wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 08:44 PM JST

PDB ID	:	8XKL / pdb_00008xkl
EMDB ID	:	EMD-38419
Title	:	Structure of ACPII-CCPII from cryptophyte algae
Authors	:	Li, X.Y.; Mao, Z.Y.; Shen, J.R.; Han, G.Y.
Deposited on	:	2023-12-23
Resolution	:	2.84 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 (1)) were used in the production of this report:

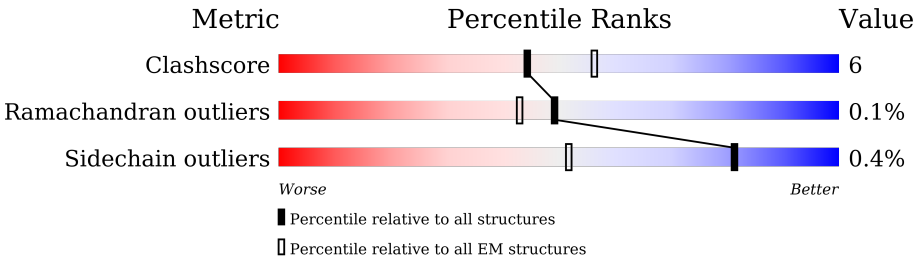
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

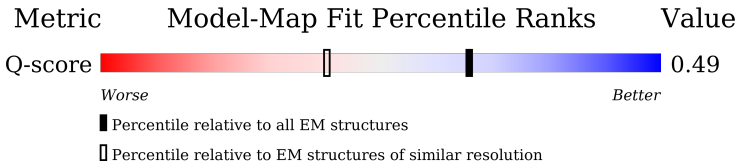
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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	0	226	5% 65% 10% 24%
2	7	235	6% 68% 14% 17%
3	8	217	63% 17% 20%
4	9	222	• 70% 10% 20%

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Mol	Chain	Length	Quality of chain
5	G	64	55% 100%
6	P	220	70% 9% 21%
7	p	218	6% 72% 14% 14%
8	s	285	42% 63% 8% 29%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 15357 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 ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	172	1308	845	225	229	9	0	0

- Molecule 2 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	7	194	1472	946	256	262	8	0	0

- Molecule 3 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	8	173	1362	899	222	238	3	0	0

- Molecule 4 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	9	178	1371	885	230	247	9	0	0

- Molecule 5 is a protein called Photosystem II reaction center protein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	G	64	320	192	64	64	0	0

- Molecule 6 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	P	173	1344	878	221	237	8	0	0

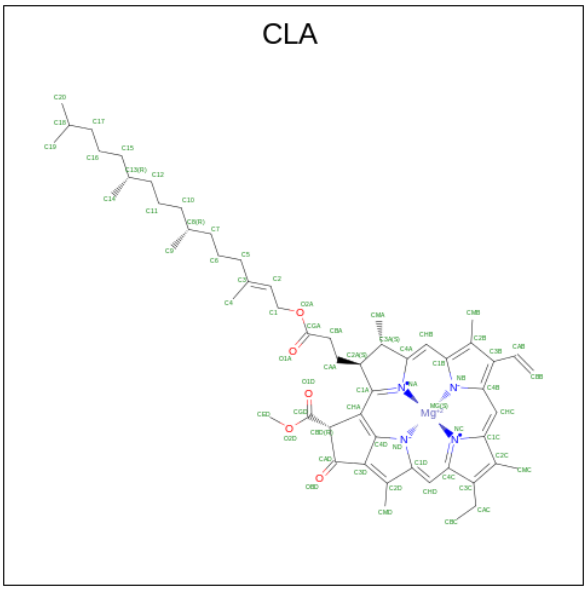
- Molecule 7 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	p	187	1471	956	243	267	5	0	0

- Molecule 8 is a protein called CCPII-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	s	203	1563	1005	255	299	4	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	0	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
9	0	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
9	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
9	7	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
9	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
9	8	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
9	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
9	9	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
9	9	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	9	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	P	1	42	34	1	4	3	0

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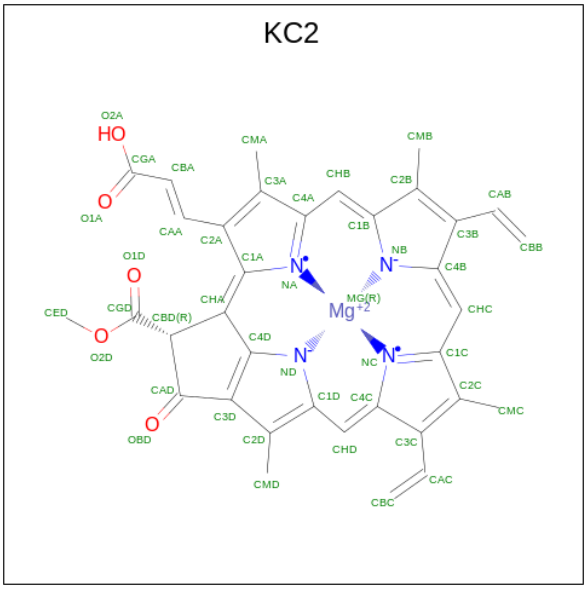
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	P	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
9	P	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
9	P	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
9	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	P	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
9	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
9	p	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
9	p	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	p	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	s	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
9	s	1	65	55	1	4	5	0

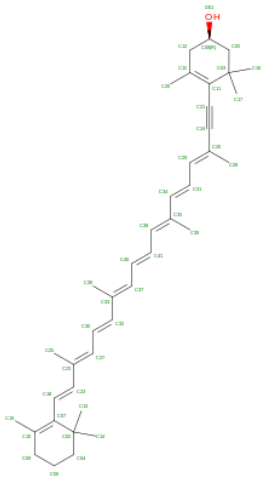
- Molecule 10 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
10	0	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
10	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
10	8	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
10	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
10	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
10	p	1	45	35	1	4	5	0

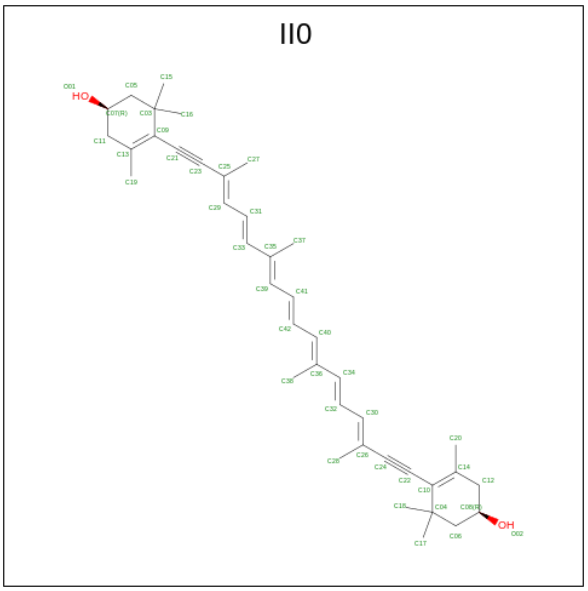
- Molecule 11 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$).

IHT



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	0	1	41	40	1	0
			Total	C	O	
11	0	1	41	40	1	0
			Total	C	O	
11	7	1	41	40	1	0
			Total	C	O	
11	8	1	41	40	1	0
			Total	C	O	
11	p	1	41	40	1	0

- Molecule 12 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
12	0	1	42	40	2	0
			Total	C	O	
12	0	1	42	40	2	0
			Total	C	O	
12	0	1	42	40	2	0
			Total	C	O	
12	7	1	42	40	2	0
			Total	C	O	
12	7	1	42	40	2	0
			Total	C	O	
12	7	1	42	40	2	0
			Total	C	O	
12	7	1	42	40	2	0
			Total	C	O	
12	8	1	42	40	2	0
			Total	C	O	
12	8	1	42	40	2	0
			Total	C	O	
12	8	1	42	40	2	0
			Total	C	O	
12	8	1	42	40	2	0
			Total	C	O	
12	9	1	42	40	2	0
			Total	C	O	
12	9	1	42	40	2	0
			Total	C	O	
12	9	1	42	40	2	0

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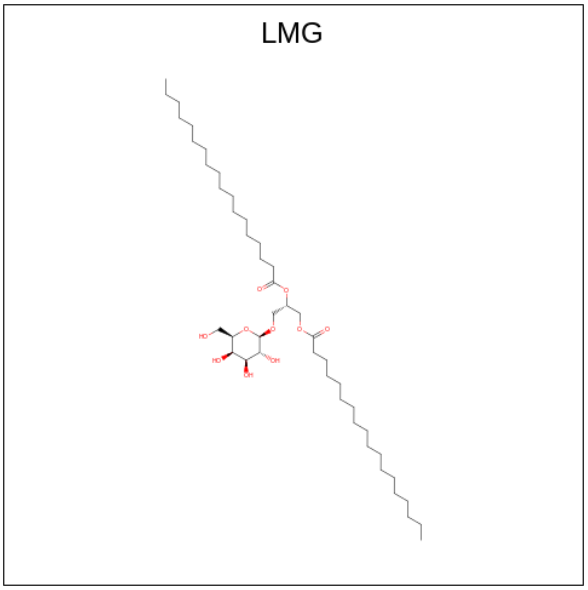
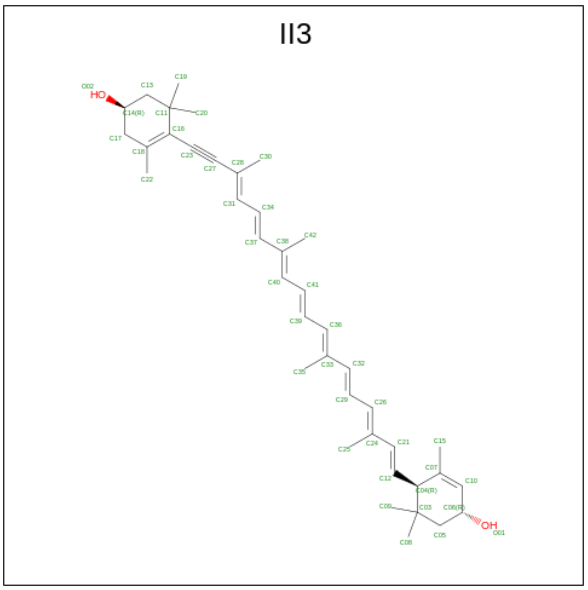
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
12	P	1	42	40	2	0
			Total	C	O	
12	P	1	42	40	2	0
			Total	C	O	
12	p	1	42	40	2	0
			Total	C	O	
12	p	1	42	40	2	0
			Total	C	O	
12	p	1	42	40	2	0
			Total	C	O	
12	p	1	42	40	2	0
			Total	C	O	
12	p	1	42	40	2	0

- Molecule 13 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



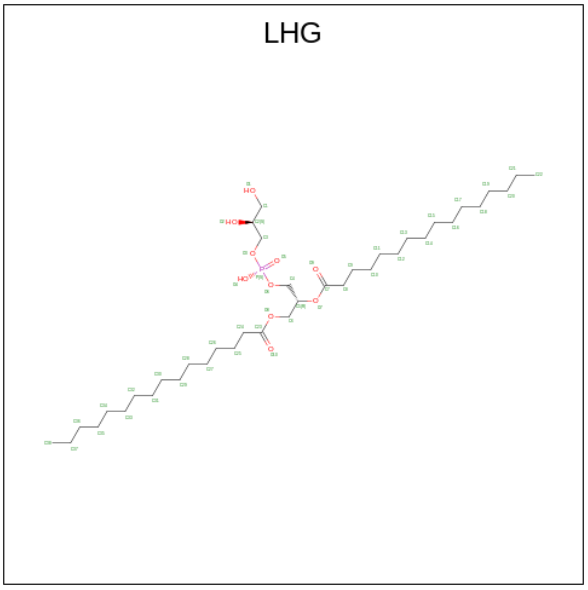
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	0	1	36	26	10	0
			Total	C	O	
13	8	1	36	26	10	0
			Total	C	O	
13	G	1	28	18	10	0
			Total	C	O	
13	G	1	28	18	10	0

- Molecule 14 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: $C_{40}H_{54}O_2$).



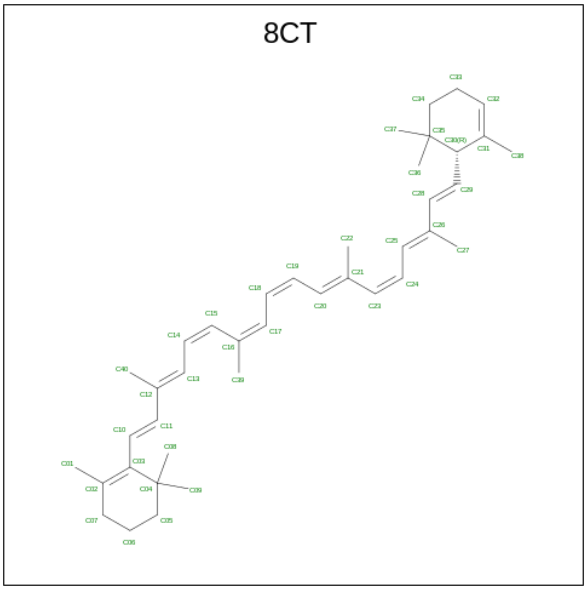
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	7	1	42	40	2	0
			Total	C	O	
14	P	1	42	40	2	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



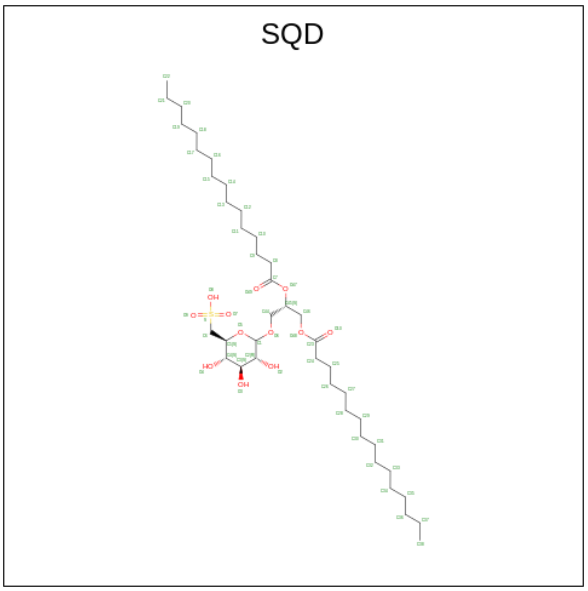
Mol	Chain	Residues	Atoms				AltConf
15	8	1	Total	C	O	P	0
			22	12	9	1	
15	s	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 16 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
16	9	1	Total	C	0
			40	40	
16	P	1	Total	C	0
			40	40	

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



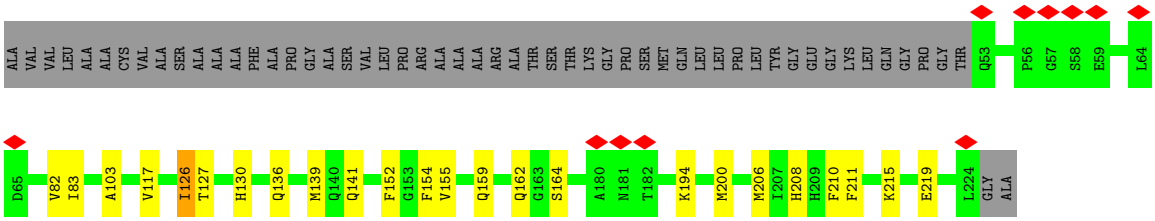
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
17	p	1	35	22	12	1	0

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.

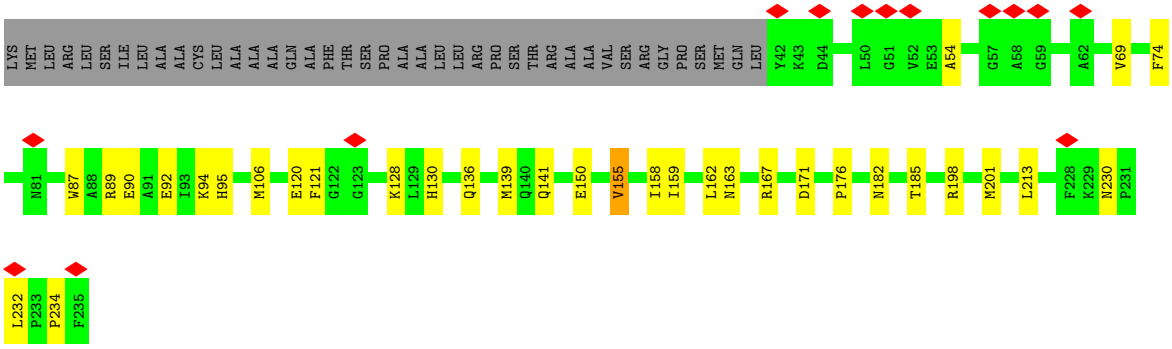
- Molecule 1: ACPII-4

Chain 0:



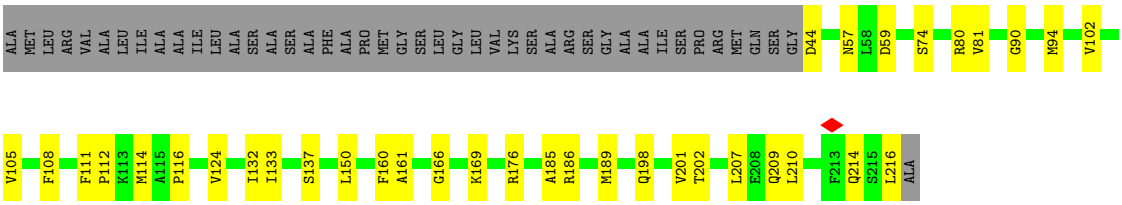
- Molecule 2: ACPII-1

Chain 7:



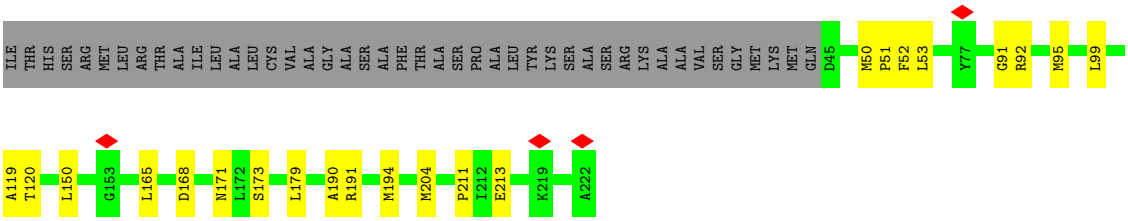
- Molecule 3: ACPII-2

Chain 8:



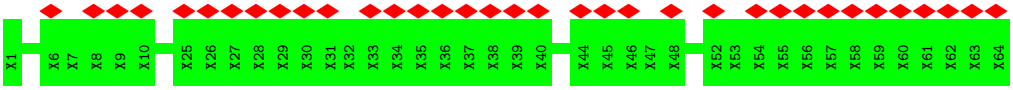
- Molecule 4: ACPII-3

Chain 9:



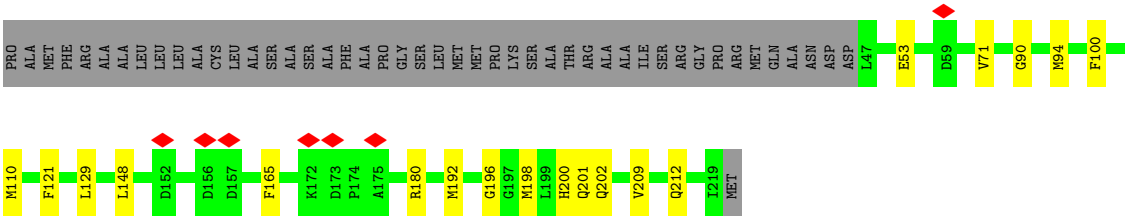
- Molecule 5: Photosystem II reaction center protein G

Chain G:



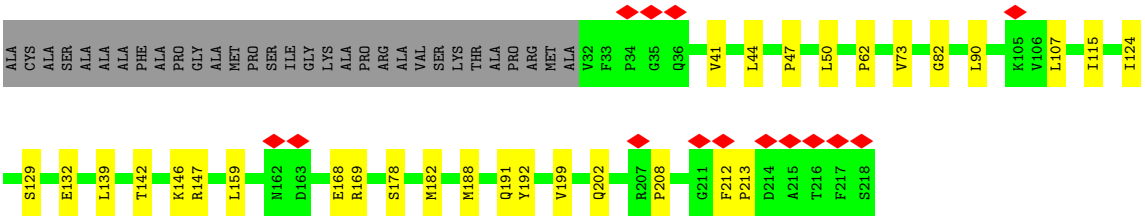
- Molecule 6: ACPII-6

Chain P:



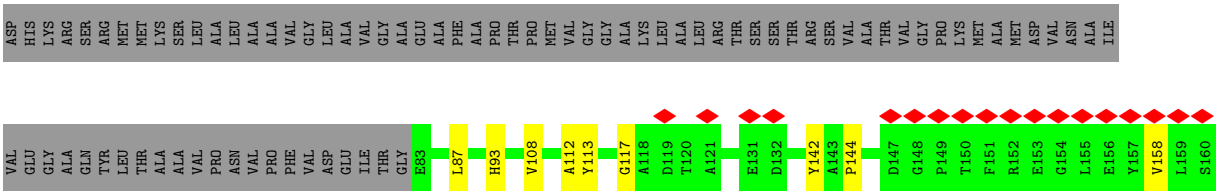
- Molecule 7: ACPII-5

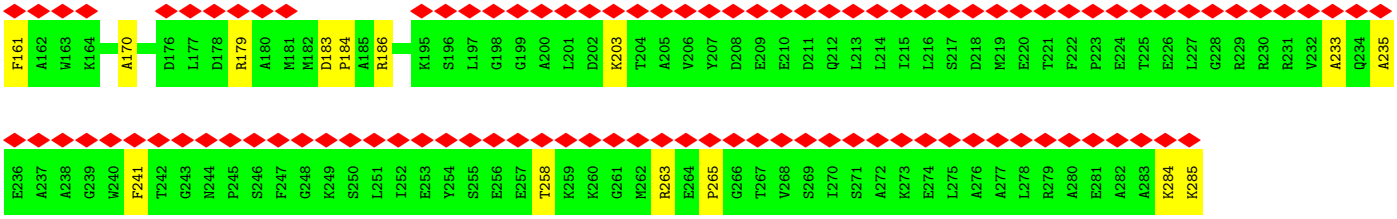
Chain p:



- Molecule 8: CCPII-S

Chain s:




F161 A162 W163 K164 A170 D176 L177 D178 R179 A180 M181 M182 D183 P184 A185 R186 K195 S196 L197 G198 G199 A200 L201 D202 K203 T204 A205 V206 Y207 D208 E209 E210 D211 Q212 L213 L214 I215 L216 S217 D218 M219 E220 T221 F222 P223 E224 T225 E226 L227 G228 R229 R230 R231 V232 A233 Q234 A235

E236 A237 A238 G239 W240 F241 T242 G243 N244 P245 S246 F247 G248 K249 S250 L251 T252 E253 Y254 S255 E256 E257 T258 K259 K260 G261 M262 R263 E264 P265 G266 T267 V268 S269 T270 S271 A272 K273 E274 L275 A276 A277 L278 R279 A280 E281 A282 A283 K284 K285

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	610800	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	1.131	Depositor
Minimum map value	-0.417	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.266	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, IHT, KC2, CLA, LMG, II0, 8CT, LHG, II3

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	0	0.19	0/1339	0.29	0/1814
2	7	0.21	0/1507	0.34	0/2043
3	8	0.23	0/1399	0.29	0/1893
4	9	0.19	0/1404	0.24	0/1895
6	P	0.20	0/1380	0.27	0/1870
7	p	0.22	0/1510	0.30	0/2046
8	s	0.15	0/1603	0.31	0/2180
All	All	0.20	0/10142	0.29	0/13741

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1308	0	1323	19	0
2	7	1472	0	1473	23	0
3	8	1362	0	1348	25	0
4	9	1371	0	1370	16	0
5	G	320	0	70	0	0
6	P	1344	0	1329	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	p	1471	0	1445	26	0
8	s	1563	0	1540	21	0
9	0	582	0	469	13	0
9	7	582	0	469	17	0
9	8	547	0	456	14	0
9	9	548	0	456	13	0
9	G	45	0	33	2	0
9	P	442	0	364	10	0
9	p	547	0	456	13	0
9	s	110	0	105	6	0
10	0	45	0	0	0	0
10	7	45	0	0	0	0
10	8	45	0	0	0	0
10	P	90	0	0	0	0
10	p	45	0	0	0	0
11	0	82	0	0	0	0
11	7	41	0	0	0	0
11	8	41	0	0	0	0
11	p	41	0	0	0	0
12	0	126	0	0	1	0
12	7	168	0	0	1	0
12	8	168	0	0	2	0
12	9	126	0	0	0	0
12	P	84	0	0	0	0
12	p	210	0	0	0	0
13	0	36	0	42	0	0
13	8	36	0	42	2	0
13	G	56	0	52	0	0
14	7	42	0	0	0	0
14	P	42	0	0	0	0
15	8	22	0	20	0	0
15	s	37	0	44	2	0
16	9	40	0	0	0	0
16	P	40	0	0	0	0
17	p	35	0	34	4	0
All	All	15357	0	12940	180	0

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

The worst 5 of 180 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)
7:p:182:MET:HE1	9:p:304:CLA:HAB	1.65	0.77
3:8:90:GLY:HA3	3:8:185:ALA:HB1	1.69	0.74
7:p:82:GLY:HA3	7:p:178:SER:HB3	1.70	0.73
4:9:91:GLY:HA3	4:9:190:ALA:HB1	1.70	0.72
2:7:155:VAL:HG22	9:7:607:CLA:HMA1	1.72	0.72

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	0	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	39
2	7	192/235 (82%)	183 (95%)	9 (5%)	0	100	100
3	8	171/217 (79%)	170 (99%)	1 (1%)	0	100	100
4	9	176/222 (79%)	172 (98%)	4 (2%)	0	100	100
6	P	171/220 (78%)	171 (100%)	0	0	100	100
7	p	185/218 (85%)	183 (99%)	2 (1%)	0	100	100
8	s	201/285 (70%)	180 (90%)	21 (10%)	0	100	100
All	All	1266/1623 (78%)	1226 (97%)	39 (3%)	1 (0%)	49	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	126	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	0	136/169 (80%)	136 (100%)	0	100	100
2	7	149/179 (83%)	147 (99%)	2 (1%)	61	79
3	8	139/167 (83%)	139 (100%)	0	100	100
4	9	143/175 (82%)	143 (100%)	0	100	100
6	P	141/174 (81%)	140 (99%)	1 (1%)	76	88
7	p	157/175 (90%)	156 (99%)	1 (1%)	78	89
8	s	159/219 (73%)	159 (100%)	0	100	100
All	All	1024/1258 (81%)	1020 (100%)	4 (0%)	81	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	7	106	MET
2	7	155	VAL
6	P	71	VAL
7	p	41	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
6	P	215	ASN
7	p	202	GLN
7	p	210	ASN
7	p	205	ASN
3	8	131	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

112 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	II0	7	616	-	39,43,43	2.76	4 (10%)	50,60,60	1.76	11 (22%)
12	II0	7	614	-	39,43,43	2.73	4 (10%)	50,60,60	1.75	10 (20%)
9	CLA	9	610	4	49,53,73	1.46	9 (18%)	59,89,113	1.49	5 (8%)
9	CLA	P	604	6	59,63,73	1.34	10 (16%)	71,101,113	1.41	6 (8%)
9	CLA	8	601	3	46,50,73	1.48	9 (19%)	55,85,113	1.47	4 (7%)
16	8CT	9	615	-	40,41,41	4.64	23 (57%)	50,56,56	2.87	20 (40%)
9	CLA	0	612	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	6 (10%)
9	CLA	P	607	6	64,68,73	1.29	10 (15%)	77,107,113	1.33	5 (6%)
15	LHG	8	618	9	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
9	CLA	8	609	15	45,49,73	1.51	10 (22%)	54,84,113	1.51	5 (9%)
11	IHT	7	618	-	40,42,42	2.01	2 (5%)	53,58,58	1.95	13 (24%)
10	KC2	7	610	2	49,53,53	1.77	11 (22%)	62,89,89	2.17	16 (25%)
9	CLA	0	613	1	49,53,73	1.49	10 (20%)	59,89,113	1.43	6 (10%)
9	CLA	8	602	3	63,67,73	1.29	9 (14%)	75,105,113	1.37	8 (10%)
12	II0	7	617	-	39,43,43	2.75	4 (10%)	50,60,60	1.72	10 (20%)
9	CLA	8	604	-	59,63,73	1.33	9 (15%)	71,101,113	1.38	7 (9%)
9	CLA	9	606	-	49,53,73	1.50	10 (20%)	59,89,113	1.35	5 (8%)
12	II0	9	612	-	39,43,43	2.73	4 (10%)	50,60,60	1.70	10 (20%)
9	CLA	9	602	4	63,67,73	1.30	10 (15%)	75,105,113	1.37	7 (9%)
9	CLA	0	604	1	59,63,73	1.36	10 (16%)	71,101,113	1.36	8 (11%)
9	CLA	8	605	3	64,68,73	1.29	9 (14%)	77,107,113	1.32	6 (7%)
9	CLA	P	601	6	46,50,73	1.49	9 (19%)	55,85,113	1.44	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	CLA	8	611	3	49,53,73	1.46	10 (20%)	59,89,113	1.48	5 (8%)
12	II0	8	613	-	39,43,43	2.75	4 (10%)	50,60,60	1.77	10 (20%)
9	CLA	0	603	1	54,58,73	1.39	10 (18%)	65,95,113	1.42	6 (9%)
9	CLA	0	608	-	64,68,73	1.28	9 (14%)	77,107,113	1.34	6 (7%)
10	KC2	P	605	6	49,53,53	1.83	11 (22%)	62,89,89	2.11	15 (24%)
9	CLA	0	607	1	49,53,73	1.47	9 (18%)	59,89,113	1.37	6 (10%)
9	CLA	8	612	3	49,53,73	1.46	10 (20%)	59,89,113	1.41	5 (8%)
9	CLA	7	607	-	49,53,73	1.47	10 (20%)	59,89,113	1.40	5 (8%)
14	II3	P	613	-	40,43,43	2.00	2 (5%)	47,60,60	1.59	10 (21%)
9	CLA	s	303	8	69,73,73	1.27	9 (13%)	83,113,113	1.29	6 (7%)
9	CLA	P	606	6	49,53,73	1.48	8 (16%)	59,89,113	1.35	6 (10%)
12	II0	P	612	-	39,43,43	2.70	4 (10%)	50,60,60	1.77	10 (20%)
9	CLA	9	609	4	64,68,73	1.29	10 (15%)	77,107,113	1.34	6 (7%)
9	CLA	7	602	2	63,67,73	1.30	10 (15%)	75,105,113	1.32	6 (8%)
9	CLA	P	603	-	54,58,73	1.40	10 (18%)	65,95,113	1.47	7 (10%)
13	LMG	0	618	-	36,36,55	0.89	1 (2%)	44,44,63	1.29	6 (13%)
9	CLA	7	612	2	49,53,73	1.48	10 (20%)	59,89,113	1.42	4 (6%)
9	CLA	0	611	1	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
9	CLA	p	310	7	64,68,73	1.30	10 (15%)	77,107,113	1.35	5 (6%)
9	CLA	7	609	-	45,49,73	1.52	9 (20%)	54,84,113	1.50	6 (11%)
10	KC2	0	610	1	49,53,53	1.79	11 (22%)	62,89,89	2.21	18 (29%)
12	II0	9	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.69	11 (22%)
9	CLA	9	608	-	45,49,73	1.49	9 (20%)	54,84,113	1.52	7 (12%)
9	CLA	7	605	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	6 (9%)
16	8CT	P	615	-	40,41,41	4.66	23 (57%)	50,56,56	2.68	19 (38%)
12	II0	p	301	-	39,43,43	2.71	4 (10%)	50,60,60	1.79	11 (22%)
12	II0	8	619	-	39,43,43	2.74	4 (10%)	50,60,60	1.73	8 (16%)
9	CLA	7	606	2	49,53,73	1.46	8 (16%)	59,89,113	1.50	6 (10%)
9	CLA	9	604	4	59,63,73	1.36	10 (16%)	71,101,113	1.37	8 (11%)
9	CLA	p	314	7	49,53,73	1.47	10 (20%)	59,89,113	1.40	4 (6%)
12	II0	p	315	-	39,43,43	2.69	4 (10%)	50,60,60	1.75	12 (24%)
13	LMG	G	102	-	28,28,55	0.94	0	36,36,63	1.30	5 (13%)
9	CLA	7	603	2	54,58,73	1.38	9 (16%)	65,95,113	1.45	6 (9%)
9	CLA	8	606	3	49,53,73	1.47	9 (18%)	59,89,113	1.44	5 (8%)
9	CLA	p	309	7	49,53,73	1.48	10 (20%)	59,89,113	1.48	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	II0	p	316	-	39,43,43	2.71	4 (10%)	50,60,60	1.60	10 (20%)
12	II0	p	317	-	39,43,43	2.74	4 (10%)	50,60,60	1.70	9 (18%)
12	II0	9	613	-	39,43,43	2.73	4 (10%)	50,60,60	1.74	9 (18%)
11	IHT	0	614	-	40,42,42	1.98	2 (5%)	53,58,58	1.79	13 (24%)
15	LHG	s	301	-	36,36,48	0.72	1 (2%)	39,42,54	1.24	4 (10%)
9	CLA	P	602	6	63,67,73	1.31	10 (15%)	75,105,113	1.32	8 (10%)
9	CLA	p	308	7	49,53,73	1.49	9 (18%)	59,89,113	1.46	6 (10%)
9	CLA	9	607	4	64,68,73	1.30	10 (15%)	77,107,113	1.32	5 (6%)
9	CLA	P	610	-	49,53,73	1.46	10 (20%)	59,89,113	1.51	7 (11%)
9	CLA	7	601	-	46,50,73	1.50	8 (17%)	55,85,113	1.42	4 (7%)
13	LMG	G	103	-	28,28,55	1.00	0	36,36,63	1.33	5 (13%)
9	CLA	p	307	7	64,68,73	1.29	9 (14%)	77,107,113	1.31	6 (7%)
12	II0	8	615	-	39,43,43	2.72	5 (12%)	50,60,60	1.84	10 (20%)
9	CLA	0	601	1	46,50,73	1.50	9 (19%)	55,85,113	1.45	4 (7%)
12	II0	P	614	-	39,43,43	2.74	4 (10%)	50,60,60	1.71	11 (22%)
12	II0	0	616	-	39,43,43	2.77	4 (10%)	50,60,60	1.75	12 (24%)
9	CLA	0	606	-	49,53,73	1.47	9 (18%)	59,89,113	1.39	5 (8%)
13	LMG	8	617	-	36,36,55	0.89	1 (2%)	44,44,63	1.30	6 (13%)
9	CLA	9	605	4	50,54,73	1.45	10 (20%)	60,90,113	1.39	4 (6%)
9	CLA	7	604	2	59,63,73	1.34	10 (16%)	71,101,113	1.42	7 (9%)
9	CLA	p	304	7	63,67,73	1.31	10 (15%)	75,105,113	1.30	9 (12%)
9	CLA	p	306	7	59,63,73	1.33	9 (15%)	71,101,113	1.39	6 (8%)
9	CLA	9	611	4	49,53,73	1.47	10 (20%)	59,89,113	1.44	5 (8%)
9	CLA	0	609	-	45,49,73	1.51	9 (20%)	54,84,113	1.48	7 (12%)
9	CLA	p	303	7	46,50,73	1.49	10 (21%)	55,85,113	1.45	4 (7%)
9	CLA	8	607	3	49,53,73	1.46	10 (20%)	59,89,113	1.43	5 (8%)
14	II3	7	615	-	40,43,43	1.99	2 (5%)	47,60,60	1.63	9 (19%)
10	KC2	p	312	7	49,53,53	1.80	11 (22%)	62,89,89	2.19	18 (29%)
9	CLA	p	305	-	54,58,73	1.41	10 (18%)	65,95,113	1.45	7 (10%)
12	II0	p	302	-	39,43,43	2.72	4 (10%)	50,60,60	1.76	11 (22%)
12	II0	0	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.75	12 (24%)
9	CLA	P	608	-	45,49,73	1.50	10 (22%)	54,84,113	1.48	5 (9%)
9	CLA	9	601	4	46,50,73	1.48	10 (21%)	55,85,113	1.49	4 (7%)
11	IHT	0	617	-	40,42,42	1.99	3 (7%)	53,58,58	2.04	15 (28%)
12	II0	8	614	-	39,43,43	2.72	4 (10%)	50,60,60	1.69	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	CLA	9	603	4	54,58,73	1.39	10 (18%)	65,95,113	1.46	6 (9%)
9	CLA	7	611	2	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
17	SQD	p	319	-	34,35,54	1.73	7 (20%)	43,46,65	1.60	7 (16%)
9	CLA	0	602	1	63,67,73	1.30	10 (15%)	75,105,113	1.32	7 (9%)
10	KC2	8	610	3	49,53,53	1.82	12 (24%)	62,89,89	2.21	17 (27%)
9	CLA	G	101	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)
11	IHT	8	616	-	40,42,42	2.04	3 (7%)	53,58,58	2.03	15 (28%)
9	CLA	s	302	-	49,53,73	1.50	9 (18%)	59,89,113	1.50	7 (11%)
9	CLA	P	611	6	49,53,73	1.48	10 (20%)	59,89,113	1.46	6 (10%)
12	II0	0	619	-	39,43,43	2.68	4 (10%)	50,60,60	1.69	13 (26%)
9	CLA	8	603	3	54,58,73	1.40	10 (18%)	65,95,113	1.43	7 (10%)
9	CLA	8	608	3	64,68,73	1.29	9 (14%)	77,107,113	1.33	7 (9%)
12	II0	7	619	-	39,43,43	2.69	4 (10%)	50,60,60	1.67	11 (22%)
9	CLA	0	605	1	54,58,73	1.40	9 (16%)	65,95,113	1.38	5 (7%)
9	CLA	p	311	-	45,49,73	1.51	9 (20%)	54,84,113	1.47	7 (12%)
10	KC2	P	609	6	49,53,53	1.80	11 (22%)	62,89,89	2.18	17 (27%)
9	CLA	p	313	-	49,53,73	1.46	10 (20%)	59,89,113	1.49	5 (8%)
11	IHT	p	318	-	40,42,42	1.99	2 (5%)	53,58,58	1.81	11 (20%)
9	CLA	7	608	2	64,68,73	1.29	10 (15%)	77,107,113	1.34	6 (7%)
9	CLA	7	613	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	II0	7	616	-	-	5/21/67/67	0/2/2/2
12	II0	7	614	-	-	0/21/67/67	0/2/2/2
9	CLA	9	610	4	-	9/15/91/115	-
9	CLA	P	604	6	-	6/27/103/115	-
9	CLA	8	601	3	-	6/12/88/115	-
16	8CT	9	615	-	-	9/29/63/63	0/2/2/2
9	CLA	0	612	-	-	7/15/91/115	-
9	CLA	P	607	6	-	7/33/109/115	-
15	LHG	8	618	9	-	11/24/24/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	8	609	15	-	4/10/86/115	-
11	IHT	7	618	-	-	2/25/65/65	0/2/2/2
10	KC2	7	610	2	-	11/15/71/71	-
9	CLA	0	613	1	-	8/15/91/115	-
9	CLA	8	602	3	-	13/32/108/115	-
12	II0	7	617	-	-	4/21/67/67	0/2/2/2
9	CLA	8	604	-	-	3/27/103/115	-
9	CLA	9	606	-	-	1/15/91/115	-
12	II0	9	612	-	-	2/21/67/67	0/2/2/2
9	CLA	9	602	4	-	11/32/108/115	-
9	CLA	0	604	1	-	9/27/103/115	-
9	CLA	8	605	3	-	13/33/109/115	-
9	CLA	P	601	6	-	2/12/88/115	-
9	CLA	8	611	3	-	6/15/91/115	-
12	II0	8	613	-	-	0/21/67/67	0/2/2/2
9	CLA	0	603	1	-	5/21/97/115	-
9	CLA	0	608	-	-	11/33/109/115	-
10	KC2	P	605	6	-	10/15/71/71	-
9	CLA	0	607	1	-	2/15/91/115	-
9	CLA	8	612	3	-	8/15/91/115	-
9	CLA	7	607	-	-	9/15/91/115	-
14	II3	P	613	-	-	1/25/67/67	0/2/2/2
9	CLA	s	303	8	-	17/39/115/115	-
9	CLA	P	606	6	-	6/15/91/115	-
12	II0	P	612	-	-	0/21/67/67	0/2/2/2
9	CLA	9	609	4	-	9/33/109/115	-
9	CLA	7	602	2	-	12/32/108/115	-
9	CLA	P	603	-	-	3/21/97/115	-
13	LMG	0	618	-	-	10/31/51/70	0/1/1/1
9	CLA	7	612	2	-	7/15/91/115	-
9	CLA	0	611	1	-	9/15/91/115	-
9	CLA	p	310	7	-	9/33/109/115	-
9	CLA	7	609	-	-	3/10/86/115	-
10	KC2	0	610	1	-	11/15/71/71	-
12	II0	9	614	-	-	4/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	9	608	-	-	3/10/86/115	-
9	CLA	7	605	-	-	8/21/97/115	-
16	8CT	P	615	-	-	4/29/63/63	0/2/2/2
12	II0	p	301	-	-	2/21/67/67	0/2/2/2
12	II0	8	619	-	-	1/21/67/67	0/2/2/2
9	CLA	7	606	2	-	9/15/91/115	-
9	CLA	9	604	4	-	8/27/103/115	-
9	CLA	p	314	7	-	5/15/91/115	-
12	II0	p	315	-	-	1/21/67/67	0/2/2/2
13	LMG	G	102	-	-	9/23/43/70	0/1/1/1
9	CLA	7	603	2	-	8/21/97/115	-
9	CLA	8	606	3	-	2/15/91/115	-
9	CLA	p	309	7	-	4/15/91/115	-
12	II0	p	316	-	-	4/21/67/67	0/2/2/2
12	II0	p	317	-	-	5/21/67/67	0/2/2/2
12	II0	9	613	-	-	1/21/67/67	0/2/2/2
11	IHT	0	614	-	-	5/25/65/65	0/2/2/2
15	LHG	s	301	-	-	20/41/41/53	-
9	CLA	P	602	6	-	16/32/108/115	-
9	CLA	p	308	7	-	6/15/91/115	-
9	CLA	9	607	4	-	6/33/109/115	-
9	CLA	P	610	-	-	6/15/91/115	-
9	CLA	7	601	-	-	5/12/88/115	-
13	LMG	G	103	-	-	7/23/43/70	0/1/1/1
9	CLA	p	307	7	-	15/33/109/115	-
12	II0	8	615	-	-	3/21/67/67	0/2/2/2
9	CLA	0	601	1	-	7/12/88/115	-
12	II0	P	614	-	-	3/21/67/67	0/2/2/2
12	II0	0	616	-	-	4/21/67/67	0/2/2/2
9	CLA	0	606	-	-	7/15/91/115	-
13	LMG	8	617	-	-	10/31/51/70	0/1/1/1
9	CLA	9	605	4	-	7/17/93/115	-
9	CLA	7	604	2	-	5/27/103/115	-
9	CLA	p	304	7	-	14/32/108/115	-
9	CLA	p	306	7	-	11/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	9	611	4	-	6/15/91/115	-
9	CLA	0	609	-	-	4/10/86/115	-
9	CLA	p	303	7	-	8/12/88/115	-
9	CLA	8	607	3	-	5/15/91/115	-
14	II3	7	615	-	-	1/25/67/67	0/2/2/2
10	KC2	p	312	7	-	10/15/71/71	-
9	CLA	p	305	-	-	12/21/97/115	-
12	II0	p	302	-	-	1/21/67/67	0/2/2/2
12	II0	0	615	-	-	0/21/67/67	0/2/2/2
9	CLA	P	608	-	-	2/10/86/115	-
9	CLA	9	601	4	-	5/12/88/115	-
11	IHT	0	617	-	-	5/25/65/65	0/2/2/2
12	II0	8	614	-	-	0/21/67/67	0/2/2/2
9	CLA	9	603	4	-	6/21/97/115	-
9	CLA	7	611	2	-	7/15/91/115	-
17	SQD	p	319	-	-	19/30/50/69	0/1/1/1
9	CLA	0	602	1	-	13/32/108/115	-
10	KC2	8	610	3	-	9/15/71/71	-
9	CLA	G	101	-	-	9/15/91/115	-
11	IHT	8	616	-	-	1/25/65/65	0/2/2/2
9	CLA	s	302	-	-	5/15/91/115	-
9	CLA	P	611	6	-	7/15/91/115	-
12	II0	0	619	-	-	2/21/67/67	0/2/2/2
9	CLA	8	603	3	-	8/21/97/115	-
9	CLA	8	608	3	-	8/33/109/115	-
12	II0	7	619	-	-	2/21/67/67	0/2/2/2
9	CLA	0	605	1	-	9/21/97/115	-
9	CLA	p	311	-	-	5/10/86/115	-
10	KC2	P	609	6	-	12/15/71/71	-
9	CLA	p	313	-	-	8/15/91/115	-
11	IHT	p	318	-	-	0/25/65/65	0/2/2/2
9	CLA	7	608	2	-	10/33/109/115	-
9	CLA	7	613	-	-	9/15/91/115	-

The worst 5 of 878 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	615	8CT	C02-C03	13.96	1.58	1.34
16	P	615	8CT	C02-C03	13.88	1.58	1.34
16	P	615	8CT	C32-C31	13.81	1.59	1.32
16	9	615	8CT	C32-C31	13.63	1.59	1.32
12	0	616	II0	C24-C26	-8.78	1.25	1.42

The worst 5 of 881 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	9	615	8CT	C33-C32-C31	-8.64	116.57	124.85
16	P	615	8CT	C33-C32-C31	-8.01	117.17	124.85
10	0	610	KC2	CHB-C1B-NB	7.41	131.26	124.45
10	8	610	KC2	CHC-C4B-NB	7.14	131.02	124.45
10	8	610	KC2	CHB-C1B-NB	7.13	131.01	124.45

There are no chirality outliers.

