wwPDB EM Validation Summary Report (i)

Aug 13, 2026 – 07:53 AM JST

PDB ID	:	9UNU / pdb_00009unu
EMDB ID	:	EMD-64362
Title	:	PSI-1 FCPI supercomplex from haptophyte Chrysotila roscoffensis
Authors	:	La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on	:	2025-04-24
Resolution	:	2.18 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:

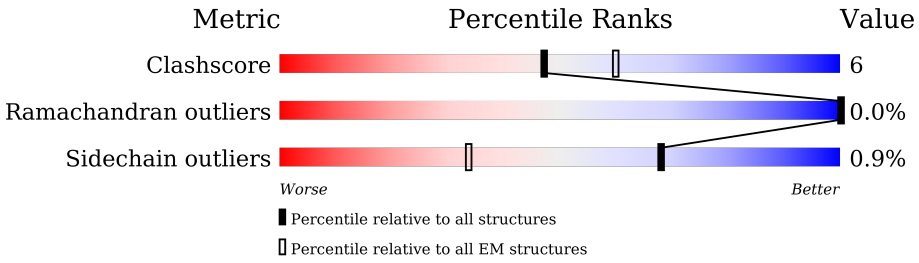
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.50

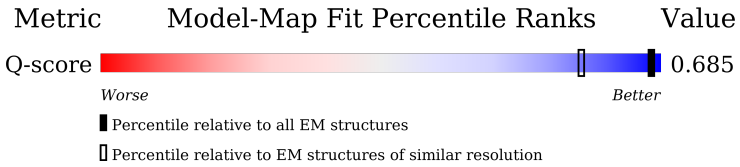
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 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.





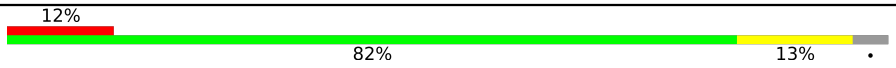
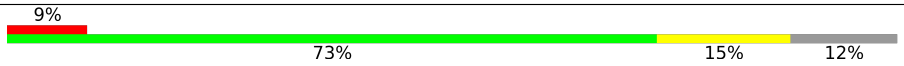
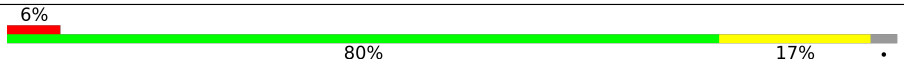
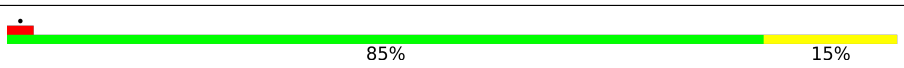
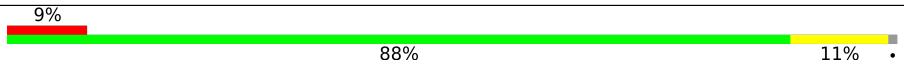
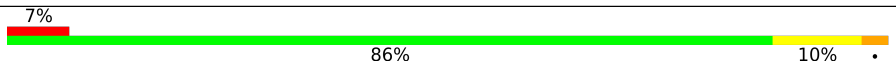
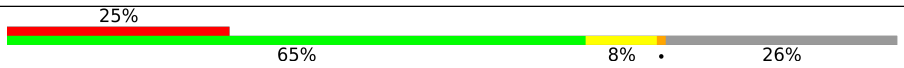
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2701 (1.70 - 2.68)

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	752	89% 9%
2	B	734	90% 9%
3	C	81	90% 9%
4	D	142	9% 89% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	67	
6	F	184	
7	I	35	
8	J	39	
9	L	141	
10	M	29	
11	U	191	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 25464 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 (psaA).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5813	3807	984	994	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5805	3823	977	984	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	599	366	106	116	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	138	1092	697	188	204	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	64	494	314	86	93	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1246	802	209	229	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	34	Total	C	N	O	S	0	0
			266	183	35	46	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			305	204	45	54	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit XI (psaL).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	140	Total	C	N	O	S	0	0
			1056	693	168	194	1		

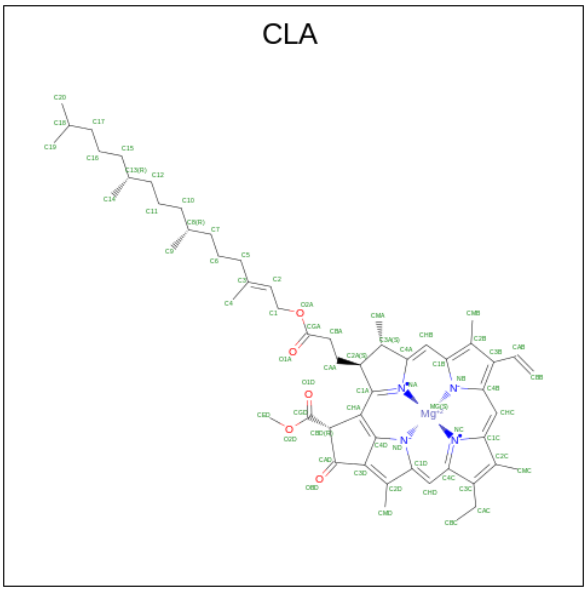
- Molecule 10 is a protein called Photosystem I reaction center subunit XII (psaM).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	29	Total	C	N	O	S	0	0
			216	144	34	37	1		

- Molecule 11 is a protein called Fucoxanthin chlorophyll a/c binding protein I (FCPI-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	141	Total	C	N	O	S	0	0
			1082	692	183	198	9		

- Molecule 12 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
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

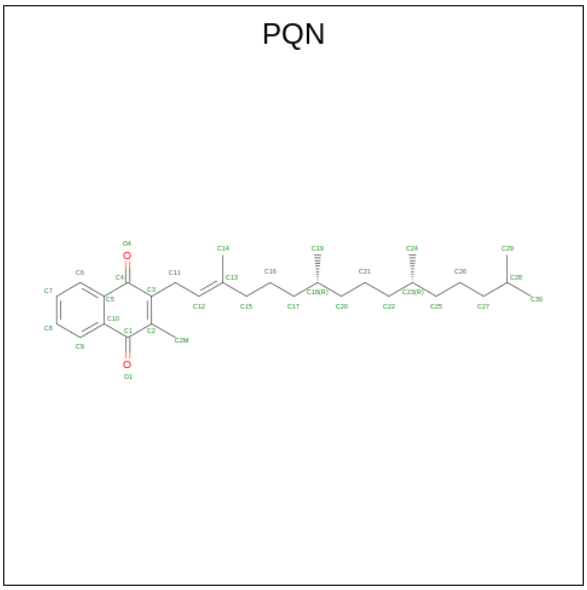
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	L	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	U	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	U	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
12	U	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

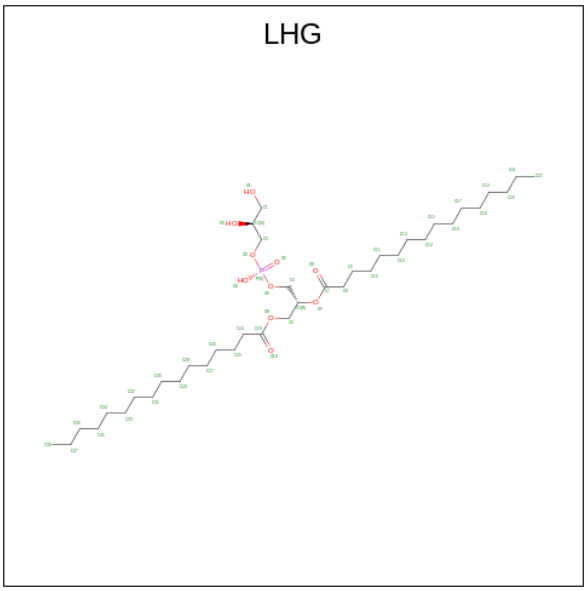
Mol	Chain	Residues	Atoms					AltConf
12	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



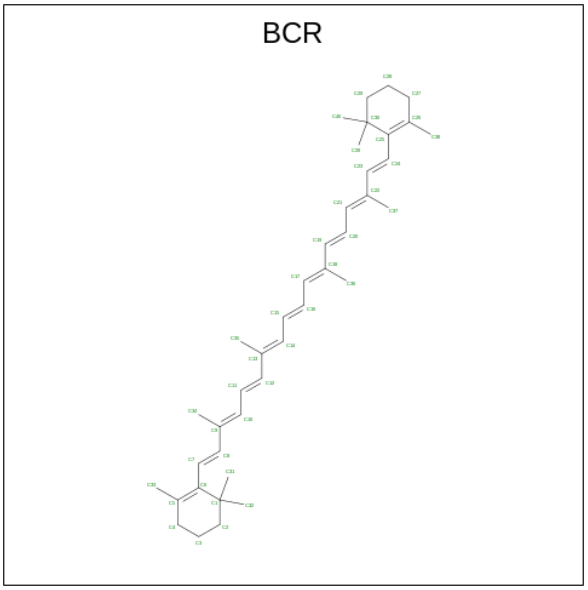
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			48	37	10	1	
14	A	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



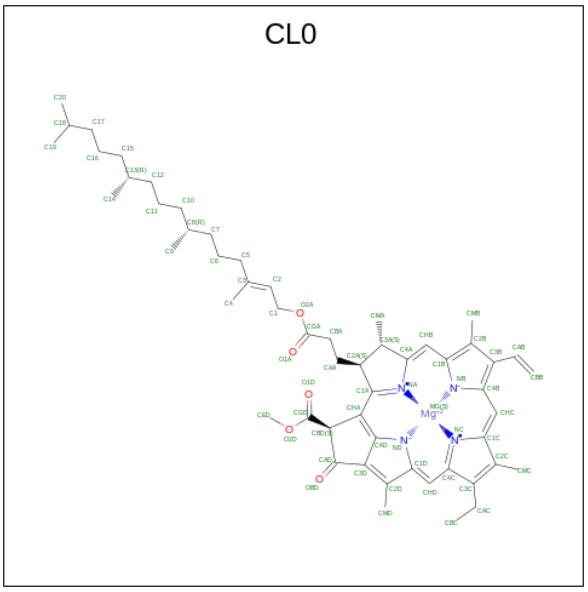
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

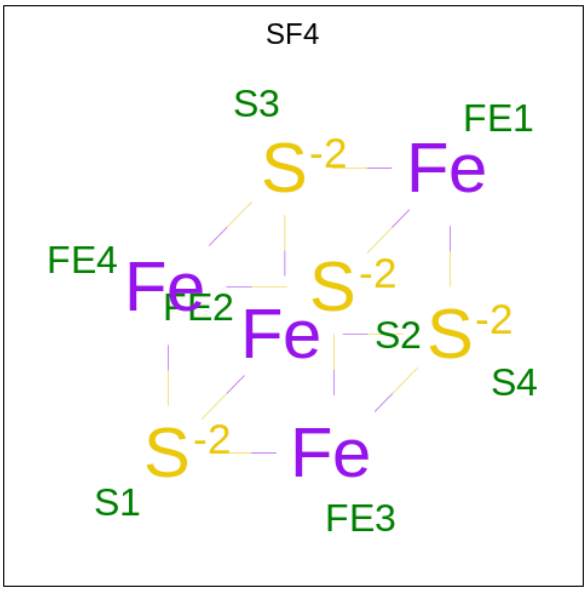
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	M	1	Total C 40 40	0

- Molecule 16 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
16	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



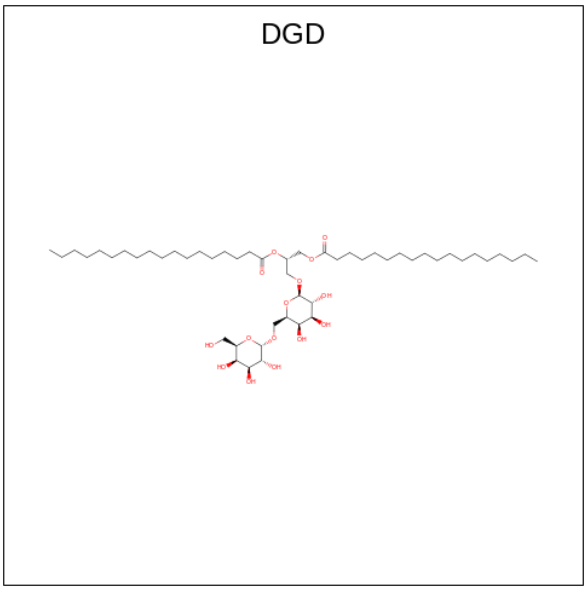
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	Fe	S		0
			8	4	4		
17	C	1	Total	Fe	S		0
			8	4	4		

Continued on next page...

Continued from previous page...

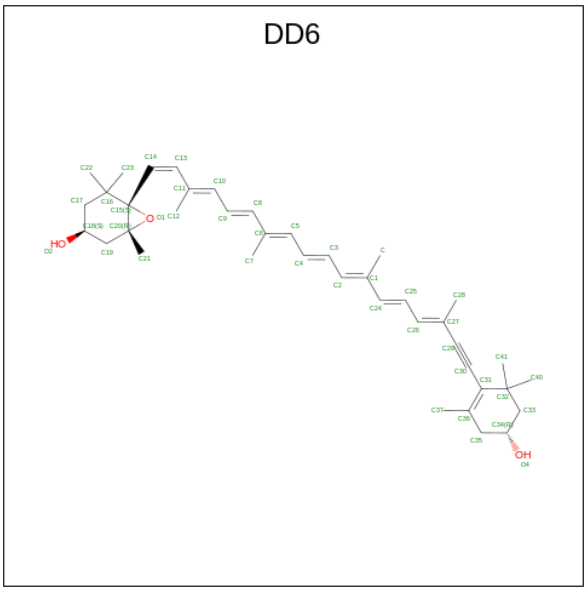
Mol	Chain	Residues	Atoms			AltConf
17	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



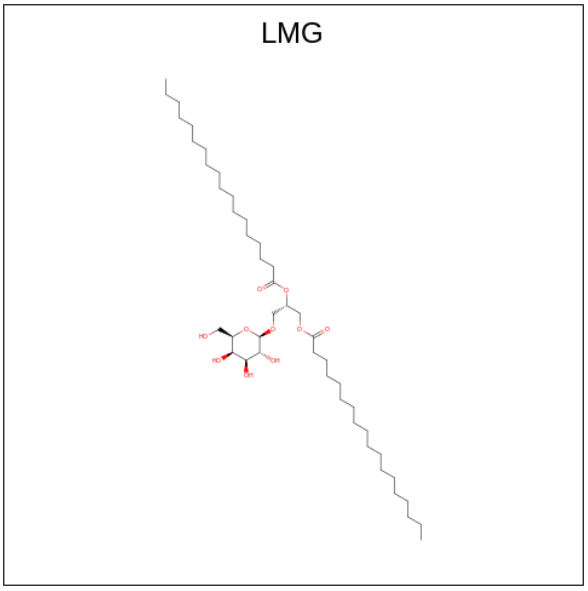
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			60	45	15	

- Molecule 19 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



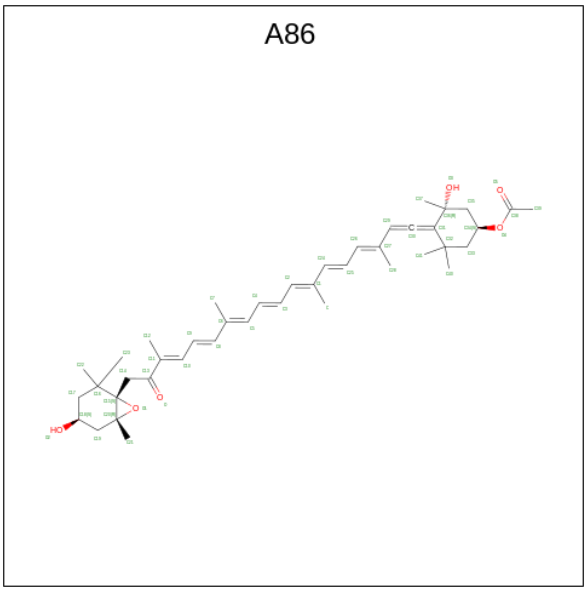
Mol	Chain	Residues	Atoms			AltConf
19	J	1	Total	C	O	0
			43	40	3	
19	U	1	Total	C	O	0
			43	40	3	
19	U	1	Total	C	O	0
			43	40	3	
19	U	1	Total	C	O	0
			26	25	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



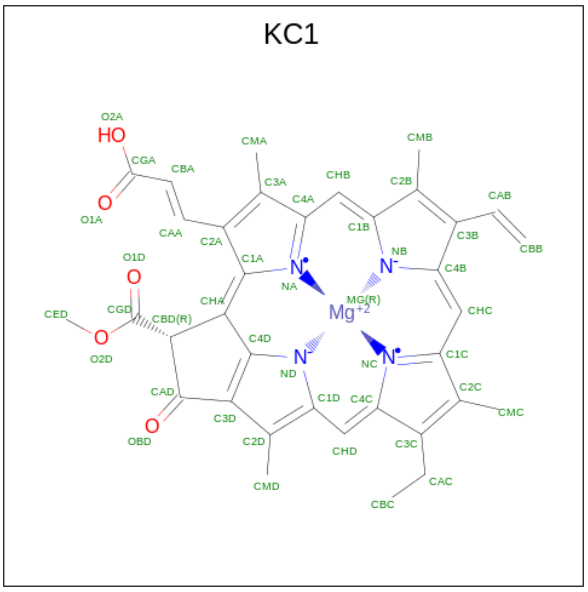
Mol	Chain	Residues	Atoms	AltConf
20	J	1	Total C O 39 29 10	0
20	U	1	Total C O 32 22 10	0

- Molecule 21 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
21	U	1	Total C O 48 42 6	0

- Molecule 22 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	U	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	110	Total	O	0
			110	110	
23	B	179	Total	O	0
			179	179	
23	C	33	Total	O	0
			33	33	
23	D	19	Total	O	0
			19	19	
23	E	10	Total	O	0
			10	10	
23	F	15	Total	O	0
			15	15	
23	J	2	Total	O	0
			2	2	
23	L	18	Total	O	0
			18	18	
23	M	2	Total	O	0
			2	2	
23	U	3	Total	O	0
			3	3	

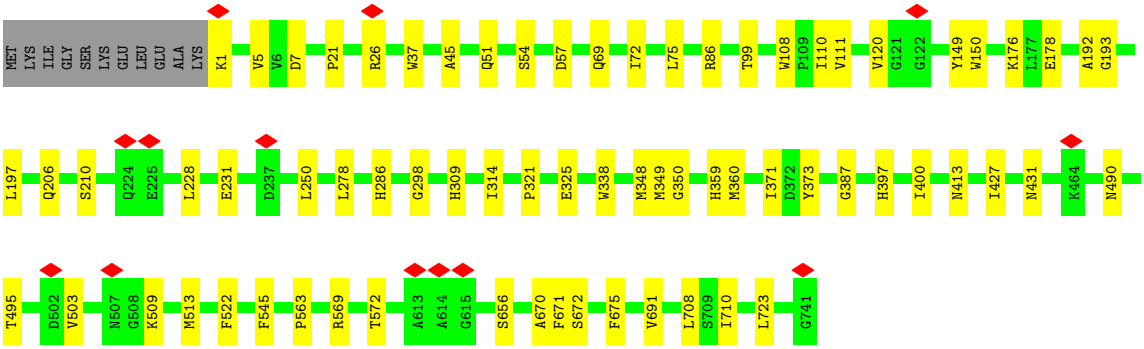
3 Residue-property plots (i)

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 (psaA)

Chain A:

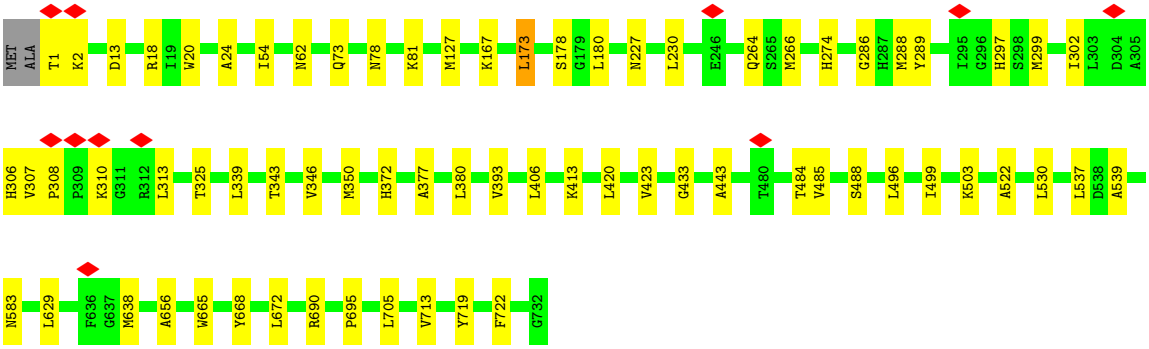




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)

Chain B:





• Molecule 3: Photosystem I iron-sulfur center (psaC)

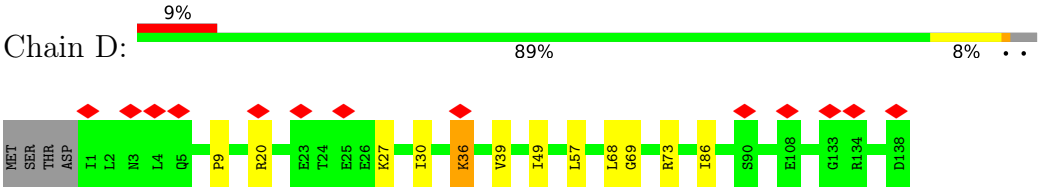
Chain C:





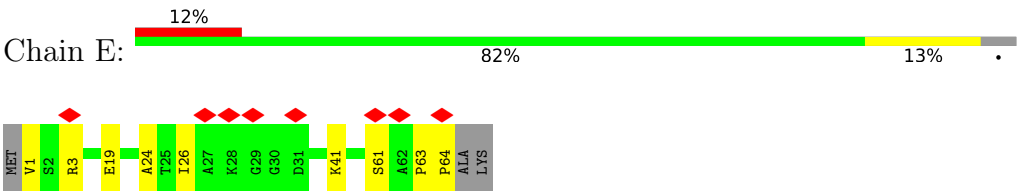
• Molecule 4: Photosystem I reaction center subunit II (psaD)

Chain D:



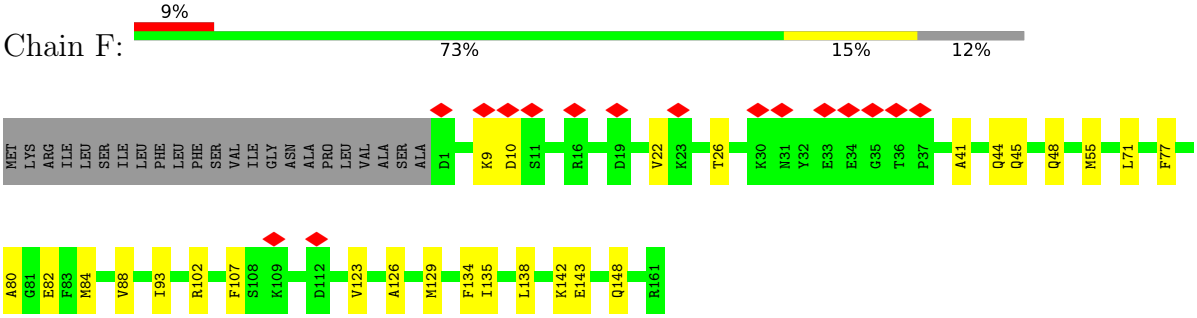
• Molecule 5: Photosystem I reaction center subunit IV (psaE)

Chain E:



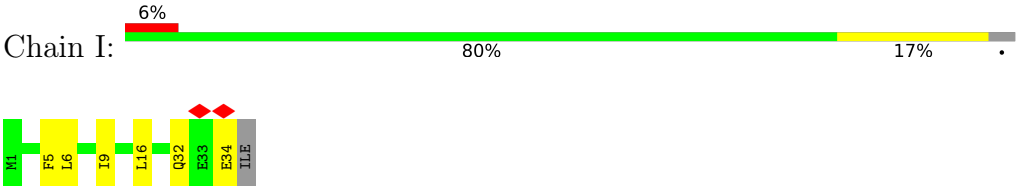
• Molecule 6: Photosystem I reaction center subunit III (psaF)

Chain F:



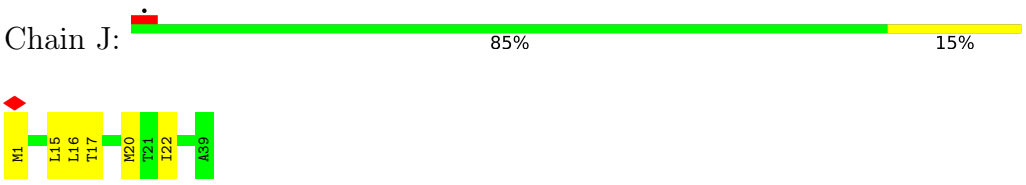
• Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I:



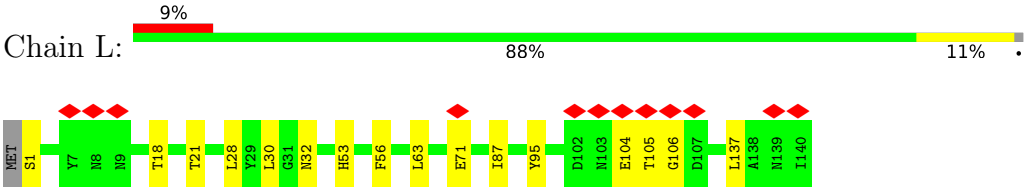
• Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J:



• Molecule 9: Photosystem I reaction center subunit XI (psaL)

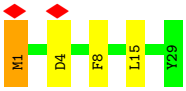
Chain L:



• Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M:

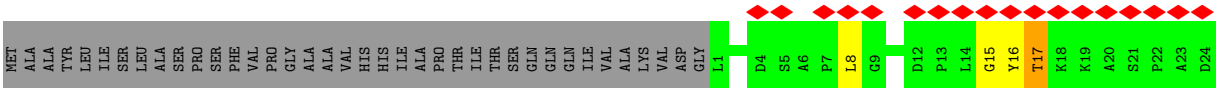


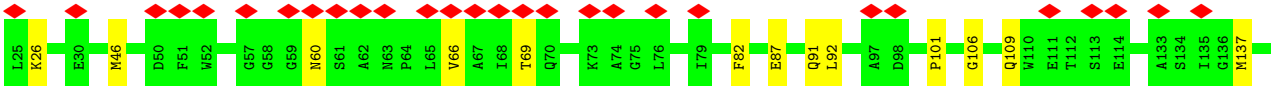


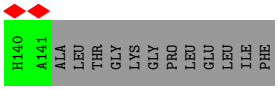
• Molecule 11: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18827	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.531	Depositor
Minimum map value	-0.210	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CL0, PQN, LMG, KC1, DD6, LHG, A86, CLA, DGD, 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	0.20	0/6007	0.43	2/8185 (0.0%)
2	B	0.19	0/6015	0.42	0/8205
3	C	0.15	0/609	0.45	0/826
4	D	0.15	0/1116	0.43	0/1503
5	E	0.14	0/505	0.34	0/689
6	F	0.24	0/1275	0.45	0/1728
7	I	0.24	0/273	0.56	0/373
8	J	0.19	0/313	0.47	0/427
9	L	0.17	0/1081	0.41	0/1470
10	M	0.18	0/218	0.33	0/295
11	U	0.20	0/1109	0.49	0/1499
All	All	0.19	0/18521	0.43	2/25200 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	LEU	CA-C-N	6.66	124.43	120.24
1	A	250	LEU	C-N-CA	6.66	124.43	120.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	665	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5698	51	0
2	B	5805	0	5634	55	0
3	C	599	0	577	4	0
4	D	1092	0	1096	8	0
5	E	494	0	488	4	0
6	F	1246	0	1256	20	0
7	I	266	0	278	6	0
8	J	305	0	310	7	0
9	L	1056	0	1068	13	0
10	M	216	0	234	2	0
11	U	1082	0	1058	19	0
12	A	2563	0	2608	65	0
12	B	2454	0	2490	69	0
12	F	94	0	69	3	0
12	J	42	0	31	0	0
12	L	164	0	150	6	0
12	U	493	0	460	17	0
13	A	33	0	46	5	0
13	B	33	0	46	0	0
14	A	75	0	93	1	0
15	A	160	0	224	6	0
15	B	200	0	280	10	0
15	F	80	0	112	2	0
15	I	80	0	112	4	0
15	J	40	0	56	1	0
15	L	80	0	112	1	0
15	M	40	0	56	3	0
16	A	65	0	72	1	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
18	B	60	0	81	3	0
19	J	43	0	0	0	0
19	U	112	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	J	39	0	48	1	0
20	U	32	0	34	1	0
21	U	48	0	0	0	0
22	U	45	0	0	0	0
23	A	110	0	0	1	0
23	B	179	0	0	1	0
23	C	33	0	0	0	0
23	D	19	0	0	0	0
23	E	10	0	0	0	0
23	F	15	0	0	0	0
23	J	2	0	0	0	0
23	L	18	0	0	0	0
23	M	2	0	0	0	0
23	U	3	0	0	0	0
All	All	25464	0	24877	299	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 299 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)
11:U:46:MET:HE2	11:U:137:MET:CE	1.56	1.35
11:U:46:MET:HE2	11:U:137:MET:HE2	1.25	1.14
11:U:46:MET:CE	11:U:137:MET:CE	2.27	1.12
11:U:46:MET:CE	11:U:137:MET:HE3	1.89	1.03
11:U:46:MET:CE	11:U:137:MET:HE2	1.93	0.95

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	739/752 (98%)	719 (97%)	20 (3%)	0	100	100
2	B	730/734 (100%)	716 (98%)	14 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	136/142 (96%)	129 (95%)	7 (5%)	0	100	100
5	E	62/67 (92%)	60 (97%)	2 (3%)	0	100	100
6	F	159/184 (86%)	155 (98%)	4 (2%)	0	100	100
7	I	32/35 (91%)	30 (94%)	2 (6%)	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
9	L	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	U	139/191 (73%)	132 (95%)	6 (4%)	1 (1%)	18	17
All	All	2277/2395 (95%)	2218 (97%)	58 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	U	16	TYR

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	603/612 (98%)	599 (99%)	4 (1%)	76	86
2	B	590/591 (100%)	586 (99%)	4 (1%)	76	86
3	C	68/69 (99%)	66 (97%)	2 (3%)	37	47
4	D	118/122 (97%)	117 (99%)	1 (1%)	73	83
5	E	53/55 (96%)	52 (98%)	1 (2%)	50	63
6	F	133/152 (88%)	133 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	32/32 (100%)	32 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	L	111/112 (99%)	111 (100%)	0	100 100
10	M	21/21 (100%)	18 (86%)	3 (14%)	3 2
11	U	110/148 (74%)	108 (98%)	2 (2%)	51 65
All	All	1870/1946 (96%)	1853 (99%)	17 (1%)	68 81

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	M	15	LEU
11	U	17	THR
2	B	485	VAL
3	C	70	SER
3	C	79	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	31	ASN
11	U	120	GLN
8	J	4	ASN
2	B	227	ASN
6	F	15	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

133 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CLA	B	835	-	69,73,73	1.19	8 (11%)	83,113,113	1.01	5 (6%)
12	CLA	B	830	2	62,66,73	1.32	7 (11%)	74,104,113	1.03	3 (4%)
12	CLA	U	201	14	56,60,73	1.31	8 (14%)	67,97,113	1.12	4 (5%)
12	CLA	U	206	11	69,73,73	1.18	7 (10%)	83,113,113	0.95	3 (3%)
15	BCR	B	840	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	4 (7%)
16	CL0	A	847	1	69,73,73	1.45	9 (13%)	83,113,113	0.85	3 (3%)
12	CLA	L	203	9	69,73,73	1.18	6 (8%)	83,113,113	0.92	3 (3%)
12	CLA	B	814	2	59,63,73	1.33	7 (11%)	71,101,113	0.97	3 (4%)
15	BCR	M	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.34	8 (14%)
12	CLA	A	819	1	47,51,73	1.42	7 (14%)	56,86,113	1.13	5 (8%)
12	CLA	B	833	23	69,73,73	1.19	7 (10%)	83,113,113	1.02	7 (8%)
17	SF4	A	849	1,2	0,12,12	-	-	-		
12	CLA	U	207	11	49,53,73	1.45	6 (12%)	59,89,113	1.04	3 (5%)
12	CLA	B	810	2	58,62,73	1.41	8 (13%)	73,100,113	0.99	4 (5%)
12	CLA	B	827	2	53,57,73	1.38	7 (13%)	62,93,113	1.02	3 (4%)
12	CLA	A	833	1	69,73,73	1.21	7 (10%)	83,113,113	1.06	6 (7%)
15	BCR	J	104	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	5 (8%)
12	CLA	B	806	2	69,73,73	1.20	7 (10%)	83,113,113	0.95	5 (6%)
12	CLA	A	806	1	69,73,73	1.17	7 (10%)	83,113,113	1.02	6 (7%)
12	CLA	B	829	23	69,73,73	1.16	6 (8%)	83,113,113	1.02	5 (6%)
12	CLA	B	821	23	68,72,73	1.17	6 (8%)	81,111,113	0.97	4 (4%)
12	CLA	B	802	2	69,73,73	1.25	7 (10%)	83,113,113	0.84	5 (6%)
12	CLA	A	813	1	54,58,73	1.39	7 (12%)	65,95,113	1.06	5 (7%)
12	CLA	A	831	1	49,53,73	1.39	6 (12%)	59,89,113	1.22	5 (8%)
17	SF4	C	101	3	0,12,12	-	-	-		
12	CLA	U	209	11	50,54,73	1.36	5 (10%)	60,90,113	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	B	807	2	69,73,73	1.20	7 (10%)	83,113,113	0.94	3 (3%)
12	CLA	A	807	1	69,73,73	1.19	8 (11%)	83,113,113	1.03	5 (6%)
15	BCR	A	843	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
12	CLA	A	835	1	69,73,73	1.25	7 (10%)	83,113,113	0.95	4 (4%)
12	CLA	A	836	23	69,73,73	1.19	7 (10%)	83,113,113	1.00	3 (3%)
15	BCR	A	841	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	4 (7%)
12	CLA	B	823	2	69,73,73	1.22	8 (11%)	83,113,113	1.00	3 (3%)
15	BCR	F	804	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	7 (12%)
12	CLA	L	202	9	53,57,73	1.36	8 (15%)	62,93,113	1.18	6 (9%)
19	DD6	U	204	-	39,45,45	1.63	8 (20%)	52,67,67	1.73	12 (23%)
12	CLA	B	846	2	69,73,73	1.18	7 (10%)	83,113,113	1.20	7 (8%)
15	BCR	L	205	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	7 (12%)
12	CLA	L	204	23	54,58,73	1.32	7 (12%)	65,95,113	1.08	4 (6%)
12	CLA	A	810	1	58,62,73	1.31	7 (12%)	69,99,113	1.09	5 (7%)
13	PQN	B	836	-	34,34,34	0.39	0	42,45,45	0.41	0
20	LMG	J	102	-	39,39,55	0.85	1 (2%)	47,47,63	1.20	4 (8%)
12	CLA	A	830	1	54,58,73	1.33	7 (12%)	65,95,113	1.02	4 (6%)
12	CLA	A	815	1	69,73,73	1.21	7 (10%)	83,113,113	1.02	5 (6%)
20	LMG	U	202	-	32,32,55	0.96	1 (3%)	40,40,63	1.19	5 (12%)
12	CLA	B	828	2	62,66,73	1.31	8 (12%)	74,104,113	1.04	5 (6%)
12	CLA	B	804	2	49,53,73	1.46	8 (16%)	59,89,113	1.05	3 (5%)
12	CLA	A	850	1	69,73,73	1.17	7 (10%)	83,113,113	0.94	3 (3%)
15	BCR	A	842	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	7 (12%)
12	CLA	B	844	2	69,73,73	1.18	8 (11%)	83,113,113	1.08	6 (7%)
15	BCR	L	201	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
18	DGD	B	842	-	61,61,67	0.91	2 (3%)	75,75,81	1.34	8 (10%)
12	CLA	U	208	23	69,73,73	1.15	5 (7%)	83,113,113	1.15	8 (9%)
12	CLA	A	848	1	69,73,73	1.23	8 (11%)	83,113,113	0.92	3 (3%)
12	CLA	B	817	23	69,73,73	1.19	6 (8%)	83,113,113	1.04	6 (7%)
12	CLA	B	803	-	69,73,73	1.16	7 (10%)	83,113,113	0.98	4 (4%)
12	CLA	B	818	2	50,54,73	1.37	6 (12%)	60,90,113	1.17	5 (8%)
12	CLA	B	832	2	51,55,73	1.41	7 (13%)	61,91,113	1.11	5 (8%)
15	BCR	B	841	-	41,41,41	1.11	2 (4%)	56,56,56	1.13	3 (5%)
12	CLA	A	808	1	60,64,73	1.32	7 (11%)	72,102,113	0.94	3 (4%)
12	CLA	A	811	1	69,73,73	1.22	7 (10%)	83,113,113	0.94	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	A	803	1	69,73,73	1.19	8 (11%)	83,113,113	0.94	4 (4%)
12	CLA	A	823	1	69,73,73	1.26	8 (11%)	83,113,113	0.91	4 (4%)
12	CLA	B	826	2	54,58,73	1.35	7 (12%)	65,95,113	1.04	4 (6%)
12	CLA	A	846	1	69,73,73	1.22	8 (11%)	83,113,113	1.05	5 (6%)
12	CLA	A	822	23	69,73,73	1.16	7 (10%)	83,113,113	0.98	4 (4%)
12	CLA	J	103	8	46,50,73	1.40	6 (13%)	55,85,113	1.22	5 (9%)
19	DD6	U	215	-	24,26,45	1.71	6 (25%)	30,35,67	1.61	6 (20%)
12	CLA	B	848	-	49,53,73	1.44	8 (16%)	59,89,113	1.28	7 (11%)
14	LHG	A	839	12	26,26,48	0.80	0	29,32,54	1.34	3 (10%)
12	CLA	A	826	1	69,73,73	1.29	9 (13%)	83,113,113	0.86	3 (3%)
12	CLA	U	205	23	65,69,73	1.23	8 (12%)	78,108,113	1.01	4 (5%)
12	CLA	B	819	2	57,61,73	1.28	8 (14%)	68,98,113	1.01	5 (7%)
12	CLA	B	809	2	69,73,73	1.21	8 (11%)	83,113,113	0.92	4 (4%)
12	CLA	A	820	1	55,59,73	1.34	7 (12%)	66,96,113	1.17	6 (9%)
12	CLA	B	825	2	69,73,73	1.21	7 (10%)	83,113,113	0.97	5 (6%)
12	CLA	B	834	2	69,73,73	1.27	8 (11%)	83,113,113	0.99	4 (4%)
12	CLA	A	828	1	69,73,73	1.26	7 (10%)	83,113,113	0.91	3 (3%)
12	CLA	A	812	1	49,53,73	1.46	7 (14%)	59,89,113	1.17	5 (8%)
12	CLA	F	803	6	50,54,73	1.38	7 (14%)	60,90,113	1.14	5 (8%)
12	CLA	A	844	23	69,73,73	1.17	7 (10%)	83,113,113	0.96	3 (3%)
12	CLA	A	802	1	59,63,73	1.27	6 (10%)	71,101,113	1.13	6 (8%)
19	DD6	U	213	-	39,45,45	1.60	6 (15%)	52,67,67	1.80	13 (25%)
12	CLA	A	827	1	54,58,73	1.40	7 (12%)	65,95,113	0.99	3 (4%)
14	LHG	A	838	-	47,47,48	0.63	1 (2%)	50,53,54	1.24	6 (12%)
12	CLA	B	847	2	54,58,73	1.36	7 (12%)	65,95,113	1.14	6 (9%)
19	DD6	J	101	-	39,45,45	1.60	7 (17%)	52,67,67	1.63	9 (17%)
12	CLA	A	801	-	69,73,73	1.17	7 (10%)	83,113,113	0.95	5 (6%)
12	CLA	B	831	2	69,73,73	1.19	7 (10%)	83,113,113	0.94	4 (4%)
12	CLA	A	817	1	49,53,73	1.43	7 (14%)	59,89,113	1.17	5 (8%)
12	CLA	A	829	1	69,73,73	1.21	6 (8%)	83,113,113	0.96	4 (4%)
12	CLA	A	852	23	69,73,73	1.20	7 (10%)	83,113,113	1.03	5 (6%)
12	CLA	A	814	23	49,53,73	1.41	7 (14%)	59,89,113	1.17	6 (10%)
12	CLA	A	821	23	69,73,73	1.22	8 (11%)	83,113,113	0.99	6 (7%)
12	CLA	B	815	2	63,67,73	1.23	6 (9%)	75,105,113	1.06	6 (8%)
12	CLA	A	851	1	69,73,73	1.19	7 (10%)	83,113,113	0.93	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	B	805	2	69,73,73	1.20	8 (11%)	83,113,113	0.92	4 (4%)
15	BCR	I	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	6 (10%)
12	CLA	A	809	1	66,70,73	1.25	7 (10%)	79,109,113	0.89	3 (3%)
21	A86	U	203	-	44,50,50	1.67	4 (9%)	51,76,76	1.77	10 (19%)
12	CLA	B	824	2	69,73,73	1.22	7 (10%)	83,113,113	0.97	5 (6%)
12	CLA	B	845	2	69,73,73	1.29	8 (11%)	83,113,113	1.01	5 (6%)
12	CLA	U	212	11	56,60,73	1.35	7 (12%)	67,97,113	1.15	5 (7%)
12	CLA	A	825	1	69,73,73	1.24	7 (10%)	83,113,113	0.94	3 (3%)
13	PQN	A	837	-	34,34,34	0.38	0	42,45,45	0.41	0
12	CLA	B	843	2	69,73,73	1.23	7 (10%)	83,113,113	0.93	4 (4%)
12	CLA	B	816	2	64,68,73	1.24	8 (12%)	77,107,113	0.96	4 (5%)
12	CLA	B	801	23	69,73,73	1.19	7 (10%)	83,113,113	0.97	4 (4%)
12	CLA	A	845	1	64,68,73	1.34	7 (10%)	77,107,113	1.00	4 (5%)
12	CLA	A	818	23	69,73,73	1.18	8 (11%)	83,113,113	1.00	5 (6%)
12	CLA	A	804	1	69,73,73	1.18	8 (11%)	83,113,113	0.94	4 (4%)
15	BCR	B	838	-	41,41,41	1.01	2 (4%)	56,56,56	1.26	6 (10%)
12	CLA	A	816	1	69,73,73	1.19	7 (10%)	83,113,113	1.00	4 (4%)
12	CLA	B	822	2	69,73,73	1.28	7 (10%)	83,113,113	1.01	5 (6%)
12	CLA	F	802	23	52,56,73	1.38	7 (13%)	62,92,113	1.10	4 (6%)
12	CLA	A	832	1	55,59,73	1.38	8 (14%)	66,96,113	1.08	4 (6%)
15	BCR	I	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.25	6 (10%)
12	CLA	B	808	2	69,73,73	1.22	7 (10%)	83,113,113	0.95	3 (3%)
12	CLA	U	211	11	69,73,73	1.16	6 (8%)	83,113,113	1.02	5 (6%)
15	BCR	B	837	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	U	210	11	46,50,73	1.43	8 (17%)	55,85,113	1.19	4 (7%)
15	BCR	F	801	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	5 (8%)
12	CLA	A	805	1	53,57,73	1.38	7 (13%)	62,93,113	1.10	4 (6%)
12	CLA	A	834	1	69,73,73	1.30	8 (11%)	83,113,113	1.01	5 (6%)
12	CLA	B	812	2	58,62,73	1.29	7 (12%)	69,99,113	1.03	5 (7%)
12	CLA	B	820	23	67,71,73	1.22	8 (11%)	80,110,113	1.05	6 (7%)
17	SF4	C	102	3	0,12,12	-	-	-		
12	CLA	B	811	2	59,63,73	1.24	6 (10%)	71,101,113	1.15	5 (7%)
12	CLA	B	813	2	63,67,73	1.27	7 (11%)	75,105,113	0.98	4 (5%)
12	CLA	A	824	1	66,70,73	1.24	7 (10%)	79,109,113	1.06	5 (6%)
15	BCR	A	840	-	41,41,41	1.03	2 (4%)	56,56,56	1.28	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BCR	B	839	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
22	KC1	U	214	11	49,53,53	1.76	10 (20%)	63,89,89	1.09	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	835	-	-	9/39/115/115	-
12	CLA	B	830	2	-	1/31/107/115	-
12	CLA	U	201	14	-	5/24/100/115	-
12	CLA	U	206	11	-	5/39/115/115	-
15	BCR	B	840	-	-	7/29/63/63	0/2/2/2
16	CL0	A	847	1	-	1/39/115/115	-
12	CLA	L	203	9	-	0/39/115/115	-
12	CLA	B	814	2	-	0/27/103/115	-
15	BCR	M	101	-	-	13/29/63/63	0/2/2/2
12	CLA	A	819	1	-	1/13/89/115	-
12	CLA	B	833	23	-	5/39/115/115	-
17	SF4	A	849	1,2	-	-	0/6/5/5
12	CLA	U	207	11	-	3/15/91/115	-
12	CLA	B	810	2	-	2/25/101/115	-
12	CLA	B	827	2	-	4/20/96/115	-
12	CLA	A	833	1	-	9/39/115/115	-
15	BCR	J	104	-	-	10/29/63/63	0/2/2/2
12	CLA	B	806	2	-	4/39/115/115	-
12	CLA	A	806	1	-	9/39/115/115	-
12	CLA	B	829	23	-	8/39/115/115	-
12	CLA	B	821	23	-	5/38/114/115	-
12	CLA	B	802	2	-	4/39/115/115	-
12	CLA	A	813	1	-	1/21/97/115	-
12	CLA	A	831	1	-	2/15/91/115	-
17	SF4	C	101	3	-	-	0/6/5/5
12	CLA	U	209	11	-	4/17/93/115	-
12	CLA	B	807	2	-	6/39/115/115	-
12	CLA	A	807	1	-	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	A	843	-	-	11/29/63/63	0/2/2/2
12	CLA	A	835	1	-	1/39/115/115	-
12	CLA	A	836	23	-	6/39/115/115	-
15	BCR	A	841	-	-	8/29/63/63	0/2/2/2
12	CLA	B	823	2	-	10/39/115/115	-
15	BCR	F	804	-	-	8/29/63/63	0/2/2/2
12	CLA	L	202	9	-	6/20/96/115	-
19	DD6	U	204	-	-	5/26/80/80	0/3/3/3
12	CLA	B	846	2	-	9/39/115/115	-
15	BCR	L	205	-	-	8/29/63/63	0/2/2/2
12	CLA	L	204	23	-	2/21/97/115	-
12	CLA	A	810	1	-	3/26/102/115	-
13	PQN	B	836	-	-	1/23/43/43	0/2/2/2
20	LMG	J	102	-	-	16/34/54/70	0/1/1/1
12	CLA	A	830	1	-	0/21/97/115	-
12	CLA	A	815	1	-	5/39/115/115	-
20	LMG	U	202	-	-	12/27/47/70	0/1/1/1
12	CLA	B	828	2	-	6/31/107/115	-
12	CLA	B	804	2	-	5/15/91/115	-
12	CLA	A	850	1	-	10/39/115/115	-
15	BCR	A	842	-	-	5/29/63/63	0/2/2/2
12	CLA	B	844	2	-	8/39/115/115	-
15	BCR	L	201	-	-	9/29/63/63	0/2/2/2
18	DGD	B	842	-	-	24/49/89/95	0/2/2/2
12	CLA	U	208	23	-	3/39/115/115	-
12	CLA	A	848	1	-	9/39/115/115	-
12	CLA	B	817	23	-	4/39/115/115	-
12	CLA	B	803	-	-	5/39/115/115	-
12	CLA	B	818	2	-	1/17/93/115	-
12	CLA	B	832	2	-	0/18/94/115	-
15	BCR	B	841	-	-	7/29/63/63	0/2/2/2
12	CLA	A	808	1	-	3/29/105/115	-
12	CLA	A	811	1	-	3/39/115/115	-
12	CLA	A	803	1	-	5/39/115/115	-
12	CLA	A	823	1	-	6/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	826	2	-	3/21/97/115	-
12	CLA	A	846	1	-	5/39/115/115	-
12	CLA	A	822	23	-	6/39/115/115	-
12	CLA	J	103	8	-	5/12/88/115	-
19	DD6	U	215	-	-	8/14/37/80	0/1/1/3
12	CLA	B	848	-	-	3/15/91/115	-
14	LHG	A	839	12	-	7/31/31/53	-
12	CLA	A	826	1	-	2/39/115/115	-
12	CLA	U	205	23	-	3/35/111/115	-
12	CLA	B	819	2	-	4/25/101/115	-
12	CLA	B	809	2	-	6/39/115/115	-
12	CLA	A	820	1	-	2/23/99/115	-
12	CLA	B	825	2	-	6/39/115/115	-
12	CLA	B	834	2	-	4/39/115/115	-
12	CLA	A	828	1	-	5/39/115/115	-
12	CLA	A	812	1	-	1/15/91/115	-
12	CLA	F	803	6	-	3/17/93/115	-
12	CLA	A	844	23	-	7/39/115/115	-
12	CLA	A	802	1	-	4/27/103/115	-
19	DD6	U	213	-	-	13/26/80/80	0/3/3/3
12	CLA	A	827	1	-	3/21/97/115	-
14	LHG	A	838	-	-	22/52/52/53	-
12	CLA	B	847	2	-	5/21/97/115	-
19	DD6	J	101	-	-	6/26/80/80	0/3/3/3
12	CLA	A	801	-	-	3/39/115/115	-
12	CLA	B	831	2	-	7/39/115/115	-
12	CLA	A	817	1	-	3/15/91/115	-
12	CLA	A	829	1	-	3/39/115/115	-
12	CLA	A	852	23	-	2/39/115/115	-
12	CLA	A	814	23	-	2/15/91/115	-
12	CLA	A	821	23	-	12/39/115/115	-
12	CLA	B	815	2	-	5/32/108/115	-
12	CLA	A	851	1	-	7/39/115/115	-
12	CLA	B	805	2	-	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	I	102	-	-	11/29/63/63	0/2/2/2
12	CLA	A	809	1	-	6/36/112/115	-
21	A86	U	203	-	-	21/34/90/90	0/3/3/3
12	CLA	B	824	2	-	4/39/115/115	-
12	CLA	B	845	2	-	3/39/115/115	-
12	CLA	U	212	11	-	2/24/100/115	-
12	CLA	A	825	1	-	6/39/115/115	-
13	PQN	A	837	-	-	3/23/43/43	0/2/2/2
12	CLA	B	843	2	-	6/39/115/115	-
12	CLA	B	816	2	-	2/33/109/115	-
12	CLA	B	801	23	-	3/39/115/115	-
12	CLA	A	845	1	-	12/33/109/115	-
12	CLA	A	818	23	-	2/39/115/115	-
12	CLA	A	804	1	-	10/39/115/115	-
15	BCR	B	838	-	-	10/29/63/63	0/2/2/2
12	CLA	A	816	1	-	2/39/115/115	-
12	CLA	B	822	2	-	1/39/115/115	-
12	CLA	F	802	23	-	3/19/95/115	-
12	CLA	A	832	1	-	3/23/99/115	-
15	BCR	I	101	-	-	9/29/63/63	0/2/2/2
12	CLA	B	808	2	-	5/39/115/115	-
12	CLA	U	211	11	-	8/39/115/115	-
15	BCR	B	837	-	-	11/29/63/63	0/2/2/2
12	CLA	U	210	11	-	1/12/88/115	-
15	BCR	F	801	-	-	8/29/63/63	0/2/2/2
12	CLA	A	805	1	-	3/20/96/115	-
12	CLA	A	834	1	-	7/39/115/115	-
12	CLA	B	812	2	-	3/26/102/115	-
12	CLA	B	820	23	-	8/37/113/115	-
17	SF4	C	102	3	-	-	0/6/5/5
12	CLA	B	811	2	-	5/27/103/115	-
12	CLA	B	813	2	-	8/32/108/115	-
12	CLA	A	824	1	-	5/36/112/115	-
15	BCR	A	840	-	-	9/29/63/63	0/2/2/2
15	BCR	B	839	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	KC1	U	214	11	-	1/15/71/71	-

The worst 5 of 795 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	203	A86	C13-C11	-6.19	1.37	1.49
16	A	847	CL0	MG-NC	5.40	2.19	2.06
16	A	847	CL0	MG-NA	5.37	2.19	2.06
12	B	845	CLA	MG-NA	5.09	2.18	2.06
12	B	822	CLA	MG-NA	4.91	2.17	2.06

The worst 5 of 626 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	U	213	DD6	C3-C4-C5	5.17	134.07	123.47
21	U	203	A86	C3-C4-C5	4.97	133.65	123.47
12	U	208	CLA	CHD-C1D-ND	-4.63	120.20	124.45
19	U	213	DD6	C14-C13-C11	4.56	132.61	125.53
19	U	204	DD6	C12-C11-C10	-4.34	116.84	122.92

There are no chirality outliers.

