wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 11:33 AM EDT

PDB ID	:	4LCZ / pdb_00004lcz
Title	:	Crystal structure of a multilayer-packed major light-harvesting complex
Authors	:	Wan, T.; Li, M.; Chang, W.R.
Deposited on	:	2013-06-24
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

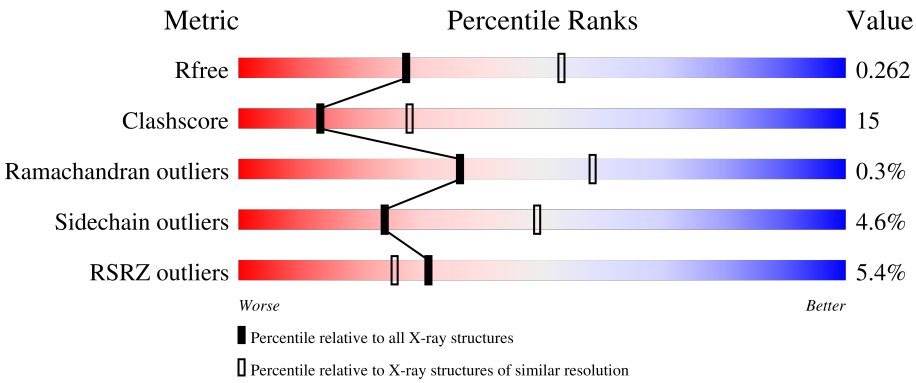
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	224	8% 71% 20% • 7%
1	B	224	% 74% 19% 7%
1	C	224	7% 76% 17% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CHL	A	305	X	-	-	-
5	CHL	A	311	X	-	-	-
5	CHL	A	312	X	-	-	-
5	CHL	A	313	X	-	-	-
5	CHL	B	305	X	-	-	-
5	CHL	B	311	X	-	-	-
5	CHL	B	312	X	-	-	-
5	CHL	B	313	X	-	-	-
5	CHL	C	305	X	-	-	-
5	CHL	C	311	X	-	-	-
5	CHL	C	312	X	-	-	-
5	CHL	C	313	X	-	-	-
6	CLA	C	307	-	-	X	-
7	CAC	A	319	-	X	-	-
7	CAC	B	319	-	X	-	-
7	CAC	C	319	-	X	-	-

2 Entry composition (i)

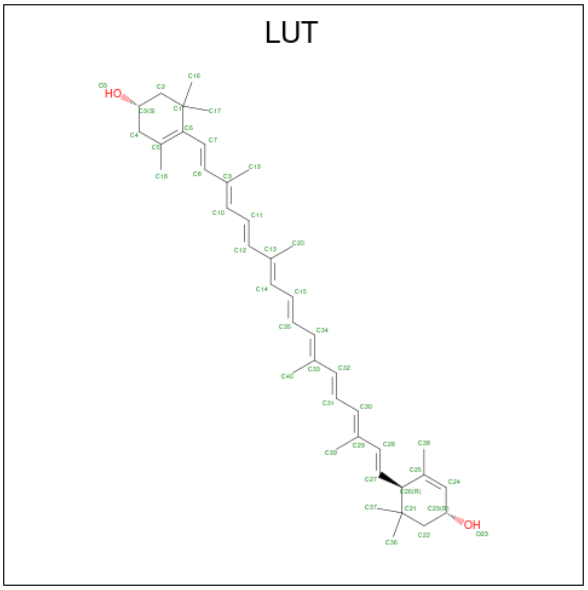
There are 10 unique types of molecules in this entry. The entry contains 8016 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Major chlorophyll a/b binding protein LHCb1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1579	1023	257	292	7	0	0	0
1	B	208	1579	1023	257	292	7	0	0	0
1	C	208	1579	1023	257	292	7	0	0	0

- Molecule 2 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			ZeroOcc	AltConf
			Total	C	O		
2	A	1	42	40	2	0	0
2	A	1	42	40	2	0	0
2	B	1	42	40	2	0	0

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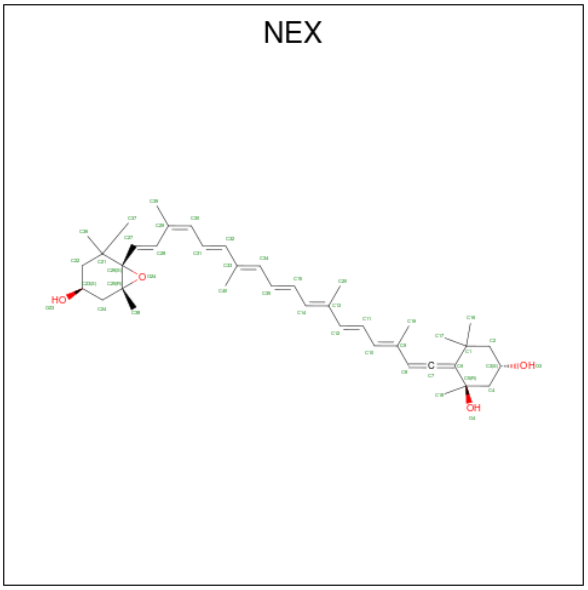
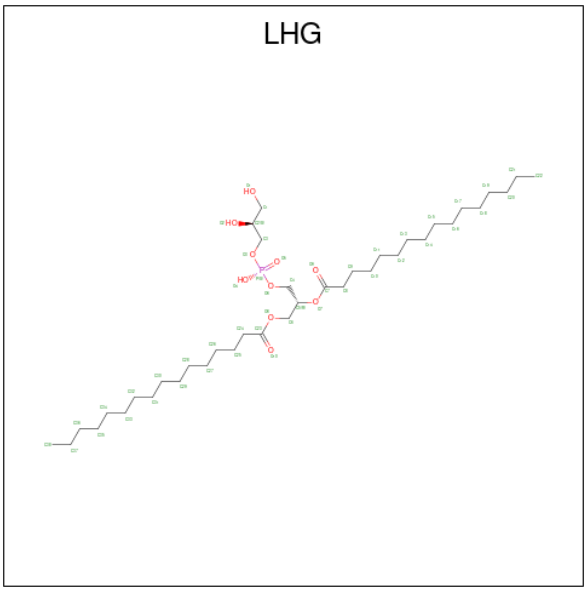
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	B	1	42	40	2	0	0
			Total	C	O		
2	C	1	42	40	2	0	0
			Total	C	O		
2	C	1	42	40	2	0	0

- Molecule 3 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: $C_{40}H_{56}O_4$).



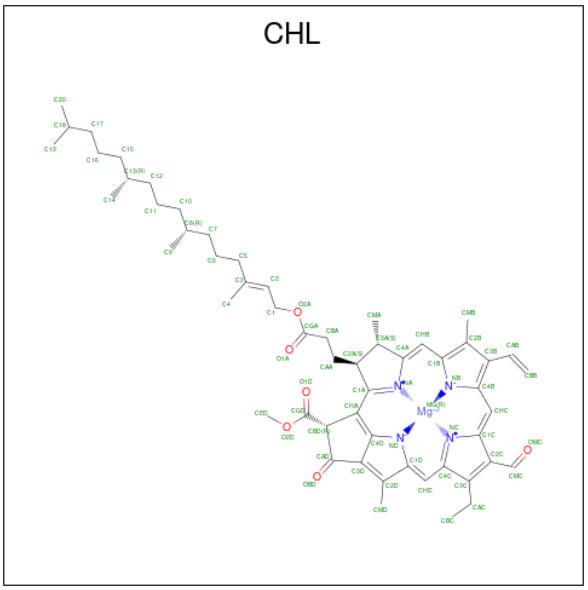
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	44	40	4	0	0
			Total	C	O		
3	B	1	44	40	4	0	0
			Total	C	O		
3	C	1	44	40	4	0	0

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	A	1	49	38	10	1	0	0
			Total	C	O	P		
4	B	1	49	38	10	1	0	0
			Total	C	O	P		
4	C	1	49	38	10	1	0	0

- Molecule 5 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0

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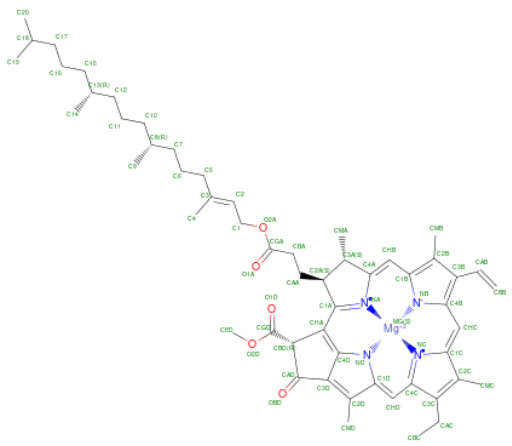
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	A	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	A	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	B	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	C	1	66	55	1	4	6	0	0

- Molecule 6 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).

CLA



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	A	1	62	52	1	4	5	0	0
			Total	C	Mg	N	O		
6	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	A	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
6	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	B	1	62	52	1	4	5	0	0
			Total	C	Mg	N	O		
6	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	B	1	65	55	1	4	5	0	0

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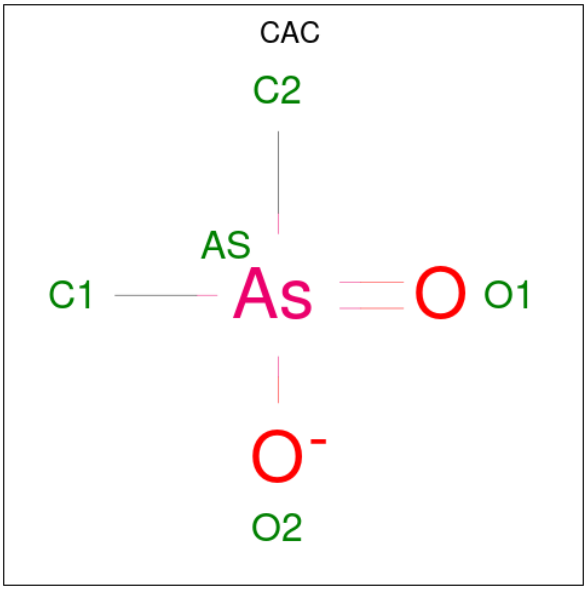
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	B	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	62	52	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
6	C	1	40	32	1	4	3	0	0

- Molecule 7 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
7	A	1	5	1	2	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	As	C	O		
7	B	1	5	1	2	2	0	0
7	C	1	5	1	2	2	0	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
8	A	3	3	3	0	0
8	B	1	1	1	0	0
8	C	1	1	1	0	0

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
9	B	2	2	2	0	0
9	C	3	3	3	0	0

- Molecule 10 is water.

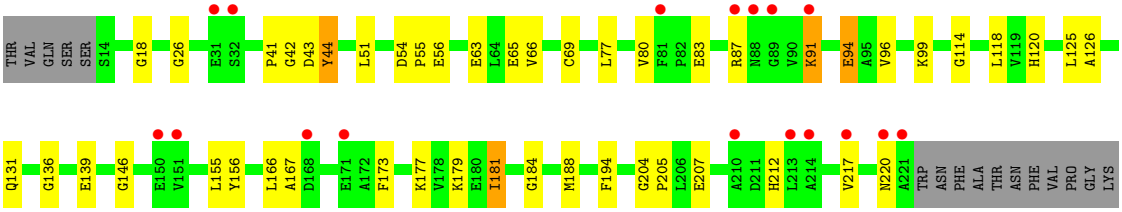
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	58	58	58	0	0
10	B	46	46	46	0	0
10	C	52	52	52	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

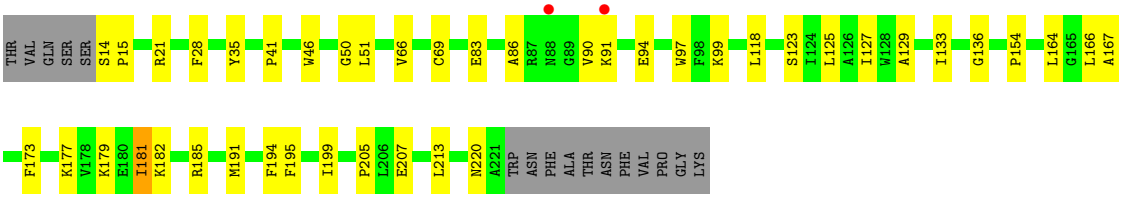
• Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain A:



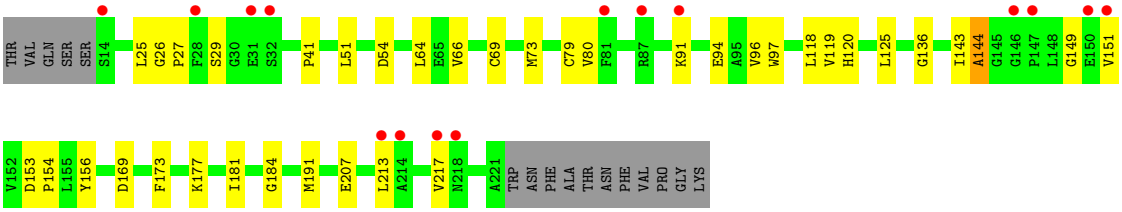
• Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain B:



• Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	199.19Å 115.10Å 109.60Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	43.45 – 2.60 43.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.4 (43.45-2.60) 83.7 (43.45-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.250 , 0.258 0.242 , 0.262	Depositor DCC
R_{free} test set	3046 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 70.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	8016	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.64	0/1626	0.97	9/2212 (0.4%)
1	B	0.61	0/1626	0.93	0/2212
1	C	0.65	0/1626	0.98	6/2212 (0.3%)
All	All	0.63	0/4878	0.96	15/6636 (0.2%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	54	ASP	CA-C-N	6.47	126.40	119.28
1	C	54	ASP	C-N-CA	6.47	126.40	119.28
1	A	204	GLY	CA-C-N	5.89	126.30	119.47
1	A	204	GLY	C-N-CA	5.89	126.30	119.47
1	A	146	GLY	CA-C-N	5.68	125.35	119.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1579	0	1520	33	0
1	B	1579	0	1521	30	0
1	C	1579	0	1521	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	84	0	112	4	0
2	B	84	0	112	13	0
2	C	84	0	112	7	0
3	A	44	0	56	3	0
3	B	44	0	56	3	0
3	C	44	0	56	3	0
4	A	49	0	74	9	0
4	B	49	0	74	5	0
4	C	49	0	74	5	0
5	A	363	0	350	21	0
5	B	363	0	350	20	0
5	C	363	0	350	17	0
6	A	493	0	522	37	0
6	B	493	0	524	36	0
6	C	492	0	521	43	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	A	3	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	2	0	0	0	0
9	C	3	0	0	0	0
10	A	58	0	0	1	0
10	B	46	0	0	2	0
10	C	52	0	0	2	0
All	All	8016	0	7905	231	0

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

The worst 5 of 231 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:C:304:LHG:C14	6:C:317:CLA:H93	1.72	1.19
6:C:306:CLA:H92	6:C:307:CLA:HMA3	1.29	1.13
4:A:304:LHG:H142	6:A:317:CLA:H93	1.22	1.12
4:A:304:LHG:C14	6:A:317:CLA:H93	1.83	1.08
6:A:307:CLA:C9	6:C:307:CLA:H92	1.85	1.06

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/224 (92%)	199 (97%)	6 (3%)	1 (0%)	24	46
1	B	206/224 (92%)	199 (97%)	7 (3%)	0	100	100
1	C	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	24	46
All	All	618/672 (92%)	596 (96%)	20 (3%)	2 (0%)	36	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	C	119	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/174 (92%)	151 (94%)	9 (6%)	19	40
1	B	160/174 (92%)	155 (97%)	5 (3%)	35	63
1	C	160/174 (92%)	152 (95%)	8 (5%)	22	46
All	All	480/522 (92%)	458 (95%)	22 (5%)	24	49

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	80	VAL

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Mol	Chain	Res	Type
1	C	96	VAL
1	C	94	GLU
1	C	125	LEU
1	A	181	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	183	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)

