wwPDB EM Validation Summary Report

Nov 2, 2026 – 07:08 PM JST

PDB ID	:	9XKK / pdb_00009xkk
EMDB ID	:	EMD-66967
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	:	2025-11-05
Resolution	:	2.50 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:

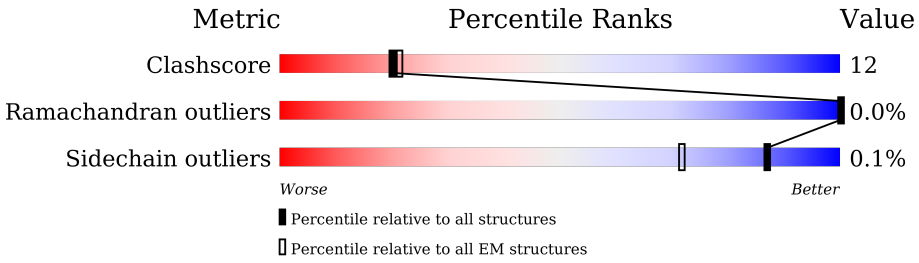
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

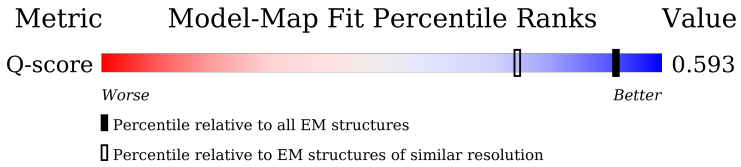
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	75% 25%
2	B	733	79% 21%
3	C	80	84% 16%
4	E	65	91% 9%

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Mol	Chain	Length	Quality of chain
5	H	95	
6	I	35	
7	L	159	
8	D	142	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 21338 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
			Total	C	N	O	S		
1	A	708	5564	3650	944	952	18	0	0

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

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

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

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

- Molecule 4 is a protein called PsaE.

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

- Molecule 5 is a protein called PsaH.

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

- Molecule 6 is a protein called Photosystem I reaction center subunit VIII.

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

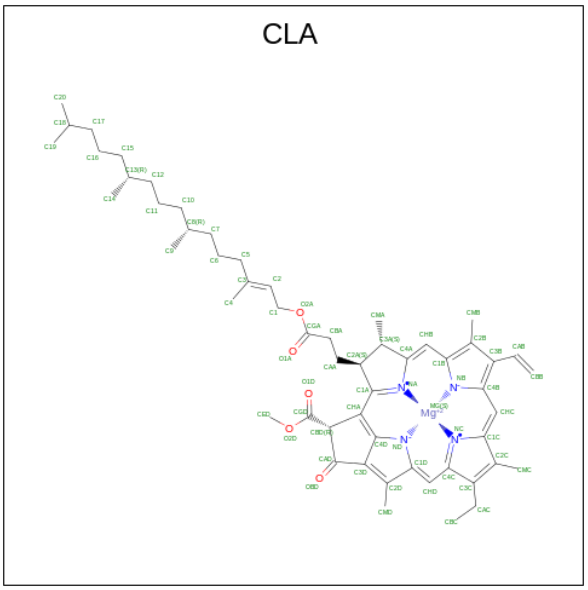
- Molecule 7 is a protein called PsaL.

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

- Molecule 8 is a protein called PsaD.

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

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
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	

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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
			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
			49	39	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
			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	

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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
			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
			45	35	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
			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	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	

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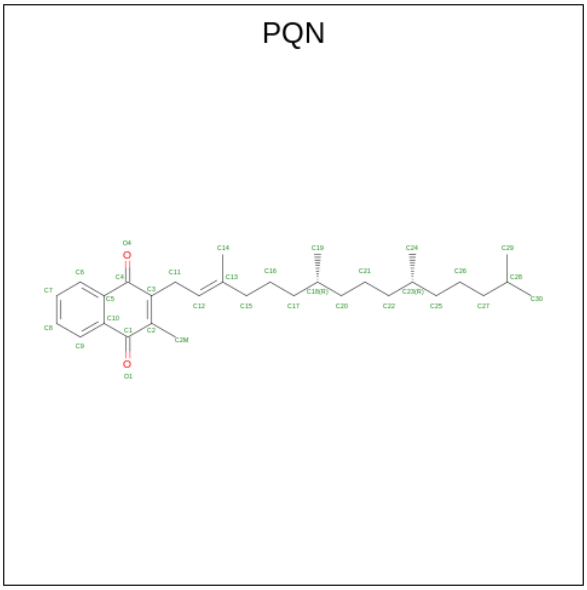
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			44	34	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	
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	

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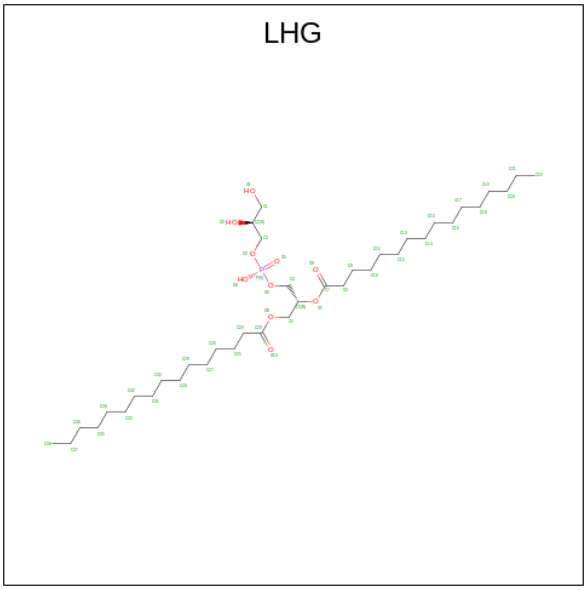
Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
9	B	1	Total	C	Mg	N	O	0
			48	38	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	

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



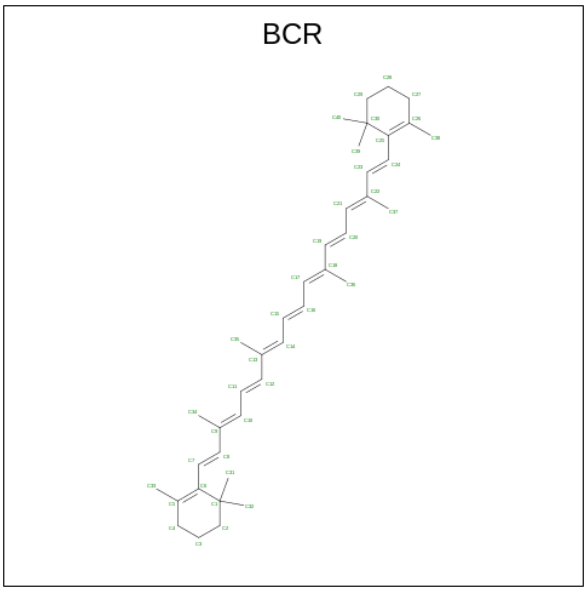
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			33	31	2	
10	B	1	Total	C	O	0
			33	31	2	

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



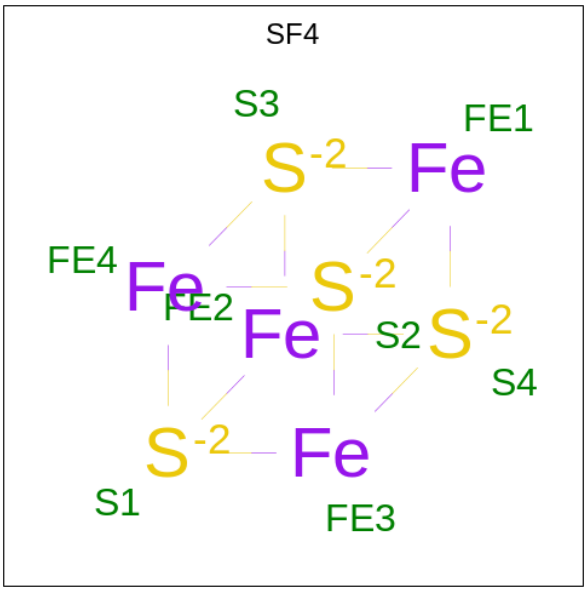
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			49	38	10	1	
11	A	1	Total	C	O	P	0
			27	16	10	1	
11	L	1	Total	C	O	P	0
			49	38	10	1	

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



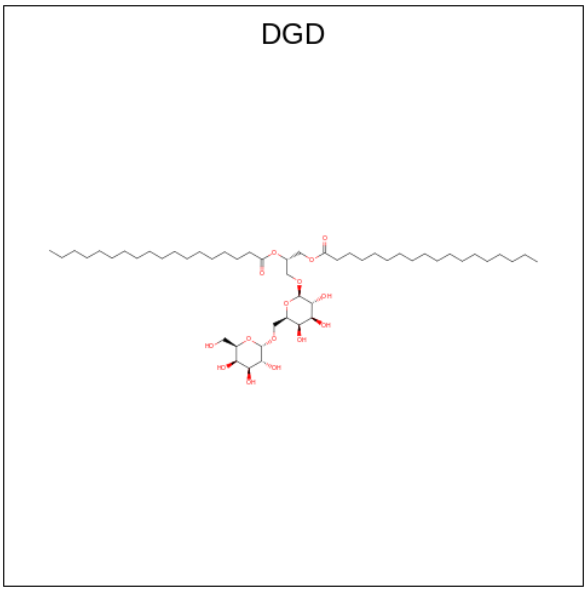
Mol	Chain	Residues	Atoms	AltConf
12	A	1	Total C 40 40	0
12	A	1	Total C 40 40	0
12	A	1	Total C 40 40	0
12	A	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	B	1	Total C 40 40	0
12	I	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C 40 40	0
12	L	1	Total C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

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



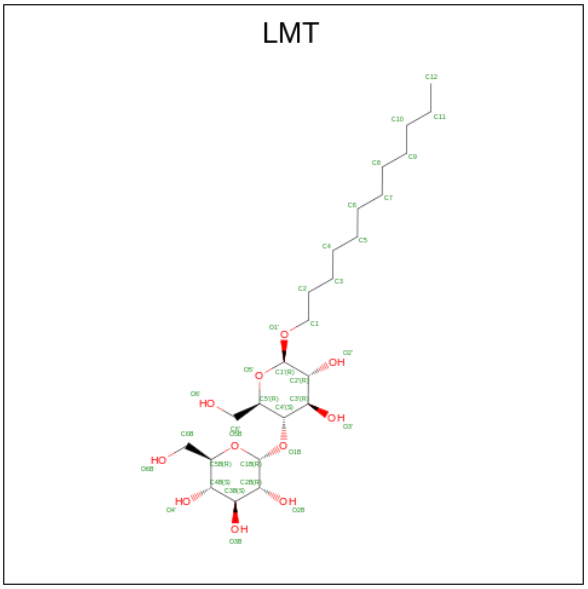
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Fe	S	0
			8	4	4	
13	C	1	Total	Fe	S	0
			8	4	4	
13	C	1	Total	Fe	S	0
			8	4	4	

- 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	

- 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	

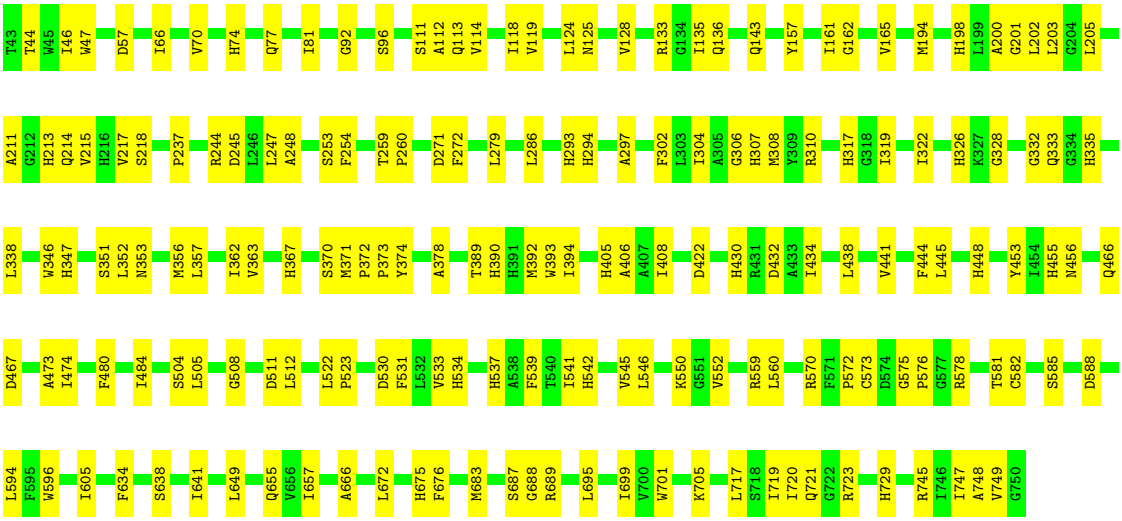
3 Residue-property plots (i)

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:

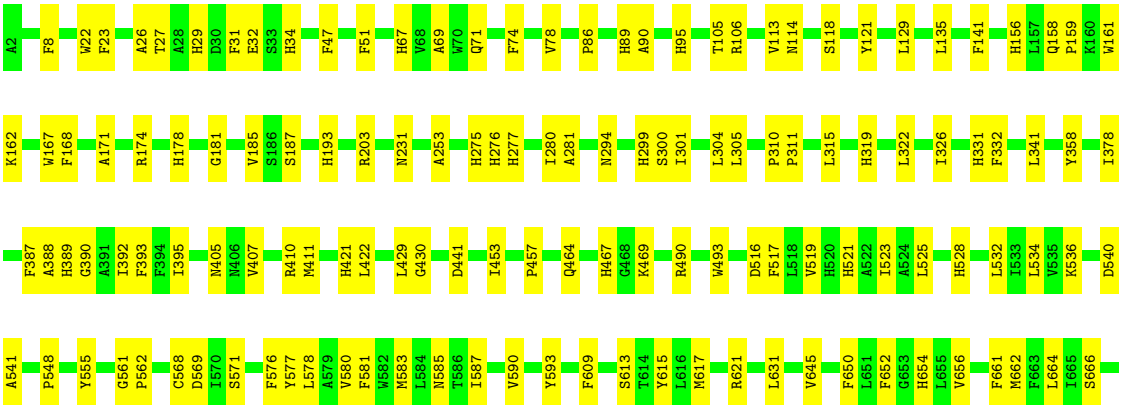


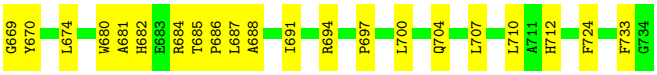


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:







• Molecule 3: Photosystem I iron-sulfur center

Chain C:

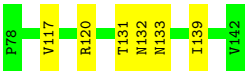




• Molecule 4: PsaE

Chain E:

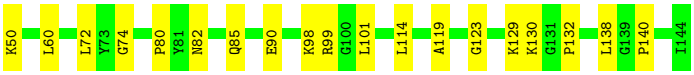




• Molecule 5: PsaH

Chain H:

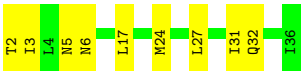




• Molecule 6: Photosystem I reaction center subunit VIII

Chain I:



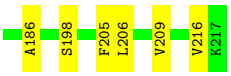


• Molecule 7: PsaL

Chain L:



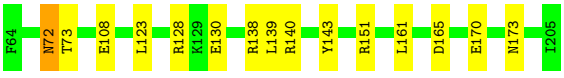




• Molecule 8: PsaD

Chain D:





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	1.681	Depositor
Minimum map value	-0.385	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.0233	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: PQN, BCR, SF4, LHG, DGD, 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	0.14	0/5754	0.30	0/7852
2	B	0.14	0/6063	0.29	0/8280
3	C	0.15	0/630	0.31	0/853
4	E	0.11	0/537	0.24	0/728
5	H	0.13	0/748	0.28	0/1014
6	I	0.19	0/272	0.35	0/371
7	L	0.17	0/1218	0.35	0/1664
8	D	0.12	0/1159	0.29	0/1565
All	All	0.14	0/16381	0.30	0/22327

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	160	0
2	B	5851	0	5636	149	0
3	C	617	0	592	13	0
4	E	525	0	526	4	0
5	H	727	0	734	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	267	0	296	7	0
7	L	1185	0	1199	40	0
8	D	1129	0	1134	11	0
9	A	2482	0	2502	124	0
9	B	1966	0	1928	129	0
9	H	65	0	72	2	0
9	L	164	0	150	11	0
10	A	33	0	46	5	0
10	B	33	0	46	4	0
11	A	76	0	98	2	0
11	L	49	0	74	9	0
12	A	160	0	224	10	0
12	B	120	0	168	7	0
12	I	40	0	56	2	0
12	L	160	0	224	15	0
13	A	8	0	0	0	0
13	C	16	0	0	2	0
14	B	66	0	96	8	0
15	B	35	0	45	3	0
All	All	21338	0	21264	523	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 523 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)
1:A:405:HIS:HE1	9:A:828:CLA:NA	1.70	0.89
1:A:390:HIS:HE1	9:A:826:CLA:ND	1.74	0.86
1:A:96:SER:HA	1:A:112:ALA:HB3	1.63	0.80
1:A:550:LYS:NZ	2:B:670:TYR:O	2.14	0.80
9:A:849:CLA:HBB1	9:B:802:CLA:C4B	2.11	0.78

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%)	681 (96%)	24 (3%)	1 (0%)	48	68
2	B	731/733 (100%)	713 (98%)	18 (2%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	E	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
5	H	93/95 (98%)	92 (99%)	1 (1%)	0	100	100
6	I	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
7	L	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
8	D	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
All	All	2001/2017 (99%)	1941 (97%)	59 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	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%)	571 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	71/71 (100%)	71 (100%)	0	100	100
4	E	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	H	77/77 (100%)	77 (100%)	0	100 100
6	I	31/31 (100%)	31 (100%)	0	100 100
7	L	123/123 (100%)	123 (100%)	0	100 100
8	D	121/121 (100%)	120 (99%)	1 (1%)	73 88
All	All	1648/1648 (100%)	1647 (100%)	1 (0%)	87 96

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

Mol	Chain	Res	Type
8	D	72	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	248	GLN
2	B	294	ASN
8	D	181	GLN
2	B	328	ASN
1	A	439	ASN

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)

102 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	$\#\|Z\| > 2$
12	BCR	A	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	10 (17%)
9	CLA	B	829	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	8 (9%)
9	CLA	A	819	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	8 (9%)
9	CLA	A	825	1	69,73,73	1.25	10 (14%)	83,113,113	1.30	6 (7%)
9	CLA	B	839	2	52,56,73	1.44	9 (17%)	62,92,113	1.36	7 (11%)
9	CLA	A	828	1	69,73,73	1.26	9 (13%)	83,113,113	1.28	7 (8%)
9	CLA	A	814	-	49,53,73	1.49	9 (18%)	59,89,113	1.44	5 (8%)
9	CLA	B	826	2	52,56,73	1.44	7 (13%)	62,92,113	1.41	7 (11%)
9	CLA	A	824	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	8 (9%)
12	BCR	B	835	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
9	CLA	A	801	1	69,73,73	1.24	9 (13%)	83,113,113	1.23	6 (7%)
9	CLA	L	305	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	6 (9%)
9	CLA	B	828	2	55,59,73	1.40	8 (14%)	66,96,113	1.39	8 (12%)
9	CLA	B	816	-	50,54,73	1.44	9 (18%)	60,90,113	1.42	4 (6%)
9	CLA	A	816	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
9	CLA	B	822	2	51,55,73	1.44	10 (19%)	61,91,113	1.44	5 (8%)
9	CLA	A	831	1	69,73,73	1.25	8 (11%)	83,113,113	1.33	7 (8%)
9	CLA	B	824	-	64,68,73	1.30	9 (14%)	77,107,113	1.23	6 (7%)
9	CLA	A	830	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	9 (10%)
9	CLA	A	834	1	55,59,73	1.41	9 (16%)	66,96,113	1.37	8 (12%)
9	CLA	B	803	2	69,73,73	1.23	9 (13%)	83,113,113	1.22	6 (7%)
9	CLA	A	808	1	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
9	CLA	L	303	7	53,57,73	1.41	9 (16%)	62,93,113	1.46	6 (9%)
9	CLA	B	840	-	52,56,73	1.44	7 (13%)	62,92,113	1.41	4 (6%)
9	CLA	A	812	1	49,53,73	1.48	8 (16%)	59,89,113	1.44	7 (11%)
9	CLA	A	820	1	53,57,73	1.43	8 (15%)	62,93,113	1.43	5 (8%)
9	CLA	B	819	2	64,68,73	1.29	9 (14%)	77,107,113	1.27	8 (10%)
9	CLA	A	822	1	59,63,73	1.35	9 (15%)	71,101,113	1.35	5 (7%)
9	CLA	A	833	1	49,53,73	1.49	9 (18%)	59,89,113	1.44	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	A	839	1	52,56,73	1.44	8 (15%)	62,92,113	1.41	5 (8%)
9	CLA	A	817	1	69,73,73	1.25	9 (13%)	83,113,113	1.26	6 (7%)
9	CLA	B	813	2	47,52,73	1.58	7 (14%)	55,87,113	1.45	5 (9%)
9	CLA	L	304	7	69,73,73	1.24	9 (13%)	83,113,113	1.31	6 (7%)
12	BCR	L	302	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	5 (8%)
11	LHG	A	843	9	26,26,48	0.80	0	29,32,54	1.36	4 (13%)
9	CLA	B	831	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
9	CLA	B	802	-	69,73,73	1.24	9 (13%)	83,113,113	1.25	7 (8%)
9	CLA	B	825	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
9	CLA	B	809	2	69,73,73	1.23	10 (14%)	83,113,113	1.32	6 (7%)
9	CLA	A	827	1	69,73,73	1.24	10 (14%)	83,113,113	1.26	6 (7%)
9	CLA	H	201	5	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
15	LMT	B	838	-	36,36,36	1.17	6 (16%)	47,47,47	0.95	1 (2%)
9	CLA	A	811	1	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
12	BCR	I	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.16	4 (7%)
9	CLA	B	810	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	6 (7%)
9	CLA	A	813	-	54,58,73	1.41	9 (16%)	65,95,113	1.39	8 (12%)
9	CLA	B	820	-	54,58,73	1.41	7 (12%)	65,95,113	1.40	5 (7%)
9	CLA	B	821	-	68,72,73	1.31	10 (14%)	85,112,113	1.33	9 (10%)
9	CLA	B	801	-	69,73,73	1.25	10 (14%)	83,113,113	1.37	9 (10%)
9	CLA	B	817	2	59,63,73	1.35	9 (15%)	71,101,113	1.33	6 (8%)
9	CLA	A	818	1	49,53,73	1.48	8 (16%)	59,89,113	1.42	4 (6%)
9	CLA	A	807	-	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
11	LHG	L	301	-	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
9	CLA	A	805	1	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
12	BCR	A	845	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	6 (10%)
9	CLA	A	823	-	69,73,73	1.26	9 (13%)	83,113,113	1.29	5 (6%)
9	CLA	B	811	2	69,73,73	1.25	9 (13%)	83,113,113	1.29	4 (4%)
9	CLA	A	835	-	69,73,73	1.24	9 (13%)	83,113,113	1.32	7 (8%)
9	CLA	A	803	-	59,63,73	1.36	7 (11%)	71,101,113	1.35	7 (9%)
9	CLA	B	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.37	6 (8%)
9	CLA	B	830	2	51,55,73	1.44	8 (15%)	61,91,113	1.38	6 (9%)
9	CLA	A	806	-	69,73,73	1.27	8 (11%)	83,113,113	1.27	6 (7%)
12	BCR	L	306	-	41,41,41	1.14	2 (4%)	56,56,56	1.30	8 (14%)
12	BCR	A	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	BCR	L	308	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	8 (14%)
9	CLA	B	823	2	69,73,73	1.24	8 (11%)	83,113,113	1.26	7 (8%)
9	CLA	B	827	2	49,53,73	1.49	9 (18%)	59,89,113	1.47	7 (11%)
13	SF4	C	101	3	0,12,12	-	-	-		
9	CLA	A	836	1	69,73,73	1.23	7 (10%)	83,113,113	1.36	7 (8%)
12	BCR	B	834	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
9	CLA	A	810	1	58,62,73	1.38	9 (15%)	69,99,113	1.34	7 (10%)
11	LHG	A	842	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
9	CLA	B	808	2	59,63,73	1.34	9 (15%)	71,101,113	1.35	6 (8%)
10	PQN	B	833	-	34,34,34	0.36	0	42,45,45	0.58	1 (2%)
9	CLA	B	807	2	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
9	CLA	B	805	2	49,53,73	1.48	10 (20%)	59,89,113	1.44	5 (8%)
9	CLA	A	802	-	69,73,73	1.26	8 (11%)	83,113,113	1.24	7 (8%)
9	CLA	A	804	1	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
9	CLA	B	806	2	69,73,73	1.24	7 (10%)	83,113,113	1.33	7 (8%)
9	CLA	B	812	2	58,62,73	1.41	9 (15%)	73,100,113	1.34	7 (9%)
9	CLA	A	841	11	56,60,73	1.41	6 (10%)	67,97,113	1.38	5 (7%)
12	BCR	B	836	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	5 (8%)
14	DGD	B	837	-	67,67,67	0.87	2 (2%)	81,81,81	1.45	12 (14%)
9	CLA	A	849	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
10	PQN	A	840	-	34,34,34	0.36	0	42,45,45	0.54	0
12	BCR	L	307	-	41,41,41	1.16	2 (4%)	56,56,56	1.26	7 (12%)
9	CLA	B	832	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
9	CLA	B	814	2	69,73,73	1.25	9 (13%)	83,113,113	1.27	5 (6%)
9	CLA	A	838	-	69,73,73	1.27	9 (13%)	83,113,113	1.27	5 (6%)
9	CLA	A	837	1	51,55,73	1.44	7 (13%)	61,91,113	1.43	6 (9%)
9	CLA	A	832	1	54,58,73	1.42	6 (11%)	65,95,113	1.44	7 (10%)
9	CLA	B	815	2	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
9	CLA	B	804	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	4 (4%)
9	CLA	A	815	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
12	BCR	A	844	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
9	CLA	A	809	-	69,73,73	1.27	8 (11%)	83,113,113	1.28	7 (8%)
9	CLA	A	826	1	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
9	CLA	A	829	1	54,58,73	1.40	9 (16%)	65,95,113	1.40	6 (9%)
13	SF4	C	102	3	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CLA	A	821	1	55,59,73	1.40	8 (14%)	66,96,113	1.36	6 (9%)
13	SF4	A	848	2,1	0,12,12	-	-	-		
9	CLA	A	850	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)

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
12	BCR	A	846	-	-	7/29/63/63	0/2/2/2
9	CLA	B	829	2	-	10/39/115/115	-
9	CLA	A	819	-	-	4/39/115/115	-
9	CLA	A	825	1	-	10/39/115/115	-
9	CLA	B	839	2	-	6/19/95/115	-
9	CLA	A	828	1	-	9/39/115/115	-
9	CLA	A	814	-	-	1/15/91/115	-
9	CLA	B	826	2	-	9/19/95/115	-
9	CLA	A	824	-	-	7/39/115/115	-
12	BCR	B	835	-	-	21/29/63/63	0/2/2/2
9	CLA	A	801	1	-	12/39/115/115	-
9	CLA	L	305	-	-	2/21/97/115	-
9	CLA	B	828	2	-	6/23/99/115	-
9	CLA	B	816	-	-	7/17/93/115	-
9	CLA	A	816	1	-	18/39/115/115	-
9	CLA	B	822	2	-	10/18/94/115	-
9	CLA	A	831	1	-	24/39/115/115	-
9	CLA	B	824	-	-	16/33/109/115	-
9	CLA	A	830	1	-	9/39/115/115	-
9	CLA	A	834	1	-	11/23/99/115	-
9	CLA	B	803	2	-	9/39/115/115	-
9	CLA	A	808	1	-	14/39/115/115	-
9	CLA	L	303	7	-	8/20/96/115	-
9	CLA	B	840	-	-	10/19/95/115	-
9	CLA	A	812	1	-	4/15/91/115	-
9	CLA	A	820	1	-	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	819	2	-	15/33/109/115	-
9	CLA	A	822	1	-	9/27/103/115	-
9	CLA	A	833	1	-	5/15/91/115	-
9	CLA	A	839	1	-	5/19/95/115	-
9	CLA	A	817	1	-	15/39/115/115	-
9	CLA	B	813	2	-	4/14/91/115	-
9	CLA	L	304	7	-	8/39/115/115	-
12	BCR	L	302	-	-	7/29/63/63	0/2/2/2
11	LHG	A	843	9	-	13/31/31/53	-
9	CLA	B	831	-	-	8/39/115/115	-
9	CLA	B	802	-	-	15/39/115/115	-
9	CLA	B	825	2	-	8/39/115/115	-
9	CLA	B	809	2	-	10/39/115/115	-
9	CLA	A	827	1	-	13/39/115/115	-
9	CLA	H	201	5	-	10/39/115/115	-
15	LMT	B	838	-	-	13/21/61/61	0/2/2/2
9	CLA	A	811	1	-	13/39/115/115	-
12	BCR	I	101	-	-	7/29/63/63	0/2/2/2
9	CLA	B	810	2	-	9/39/115/115	-
9	CLA	A	813	-	-	7/21/97/115	-
9	CLA	B	820	-	-	8/21/97/115	-
9	CLA	B	821	-	-	12/37/113/115	-
9	CLA	B	801	-	-	20/39/115/115	-
9	CLA	B	817	2	-	8/27/103/115	-
9	CLA	A	818	1	-	6/15/91/115	-
9	CLA	A	807	-	-	21/39/115/115	-
11	LHG	L	301	-	-	24/53/53/53	-
9	CLA	A	805	1	-	10/39/115/115	-
12	BCR	A	845	-	-	10/29/63/63	0/2/2/2
9	CLA	A	823	-	-	8/39/115/115	-
9	CLA	B	811	2	-	21/39/115/115	-
9	CLA	A	835	-	-	11/39/115/115	-
9	CLA	A	803	-	-	7/27/103/115	-
9	CLA	B	818	2	-	9/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	B	830	2	-	1/18/94/115	-
9	CLA	A	806	-	-	15/39/115/115	-
12	BCR	L	306	-	-	8/29/63/63	0/2/2/2
12	BCR	A	847	-	-	9/29/63/63	0/2/2/2
12	BCR	L	308	-	-	10/29/63/63	0/2/2/2
9	CLA	B	823	2	-	12/39/115/115	-
9	CLA	B	827	2	-	4/15/91/115	-
13	SF4	C	101	3	-	-	0/6/5/5
9	CLA	A	836	1	-	12/39/115/115	-
12	BCR	B	834	-	-	9/29/63/63	0/2/2/2
9	CLA	A	810	1	-	8/26/102/115	-
11	LHG	A	842	-	-	24/53/53/53	-
9	CLA	B	808	2	-	5/27/103/115	-
10	PQN	B	833	-	-	2/23/43/43	0/2/2/2
9	CLA	B	807	2	-	13/39/115/115	-
9	CLA	B	805	2	-	3/15/91/115	-
9	CLA	A	802	-	-	8/39/115/115	-
9	CLA	A	804	1	-	7/39/115/115	-
9	CLA	B	806	2	-	14/39/115/115	-
9	CLA	B	812	2	-	8/25/101/115	-
9	CLA	A	841	11	-	9/24/100/115	-
12	BCR	B	836	-	-	8/29/63/63	0/2/2/2
14	DGD	B	837	-	-	24/55/95/95	0/2/2/2
9	CLA	A	849	-	-	19/39/115/115	-
10	PQN	A	840	-	-	12/23/43/43	0/2/2/2
12	BCR	L	307	-	-	8/29/63/63	0/2/2/2
9	CLA	B	832	2	-	12/39/115/115	-
9	CLA	B	814	2	-	16/39/115/115	-
9	CLA	A	838	-	-	16/39/115/115	-
9	CLA	A	837	1	-	11/18/94/115	-
9	CLA	A	832	1	-	7/21/97/115	-
9	CLA	B	815	2	-	10/39/115/115	-
9	CLA	B	804	-	-	13/39/115/115	-
9	CLA	A	815	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BCR	A	844	-	-	7/29/63/63	0/2/2/2
9	CLA	A	809	-	-	16/39/115/115	-
9	CLA	A	826	1	-	18/39/115/115	-
9	CLA	A	829	1	-	6/21/97/115	-
13	SF4	C	102	3	-	-	0/6/5/5
9	CLA	A	821	1	-	9/23/99/115	-
13	SF4	A	848	2,1	-	-	0/6/5/5
9	CLA	A	850	1	-	13/39/115/115	-

The worst 5 of 714 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	813	CLA	C2B-C1B	4.83	1.49	1.39
9	A	826	CLA	C1D-ND	4.01	1.42	1.37
9	A	838	CLA	C1D-ND	3.97	1.42	1.37
9	A	841	CLA	C1D-ND	3.95	1.42	1.37
9	B	818	CLA	C1D-ND	3.90	1.42	1.37

The worst 5 of 613 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	818	CLA	C4A-NA-C1A	7.21	109.95	106.71
9	B	809	CLA	C4A-NA-C1A	7.12	109.91	106.71
9	B	806	CLA	C4A-NA-C1A	7.05	109.88	106.71
9	B	832	CLA	C4A-NA-C1A	7.03	109.86	106.71
9	A	832	CLA	C4A-NA-C1A	7.01	109.86	106.71

There are no chirality outliers.

5 of 1044 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	801	CLA	CBD-CGD-O2D-CED
9	A	803	CLA	C1A-C2A-CAA-CBA
9	A	803	CLA	CHA-CBD-CGD-O1D
9	A	803	CLA	CHA-CBD-CGD-O2D
9	A	804	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

93 monomers are involved in 308 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	846	BCR	3	0
9	B	829	CLA	8	0
9	A	825	CLA	5	0
9	A	828	CLA	4	0
9	A	814	CLA	1	0
9	B	826	CLA	1	0
9	A	824	CLA	1	0
12	B	835	BCR	3	0
9	A	801	CLA	5	0
9	L	305	CLA	1	0
9	B	828	CLA	1	0
9	A	816	CLA	6	0
9	B	822	CLA	3	0
9	A	831	CLA	12	0
9	B	824	CLA	7	0
9	A	830	CLA	3	0
9	A	834	CLA	4	0
9	B	803	CLA	5	0
9	A	808	CLA	2	0
9	L	303	CLA	2	0
9	A	812	CLA	2	0
9	A	820	CLA	2	0
9	B	819	CLA	5	0
9	A	822	CLA	2	0
9	A	833	CLA	1	0
9	A	839	CLA	3	0
9	A	817	CLA	6	0
9	L	304	CLA	8	0
12	L	302	BCR	2	0
11	A	843	LHG	2	0
9	B	831	CLA	9	0
9	B	802	CLA	7	0
9	B	825	CLA	7	0
9	B	809	CLA	7	0
9	A	827	CLA	3	0
9	H	201	CLA	2	0
15	B	838	LMT	3	0
9	A	811	CLA	4	0
12	I	101	BCR	2	0
9	B	810	CLA	4	0
9	B	820	CLA	1	0
9	B	821	CLA	4	0
9	B	801	CLA	10	0

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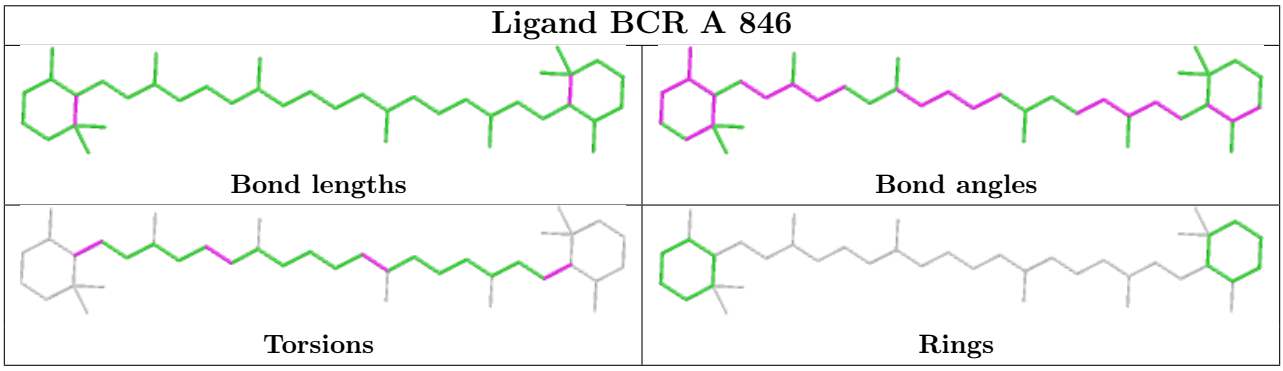
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	817	CLA	3	0
9	A	818	CLA	1	0
9	A	807	CLA	5	0
11	L	301	LHG	9	0
9	A	805	CLA	2	0
12	A	845	BCR	2	0
9	A	823	CLA	4	0
9	B	811	CLA	5	0
9	A	835	CLA	5	0
9	A	803	CLA	1	0
9	B	818	CLA	5	0
9	B	830	CLA	4	0
9	A	806	CLA	2	0
12	L	306	BCR	6	0
12	A	847	BCR	3	0
12	L	308	BCR	1	0
9	B	823	CLA	3	0
9	B	827	CLA	2	0
13	C	101	SF4	1	0
9	A	836	CLA	2	0
12	B	834	BCR	1	0
9	A	810	CLA	1	0
9	B	808	CLA	2	0
10	B	833	PQN	4	0
9	B	807	CLA	5	0
9	B	805	CLA	2	0
9	A	802	CLA	6	0
9	A	804	CLA	6	0
9	B	806	CLA	5	0
9	B	812	CLA	3	0
9	A	841	CLA	1	0
12	B	836	BCR	3	0
14	B	837	DGD	8	0
9	A	849	CLA	4	0
10	A	840	PQN	5	0
12	L	307	BCR	6	0
9	B	832	CLA	9	0
9	B	814	CLA	6	0
9	A	838	CLA	4	0
9	A	837	CLA	1	0
9	A	832	CLA	1	0
9	B	815	CLA	6	0

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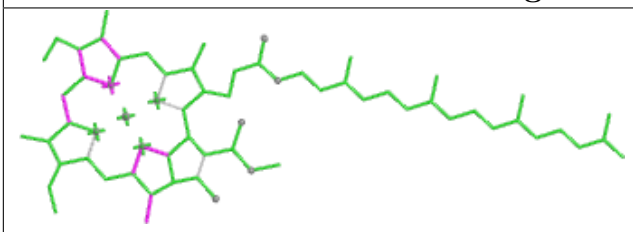
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	804	CLA	10	0
9	A	815	CLA	2	0
12	A	844	BCR	2	0
9	A	826	CLA	11	0
9	A	829	CLA	1	0
13	C	102	SF4	1	0
9	A	821	CLA	1	0
9	A	850	CLA	5	0

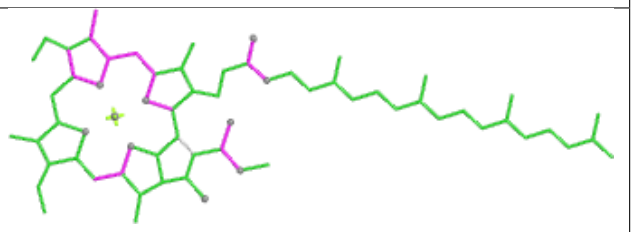
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