5 of 740 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	804	CLA	C1A-C2A-CAA-CBA
12	A	804	CLA	C3A-C2A-CAA-CBA
12	A	806	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	O1A-CGA-O2A-C1
12	A	815	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

100 monomers are involved in 178 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	835	CLA	4	0
12	B	830	CLA	2	0
12	U	201	CLA	2	0
12	U	206	CLA	3	0
15	B	840	BCR	3	0
16	A	847	CL0	1	0
12	L	203	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	M	101	BCR	3	0
12	B	833	CLA	2	0
12	U	207	CLA	2	0
12	B	810	CLA	1	0
12	B	827	CLA	2	0
12	A	833	CLA	4	0
15	J	104	BCR	1	0
12	B	806	CLA	2	0
12	A	806	CLA	2	0
12	B	829	CLA	1	0
12	B	802	CLA	2	0
12	A	831	CLA	2	0
12	U	209	CLA	2	0
12	B	807	CLA	2	0
12	A	807	CLA	3	0
15	A	843	BCR	3	0
12	A	835	CLA	5	0
12	A	836	CLA	3	0
15	A	841	BCR	2	0
12	B	823	CLA	2	0
15	F	804	BCR	2	0
12	L	202	CLA	1	0
12	B	846	CLA	4	0
15	L	205	BCR	1	0
12	L	204	CLA	3	0
12	A	810	CLA	1	0
20	J	102	LMG	1	0
12	A	830	CLA	1	0
12	A	815	CLA	6	0
20	U	202	LMG	1	0
12	B	828	CLA	1	0
12	A	850	CLA	1	0
15	A	842	BCR	1	0
12	B	844	CLA	4	0
18	B	842	DGD	3	0
12	U	208	CLA	3	0
12	A	848	CLA	2	0
12	B	817	CLA	3	0
12	B	803	CLA	2	0
12	B	818	CLA	4	0
15	B	841	BCR	2	0
12	A	808	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	811	CLA	1	0
12	A	803	CLA	3	0
12	A	823	CLA	1	0
12	A	846	CLA	2	0
12	A	822	CLA	1	0
12	B	848	CLA	2	0
12	A	826	CLA	2	0
12	U	205	CLA	1	0
12	B	819	CLA	2	0
12	B	809	CLA	1	0
12	A	820	CLA	1	0
12	B	825	CLA	3	0
12	B	834	CLA	5	0
12	A	828	CLA	5	0
12	F	803	CLA	2	0
12	A	844	CLA	2	0
14	A	838	LHG	1	0
12	B	847	CLA	2	0
12	A	801	CLA	1	0
12	B	831	CLA	2	0
12	A	817	CLA	1	0
12	A	829	CLA	1	0
12	A	852	CLA	4	0
12	A	814	CLA	2	0
12	A	821	CLA	1	0
12	B	815	CLA	3	0
12	A	851	CLA	3	0
12	B	805	CLA	3	0
15	I	102	BCR	4	0
12	B	824	CLA	3	0
12	B	845	CLA	2	0
12	U	212	CLA	3	0
12	A	825	CLA	3	0
13	A	837	PQN	5	0
12	B	843	CLA	4	0
12	B	801	CLA	1	0
12	A	818	CLA	1	0
15	B	838	BCR	2	0
12	A	816	CLA	1	0
12	B	822	CLA	3	0
12	F	802	CLA	1	0
12	B	808	CLA	4	0

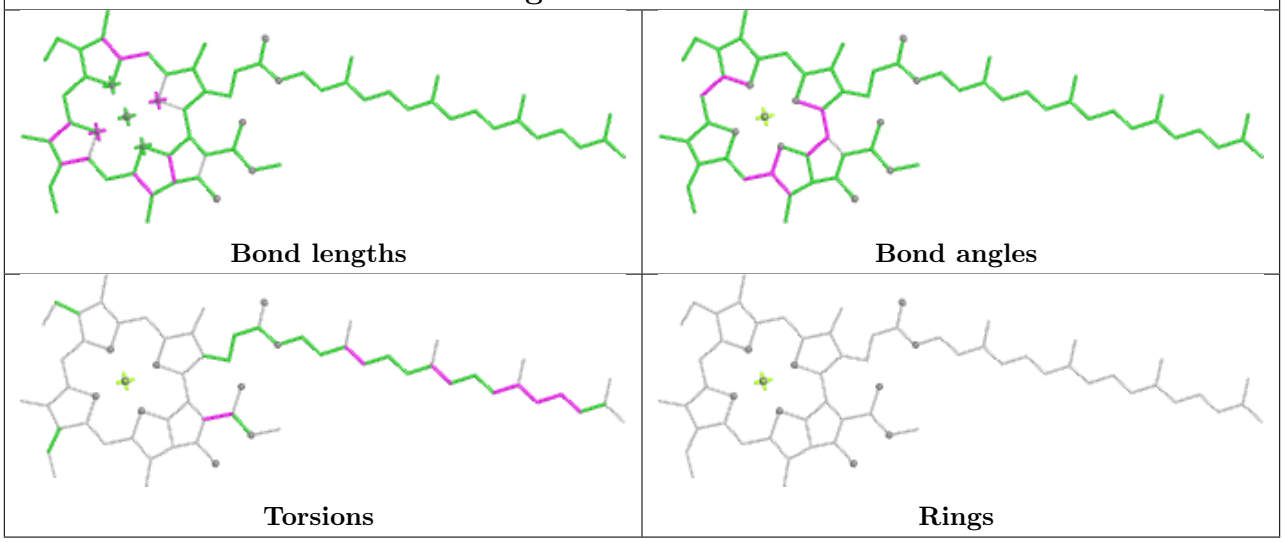
Continued on next page...

Continued from previous page...

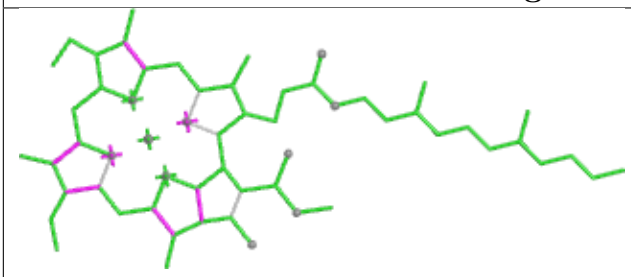
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	U	211	CLA	3	0
15	B	837	BCR	2	0
12	U	210	CLA	2	0
12	A	834	CLA	2	0
12	B	812	CLA	2	0
12	B	820	CLA	1	0
12	B	813	CLA	1	0
12	A	824	CLA	5	0
15	B	839	BCR	1	0

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.