Of 67 ligands modelled in this entry, 10 are monoatomic - leaving 57 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CLA	B	308	10	66,70,73	2.57	17 (25%)	78,109,113	2.03	16 (20%)
6	CLA	B	315	4	69,73,73	2.51	16 (23%)	82,113,113	2.16	22 (26%)
7	CAC	A	319	8	2,4,4	3.60	2 (100%)	4,6,6	4.68	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	CLA	B	316	1	69,73,73	2.65	16 (23%)	82,113,113	2.10	21 (25%)
5	CHL	C	305	1	70,74,74	2.18	18 (25%)	79,114,114	2.02	22 (27%)
5	CHL	C	312	10	70,74,74	2.16	18 (25%)	79,114,114	2.04	25 (31%)
2	LUT	C	301	-	42,43,43	1.01	2 (4%)	51,60,60	1.95	17 (33%)
6	CLA	B	307	1	69,73,73	2.35	19 (27%)	82,113,113	2.08	21 (25%)
6	CLA	B	314	1	69,73,73	2.18	17 (24%)	82,113,113	1.82	18 (21%)
6	CLA	A	308	10	66,70,73	2.68	14 (21%)	78,109,113	2.08	19 (24%)
3	NEX	A	303	-	40,46,46	1.05	3 (7%)	50,70,70	2.69	16 (32%)
5	CHL	A	305	1	70,74,74	2.06	16 (22%)	79,114,114	2.07	20 (25%)
5	CHL	B	310	10	55,59,74	2.58	15 (27%)	61,96,114	2.24	17 (27%)
4	LHG	A	304	6	48,48,48	0.93	2 (4%)	51,54,54	1.02	2 (3%)
7	CAC	C	319	8	2,4,4	3.40	2 (100%)	4,6,6	5.18	3 (75%)
5	CHL	A	313	1	70,74,74	2.28	17 (24%)	79,114,114	1.85	18 (22%)
5	CHL	C	311	10	70,74,74	2.04	19 (27%)	79,114,114	2.01	23 (29%)
2	LUT	A	302	-	42,43,43	0.89	2 (4%)	51,60,60	1.67	10 (19%)
6	CLA	C	306	1	69,73,73	2.54	19 (27%)	82,113,113	2.03	24 (29%)
5	CHL	A	311	10	70,74,74	2.29	15 (21%)	79,114,114	1.90	17 (21%)
5	CHL	B	305	1	70,74,74	2.26	18 (25%)	79,114,114	2.16	20 (25%)
5	CHL	B	312	10	70,74,74	2.11	19 (27%)	79,114,114	1.86	20 (25%)
4	LHG	C	304	6	48,48,48	0.95	2 (4%)	51,54,54	1.04	4 (7%)
5	CHL	C	313	1	70,74,74	2.18	16 (22%)	79,114,114	1.93	21 (26%)
2	LUT	A	301	-	42,43,43	0.91	1 (2%)	51,60,60	1.62	10 (19%)
2	LUT	C	302	-	42,43,43	0.84	1 (2%)	51,60,60	1.87	13 (25%)
5	CHL	A	309	1	52,56,74	2.51	19 (36%)	57,92,114	2.26	17 (29%)
6	CLA	A	315	4	69,73,73	2.53	16 (23%)	82,113,113	1.98	24 (29%)
6	CLA	A	317	1	69,73,73	2.19	16 (23%)	82,113,113	1.76	18 (21%)
2	LUT	B	301	-	42,43,43	0.87	1 (2%)	51,60,60	1.83	14 (27%)
6	CLA	C	308	10	66,70,73	2.19	18 (27%)	78,109,113	1.90	18 (23%)
6	CLA	C	318	1	44,48,73	2.95	18 (40%)	51,82,113	2.21	17 (33%)
6	CLA	A	306	1	69,73,73	2.18	17 (24%)	82,113,113	2.03	20 (24%)
5	CHL	B	309	1	52,56,74	2.52	18 (34%)	57,92,114	2.12	16 (28%)
3	NEX	C	303	-	40,46,46	1.13	3 (7%)	50,70,70	2.78	16 (32%)
5	CHL	A	310	10	55,59,74	2.80	15 (27%)	61,96,114	2.26	21 (34%)
6	CLA	A	316	1	69,73,73	2.88	16 (23%)	82,113,113	1.98	19 (23%)
5	CHL	B	311	10	70,74,74	2.04	18 (25%)	79,114,114	2.03	16 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	CAC	B	319	8	2,4,4	3.74	2 (100%)	4,6,6	4.54	2 (50%)
5	CHL	C	309	1	52,56,74	2.57	20 (38%)	57,92,114	2.13	18 (31%)
6	CLA	A	314	1	69,73,73	2.36	18 (26%)	82,113,113	1.92	19 (23%)
6	CLA	A	318	1	45,49,73	3.02	19 (42%)	54,84,113	2.08	15 (27%)
6	CLA	C	315	4	69,73,73	2.56	19 (27%)	82,113,113	1.90	22 (26%)
6	CLA	C	317	1	69,73,73	2.36	19 (27%)	82,113,113	1.92	21 (25%)
6	CLA	A	307	1	69,73,73	2.20	16 (23%)	82,113,113	2.10	25 (30%)
3	NEX	B	303	-	40,46,46	1.03	3 (7%)	50,70,70	2.75	17 (34%)
6	CLA	C	316	1	69,73,73	2.57	16 (23%)	82,113,113	2.00	20 (24%)
6	CLA	B	306	1	69,73,73	2.26	17 (24%)	82,113,113	2.02	21 (25%)
4	LHG	B	304	6	48,48,48	0.98	2 (4%)	51,54,54	1.11	3 (5%)
5	CHL	B	313	1	70,74,74	2.31	14 (20%)	79,114,114	1.86	18 (22%)
6	CLA	C	314	1	69,73,73	2.34	17 (24%)	82,113,113	1.93	20 (24%)
6	CLA	B	318	1	45,49,73	3.06	19 (42%)	54,84,113	2.13	14 (25%)
2	LUT	B	302	-	42,43,43	1.00	3 (7%)	51,60,60	1.87	14 (27%)
6	CLA	B	317	1	69,73,73	2.27	15 (21%)	82,113,113	1.80	19 (23%)
6	CLA	C	307	1	69,73,73	2.28	19 (27%)	82,113,113	2.05	26 (31%)
5	CHL	C	310	10	55,59,74	2.55	18 (32%)	61,96,114	2.23	20 (32%)
5	CHL	A	312	10	70,74,74	2.27	18 (25%)	79,114,114	2.00	22 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	B	308	10	-	12/36/112/115	-
6	CLA	B	315	4	-	13/39/115/115	-
6	CLA	B	316	1	-	12/39/115/115	-
5	CHL	C	305	1	1/1/15/21	22/41/117/117	-
5	CHL	C	312	10	1/1/15/21	12/41/117/117	-
2	LUT	C	301	-	-	3/29/67/67	0/2/2/2
6	CLA	B	307	1	-	12/39/115/115	-
6	CLA	B	314	1	-	4/39/115/115	-
6	CLA	A	308	10	-	14/36/112/115	-
3	NEX	A	303	-	-	4/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	A	305	1	1/1/15/21	24/41/117/117	-
5	CHL	B	310	10	-	7/23/99/117	-
4	LHG	A	304	6	-	16/53/53/53	-
5	CHL	A	313	1	1/1/15/21	16/41/117/117	-
5	CHL	C	311	10	1/1/15/21	20/41/117/117	-
2	LUT	A	302	-	-	2/29/67/67	0/2/2/2
6	CLA	C	306	1	-	9/39/115/115	-
5	CHL	A	311	10	1/1/15/21	20/41/117/117	-
5	CHL	B	305	1	1/1/15/21	22/41/117/117	-
5	CHL	B	312	10	1/1/15/21	10/41/117/117	-
4	LHG	C	304	6	-	13/53/53/53	-
5	CHL	C	313	1	1/1/15/21	17/41/117/117	-
2	LUT	A	301	-	-	2/29/67/67	0/2/2/2
2	LUT	C	302	-	-	2/29/67/67	0/2/2/2
5	CHL	A	309	1	-	5/20/96/117	-
6	CLA	A	315	4	-	14/39/115/115	-
6	CLA	A	317	1	-	16/39/115/115	-
2	LUT	B	301	-	-	0/29/67/67	0/2/2/2
6	CLA	C	308	10	-	10/36/112/115	-
6	CLA	C	318	1	-	2/10/82/115	-
6	CLA	A	306	1	-	7/39/115/115	-
5	CHL	B	309	1	-	7/20/96/117	-
3	NEX	C	303	-	-	6/27/83/83	0/3/3/3
5	CHL	A	310	10	-	10/23/99/117	-
6	CLA	A	316	1	-	13/39/115/115	-
5	CHL	B	311	10	1/1/15/21	21/41/117/117	-
5	CHL	C	309	1	-	1/20/96/117	-
6	CLA	A	314	1	-	3/39/115/115	-
6	CLA	A	318	1	-	0/10/86/115	-
6	CLA	C	315	4	-	11/39/115/115	-
6	CLA	C	317	1	-	11/39/115/115	-
6	CLA	A	307	1	-	12/39/115/115	-
3	NEX	B	303	-	-	4/27/83/83	0/3/3/3
6	CLA	C	316	1	-	12/39/115/115	-
6	CLA	B	306	1	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LHG	B	304	6	-	16/53/53/53	-
5	CHL	B	313	1	1/1/15/21	15/41/117/117	-
6	CLA	C	314	1	-	8/39/115/115	-
6	CLA	B	318	1	-	2/10/86/115	-
2	LUT	B	302	-	-	2/29/67/67	0/2/2/2
6	CLA	B	317	1	-	18/39/115/115	-
6	CLA	C	307	1	-	13/39/115/115	-
5	CHL	C	310	10	-	8/23/99/117	-
5	CHL	A	312	10	1/1/15/21	11/41/117/117	-

The worst 5 of 755 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	316	CLA	MG-NA	18.03	2.49	2.06
6	A	308	CLA	MG-NA	15.46	2.43	2.06
6	B	316	CLA	MG-NA	15.07	2.42	2.06
6	C	316	CLA	MG-NA	14.04	2.39	2.06
5	A	310	CHL	MG-NA	13.49	2.38	2.06

The worst 5 of 974 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	303	NEX	O24-C25-C24	13.00	125.68	113.49
3	B	303	NEX	O24-C25-C24	12.59	125.29	113.49
3	A	303	NEX	O24-C25-C24	11.71	124.46	113.49
7	A	319	CAC	O2-AS-C2	-7.82	86.90	105.84
6	A	314	CLA	C4A-NA-C1A	7.50	110.10	106.68

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	305	CHL	C8
5	A	311	CHL	C8
5	A	312	CHL	C8
5	A	313	CHL	C8
5	B	305	CHL	C8

5 of 552 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	NEX	C11-C12-C13-C14
3	B	303	NEX	O24-C26-C27-C28
4	A	304	LHG	C4-O6-P-O3
4	A	304	LHG	C4-O6-P-O4
4	A	304	LHG	C4-O6-P-O5

There are no ring outliers.

51 monomers are involved in 184 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	315	CLA	5	0
6	B	316	CLA	5	0
5	C	305	CHL	6	0
5	C	312	CHL	3	0
2	C	301	LUT	2	0
6	B	307	CLA	16	0
6	B	314	CLA	5	0
3	A	303	NEX	3	0
5	A	305	CHL	7	0
5	B	310	CHL	2	0
4	A	304	LHG	9	0
5	A	313	CHL	6	0
5	C	311	CHL	3	0
2	A	302	LUT	1	0
6	C	306	CLA	13	0
5	A	311	CHL	4	0
5	B	305	CHL	9	0
5	B	312	CHL	2	0
4	C	304	LHG	5	0
5	C	313	CHL	4	0
2	A	301	LUT	3	0
2	C	302	LUT	5	0
5	A	309	CHL	2	0
6	A	315	CLA	3	0
6	A	317	CLA	7	0
2	B	301	LUT	7	0
6	C	308	CLA	1	0
6	C	318	CLA	2	0
6	A	306	CLA	6	0
5	B	309	CHL	1	0
3	C	303	NEX	3	0
5	A	310	CHL	3	0
6	A	316	CLA	4	0

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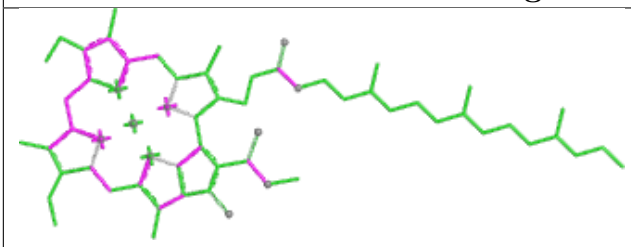
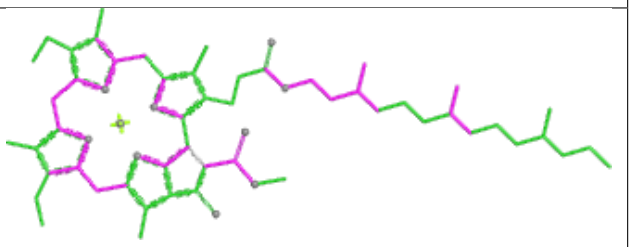
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	311	CHL	5	0
6	A	314	CLA	6	0
6	A	318	CLA	1	0
6	C	315	CLA	2	0
6	C	317	CLA	4	0
6	A	307	CLA	17	0
3	B	303	NEX	3	0
6	C	316	CLA	2	0
6	B	306	CLA	11	0
4	B	304	LHG	5	0
5	B	313	CHL	2	0
6	C	314	CLA	5	0
6	B	318	CLA	1	0
2	B	302	LUT	6	0
6	B	317	CLA	3	0
6	C	307	CLA	22	0
5	C	310	CHL	2	0
5	A	312	CHL	2	0