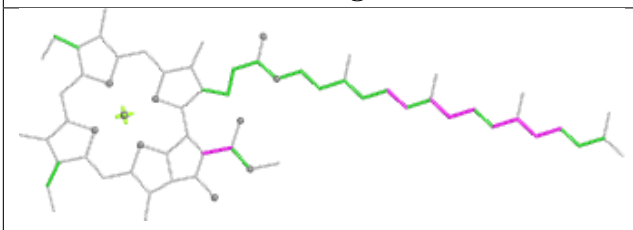
Ligand CLA B 829



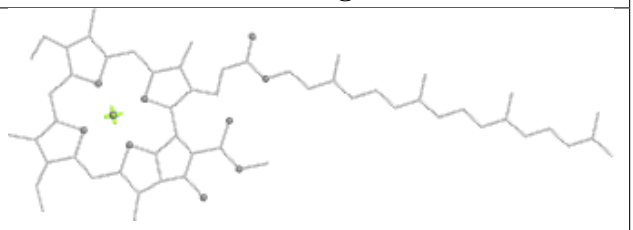
Bond lengths



Bond angles

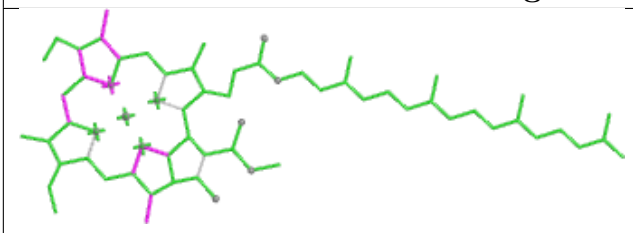


Torsions

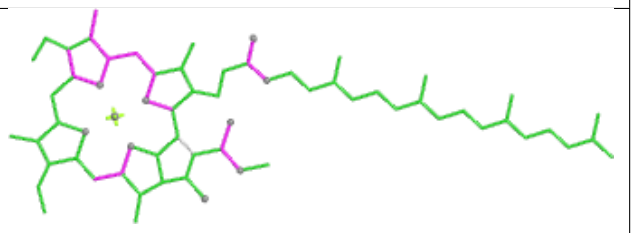


Rings

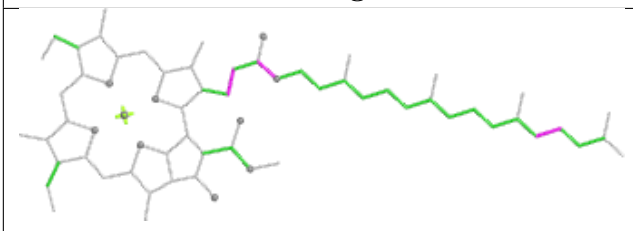
Ligand CLA A 819



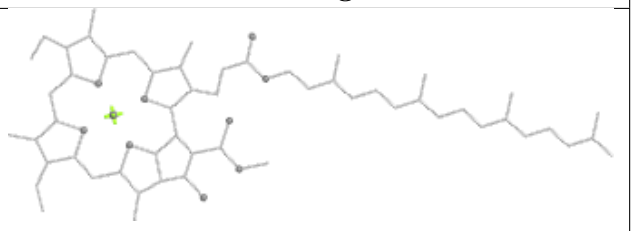
Bond lengths



Bond angles

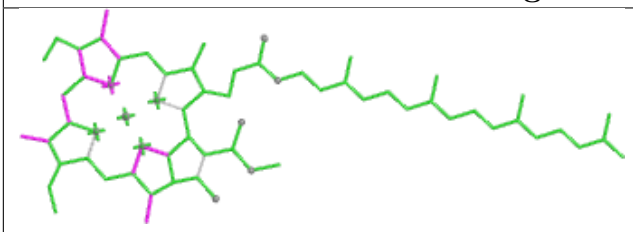


Torsions

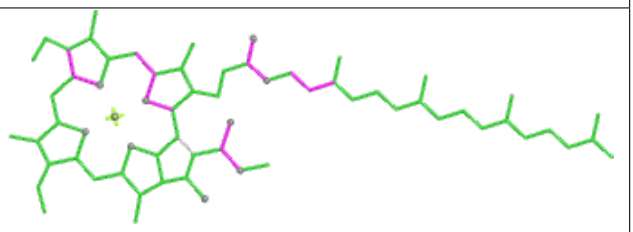


Rings

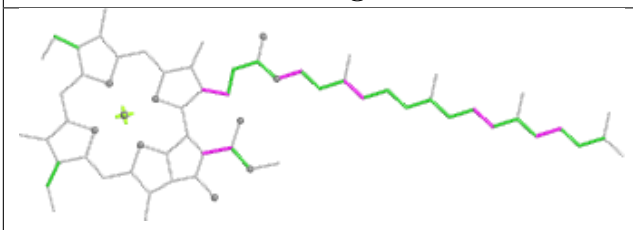
Ligand CLA A 825



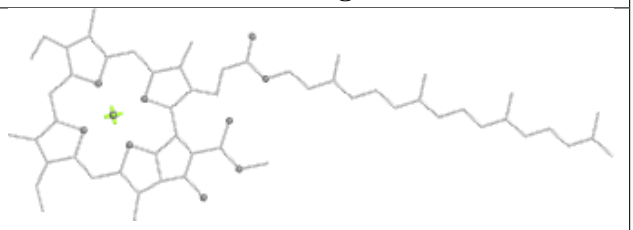
Bond lengths



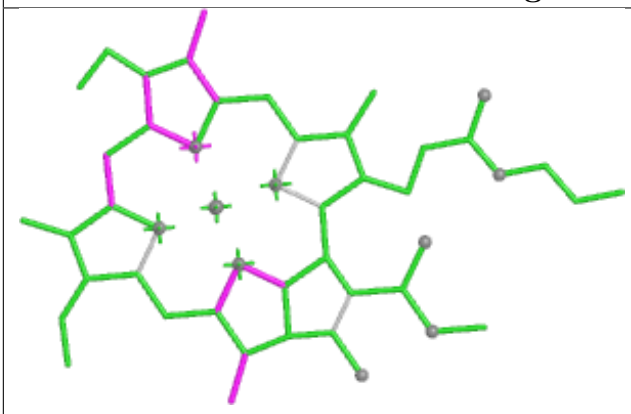
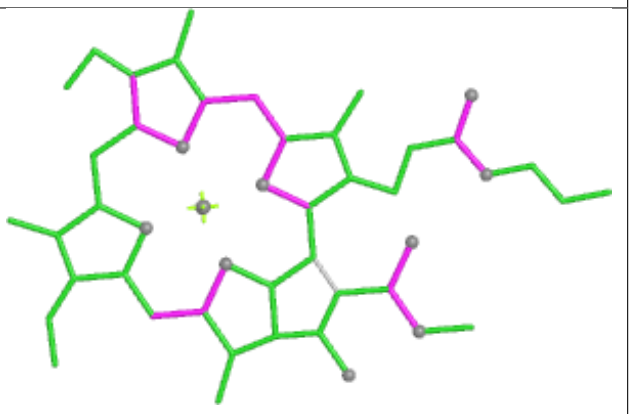
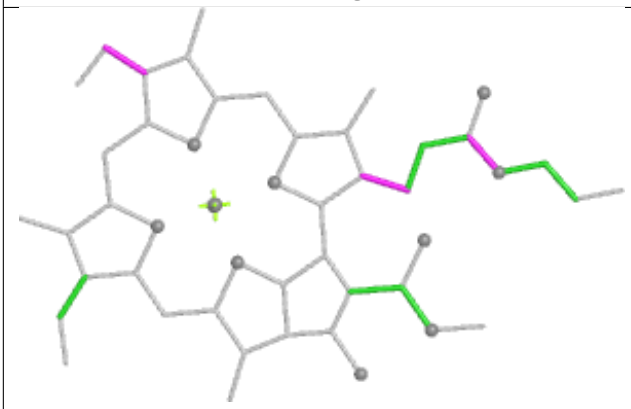
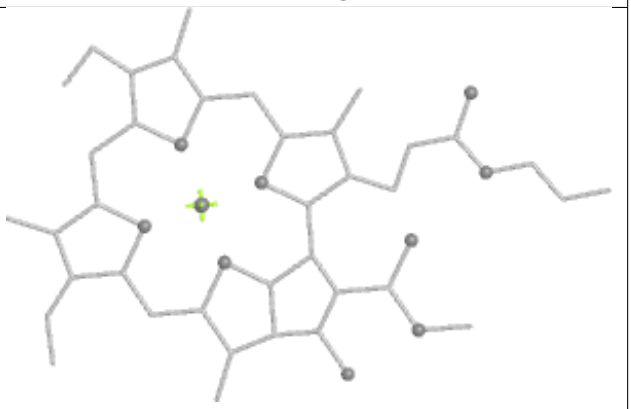
Bond angles

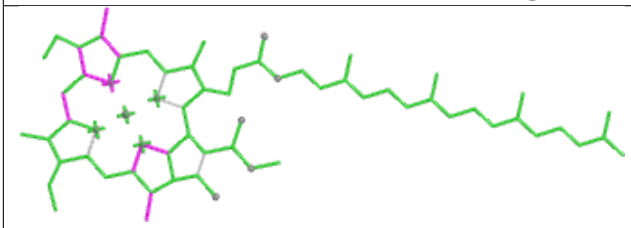
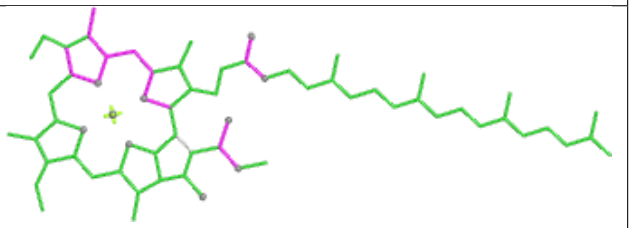
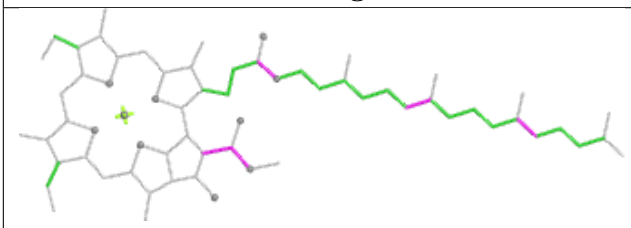
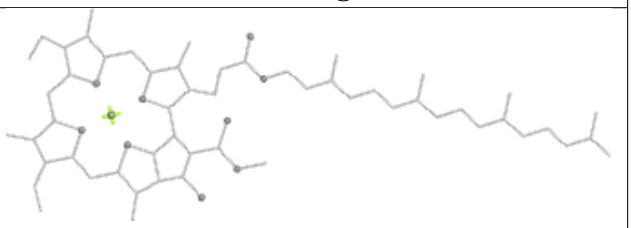


Torsions

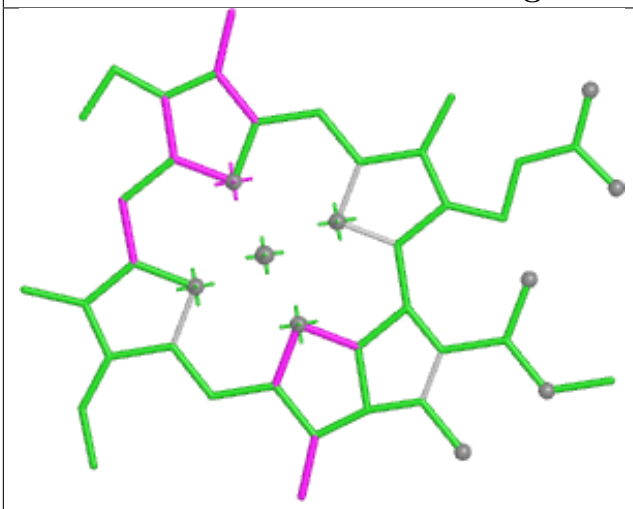


Rings

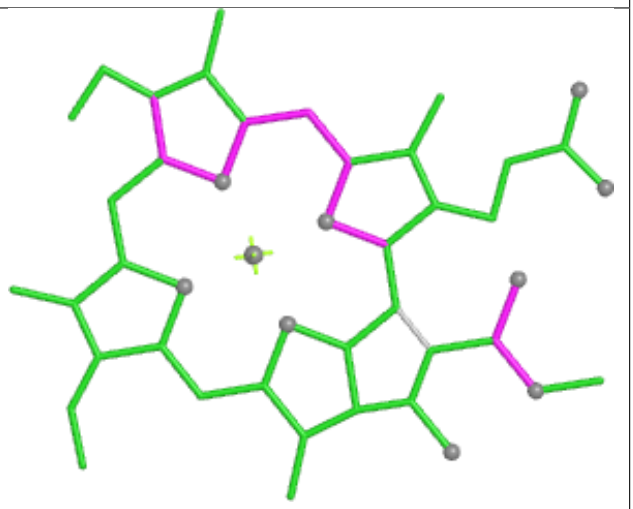
Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

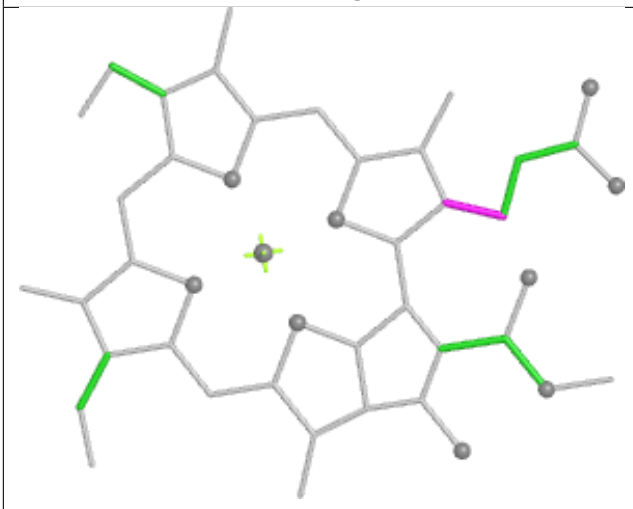
Ligand CLA A 814



Bond lengths



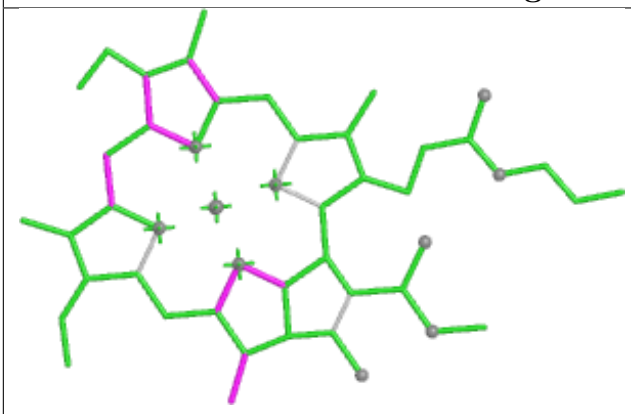
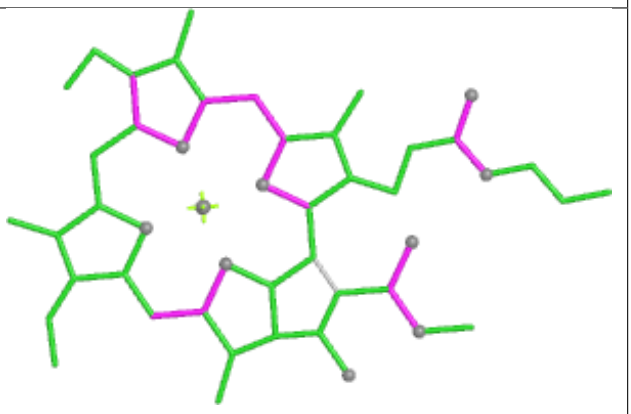
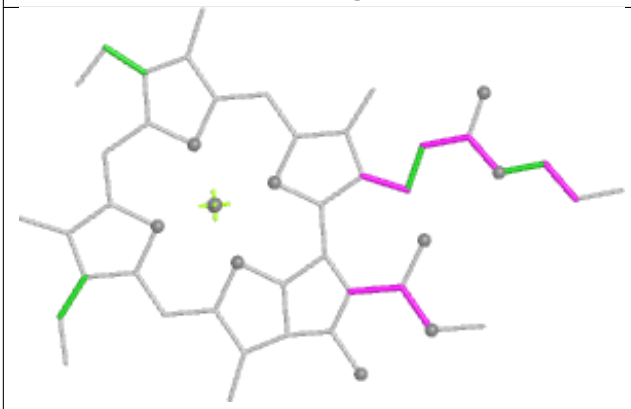
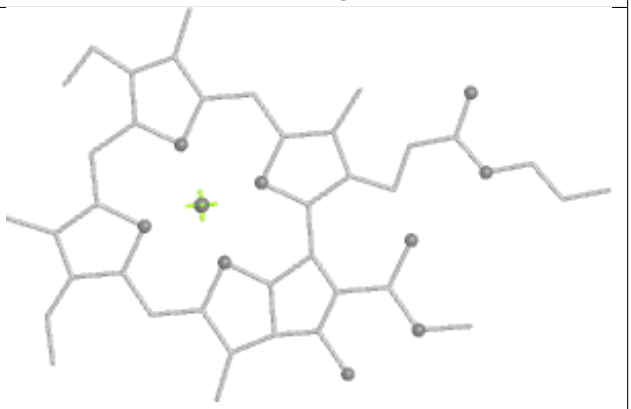
Bond angles

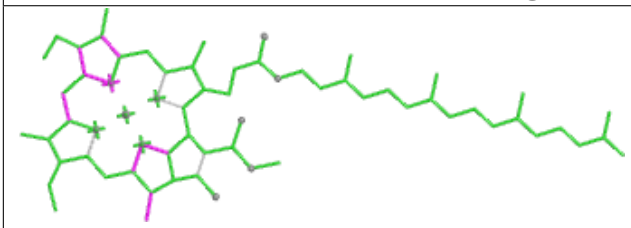
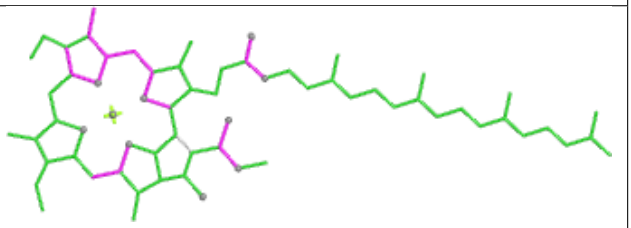
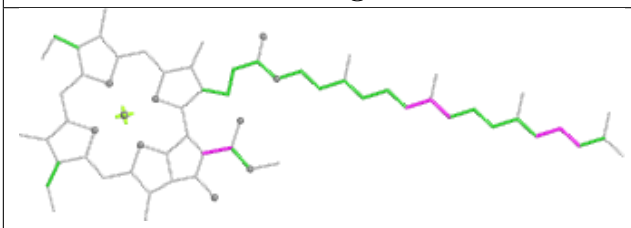
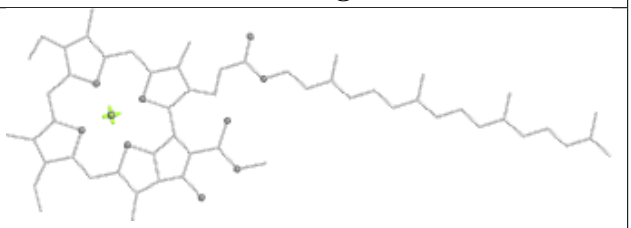


Torsions

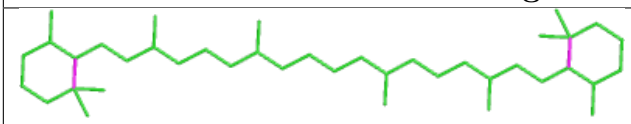


Rings

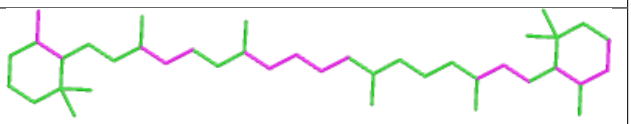
Ligand CLA B 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

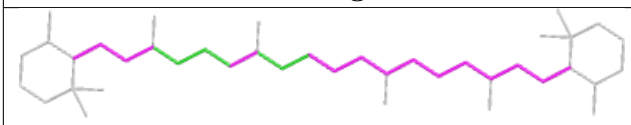
Ligand BCR B 835



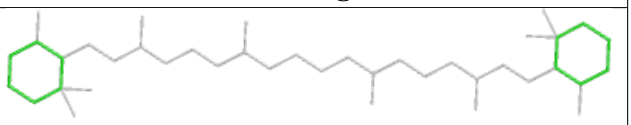
Bond lengths



Bond angles

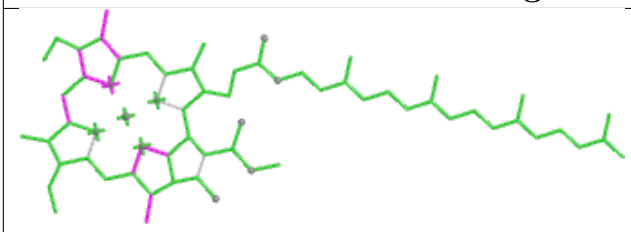


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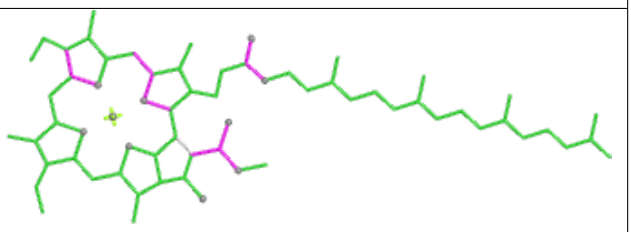


Rings

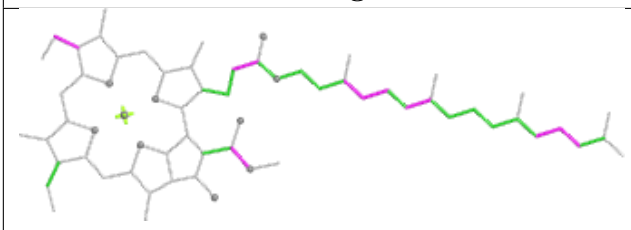
Ligand CLA A 801



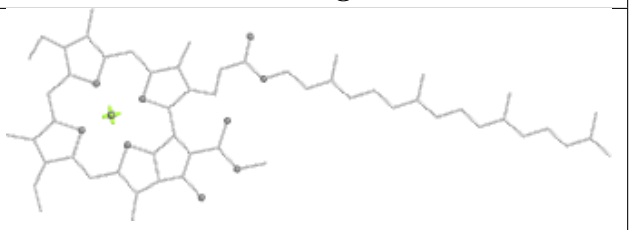
Bond lengths



Bond angles

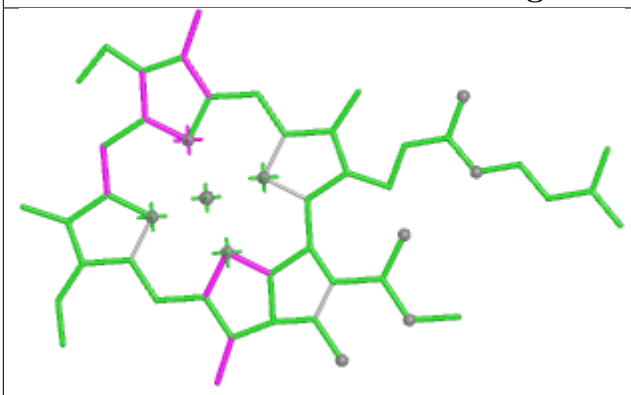


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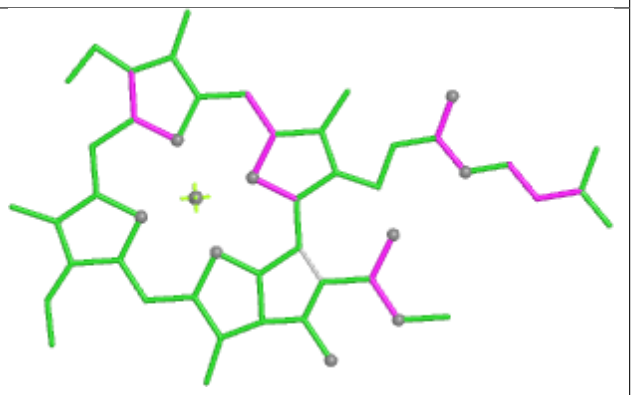


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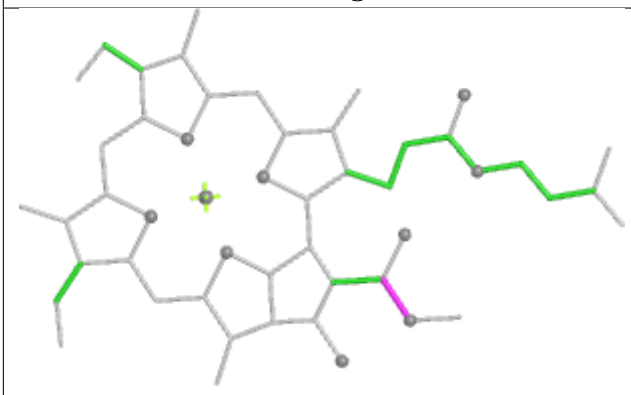
Ligand CLA L 305



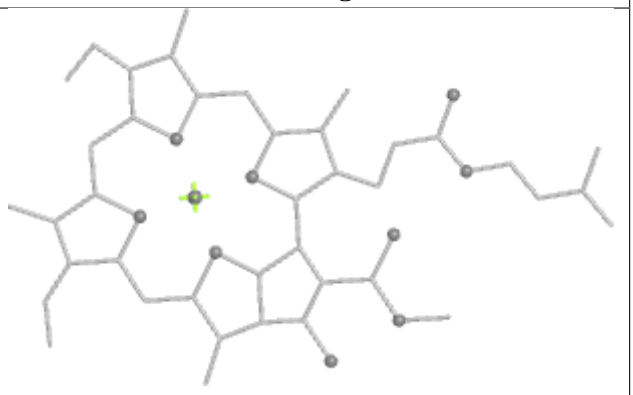
Bond lengths



Bond angles

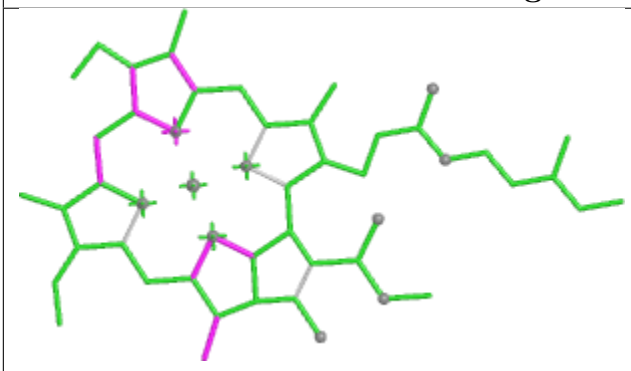


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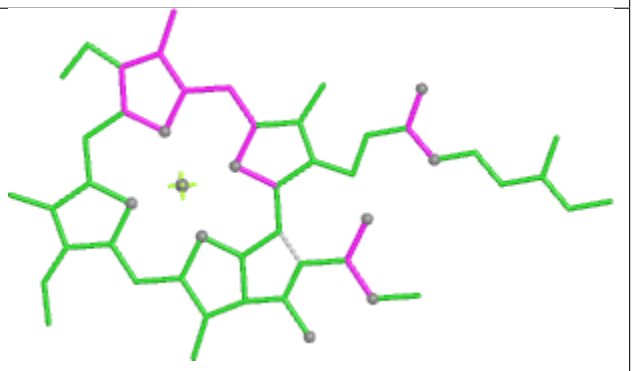


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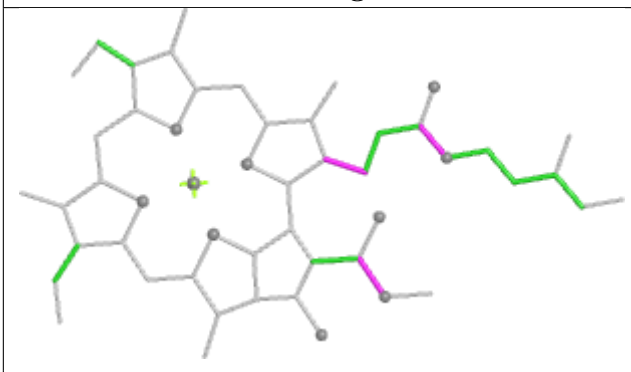
Ligand CLA B 828



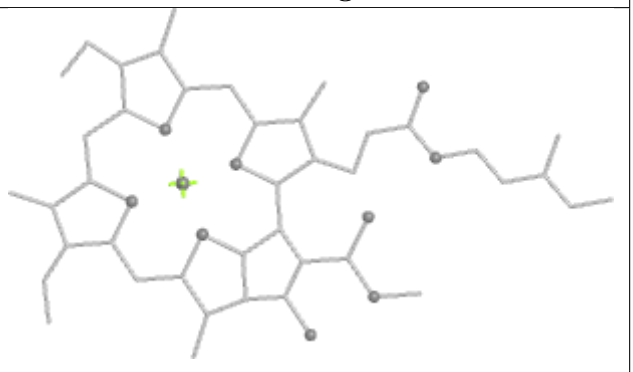
Bond lengths



Bond angles

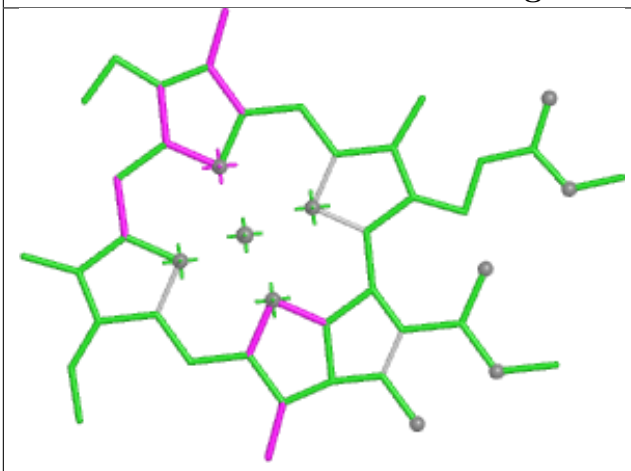


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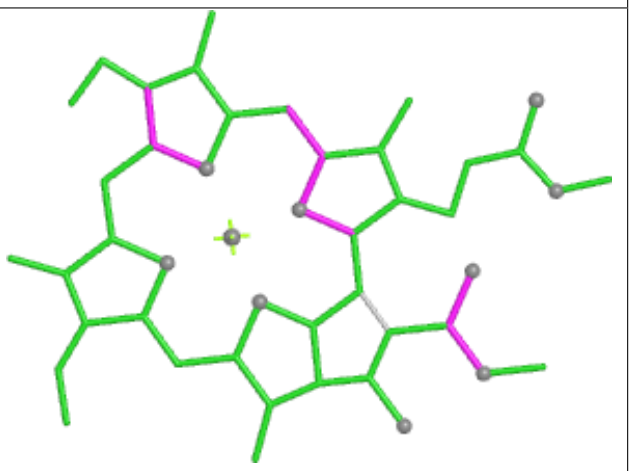


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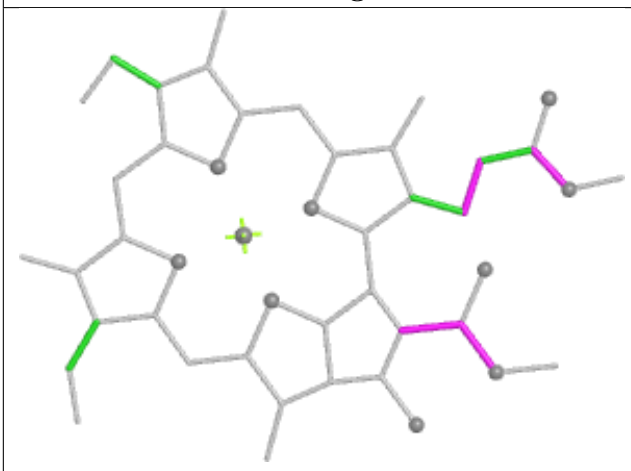
Ligand CLA B 816



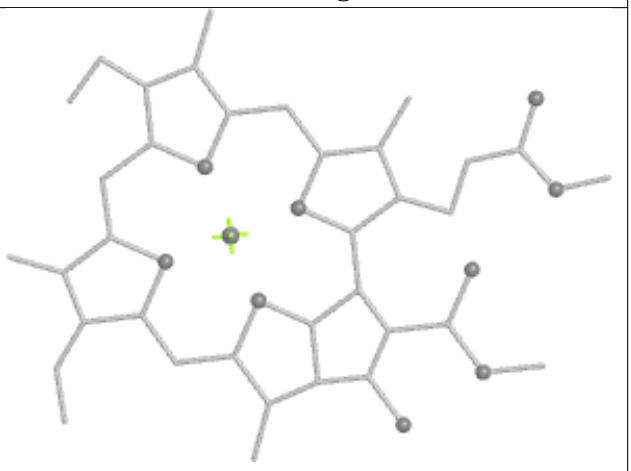
Bond lengths



Bond angles

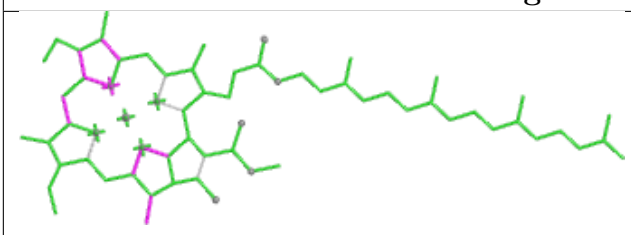


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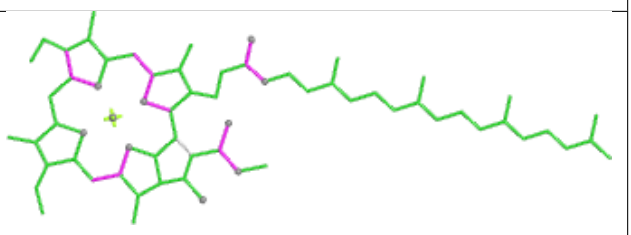


Rings

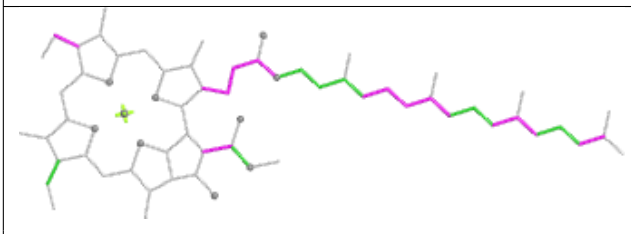
Ligand CLA A 816



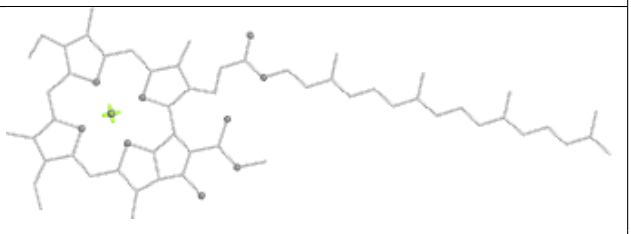
Bond lengths



Bond angles

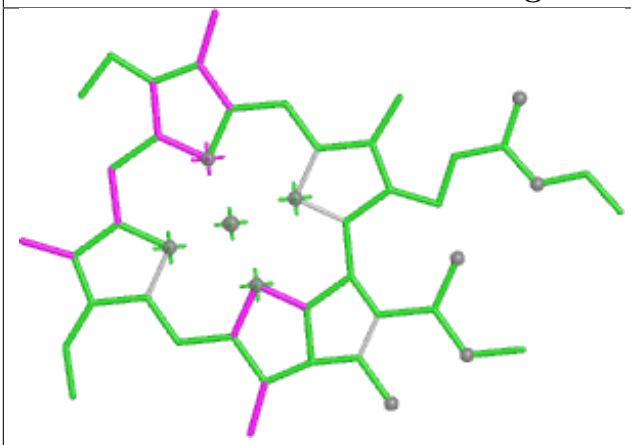


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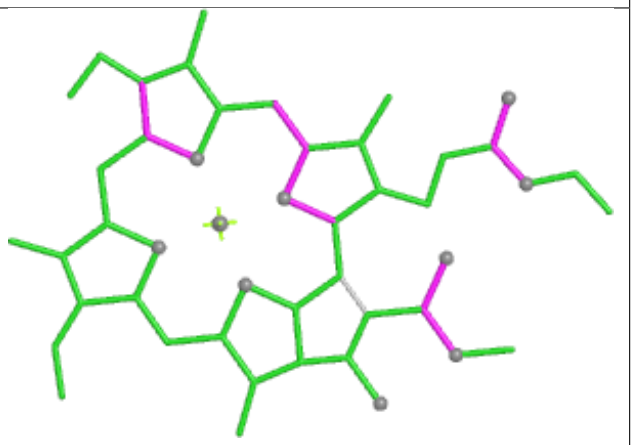


Rings

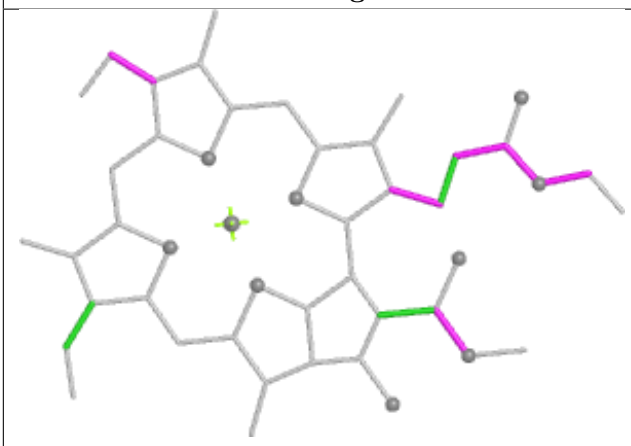
Ligand CLA B 822



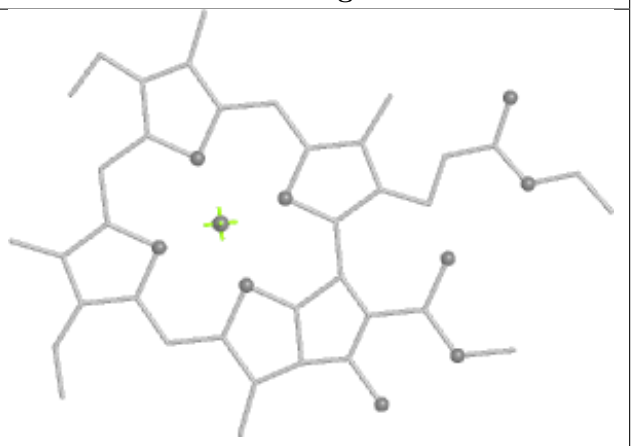
Bond lengths



Bond angles

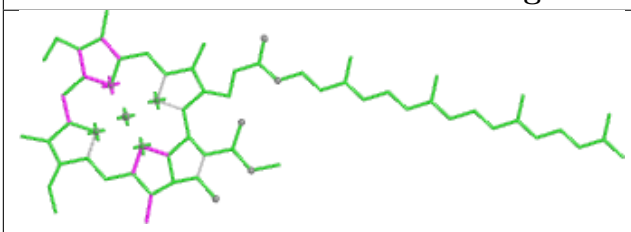


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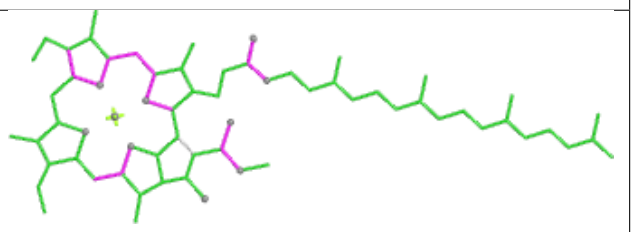


