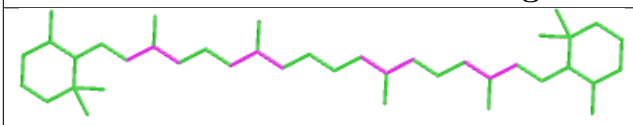


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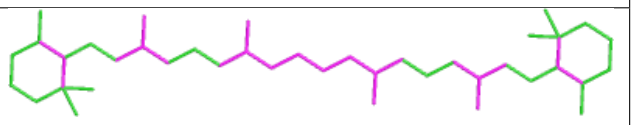


Rings

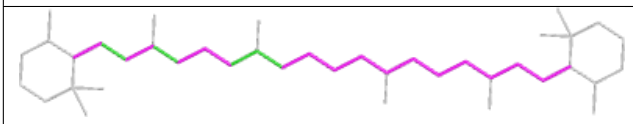
Ligand BCR O 106



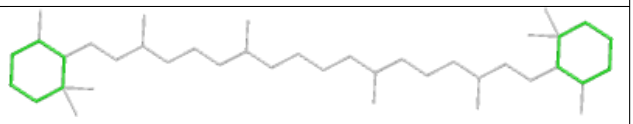
Bond lengths



Bond angles

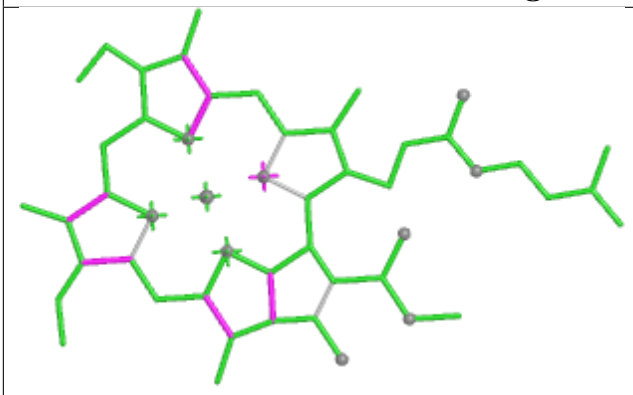


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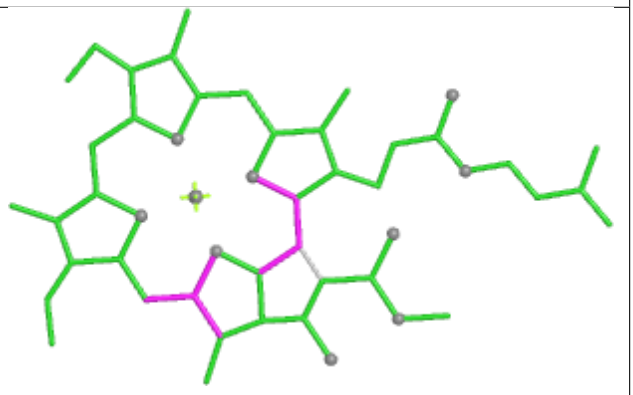


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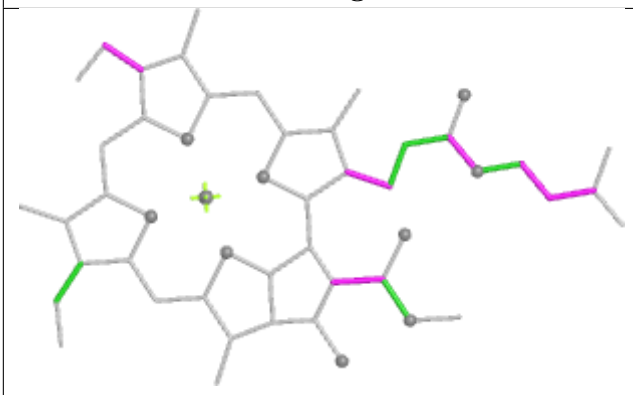
Ligand CLA B 830



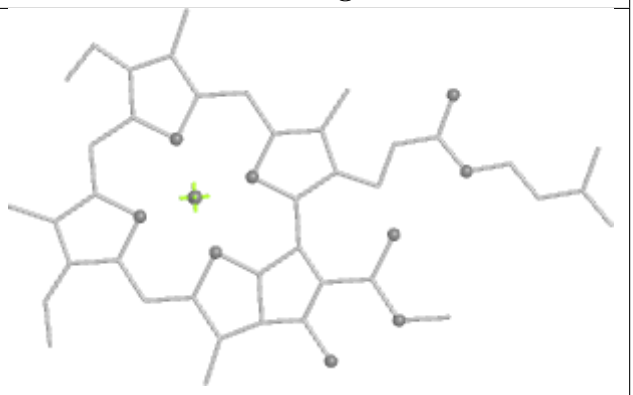
Bond lengths



Bond angles

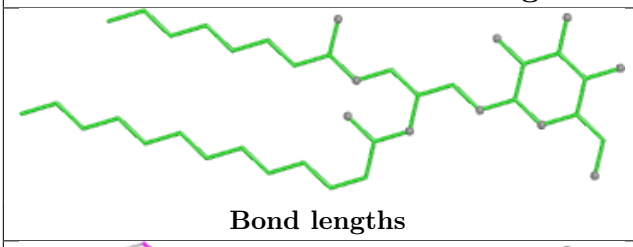


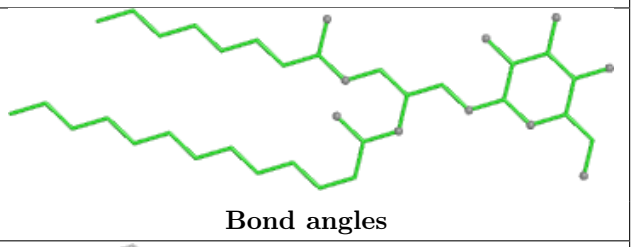
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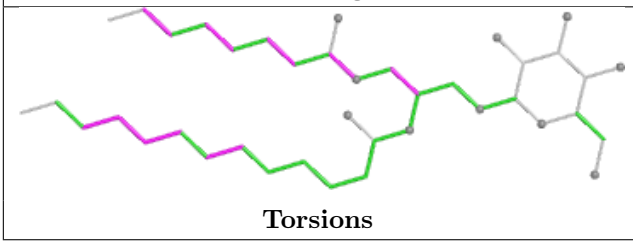


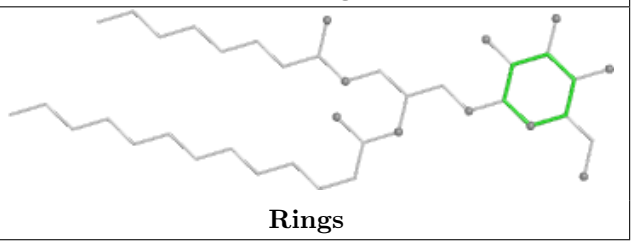
Rings

Ligand LMG F 309

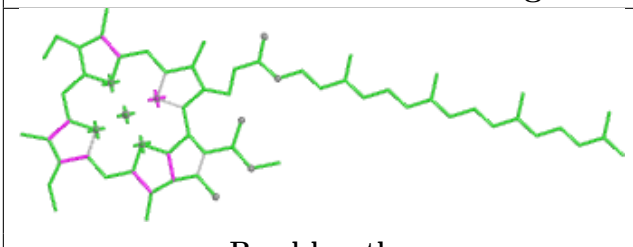

Bond lengths

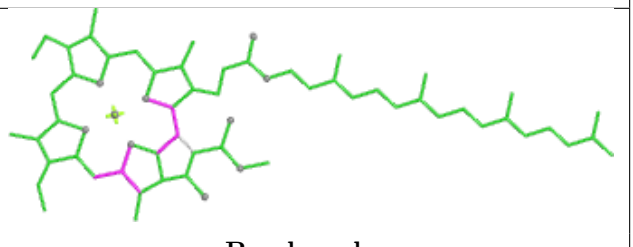

Bond angles

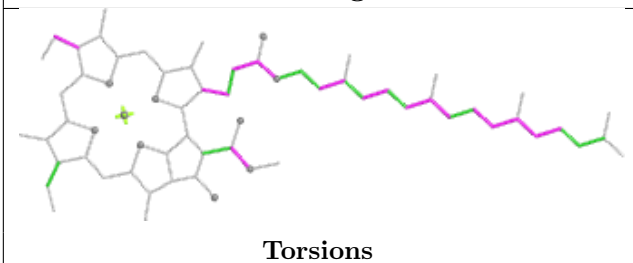

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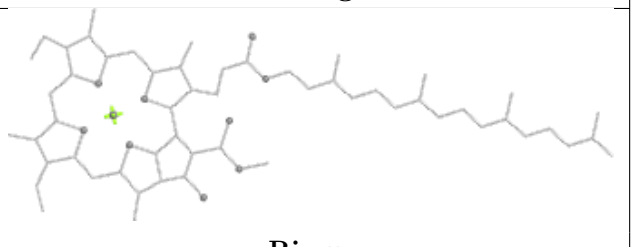

Rings

Ligand CLA B 833

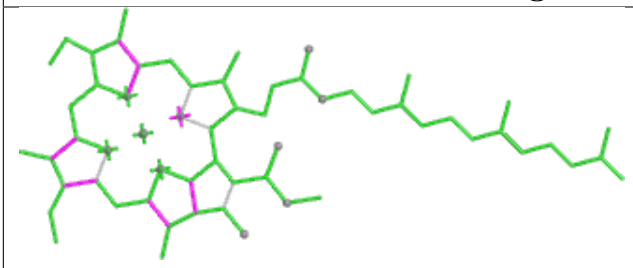

Bond lengths

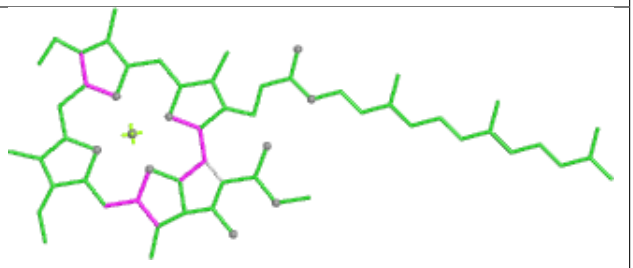

Bond angles

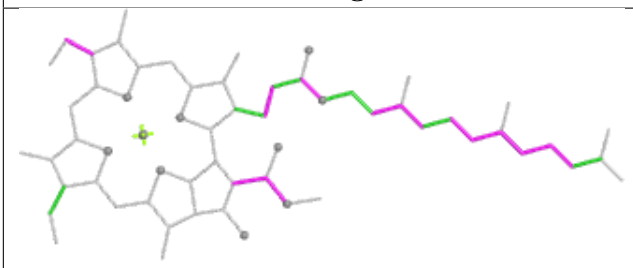

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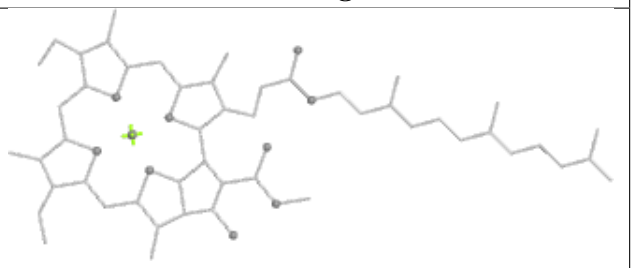

Rings

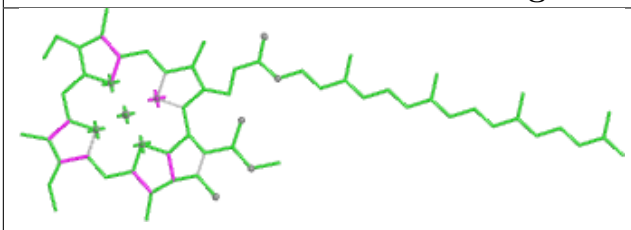
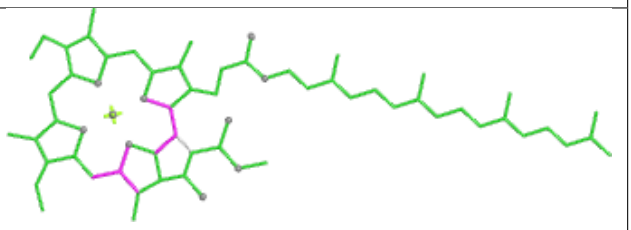
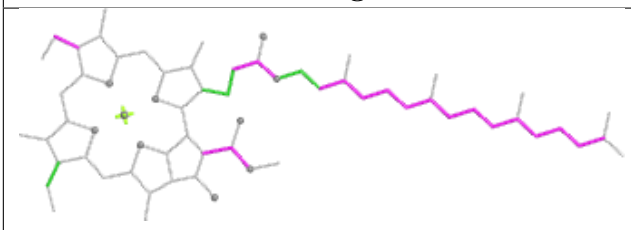
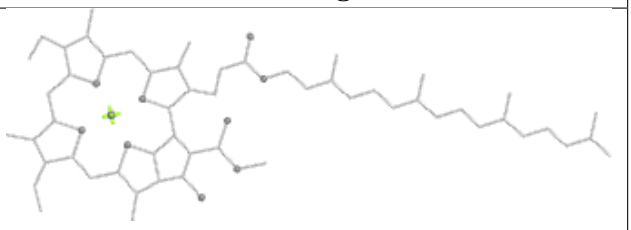
Ligand CLA 3 301

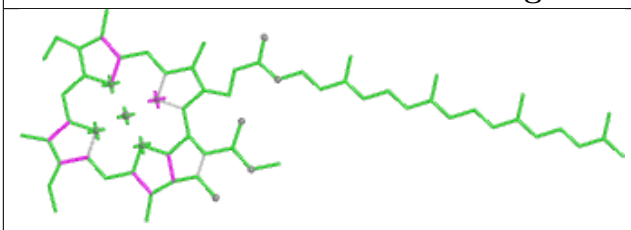
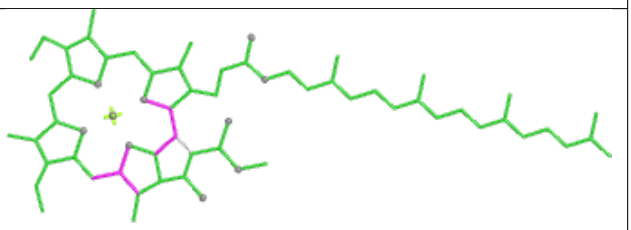
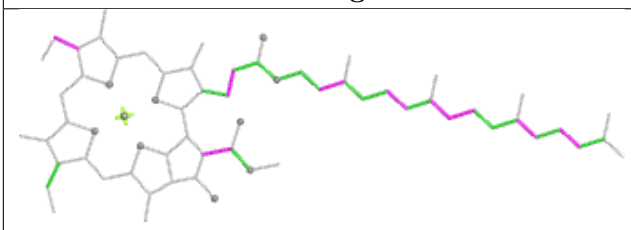
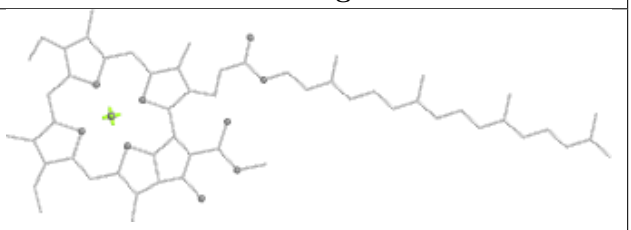

Bond lengths


Bond angles

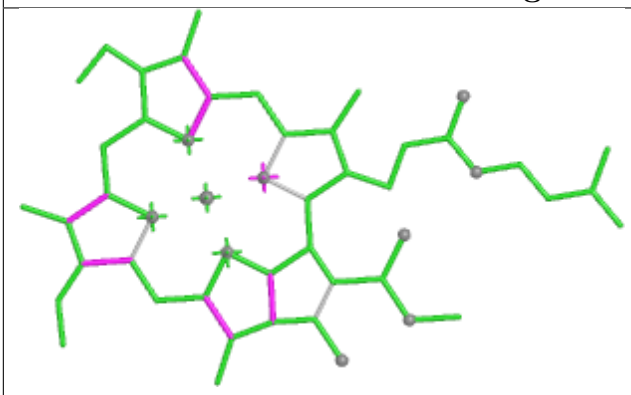

Torsions


Rings

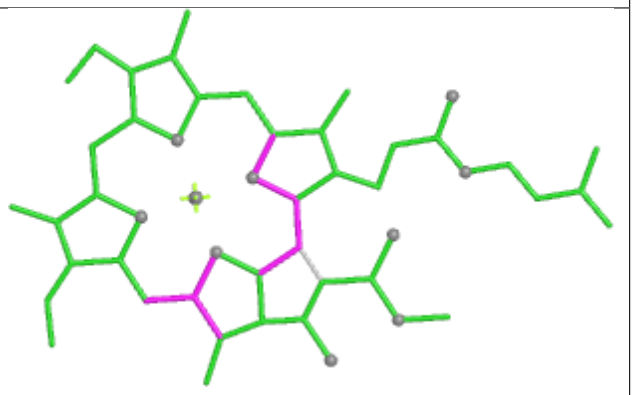
Ligand CLA 1 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

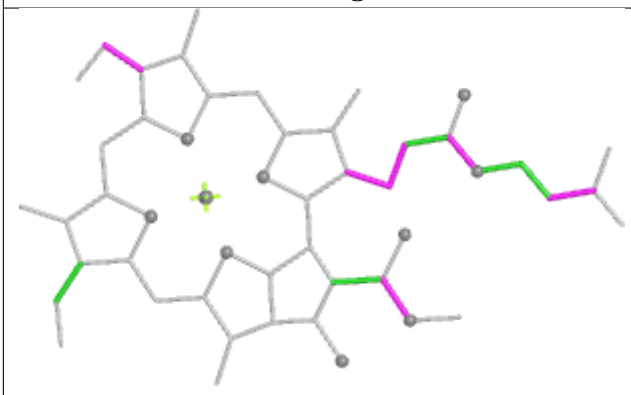
Ligand CLA A 813



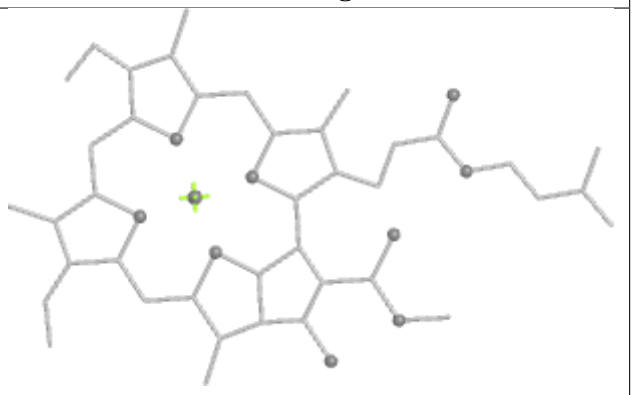
Bond lengths



Bond angles

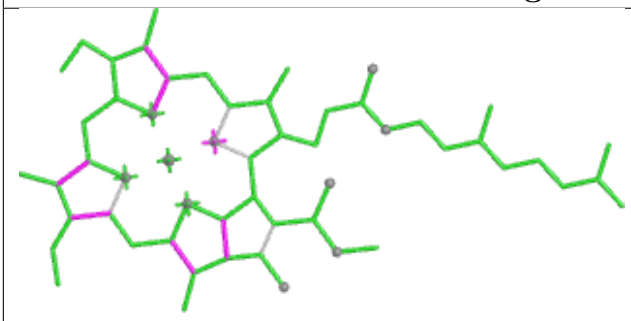


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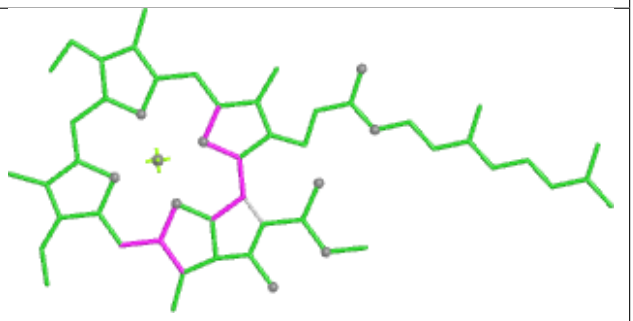