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

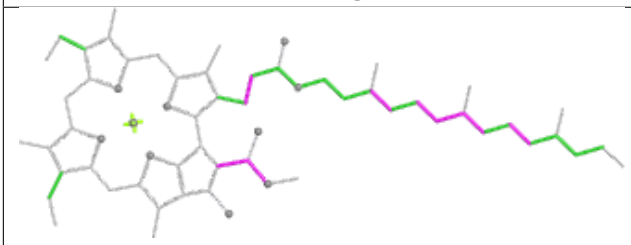
Ligand CLA B 308



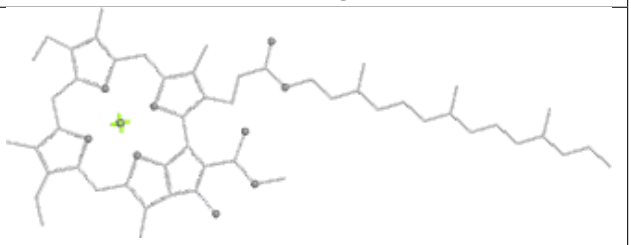
Bond lengths



Bond angles

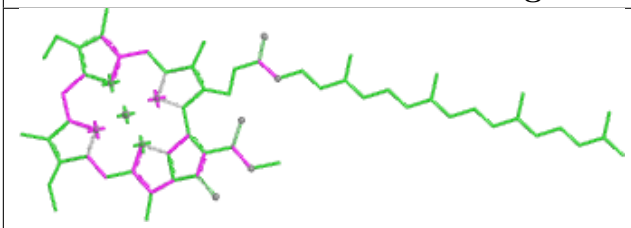


Torsions

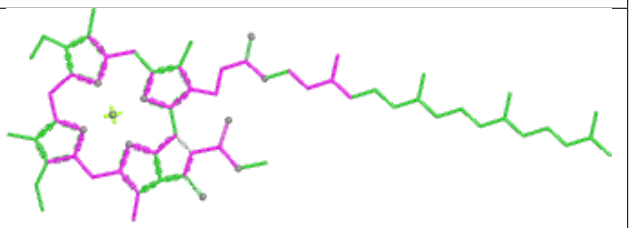


Rings

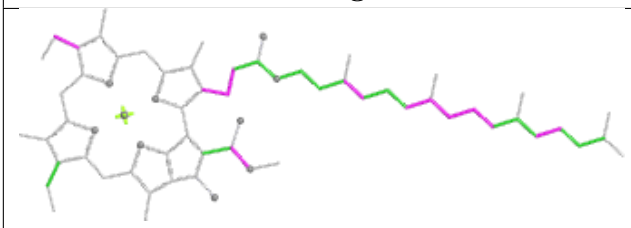
Ligand CLA B 315



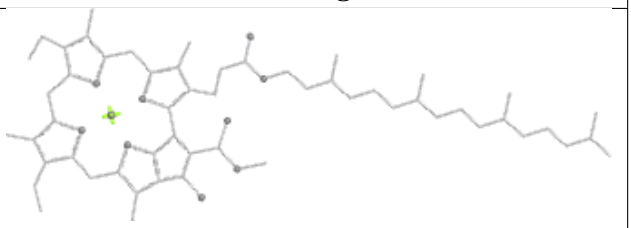
Bond lengths



Bond angles

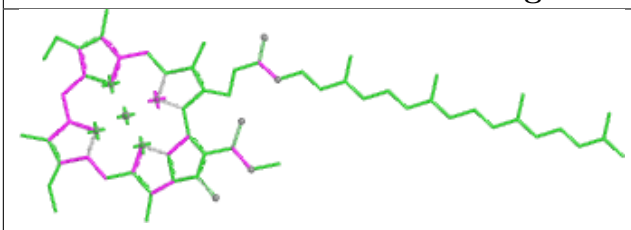


Torsions

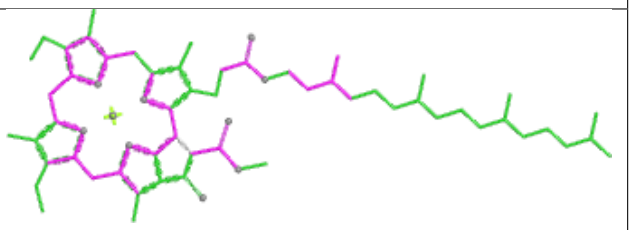


Rings

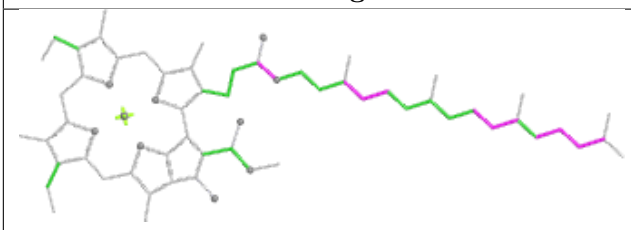
Ligand CLA B 316



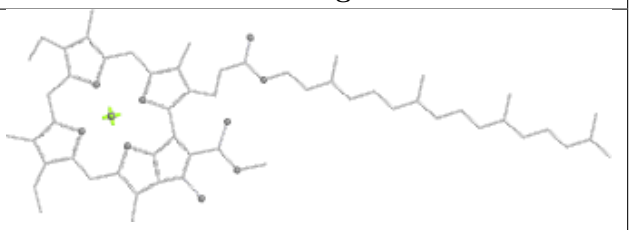
Bond lengths



Bond angles

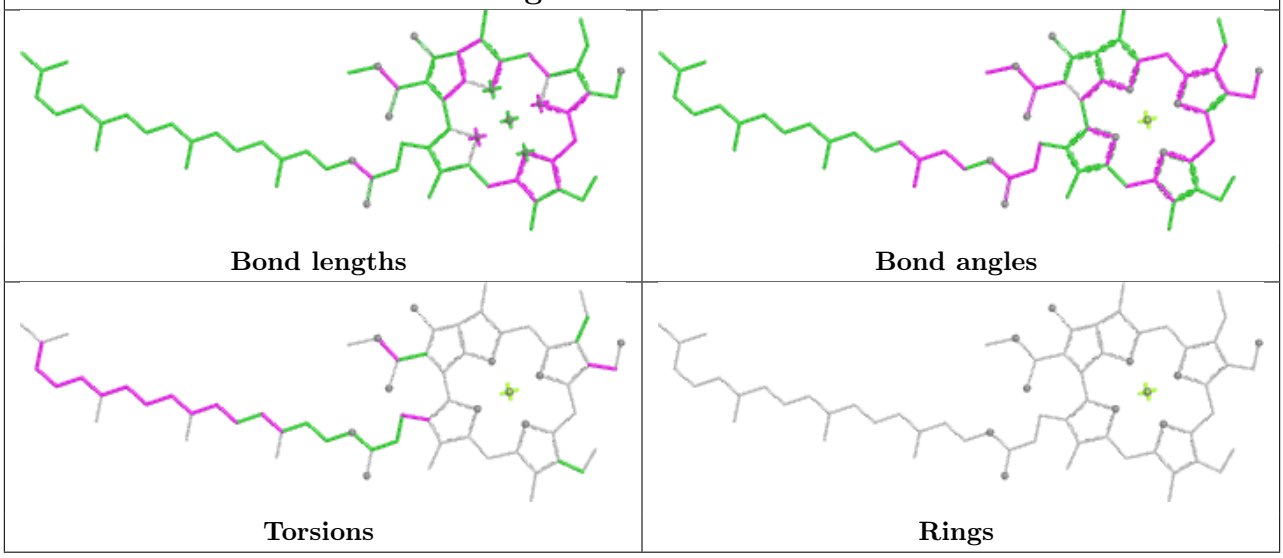


Torsions

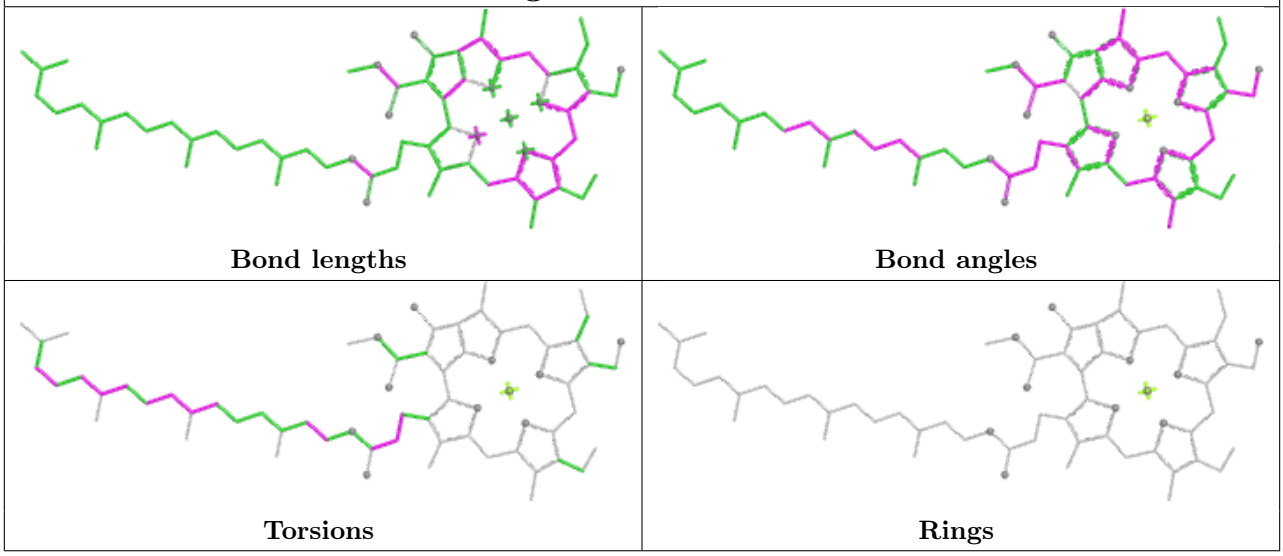


Rings

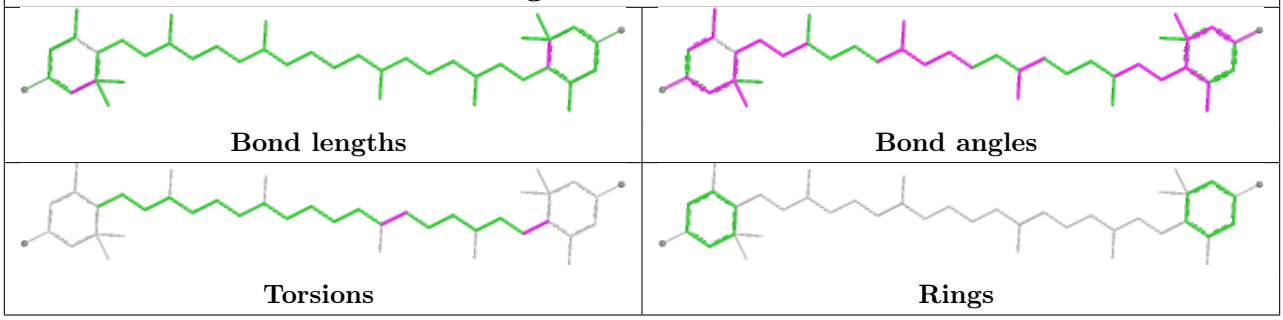
Ligand CHL C 305



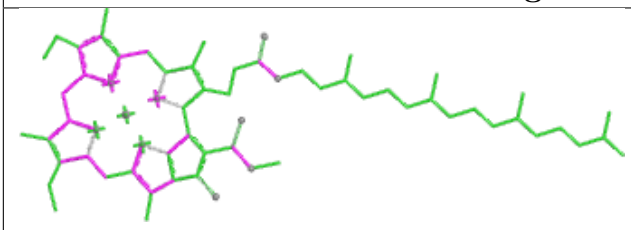
Ligand CHL C 312



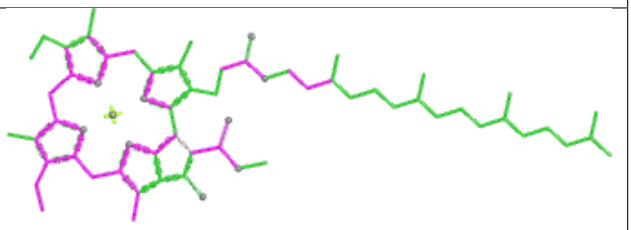
Ligand LUT C 301



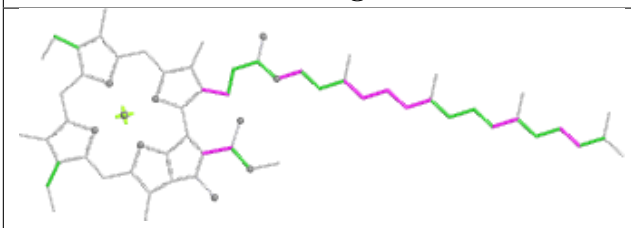
Ligand CLA B 307



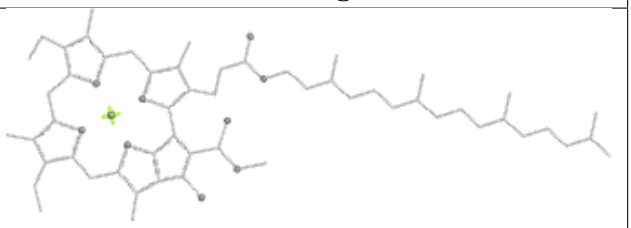
Bond lengths



Bond angles

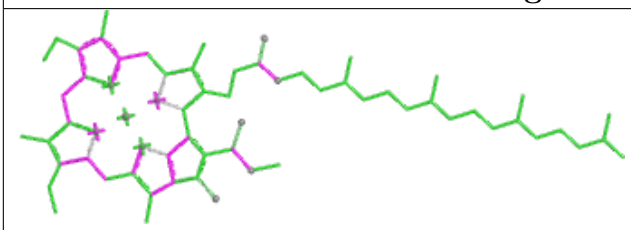


Torsions

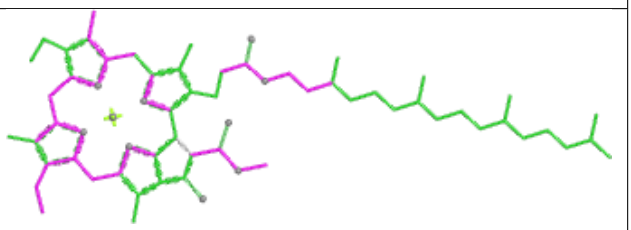


Rings

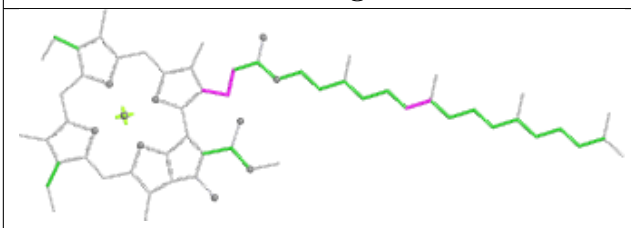
Ligand CLA B 314



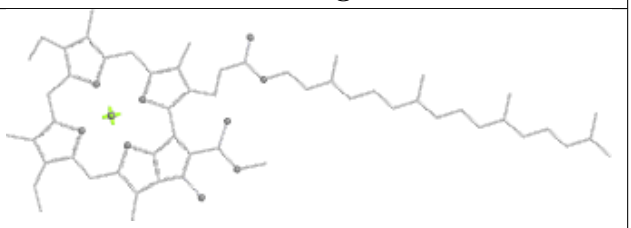
Bond lengths



Bond angles

