wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 11:01 PM JST

PDB ID	:	8W4O / pdb_00008w4o
EMDB ID	:	EMD-37267
Title	:	Structure of PSII-FCPII-G/H complex in the PSII-FCPII supercomplex from Cyclotella meneghiniana
Authors	:	Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on	:	2023-08-24
Resolution	:	3.23 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:

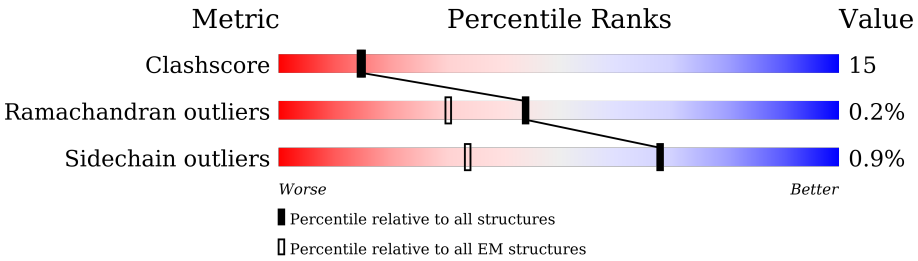
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

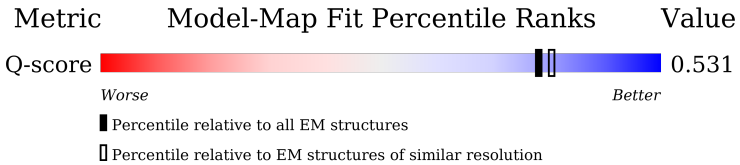
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.23 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	14612 (2.73 - 3.73)

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	5	169	13% 75% 25%
2	7	164	21% 70% 30%
3	6	164	12% 71% 27% •

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 6046 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 FCPII-G, Fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	5	169	1280	827	211	239	3	0	0

- Molecule 2 is a protein called FCPII-H2, Fucoxanthin chlorophyll a/c binding protein.

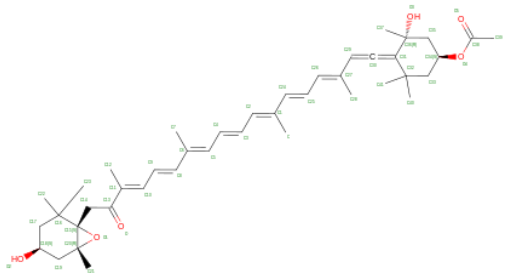
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	7	164	1222	808	198	212	4	0	0

- Molecule 3 is a protein called FCPII-H1, Fucoxanthin chlorophyll a/c binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	6	164	1209	796	210	201	2	0	0

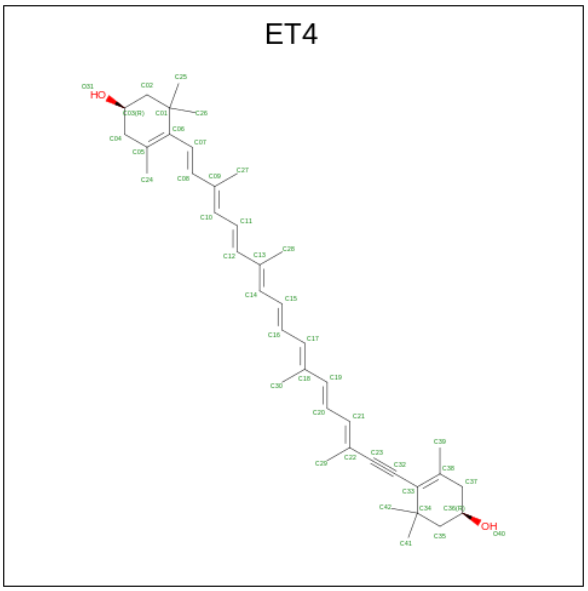
- Molecule 4 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).

A86



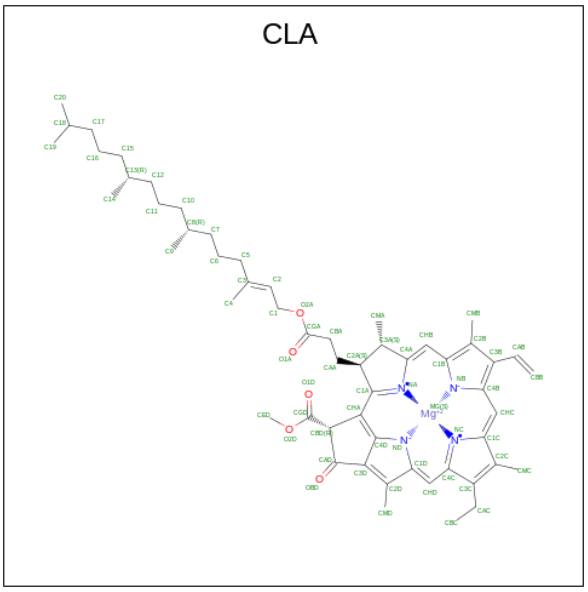
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	5	1	48	42	6	0
			Total	C	O	
4	5	1	48	42	6	0
			Total	C	O	
4	5	1	48	42	6	0
			Total	C	O	
4	7	1	48	42	6	0
			Total	C	O	
4	7	1	48	42	6	0
			Total	C	O	
4	6	1	48	42	6	0

- Molecule 5 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: $C_{40}H_{54}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	5	1	42	40	2	0

- Molecule 6 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
			Total	C	Mg	N	O	
6	5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
6	5	1	61	51	1	4	5	0

Continued on next page...

Continued from previous page...

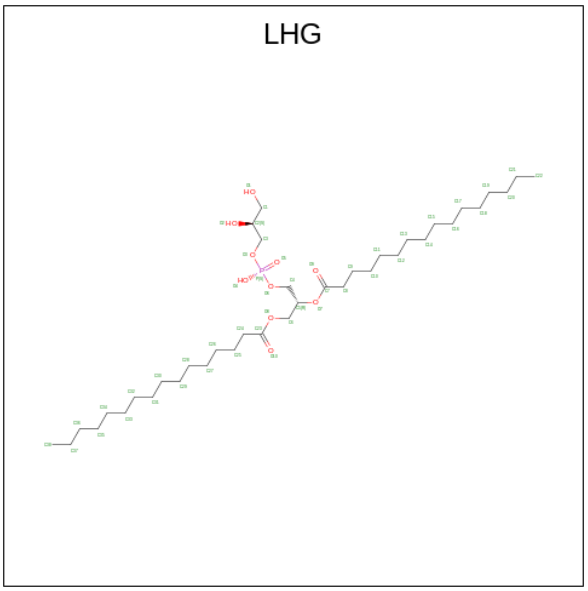
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
6	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
6	5	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
6	5	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
6	5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
6	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
6	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
6	5	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
6	5	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
6	5	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
6	7	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
6	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
6	7	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
6	7	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
6	7	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
6	7	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
6	7	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
6	7	1	36	30	1	4	1	0
			Total	C	Mg	N	O	
6	7	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
6	7	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
6	7	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
6	7	1	41	33	1	4	3	0

Continued on next page...

Continued from previous page...

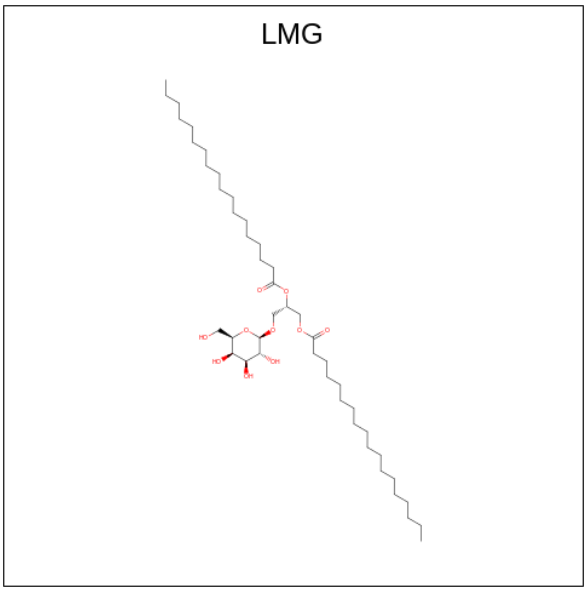
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
6	6	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
6	6	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	44	34	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
6	6	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
6	6	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
6	6	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
6	6	1	38	32	1	4	1	0

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



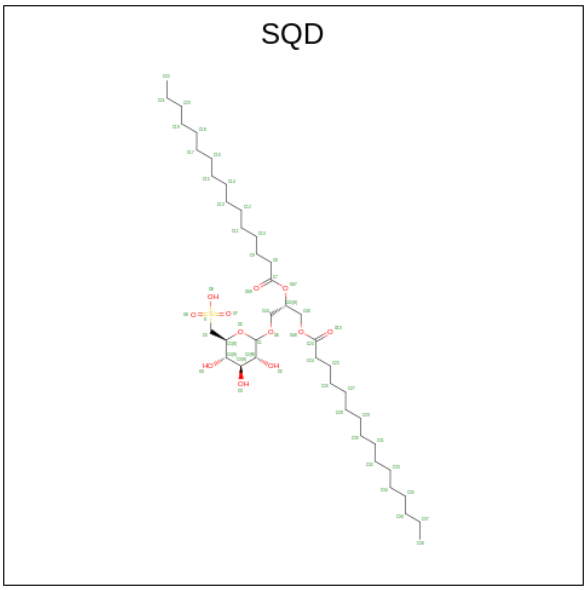
Mol	Chain	Residues	Atoms				AltConf
7	5	1	Total	C	O	P	0
			42	31	10	1	
7	5	1	Total	C	O	P	0
			34	23	10	1	
7	5	1	Total	C	O	P	0
			28	19	8	1	

- Molecule 8 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



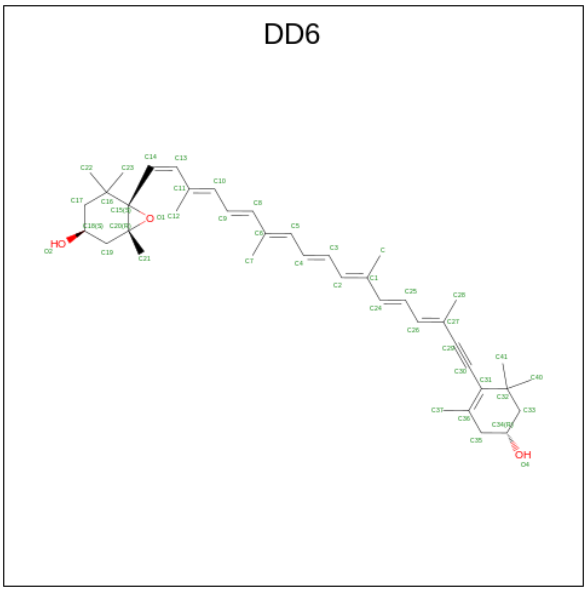
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	5	1	48	38	10	0

- Molecule 9 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
9	5	1	48	35	12	1	0

- Molecule 10 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: $C_{40}H_{54}O_3$).



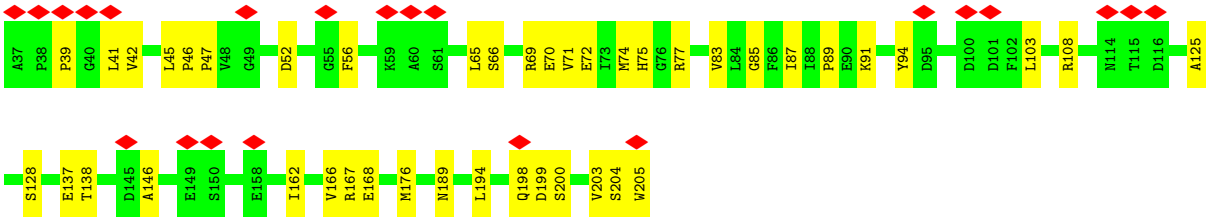
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	7	1	43	40	3	0
			Total	C	O	
10	7	1	43	40	3	0
			Total	C	O	
10	6	1	43	40	3	0
			Total	C	O	
10	6	1	43	40	3	0

3 Residue-property plots (i)

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

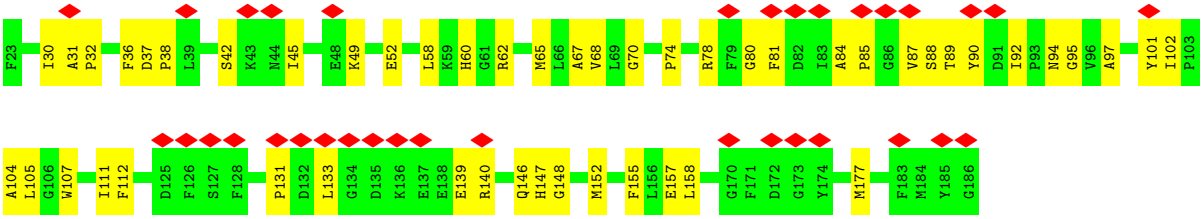
• Molecule 1: FCPII-G, Fucoxanthin chlorophyll a/c binding protein

Chain 5:



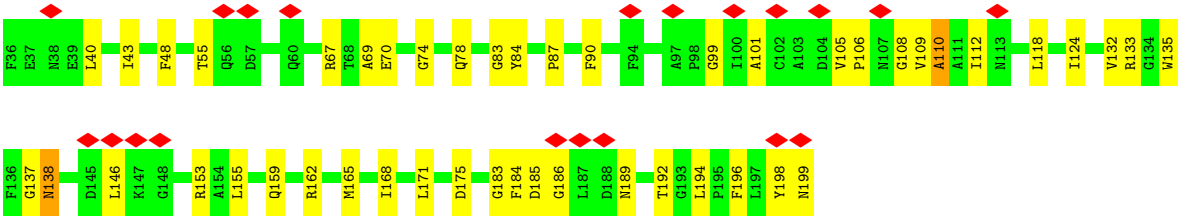
• Molecule 2: FCPII-H2, Fucoxanthin chlorophyll a/c binding protein

Chain 7:



• Molecule 3: FCPII-H1, Fucoxanthin chlorophyll a/c binding protein

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	314409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.873	Depositor
Minimum map value	-0.442	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.313	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, DD6, LHG, ET4, A86, SQD, LMG

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	5	0.27	0/1312	0.49	0/1792
2	7	0.24	0/1258	0.44	0/1714
3	6	0.31	0/1242	0.47	0/1697
All	All	0.27	0/3812	0.47	0/5203

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	5	1280	0	1242	39	0
2	7	1222	0	1142	64	0
3	6	1209	0	1150	40	0
4	5	144	0	0	1	0
4	6	48	0	0	1	0
4	7	96	0	0	0	0
5	5	42	0	0	0	0
6	5	528	0	439	16	0
6	6	580	0	441	15	0
6	7	525	0	395	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	5	104	0	121	2	0
8	5	48	0	69	1	0
9	5	48	0	63	5	0
10	6	86	0	0	3	0
10	7	86	0	0	26	0
All	All	6046	0	5062	168	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 168 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)
2:7:65:MET:HG2	10:7:304:DD6:C3	1.71	1.19
2:7:37:ASP:HA	10:7:303:DD6:O2	1.54	1.06
2:7:155:PHE:CE2	10:7:303:DD6:C24	2.39	1.05
2:7:68:VAL:HG11	10:7:304:DD6:C26	1.89	1.01
10:7:304:DD6:C8	6:7:310:CLA:HHC	1.92	1.00

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	5	167/169 (99%)	144 (86%)	23 (14%)	0	100 100
2	7	162/164 (99%)	143 (88%)	19 (12%)	0	100 100
3	6	162/164 (99%)	135 (83%)	26 (16%)	1 (1%)	21 53
All	All	491/497 (99%)	422 (86%)	68 (14%)	1 (0%)	44 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	6	110	ALA

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	5	129/136 (95%)	129 (100%)	0	100	100
2	7	110/131 (84%)	109 (99%)	1 (1%)	70	79
3	6	107/129 (83%)	105 (98%)	2 (2%)	50	70
All	All	346/396 (87%)	343 (99%)	3 (1%)	68	79

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

Mol	Chain	Res	Type
2	7	139	GLU
3	6	138	ASN
3	6	192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	5	171	GLN
1	5	185	GLN
1	5	189	ASN
1	5	196	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)

52 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	$\#\|Z\| > 2$
6	CLA	7	311	2	47,51,73	1.48	8 (17%)	56,86,113	1.41	6 (10%)
10	DD6	7	303	-	39,45,45	1.99	3 (7%)	52,67,67	2.20	17 (32%)
10	DD6	7	304	-	39,45,45	2.05	3 (7%)	52,67,67	2.51	17 (32%)
6	CLA	5	306	-	49,53,73	1.47	8 (16%)	59,89,113	1.44	5 (8%)
4	A86	5	303	-	44,50,50	1.27	4 (9%)	51,76,76	2.43	20 (39%)
6	CLA	7	307	-	51,55,73	1.44	9 (17%)	61,91,113	1.46	7 (11%)
6	CLA	6	210	3	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
6	CLA	5	308	-	65,69,73	1.30	9 (13%)	78,108,113	1.34	7 (8%)
6	CLA	6	216	3	41,46,73	1.55	7 (17%)	51,80,113	1.50	5 (9%)
6	CLA	6	215	3	41,46,73	1.54	8 (19%)	51,80,113	1.54	6 (11%)
5	ET4	5	302	-	41,43,43	1.73	11 (26%)	54,60,60	2.22	17 (31%)
6	CLA	7	306	2	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)
6	CLA	7	305	-	45,49,73	1.52	9 (20%)	54,84,113	1.53	7 (12%)
6	CLA	6	213	3	43,48,73	1.54	8 (18%)	51,83,113	1.48	5 (9%)
7	LHG	5	318	-	27,27,48	0.87	2 (7%)	31,32,54	1.72	4 (12%)
6	CLA	7	315	2	41,46,73	1.56	7 (17%)	51,80,113	1.53	5 (9%)
6	CLA	6	211	3	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)
6	CLA	6	209	3	48,52,73	1.56	10 (20%)	61,88,113	1.50	8 (13%)
10	DD6	6	203	-	39,45,45	1.99	3 (7%)	52,67,67	2.20	17 (32%)
6	CLA	7	308	2	48,52,73	1.56	9 (18%)	61,88,113	1.49	6 (9%)
6	CLA	5	307	-	65,69,73	1.29	8 (12%)	78,108,113	1.34	5 (6%)
6	CLA	6	208	-	51,55,73	1.44	7 (13%)	61,91,113	1.43	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	A86	5	301	-	44,50,50	1.29	3 (6%)	51,76,76	2.93	19 (37%)
7	LHG	5	317	-	33,33,48	0.73	0	36,39,54	1.35	4 (11%)
6	CLA	5	312	-	46,50,73	1.50	9 (19%)	55,85,113	1.46	4 (7%)
6	CLA	7	313	2	41,46,73	1.57	8 (19%)	51,80,113	1.52	6 (11%)
9	SQD	5	319	-	47,48,54	1.03	5 (10%)	56,59,65	1.45	8 (14%)
6	CLA	5	311	-	49,53,73	1.47	8 (16%)	59,89,113	1.49	4 (6%)
6	CLA	7	314	2	41,46,73	1.56	9 (21%)	51,80,113	1.55	8 (15%)
6	CLA	6	214	3	41,46,73	1.55	8 (19%)	51,80,113	1.56	6 (11%)
4	A86	5	320	-	44,50,50	1.29	3 (6%)	51,76,76	2.94	18 (35%)
4	A86	6	202	-	44,50,50	1.32	4 (9%)	51,76,76	2.90	16 (31%)
6	CLA	6	201	2	48,52,73	1.56	10 (20%)	61,88,113	1.53	8 (13%)
8	LMG	5	316	-	48,48,55	0.77	0	56,56,63	1.29	6 (10%)
6	CLA	7	312	2	40,44,73	1.70	9 (22%)	49,77,113	1.62	8 (16%)
4	A86	7	301	-	44,50,50	1.30	3 (6%)	51,76,76	2.97	19 (37%)
6	CLA	5	309	1	45,49,73	1.51	9 (20%)	54,84,113	1.53	7 (12%)
6	CLA	5	310	1	59,63,73	1.34	8 (13%)	71,101,113	1.36	7 (9%)
6	CLA	5	313	1	41,46,73	1.55	8 (19%)	51,80,113	1.56	7 (13%)
4	A86	7	302	-	44,50,50	1.52	6 (13%)	51,76,76	3.25	18 (35%)
6	CLA	6	206	3	49,53,73	1.46	8 (16%)	59,89,113	1.51	6 (10%)
6	CLA	6	212	3	45,49,73	1.51	8 (17%)	54,84,113	1.51	6 (11%)
6	CLA	7	309	2	63,67,73	1.30	9 (14%)	75,105,113	1.34	8 (10%)
6	CLA	7	310	2	59,63,73	1.35	9 (15%)	71,101,113	1.38	8 (11%)
10	DD6	6	204	-	39,45,45	2.22	4 (10%)	52,67,67	2.34	17 (32%)
6	CLA	5	304	-	45,49,73	1.51	9 (20%)	54,84,113	1.53	6 (11%)
6	CLA	6	207	3	48,52,73	1.56	9 (18%)	61,88,113	1.48	8 (13%)
6	CLA	6	205	-	45,49,73	1.52	8 (17%)	54,84,113	1.50	7 (12%)
7	LHG	5	315	-	41,41,48	0.65	1 (2%)	44,47,54	1.14	3 (6%)
6	CLA	5	314	1	41,46,73	1.56	8 (19%)	51,80,113	1.53	5 (9%)
6	CLA	5	305	1	65,69,73	1.31	10 (15%)	78,108,113	1.35	8 (10%)
6	CLA	7	316	-	45,49,73	1.52	7 (15%)	54,84,113	1.51	7 (12%)

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
6	CLA	7	311	2	-	7/13/89/115	-
10	DD6	7	303	-	-	2/26/80/80	0/3/3/3
10	DD6	7	304	-	-	10/26/80/80	0/3/3/3
6	CLA	5	306	-	-	4/15/91/115	-
4	A86	5	303	-	-	5/34/90/90	0/3/3/3
6	CLA	7	307	-	-	5/18/94/115	-
6	CLA	6	210	3	-	16/39/115/115	-
6	CLA	5	308	-	-	14/35/111/115	-
6	CLA	6	216	3	-	2/4/80/115	-
6	CLA	6	215	3	-	0/4/80/115	-
5	ET4	5	302	-	-	9/25/67/67	0/2/2/2
6	CLA	7	306	2	-	3/15/91/115	-
6	CLA	7	305	-	-	6/10/86/115	-
6	CLA	6	213	3	-	6/8/84/115	-
7	LHG	5	318	-	-	17/29/29/53	-
6	CLA	7	315	2	-	2/4/80/115	-
6	CLA	6	211	3	-	5/27/103/115	-
6	CLA	6	209	3	-	6/13/89/115	-
10	DD6	6	203	-	-	2/26/80/80	0/3/3/3
6	CLA	7	308	2	-	7/13/89/115	-
6	CLA	5	307	-	-	21/35/111/115	-
6	CLA	6	208	-	-	7/18/94/115	-
4	A86	5	301	-	-	10/34/90/90	0/3/3/3
7	LHG	5	317	-	-	26/38/38/53	-
6	CLA	5	312	-	-	9/12/88/115	-
6	CLA	7	313	2	-	2/4/80/115	-
9	SQD	5	319	-	-	18/43/63/69	0/1/1/1
6	CLA	5	311	-	-	9/15/91/115	-
6	CLA	7	314	2	-	0/4/80/115	-
6	CLA	6	214	3	-	0/4/80/115	-
4	A86	5	320	-	-	8/34/90/90	0/3/3/3
4	A86	6	202	-	-	7/34/90/90	0/3/3/3
6	CLA	6	201	2	-	4/13/89/115	-
8	LMG	5	316	-	-	25/43/63/70	0/1/1/1
6	CLA	7	312	2	-	0/2/78/115	-
4	A86	7	301	-	-	8/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	5	309	1	-	4/10/86/115	-
6	CLA	5	310	1	-	5/27/103/115	-
6	CLA	5	313	1	-	2/4/80/115	-
4	A86	7	302	-	-	8/34/90/90	0/3/3/3
6	CLA	6	206	3	-	8/15/91/115	-
6	CLA	6	212	3	-	4/10/86/115	-
6	CLA	7	309	2	-	10/32/108/115	-
6	CLA	7	310	2	-	10/27/103/115	-
10	DD6	6	204	-	-	5/26/80/80	0/3/3/3
6	CLA	5	304	-	-	4/10/86/115	-
6	CLA	6	207	3	-	6/13/89/115	-
6	CLA	6	205	-	-	4/10/86/115	-
7	LHG	5	315	-	-	10/46/46/53	-
6	CLA	5	314	1	-	0/4/80/115	-
6	CLA	5	305	1	-	17/35/111/115	-
6	CLA	7	316	-	-	2/10/86/115	-

The worst 5 of 358 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	6	204	DD6	C29-C27	-9.29	1.24	1.42
10	7	304	DD6	C29-C27	-8.70	1.25	1.42
10	6	204	DD6	C30-C31	-8.46	1.24	1.42
10	6	203	DD6	C29-C27	-8.37	1.26	1.42
10	7	303	DD6	C29-C27	-8.36	1.26	1.42

The worst 5 of 451 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	7	302	A86	O1-C15-C14	-13.42	86.28	113.21
4	7	301	A86	O1-C15-C14	-12.11	88.91	113.21
4	5	320	A86	O1-C15-C14	-12.00	89.12	113.21
4	6	202	A86	O1-C15-C14	-11.25	90.63	113.21
4	5	301	A86	O1-C15-C14	8.62	130.51	113.21

There are no chirality outliers.

5 of 381 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5	301	A86	C10-C11-C13-O
4	5	301	A86	C10-C11-C13-C14
4	5	301	A86	C12-C11-C13-O
4	5	301	A86	C13-C14-C15-C16
4	5	301	A86	C13-C14-C15-O1

There are no ring outliers.

