wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 12:45 AM JST

PDB ID	:	5XNO / pdb_00005xno
EMDB ID	:	EMD-6744
Title	:	Structure of M-LHCII and CP24 complexes in the unstacked C2S2M2-type PSII-LHCII supercomplex from Pisum sativum
Authors	:	Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on	:	2017-05-23
Resolution	:	3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

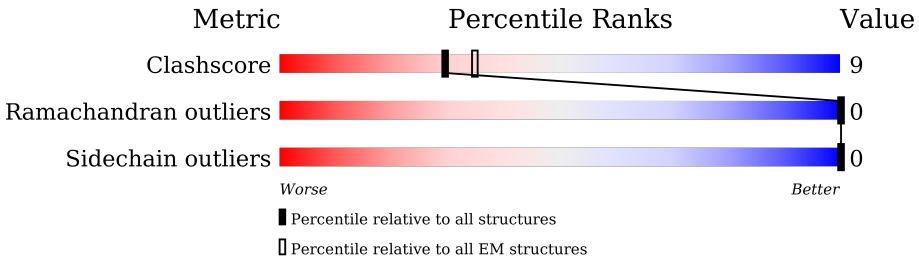
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

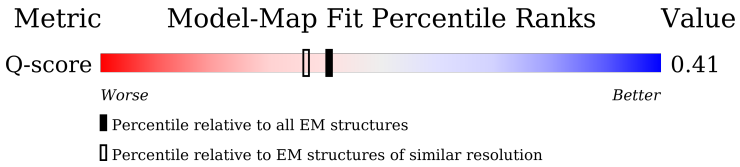
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	1	232	31% 78% 16% 6%
1	2	232	44% 77% 17% 6%
2	3	243	26% 75% 15% 9%
3	4	210	47% 76% 18% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CHL	1	607	X	-	-	-
4	CHL	1	609	X	-	-	-
4	CHL	2	607	X	-	-	-
4	CHL	2	609	X	-	-	-
4	CHL	3	601	X	-	-	-
4	CHL	3	609	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10020 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 Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		

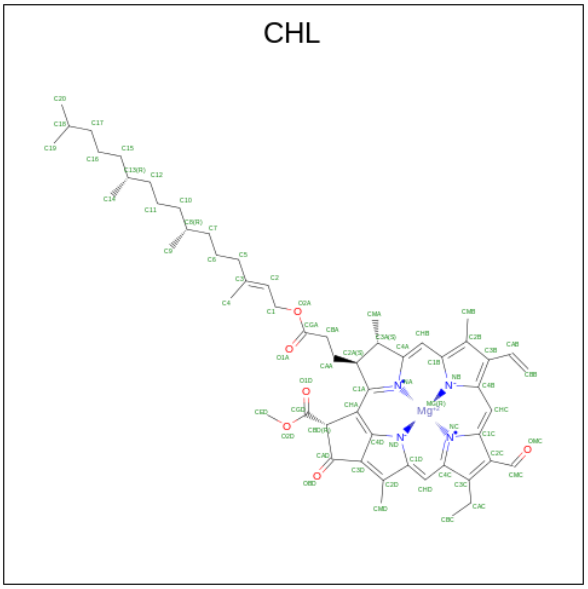
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
4	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
4	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
4	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
4	3	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
4	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	3	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
4	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
4	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
4	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
4	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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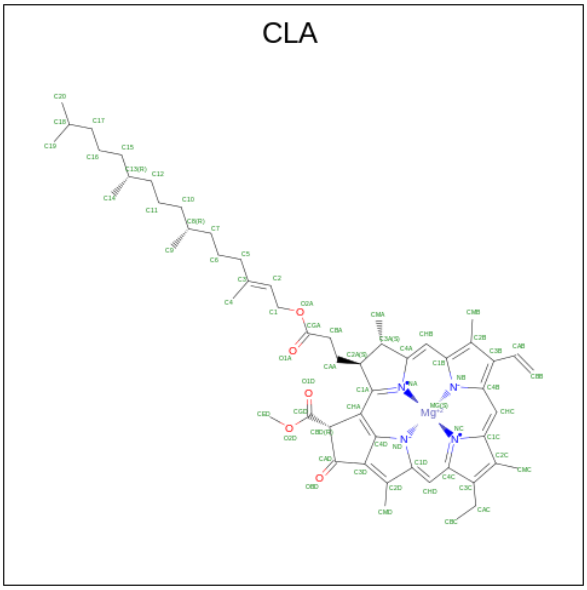
Mol	Chain	Residues	Atoms					AltConf
4	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 5 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
5	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
5	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
5	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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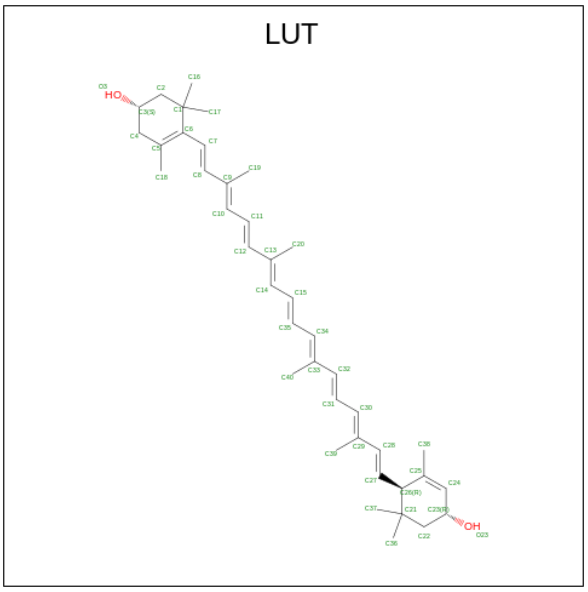
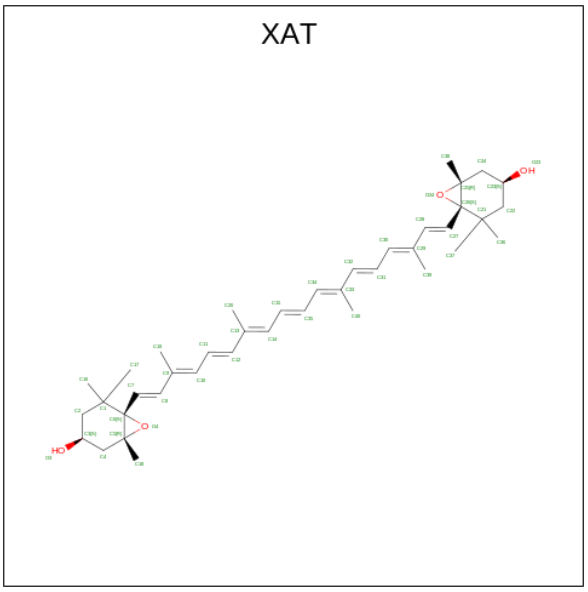
Mol	Chain	Residues	Atoms					AltConf
5	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
5	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
5	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
5	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
5	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
5	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	3	1	Total 58	C 48	Mg 1	N 4	O 5	0
5	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
5	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
5	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 6 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



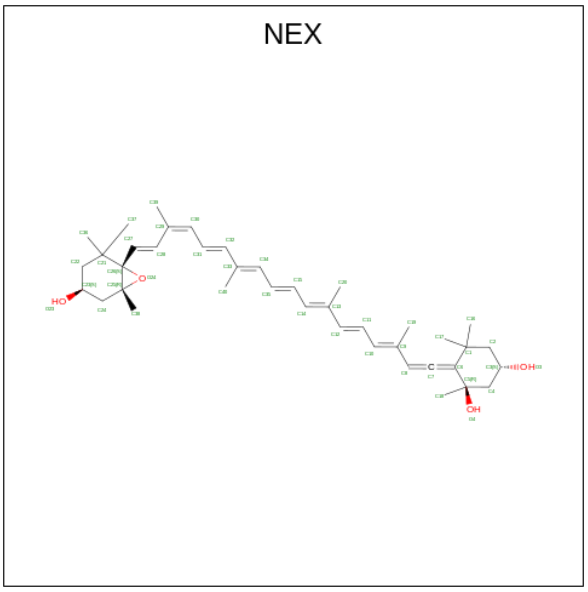
Mol	Chain	Residues	Atoms	AltConf
6	1	1	Total C O 42 40 2	0
6	1	1	Total C O 42 40 2	0
6	2	1	Total C O 42 40 2	0
6	2	1	Total C O 42 40 2	0
6	3	1	Total C O 42 40 2	0
6	3	1	Total C O 42 40 2	0
6	4	1	Total C O 42 40 2	0

- Molecule 7 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



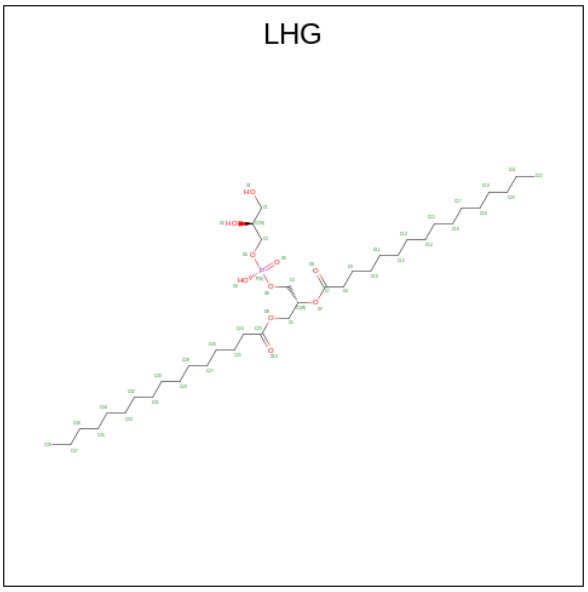
Mol	Chain	Residues	Atoms			AltConf
7	1	1	Total	C	O	0
			44	40	4	
7	2	1	Total	C	O	0
			44	40	4	
7	3	1	Total	C	O	0
			44	40	4	
7	4	1	Total	C	O	0
			44	40	4	

- Molecule 8 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



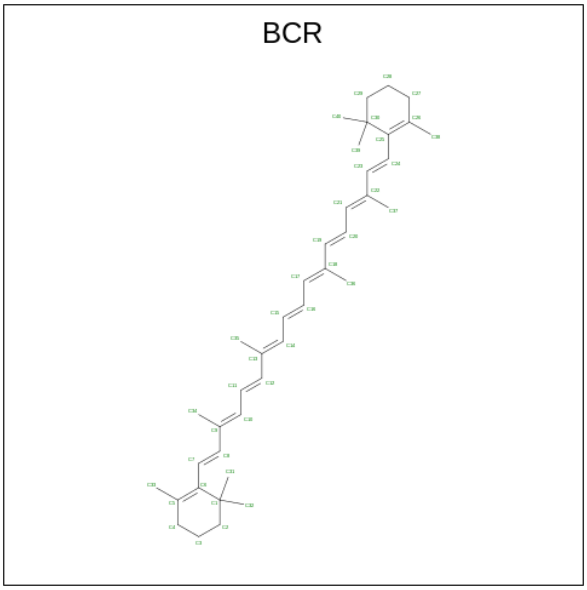
Mol	Chain	Residues	Atoms			AltConf
8	1	1	Total	C	O	0
			44	40	4	
8	2	1	Total	C	O	0
			44	40	4	
8	3	1	Total	C	O	0
			44	40	4	

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
9	1	1	Total	C	O	P	0
			41	30	10	1	
9	2	1	Total	C	O	P	0
			37	26	10	1	
9	3	1	Total	C	O	P	0
			47	36	10	1	
9	4	1	Total	C	O	P	0
			21	10	10	1	

- Molecule 10 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



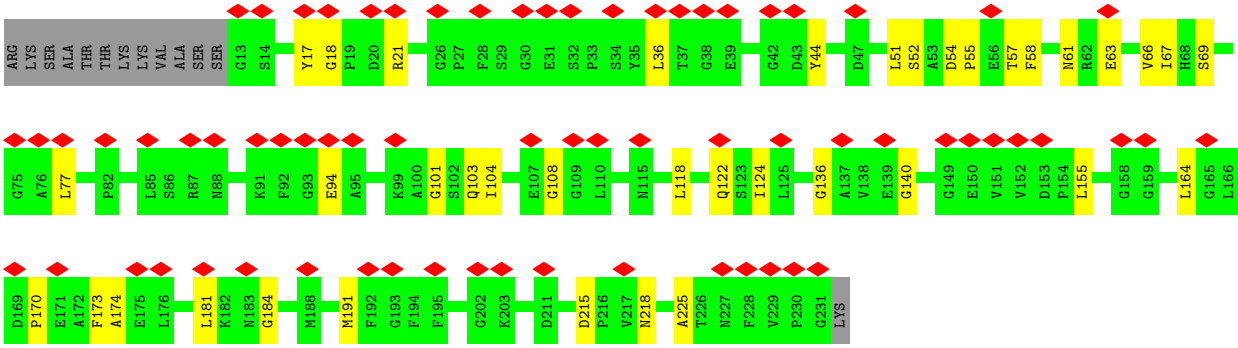
Mol	Chain	Residues	Atoms		AltConf
10	4	1	Total	C	0
			40	40	

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.

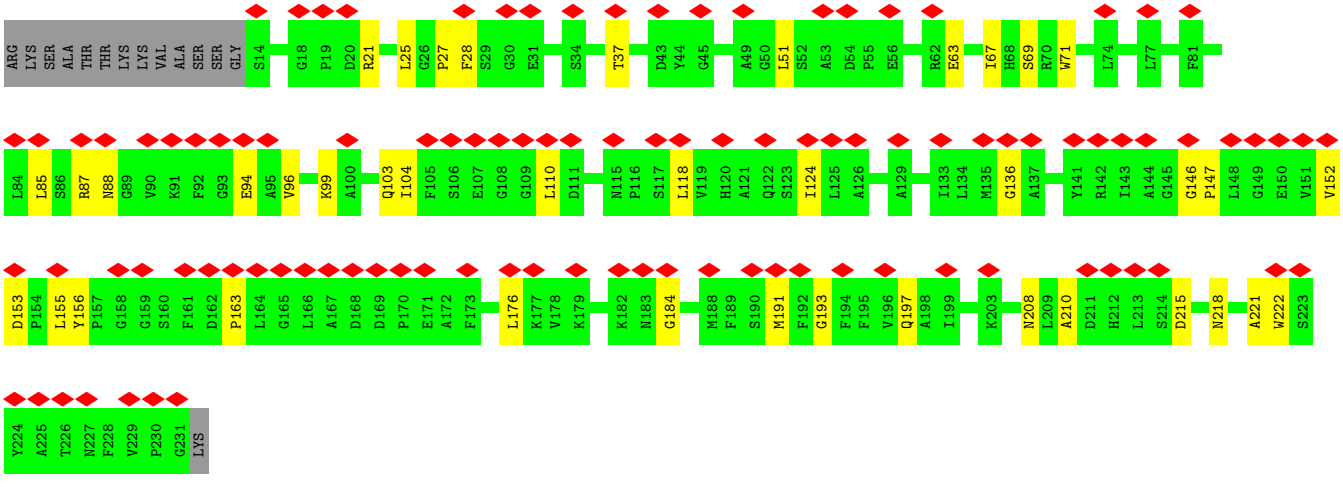
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain 1:



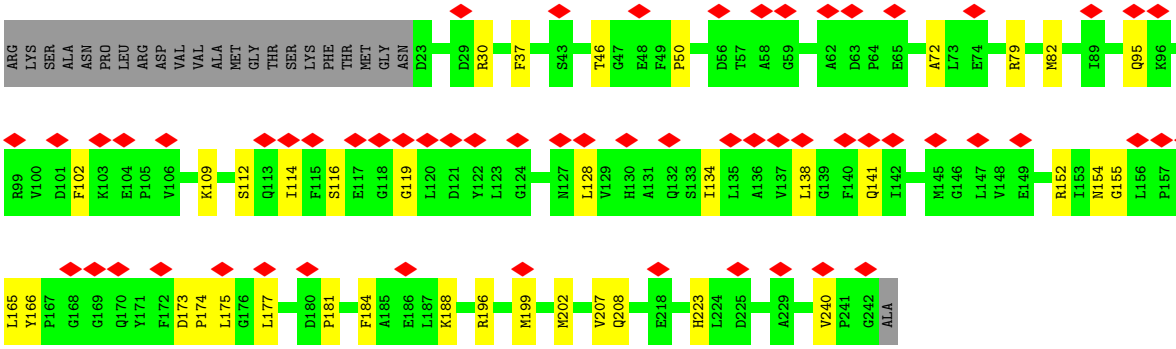
• Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

Chain 2:



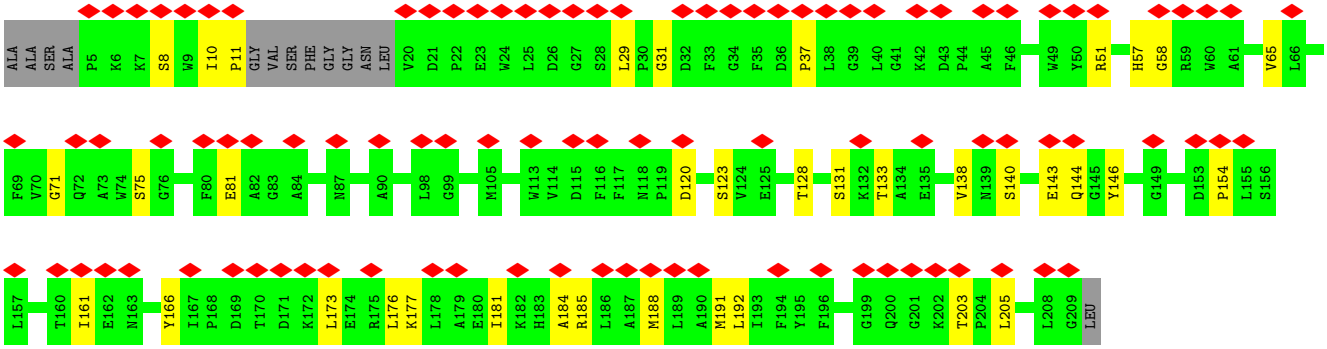
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50237	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	156.0, 156.0, 156.0	wwPDB
Map dimensions	150, 150, 150	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, NEX, CLA, LUT, CHL, LHG, BCR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1	0.42	0/1720	0.55	0/2342
1	2	0.36	0/1716	0.57	1/2337 (0.0%)
2	3	0.42	0/1759	0.58	0/2396
3	4	0.38	0/1586	0.65	0/2158
All	All	0.40	0/6781	0.59	1/9233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	152	VAL	N-CA-C	-5.02	106.76	111.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	27	0
1	2	1664	0	1593	29	0
2	3	1707	0	1659	30	0
3	4	1534	0	1486	25	0
4	1	309	0	244	11	0
4	2	306	0	238	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	316	0	254	17	0
4	4	229	0	152	4	0
5	1	412	0	348	12	0
5	2	391	0	314	12	0
5	3	426	0	373	12	0
5	4	270	0	198	4	0
6	1	84	0	112	9	0
6	2	84	0	112	8	0
6	3	84	0	112	10	0
6	4	42	0	56	4	0
7	1	44	0	56	4	0
7	2	44	0	56	6	0
7	3	44	0	56	5	0
7	4	44	0	56	4	0
8	1	44	0	56	2	0
8	2	44	0	56	1	0
8	3	44	0	56	3	0
9	1	41	0	55	0	0
9	2	37	0	44	2	0
9	3	47	0	67	3	0
9	4	21	0	12	1	0
10	4	40	0	56	3	0
All	All	10020	0	9473	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 9.

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)
4:3:606:CHL:HBB2	4:3:607:CHL:HBB1	1.57	0.86
5:1:602:CLA:HAB	6:1:1621:LUT:H32	1.66	0.77
1:2:191:MET:HE2	6:2:1621:LUT:H10	1.69	0.74
2:3:202:MET:HE2	6:3:1621:LUT:H10	1.69	0.73
5:2:610:CLA:H2	6:2:1620:LUT:H28	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	1	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	2	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
2	3	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
All	All	844/917 (92%)	809 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
All	All	671/719 (93%)	671 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	3	95	GLN
2	3	219	ASN
3	4	122	GLN
3	4	72	GLN
1	2	88	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

72 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	$\#\|Z\| > 2$
4	CHL	2	609	1	65,69,74	1.97	16 (24%)	74,108,114	2.90	25 (33%)
4	CHL	2	605	1	50,54,74	2.29	19 (38%)	56,90,114	3.29	23 (41%)
4	CHL	4	607	-	50,54,74	2.27	19 (38%)	56,90,114	3.27	22 (39%)
6	LUT	3	1621	-	42,43,43	0.94	1 (2%)	51,60,60	1.61	11 (21%)
8	NEX	1	1623	-	38,46,46	1.13	4 (10%)	50,70,70	2.61	18 (36%)
5	CLA	1	613	1	59,63,73	1.35	11 (18%)	71,101,113	1.35	7 (9%)
5	CLA	4	604	-	49,53,73	1.49	10 (20%)	59,89,113	1.41	7 (11%)
6	LUT	3	1620	-	42,43,43	0.97	3 (7%)	51,60,60	2.03	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CHL	3	605	2	50,54,74	2.24	18 (36%)	56,90,114	3.34	25 (44%)
4	CHL	4	606	-	50,54,74	2.24	17 (34%)	56,90,114	3.35	25 (44%)
5	CLA	4	612	3	49,53,73	1.48	10 (20%)	59,89,113	1.42	8 (13%)
4	CHL	4	609	3	50,54,74	2.20	19 (38%)	56,90,114	3.46	23 (41%)
4	CHL	1	606	-	50,54,74	2.23	17 (34%)	56,90,114	3.19	22 (39%)
4	CHL	4	601	3	48,53,74	2.43	19 (39%)	53,89,114	3.23	20 (37%)
5	CLA	2	613	1	49,53,73	1.47	9 (18%)	59,89,113	1.34	8 (13%)
4	CHL	3	609	2	65,69,74	2.05	20 (30%)	74,108,114	2.85	24 (32%)
5	CLA	4	602	3	49,53,73	1.44	10 (20%)	59,89,113	1.49	9 (15%)
5	CLA	4	603	3	49,53,73	1.48	11 (22%)	59,89,113	1.38	5 (8%)
4	CHL	1	601	1	50,54,74	2.27	17 (34%)	56,90,114	3.35	23 (41%)
5	CLA	4	610	3	49,53,73	1.49	10 (20%)	59,89,113	1.27	8 (13%)
7	XAT	3	1622	-	39,47,47	1.19	5 (12%)	54,74,74	3.06	27 (50%)
6	LUT	4	620	-	42,43,43	0.95	3 (7%)	51,60,60	2.09	15 (29%)
7	XAT	4	622	-	39,47,47	0.98	2 (5%)	54,74,74	2.70	20 (37%)
8	NEX	2	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.41	14 (28%)
7	XAT	1	1622	-	39,47,47	0.95	2 (5%)	54,74,74	2.85	22 (40%)
9	LHG	1	2630	5	40,40,48	0.74	1 (2%)	43,46,54	1.33	6 (13%)
4	CHL	2	608	-	50,54,74	2.21	18 (36%)	56,90,114	3.38	20 (35%)
4	CHL	2	607	-	65,69,74	2.07	21 (32%)	74,108,114	2.85	25 (33%)
5	CLA	1	602	1	65,69,73	1.34	11 (16%)	78,108,113	1.22	9 (11%)
4	CHL	2	601	1	50,54,74	2.26	18 (36%)	56,90,114	3.36	25 (44%)
5	CLA	2	602	1	65,69,73	1.31	10 (15%)	78,108,113	1.22	9 (11%)
5	CLA	1	603	1	59,63,73	1.38	12 (20%)	71,101,113	1.45	9 (12%)
5	CLA	2	604	-	49,53,73	1.47	11 (22%)	59,89,113	1.47	10 (16%)
5	CLA	3	613	2	62,66,73	1.33	11 (17%)	74,104,113	1.33	8 (10%)
5	CLA	3	602	2	64,68,73	1.31	11 (17%)	77,107,113	1.20	7 (9%)
5	CLA	4	611	9	49,53,73	1.46	8 (16%)	59,89,113	1.31	8 (13%)
9	LHG	2	2630	5	36,36,48	0.74	1 (2%)	39,42,54	1.26	4 (10%)
8	NEX	3	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.46	16 (32%)
4	CHL	3	607	-	57,61,74	2.13	20 (35%)	64,98,114	3.19	23 (35%)
7	XAT	2	1622	-	39,47,47	1.03	0	54,74,74	2.98	24 (44%)
5	CLA	1	610	1	60,64,73	1.29	8 (13%)	72,102,113	1.23	9 (12%)
5	CLA	3	612	2	49,53,73	1.49	12 (24%)	59,89,113	1.41	8 (13%)
5	CLA	1	611	9	49,53,73	1.48	12 (24%)	59,89,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CLA	1	612	1	49,53,73	1.48	11 (22%)	59,89,113	1.54	11 (18%)
5	CLA	2	610	1	54,58,73	1.38	9 (16%)	65,95,113	1.16	6 (9%)
4	CHL	4	608	-	50,54,74	2.18	18 (36%)	56,90,114	3.32	27 (48%)
6	LUT	2	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.79	16 (31%)
5	CLA	3	604	-	49,53,73	1.48	11 (22%)	59,89,113	1.30	4 (6%)
4	CHL	3	601	2	68,72,74	1.92	17 (25%)	77,111,114	3.03	28 (36%)
5	CLA	2	611	9	49,53,73	1.46	10 (20%)	59,89,113	1.45	7 (11%)
10	BCR	4	623	-	41,41,41	0.78	0	56,56,56	2.18	15 (26%)
4	CHL	1	607	-	67,71,74	1.93	19 (28%)	76,110,114	3.11	27 (35%)
4	CHL	3	608	-	50,54,74	2.23	18 (36%)	56,90,114	3.42	22 (39%)
9	LHG	3	2630	5	46,46,48	0.79	1 (2%)	49,52,54	1.30	4 (8%)
4	CHL	3	606	-	50,54,74	2.33	17 (34%)	56,90,114	3.36	25 (44%)
5	CLA	3	614	2	52,56,73	1.46	7 (13%)	62,92,113	1.33	8 (12%)
5	CLA	1	604	-	54,58,73	1.43	11 (20%)	65,95,113	1.40	9 (13%)
5	CLA	1	614	1	49,53,73	1.48	10 (20%)	59,89,113	1.35	9 (15%)
9	LHG	4	2630	5	20,20,48	0.87	0	23,26,54	1.32	1 (4%)
5	CLA	3	603	2	59,63,73	1.35	12 (20%)	71,101,113	1.46	8 (11%)
5	CLA	3	610	2	64,68,73	1.30	10 (15%)	77,107,113	1.18	9 (11%)
6	LUT	1	1620	-	42,43,43	0.93	2 (4%)	51,60,60	1.87	14 (27%)
4	CHL	1	608	-	50,54,74	2.22	18 (36%)	56,90,114	3.35	23 (41%)
4	CHL	2	606	-	50,54,74	2.24	18 (36%)	56,90,114	3.27	23 (41%)
5	CLA	2	612	1	49,53,73	1.48	9 (18%)	59,89,113	1.39	9 (15%)
5	CLA	3	611	9	59,63,73	1.40	11 (18%)	71,101,113	1.37	9 (12%)
4	CHL	1	605	1	50,54,74	2.28	21 (42%)	56,90,114	3.32	20 (35%)
6	LUT	2	1620	-	42,43,43	0.81	0	51,60,60	1.72	15 (29%)
6	LUT	1	1621	-	42,43,43	1.02	3 (7%)	51,60,60	1.91	17 (33%)
5	CLA	2	603	1	59,63,73	1.37	10 (16%)	71,101,113	1.40	8 (11%)
4	CHL	1	609	1	66,70,74	2.05	17 (25%)	75,109,114	2.85	23 (30%)
5	CLA	2	614	1	49,53,73	1.47	10 (20%)	59,89,113	1.32	8 (13%)

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
4	CHL	2	609	1	1/1/14/21	17/35/111/117	-
4	CHL	2	605	1	-	10/17/93/117	-
4	CHL	4	607	-	-	10/17/93/117	-
6	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
8	NEX	1	1623	-	-	9/27/83/83	0/3/3/3
5	CLA	1	613	1	-	9/27/103/115	-
5	CLA	4	604	-	-	11/15/91/115	-
6	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
4	CHL	3	605	2	-	12/17/93/117	-
4	CHL	4	606	-	-	7/17/93/117	-
5	CLA	4	612	3	-	8/15/91/115	-
4	CHL	4	609	3	-	9/17/93/117	-
4	CHL	1	606	-	-	9/17/93/117	-
4	CHL	4	601	3	-	6/15/91/117	-
5	CLA	2	613	1	-	7/15/91/115	-
4	CHL	3	609	2	1/1/14/21	14/35/111/117	-
5	CLA	4	602	3	-	4/15/91/115	-
5	CLA	4	603	3	-	6/15/91/115	-
4	CHL	1	601	1	-	7/17/93/117	-
5	CLA	4	610	3	-	8/15/91/115	-
7	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
6	LUT	4	620	-	-	5/29/67/67	0/2/2/2
7	XAT	4	622	-	-	3/31/93/93	0/4/4/4
8	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
7	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
9	LHG	1	2630	5	-	9/45/45/53	-
4	CHL	2	608	-	-	10/17/93/117	-
4	CHL	2	607	-	1/1/14/21	20/35/111/117	-
5	CLA	1	602	1	-	10/35/111/115	-
4	CHL	2	601	1	-	8/17/93/117	-
5	CLA	2	602	1	-	15/35/111/115	-
5	CLA	1	603	1	-	12/27/103/115	-
5	CLA	2	604	-	-	9/15/91/115	-
5	CLA	3	613	2	-	10/31/107/115	-
5	CLA	3	602	2	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	4	611	9	-	8/15/91/115	-
9	LHG	2	2630	5	-	14/41/41/53	-
8	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
4	CHL	3	607	-	-	12/26/102/117	-
7	XAT	2	1622	-	-	4/31/93/93	0/4/4/4
5	CLA	1	610	1	-	5/29/105/115	-
5	CLA	3	612	2	-	8/15/91/115	-
5	CLA	1	611	9	-	7/15/91/115	-
5	CLA	1	612	1	-	6/15/91/115	-
5	CLA	2	610	1	-	5/21/97/115	-
4	CHL	4	608	-	-	8/17/93/117	-
6	LUT	2	1621	-	-	1/29/67/67	0/2/2/2
5	CLA	3	604	-	-	11/15/91/115	-
4	CHL	3	601	2	1/1/14/21	15/39/115/117	-
5	CLA	2	611	9	-	5/15/91/115	-
10	BCR	4	623	-	-	12/29/63/63	0/2/2/2
4	CHL	1	607	-	1/1/14/21	19/38/114/117	-
4	CHL	3	608	-	-	8/17/93/117	-
9	LHG	3	2630	5	-	25/51/51/53	-
4	CHL	3	606	-	-	5/17/93/117	-
5	CLA	3	614	2	-	5/19/95/115	-
5	CLA	1	604	-	-	12/21/97/115	-
5	CLA	1	614	1	-	6/15/91/115	-
9	LHG	4	2630	5	-	8/23/23/53	-
5	CLA	3	603	2	-	11/27/103/115	-
5	CLA	3	610	2	-	6/33/109/115	-
6	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
4	CHL	1	608	-	-	3/17/93/117	-
4	CHL	2	606	-	-	5/17/93/117	-
5	CLA	2	612	1	-	8/15/91/115	-
5	CLA	3	611	9	-	12/27/103/115	-
4	CHL	1	605	1	-	10/17/93/117	-
6	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
6	LUT	1	1621	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	2	603	1	-	15/27/103/115	-
4	CHL	1	609	1	1/1/14/21	13/37/113/117	-
5	CLA	2	614	1	-	8/15/91/115	-

The worst 5 of 761 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	606	CHL	C3D-C4D	-5.65	1.31	1.44
4	3	601	CHL	C3D-C4D	-5.64	1.31	1.44
4	1	601	CHL	C3D-C4D	-5.61	1.31	1.44
4	1	608	CHL	C3D-C4D	-5.58	1.31	1.44
4	1	609	CHL	C3D-C4D	-5.53	1.31	1.44

The worst 5 of 1060 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1	1622	XAT	O24-C25-C24	10.49	121.26	113.38
4	1	607	CHL	C2B-C1B-NB	10.36	117.17	110.23
4	2	601	CHL	CMD-C2D-C1D	9.95	142.25	124.71
4	1	601	CHL	CMD-C2D-C1D	9.90	142.16	124.71
7	2	1622	XAT	O4-C5-C4	9.86	120.79	113.38

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	1	607	CHL	C8
4	1	609	CHL	C8
4	2	607	CHL	C8
4	2	609	CHL	C8
4	3	601	CHL	C8

5 of 613 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1	605	CHL	C1C-C2C-CMC-OMC
4	1	605	CHL	C3C-C2C-CMC-OMC
4	1	606	CHL	C2B-C3B-CAB-CBB
4	1	606	CHL	C4B-C3B-CAB-CBB
4	1	606	CHL	C3C-C2C-CMC-OMC

There are no ring outliers.