5 of 734 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	602	CLA	C1A-C2A-CAA-CBA
9	0	602	CLA	C3A-C2A-CAA-CBA
9	0	602	CLA	CHA-CBD-CGD-O1D
9	0	602	CLA	CHA-CBD-CGD-O2D
9	0	603	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

54 monomers are involved in 91 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	7	614	II0	1	0
9	9	610	CLA	1	0
9	P	604	CLA	1	0
9	0	612	CLA	2	0
9	P	607	CLA	2	0
9	8	609	CLA	1	0
9	0	613	CLA	1	0
9	8	602	CLA	1	0
9	9	606	CLA	2	0
9	9	602	CLA	1	0
9	8	605	CLA	2	0
9	8	611	CLA	1	0
9	0	603	CLA	1	0

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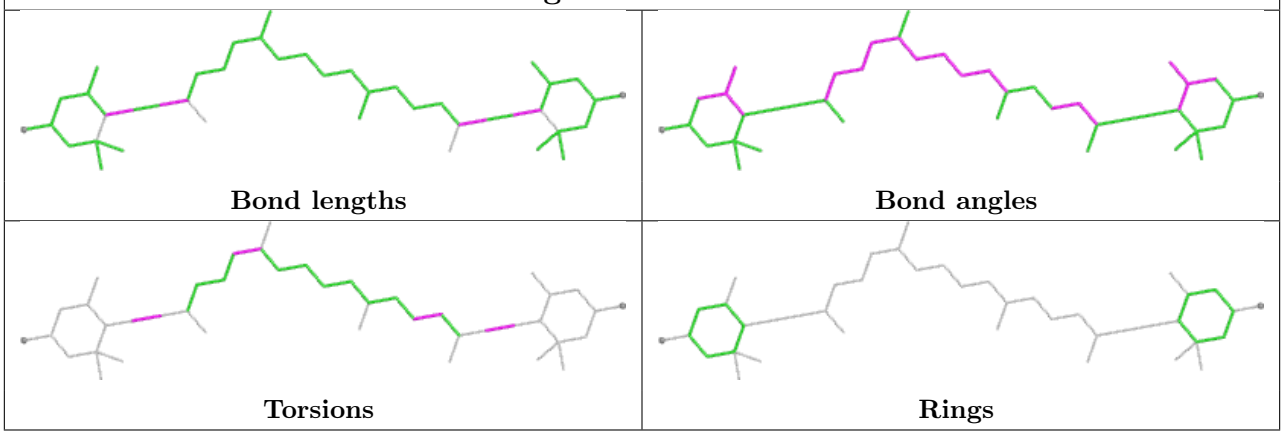
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	0	608	CLA	3	0
9	0	607	CLA	3	0
9	7	607	CLA	2	0
9	s	303	CLA	2	0
9	P	606	CLA	2	0
9	9	609	CLA	3	0
9	7	602	CLA	4	0
9	7	612	CLA	2	0
9	p	310	CLA	1	0
9	7	605	CLA	3	0
12	8	619	II0	1	0
9	7	606	CLA	1	0
9	9	604	CLA	1	0
9	7	603	CLA	1	0
9	8	606	CLA	4	0
9	p	309	CLA	4	0
15	s	301	LHG	2	0
9	P	602	CLA	3	0
9	9	607	CLA	4	0
9	P	610	CLA	1	0
9	p	307	CLA	3	0
9	0	601	CLA	1	0
12	0	616	II0	1	0
13	8	617	LMG	2	0
9	9	605	CLA	1	0
9	7	604	CLA	1	0
9	p	304	CLA	3	0
9	p	306	CLA	2	0
9	8	607	CLA	2	0
12	8	614	II0	1	0
9	7	611	CLA	2	0
17	p	319	SQD	4	0
9	0	602	CLA	2	0
9	G	101	CLA	2	0
9	s	302	CLA	4	0
9	P	611	CLA	1	0
9	8	603	CLA	2	0
9	8	608	CLA	2	0
9	0	605	CLA	1	0
9	7	608	CLA	1	0
9	7	613	CLA	1	0

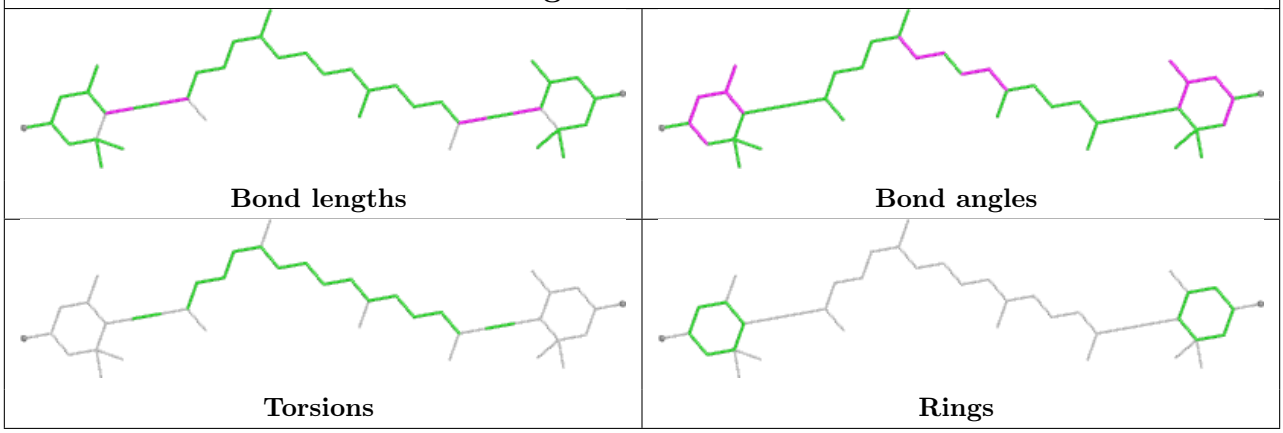
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

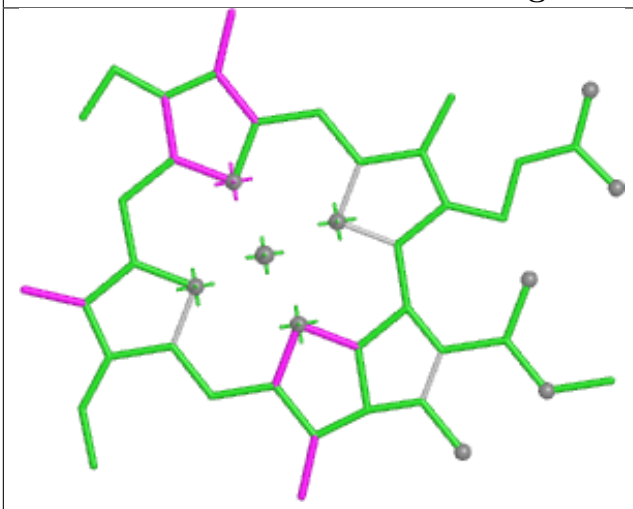
Ligand II0 7 616



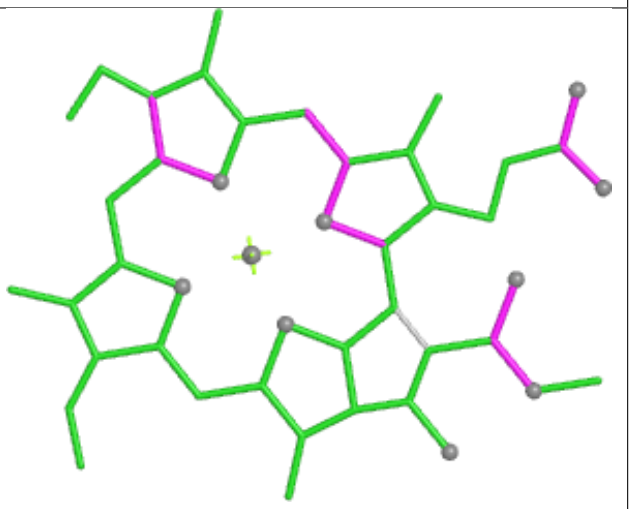
Ligand II0 7 614



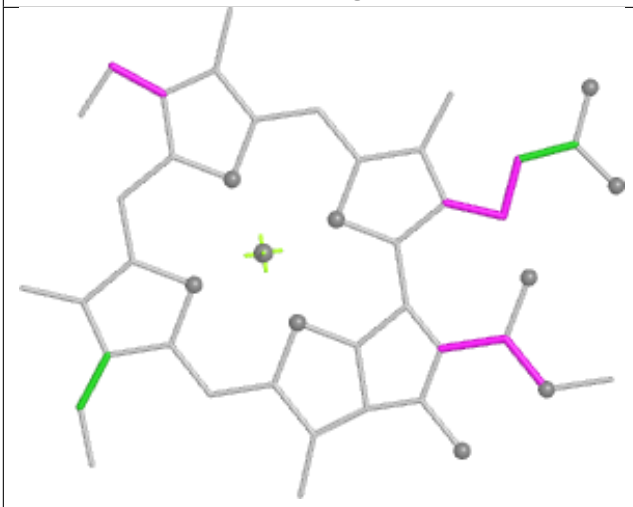
Ligand CLA 9 610



Bond lengths

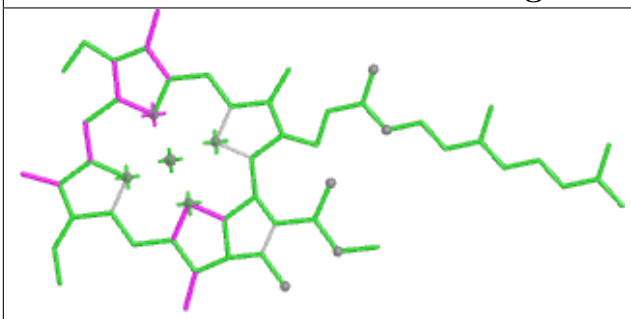
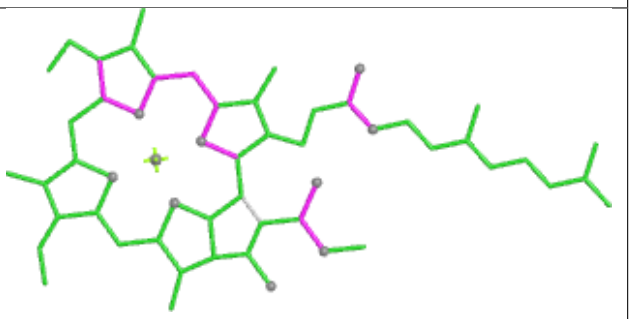
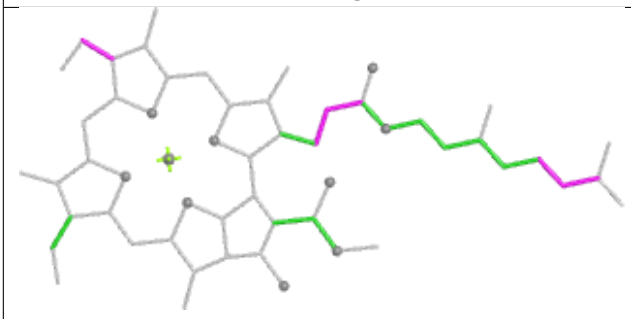
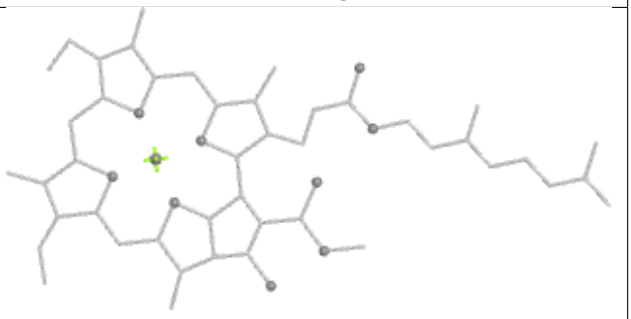


Bond angles

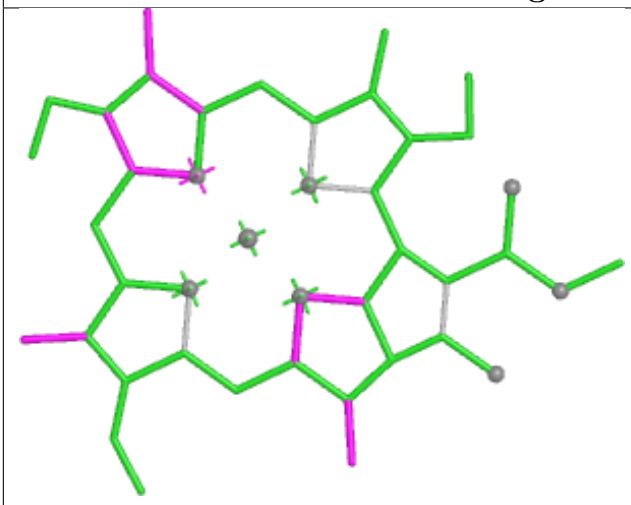


Torsions

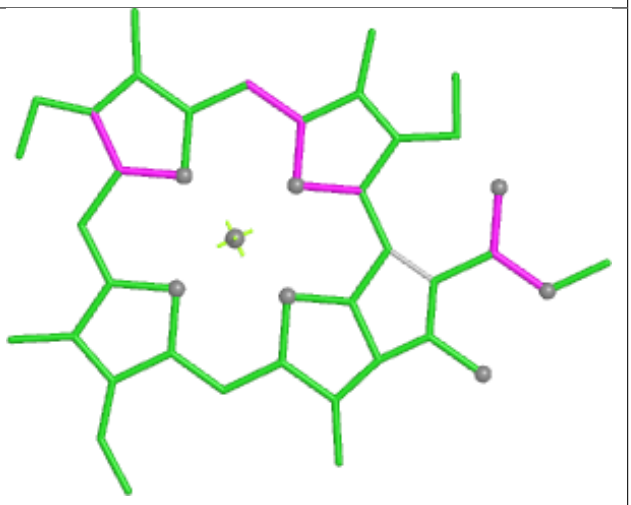
Rings

Ligand CLA P 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

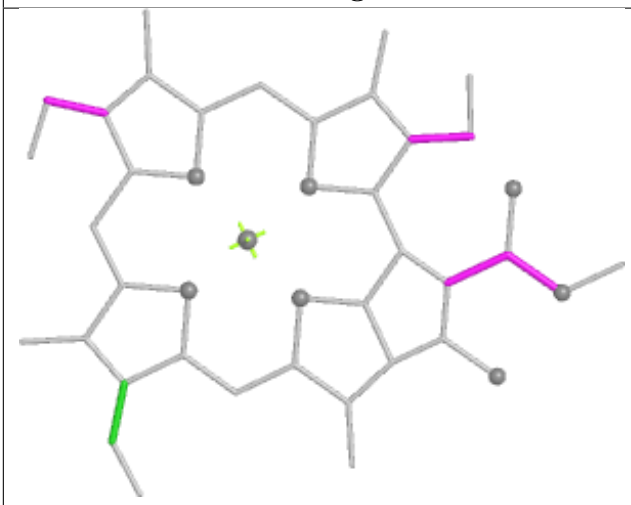
Ligand CLA 8 601



Bond lengths



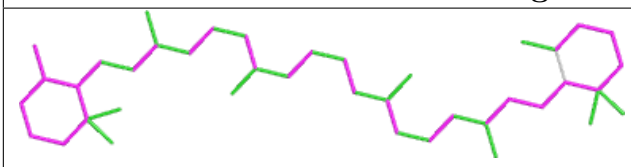
Bond angles



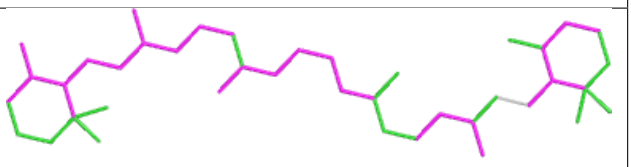
Torsions

Rings

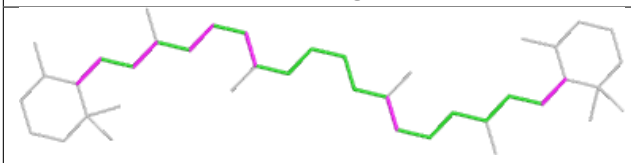
Ligand 8CT 9 615



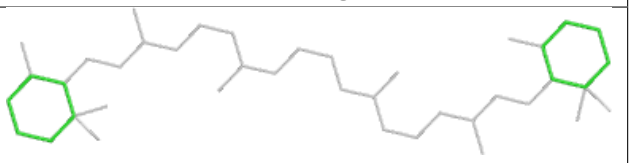
Bond lengths



Bond angles

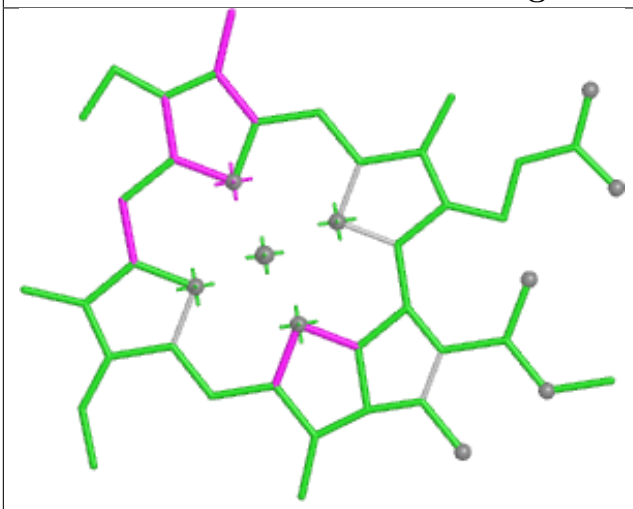


Torsions

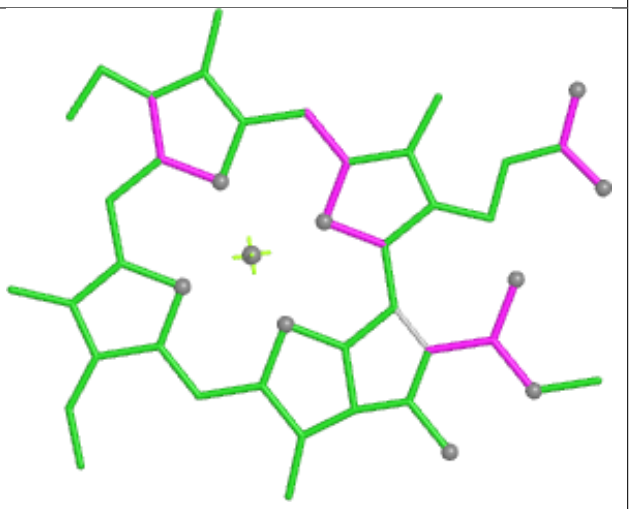


Rings

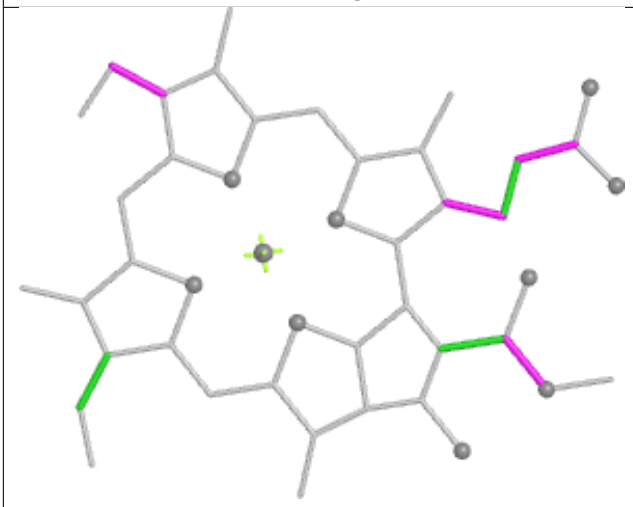
Ligand CLA 0 612



Bond lengths



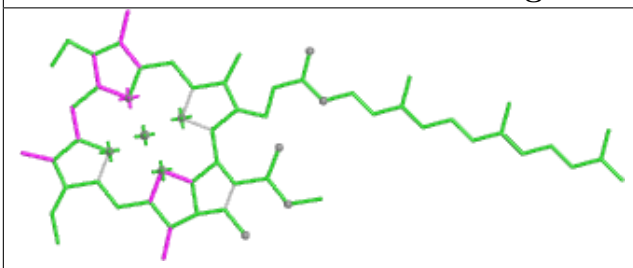
Bond angles



Torsions

Rings

Ligand CLA P 607



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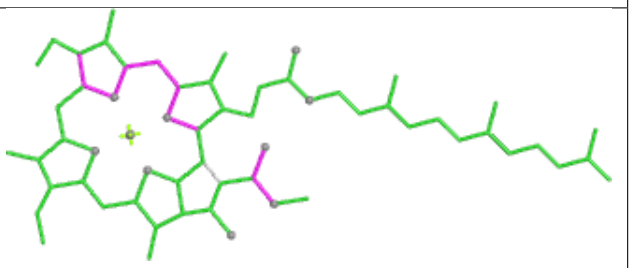
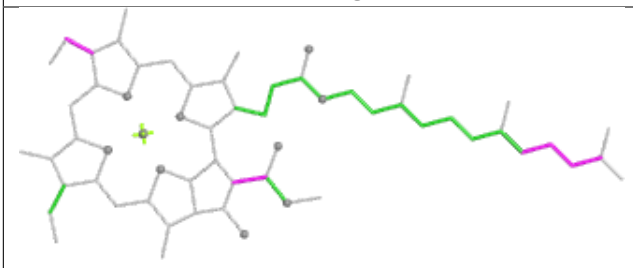
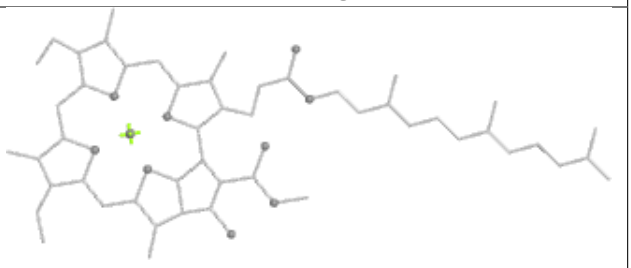


Bond angles

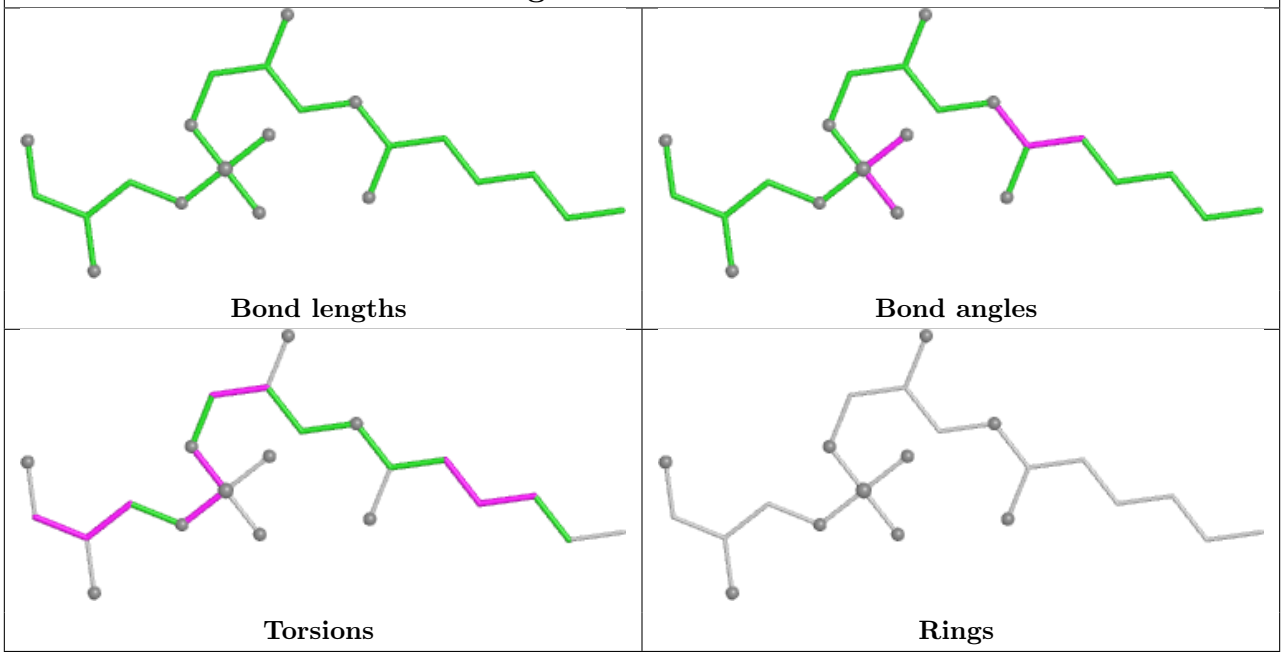


Torsions



Rings

Ligand LHG 8 618



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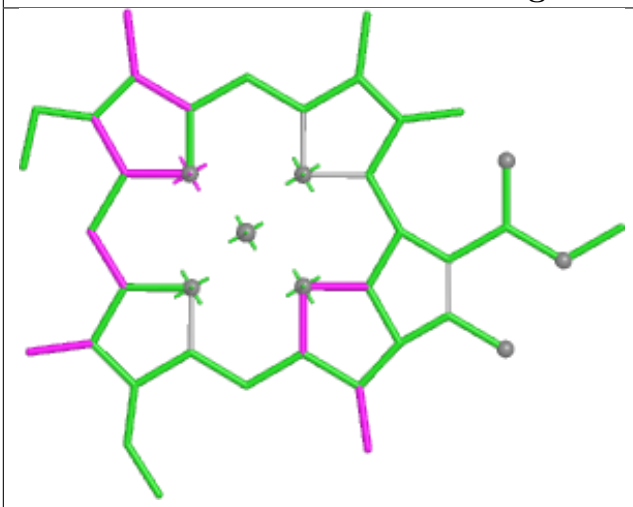
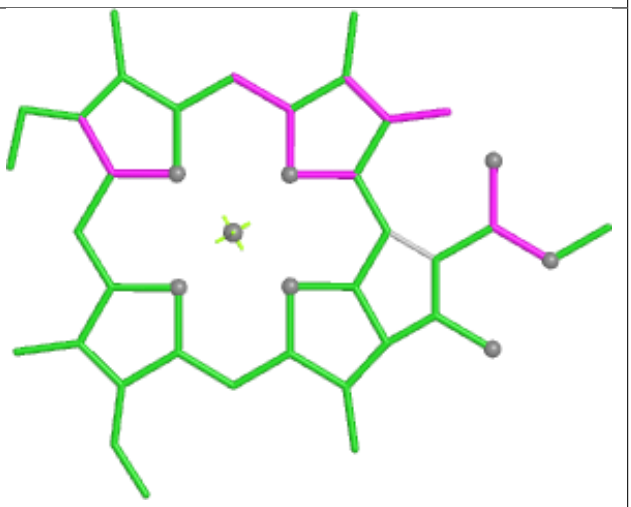
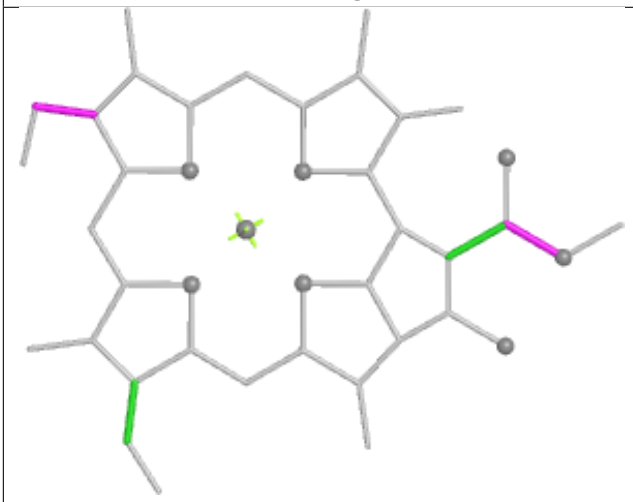


Bond lengths



Bond angles



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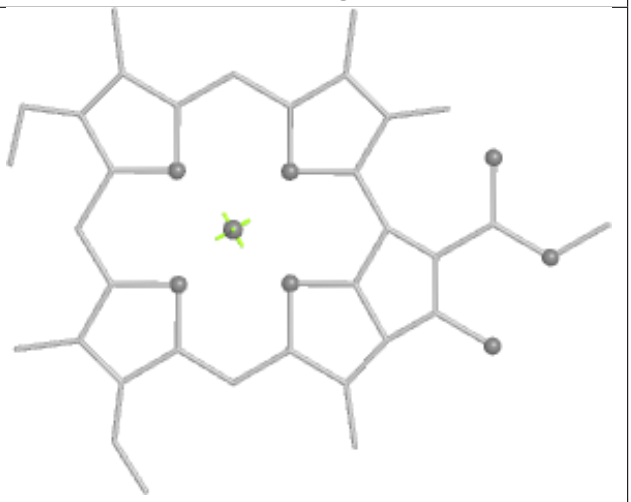
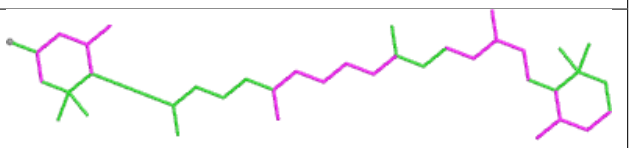


Rings

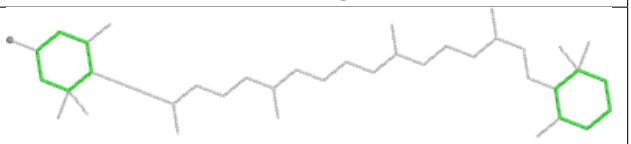
Ligand IHT 7 618

Bond lengths

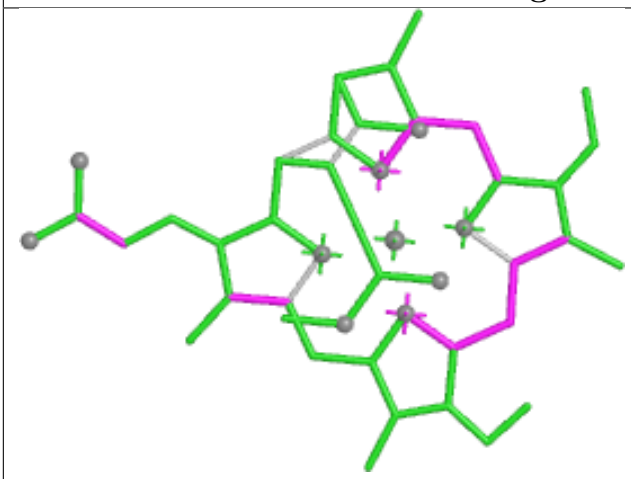
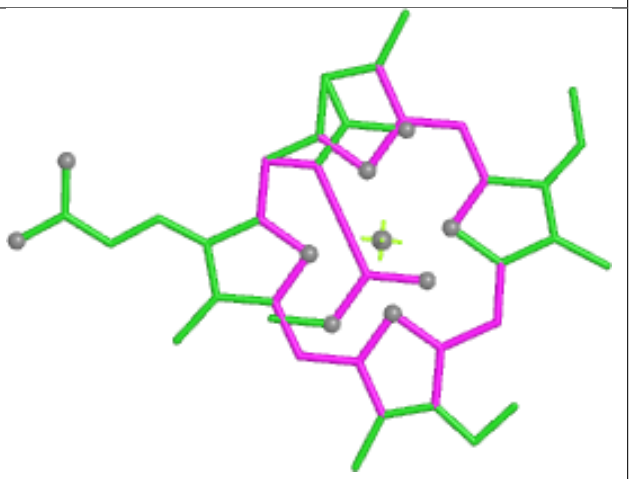
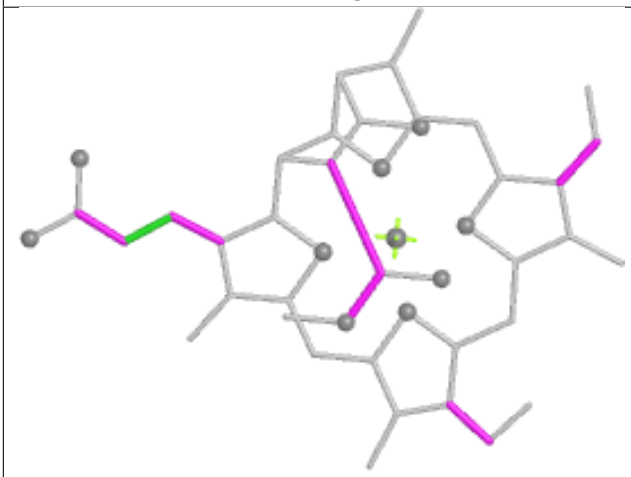
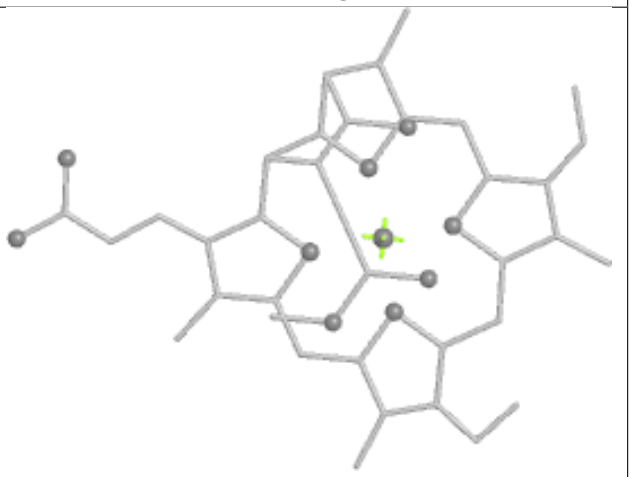


Bond angles

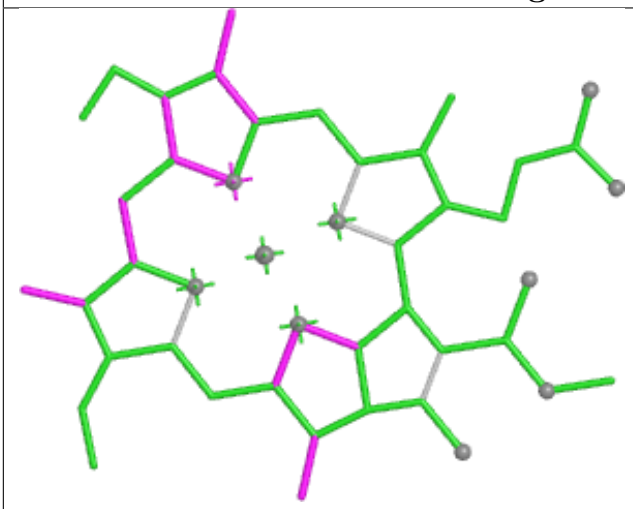
Torsions



Rings

Ligand KC2 7 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 613



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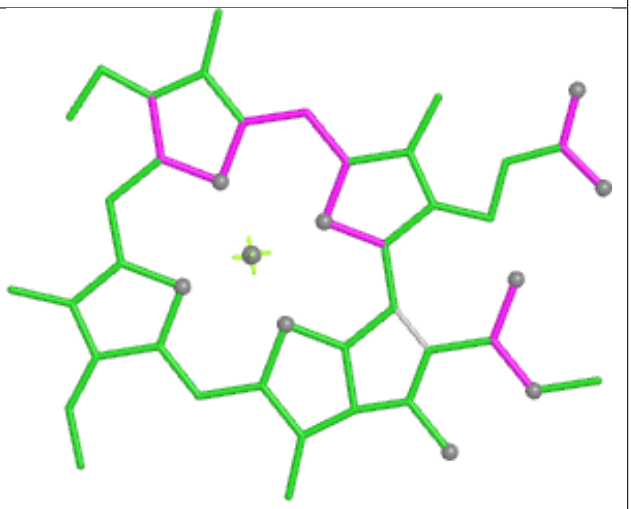

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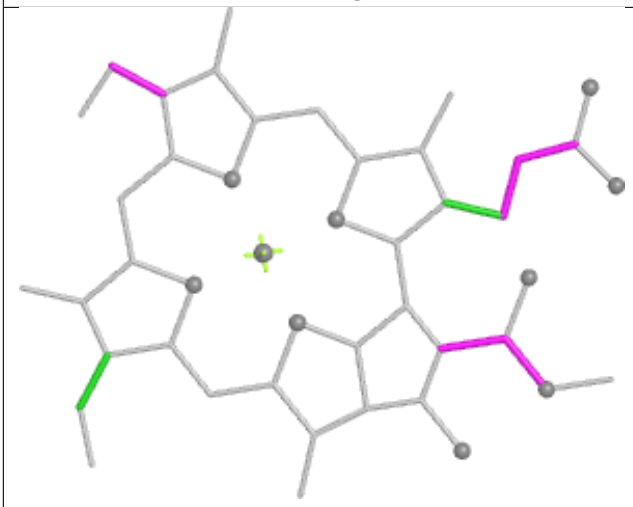
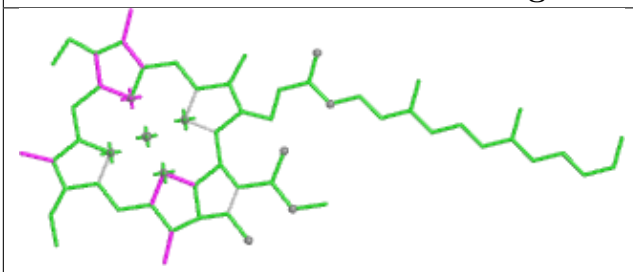


Torsions

Rings

Ligand CLA 8 602



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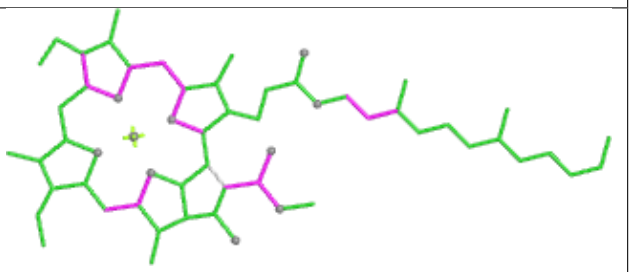

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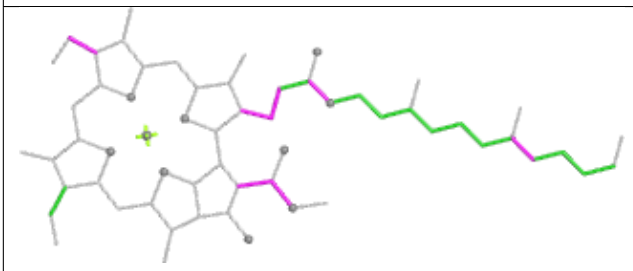

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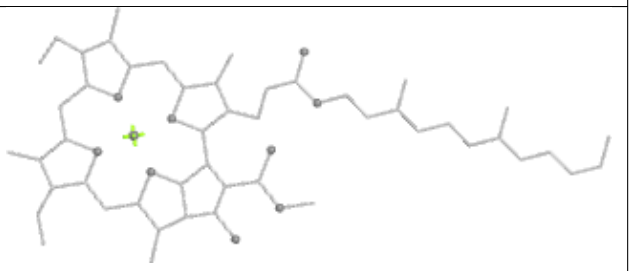
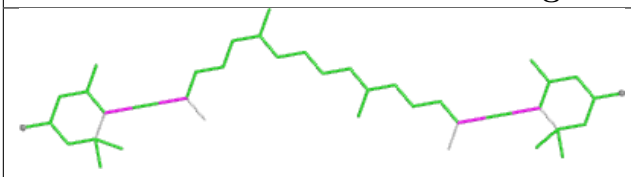
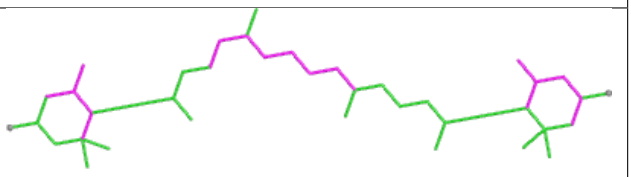
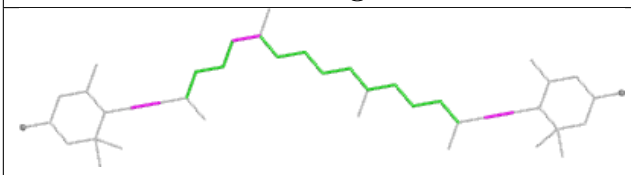
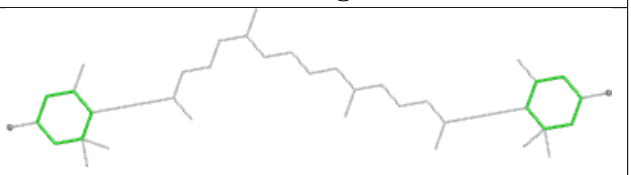


Rings

Ligand II0 7 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

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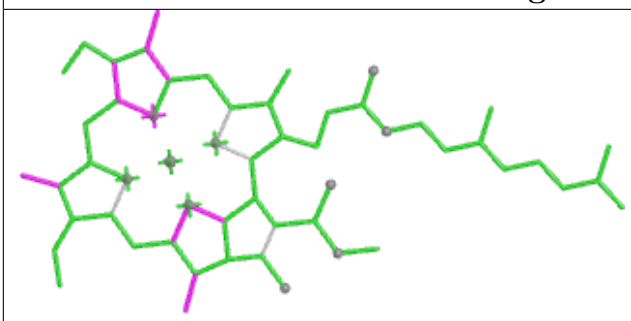
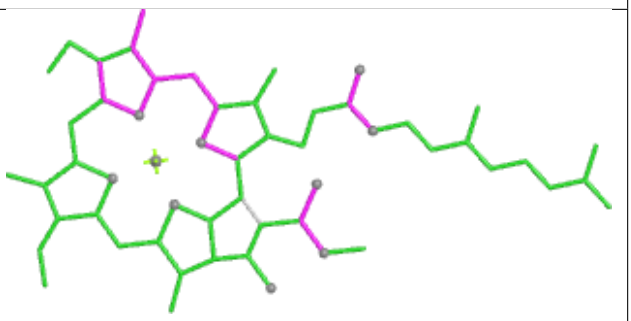
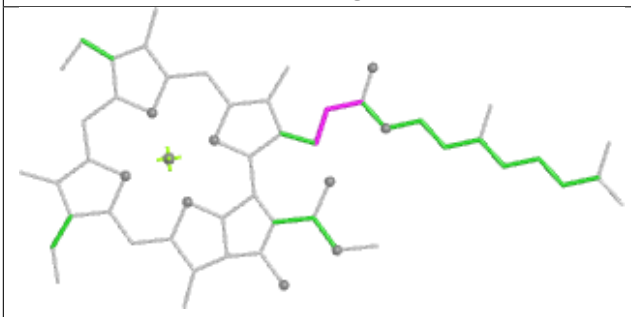
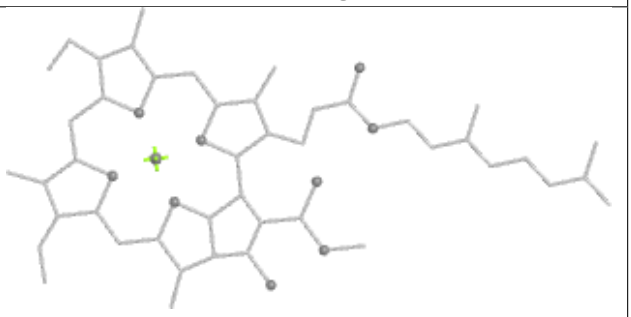
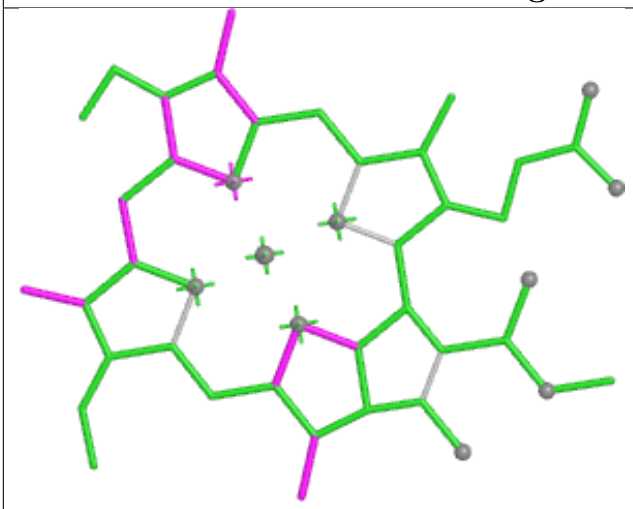
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 606



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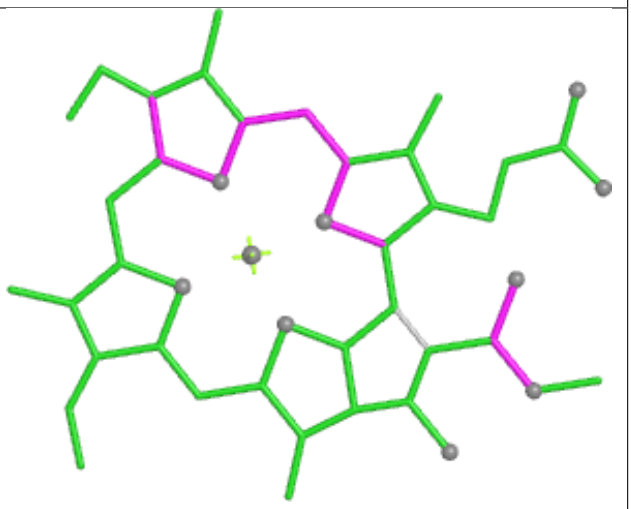
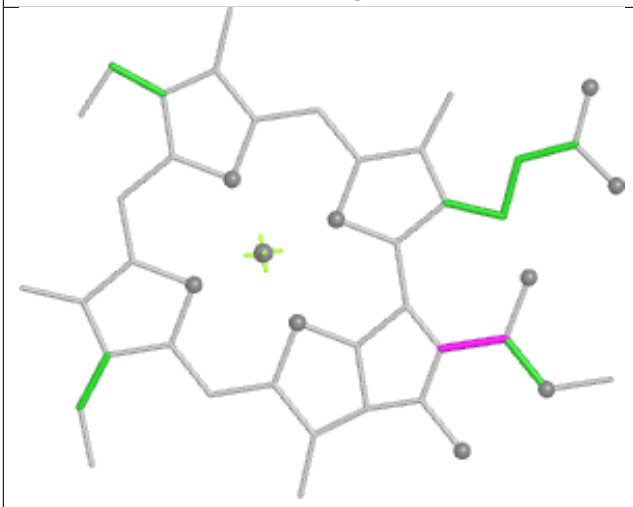


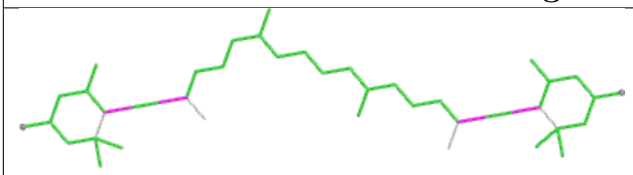
Bond angles



Torsions

Rings

Ligand II0 9 612



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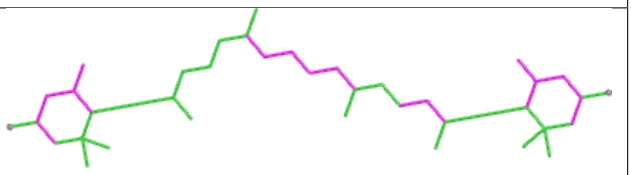

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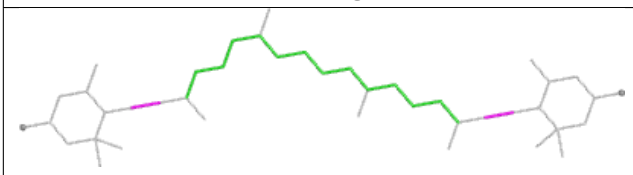

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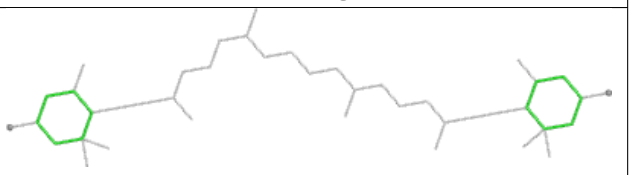
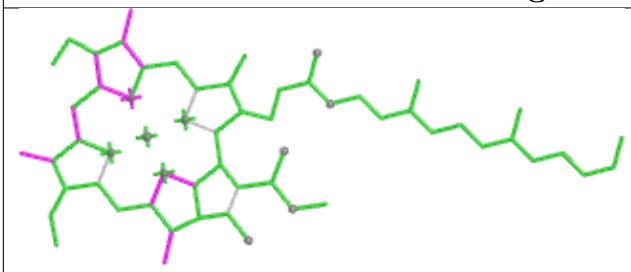
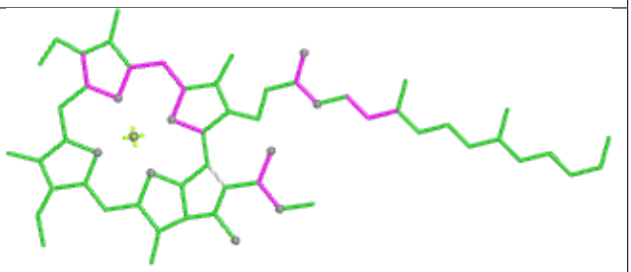
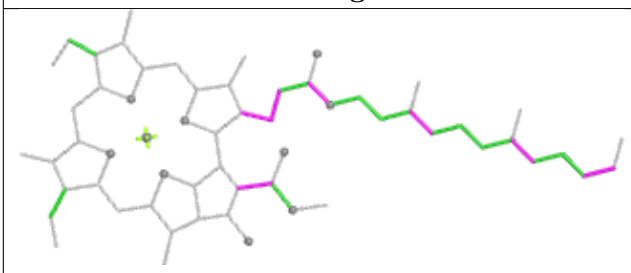
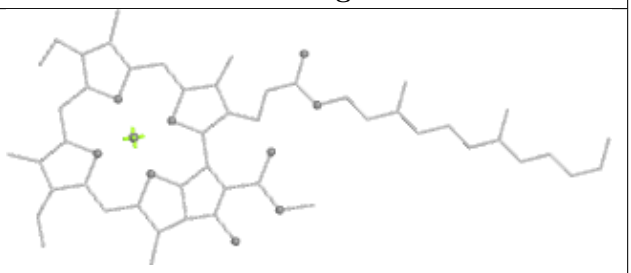