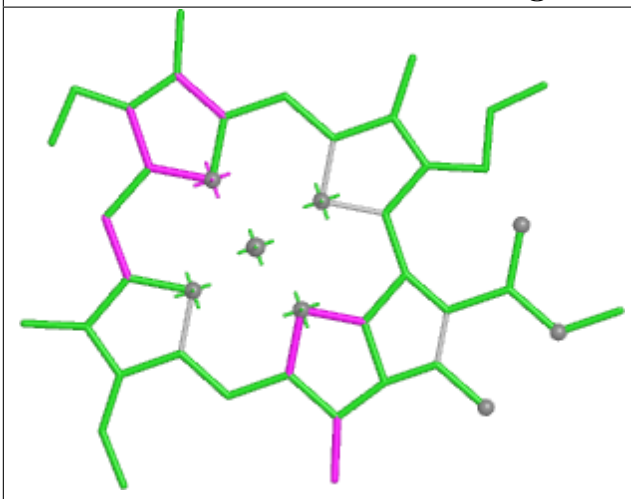
29 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	7	303	DD6	18	0
10	7	304	DD6	8	0
4	5	303	A86	1	0
6	7	307	CLA	3	0
6	6	210	CLA	5	0
6	5	308	CLA	6	0
6	7	306	CLA	4	0
6	7	305	CLA	1	0
7	5	318	LHG	1	0
6	6	211	CLA	2	0
6	6	209	CLA	1	0
10	6	203	DD6	1	0
6	5	307	CLA	1	0
9	5	319	SQD	5	0
6	5	311	CLA	2	0
6	6	214	CLA	1	0
4	6	202	A86	1	0
6	6	201	CLA	2	0
8	5	316	LMG	1	0
6	7	312	CLA	1	0
6	5	310	CLA	1	0
6	5	313	CLA	1	0
6	6	206	CLA	4	0
6	7	309	CLA	6	0
6	7	310	CLA	7	0
10	6	204	DD6	2	0
6	5	304	CLA	3	0
7	5	315	LHG	2	0
6	5	305	CLA	3	0

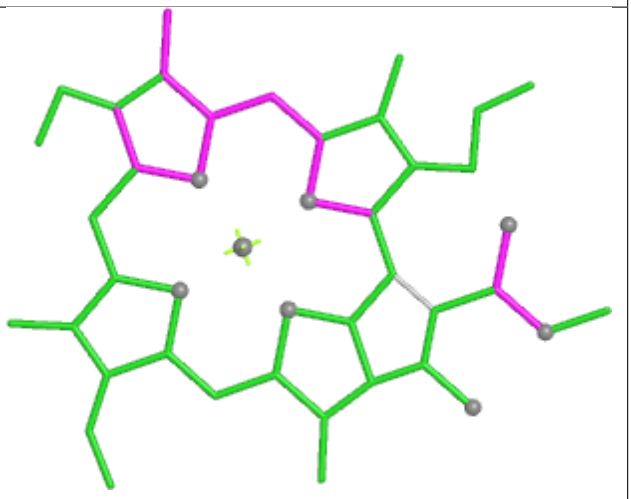
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

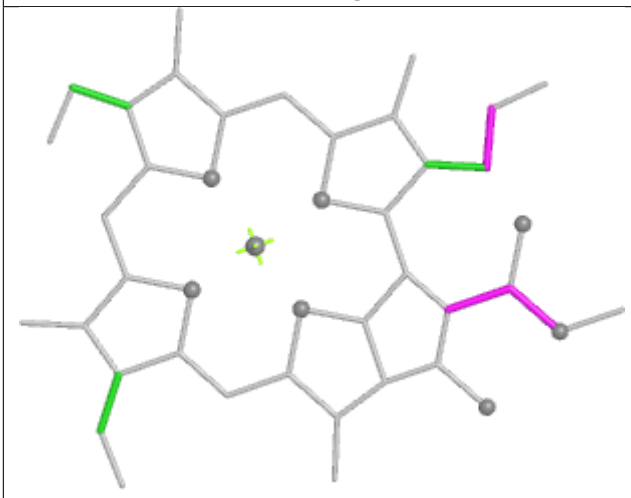
Ligand CLA 7 311



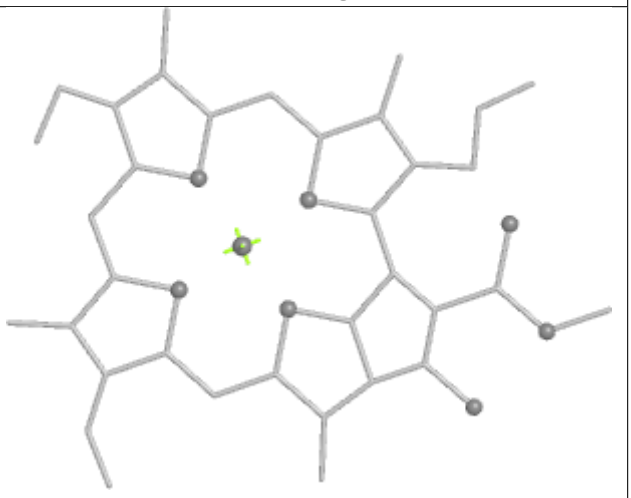
Bond lengths



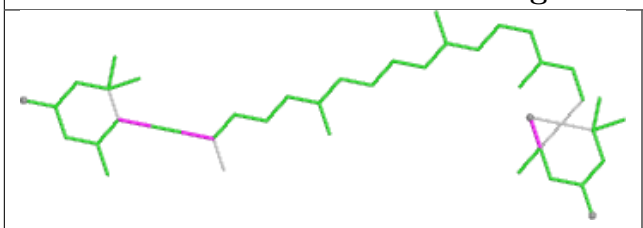
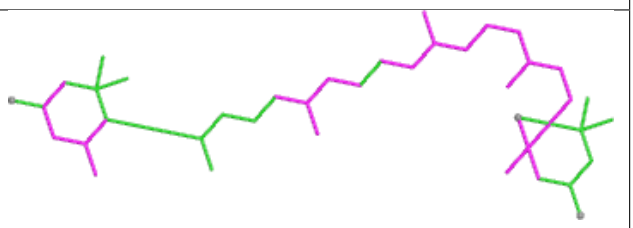
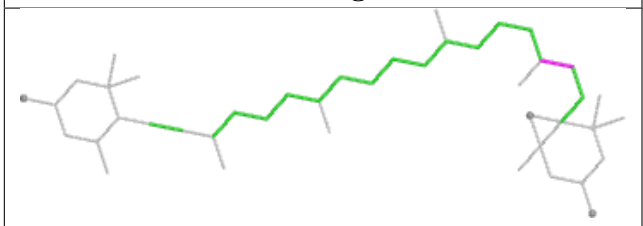
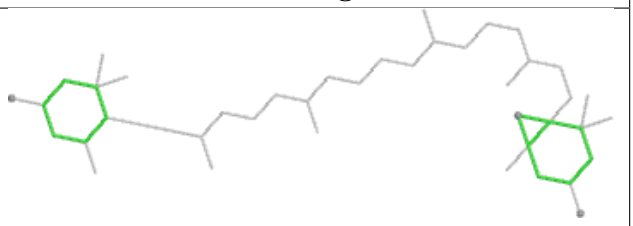
Bond angles

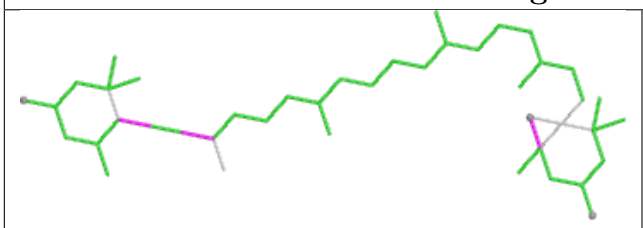
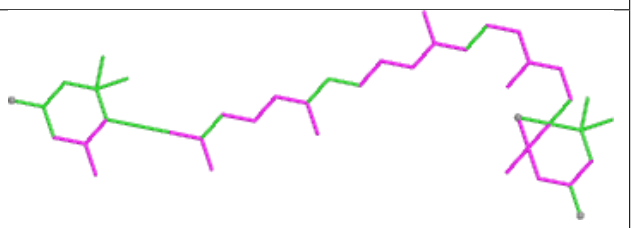
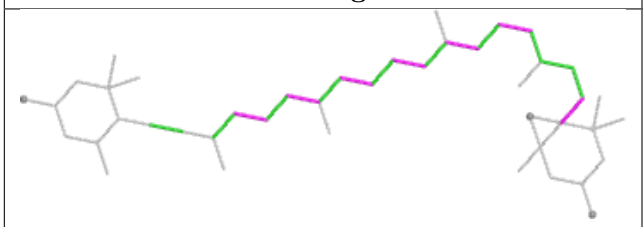
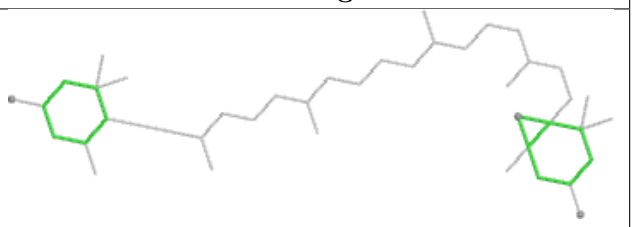


Torsions

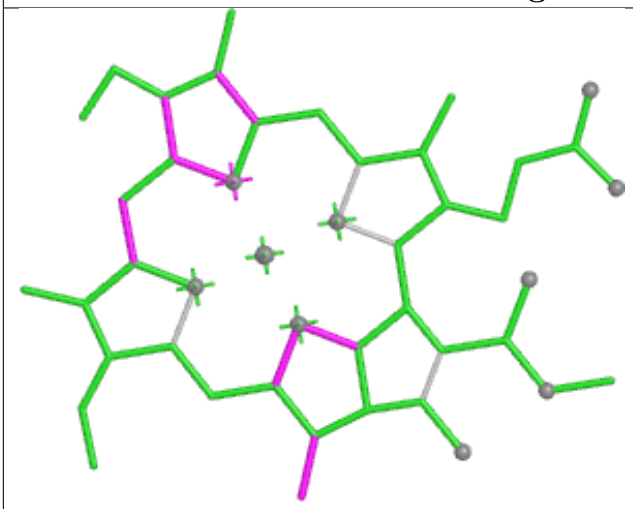


Rings

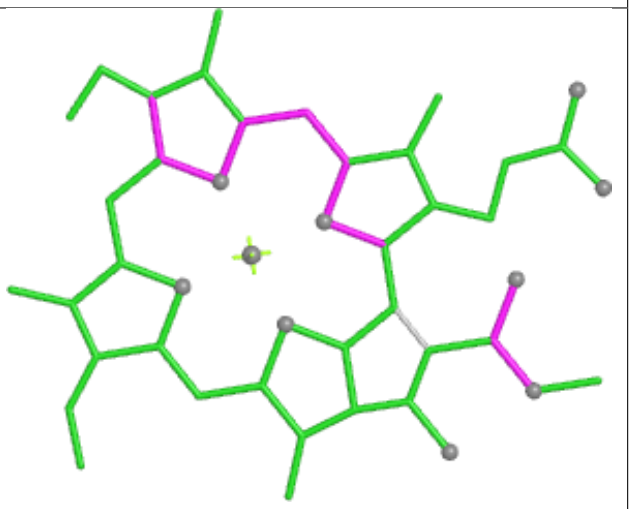
Ligand DD6 7 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 7 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

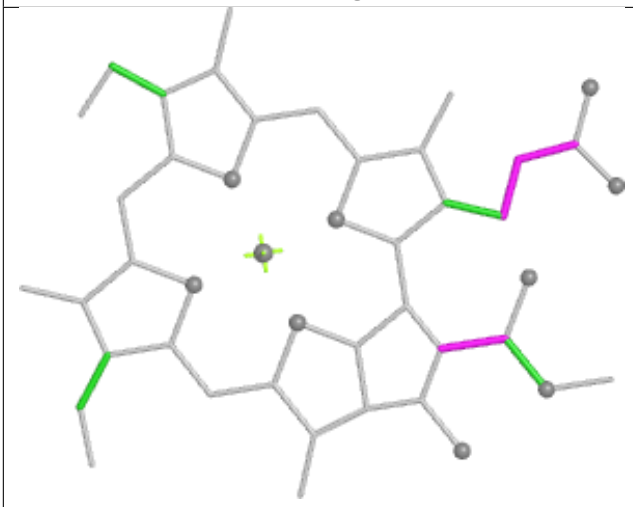
Ligand CLA 5 306



Bond lengths



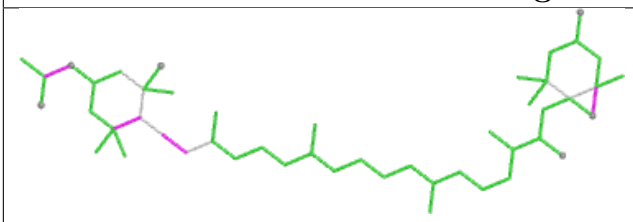
Bond angles



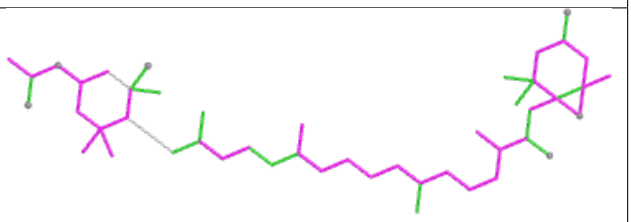
Torsions

Rings

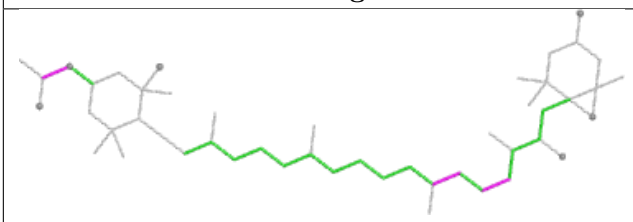
Ligand A86 5 303



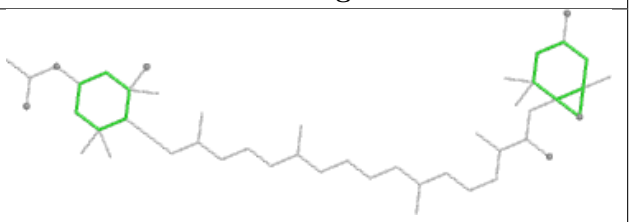
Bond lengths



Bond angles

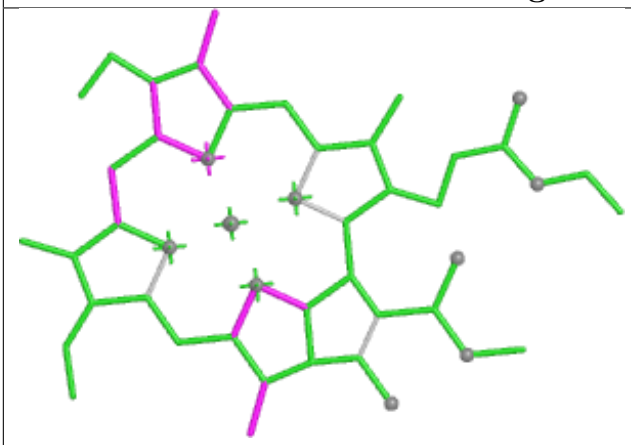


Torsions

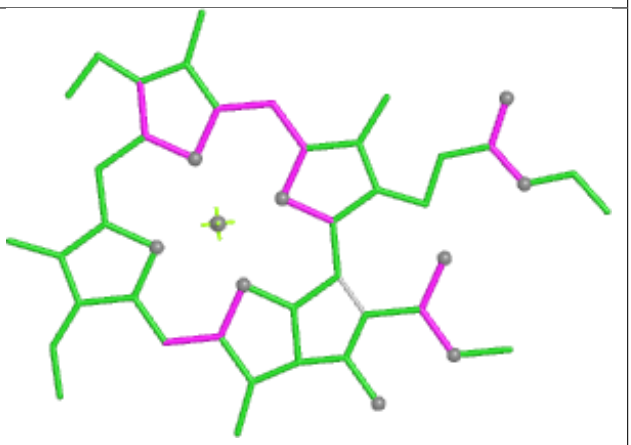


Rings

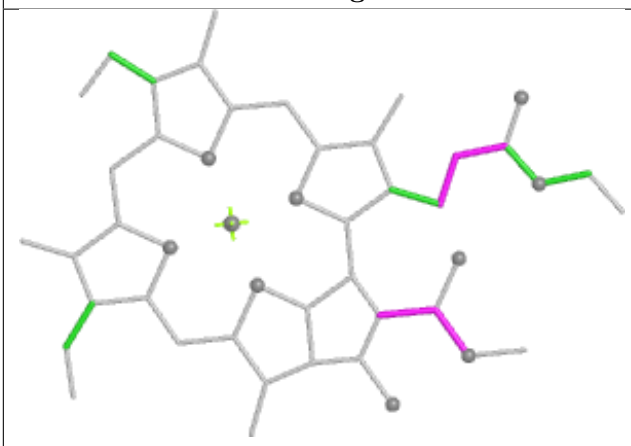
Ligand CLA 7 307



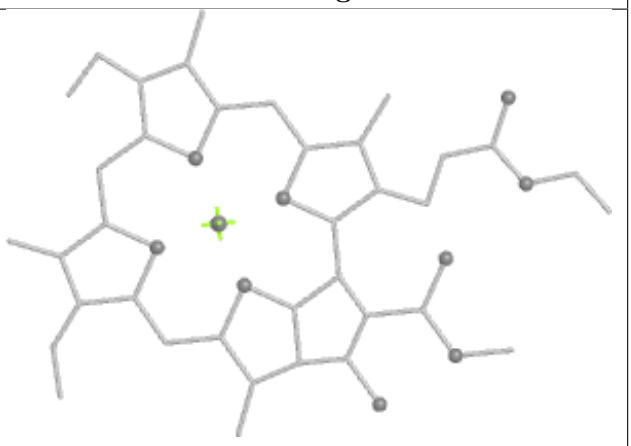
Bond lengths



Bond angles

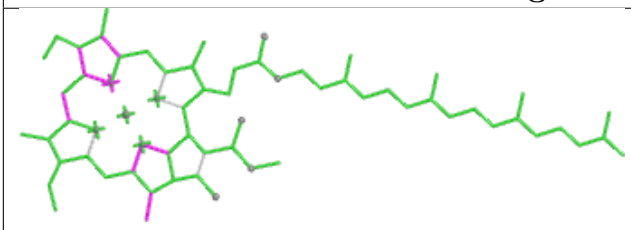


Torsions

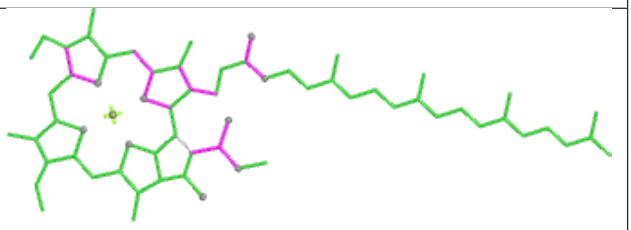


Rings

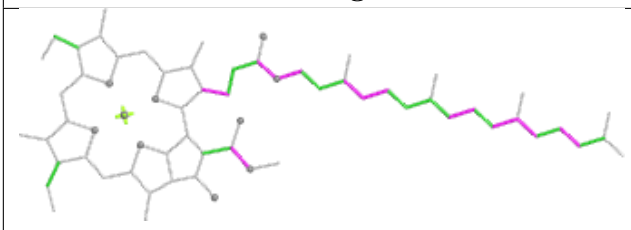
Ligand CLA 6 210



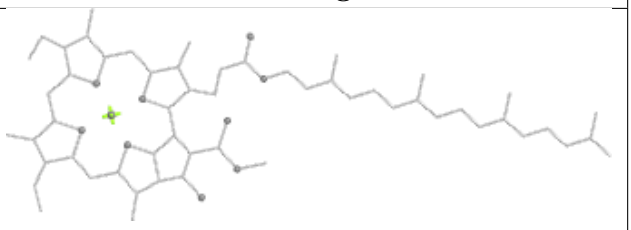
Bond lengths



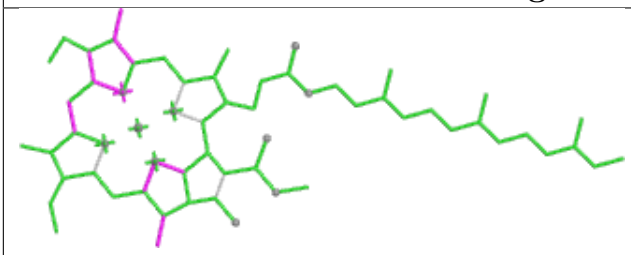
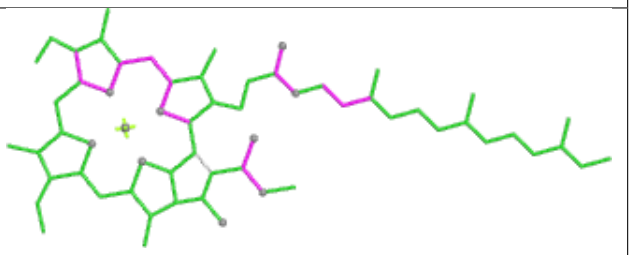
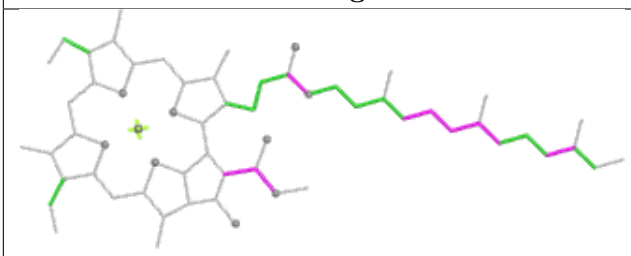
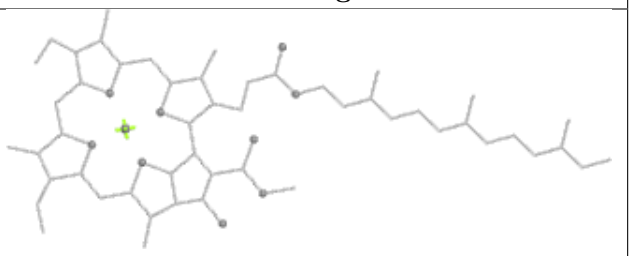
Bond angles



