wwPDB EM Validation Summary Report (i)

Aug 5, 2026 – 08:12 PM JST

PDB ID	:	8J0D / pdb_00008j0d
EMDB ID	:	EMD-35899
Title	:	FCP heterodimer, Lhca2, and Lhcf5 together as the M1 side binds to the PSII core in the diatom Thalassiosira pseudonana
Authors	:	Li, Z.; Feng, Y.; Wang, W.; Shen, J.R.
Deposited on	:	2023-04-10
Resolution	:	3.19 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:

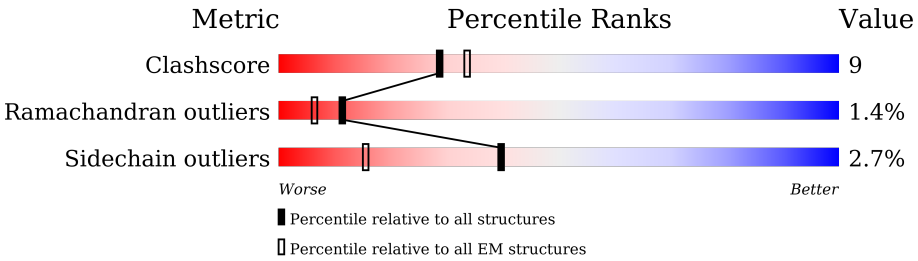
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

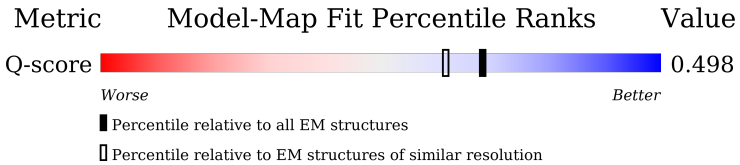
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.19 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	14455 (2.69 - 3.69)

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	3	220	14% 87% 11% •
2	4	163	• 87% 13% •
3	5	160	7% 76% 20% •
4	6	168	18% 77% 21% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	5	314	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 9105 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 Fucoxanthin chl a/c protein, lhca clade.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3	220	1710	1110	281	315	4	0	0

- Molecule 2 is a protein called Fucoxanthin-chlorophyll a-c binding protein, plastid.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	4	163	1249	809	204	232	4	0	0

- Molecule 3 is a protein called Fucoxanthin chlorophyll a/c protein 6.

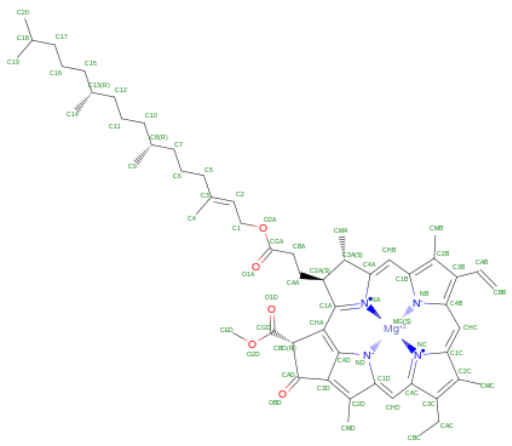
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	5	160	1229	780	217	227	5	0	0

- Molecule 4 is a protein called Fucoxanthin chlorophyll a/c protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	6	168	1296	833	219	238	6	0	0

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).

CLA



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	3	1	65	55	1	4	5	0
5	3	1	65	55	1	4	5	0
5	3	1	65	55	1	4	5	0
5	3	1	48	38	1	4	5	0
5	3	1	65	55	1	4	5	0
5	3	1	65	55	1	4	5	0
5	3	1	65	55	1	4	5	0
5	3	1	51	41	1	4	5	0
5	3	1	41	33	1	4	3	0
5	3	1	56	46	1	4	5	0
5	3	1	61	51	1	4	5	0
5	3	1	55	45	1	4	5	0
5	4	1	55	45	1	4	5	0
5	4	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
5	4	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
5	4	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
5	4	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
5	4	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
5	4	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
5	4	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
5	4	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
5	4	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
5	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
5	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
5	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
5	5	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
5	5	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
5	5	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
5	5	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
5	5	1	38	32	1	4	1	0
			Total	C	Mg	N	O	
5	6	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
5	6	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
5	6	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
5	6	1	46	36	1	4	5	0

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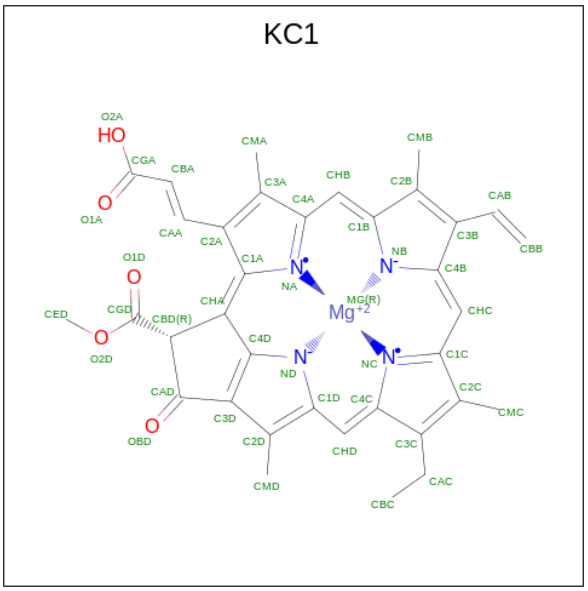
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
5	6	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
5	6	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
5	6	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
5	6	1	39	30	1	4	4	0

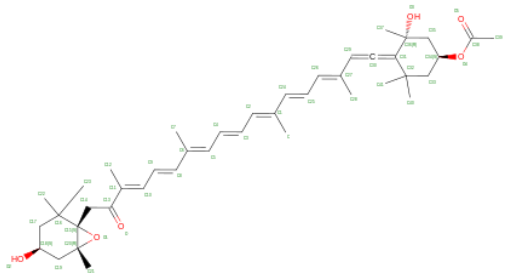
- Molecule 6 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
6	3	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
6	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
6	6	1	45	35	1	4	5	0

- Molecule 7 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	
7	3	1	48	42	6	0
7	4	1	48	42	6	0
7	4	1	48	42	6	0
7	4	1	48	42	6	0
7	5	1	48	42	6	0
7	5	1	48	42	6	0
7	5	1	48	42	6	0
7	5	1	48	42	6	0
7	5	1	47	41	6	0
7	5	1	48	42	6	0
7	5	1	48	42	6	0
7	5	1	48	42	6	0
7	6	1	48	42	6	0
7	6	1	48	42	6	0

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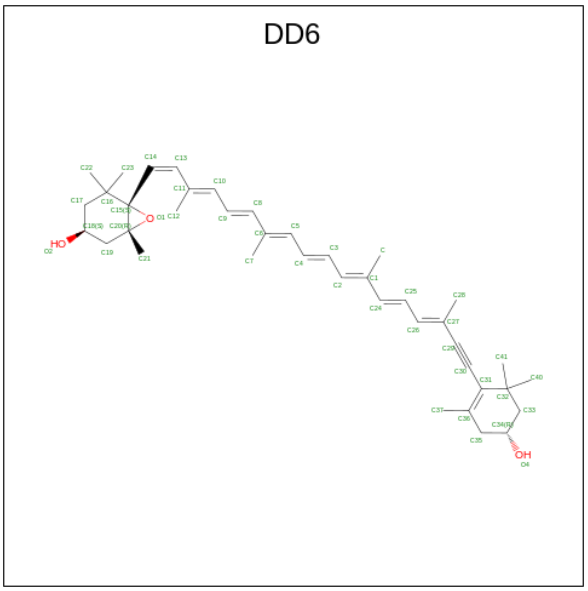
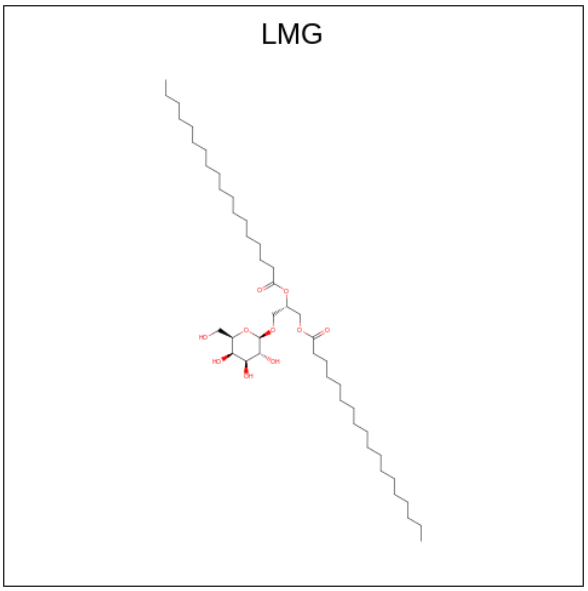
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
7	6	1	48	42	6	0
			Total	C	O	
7	6	1	48	42	6	0
			Total	C	O	
7	6	1	48	42	6	0

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



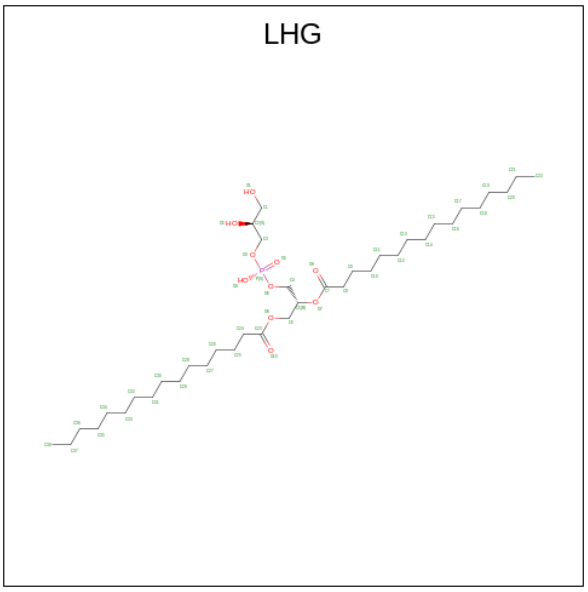
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	3	1	43	40	3	0
			Total	C	O	
8	4	1	43	40	3	0

- Molecule 9 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



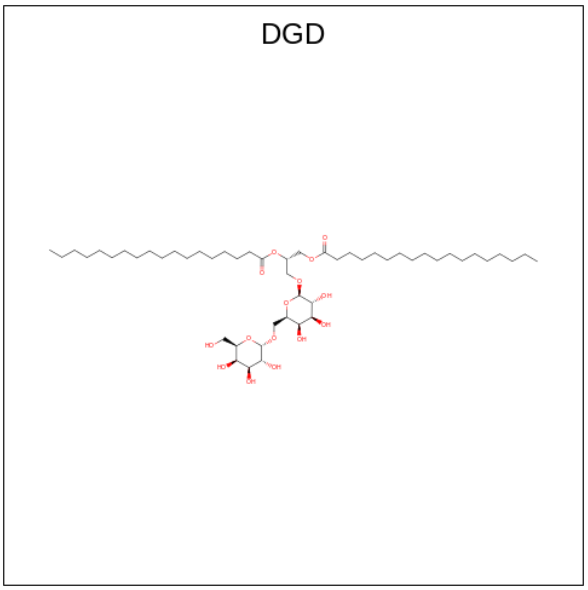
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	3	1	31	21	10	0
			Total	C	O	
9	3	1	23	13	10	0
			Total	C	O	
9	5	1	31	21	10	0

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



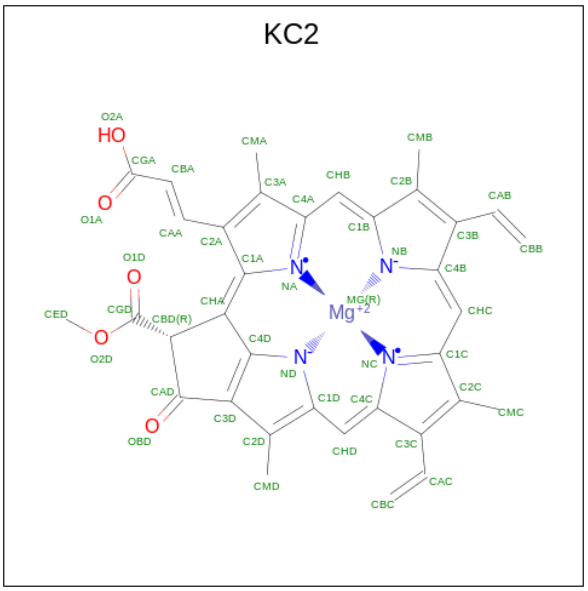
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	3	1	27	16	10	1	0
10	3	1	49	38	10	1	0
10	4	1	49	38	10	1	0
10	5	1	33	24	8	1	0

- Molecule 11 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



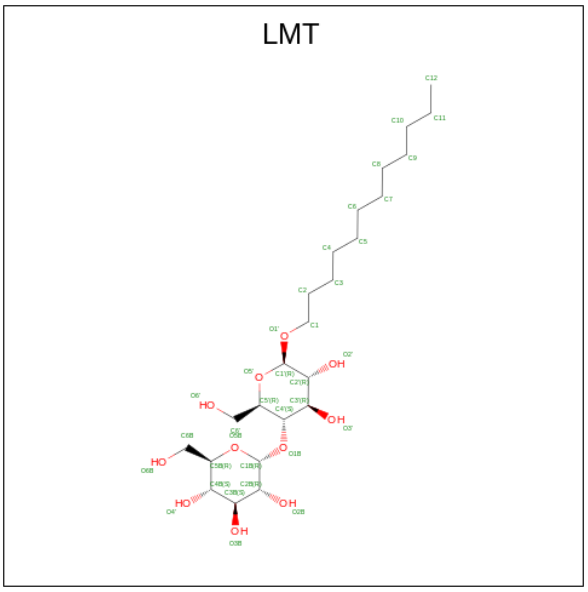
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	3	1	39	34	5	0

- Molecule 12 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	4	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
12	5	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
12	6	1	45	35	1	4	5	0

- Molecule 13 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



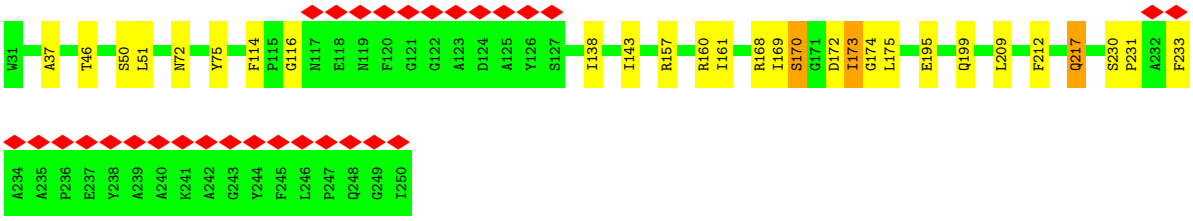
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	4	1	35	24	11	0
			Total	C	O	
13	5	1	31	20	11	0

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: Fucoxanthin chl a/c protein, lhca clade

Chain 3:

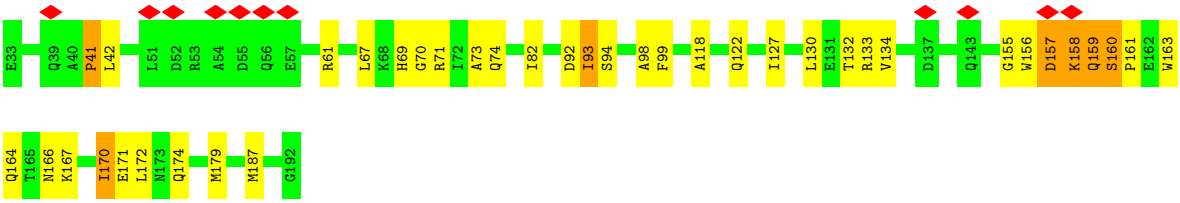


- Molecule 2: Fucoxanthin-chlorophyll a-c binding protein, plastid

Chain 4:

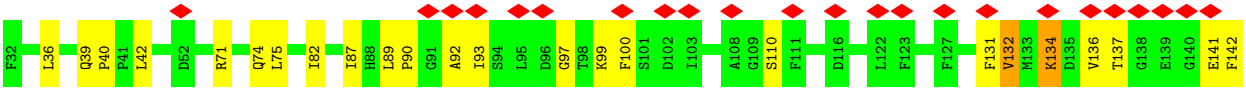
- Molecule 3: Fucoxanthin chlorophyll a/c protein 6

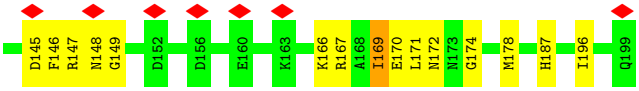
Chain 5:



- Molecule 4: Fucoxanthin chlorophyll a/c protein 5

Chain 6:




D145
F146
R147
N148
G149
D152
D156
E160
K163
K166
R167
A168
I169
E170
L171
N172
N173
G174
M178
H187
I196
Q199

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97098	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.598	Depositor
Minimum map value	-0.249	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	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: DD6, LHG, DGD, KC2, CLA, KC1, LMG, A86, LMT

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	3	0.20	0/1765	0.37	0/2405
2	4	0.26	0/1282	0.42	0/1746
3	5	0.22	0/1255	0.48	1/1696 (0.1%)
4	6	0.22	0/1324	0.40	0/1780
All	All	0.22	0/5626	0.41	1/7627 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	5	41	PRO	N-CA-CB	7.68	111.32	103.25

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	3	1710	0	1624	19	0
2	4	1249	0	1219	16	0
3	5	1229	0	1184	47	0
4	6	1296	0	1268	27	0
5	3	702	0	698	27	0
5	4	603	0	556	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	5	401	0	340	33	0
5	6	396	0	328	11	0
6	3	45	0	0	0	0
6	5	45	0	0	0	0
6	6	45	0	0	3	0
7	3	48	0	0	1	0
7	4	144	0	0	0	0
7	5	383	0	0	5	0
7	6	240	0	0	1	0
8	3	43	0	0	0	0
8	4	43	0	0	0	0
9	3	54	0	48	1	0
9	5	31	0	32	1	0
10	3	76	0	98	3	0
10	4	49	0	74	2	0
10	5	33	0	42	0	0
11	3	39	0	62	1	0
12	4	45	0	0	0	0
12	5	45	0	0	3	0
12	6	45	0	0	1	0
13	4	35	0	45	0	0
13	5	31	0	34	0	0
All	All	9105	0	7652	157	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 9.

The worst 5 of 157 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)
3:5:156:TRP:CE3	5:5:314:CLA:HBA1	1.79	1.16
3:5:156:TRP:HE3	5:5:314:CLA:HBA1	1.06	1.13
3:5:167:LYS:CD	5:5:314:CLA:HMA3	1.82	1.07
3:5:167:LYS:CE	5:5:314:CLA:HMA3	1.91	1.00
3:5:156:TRP:HE3	5:5:314:CLA:CBA	1.78	0.95

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	218/220 (99%)	196 (90%)	19 (9%)	3 (1%)	9	39
2	4	161/163 (99%)	143 (89%)	16 (10%)	2 (1%)	10	42
3	5	158/160 (99%)	141 (89%)	14 (9%)	3 (2%)	6	33
4	6	166/168 (99%)	148 (89%)	16 (10%)	2 (1%)	10	42
All	All	703/711 (99%)	628 (89%)	65 (9%)	10 (1%)	11	39

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	173	ILE
3	5	41	PRO
2	4	54	ILE
3	5	157	ASP
4	6	196	ILE

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	3	171/171 (100%)	169 (99%)	2 (1%)	63	79
2	4	128/129 (99%)	127 (99%)	1 (1%)	73	82
3	5	120/123 (98%)	114 (95%)	6 (5%)	22	55
4	6	131/131 (100%)	125 (95%)	6 (5%)	24	58
All	All	550/554 (99%)	535 (97%)	15 (3%)	40	68

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	5	170	ILE
4	6	170	GLU
3	5	172	LEU
4	6	171	LEU
4	6	136	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	3	248	GLN
2	4	56	GLN
3	5	173	ASN
1	3	99	GLN
1	3	71	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)

74 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	$\#\|Z\| > 2$
5	CLA	5	312	3	50,54,73	1.46	10 (20%)	60,90,113	1.41	6 (10%)
5	CLA	3	601	-	69,73,73	1.25	10 (14%)	83,113,113	1.33	6 (7%)
7	A86	5	306	-	44,50,50	1.24	4 (9%)	51,76,76	7.71	25 (49%)
7	A86	6	305	-	44,50,50	1.21	3 (6%)	51,76,76	8.91	23 (45%)
5	CLA	5	314	3	59,63,73	1.37	8 (13%)	71,101,113	1.41	6 (8%)
9	LMG	3	615	-	31,31,55	0.97	0	39,39,63	1.28	5 (12%)
5	CLA	3	607	1	69,73,73	1.25	10 (14%)	83,113,113	1.31	9 (10%)
5	CLA	4	314	2	60,64,73	1.33	9 (15%)	72,102,113	1.36	8 (11%)
7	A86	4	301	-	44,50,50	1.25	4 (9%)	51,76,76	9.56	27 (52%)
13	LMT	4	317	-	36,36,36	1.19	6 (16%)	47,47,47	1.00	1 (2%)
5	CLA	5	308	-	50,54,73	1.45	8 (16%)	60,90,113	1.42	4 (6%)
5	CLA	6	311	4	69,73,73	1.26	8 (11%)	83,113,113	1.23	4 (4%)
5	CLA	5	309	3	59,63,73	1.34	10 (16%)	71,101,113	1.40	8 (11%)
5	CLA	4	305	-	59,63,73	1.34	10 (16%)	71,101,113	1.38	6 (8%)
5	CLA	3	612	-	65,69,73	1.28	9 (13%)	78,108,113	1.30	5 (6%)
6	KC1	5	315	3	49,53,53	1.43	7 (14%)	63,89,89	1.99	14 (22%)
5	CLA	4	311	2	64,68,73	1.29	10 (15%)	77,107,113	1.33	9 (11%)
7	A86	5	307	-	44,50,50	1.23	4 (9%)	51,76,76	11.49	23 (45%)
7	A86	6	303	-	44,50,50	1.24	4 (9%)	51,76,76	8.48	24 (47%)
8	DD6	3	614	-	39,45,45	1.99	3 (7%)	52,67,67	1.98	15 (28%)
5	CLA	3	611	-	60,64,73	1.35	10 (16%)	72,102,113	1.38	7 (9%)
7	A86	5	304	-	44,50,50	1.22	3 (6%)	51,76,76	11.21	23 (45%)
13	LMT	5	320	-	32,32,36	1.23	5 (15%)	43,43,47	0.93	1 (2%)
11	DGD	3	620	-	38,38,67	0.65	1 (2%)	40,40,81	1.48	6 (15%)
5	CLA	3	602	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
12	KC2	4	307	2	49,53,53	1.72	9 (18%)	62,89,89	2.38	19 (30%)
5	CLA	6	307	4	58,62,73	1.36	10 (17%)	69,99,113	1.37	5 (7%)
12	KC2	5	310	3	49,53,53	1.72	10 (20%)	62,89,89	2.36	19 (30%)
6	KC1	6	313	4	49,53,53	1.38	7 (14%)	63,89,89	1.95	14 (22%)
5	CLA	4	306	2	69,73,73	1.25	10 (14%)	83,113,113	1.28	6 (7%)
5	CLA	5	313	-	69,73,73	1.25	9 (13%)	83,113,113	1.26	7 (8%)
5	CLA	5	317	-	41,46,73	1.56	8 (19%)	51,80,113	1.58	6 (11%)
5	CLA	3	610	1	45,49,73	1.47	10 (22%)	54,84,113	1.58	6 (11%)
5	CLA	6	312	4	50,54,73	1.46	8 (16%)	60,90,113	1.50	8 (13%)
5	CLA	4	315	-	51,55,73	1.44	10 (19%)	61,91,113	1.42	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	CLA	4	312	2	55,59,73	1.40	9 (16%)	66,96,113	1.49	9 (13%)
5	CLA	3	605	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	7 (8%)
10	LHG	3	617	5	26,26,48	0.85	1 (3%)	29,32,54	1.38	3 (10%)
6	KC1	3	609	1	49,53,53	1.42	7 (14%)	63,89,89	2.01	12 (19%)
9	LMG	5	319	-	31,31,55	0.96	1 (3%)	39,39,63	1.34	6 (15%)
5	CLA	6	314	4	45,49,73	1.54	9 (20%)	54,84,113	1.75	8 (14%)
5	CLA	3	604	-	52,56,73	1.41	10 (19%)	62,92,113	1.43	7 (11%)
7	A86	6	301	-	44,50,50	1.25	5 (11%)	51,76,76	11.60	24 (47%)
7	A86	5	305	-	43,49,50	1.42	5 (11%)	48,74,76	7.05	25 (52%)
7	A86	5	302	-	44,50,50	1.25	5 (11%)	51,76,76	12.11	24 (47%)
12	KC2	6	308	-	49,53,53	1.80	9 (18%)	62,89,89	2.27	21 (33%)
5	CLA	4	308	-	69,73,73	1.24	10 (14%)	83,113,113	1.31	5 (6%)
7	A86	3	613	-	44,50,50	1.25	3 (6%)	51,76,76	2.32	17 (33%)
5	CLA	6	306	-	57,61,73	1.37	8 (14%)	68,98,113	1.41	6 (8%)
5	CLA	5	311	-	59,63,73	1.34	8 (13%)	71,101,113	1.37	5 (7%)
7	A86	5	301	-	44,50,50	1.24	4 (9%)	51,76,76	11.32	26 (50%)
7	A86	5	321	-	44,50,50	1.25	4 (9%)	51,76,76	9.10	23 (45%)
7	A86	6	302	-	44,50,50	1.19	3 (6%)	51,76,76	11.15	25 (49%)
5	CLA	6	315	-	40,46,73	1.72	7 (17%)	52,79,113	1.60	9 (17%)
5	CLA	3	608	10	55,59,73	1.41	9 (16%)	66,96,113	1.37	6 (9%)
10	LHG	3	618	-	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
7	A86	4	302	-	44,50,50	1.24	4 (9%)	51,76,76	12.51	28 (54%)
5	CLA	5	316	-	45,49,73	1.52	8 (17%)	54,84,113	1.52	8 (14%)
7	A86	6	304	-	44,50,50	1.24	3 (6%)	51,76,76	11.87	21 (41%)
5	CLA	3	603	1	69,73,73	1.25	10 (14%)	83,113,113	1.26	7 (8%)
9	LMG	3	616	-	23,23,55	1.25	3 (13%)	31,31,63	1.31	5 (16%)
5	CLA	4	310	-	50,54,73	1.43	9 (18%)	60,90,113	1.42	6 (10%)
5	CLA	4	313	2	45,49,73	1.48	9 (20%)	54,84,113	1.53	7 (12%)
7	A86	5	303	-	44,50,50	1.23	3 (6%)	51,76,76	11.73	23 (45%)
5	CLA	4	309	2	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
10	LHG	4	318	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
5	CLA	3	619	-	59,63,73	1.33	10 (16%)	71,101,113	1.37	6 (8%)
8	DD6	4	303	-	39,45,45	2.02	3 (7%)	52,67,67	2.77	15 (28%)
10	LHG	5	318	-	32,32,48	0.83	2 (6%)	36,37,54	1.70	6 (16%)
5	CLA	6	310	4	50,54,73	1.47	8 (16%)	60,90,113	1.31	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CLA	3	606	1	69,73,73	1.25	10 (14%)	83,113,113	1.26	6 (7%)
5	CLA	4	316	-	56,60,73	1.38	10 (17%)	67,97,113	1.41	6 (8%)
5	CLA	6	309	-	56,60,73	1.38	8 (14%)	67,97,113	1.40	7 (10%)
7	A86	4	304	-	44,50,50	1.26	5 (11%)	51,76,76	11.03	27 (52%)

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
5	CLA	5	312	3	-	11/17/93/115	-
5	CLA	3	601	-	-	17/39/115/115	-
7	A86	5	306	-	-	8/34/90/90	0/3/3/3
7	A86	6	305	-	-	8/34/90/90	0/3/3/3
5	CLA	5	314	3	-	9/27/103/115	-
9	LMG	3	615	-	-	8/26/46/70	0/1/1/1
5	CLA	3	607	1	-	15/39/115/115	-
5	CLA	4	314	2	-	9/29/105/115	-
7	A86	4	301	-	-	10/34/90/90	0/3/3/3
13	LMT	4	317	-	-	11/21/61/61	0/2/2/2
5	CLA	5	308	-	-	7/17/93/115	-
5	CLA	6	311	4	-	7/39/115/115	-
5	CLA	5	309	3	-	6/27/103/115	-
5	CLA	4	305	-	-	9/27/103/115	-
5	CLA	3	612	-	-	16/35/111/115	-
6	KC1	5	315	3	-	6/15/71/71	-
5	CLA	4	311	2	-	15/33/109/115	-
7	A86	5	307	-	-	8/34/90/90	0/3/3/3
7	A86	6	303	-	-	8/34/90/90	0/3/3/3
8	DD6	3	614	-	-	5/26/80/80	0/3/3/3
5	CLA	3	611	-	-	9/29/105/115	-
7	A86	5	304	-	-	8/34/90/90	0/3/3/3
13	LMT	5	320	-	-	8/17/57/61	0/2/2/2
11	DGD	3	620	-	-	22/40/40/95	-
5	CLA	3	602	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	KC2	4	307	2	-	8/15/71/71	-
5	CLA	6	307	4	-	5/26/102/115	-
12	KC2	5	310	3	-	3/15/71/71	-
6	KC1	6	313	4	-	5/15/71/71	-
5	CLA	4	306	2	-	8/39/115/115	-
5	CLA	5	313	-	-	11/39/115/115	-
5	CLA	5	317	-	-	0/4/80/115	-
5	CLA	3	610	1	-	0/10/86/115	-
5	CLA	6	312	4	-	6/17/93/115	-
5	CLA	4	315	-	-	4/18/94/115	-
5	CLA	4	312	2	-	5/23/99/115	-
5	CLA	3	605	-	-	15/39/115/115	-
10	LHG	3	617	5	-	13/31/31/53	-
6	KC1	3	609	1	-	9/15/71/71	-
9	LMG	5	319	-	-	13/26/46/70	0/1/1/1
5	CLA	6	314	4	-	0/10/86/115	-
5	CLA	3	604	-	-	9/19/95/115	-
7	A86	6	301	-	-	7/34/90/90	0/3/3/3
7	A86	5	305	-	-	8/33/89/90	0/3/3/3
7	A86	5	302	-	-	9/34/90/90	0/3/3/3
12	KC2	6	308	-	-	10/15/71/71	-
5	CLA	4	308	-	-	9/39/115/115	-
7	A86	3	613	-	-	5/34/90/90	0/3/3/3
5	CLA	6	306	-	-	8/25/101/115	-
5	CLA	5	311	-	-	8/27/103/115	-
7	A86	5	301	-	-	11/34/90/90	0/3/3/3
7	A86	5	321	-	-	8/34/90/90	0/3/3/3
7	A86	6	302	-	-	8/34/90/90	0/3/3/3
5	CLA	6	315	-	-	3/8/80/115	-
5	CLA	3	608	10	-	8/23/99/115	-
10	LHG	3	618	-	-	15/53/53/53	-
7	A86	4	302	-	-	9/34/90/90	0/3/3/3
5	CLA	5	316	-	-	2/10/86/115	-
7	A86	6	304	-	-	9/34/90/90	0/3/3/3
5	CLA	3	603	1	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LMG	3	616	-	-	6/16/36/70	0/1/1/1
5	CLA	4	310	-	-	6/17/93/115	-
5	CLA	4	313	2	-	4/10/86/115	-
7	A86	5	303	-	-	9/34/90/90	0/3/3/3
5	CLA	4	309	2	-	5/39/115/115	-
10	LHG	4	318	-	-	34/53/53/53	-
5	CLA	3	619	-	-	10/27/103/115	-
8	DD6	4	303	-	-	3/26/80/80	0/3/3/3
10	LHG	5	318	-	-	11/34/34/53	-
5	CLA	6	310	4	-	11/17/93/115	-
5	CLA	3	606	1	-	16/39/115/115	-
5	CLA	4	316	-	-	4/24/100/115	-
5	CLA	6	309	-	-	8/24/100/115	-
7	A86	4	304	-	-	8/34/90/90	0/3/3/3

The worst 5 of 499 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	4	303	DD6	C29-C27	-8.61	1.26	1.42
8	3	614	DD6	C29-C27	-8.43	1.26	1.42
8	3	614	DD6	C30-C31	-7.71	1.26	1.42
8	4	303	DD6	C30-C31	-7.64	1.26	1.42
7	5	305	A86	O4-C38	5.70	1.45	1.33

The worst 5 of 837 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5	302	A86	C23-C16-C22	-71.42	2.02	107.37
7	6	304	A86	C23-C16-C22	-71.27	2.25	107.37
7	5	303	A86	C23-C16-C22	-70.78	2.97	107.37
7	4	302	A86	C23-C16-C22	-70.30	3.68	107.37
7	5	307	A86	C23-C16-C22	-68.89	5.75	107.37

There are no chirality outliers.

