wwPDB EM Validation Summary Report

Nov 9, 2026 – 06:20 PM JST

PDB ID	:	9XNV / pdb_00009xnv
EMDB ID	:	EMD-67061
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	:	2025-11-13
Resolution	:	2.75 Å(reported)

This is a wwPDB EM Validation Summary 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:

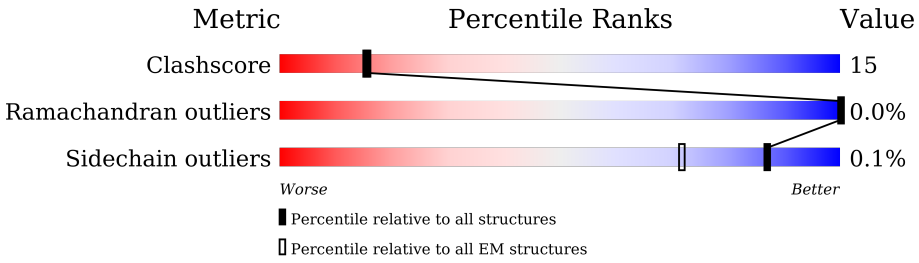
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

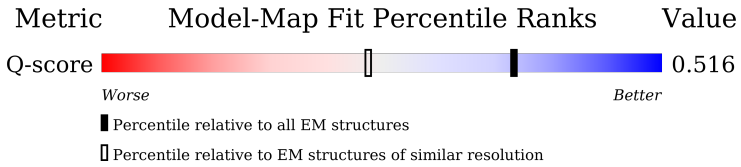
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.75 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.





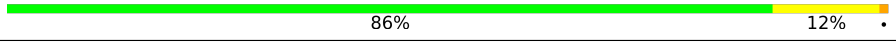
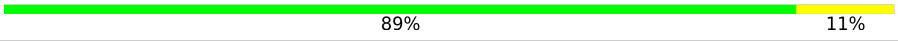
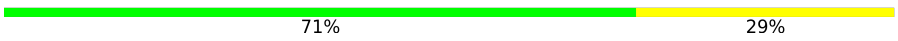
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

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

Mol	Chain	Length	Quality of chain
1	A	708	74% 26%
1	a	708	75% 25%
2	B	733	79% 21%
2	b	733	79% 21%

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Mol	Chain	Length	Quality of chain
3	C	80	
3	c	80	
4	D	142	
4	d	142	
5	E	65	
5	e	65	
6	H	95	
6	h	95	
7	I	35	
7	i	35	
8	L	159	
8	l	159	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CLA	A	819	-	-	X	-
9	CLA	a	820	-	-	X	-
9	CLA	h	201	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 42578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	708	Total	C	N	O	S	0	0
			5564	3650	944	952	18		
1	a	708	Total	C	N	O	S	0	0
			5564	3650	944	952	18		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

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

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1129	726	196	204	3		
4	d	142	Total	C	N	O	S	0	0
			1129	726	196	204	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	65	Total 525	C 335	N 92	O 98	0	0
5	e	65	Total 525	C 335	N 92	O 98	0	0

- Molecule 6 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	95	Total 727	C 477	N 116	O 134	0	0
6	h	95	Total 727	C 477	N 116	O 134	0	0

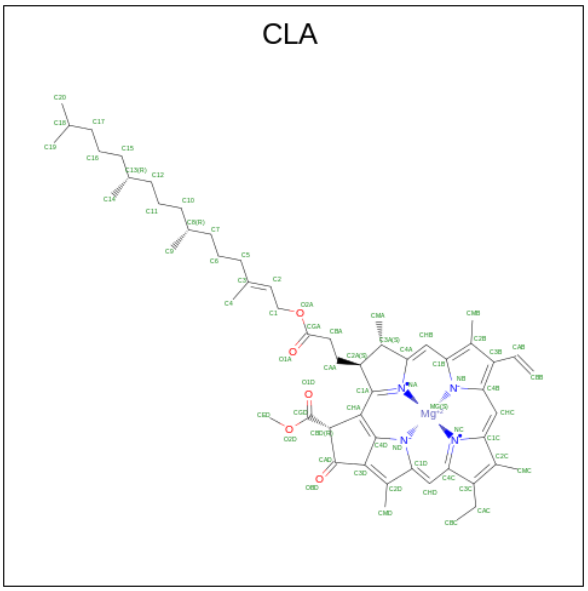
- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	35	Total 267	C 181	N 41	O 44	S 1	0	0
7	i	35	Total 267	C 181	N 41	O 44	S 1	0	0

- Molecule 8 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	159	Total 1185	C 782	N 187	O 214	S 2	0	0
8	l	159	Total 1185	C 782	N 187	O 214	S 2	0	0

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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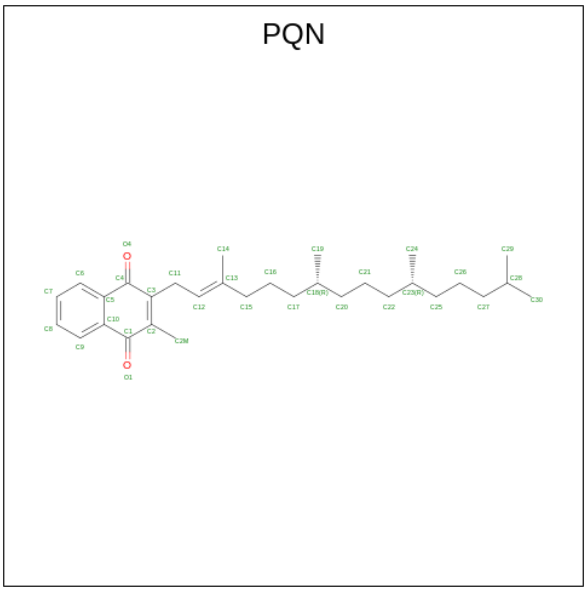
Mol	Chain	Residues	Atoms					AltConf
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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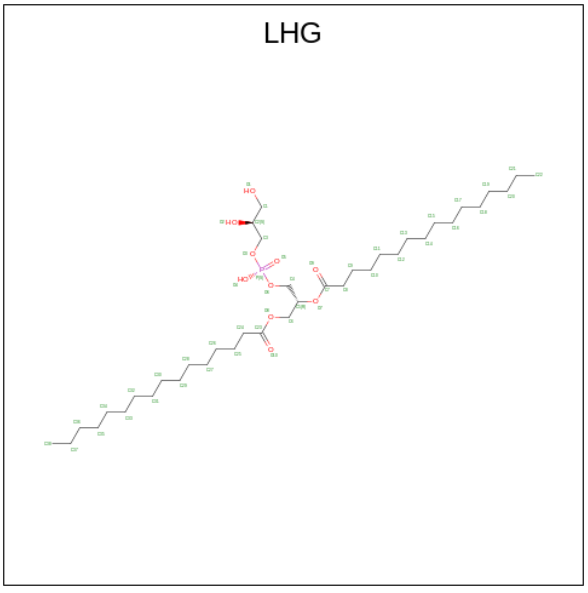
Mol	Chain	Residues	Atoms					AltConf
9	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	h	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	h	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 10 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



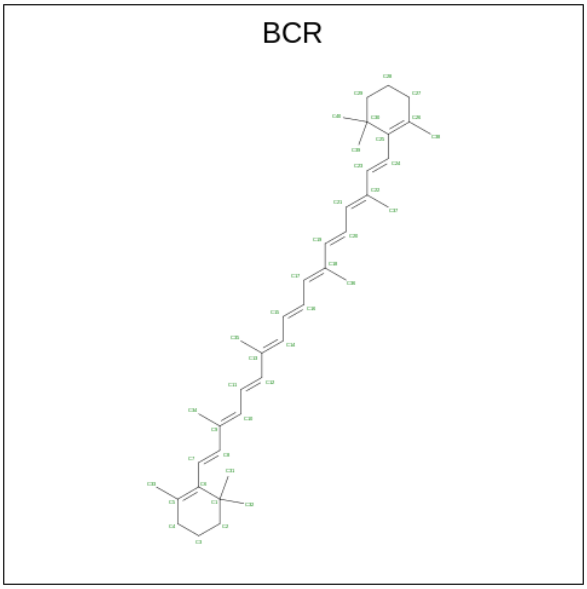
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C O 33 31 2	0
10	B	1	Total C O 33 31 2	0
10	a	1	Total C O 33 31 2	0
10	b	1	Total C O 33 31 2	0

- Molecule 11 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
11	A	1	Total	C	O	P	0
			49	38	10	1	
11	A	1	Total	C	O	P	0
			27	16	10	1	
11	A	1	Total	C	O	P	0
			49	38	10	1	
11	a	1	Total	C	O	P	0
			49	38	10	1	
11	a	1	Total	C	O	P	0
			27	16	10	1	
11	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



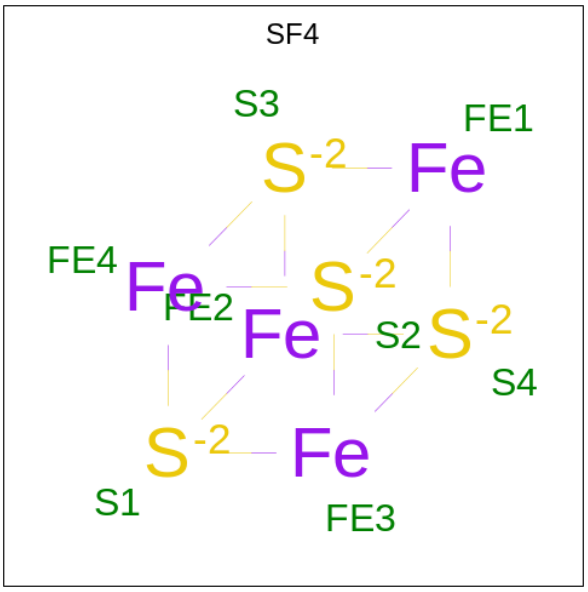
Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	A	1	Total	C	0
			40	40	
12	B	1	Total	C	0
			40	40	

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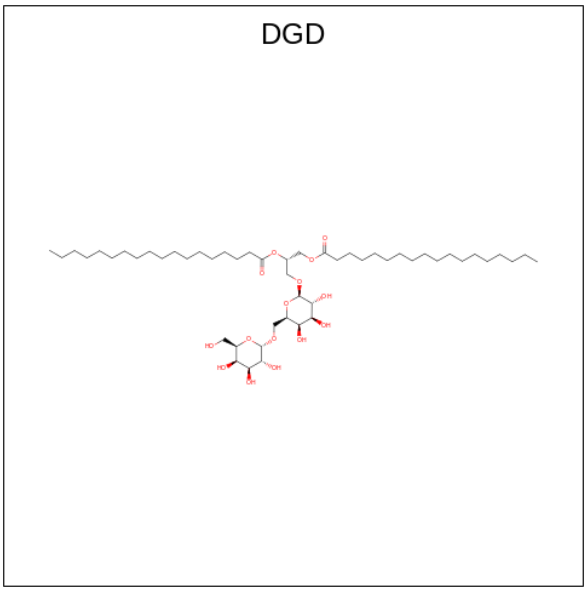
Mol	Chain	Residues	Atoms	AltConf
12	B	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	H	1	Total C 40 40	0
12	I	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	a	1	Total C 40 40	0
12	b	1	Total C 40 40	0
12	b	1	Total C 40 40	0
12	b	1	Total C 40 40	0
12	h	1	Total C 40 40	0
12	i	1	Total C 40 40	0
12	l	1	Total C 40 40	0
12	l	1	Total C 40 40	0
12	l	1	Total C 40 40	0

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



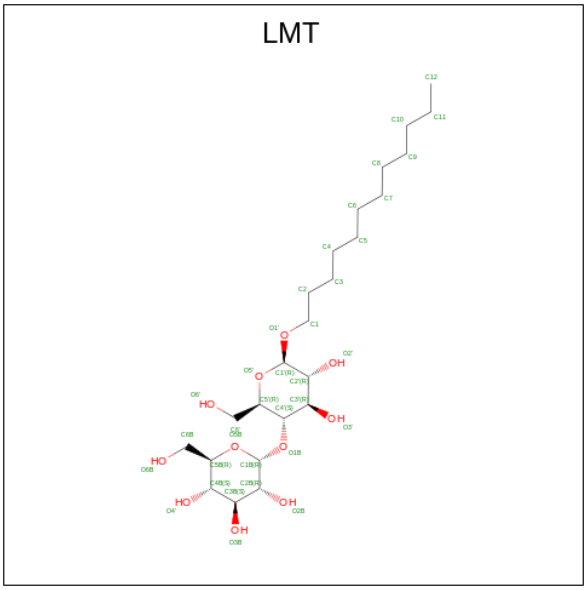
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 8 4 4	0
13	C	1	Total Fe S 8 4 4	0
13	a	1	Total Fe S 8 4 4	0
13	c	1	Total Fe S 8 4 4	0
13	c	1	Total Fe S 8 4 4	0

- Molecule 14 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	C	O	0
			66	51	15	
14	b	1	Total	C	O	0
			66	51	15	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



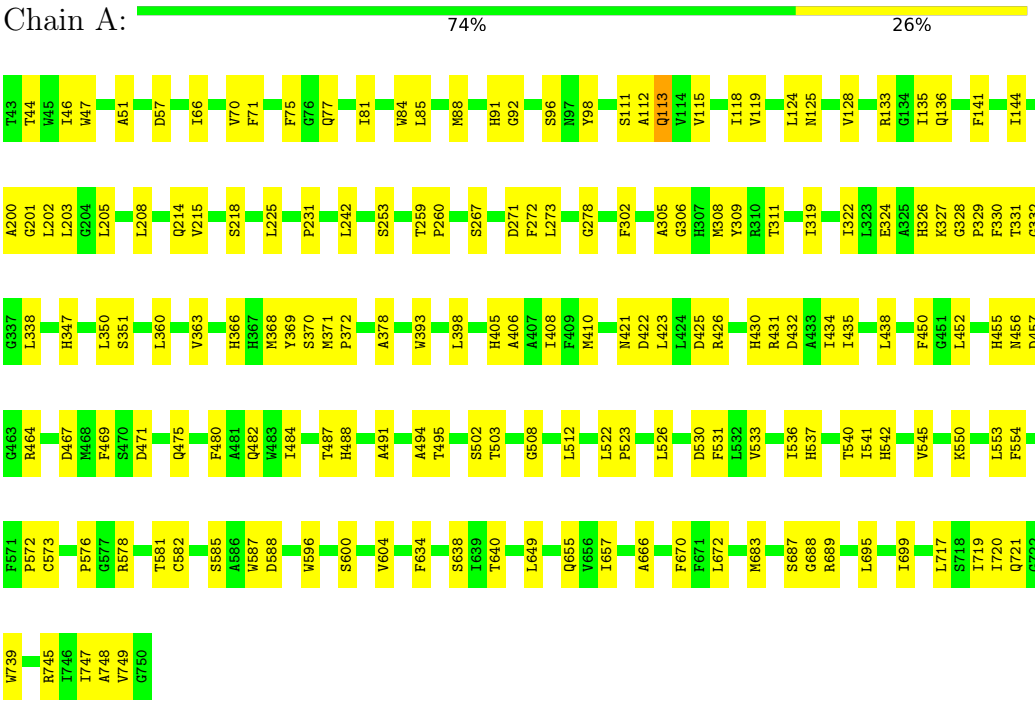
Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	C	O	0
			35	24	11	
15	b	1	Total	C	O	0
			35	24	11	

3 Residue-property plots (i)

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

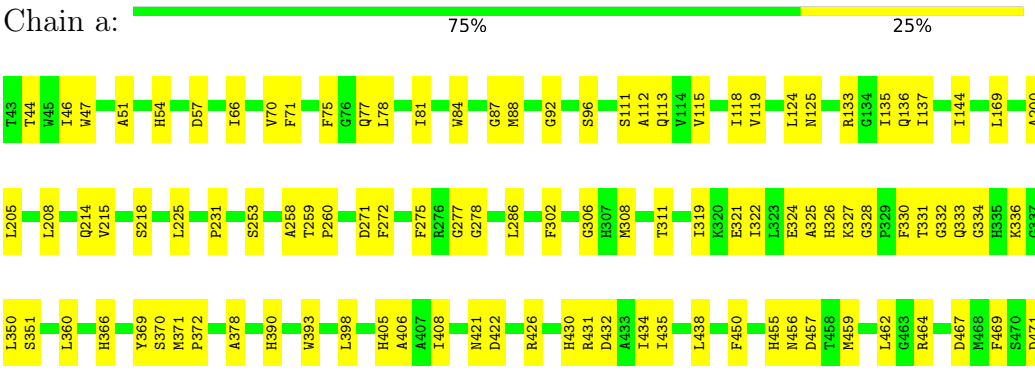
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

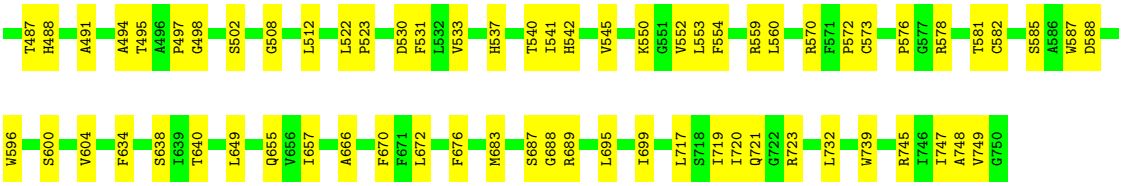
Chain A:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:

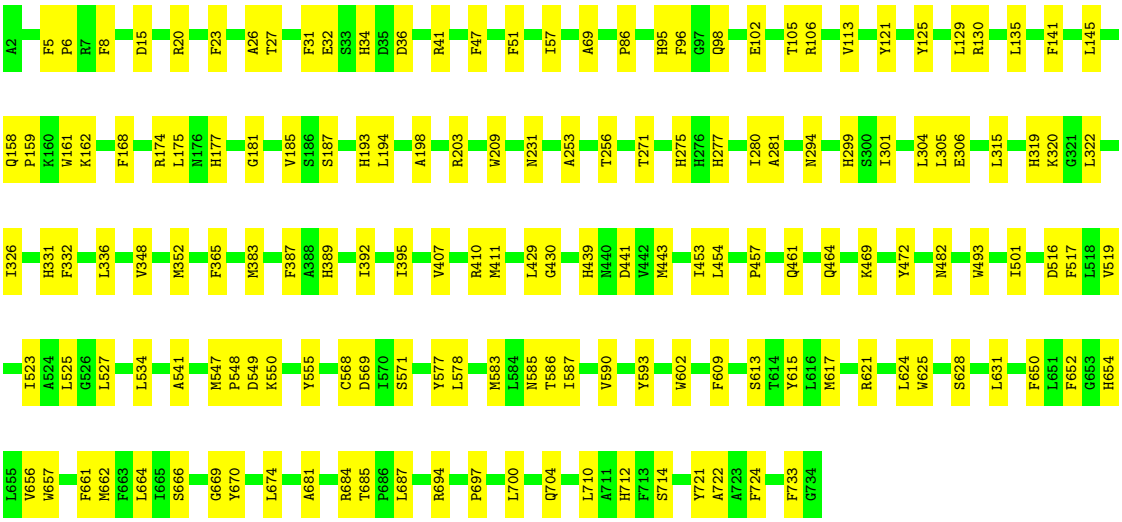




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

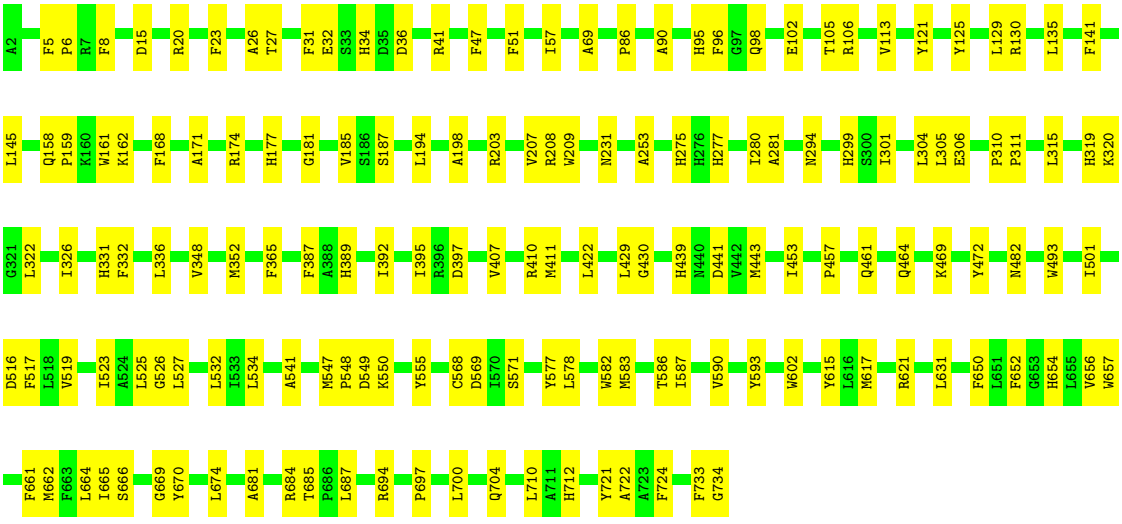




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:





• Molecule 3: Photosystem I iron-sulfur center

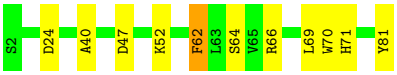
Chain C:





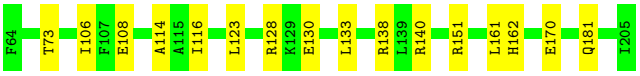
• Molecule 3: Photosystem I iron-sulfur center





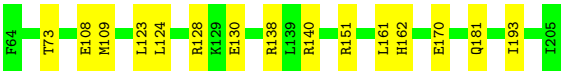
• Molecule 4: PsaD





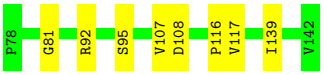
• Molecule 4: PsaD





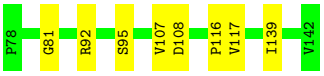
• Molecule 5: PsaE





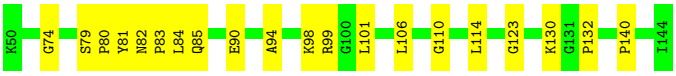
• Molecule 5: PsaE





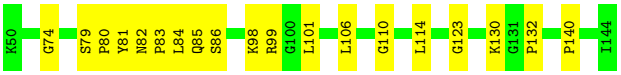
• Molecule 6: PsaH





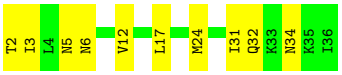
• Molecule 6: PsaH





• Molecule 7: Photosystem I reaction center subunit VIII





• Molecule 7: Photosystem I reaction center subunit VIII

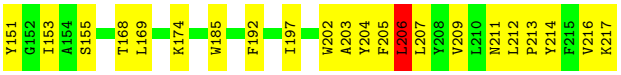




• Molecule 8: PsaL







• Molecule 8: PsaL







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3309024	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	1.526	Depositor
Minimum map value	-0.317	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0614	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: DGD, BCR, LHG, SF4, PQN, LMT, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.16	0/5754	0.31	0/7852
1	a	0.13	0/5754	0.29	0/7852
2	B	0.13	0/6063	0.28	0/8280
2	b	0.13	0/6063	0.28	0/8280
3	C	0.11	0/630	0.30	0/853
3	c	0.23	0/630	0.59	3/853 (0.4%)
4	D	0.09	0/1159	0.24	0/1565
4	d	0.10	0/1159	0.25	0/1565
5	E	0.08	0/537	0.21	0/728
5	e	0.09	0/537	0.20	0/728
6	H	0.18	0/748	0.33	0/1014
6	h	0.18	0/748	0.34	0/1014
7	I	0.18	0/272	0.31	0/371
7	i	0.18	0/272	0.31	0/371
8	L	0.32	1/1218 (0.1%)	0.60	1/1664 (0.1%)
8	l	0.19	0/1218	0.54	3/1664 (0.2%)
All	All	0.15	1/32762 (0.0%)	0.33	7/44654 (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
8	L	0	2
8	l	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	206	LEU	C-N	5.78	1.42	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	l	211	ASN	CA-C-N	-8.23	110.17	121.61
8	l	211	ASN	C-N-CA	-8.23	110.17	121.61
3	c	62	PHE	N-CA-CB	7.33	122.88	110.49
3	c	62	PHE	CA-CB-CG	-7.14	106.66	113.80
8	L	84	TRP	CA-CB-CG	7.05	127.00	113.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	L	206	LEU	Peptide,Mainchain
8	l	209	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5564	0	5418	174	0
1	a	5564	0	5417	182	0
2	B	5851	0	5636	123	0
2	b	5851	0	5636	121	0
3	C	617	0	592	9	0
3	c	617	0	592	9	0
4	D	1129	0	1134	11	0
4	d	1129	0	1134	10	0
5	E	525	0	526	4	0
5	e	525	0	526	4	0
6	H	727	0	734	42	0
6	h	727	0	734	31	0
7	I	267	0	296	10	0
7	i	267	0	296	11	0
8	L	1185	0	1199	69	0
8	l	1185	0	1199	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	2285	0	2317	225	0
9	B	1966	0	1928	86	0
9	H	65	0	72	3	0
9	L	261	0	210	40	0
9	a	2336	0	2387	238	0
9	b	1966	0	1928	90	0
9	h	116	0	109	42	0
9	l	261	0	226	35	0
10	A	33	0	46	6	0
10	B	33	0	46	2	0
10	a	33	0	46	5	0
10	b	33	0	46	2	0
11	A	125	0	172	9	0
11	a	76	0	98	5	0
11	l	49	0	74	4	0
12	A	160	0	224	12	0
12	B	120	0	168	11	0
12	H	40	0	56	3	0
12	I	40	0	56	1	0
12	L	120	0	168	11	0
12	a	160	0	224	22	0
12	b	120	0	168	12	0
12	h	40	0	56	2	0
12	i	40	0	56	1	0
12	l	120	0	168	12	0
13	A	8	0	0	0	0
13	C	16	0	0	0	0
13	a	8	0	0	0	0
13	c	16	0	0	0	0
14	B	66	0	96	8	0
14	b	66	0	96	6	0
15	B	35	0	46	5	0
15	b	35	0	46	5	0
All	All	42578	0	42402	1243	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 15.

The worst 5 of 1243 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)
9:L:307:CLA:HMD1	1:a:275:PHE:CD2	1.27	1.62
9:L:307:CLA:CMD	1:a:275:PHE:CD2	1.79	1.59
9:L:307:CLA:HMD3	1:a:275:PHE:CE2	1.39	1.57
9:A:819:CLA:CBB	9:A:821:CLA:CMA	1.84	1.52
1:A:322:ILE:HG21	9:A:819:CLA:CGA	1.45	1.44

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	706/708 (100%)	680 (96%)	25 (4%)	1 (0%)	48	71
1	a	706/708 (100%)	679 (96%)	26 (4%)	1 (0%)	48	71
2	B	731/733 (100%)	711 (97%)	20 (3%)	0	100	100
2	b	731/733 (100%)	710 (97%)	21 (3%)	0	100	100
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	D	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
4	d	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
5	E	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
5	e	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
6	H	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
6	h	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
7	I	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
7	i	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
8	L	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
8	l	157/159 (99%)	149 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4002/4034 (99%)	3871 (97%)	129 (3%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	115	VAL
1	A	115	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	571/571 (100%)	570 (100%)	1 (0%)	87 95
1	a	571/571 (100%)	571 (100%)	0	100 100
2	B	596/596 (100%)	596 (100%)	0	100 100
2	b	596/596 (100%)	596 (100%)	0	100 100
3	C	71/71 (100%)	71 (100%)	0	100 100
3	c	71/71 (100%)	71 (100%)	0	100 100
4	D	121/121 (100%)	121 (100%)	0	100 100
4	d	121/121 (100%)	121 (100%)	0	100 100
5	E	58/58 (100%)	58 (100%)	0	100 100
5	e	58/58 (100%)	58 (100%)	0	100 100
6	H	77/77 (100%)	77 (100%)	0	100 100
6	h	77/77 (100%)	77 (100%)	0	100 100
7	I	31/31 (100%)	31 (100%)	0	100 100
7	i	31/31 (100%)	31 (100%)	0	100 100
8	L	123/123 (100%)	121 (98%)	2 (2%)	55 73
8	l	123/123 (100%)	123 (100%)	0	100 100
All	All	3296/3296 (100%)	3293 (100%)	3 (0%)	87 95

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

Mol	Chain	Res	Type
1	A	113	GLN
8	L	80	PRO
8	L	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	384	GLN
2	b	158	GLN
2	b	114	ASN
2	b	294	ASN
2	B	158	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

202 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	$\#\|Z\|>2$
9	CLA	B	816	2	50,54,73	1.34	6 (12%)	60,90,113	1.13	4 (6%)
9	CLA	B	817	2	59,63,73	1.26	6 (10%)	71,101,113	1.00	4 (5%)
9	CLA	b	840	-	52,56,73	1.35	7 (13%)	62,92,113	0.99	3 (4%)
9	CLA	A	823	1	69,73,73	1.19	7 (10%)	83,113,113	0.89	5 (6%)
9	CLA	a	802	-	69,73,73	1.15	7 (10%)	83,113,113	0.98	5 (6%)
13	SF4	a	845	1,2	0,12,12	-	-	-		
14	DGD	B	837	-	67,67,67	0.81	2 (2%)	81,81,81	1.01	3 (3%)
9	CLA	A	832	1	69,73,73	1.16	6 (8%)	83,113,113	0.98	4 (4%)
10	PQN	b	833	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
13	SF4	c	102	3	0,12,12	-	-	-		
9	CLA	B	806	2	69,73,73	1.18	7 (10%)	83,113,113	0.94	3 (3%)
9	CLA	a	807	-	69,73,73	1.10	6 (8%)	83,113,113	0.98	4 (4%)
9	CLA	B	810	2	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
12	BCR	B	834	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	12 (21%)
9	CLA	A	809	-	69,73,73	1.16	6 (8%)	83,113,113	0.91	3 (3%)
13	SF4	c	101	3	0,12,12	-	-	-		
14	DGD	b	837	-	67,67,67	0.81	2 (2%)	81,81,81	1.02	4 (4%)
9	CLA	b	816	2	50,54,73	1.33	6 (12%)	60,90,113	1.15	4 (6%)
9	CLA	b	817	2	59,63,73	1.26	6 (10%)	71,101,113	1.00	4 (5%)
9	CLA	b	821	-	68,72,73	1.21	7 (10%)	85,112,113	0.96	4 (4%)
9	CLA	B	822	2	51,55,73	1.40	6 (11%)	61,91,113	1.06	4 (6%)
9	CLA	B	803	2	69,73,73	1.17	7 (10%)	83,113,113	0.89	4 (4%)
15	LMT	b	838	-	36,36,36	0.22	0	47,47,47	0.41	0
9	CLA	b	813	2	47,52,73	1.28	5 (10%)	55,87,113	1.07	3 (5%)
9	CLA	A	814	-	49,53,73	1.38	7 (14%)	59,89,113	1.18	6 (10%)
12	BCR	b	834	-	41,41,41	1.71	8 (19%)	56,56,56	1.68	13 (23%)
9	CLA	a	822	-	69,73,73	1.14	6 (8%)	83,113,113	0.94	4 (4%)
12	BCR	L	306	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	12 (21%)
9	CLA	a	815	1	69,73,73	1.18	6 (8%)	83,113,113	0.92	3 (3%)
9	CLA	a	804	1	69,73,73	1.16	7 (10%)	83,113,113	0.98	4 (4%)
9	CLA	a	836	-	69,73,73	1.13	5 (7%)	83,113,113	1.06	5 (6%)
9	CLA	b	818	2	63,67,73	1.19	6 (9%)	75,105,113	1.07	5 (6%)
9	CLA	B	819	2	64,68,73	1.24	7 (10%)	77,107,113	0.98	4 (5%)
10	PQN	A	837	-	34,34,34	0.35	0	42,45,45	0.56	0
15	LMT	B	838	-	36,36,36	0.21	0	47,47,47	0.40	0
12	BCR	B	835	-	41,41,41	1.70	8 (19%)	56,56,56	1.70	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	a	816	1	69,73,73	1.14	7 (10%)	83,113,113	1.07	8 (9%)
9	CLA	a	820	1	55,59,73	3.04	16 (29%)	66,96,113	3.57	30 (45%)
9	CLA	A	801	1	69,73,73	1.16	7 (10%)	83,113,113	1.00	5 (6%)
9	CLA	a	837	1	52,56,73	1.35	6 (11%)	62,92,113	1.08	5 (8%)
9	CLA	b	820	-	54,58,73	1.44	7 (12%)	65,95,113	1.12	5 (7%)
9	CLA	a	824	1	69,73,73	1.16	7 (10%)	83,113,113	0.91	5 (6%)
12	BCR	A	840	-	41,41,41	1.69	8 (19%)	56,56,56	1.60	12 (21%)
9	CLA	A	846	-	69,73,73	1.17	7 (10%)	83,113,113	0.99	4 (4%)
9	CLA	A	805	1	69,73,73	1.17	6 (8%)	83,113,113	0.90	3 (3%)
13	SF4	A	844	1,2	0,12,12	-	-	-		
9	CLA	B	812	2	58,62,73	1.33	8 (13%)	73,100,113	1.10	4 (5%)
9	CLA	a	818	1	49,53,73	1.36	6 (12%)	59,89,113	0.96	3 (5%)
9	CLA	a	835	1	51,55,73	1.35	6 (11%)	61,91,113	1.01	4 (6%)
9	CLA	l	305	8	53,57,73	1.37	6 (11%)	62,93,113	1.20	5 (8%)
9	CLA	B	802	-	69,73,73	1.19	7 (10%)	83,113,113	0.91	4 (4%)
13	SF4	C	102	3	0,12,12	-	-	-		
9	CLA	A	822	-	69,73,73	1.17	6 (8%)	83,113,113	0.89	3 (3%)
9	CLA	a	808	1	69,73,73	1.14	6 (8%)	83,113,113	1.02	5 (6%)
9	CLA	b	803	2	69,73,73	1.17	7 (10%)	83,113,113	0.90	4 (4%)
12	BCR	L	305	-	41,41,41	1.69	8 (19%)	56,56,56	1.59	10 (17%)
9	CLA	B	805	2	49,53,73	1.41	7 (14%)	59,89,113	1.11	4 (6%)
9	CLA	b	814	2	69,73,73	1.17	7 (10%)	83,113,113	0.93	3 (3%)
9	CLA	A	828	1	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
9	CLA	A	831	1	55,59,73	1.36	7 (12%)	66,96,113	1.05	4 (6%)
9	CLA	a	812	1	49,53,73	1.43	8 (16%)	59,89,113	1.24	5 (8%)
9	CLA	a	810	1	58,62,73	1.24	6 (10%)	69,99,113	1.03	4 (5%)
9	CLA	a	826	1	69,73,73	1.21	7 (10%)	83,113,113	0.92	4 (4%)
9	CLA	b	832	2	69,73,73	1.17	6 (8%)	83,113,113	0.98	3 (3%)
9	CLA	b	809	-	69,73,73	1.21	7 (10%)	83,113,113	0.91	4 (4%)
9	CLA	a	827	1	69,73,73	1.25	8 (11%)	83,113,113	0.95	4 (4%)
9	CLA	b	802	-	69,73,73	1.24	8 (11%)	83,113,113	0.98	5 (6%)
12	BCR	a	842	-	41,41,41	1.71	8 (19%)	56,56,56	1.58	11 (19%)
9	CLA	L	304	-	54,58,73	1.30	6 (11%)	65,95,113	1.18	5 (7%)
9	CLA	B	829	2	69,73,73	1.16	6 (8%)	83,113,113	1.02	5 (6%)
9	CLA	l	306	8	69,73,73	1.16	6 (8%)	83,113,113	0.95	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	b	824	-	64,68,73	1.26	7 (10%)	77,107,113	0.94	3 (3%)
9	CLA	B	807	2	69,73,73	1.22	8 (11%)	83,113,113	0.88	3 (3%)
12	BCR	a	841	-	41,41,41	1.70	8 (19%)	56,56,56	1.61	12 (21%)
9	CLA	b	810	2	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
9	CLA	L	308	11	56,60,73	1.40	7 (12%)	67,97,113	1.55	10 (14%)
9	CLA	b	830	2	51,55,73	1.36	7 (13%)	61,91,113	1.10	4 (6%)
9	CLA	A	833	1	69,73,73	1.17	6 (8%)	83,113,113	0.94	4 (4%)
9	CLA	b	807	2	69,73,73	1.21	8 (11%)	83,113,113	0.88	3 (3%)
9	CLA	b	806	2	69,73,73	1.19	7 (10%)	83,113,113	0.94	3 (3%)
11	LHG	a	840	9	26,26,48	0.35	0	29,32,54	0.49	0
9	CLA	A	836	1	52,56,73	1.35	6 (11%)	62,92,113	1.10	5 (8%)
9	CLA	B	832	2	69,73,73	1.18	6 (8%)	83,113,113	0.98	3 (3%)
9	CLA	B	827	2	49,53,73	1.34	7 (14%)	59,89,113	1.25	5 (8%)
12	BCR	l	308	-	41,41,41	1.68	8 (19%)	56,56,56	1.59	10 (17%)
9	CLA	a	847	1	69,73,73	1.20	8 (11%)	83,113,113	0.98	4 (4%)
11	LHG	A	838	-	48,48,48	0.28	0	51,54,54	0.32	0
9	CLA	b	826	2	52,56,73	1.34	6 (11%)	62,92,113	1.08	4 (6%)
9	CLA	b	839	2	52,56,73	1.33	6 (11%)	62,92,113	1.07	4 (6%)
9	CLA	A	808	1	69,73,73	1.13	6 (8%)	83,113,113	1.08	4 (4%)
9	CLA	b	805	2	49,53,73	1.41	7 (14%)	59,89,113	1.12	4 (6%)
9	CLA	A	825	1	69,73,73	1.21	8 (11%)	83,113,113	0.92	4 (4%)
9	CLA	B	804	-	69,73,73	1.17	7 (10%)	83,113,113	1.00	5 (6%)
12	BCR	h	203	-	41,41,41	1.70	8 (19%)	56,56,56	1.72	12 (21%)
12	BCR	a	844	-	41,41,41	1.69	8 (19%)	56,56,56	1.60	11 (19%)
9	CLA	B	814	2	69,73,73	1.17	7 (10%)	83,113,113	0.92	3 (3%)
9	CLA	A	811	1	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
9	CLA	a	833	1	69,73,73	1.16	7 (10%)	83,113,113	0.97	4 (4%)
9	CLA	A	803	-	59,63,73	1.25	7 (11%)	71,101,113	1.04	5 (7%)
9	CLA	a	825	1	69,73,73	1.13	6 (8%)	83,113,113	1.05	5 (6%)
9	CLA	a	829	1	69,73,73	1.18	7 (10%)	83,113,113	0.95	4 (4%)
9	CLA	A	835	-	69,73,73	1.13	5 (7%)	83,113,113	1.06	5 (6%)
12	BCR	b	835	-	41,41,41	1.69	8 (19%)	56,56,56	1.68	13 (23%)
9	CLA	A	834	1	51,55,73	1.35	6 (11%)	61,91,113	1.01	4 (6%)
9	CLA	A	817	1	69,73,73	1.17	7 (10%)	83,113,113	0.98	4 (4%)
9	CLA	B	808	2	59,63,73	1.28	6 (10%)	71,101,113	1.01	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	A	807	-	69,73,73	1.13	6 (8%)	83,113,113	0.94	4 (4%)
12	BCR	A	841	-	41,41,41	1.71	8 (19%)	56,56,56	1.56	11 (19%)
9	CLA	b	828	2	55,59,73	1.37	8 (14%)	66,96,113	1.05	4 (6%)
9	CLA	B	820	-	54,58,73	1.38	7 (12%)	65,95,113	1.01	4 (6%)
9	CLA	A	812	1	49,53,73	1.43	7 (14%)	59,89,113	1.29	7 (11%)
9	CLA	H	201	6	69,73,73	1.25	8 (11%)	83,113,113	0.98	4 (4%)
11	LHG	a	839	-	48,48,48	0.28	0	51,54,54	0.32	0
9	CLA	B	828	2	55,59,73	1.38	8 (14%)	66,96,113	1.06	4 (6%)
9	CLA	B	824	-	64,68,73	1.25	7 (10%)	77,107,113	0.94	3 (3%)
9	CLA	a	819	-	69,73,73	1.26	10 (14%)	83,113,113	1.17	7 (8%)
9	CLA	b	808	2	59,63,73	1.28	7 (11%)	71,101,113	1.02	4 (5%)
9	CLA	b	812	2	58,62,73	1.36	7 (12%)	73,100,113	1.09	5 (6%)
9	CLA	a	805	1	69,73,73	1.18	6 (8%)	83,113,113	0.90	4 (4%)
9	CLA	A	826	1	69,73,73	1.26	8 (11%)	83,113,113	0.95	4 (4%)
9	CLA	b	819	2	64,68,73	1.23	7 (10%)	77,107,113	1.01	4 (5%)
9	CLA	b	827	2	49,53,73	1.34	7 (14%)	59,89,113	1.26	5 (8%)
9	CLA	A	813	1	54,58,73	1.28	6 (11%)	65,95,113	1.11	4 (6%)
9	CLA	B	831	-	69,73,73	1.21	8 (11%)	83,113,113	0.93	4 (4%)
9	CLA	h	202	6	69,73,73	1.23	8 (11%)	83,113,113	0.99	5 (6%)
9	CLA	h	201	1	55,59,73	1.58	11 (20%)	66,96,113	1.86	14 (21%)
9	CLA	a	801	1	69,73,73	1.16	7 (10%)	83,113,113	1.00	5 (6%)
9	CLA	A	802	-	69,73,73	1.15	7 (10%)	83,113,113	0.98	4 (4%)
9	CLA	B	826	2	52,56,73	1.34	6 (11%)	62,92,113	1.08	4 (6%)
9	CLA	a	806	-	69,73,73	1.14	6 (8%)	83,113,113	0.91	4 (4%)
9	CLA	A	821	-	69,73,73	1.16	7 (10%)	83,113,113	1.01	5 (6%)
9	CLA	a	814	-	49,53,73	1.37	7 (14%)	59,89,113	1.18	6 (10%)
9	CLA	a	828	1	54,58,73	1.31	6 (11%)	65,95,113	1.01	3 (4%)
9	CLA	b	801	-	69,73,73	1.20	7 (10%)	83,113,113	0.97	4 (4%)
9	CLA	B	813	2	47,52,73	1.29	5 (10%)	55,87,113	1.05	3 (5%)
9	CLA	l	302	-	56,60,73	1.35	8 (14%)	67,97,113	0.98	3 (4%)
9	CLA	a	830	1	69,73,73	1.21	8 (11%)	83,113,113	1.03	4 (4%)
12	BCR	L	301	-	41,41,41	1.68	8 (19%)	56,56,56	1.46	8 (14%)
11	LHG	l	303	-	48,48,48	0.28	0	51,54,54	0.34	0
13	SF4	C	101	3	0,12,12	-	-	-		
9	CLA	a	846	-	69,73,73	1.17	7 (10%)	83,113,113	0.98	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	A	819	-	69,73,73	3.00	13 (18%)	83,113,113	10.30	14 (16%)
9	CLA	b	822	2	51,55,73	1.39	7 (13%)	61,91,113	1.09	5 (8%)
9	CLA	b	815	2	69,73,73	1.21	7 (10%)	83,113,113	0.98	5 (6%)
9	CLA	l	307	-	54,58,73	1.33	6 (11%)	65,95,113	1.09	5 (7%)
9	CLA	A	818	1	49,53,73	1.37	6 (12%)	59,89,113	0.97	3 (5%)
12	BCR	H	202	-	41,41,41	1.70	8 (19%)	56,56,56	1.78	13 (23%)
9	CLA	a	817	1	69,73,73	1.16	6 (8%)	83,113,113	0.99	4 (4%)
12	BCR	a	843	-	41,41,41	1.70	8 (19%)	56,56,56	1.56	12 (21%)
9	CLA	A	829	1	69,73,73	1.20	7 (10%)	83,113,113	1.04	4 (4%)
9	CLA	b	811	2	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
9	CLA	L	303	8	69,73,73	1.15	6 (8%)	83,113,113	0.92	4 (4%)
9	CLA	B	823	2	69,73,73	1.19	7 (10%)	83,113,113	1.05	5 (6%)
9	CLA	A	816	1	69,73,73	1.14	6 (8%)	83,113,113	1.03	5 (6%)
9	CLA	B	839	2	52,56,73	1.33	6 (11%)	62,92,113	1.08	4 (6%)
9	CLA	b	804	-	69,73,73	1.16	7 (10%)	83,113,113	0.99	5 (6%)
9	CLA	A	804	1	69,73,73	1.16	6 (8%)	83,113,113	0.97	4 (4%)
9	CLA	B	825	2	69,73,73	1.20	8 (11%)	83,113,113	0.96	4 (4%)
9	CLA	A	830	1	54,58,73	1.26	5 (9%)	65,95,113	1.05	5 (7%)
9	CLA	L	307	-	49,53,73	1.30	5 (10%)	59,89,113	1.53	11 (18%)
9	CLA	a	823	-	69,73,73	1.17	6 (8%)	83,113,113	0.91	3 (3%)
9	CLA	a	834	1	69,73,73	1.17	6 (8%)	83,113,113	0.94	4 (4%)
9	CLA	B	809	-	69,73,73	1.20	7 (10%)	83,113,113	0.89	4 (4%)
9	CLA	a	803	-	59,63,73	1.25	7 (11%)	71,101,113	1.03	5 (7%)
12	BCR	I	101	-	41,41,41	1.67	8 (19%)	56,56,56	1.53	11 (19%)
9	CLA	A	827	1	54,58,73	1.31	6 (11%)	65,95,113	1.04	3 (4%)
9	CLA	a	832	1	55,59,73	1.37	7 (12%)	66,96,113	1.04	4 (6%)
12	BCR	A	842	-	41,41,41	1.68	8 (19%)	56,56,56	1.52	11 (19%)
9	CLA	A	815	1	69,73,73	1.19	6 (8%)	83,113,113	0.91	3 (3%)
9	CLA	B	801	-	69,73,73	1.20	8 (11%)	83,113,113	0.98	5 (6%)
10	PQN	a	838	-	34,34,34	0.36	0	42,45,45	0.55	0
12	BCR	l	309	-	41,41,41	1.69	8 (19%)	56,56,56	1.69	13 (23%)
12	BCR	l	304	-	41,41,41	1.67	8 (19%)	56,56,56	1.47	9 (16%)
9	CLA	B	815	2	69,73,73	1.22	8 (11%)	83,113,113	0.96	6 (7%)
11	LHG	A	845	-	48,48,48	0.28	0	51,54,54	0.36	0
9	CLA	a	809	-	69,73,73	1.16	6 (8%)	83,113,113	0.91	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	BCR	i	101	-	41,41,41	1.66	8 (19%)	56,56,56	1.53	11 (19%)
12	BCR	A	843	-	41,41,41	1.69	8 (19%)	56,56,56	1.57	10 (17%)
9	CLA	a	831	1	54,58,73	1.22	5 (9%)	65,95,113	1.09	7 (10%)
9	CLA	b	823	2	69,73,73	1.18	6 (8%)	83,113,113	1.06	5 (6%)
9	CLA	l	301	-	49,53,73	1.40	6 (12%)	59,89,113	1.83	12 (20%)
9	CLA	A	806	-	69,73,73	1.12	7 (10%)	83,113,113	1.13	9 (10%)
9	CLA	b	829	2	69,73,73	1.16	6 (8%)	83,113,113	1.02	4 (4%)
9	CLA	A	847	1	69,73,73	1.20	8 (11%)	83,113,113	0.97	4 (4%)
9	CLA	B	830	2	51,55,73	1.35	7 (13%)	61,91,113	1.12	5 (8%)
9	CLA	a	813	1	54,58,73	1.28	6 (11%)	65,95,113	1.07	4 (6%)
9	CLA	A	820	1	59,63,73	1.20	6 (10%)	71,101,113	1.08	4 (5%)
12	BCR	B	836	-	41,41,41	1.66	8 (19%)	56,56,56	1.57	10 (17%)
9	CLA	B	818	2	63,67,73	1.19	6 (9%)	75,105,113	1.07	5 (6%)
9	CLA	b	825	2	69,73,73	1.20	8 (11%)	83,113,113	0.98	4 (4%)
11	LHG	A	839	-	26,26,48	0.36	0	29,32,54	0.46	0
9	CLA	B	821	-	68,72,73	1.21	7 (10%)	85,112,113	0.95	4 (4%)
9	CLA	B	840	-	52,56,73	1.34	7 (13%)	62,92,113	0.98	3 (4%)
9	CLA	a	811	1	69,73,73	1.16	6 (8%)	83,113,113	0.95	4 (4%)
9	CLA	b	831	-	69,73,73	1.21	8 (11%)	83,113,113	0.93	4 (4%)
10	PQN	B	833	-	34,34,34	0.36	0	42,45,45	0.55	1 (2%)
9	CLA	A	810	1	58,62,73	1.25	6 (10%)	69,99,113	1.06	4 (5%)
9	CLA	A	824	1	69,73,73	1.14	6 (8%)	83,113,113	1.05	6 (7%)
9	CLA	L	302	8	53,57,73	1.37	6 (11%)	62,93,113	1.19	5 (8%)
9	CLA	a	821	1	59,63,73	1.22	6 (10%)	71,101,113	1.07	4 (5%)
9	CLA	B	811	2	69,73,73	1.16	6 (8%)	83,113,113	0.96	4 (4%)
12	BCR	b	836	-	41,41,41	1.66	8 (19%)	56,56,56	1.57	10 (17%)

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
9	CLA	B	816	2	-	11/17/93/115	-
9	CLA	B	817	2	-	12/27/103/115	-
9	CLA	b	840	-	-	8/19/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	823	1	-	13/39/115/115	-
9	CLA	a	802	-	-	17/39/115/115	-
14	DGD	B	837	-	-	32/55/95/95	0/2/2/2
13	SF4	a	845	1,2	-	-	0/6/5/5
9	CLA	A	832	1	-	14/39/115/115	-
10	PQN	b	833	-	-	2/23/43/43	0/2/2/2
13	SF4	c	102	3	-	-	0/6/5/5
9	CLA	B	806	2	-	17/39/115/115	-
9	CLA	a	807	-	-	23/39/115/115	-
9	CLA	B	810	2	-	16/39/115/115	-
12	BCR	B	834	-	-	22/29/63/63	0/2/2/2
9	CLA	A	809	-	-	20/39/115/115	-
14	DGD	b	837	-	-	29/55/95/95	0/2/2/2
13	SF4	c	101	3	-	-	0/6/5/5
9	CLA	b	816	2	-	11/17/93/115	-
9	CLA	b	817	2	-	12/27/103/115	-
9	CLA	b	821	-	-	15/37/113/115	-
9	CLA	B	822	2	-	10/18/94/115	-
9	CLA	B	803	2	-	15/39/115/115	-
15	LMT	b	838	-	-	17/21/61/61	0/2/2/2
9	CLA	b	813	2	-	4/14/91/115	-
9	CLA	A	814	-	-	4/15/91/115	-
12	BCR	b	834	-	-	20/29/63/63	0/2/2/2
9	CLA	a	822	-	-	14/39/115/115	-
12	BCR	L	306	-	-	18/29/63/63	0/2/2/2
9	CLA	a	815	1	-	27/39/115/115	-
9	CLA	a	804	1	-	11/39/115/115	-
9	CLA	a	836	-	-	21/39/115/115	-
9	CLA	b	818	2	-	17/32/108/115	-
9	CLA	B	819	2	-	18/33/109/115	-
10	PQN	A	837	-	-	12/23/43/43	0/2/2/2
15	LMT	B	838	-	-	16/21/61/61	0/2/2/2
12	BCR	B	835	-	-	26/29/63/63	0/2/2/2
9	CLA	a	816	1	-	19/39/115/115	-
9	CLA	a	820	1	-	12/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	801	1	-	18/39/115/115	-
9	CLA	a	837	1	-	6/19/95/115	-
9	CLA	b	820	-	-	9/21/97/115	-
9	CLA	a	824	1	-	23/39/115/115	-
12	BCR	A	840	-	-	18/29/63/63	0/2/2/2
9	CLA	A	846	-	-	17/39/115/115	-
9	CLA	A	805	1	-	17/39/115/115	-
13	SF4	A	844	1,2	-	-	0/6/5/5
9	CLA	B	812	2	-	11/25/101/115	-
9	CLA	a	818	1	-	7/15/91/115	-
9	CLA	a	835	1	-	10/18/94/115	-
9	CLA	l	305	8	-	8/20/96/115	-
9	CLA	B	802	-	-	22/39/115/115	-
13	SF4	C	102	3	-	-	0/6/5/5
9	CLA	A	822	-	-	14/39/115/115	-
9	CLA	a	808	1	-	23/39/115/115	-
9	CLA	b	803	2	-	15/39/115/115	-
12	BCR	L	305	-	-	16/29/63/63	0/2/2/2
9	CLA	B	805	2	-	5/15/91/115	-
9	CLA	b	814	2	-	19/39/115/115	-
9	CLA	A	828	1	-	13/39/115/115	-
9	CLA	A	831	1	-	12/23/99/115	-
9	CLA	a	812	1	-	3/15/91/115	-
9	CLA	a	810	1	-	10/26/102/115	-
9	CLA	a	826	1	-	16/39/115/115	-
9	CLA	b	832	2	-	13/39/115/115	-
9	CLA	b	809	-	-	10/39/115/115	-
9	CLA	a	827	1	-	14/39/115/115	-
9	CLA	b	802	-	-	20/39/115/115	-
12	BCR	a	842	-	-	20/29/63/63	0/2/2/2
9	CLA	L	304	-	-	9/21/97/115	-
9	CLA	B	829	2	-	13/39/115/115	-
9	CLA	l	306	8	-	20/39/115/115	-
9	CLA	b	824	-	-	19/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	807	2	-	19/39/115/115	-
12	BCR	a	841	-	-	20/29/63/63	0/2/2/2
9	CLA	b	810	2	-	16/39/115/115	-
9	CLA	L	308	11	-	11/24/100/115	-
9	CLA	b	830	2	-	3/18/94/115	-
9	CLA	A	833	1	-	22/39/115/115	-
9	CLA	b	807	2	-	19/39/115/115	-
9	CLA	b	806	2	-	14/39/115/115	-
11	LHG	a	840	9	-	16/31/31/53	-
9	CLA	A	836	1	-	6/19/95/115	-
9	CLA	B	832	2	-	11/39/115/115	-
9	CLA	B	827	2	-	7/15/91/115	-
12	BCR	l	308	-	-	17/29/63/63	0/2/2/2
9	CLA	a	847	1	-	17/39/115/115	-
11	LHG	A	838	-	-	34/53/53/53	-
9	CLA	b	826	2	-	7/19/95/115	-
9	CLA	b	839	2	-	7/19/95/115	-
9	CLA	A	808	1	-	23/39/115/115	-
9	CLA	b	805	2	-	5/15/91/115	-
9	CLA	A	825	1	-	17/39/115/115	-
9	CLA	B	804	-	-	17/39/115/115	-
12	BCR	h	203	-	-	23/29/63/63	0/2/2/2
12	BCR	a	844	-	-	20/29/63/63	0/2/2/2
9	CLA	B	814	2	-	18/39/115/115	-
9	CLA	A	811	1	-	23/39/115/115	-
9	CLA	a	833	1	-	14/39/115/115	-
9	CLA	A	803	-	-	12/27/103/115	-
9	CLA	a	825	1	-	21/39/115/115	-
9	CLA	a	829	1	-	13/39/115/115	-
9	CLA	A	835	-	-	21/39/115/115	-
12	BCR	b	835	-	-	24/29/63/63	0/2/2/2
9	CLA	A	834	1	-	10/18/94/115	-
9	CLA	A	817	1	-	22/39/115/115	-
9	CLA	B	808	2	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	A	807	-	-	23/39/115/115	-
12	BCR	A	841	-	-	19/29/63/63	0/2/2/2
9	CLA	b	828	2	-	10/23/99/115	-
9	CLA	B	820	-	-	10/21/97/115	-
9	CLA	A	812	1	-	4/15/91/115	-
9	CLA	H	201	6	-	21/39/115/115	-
11	LHG	a	839	-	-	34/53/53/53	-
9	CLA	B	828	2	-	6/23/99/115	-
9	CLA	B	824	-	-	19/33/109/115	-
9	CLA	a	819	-	-	18/39/115/115	-
9	CLA	b	808	2	-	9/27/103/115	-
9	CLA	b	812	2	-	6/25/101/115	-
9	CLA	a	805	1	-	16/39/115/115	-
9	CLA	A	826	1	-	18/39/115/115	-
9	CLA	b	819	2	-	20/33/109/115	-
9	CLA	b	827	2	-	6/15/91/115	-
9	CLA	A	813	1	-	8/21/97/115	-
9	CLA	B	831	-	-	13/39/115/115	-
9	CLA	h	202	6	-	22/39/115/115	-
9	CLA	h	201	1	-	15/23/99/115	-
9	CLA	a	801	1	-	16/39/115/115	-
9	CLA	A	802	-	-	16/39/115/115	-
9	CLA	B	826	2	-	8/19/95/115	-
9	CLA	a	806	-	-	24/39/115/115	-
9	CLA	A	821	-	-	20/39/115/115	-
9	CLA	a	814	-	-	4/15/91/115	-
9	CLA	a	828	1	-	6/21/97/115	-
9	CLA	b	801	-	-	22/39/115/115	-
9	CLA	B	813	2	-	6/14/91/115	-
9	CLA	l	302	-	-	11/24/100/115	-
9	CLA	a	830	1	-	24/39/115/115	-
12	BCR	L	301	-	-	16/29/63/63	0/2/2/2
11	LHG	l	303	-	-	31/53/53/53	-
13	SF4	C	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	a	846	-	-	24/39/115/115	-
9	CLA	A	819	-	-	26/39/115/115	-
9	CLA	b	822	2	-	10/18/94/115	-
9	CLA	b	815	2	-	15/39/115/115	-
9	CLA	l	307	-	-	8/21/97/115	-
9	CLA	A	818	1	-	8/15/91/115	-
12	BCR	H	202	-	-	23/29/63/63	0/2/2/2
9	CLA	a	817	1	-	22/39/115/115	-
12	BCR	a	843	-	-	19/29/63/63	0/2/2/2
9	CLA	A	829	1	-	25/39/115/115	-
9	CLA	b	811	2	-	19/39/115/115	-
9	CLA	L	303	8	-	21/39/115/115	-
9	CLA	B	823	2	-	15/39/115/115	-
9	CLA	A	816	1	-	22/39/115/115	-
9	CLA	B	839	2	-	9/19/95/115	-
9	CLA	b	804	-	-	20/39/115/115	-
9	CLA	A	804	1	-	11/39/115/115	-
9	CLA	B	825	2	-	14/39/115/115	-
9	CLA	A	830	1	-	14/21/97/115	-
9	CLA	L	307	-	-	11/15/91/115	-
9	CLA	a	823	-	-	13/39/115/115	-
9	CLA	a	834	1	-	22/39/115/115	-
9	CLA	B	809	-	-	10/39/115/115	-
9	CLA	a	803	-	-	14/27/103/115	-
12	BCR	I	101	-	-	16/29/63/63	0/2/2/2
9	CLA	A	827	1	-	8/21/97/115	-
9	CLA	a	832	1	-	14/23/99/115	-
12	BCR	A	842	-	-	16/29/63/63	0/2/2/2
9	CLA	A	815	1	-	23/39/115/115	-
9	CLA	B	801	-	-	22/39/115/115	-
10	PQN	a	838	-	-	11/23/43/43	0/2/2/2
12	BCR	l	309	-	-	18/29/63/63	0/2/2/2
12	BCR	l	304	-	-	18/29/63/63	0/2/2/2
9	CLA	B	815	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LHG	A	845	-	-	35/53/53/53	-
9	CLA	a	809	-	-	20/39/115/115	-
12	BCR	i	101	-	-	17/29/63/63	0/2/2/2
12	BCR	A	843	-	-	13/29/63/63	0/2/2/2
9	CLA	a	831	1	-	10/21/97/115	-
9	CLA	b	823	2	-	18/39/115/115	-
9	CLA	l	301	-	-	8/15/91/115	-
9	CLA	A	806	-	-	24/39/115/115	-
9	CLA	b	829	2	-	14/39/115/115	-
9	CLA	A	847	1	-	23/39/115/115	-
9	CLA	B	830	2	-	3/18/94/115	-
9	CLA	a	813	1	-	6/21/97/115	-
9	CLA	A	820	1	-	13/27/103/115	-
12	BCR	B	836	-	-	16/29/63/63	0/2/2/2
9	CLA	B	818	2	-	17/32/108/115	-
9	CLA	b	825	2	-	14/39/115/115	-
11	LHG	A	839	-	-	15/31/31/53	-
9	CLA	B	821	-	-	17/37/113/115	-
9	CLA	B	840	-	-	7/19/95/115	-
9	CLA	a	811	1	-	23/39/115/115	-
9	CLA	b	831	-	-	13/39/115/115	-
10	PQN	B	833	-	-	2/23/43/43	0/2/2/2
9	CLA	A	810	1	-	10/26/102/115	-
9	CLA	A	824	1	-	19/39/115/115	-
9	CLA	L	302	8	-	8/20/96/115	-
9	CLA	a	821	1	-	14/27/103/115	-
9	CLA	B	811	2	-	18/39/115/115	-
12	BCR	b	836	-	-	16/29/63/63	0/2/2/2

The worst 5 of 1268 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	819	CLA	C1D-C2D	-16.73	1.12	1.45
9	a	820	CLA	MG-NB	12.48	2.30	2.05
9	A	819	CLA	C3D-C2D	11.31	1.70	1.39
9	a	820	CLA	MG-ND	11.03	2.27	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	819	CLA	C4D-ND	-7.44	1.27	1.37

The worst 5 of 1014 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	819	CLA	C3D-C4D-ND	-51.00	27.73	110.24
9	A	819	CLA	C3D-C2D-C1D	-47.75	40.67	105.83
9	A	819	CLA	C1D-ND-C4D	41.92	136.11	106.33
9	A	819	CLA	C2D-C1D-ND	-34.87	84.41	110.10
9	A	819	CLA	CHD-C1D-ND	22.23	144.88	124.45

There are no chirality outliers.

5 of 3012 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	801	CLA	C2B-C3B-CAB-CBB
9	A	801	CLA	C4B-C3B-CAB-CBB
9	A	801	CLA	CBD-CGD-O2D-CED
9	A	801	CLA	O1D-CGD-O2D-CED
9	A	801	CLA	C1-C2-C3-C4

There are no ring outliers.

187 monomers are involved in 793 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	817	CLA	2	0
9	b	840	CLA	2	0
9	A	823	CLA	11	0
9	a	802	CLA	4	0
14	B	837	DGD	8	0
9	A	832	CLA	5	0
10	b	833	PQN	2	0
9	B	806	CLA	5	0
9	a	807	CLA	9	0
9	B	810	CLA	2	0
12	B	834	BCR	5	0
9	A	809	CLA	5	0
14	b	837	DGD	6	0
9	b	816	CLA	1	0
9	b	817	CLA	1	0
9	b	821	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	822	CLA	3	0
9	B	803	CLA	8	0
15	b	838	LMT	5	0
9	b	813	CLA	1	0
9	A	814	CLA	2	0
12	b	834	BCR	4	0
9	a	822	CLA	2	0
12	L	306	BCR	2	0
9	a	815	CLA	1	0
9	a	804	CLA	4	0
9	a	836	CLA	3	0
9	b	818	CLA	9	0
9	B	819	CLA	2	0
10	A	837	PQN	6	0
15	B	838	LMT	5	0
12	B	835	BCR	4	0
9	a	816	CLA	10	0
9	a	820	CLA	74	0
9	A	801	CLA	9	0
9	a	837	CLA	3	0
9	b	820	CLA	2	0
9	a	824	CLA	4	0
12	A	840	BCR	3	0
9	A	846	CLA	6	0
9	A	805	CLA	6	0
9	B	812	CLA	2	0
9	a	818	CLA	1	0
9	a	835	CLA	1	0
9	l	305	CLA	6	0
9	B	802	CLA	4	0
9	A	822	CLA	3	0
9	a	808	CLA	6	0
9	b	803	CLA	8	0
12	L	305	BCR	3	0
9	b	814	CLA	2	0
9	A	828	CLA	4	0
9	A	831	CLA	5	0
9	a	812	CLA	2	0
9	a	810	CLA	3	0
9	a	826	CLA	4	0
9	b	832	CLA	3	0
9	b	809	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	827	CLA	9	0
9	b	802	CLA	5	0
12	a	842	BCR	6	0
9	L	304	CLA	1	0
9	B	829	CLA	3	0
9	l	306	CLA	7	0
9	b	824	CLA	3	0
9	B	807	CLA	3	0
12	a	841	BCR	5	0
9	b	810	CLA	3	0
9	L	308	CLA	11	0
9	b	830	CLA	2	0
9	A	833	CLA	6	0
9	b	807	CLA	4	0
9	b	806	CLA	5	0
11	a	840	LHG	4	0
9	A	836	CLA	4	0
9	B	832	CLA	3	0
9	B	827	CLA	3	0
12	l	308	BCR	3	0
9	a	847	CLA	9	0
11	A	838	LHG	1	0
9	b	839	CLA	2	0
9	A	808	CLA	3	0
9	A	825	CLA	6	0
9	B	804	CLA	7	0
12	h	203	BCR	2	0
12	a	844	BCR	7	0
9	B	814	CLA	2	0
9	A	811	CLA	5	0
9	a	833	CLA	8	0
9	A	803	CLA	4	0
9	a	825	CLA	11	0
9	a	829	CLA	3	0
9	A	835	CLA	4	0
12	b	835	BCR	6	0
9	A	817	CLA	10	0
9	B	808	CLA	2	0
9	A	807	CLA	9	0
12	A	841	BCR	5	0
9	b	828	CLA	2	0
9	B	820	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	812	CLA	1	0
9	H	201	CLA	3	0
11	a	839	LHG	1	0
9	B	824	CLA	2	0
9	a	819	CLA	13	0
9	b	808	CLA	2	0
9	b	812	CLA	1	0
9	a	805	CLA	6	0
9	A	826	CLA	8	0
9	b	819	CLA	1	0
9	b	827	CLA	5	0
9	A	813	CLA	1	0
9	B	831	CLA	2	0
9	h	202	CLA	6	0
9	h	201	CLA	36	0
9	a	801	CLA	7	0
9	A	802	CLA	6	0
9	a	806	CLA	5	0
9	A	821	CLA	18	0
9	a	814	CLA	2	0
9	b	801	CLA	2	0
9	B	813	CLA	3	0
9	l	302	CLA	10	0
9	a	830	CLA	6	0
12	L	301	BCR	6	0
11	l	303	LHG	4	0
9	a	846	CLA	7	0
9	A	819	CLA	71	0
9	b	822	CLA	4	0
9	b	815	CLA	3	0
9	l	307	CLA	3	0
9	A	818	CLA	1	0
12	H	202	BCR	3	0
9	a	817	CLA	9	0
12	a	843	BCR	5	0
9	A	829	CLA	5	0
9	b	811	CLA	4	0
9	L	303	CLA	5	0
9	B	823	CLA	4	0
9	A	816	CLA	3	0
9	B	839	CLA	3	0
9	b	804	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	804	CLA	3	0
9	B	825	CLA	5	0
9	A	830	CLA	15	0
9	L	307	CLA	19	0
9	a	823	CLA	4	0
9	a	834	CLA	7	0
9	B	809	CLA	2	0
9	a	803	CLA	2	0
12	I	101	BCR	1	0
9	a	832	CLA	3	0
12	A	842	BCR	3	0
9	A	815	CLA	5	0
9	B	801	CLA	2	0
10	a	838	PQN	5	0
12	l	309	BCR	3	0
12	l	304	BCR	6	0
9	B	815	CLA	6	0
11	A	845	LHG	5	0
9	a	809	CLA	3	0
12	i	101	BCR	1	0
12	A	843	BCR	2	0
9	a	831	CLA	8	0
9	b	823	CLA	3	0
9	l	301	CLA	11	0
9	A	806	CLA	6	0
9	b	829	CLA	3	0
9	A	847	CLA	7	0
9	B	830	CLA	2	0
9	a	813	CLA	2	0
9	A	820	CLA	11	0
12	B	836	BCR	2	0
9	B	818	CLA	6	0
9	b	825	CLA	6	0
11	A	839	LHG	3	0
9	B	821	CLA	3	0
9	B	840	CLA	3	0
9	a	811	CLA	5	0
9	b	831	CLA	1	0
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9	A	810	CLA	4	0
9	A	824	CLA	11	0
9	L	302	CLA	4	0

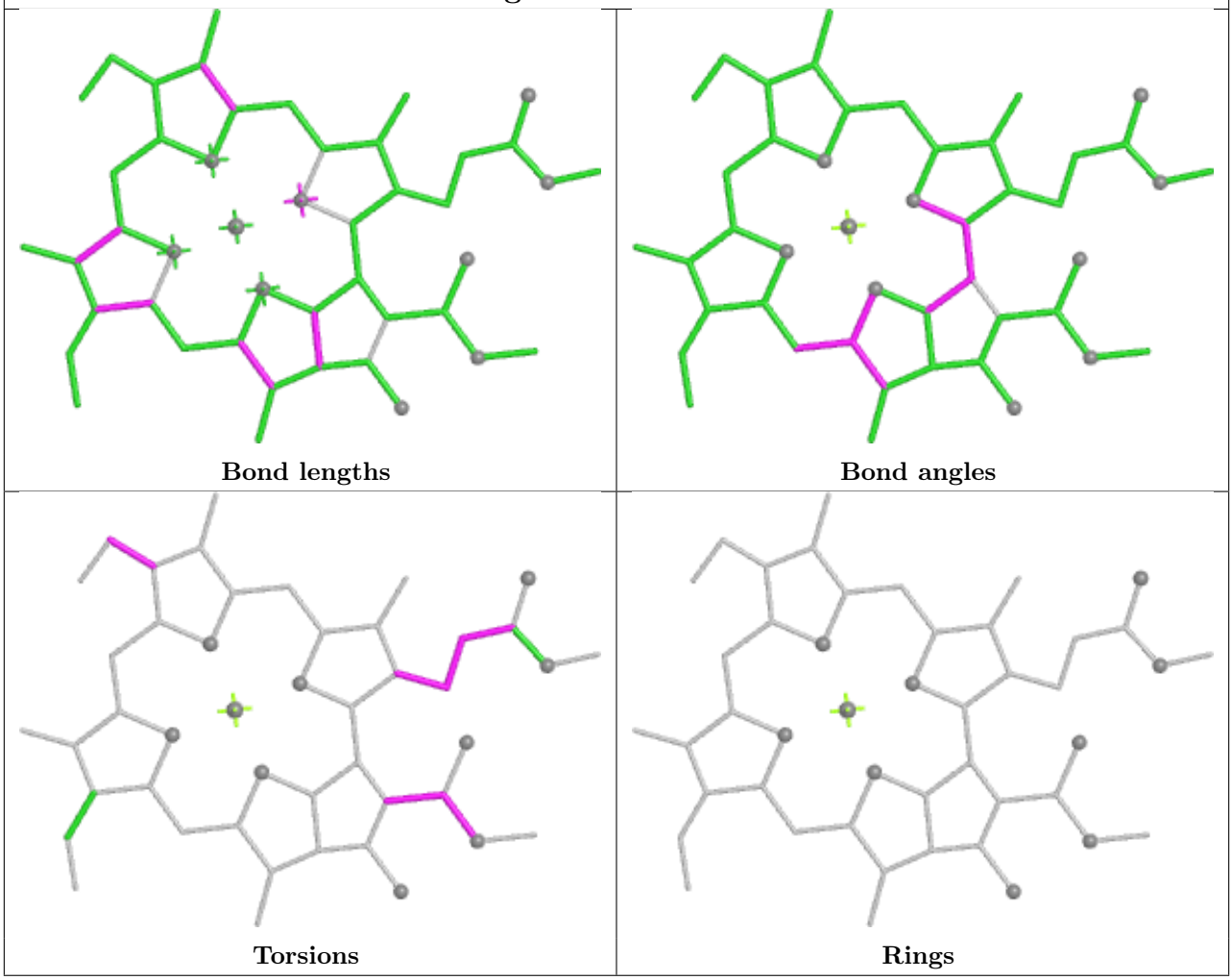
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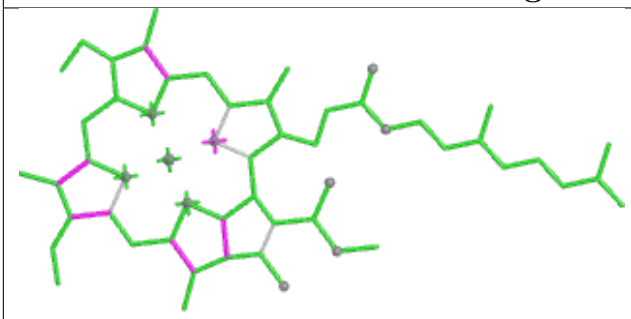
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	a	821	CLA	6	0
9	B	811	CLA	5	0
12	b	836	BCR	2	0

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.