58 monomers are involved in 119 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	2	609	CHL	4	0
4	2	605	CHL	1	0
4	4	607	CHL	1	0
6	3	1621	LUT	3	0
8	1	1623	NEX	2	0
5	1	613	CLA	1	0
6	3	1620	LUT	7	0
4	3	605	CHL	1	0
4	4	606	CHL	1	0
5	4	612	CLA	2	0
4	1	606	CHL	2	0
4	4	601	CHL	1	0
5	2	613	CLA	2	0
4	3	609	CHL	4	0
5	4	603	CLA	1	0
5	4	610	CLA	1	0
7	3	1622	XAT	5	0
6	4	620	LUT	4	0
7	4	622	XAT	4	0
8	2	1623	NEX	1	0
7	1	1622	XAT	4	0
4	2	608	CHL	2	0
4	2	607	CHL	2	0
5	1	602	CLA	4	0
5	2	602	CLA	3	0
5	1	603	CLA	2	0
5	2	604	CLA	1	0
5	3	613	CLA	3	0
5	3	602	CLA	4	0
5	4	611	CLA	1	0
9	2	2630	LHG	2	0
8	3	1623	NEX	3	0
4	3	607	CHL	6	0
7	2	1622	XAT	6	0
5	1	610	CLA	2	0
5	1	612	CLA	2	0
5	2	610	CLA	3	0
4	4	608	CHL	1	0
6	2	1621	LUT	4	0
4	3	601	CHL	2	0
10	4	623	BCR	3	0
4	1	607	CHL	4	0

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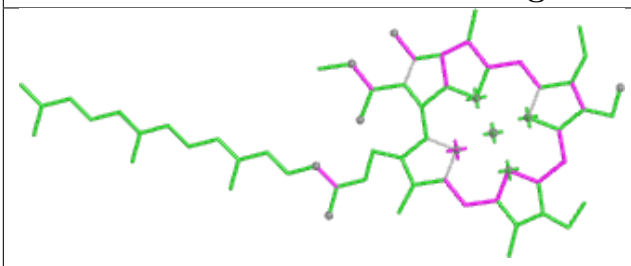
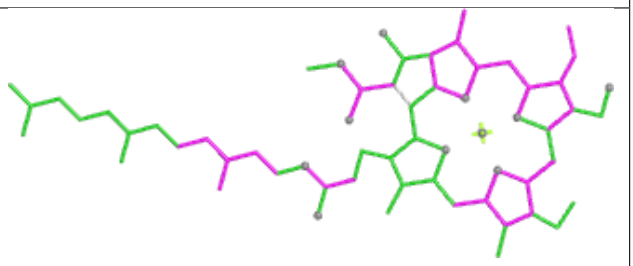
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	608	CHL	3	0
9	3	2630	LHG	3	0
4	3	606	CHL	4	0
5	1	604	CLA	1	0
9	4	2630	LHG	1	0
5	3	603	CLA	1	0
5	3	610	CLA	2	0
6	1	1620	LUT	5	0
4	1	608	CHL	1	0
4	2	606	CHL	3	0
5	2	612	CLA	2	0
5	3	611	CLA	2	0
6	2	1620	LUT	4	0
6	1	1621	LUT	4	0
5	2	603	CLA	2	0
4	1	609	CHL	5	0

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.

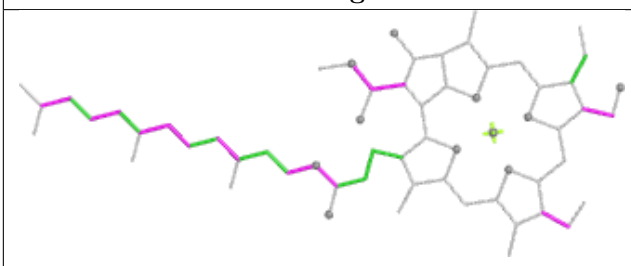
Ligand CHL 2 609



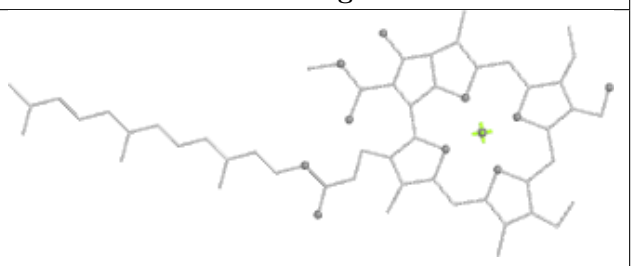
Bond lengths



Bond angles



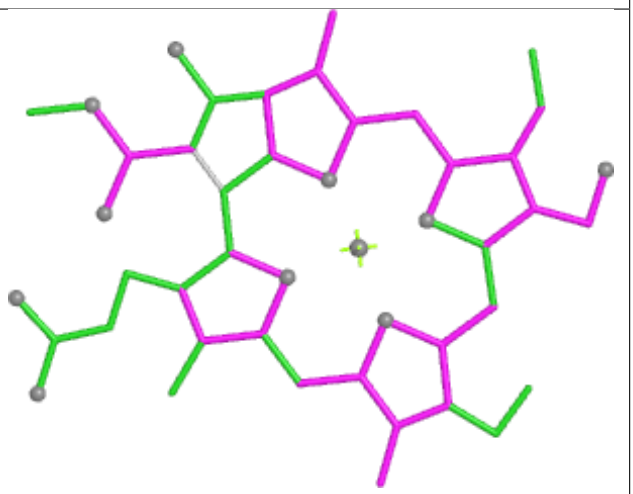
Torsions



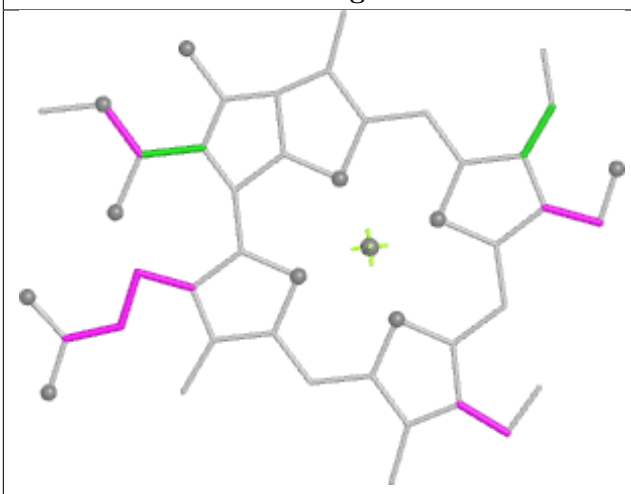
Rings

Ligand CHL 2 605

Bond lengths



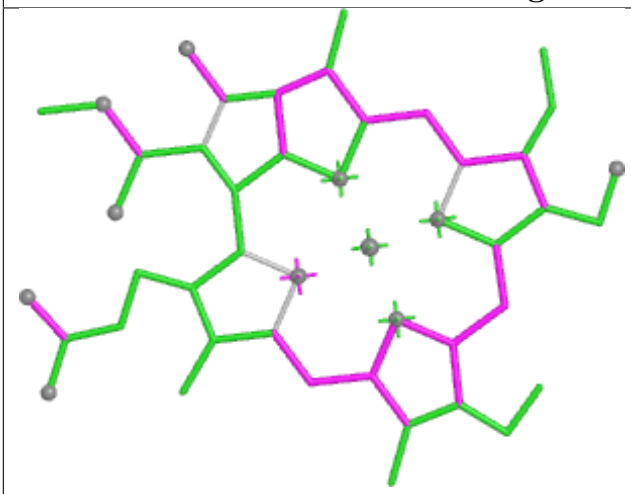
Bond angles



Torsions

Rings

Ligand CHL 4 607



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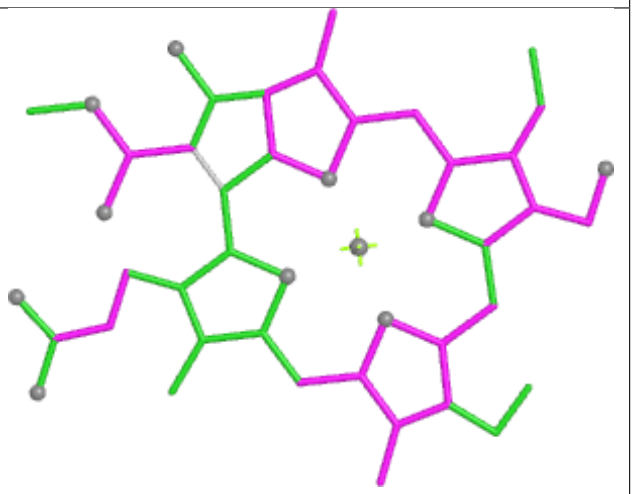

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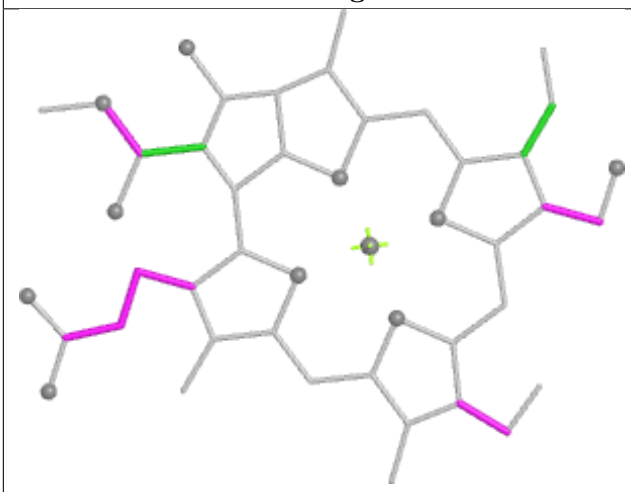

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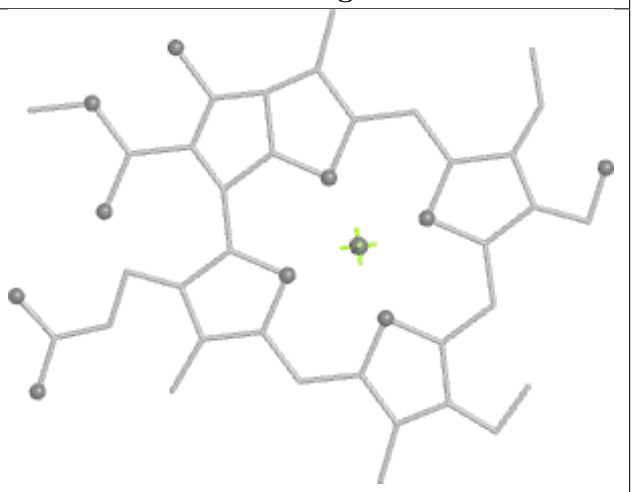
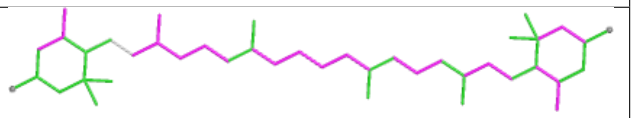


Rings

Ligand LUT 3 1621

Bond lengths



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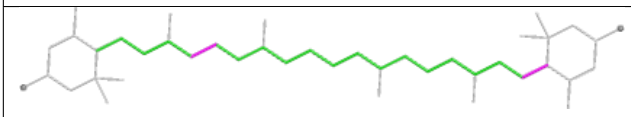

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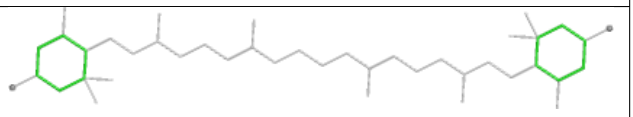
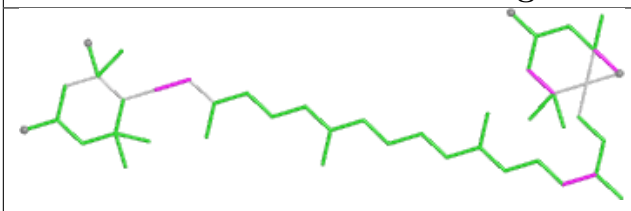


Rings

Ligand NEX 1 1623



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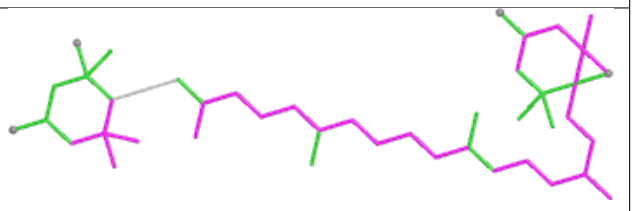
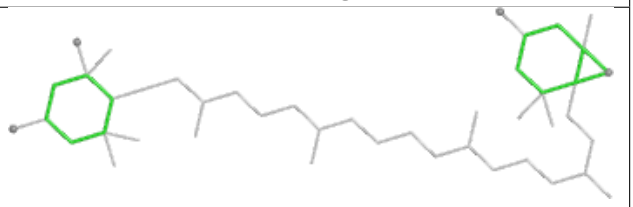


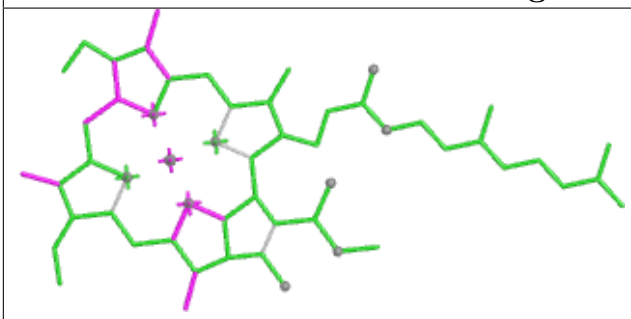
Bond angles

Torsions



Rings

Ligand CLA 1 613



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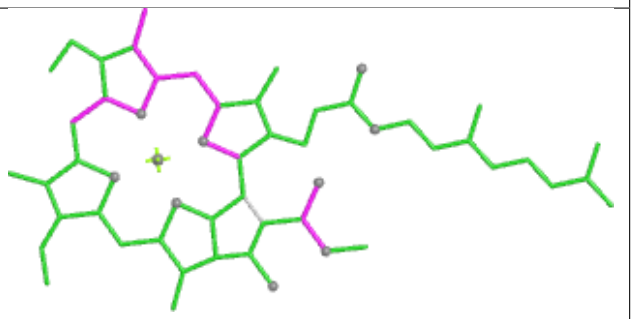
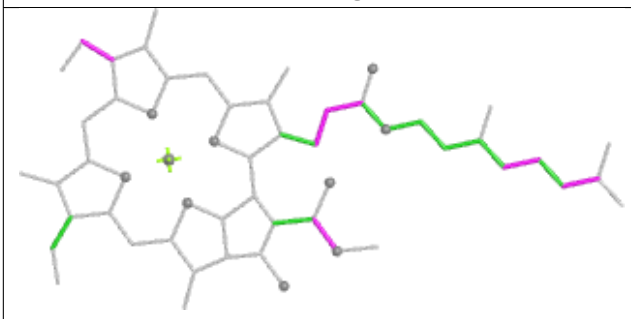


Bond angles



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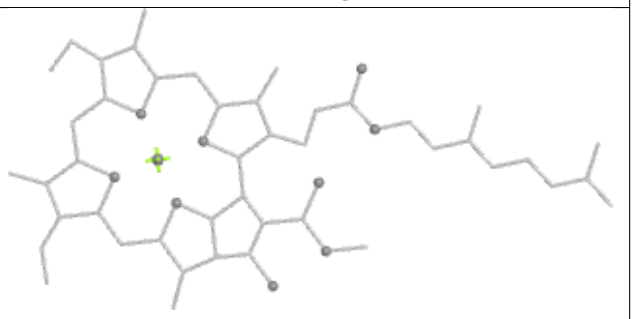
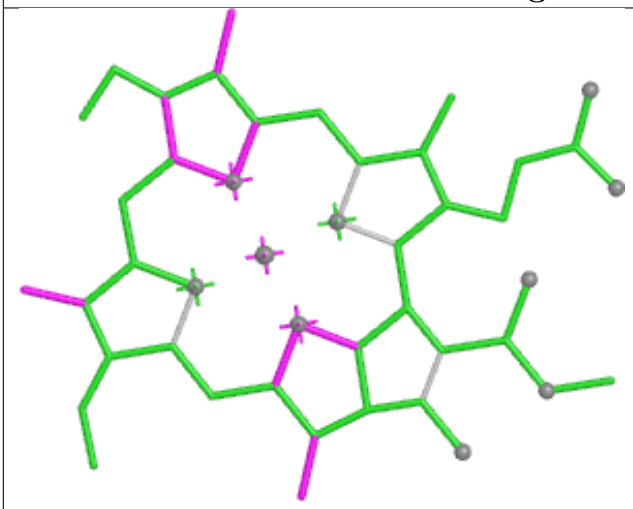


Rings

Ligand CLA 4 604



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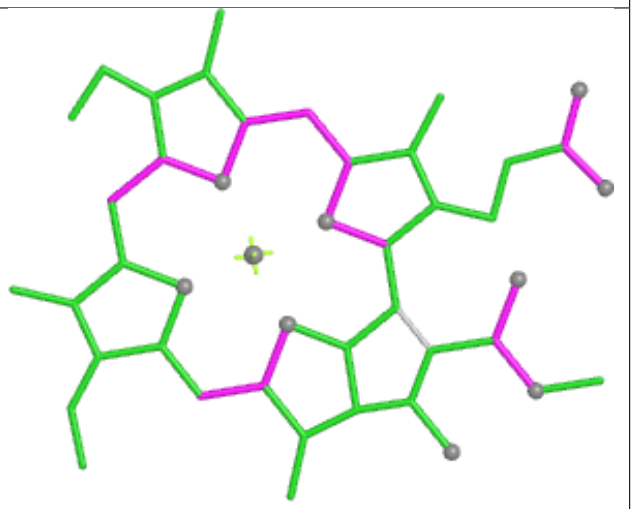
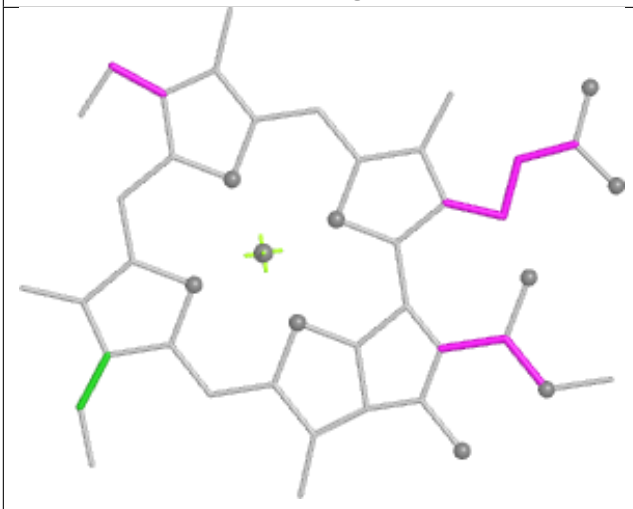


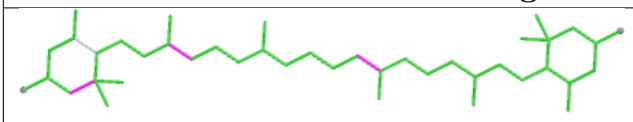
Bond angles



Torsions

Rings

Ligand LUT 3 1620



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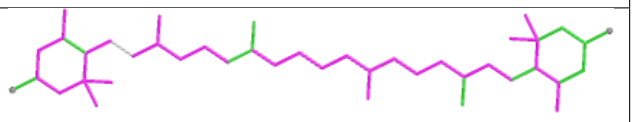
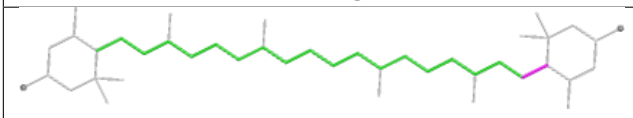
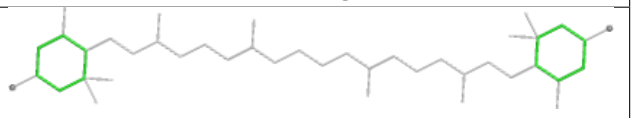


Bond angles

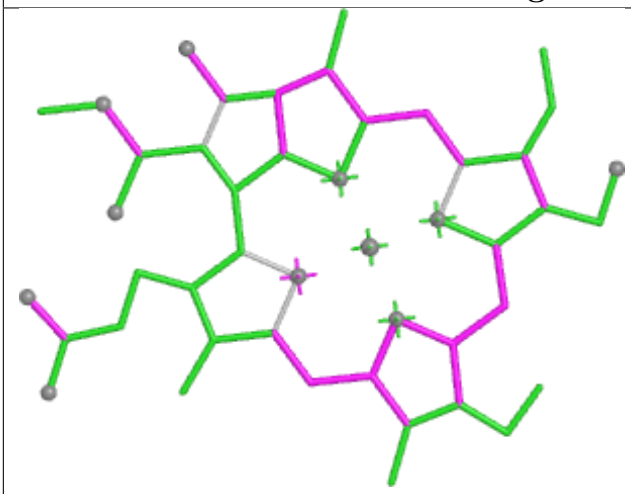


Torsions



Rings

Ligand CHL 3 605



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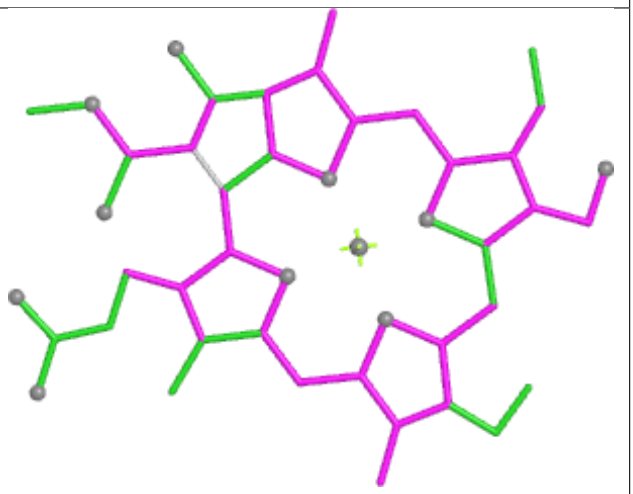

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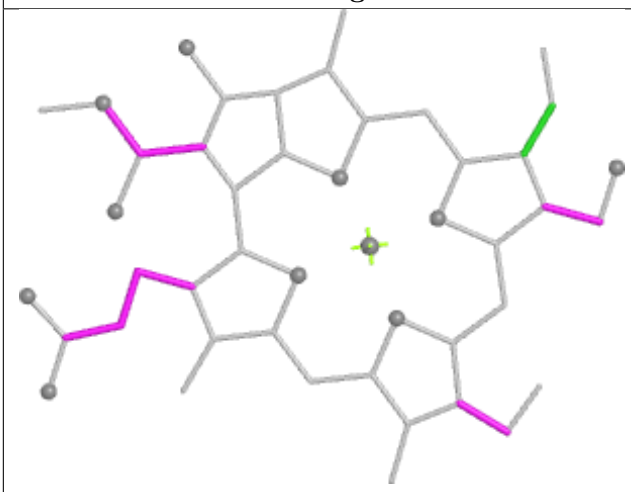

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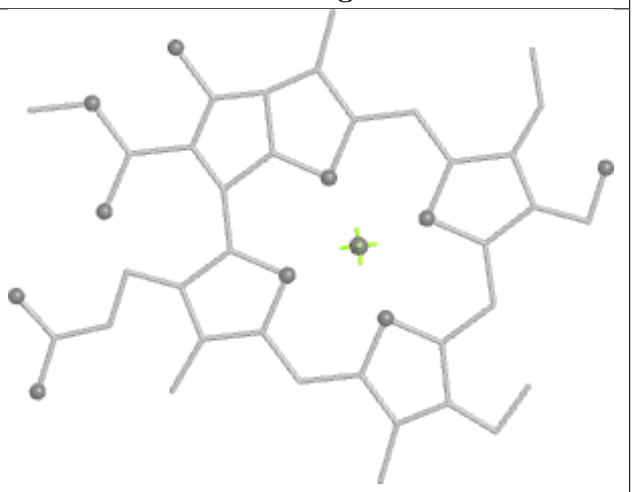
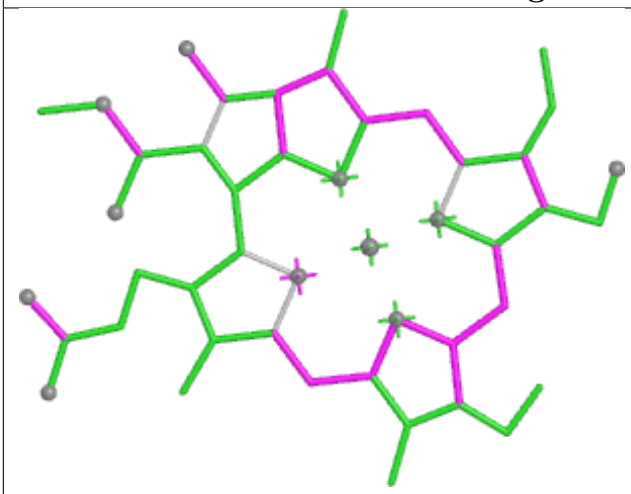


Rings

Ligand CHL 4 606



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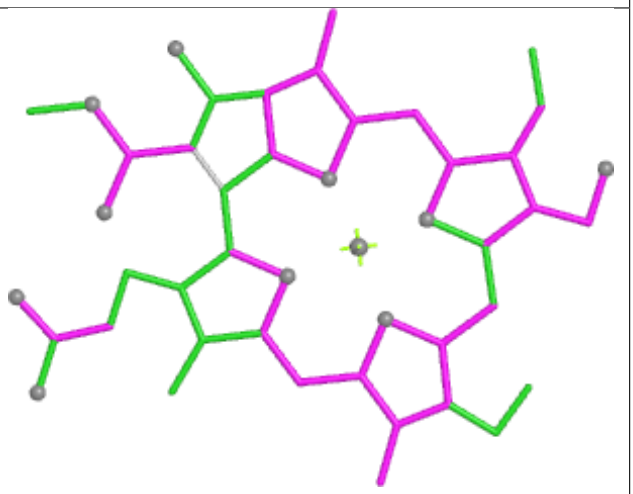
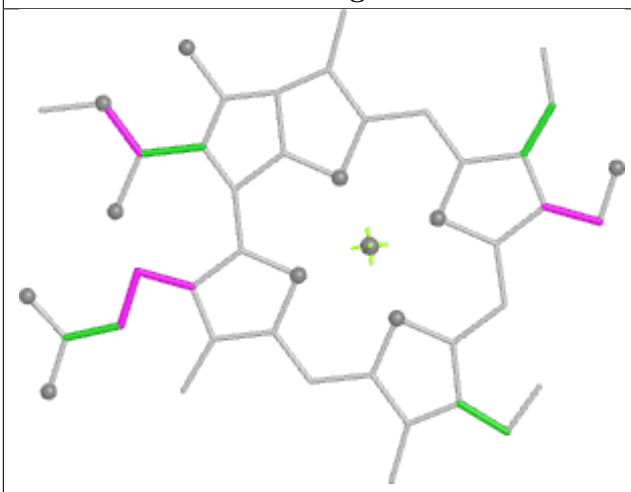


Bond angles



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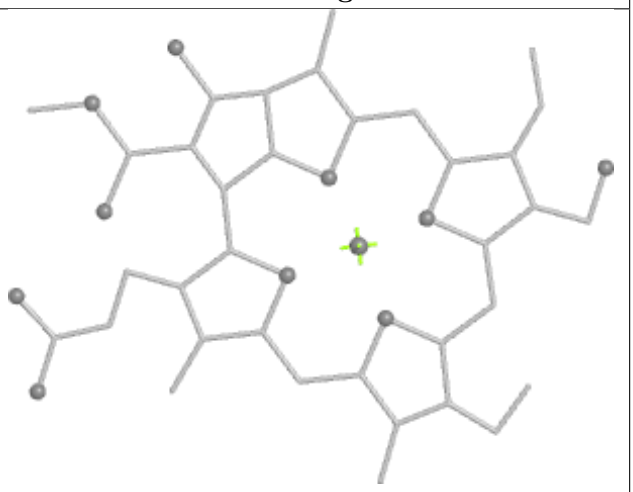
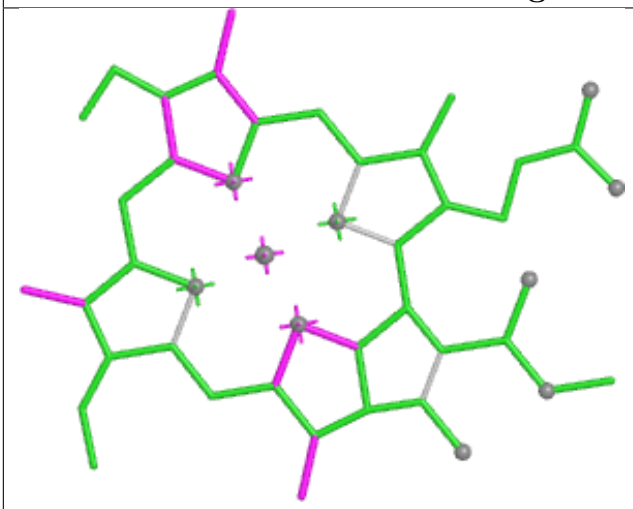


Rings

Ligand CLA 4 612



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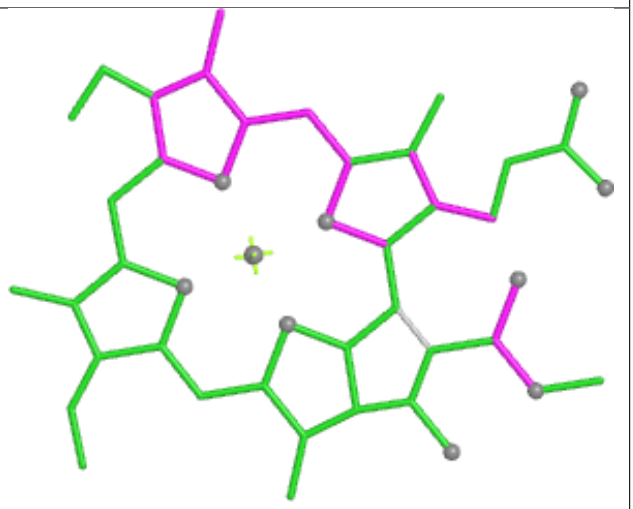
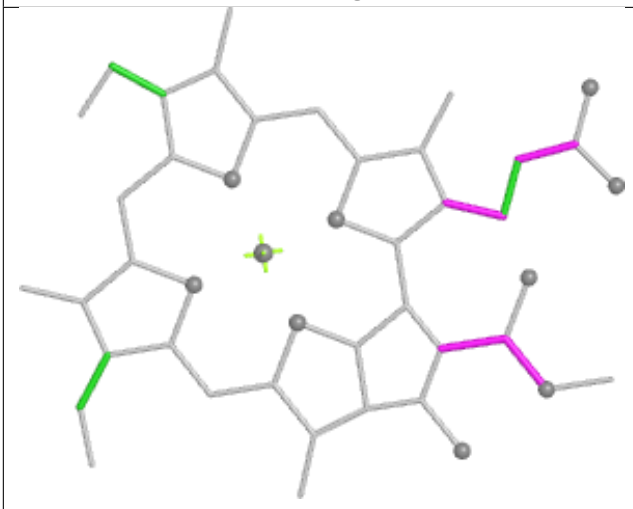