5 of 649 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	3	601	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	3	602	CLA	CHA-CBD-CGD-O1D
5	3	602	CLA	CHA-CBD-CGD-O2D
5	3	604	CLA	CHA-CBD-CGD-O1D
5	3	604	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

42 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	312	CLA	2	0
5	3	601	CLA	1	0
7	5	306	A86	1	0
5	5	314	CLA	26	0
9	3	615	LMG	1	0
5	3	607	CLA	2	0
5	4	314	CLA	4	0
5	3	612	CLA	3	0
5	4	311	CLA	1	0
5	3	611	CLA	5	0
7	5	304	A86	3	0
11	3	620	DGD	1	0
5	3	602	CLA	3	0
5	6	307	CLA	2	0
12	5	310	KC2	3	0
6	6	313	KC1	3	0
5	4	306	CLA	2	0
5	5	313	CLA	1	0
5	3	610	CLA	1	0
5	6	312	CLA	3	0
5	4	315	CLA	1	0
5	4	312	CLA	2	0
5	3	605	CLA	1	0
9	5	319	LMG	1	0
5	6	314	CLA	2	0
5	3	604	CLA	1	0
7	6	301	A86	1	0
12	6	308	KC2	1	0
5	4	308	CLA	4	0
7	3	613	A86	1	0
5	6	306	CLA	3	0
5	5	311	CLA	2	0
7	5	321	A86	1	0

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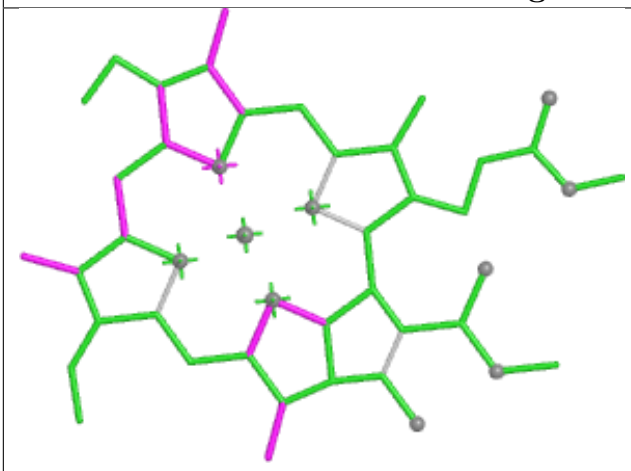
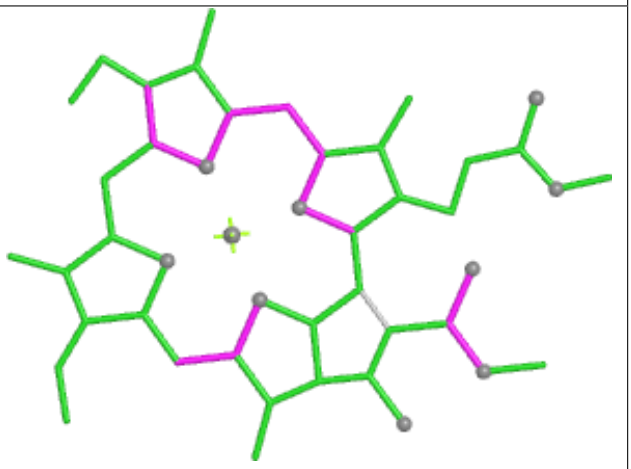
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	6	315	CLA	1	0
10	3	618	LHG	3	0
5	5	316	CLA	2	0
5	3	603	CLA	4	0
5	4	310	CLA	1	0
5	4	309	CLA	1	0
10	4	318	LHG	2	0
5	3	619	CLA	3	0
5	3	606	CLA	6	0

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.

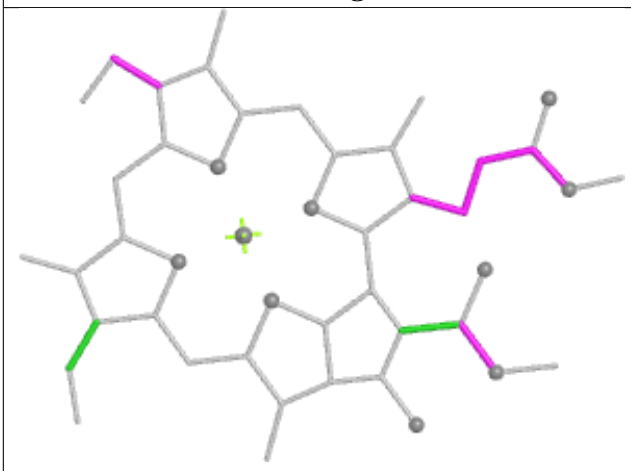
Ligand CLA 5 312



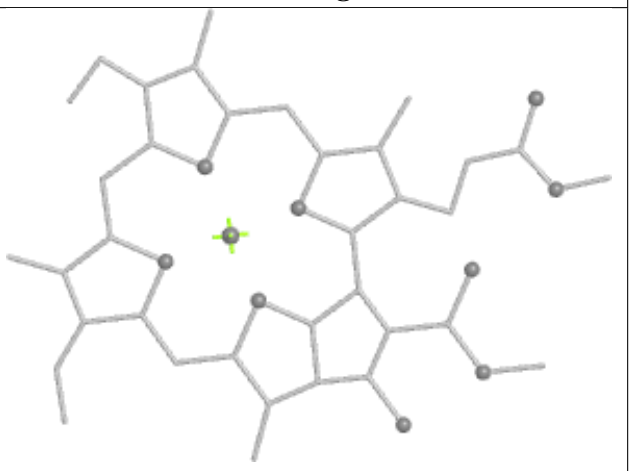
Bond lengths



Bond angles

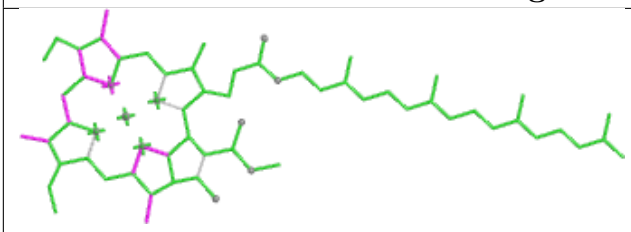


Torsions

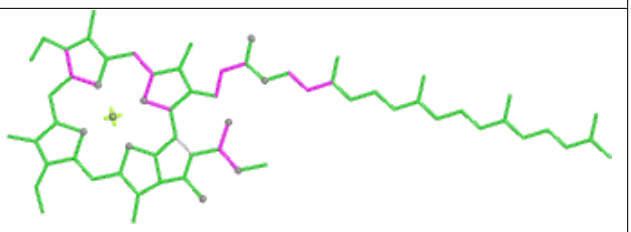


Rings

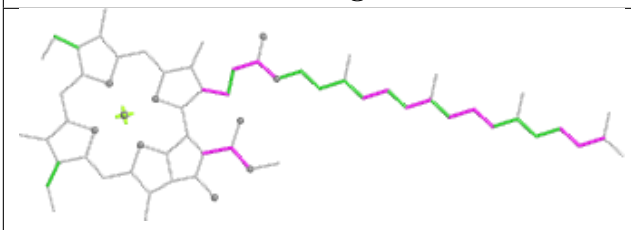
Ligand CLA 3 601



Bond lengths



Bond angles



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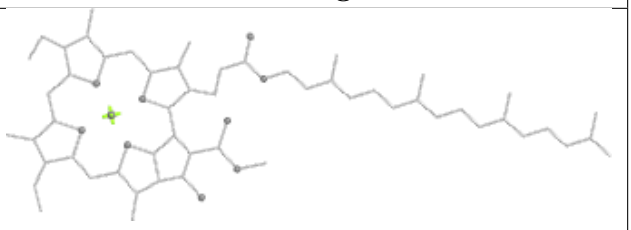
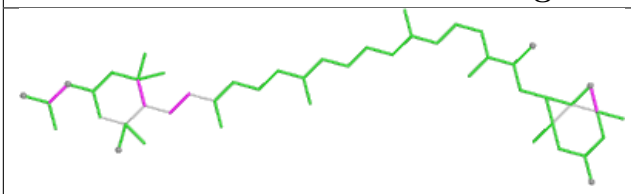
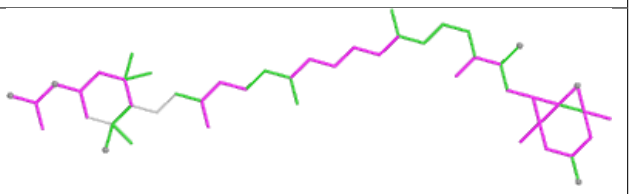
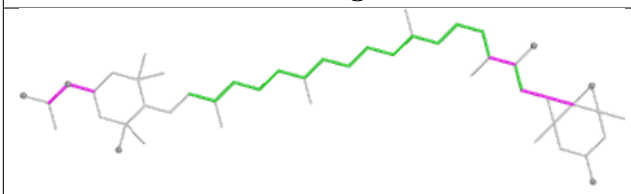
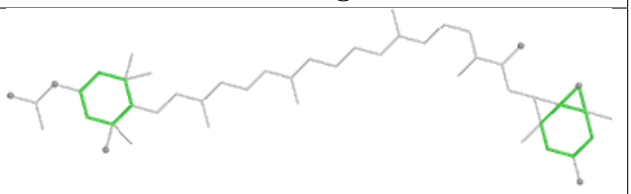
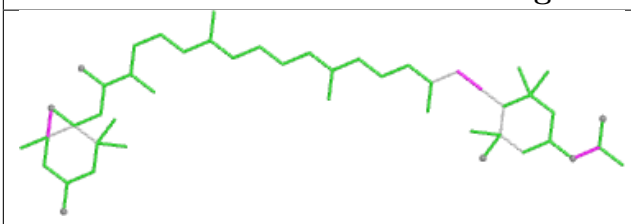
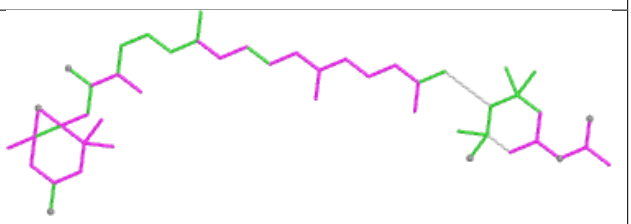
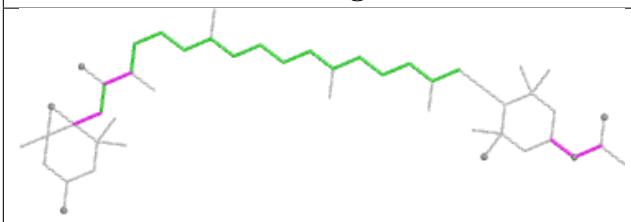
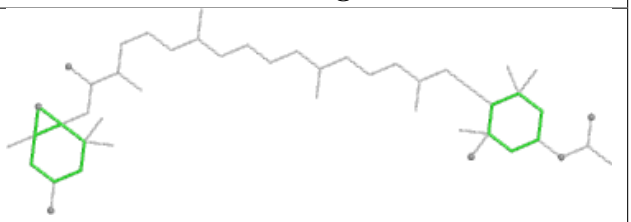
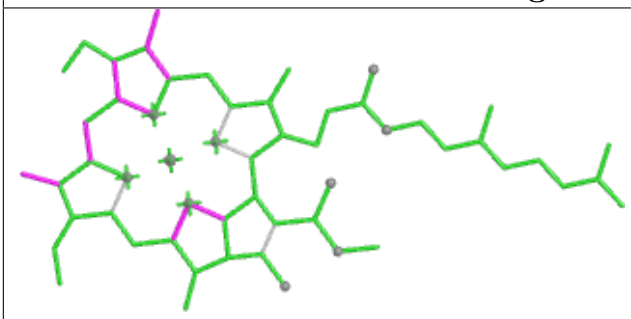
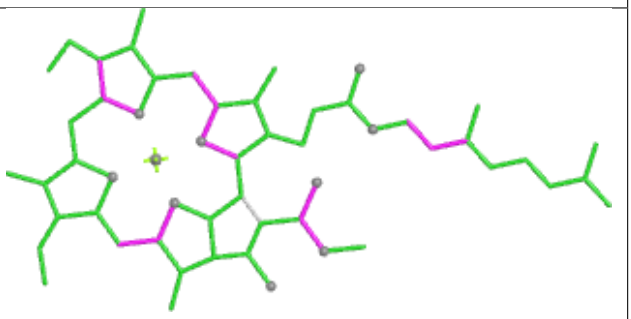
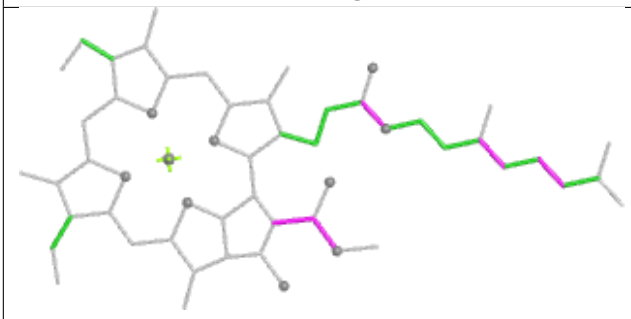
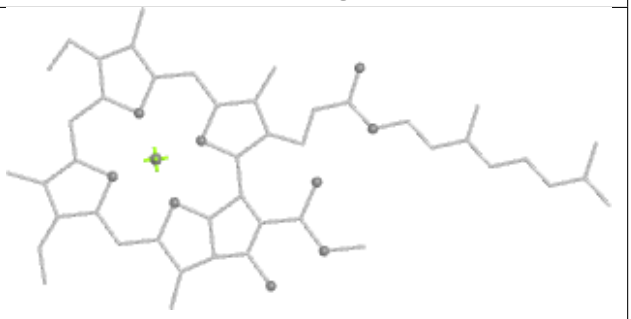


Rings

Ligand A86 5 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 6 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

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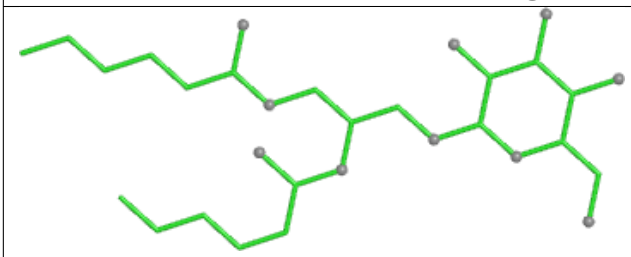
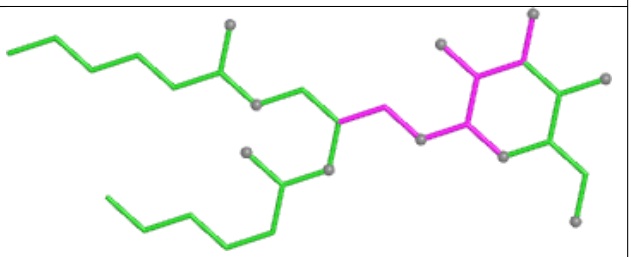
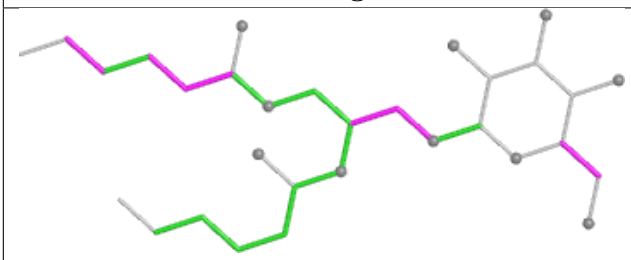
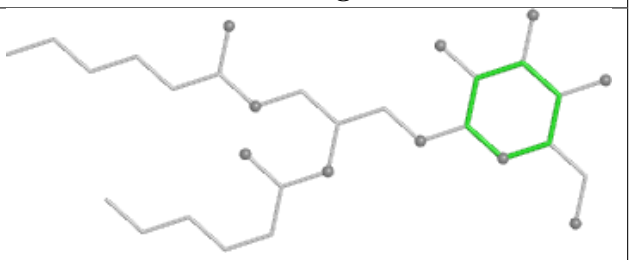
 Bond lengths	 Bond angles
 Torsions	 Rings

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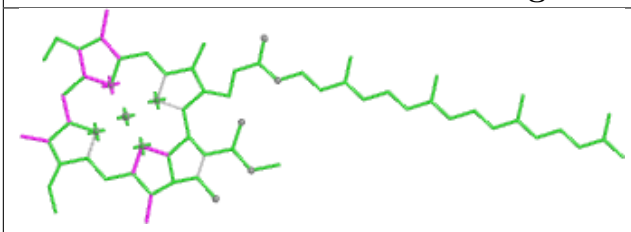
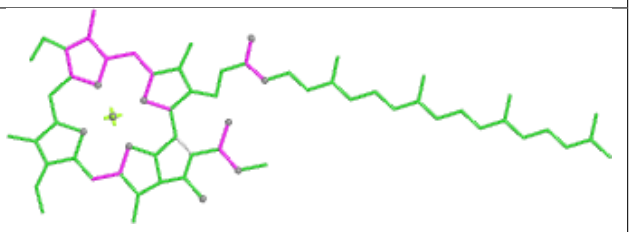
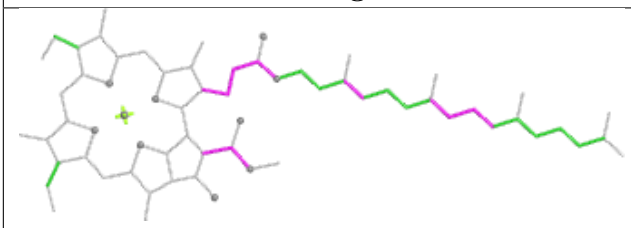
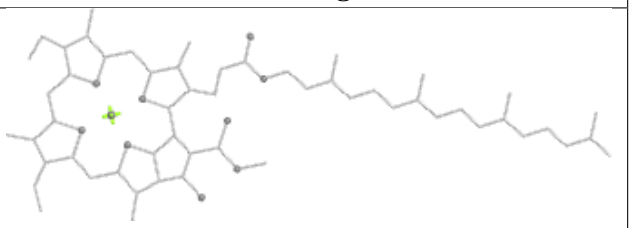
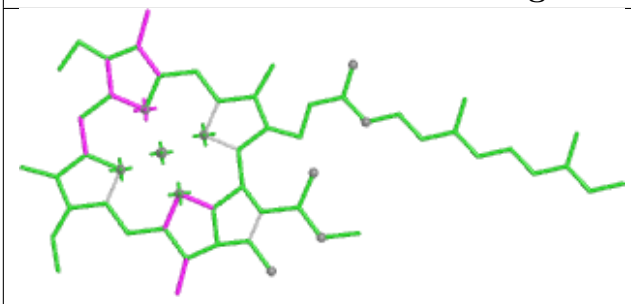
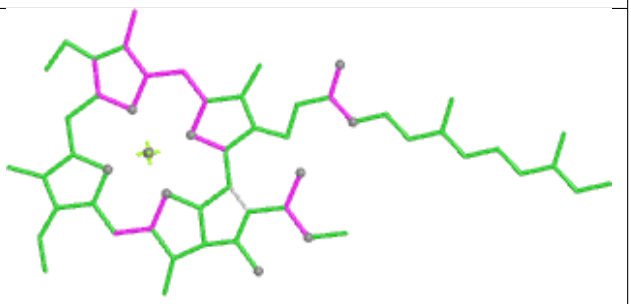
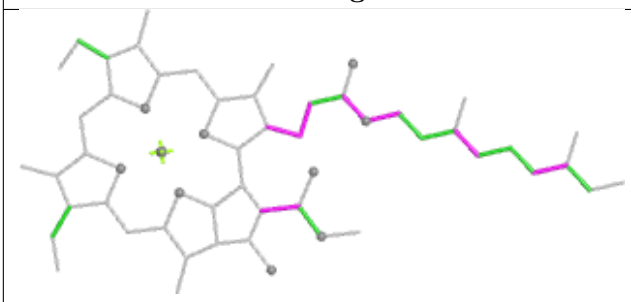
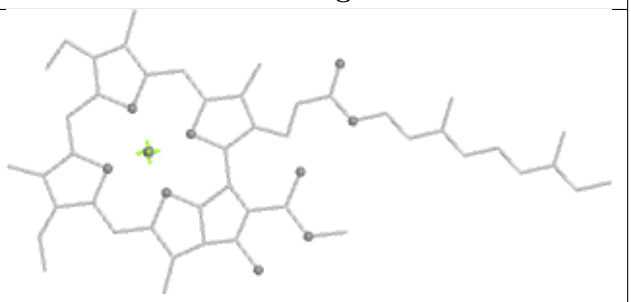
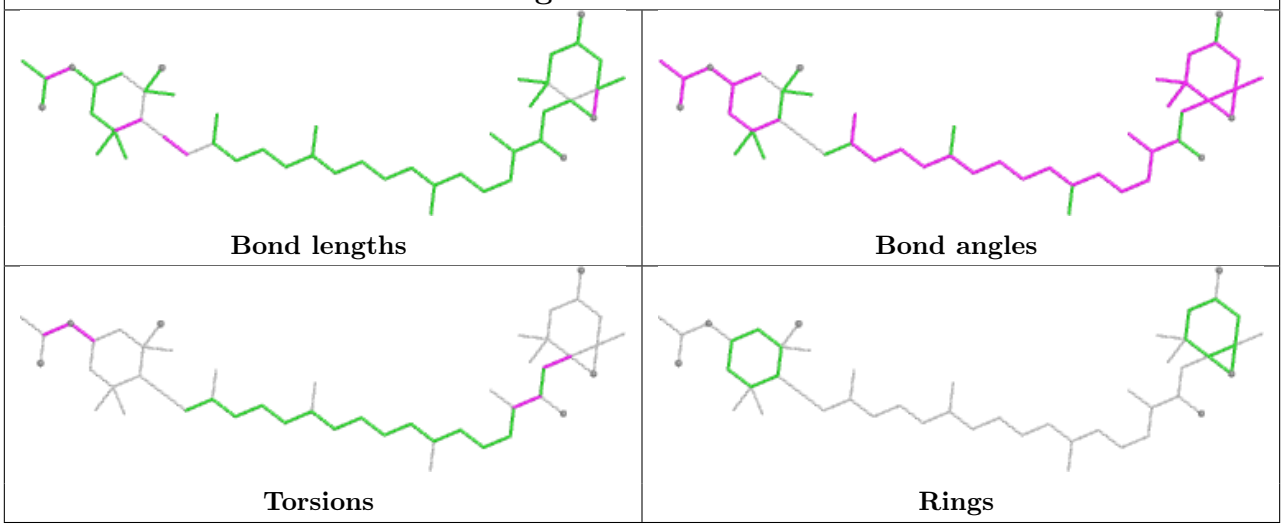
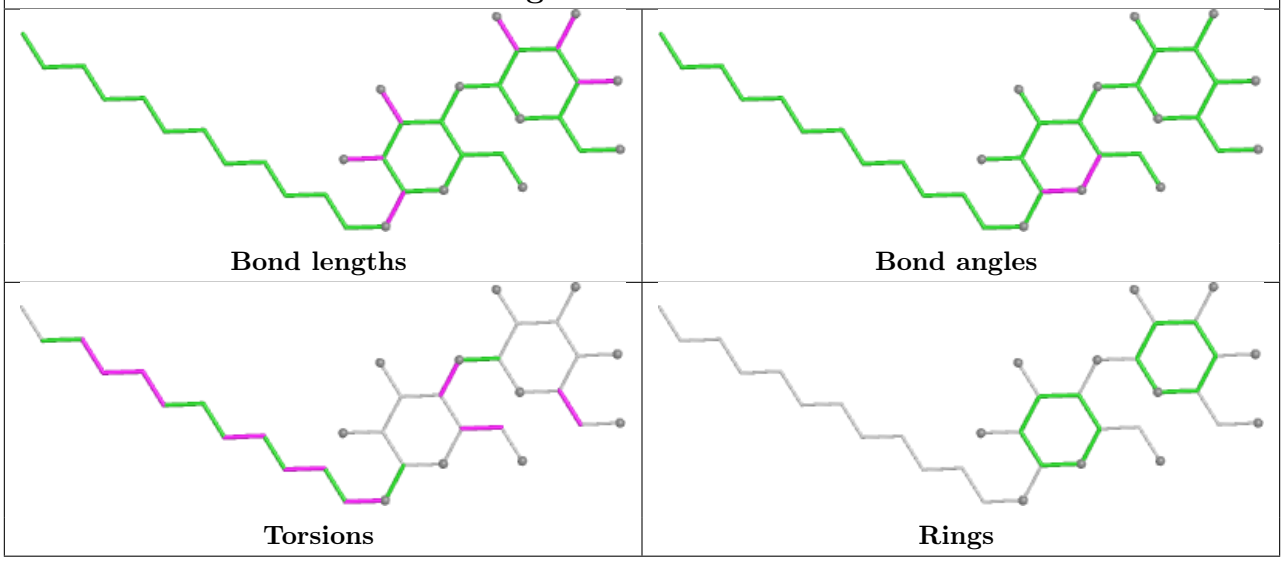
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

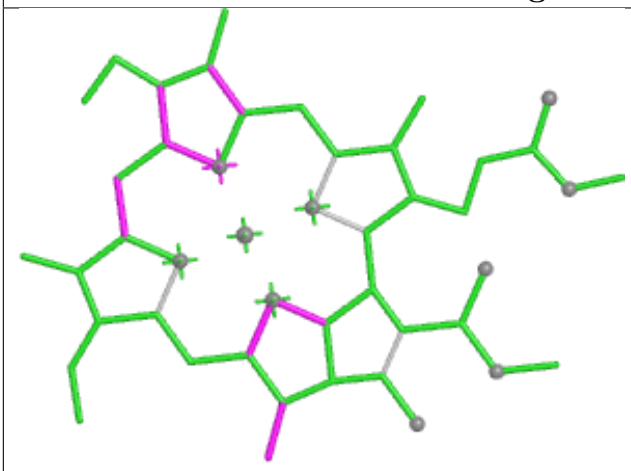
Ligand A86 4 301



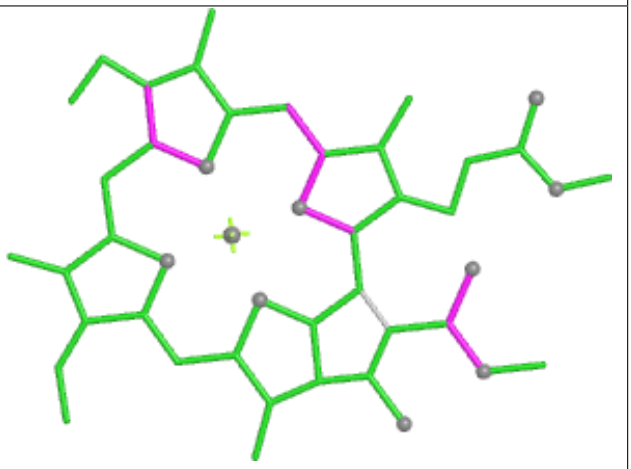
Ligand LMT 4 317



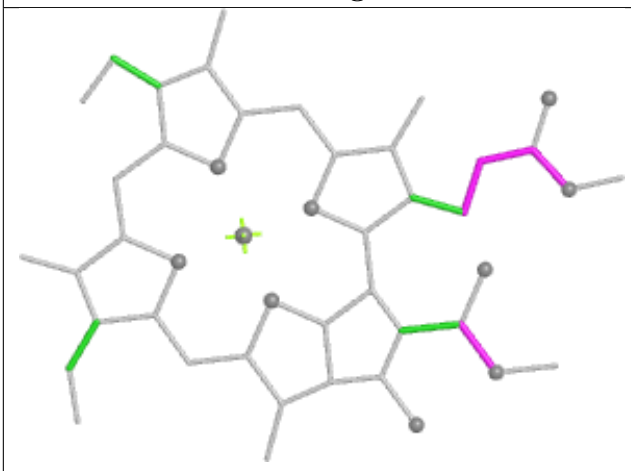
Ligand CLA 5 308



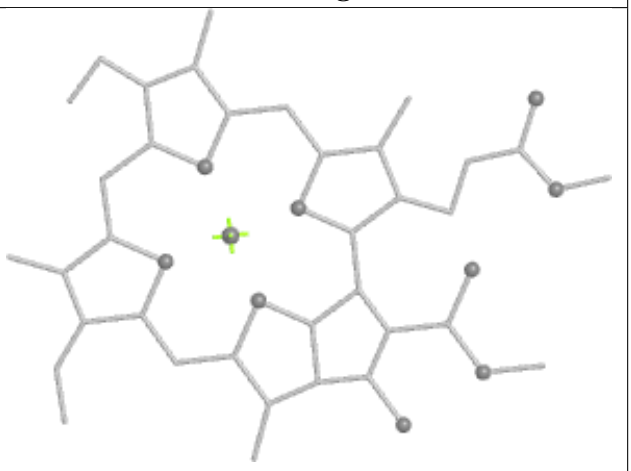
Bond lengths



Bond angles

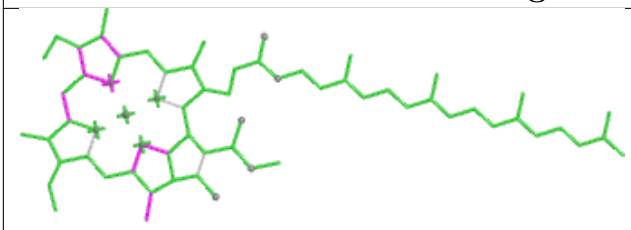


Torsions



Rings

Ligand CLA 6 311



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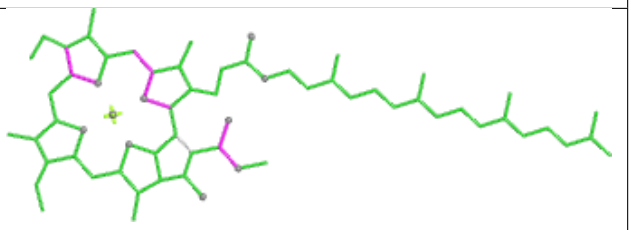

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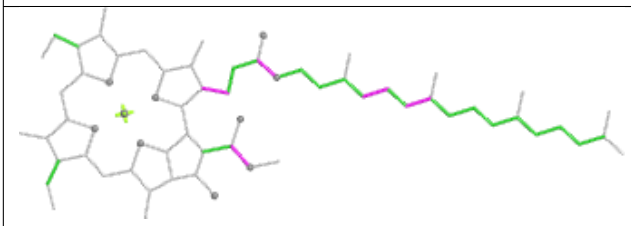

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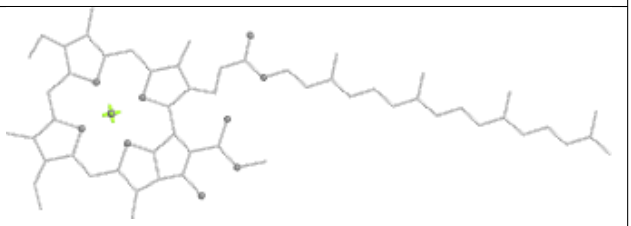
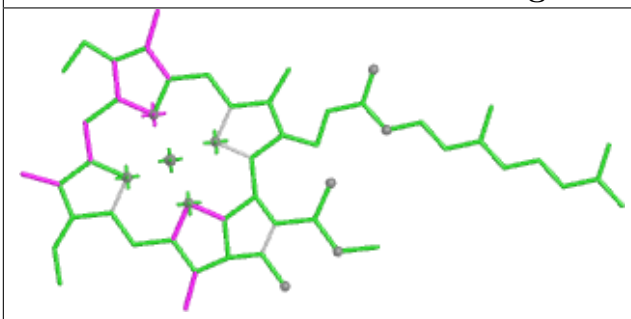
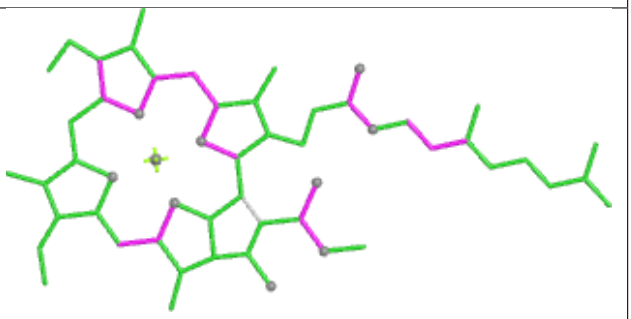
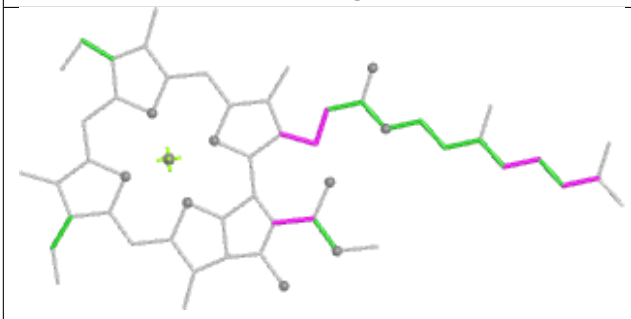
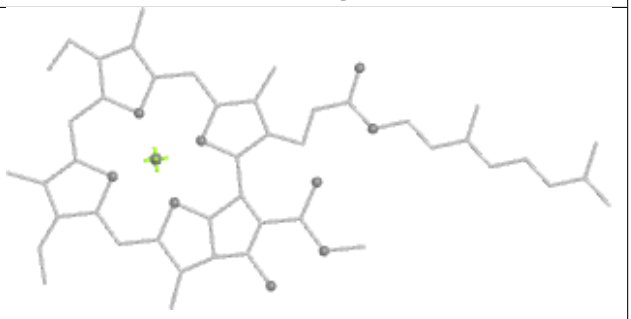
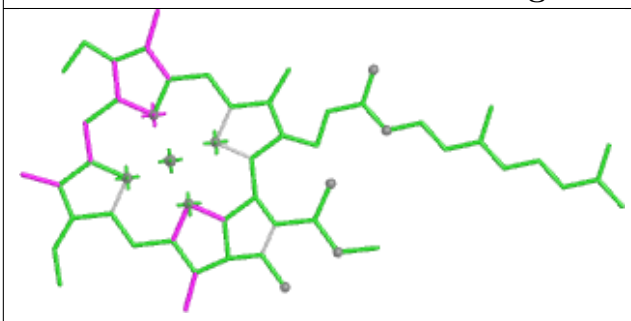
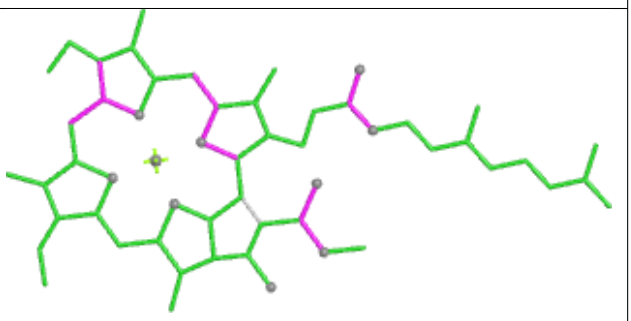
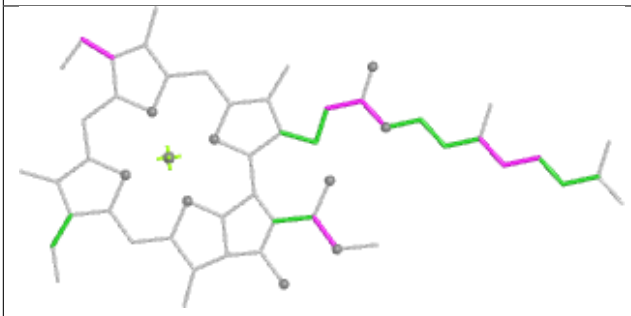
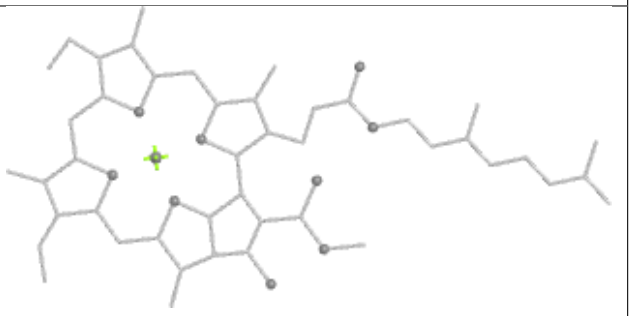
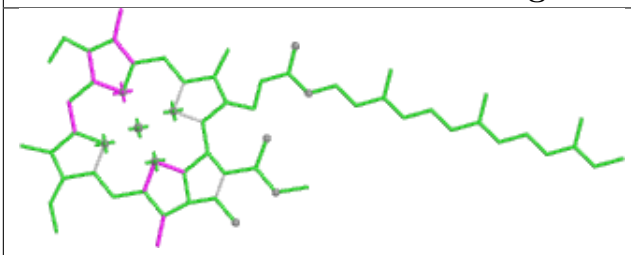