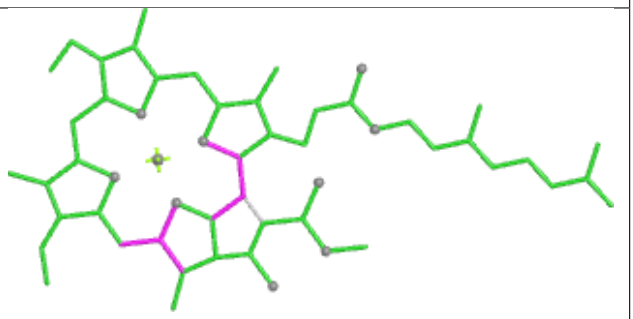
Ligand CLA B 816



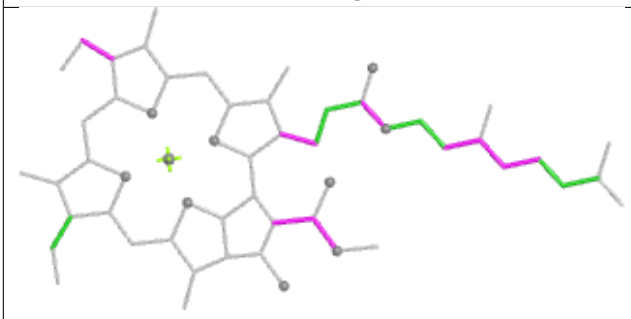
Ligand CLA B 817



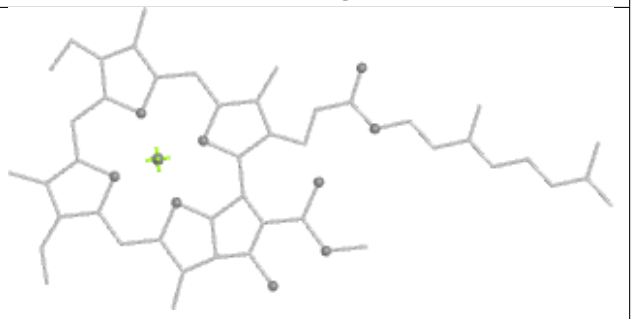
Bond lengths



Bond angles

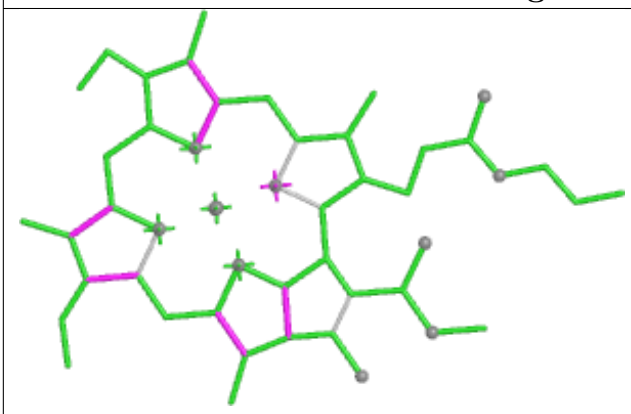


Torsions

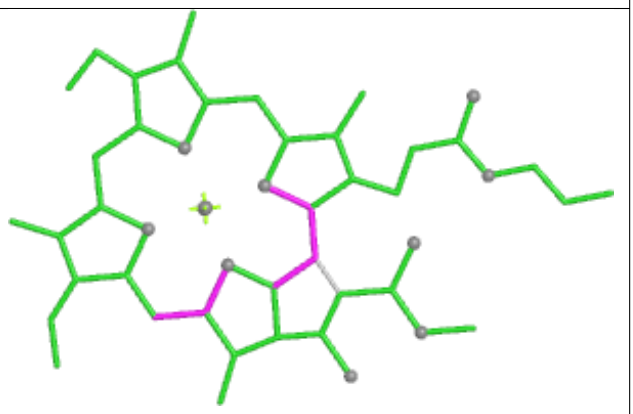


Rings

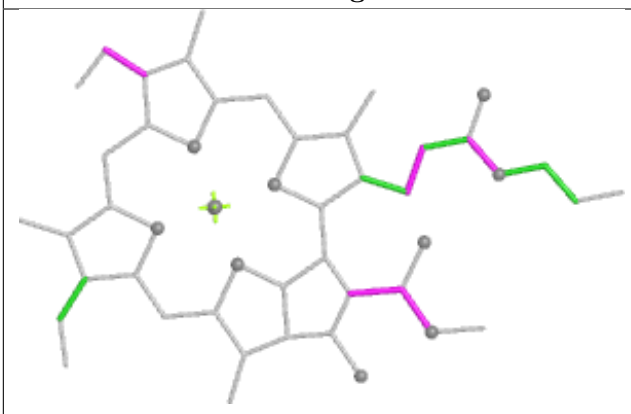
Ligand CLA b 840



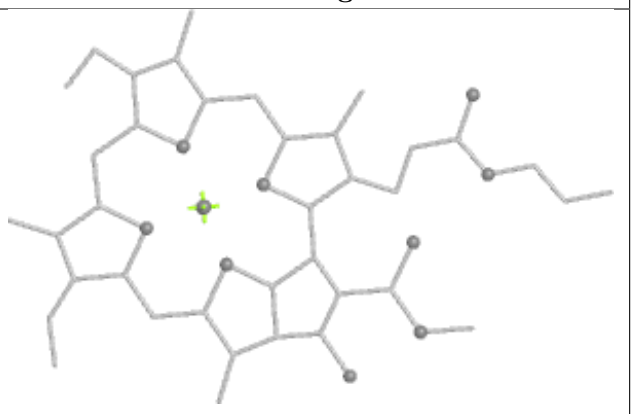
Bond lengths



Bond angles

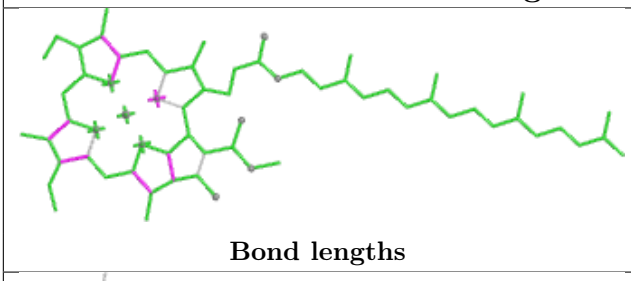


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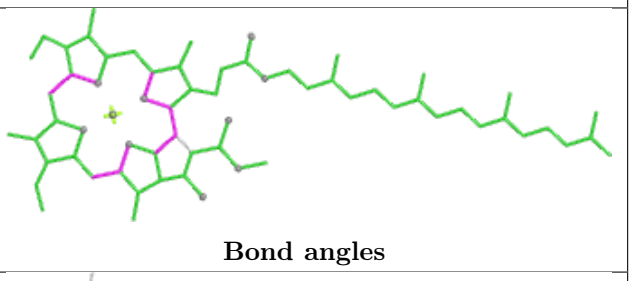


Rings

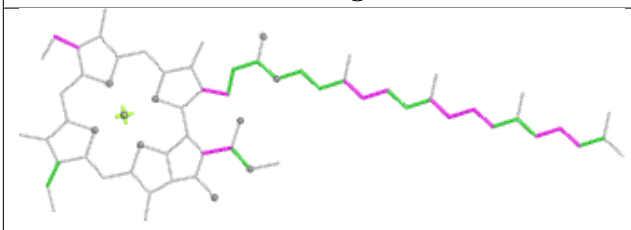
Ligand CLA A 823



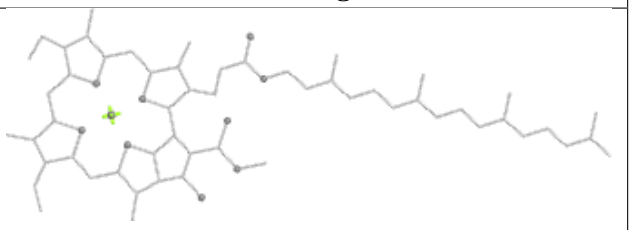
Bond lengths



Bond angles

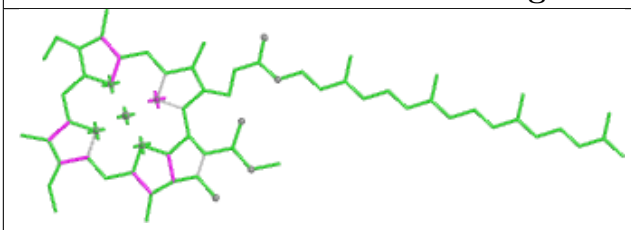


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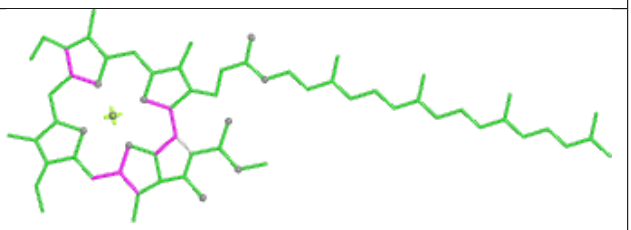


Rings

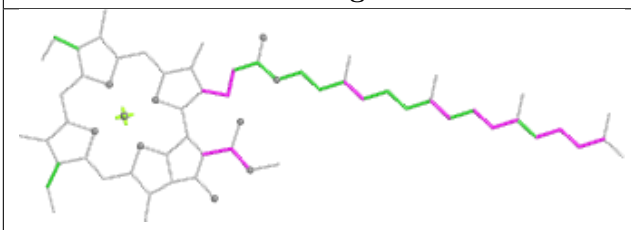
Ligand CLA a 802



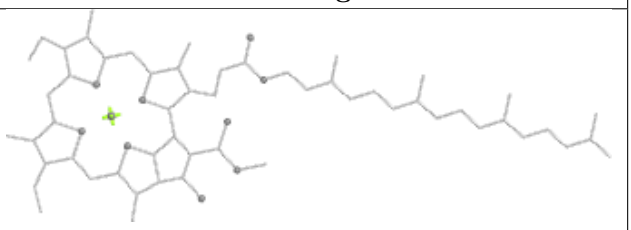
Bond lengths



Bond angles

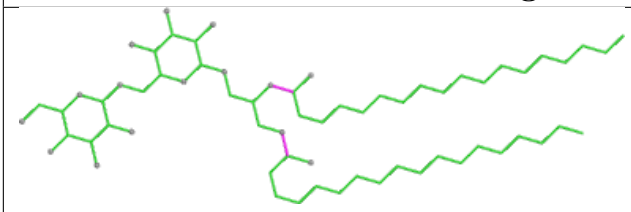


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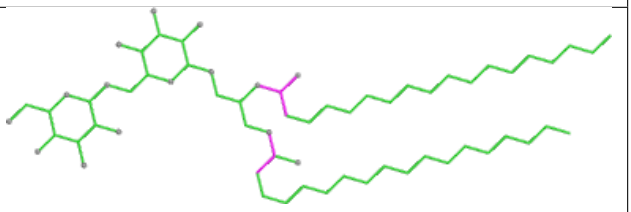


Rings

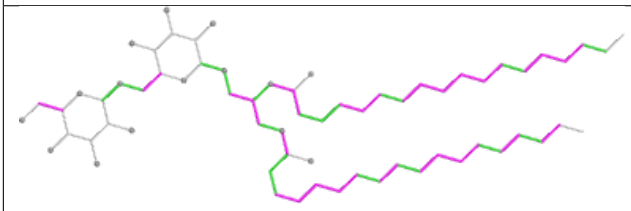
Ligand DGD B 837



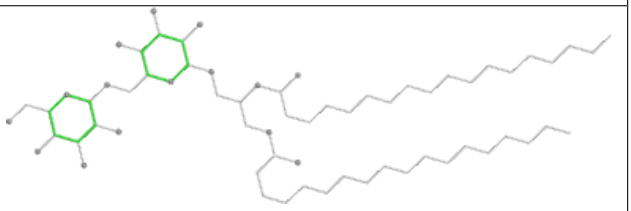
Bond lengths



Bond angles

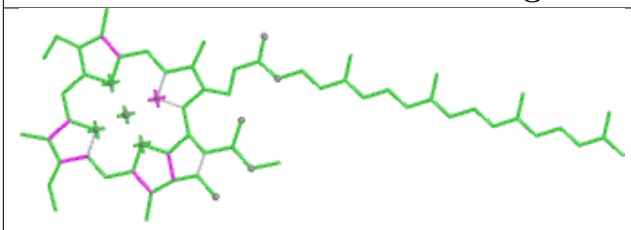


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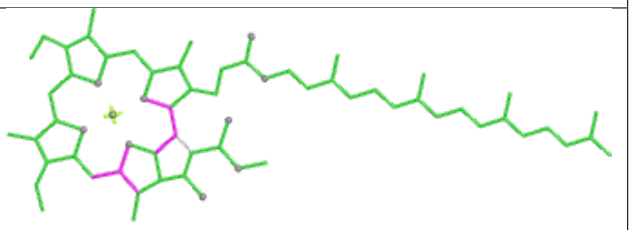


Rings

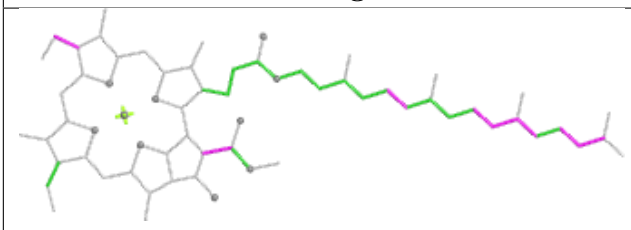
Ligand CLA A 832



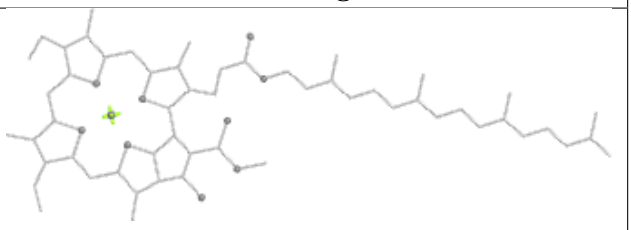
Bond lengths



Bond angles

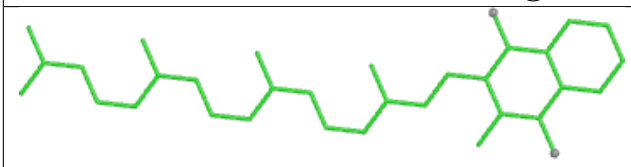


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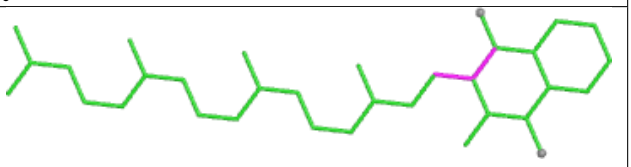


Rings

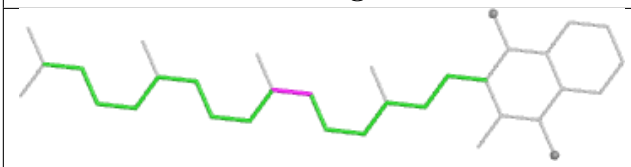
Ligand PQN b 833



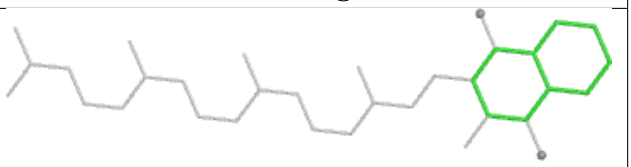
Bond lengths



Bond angles

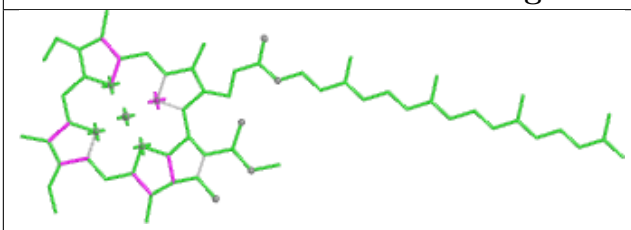


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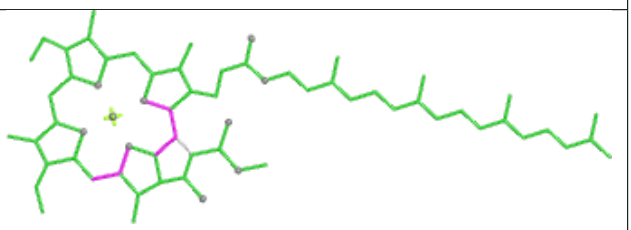


Rings

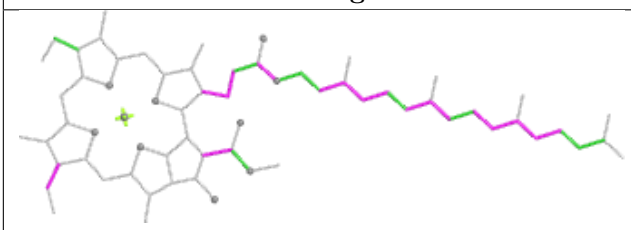
Ligand CLA B 806



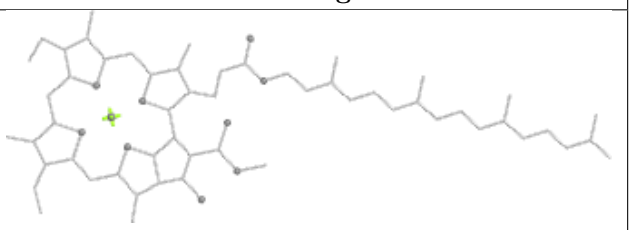
Bond lengths



Bond angles

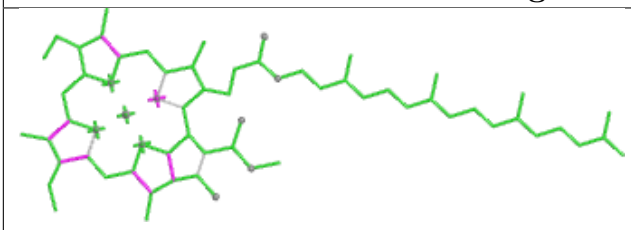


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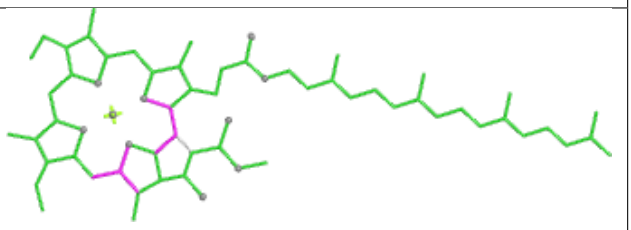


Rings

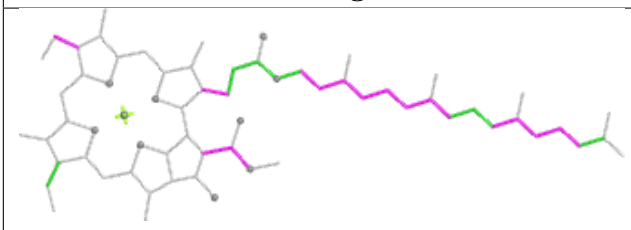
Ligand CLA a 807



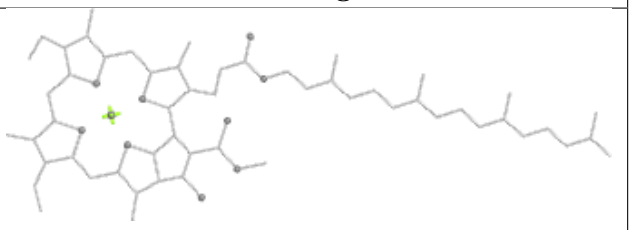
Bond lengths



Bond angles

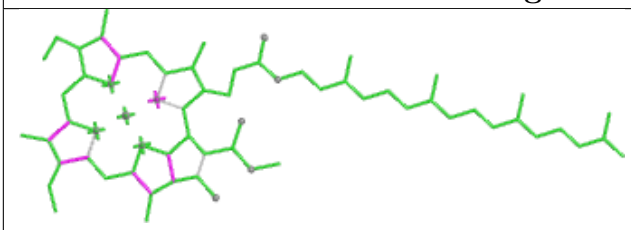


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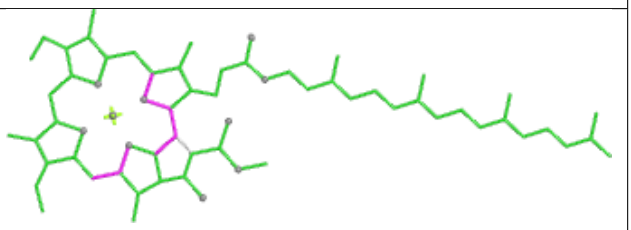


Rings

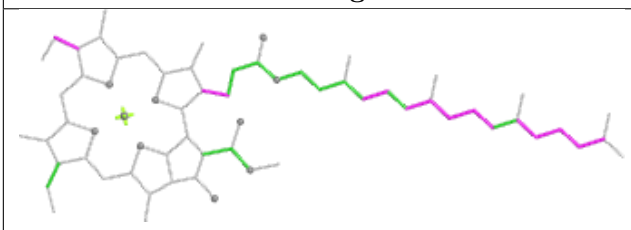
Ligand CLA B 810



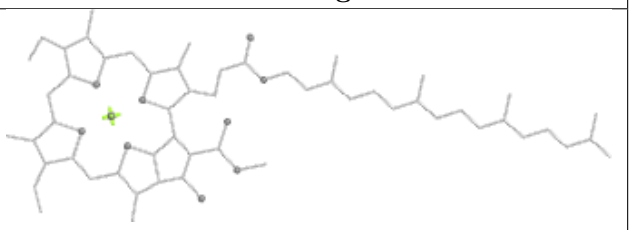
Bond lengths



Bond angles

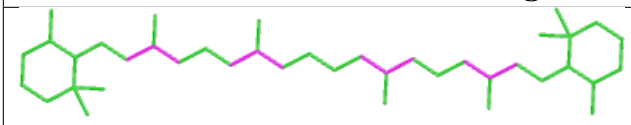


Torsions



Rings

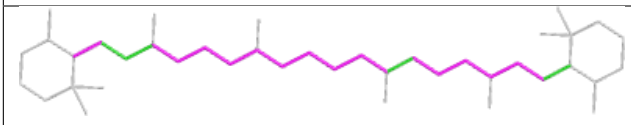
Ligand BCR B 834



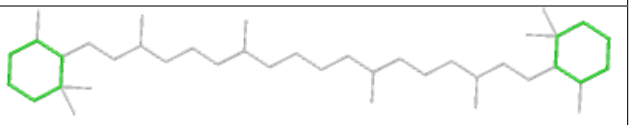
Bond lengths



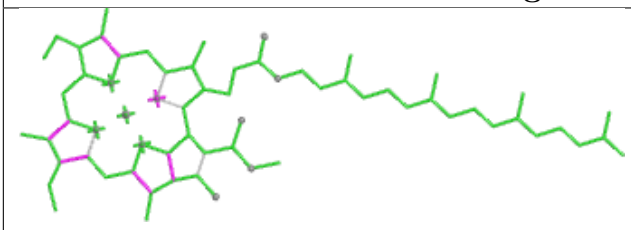
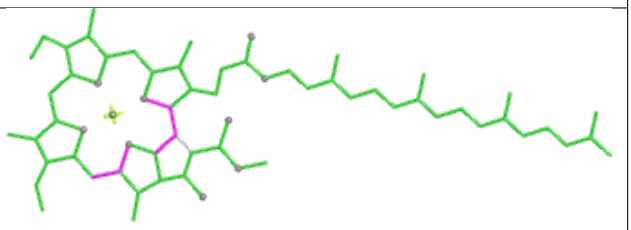
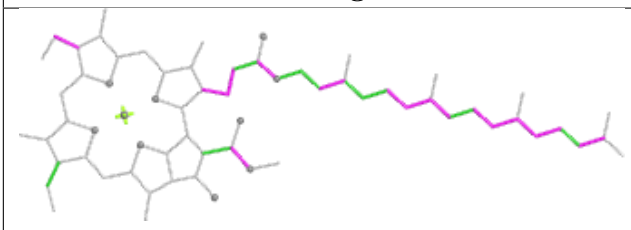
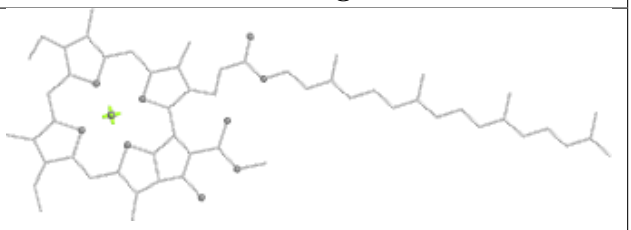
Bond angles

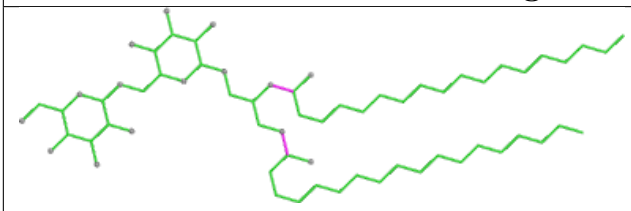
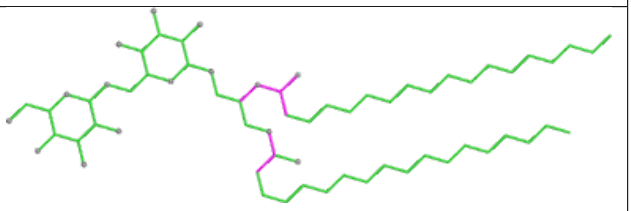
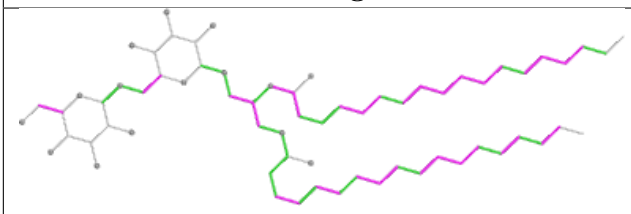
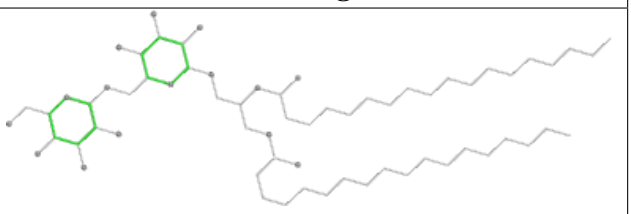


Torsions

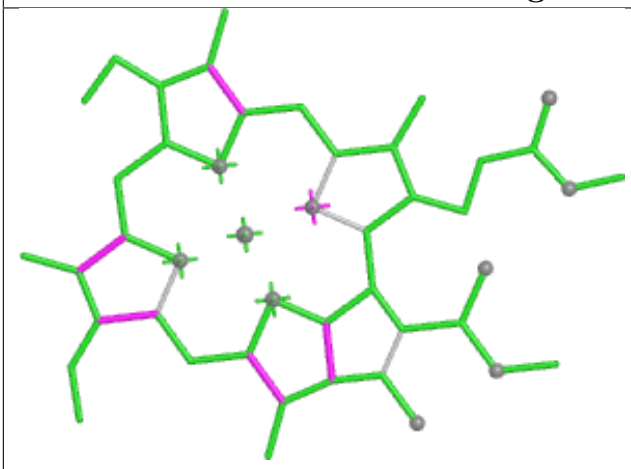


Rings

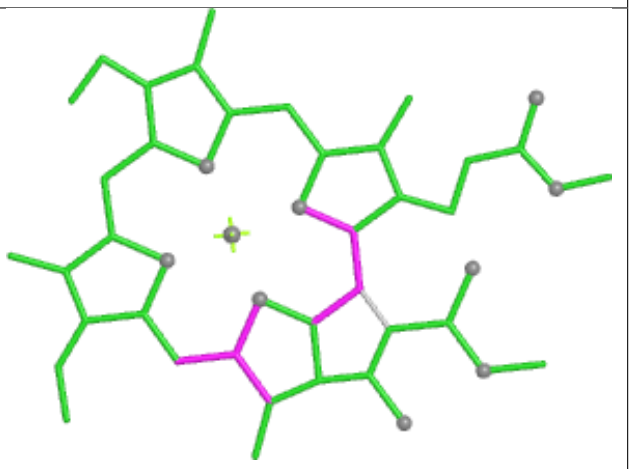
Ligand CLA A 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD b 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

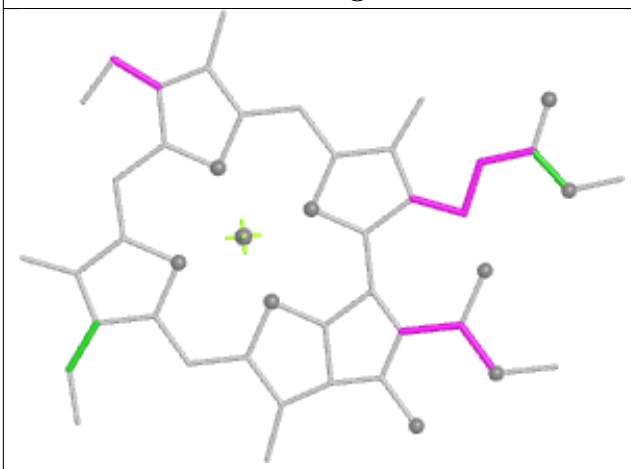
Ligand CLA b 816



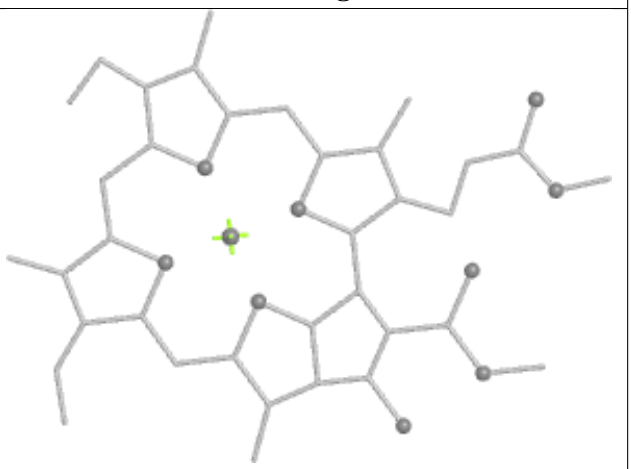
Bond lengths



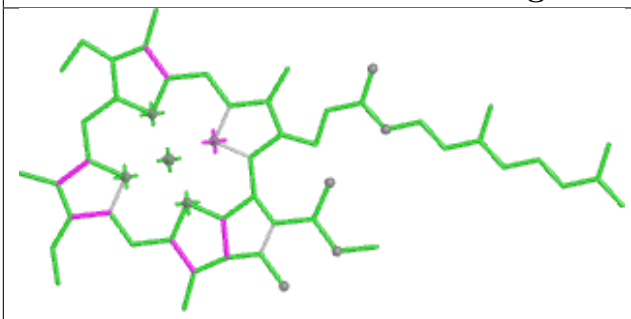
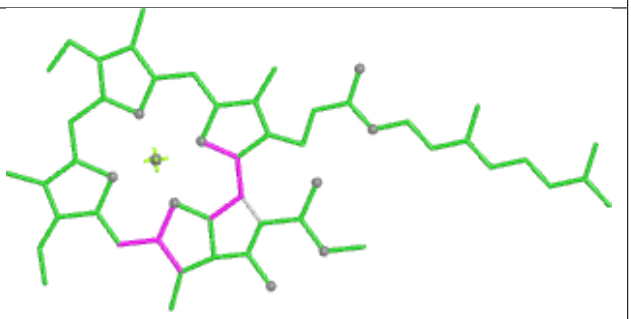
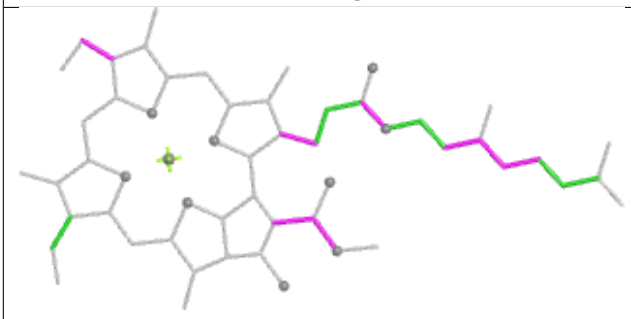
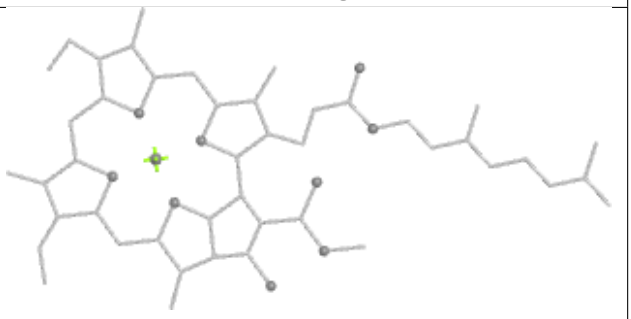
Bond angles

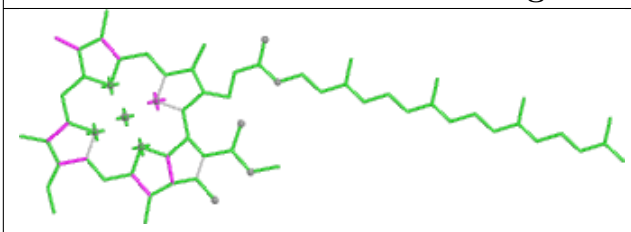
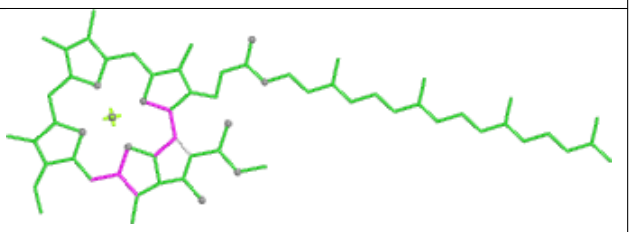
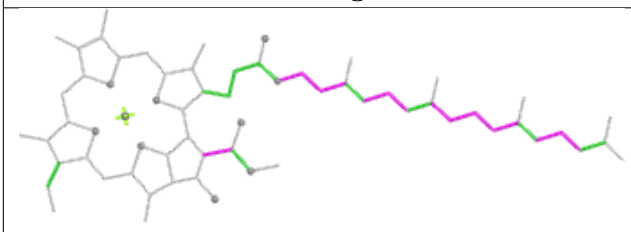
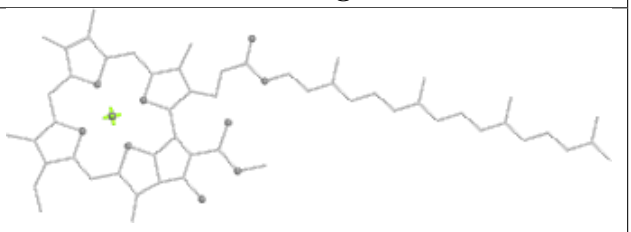


Torsions

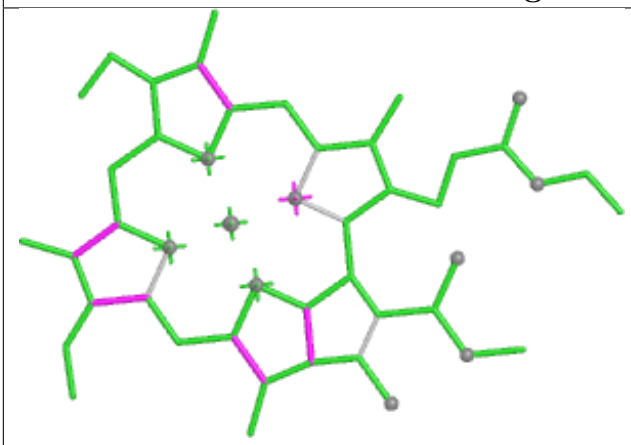


Rings

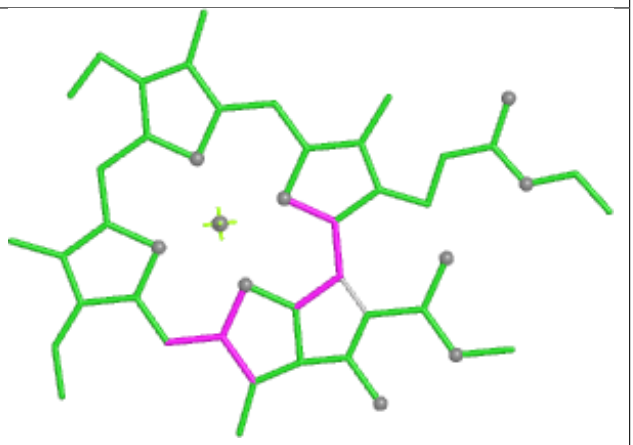
Ligand CLA b 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

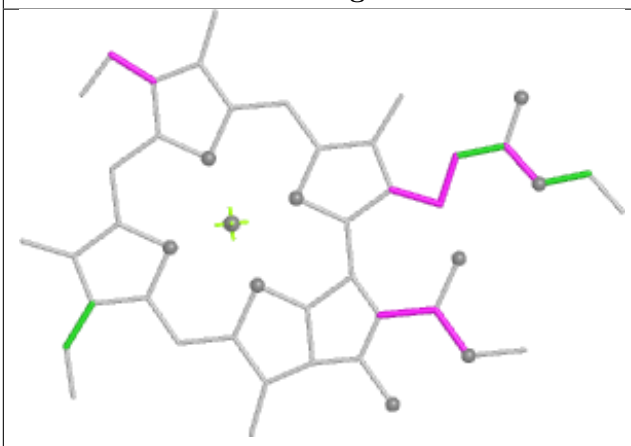
Ligand CLA B 822



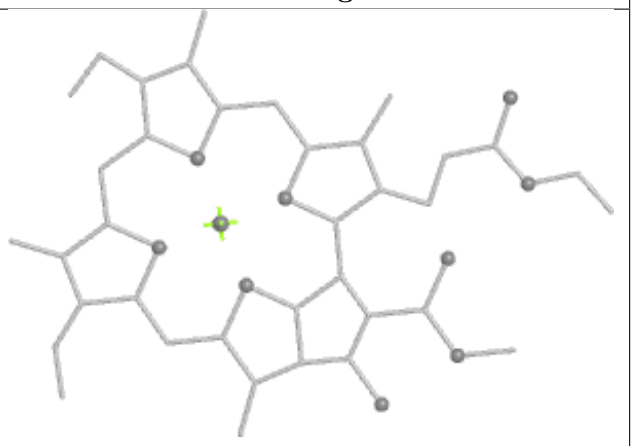
Bond lengths



Bond angles

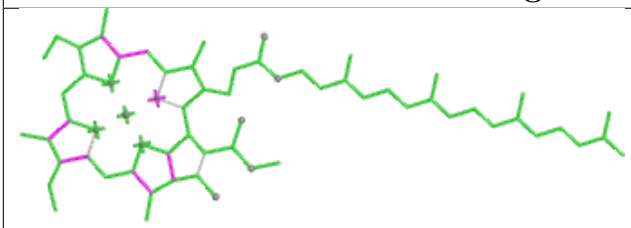


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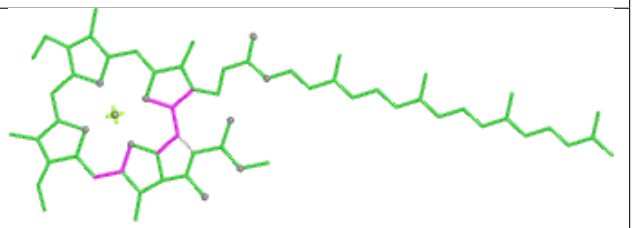


Rings

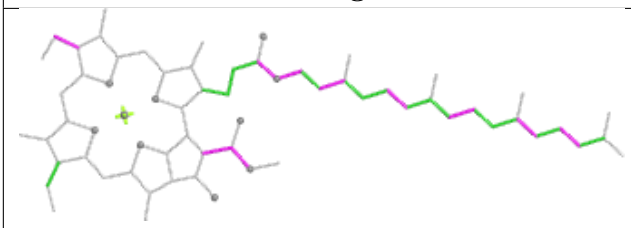
Ligand CLA B 803



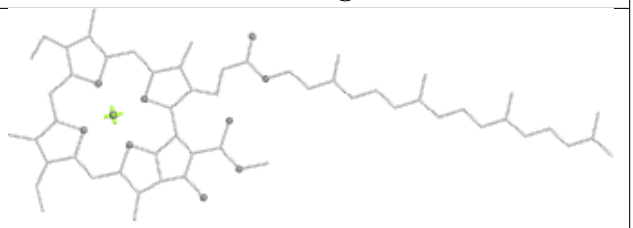
Bond lengths



Bond angles

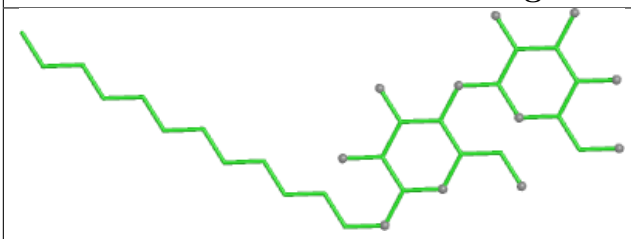


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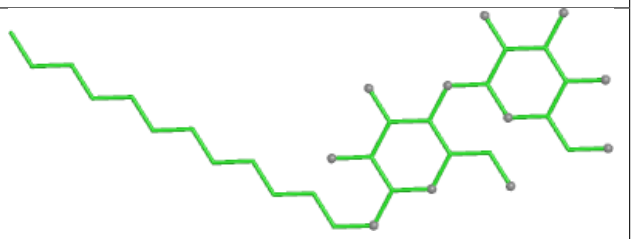


Rings

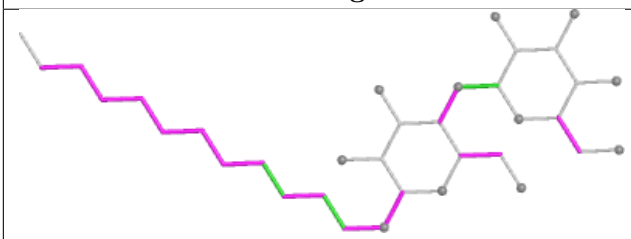
Ligand LMT b 838



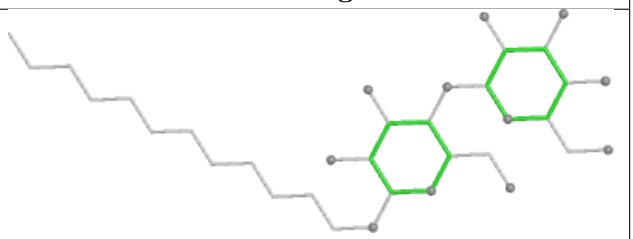
Bond lengths



Bond angles

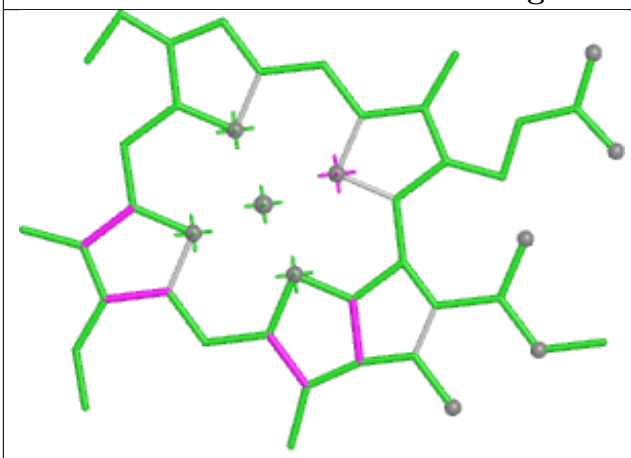


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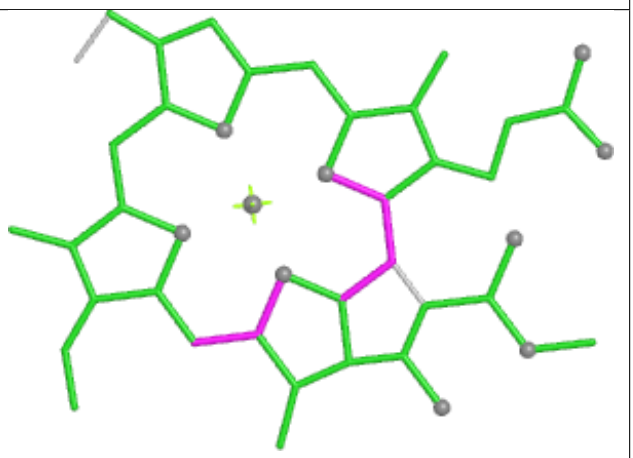


Rings

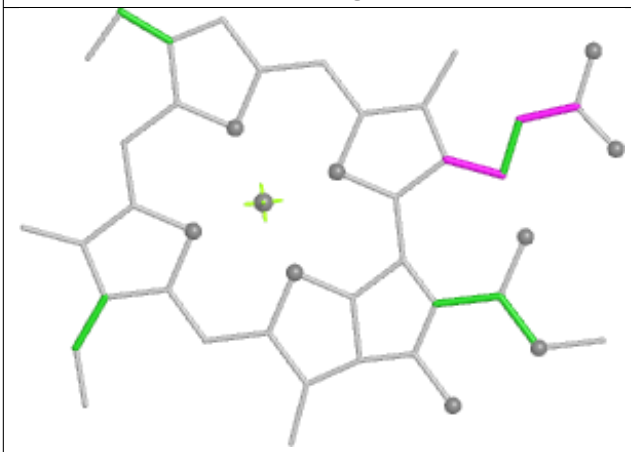
Ligand CLA b 813



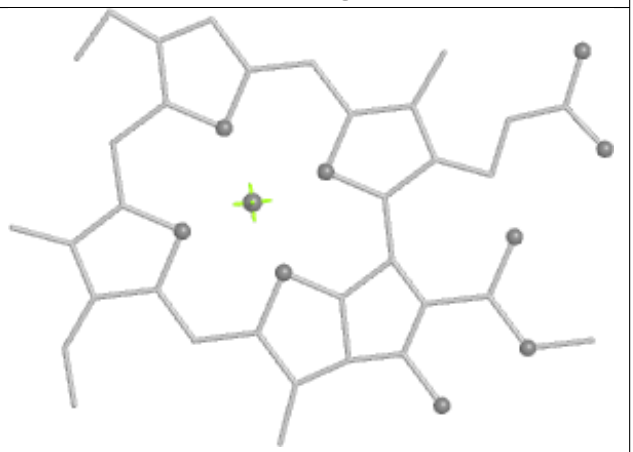
Bond lengths



Bond angles

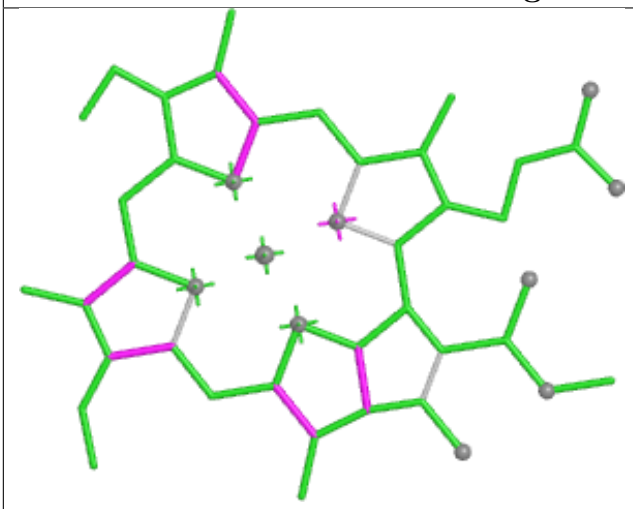


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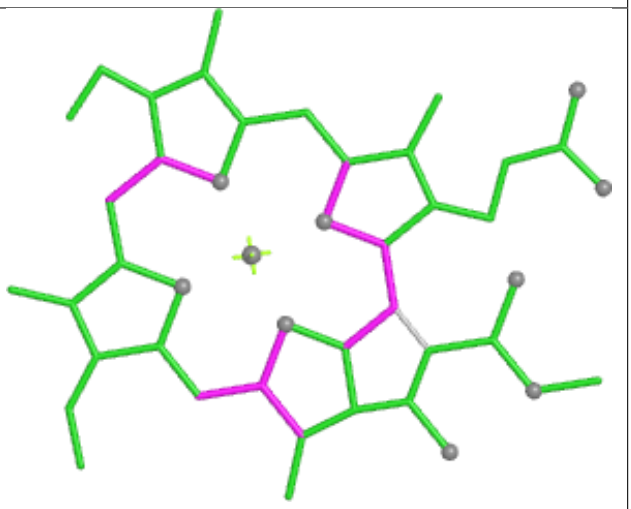


Rings

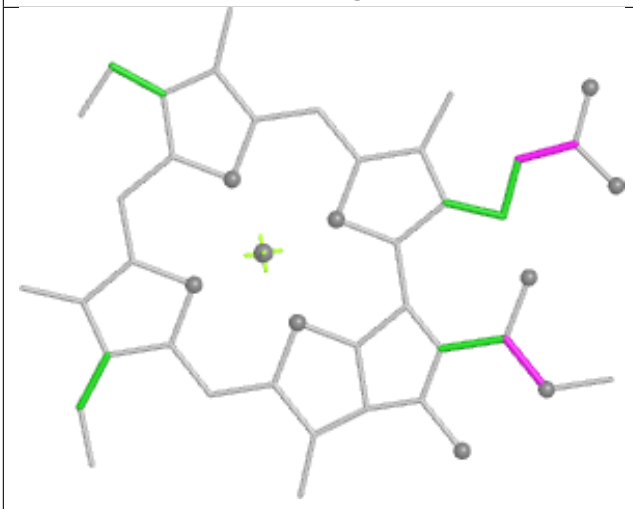
Ligand CLA A 814



Bond lengths



Bond angles

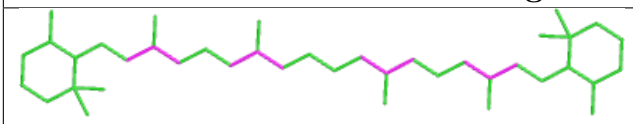


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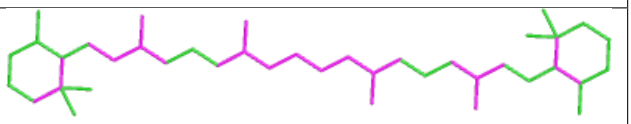


Rings

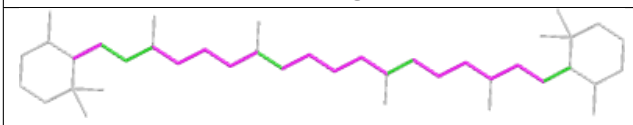
Ligand BCR b 834



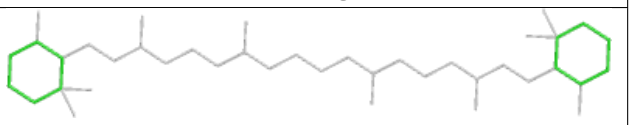
Bond lengths



Bond angles

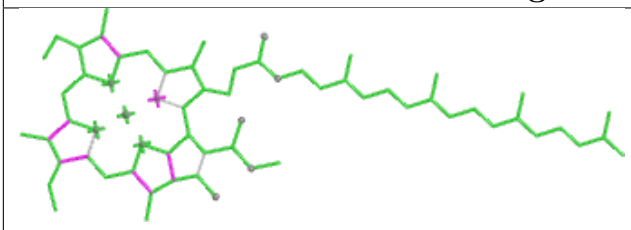


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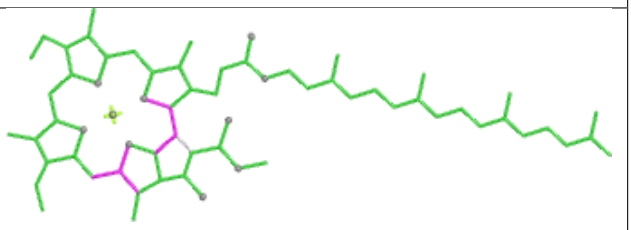


Rings

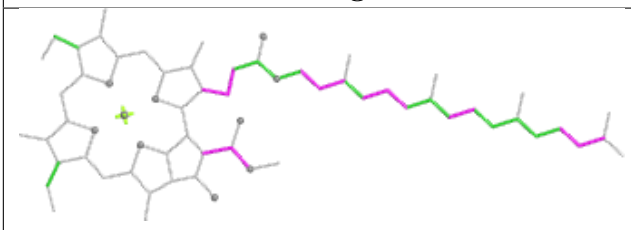
Ligand CLA a 822



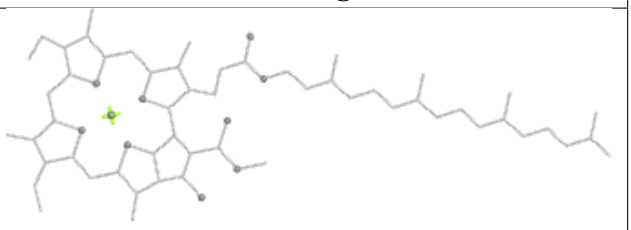
Bond lengths



Bond angles

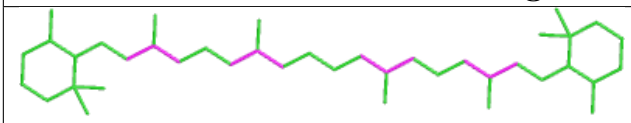


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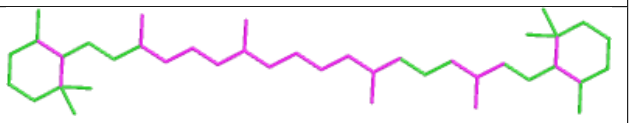


Rings

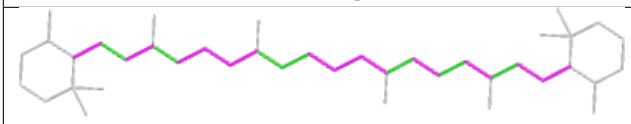
Ligand BCR L 306



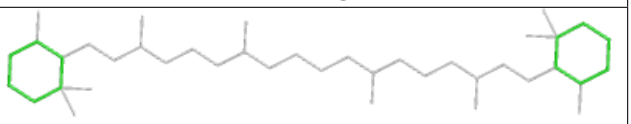
Bond lengths



Bond angles

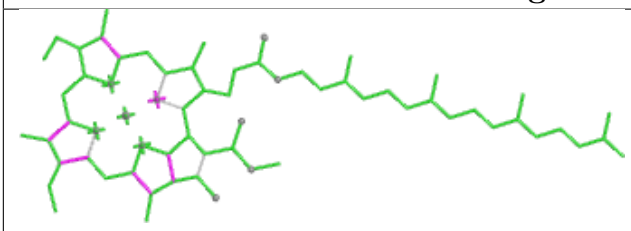


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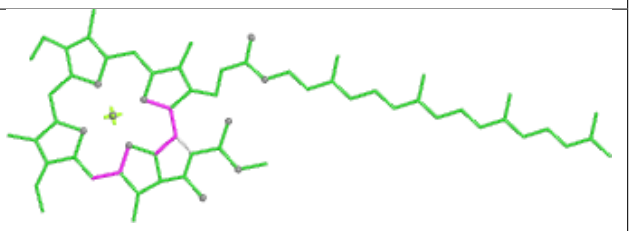


Rings

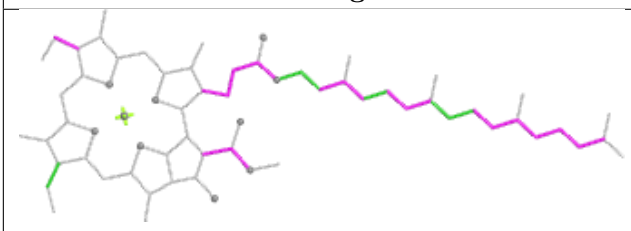
Ligand CLA a 815



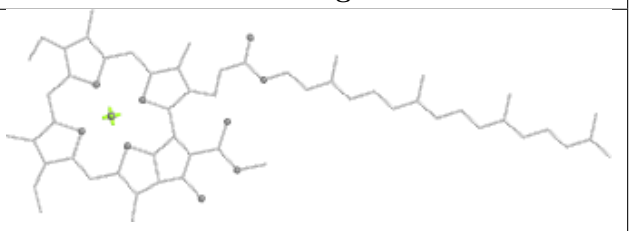
Bond lengths



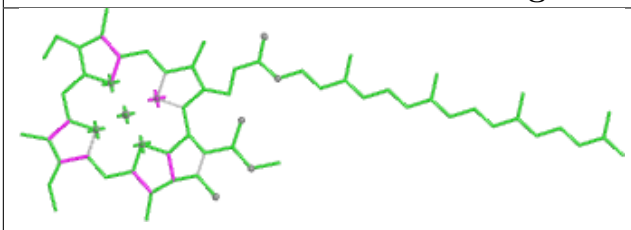
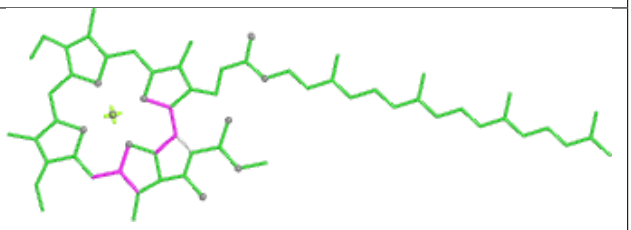
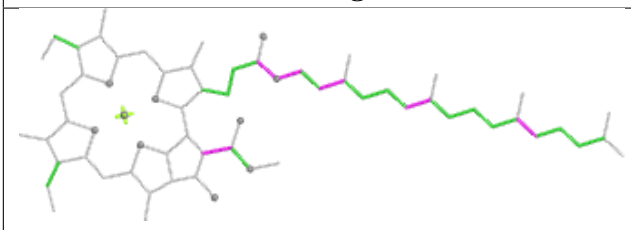
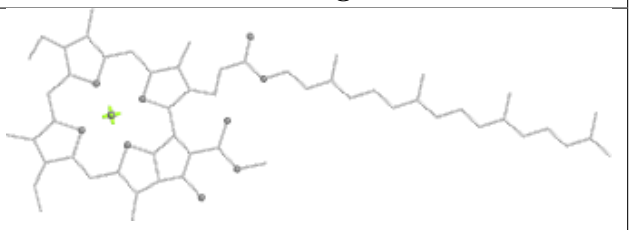
Bond angles

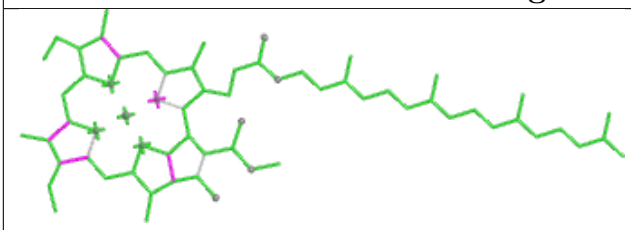
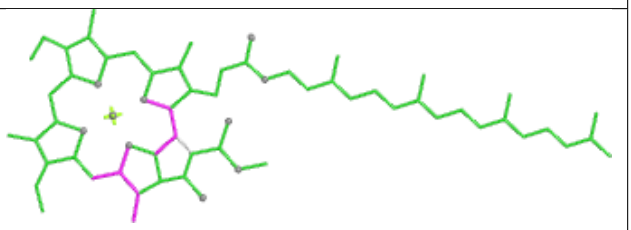
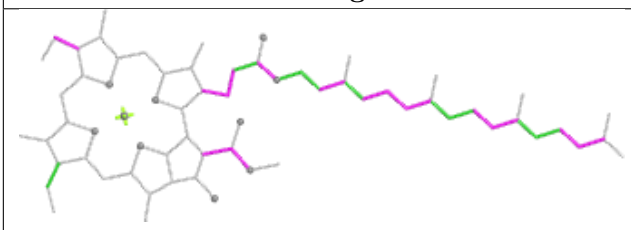
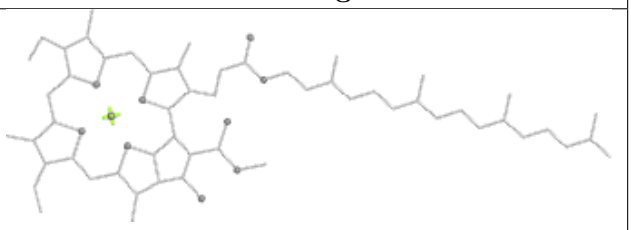


Torsions

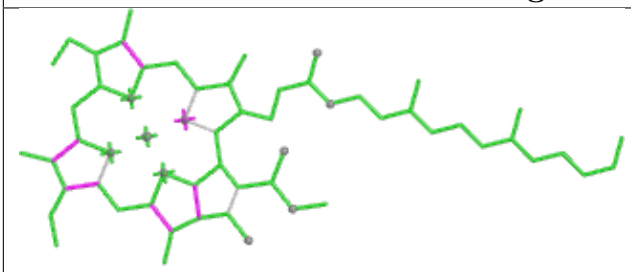


Rings

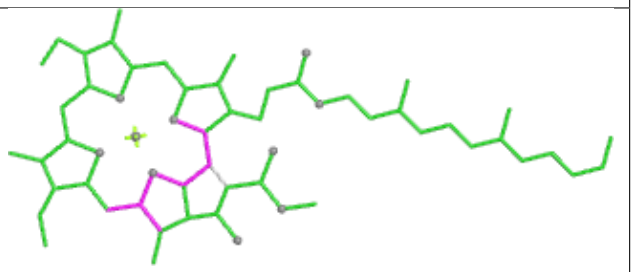
Ligand CLA a 804	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA a 836	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

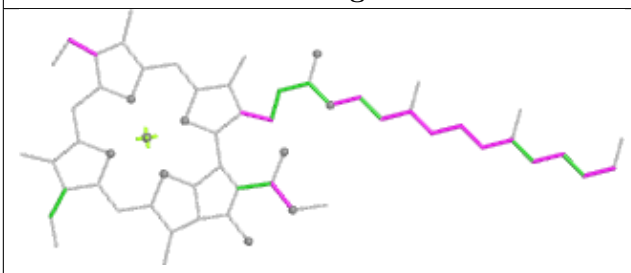
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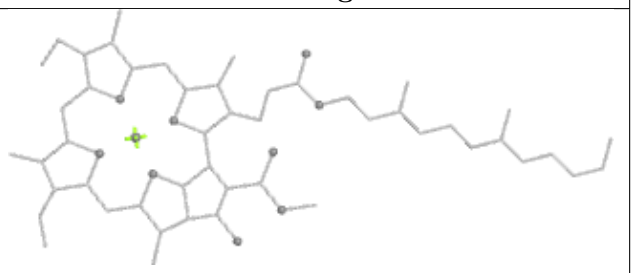
Bond lengths



Bond angles

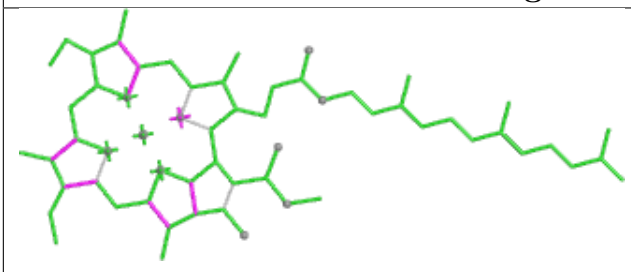


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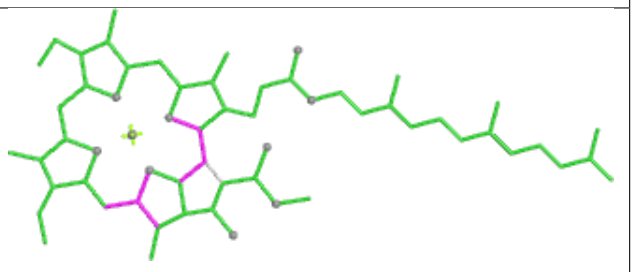


Rings

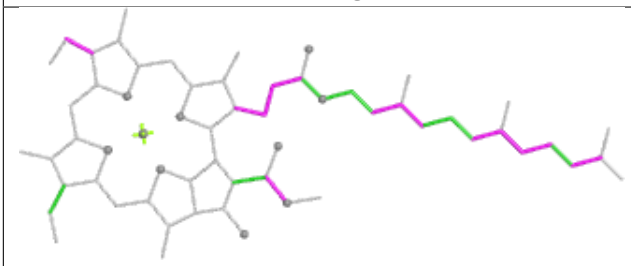
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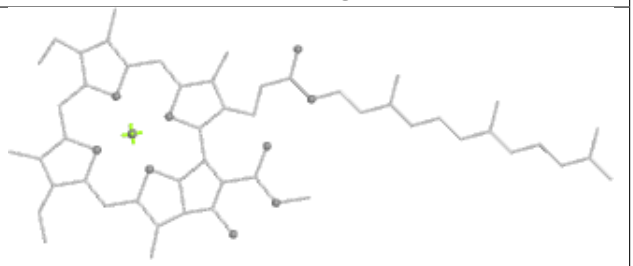
Bond lengths



Bond angles

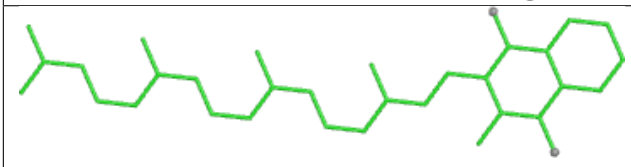


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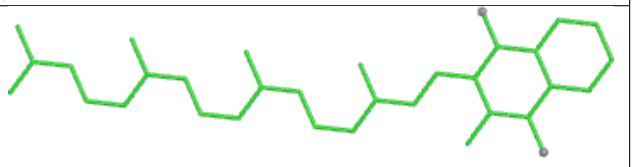


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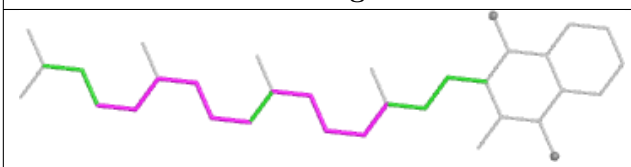
Ligand PQN A 837



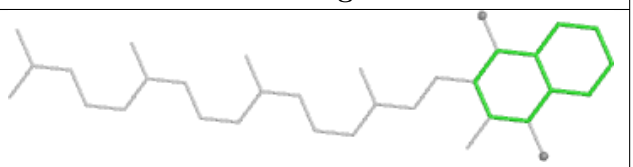
Bond lengths



Bond angles

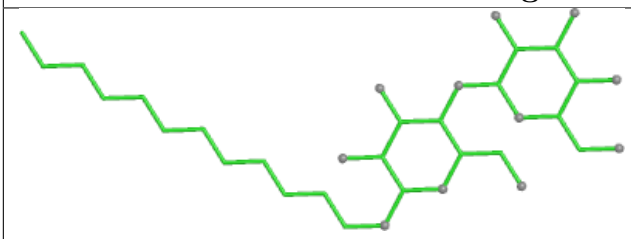


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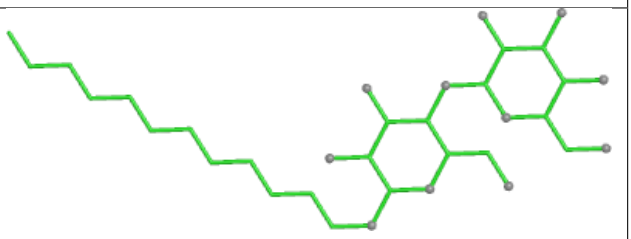


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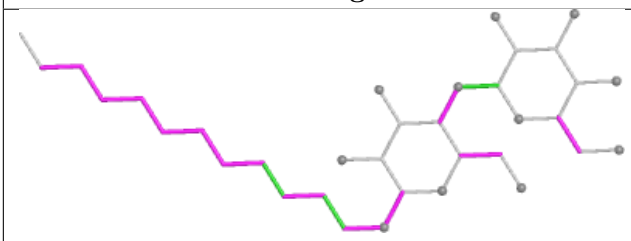
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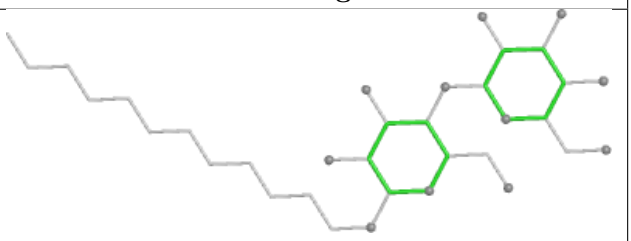
Bond lengths



Bond angles

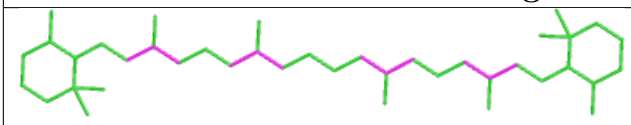


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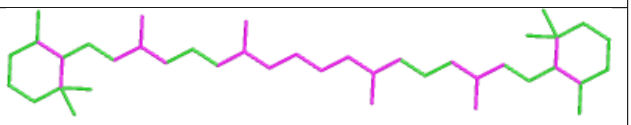


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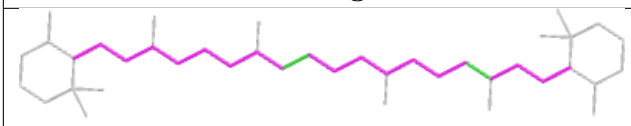
Ligand BCR B 835



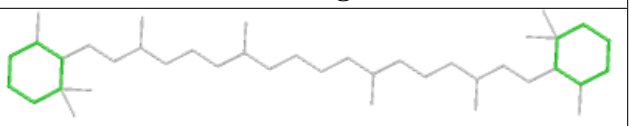
Bond lengths



Bond angles

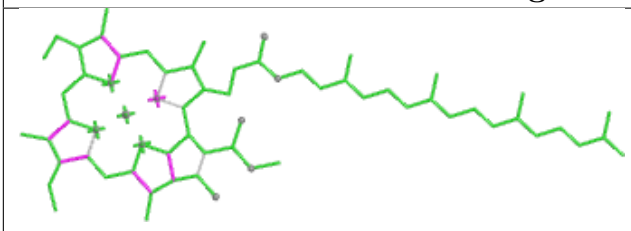


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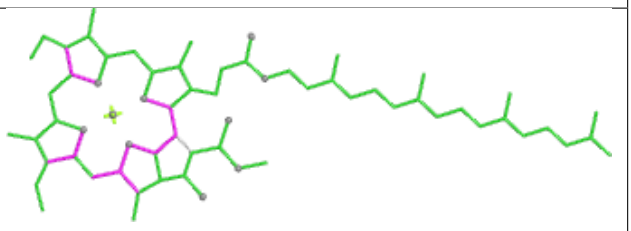


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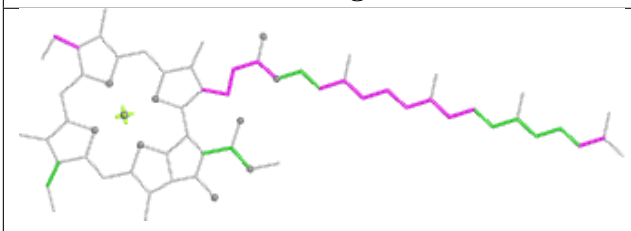
Ligand CLA a 816



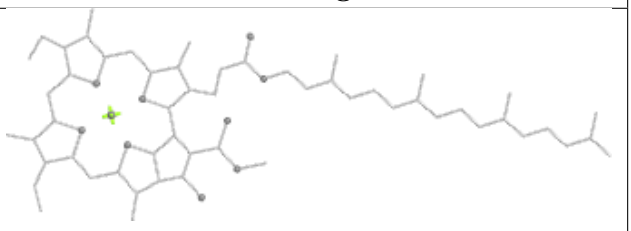
Bond lengths



Bond angles

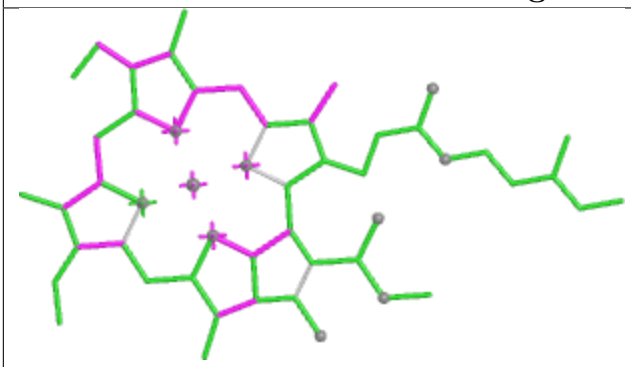


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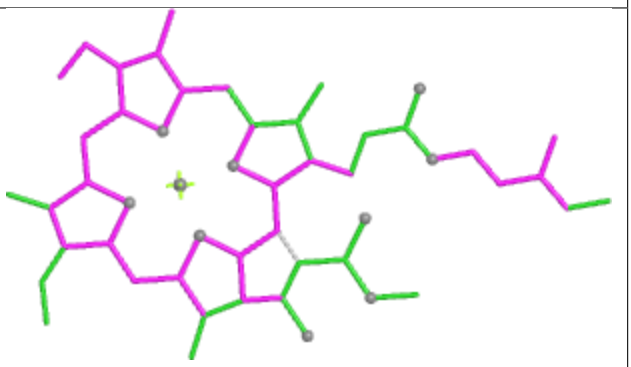