Rings

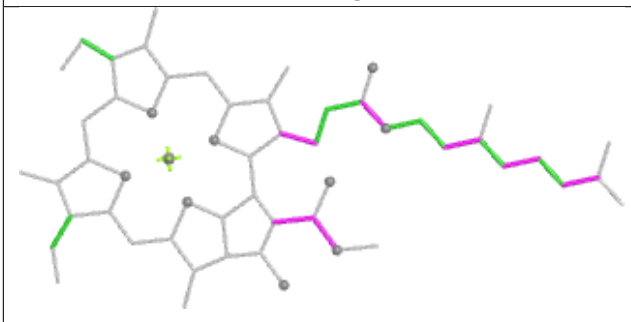
Ligand CLA B 815



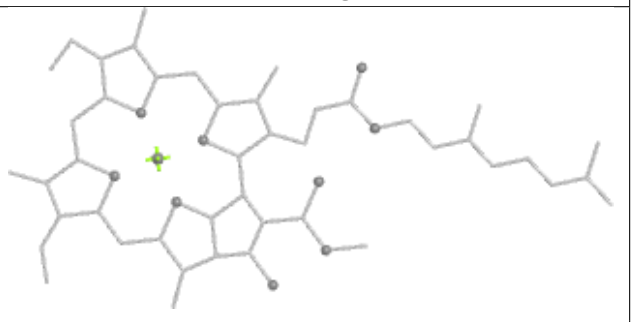
Bond lengths



Bond angles



Torsions

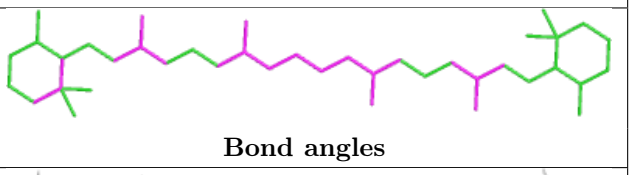


Rings

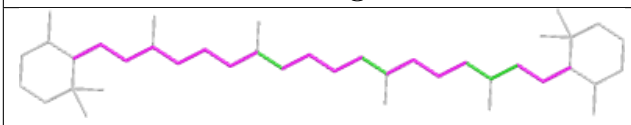
Ligand BCR G 206



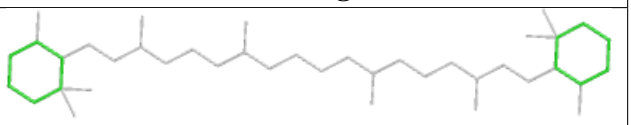
Bond lengths



Bond angles

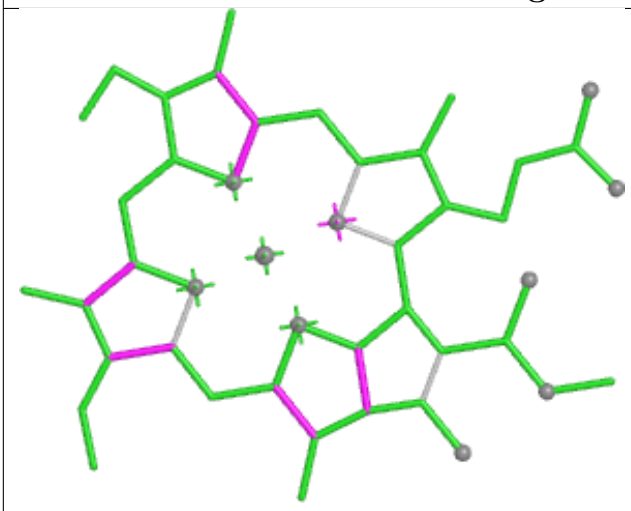


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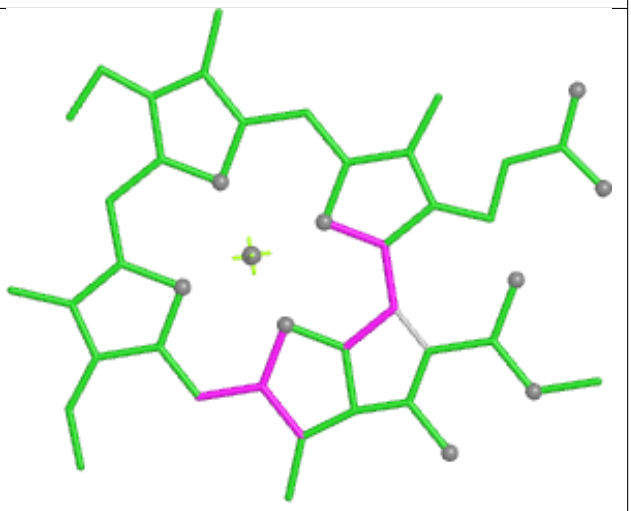


Rings

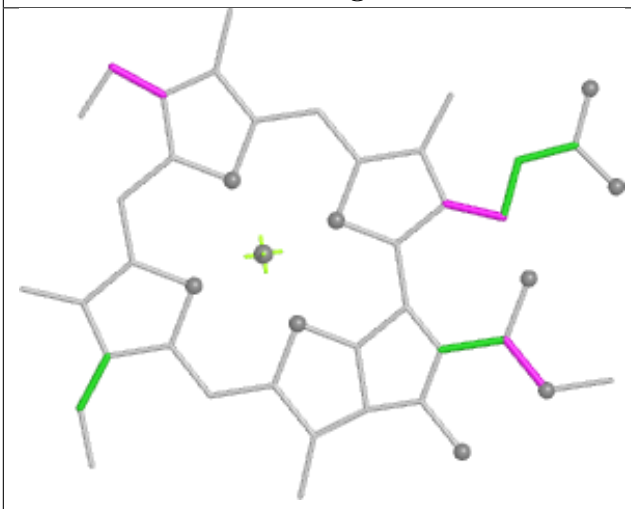
Ligand CLA 3 316



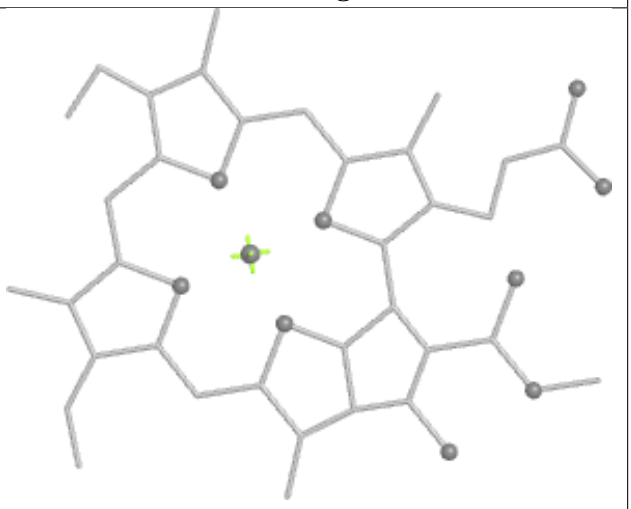
Bond lengths



Bond angles



Torsions

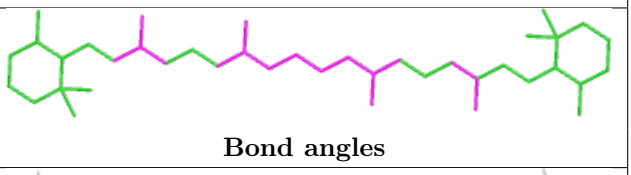


Rings

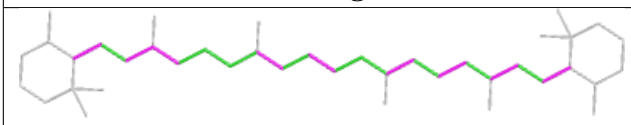
Ligand BCR A 847



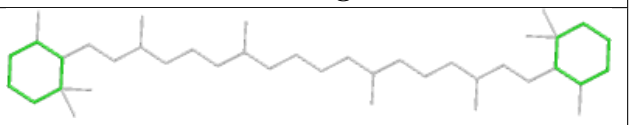
Bond lengths



Bond angles

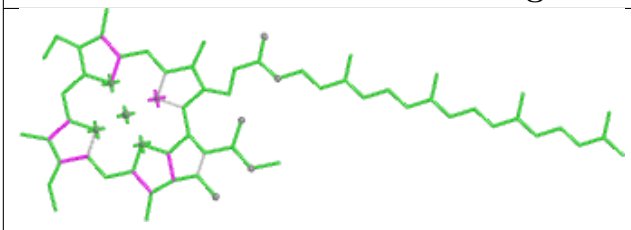


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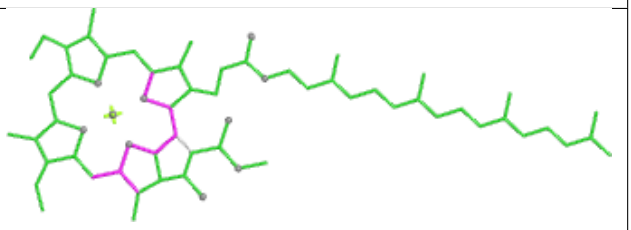


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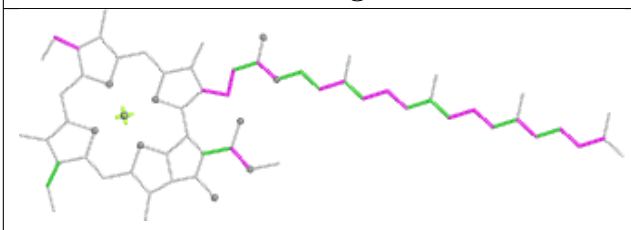
Ligand CLA L 302



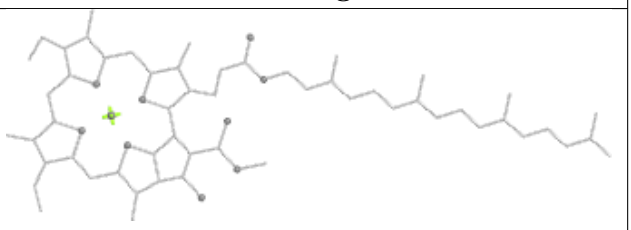
Bond lengths



Bond angles

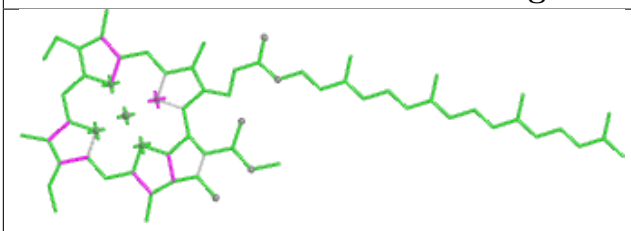


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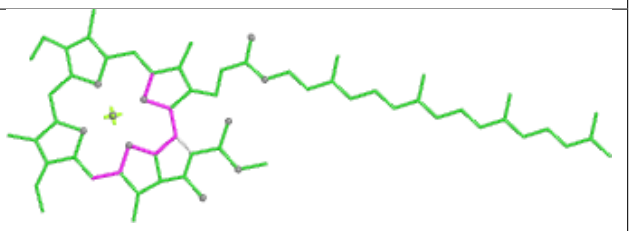


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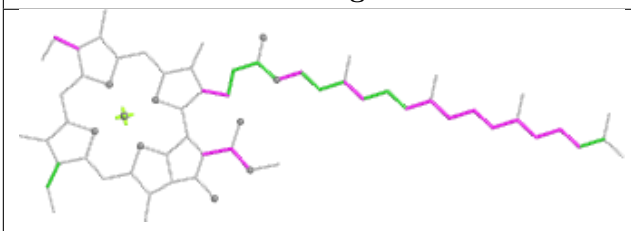
Ligand CLA 1 307



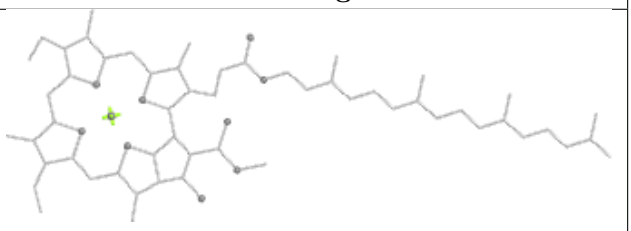
Bond lengths



Bond angles

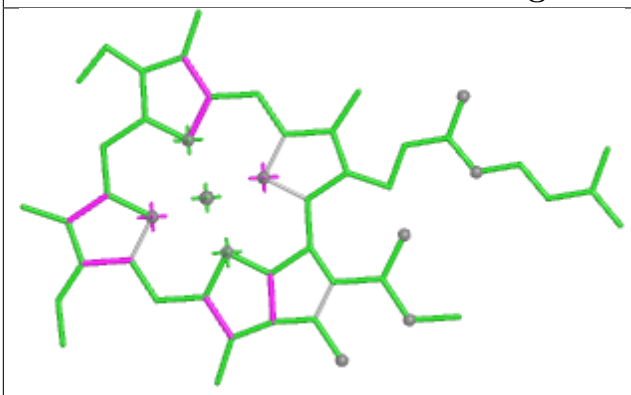


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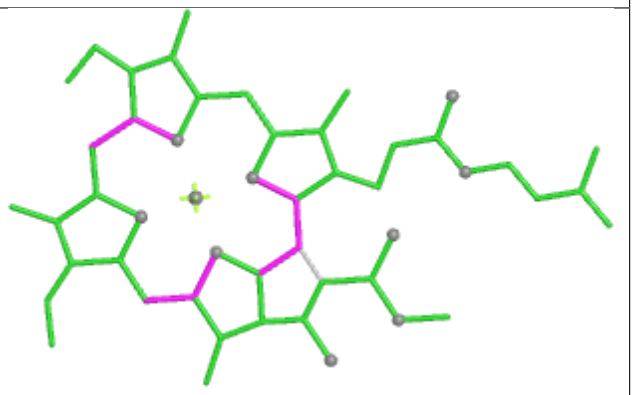


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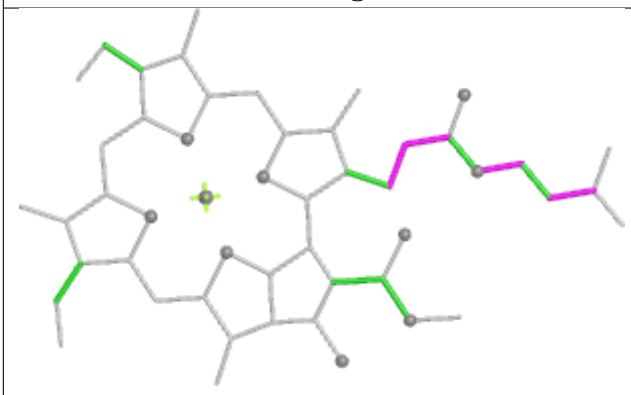
Ligand CLA 3 302



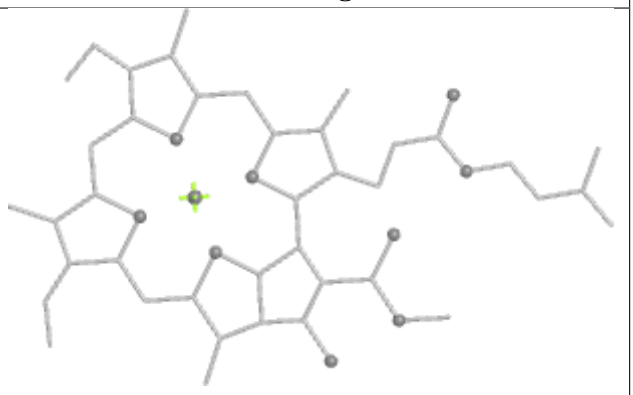
Bond lengths



Bond angles

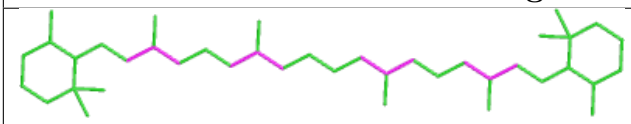


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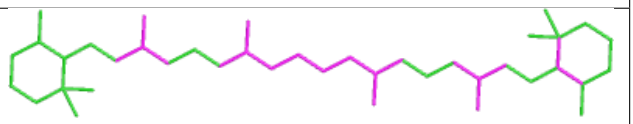


Rings

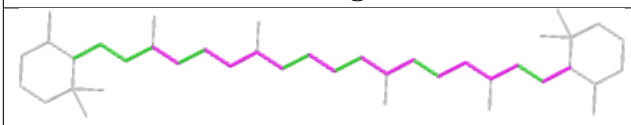
Ligand BCR J 103



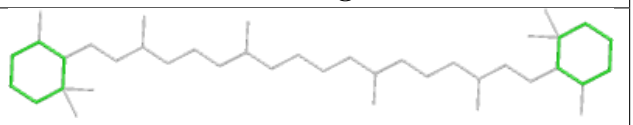
Bond lengths



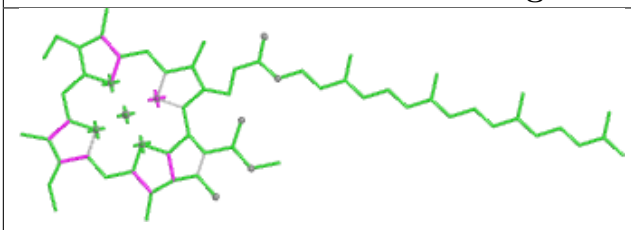
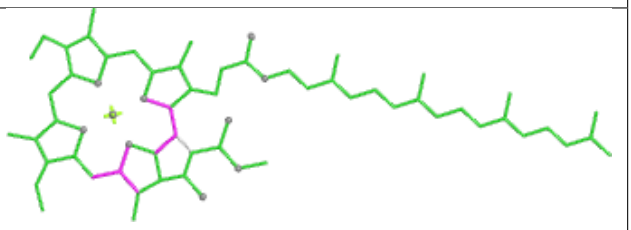
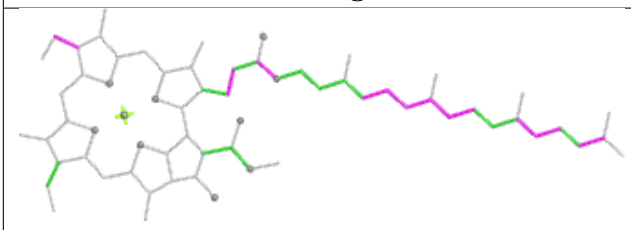
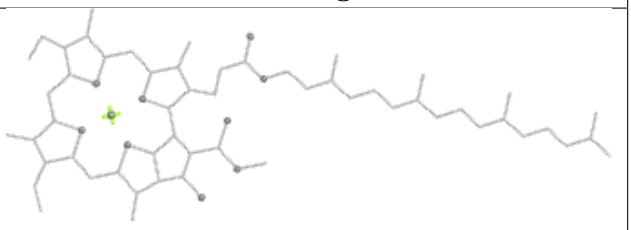
Bond angles

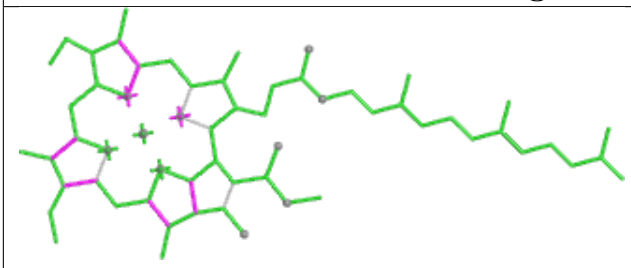
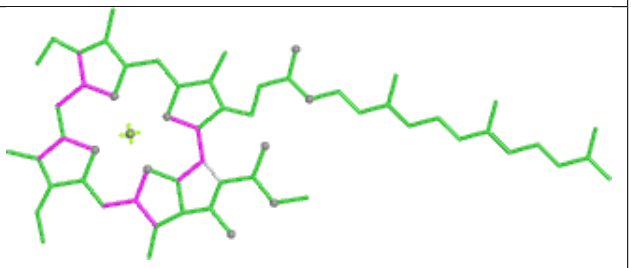
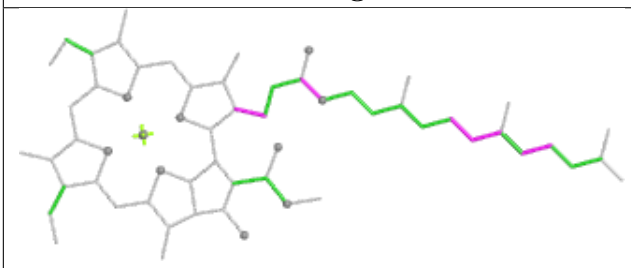
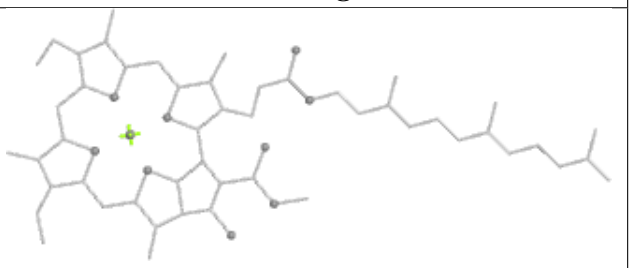


Torsions

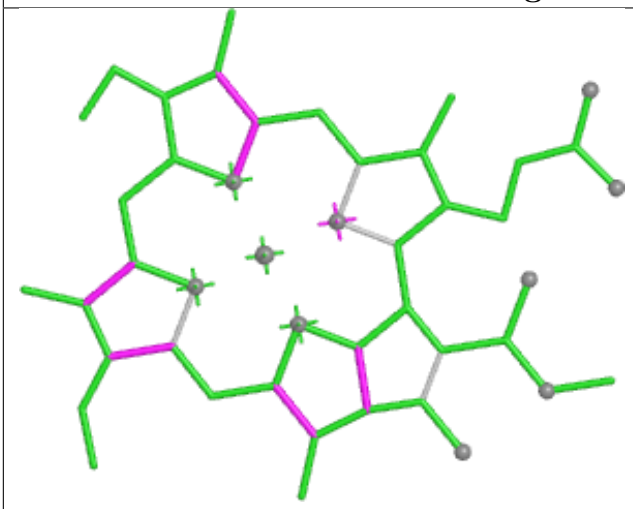


Rings

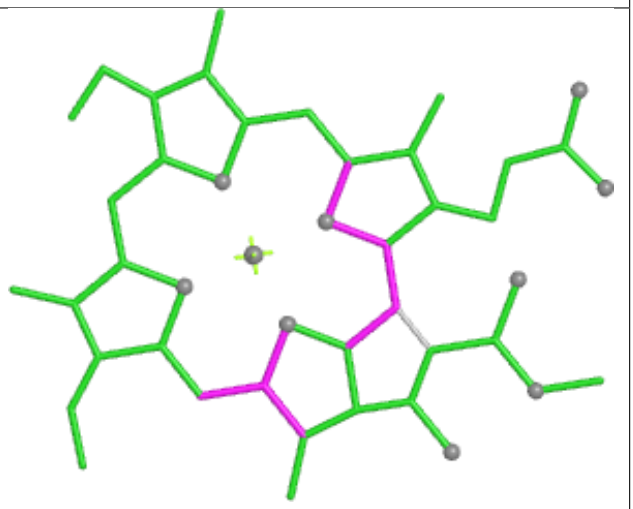
Ligand CLA L 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