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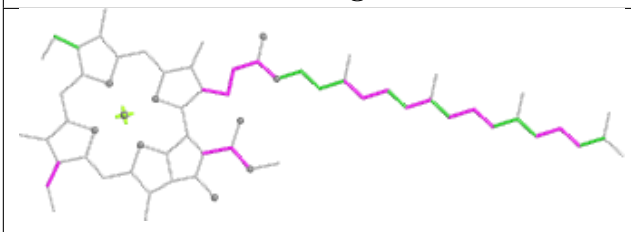
Ligand CLA A 831



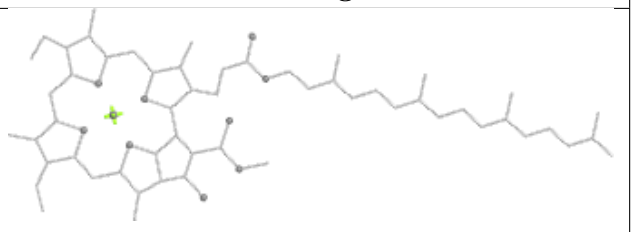
Bond lengths



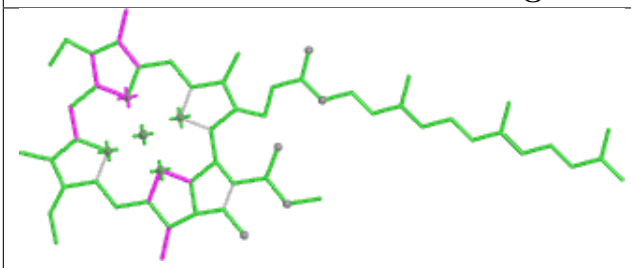
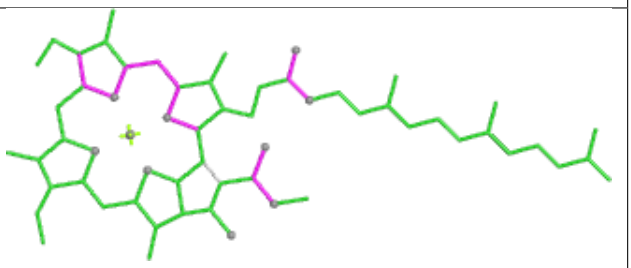
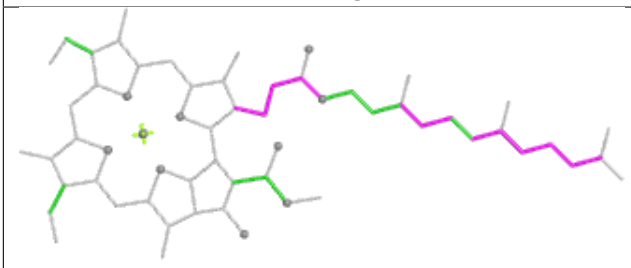
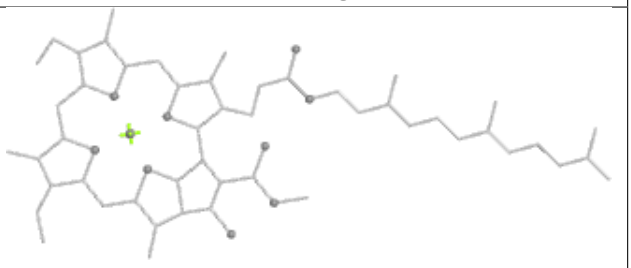
Bond angles

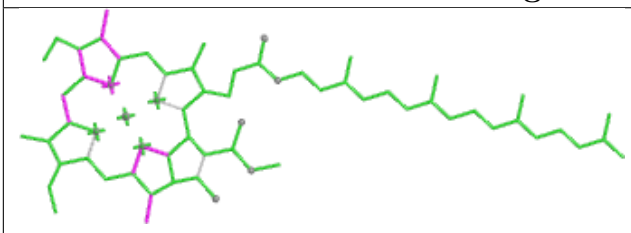
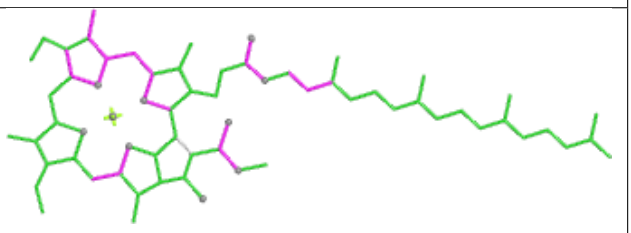
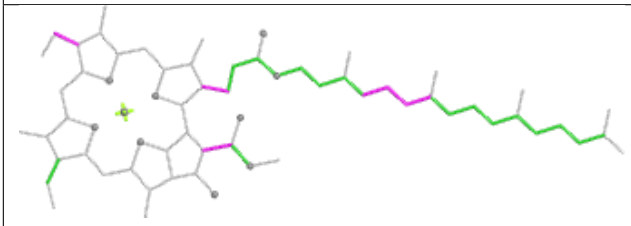
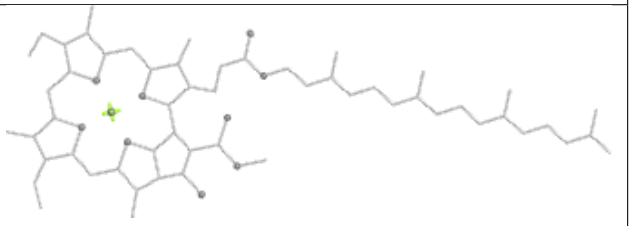


Torsions

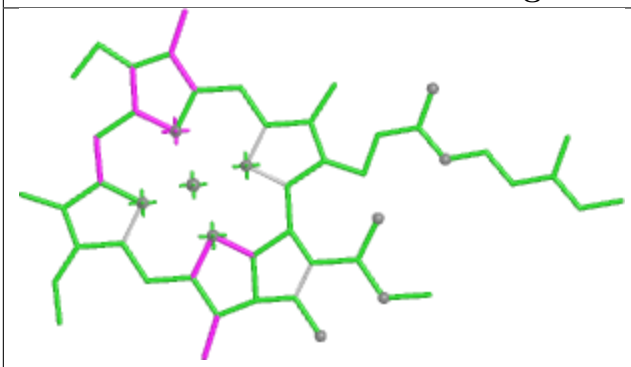


Rings

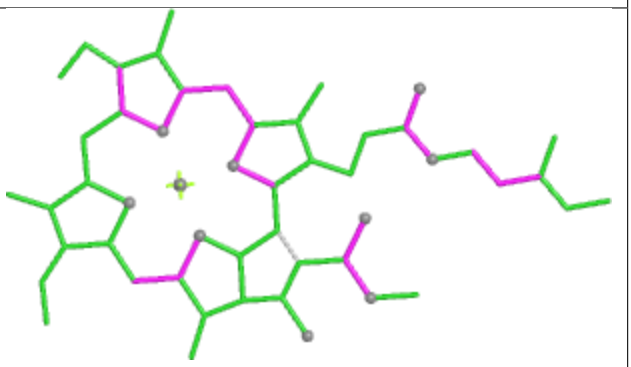
Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

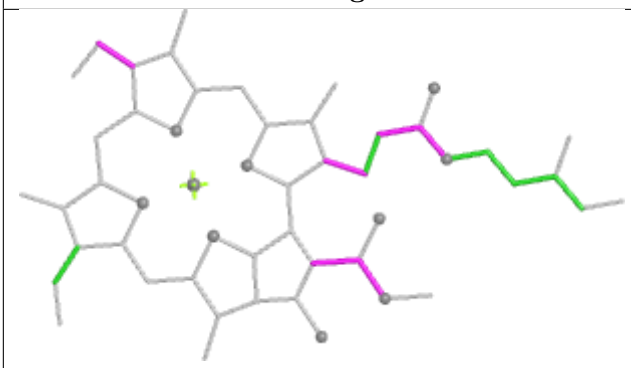
Ligand CLA A 834



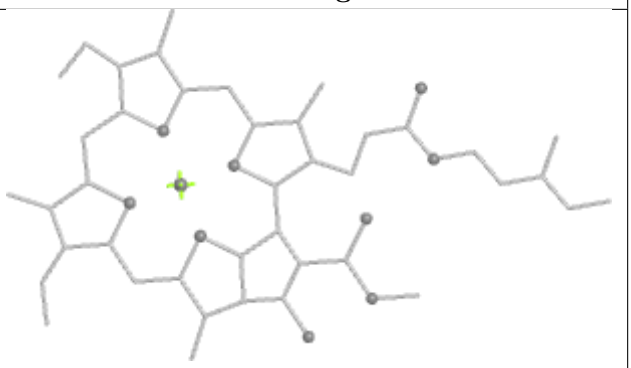
Bond lengths



Bond angles

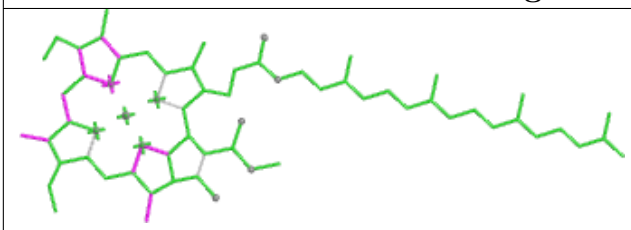


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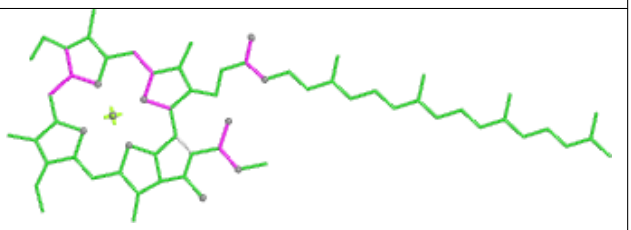


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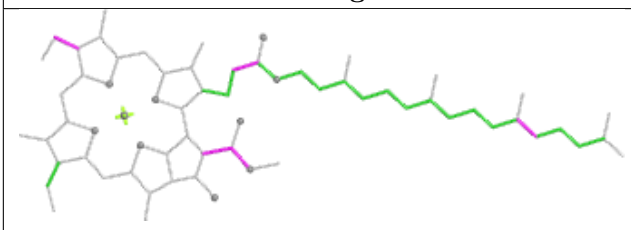
Ligand CLA B 803



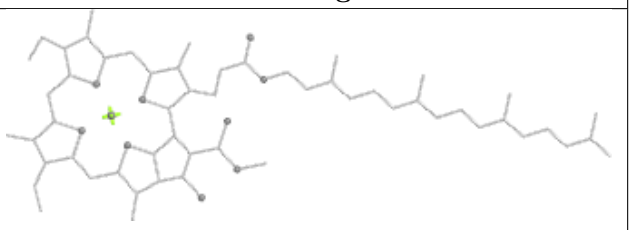
Bond lengths



Bond angles

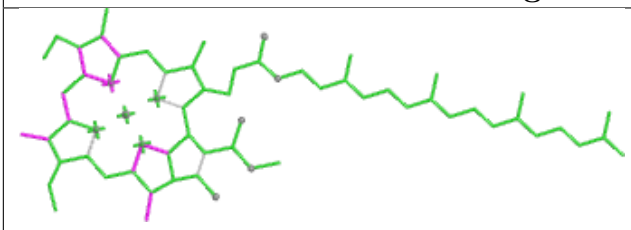


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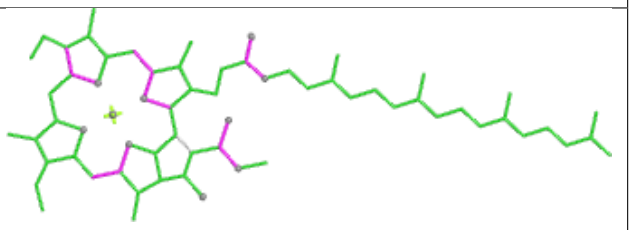


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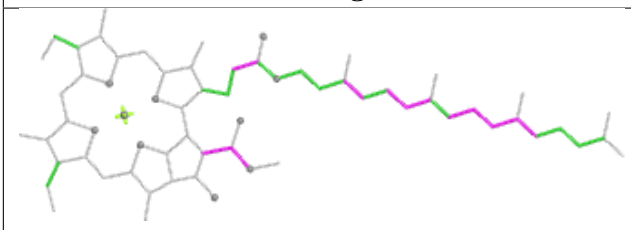
Ligand CLA A 808



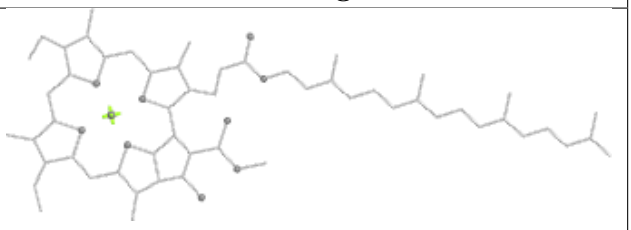
Bond lengths



Bond angles

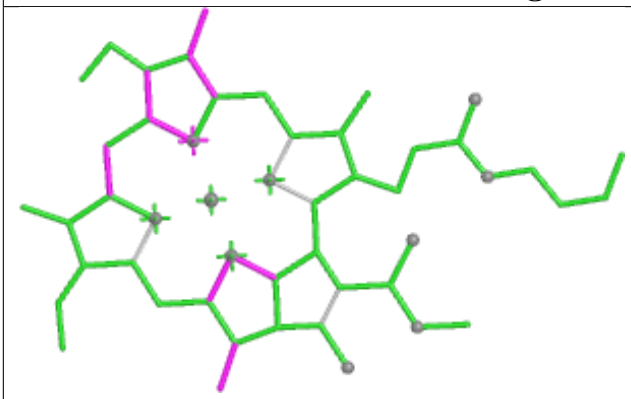


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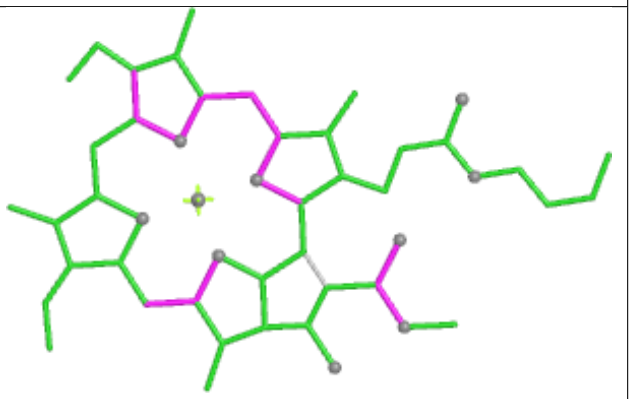


Rings

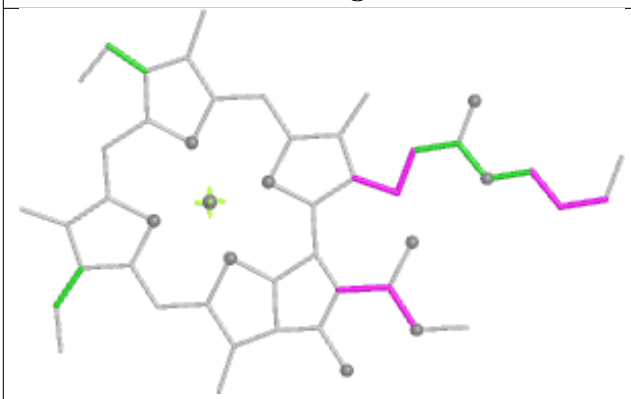
Ligand CLA L 303



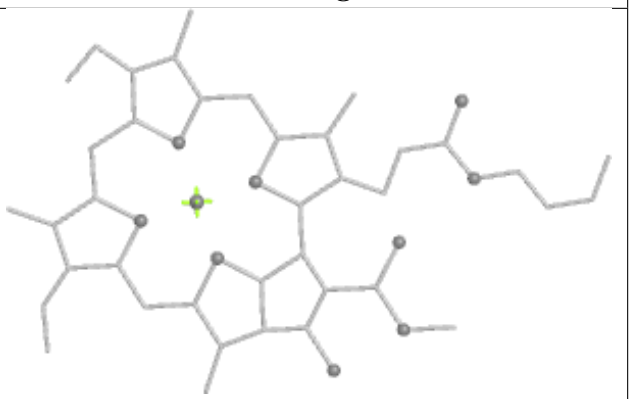
Bond lengths



Bond angles

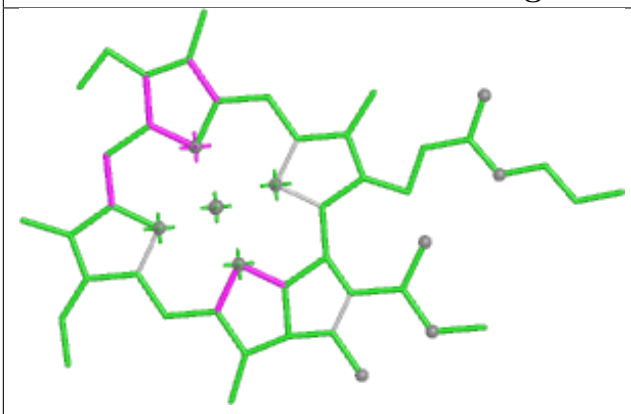


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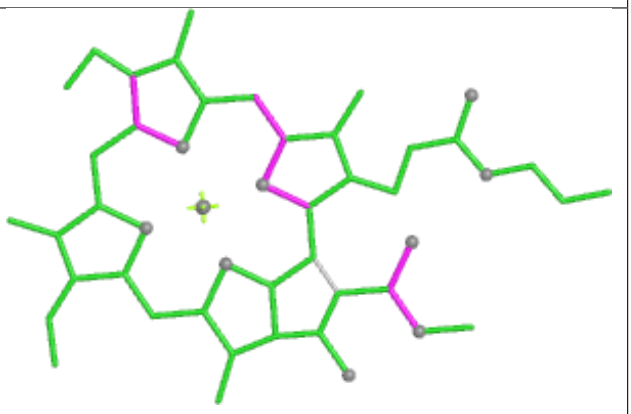


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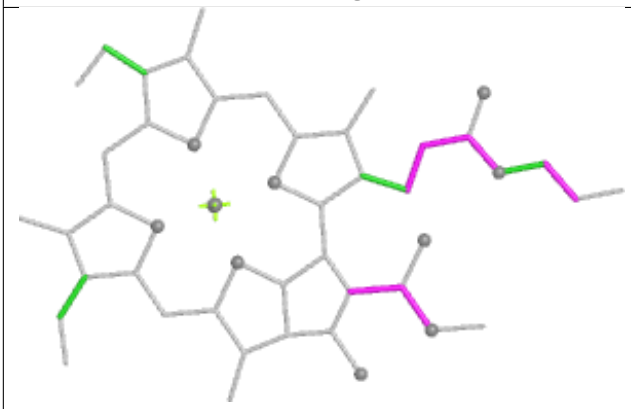
Ligand CLA B 840



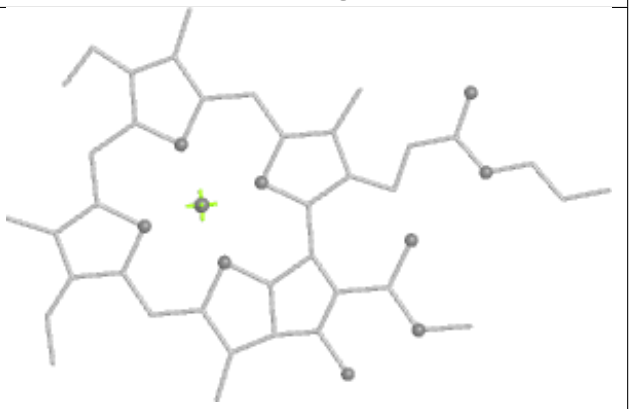
Bond lengths



Bond angles

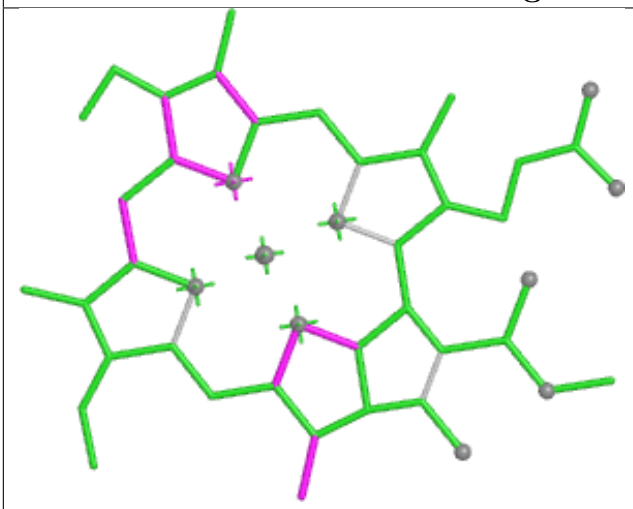


Torsions

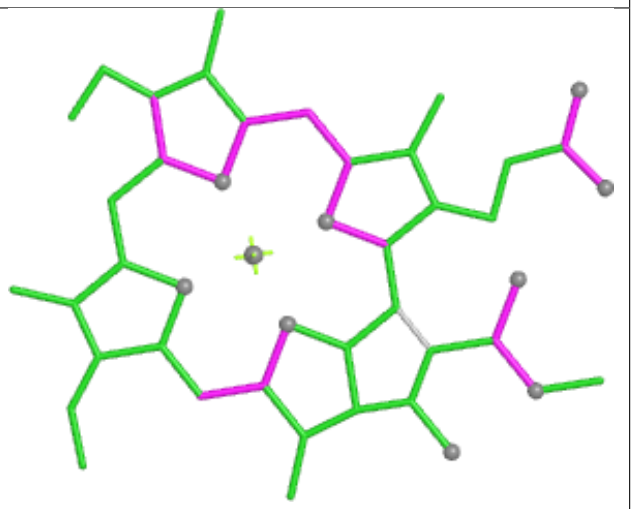


Rings

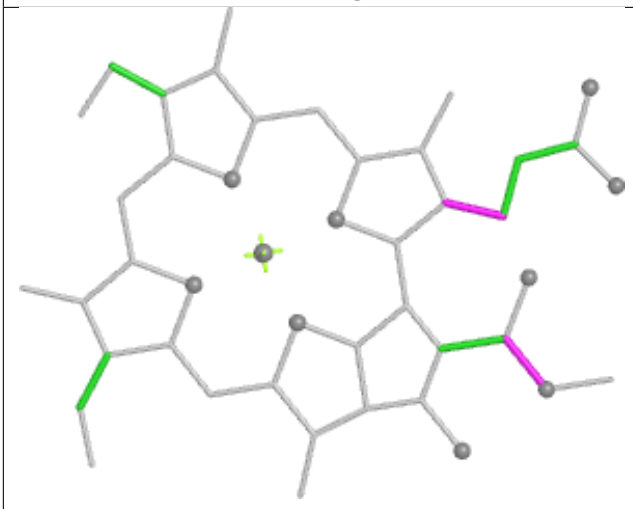
Ligand CLA A 812



Bond lengths



Bond angles

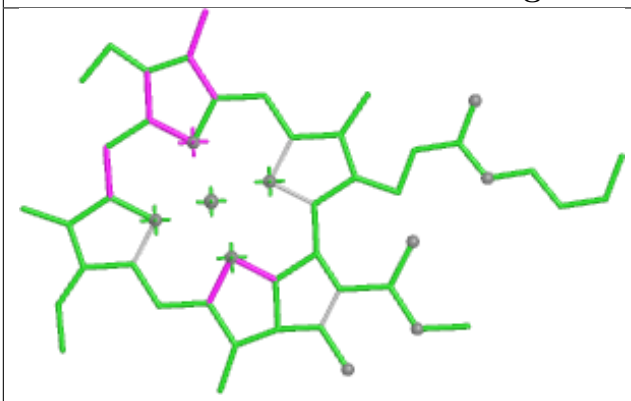


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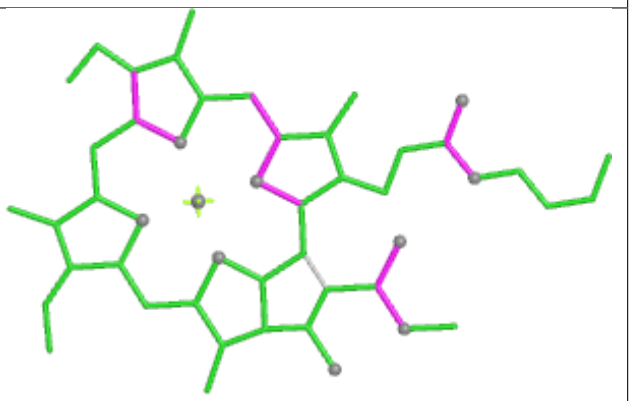


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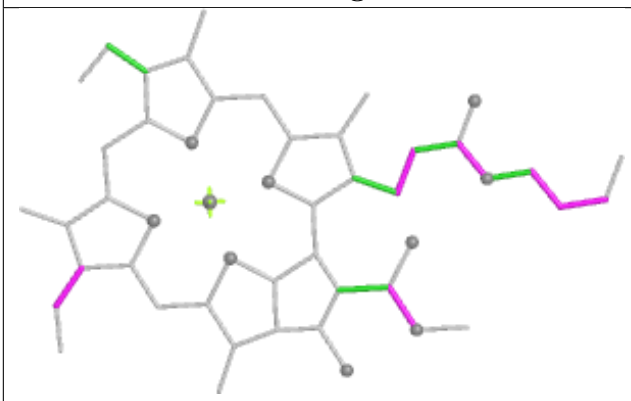
Ligand CLA A 820



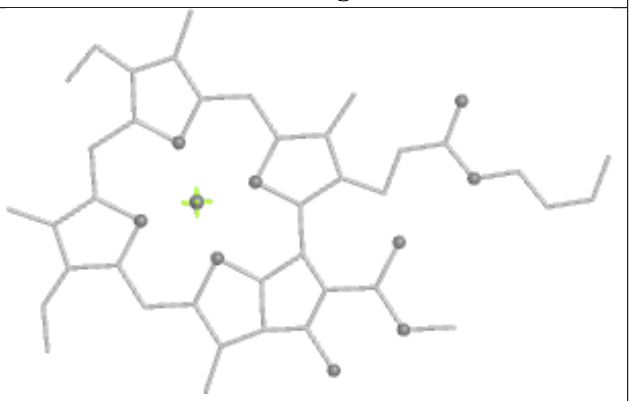
Bond lengths



Bond angles

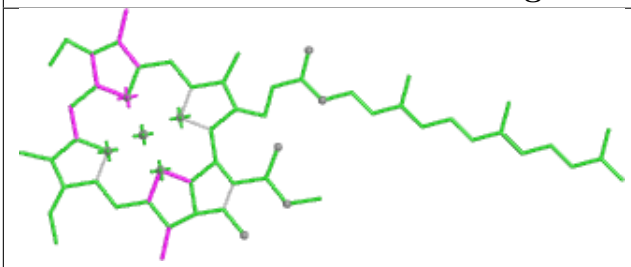


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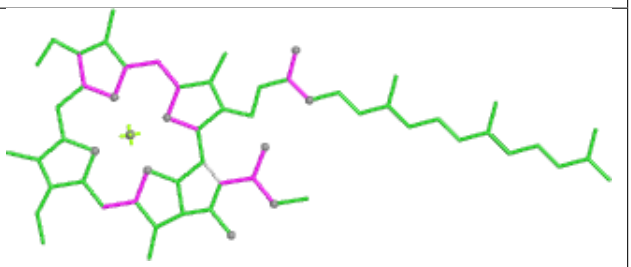


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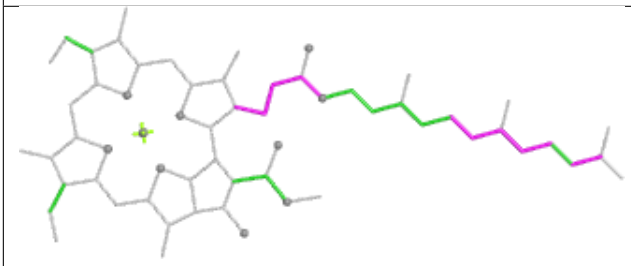
Ligand CLA B 819



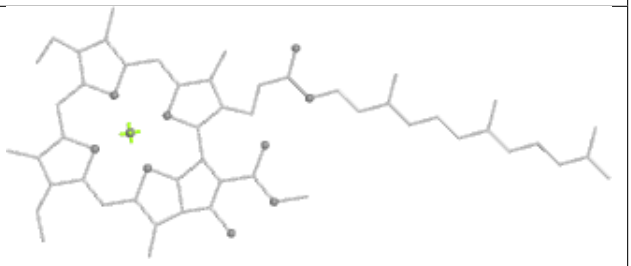
Bond lengths



Bond angles

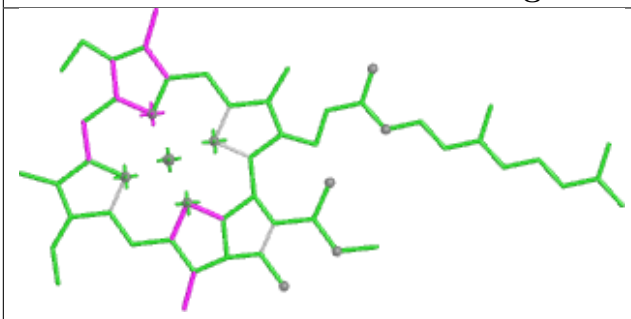


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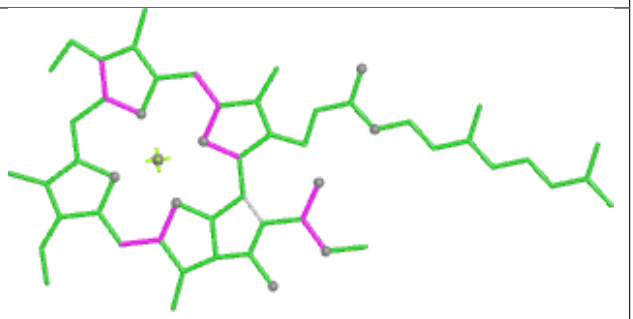


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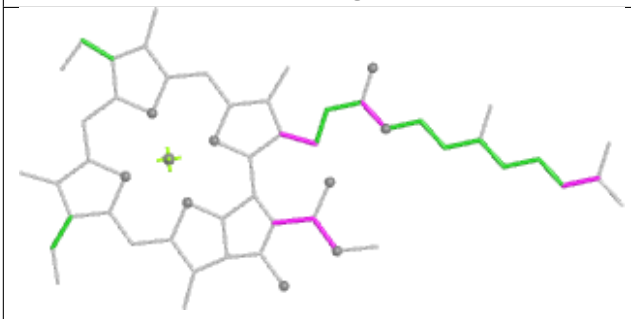
Ligand CLA A 822



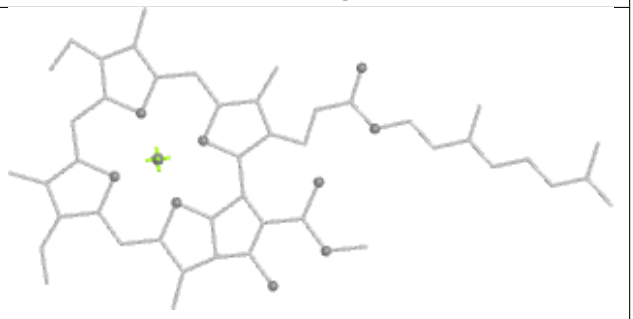
Bond lengths



Bond angles

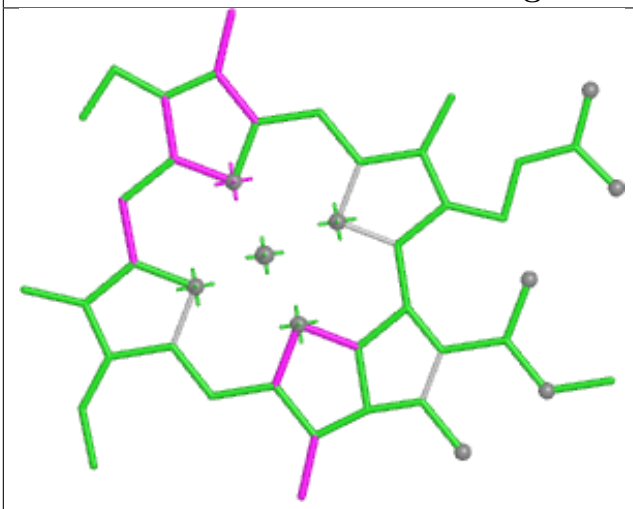


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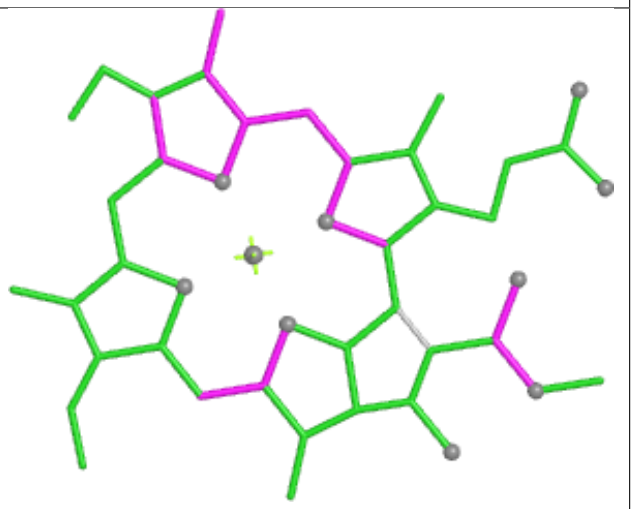


Rings

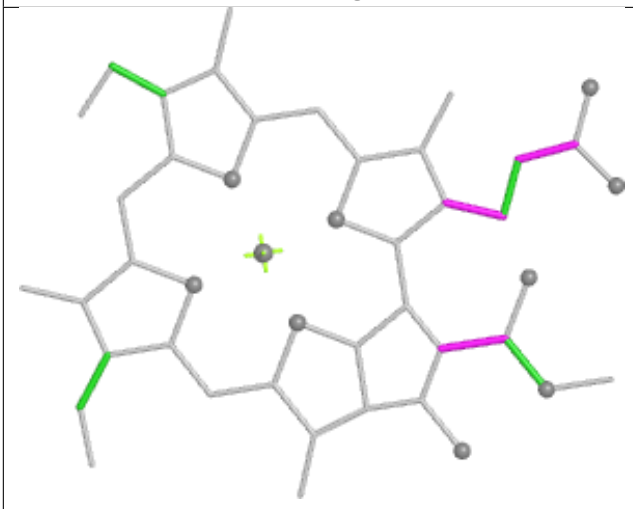
Ligand CLA A 833



Bond lengths



Bond angles

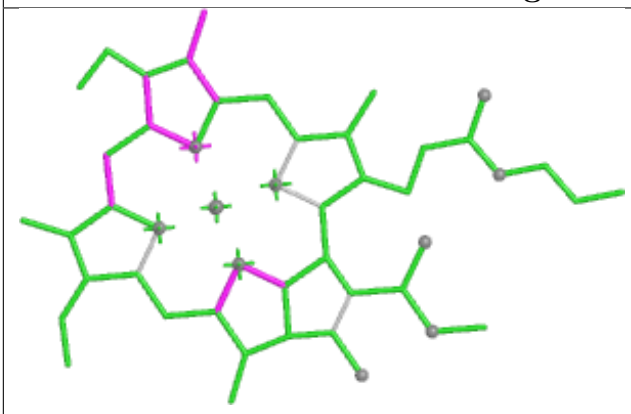


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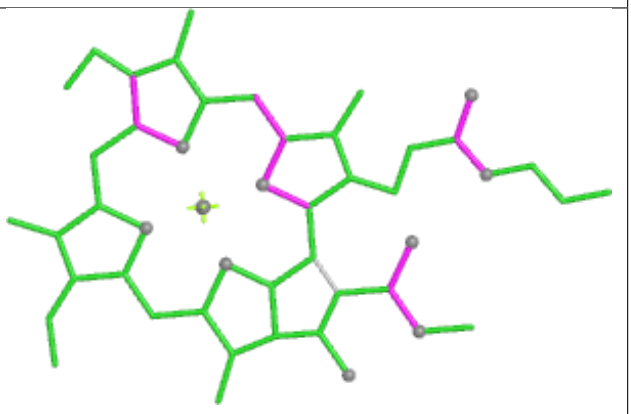


Rings

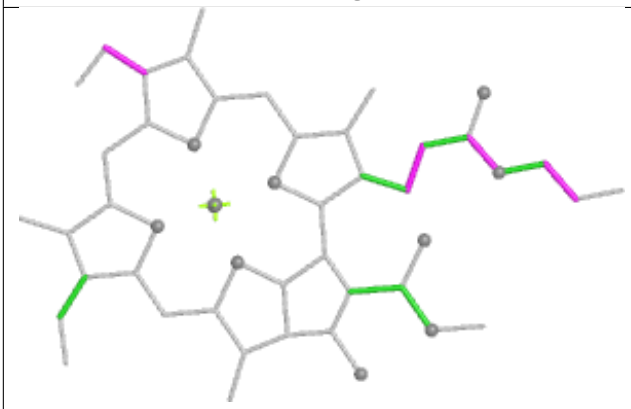
Ligand CLA A 839



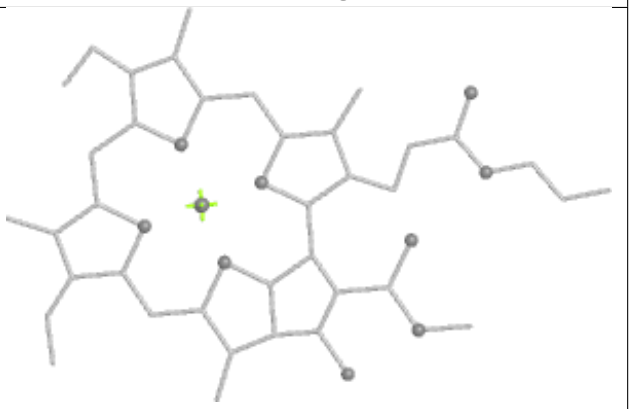
Bond lengths



Bond angles

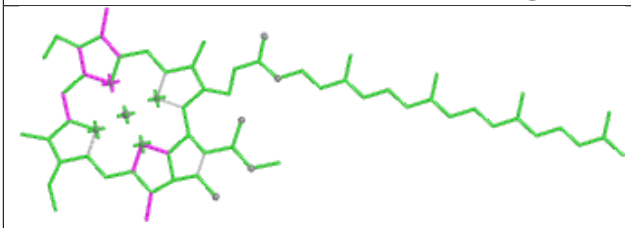


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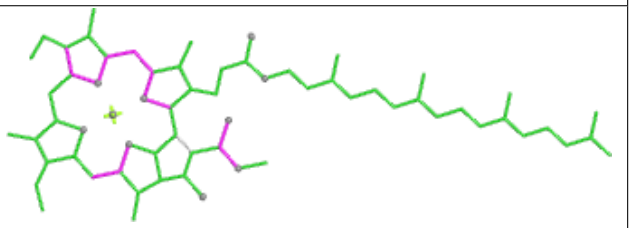