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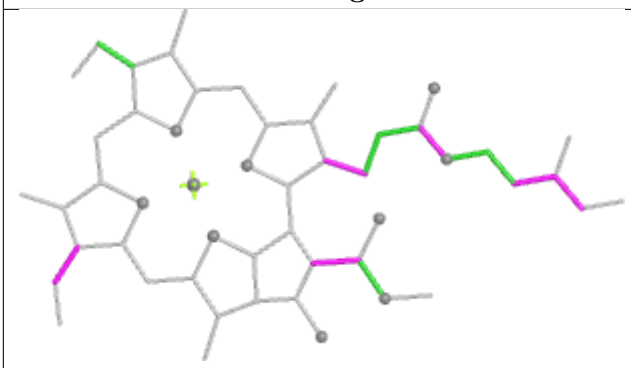
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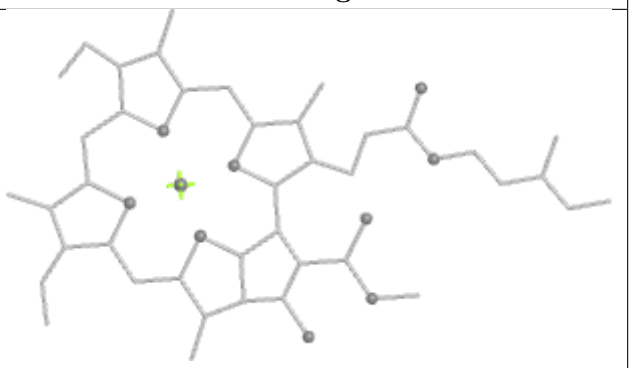
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Bond angles

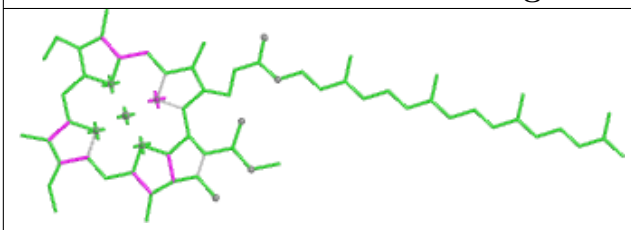


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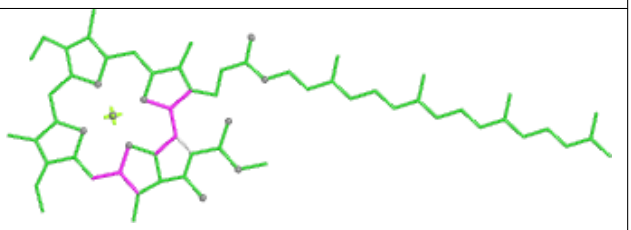


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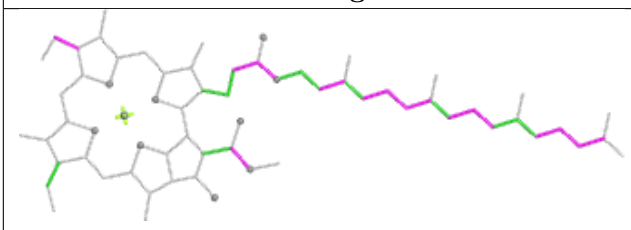
Ligand CLA A 801



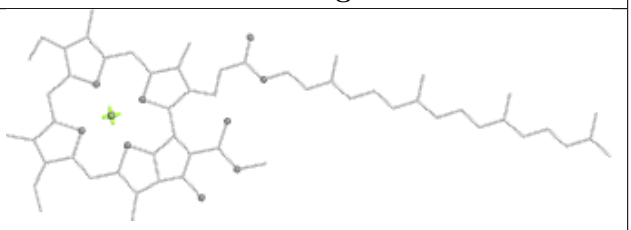
Bond lengths



Bond angles

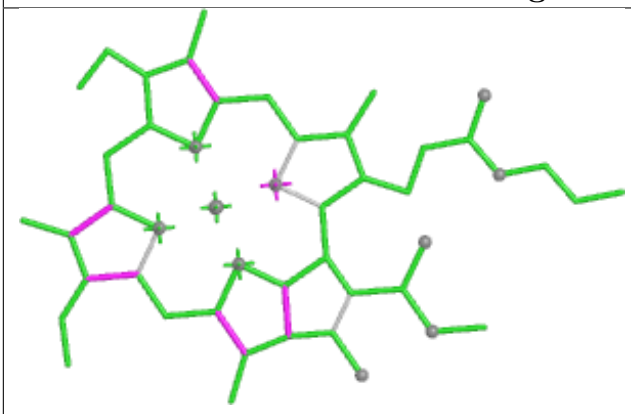


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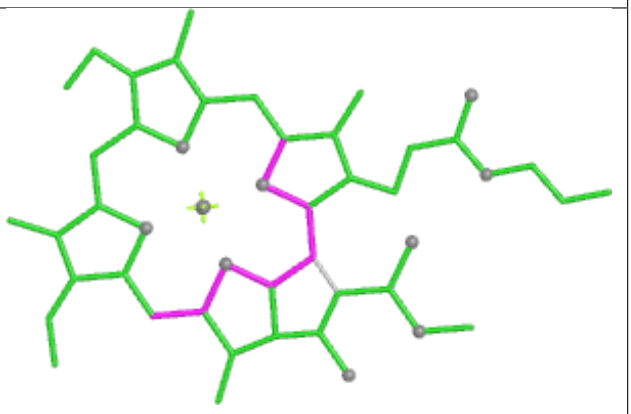


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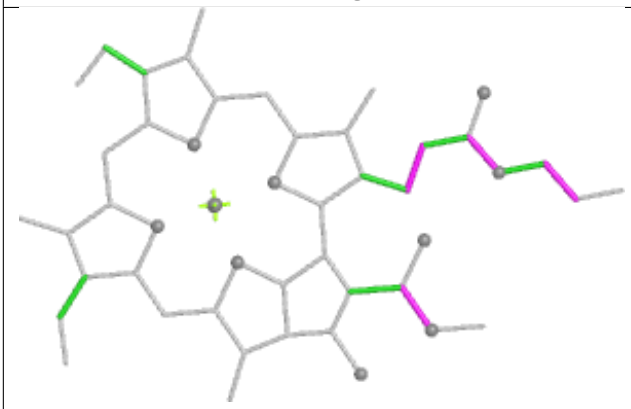
Ligand CLA a 837



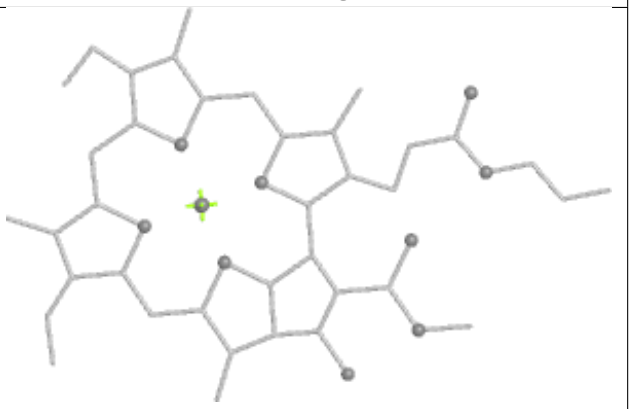
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Bond angles

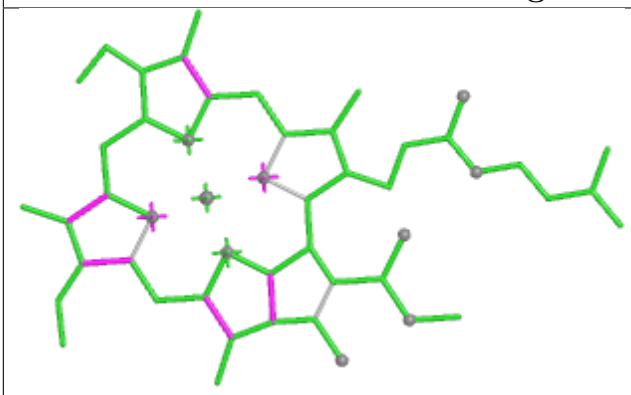


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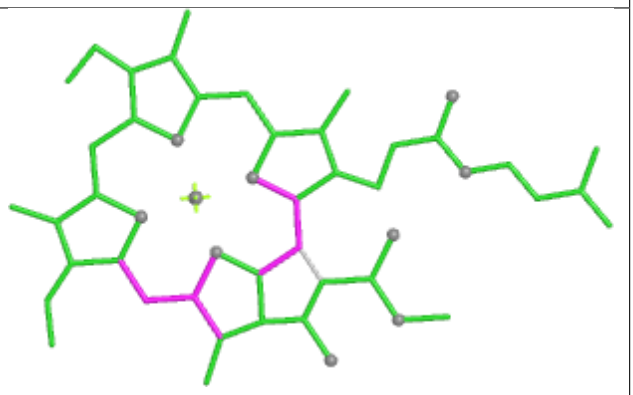


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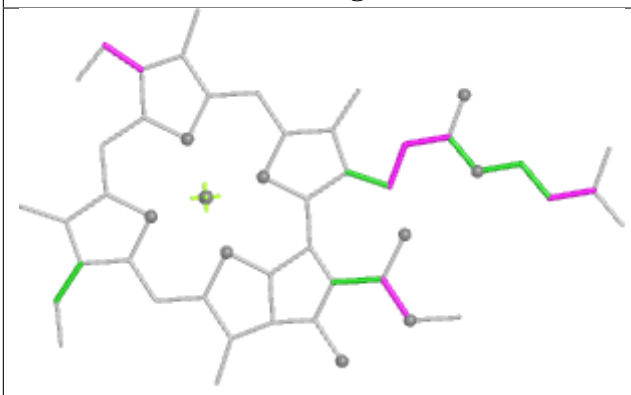
Ligand CLA b 820



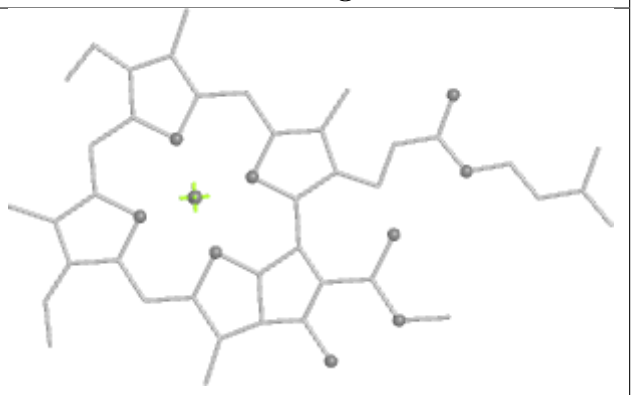
Bond lengths



Bond angles

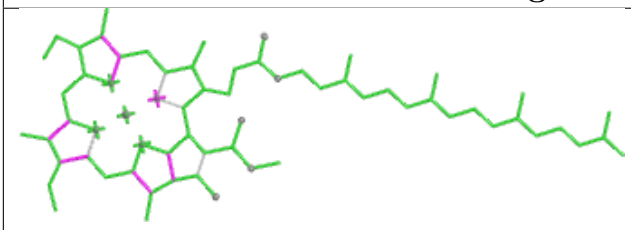


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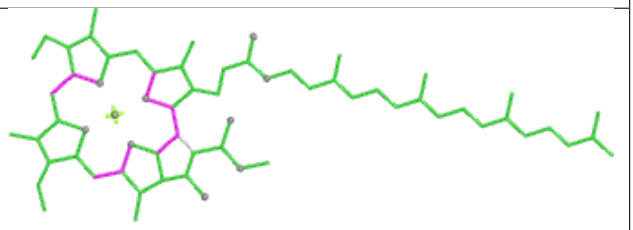


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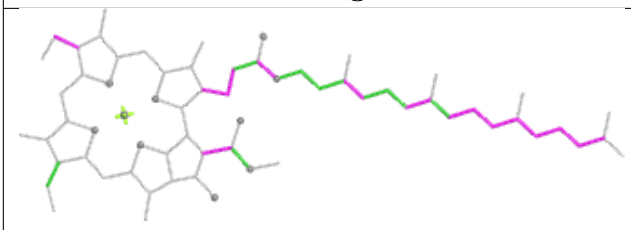
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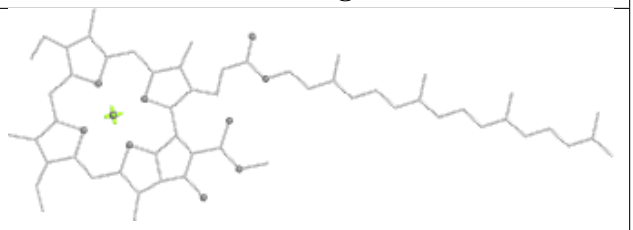
Bond lengths



Bond angles



Torsions

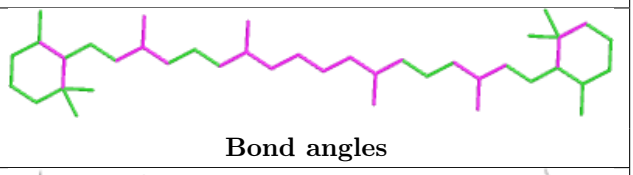


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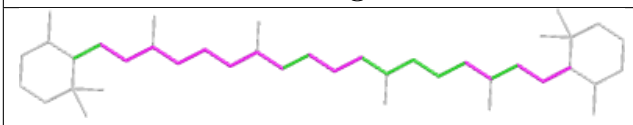
Ligand BCR A 840



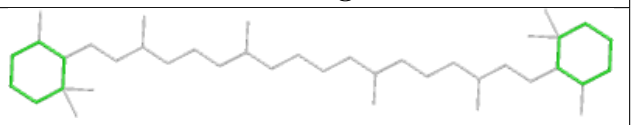
Bond lengths



Bond angles

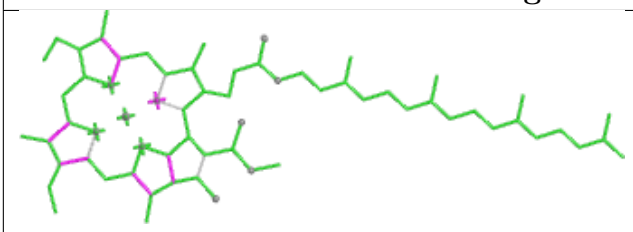


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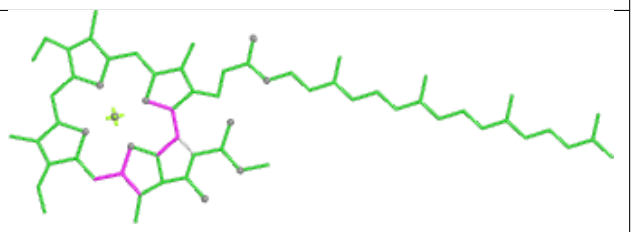


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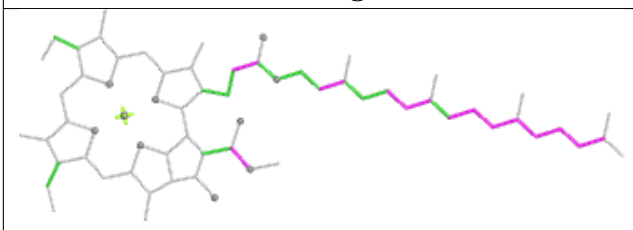
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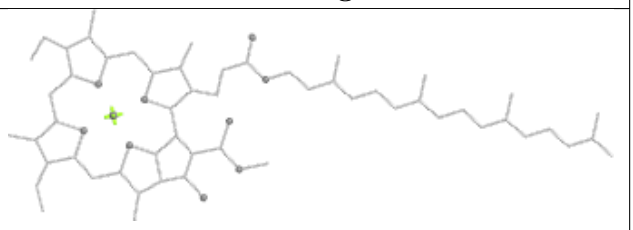
Bond lengths



Bond angles

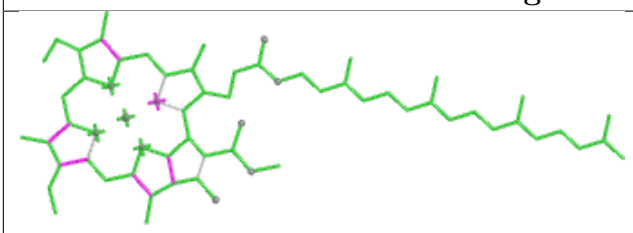


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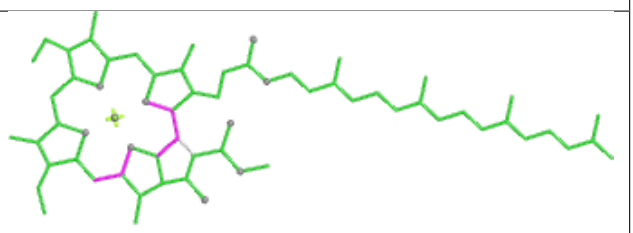


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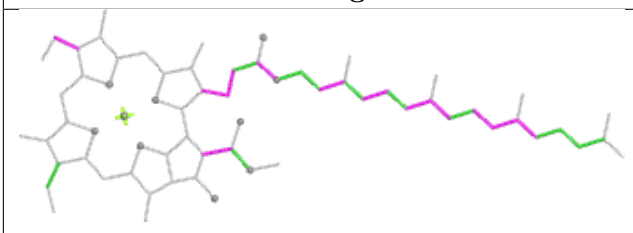
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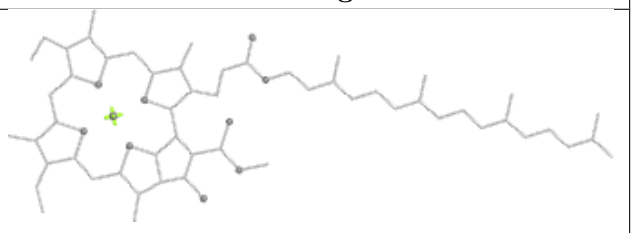
Bond lengths



Bond angles

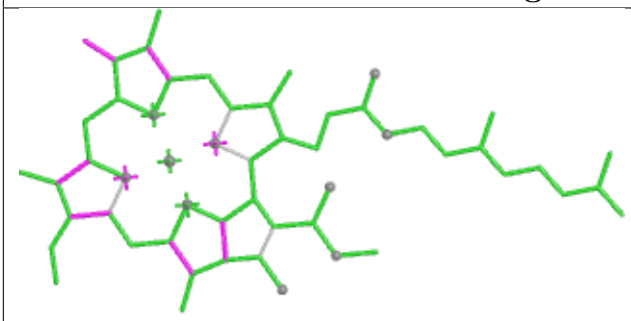


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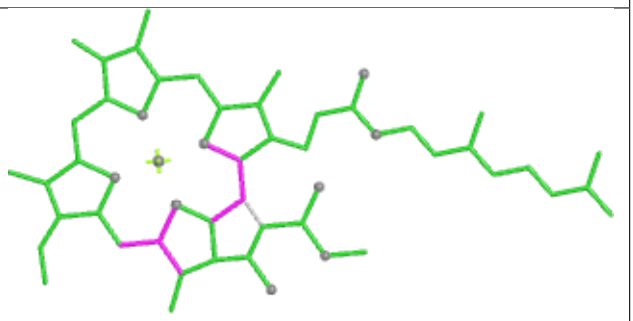


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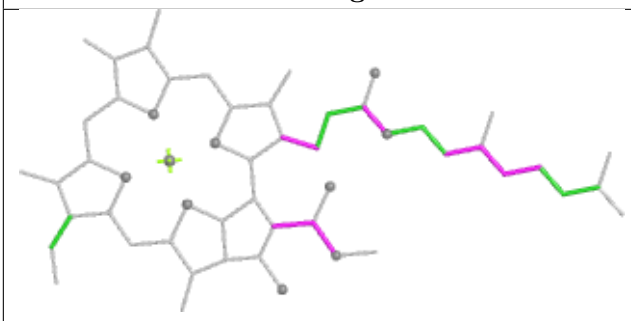
Ligand CLA B 812



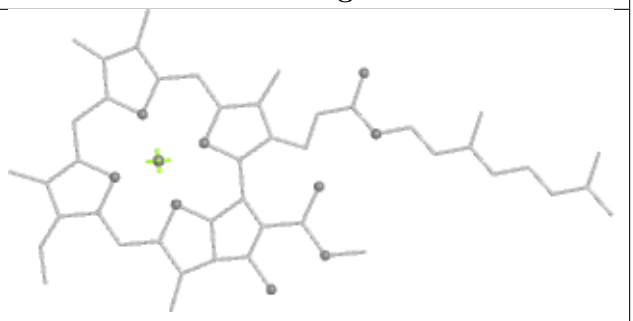
Bond lengths



Bond angles

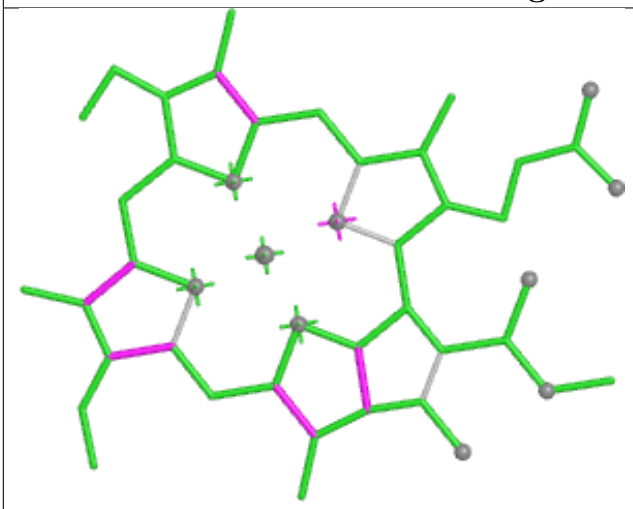


Torsions

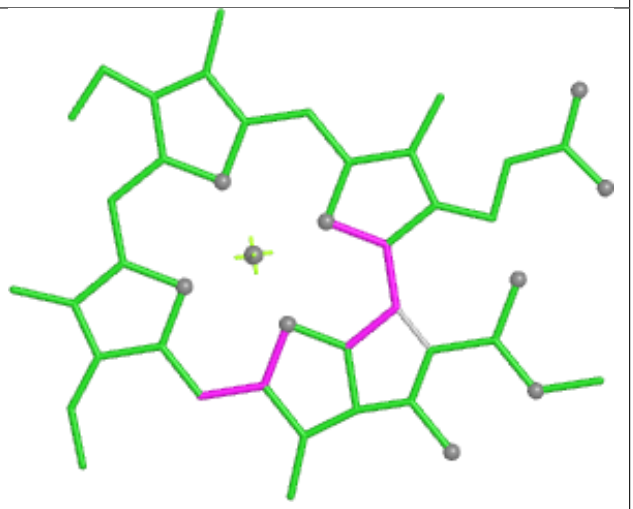


Rings

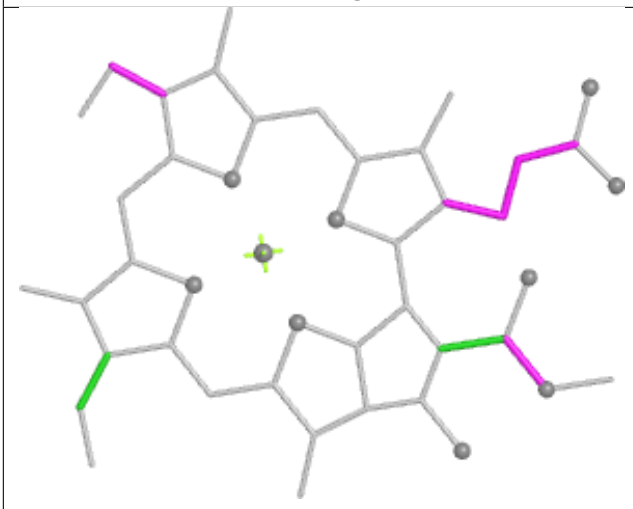
Ligand CLA a 818



Bond lengths



Bond angles

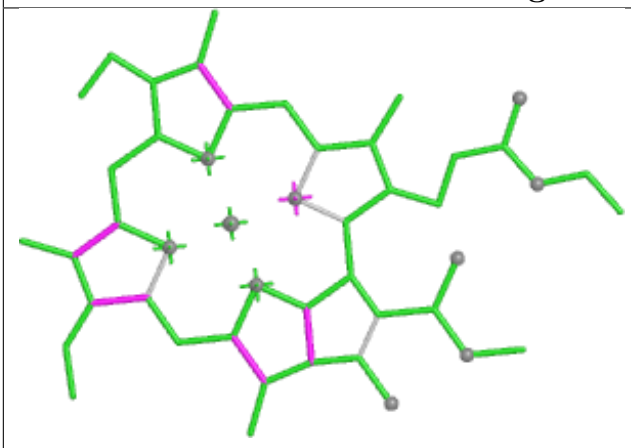


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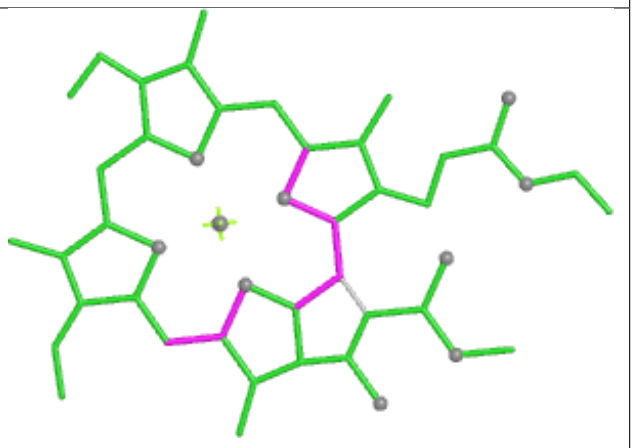


Rings

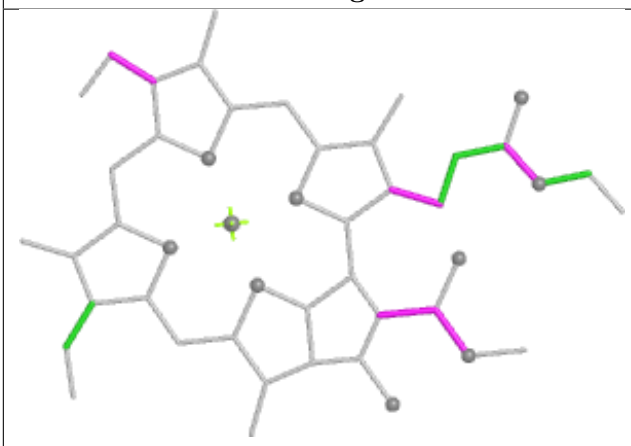
Ligand CLA a 835



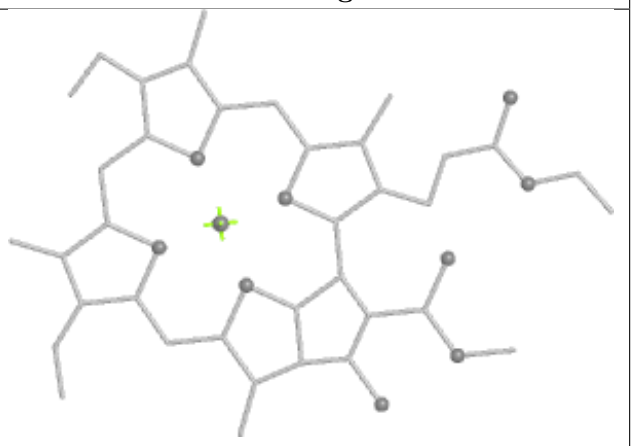
Bond lengths



Bond angles

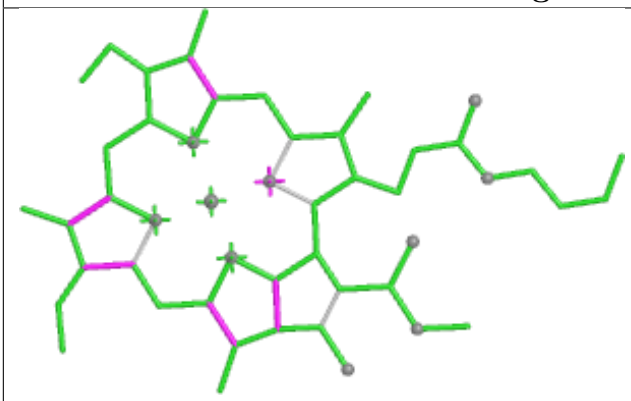


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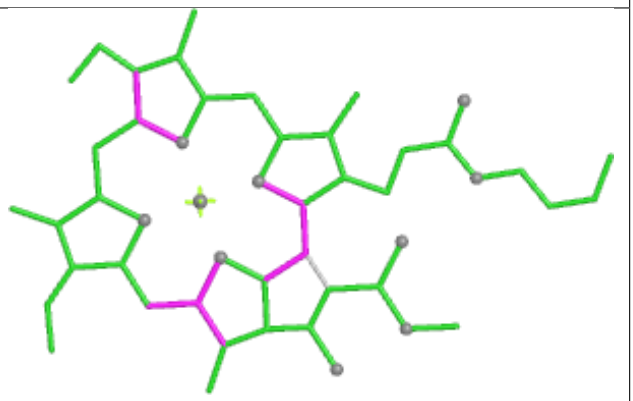


Rings

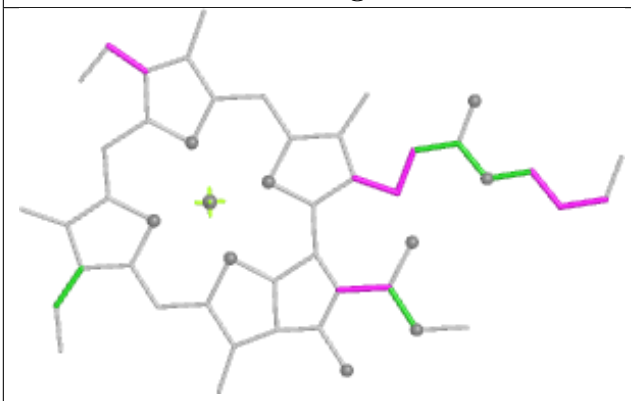
Ligand CLA l 305



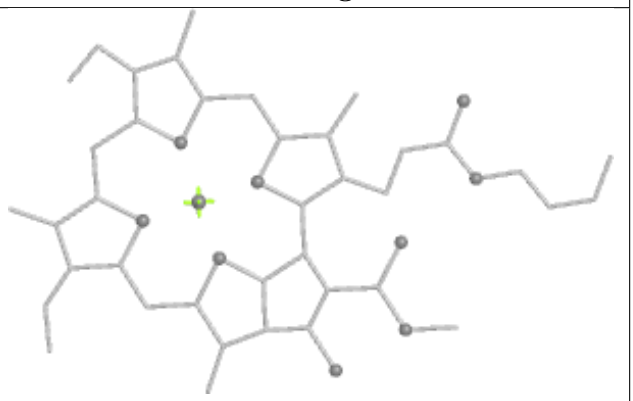
Bond lengths



Bond angles

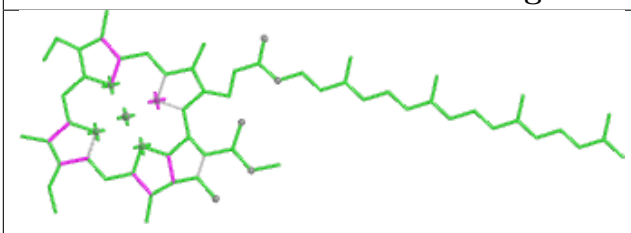


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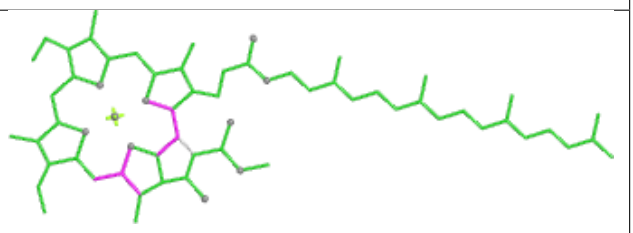


Rings

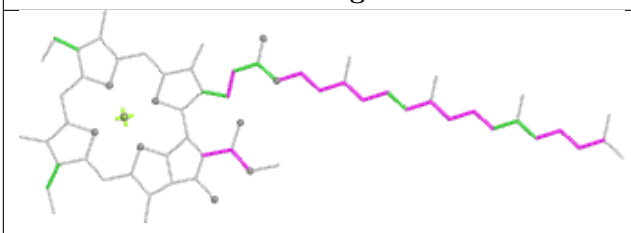
Ligand CLA B 802



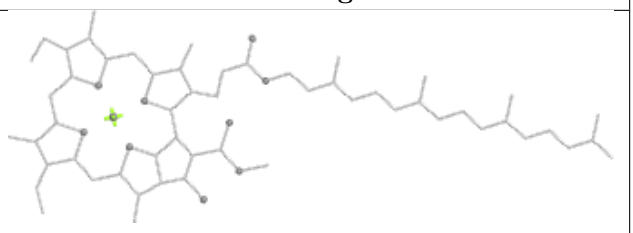
Bond lengths



Bond angles

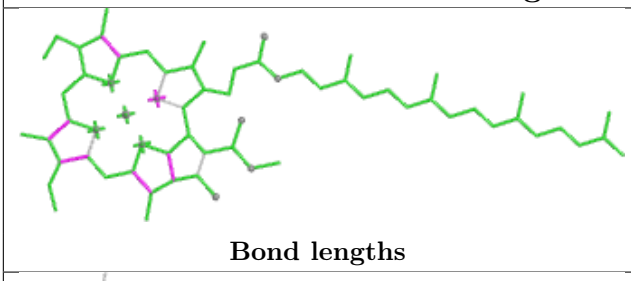


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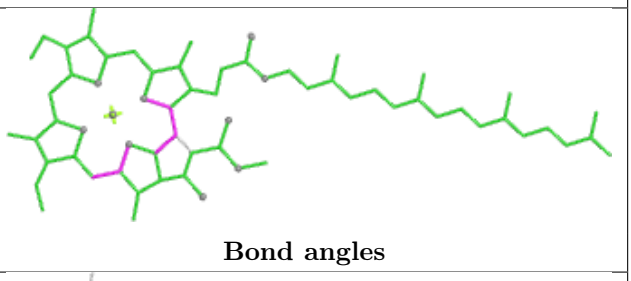


Rings

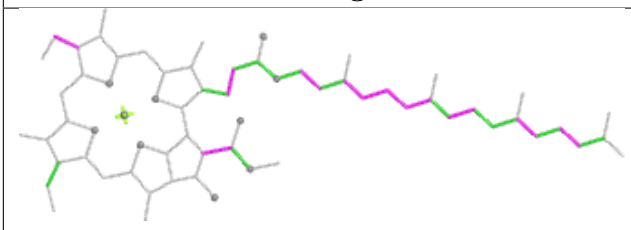
Ligand CLA A 822



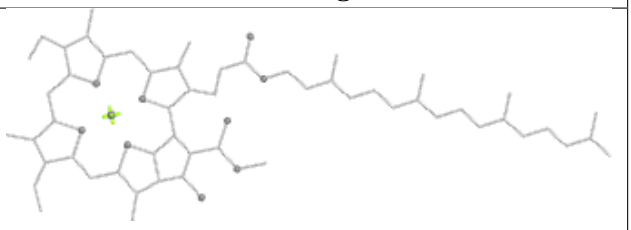
Bond lengths



Bond angles

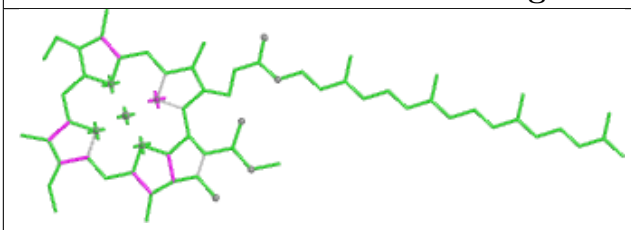


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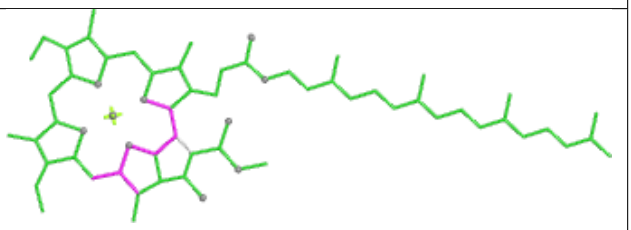


Rings

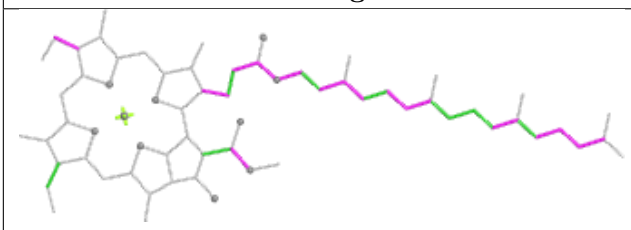
Ligand CLA a 808



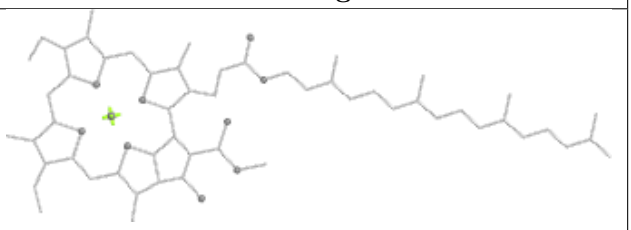
Bond lengths



Bond angles

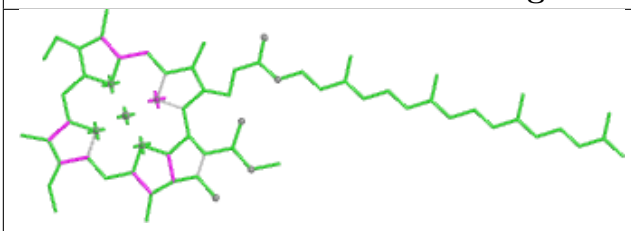


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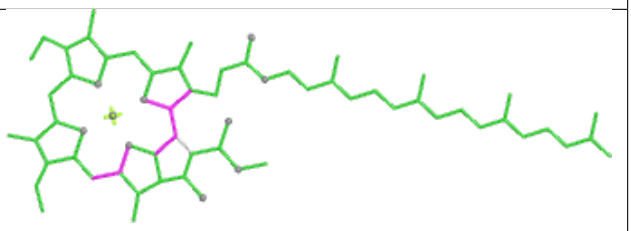


Rings

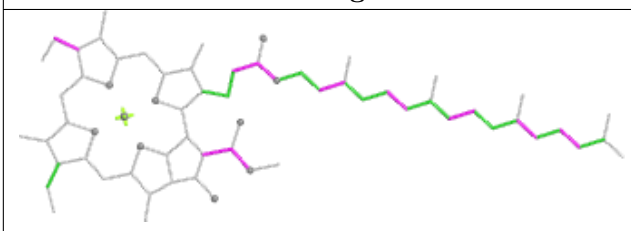
Ligand CLA b 803



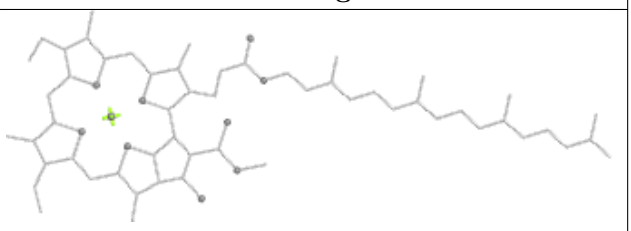
Bond lengths



Bond angles



Torsions

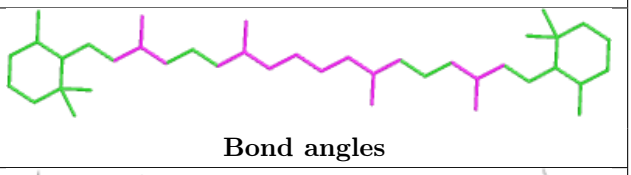


Rings

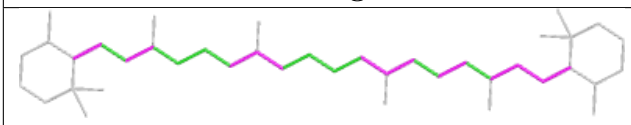
Ligand BCR L 305



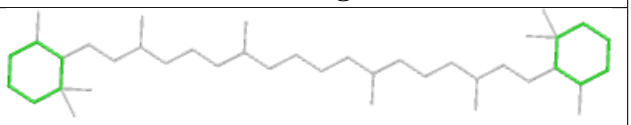
Bond lengths



Bond angles

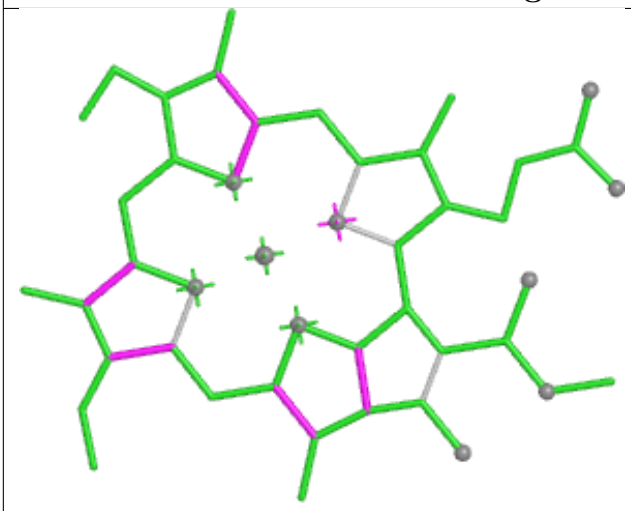


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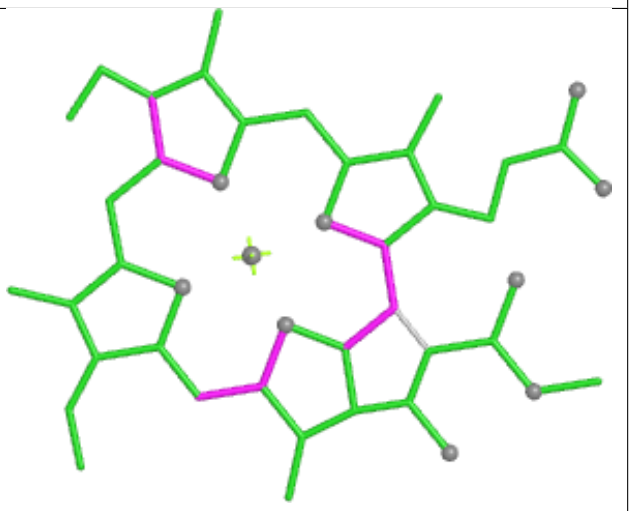


Rings

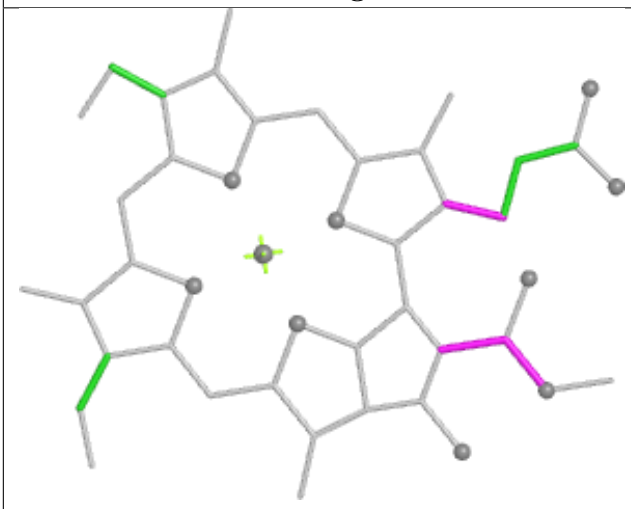
Ligand CLA B 805



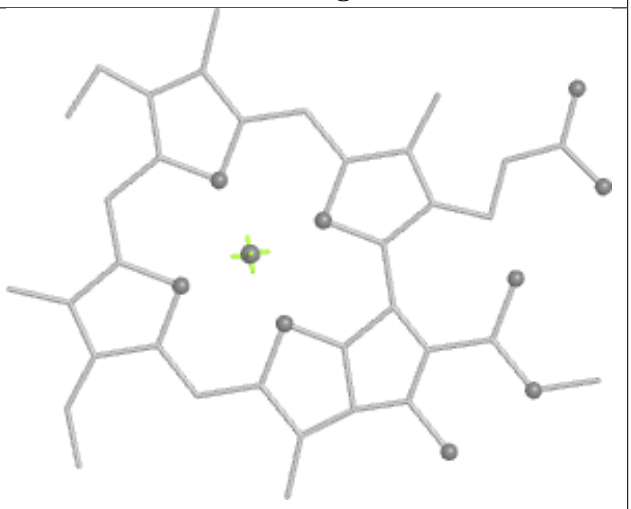
Bond lengths



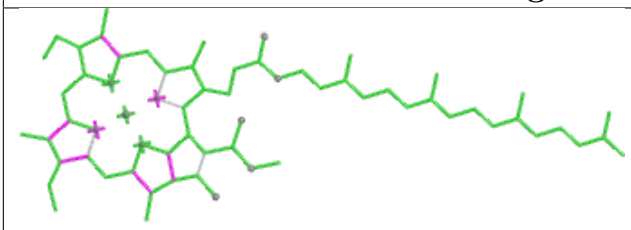
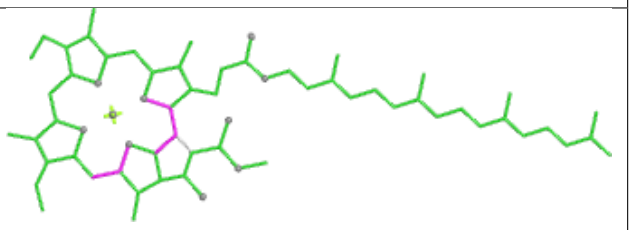
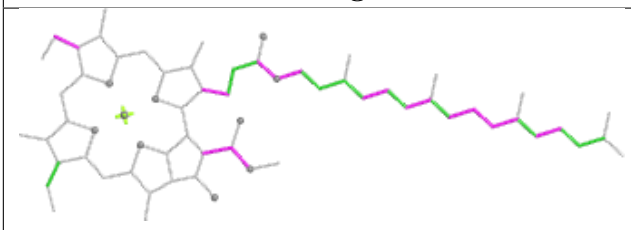
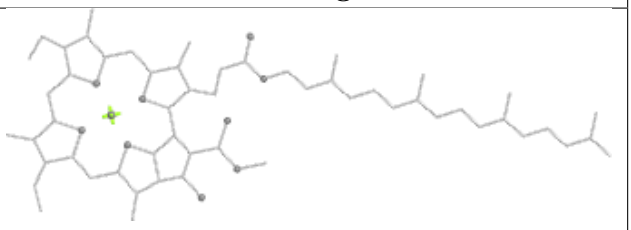
Bond angles

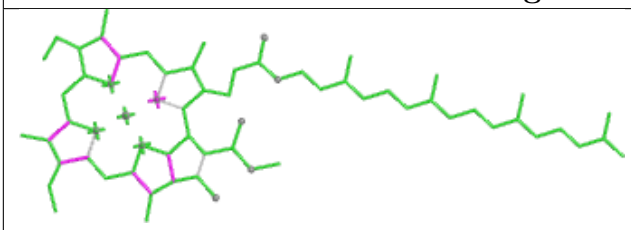
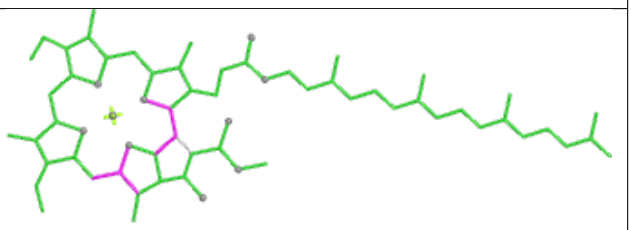
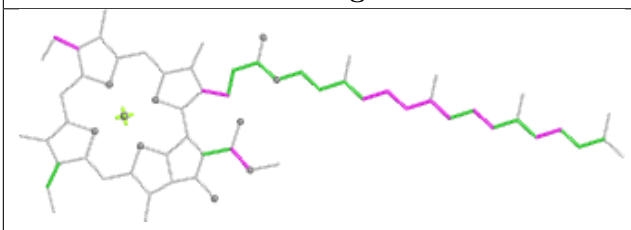
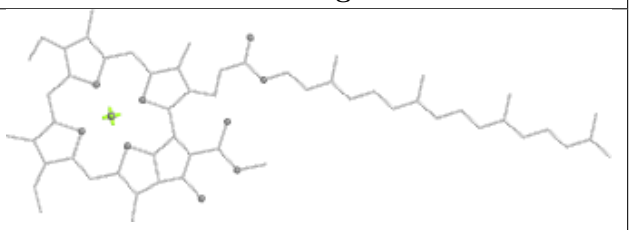


Torsions

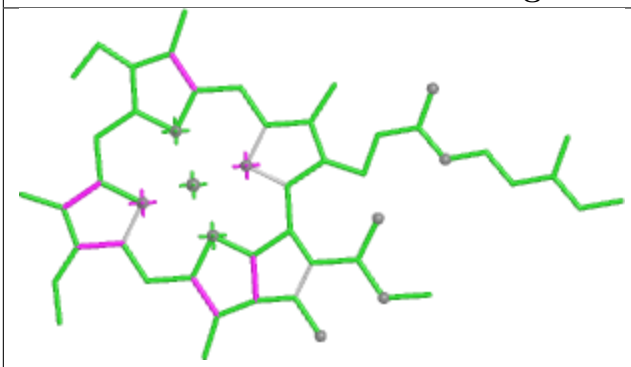


Rings

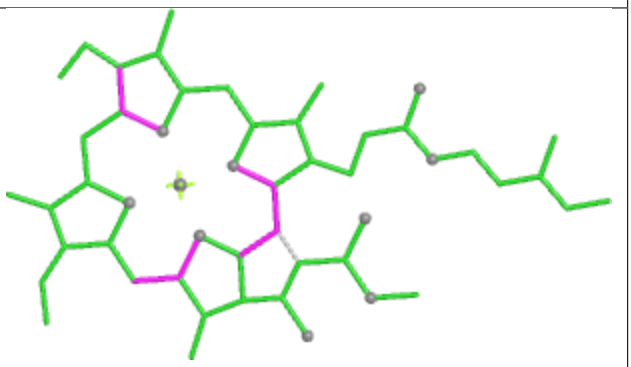
Ligand CLA b 814	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

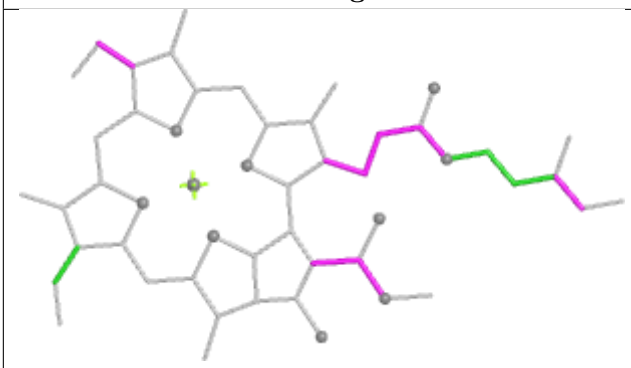
Ligand CLA A 831



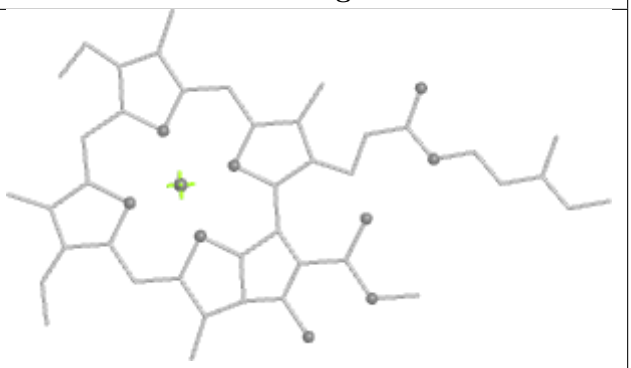
Bond lengths



Bond angles

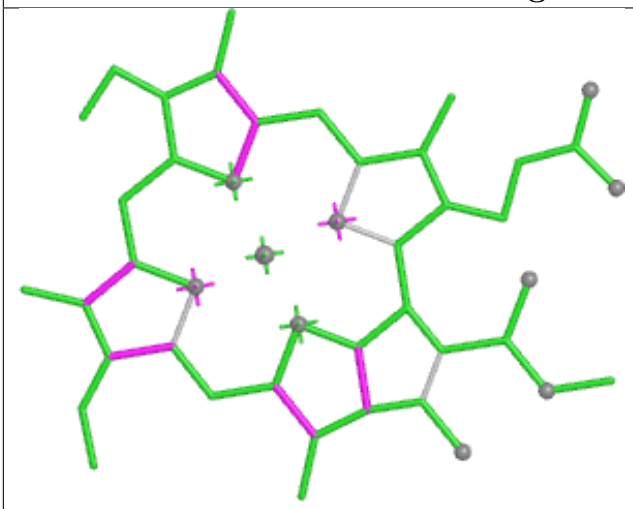


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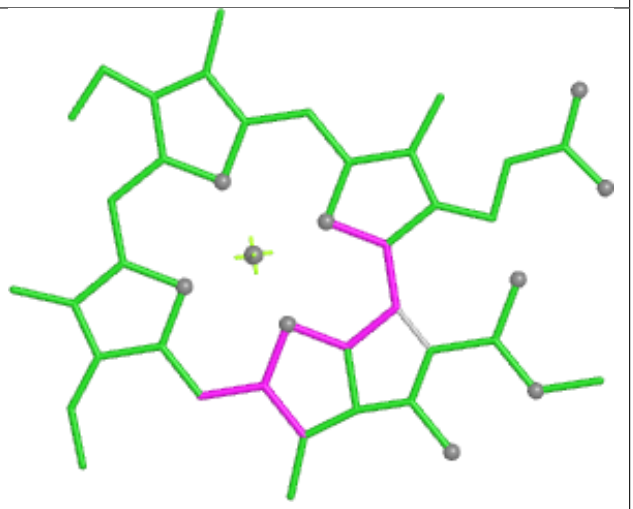


Rings

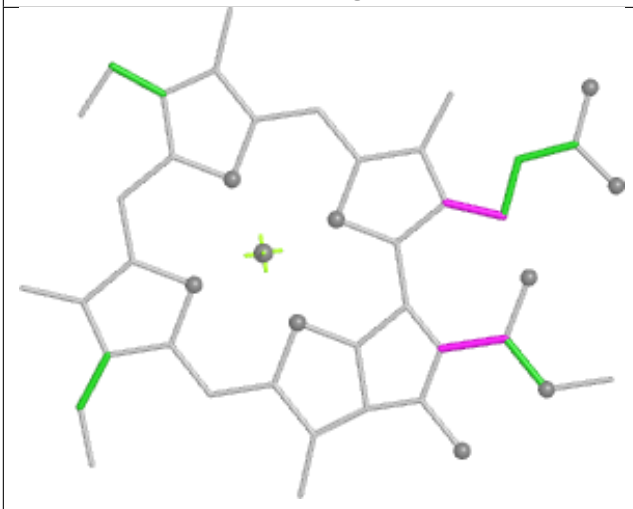
Ligand CLA a 812



Bond lengths



Bond angles

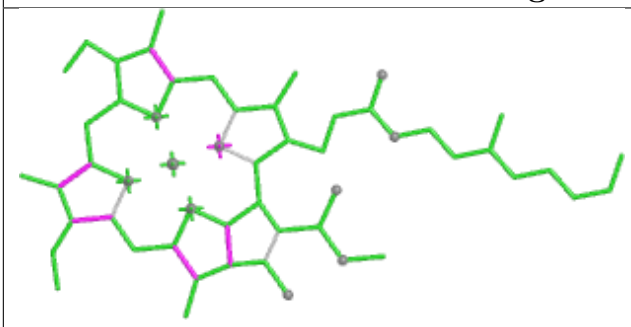


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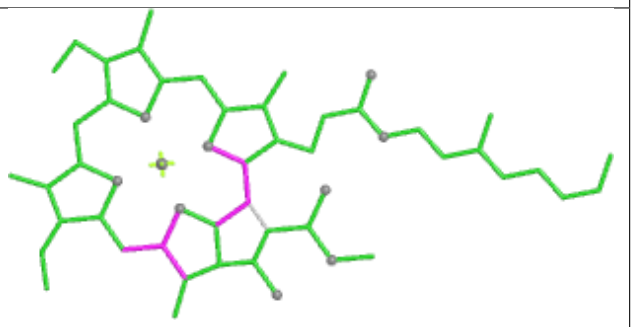


Rings

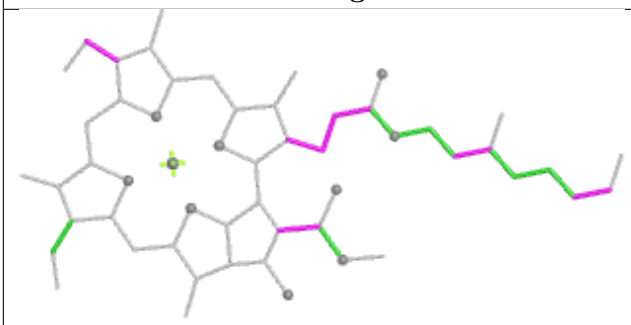
Ligand CLA a 810



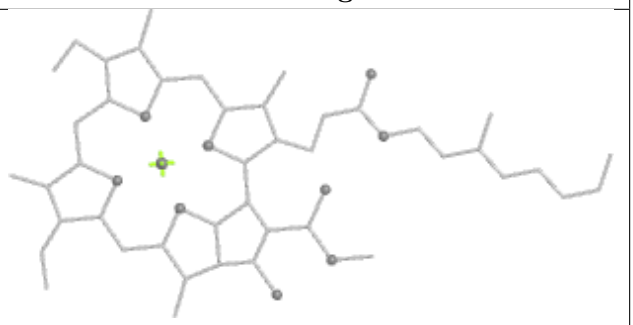
Bond lengths



Bond angles

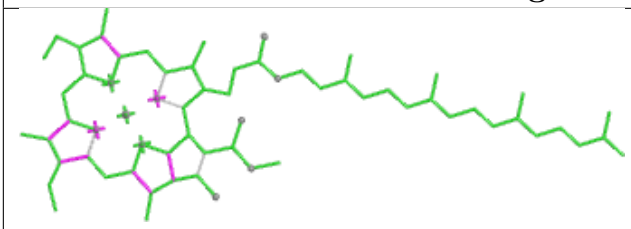


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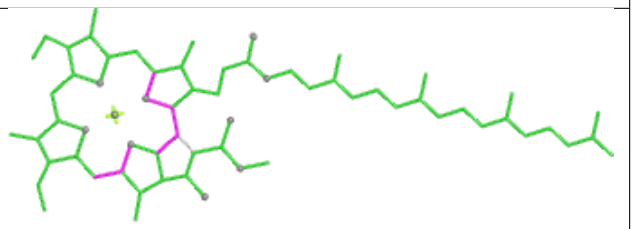


Rings

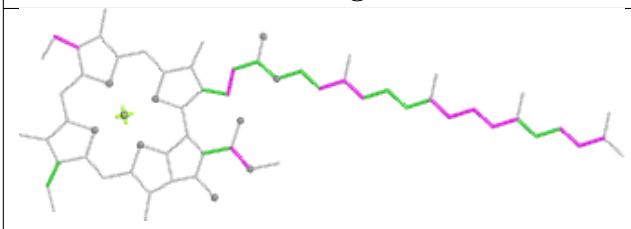
Ligand CLA a 826



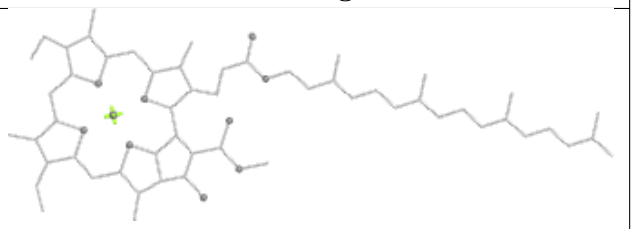
Bond lengths



Bond angles

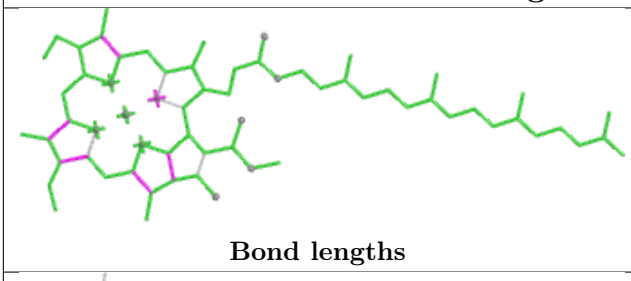


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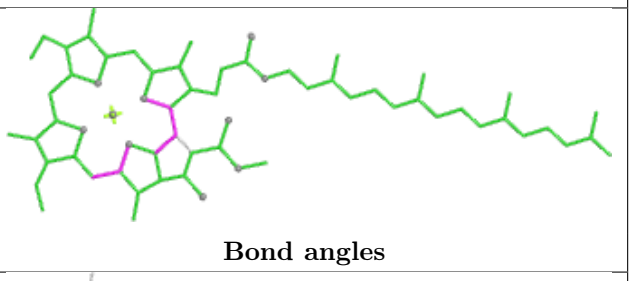


Rings

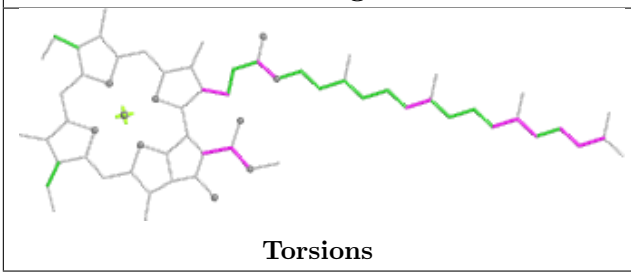
Ligand CLA b 832



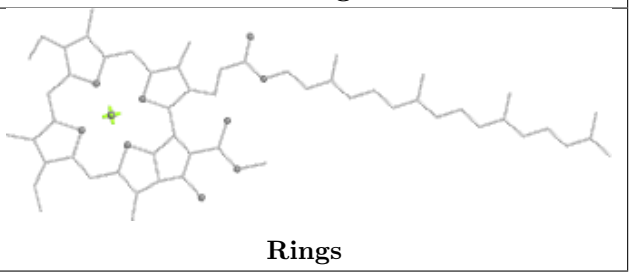
Bond lengths



Bond angles

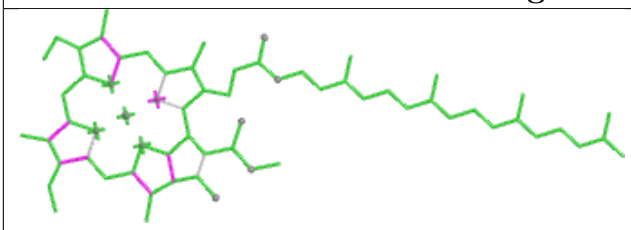


Torsions

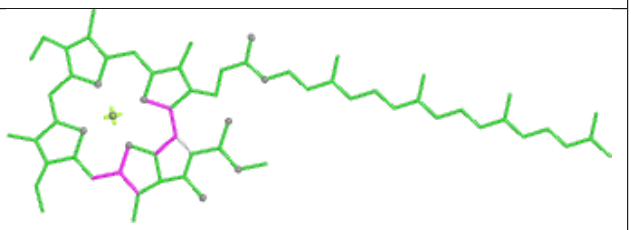


Rings

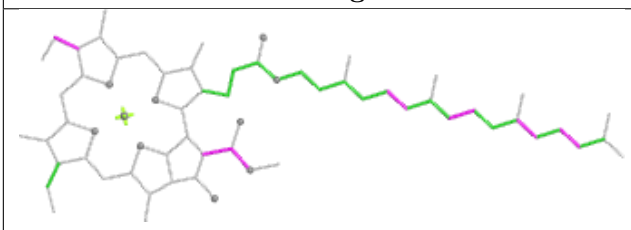
Ligand CLA b 809



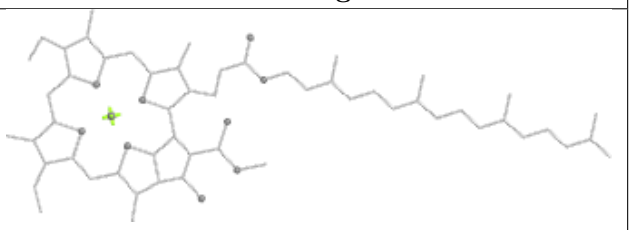
Bond lengths



Bond angles

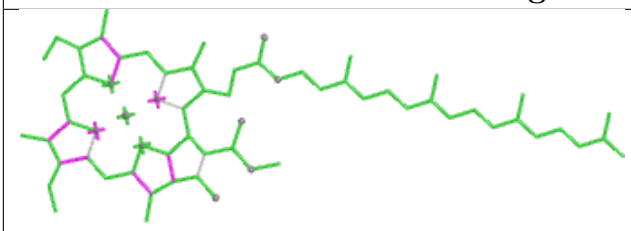


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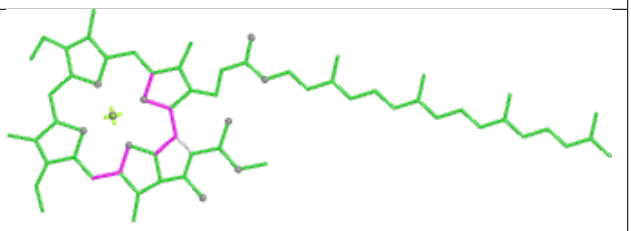


Rings

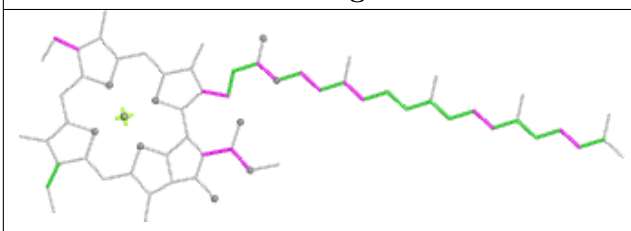
Ligand CLA a 827



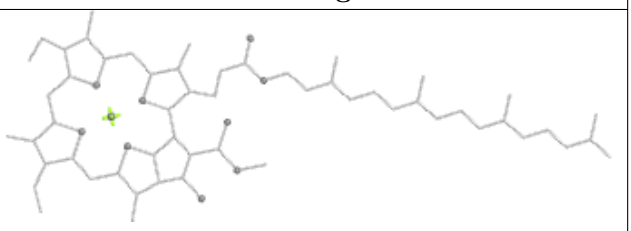
Bond lengths



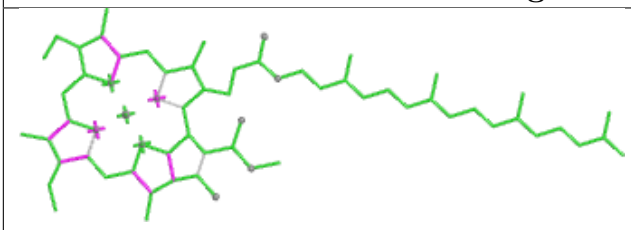
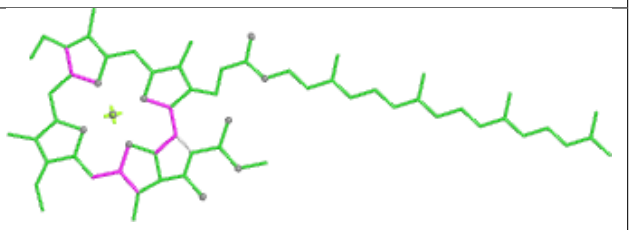
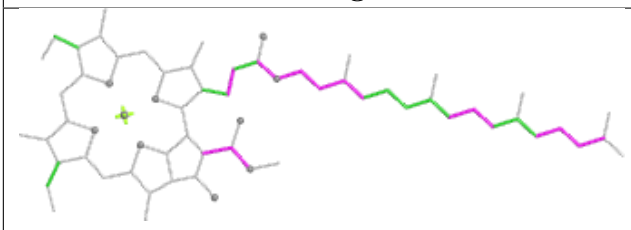
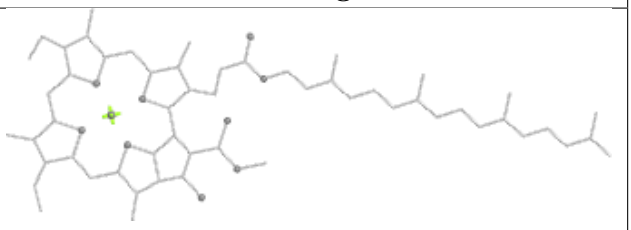
Bond angles

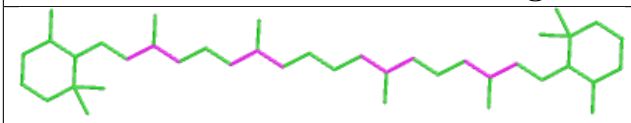
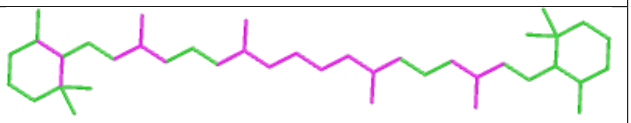
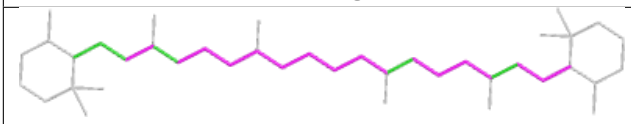
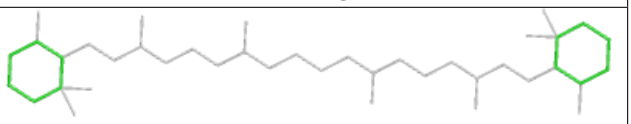


Torsions

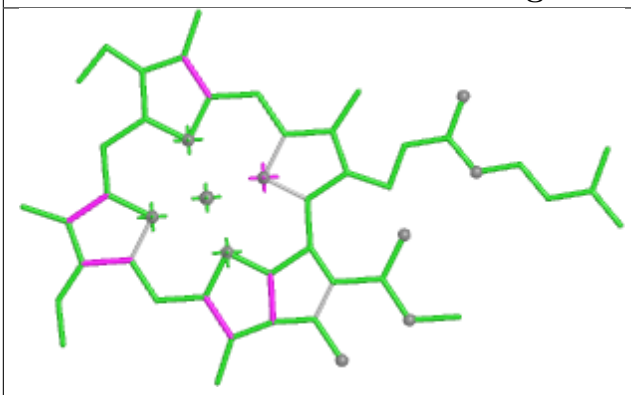


Rings

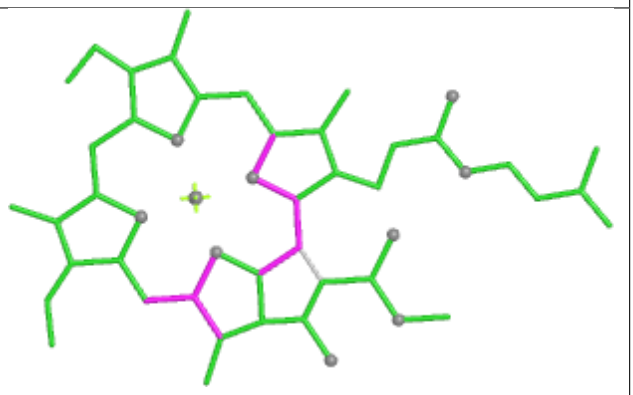
Ligand CLA b 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