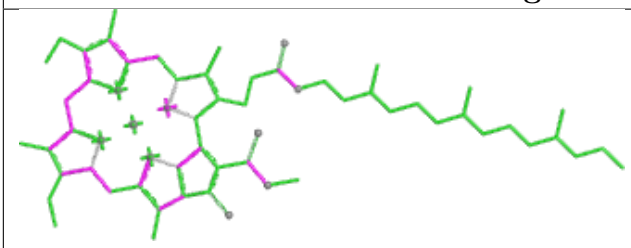


Torsions

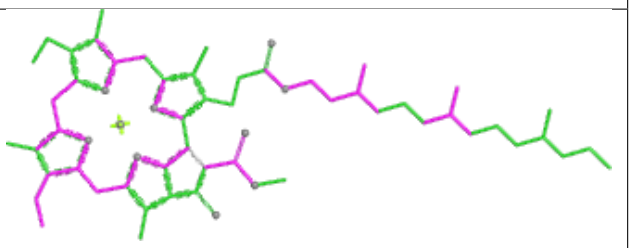


Rings

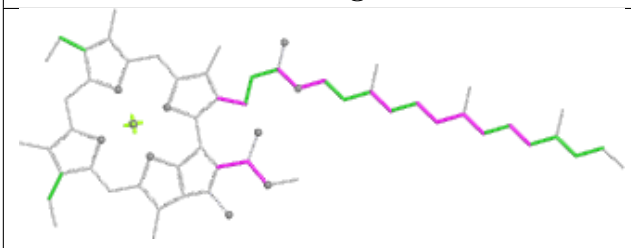
Ligand CLA A 308



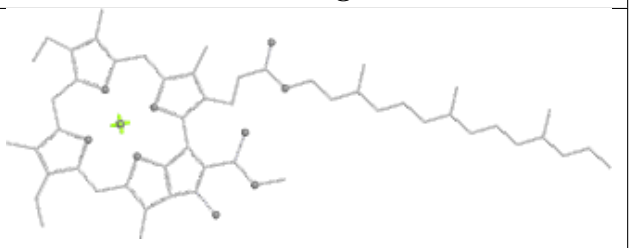
Bond lengths



Bond angles

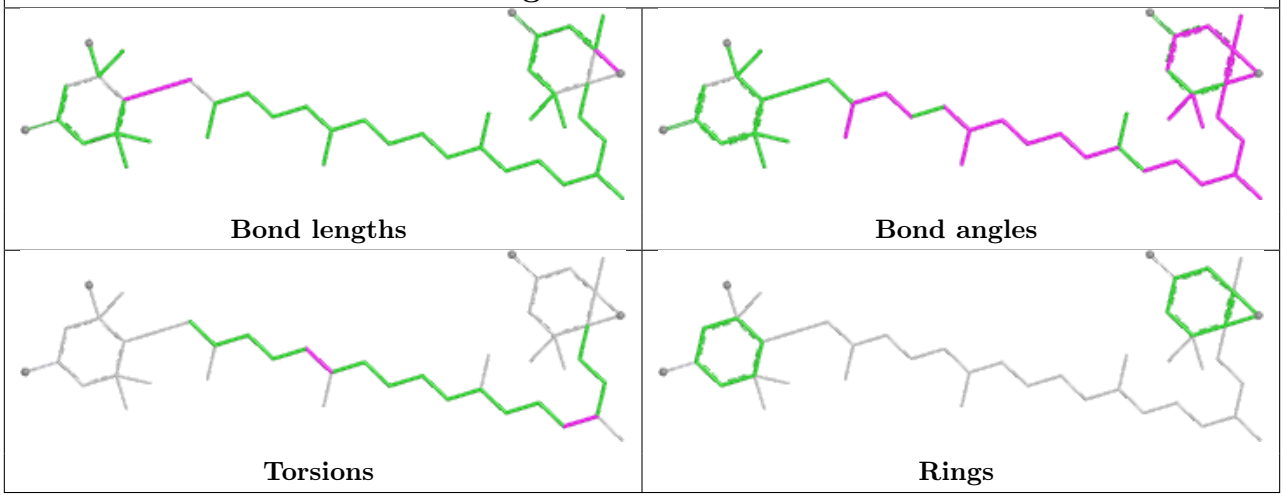


Torsions

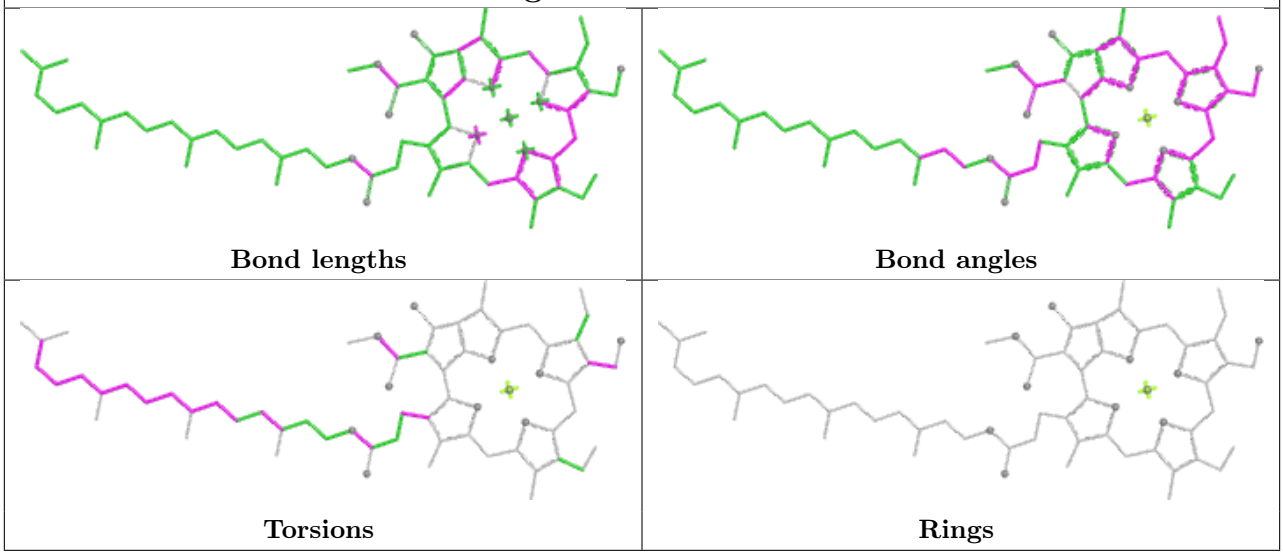


Rings

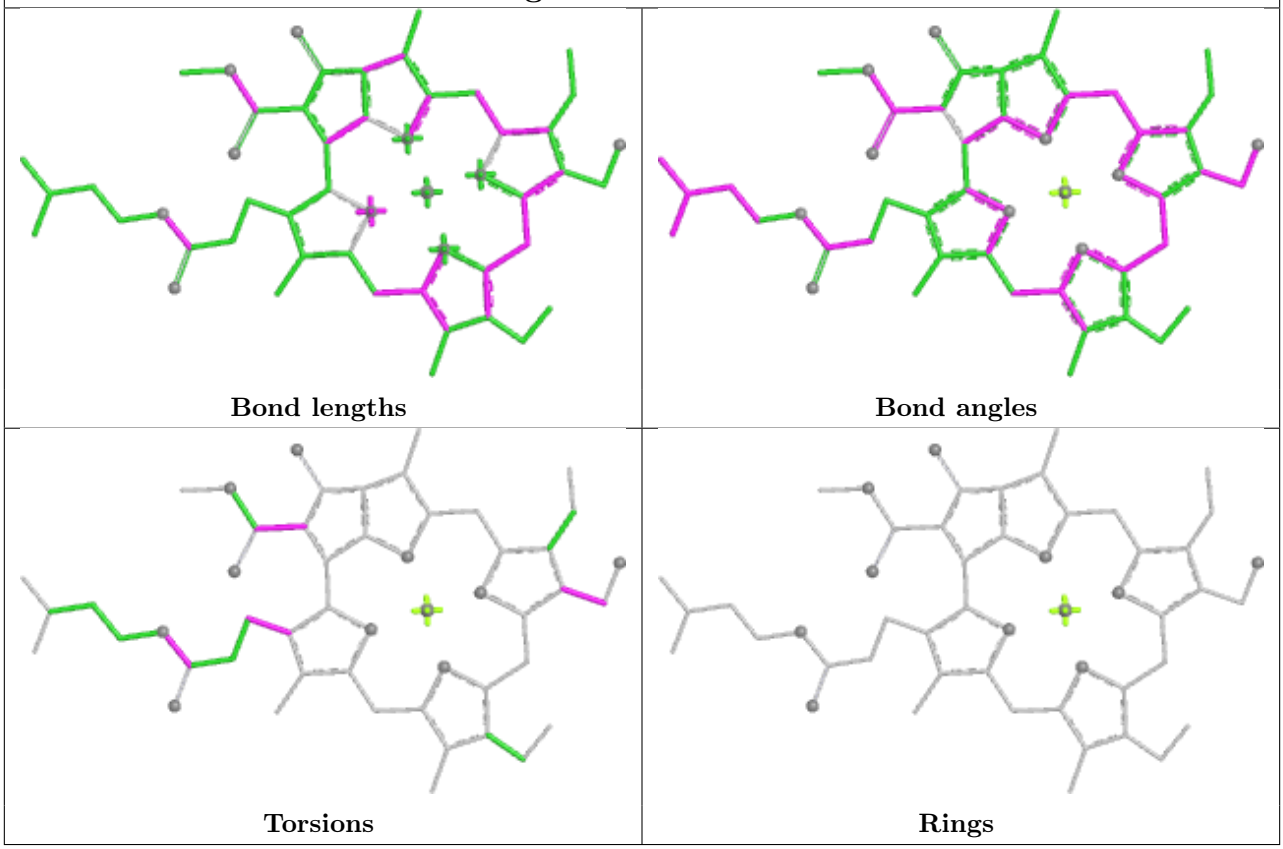
Ligand NEX A 303



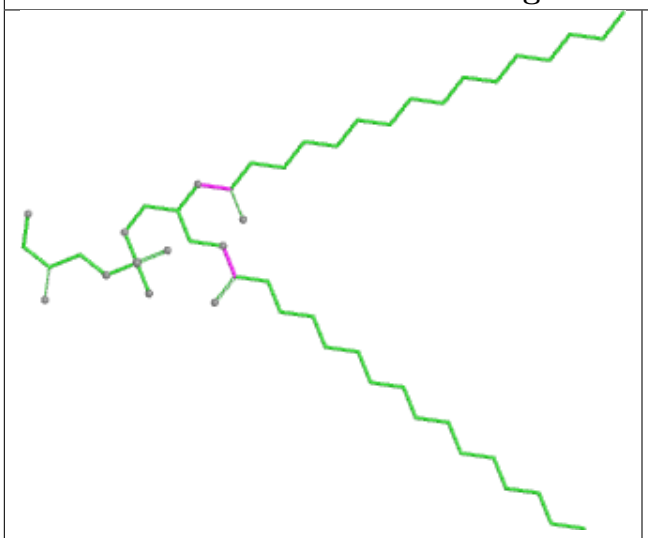
Ligand CHL A 305



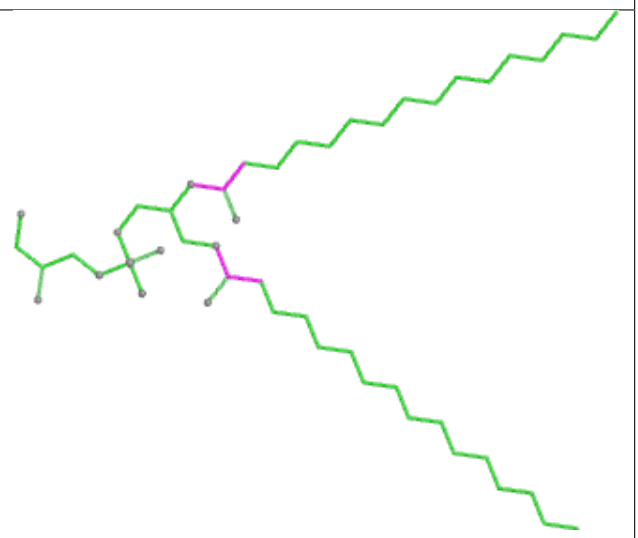
Ligand CHL B 310



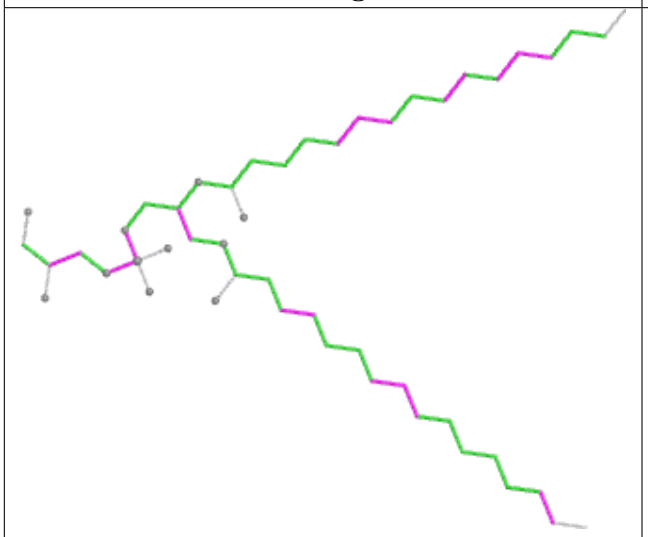
Ligand LHG A 304



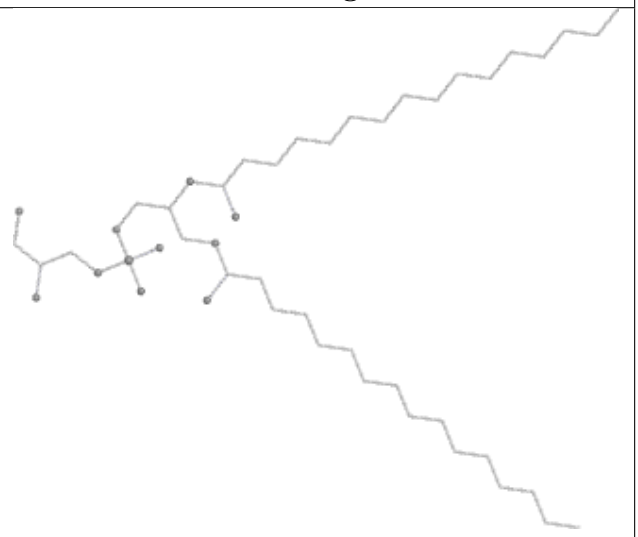
Bond lengths



Bond angles

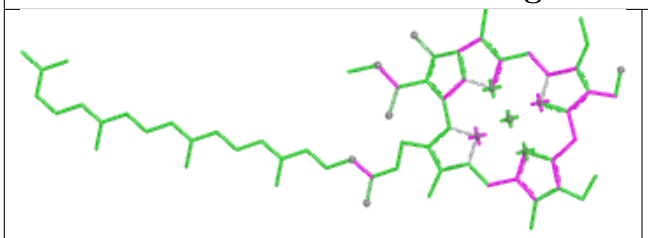


Torsions

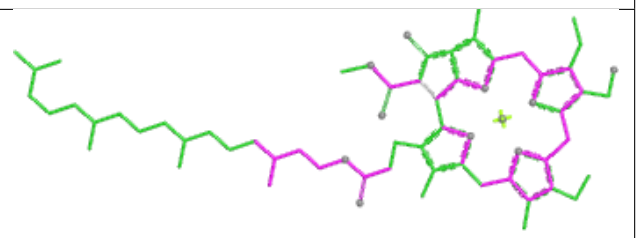


Rings

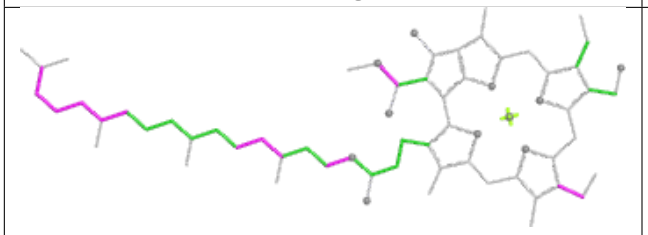
Ligand CHL A 313



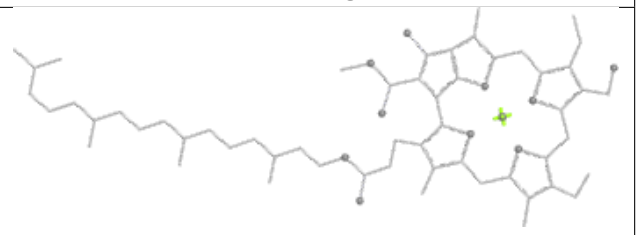
Bond lengths



Bond angles

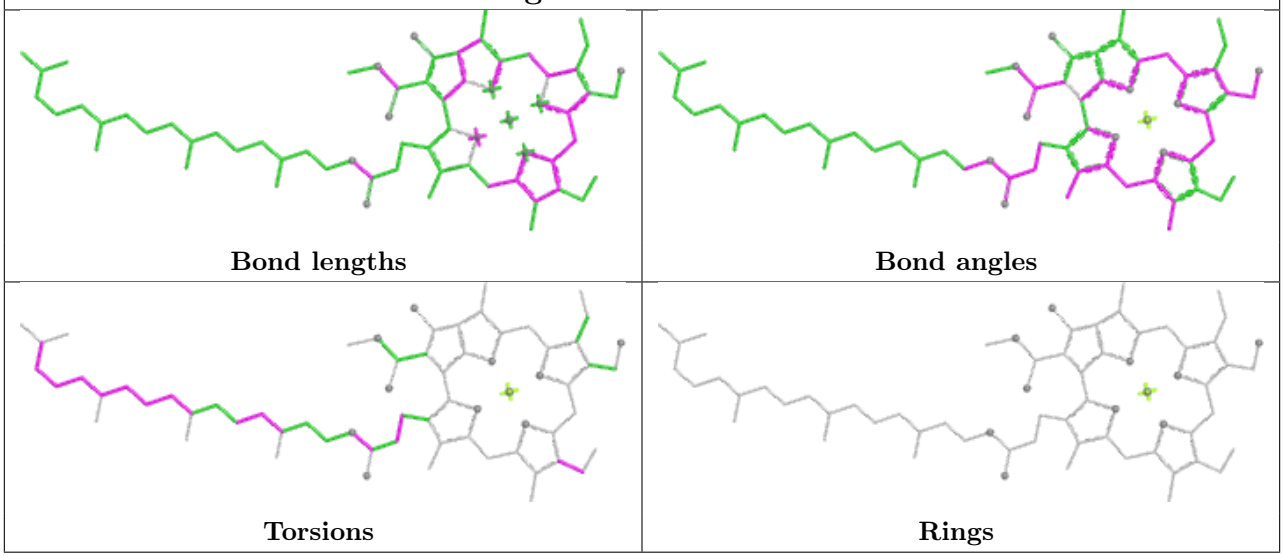


Torsions

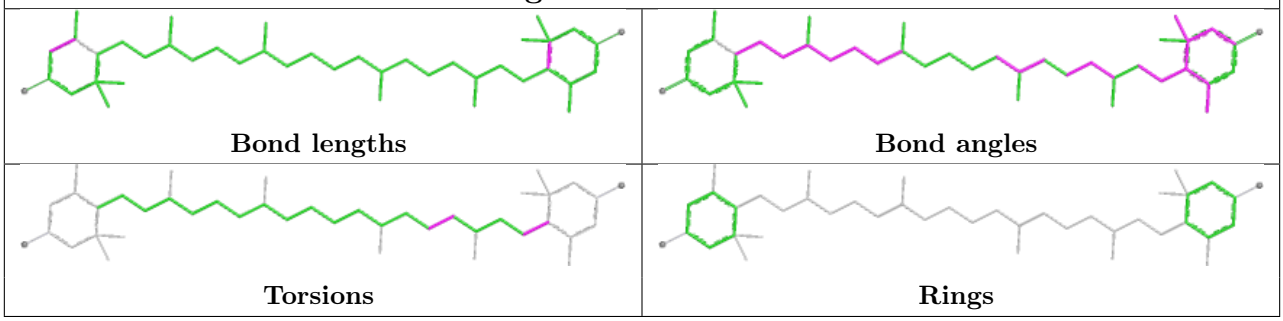


Rings

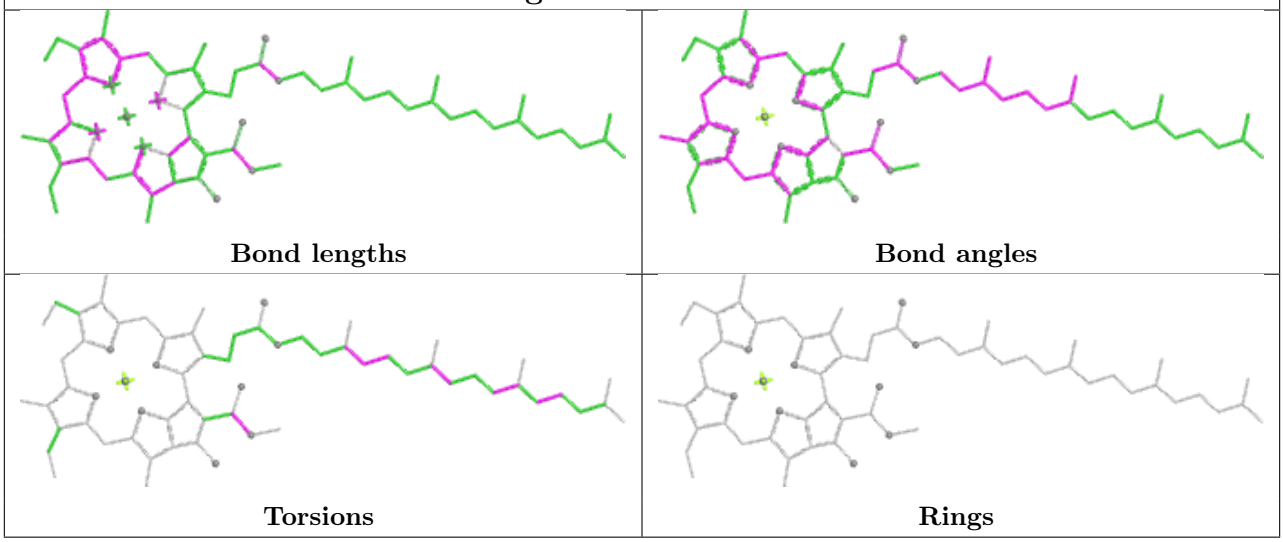
Ligand CHL C 311



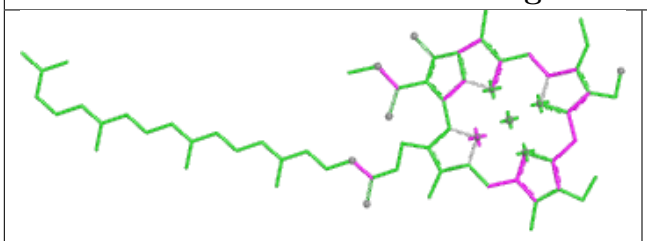
Ligand LUT A 302



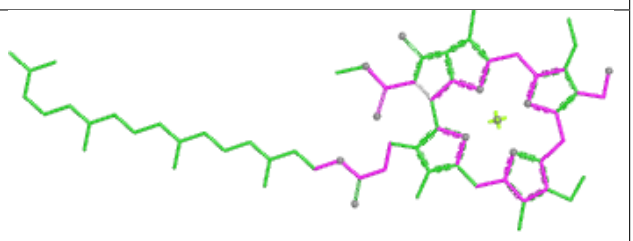
Ligand CLA C 306



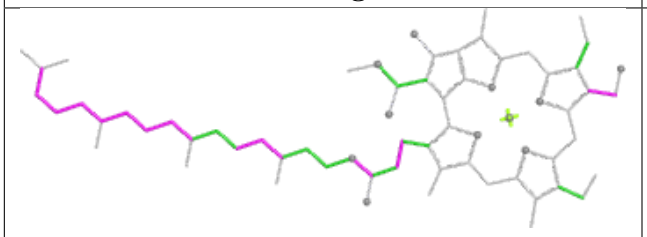
Ligand CHL A 311



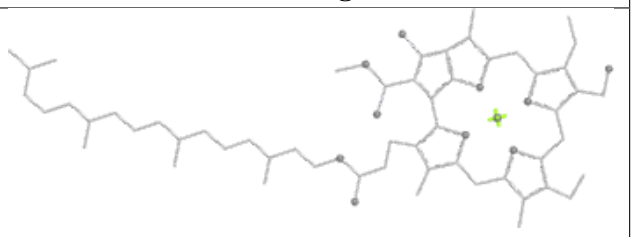
Bond lengths



Bond angles