Rings

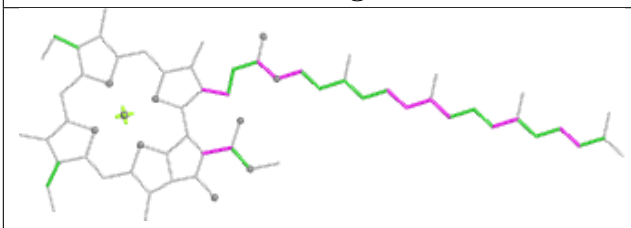
Ligand CLA A 817



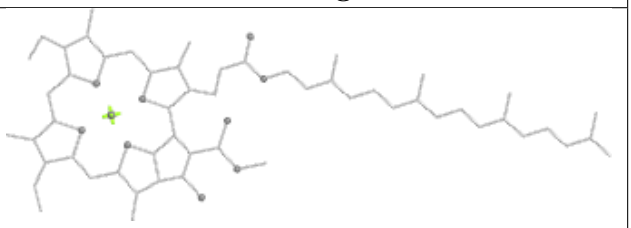
Bond lengths



Bond angles

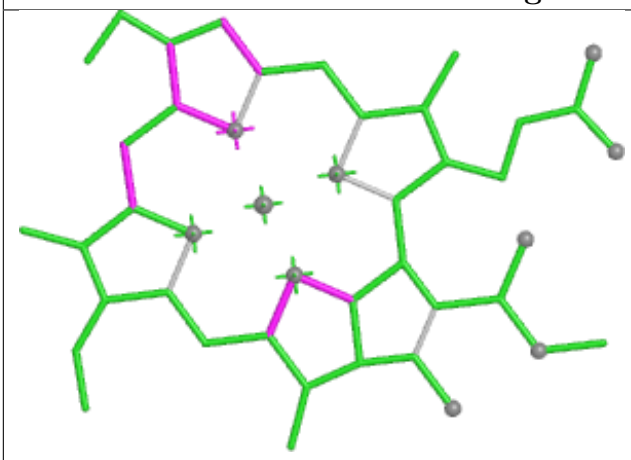


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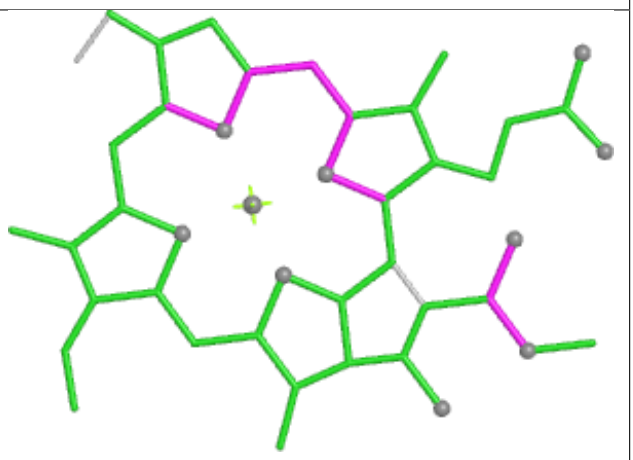


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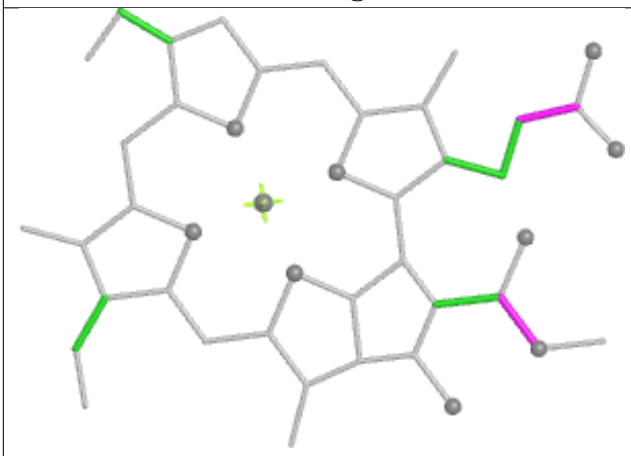
Ligand CLA B 813



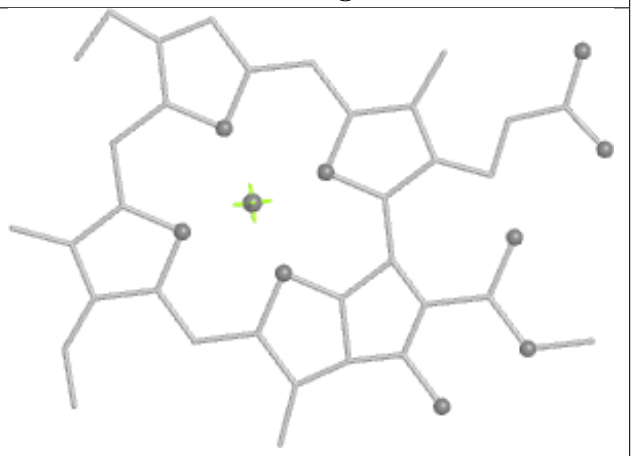
Bond lengths



Bond angles

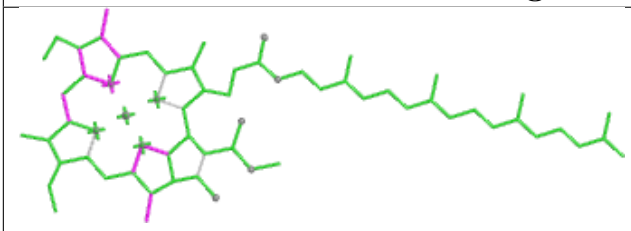


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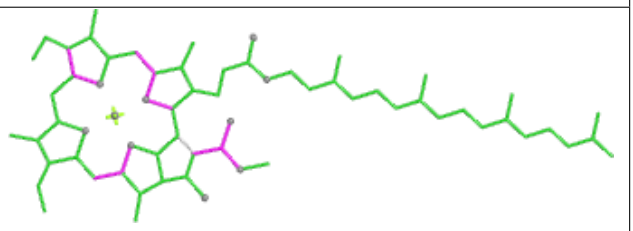


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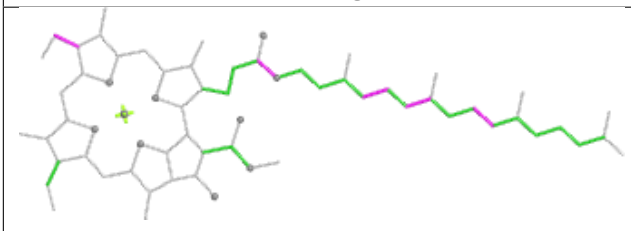
Ligand CLA L 304



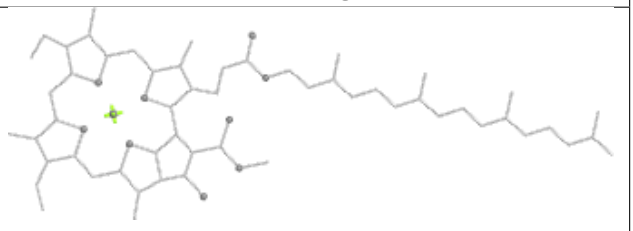
Bond lengths



Bond angles

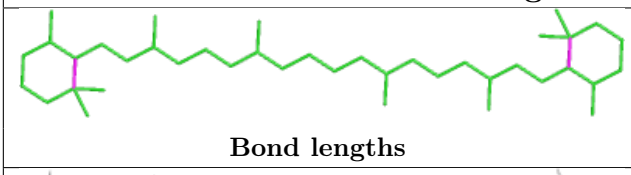


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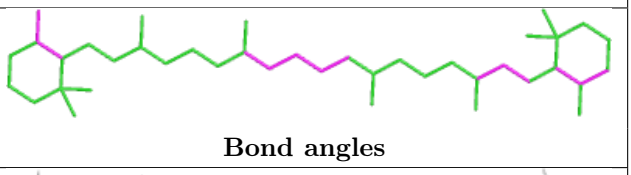


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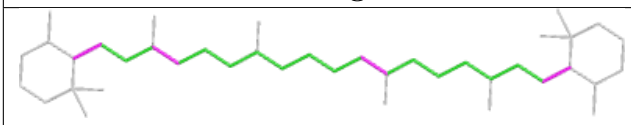
Ligand BCR L 302



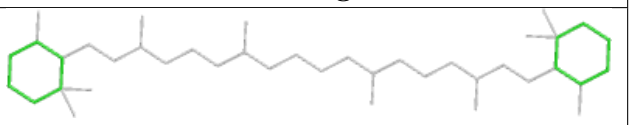
Bond lengths



Bond angles

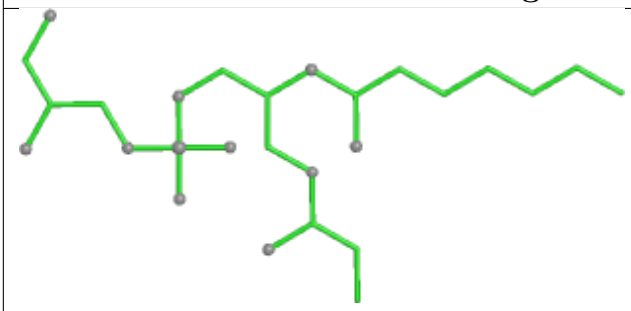


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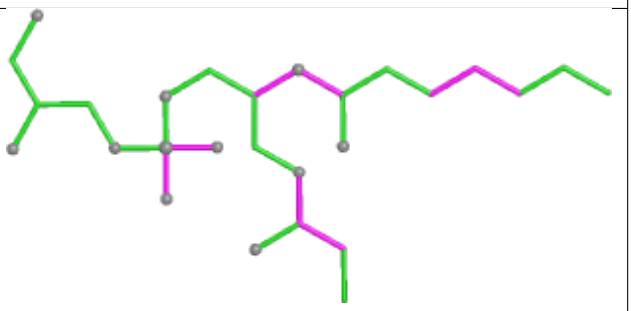


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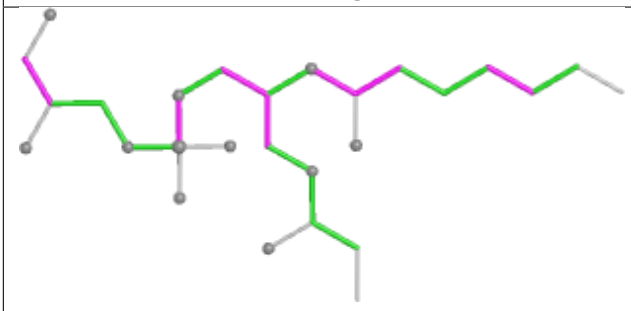
Ligand LHG A 843



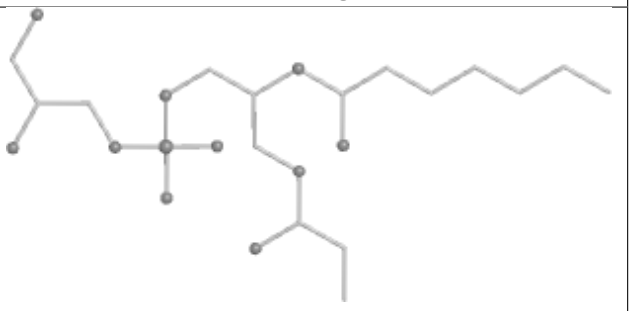
Bond lengths



Bond angles

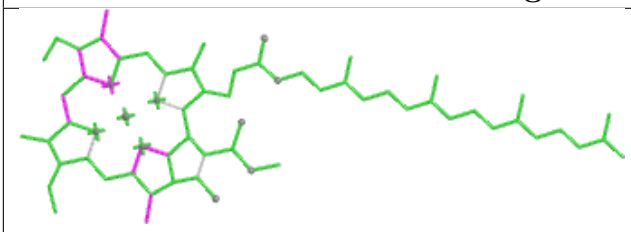


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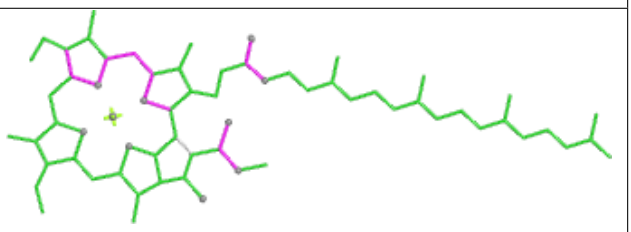


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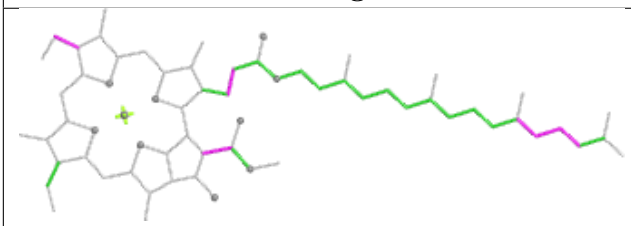
Ligand CLA B 831



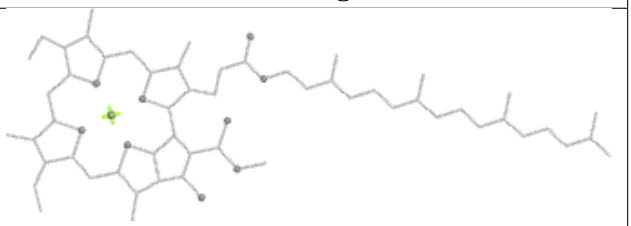
Bond lengths



Bond angles

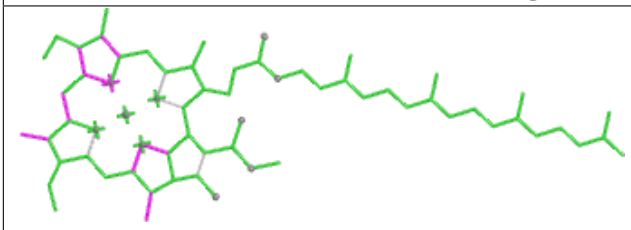


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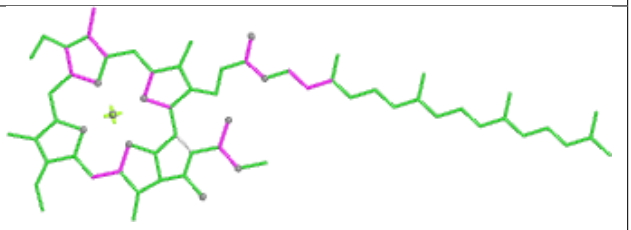


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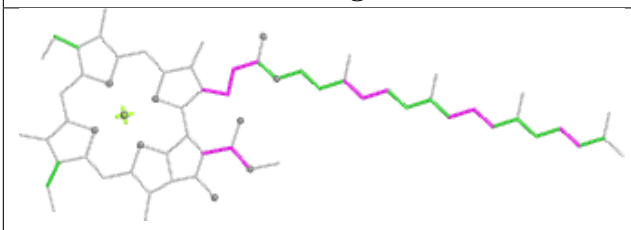
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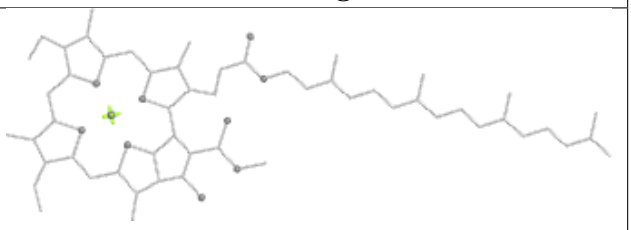
Bond lengths



Bond angles

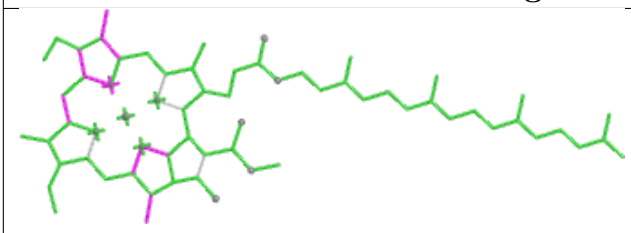


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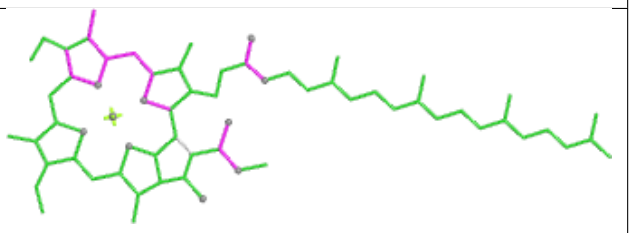


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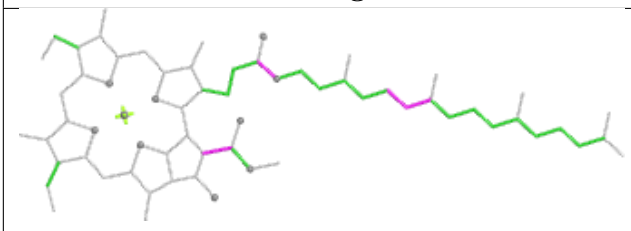
Ligand CLA B 825



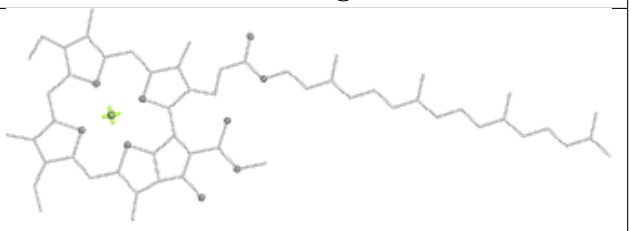
Bond lengths



Bond angles

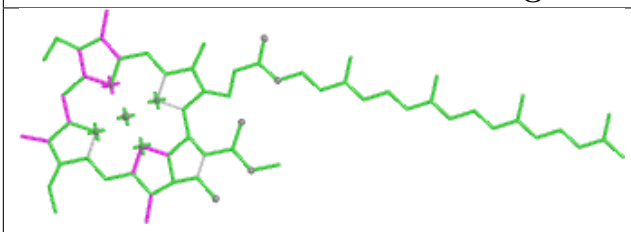


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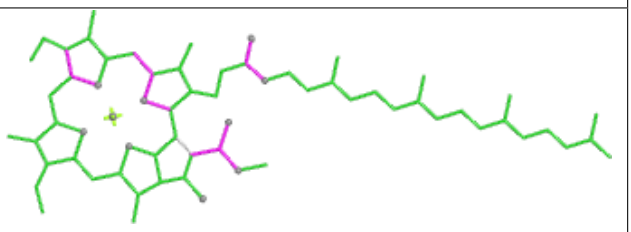


Rings

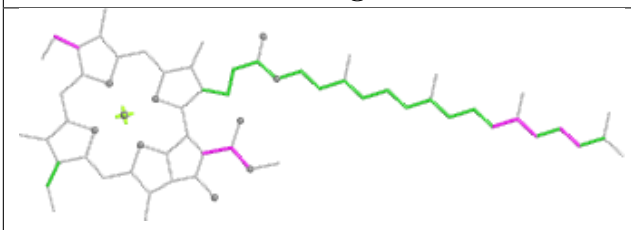
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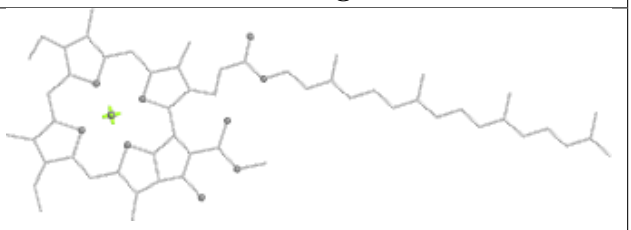
Bond lengths



Bond angles

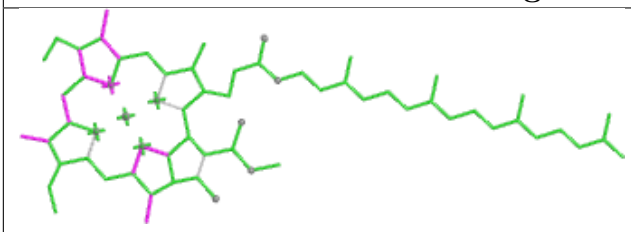


Torsions

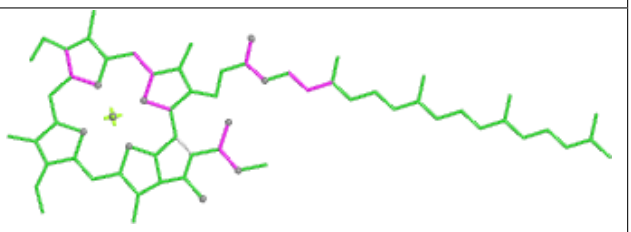


Rings

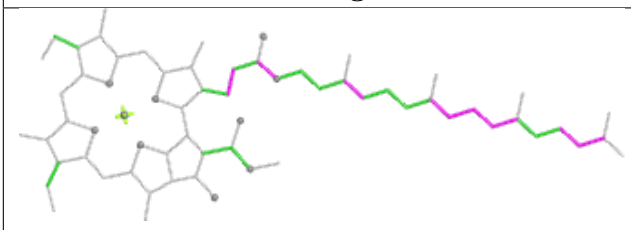
Ligand CLA A 827



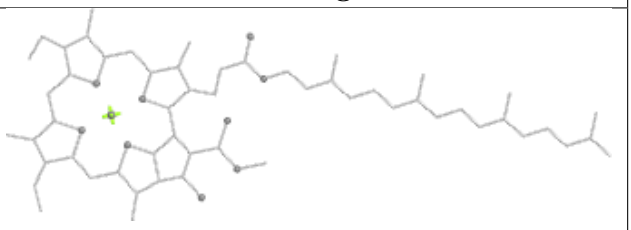
Bond lengths



Bond angles

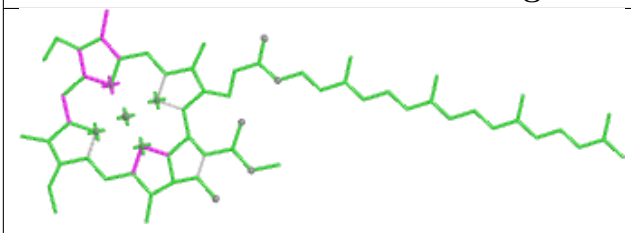


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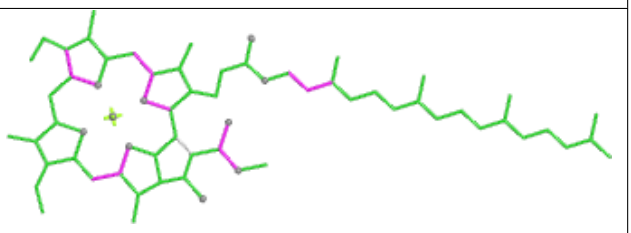


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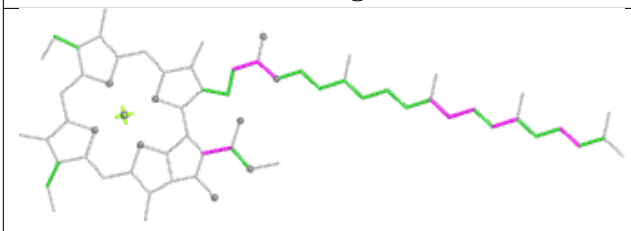
Ligand CLA H 201



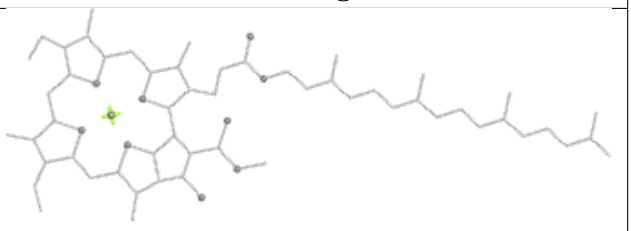
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Bond angles

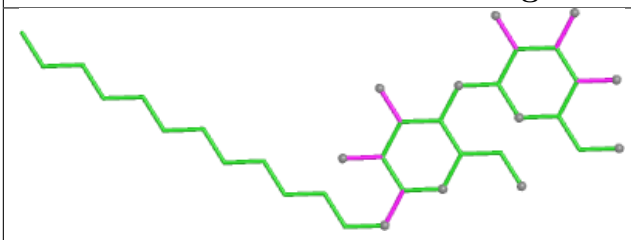


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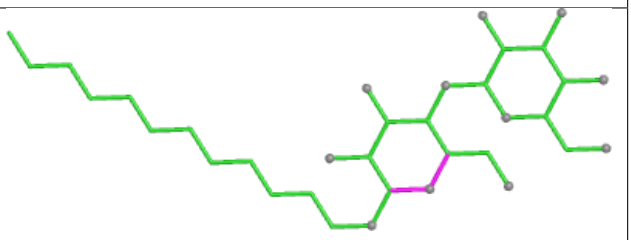


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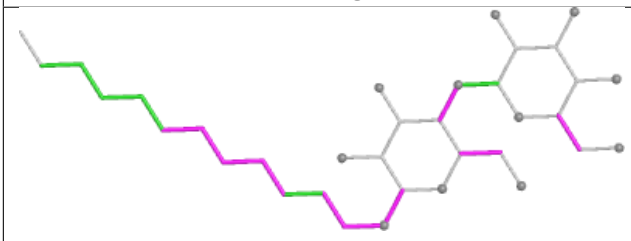
Ligand LMT B 838



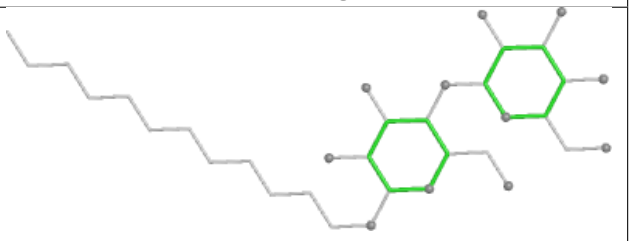
Bond lengths



Bond angles

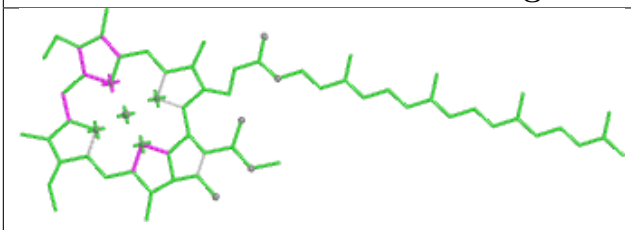


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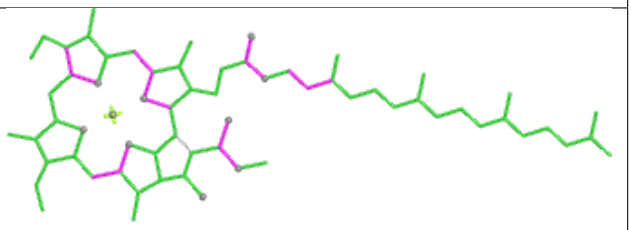


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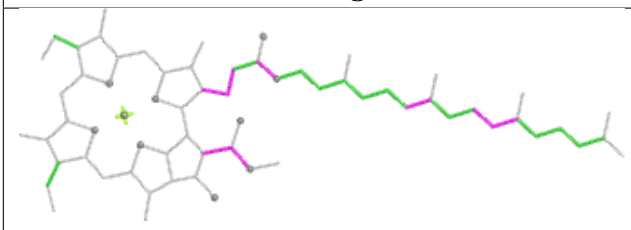
Ligand CLA A 811



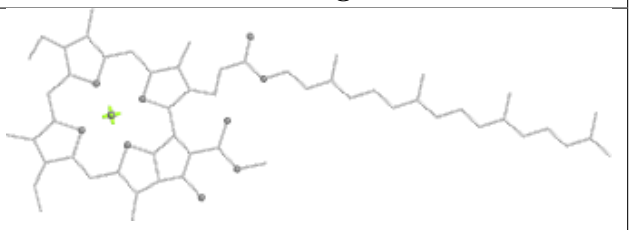
Bond lengths



Bond angles

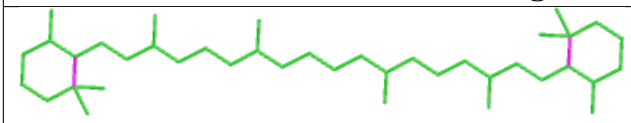


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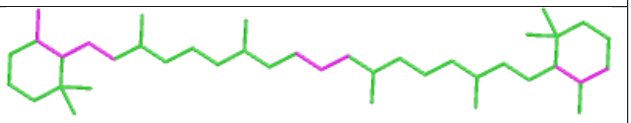


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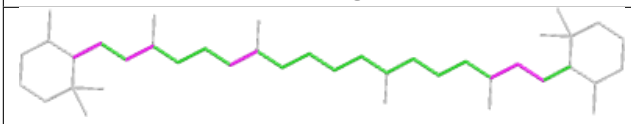
Ligand BCR I 101



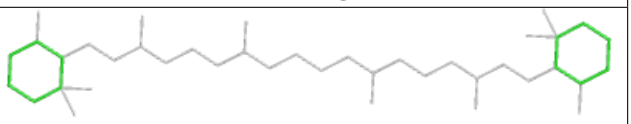
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Bond angles

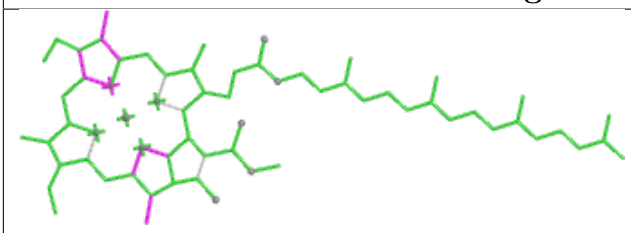


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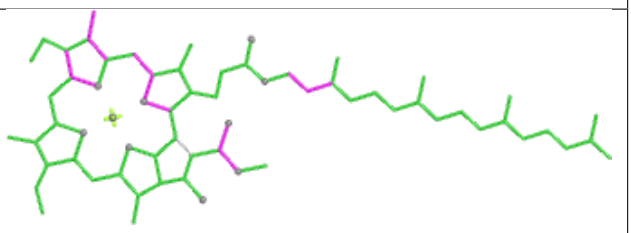


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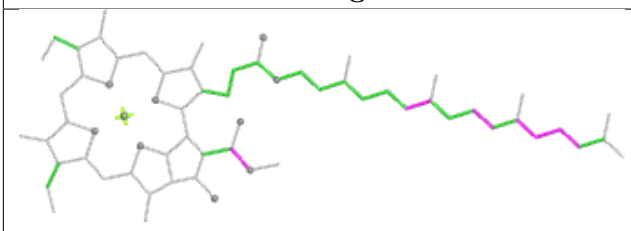
Ligand CLA B 810



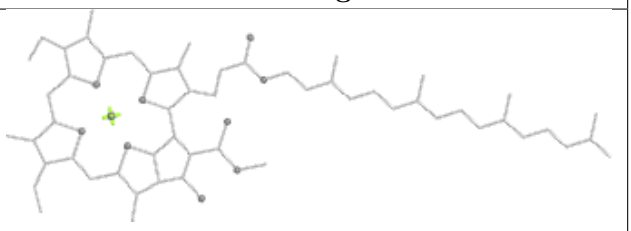
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Bond angles

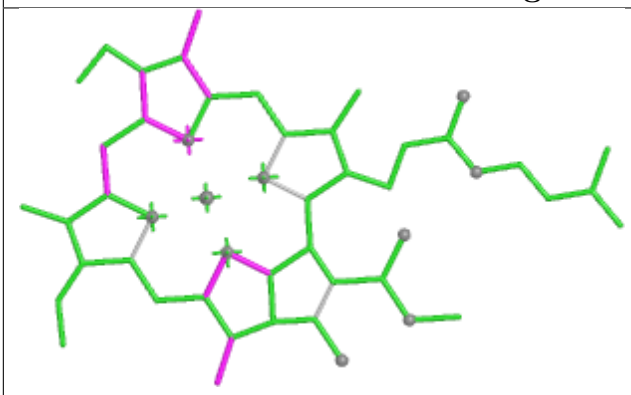


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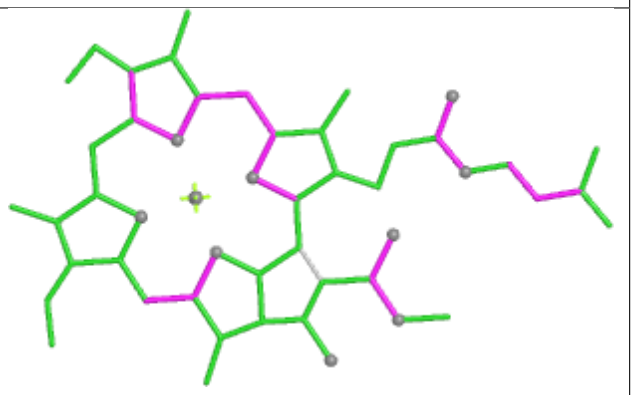


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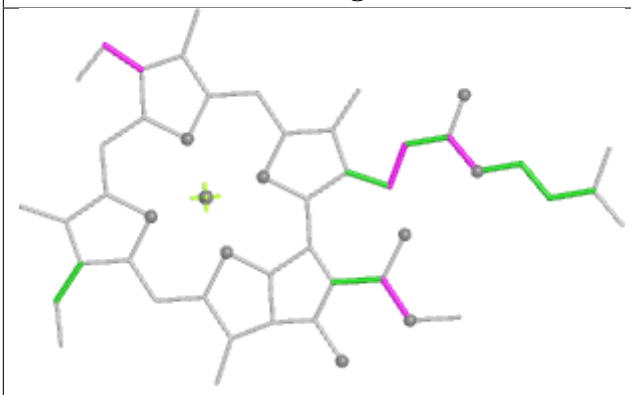
Ligand CLA A 813



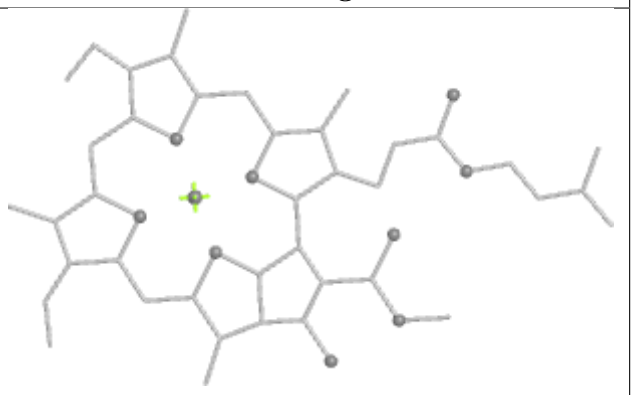
Bond lengths



Bond angles

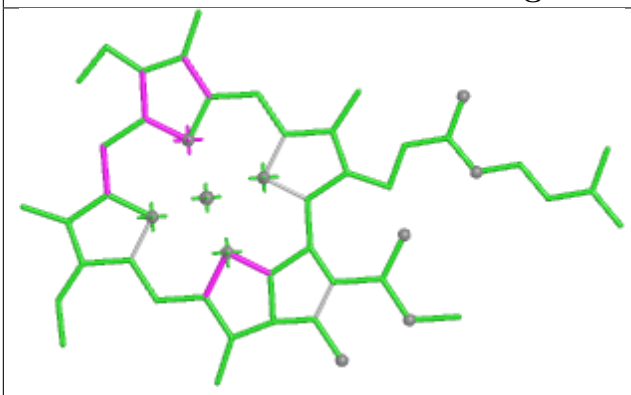


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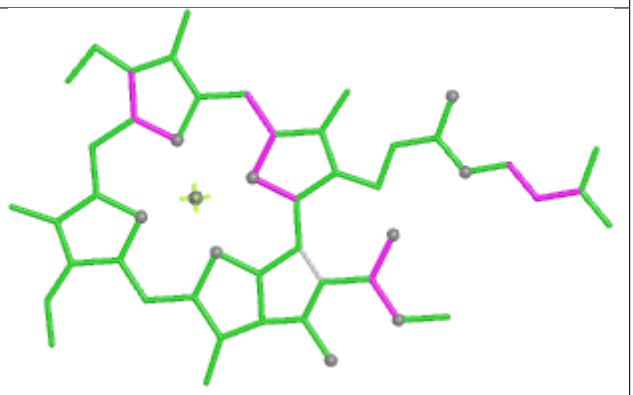


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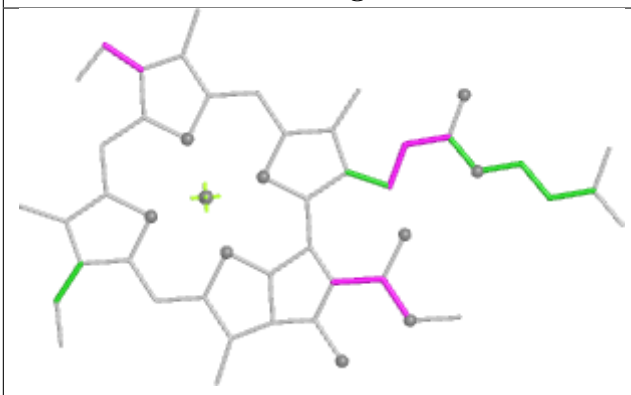
Ligand CLA B 820



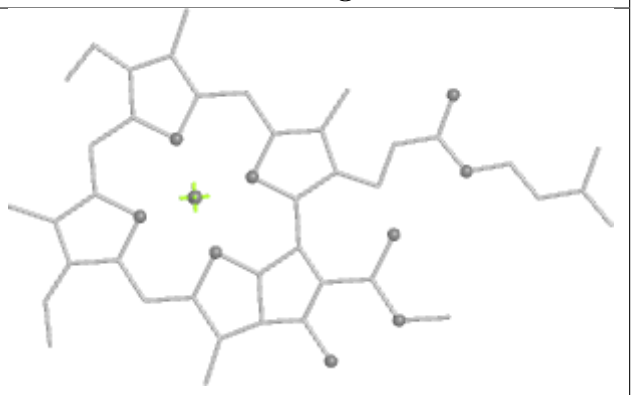
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Bond angles

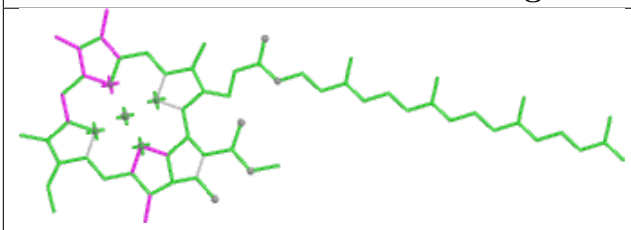


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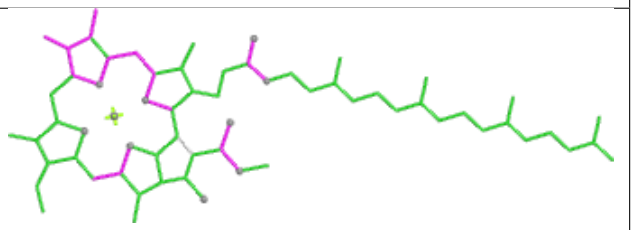


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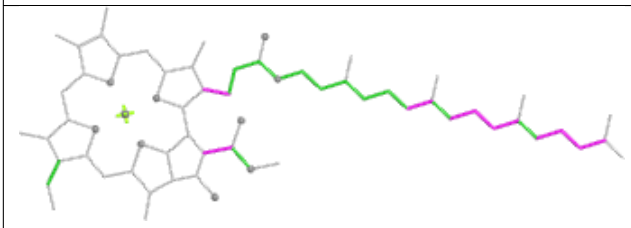
Ligand CLA B 821



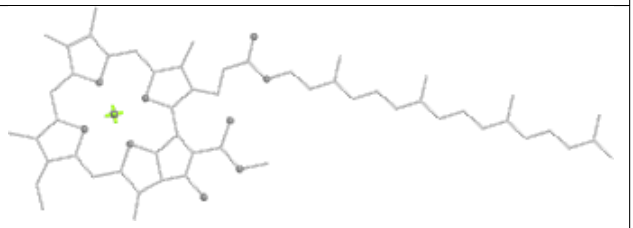
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Bond angles