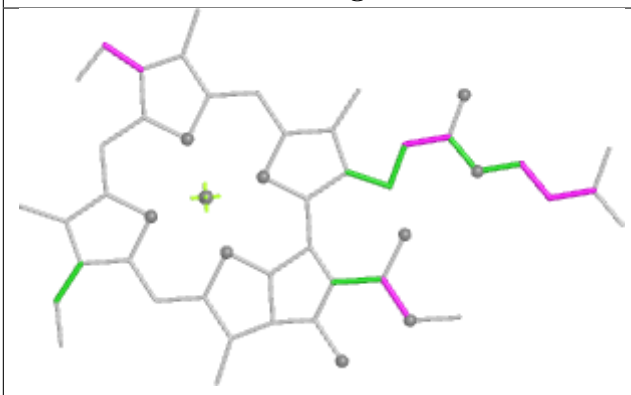
Ligand CLA L 304



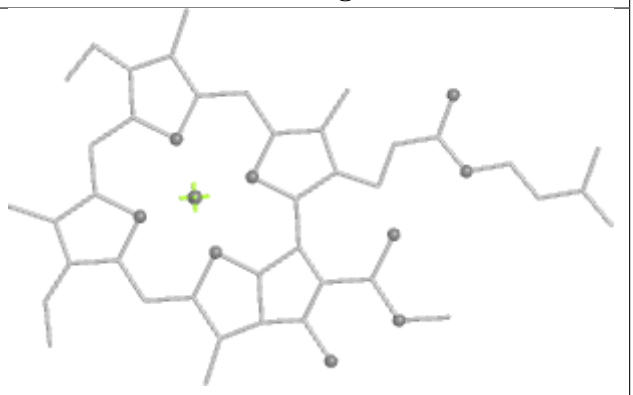
Bond lengths



Bond angles

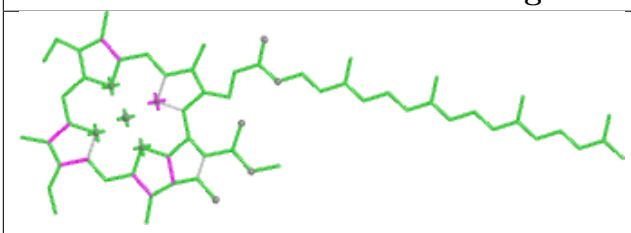


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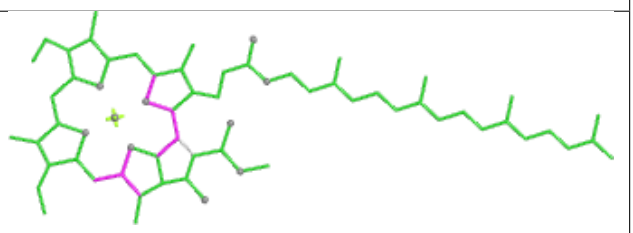


Rings

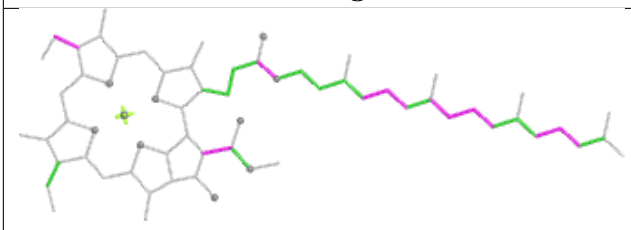
Ligand CLA B 829



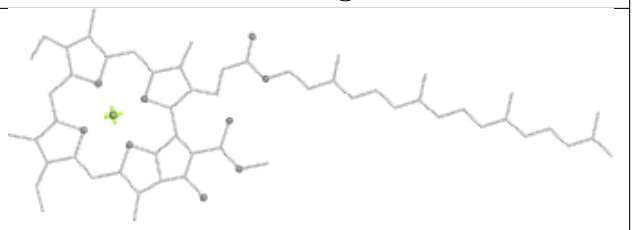
Bond lengths



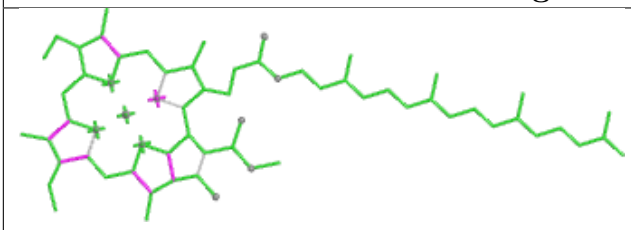
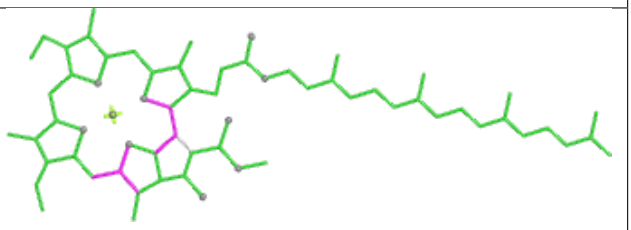
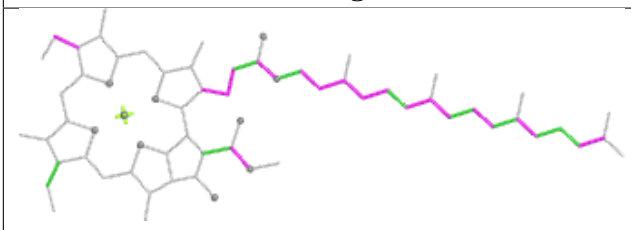
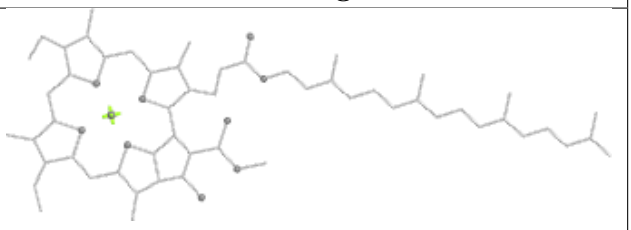
Bond angles

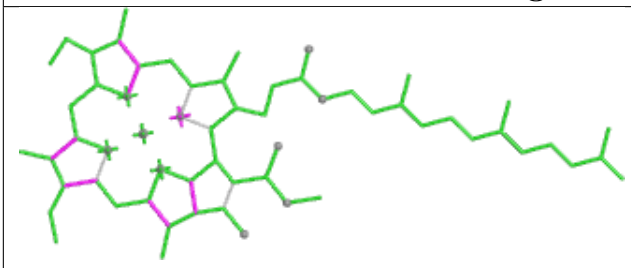
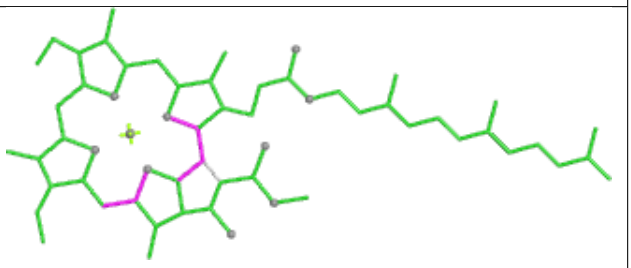
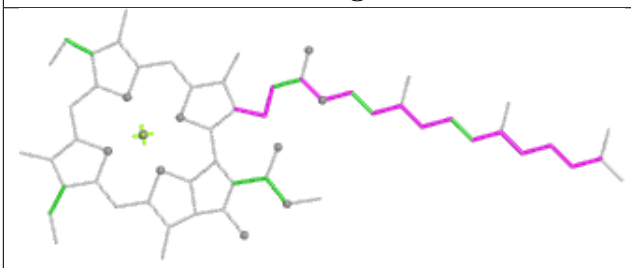
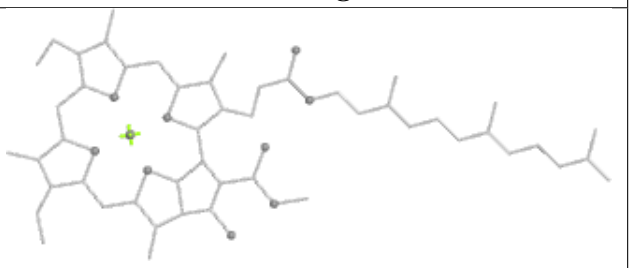


Torsions

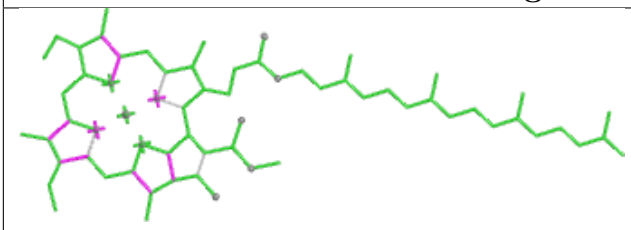


Rings

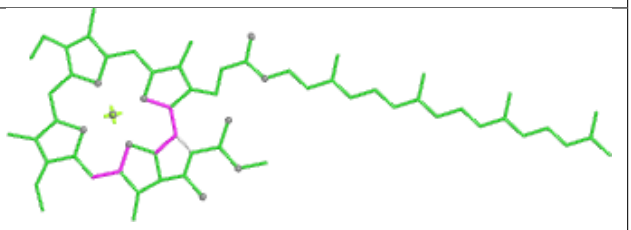
Ligand CLA l 306	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b 824	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

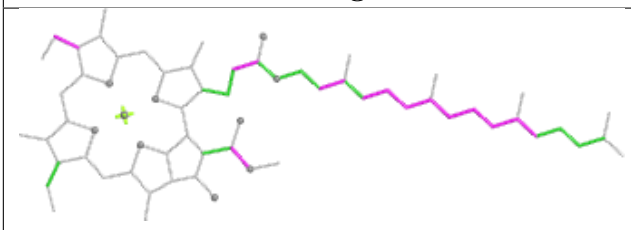
Ligand CLA B 807



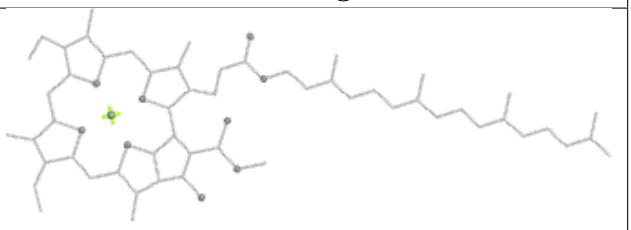
Bond lengths



Bond angles

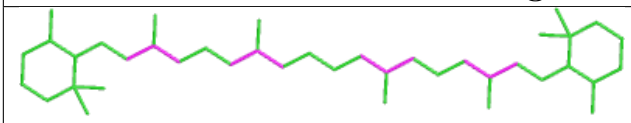


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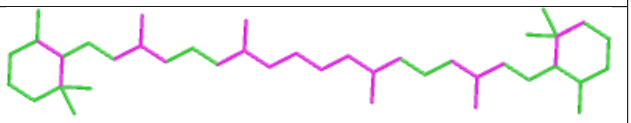


Rings

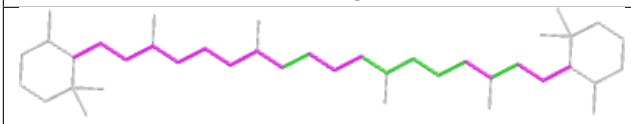
Ligand BCR a 841



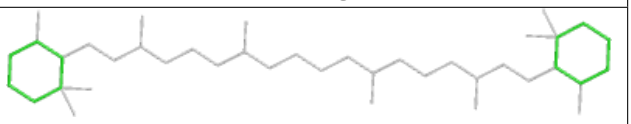
Bond lengths



Bond angles

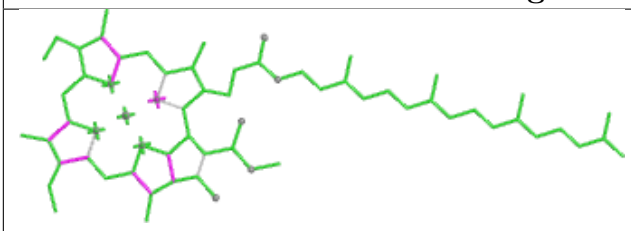


Torsions

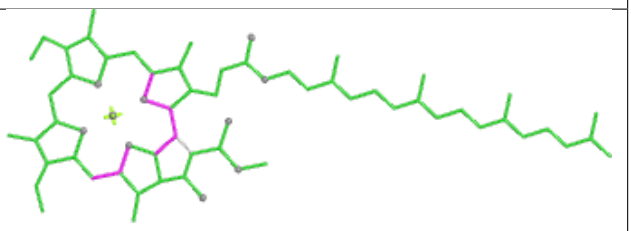


Rings

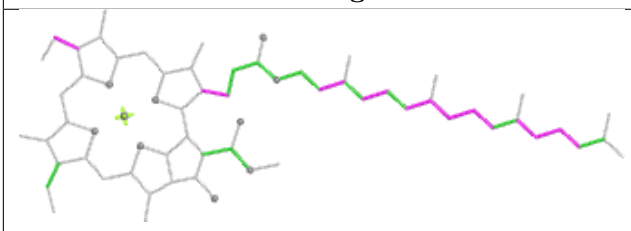
Ligand CLA b 810



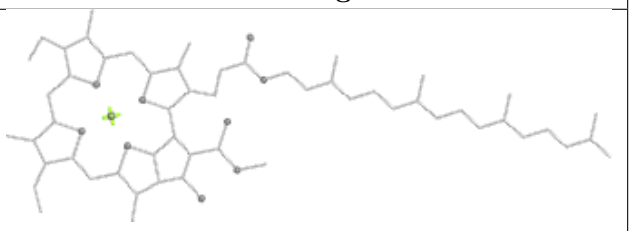
Bond lengths



Bond angles

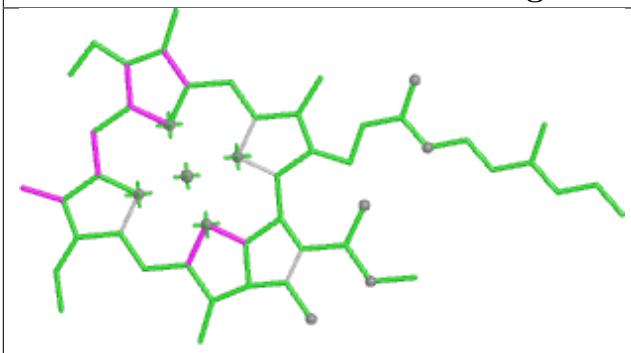


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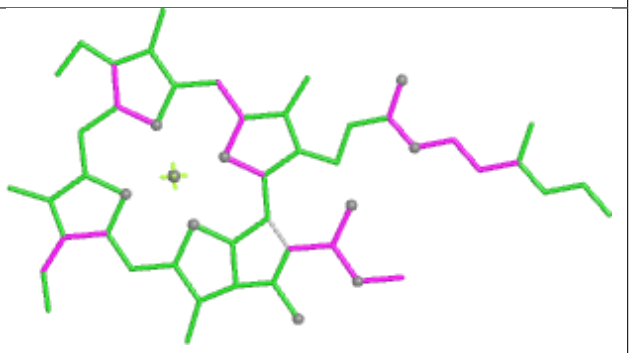


Rings

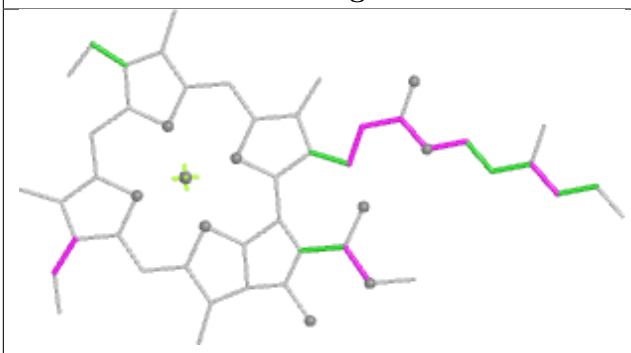
Ligand CLA L 308



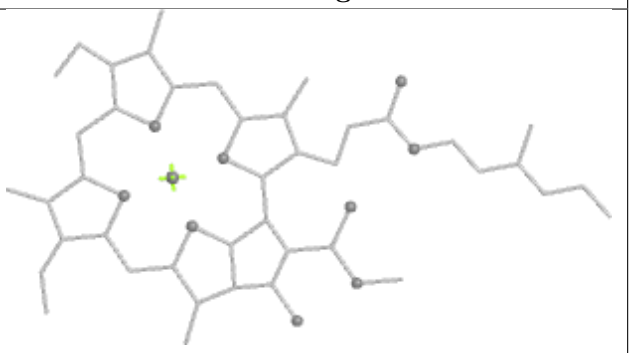
Bond lengths



Bond angles

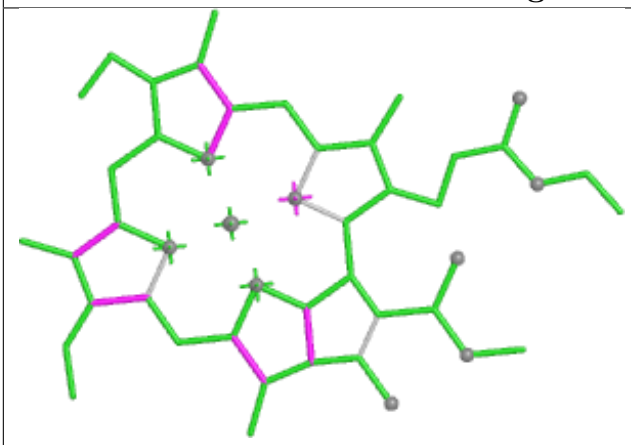


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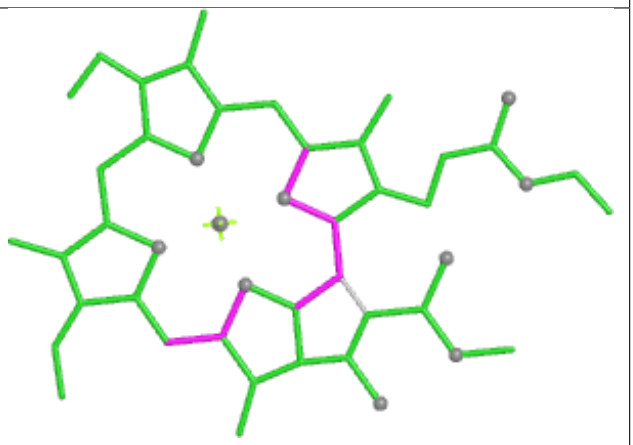


Rings

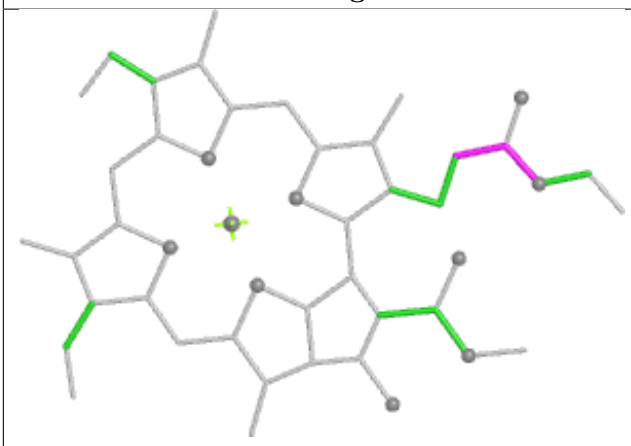
Ligand CLA b 830



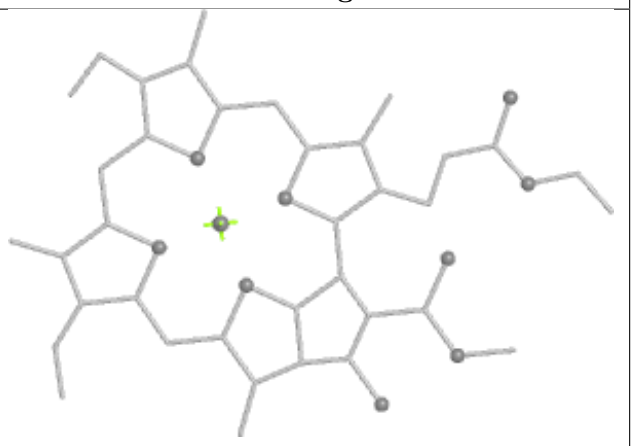
Bond lengths



Bond angles

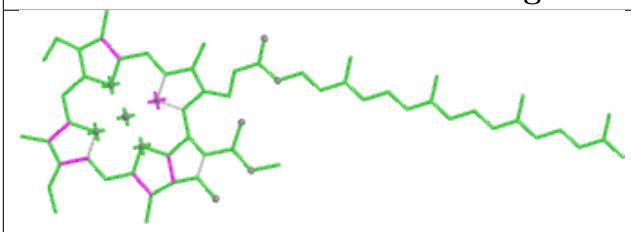


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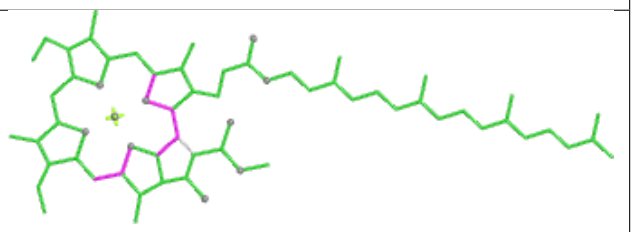


Rings

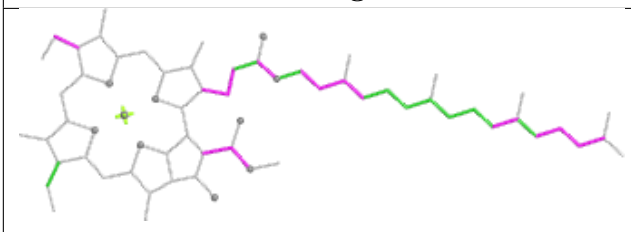
Ligand CLA A 833



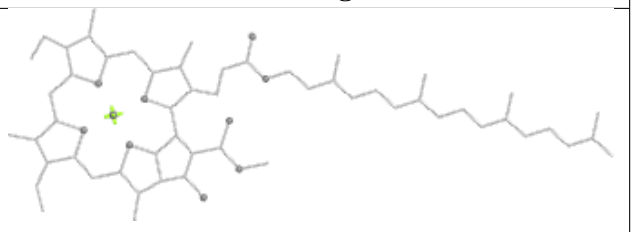
Bond lengths



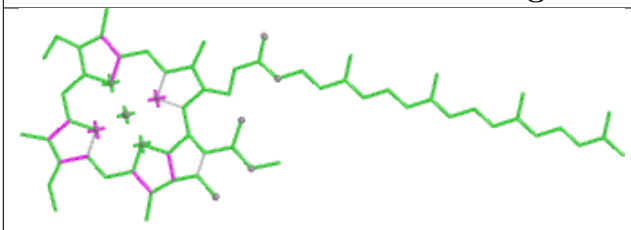
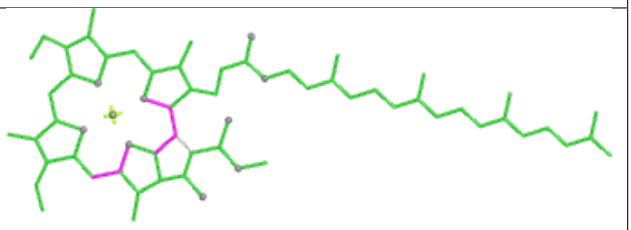
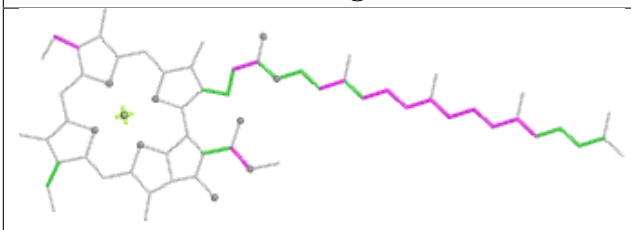
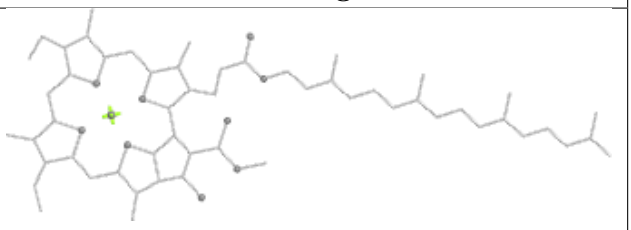
Bond angles

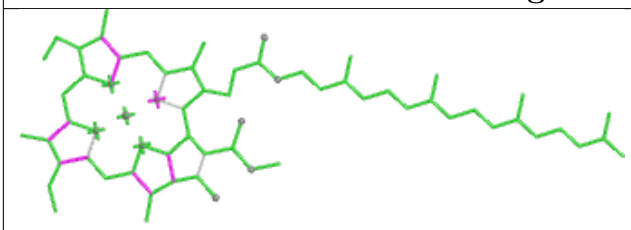
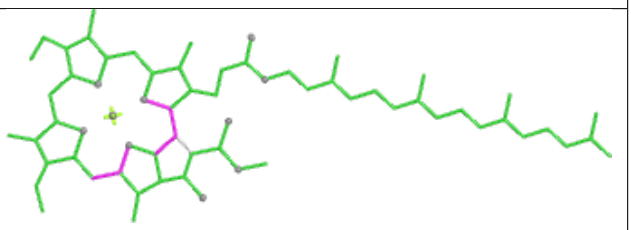
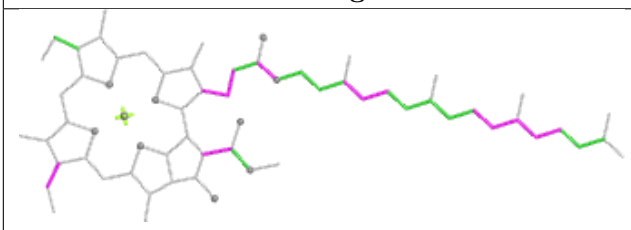
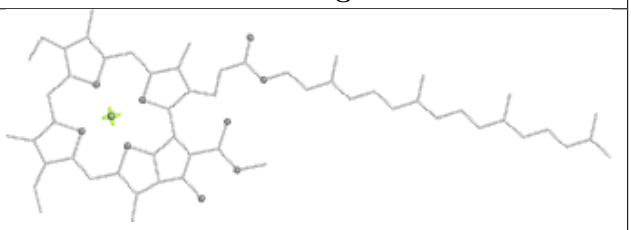


Torsions

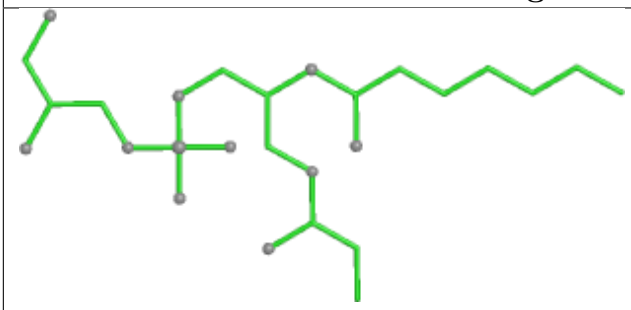


Rings

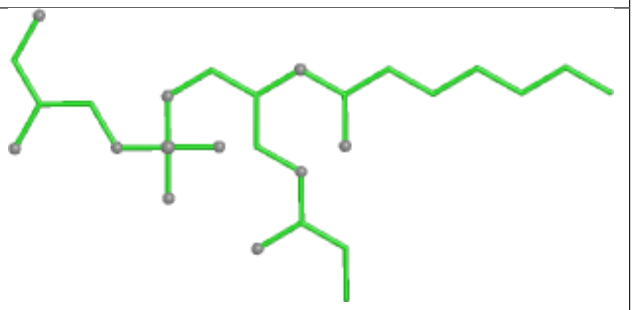
Ligand CLA b 807	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b 806	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

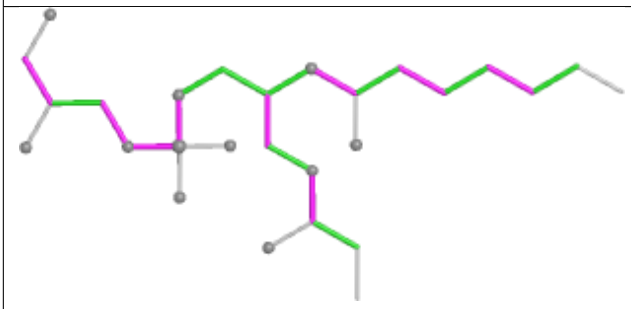
Ligand LHG a 840



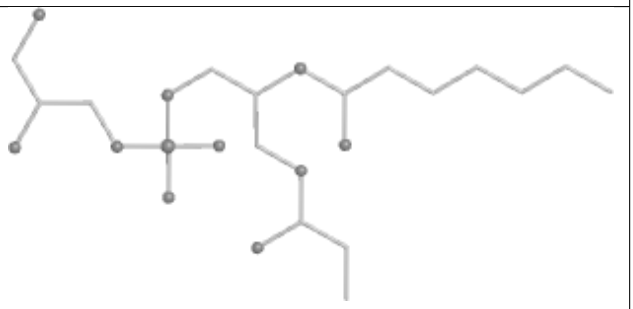
Bond lengths



Bond angles

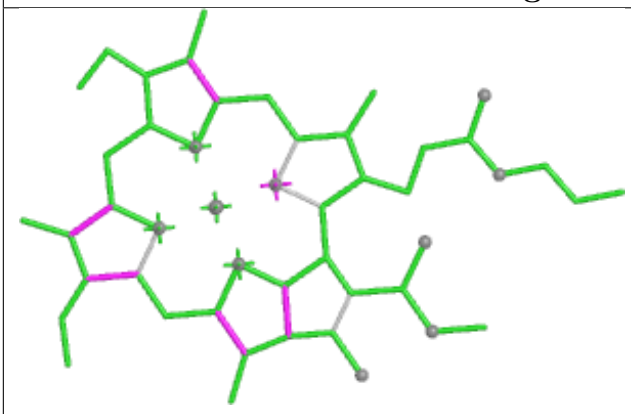


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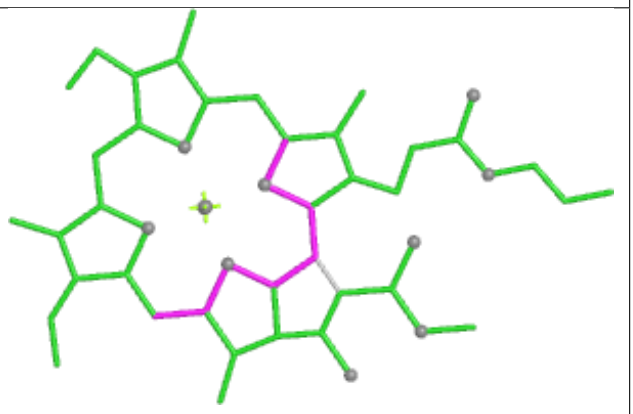


Rings

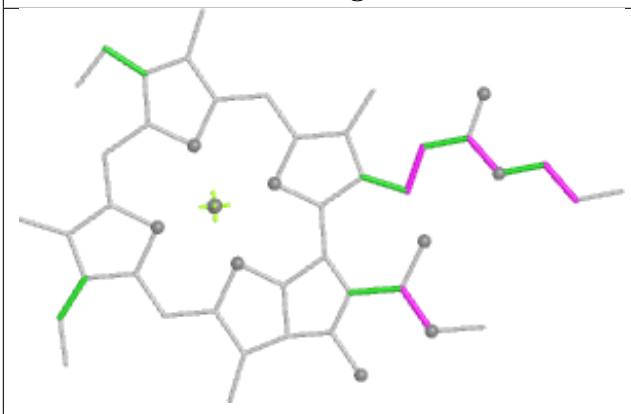
Ligand CLA A 836



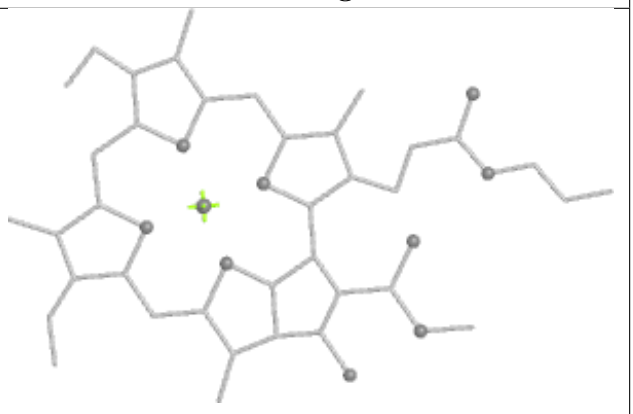
Bond lengths



Bond angles

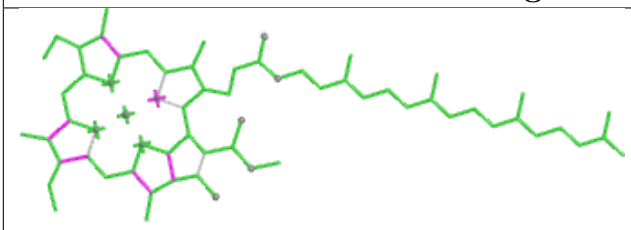


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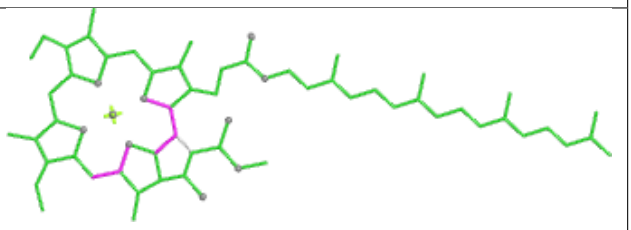


Rings

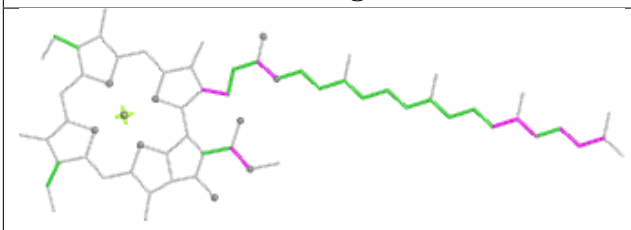
Ligand CLA B 832



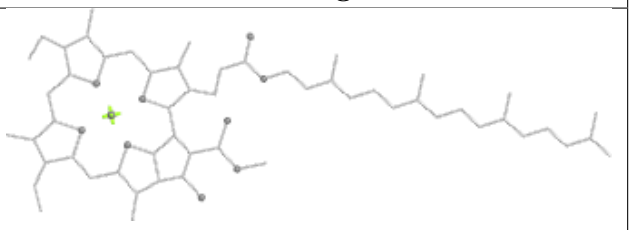
Bond lengths



Bond angles

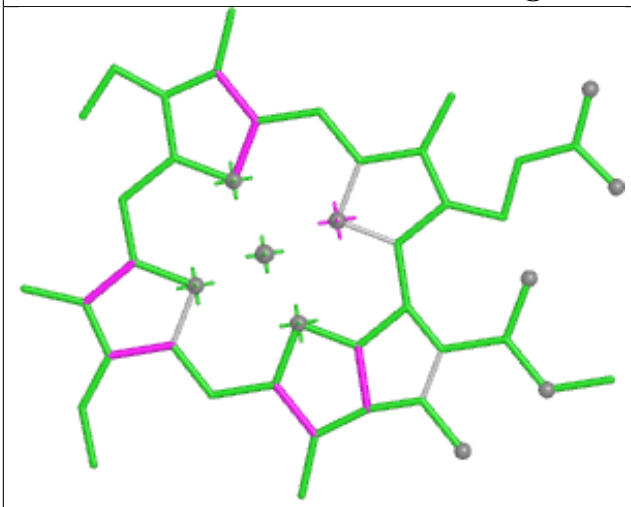


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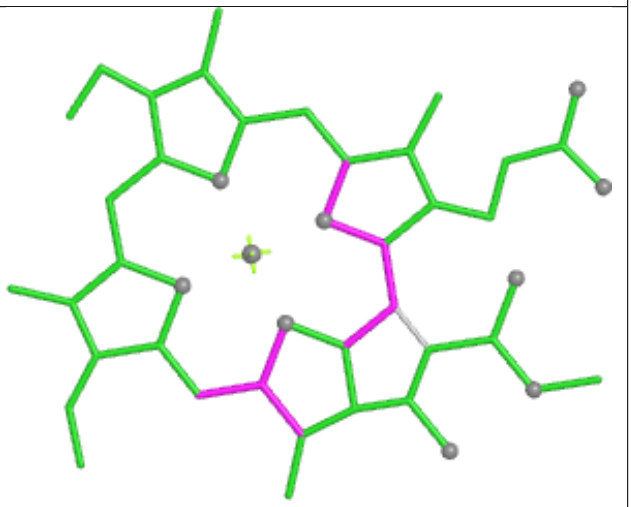


Rings

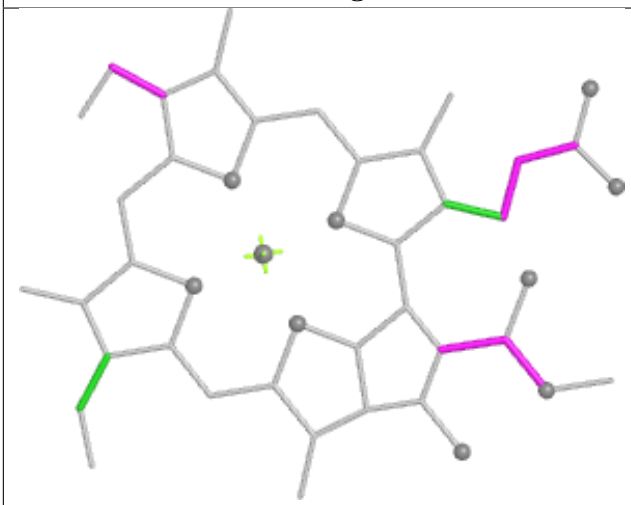
Ligand CLA B 827



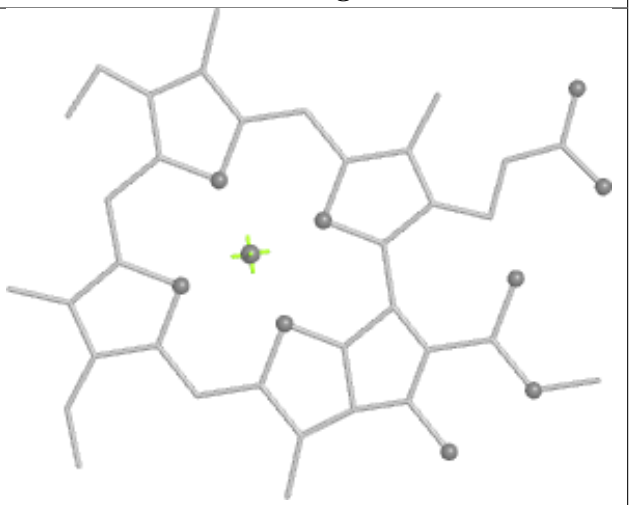
Bond lengths



Bond angles



Torsions

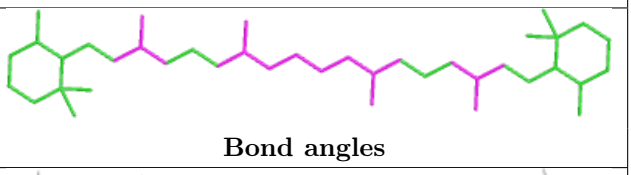


Rings

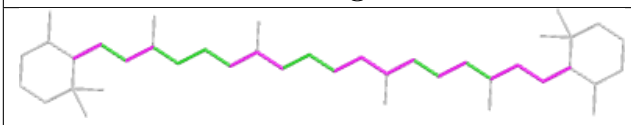
Ligand BCR l 308



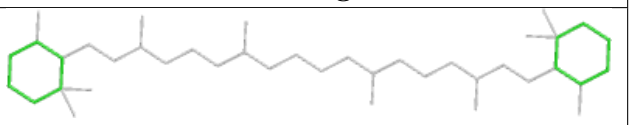
Bond lengths



Bond angles

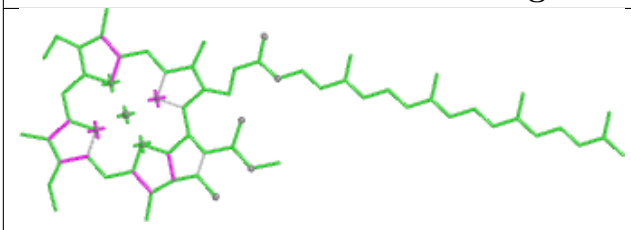


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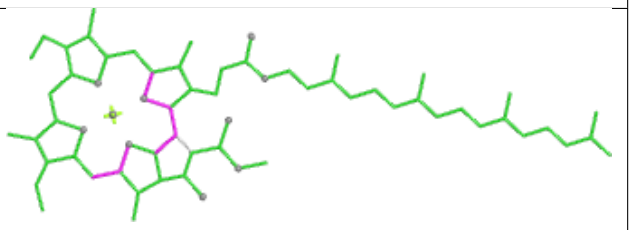


Rings

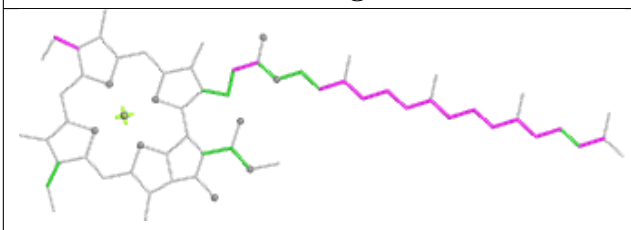
Ligand CLA a 847



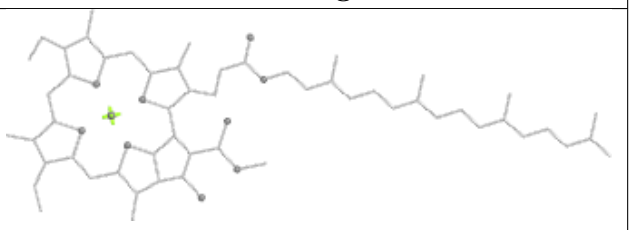
Bond lengths



Bond angles

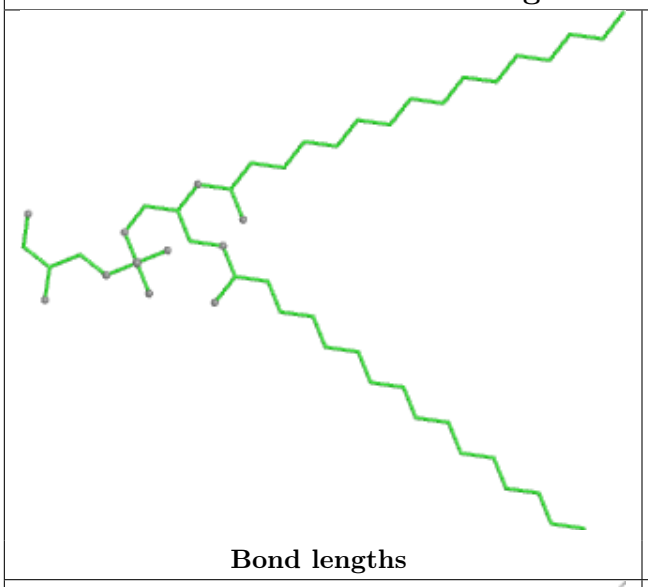


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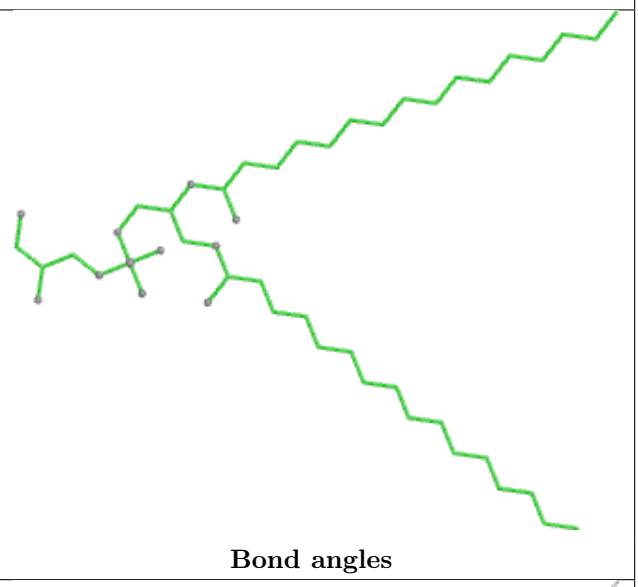


Rings

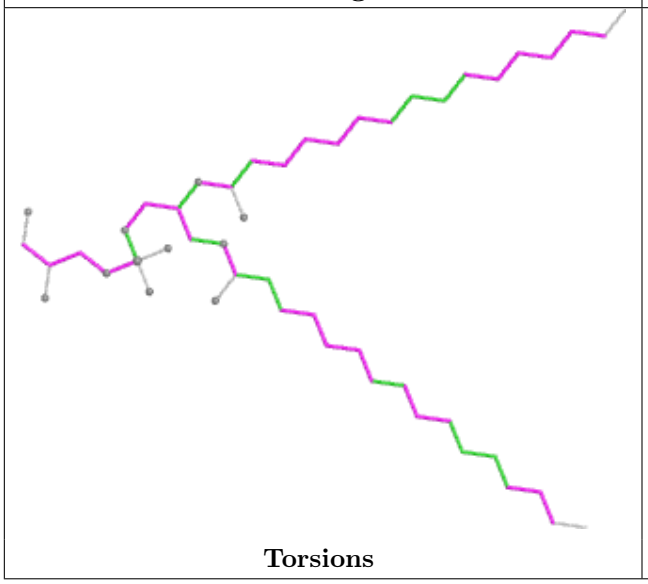
Ligand LHG A 838



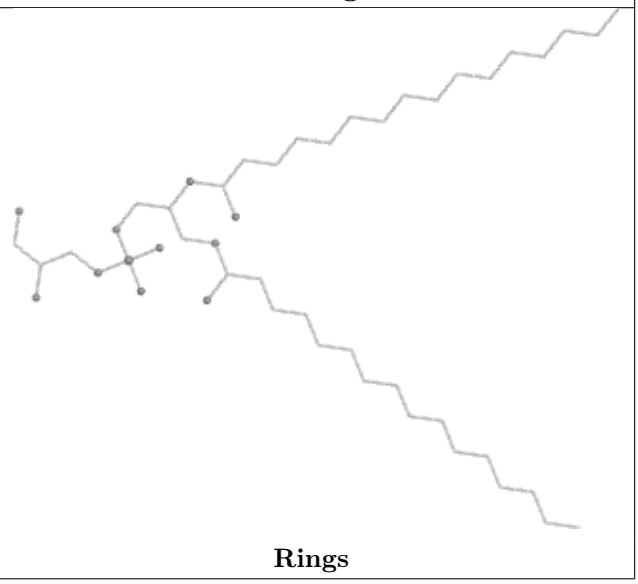
Bond lengths



Bond angles

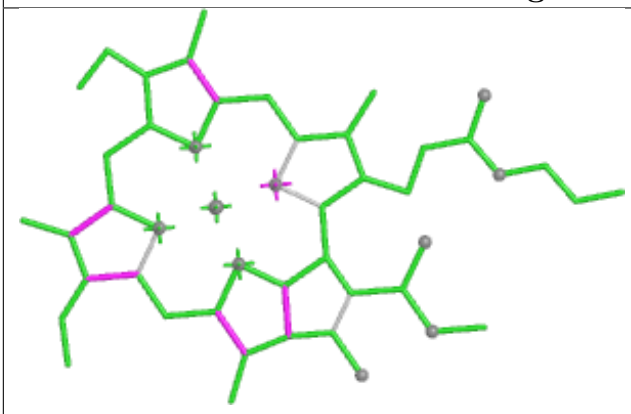


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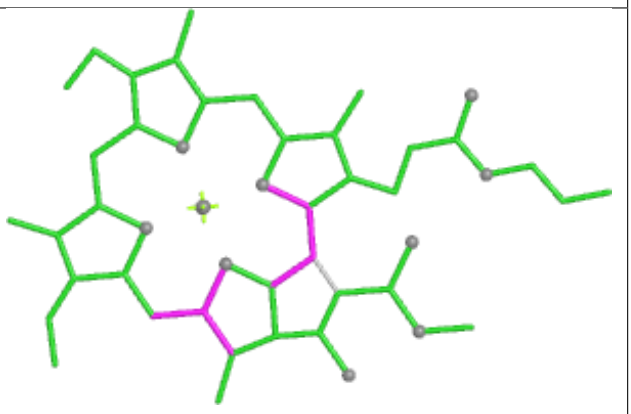


Rings

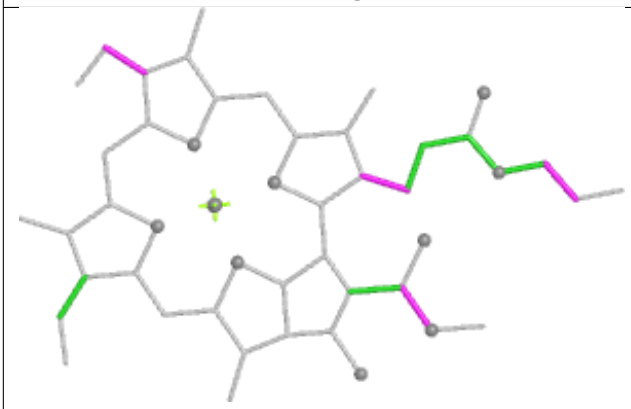
Ligand CLA b 826



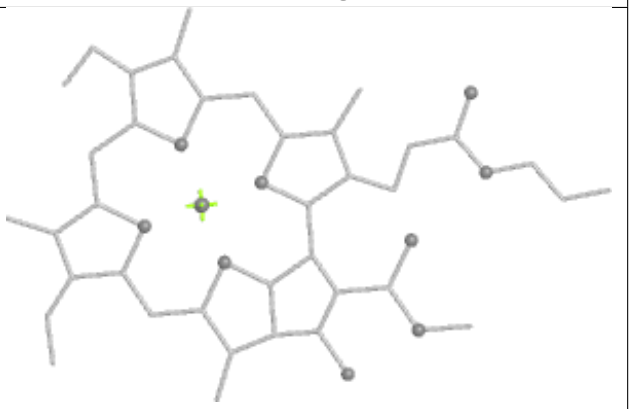
Bond lengths



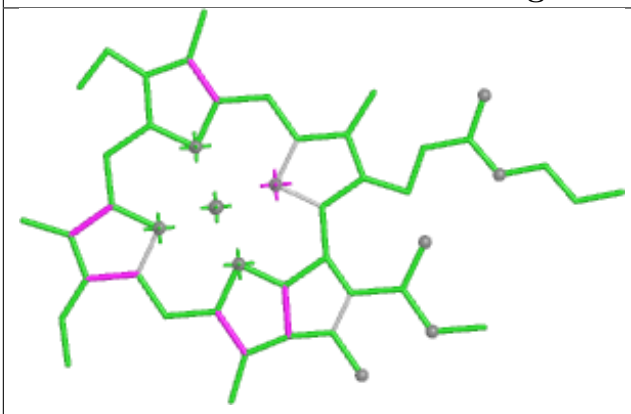
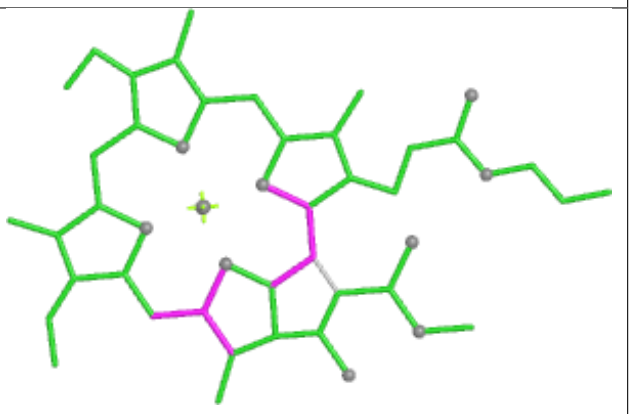
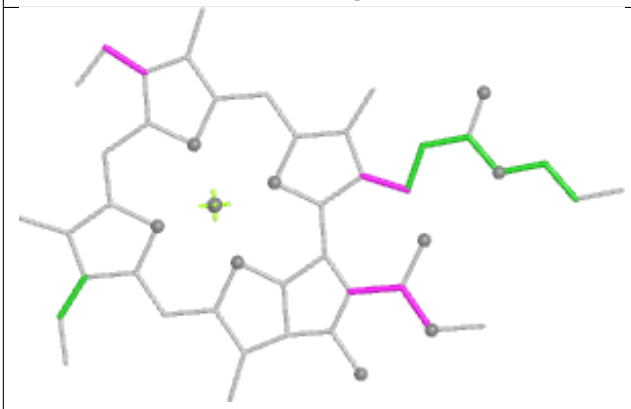
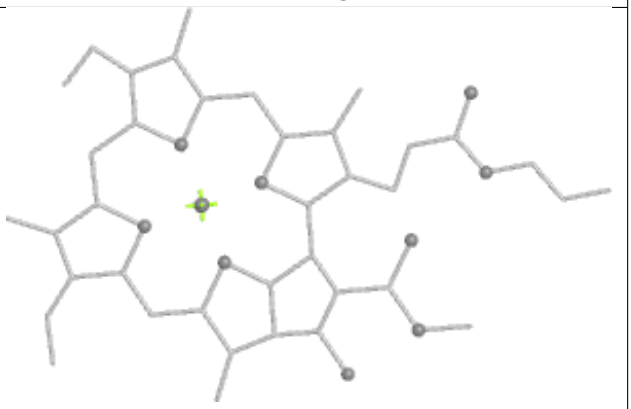
Bond angles

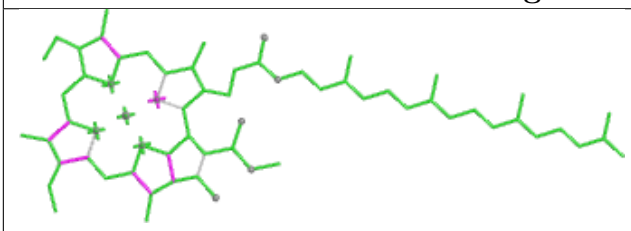
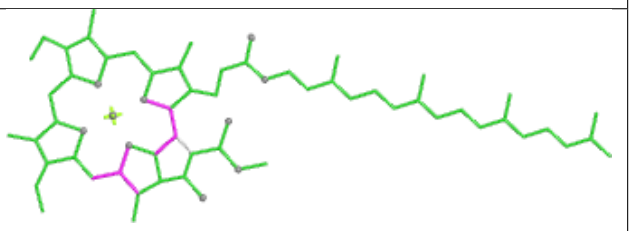
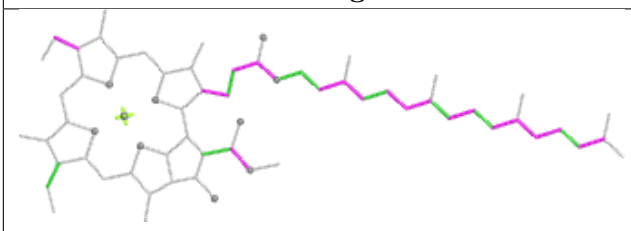
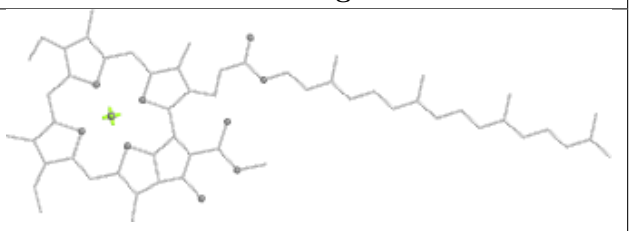


Torsions

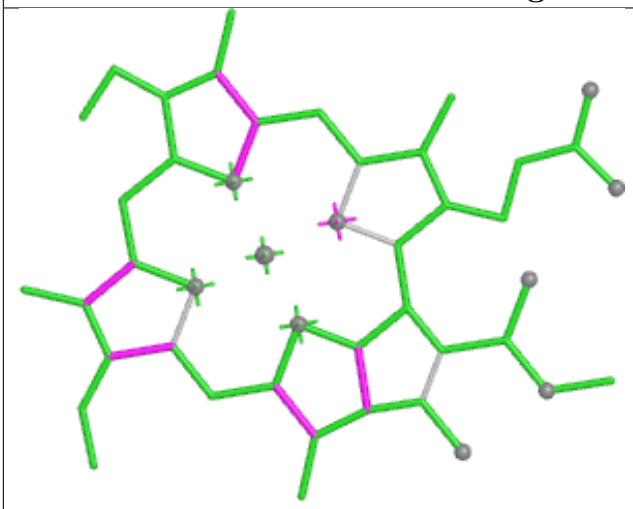


Rings

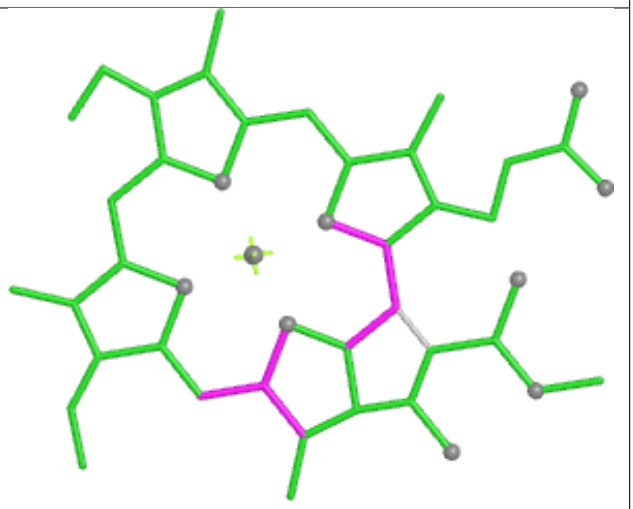
Ligand CLA b 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

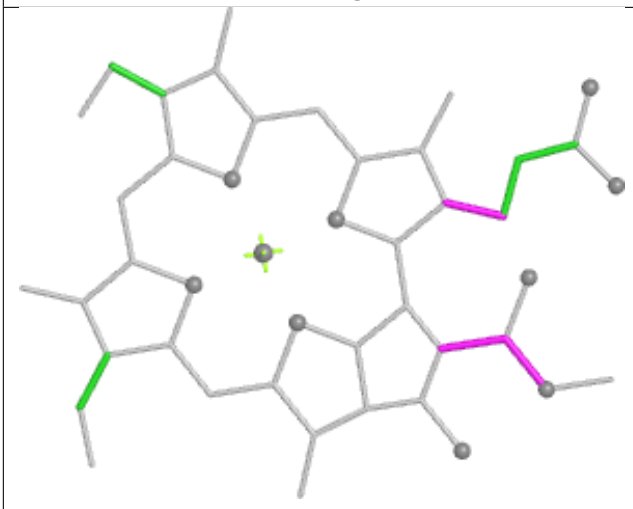
Ligand CLA b 805



Bond lengths



Bond angles

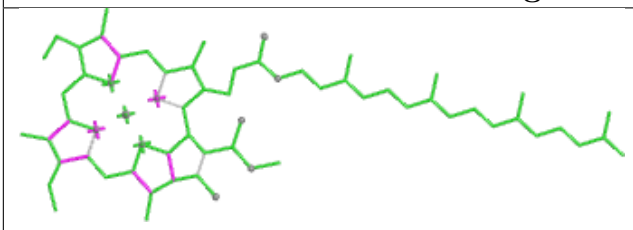


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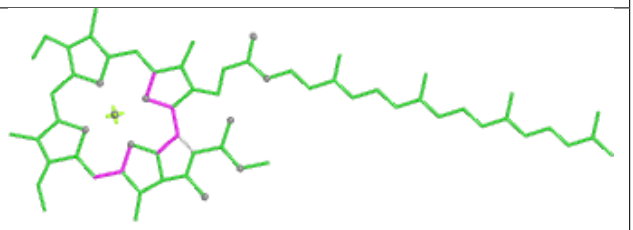


Rings

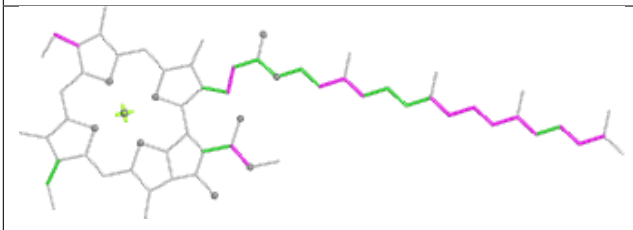
Ligand CLA A 825



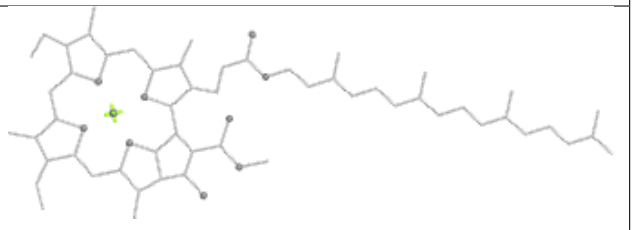
Bond lengths



Bond angles

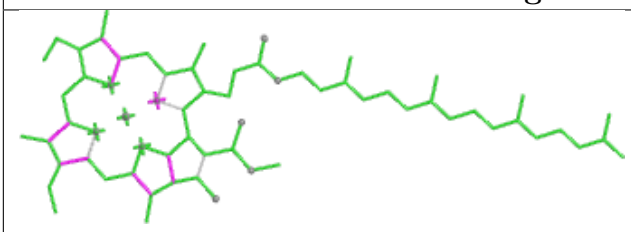


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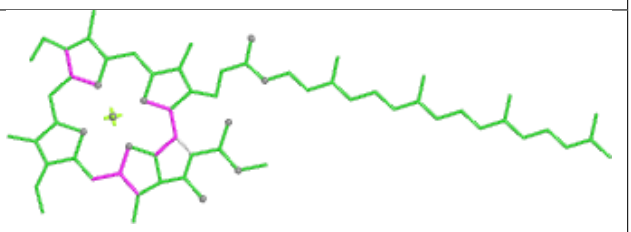


Rings

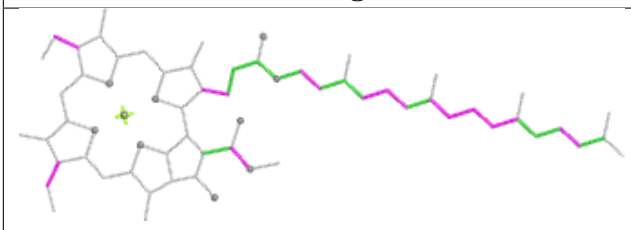
Ligand CLA B 804



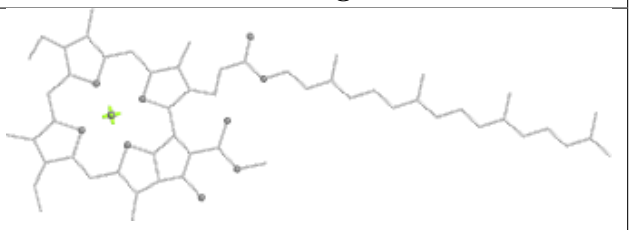
Bond lengths



Bond angles

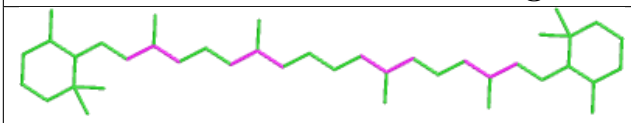


Torsions

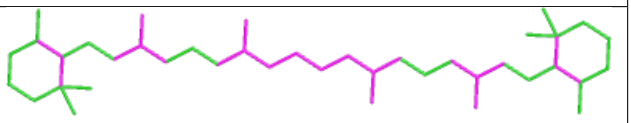


Rings

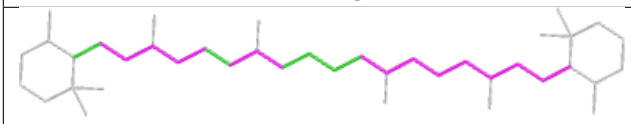
Ligand BCR h 203



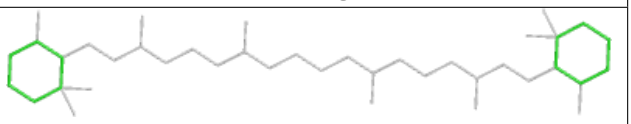
Bond lengths



Bond angles

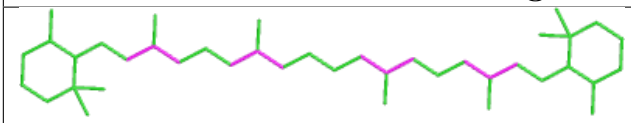


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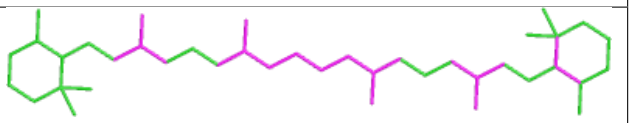


Rings

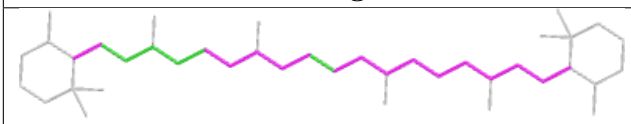
Ligand BCR a 844



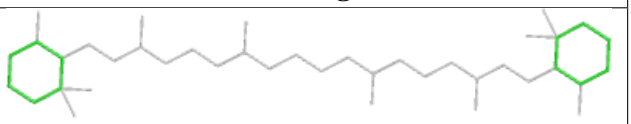
Bond lengths



Bond angles

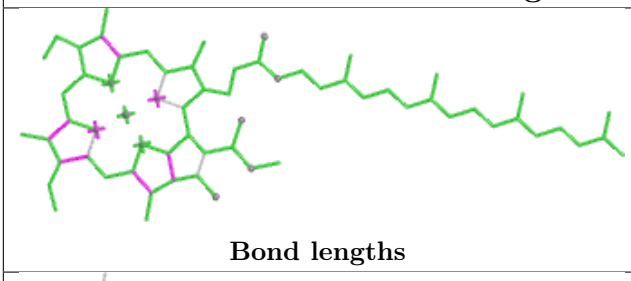


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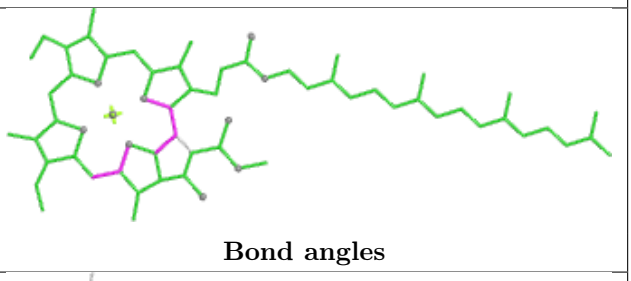


Rings

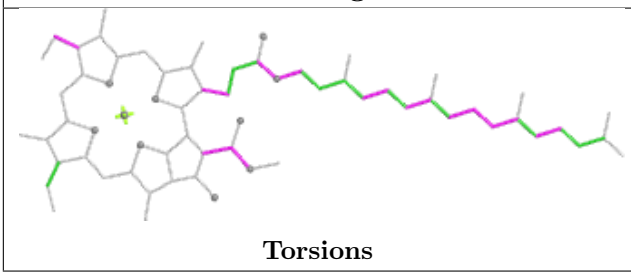
Ligand CLA B 814



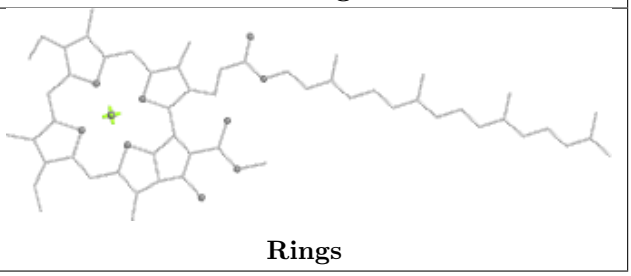
Bond lengths



Bond angles

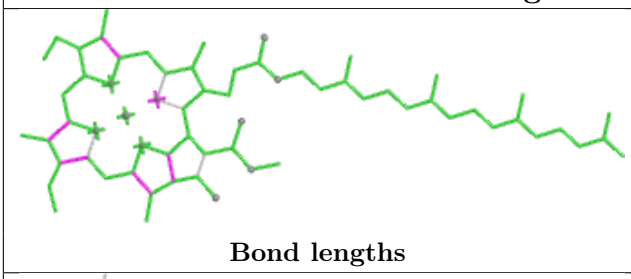


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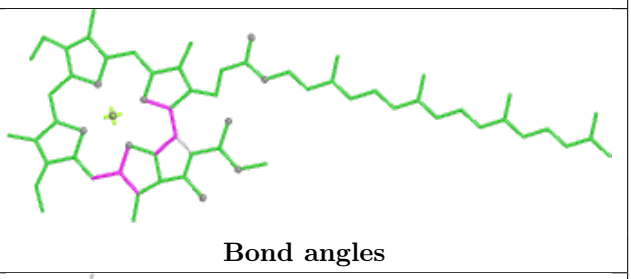


Rings

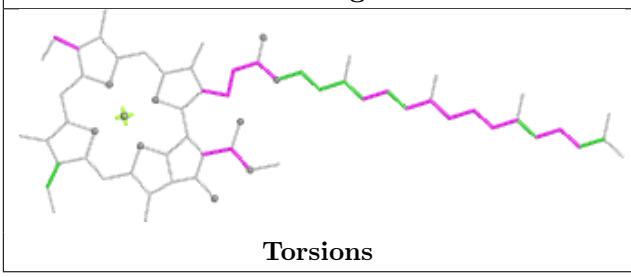
Ligand CLA A 811



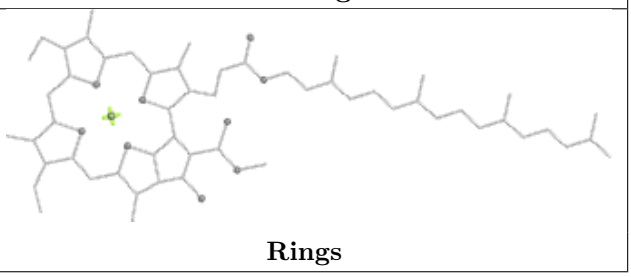
Bond lengths



Bond angles

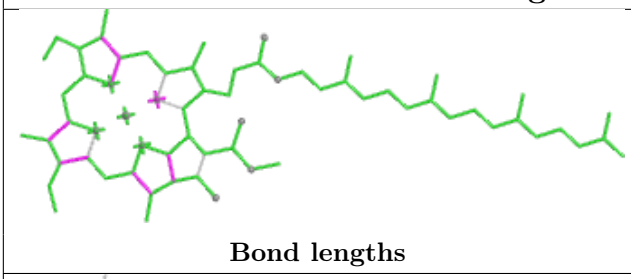


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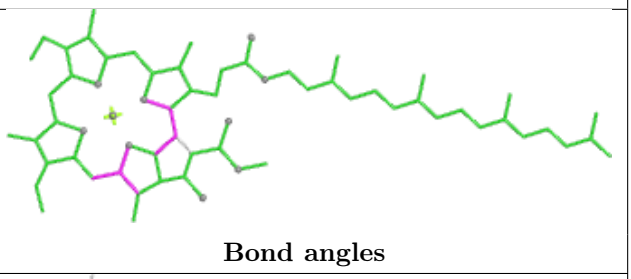


Rings

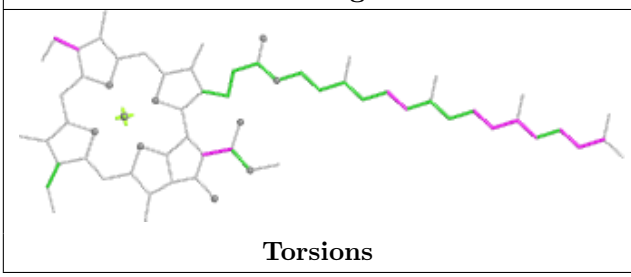
Ligand CLA a 833



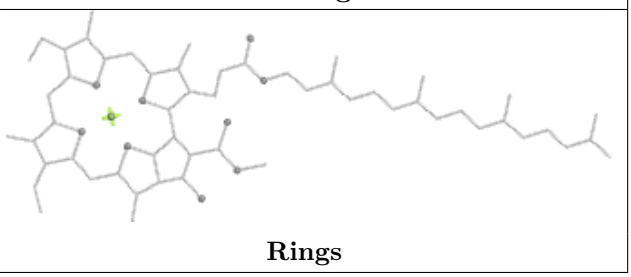
Bond lengths



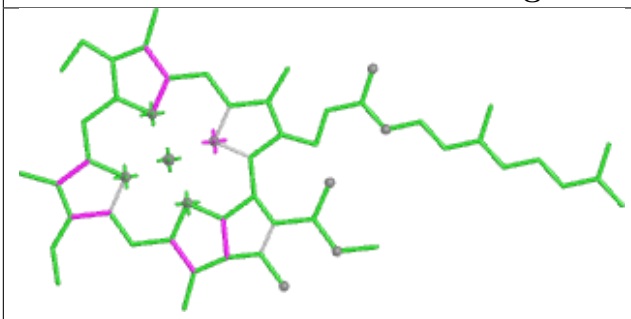
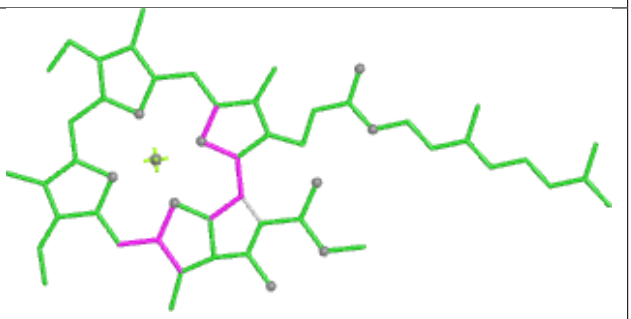
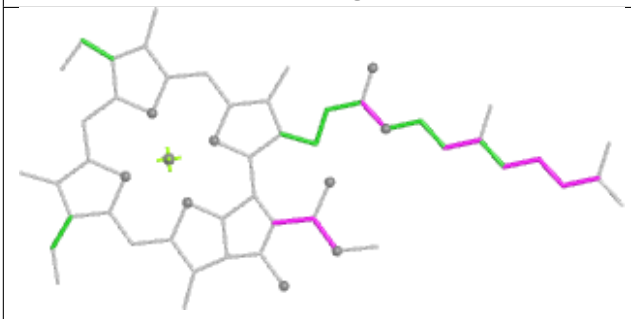
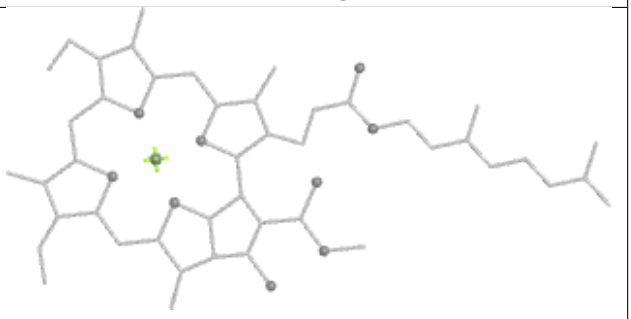
Bond angles