Rings

Ligand CLA 9 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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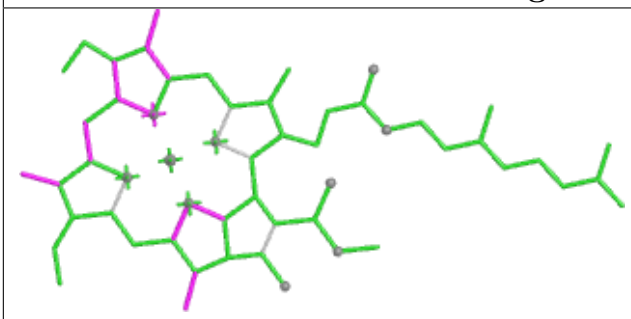
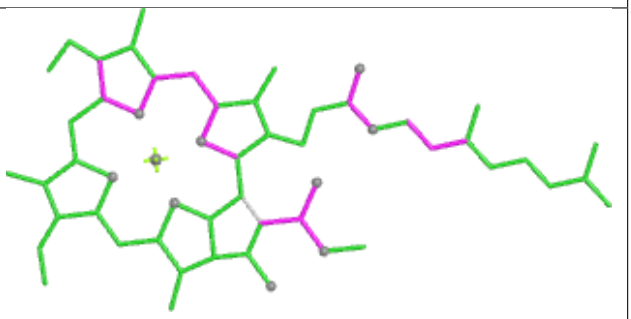
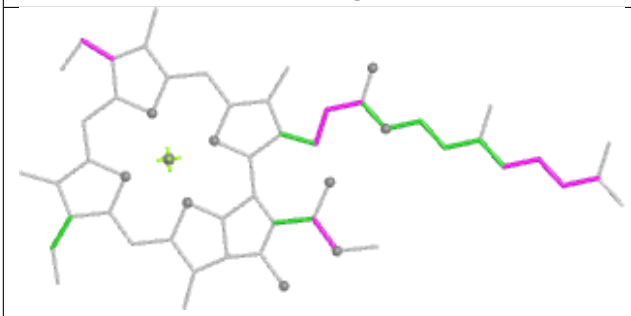
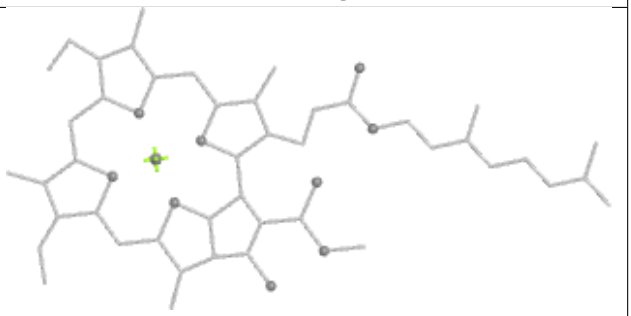
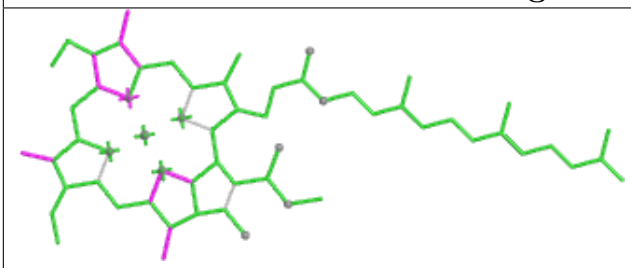
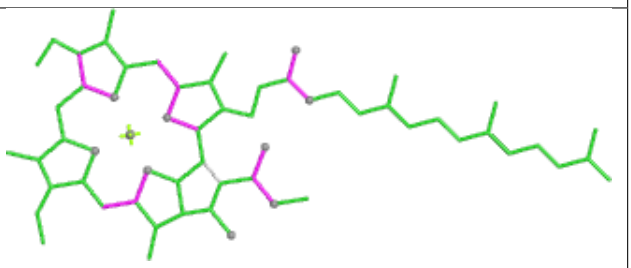
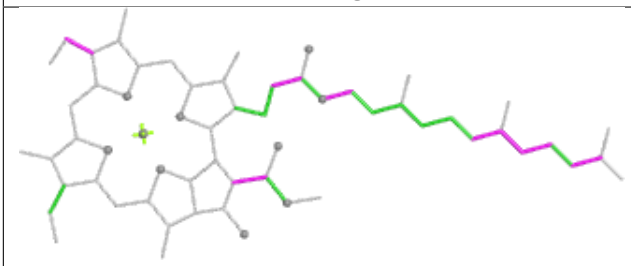
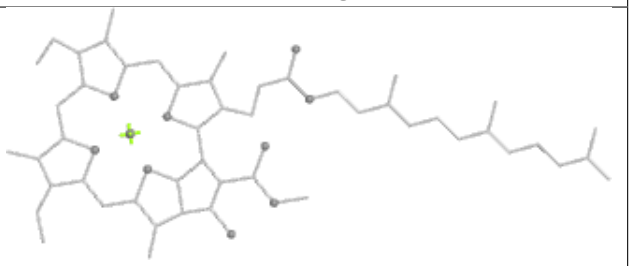
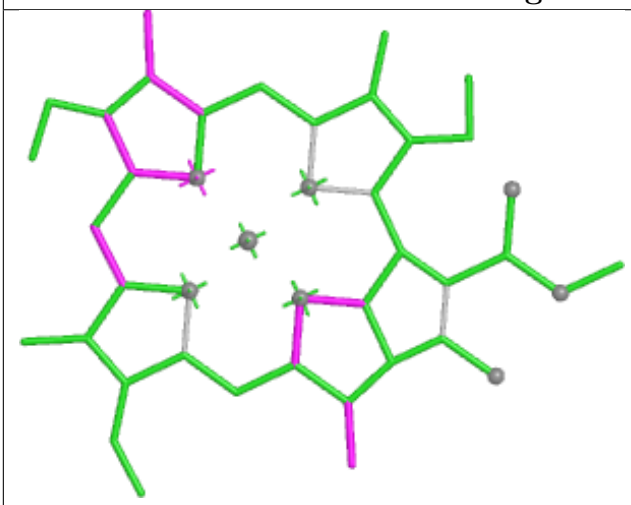
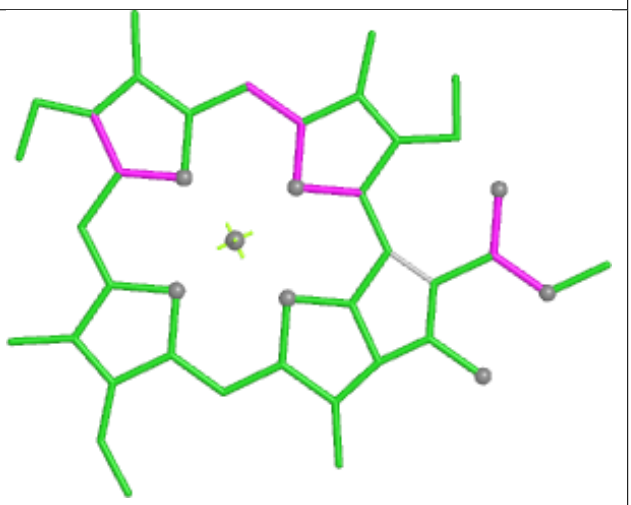
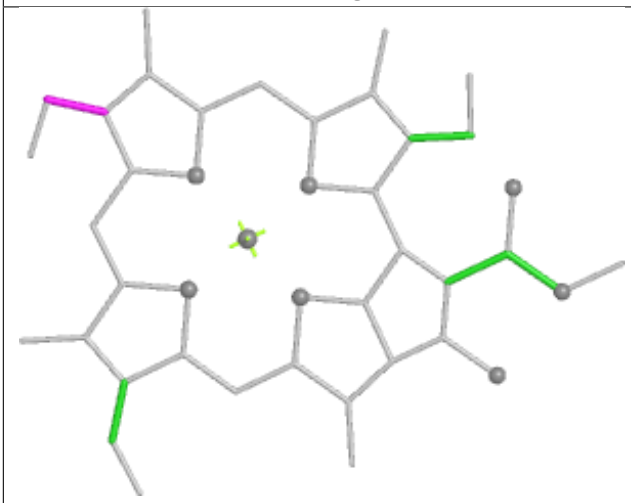
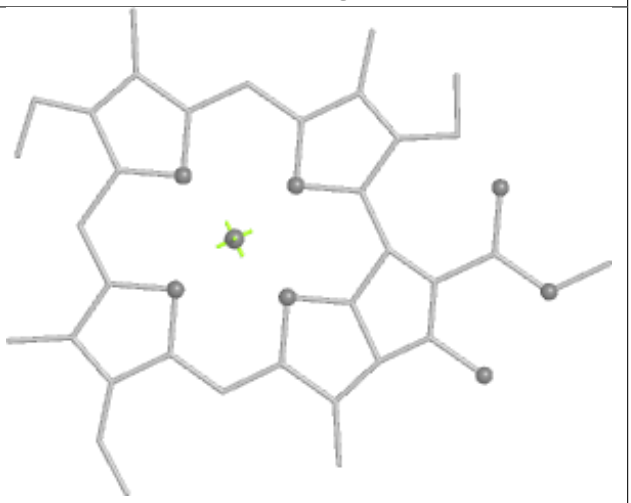
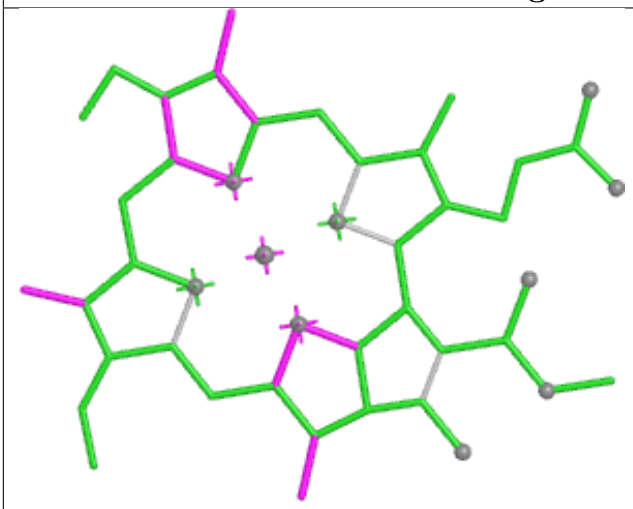
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 611



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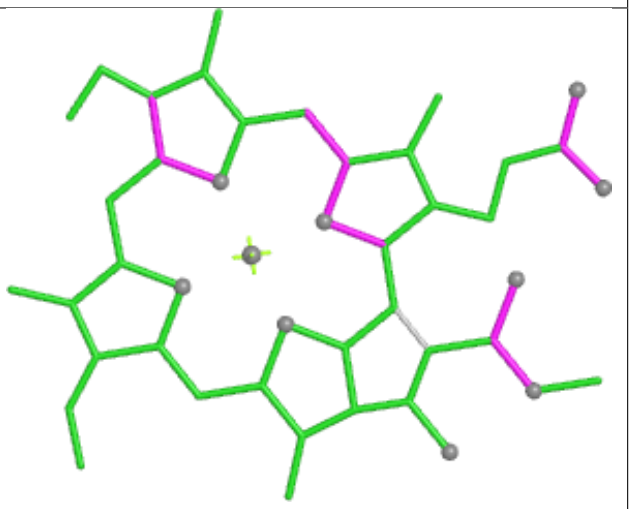

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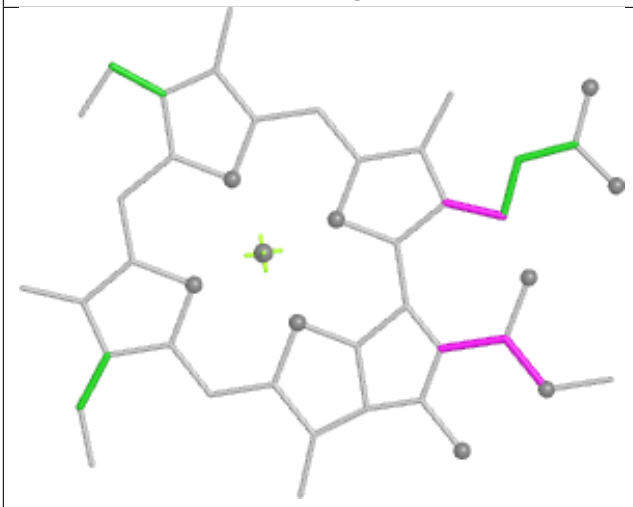
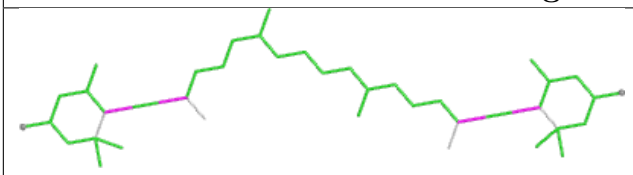


Torsions

Rings

Ligand II0 8 613



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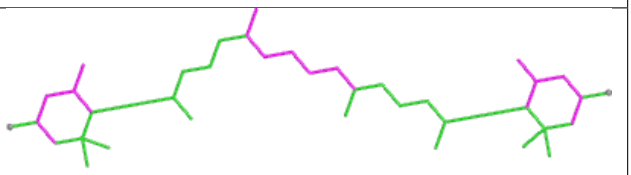

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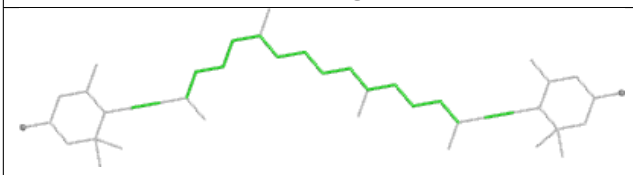
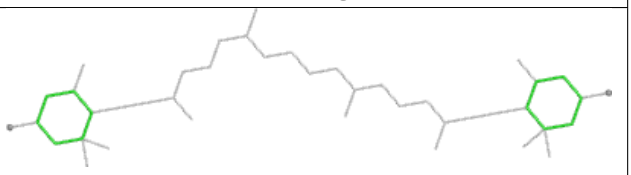
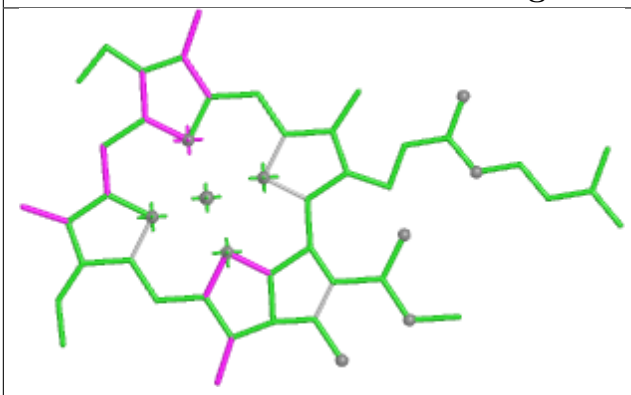
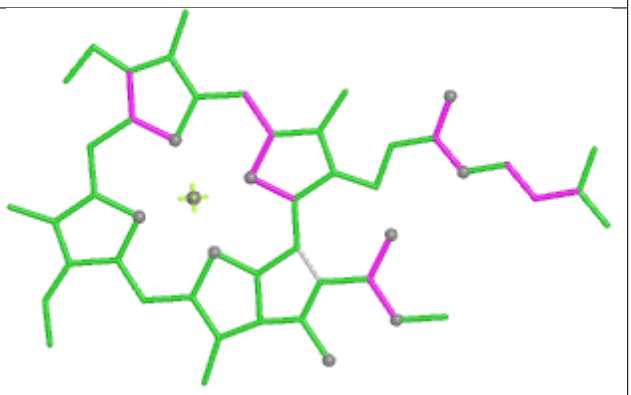
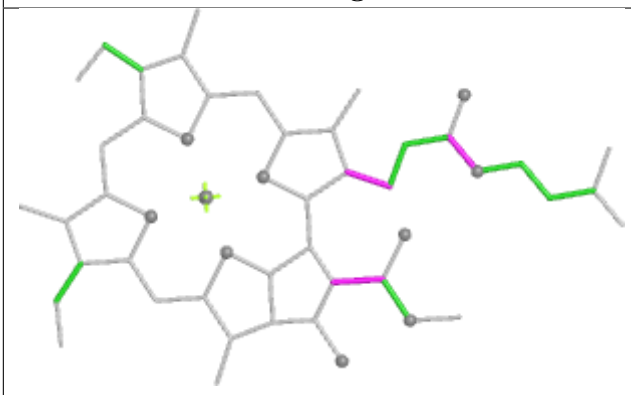
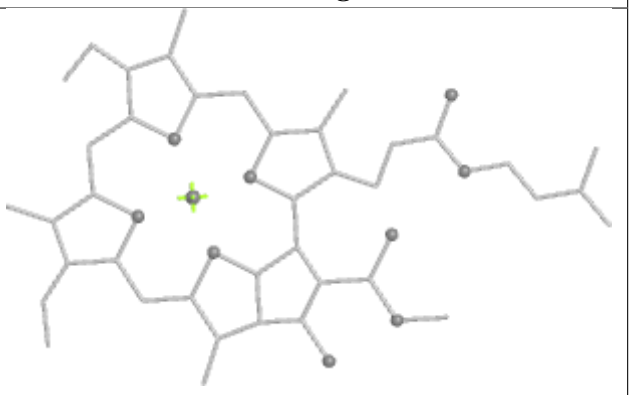
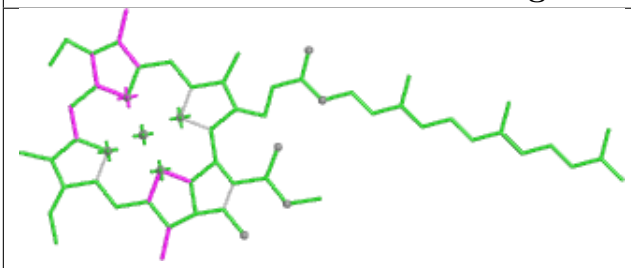
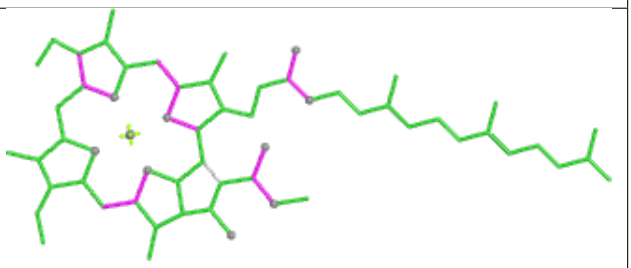
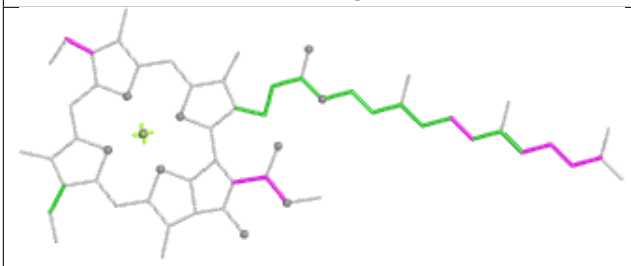
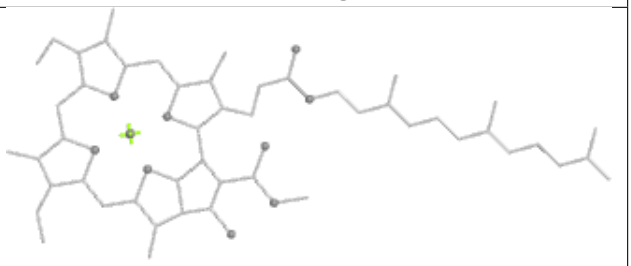


Torsions

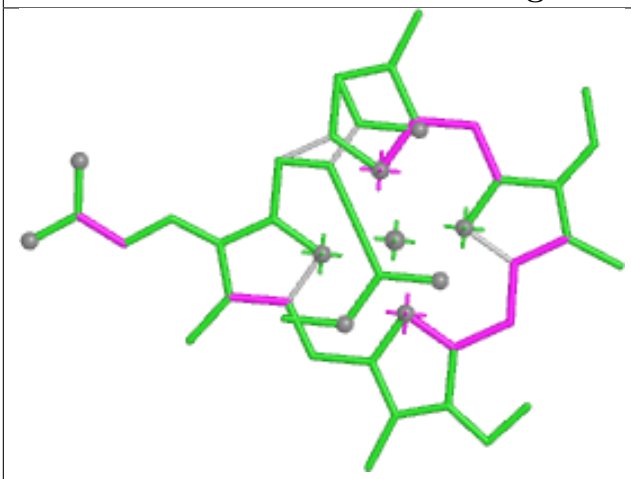


Rings

Ligand CLA 0 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC2 P 605



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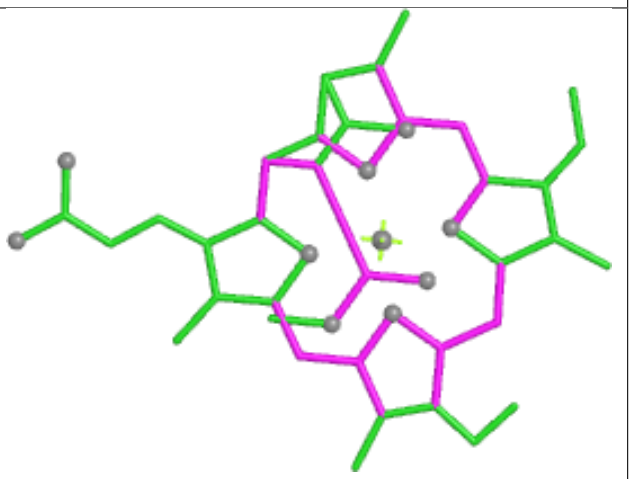

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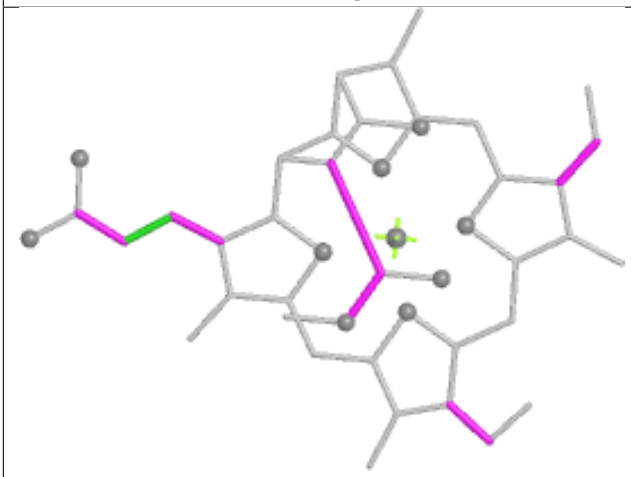

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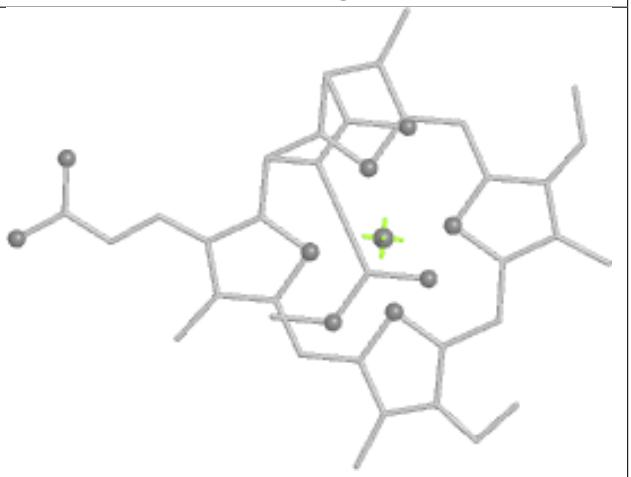
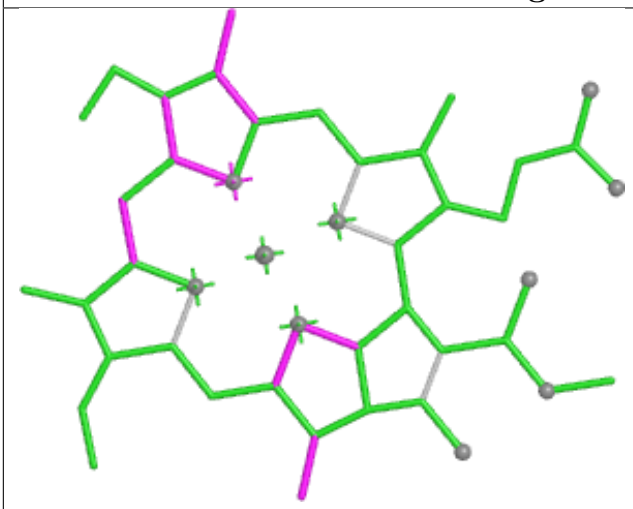


Rings

Ligand CLA 0 607



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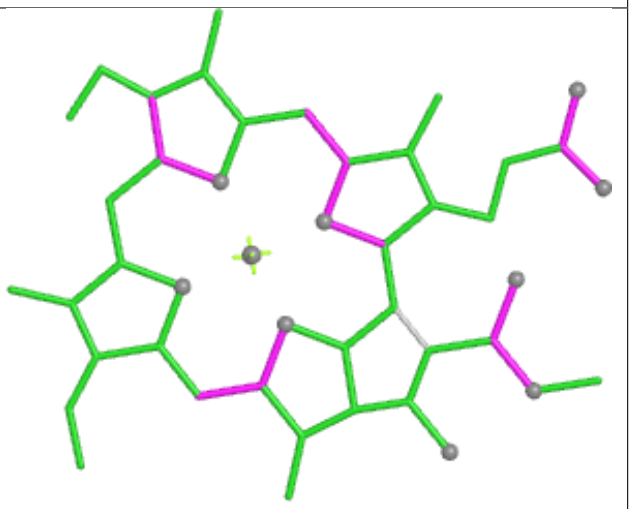

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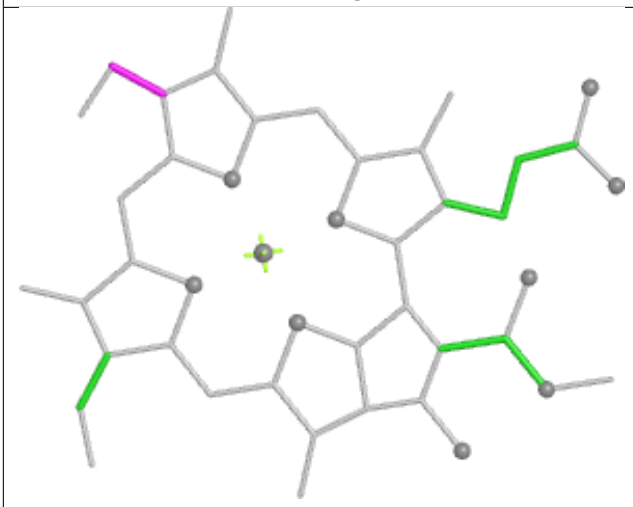
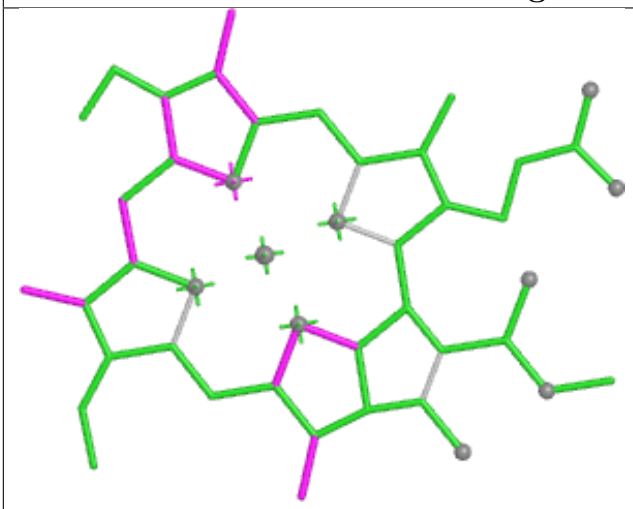


Torsions

Rings

Ligand CLA 8 612



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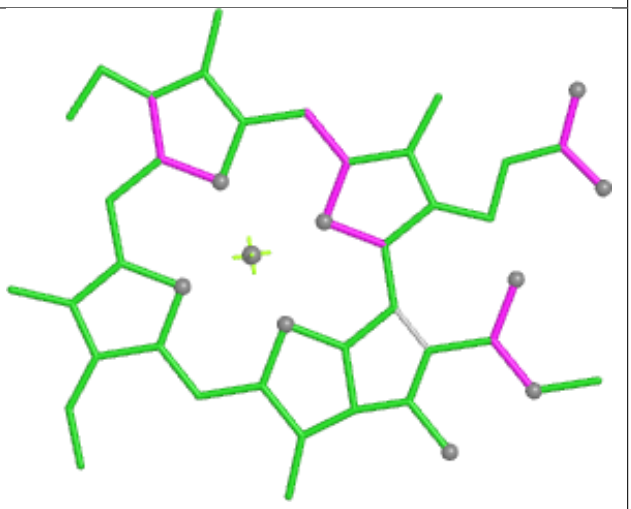

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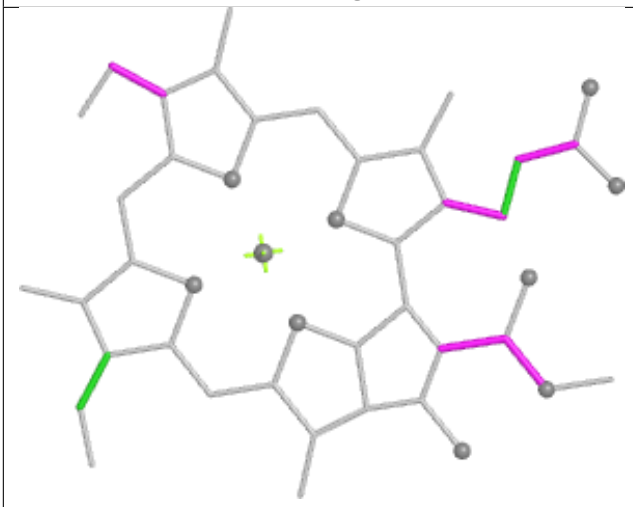
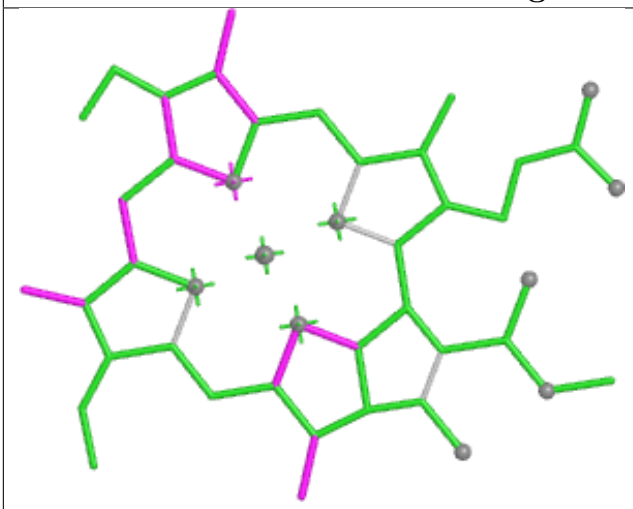


Torsions

Rings

Ligand CLA 7 607



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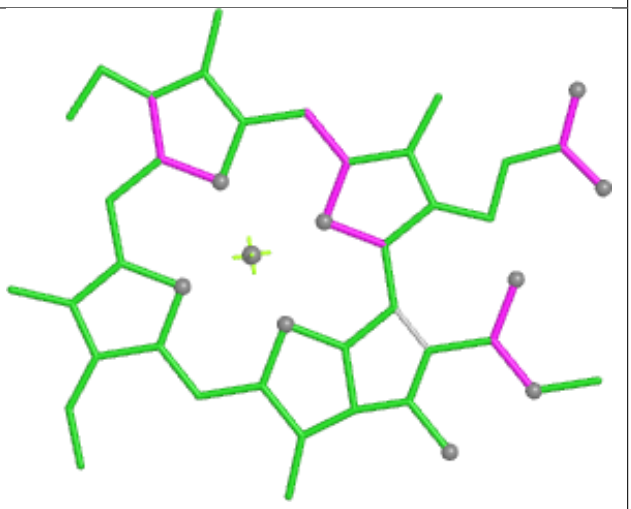

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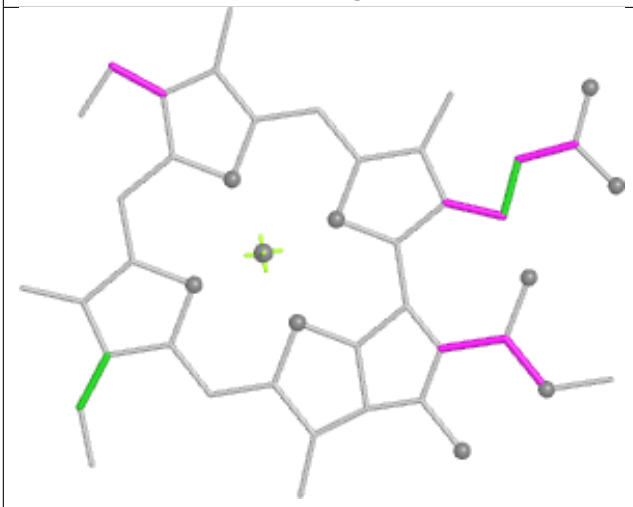
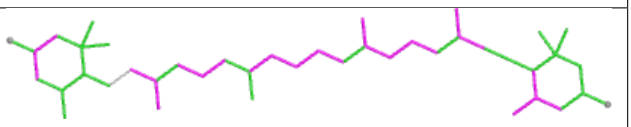


Torsions

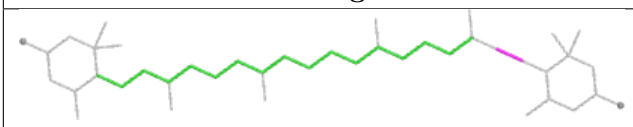
Rings

Ligand II3 P 613

Bond lengths



Bond angles



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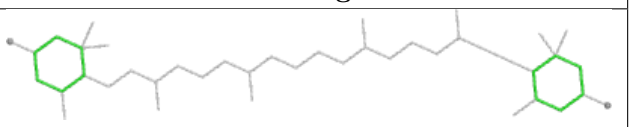
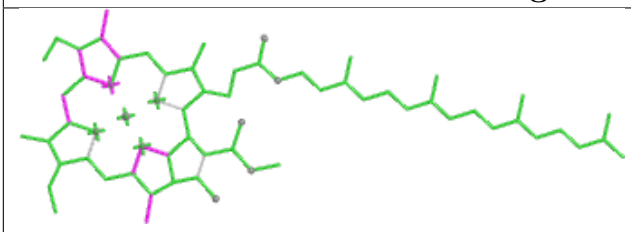


Rings

Ligand CLA s 303



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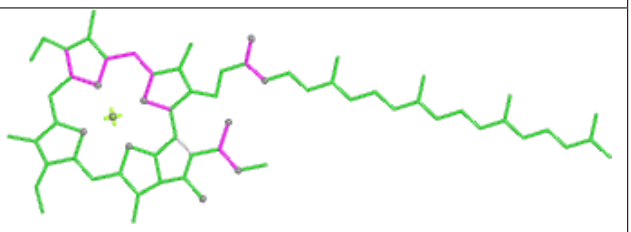

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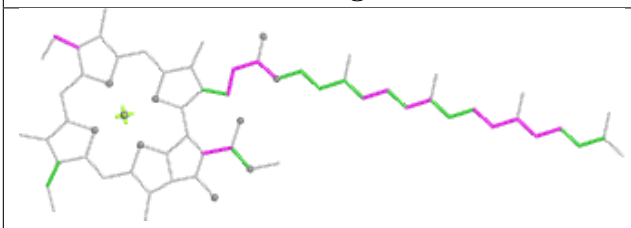

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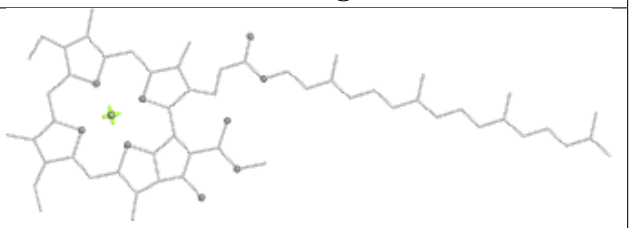
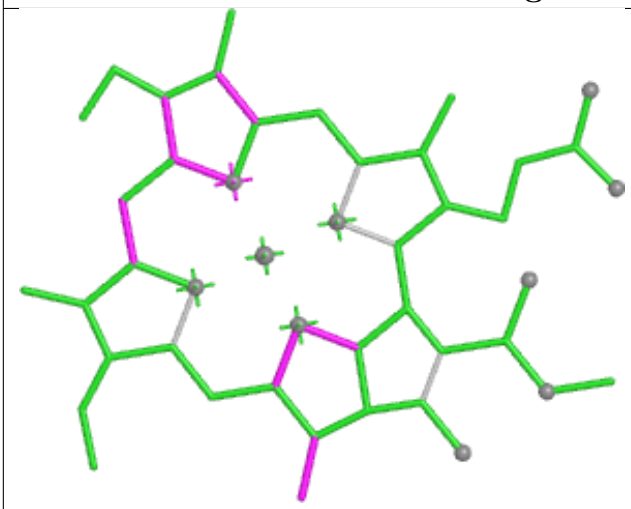


Rings

Ligand CLA P 606



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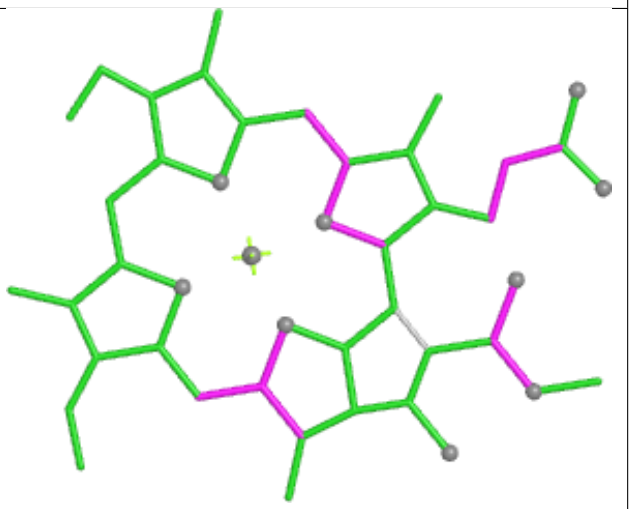
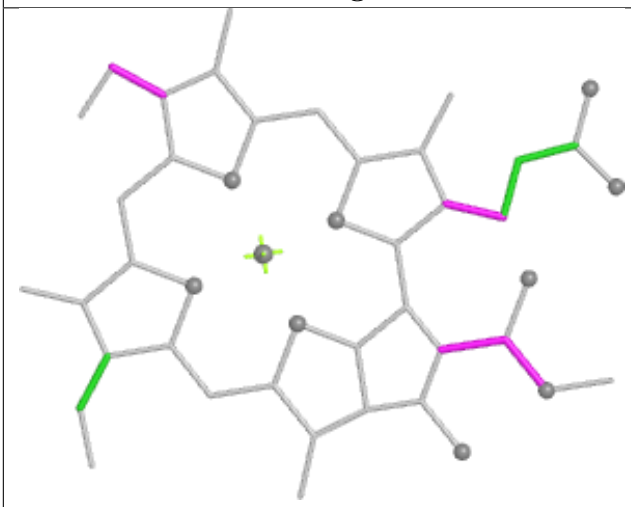


Bond angles



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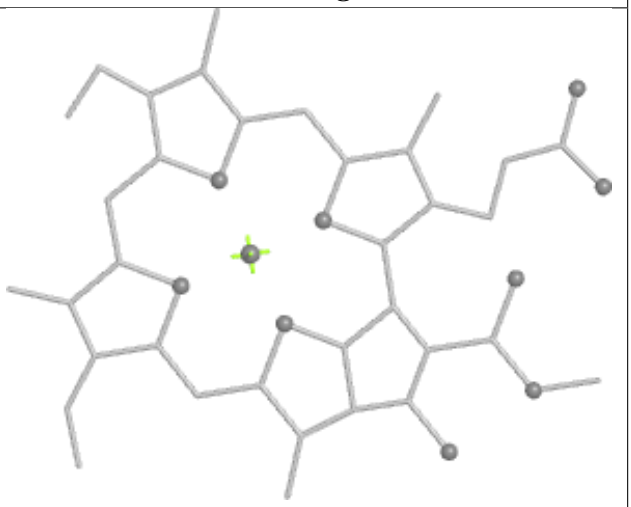
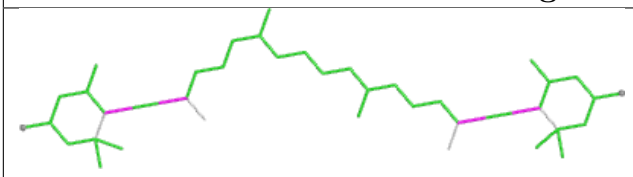


Rings

Ligand II0 P 612



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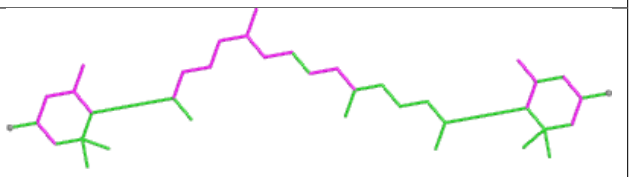

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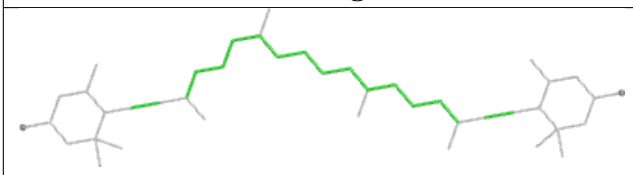

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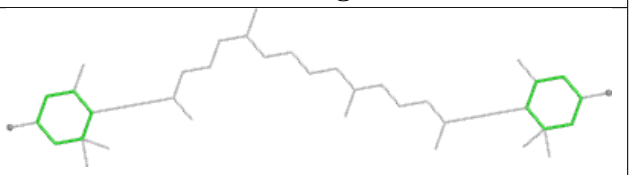
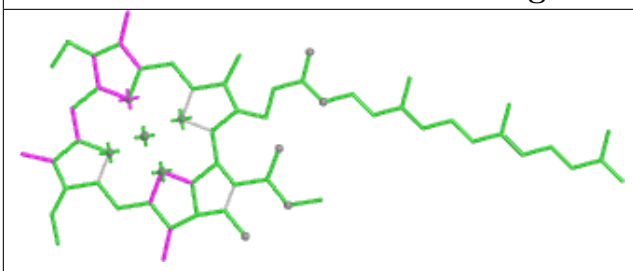


Rings

Ligand CLA 9 609



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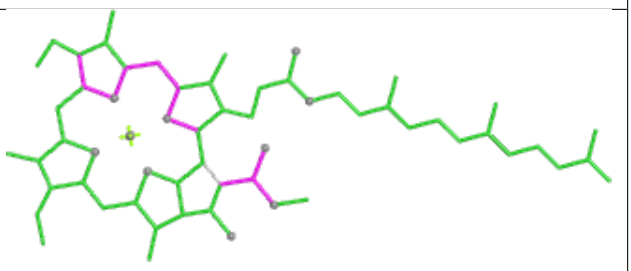

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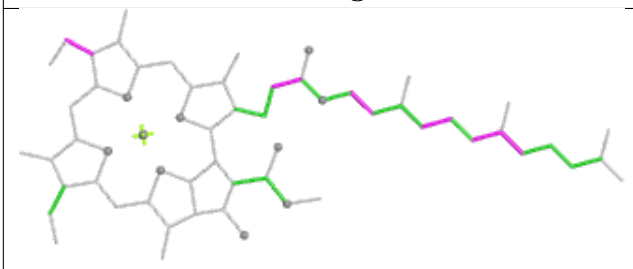

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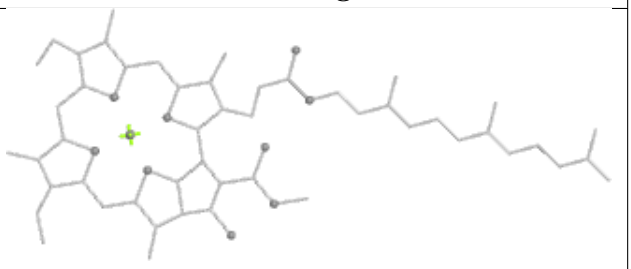
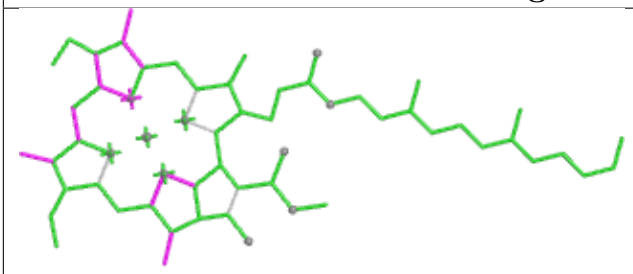


Rings

Ligand CLA 7 602



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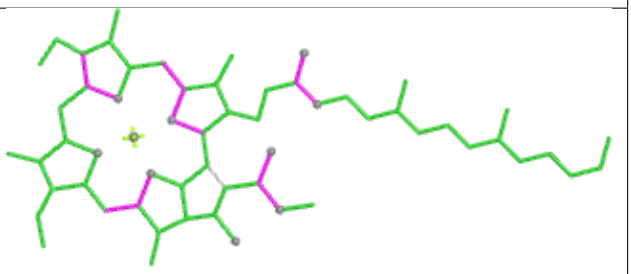
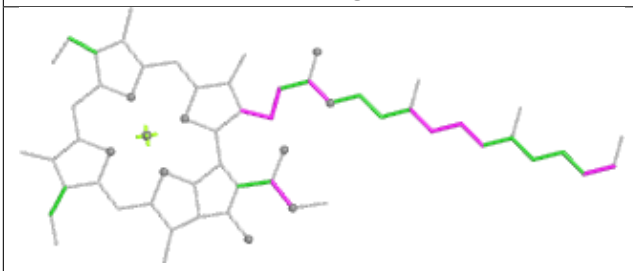


Bond angles



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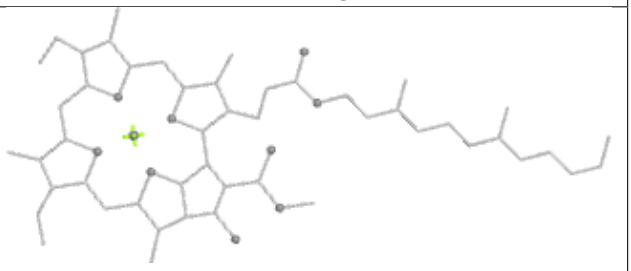
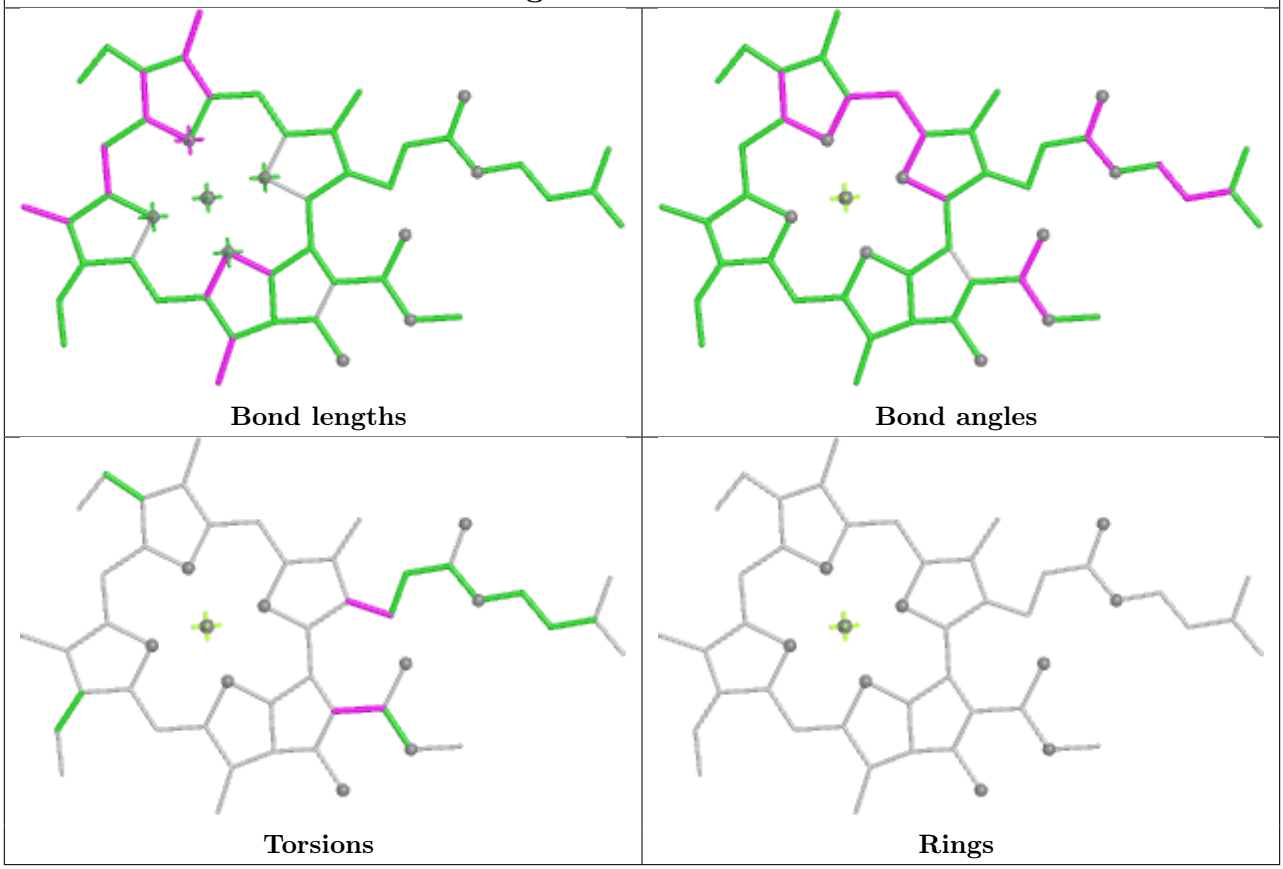
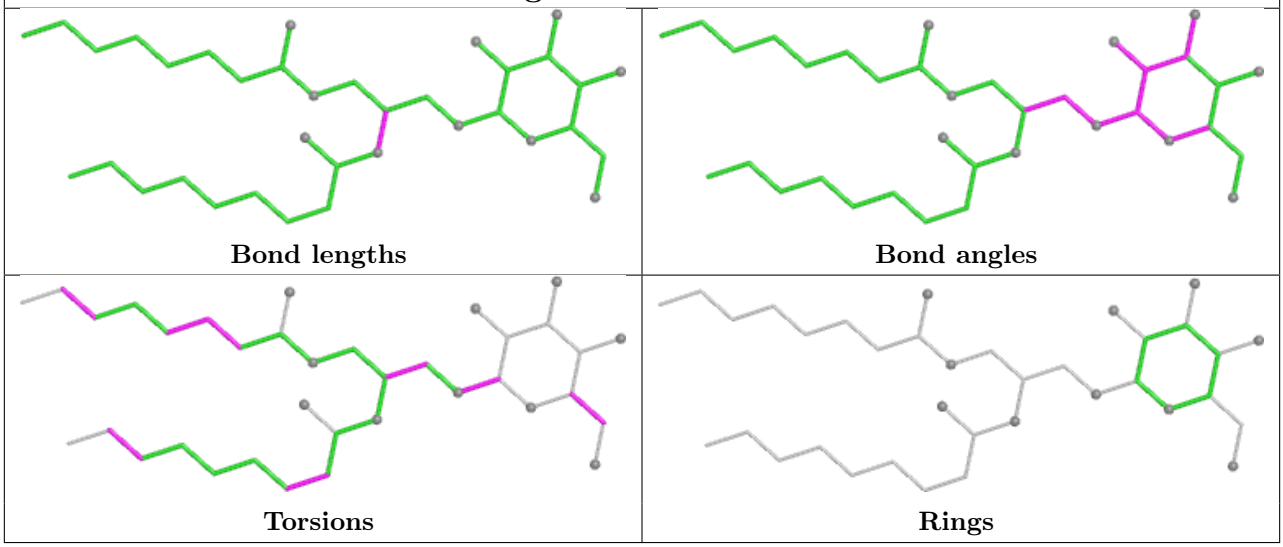