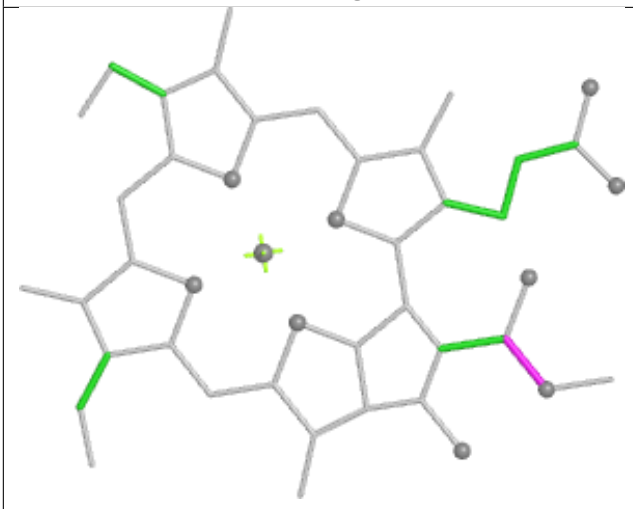
Ligand CLA B 834



Bond lengths



Bond angles

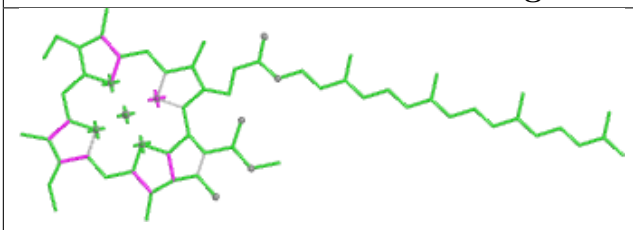


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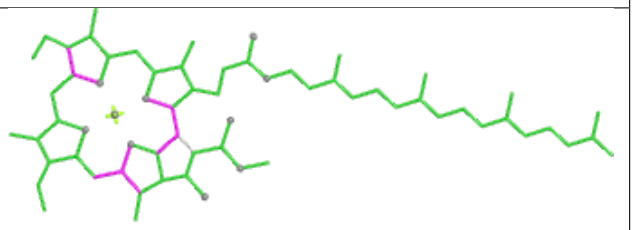


Rings

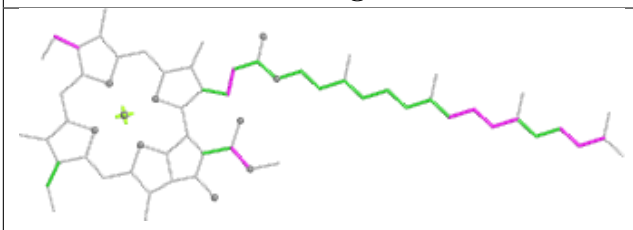
Ligand CLA B 803



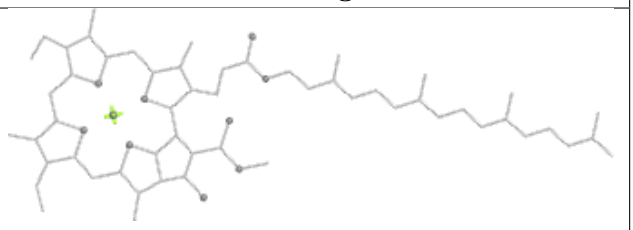
Bond lengths



Bond angles

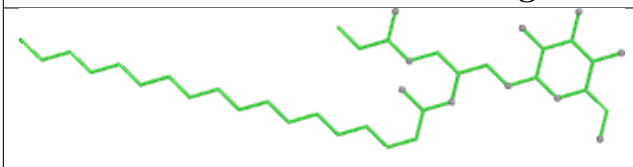


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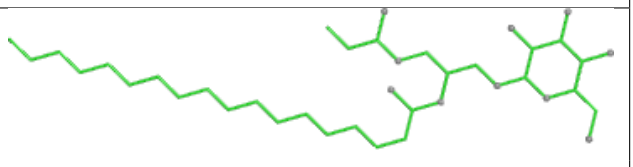


Rings

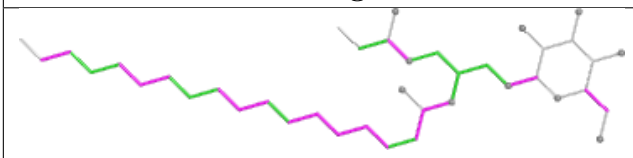
Ligand LMG G 202



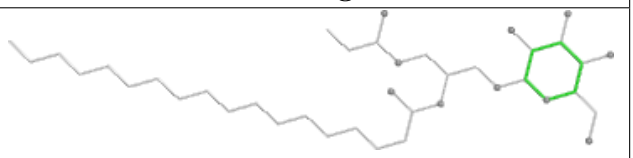
Bond lengths



Bond angles

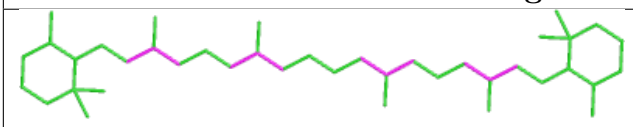


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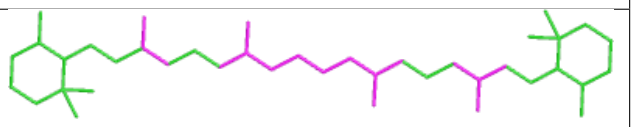


Rings

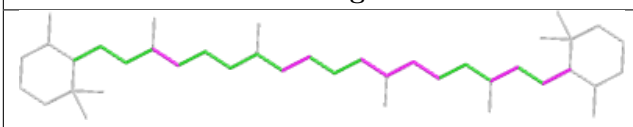
Ligand BCR L 306



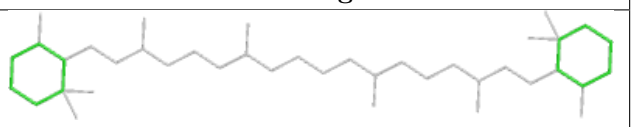
Bond lengths



Bond angles

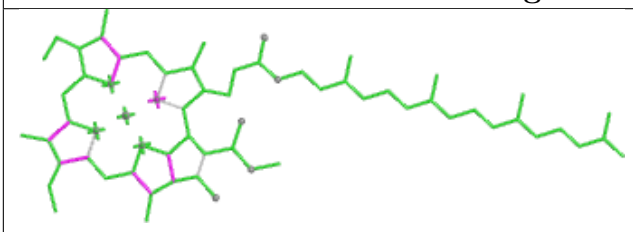


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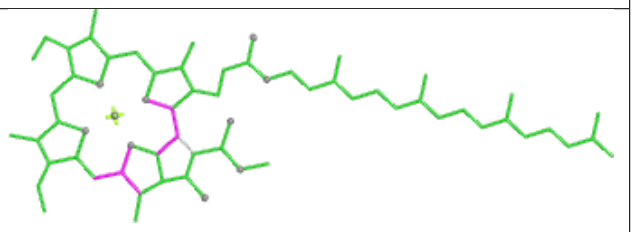


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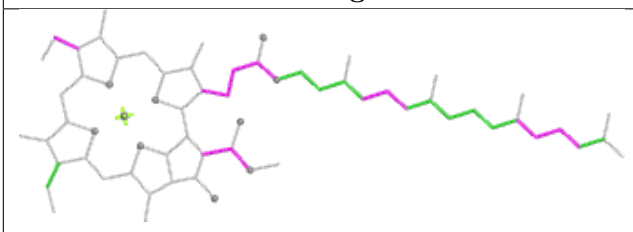
Ligand CLA A 806



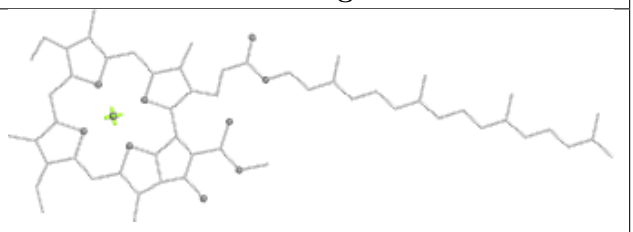
Bond lengths



Bond angles

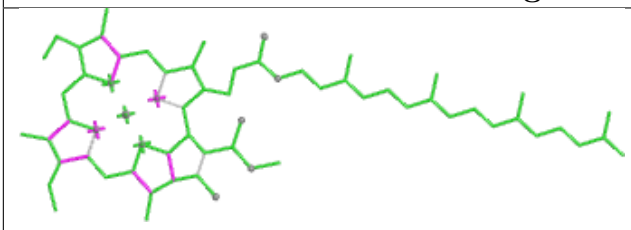


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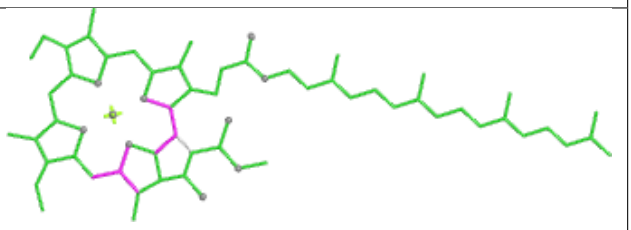


Rings

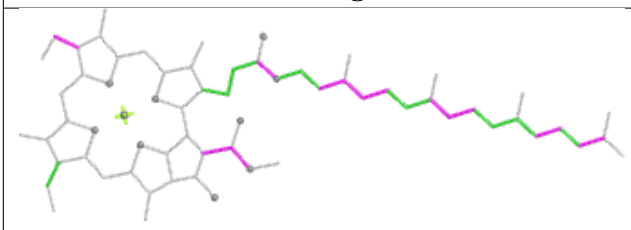
Ligand CLA A 831



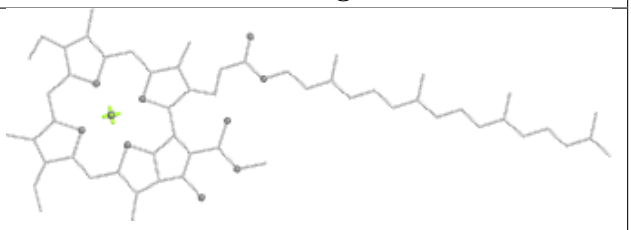
Bond lengths



Bond angles

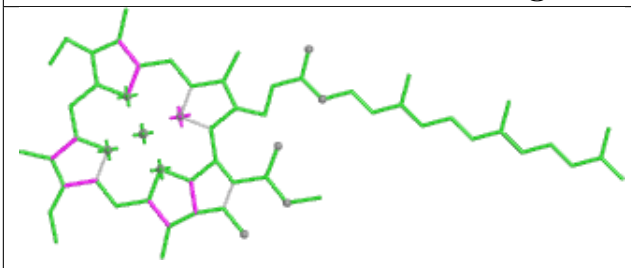


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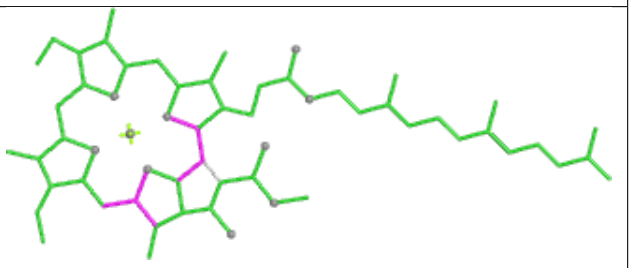


Rings

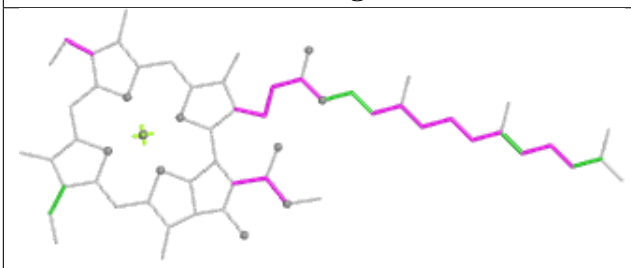
Ligand CLA 2 303



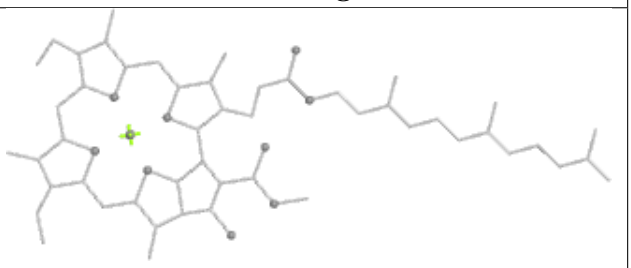
Bond lengths



Bond angles



Torsions

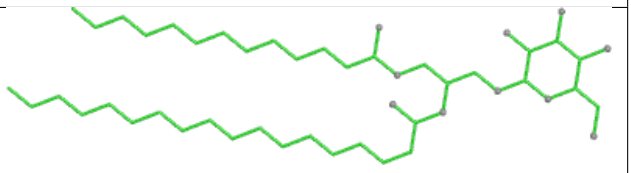


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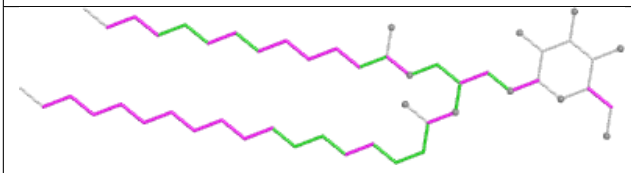
Ligand LMG 4 319



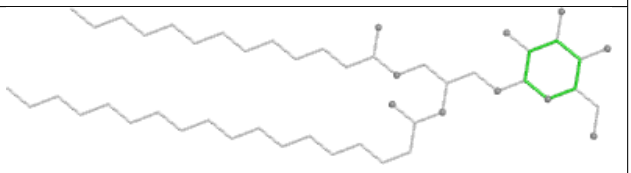
Bond lengths



Bond angles

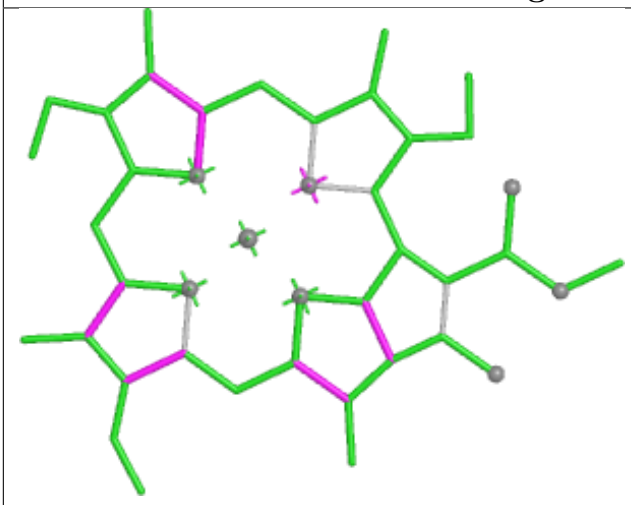


Torsions

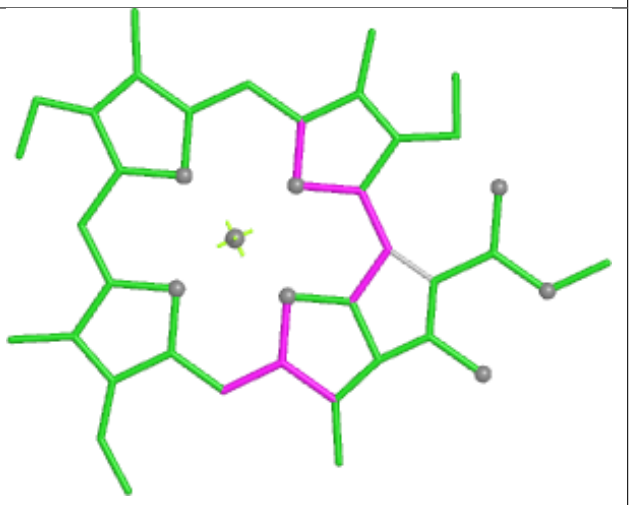


Rings

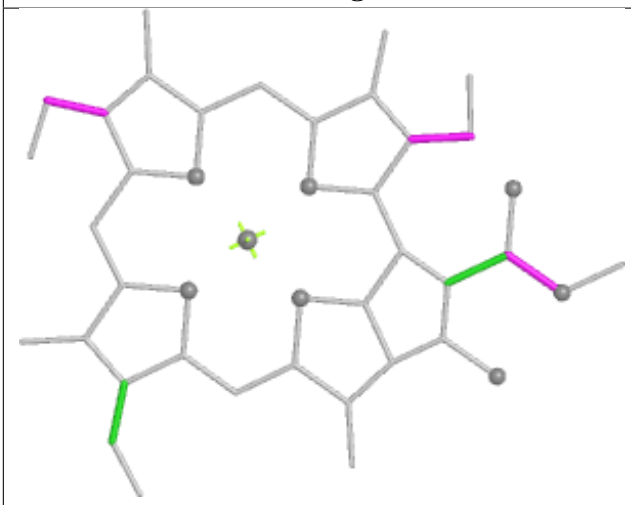
Ligand CLA J 102



Bond lengths



Bond angles

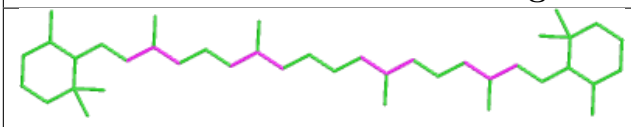


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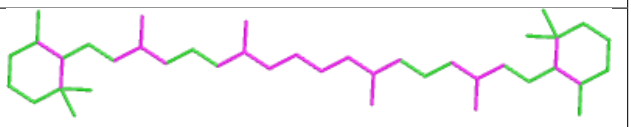


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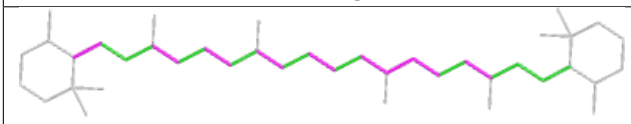
Ligand BCR I 101



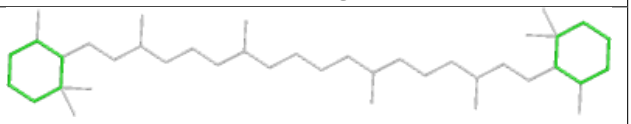
Bond lengths



Bond angles

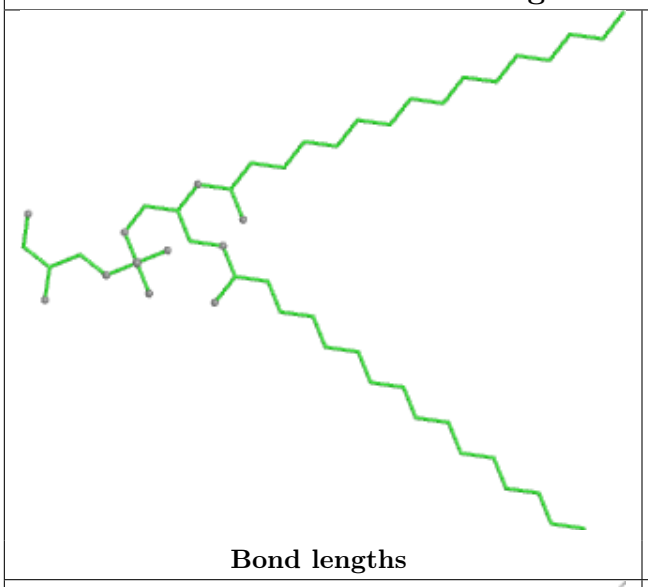


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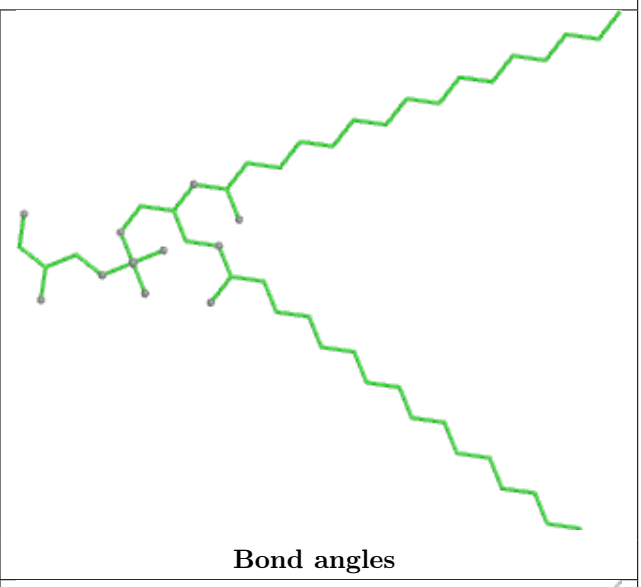


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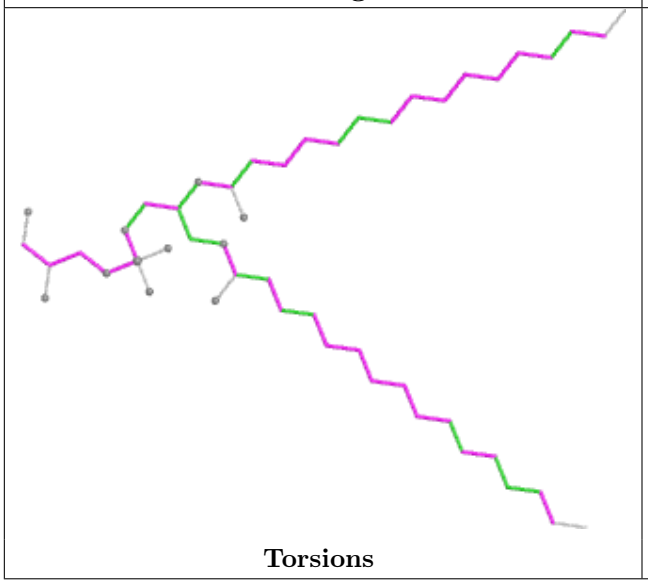
Ligand LHG 4 320