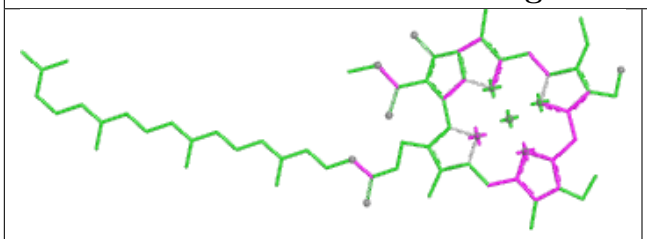


Torsions

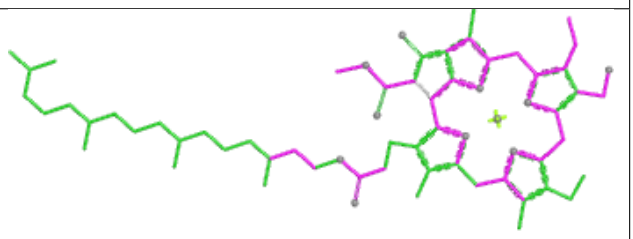


Rings

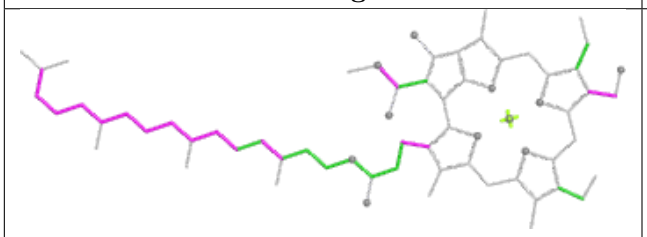
Ligand CHL B 305



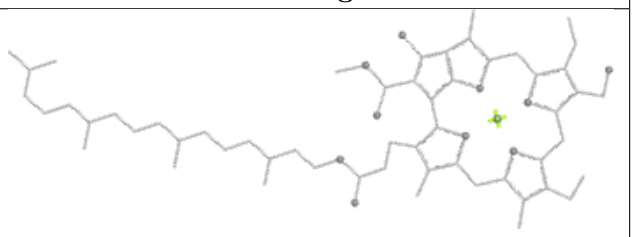
Bond lengths



Bond angles

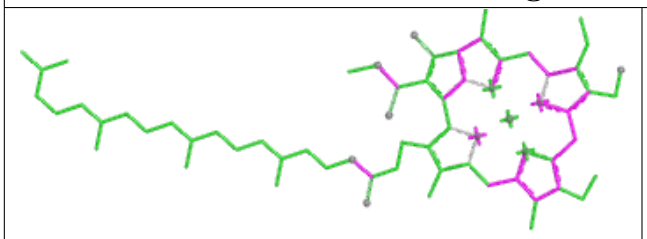


Torsions

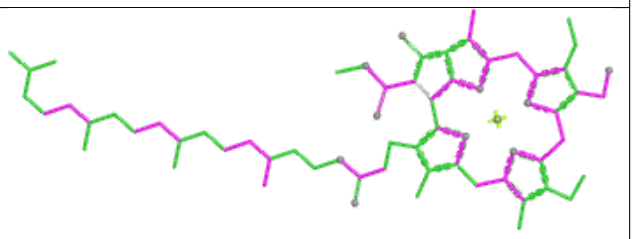


Rings

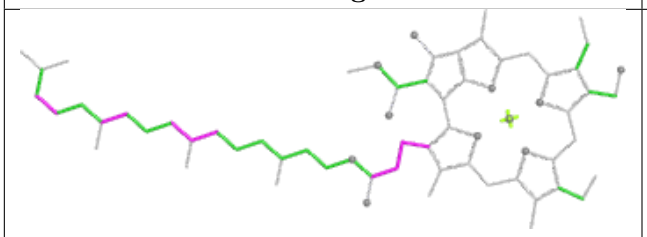
Ligand CHL B 312



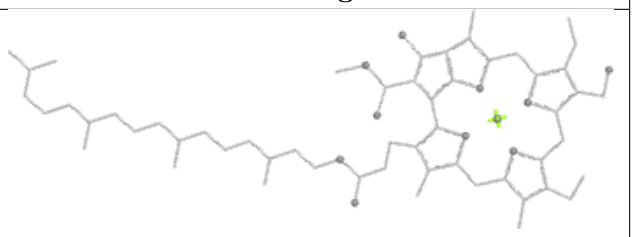
Bond lengths



Bond angles

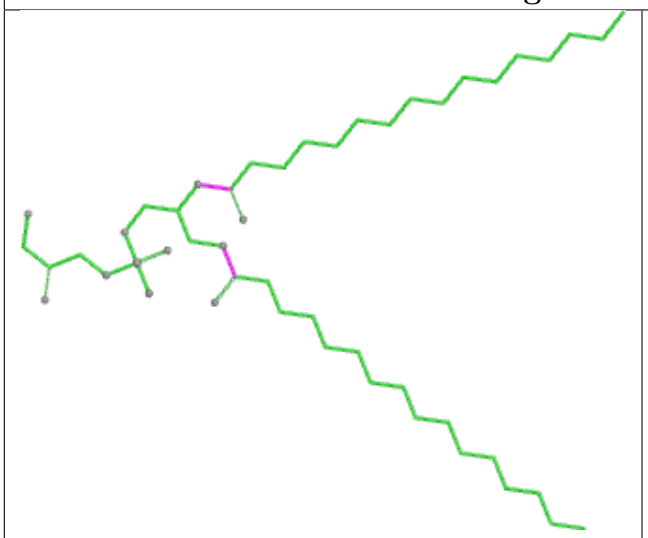


Torsions



Rings

Ligand LHG C 304



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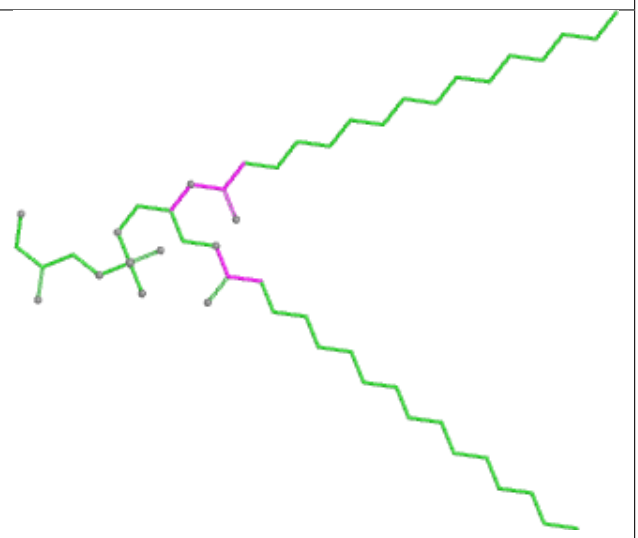
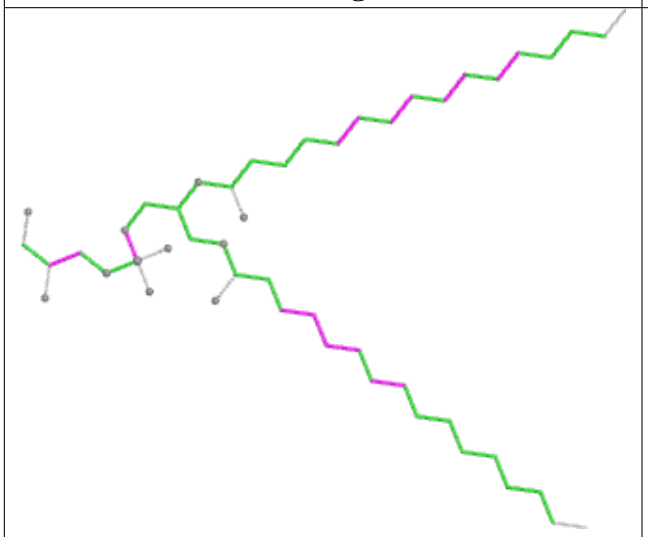
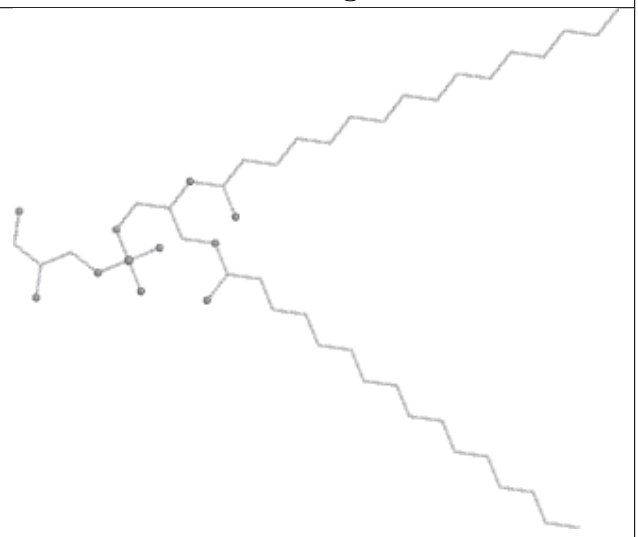


Bond angles

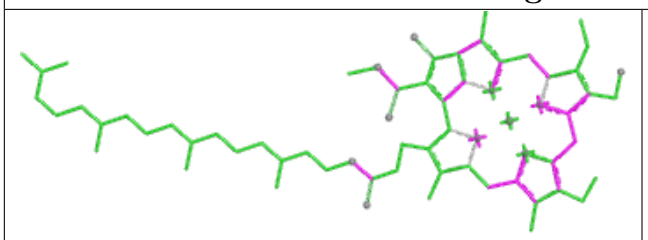


Torsions

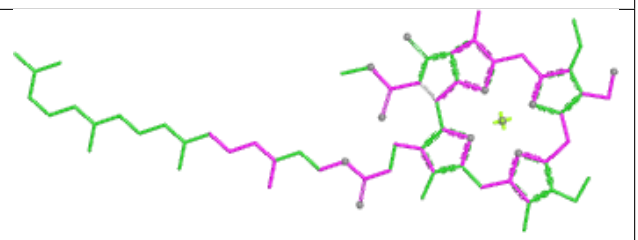


Rings

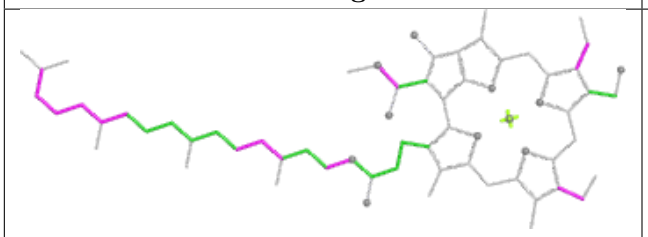
Ligand CHL C 313



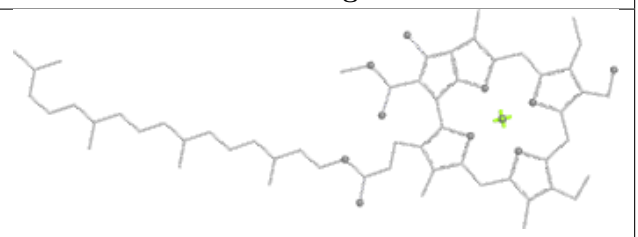
Bond lengths



Bond angles

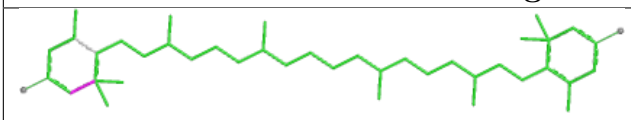


Torsions

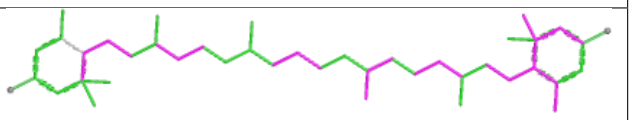


Rings

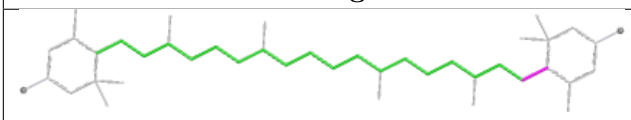
Ligand LUT A 301



Bond lengths



Bond angles



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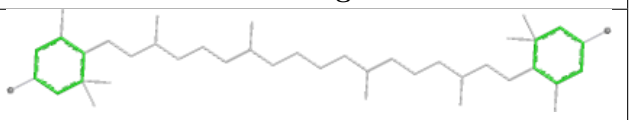
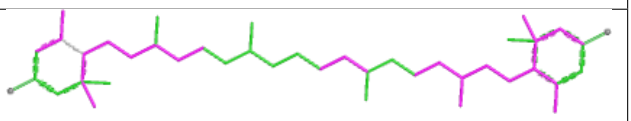