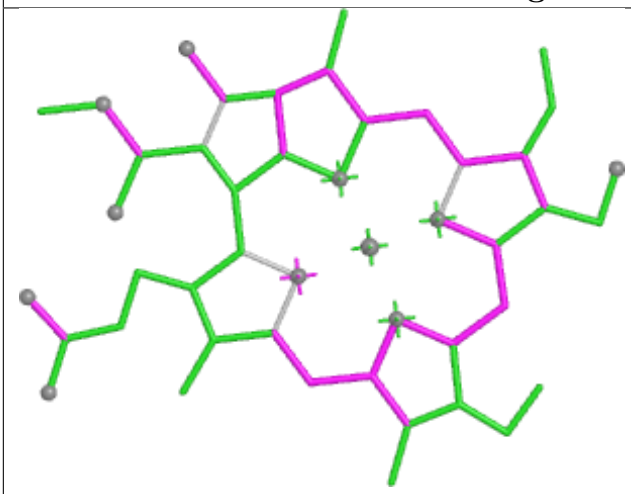
Bond angles



Torsions

Rings

Ligand CHL 4 609



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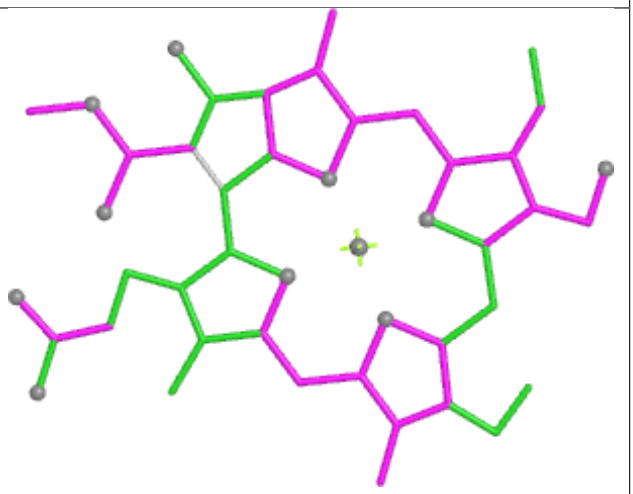
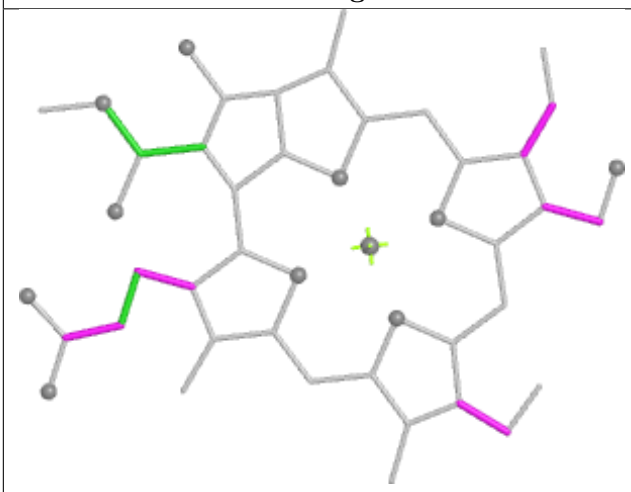


Bond angles



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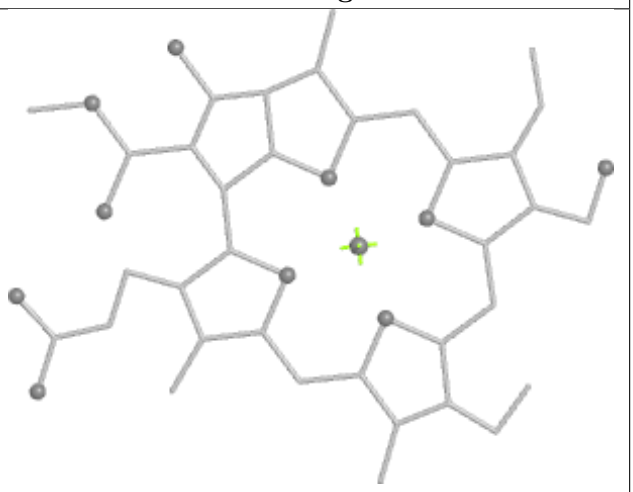
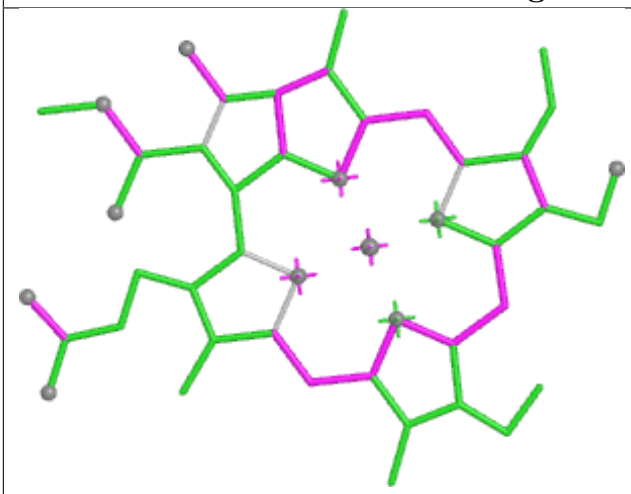


Rings

Ligand CHL 1 606



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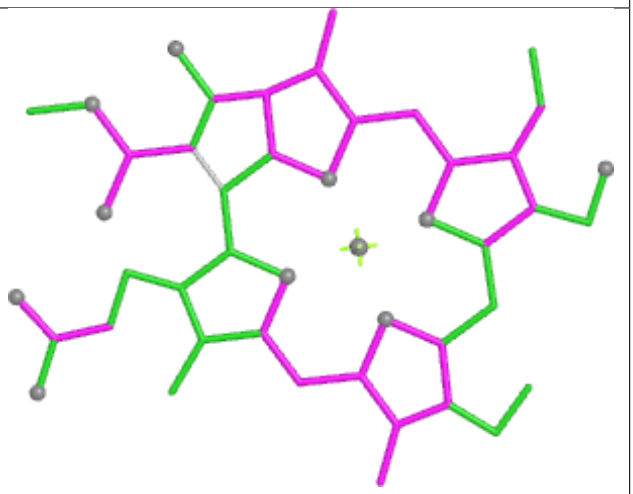

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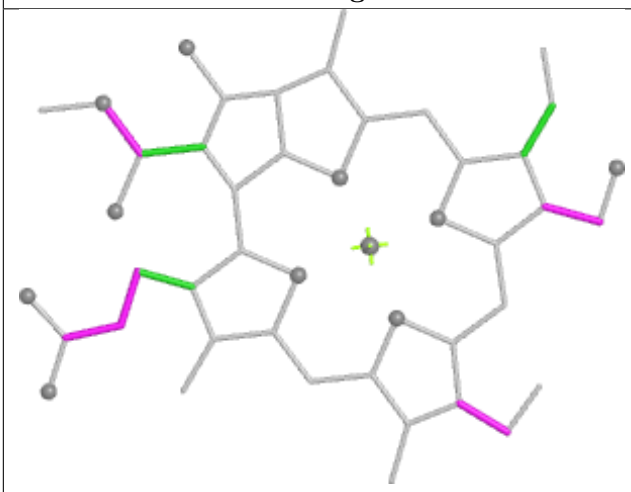

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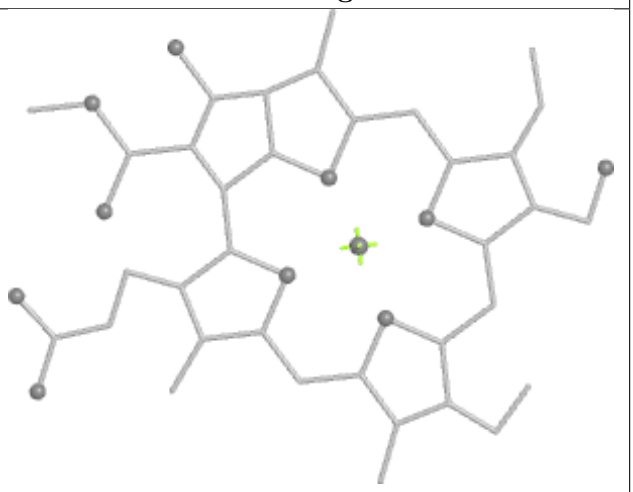
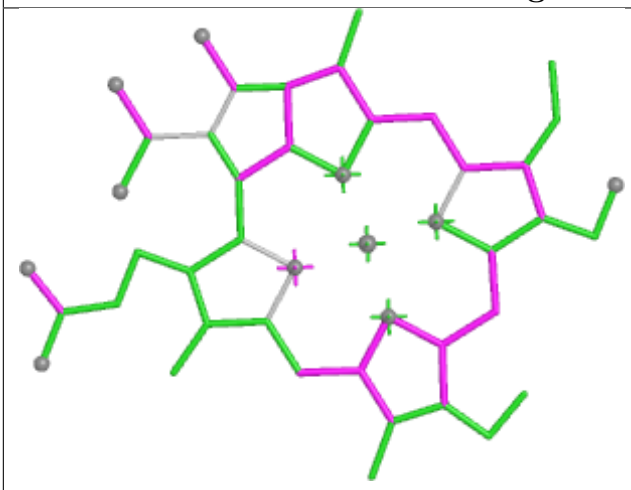


Rings

Ligand CHL 4 601



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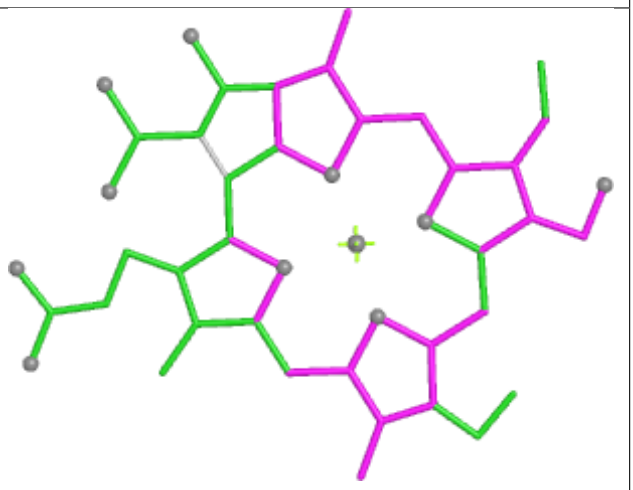
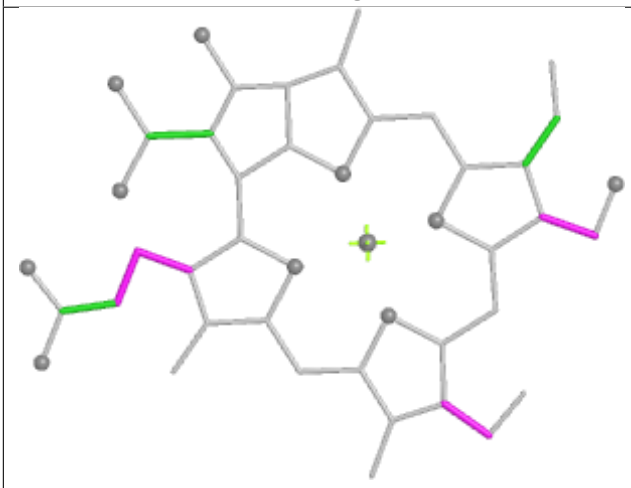


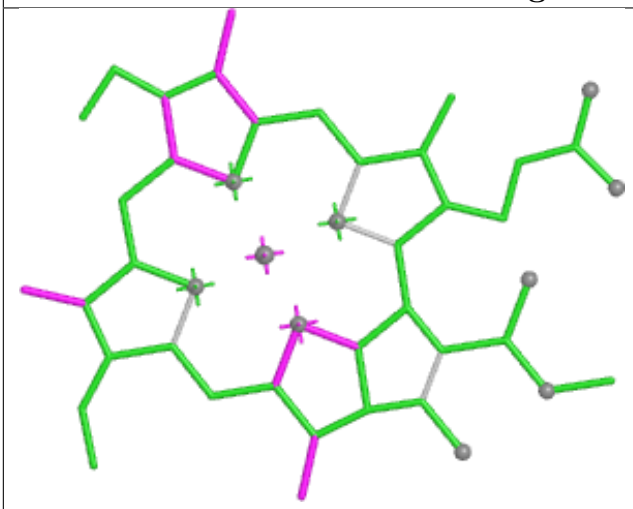
Bond angles



Torsions

Rings

Ligand CLA 2 613



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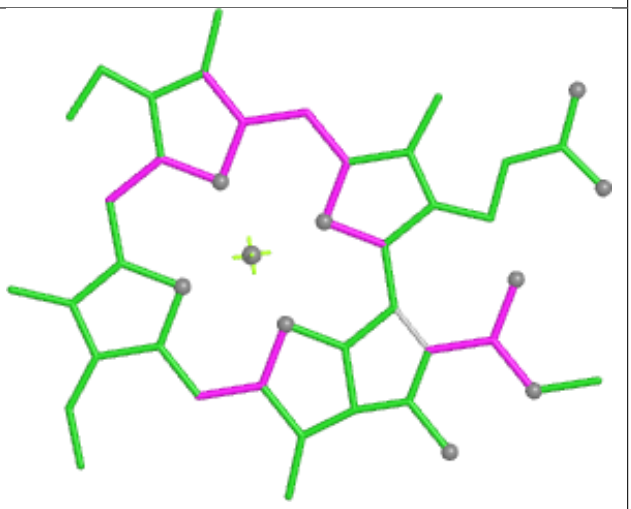
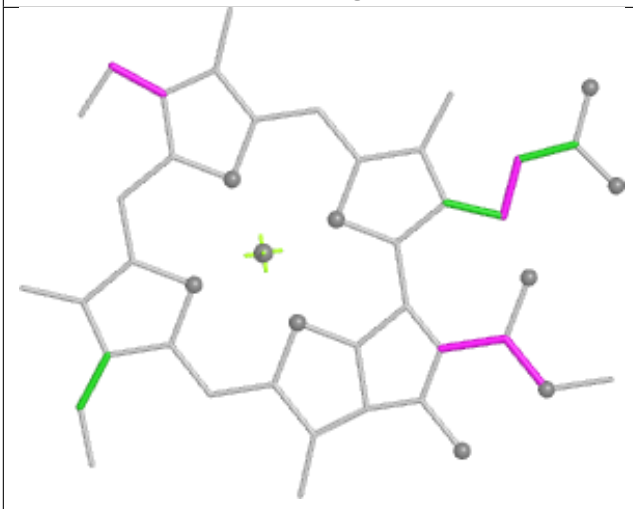


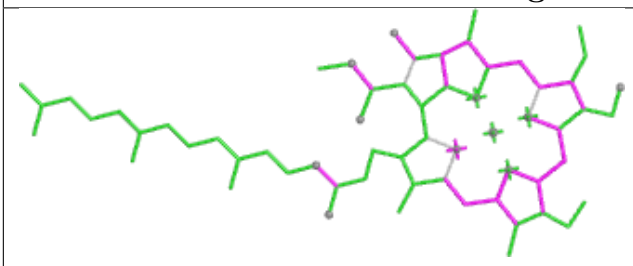
Bond angles



Torsions

Rings

Ligand CHL 3 609



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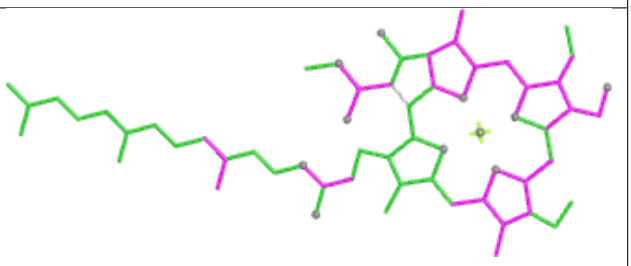
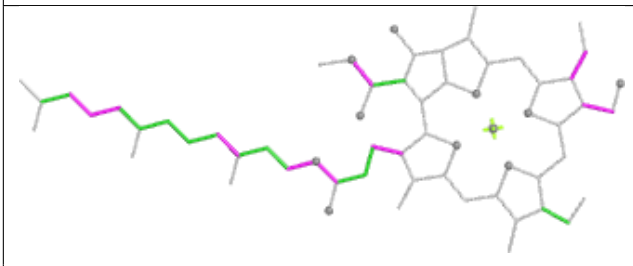


Bond angles



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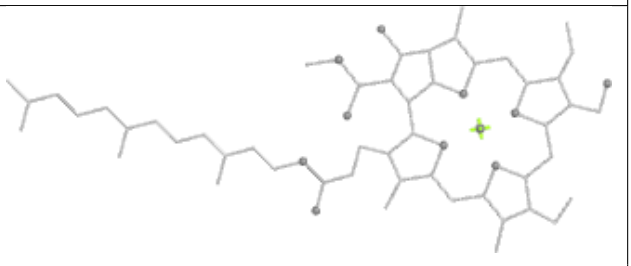
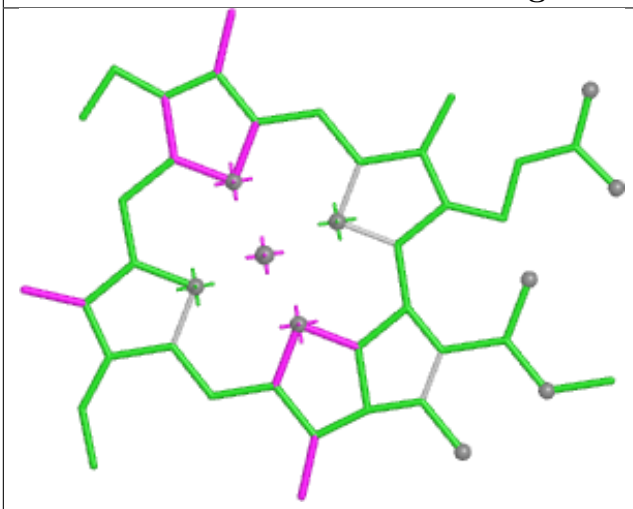


Rings

Ligand CLA 4 602



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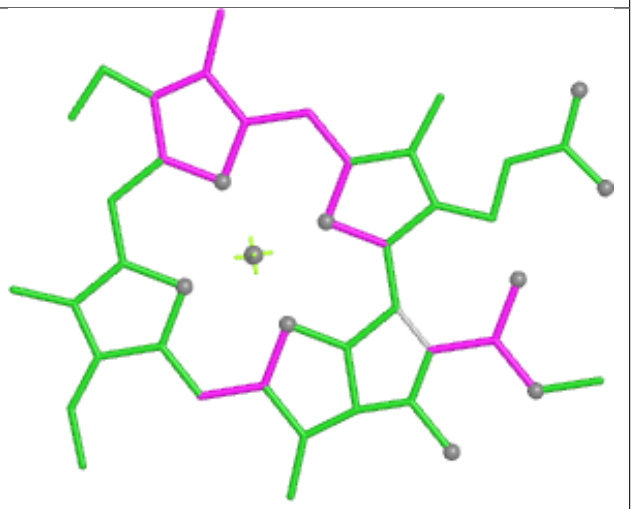
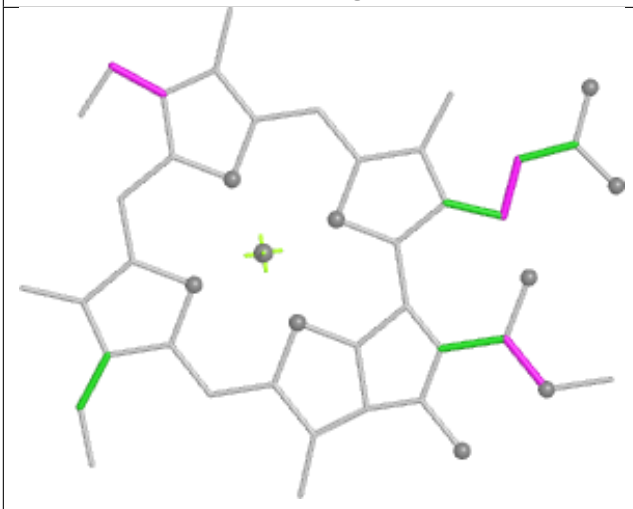


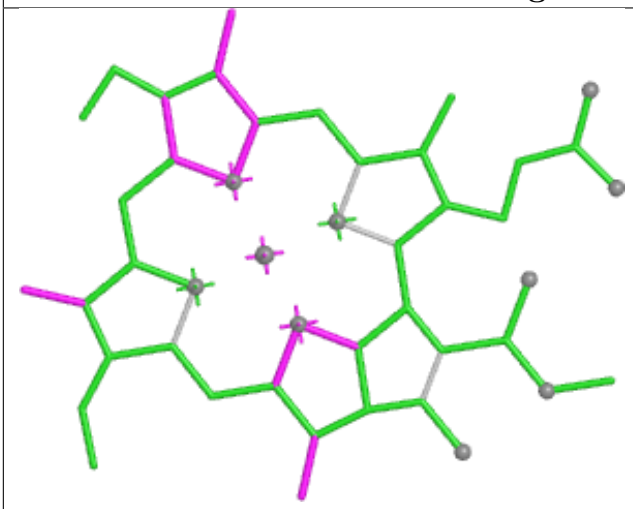
Bond angles



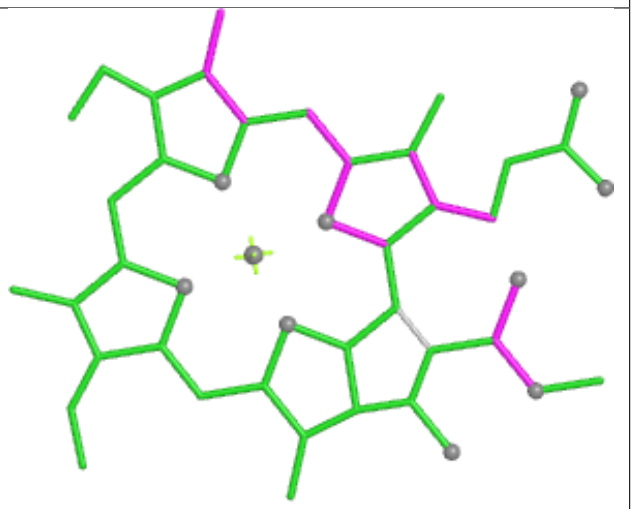
Torsions

Rings

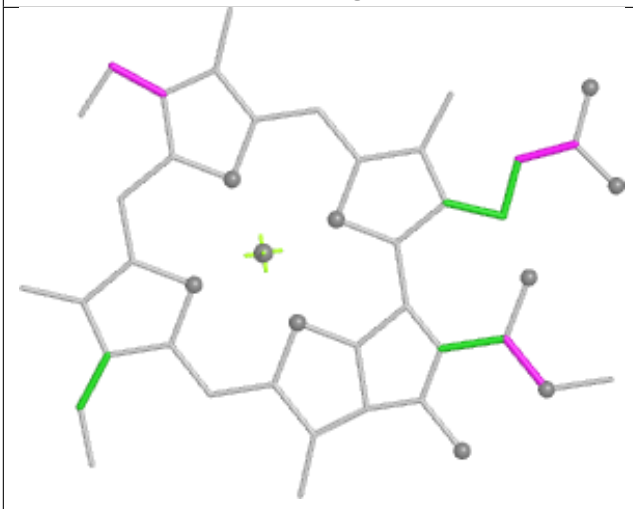
Ligand CLA 4 603



Bond lengths



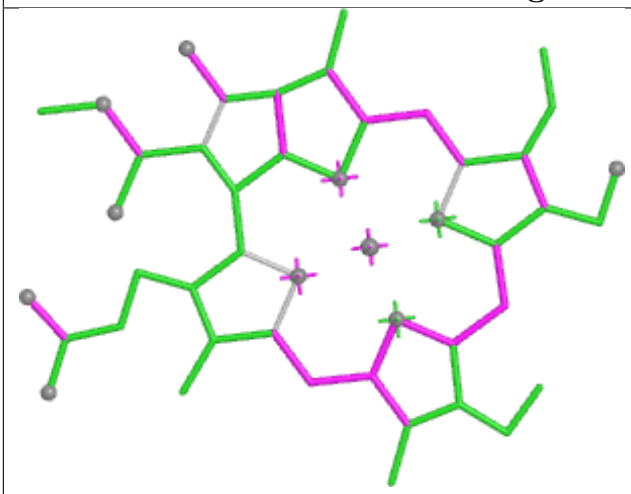
Bond angles



Torsions

Rings

Ligand CHL 1 601



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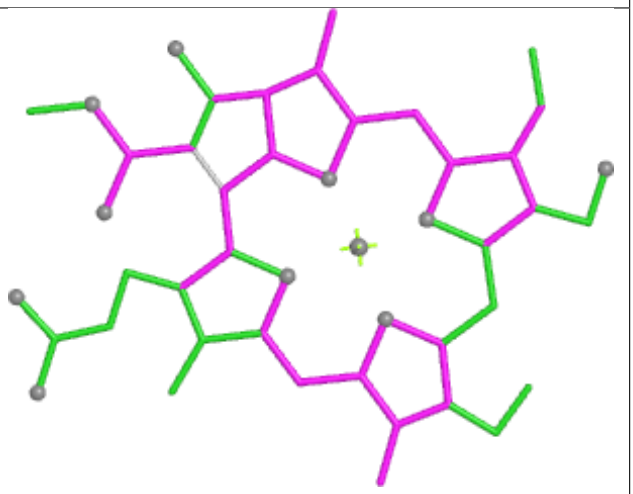

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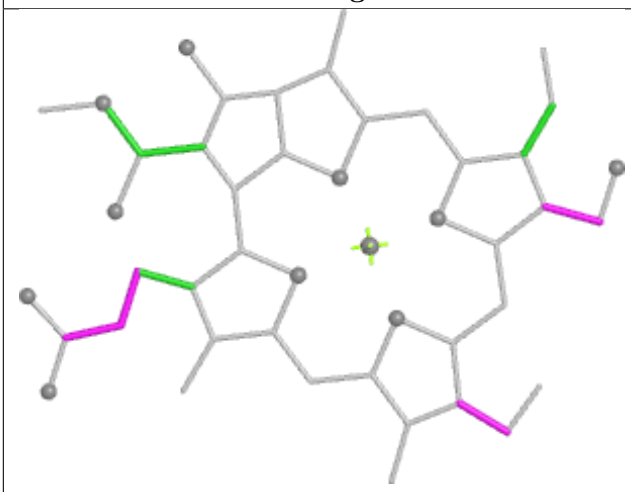

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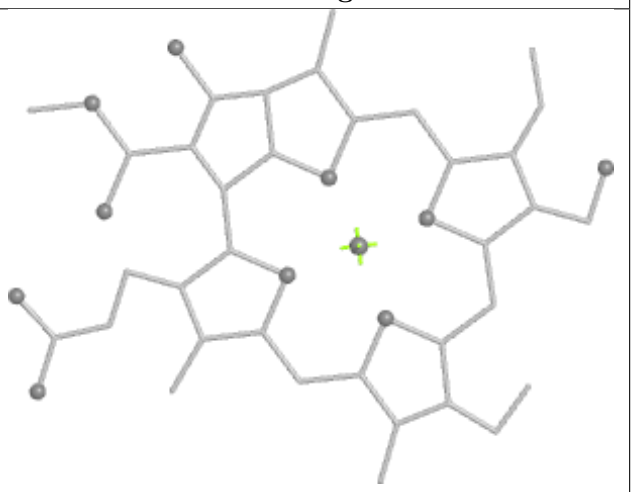
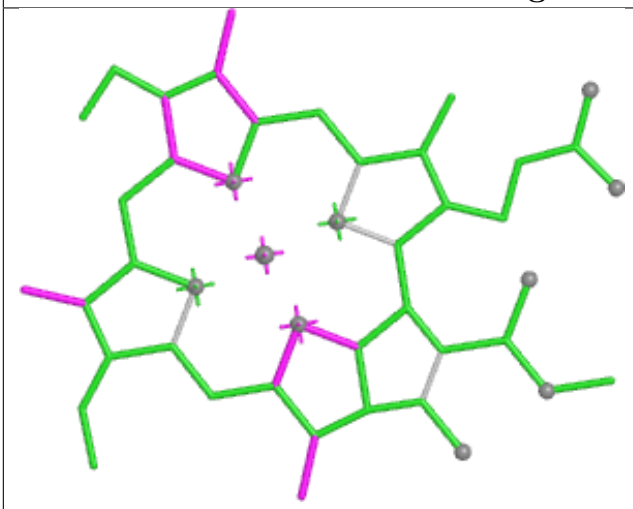


Rings

Ligand CLA 4 610



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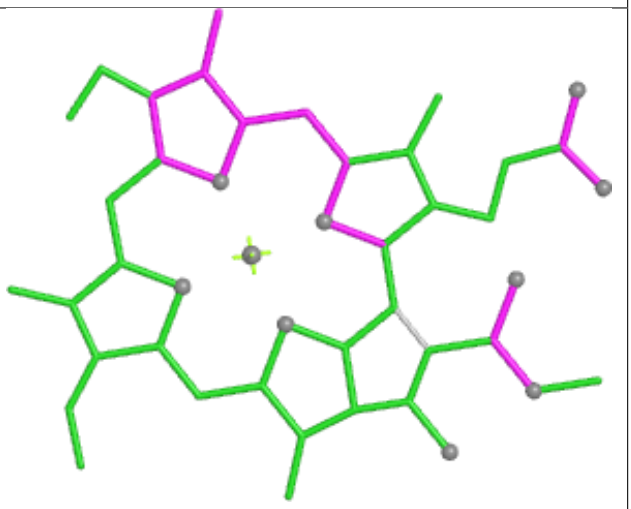

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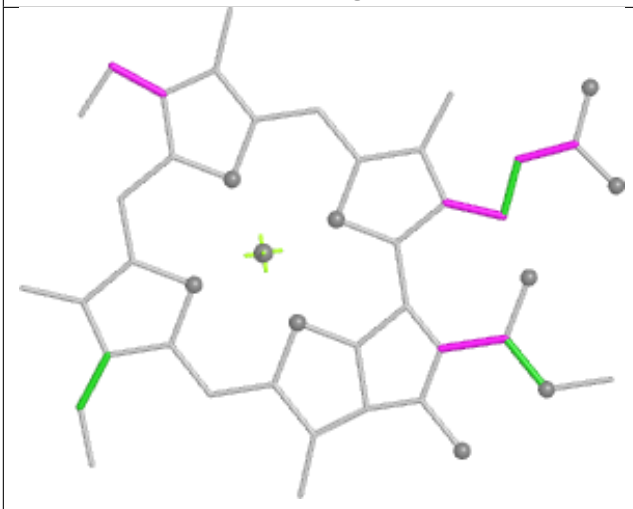
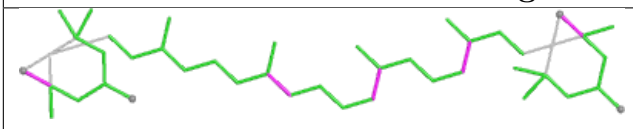


Torsions

Rings

Ligand XAT 3 1622



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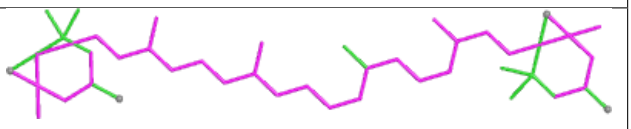

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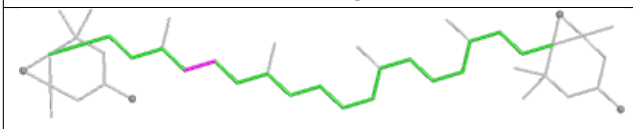

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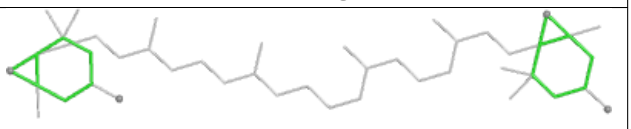
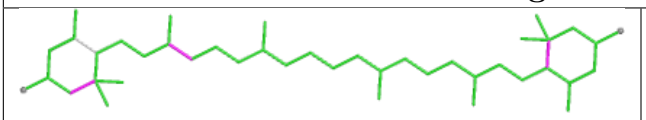


Rings

Ligand LUT 4 620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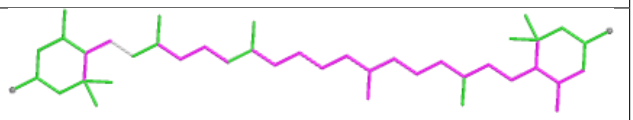
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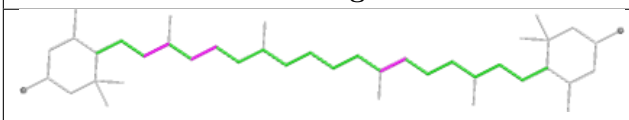
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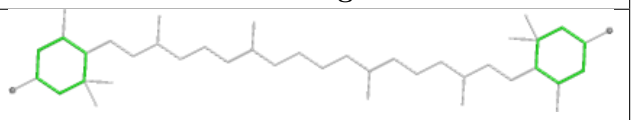
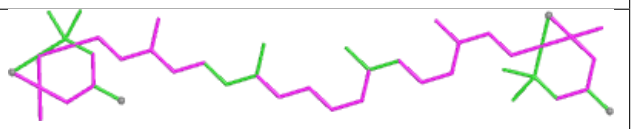