Rings

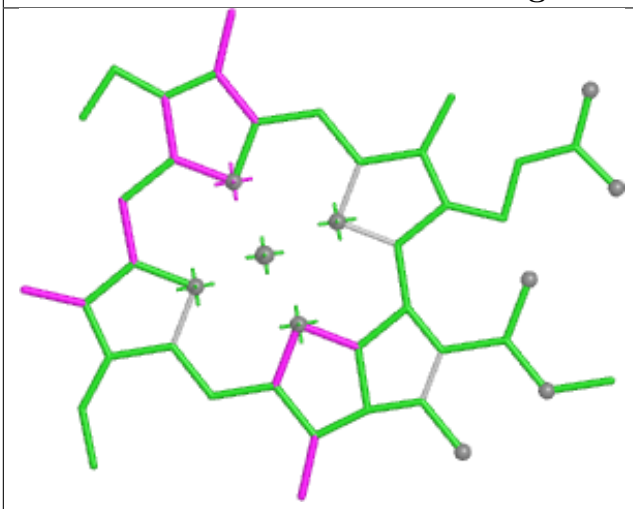
Ligand CLA P 603



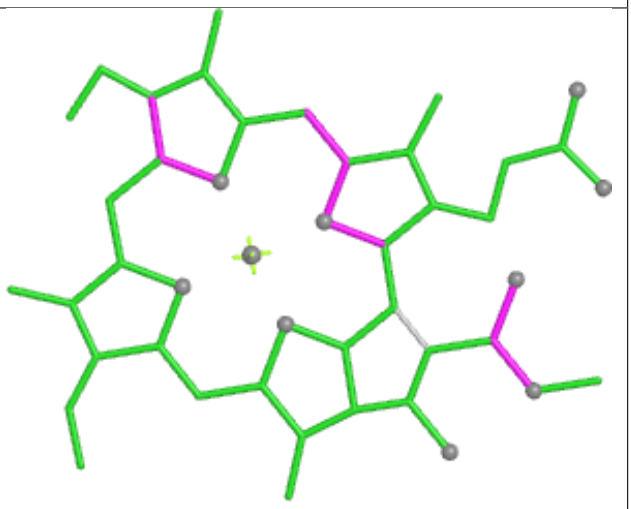
Ligand LMG 0 618



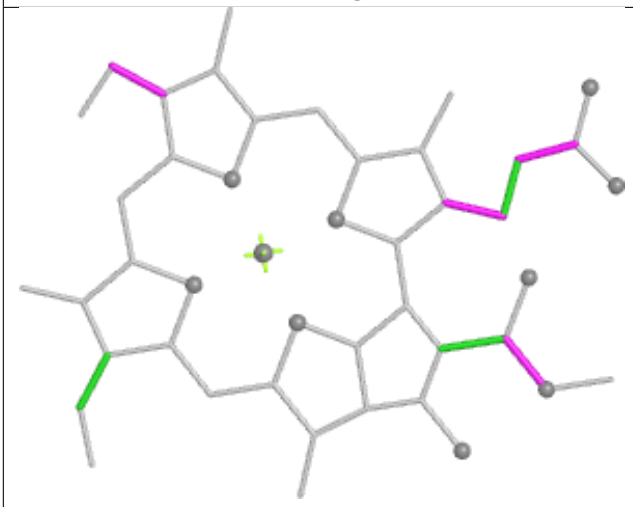
Ligand CLA 7 612



Bond lengths



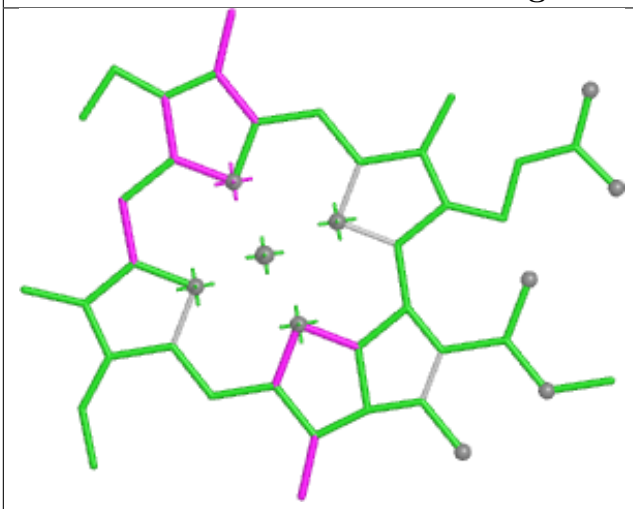
Bond angles



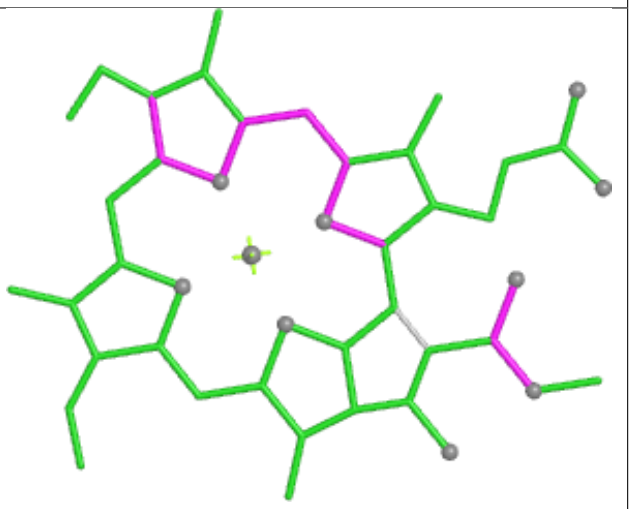
Torsions

Rings

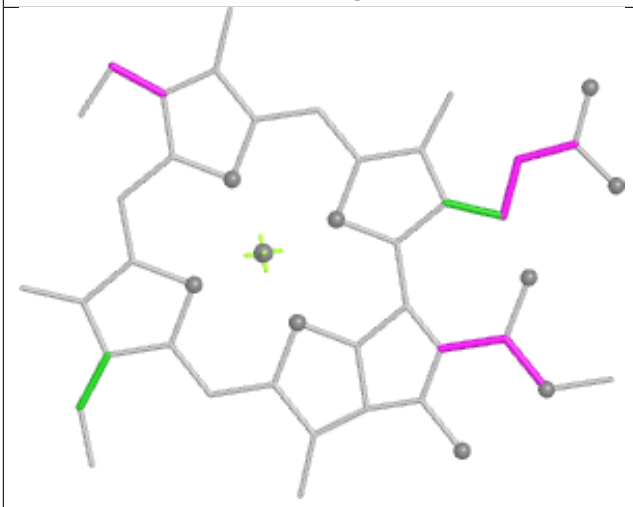
Ligand CLA 0 611



Bond lengths



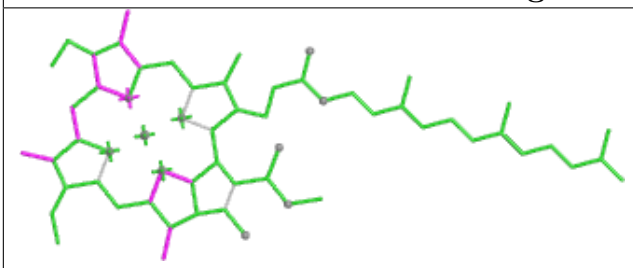
Bond angles



Torsions

Rings

Ligand CLA p 310



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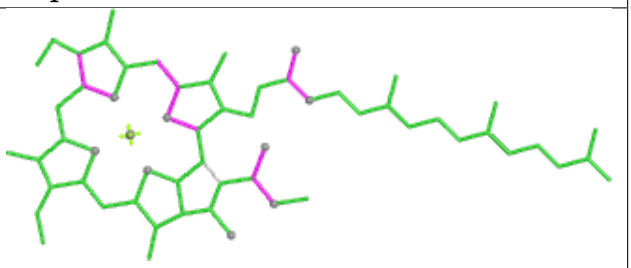
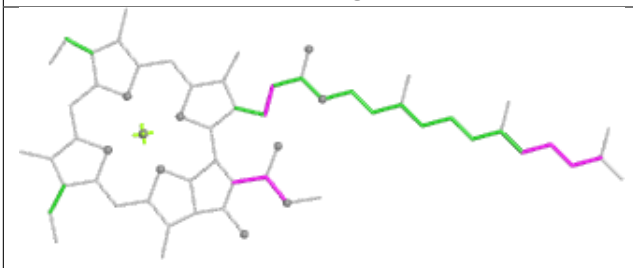
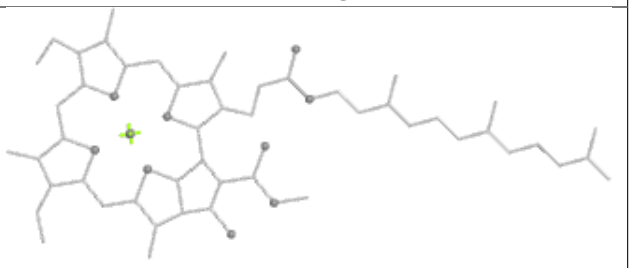


Bond angles

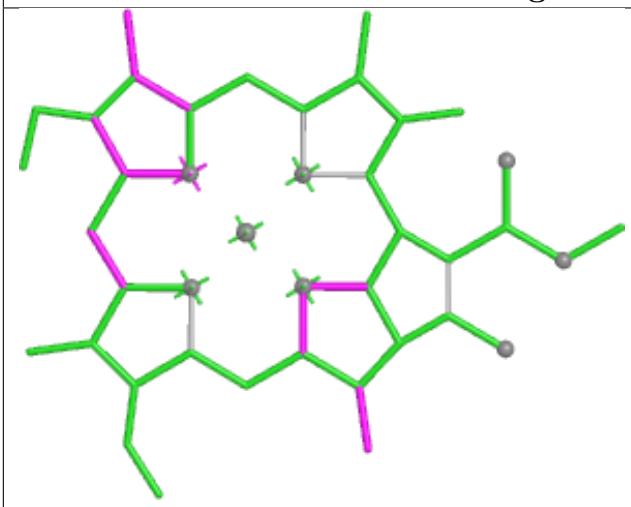


Torsions

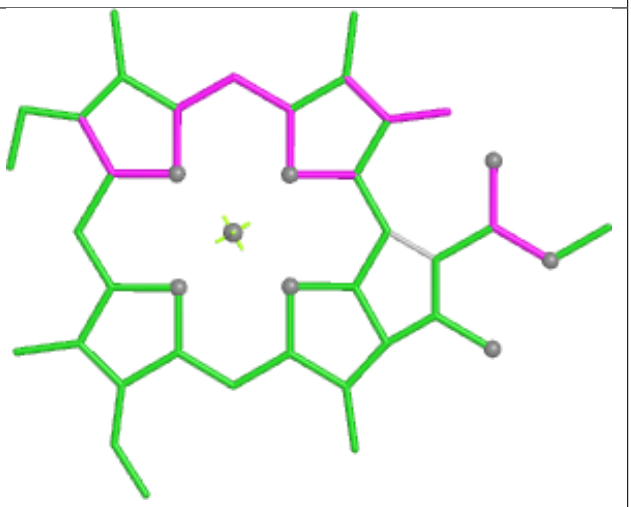


Rings

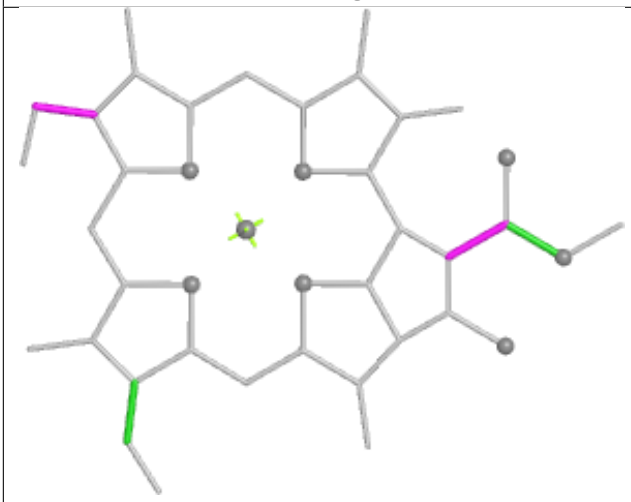
Ligand CLA 7 609



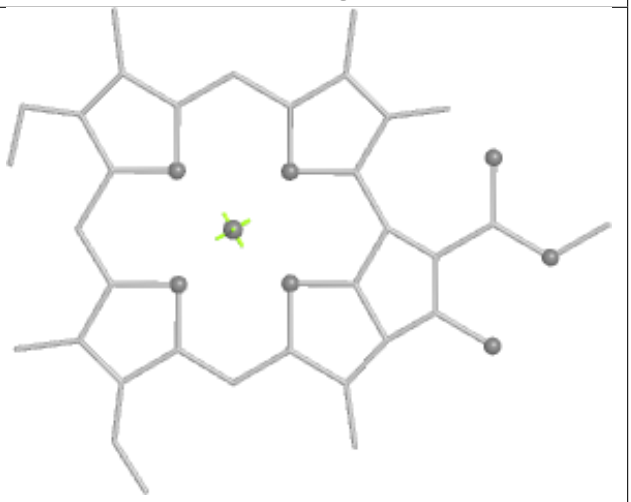
Bond lengths



Bond angles

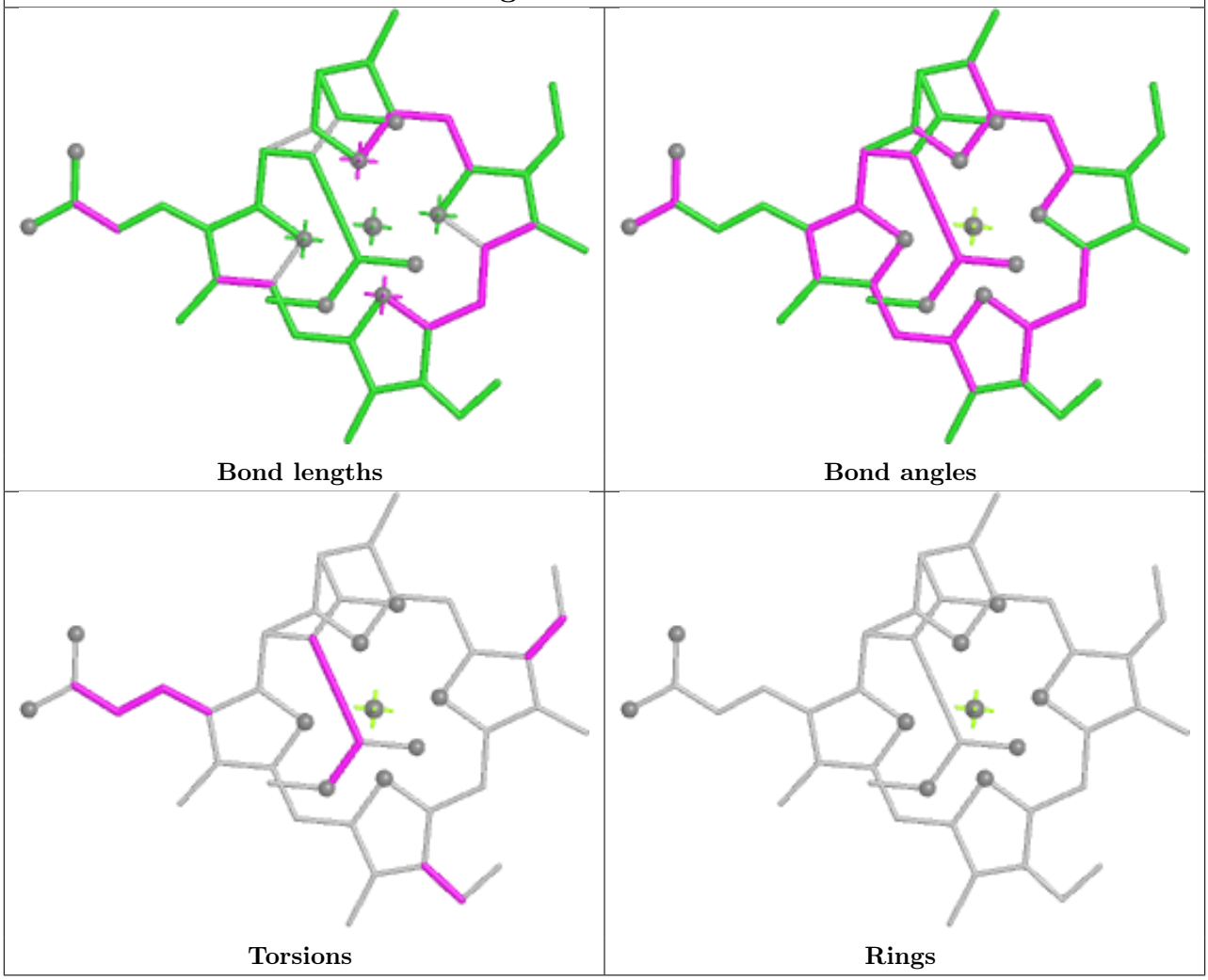


Torsions

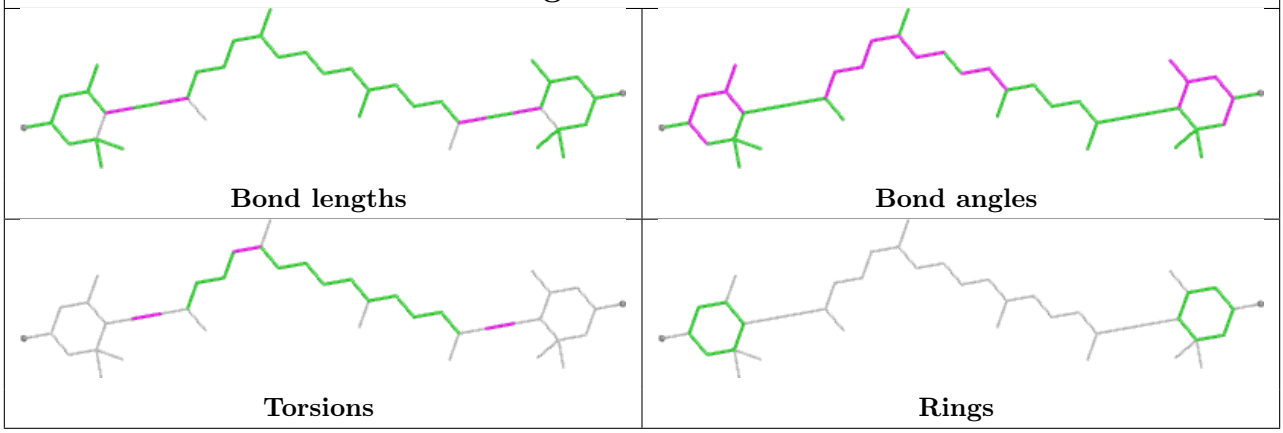


Rings

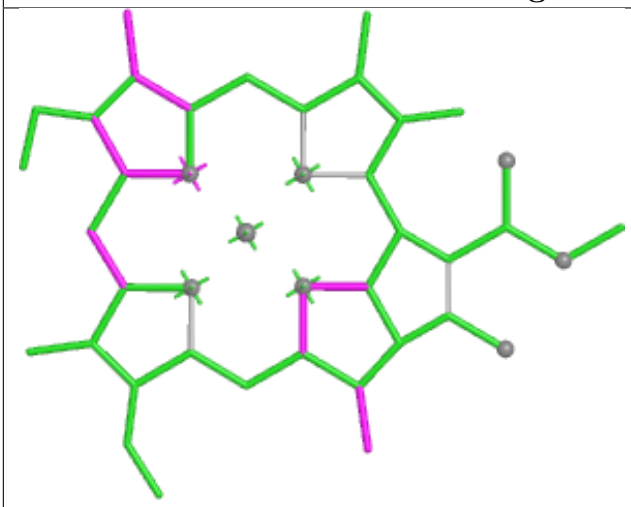
Ligand KC2 0 610



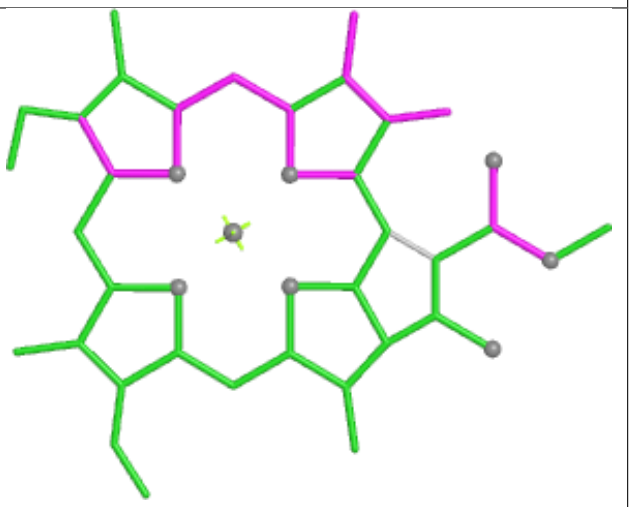
Ligand II0 9 614



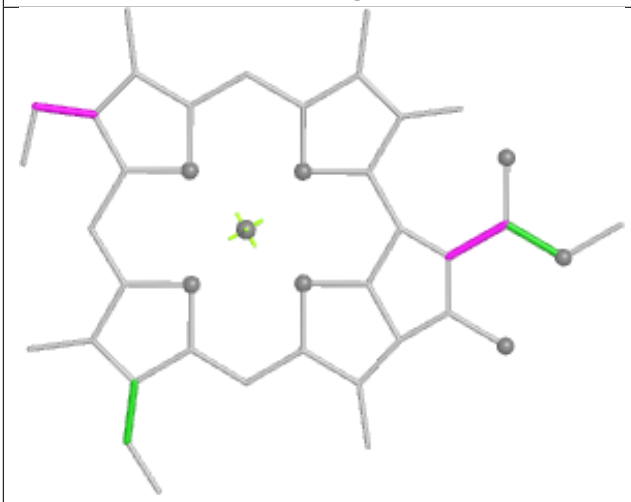
Ligand CLA 9 608



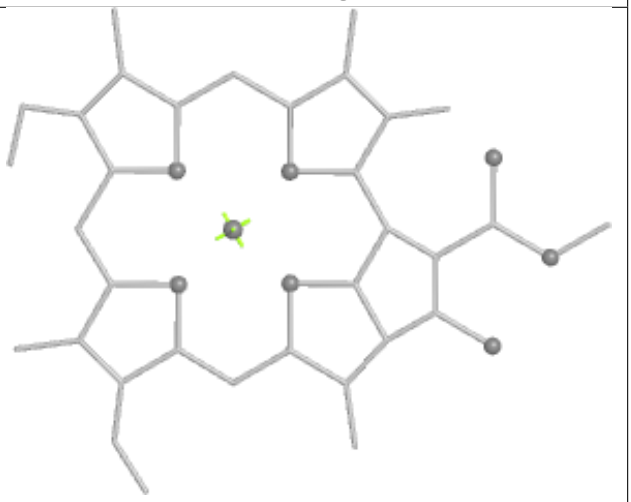
Bond lengths



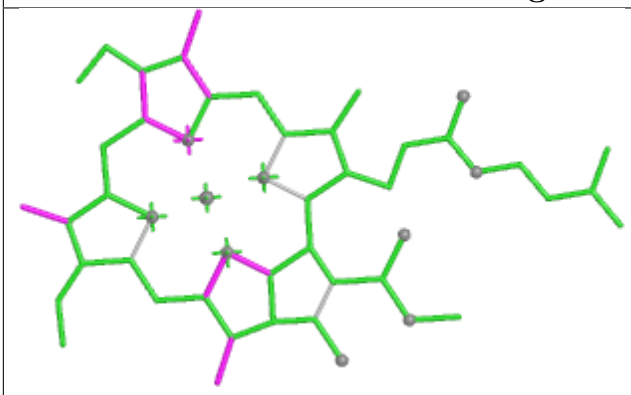
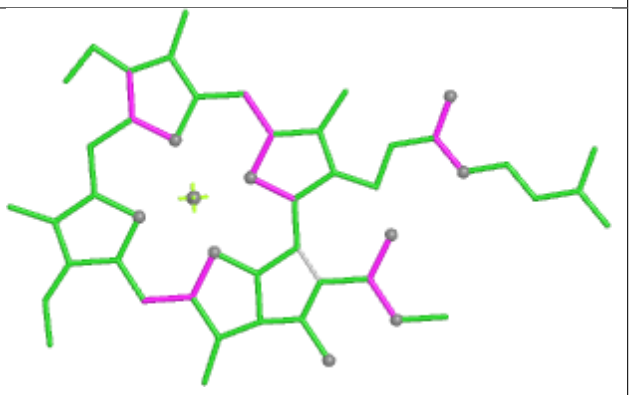
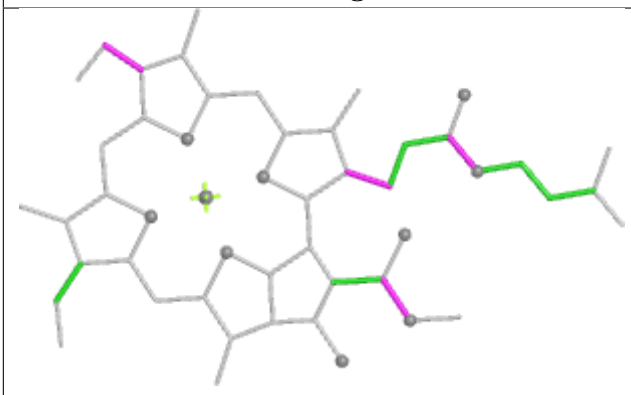
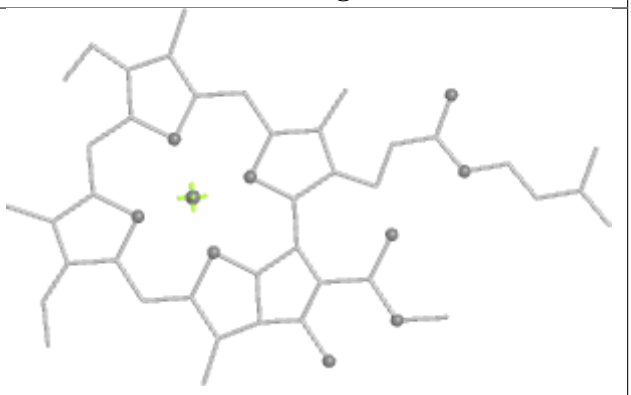
Bond angles

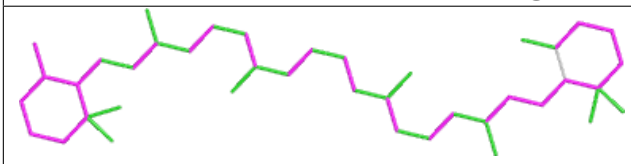
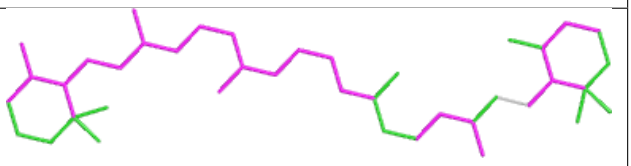
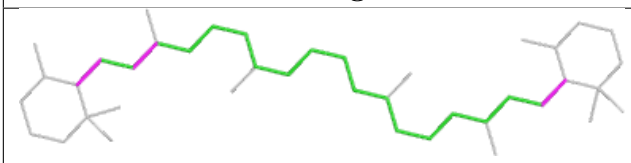
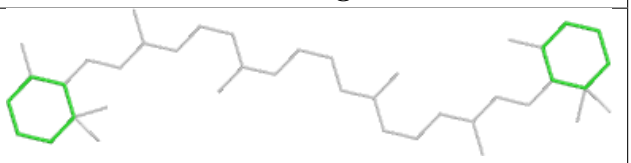


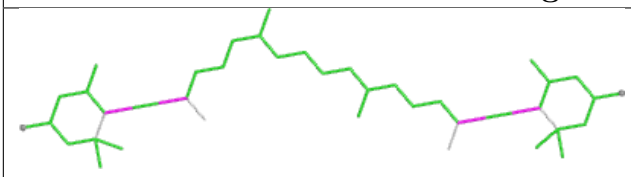
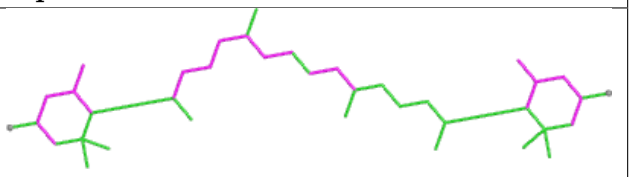
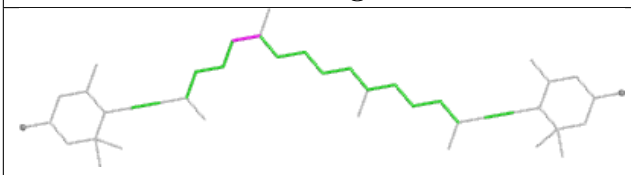
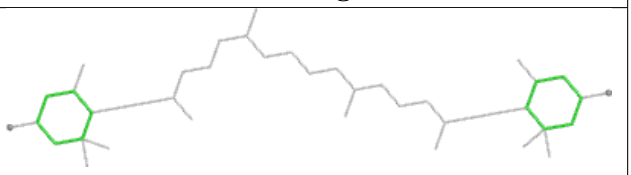
Torsions

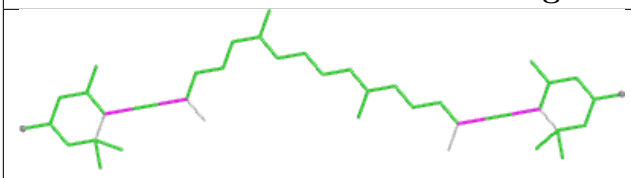
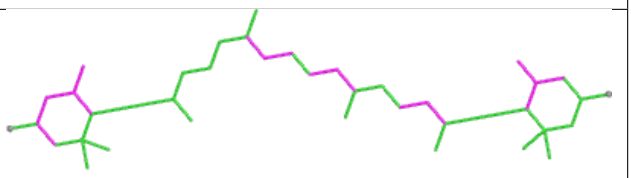
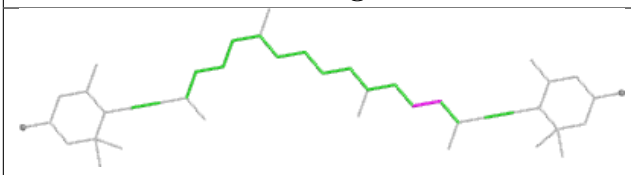
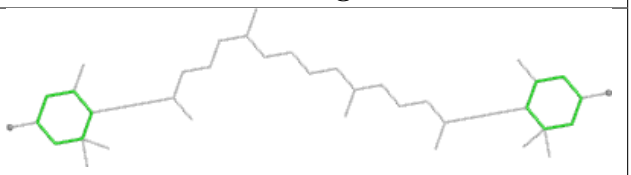


Rings

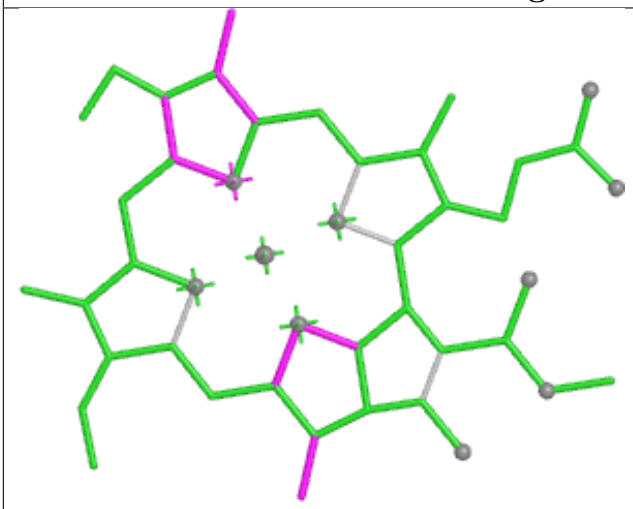
Ligand CLA 7 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT P 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

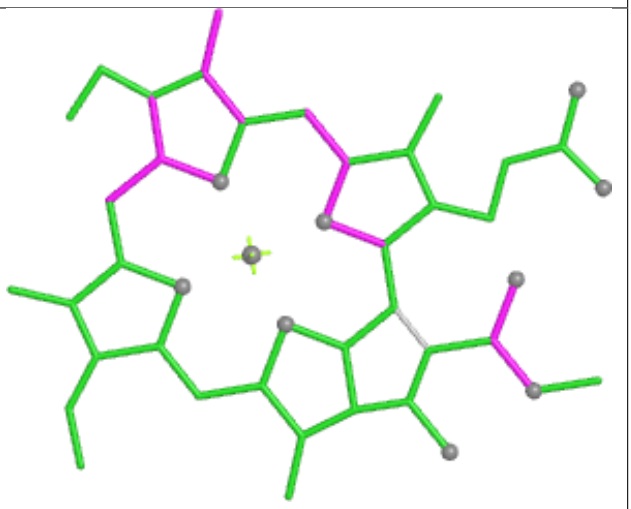
Ligand II0 p 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 8 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

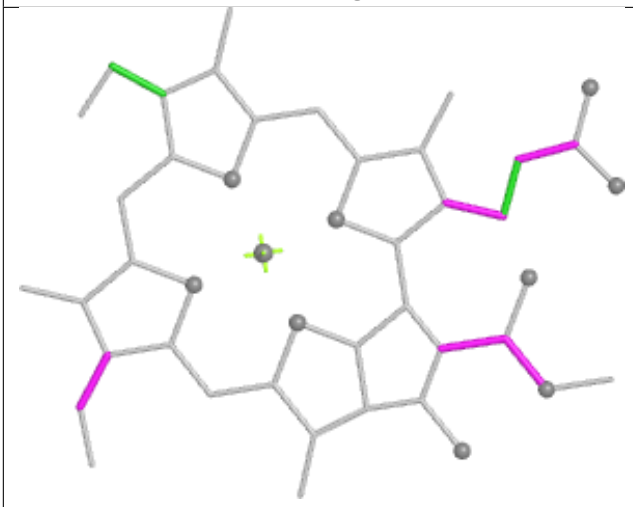
Ligand CLA 7 606



Bond lengths

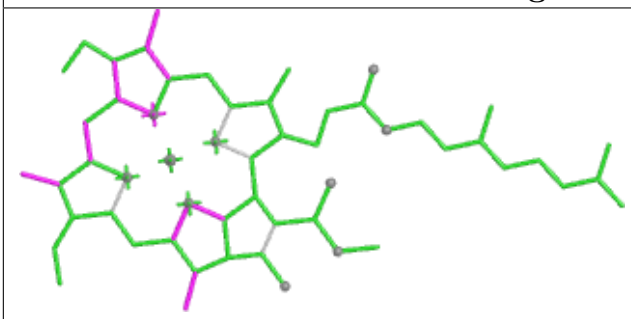
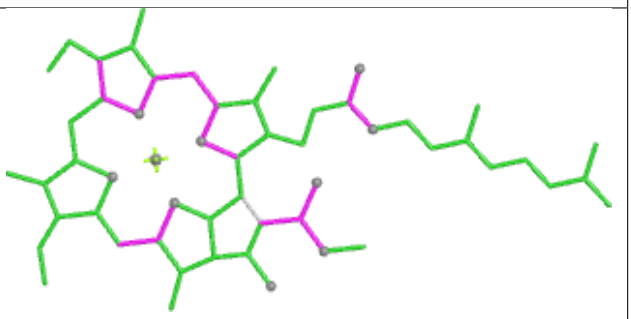
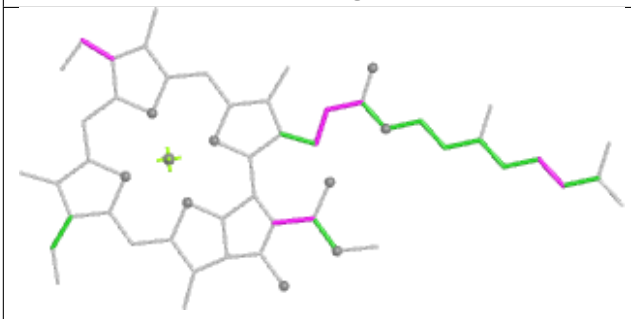
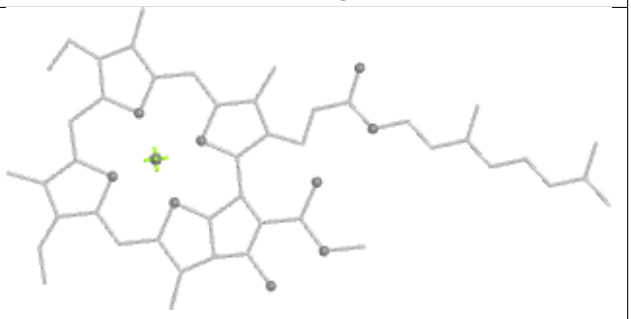


