wwPDB EM Validation Summary Report (i)

Nov 3, 2026 – 12:45 PM EST

PDB ID	:	9OY9 / pdb_00009oy9
EMDB ID	:	EMD-71005
Title	:	Structure of a red shifted PSI monomer from 6803
Authors	:	Mazor, Y.; Kahtun, H.; Asido, M.; Gorski, C.; Schlau-Cohen, G.S.
Deposited on	:	2025-06-04
Resolution	:	1.76 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 (i) 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 (i)) were used in the production of this report:

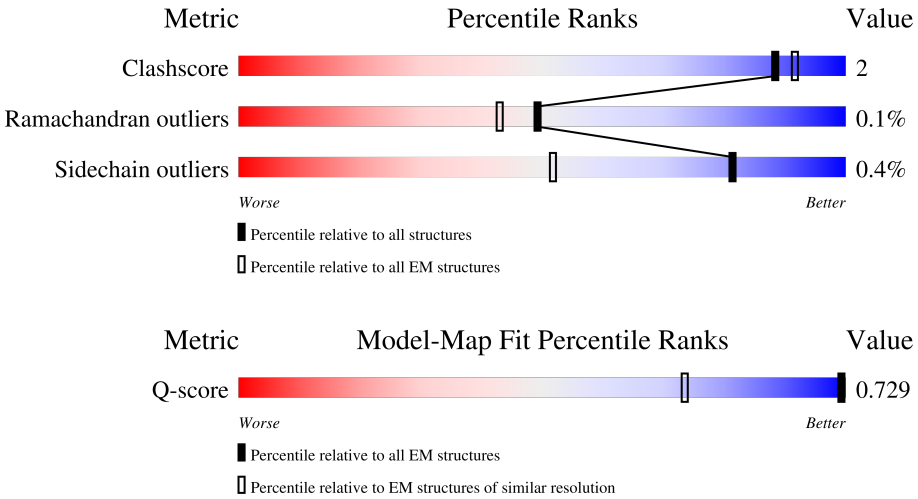
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 1.76 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.



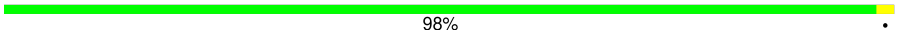
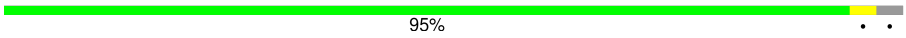
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	674 (1.27 - 2.26)

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	751	97%
2	B	735	96%
3	C	81	99%
4	D	141	98%

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Mol	Chain	Length	Quality of chain
5	E	74	
6	F	165	
7	I	40	
8	J	40	
9	K	86	
10	L	157	
11	M	31	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 25286 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5801	3800	987	987	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5818	3831	974	998	15		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	95	GLN	HIS	engineered mutation	UNP P29255
B	486	ALA	-	linker	UNP P29255
B	487	TRP	-	linker	UNP P29255
B	488	PRO	-	linker	UNP P29255
B	489	ASN	-	linker	UNP P29255
B	490	TYR	-	linker	UNP P29255
B	491	GLY	-	linker	UNP P29255
B	492	ASN	-	linker	UNP P29255
B	493	VAL	-	linker	UNP P29255

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			537	337	95	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	40	Total	C	N	O	S	0	0
			318	215	47	53	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	77	Total	C	N	O	S	0	0
			538	353	89	92	4		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

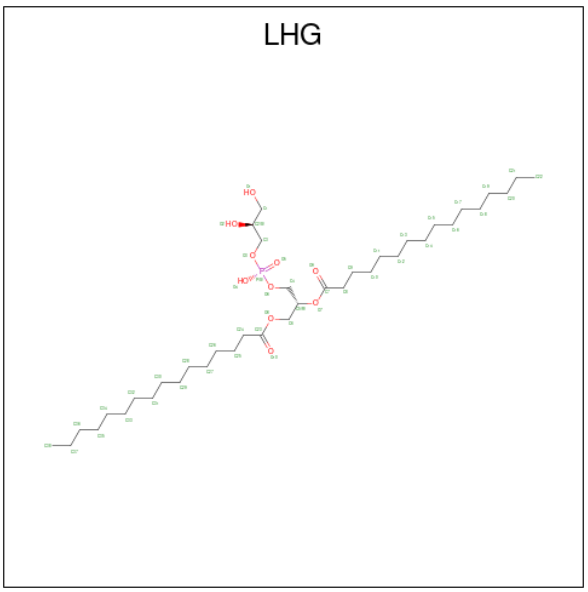
Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1150	750	187	211	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

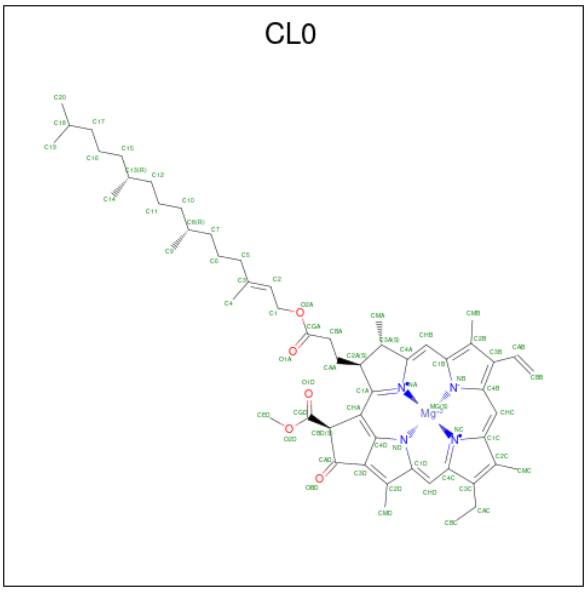
- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG)

(formula: $C_{38}H_{75}O_{10}P$).



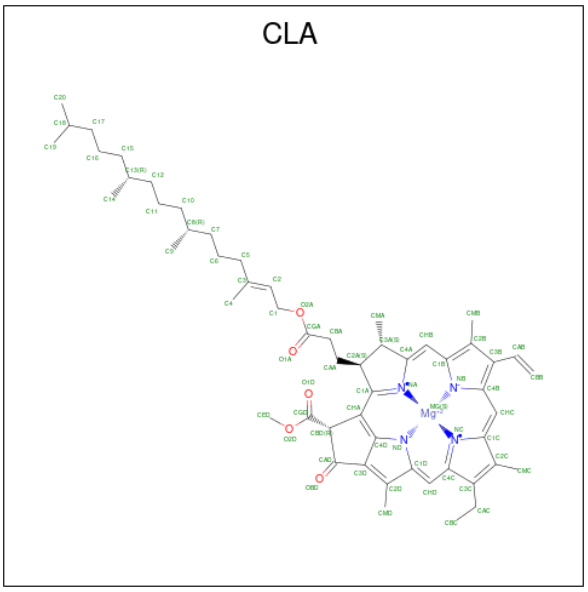
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			48	37	10	1	
12	A	1	Total	C	O	P	0
			49	38	10	1	
12	B	1	Total	C	O	P	0
			38	27	10	1	
12	M	1	Total	C	O	P	0
			40	29	10	1	

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 14 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
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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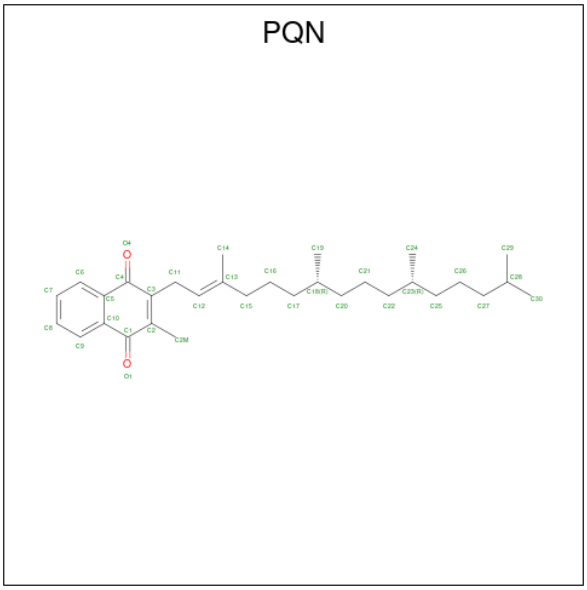
Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	J	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



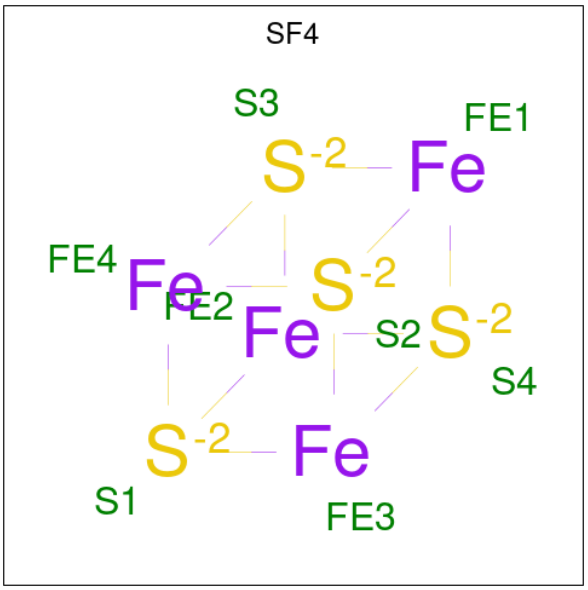
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total 33	C 31	O 2	0

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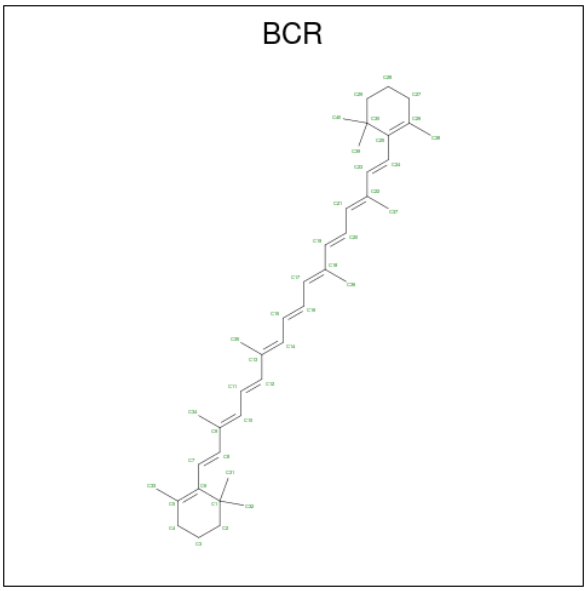
Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



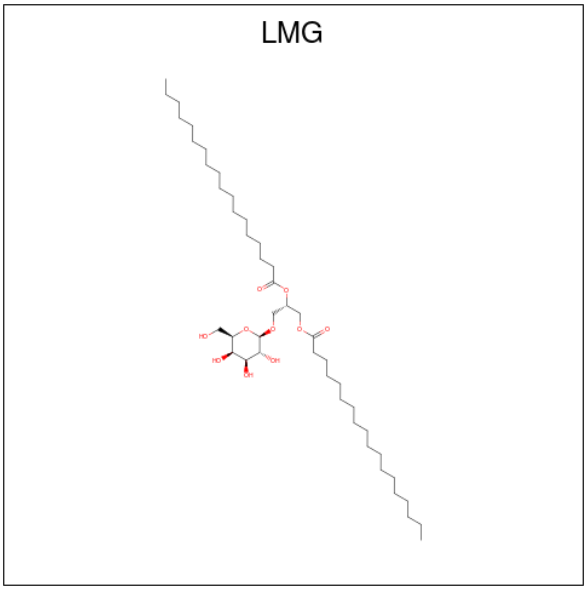
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	A	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 30 30	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	B	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	I	1	Total C 40 40	0

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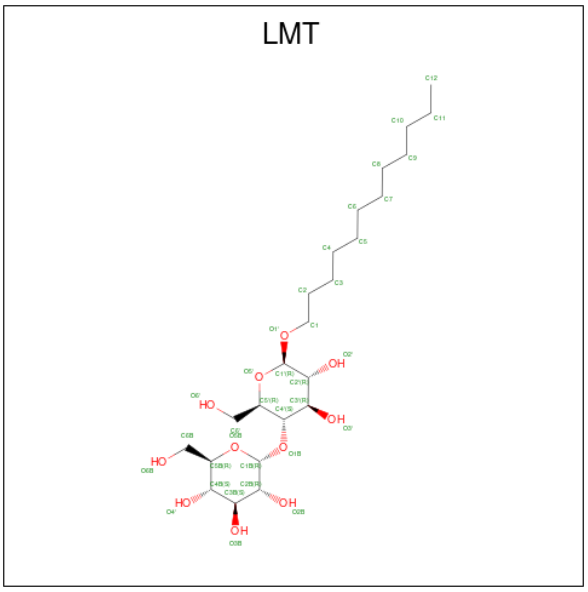
Mol	Chain	Residues	Atoms	AltConf
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total C O 46 36 10	0
18	B	1	Total C O 50 40 10	0
18	B	1	Total C O 38 28 10	0
18	I	1	Total C O 38 28 10	0

- Molecule 19 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

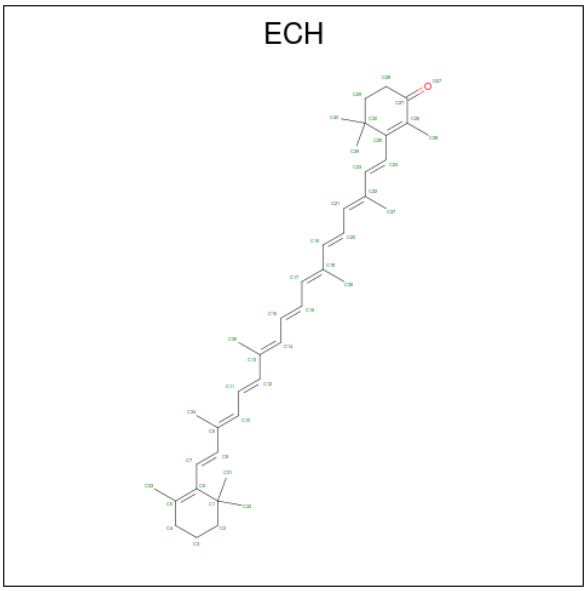


Mol	Chain	Residues	Atoms	AltConf
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	A	1	Total C O 35 24 11	0
19	F	1	Total C O 35 24 11	0
19	F	1	Total C O 35 24 11	0

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total Ca 1 1	0
20	L	1	Total Ca 1 1	0

- Molecule 21 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
21	B	1	Total C O 41 40 1	0
21	I	1	Total C O 41 40 1	0
21	M	1	Total C O 41 40 1	0

- Molecule 22 is water.

Mol	Chain	Residues	Atoms	AltConf
22	A	109	Total O 109 109	0
22	B	153	Total O 153 153	0
22	C	31	Total O 31 31	0
22	D	23	Total O 23 23	0
22	E	3	Total O 3 3	0
22	F	4	Total O 4 4	0
22	I	4	Total O 4 4	0
22	J	2	Total O 2 2	0
22	K	2	Total O 2 2	0

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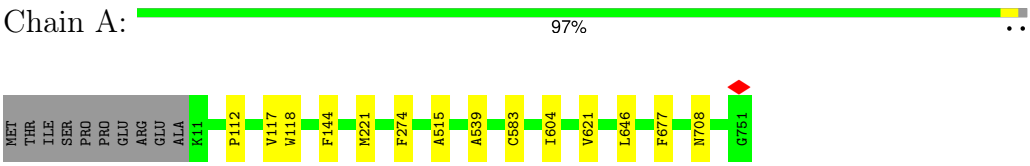
Mol	Chain	Residues	Atoms	AltConf
22	L	16	Total O 16 16	0
22	M	3	Total O 3 3	0

3 Residue-property plots (i)

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

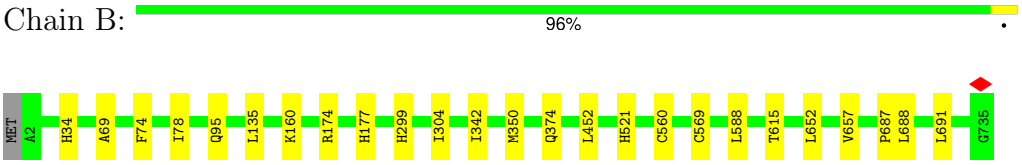
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



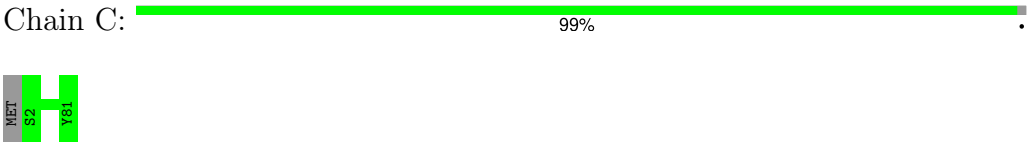
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



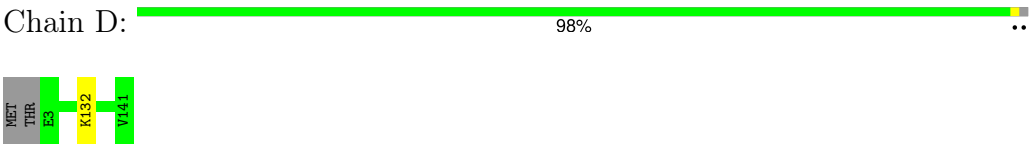
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



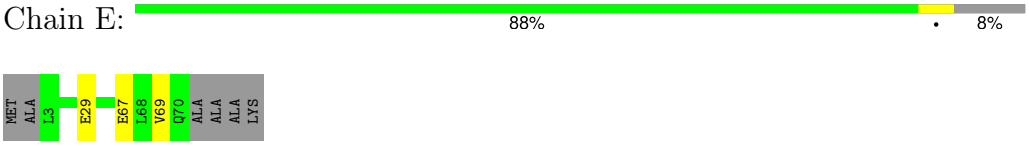
• Molecule 4: Photosystem I reaction center subunit II

Chain D:



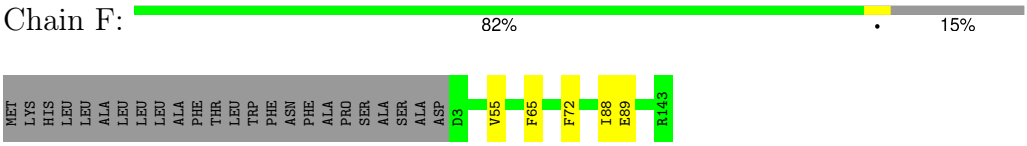
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



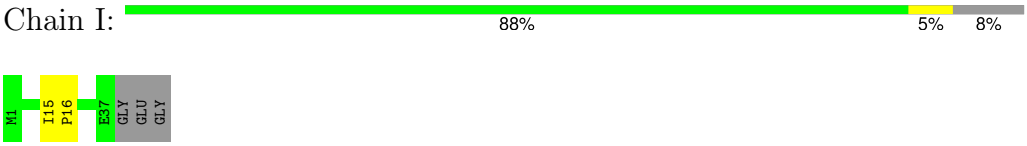
• Molecule 6: Photosystem I reaction center subunit III

Chain F:



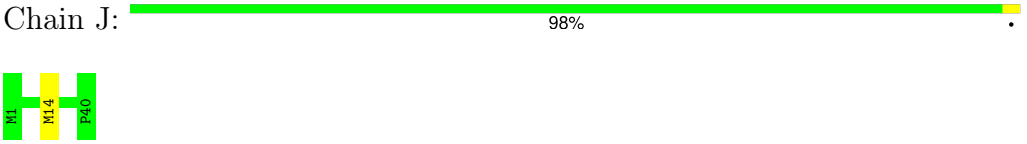
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



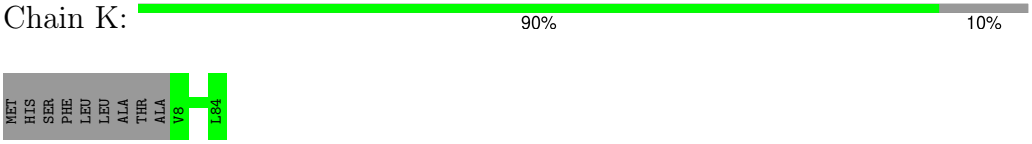
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



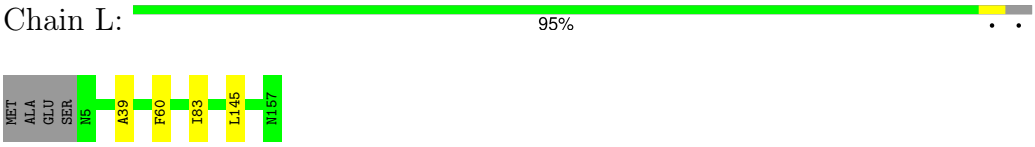
• Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:



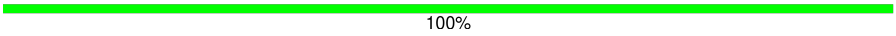
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	857484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	54.034	Depositor
Minimum map value	-12.744	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.4	Depositor
Map size (Å)	321.64, 321.64, 321.64	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.731, 0.731, 0.731	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, LMG, SF4, CLA, CA, CL0, LHG, ECH, LMT, BCR

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	0.30	0/5999	0.29	0/8176
2	B	0.31	0/6032	0.30	0/8250
3	C	0.29	0/610	0.34	0/826
4	D	0.27	0/1111	0.29	0/1497
5	E	0.23	0/546	0.28	0/738
6	F	0.22	0/1130	0.29	0/1535
7	I	0.32	0/304	0.29	0/416
8	J	0.27	0/327	0.27	0/443
9	K	0.21	0/549	0.26	0/745
10	L	0.29	0/1180	0.29	0/1603
11	M	0.29	0/241	0.24	0/326
All	All	0.29	0/18029	0.29	0/24555

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	5801	0	5664	9	0
2	B	5818	0	5588	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	600	0	581	0	0
4	D	1087	0	1082	0	0
5	E	537	0	520	2	0
6	F	1100	0	1096	3	0
7	I	293	0	292	1	0
8	J	318	0	328	1	0
9	K	538	0	565	0	0
10	L	1150	0	1122	4	0
11	M	238	0	260	0	0
12	A	97	0	143	0	0
12	B	38	0	49	0	0
12	M	40	0	50	0	0
13	A	65	0	72	3	0
14	A	2708	0	2844	20	0
14	B	2455	0	2569	31	0
14	F	156	0	138	2	0
14	J	160	0	144	1	0
14	K	155	0	138	0	0
14	L	195	0	216	1	0
15	A	33	0	46	0	0
15	B	33	0	46	0	0
16	A	8	0	0	0	0
16	C	16	0	0	0	0
17	A	200	0	280	7	0
17	B	230	0	319	3	0
17	F	80	0	112	2	0
17	I	40	0	56	0	0
17	J	80	0	112	2	0
17	K	80	0	112	1	0
17	L	80	0	112	4	0
18	A	46	0	62	0	0
18	B	88	0	119	0	0
18	I	38	0	46	0	0
19	A	140	0	184	0	0
19	F	70	0	92	0	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	B	41	0	54	1	0
21	I	41	0	54	0	0
21	M	41	0	54	3	0
22	A	109	0	0	0	0
22	B	153	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	31	0	0	0	0
22	D	23	0	0	0	0
22	E	3	0	0	0	0
22	F	4	0	0	0	0
22	I	4	0	0	0	0
22	J	2	0	0	0	0
22	K	2	0	0	0	0
22	L	16	0	0	0	0
22	M	3	0	0	0	0
All	All	25286	0	25321	95	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 2.

The worst 5 of 95 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)
14:A:804:CLA:HMB1	14:A:804:CLA:HBB1	1.74	0.69
14:A:820:CLA:HMB1	14:A:820:CLA:HBB1	1.78	0.66
14:B:837:CLA:HMB1	14:B:837:CLA:HBB1	1.77	0.66
2:B:452:LEU:HD22	2:B:615:THR:HG21	1.83	0.61
1:A:604:ILE:HD11	13:A:802:CL0:H35	1.84	0.60

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	739/751 (98%)	719 (97%)	20 (3%)	0	100 100
2	B	732/735 (100%)	716 (98%)	15 (2%)	1 (0%)	48 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	78/81 (96%)	75 (96%)	3 (4%)	0	100 100
4	D	137/141 (97%)	132 (96%)	4 (3%)	1 (1%)	18 7
5	E	66/74 (89%)	60 (91%)	6 (9%)	0	100 100
6	F	139/165 (84%)	135 (97%)	4 (3%)	0	100 100
7	I	35/40 (88%)	34 (97%)	1 (3%)	0	100 100
8	J	38/40 (95%)	37 (97%)	1 (3%)	0	100 100
9	K	75/86 (87%)	73 (97%)	2 (3%)	0	100 100
10	L	151/157 (96%)	146 (97%)	5 (3%)	0	100 100
11	M	29/31 (94%)	29 (100%)	0	0	100 100
All	All	2219/2301 (96%)	2156 (97%)	61 (3%)	2 (0%)	49 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	132	LYS
2	B	560	CYS

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	594/603 (98%)	592 (100%)	2 (0%)	86 83
2	B	587/588 (100%)	584 (100%)	3 (0%)	81 75
3	C	68/69 (99%)	68 (100%)	0	100 100
4	D	114/116 (98%)	114 (100%)	0	100 100
5	E	58/60 (97%)	56 (97%)	2 (3%)	32 13
6	F	118/137 (86%)	117 (99%)	1 (1%)	73 64
7	I	31/32 (97%)	31 (100%)	0	100 100
8	J	35/35 (100%)	35 (100%)	0	100 100
9	K	55/62 (89%)	55 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	L	115/118 (98%)	115 (100%)	0	100 100
11	M	25/25 (100%)	25 (100%)	0	100 100
All	All	1800/1845 (98%)	1792 (100%)	8 (0%)	81 80

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	89	GLU
5	E	67	GLU
2	B	569	CYS
2	B	342	ILE
5	E	29	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
10	L	9	GLN
10	L	122	GLN
2	B	373	HIS
2	B	705	GLN
3	C	38	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 141 ligands modelled in this entry, 2 are monoatomic - leaving 139 for Mogul analysis.

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	$\#\|Z\| > 2$
14	CLA	B	821	2	69,73,73	0.97	4 (5%)	82,113,113	0.96	4 (4%)
14	CLA	K	4002	9	49,53,73	1.15	4 (8%)	58,89,113	0.92	3 (5%)
14	CLA	A	843	1	69,73,73	0.95	4 (5%)	82,113,113	1.06	6 (7%)
17	BCR	A	850	-	41,41,41	0.32	0	56,56,56	0.50	0
14	CLA	B	817	2	64,68,73	1.00	4 (6%)	76,107,113	1.08	4 (5%)
14	CLA	L	202	10	69,73,73	0.96	3 (4%)	82,113,113	1.11	3 (3%)
21	ECH	B	846	-	42,42,42	0.39	0	55,58,58	0.65	0
14	CLA	B	827	2	69,73,73	0.97	4 (5%)	82,113,113	0.95	3 (3%)
14	CLA	A	816	1	49,53,73	1.13	4 (8%)	58,89,113	1.09	2 (3%)
14	CLA	A	811	1	49,53,73	1.15	5 (10%)	58,89,113	1.14	3 (5%)
14	CLA	B	818	2	69,73,73	0.97	4 (5%)	82,113,113	1.01	6 (7%)
15	PQN	B	843	-	34,34,34	0.50	0	43,45,45	0.68	1 (2%)
17	BCR	J	1104	-	41,41,41	0.33	0	56,56,56	0.58	0
14	CLA	J	1103	8	54,58,73	1.10	5 (9%)	64,95,113	1.04	5 (7%)
14	CLA	B	832	2	59,63,73	1.05	3 (5%)	70,101,113	1.07	6 (8%)
14	CLA	A	834	1	69,73,73	0.96	3 (4%)	82,113,113	1.01	7 (8%)
14	CLA	B	838	2	69,73,73	0.97	4 (5%)	82,113,113	0.95	4 (4%)
14	CLA	A	825	1	69,73,73	0.98	4 (5%)	82,113,113	1.00	4 (4%)
14	CLA	A	844	22	69,73,73	0.96	4 (5%)	82,113,113	1.01	4 (4%)
14	CLA	K	4003	9	49,53,73	1.17	5 (10%)	58,89,113	1.09	2 (3%)
18	LMG	I	101	-	38,38,55	0.62	0	46,46,63	0.70	0
16	SF4	C	102	3	0,12,12	-	-	-		
14	CLA	A	819	1	69,73,73	0.95	4 (5%)	82,113,113	0.95	3 (3%)
14	CLA	B	840	22	69,73,73	0.96	3 (4%)	82,113,113	0.93	5 (6%)
14	CLA	A	820	1	69,73,73	0.96	4 (5%)	82,113,113	1.18	6 (7%)
17	BCR	F	202	-	41,41,41	0.33	0	56,56,56	0.94	1 (1%)
14	CLA	B	841	2	69,73,73	0.96	4 (5%)	82,113,113	1.14	6 (7%)
14	CLA	A	808	1	69,73,73	0.95	4 (5%)	82,113,113	1.01	4 (4%)
14	CLA	B	814	2	69,73,73	0.98	4 (5%)	82,113,113	0.93	3 (3%)
14	CLA	B	820	22	69,73,73	0.98	6 (8%)	82,113,113	0.94	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	813	2	59,63,73	1.04	5 (8%)	70,101,113	0.99	3 (4%)
14	CLA	B	823	2	49,53,73	1.14	4 (8%)	58,89,113	0.99	3 (5%)
14	CLA	B	835	22	49,53,73	1.15	4 (8%)	58,89,113	1.22	3 (5%)
14	CLA	J	1101	1	69,73,73	0.96	3 (4%)	82,113,113	0.90	1 (1%)
14	CLA	A	833	1	64,68,73	1.00	4 (6%)	76,107,113	0.97	3 (3%)
17	BCR	I	102	-	41,41,41	0.37	0	56,56,56	0.84	1 (1%)
21	ECH	M	102	-	42,42,42	0.39	0	55,58,58	0.70	0
14	CLA	A	822	22	69,73,73	0.97	3 (4%)	82,113,113	0.94	4 (4%)
14	CLA	B	822	2	69,73,73	0.97	4 (5%)	82,113,113	0.93	3 (3%)
14	CLA	A	806	1	69,73,73	0.99	4 (5%)	82,113,113	1.14	7 (8%)
14	CLA	B	836	22	50,54,73	1.12	5 (10%)	59,90,113	0.97	1 (1%)
18	LMG	B	802	-	50,50,55	0.59	0	58,58,63	0.64	0
14	CLA	A	827	22	64,68,73	1.01	3 (4%)	76,107,113	0.96	2 (2%)
14	CLA	A	803	-	69,73,73	0.95	4 (5%)	82,113,113	1.01	3 (3%)
14	CLA	B	808	2	69,73,73	0.97	5 (7%)	82,113,113	1.21	5 (6%)
12	LHG	M	101	-	39,39,48	0.57	0	42,45,54	0.55	0
19	LMT	A	858	-	36,36,36	0.58	0	47,47,47	0.85	1 (2%)
17	BCR	A	848	-	41,41,41	0.34	0	56,56,56	0.54	0
14	CLA	A	815	1	59,63,73	1.04	4 (6%)	70,101,113	1.02	4 (5%)
14	CLA	B	801	22	69,73,73	0.95	4 (5%)	82,113,113	1.04	5 (6%)
14	CLA	B	809	2	69,73,73	0.95	3 (4%)	82,113,113	1.06	4 (4%)
14	CLA	B	828	2	69,73,73	0.96	4 (5%)	82,113,113	1.01	5 (6%)
14	CLA	B	834	22	59,63,73	1.03	4 (6%)	70,101,113	1.05	6 (8%)
14	CLA	A	810	1	54,58,73	1.10	4 (7%)	64,95,113	1.03	2 (3%)
14	CLA	A	821	1	69,73,73	0.98	4 (5%)	82,113,113	0.98	4 (4%)
19	LMT	A	854	-	36,36,36	0.64	0	47,47,47	0.66	0
14	CLA	A	859	-	69,73,73	0.97	5 (7%)	82,113,113	1.10	5 (6%)
14	CLA	B	839	2	69,73,73	0.98	4 (5%)	82,113,113	0.99	5 (6%)
14	CLA	F	203	22	49,53,73	1.14	3 (6%)	58,89,113	1.01	4 (6%)
14	CLA	A	807	1	69,73,73	0.99	4 (5%)	82,113,113	0.95	2 (2%)
14	CLA	A	840	1	69,73,73	0.96	3 (4%)	82,113,113	1.13	5 (6%)
14	CLA	B	829	-	69,73,73	0.96	4 (5%)	82,113,113	1.00	4 (4%)
14	CLA	B	826	22	69,73,73	0.97	4 (5%)	82,113,113	0.99	3 (3%)
14	CLA	A	817	22	50,54,73	1.12	5 (10%)	59,90,113	1.09	6 (10%)
14	CLA	A	828	1	69,73,73	0.96	4 (5%)	82,113,113	0.99	4 (4%)
14	CLA	A	814	1	69,73,73	0.97	5 (7%)	82,113,113	0.98	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	835	1	69,73,73	0.96	3 (4%)	82,113,113	1.02	7 (8%)
17	BCR	B	845	-	41,41,41	0.33	0	56,56,56	0.69	0
14	CLA	B	810	2	69,73,73	0.96	3 (4%)	82,113,113	0.96	3 (3%)
18	LMG	B	851	-	38,38,55	0.59	0	46,46,63	0.61	0
14	CLA	A	838	1	55,59,73	1.07	3 (5%)	64,96,113	0.98	2 (3%)
14	CLA	B	824	2	57,61,73	1.06	4 (7%)	67,98,113	1.17	4 (5%)
14	CLA	K	4004	22	69,73,73	0.97	4 (5%)	82,113,113	1.01	2 (2%)
17	BCR	K	4001	-	41,41,41	0.35	0	56,56,56	0.83	2 (3%)
19	LMT	F	206	-	36,36,36	0.57	0	47,47,47	0.90	2 (4%)
17	BCR	A	849	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
14	CLA	B	815	2	69,73,73	0.94	3 (4%)	82,113,113	0.97	5 (6%)
13	CL0	A	802	1	69,73,73	0.98	6 (8%)	82,113,113	1.01	4 (4%)
14	CLA	A	805	1	69,73,73	0.96	5 (7%)	82,113,113	1.00	5 (6%)
14	CLA	A	837	1	69,73,73	0.97	4 (5%)	82,113,113	0.94	3 (3%)
14	CLA	A	841	1	69,73,73	0.95	4 (5%)	82,113,113	1.01	6 (7%)
17	BCR	F	205	-	41,41,41	0.31	0	56,56,56	0.56	0
14	CLA	F	204	6	50,54,73	1.12	4 (8%)	59,90,113	0.96	2 (3%)
14	CLA	F	201	2	69,73,73	0.97	3 (4%)	82,113,113	1.00	2 (2%)
17	BCR	J	1105	-	41,41,41	0.31	0	56,56,56	0.61	0
14	CLA	A	845	12	50,54,73	1.11	3 (6%)	59,90,113	0.98	2 (3%)
17	BCR	B	852	-	41,41,41	0.31	0	56,56,56	0.55	1 (1%)
14	CLA	B	842	12	50,54,73	1.12	4 (8%)	59,90,113	1.00	3 (5%)
17	BCR	L	206	-	41,41,41	0.34	0	56,56,56	0.74	1 (1%)
21	ECH	I	103	-	42,42,42	0.42	0	55,58,58	0.58	0
14	CLA	B	804	2	69,73,73	0.98	3 (4%)	82,113,113	0.90	2 (2%)
16	SF4	A	847	1,2	0,12,12	-	-	-		
14	CLA	B	805	2	69,73,73	0.97	3 (4%)	82,113,113	0.96	4 (4%)
14	CLA	A	832	1	69,73,73	0.98	6 (8%)	82,113,113	0.98	4 (4%)
14	CLA	B	812	2	69,73,73	0.96	4 (5%)	82,113,113	1.04	3 (3%)
14	CLA	L	204	-	69,73,73	0.96	4 (5%)	82,113,113	1.00	5 (6%)
17	BCR	B	849	-	41,41,41	0.35	0	56,56,56	0.79	1 (1%)
17	BCR	A	852	-	41,41,41	0.32	0	56,56,56	0.62	1 (1%)
12	LHG	A	855	14	48,48,48	0.56	0	51,54,54	0.51	0
14	CLA	A	830	1	69,73,73	1.01	5 (7%)	82,113,113	1.05	7 (8%)
12	LHG	A	801	-	47,47,48	0.53	0	50,53,54	0.59	0
17	BCR	B	847	-	30,30,41	0.45	0	39,39,56	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	813	1	58,62,73	1.05	5 (8%)	68,99,113	0.99	2 (2%)
17	BCR	B	848	-	41,41,41	0.34	0	56,56,56	0.82	2 (3%)
14	CLA	B	806	2	69,73,73	0.95	3 (4%)	82,113,113	1.03	5 (6%)
14	CLA	B	811	2	69,73,73	0.96	4 (5%)	82,113,113	1.02	1 (1%)
14	CLA	A	836	1	69,73,73	0.95	5 (7%)	82,113,113	1.01	4 (4%)
14	CLA	B	825	22	69,73,73	0.99	4 (5%)	82,113,113	1.16	5 (6%)
14	CLA	B	807	2	69,73,73	0.98	3 (4%)	82,113,113	0.96	3 (3%)
17	BCR	B	844	-	41,41,41	0.32	0	56,56,56	0.62	0
14	CLA	J	1102	8	49,53,73	1.15	5 (10%)	58,89,113	0.97	2 (3%)
16	SF4	C	101	3	0,12,12	-	-	-		
14	CLA	B	819	2	69,73,73	0.95	4 (5%)	82,113,113	1.02	5 (6%)
18	LMG	A	853	-	46,46,55	0.58	0	54,54,63	0.68	0
14	CLA	A	824	1	55,59,73	1.07	4 (7%)	64,96,113	1.03	4 (6%)
14	CLA	A	804	22	69,73,73	0.97	3 (4%)	82,113,113	0.94	3 (3%)
12	LHG	B	850	14	37,37,48	0.59	0	40,43,54	0.57	0
17	BCR	A	851	-	41,41,41	0.34	0	56,56,56	0.71	1 (1%)
14	CLA	A	812	1	69,73,73	0.96	3 (4%)	82,113,113	0.94	2 (2%)
14	CLA	A	839	1	69,73,73	0.95	4 (5%)	82,113,113	0.99	4 (4%)
14	CLA	B	830	2	69,73,73	0.97	5 (7%)	82,113,113	0.95	5 (6%)
17	BCR	L	205	-	41,41,41	0.33	0	56,56,56	0.56	0
14	CLA	A	809	1	69,73,73	0.95	4 (5%)	82,113,113	1.17	4 (4%)
14	CLA	A	818	1	69,73,73	0.96	4 (5%)	82,113,113	1.08	5 (6%)
14	CLA	B	837	2	54,58,73	1.10	4 (7%)	64,95,113	0.99	3 (4%)
14	CLA	A	826	22	69,73,73	0.97	4 (5%)	82,113,113	1.01	2 (2%)
14	CLA	B	833	2	69,73,73	0.96	5 (7%)	82,113,113	0.98	4 (4%)
19	LMT	A	857	-	36,36,36	0.55	0	47,47,47	0.78	1 (2%)
19	LMT	F	207	-	36,36,36	0.57	0	47,47,47	0.71	0
14	CLA	A	831	1	69,73,73	0.95	3 (4%)	82,113,113	0.97	2 (2%)
14	CLA	A	842	22	69,73,73	0.98	3 (4%)	82,113,113	0.98	3 (3%)
14	CLA	B	831	2	69,73,73	0.97	4 (5%)	82,113,113	0.98	4 (4%)
17	BCR	K	4005	-	41,41,41	0.30	0	56,56,56	0.53	0
14	CLA	L	203	10	69,73,73	0.95	4 (5%)	82,113,113	1.00	2 (2%)
14	CLA	A	823	1	69,73,73	0.97	4 (5%)	82,113,113	0.95	4 (4%)
14	CLA	A	829	1	69,73,73	0.97	5 (7%)	82,113,113	1.04	6 (7%)
14	CLA	B	816	2	64,68,73	0.99	3 (4%)	76,107,113	1.11	4 (5%)
19	LMT	A	856	-	36,36,36	0.57	0	47,47,47	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	PQN	A	846	-	34,34,34	0.46	0	43,45,45	0.66	1 (2%)

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
14	CLA	B	821	2	-	9/39/115/115	-
14	CLA	K	4002	9	-	3/15/91/115	-
14	CLA	A	843	1	-	8/39/115/115	-
17	BCR	A	850	-	-	4/29/63/63	0/2/2/2
14	CLA	B	817	2	-	7/33/109/115	-
14	CLA	L	202	10	-	8/39/115/115	-
21	ECH	B	846	-	-	6/29/66/66	0/2/2/2
14	CLA	B	827	2	-	6/39/115/115	-
14	CLA	A	816	1	-	0/15/91/115	-
14	CLA	A	811	1	-	4/15/91/115	-
14	CLA	B	818	2	-	7/39/115/115	-
15	PQN	B	843	-	-	4/23/43/43	0/2/2/2
17	BCR	J	1104	-	-	7/29/63/63	0/2/2/2
14	CLA	J	1103	8	-	7/21/97/115	-
14	CLA	B	832	2	-	2/27/103/115	-
14	CLA	A	834	1	-	5/39/115/115	-
14	CLA	B	838	2	-	10/39/115/115	-
14	CLA	A	825	1	-	12/39/115/115	-
14	CLA	A	844	22	-	15/39/115/115	-
14	CLA	K	4003	9	-	7/15/91/115	-
18	LMG	I	101	-	-	8/33/53/70	0/1/1/1
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	819	1	-	9/39/115/115	-
14	CLA	B	840	22	-	3/39/115/115	-
14	CLA	A	820	1	-	6/39/115/115	-
17	BCR	F	202	-	-	4/29/63/63	0/2/2/2
14	CLA	B	841	2	-	12/39/115/115	-
14	CLA	A	808	1	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	814	2	-	9/39/115/115	-
14	CLA	B	820	22	-	9/39/115/115	-
14	CLA	B	813	2	-	9/27/103/115	-
14	CLA	B	823	2	-	3/15/91/115	-
14	CLA	B	835	22	-	1/15/91/115	-
14	CLA	J	1101	1	-	2/39/115/115	-
14	CLA	A	833	1	-	2/33/109/115	-
17	BCR	I	102	-	-	5/29/63/63	0/2/2/2
21	ECH	M	102	-	-	8/29/66/66	0/2/2/2
14	CLA	A	822	22	-	6/39/115/115	-
14	CLA	B	822	2	-	14/39/115/115	-
14	CLA	A	806	1	-	14/39/115/115	-
14	CLA	B	836	22	-	3/17/93/115	-
18	LMG	B	802	-	-	12/45/65/70	0/1/1/1
14	CLA	A	827	22	-	2/33/109/115	-
14	CLA	A	803	-	-	4/39/115/115	-
14	CLA	B	808	2	-	3/39/115/115	-
12	LHG	M	101	-	-	9/44/44/53	-
19	LMT	A	858	-	-	7/21/61/61	0/2/2/2
17	BCR	A	848	-	-	2/29/63/63	0/2/2/2
14	CLA	A	815	1	-	6/27/103/115	-
14	CLA	B	801	22	-	7/39/115/115	-
14	CLA	B	809	2	-	7/39/115/115	-
14	CLA	B	828	2	-	7/39/115/115	-
14	CLA	B	834	22	-	6/27/103/115	-
14	CLA	A	810	1	-	4/21/97/115	-
14	CLA	A	821	1	-	5/39/115/115	-
19	LMT	A	854	-	-	5/21/61/61	0/2/2/2
14	CLA	A	859	-	-	5/39/115/115	-
14	CLA	B	839	2	-	8/39/115/115	-
14	CLA	F	203	22	-	5/15/91/115	-
14	CLA	A	807	1	-	13/39/115/115	-
14	CLA	A	840	1	-	8/39/115/115	-
14	CLA	B	829	-	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	826	22	-	9/39/115/115	-
14	CLA	A	817	22	-	7/17/93/115	-
14	CLA	A	828	1	-	6/39/115/115	-
14	CLA	A	814	1	-	11/39/115/115	-
14	CLA	A	835	1	-	5/39/115/115	-
17	BCR	B	845	-	-	2/29/63/63	0/2/2/2
14	CLA	B	810	2	-	7/39/115/115	-
18	LMG	B	851	-	-	10/33/53/70	0/1/1/1
14	CLA	A	838	1	-	2/23/99/115	-
14	CLA	B	824	2	-	5/25/101/115	-
14	CLA	K	4004	22	-	11/39/115/115	-
17	BCR	K	4001	-	-	4/29/63/63	0/2/2/2
19	LMT	F	206	-	-	4/21/61/61	0/2/2/2
17	BCR	A	849	-	-	6/29/63/63	0/2/2/2
14	CLA	B	815	2	-	6/39/115/115	-
13	CL0	A	802	1	-	4/39/115/115	-
14	CLA	A	805	1	-	17/39/115/115	-
14	CLA	A	837	1	-	7/39/115/115	-
14	CLA	A	841	1	-	5/39/115/115	-
17	BCR	F	205	-	-	2/29/63/63	0/2/2/2
14	CLA	F	204	6	-	3/17/93/115	-
14	CLA	F	201	2	-	8/39/115/115	-
17	BCR	J	1105	-	-	5/29/63/63	0/2/2/2
14	CLA	A	845	12	-	4/17/93/115	-
17	BCR	B	852	-	-	4/29/63/63	0/2/2/2
14	CLA	B	842	12	-	1/17/93/115	-
17	BCR	L	206	-	-	7/29/63/63	0/2/2/2
21	ECH	I	103	-	-	5/29/66/66	0/2/2/2
14	CLA	B	804	2	-	4/39/115/115	-
16	SF4	A	847	1,2	-	-	0/6/5/5
14	CLA	B	805	2	-	3/39/115/115	-
14	CLA	A	832	1	-	7/39/115/115	-
14	CLA	B	812	2	-	11/39/115/115	-
14	CLA	L	204	-	-	9/39/115/115	-
17	BCR	B	849	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	A	852	-	-	11/29/63/63	0/2/2/2
12	LHG	A	855	14	-	8/53/53/53	-
14	CLA	A	830	1	-	7/39/115/115	-
12	LHG	A	801	-	-	15/52/52/53	-
17	BCR	B	847	-	-	1/24/41/63	0/1/1/2
14	CLA	A	813	1	-	6/26/102/115	-
17	BCR	B	848	-	-	2/29/63/63	0/2/2/2
14	CLA	B	806	2	-	8/39/115/115	-
14	CLA	B	811	2	-	3/39/115/115	-
14	CLA	A	836	1	-	4/39/115/115	-
14	CLA	B	825	22	-	18/39/115/115	-
14	CLA	B	807	2	-	4/39/115/115	-
17	BCR	B	844	-	-	4/29/63/63	0/2/2/2
14	CLA	J	1102	8	-	4/15/91/115	-
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	819	2	-	9/39/115/115	-
18	LMG	A	853	-	-	16/41/61/70	0/1/1/1
14	CLA	A	824	1	-	4/23/99/115	-
14	CLA	A	804	22	-	7/39/115/115	-
12	LHG	B	850	14	-	4/42/42/53	-
17	BCR	A	851	-	-	4/29/63/63	0/2/2/2
14	CLA	A	812	1	-	17/39/115/115	-
14	CLA	A	839	1	-	7/39/115/115	-
14	CLA	B	830	2	-	12/39/115/115	-
17	BCR	L	205	-	-	6/29/63/63	0/2/2/2
14	CLA	A	809	1	-	5/39/115/115	-
14	CLA	A	818	1	-	8/39/115/115	-
14	CLA	B	837	2	-	1/21/97/115	-
14	CLA	A	826	22	-	16/39/115/115	-
14	CLA	B	833	2	-	8/39/115/115	-
19	LMT	A	857	-	-	3/21/61/61	0/2/2/2
19	LMT	F	207	-	-	10/21/61/61	0/2/2/2
14	CLA	A	831	1	-	12/39/115/115	-
14	CLA	A	842	22	-	6/39/115/115	-
14	CLA	B	831	2	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	K	4005	-	-	3/29/63/63	0/2/2/2
14	CLA	L	203	10	-	6/39/115/115	-
14	CLA	A	823	1	-	14/39/115/115	-
14	CLA	A	829	1	-	12/39/115/115	-
14	CLA	B	816	2	-	13/33/109/115	-
19	LMT	A	856	-	-	5/21/61/61	0/2/2/2
15	PQN	A	846	-	-	0/23/43/43	0/2/2/2

The worst 5 of 386 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	836	CLA	C1D-ND	3.13	1.42	1.37
14	J	1103	CLA	C1D-ND	3.13	1.42	1.37
14	K	4002	CLA	C1D-ND	3.12	1.42	1.37
14	A	838	CLA	C1D-ND	3.11	1.41	1.37
14	K	4003	CLA	C1D-ND	3.11	1.41	1.37

The worst 5 of 387 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	809	CLA	C4A-NA-C1A	6.17	109.49	106.68
14	B	835	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	B	825	CLA	C4A-NA-C1A	5.73	109.30	106.68
14	L	202	CLA	C4A-NA-C1A	5.68	109.27	106.68
14	A	859	CLA	C4A-NA-C1A	5.32	109.11	106.68

There are no chirality outliers.

5 of 905 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	801	LHG	C3-O3-P-O5
12	A	801	LHG	C4-O6-P-O5
12	A	801	LHG	O9-C7-O7-C5
12	A	855	LHG	C3-O3-P-O5
12	B	850	LHG	C3-O3-P-O5

There are no ring outliers.