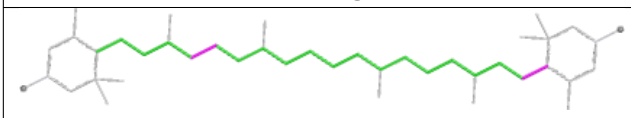
Rings

Ligand LUT C 302

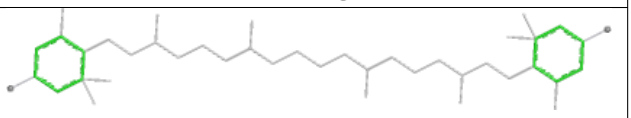
Bond lengths



Bond angles

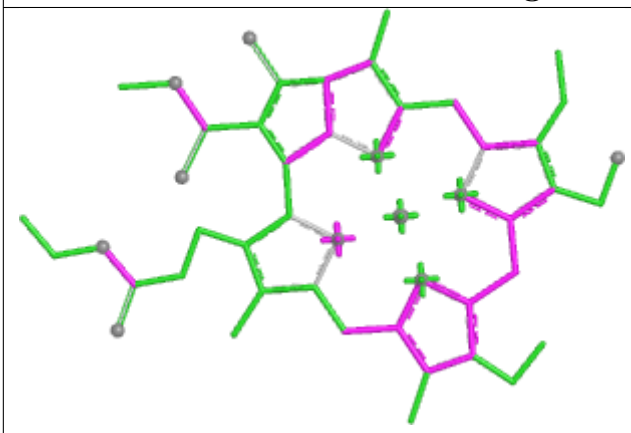


Torsions

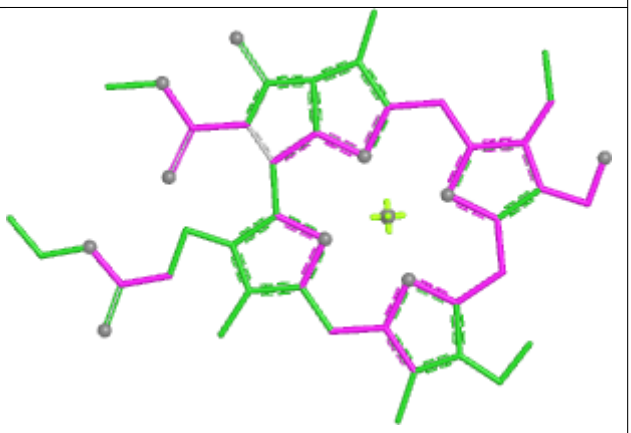


Rings

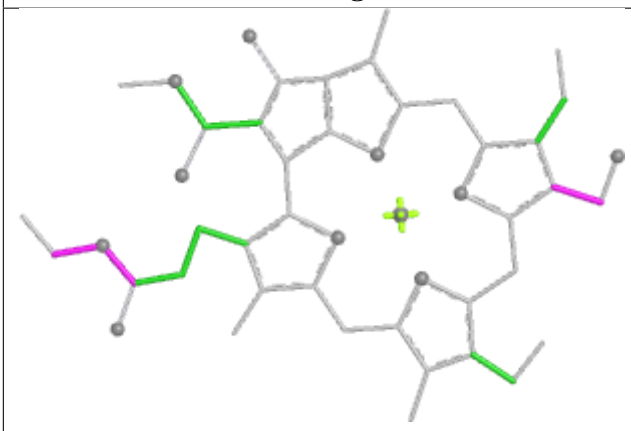
Ligand CHL A 309



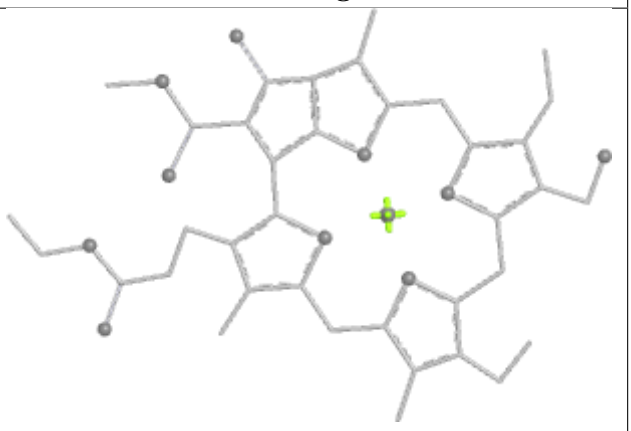
Bond lengths



Bond angles

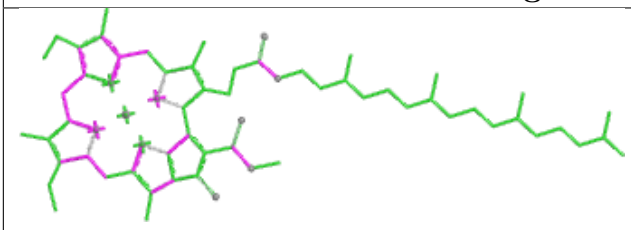


Torsions

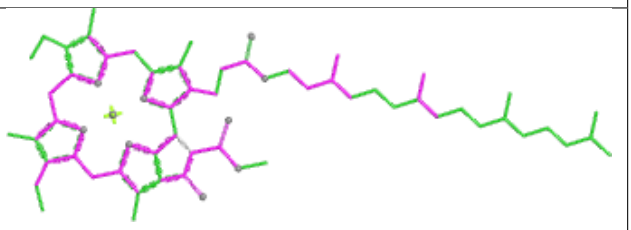


Rings

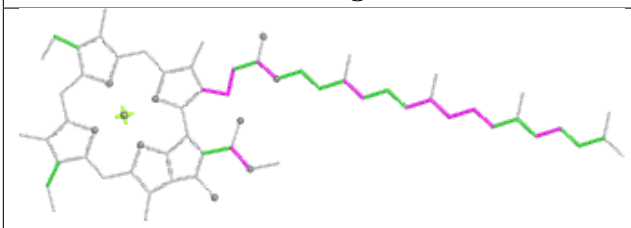
Ligand CLA A 315



Bond lengths



Bond angles



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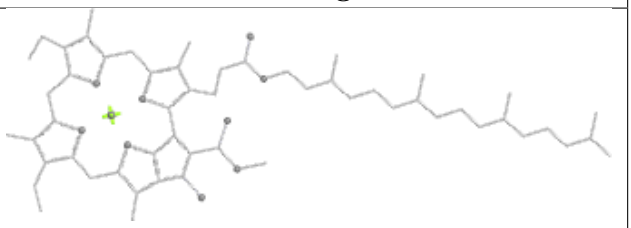
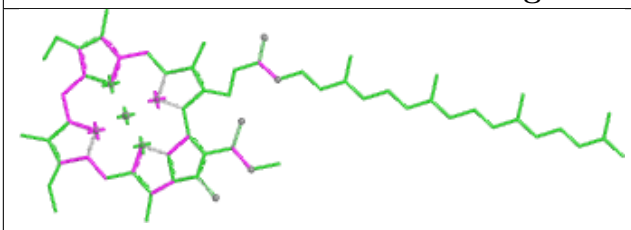


Rings

Ligand CLA A 317



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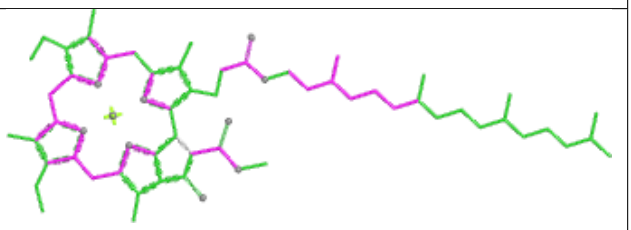
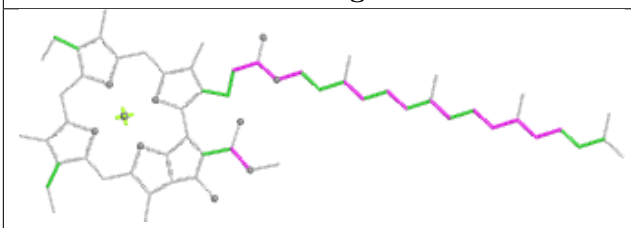


Bond angles



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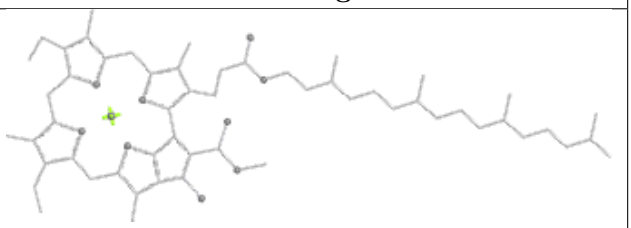
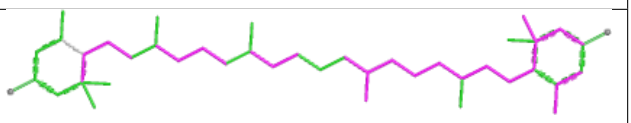


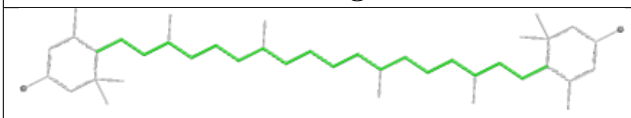
Rings

Ligand LUT B 301

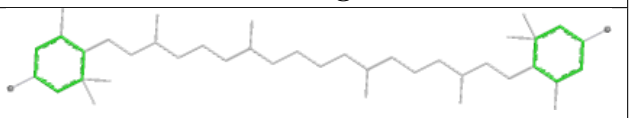
Bond lengths



Bond angles

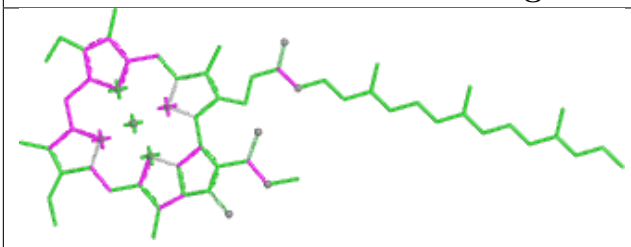


Torsions

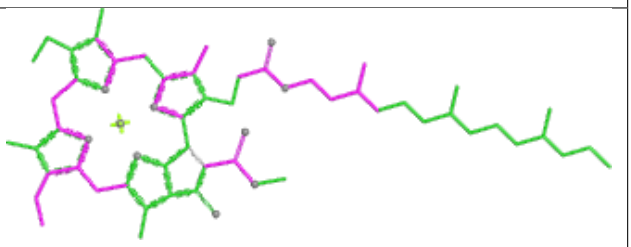


Rings

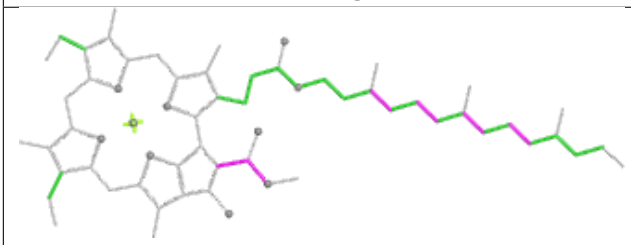
Ligand CLA C 308



Bond lengths



Bond angles



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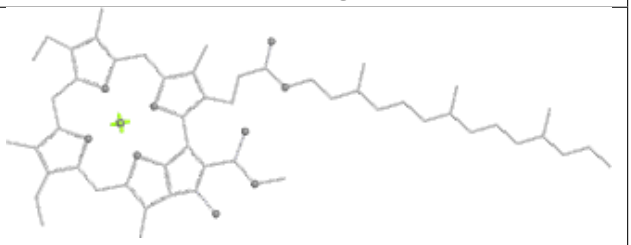
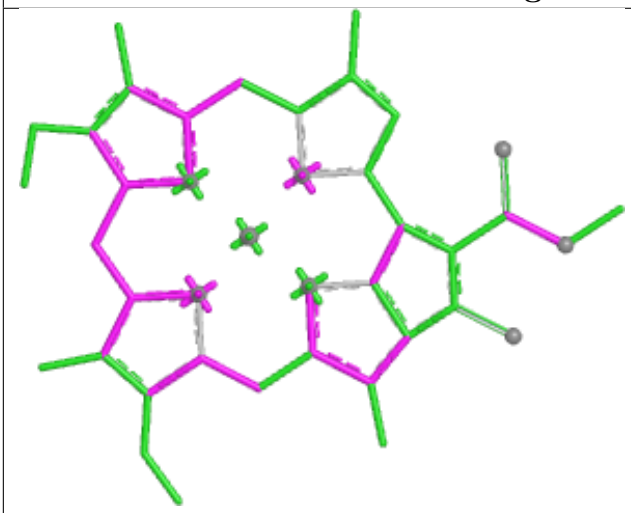


Rings

Ligand CLA C 318



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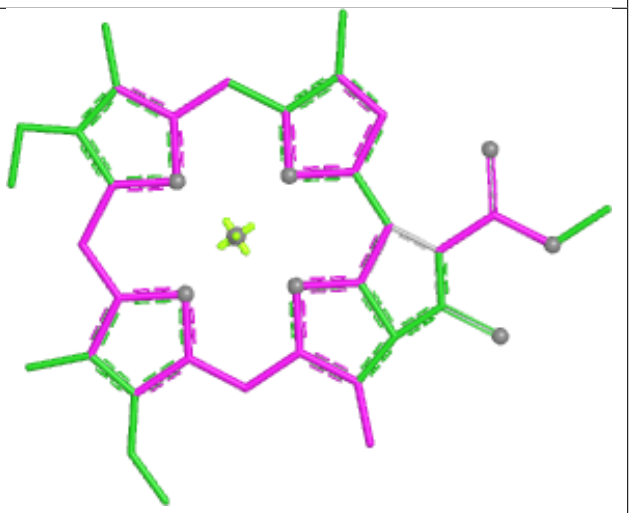
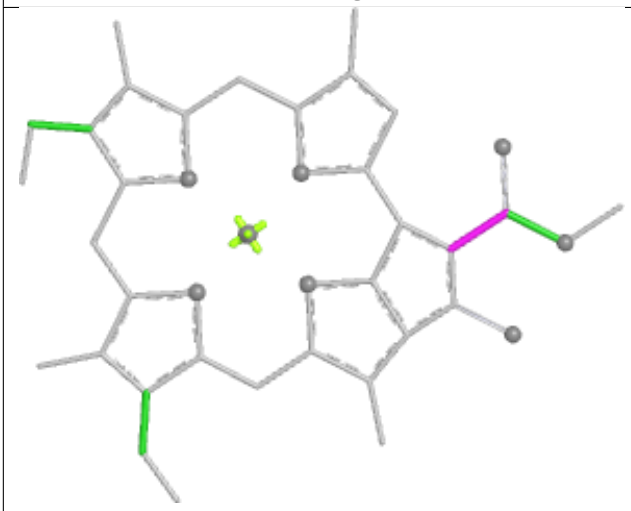


Bond angles



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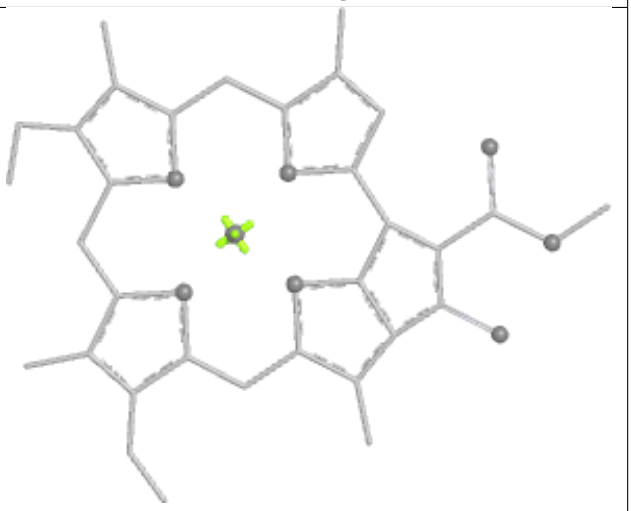
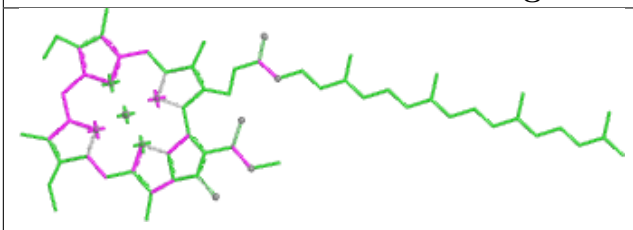
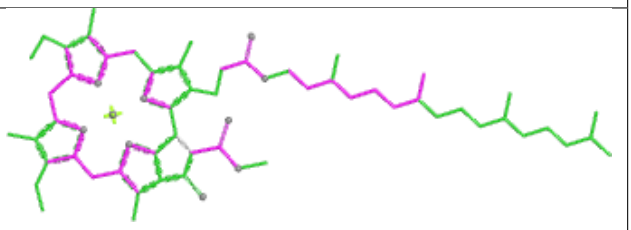