Bond angles

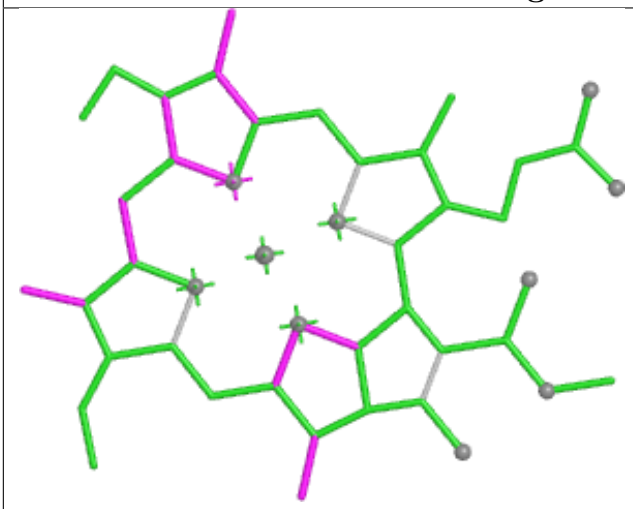


Torsions

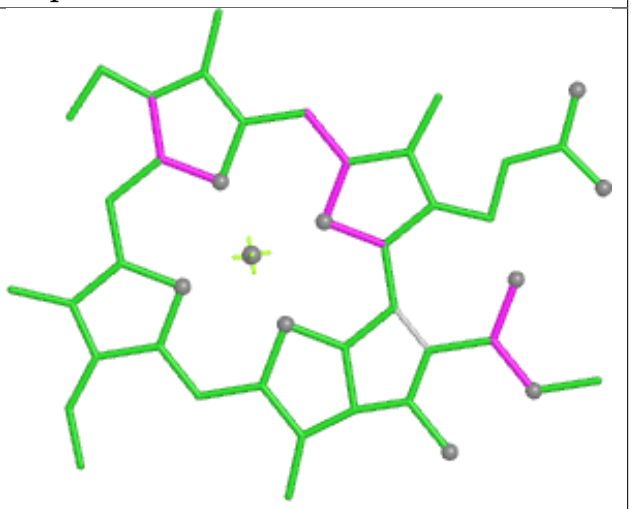
Rings

Ligand CLA 9 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

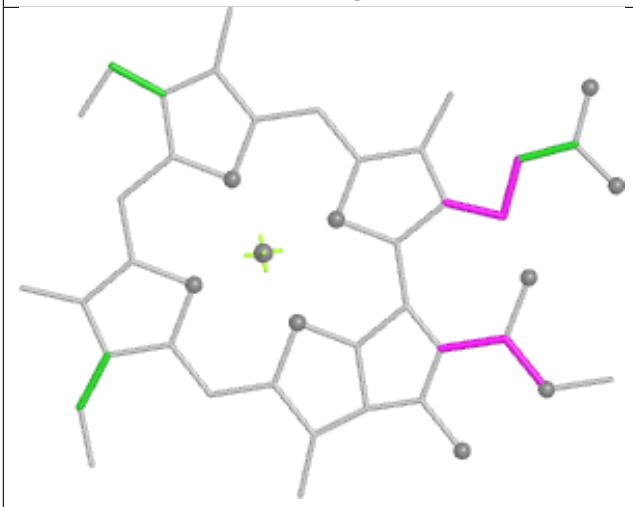
Ligand CLA p 314



Bond lengths



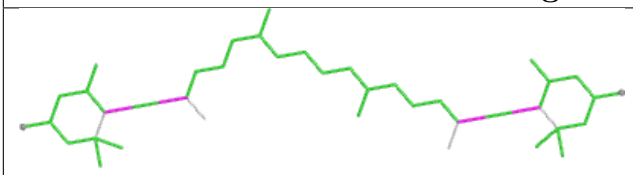
Bond angles



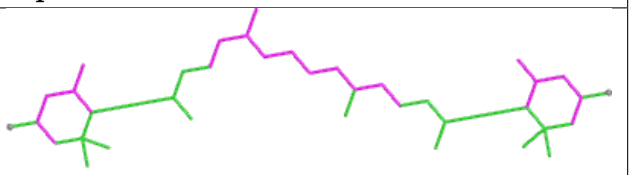
Torsions

Rings

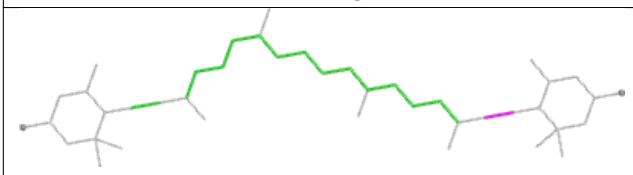
Ligand II0 p 315



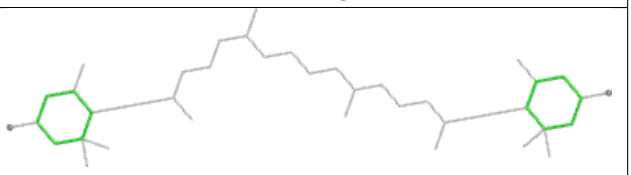
Bond lengths



Bond angles

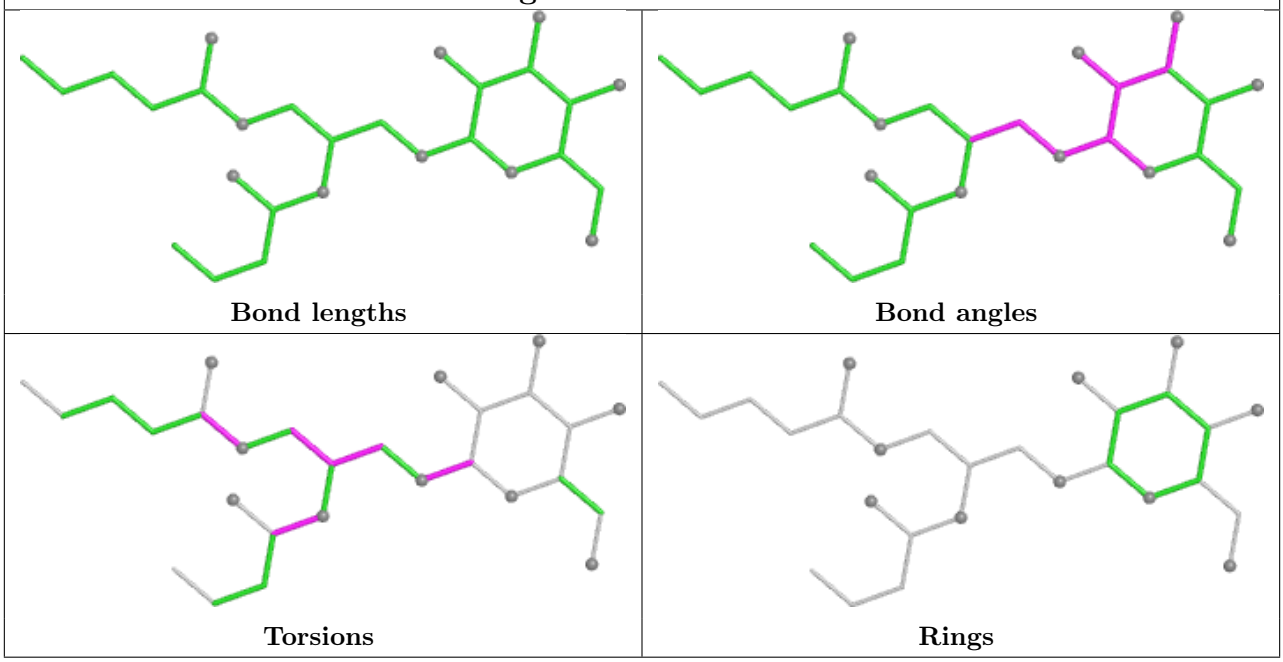


Torsions

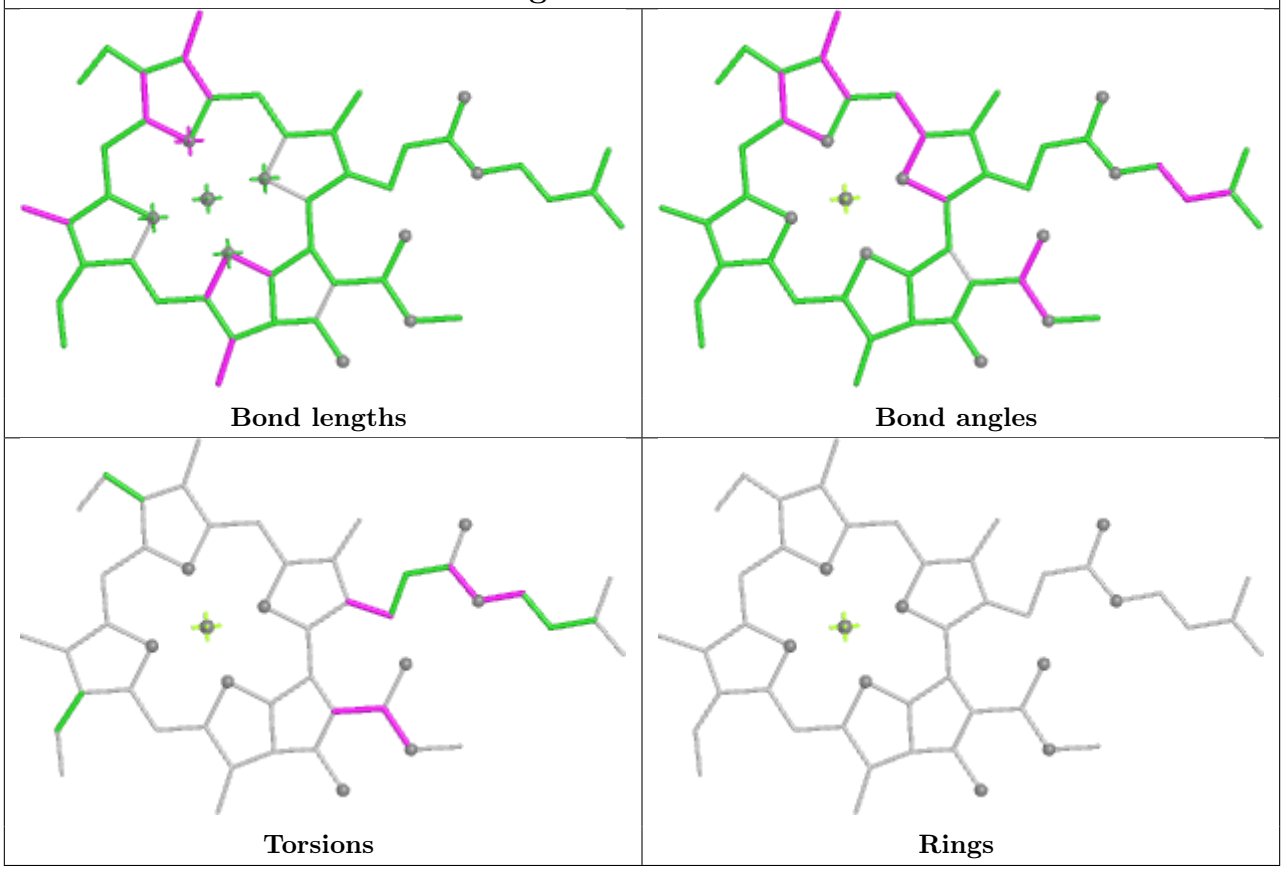


Rings

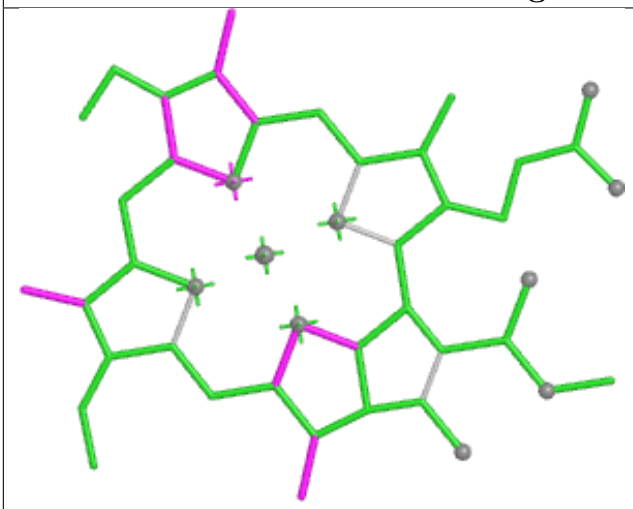
Ligand LMG G 102



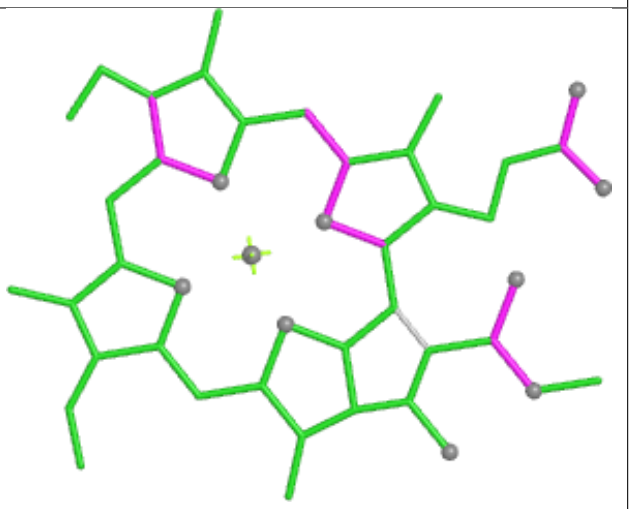
Ligand CLA 7 603



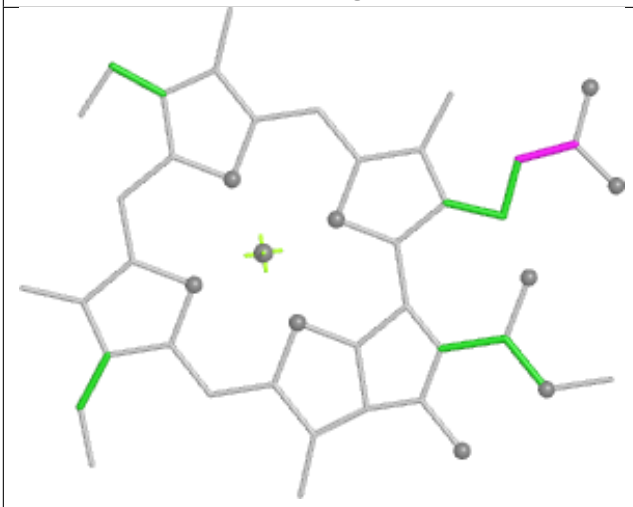
Ligand CLA 8 606



Bond lengths



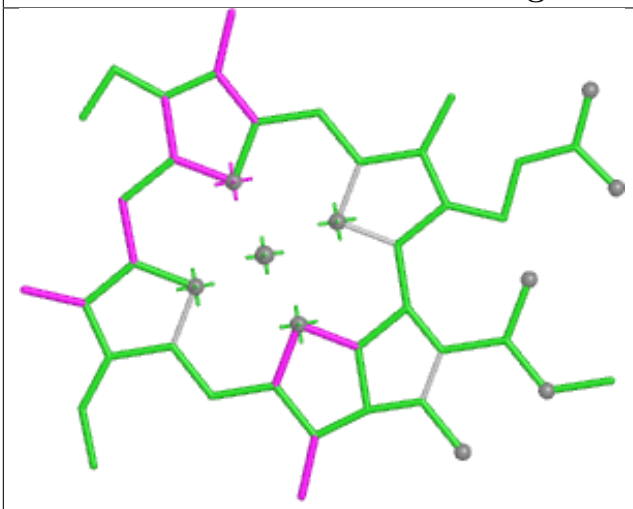
Bond angles



Torsions

Rings

Ligand CLA p 309



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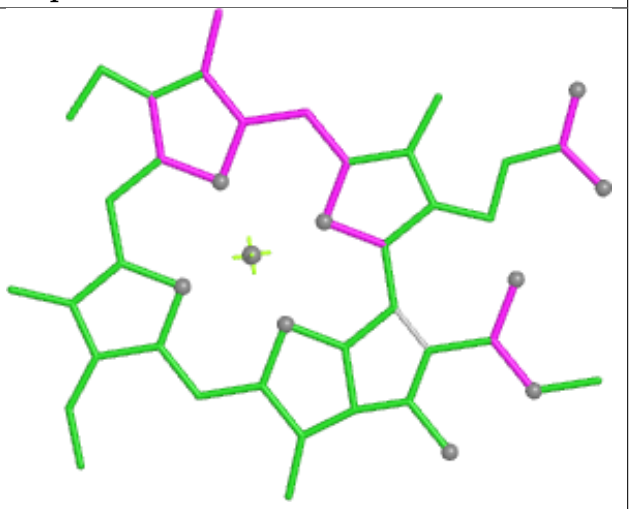
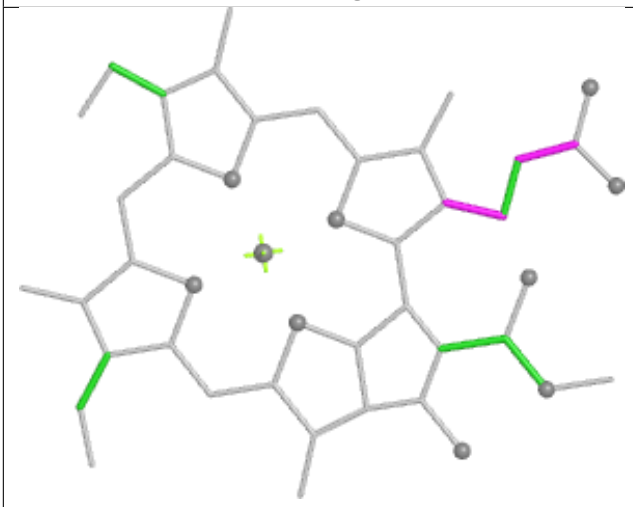


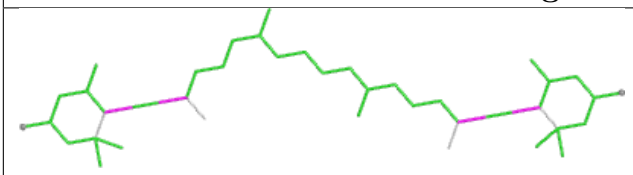
Bond angles



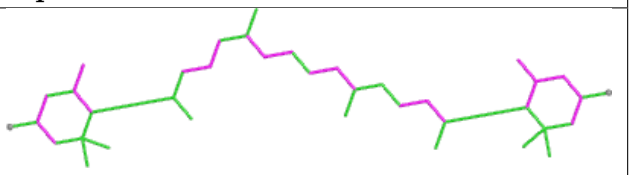
Torsions

Rings

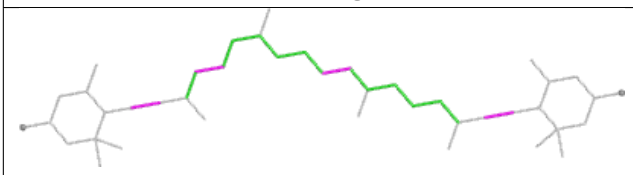
Ligand II0 p 316



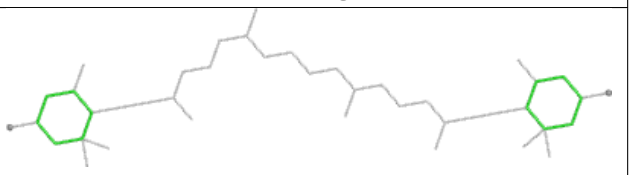
Bond lengths



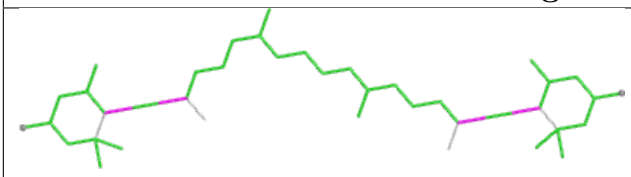
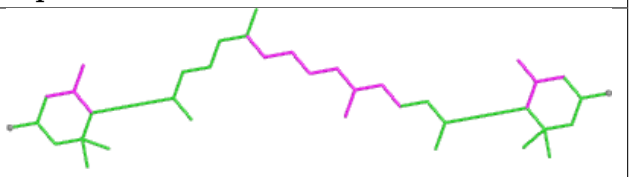
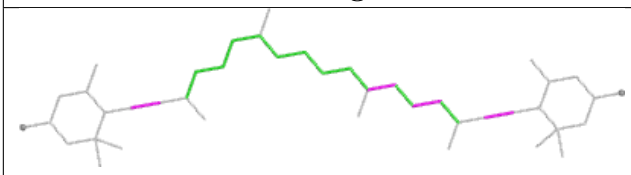
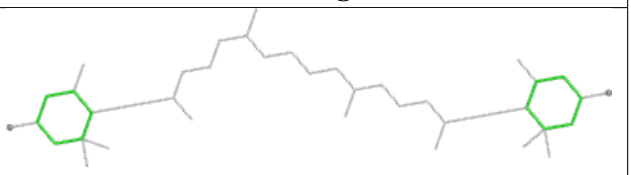
Bond angles

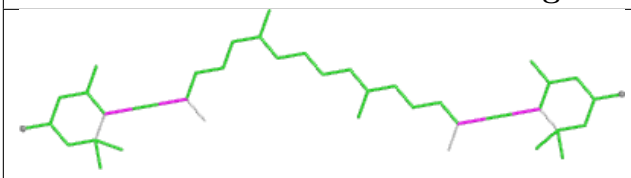
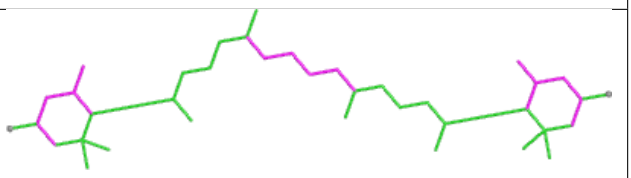
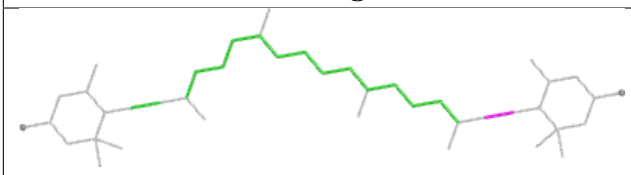
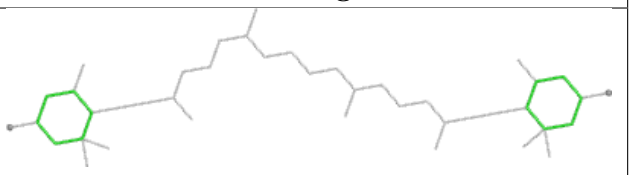


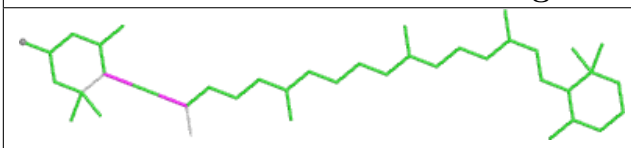
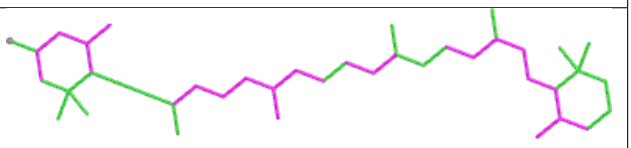
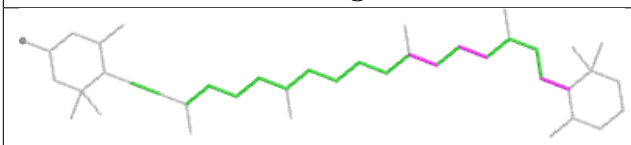
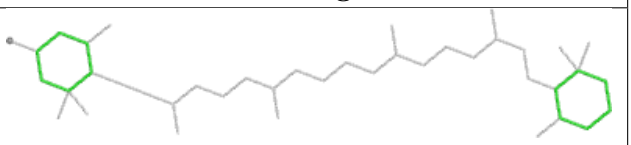
Torsions



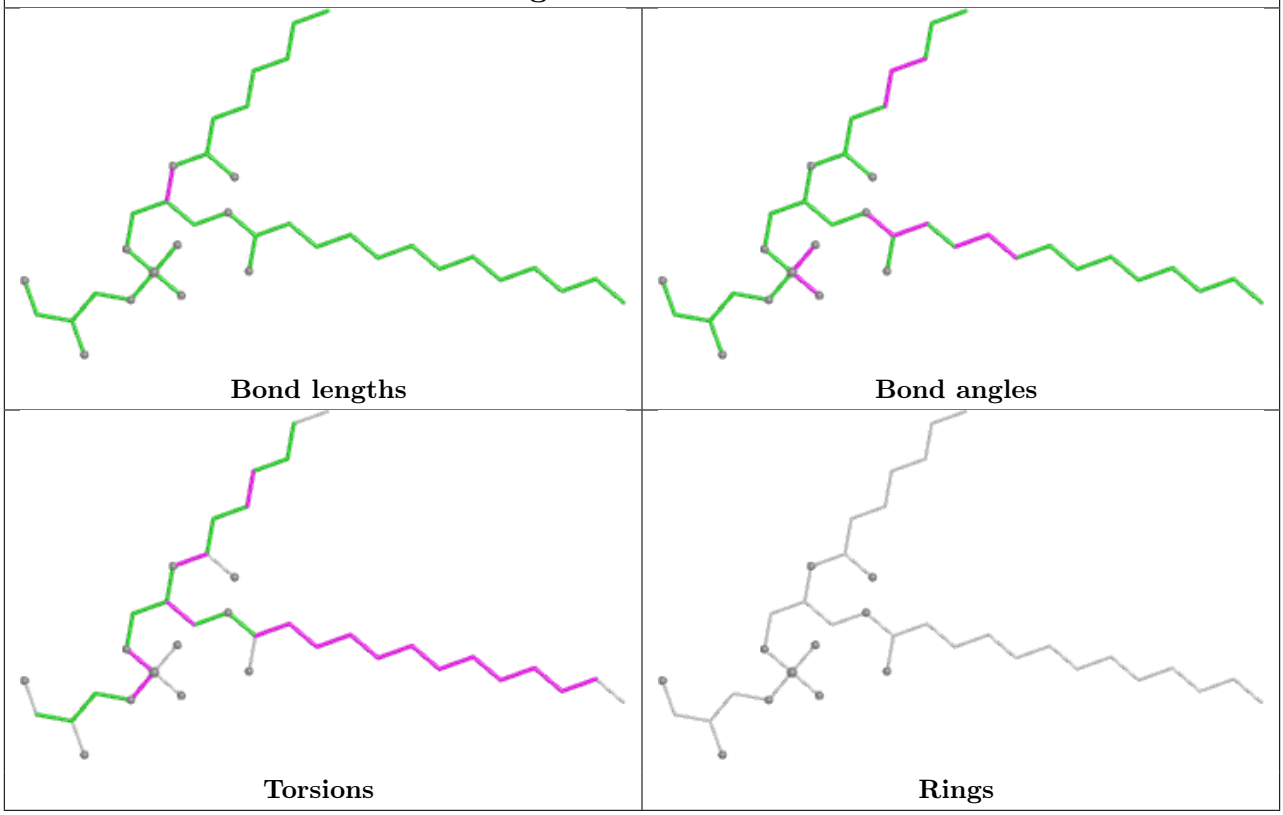
Rings

Ligand II0 p 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

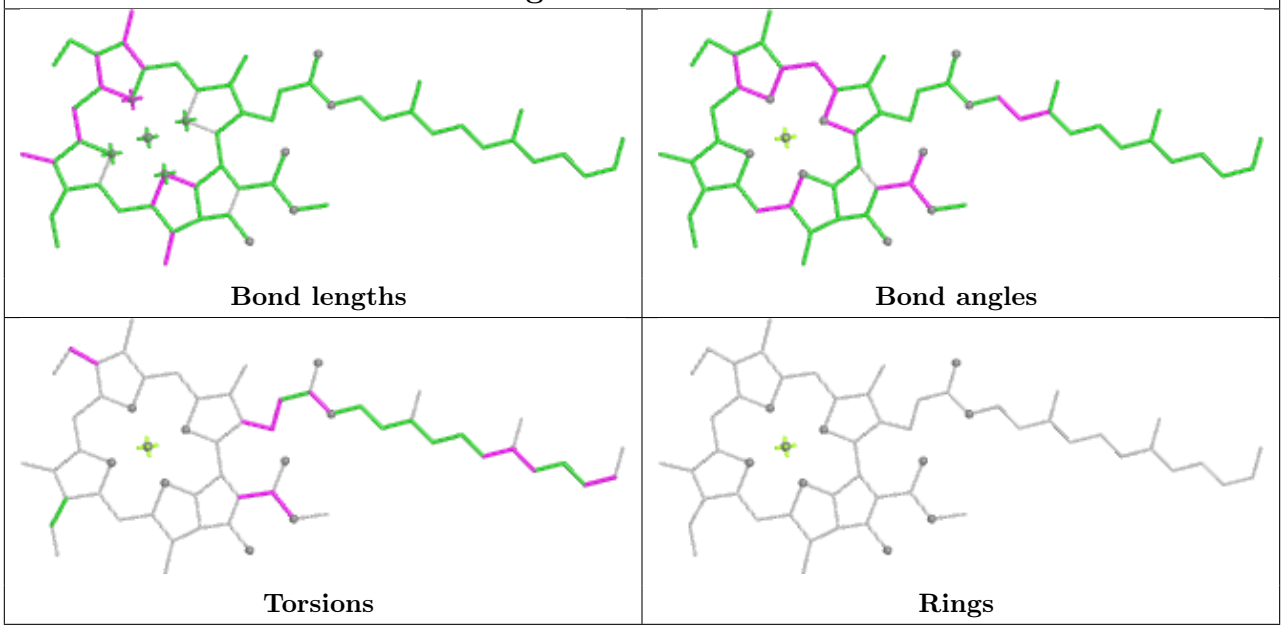
Ligand II0 9 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHT 0 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

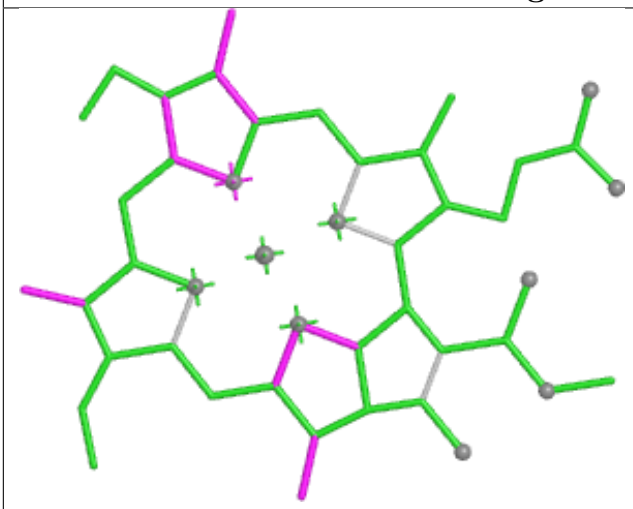
Ligand LHG s 301



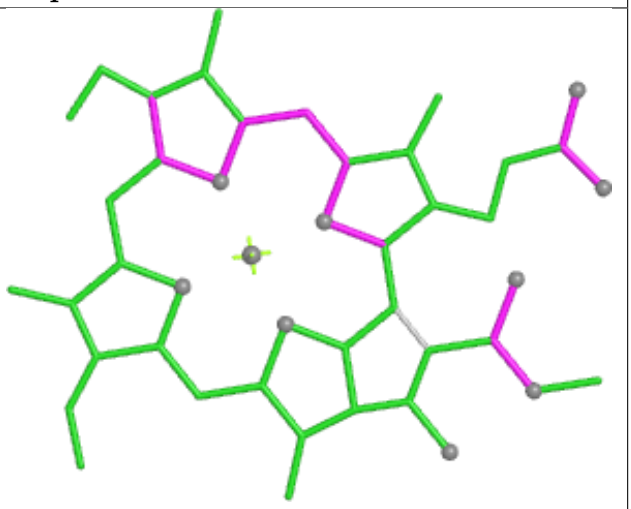
Ligand CLA P 602



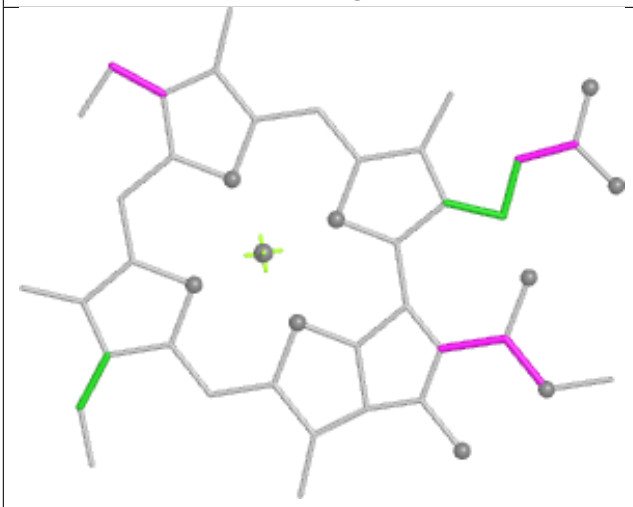
Ligand CLA p 308



Bond lengths



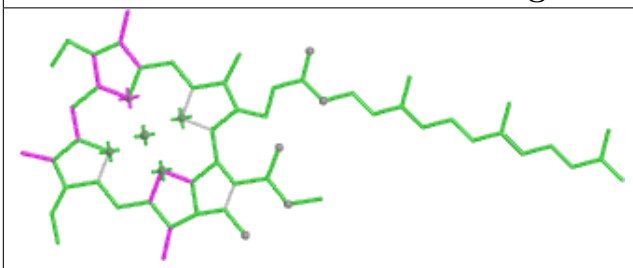
Bond angles



Torsions

Rings

Ligand CLA 9 607



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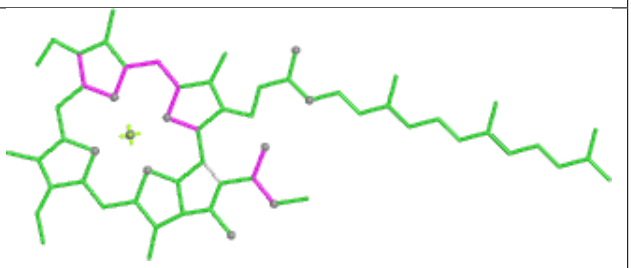
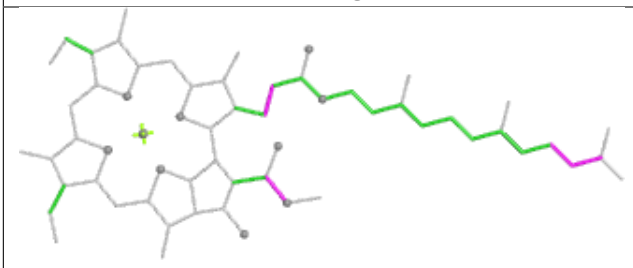
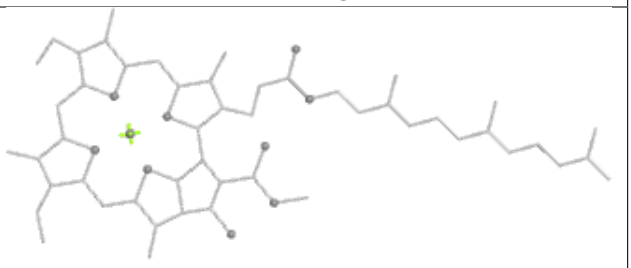


Bond angles

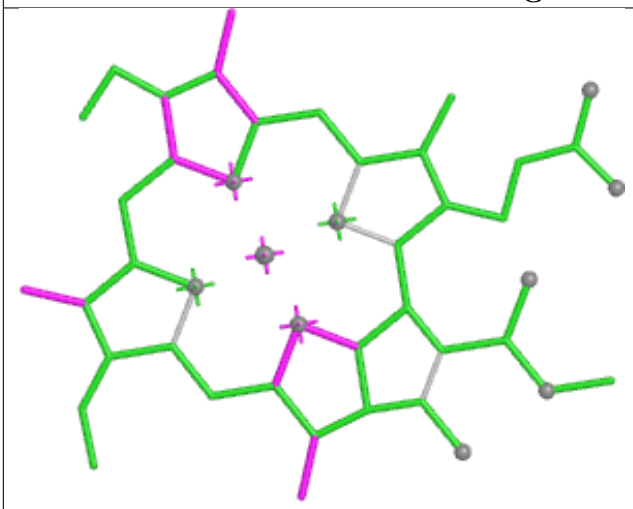


Torsions

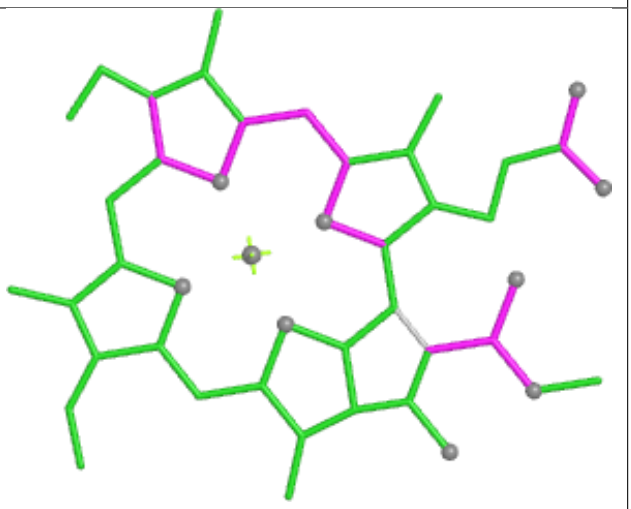


Rings

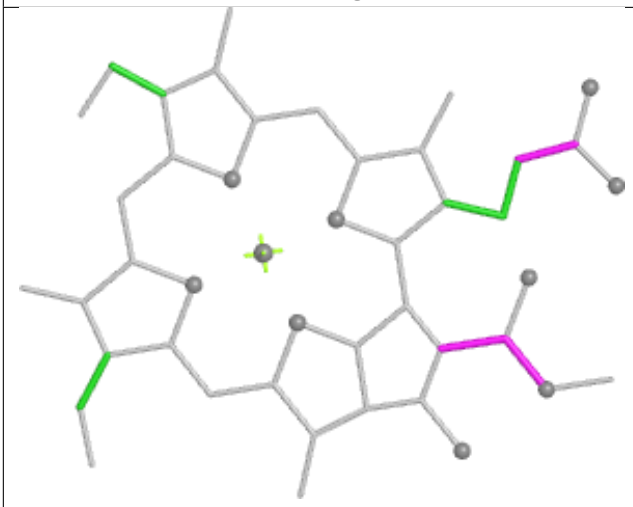
Ligand CLA P 610



Bond lengths



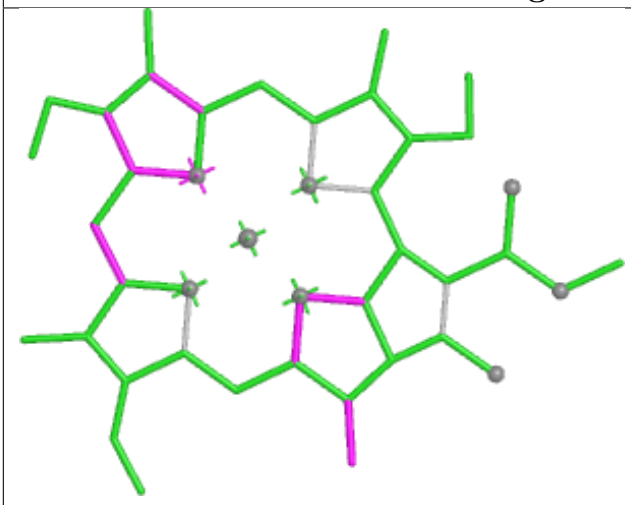
Bond angles



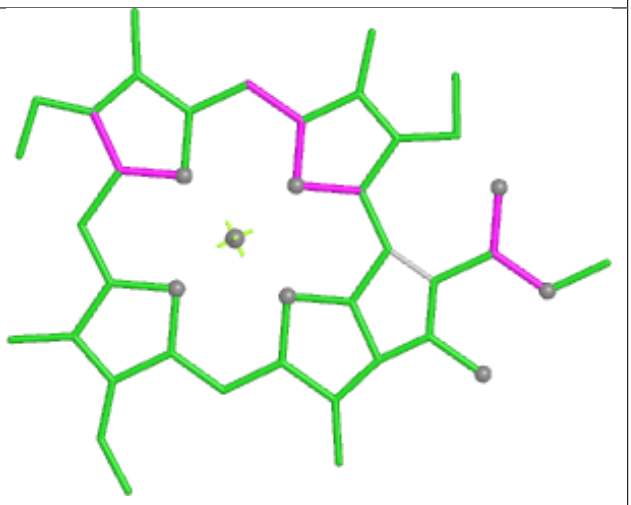
Torsions

Rings

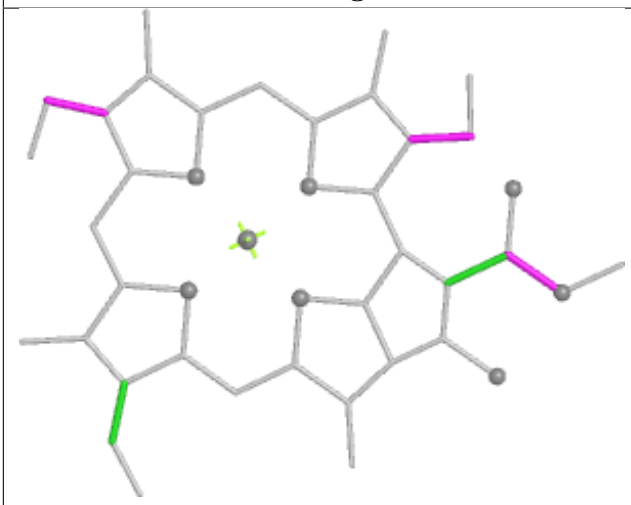
Ligand CLA 7 601



Bond lengths

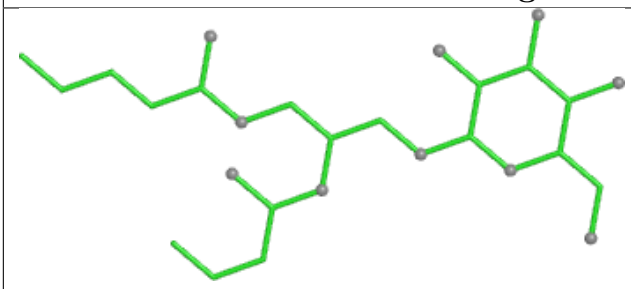
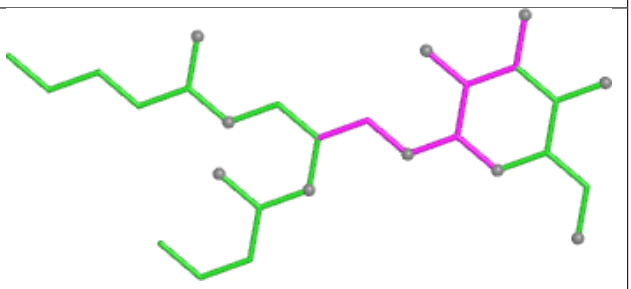
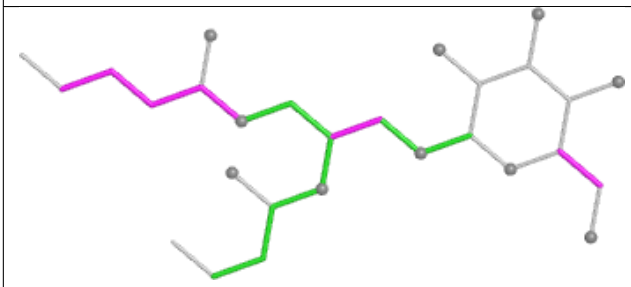
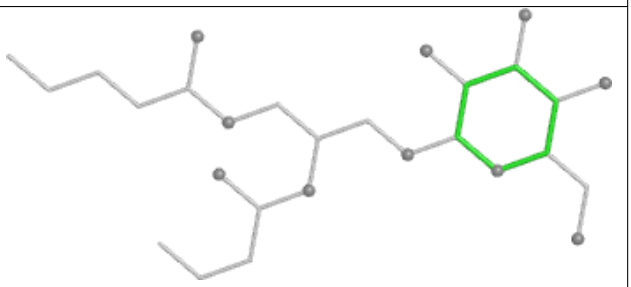


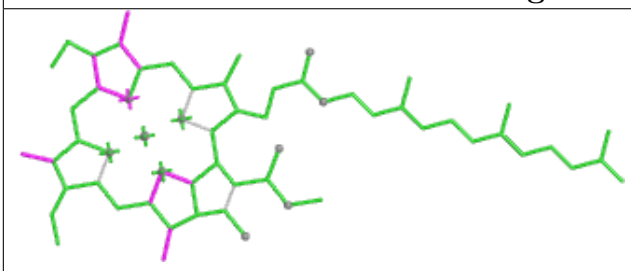
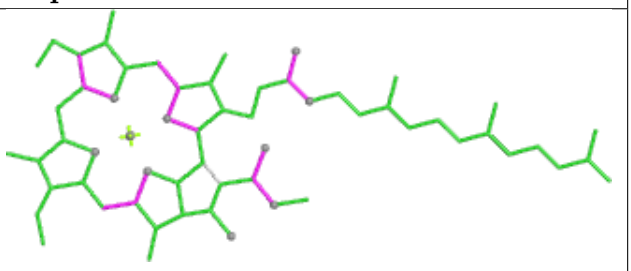
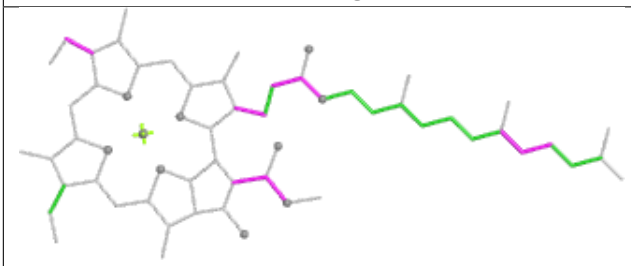
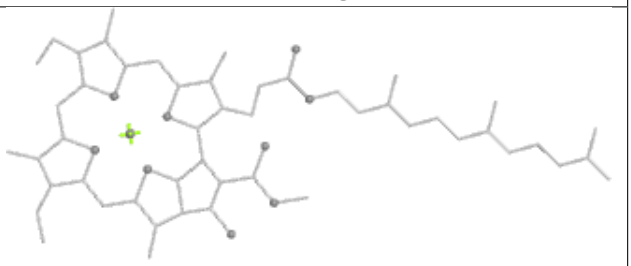
Bond angles



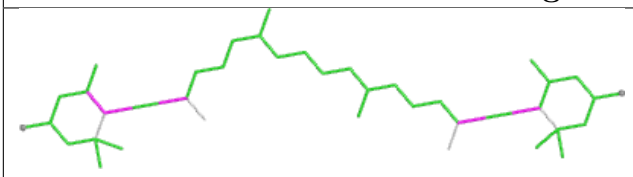
Torsions

Rings

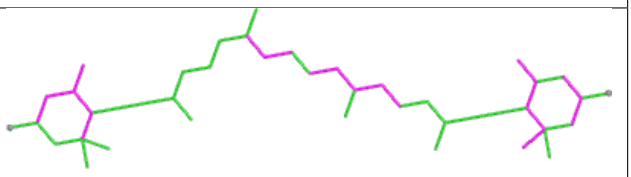
Ligand LMG G 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

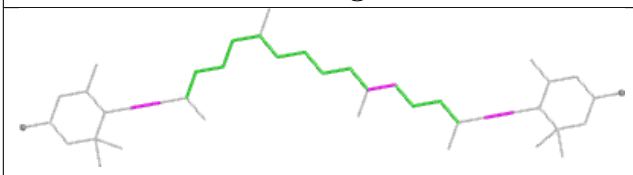
Ligand II0 8 615



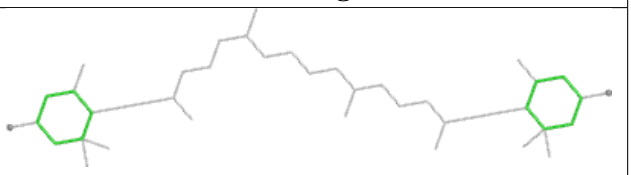
Bond lengths



Bond angles

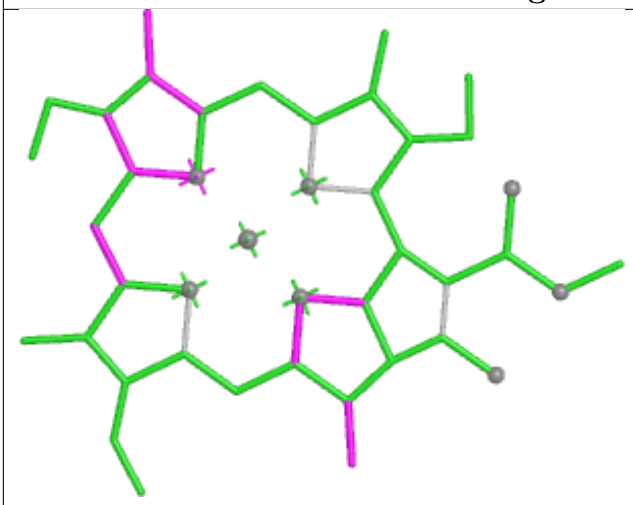


Torsions

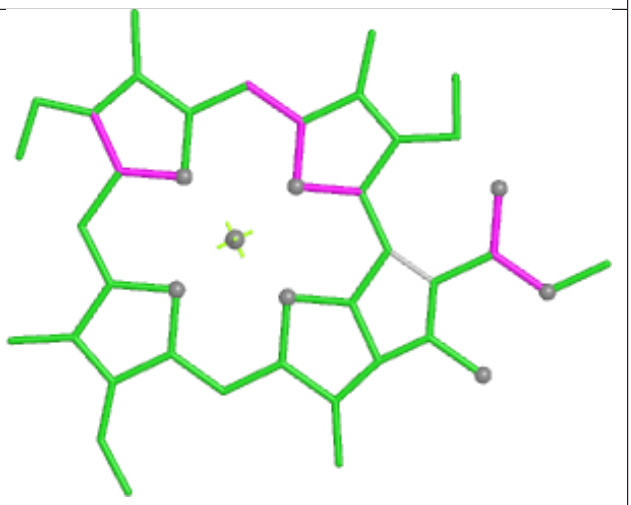


Rings

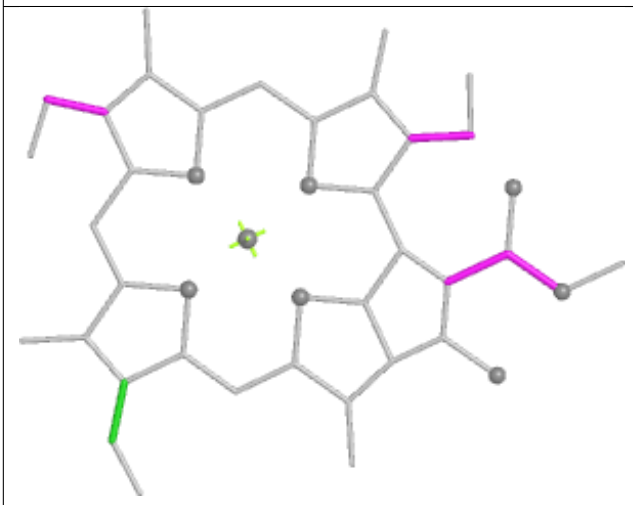
Ligand CLA 0 601



Bond lengths

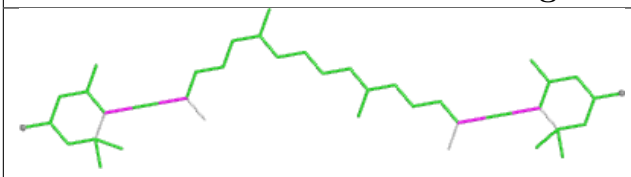
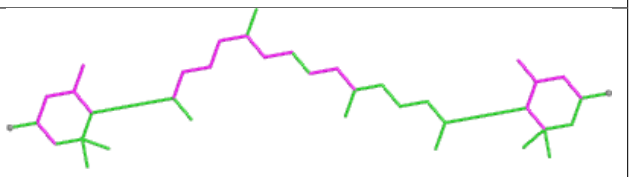
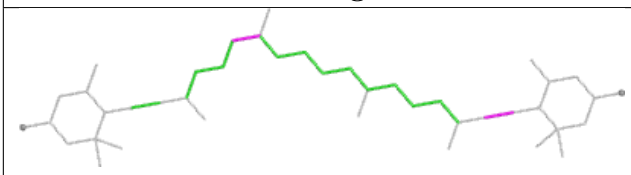
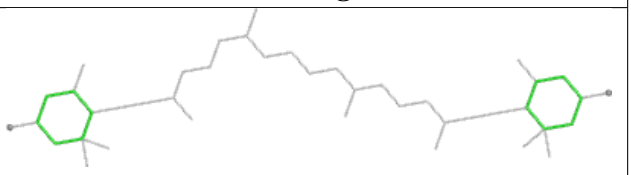


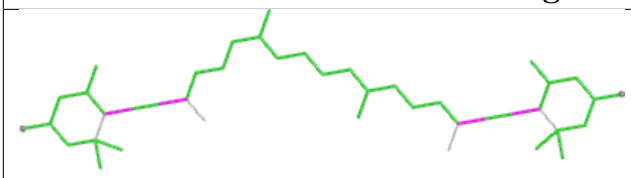
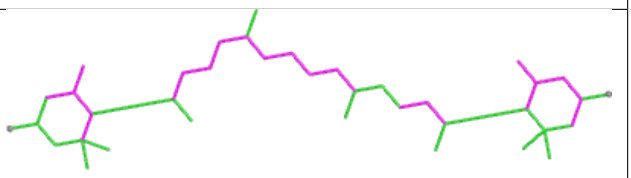
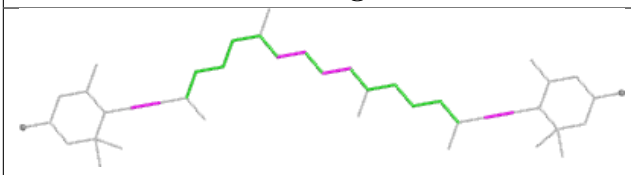
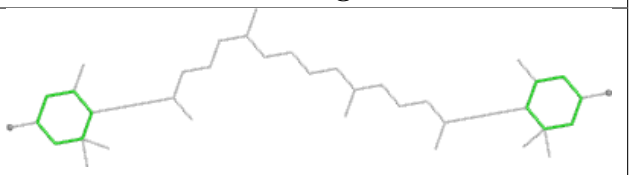
Bond angles



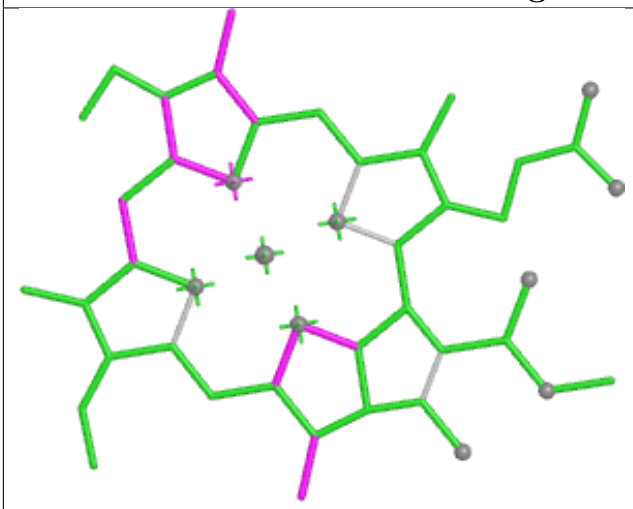
Torsions

Rings

Ligand II0 P 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 0 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 606



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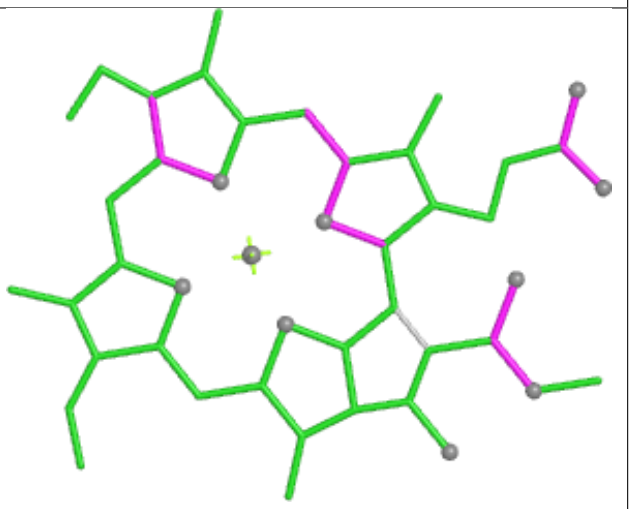

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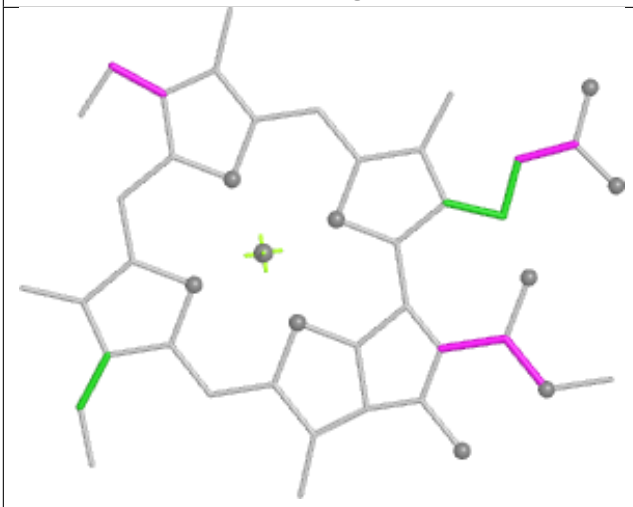
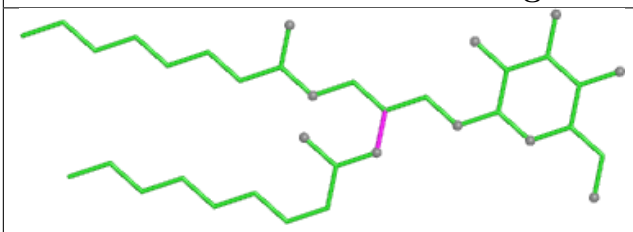