60 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	846	ECH	1	0
14	B	827	CLA	2	0
14	A	816	CLA	1	0
17	J	1104	BCR	2	0
14	B	838	CLA	1	0
14	A	825	CLA	2	0
14	A	819	CLA	1	0
14	A	820	CLA	2	0
17	F	202	BCR	2	0
14	B	841	CLA	2	0
14	B	814	CLA	2	0
14	B	820	CLA	1	0
14	B	813	CLA	2	0
14	J	1101	CLA	1	0
21	M	102	ECH	3	0
14	A	822	CLA	1	0
14	A	803	CLA	1	0
14	A	815	CLA	1	0
14	B	801	CLA	2	0
14	B	809	CLA	1	0
14	A	810	CLA	1	0
14	A	859	CLA	1	0
14	B	839	CLA	3	0
14	F	203	CLA	1	0
14	A	807	CLA	1	0
14	A	840	CLA	1	0
14	B	829	CLA	1	0
14	B	826	CLA	4	0
14	A	817	CLA	1	0
14	A	828	CLA	1	0
17	B	845	BCR	2	0
14	B	810	CLA	1	0
17	K	4001	BCR	1	0
17	A	849	BCR	1	0
13	A	802	CL0	3	0
14	A	837	CLA	1	0
14	F	201	CLA	1	0
17	L	206	BCR	2	0
14	B	805	CLA	1	0
14	A	832	CLA	1	0
14	L	204	CLA	1	0
17	B	849	BCR	1	0
17	A	852	BCR	4	0

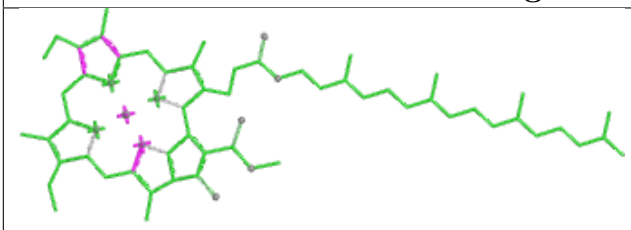
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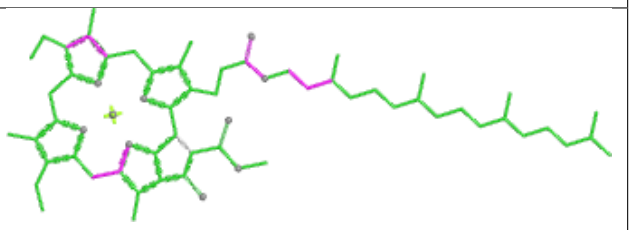
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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14	B	806	CLA	1	0
14	B	811	CLA	2	0
14	B	825	CLA	2	0
14	B	807	CLA	1	0
14	B	819	CLA	2	0
14	A	804	CLA	2	0
17	A	851	BCR	2	0
14	A	839	CLA	1	0
14	B	830	CLA	1	0
17	L	205	BCR	2	0
14	A	818	CLA	1	0
14	B	837	CLA	3	0
14	A	826	CLA	1	0
14	B	833	CLA	1	0
14	A	829	CLA	1	0
14	B	816	CLA	1	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.

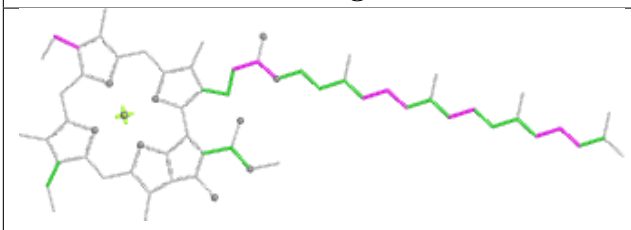
Ligand CLA B 821



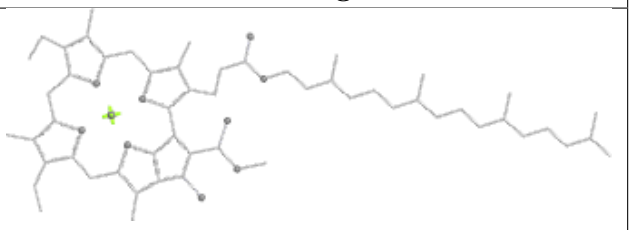
Bond lengths



Bond angles

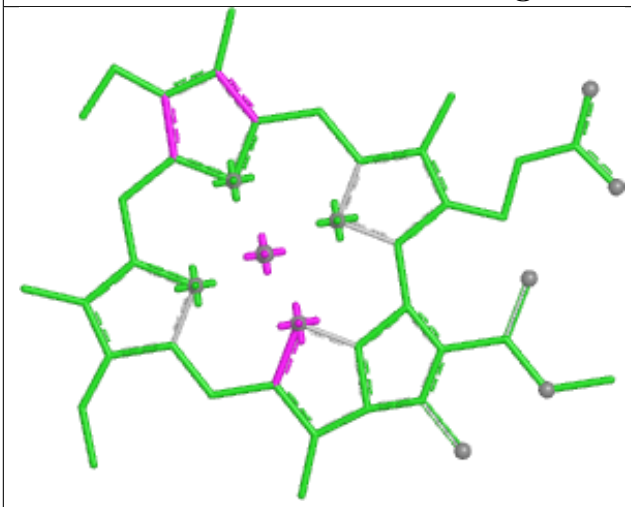


Torsions

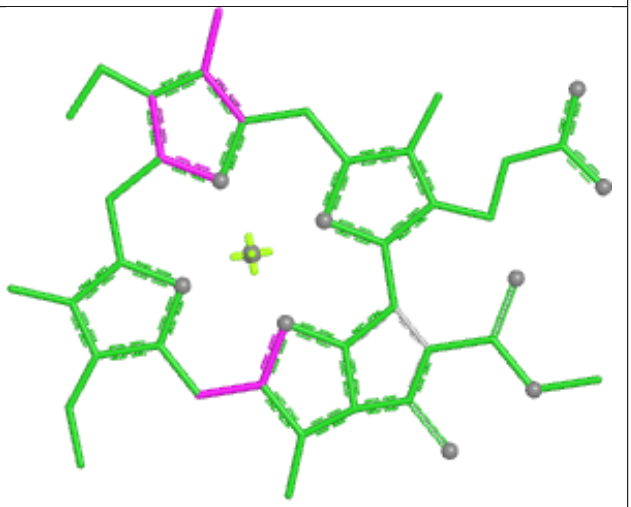


Rings

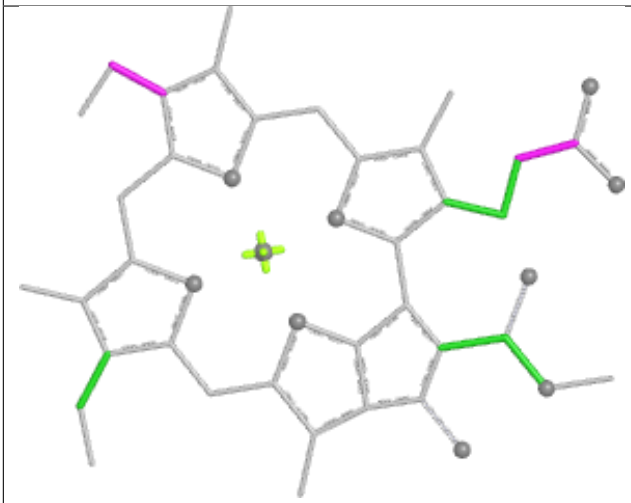
Ligand CLA K 4002



Bond lengths



Bond angles

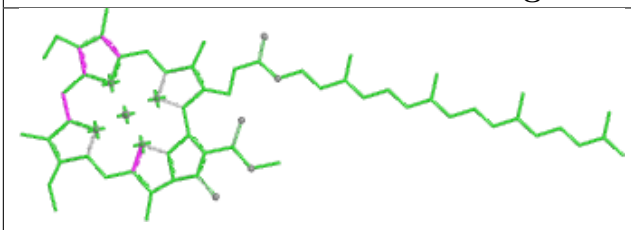


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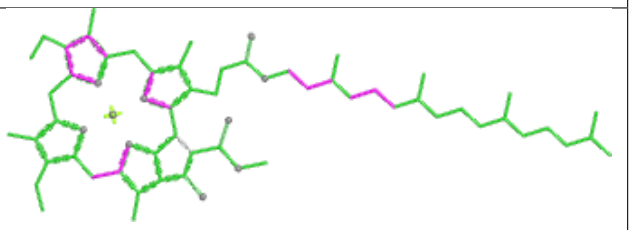


Rings

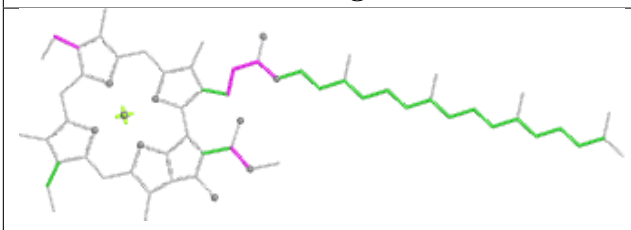
Ligand CLA A 843



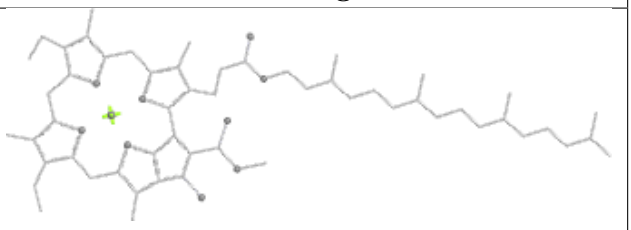
Bond lengths



Bond angles

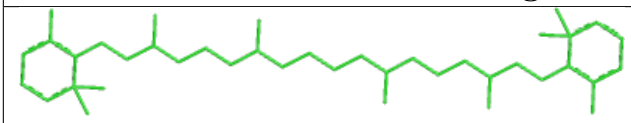


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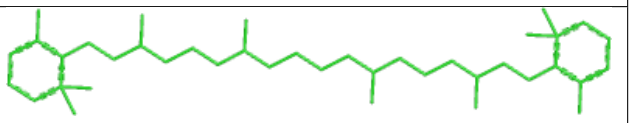


Rings

Ligand BCR A 850



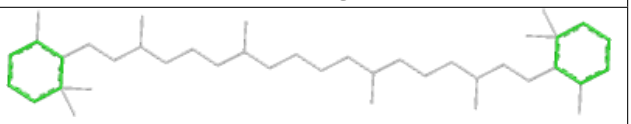
Bond lengths



Bond angles

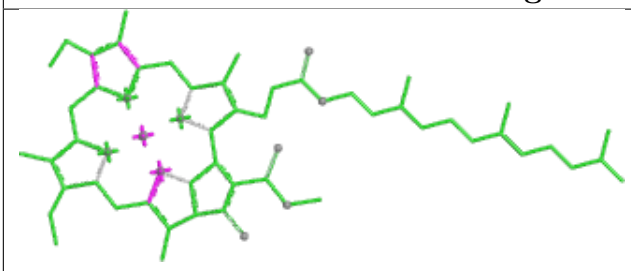


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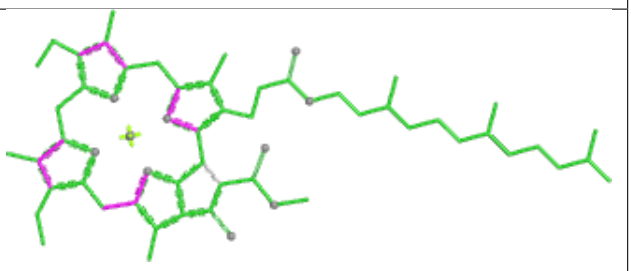


Rings

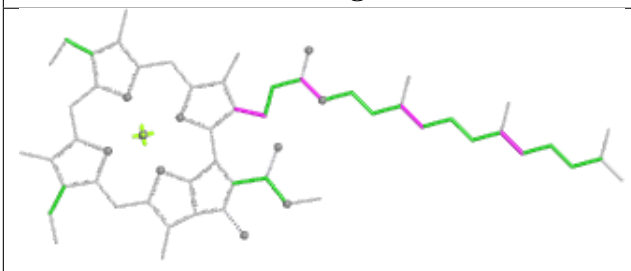
Ligand CLA B 817



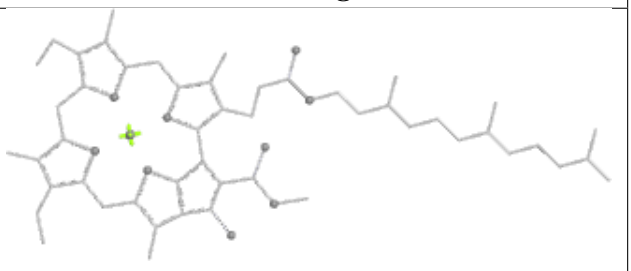
Bond lengths



Bond angles

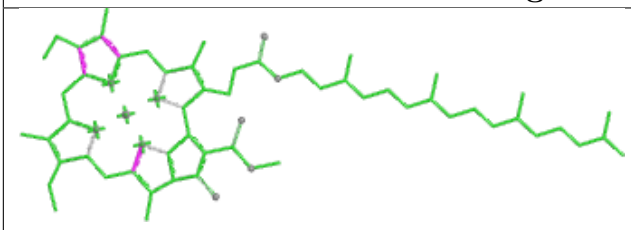


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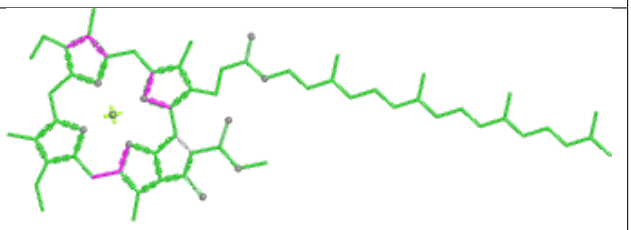


Rings

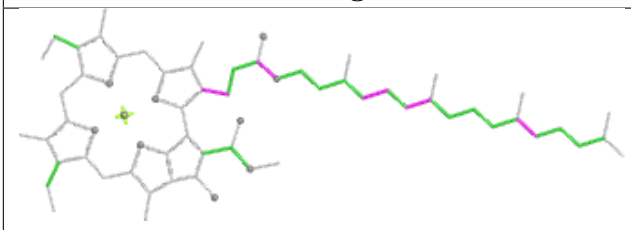
Ligand CLA L 202



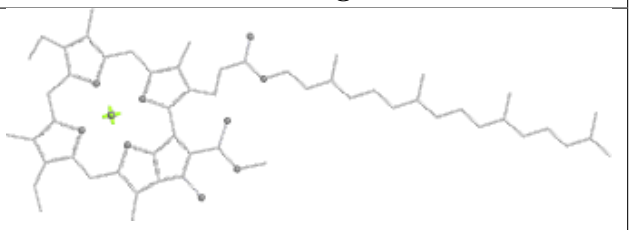
Bond lengths



Bond angles

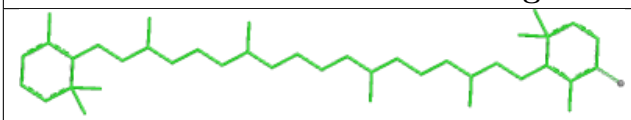


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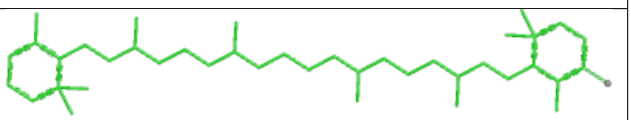


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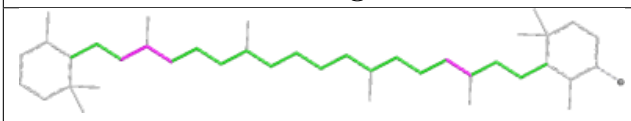
Ligand ECH B 846



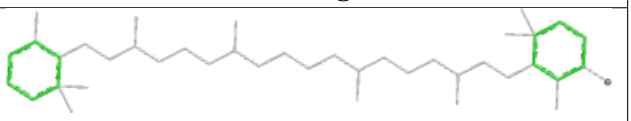
Bond lengths



Bond angles

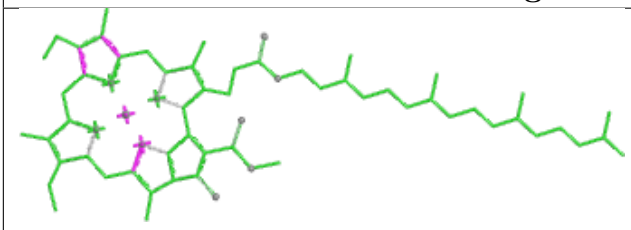


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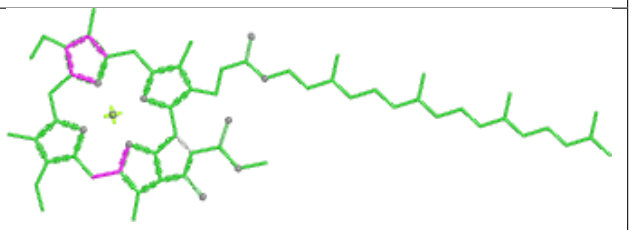


Rings

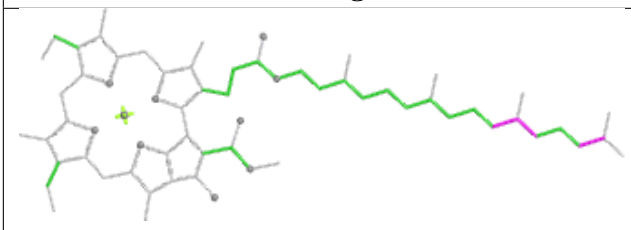
Ligand CLA B 827



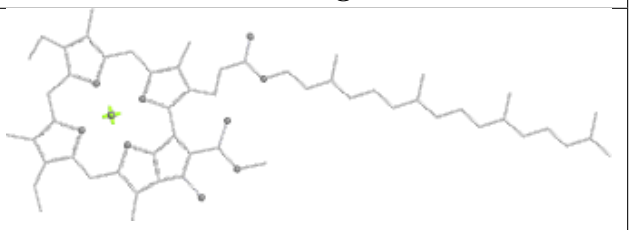
Bond lengths



Bond angles

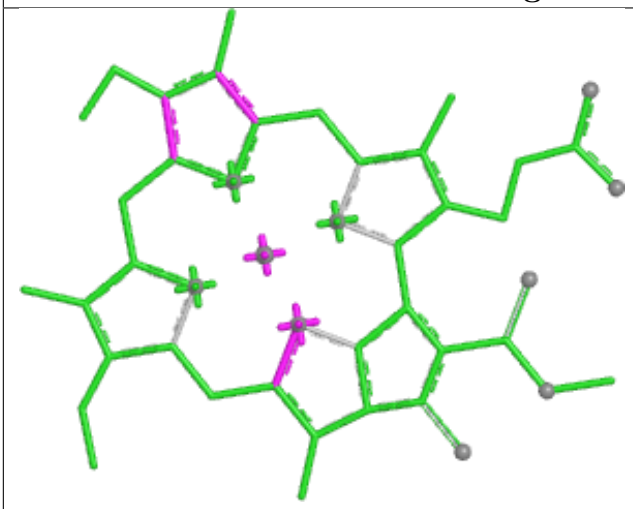


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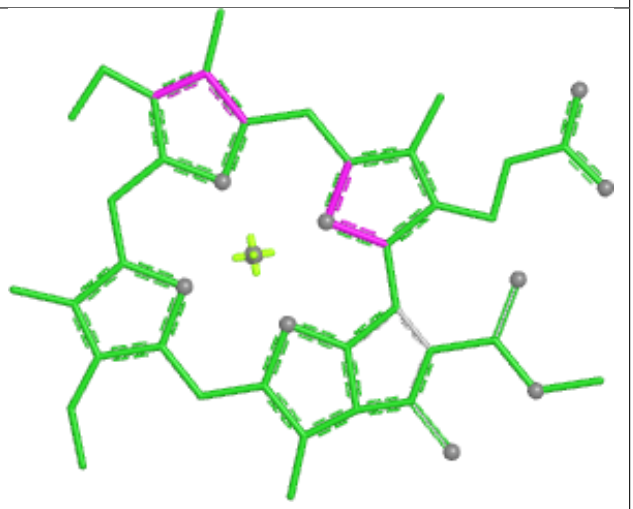


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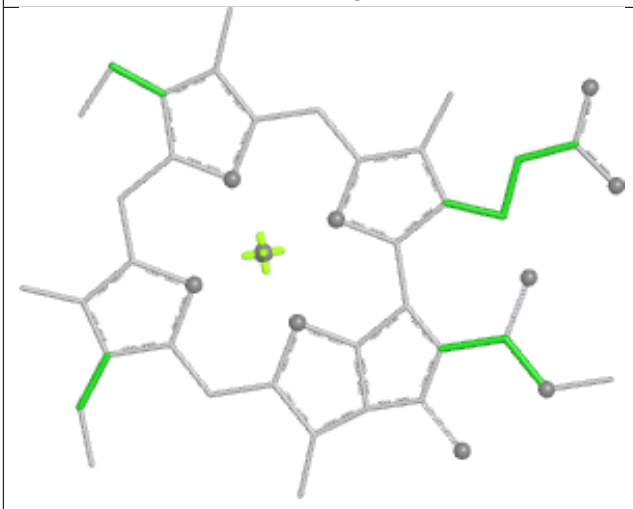
Ligand CLA A 816



Bond lengths



Bond angles

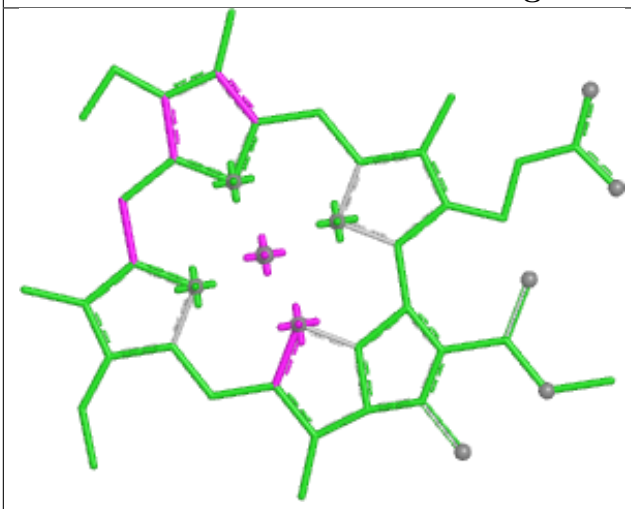


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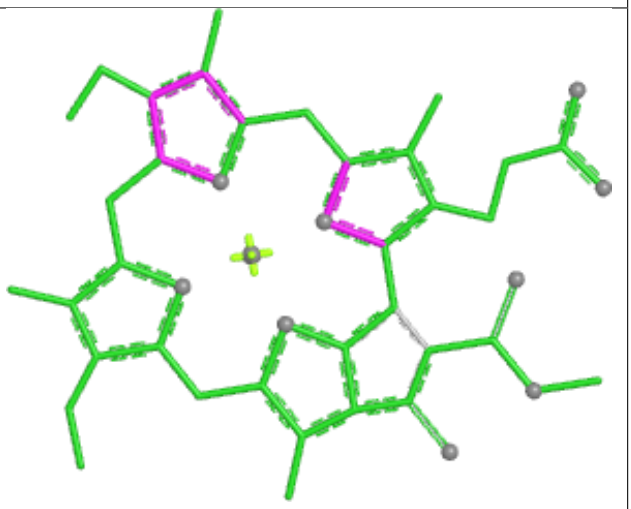


Rings

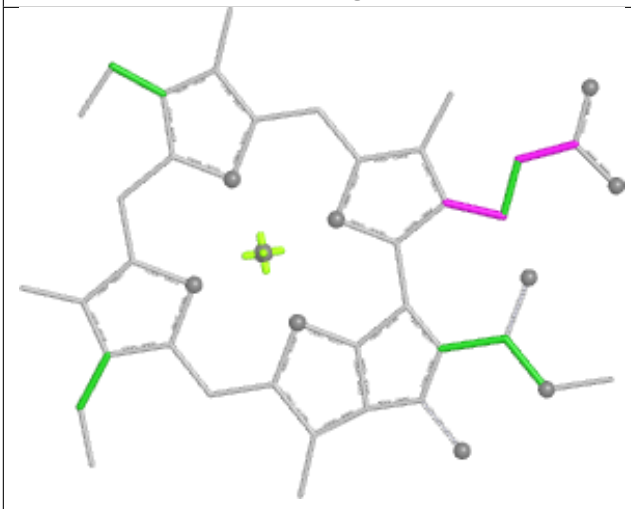
Ligand CLA A 811



Bond lengths



Bond angles

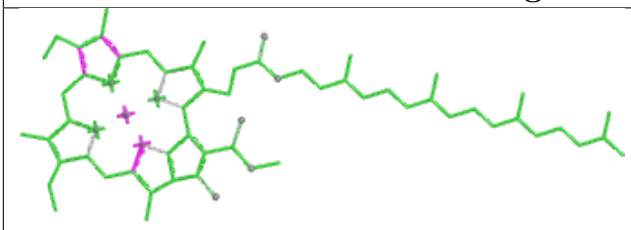


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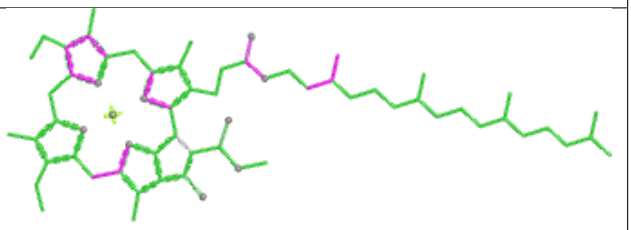


Rings

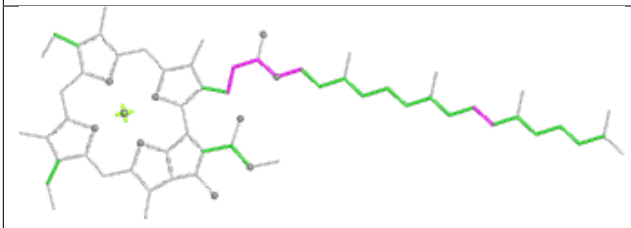
Ligand CLA B 818



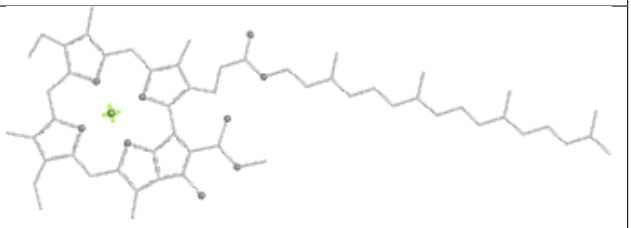
Bond lengths



Bond angles

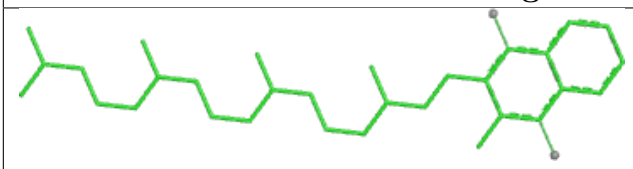


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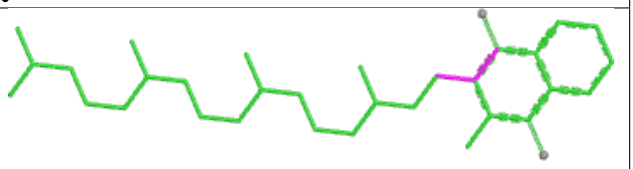


Rings

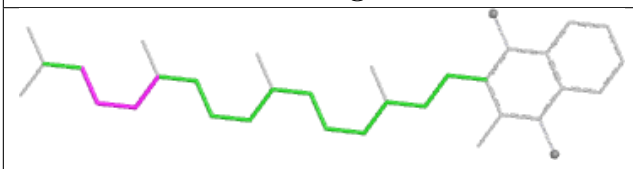
Ligand PQN B 843



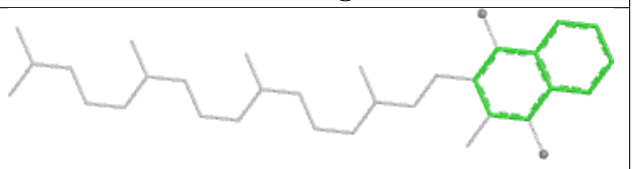
Bond lengths



Bond angles



Torsions

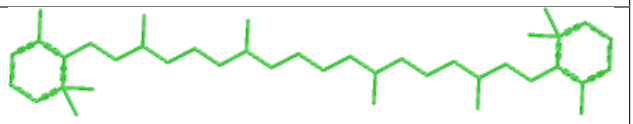


Rings

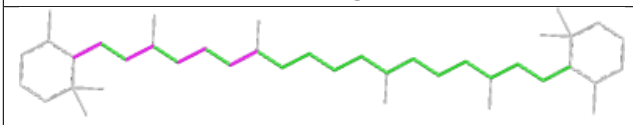
Ligand BCR J 1104



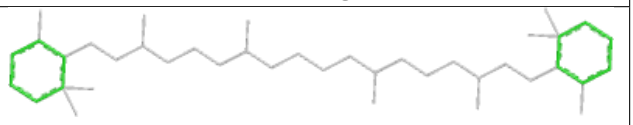
Bond lengths



Bond angles

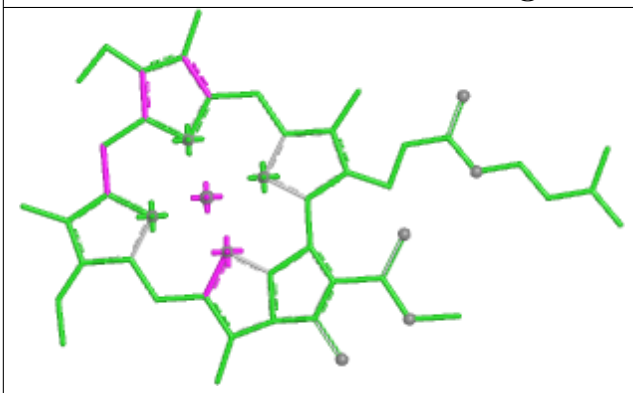


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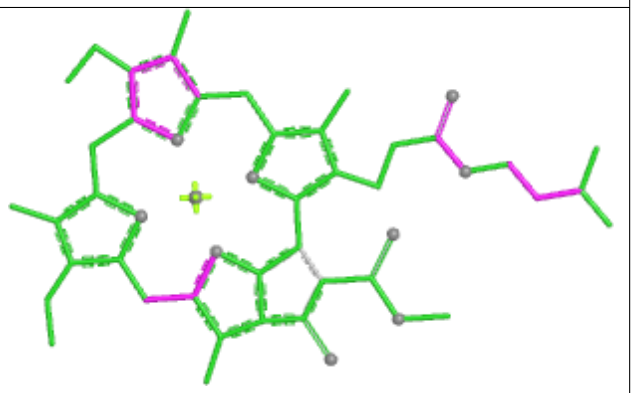


Rings

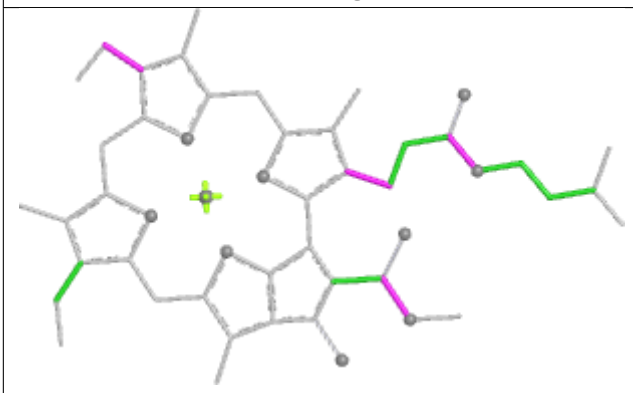
Ligand CLA J 1103



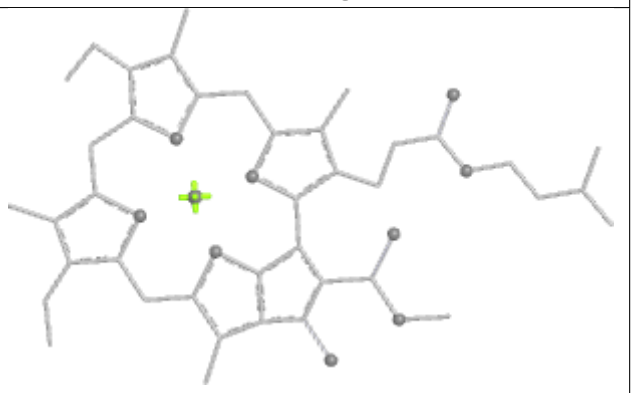
Bond lengths



Bond angles

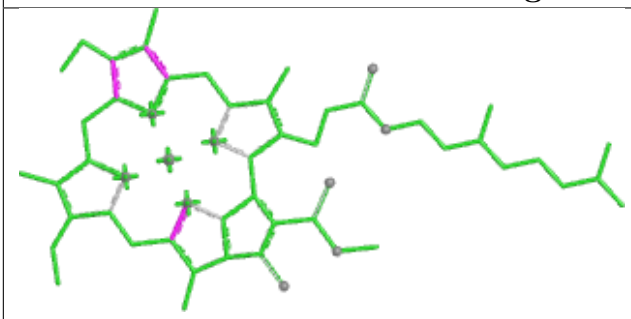


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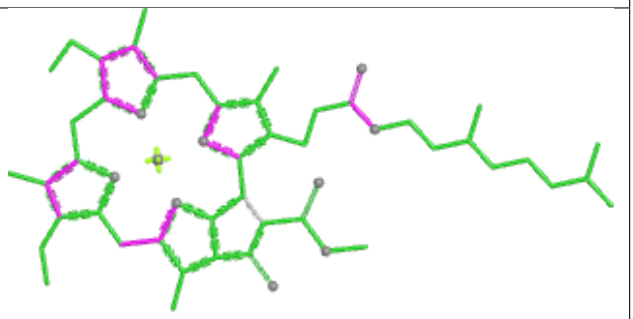


Rings

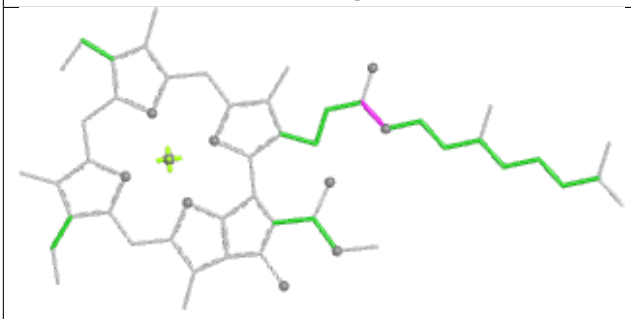
Ligand CLA B 832



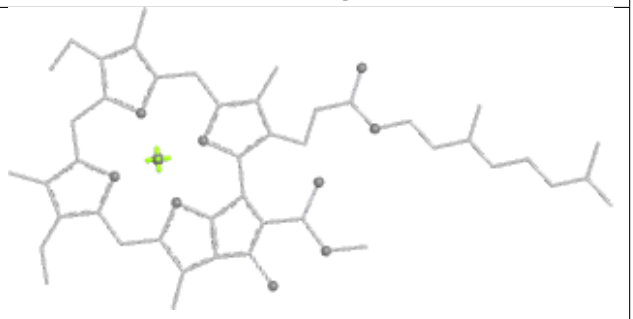
Bond lengths



Bond angles

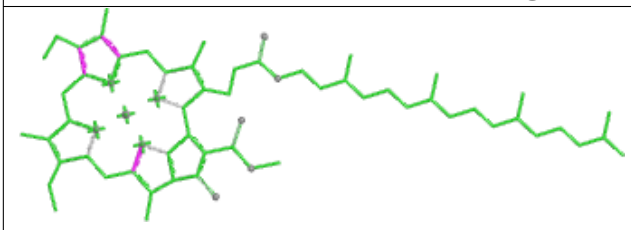


Torsions

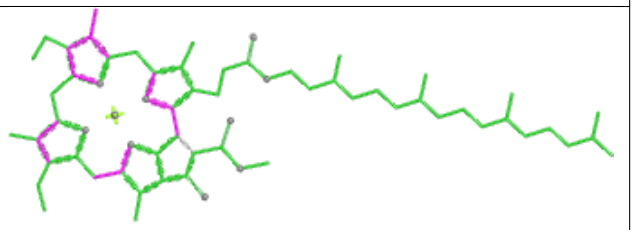


Rings

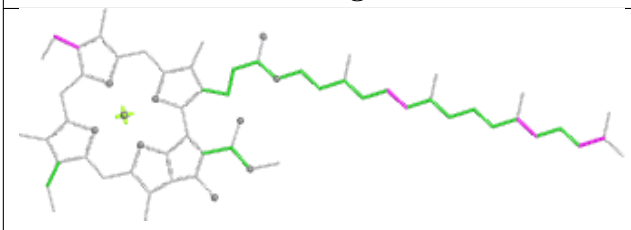
Ligand CLA A 834



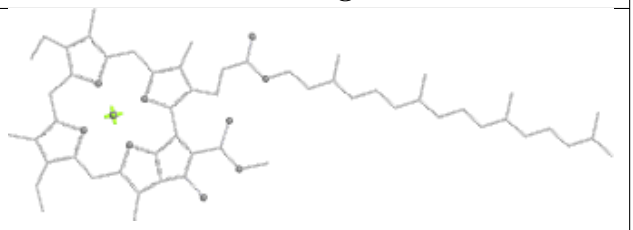
Bond lengths



Bond angles

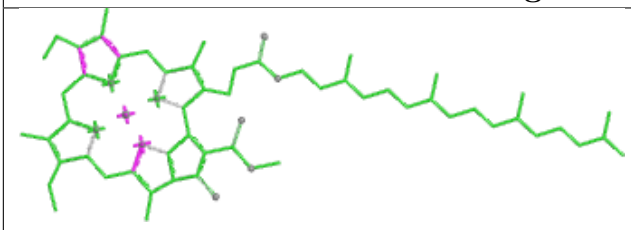


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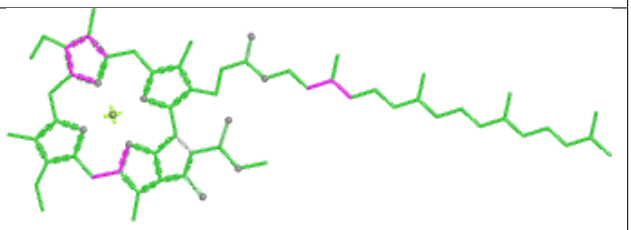


Rings

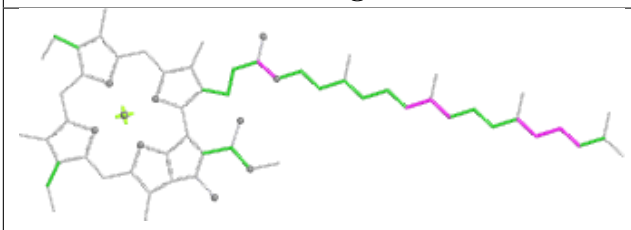
Ligand CLA B 838



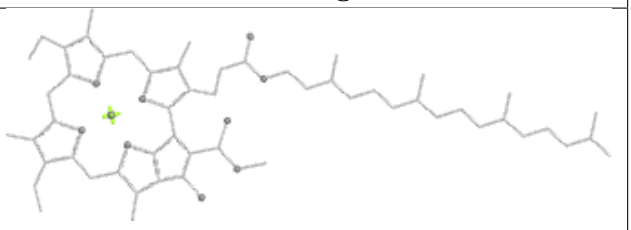
Bond lengths



Bond angles

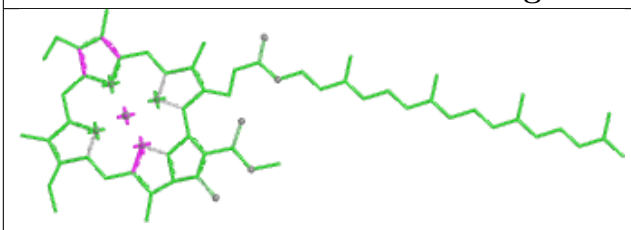


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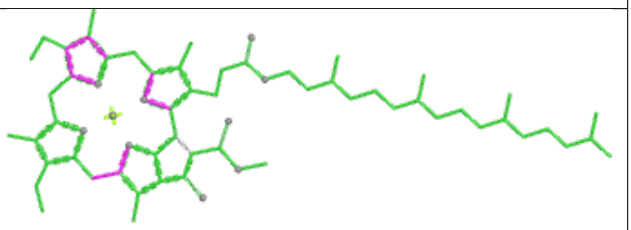


Rings

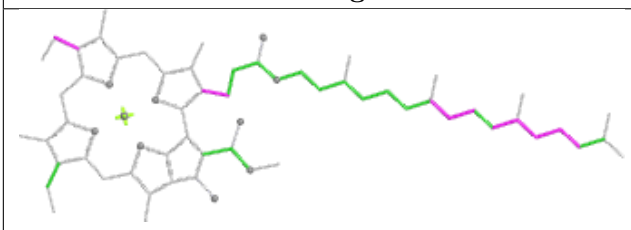
Ligand CLA A 825



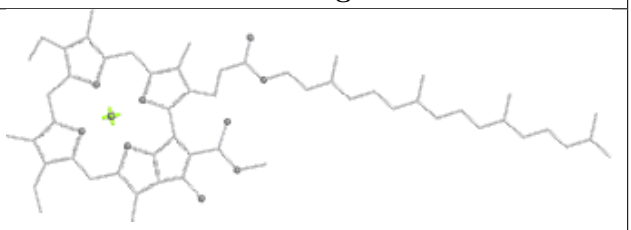
Bond lengths



Bond angles

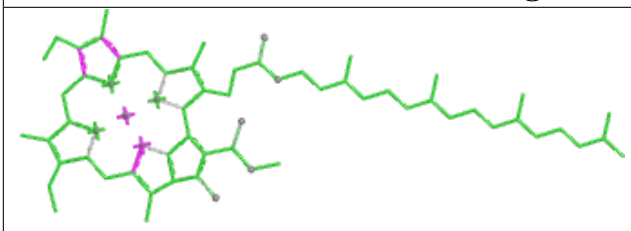


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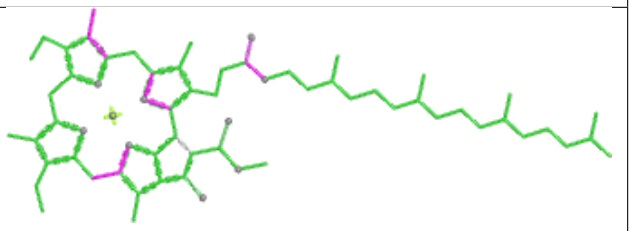


Rings

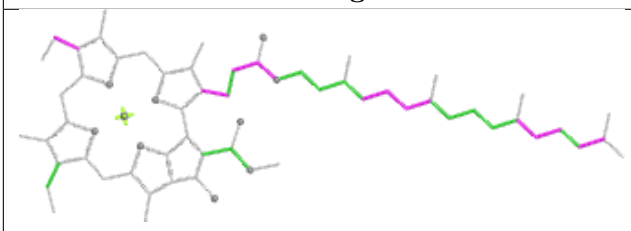
Ligand CLA A 844



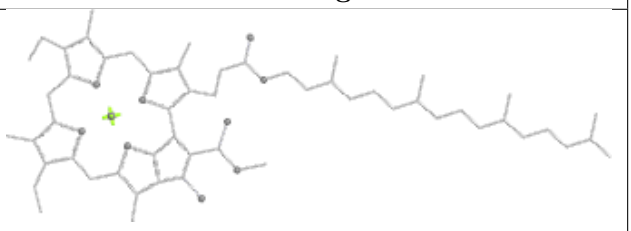
Bond lengths



Bond angles

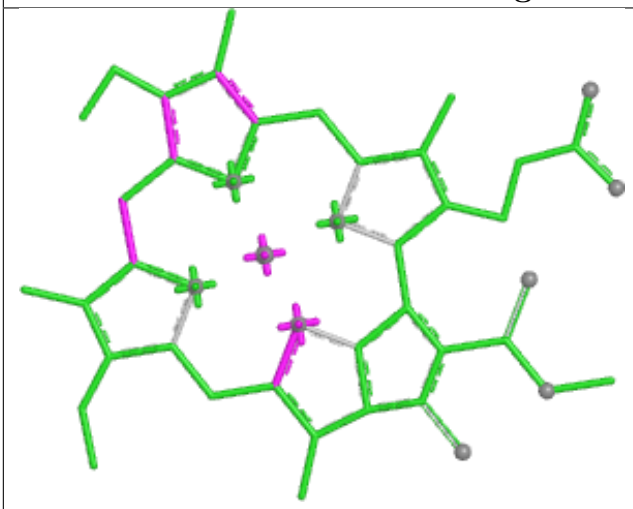


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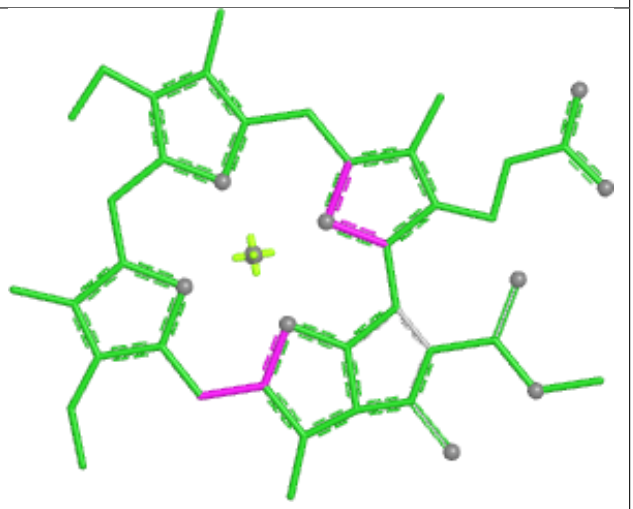


Rings

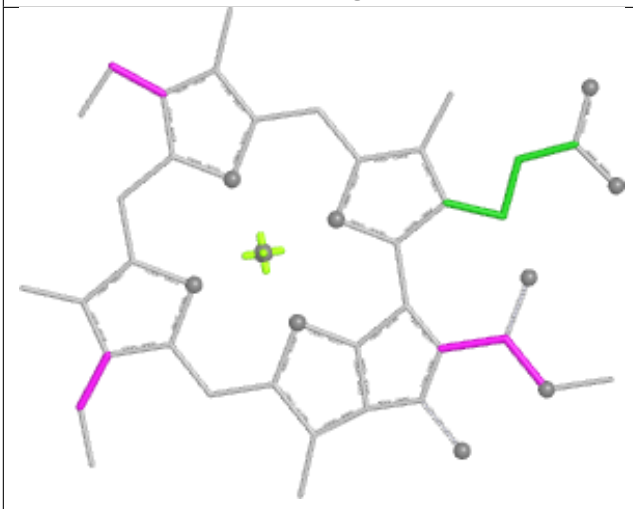
Ligand CLA K 4003



Bond lengths



Bond angles

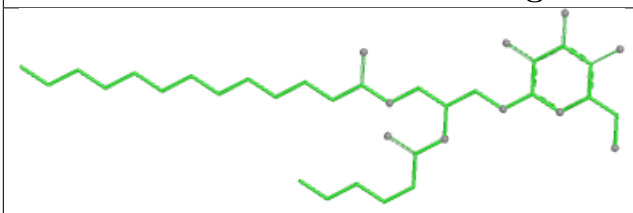


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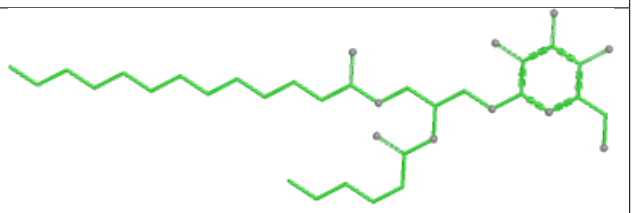


Rings

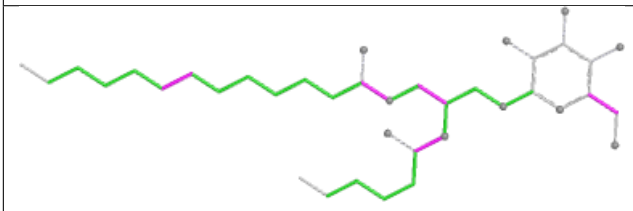
Ligand LMG I 101



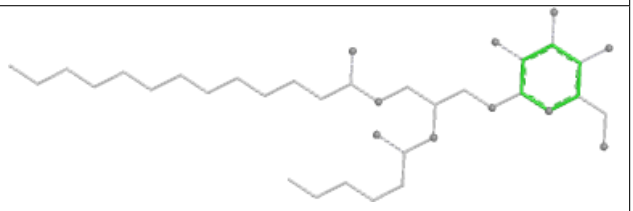
Bond lengths



Bond angles

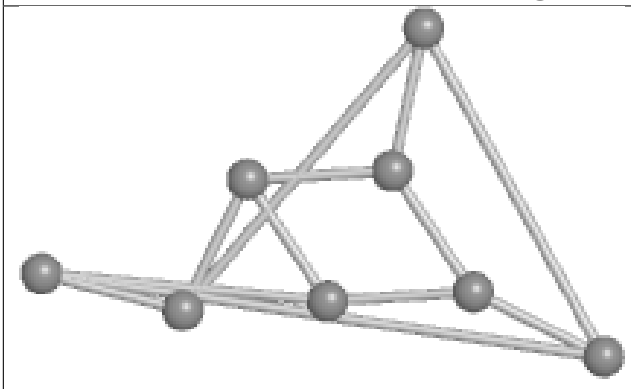


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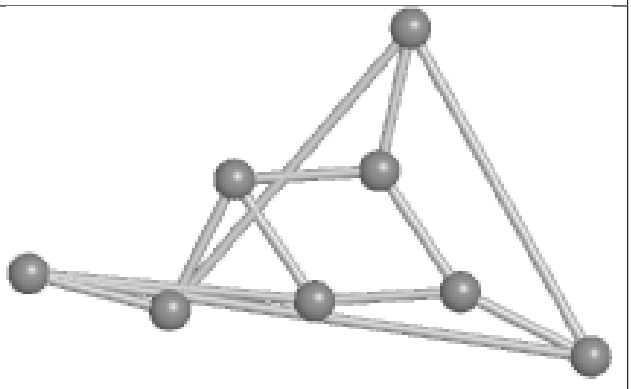