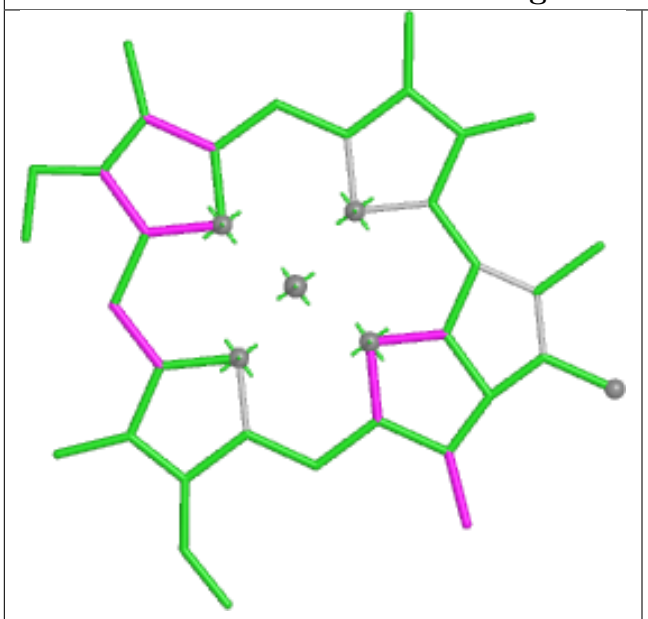
Torsions



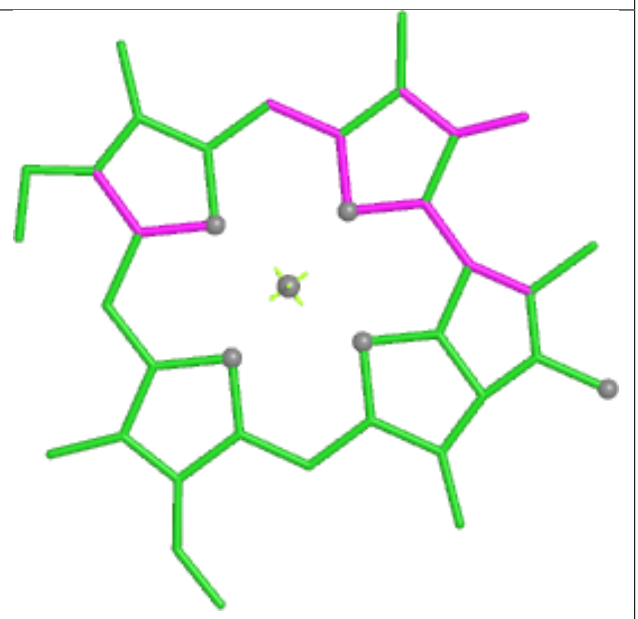
Rings

Ligand CLA 5 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

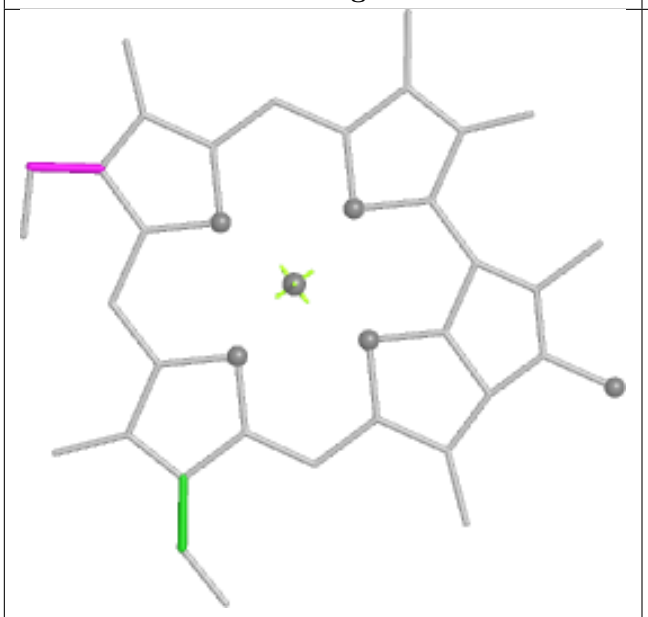
Ligand CLA 6 216



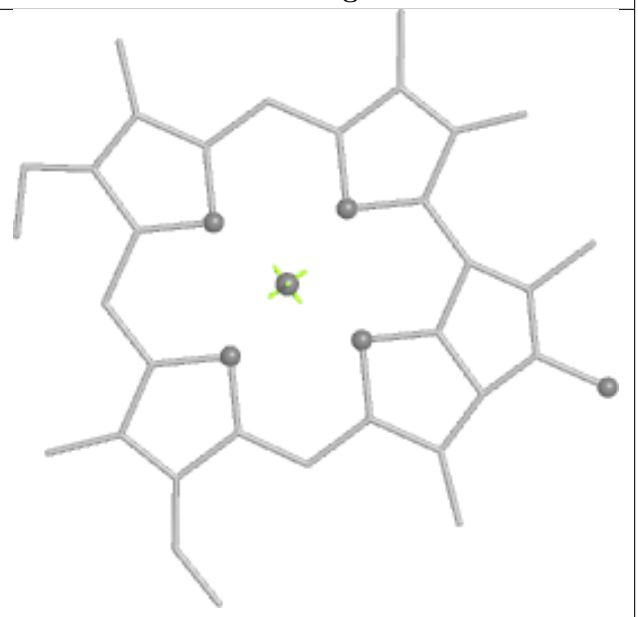
Bond lengths



Bond angles

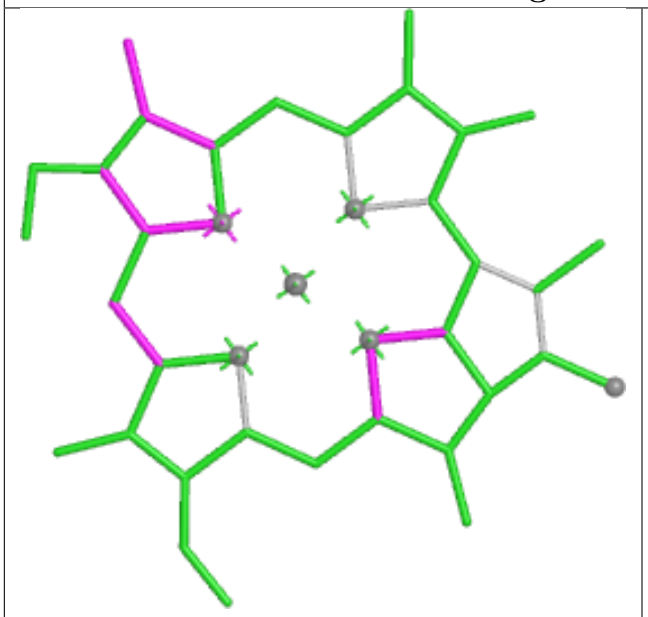


Torsions

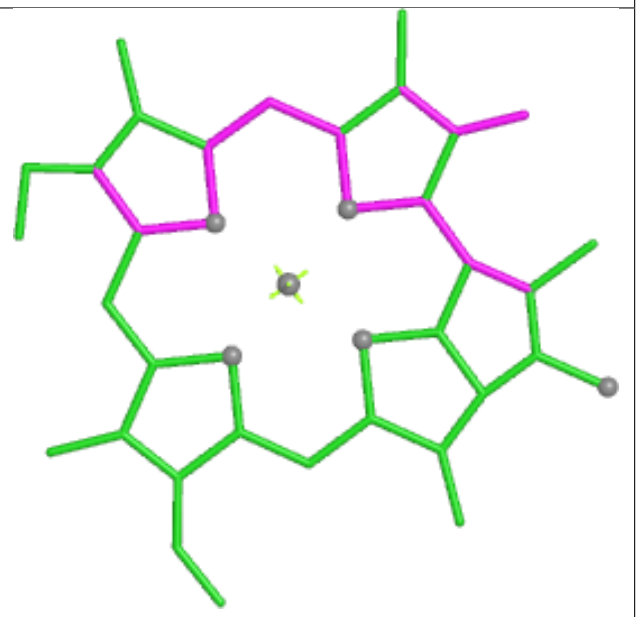


Rings

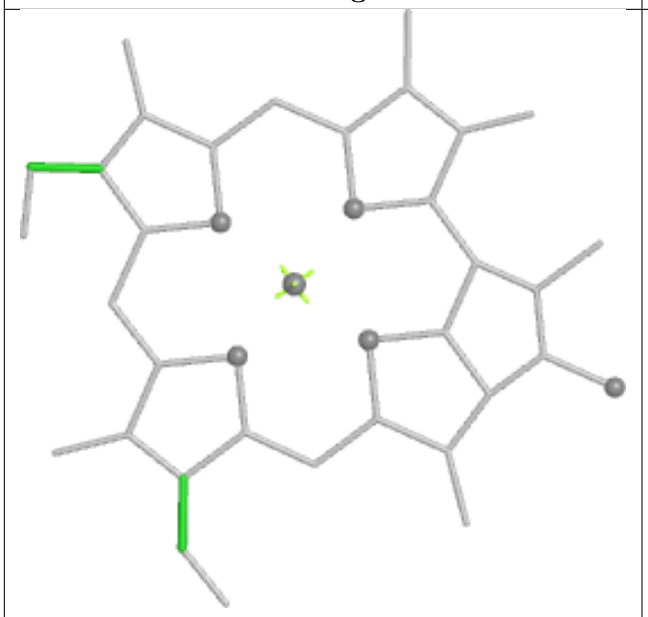
Ligand CLA 6 215



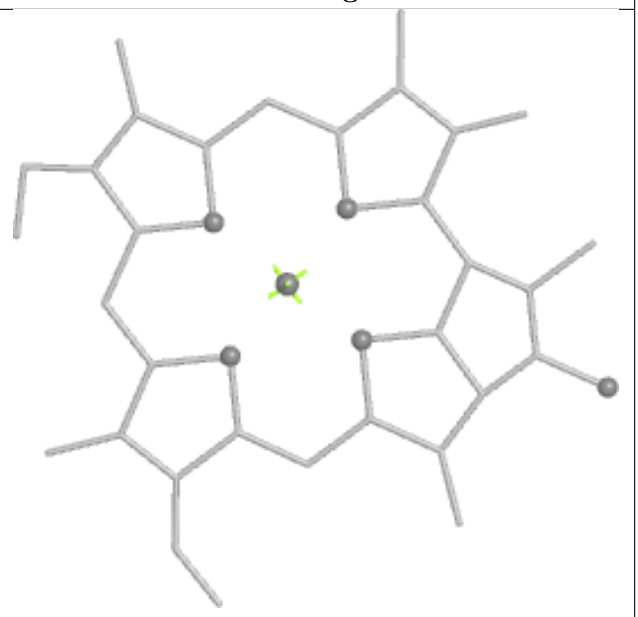
Bond lengths



Bond angles

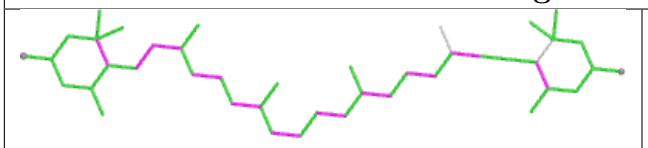


Torsions

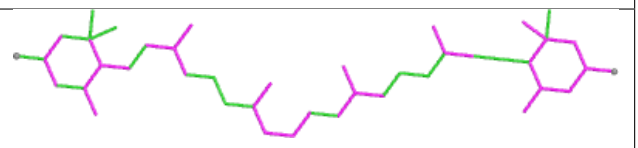


Rings

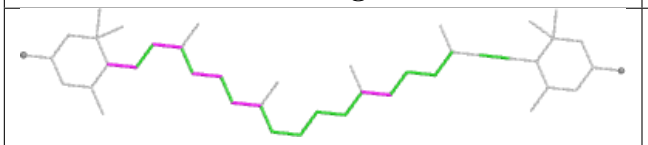
Ligand ET4 5 302



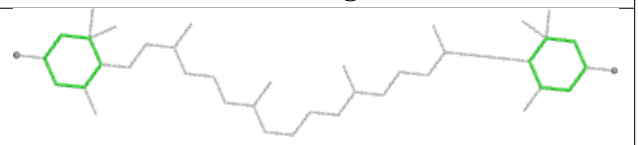
Bond lengths



Bond angles

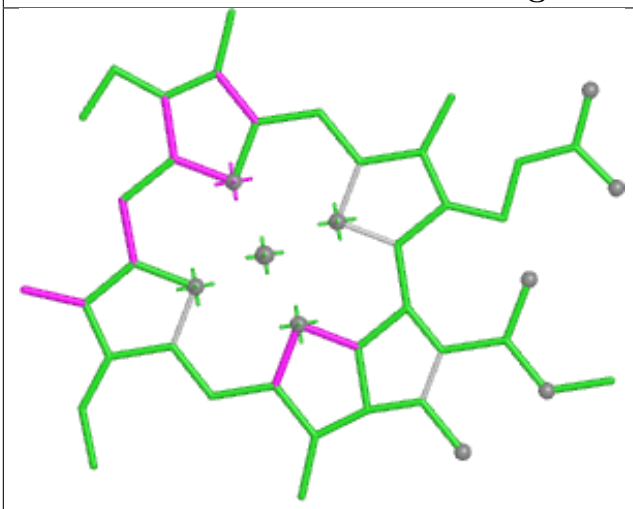


Torsions

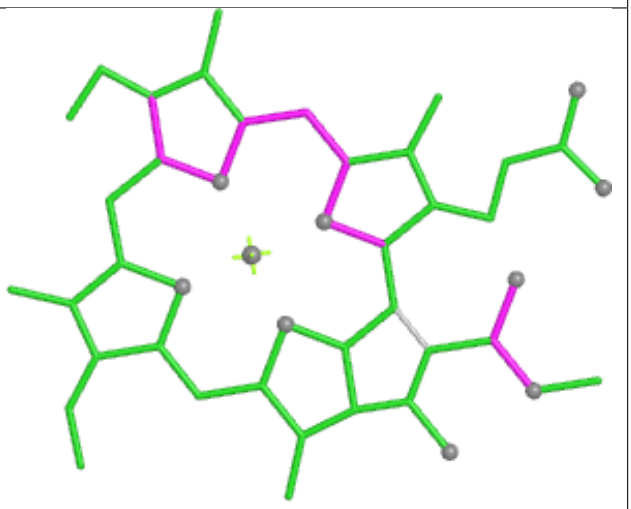


Rings

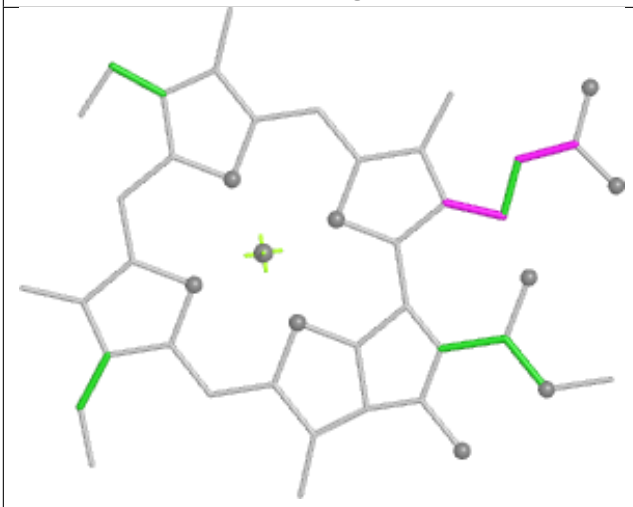
Ligand CLA 7 306



Bond lengths



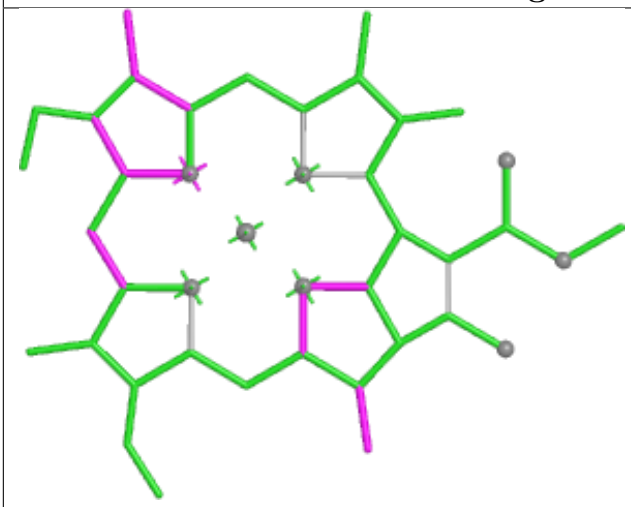
Bond angles



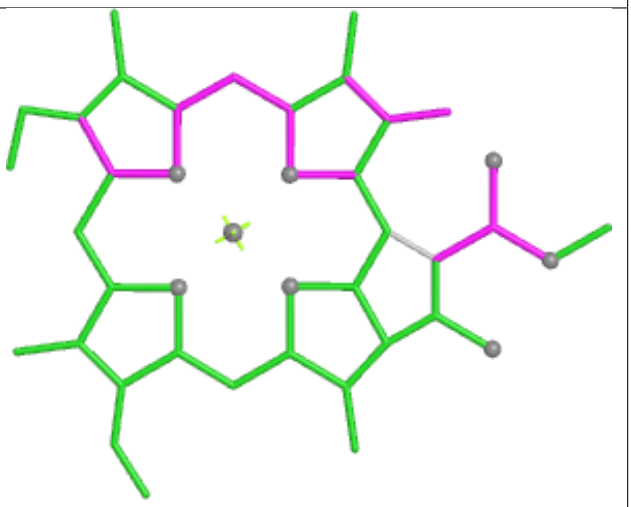
Torsions

Rings

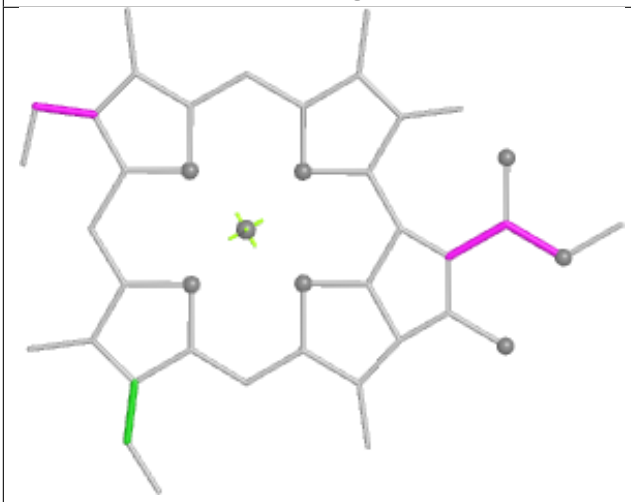
Ligand CLA 7 305



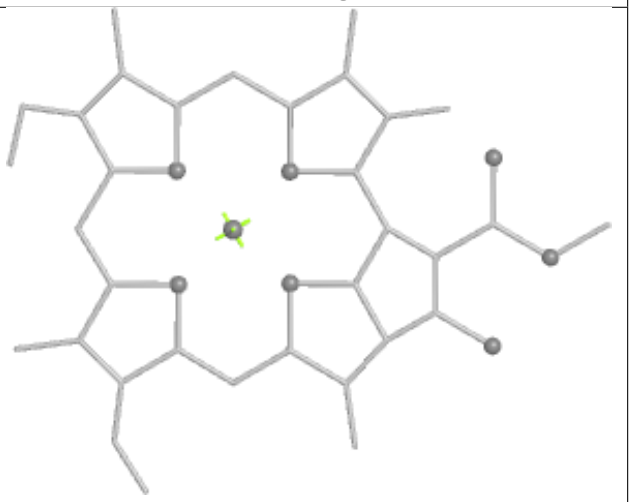
Bond lengths



Bond angles

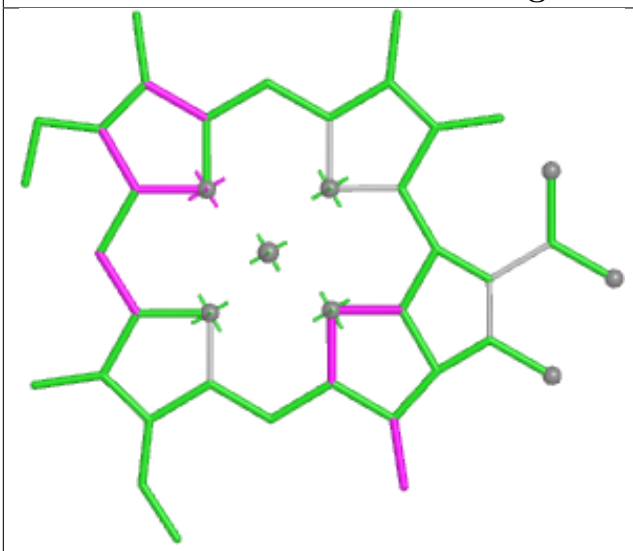


Torsions

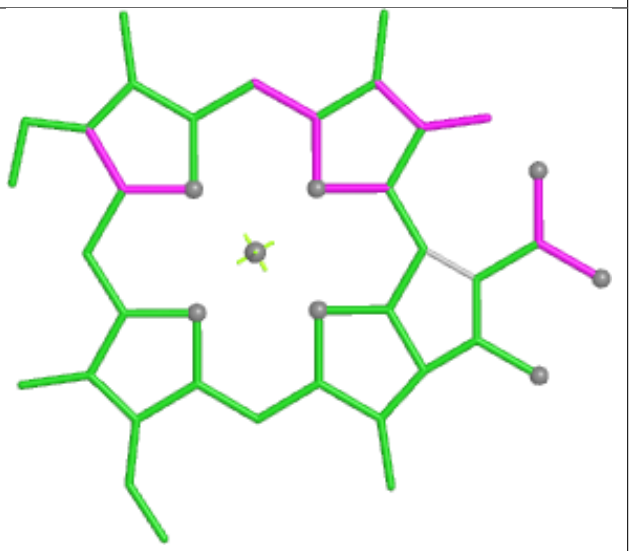


Rings

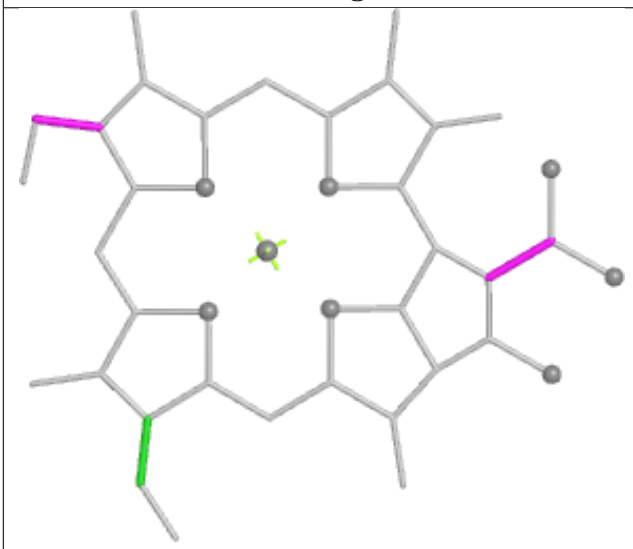
Ligand CLA 6 213



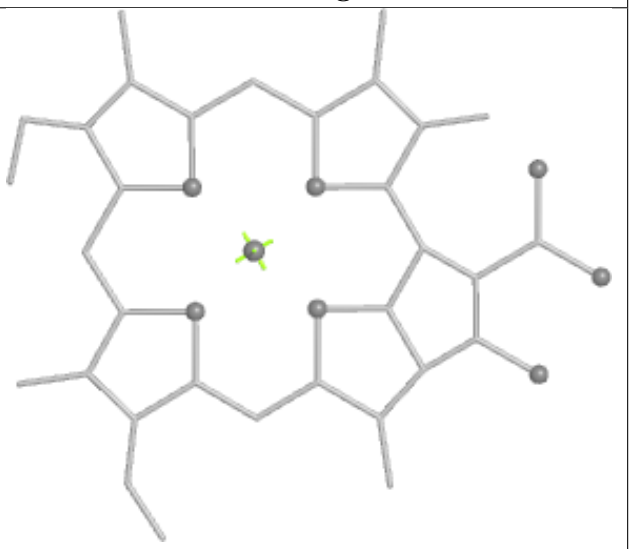
Bond lengths



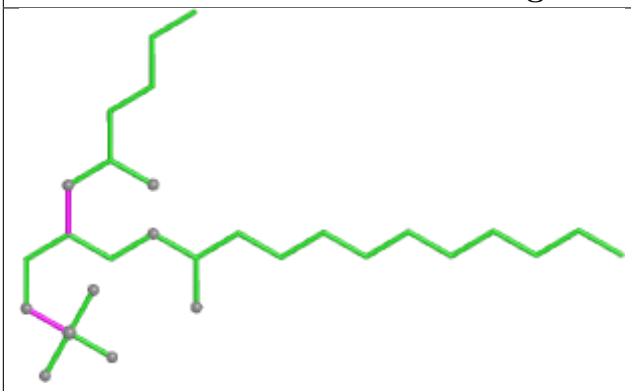
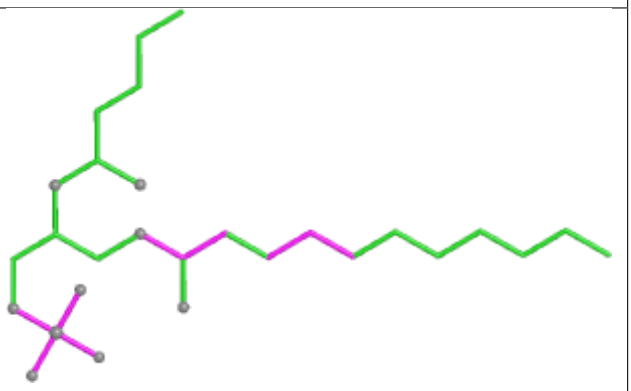
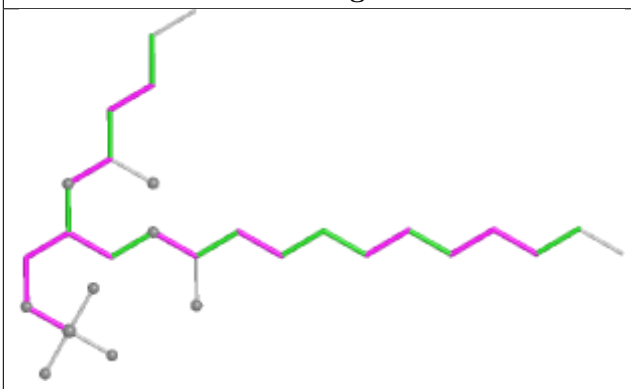
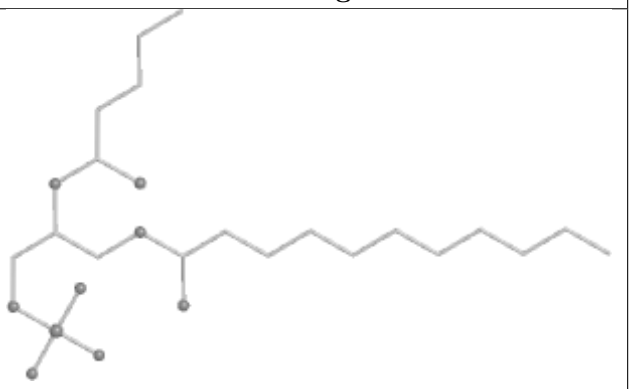
Bond angles



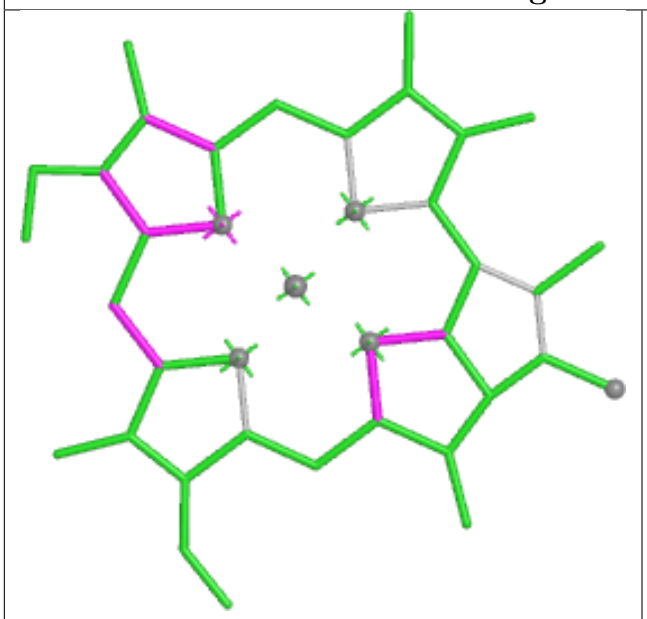
Torsions



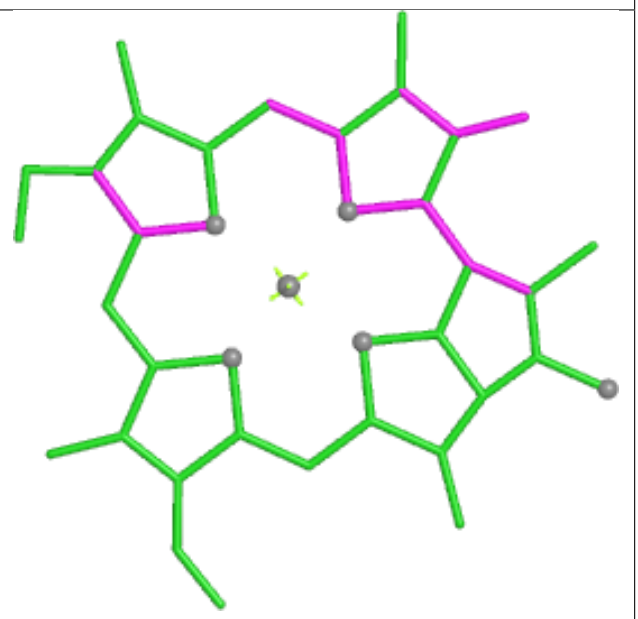
Rings

Ligand LHG 5 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

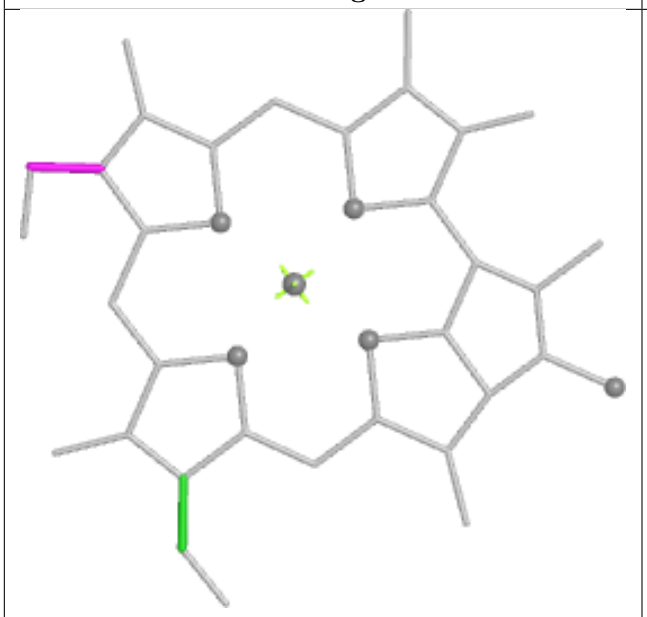
Ligand CLA 7 315



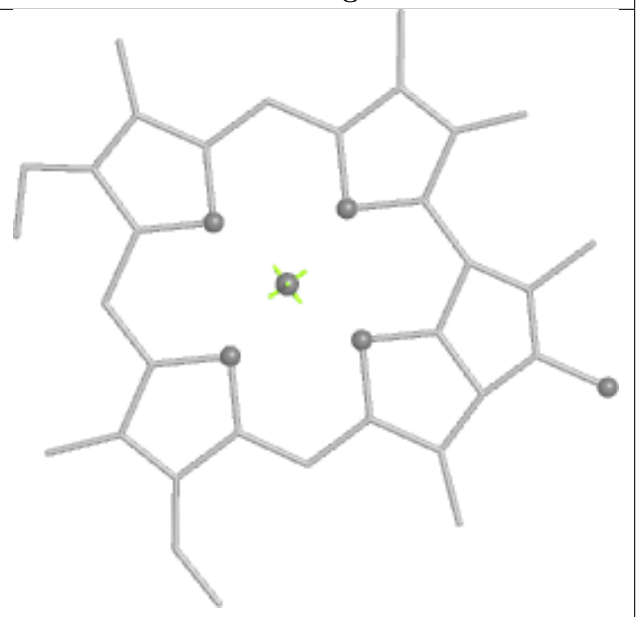
Bond lengths



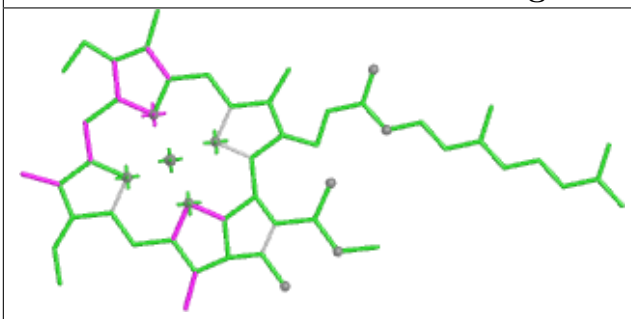
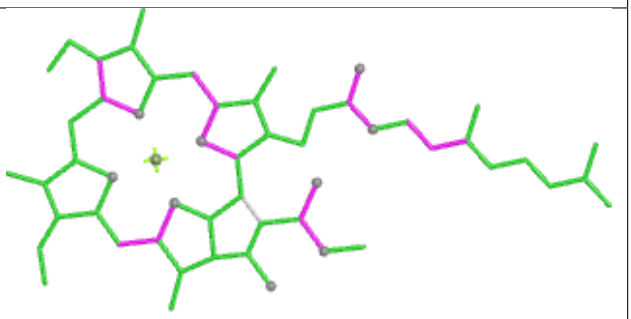
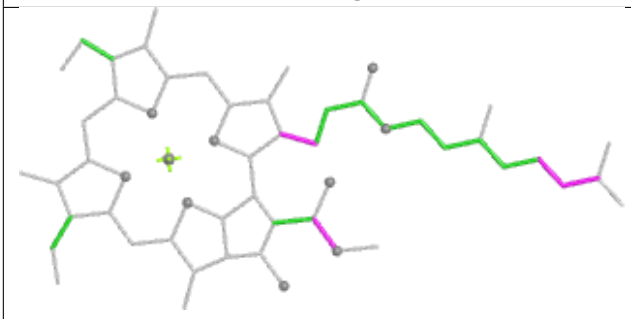
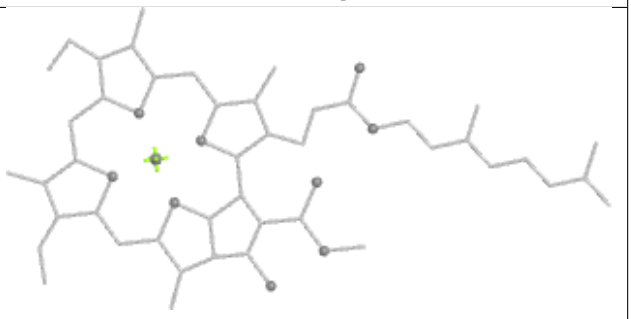
Bond angles