Rings

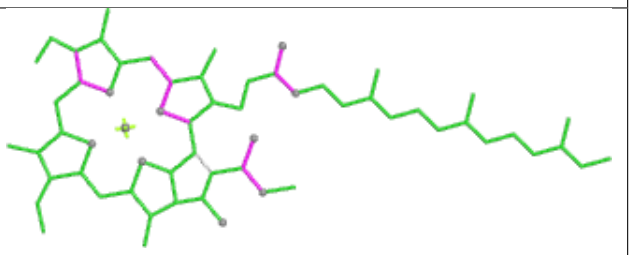
Ligand CLA 5 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

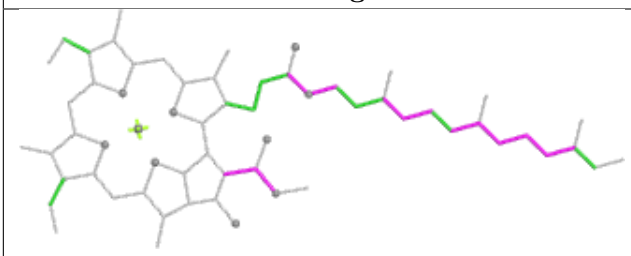
Ligand CLA 3 612



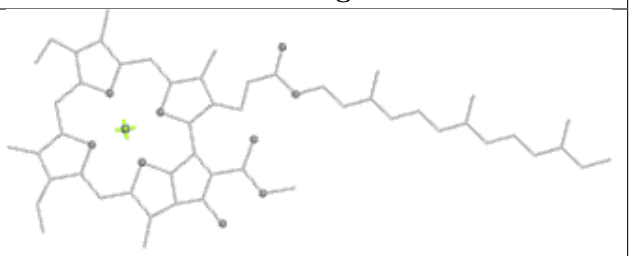
Bond lengths



Bond angles

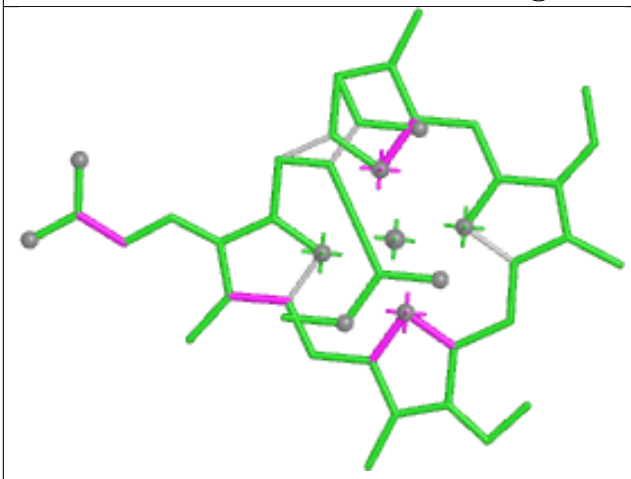


Torsions



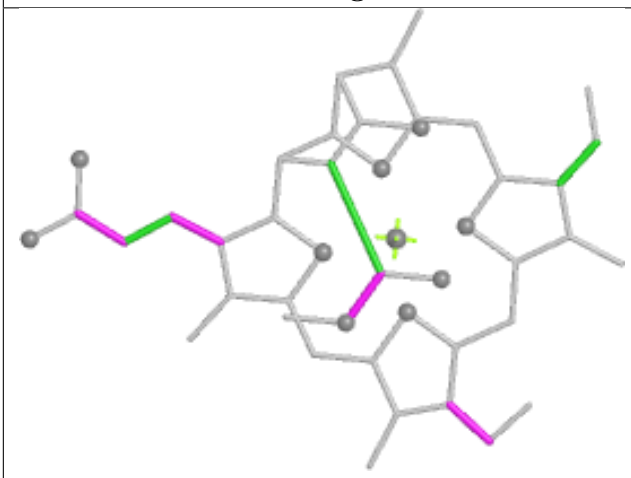
Rings

Ligand KC1 5 315

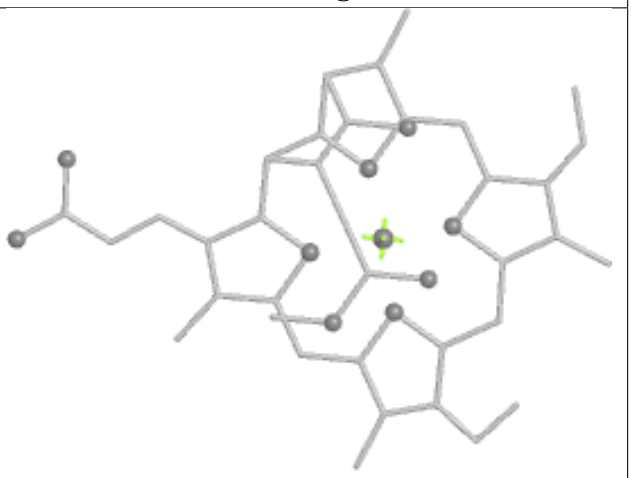


Bond lengths

Bond angles

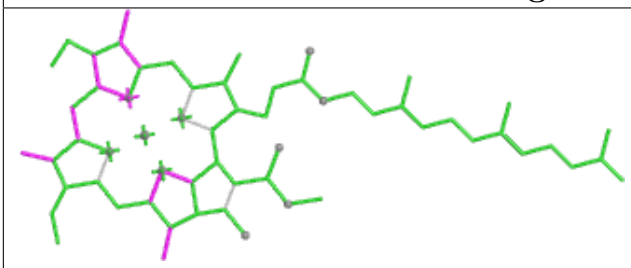


Torsions

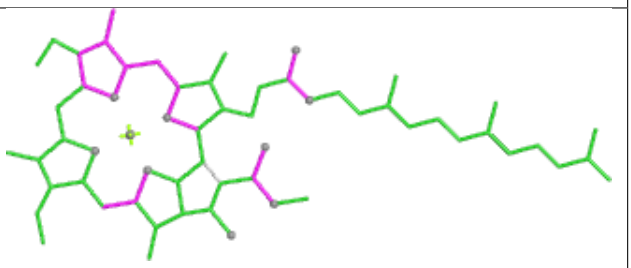


Rings

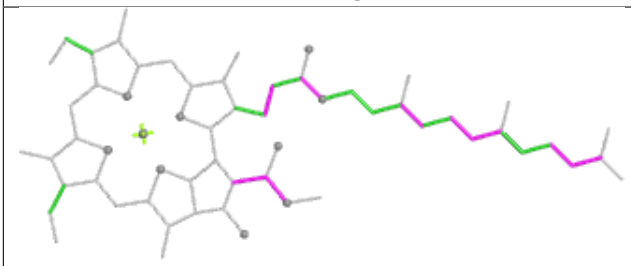
Ligand CLA 4 311



Bond lengths



Bond angles



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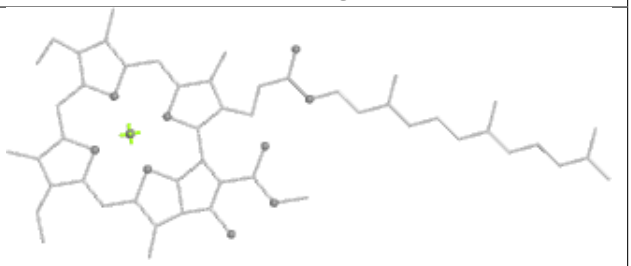
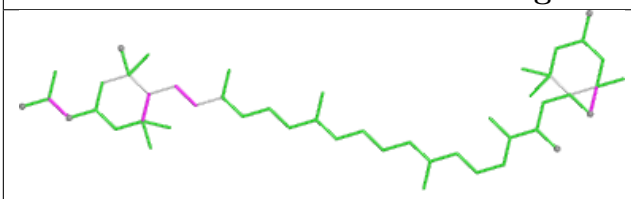


Rings

Ligand A86 5 307



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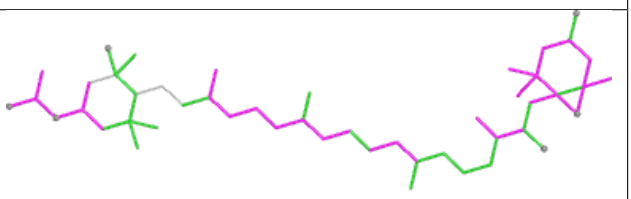
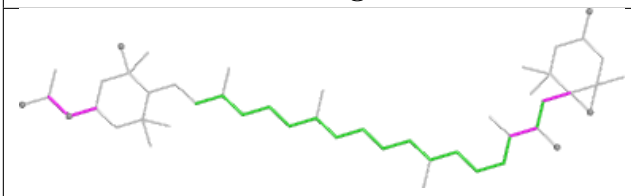


Bond angles



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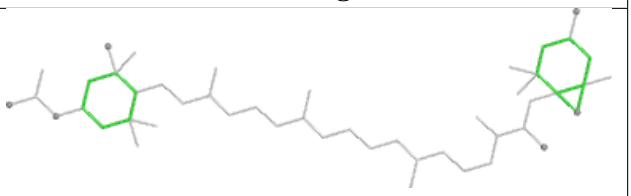
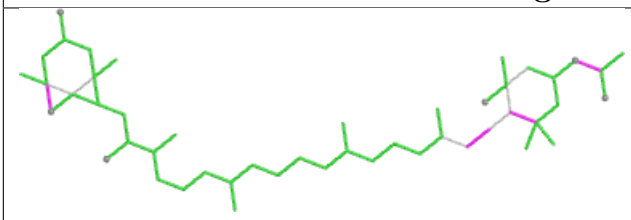


Rings

Ligand A86 6 303



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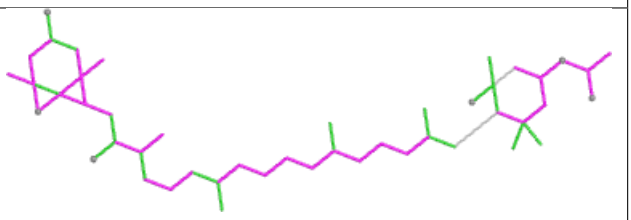
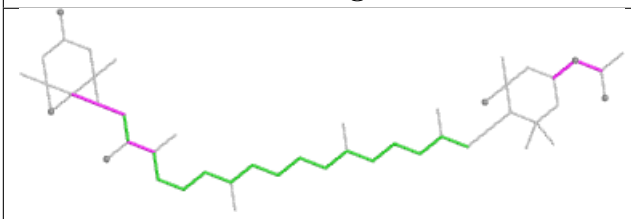


Bond angles



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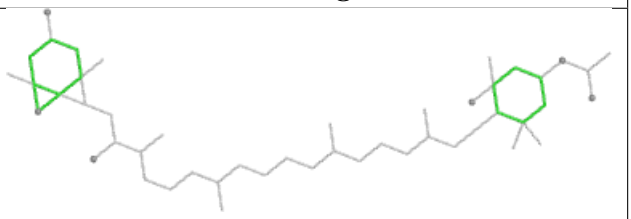
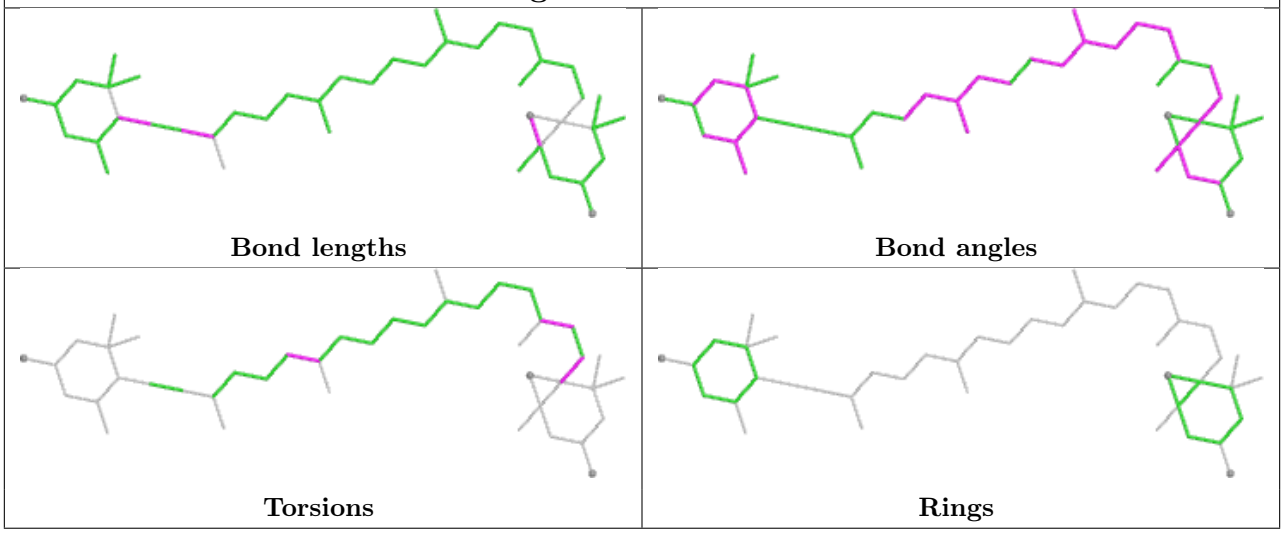
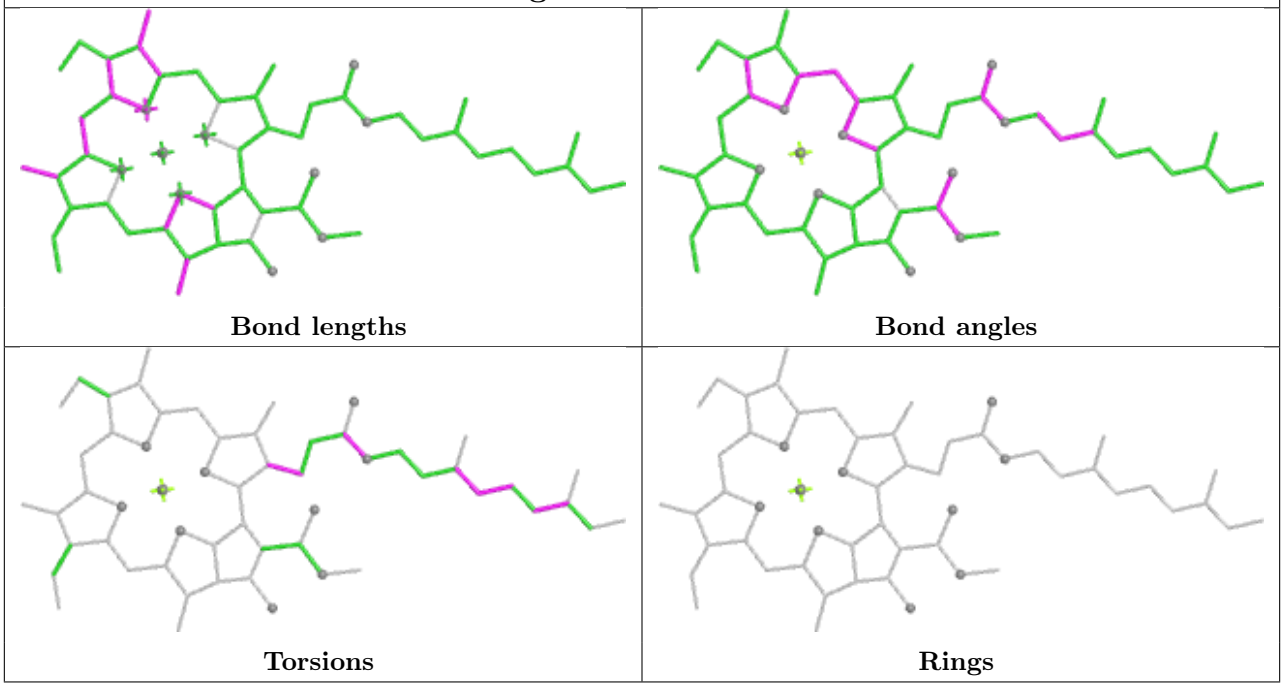


Rings

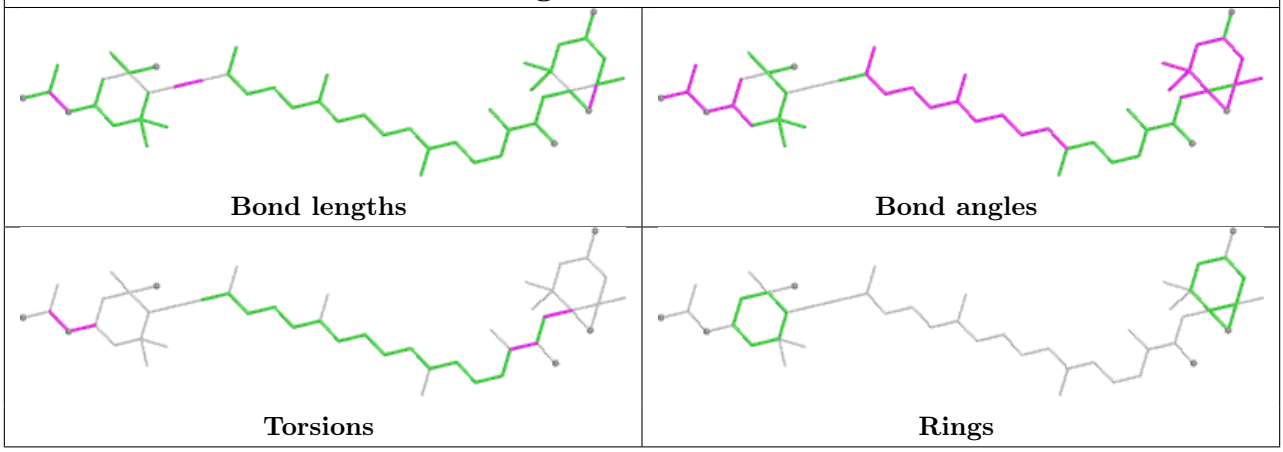
Ligand DD6 3 614



Ligand CLA 3 611



Ligand A86 5 304



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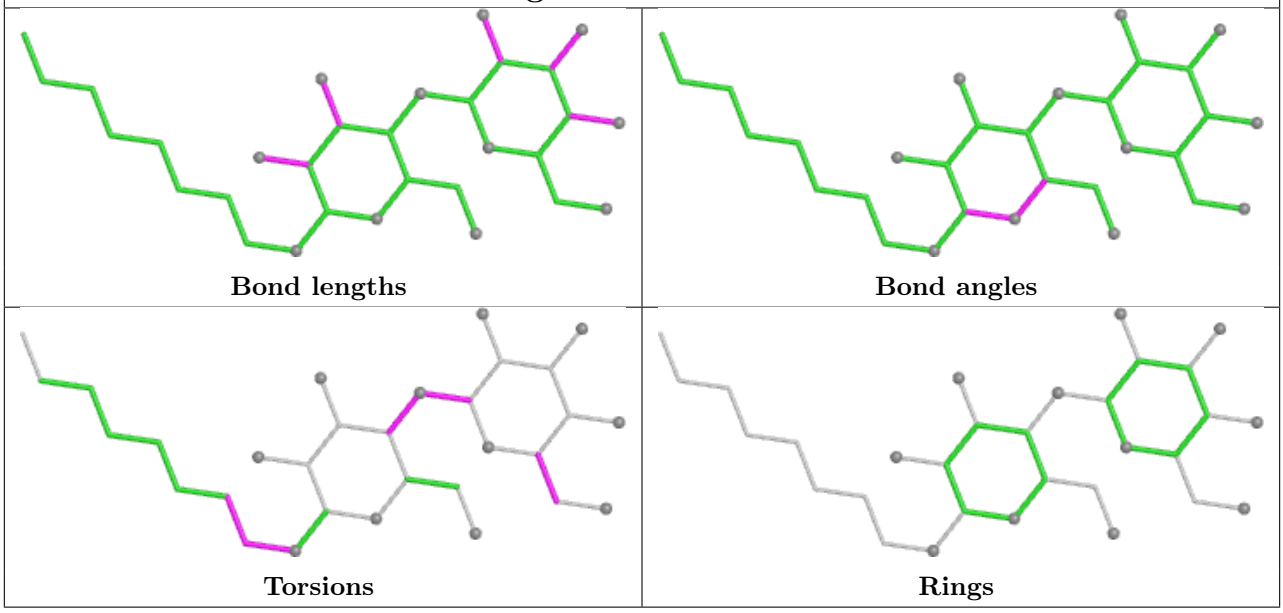

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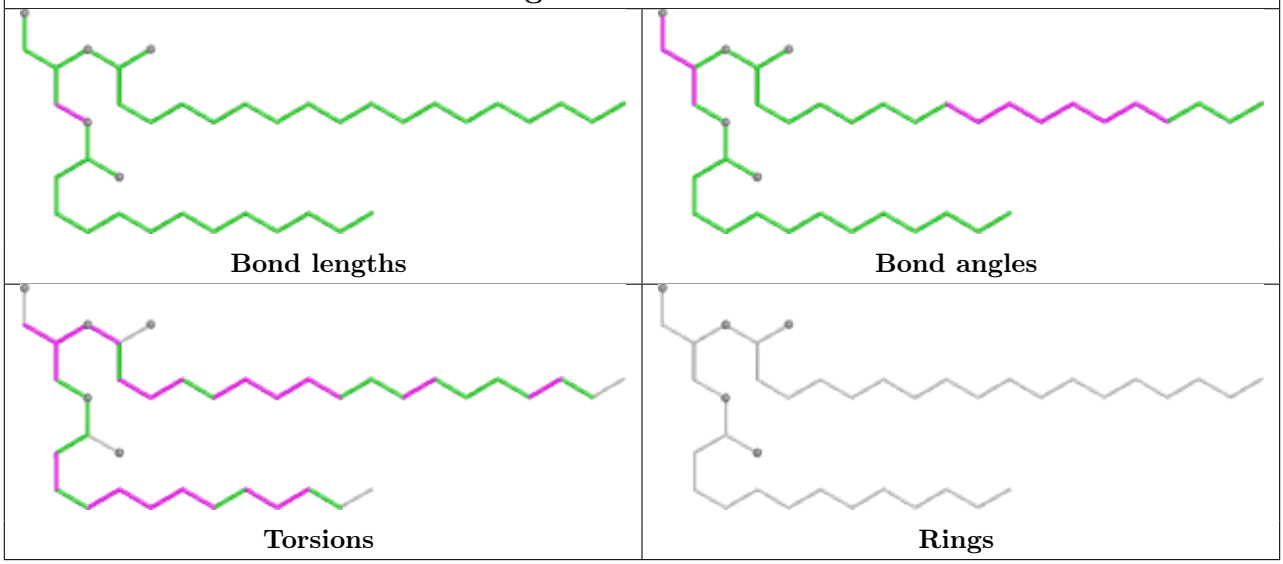

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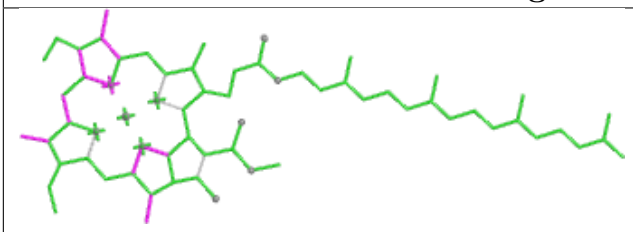
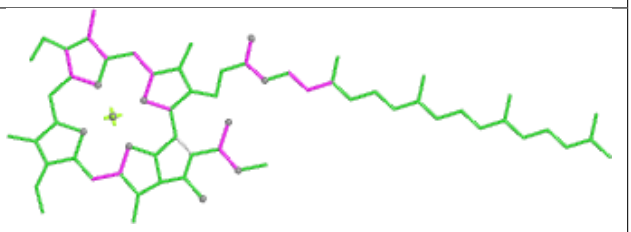
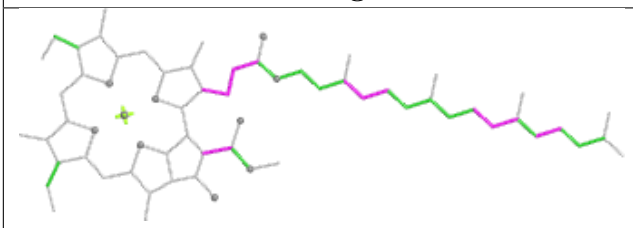


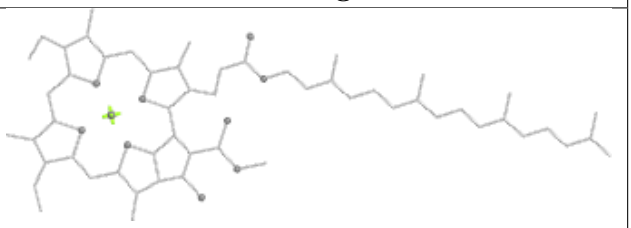
Bond lengths



Bond angles

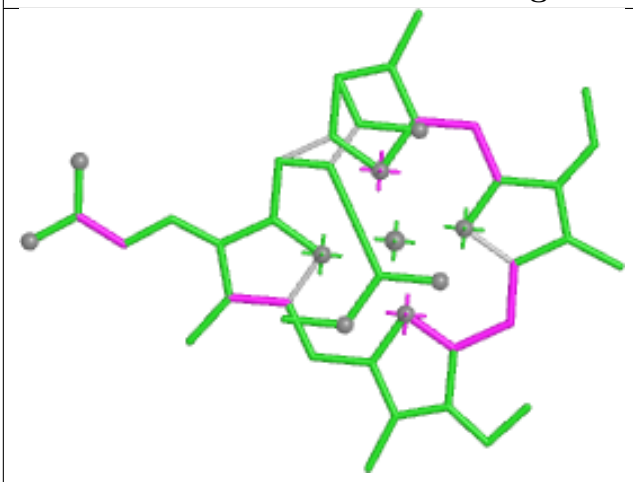


Torsions



Rings

Ligand KC2 4 307



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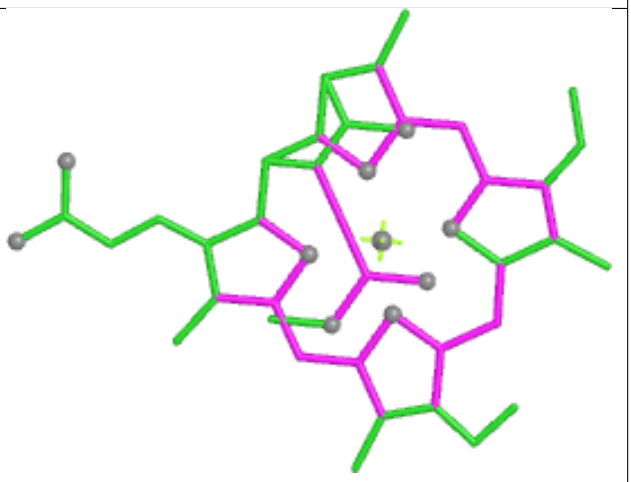
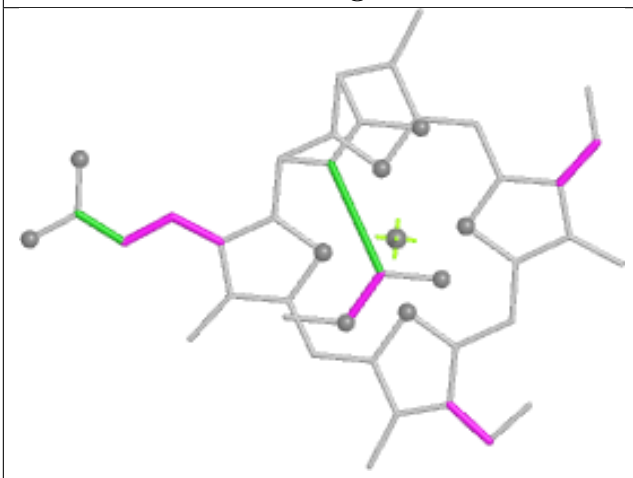


Bond angles



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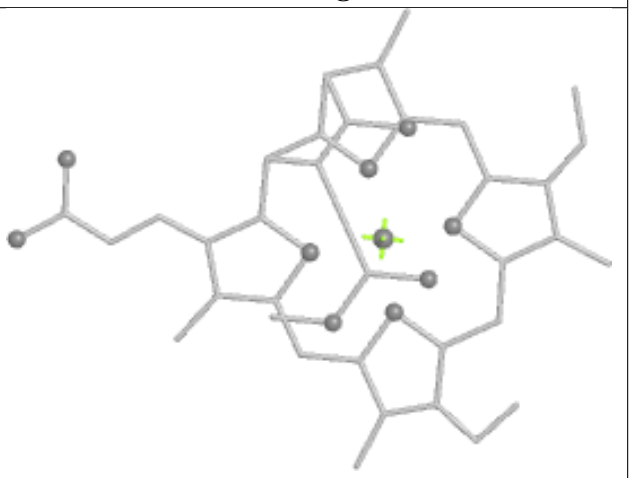
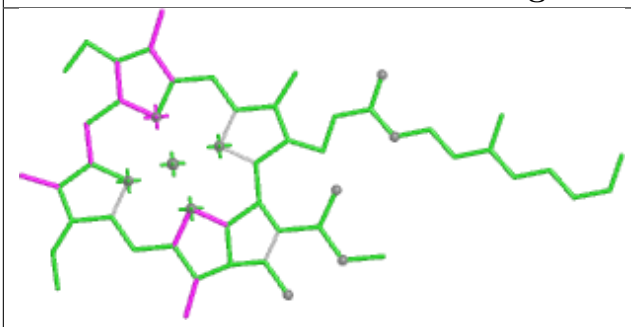
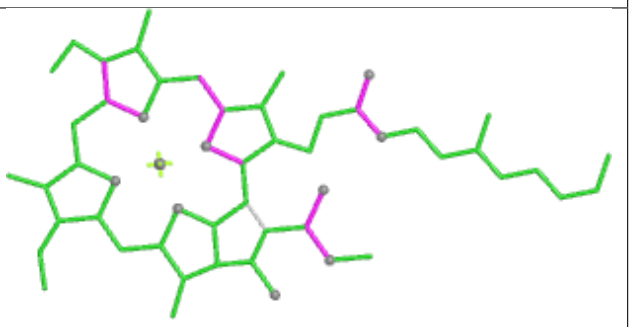
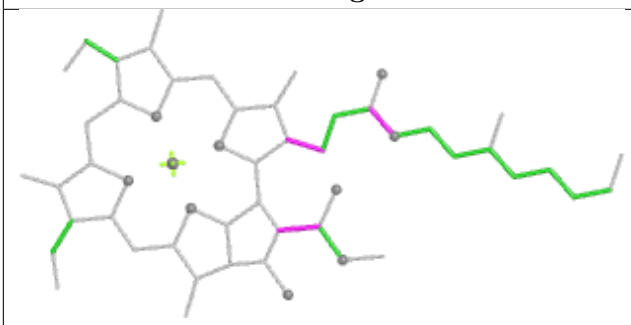
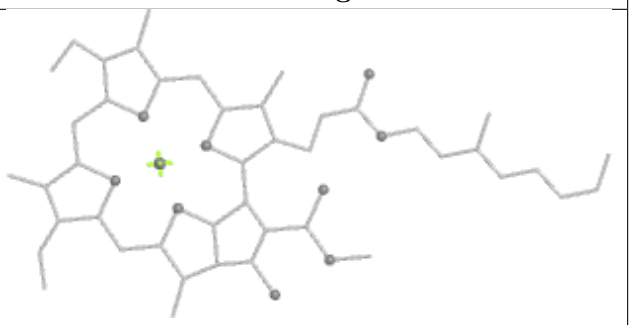
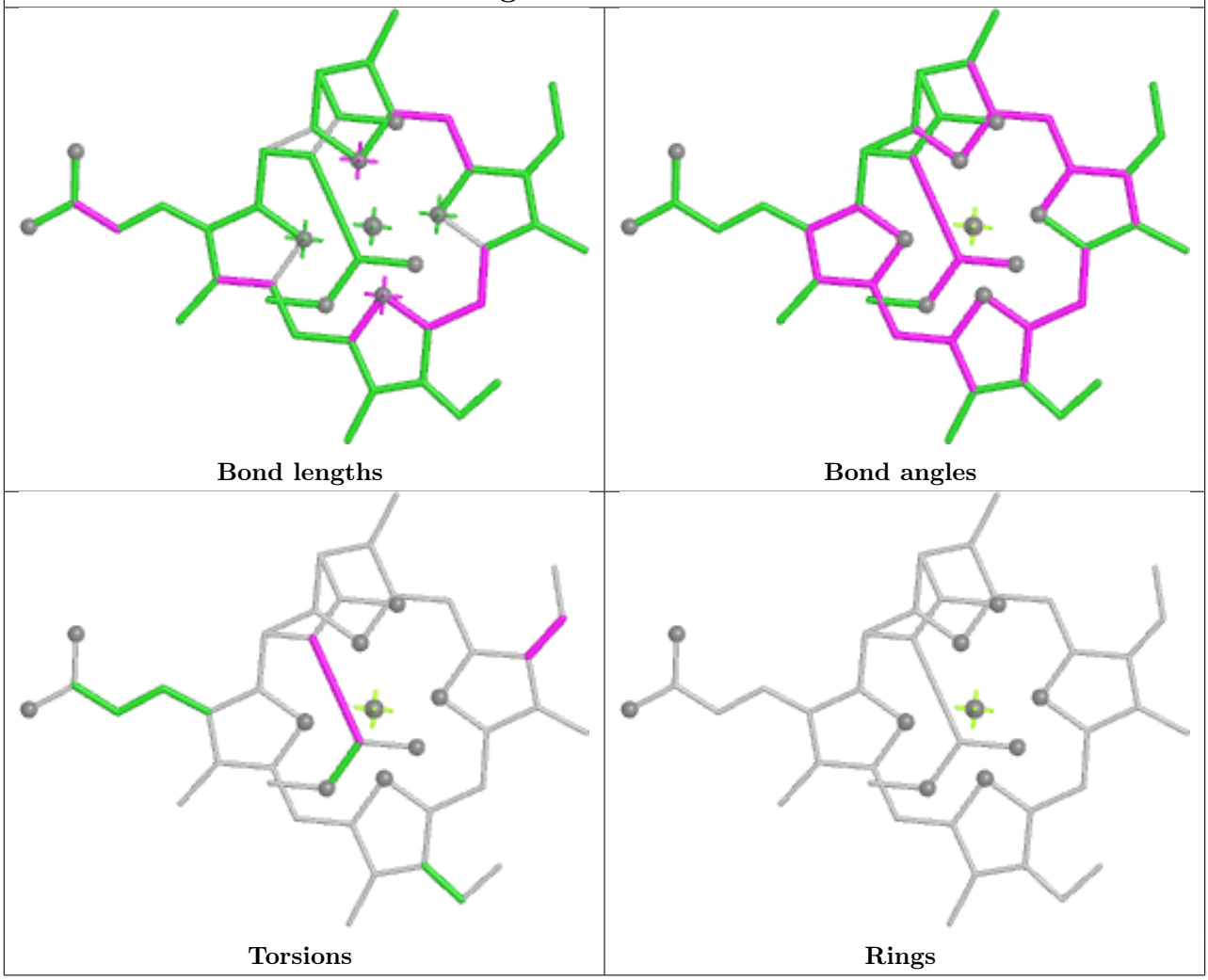