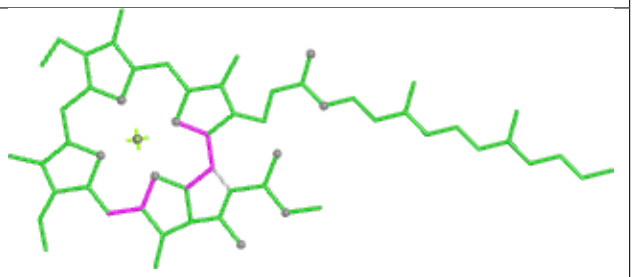
Ligand CLA B 835



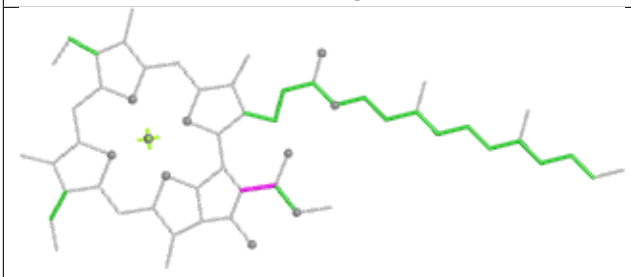
Ligand CLA B 830



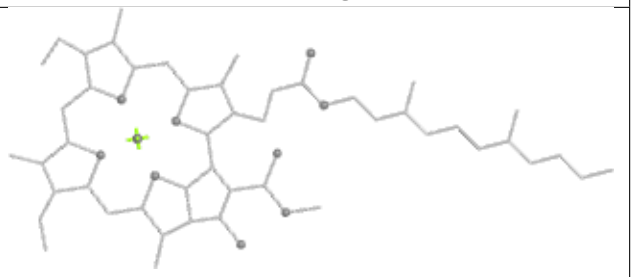
Bond lengths



Bond angles

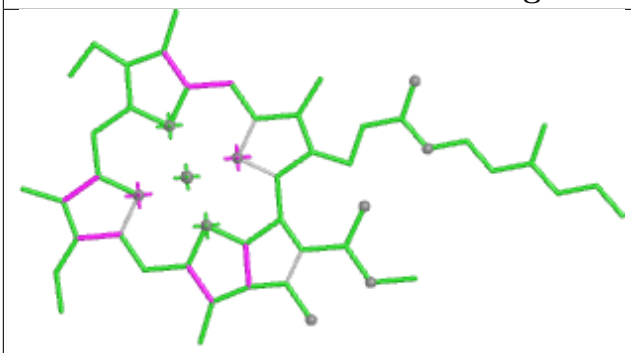


Torsions

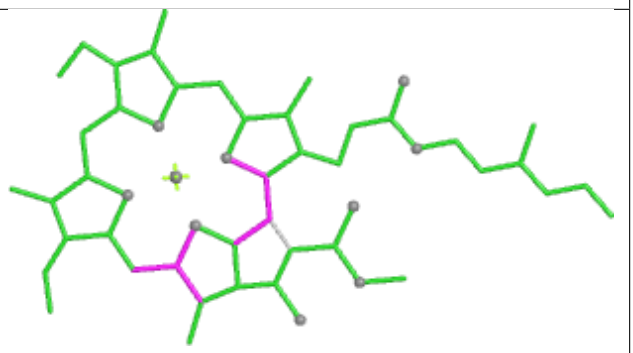


Rings

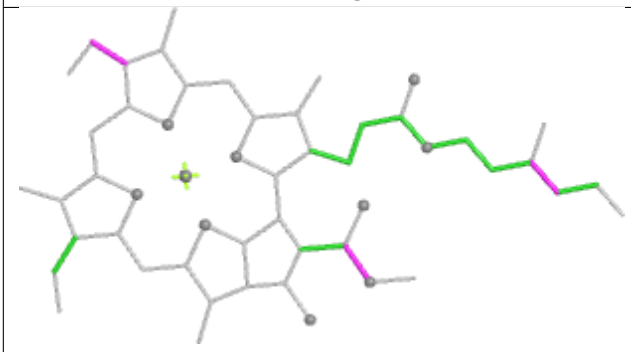
Ligand CLA U 201



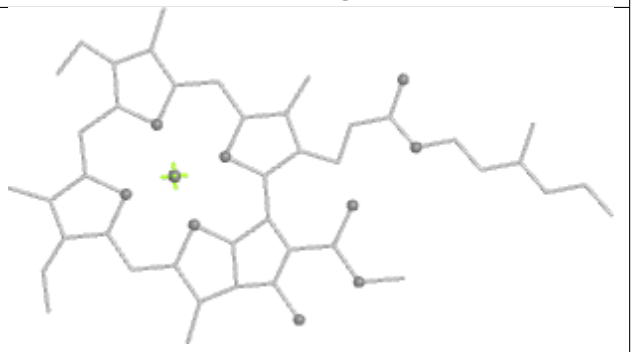
Bond lengths



Bond angles

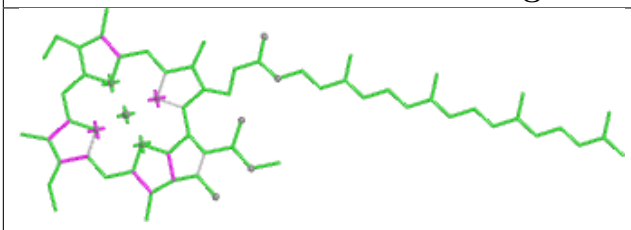


Torsions

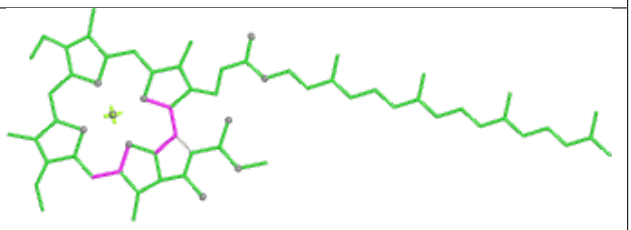


Rings

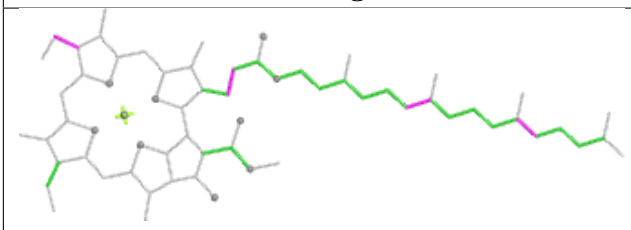
Ligand CLA U 206



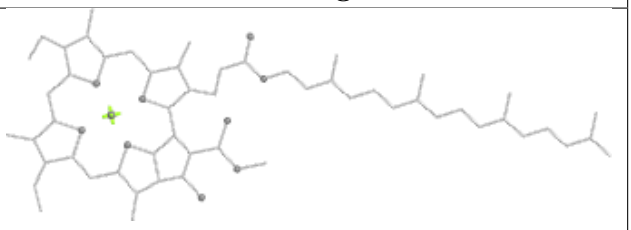
Bond lengths



Bond angles

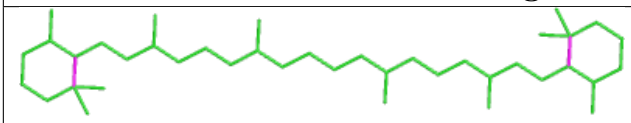


Torsions

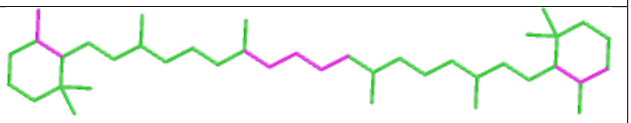


Rings

Ligand BCR B 840



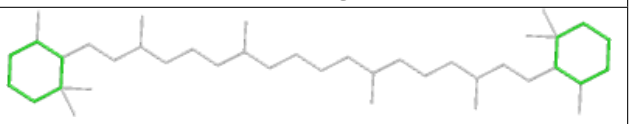
Bond lengths



Bond angles

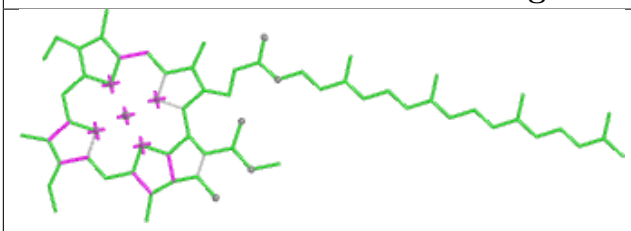


Torsions

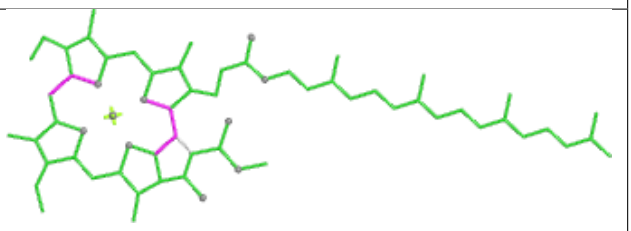


Rings

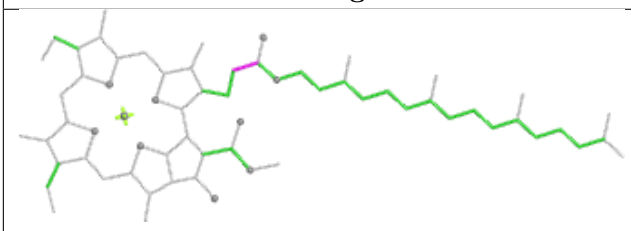
Ligand CL0 A 847



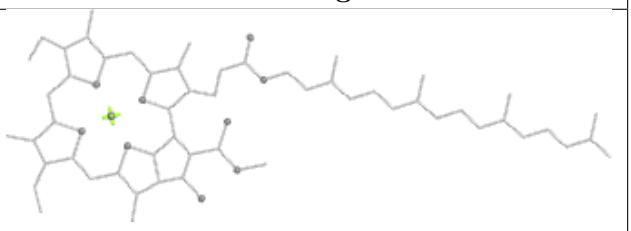
Bond lengths



Bond angles

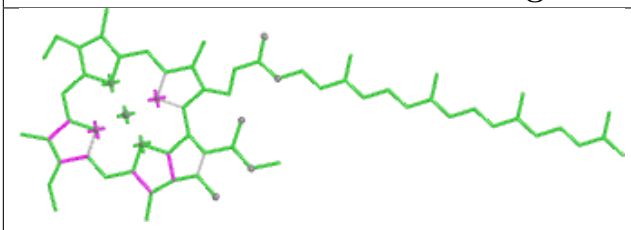


Torsions

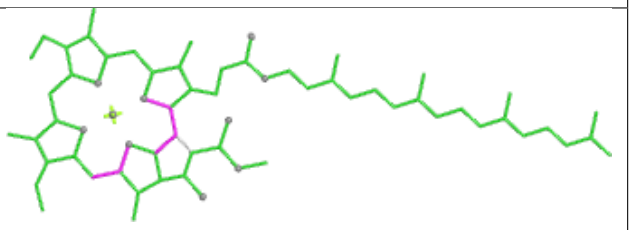


Rings

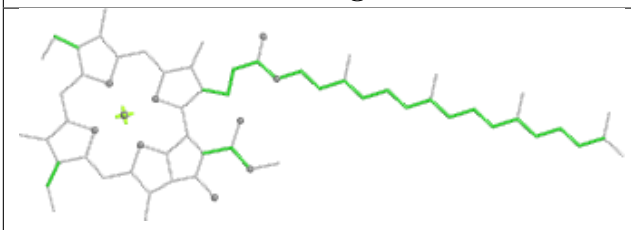
Ligand CLA L 203



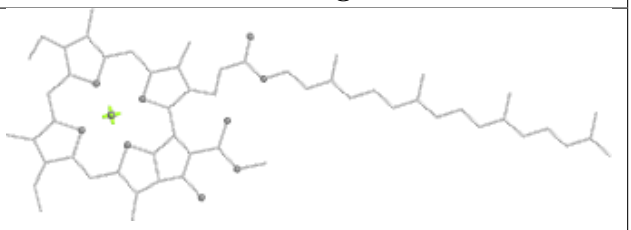
Bond lengths



Bond angles

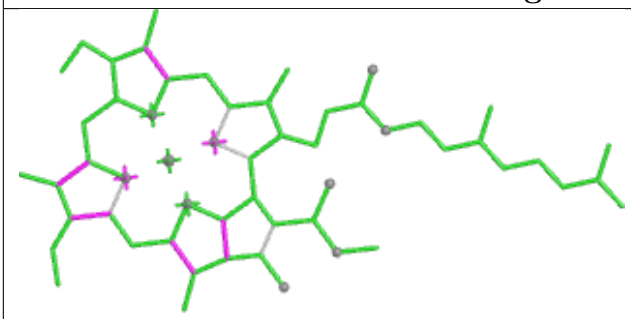


Torsions

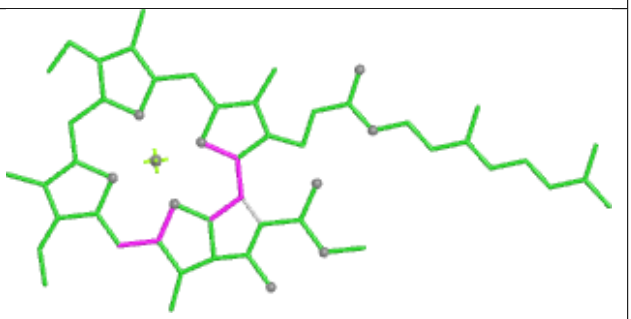


Rings

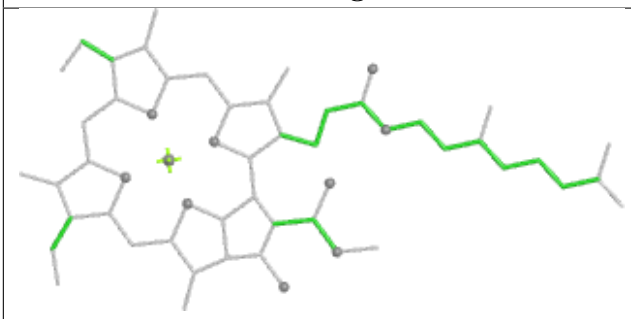
Ligand CLA B 814



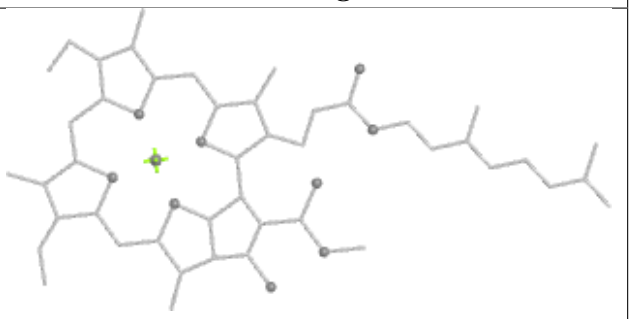
Bond lengths



Bond angles

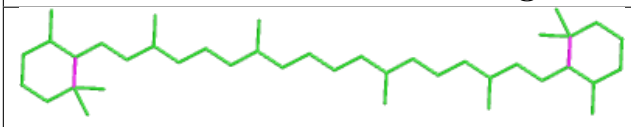


Torsions

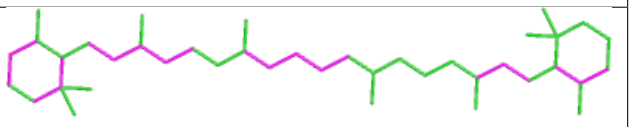


Rings

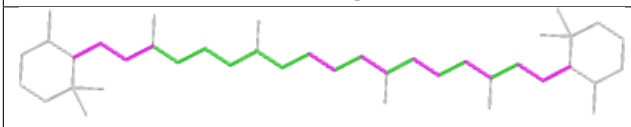
Ligand BCR M 101



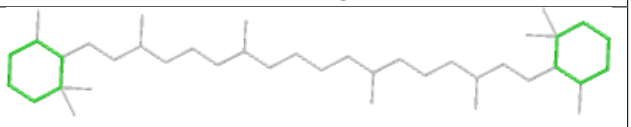
Bond lengths



Bond angles

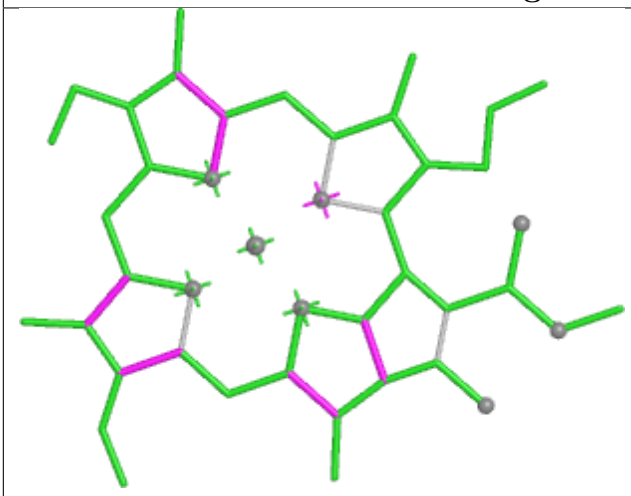


Torsions

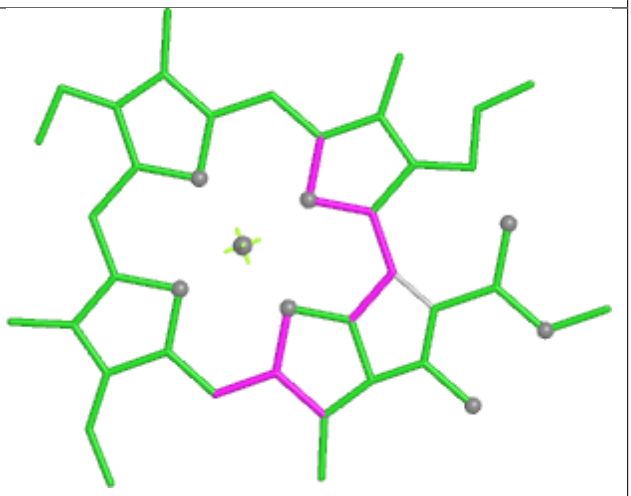


Rings

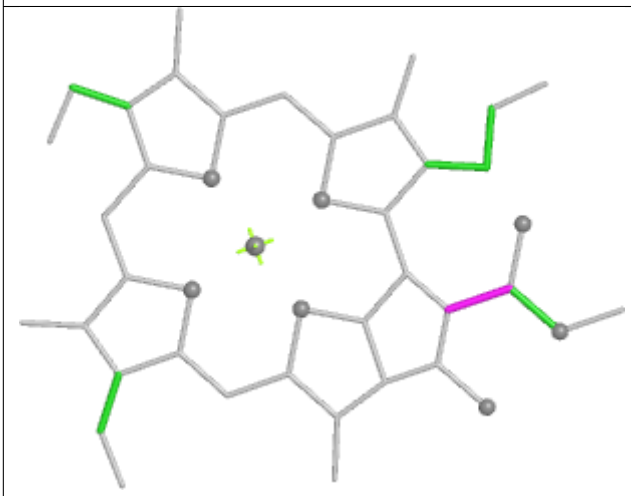
Ligand CLA A 819



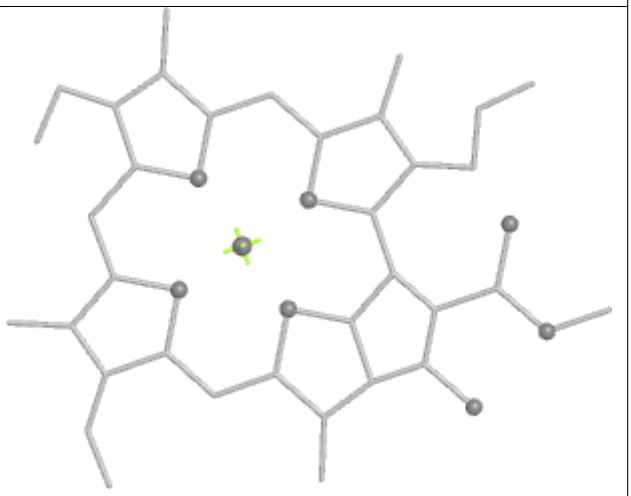
Bond lengths



Bond angles

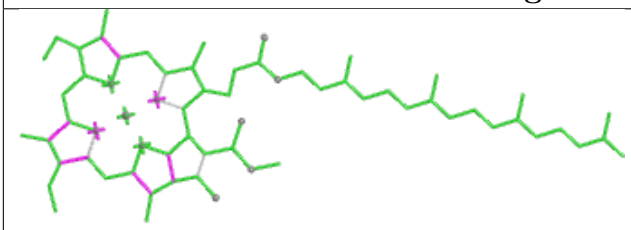


Torsions

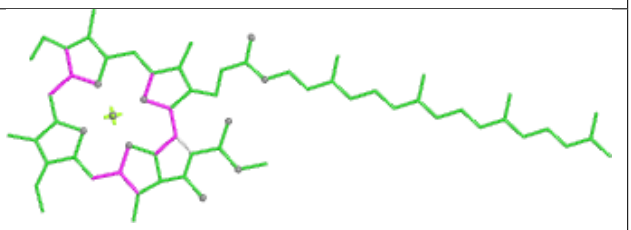


Rings

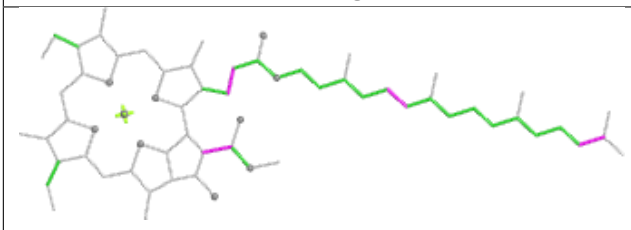
Ligand CLA B 833



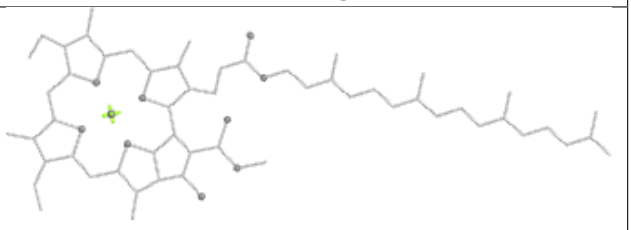
Bond lengths



Bond angles

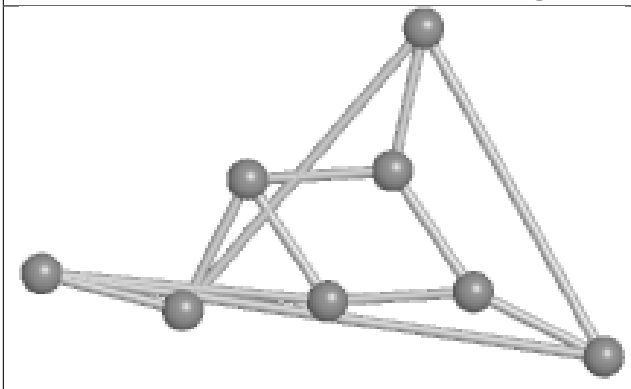


Torsions

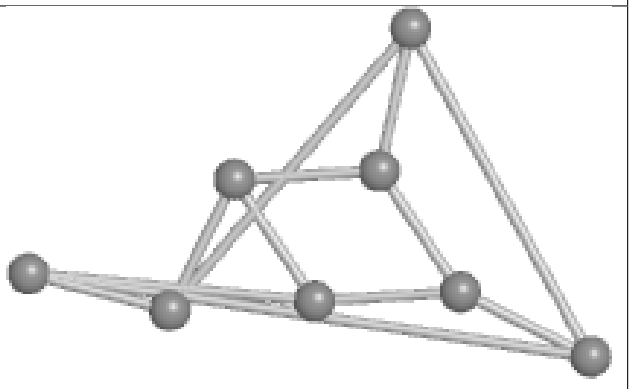


Rings

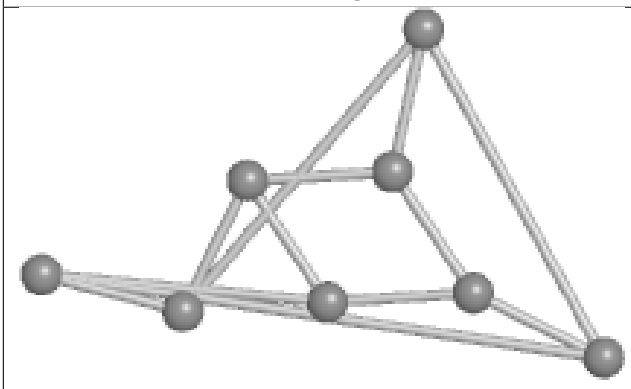
Ligand SF4 A 849



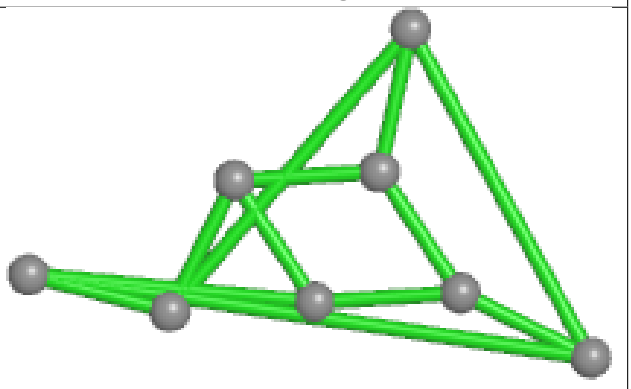
Bond lengths



Bond angles

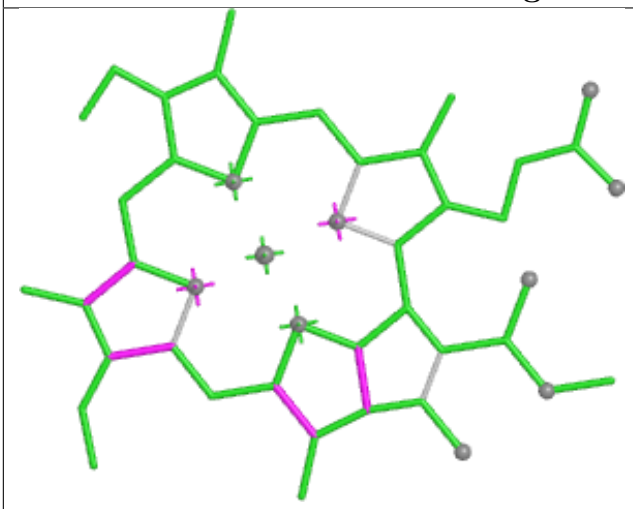


Torsions

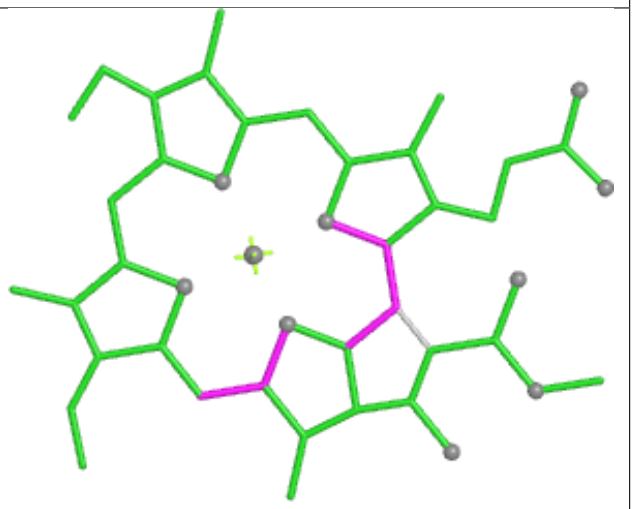


Rings

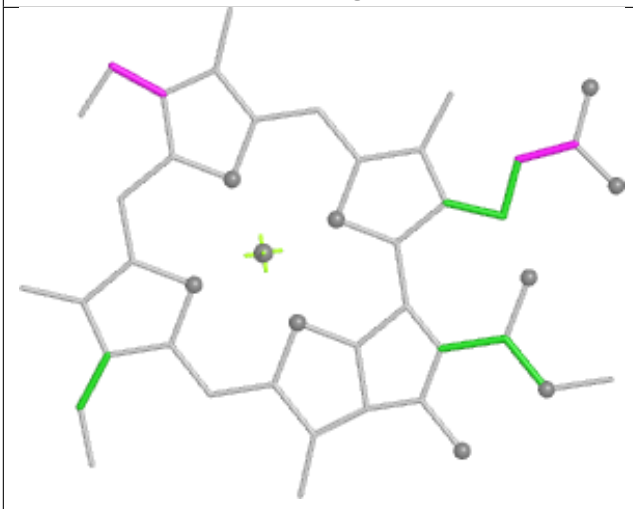
Ligand CLA U 207



Bond lengths



Bond angles

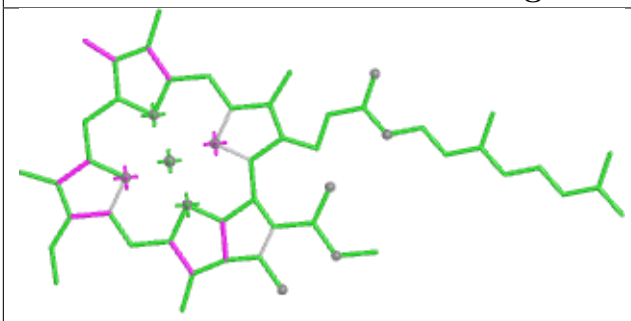


Torsions

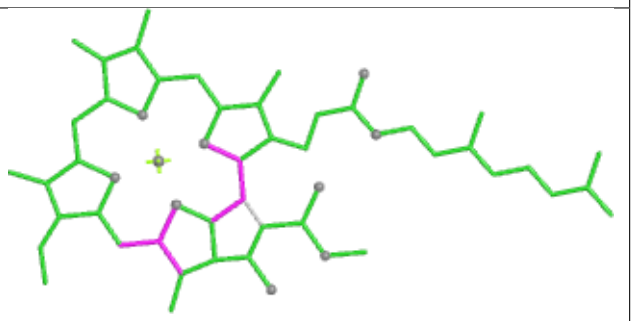


Rings

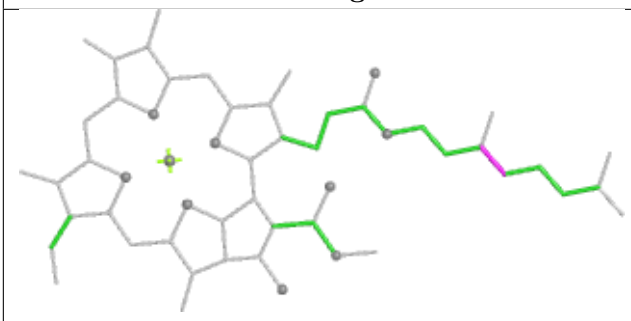
Ligand CLA B 810



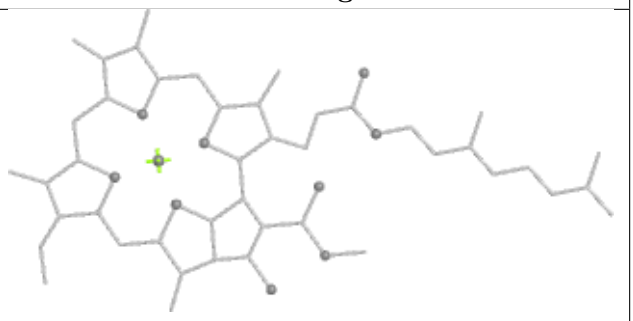
Bond lengths



Bond angles

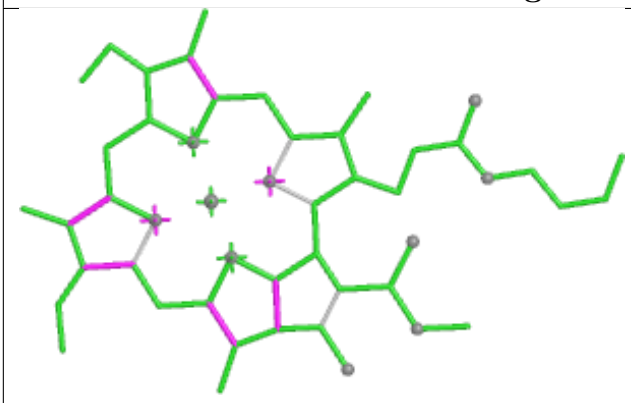


Torsions

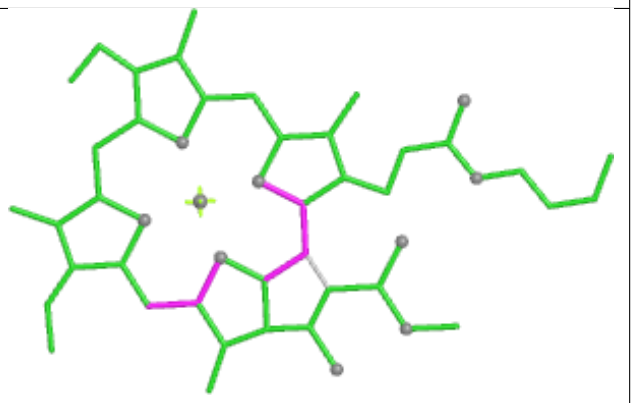


Rings

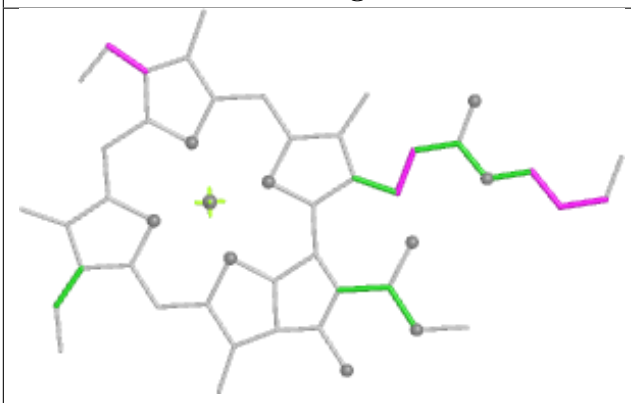
Ligand CLA B 827



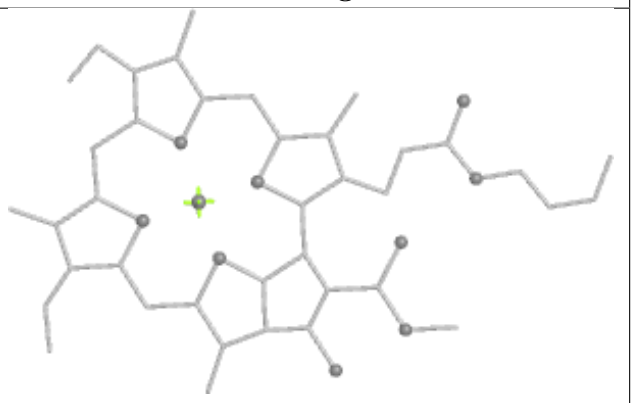
Bond lengths



Bond angles

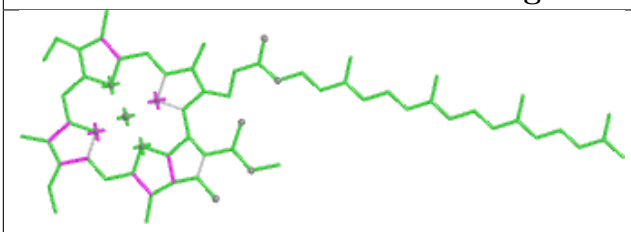


Torsions

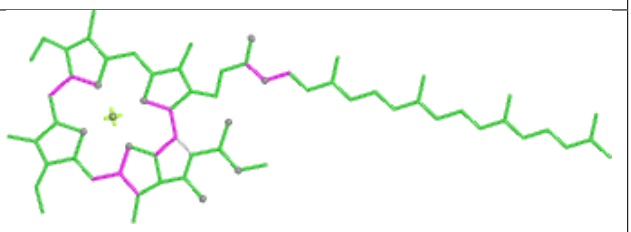


Rings

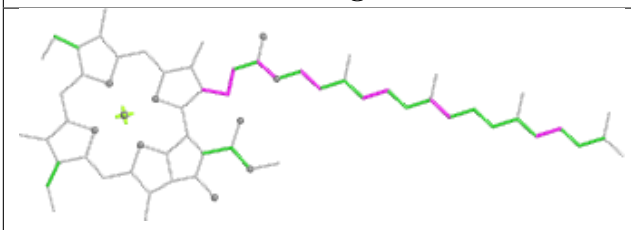
Ligand CLA A 833



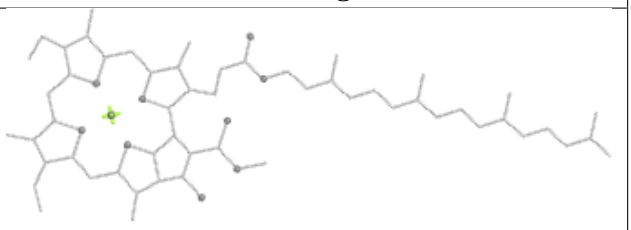
Bond lengths



Bond angles

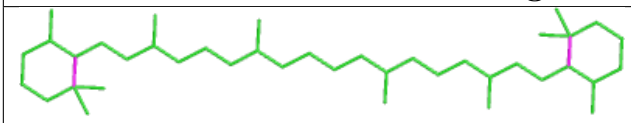


Torsions

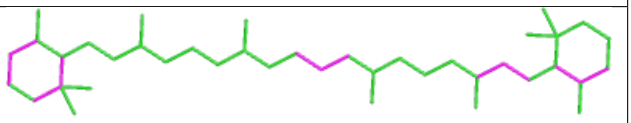


Rings

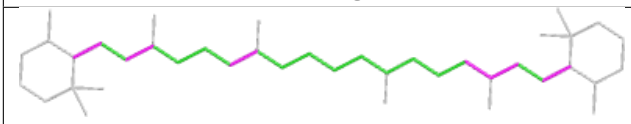
Ligand BCR J 104



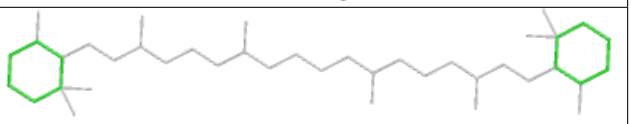
Bond lengths



Bond angles

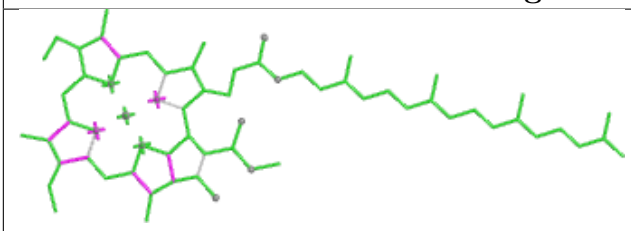


Torsions

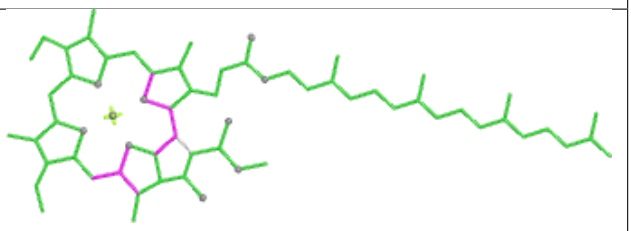


Rings

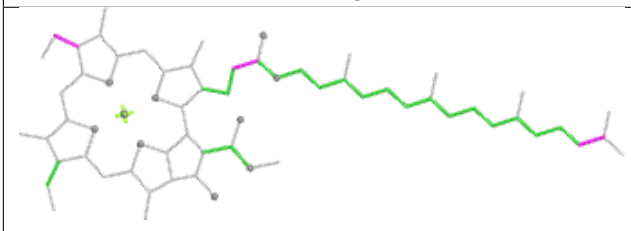
Ligand CLA B 806



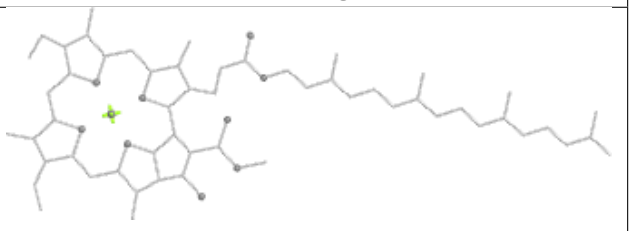
Bond lengths



Bond angles

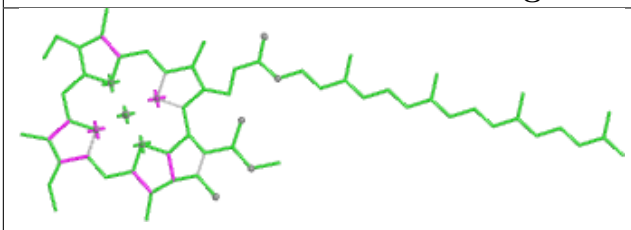


Torsions

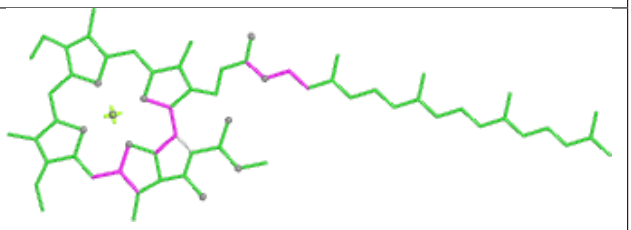


Rings

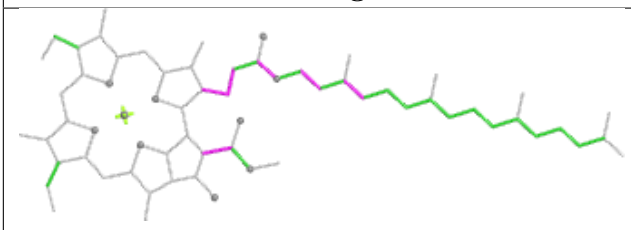
Ligand CLA A 806



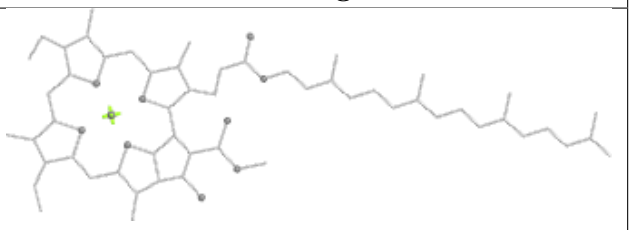
Bond lengths



Bond angles

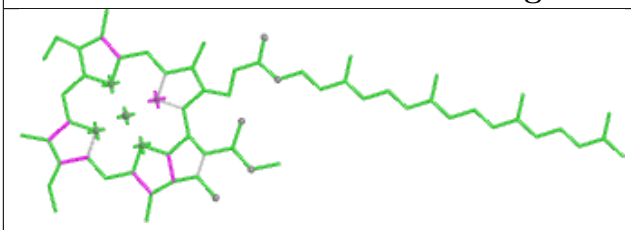


Torsions

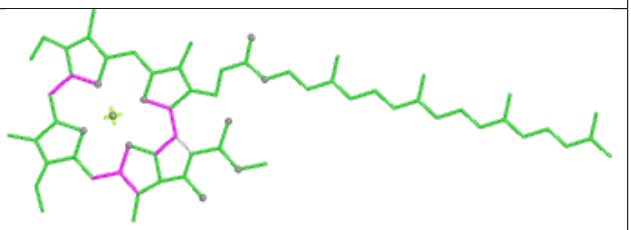


Rings

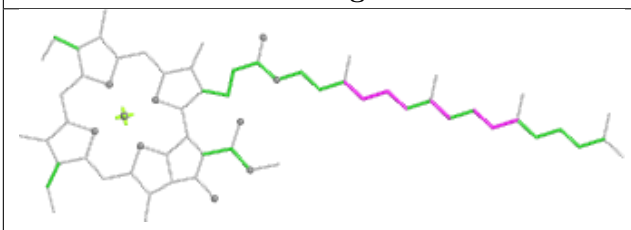
Ligand CLA B 829



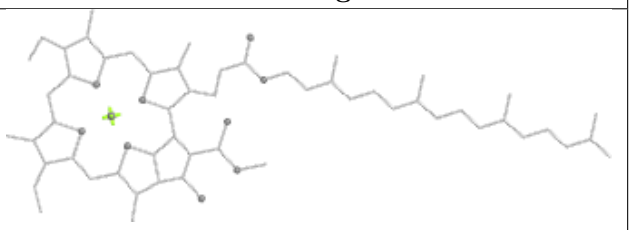
Bond lengths



Bond angles

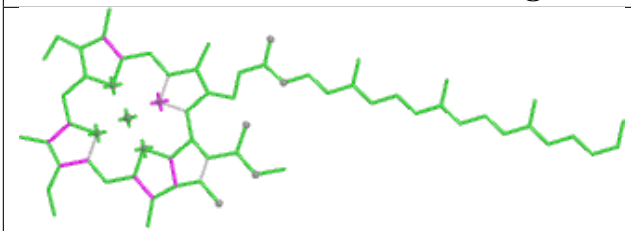


Torsions

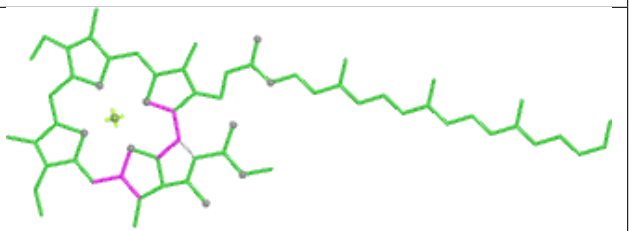


Rings

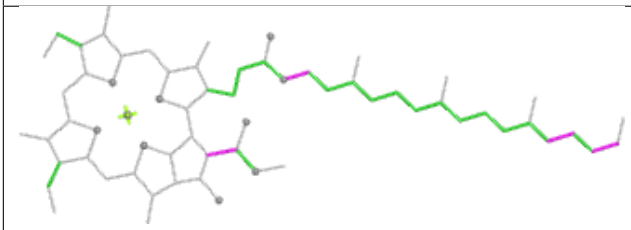
Ligand CLA B 821



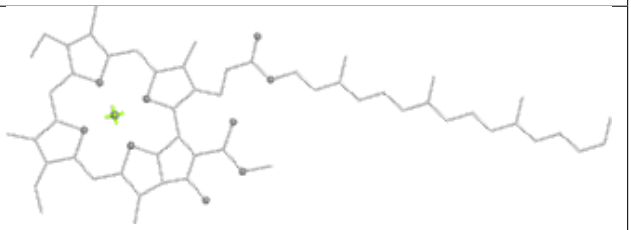
Bond lengths



Bond angles

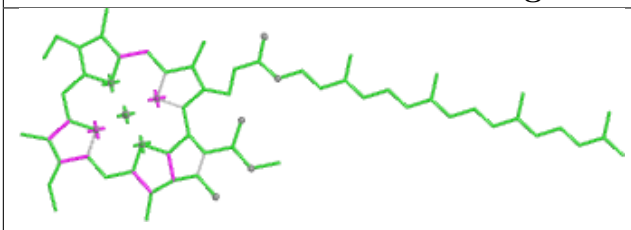


Torsions

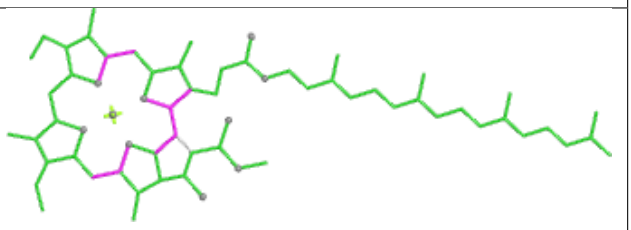


Rings

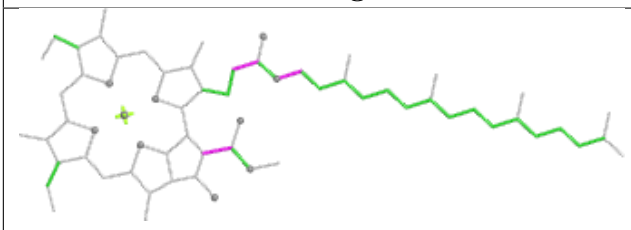
Ligand CLA B 802



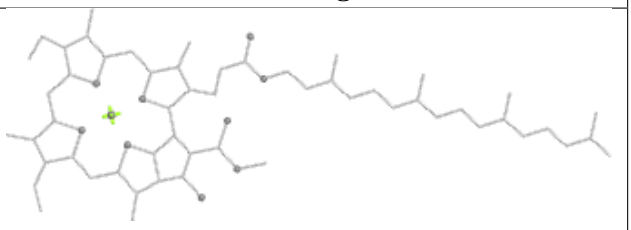
Bond lengths



Bond angles

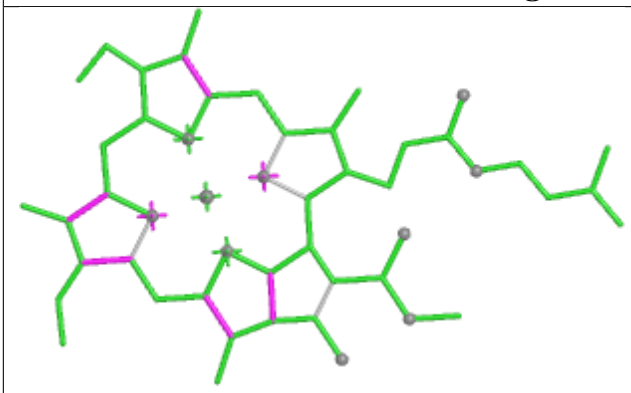


Torsions

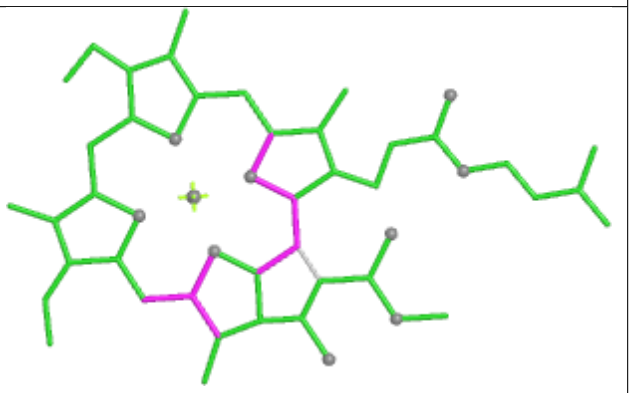


Rings

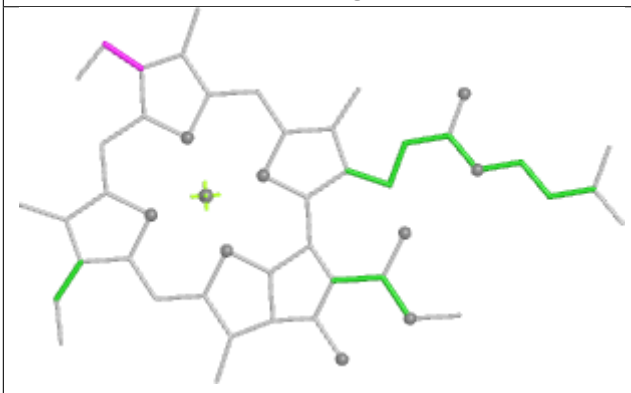
Ligand CLA A 813



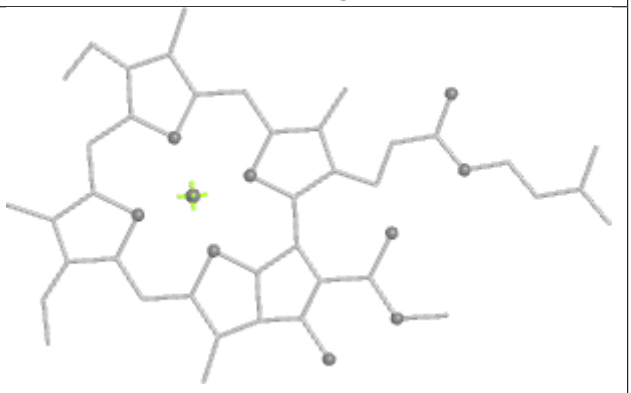
Bond lengths



Bond angles

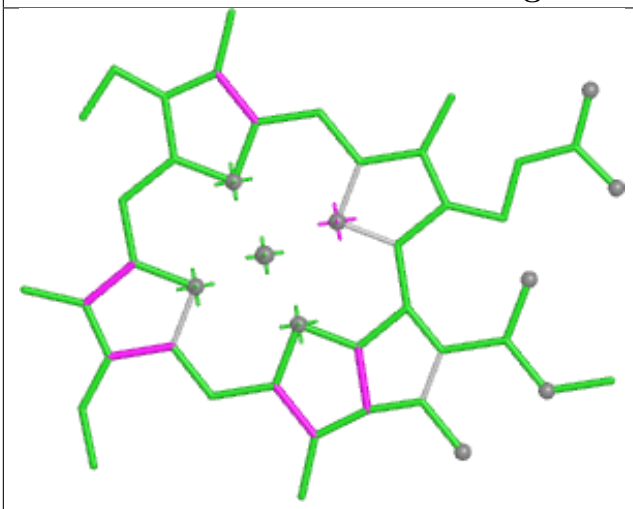


Torsions

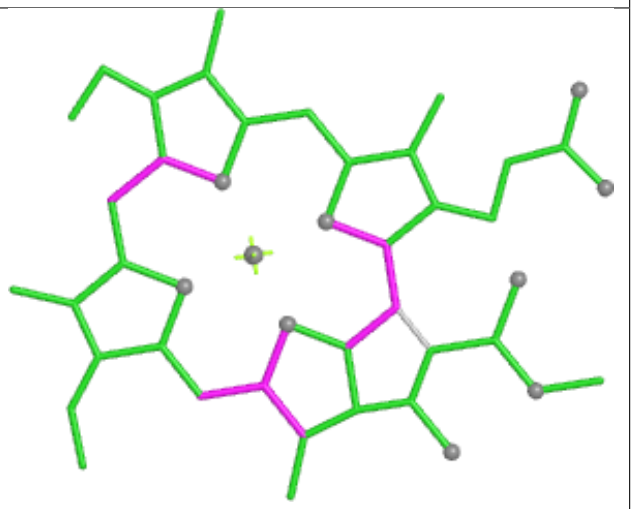


Rings

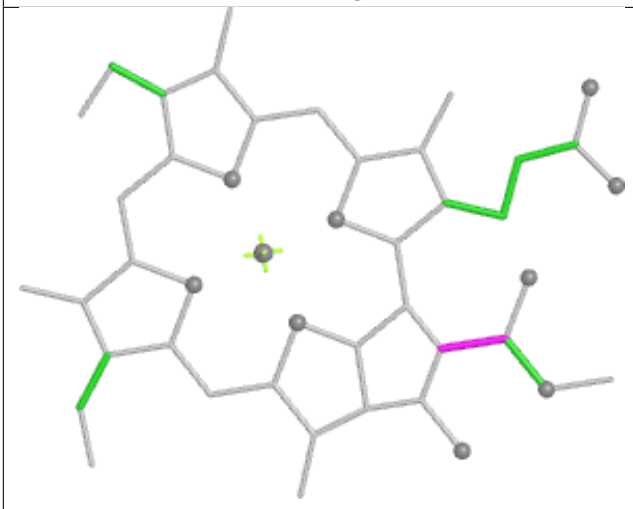
Ligand CLA A 831



Bond lengths



Bond angles

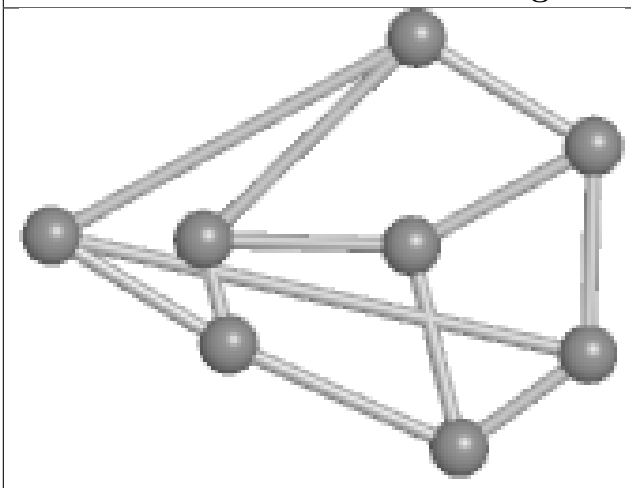


Torsions

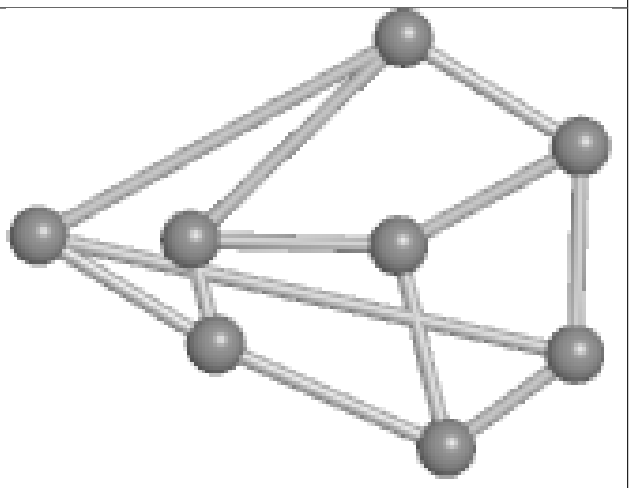


Rings

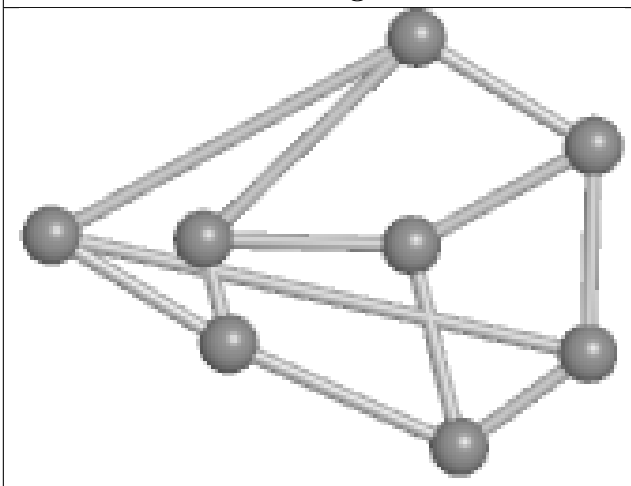
Ligand SF4 C 101



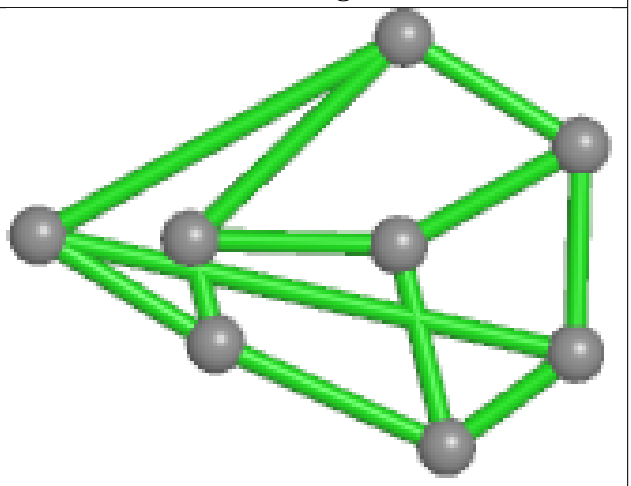
Bond lengths



Bond angles

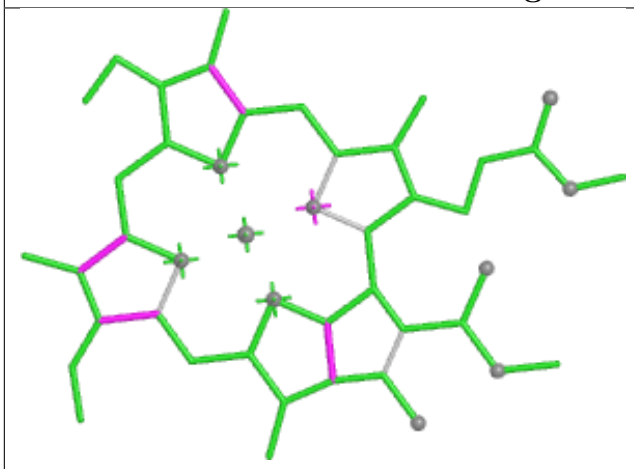


Torsions

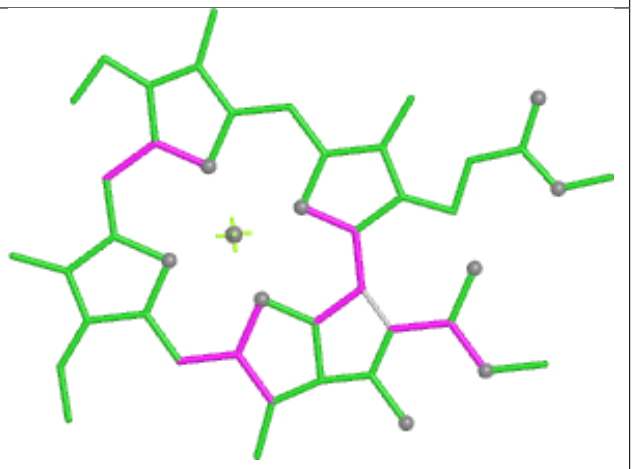


Rings

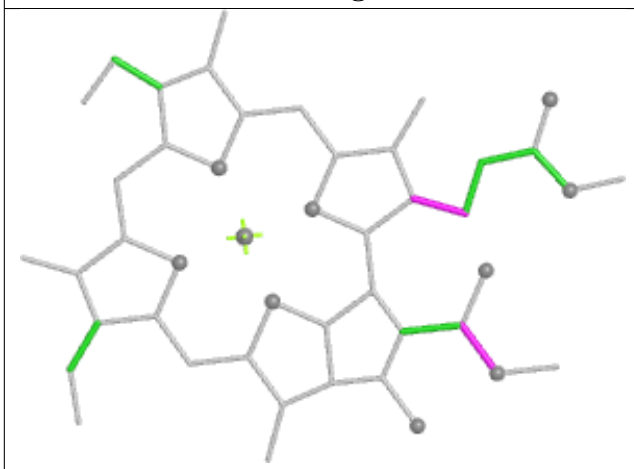
Ligand CLA U 209



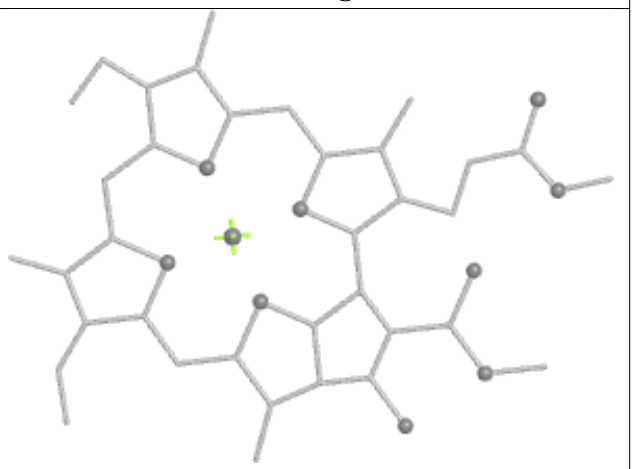
Bond lengths



Bond angles

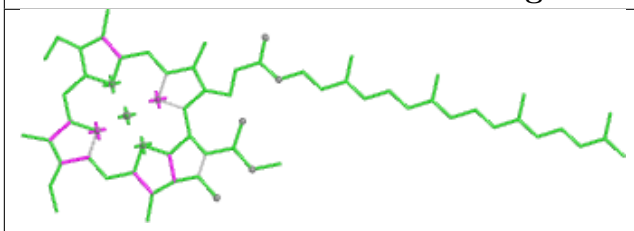


Torsions

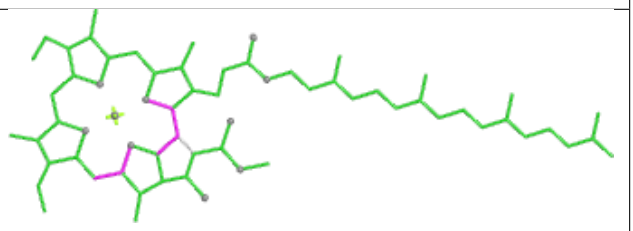


Rings

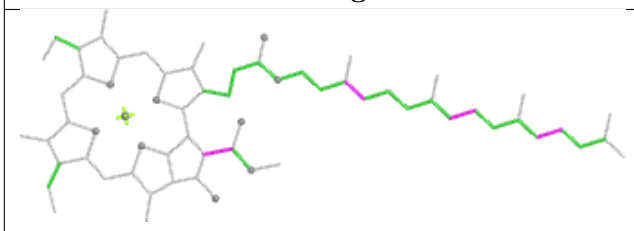
Ligand CLA B 807



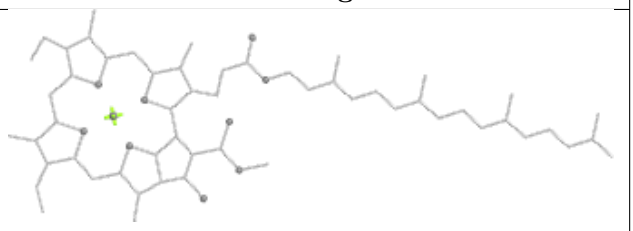
Bond lengths



Bond angles

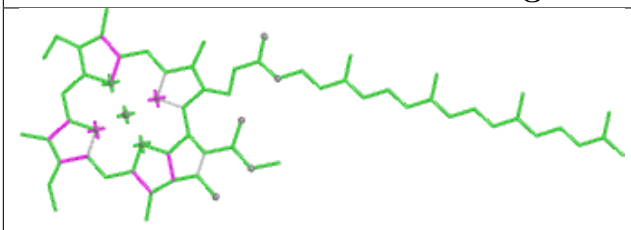


Torsions

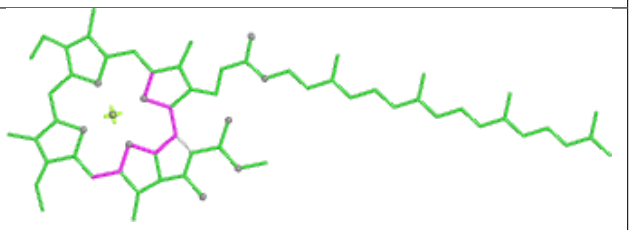


Rings

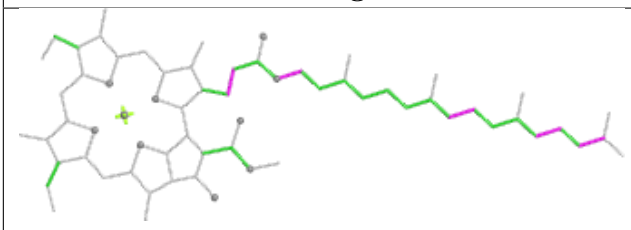
Ligand CLA A 807



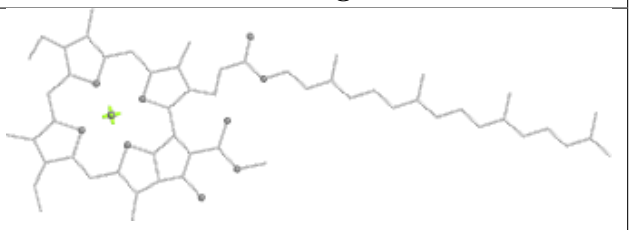
Bond lengths



Bond angles

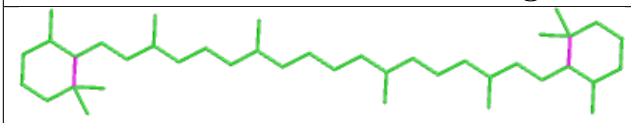


Torsions

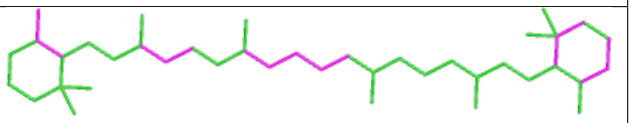


Rings

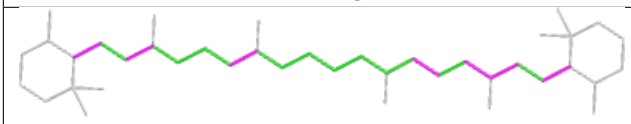
Ligand BCR A 843



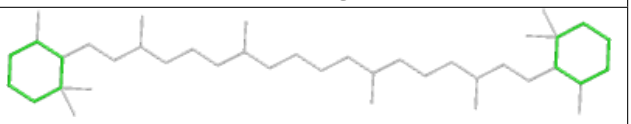
Bond lengths



Bond angles

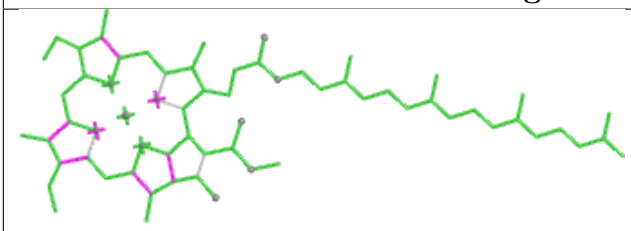


Torsions

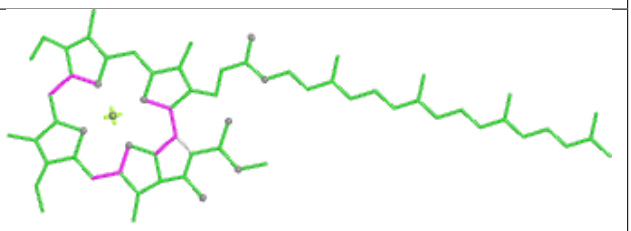


Rings

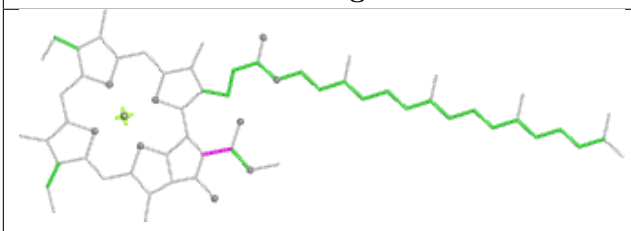
Ligand CLA A 835



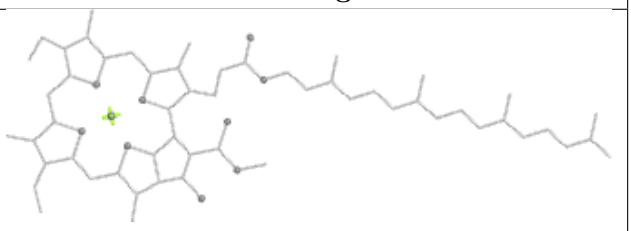
Bond lengths



Bond angles

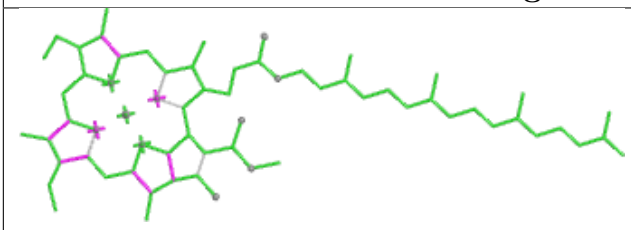


Torsions

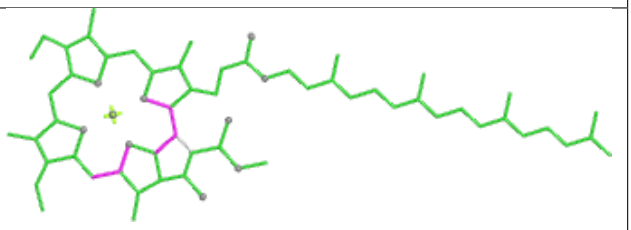


Rings

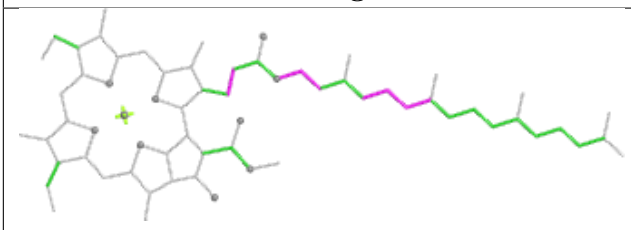
Ligand CLA A 836



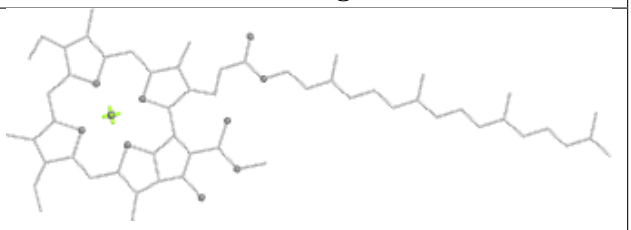
Bond lengths



Bond angles

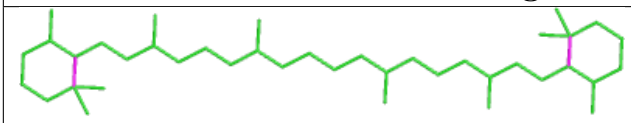


Torsions

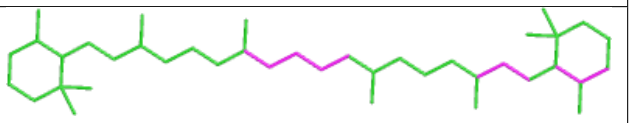


Rings

Ligand BCR A 841



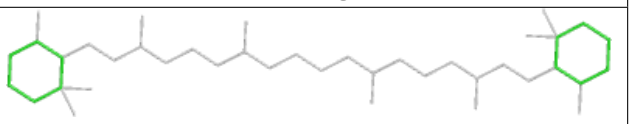