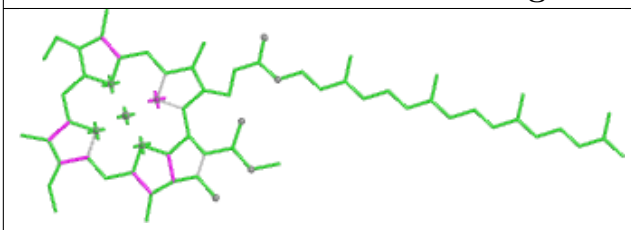
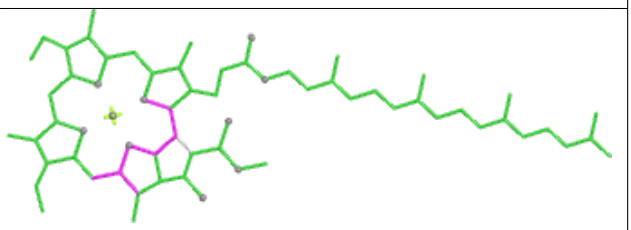
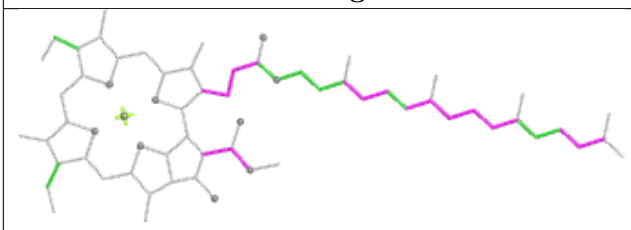
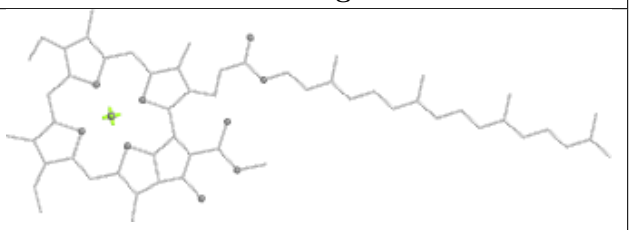


Torsions

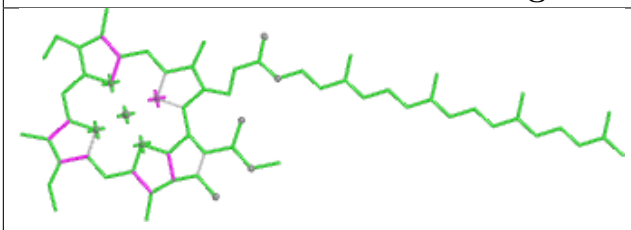


Rings

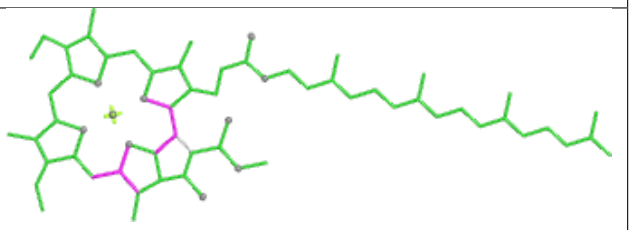
Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

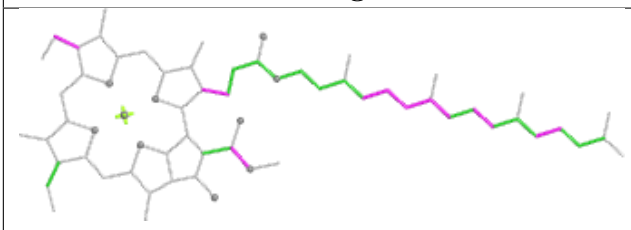
Ligand CLA a 829



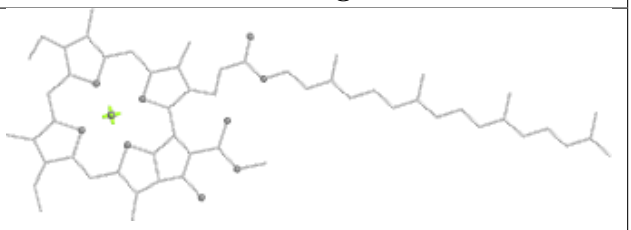
Bond lengths



Bond angles

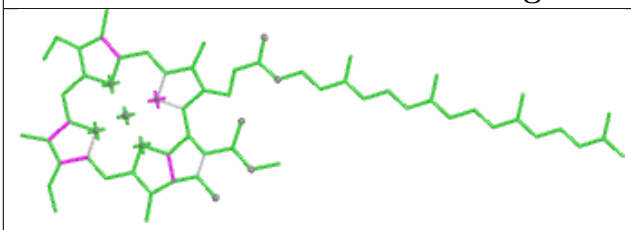


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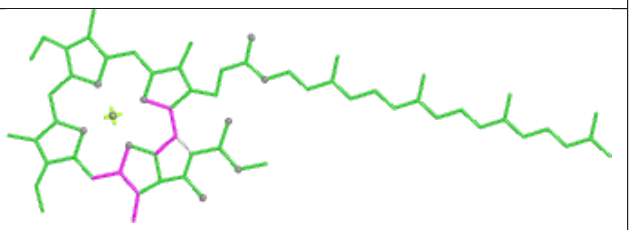


Rings

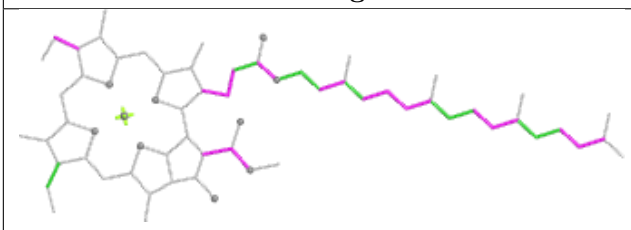
Ligand CLA A 835



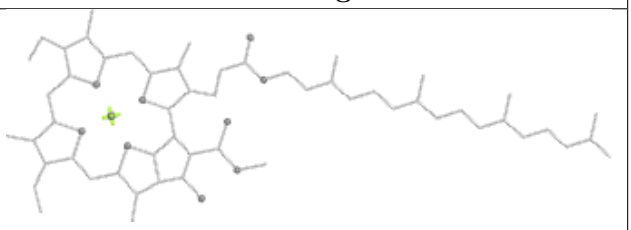
Bond lengths



Bond angles

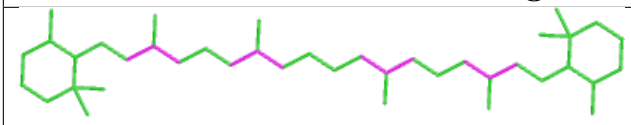


Torsions



Rings

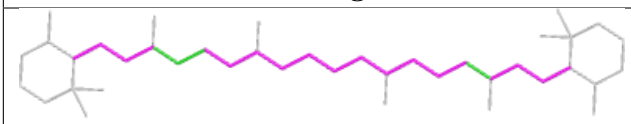
Ligand BCR b 835



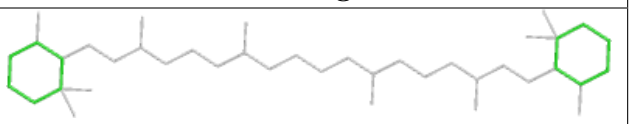
Bond lengths



Bond angles

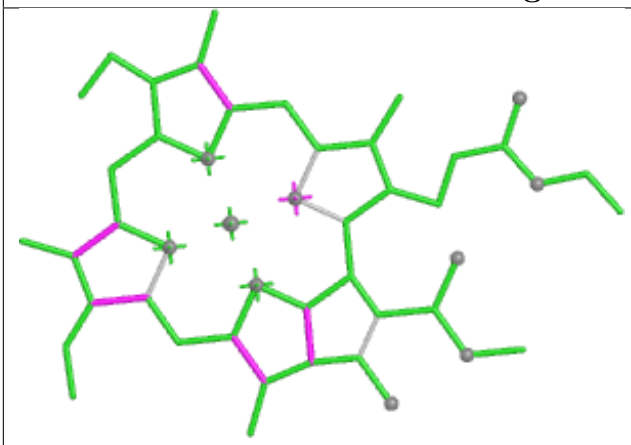


Torsions

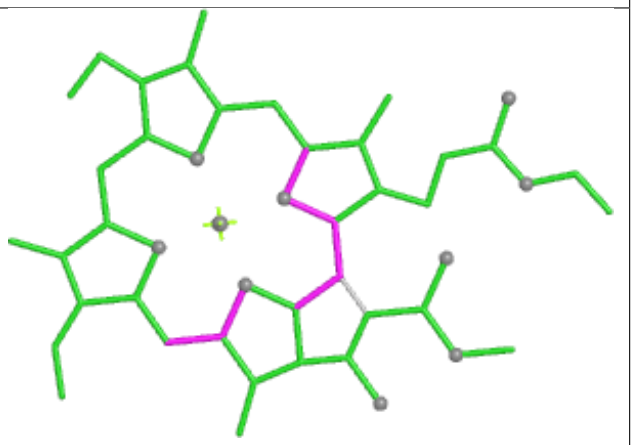


Rings

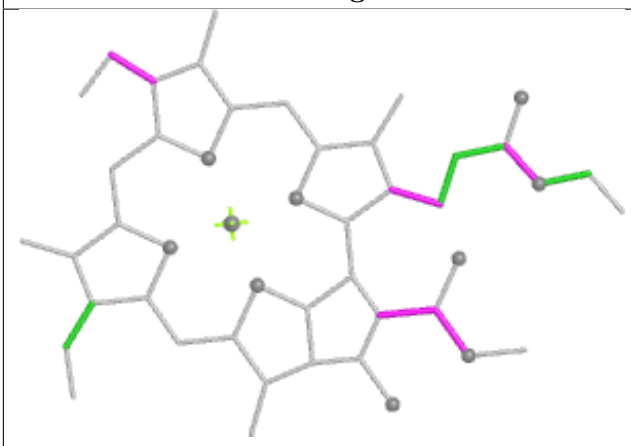
Ligand CLA A 834



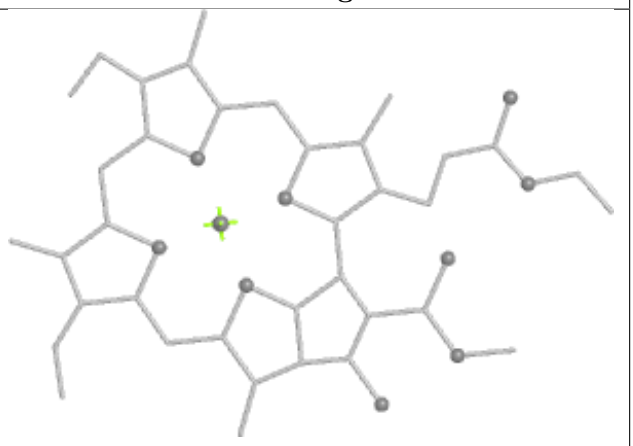
Bond lengths



Bond angles

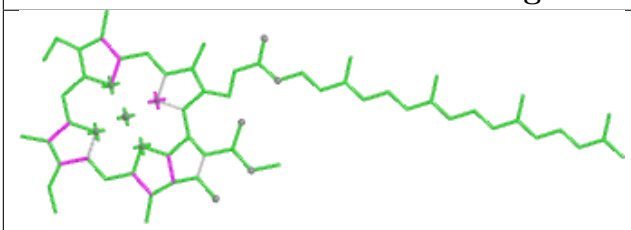


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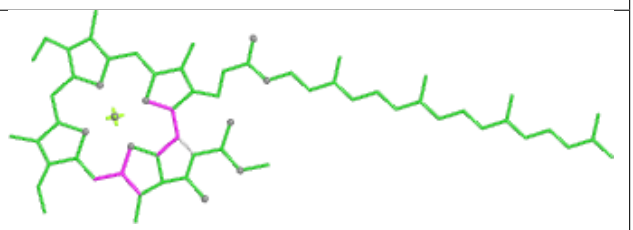


Rings

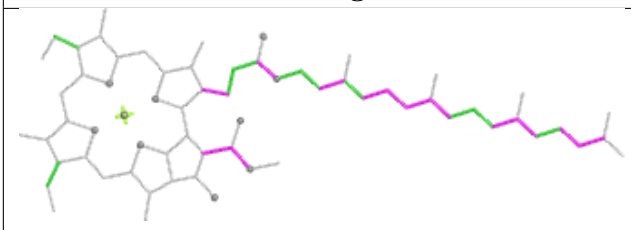
Ligand CLA A 817



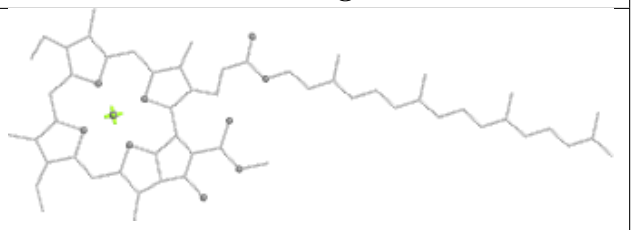
Bond lengths



Bond angles

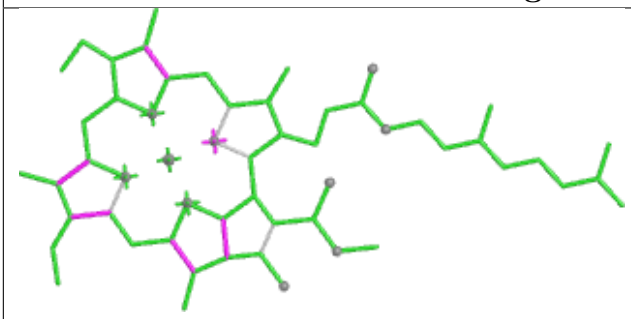


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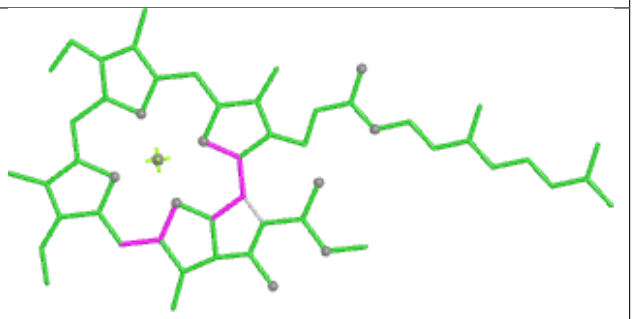


Rings

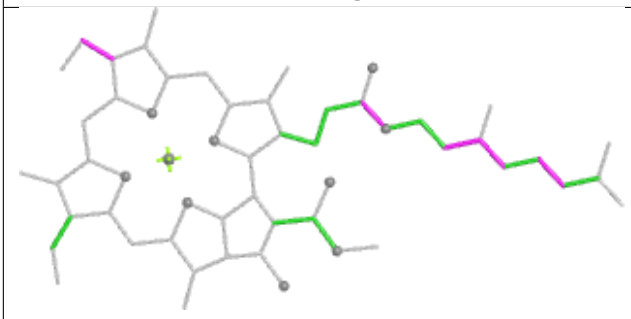
Ligand CLA B 808



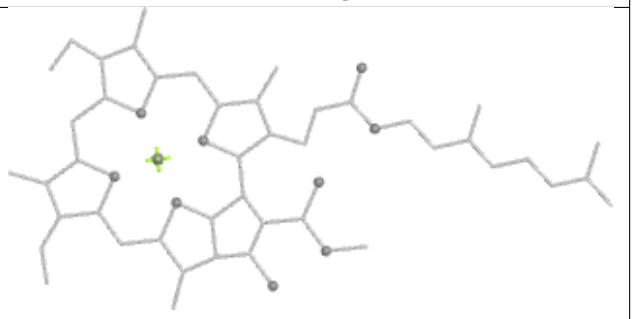
Bond lengths



Bond angles

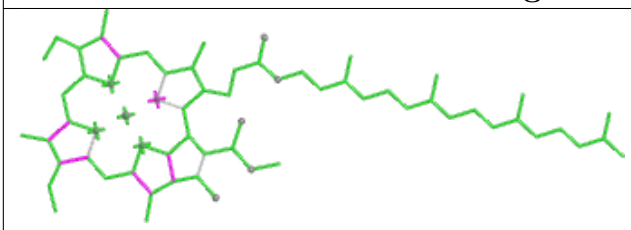


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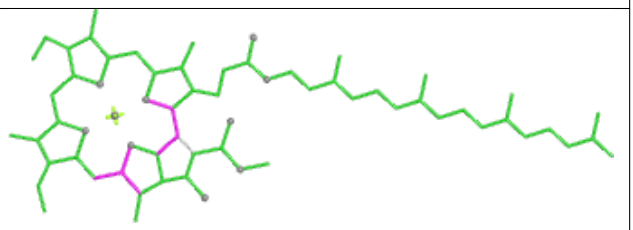


Rings

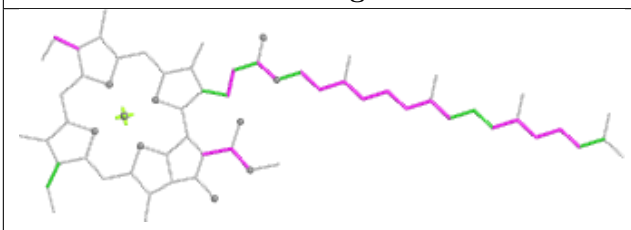
Ligand CLA A 807



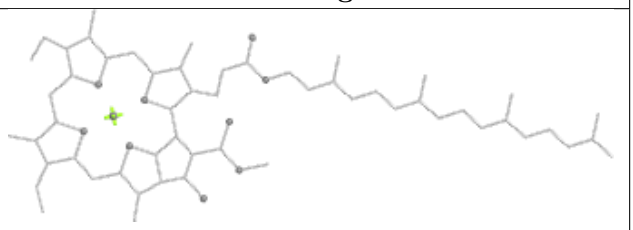
Bond lengths



Bond angles

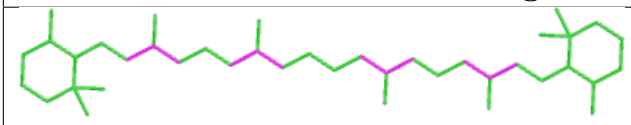


Torsions

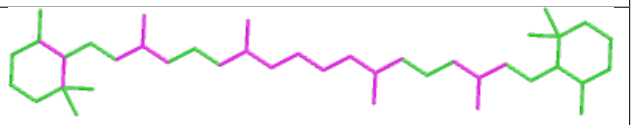


Rings

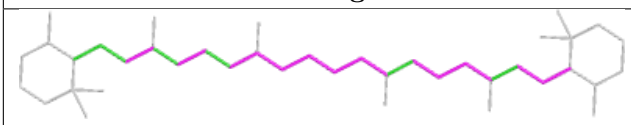
Ligand BCR A 841



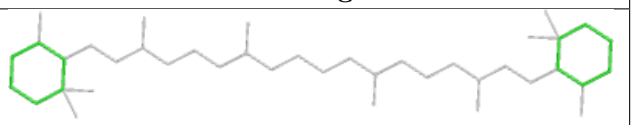
Bond lengths



Bond angles

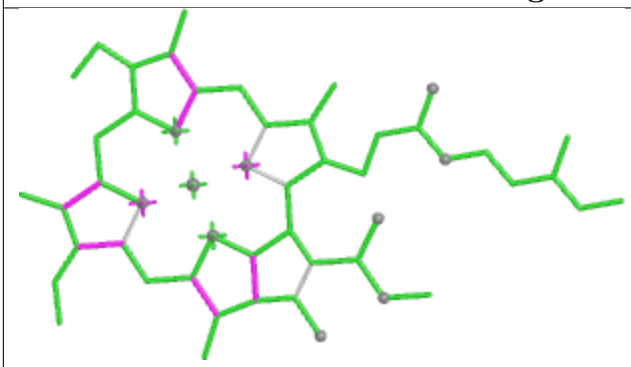


Torsions

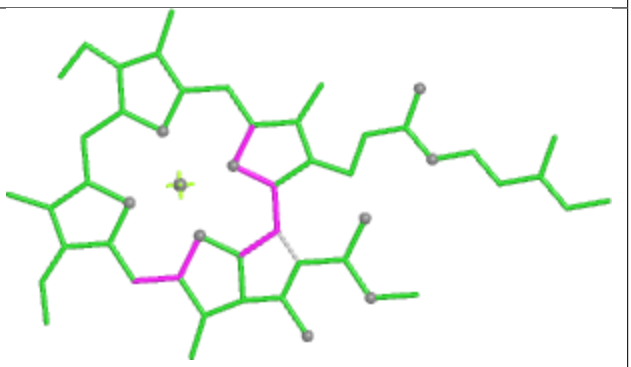


Rings

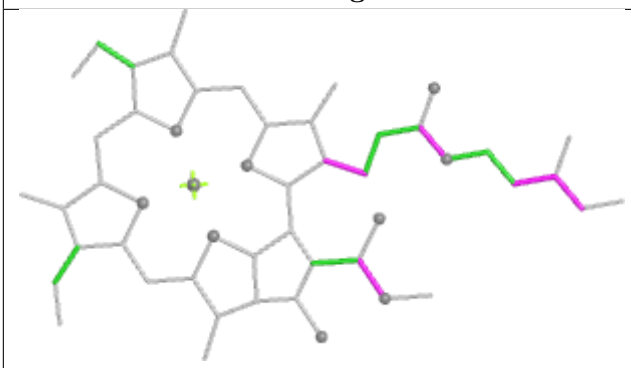
Ligand CLA b 828



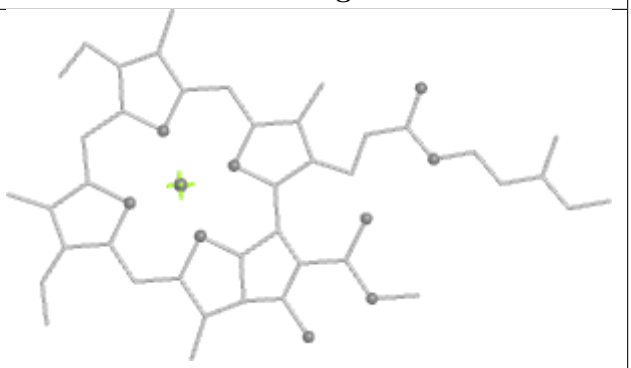
Bond lengths



Bond angles

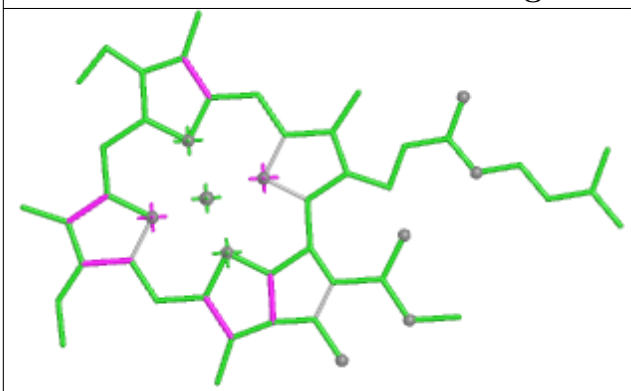


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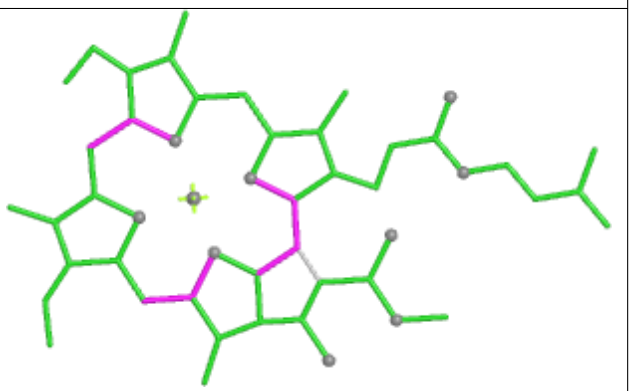


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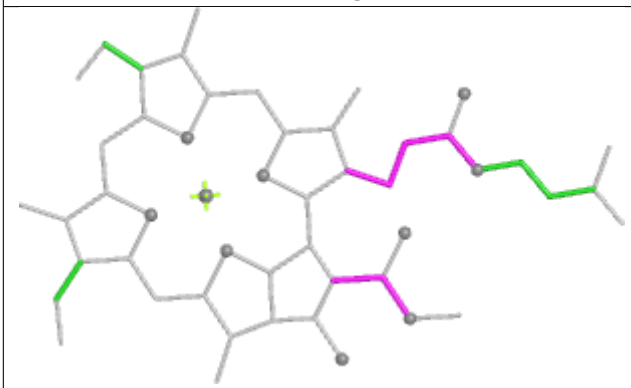
Ligand CLA B 820



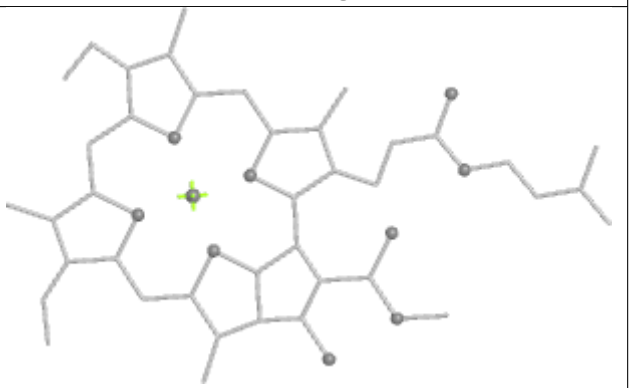
Bond lengths



Bond angles

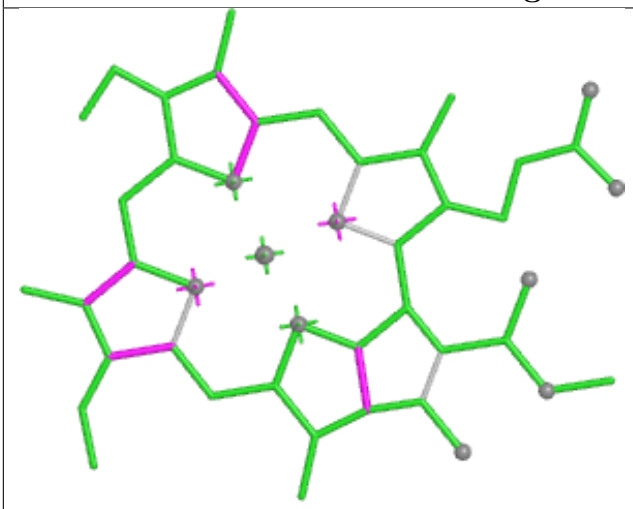


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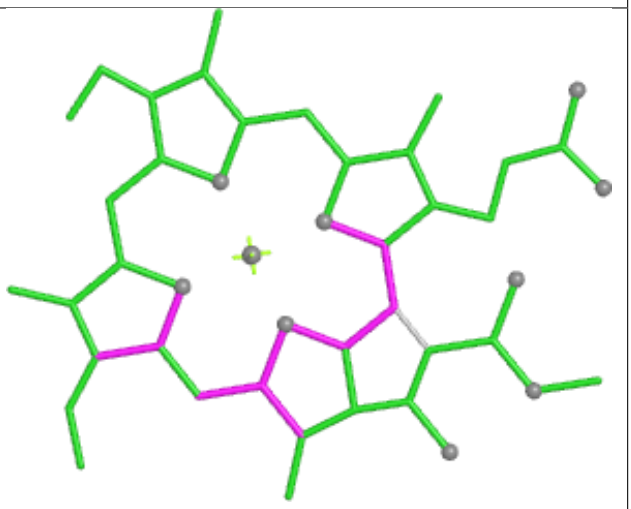


Rings

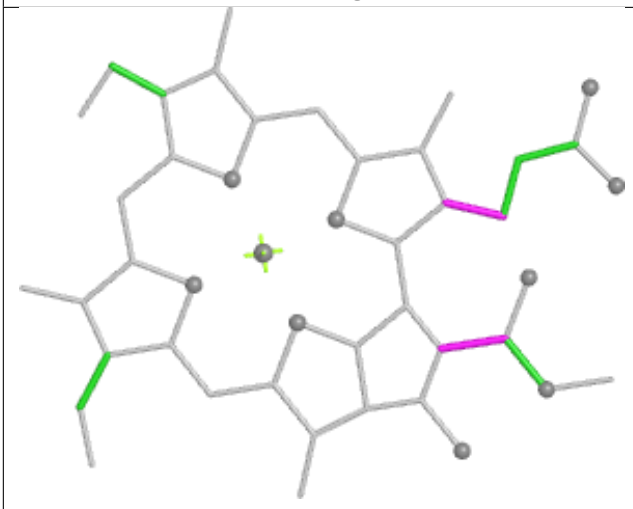
Ligand CLA A 812



Bond lengths



Bond angles

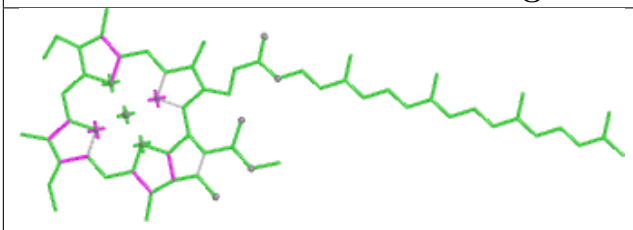


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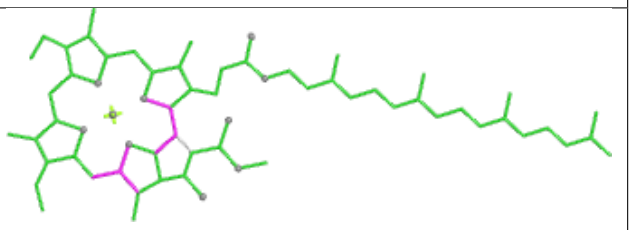


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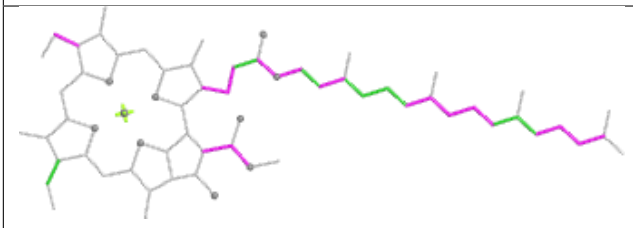
Ligand CLA H 201



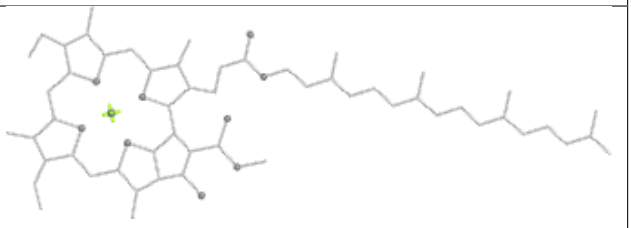
Bond lengths



Bond angles

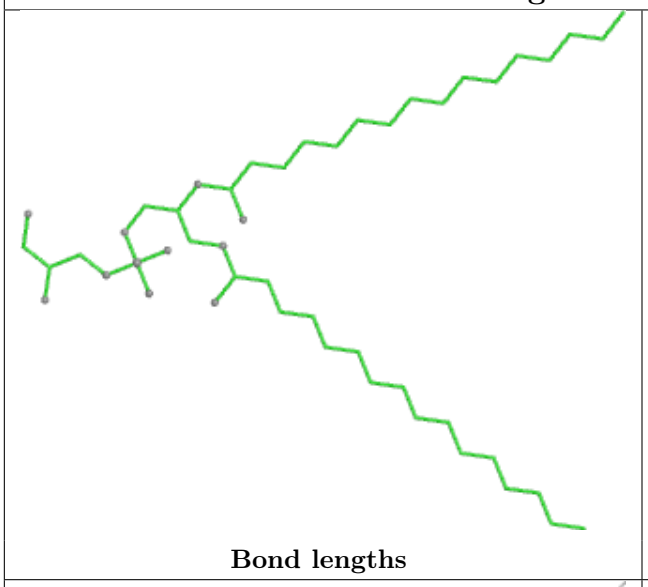


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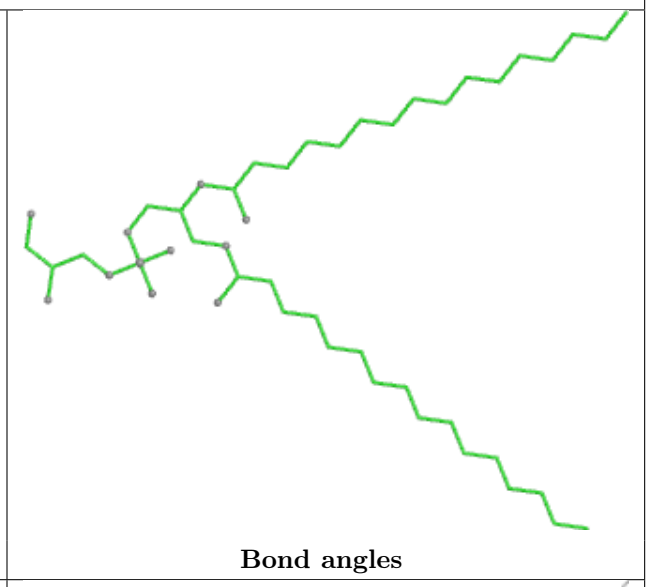


Rings

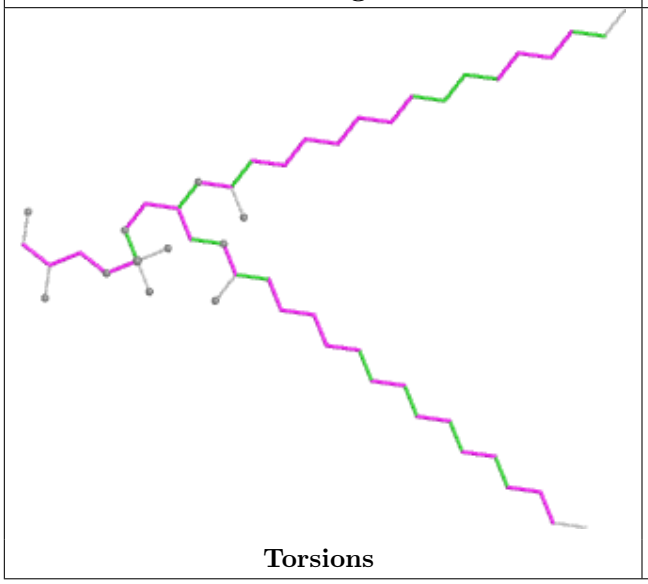
Ligand LHG a 839



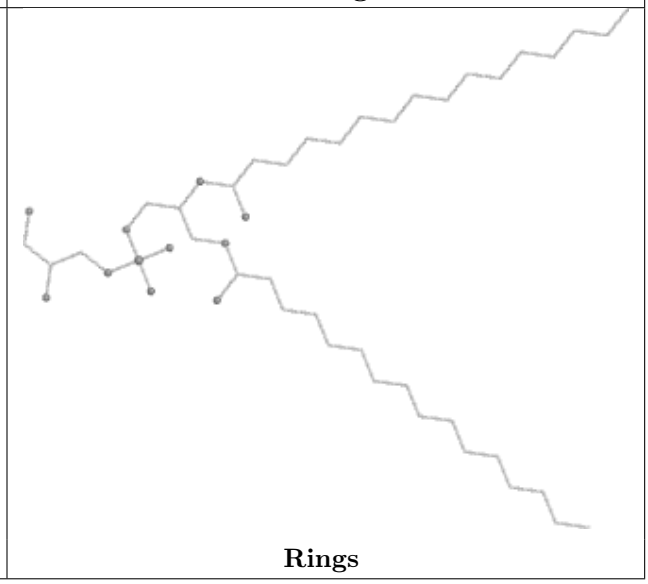
Bond lengths



Bond angles

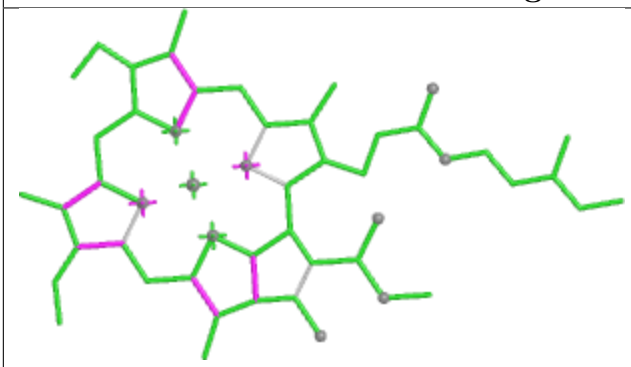


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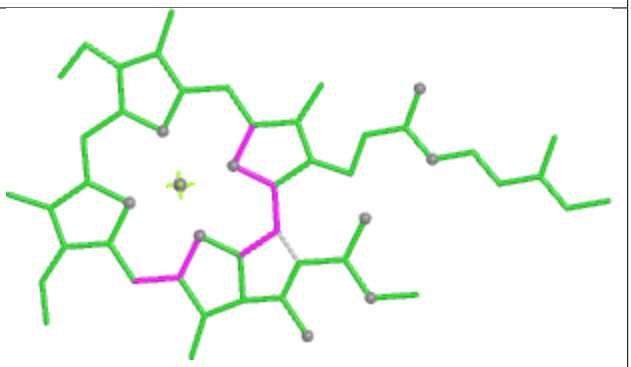


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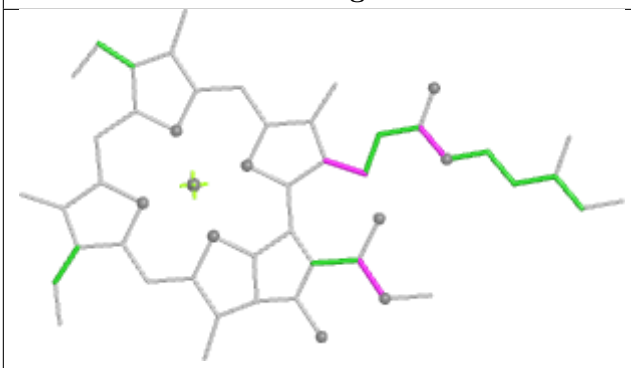
Ligand CLA B 828



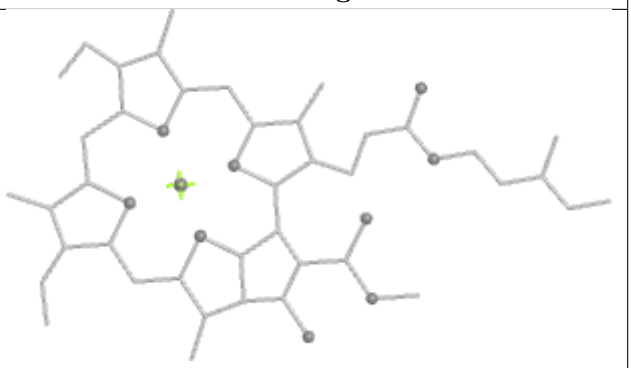
Bond lengths



Bond angles

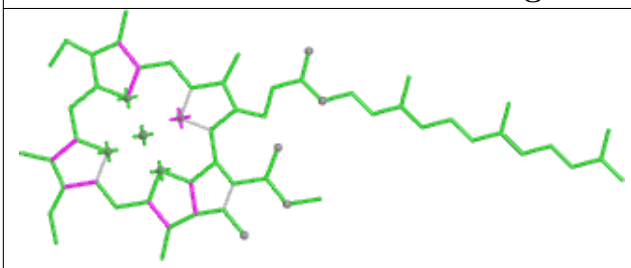


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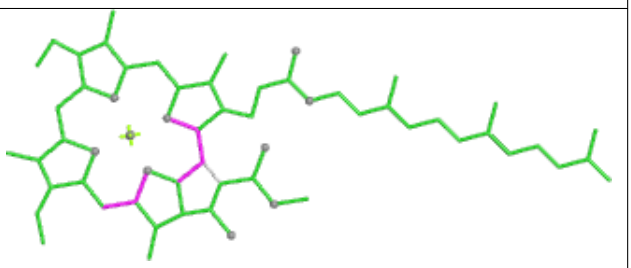


Rings

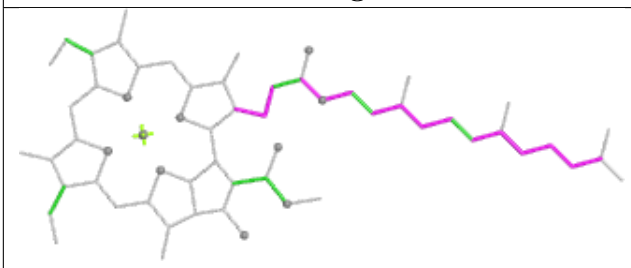
Ligand CLA B 824



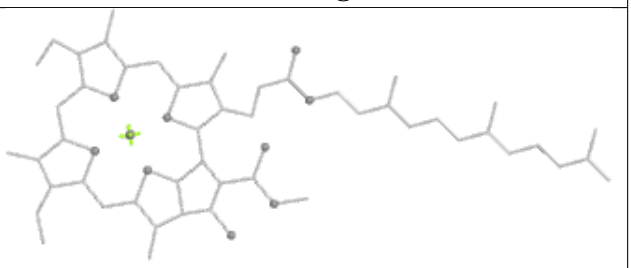
Bond lengths



Bond angles

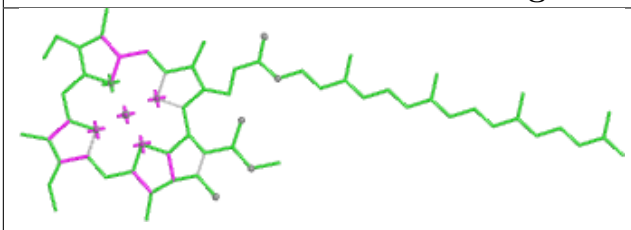


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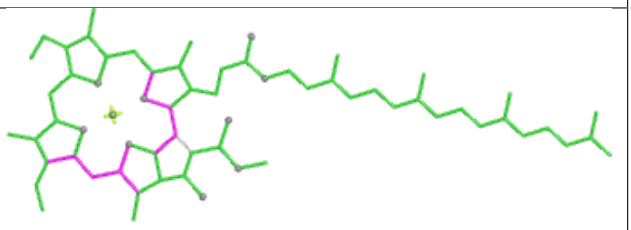


Rings

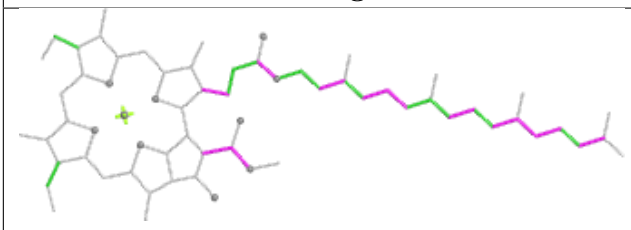
Ligand CLA a 819



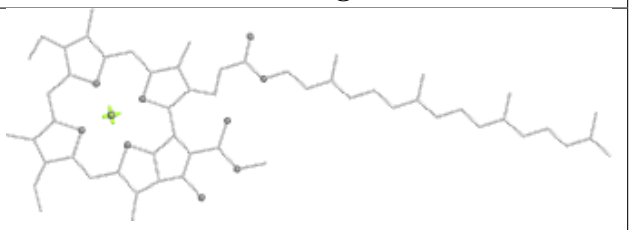
Bond lengths



Bond angles

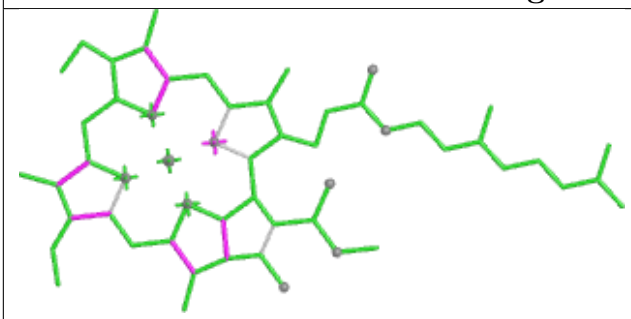


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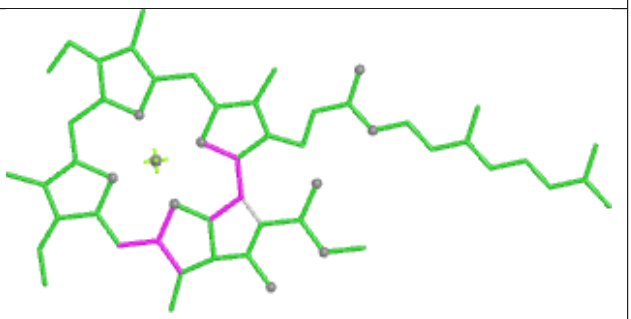


Rings

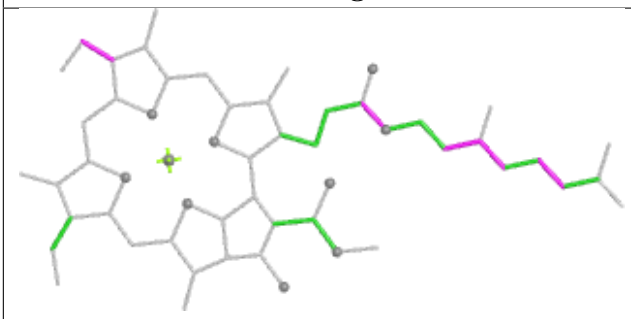
Ligand CLA b 808



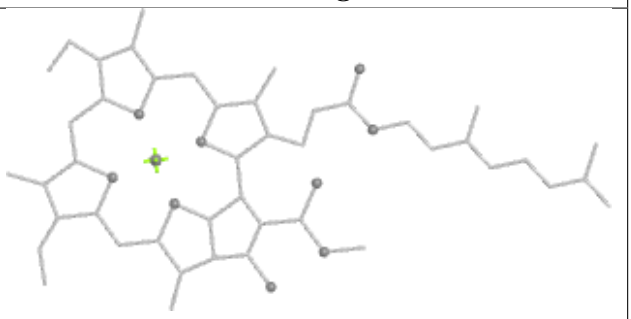
Bond lengths



Bond angles

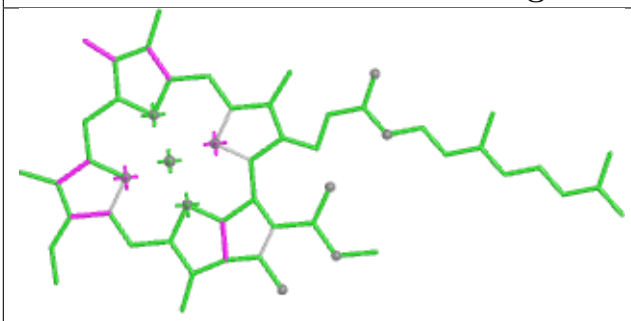


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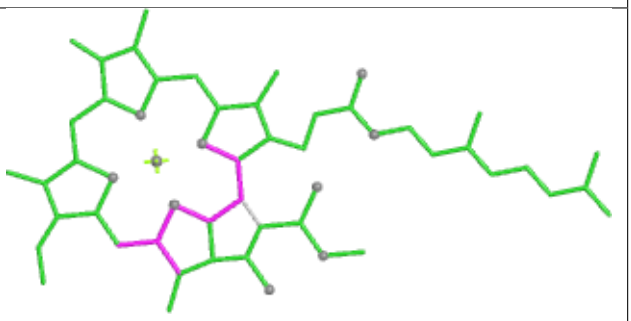


Rings

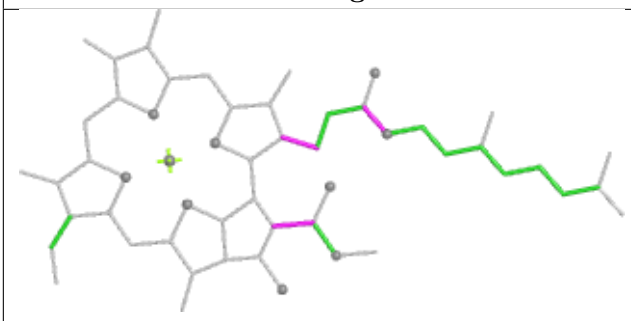
Ligand CLA b 812



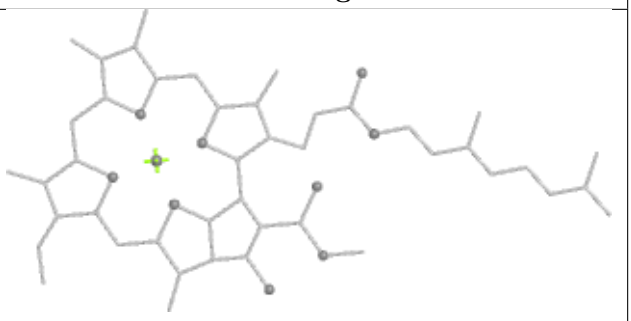
Bond lengths



Bond angles

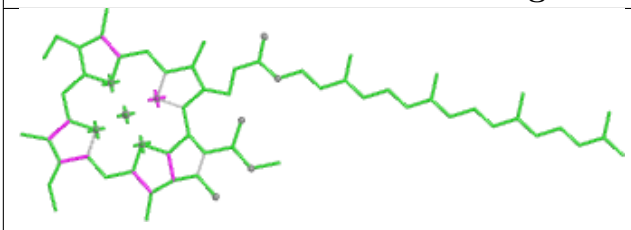


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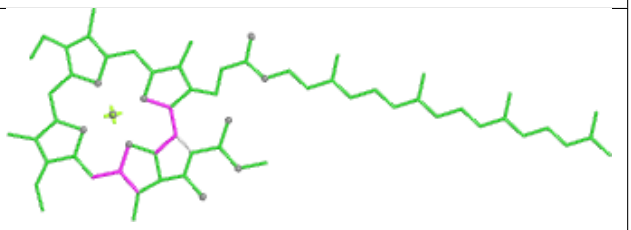


Rings

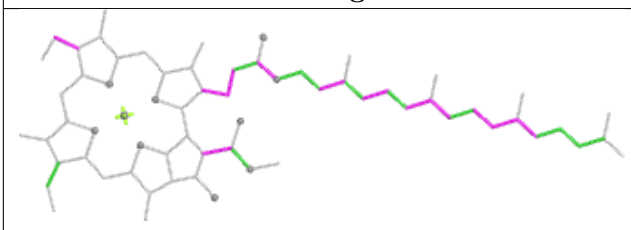
Ligand CLA a 805



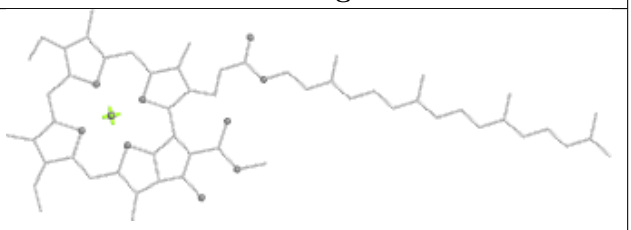
Bond lengths



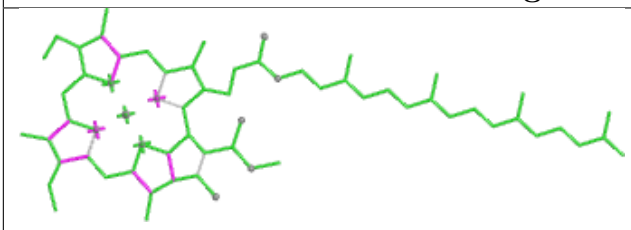
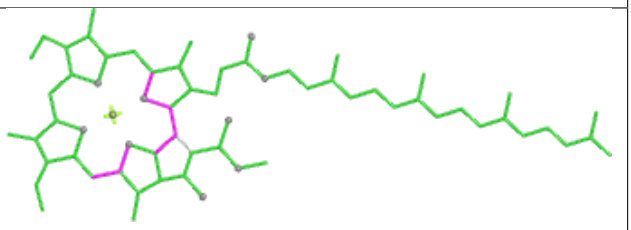
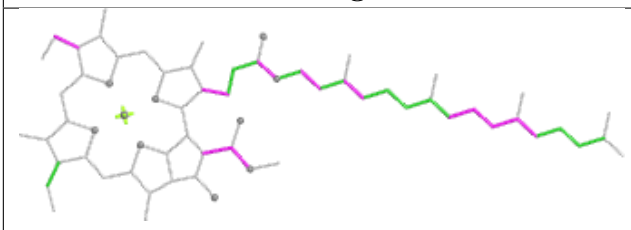
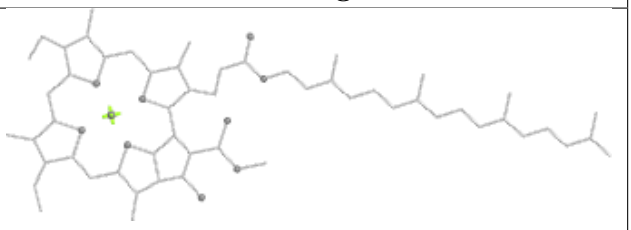
Bond angles

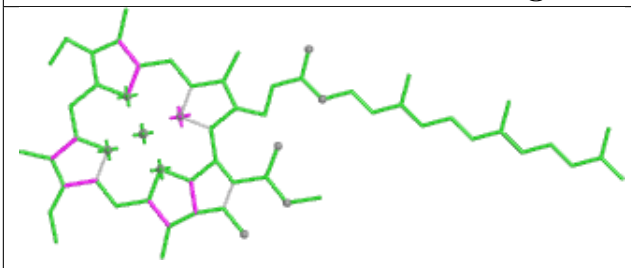
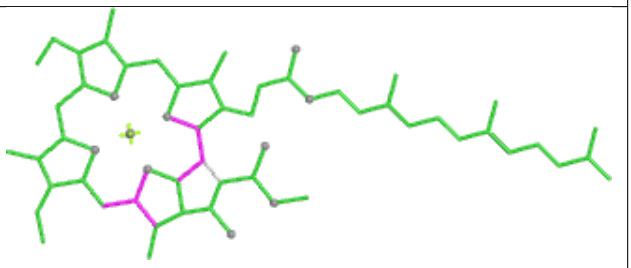
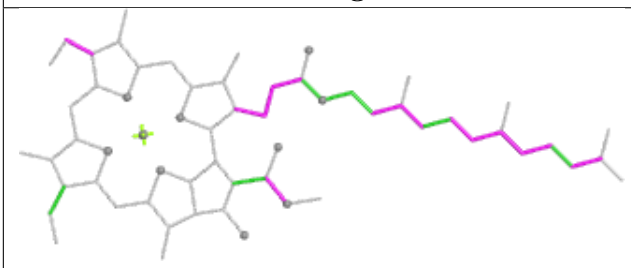
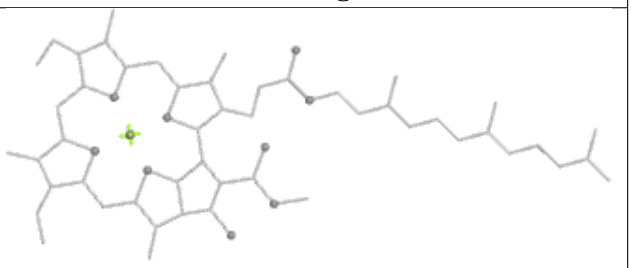


Torsions

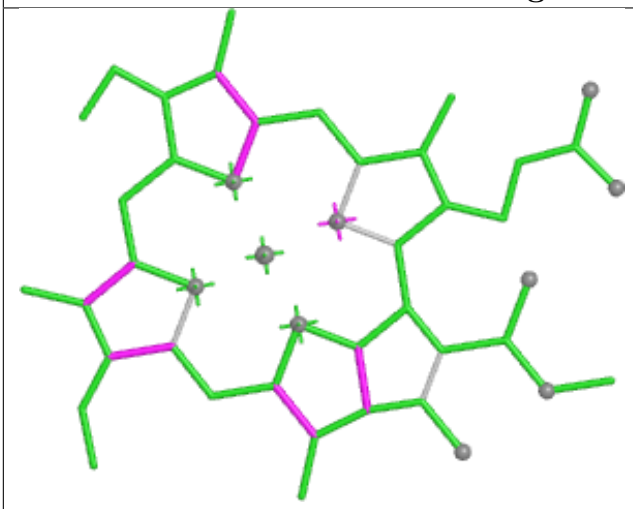


Rings

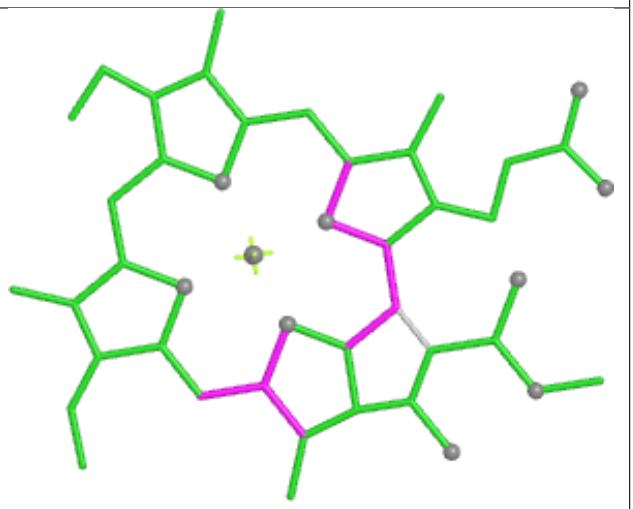
Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

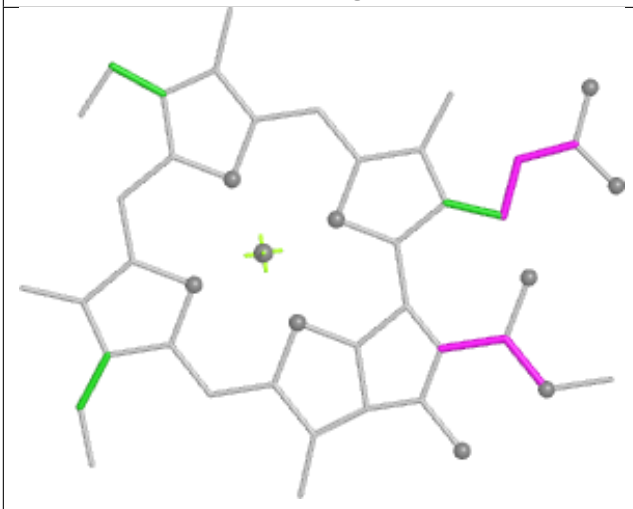
Ligand CLA b 827



Bond lengths



Bond angles

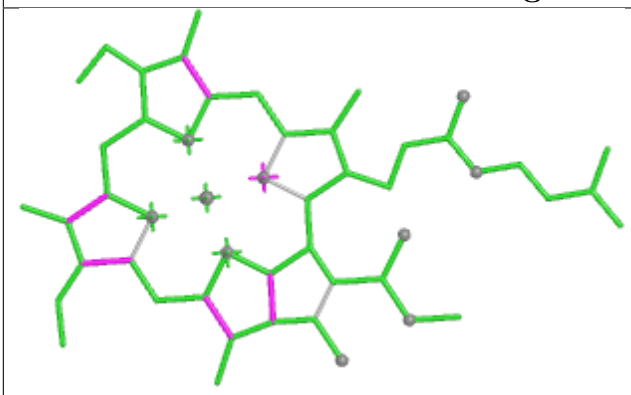


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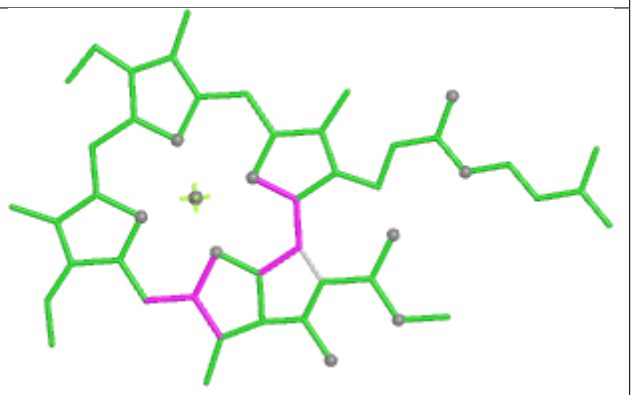


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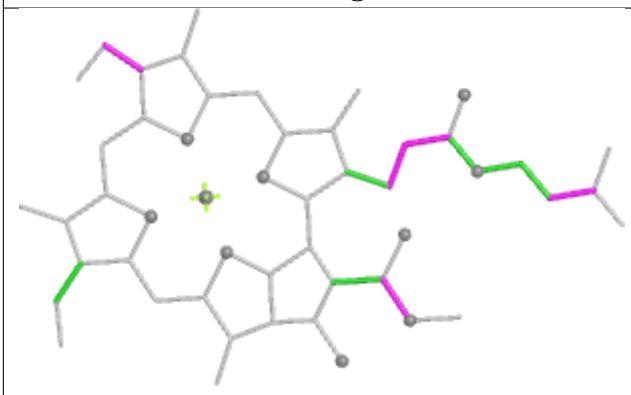
Ligand CLA A 813



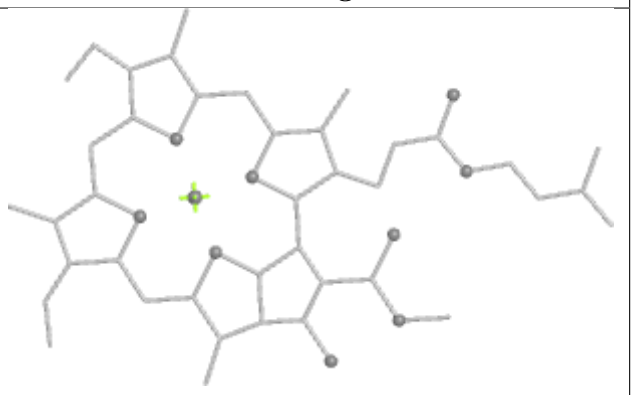
Bond lengths



Bond angles

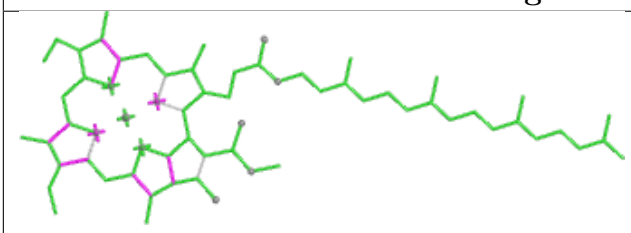


Torsions

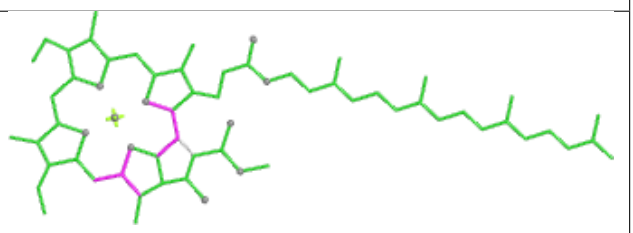


Rings

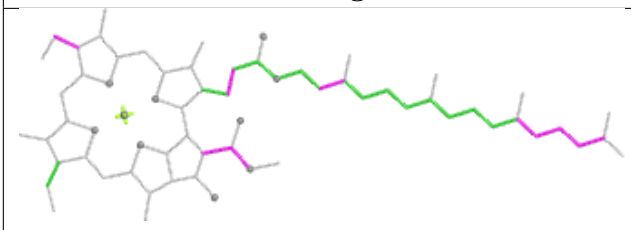
Ligand CLA B 831



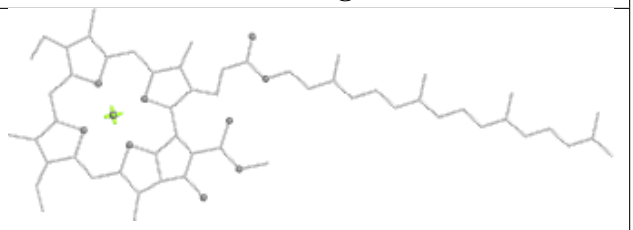
Bond lengths



Bond angles

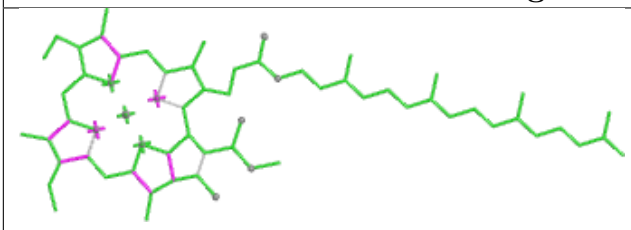


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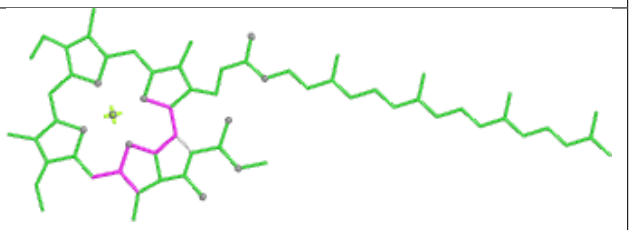


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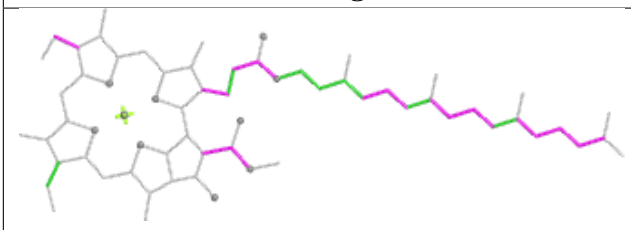
Ligand CLA h 202



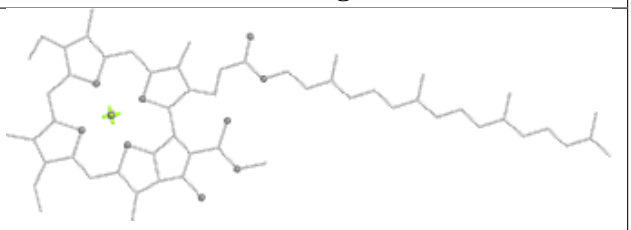
Bond lengths



Bond angles

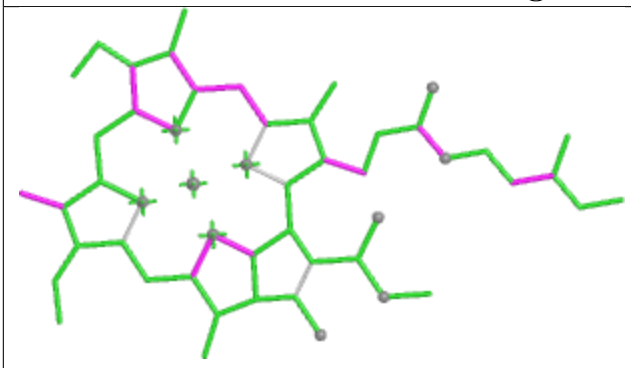


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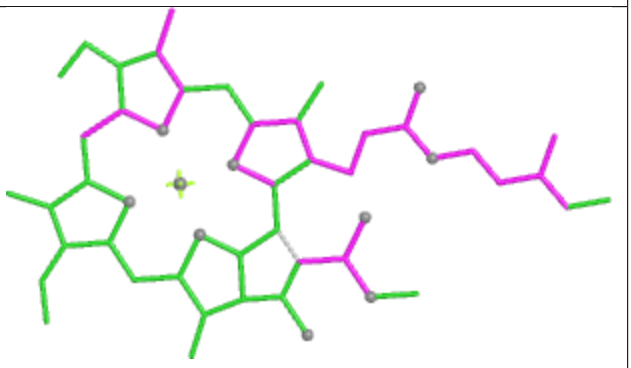


Rings

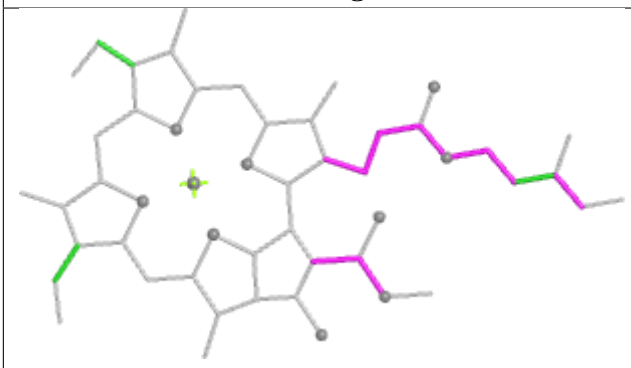
Ligand CLA h 201



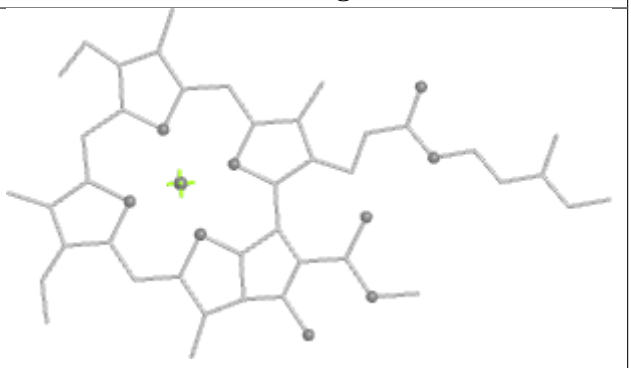
Bond lengths



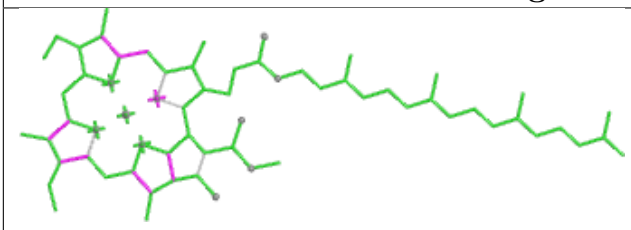
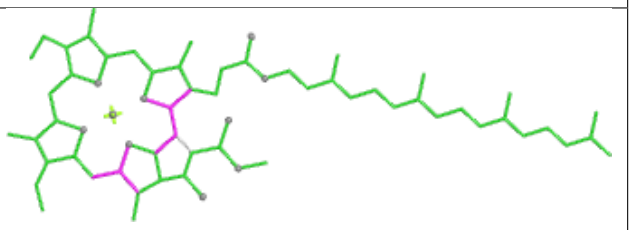
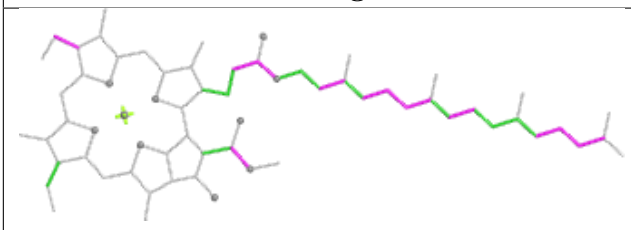
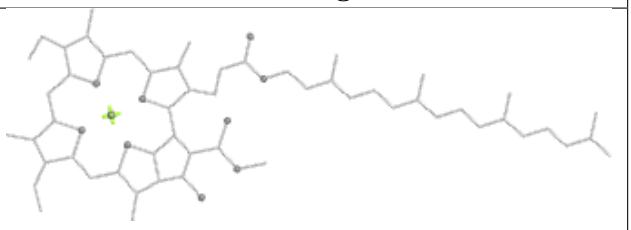
Bond angles