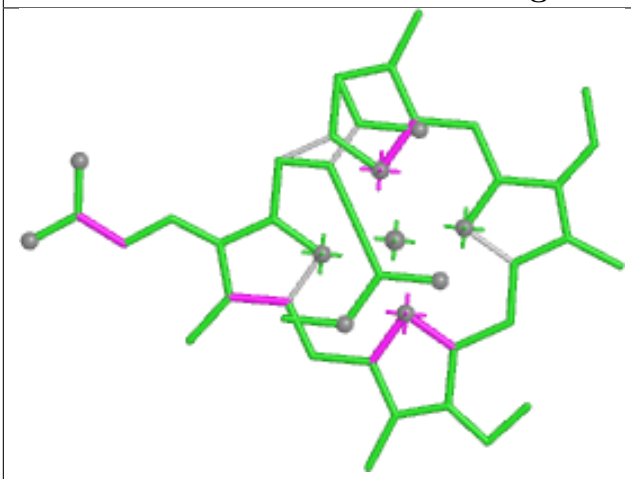
Rings

Ligand CLA 6 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

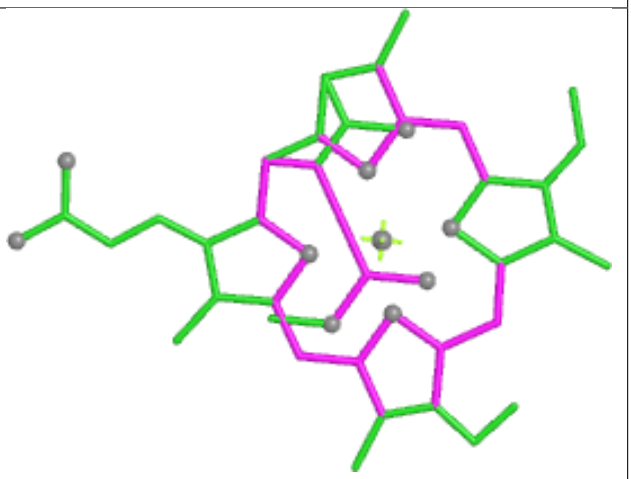
Ligand KC2 5 310



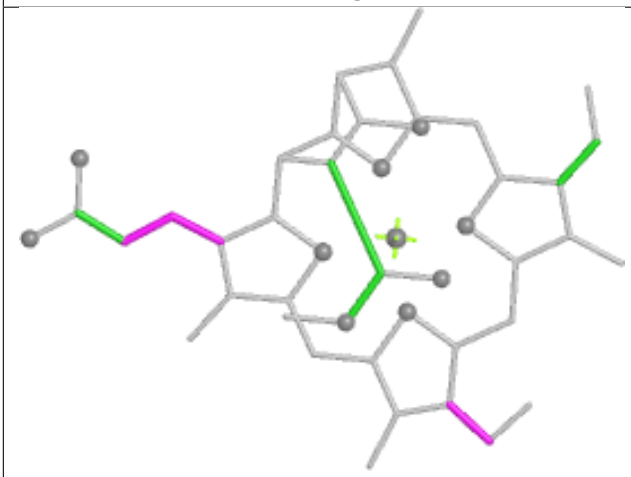
Ligand KC1 6 313



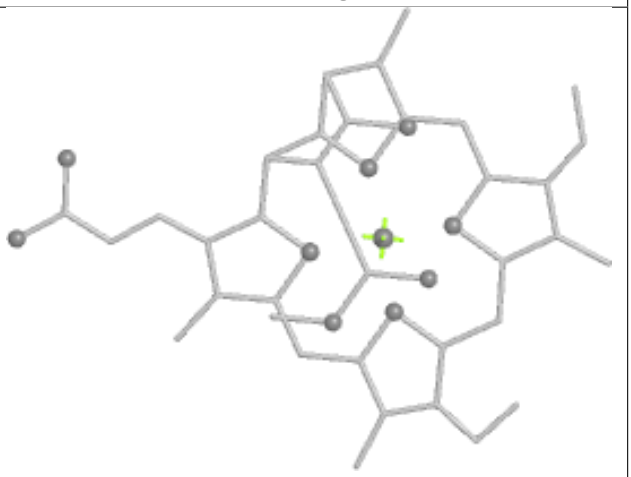
Bond lengths



Bond angles

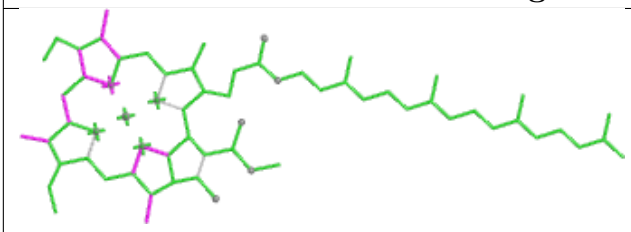


Torsions

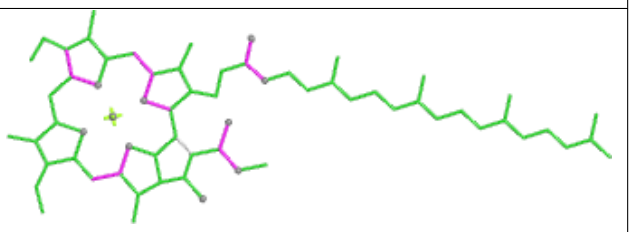


Rings

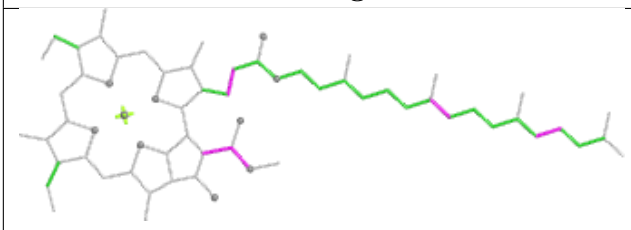
Ligand CLA 4 306



Bond lengths



Bond angles



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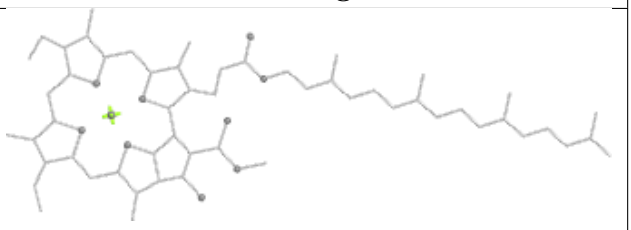
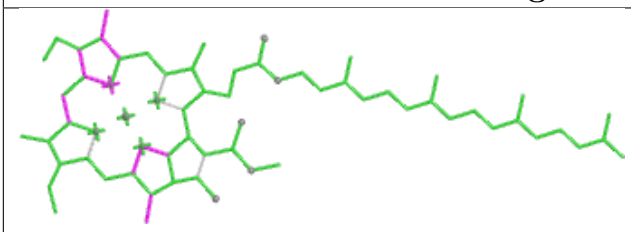
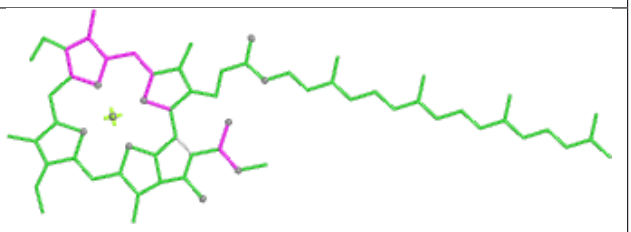
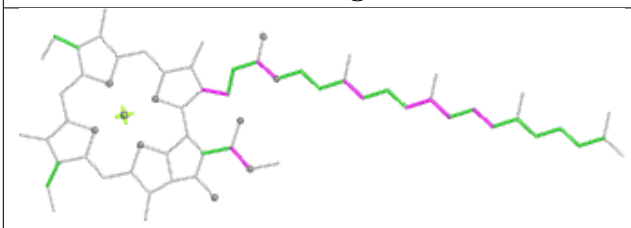
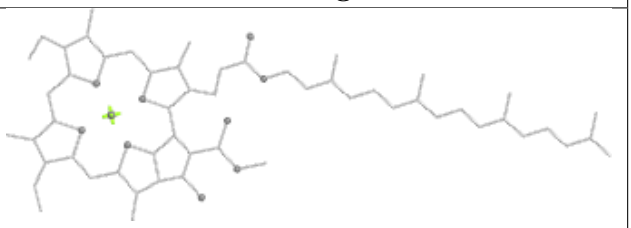
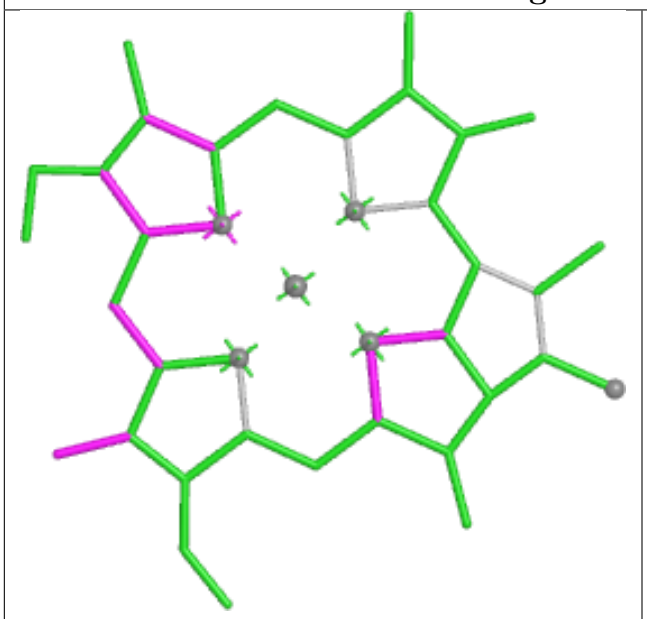


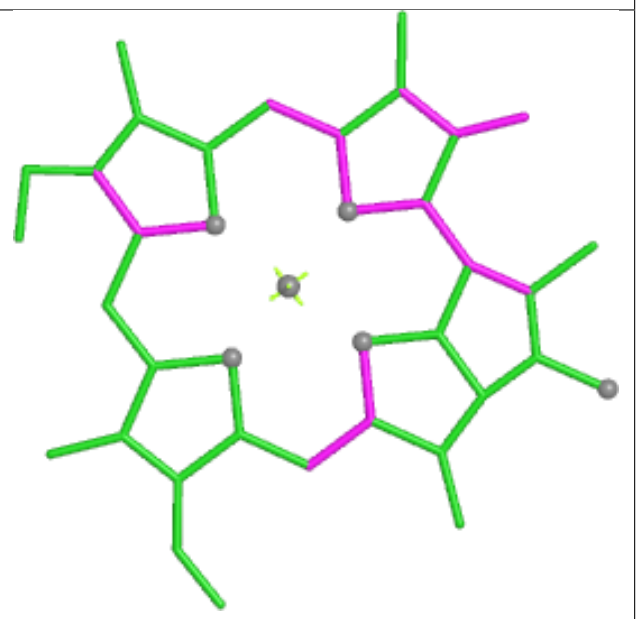
Rings

Ligand CLA 5 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

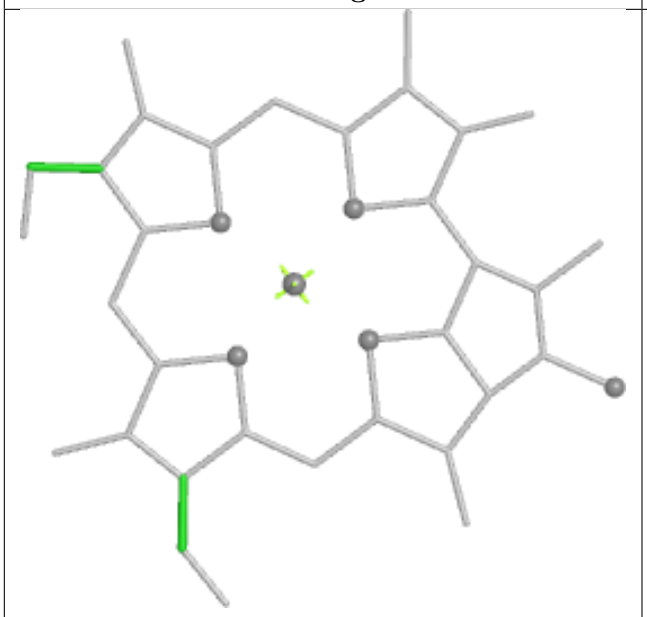
Ligand CLA 5 317



Bond lengths



Bond angles



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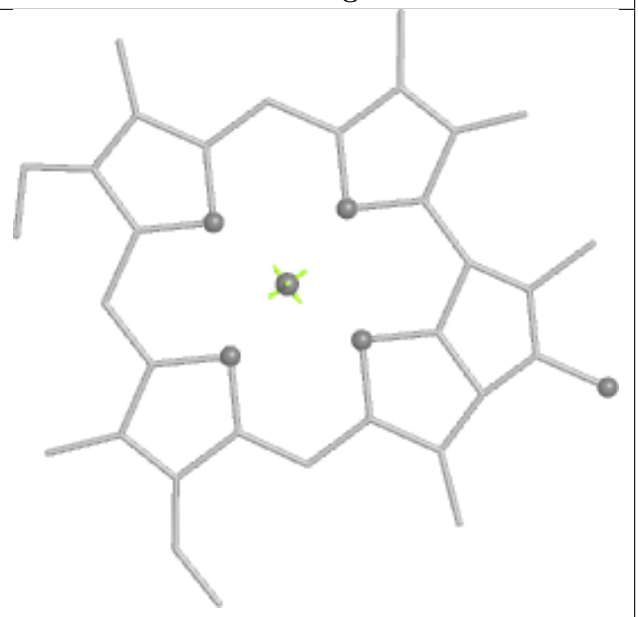
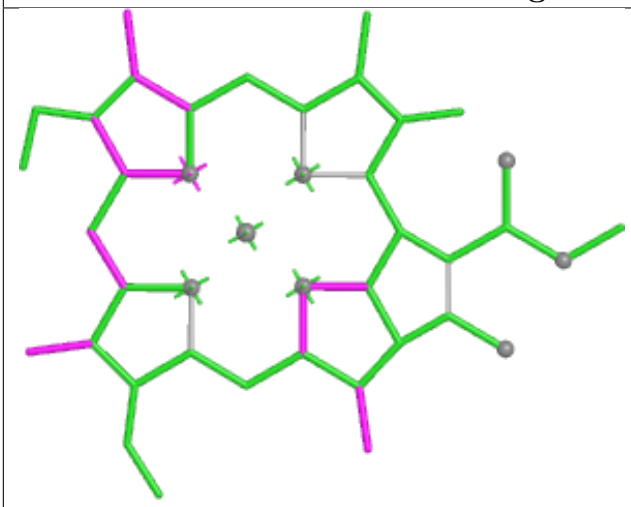
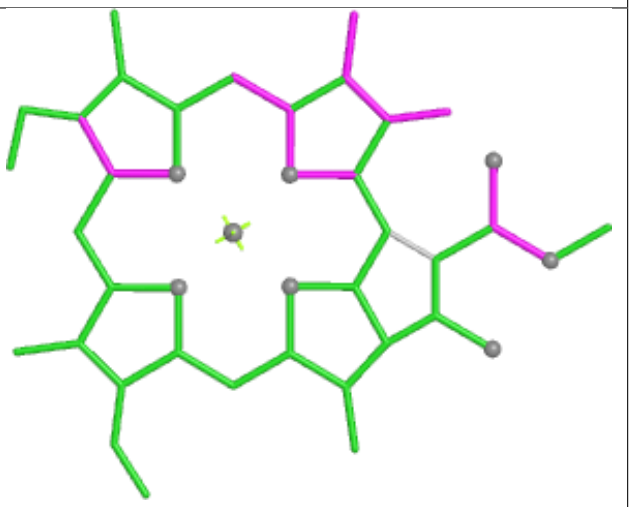


Rings

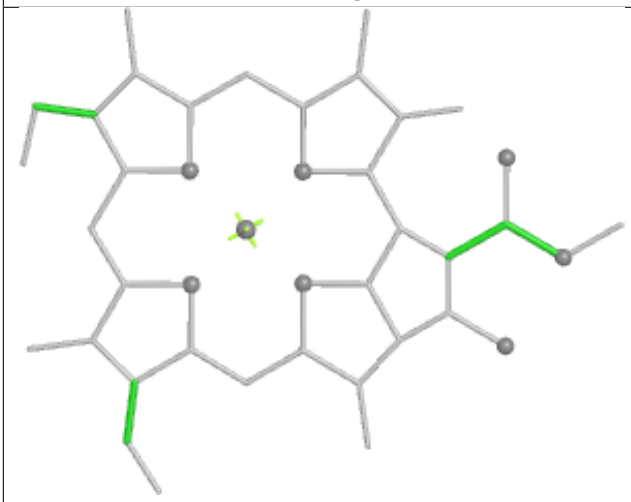
Ligand CLA 3 610



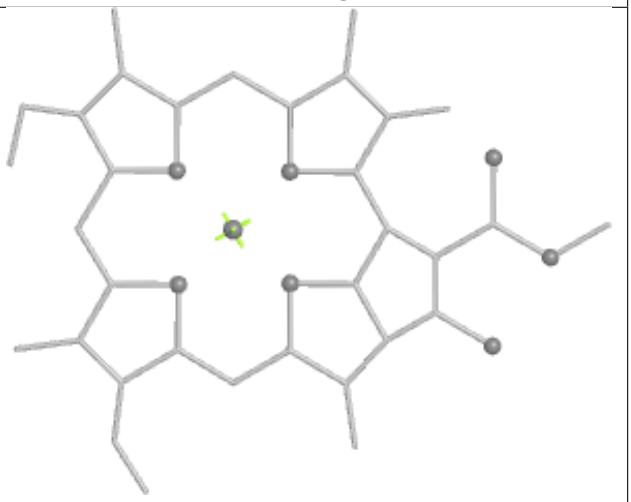
Bond lengths



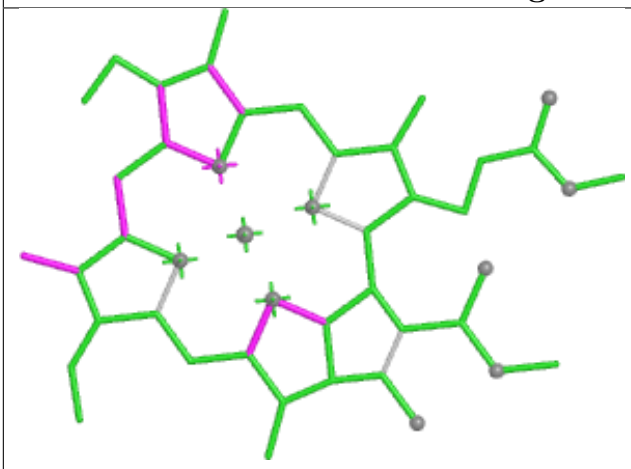
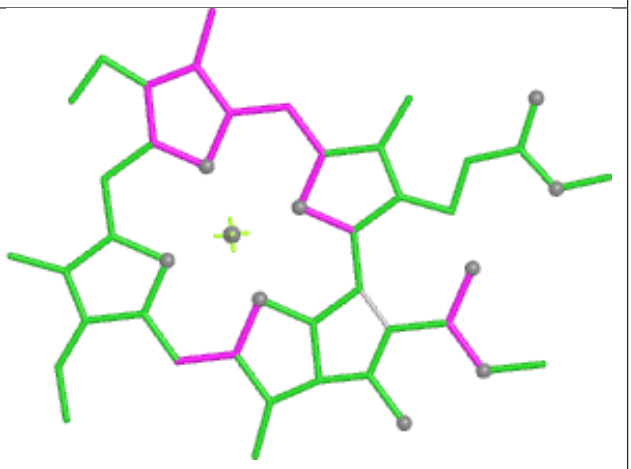
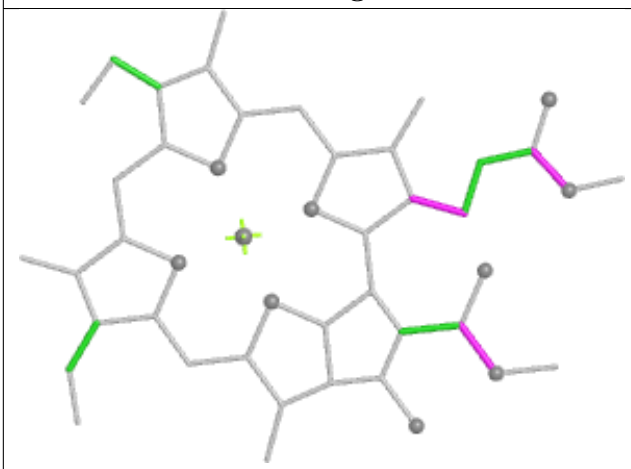
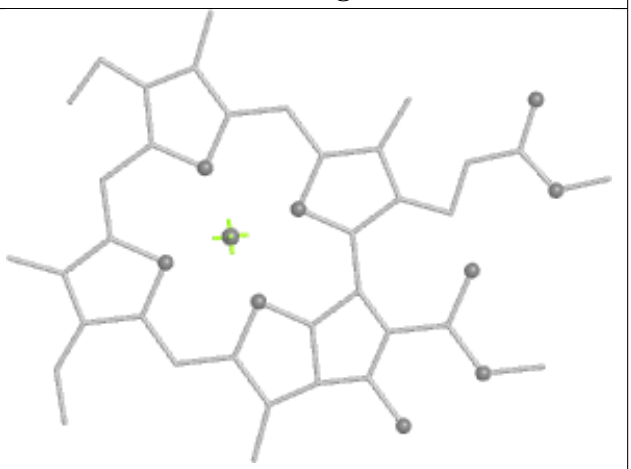
Bond angles

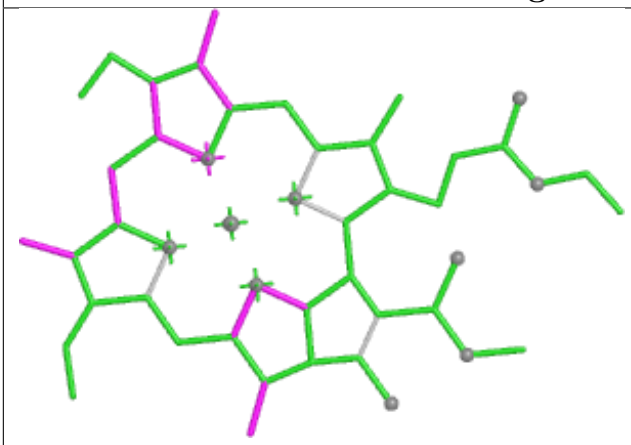
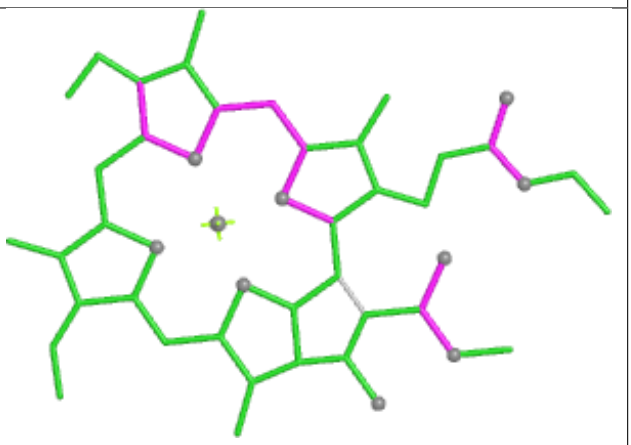
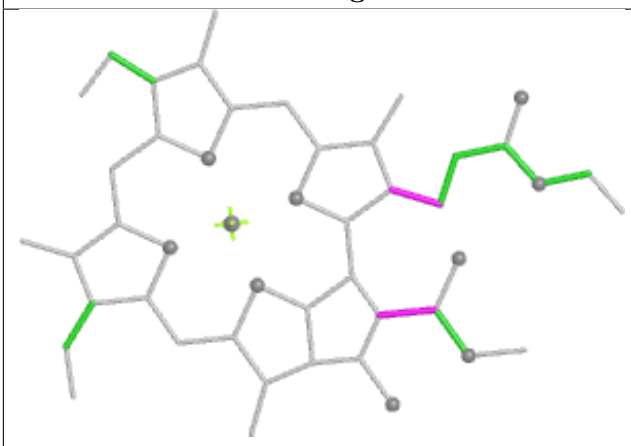
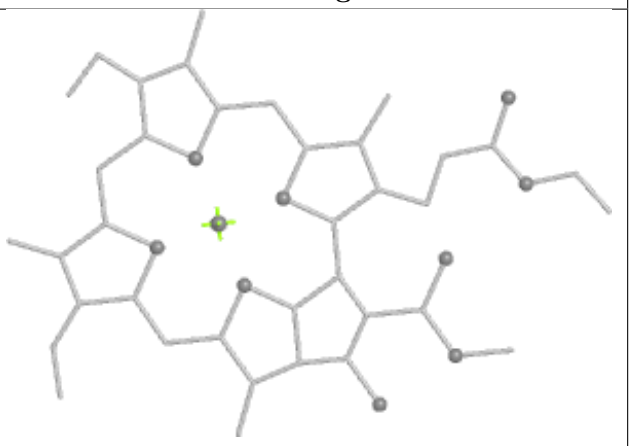


Torsions



Rings

Ligand CLA 6 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

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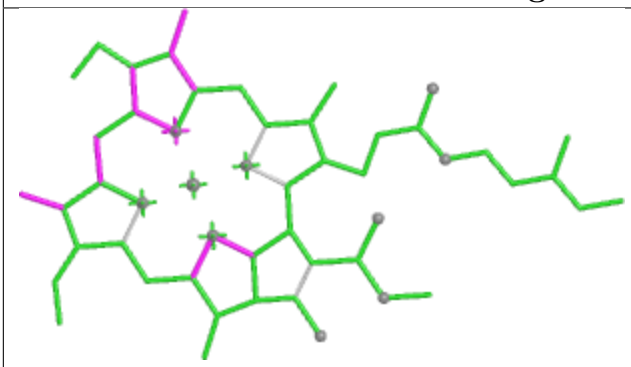
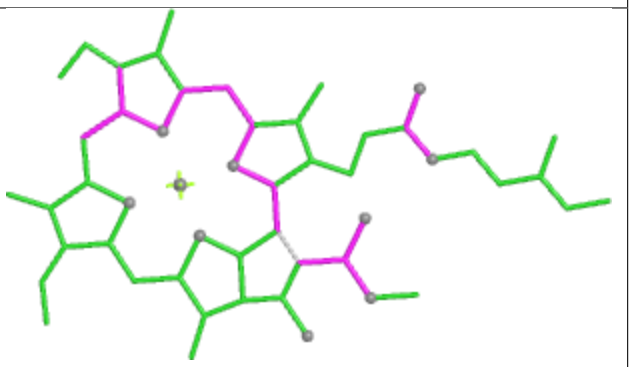
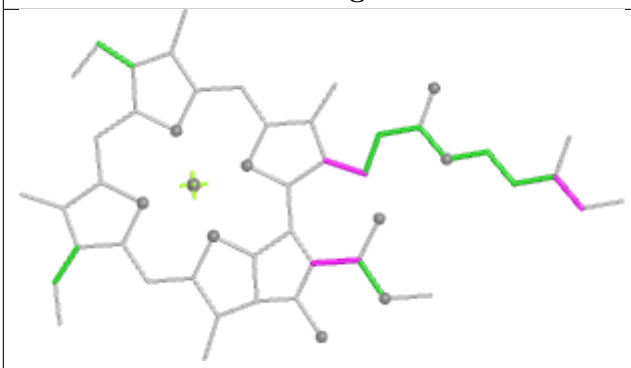
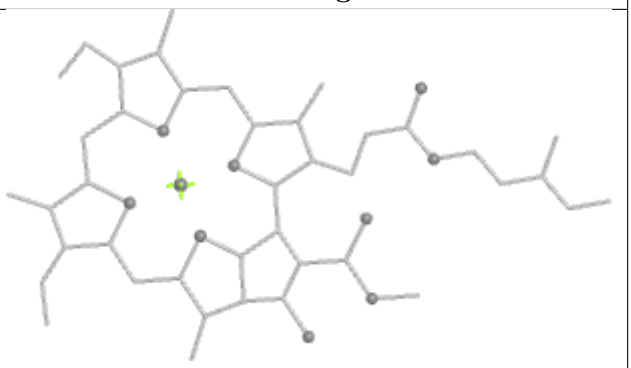
 Bond lengths	 Bond angles
 Torsions	 Rings

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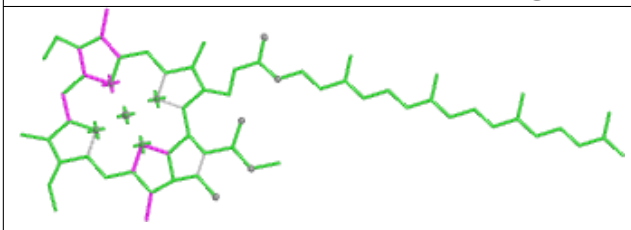
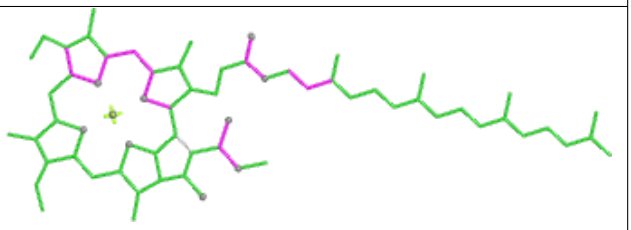
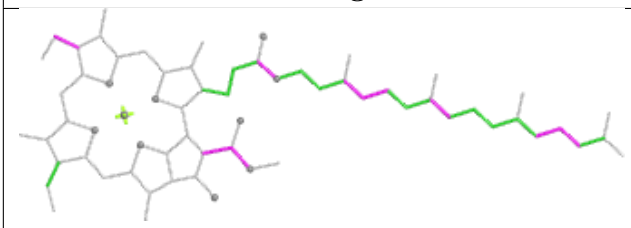
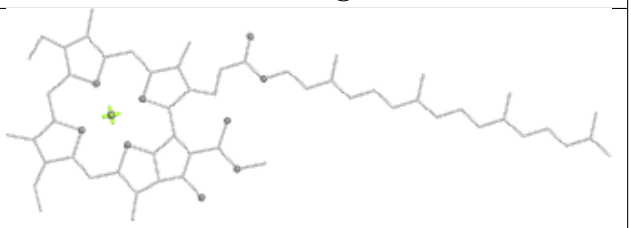
 Bond lengths	 Bond angles
 Torsions	 Rings