Rings

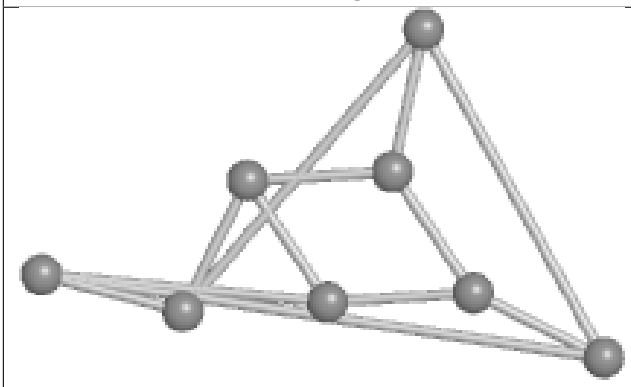
Ligand SF4 C 102



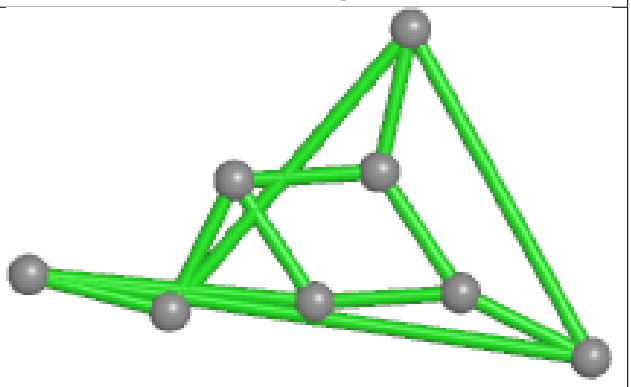
Bond lengths



Bond angles

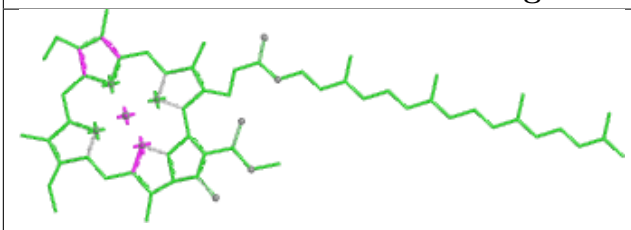


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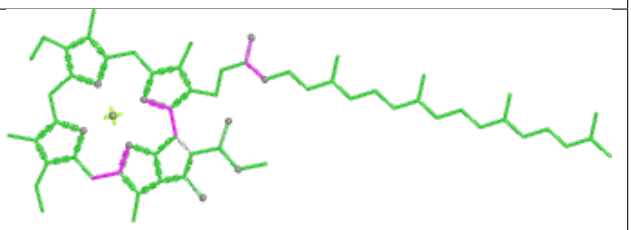


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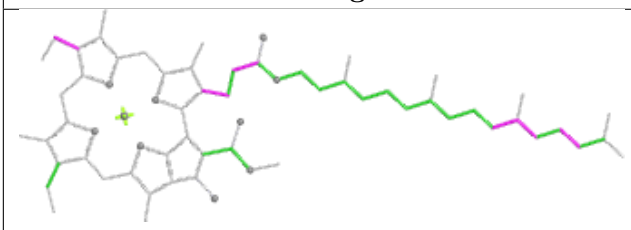
Ligand CLA A 819



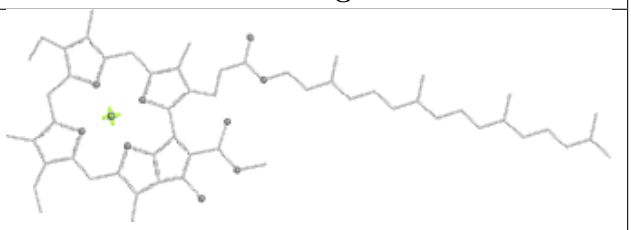
Bond lengths



Bond angles

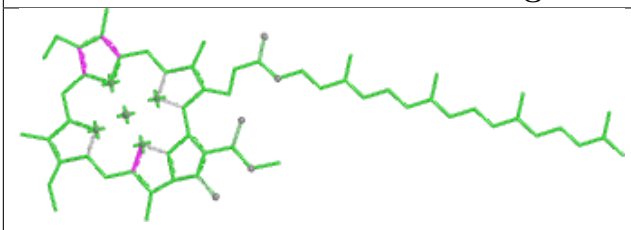


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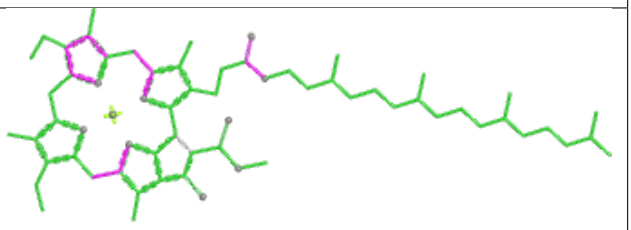


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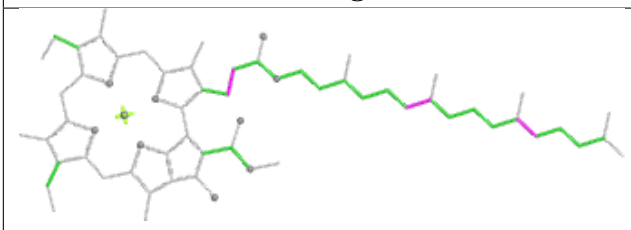
Ligand CLA B 840



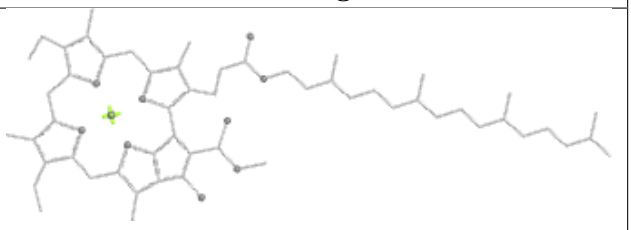
Bond lengths



Bond angles

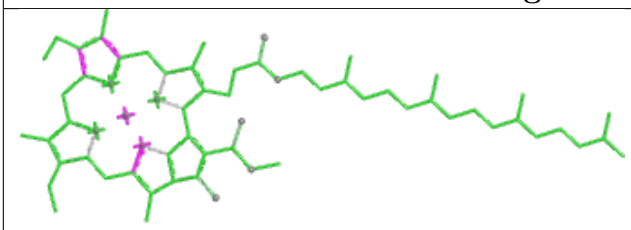


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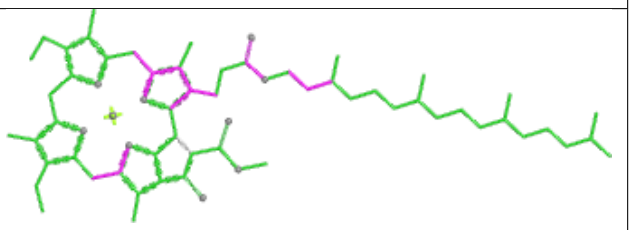


Rings

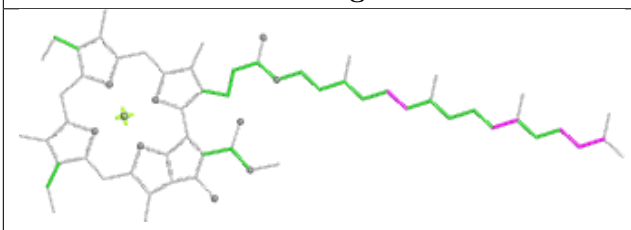
Ligand CLA A 820



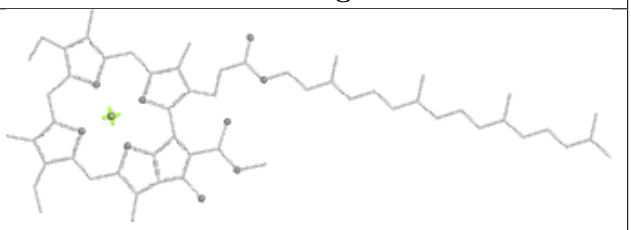
Bond lengths



Bond angles



Torsions

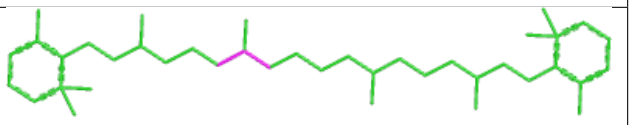


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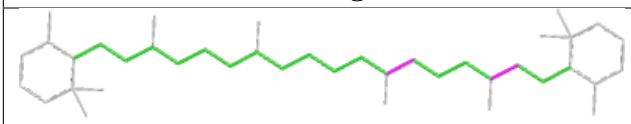
Ligand BCR F 202



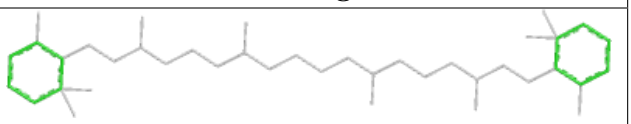
Bond lengths



Bond angles

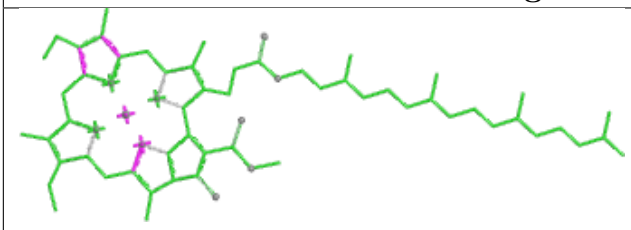


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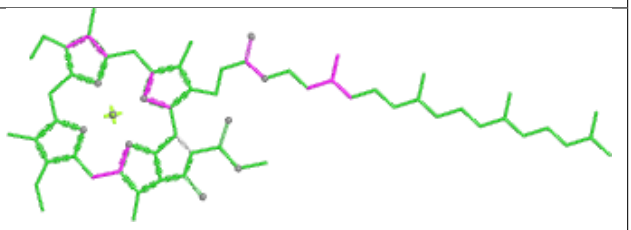


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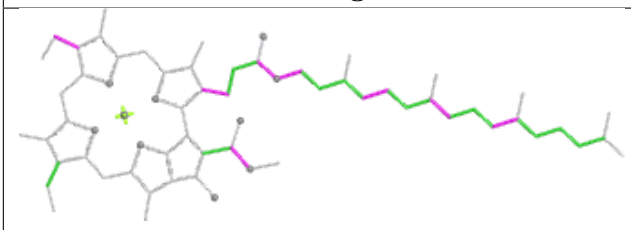
Ligand CLA B 841



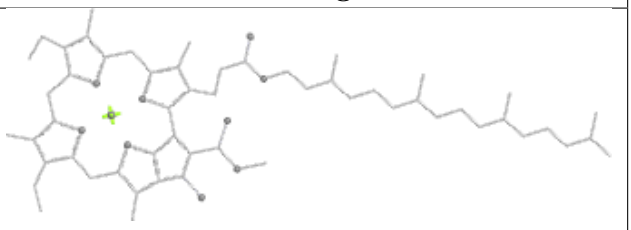
Bond lengths



Bond angles

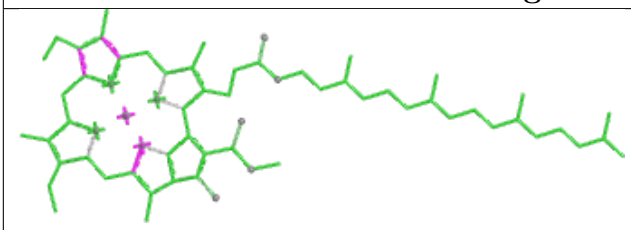


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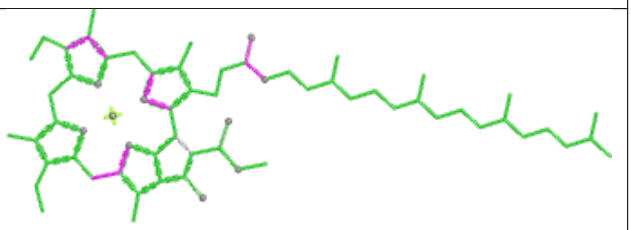


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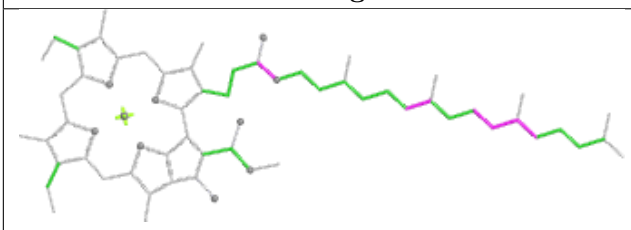
Ligand CLA A 808



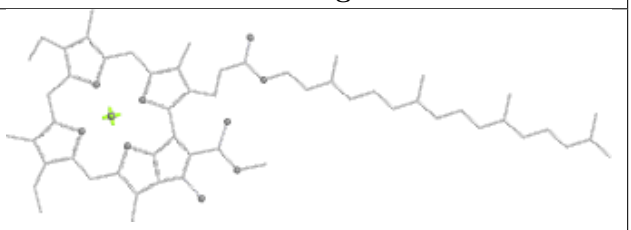
Bond lengths



Bond angles

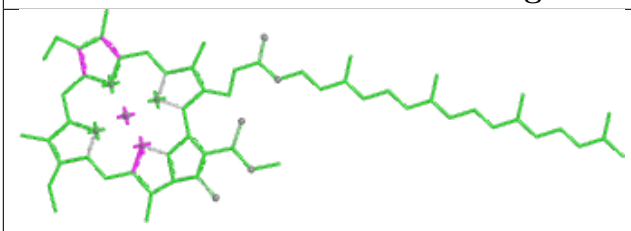


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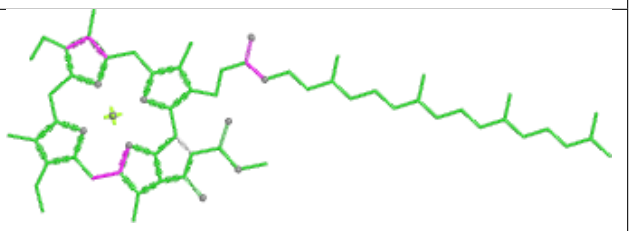


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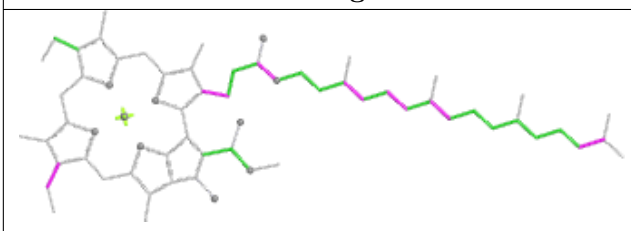
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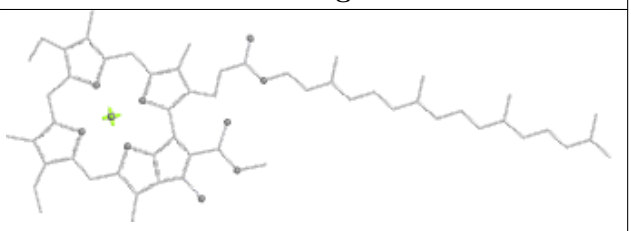
Bond lengths



Bond angles

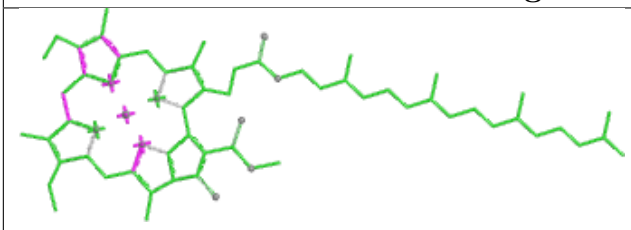


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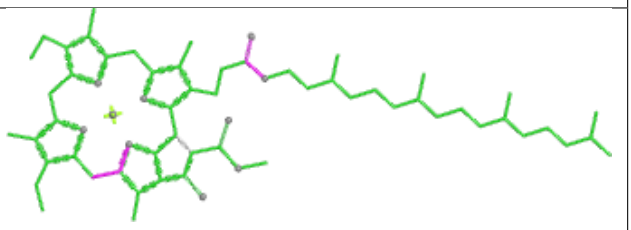


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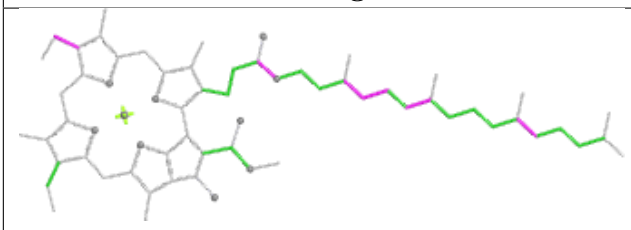
Ligand CLA B 820



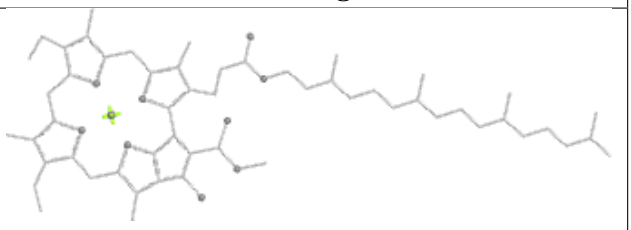
Bond lengths



Bond angles

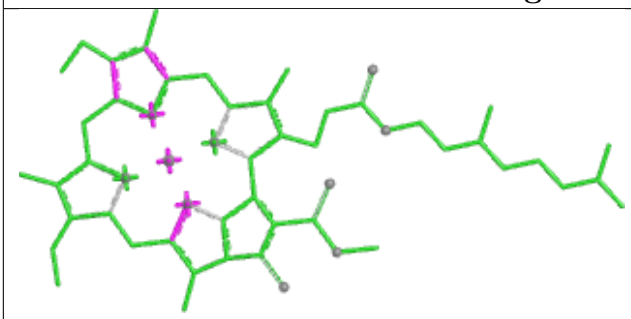


Torsions

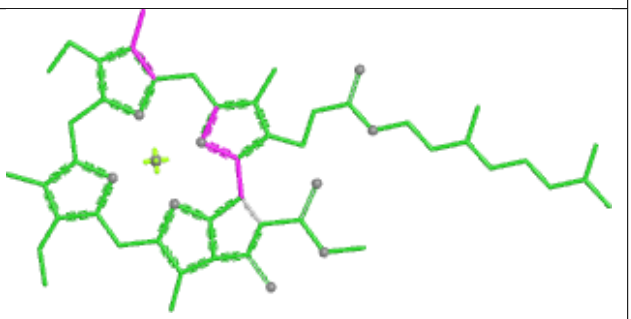


Rings

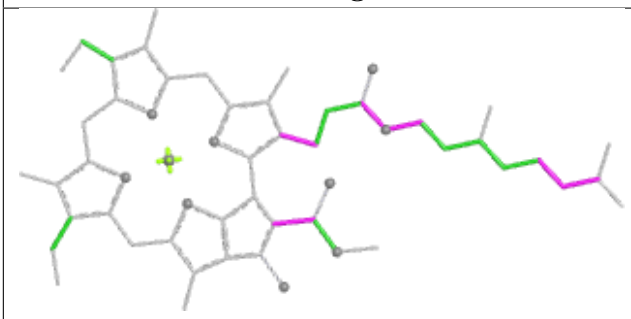
Ligand CLA B 813



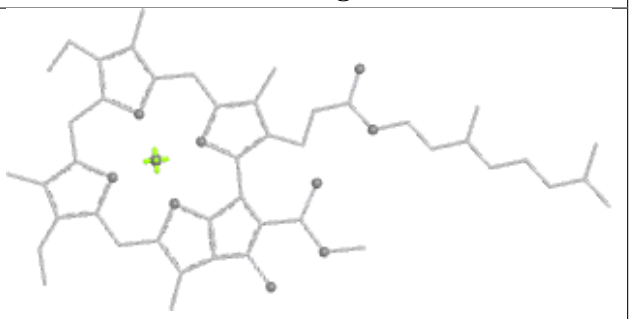
Bond lengths



Bond angles

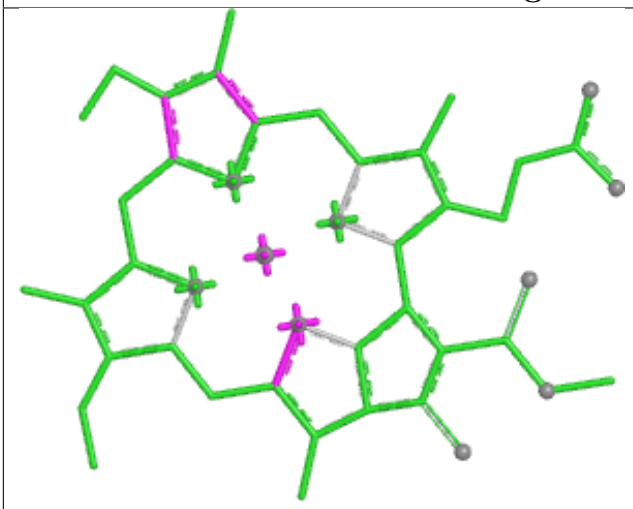


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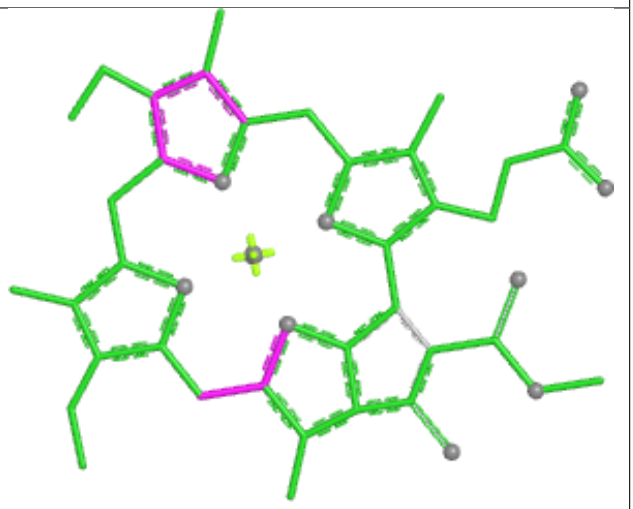


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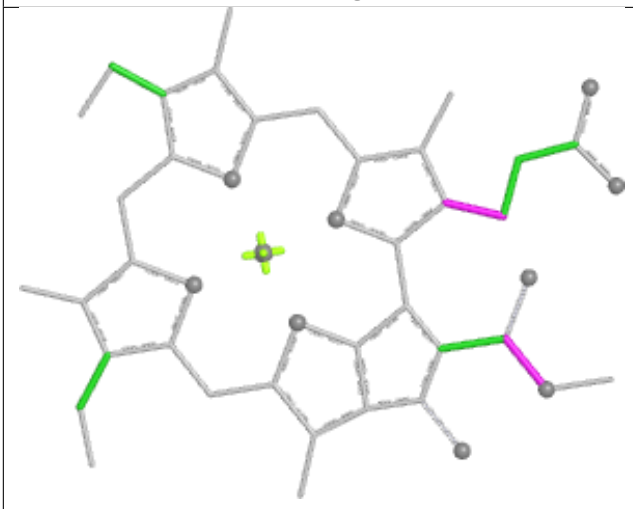
Ligand CLA B 823



Bond lengths



Bond angles

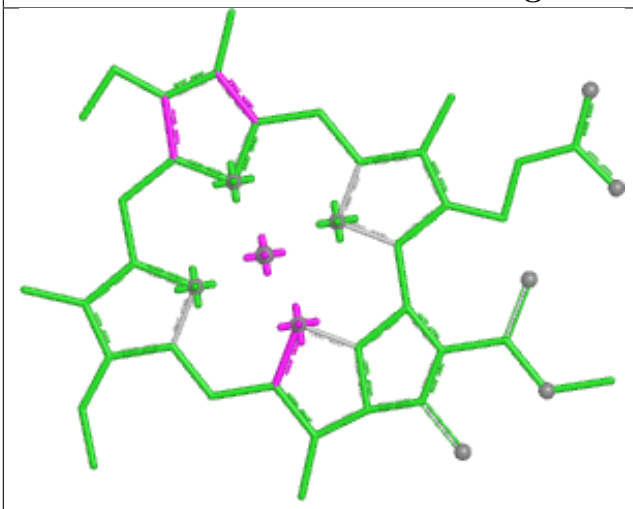


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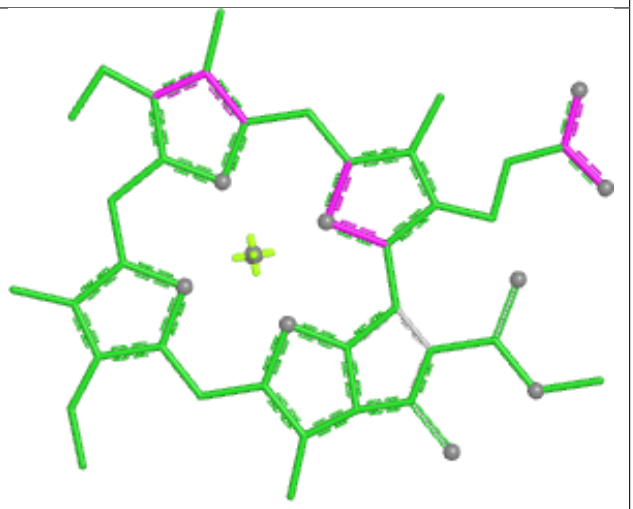


Rings

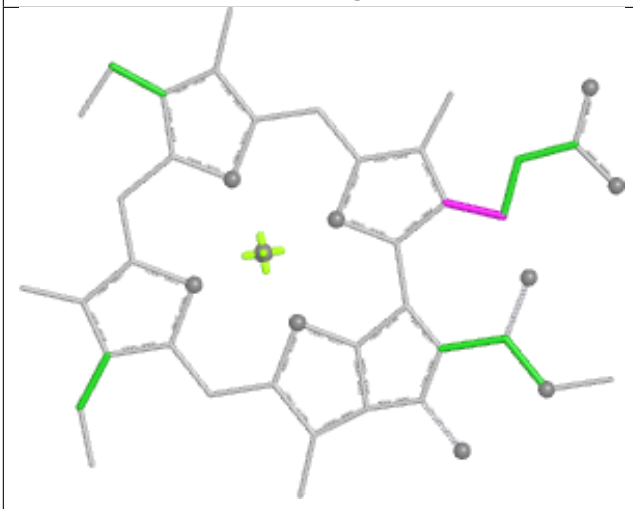
Ligand CLA B 835



Bond lengths



Bond angles

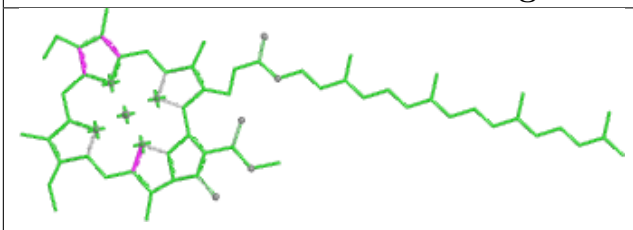


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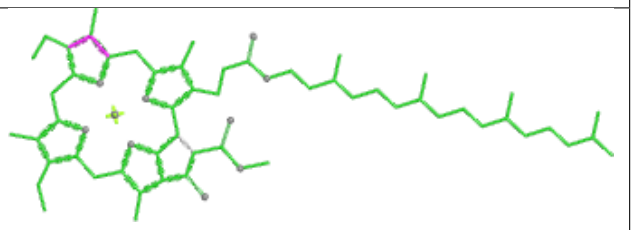


Rings

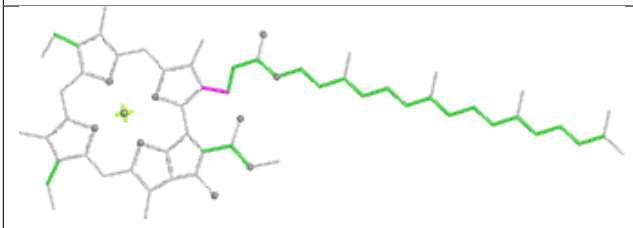
Ligand CLA J 1101



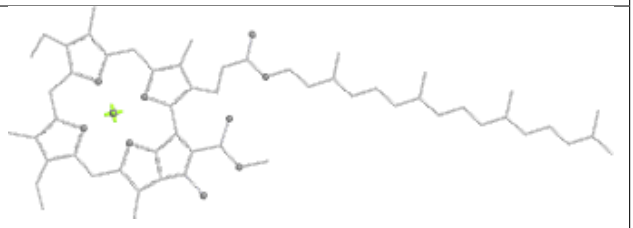
Bond lengths



Bond angles

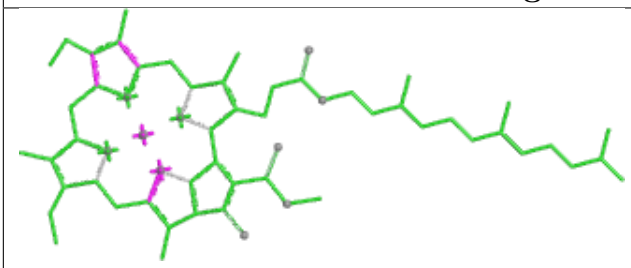


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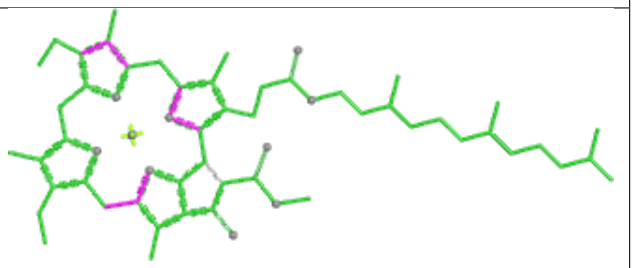


Rings

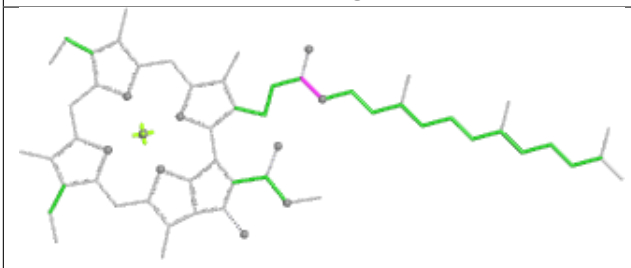
Ligand CLA A 833



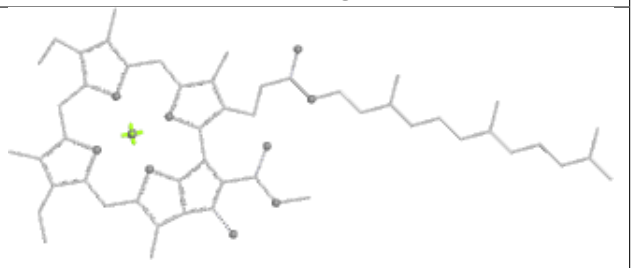
Bond lengths



Bond angles

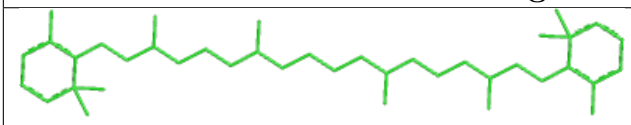


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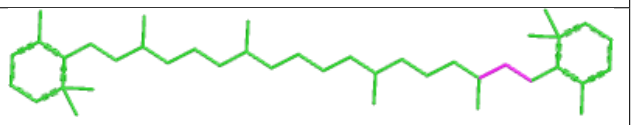


Rings

Ligand BCR I 102



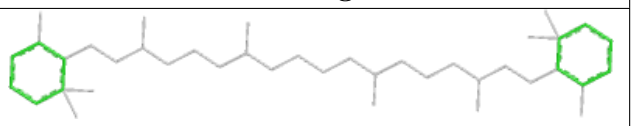
Bond lengths



Bond angles



Torsions



Rings

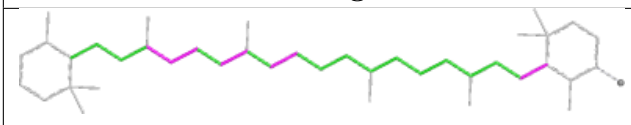
Ligand ECH M 102



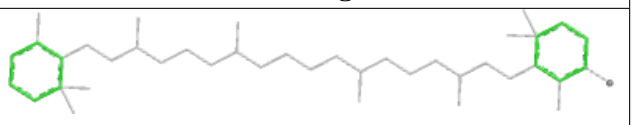
Bond lengths



Bond angles

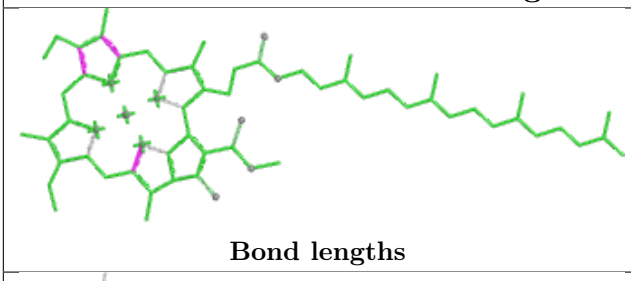


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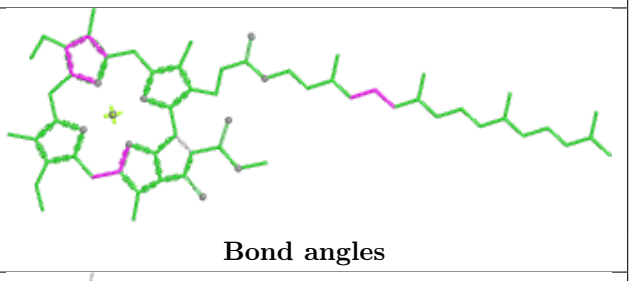


Rings

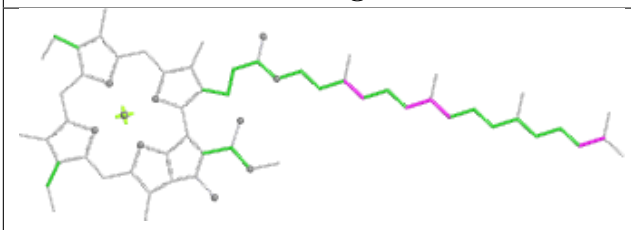
Ligand CLA A 822



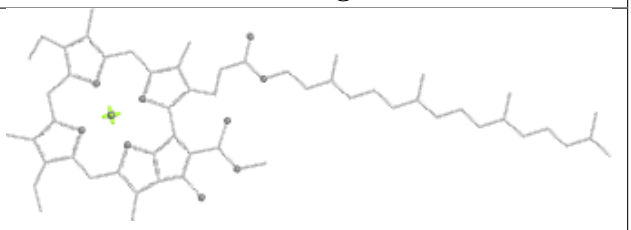
Bond lengths



Bond angles

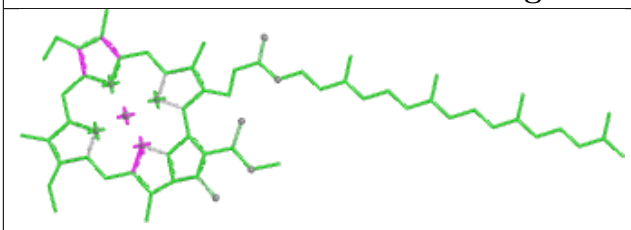


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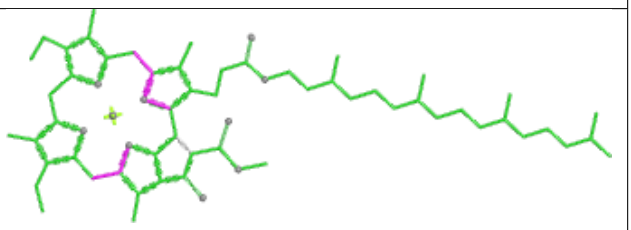


Rings

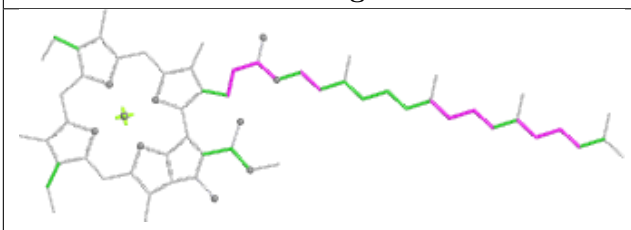
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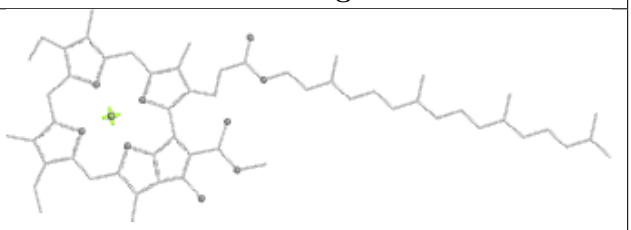
Bond lengths



Bond angles

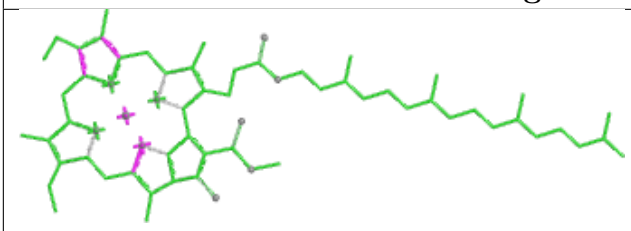


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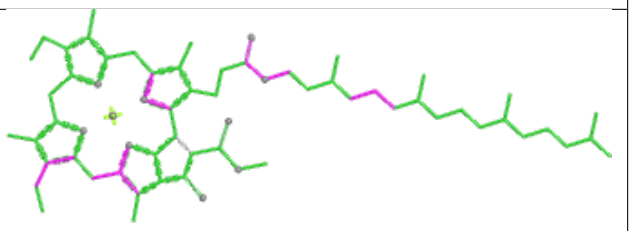


Rings

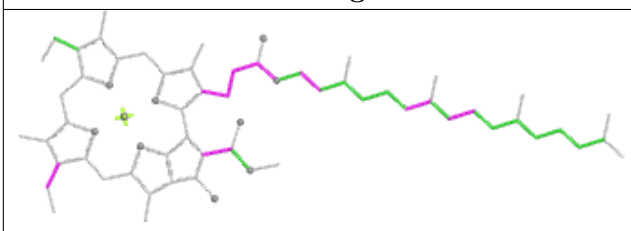
Ligand CLA A 806



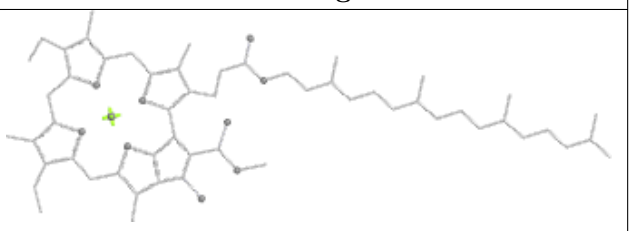
Bond lengths



Bond angles

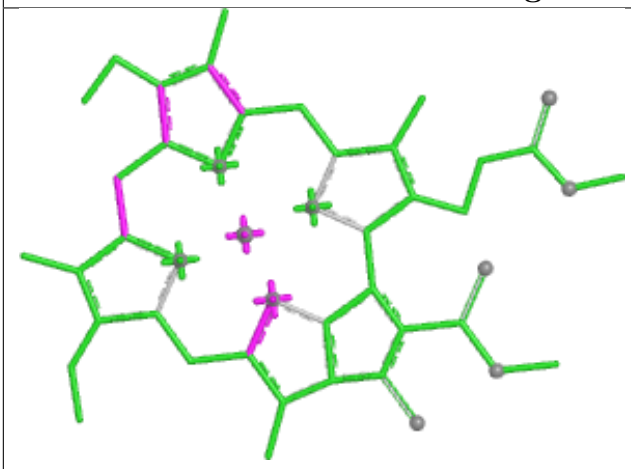


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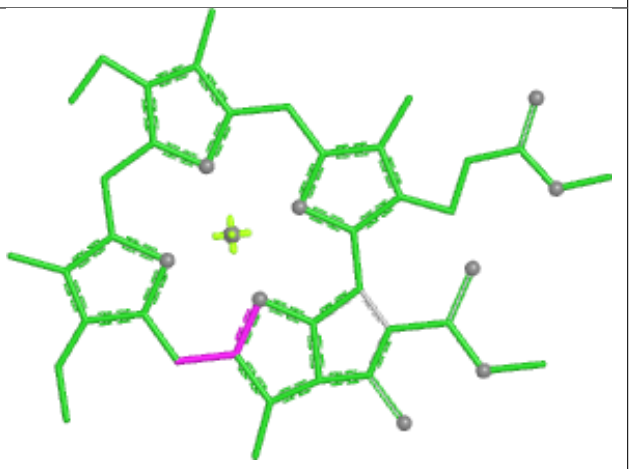


Rings

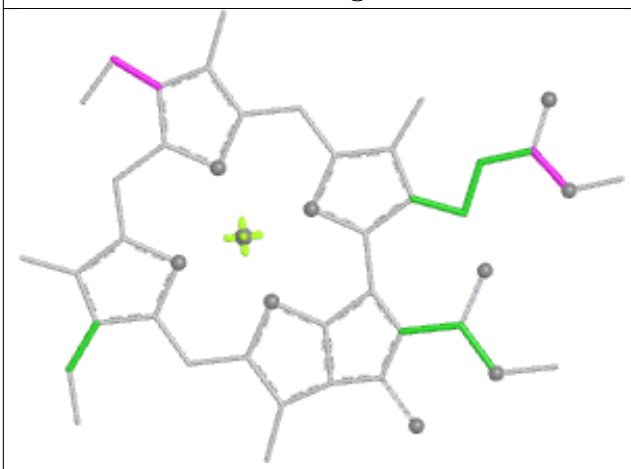
Ligand CLA B 836



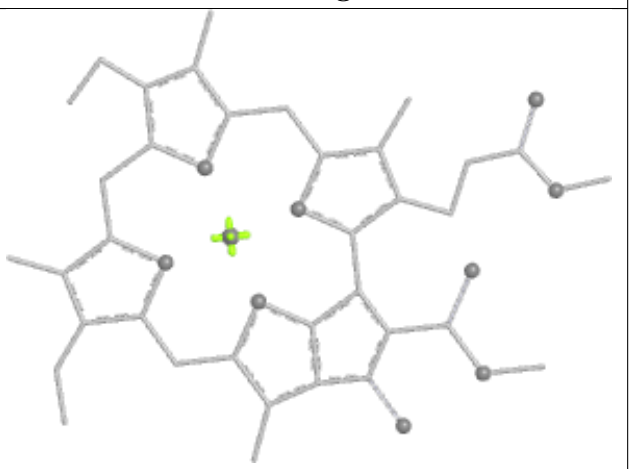
Bond lengths



Bond angles

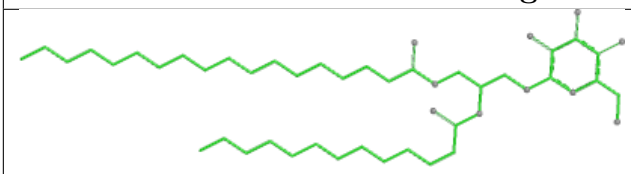


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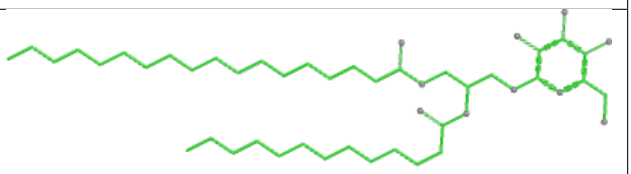


Rings

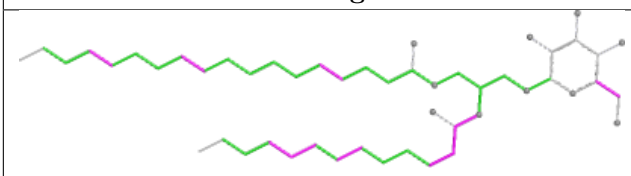
Ligand LMG B 802



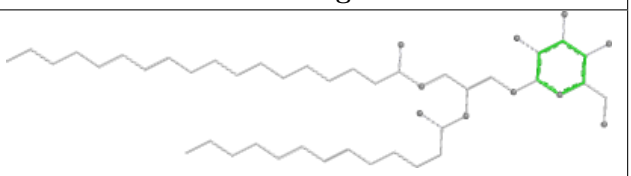
Bond lengths



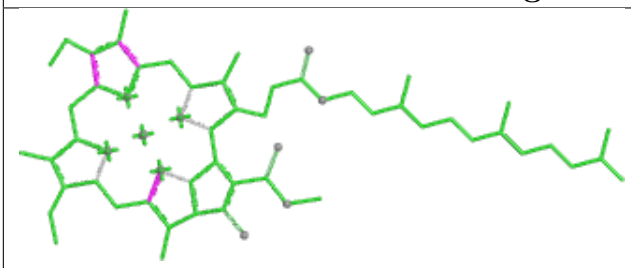
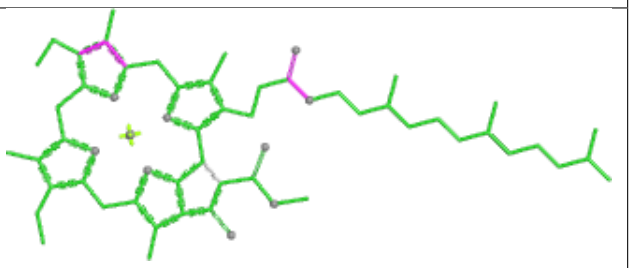
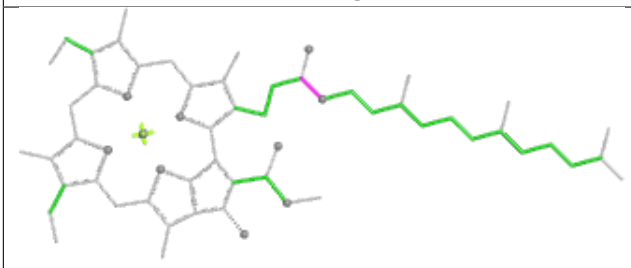
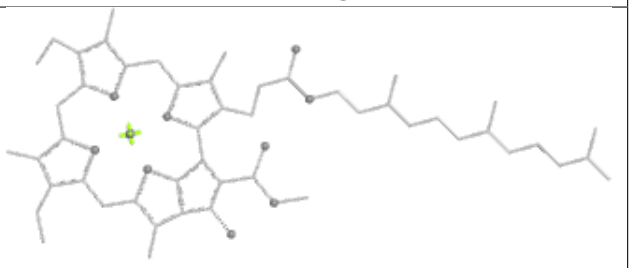
Bond angles

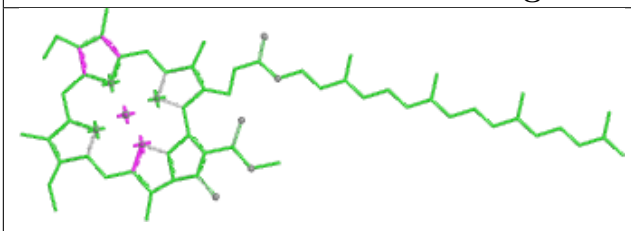
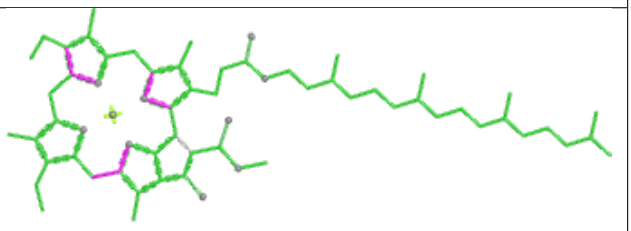
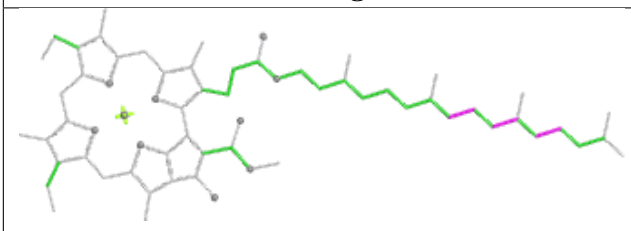
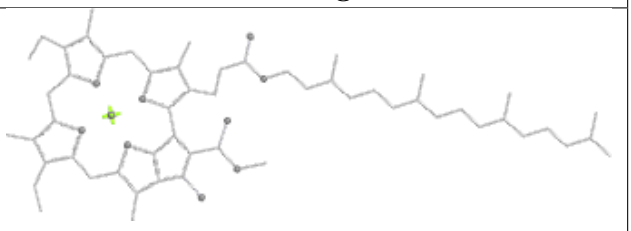