Bond lengths



Bond angles

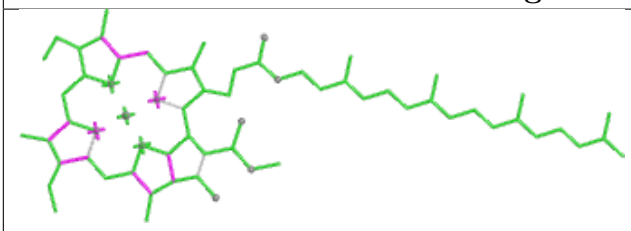


Torsions

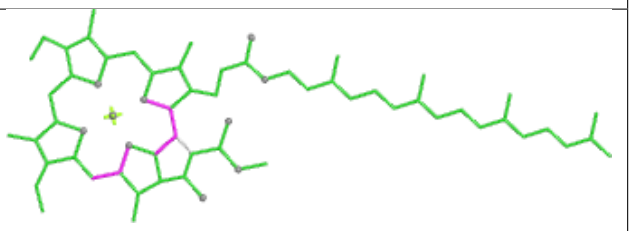


Rings

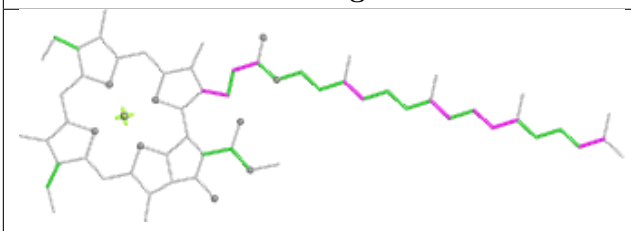
Ligand CLA B 823



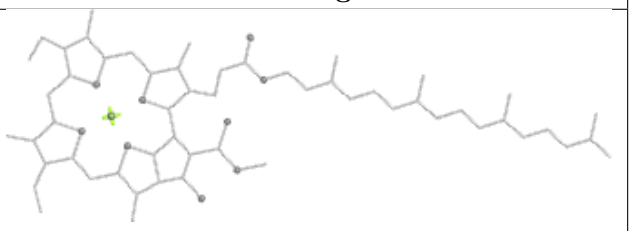
Bond lengths



Bond angles

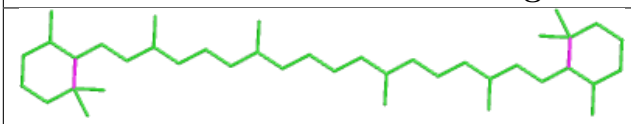


Torsions

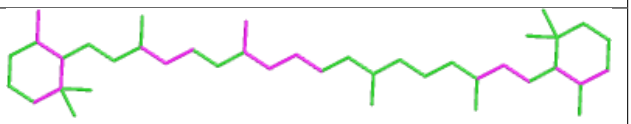


Rings

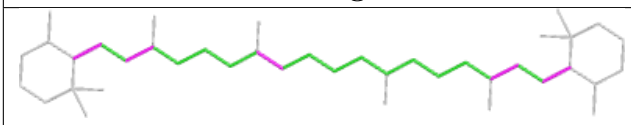
Ligand BCR F 804



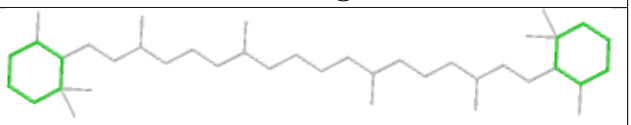
Bond lengths



Bond angles

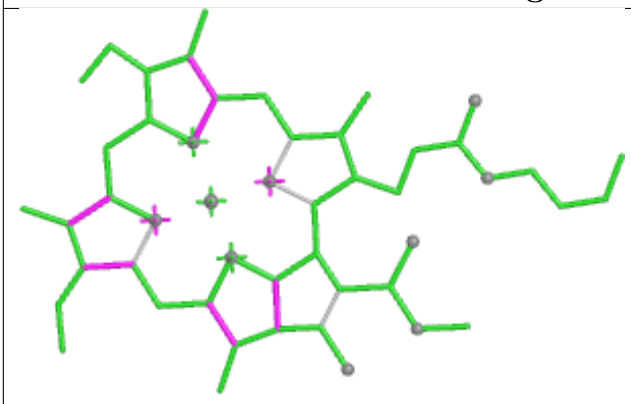


Torsions

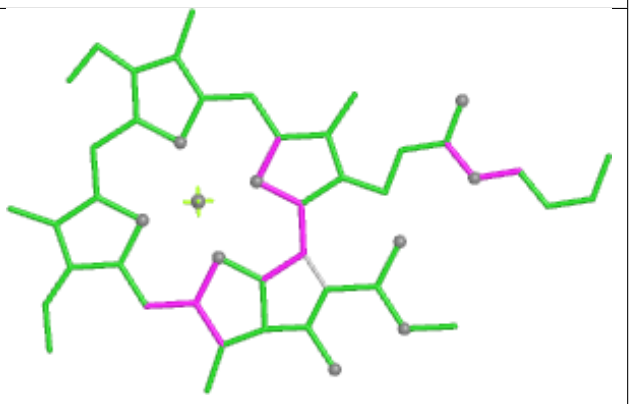


Rings

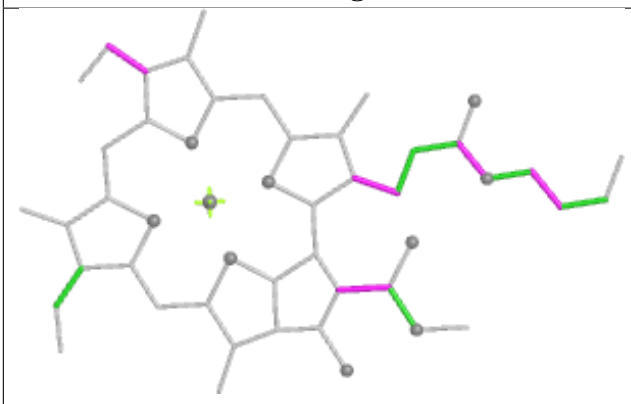
Ligand CLA L 202



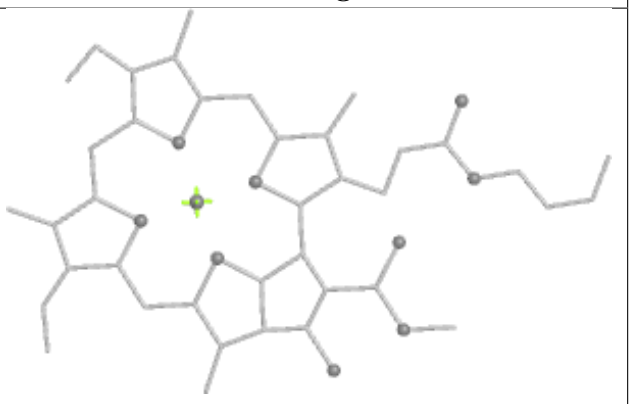
Bond lengths



Bond angles

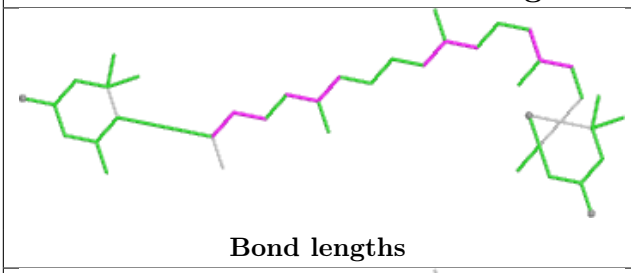


Torsions

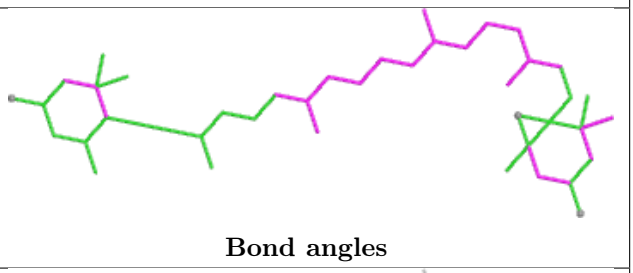


Rings

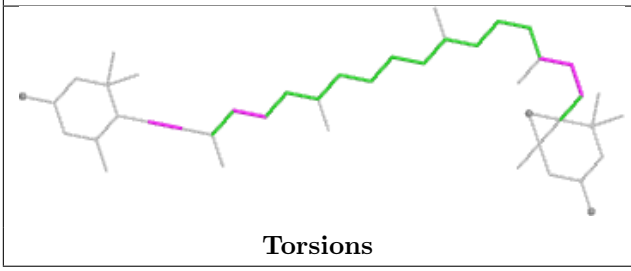
Ligand DD6 U 204



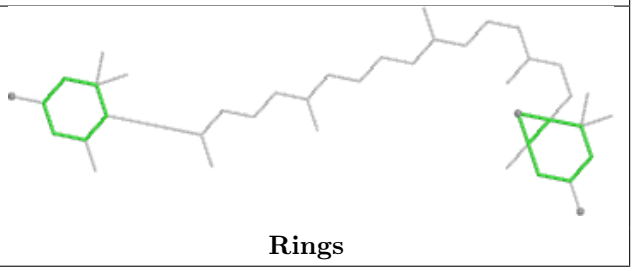
Bond lengths



Bond angles

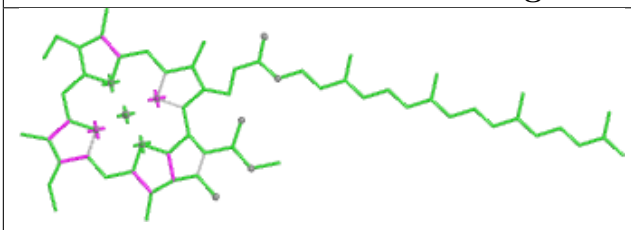


Torsions

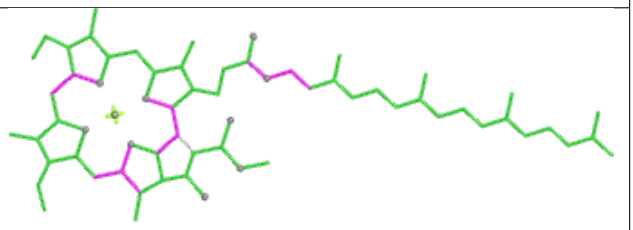


Rings

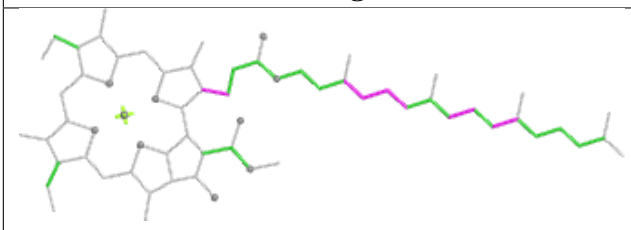
Ligand CLA B 846



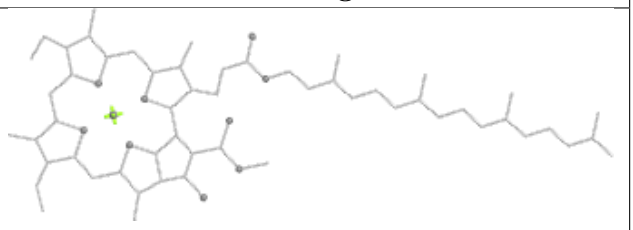
Bond lengths



Bond angles

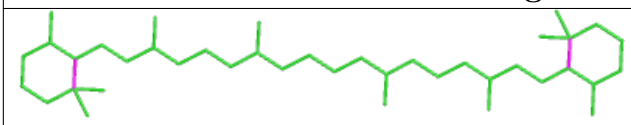


Torsions

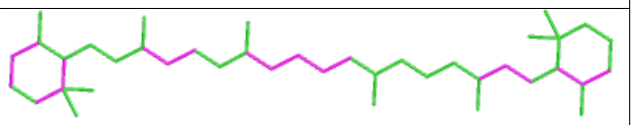


Rings

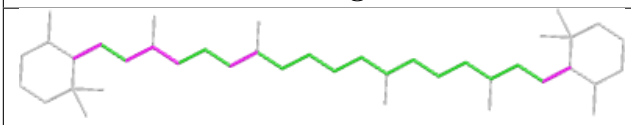
Ligand BCR L 205



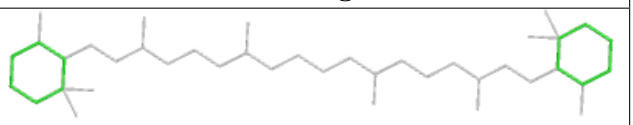
Bond lengths



Bond angles

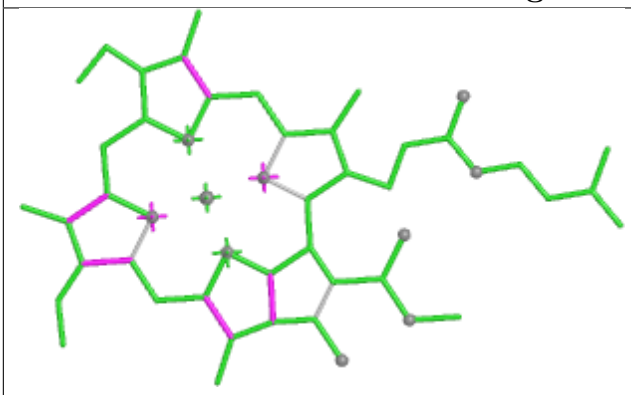


Torsions

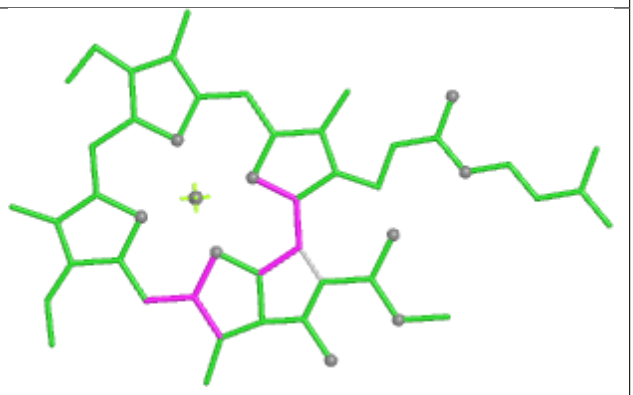


Rings

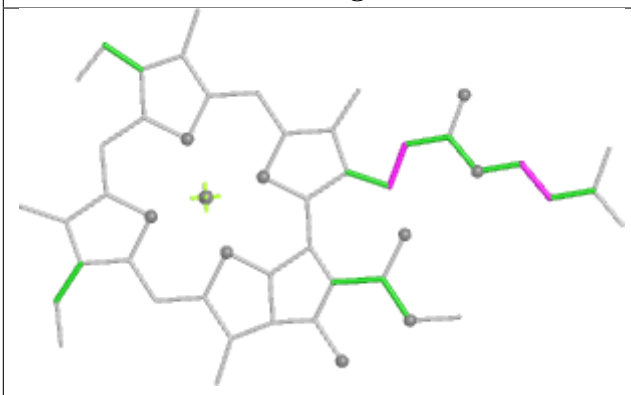
Ligand CLA L 204



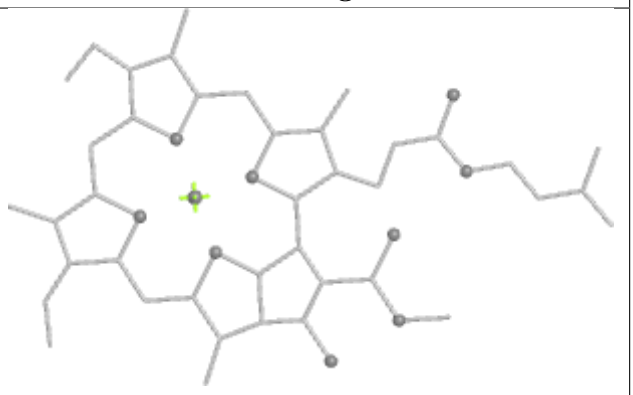
Bond lengths



Bond angles

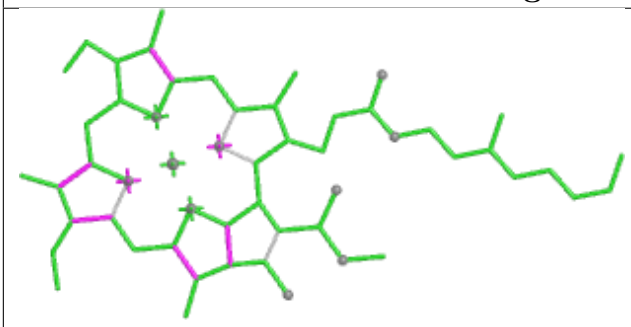


Torsions

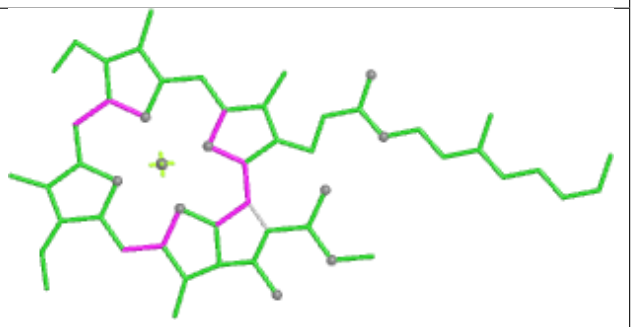


Rings

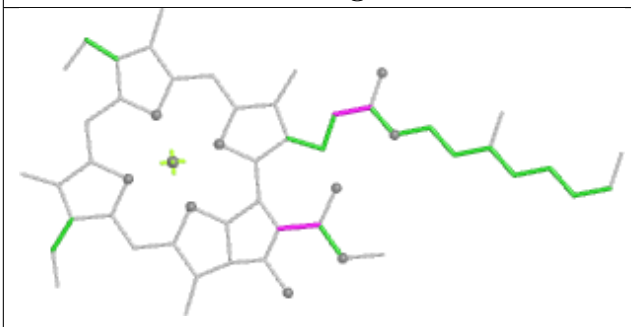
Ligand CLA A 810



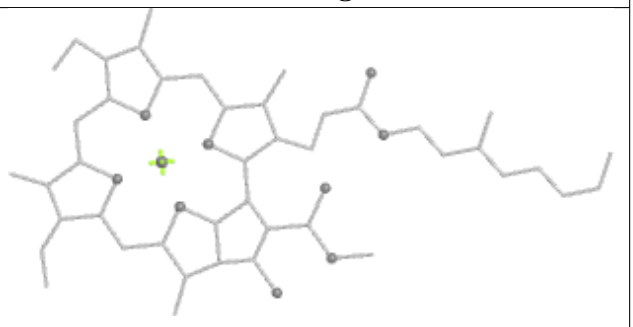
Bond lengths



Bond angles

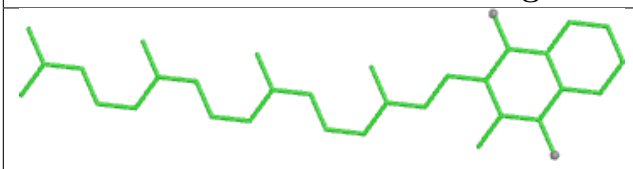


Torsions

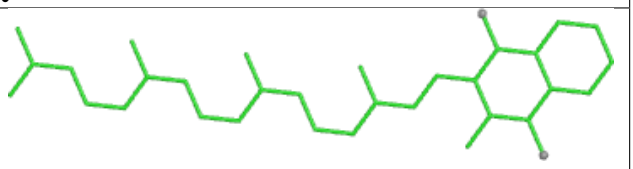


Rings

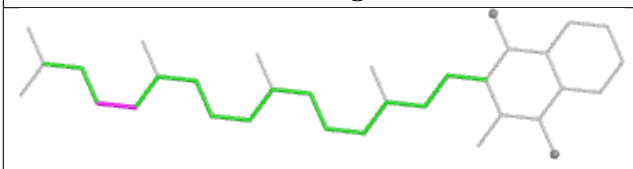
Ligand PQN B 836



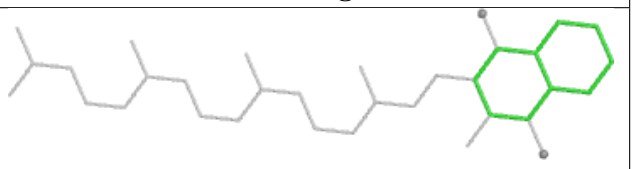
Bond lengths



Bond angles

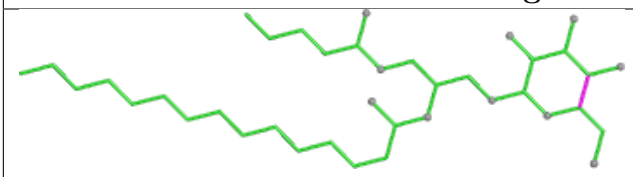


Torsions

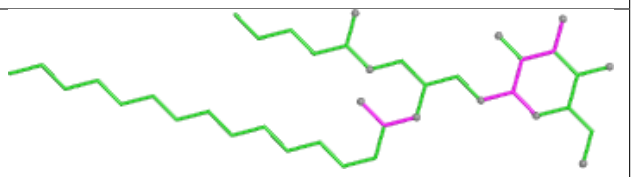


Rings

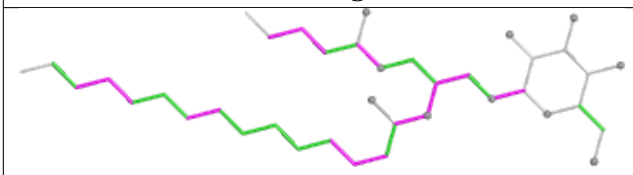
Ligand LMG J 102



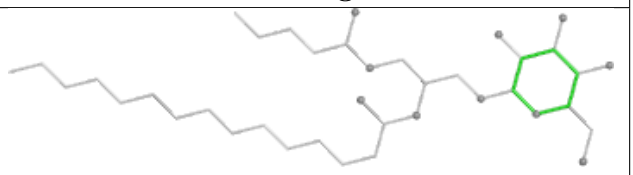
Bond lengths



Bond angles

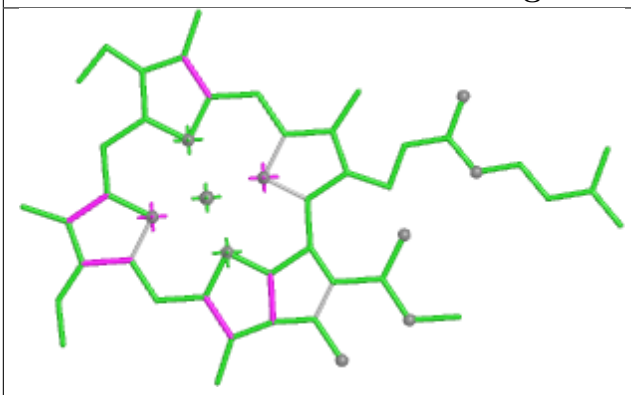


Torsions

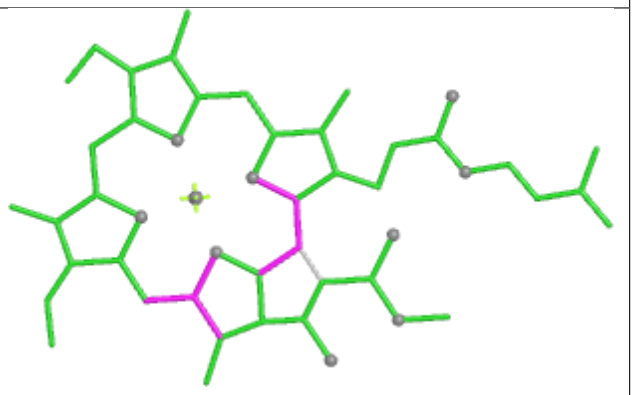


Rings

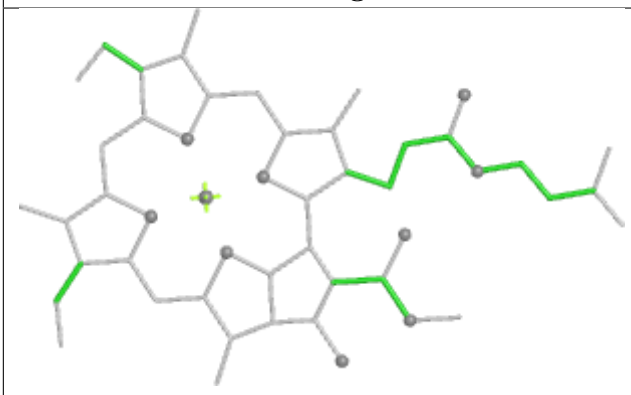
Ligand CLA A 830



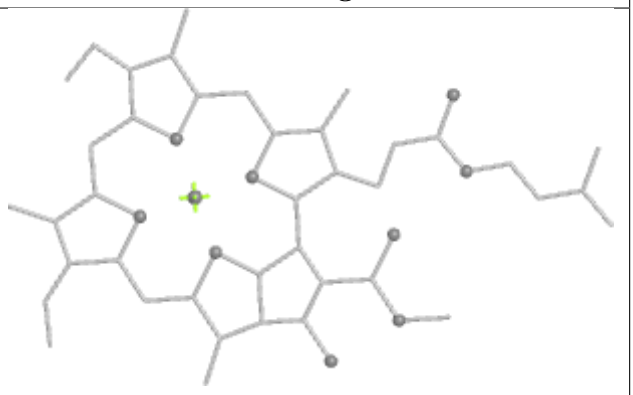
Bond lengths



Bond angles

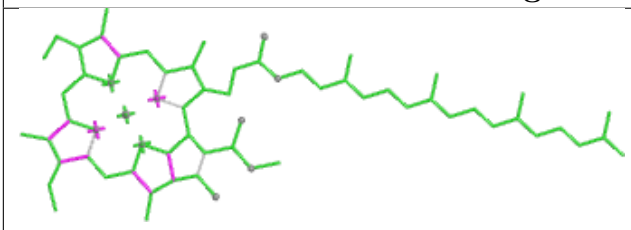


Torsions

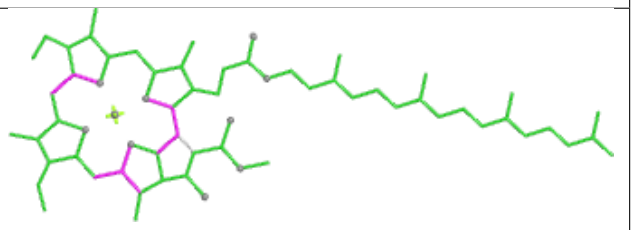


Rings

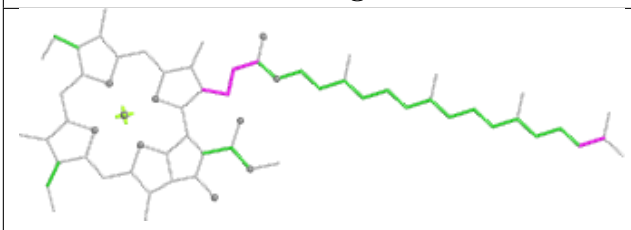
Ligand CLA A 815



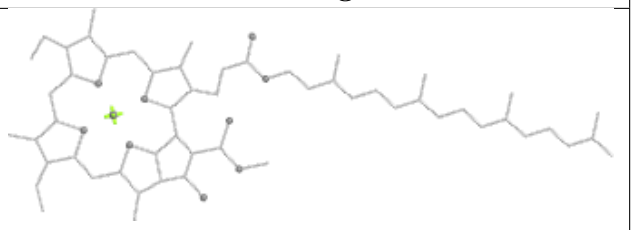
Bond lengths



Bond angles

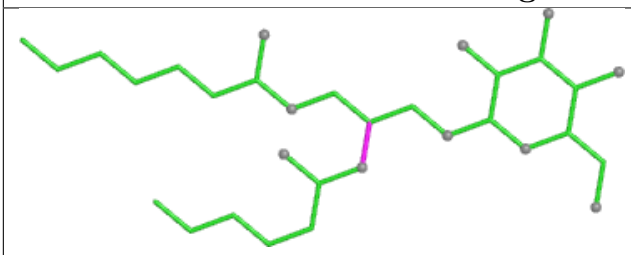


Torsions

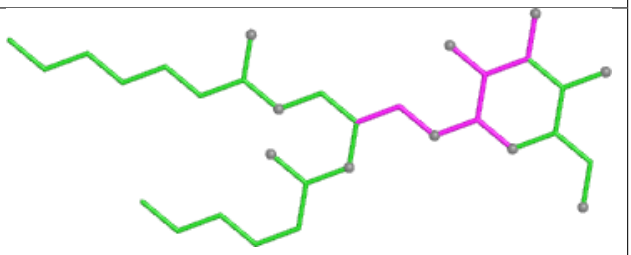


Rings

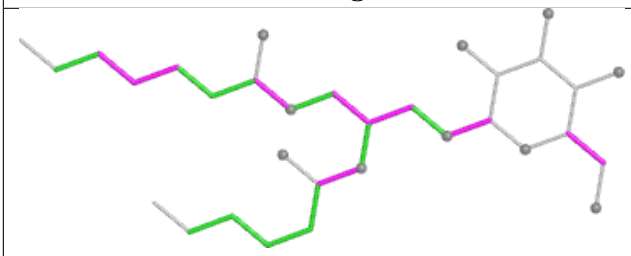
Ligand LMG U 202



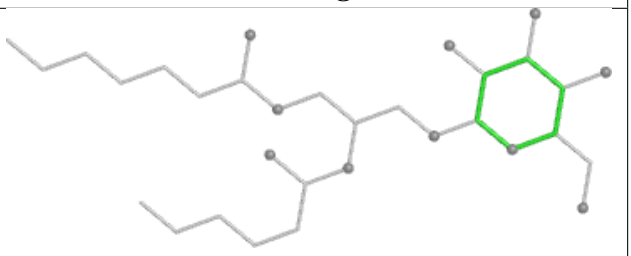
Bond lengths



Bond angles

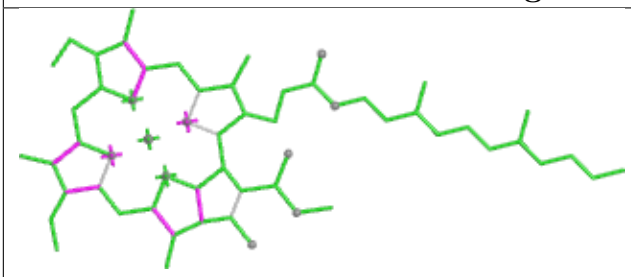


Torsions

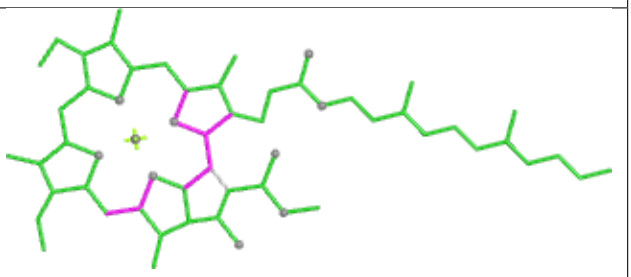


Rings

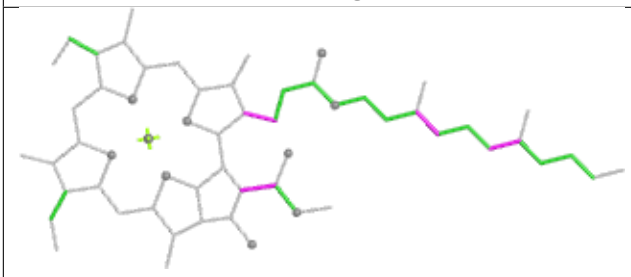
Ligand CLA B 828



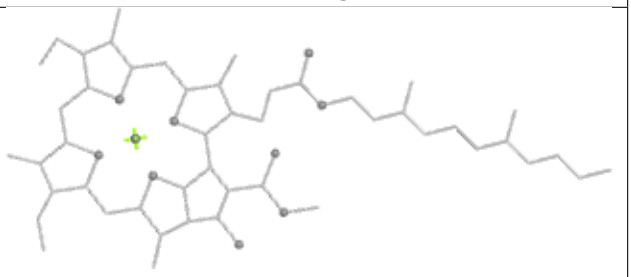
Bond lengths



Bond angles

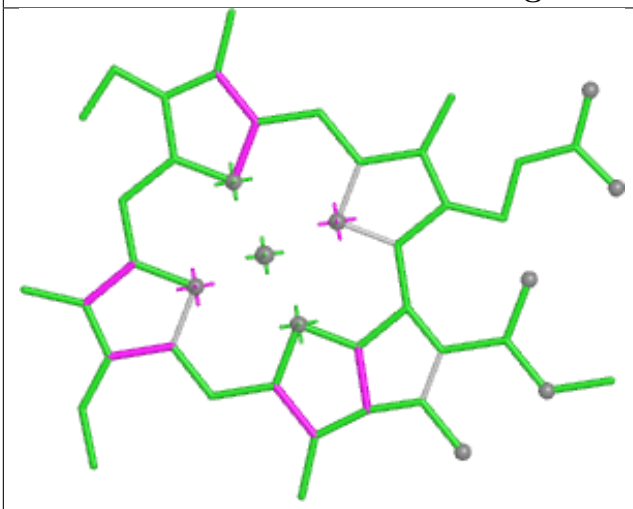


Torsions

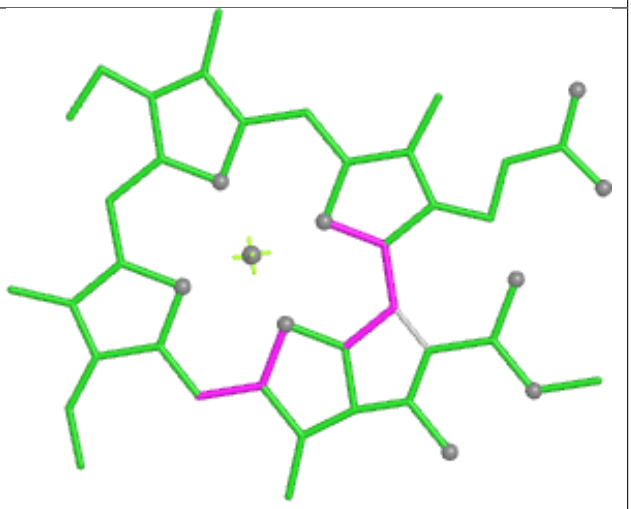


Rings

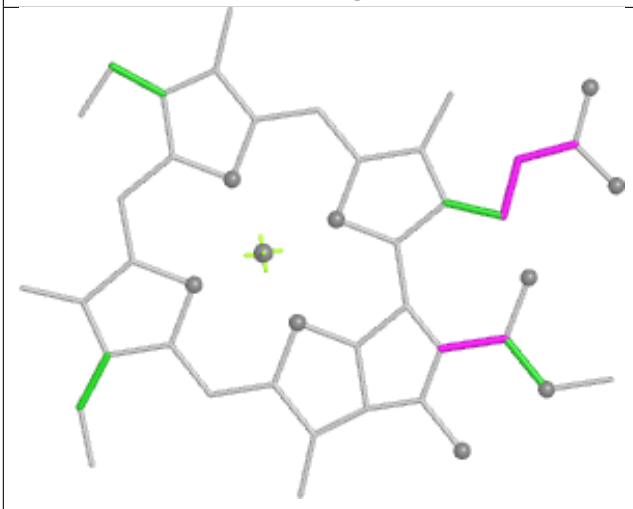
Ligand CLA B 804



Bond lengths



Bond angles

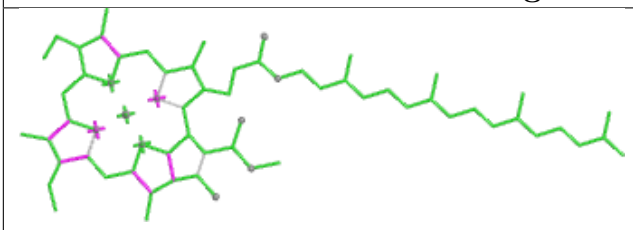


Torsions

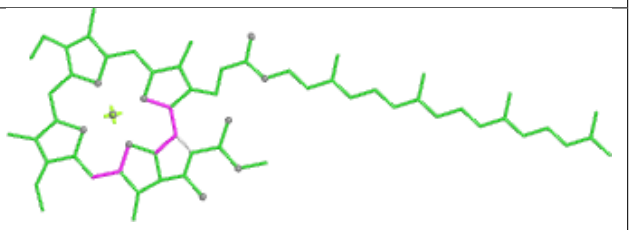


Rings

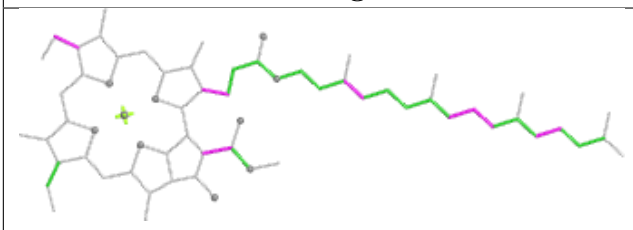
Ligand CLA A 850



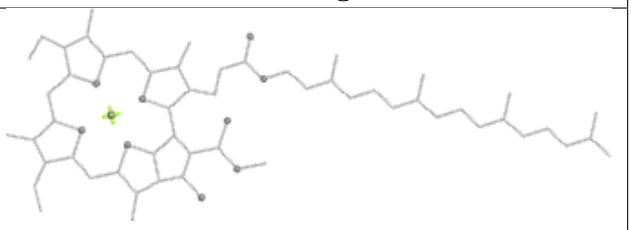
Bond lengths



Bond angles

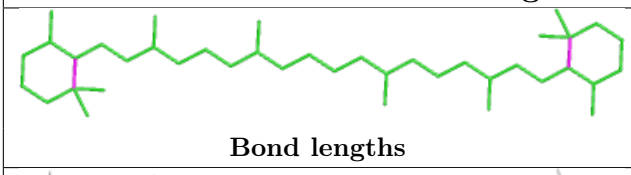


Torsions

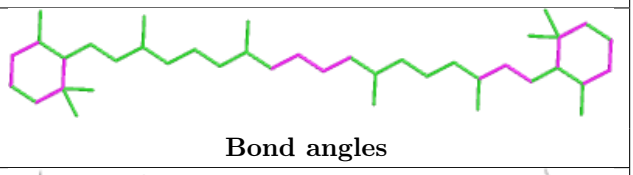


Rings

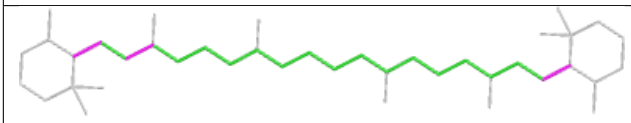
Ligand BCR A 842



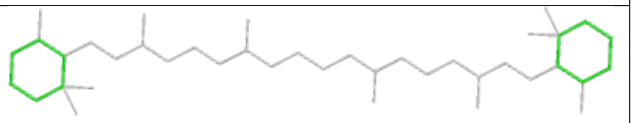
Bond lengths



Bond angles

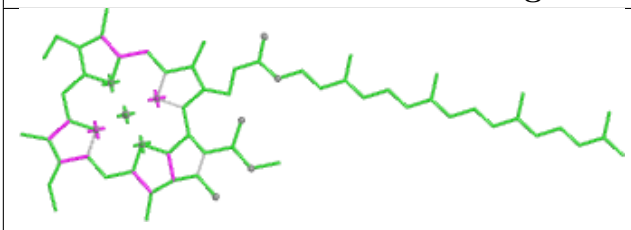


Torsions

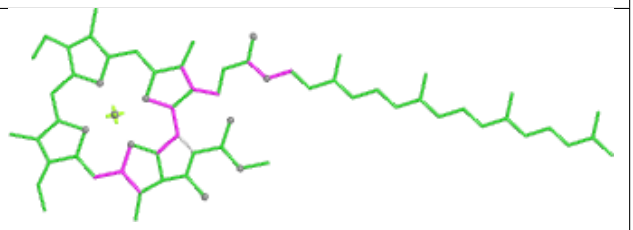


Rings

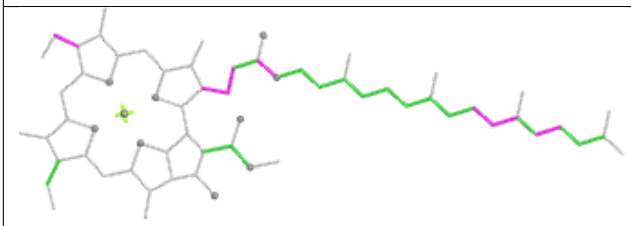
Ligand CLA B 844



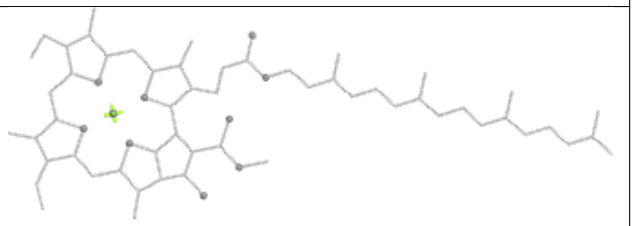
Bond lengths



Bond angles



Torsions

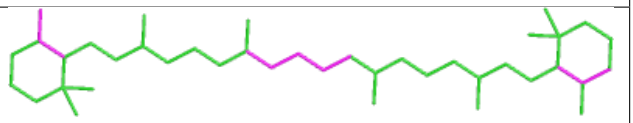


Rings

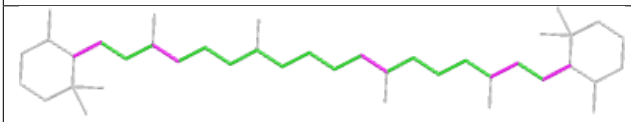
Ligand BCR L 201



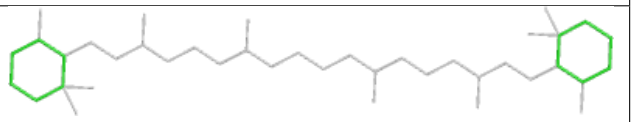
Bond lengths



Bond angles

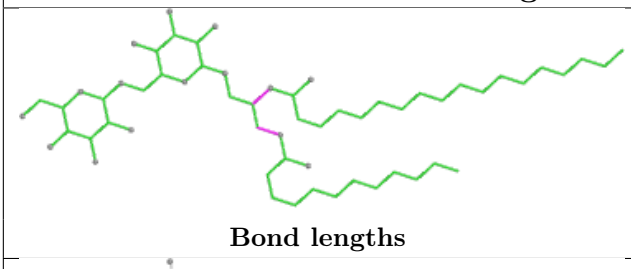


Torsions

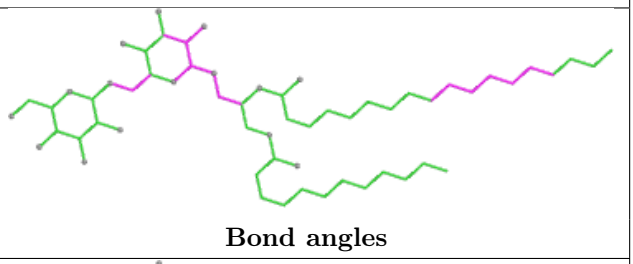


Rings

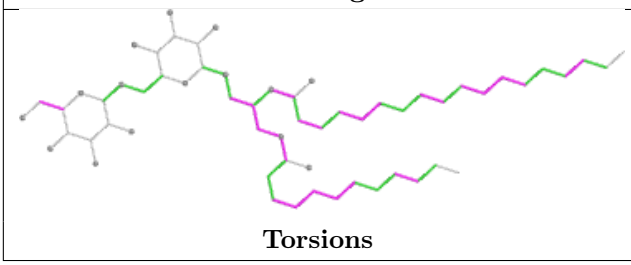
Ligand DGD B 842



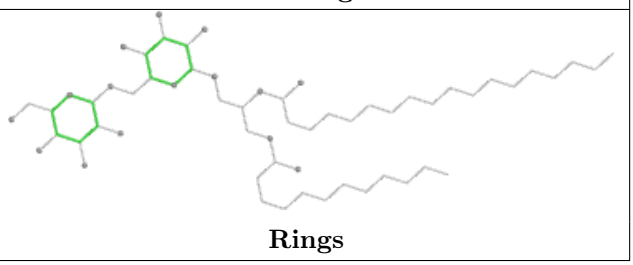
Bond lengths



Bond angles

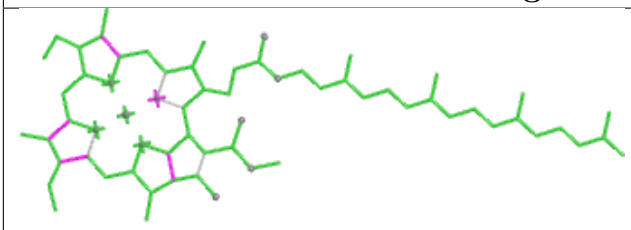


Torsions

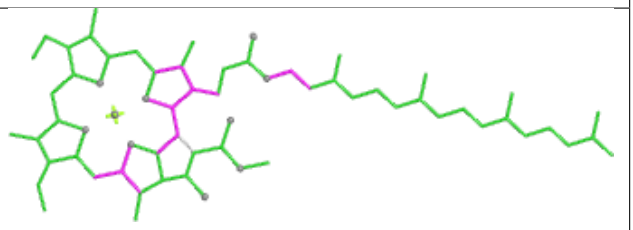


Rings

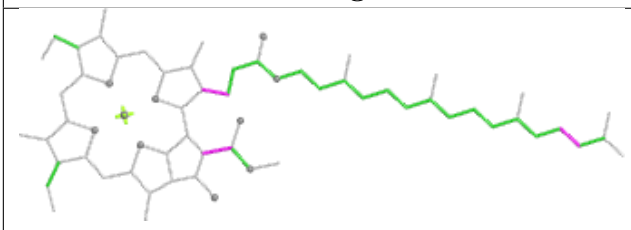
Ligand CLA U 208



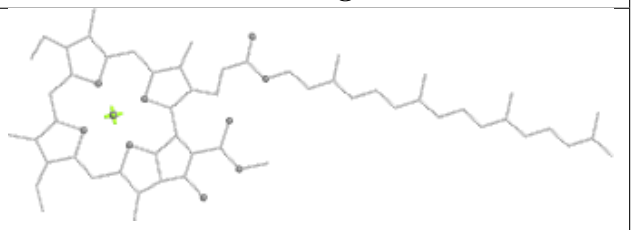
Bond lengths



Bond angles

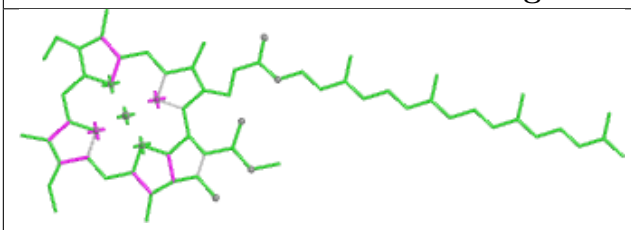


Torsions

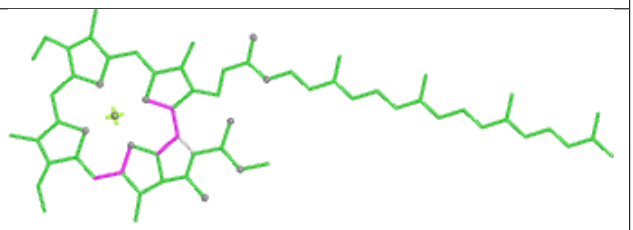


Rings

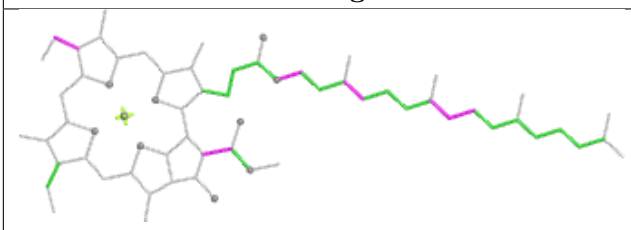
Ligand CLA A 848



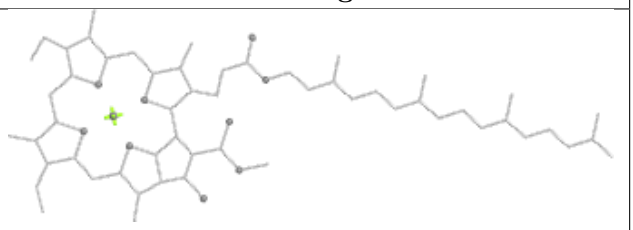
Bond lengths



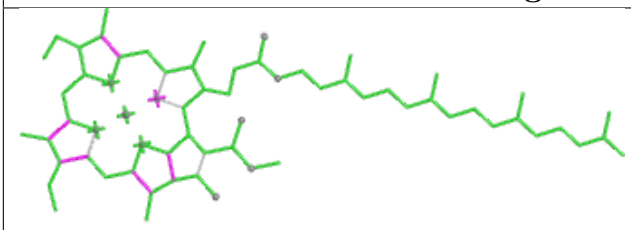
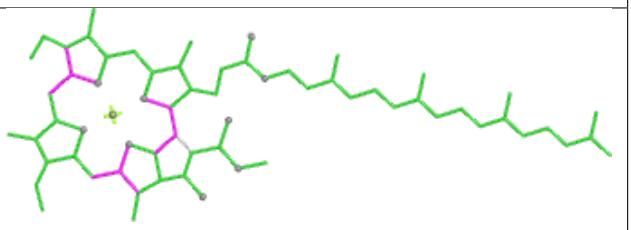
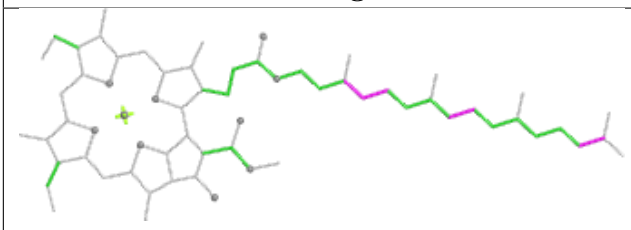
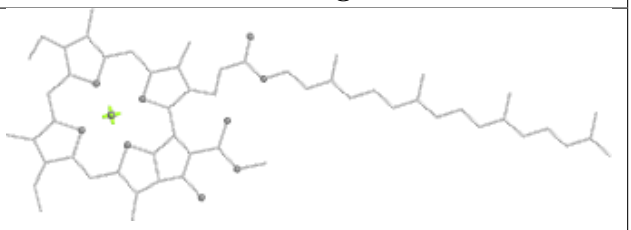
Bond angles

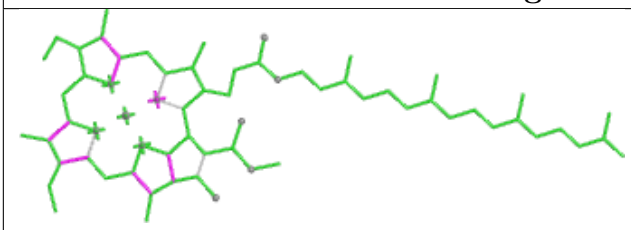
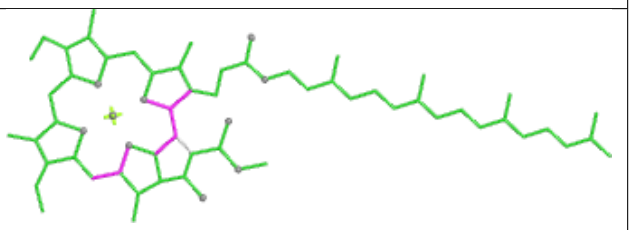
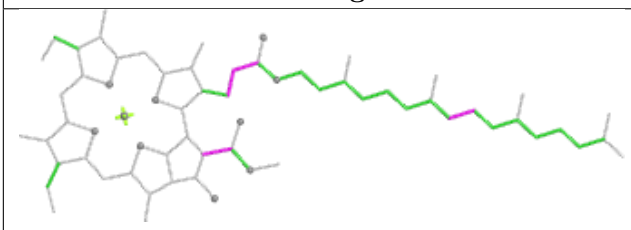
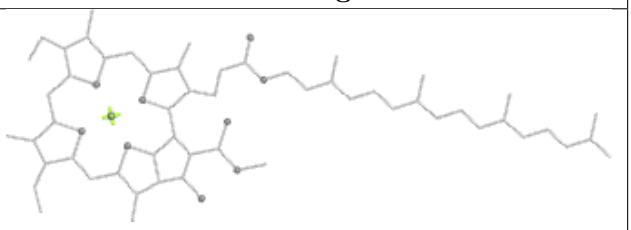


Torsions

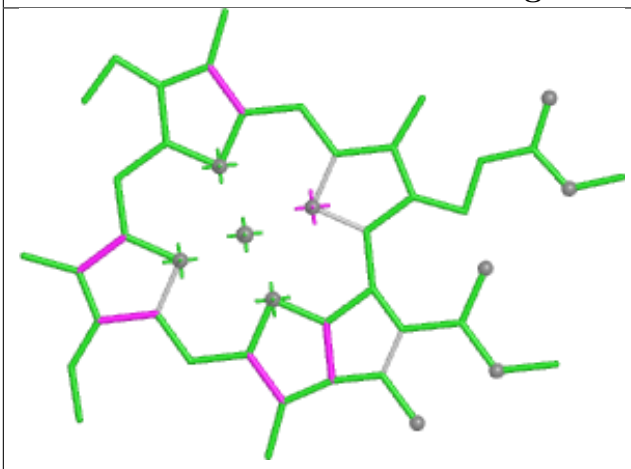


Rings

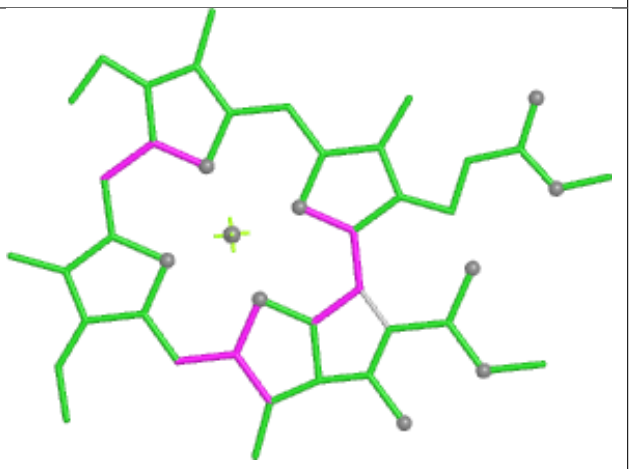
Ligand CLA B 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

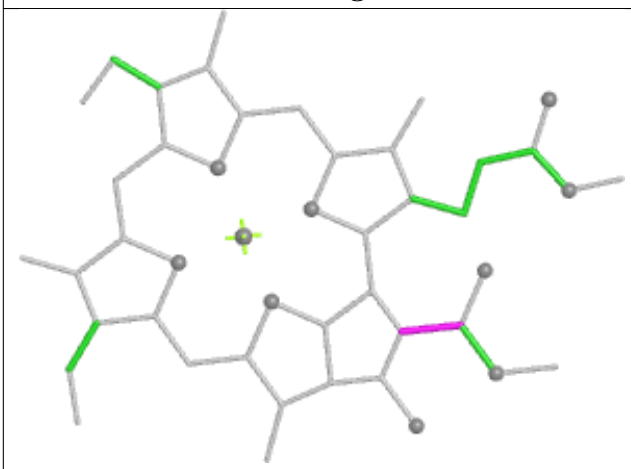
Ligand CLA B 818



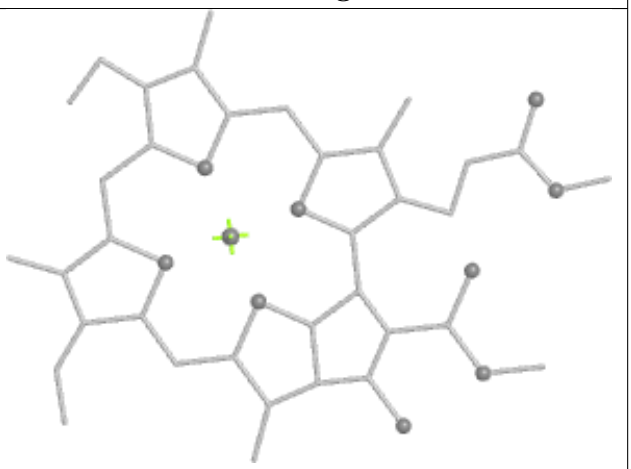
Bond lengths



Bond angles

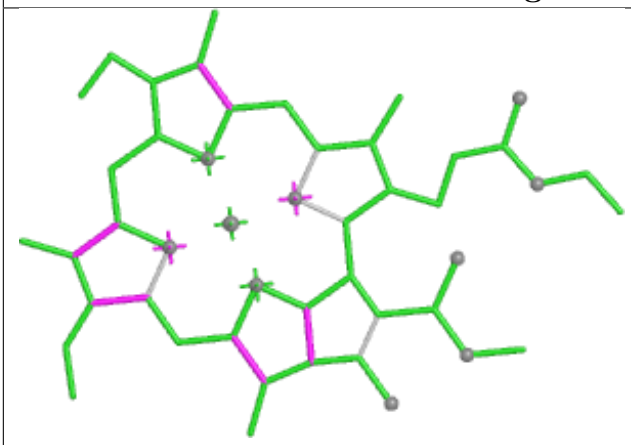


Torsions

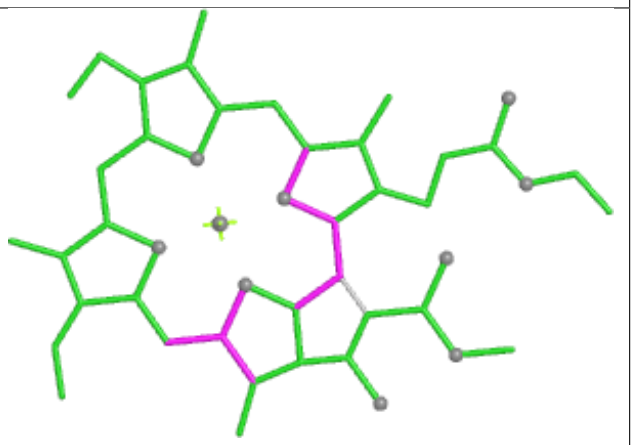


Rings

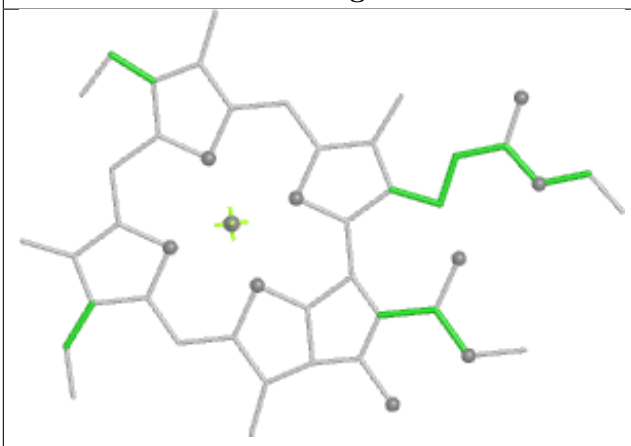
Ligand CLA B 832



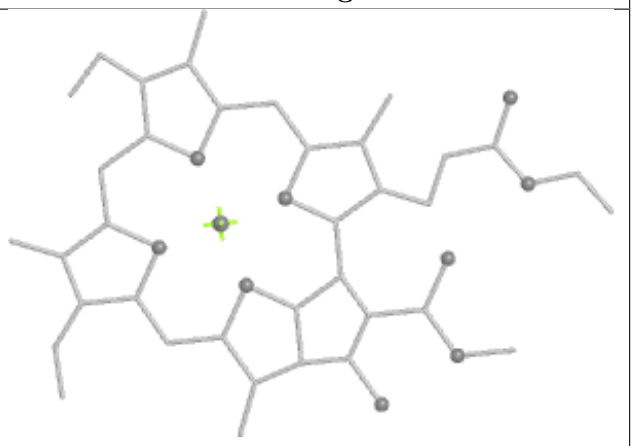
Bond lengths



Bond angles



Torsions

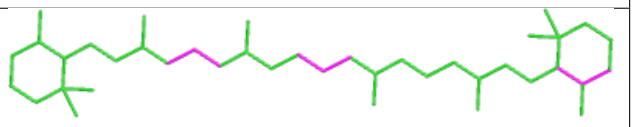


Rings

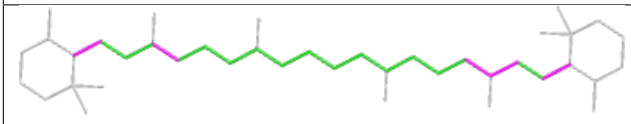
Ligand BCR B 841



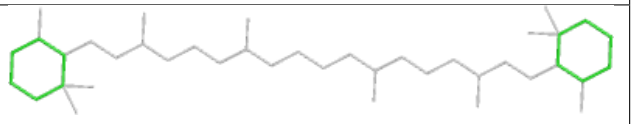
Bond lengths



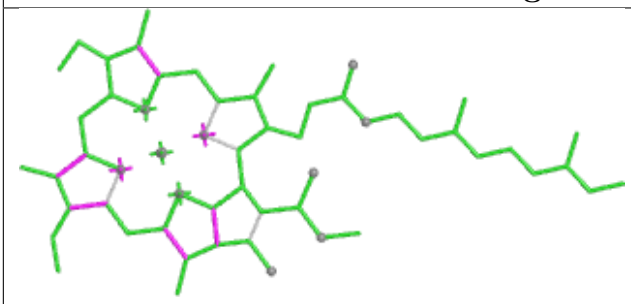
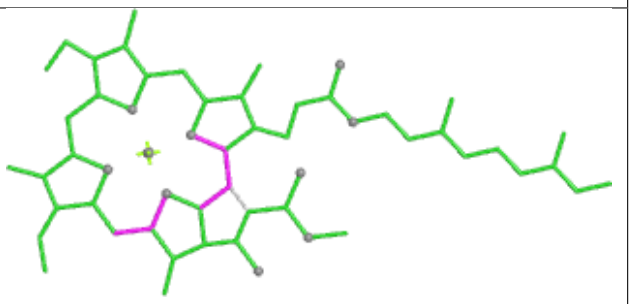
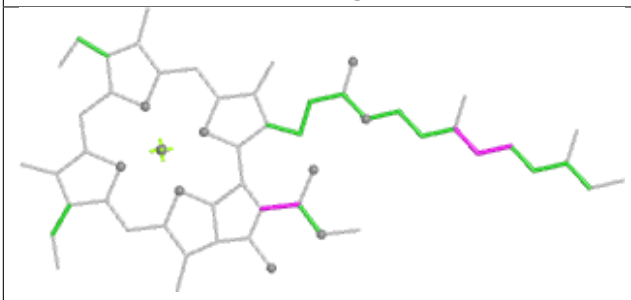
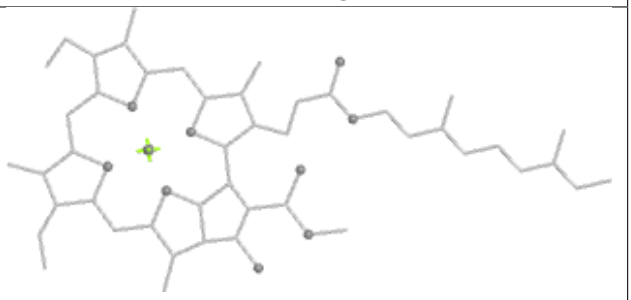
Bond angles

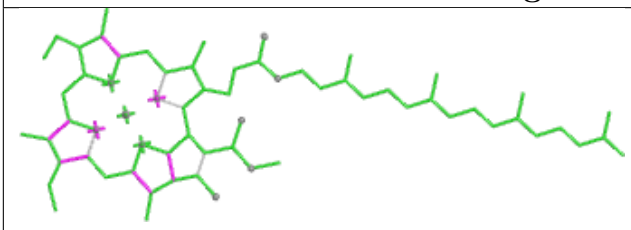
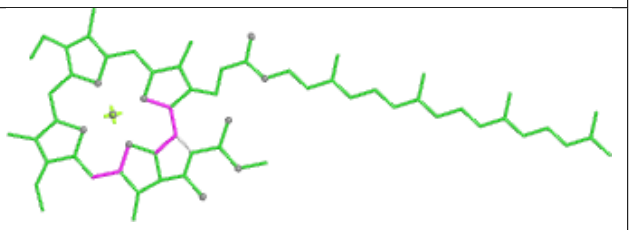
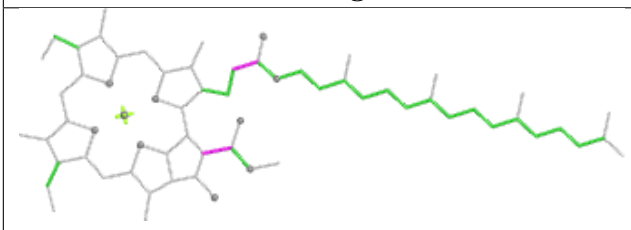
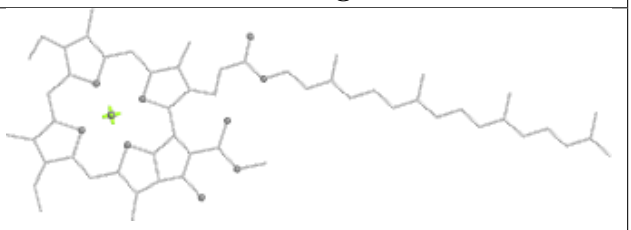


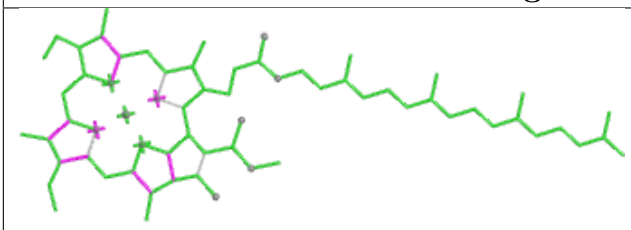
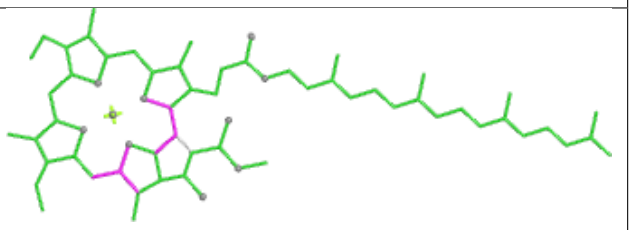
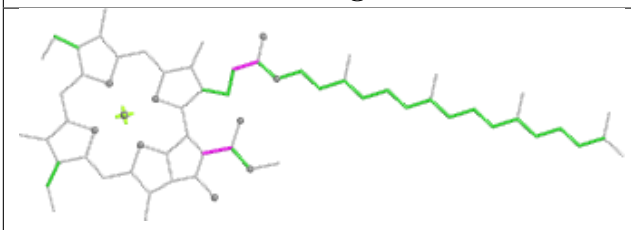
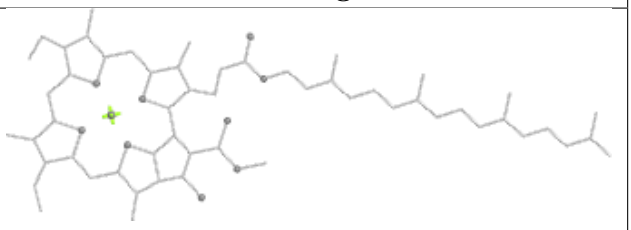
Torsions

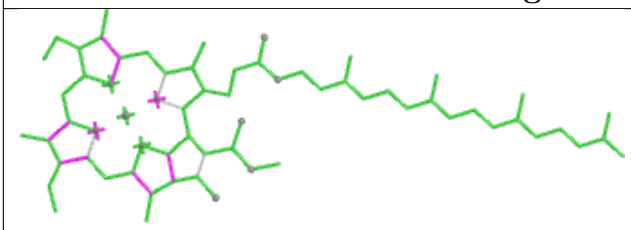
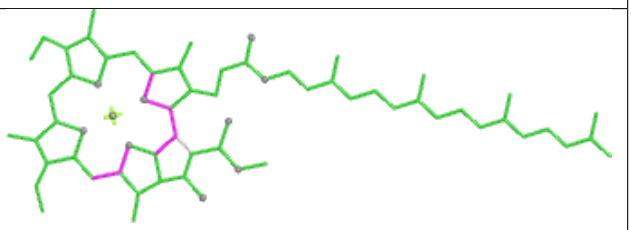
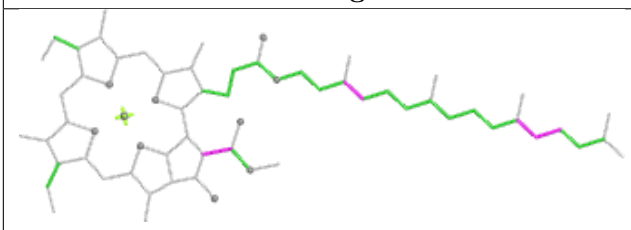
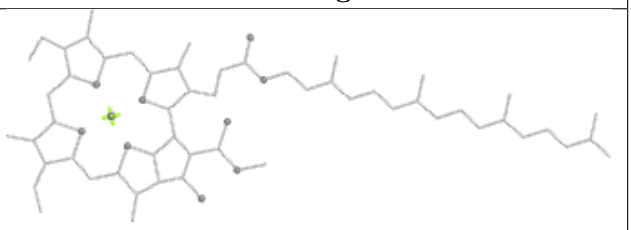


Rings

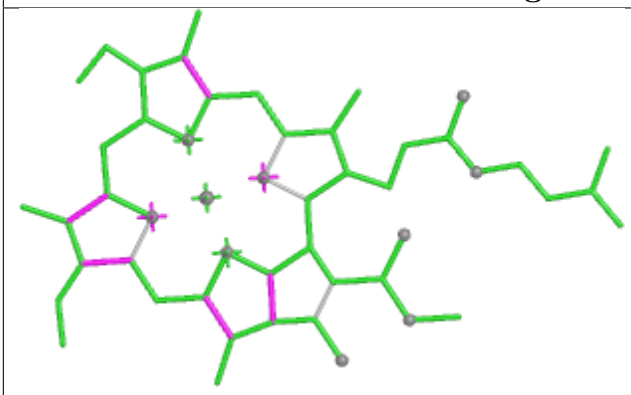
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

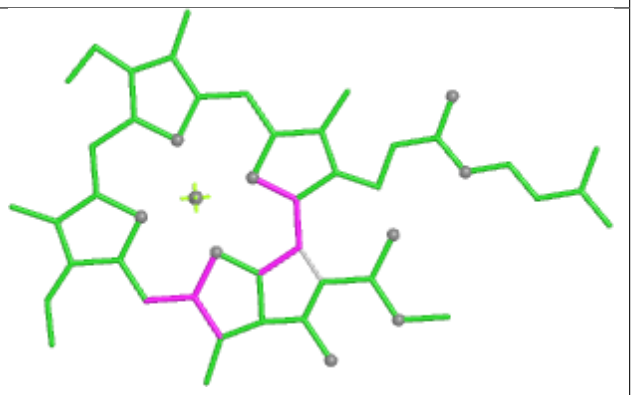
Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