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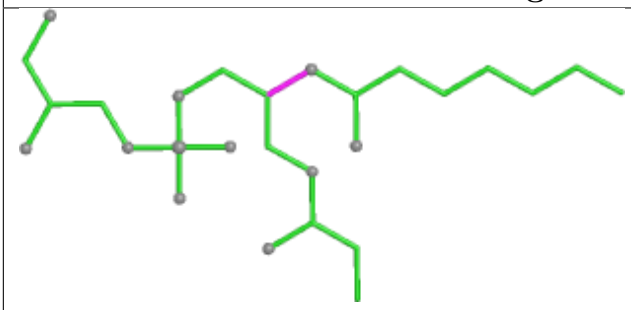	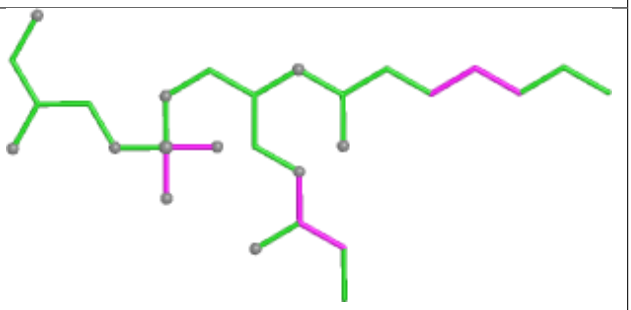
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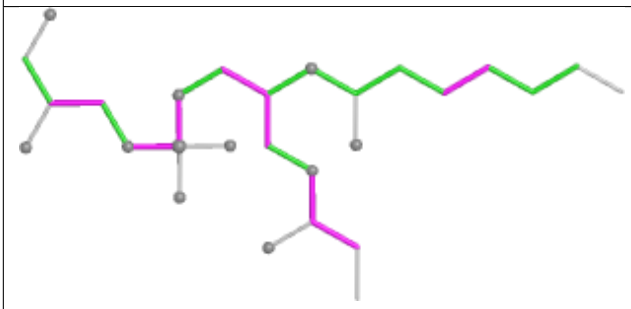
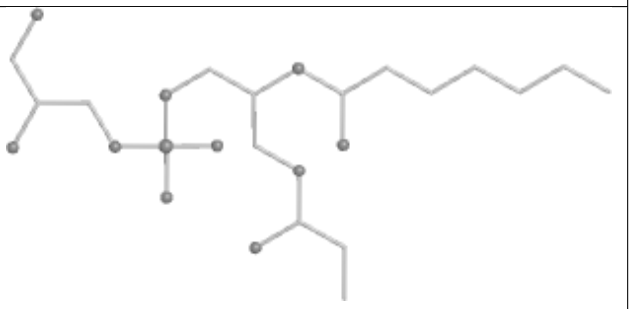
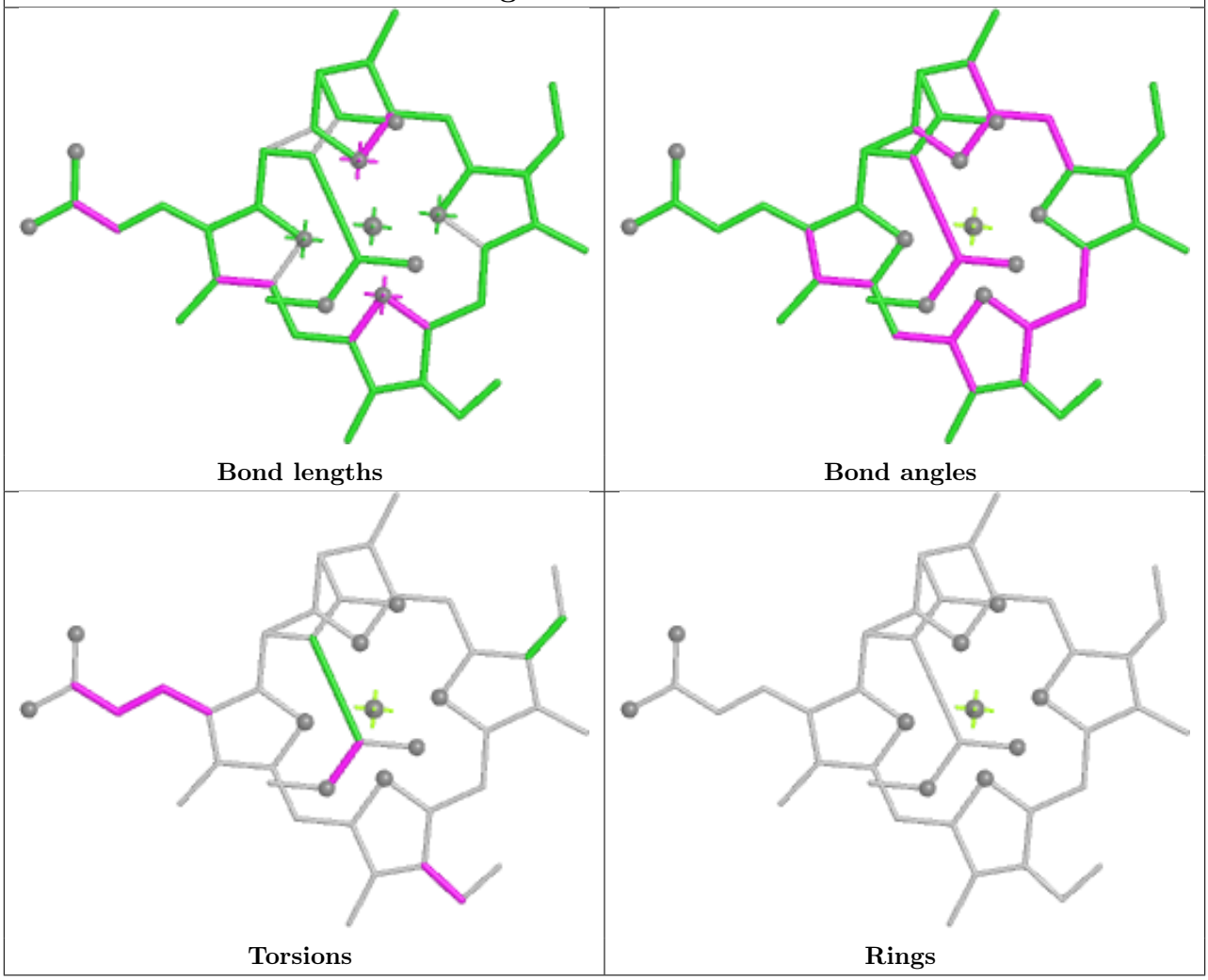
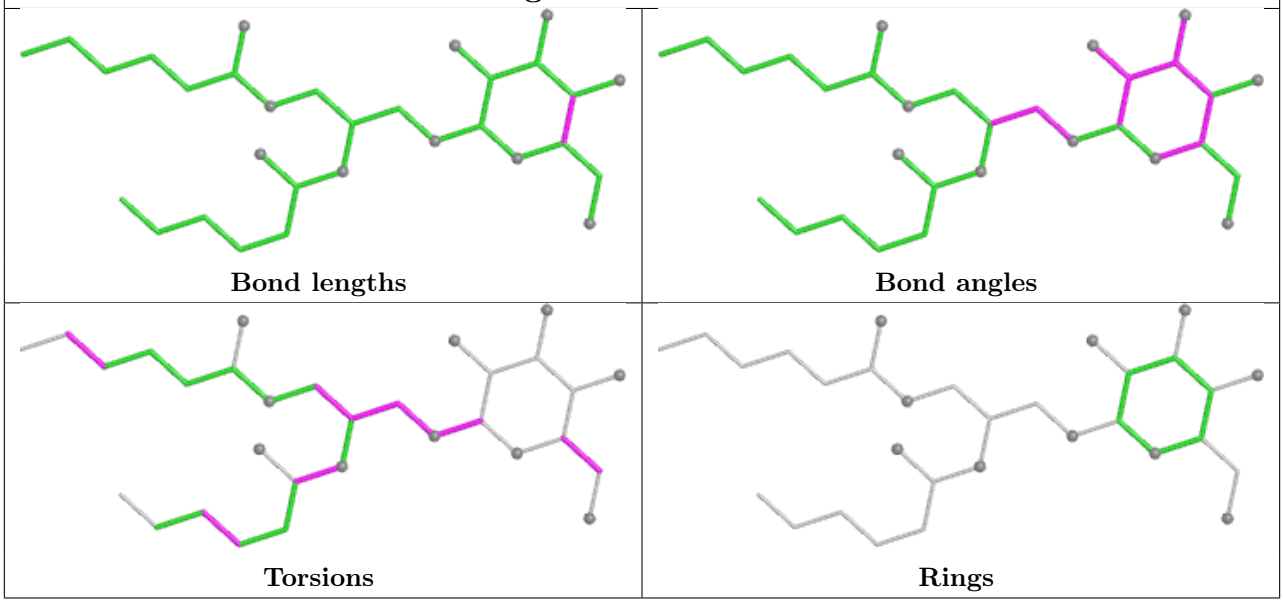
	
Torsions	**Rings**

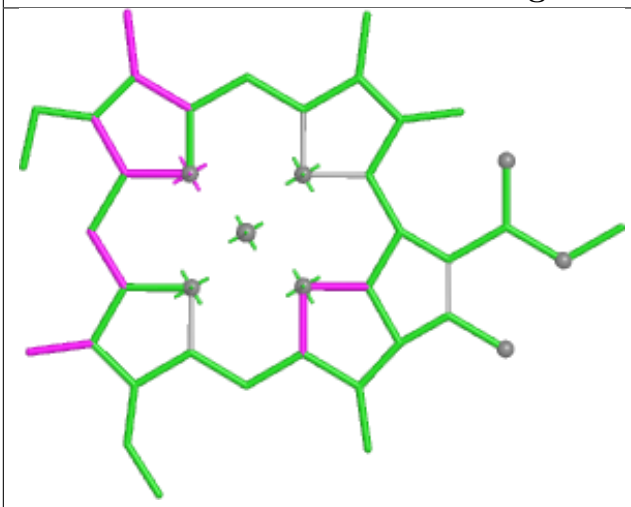
Ligand KC1 3 609



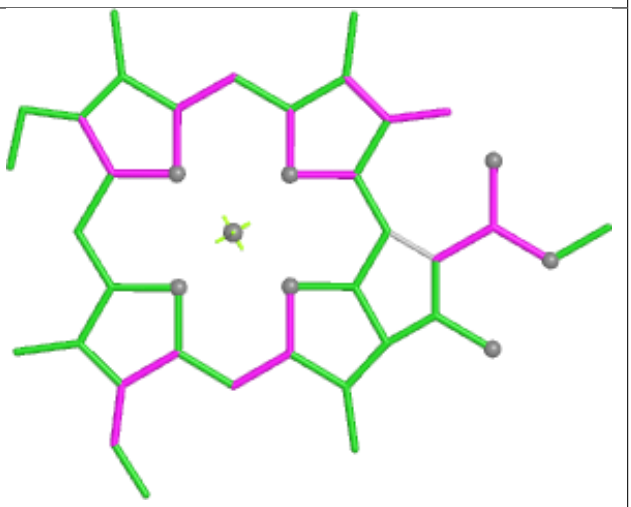
Ligand LMG 5 319



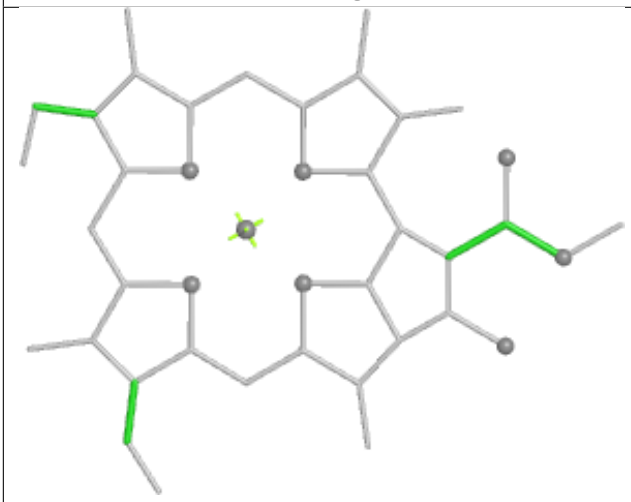
Ligand CLA 6 314



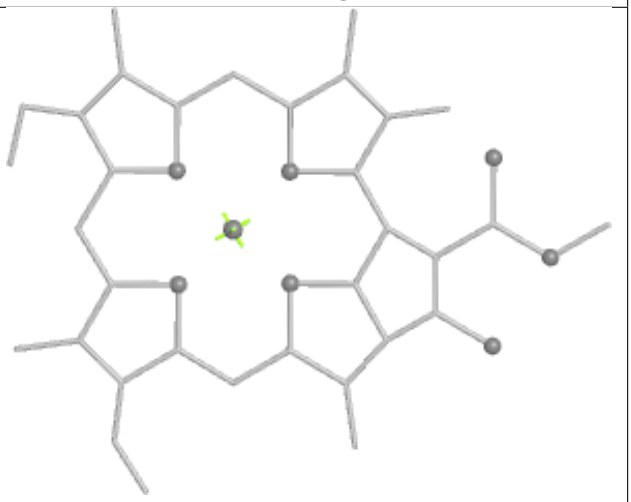
Bond lengths



Bond angles

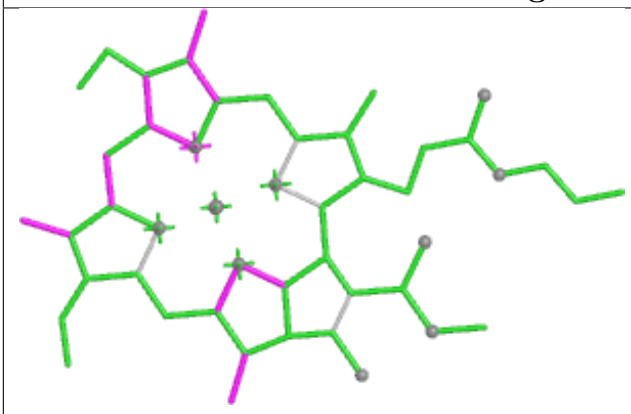


Torsions



Rings

Ligand CLA 3 604



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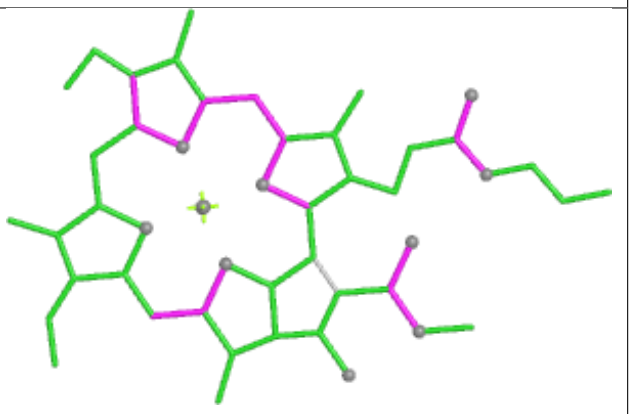

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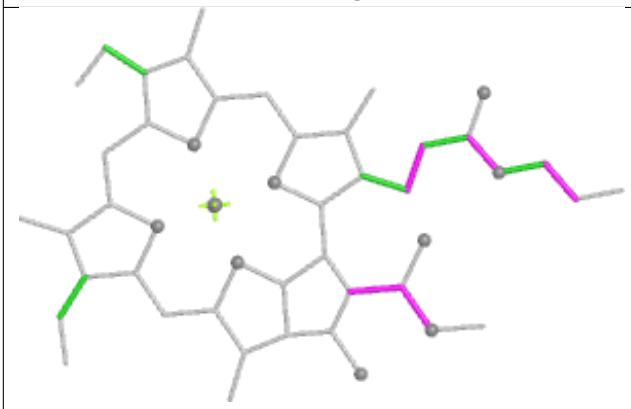

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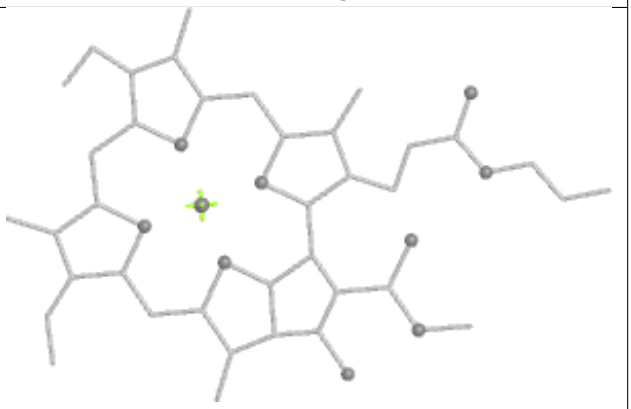
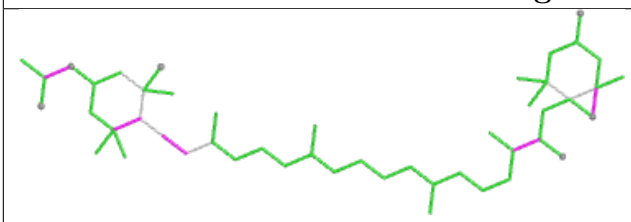


Rings

Ligand A86 6 301



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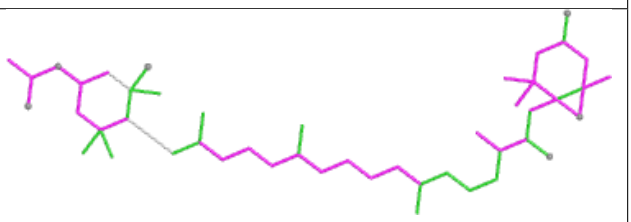

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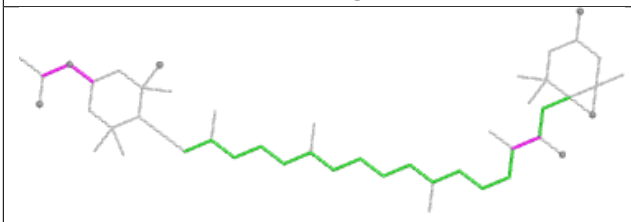

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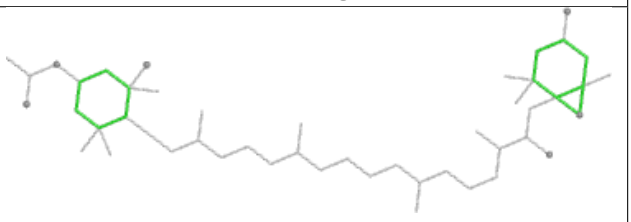
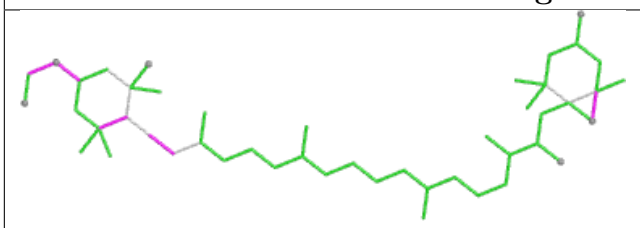
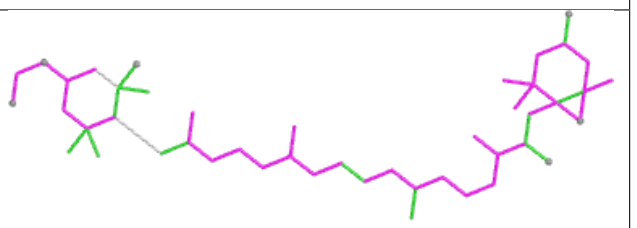
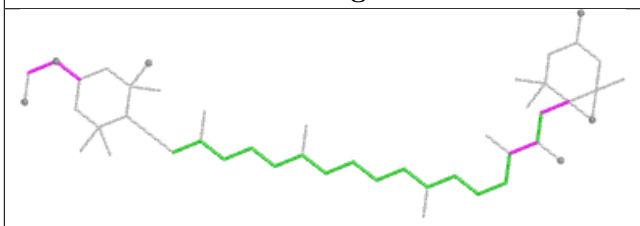
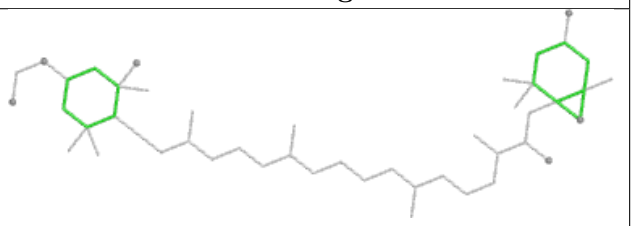
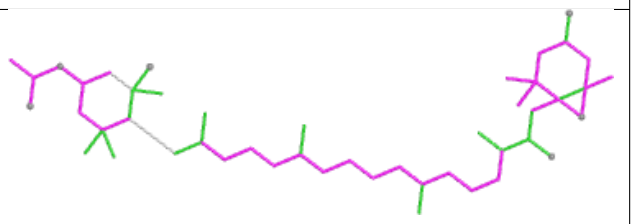
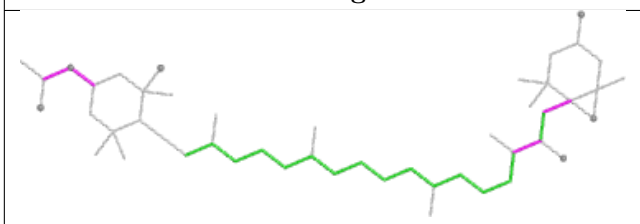
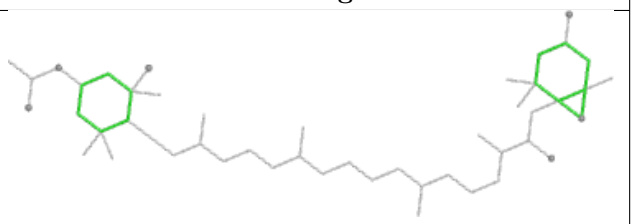
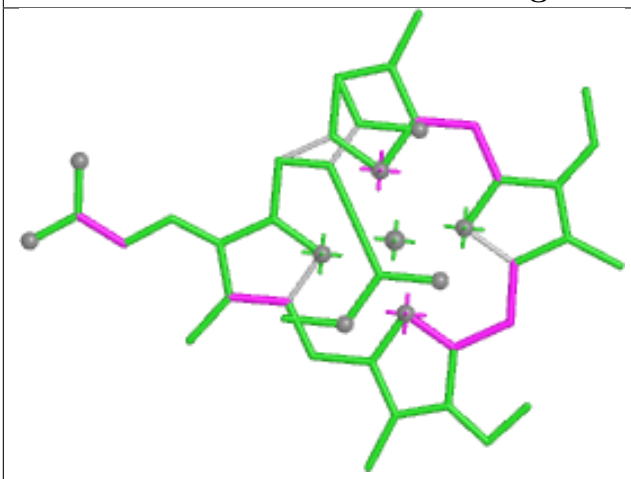


Rings

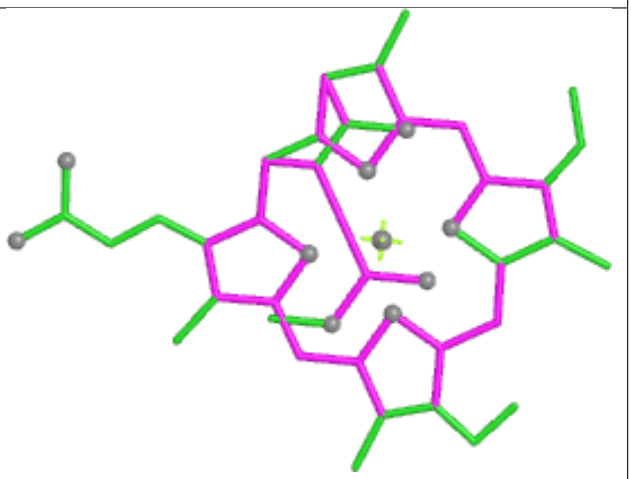
Ligand A86 5 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 5 302	
Bond lengths	 Bond angles
 Torsions	 Rings

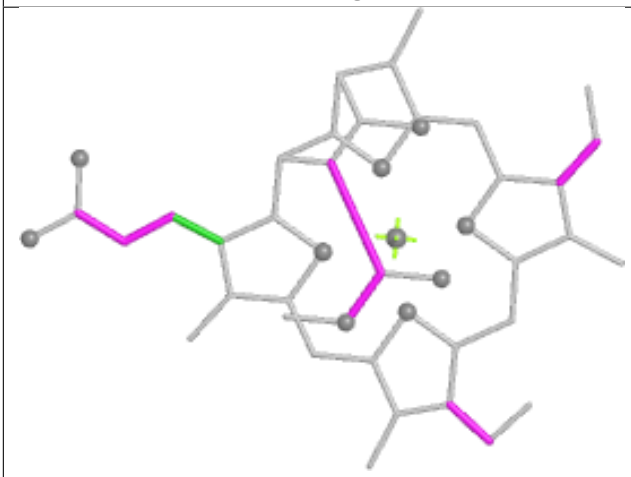
Ligand KC2 6 308



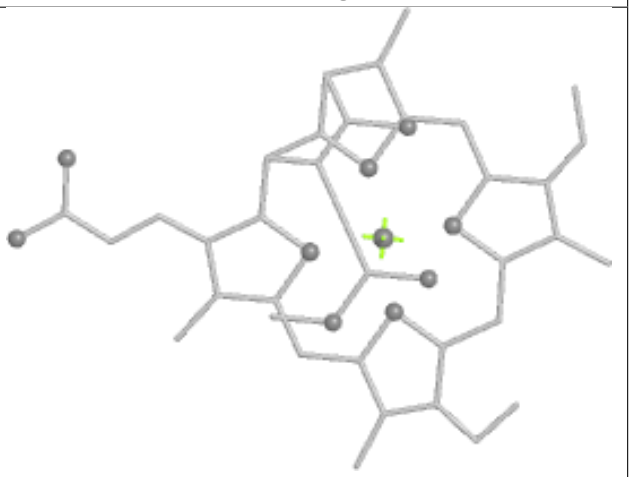
Bond lengths



Bond angles

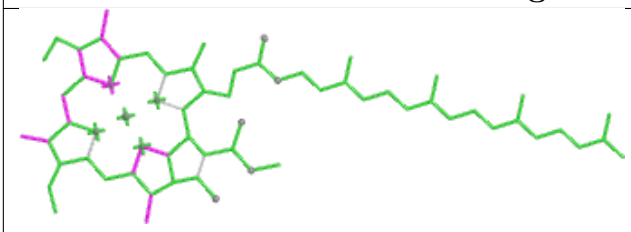


Torsions



Rings

Ligand CLA 4 308



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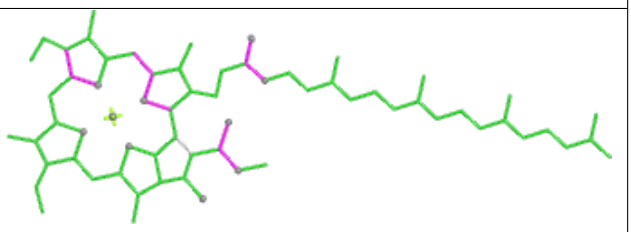
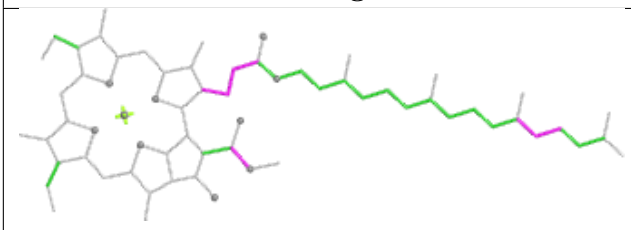


Bond angles



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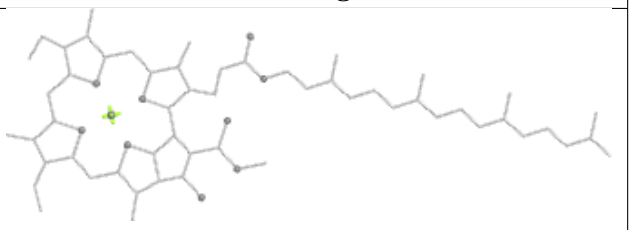
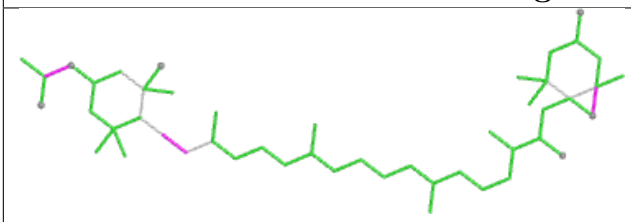
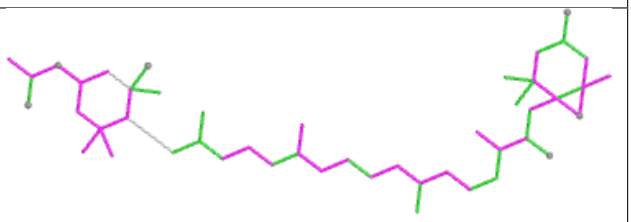


Rings

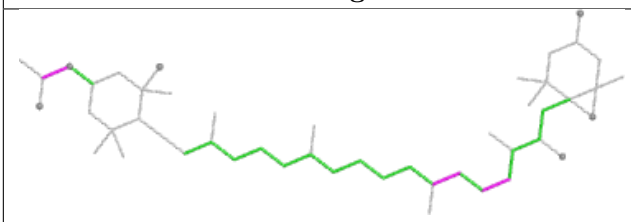
Ligand A86 3 613



Bond lengths



Bond angles



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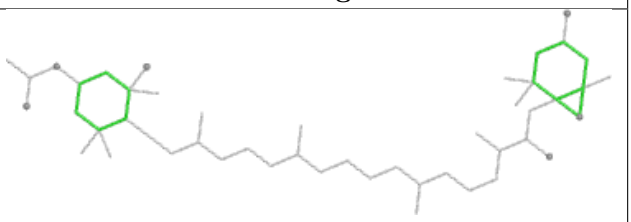
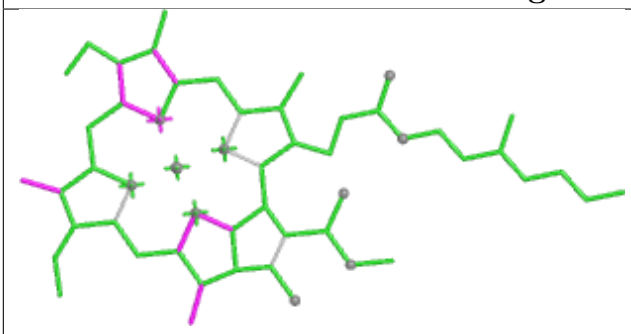
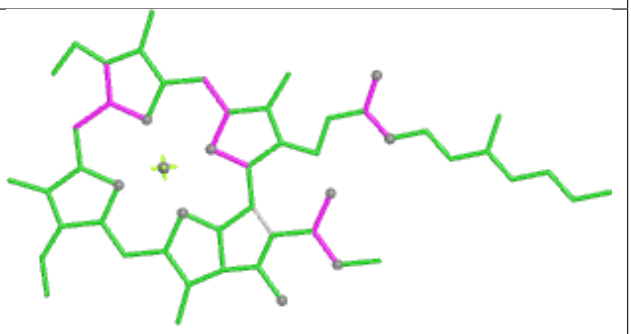


Rings

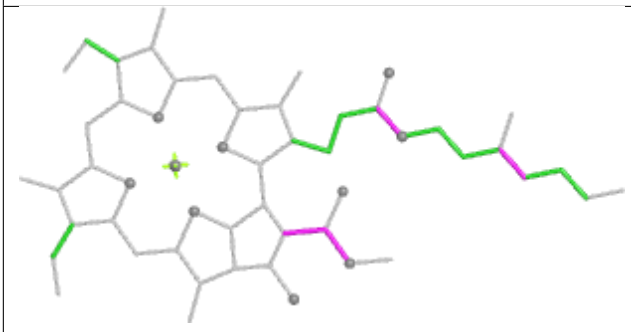
Ligand CLA 6 306



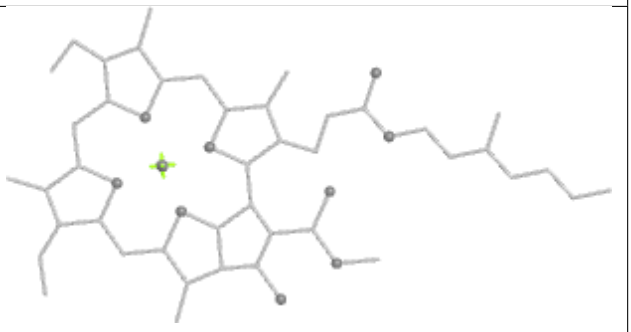
Bond lengths



Bond angles

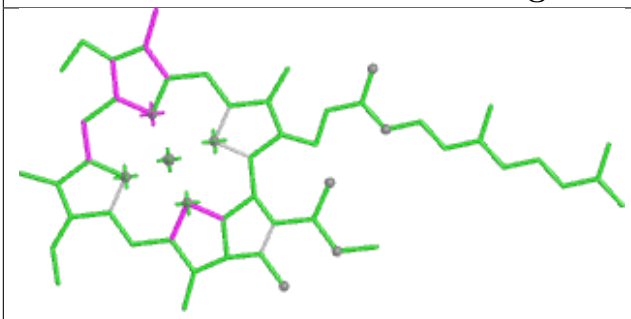


Torsions

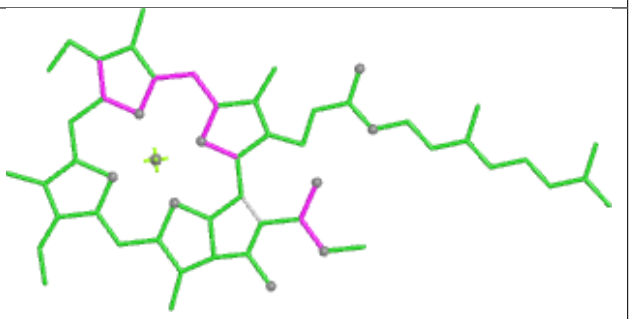


Rings

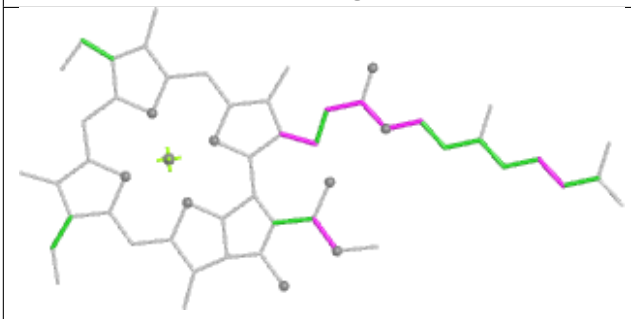
Ligand CLA 5 311



Bond lengths



Bond angles



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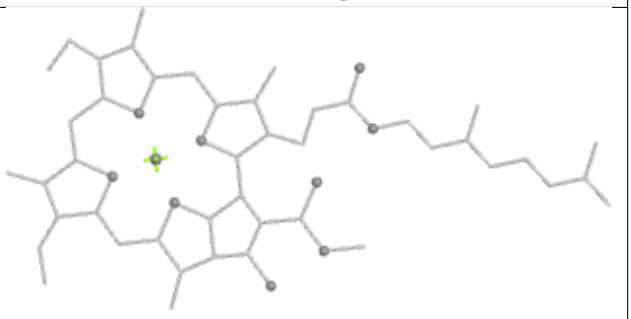
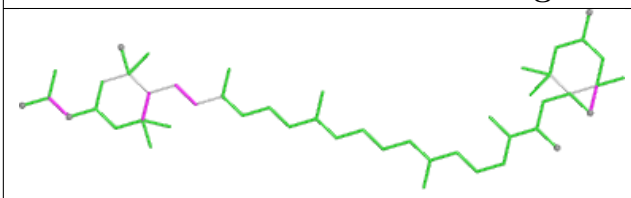


Rings

Ligand A86 5 301



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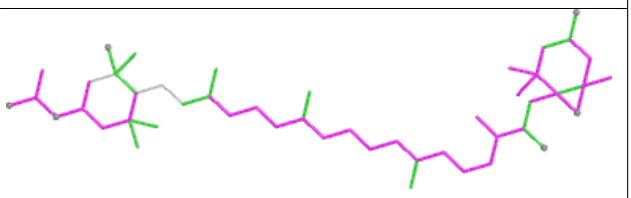

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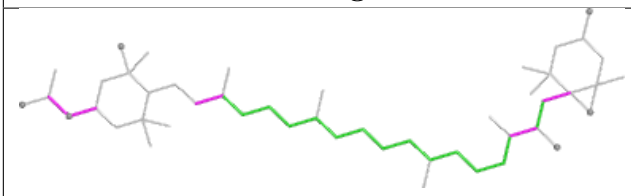

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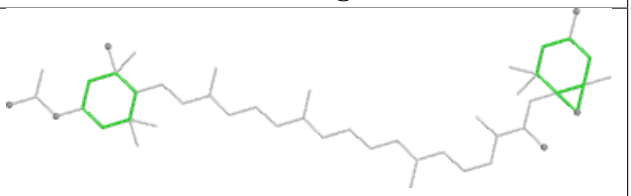