Torsions

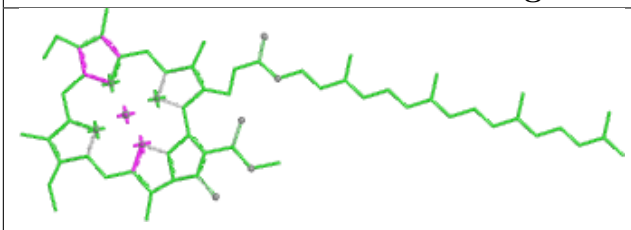


Rings

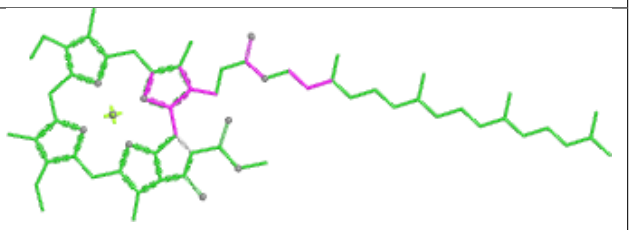
Ligand CLA A 827	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 803	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

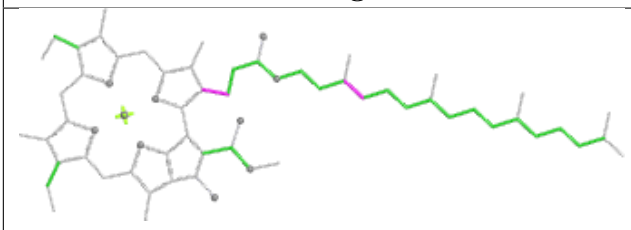
Ligand CLA B 808



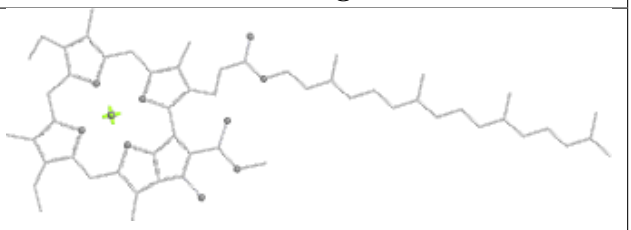
Bond lengths



Bond angles

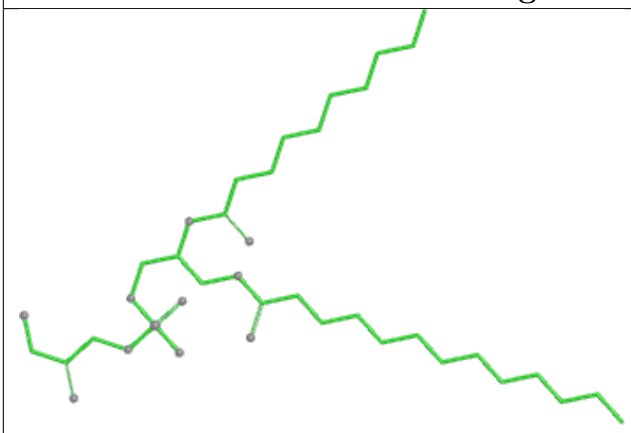


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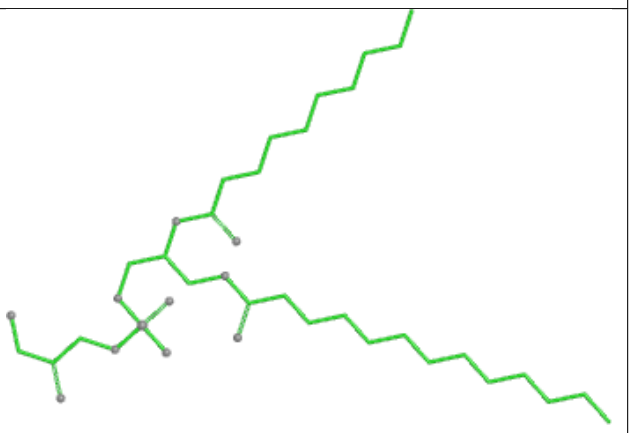


Rings

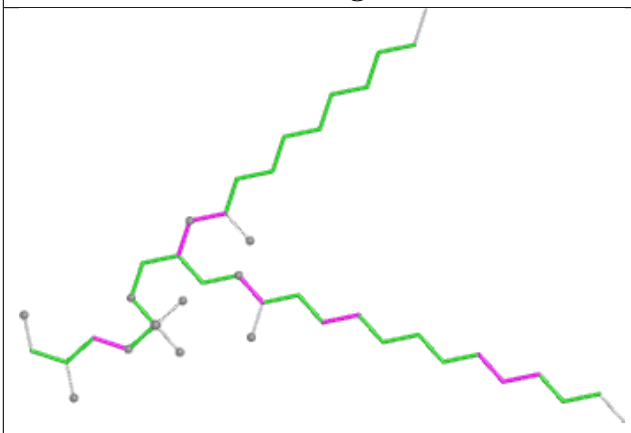
Ligand LHG M 101



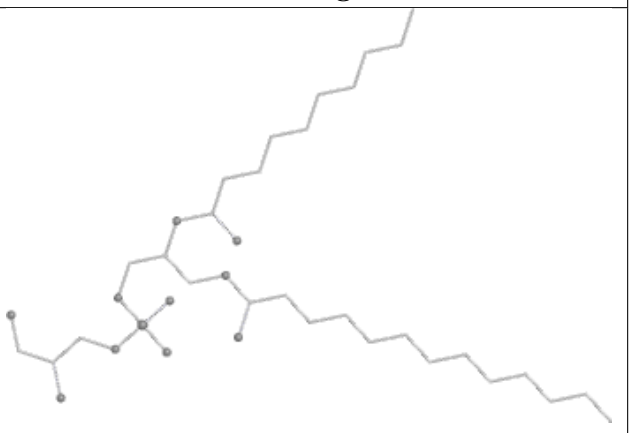
Bond lengths



Bond angles

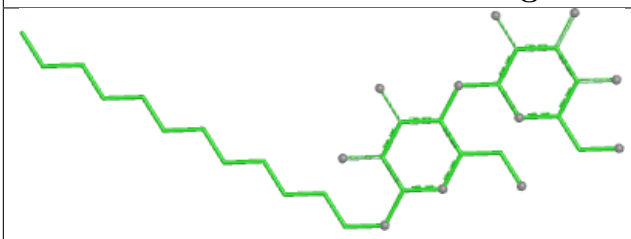


Torsions

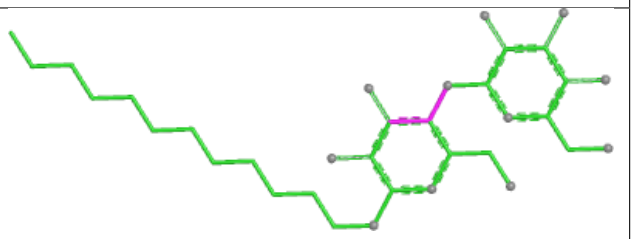


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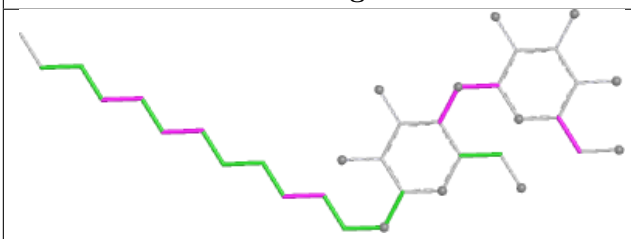
Ligand LMT A 858



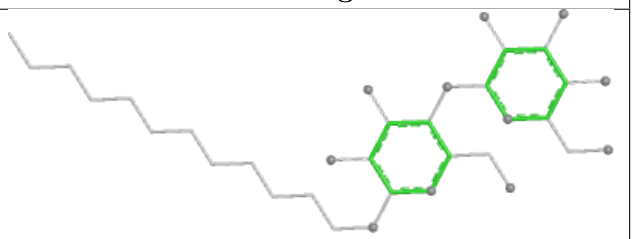
Bond lengths



Bond angles

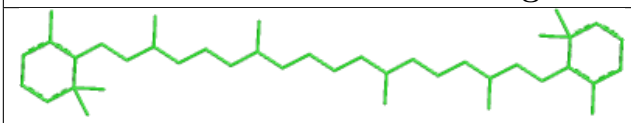


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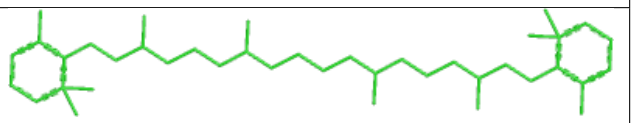


Rings

Ligand BCR A 848



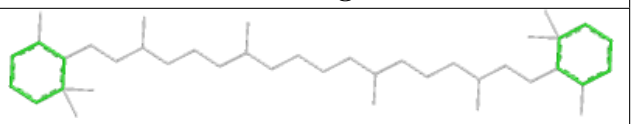
Bond lengths



Bond angles

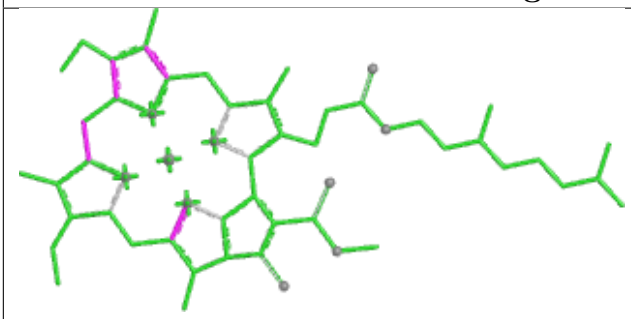


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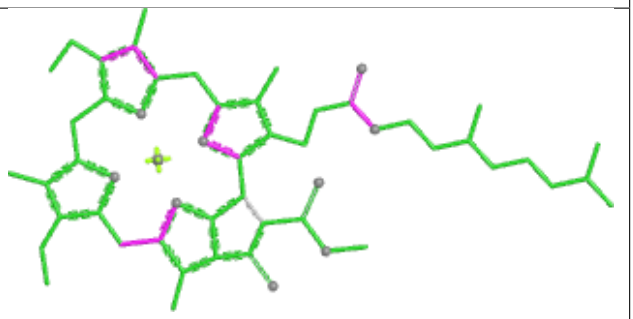


Rings

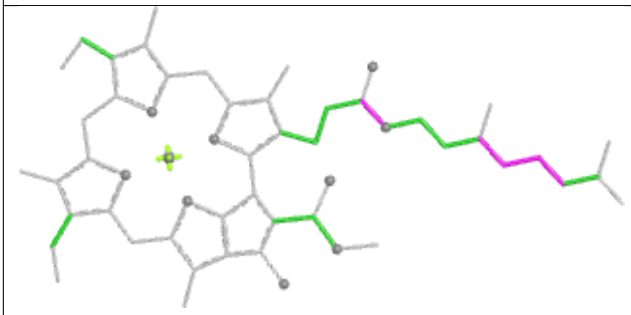
Ligand CLA A 815



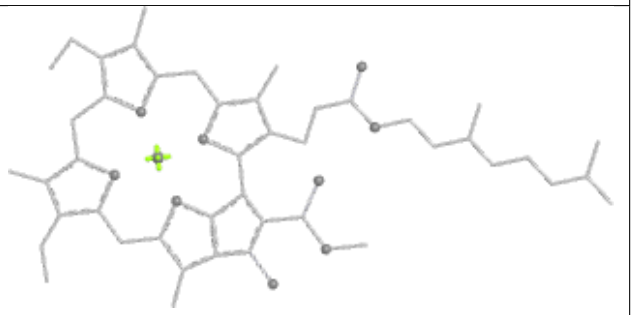
Bond lengths



Bond angles

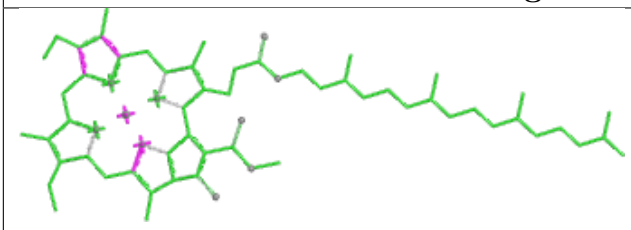


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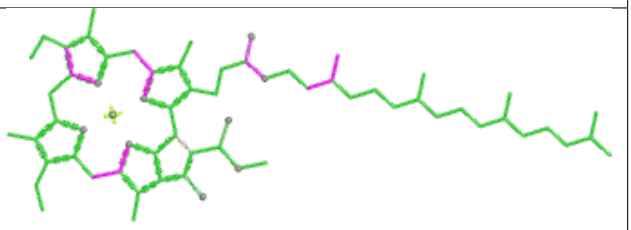


Rings

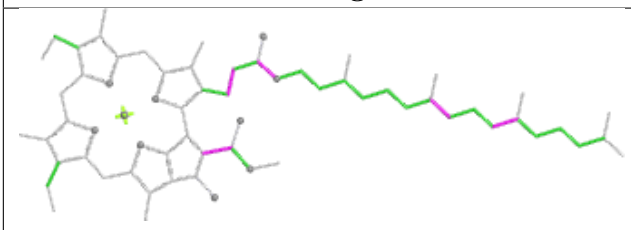
Ligand CLA B 801



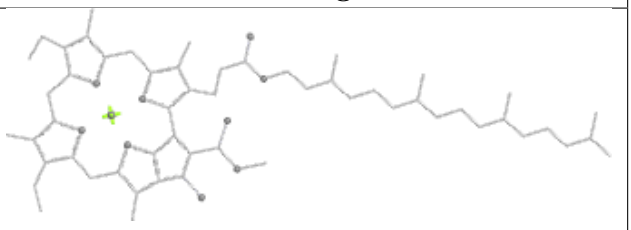
Bond lengths



Bond angles

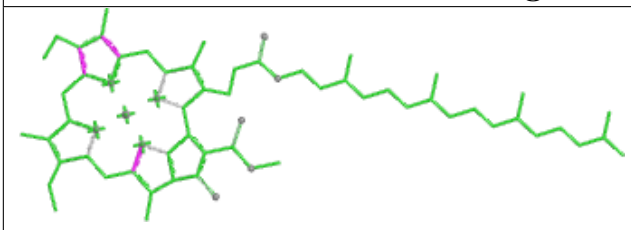


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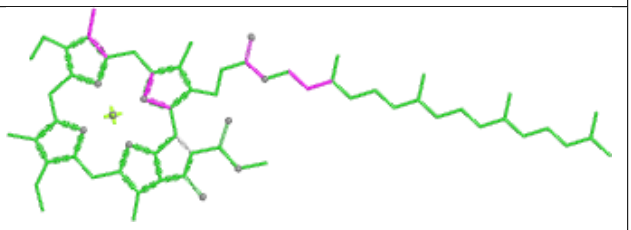


Rings

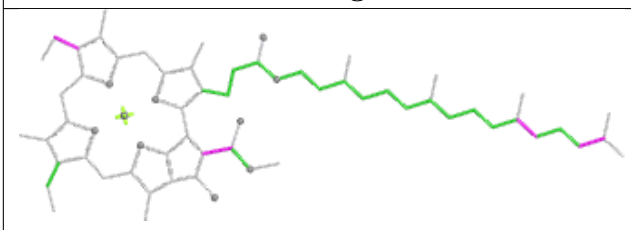
Ligand CLA B 809



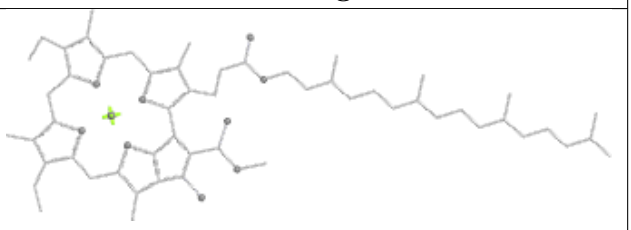
Bond lengths



Bond angles

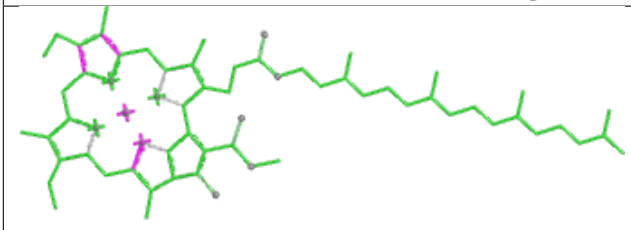


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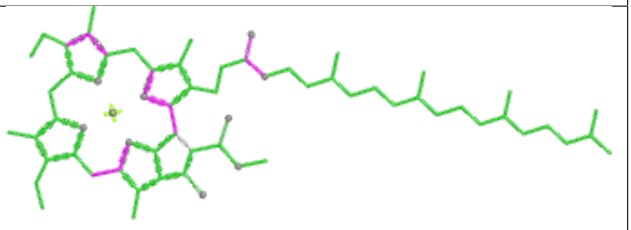


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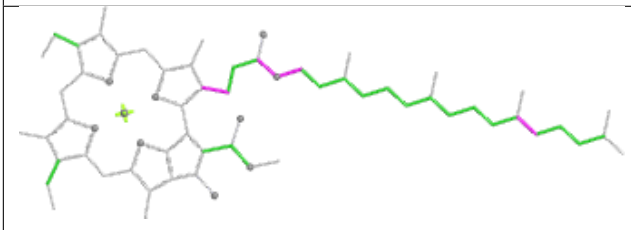
Ligand CLA B 828



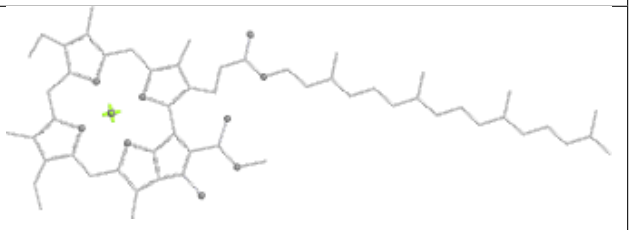
Bond lengths



Bond angles

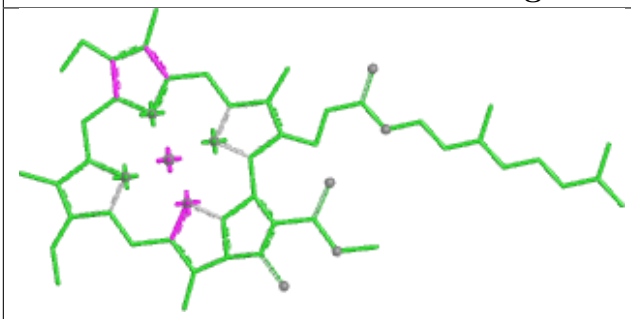


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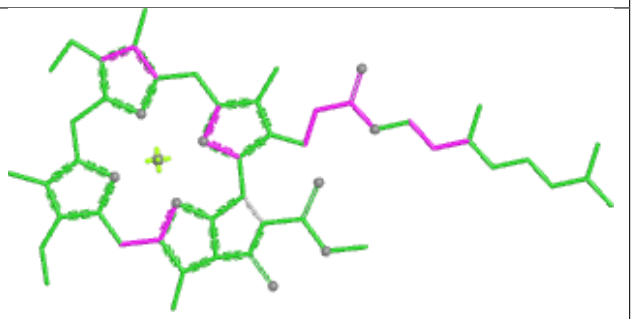


Rings

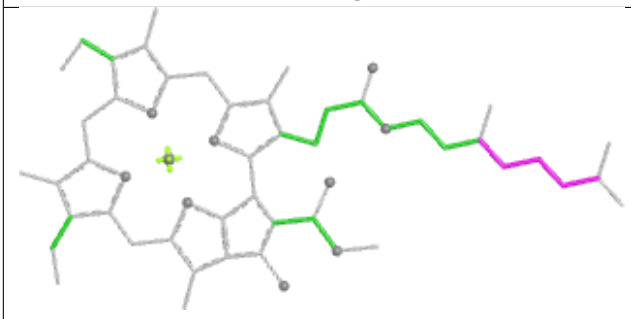
Ligand CLA B 834



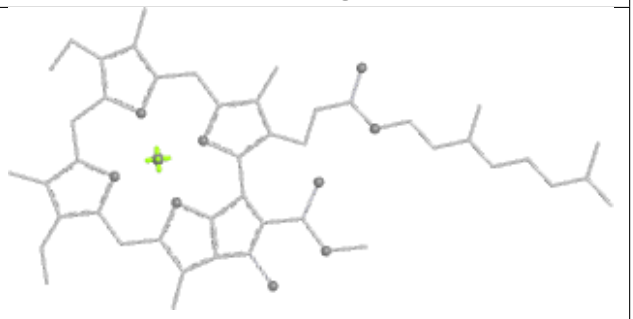
Bond lengths



Bond angles

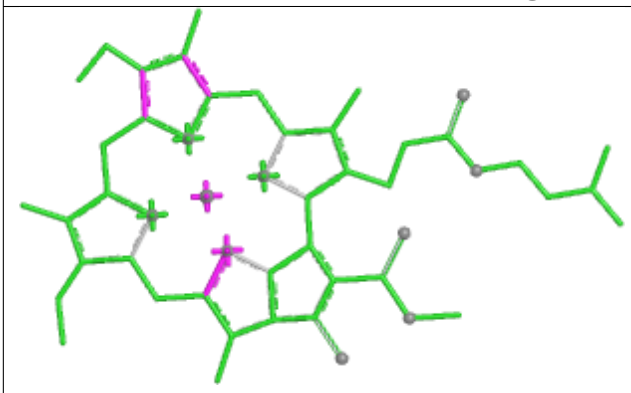


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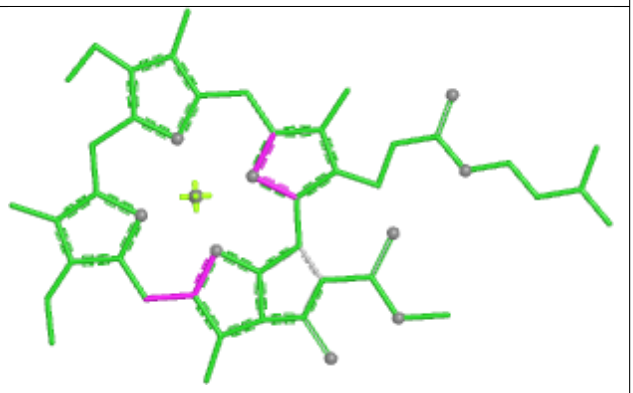


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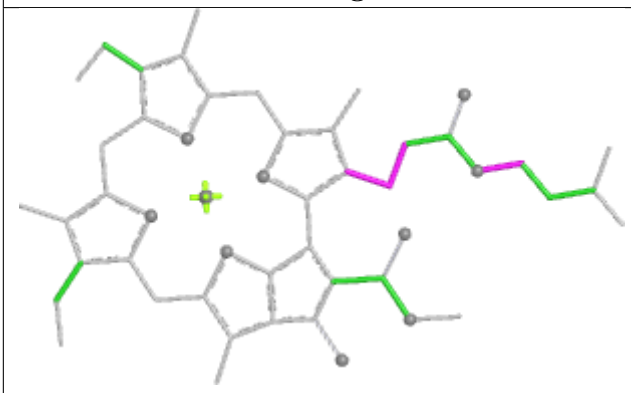
Ligand CLA A 810



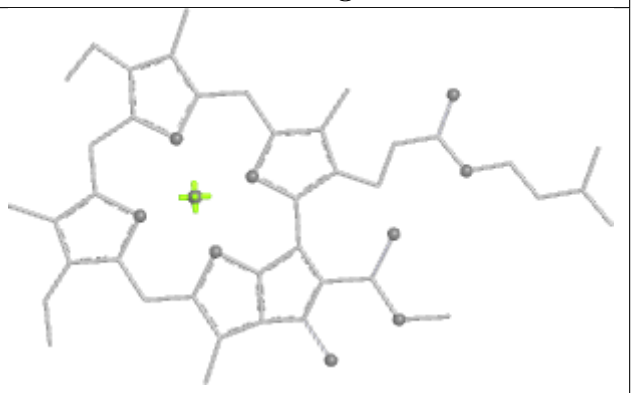
Bond lengths



Bond angles

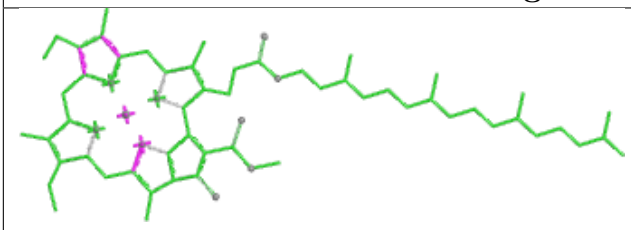


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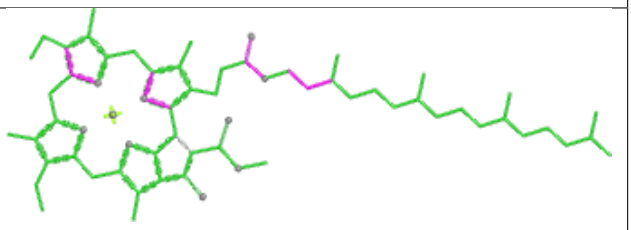


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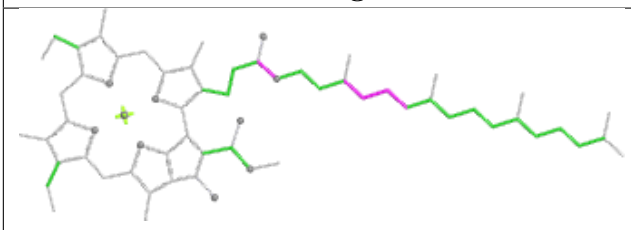
Ligand CLA A 821



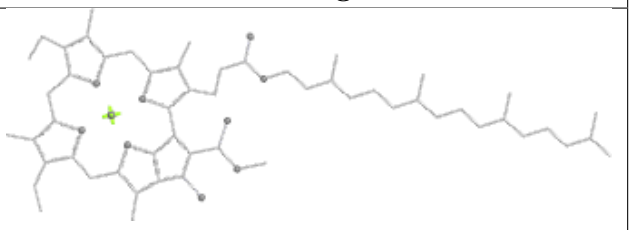
Bond lengths



Bond angles

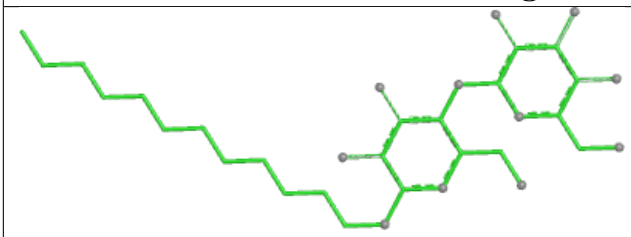


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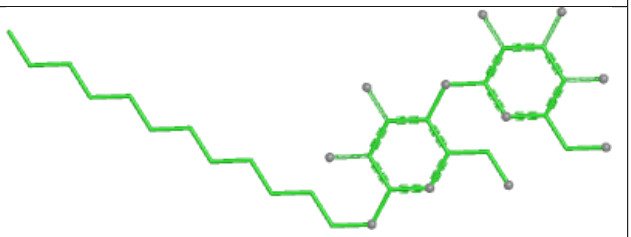


Rings

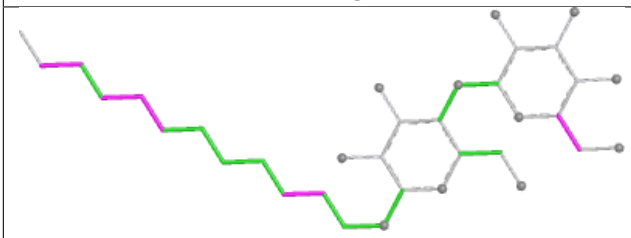
Ligand LMT A 854



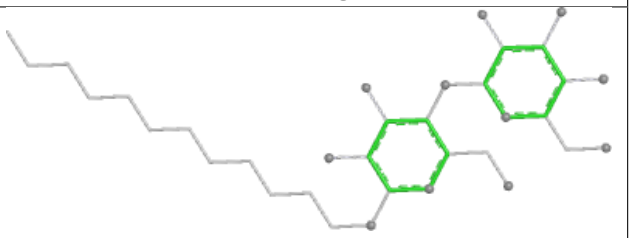
Bond lengths



Bond angles

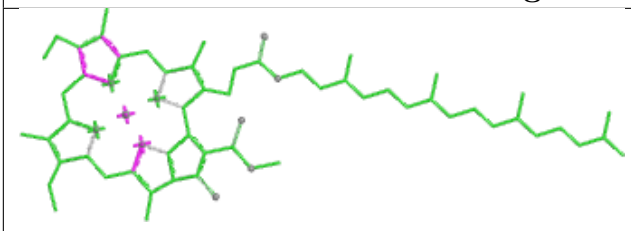


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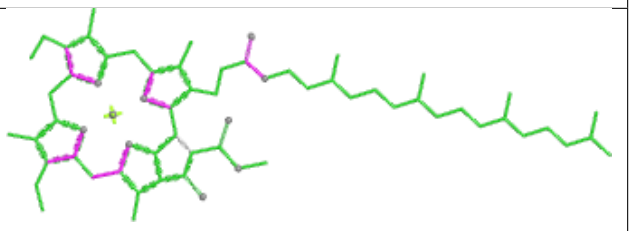


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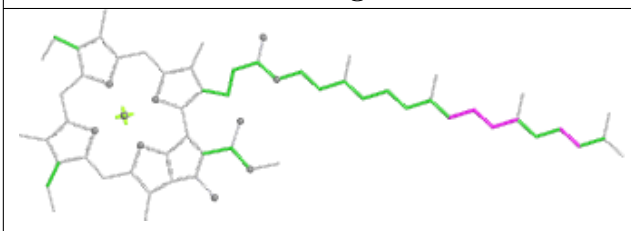
Ligand CLA A 859



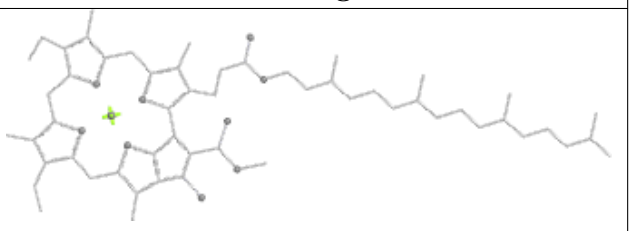
Bond lengths



Bond angles

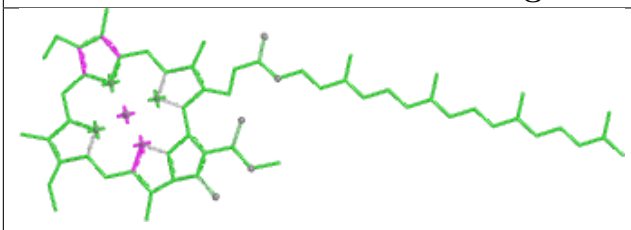


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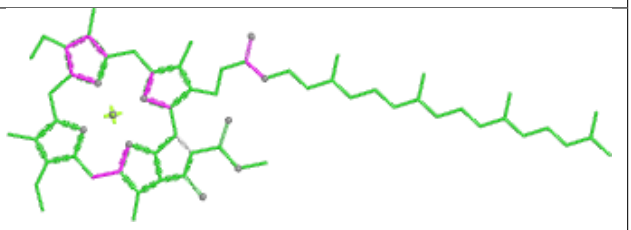


Rings

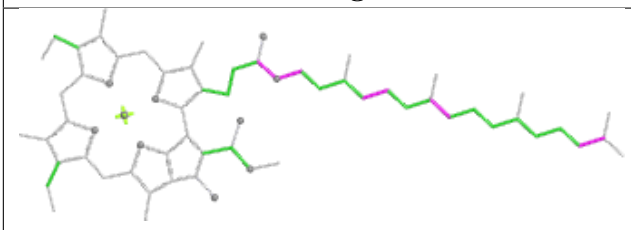
Ligand CLA B 839



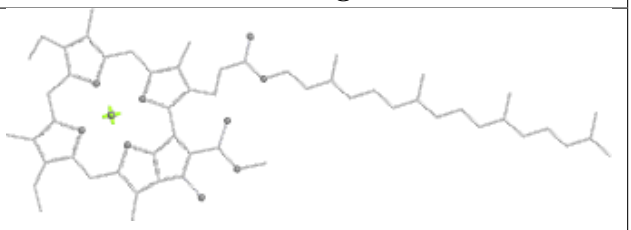
Bond lengths



Bond angles

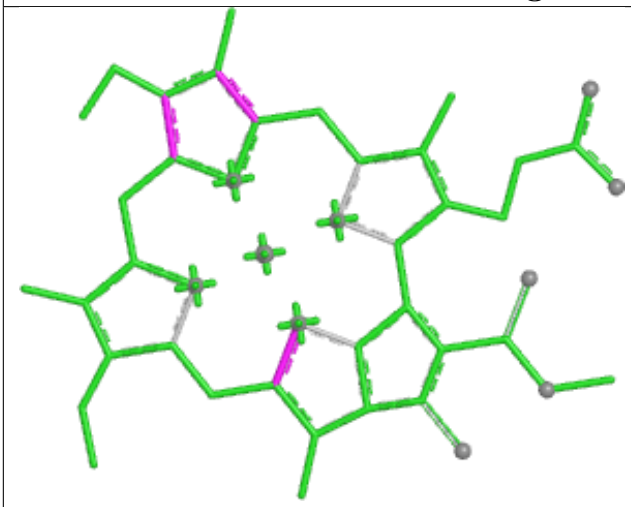


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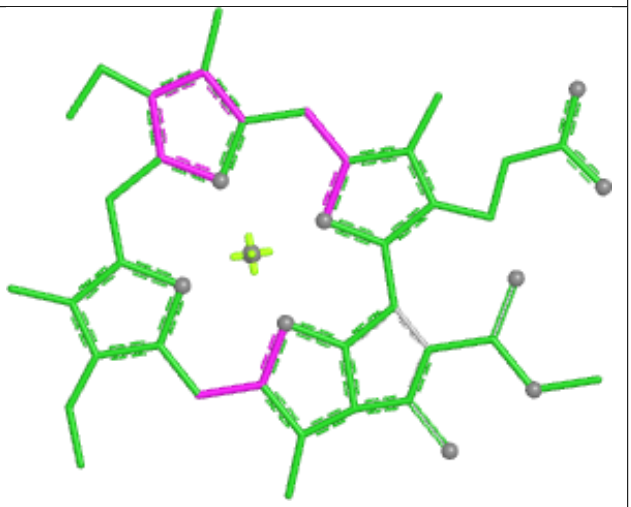


Rings

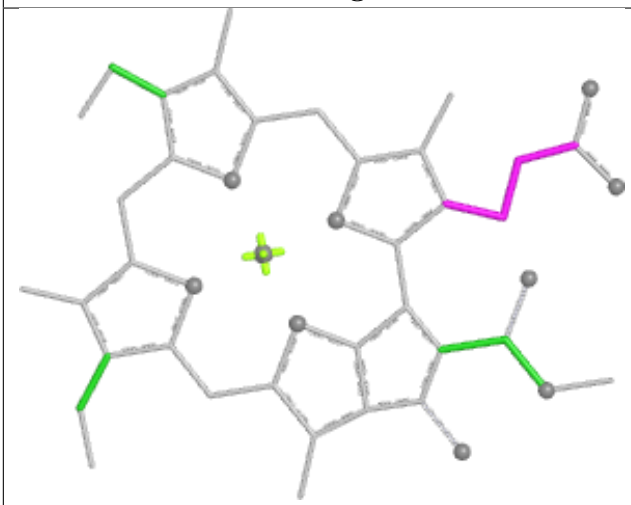
Ligand CLA F 203



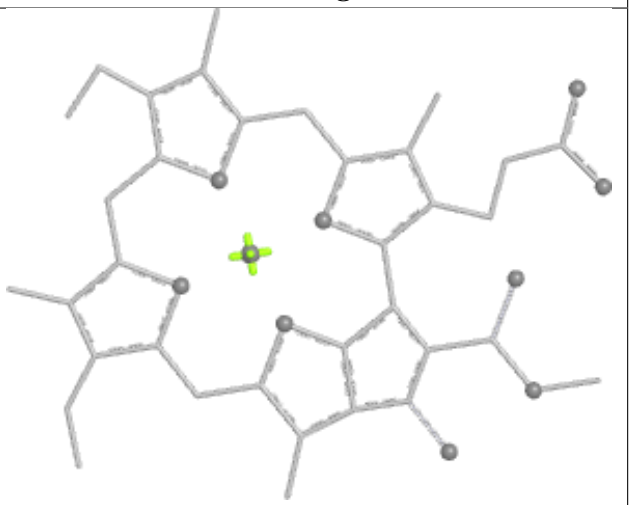
Bond lengths



Bond angles

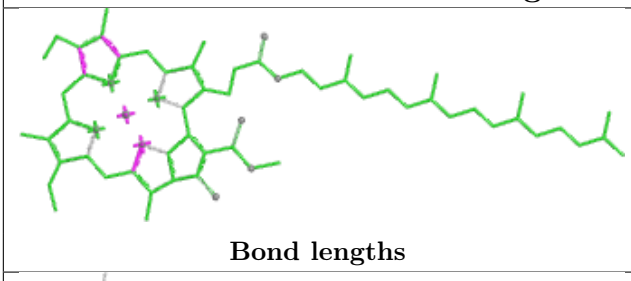


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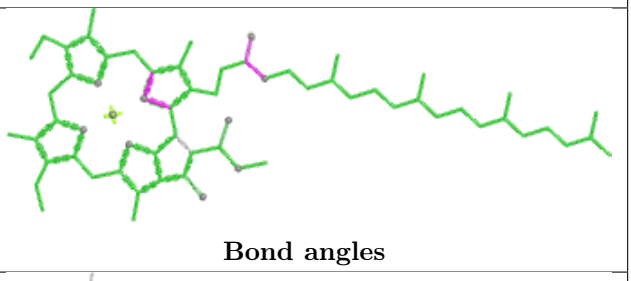


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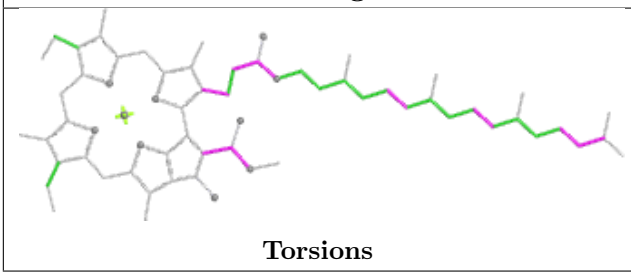
Ligand CLA A 807



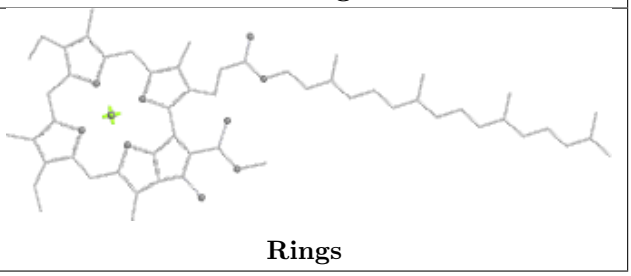
Bond lengths



Bond angles

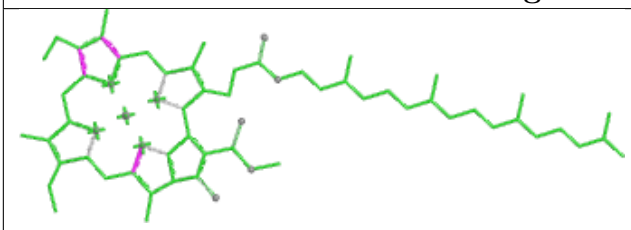


Torsions

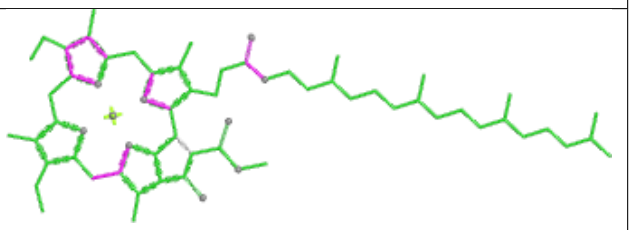


Rings

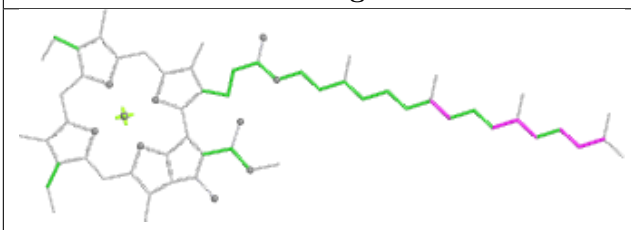
Ligand CLA A 840



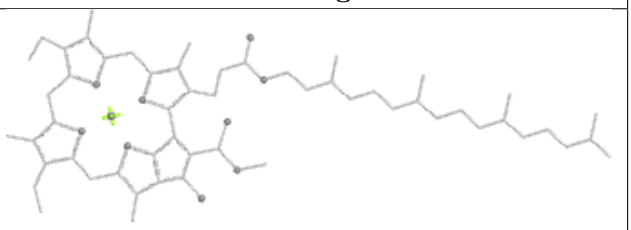
Bond lengths



Bond angles

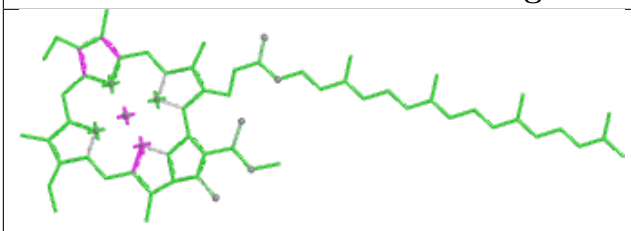


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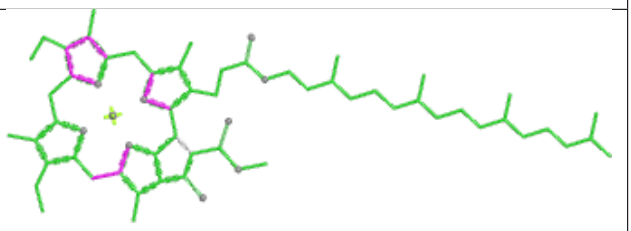


Rings

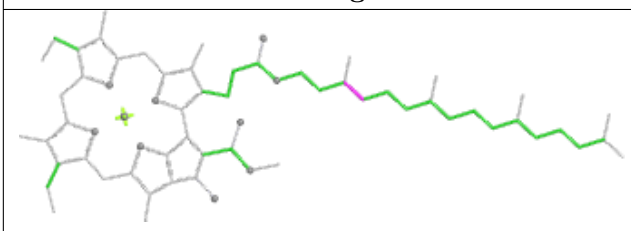
Ligand CLA B 829



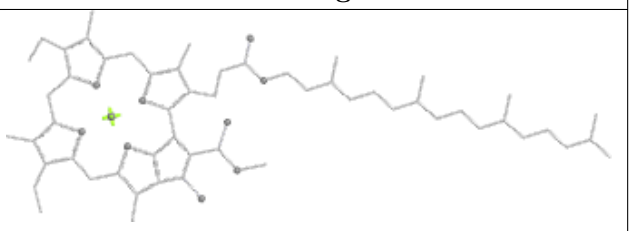
Bond lengths



Bond angles

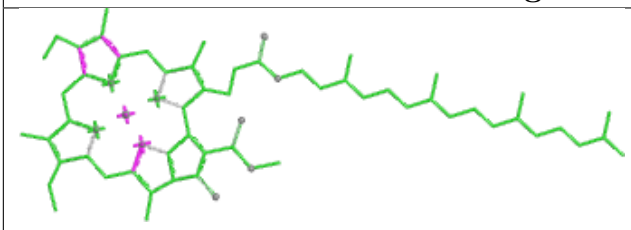


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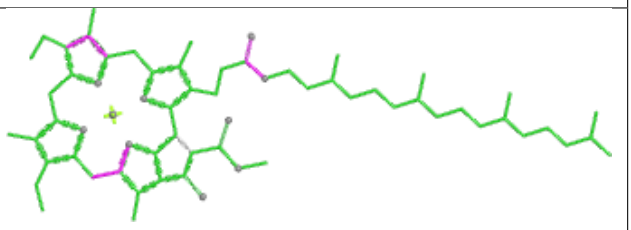


Rings

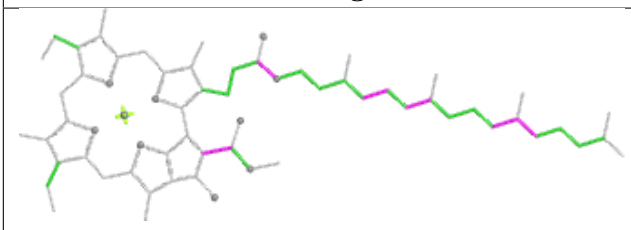
Ligand CLA B 826



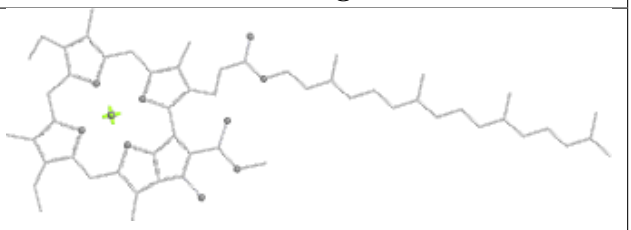
Bond lengths



Bond angles

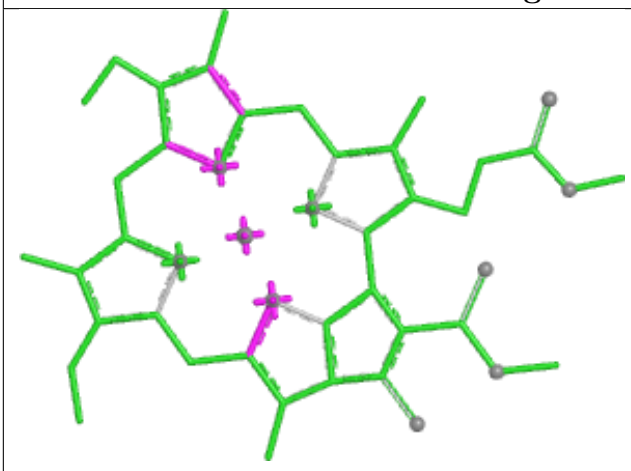


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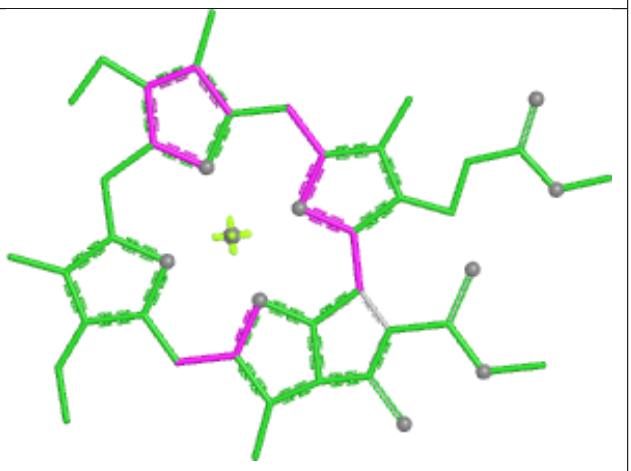


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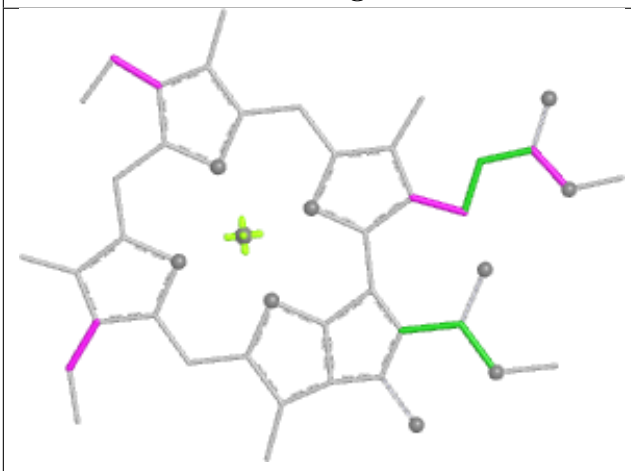
Ligand CLA A 817



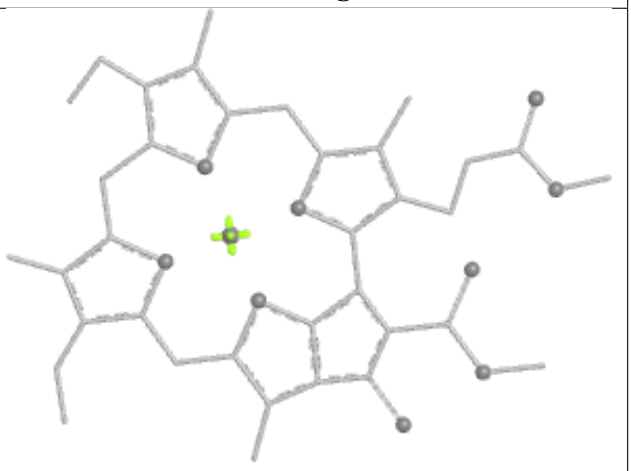
Bond lengths



Bond angles

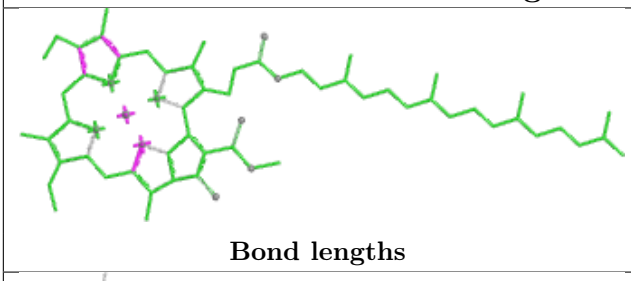


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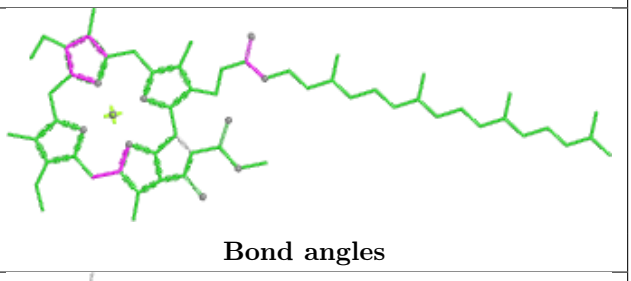