Rings

Ligand XAT 4 622

Bond lengths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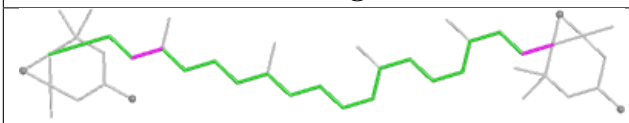
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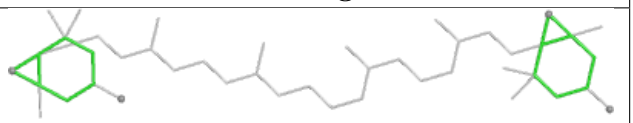
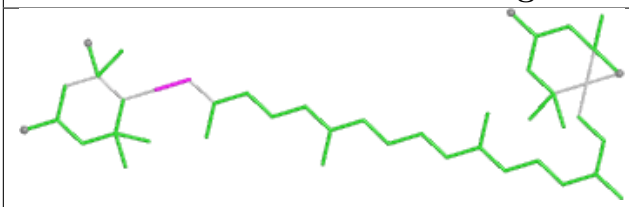

Rings

Ligand NEX 2 1623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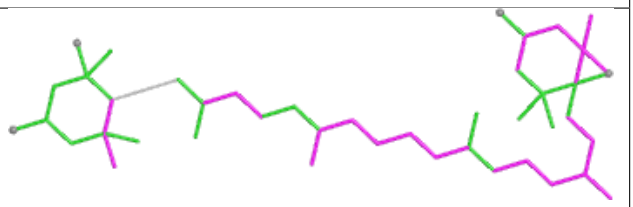
Bond angles

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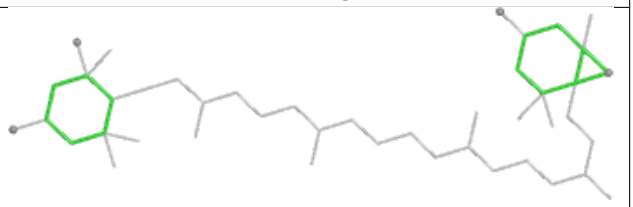
Rings

Ligand XAT 1 1622

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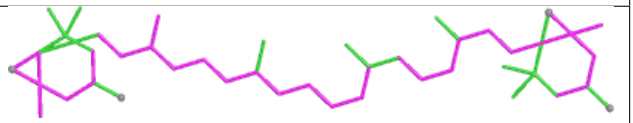
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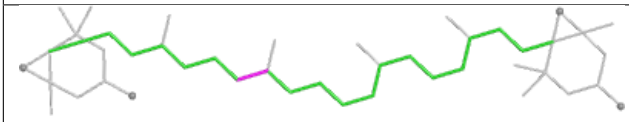
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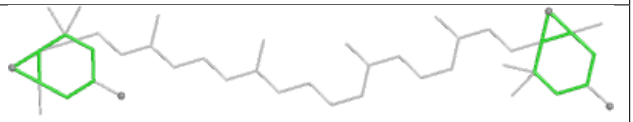
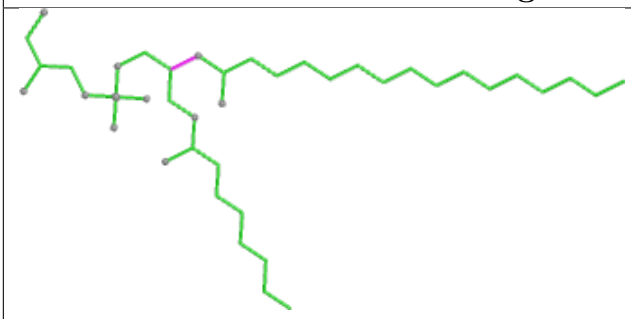

Rings

Ligand LHG 1 2630



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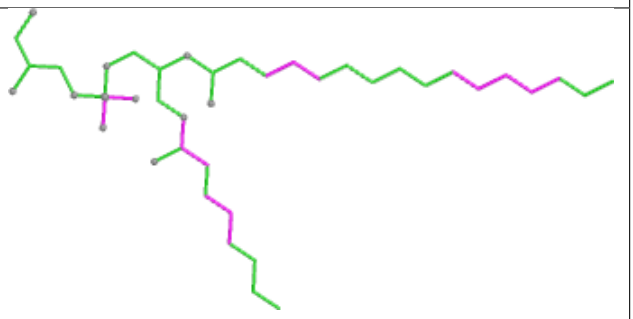

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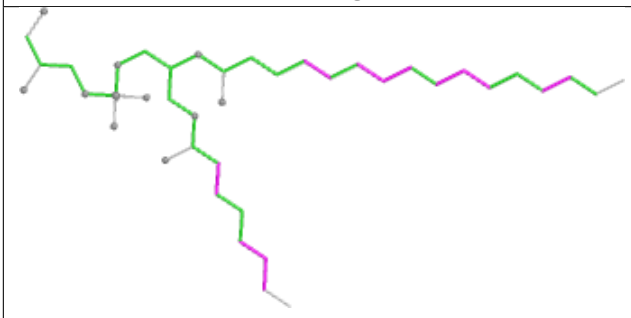

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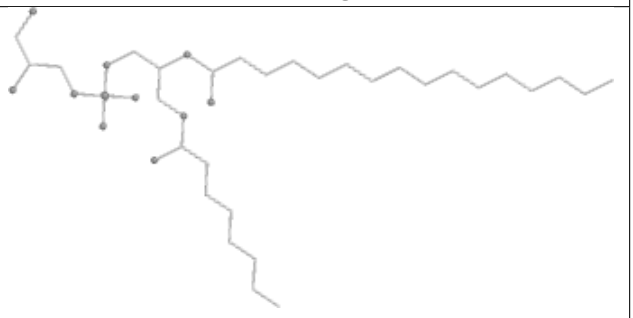
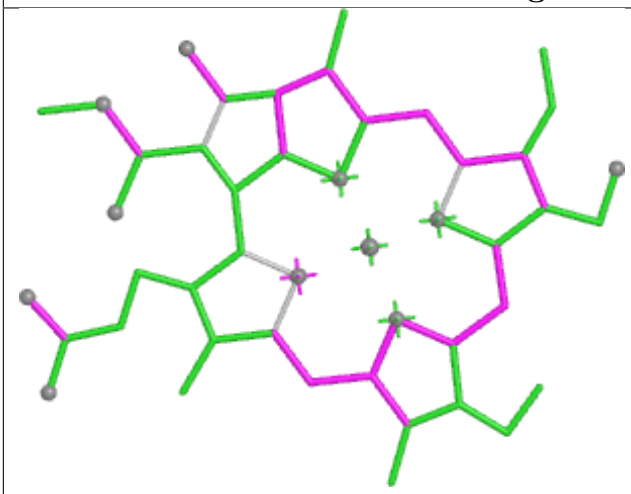


Rings

Ligand CHL 2 608



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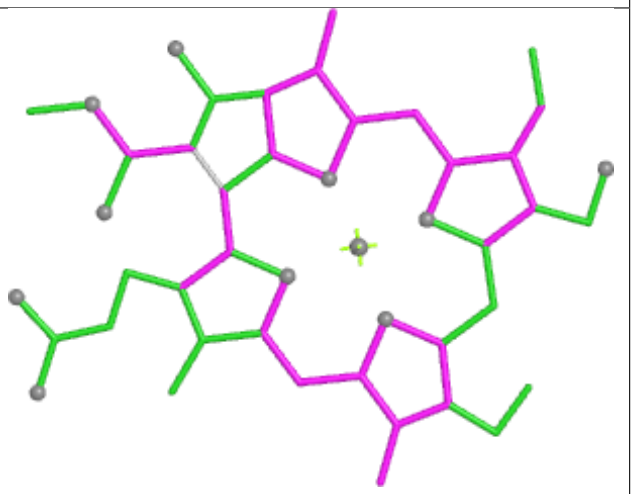

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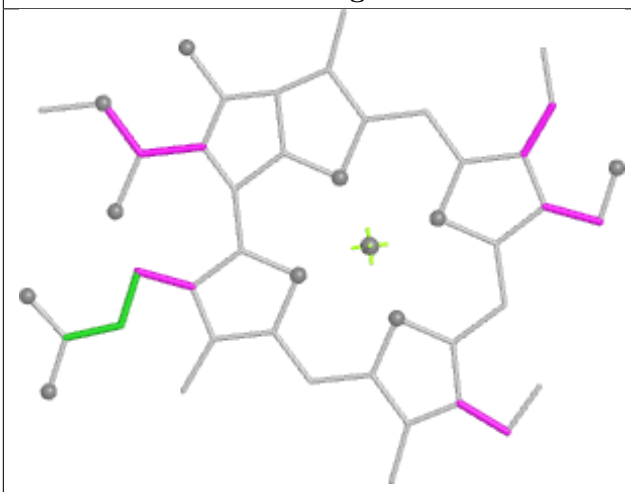

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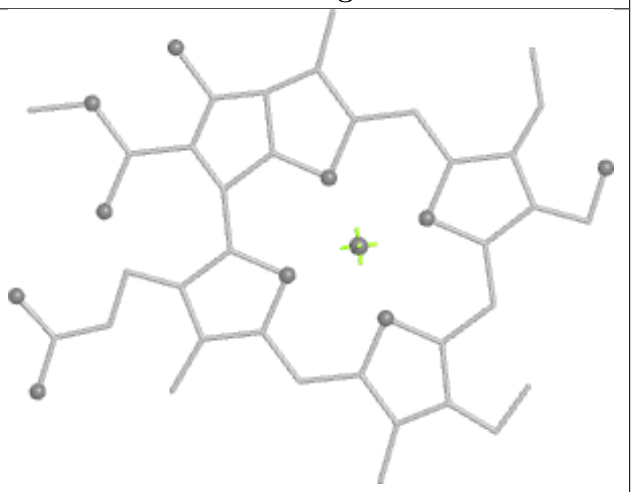

Rings

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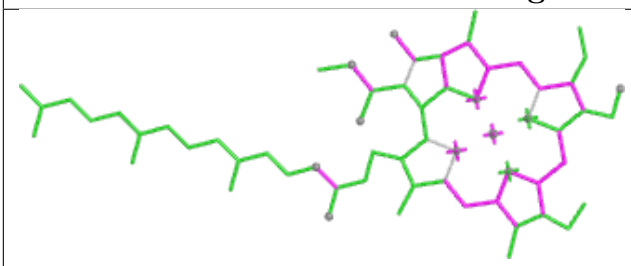

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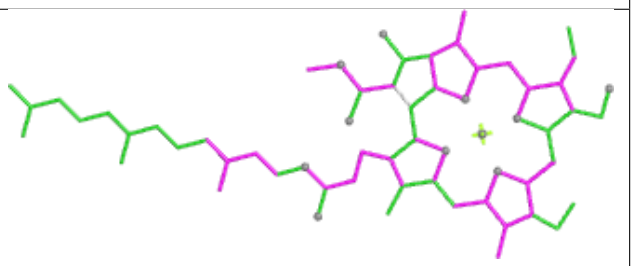

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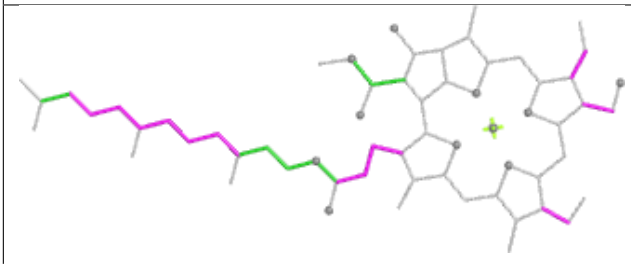

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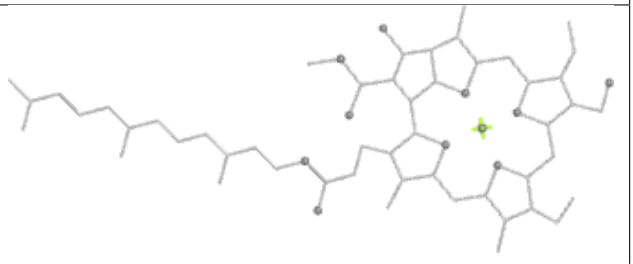
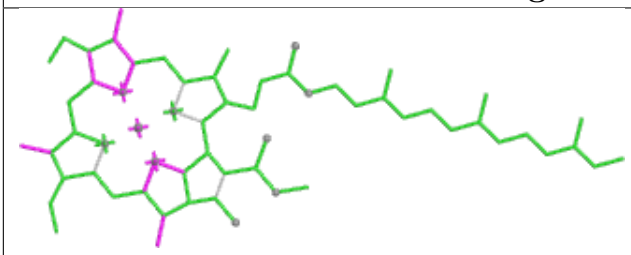


Rings

Ligand CLA 1 602



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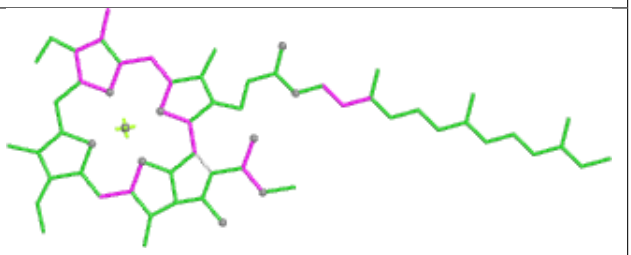
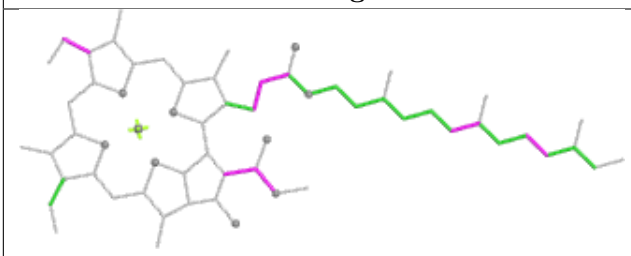


Bond angles



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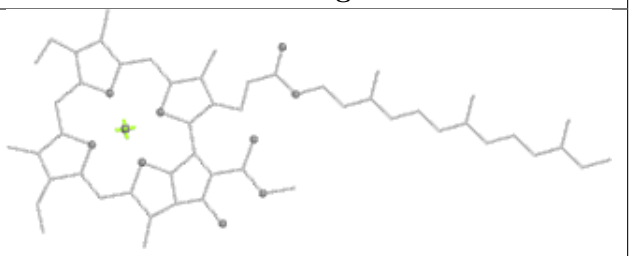
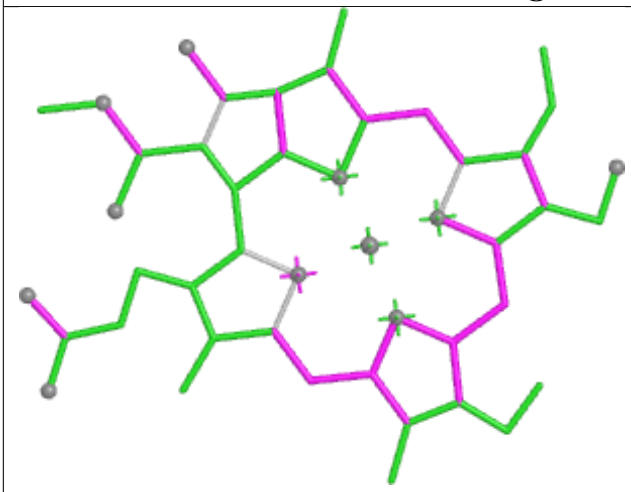


Rings

Ligand CHL 2 601



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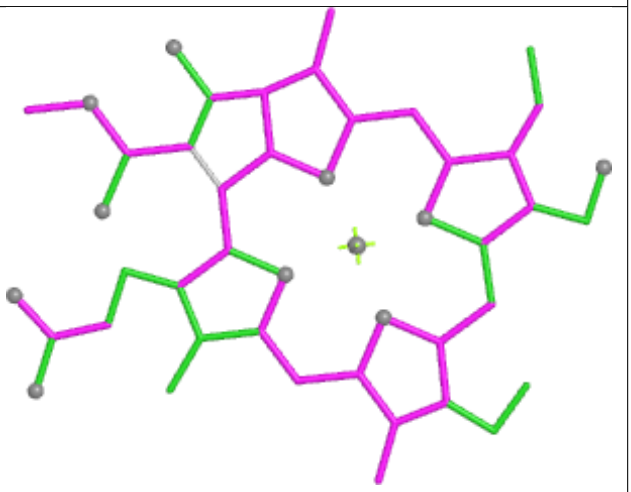
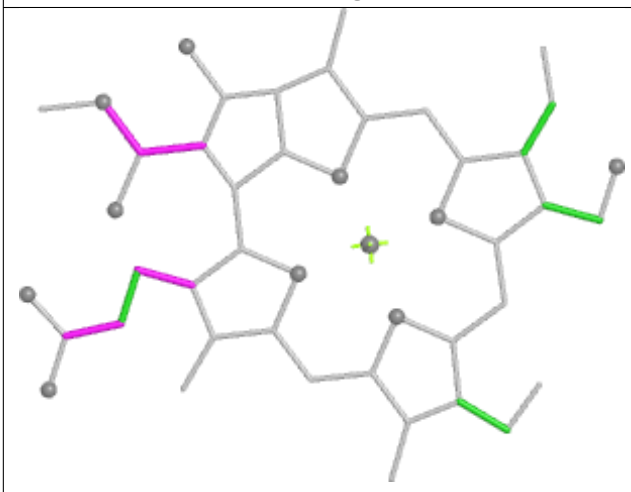


Bond angles



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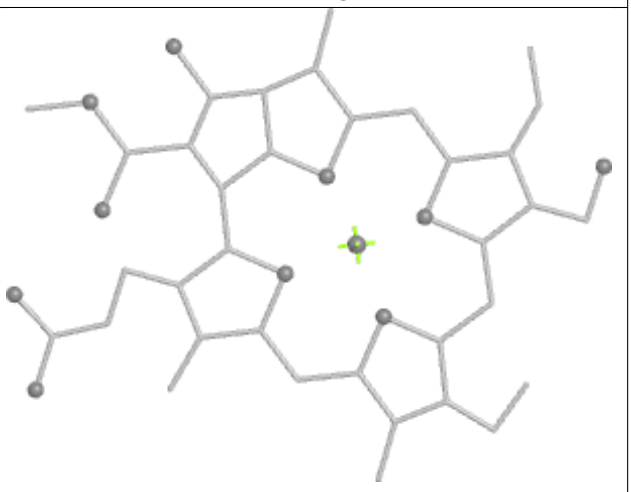

Rings

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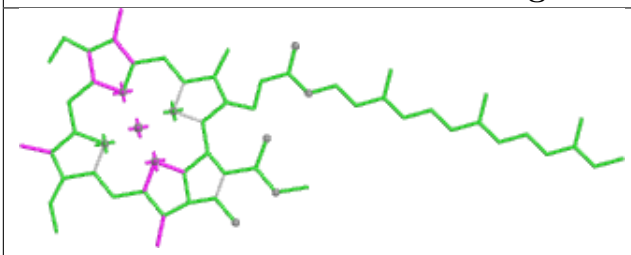
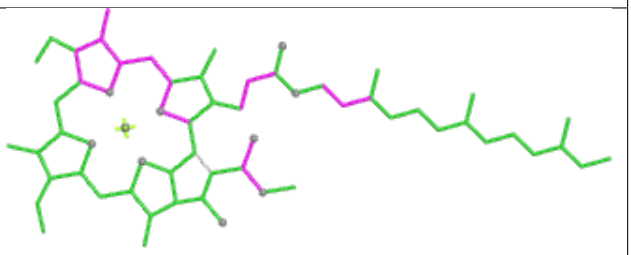
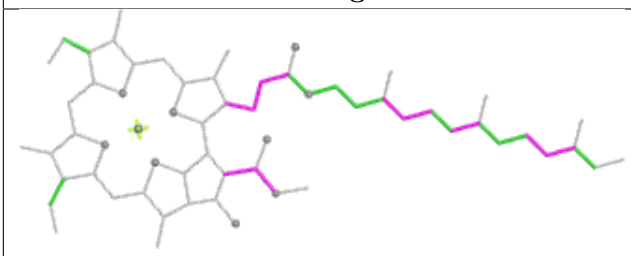
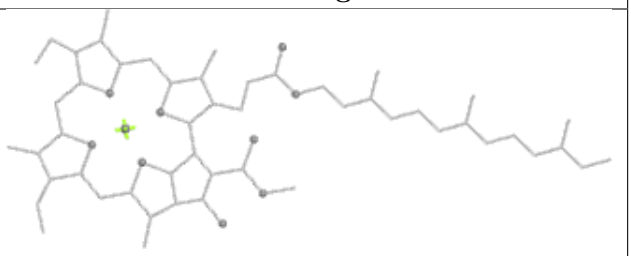
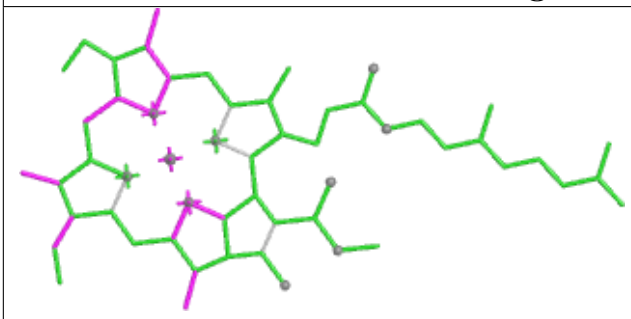
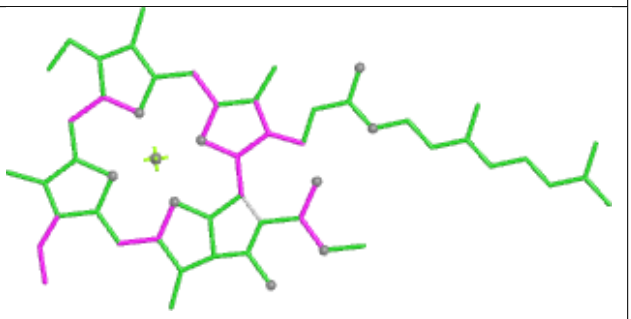
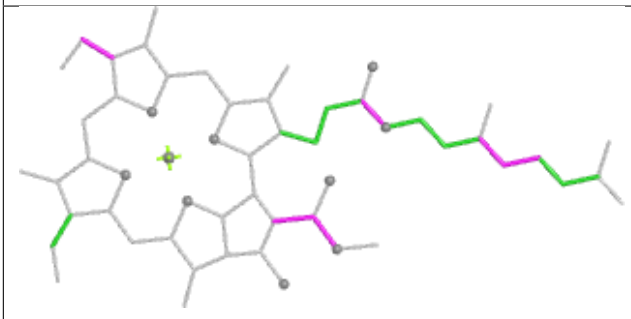
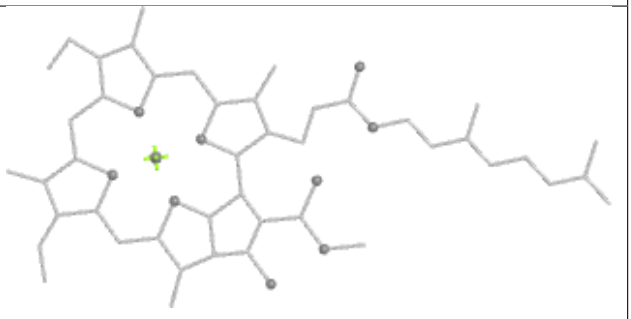
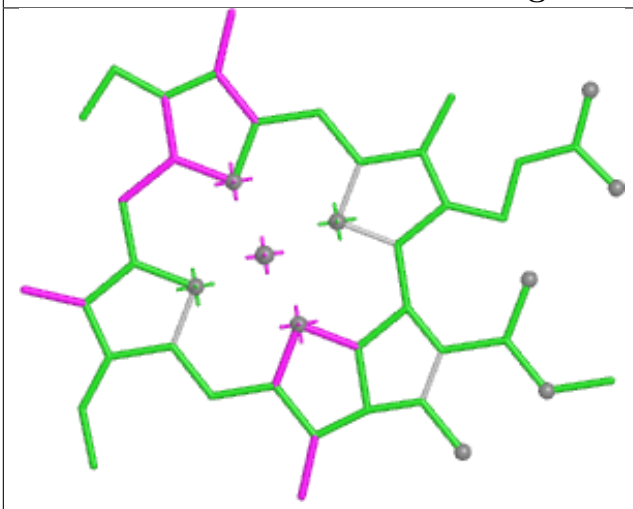
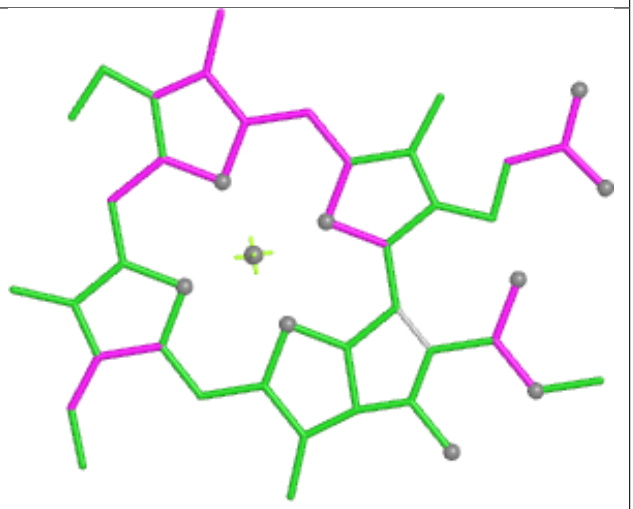
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

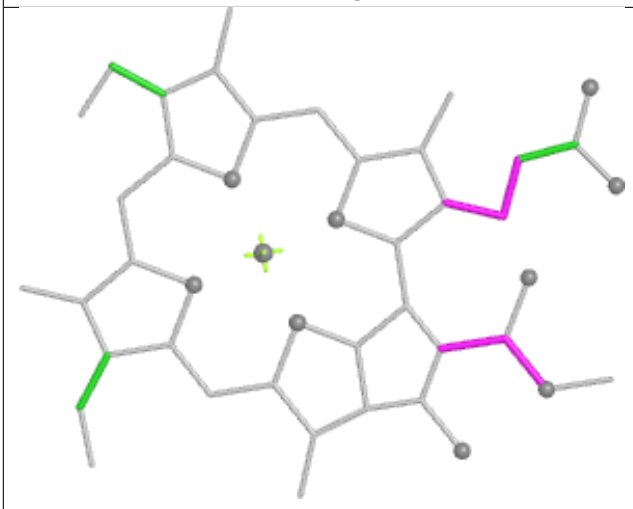
Ligand CLA 2 604



Bond lengths



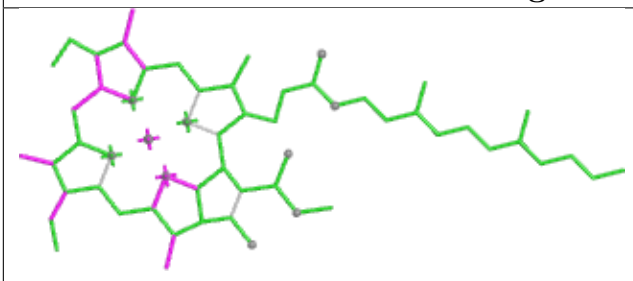
Bond angles



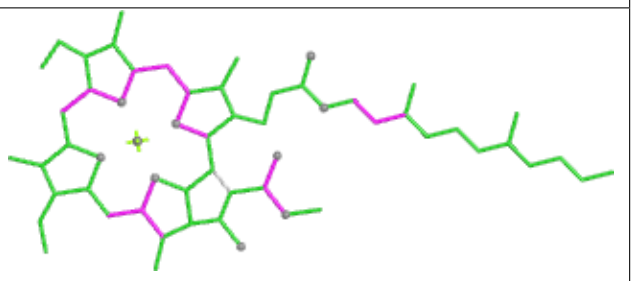
Torsions

Rings

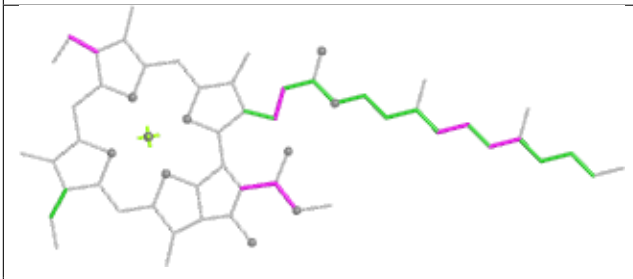
Ligand CLA 3 613



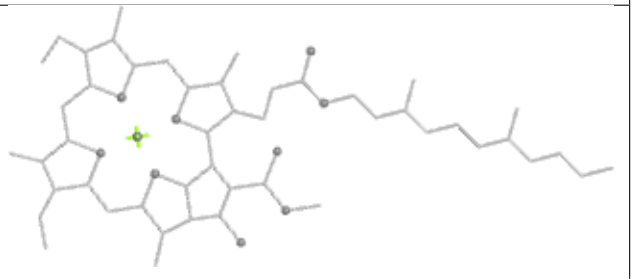
Bond lengths



Bond angles

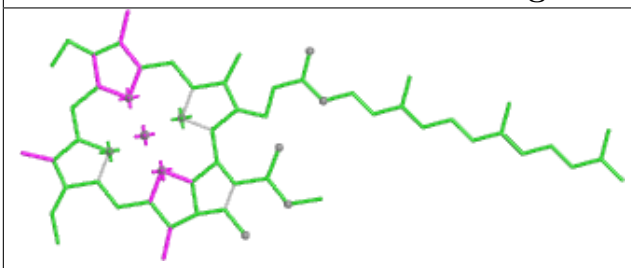


Torsions



Rings

Ligand CLA 3 602



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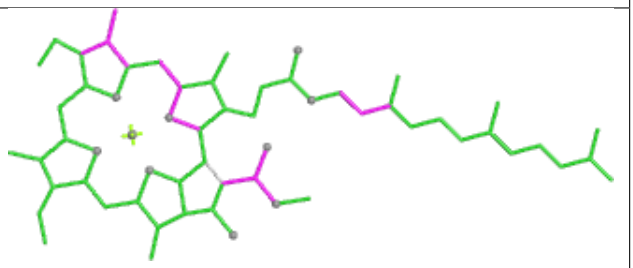
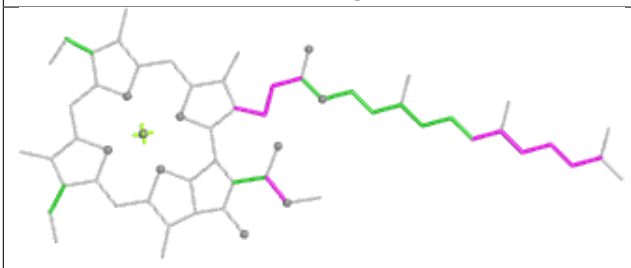


Bond angles



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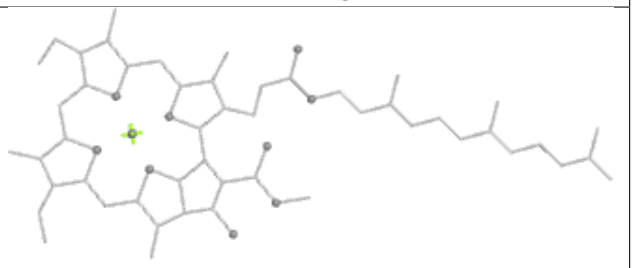
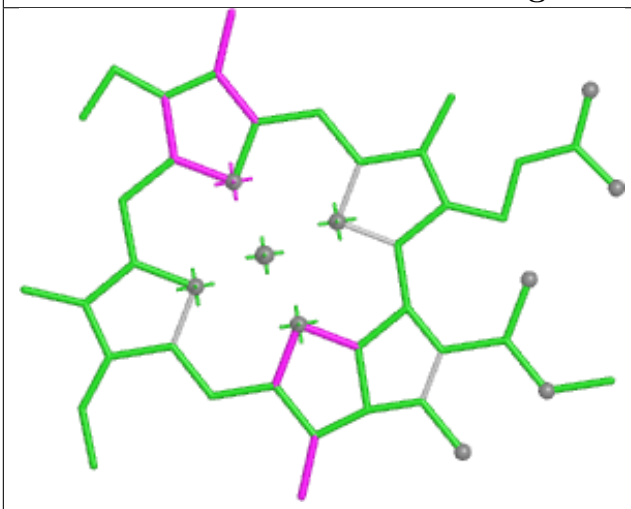