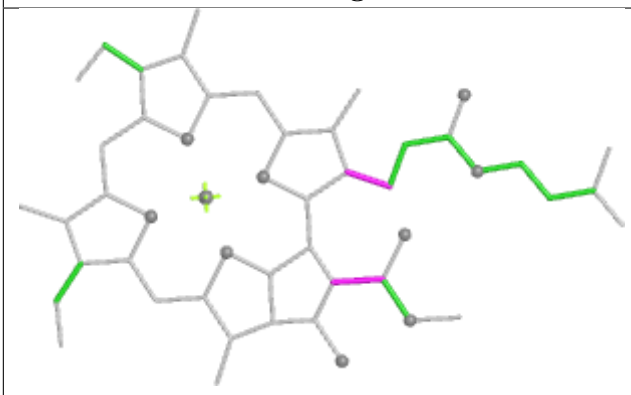
Ligand CLA B 826



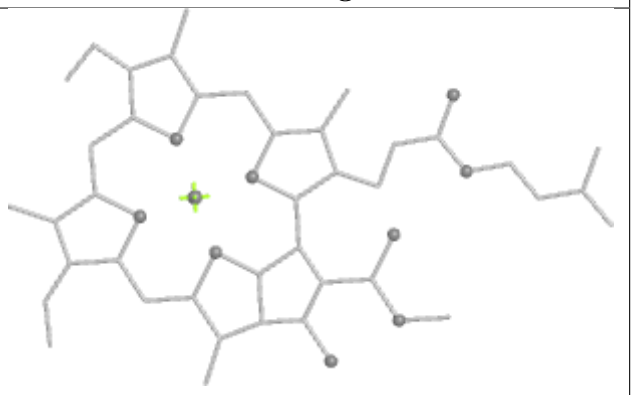
Bond lengths



Bond angles

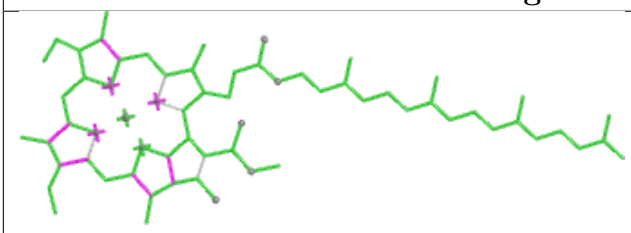


Torsions

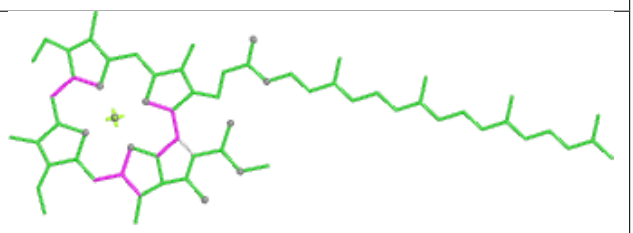


Rings

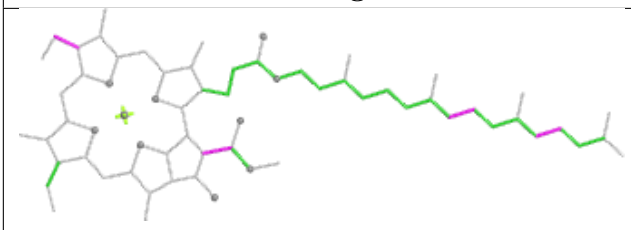
Ligand CLA A 846



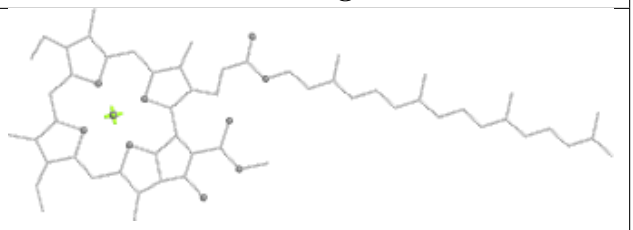
Bond lengths



Bond angles

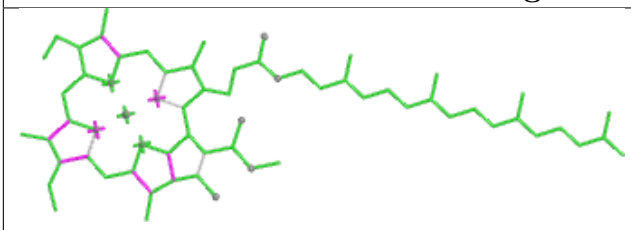


Torsions

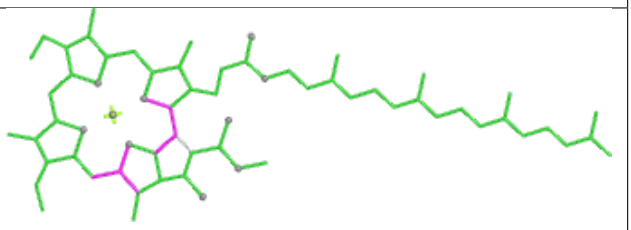


Rings

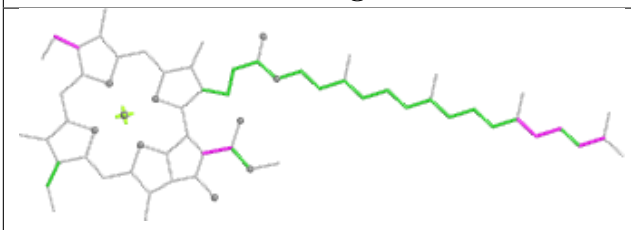
Ligand CLA A 822



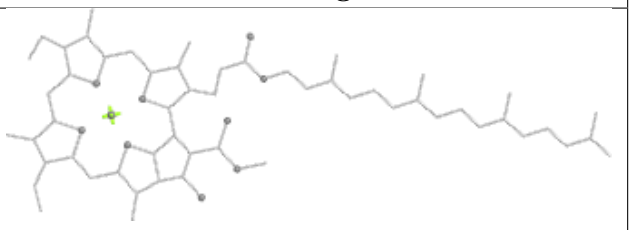
Bond lengths



Bond angles

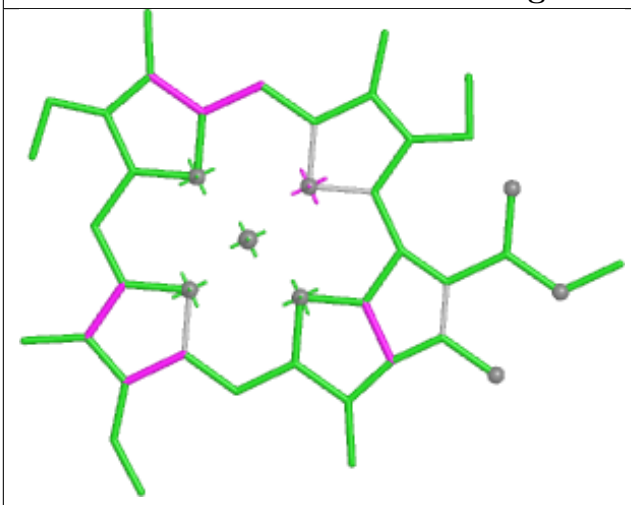


Torsions

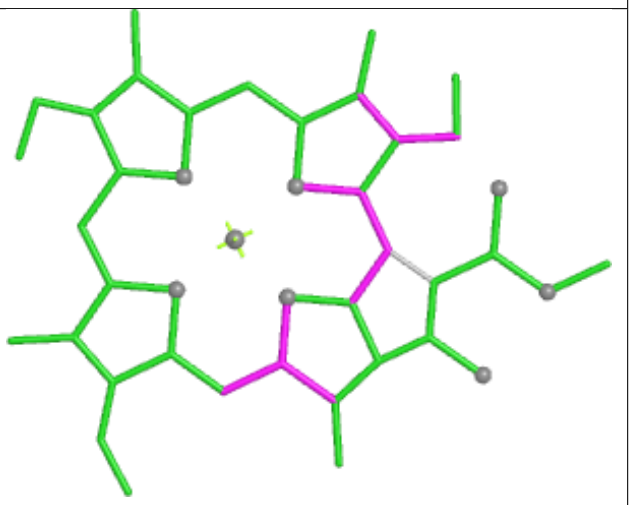


Rings

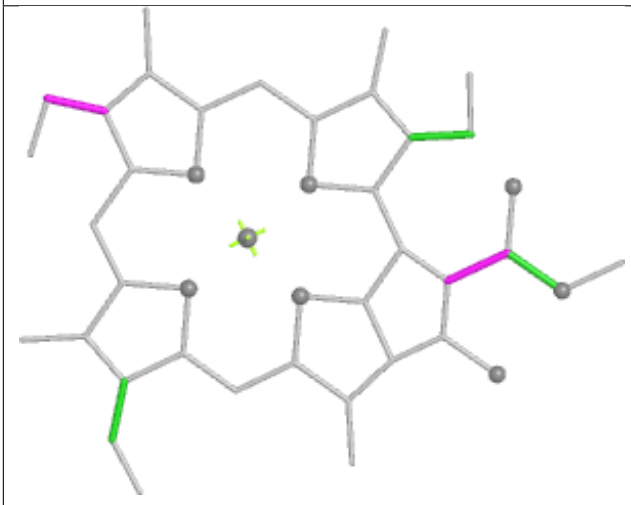
Ligand CLA J 103



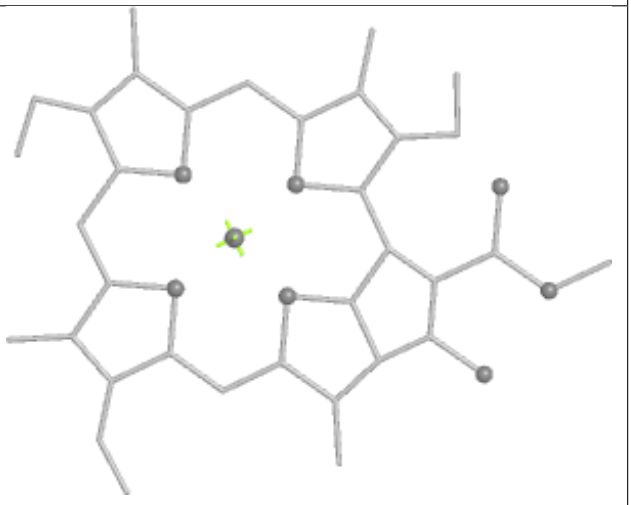
Bond lengths



Bond angles

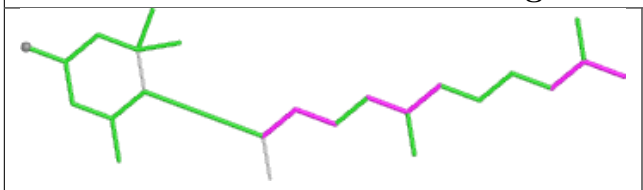


Torsions

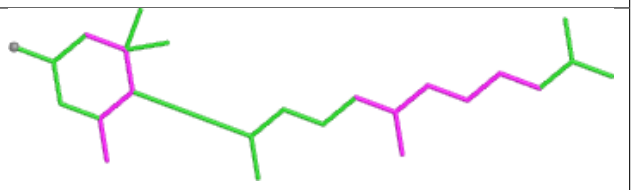


Rings

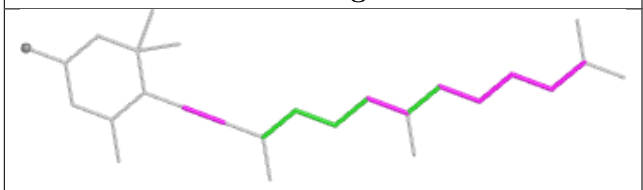
Ligand DD6 U 215



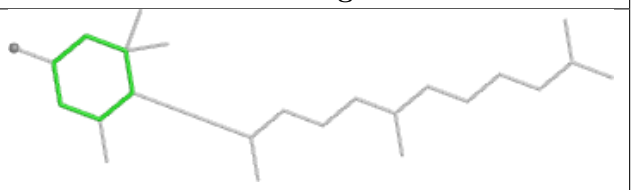
Bond lengths



Bond angles

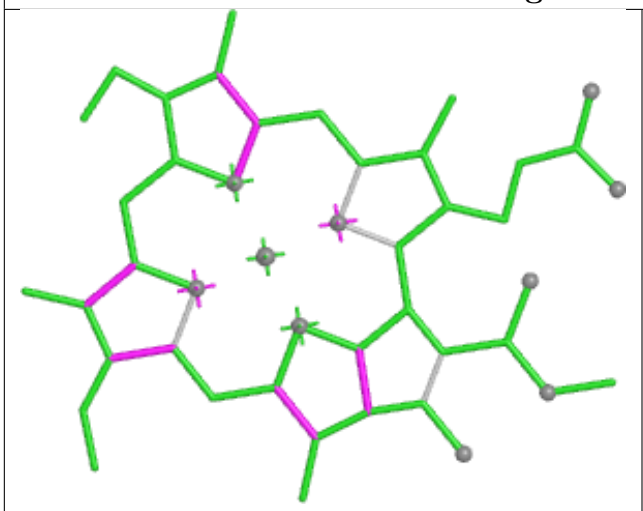


Torsions

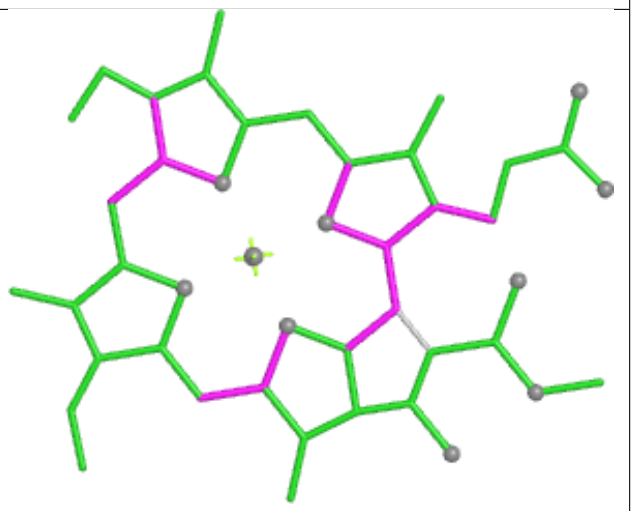


Rings

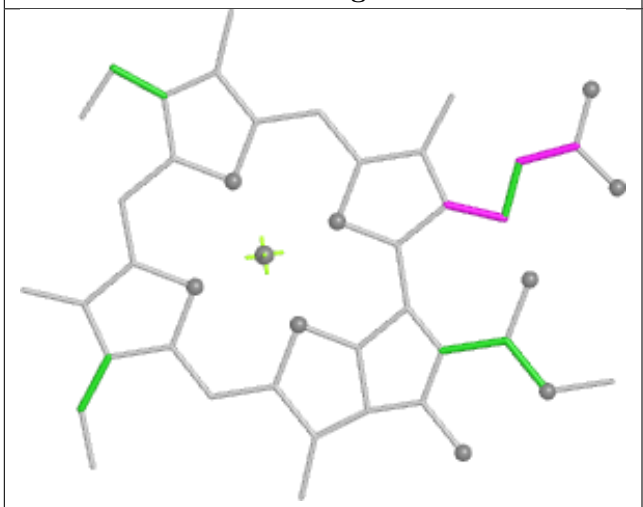
Ligand CLA B 848



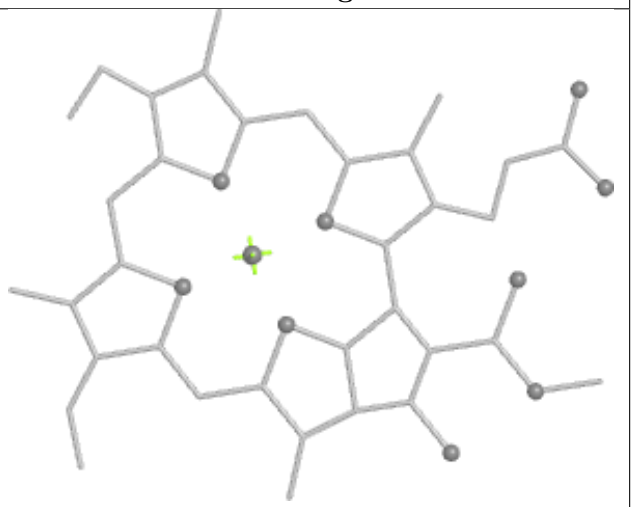
Bond lengths



Bond angles

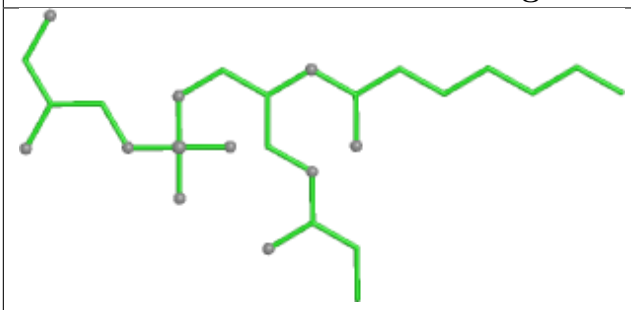


Torsions

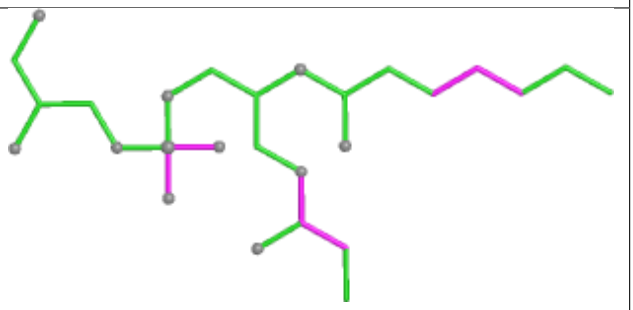


Rings

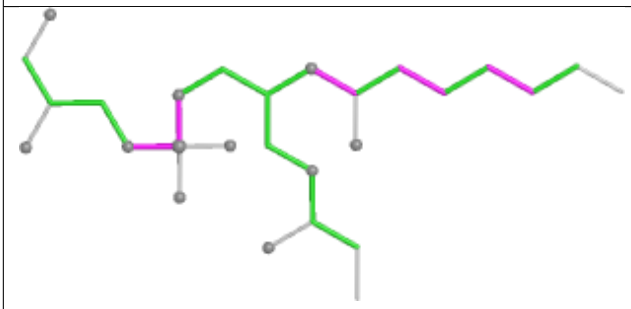
Ligand LHG A 839



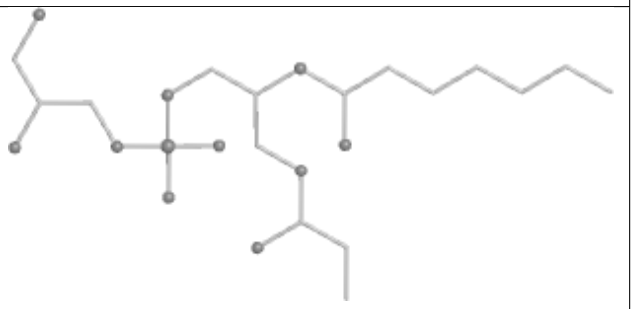
Bond lengths



Bond angles

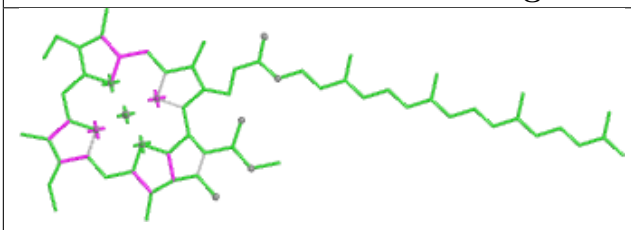


Torsions

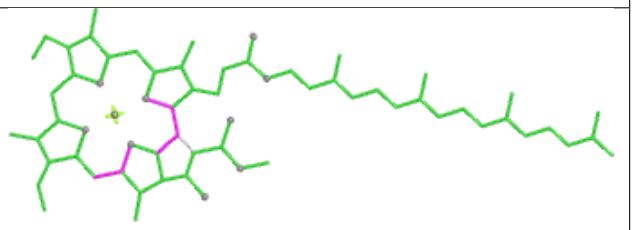


Rings

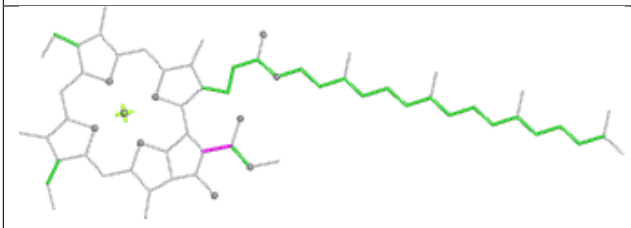
Ligand CLA A 826



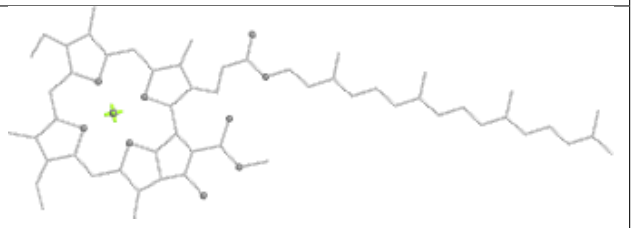
Bond lengths



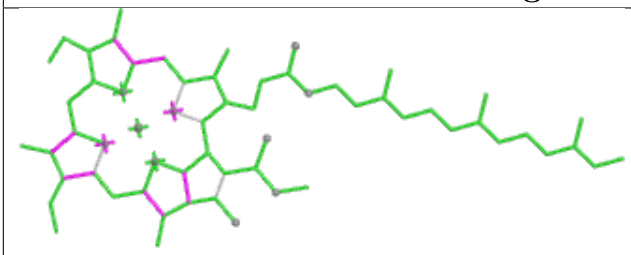
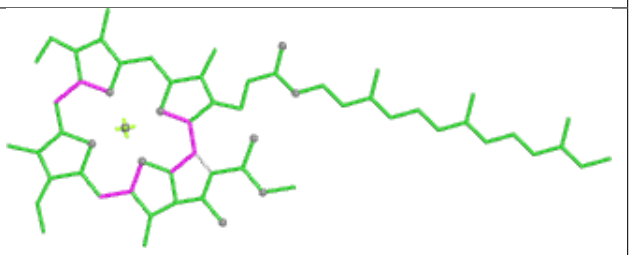
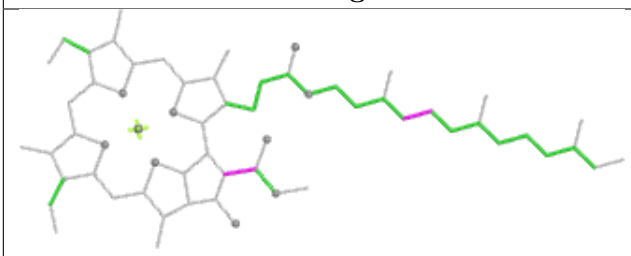
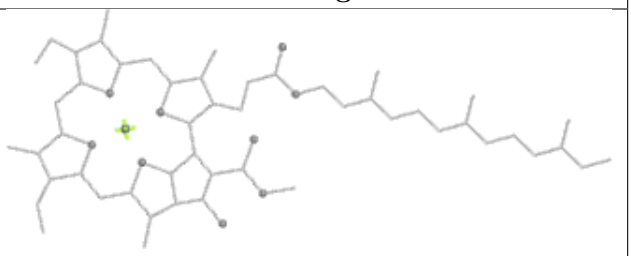
Bond angles

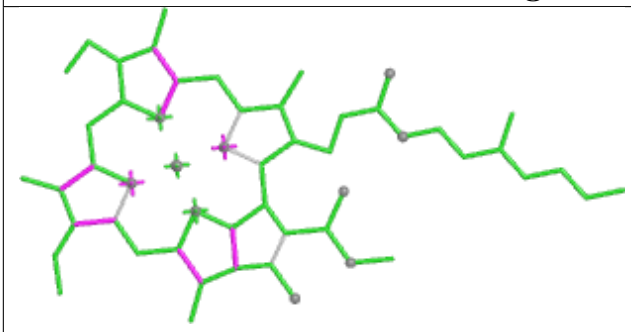
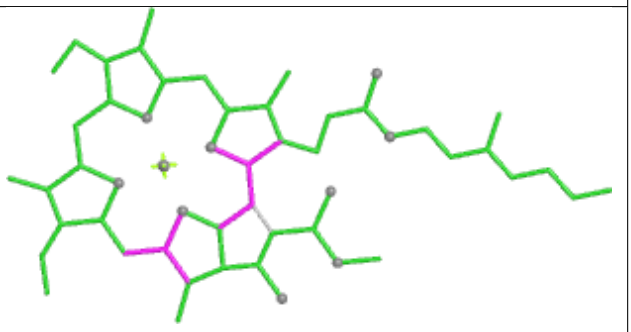
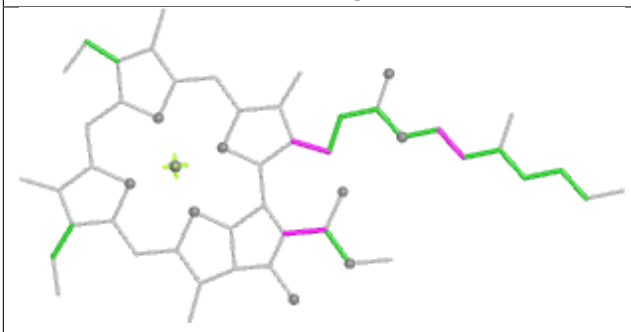
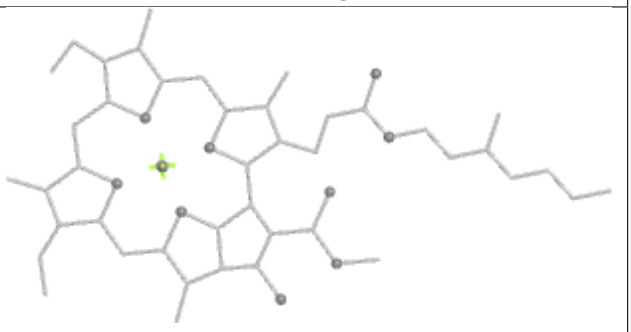


Torsions

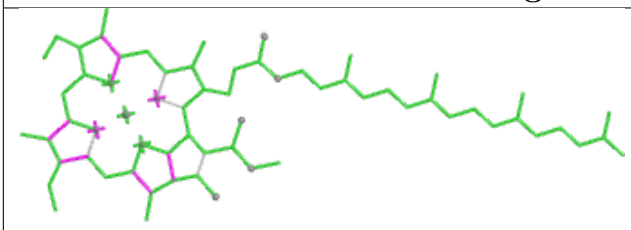


Rings

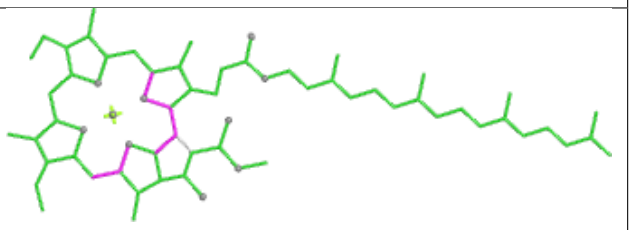
Ligand CLA U 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