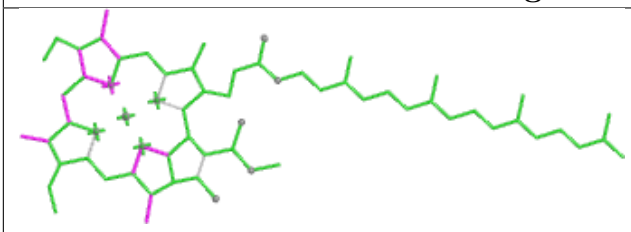


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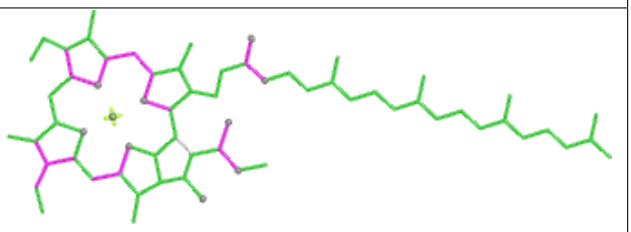


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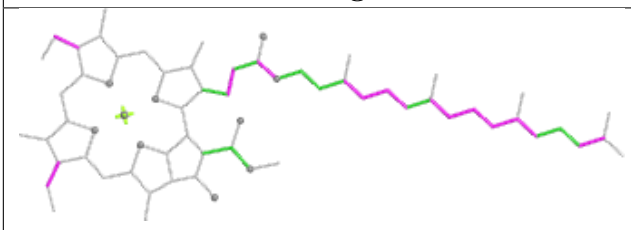
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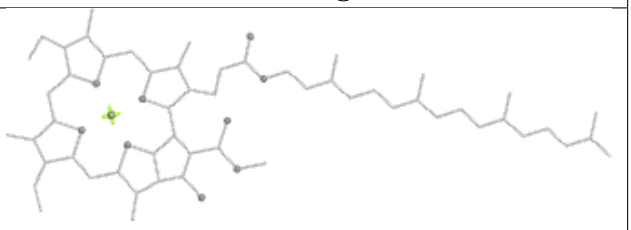
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Bond angles

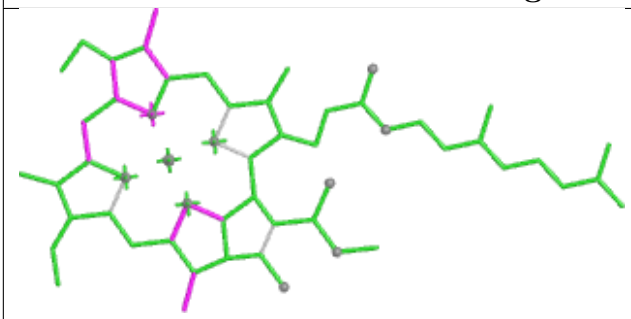


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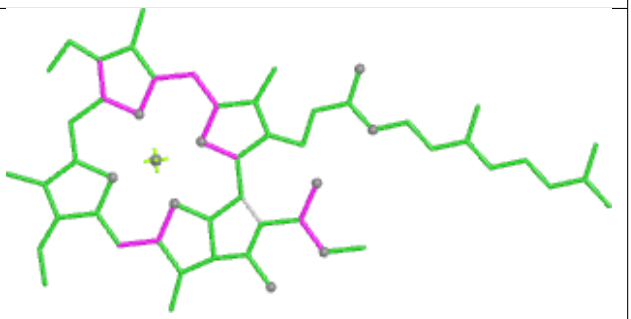


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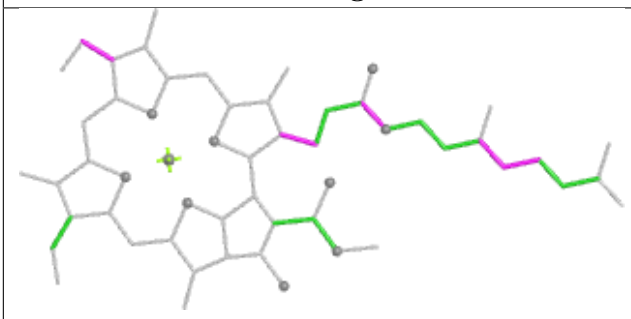
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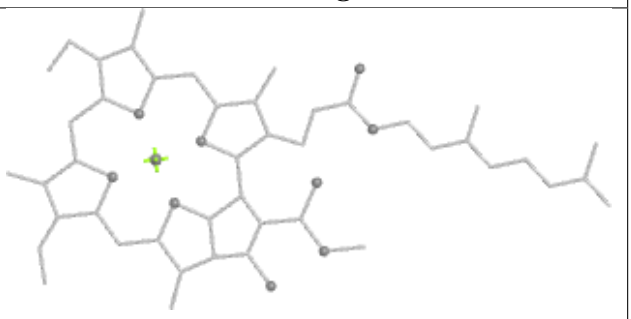
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Bond angles

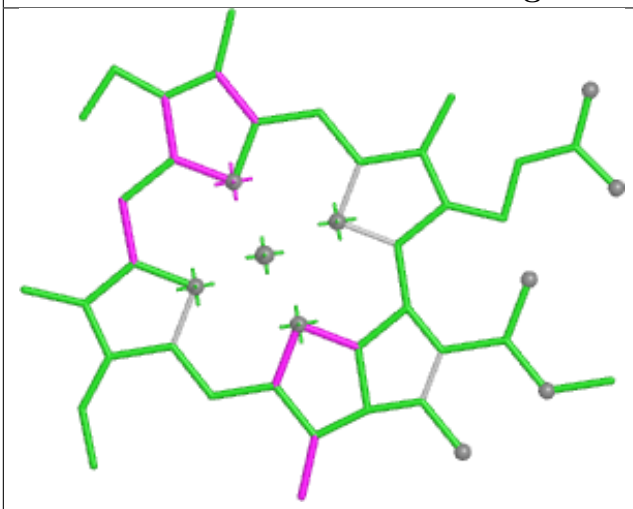


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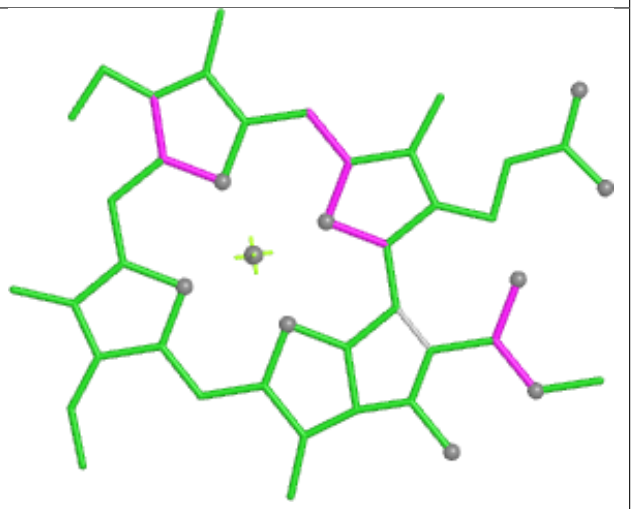


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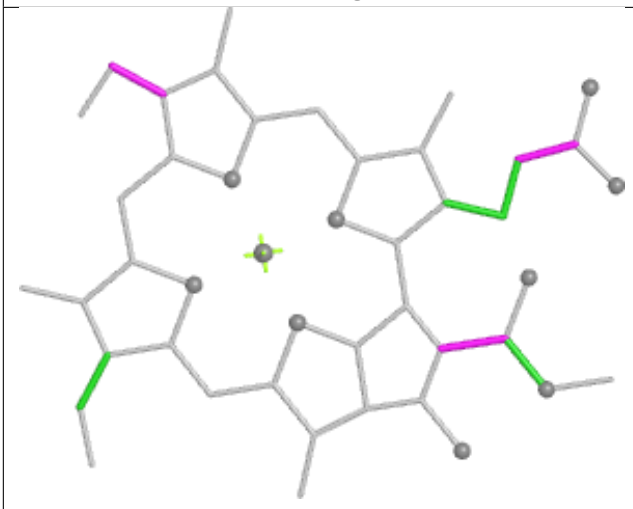
Ligand CLA A 818



Bond lengths



Bond angles

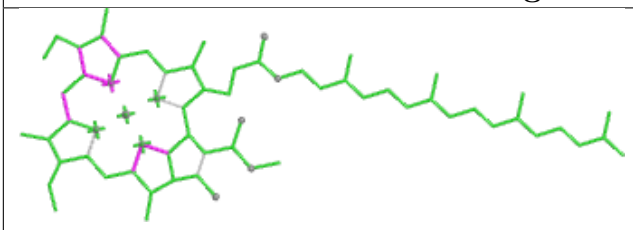


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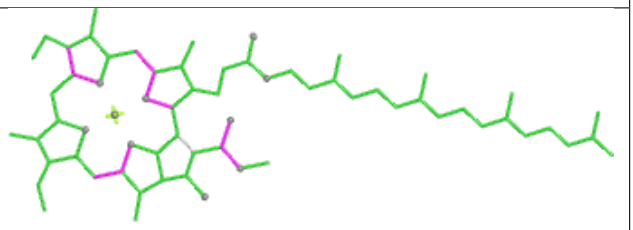


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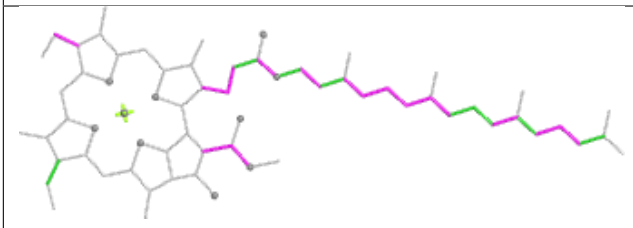
Ligand CLA A 807



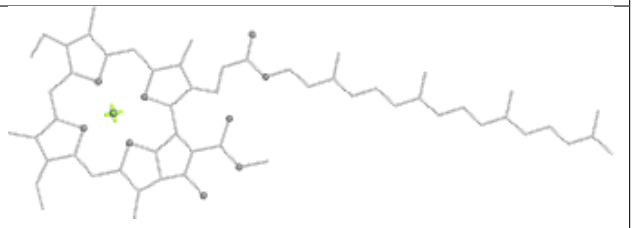
Bond lengths



Bond angles

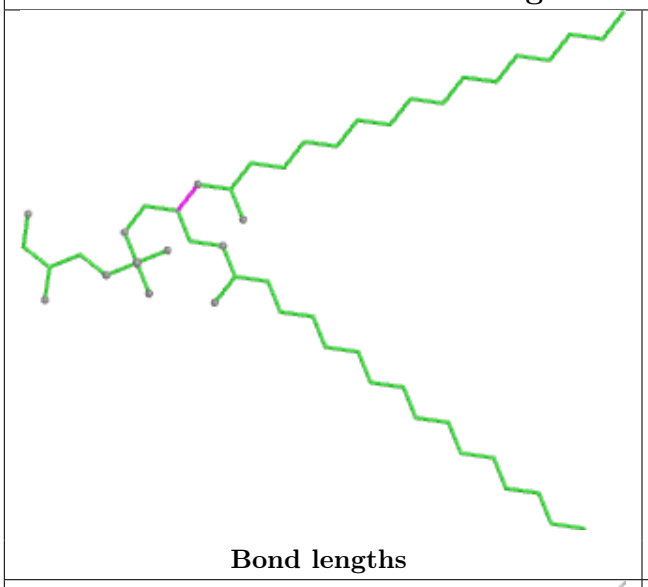


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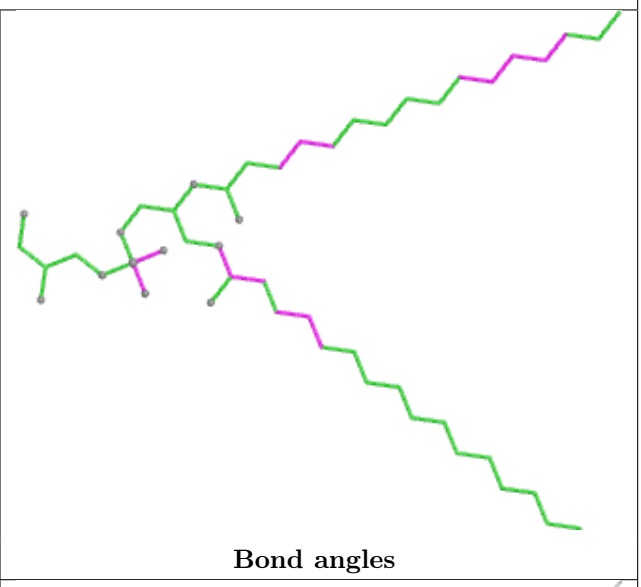


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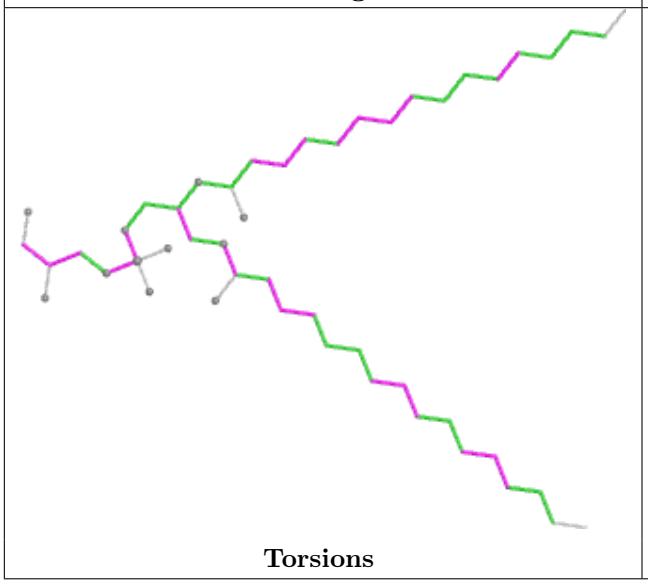
Ligand LHG L 301



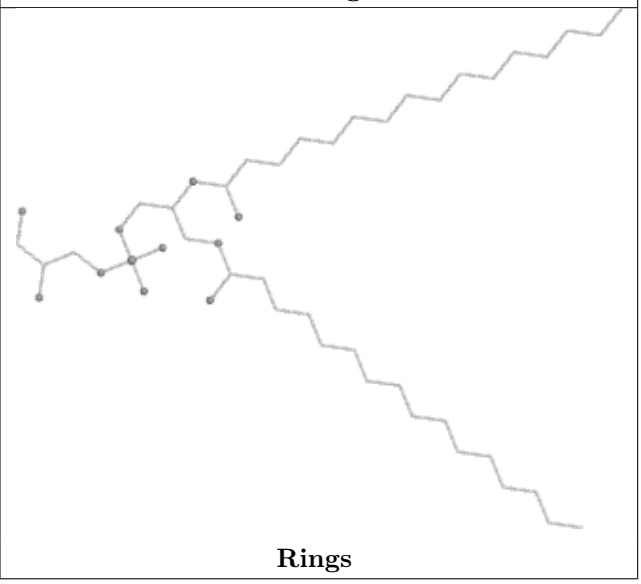
Bond lengths



Bond angles

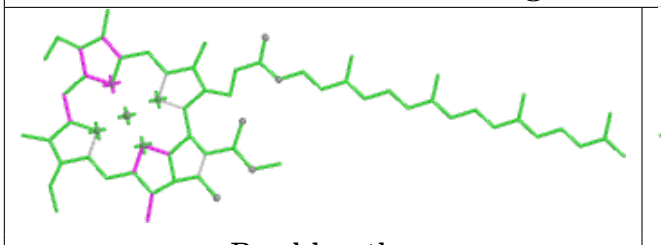


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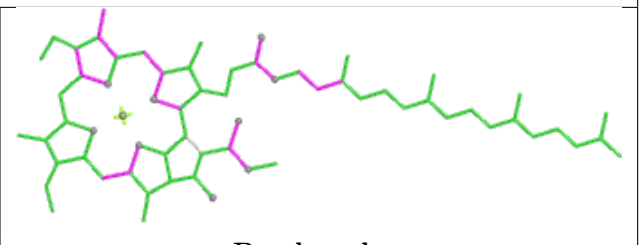


Rings

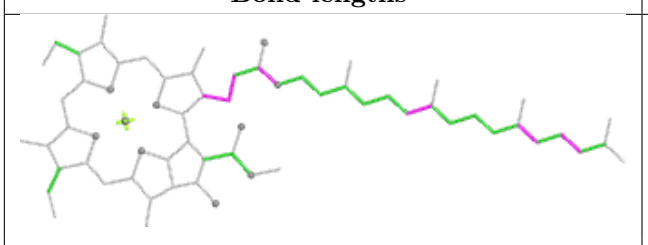
Ligand CLA A 805



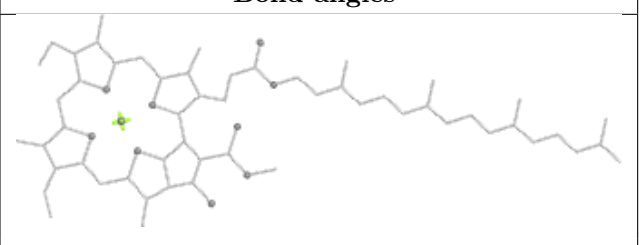
Bond lengths



Bond angles

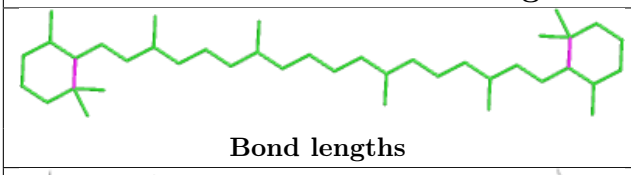


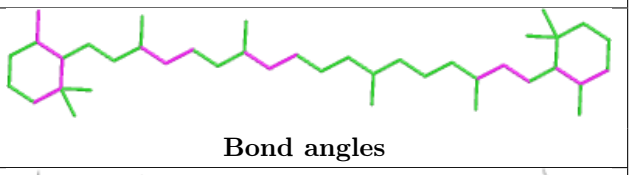
Torsions

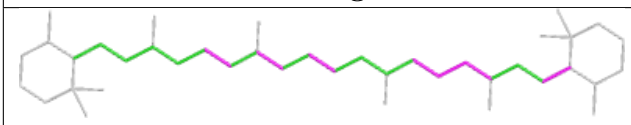


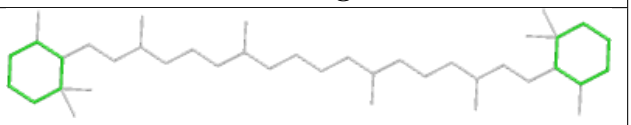
Rings

Ligand BCR A 845

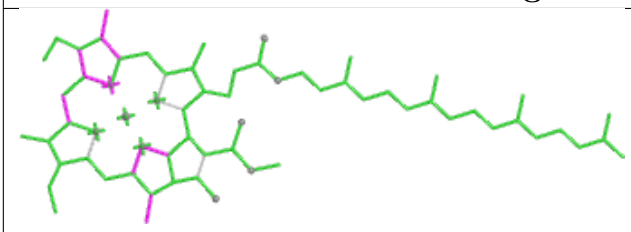

Bond lengths

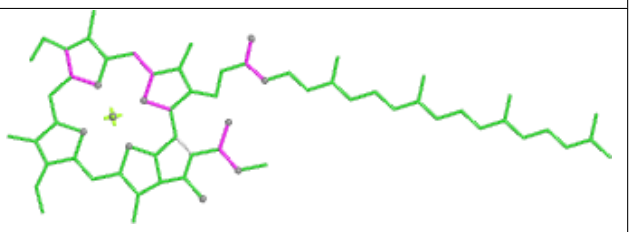

Bond angles

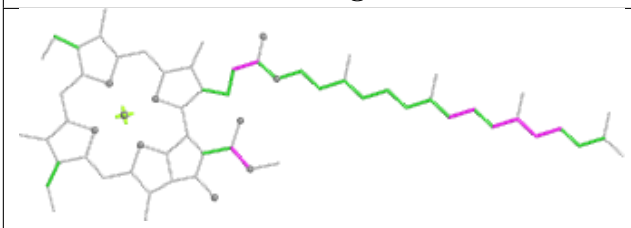

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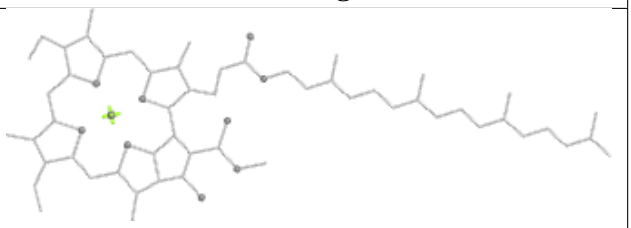

Rings

Ligand CLA A 823

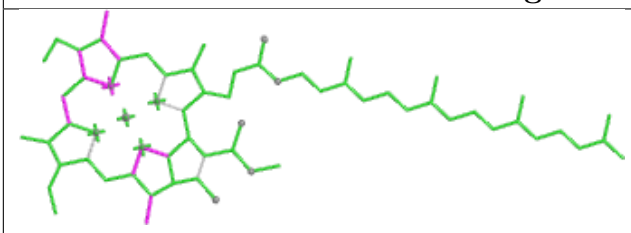

Bond lengths

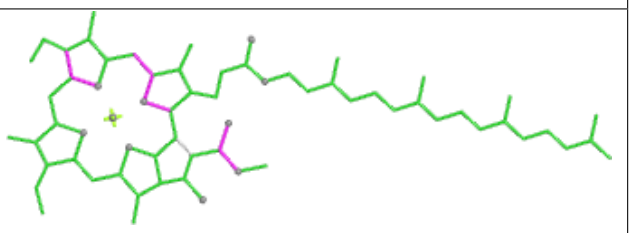

Bond angles

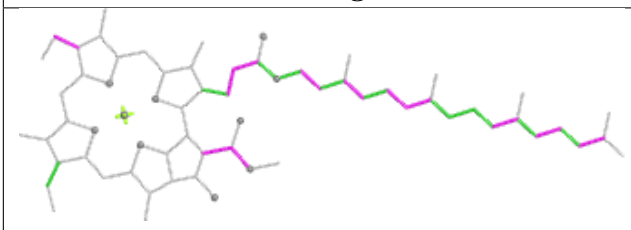

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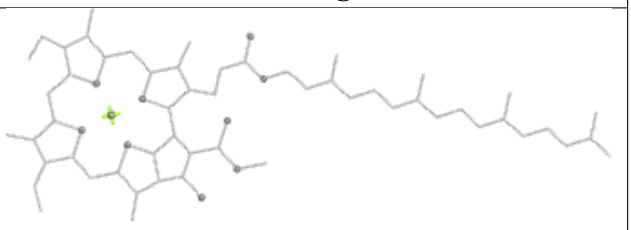

Rings

Ligand CLA B 811

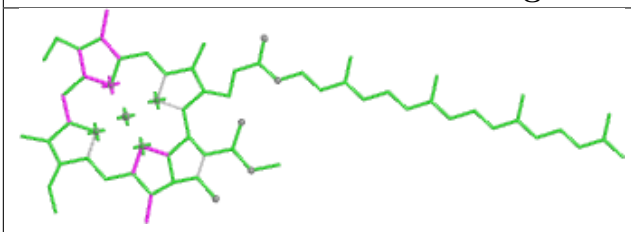

Bond lengths


Bond angles

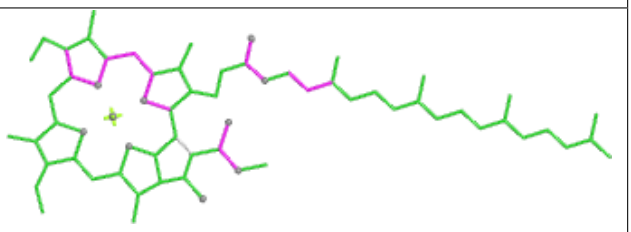

Torsions


Rings

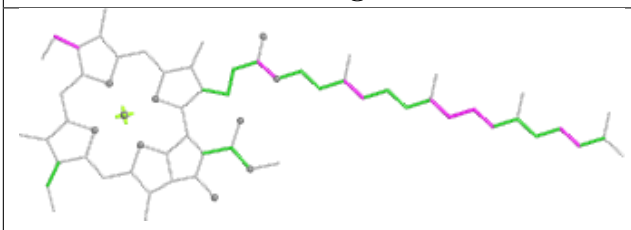
Ligand CLA A 835



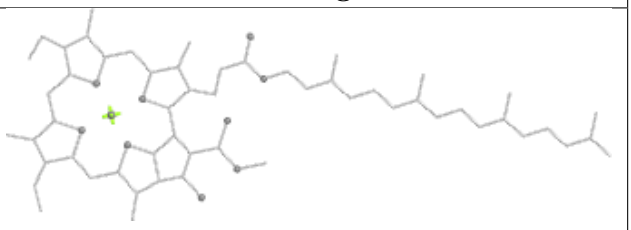
Bond lengths



Bond angles

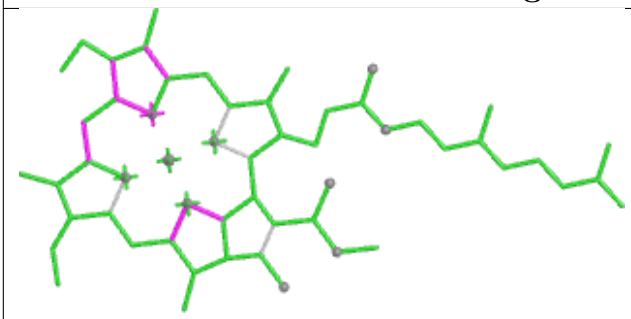


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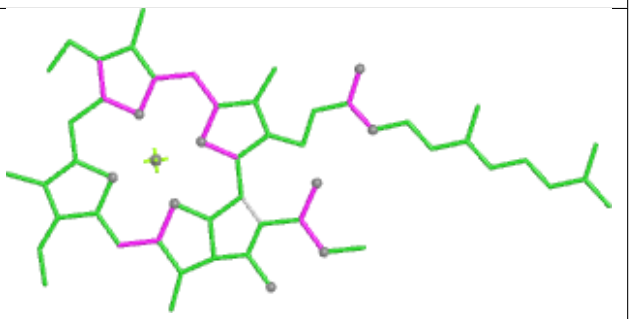


Rings

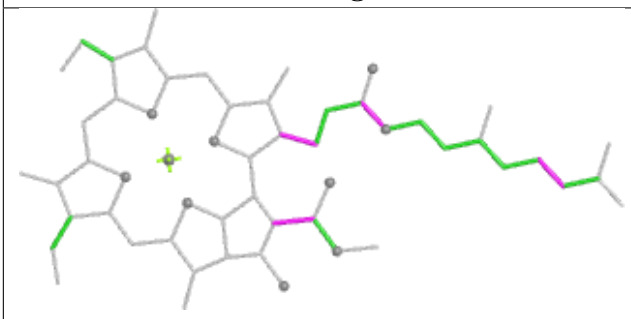
Ligand CLA A 803



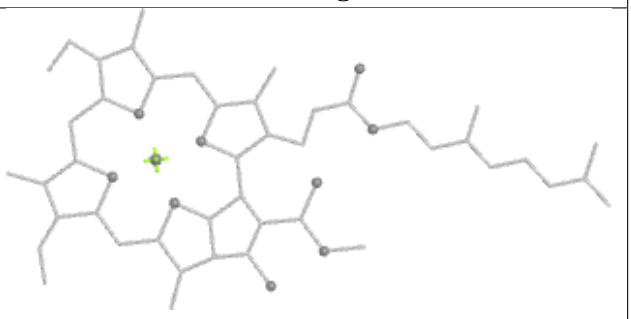
Bond lengths



Bond angles

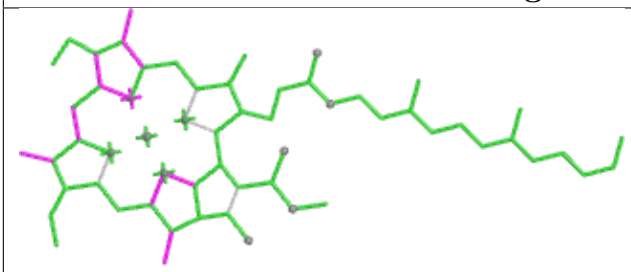


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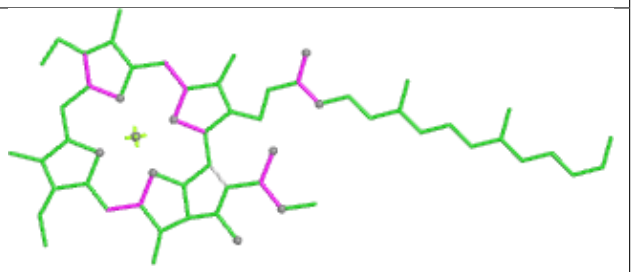


Rings

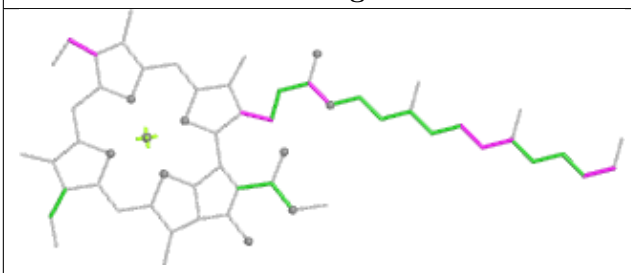
Ligand CLA B 818



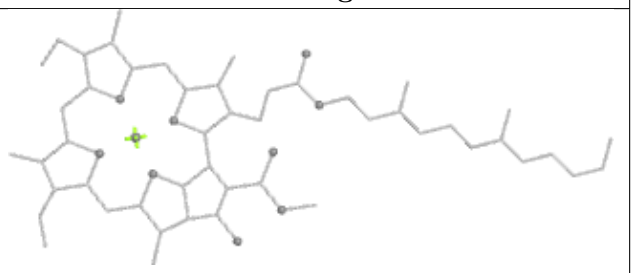
Bond lengths



Bond angles

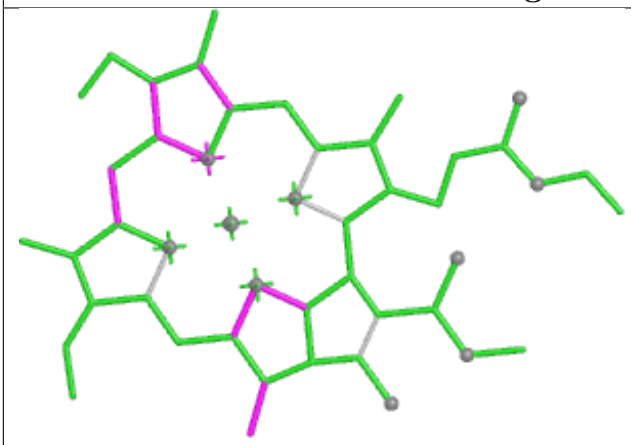


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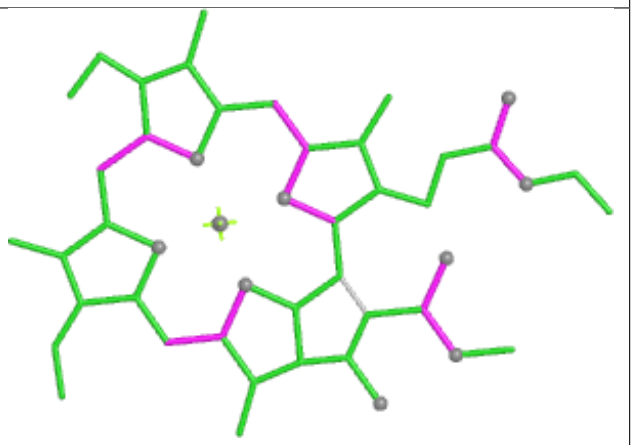


Rings

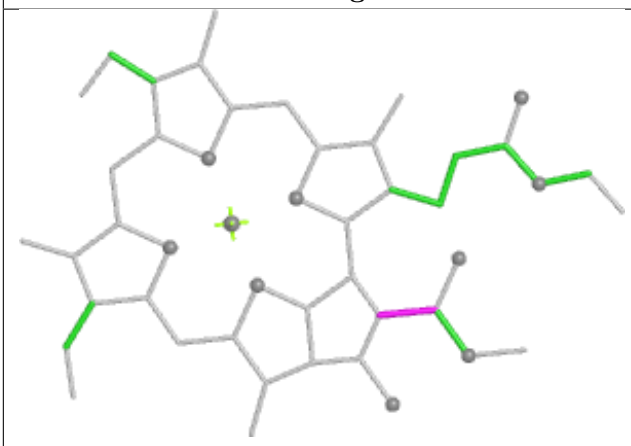
Ligand CLA B 830



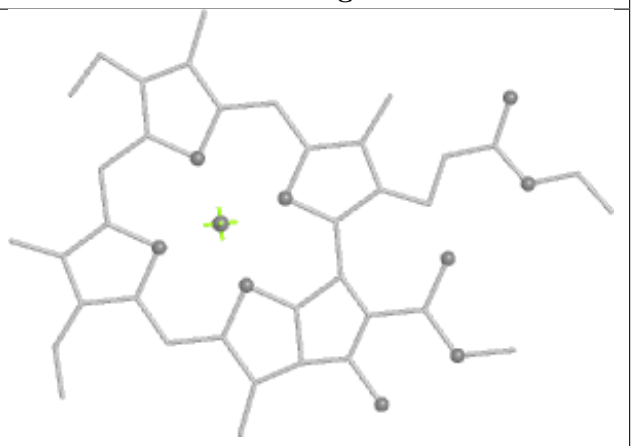
Bond lengths



Bond angles

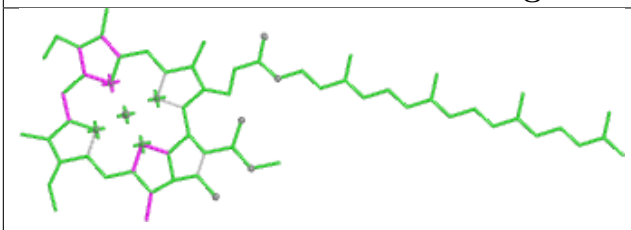


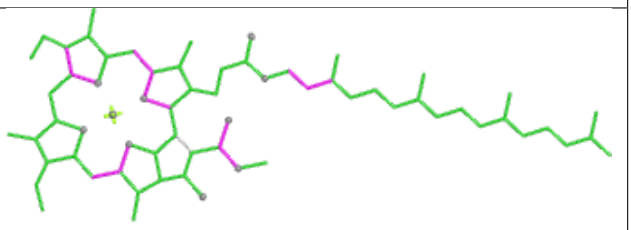
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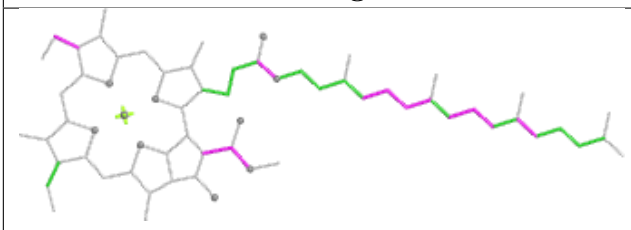


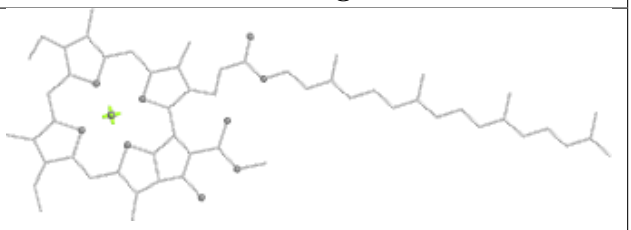
Rings

Ligand CLA A 806

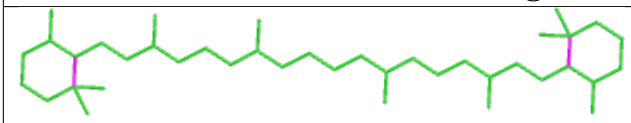

Bond lengths

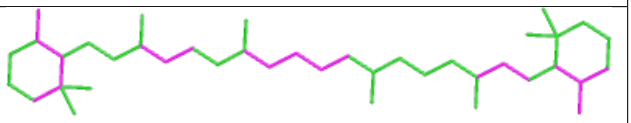

Bond angles


Torsions

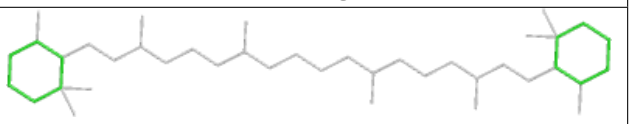

Rings

Ligand BCR L 306

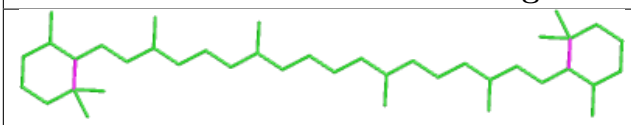

Bond lengths

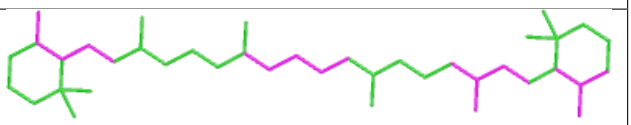

Bond angles

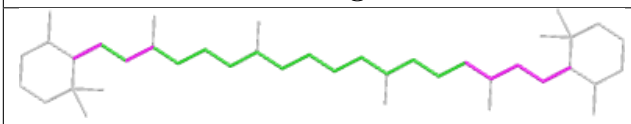

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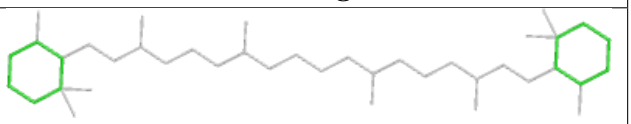

Rings

Ligand BCR A 847

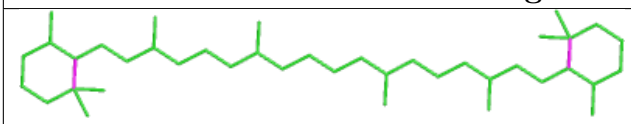

Bond lengths

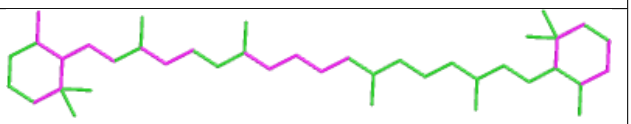

Bond angles

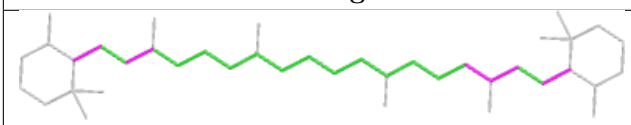

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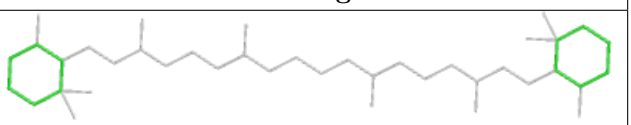