Rings

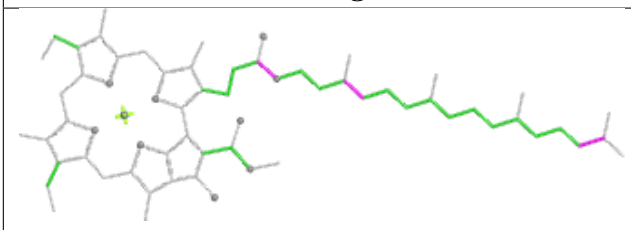
Ligand CLA A 828



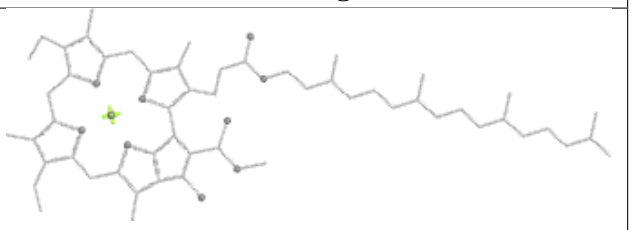
Bond lengths



Bond angles

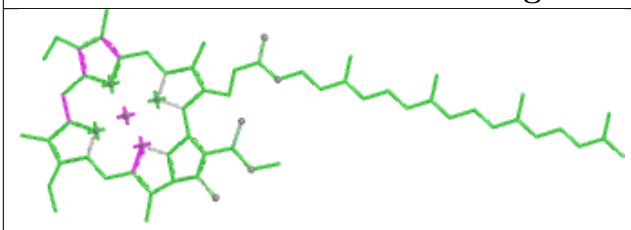


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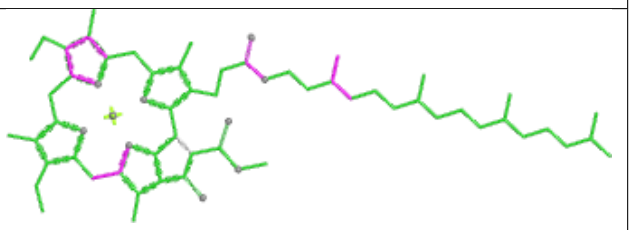


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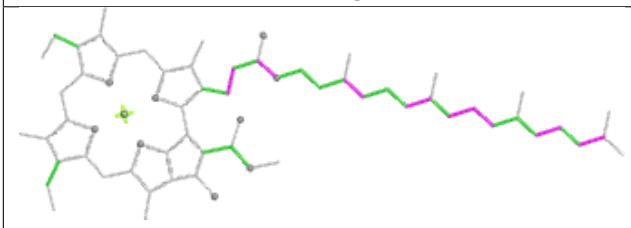
Ligand CLA A 814



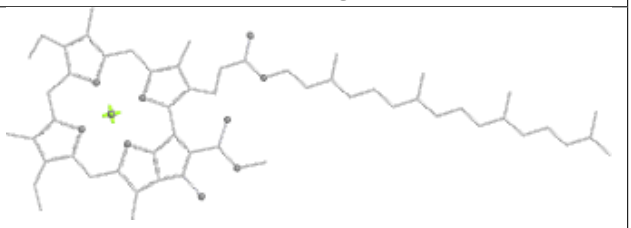
Bond lengths



Bond angles

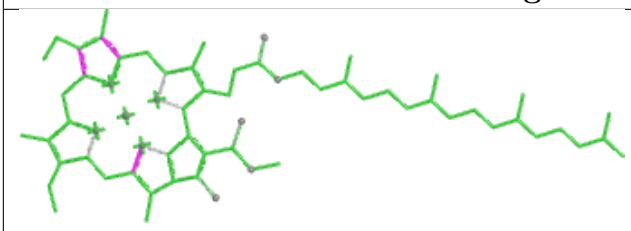


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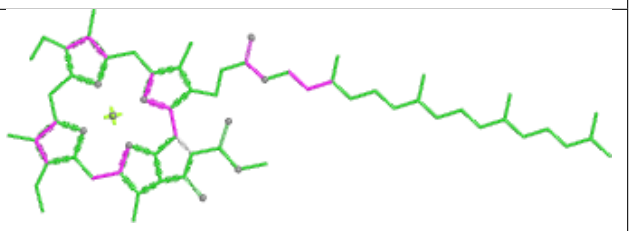


Rings

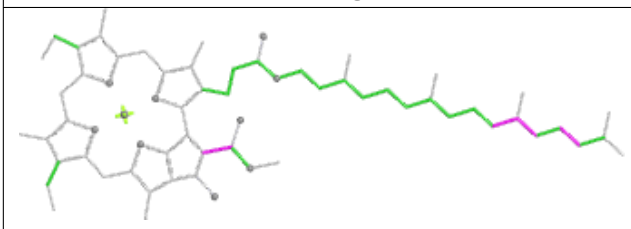
Ligand CLA A 835



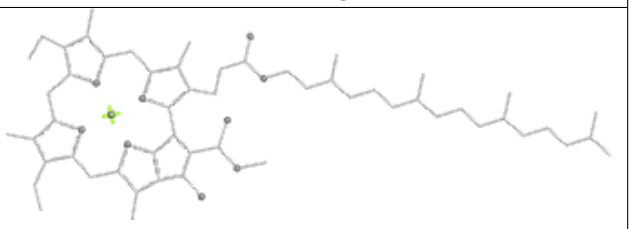
Bond lengths



Bond angles

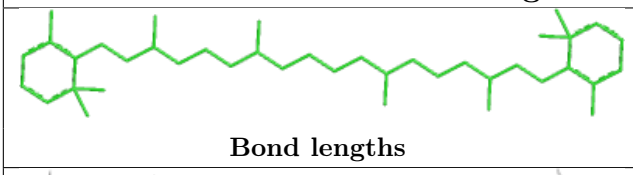


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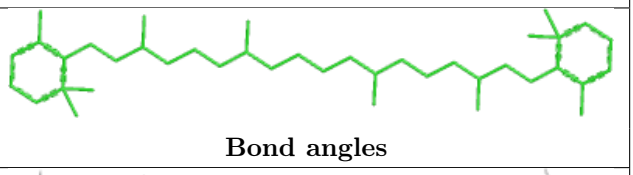


Rings

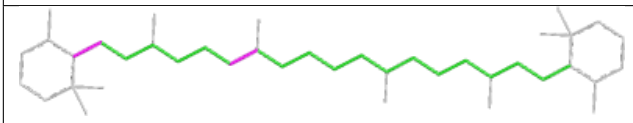
Ligand BCR B 845



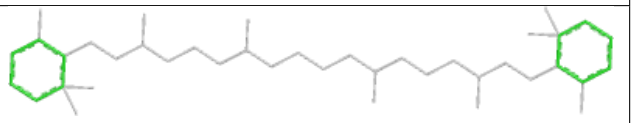
Bond lengths



Bond angles

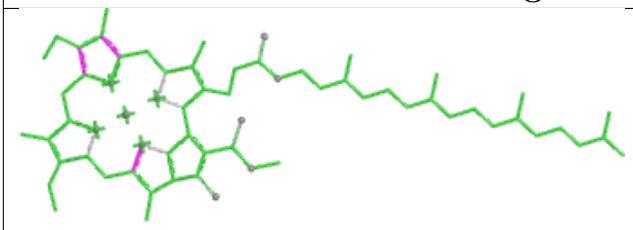


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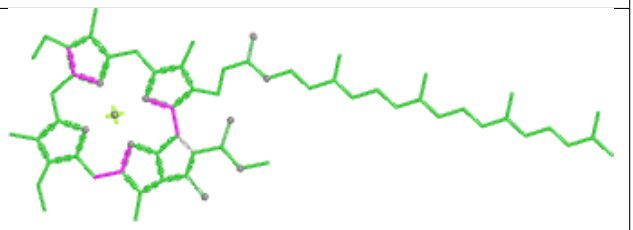


Rings

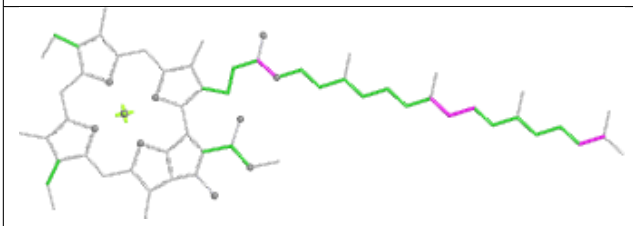
Ligand CLA B 810



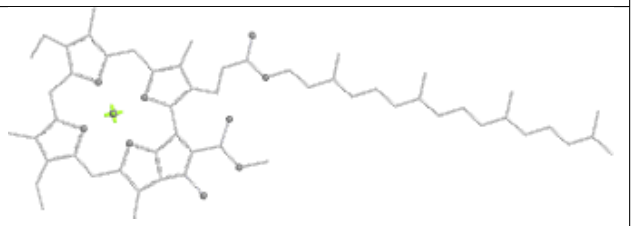
Bond lengths



Bond angles

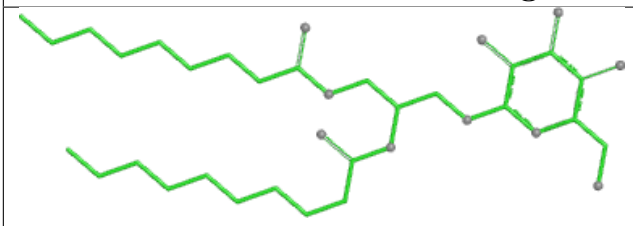


Torsions

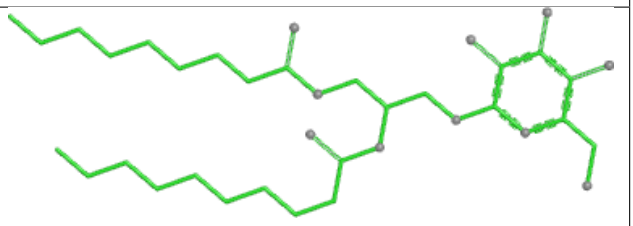


Rings

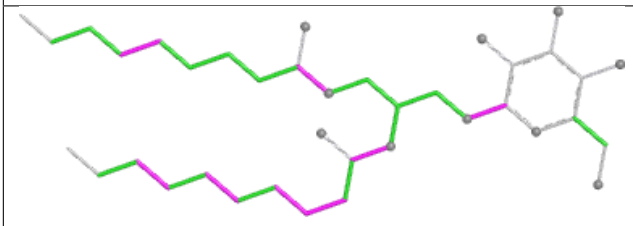
Ligand LMG B 851



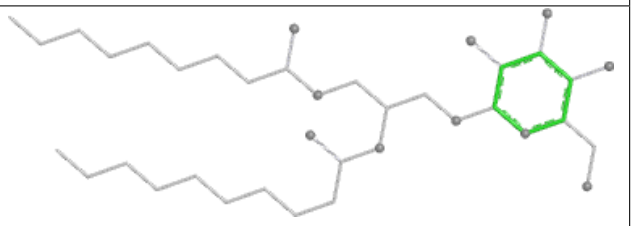
Bond lengths



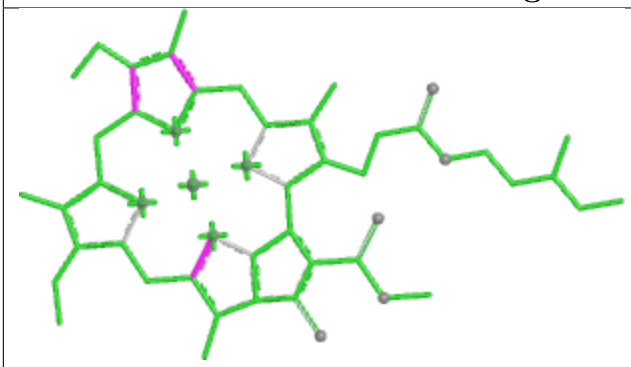
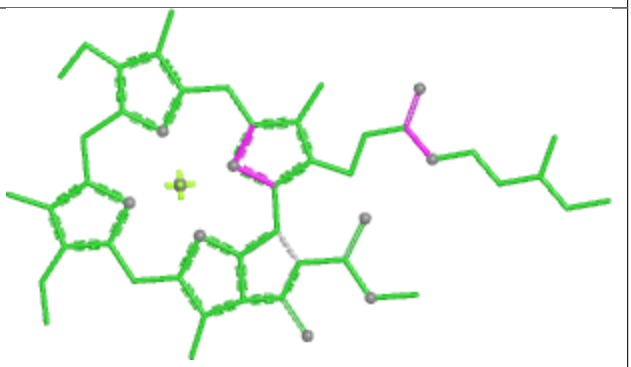
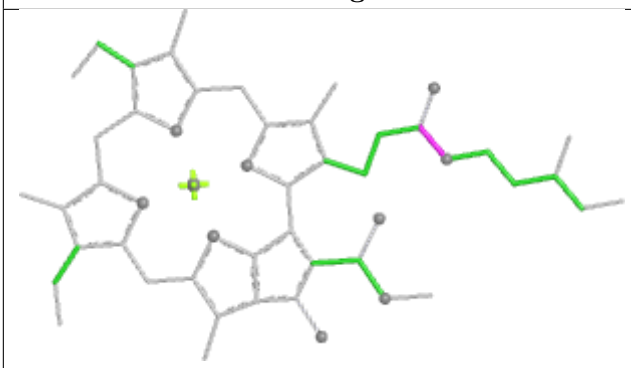
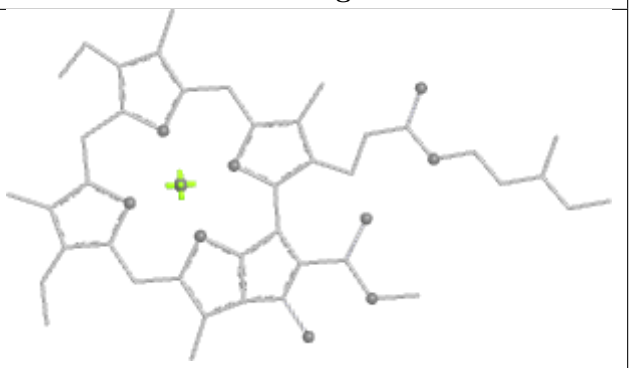
Bond angles

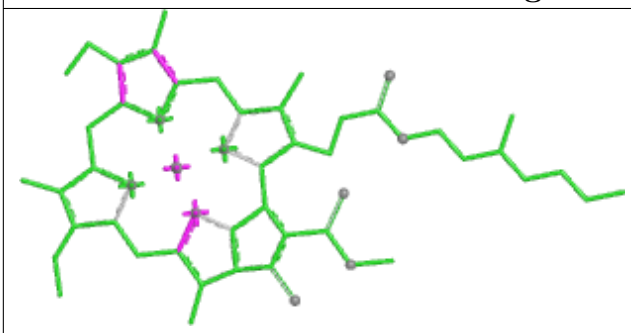
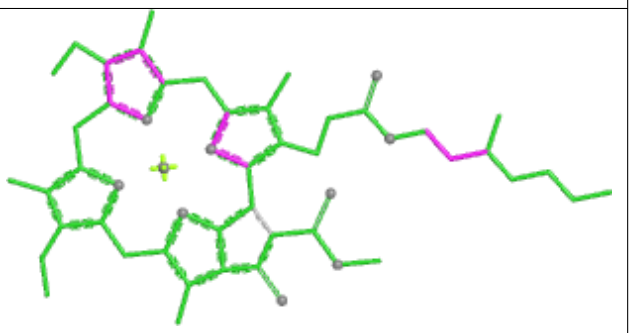
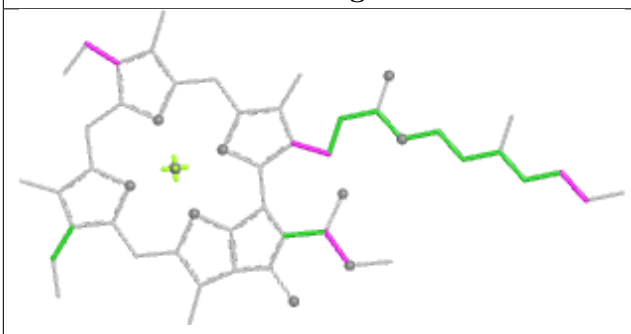
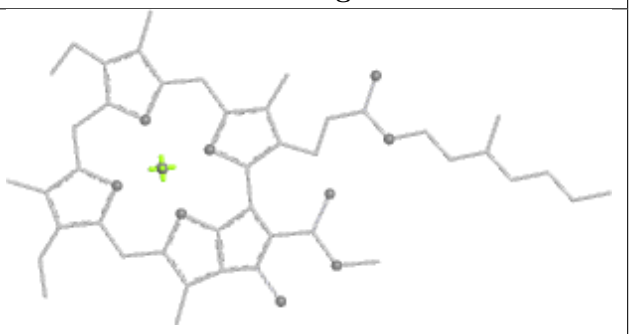


Torsions

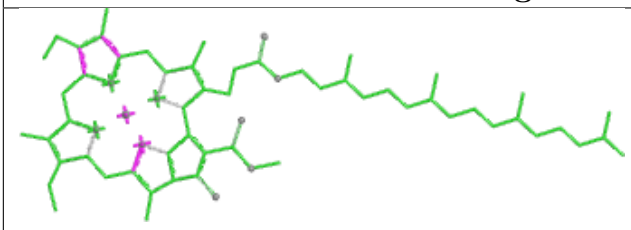


Rings

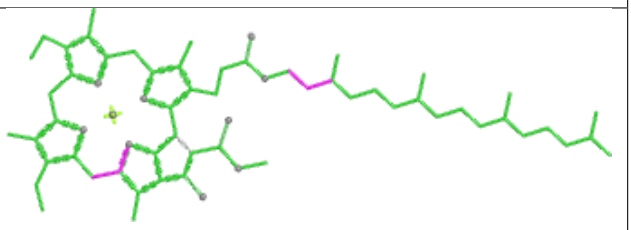
Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

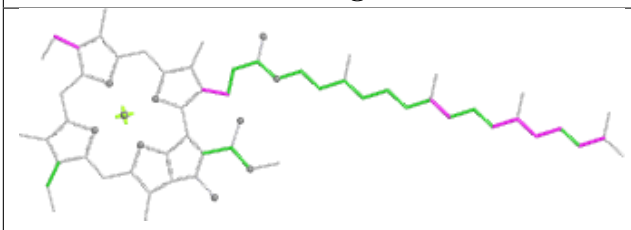
Ligand CLA K 4004



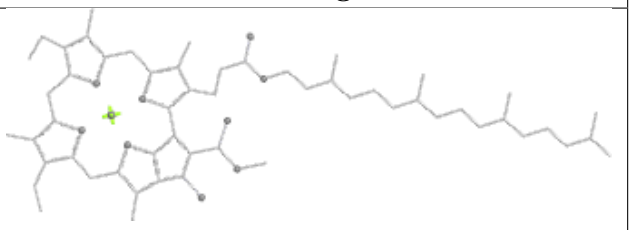
Bond lengths



Bond angles

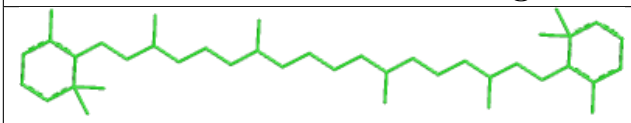


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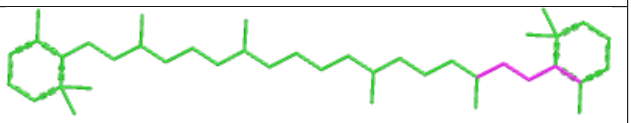


Rings

Ligand BCR K 4001



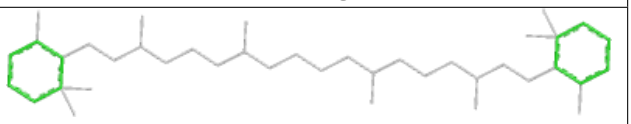
Bond lengths



Bond angles

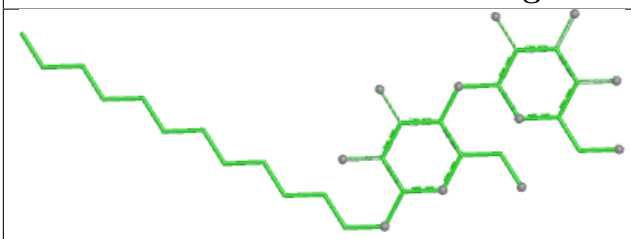


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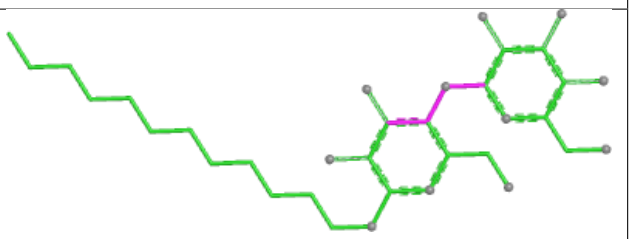


Rings

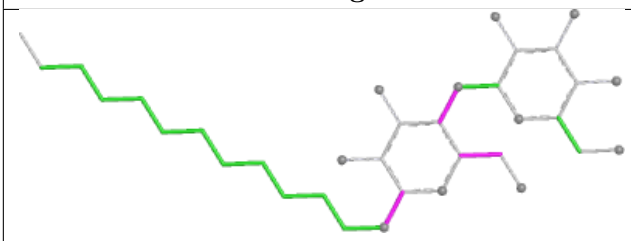
Ligand LMT F 206



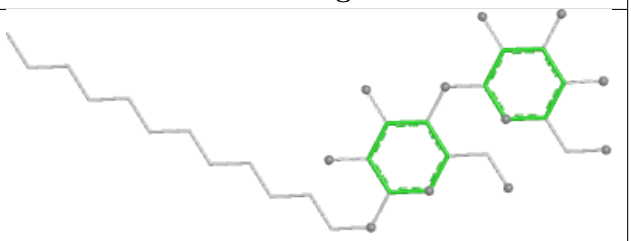
Bond lengths



Bond angles

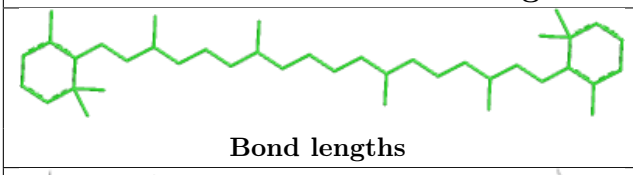


Torsions

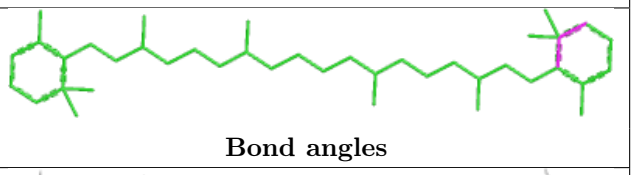


Rings

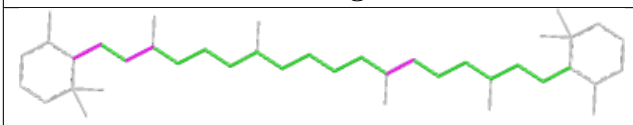
Ligand BCR A 849



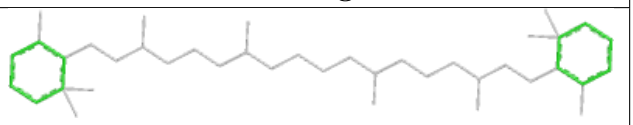
Bond lengths



Bond angles

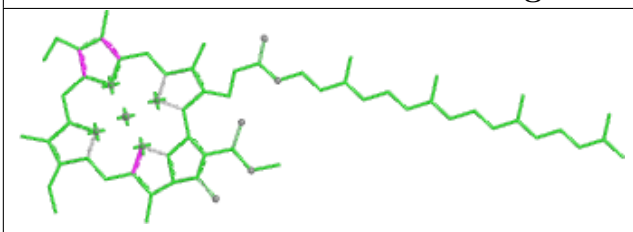


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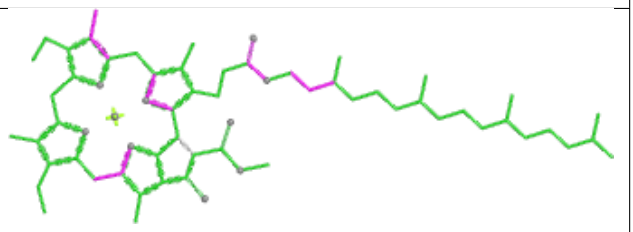


Rings

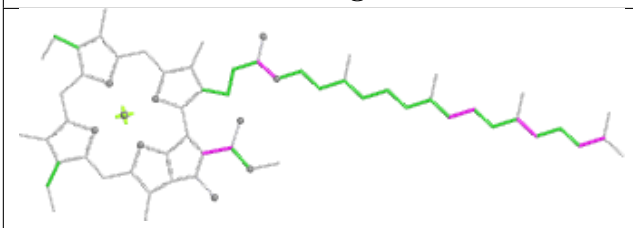
Ligand CLA B 815



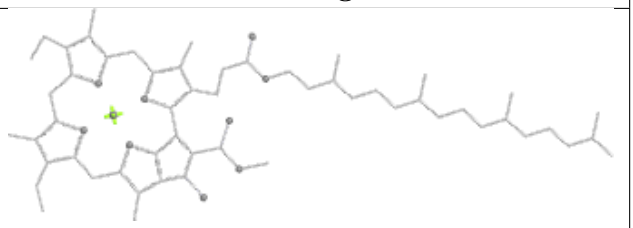
Bond lengths



Bond angles

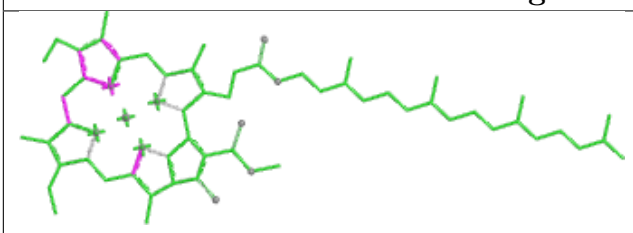


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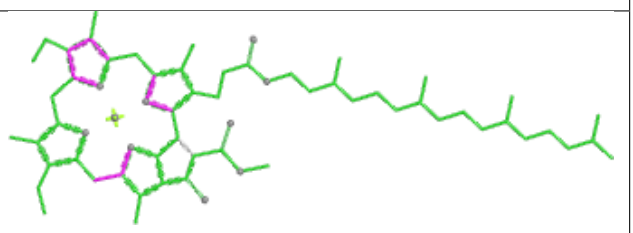


Rings

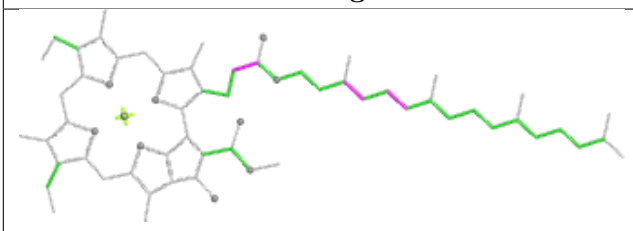
Ligand CL0 A 802



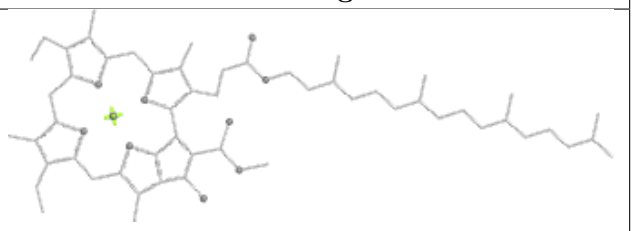
Bond lengths



Bond angles

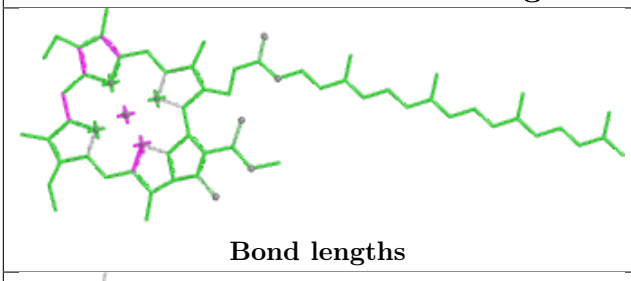


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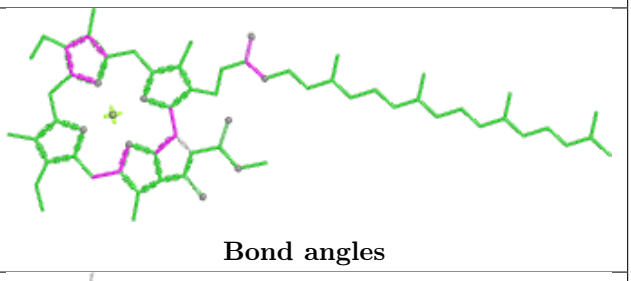


Rings

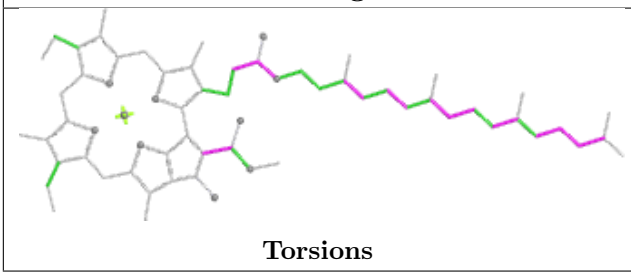
Ligand CLA A 805



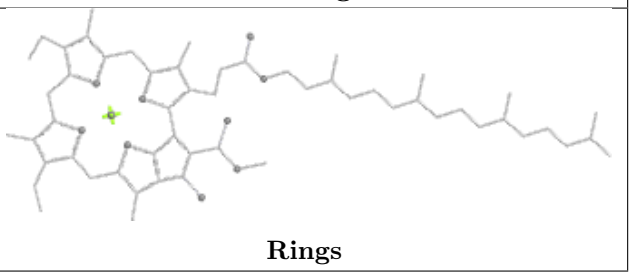
Bond lengths



Bond angles

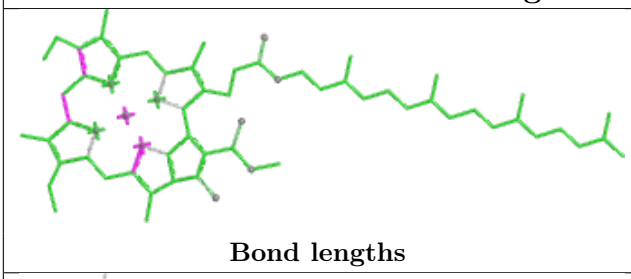


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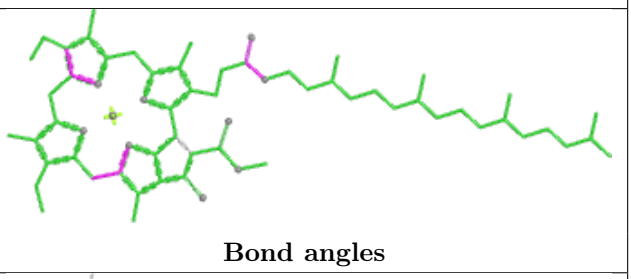


Rings

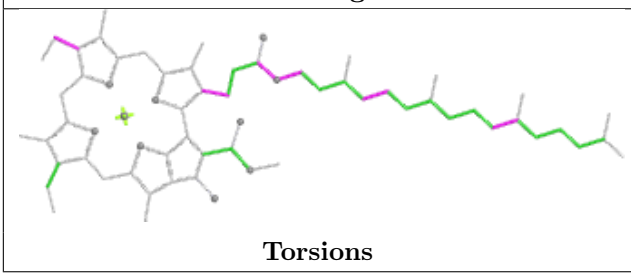
Ligand CLA A 837



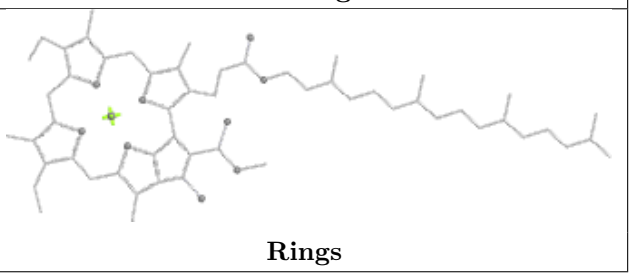
Bond lengths



Bond angles

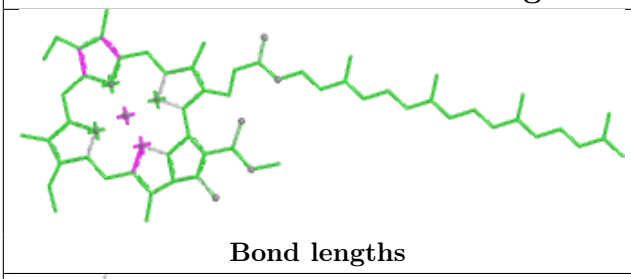


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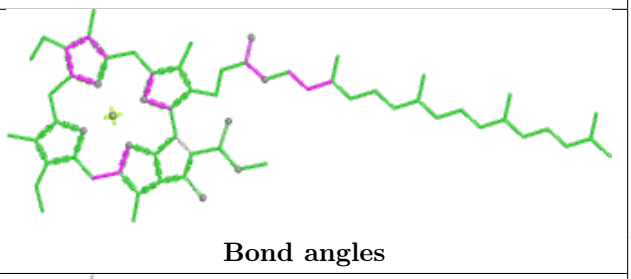


Rings

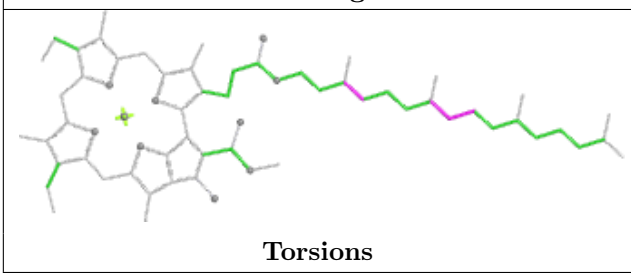
Ligand CLA A 841



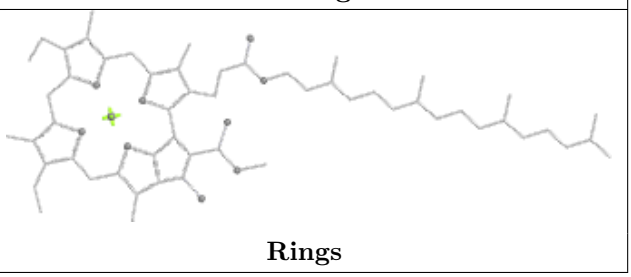
Bond lengths



Bond angles

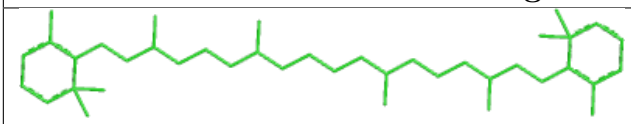


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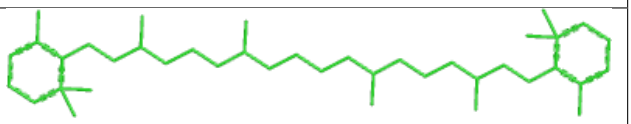


Rings

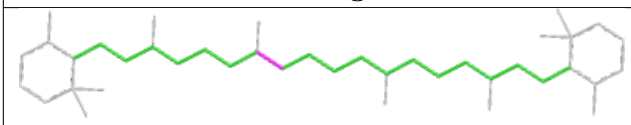
Ligand BCR F 205



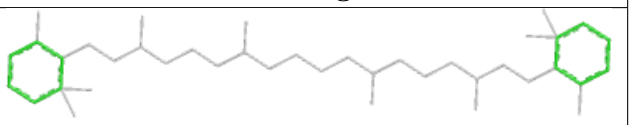
Bond lengths



Bond angles

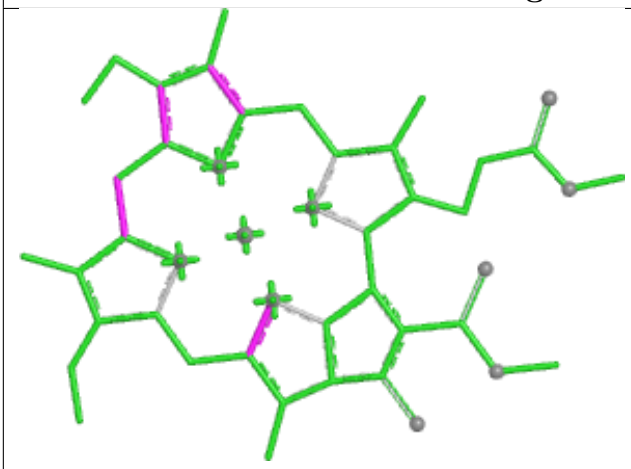


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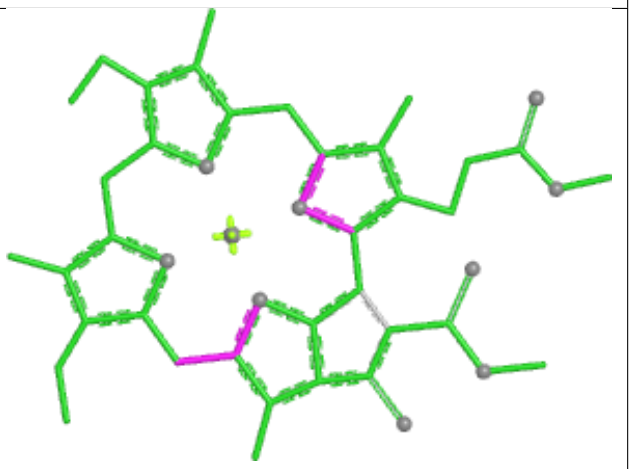


Rings

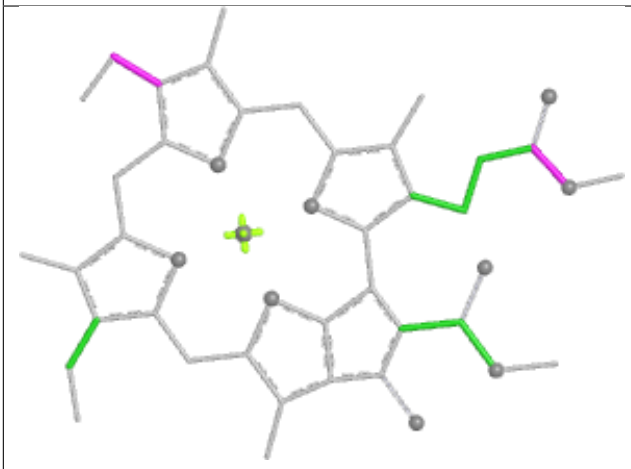
Ligand CLA F 204



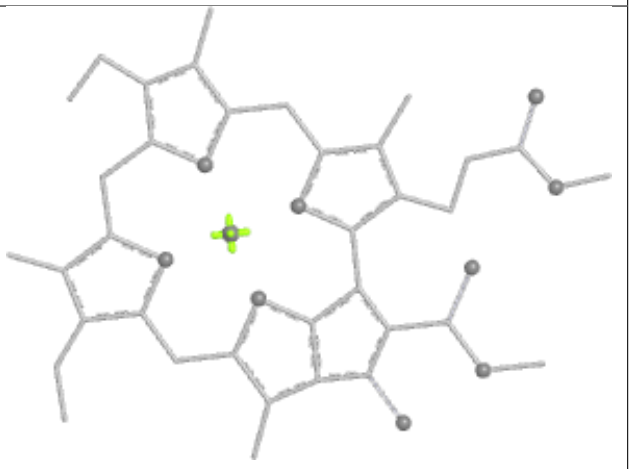
Bond lengths



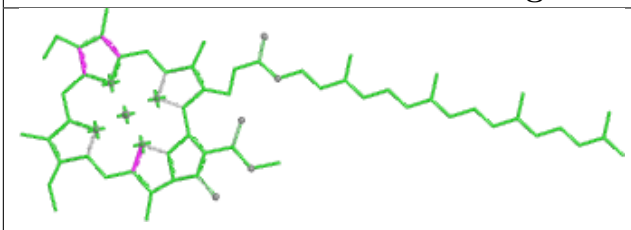
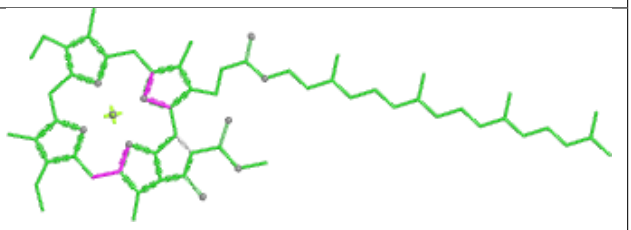
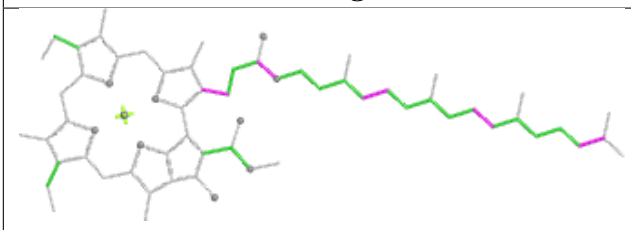
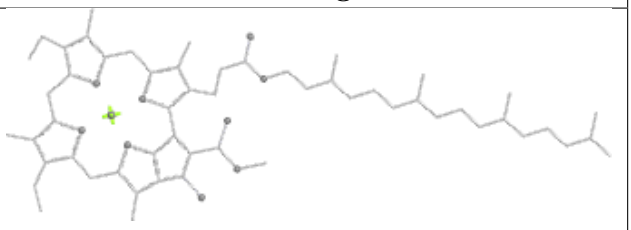
Bond angles

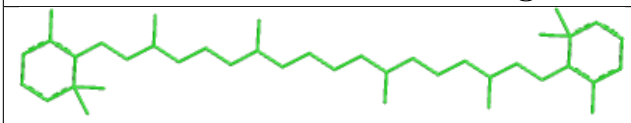
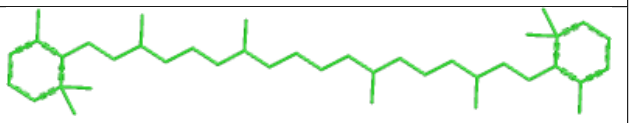
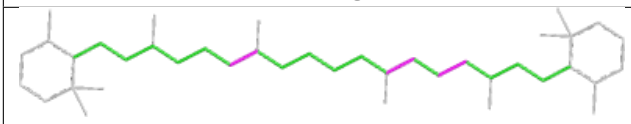
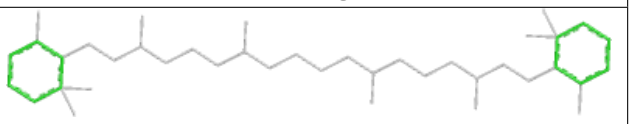


Torsions

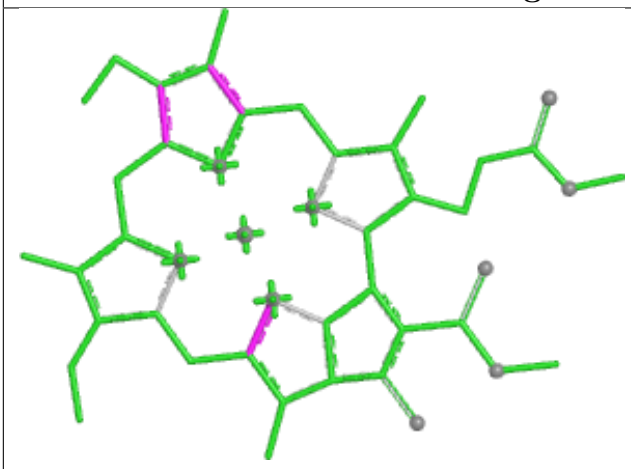


Rings

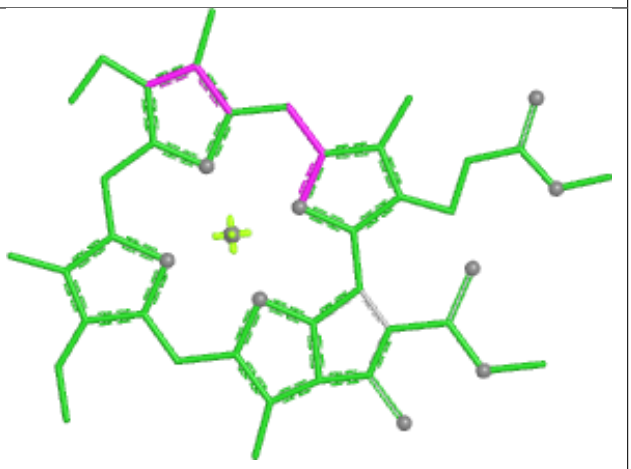
Ligand CLA F 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR J 1105	
	
Bond lengths	Bond angles
	
Torsions	Rings

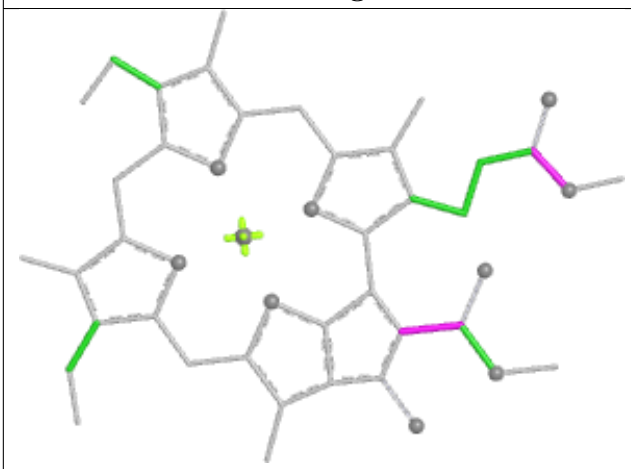
Ligand CLA A 845



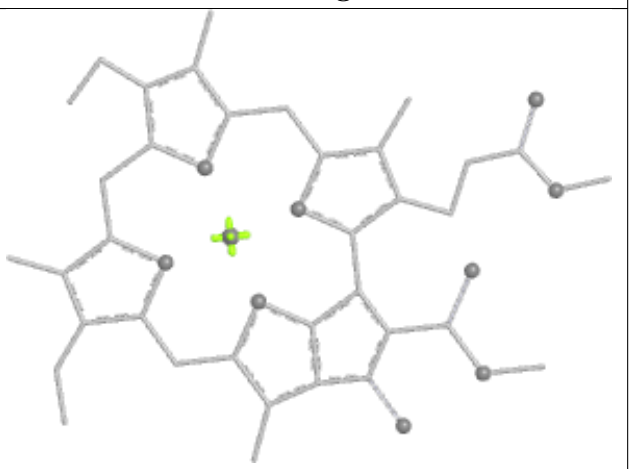
Bond lengths



Bond angles



Torsions



Rings

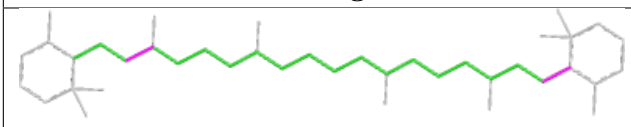
Ligand BCR B 852



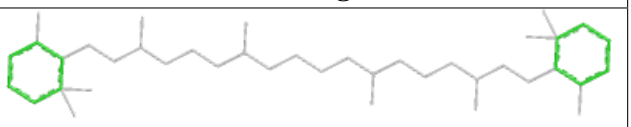
Bond lengths



Bond angles

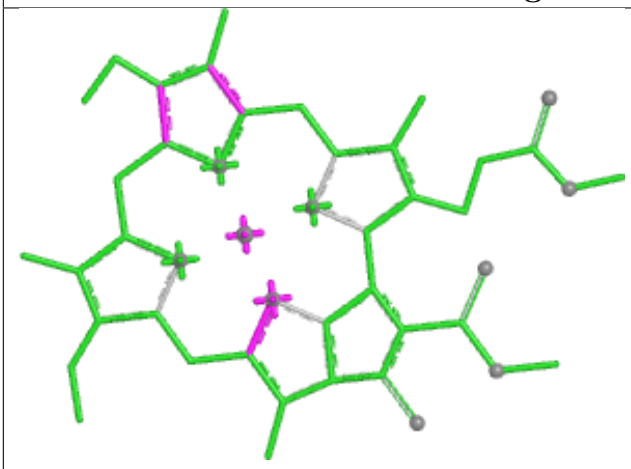


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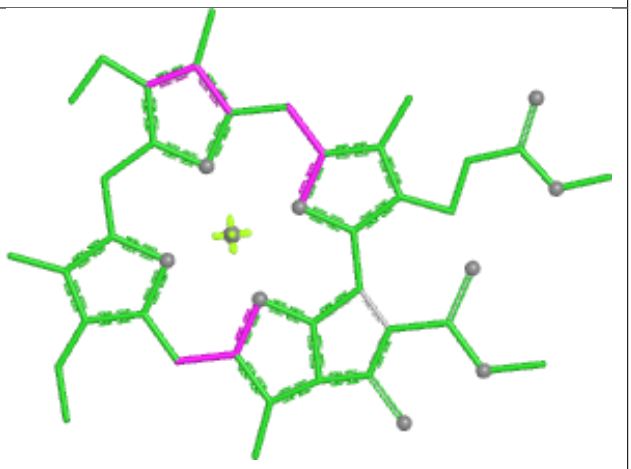