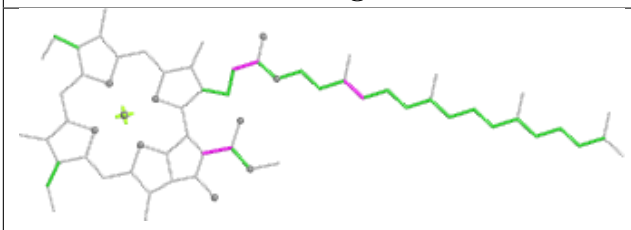
Ligand CLA B 809



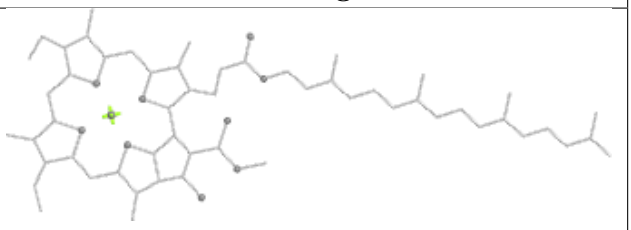
Bond lengths



Bond angles

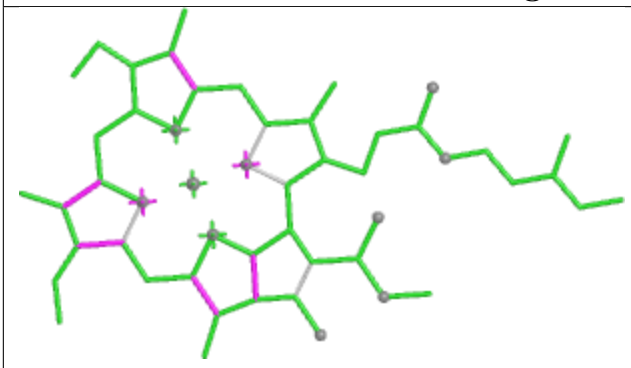


Torsions

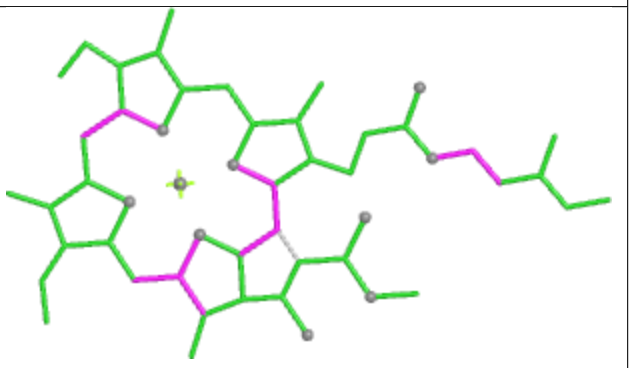


Rings

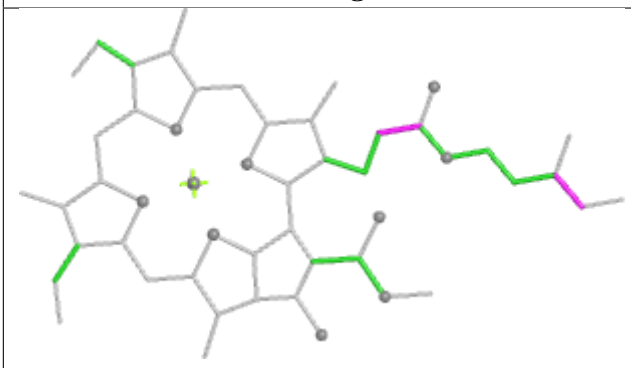
Ligand CLA A 820



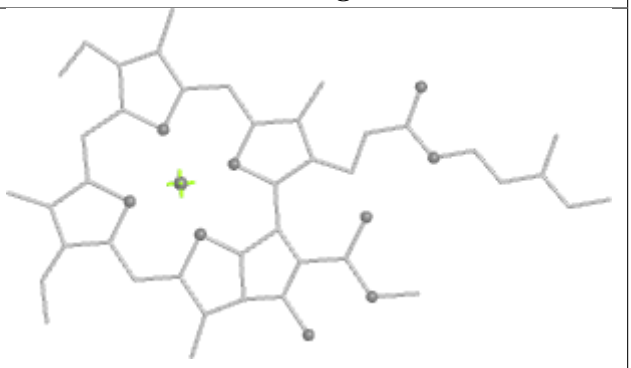
Bond lengths



Bond angles

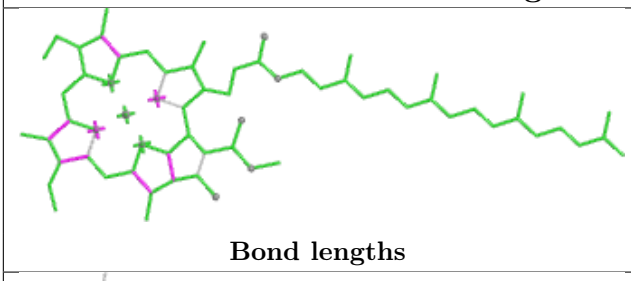


Torsions

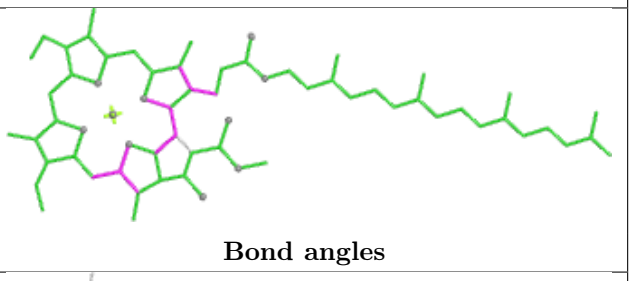


Rings

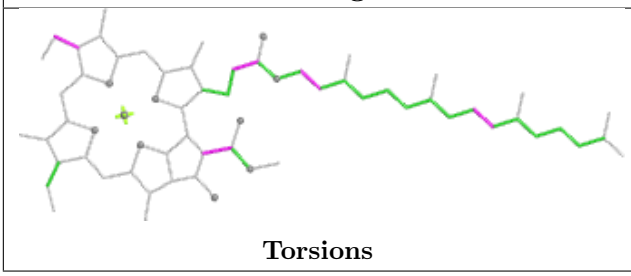
Ligand CLA B 825



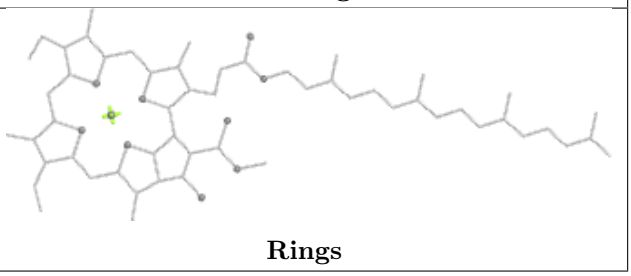
Bond lengths



Bond angles

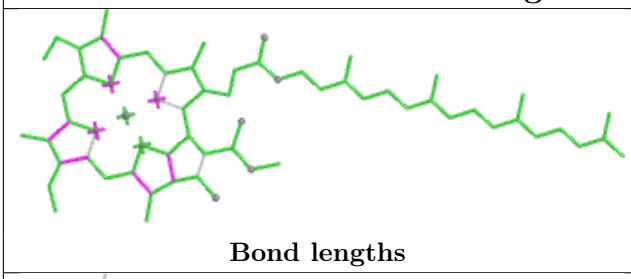


Torsions

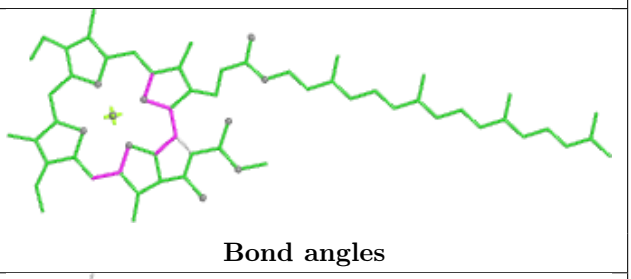


Rings

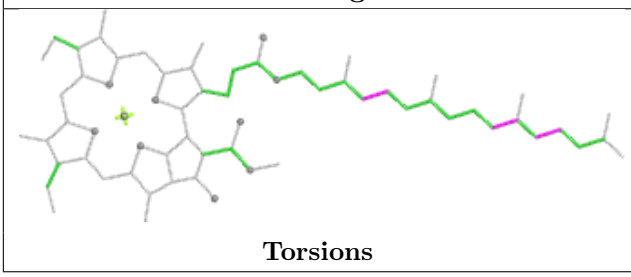
Ligand CLA B 834



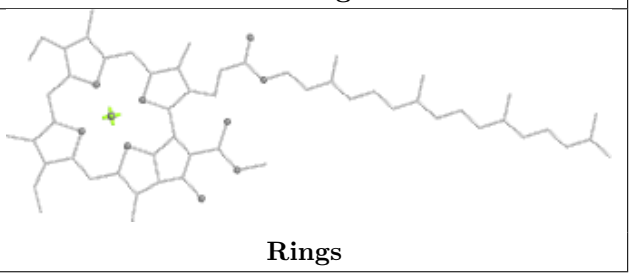
Bond lengths



Bond angles

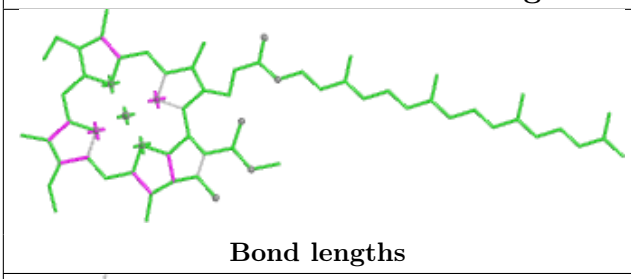


Torsions

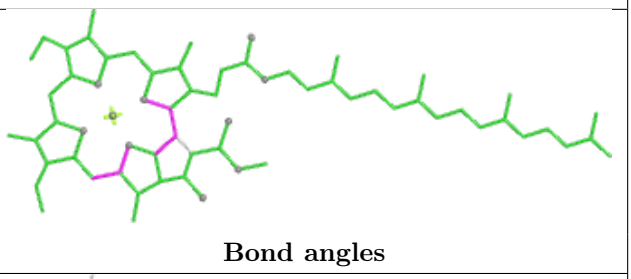


Rings

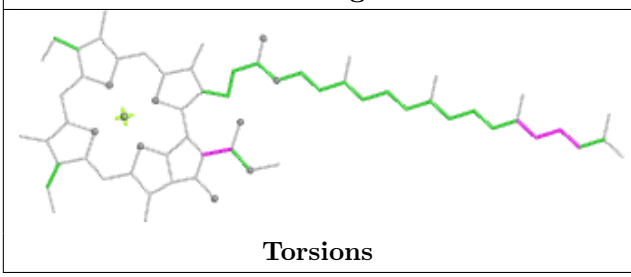
Ligand CLA A 828



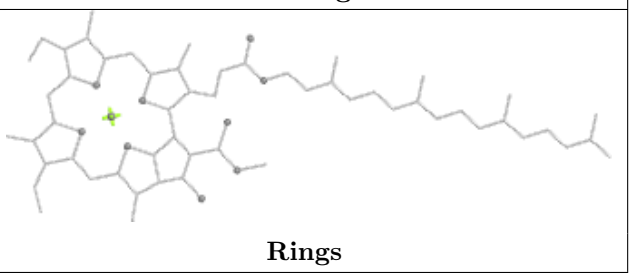
Bond lengths



Bond angles

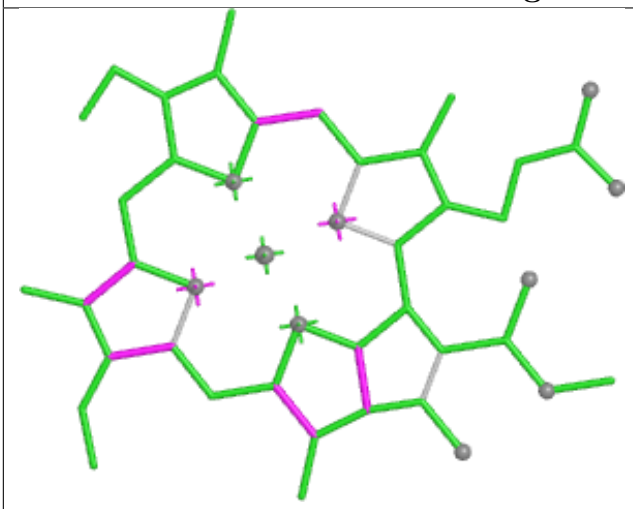


Torsions

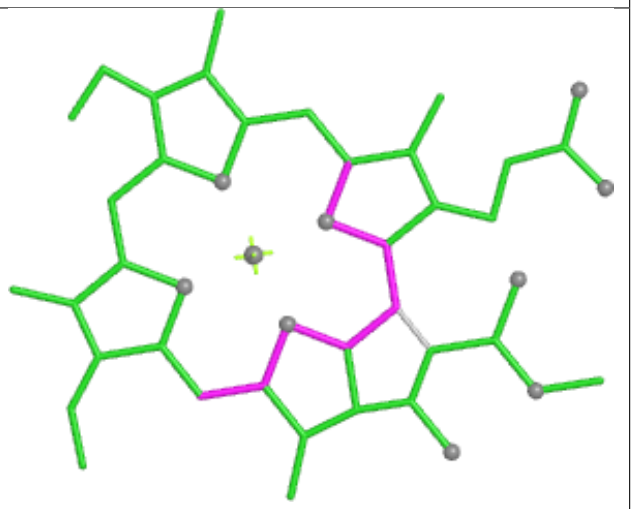


Rings

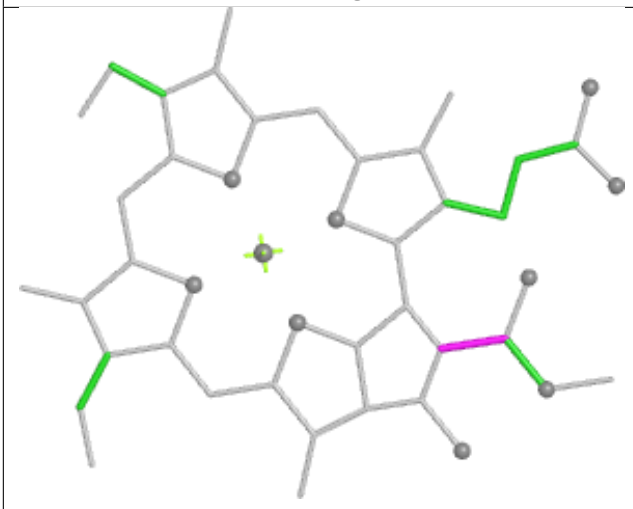
Ligand CLA A 812



Bond lengths



Bond angles

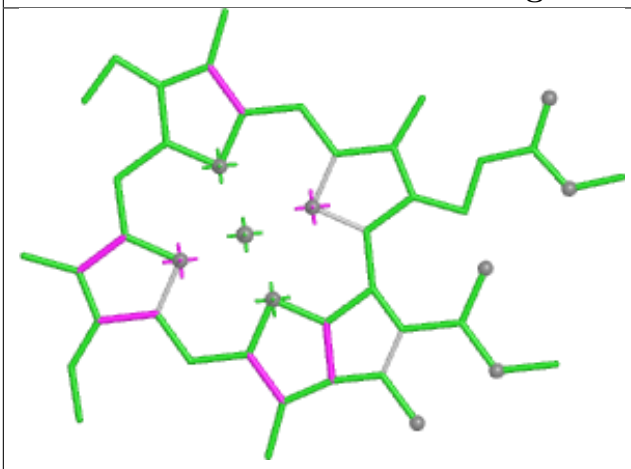


Torsions

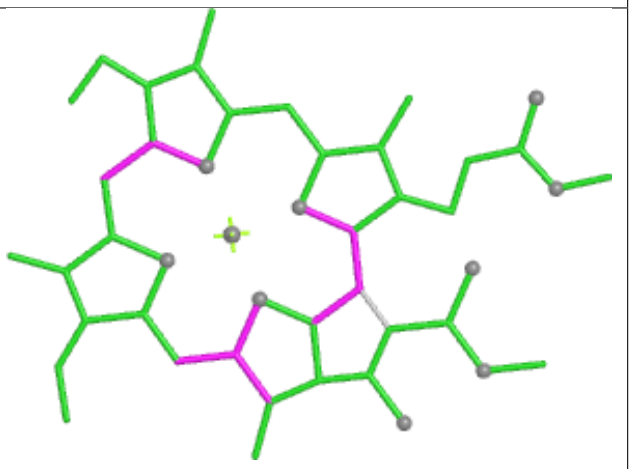


Rings

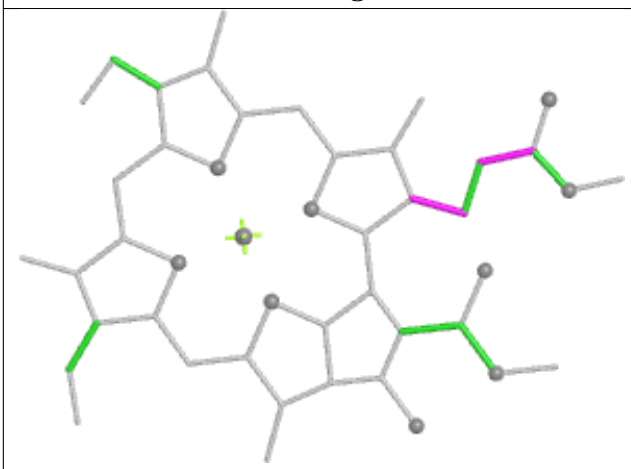
Ligand CLA F 803



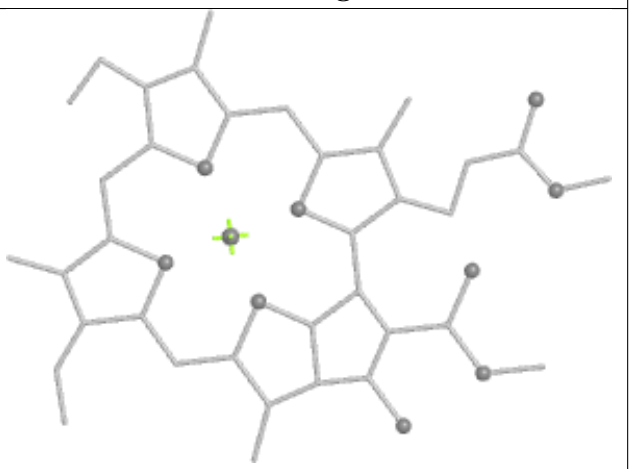
Bond lengths



Bond angles

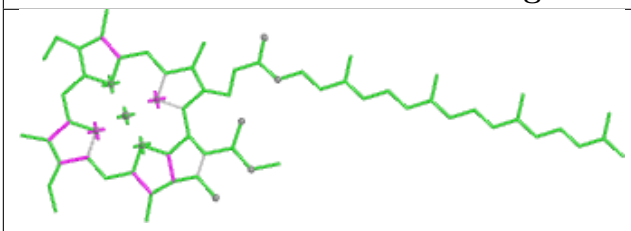


Torsions

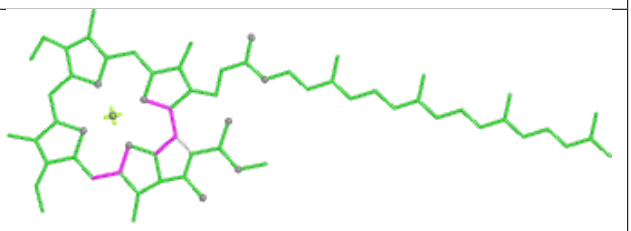


Rings

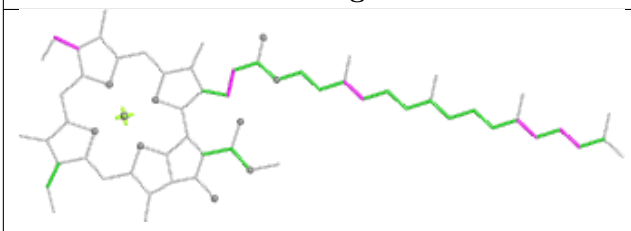
Ligand CLA A 844



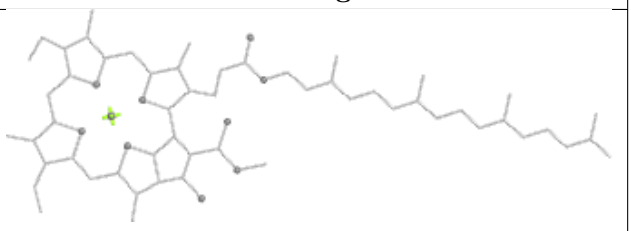
Bond lengths



Bond angles

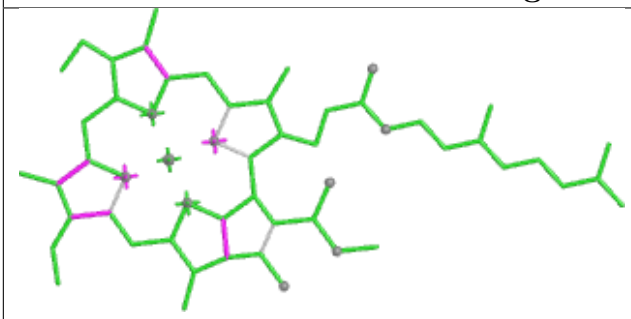


Torsions

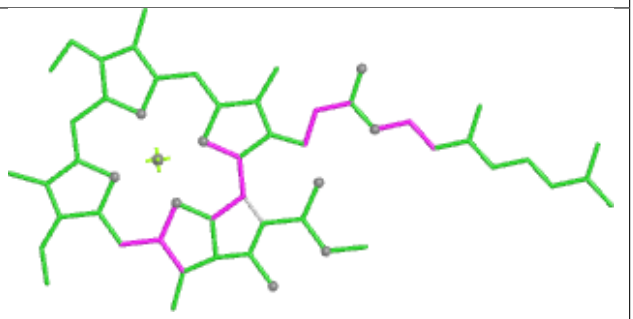


Rings

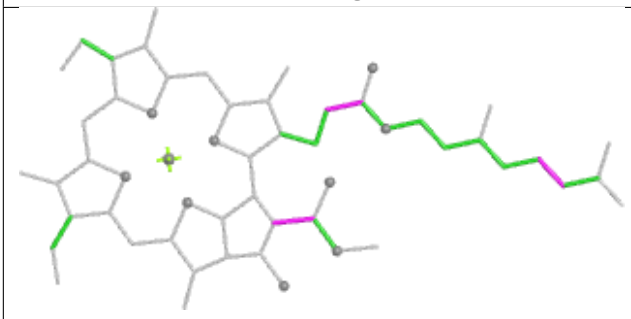
Ligand CLA A 802



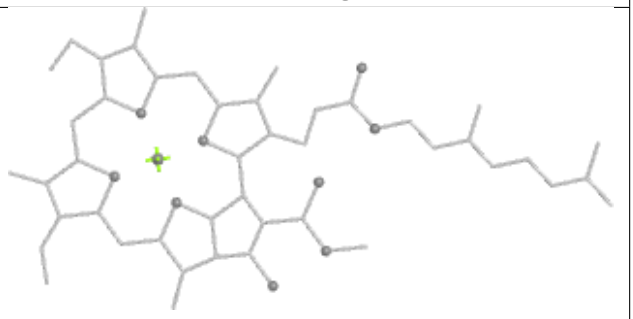
Bond lengths



Bond angles

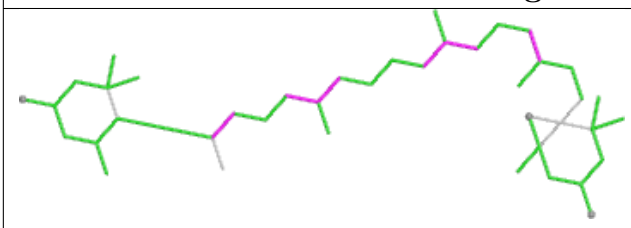


Torsions

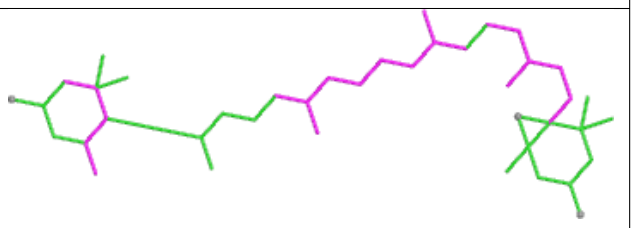


Rings

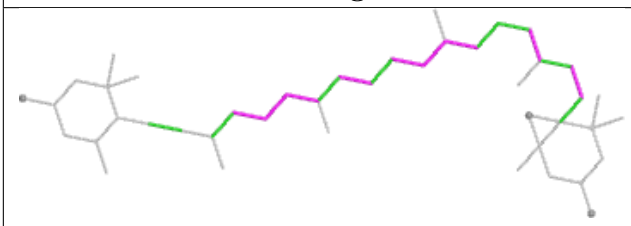
Ligand DD6 U 213



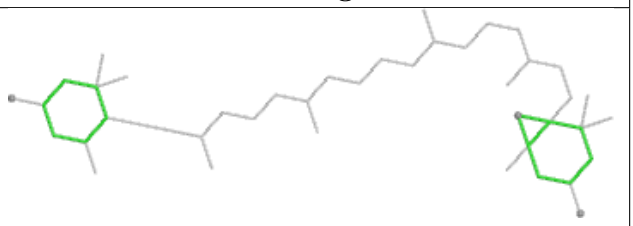
Bond lengths



Bond angles

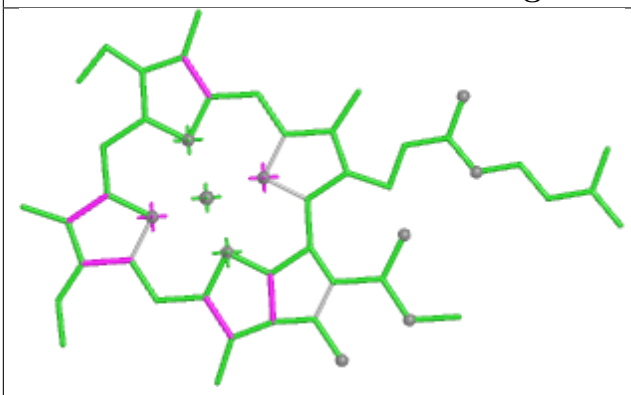


Torsions

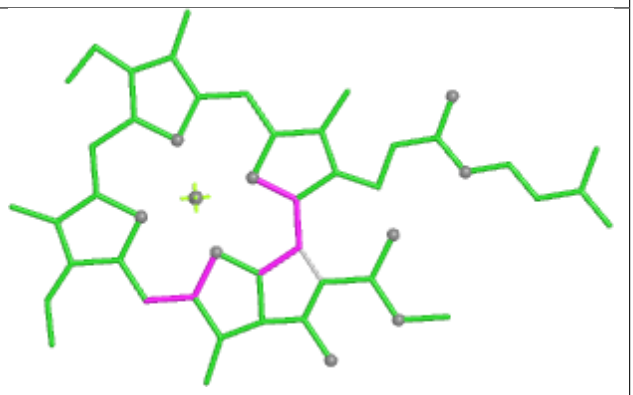


Rings

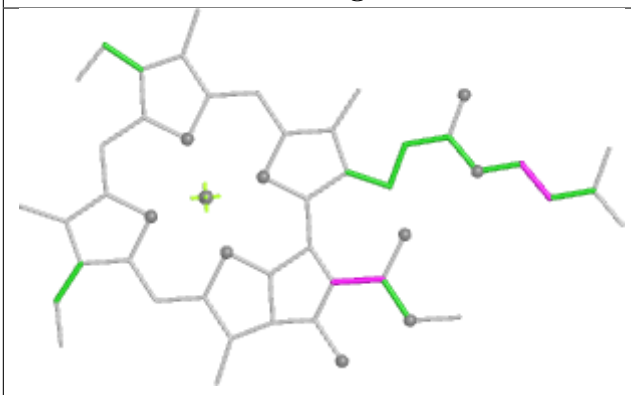
Ligand CLA A 827



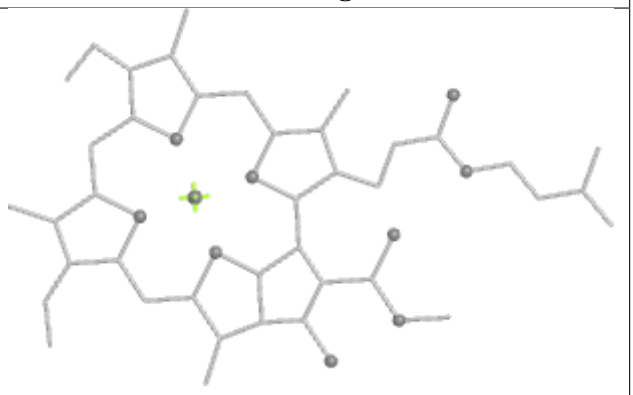
Bond lengths



Bond angles

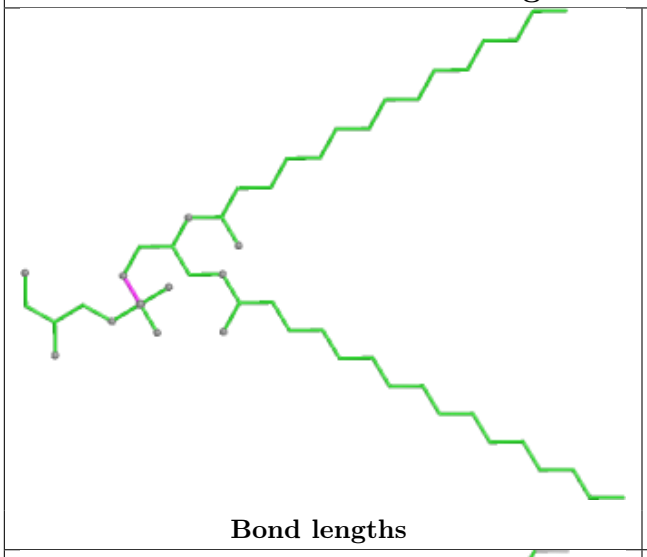


Torsions

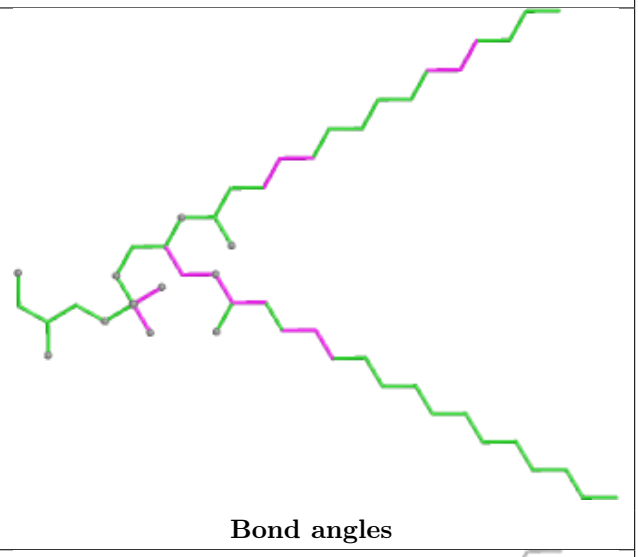


Rings

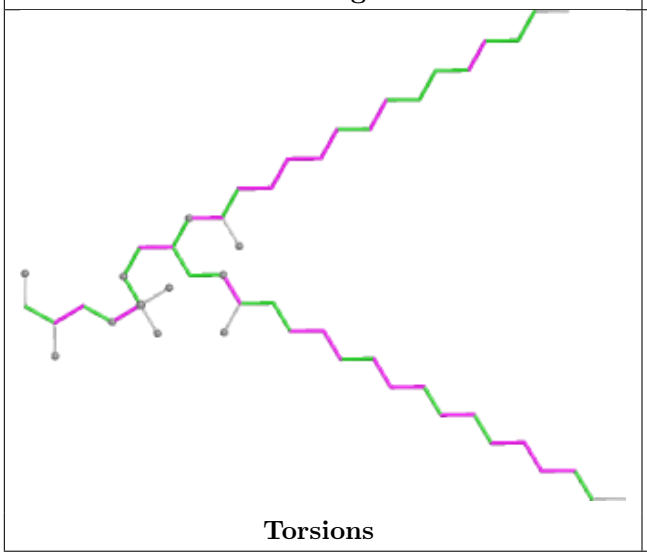
Ligand LHG A 838



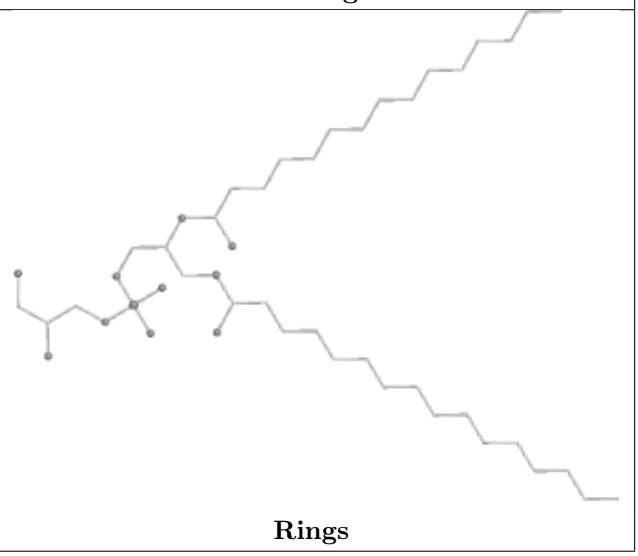
Bond lengths



Bond angles

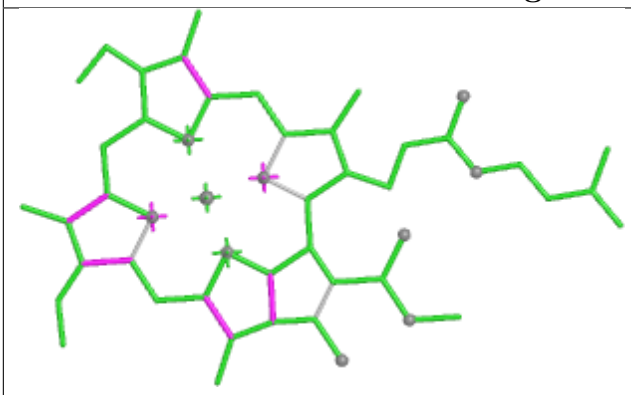


Torsions

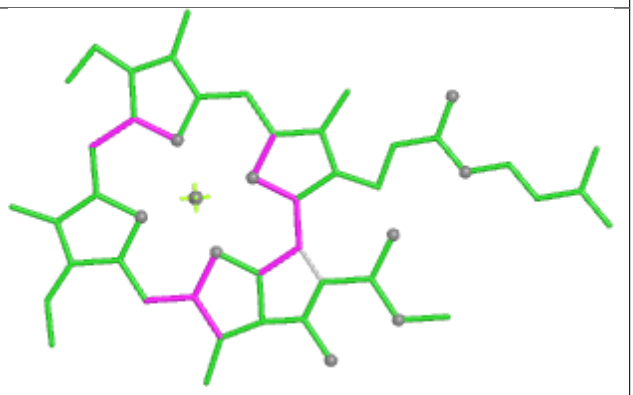


Rings

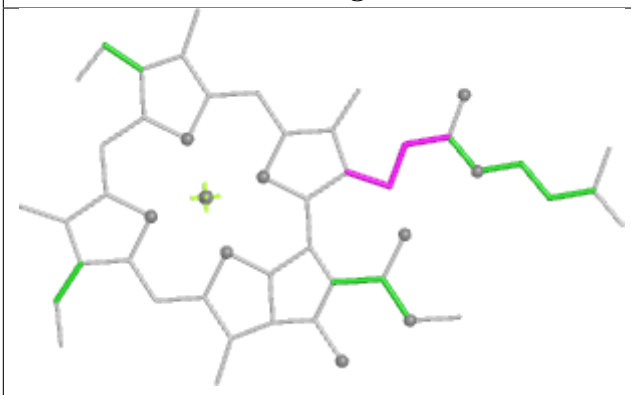
Ligand CLA B 847



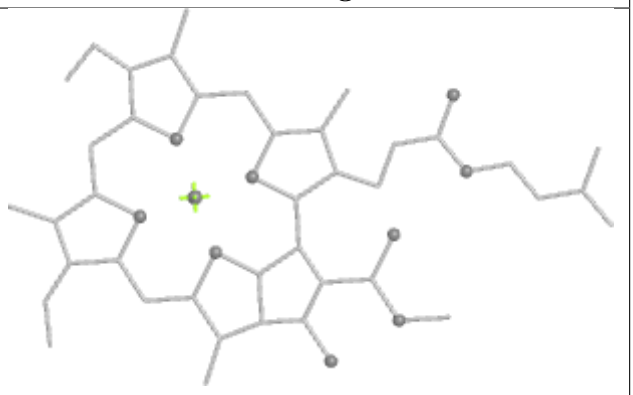
Bond lengths



Bond angles

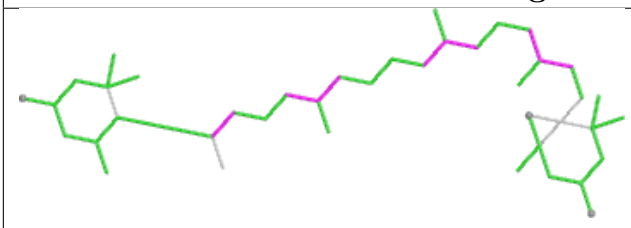


Torsions

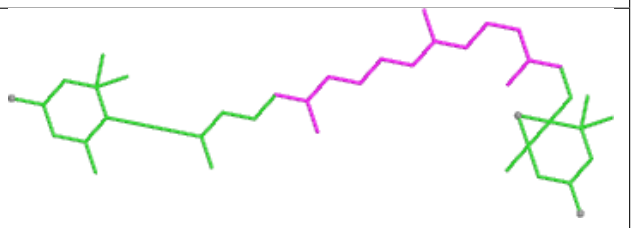


Rings

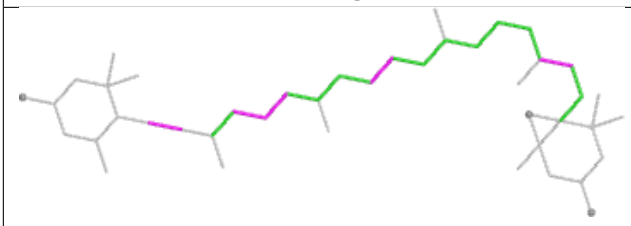
Ligand DD6 J 101



Bond lengths



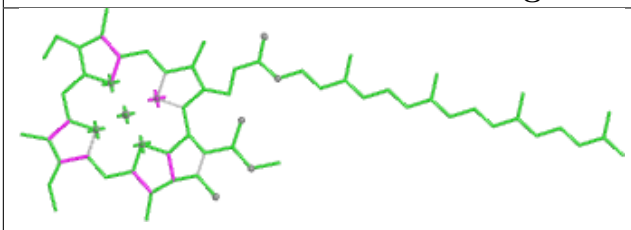
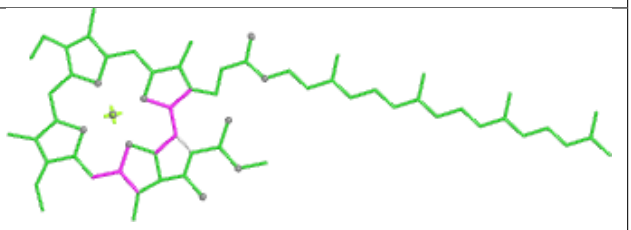
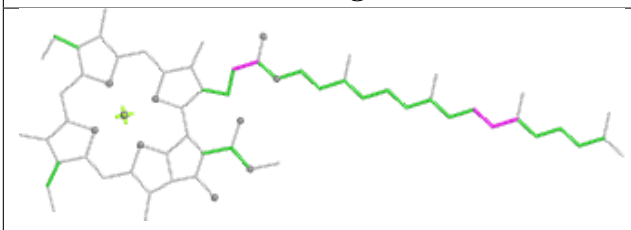
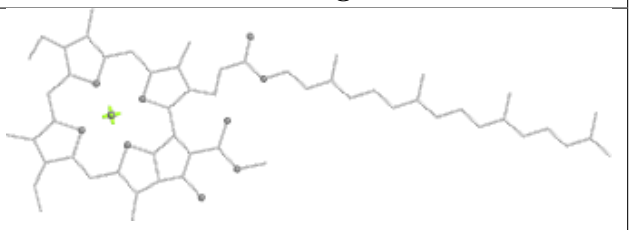
Bond angles

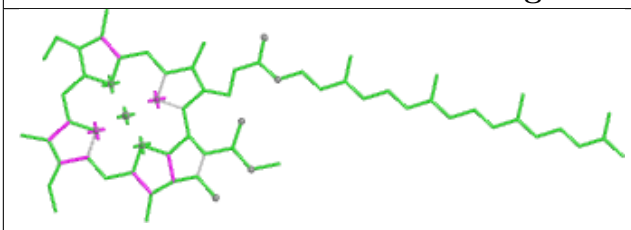
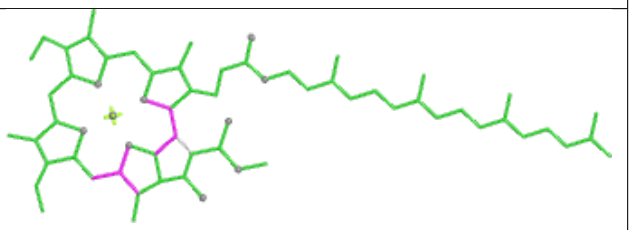
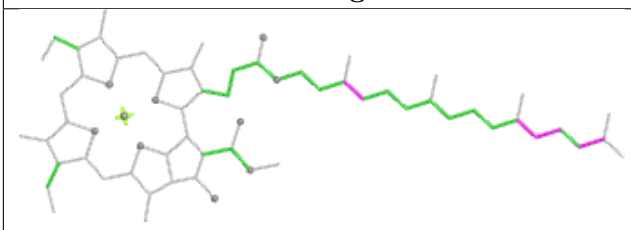
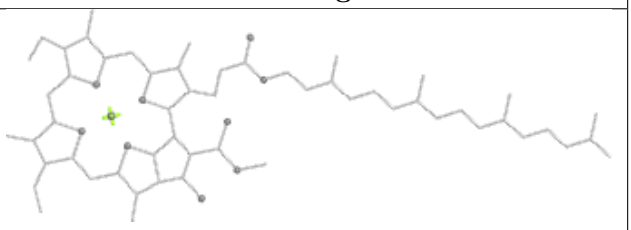


Torsions

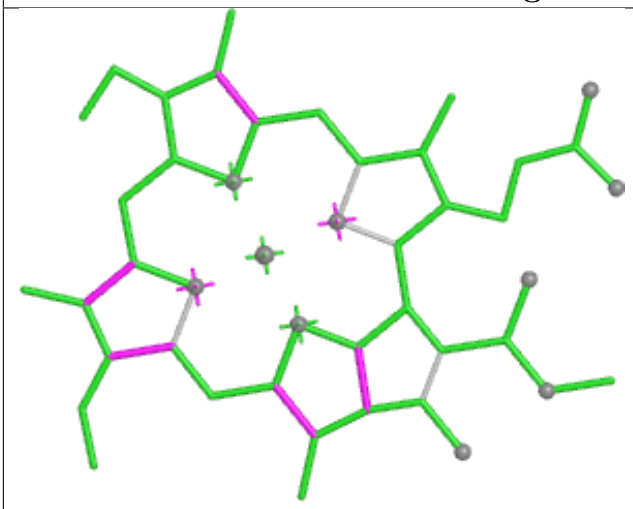


Rings

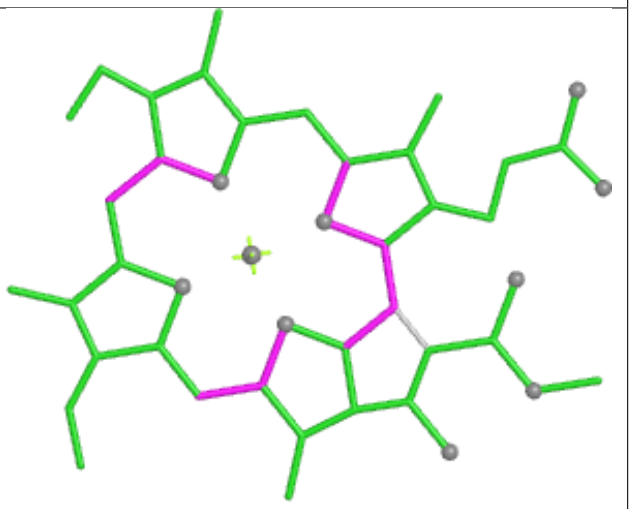
Ligand CLA A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

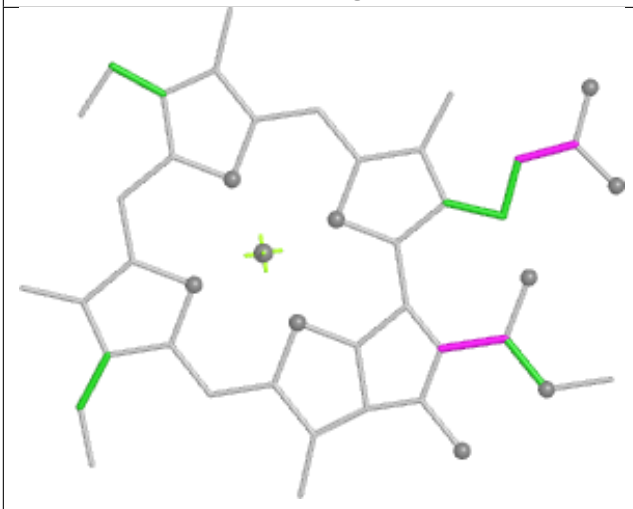
Ligand CLA A 817



Bond lengths



Bond angles

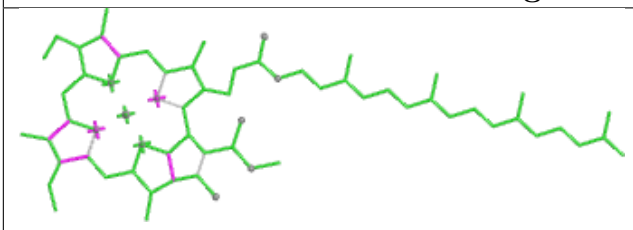


Torsions

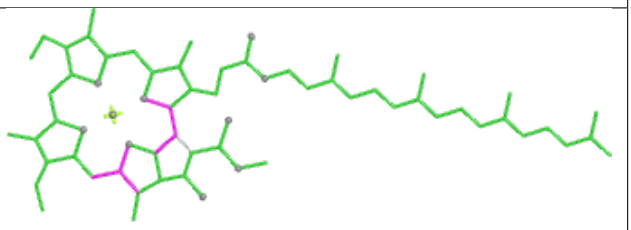


Rings

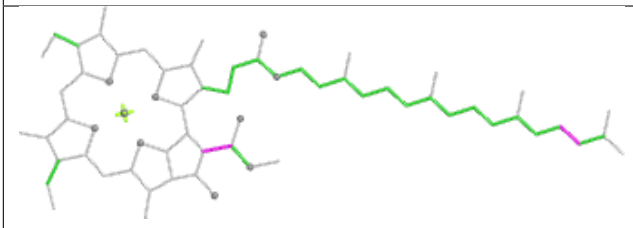
Ligand CLA A 829



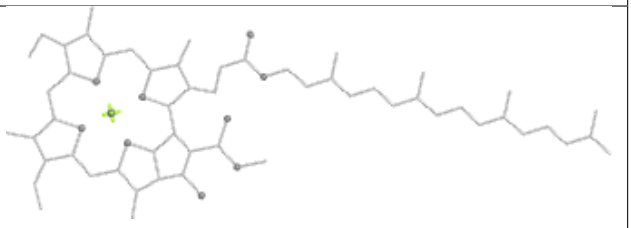
Bond lengths



Bond angles

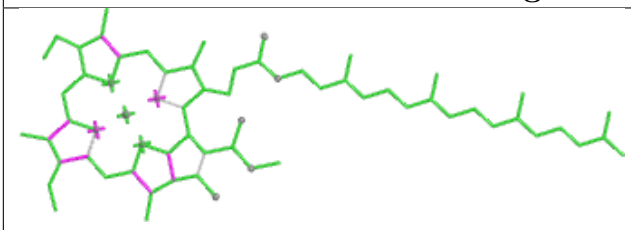


Torsions

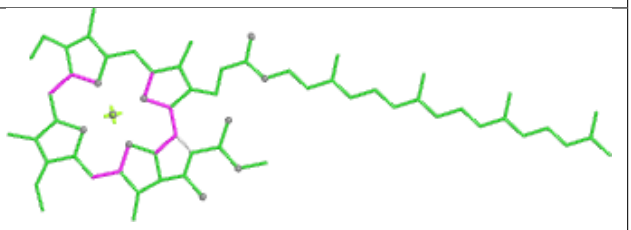


Rings

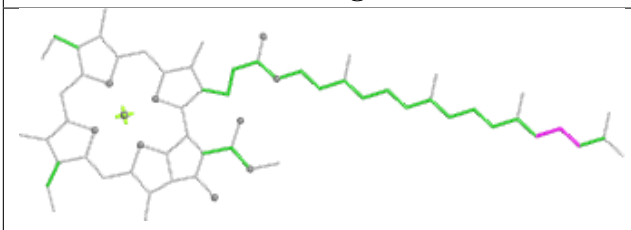
Ligand CLA A 852



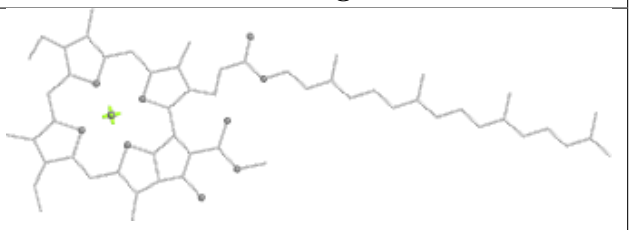
Bond lengths



Bond angles

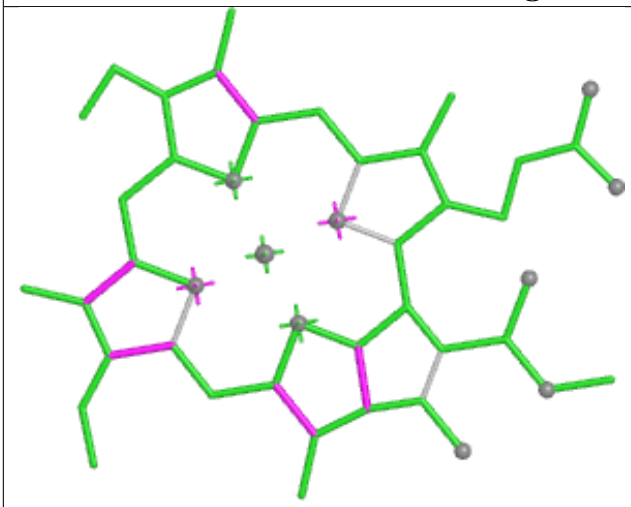


Torsions

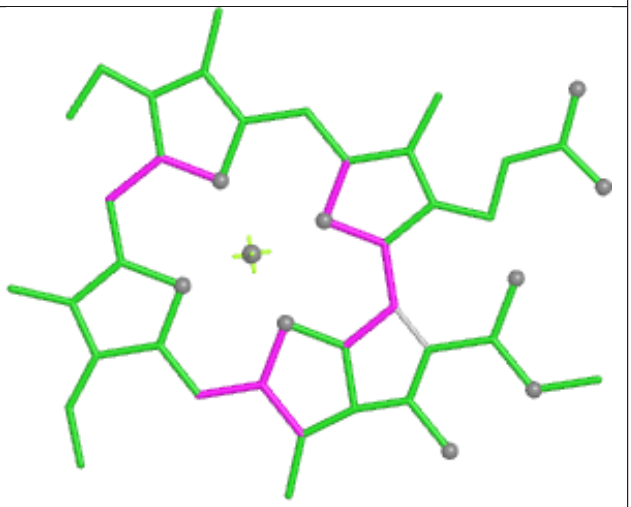


Rings

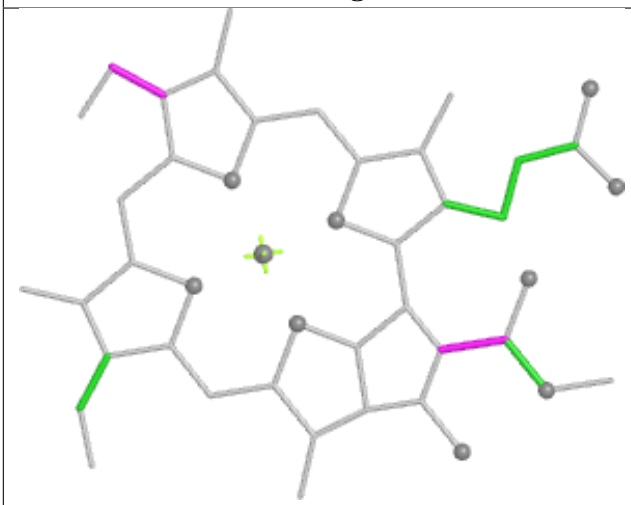
Ligand CLA A 814



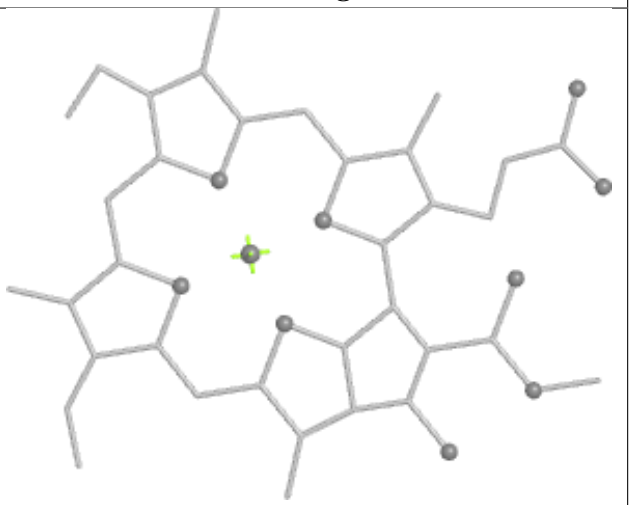
Bond lengths



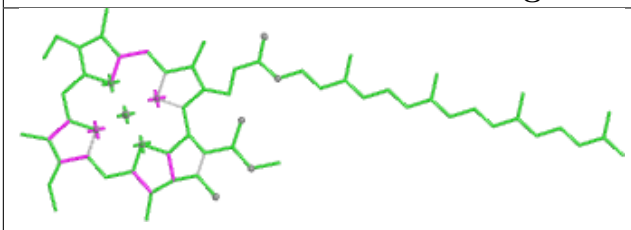
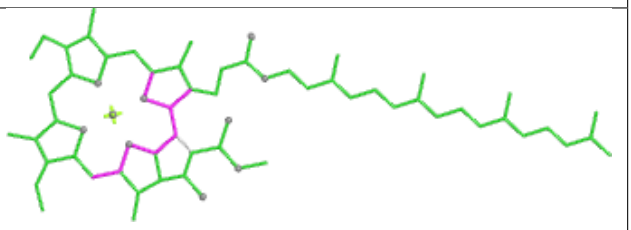
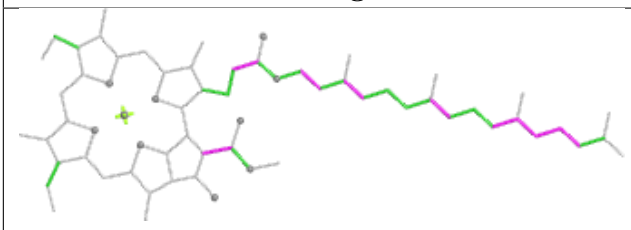
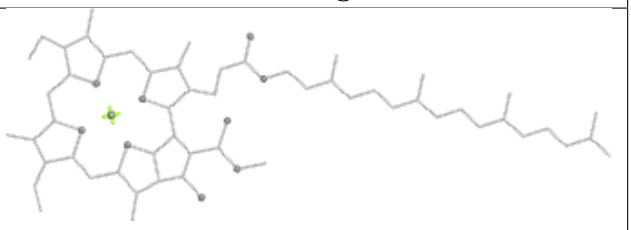
Bond angles

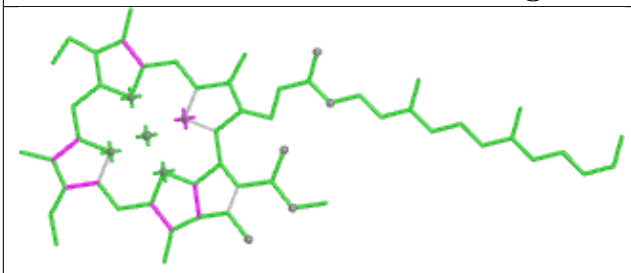
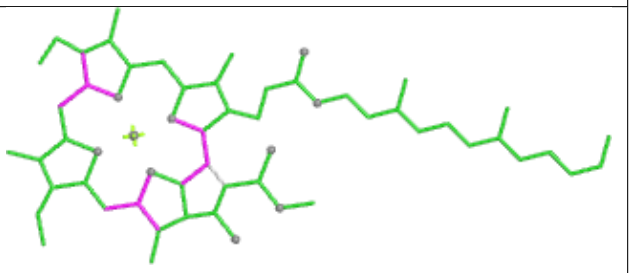
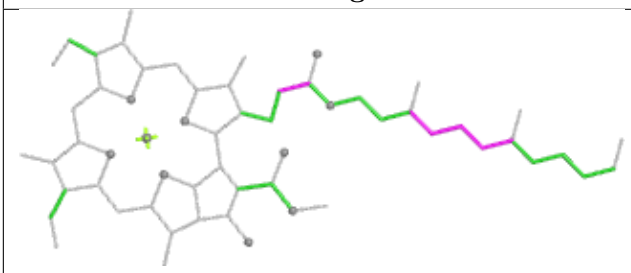
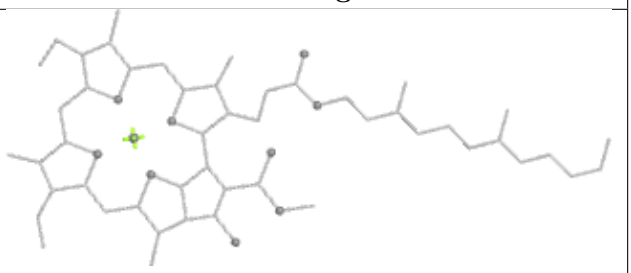


Torsions

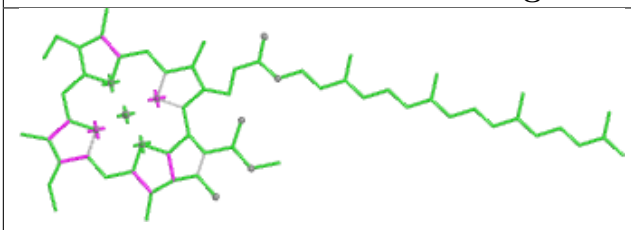


Rings

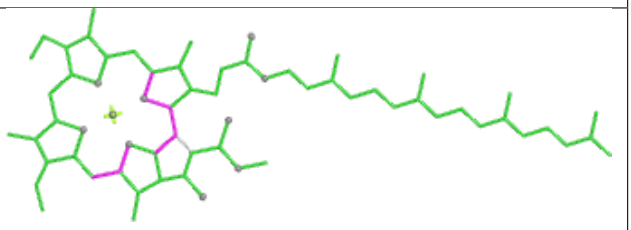
Ligand CLA A 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 815	
	
Bond lengths	Bond angles
	
Torsions	Rings

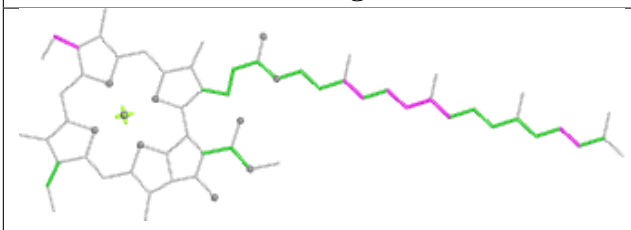
Ligand CLA A 851



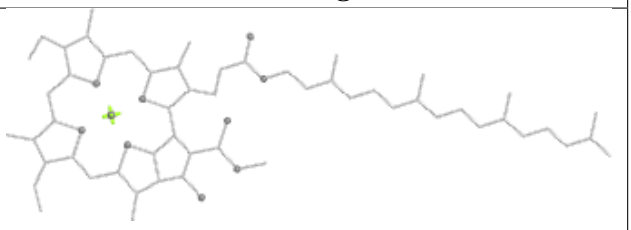
Bond lengths



Bond angles

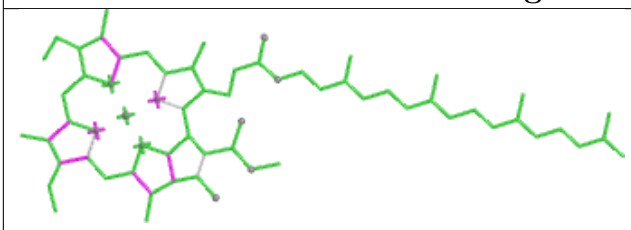


Torsions

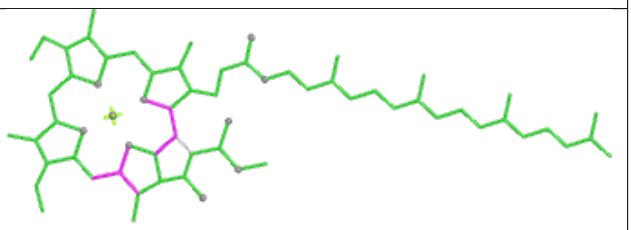


Rings

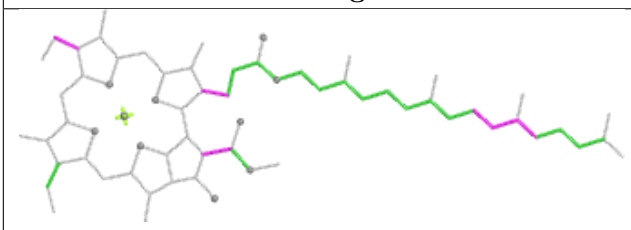
Ligand CLA B 805



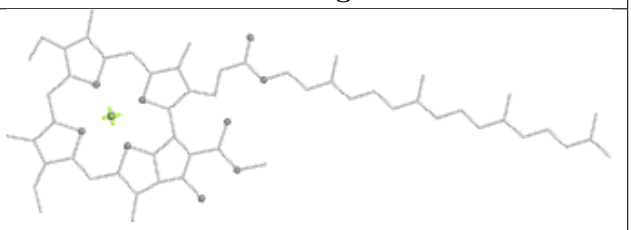
Bond lengths



Bond angles



Torsions

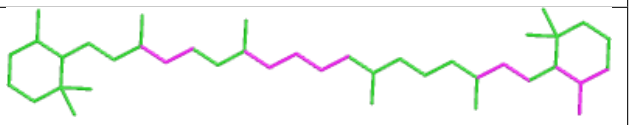


Rings

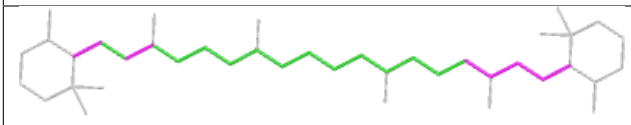
Ligand BCR I 102



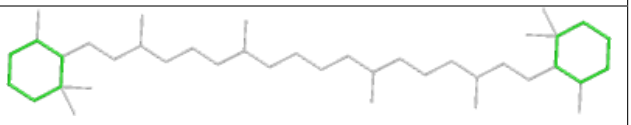
Bond lengths



Bond angles

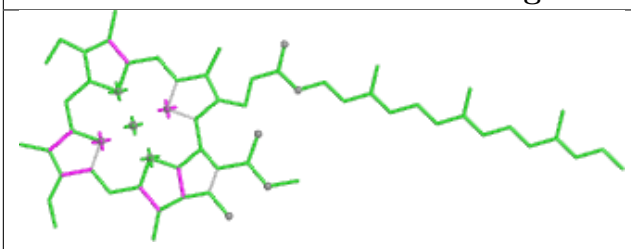


Torsions

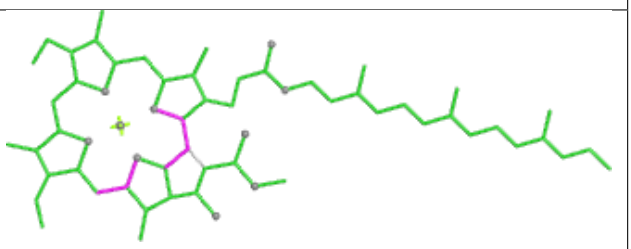


Rings

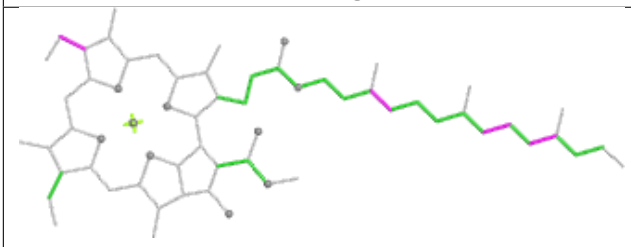
Ligand CLA A 809



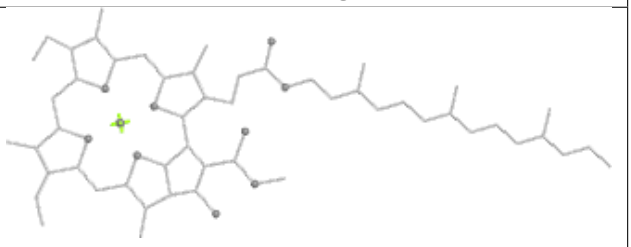
Bond lengths



Bond angles

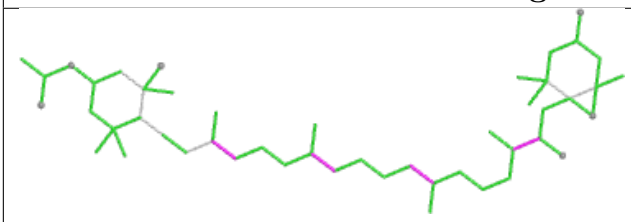


Torsions

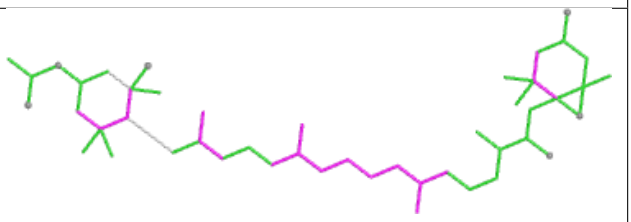


Rings

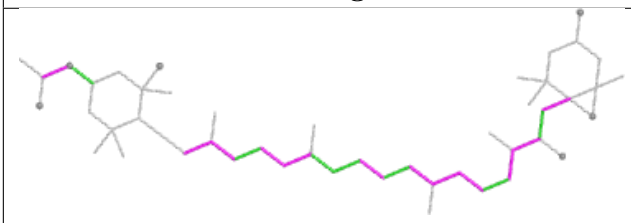
Ligand A86 U 203



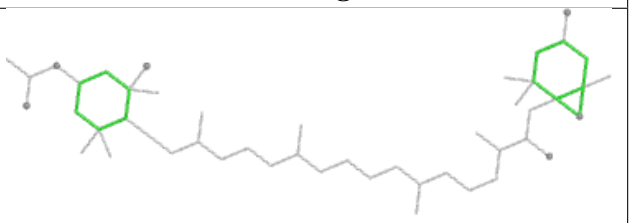
Bond lengths



Bond angles

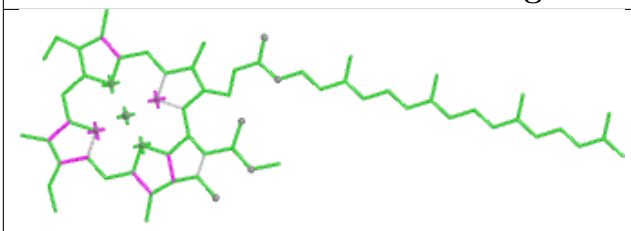


Torsions

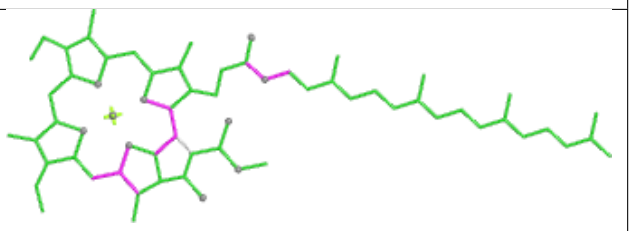


Rings

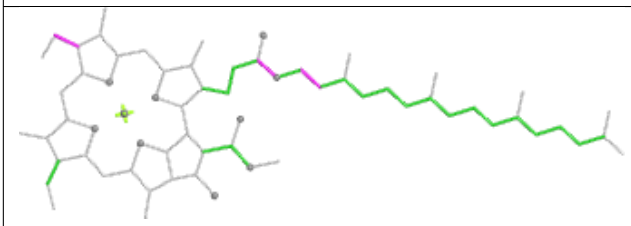
Ligand CLA B 824



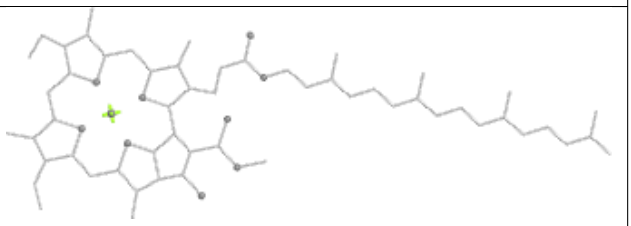
Bond lengths



Bond angles

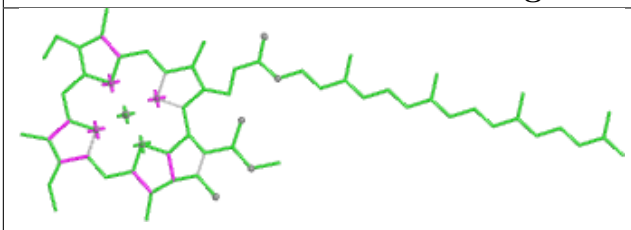


Torsions

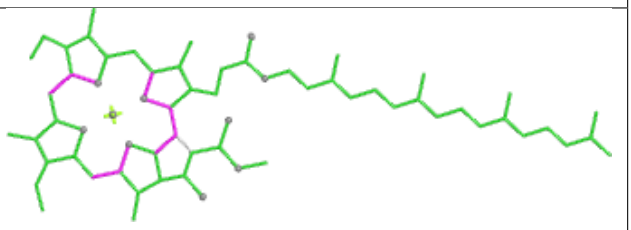


Rings

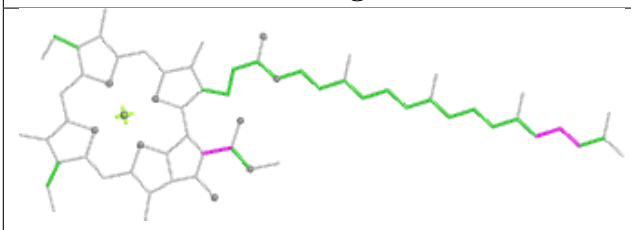
Ligand CLA B 845



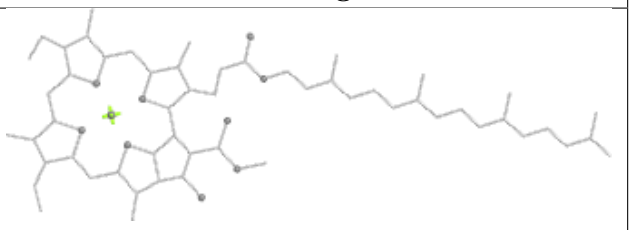
Bond lengths



Bond angles

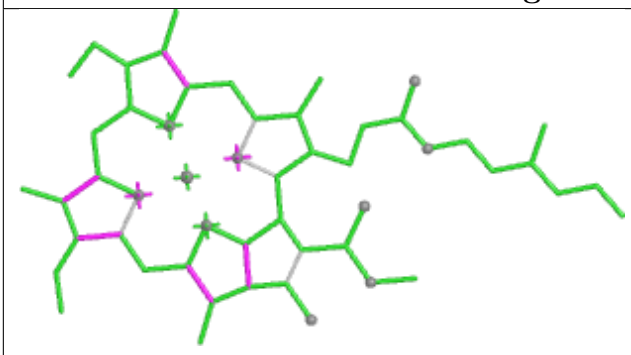


Torsions

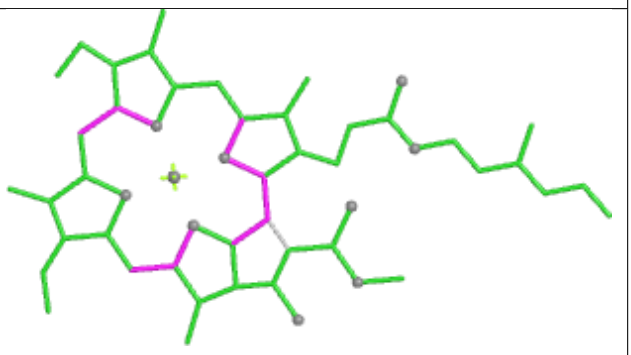


Rings

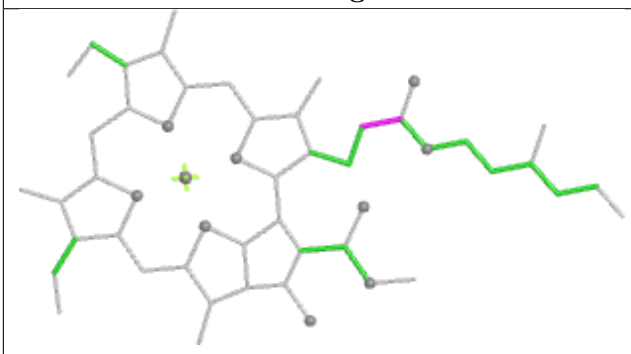
Ligand CLA U 212



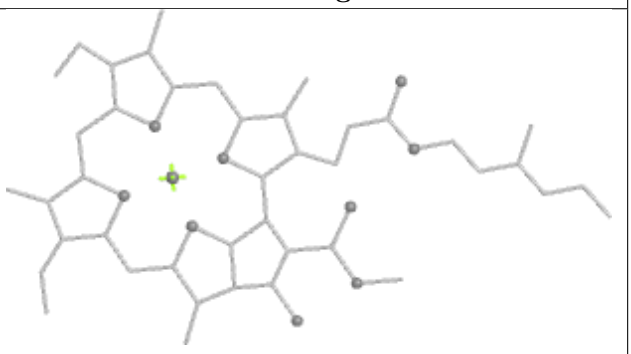
Bond lengths



Bond angles

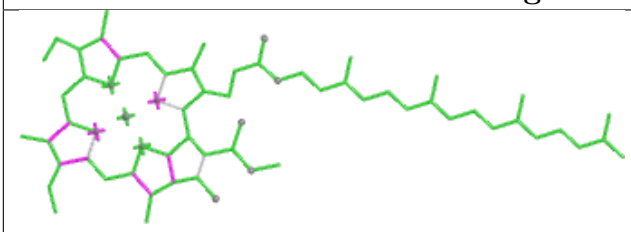


Torsions

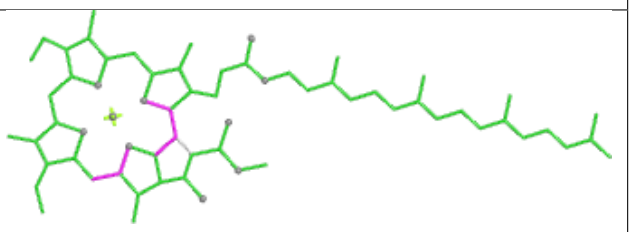


Rings

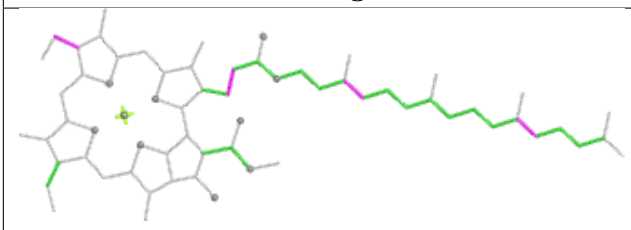
Ligand CLA A 825



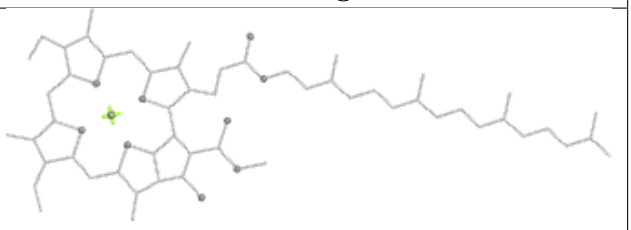
Bond lengths



Bond angles

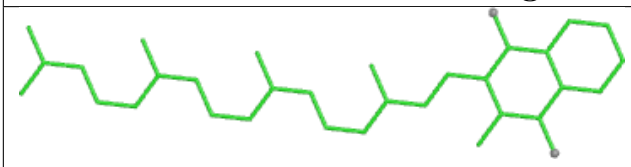


Torsions

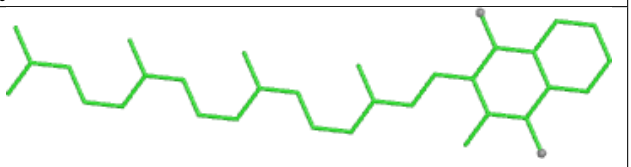


Rings

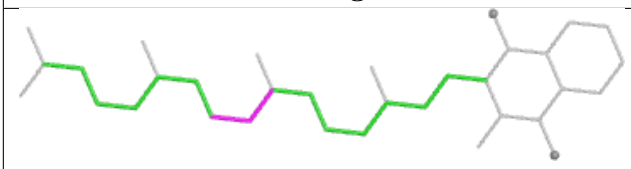
Ligand PQN A 837



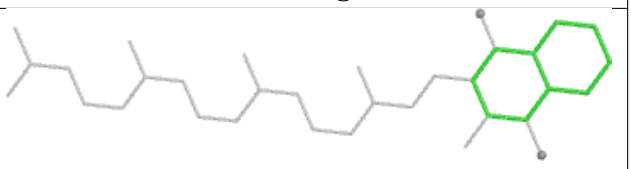
Bond lengths



Bond angles

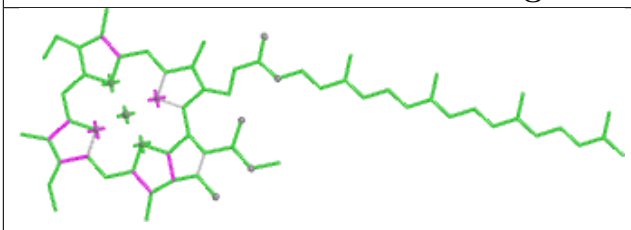


Torsions

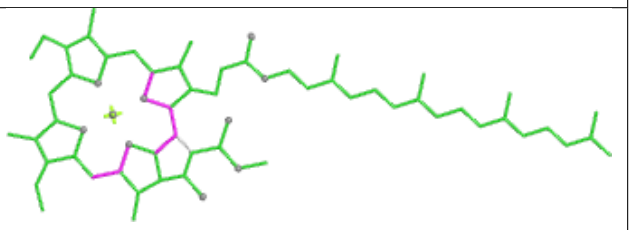


Rings

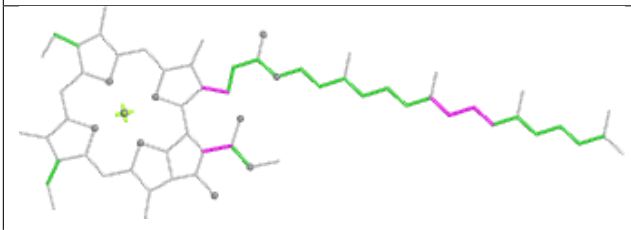
Ligand CLA B 843



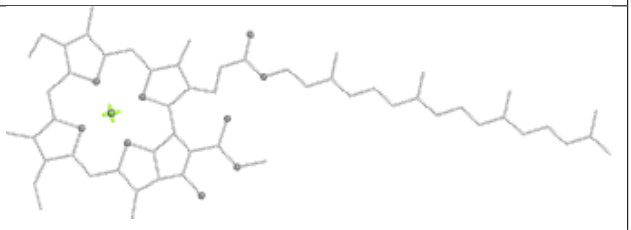
Bond lengths



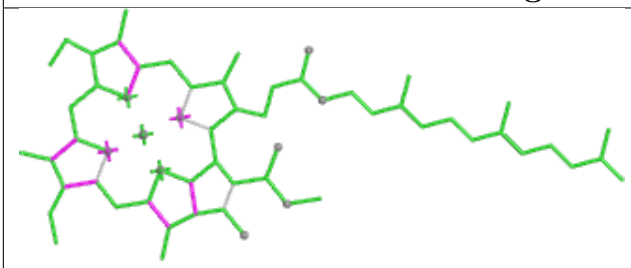
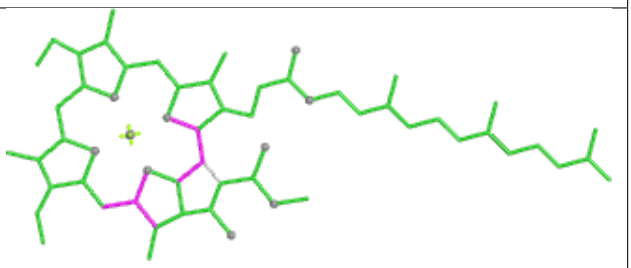
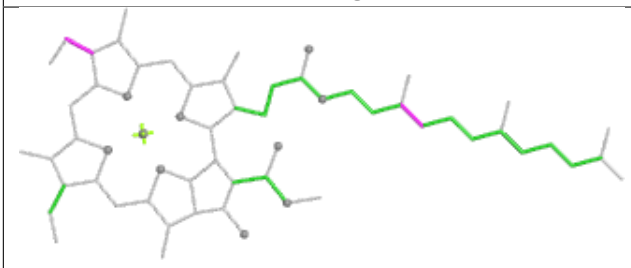
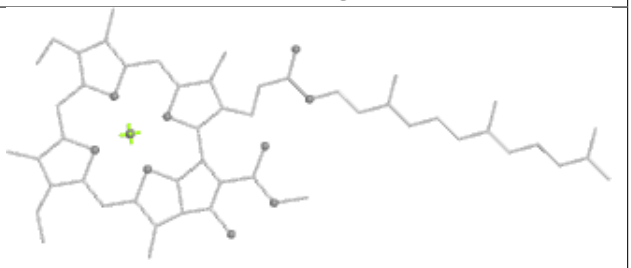
Bond angles