Torsions

Rings

Ligand LMG 8 617



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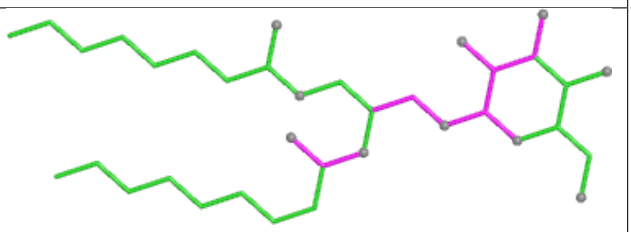

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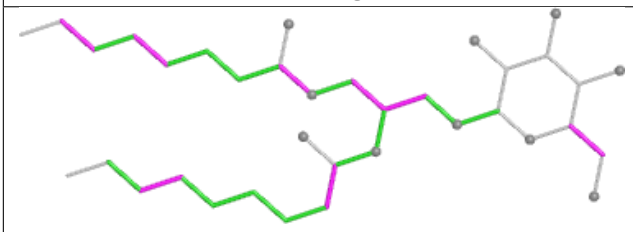
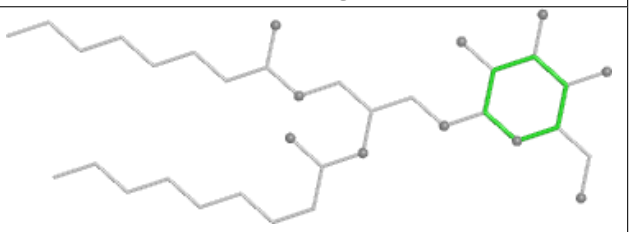
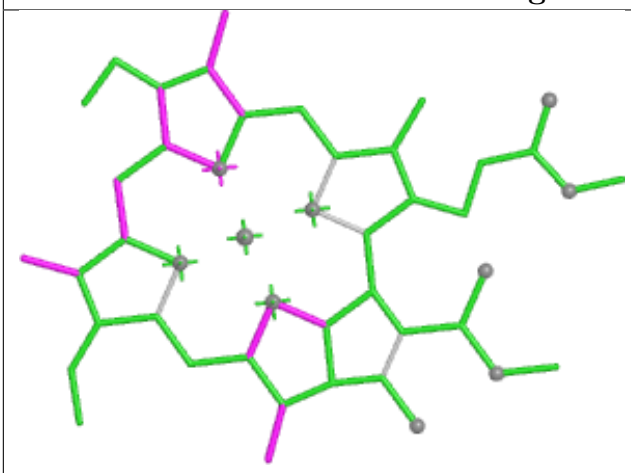
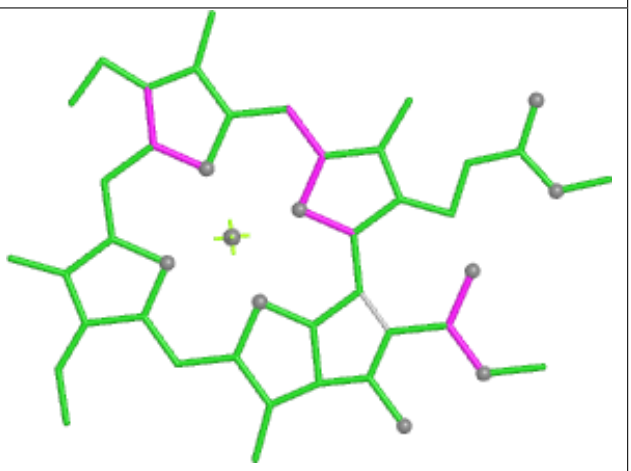
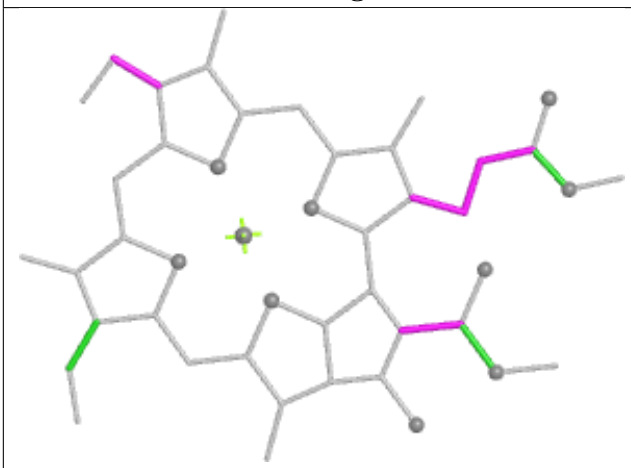
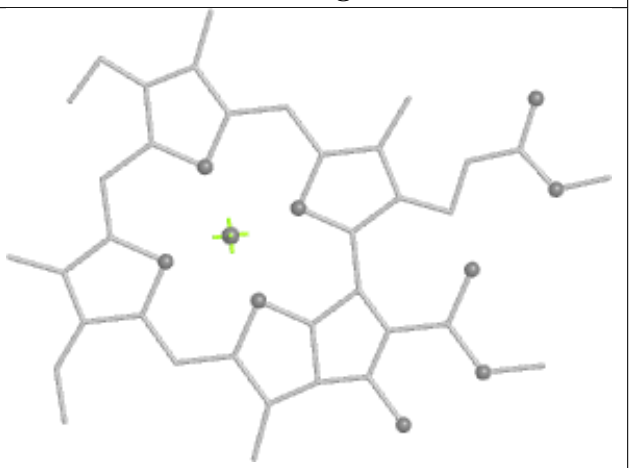
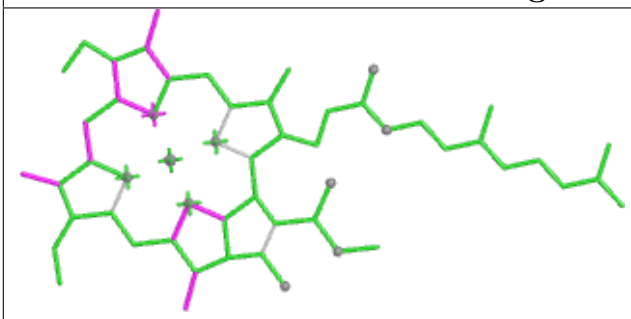
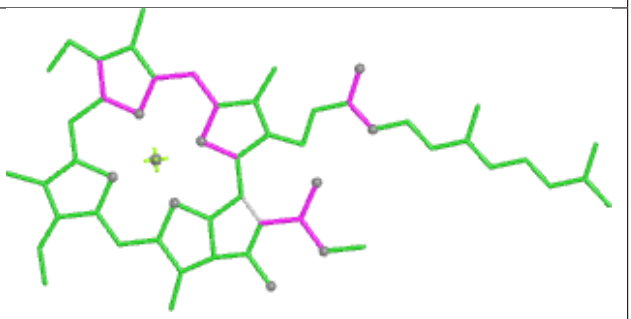
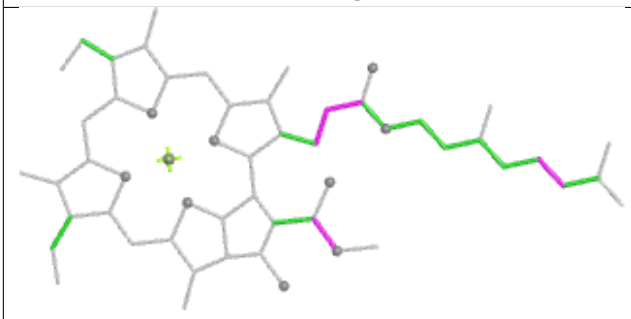
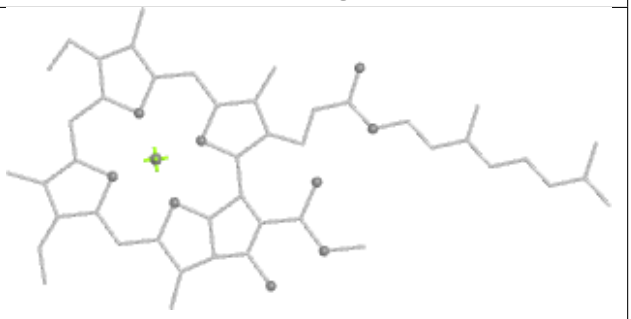


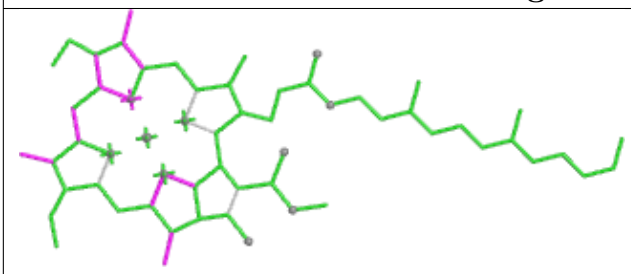
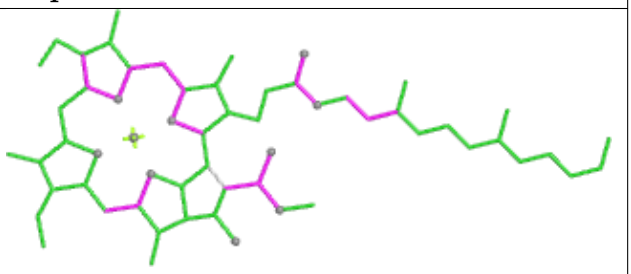
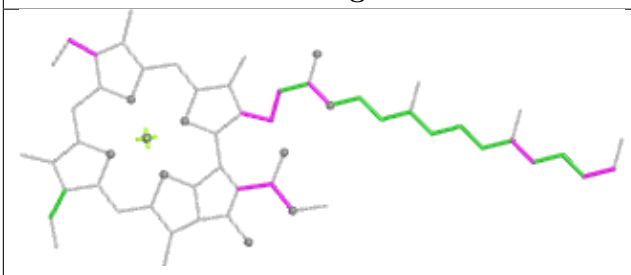
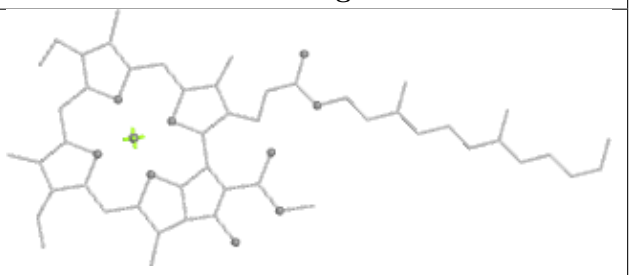
Torsions

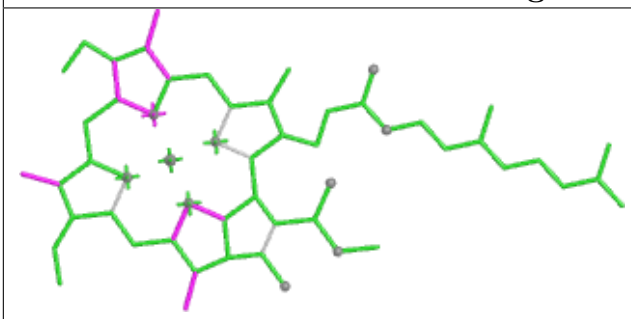
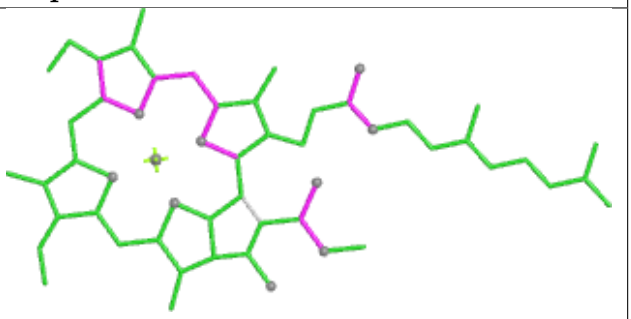
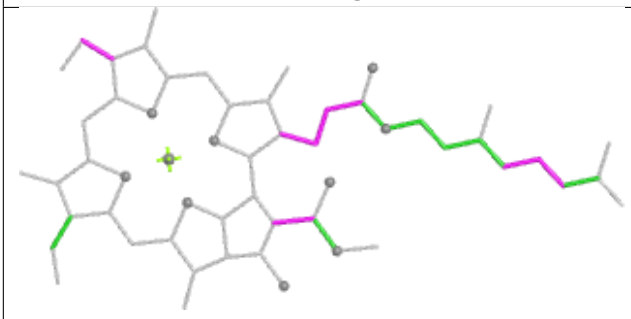
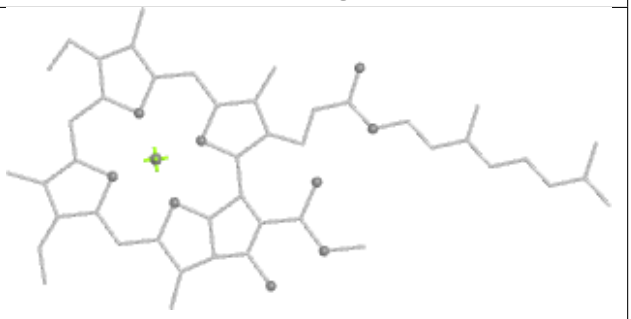


Rings

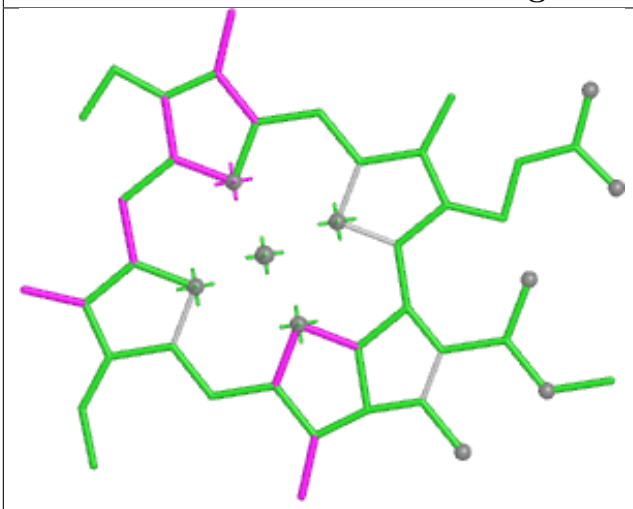
Ligand CLA 9 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 611



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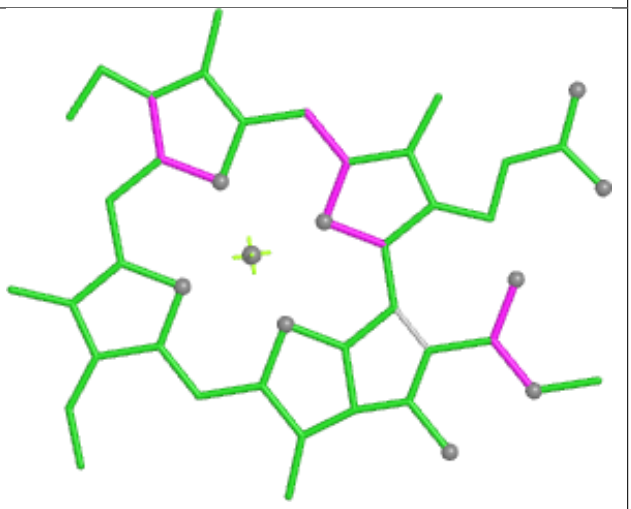
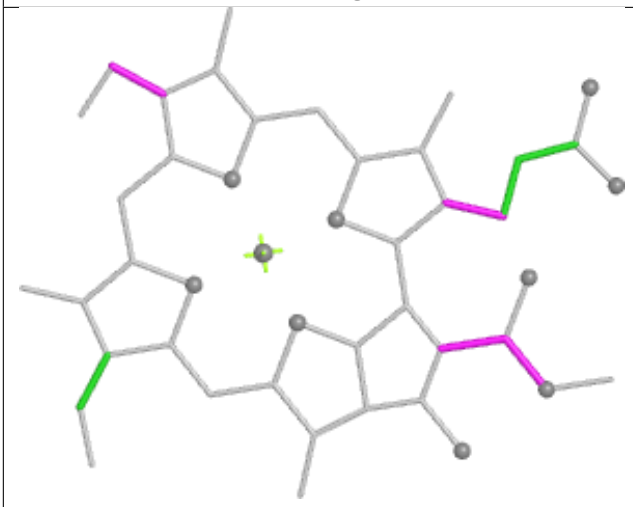


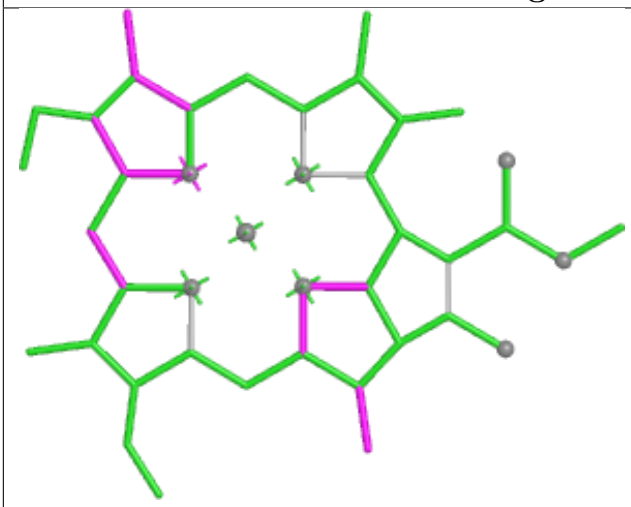
Bond angles



Torsions

Rings

Ligand CLA 0 609



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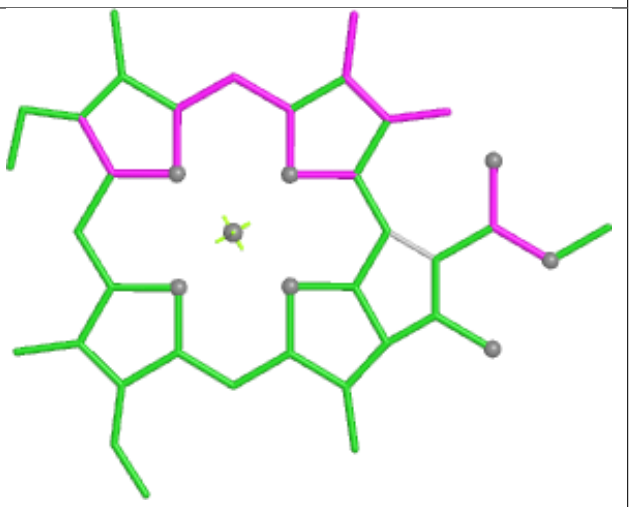
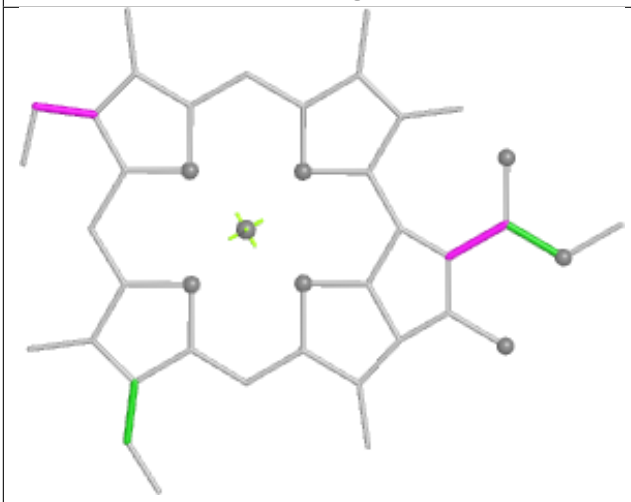
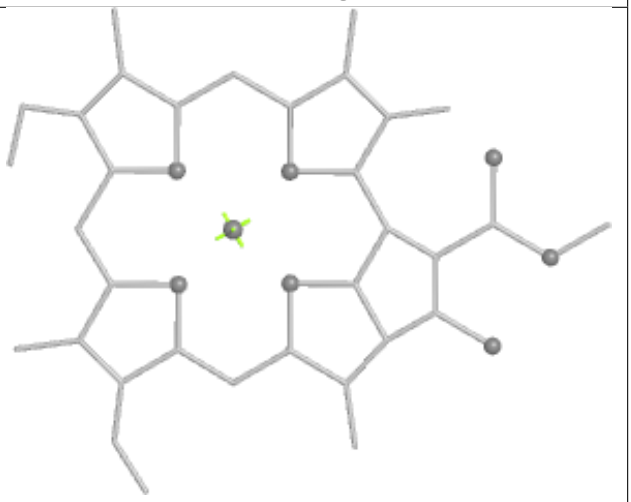


Bond angles

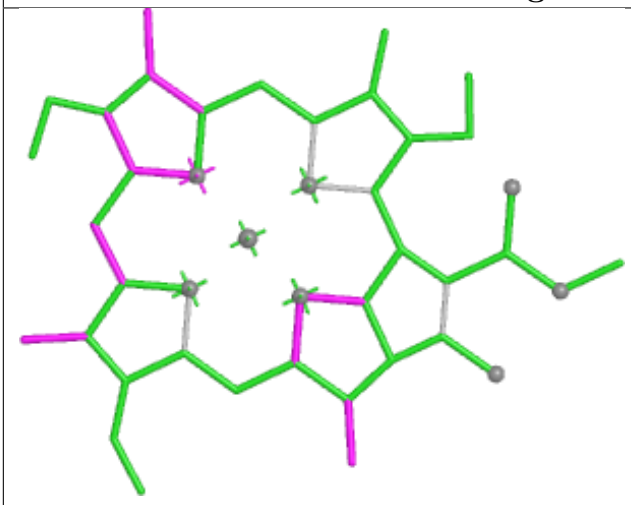


Torsions



Rings

Ligand CLA p 303



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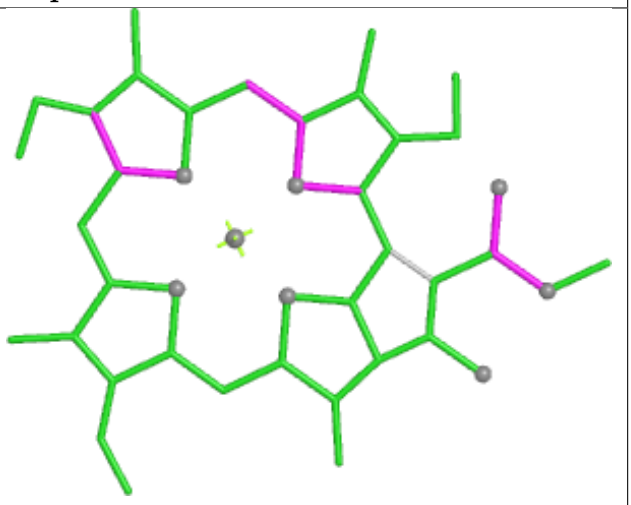
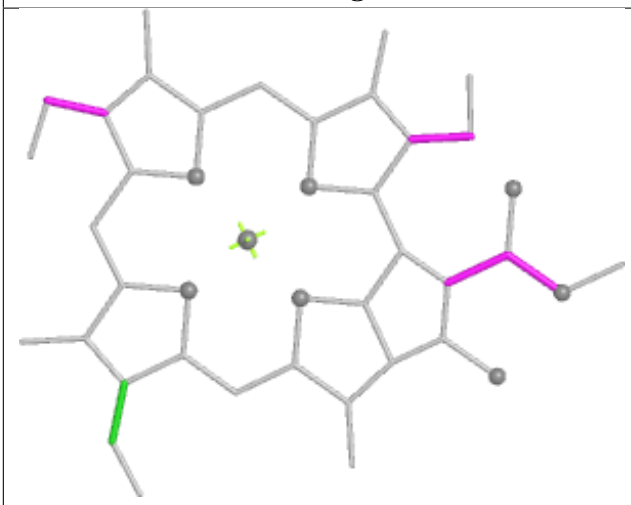


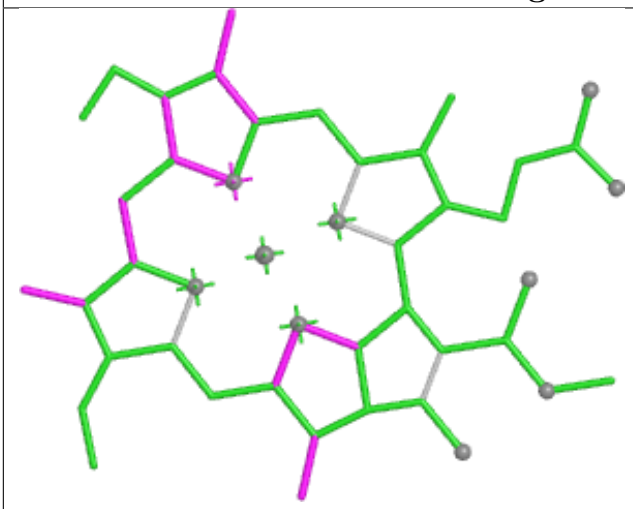
Bond angles



Torsions

Rings

Ligand CLA 8 607



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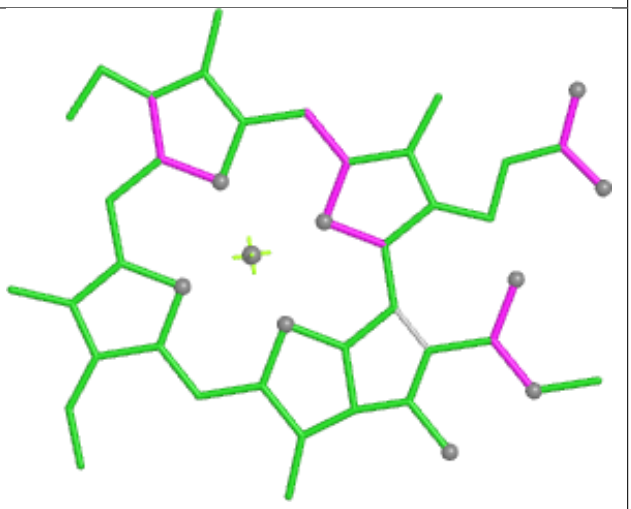
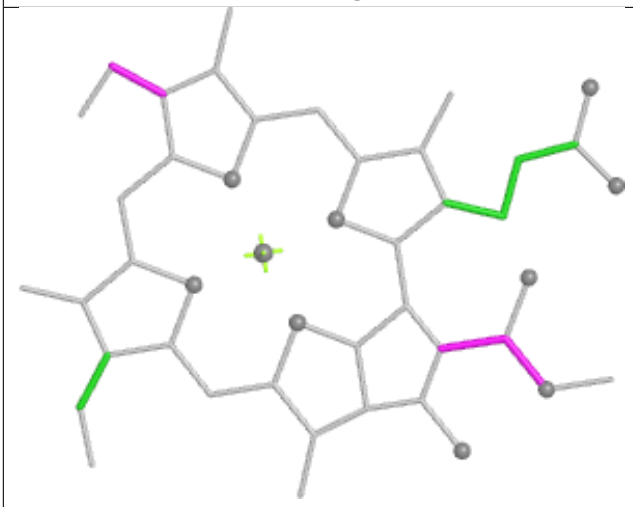


Bond angles

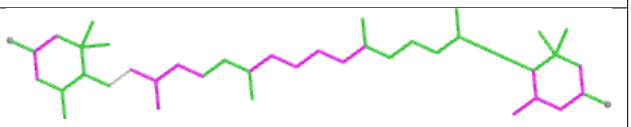


Torsions

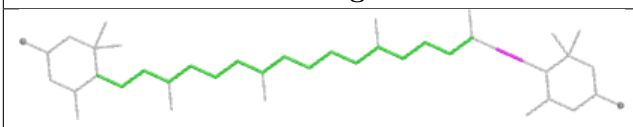
Rings

Ligand II3 7 615

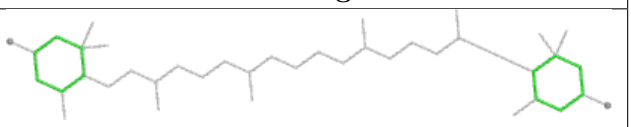
Bond lengths



Bond angles

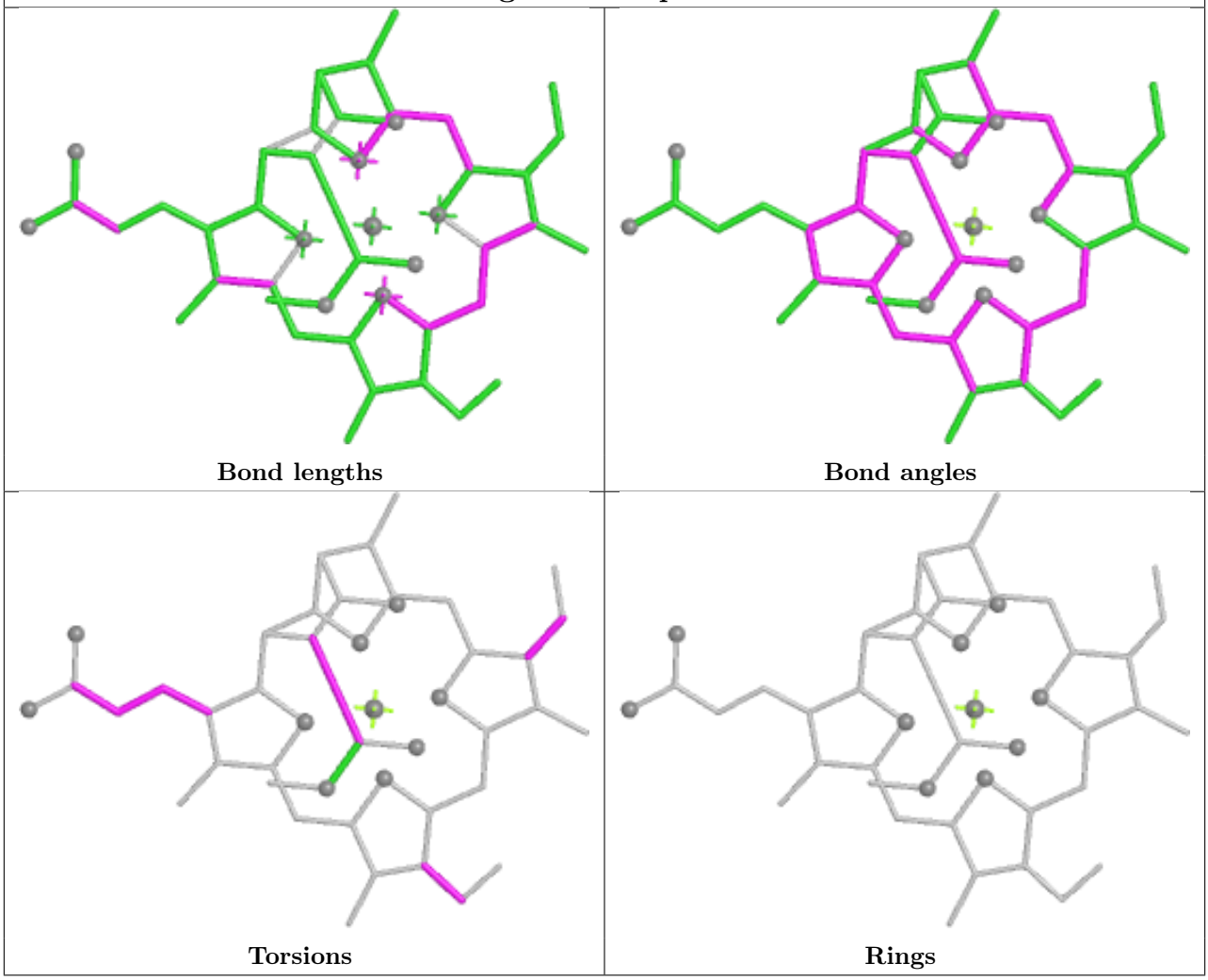


Torsions

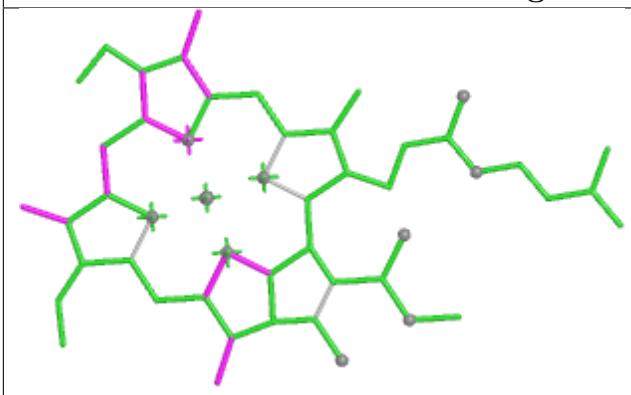


Rings

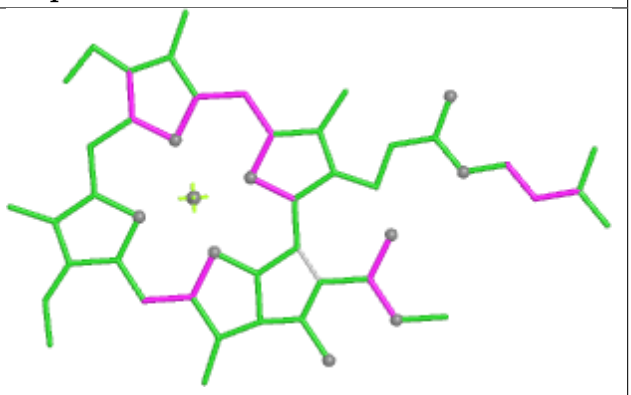
Ligand KC2 p 312



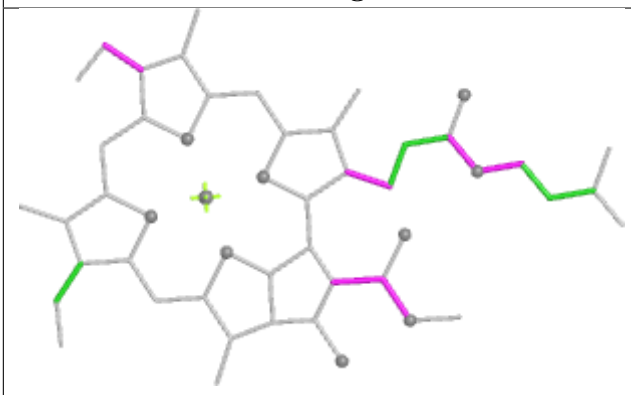
Ligand CLA p 305



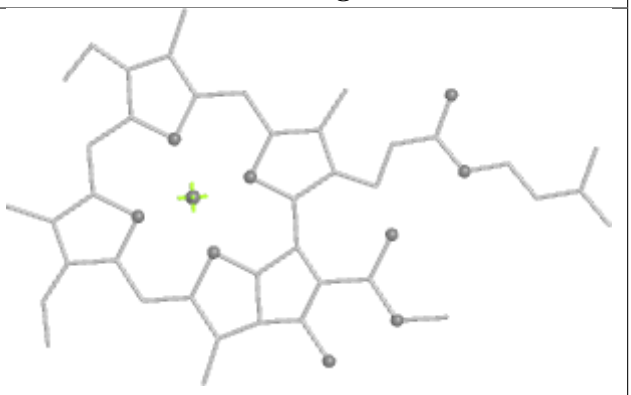
Bond lengths



Bond angles

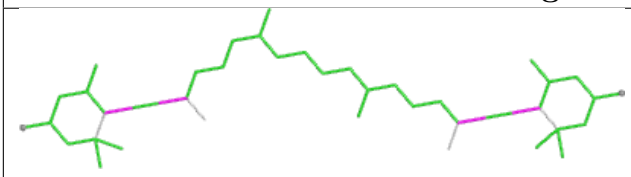


Torsions

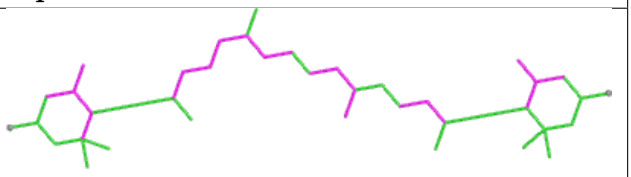


Rings

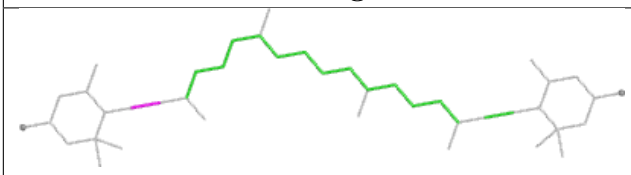
Ligand II0 p 302



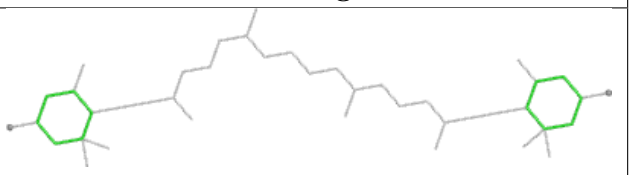
Bond lengths



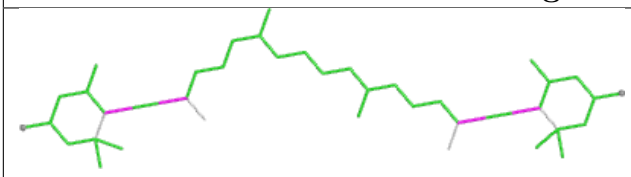
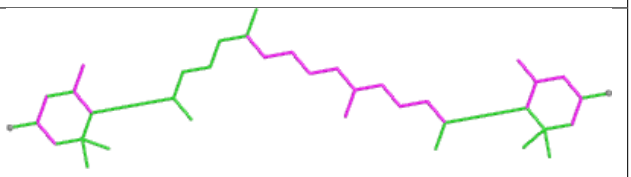
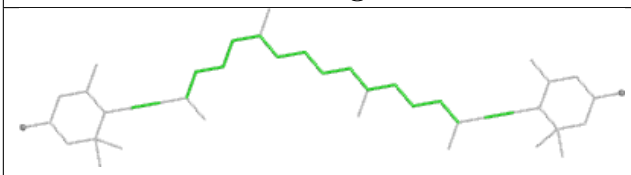
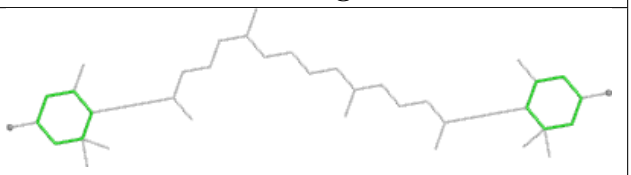
Bond angles



Torsions



Rings

Ligand II0 0 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

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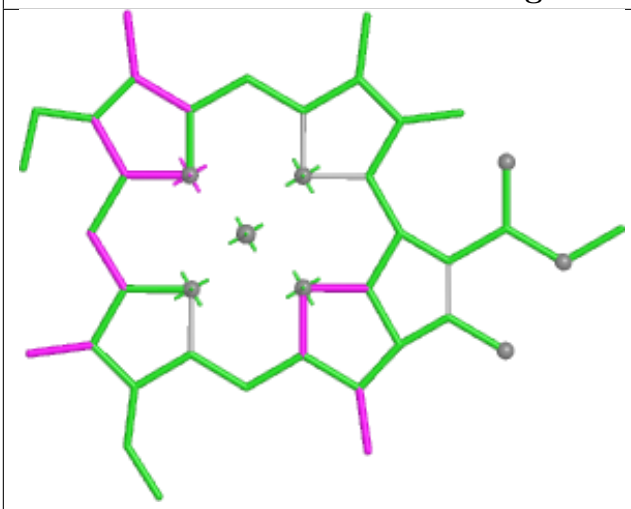
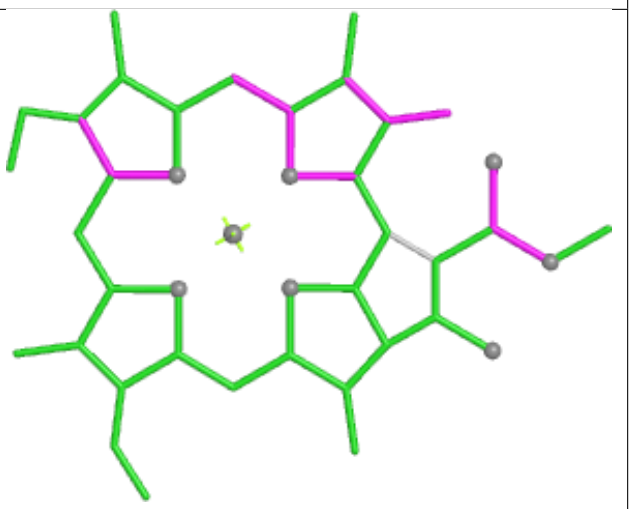
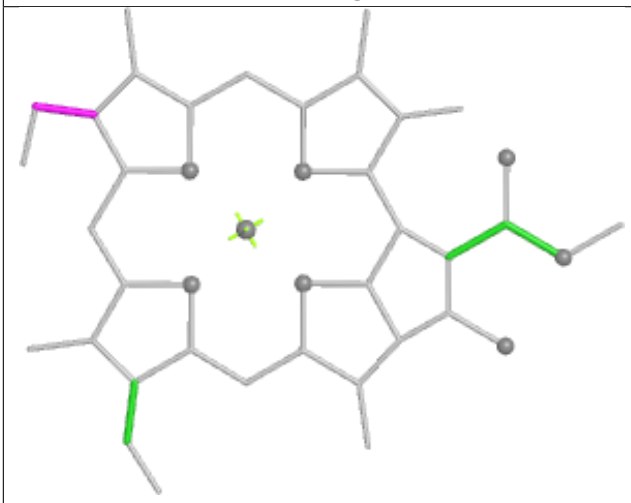
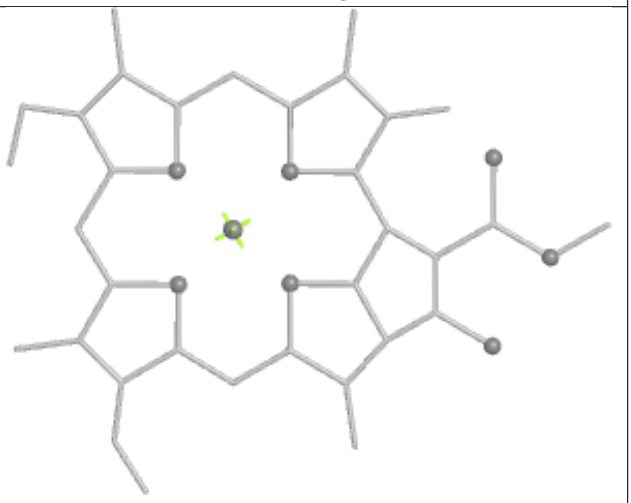
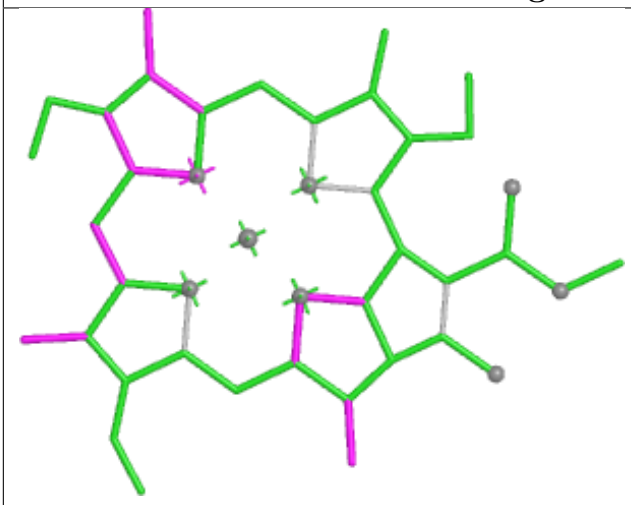
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 601



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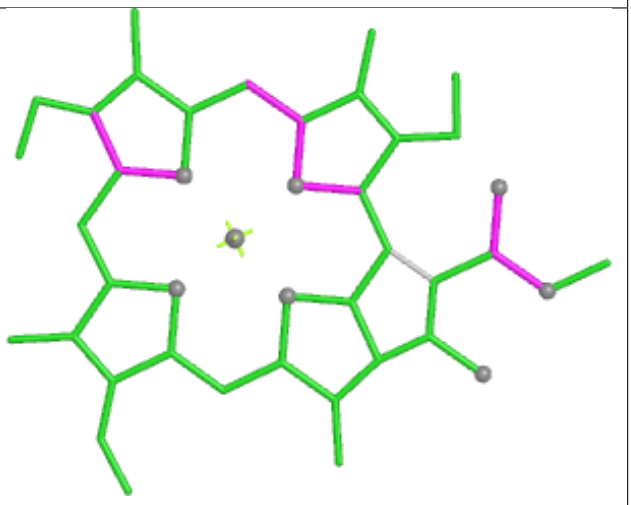

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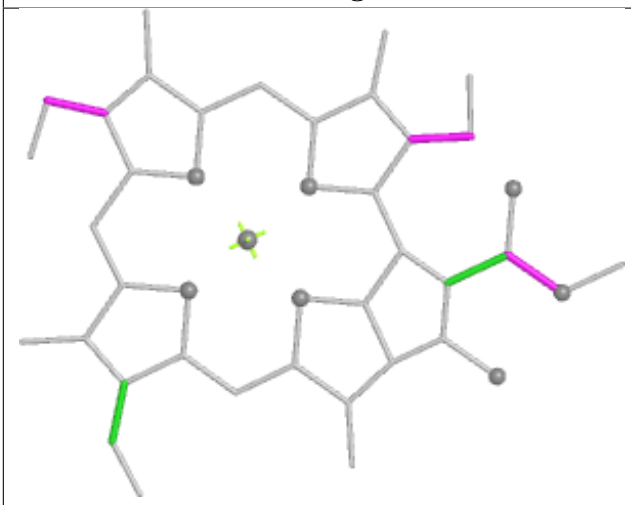
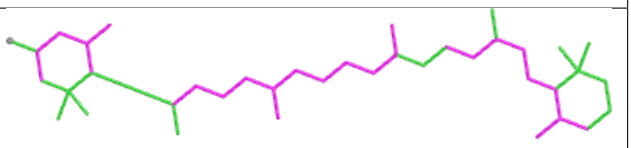


Torsions

Rings

Ligand IHT 0 617

Bond lengths



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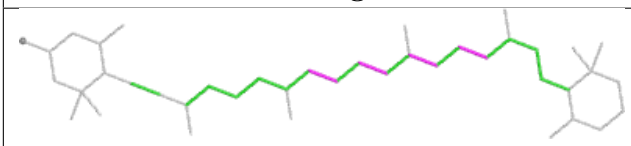
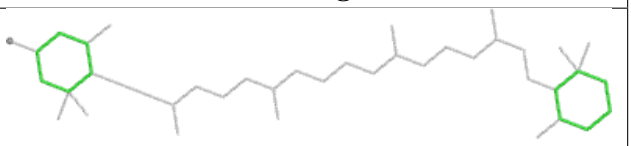
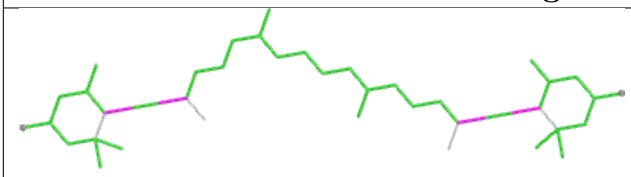
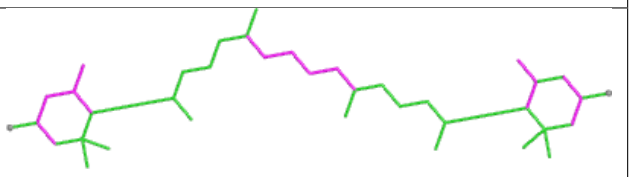
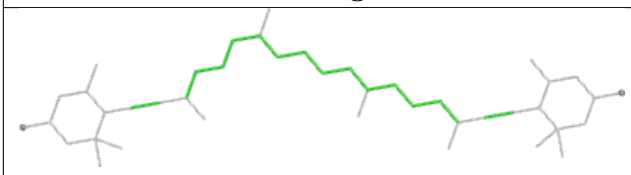
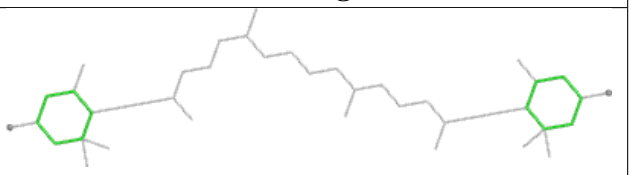