Rings

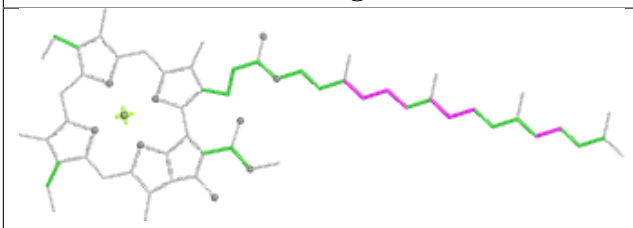
Ligand CLA A 306



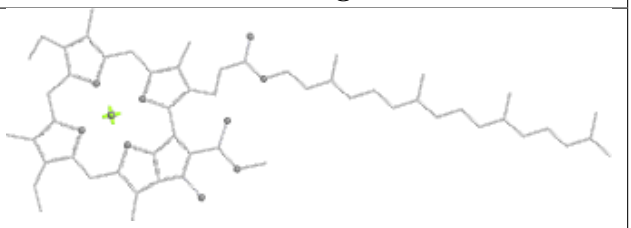
Bond lengths



Bond angles

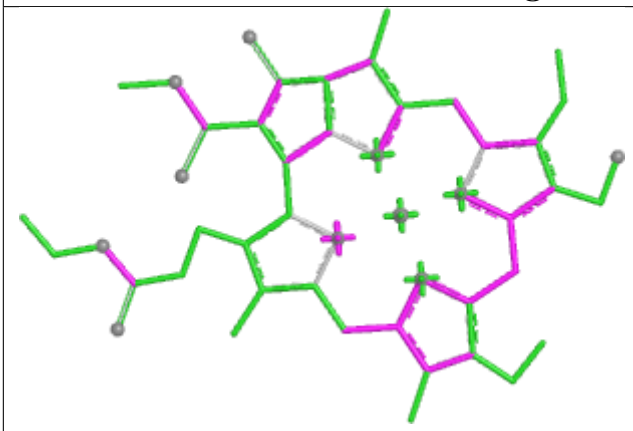


Torsions

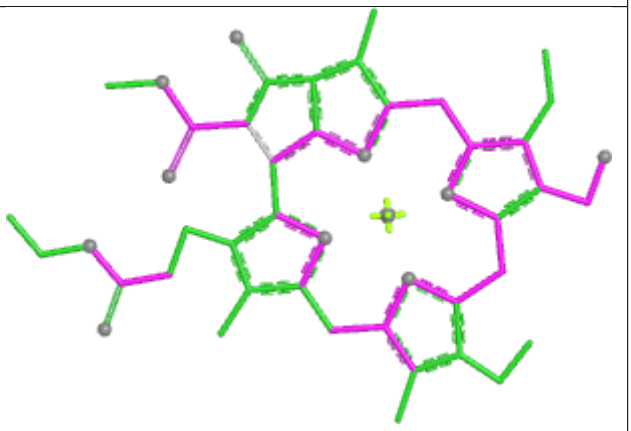


Rings

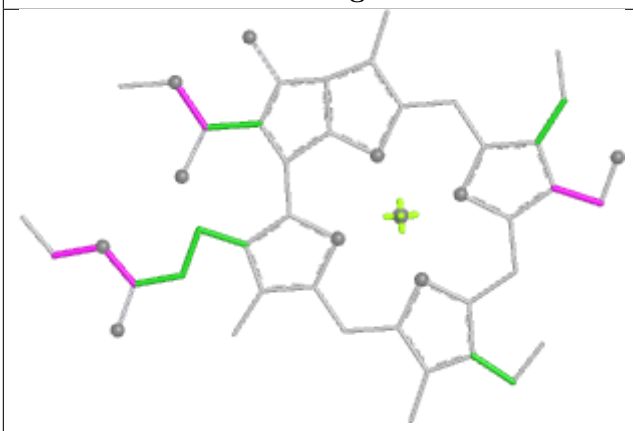
Ligand CHL B 309



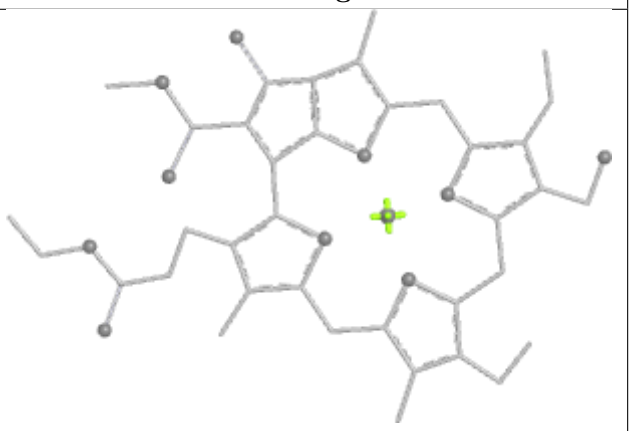
Bond lengths



Bond angles

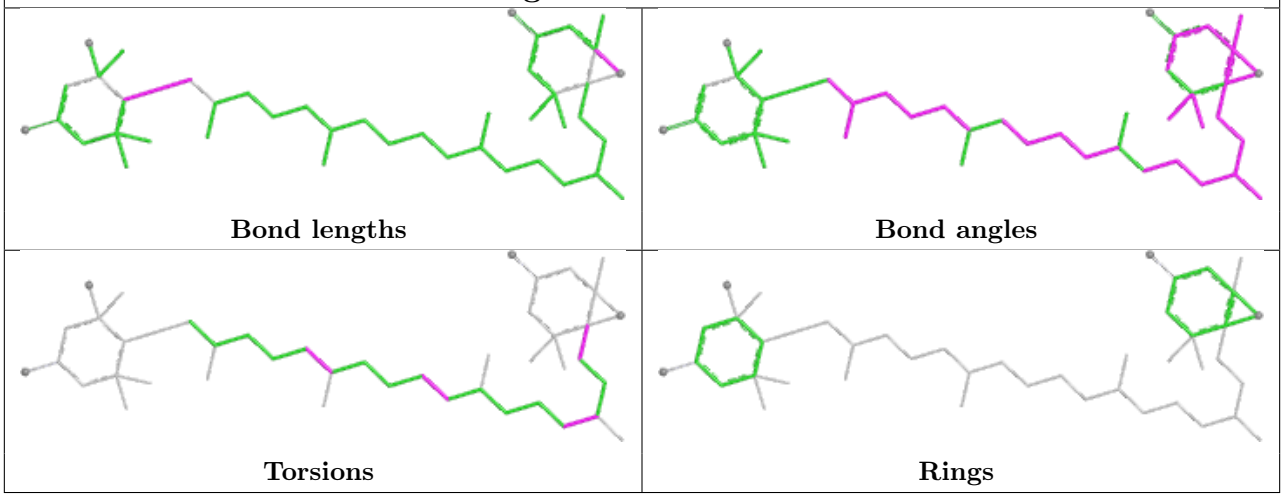


Torsions

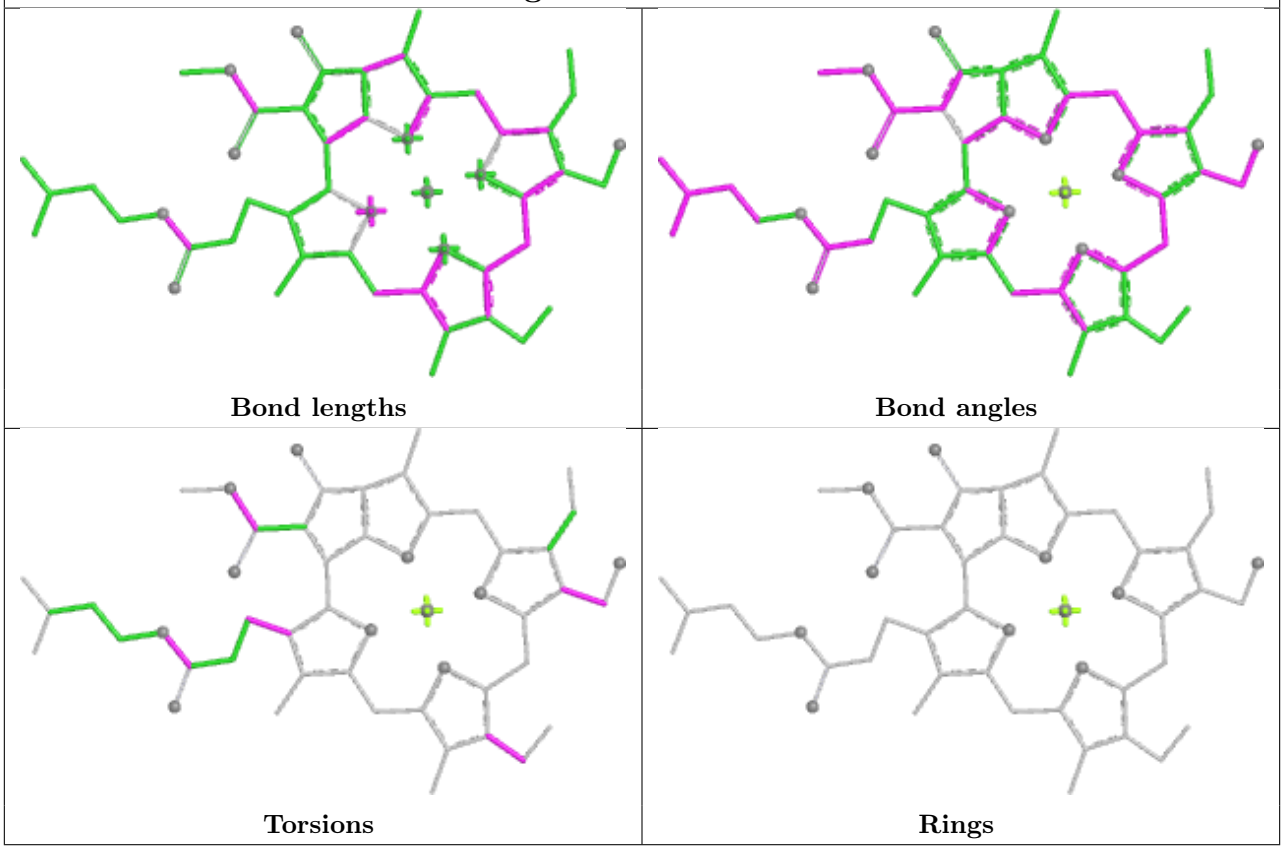


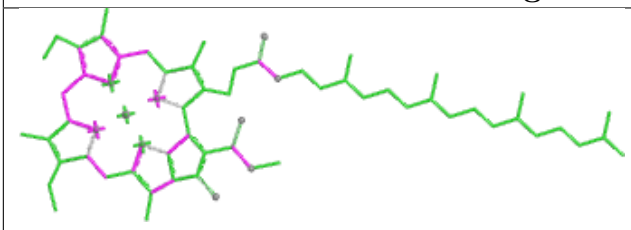
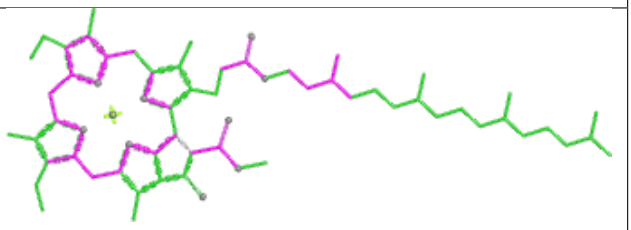
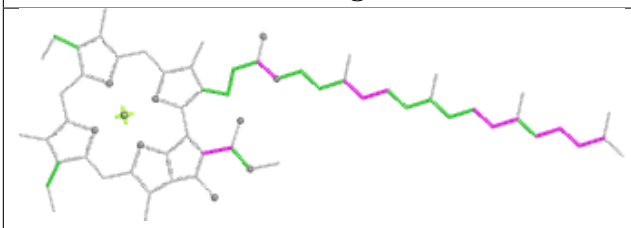
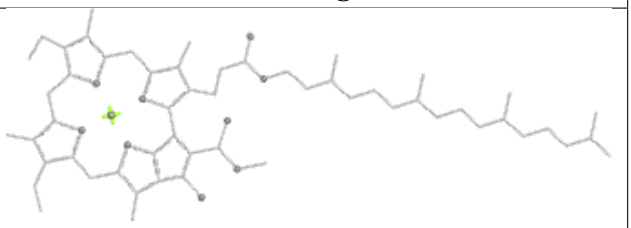
Rings

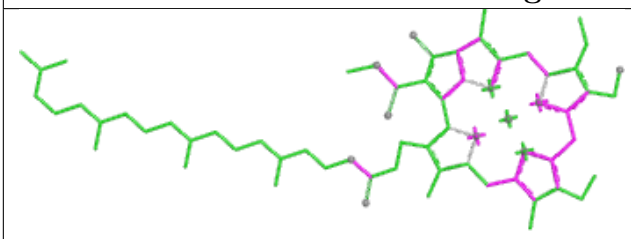
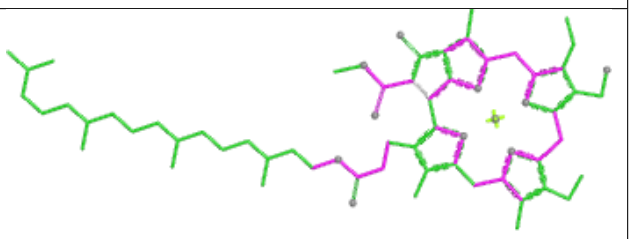
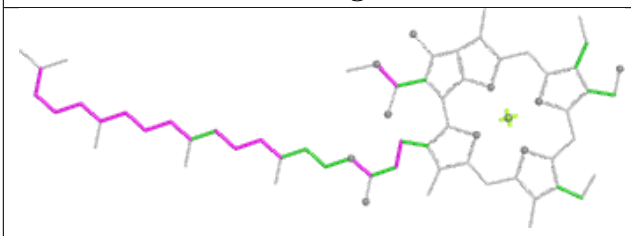
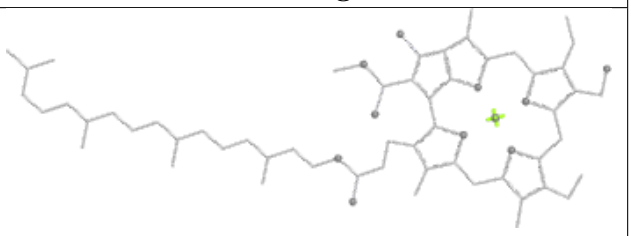
Ligand NEX C 303



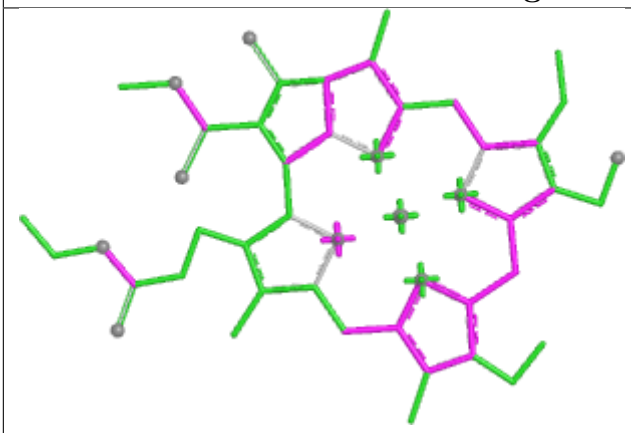
Ligand CHL A 310



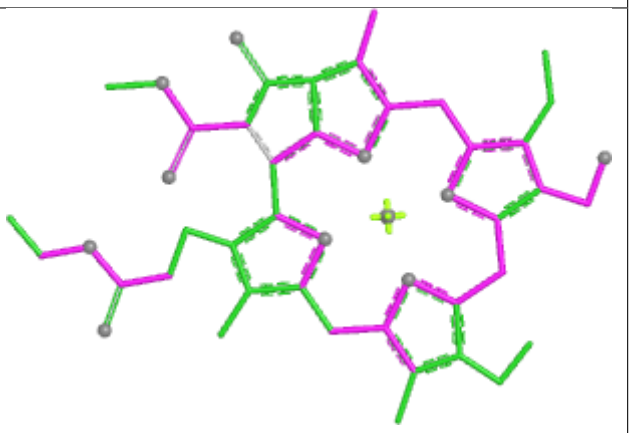
Ligand CLA A 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL B 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