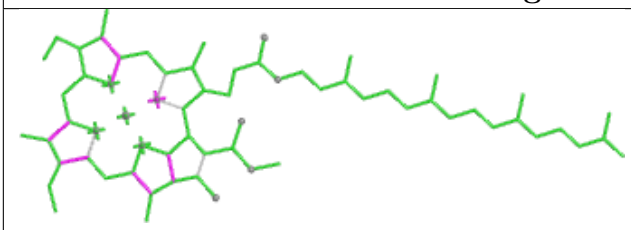
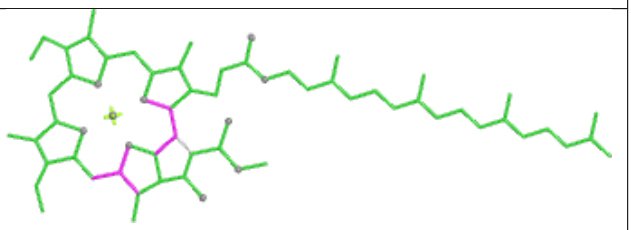
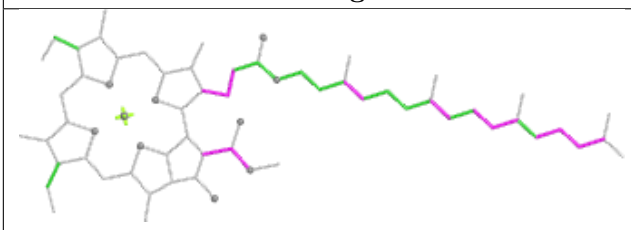
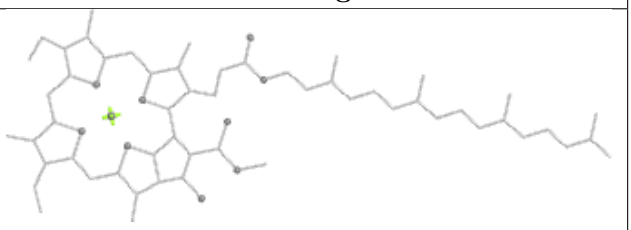


Torsions

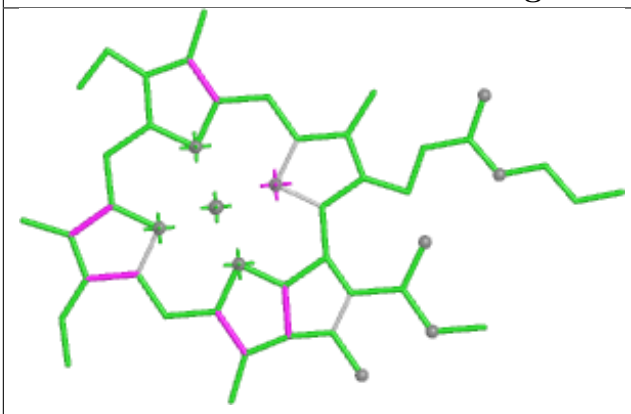


Rings

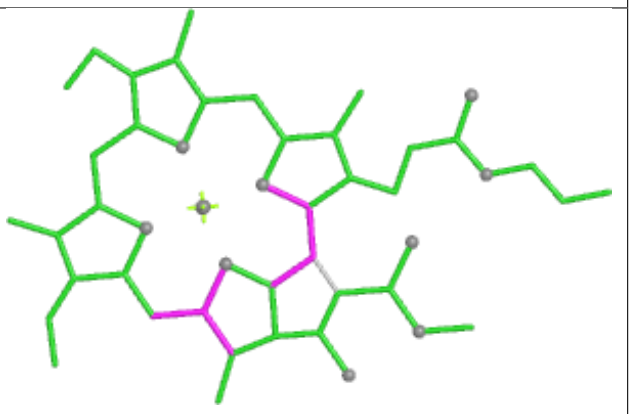
Ligand CLA a 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

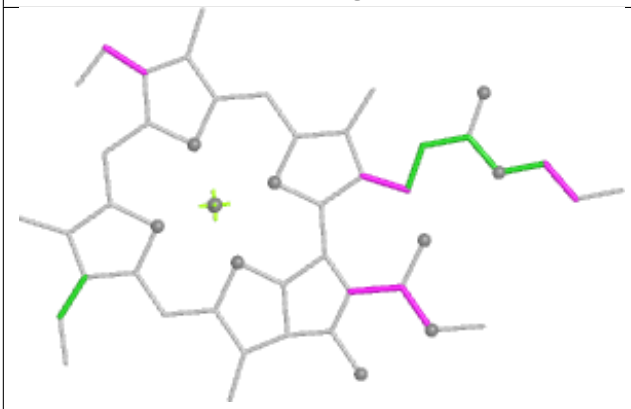
Ligand CLA B 826



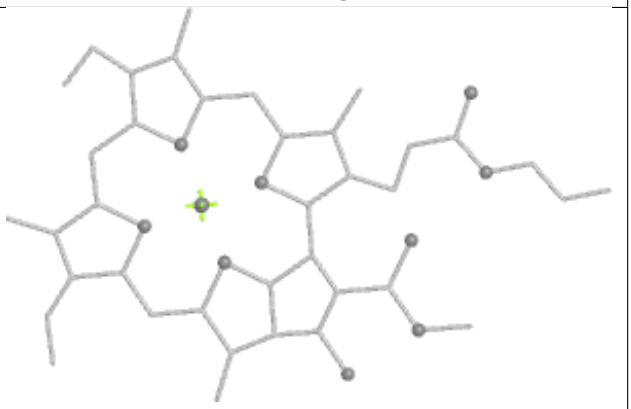
Bond lengths



Bond angles

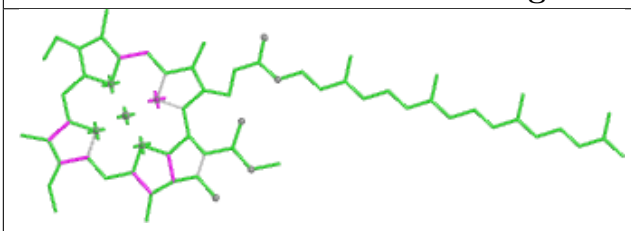


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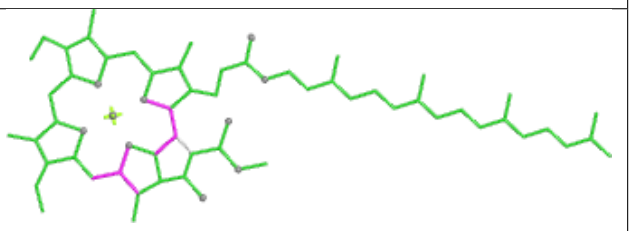


Rings

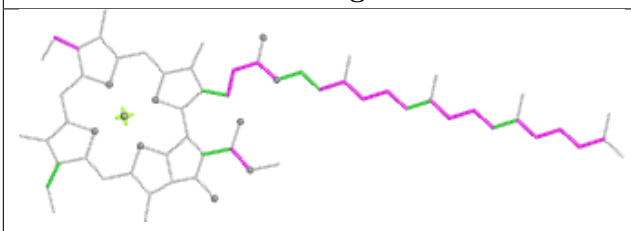
Ligand CLA a 806



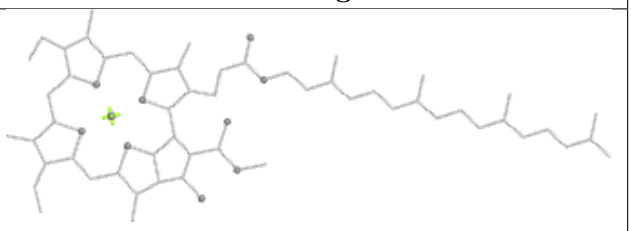
Bond lengths



Bond angles

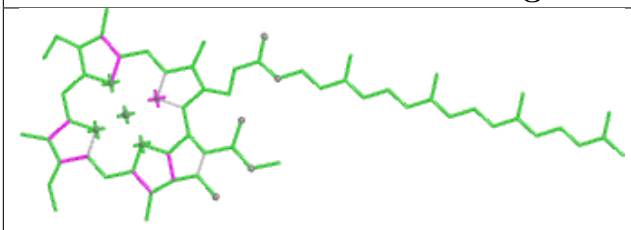


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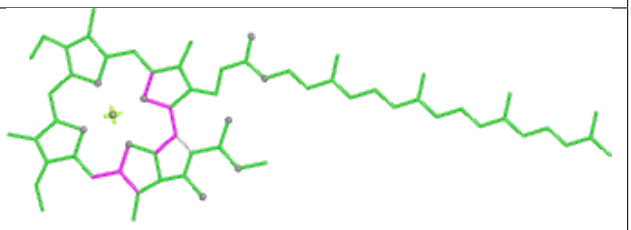


Rings

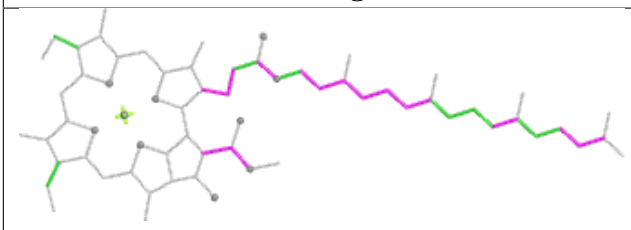
Ligand CLA A 821



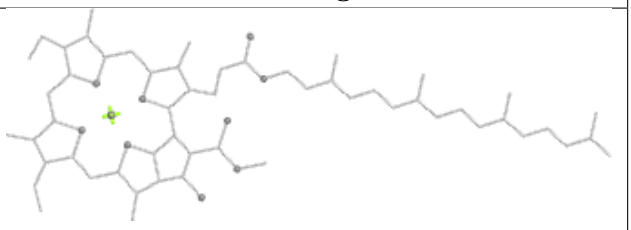
Bond lengths



Bond angles

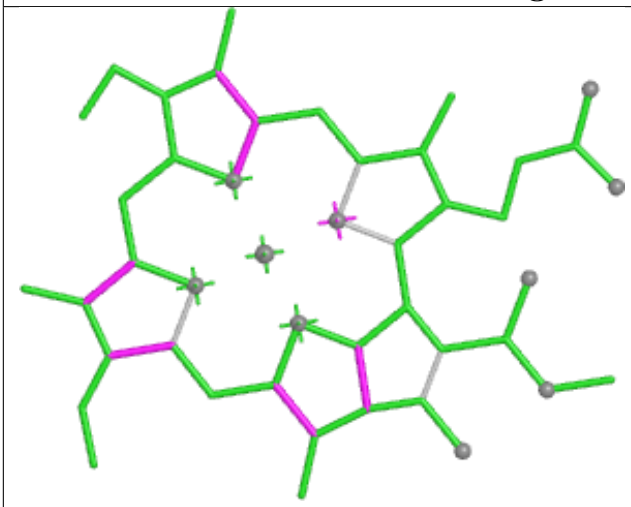


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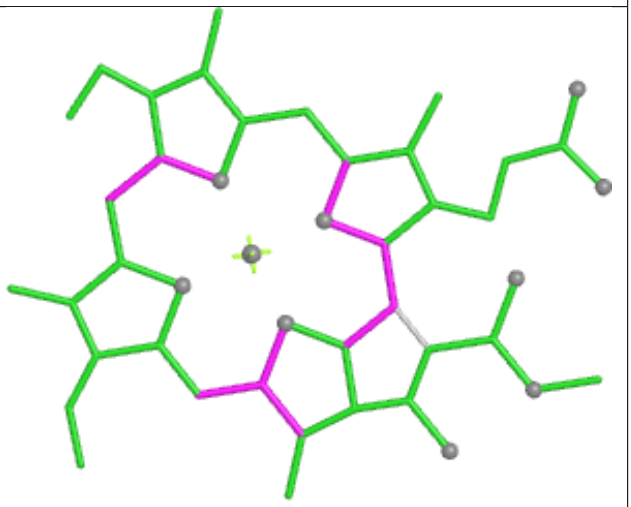


Rings

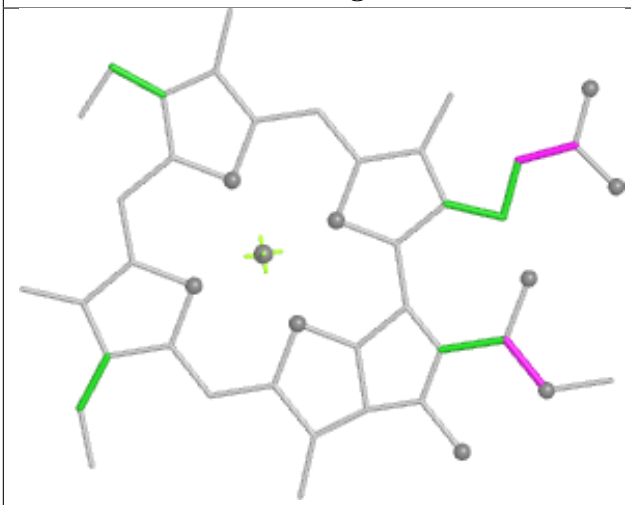
Ligand CLA a 814



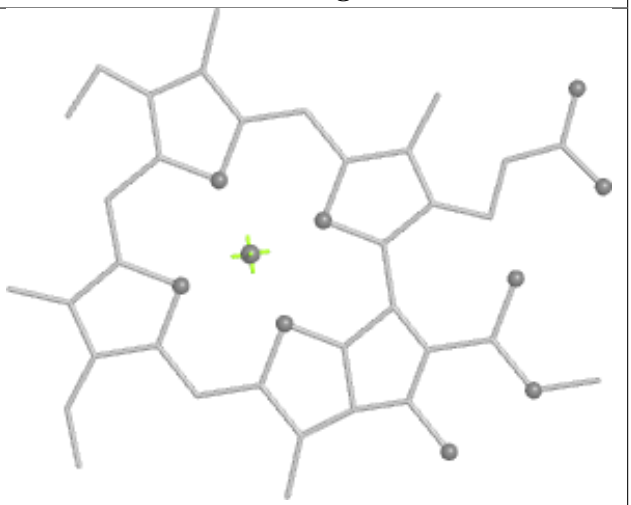
Bond lengths



Bond angles

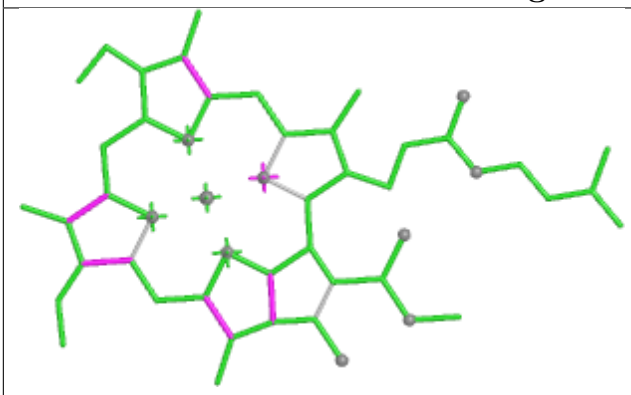


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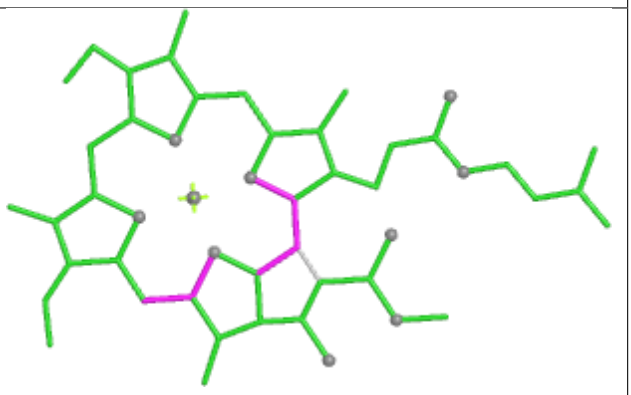


Rings

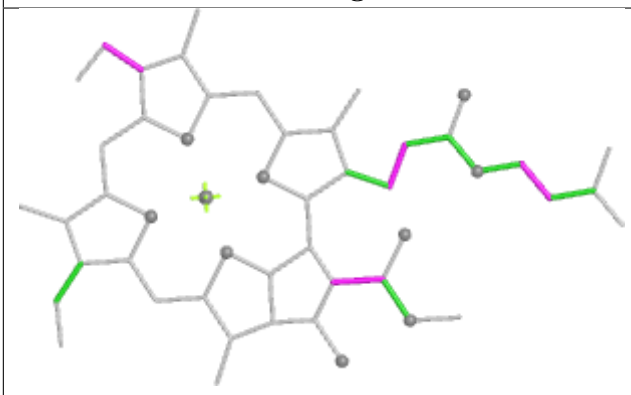
Ligand CLA a 828



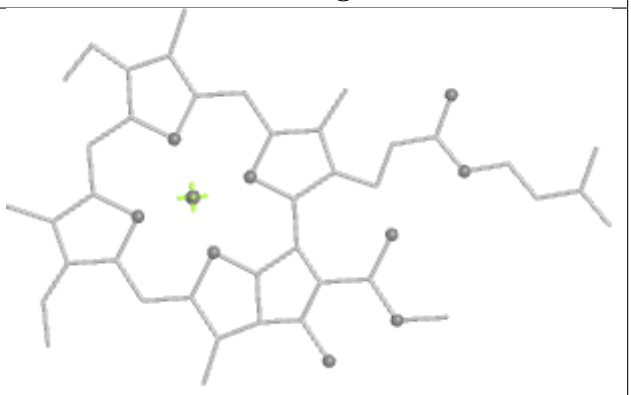
Bond lengths



Bond angles

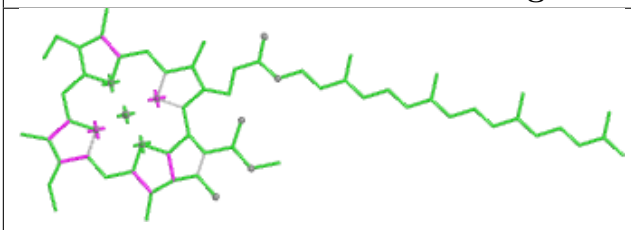


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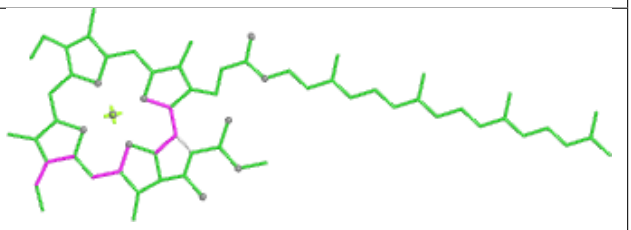


Rings

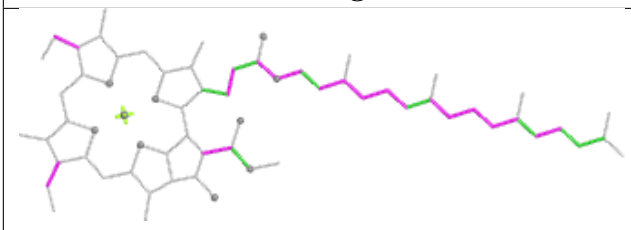
Ligand CLA b 801



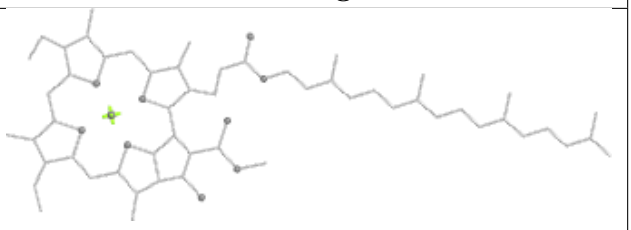
Bond lengths



Bond angles

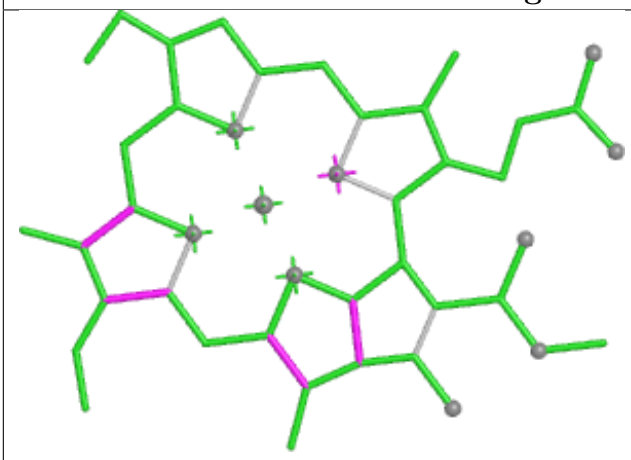


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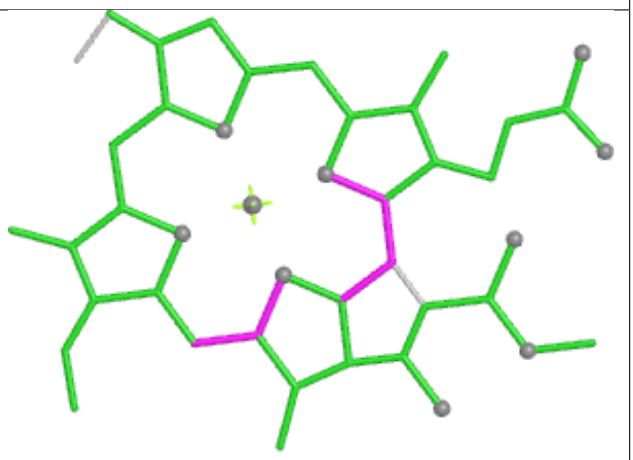


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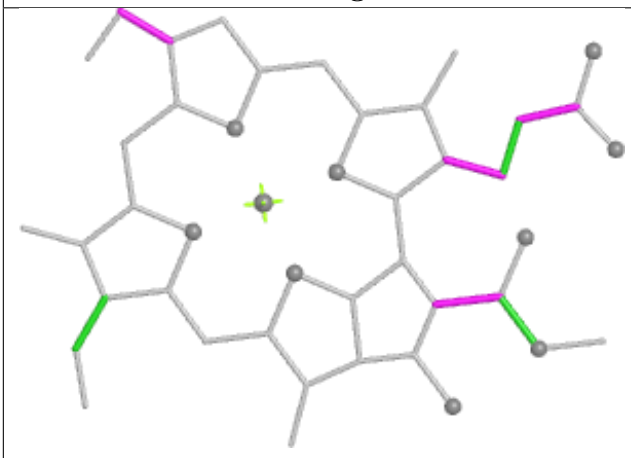
Ligand CLA B 813



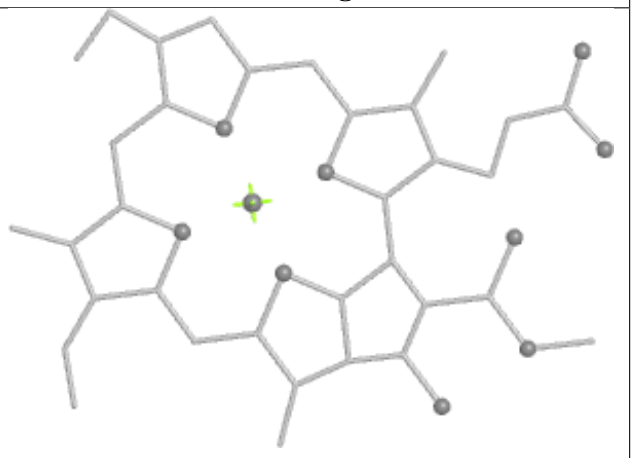
Bond lengths



Bond angles

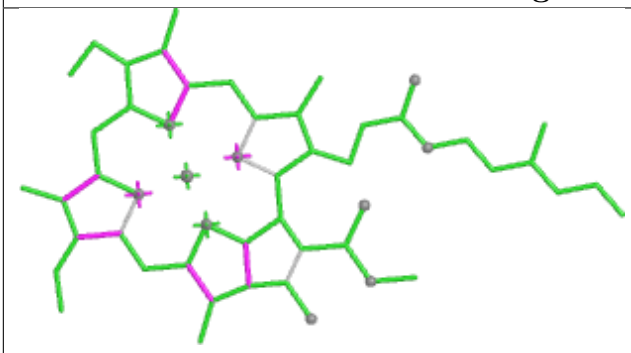


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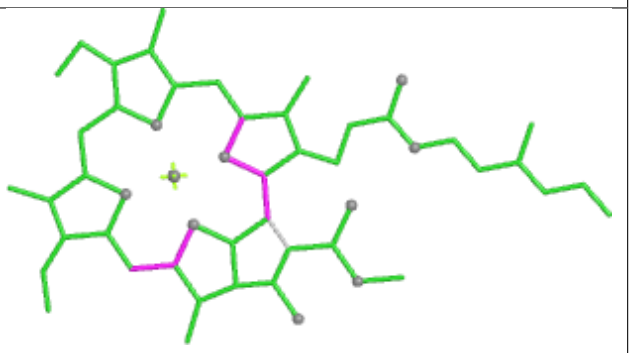


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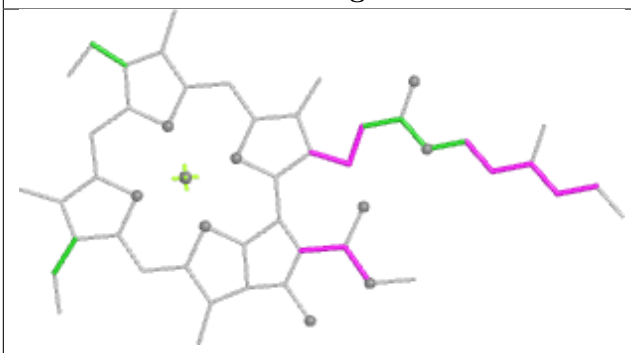
Ligand CLA l 302



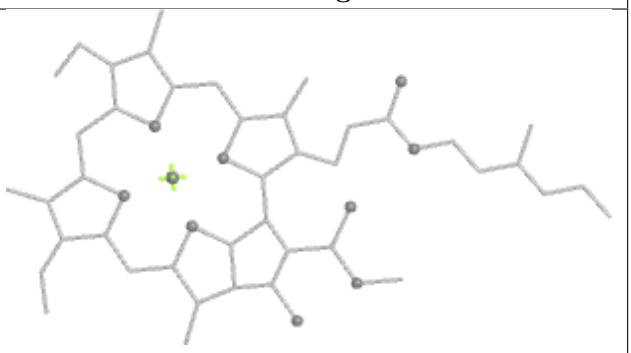
Bond lengths



Bond angles

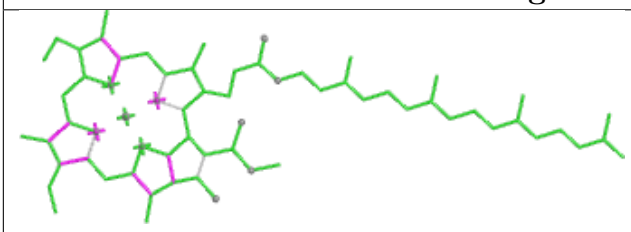


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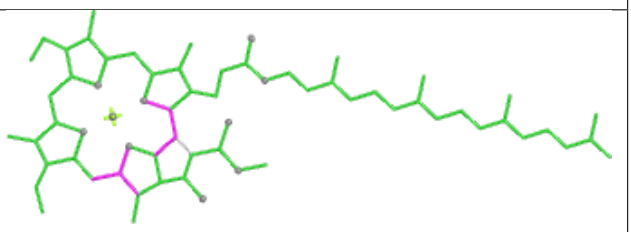


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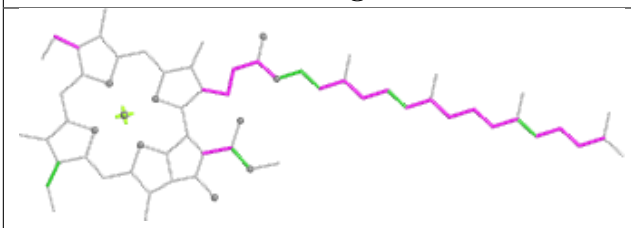
Ligand CLA a 830



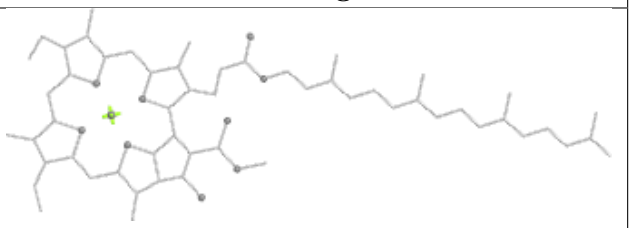
Bond lengths



Bond angles

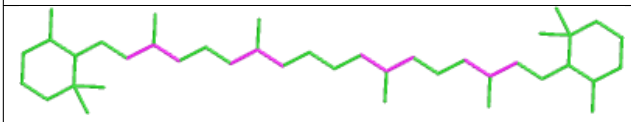


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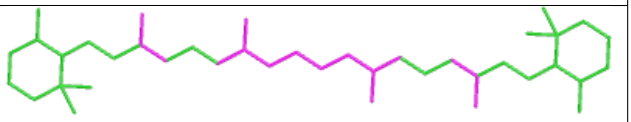


Rings

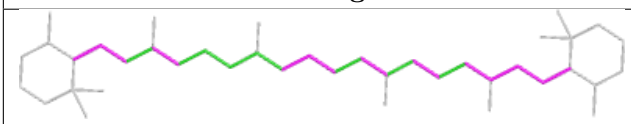
Ligand BCR L 301



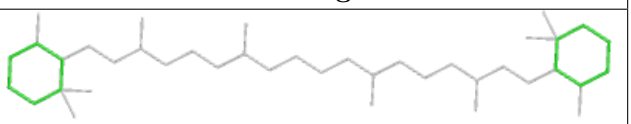
Bond lengths



Bond angles

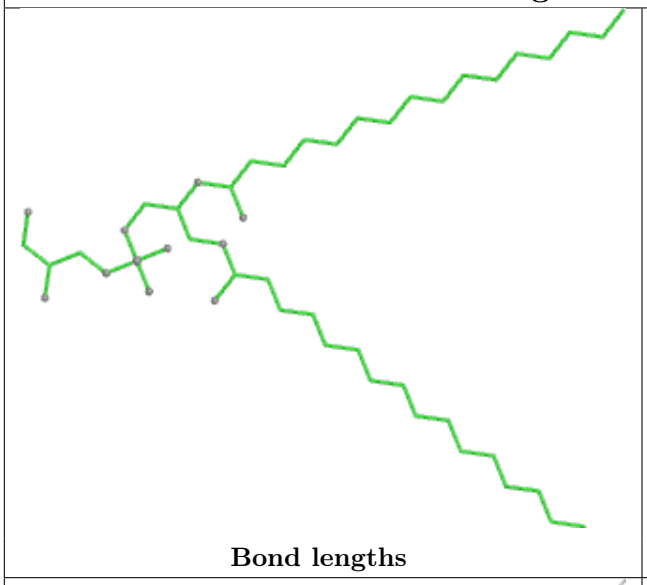


Torsions

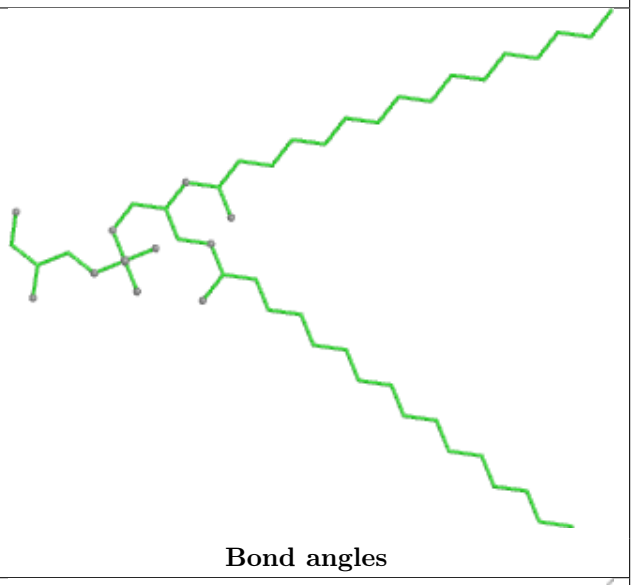


Rings

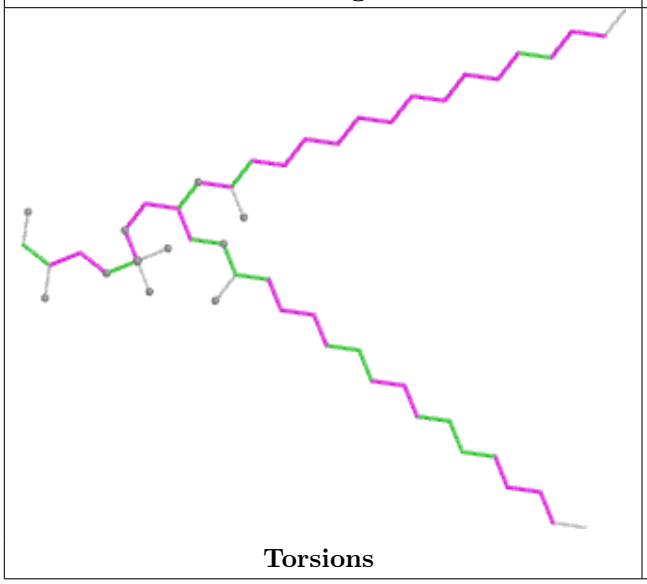
Ligand LHG l 303



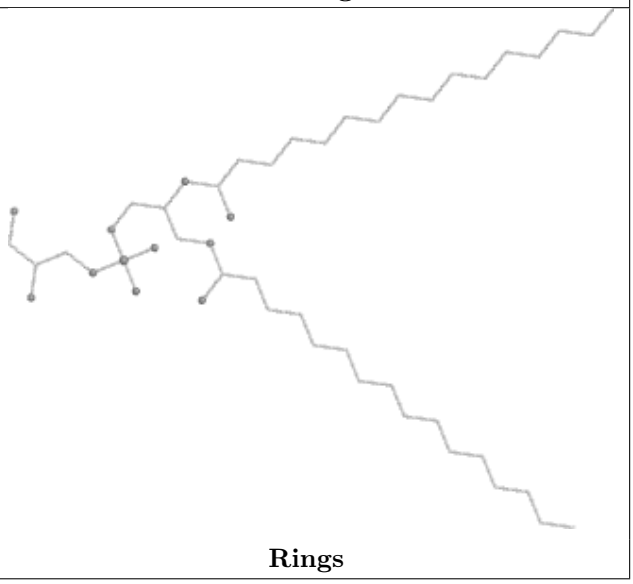
Bond lengths



Bond angles

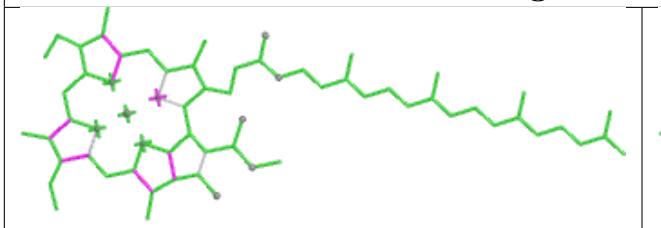


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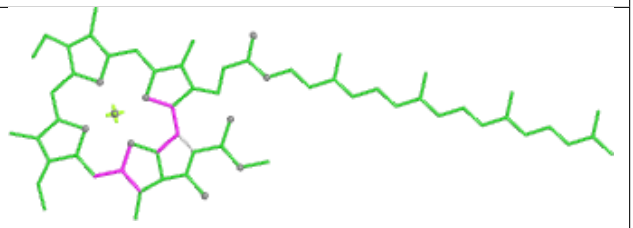


Rings

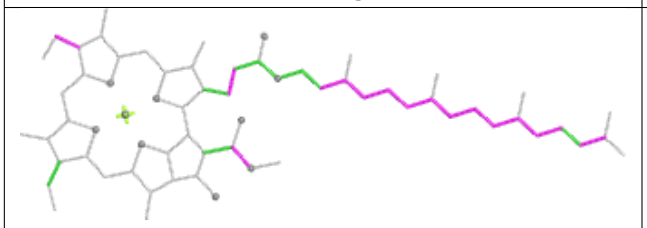
Ligand CLA a 846



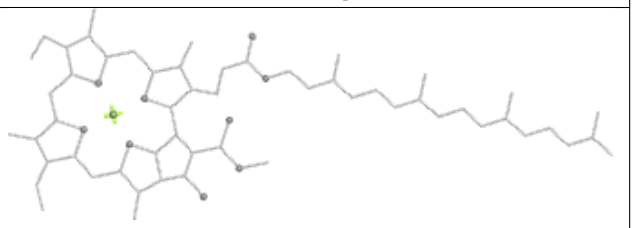
Bond lengths



Bond angles

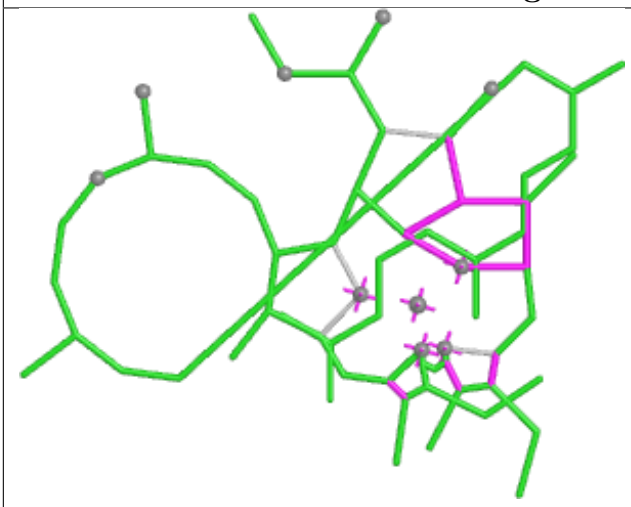


Torsions



Rings

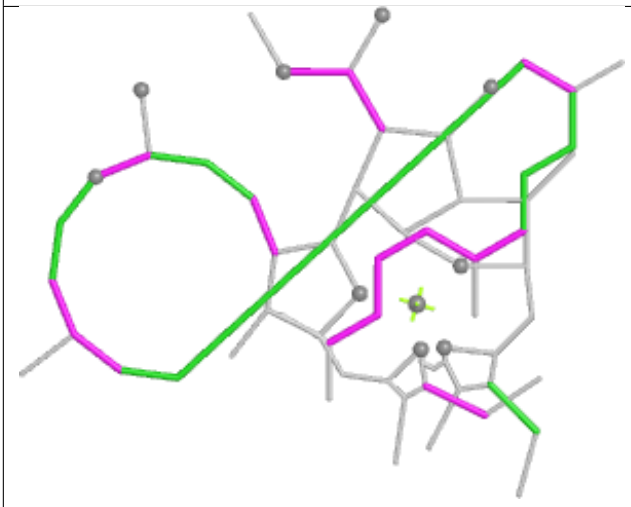
Ligand CLA A 819



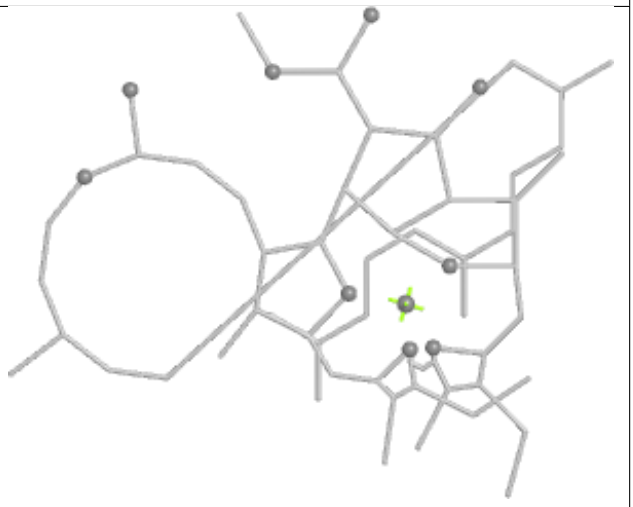
Bond lengths



Bond angles

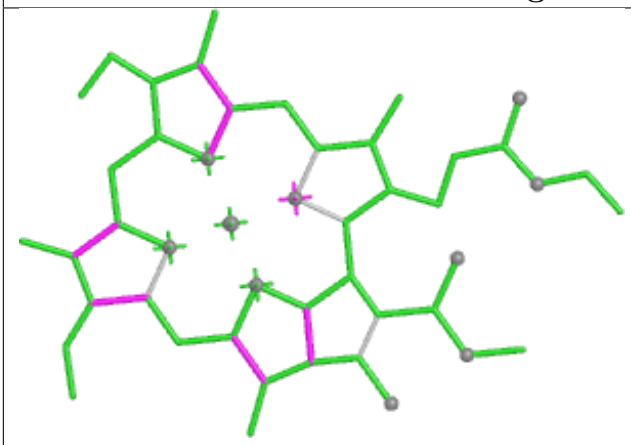


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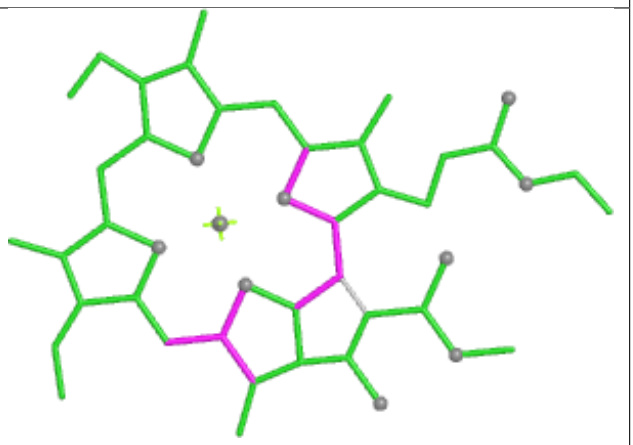


Rings

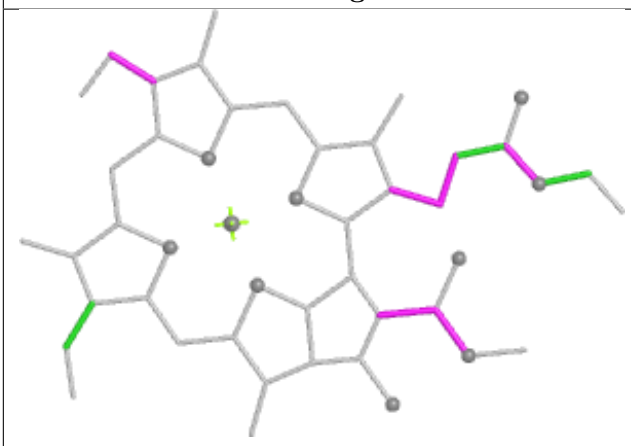
Ligand CLA b 822



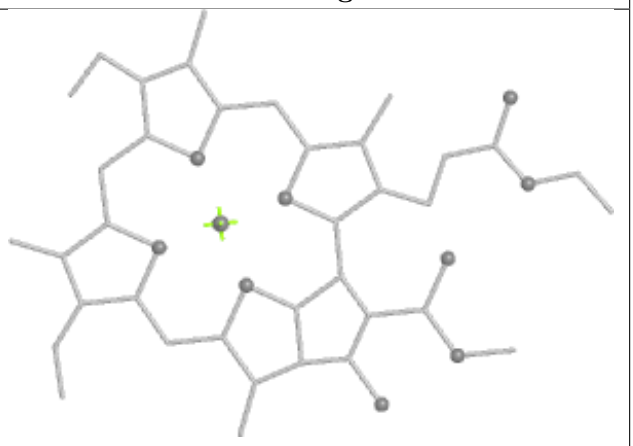
Bond lengths



Bond angles

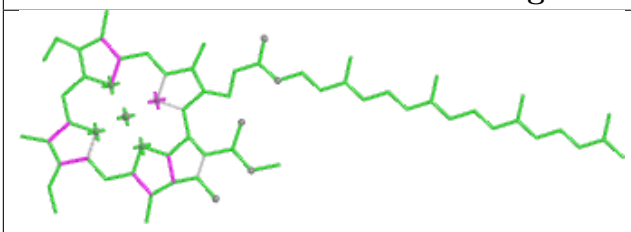


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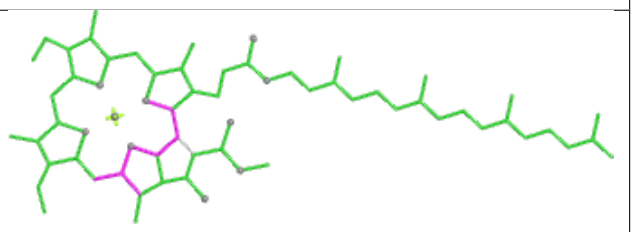


Rings

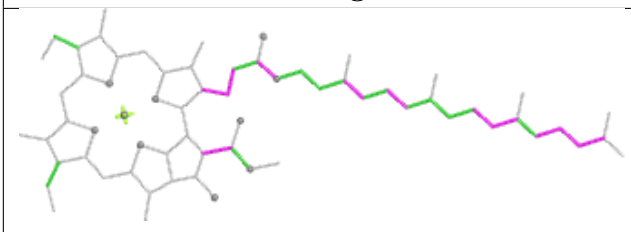
Ligand CLA b 815



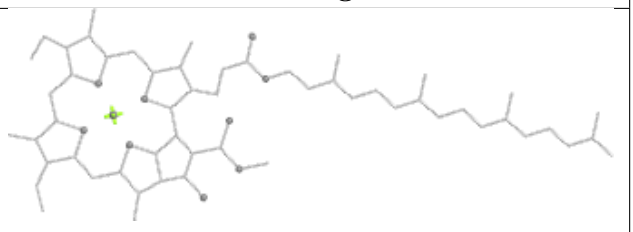
Bond lengths



Bond angles

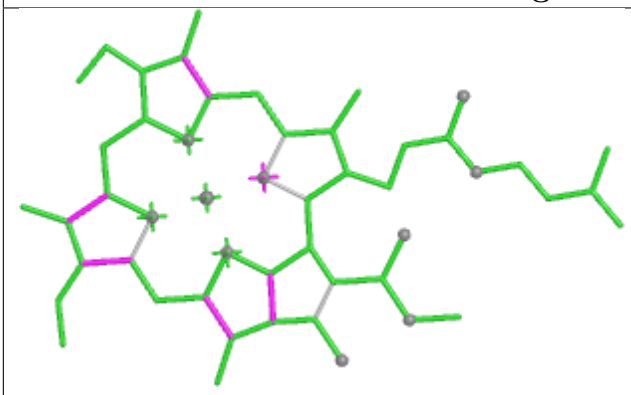


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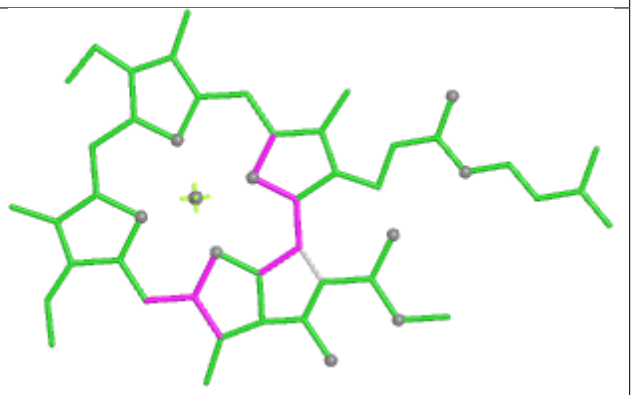


Rings

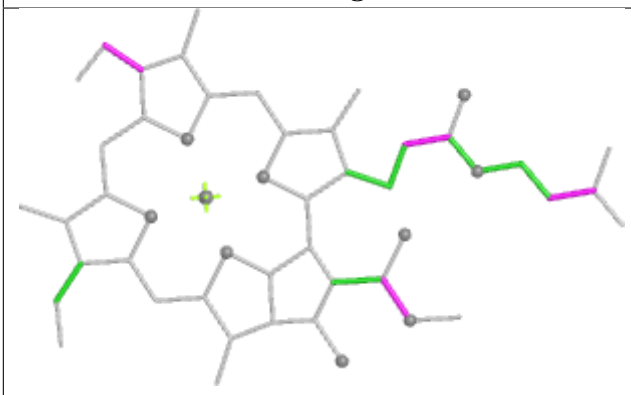
Ligand CLA l 307



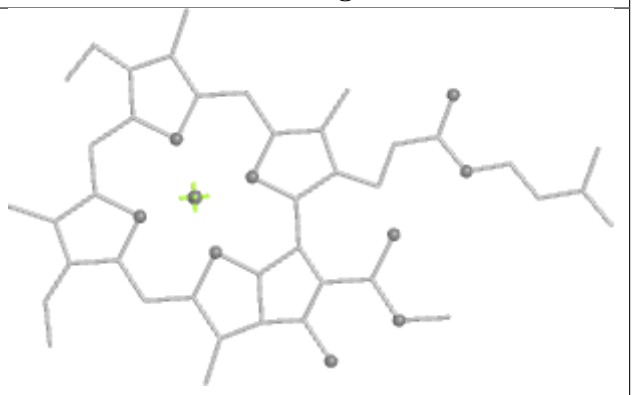
Bond lengths



Bond angles

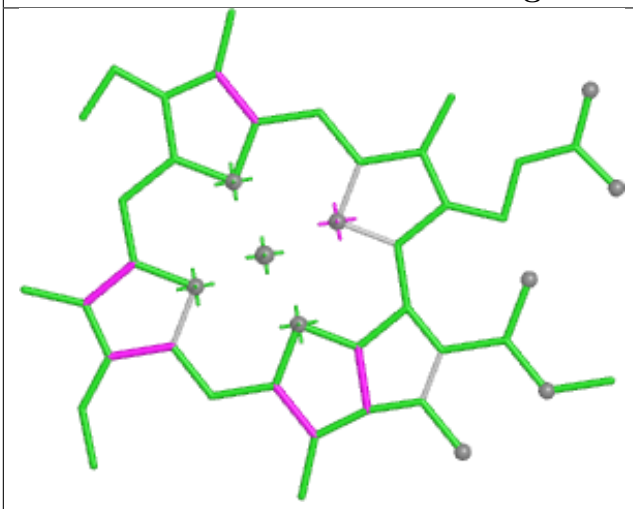


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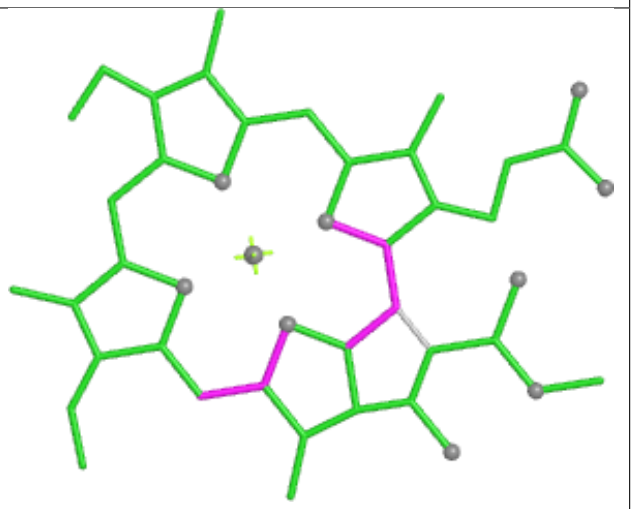


Rings

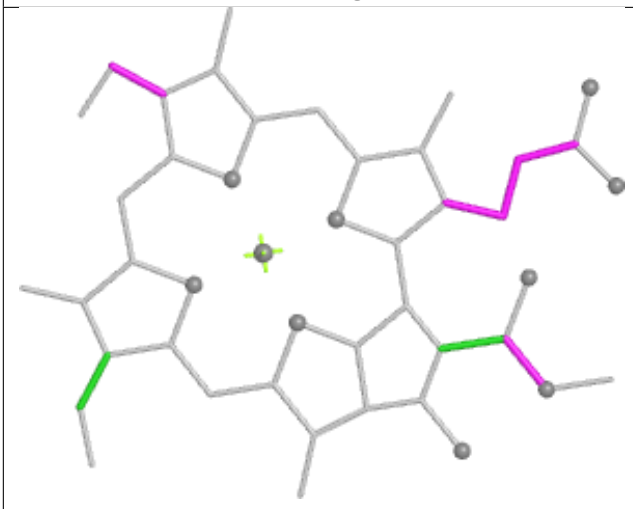
Ligand CLA A 818



Bond lengths



Bond angles

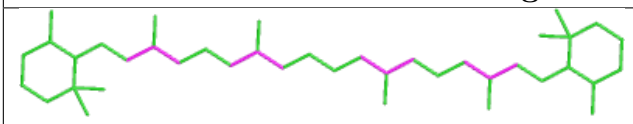


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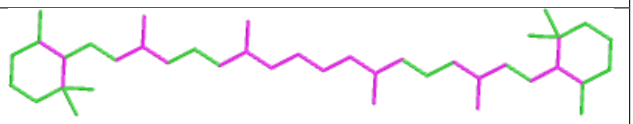


Rings

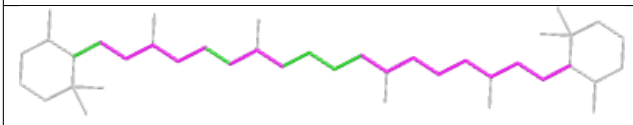
Ligand BCR H 202



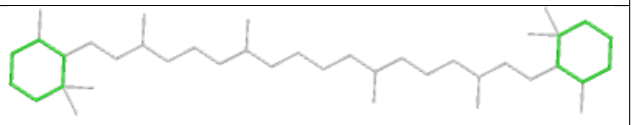
Bond lengths



Bond angles

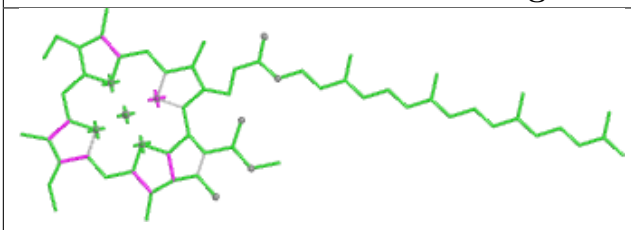


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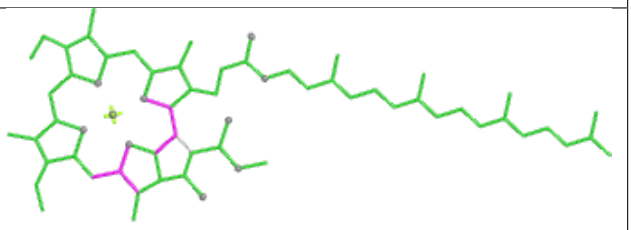


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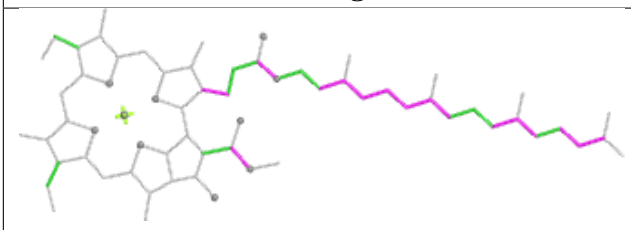
Ligand CLA a 817



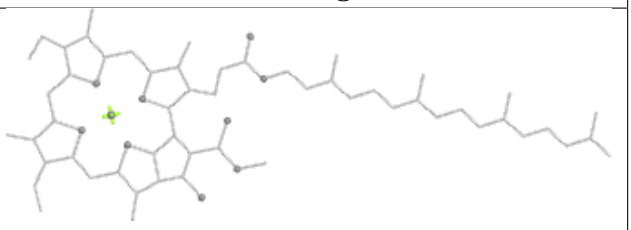
Bond lengths



Bond angles

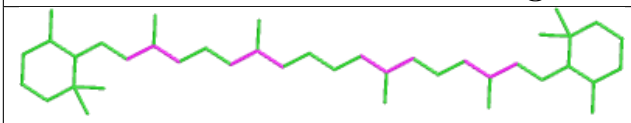


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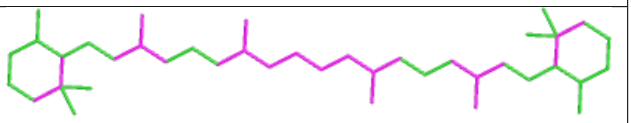


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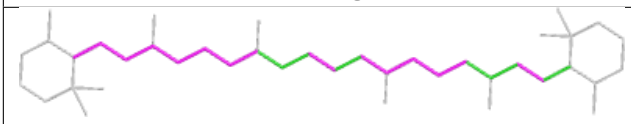
Ligand BCR a 843



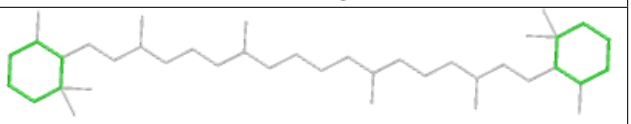
Bond lengths



Bond angles

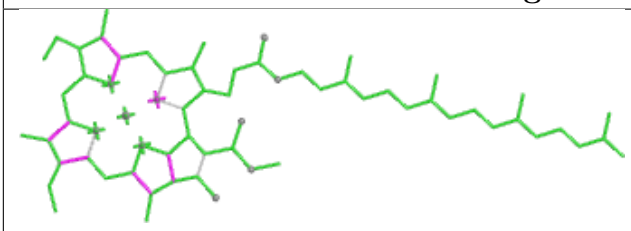


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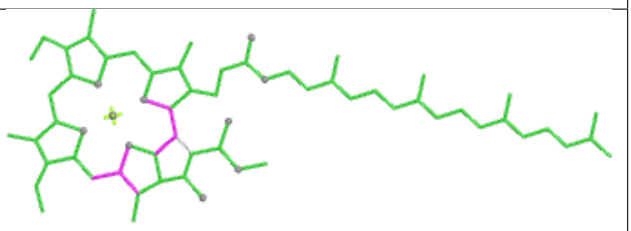


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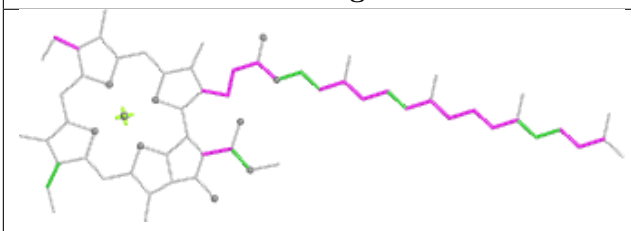
Ligand CLA A 829



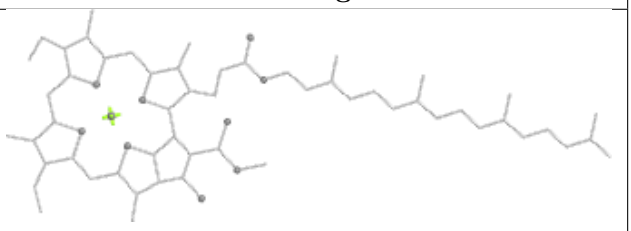
Bond lengths



Bond angles

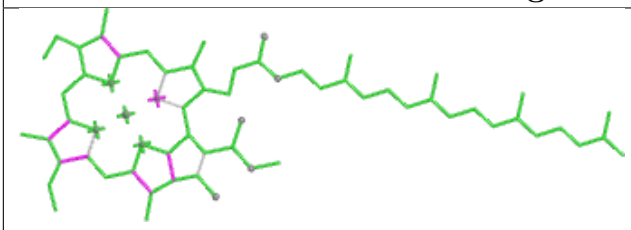


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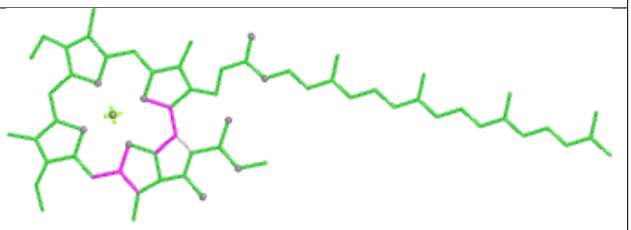


Rings

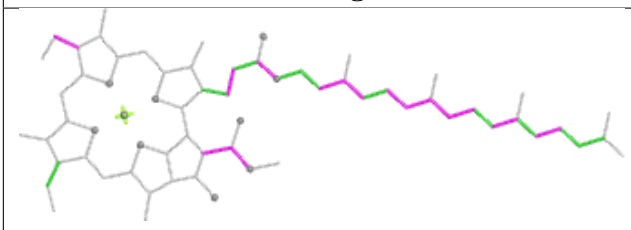
Ligand CLA b 811



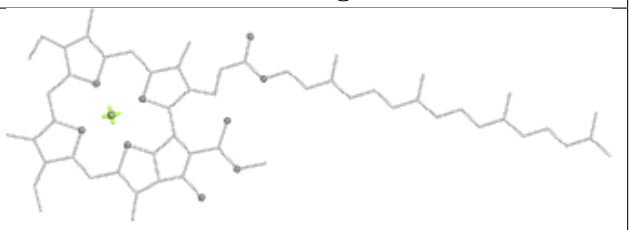
Bond lengths



Bond angles

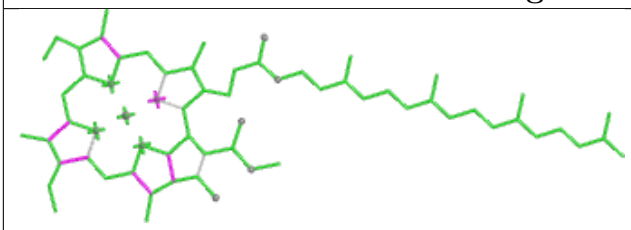


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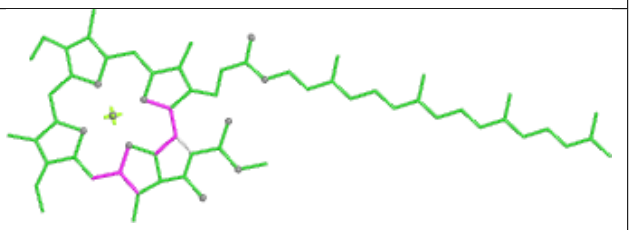


Rings

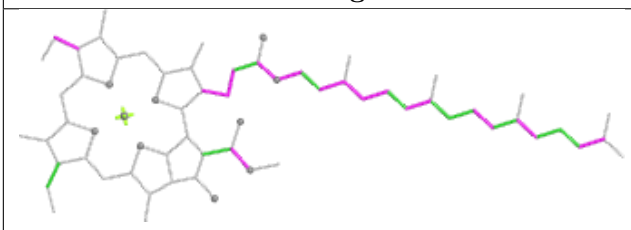
Ligand CLA L 303



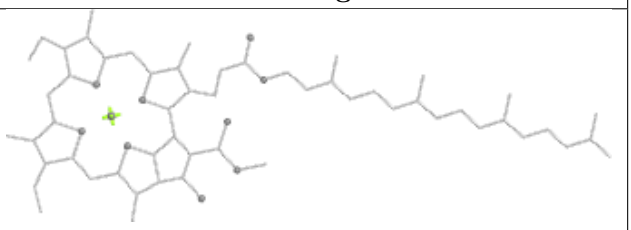
Bond lengths



Bond angles

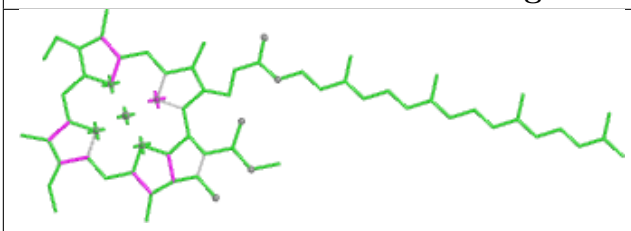


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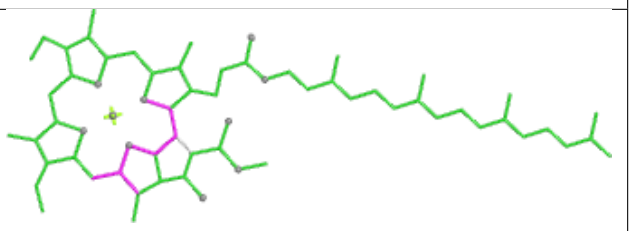


Rings

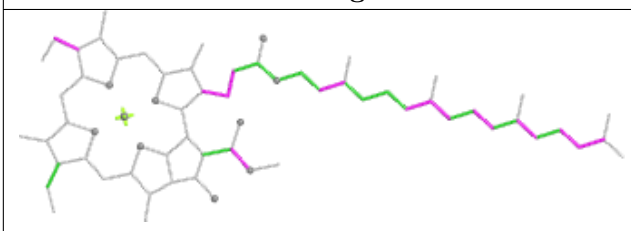
Ligand CLA B 823



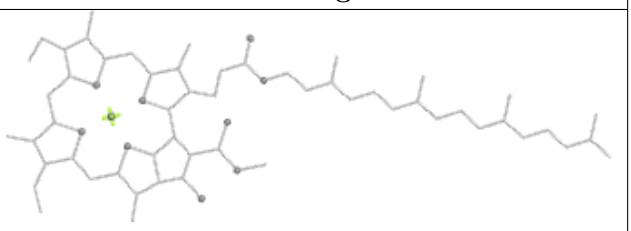
Bond lengths



Bond angles

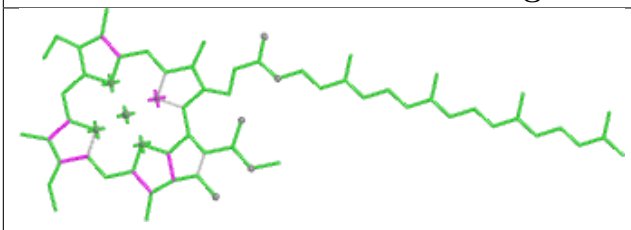


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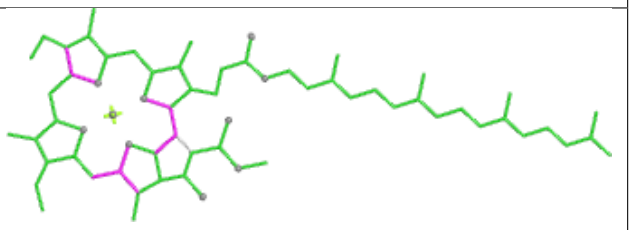


Rings

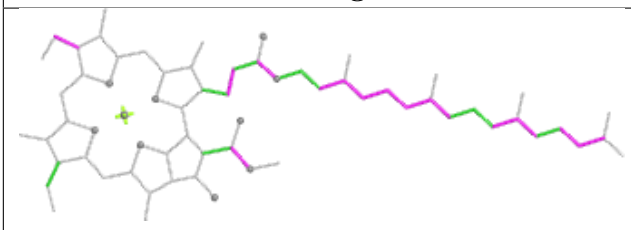
Ligand CLA A 816



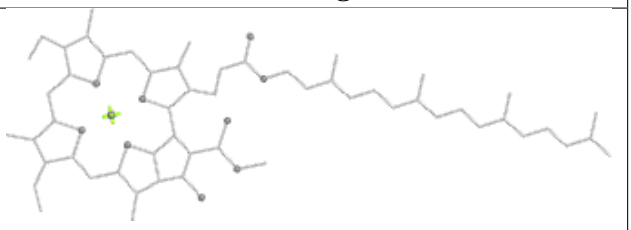
Bond lengths



Bond angles

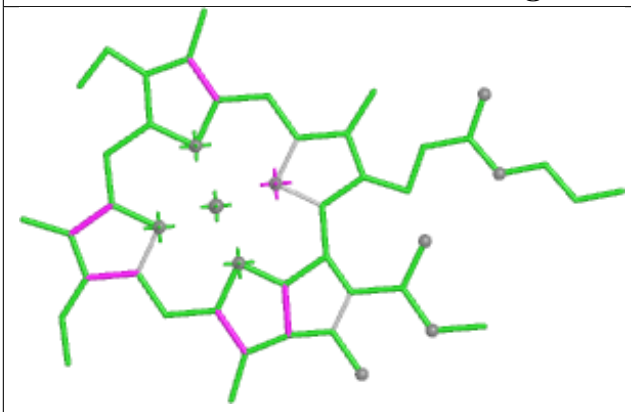


Torsions

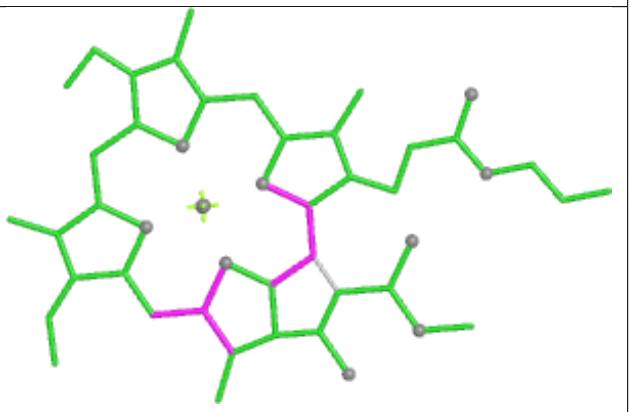


Rings

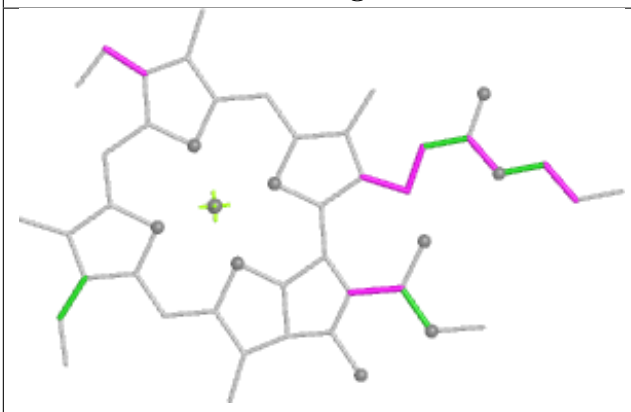
Ligand CLA B 839



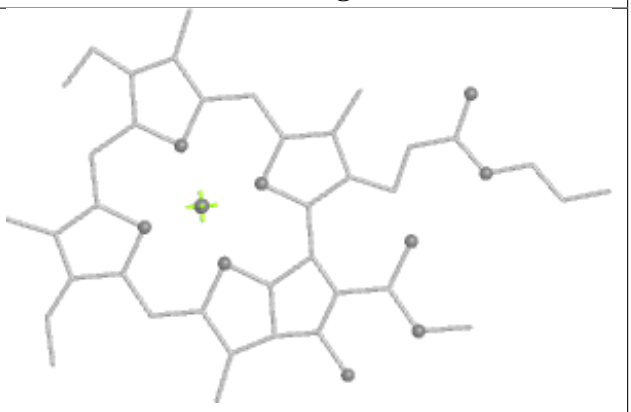
Bond lengths



Bond angles

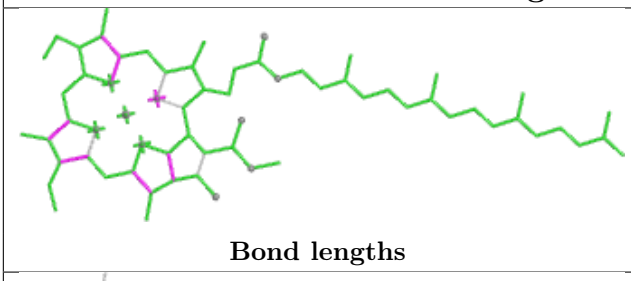


Torsions

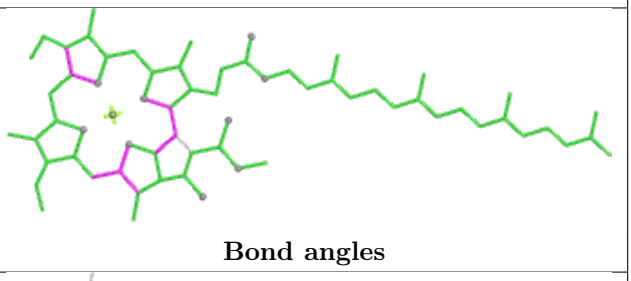


Rings

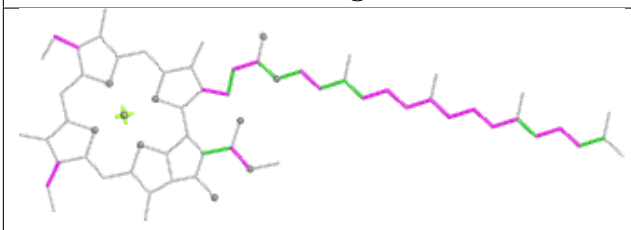
Ligand CLA b 804



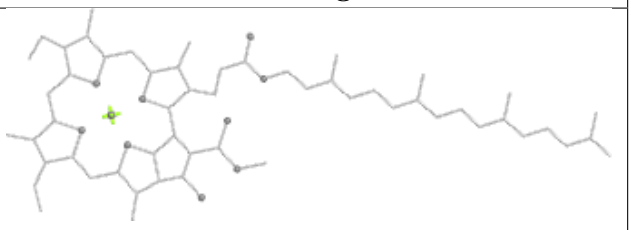
Bond lengths



Bond angles

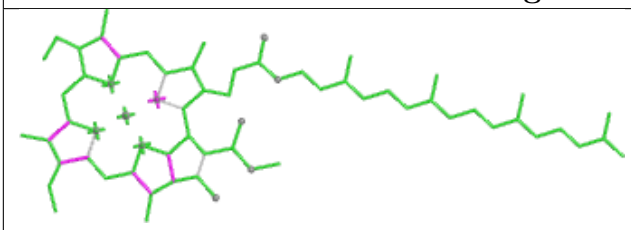


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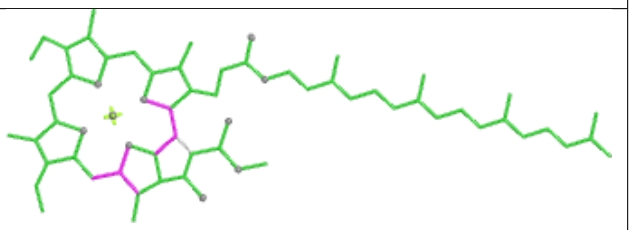