Rings

Ligand CLA 4 611



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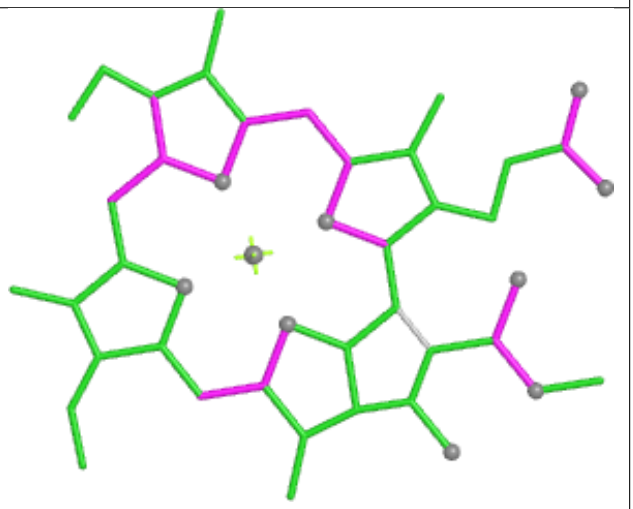
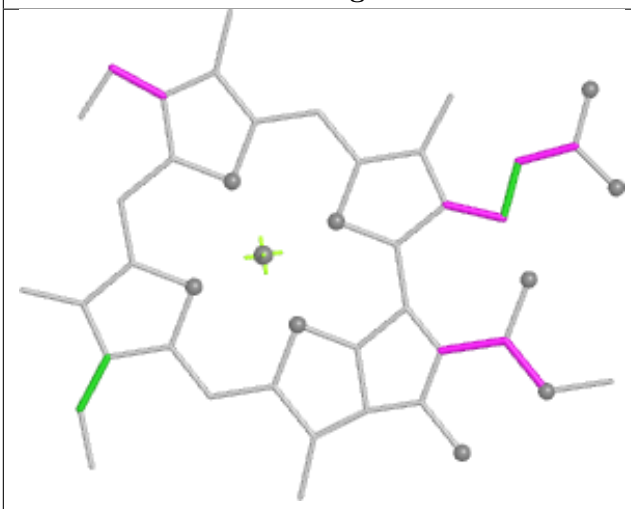


Bond angles



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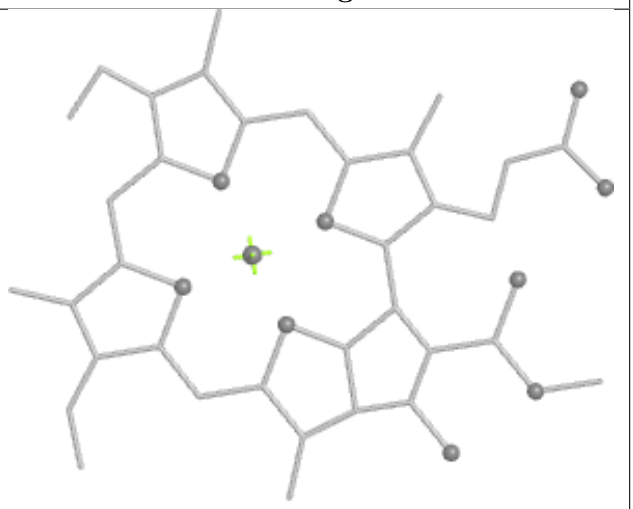
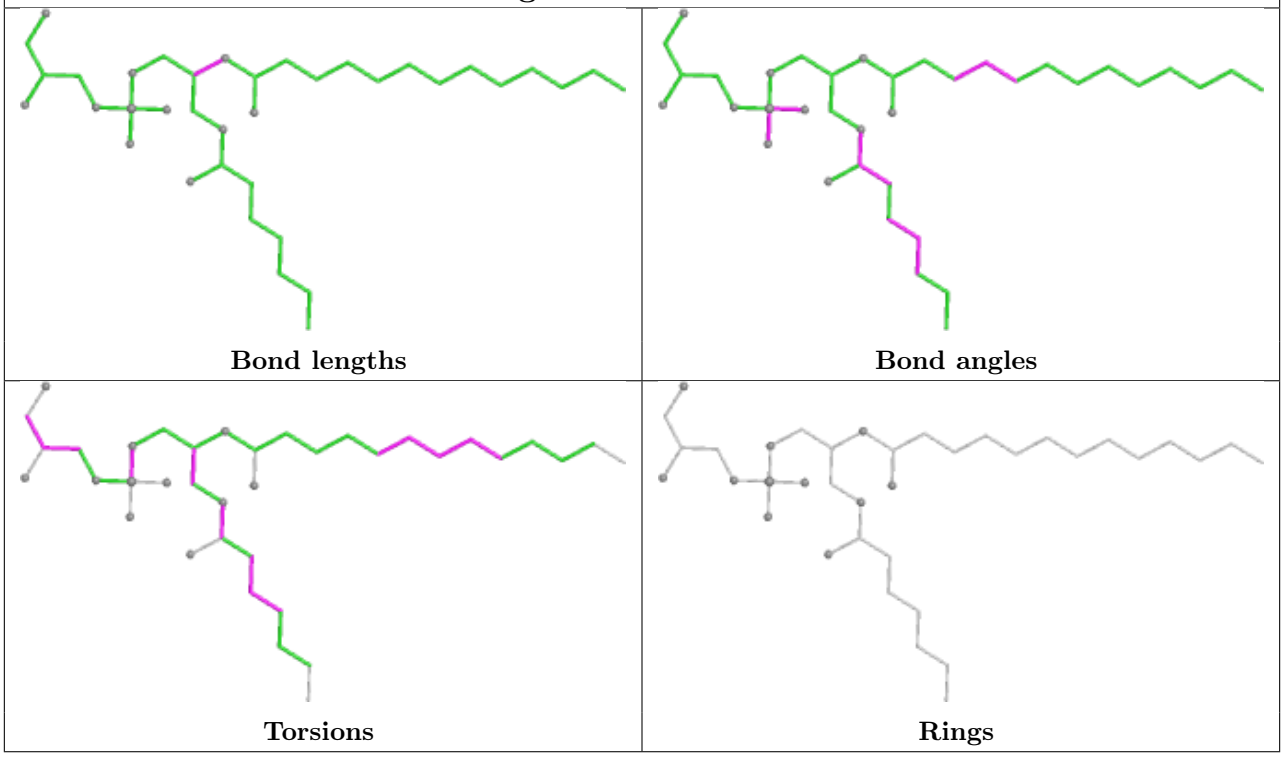
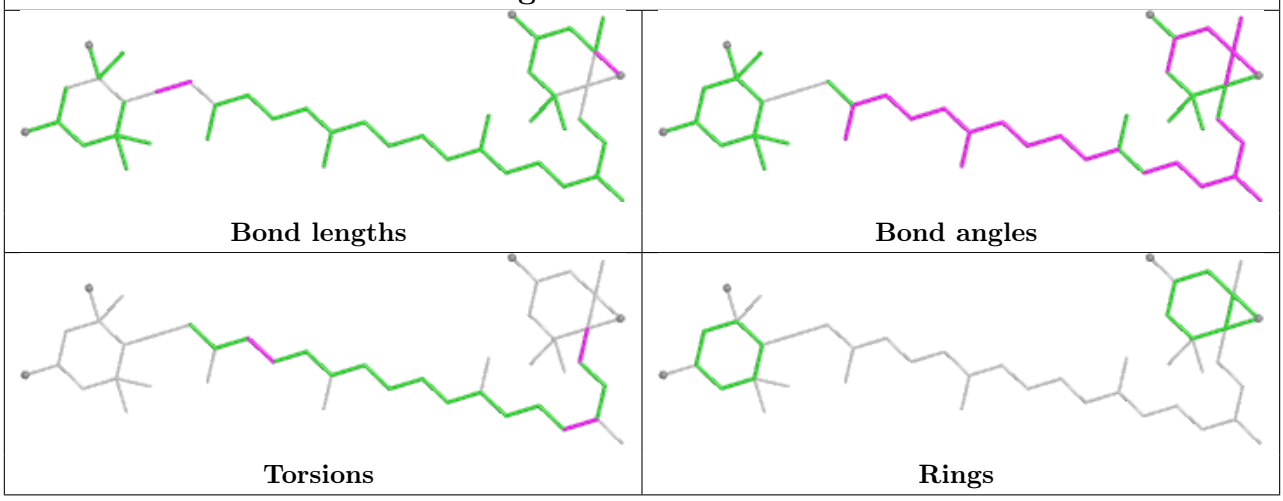


Rings

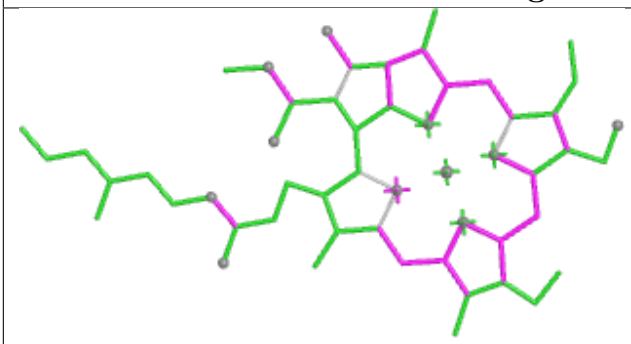
Ligand LHG 2 2630



Ligand NEX 3 1623



Ligand CHL 3 607



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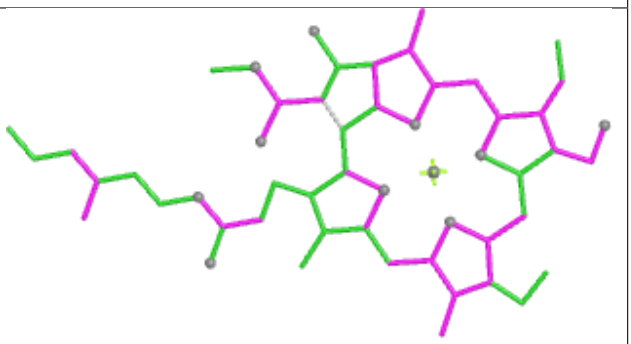
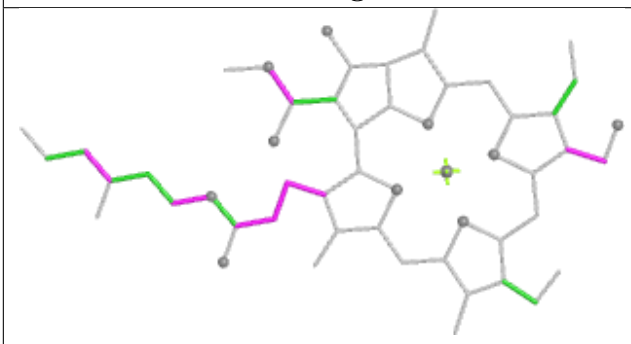


Bond angles



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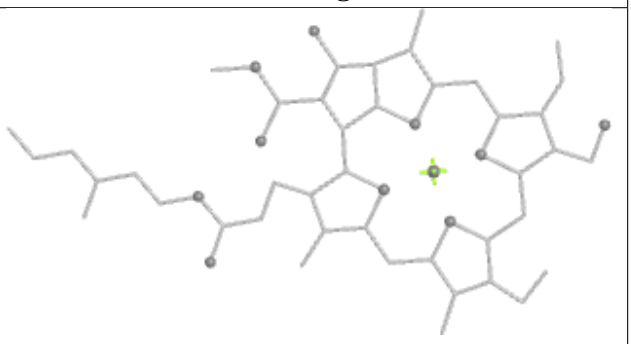
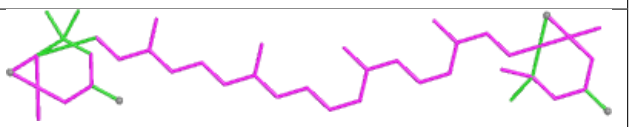


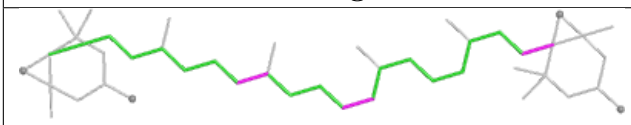
Rings

Ligand XAT 2 1622

Bond lengths



Bond angles



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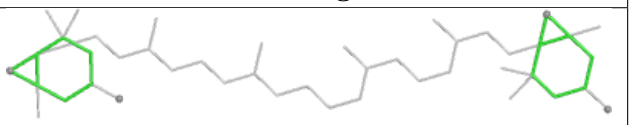
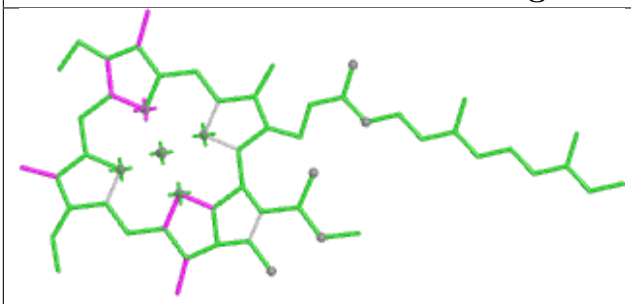
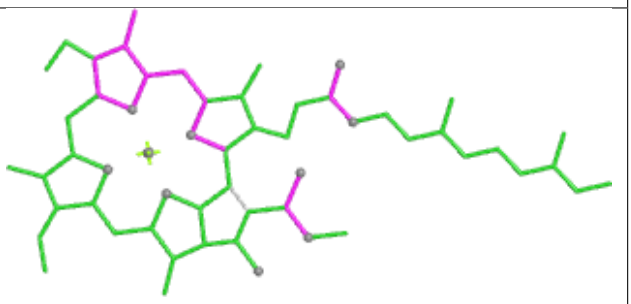
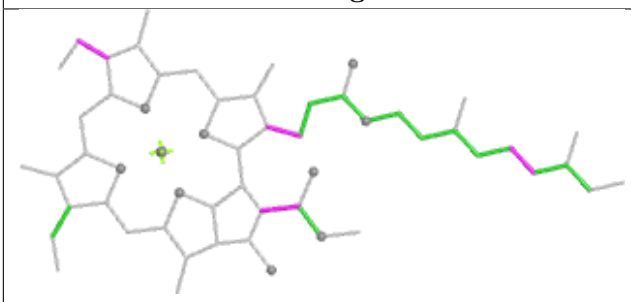
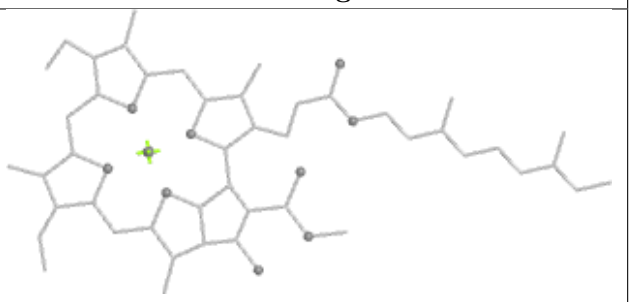
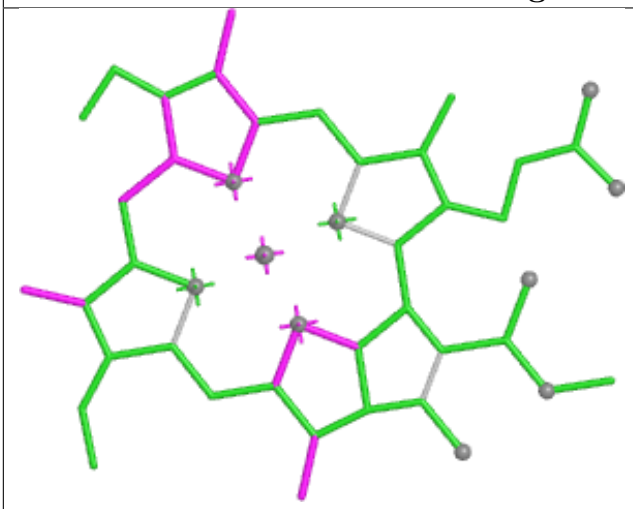


Rings

Ligand CLA 1 610	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 3 612



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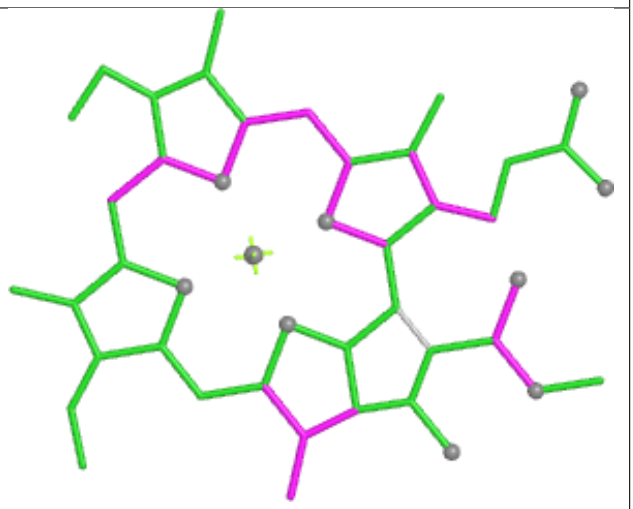
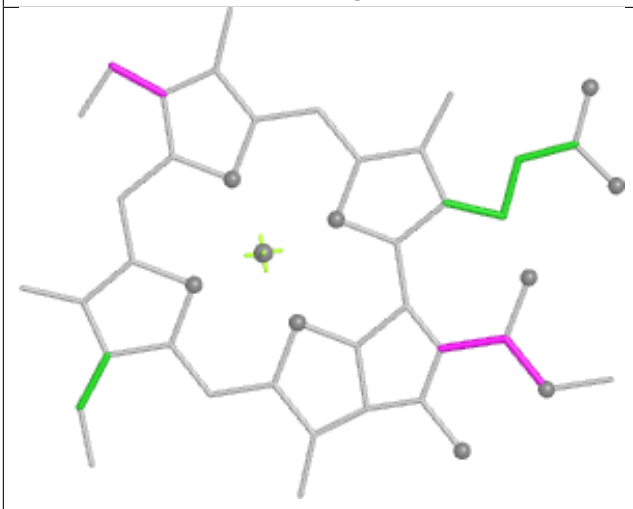


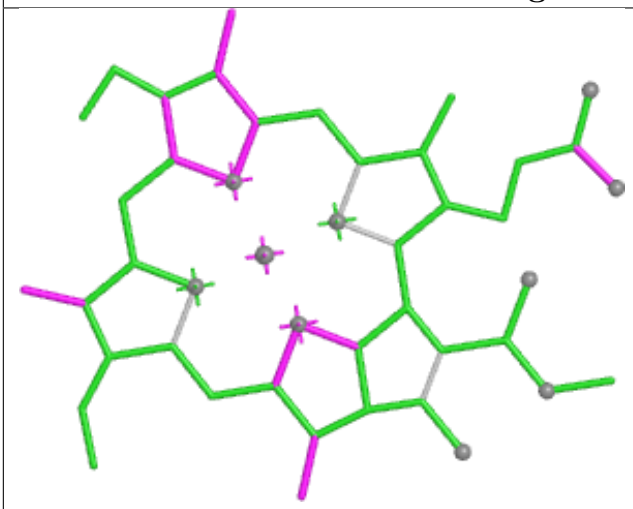
Bond angles



Torsions

Rings

Ligand CLA 1 611



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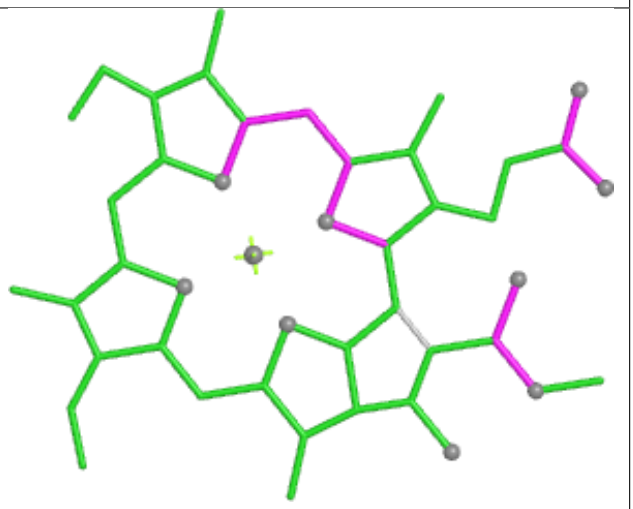

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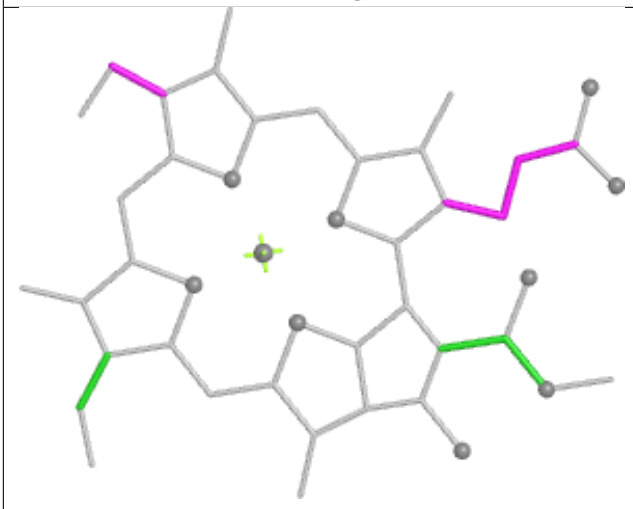

Torsions

Rings

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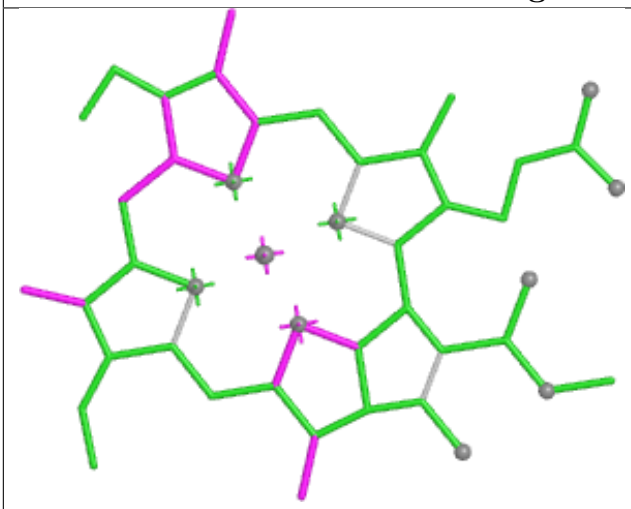

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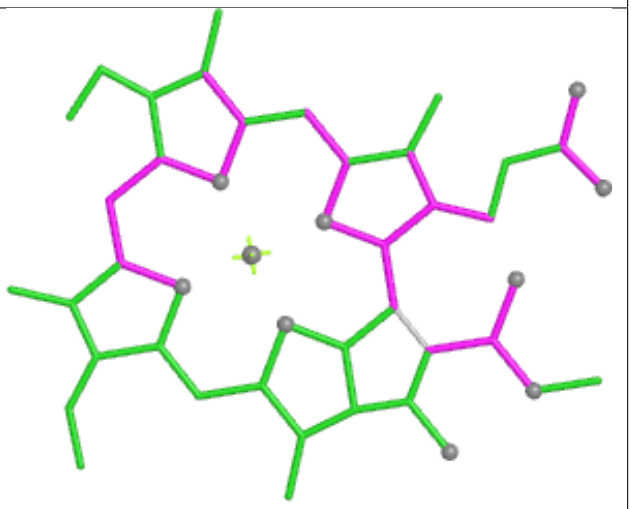

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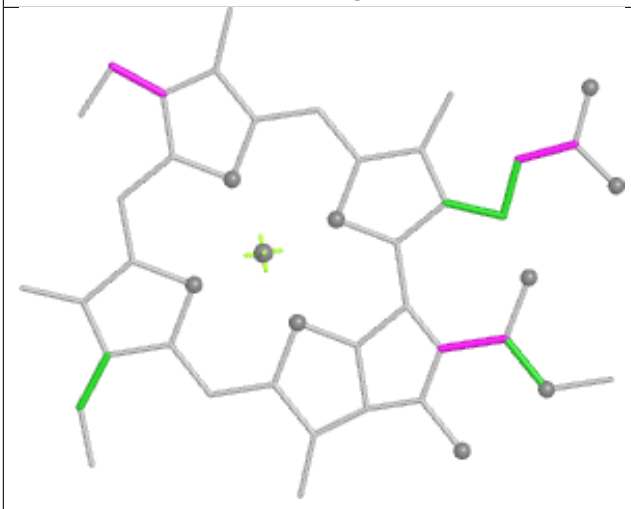
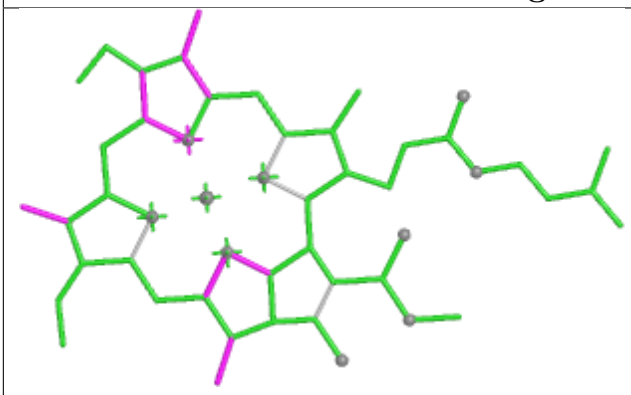


Torsions

Rings

Ligand CLA 2 610



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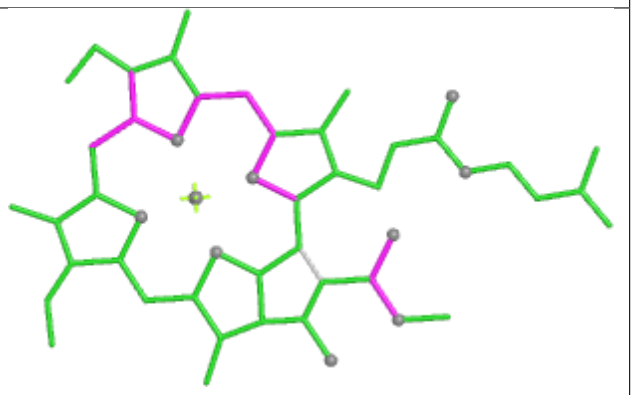

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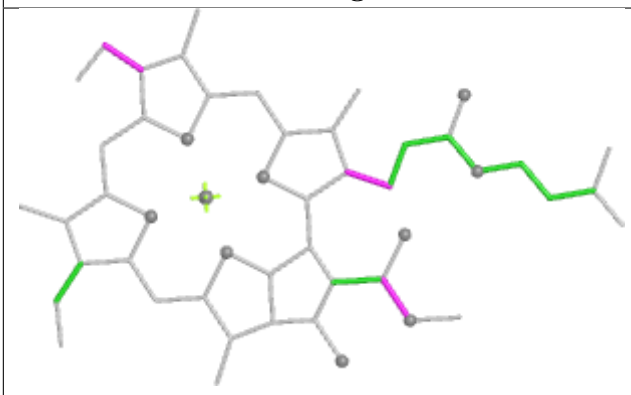

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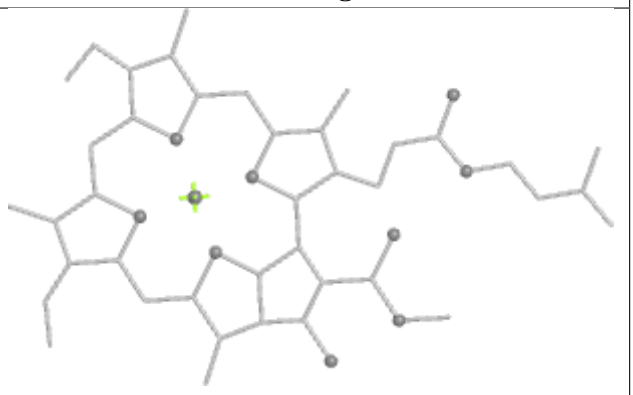
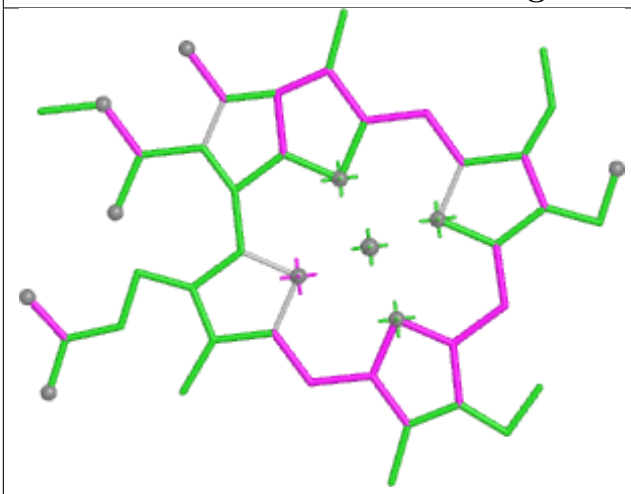


Rings

Ligand CHL 4 608



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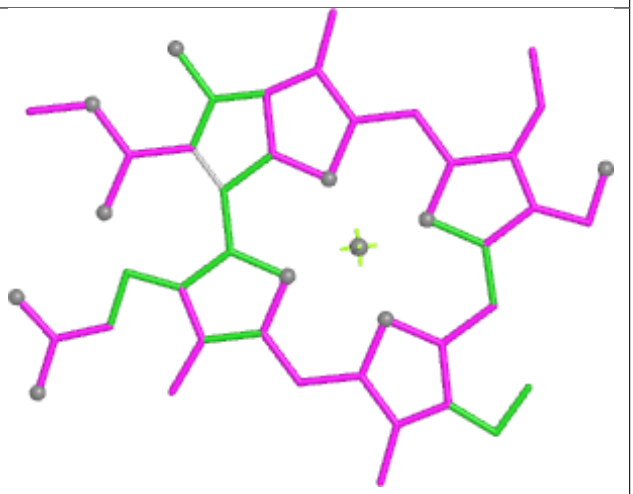
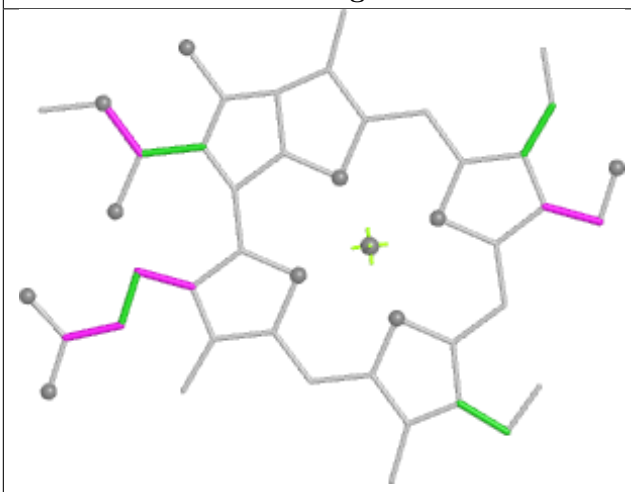


Bond angles



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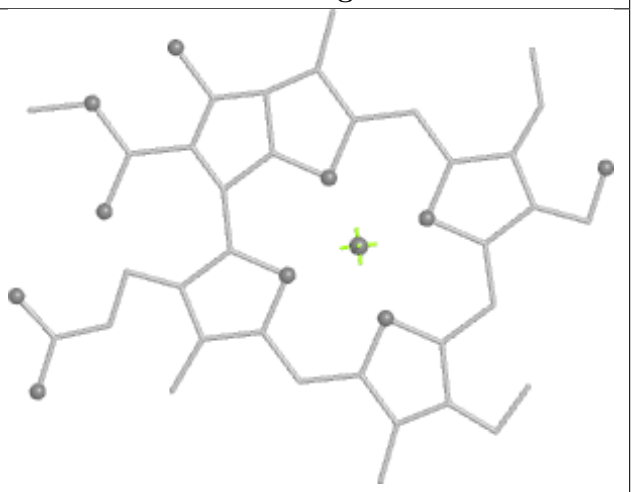
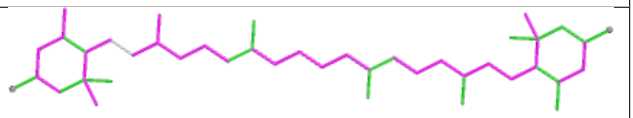


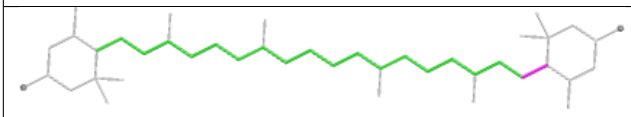
Rings

Ligand LUT 2 1621

Bond lengths



Bond angles



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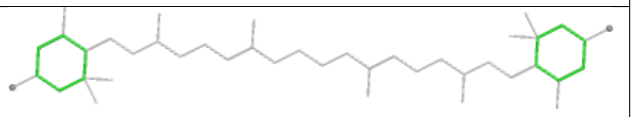
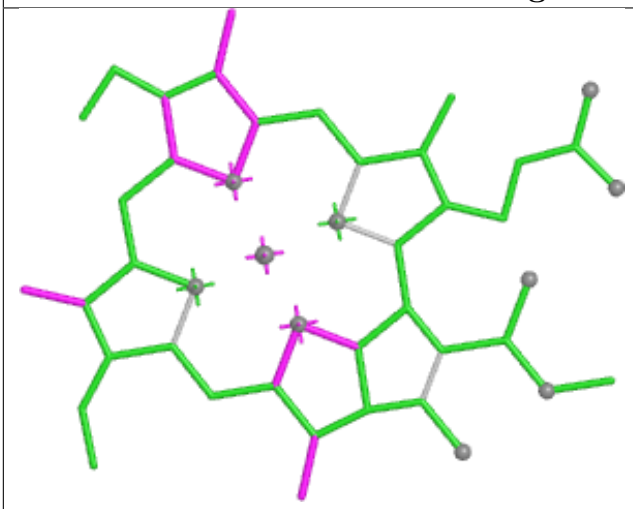