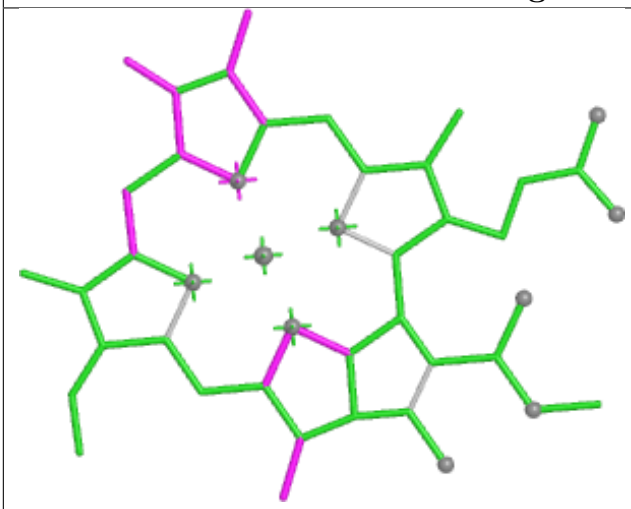
Torsions



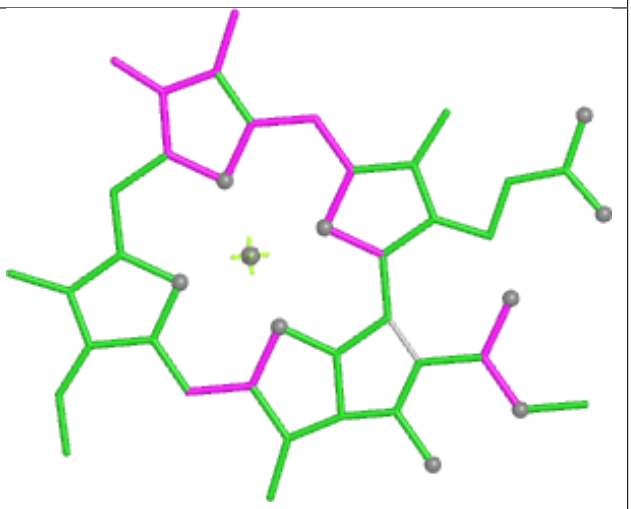
Rings

Ligand CLA 6 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

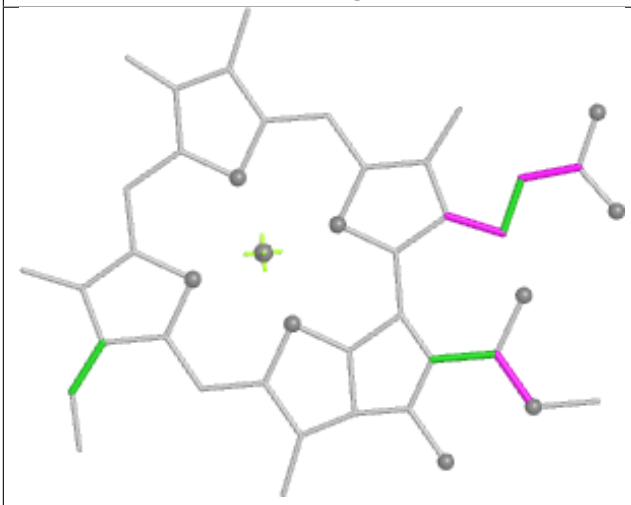
Ligand CLA 6 209



Bond lengths



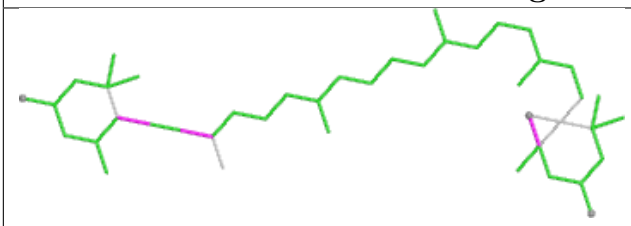
Bond angles



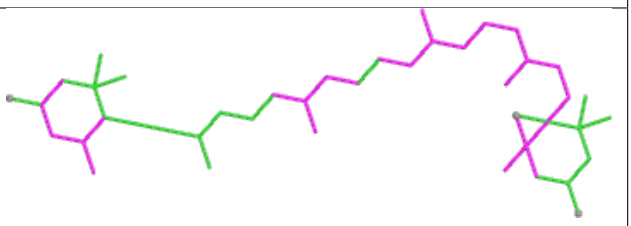
Torsions

Rings

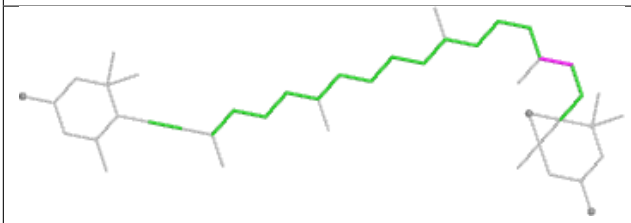
Ligand DD6 6 203



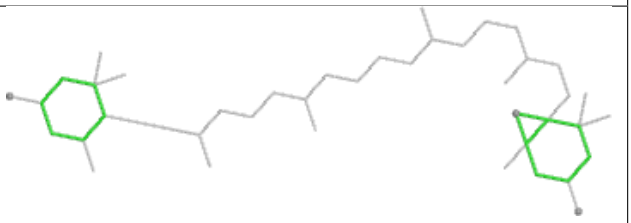
Bond lengths



Bond angles

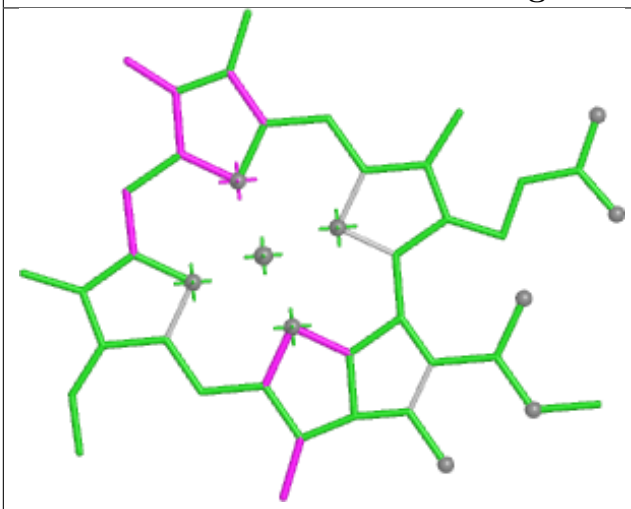


Torsions

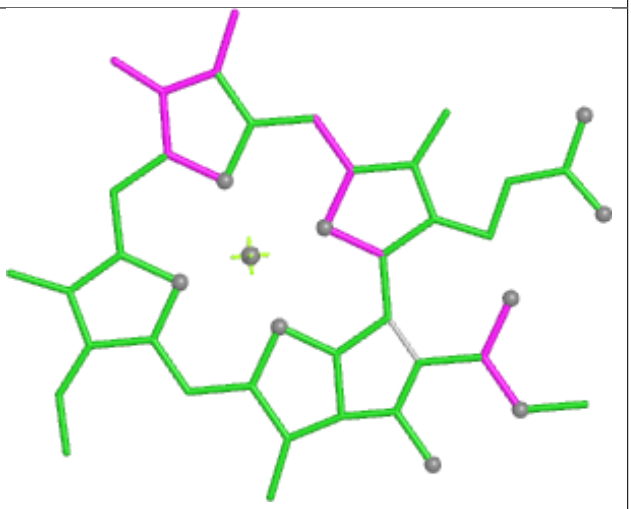


Rings

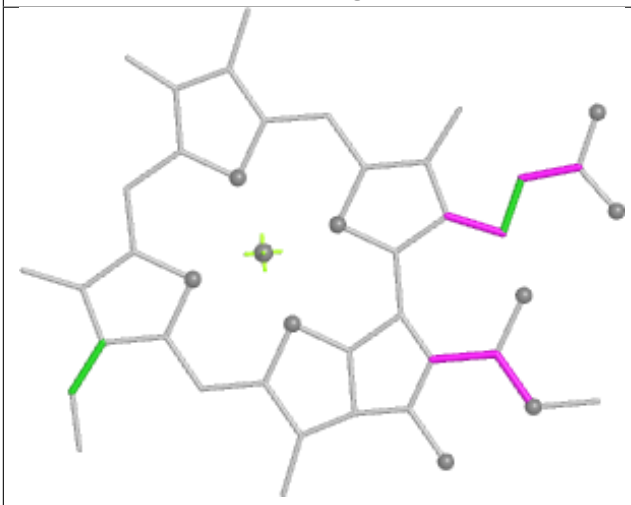
Ligand CLA 7 308



Bond lengths



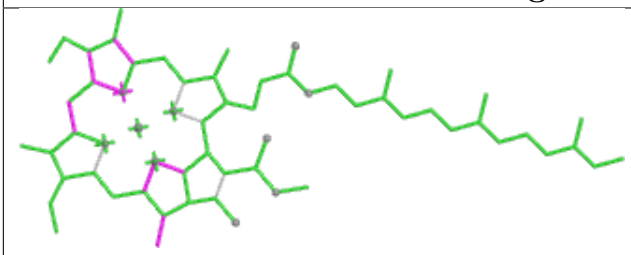
Bond angles



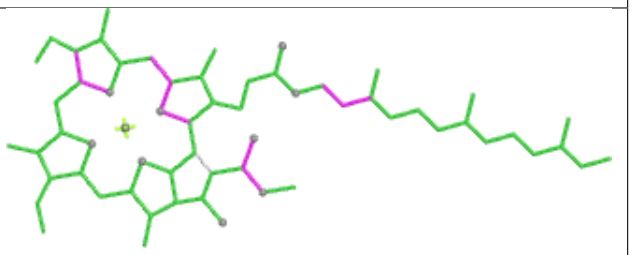
Torsions

Rings

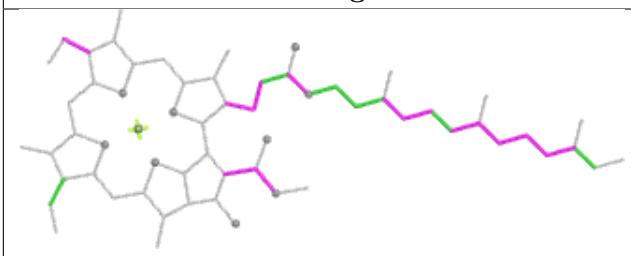
Ligand CLA 5 307



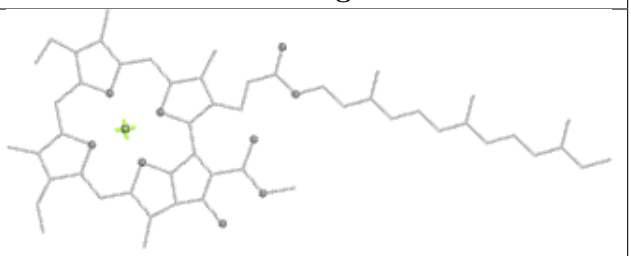
Bond lengths



Bond angles

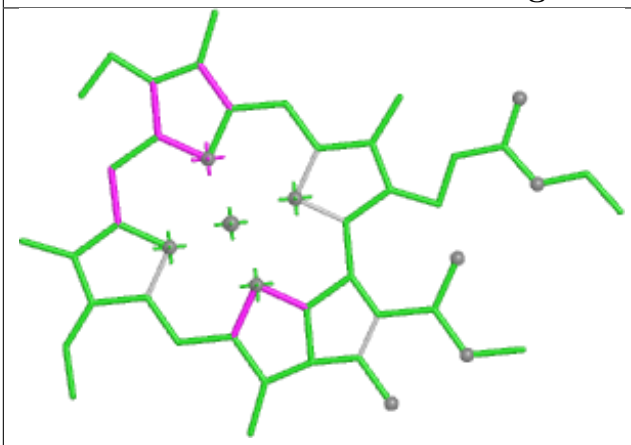


Torsions

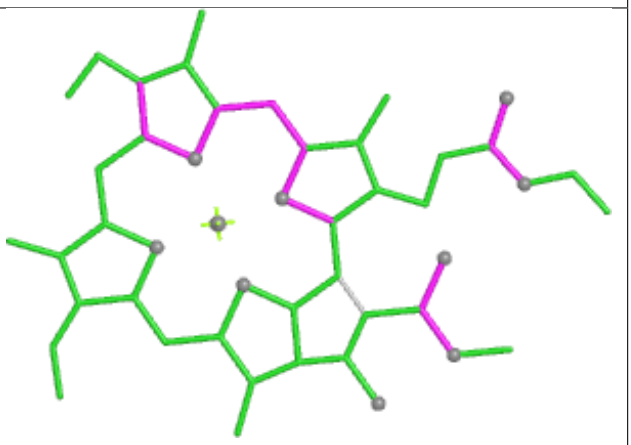


Rings

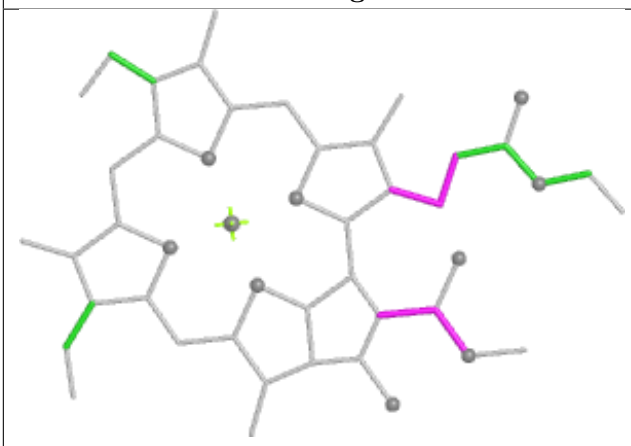
Ligand CLA 6 208



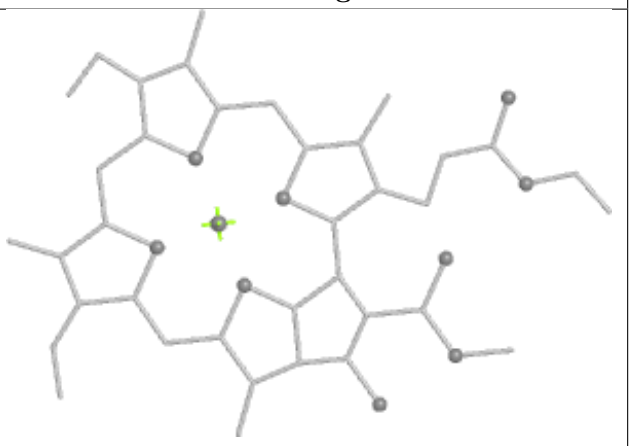
Bond lengths



Bond angles

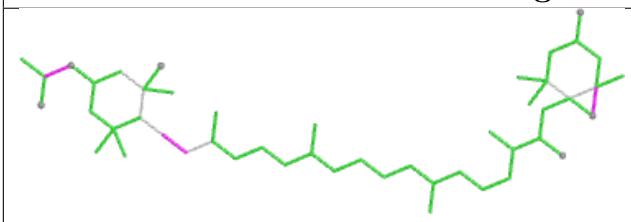


Torsions

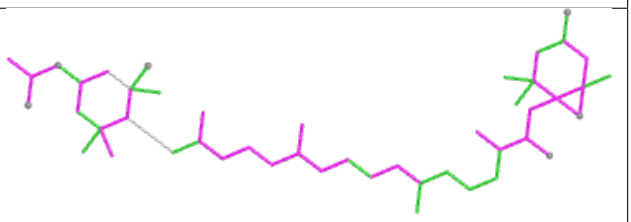


Rings

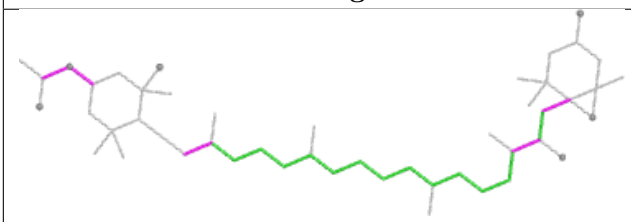
Ligand A86 5 301



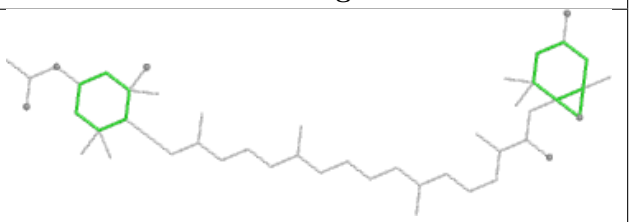
Bond lengths



Bond angles

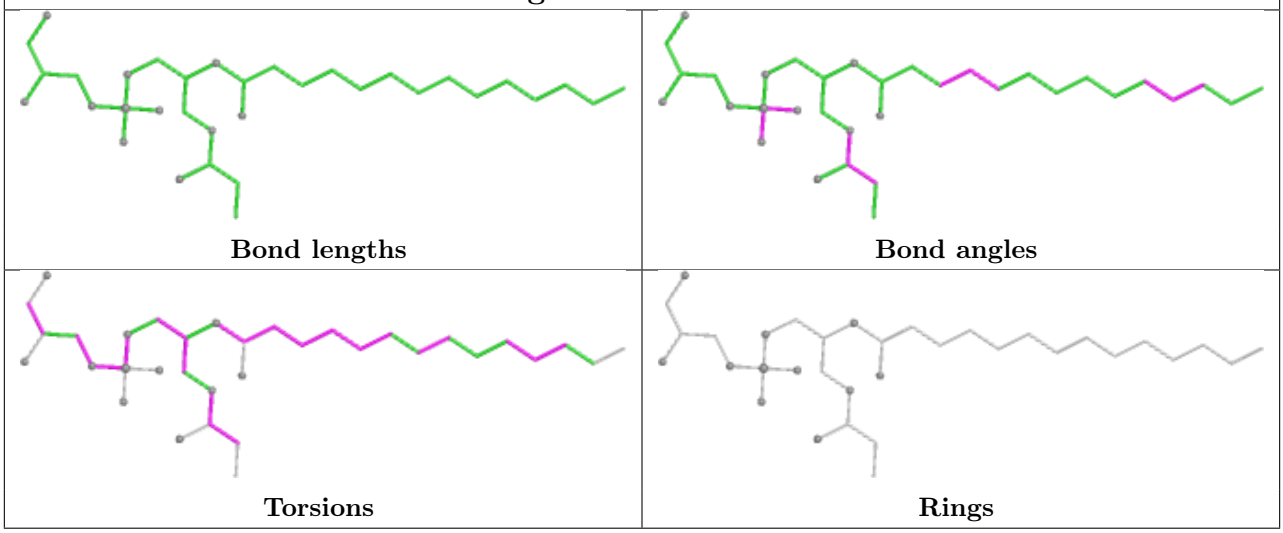


Torsions

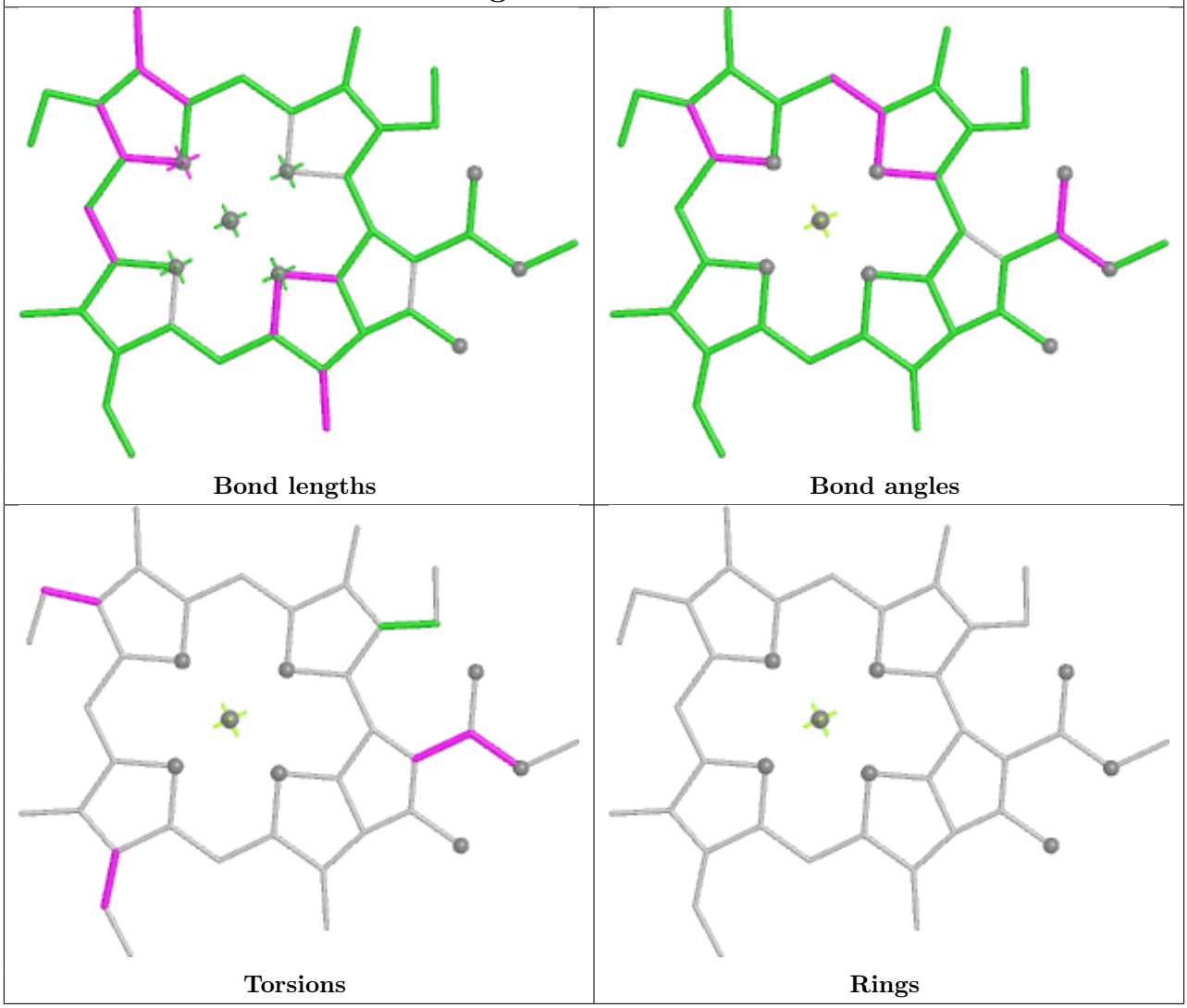


Rings

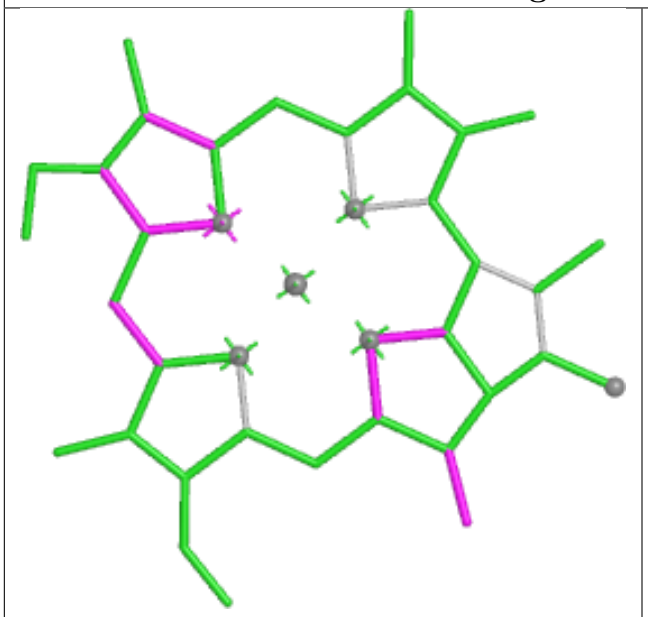
Ligand LHG 5 317



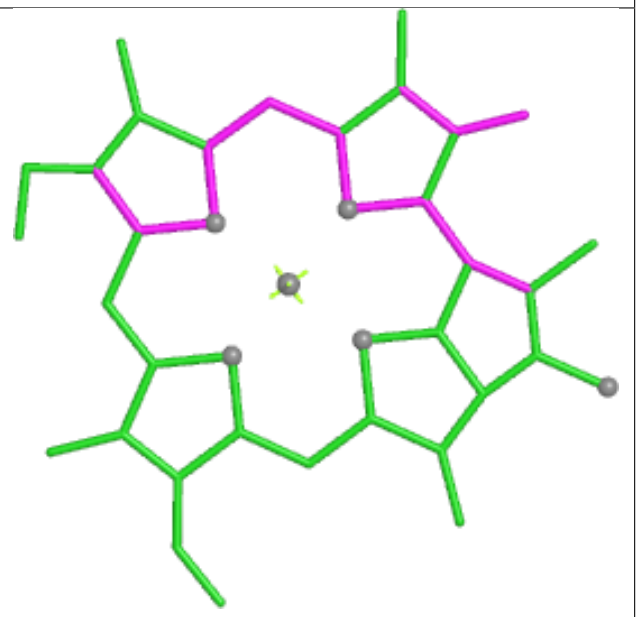
Ligand CLA 5 312



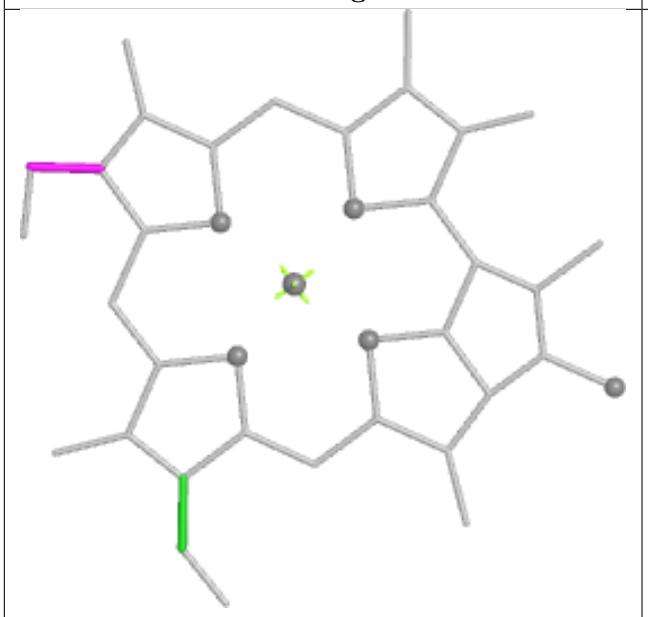
Ligand CLA 7 313



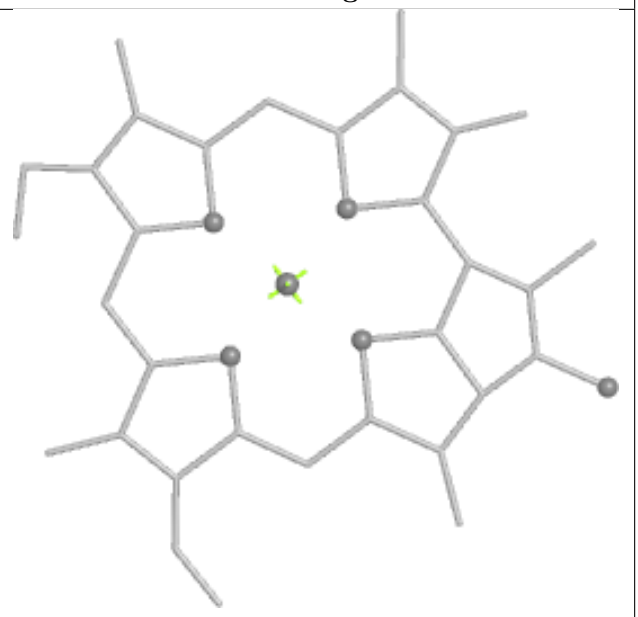
Bond lengths



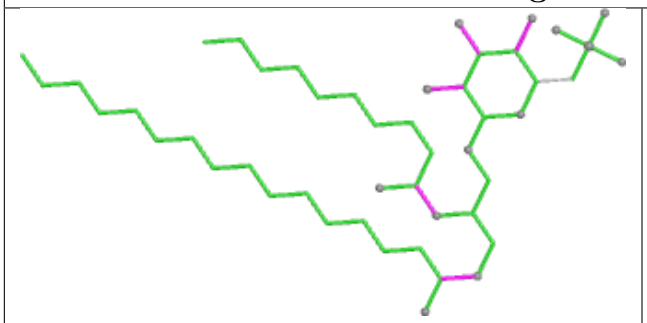
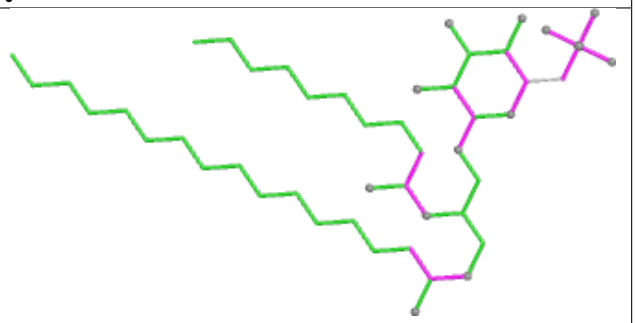
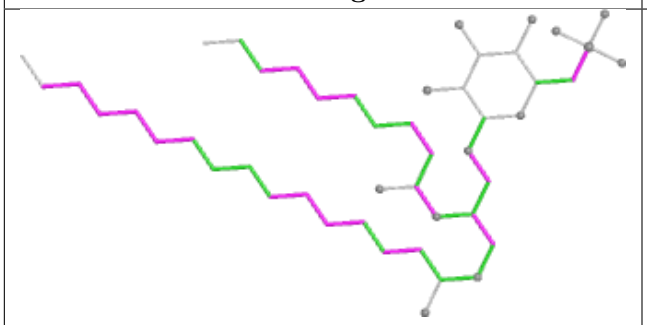
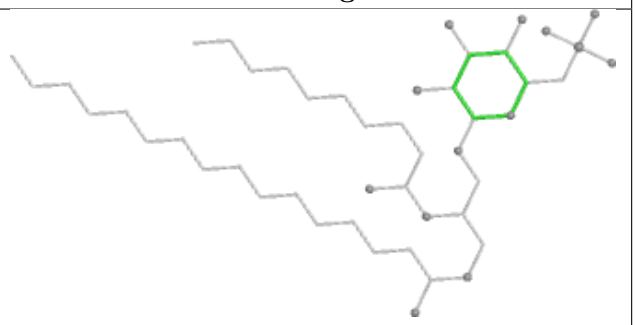
Bond angles