Rings

Ligand BCR L 308

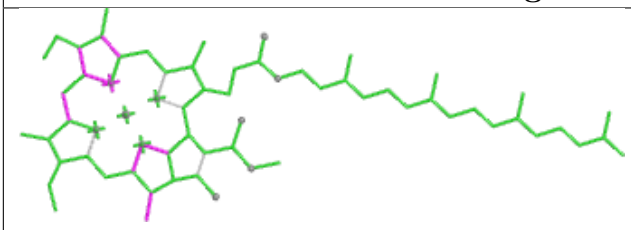

Bond lengths


Bond angles

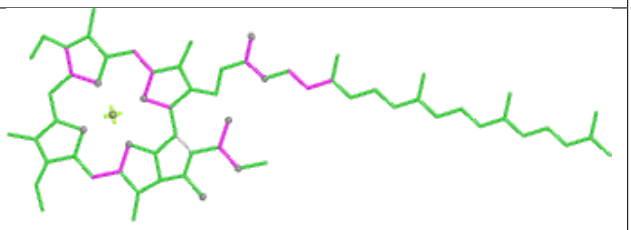

Torsions


Rings

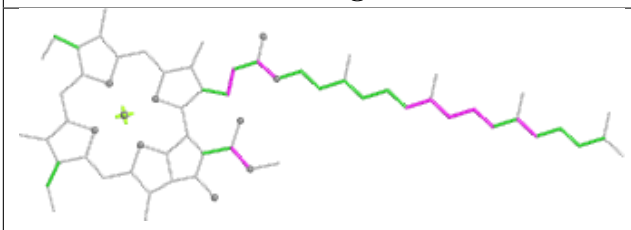
Ligand CLA B 823



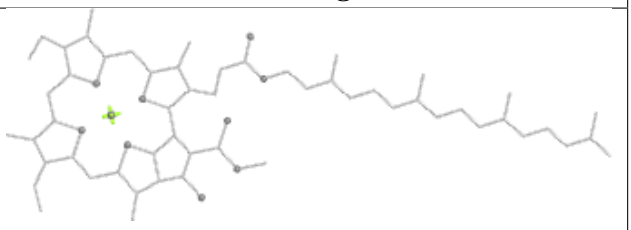
Bond lengths



Bond angles

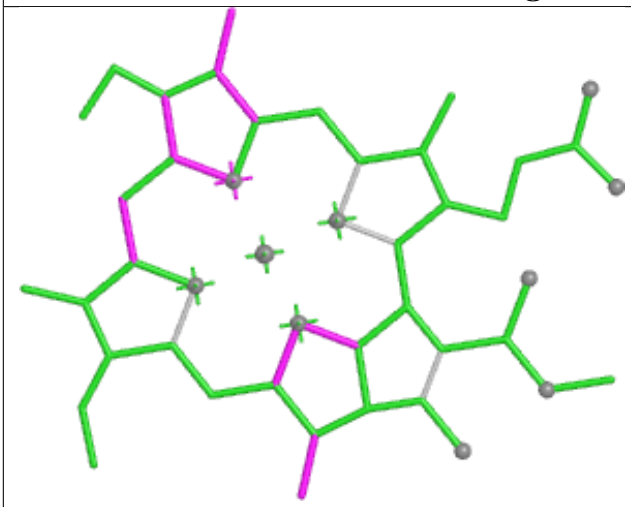


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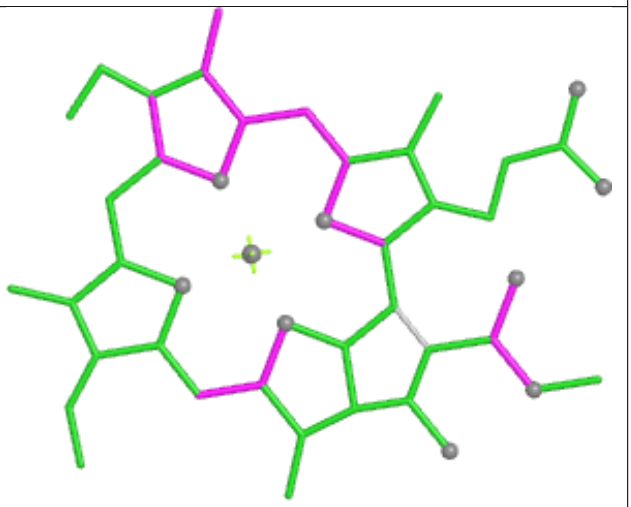


Rings

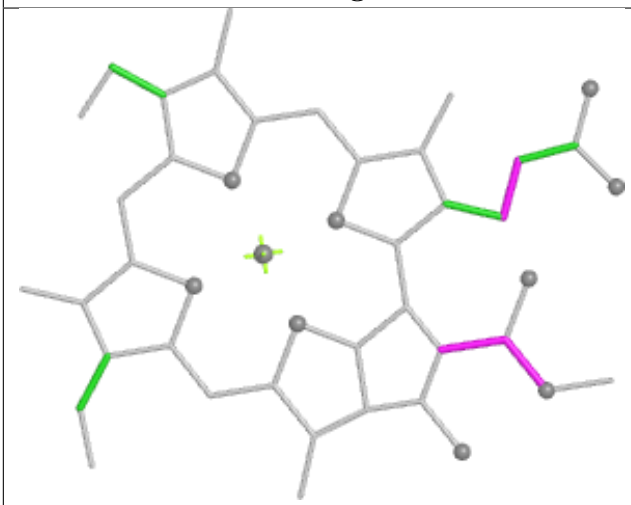
Ligand CLA B 827



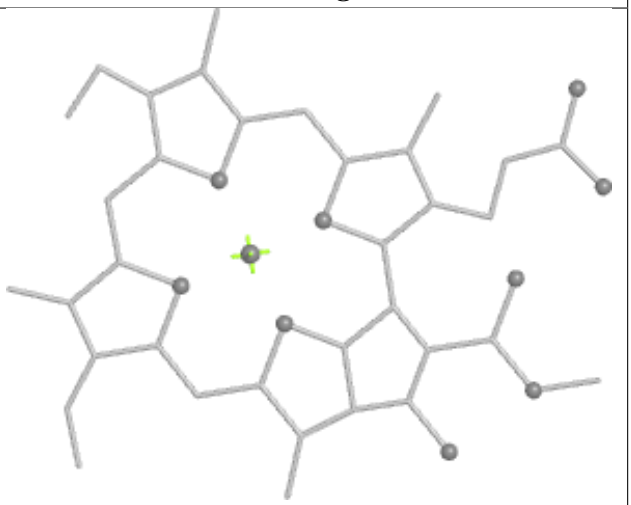
Bond lengths



Bond angles

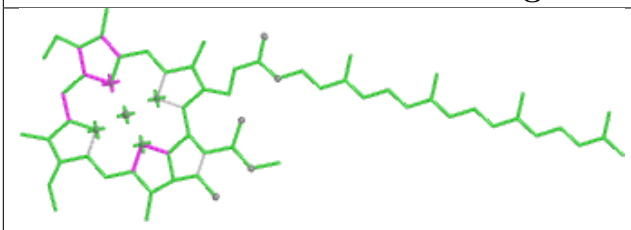


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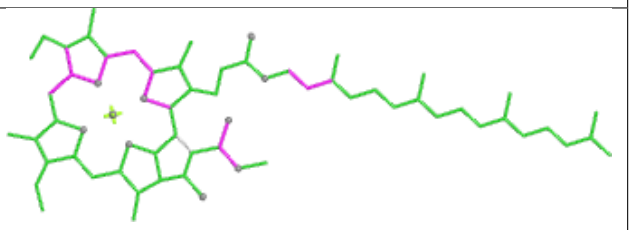


Rings

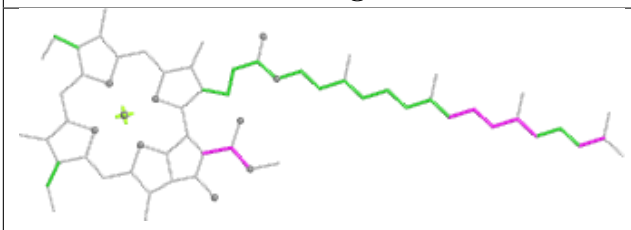
Ligand CLA A 836



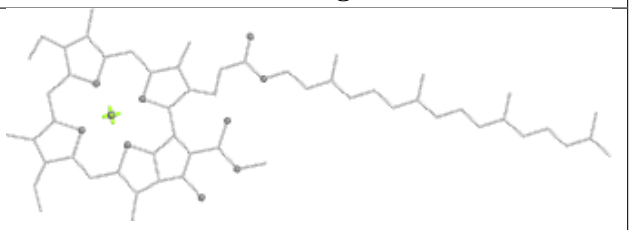
Bond lengths



Bond angles

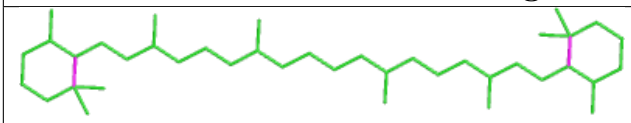


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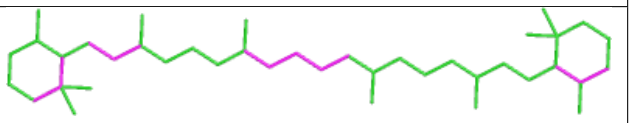


Rings

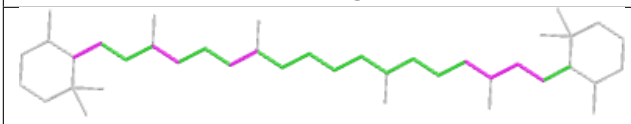
Ligand BCR B 834



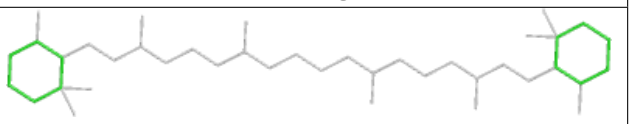
Bond lengths



Bond angles

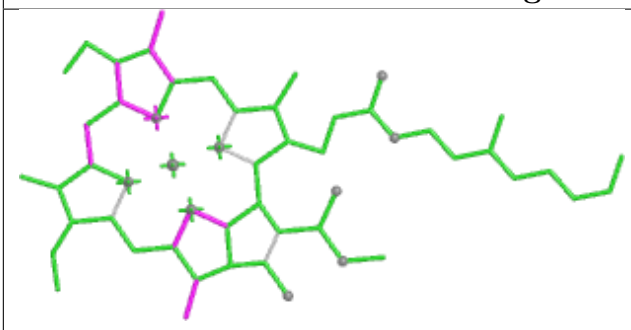


Torsions

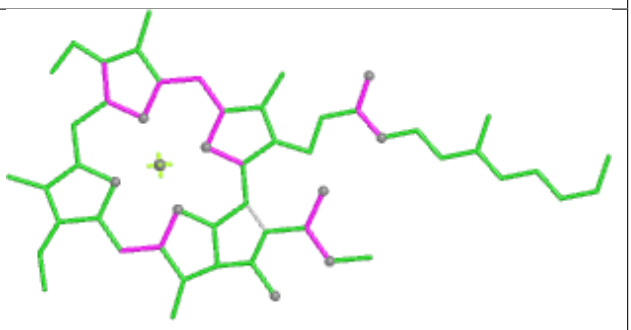


Rings

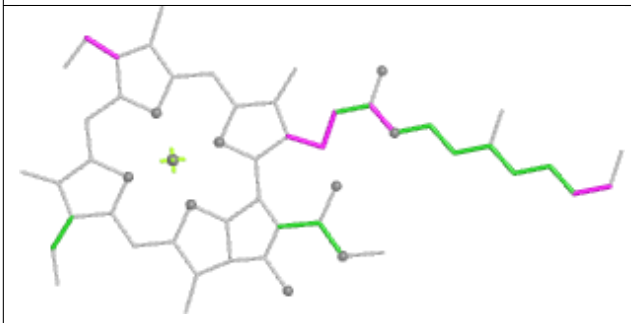
Ligand CLA A 810



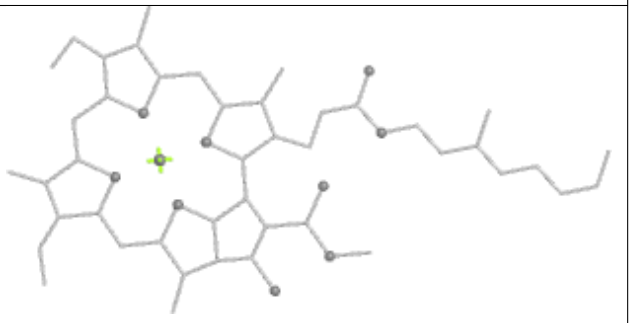
Bond lengths



Bond angles

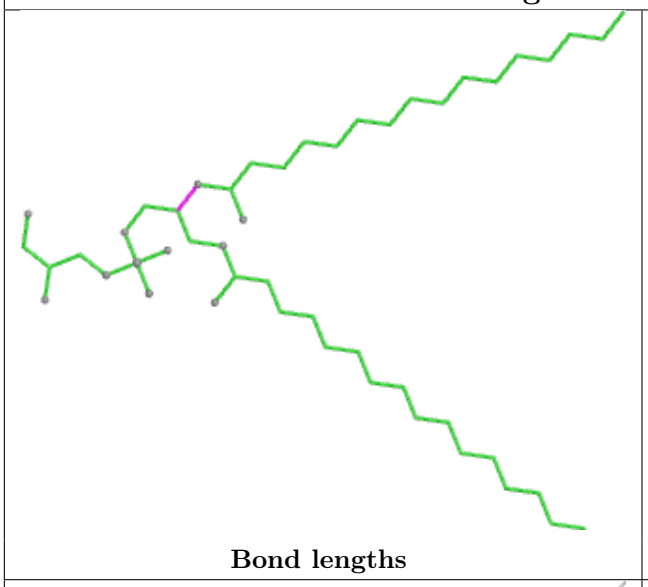


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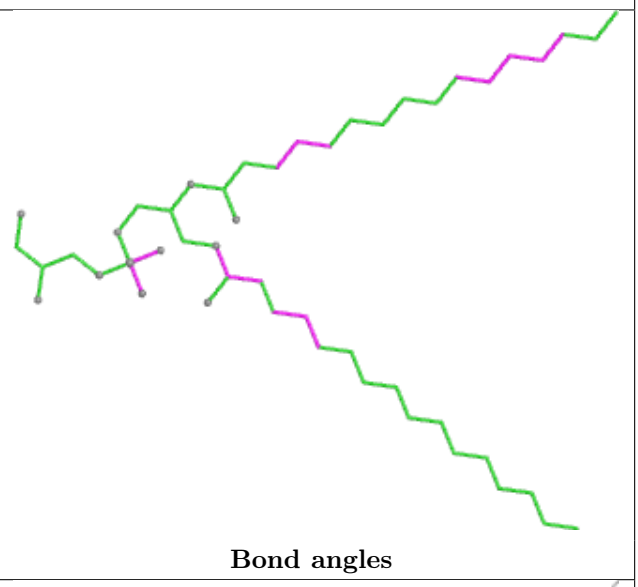


Rings

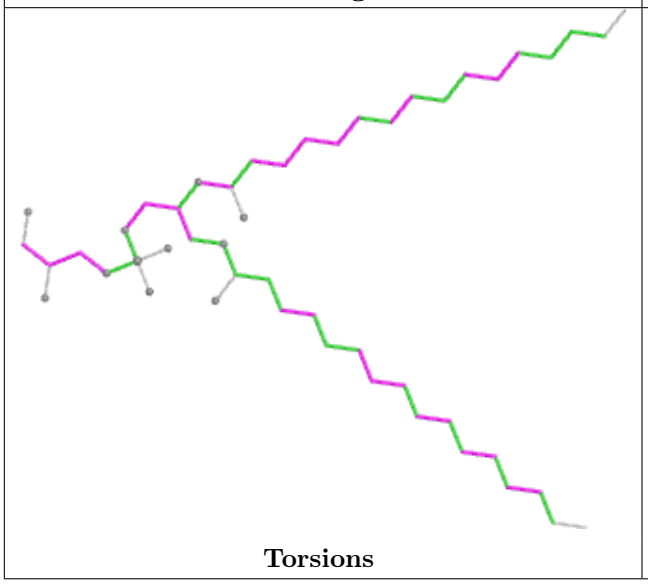
Ligand LHG A 842



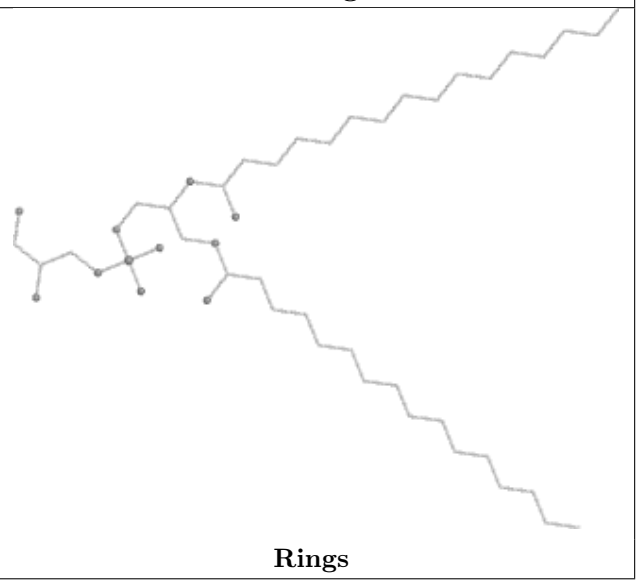
Bond lengths



Bond angles

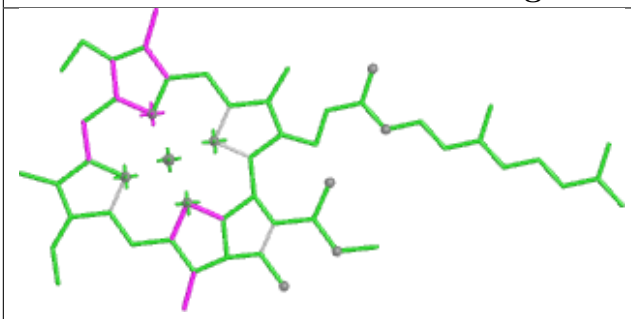


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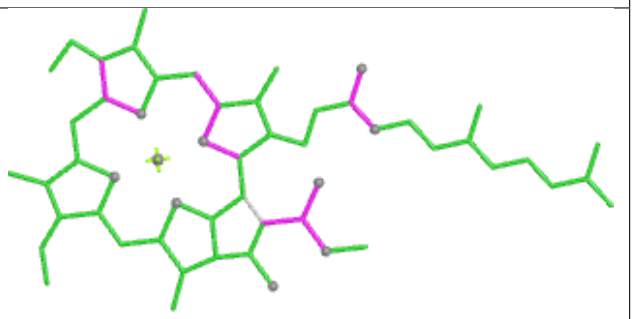


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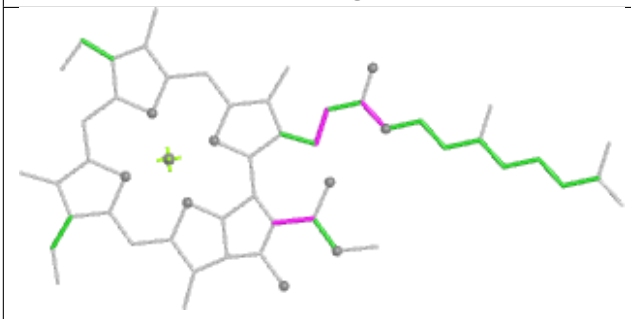
Ligand CLA B 808



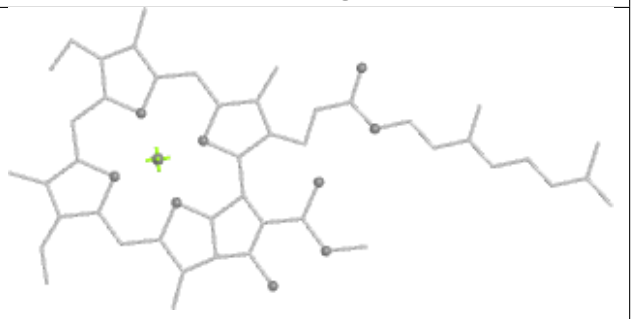
Bond lengths



Bond angles

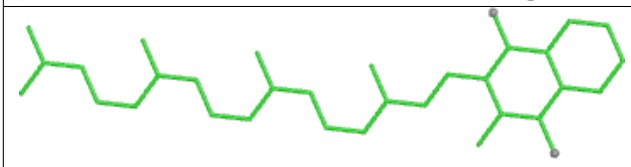


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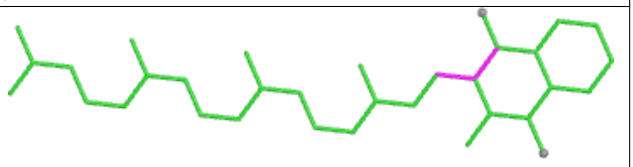


Rings

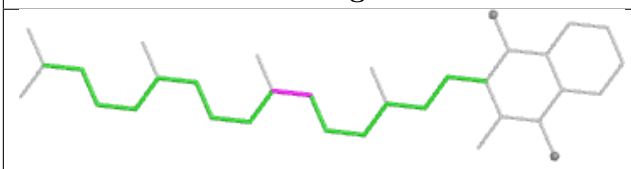
Ligand PQN B 833



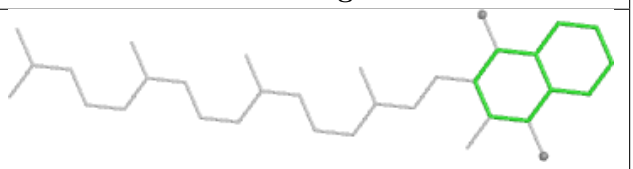
Bond lengths



Bond angles

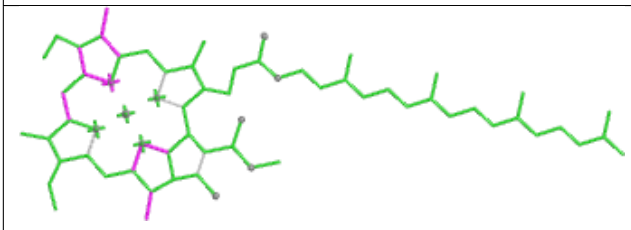


Torsions

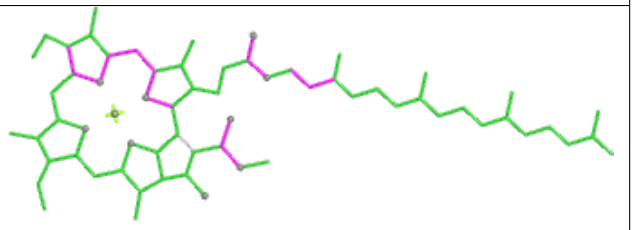


Rings

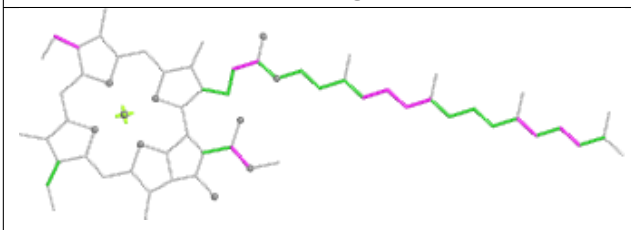
Ligand CLA B 807



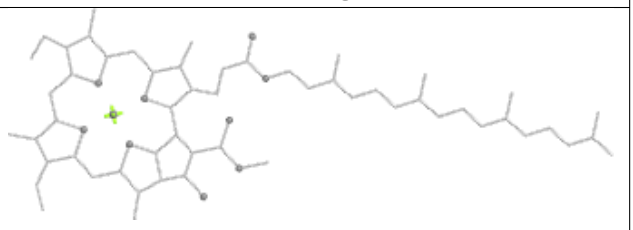
Bond lengths



Bond angles

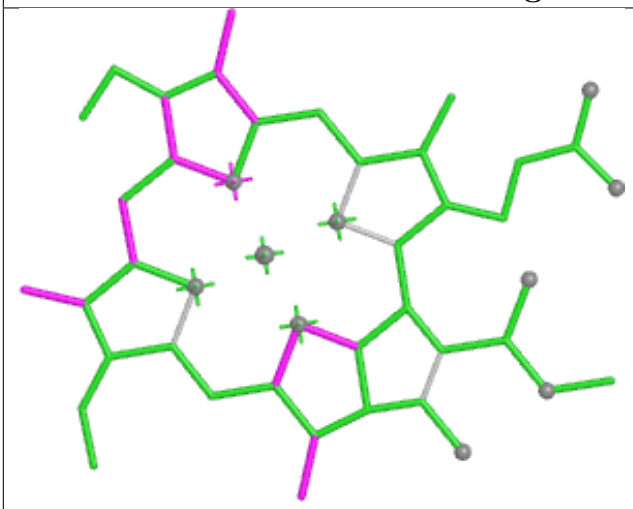


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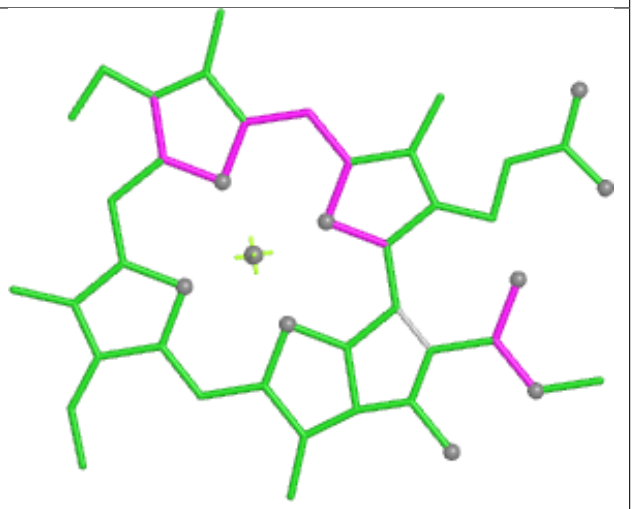


Rings

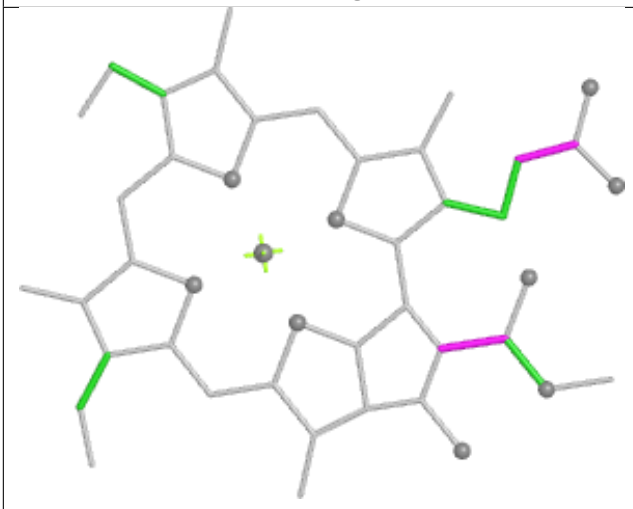
Ligand CLA B 805



Bond lengths



Bond angles

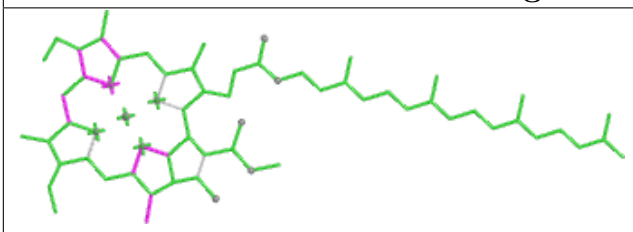


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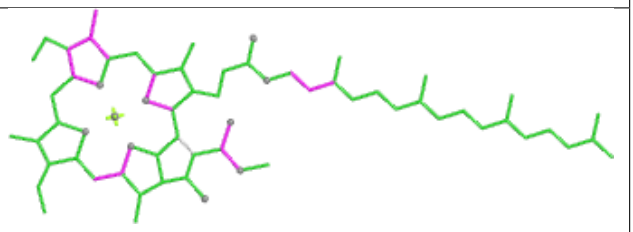


Rings

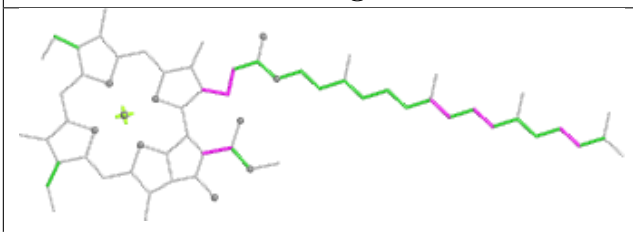
Ligand CLA A 802



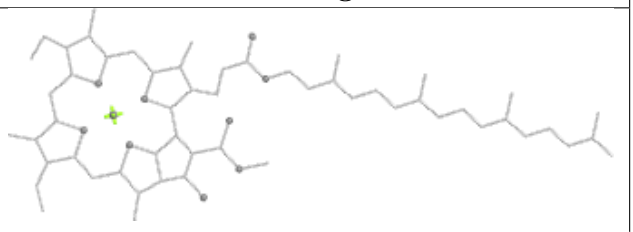
Bond lengths



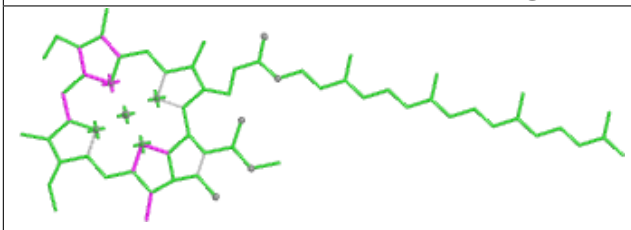
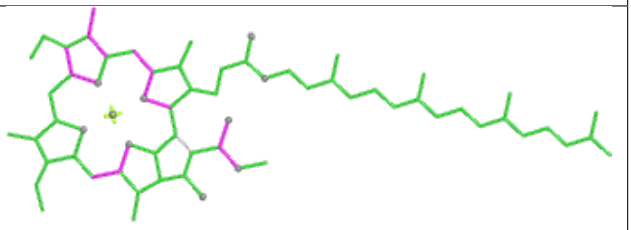
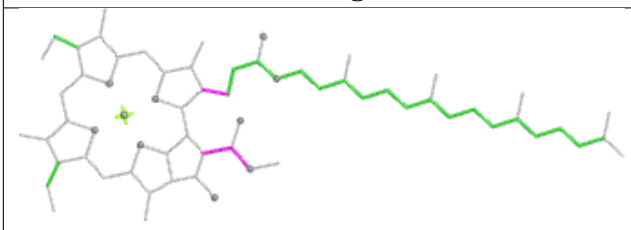
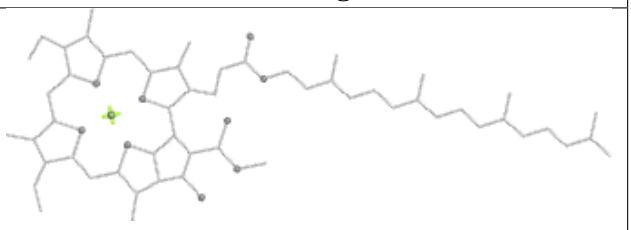
Bond angles

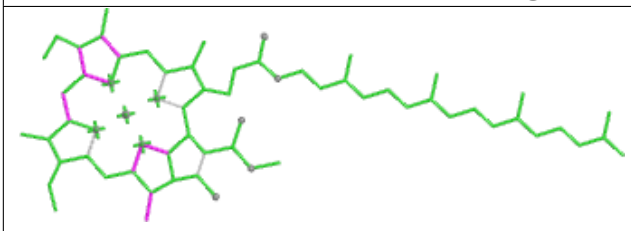
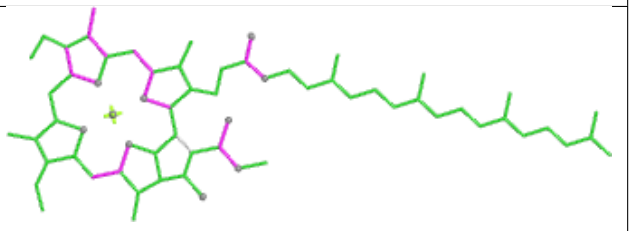
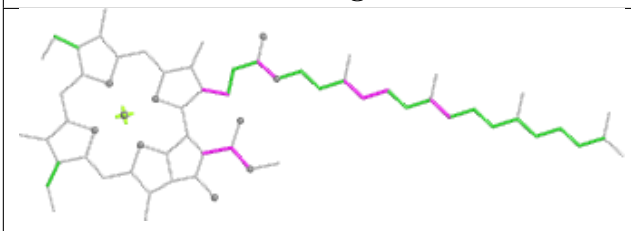
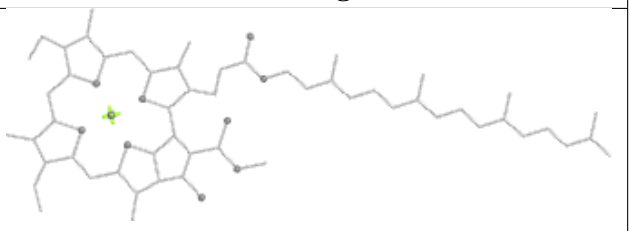


Torsions

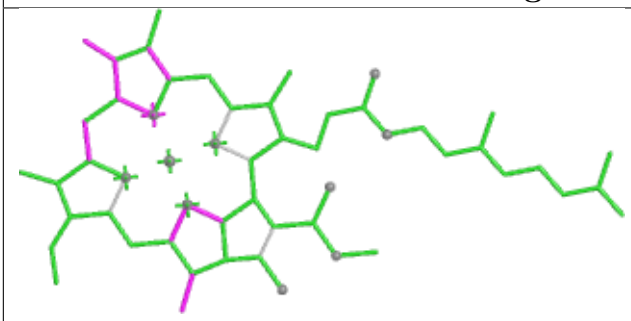


Rings

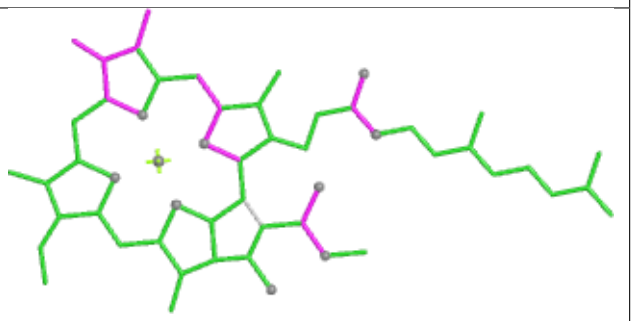
Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

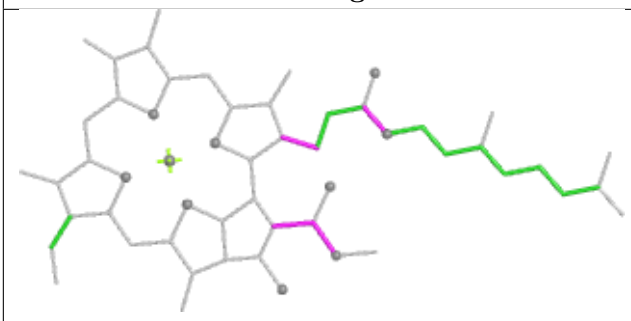
Ligand CLA B 812



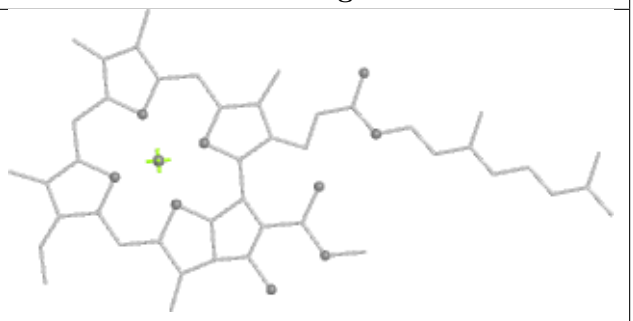
Bond lengths



Bond angles

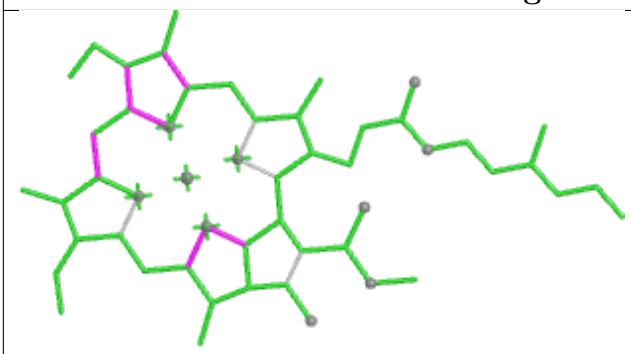


Torsions

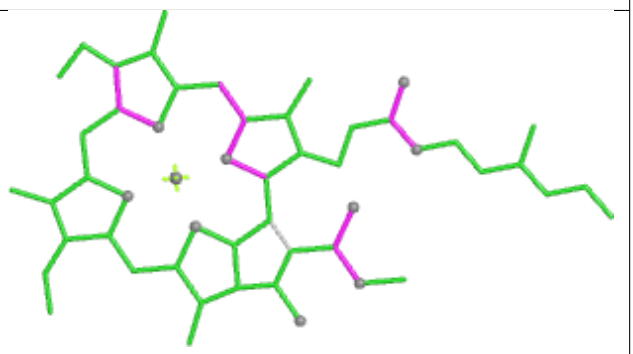


Rings

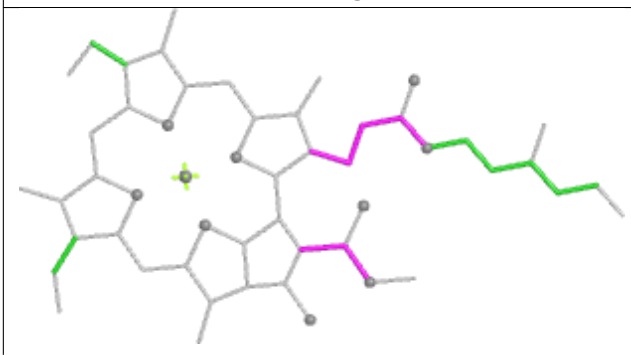
Ligand CLA A 841



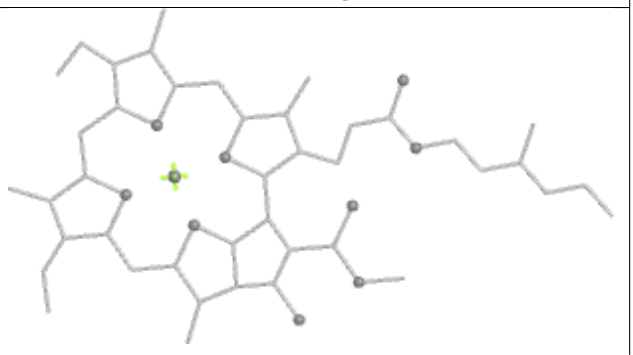
Bond lengths



Bond angles

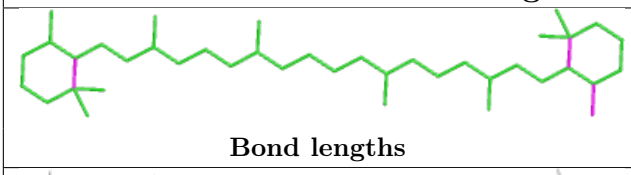


Torsions

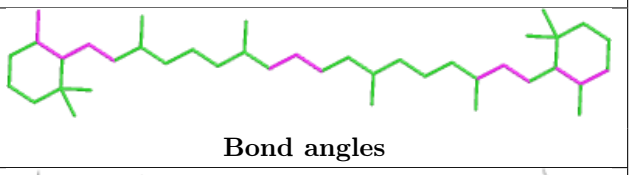


Rings

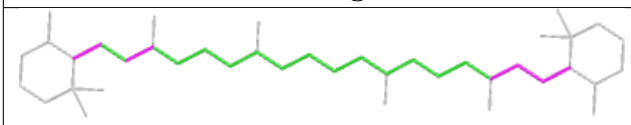
Ligand BCR B 836



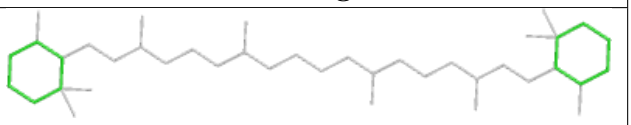
Bond lengths



Bond angles

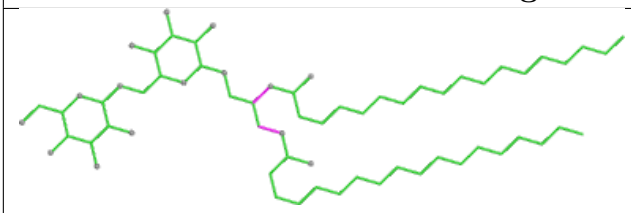


Torsions

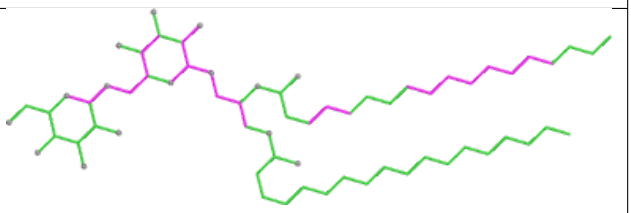


Rings

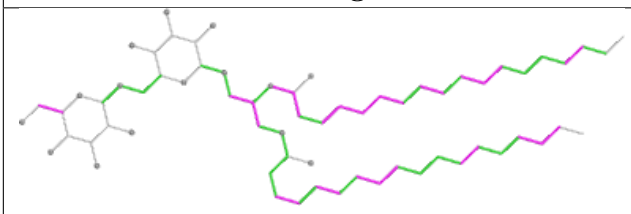
Ligand DGD B 837



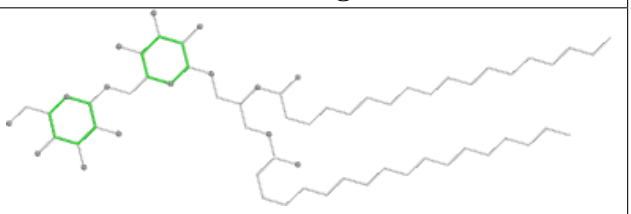
Bond lengths



Bond angles

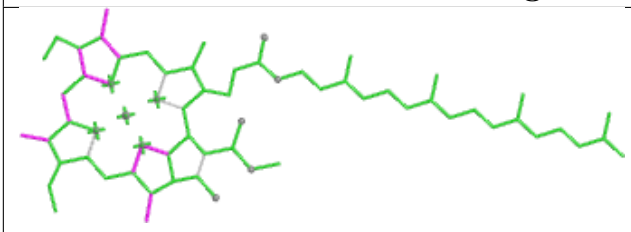


Torsions

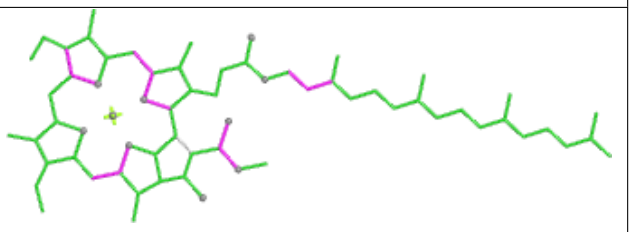


Rings

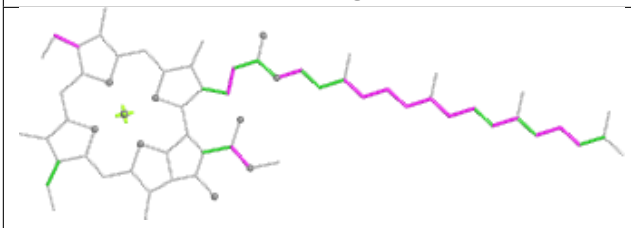
Ligand CLA A 849



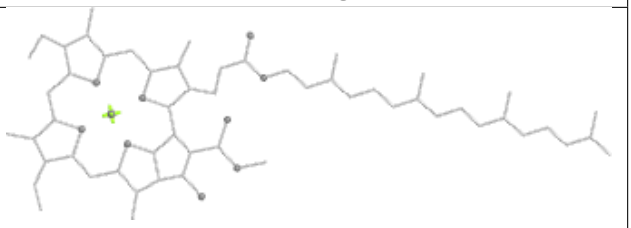
Bond lengths



Bond angles

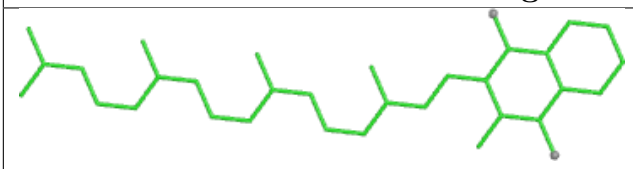


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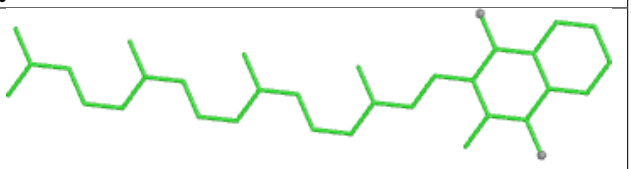