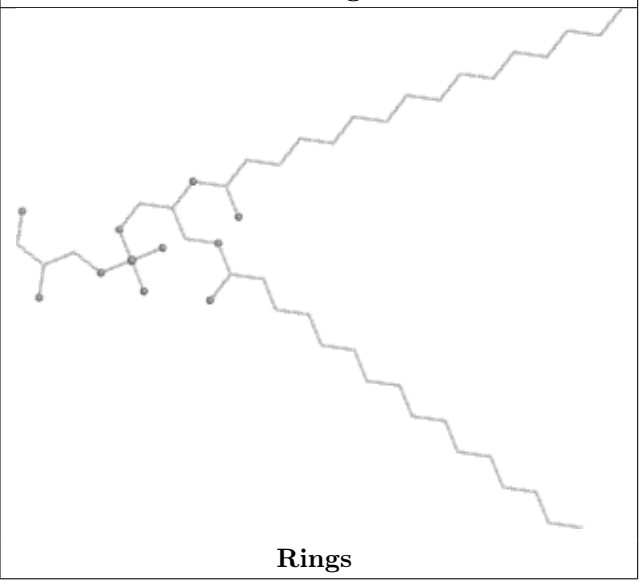
Bond lengths



Bond angles

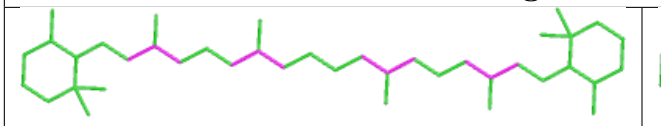


Torsions



Rings

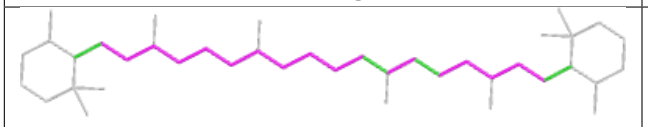
Ligand BCR K 304



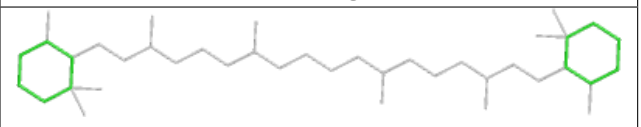
Bond lengths



Bond angles

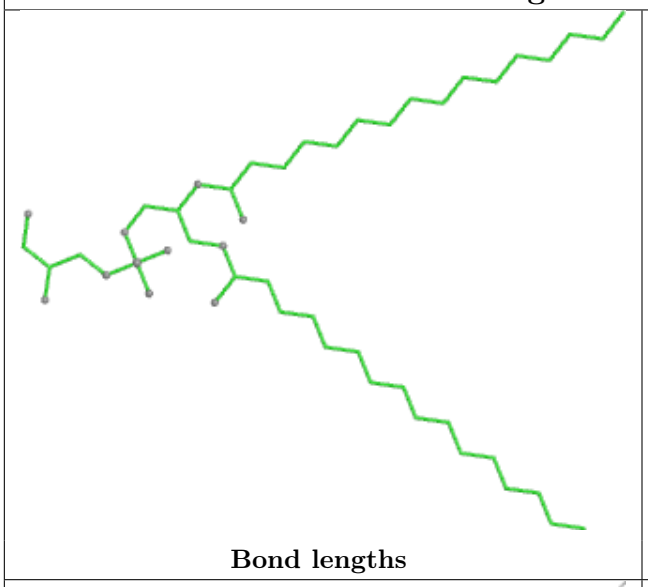


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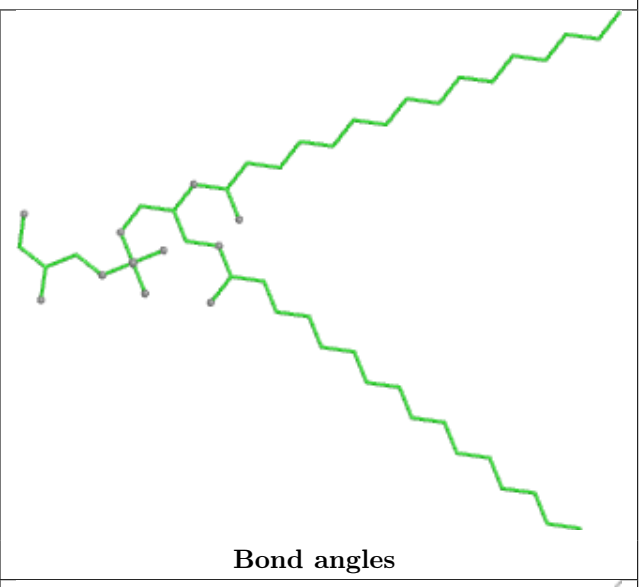


Rings

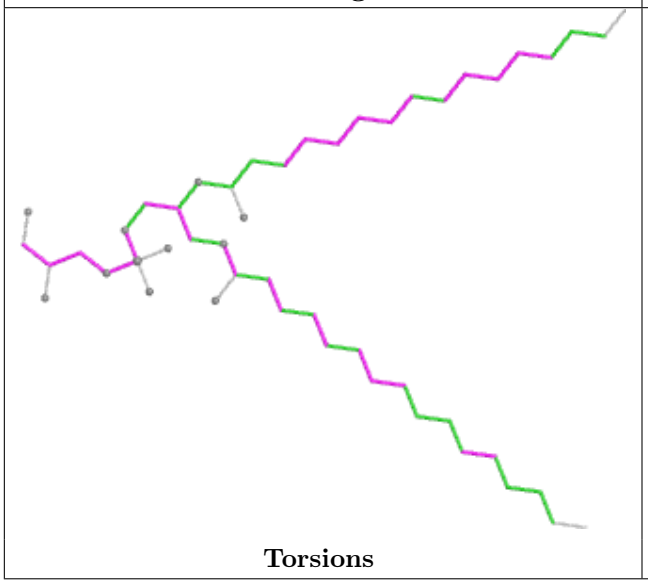
Ligand LHG 1 317



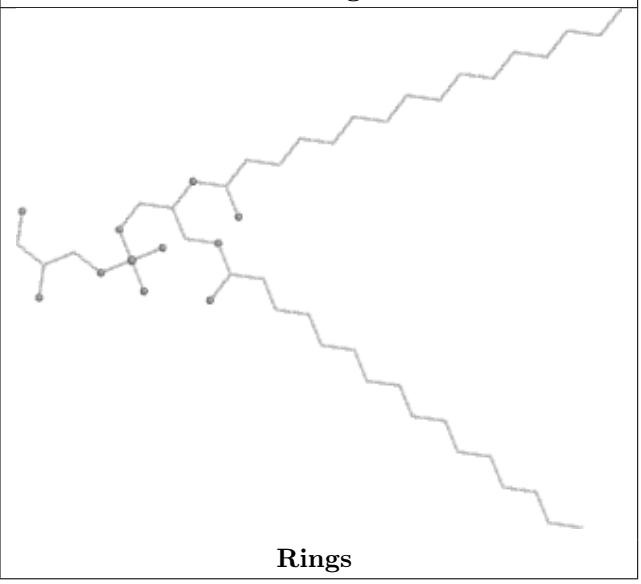
Bond lengths



Bond angles

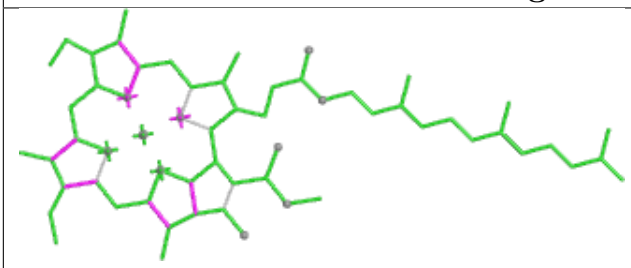


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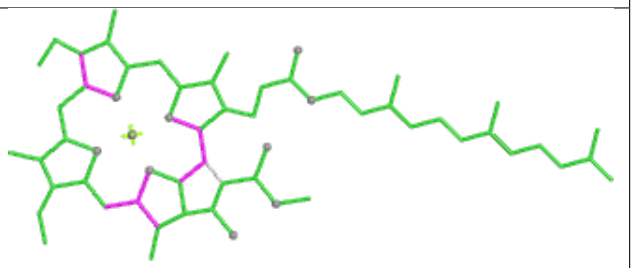


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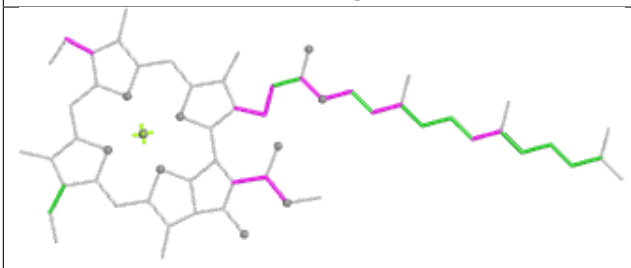
Ligand CLA 4 302



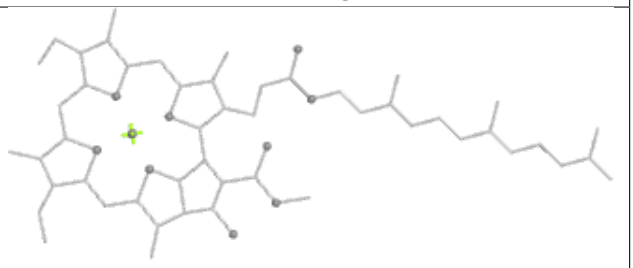
Bond lengths



Bond angles

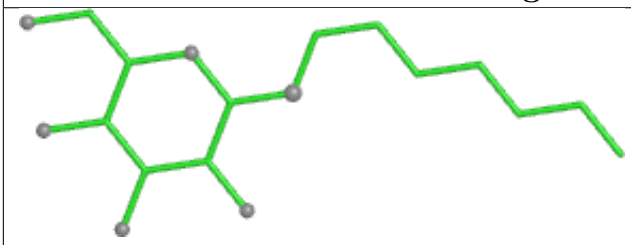


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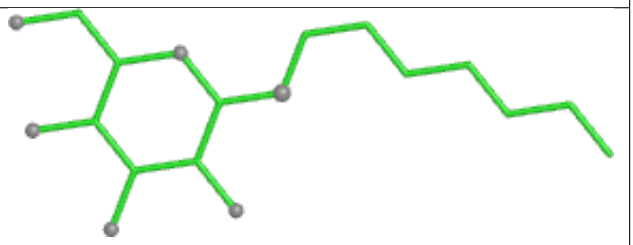


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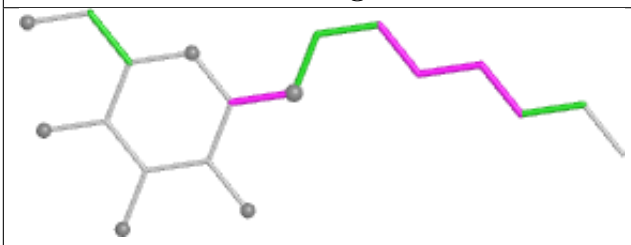
Ligand HTG F 305



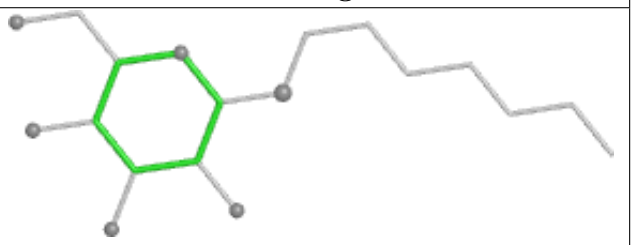
Bond lengths



Bond angles

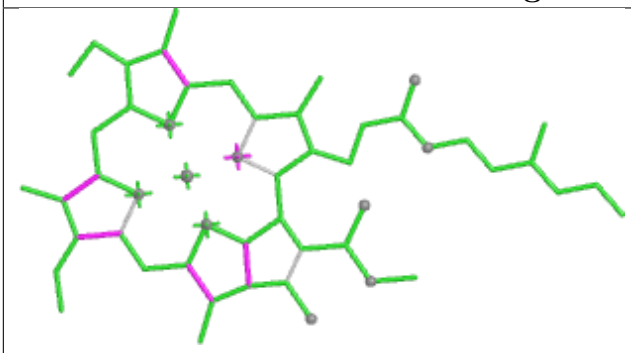


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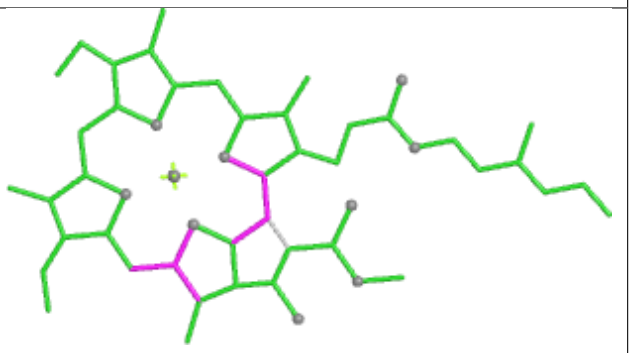


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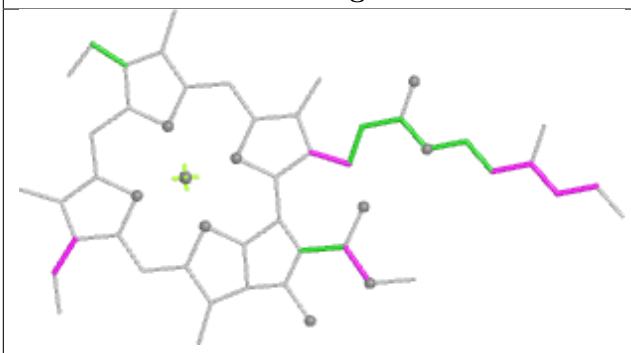
Ligand CLA O 103



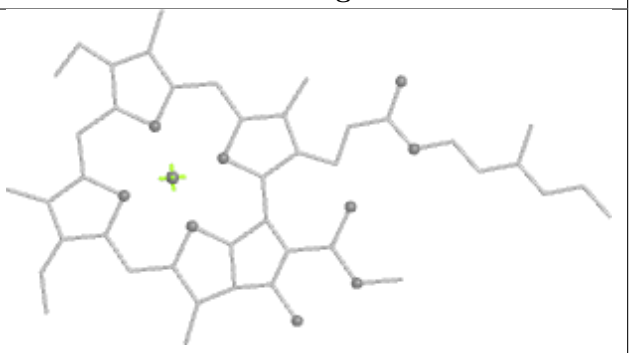
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Bond angles

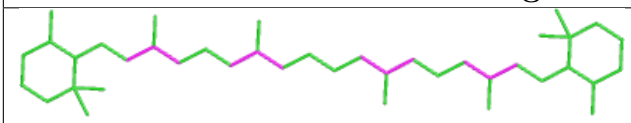


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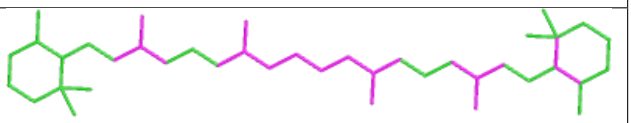


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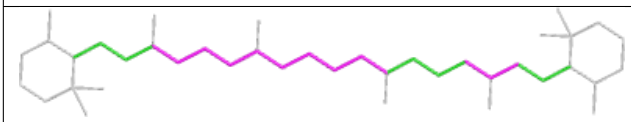
Ligand BCR B 843



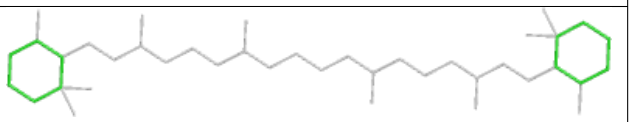
Bond lengths



Bond angles

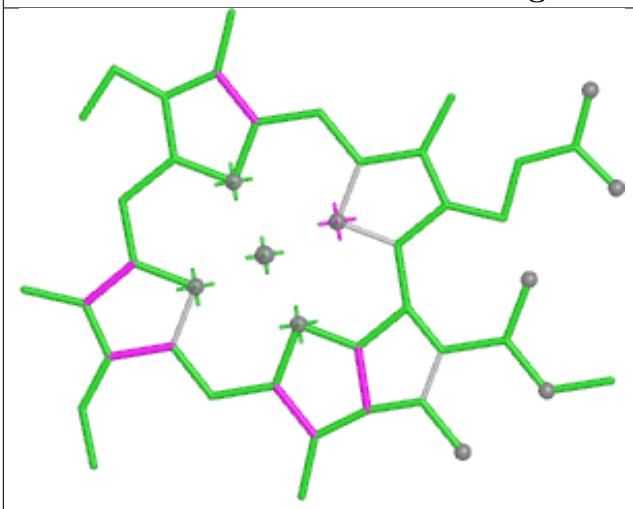


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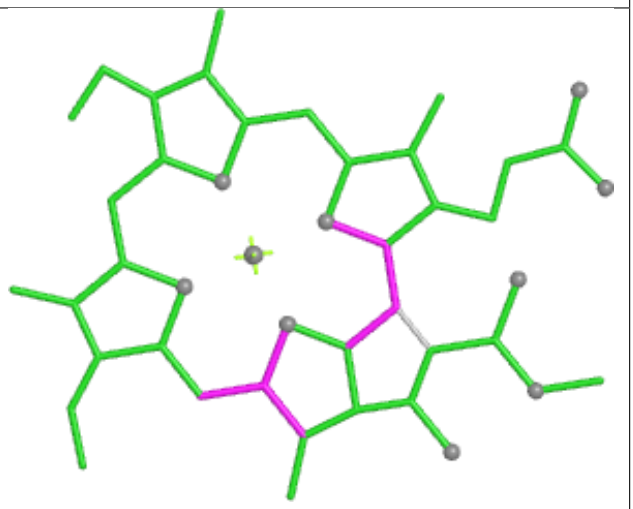


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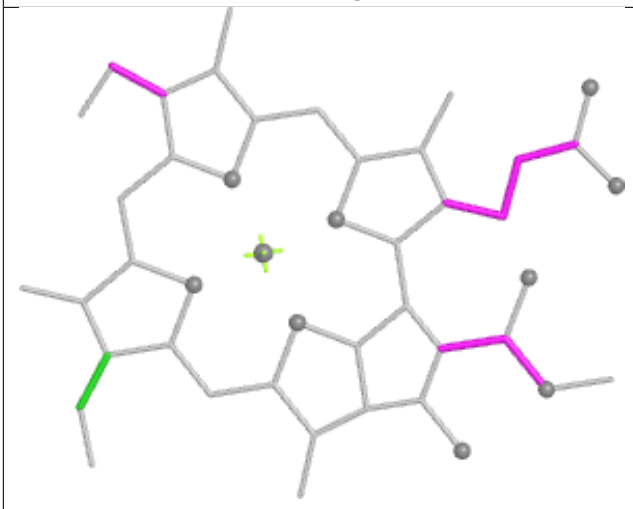
Ligand CLA 4 313



Bond lengths



Bond angles

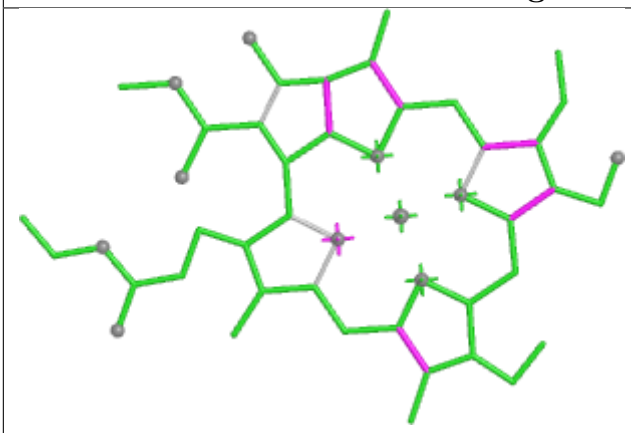


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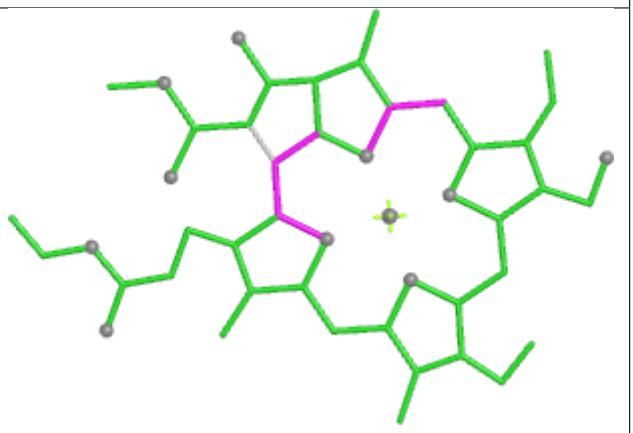