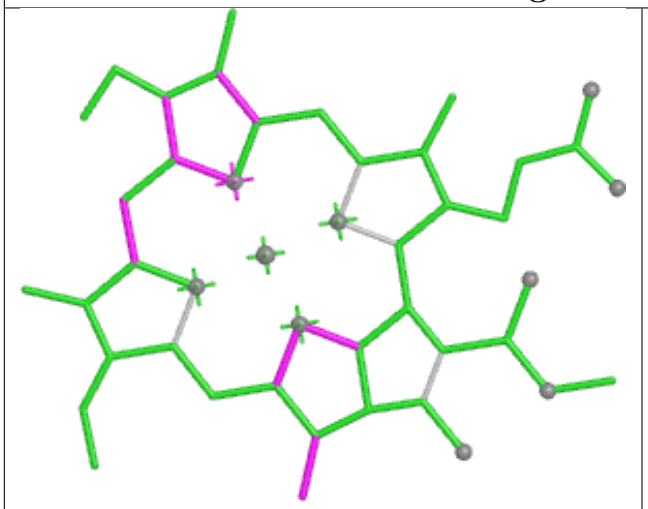
Torsions



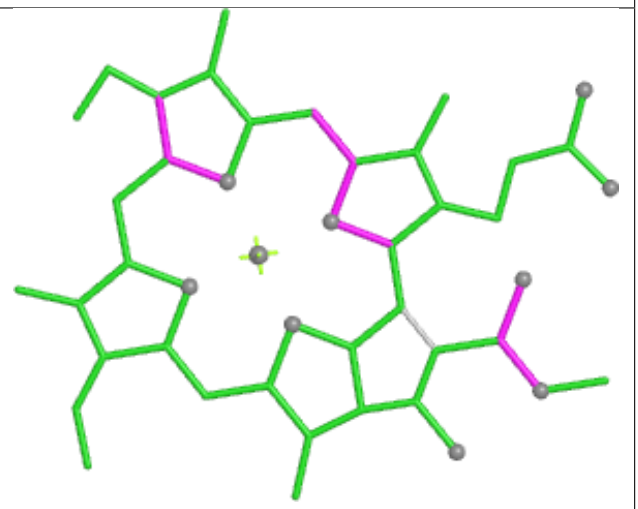
Rings

Ligand SQD 5 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

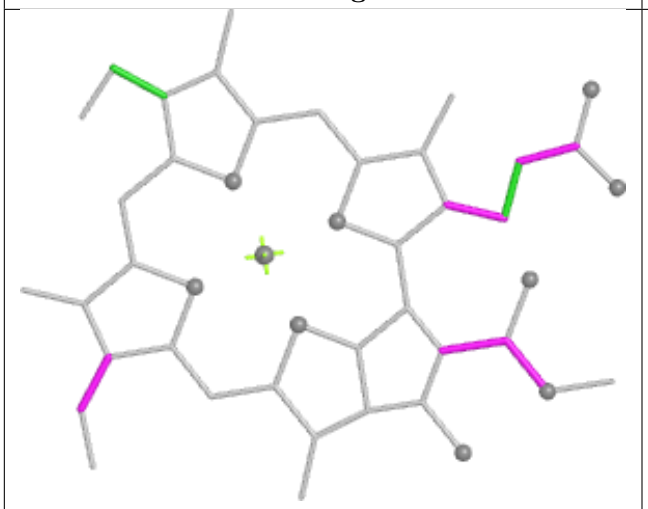
Ligand CLA 5 311



Bond lengths



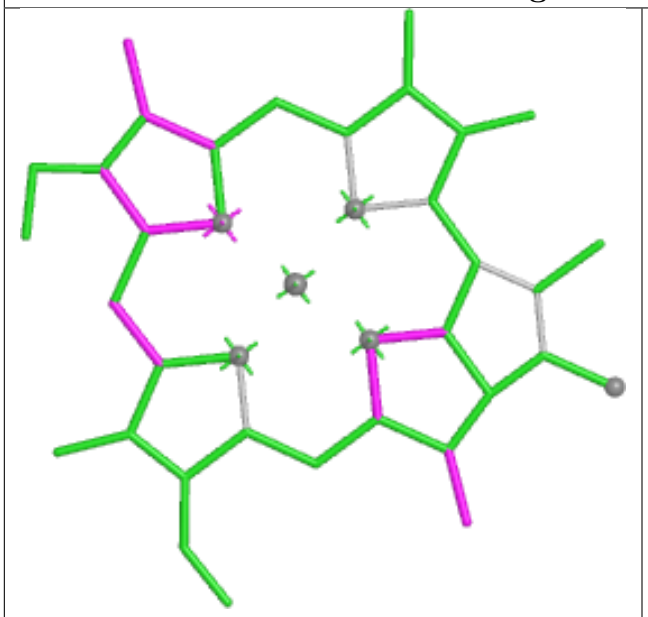
Bond angles



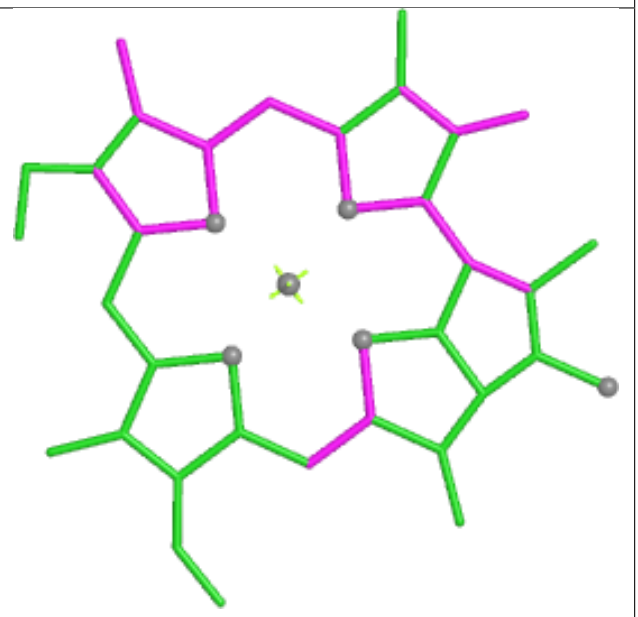
Torsions

Rings

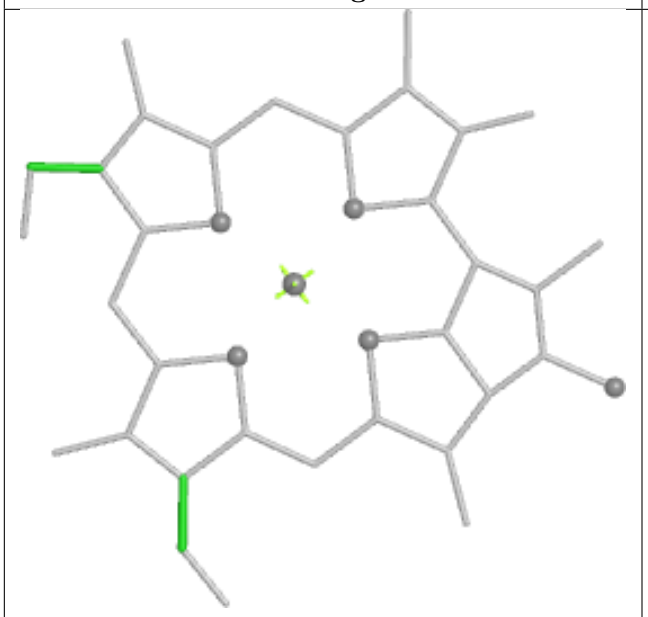
Ligand CLA 7 314



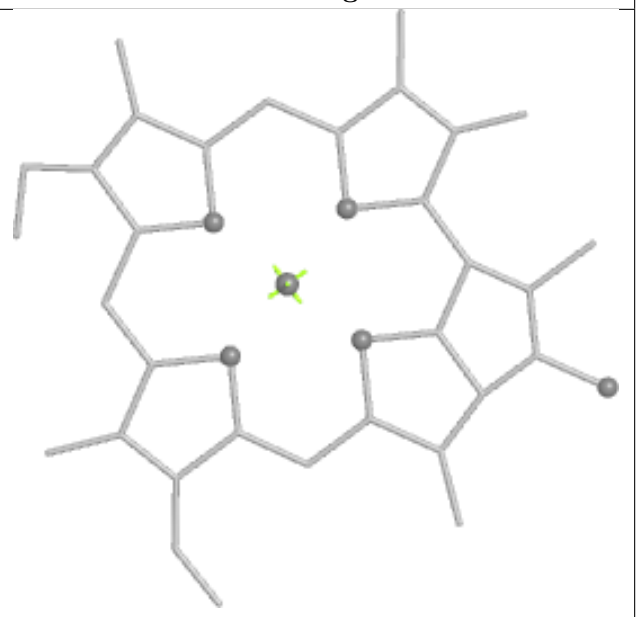
Bond lengths



Bond angles

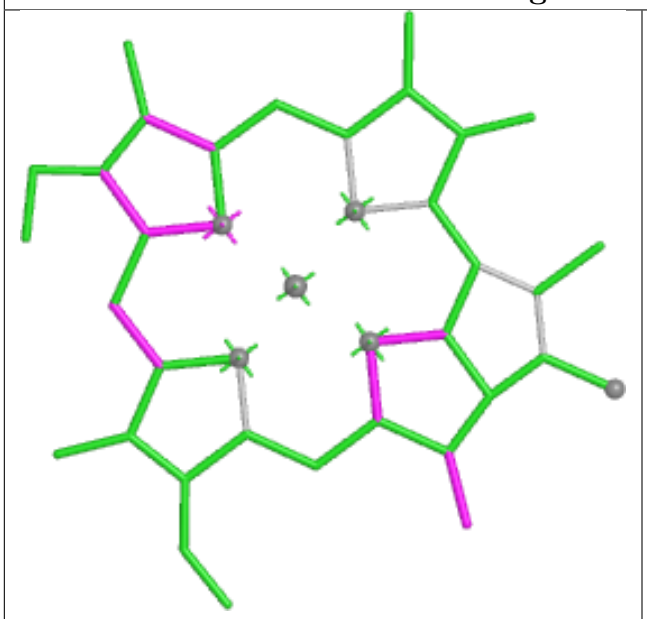


Torsions

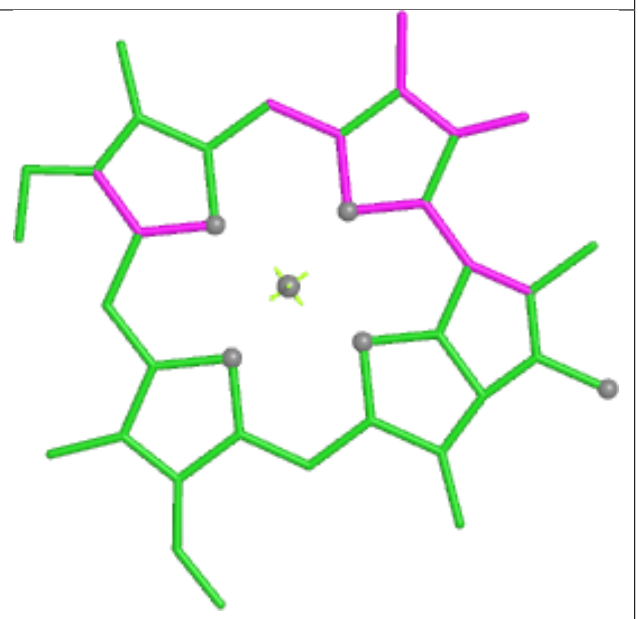


Rings

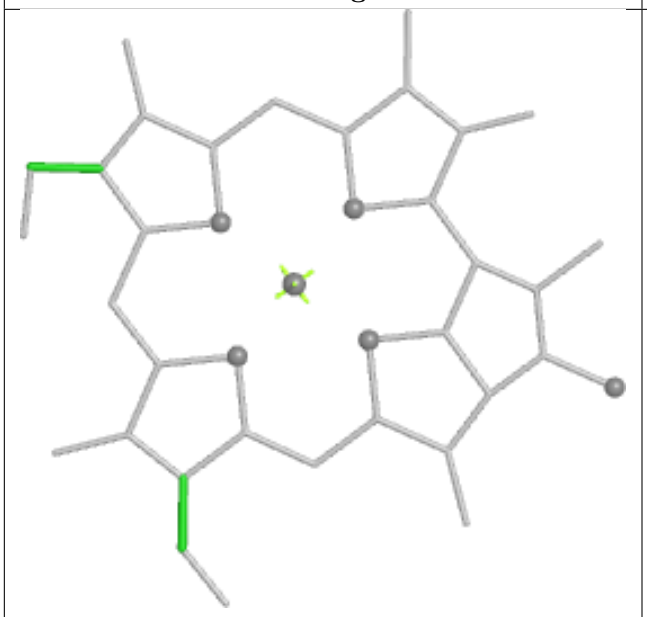
Ligand CLA 6 214



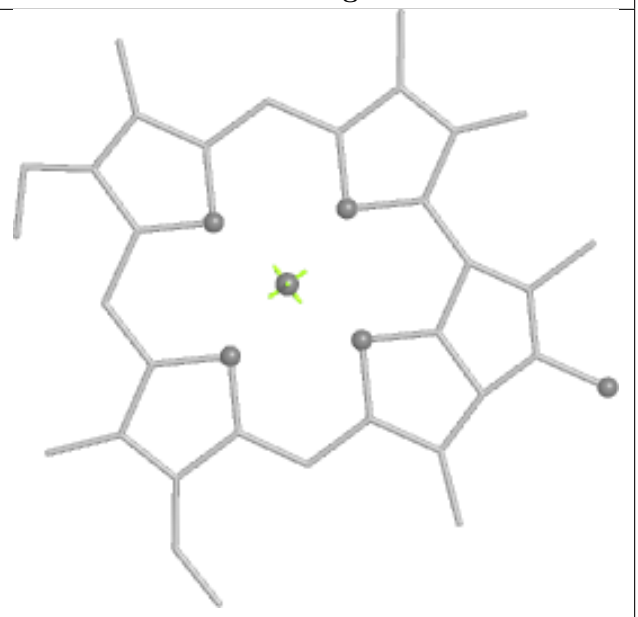
Bond lengths



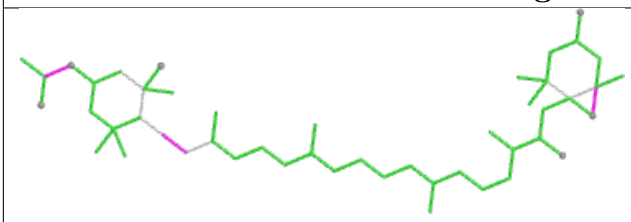
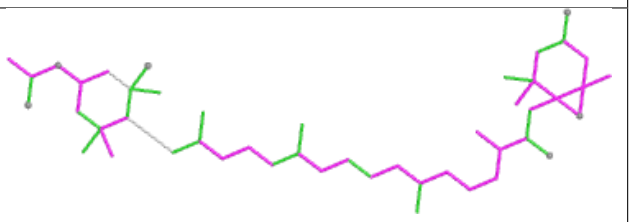
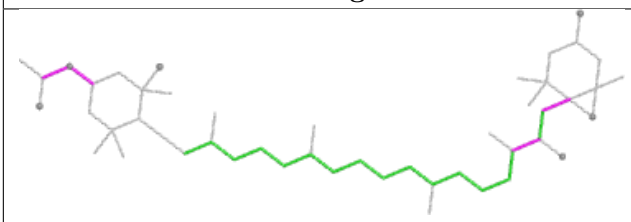
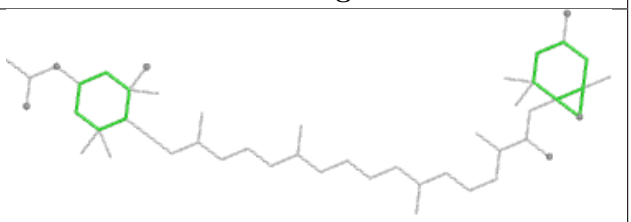
Bond angles

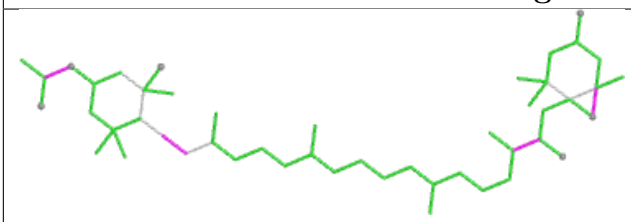
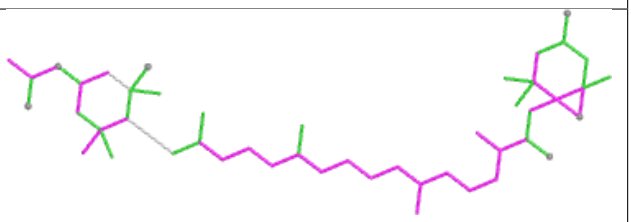
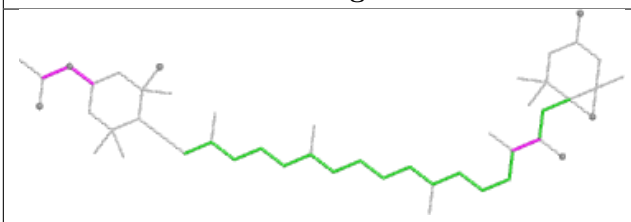
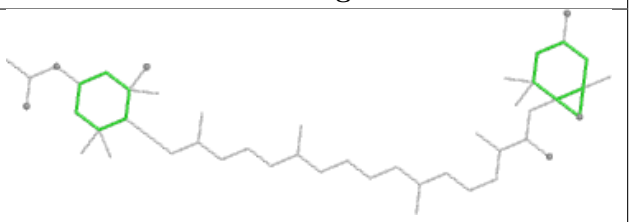


Torsions

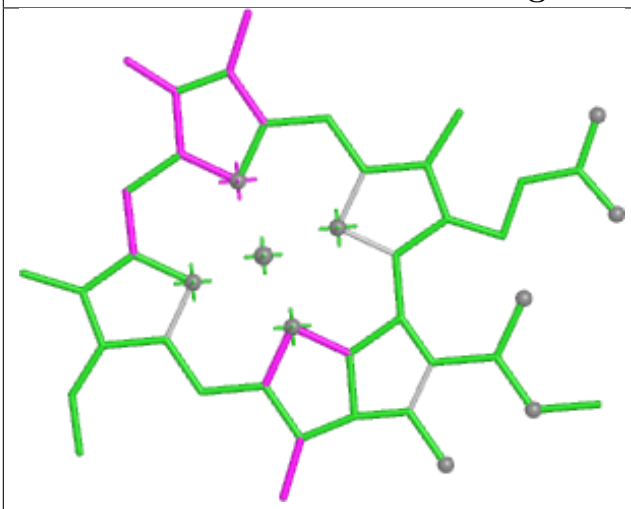


Rings

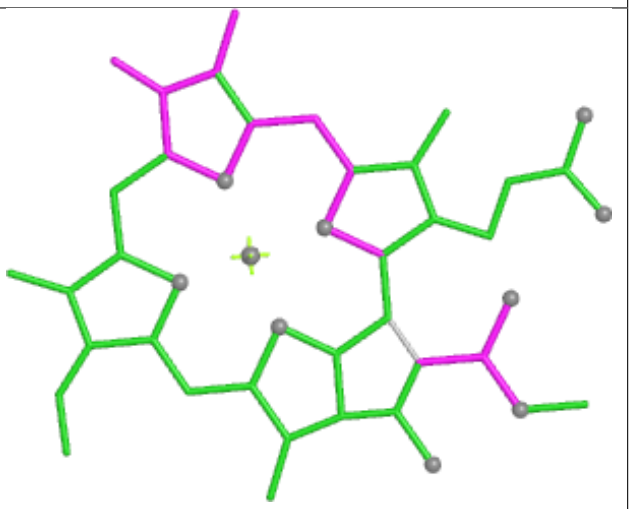
Ligand A86 5 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 6 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

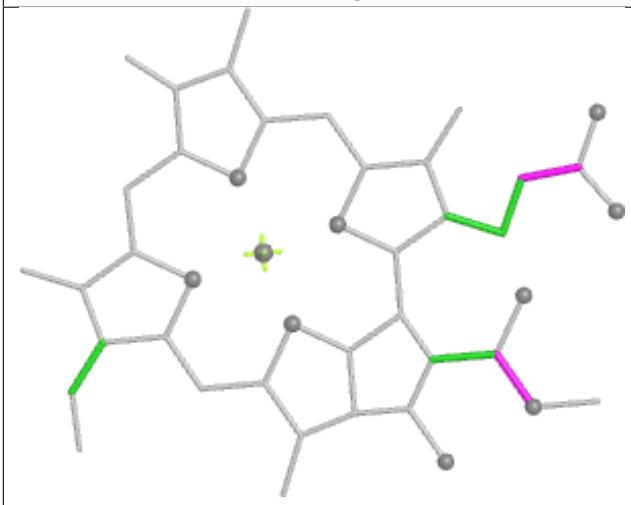
Ligand CLA 6 201



Bond lengths



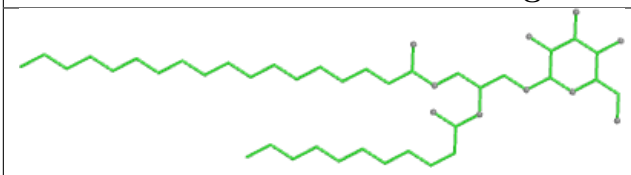
Bond angles



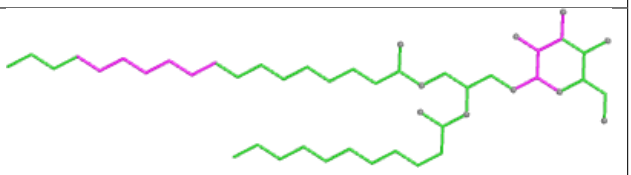
Torsions

Rings

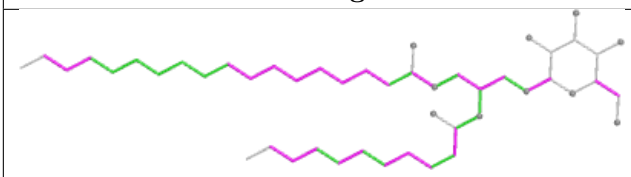
Ligand LMG 5 316



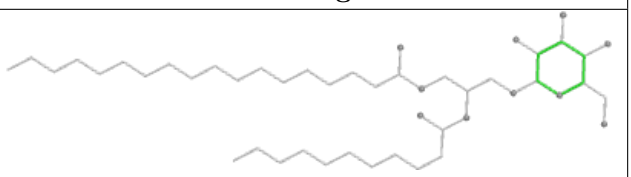
Bond lengths



Bond angles

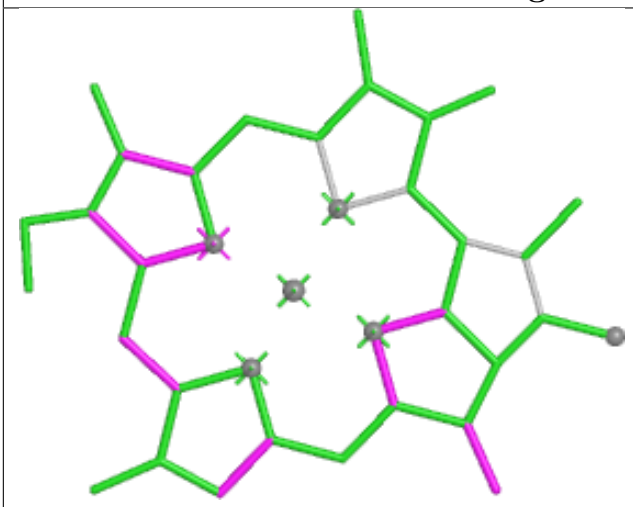


Torsions

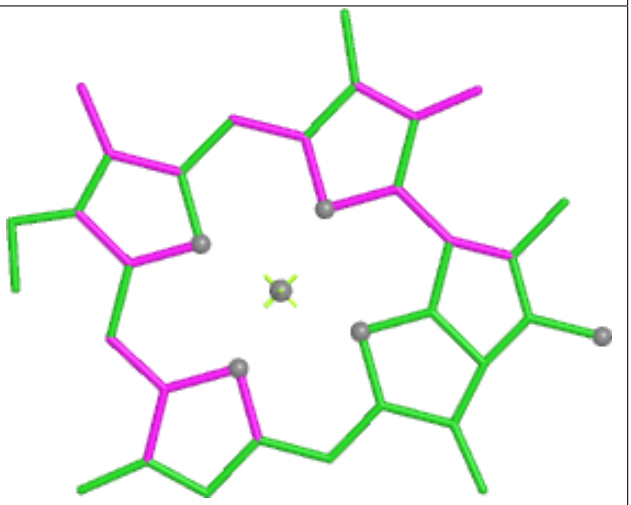


Rings

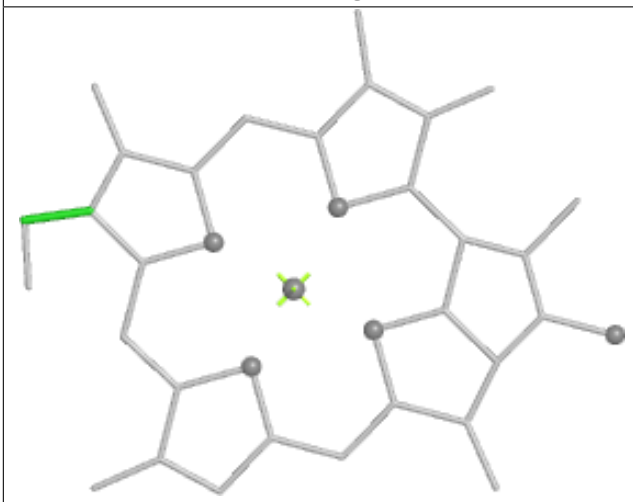
Ligand CLA 7 312



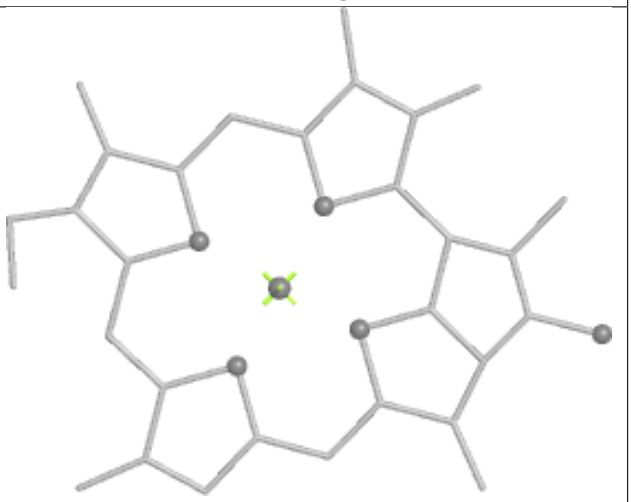
Bond lengths



Bond angles

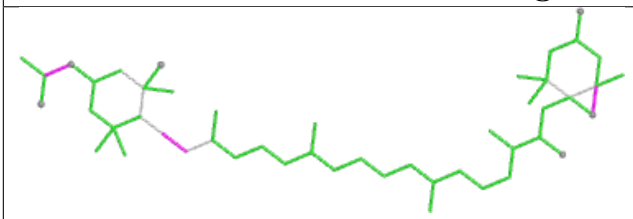


Torsions

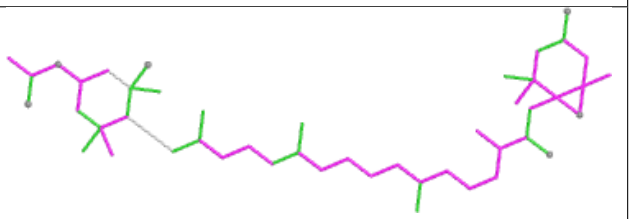


Rings

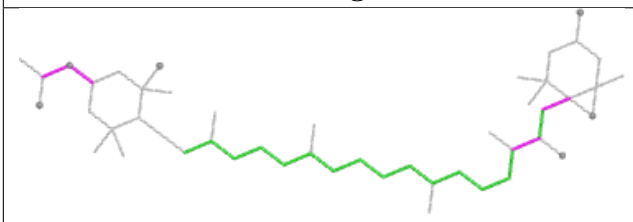
Ligand A86 7 301



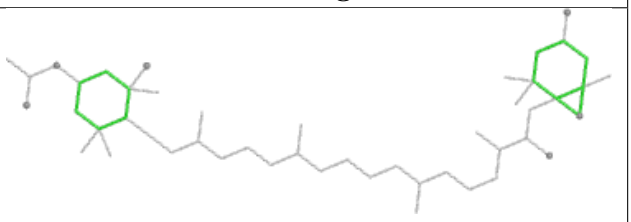
Bond lengths



Bond angles

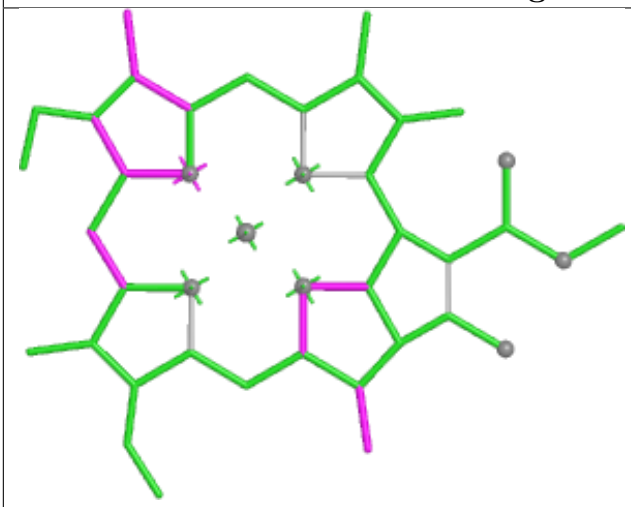


Torsions

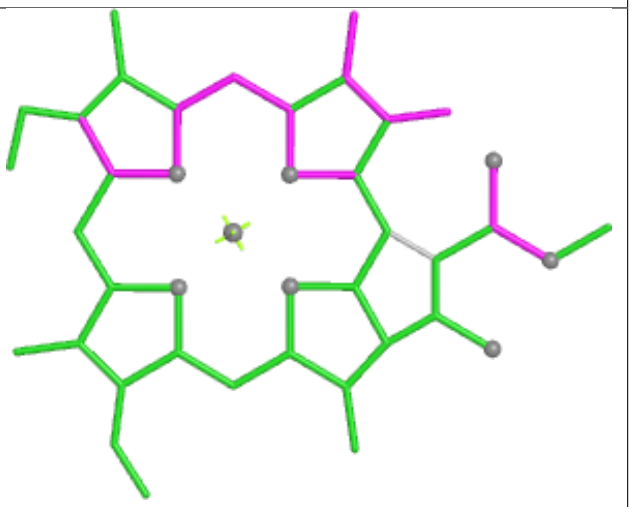


Rings

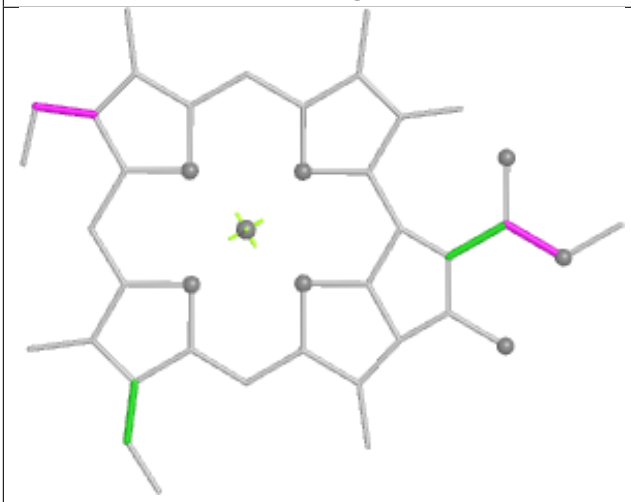
Ligand CLA 5 309



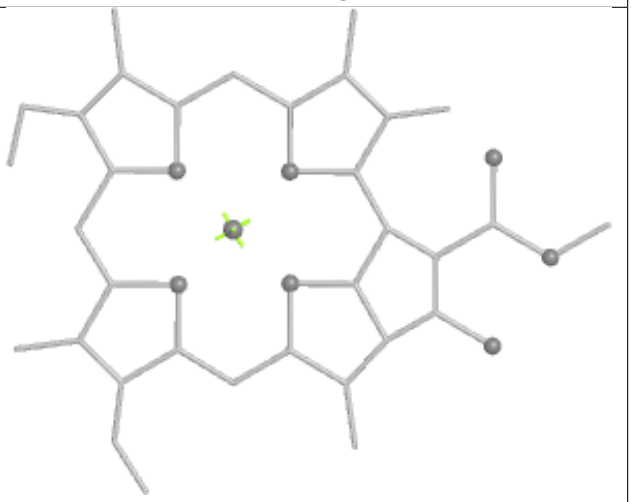
Bond lengths



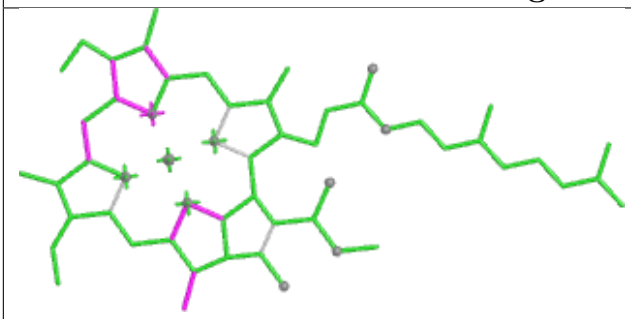
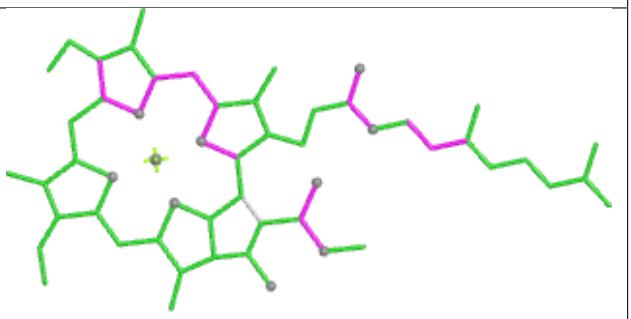
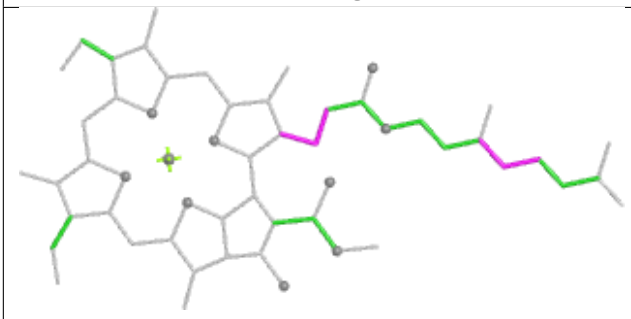
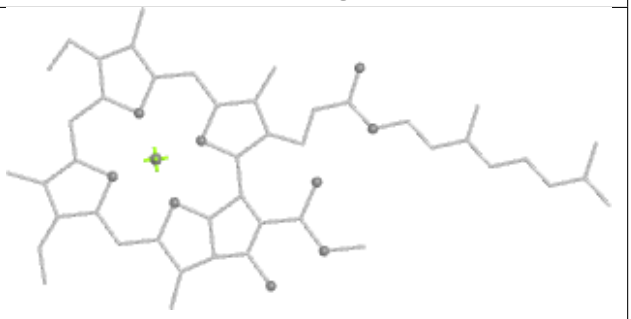
Bond angles