Torsions



Rings

Ligand II0 8 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

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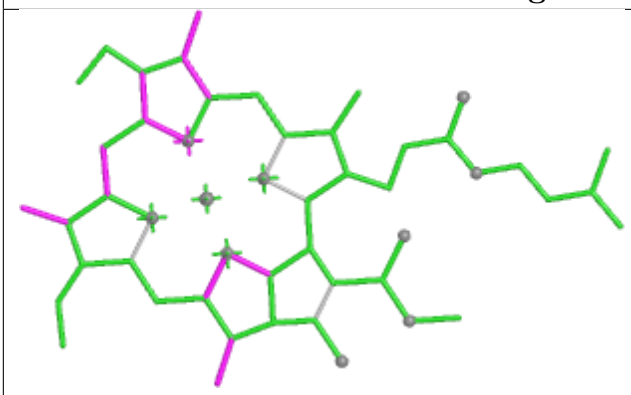
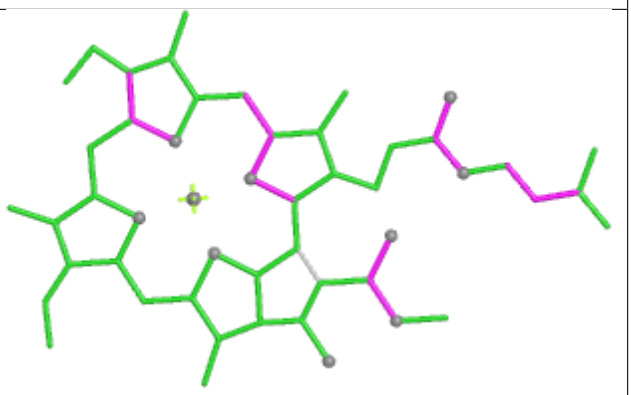
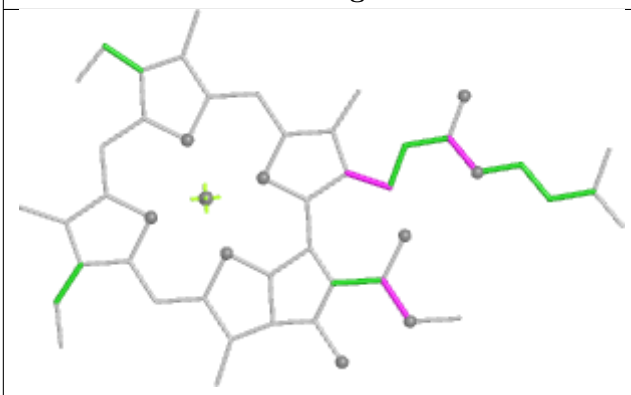
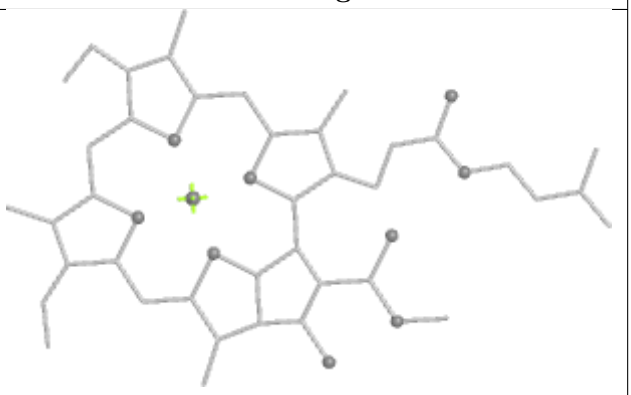
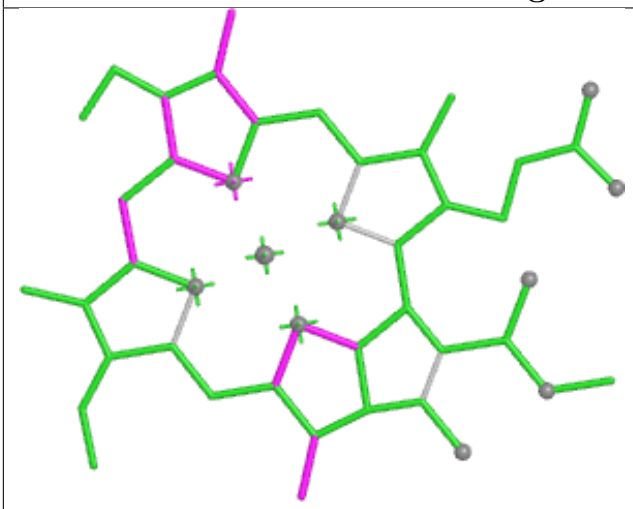
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 611



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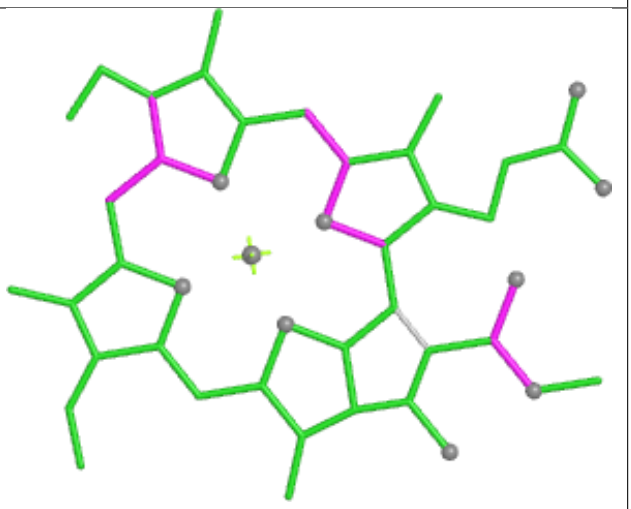
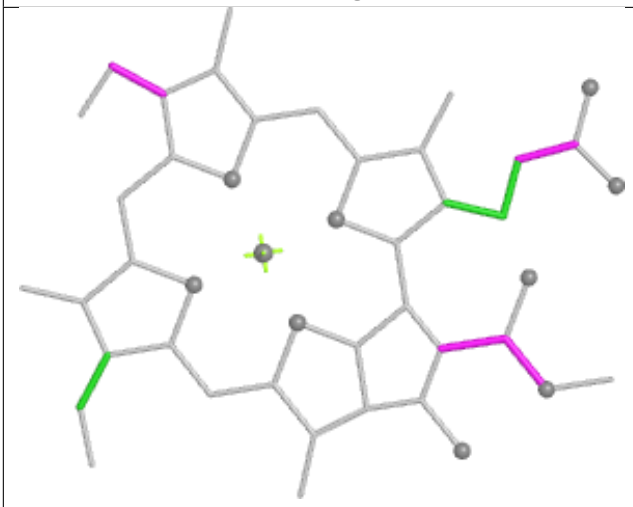


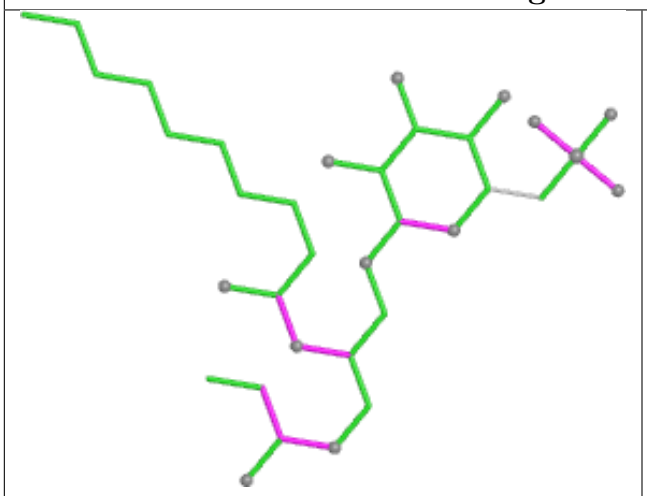
Bond angles



Torsions

Rings

Ligand SQD p 319



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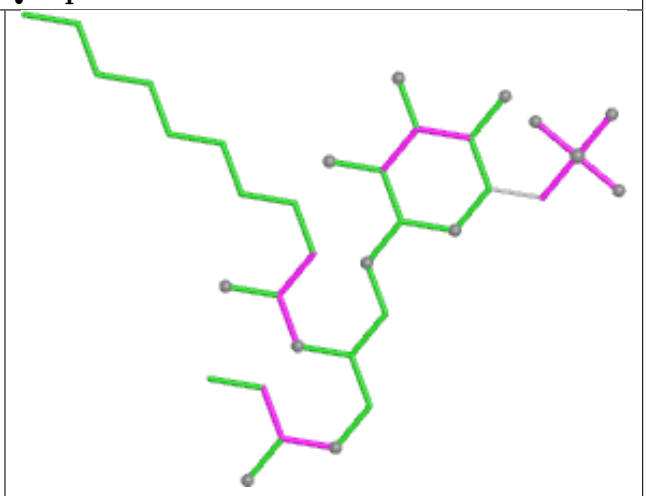

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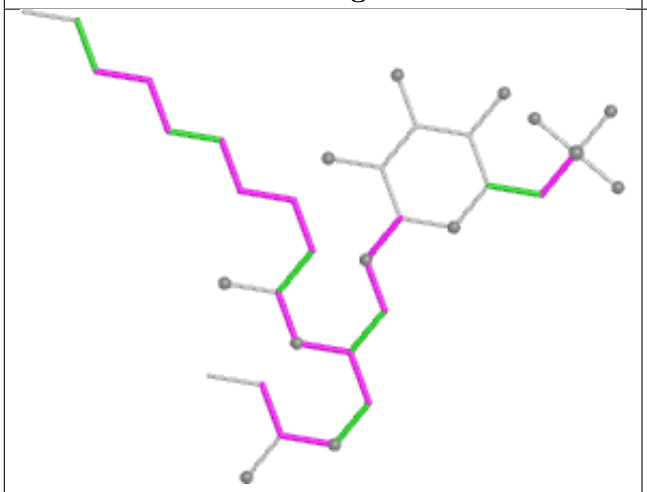

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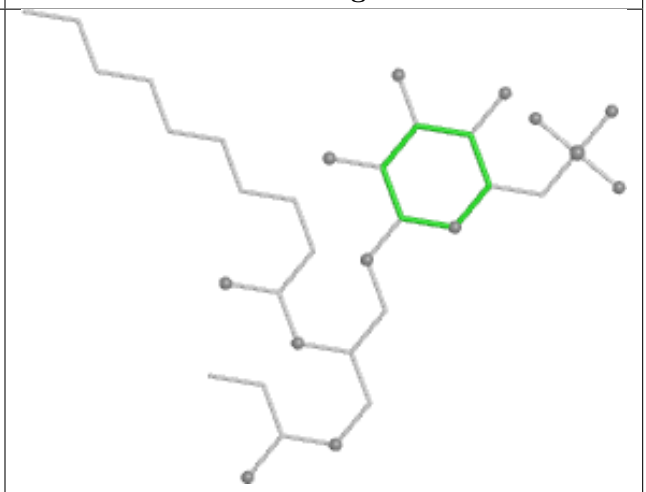
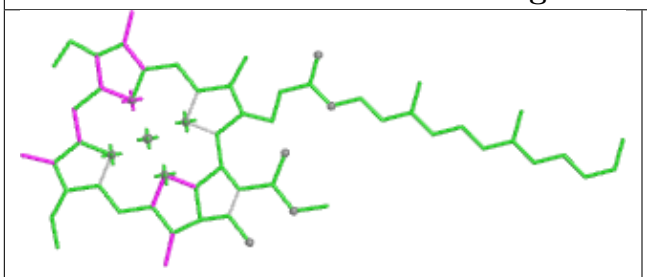


Rings

Ligand CLA 0 602



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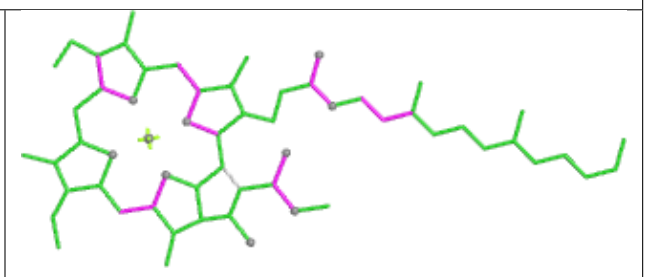

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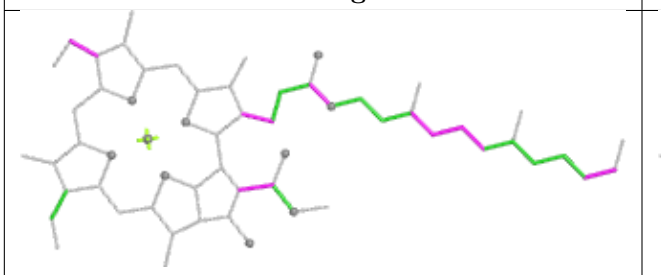

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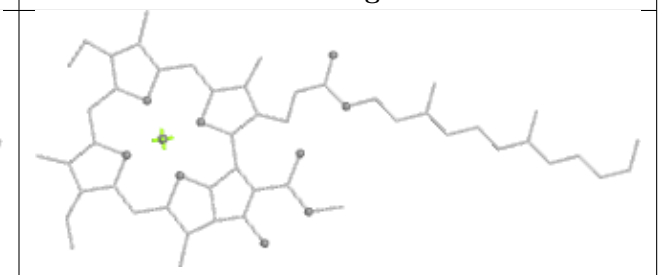
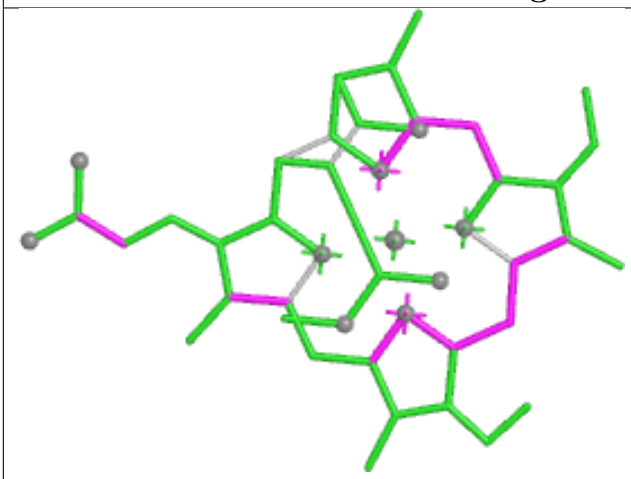


Rings

Ligand KC2 8 610



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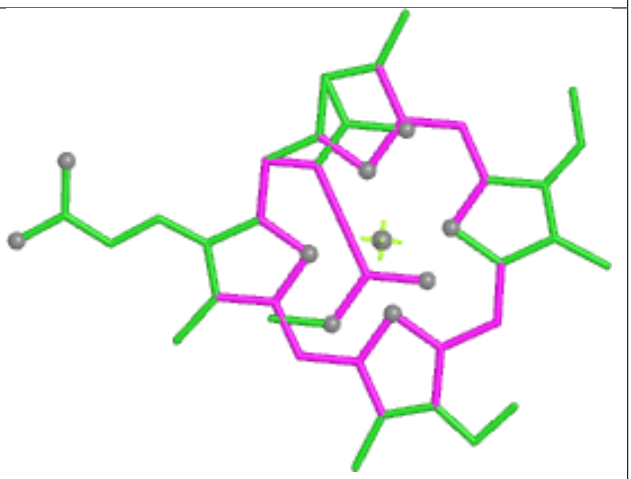

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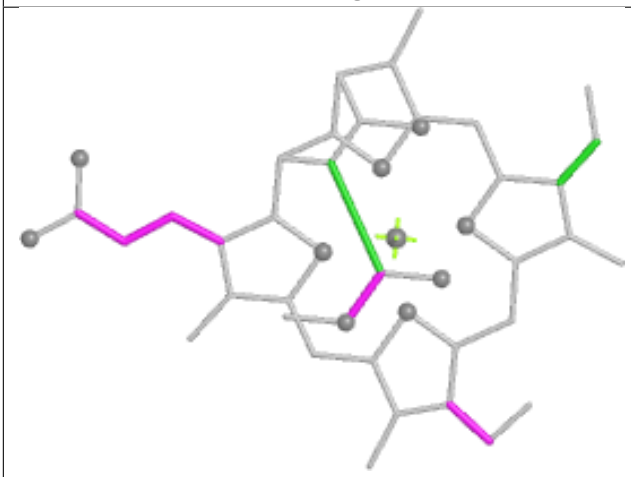

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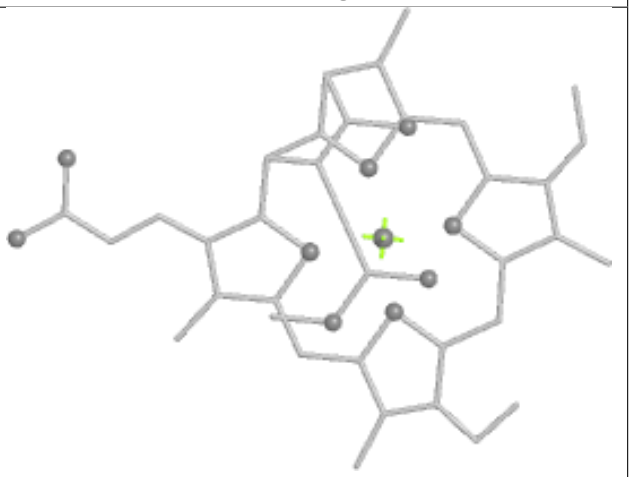
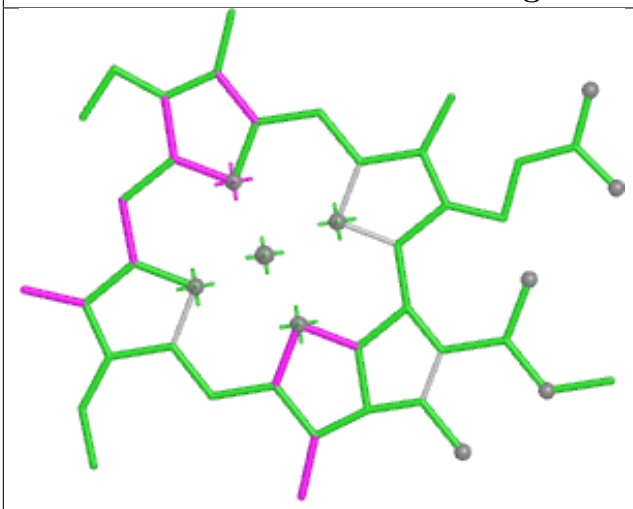


Rings

Ligand CLA G 101



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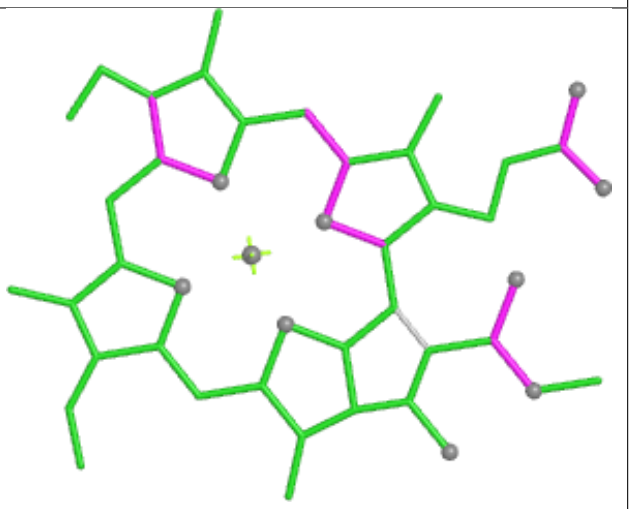
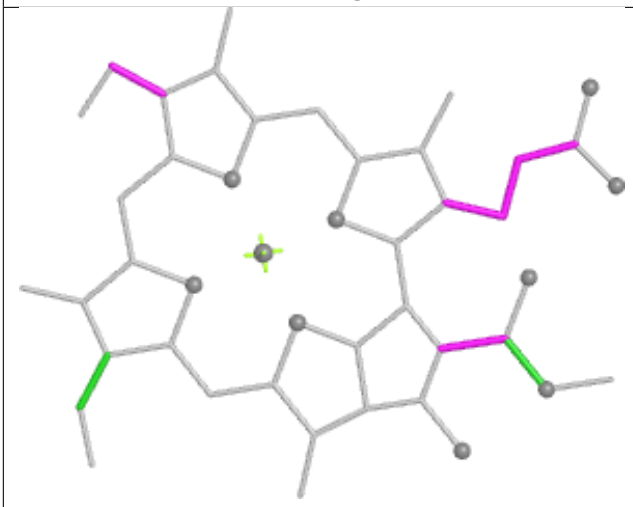


Bond angles

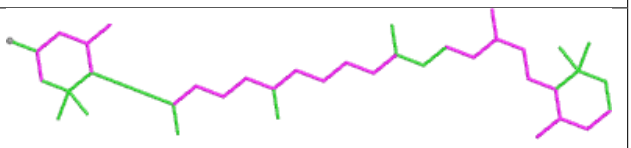


Torsions

Rings

Ligand IHT 8 616

Bond lengths



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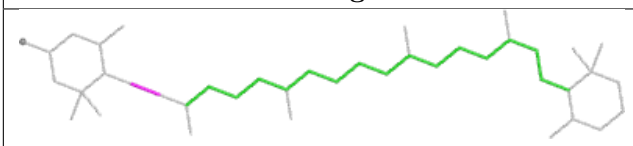
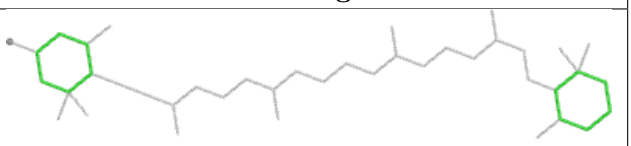
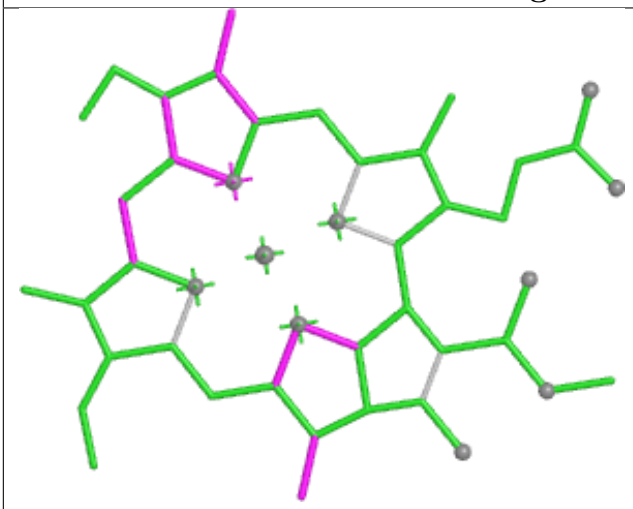


Torsions



Rings

Ligand CLA s 302



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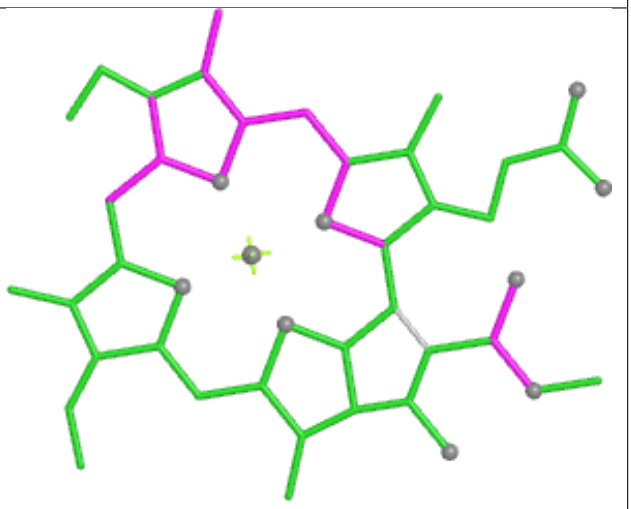
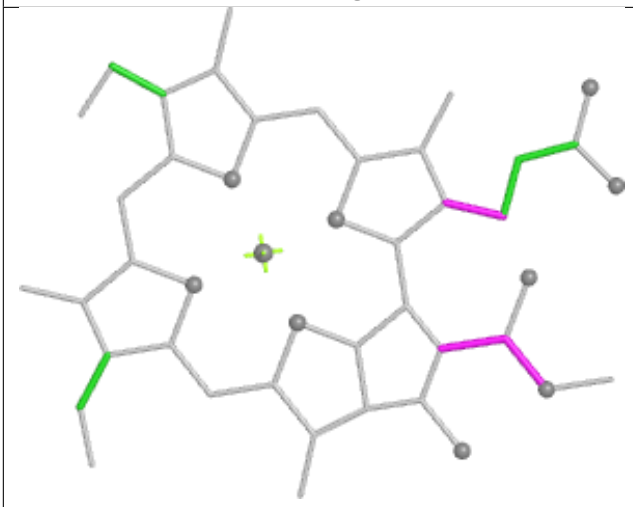


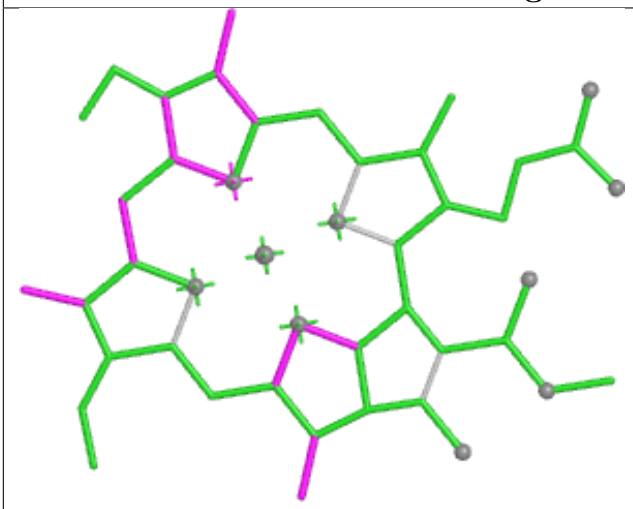
Bond angles



Torsions

Rings

Ligand CLA P 611



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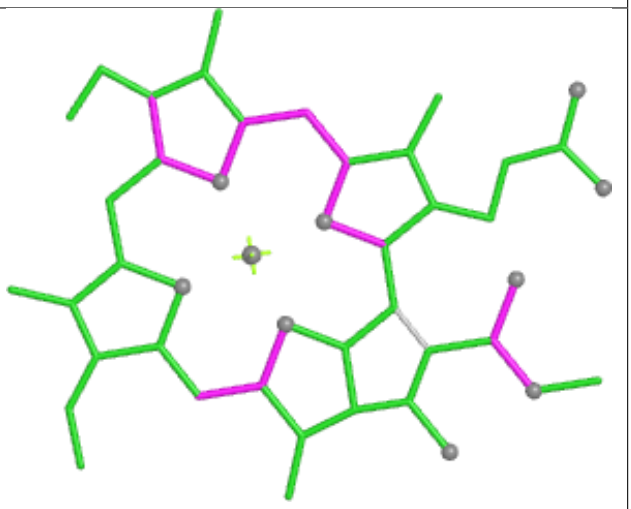
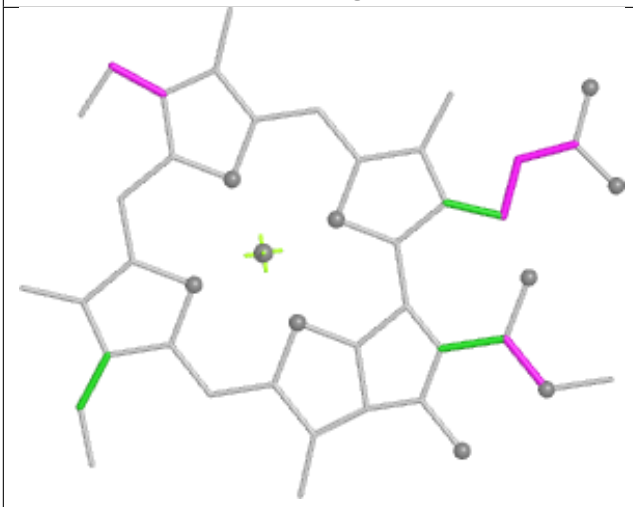


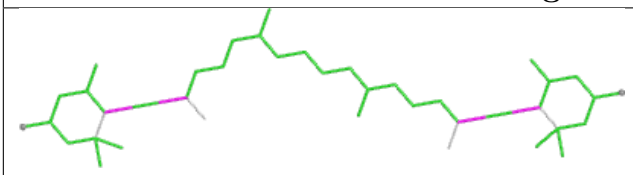
Bond angles



Torsions

Rings

Ligand II0 0 619



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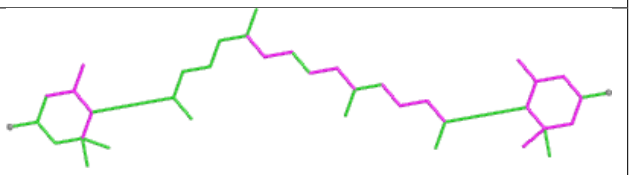
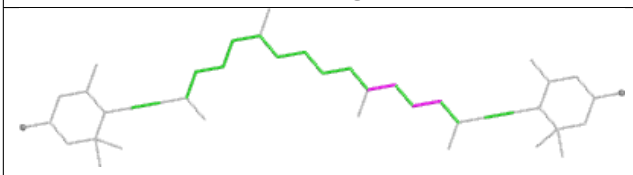
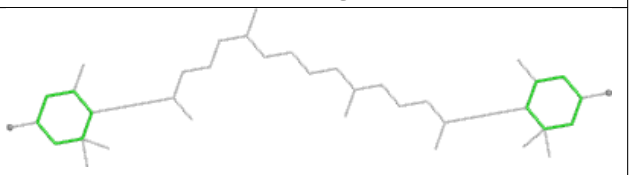