Rings

Ligand CLA 3 604



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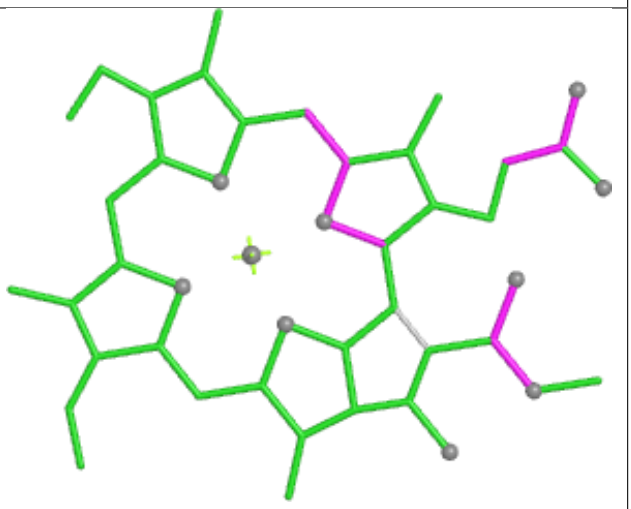
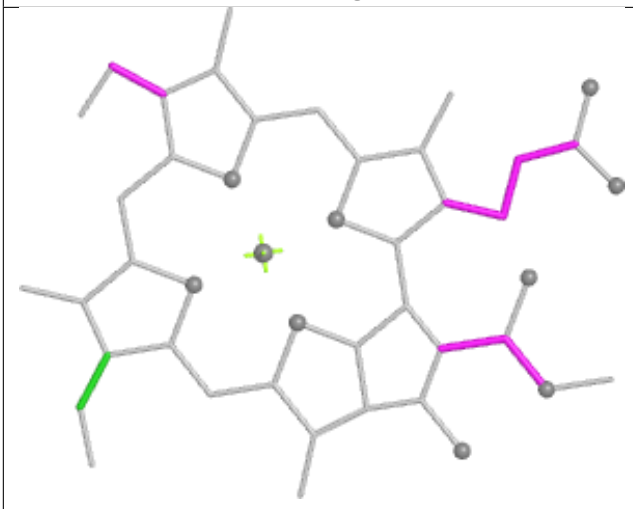


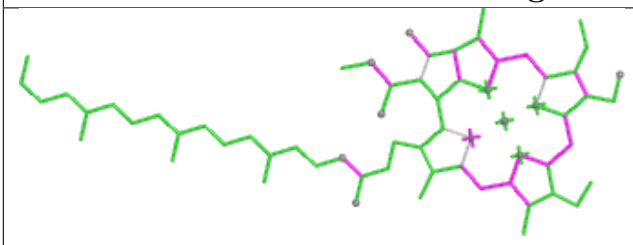
Bond angles



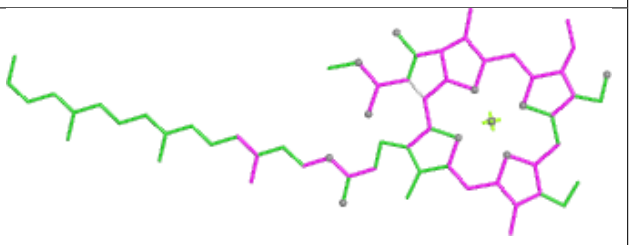
Torsions

Rings

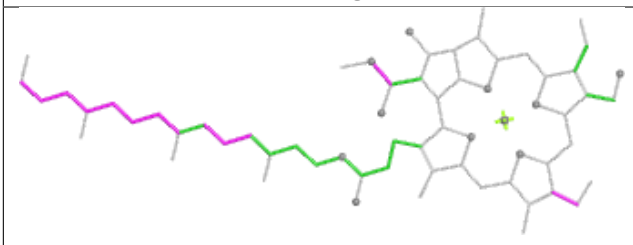
Ligand CHL 3 601



Bond lengths



Bond angles



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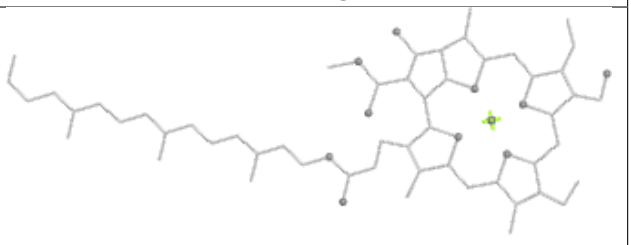
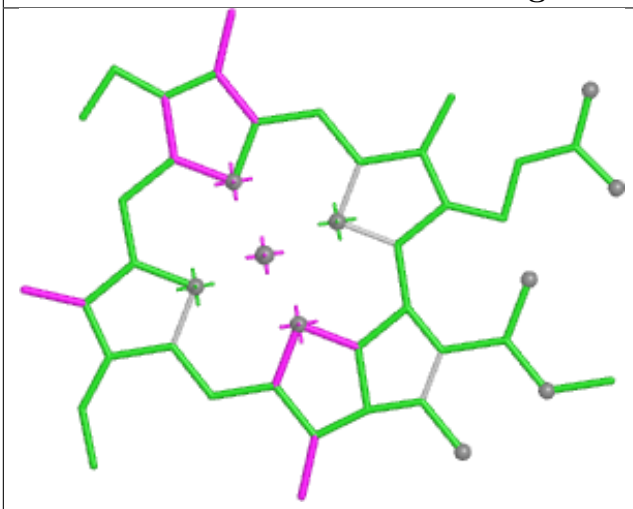


Rings

Ligand CLA 2 611



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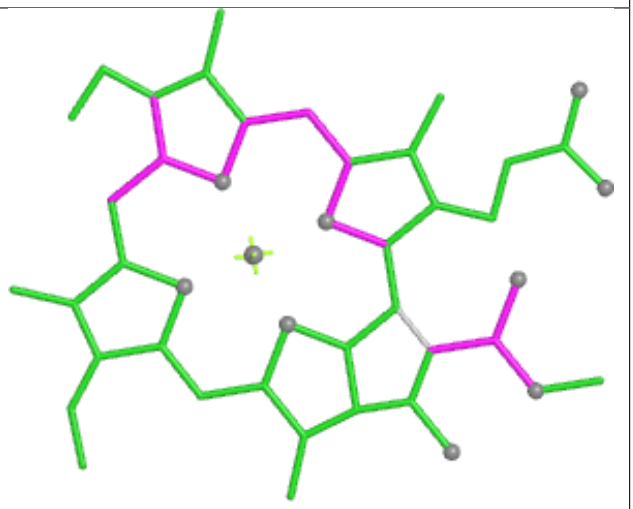
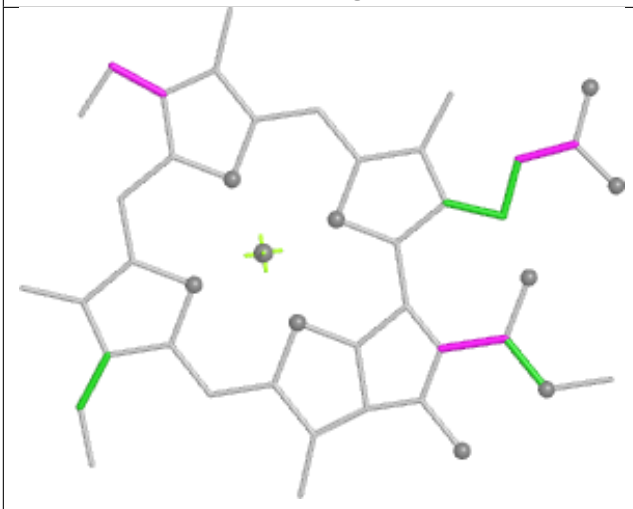


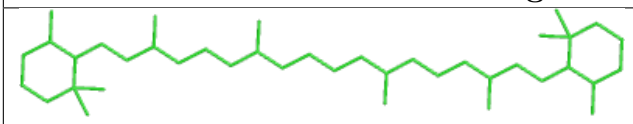
Bond angles



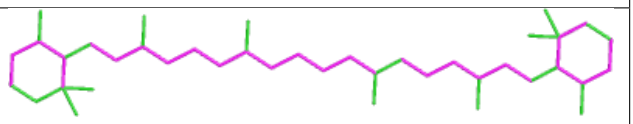
Torsions

Rings

Ligand BCR 4 623



Bond lengths



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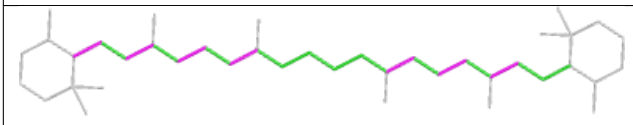
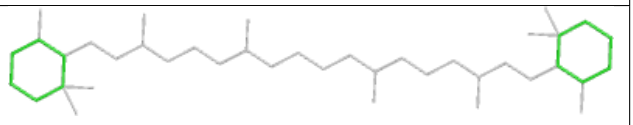
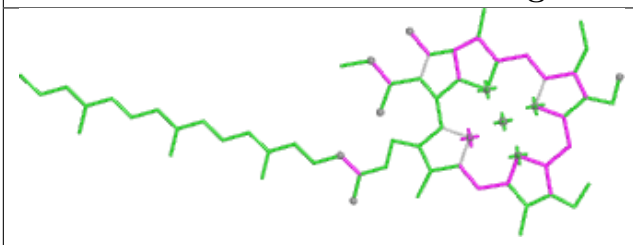


Torsions



Rings

Ligand CHL 1 607



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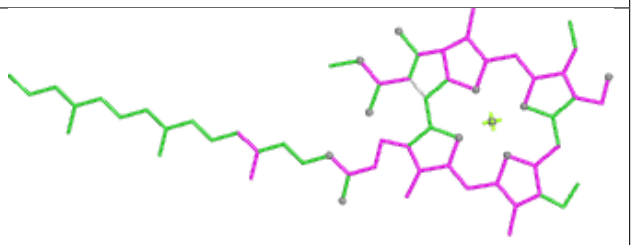
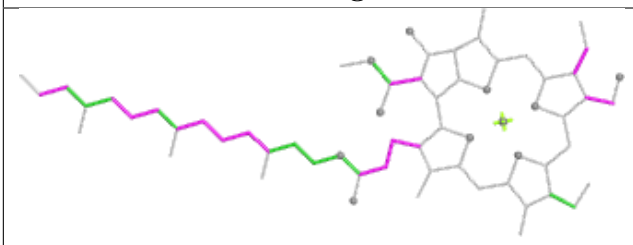


Bond angles



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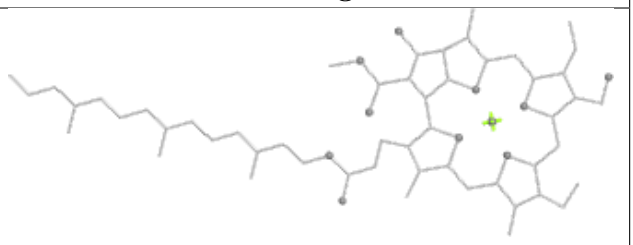
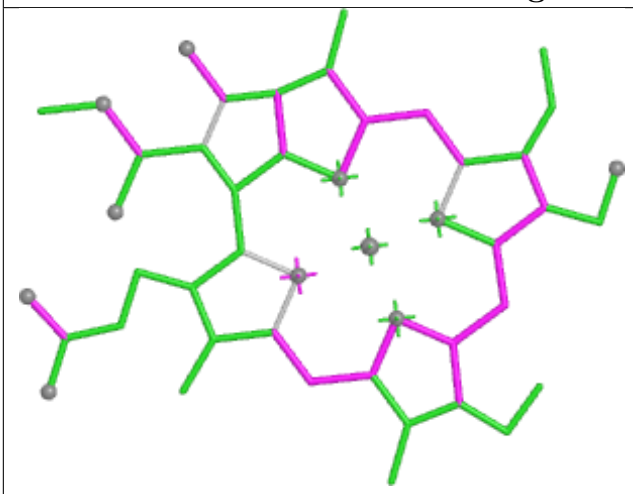


Rings

Ligand CHL 3 608



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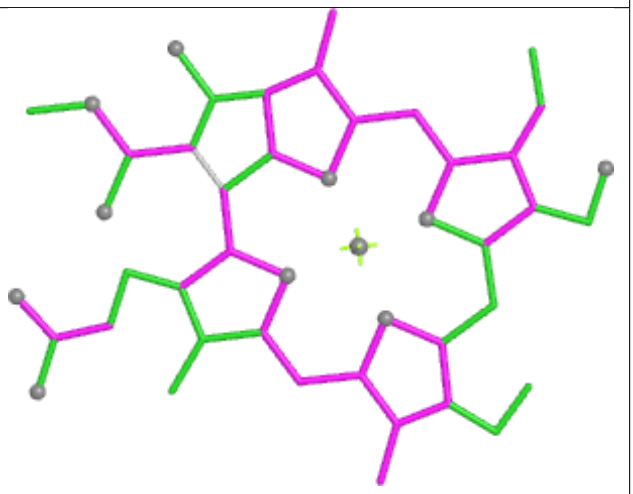

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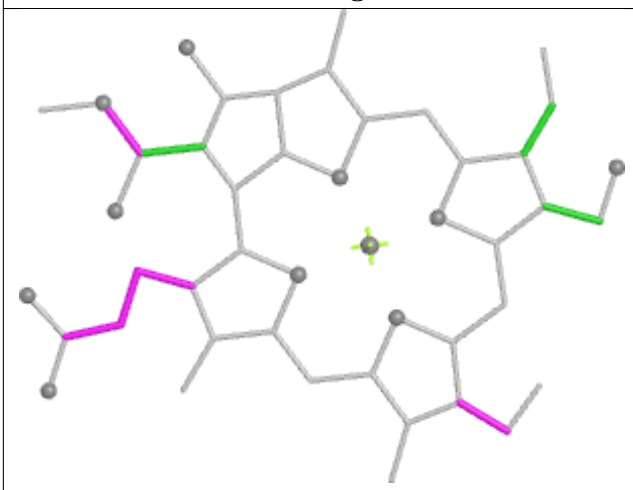

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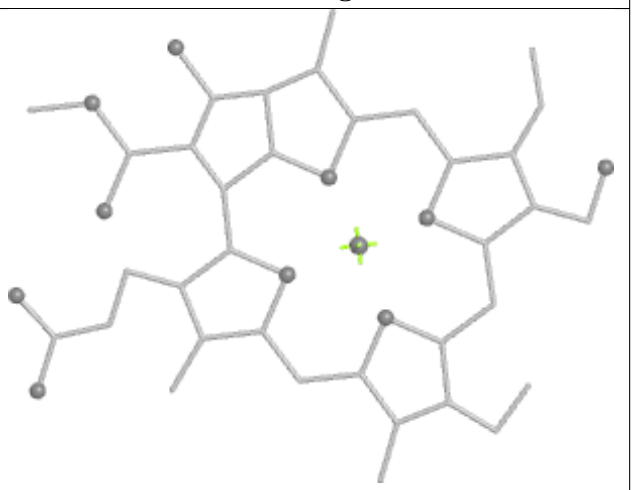
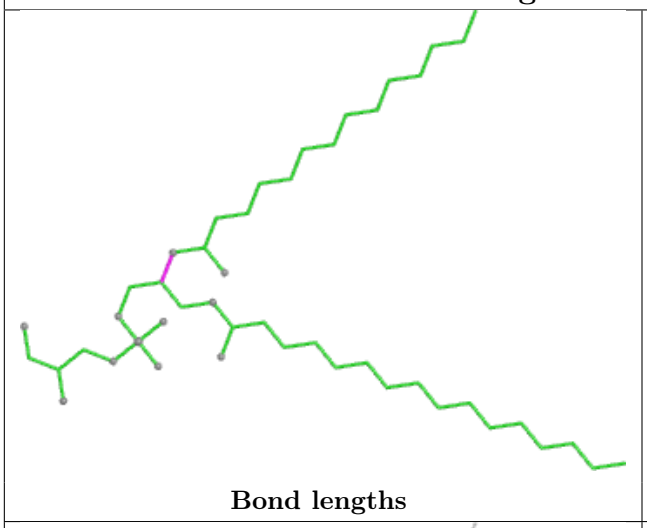


Rings

Ligand LHG 3 2630



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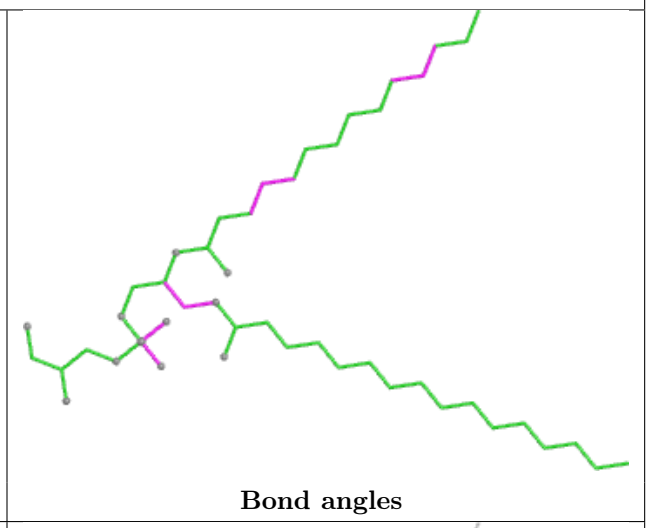

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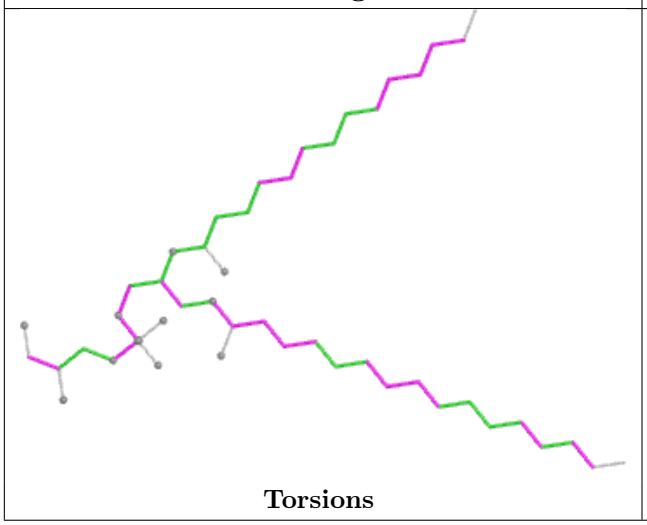

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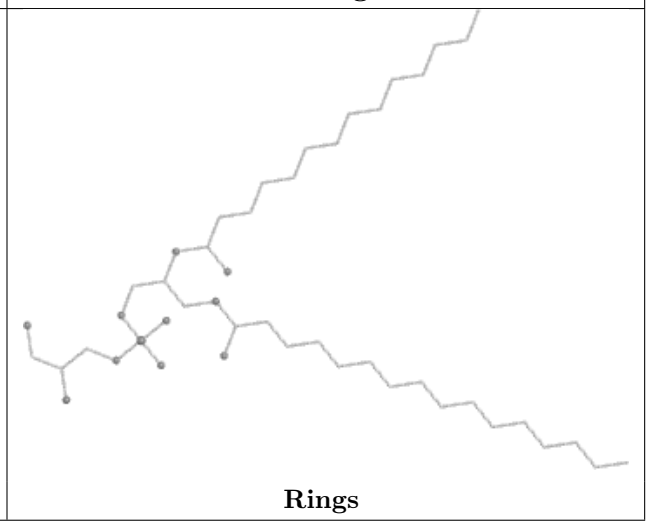

Rings

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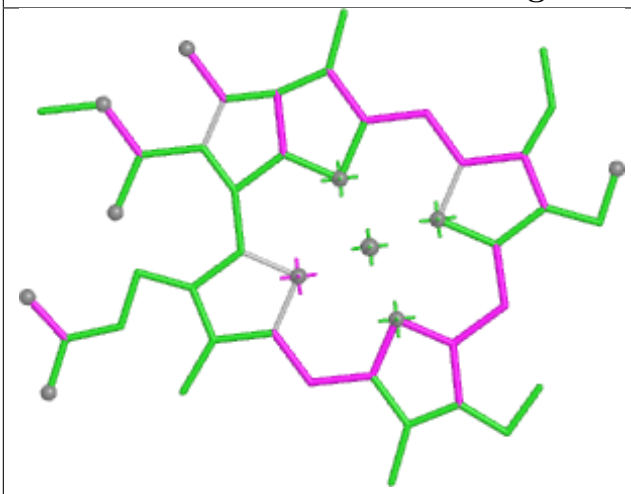

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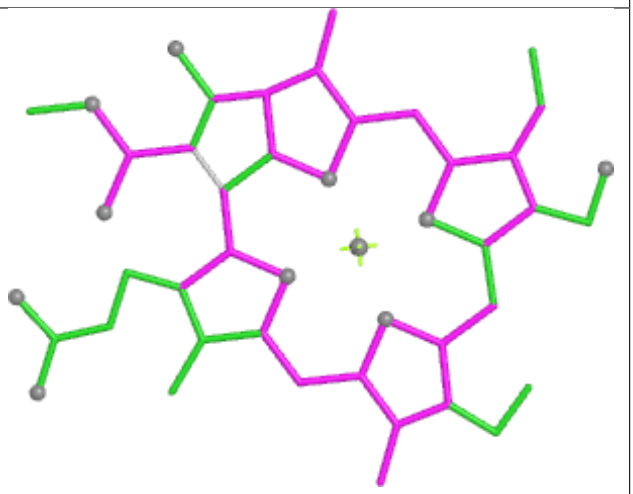

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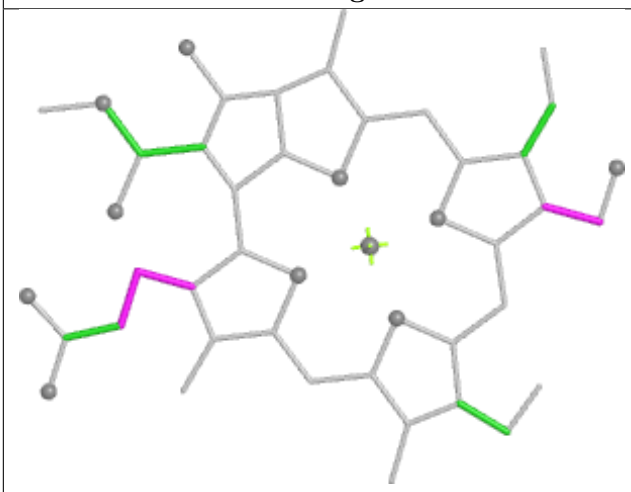

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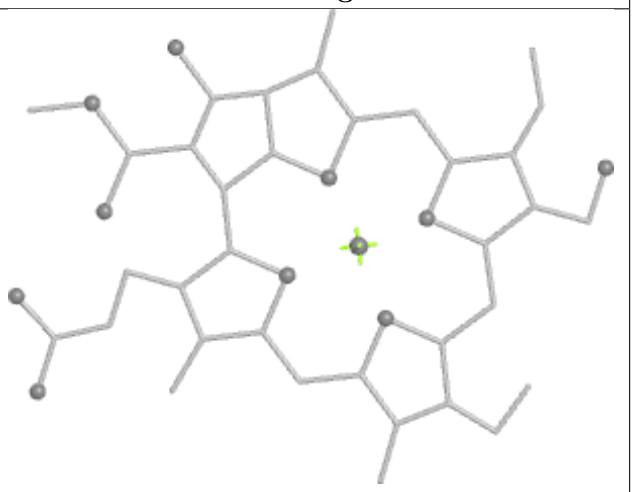
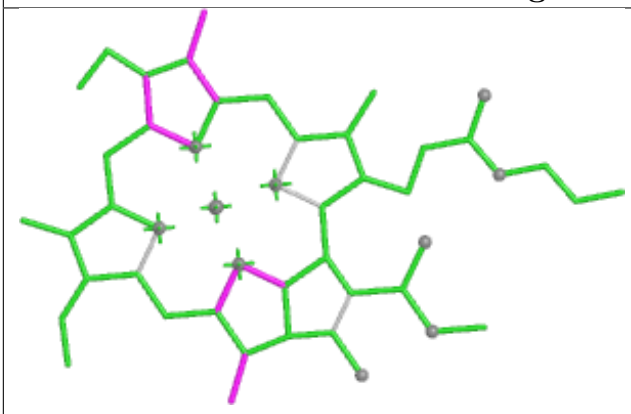


Rings

Ligand CLA 3 614



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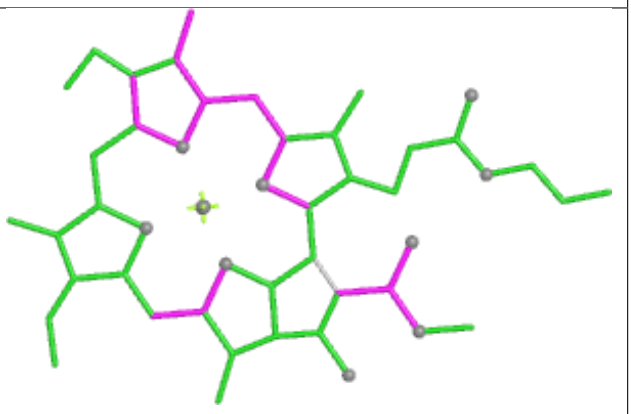

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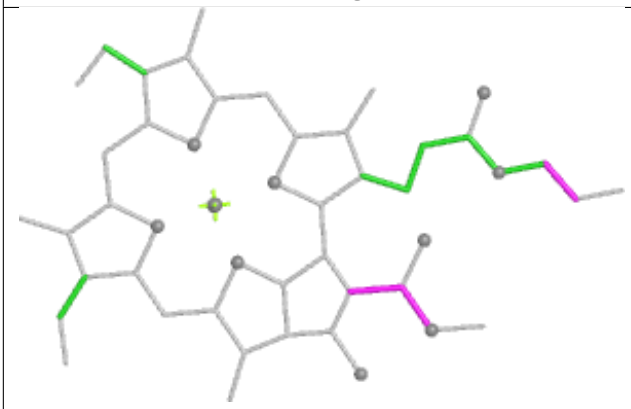

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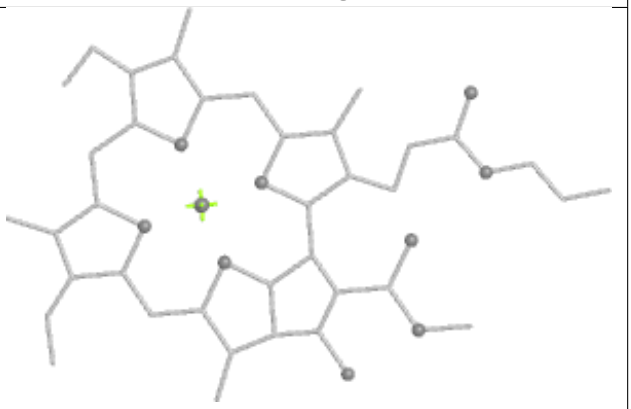

Rings

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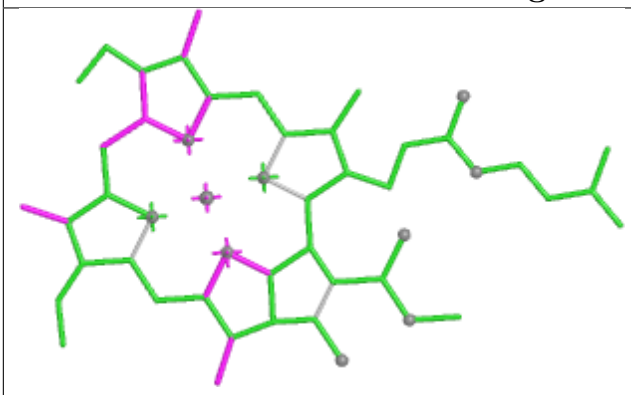

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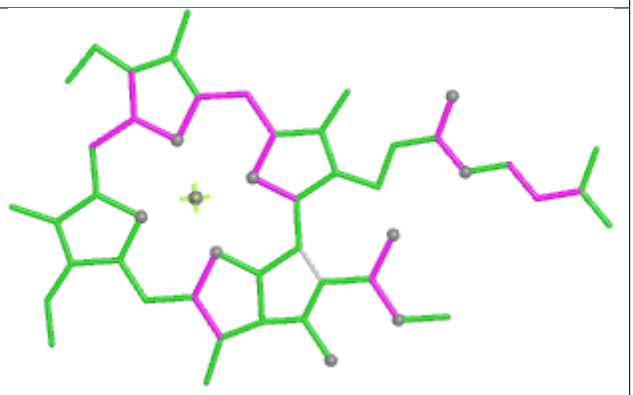

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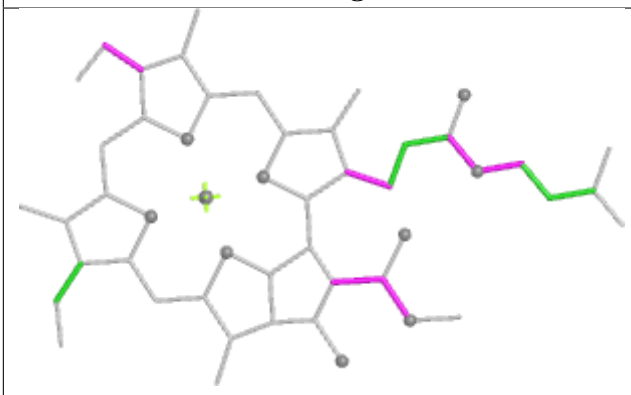

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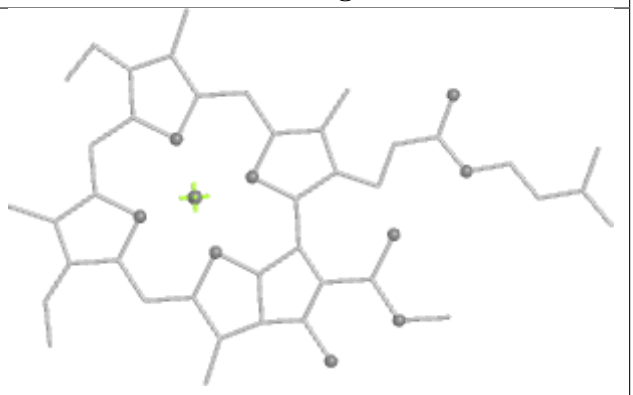

Rings

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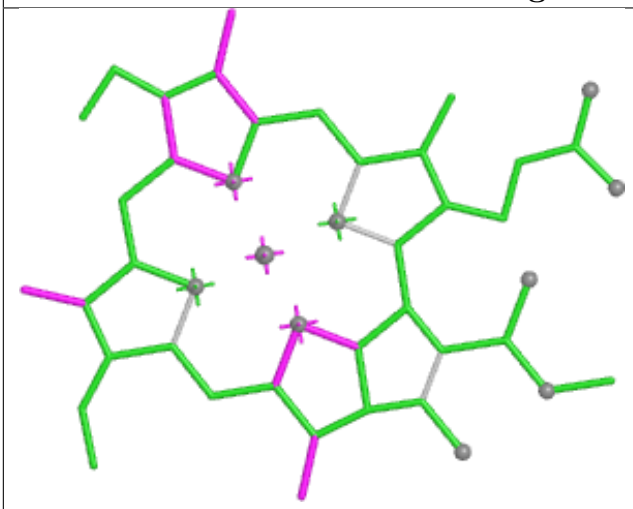

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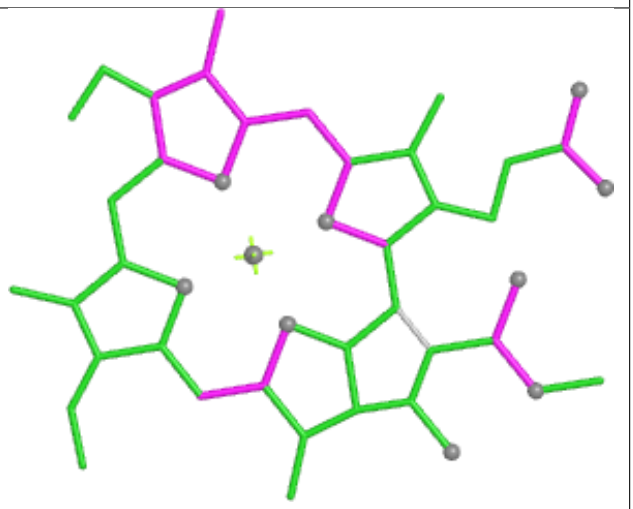