Rings

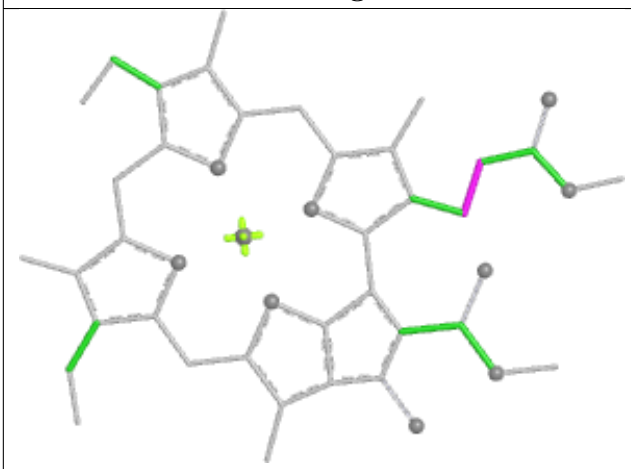
Ligand CLA B 842



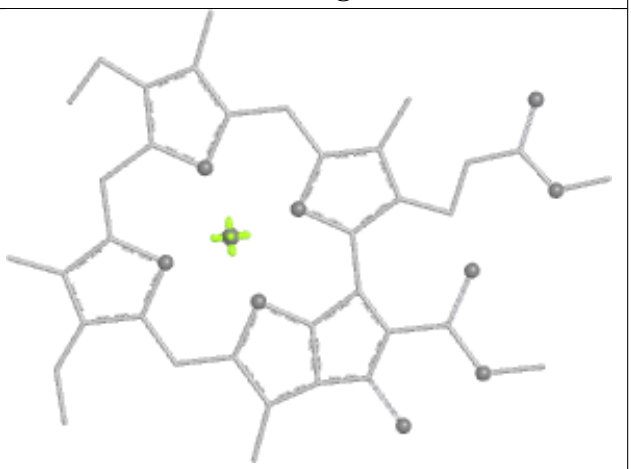
Bond lengths



Bond angles



Torsions



Rings

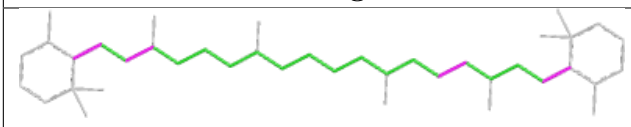
Ligand BCR L 206



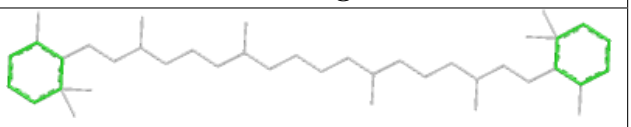
Bond lengths



Bond angles

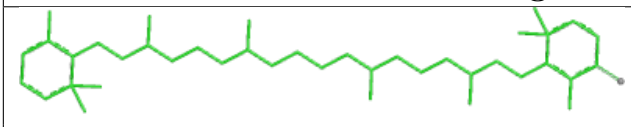


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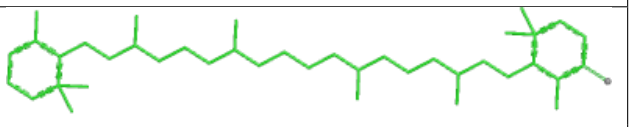


Rings

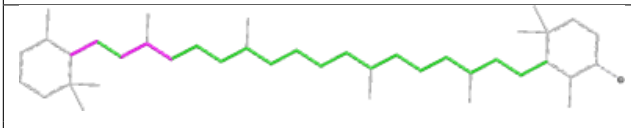
Ligand ECH I 103



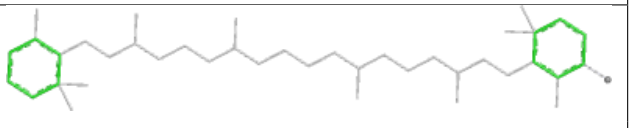
Bond lengths



Bond angles

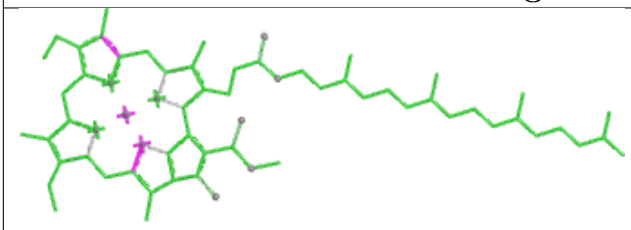


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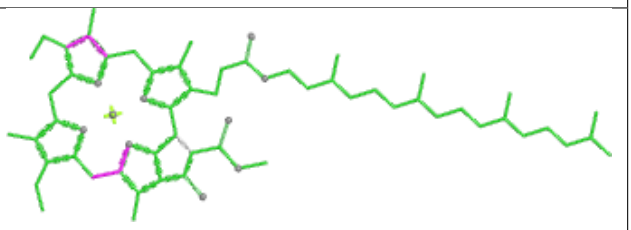


Rings

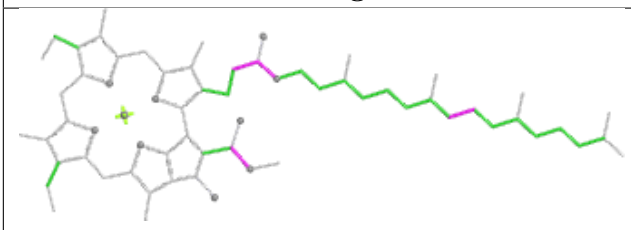
Ligand CLA B 804



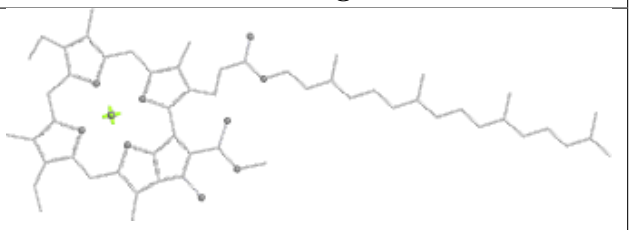
Bond lengths



Bond angles

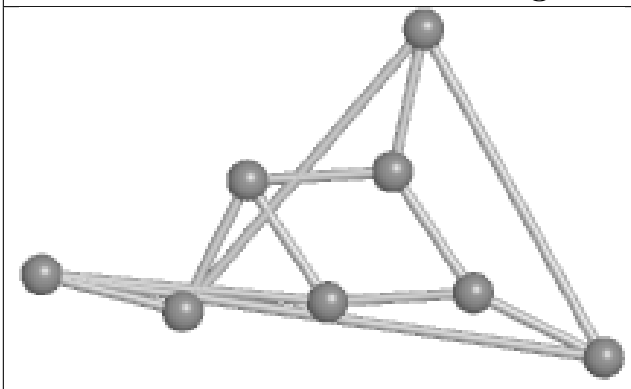


Torsions

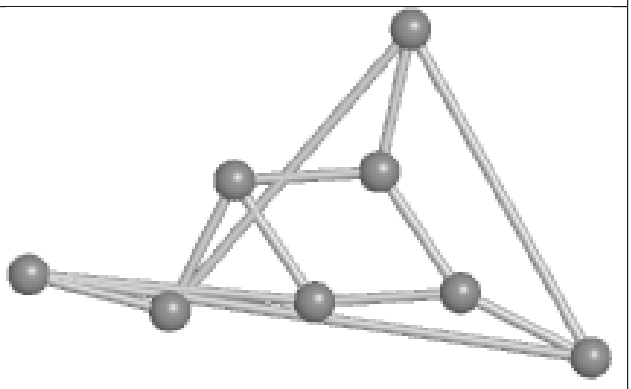


Rings

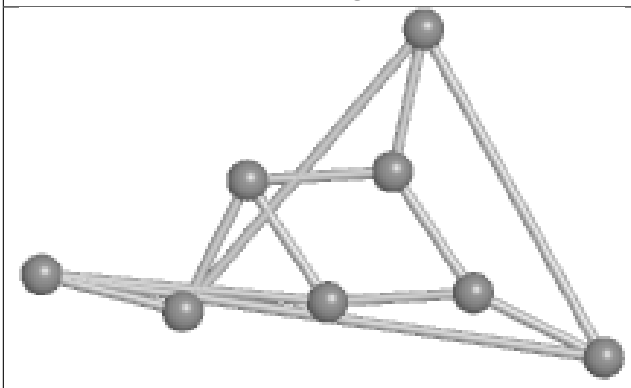
Ligand SF4 A 847



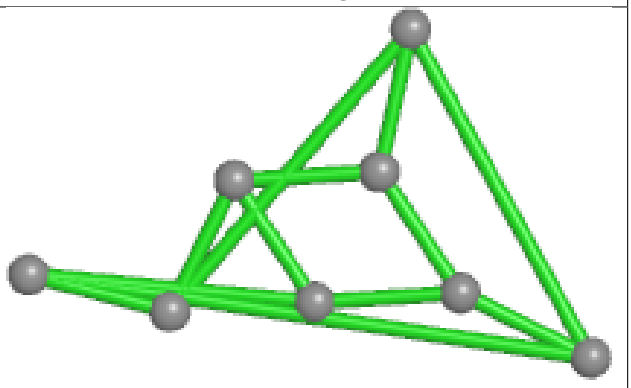
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Bond angles

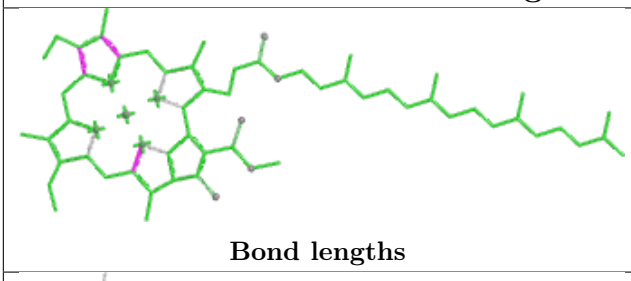


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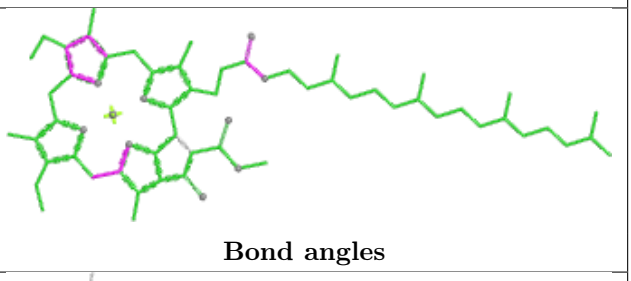


Rings

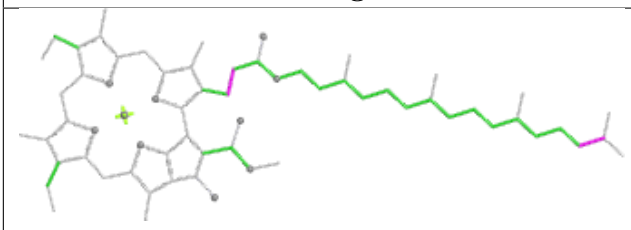
Ligand CLA B 805



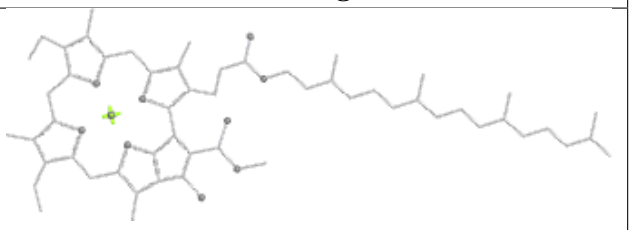
Bond lengths



Bond angles

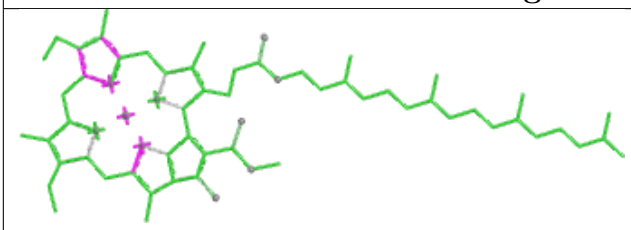


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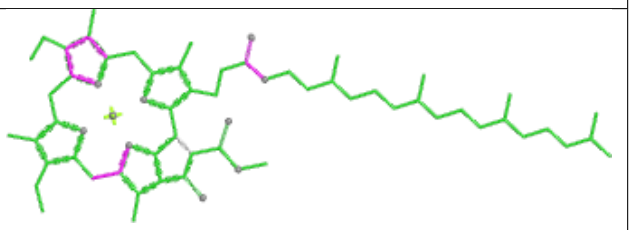


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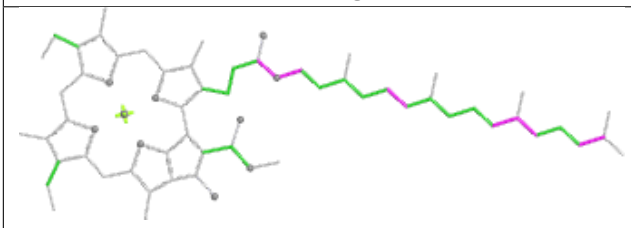
Ligand CLA A 832



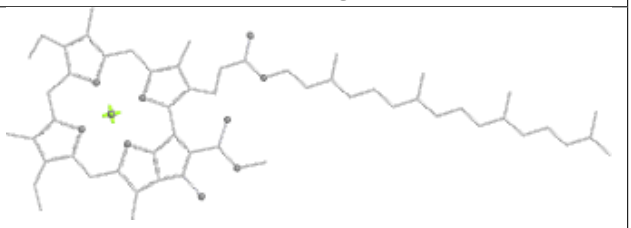
Bond lengths



Bond angles

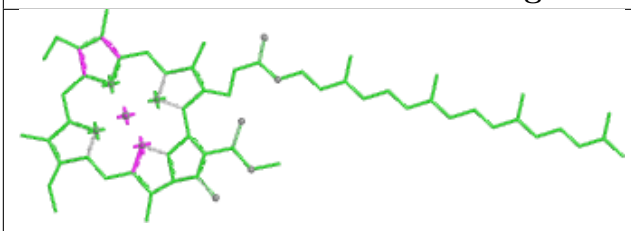


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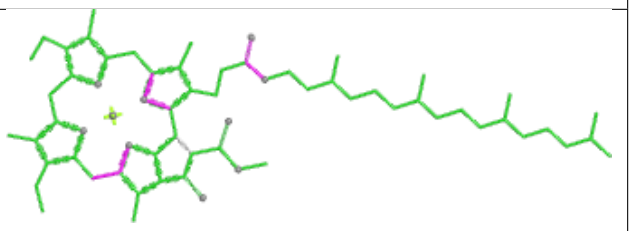


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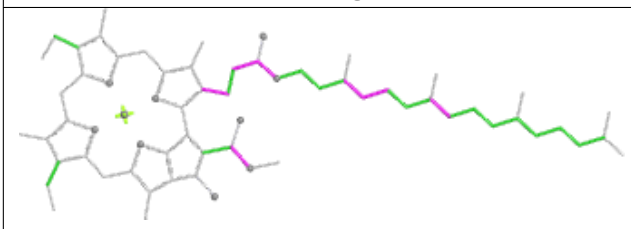
Ligand CLA B 812



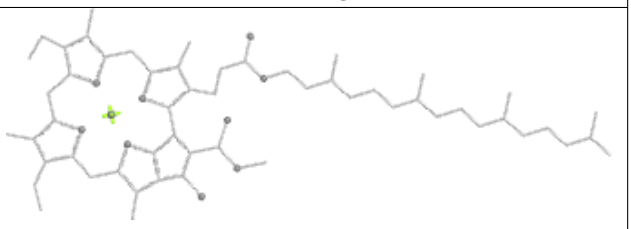
Bond lengths



Bond angles

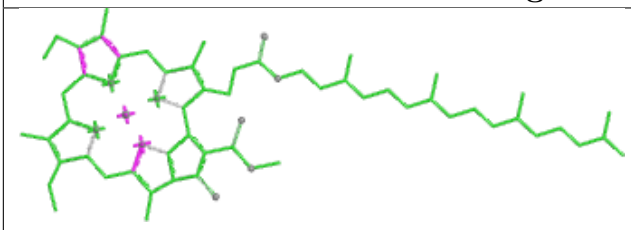


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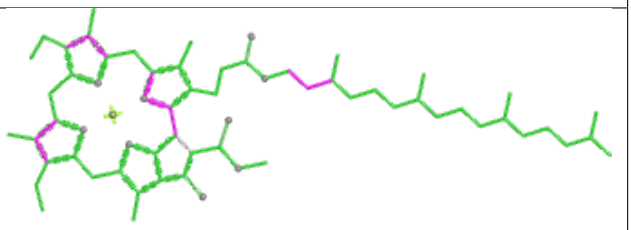


Rings

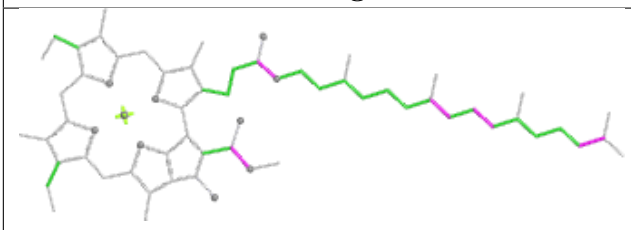
Ligand CLA L 204



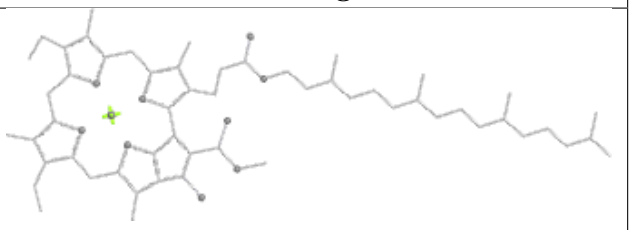
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Bond angles

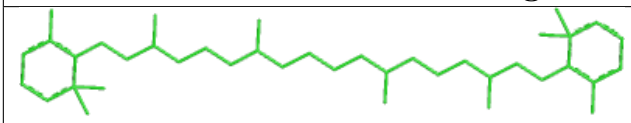


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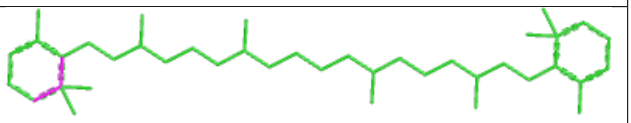


Rings

Ligand BCR B 849



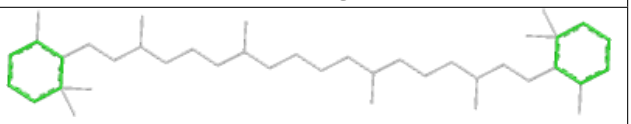
Bond lengths



Bond angles



Torsions



Rings

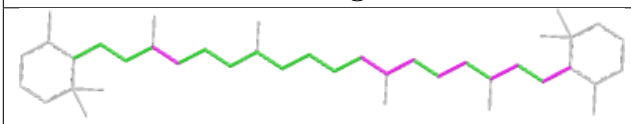
Ligand BCR A 852



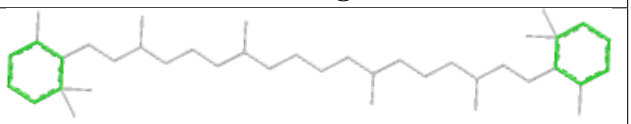
Bond lengths



Bond angles

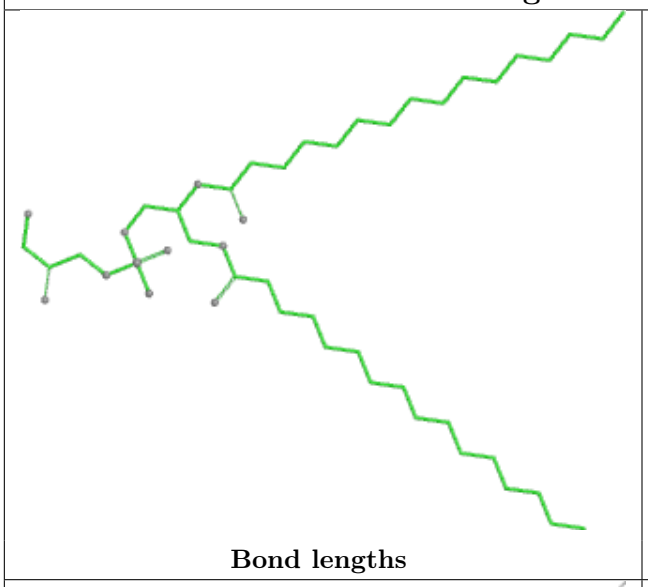


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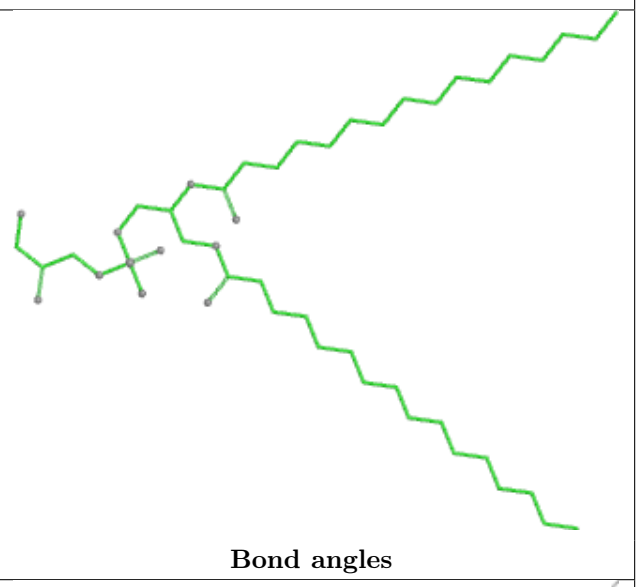


Rings

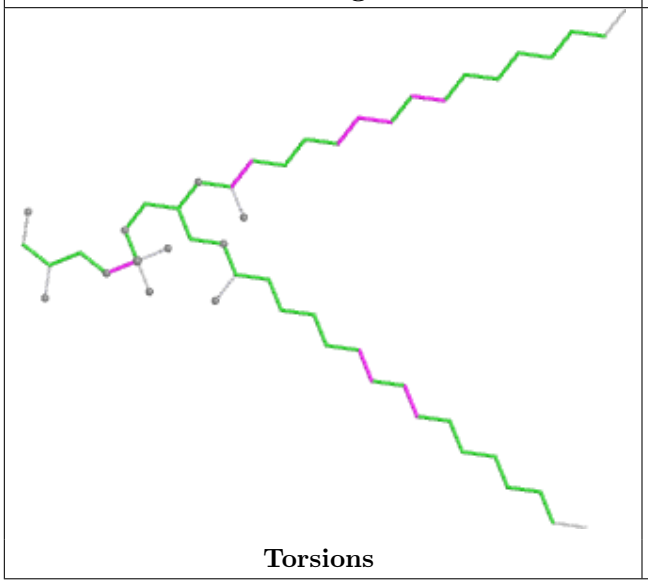
Ligand LHG A 855



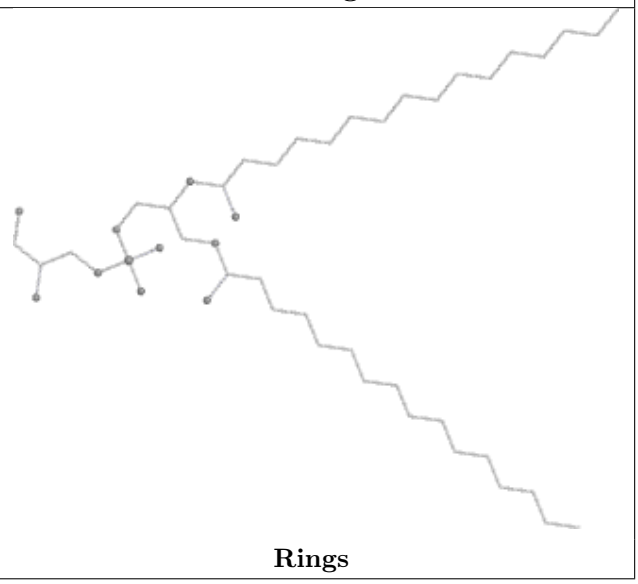
Bond lengths



Bond angles

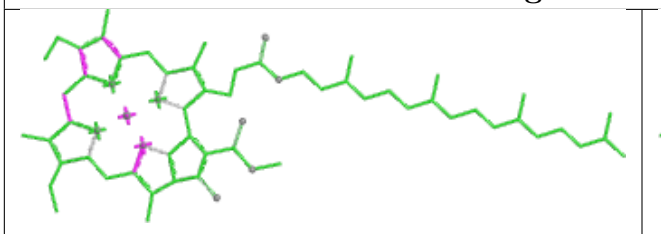


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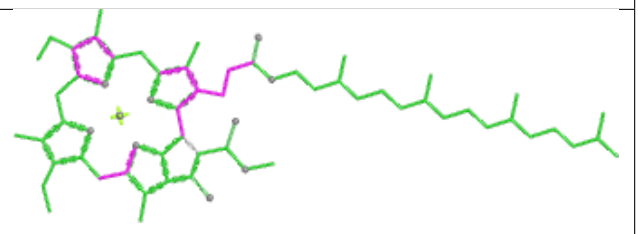


Rings

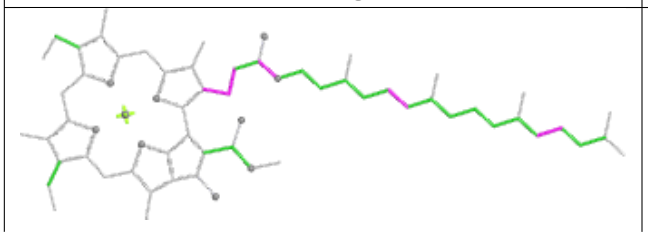
Ligand CLA A 830



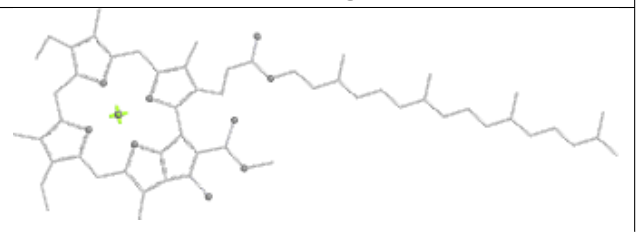
Bond lengths



Bond angles

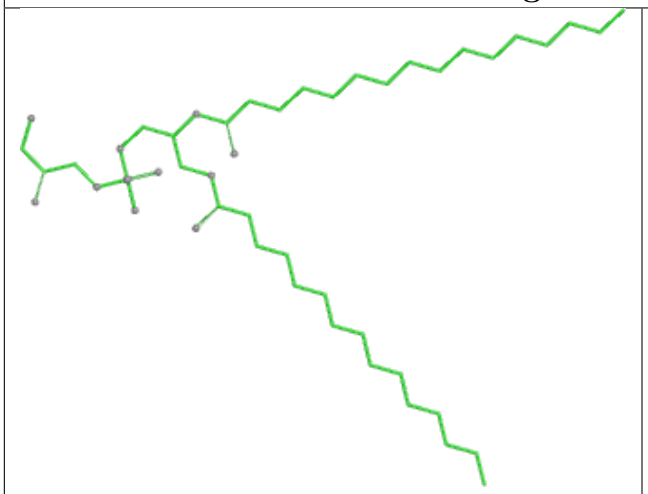


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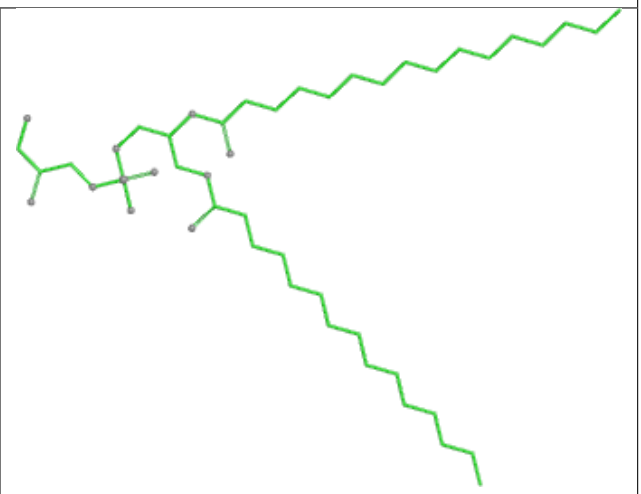


Rings

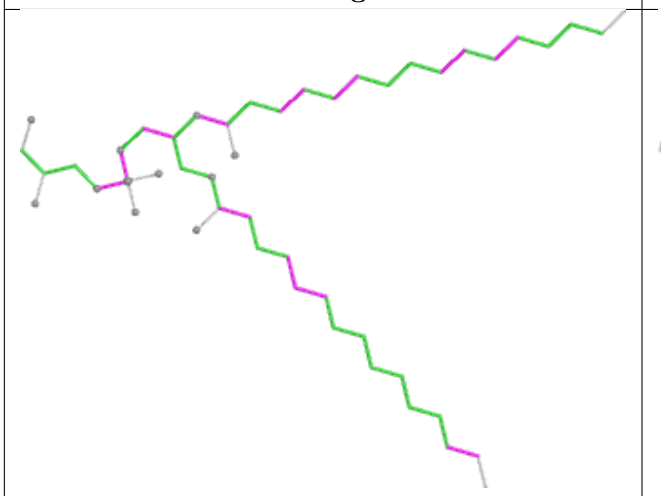
Ligand LHG A 801



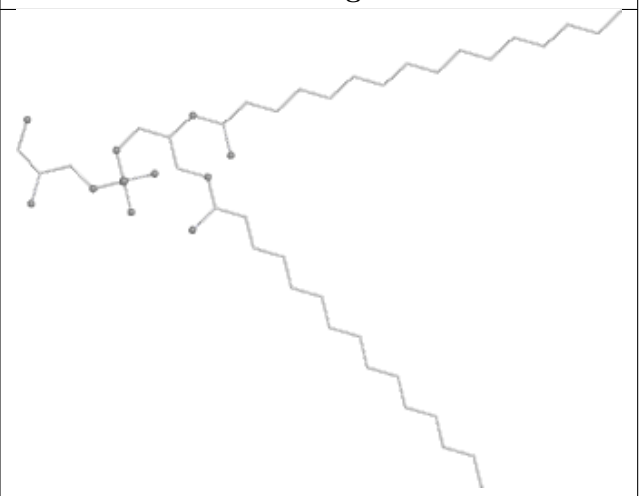
Bond lengths



Bond angles

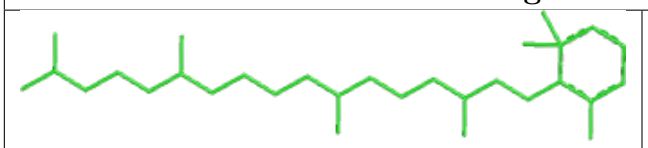


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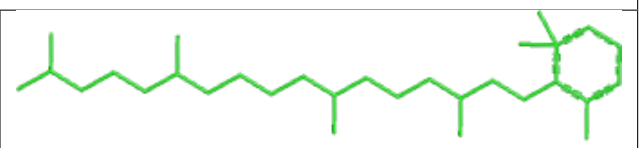


Rings

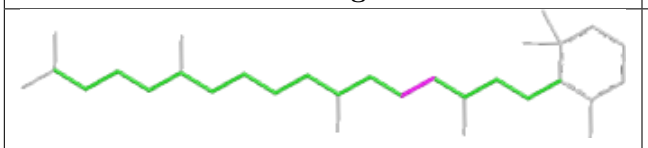
Ligand BCR B 847



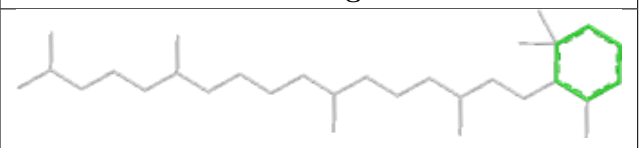
Bond lengths



Bond angles

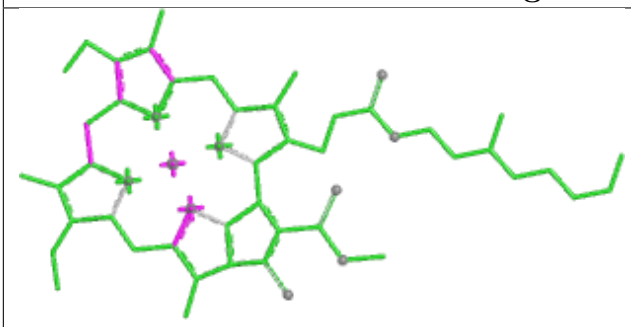


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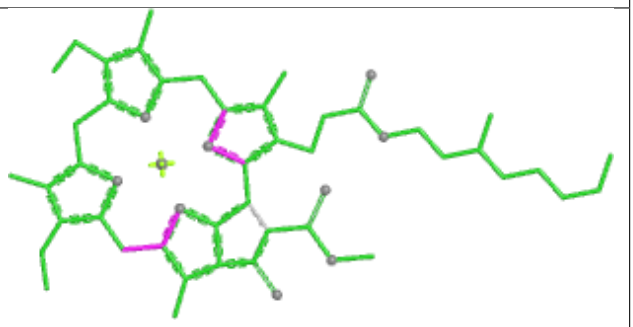


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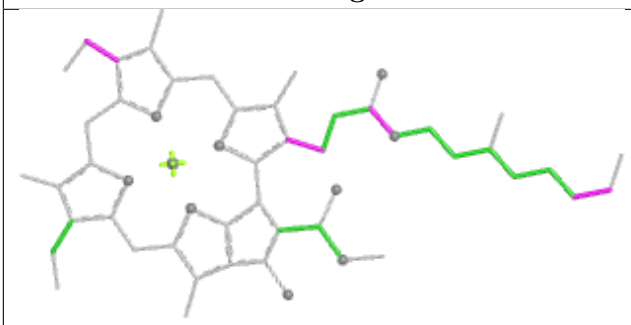
Ligand CLA A 813



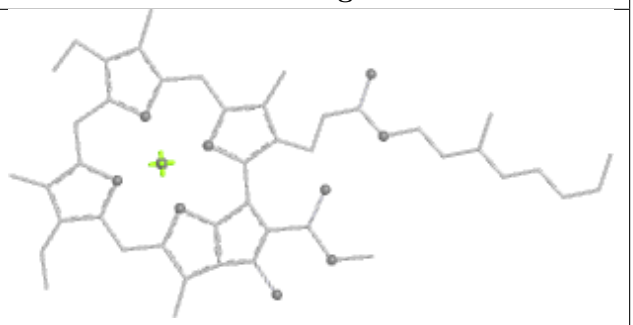
Bond lengths



Bond angles



Torsions

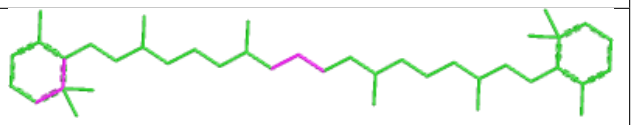


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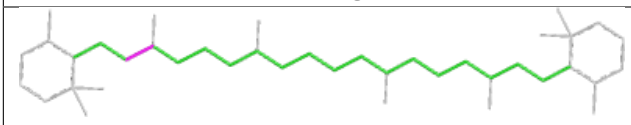
Ligand BCR B 848



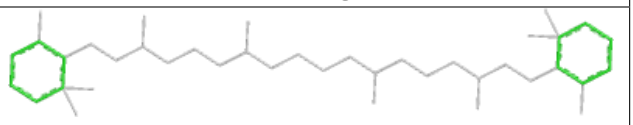
Bond lengths



Bond angles

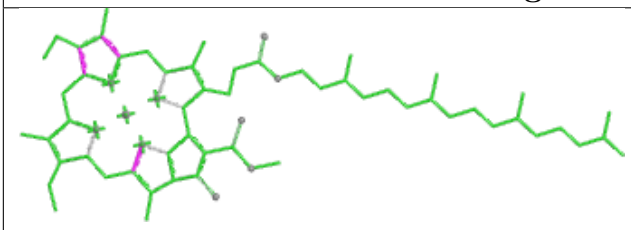


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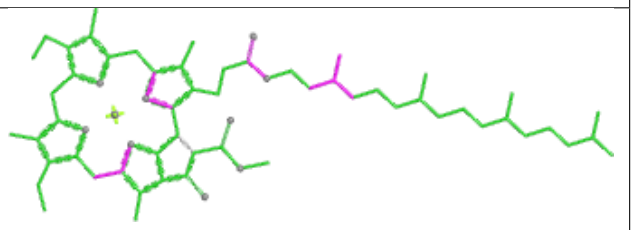


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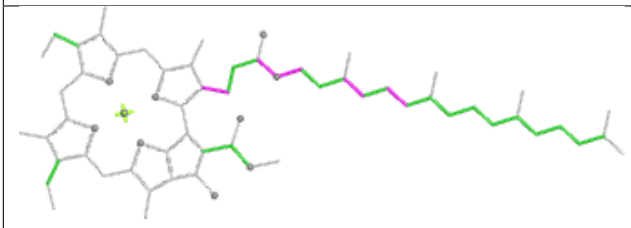
Ligand CLA B 806



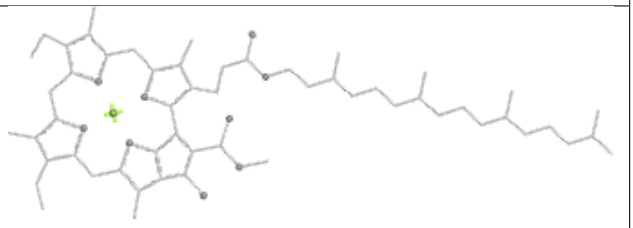
Bond lengths



Bond angles

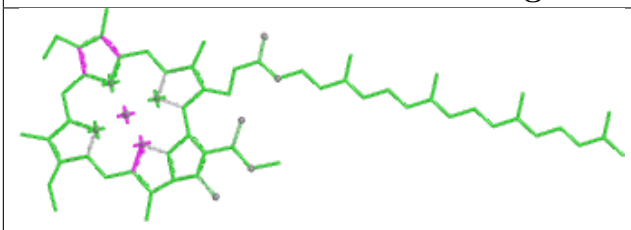


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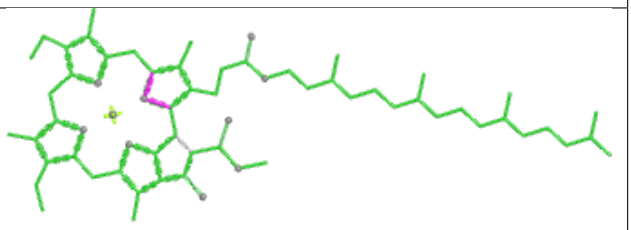


Rings

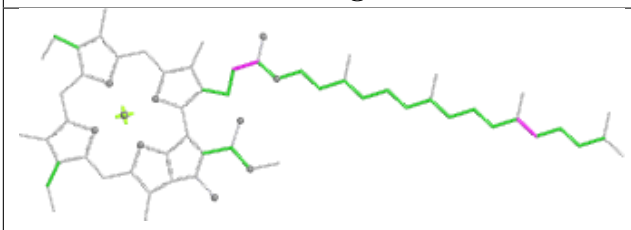
Ligand CLA B 811



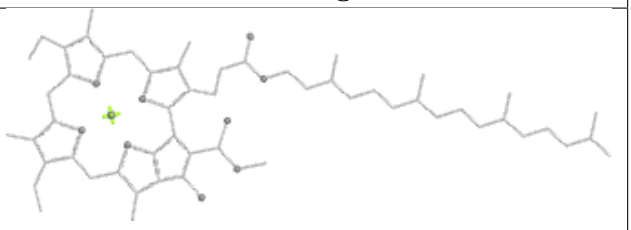
Bond lengths



Bond angles

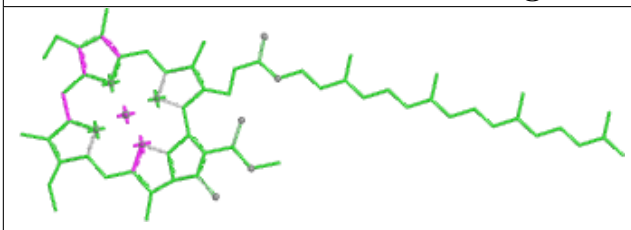


Torsions

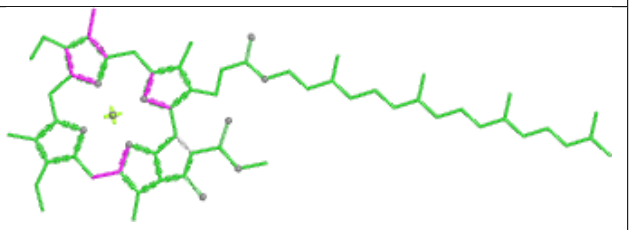


Rings

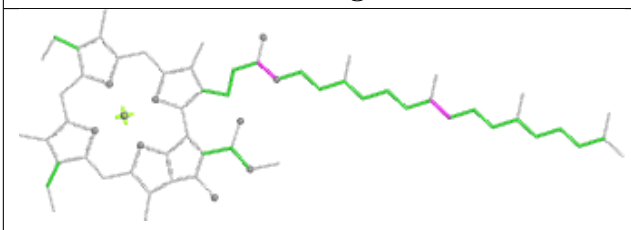
Ligand CLA A 836



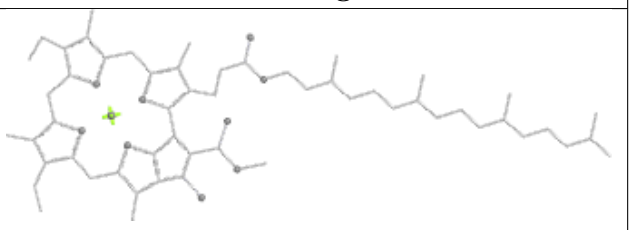
Bond lengths



Bond angles

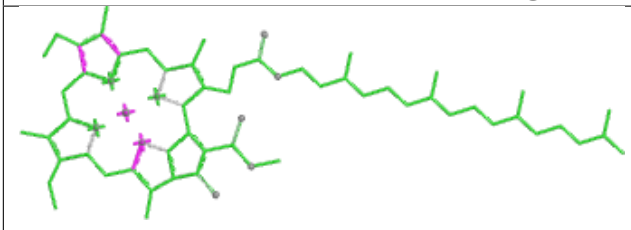


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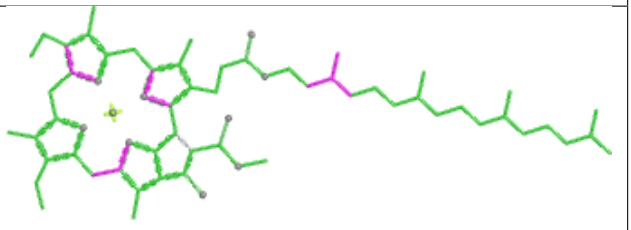


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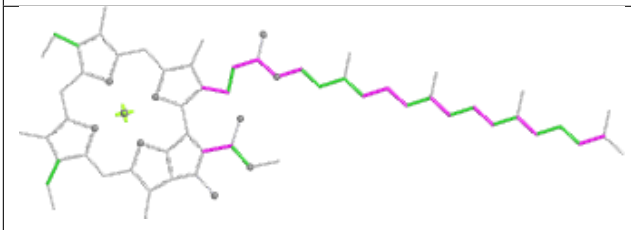
Ligand CLA B 825



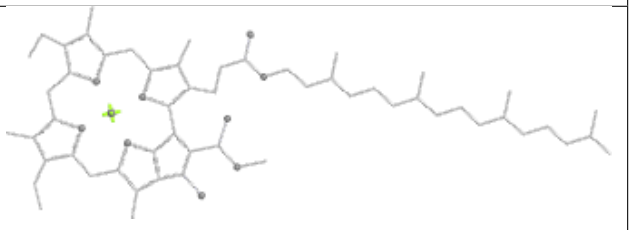
Bond lengths



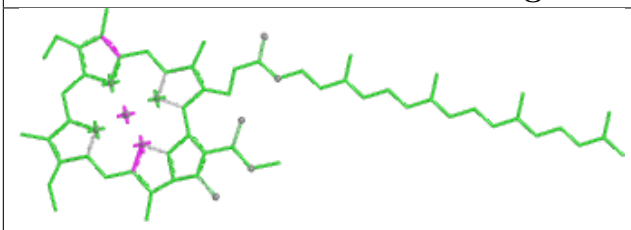
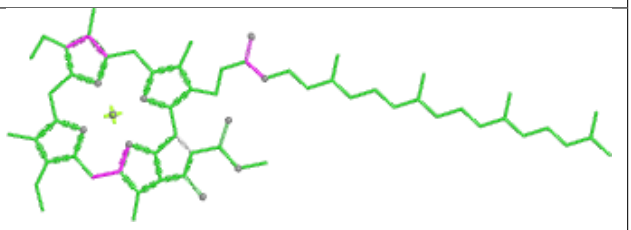
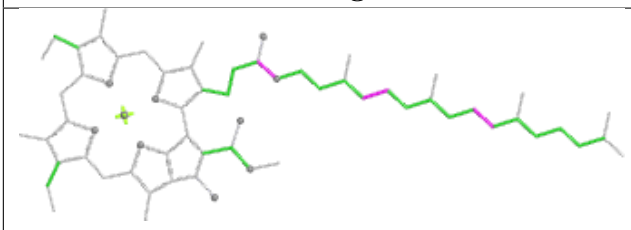
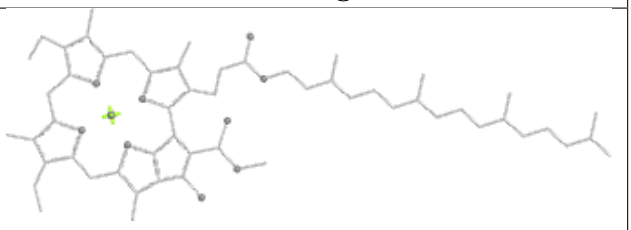
Bond angles

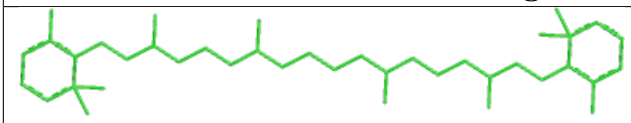
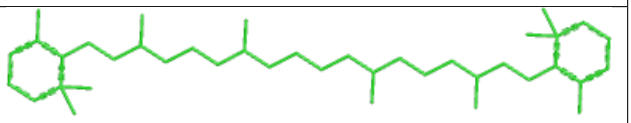
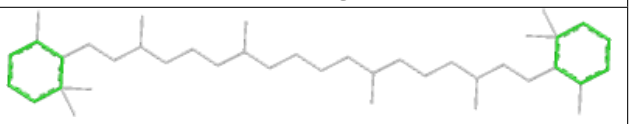


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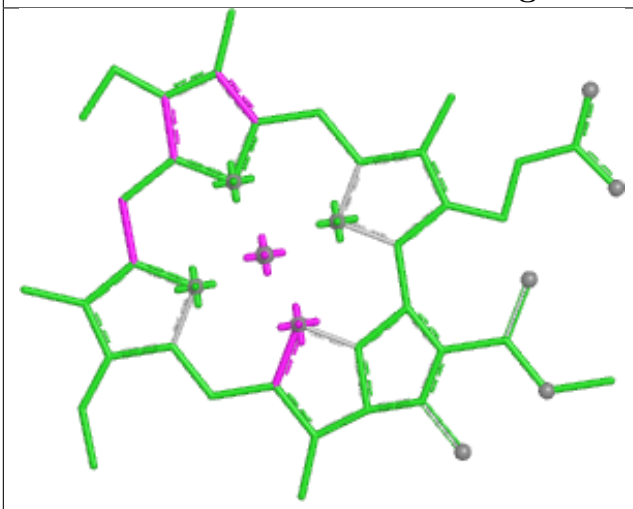


Rings

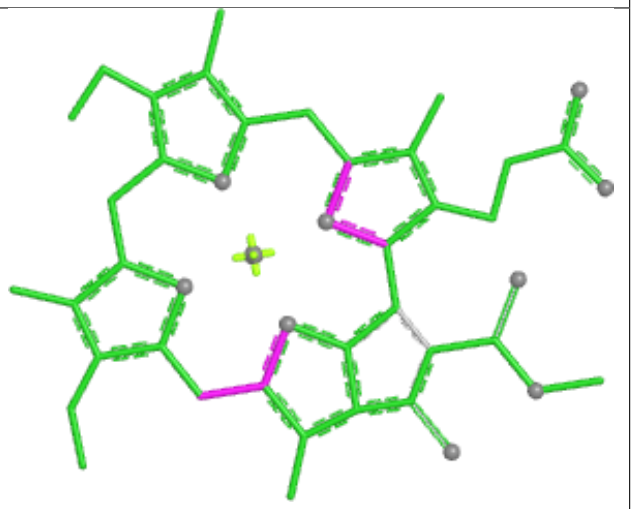
Ligand CLA B 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