Rings

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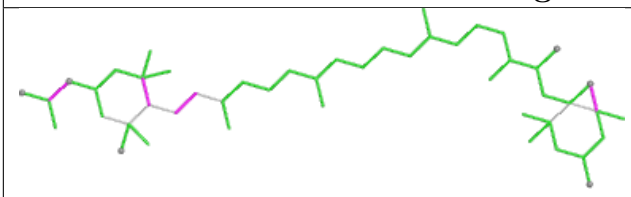

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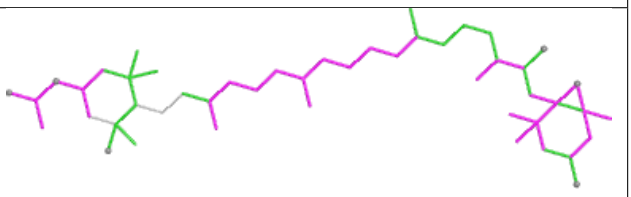

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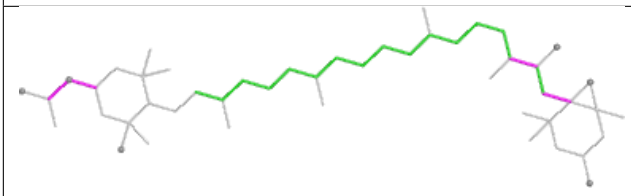
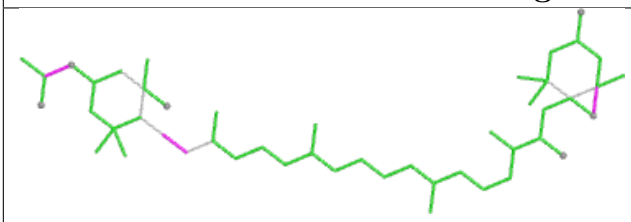


Torsions

Rings

Ligand A86 6 302



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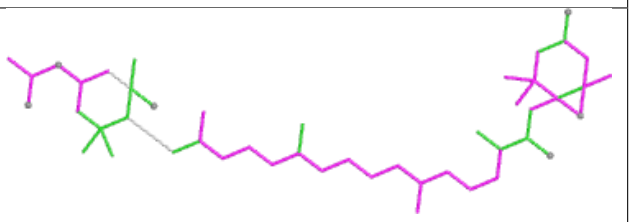

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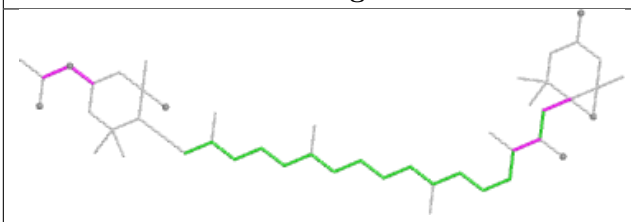

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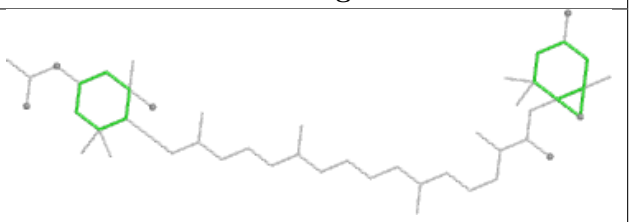

Rings

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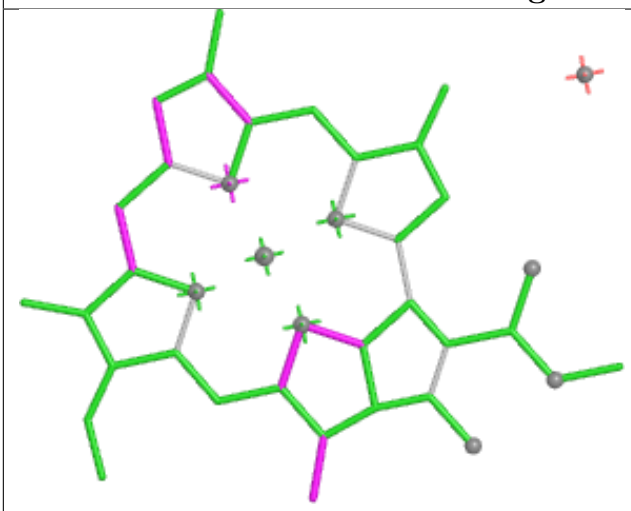

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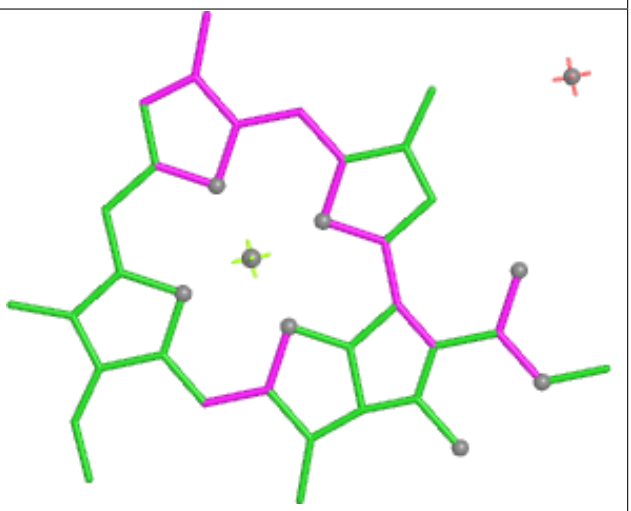

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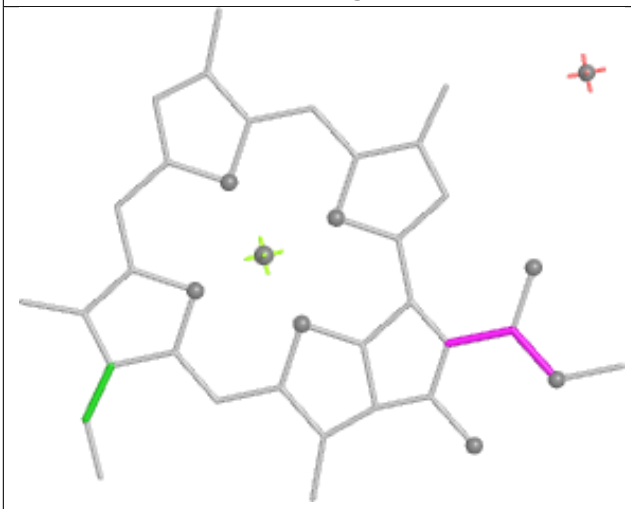

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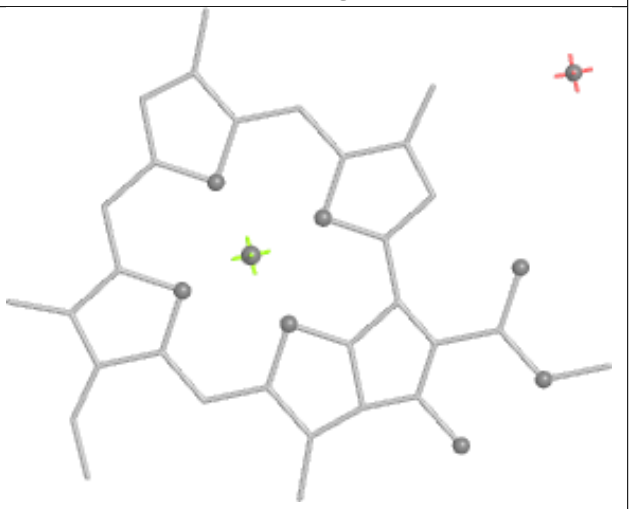
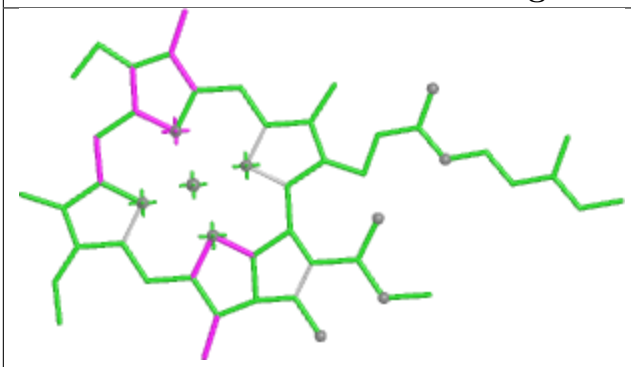
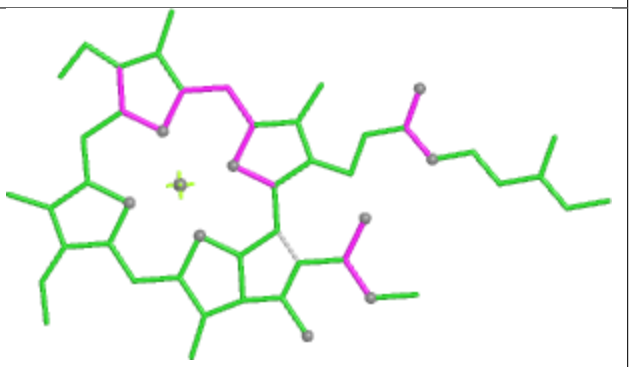


Rings

Ligand CLA 3 608	
	
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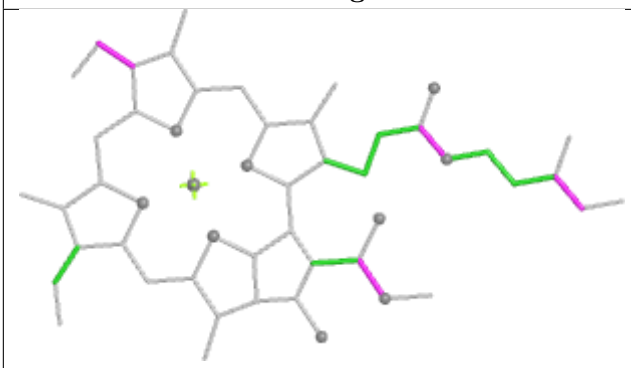
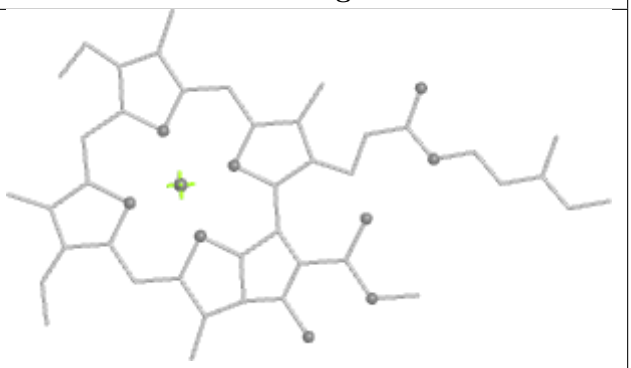
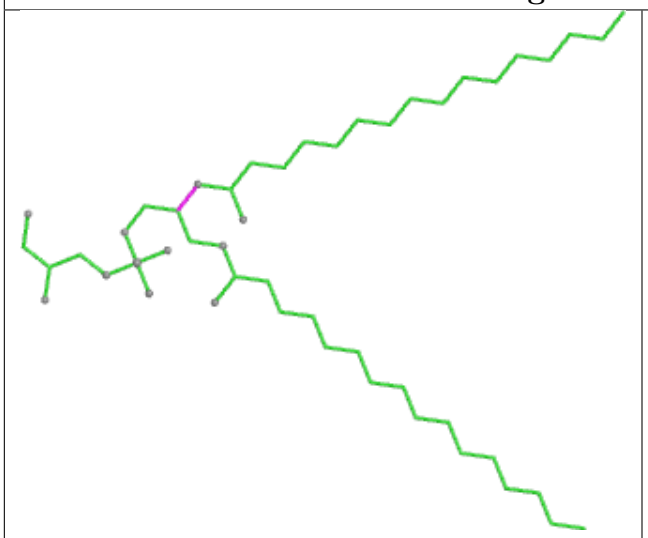
	
Torsions	**Rings**

Ligand LHG 3 618



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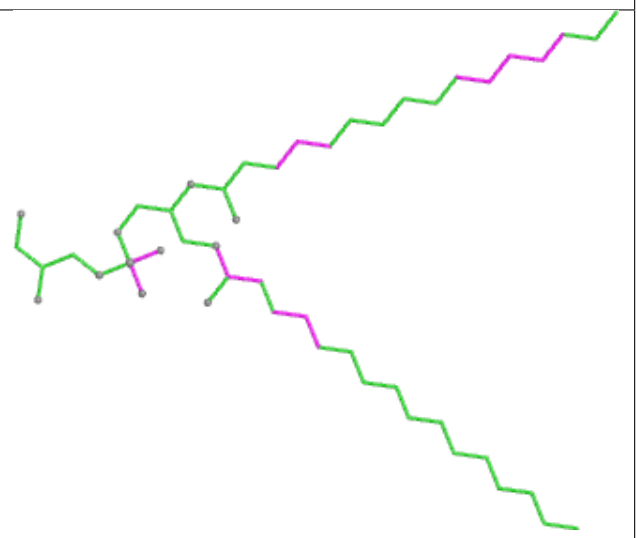
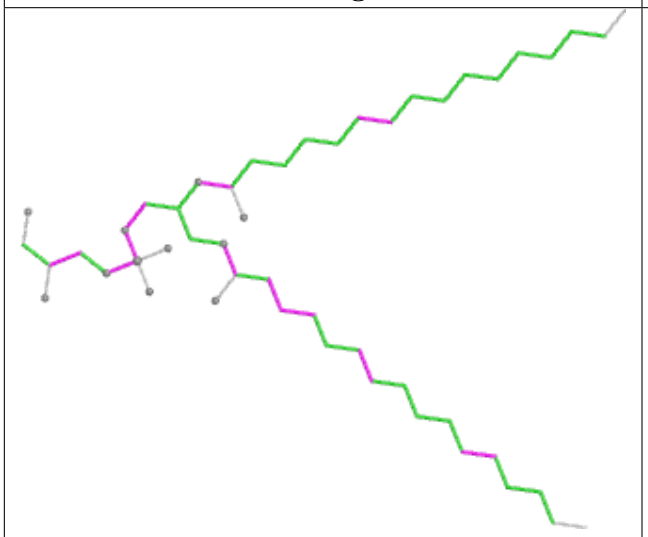


Bond angles



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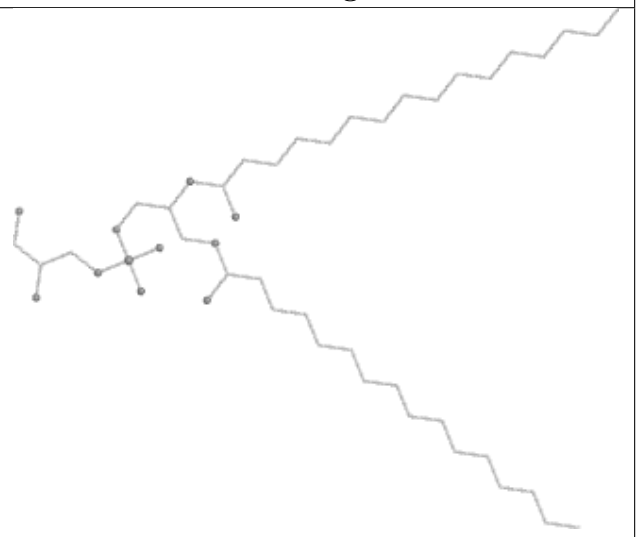
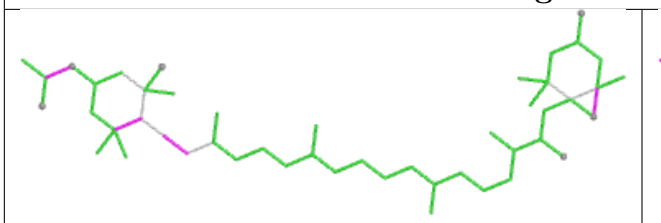


Rings

Ligand A86 4 302



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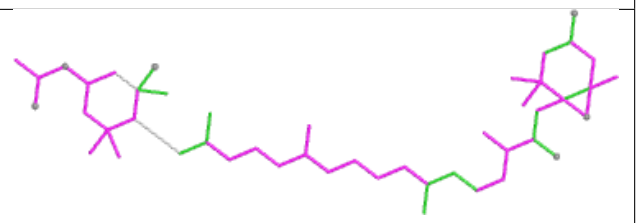

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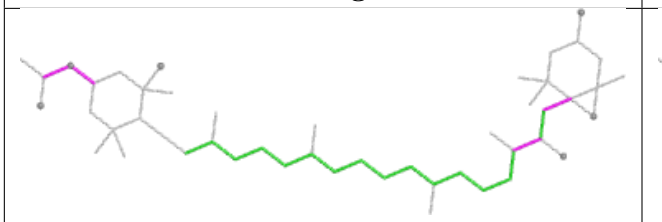

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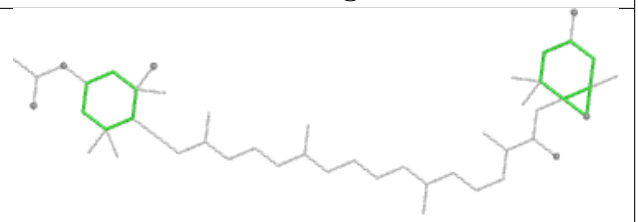
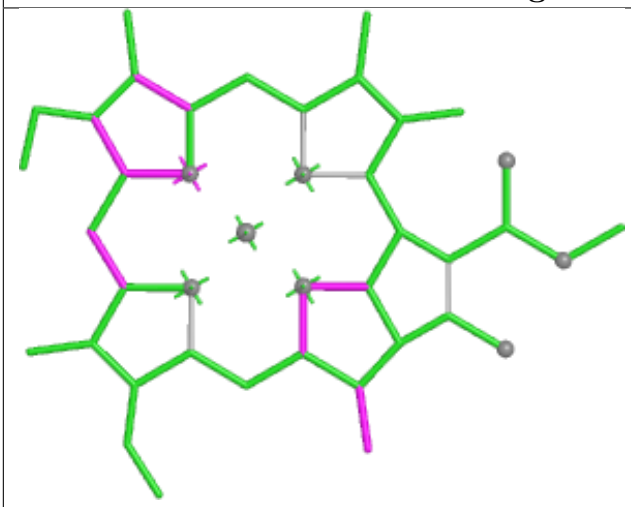


Rings

Ligand CLA 5 316



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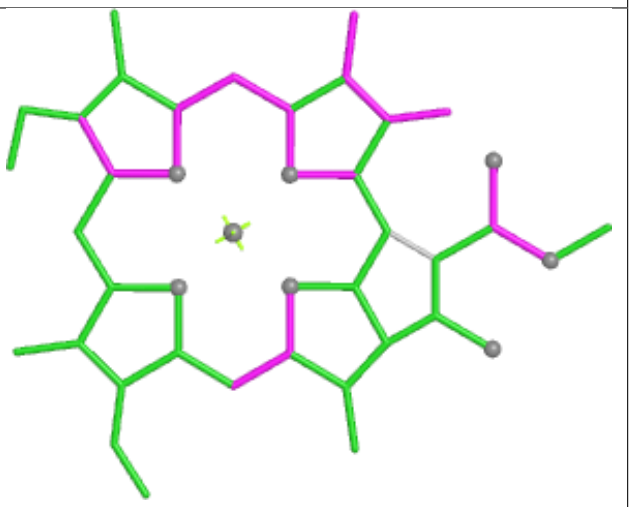
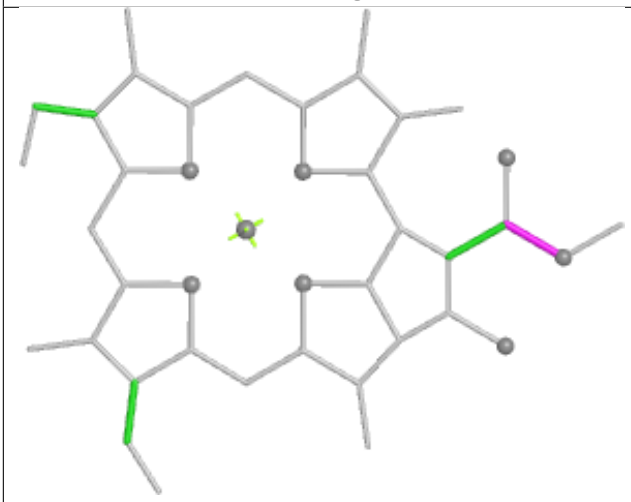


Bond angles



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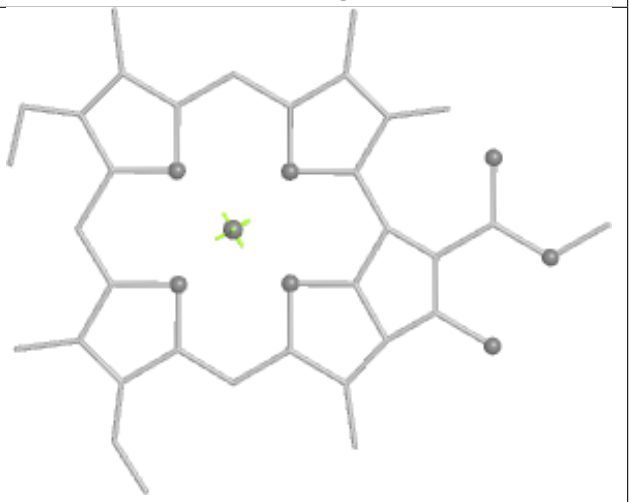
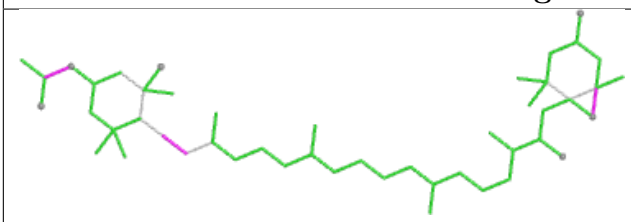


Rings

Ligand A86 6 304



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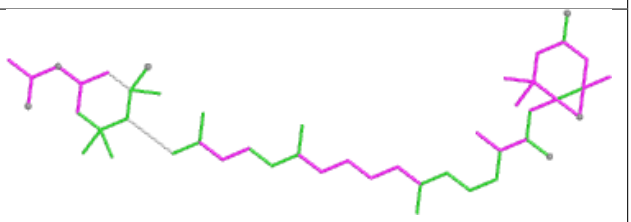
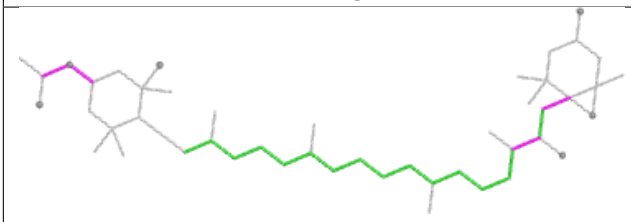


Bond angles



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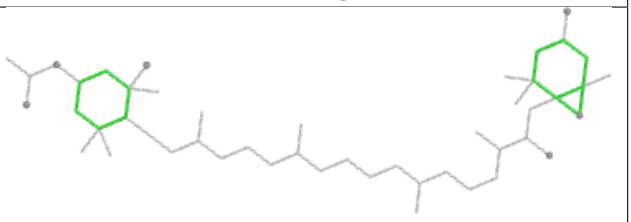
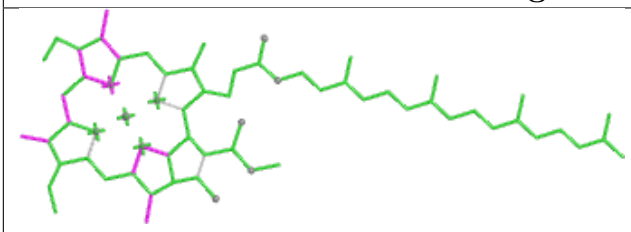


Rings

Ligand CLA 3 603



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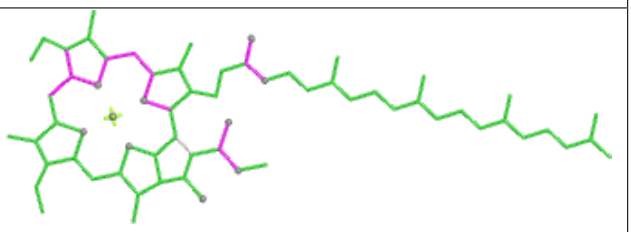
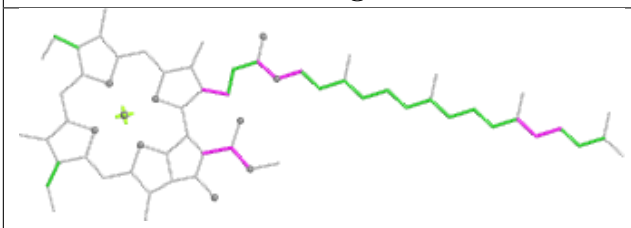


Bond angles



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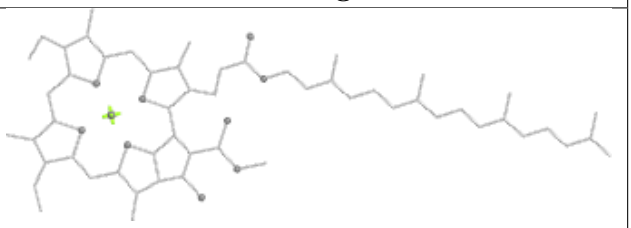
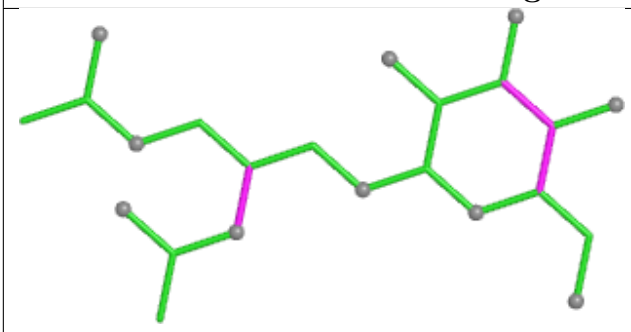


Rings

Ligand LMG 3 616



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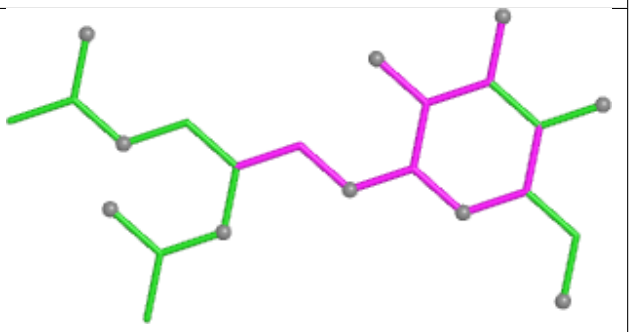
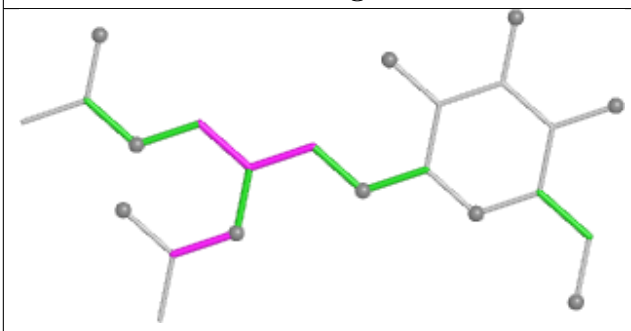


Bond angles



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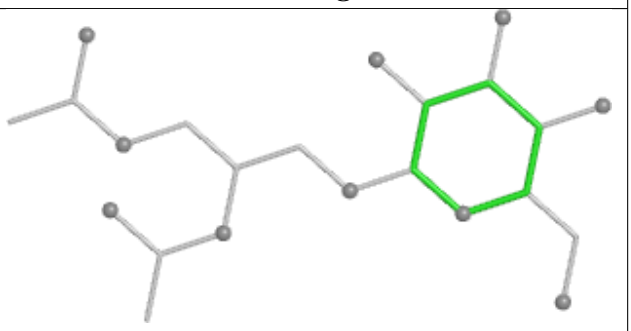
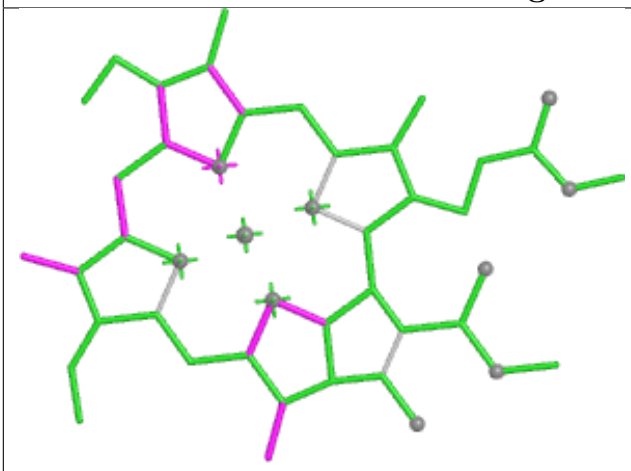


Rings

Ligand CLA 4 310



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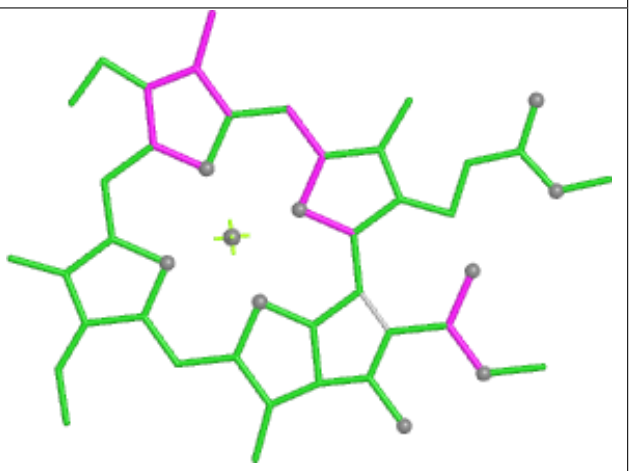
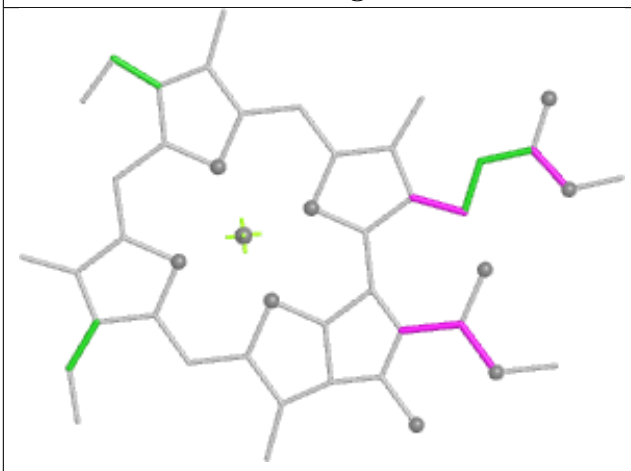


Bond angles



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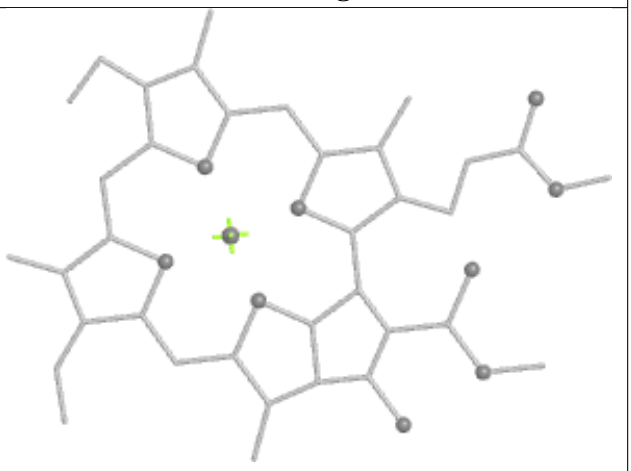
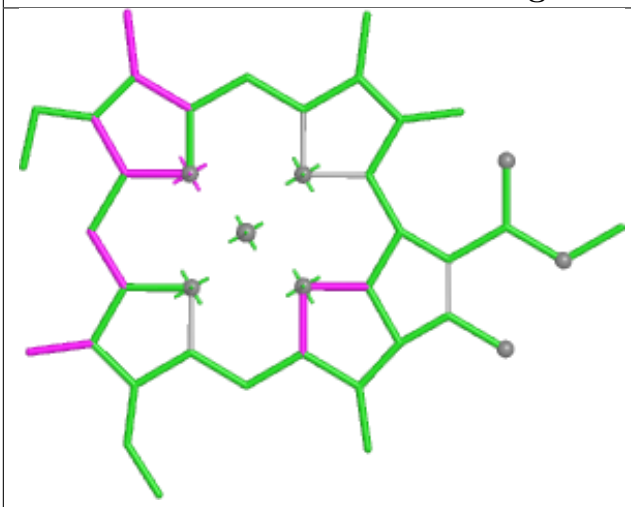


Rings

Ligand CLA 4 313



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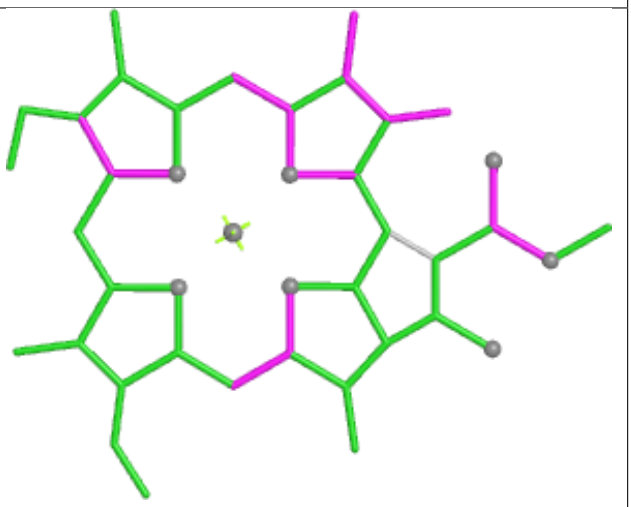
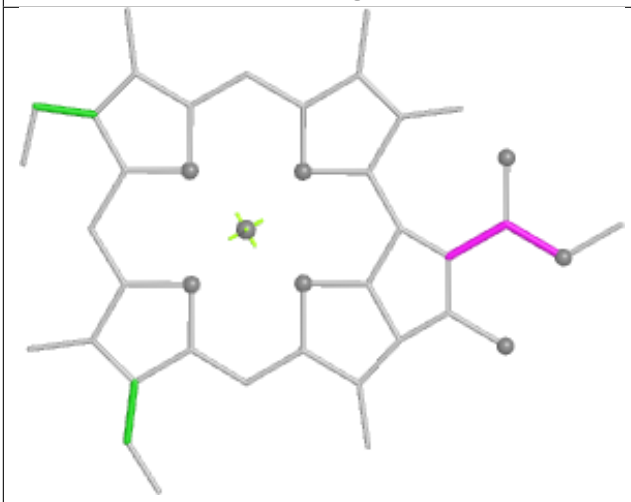
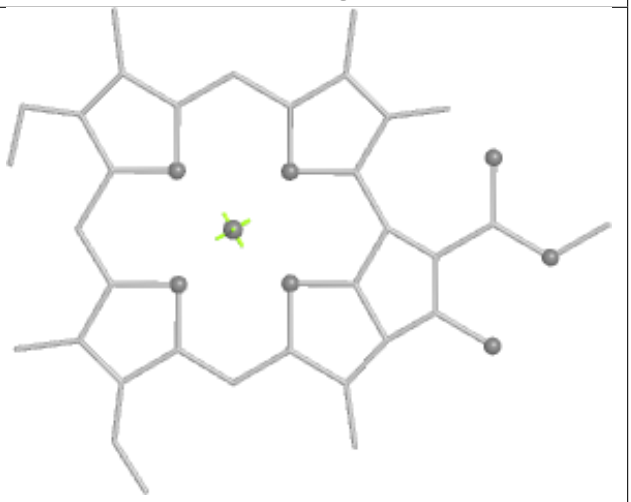