Rings

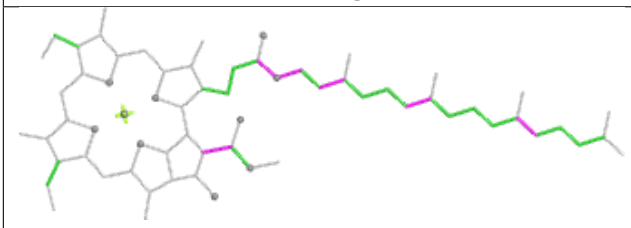
Ligand CLA A 804



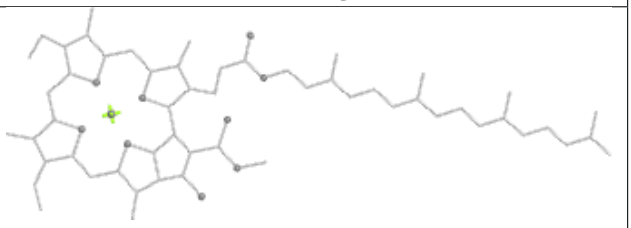
Bond lengths



Bond angles

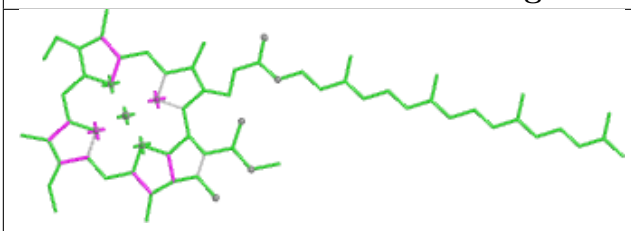


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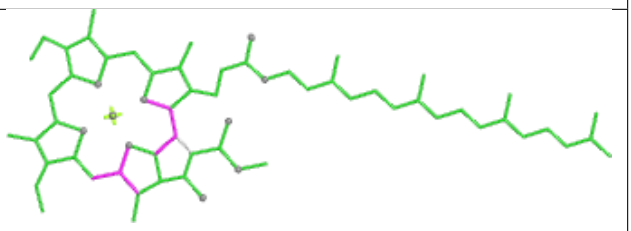


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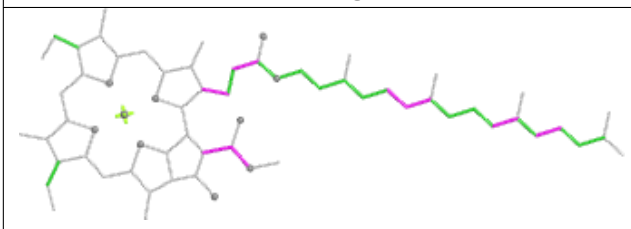
Ligand CLA B 825



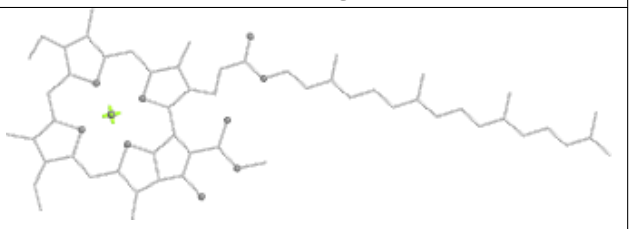
Bond lengths



Bond angles

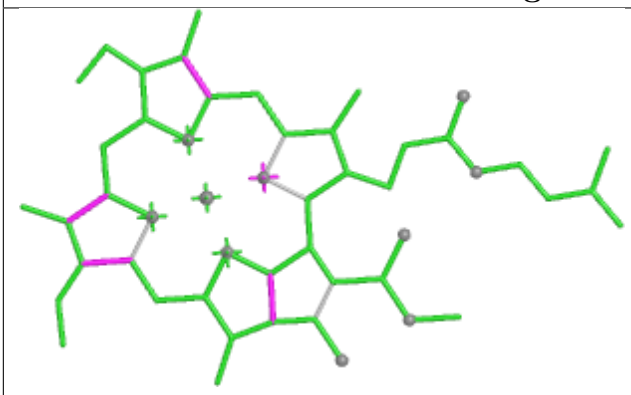


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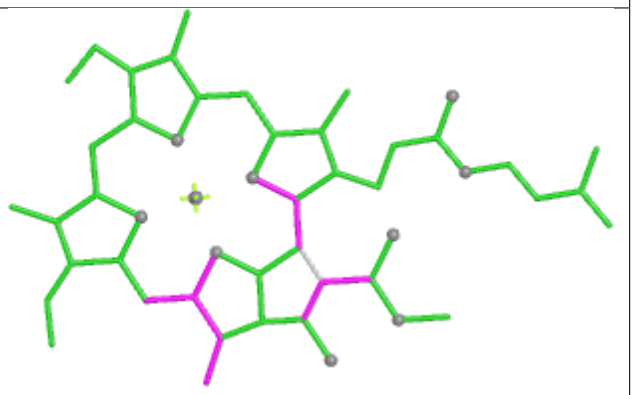


Rings

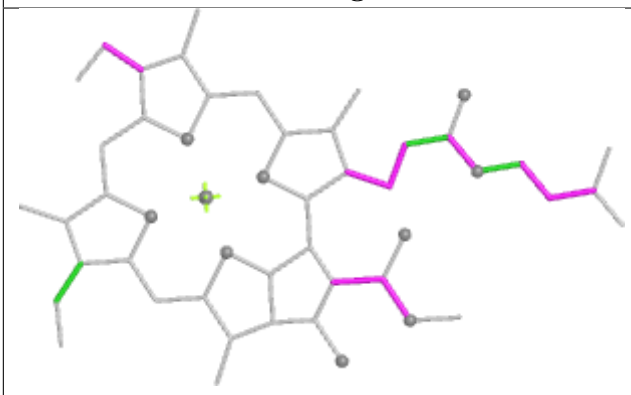
Ligand CLA A 830



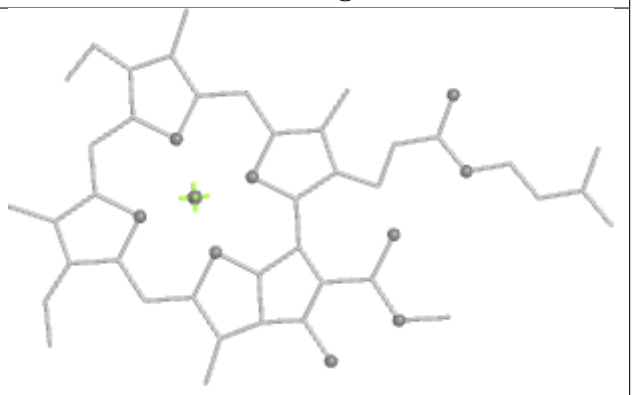
Bond lengths



Bond angles

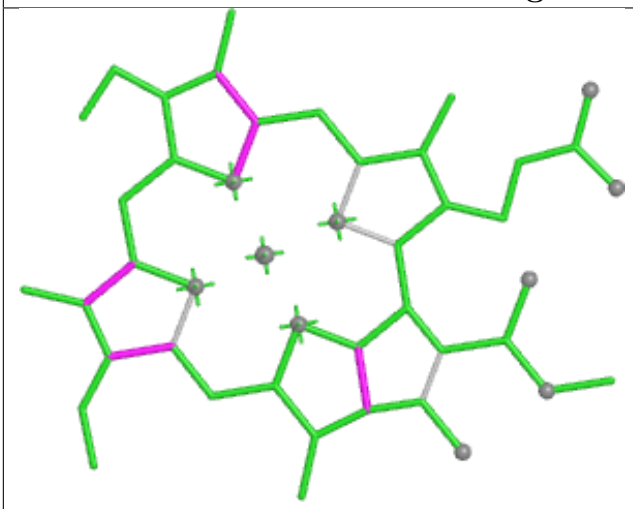


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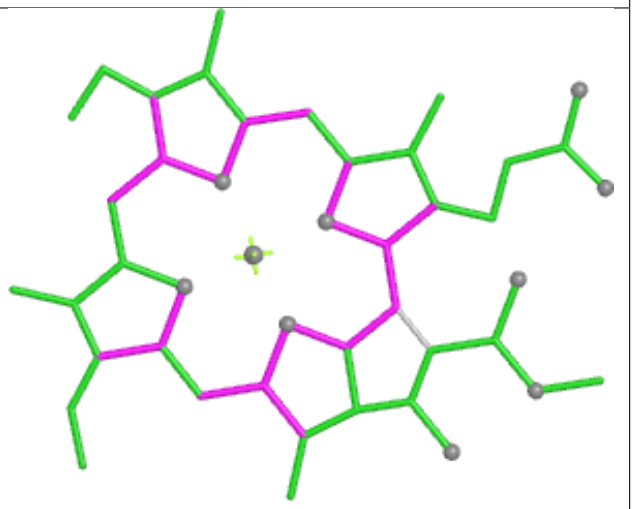


Rings

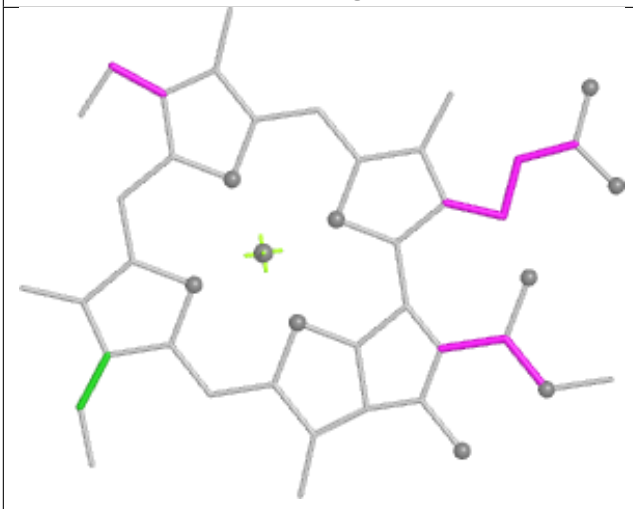
Ligand CLA L 307



Bond lengths



Bond angles

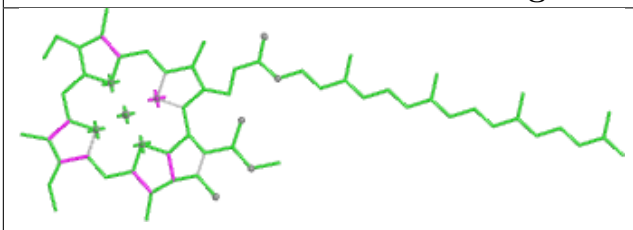


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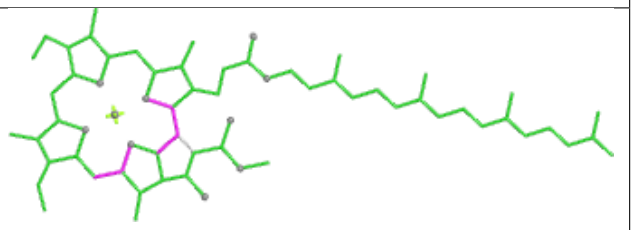


Rings

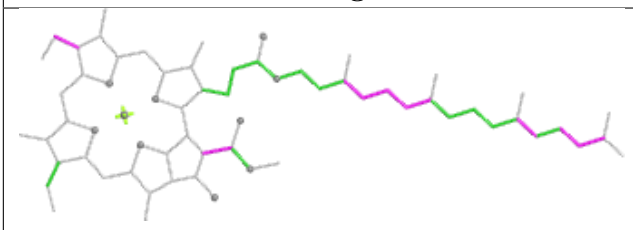
Ligand CLA a 823



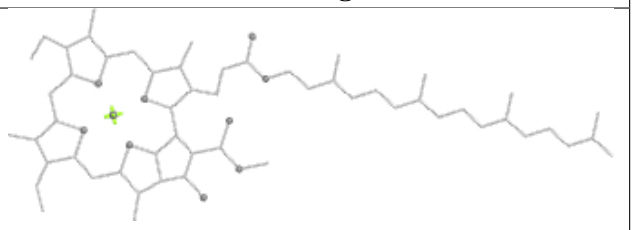
Bond lengths



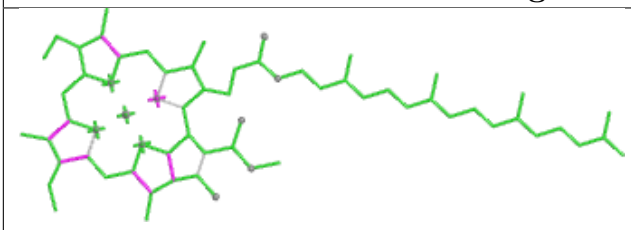
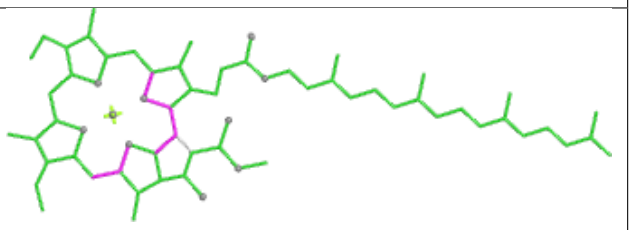
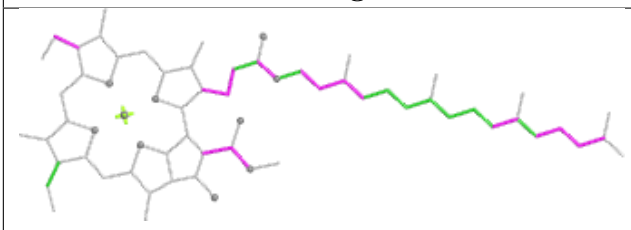
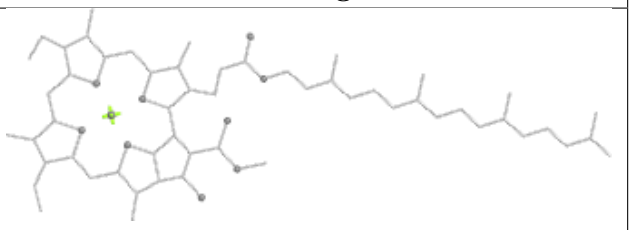
Bond angles

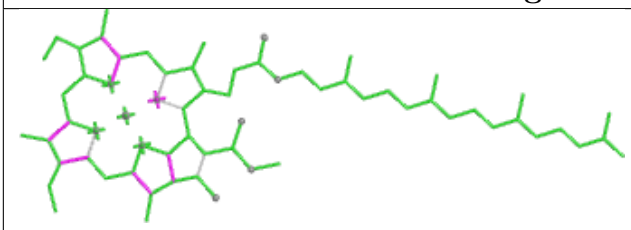
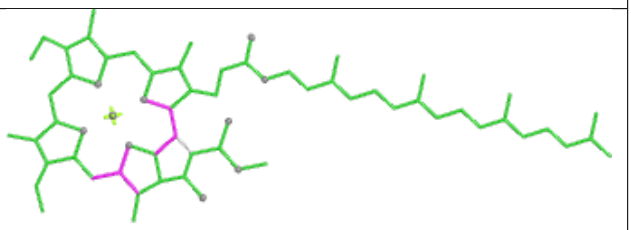
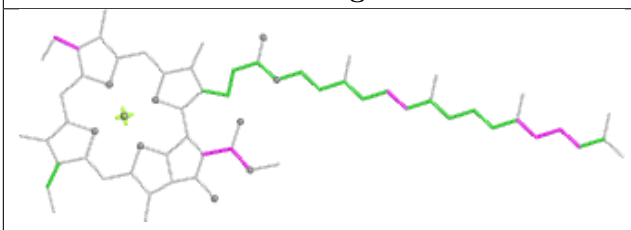
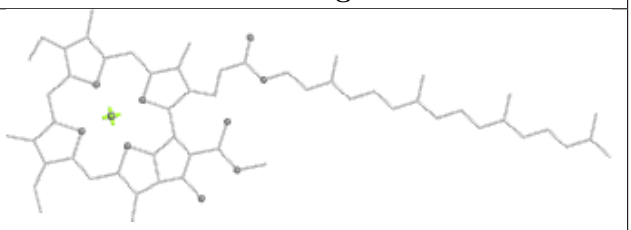


Torsions

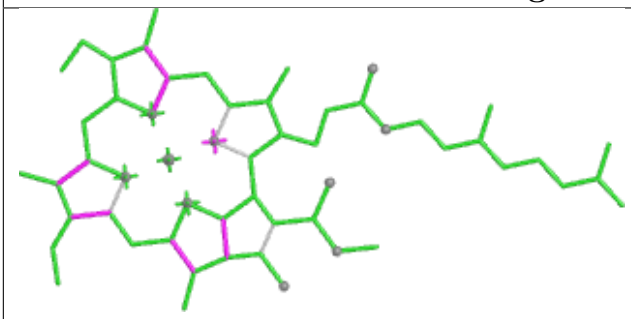


Rings

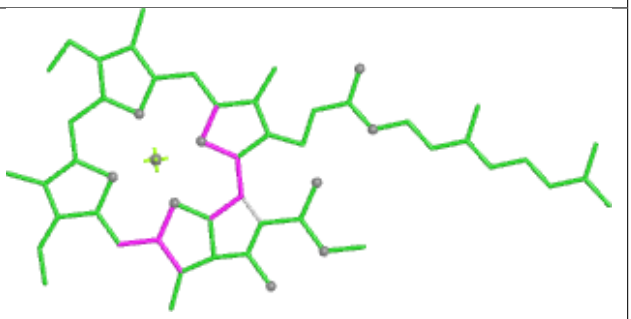
Ligand CLA a 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

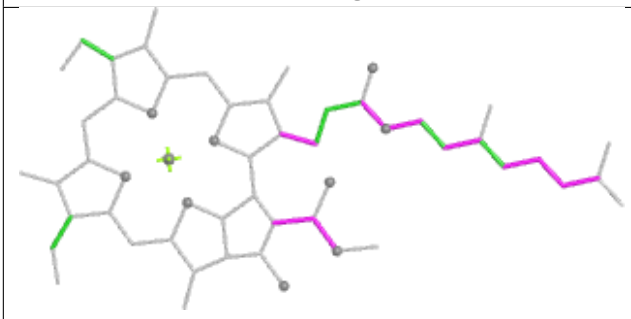
Ligand CLA a 803



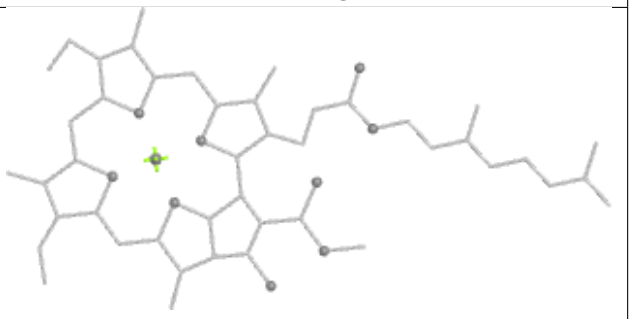
Bond lengths



Bond angles

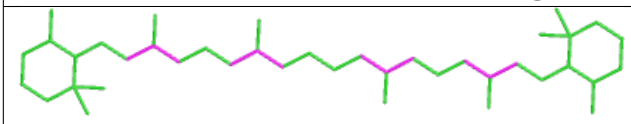


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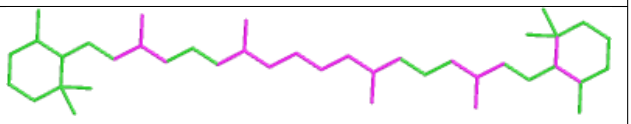


Rings

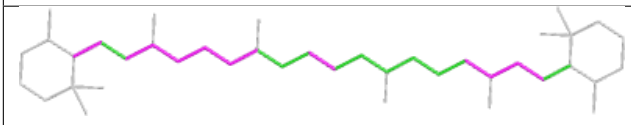
Ligand BCR I 101



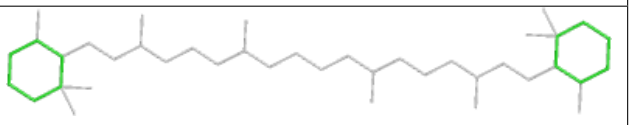
Bond lengths



Bond angles

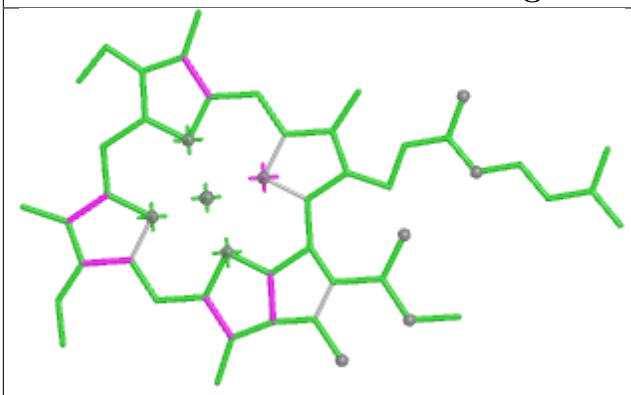


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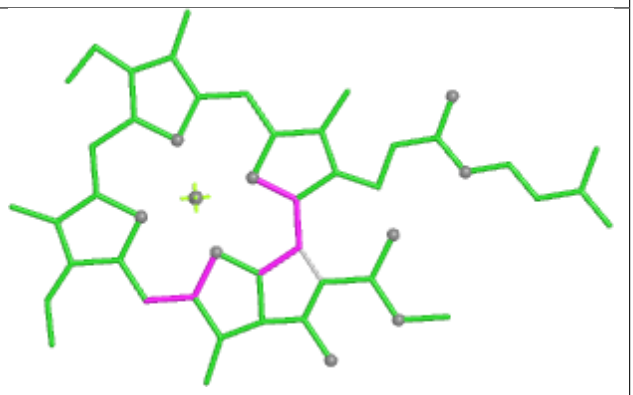


Rings

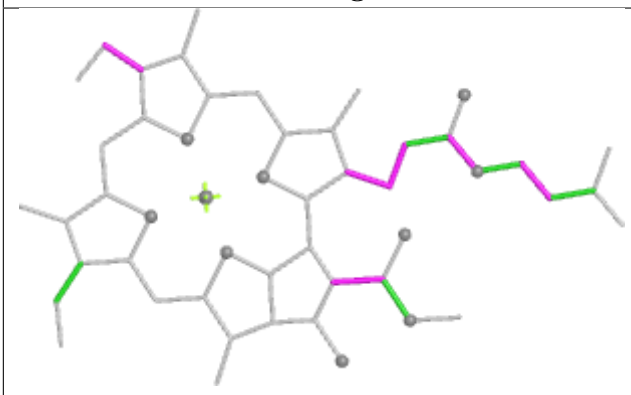
Ligand CLA A 827



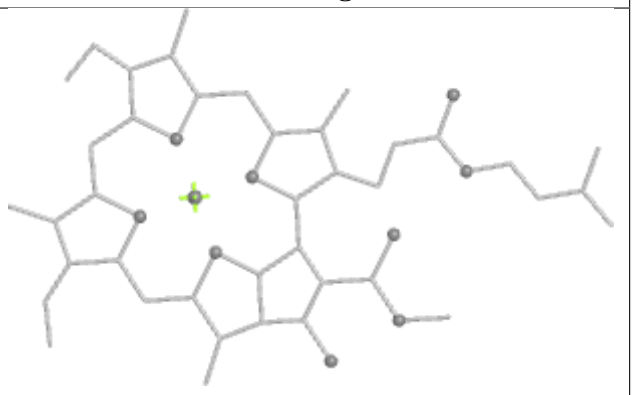
Bond lengths



Bond angles

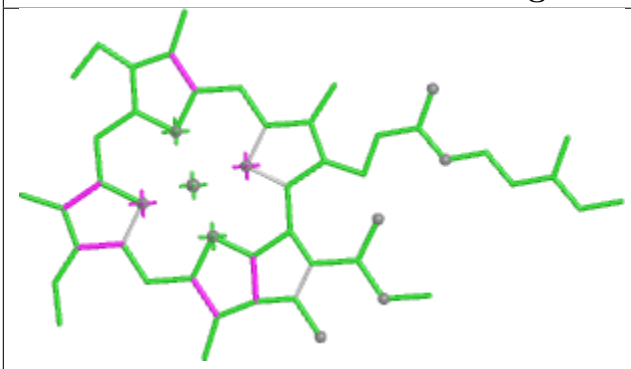


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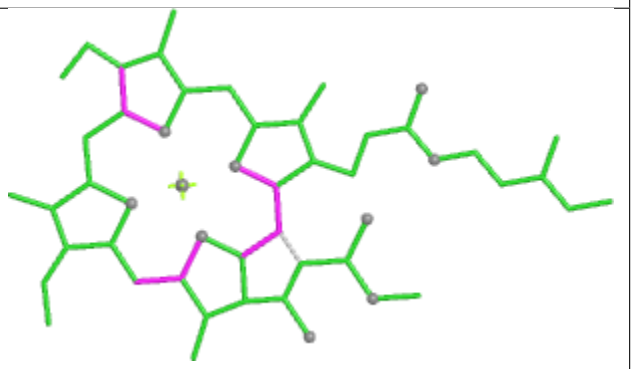


Rings

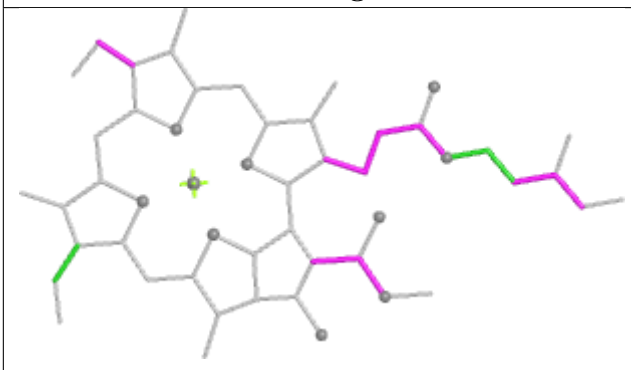
Ligand CLA a 832



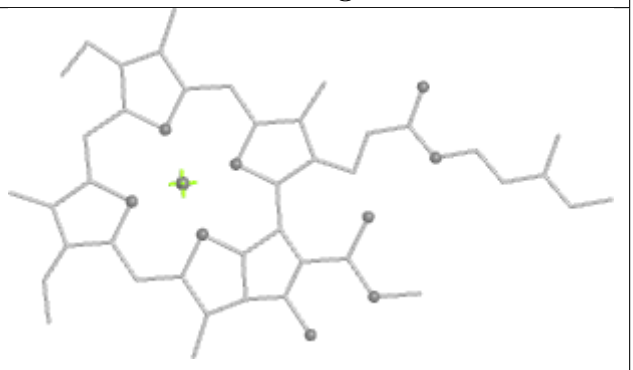
Bond lengths



Bond angles



Torsions

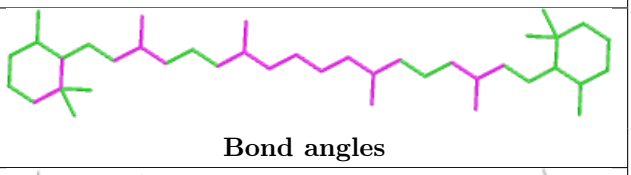


Rings

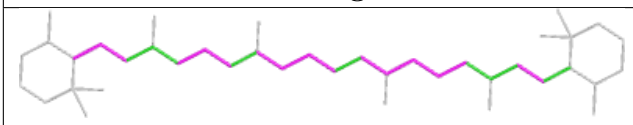
Ligand BCR A 842



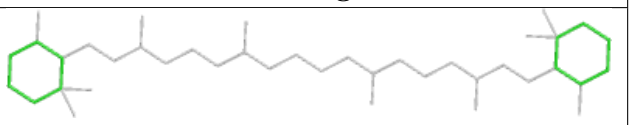
Bond lengths



Bond angles

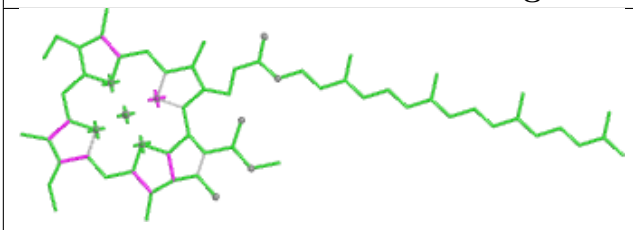


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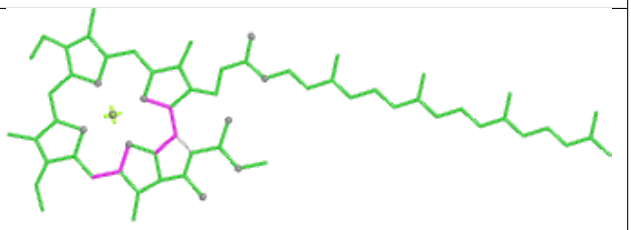


Rings

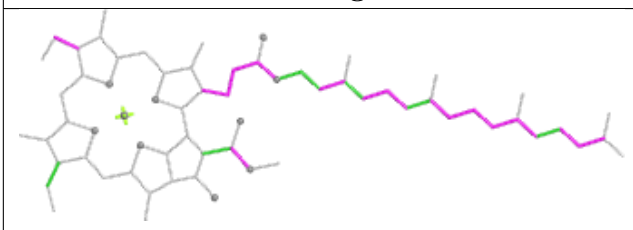
Ligand CLA A 815



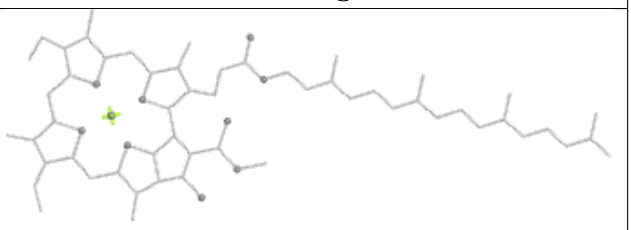
Bond lengths



Bond angles

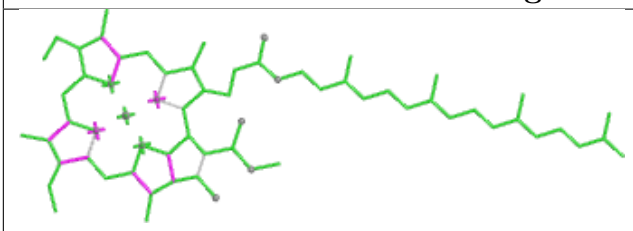


Torsions

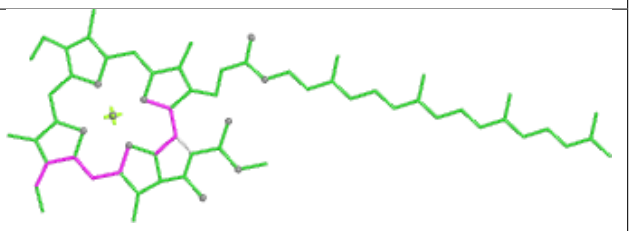


Rings

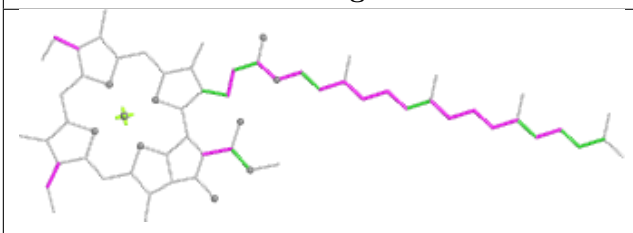
Ligand CLA B 801



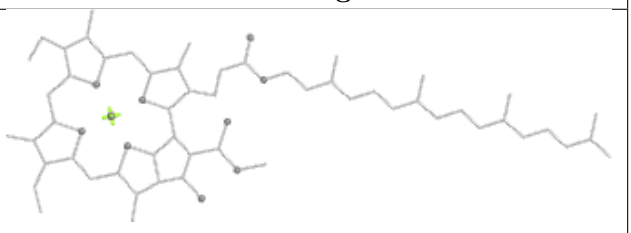
Bond lengths



Bond angles

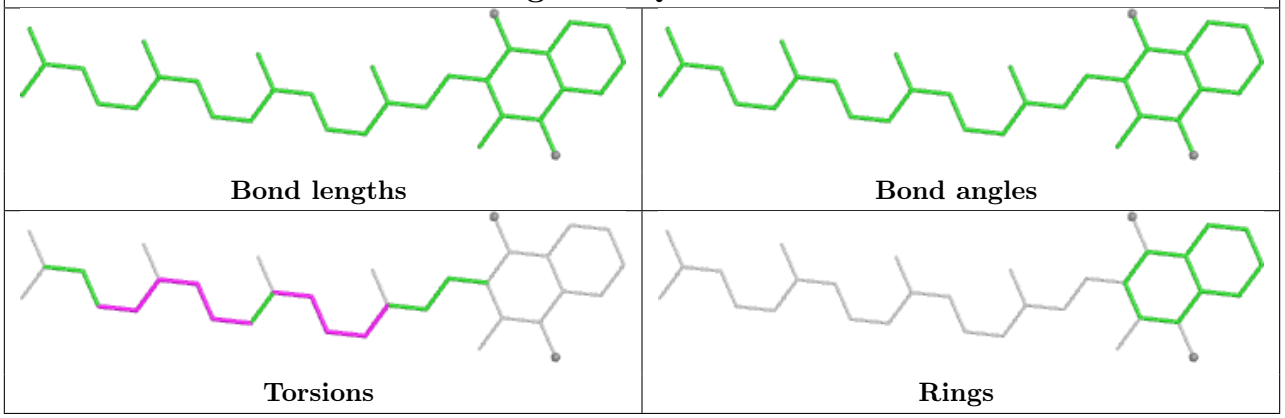


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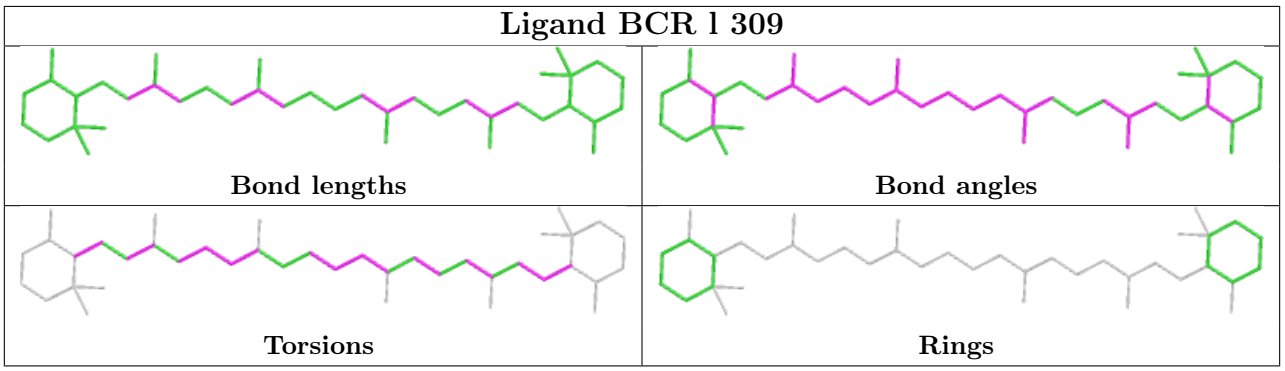


Rings

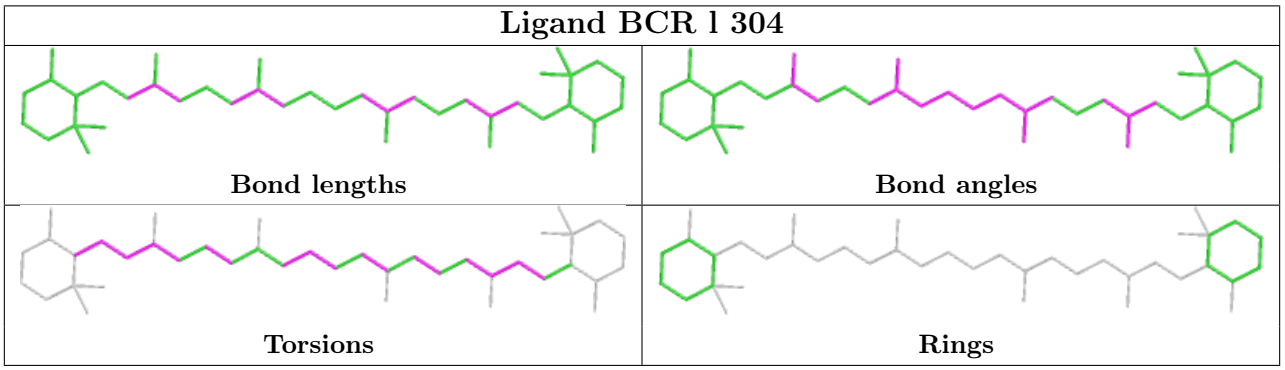
Ligand PQN a 838



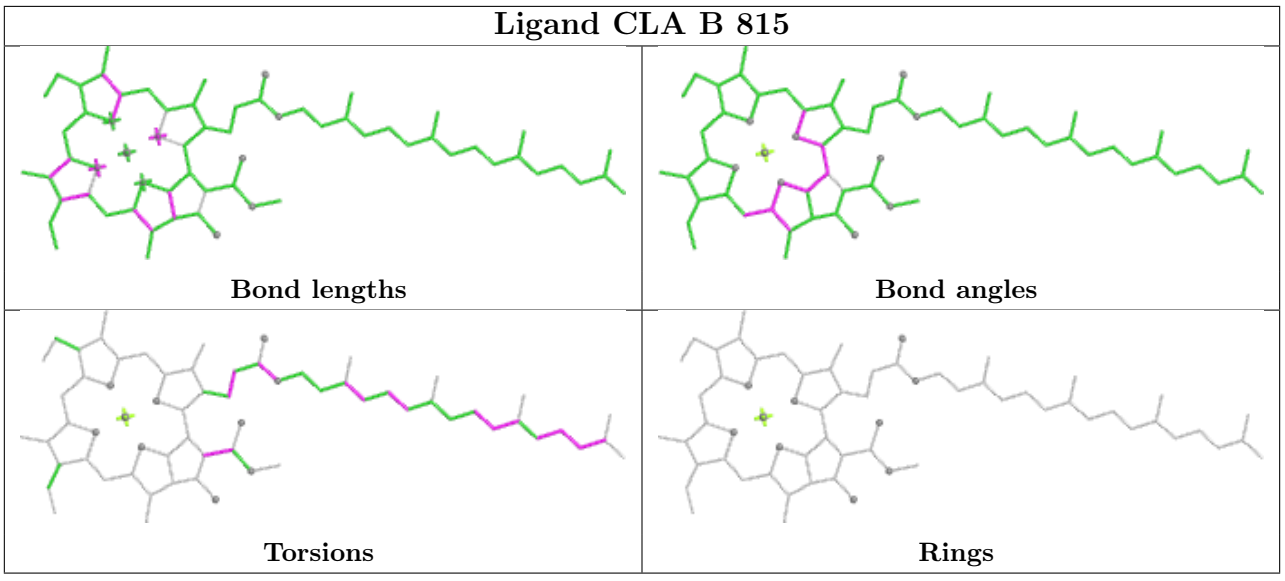
Ligand BCR l 309



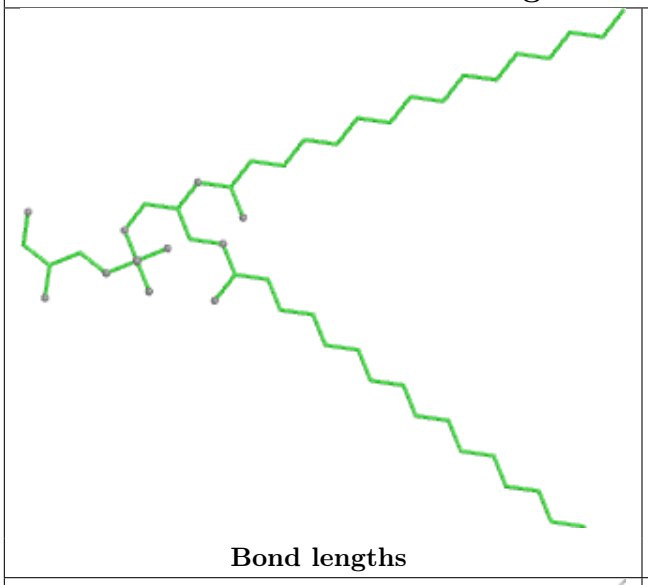
Ligand BCR l 304



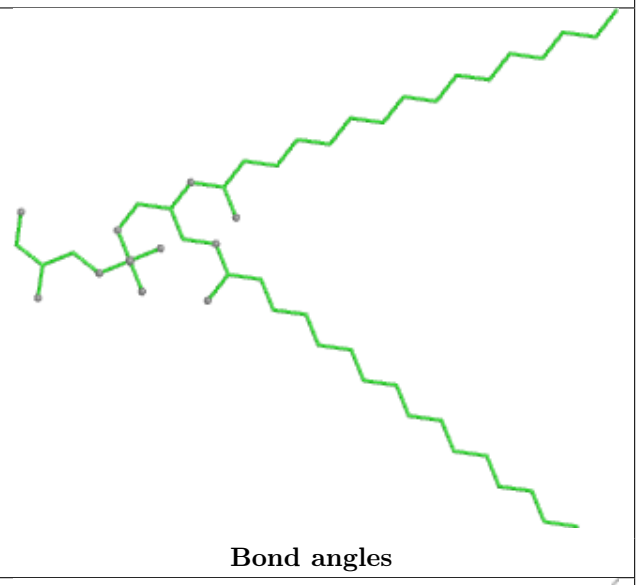
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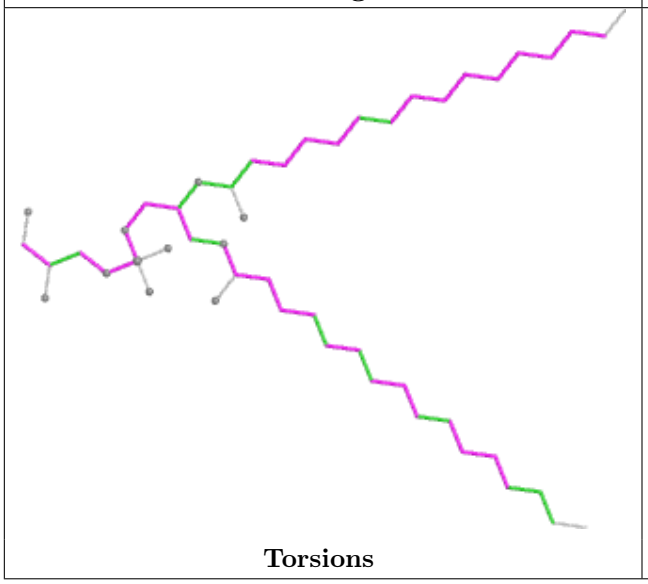
Ligand LHG A 845



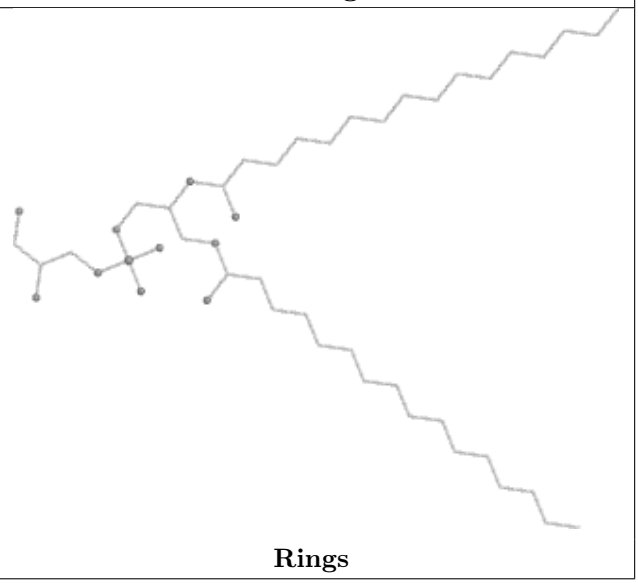
Bond lengths



Bond angles

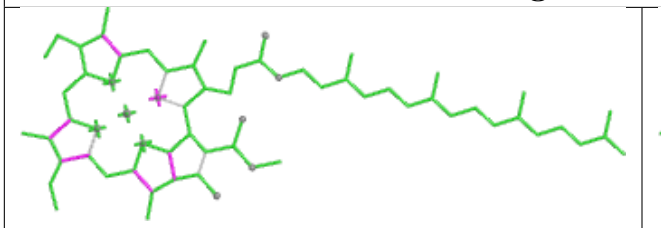


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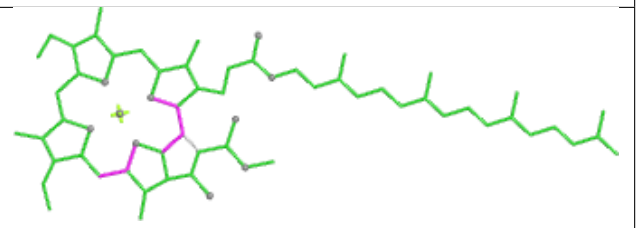


Rings

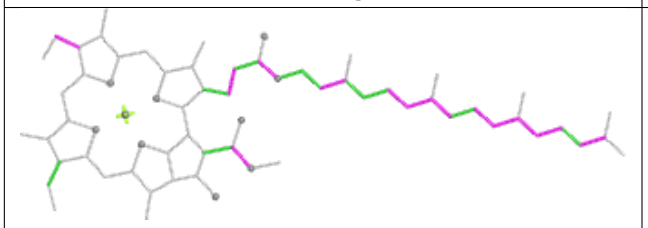
Ligand CLA a 809



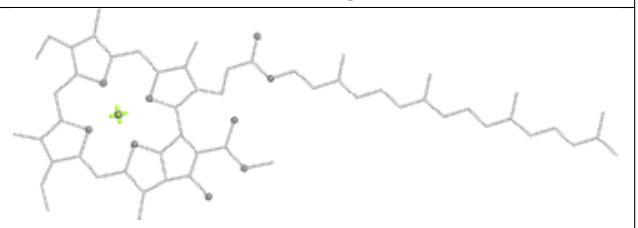
Bond lengths



Bond angles



Torsions

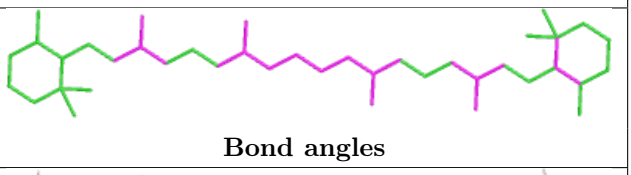


Rings

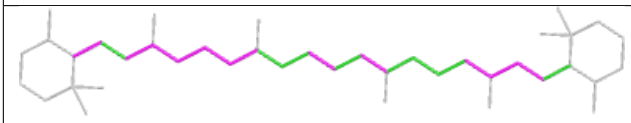
Ligand BCR i 101



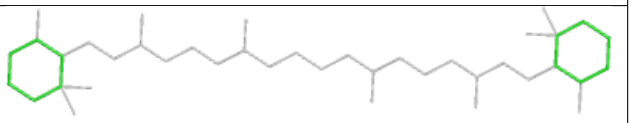
Bond lengths



Bond angles

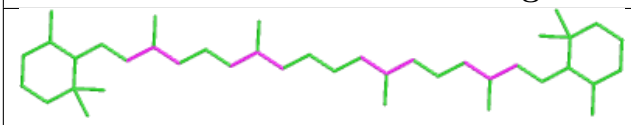


Torsions



Rings

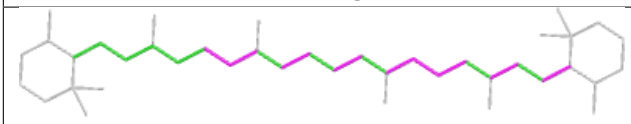
Ligand BCR A 843



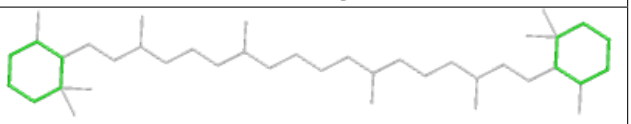
Bond lengths



Bond angles

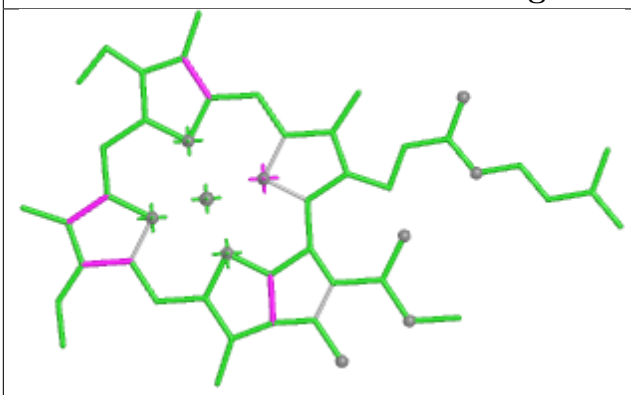


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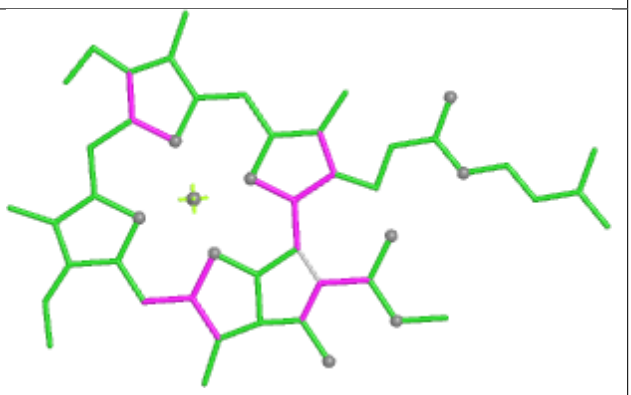


Rings

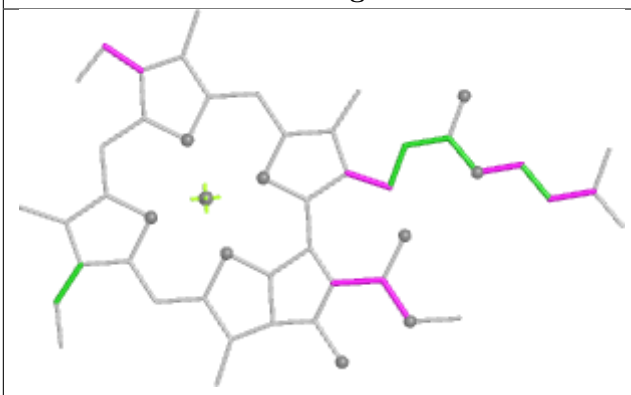
Ligand CLA a 831



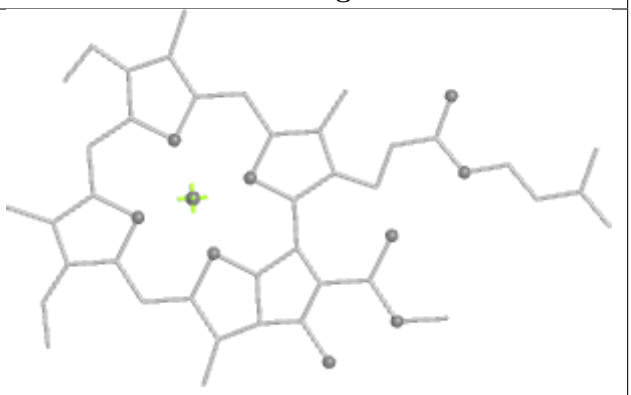
Bond lengths



Bond angles

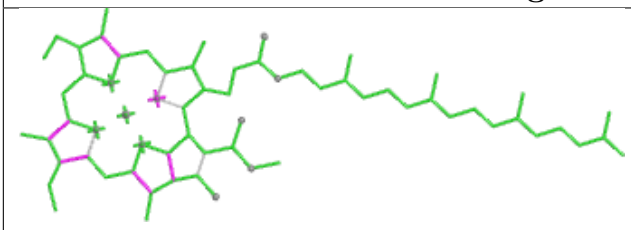


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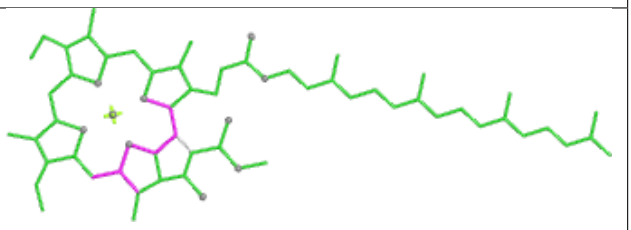


Rings

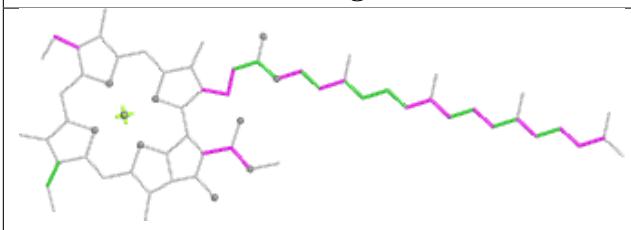
Ligand CLA b 823



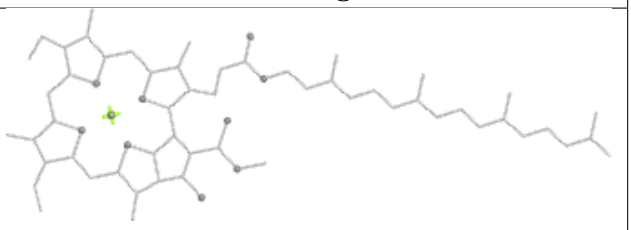
Bond lengths



Bond angles

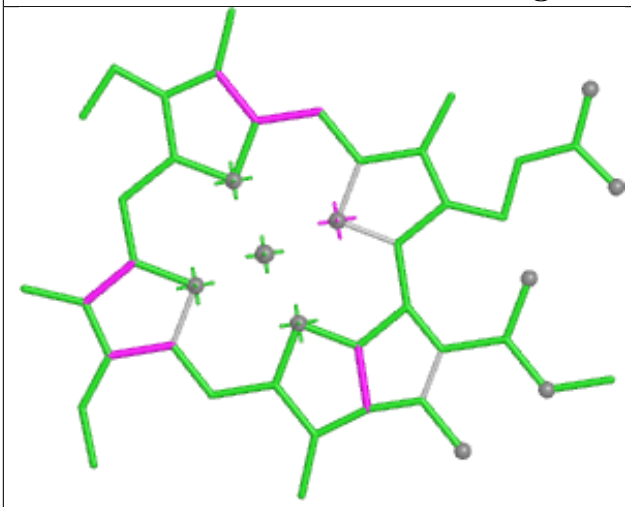


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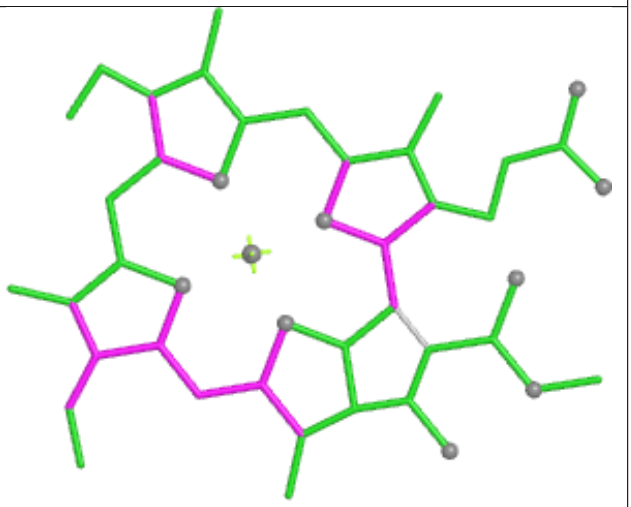


Rings

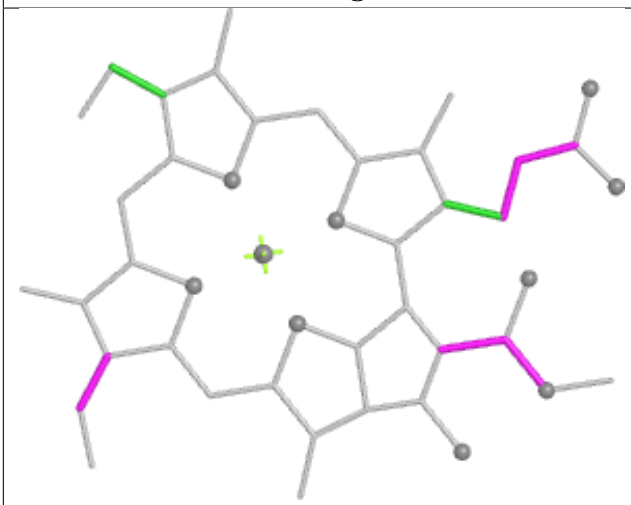
Ligand CLA l 301



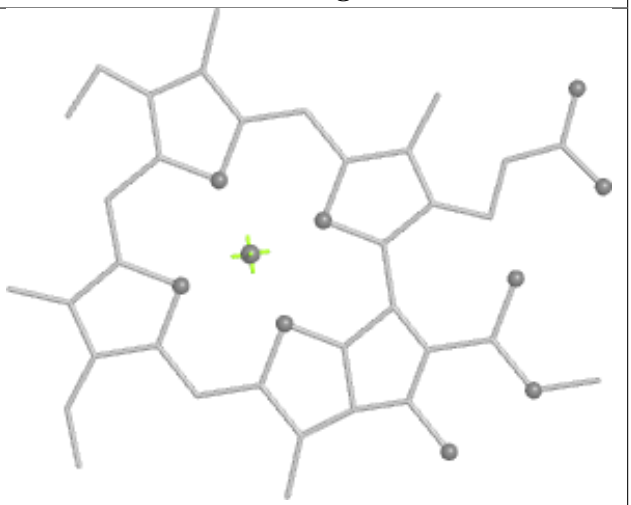
Bond lengths



Bond angles

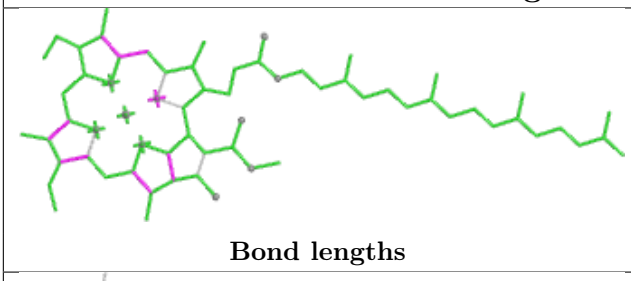


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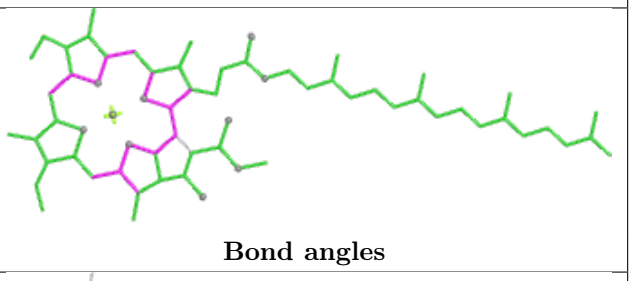


Rings

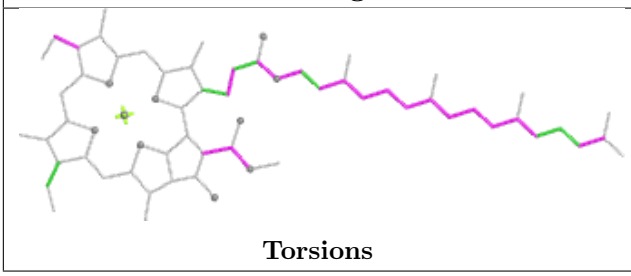
Ligand CLA A 806



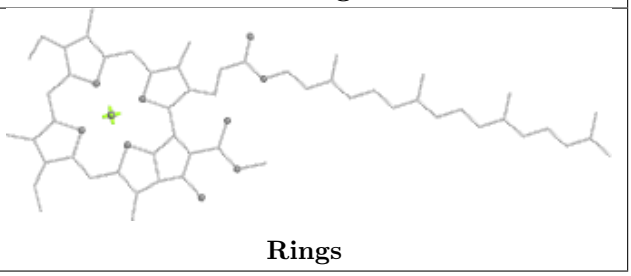
Bond lengths



Bond angles

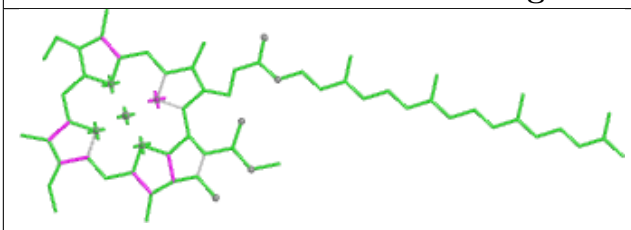


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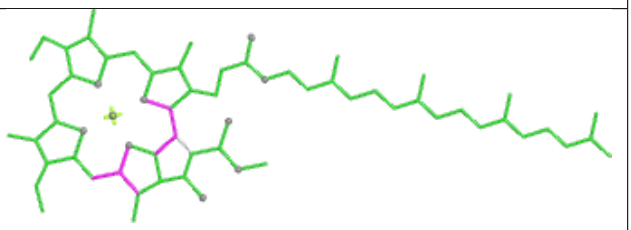


Rings

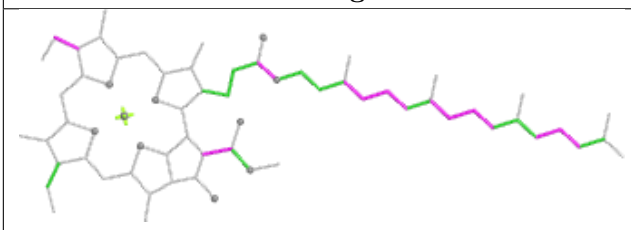
Ligand CLA b 829



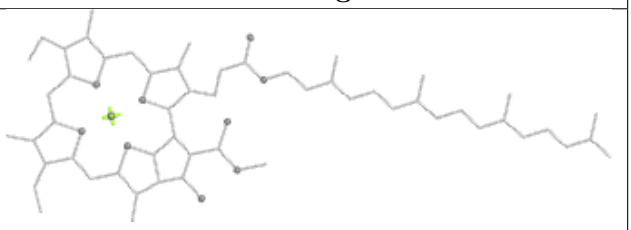
Bond lengths



Bond angles

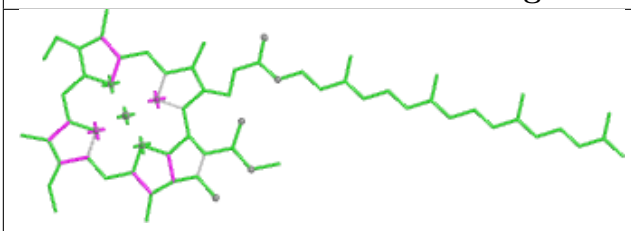


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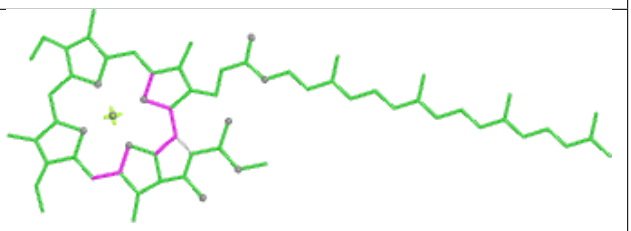


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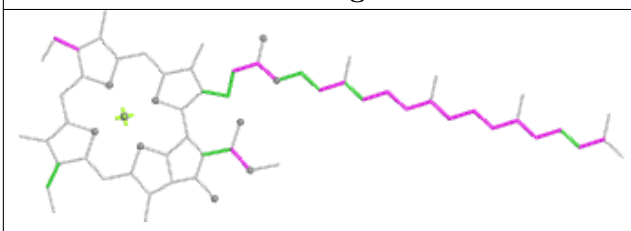
Ligand CLA A 847



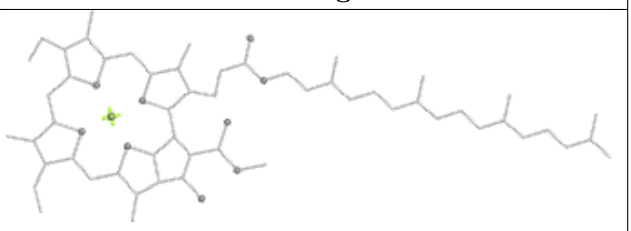
Bond lengths



Bond angles

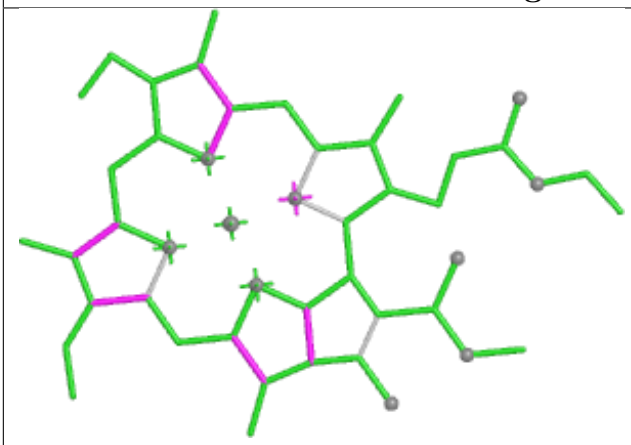


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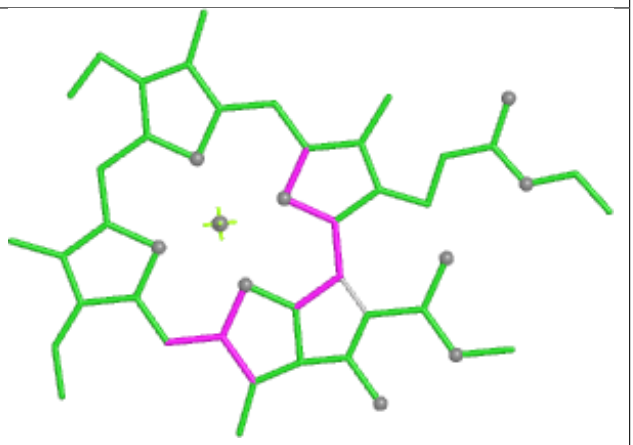


Rings

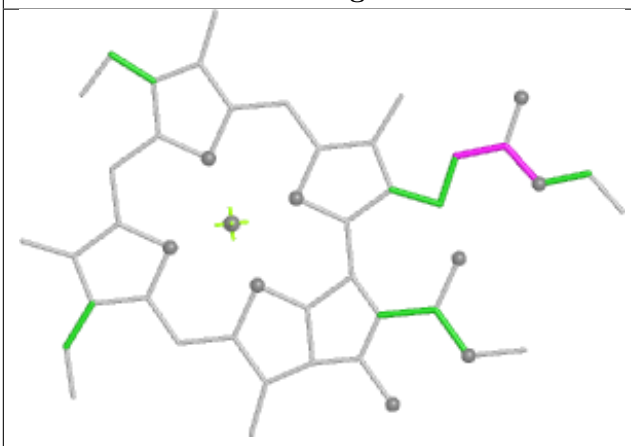
Ligand CLA B 830



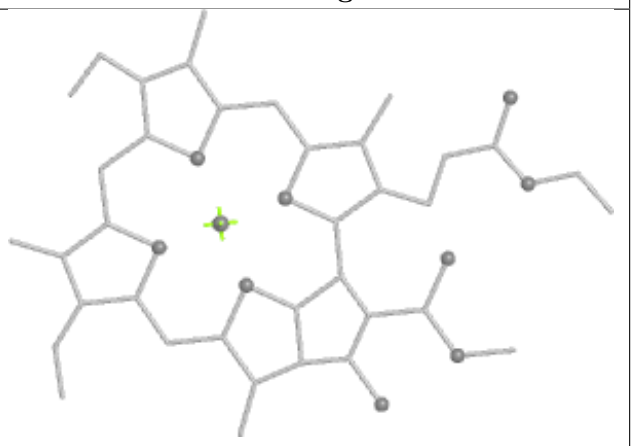
Bond lengths



Bond angles

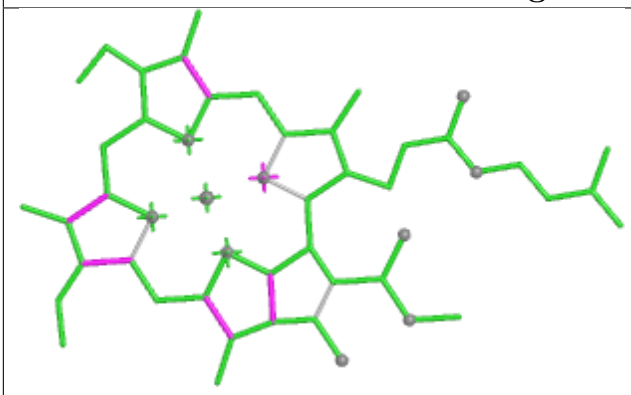


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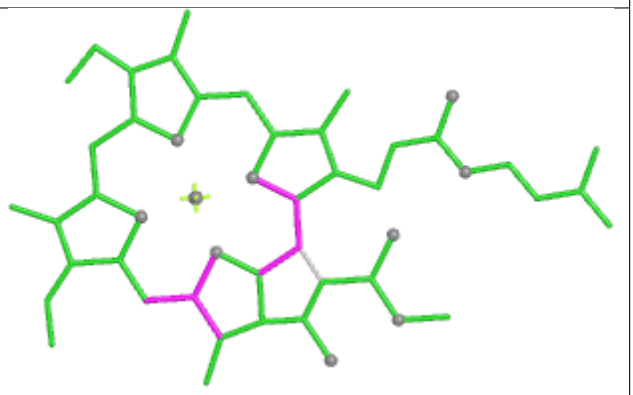


Rings

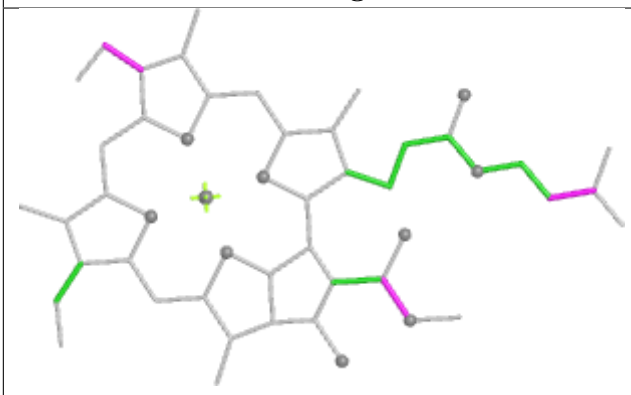
Ligand CLA a 813



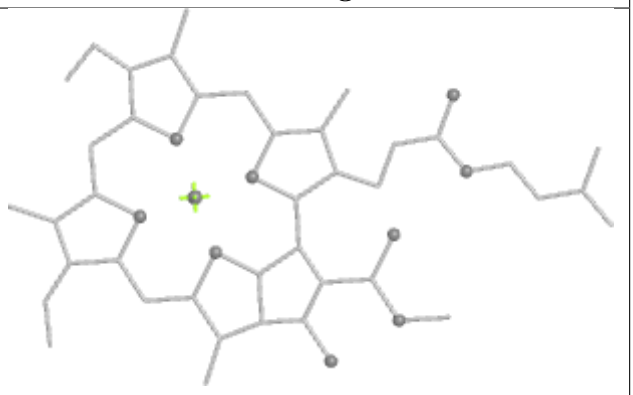
Bond lengths



Bond angles

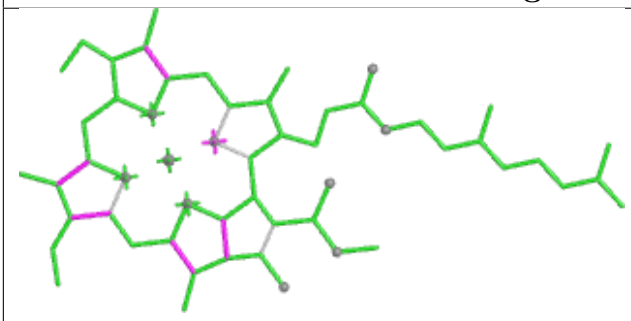


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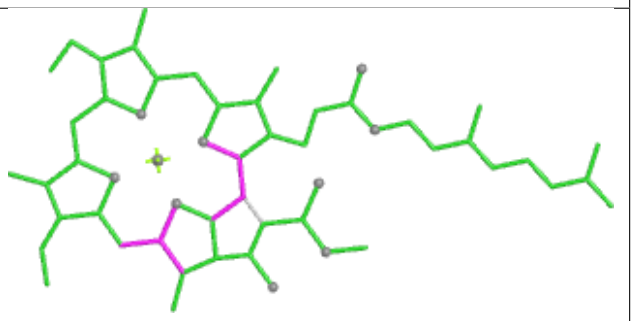