Rings

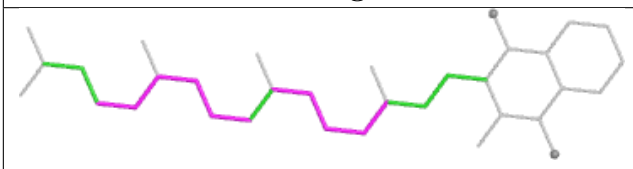
Ligand PQN A 840



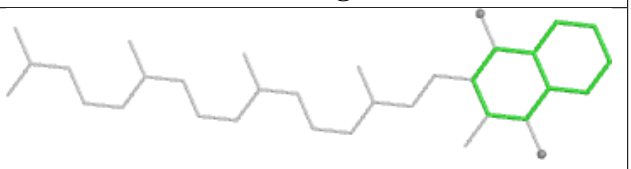
Bond lengths



Bond angles



Torsions

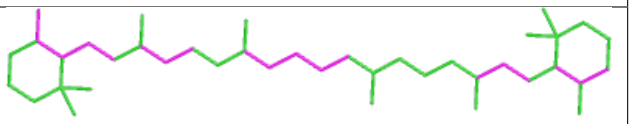


Rings

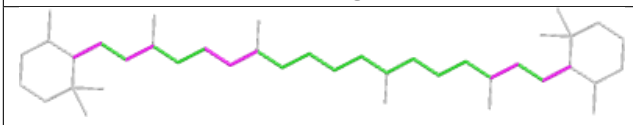
Ligand BCR L 307



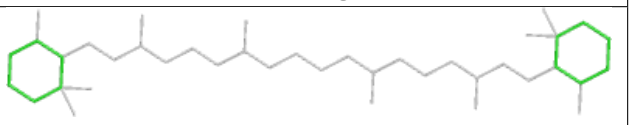
Bond lengths



Bond angles

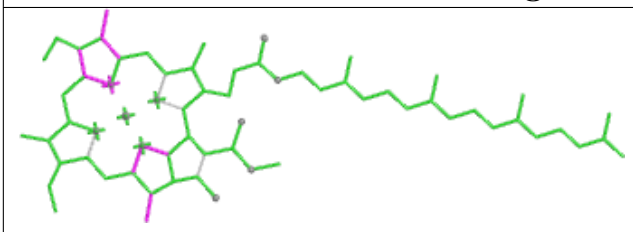


Torsions

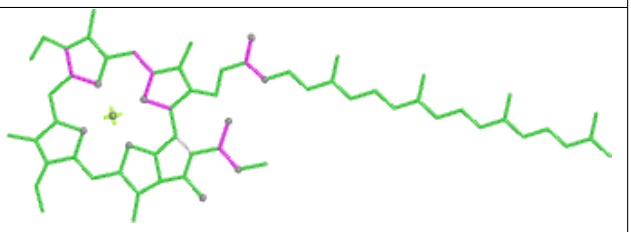


Rings

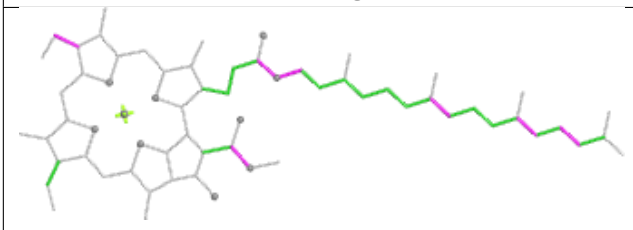
Ligand CLA B 832



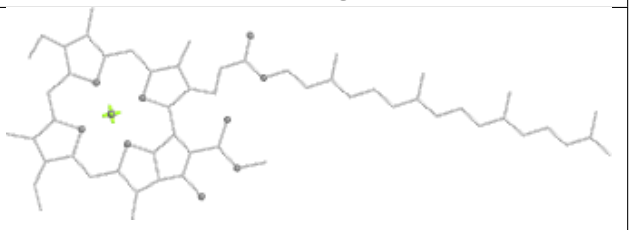
Bond lengths



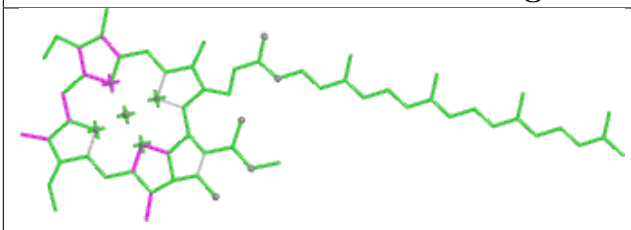
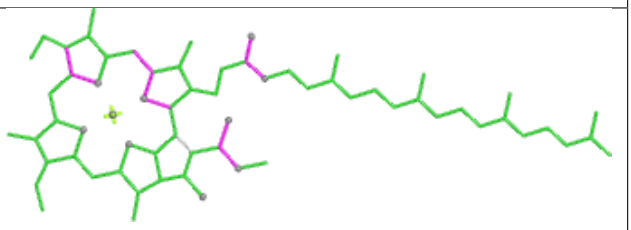
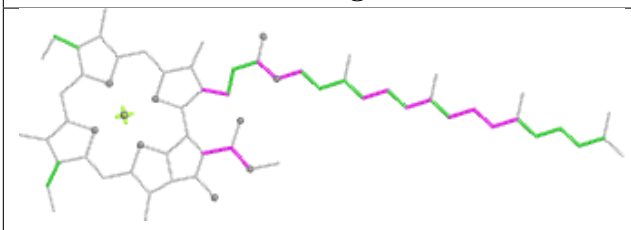
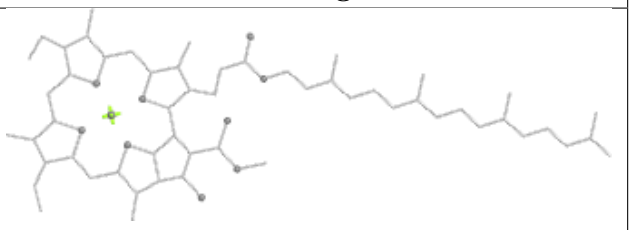
Bond angles

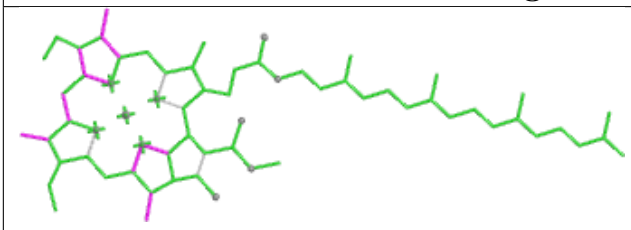
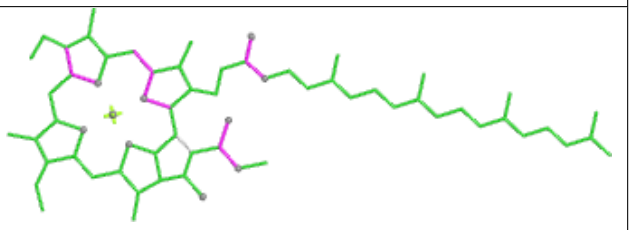
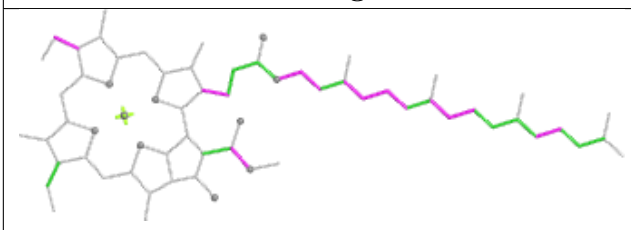
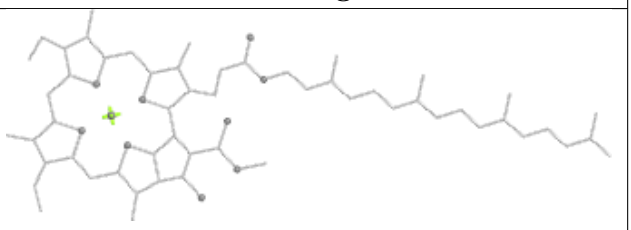


Torsions

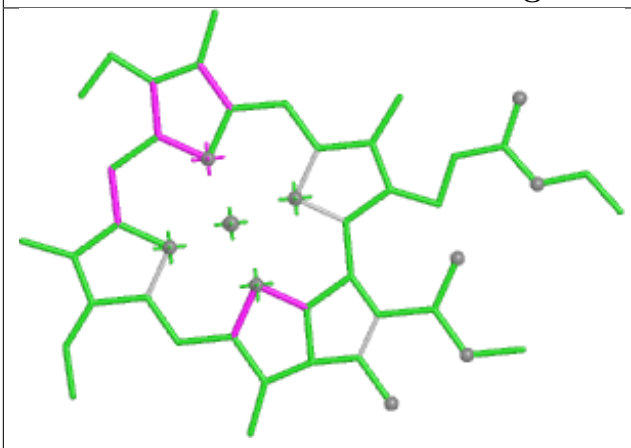


Rings

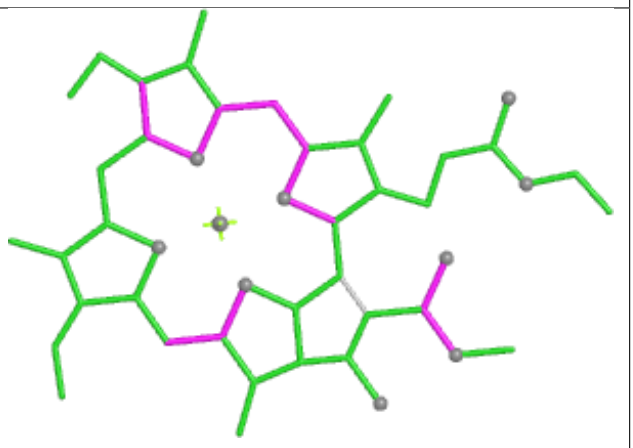
Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

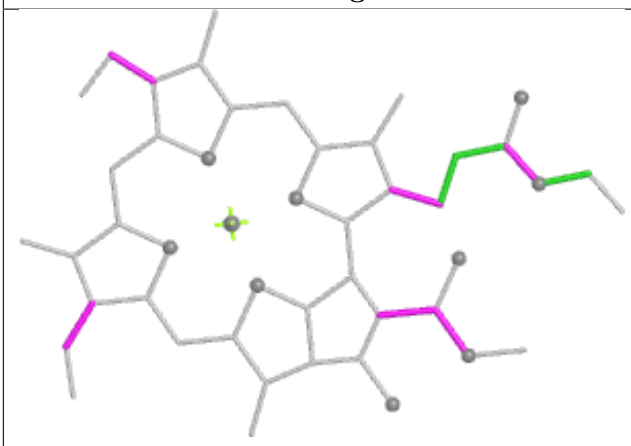
Ligand CLA A 837



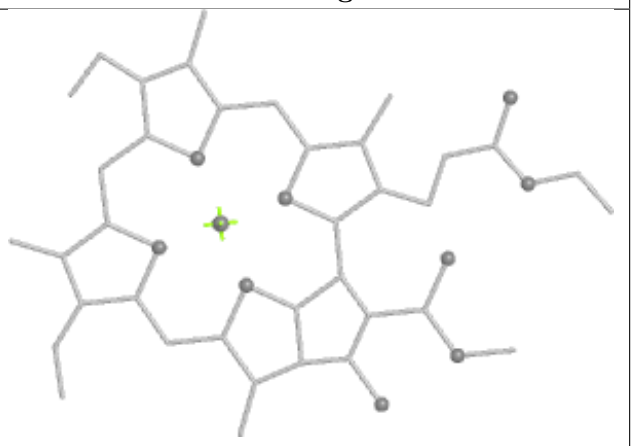
Bond lengths



Bond angles

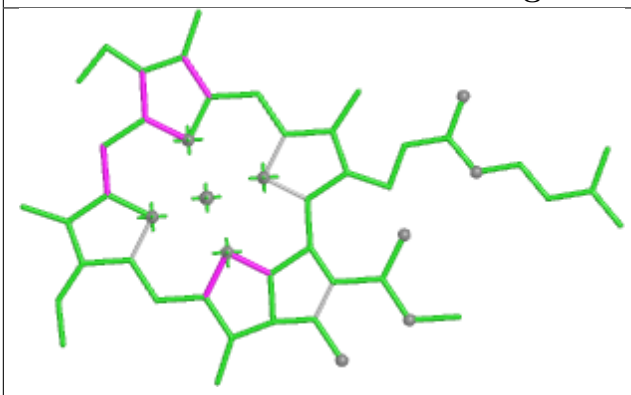


Torsions

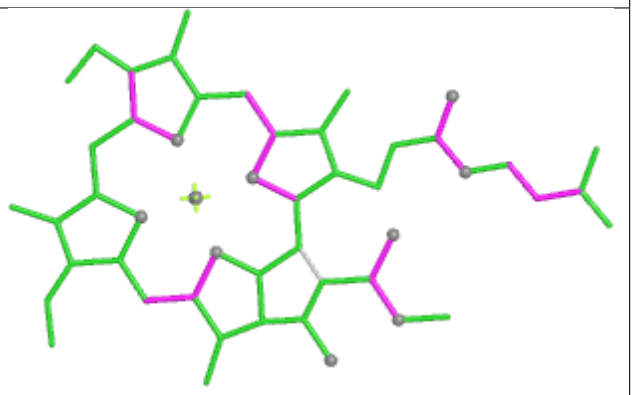


Rings

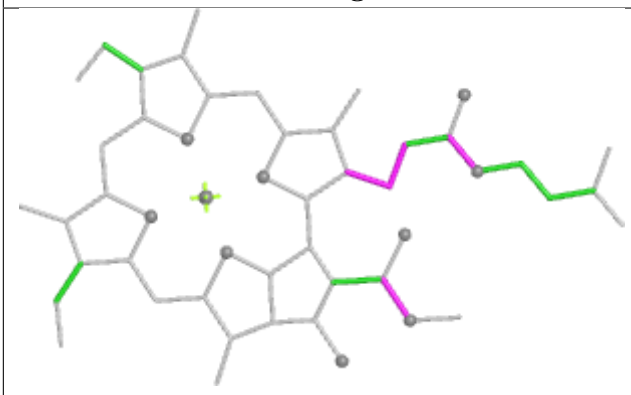
Ligand CLA A 832



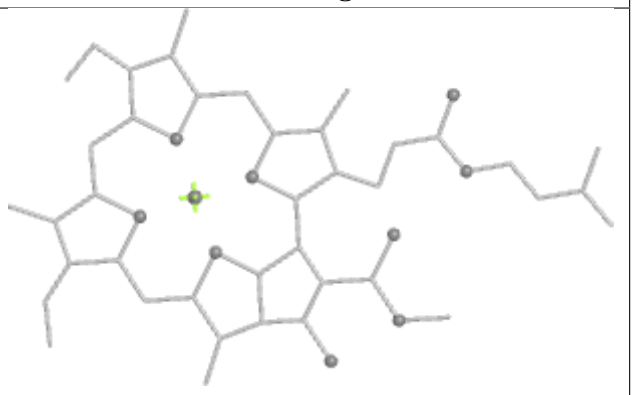
Bond lengths



Bond angles

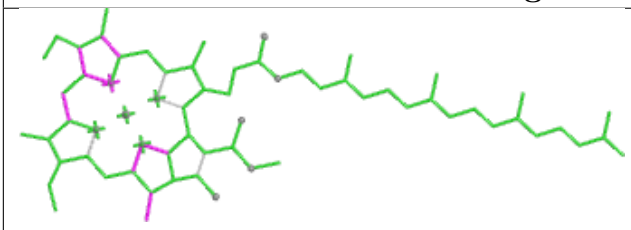


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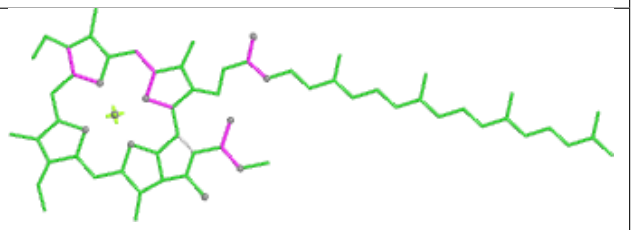


Rings

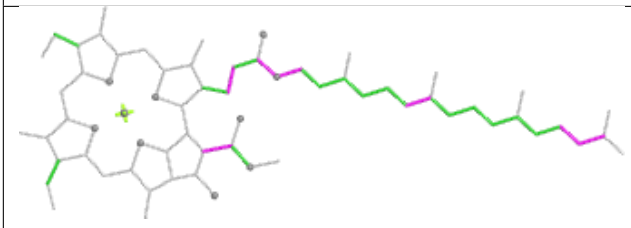
Ligand CLA B 815



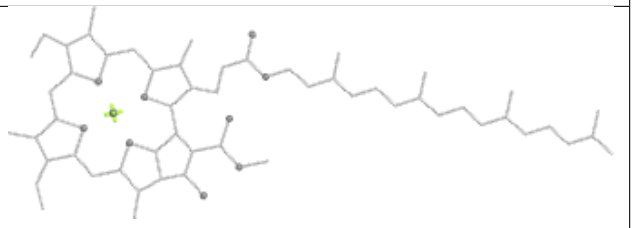
Bond lengths



Bond angles

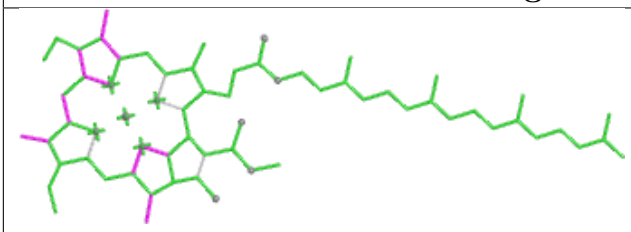


Torsions

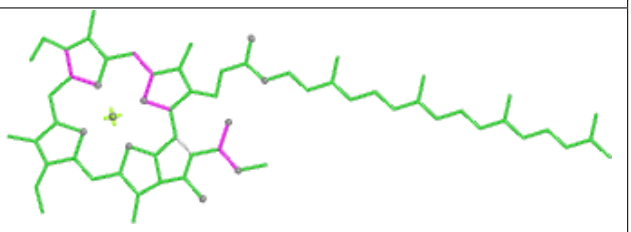


Rings

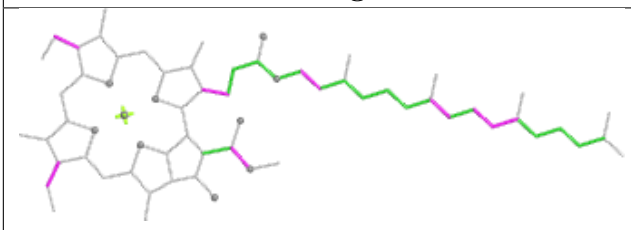
Ligand CLA B 804



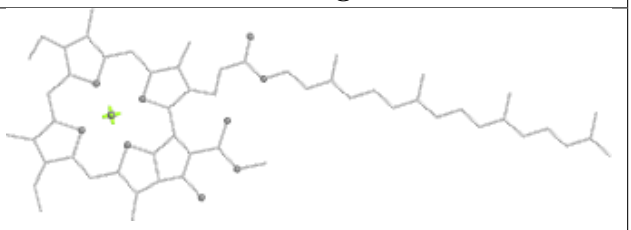
Bond lengths



Bond angles

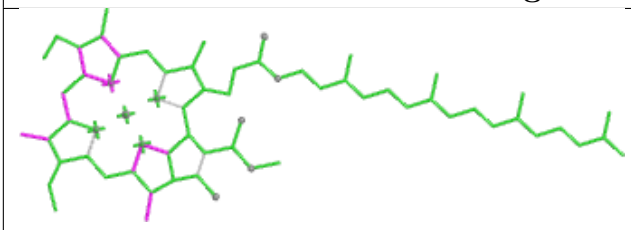


Torsions

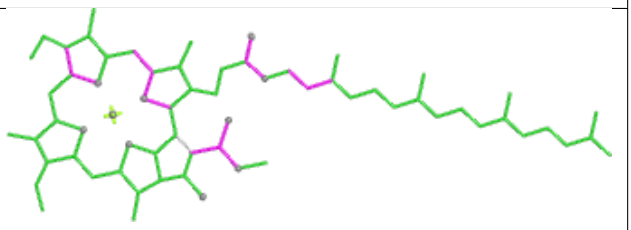


Rings

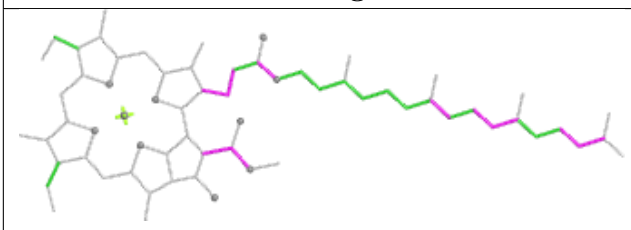
Ligand CLA A 815



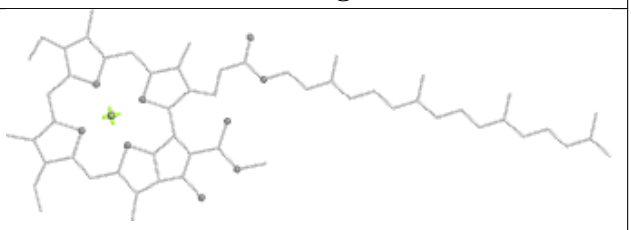
Bond lengths



Bond angles

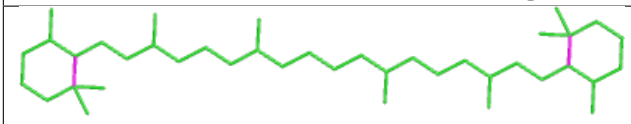


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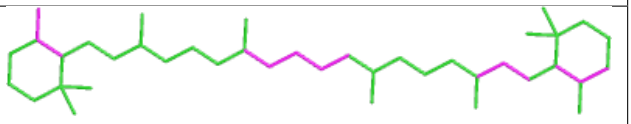


Rings

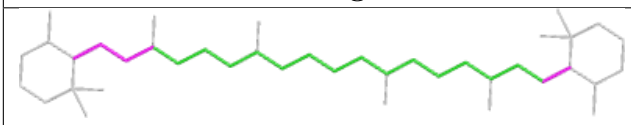
Ligand BCR A 844



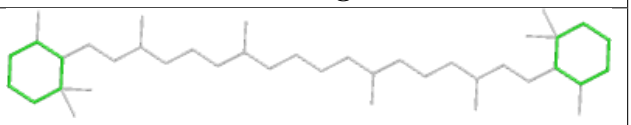
Bond lengths



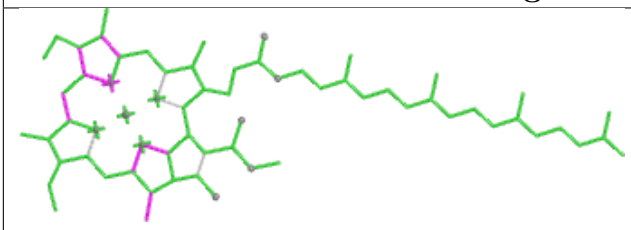
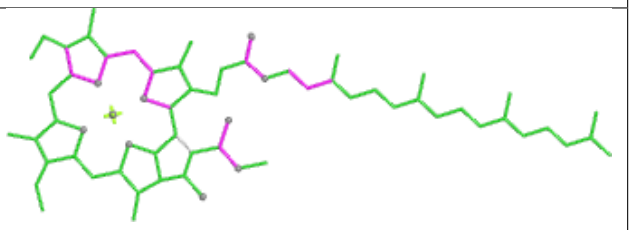
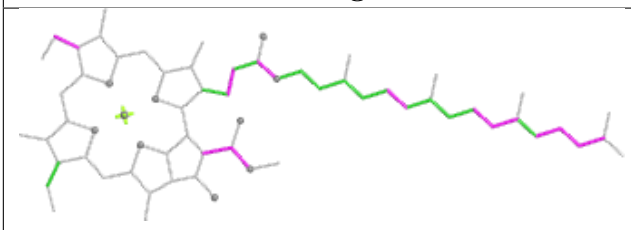
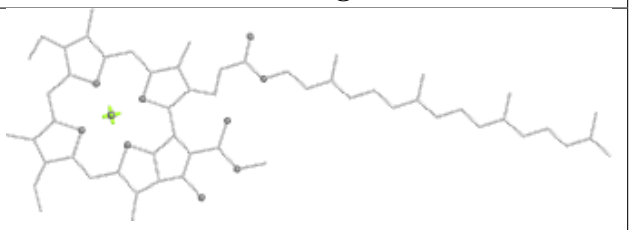
Bond angles

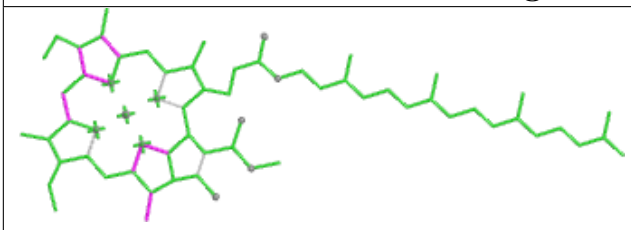
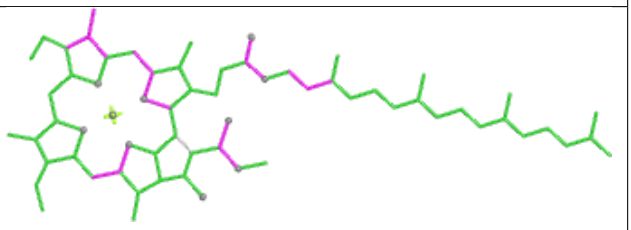
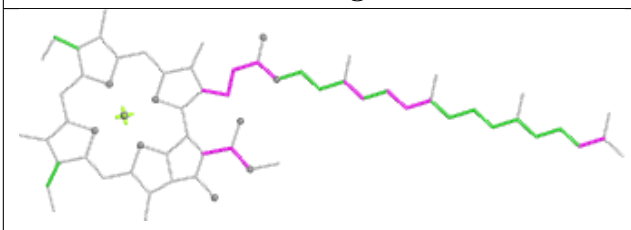
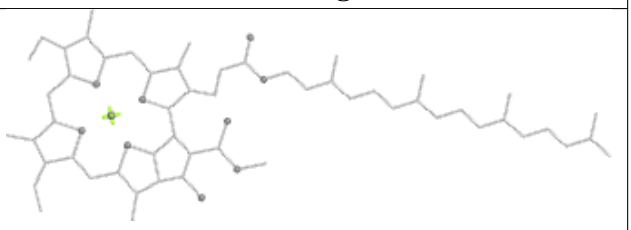


Torsions

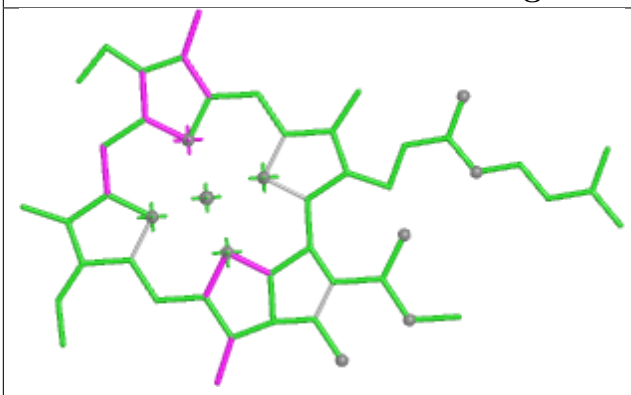


Rings

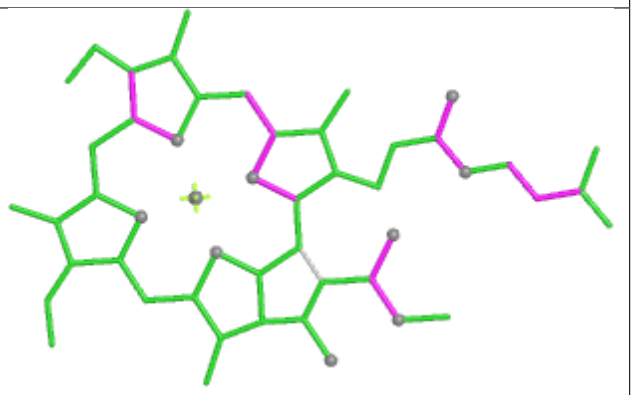
Ligand CLA A 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

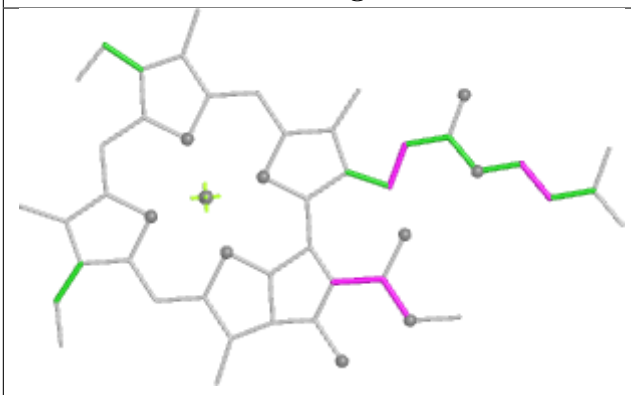
Ligand CLA A 829



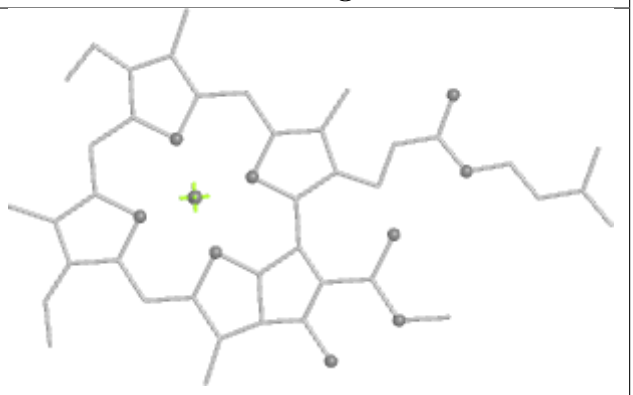
Bond lengths



Bond angles

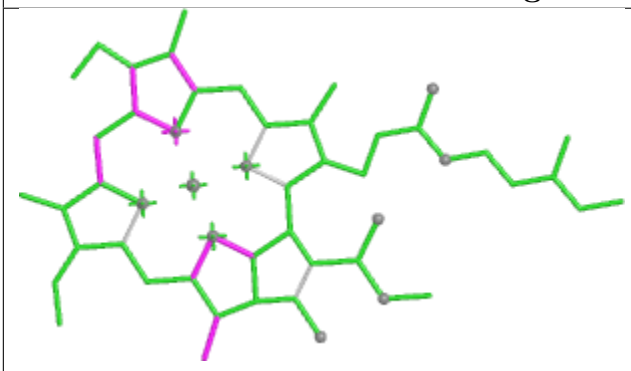


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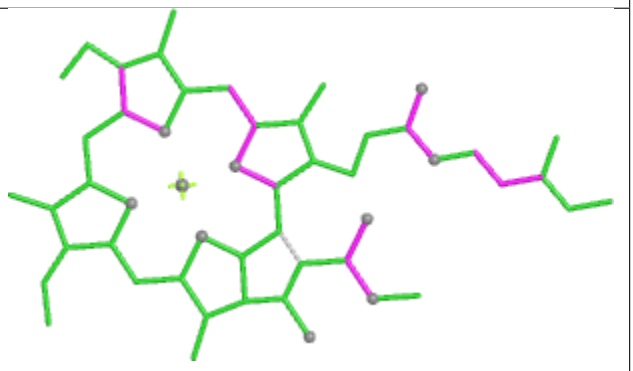


Rings

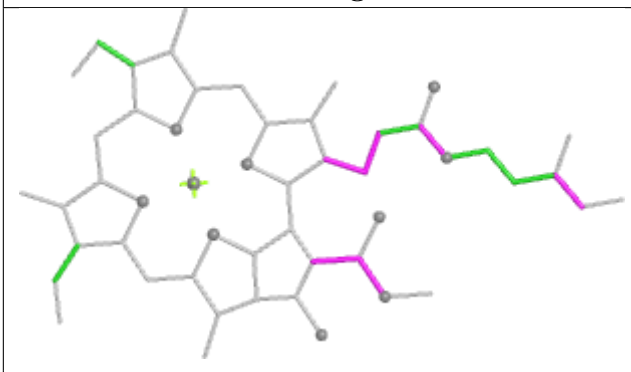
Ligand CLA A 821



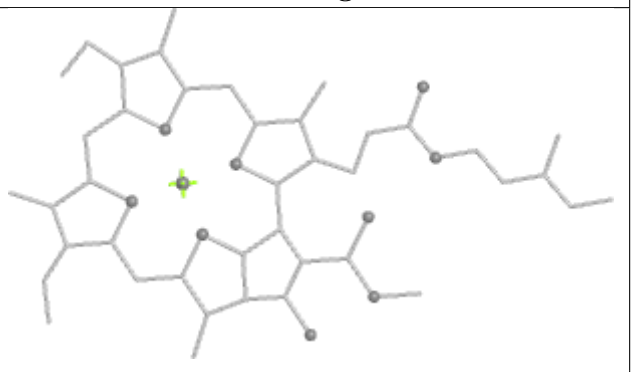
Bond lengths



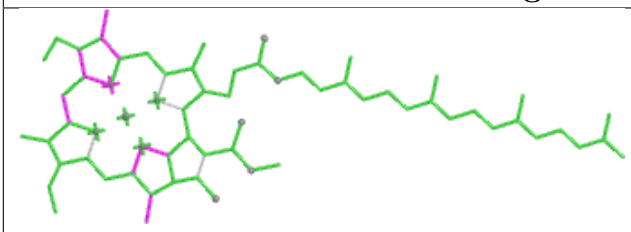
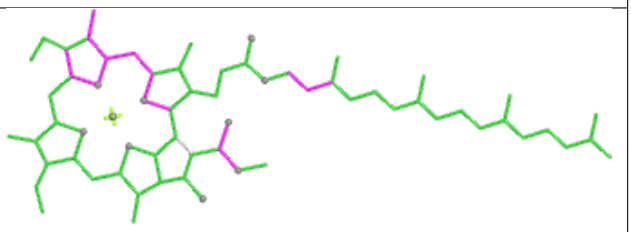
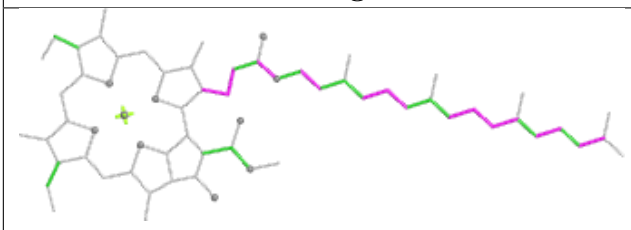
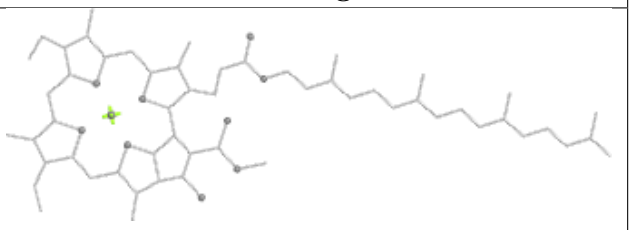
Bond angles



Torsions



Rings

Ligand CLA A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

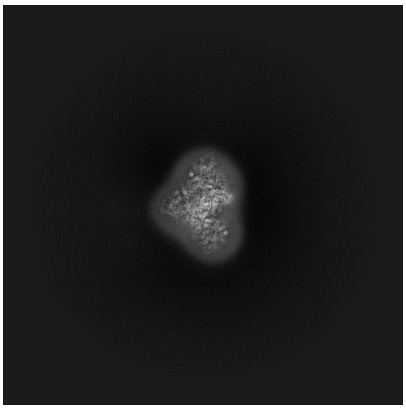
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66967. These allow visual inspection of the internal detail of the map and identification of artifacts.