Bond angles

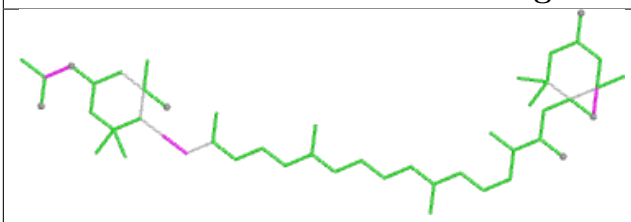


Torsions

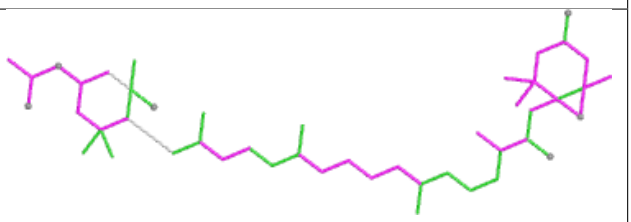


Rings

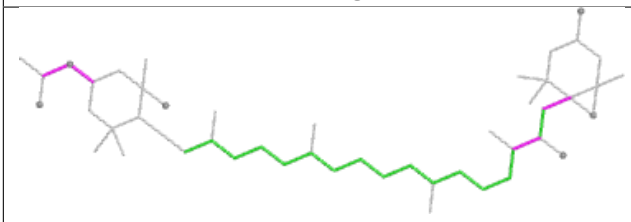
Ligand A86 5 303



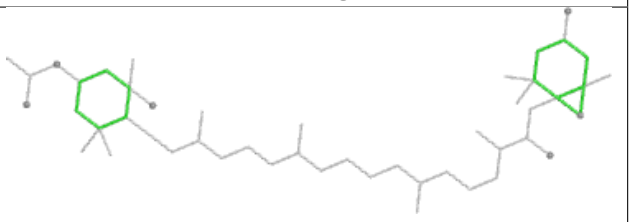
Bond lengths



Bond angles

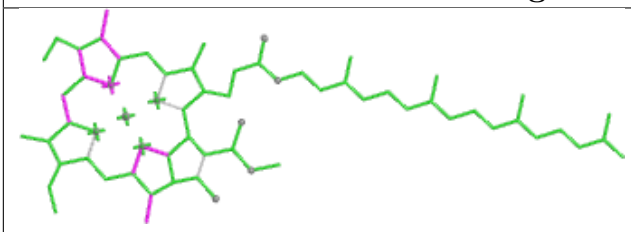


Torsions

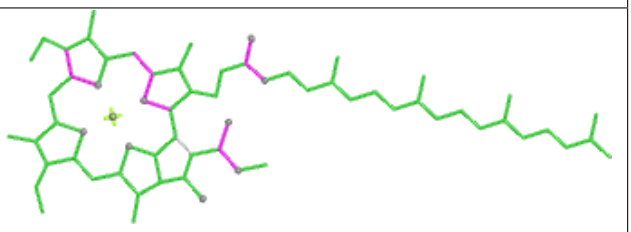


Rings

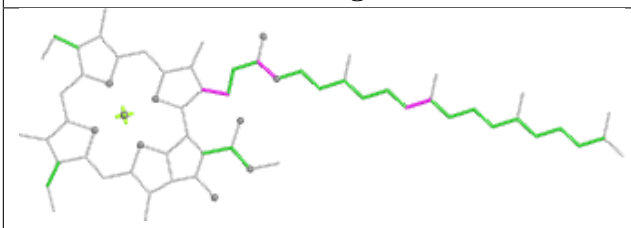
Ligand CLA 4 309



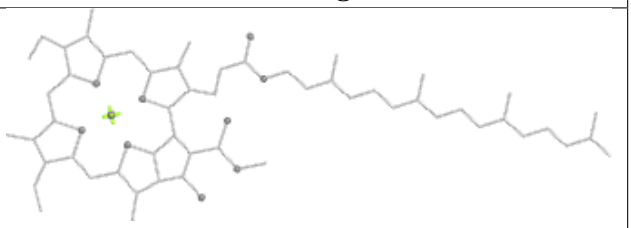
Bond lengths



Bond angles

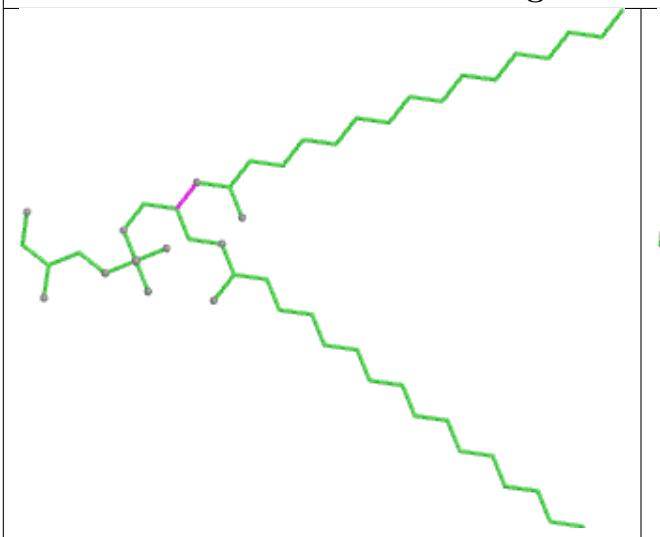


Torsions

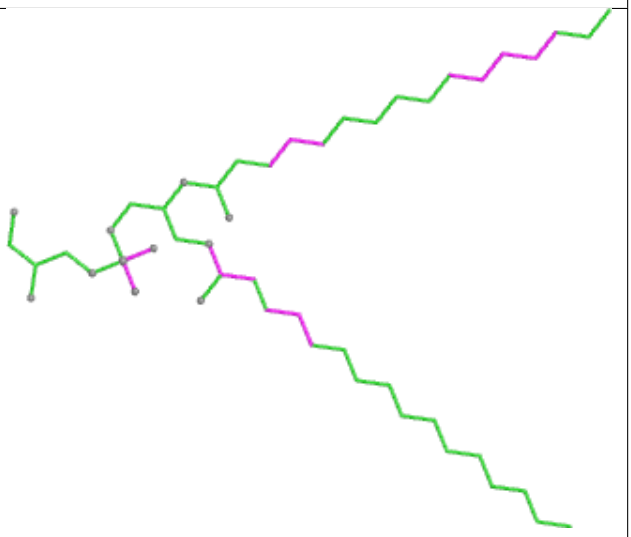


Rings

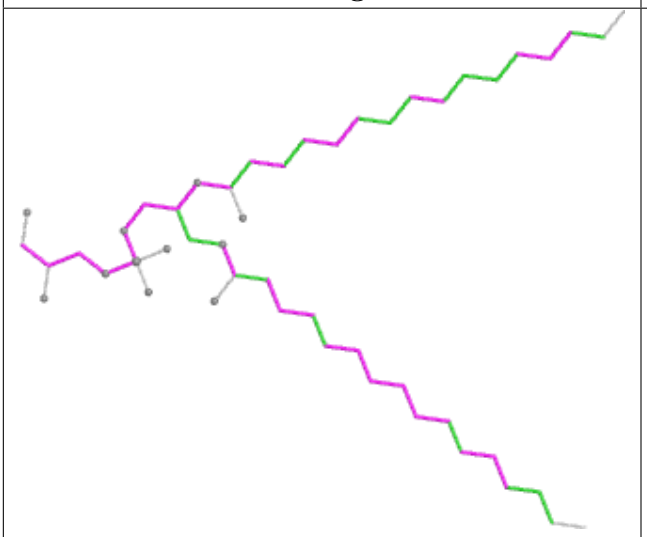
Ligand LHG 4 318



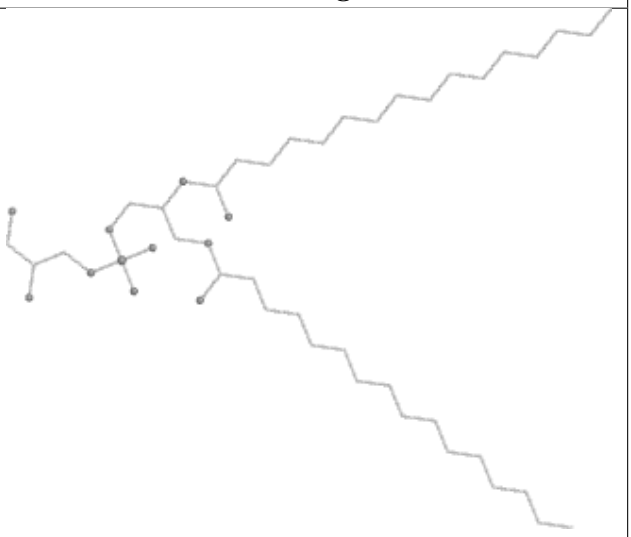
Bond lengths



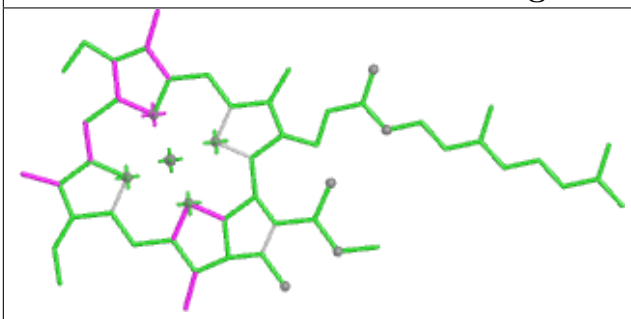
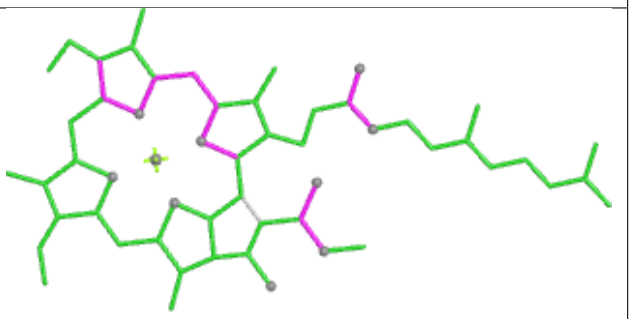
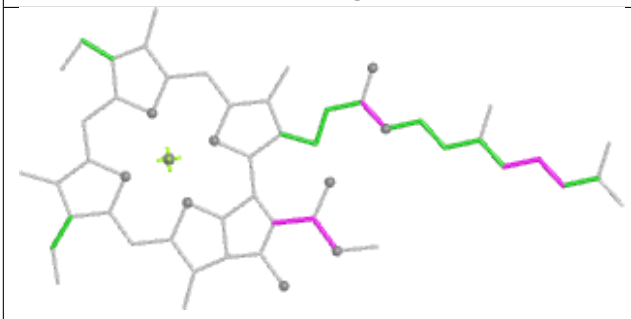
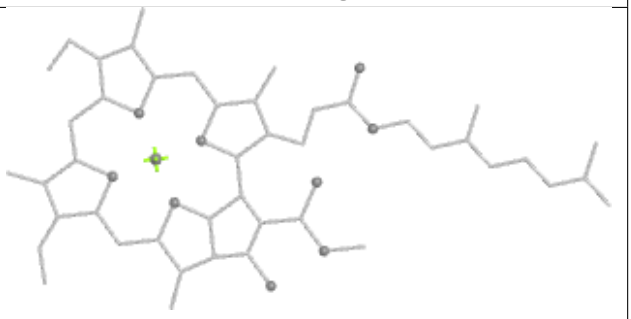
Bond angles

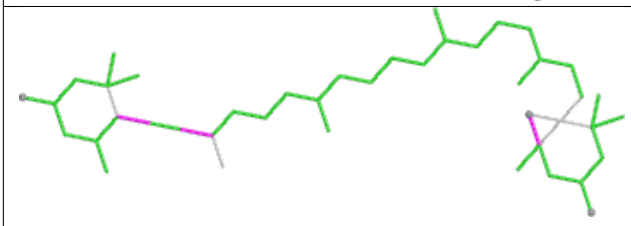
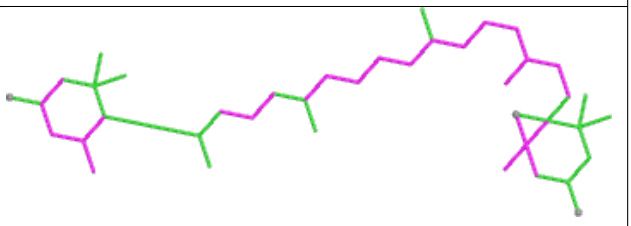
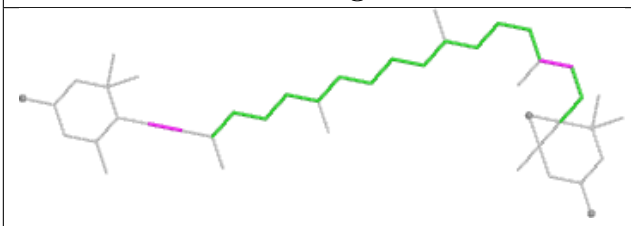
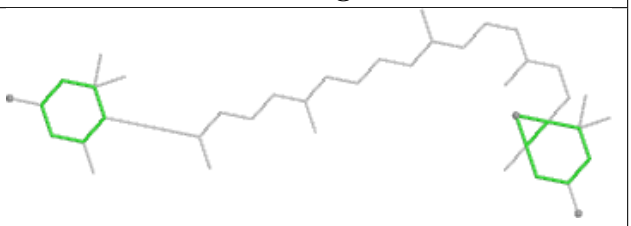


Torsions

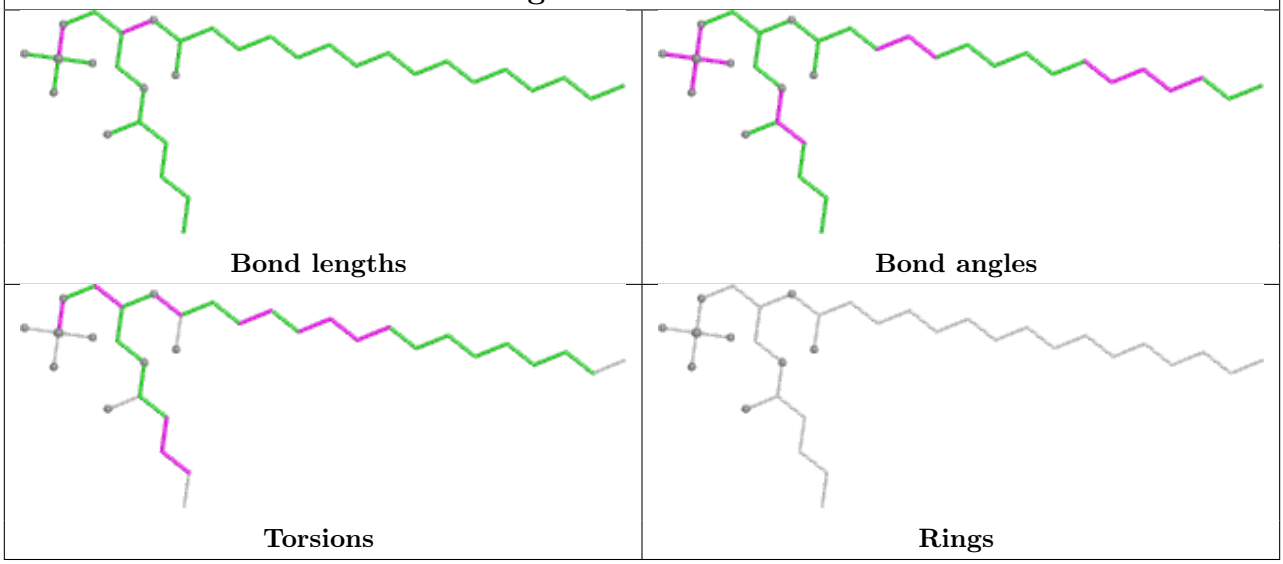


Rings

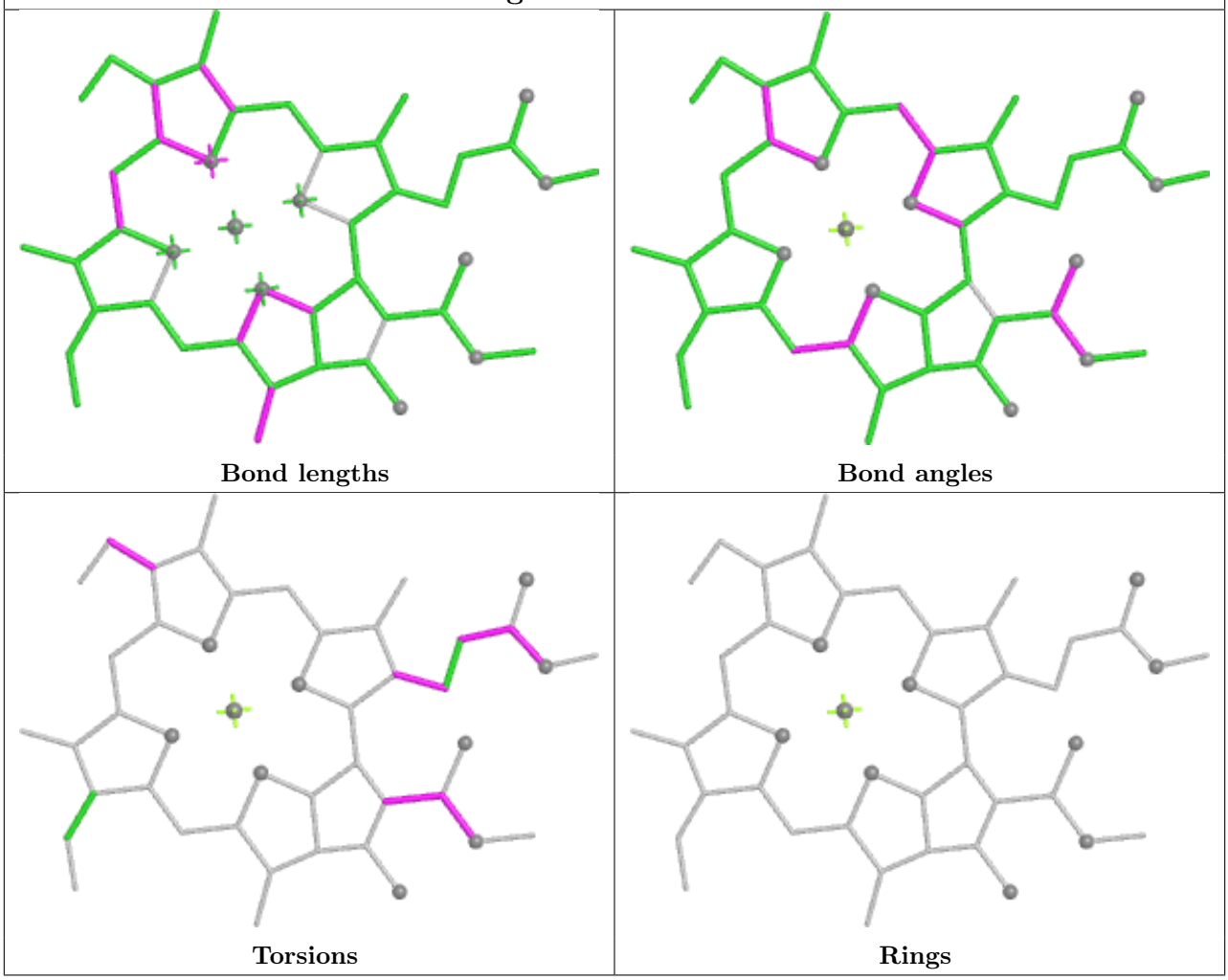
Ligand CLA 3 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

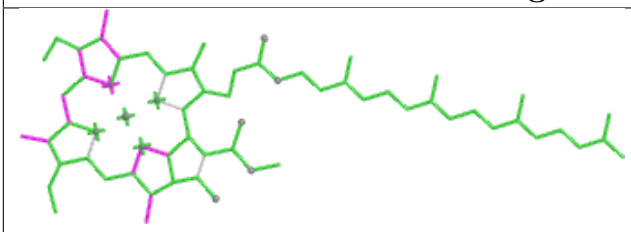
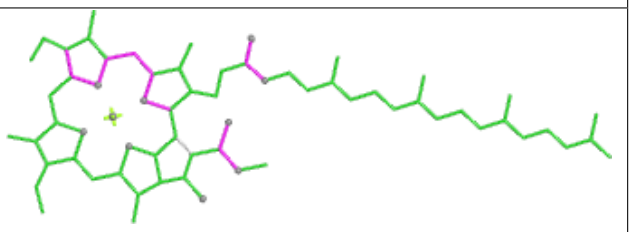
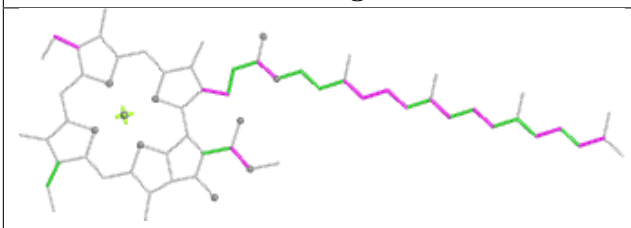
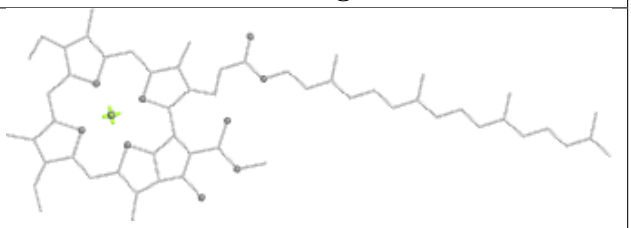
Ligand DD6 4 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

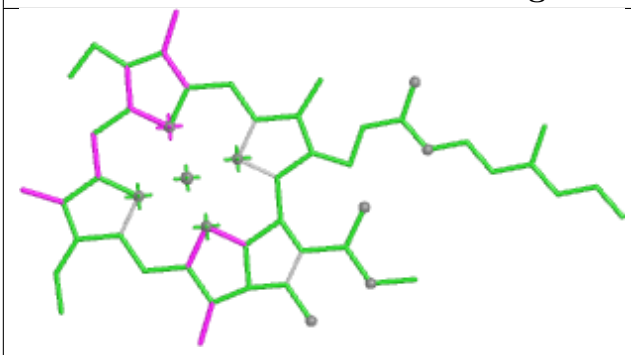
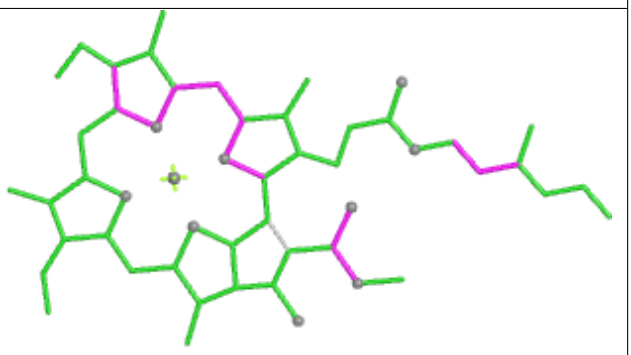
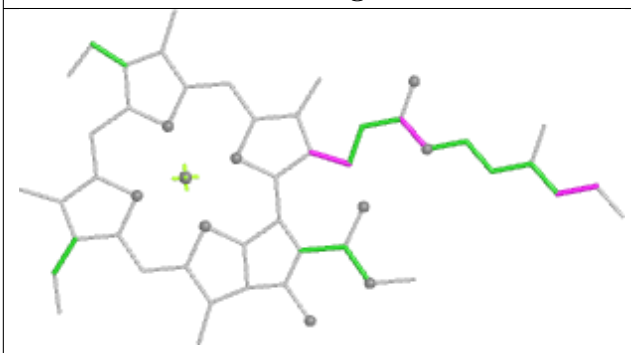
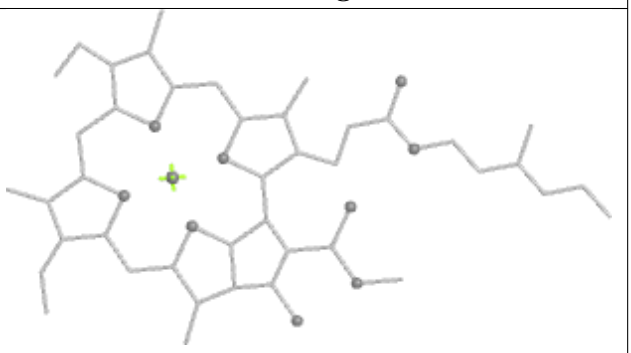
Ligand LHG 5 318



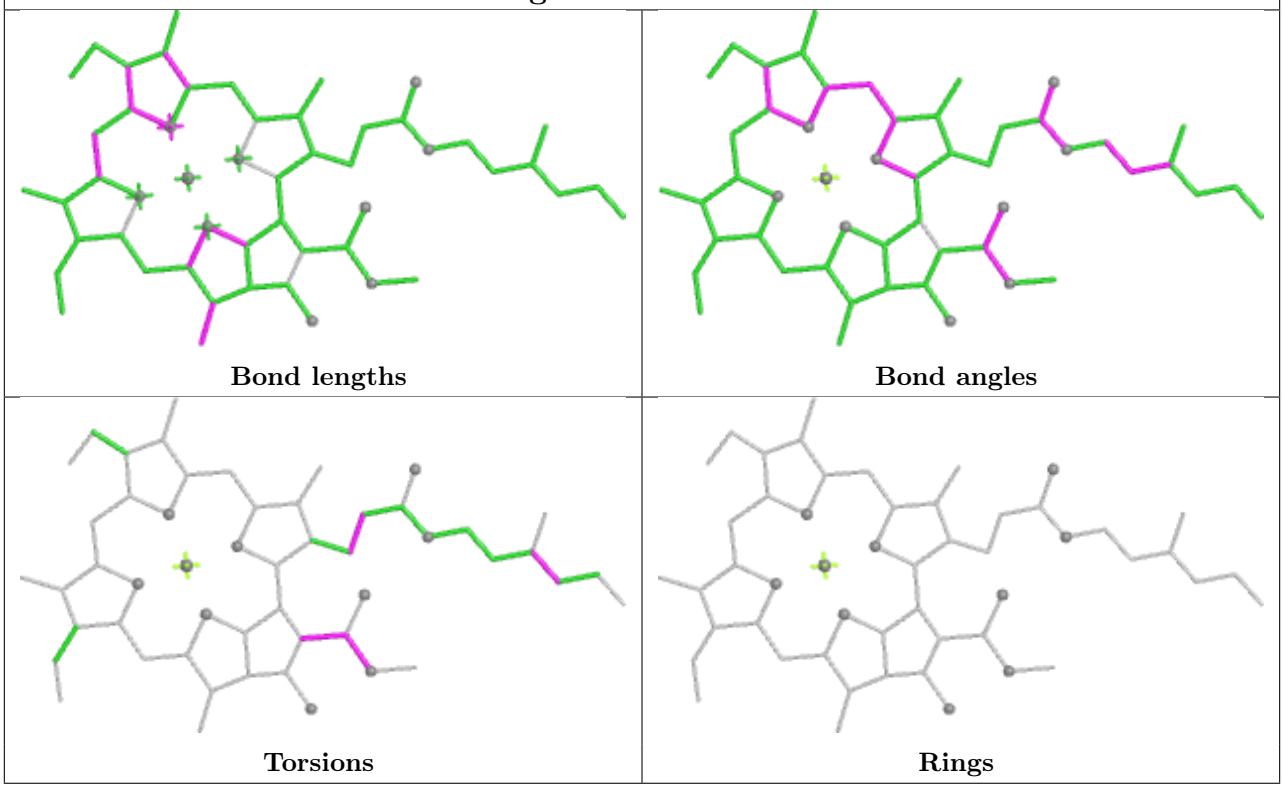
Ligand CLA 6 310



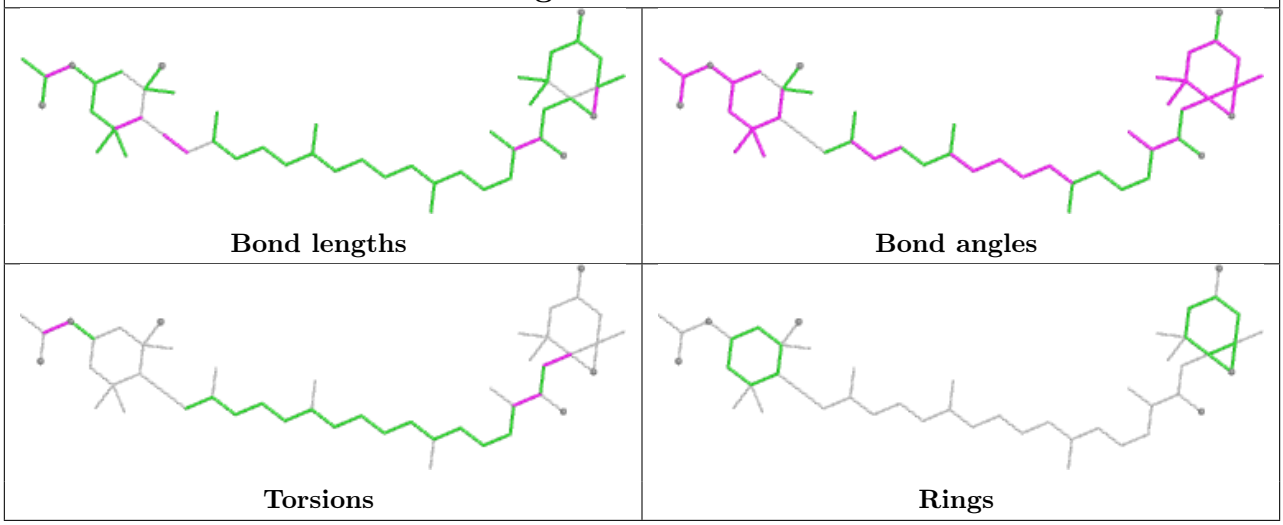
Ligand CLA 3 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 309



Ligand A86 4 304



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.

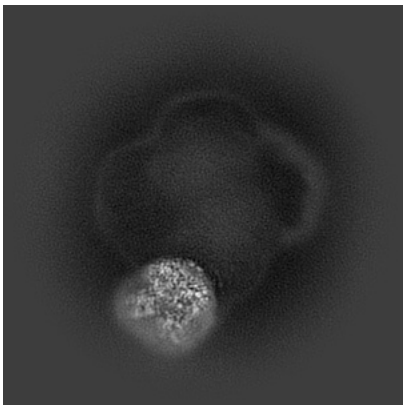
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35899. These allow visual inspection of the internal detail of the map and identification of artifacts.