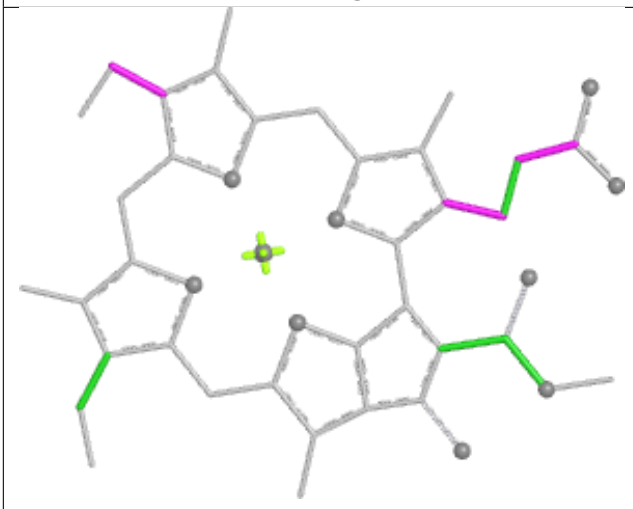
Ligand CLA J 1102



Bond lengths



Bond angles

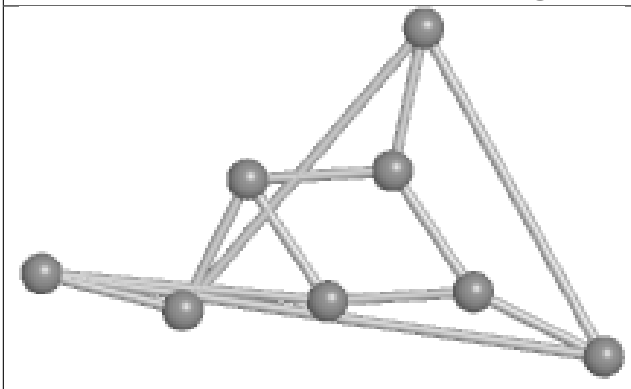


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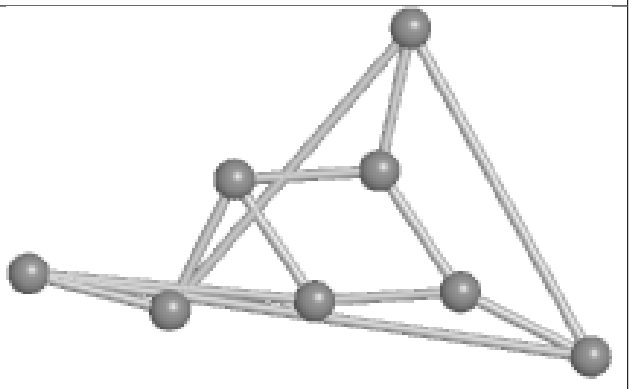


Rings

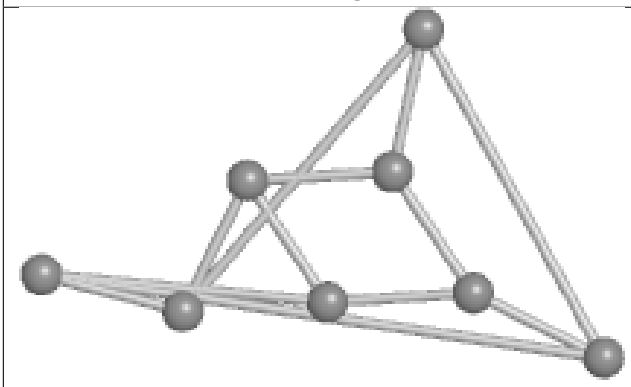
Ligand SF4 C 101



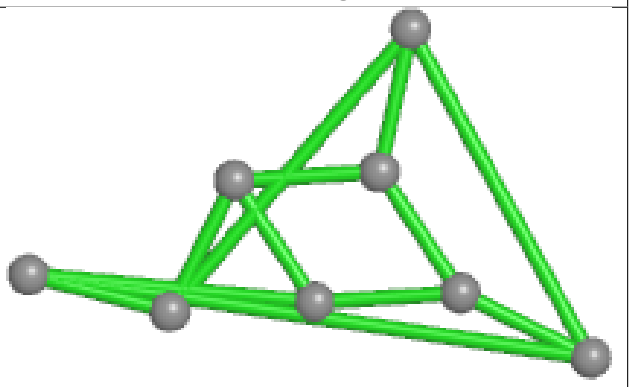
Bond lengths



Bond angles

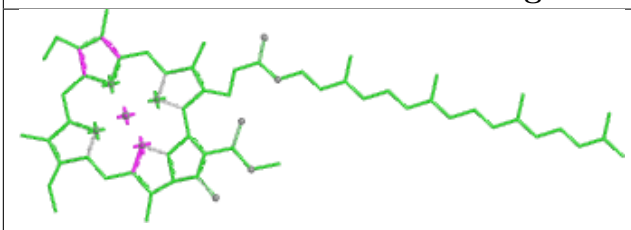


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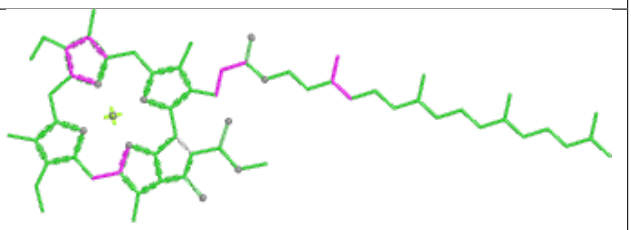


Rings

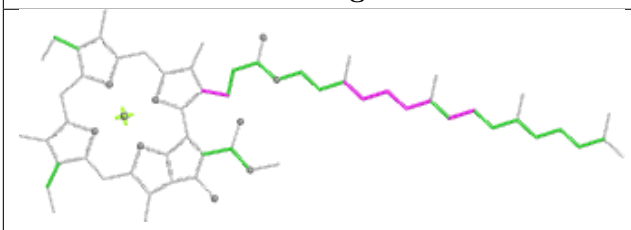
Ligand CLA B 819



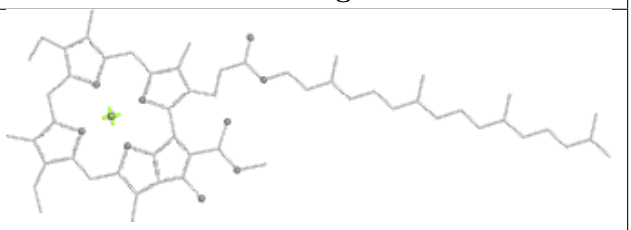
Bond lengths



Bond angles

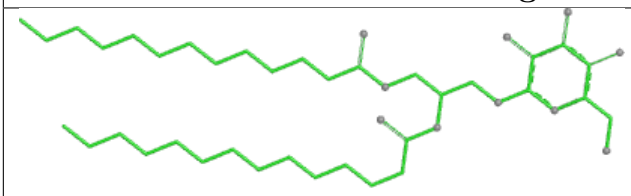


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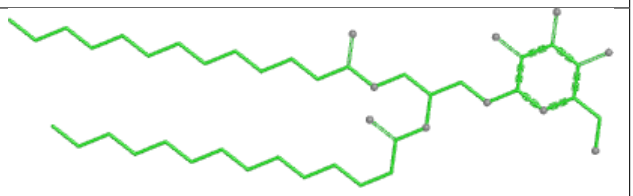


Rings

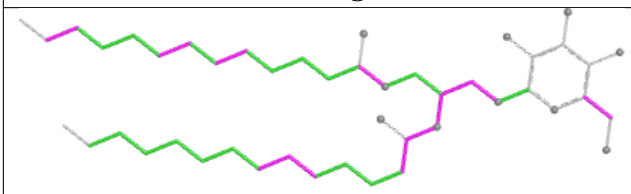
Ligand LMG A 853



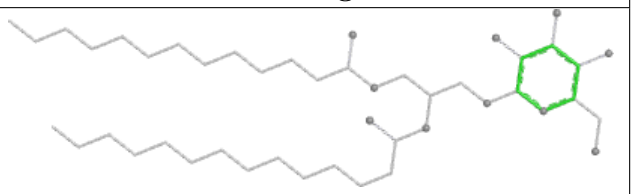
Bond lengths



Bond angles

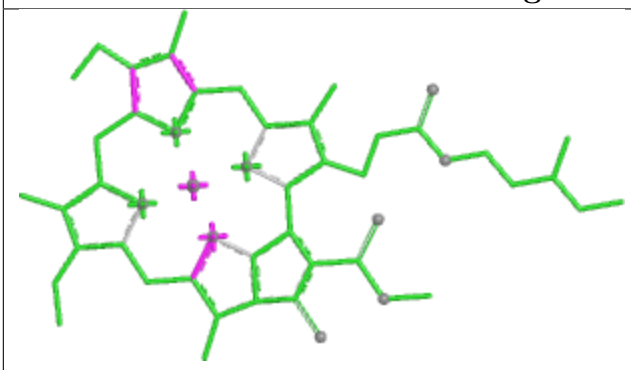


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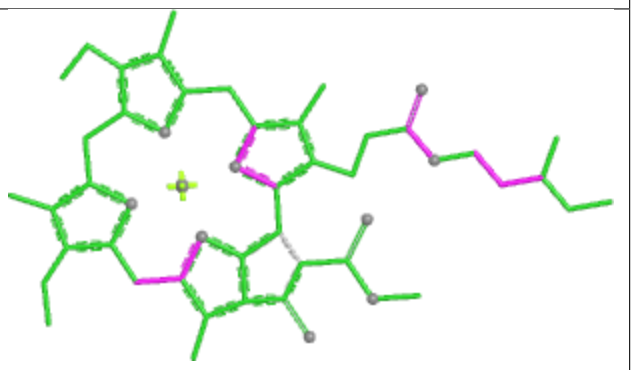


Rings

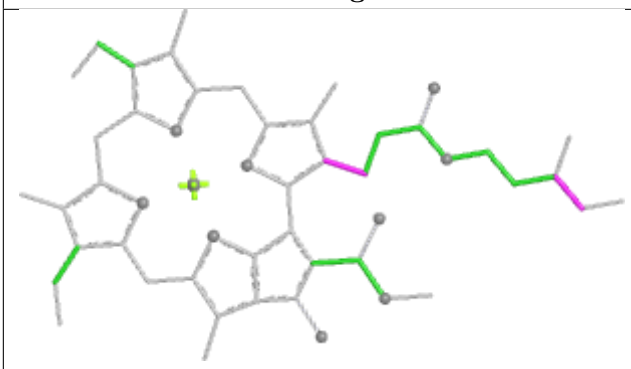
Ligand CLA A 824



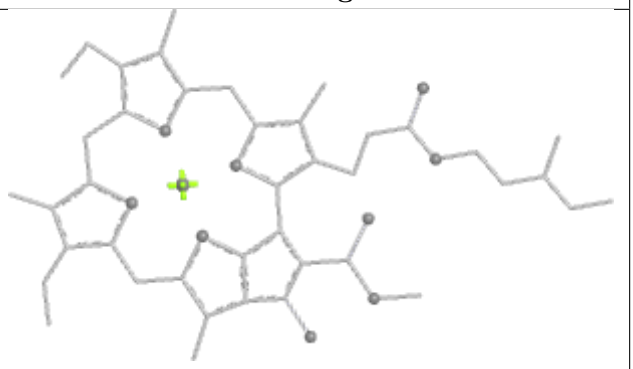
Bond lengths



Bond angles

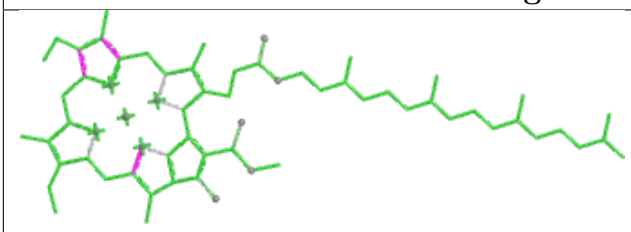


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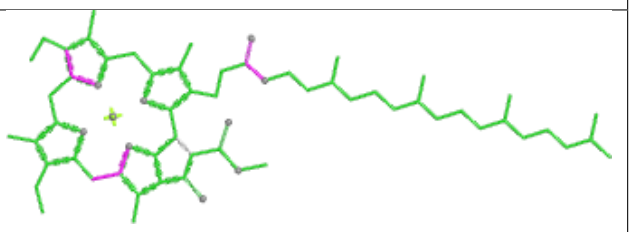


Rings

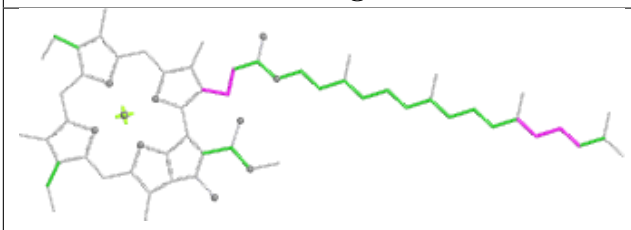
Ligand CLA A 804



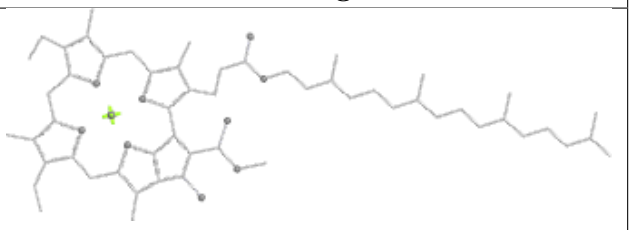
Bond lengths



Bond angles

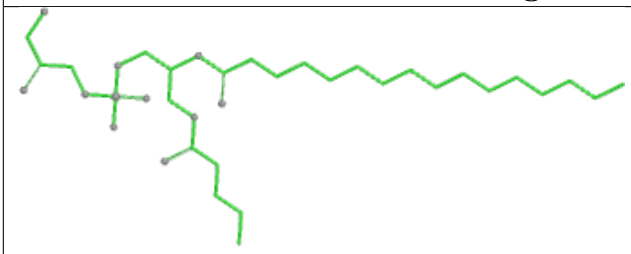


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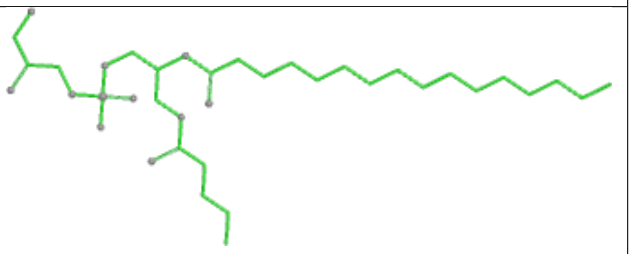


Rings

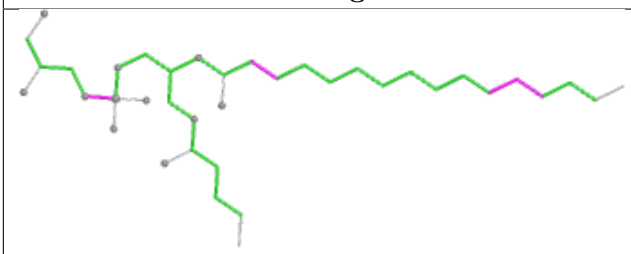
Ligand LHG B 850



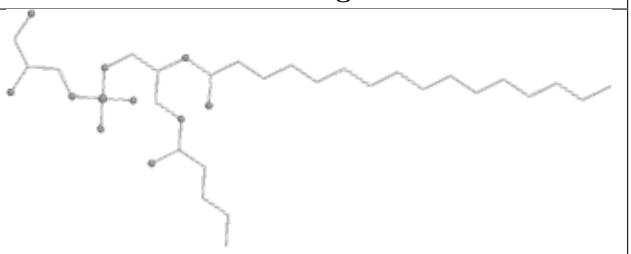
Bond lengths



Bond angles

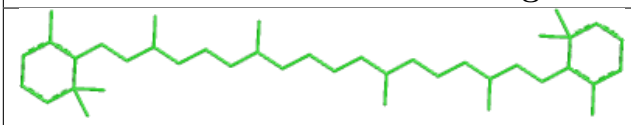


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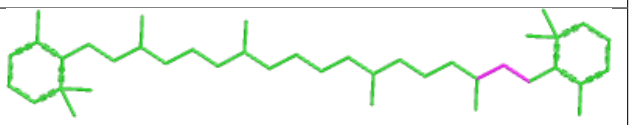


Rings

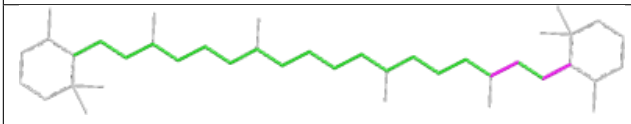
Ligand BCR A 851



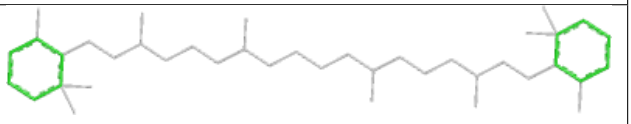
Bond lengths



Bond angles

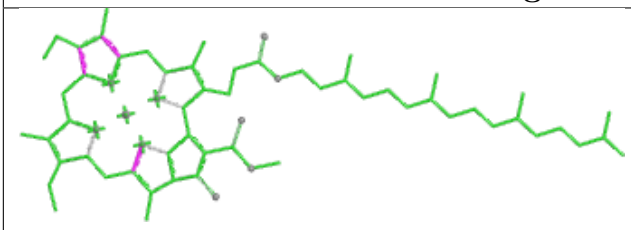


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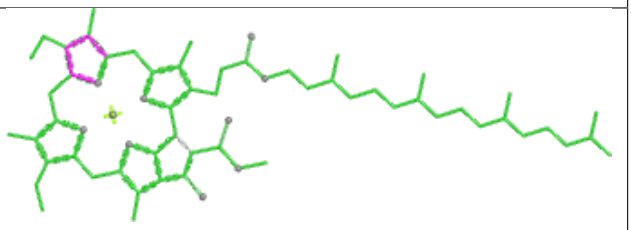


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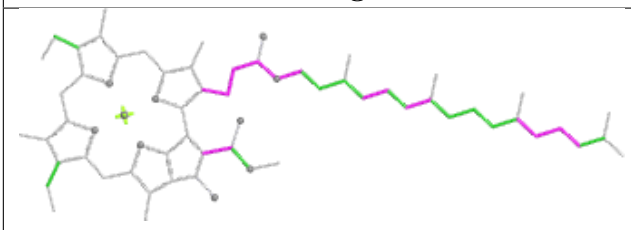
Ligand CLA A 812



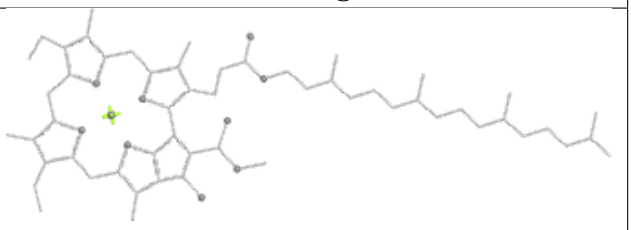
Bond lengths



Bond angles

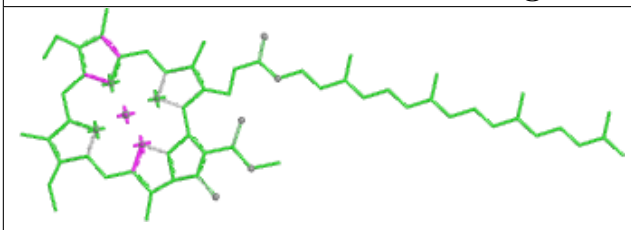


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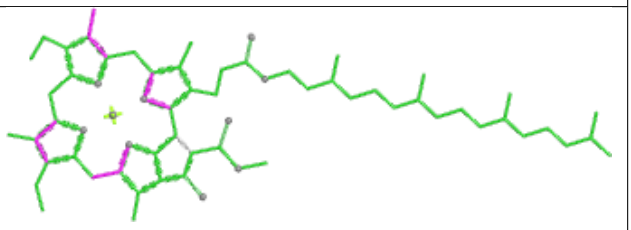


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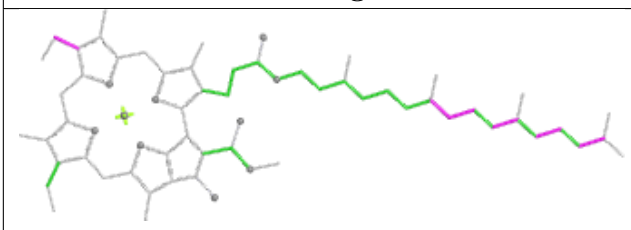
Ligand CLA A 839



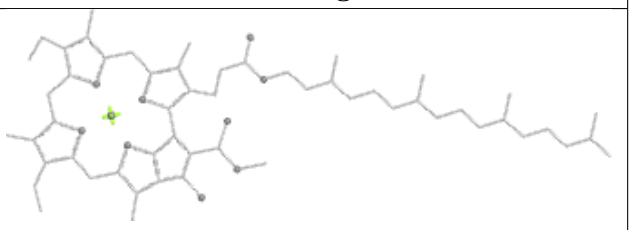
Bond lengths



Bond angles

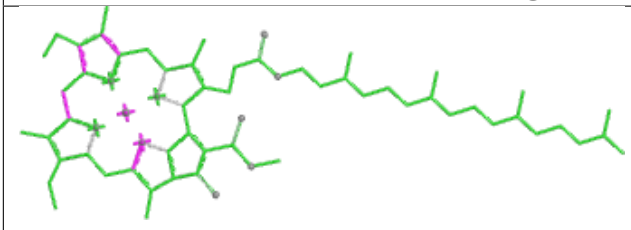


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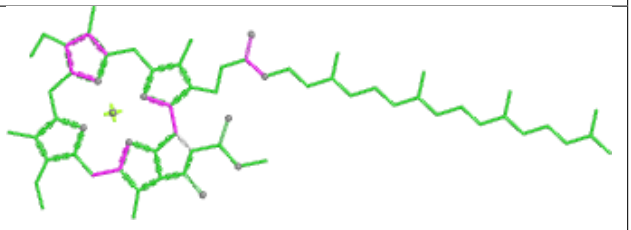


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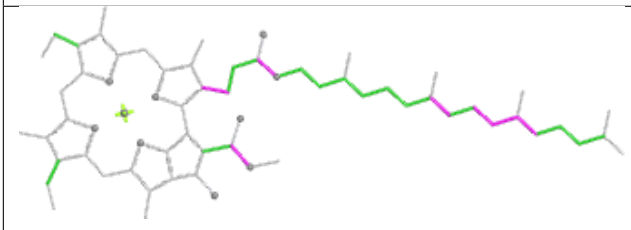
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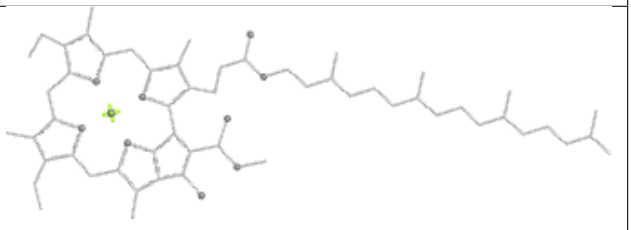
Bond lengths



Bond angles

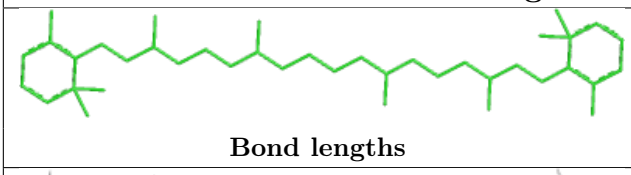


Torsions

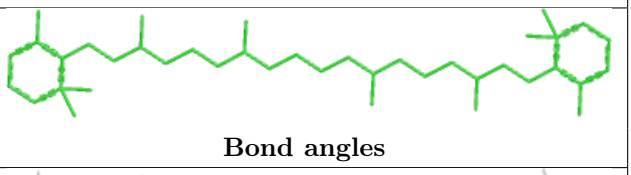


Rings

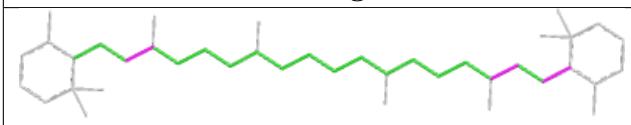
Ligand BCR L 205



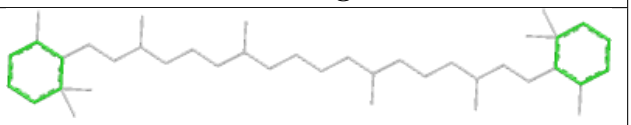
Bond lengths



Bond angles

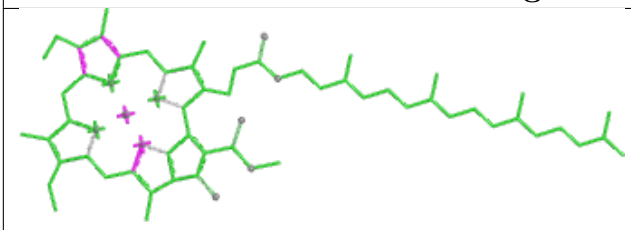


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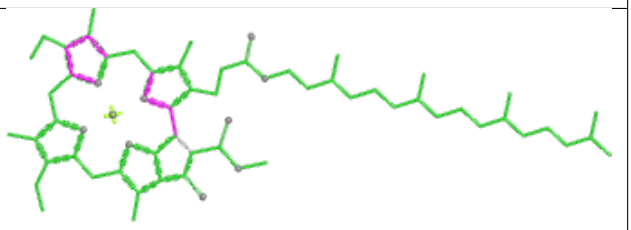


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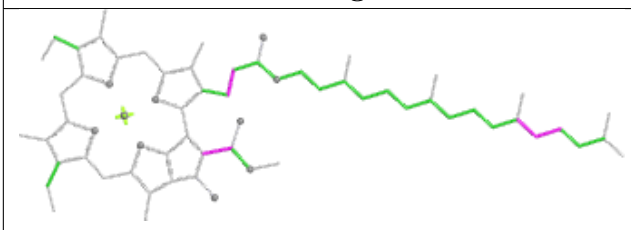
Ligand CLA A 809



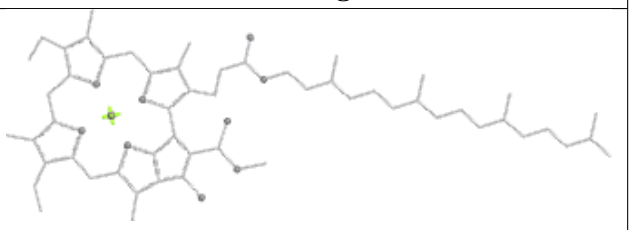
Bond lengths



Bond angles

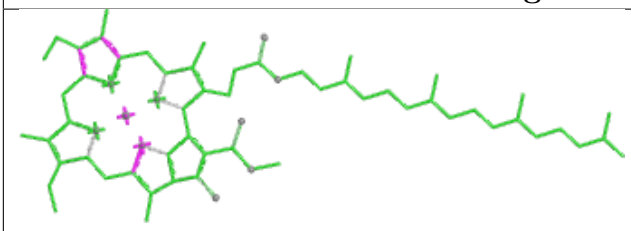


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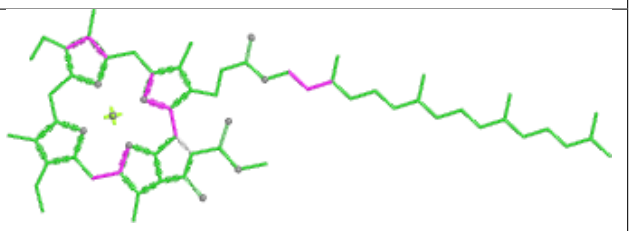


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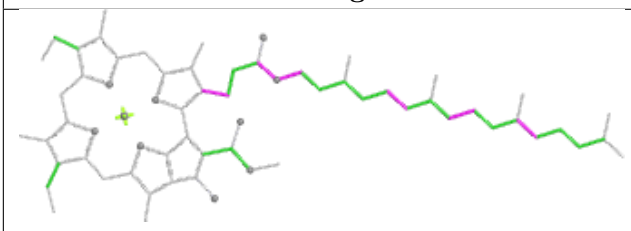
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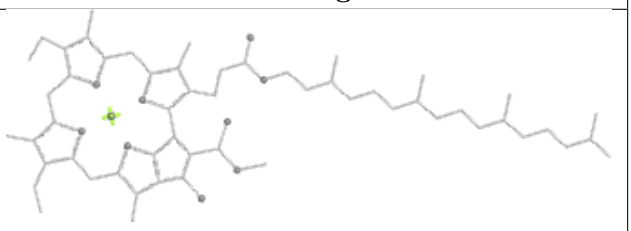
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Bond angles

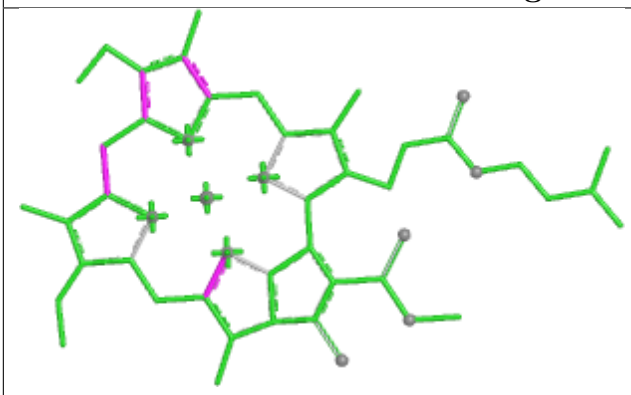


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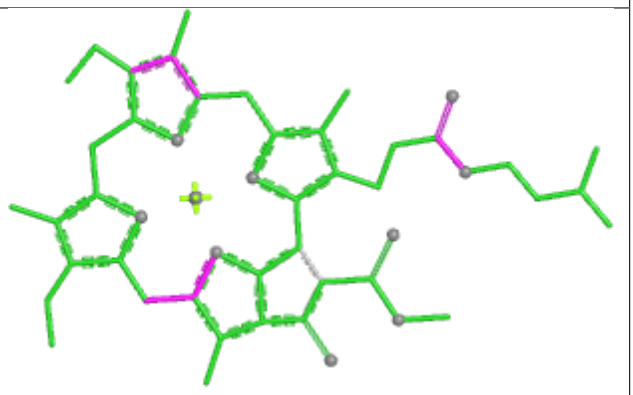


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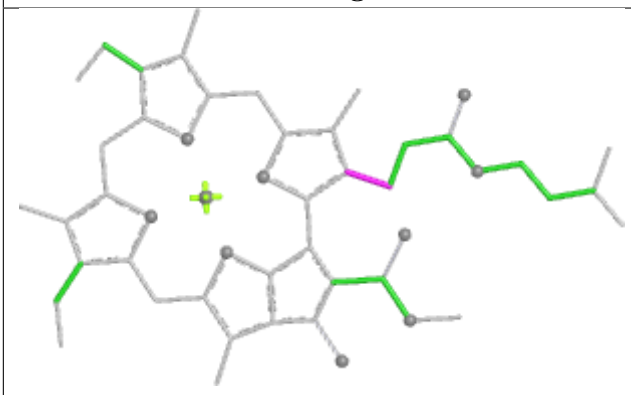
Ligand CLA B 837



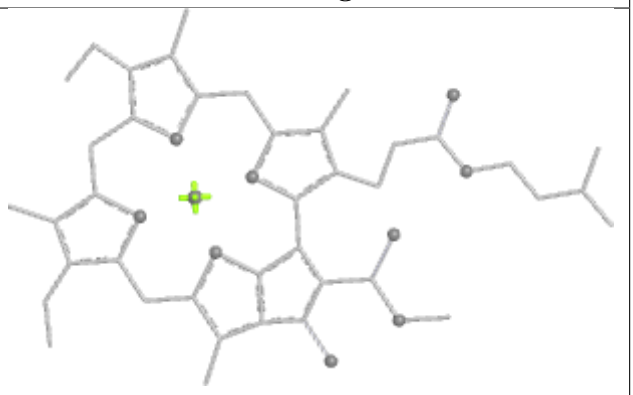
Bond lengths



Bond angles

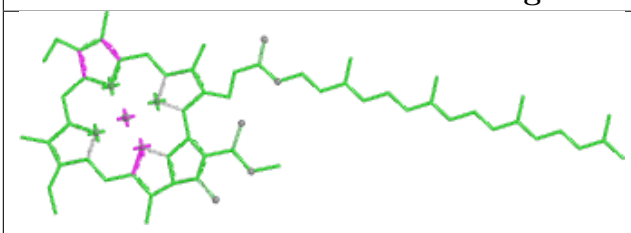


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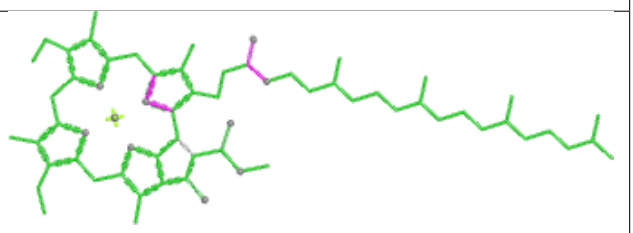


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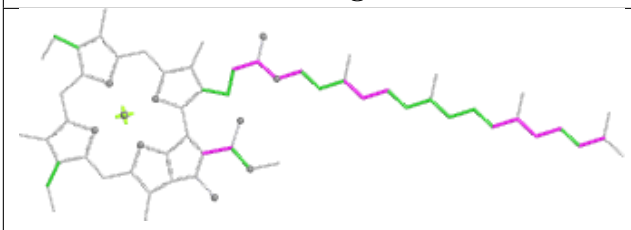
Ligand CLA A 826



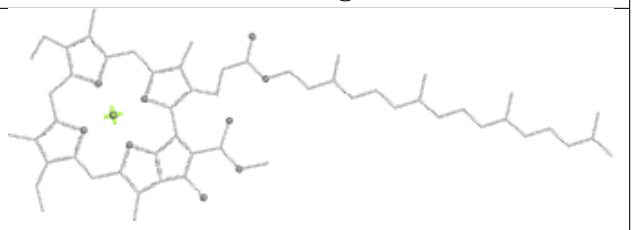
Bond lengths



Bond angles

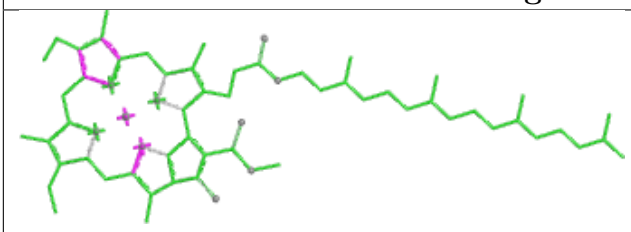


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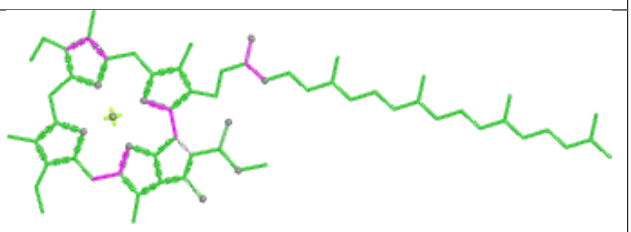


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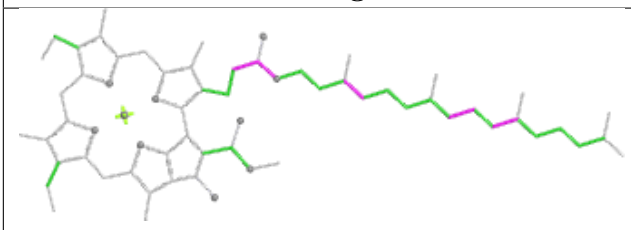
Ligand CLA B 833



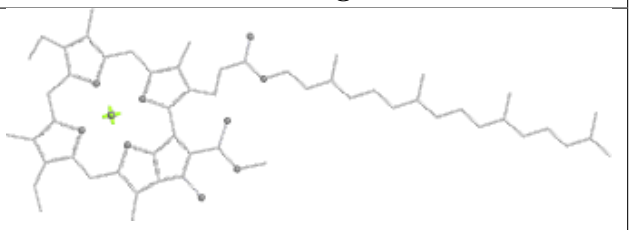
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Bond angles

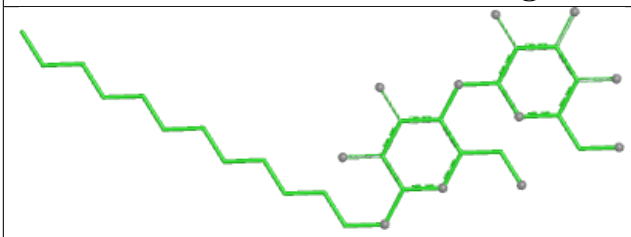


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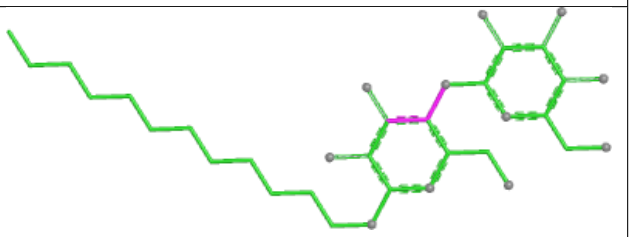


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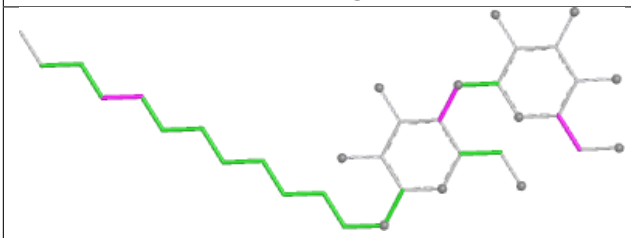
Ligand LMT A 857



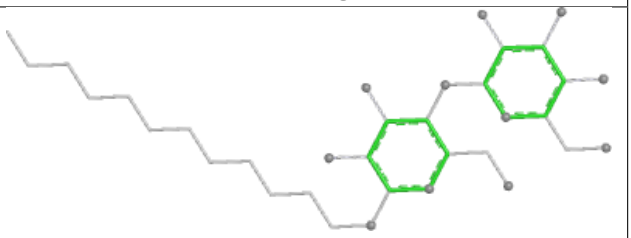
Bond lengths



Bond angles

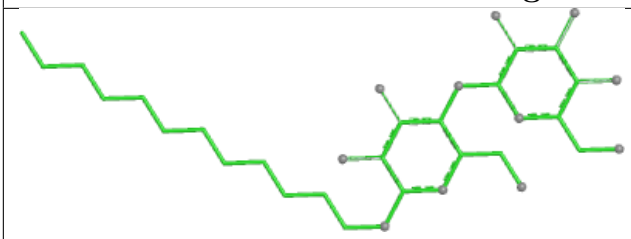


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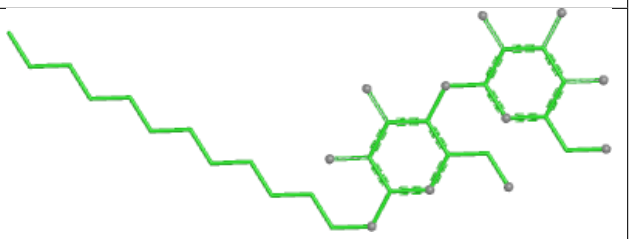


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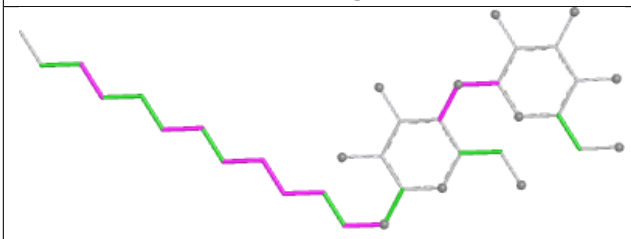
Ligand LMT F 207



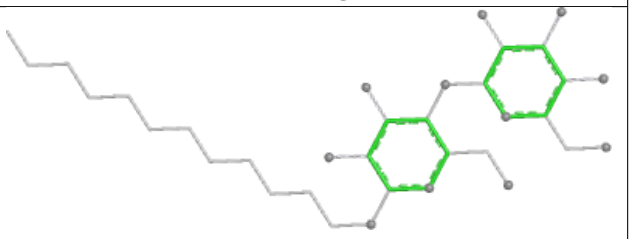
Bond lengths



Bond angles

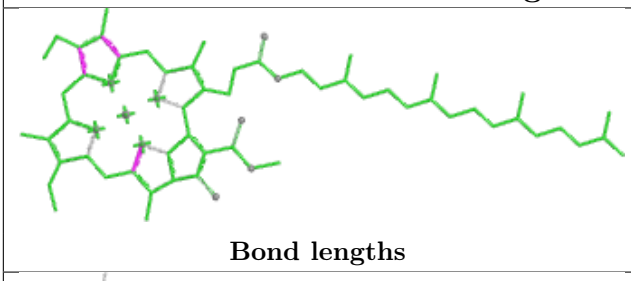


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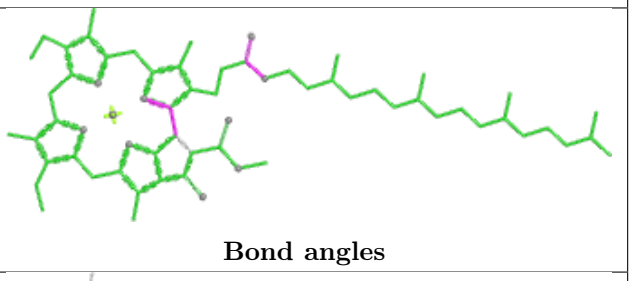


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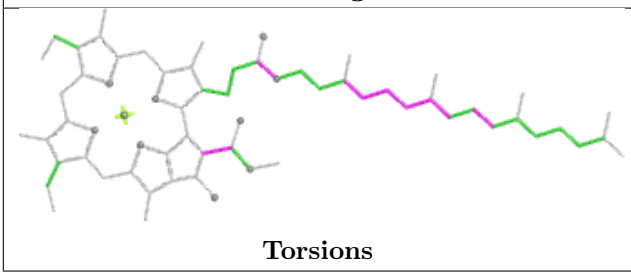
Ligand CLA A 831



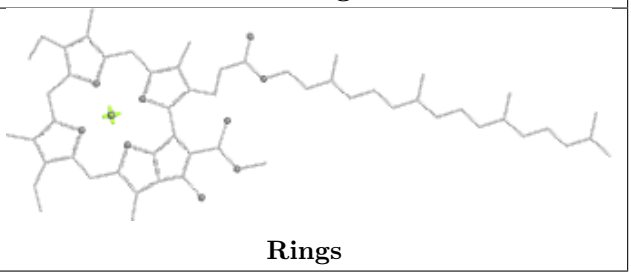
Bond lengths



Bond angles

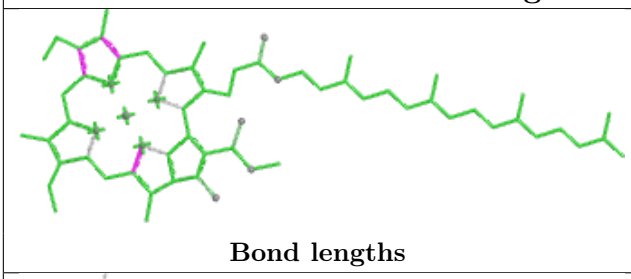


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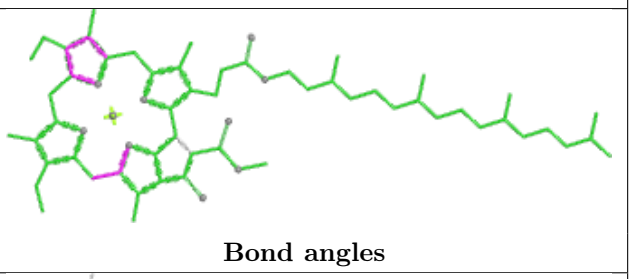


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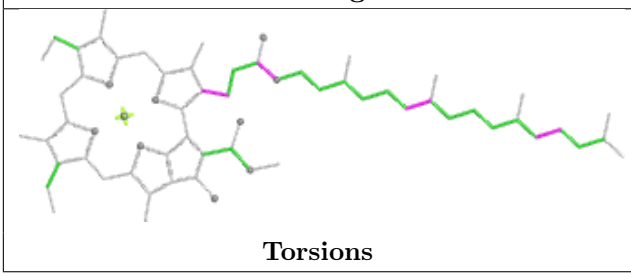
Ligand CLA A 842



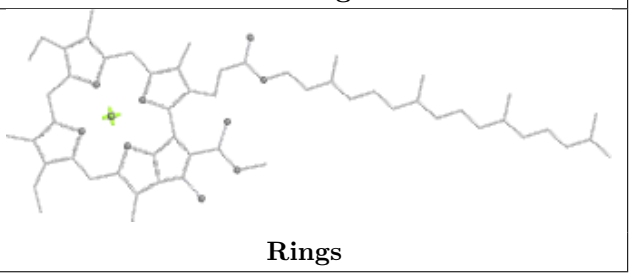
Bond lengths



Bond angles

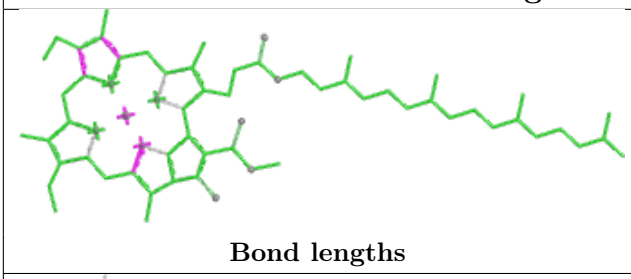


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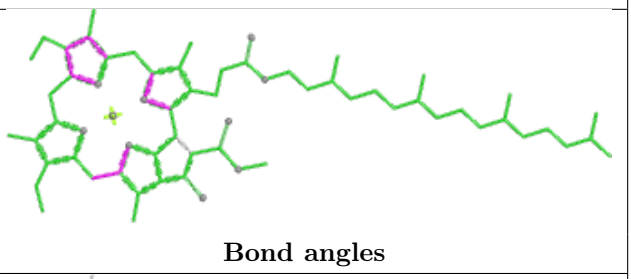


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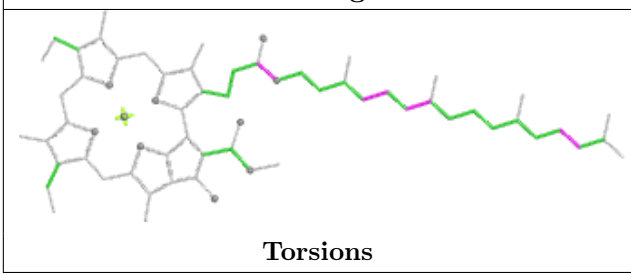
Ligand CLA B 831



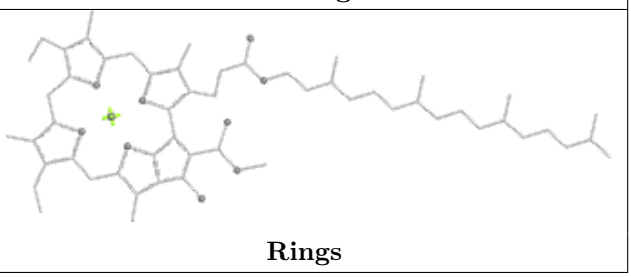
Bond lengths



Bond angles

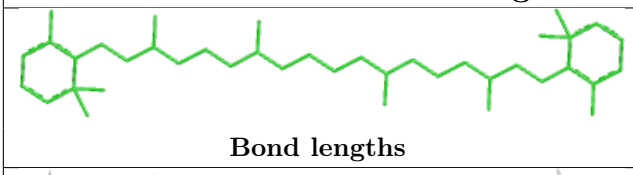


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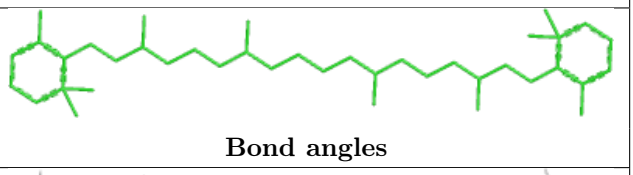


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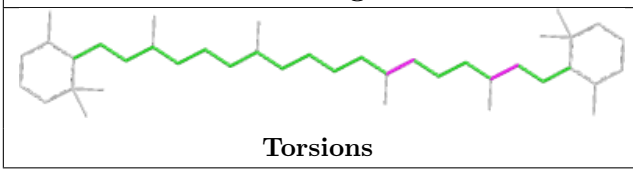
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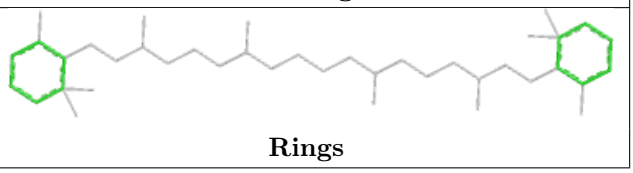
Bond lengths



Bond angles

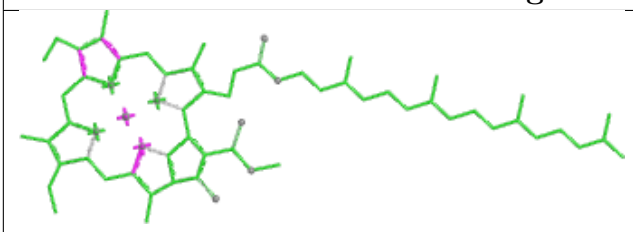


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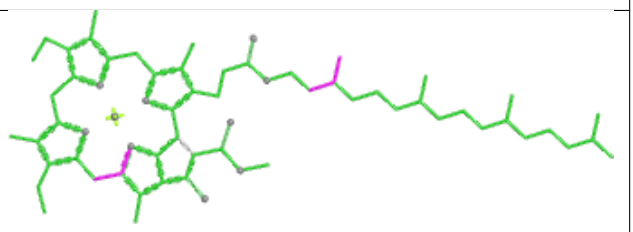


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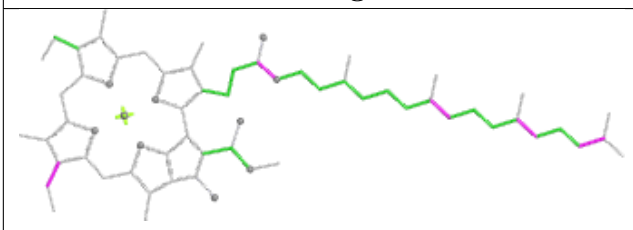
Ligand CLA L 203