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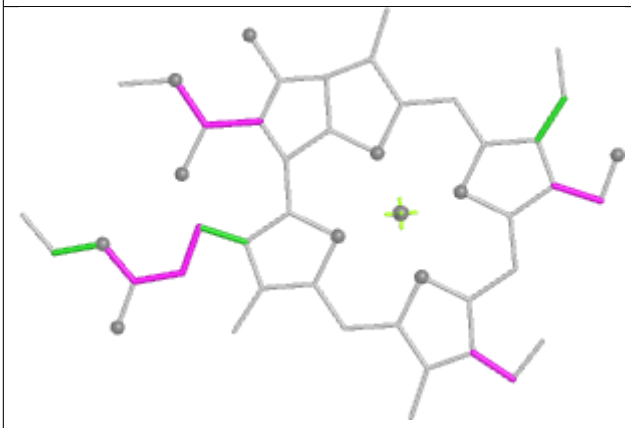
Ligand CHL 2 305



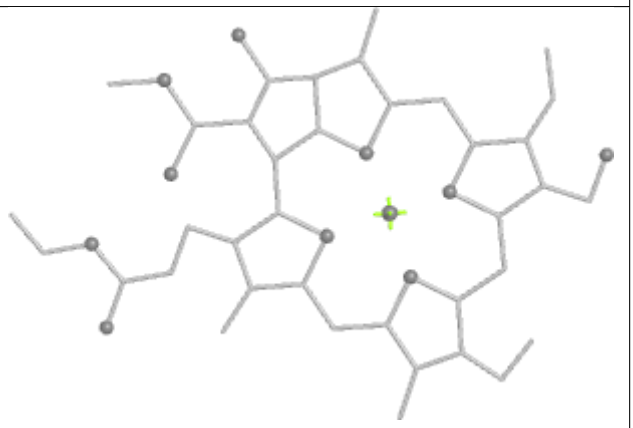
Bond lengths



Bond angles

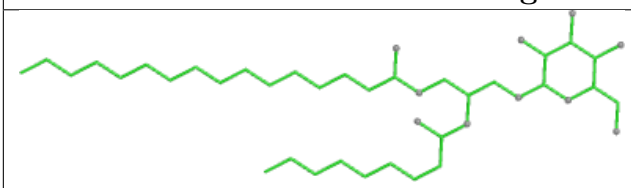


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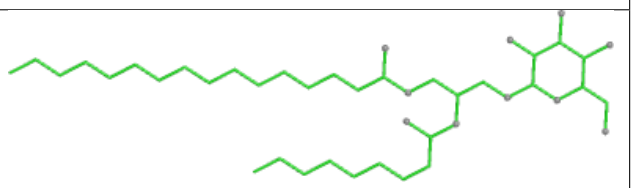


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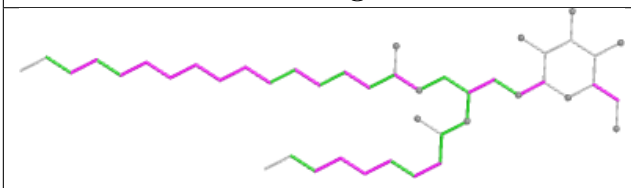
Ligand LMG B 849



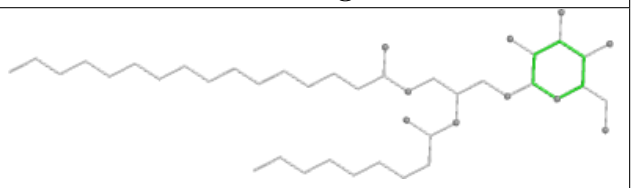
Bond lengths



Bond angles



Torsions

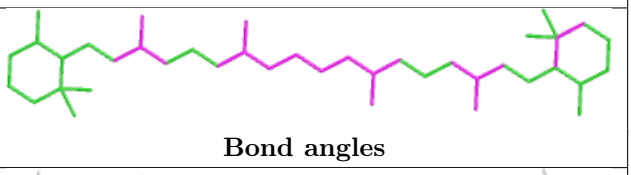


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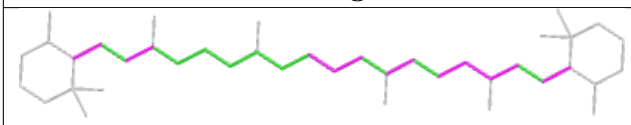
Ligand BCR L 305



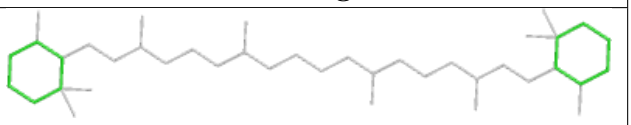
Bond lengths



Bond angles

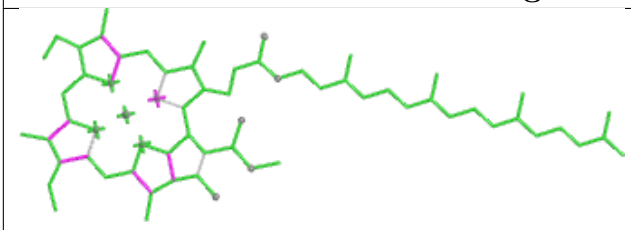


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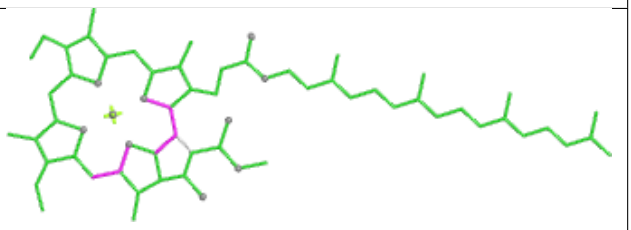


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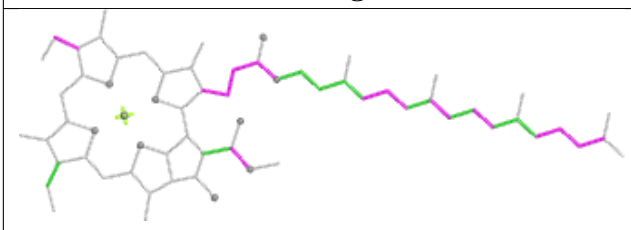
Ligand CLA A 807



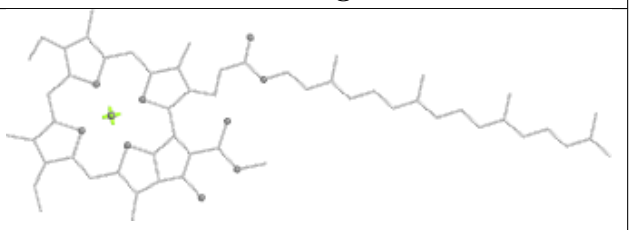
Bond lengths



Bond angles

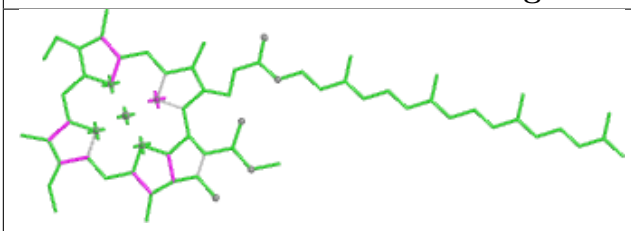


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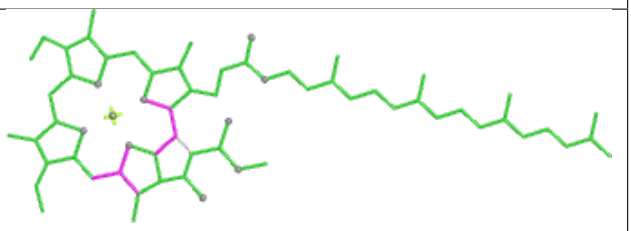


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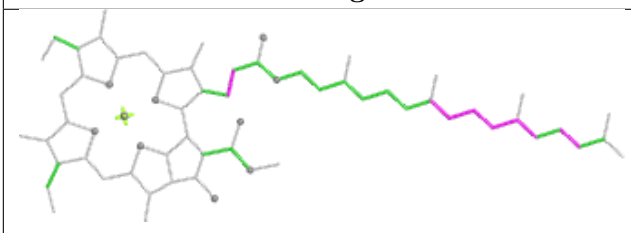
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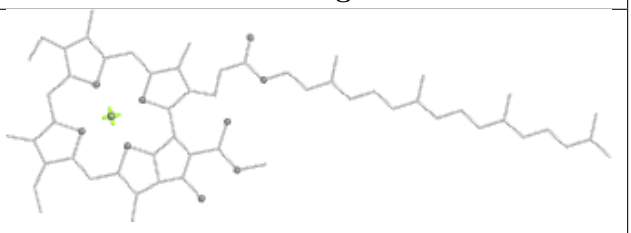
Bond lengths



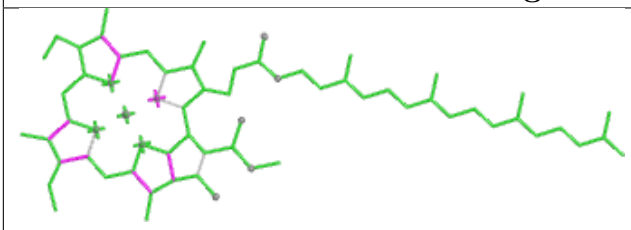
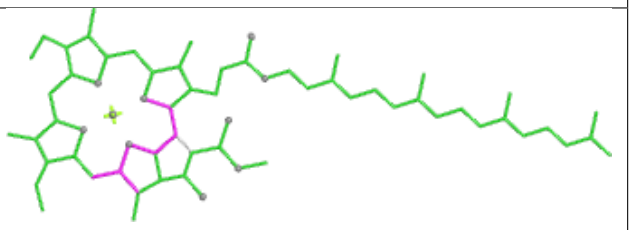
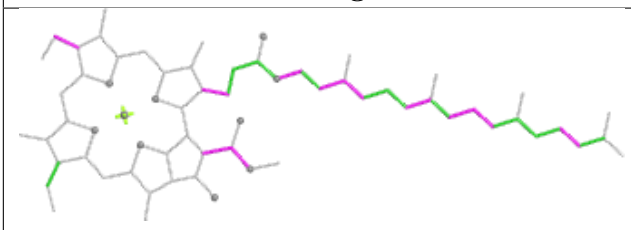
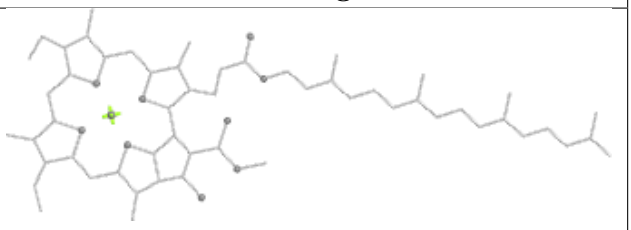
Bond angles

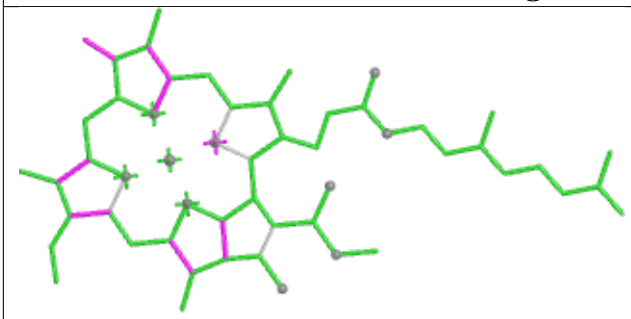
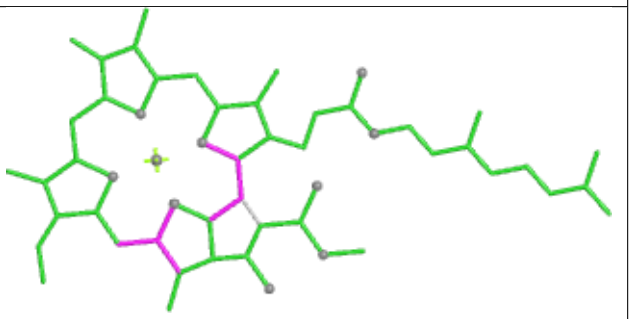
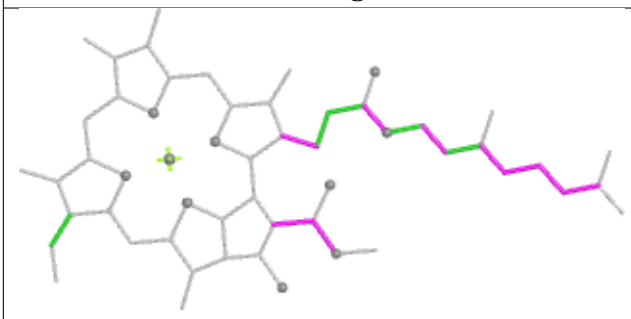
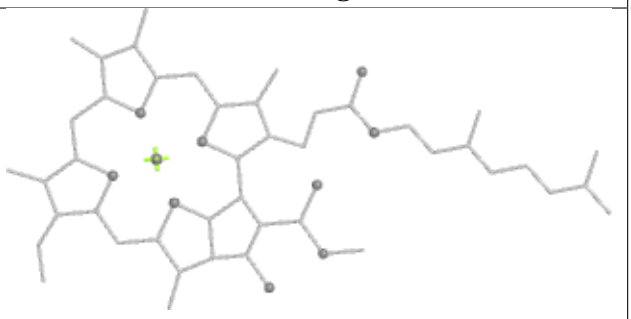


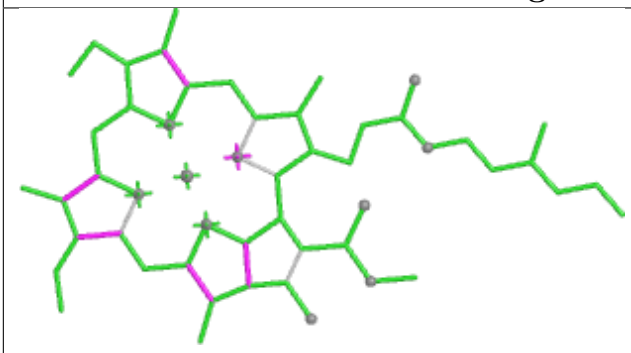
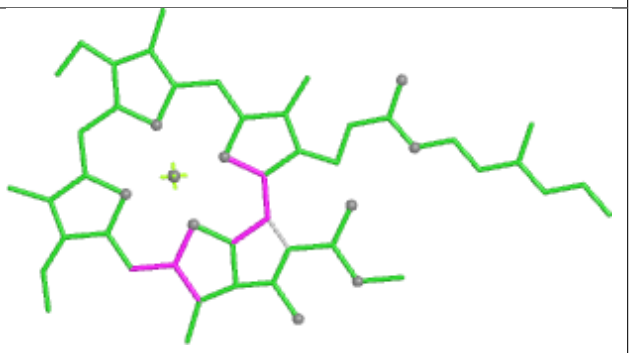
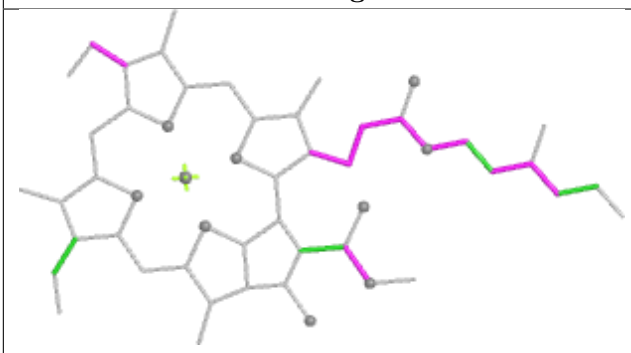
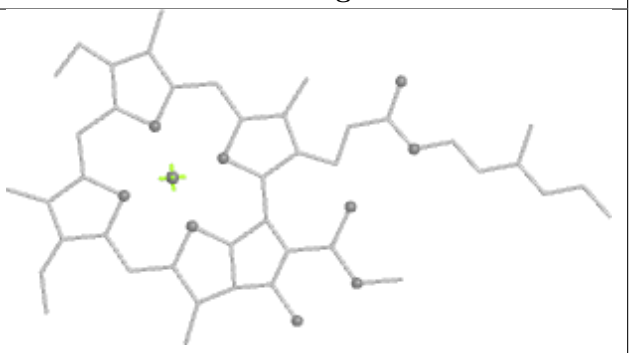
Torsions

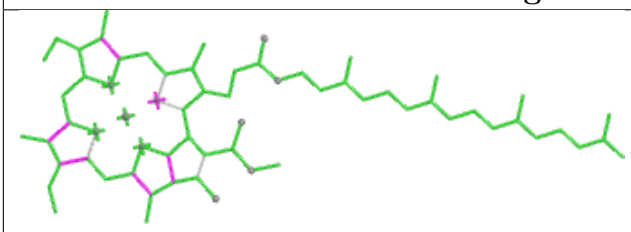
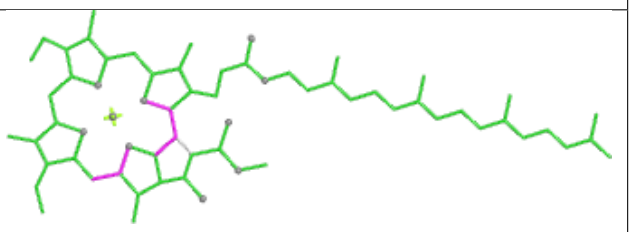
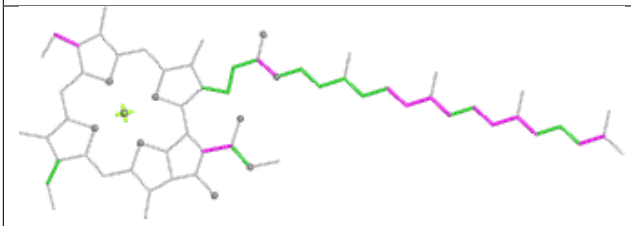
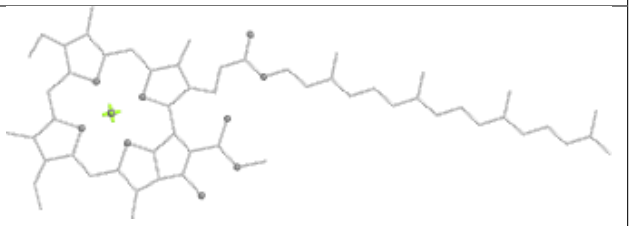


Rings

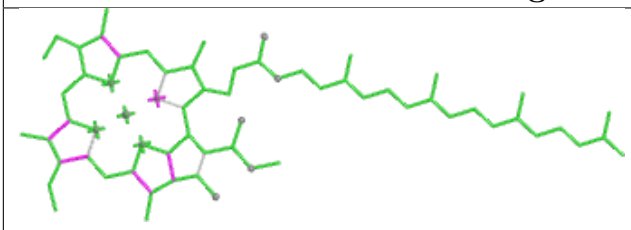
Ligand CLA A 854	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

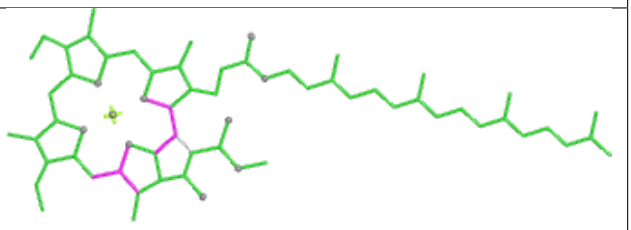
Ligand CLA 1 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

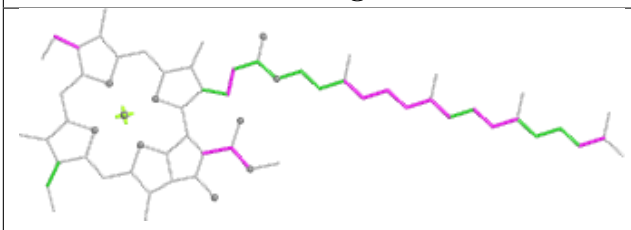
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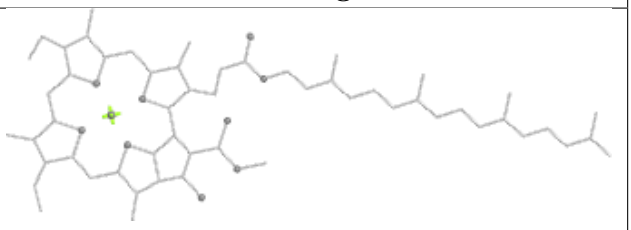
Bond lengths



Bond angles

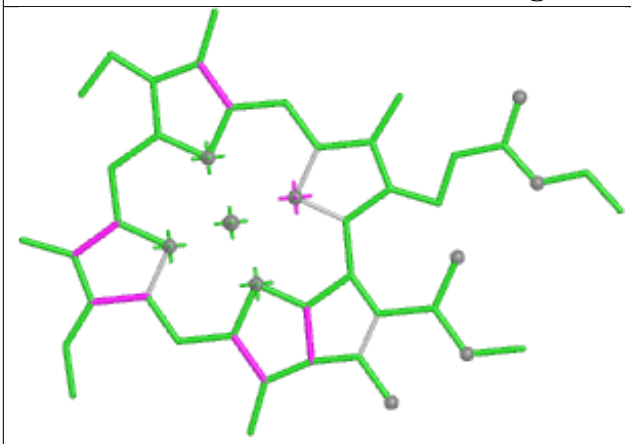


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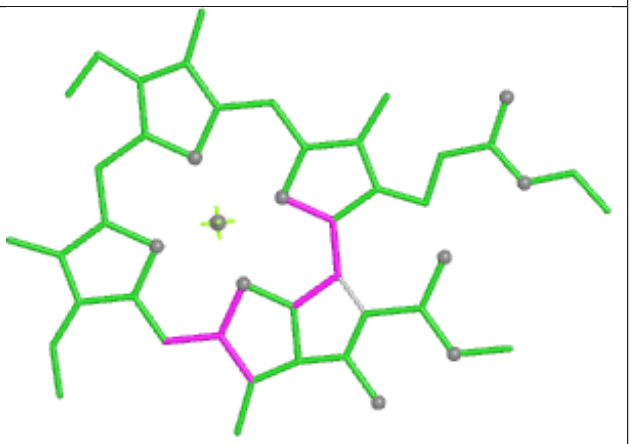