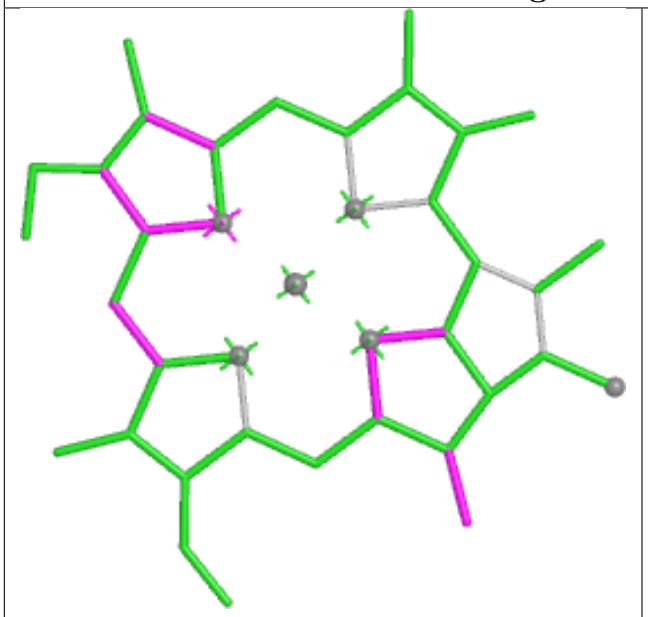
Torsions



Rings

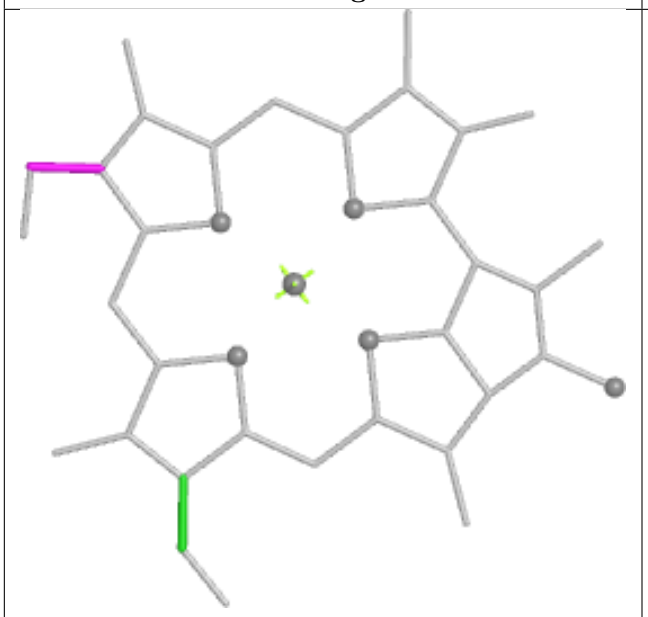
Ligand CLA 5 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 313

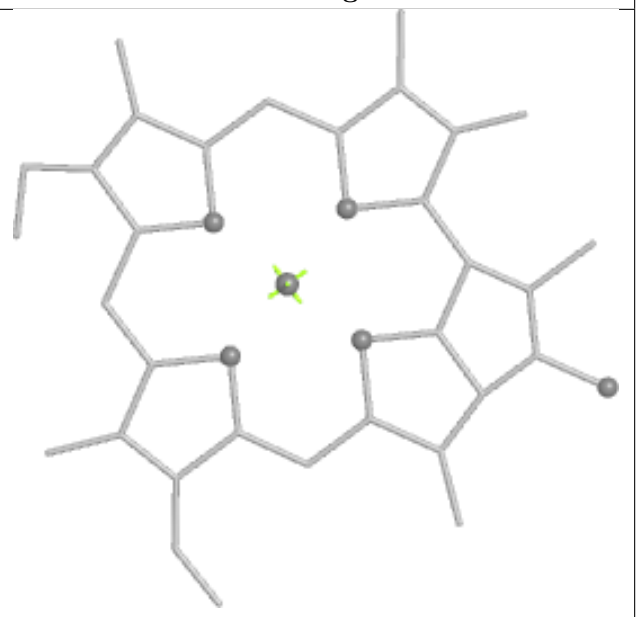


Bond lengths

Bond angles

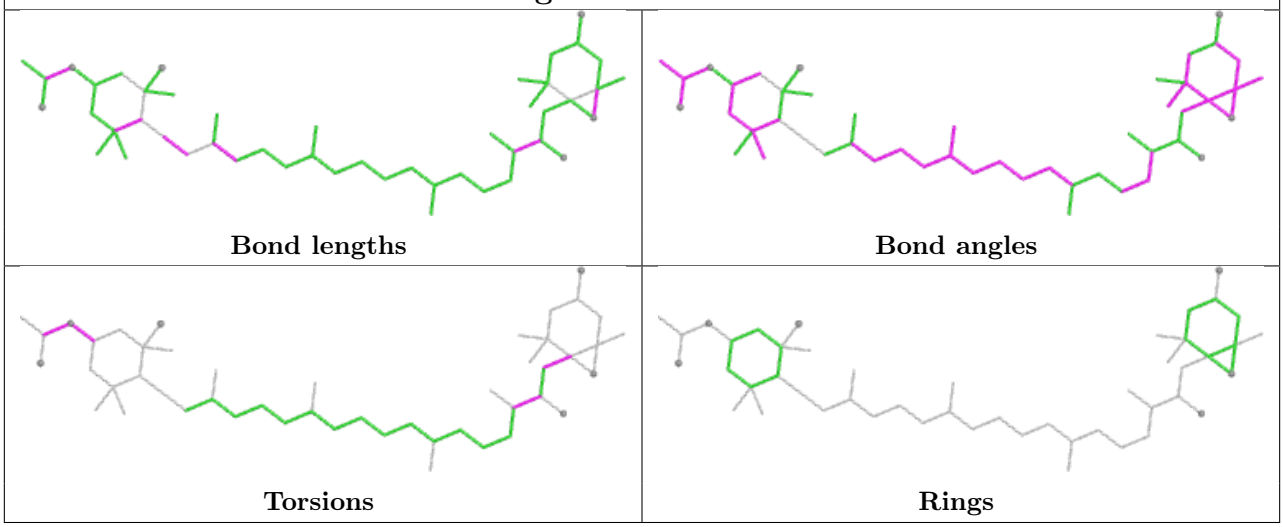


Torsions

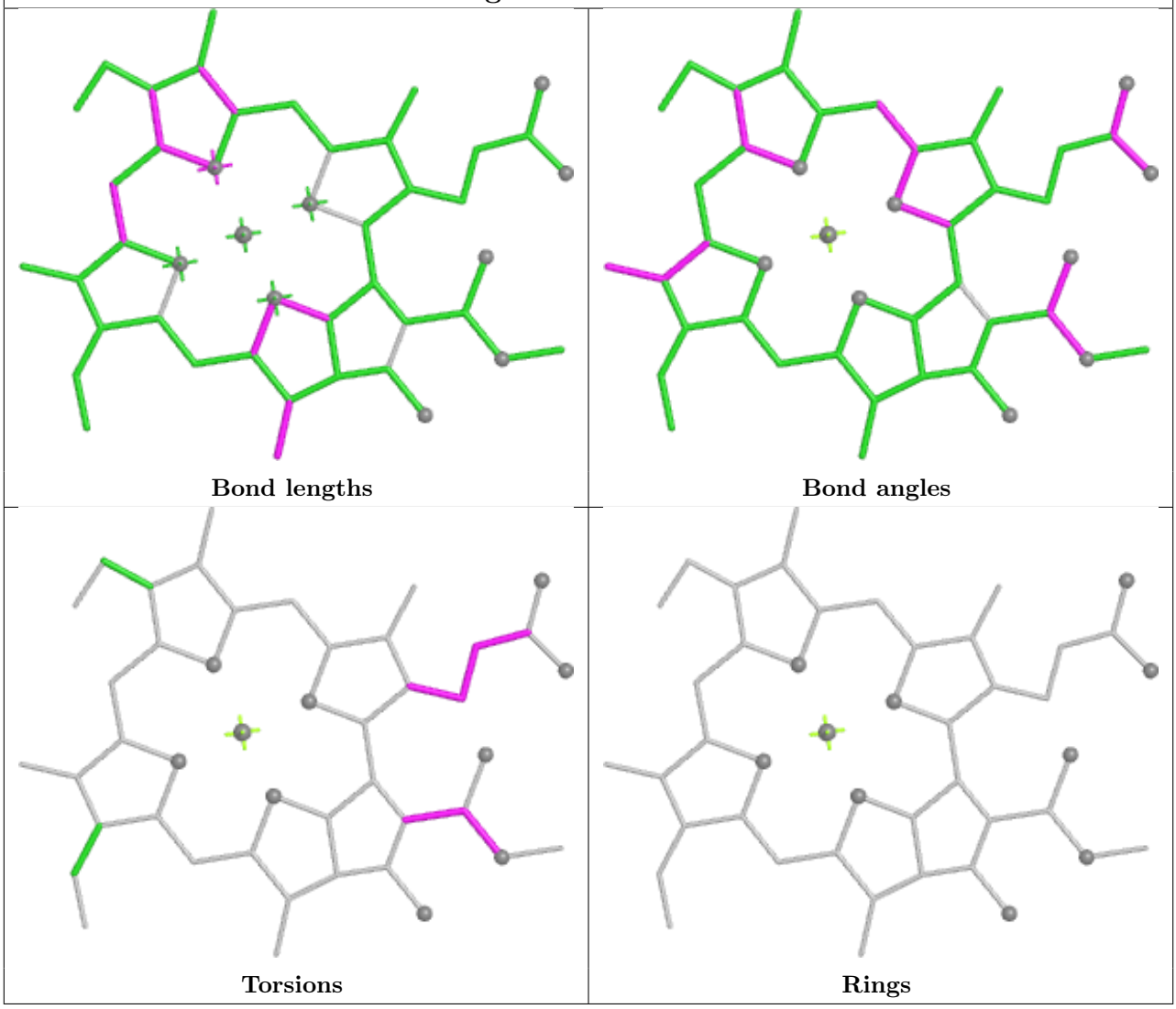


Rings

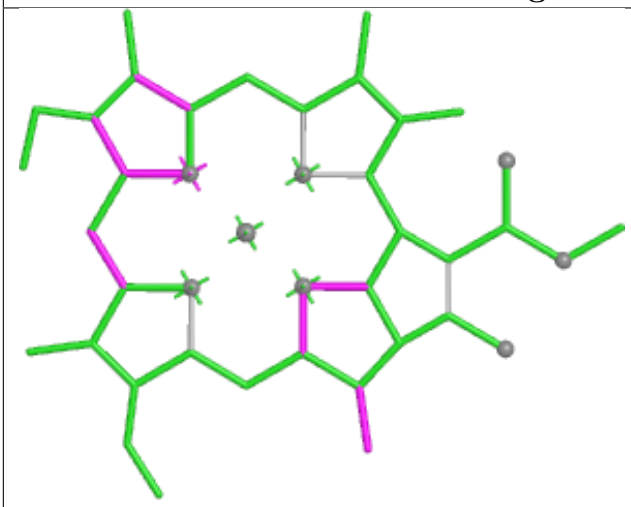
Ligand A86 7 302



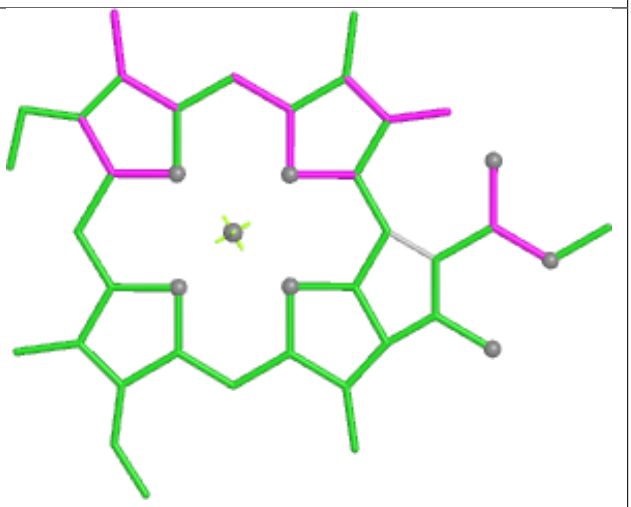
Ligand CLA 6 206



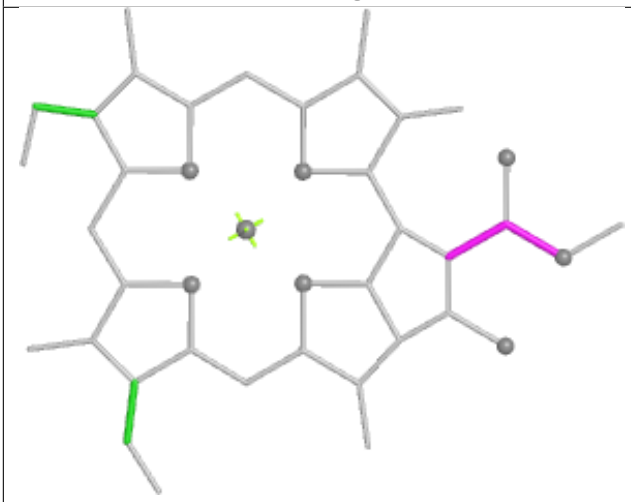
Ligand CLA 6 212



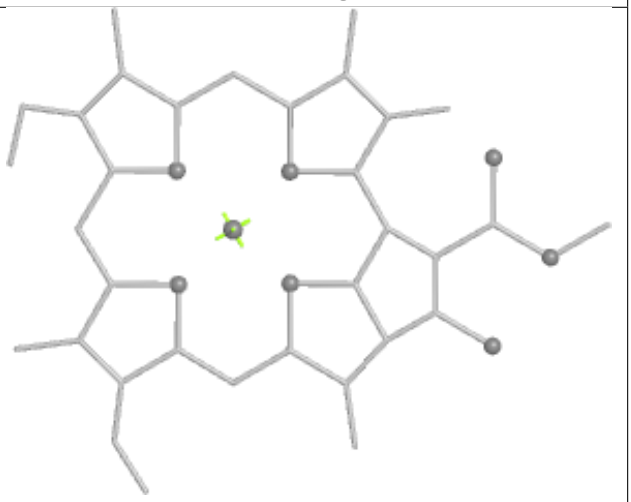
Bond lengths



Bond angles

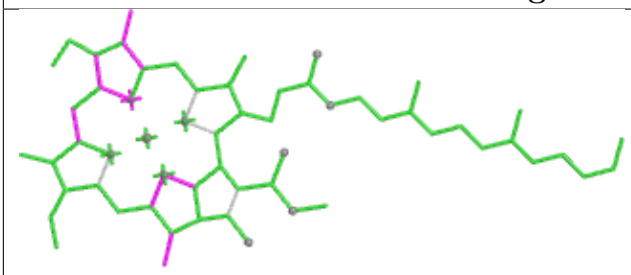


Torsions

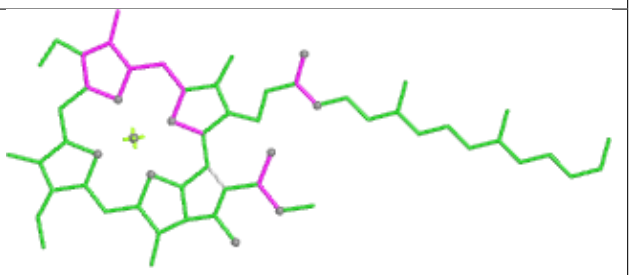


Rings

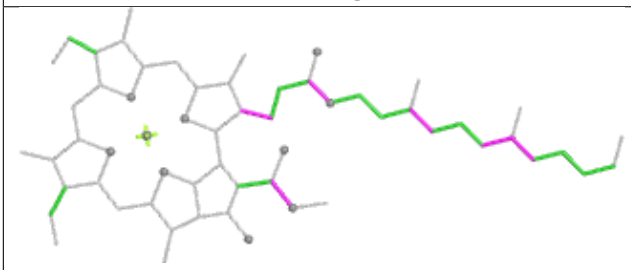
Ligand CLA 7 309



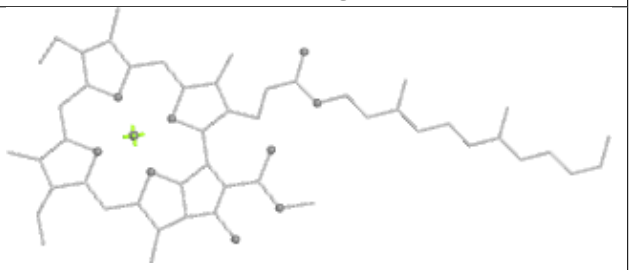
Bond lengths



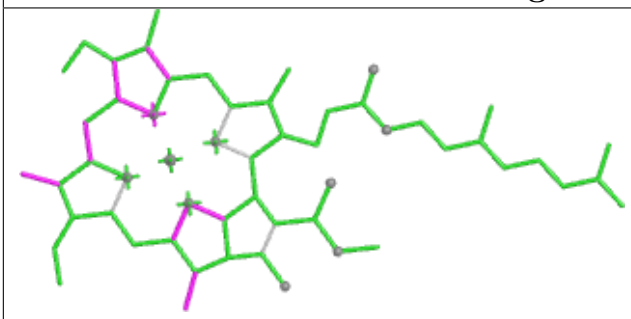
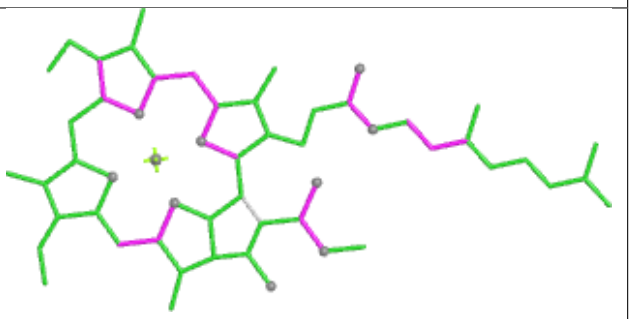
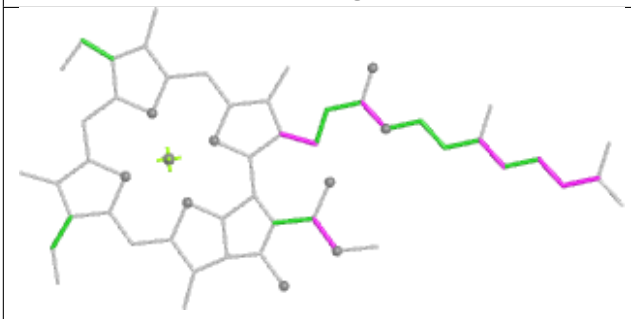
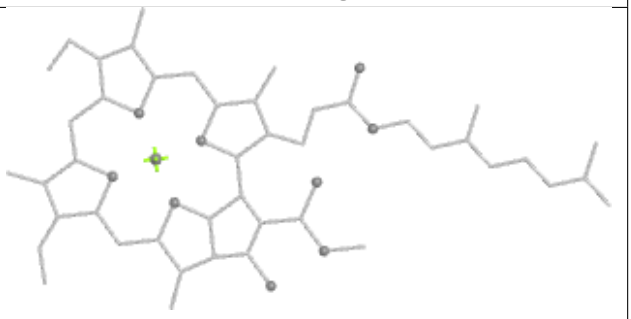
Bond angles

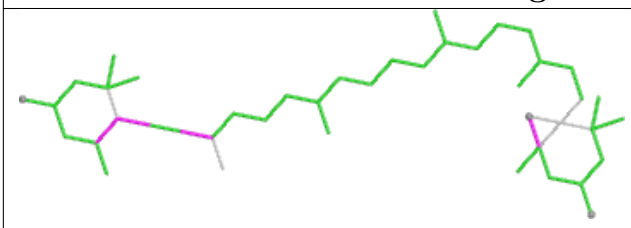
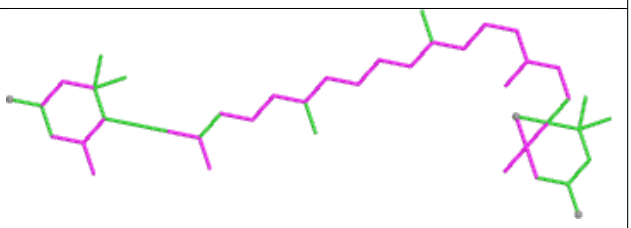
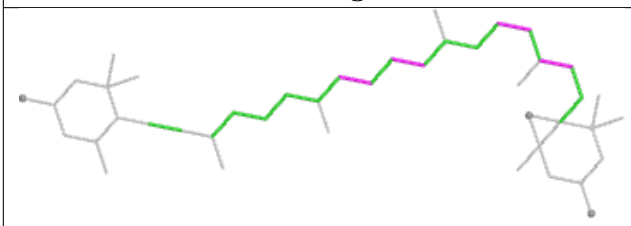
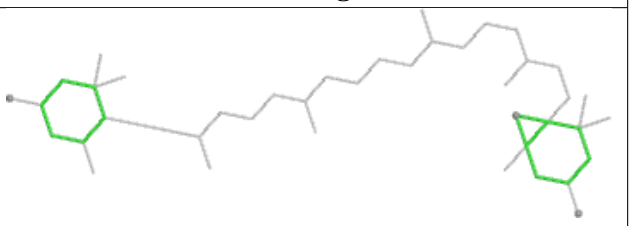


Torsions

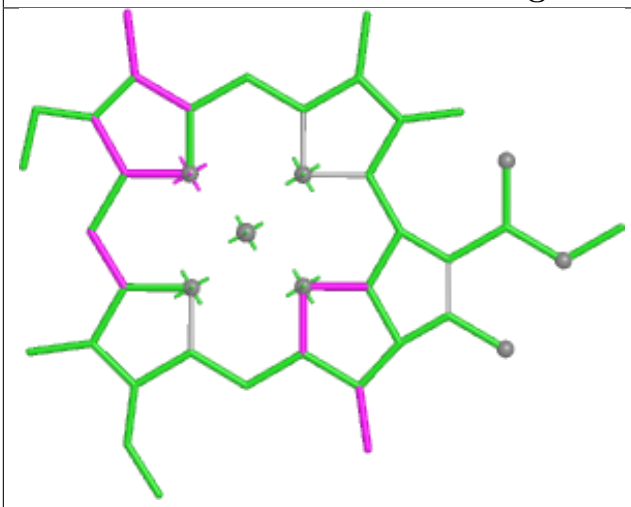


Rings

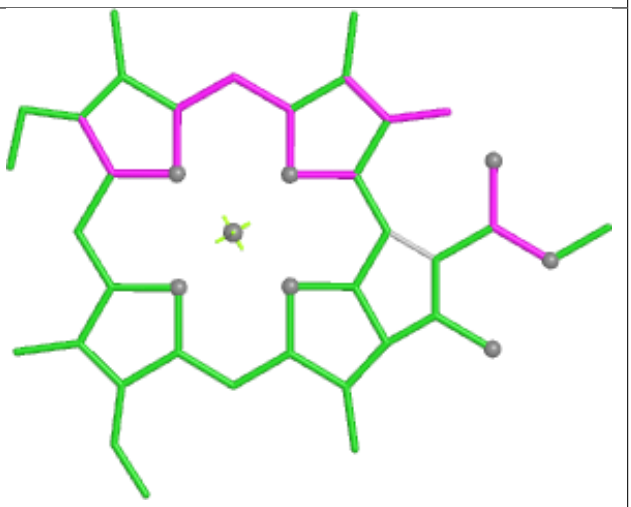
Ligand CLA 7 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 6 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