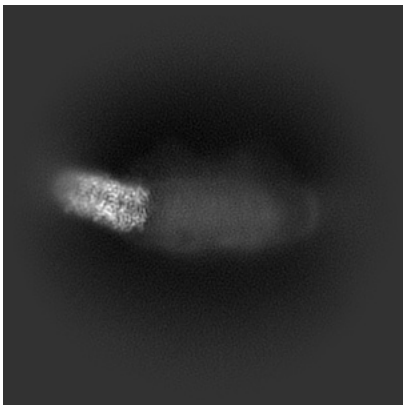
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

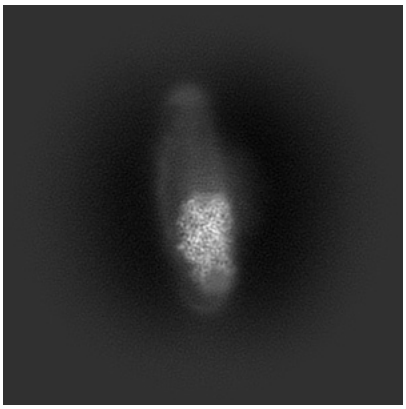
6.1.1 Primary map



X

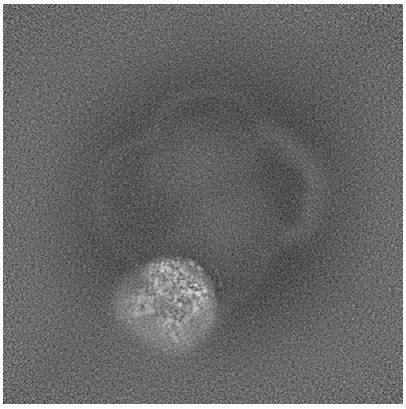


Y

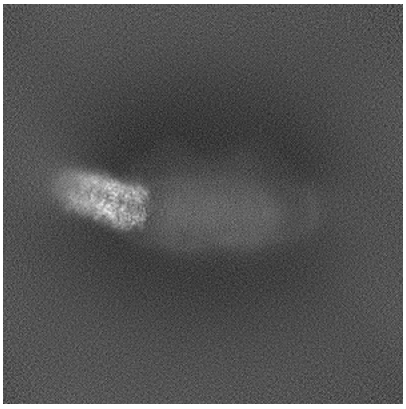


Z

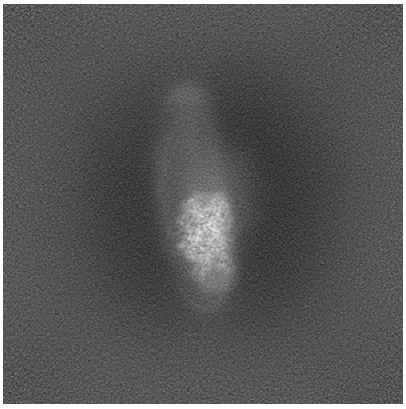
6.1.2 Raw map



X



Y

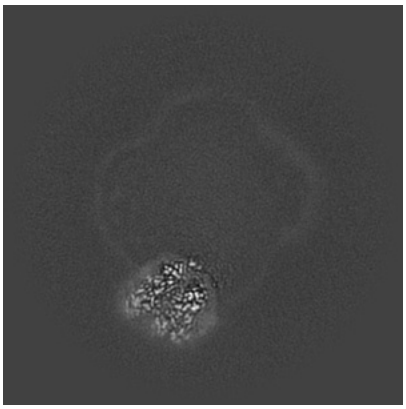


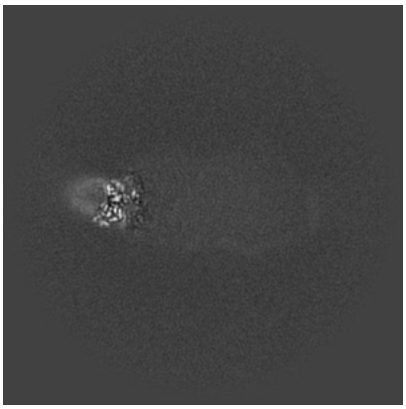
Z

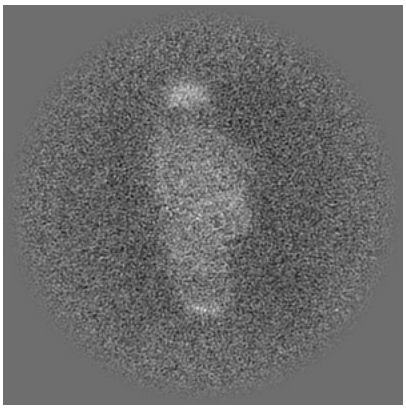
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

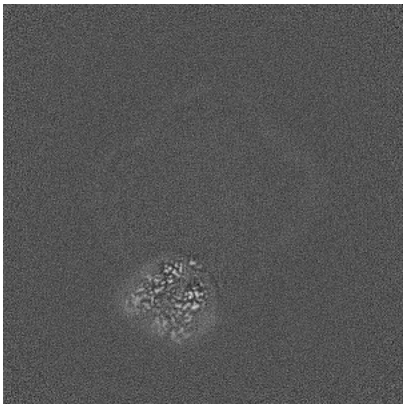
6.2.1 Primary map

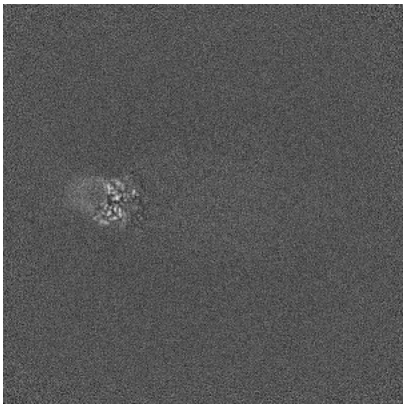

X Index: 250

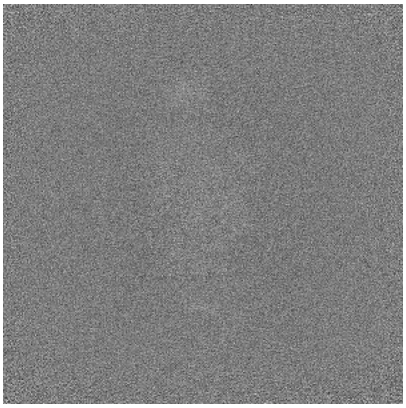

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

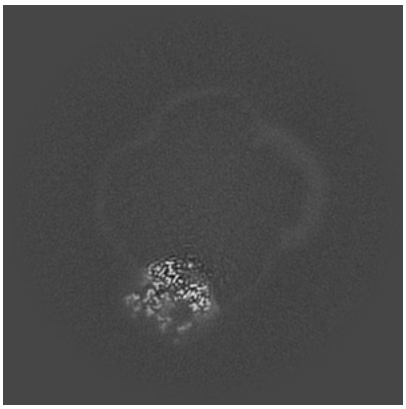

Y Index: 250


Z Index: 250

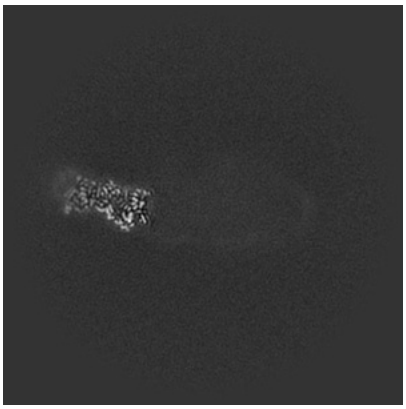
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

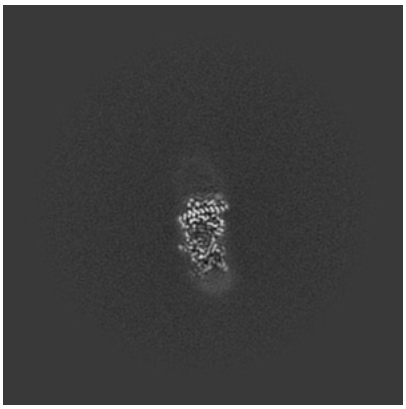
6.3.1 Primary map



X Index: 238

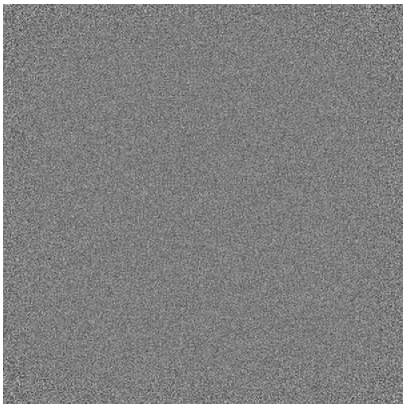


Y Index: 216

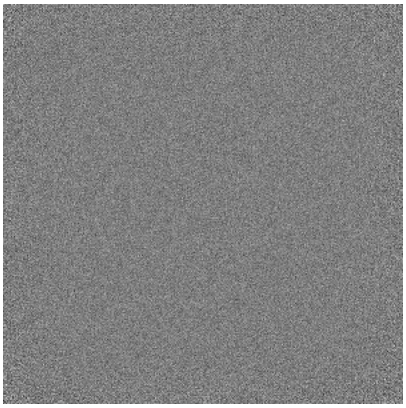


Z Index: 139

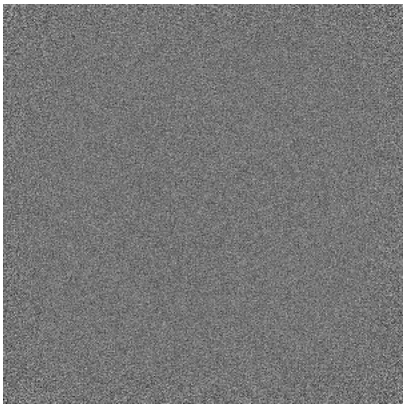
6.3.2 Raw map



X Index: 0



Y Index: 0

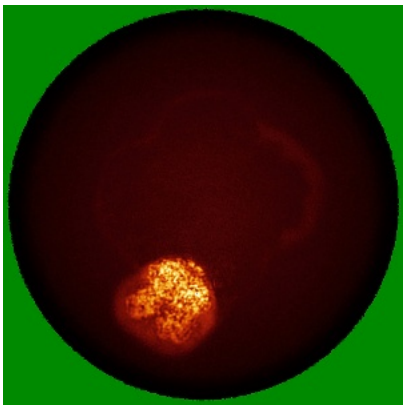


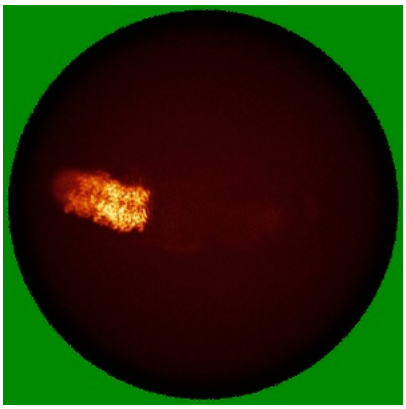
Z Index: 0

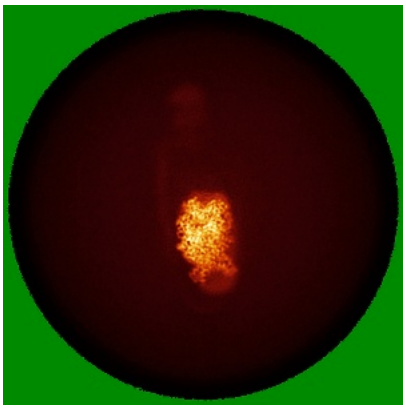
The images above show the largest variance slices of the map in three orthogonal directions.

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

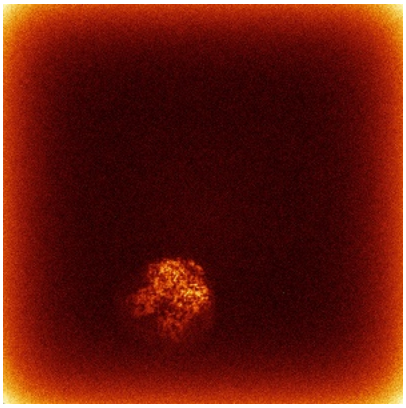
6.4.1 Primary map

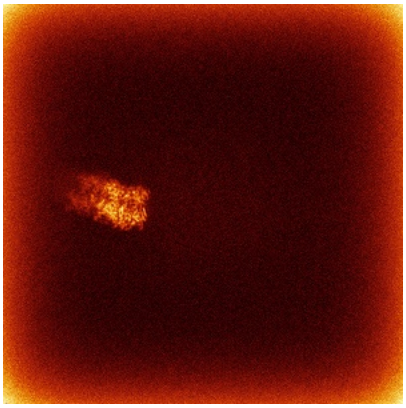

X

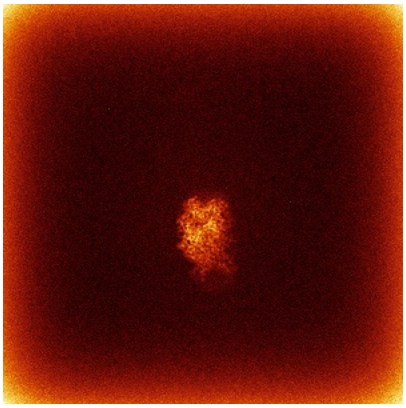

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

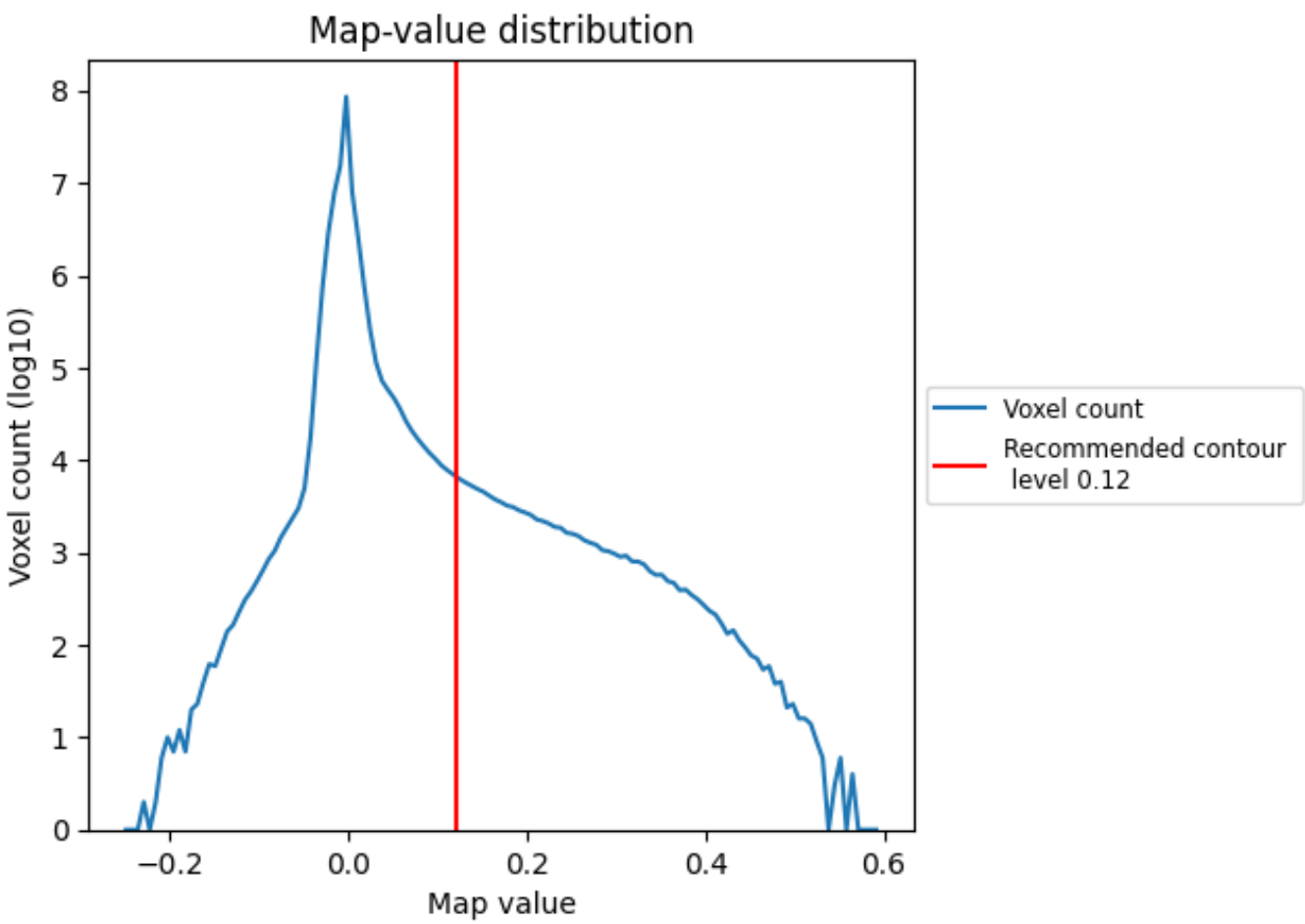
6.6 Mask visualisation (i)

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

7 Map analysis (i)

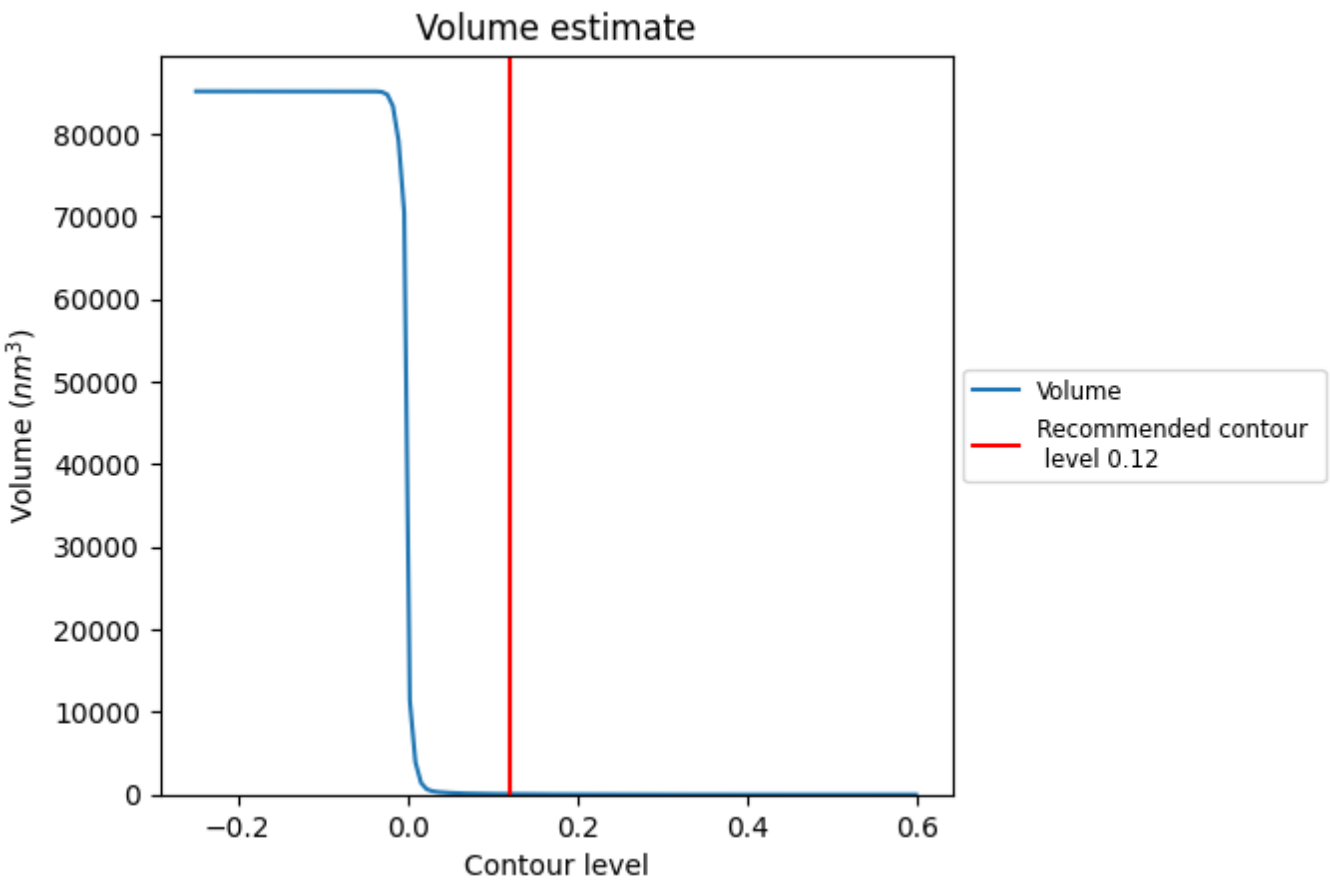
This section contains the results of statistical analysis of the map.

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.

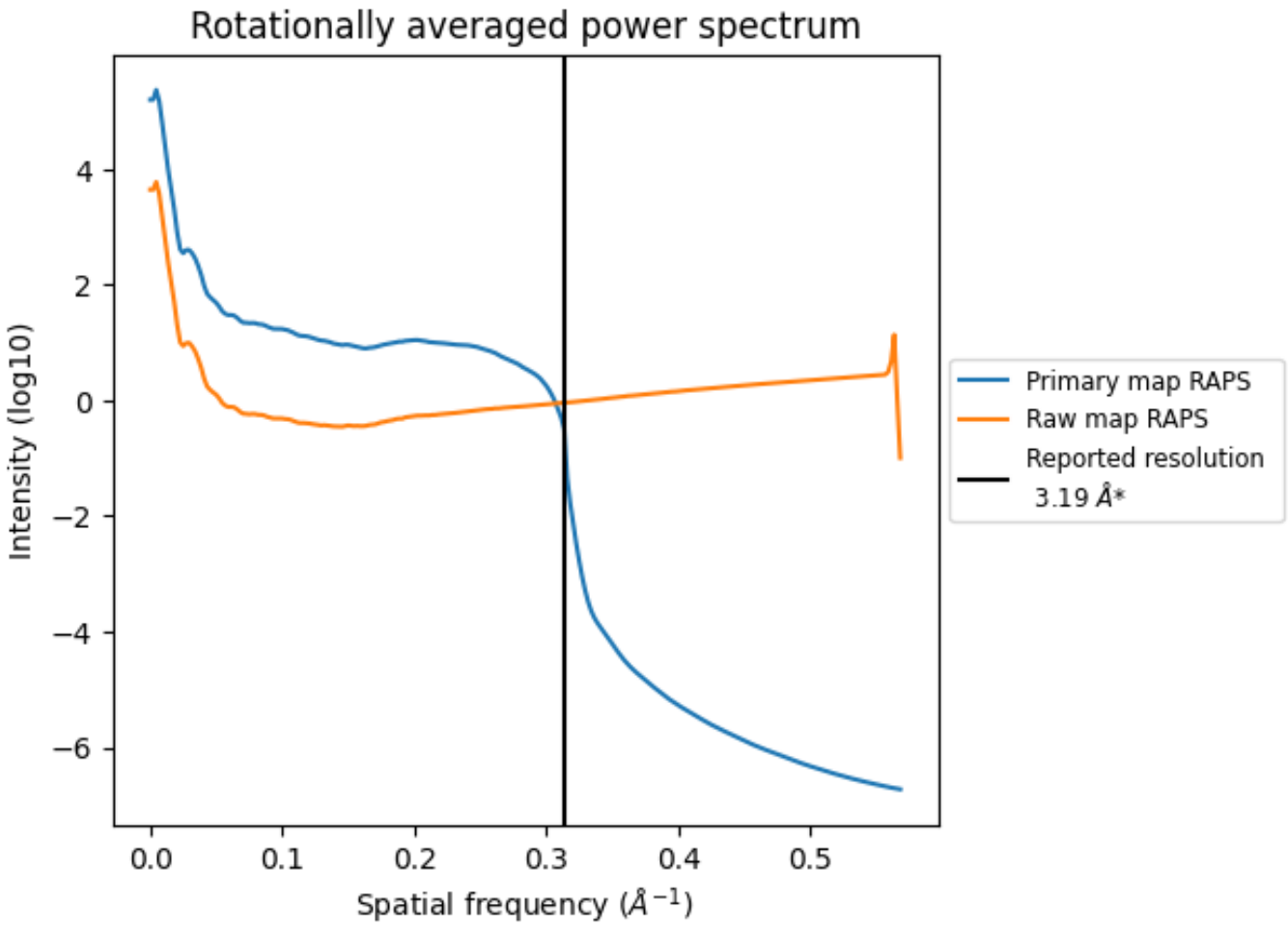
7.2 Volume estimate (i)



The volume at the recommended contour level is 61 nm^3; this corresponds to an approximate mass of 55 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)

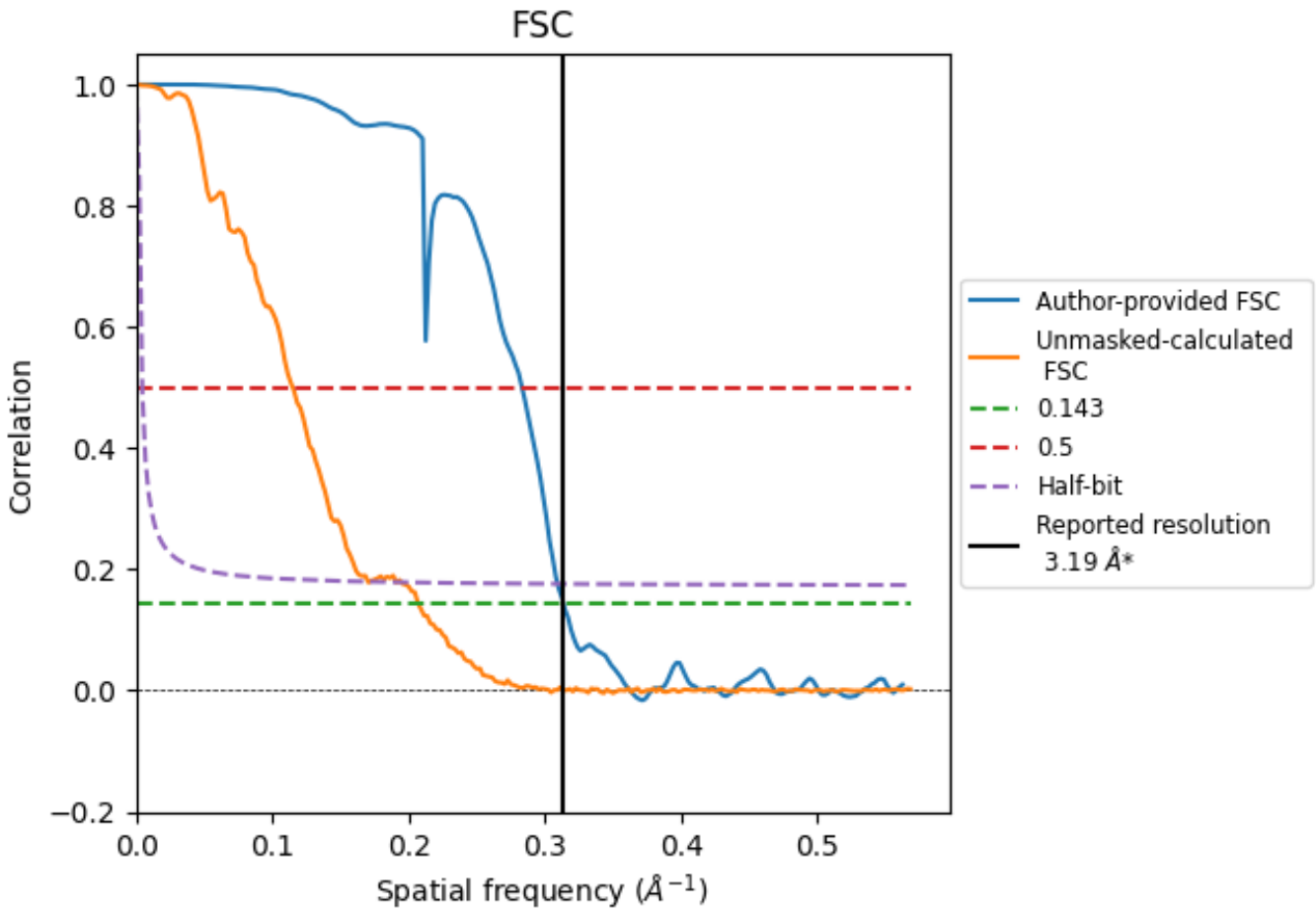


*Reported resolution corresponds to spatial frequency of 0.313 Å^{-1}

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 0.313 Å^{-1}

8.2 Resolution estimates (i)

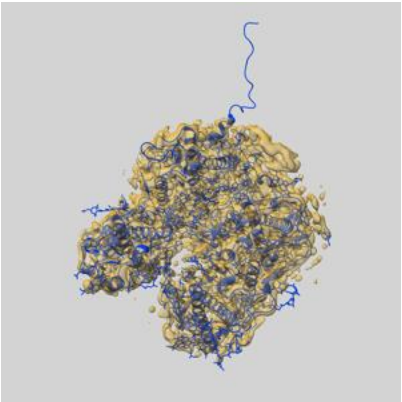
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.19	3.53	3.23
Unmasked-calculated*	4.83	8.70	5.88

*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 4.83 differs from the reported value 3.19 by more than 10 %

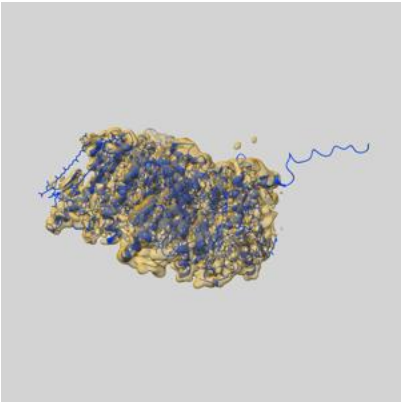
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35899 and PDB model 8J0D. Per-residue inclusion information can be found in section 3 on page 14.

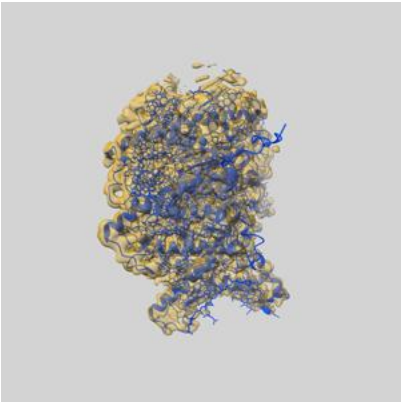
9.1 Map-model overlay (i)



X



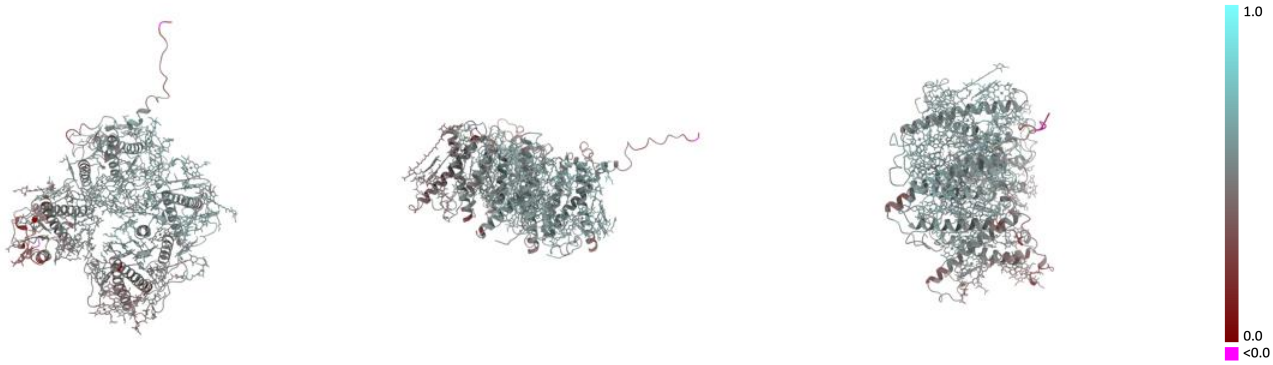
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

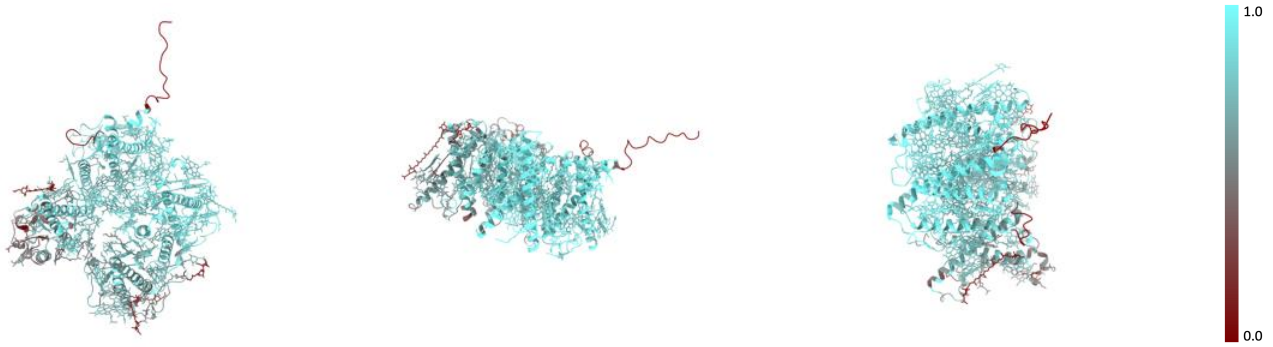
9.2 Q-score mapped to coordinate model (i)



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.

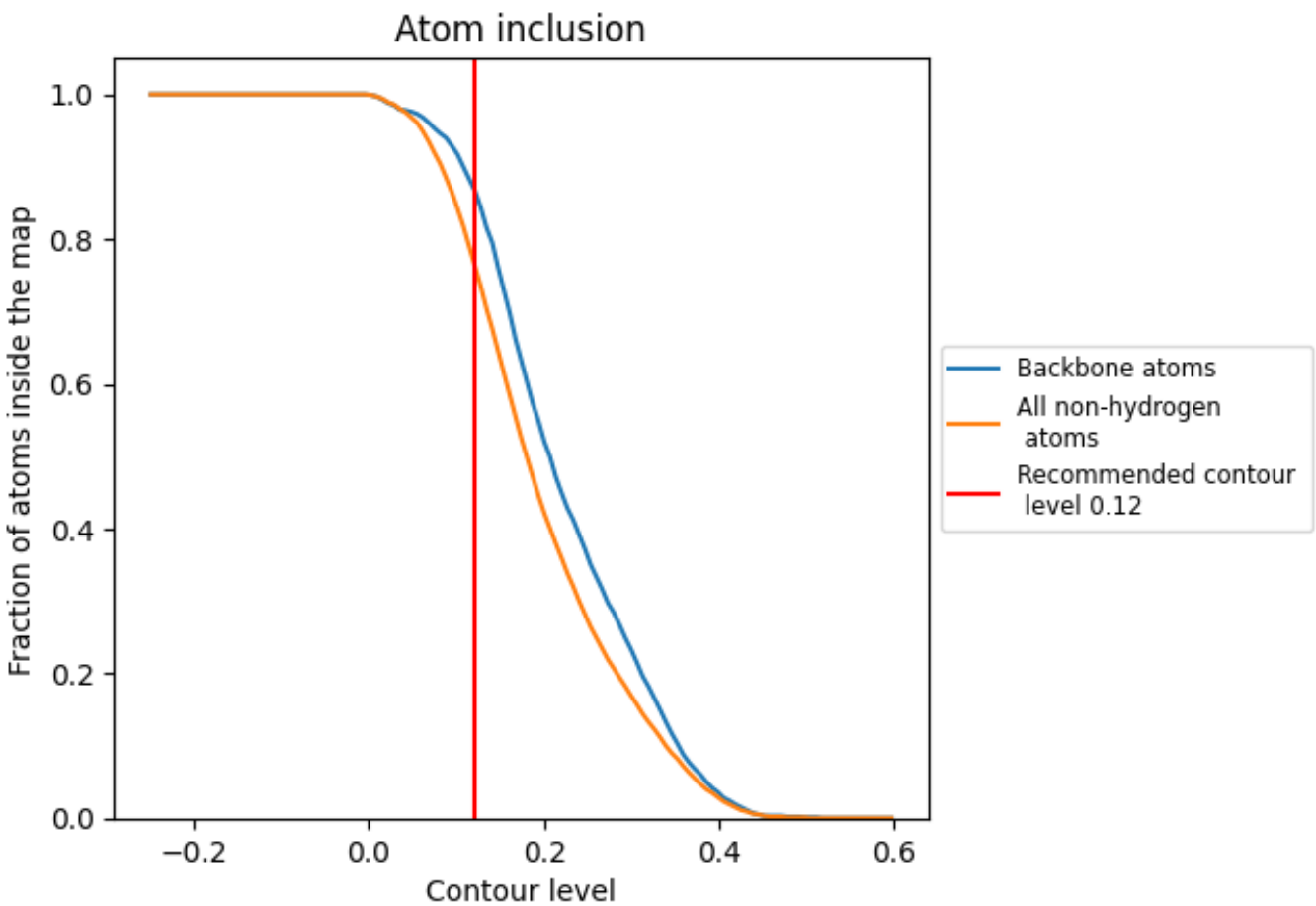
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 77% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7690	0.4980
3	0.8220	0.5230
4	0.9060	0.5420
5	0.6710	0.4700
6	0.6570	0.4470