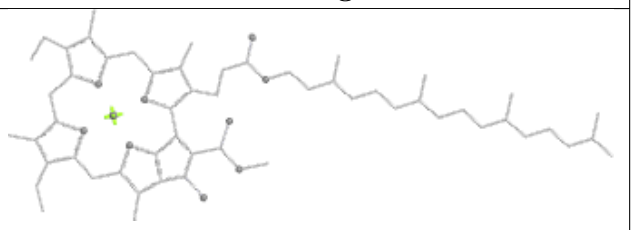
Bond lengths



Bond angles

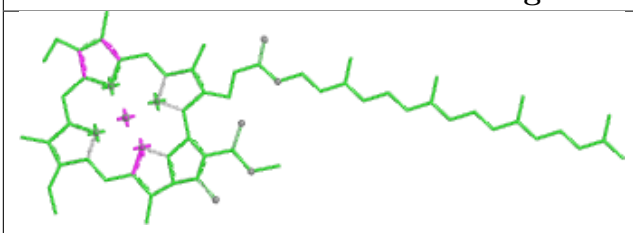


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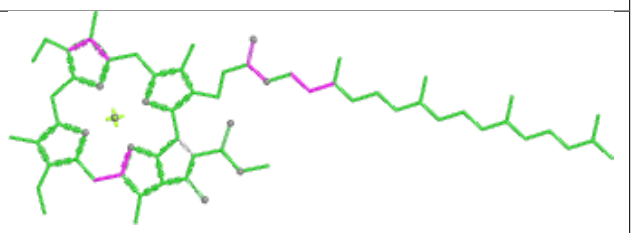


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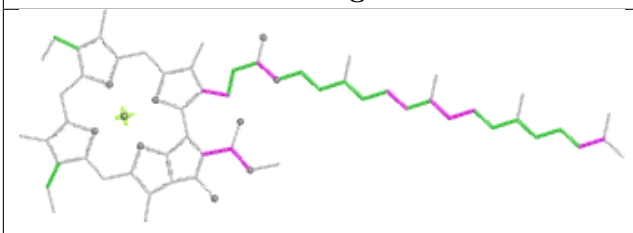
Ligand CLA A 823



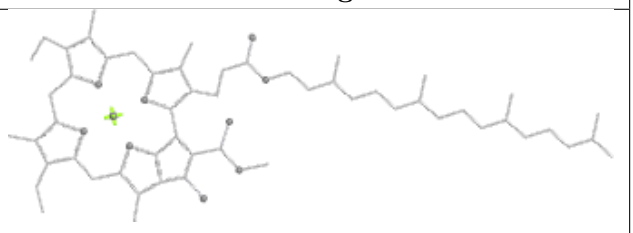
Bond lengths



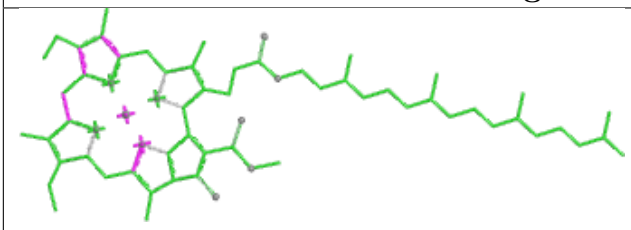
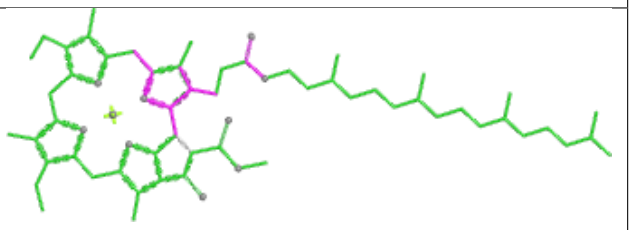
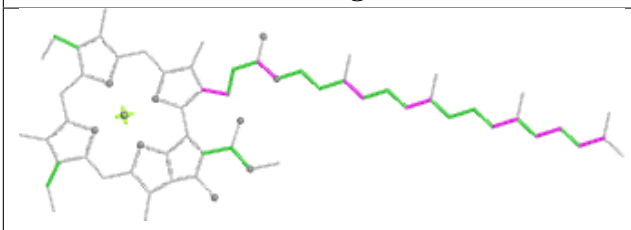
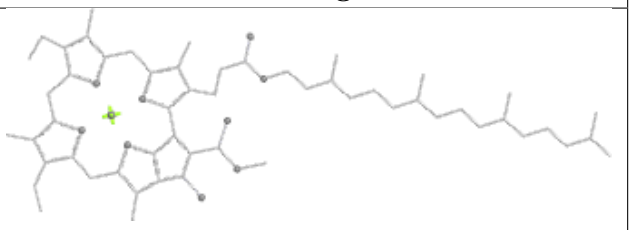
Bond angles

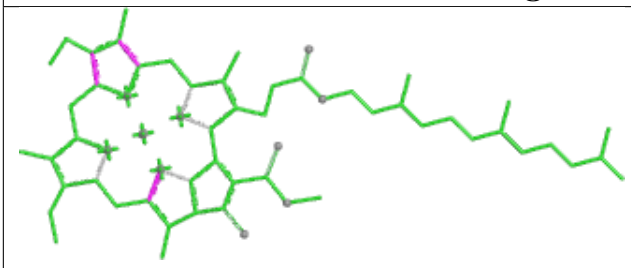
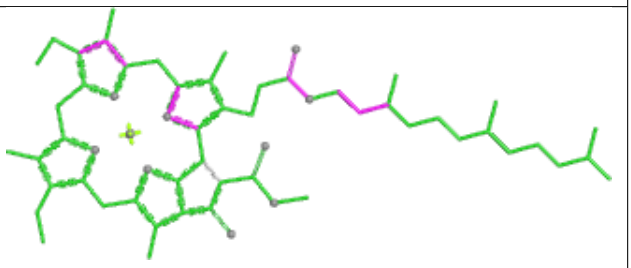
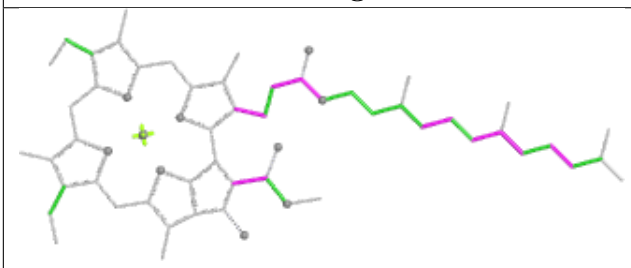
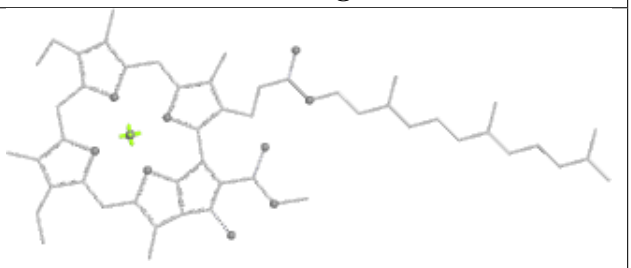


Torsions

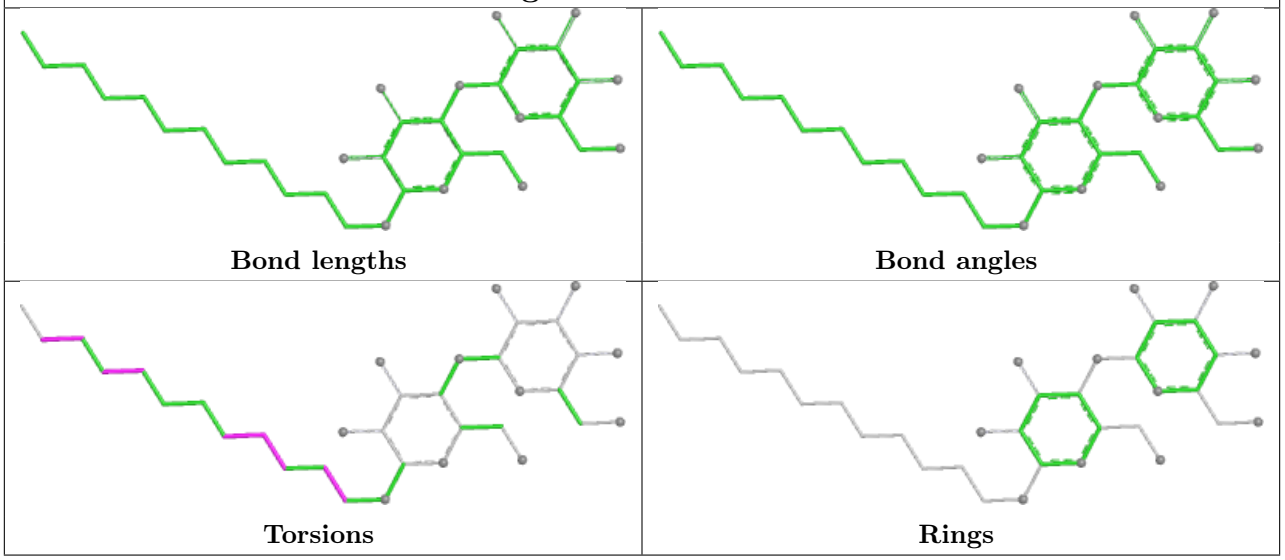


Rings

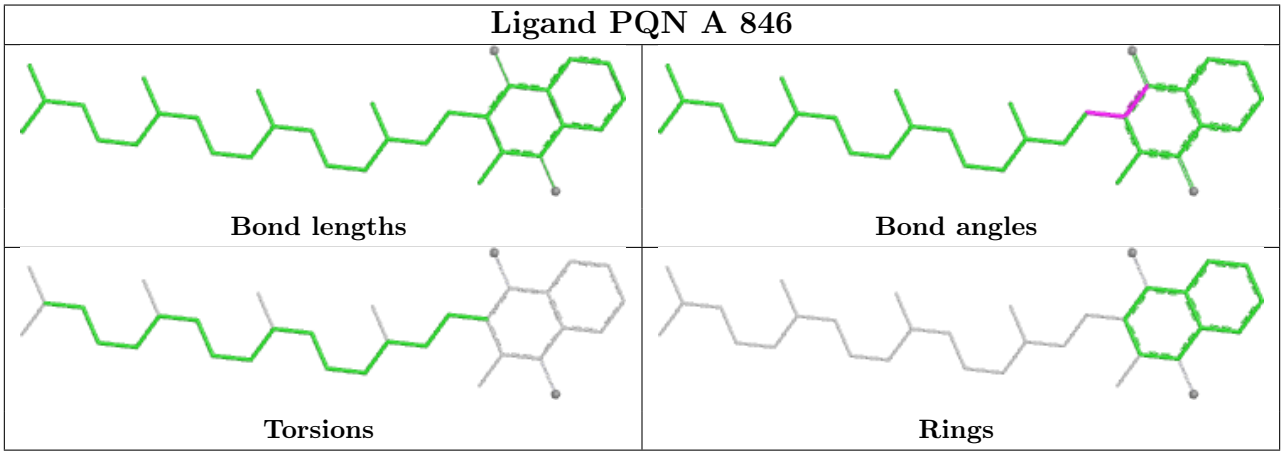
Ligand CLA A 829	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMT A 856



Ligand PQN A 846



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

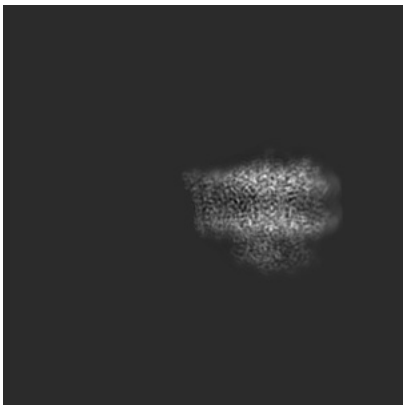
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71005. These allow visual inspection of the internal detail of the map and identification of artifacts.

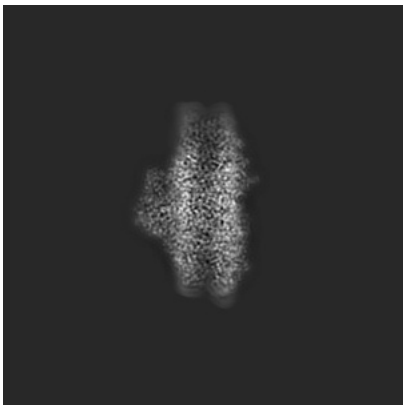
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

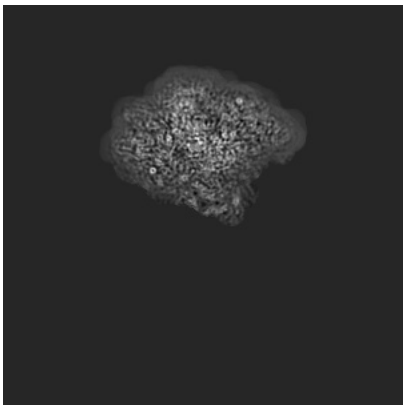
6.1.1 Primary map



X

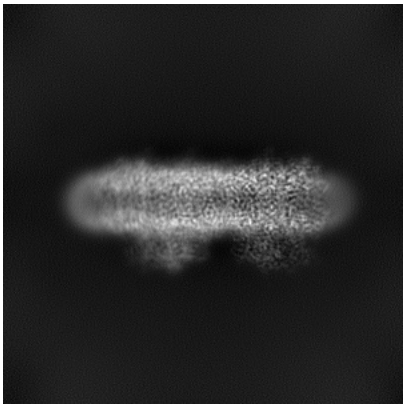


Y

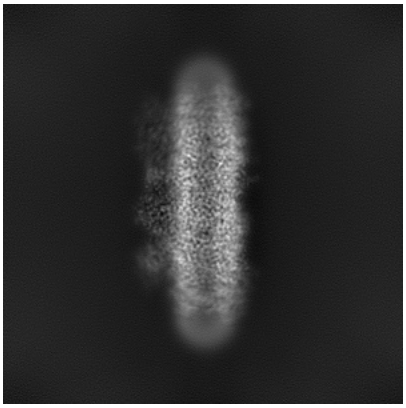


Z

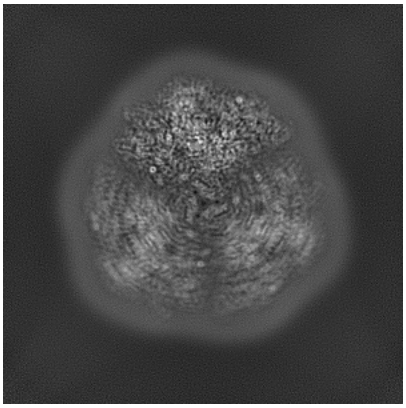
6.1.2 Raw map



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: 220

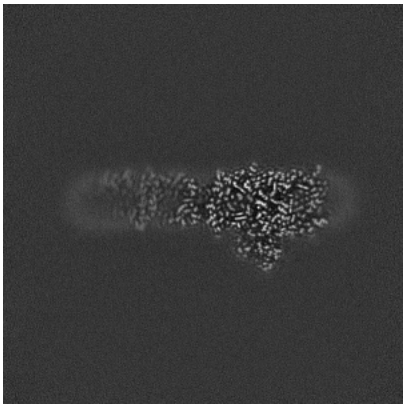


Y Index: 220

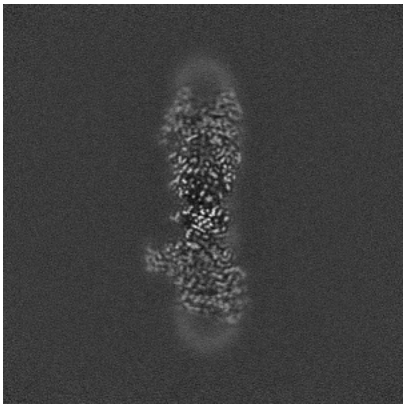


Z Index: 220

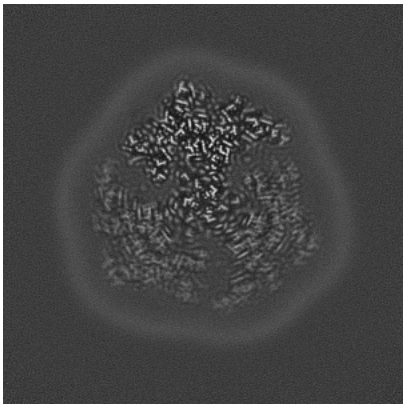
6.2.2 Raw map



X Index: 220



Y Index: 220



Z Index: 220

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

6.3 Largest variance slices (i)

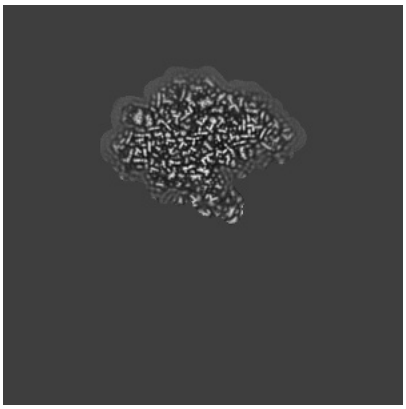
6.3.1 Primary map



X Index: 213

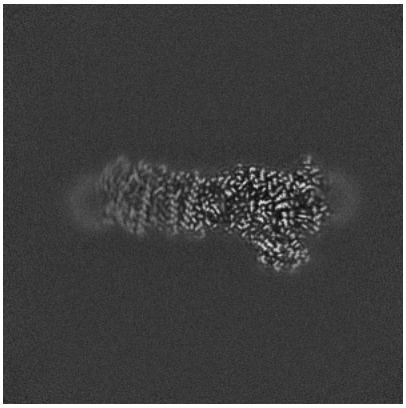


Y Index: 293

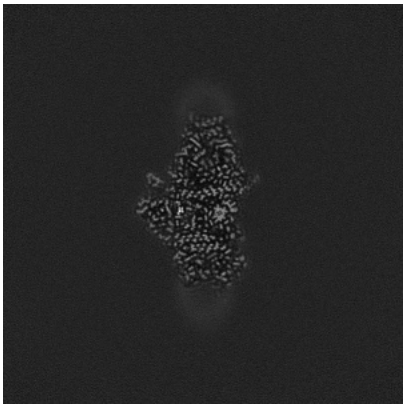


Z Index: 238

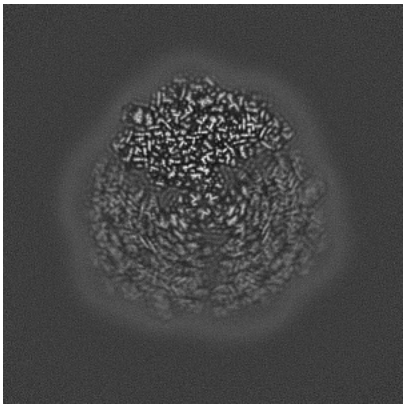
6.3.2 Raw map



X Index: 204



Y Index: 293

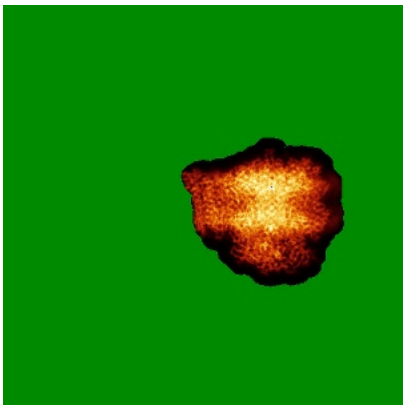


Z Index: 238

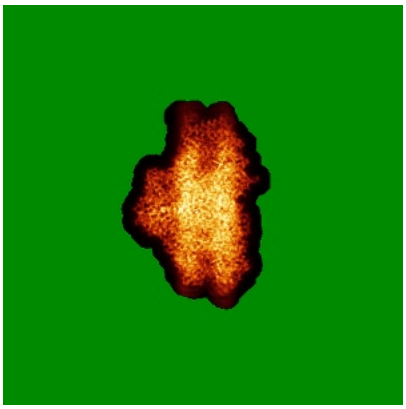
The images above show the largest variance slices of the map in three orthogonal directions.

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

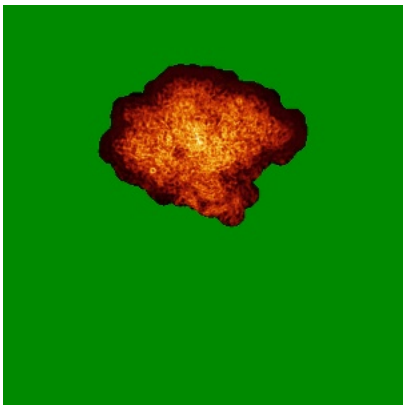
6.4.1 Primary map



X

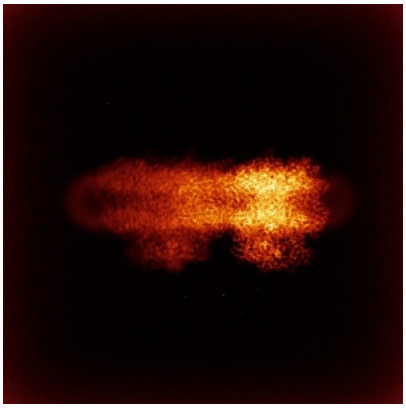


Y

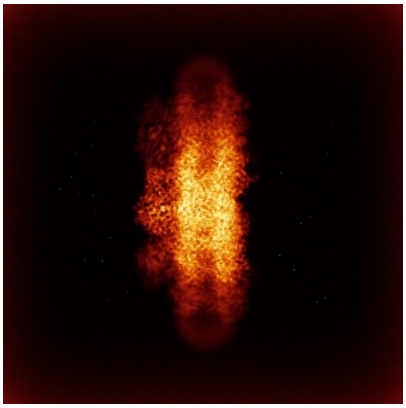


Z

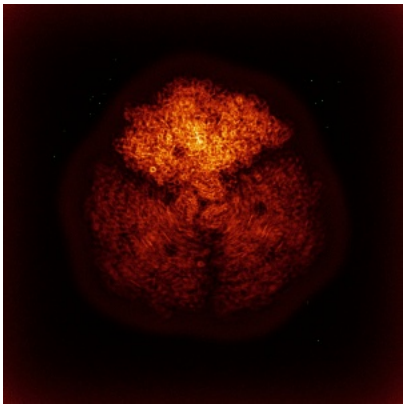
6.4.2 Raw map



X



Y

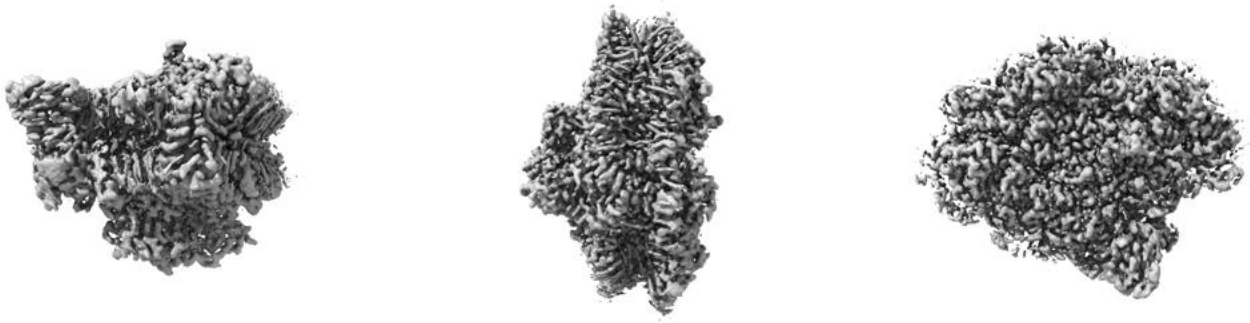


Z

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 4.4. 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.

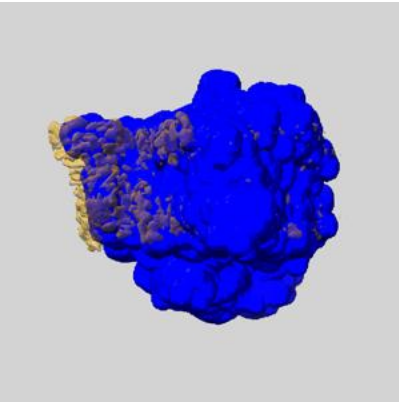
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

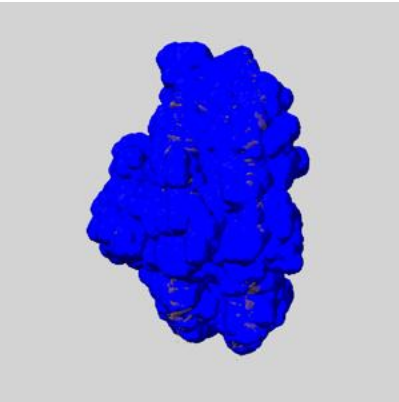
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

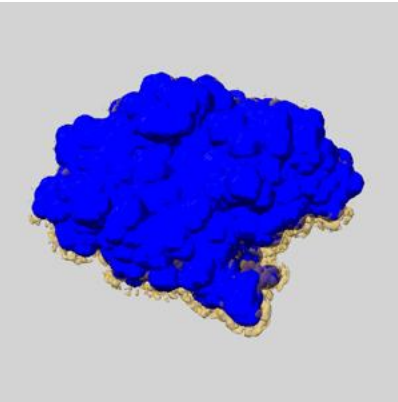
6.6.1 emd_71005_msk_1.map



X



Y

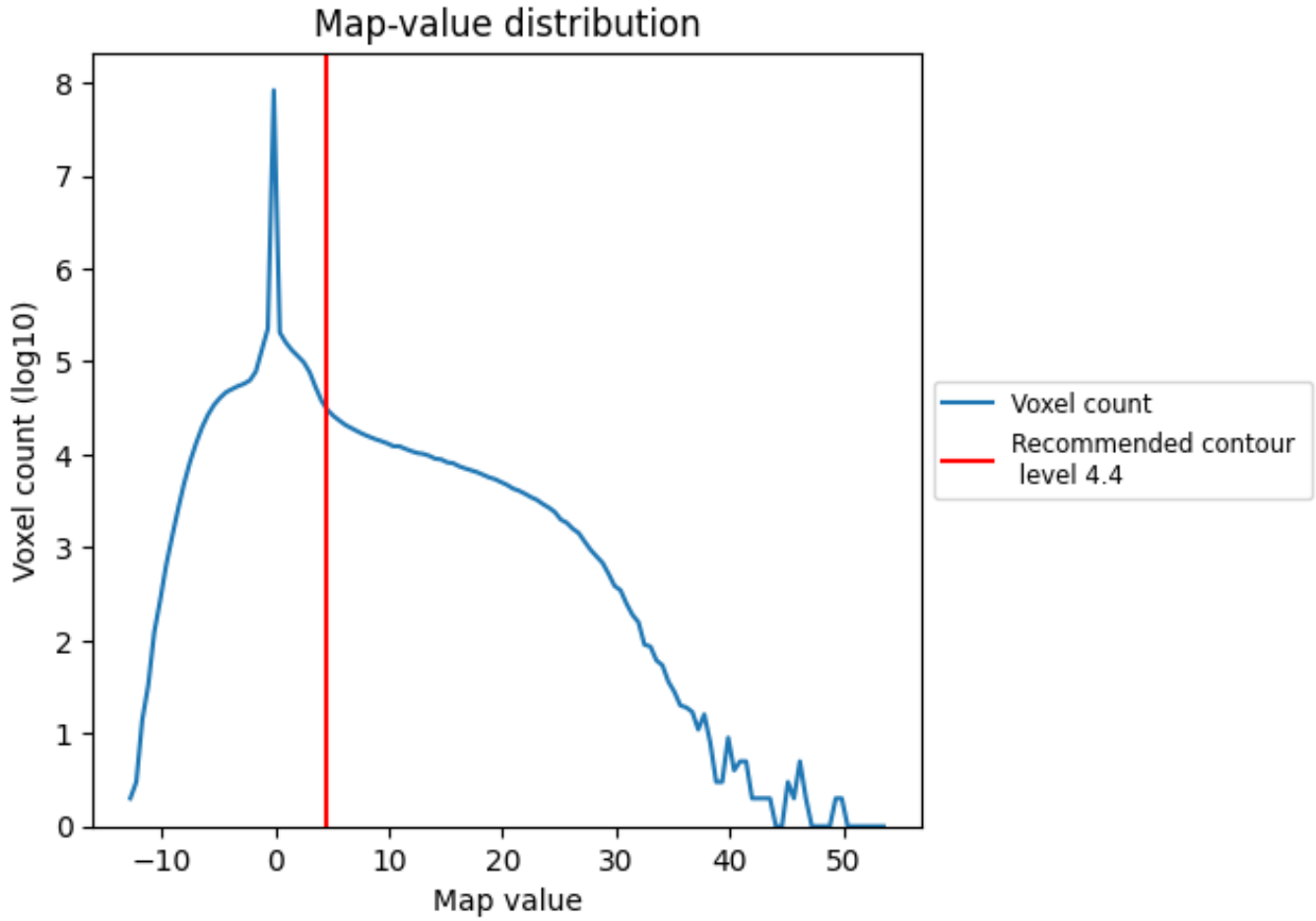


Z

7 Map analysis

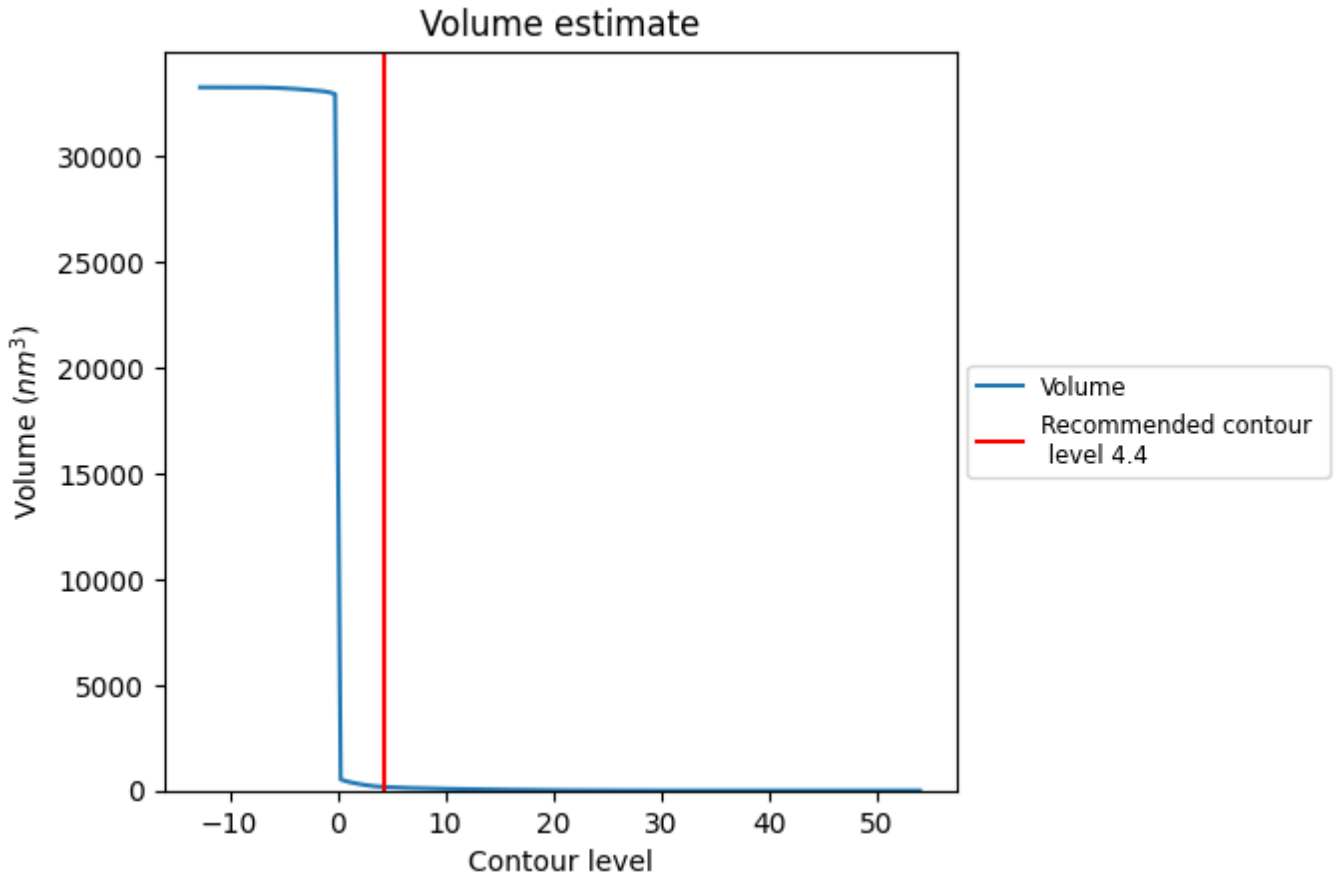
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

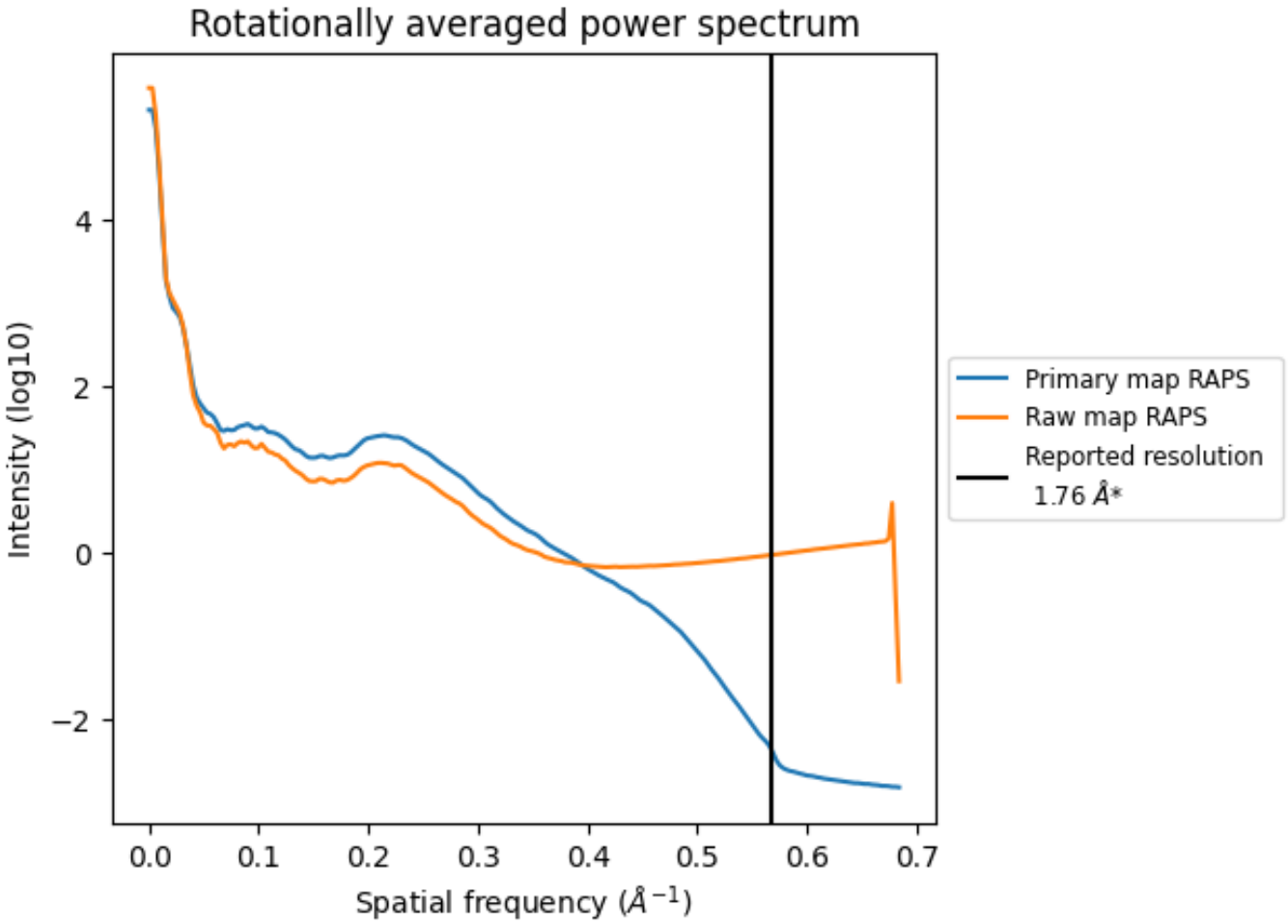
7.2 Volume estimate



The volume at the recommended contour level is 168 nm^3; this corresponds to an approximate mass of 152 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)

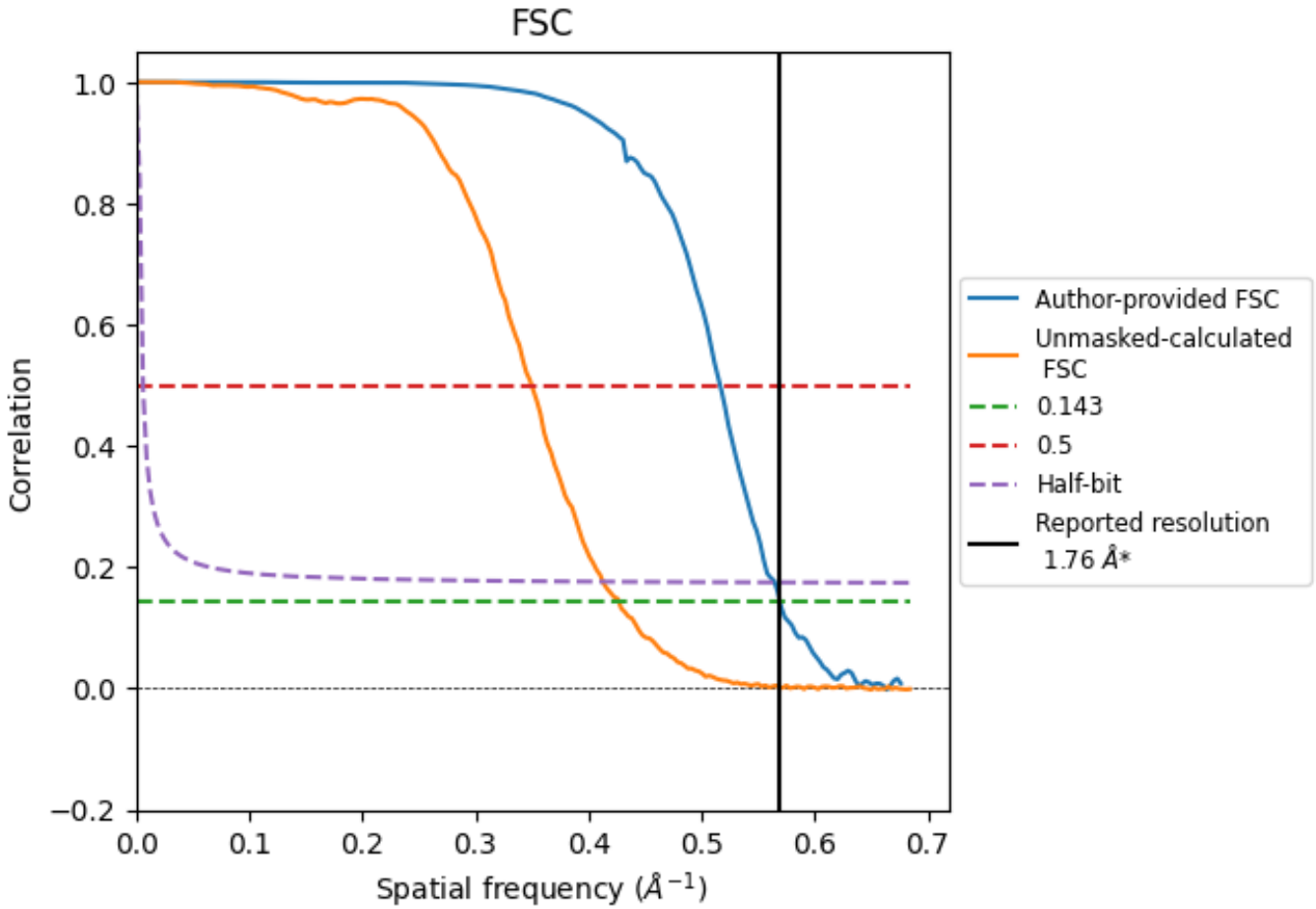


*Reported resolution corresponds to spatial frequency of 0.568 Å^{-1}

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 0.568 Å^{-1}

8.2 Resolution estimates (i)

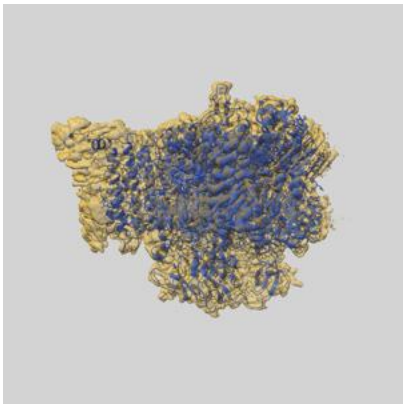
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.76	-	-
Author-provided FSC curve	1.76	1.94	1.77
Unmasked-calculated*	2.34	2.86	2.42

*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 2.34 differs from the reported value 1.76 by more than 10 %

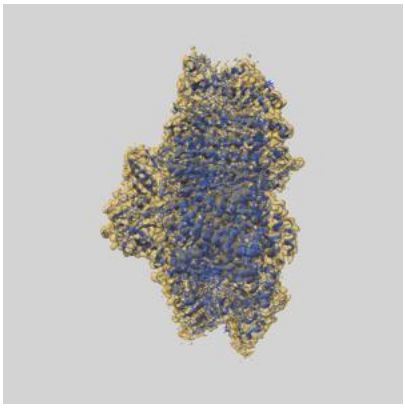
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71005 and PDB model 9OY9. Per-residue inclusion information can be found in section 3 on page 19.

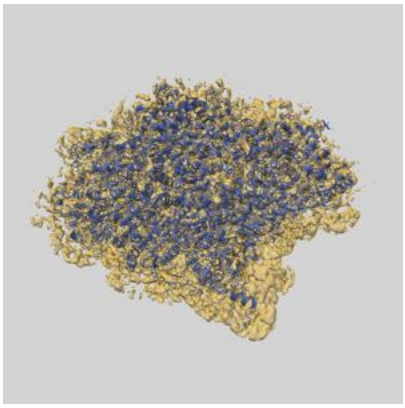
9.1 Map-model overlay



X



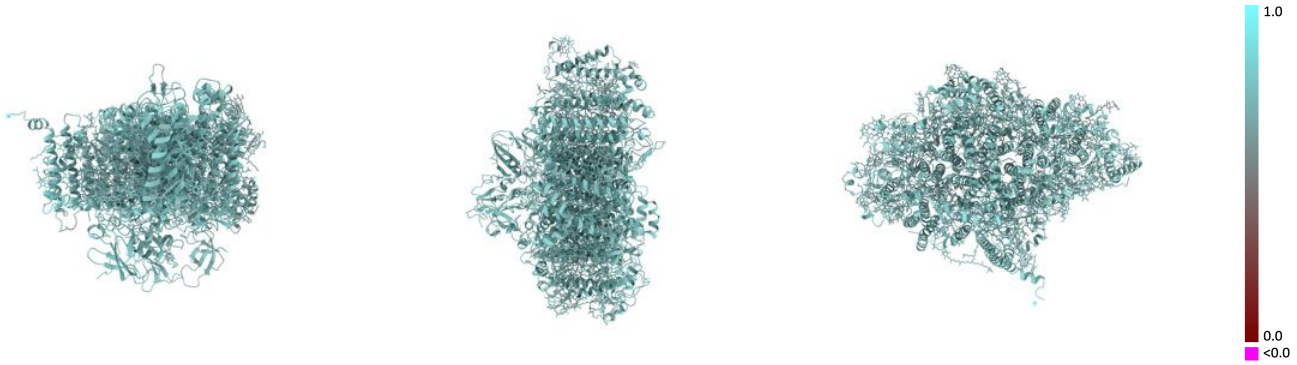
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.4 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.

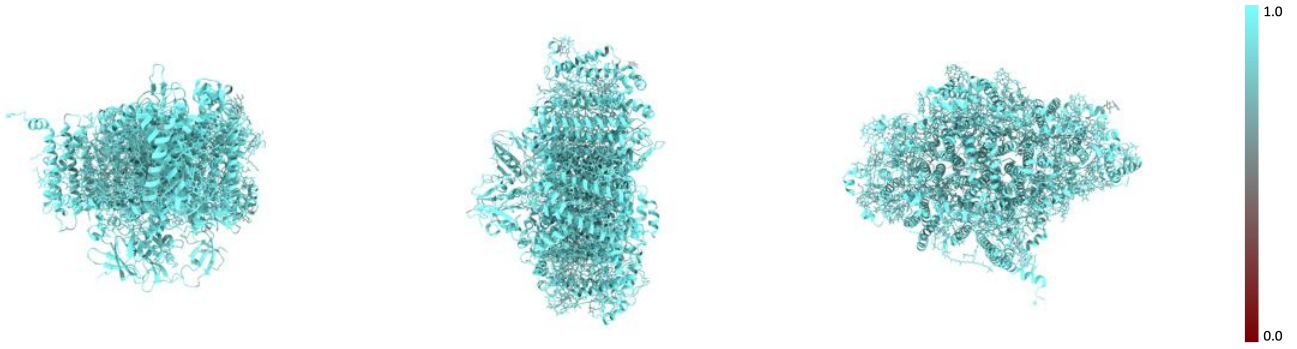
9.2 Q-score mapped to coordinate model (i)



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.

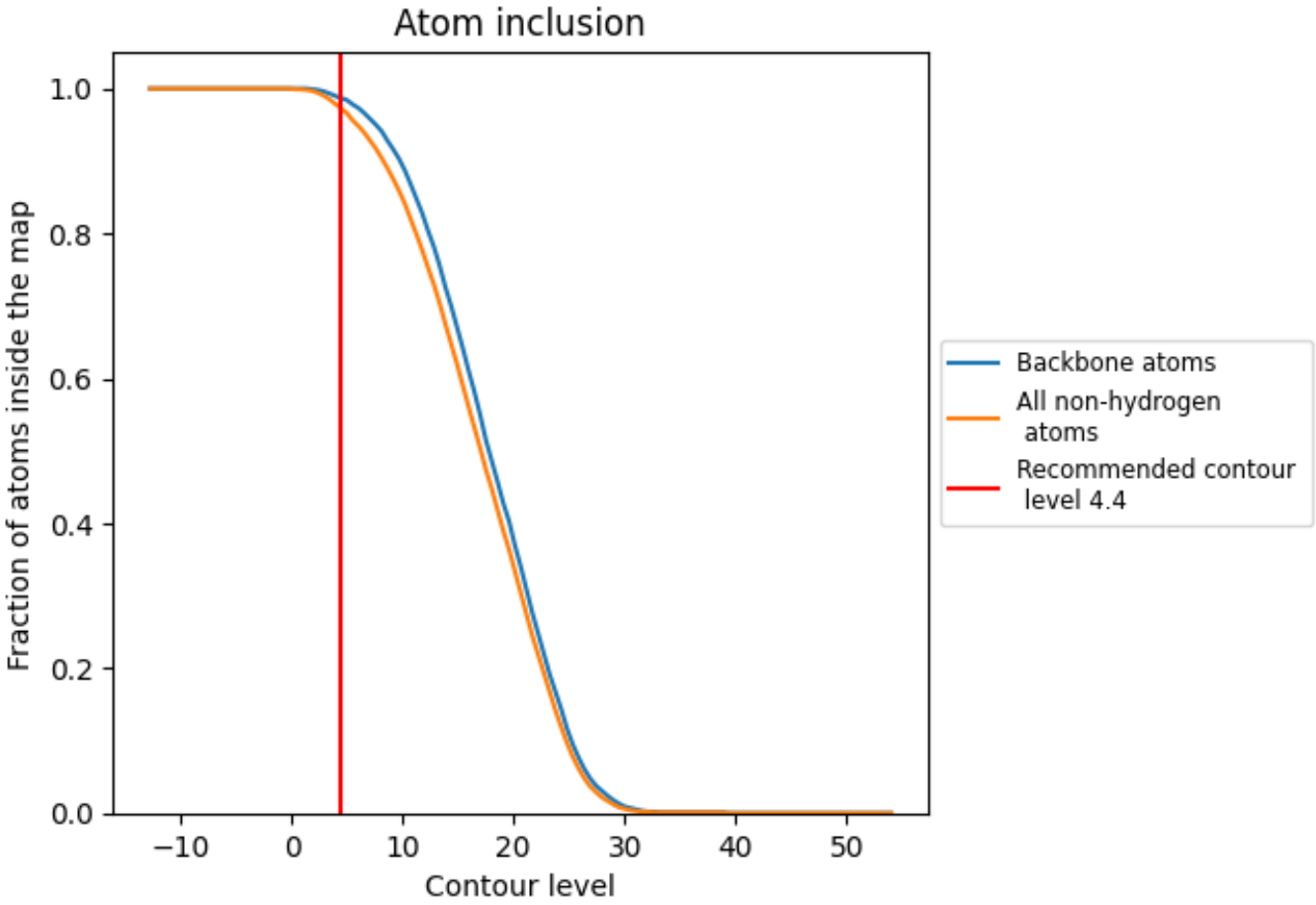
9.3 Atom inclusion mapped to coordinate model (i)



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 (4.4).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (4.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9730	0.7290
A	0.9740	0.7330
B	0.9740	0.7350
C	0.9950	0.7480
D	0.9750	0.7270
E	0.9620	0.7060
F	0.9550	0.7020
I	0.9830	0.7350
J	0.9670	0.6990
K	0.9410	0.6910
L	0.9760	0.7320
M	0.9810	0.7270