Rings

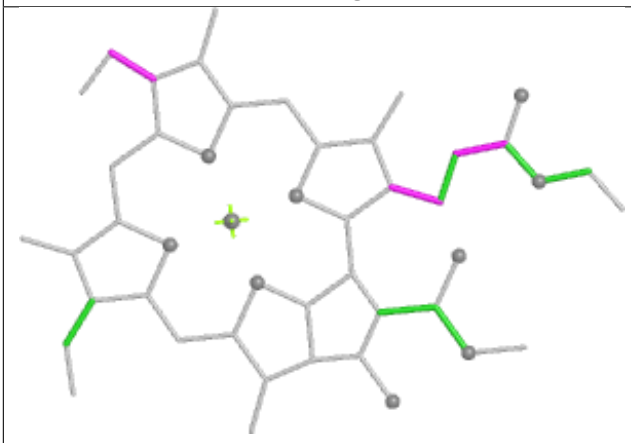
Ligand CLA 4 314



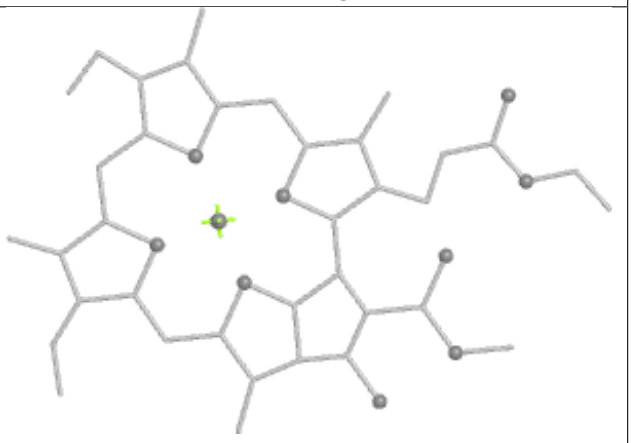
Bond lengths



Bond angles

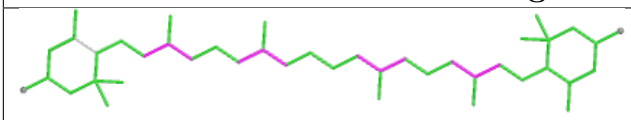


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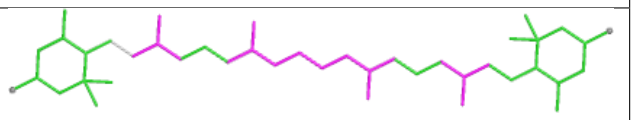


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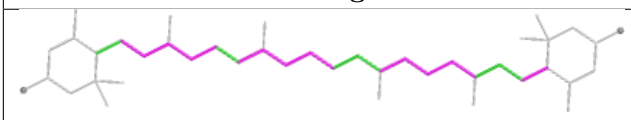
Ligand LUT 3 313



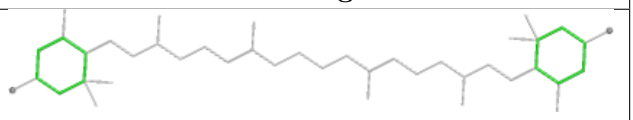
Bond lengths



Bond angles

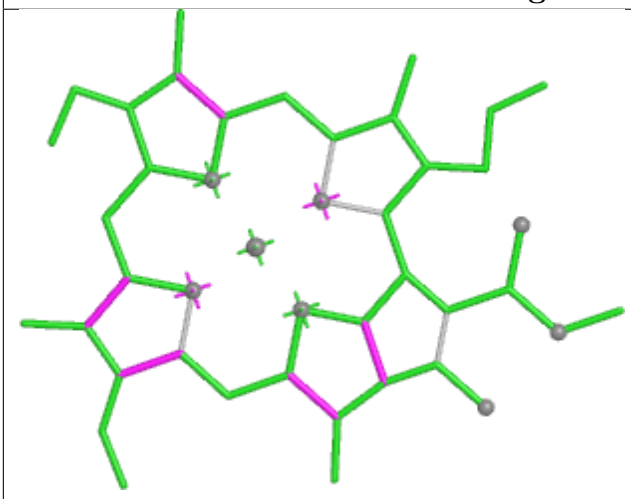


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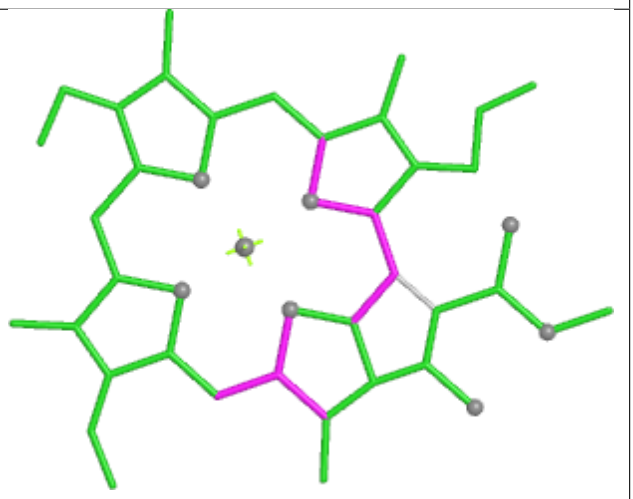


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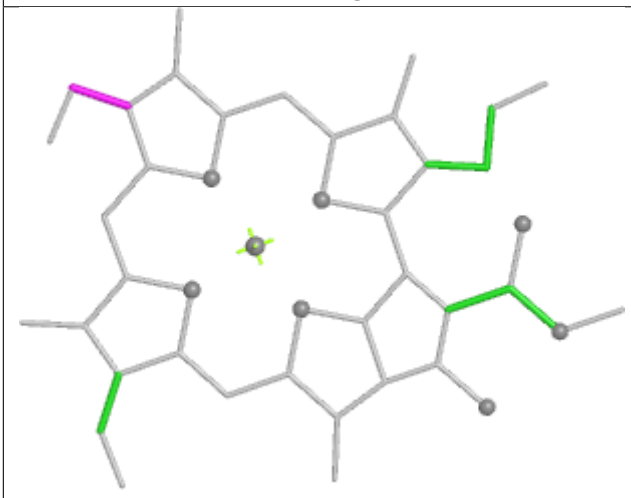
Ligand CLA 2 312



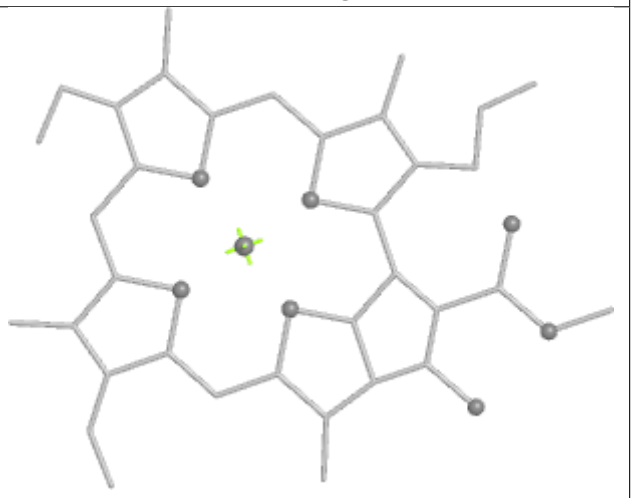
Bond lengths



Bond angles

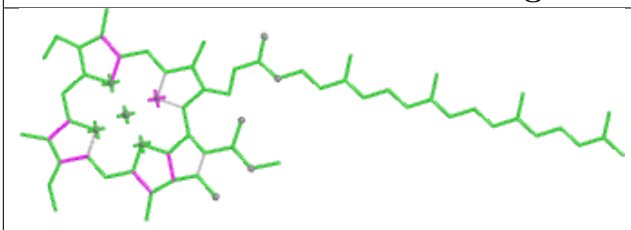


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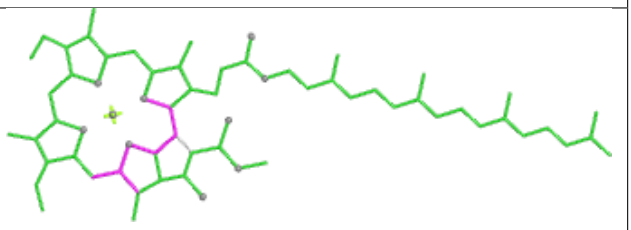


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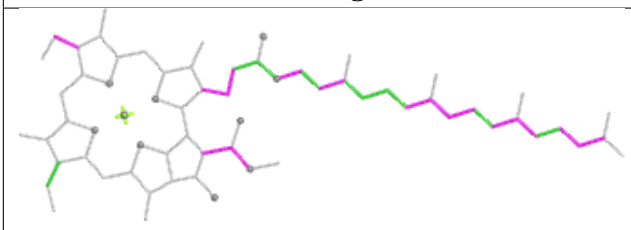
Ligand CLA B 827



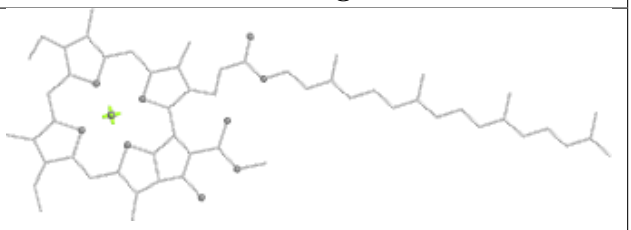
Bond lengths



Bond angles

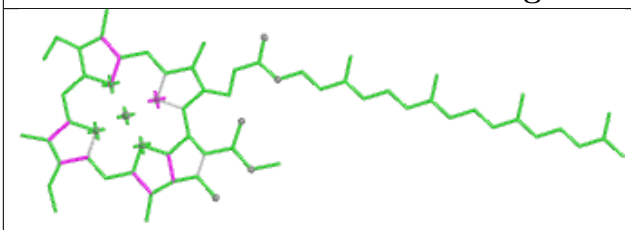


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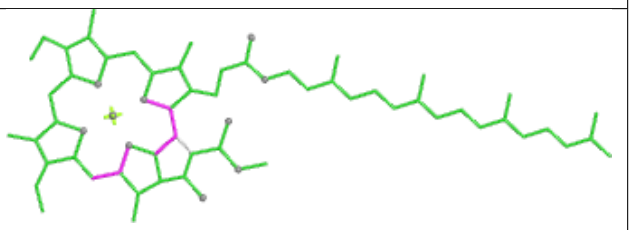


Rings

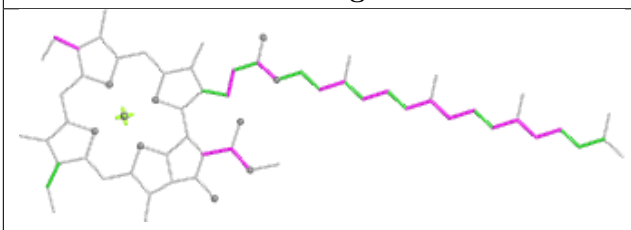
Ligand CLA A 815



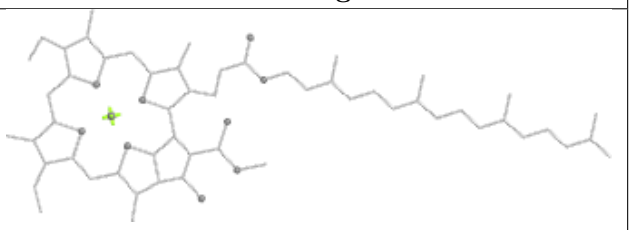
Bond lengths



Bond angles

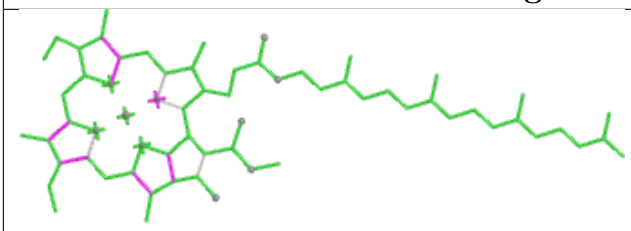


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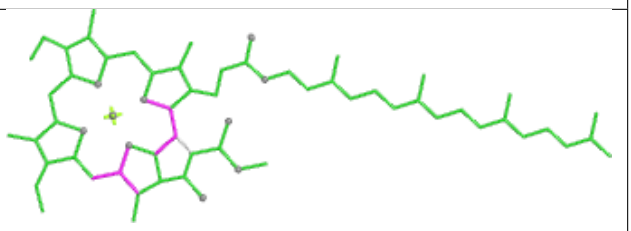


Rings

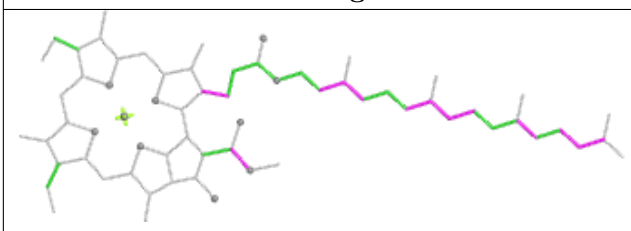
Ligand CLA B 829



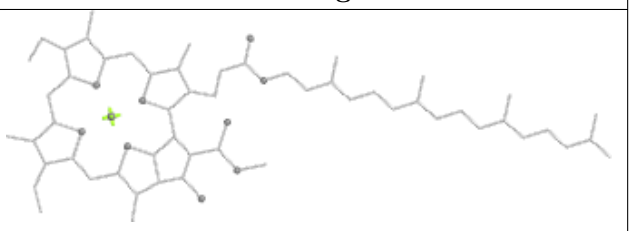
Bond lengths



Bond angles

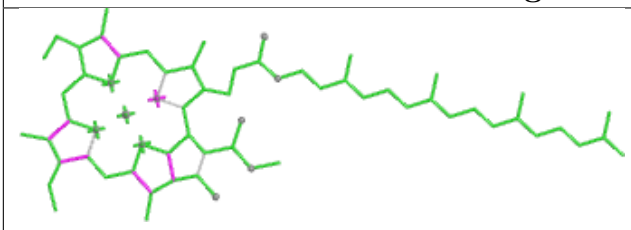


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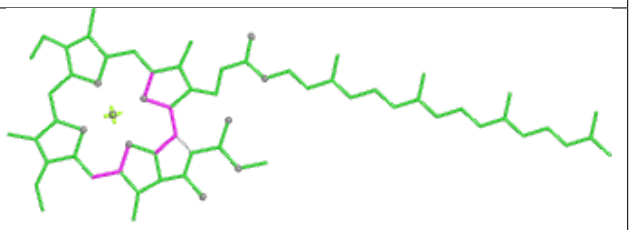


Rings

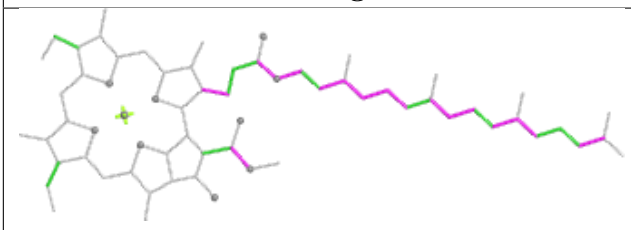
Ligand CLA B 839



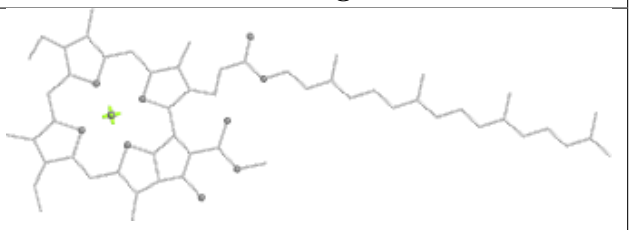
Bond lengths



Bond angles

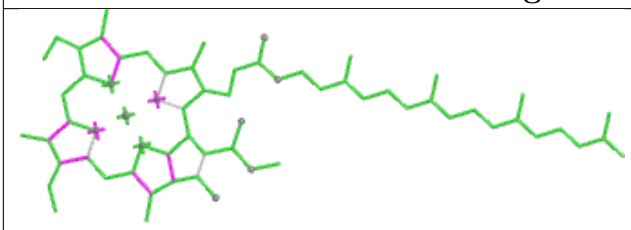


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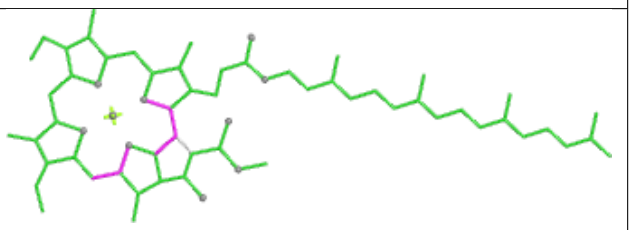


Rings

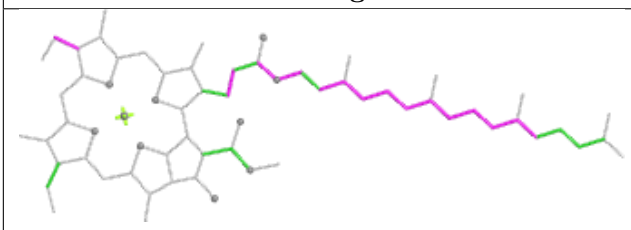
Ligand CLA A 840



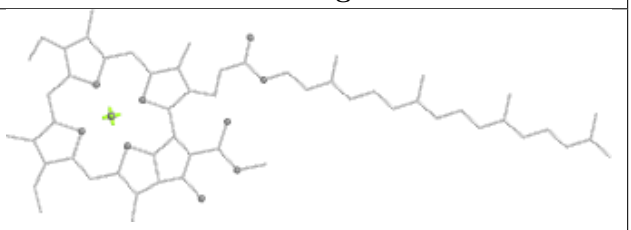
Bond lengths



Bond angles

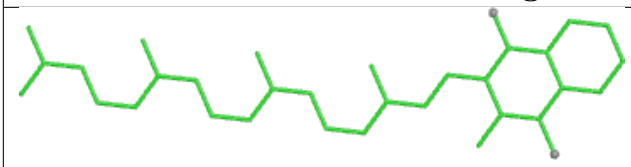


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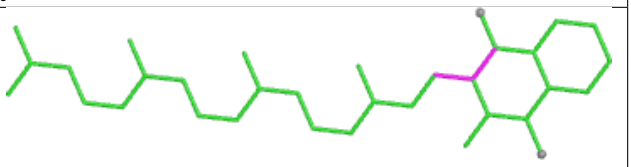


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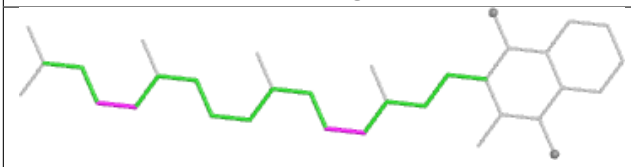
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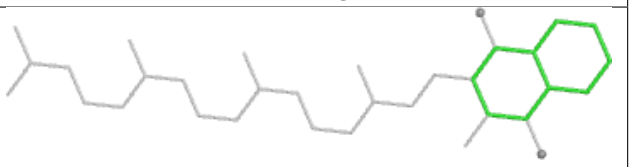
Bond lengths



Bond angles



Torsions

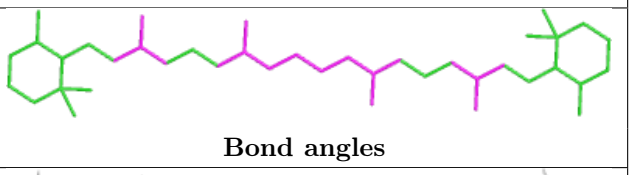


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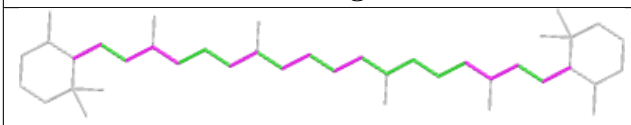
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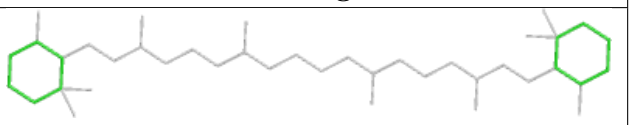
Bond lengths



Bond angles

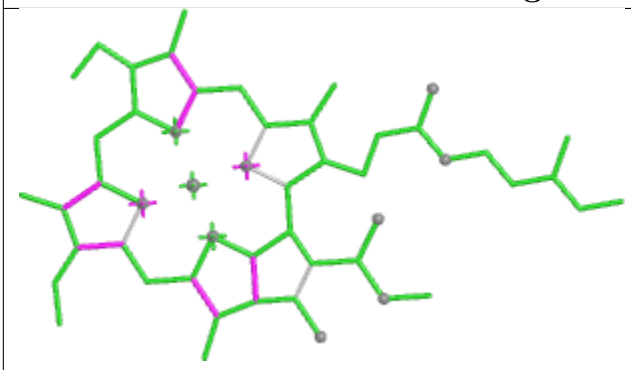


Torsions

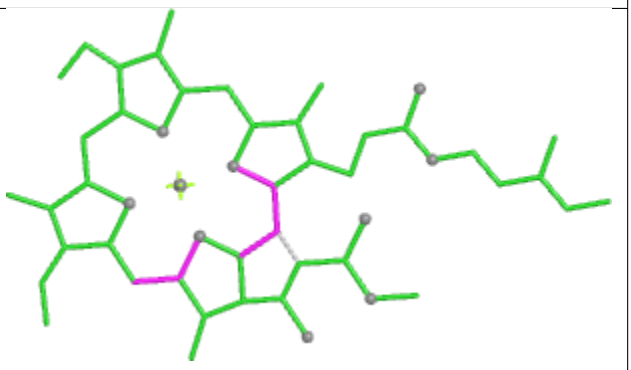


Rings

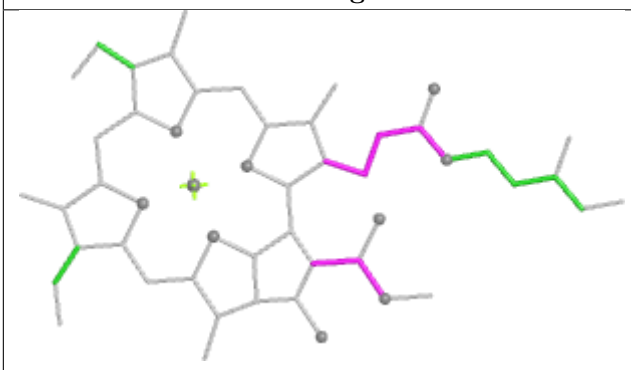
Ligand CLA A 834



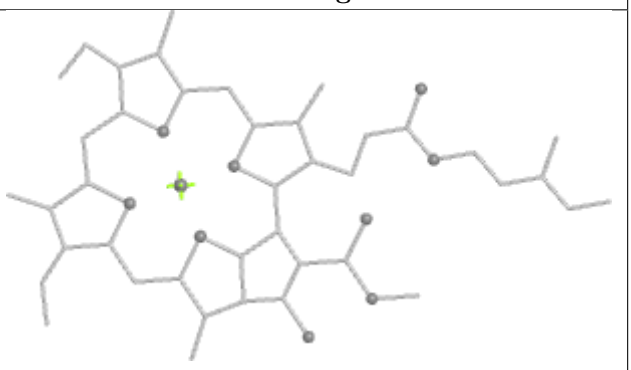
Bond lengths



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.