Bond angles

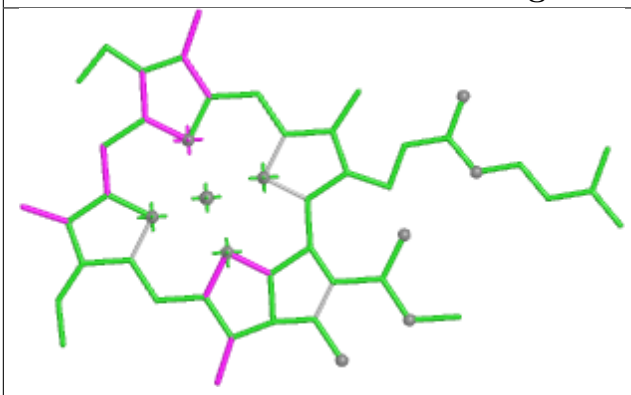


Torsions

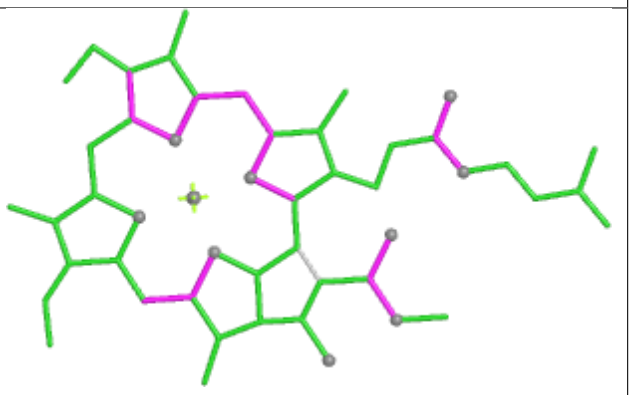


Rings

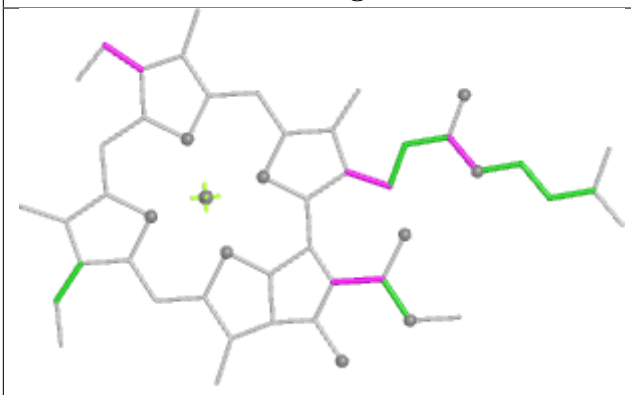
Ligand CLA 8 603



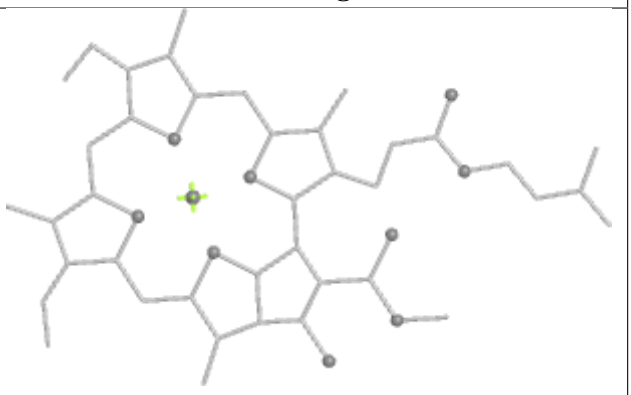
Bond lengths



Bond angles

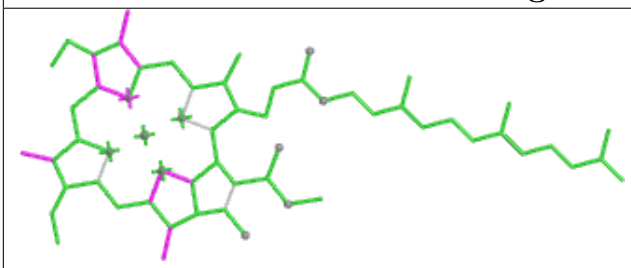


Torsions

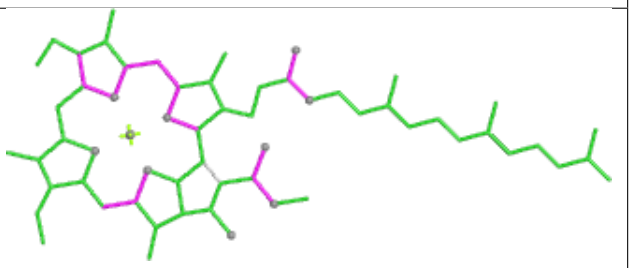


Rings

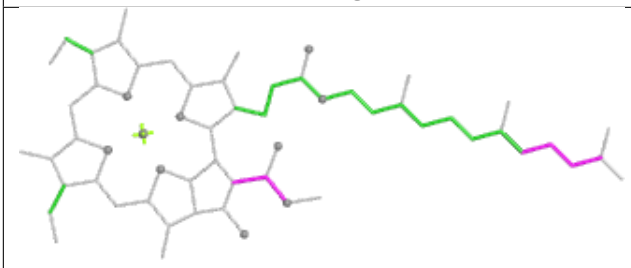
Ligand CLA 8 608



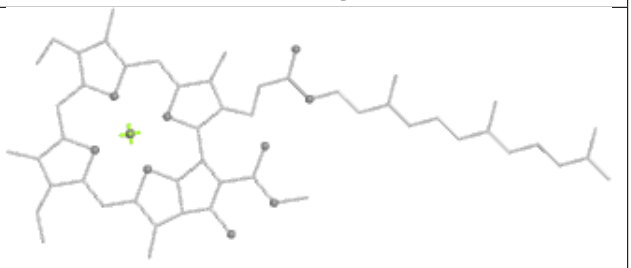
Bond lengths



Bond angles

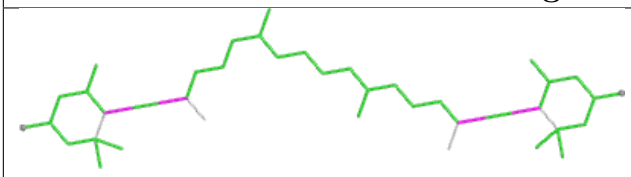


Torsions

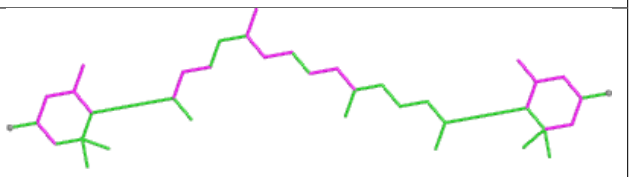


Rings

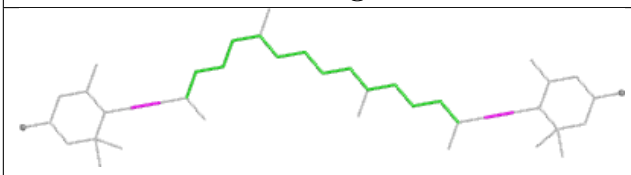
Ligand II0 7 619



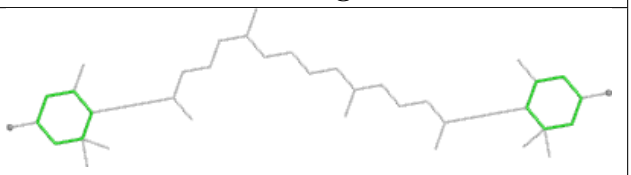
Bond lengths



Bond angles

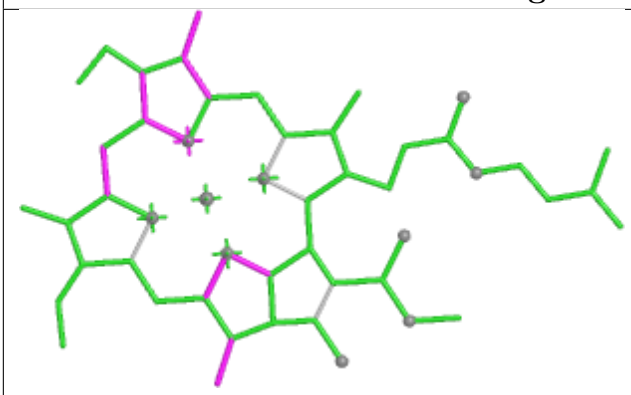


Torsions

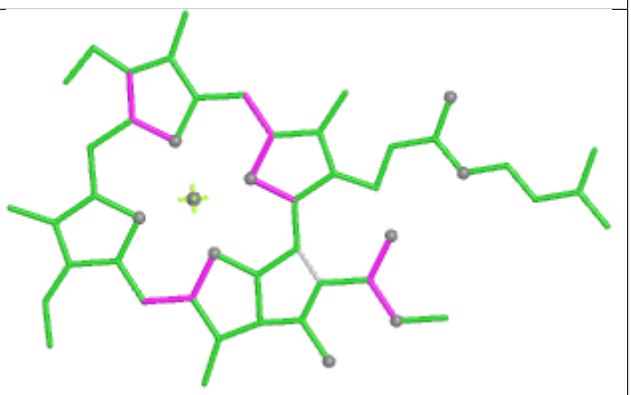


Rings

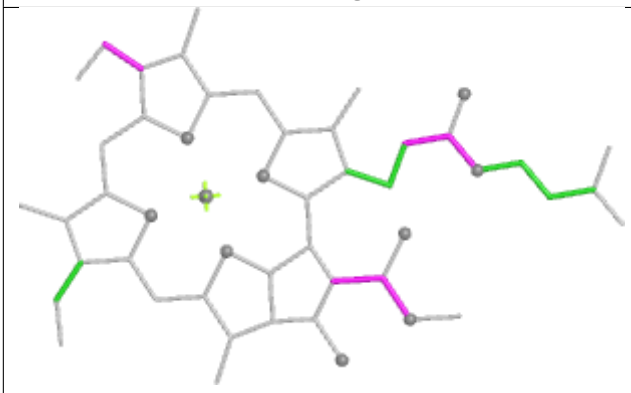
Ligand CLA 0 605



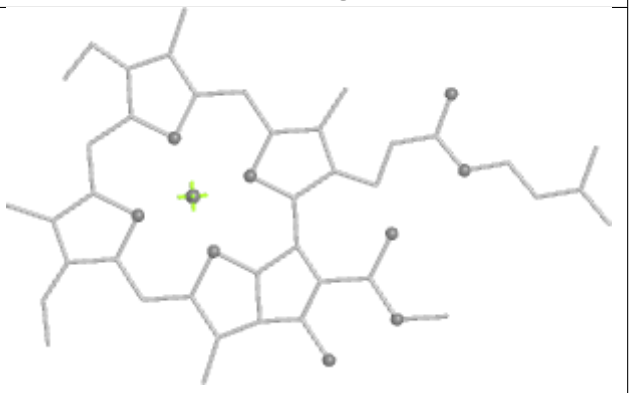
Bond lengths



Bond angles

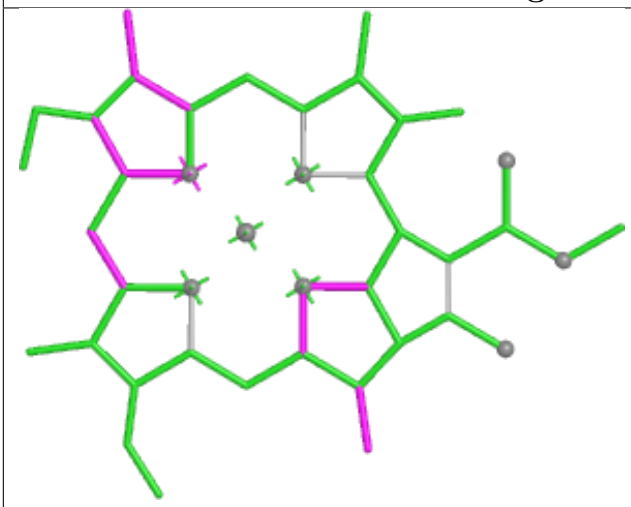


Torsions

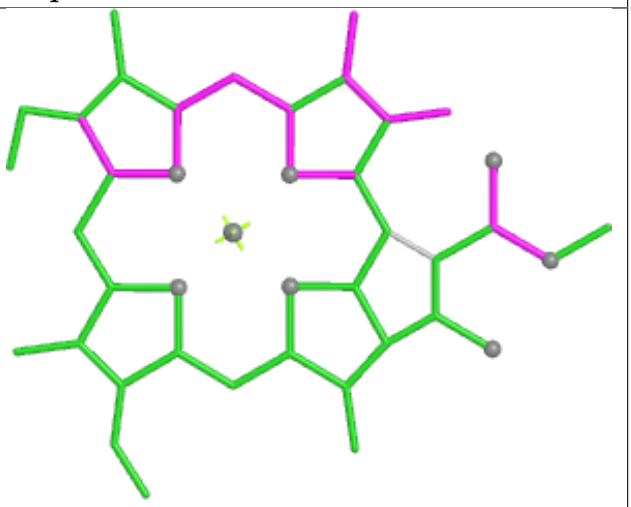


Rings

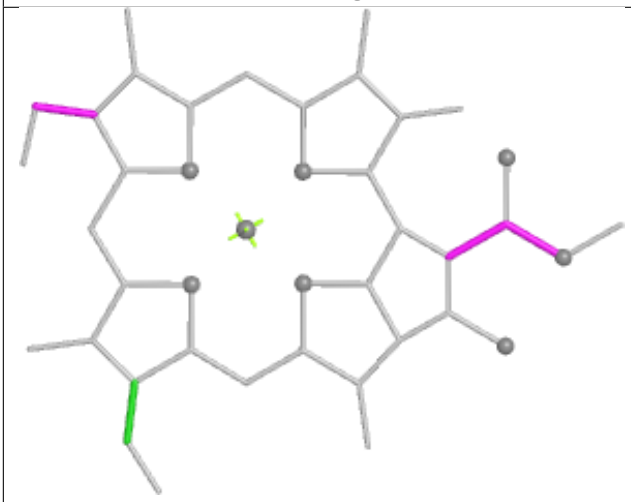
Ligand CLA p 311



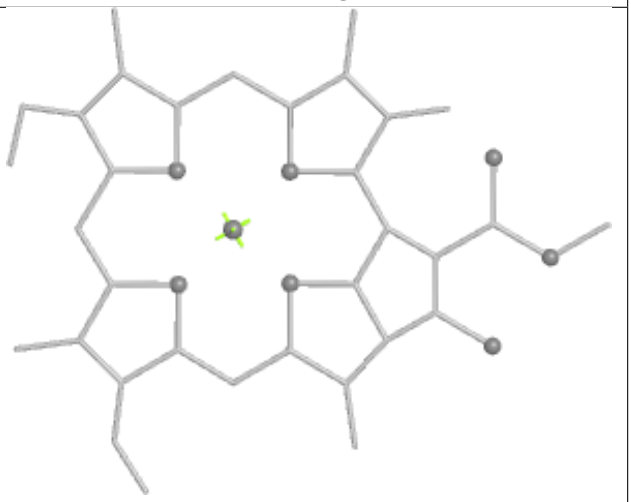
Bond lengths



Bond angles

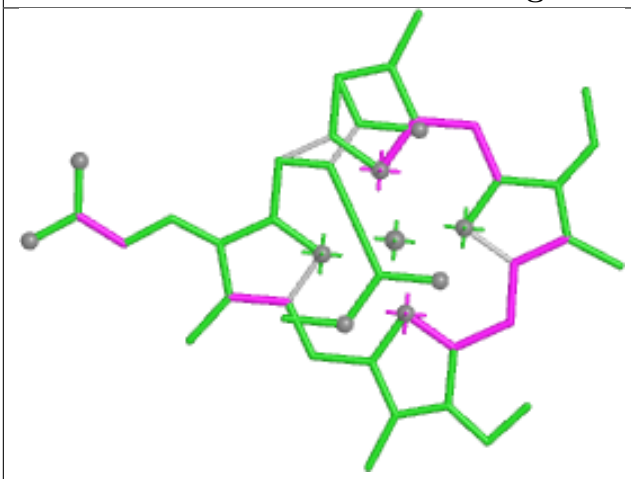


Torsions

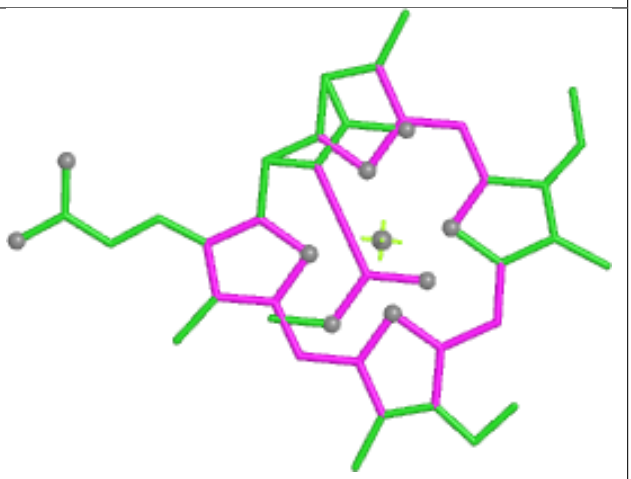


Rings

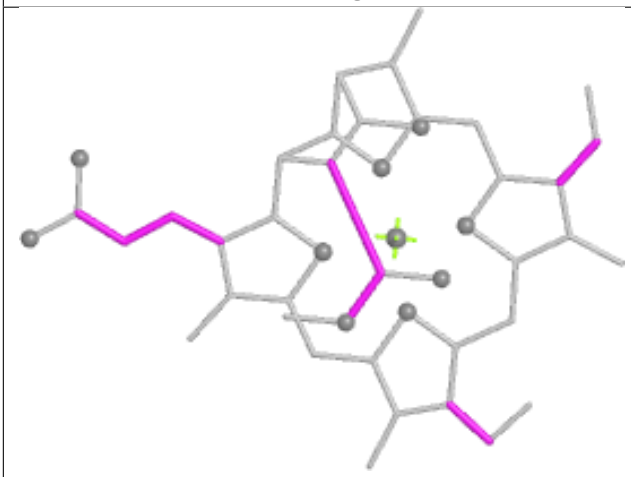
Ligand KC2 P 609



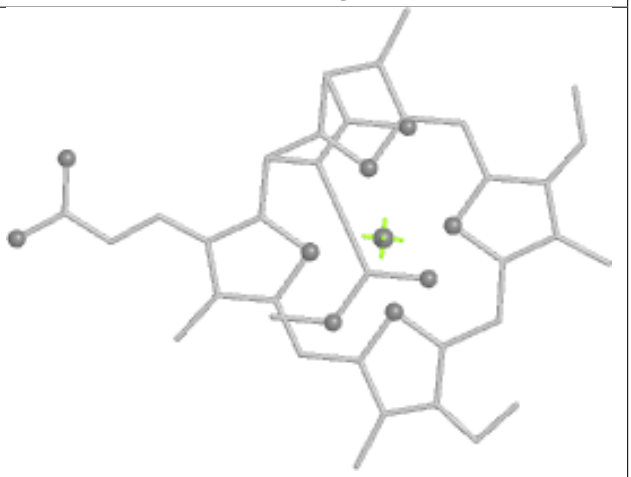
Bond lengths



Bond angles

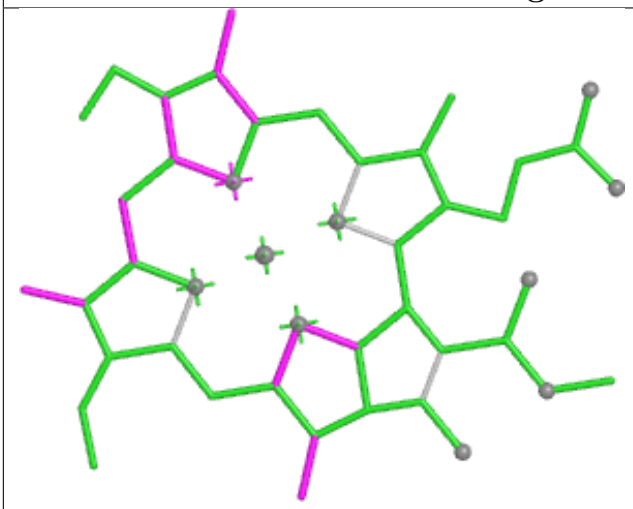


Torsions

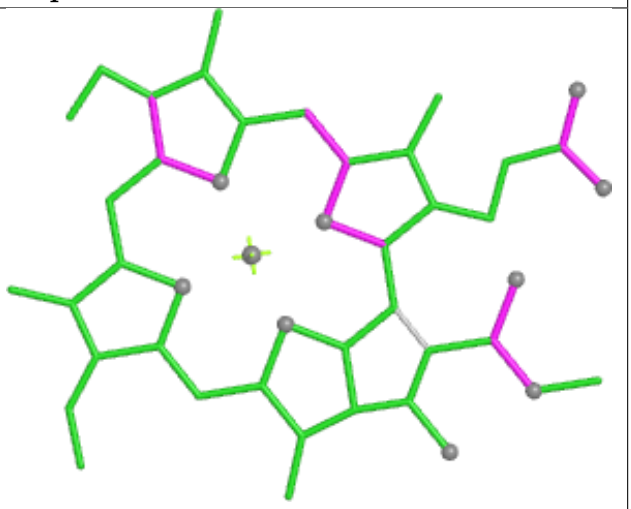


Rings

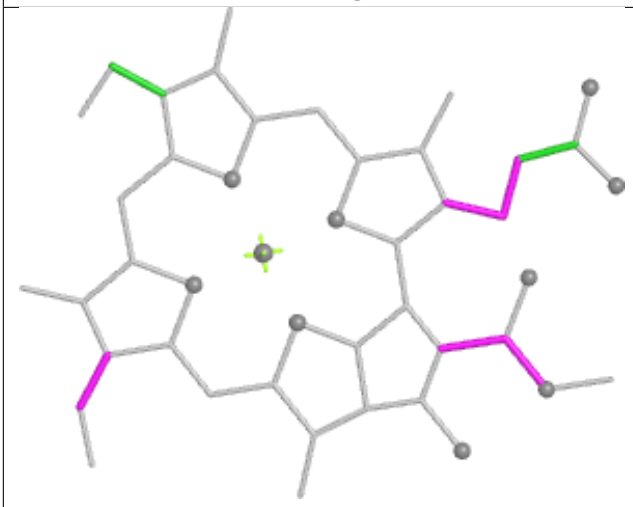
Ligand CLA p 313



Bond lengths



Bond angles

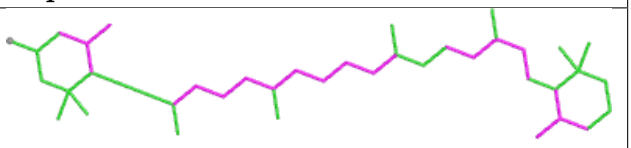


Torsions

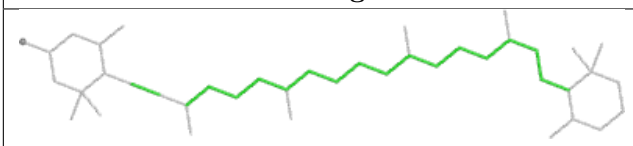
Rings

Ligand IHT p 318

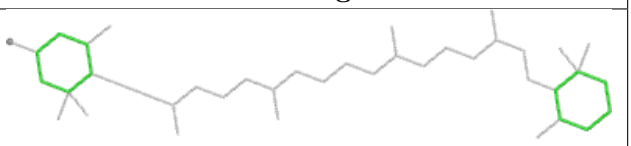
Bond lengths



Bond angles

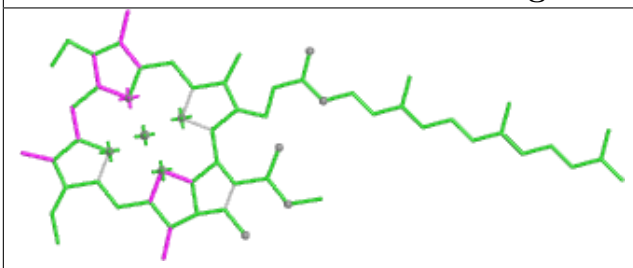


Torsions

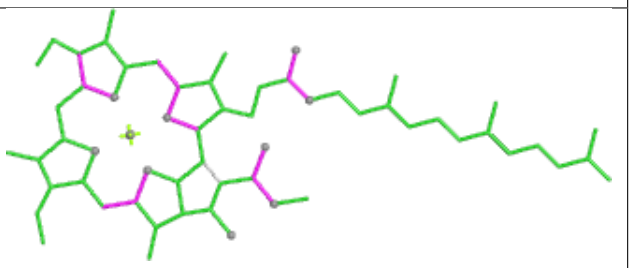


Rings

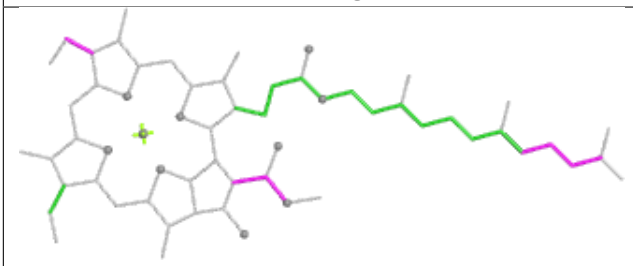
Ligand CLA 7 608



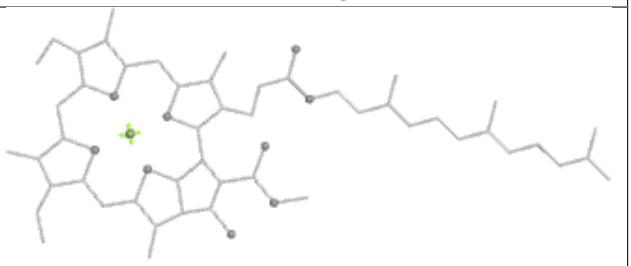
Bond lengths



Bond angles

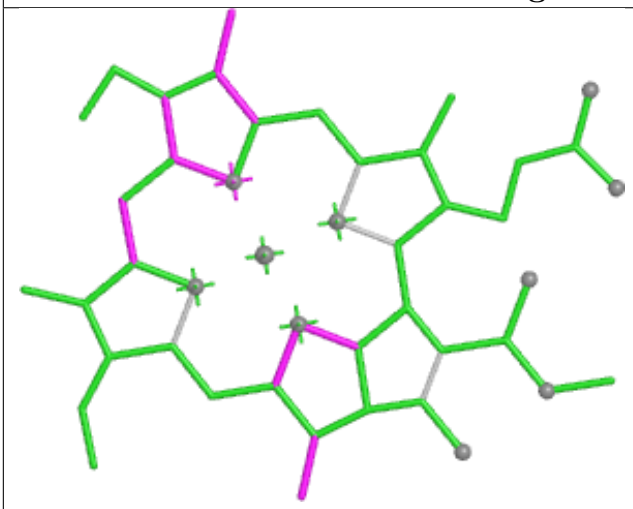


Torsions

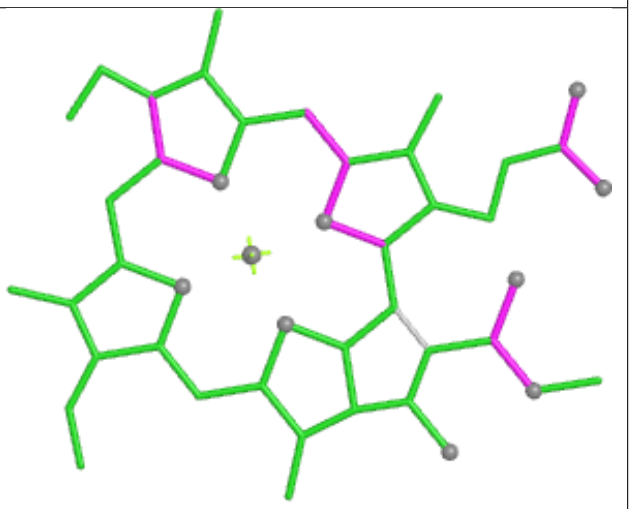


Rings

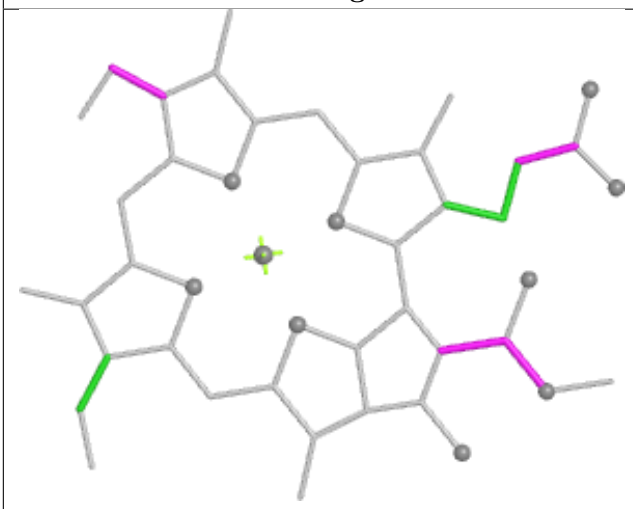
Ligand CLA 7 613



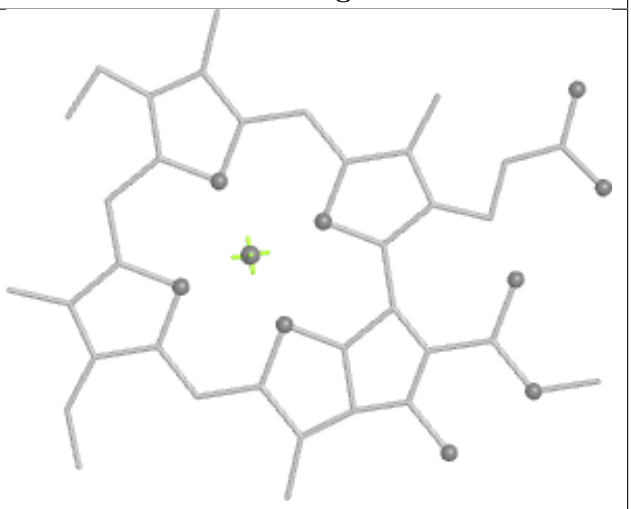
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

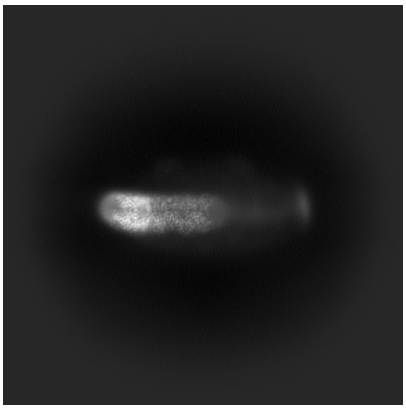
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-38419. These allow visual inspection of the internal detail of the map and identification of artifacts.

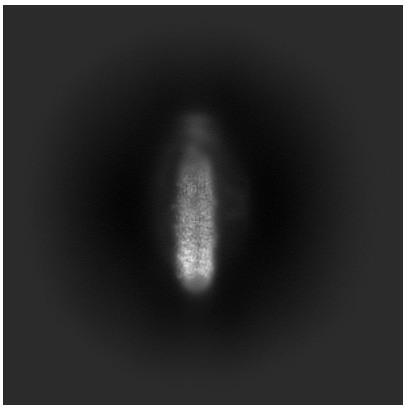
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

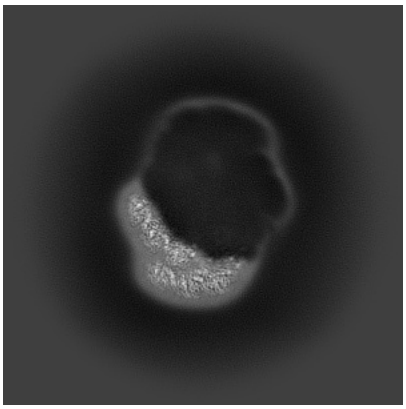
6.1.1 Primary map



X

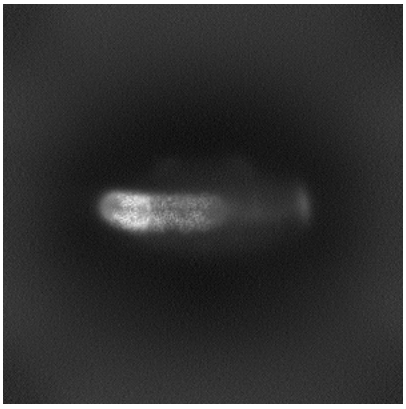


Y

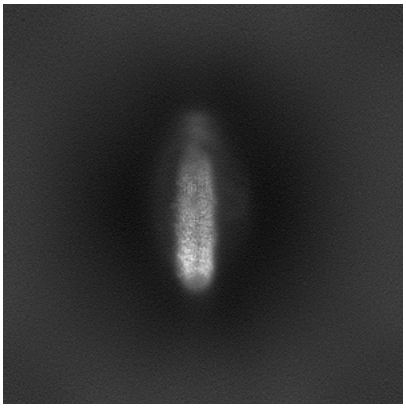


Z

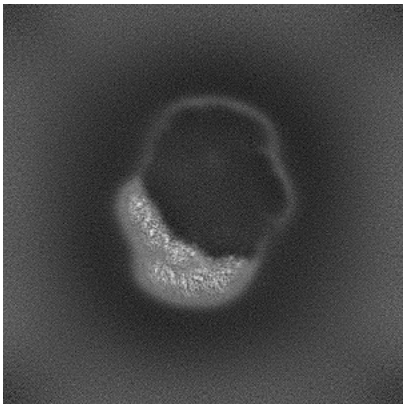
6.1.2 Raw map



X



Y

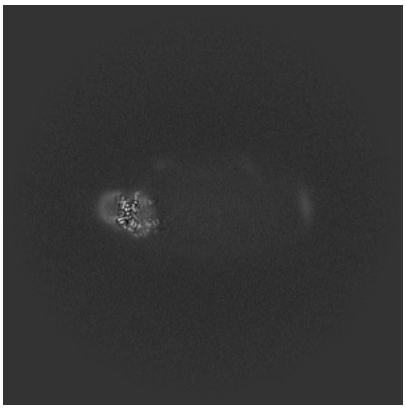


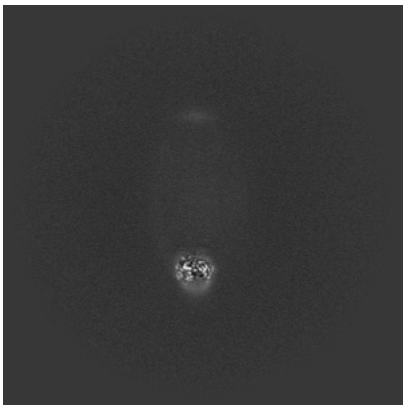
Z

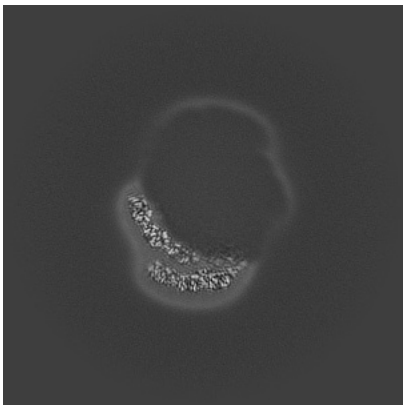
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

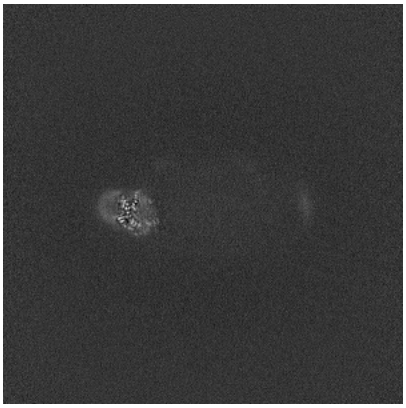
6.2.1 Primary map

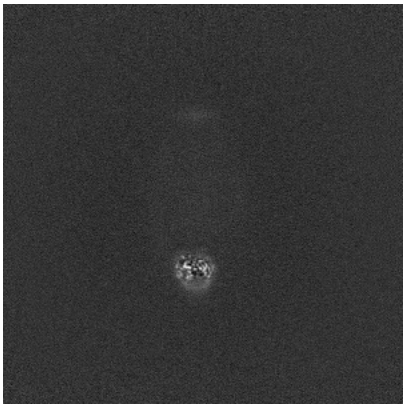

X Index: 256

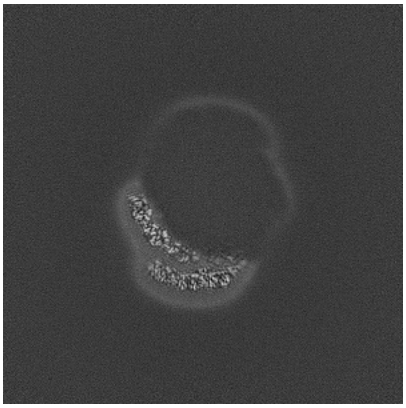

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

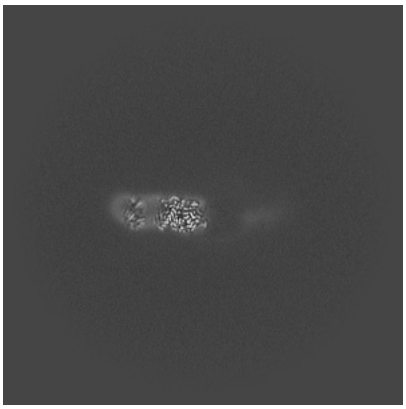

Y Index: 256


Z Index: 256

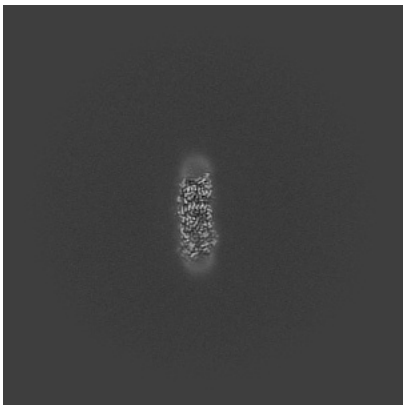
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

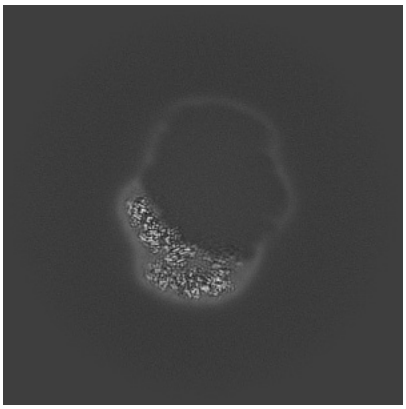
6.3.1 Primary map



X Index: 188

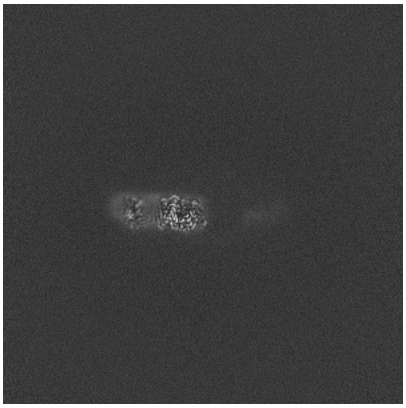


Y Index: 159

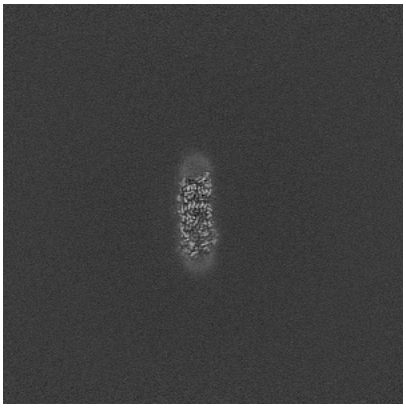


Z Index: 237

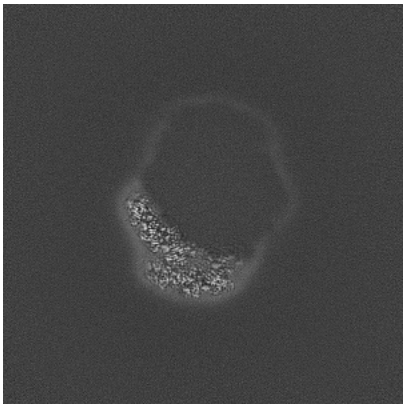
6.3.2 Raw map



X Index: 189



Y Index: 159

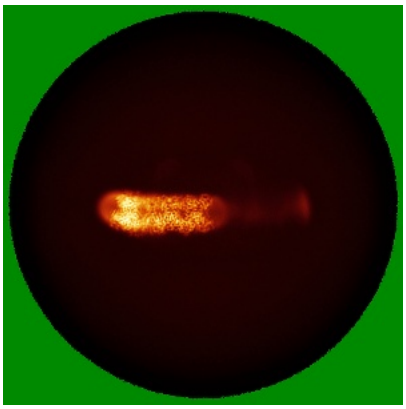


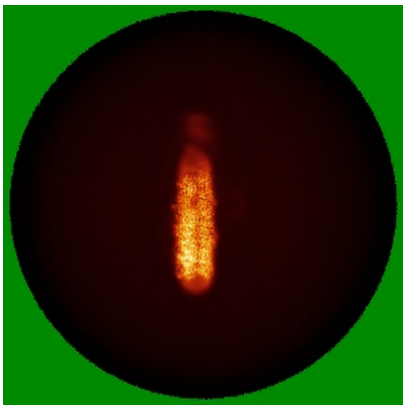
Z Index: 236

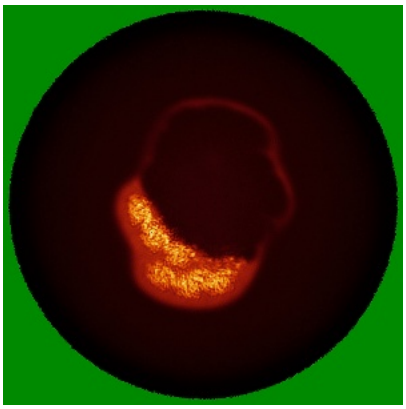
The images above show the largest variance slices of the map in three orthogonal directions.

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

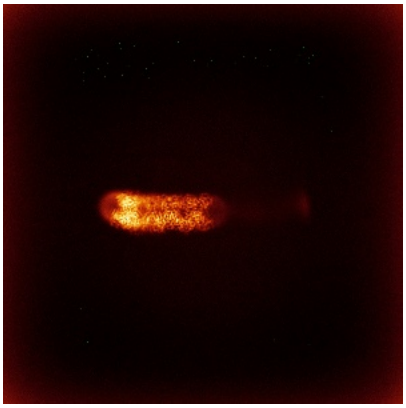
6.4.1 Primary map

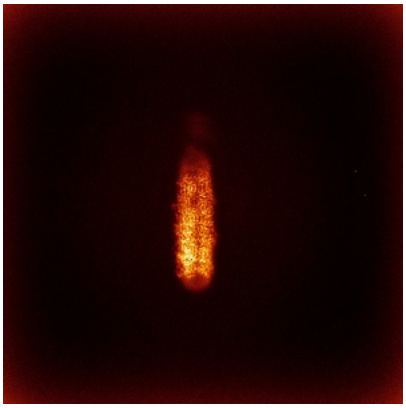

X

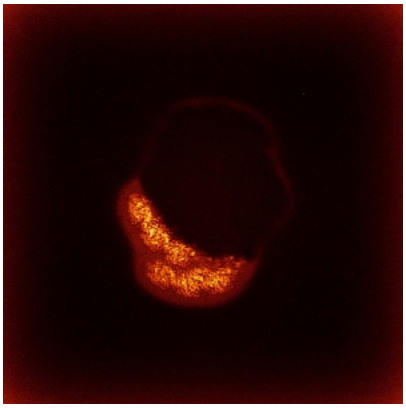

Y


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 0.266. 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.

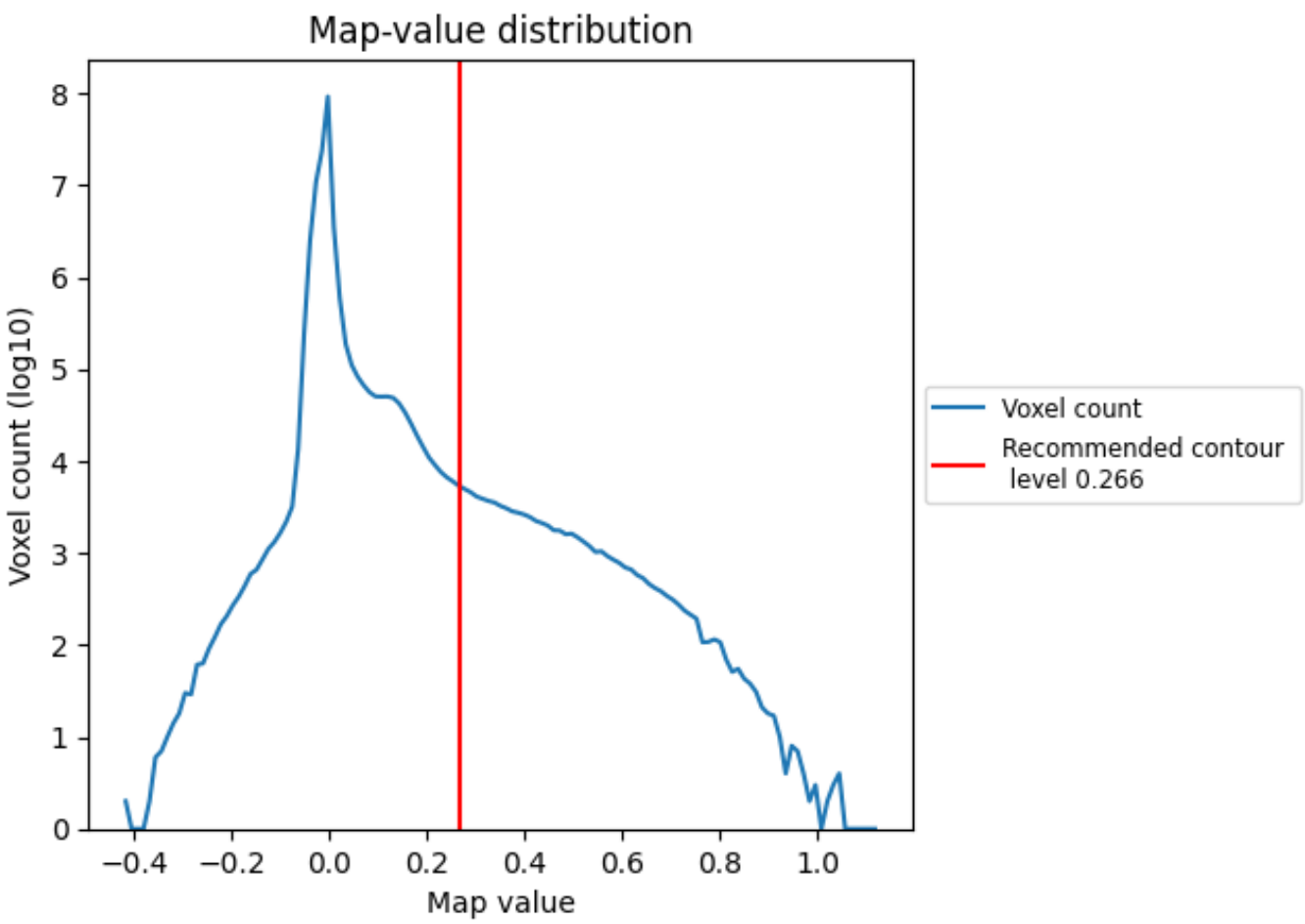
6.6 Mask visualisation (i)

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

7 Map analysis (i)

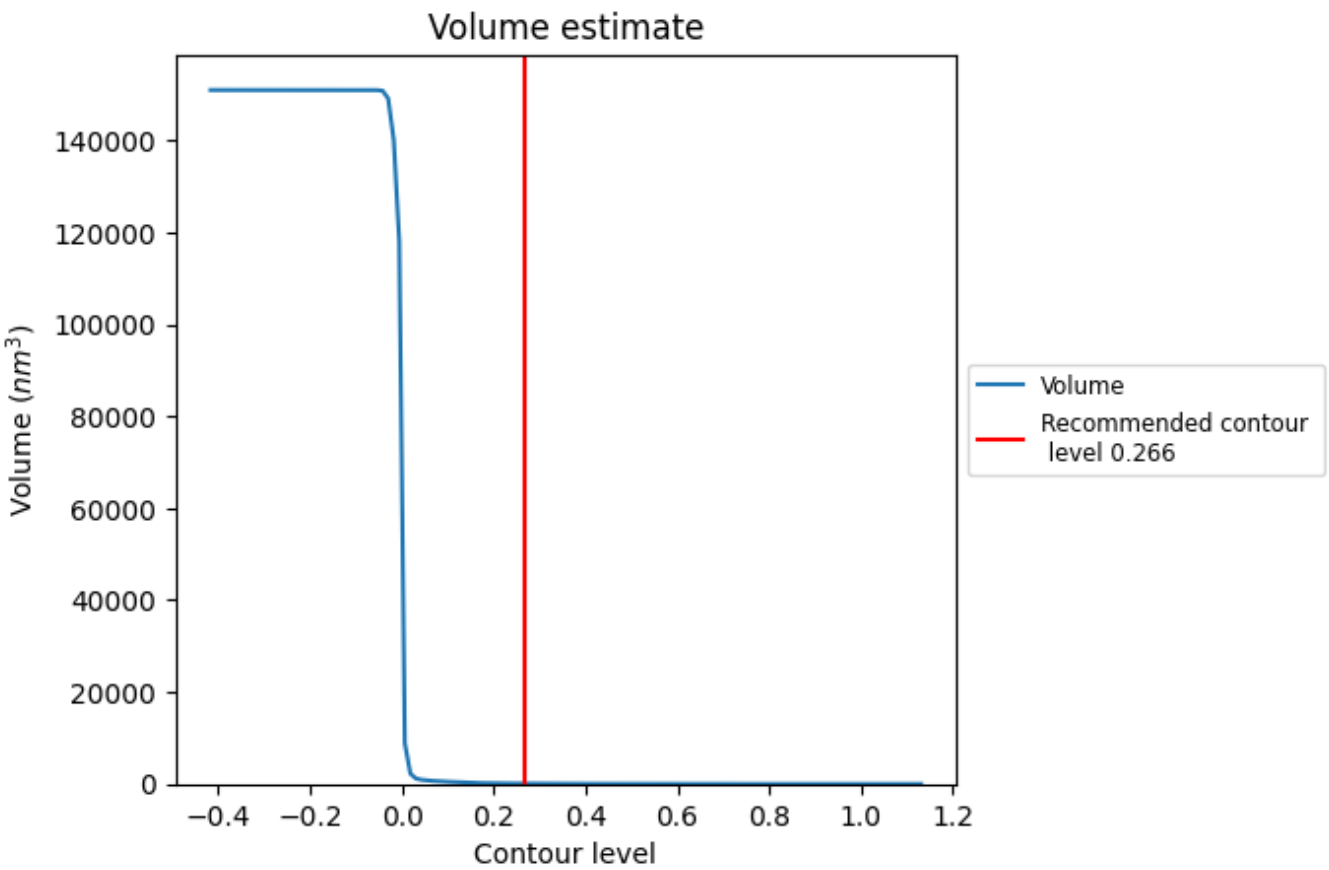
This section contains the results of statistical analysis of the map.

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.

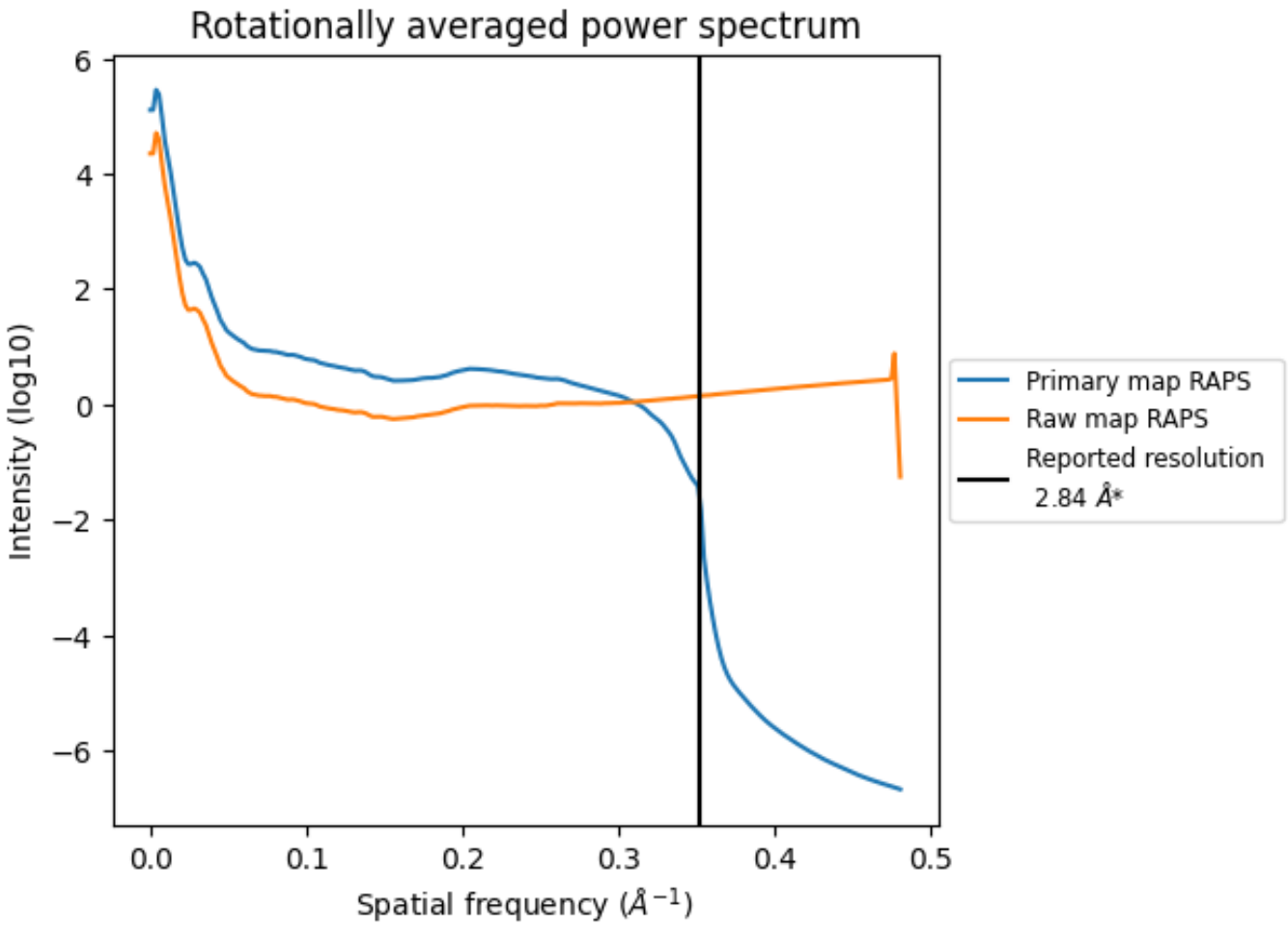
7.2 Volume estimate (i)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

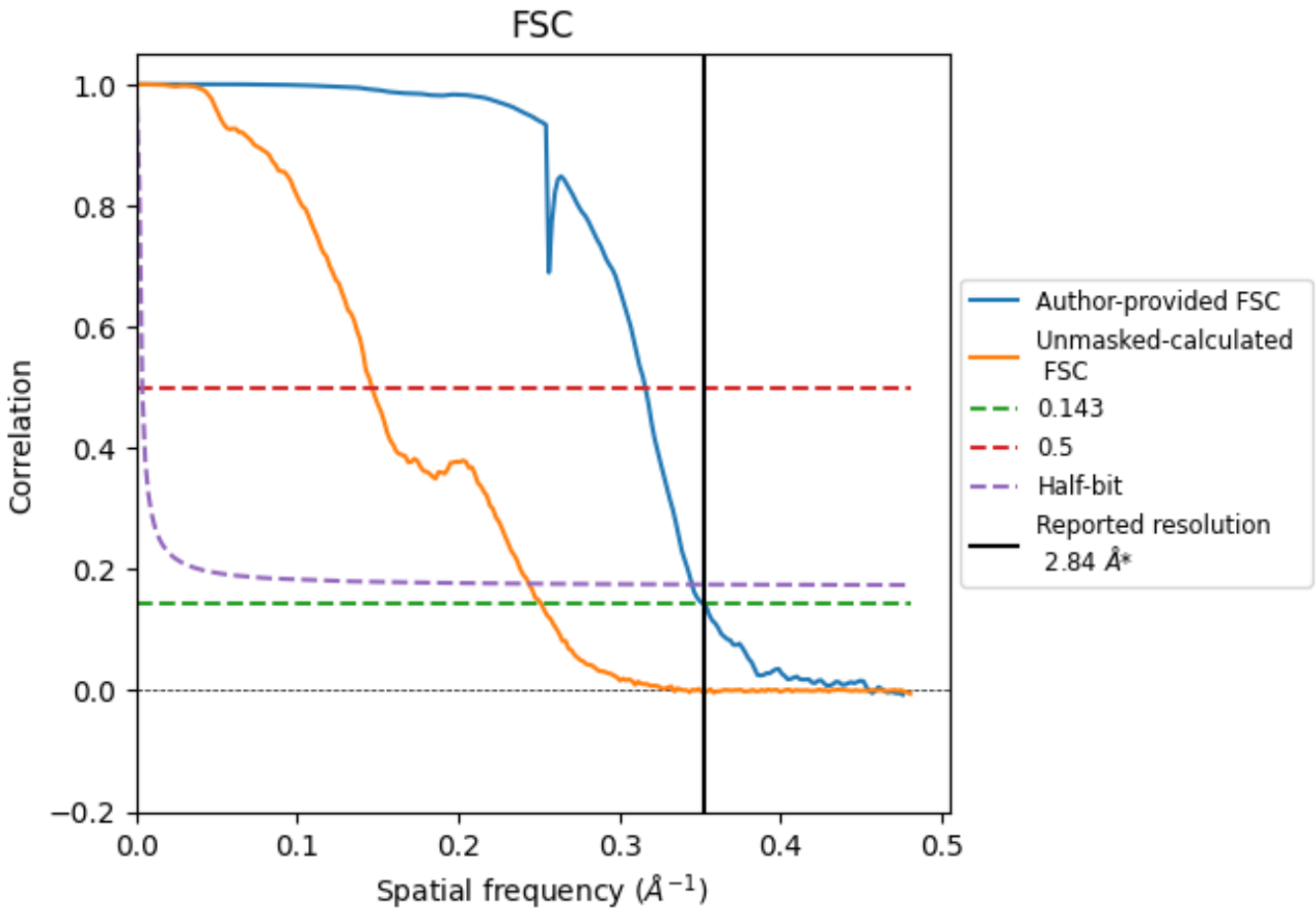


*Reported resolution corresponds to spatial frequency of 0.352 Å^{-1}

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 0.352 Å^{-1}

8.2 Resolution estimates (i)

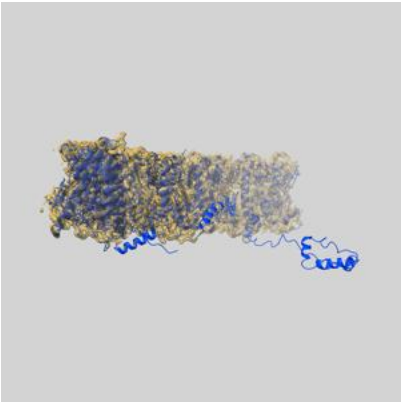
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.16	2.90
Unmasked-calculated*	3.98	6.83	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.84 by more than 10 %

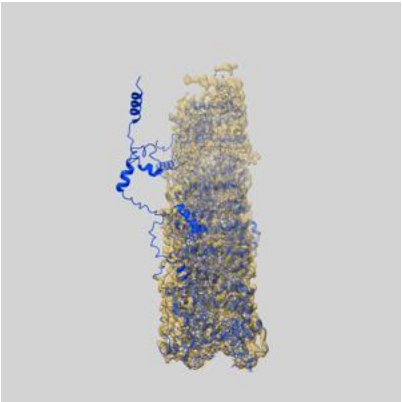
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-38419 and PDB model 8XKL. Per-residue inclusion information can be found in section 3 on page 16.

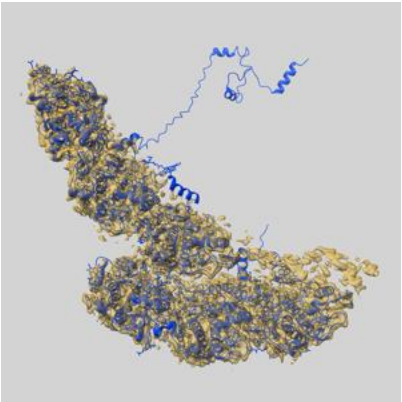
9.1 Map-model overlay (i)



X



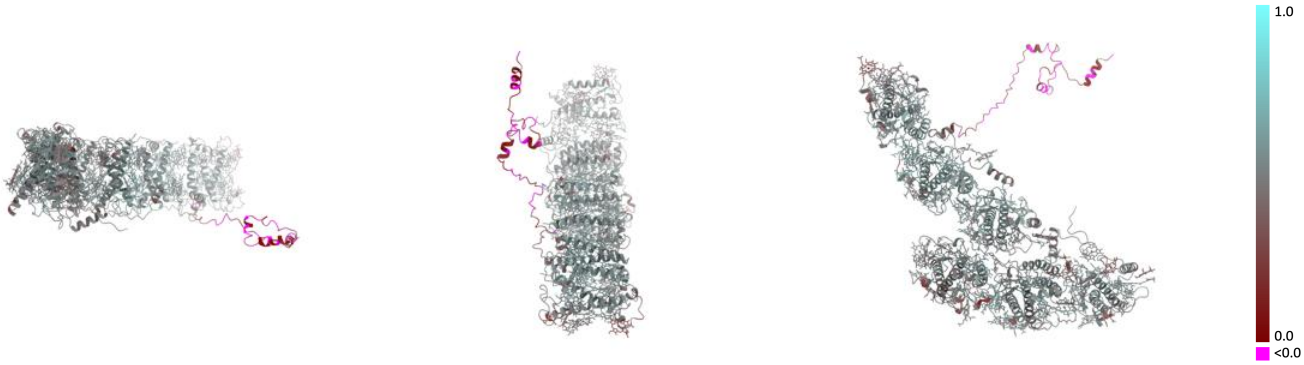
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.266 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.

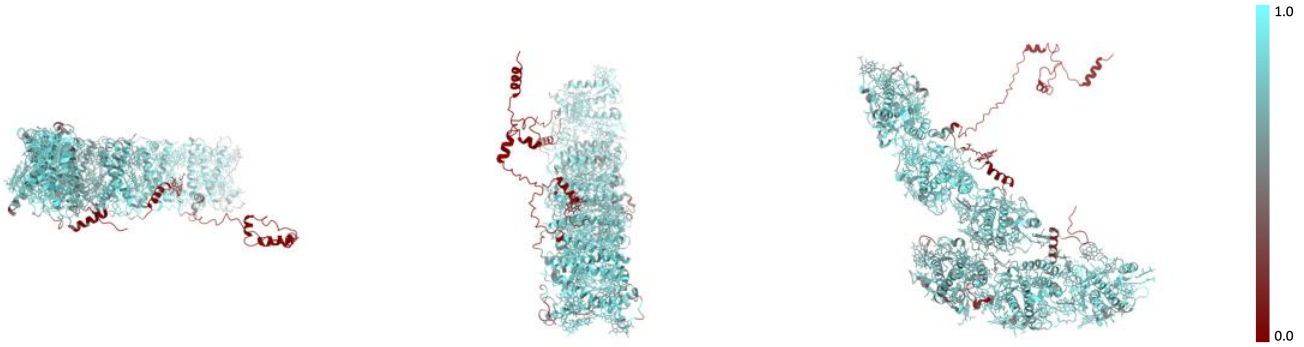
9.2 Q-score mapped to coordinate model (i)



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.

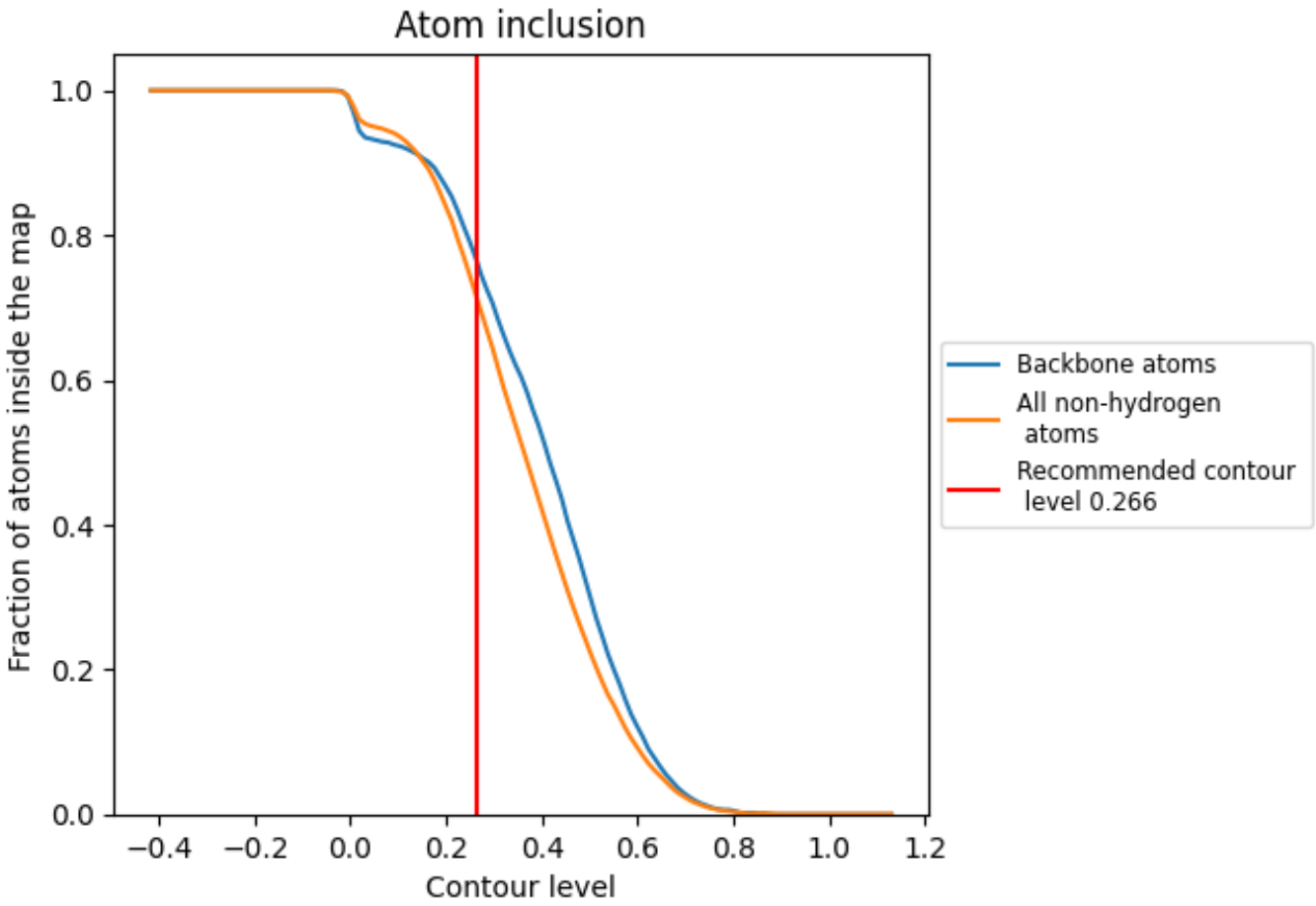
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.266).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.4900
0	0.7050	0.4920
7	0.7430	0.5020
8	0.8400	0.5470
9	0.7770	0.5340
G	0.4410	0.4780
P	0.7690	0.4930
p	0.7700	0.5160
s	0.3310	0.3040