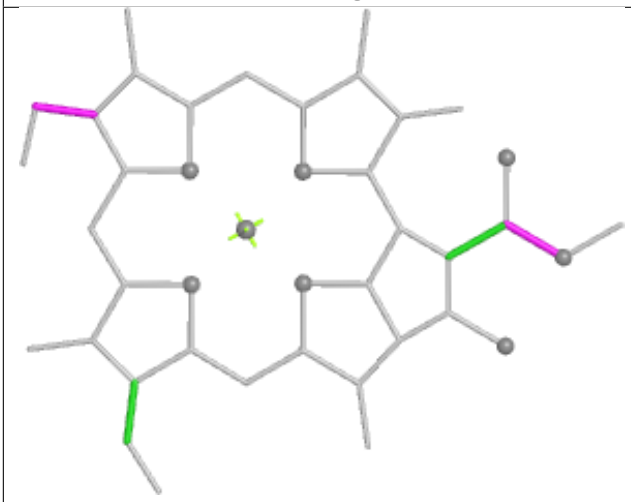
Ligand CLA 5 304



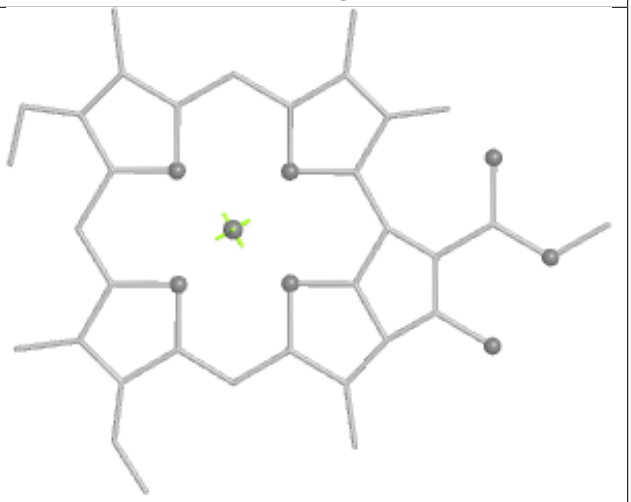
Bond lengths



Bond angles

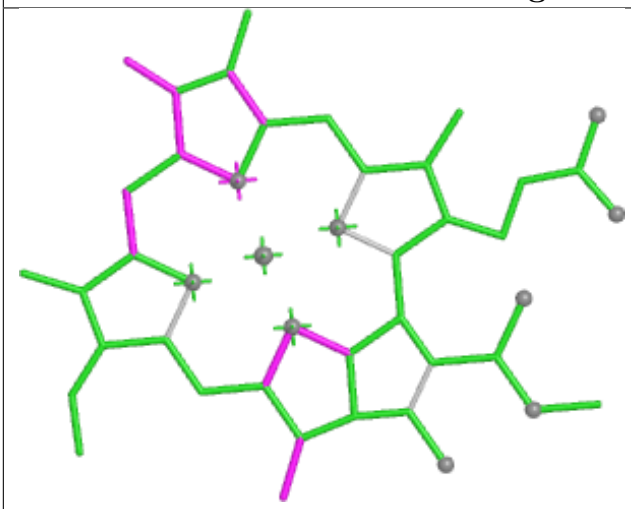


Torsions

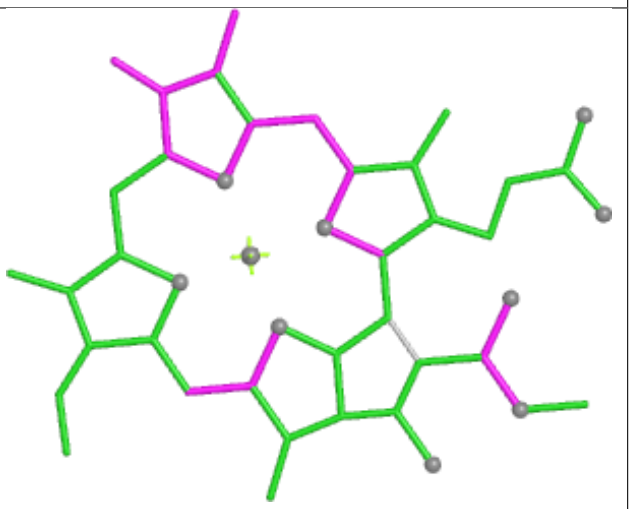


Rings

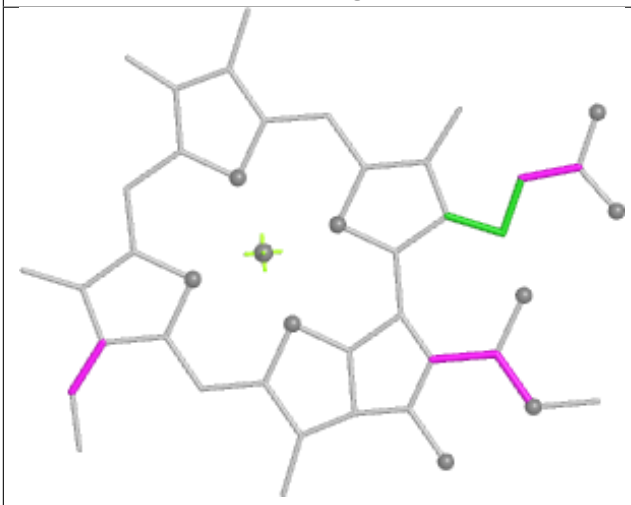
Ligand CLA 6 207



Bond lengths



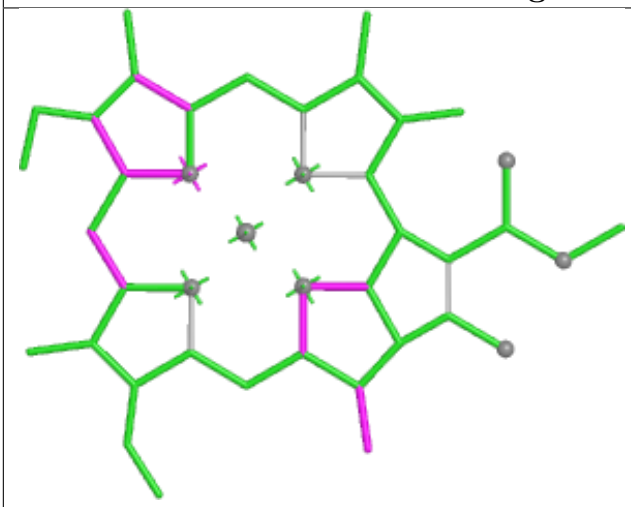
Bond angles



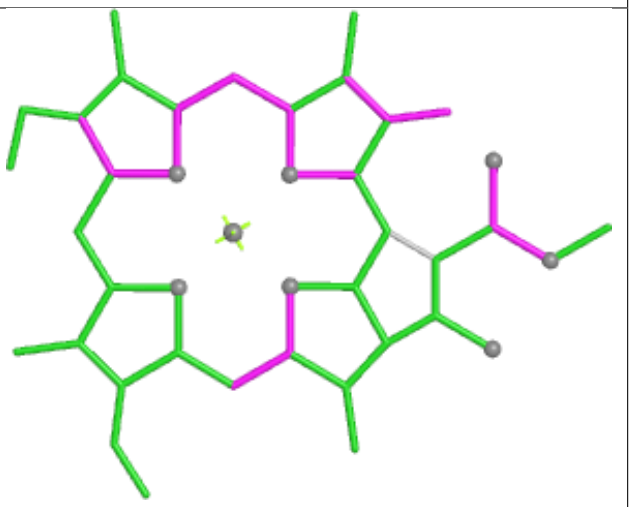
Torsions

Rings

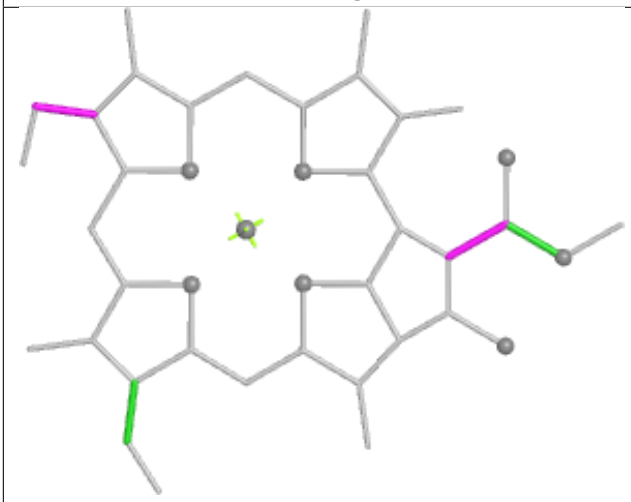
Ligand CLA 6 205



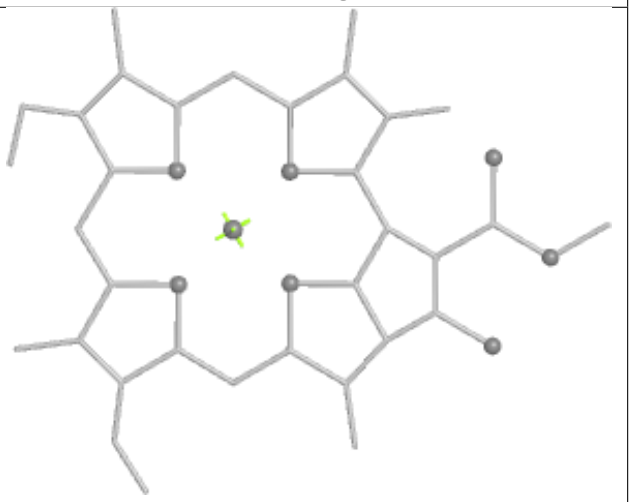
Bond lengths



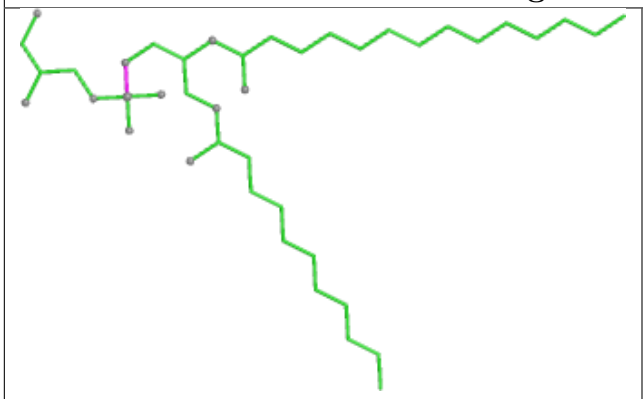
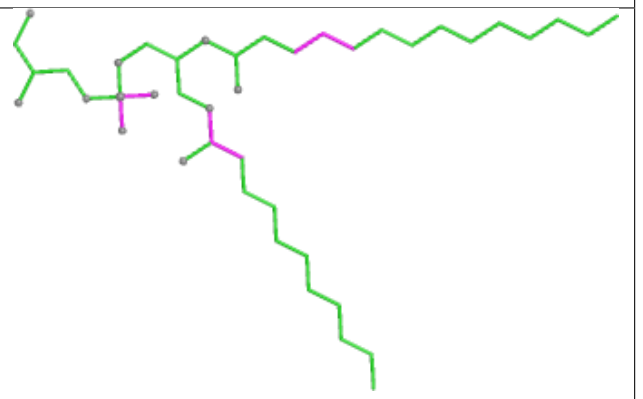
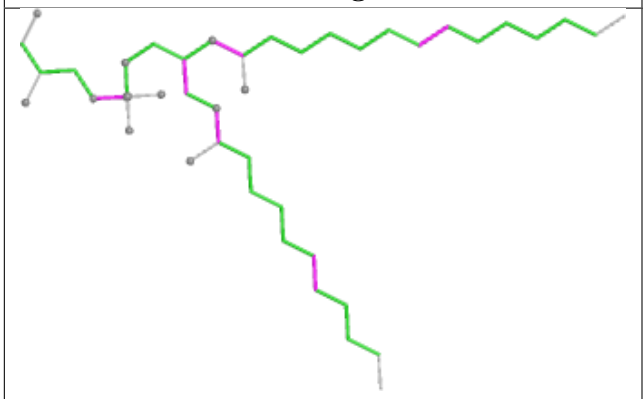
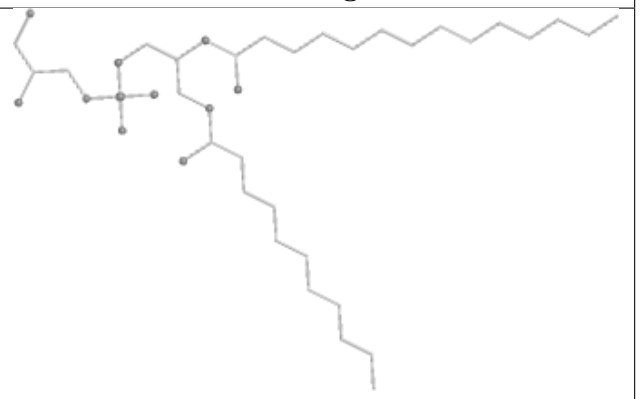
Bond angles



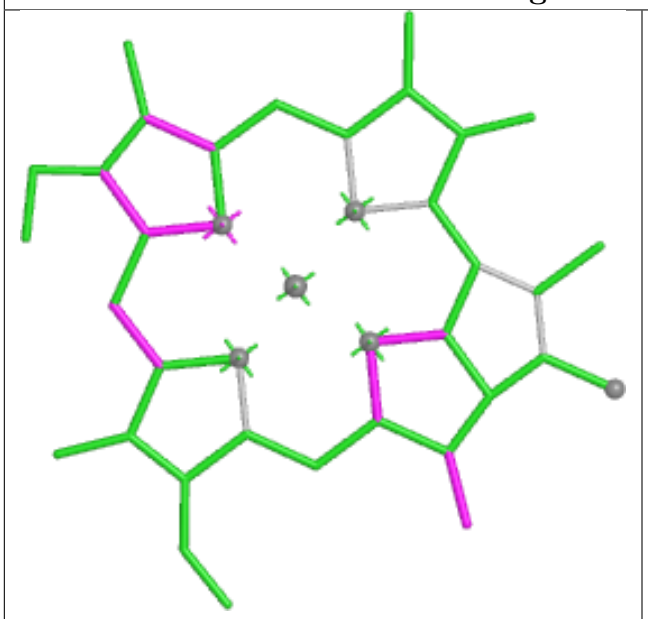
Torsions



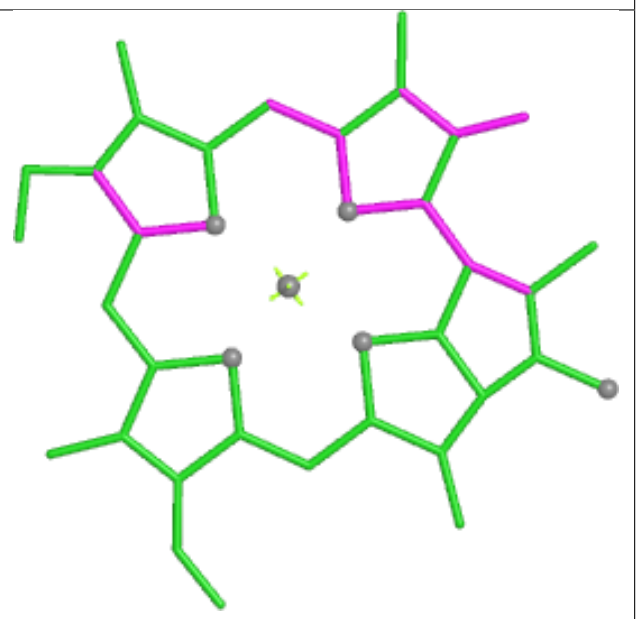
Rings

Ligand LHG 5 315	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

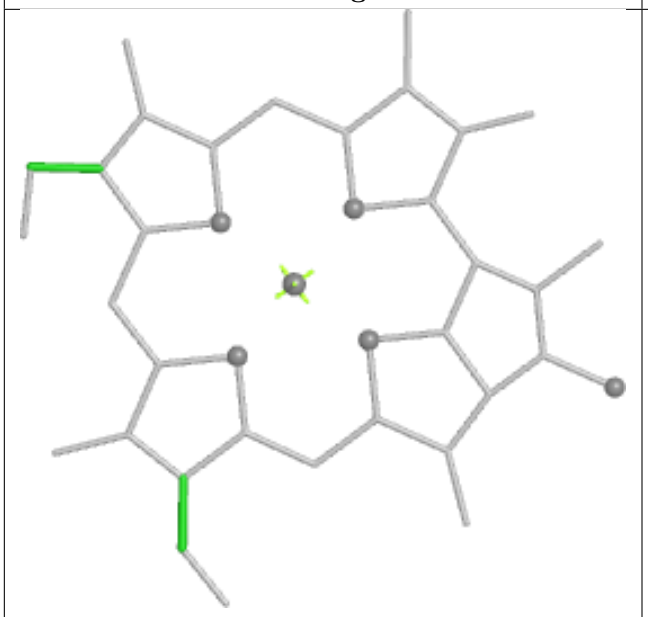
Ligand CLA 5 314



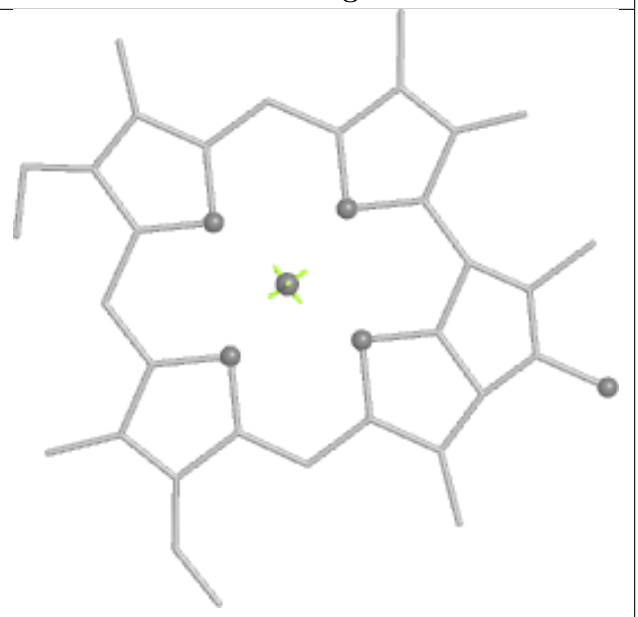
Bond lengths



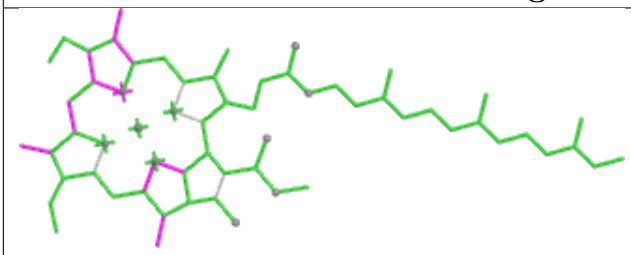
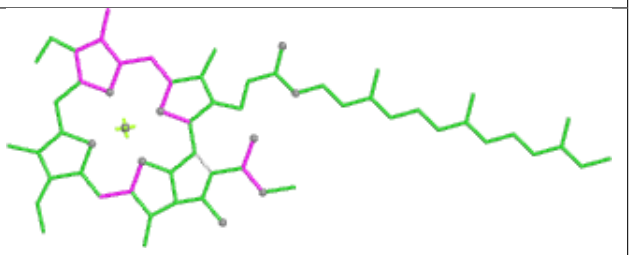
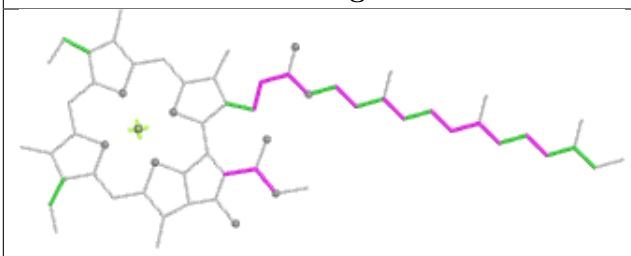
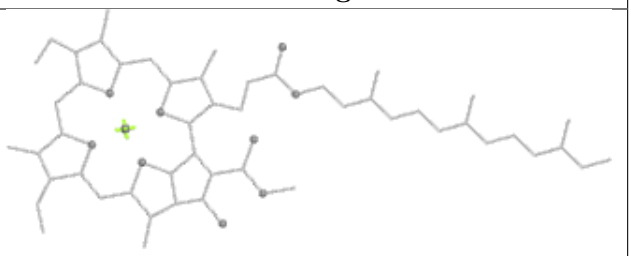
Bond angles

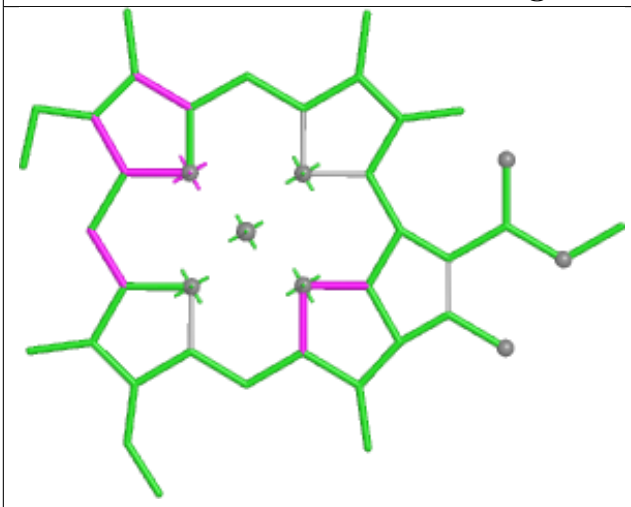
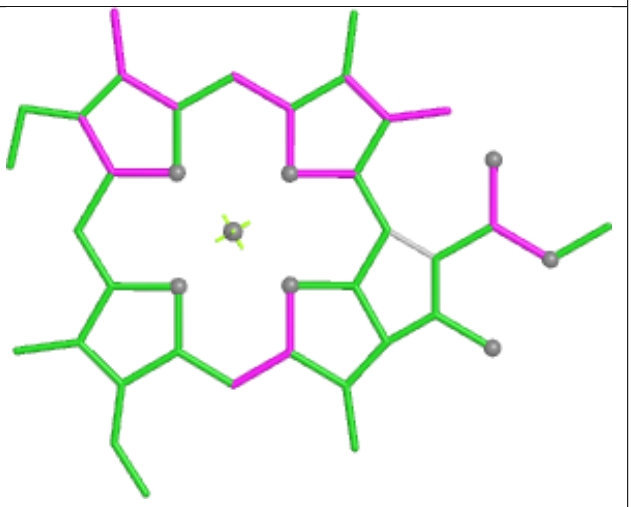
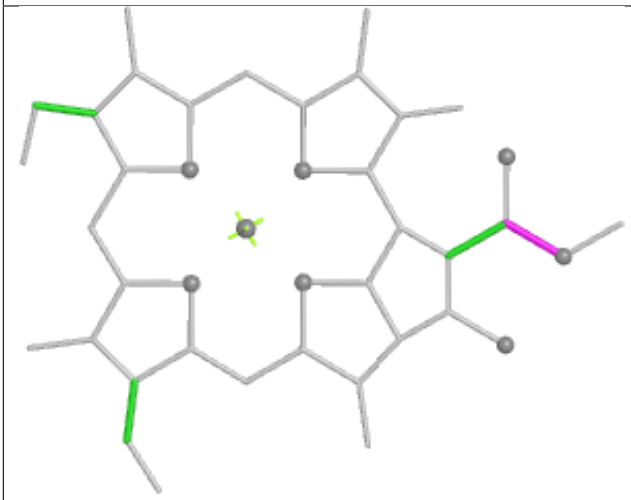
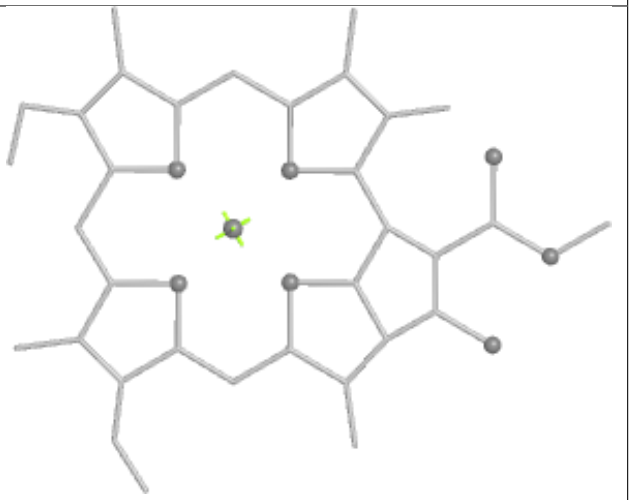


Torsions



Rings

Ligand CLA 5 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 316	
 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.

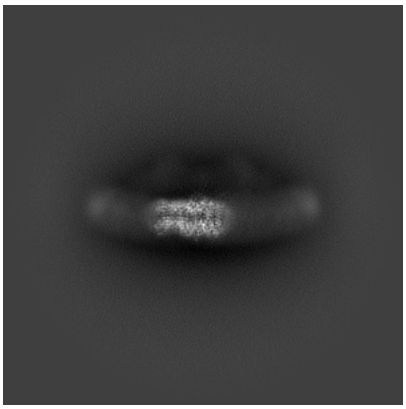
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37267. These allow visual inspection of the internal detail of the map and identification of artifacts.

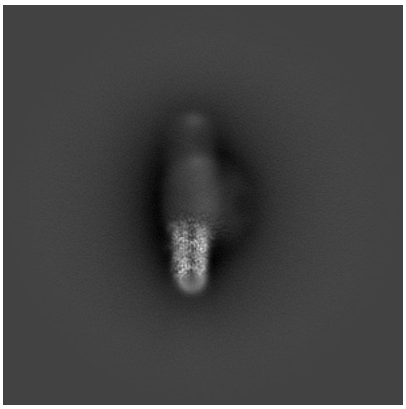
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

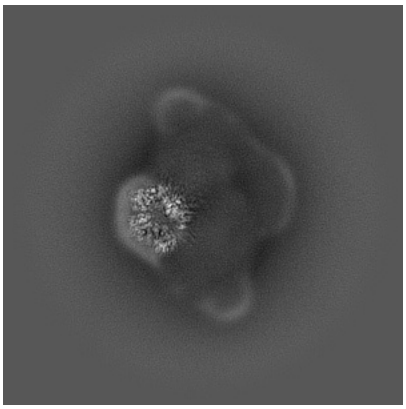
6.1.1 Primary map



X

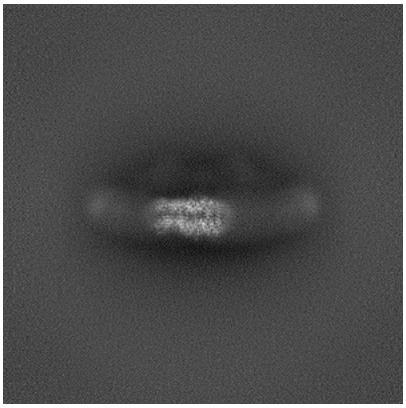


Y

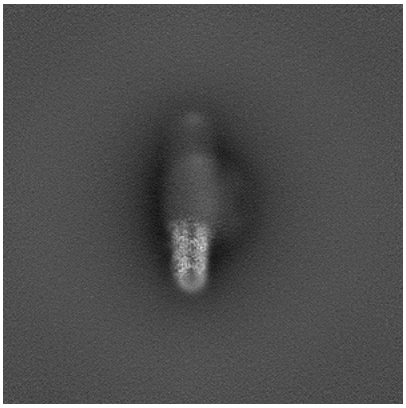


Z

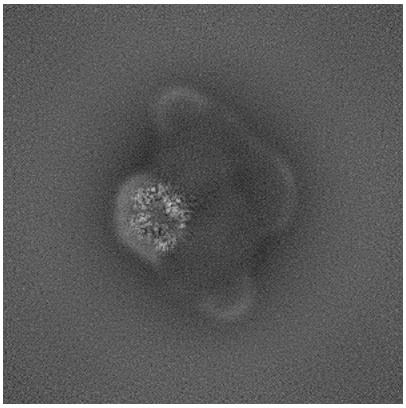
6.1.2 Raw map



X



Y

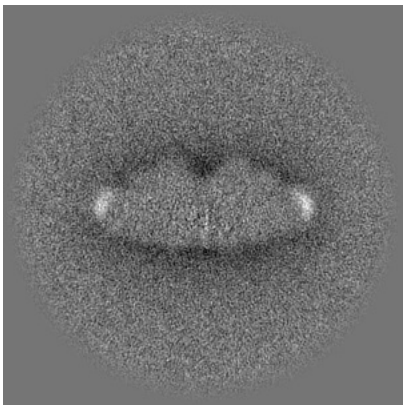


Z

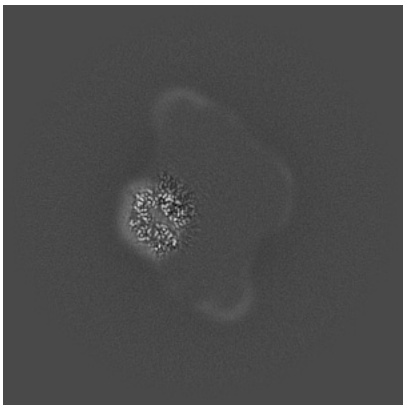
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

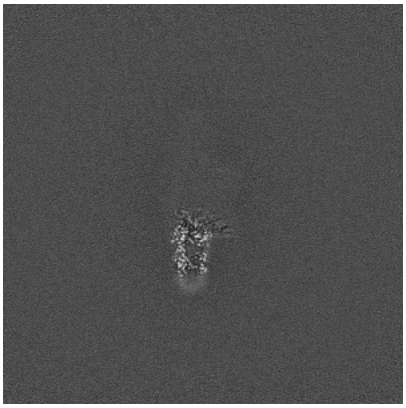

X Index: 256

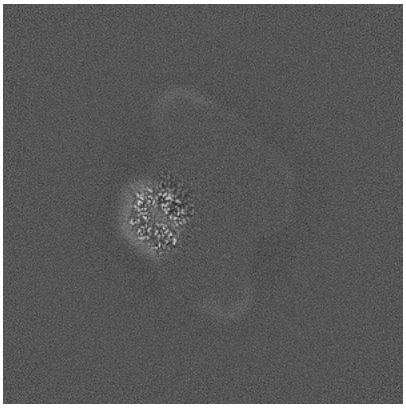
Y Index: 256


Z Index: 256

6.2.2 Raw map

X Index: 256

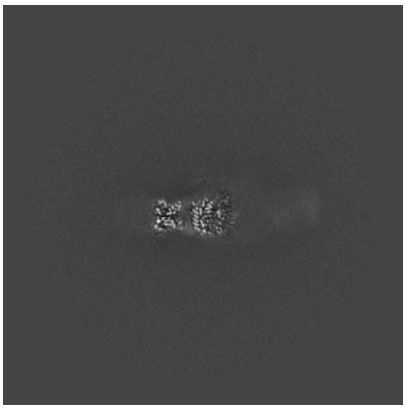

Y Index: 256


Z Index: 256

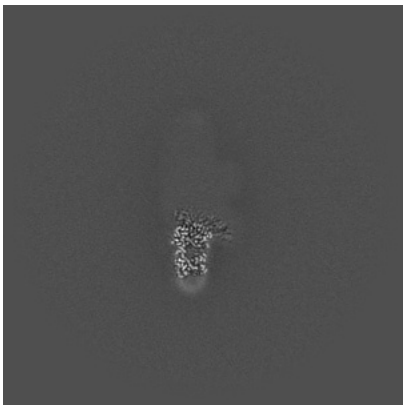
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

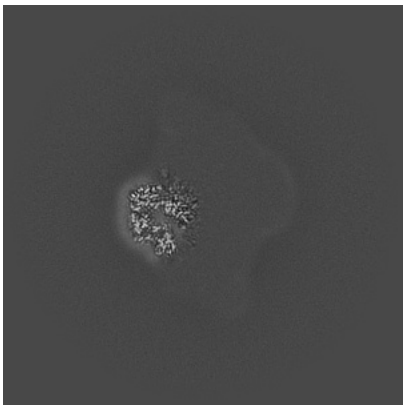
6.3.1 Primary map



X Index: 210

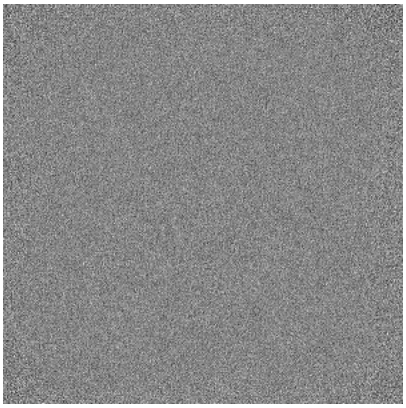


Y Index: 257

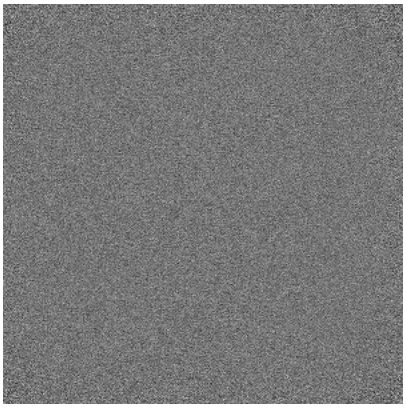


Z Index: 230

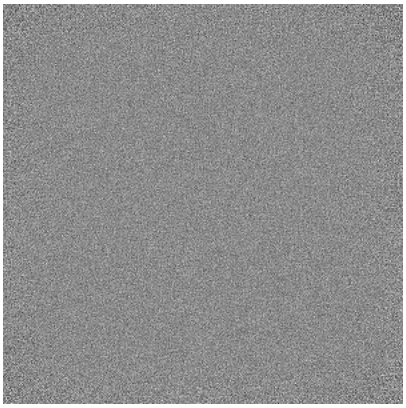
6.3.2 Raw map



X Index: 0



Y Index: 0

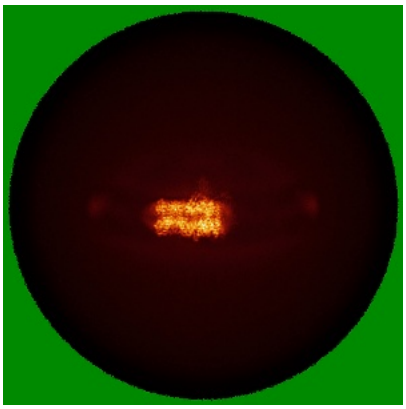


Z Index: 511

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

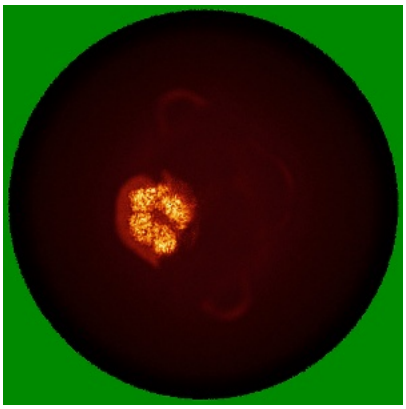
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