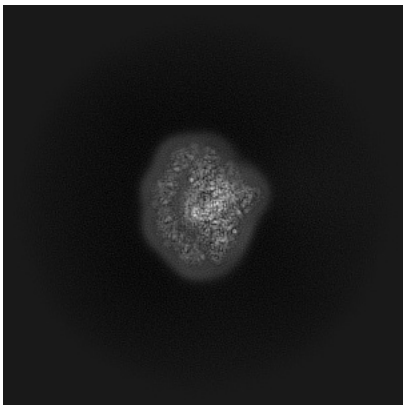
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67007. These allow visual inspection of the internal detail of the map and identification of artifacts.

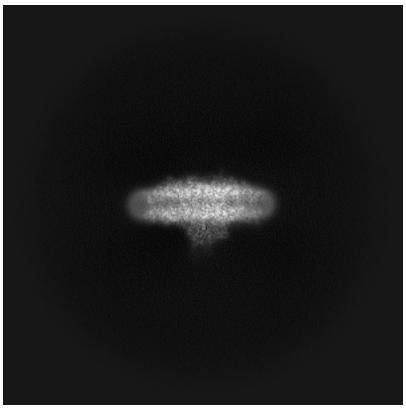
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X

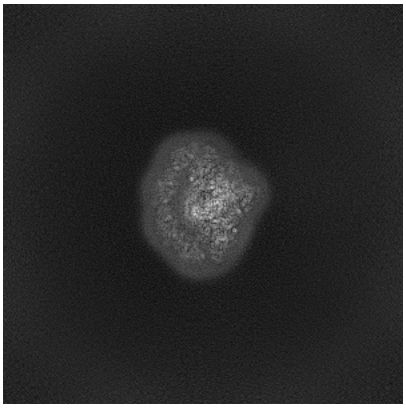


Y

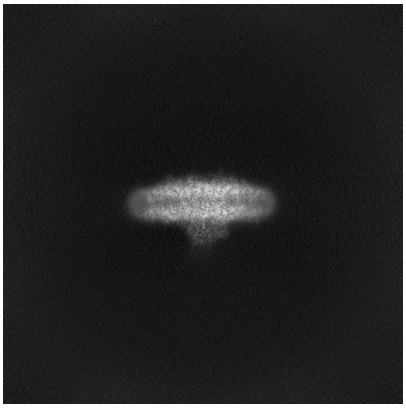


Z

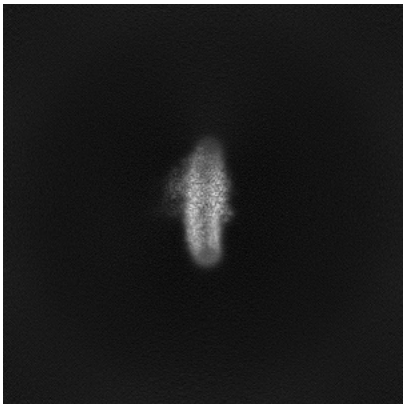
6.1.2 Raw map



X



Y

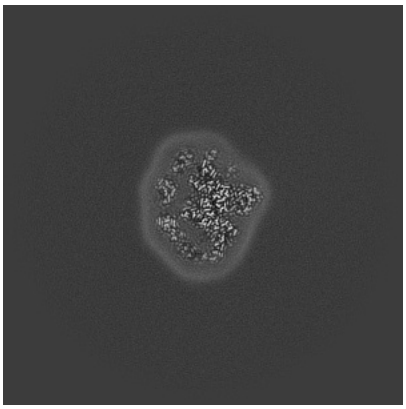


Z

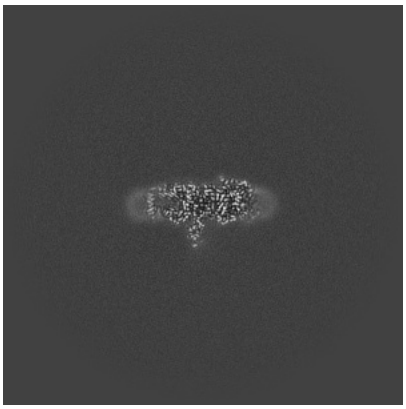
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

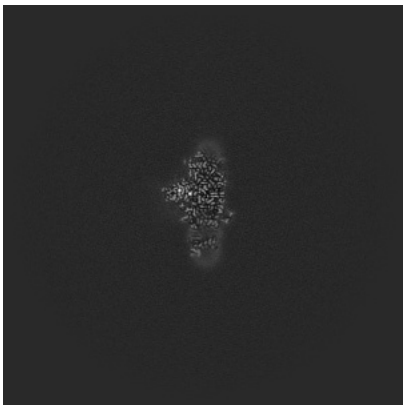
6.2.1 Primary map



X Index: 256

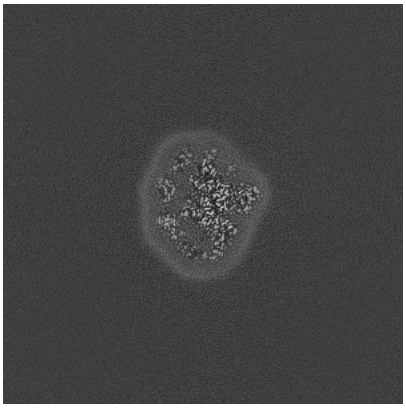


Y Index: 256

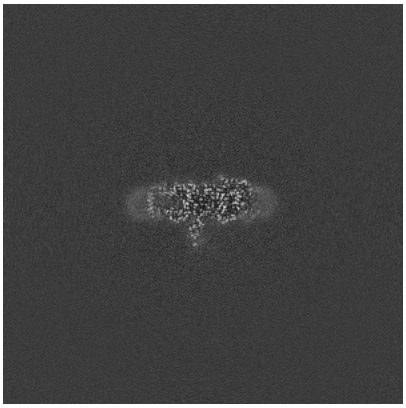


Z Index: 256

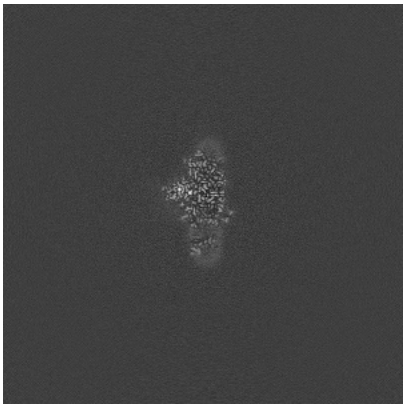
6.2.2 Raw map



X Index: 256



Y Index: 256

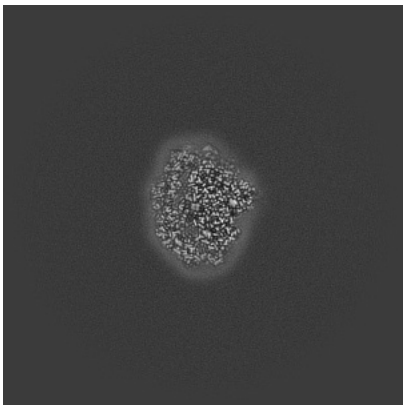


Z Index: 256

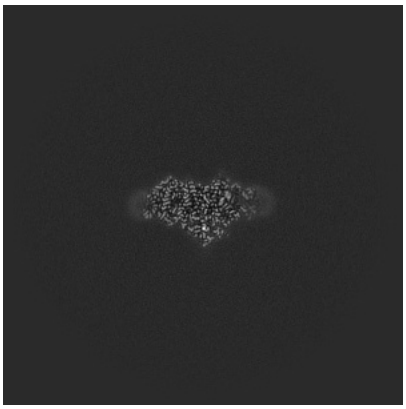
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

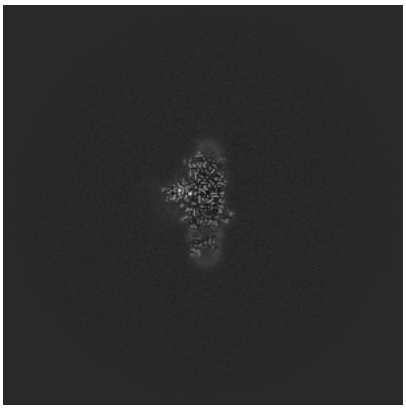
6.3.1 Primary map



X Index: 245

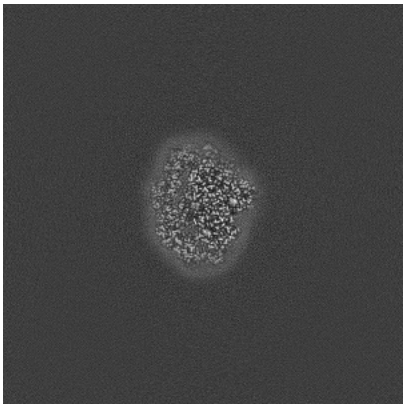


Y Index: 274

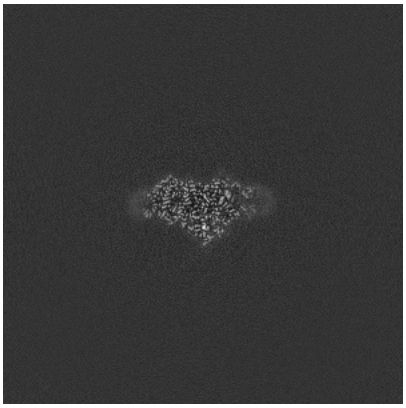


Z Index: 256

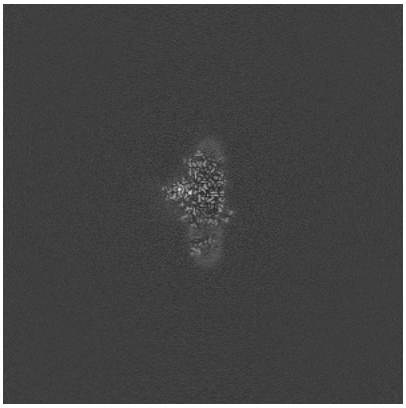
6.3.2 Raw map



X Index: 245



Y Index: 274

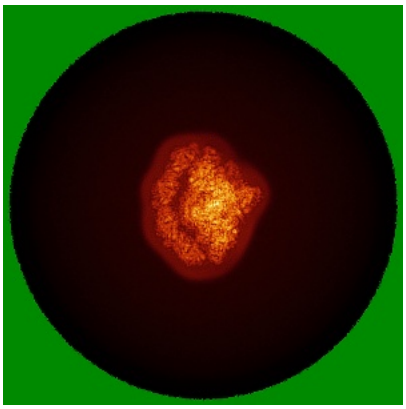


Z Index: 256

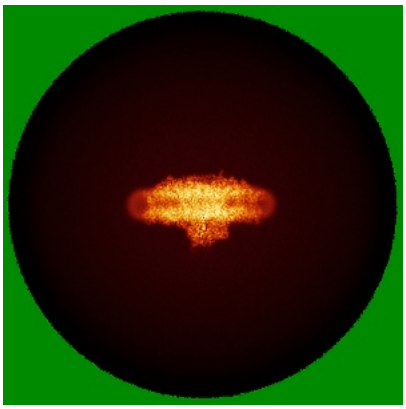
The images above show the largest variance slices of the map in three orthogonal directions.

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

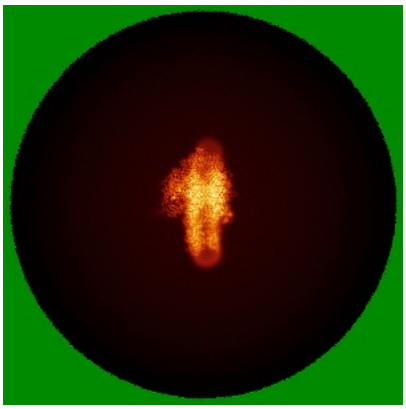
6.4.1 Primary map



X

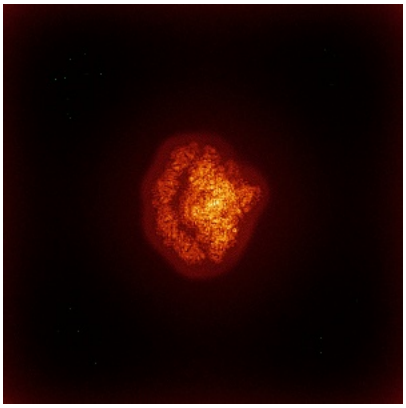


Y

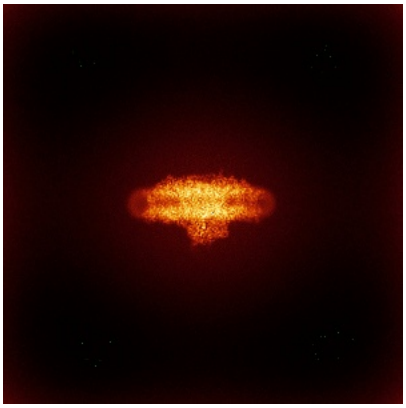


Z

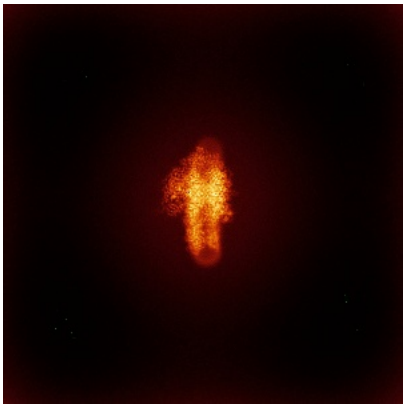
6.4.2 Raw map



X



Y

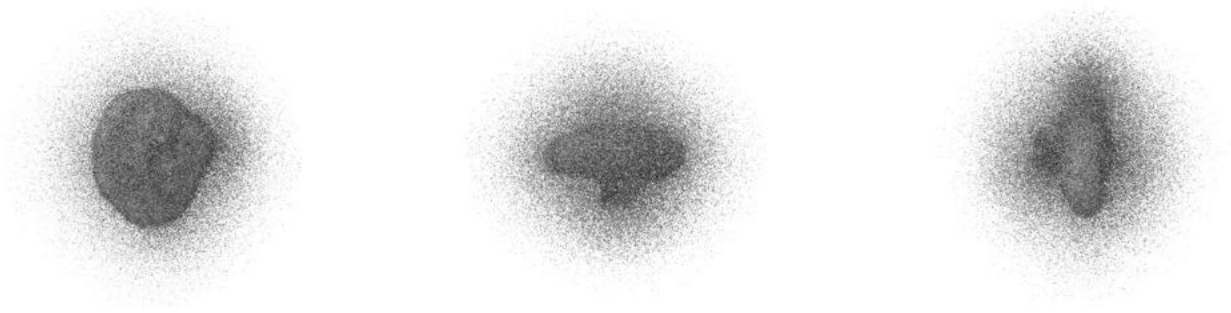


Z

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)

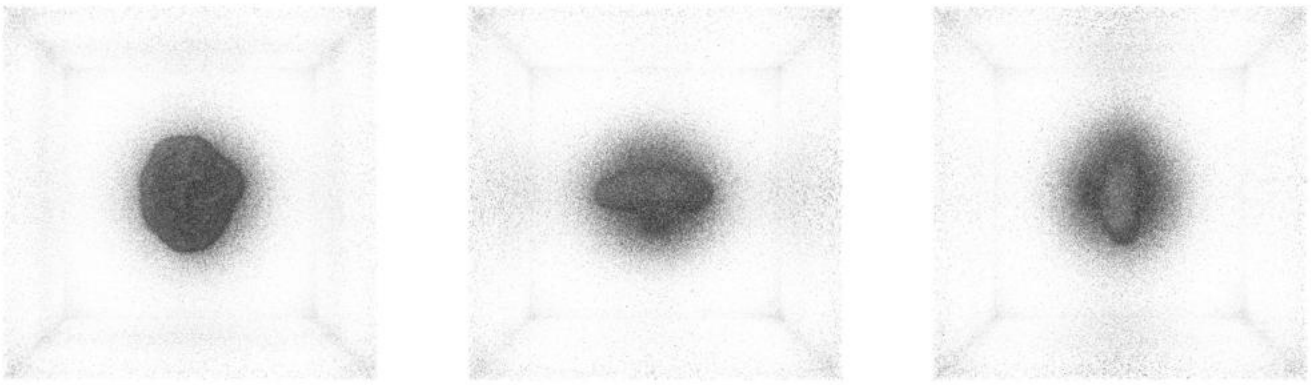
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0418. 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.