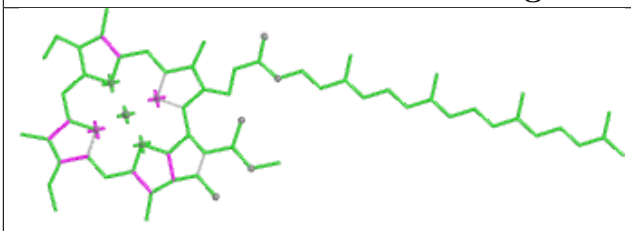
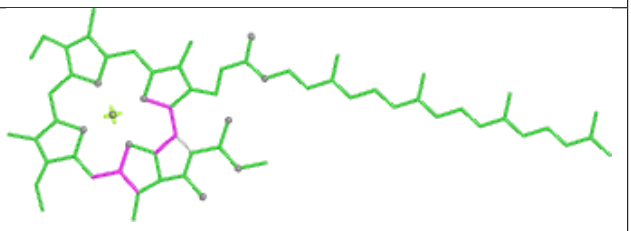
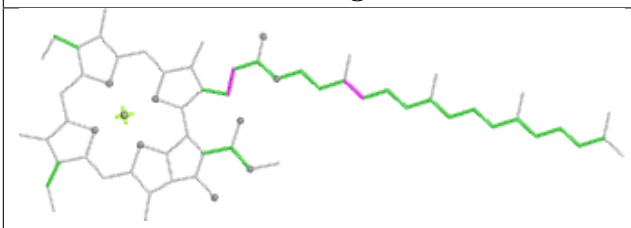
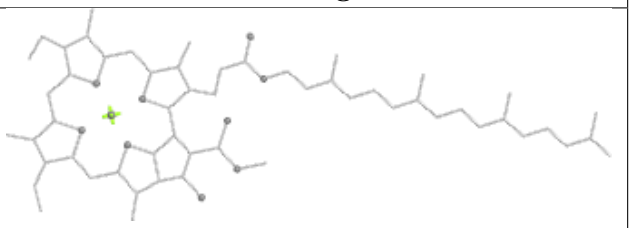


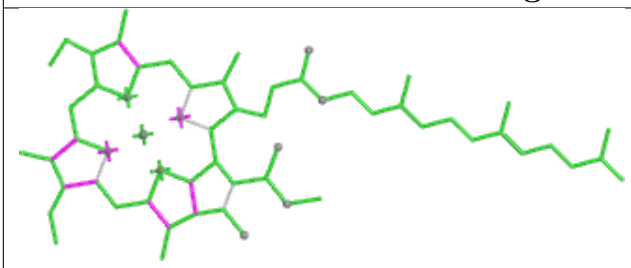
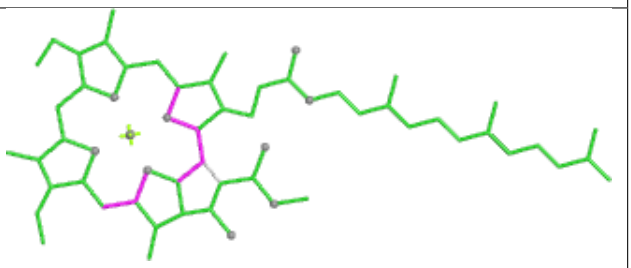
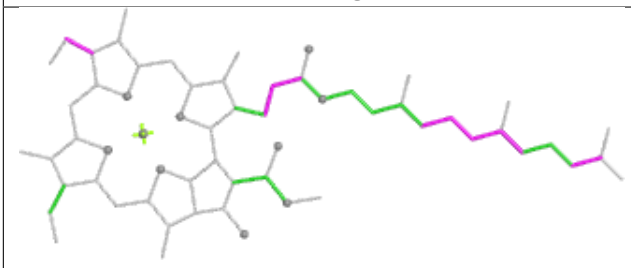
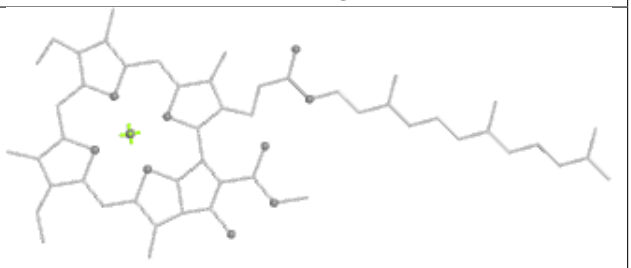
Torsions

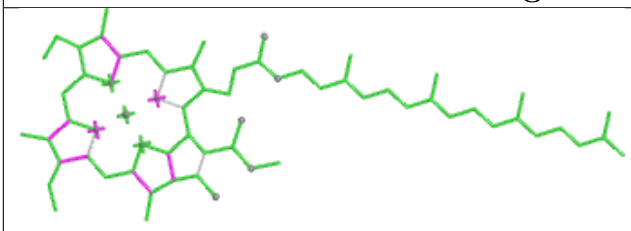
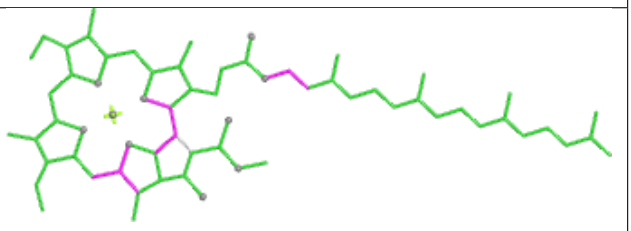
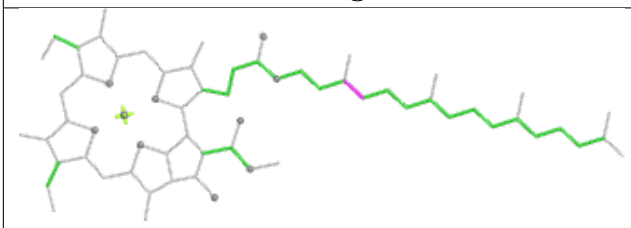
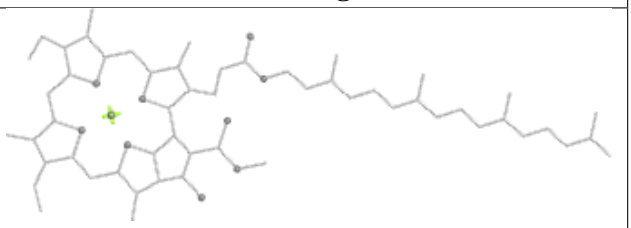


Rings

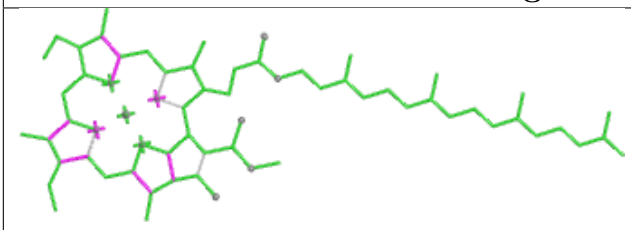
Ligand CLA B 816	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 801	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

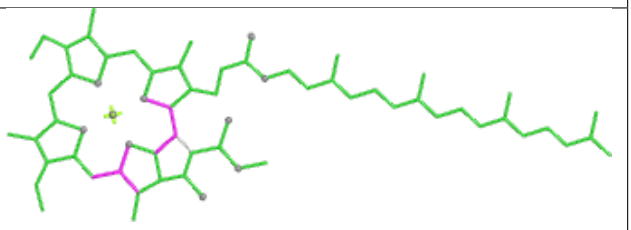
Ligand CLA A 845	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 818	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