Rings

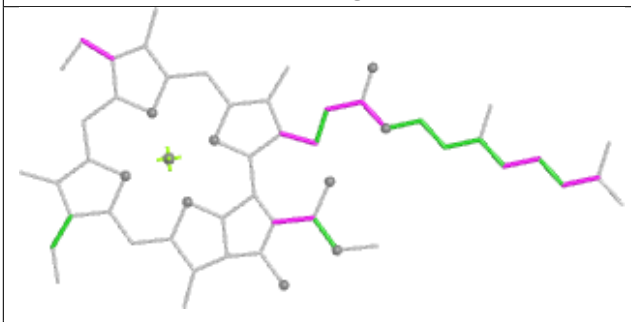
Ligand CLA A 820



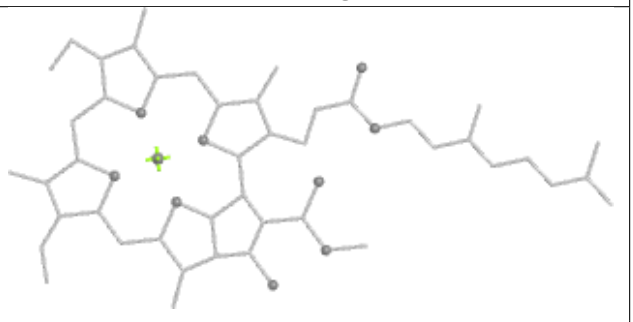
Bond lengths



Bond angles



Torsions

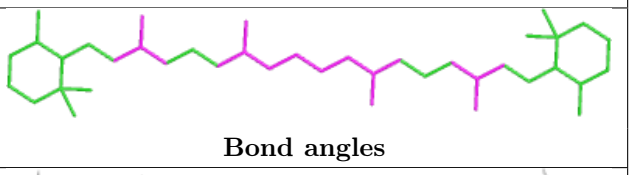


Rings

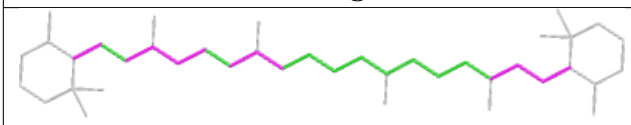
Ligand BCR B 836



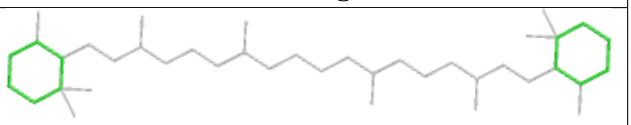
Bond lengths



Bond angles

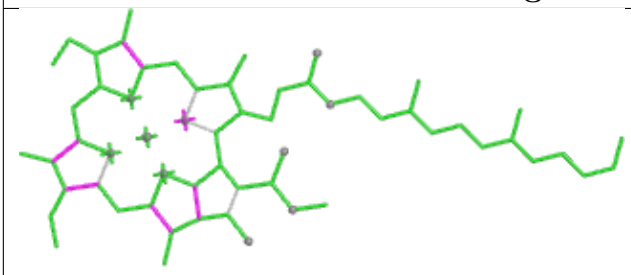


Torsions

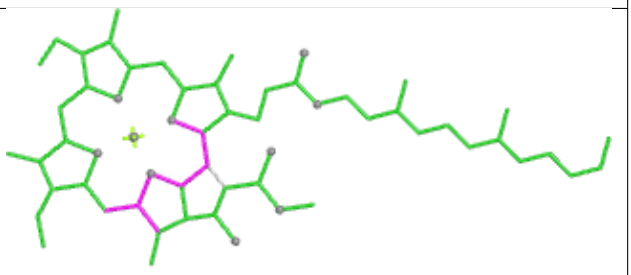


Rings

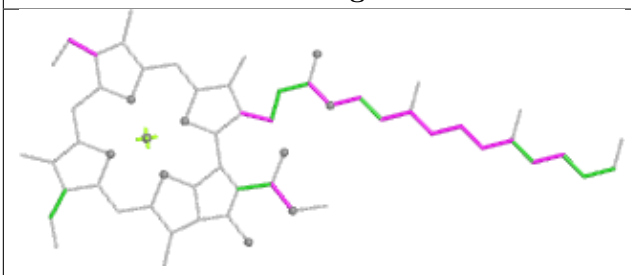
Ligand CLA B 818



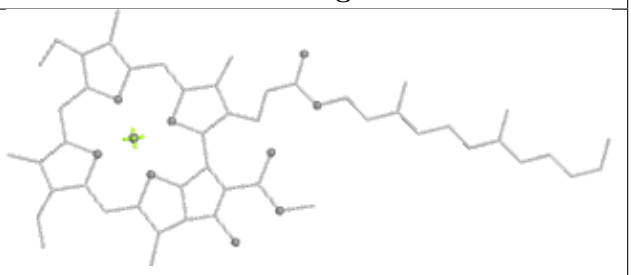
Bond lengths



Bond angles

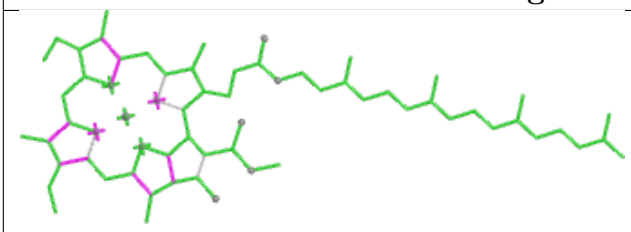


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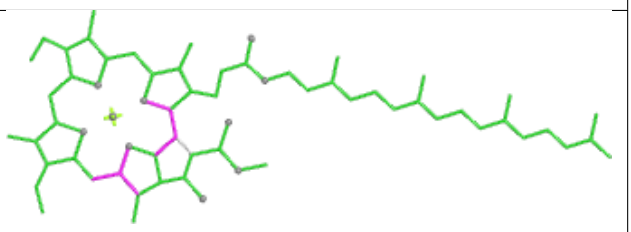


Rings

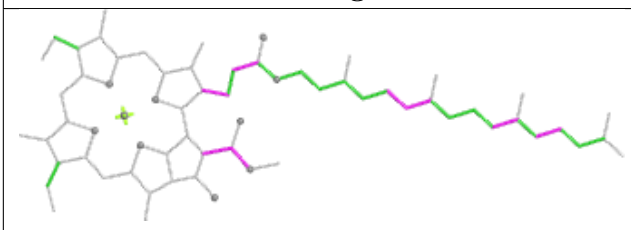
Ligand CLA b 825



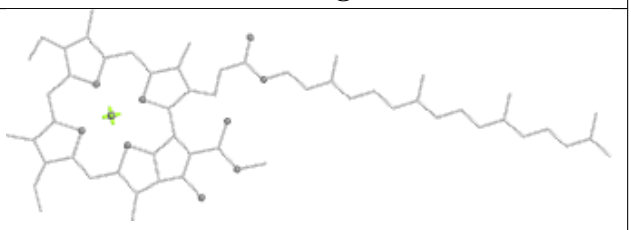
Bond lengths



Bond angles

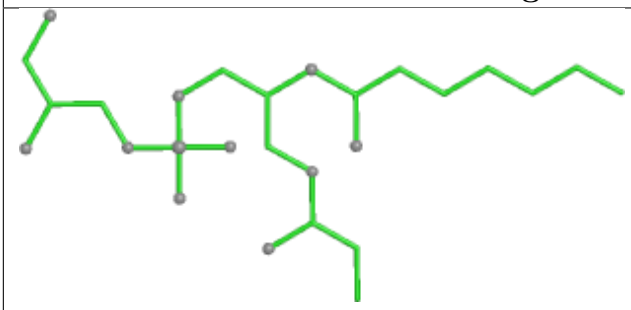


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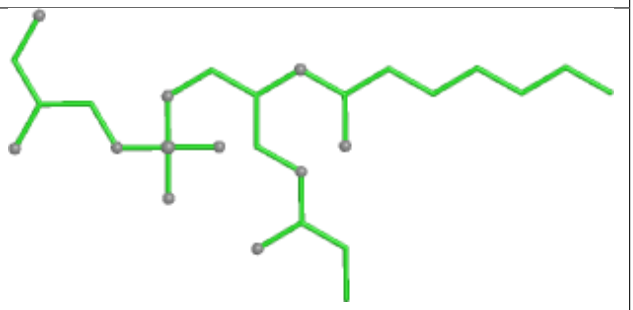


Rings

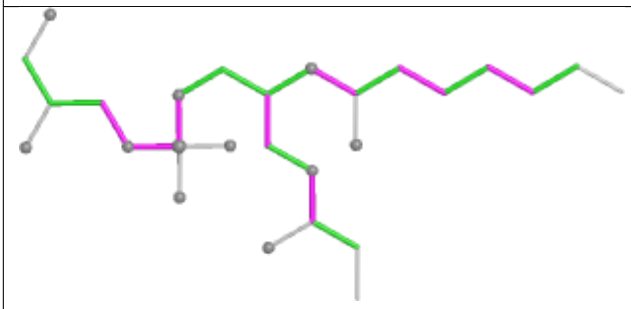
Ligand LHG A 839



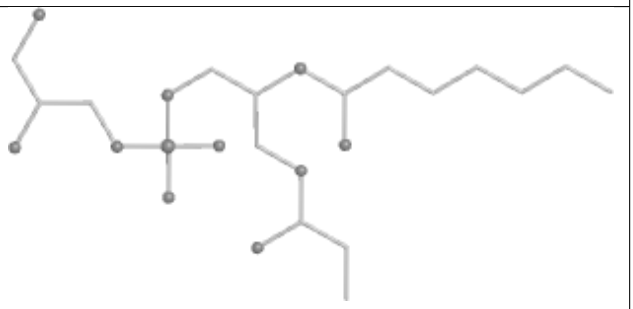
Bond lengths



Bond angles

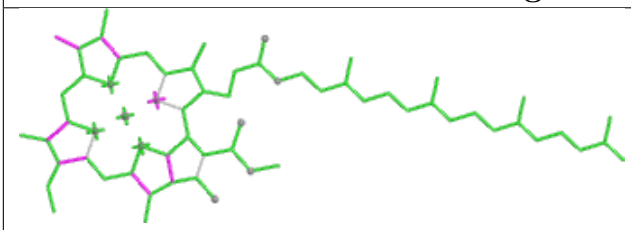


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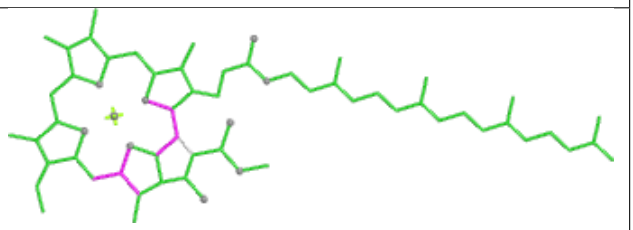


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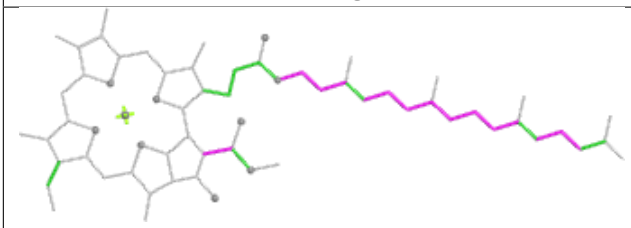
Ligand CLA B 821



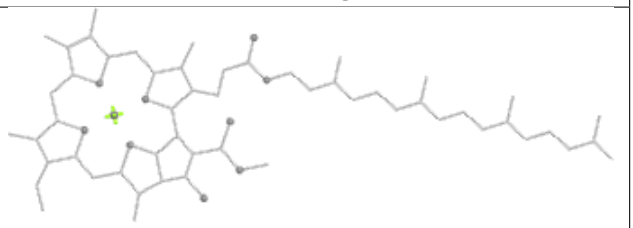
Bond lengths



Bond angles

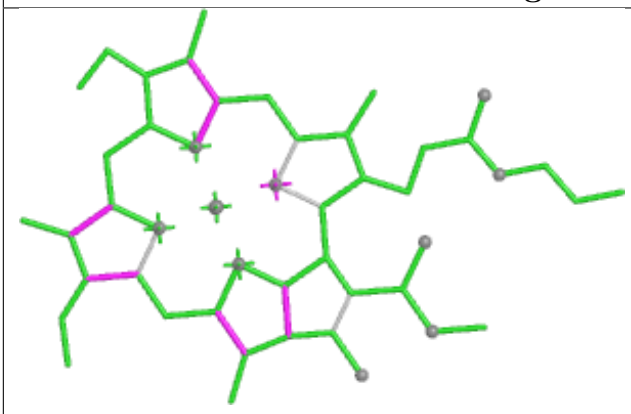


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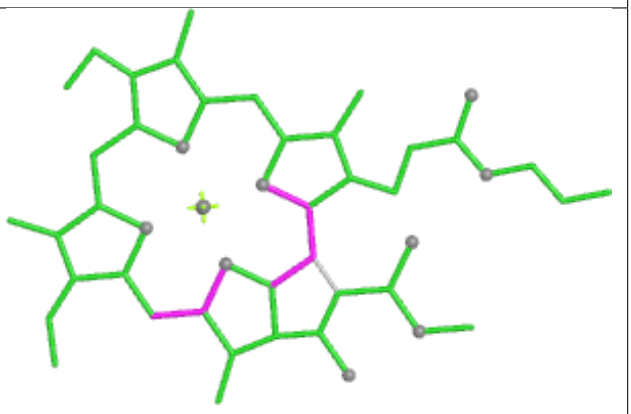


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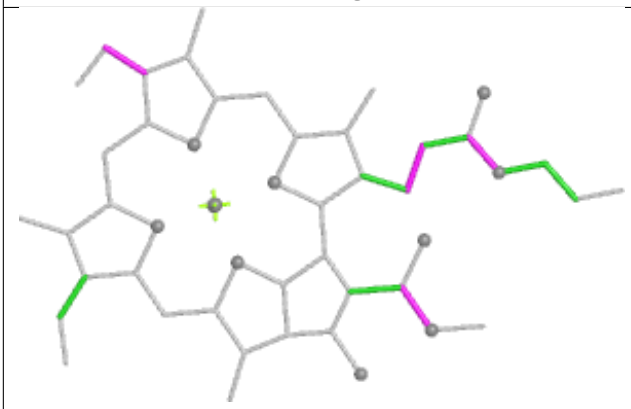
Ligand CLA B 840



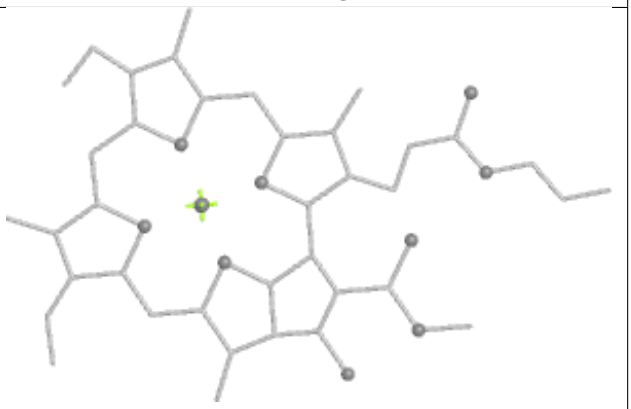
Bond lengths



Bond angles

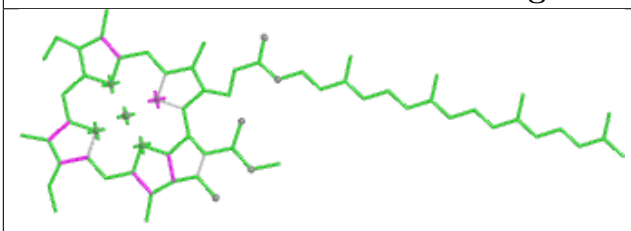


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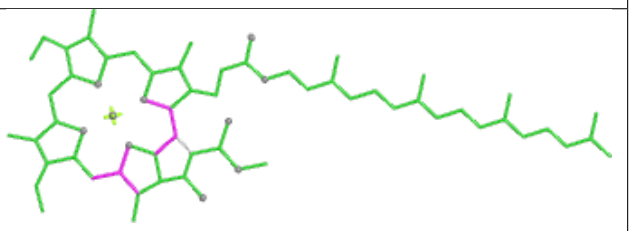


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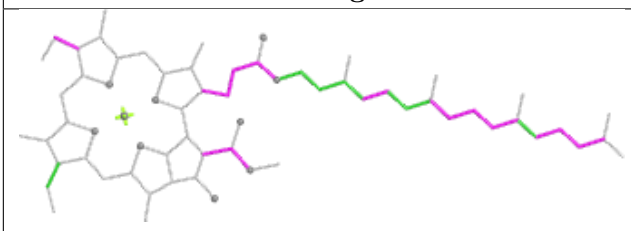
Ligand CLA a 811



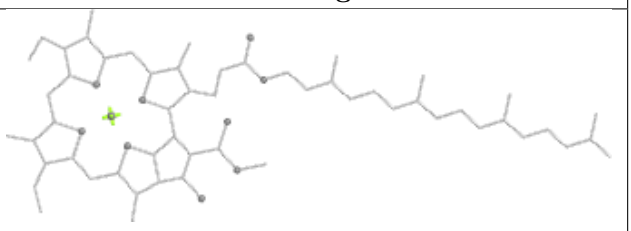
Bond lengths



Bond angles

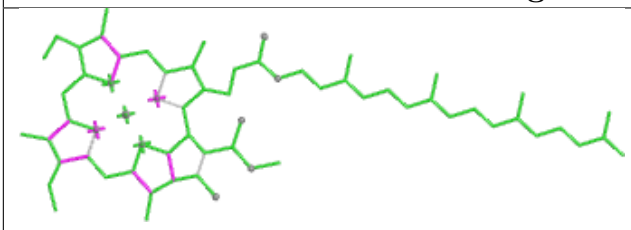


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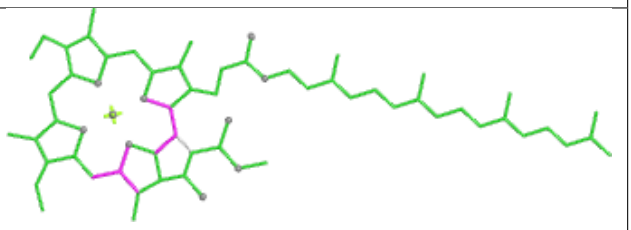


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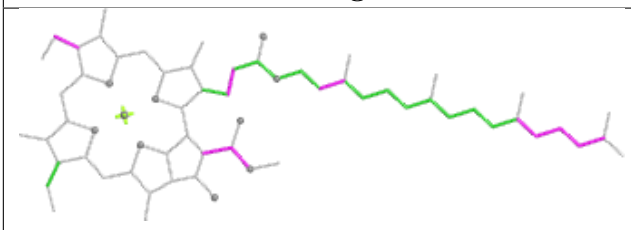
Ligand CLA b 831



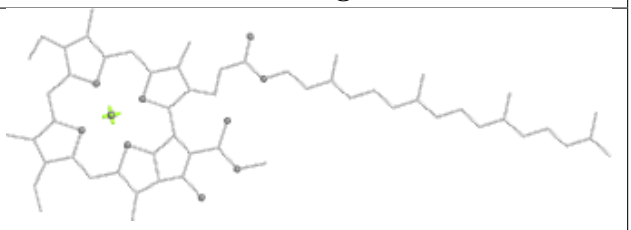
Bond lengths



Bond angles

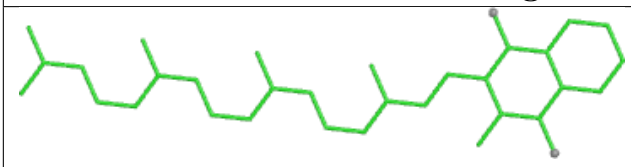


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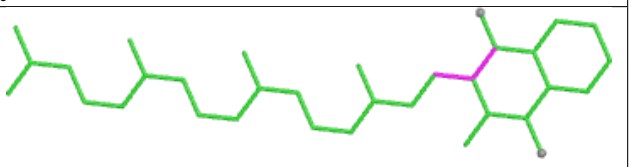


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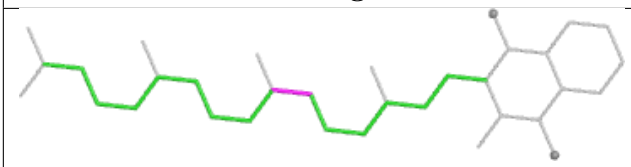
Ligand PQN B 833



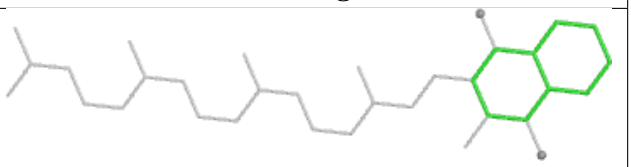
Bond lengths



Bond angles

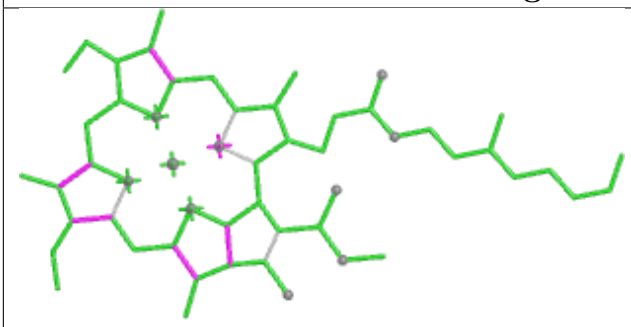


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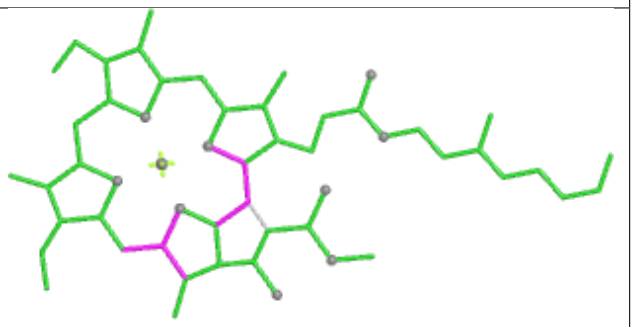


Rings

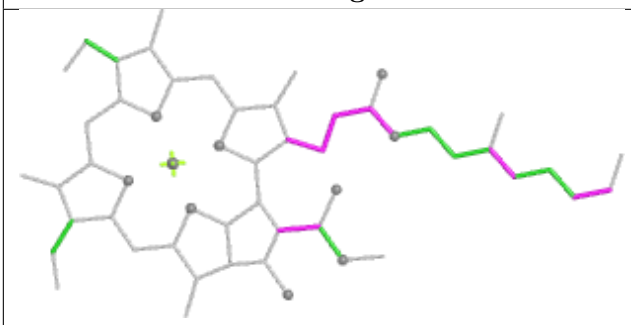
Ligand CLA A 810



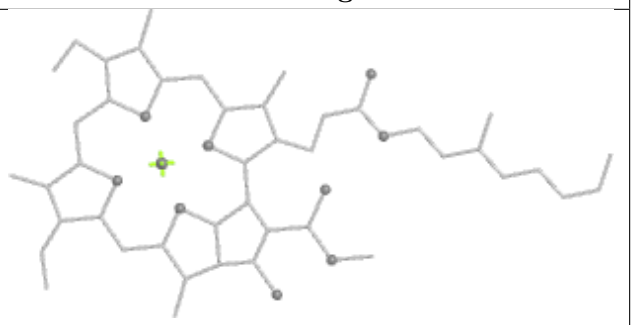
Bond lengths



Bond angles

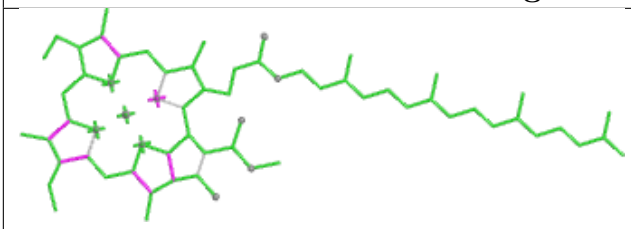


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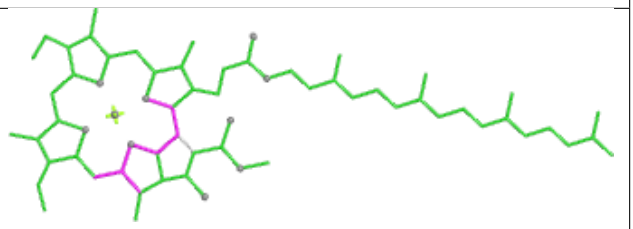


Rings

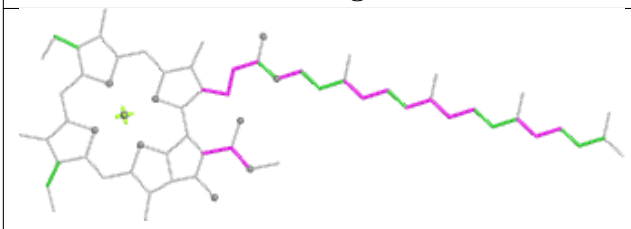
Ligand CLA A 824



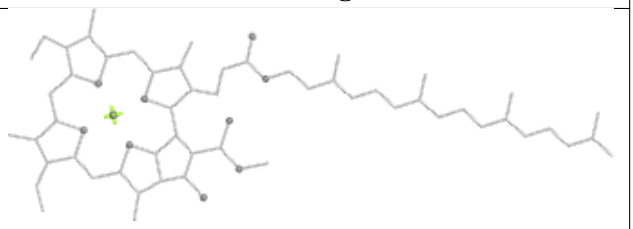
Bond lengths



Bond angles

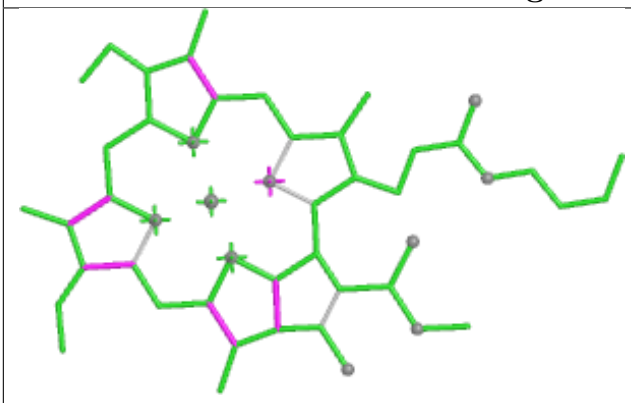


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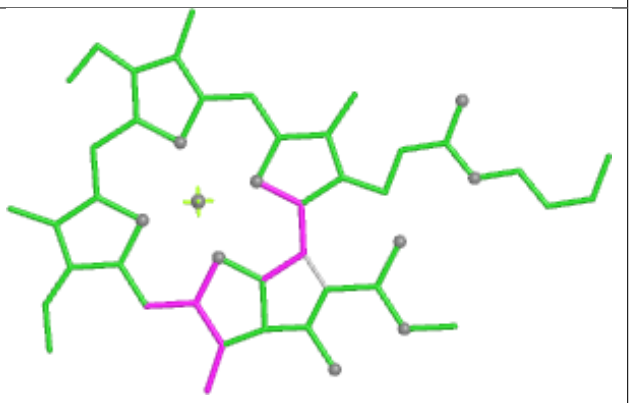


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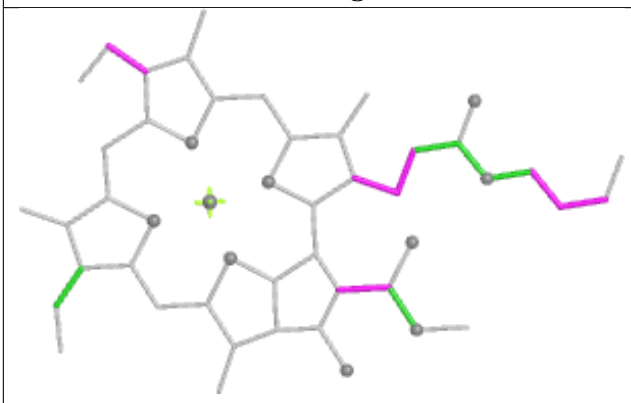
Ligand CLA L 302



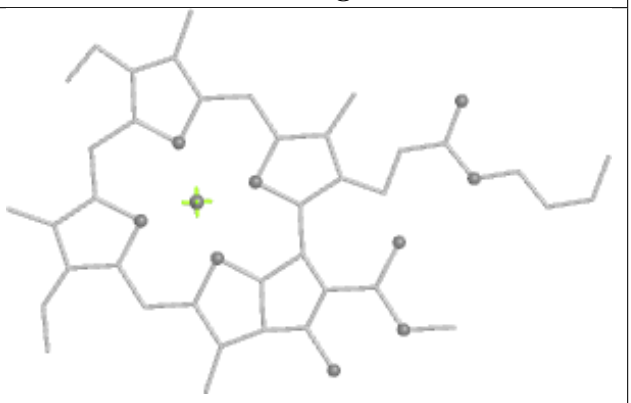
Bond lengths



Bond angles

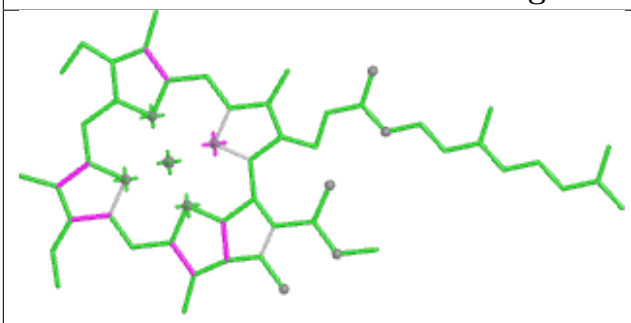


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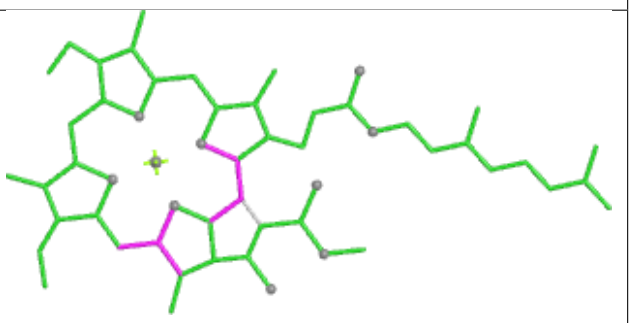


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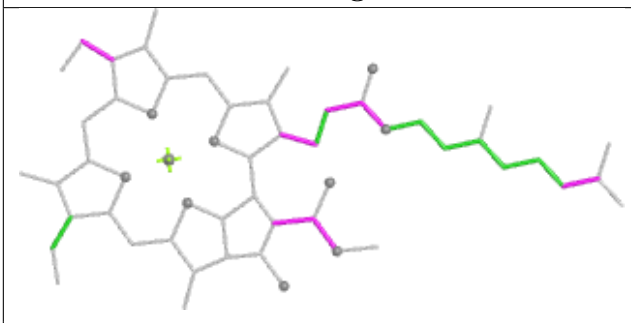
Ligand CLA a 821



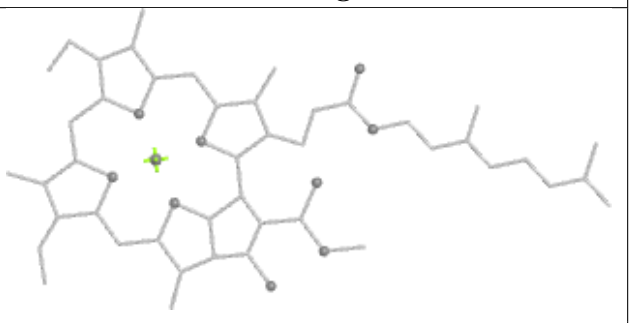
Bond lengths



Bond angles

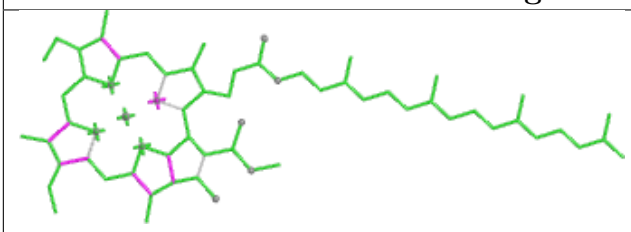


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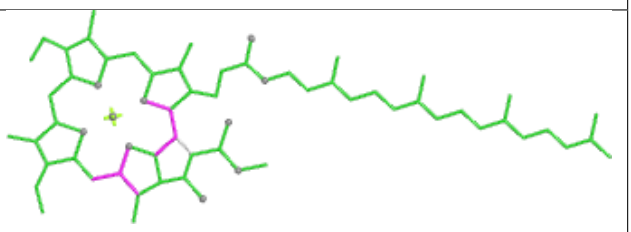


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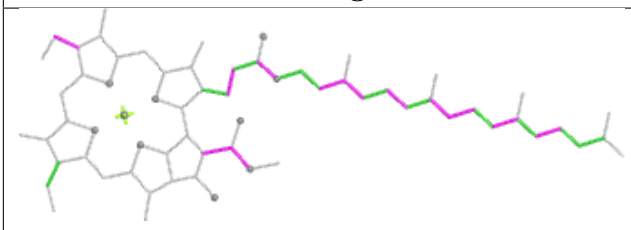
Ligand CLA B 811



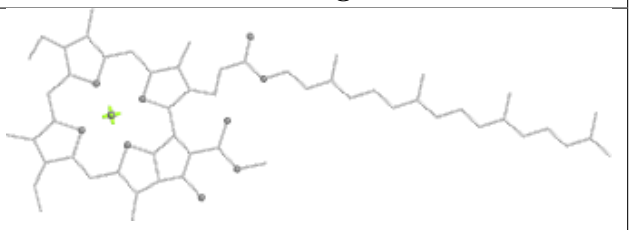
Bond lengths



Bond angles

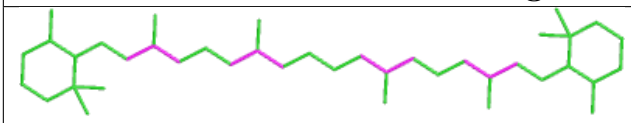


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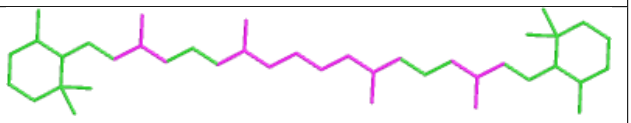


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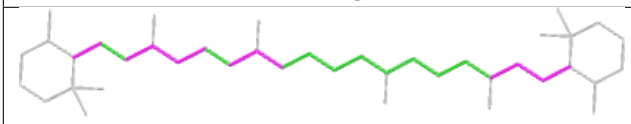
Ligand BCR b 836



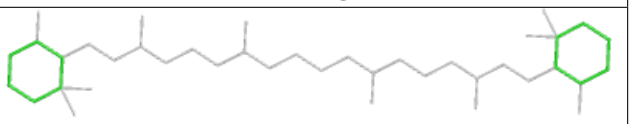
Bond lengths



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.

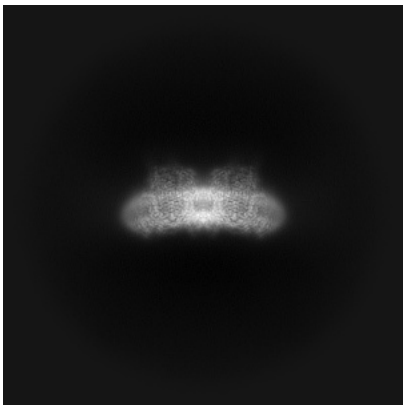
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-67061. These allow visual inspection of the internal detail of the map and identification of artifacts.

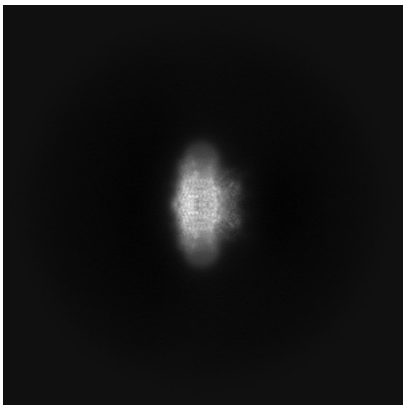
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

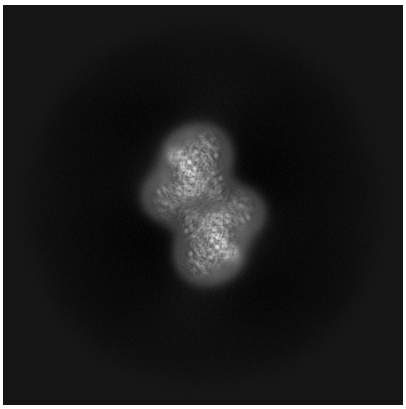
6.1.1 Primary map



X

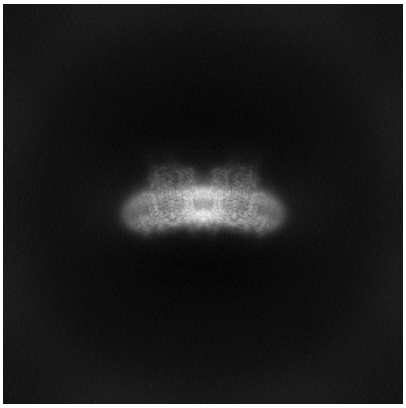


Y

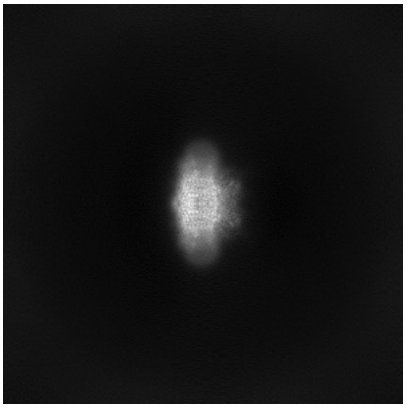


Z

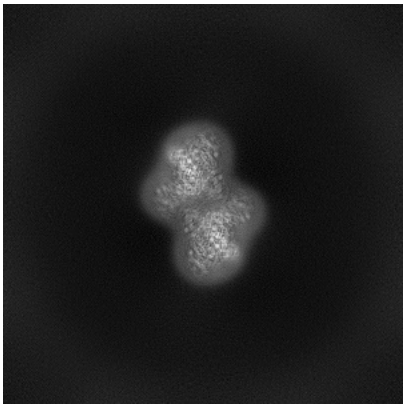
6.1.2 Raw map



X



Y

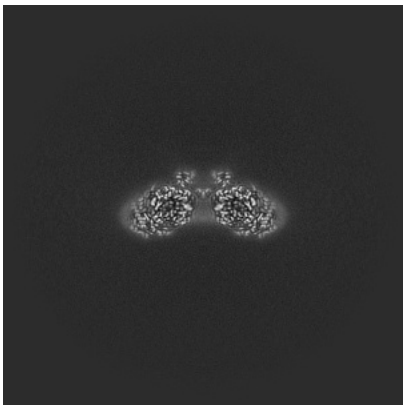


Z

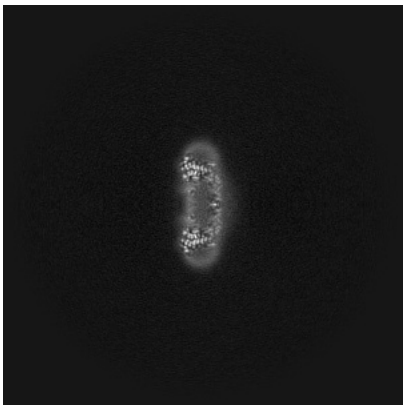
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

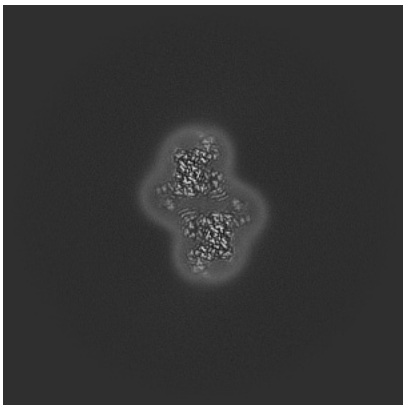
6.2.1 Primary map



X Index: 256

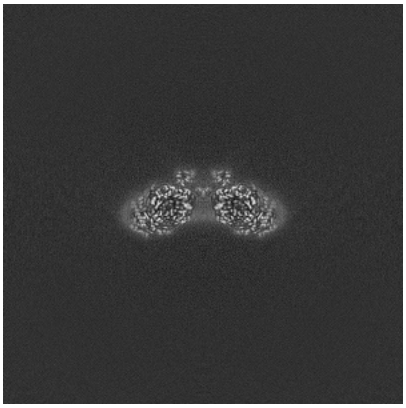


Y Index: 256

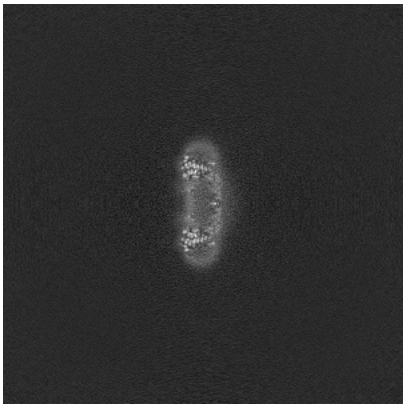


Z Index: 256

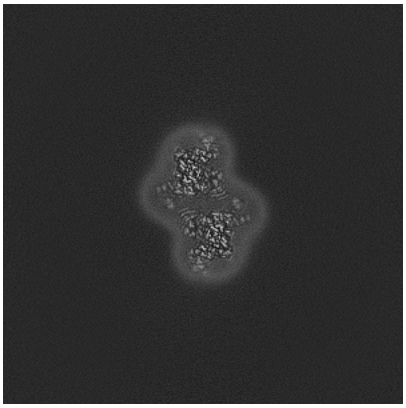
6.2.2 Raw map



X Index: 256



Y Index: 256

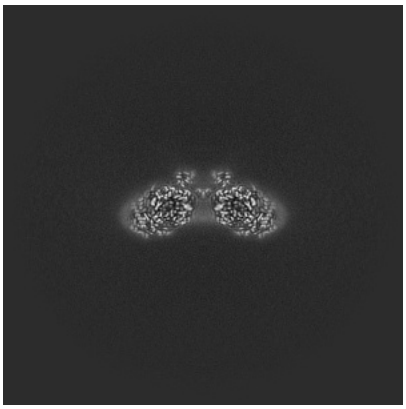


Z Index: 256

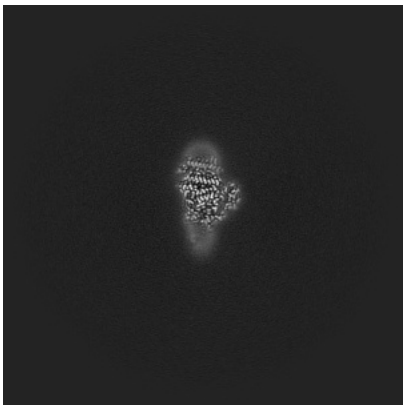
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

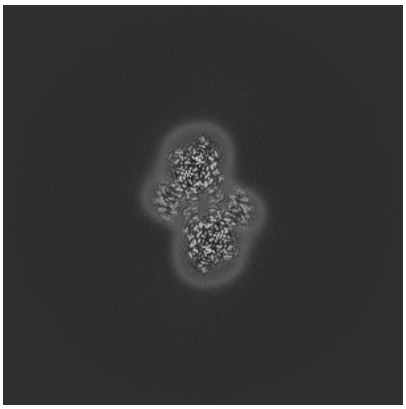
6.3.1 Primary map



X Index: 256

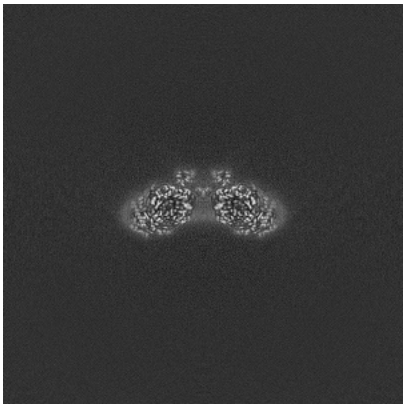


Y Index: 235

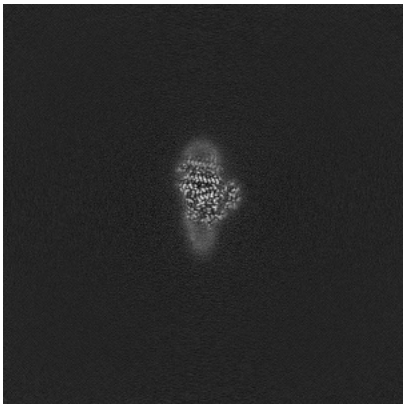


Z Index: 243

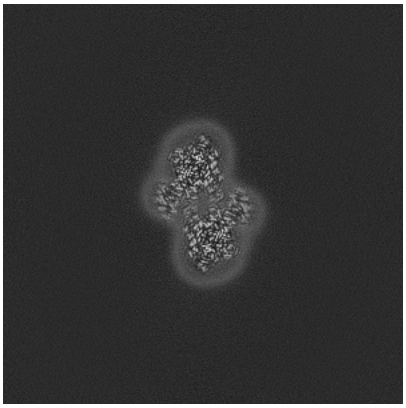
6.3.2 Raw map



X Index: 256



Y Index: 235

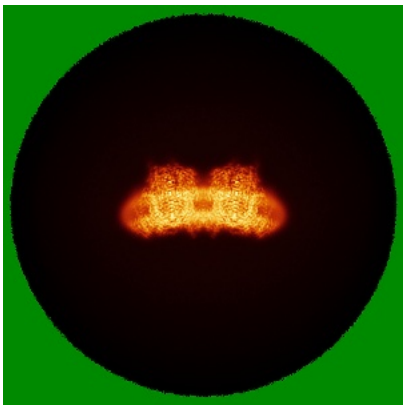


Z Index: 243

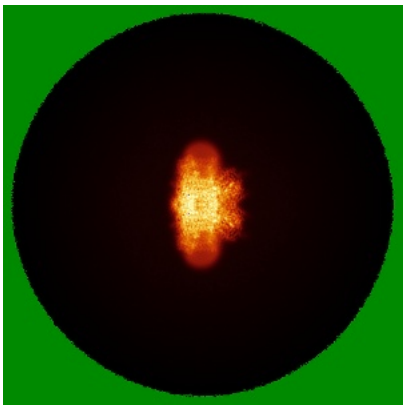
The images above show the largest variance slices of the map in three orthogonal directions.

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

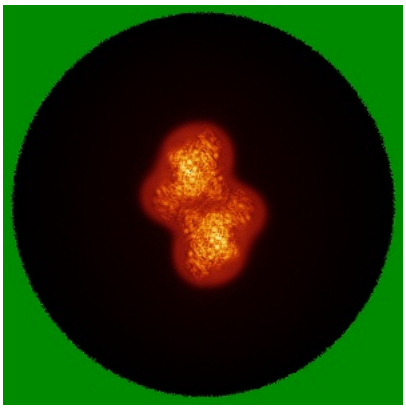
6.4.1 Primary map



X

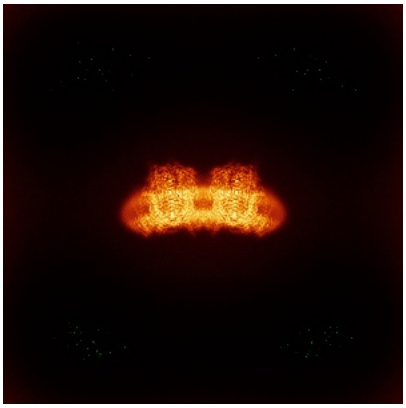


Y

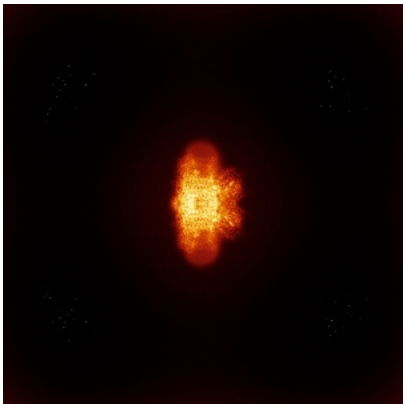


Z

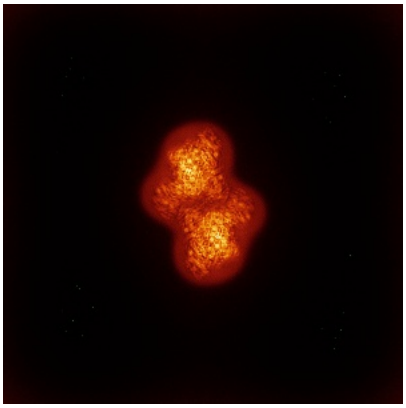
6.4.2 Raw map



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 0.0614. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

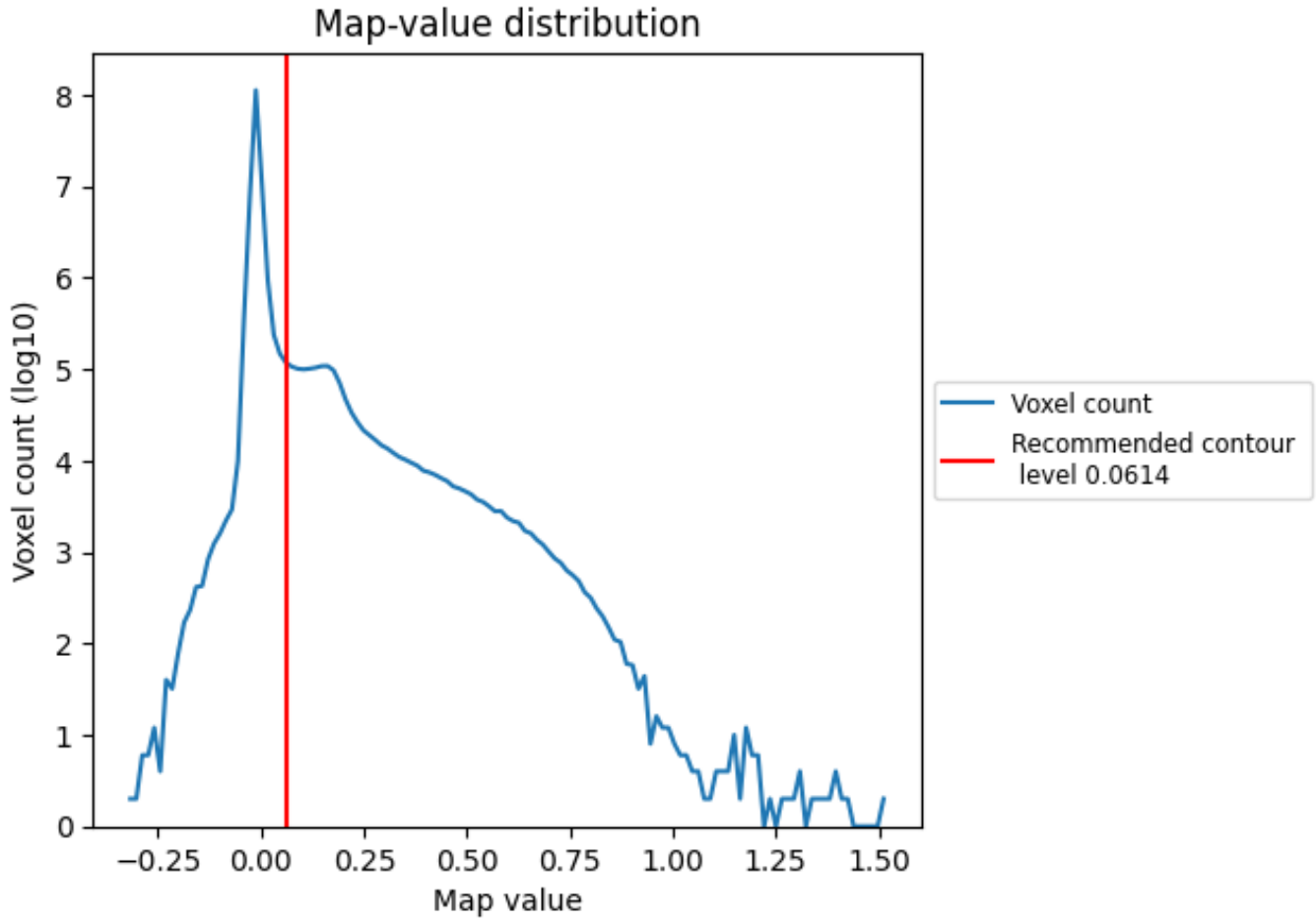
6.6 Mask visualisation (i)

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

7 Map analysis

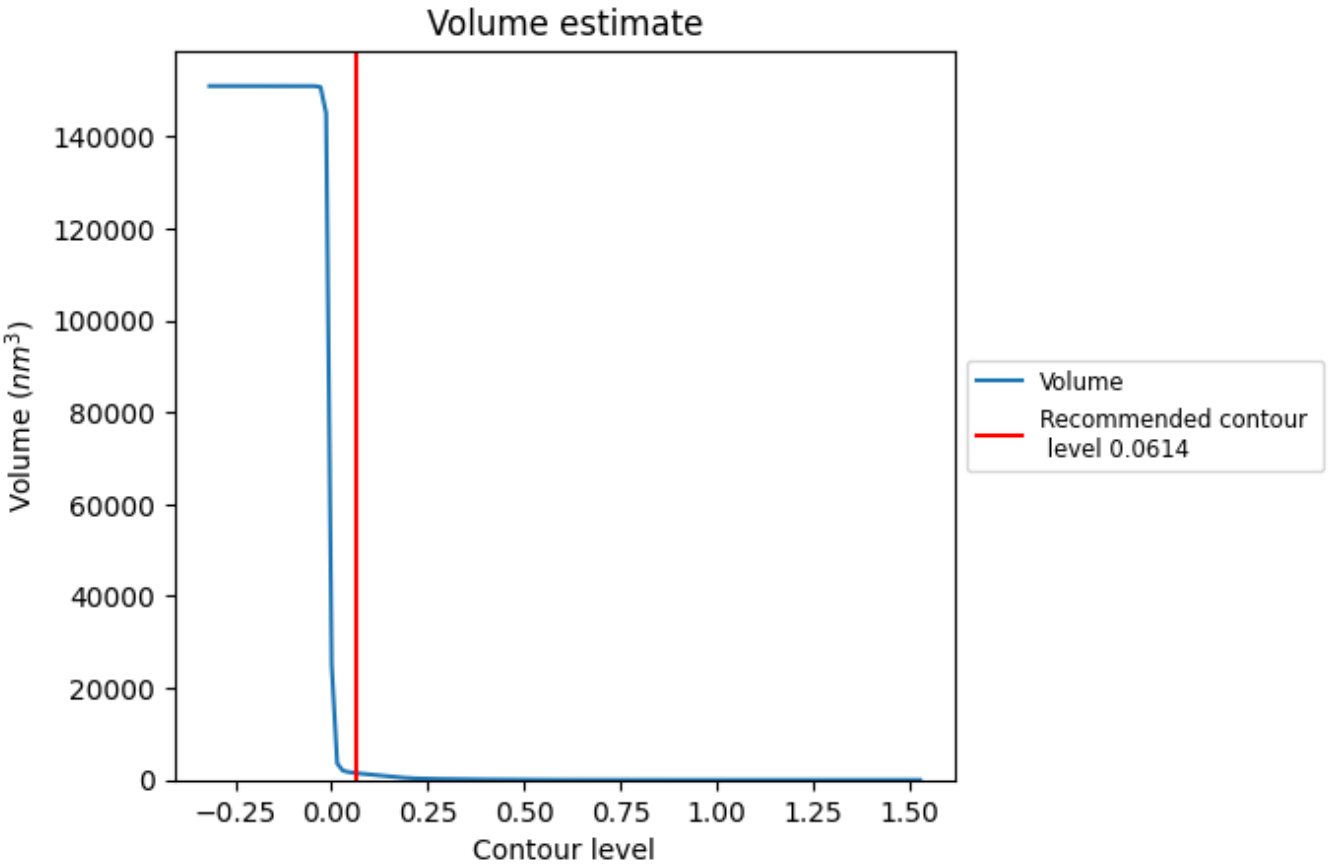
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

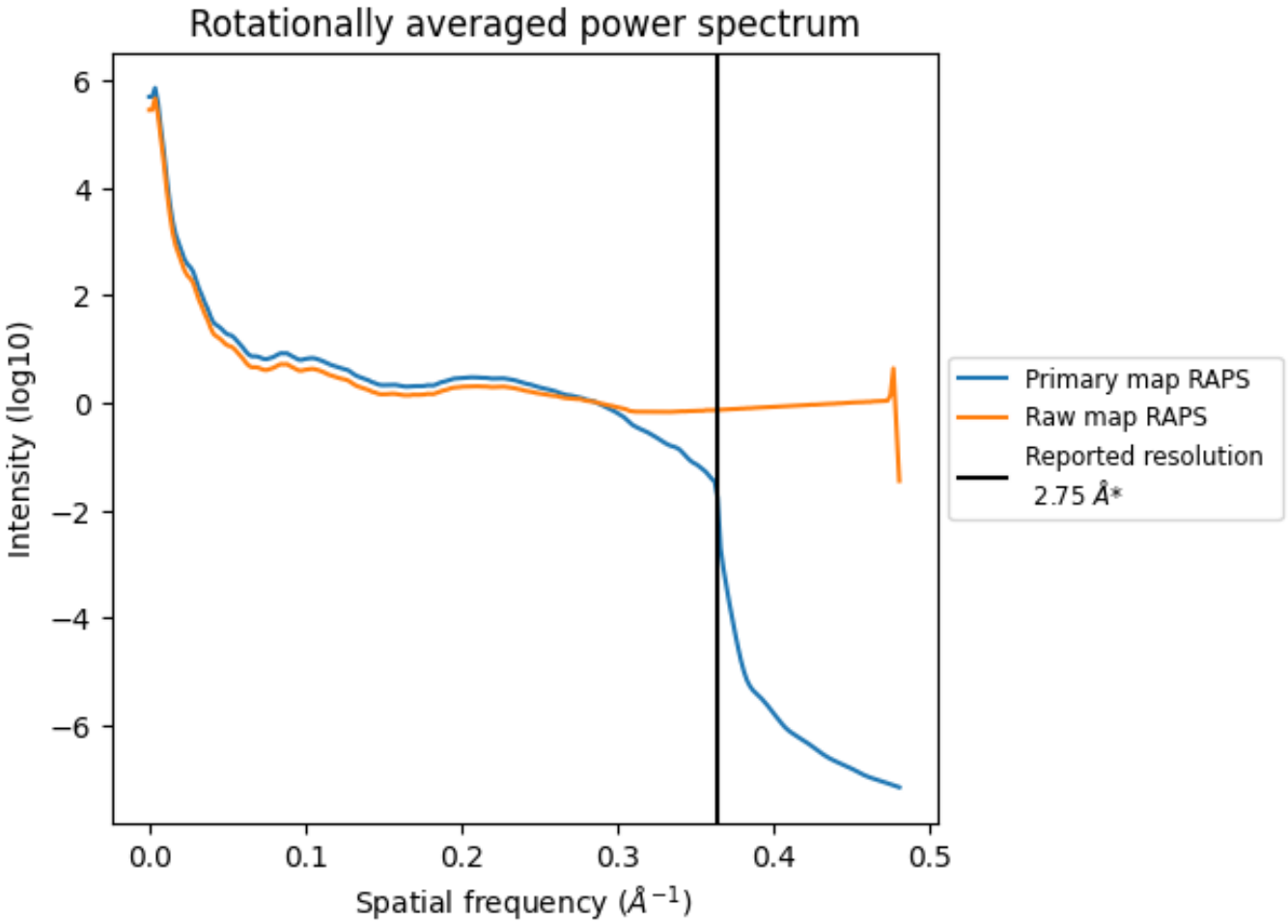
7.2 Volume estimate



The volume at the recommended contour level is 1511 nm^3; this corresponds to an approximate mass of 1365 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)

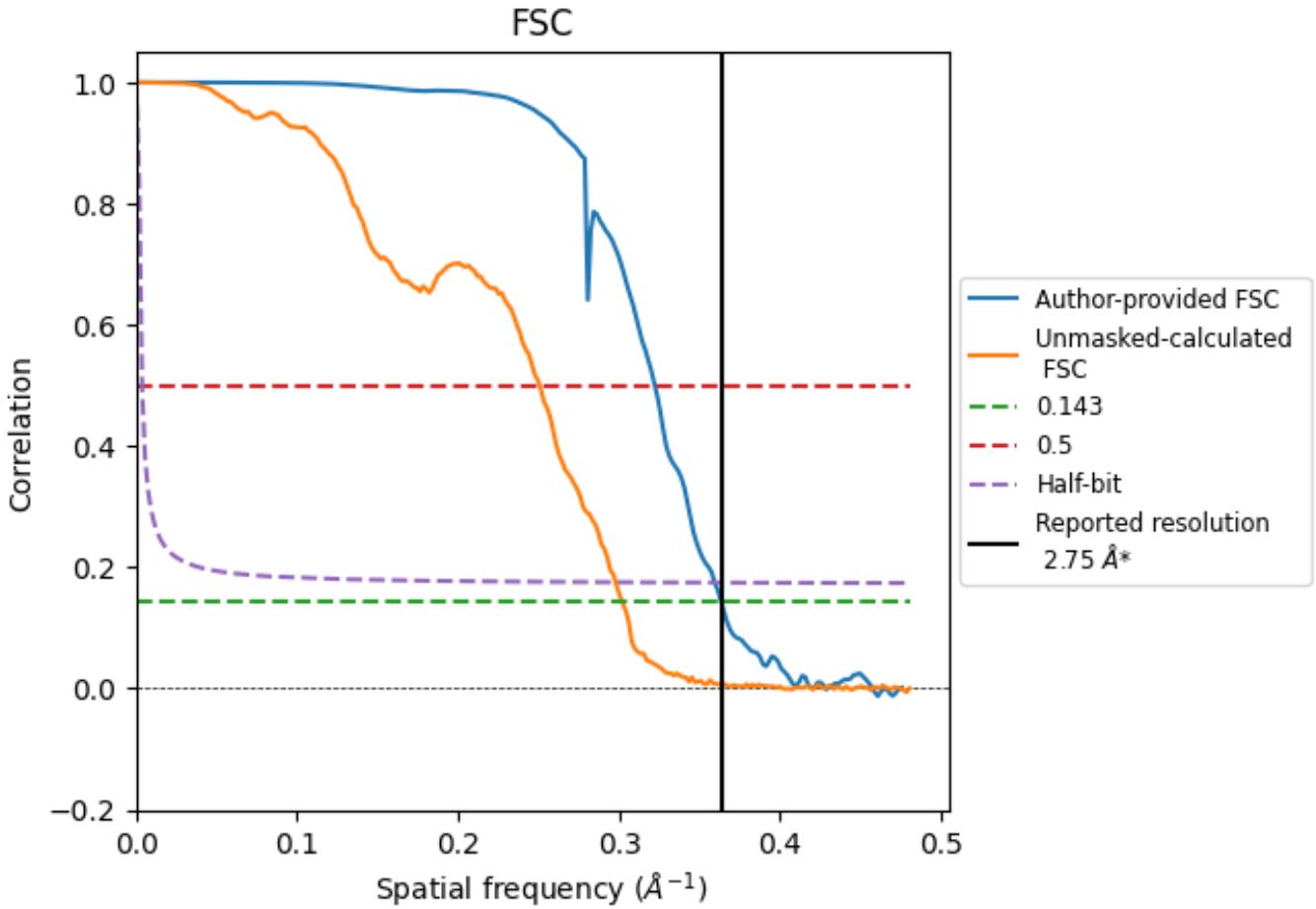


*Reported resolution corresponds to spatial frequency of 0.364 Å^{-1}

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 0.364 Å^{-1}

8.2 Resolution estimates (i)

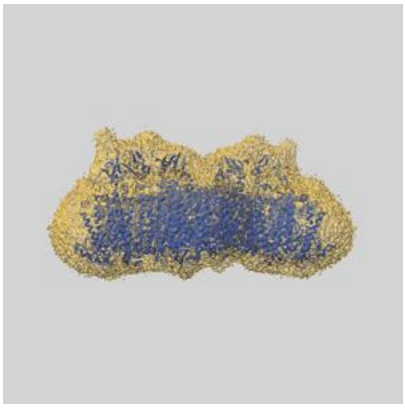
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.75	-	-
Author-provided FSC curve	2.75	3.10	2.78
Unmasked-calculated*	3.31	3.99	3.35

*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 3.31 differs from the reported value 2.75 by more than 10 %

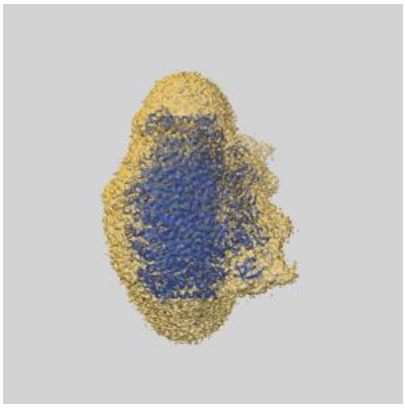
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-67061 and PDB model 9XNV. Per-residue inclusion information can be found in section 3 on page 19.

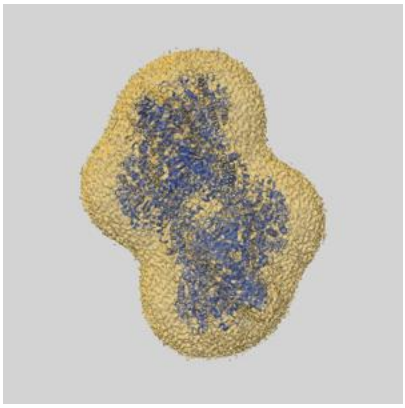
9.1 Map-model overlay



X



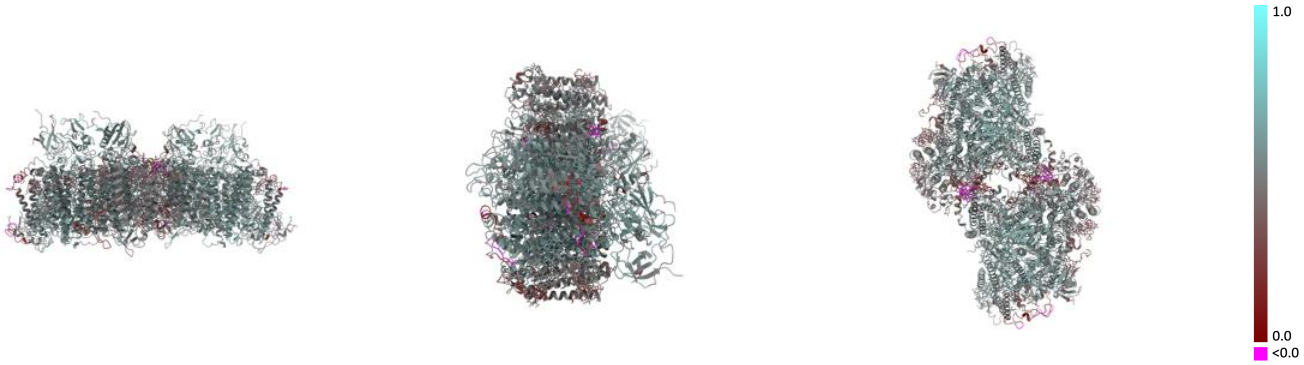
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0614 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

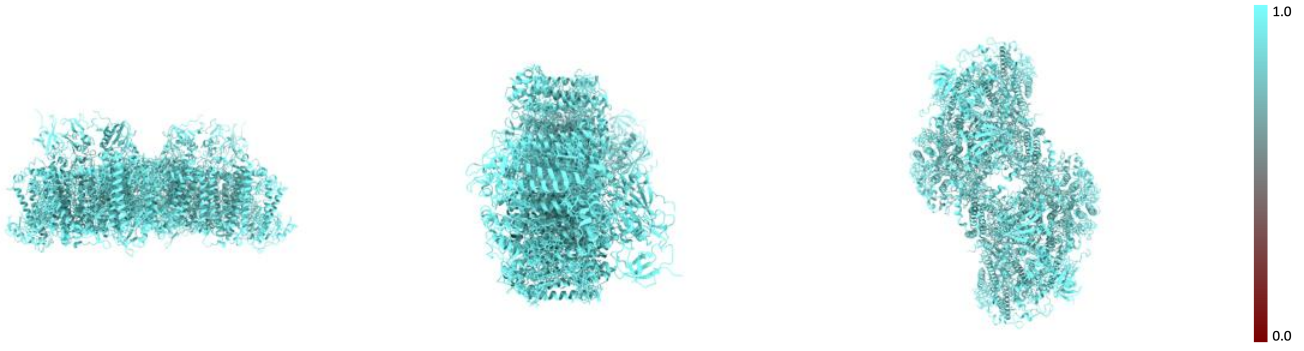
9.2 Q-score mapped to coordinate model



X Y Z

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

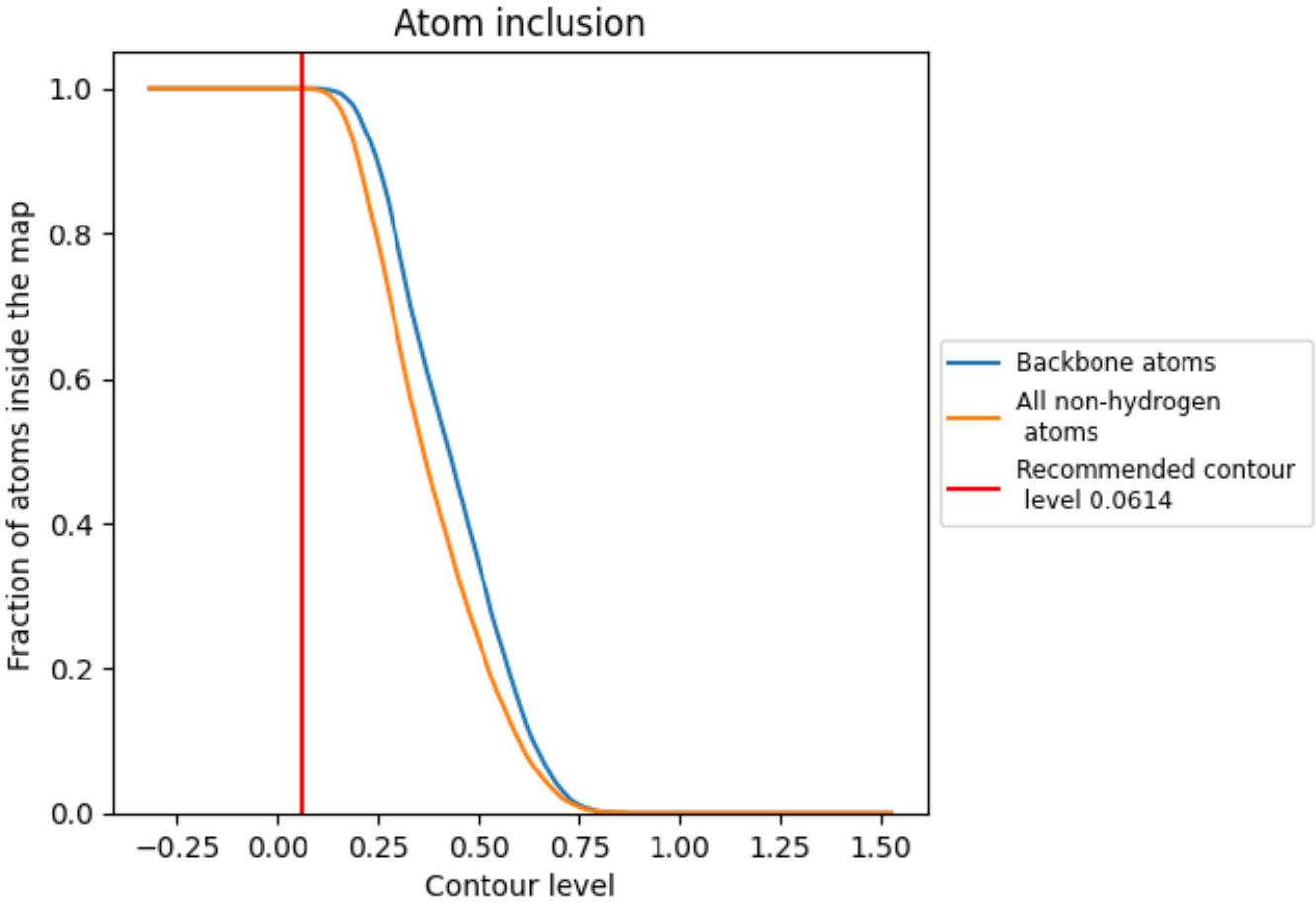
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0614).

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 (0.0614) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	1.0000	0.5160
A	1.0000	0.4900
B	1.0000	0.5410
C	1.0000	0.5670
D	1.0000	0.5660
E	1.0000	0.5280
H	1.0000	0.4870
I	1.0000	0.5450
L	0.9990	0.4810
a	1.0000	0.4890
b	1.0000	0.5420
c	1.0000	0.5690
d	1.0000	0.5620
e	1.0000	0.5280
h	1.0000	0.4580
i	1.0000	0.5470
l	0.9990	0.4700