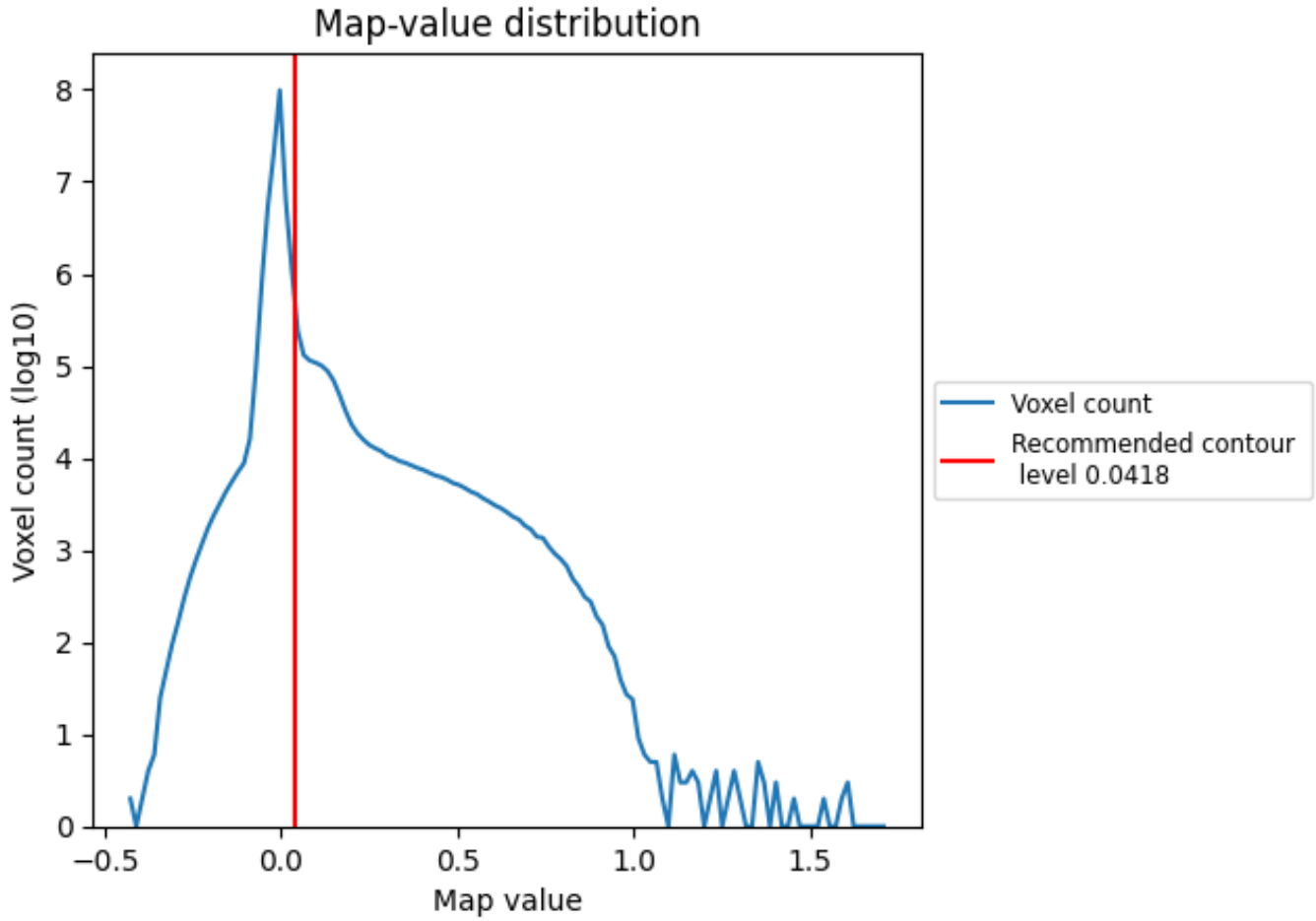
6.6 Mask visualisation (i)

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

7 Map analysis

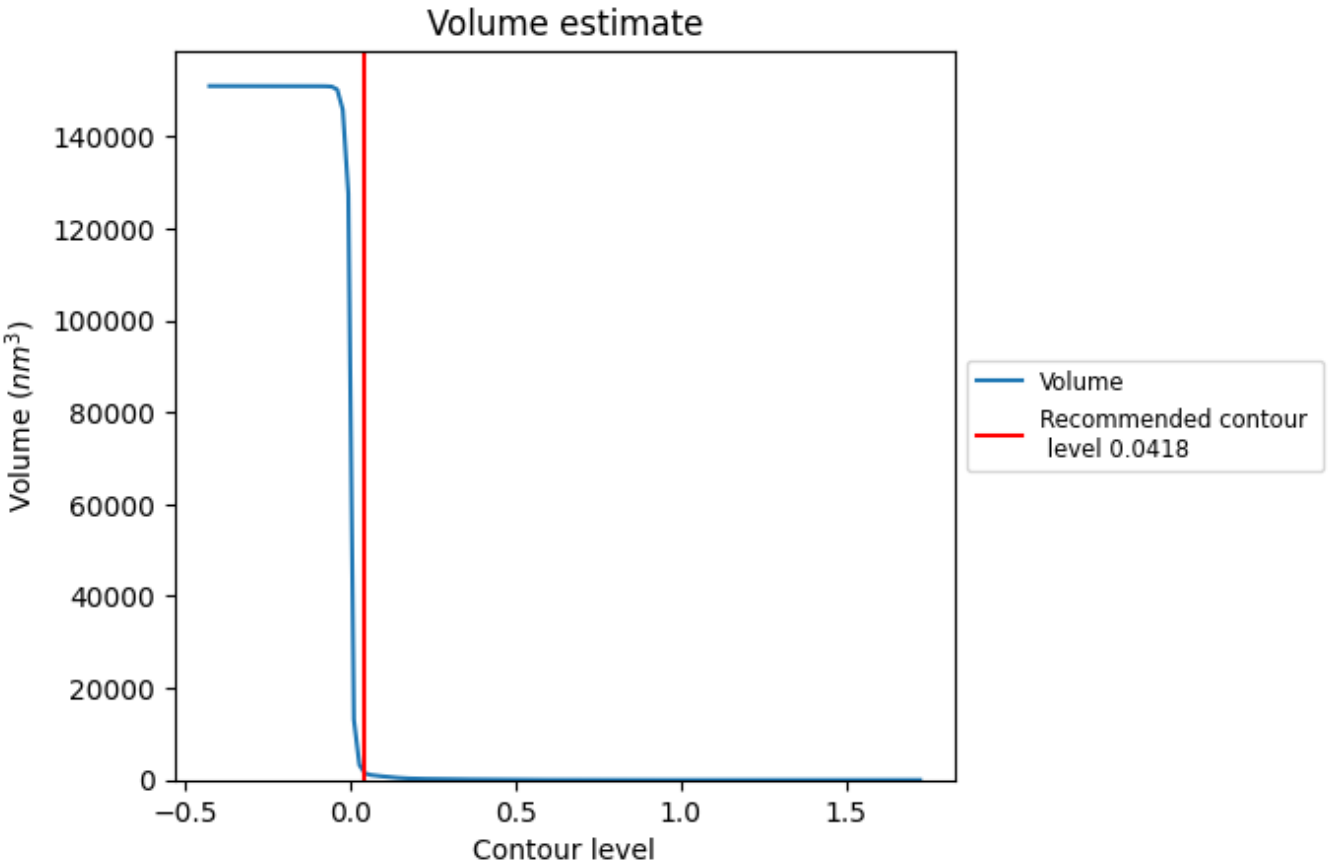
This section contains the results of statistical analysis of the map.

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.

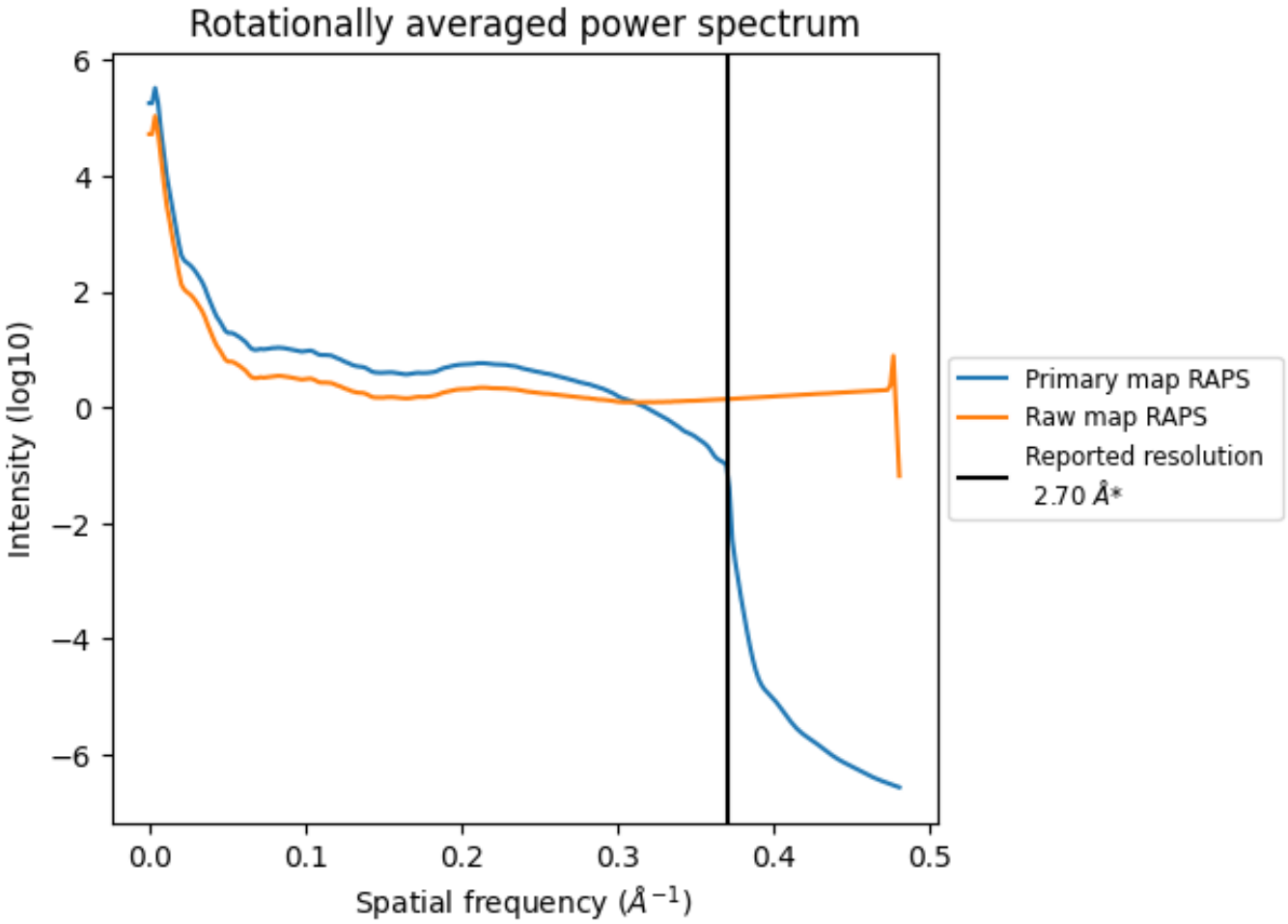
7.2 Volume estimate (i)



The volume at the recommended contour level is 1604 nm^3; this corresponds to an approximate mass of 1449 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)

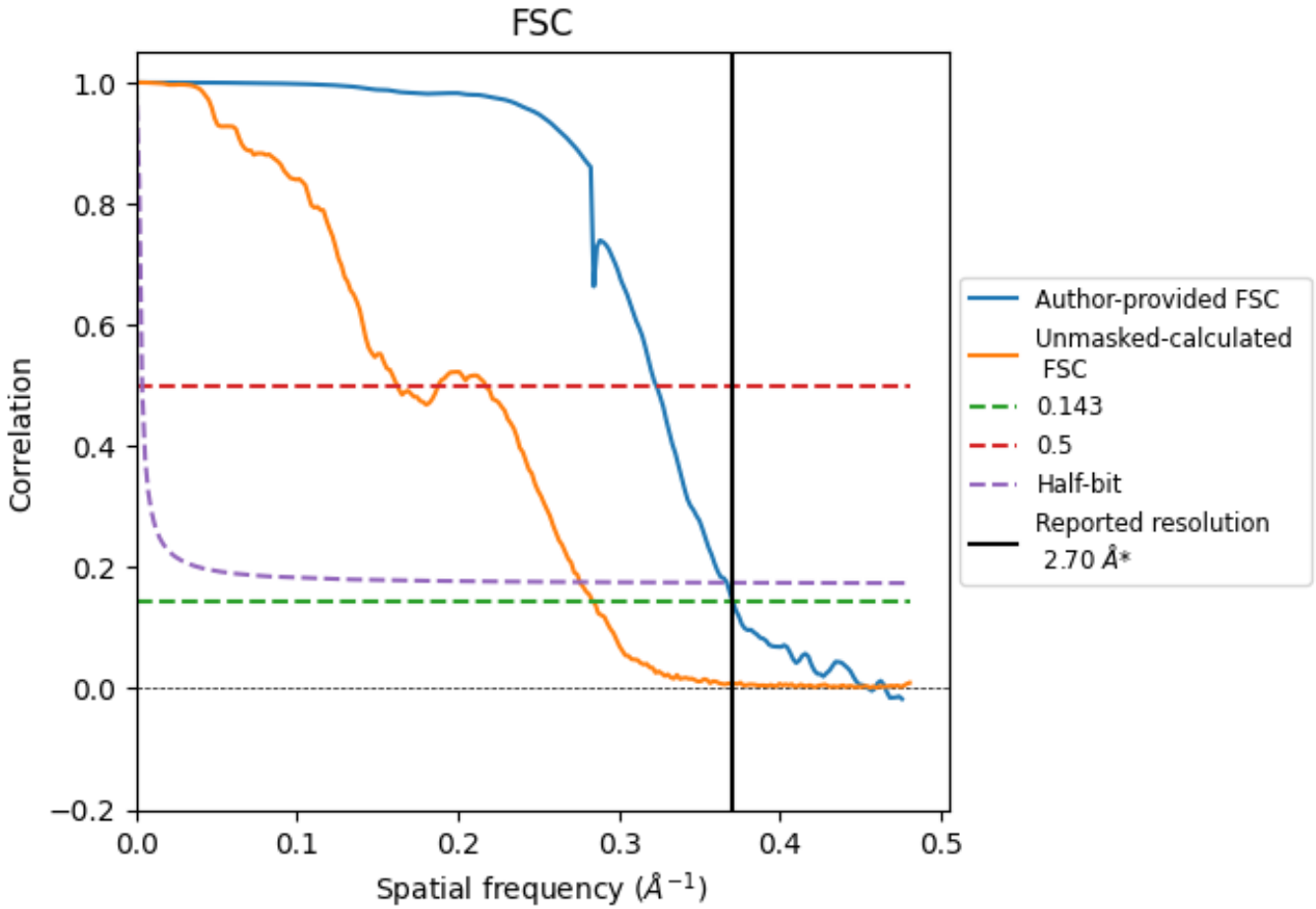


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

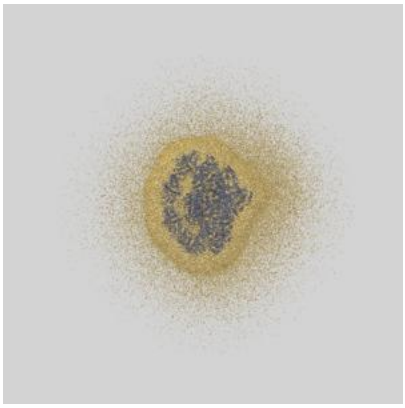
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.09	2.72
Unmasked-calculated*	3.52	6.17	3.63

*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 3.52 differs from the reported value 2.7 by more than 10 %

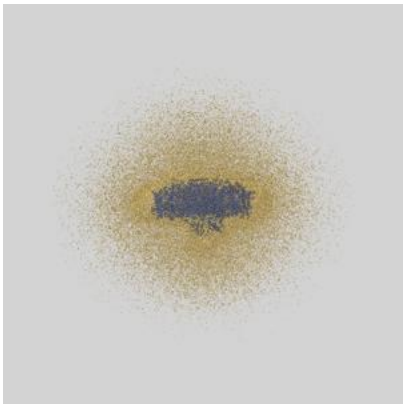
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67007 and PDB model 9XLV. Per-residue inclusion information can be found in section 3 on page 24.

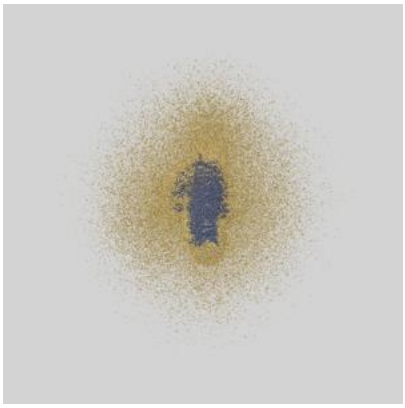
9.1 Map-model overlay



X



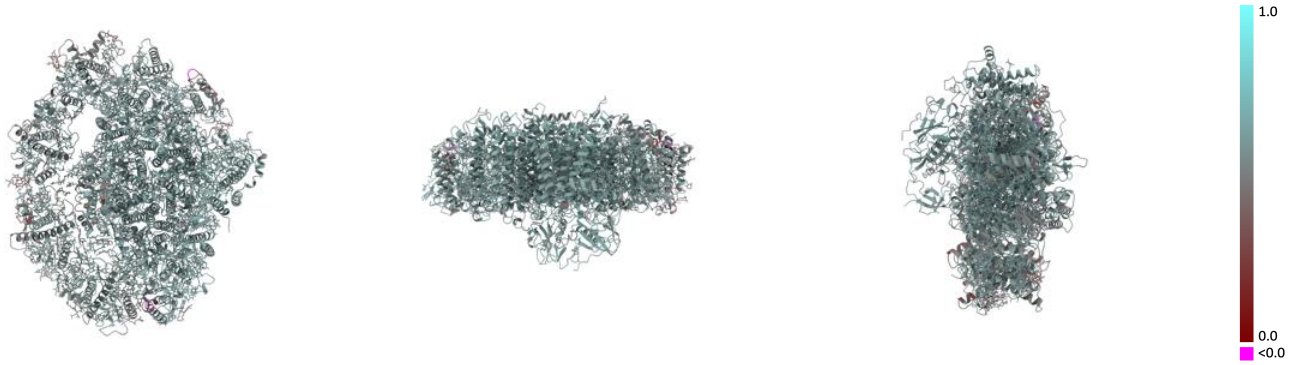
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0418 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.

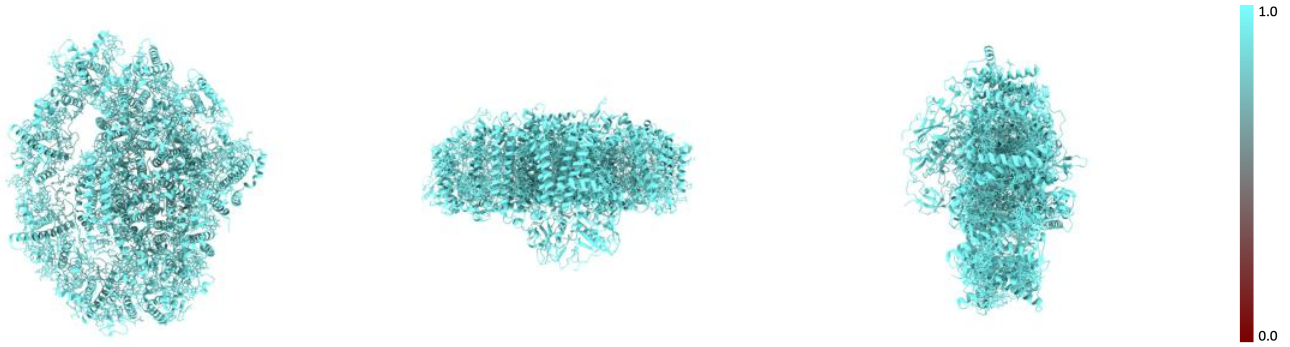
9.2 Q-score mapped to coordinate model (i)



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.

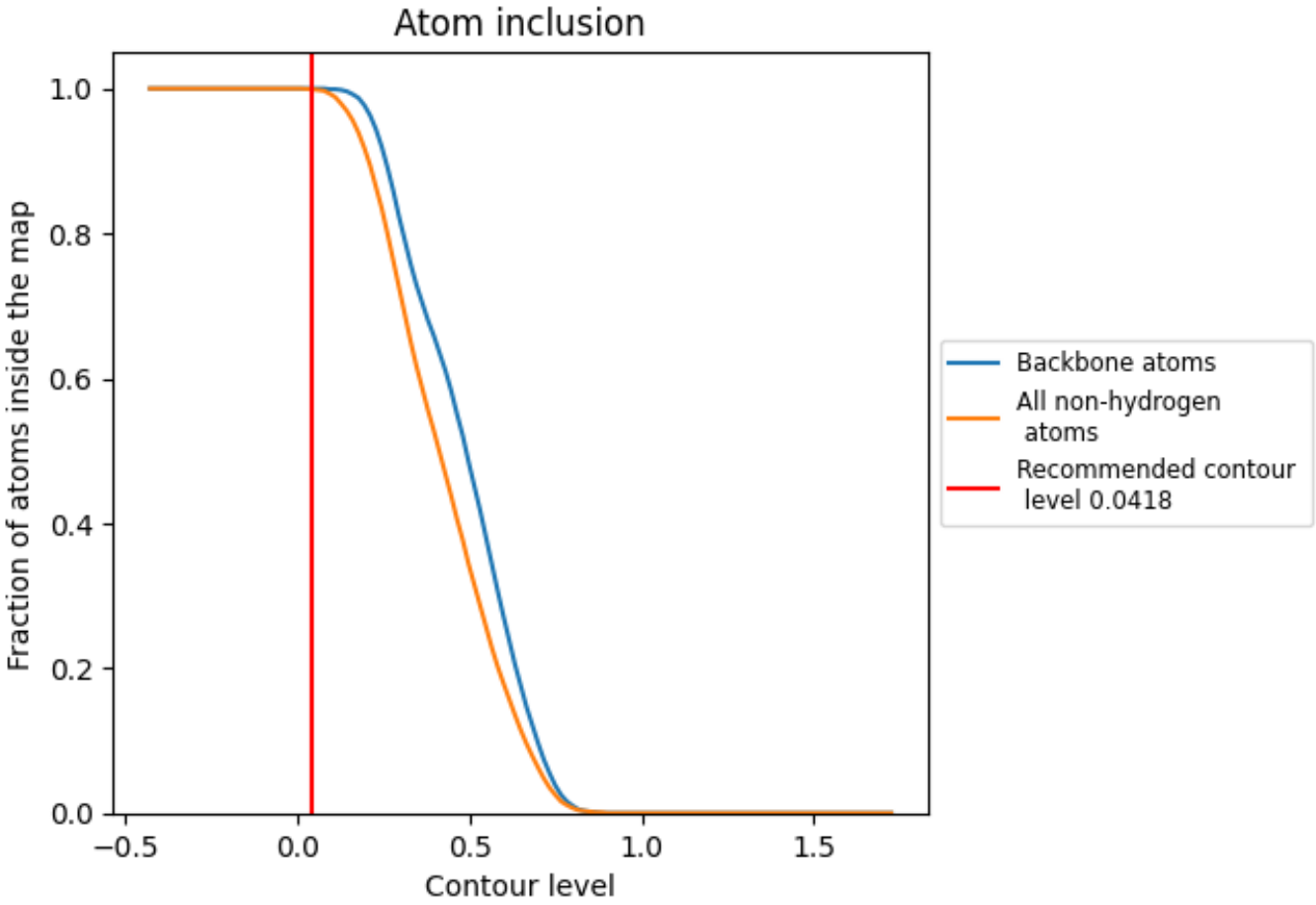
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0418).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0418) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9990	0.5710
1	0.9980	0.5490
2	0.9980	0.5340
3	1.0000	0.5230
4	0.9970	0.5370
A	0.9990	0.5980
B	1.0000	0.6010
C	0.9970	0.5710
D	0.9990	0.5780
E	1.0000	0.5760
F	0.9980	0.5600
G	0.9930	0.5340
H	1.0000	0.5660
I	1.0000	0.5780
J	1.0000	0.5670
K	0.9990	0.5220
L	1.0000	0.5770
O	0.9990	0.4960