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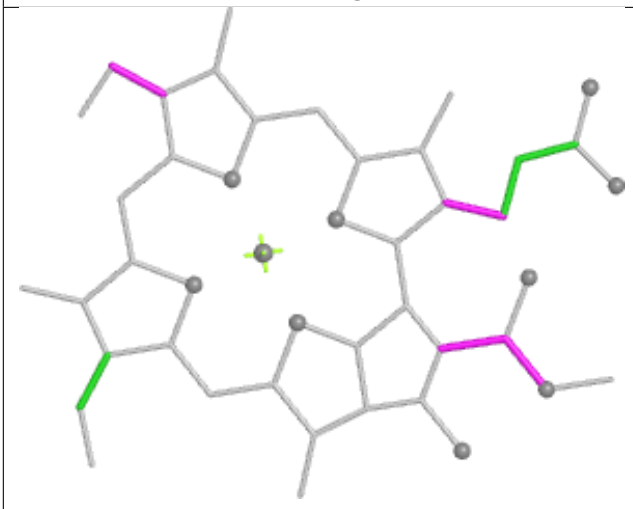
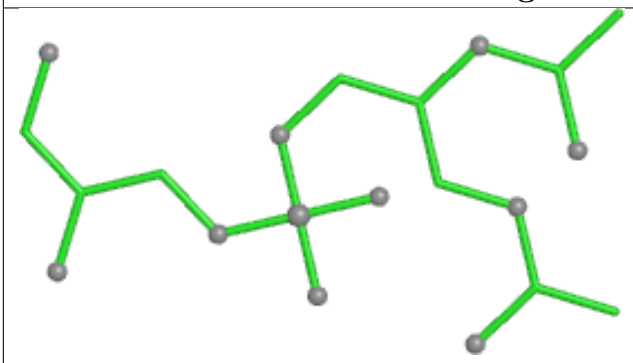


Torsions

Rings

Ligand LHG 4 2630



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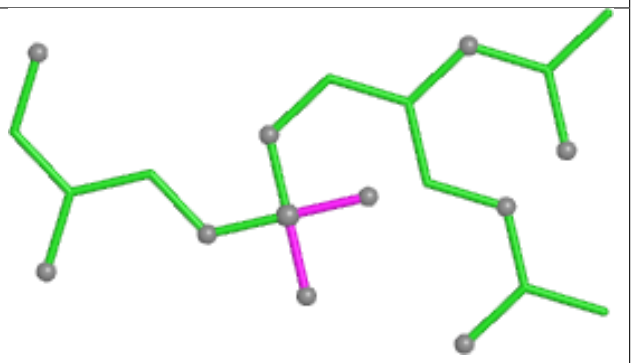

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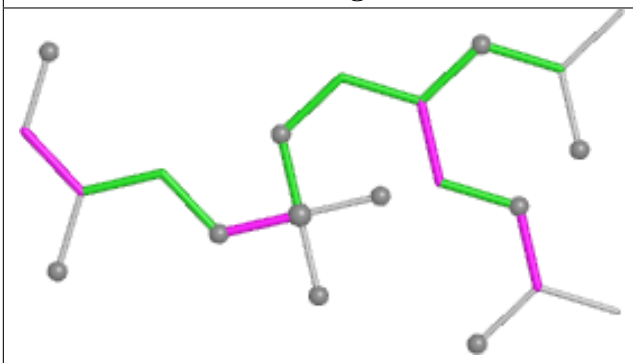

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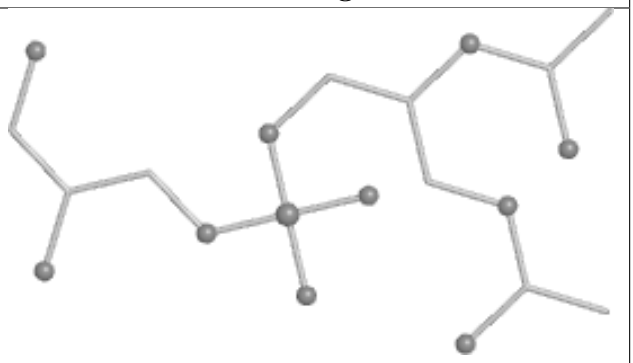
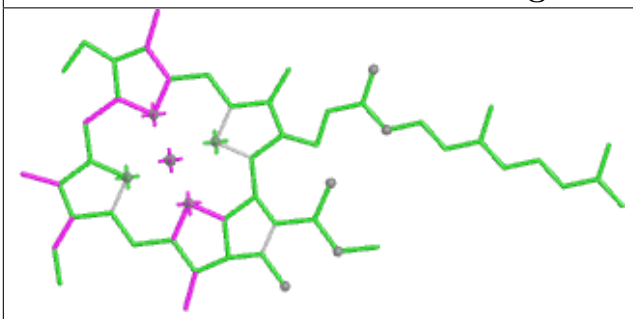


Rings

Ligand CLA 3 603



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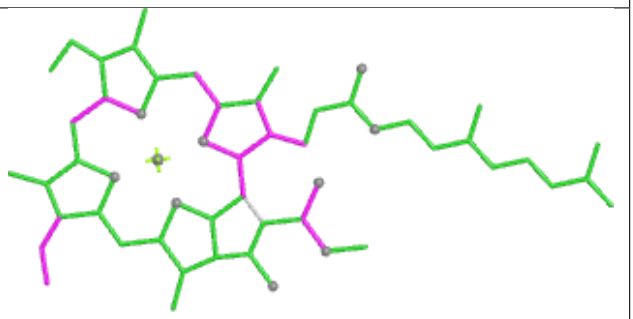
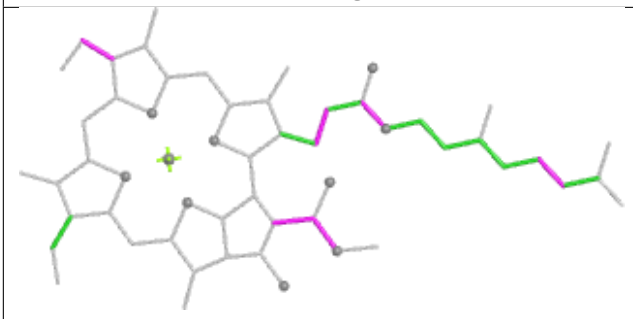


Bond angles



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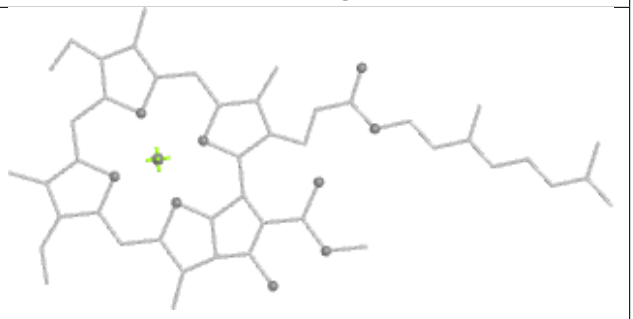
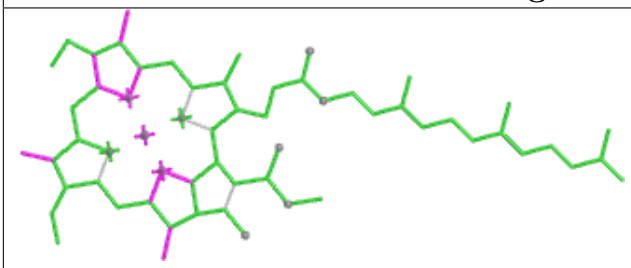
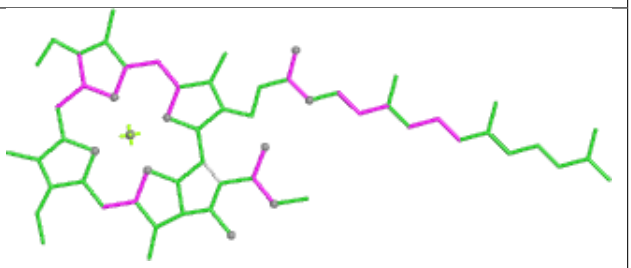
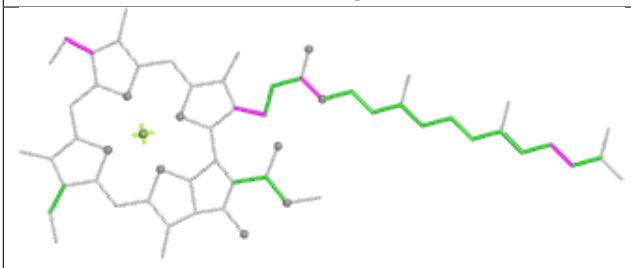
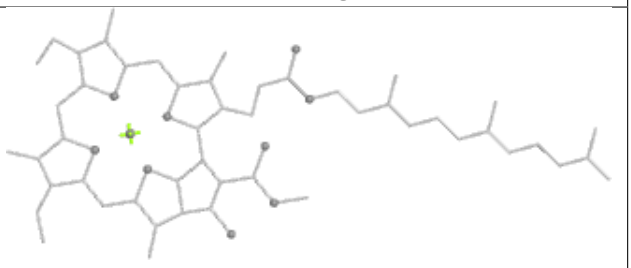
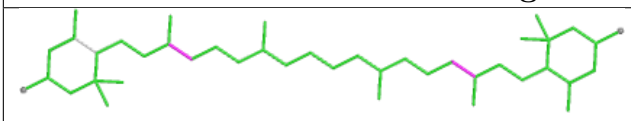
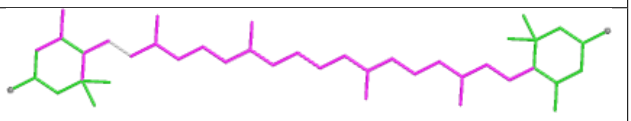
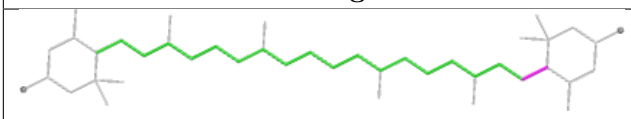
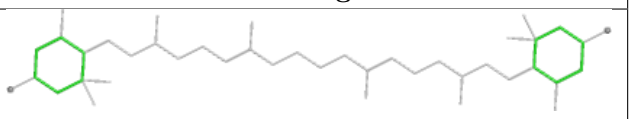
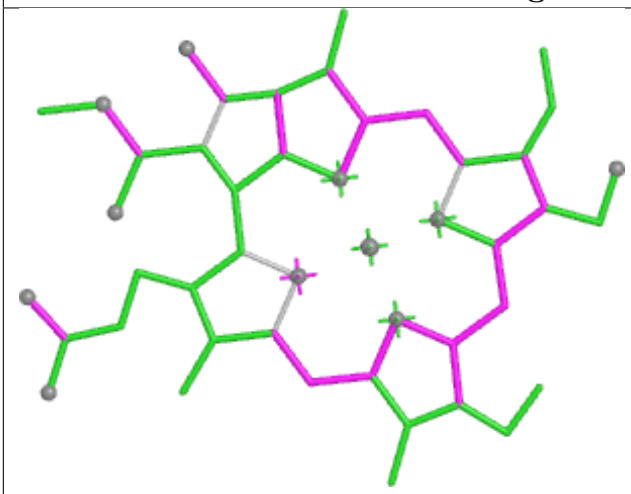


Rings

Ligand CLA 3 610	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand LUT 1 1620	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CHL 1 608



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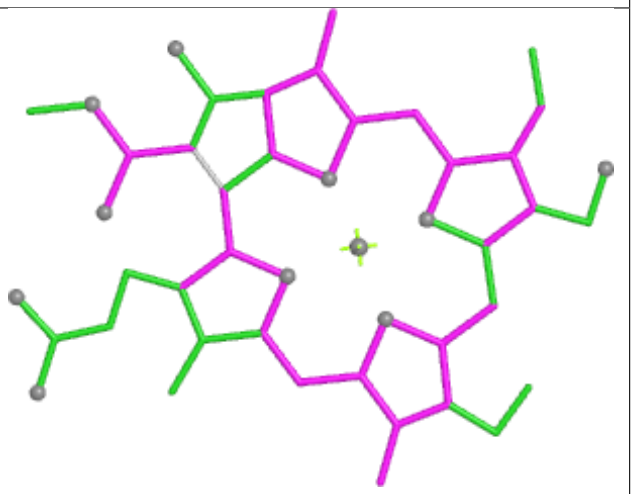
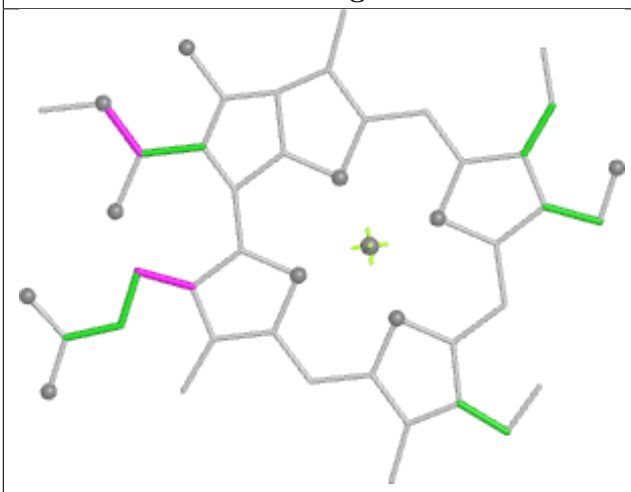
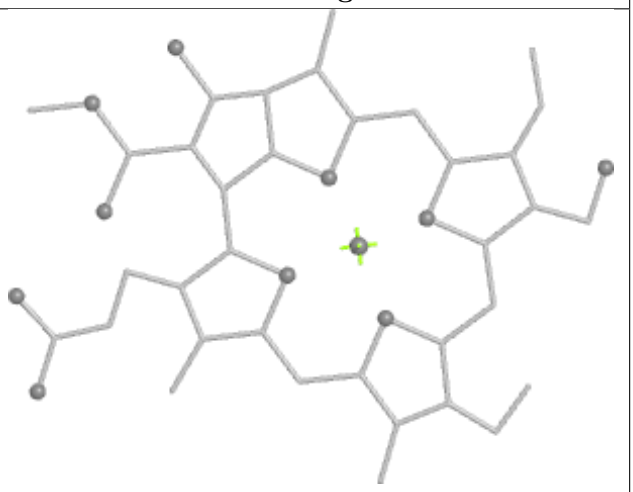


Bond angles

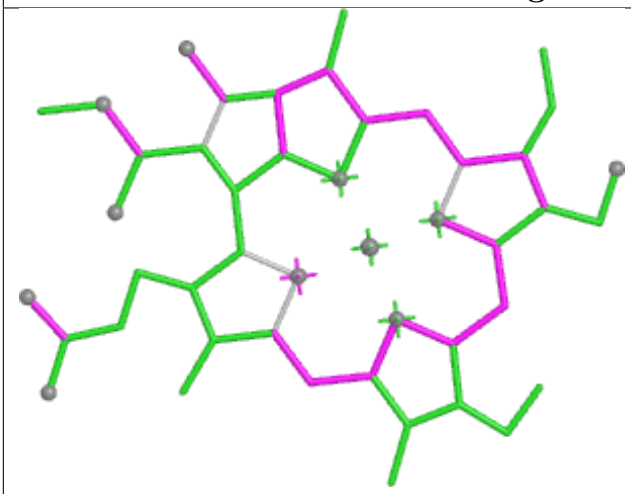


Torsions



Rings

Ligand CHL 2 606



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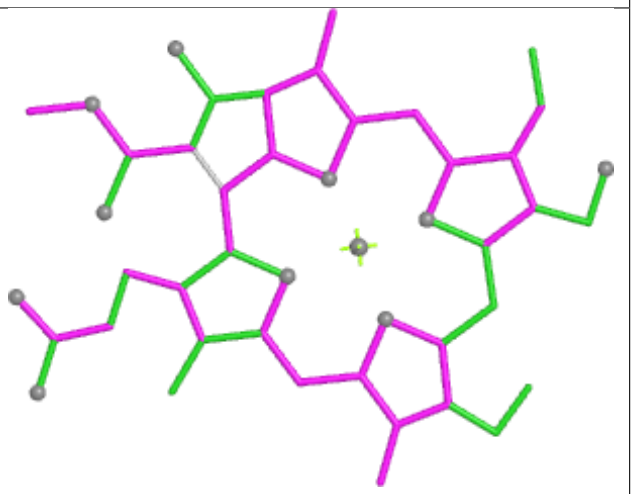
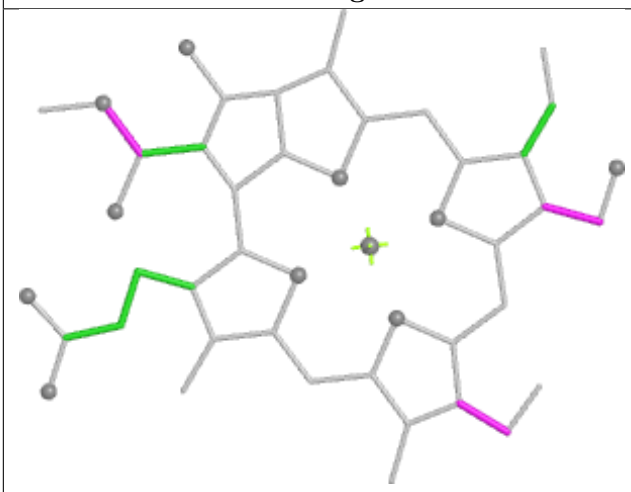


Bond angles



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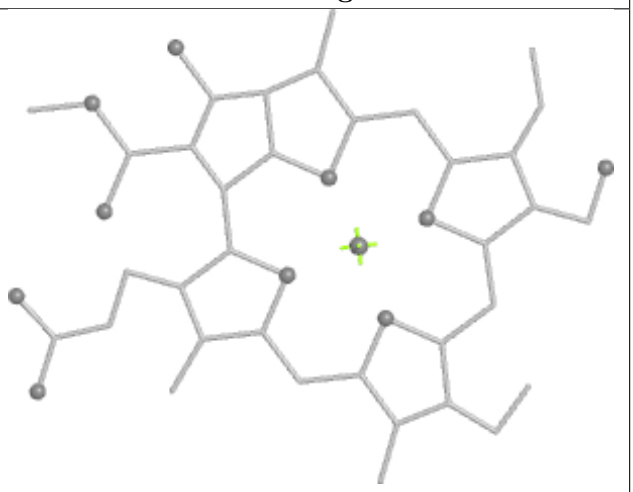
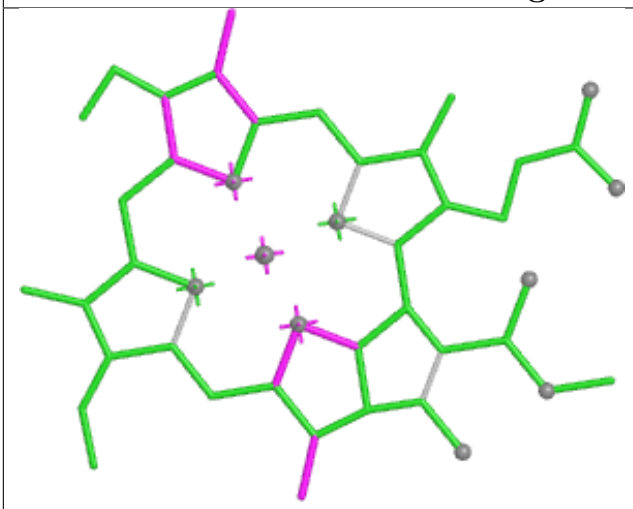


Rings

Ligand CLA 2 612



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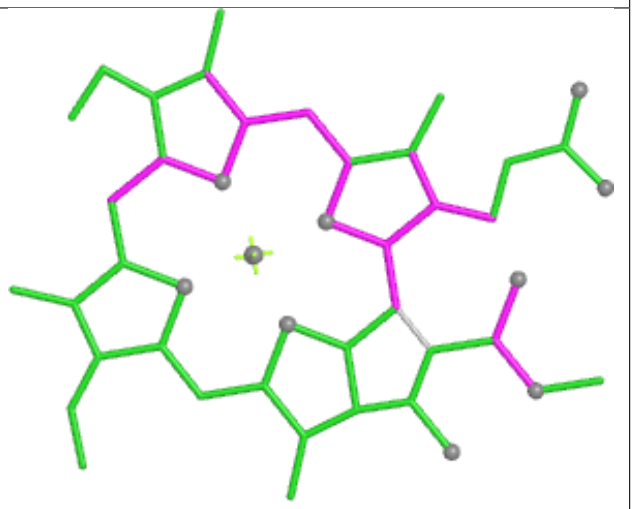
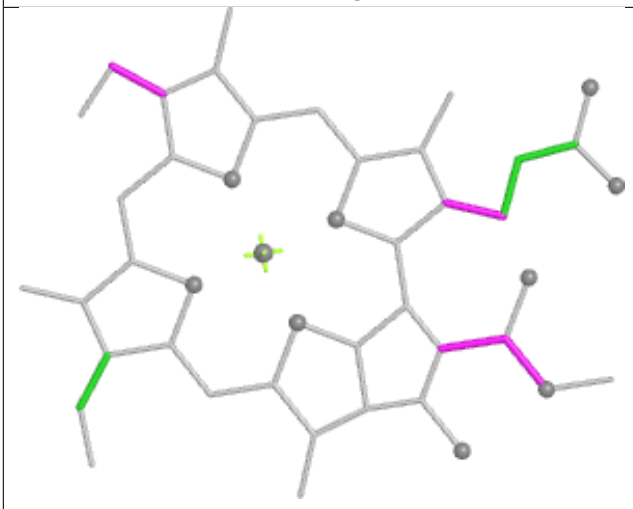