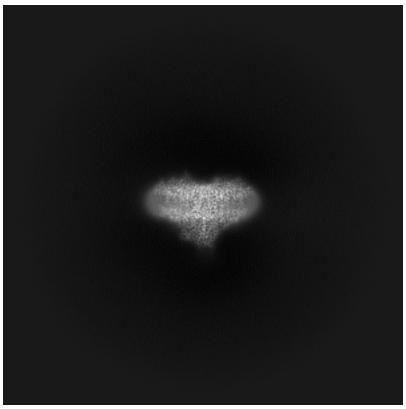
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

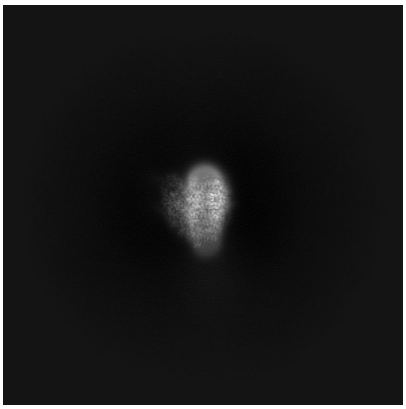
6.1.1 Primary map



X

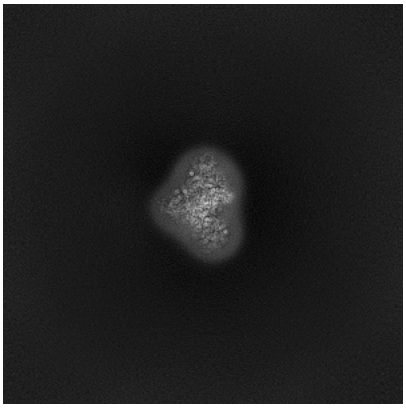


Y

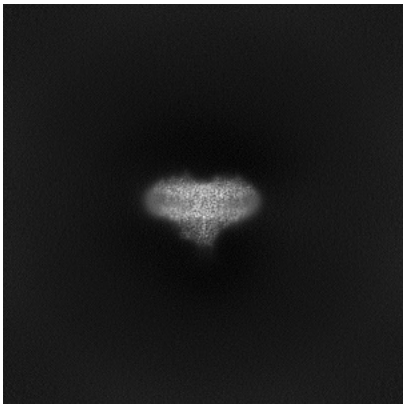


Z

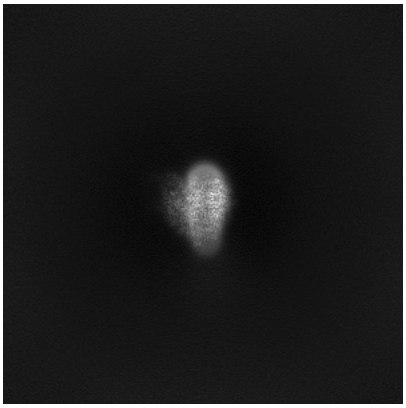
6.1.2 Raw map



X



Y

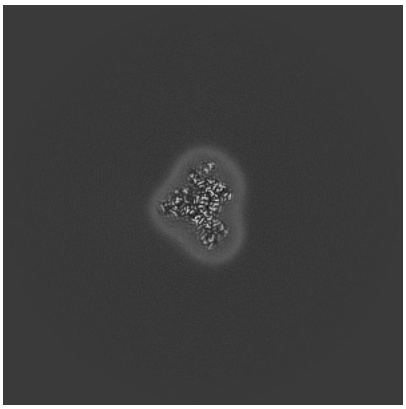


Z

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

6.2 Central slices (i)

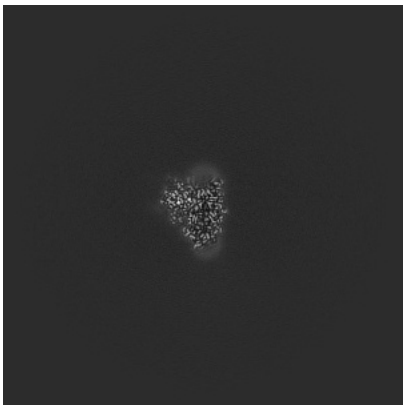
6.2.1 Primary map



X Index: 256

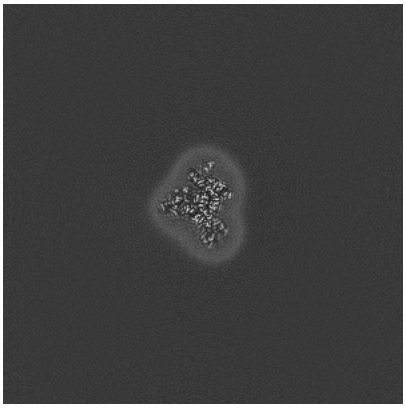


Y Index: 256



Z Index: 256

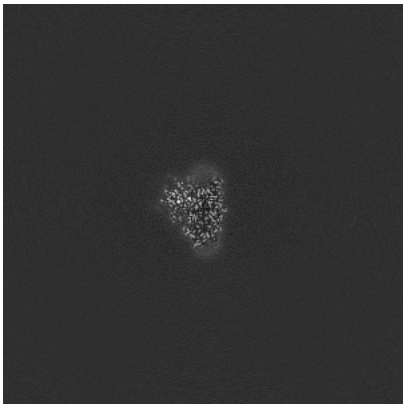
6.2.2 Raw map



X Index: 256



Y Index: 256

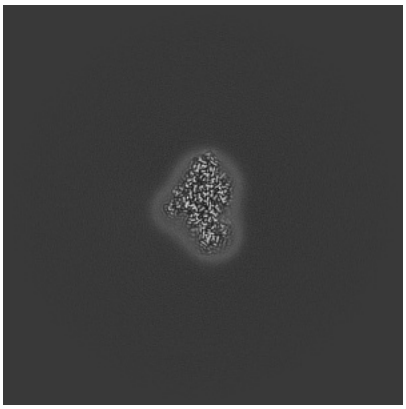


Z Index: 256

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

6.3 Largest variance slices (i)

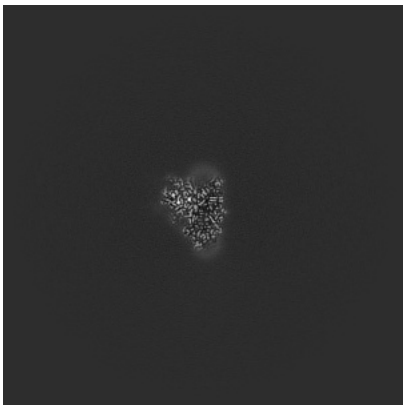
6.3.1 Primary map



X Index: 268

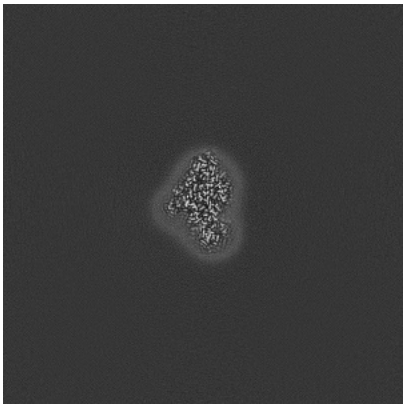


Y Index: 258

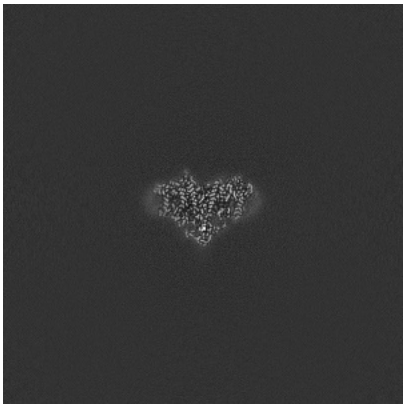


Z Index: 257

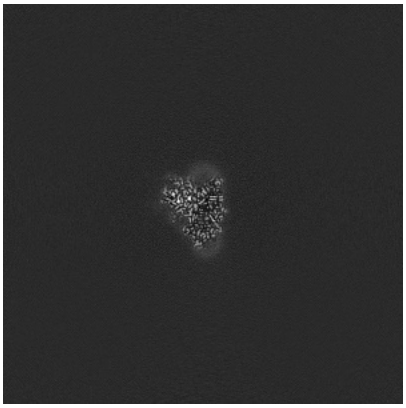
6.3.2 Raw map



X Index: 268



Y Index: 258

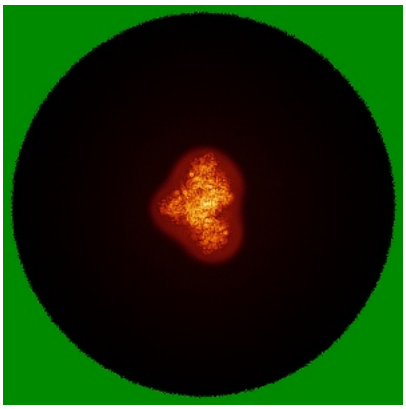


Z Index: 257

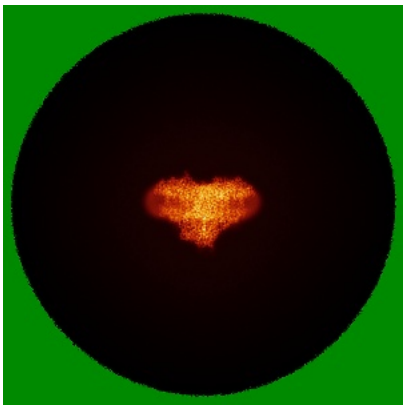
The images above show the largest variance slices of the map in three orthogonal directions.

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

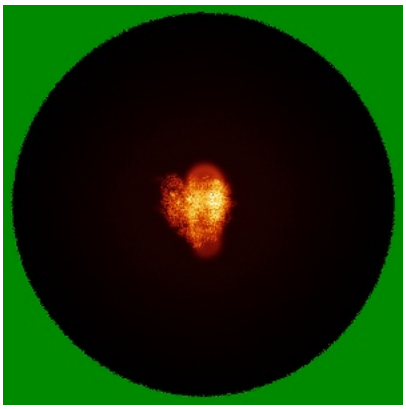
6.4.1 Primary map



X

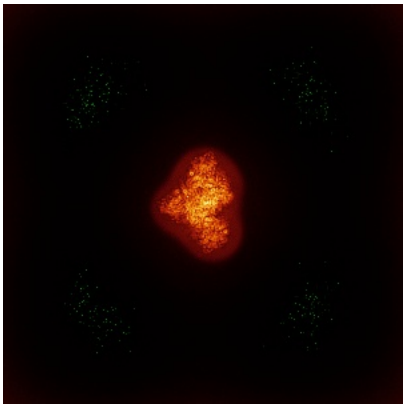


Y

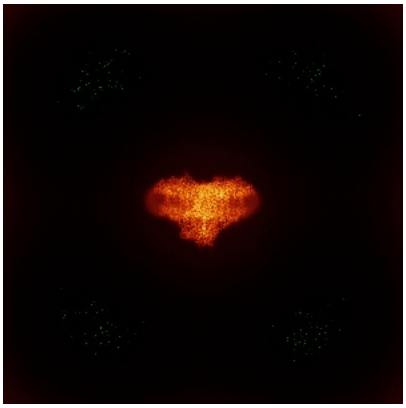


Z

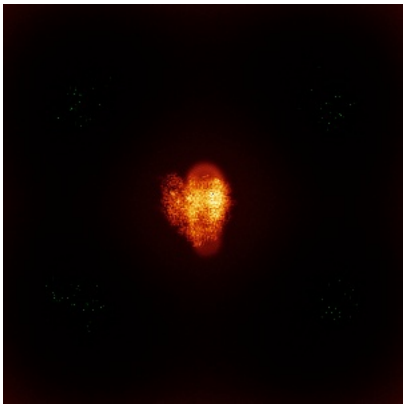
6.4.2 Raw map



X



Y

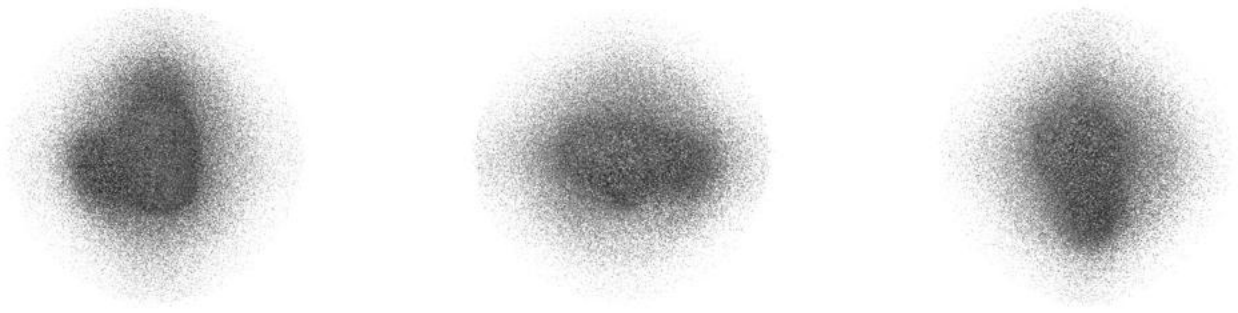


Z

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)

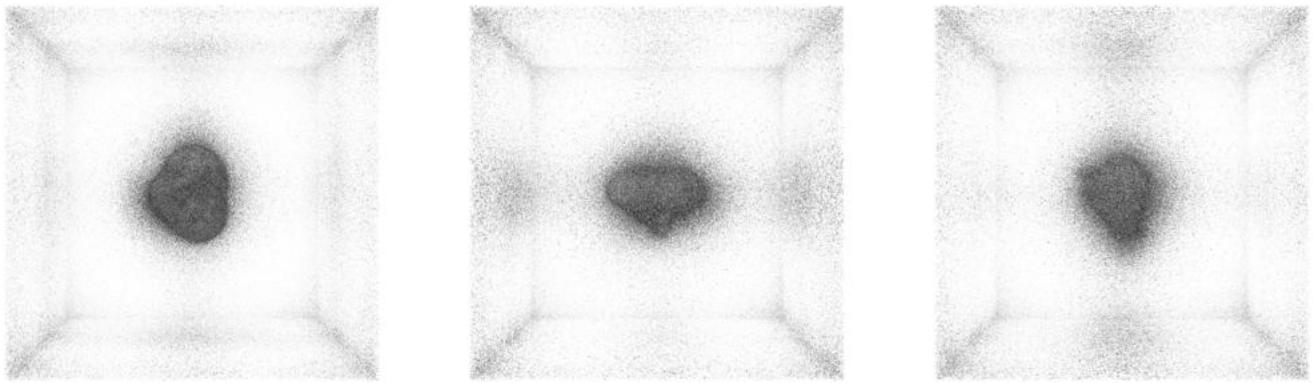
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0233. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

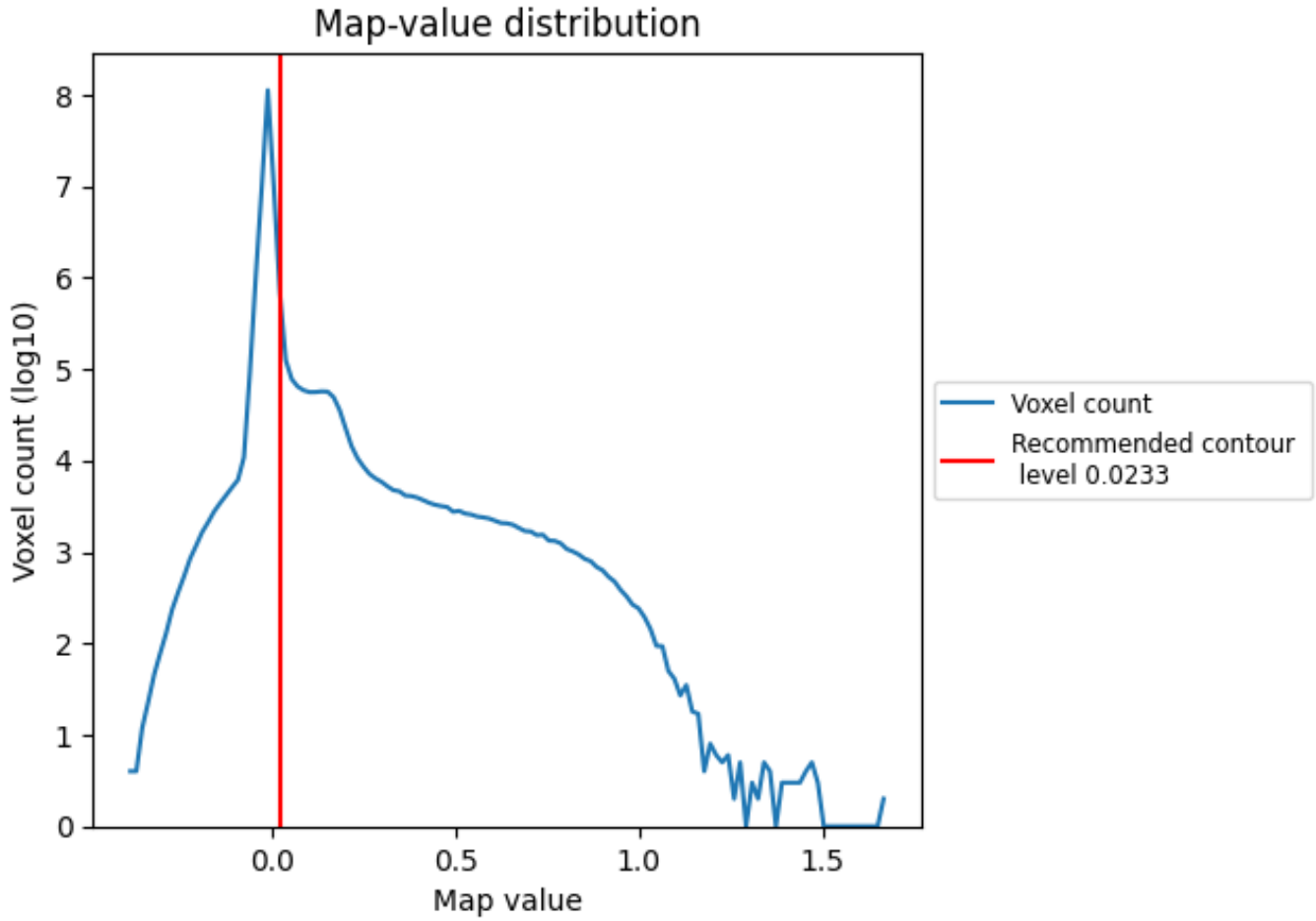
6.6 Mask visualisation (i)

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

7 Map analysis

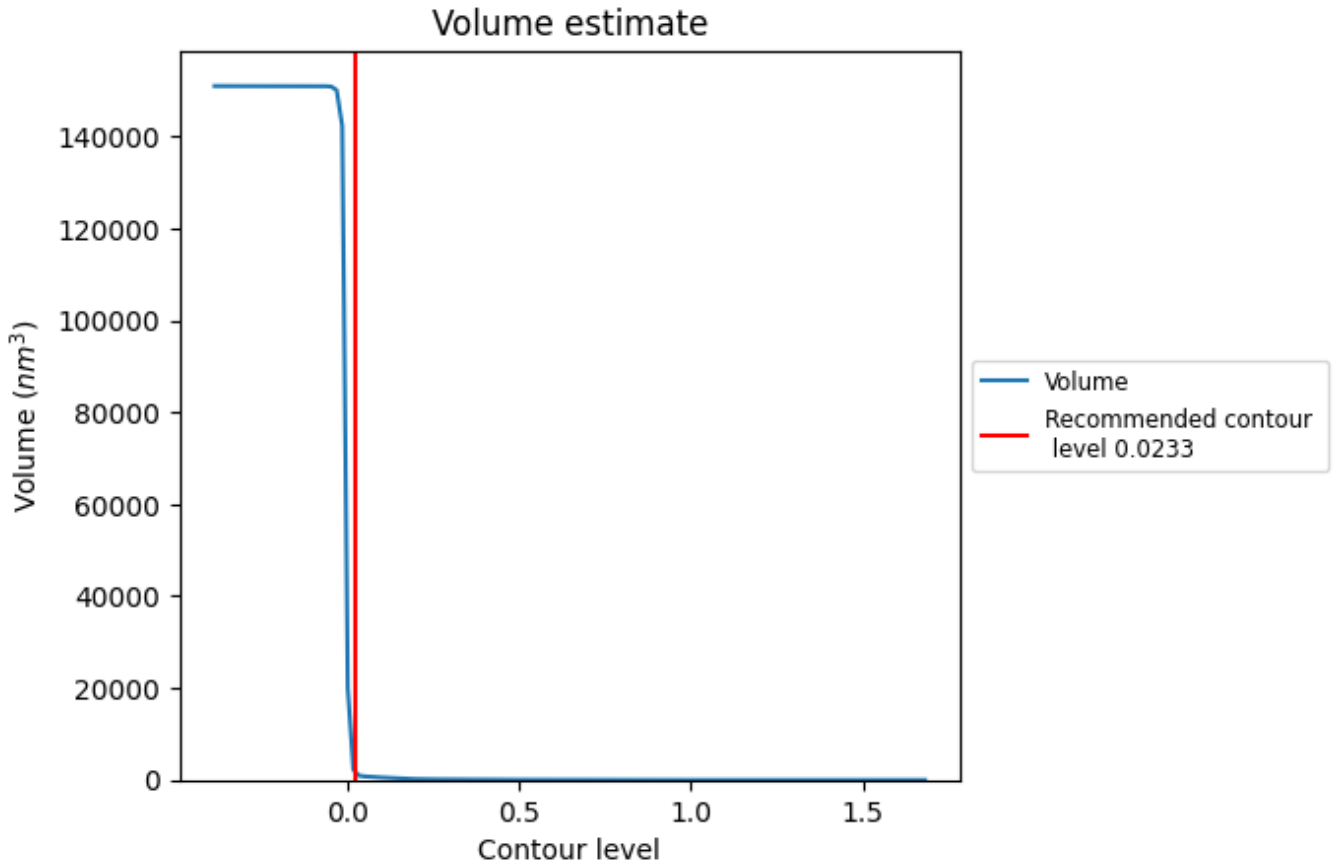
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

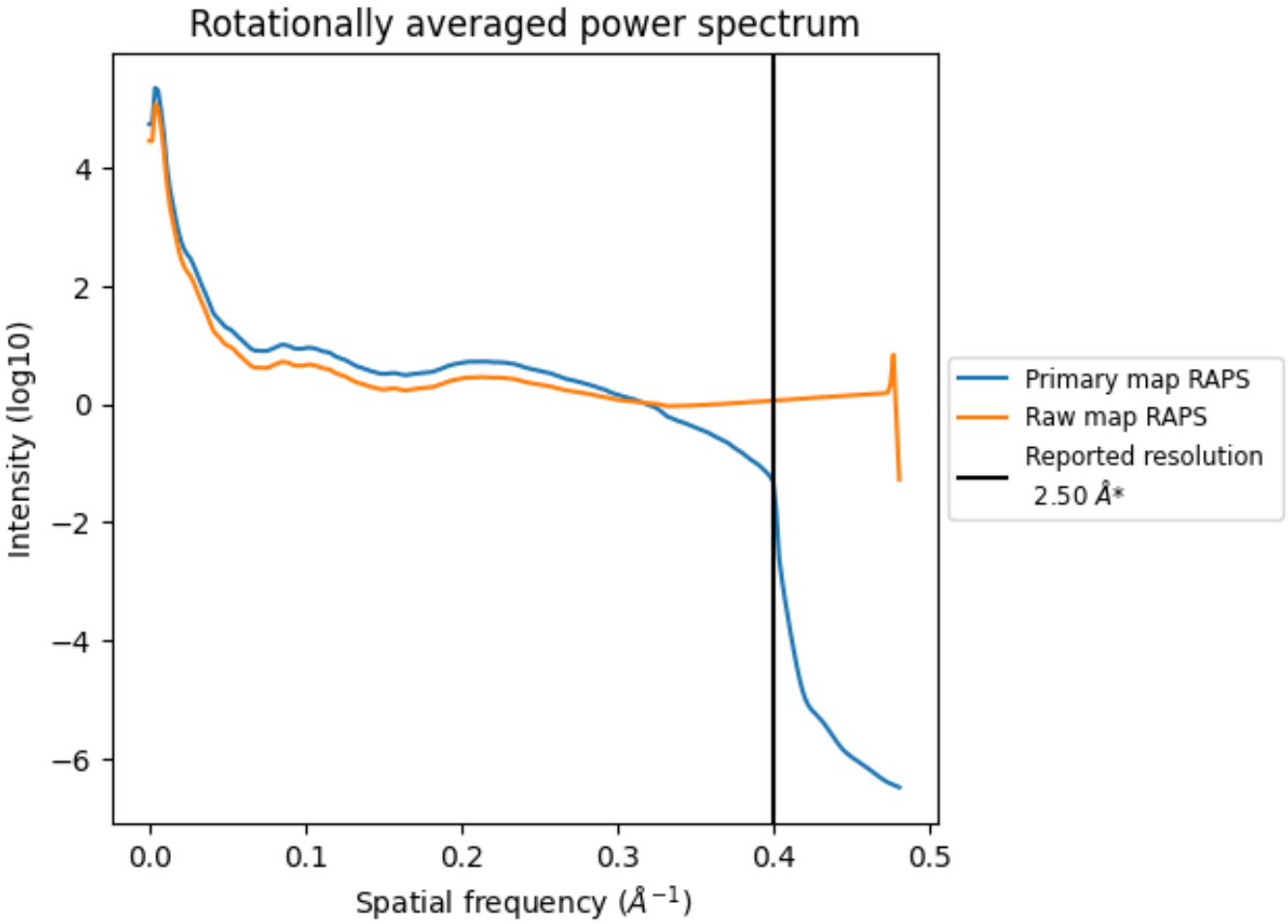
7.2 Volume estimate (i)



The volume at the recommended contour level is 1872 nm^3; this corresponds to an approximate mass of 1691 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)

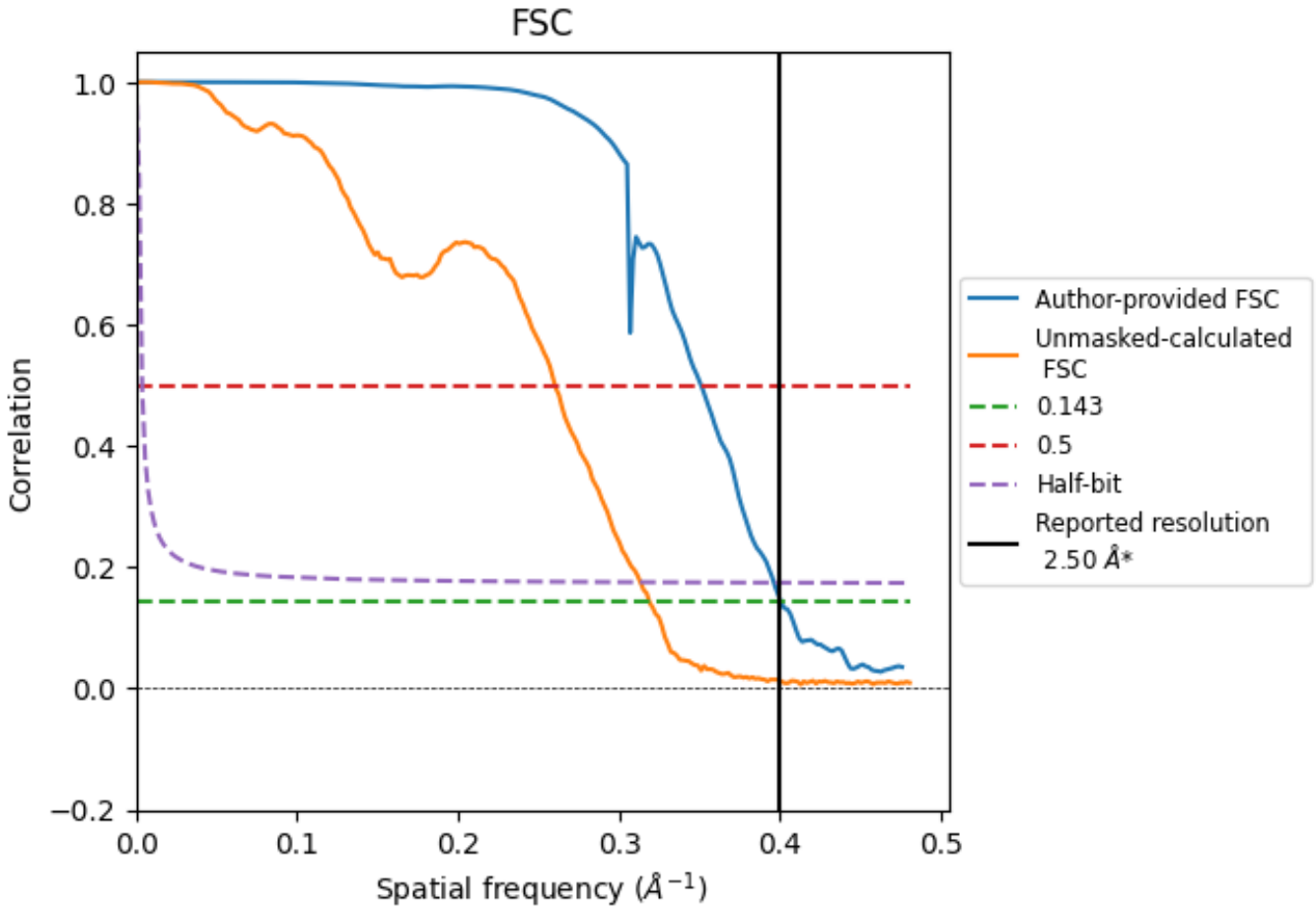


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

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 0.400 Å^{-1}

8.2 Resolution estimates (i)

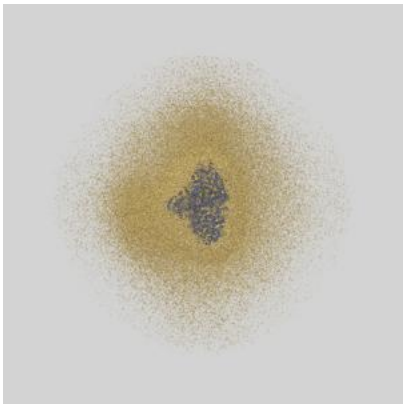
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.85	2.52
Unmasked-calculated*	3.13	3.84	3.19

*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 3.13 differs from the reported value 2.5 by more than 10 %

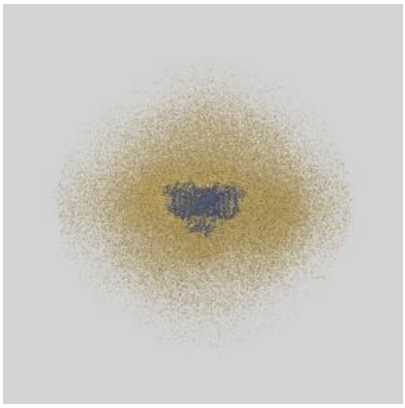
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66967 and PDB model 9XKK. Per-residue inclusion information can be found in section 3 on page 14.

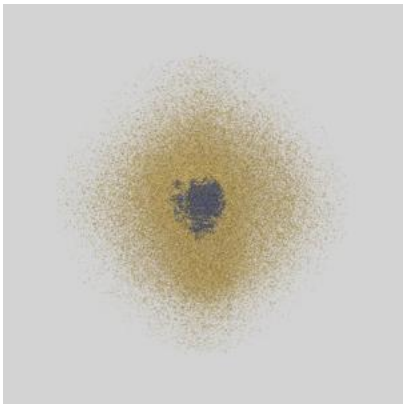
9.1 Map-model overlay



X



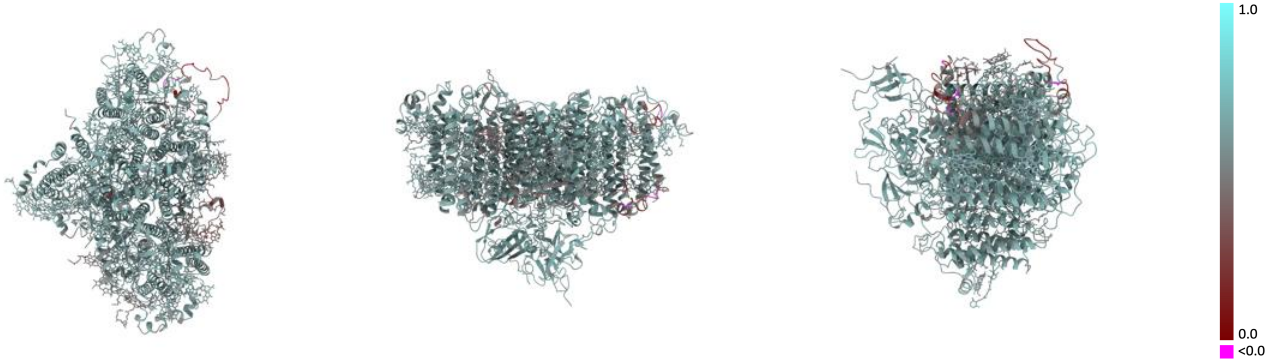
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0233 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

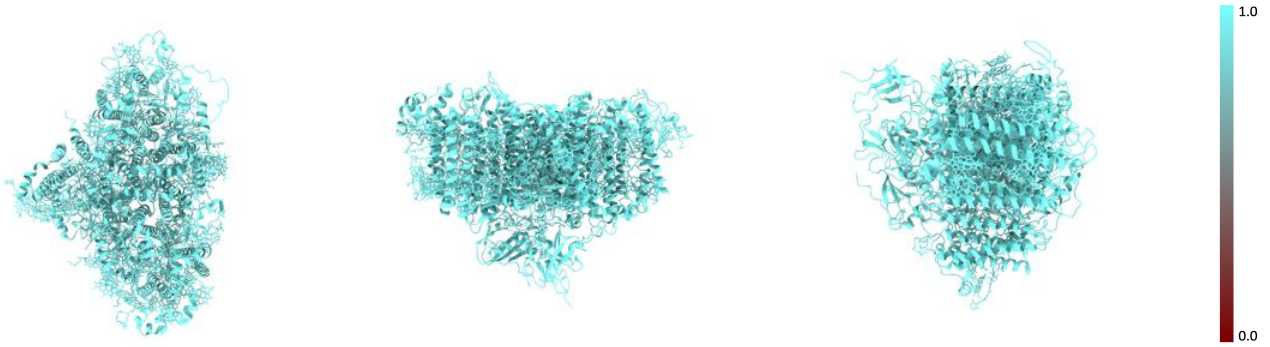
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

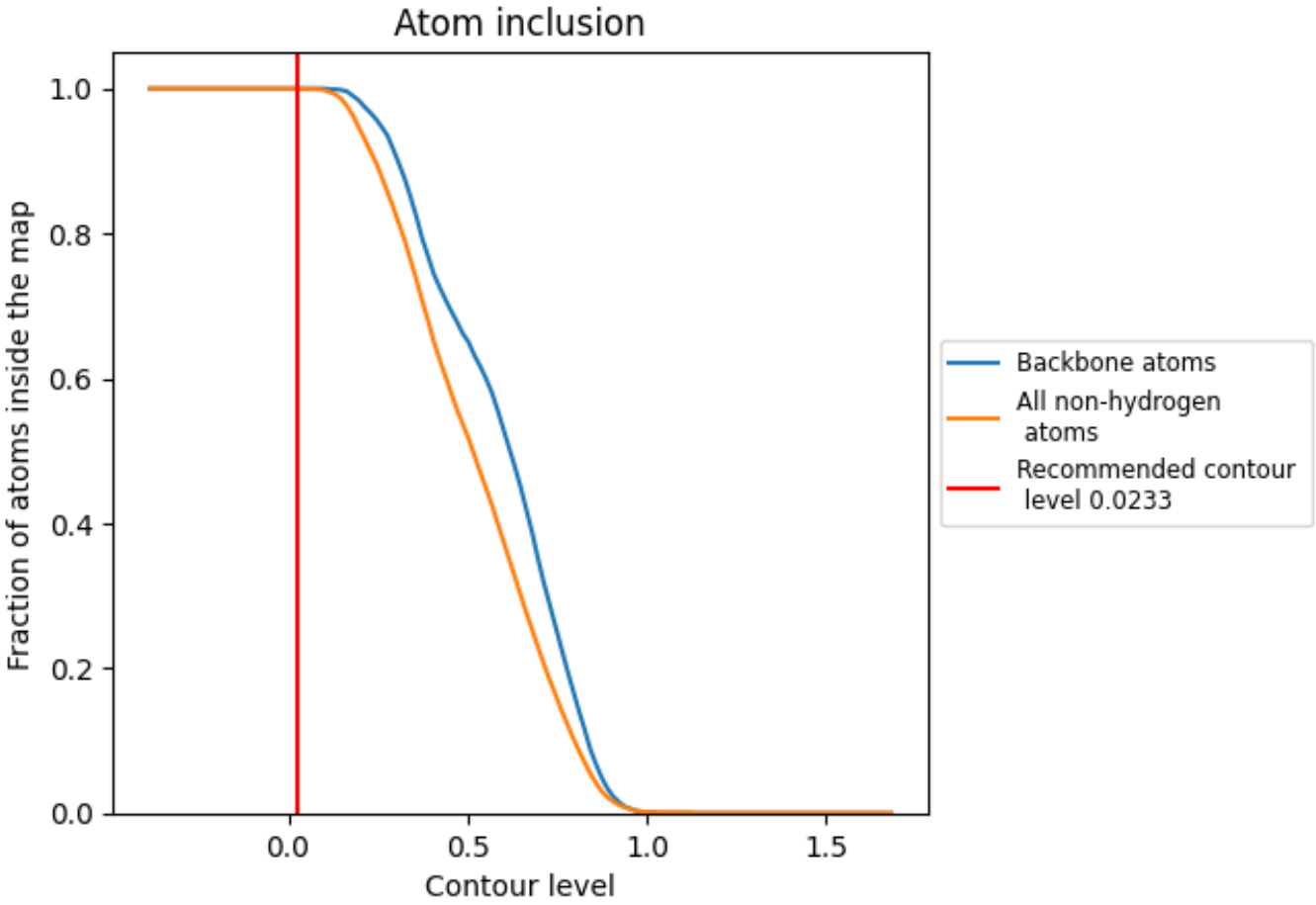
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0233).

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 (0.0233) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	1.0000	0.5930
A	0.9990	0.5840
B	1.0000	0.5960
C	0.9980	0.6180
D	1.0000	0.6210
E	1.0000	0.5930
H	1.0000	0.5990
I	1.0000	0.5890
L	1.0000	0.5960