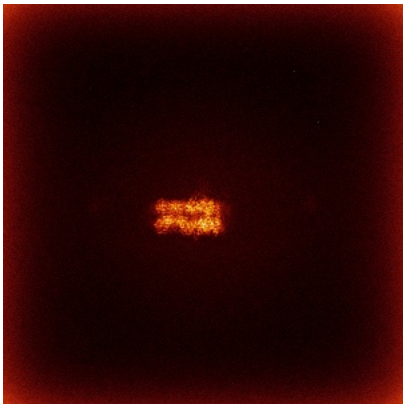
X

Y

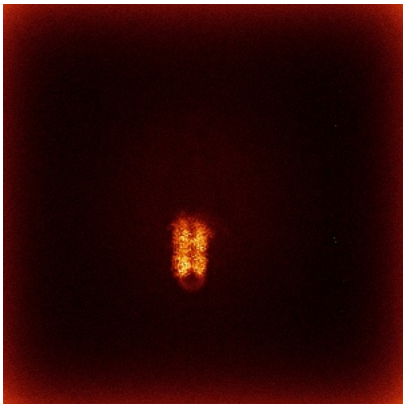


Z

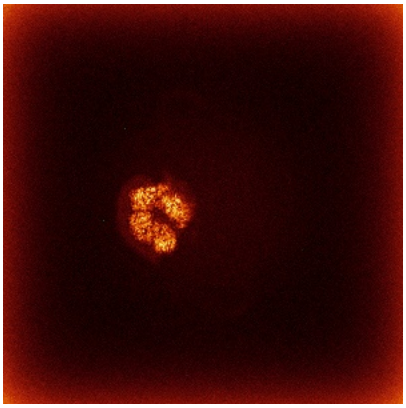
6.4.2 Raw map



X



Y

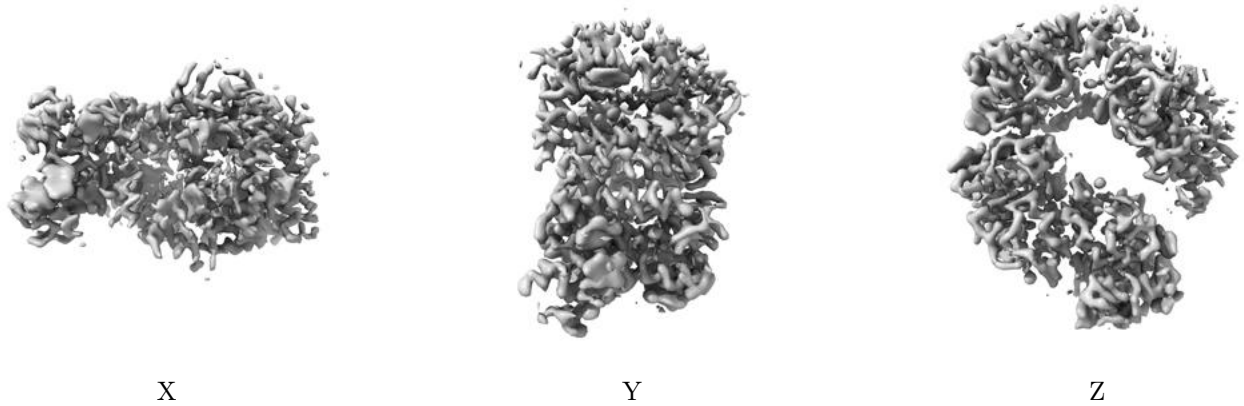


Z

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.

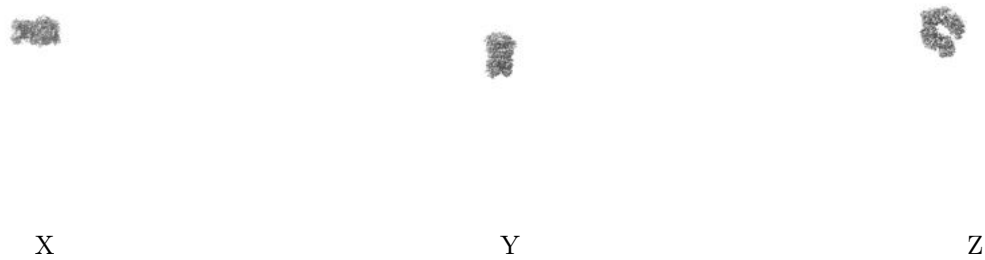
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.313. 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



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

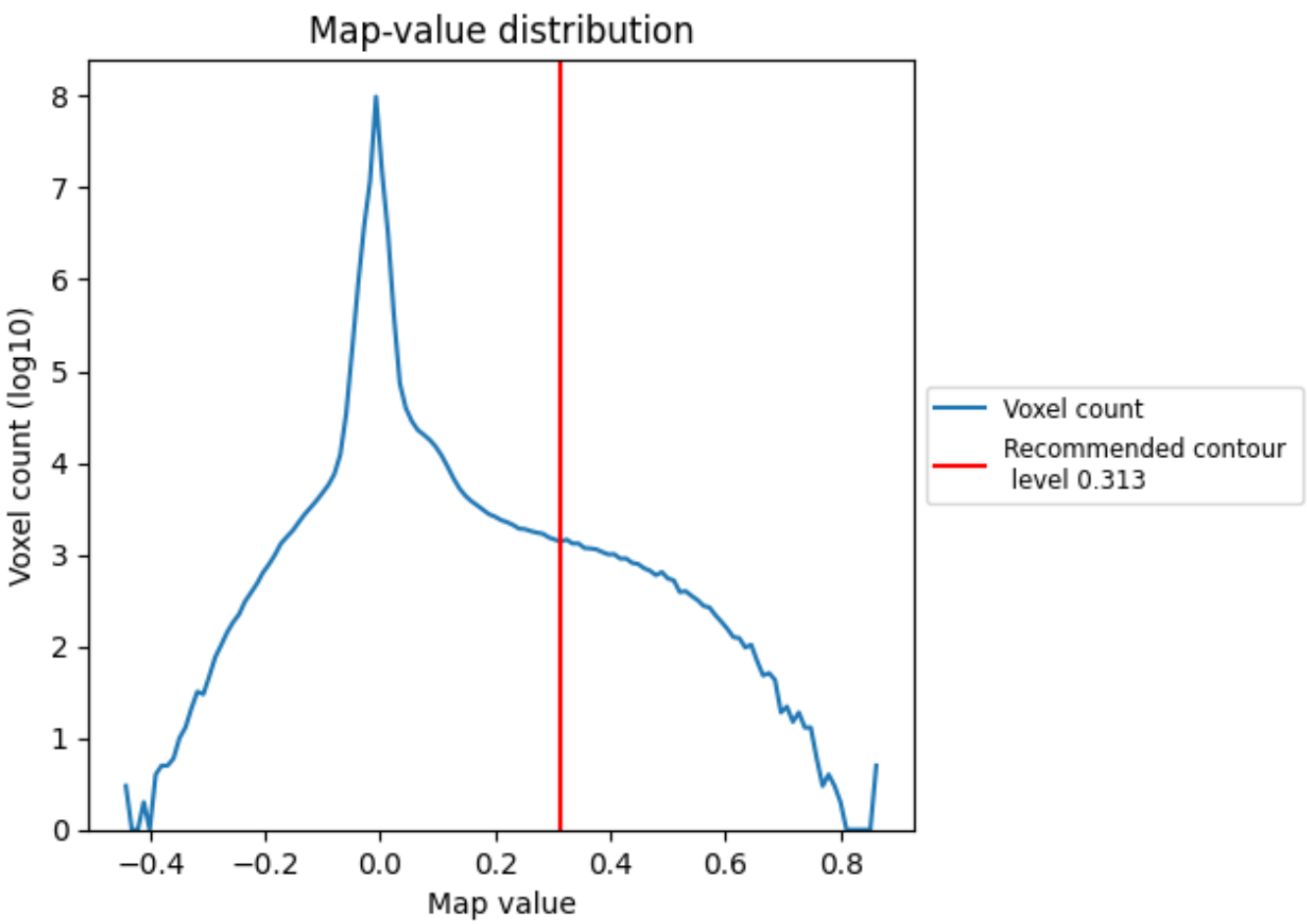
6.6 Mask visualisation (i)

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

7 Map analysis (i)

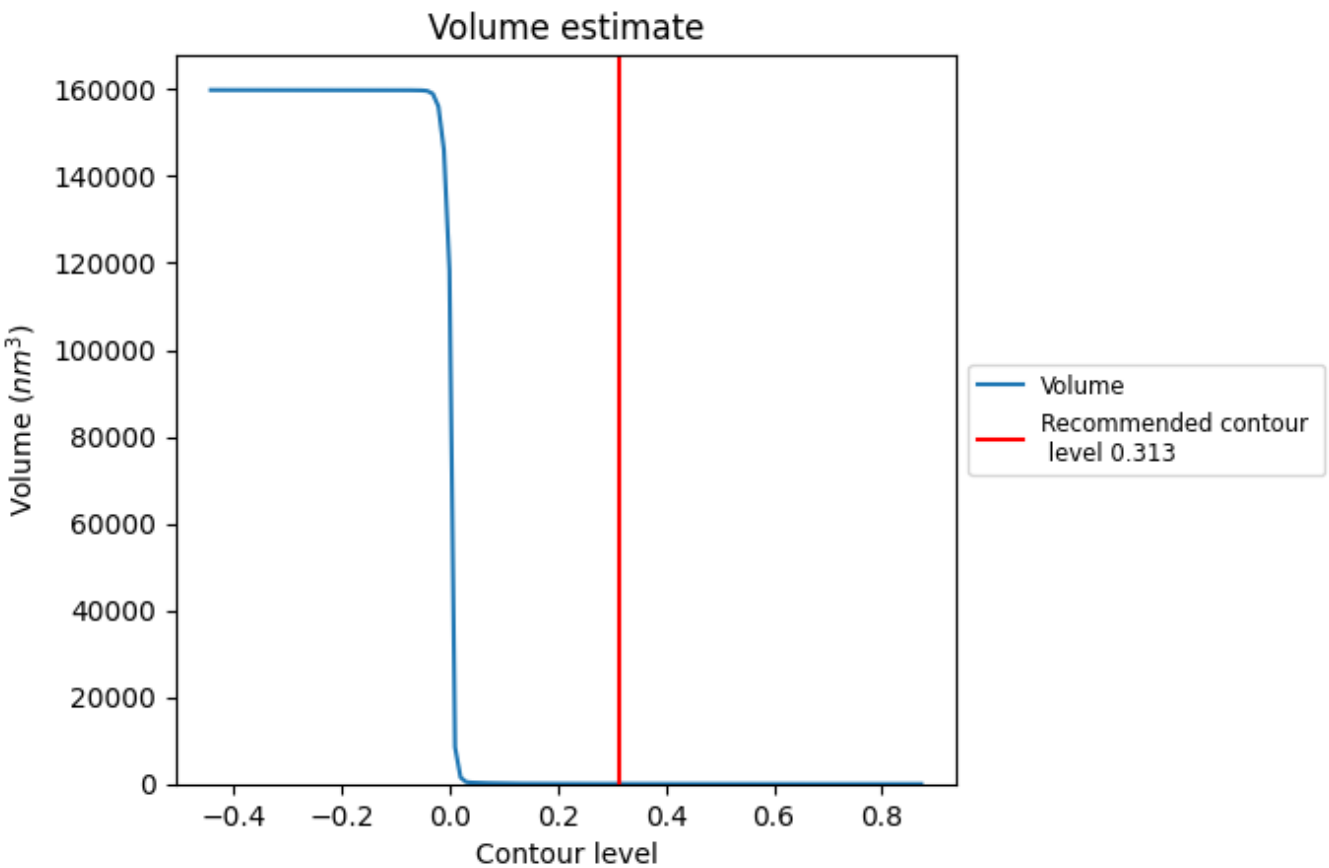
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

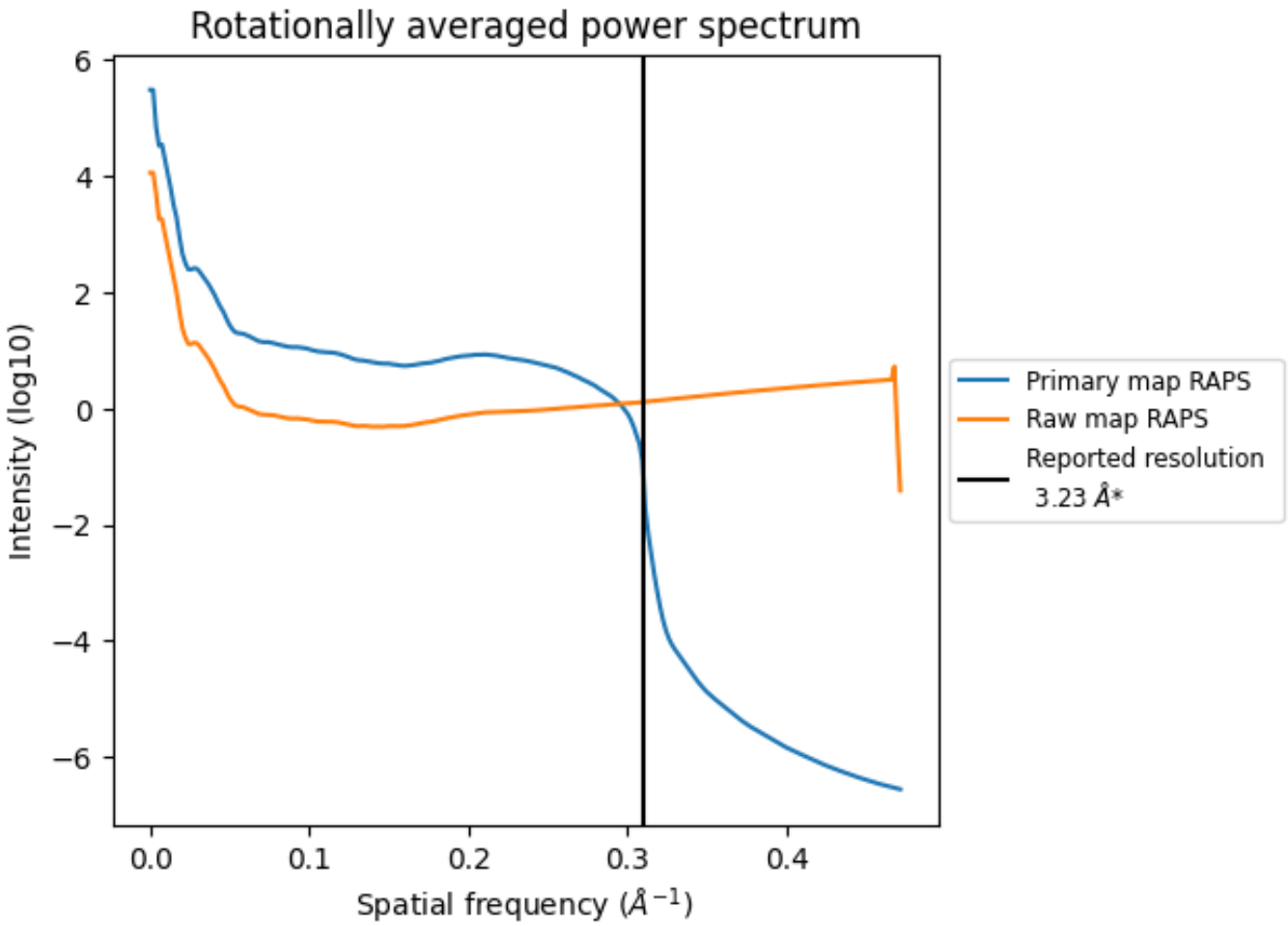
7.2 Volume estimate (i)



The volume at the recommended contour level is 27 nm^3; this corresponds to an approximate mass of 24 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)

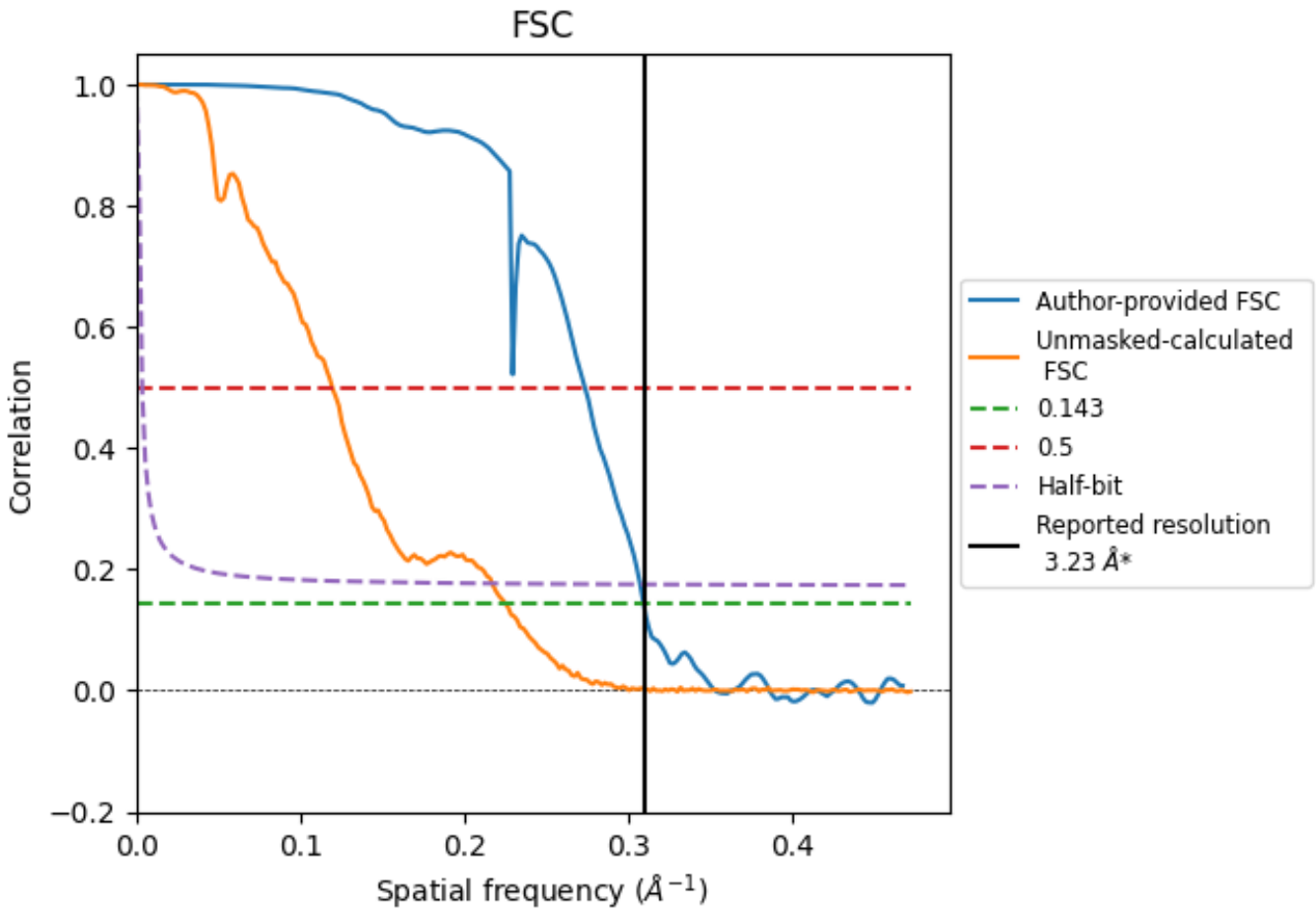


*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

8.2 Resolution estimates (i)

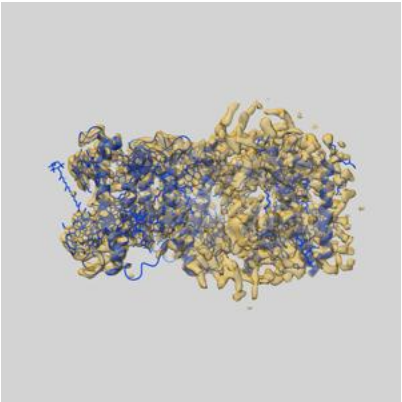
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.23	3.66	3.26
Unmasked-calculated*	4.44	8.37	4.61

*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 4.44 differs from the reported value 3.23 by more than 10 %

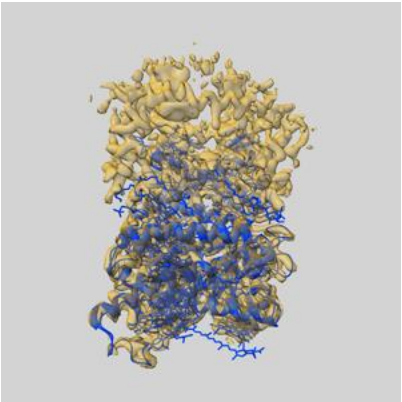
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37267 and PDB model 8W4O. Per-residue inclusion information can be found in section 3 on page 11.

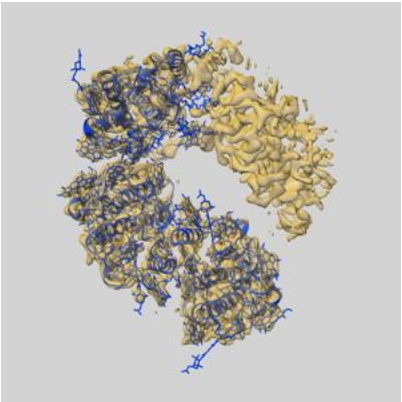
9.1 Map-model overlay (i)



X



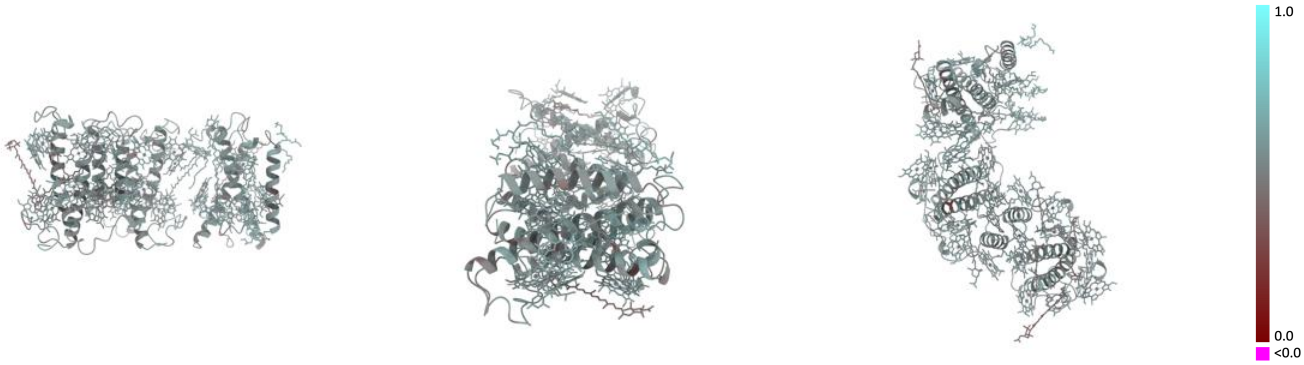
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.313 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

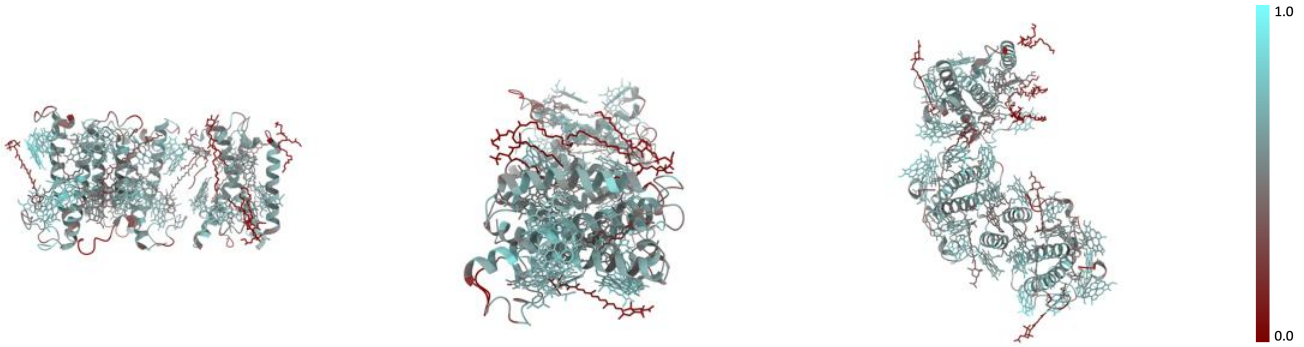
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

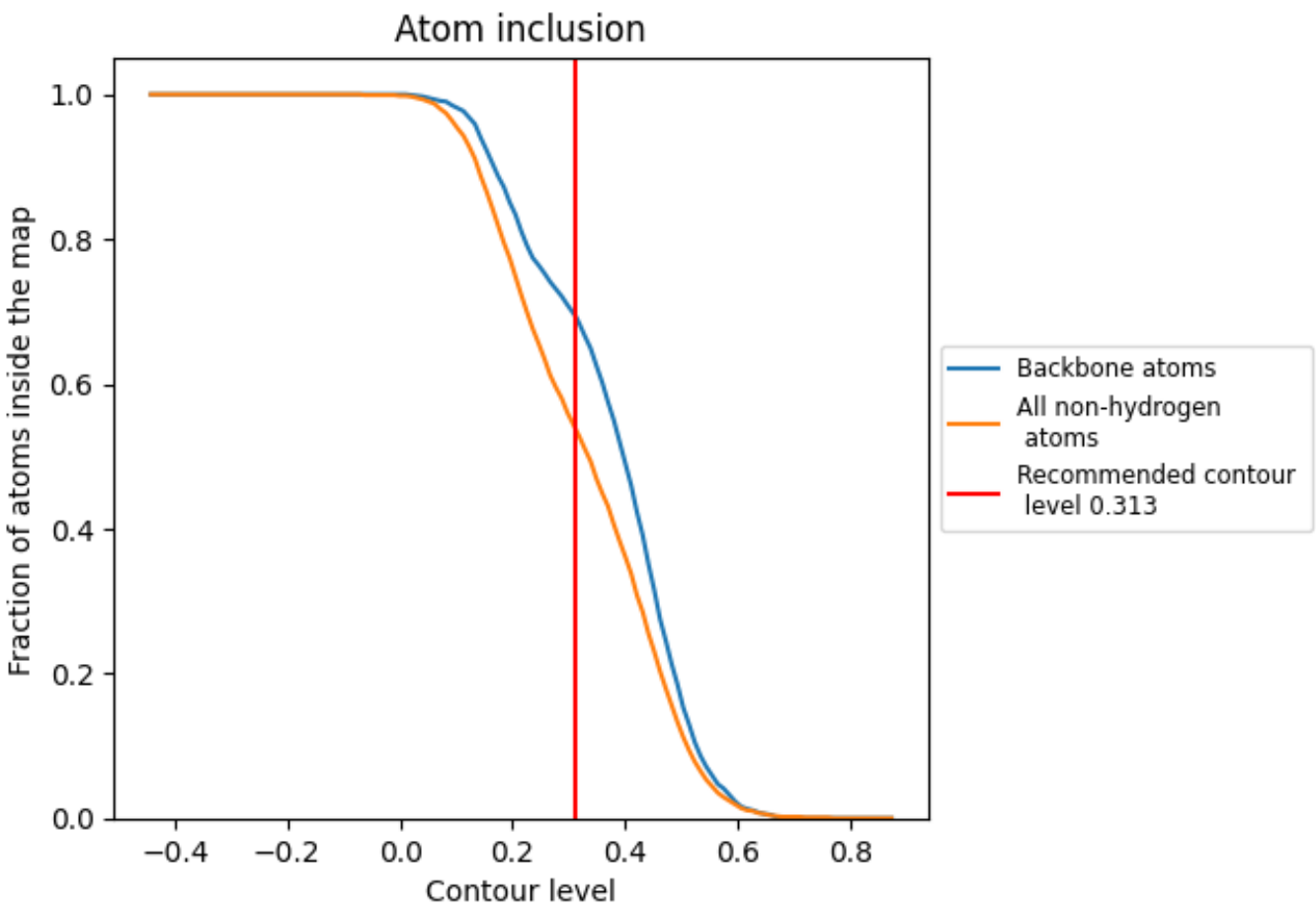
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.313).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.313) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5360	0.5310
5	0.5040	0.5380
6	0.5690	0.5340
7	0.5380	0.5200