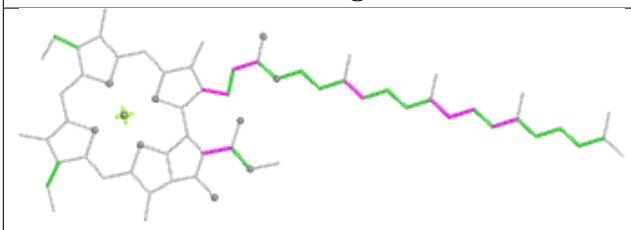
Ligand CLA A 804



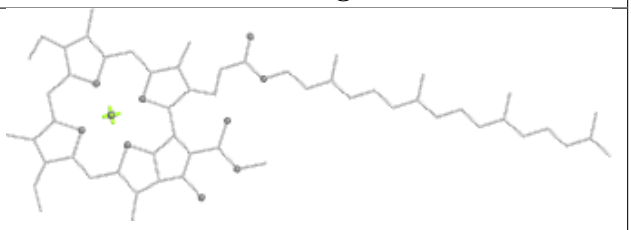
Bond lengths



Bond angles

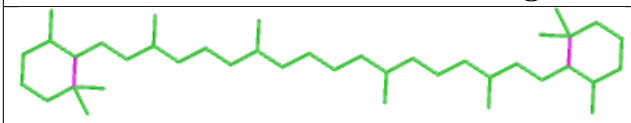


Torsions

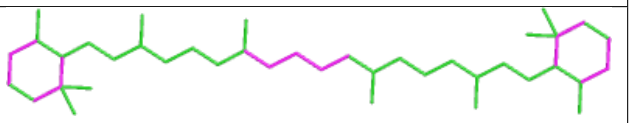


Rings

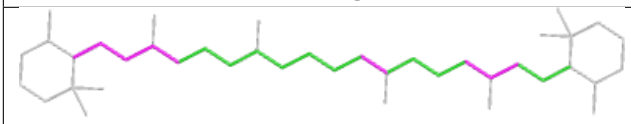
Ligand BCR B 838



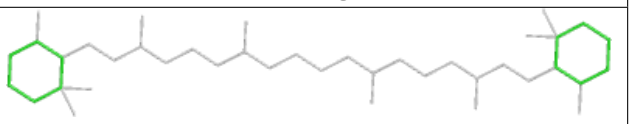
Bond lengths



Bond angles

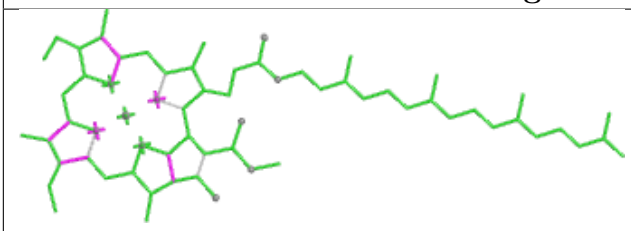


Torsions

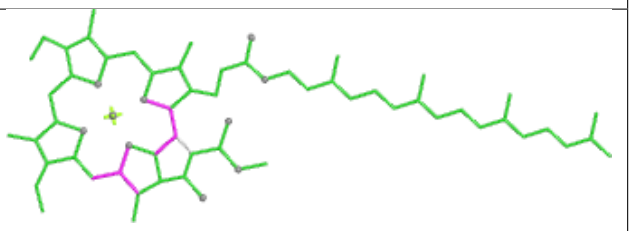


Rings

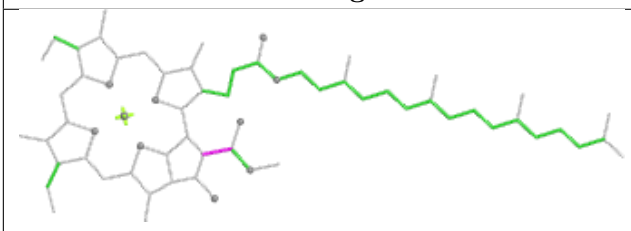
Ligand CLA A 816



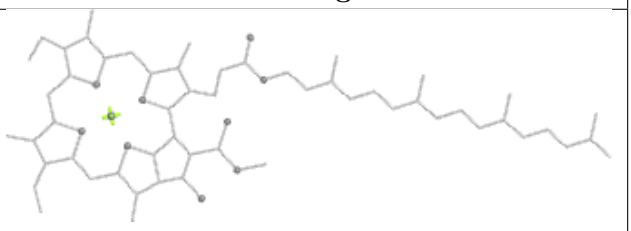
Bond lengths



Bond angles

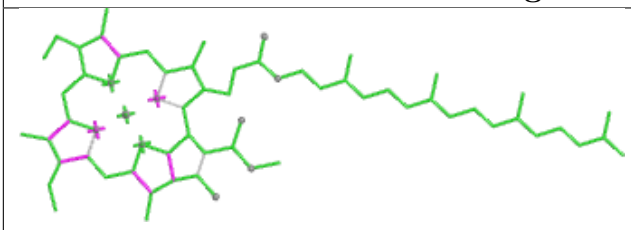


Torsions

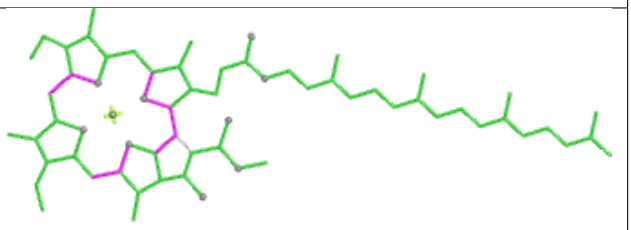


Rings

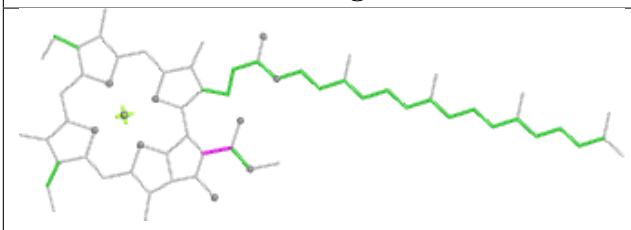
Ligand CLA B 822



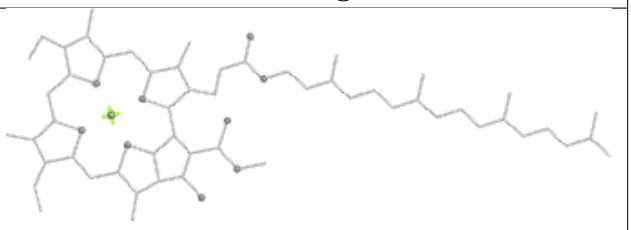
Bond lengths



Bond angles

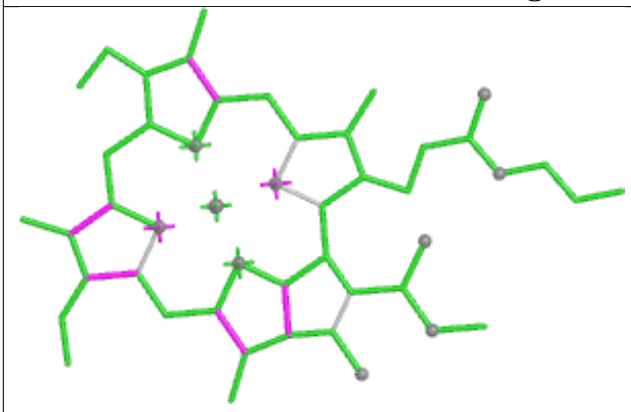


Torsions

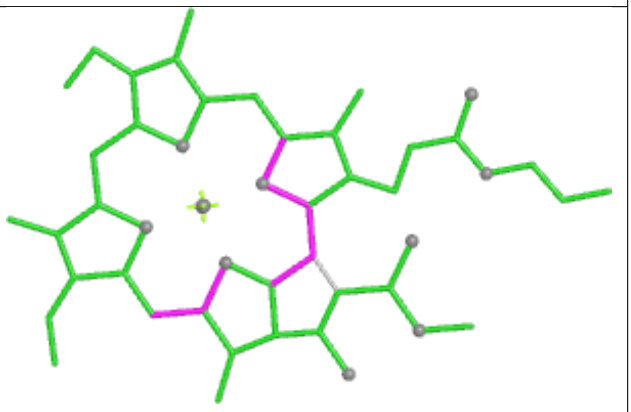


Rings

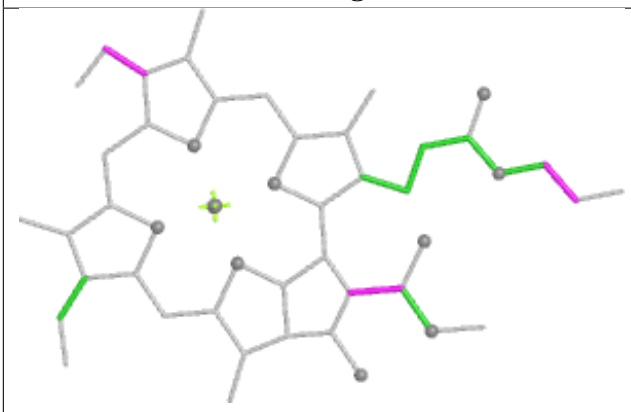
Ligand CLA F 802



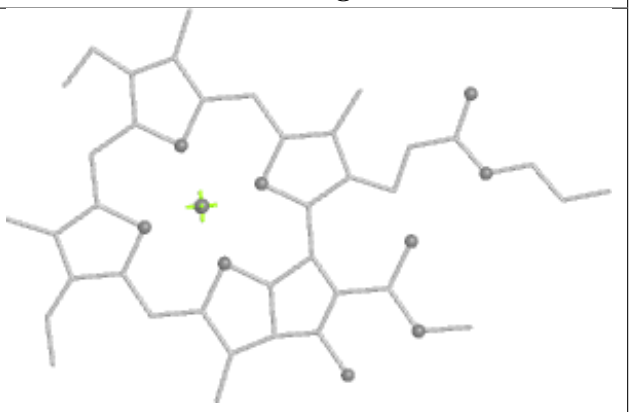
Bond lengths



Bond angles

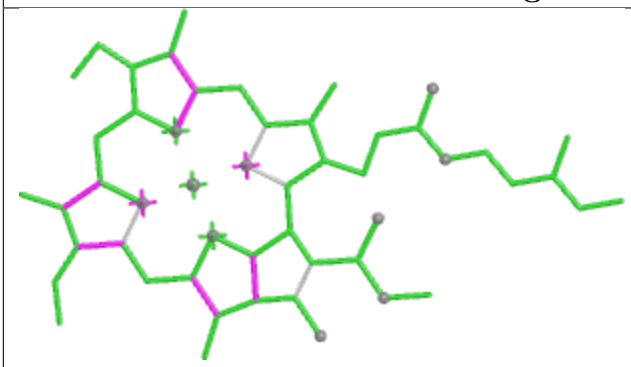


Torsions

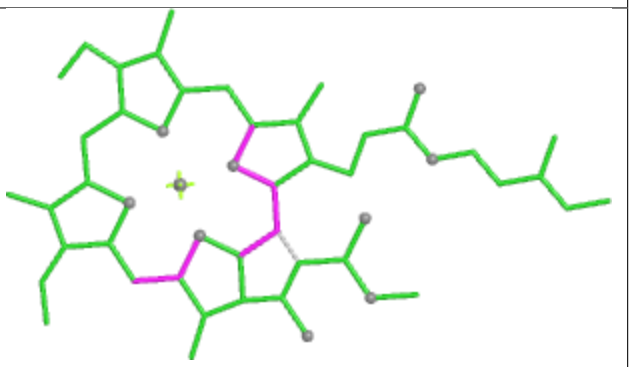


Rings

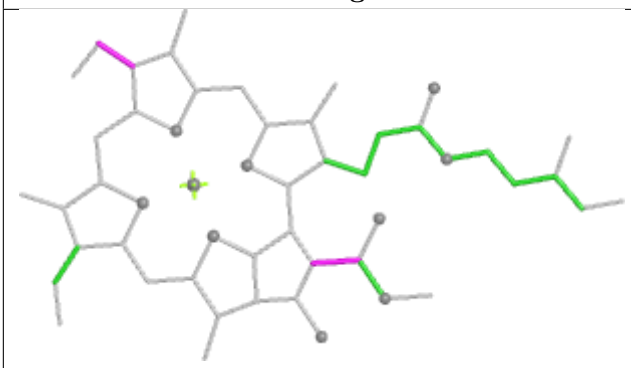
Ligand CLA A 832



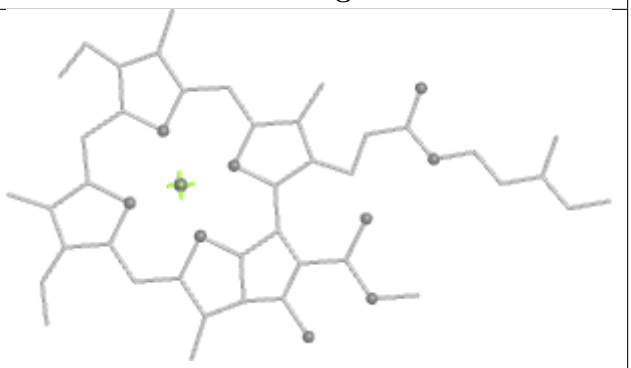
Bond lengths



Bond angles

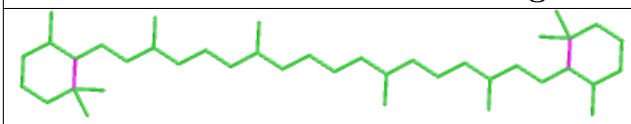


Torsions

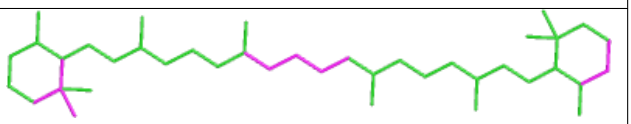


Rings

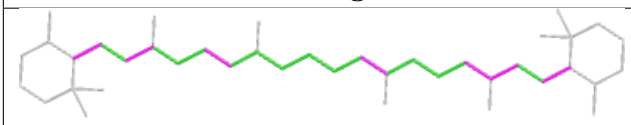
Ligand BCR I 101



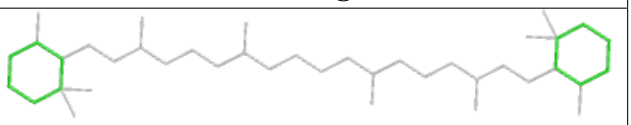
Bond lengths



Bond angles

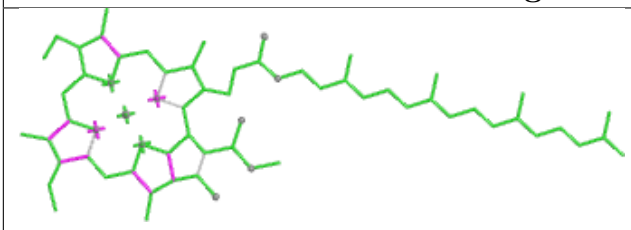


Torsions

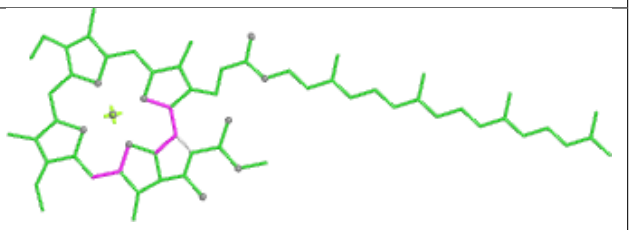


Rings

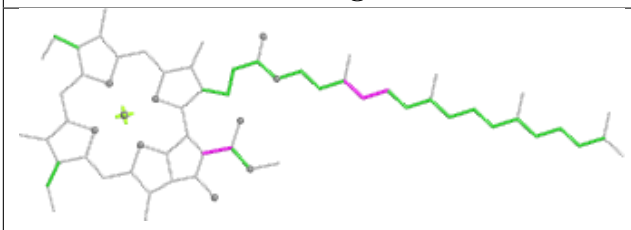
Ligand CLA B 808



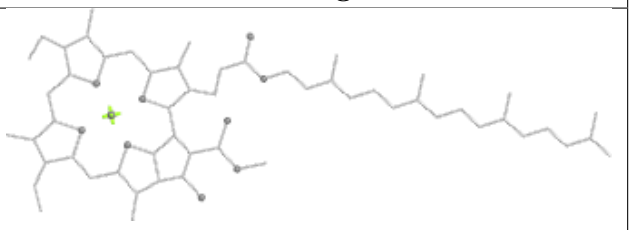
Bond lengths



Bond angles

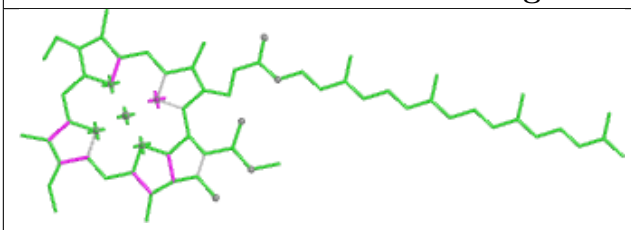


Torsions

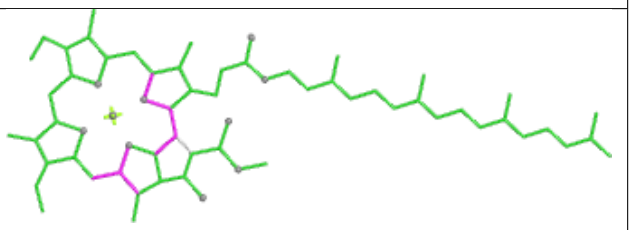


Rings

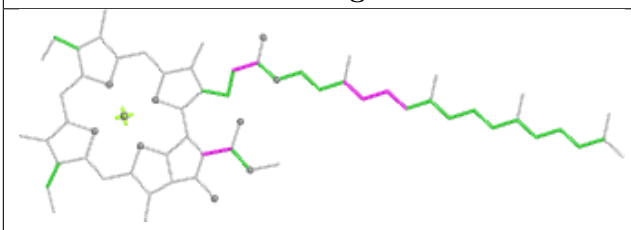
Ligand CLA U 211



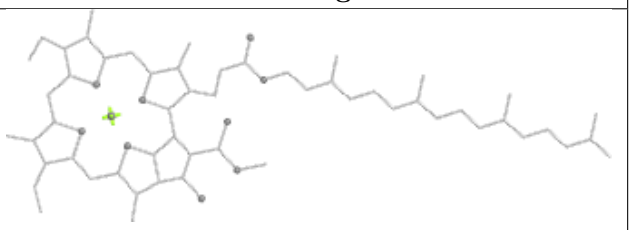
Bond lengths



Bond angles



Torsions

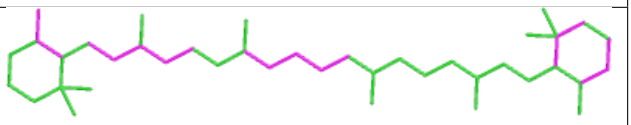


Rings

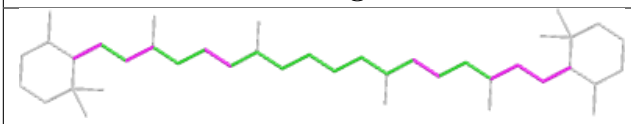
Ligand BCR B 837



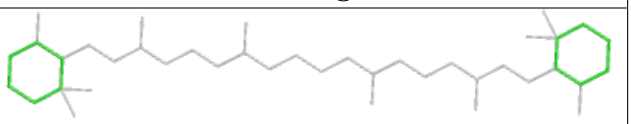
Bond lengths



Bond angles

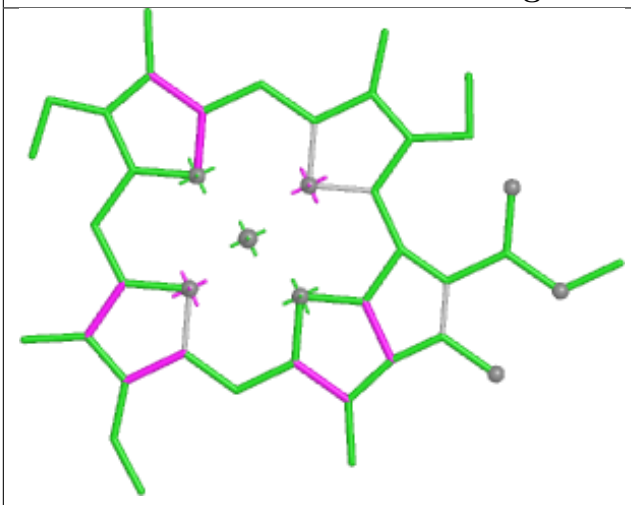


Torsions

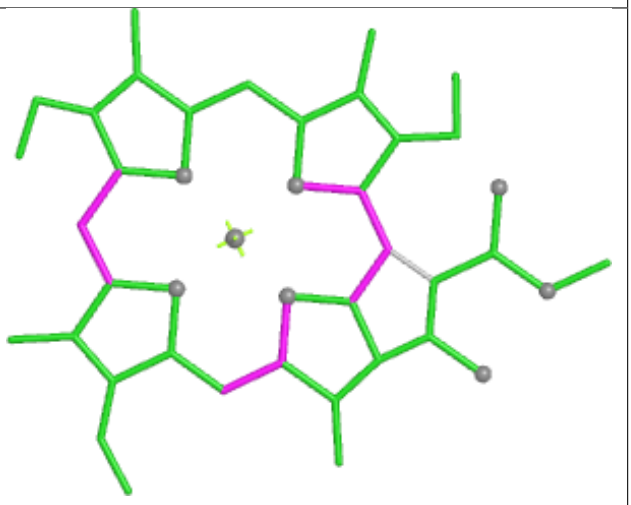


Rings

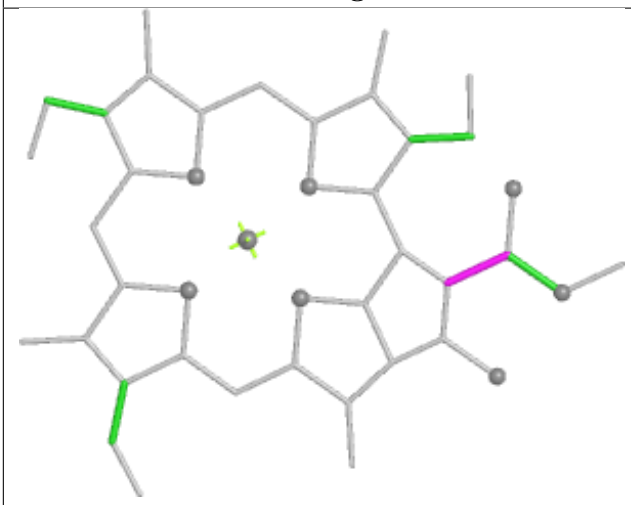
Ligand CLA U 210



Bond lengths



Bond angles



Torsions

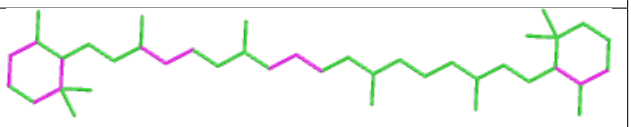


Rings

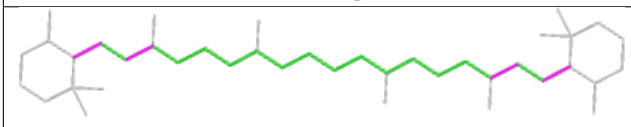
Ligand BCR F 801



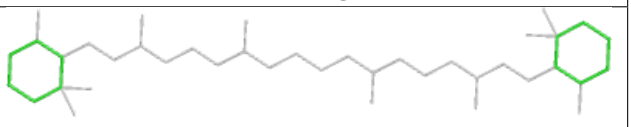
Bond lengths



Bond angles

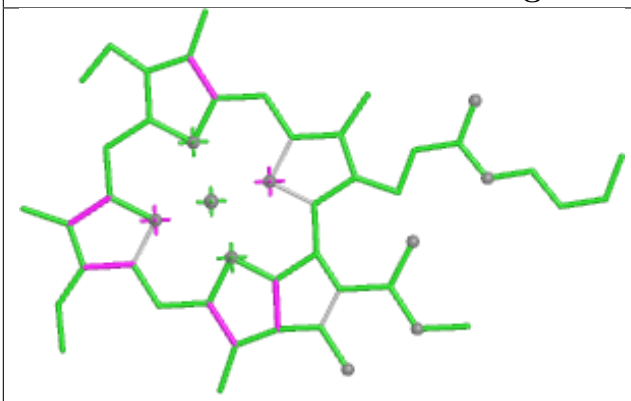


Torsions

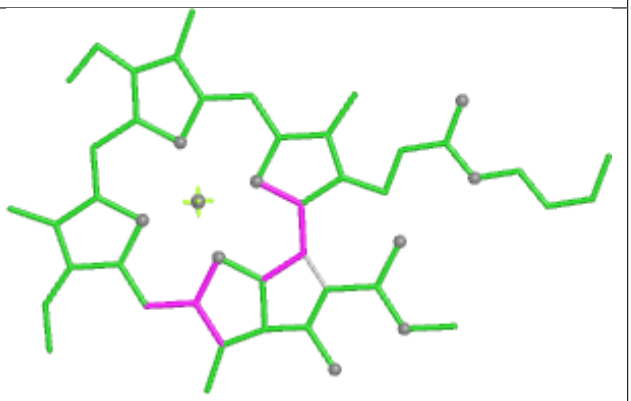


Rings

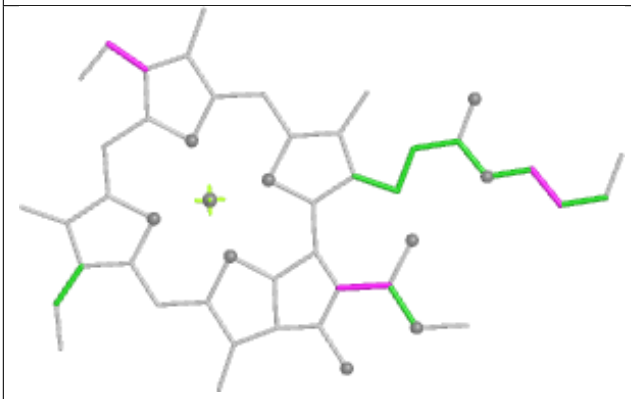
Ligand CLA A 805



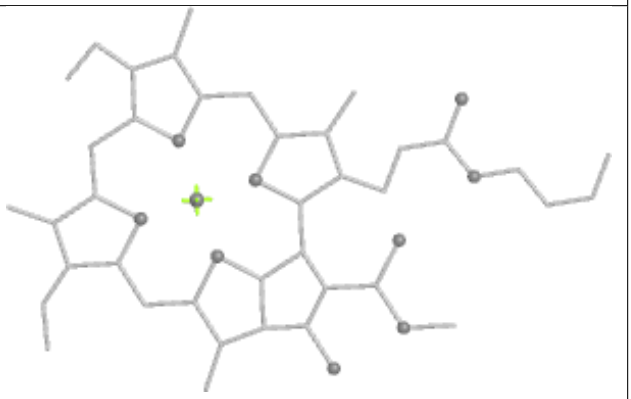
Bond lengths



Bond angles

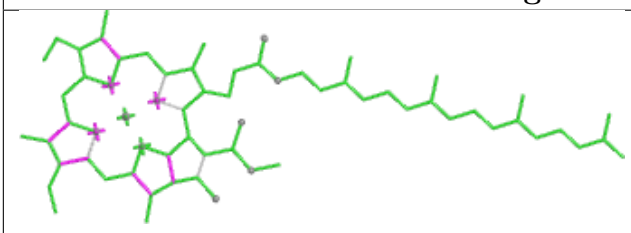


Torsions

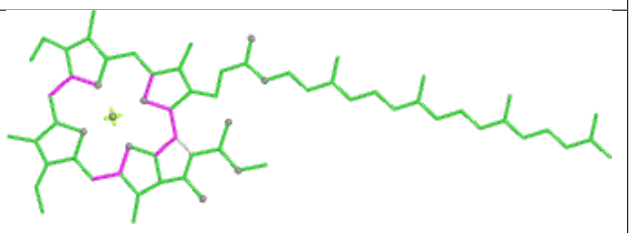


Rings

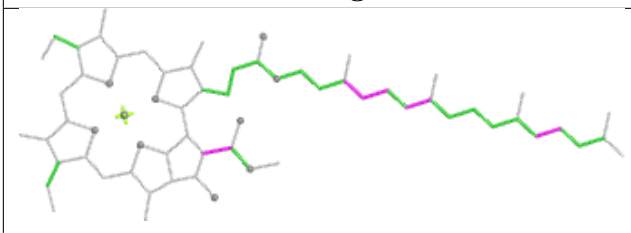
Ligand CLA A 834



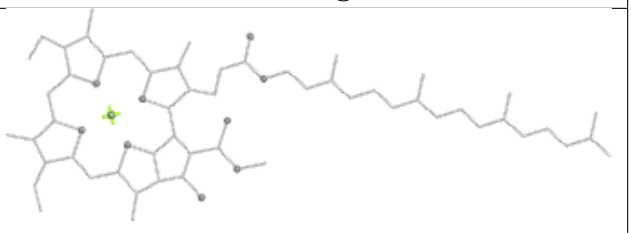
Bond lengths



Bond angles

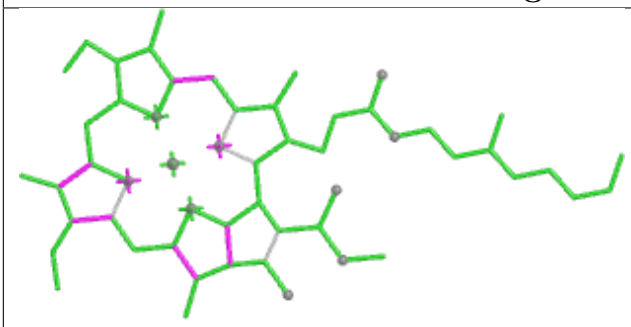


Torsions

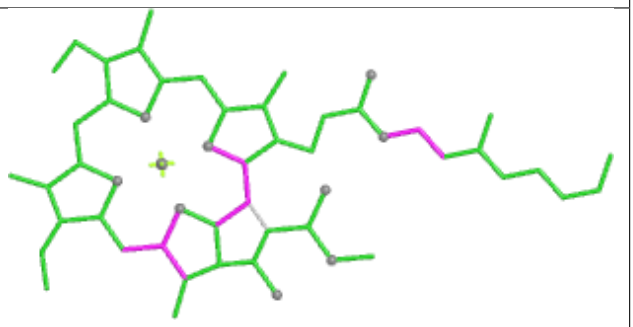


Rings

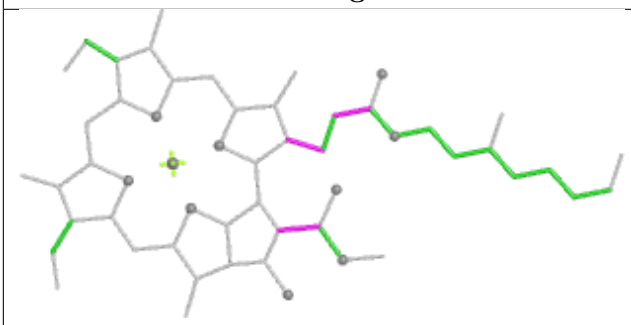
Ligand CLA B 812



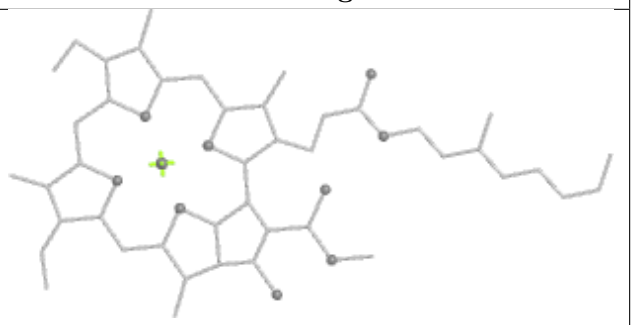
Bond lengths



Bond angles

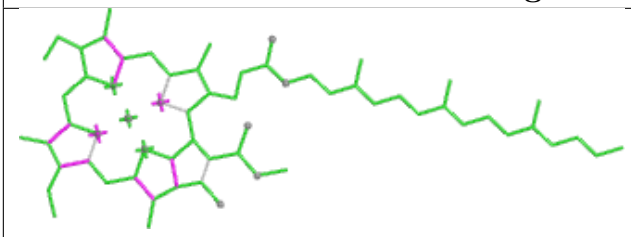


Torsions

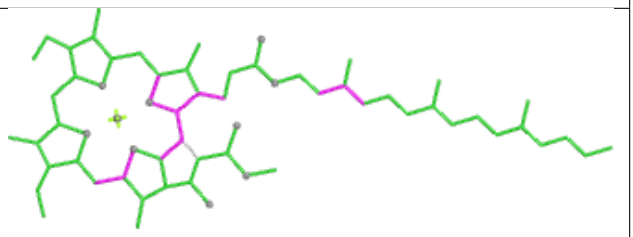


Rings

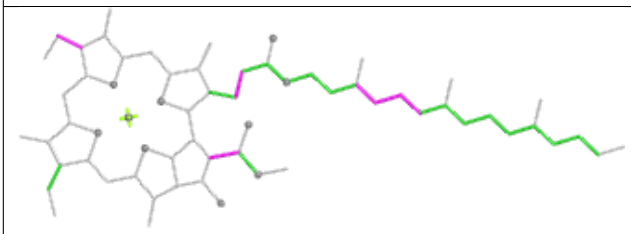
Ligand CLA B 820



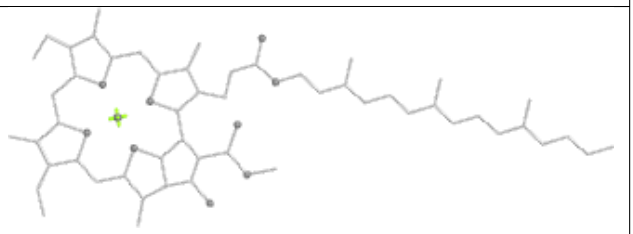
Bond lengths



Bond angles

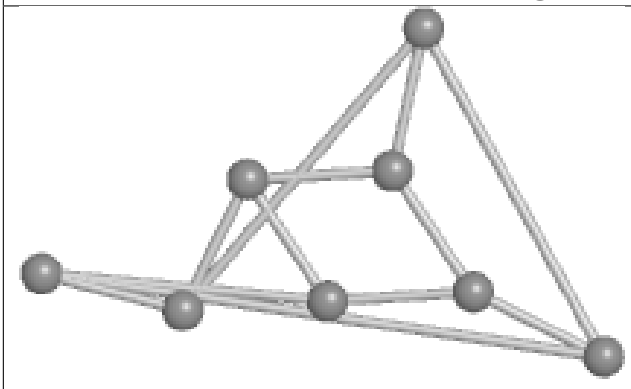


Torsions

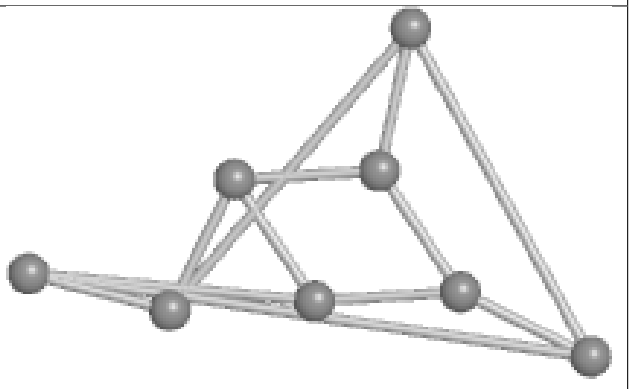


Rings

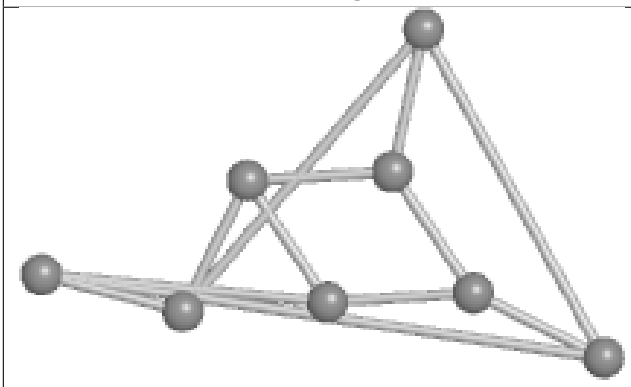
Ligand SF4 C 102



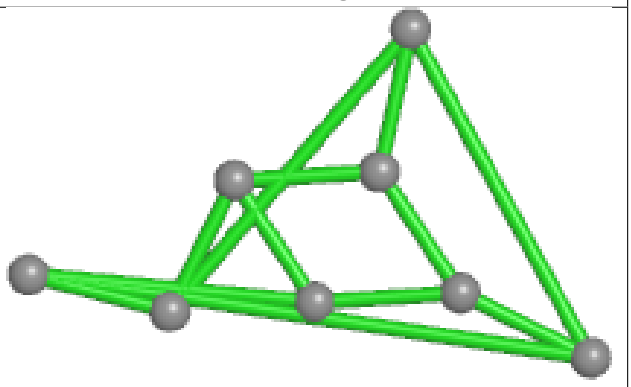
Bond lengths



Bond angles

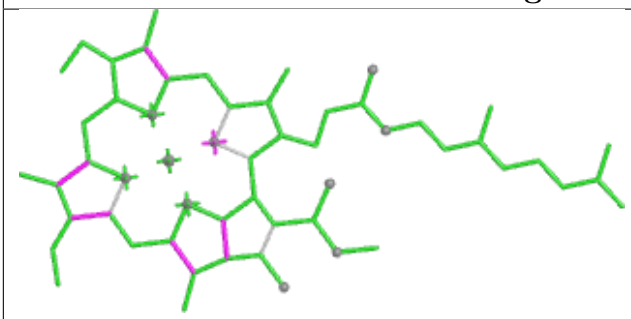


Torsions

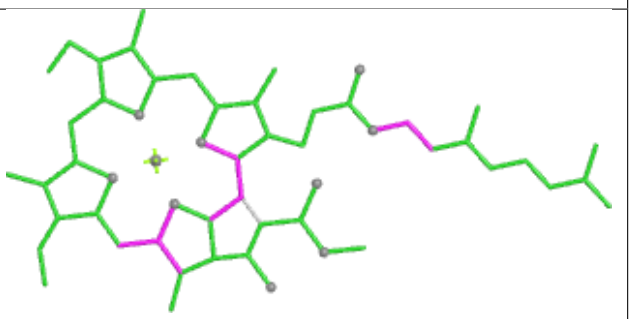


Rings

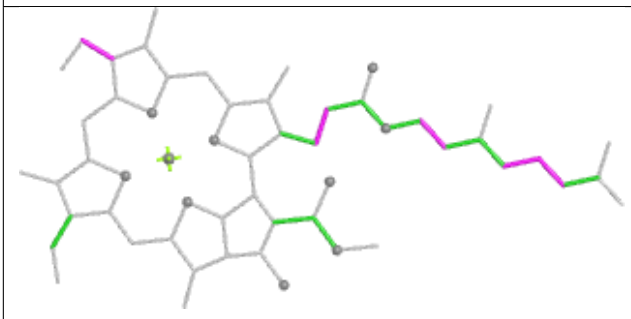
Ligand CLA B 811



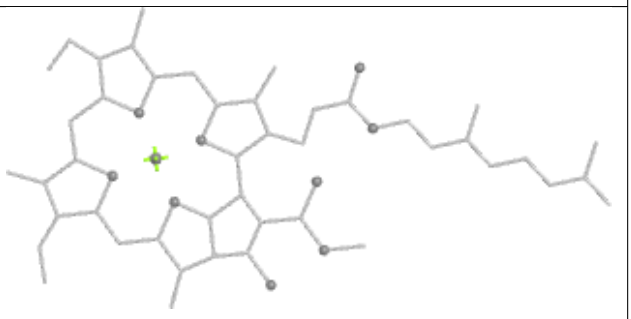
Bond lengths



Bond angles

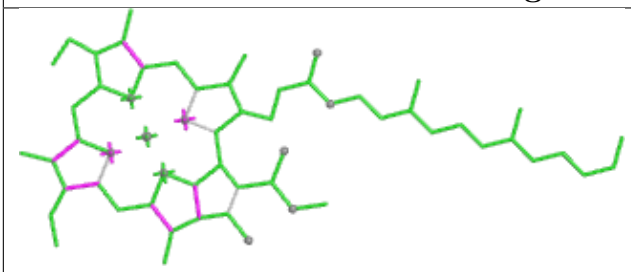


Torsions

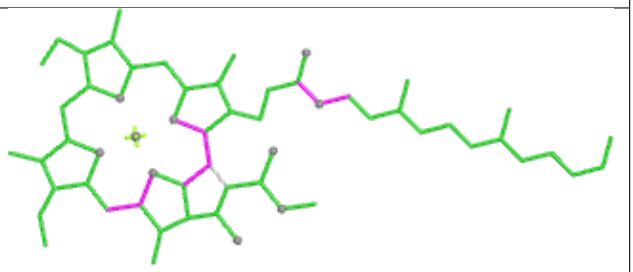


Rings

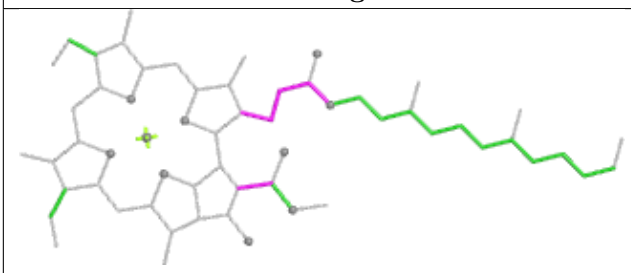
Ligand CLA B 813



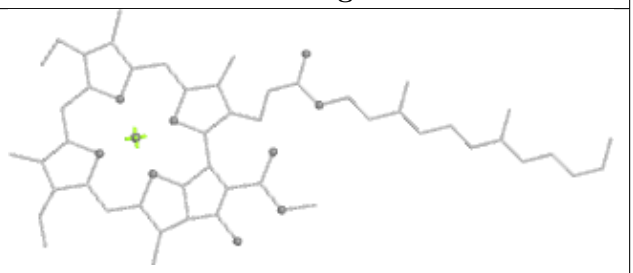
Bond lengths



Bond angles

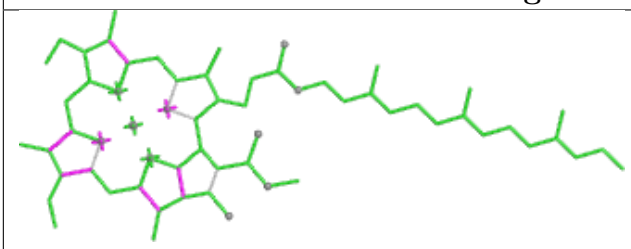


Torsions

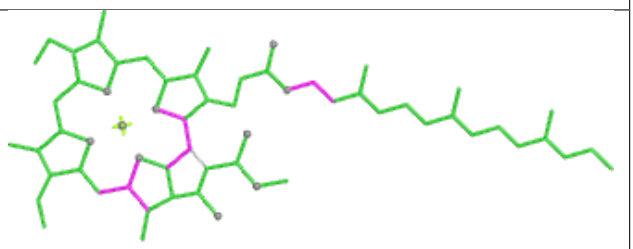


Rings

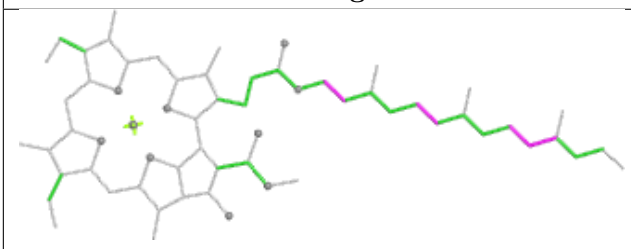
Ligand CLA A 824



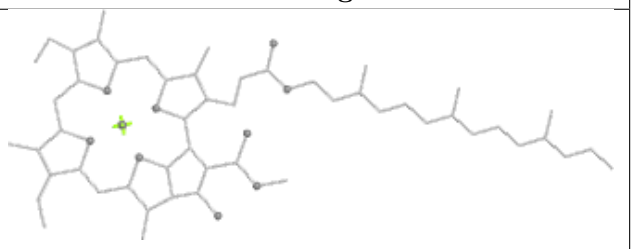
Bond lengths



Bond angles



Torsions

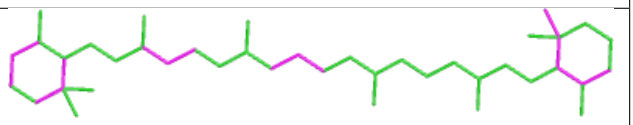


Rings

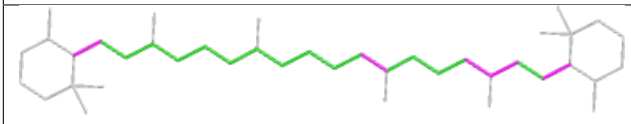
Ligand BCR A 840



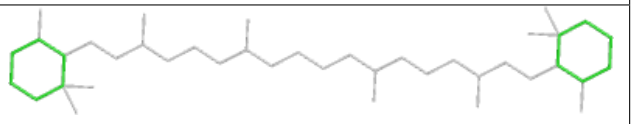
Bond lengths



Bond angles

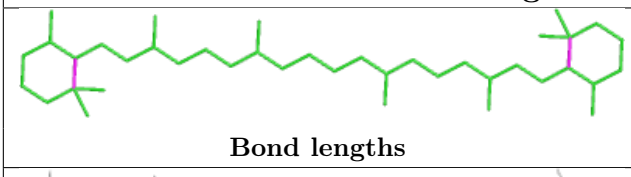


Torsions

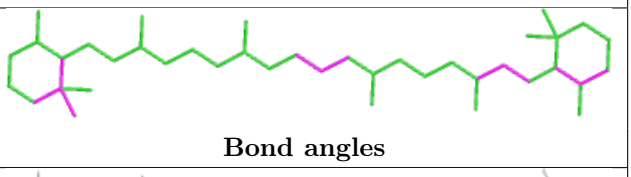


Rings

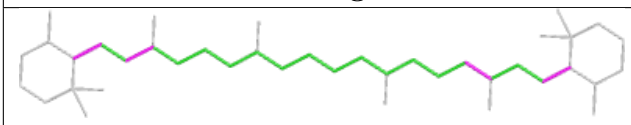
Ligand BCR B 839



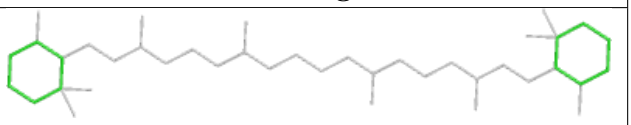
Bond lengths



Bond angles

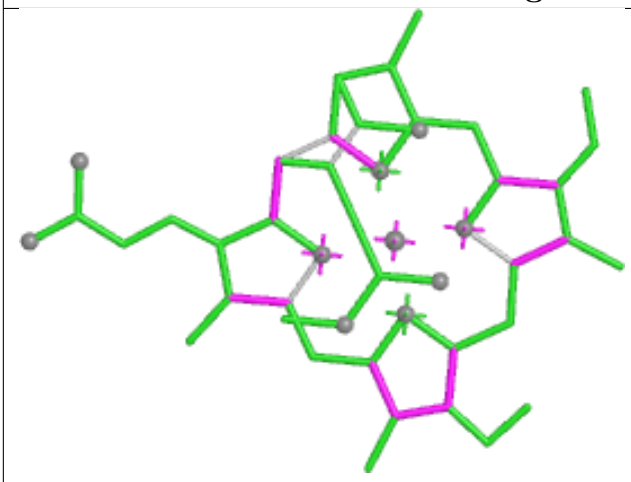


Torsions

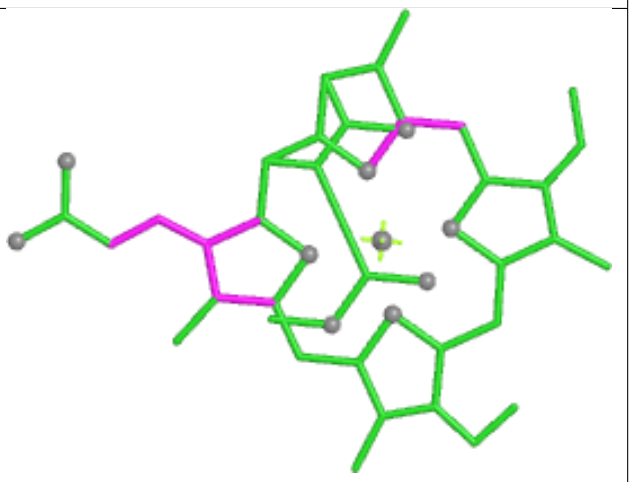


Rings

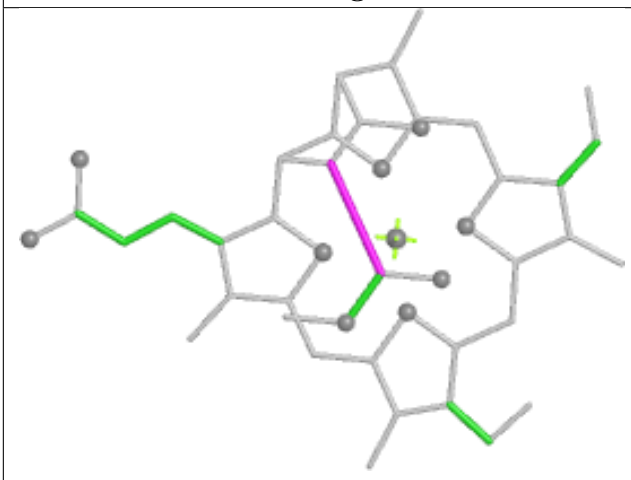
Ligand KC1 U 214



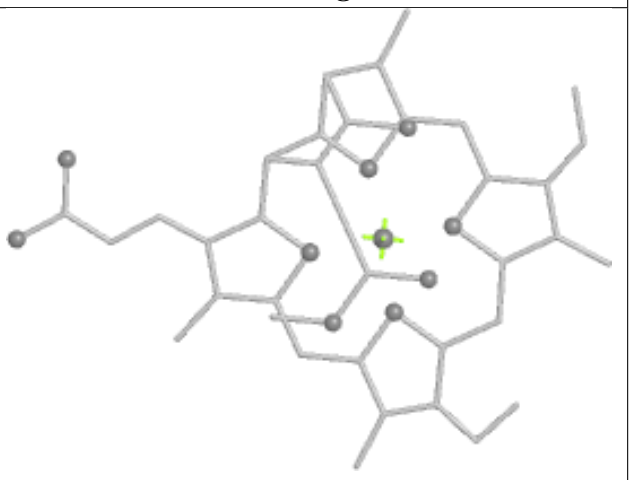
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

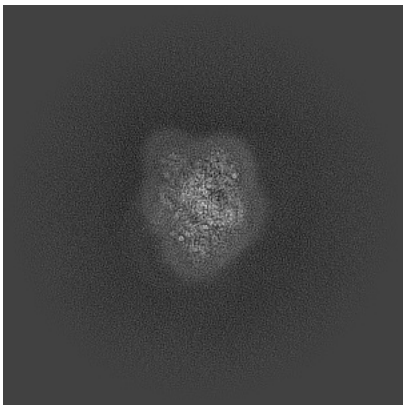
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64362. These allow visual inspection of the internal detail of the map and identification of artifacts.

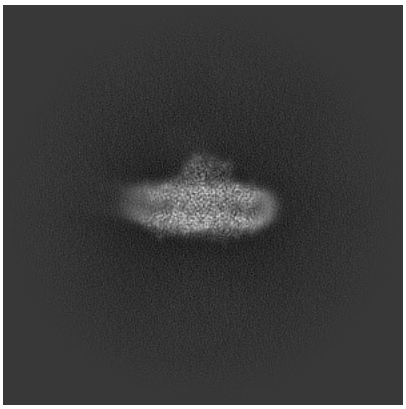
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

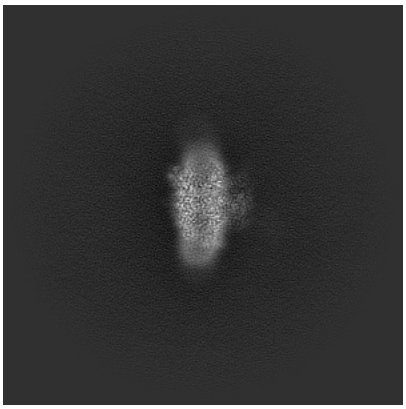
6.1.1 Primary map



X

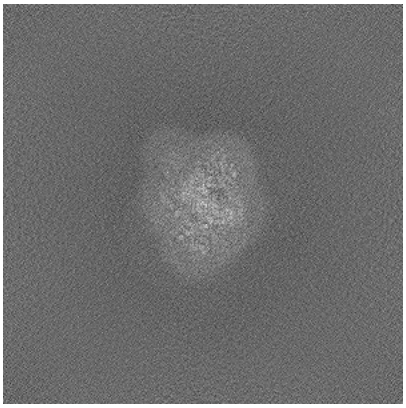


Y

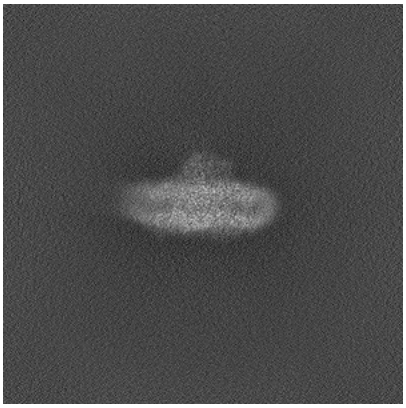


Z

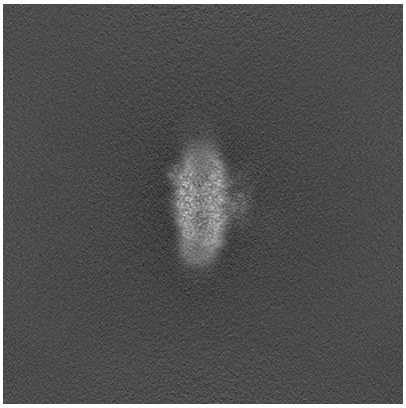
6.1.2 Raw map



X



Y

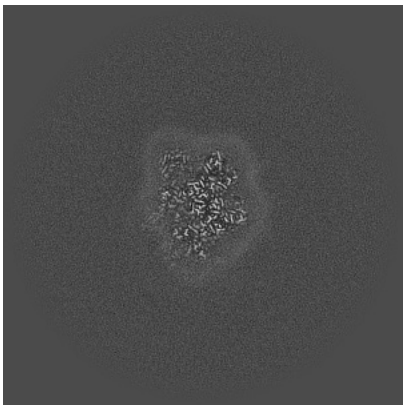


Z

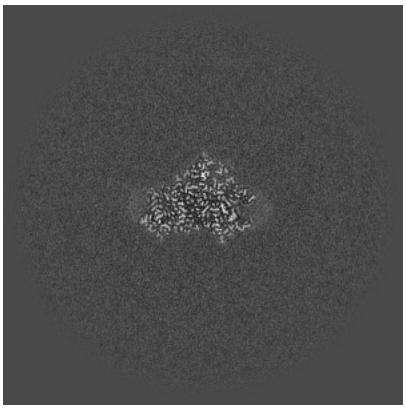
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

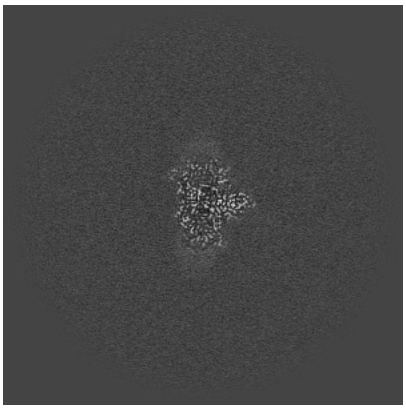
6.2.1 Primary map



X Index: 300

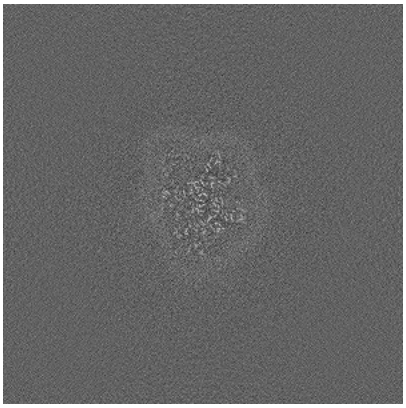


Y Index: 300

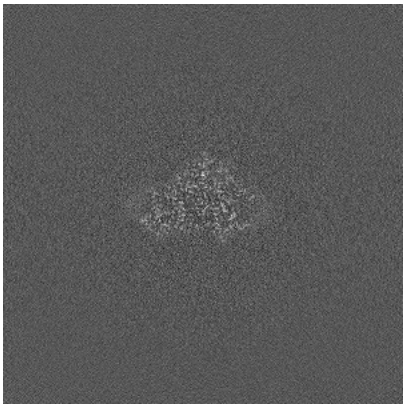


Z Index: 300

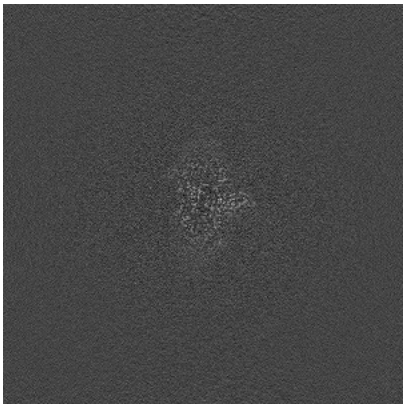
6.2.2 Raw map



X Index: 300



Y Index: 300

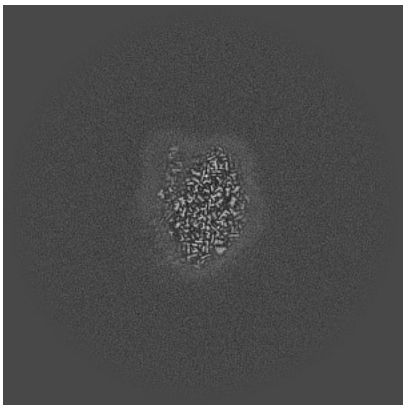


Z Index: 300

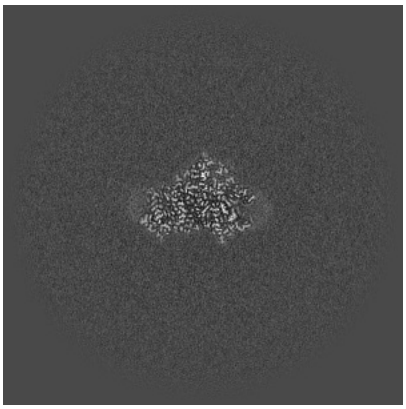
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

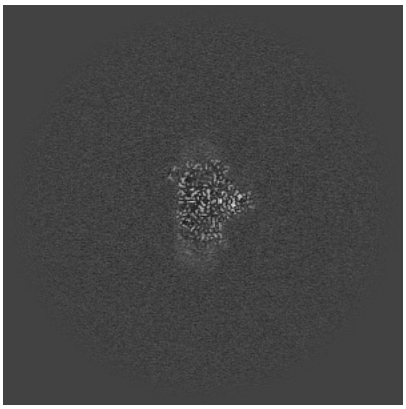
6.3.1 Primary map



X Index: 282

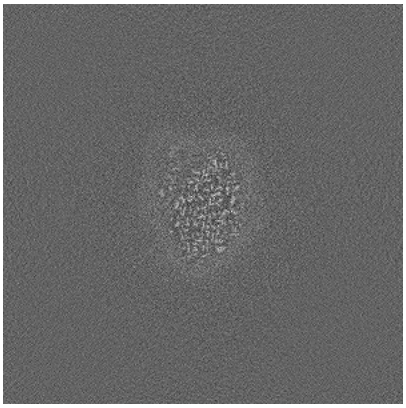


Y Index: 300

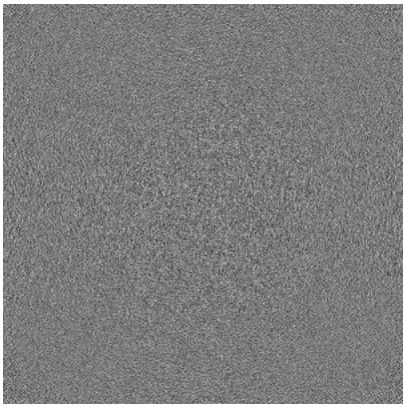


Z Index: 298

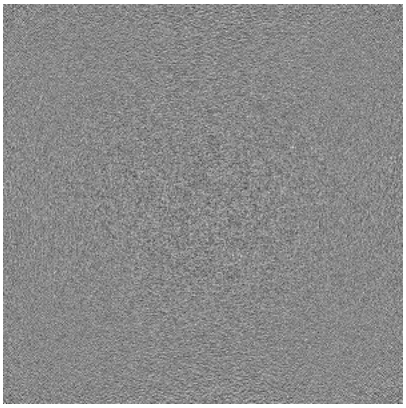
6.3.2 Raw map



X Index: 282



Y Index: 0

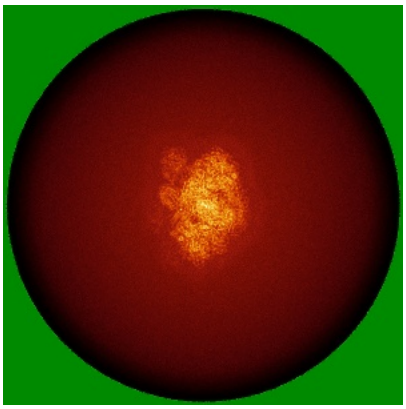


Z Index: 599

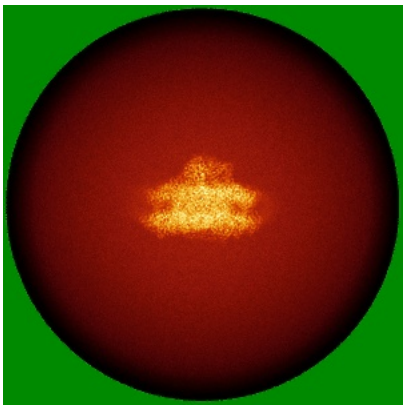
The images above show the largest variance slices of the map in three orthogonal directions.

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

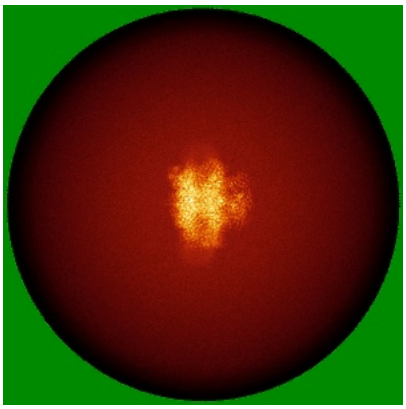
6.4.1 Primary map



X

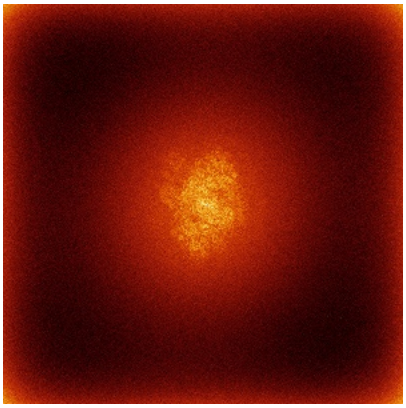


Y

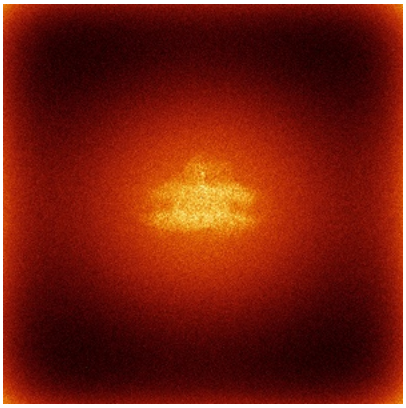


Z

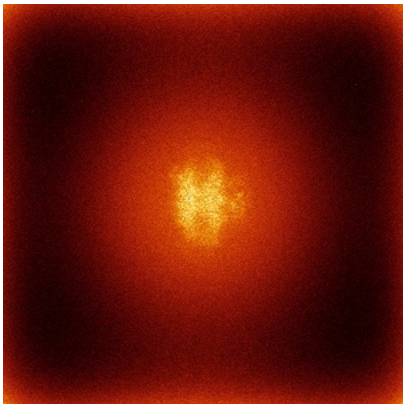
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

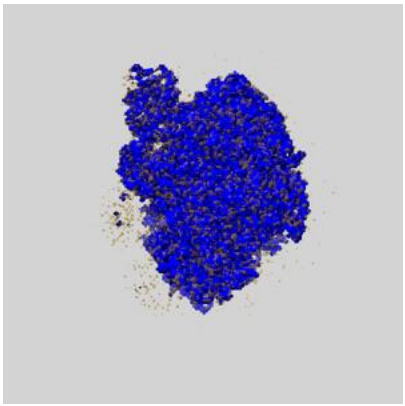
6.6 Mask visualisation (i)

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

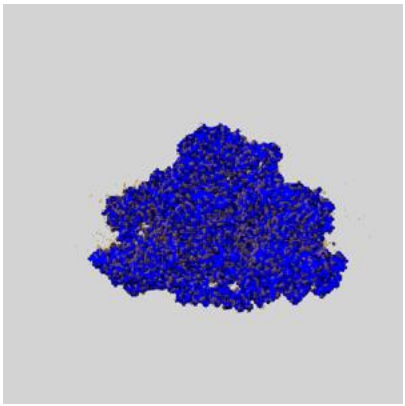
A mask typically either:

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

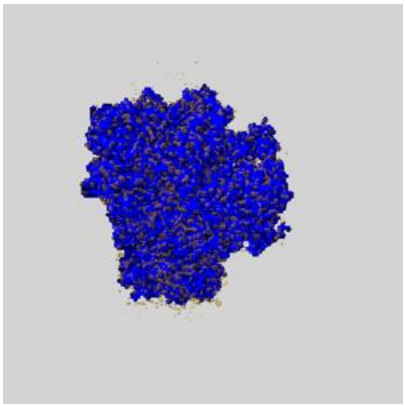
6.6.1 emd_64362_msk_1.map (i)



X



Y

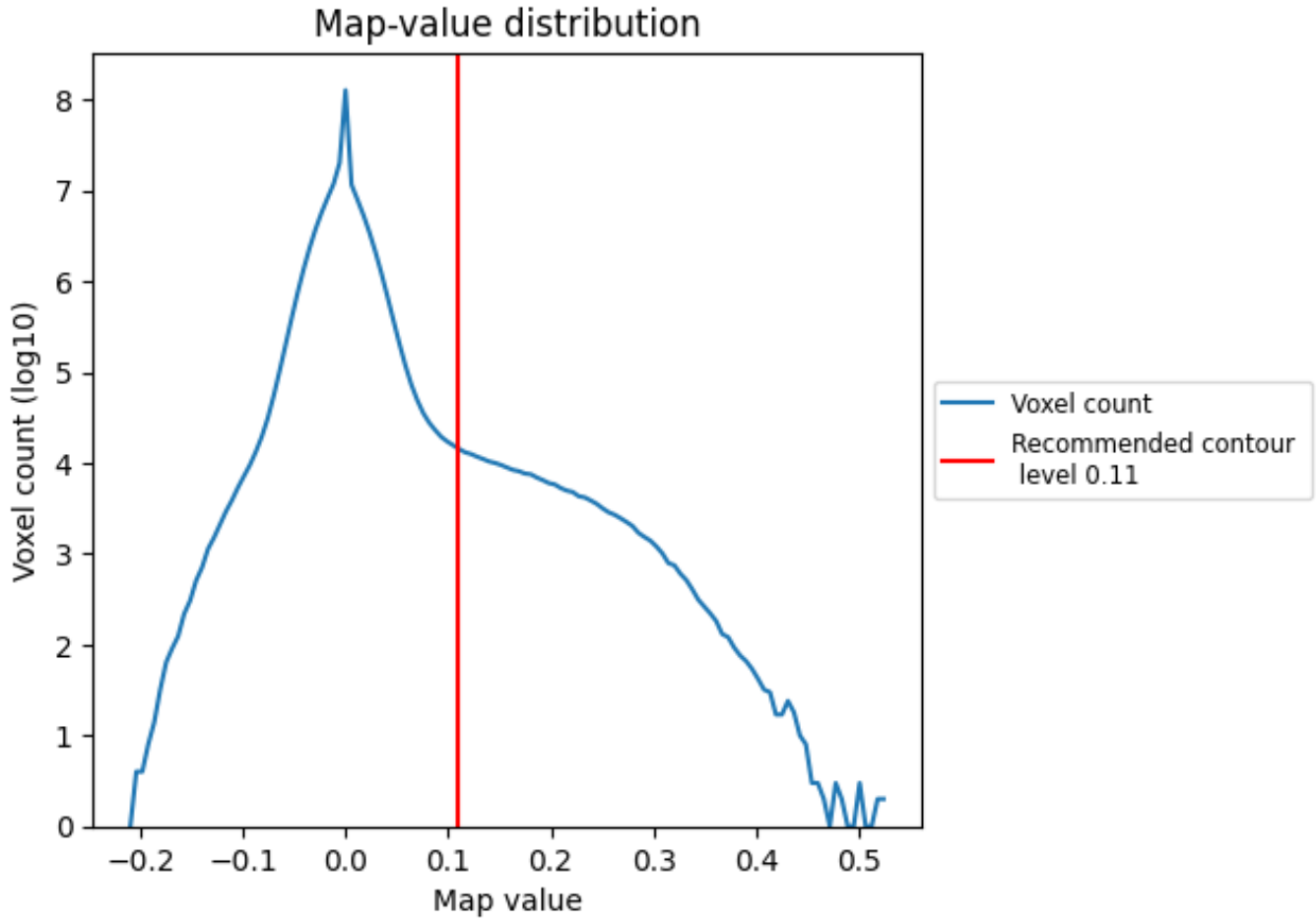


Z

7 Map analysis

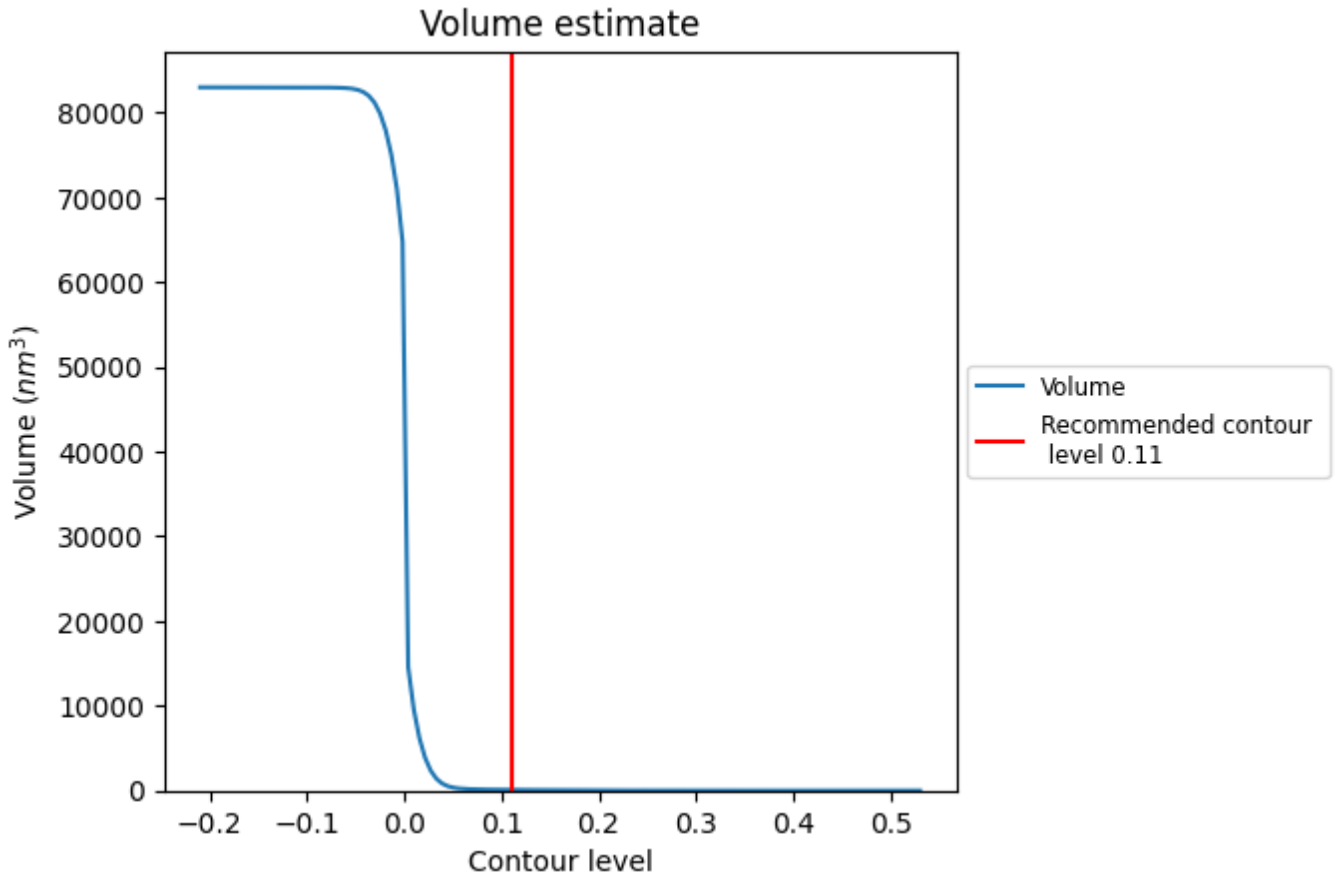
This section contains the results of statistical analysis of the map.

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.

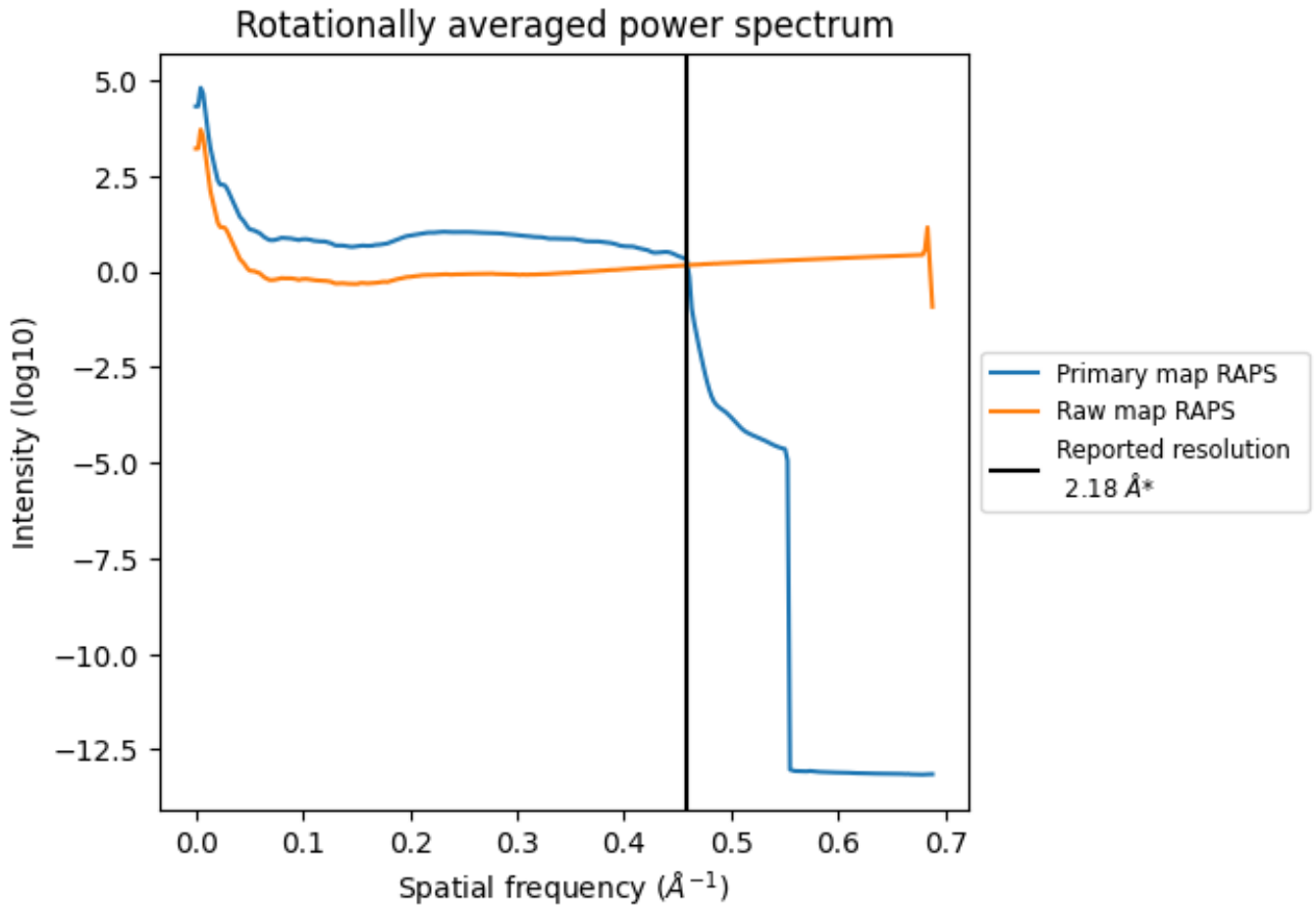
7.2 Volume estimate (i)



The volume at the recommended contour level is 84 nm^3; this corresponds to an approximate mass of 76 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)

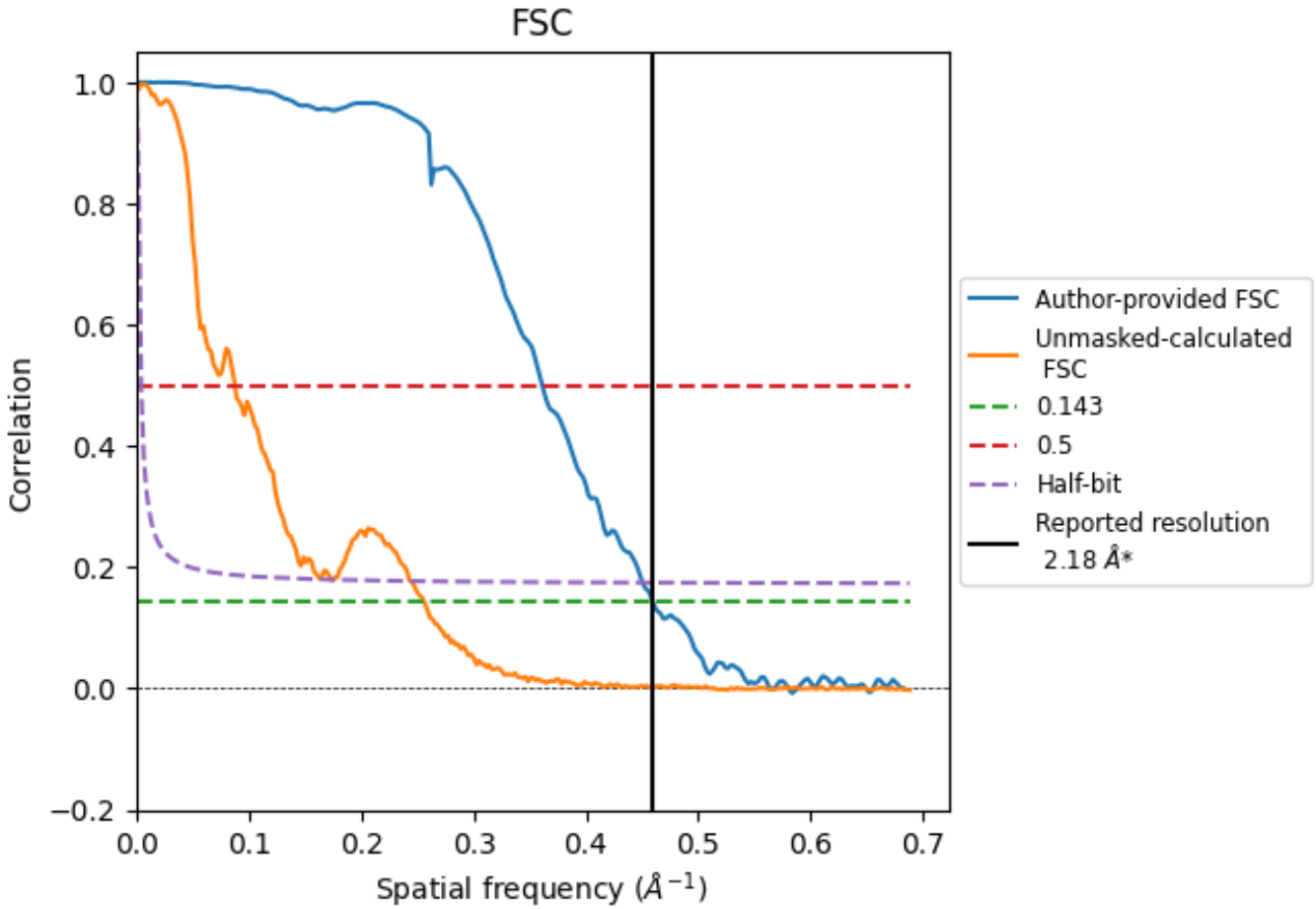


*Reported resolution corresponds to spatial frequency of 0.459 $Å^{-1}$

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 0.459 $Å^{-1}$

8.2 Resolution estimates (i)

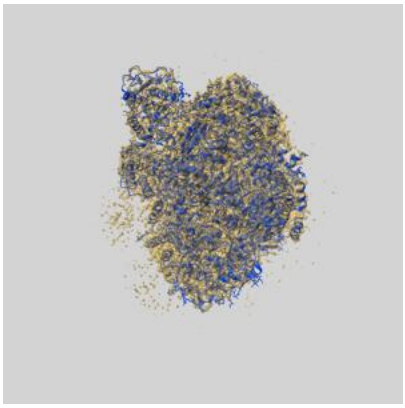
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.18	-	-
Author-provided FSC curve	2.18	2.77	2.22
Unmasked-calculated*	3.91	11.39	5.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 2.18 by more than 10 %

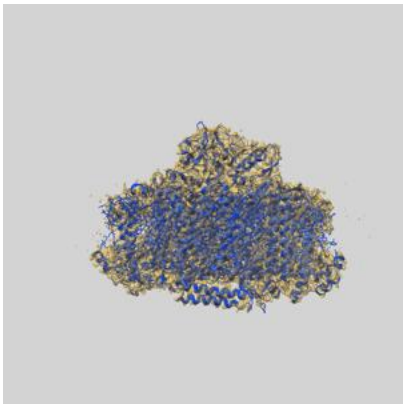
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64362 and PDB model 9UNU. Per-residue inclusion information can be found in section 3 on page 19.

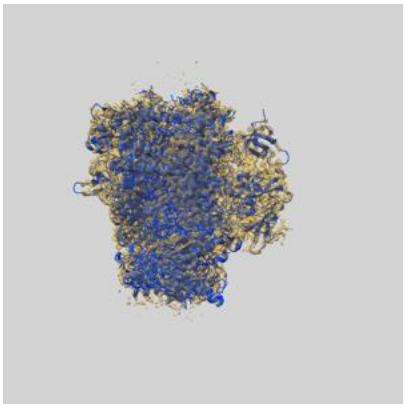
9.1 Map-model overlay



X



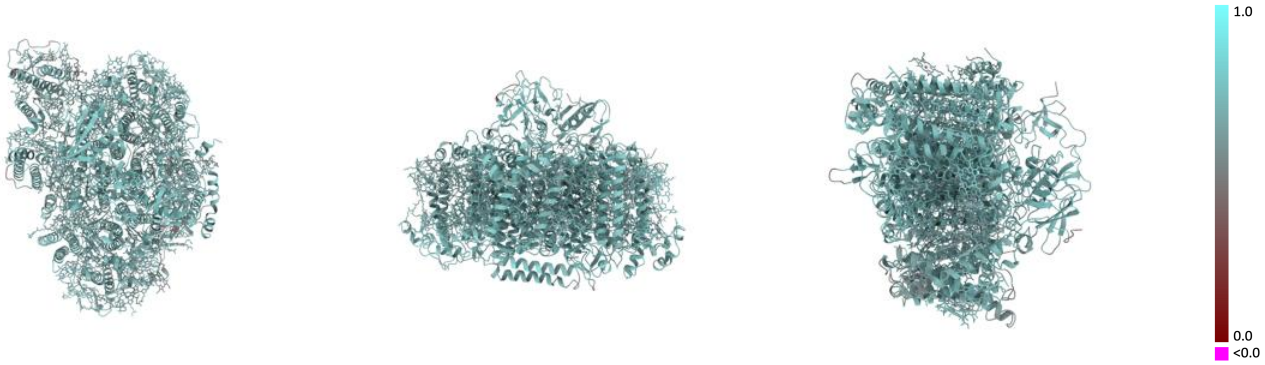
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

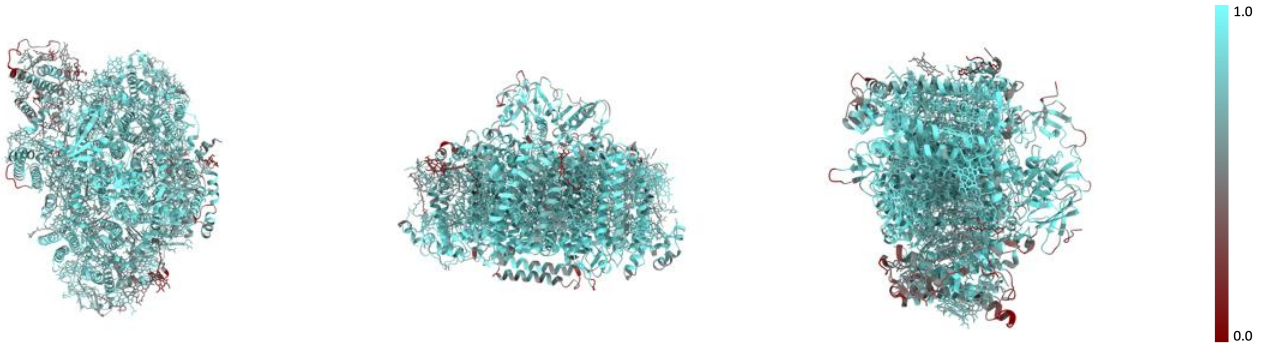
9.2 Q-score mapped to coordinate model



X Y Z

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

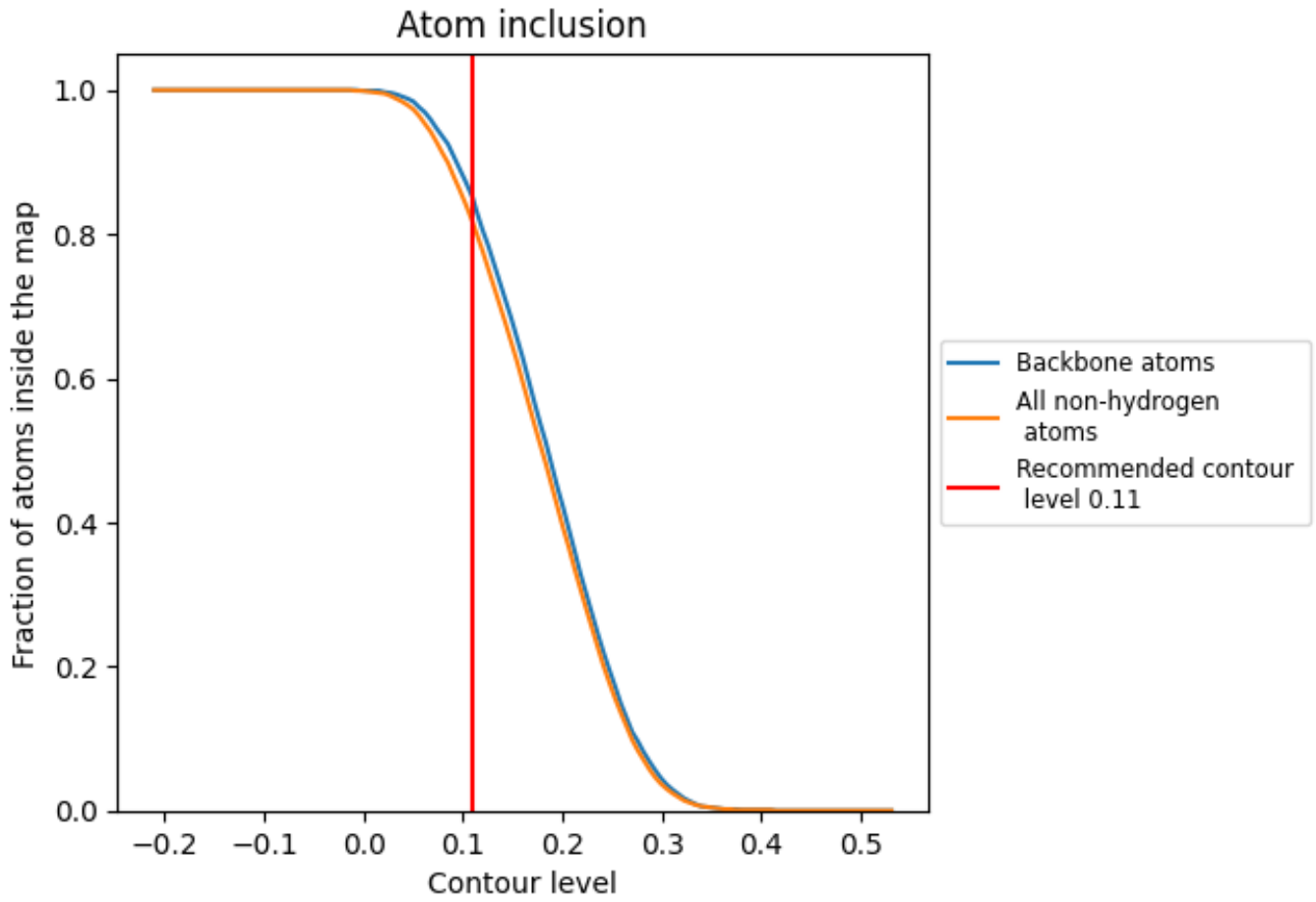
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.6850
A	0.8700	0.6970
B	0.8510	0.6940
C	0.9180	0.7110
D	0.7640	0.6730
E	0.7560	0.6610
F	0.7180	0.6660
I	0.7800	0.6710
J	0.6750	0.6620
L	0.7720	0.6720
M	0.7550	0.6740
U	0.5340	0.6190