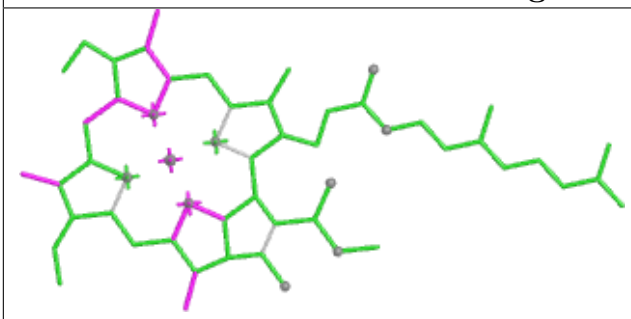
Bond angles



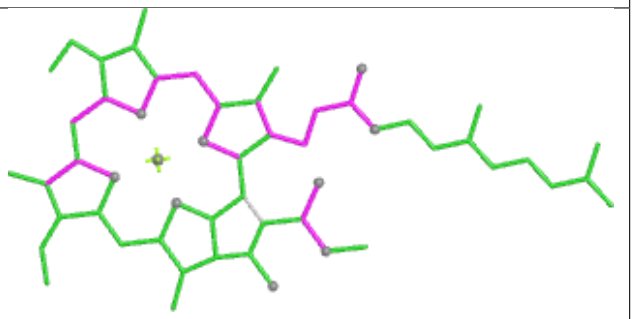
Torsions

Rings

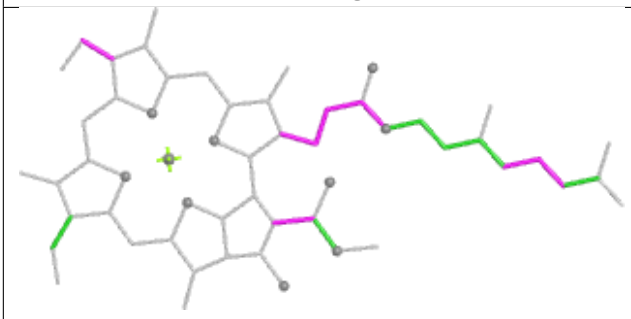
Ligand CLA 3 611



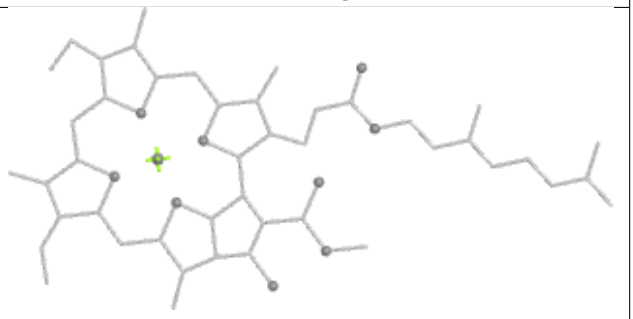
Bond lengths



Bond angles

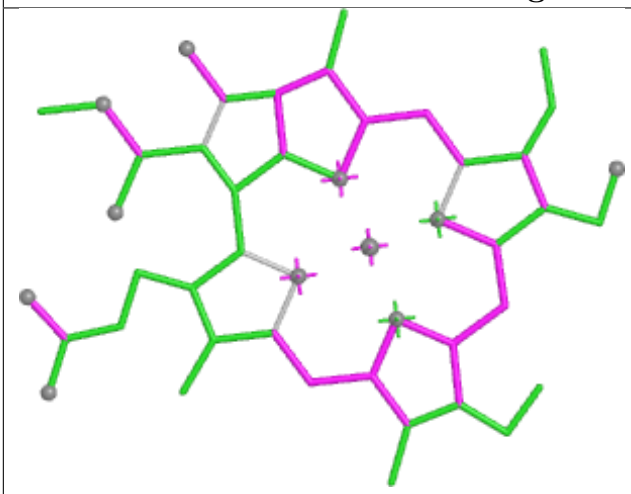


Torsions

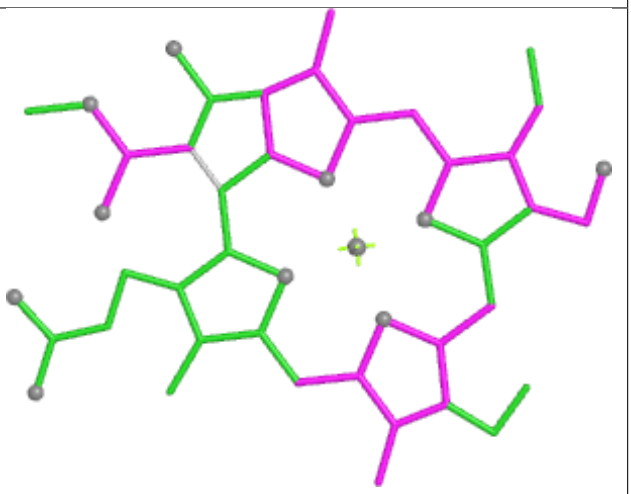


Rings

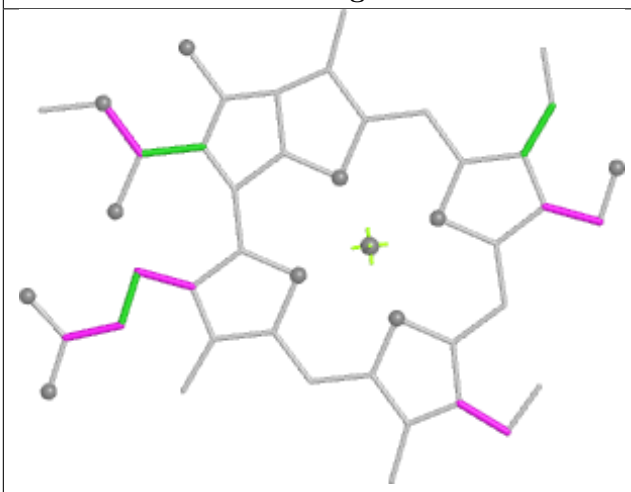
Ligand CHL 1 605



Bond lengths



Bond angles

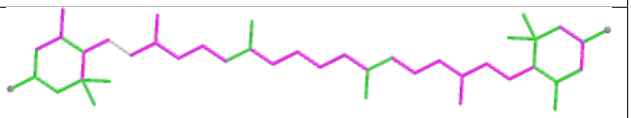


Torsions

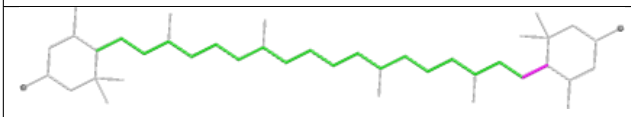
Rings

Ligand LUT 2 1620

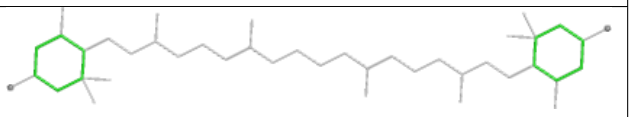
Bond lengths



Bond angles

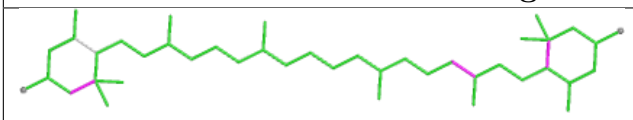


Torsions

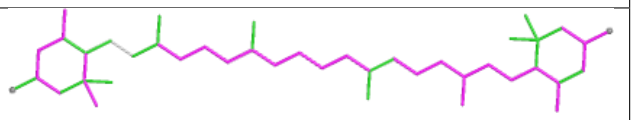


Rings

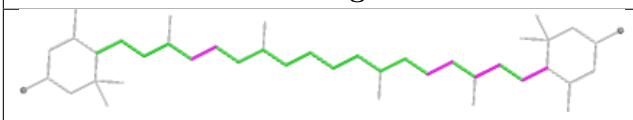
Ligand LUT 1 1621



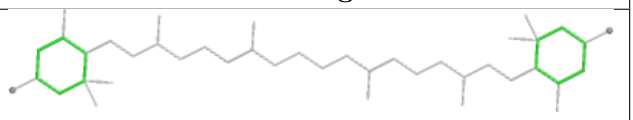
Bond lengths



Bond angles

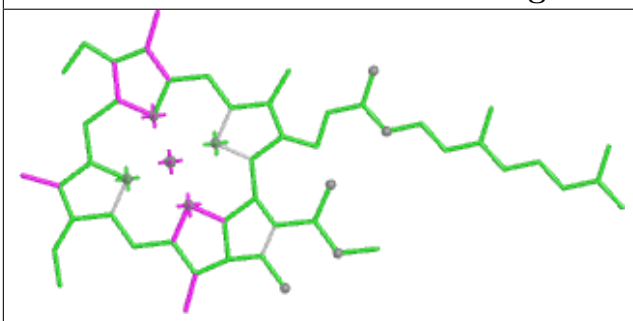


Torsions

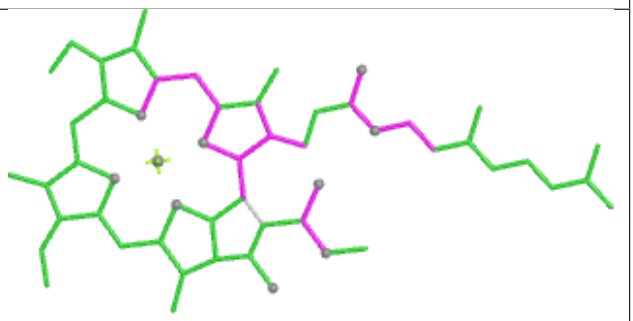


Rings

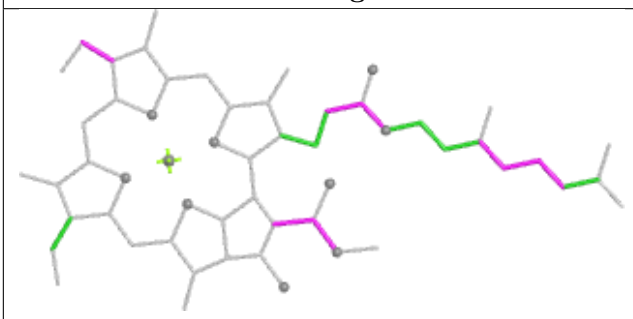
Ligand CLA 2 603



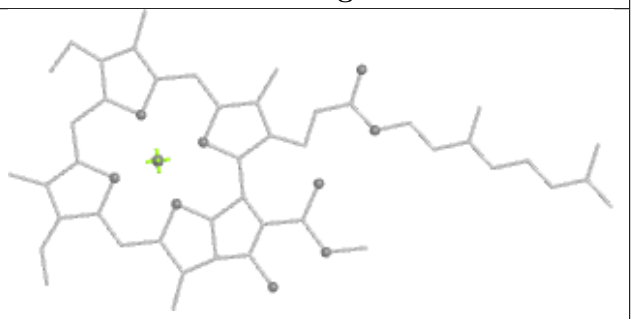
Bond lengths



Bond angles

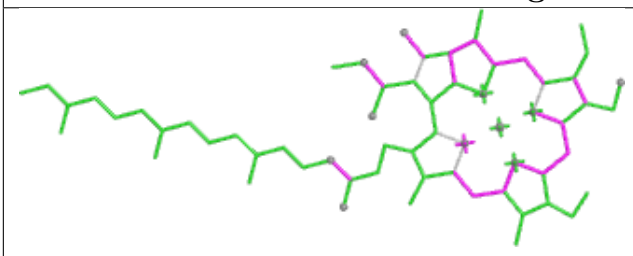


Torsions

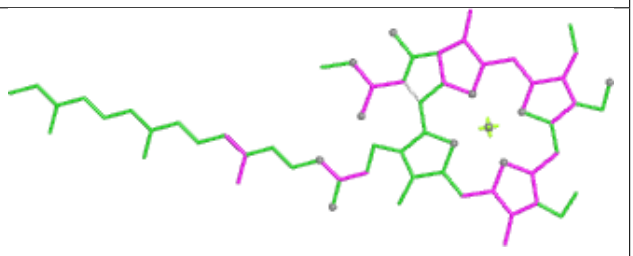


Rings

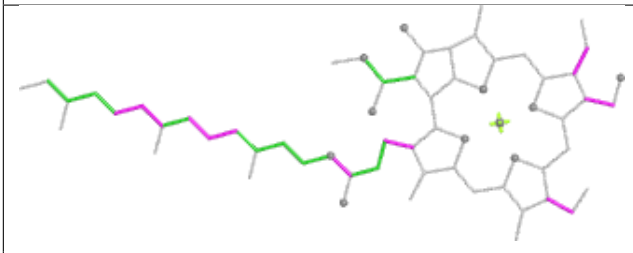
Ligand CHL 1 609



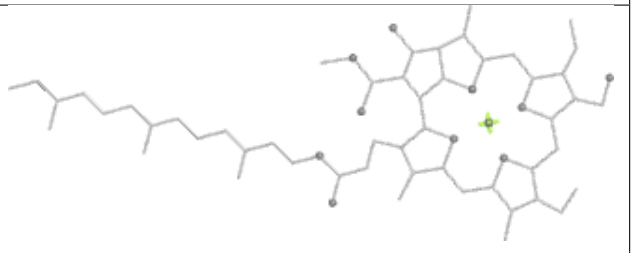
Bond lengths



Bond angles

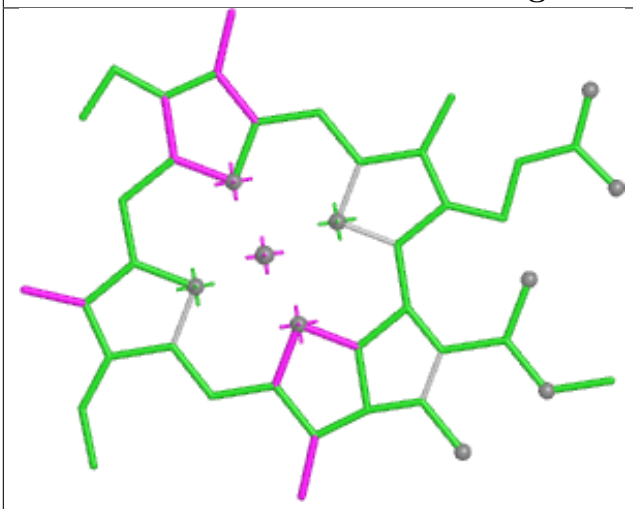


Torsions

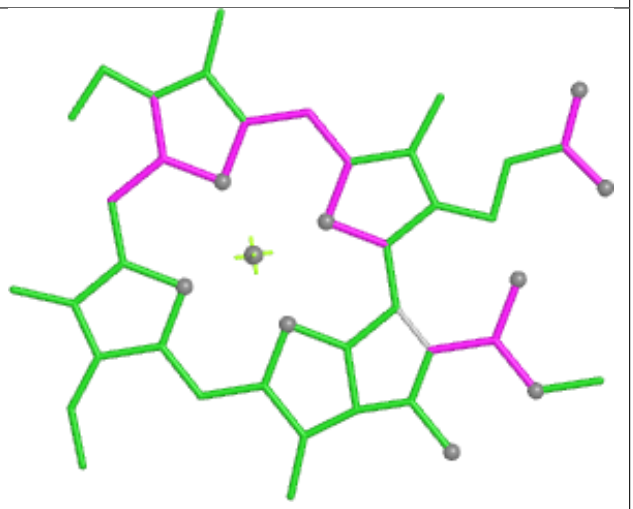


Rings

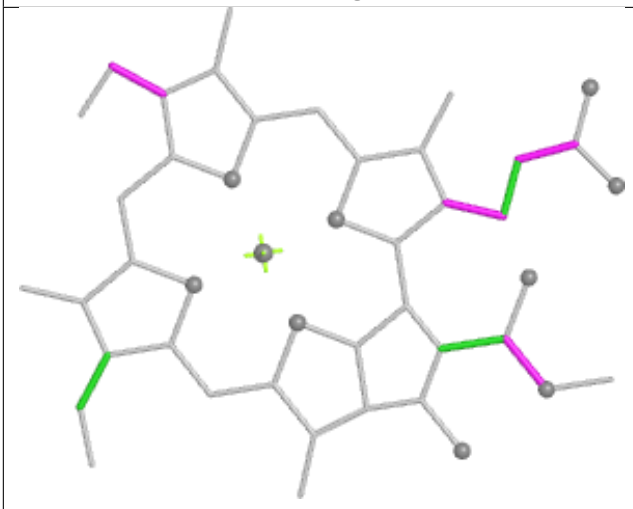
Ligand CLA 2 614



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

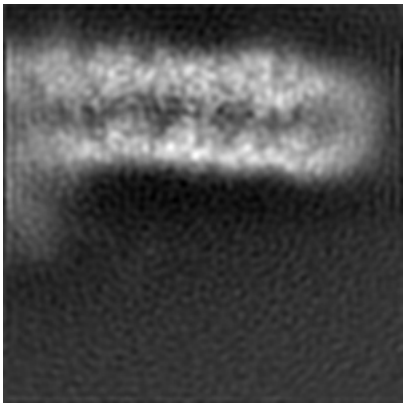
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6744. These allow visual inspection of the internal detail of the map and identification of artifacts.

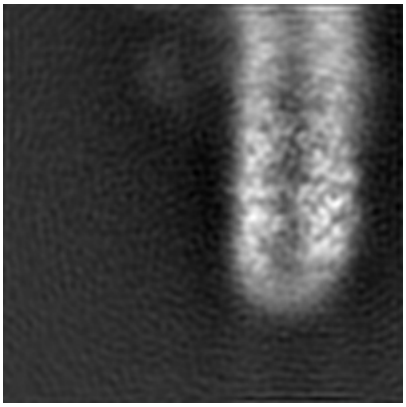
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

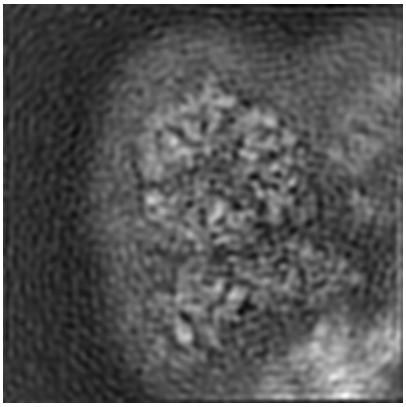
6.1.1 Primary map



X



Y

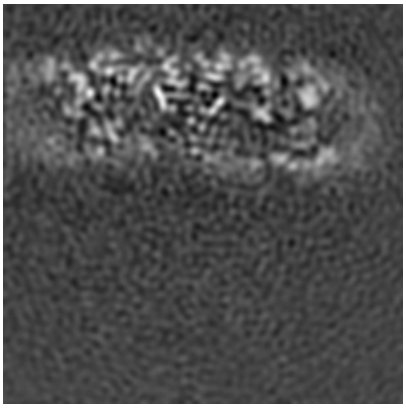


Z

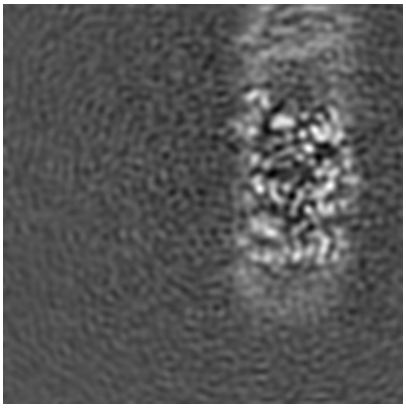
The images above show the map projected in three orthogonal directions.

6.2 Central slices

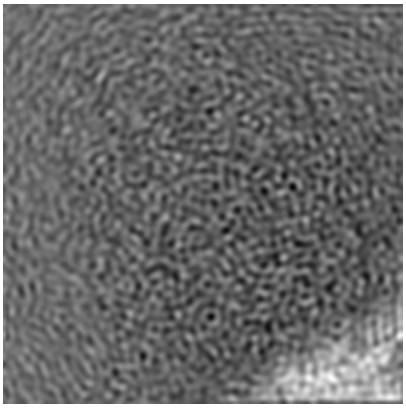
6.2.1 Primary map



X Index: 75



Y Index: 75

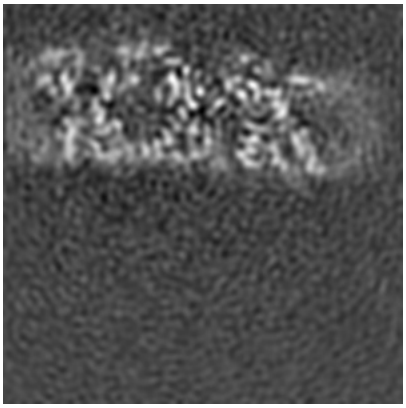


Z Index: 75

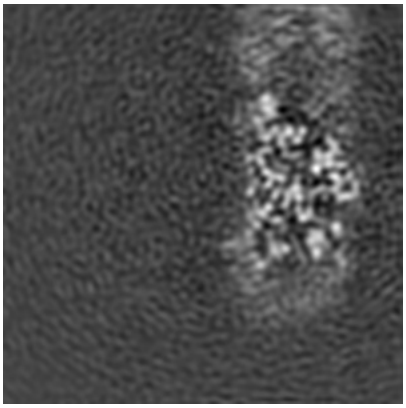
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

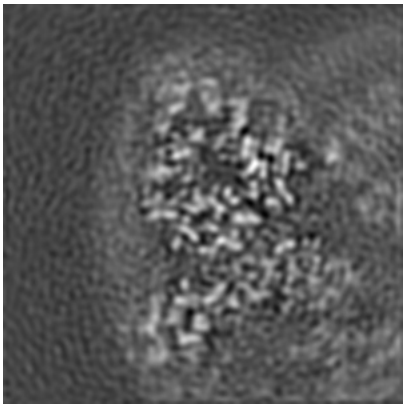
6.3.1 Primary map



X Index: 69



Y Index: 70

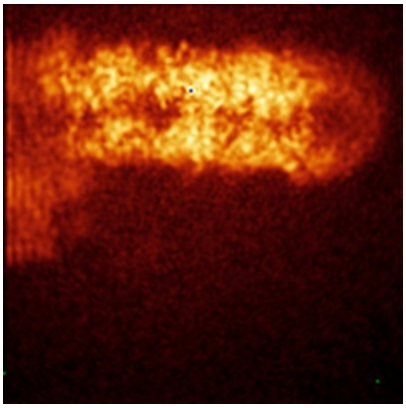


Z Index: 118

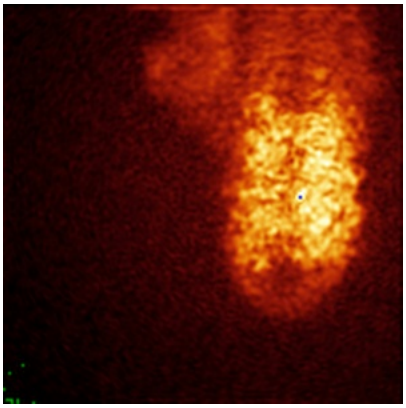
The images above show the largest variance slices of the map in three orthogonal directions.

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

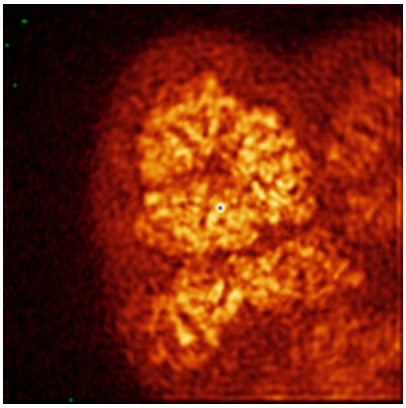
6.4.1 Primary map



X



Y



Z

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 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

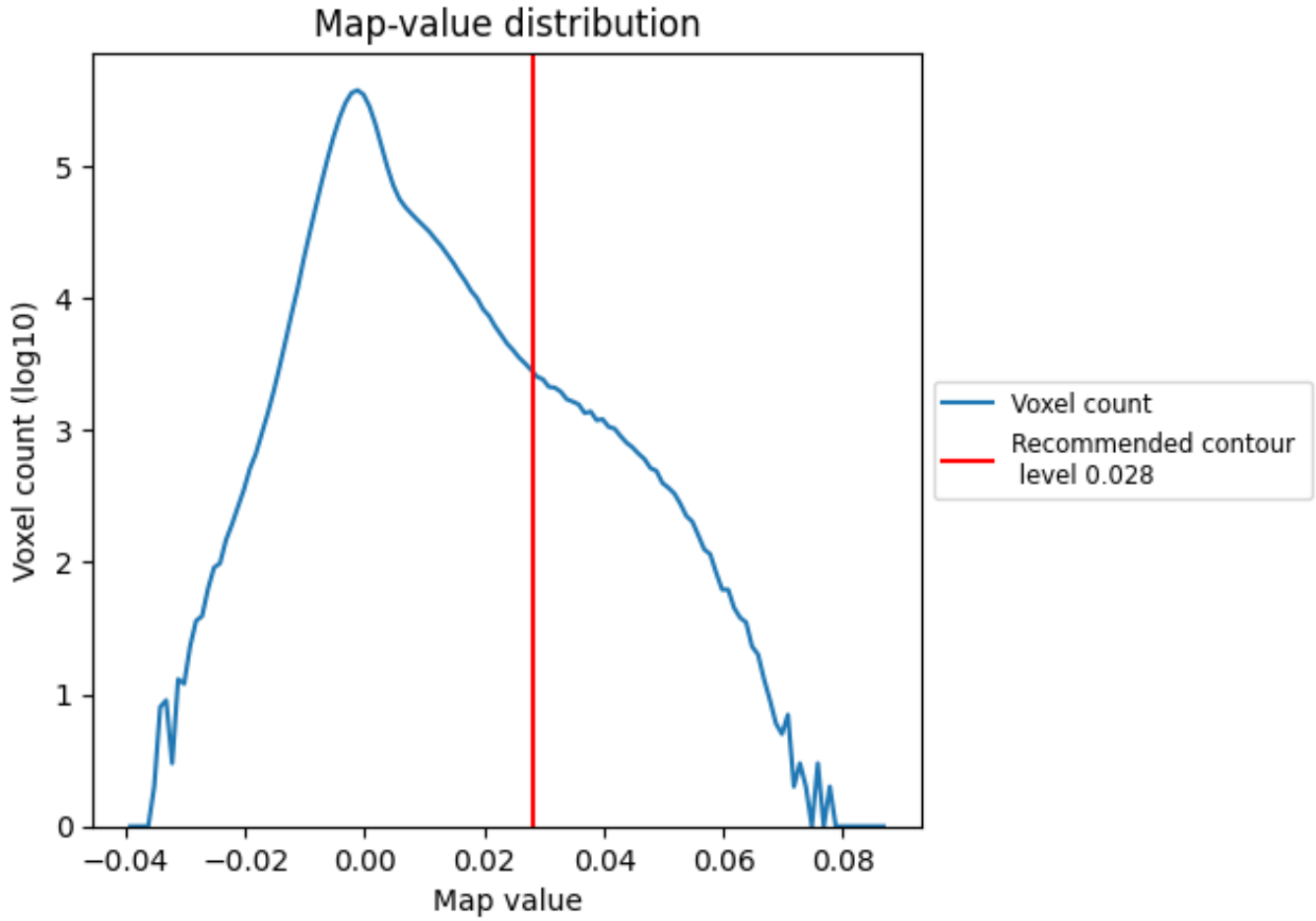
6.6 Mask visualisation (i)

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

7 Map analysis

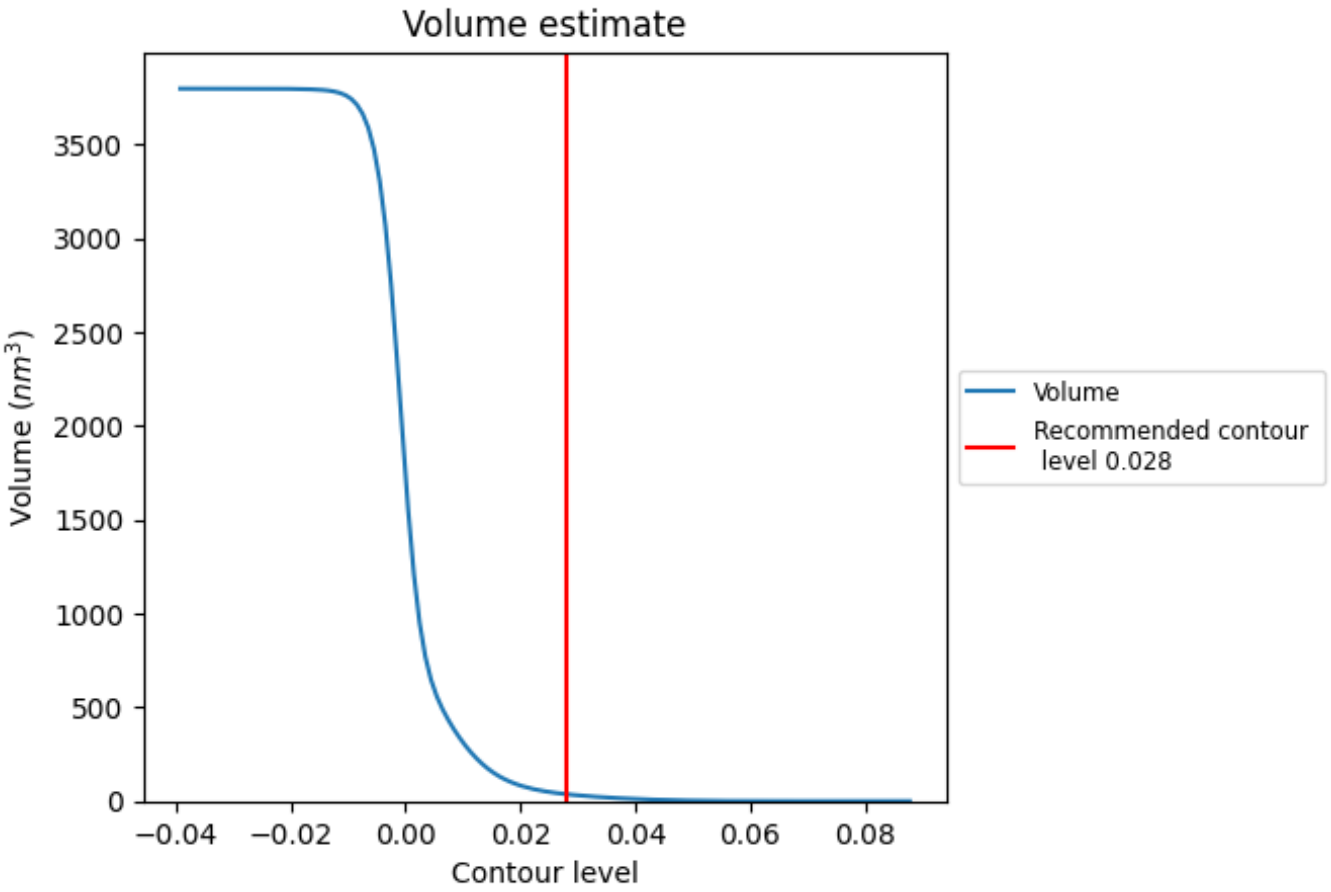
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

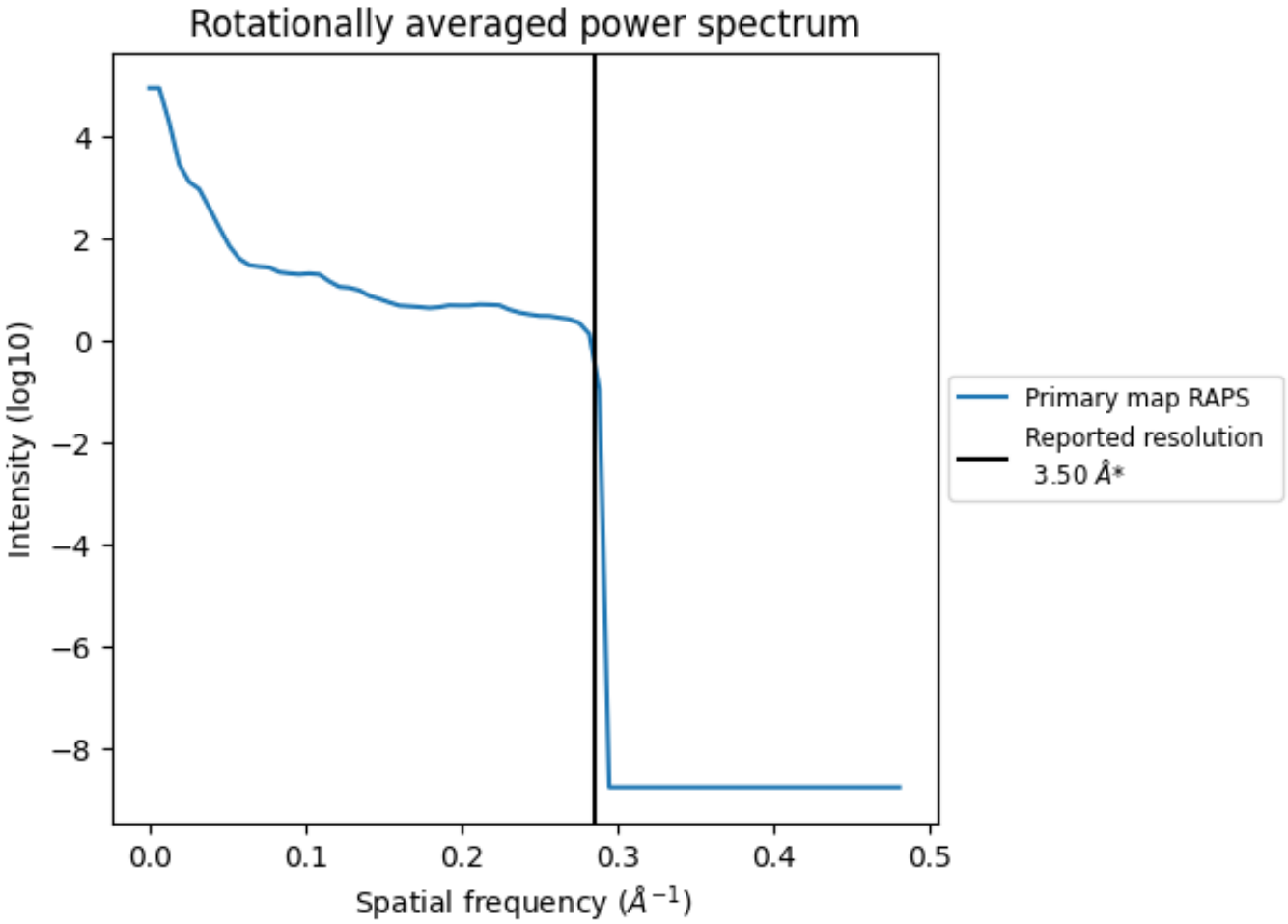
7.2 Volume estimate (i)



The volume at the recommended contour level is 37 nm^3; this corresponds to an approximate mass of 33 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 0.286 Å^{-1}

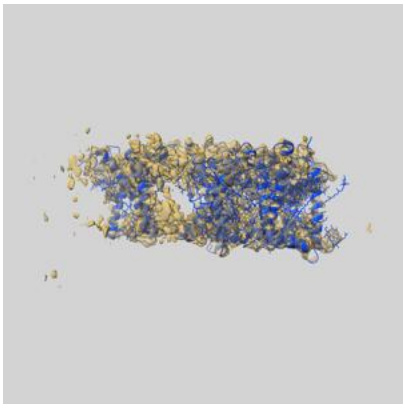
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

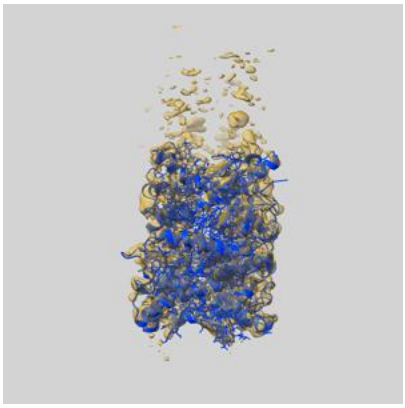
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6744 and PDB model 5XNO. Per-residue inclusion information can be found in section 3 on page 12.

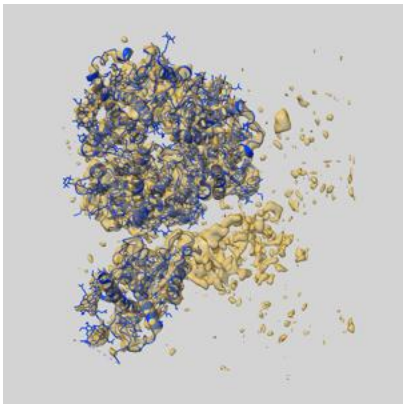
9.1 Map-model overlay



X



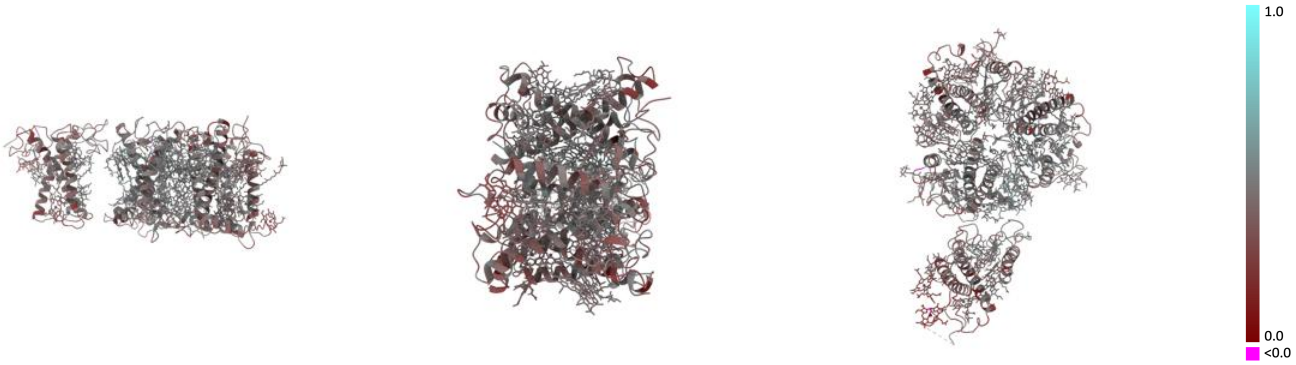
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

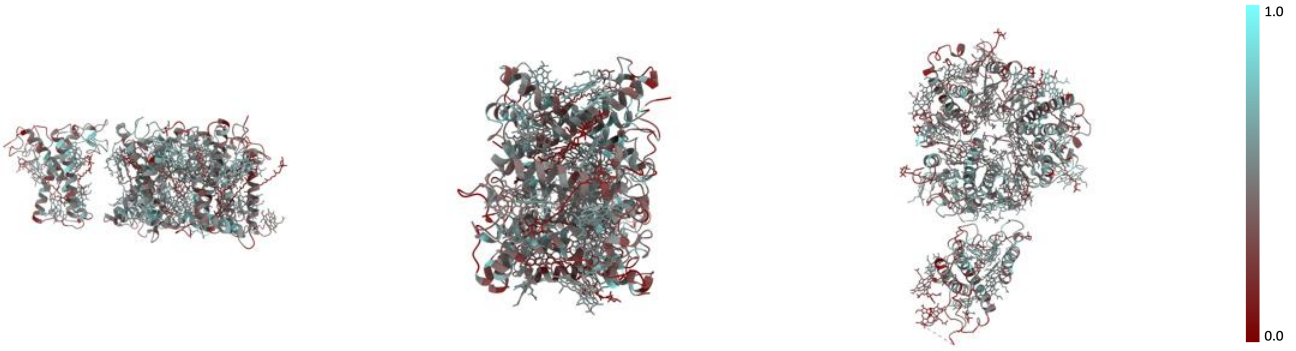
9.2 Q-score mapped to coordinate model (i)



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.

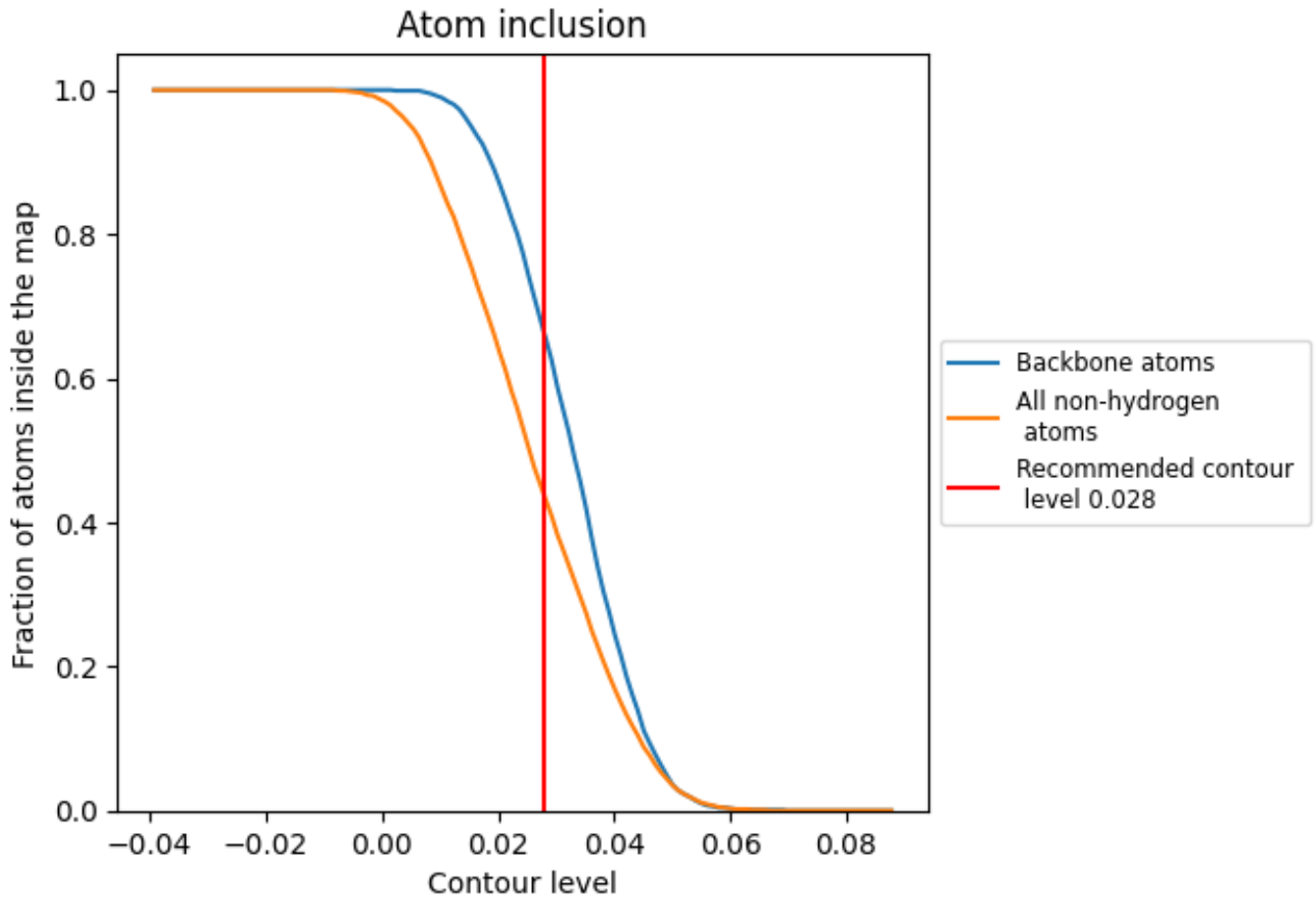
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4360	0.4100
1	0.4500	0.4300
2	0.4070	0.3980
3	0.4720	0.4390
4	0.4080	0.3640