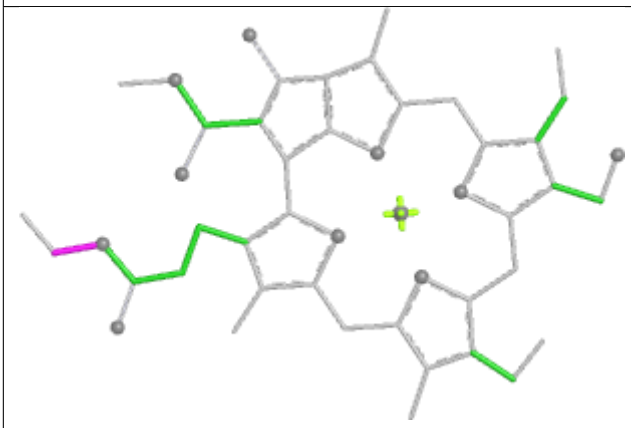
Ligand CHL C 309



Bond lengths



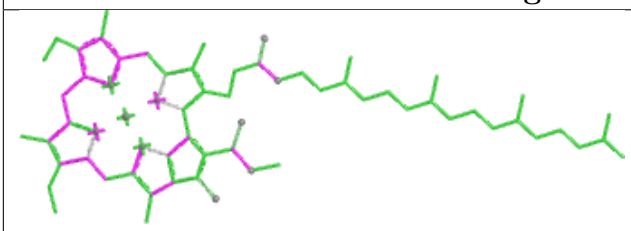
Bond angles



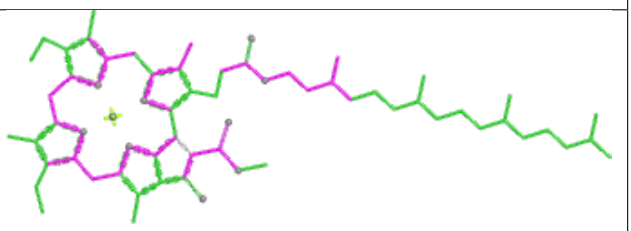
Torsions

Rings

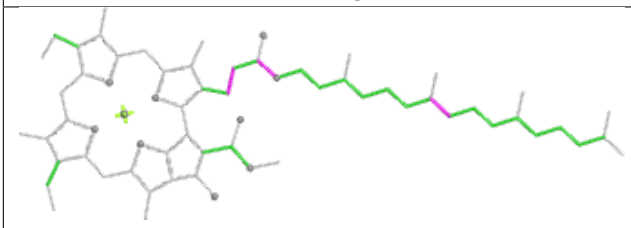
Ligand CLA A 314



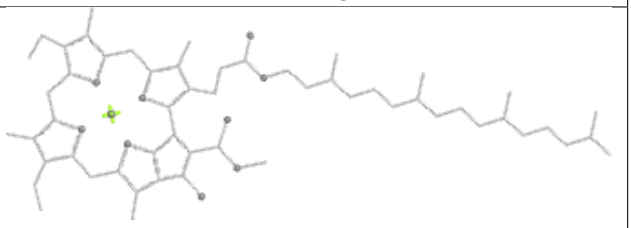
Bond lengths



Bond angles

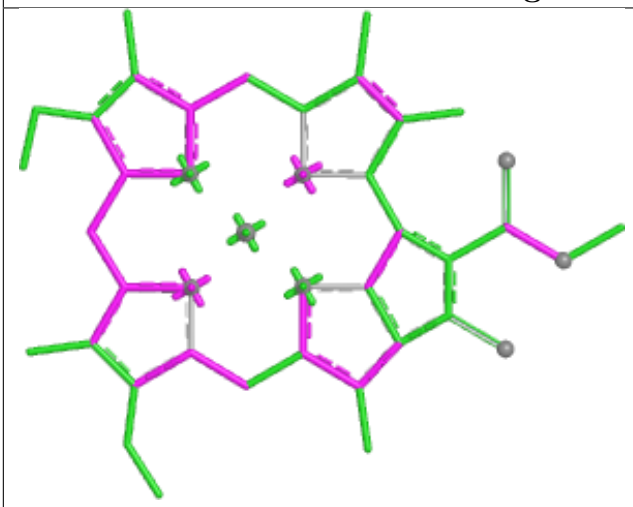


Torsions

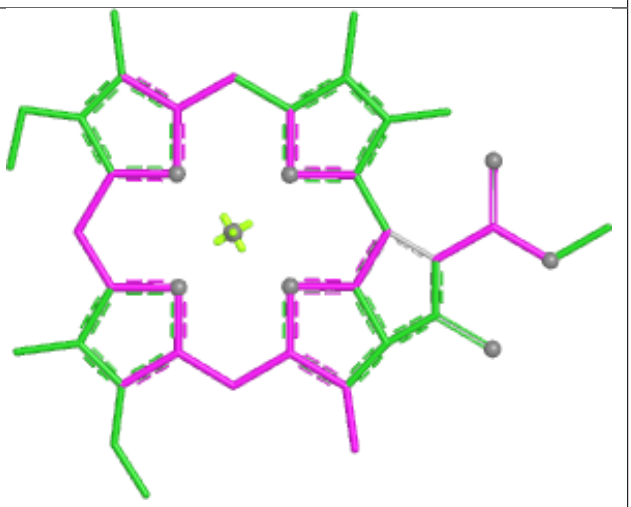


Rings

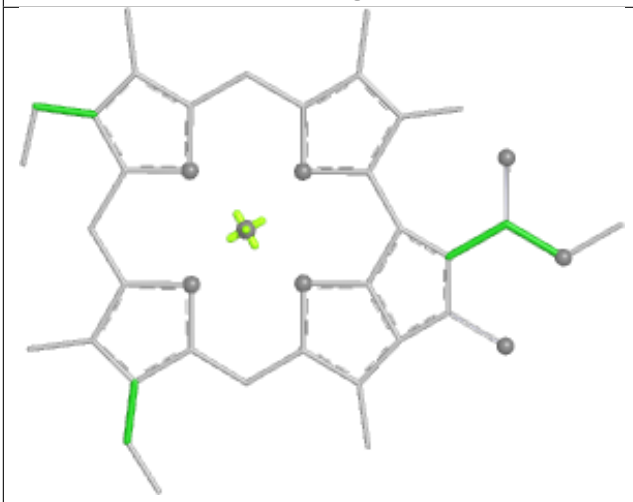
Ligand CLA A 318



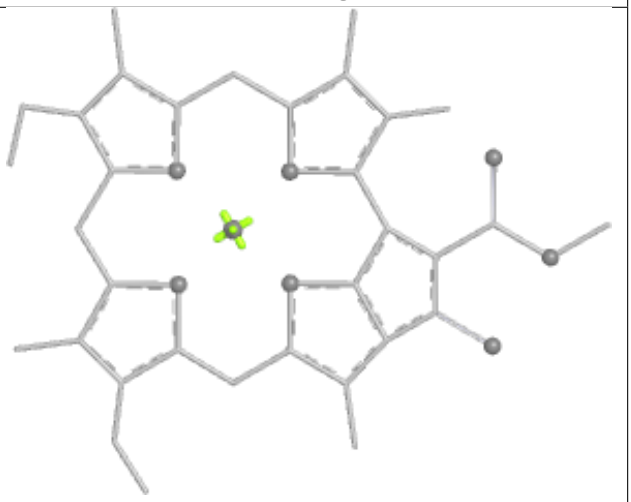
Bond lengths



Bond angles

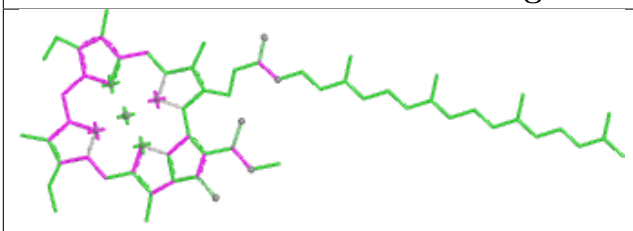


Torsions

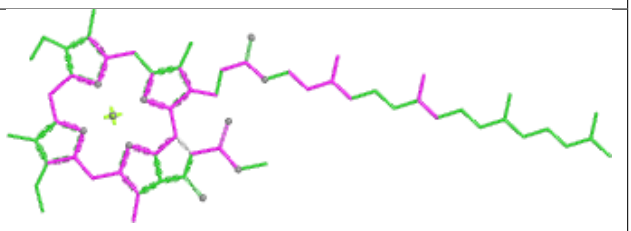


Rings

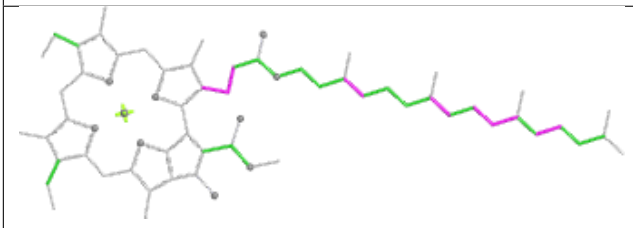
Ligand CLA C 315



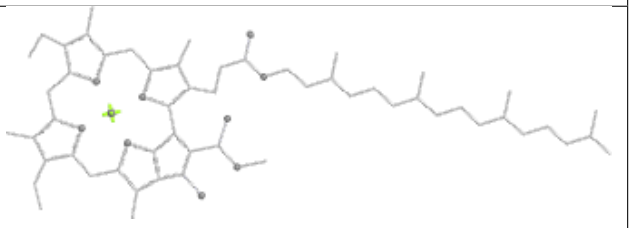
Bond lengths



Bond angles

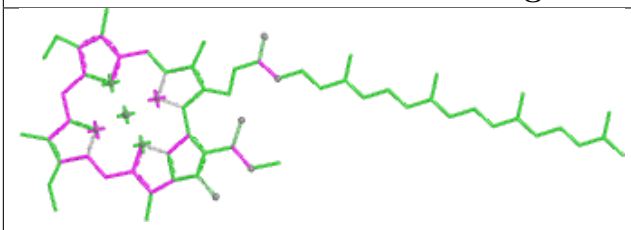


Torsions

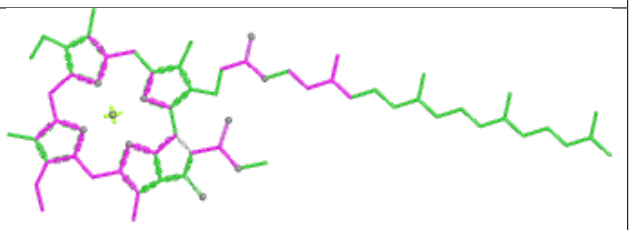


Rings

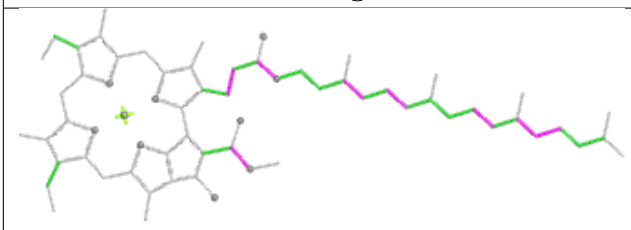
Ligand CLA C 317



Bond lengths



Bond angles



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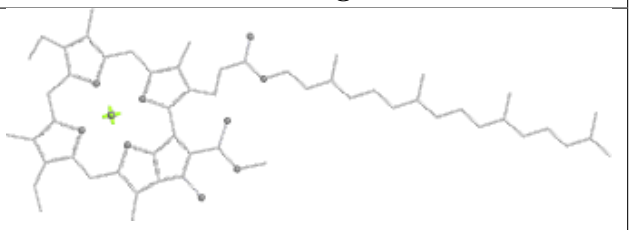
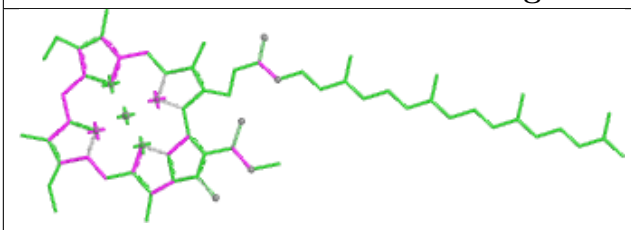
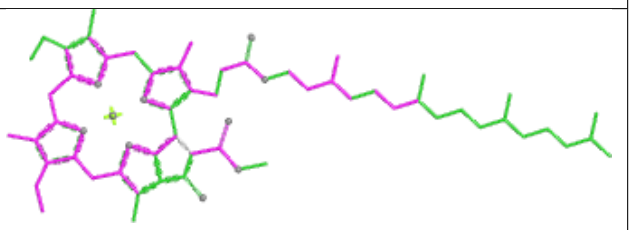


Rings

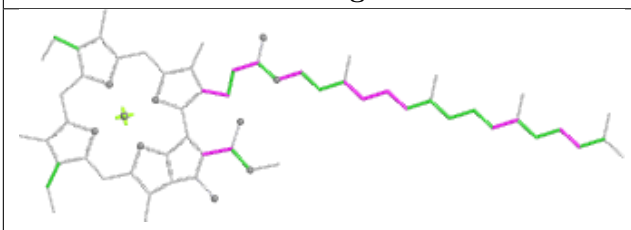
Ligand CLA A 307



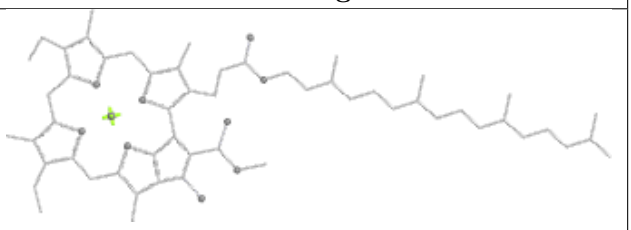
Bond lengths



Bond angles

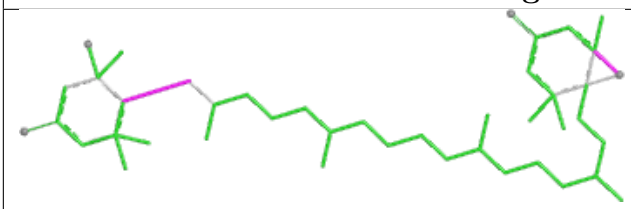


Torsions

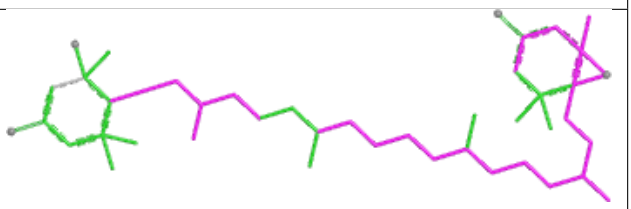


Rings

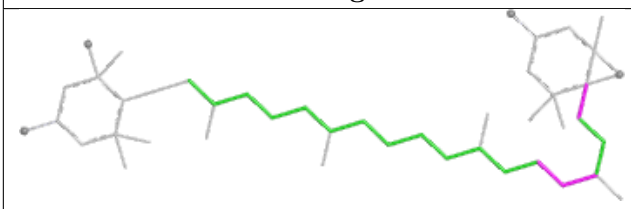
Ligand NEX B 303



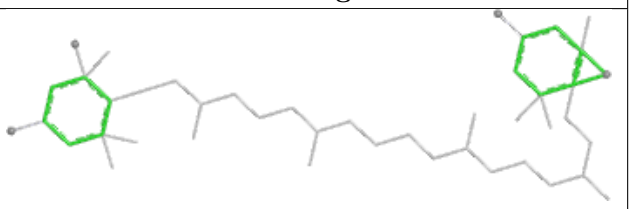
Bond lengths



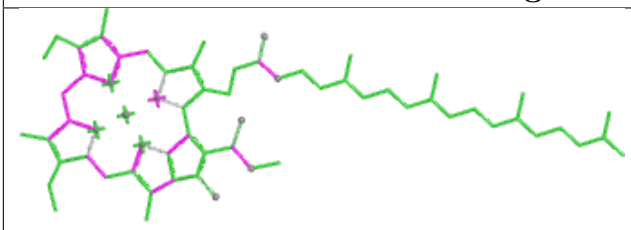
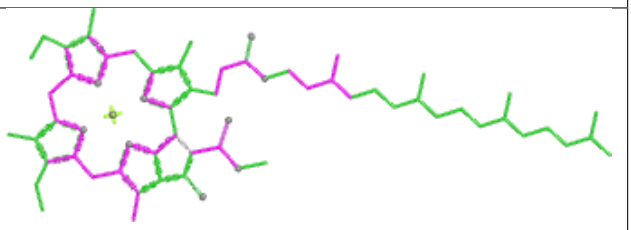
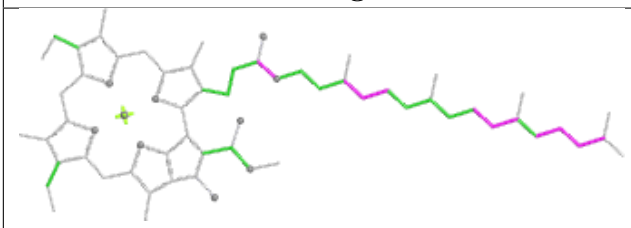
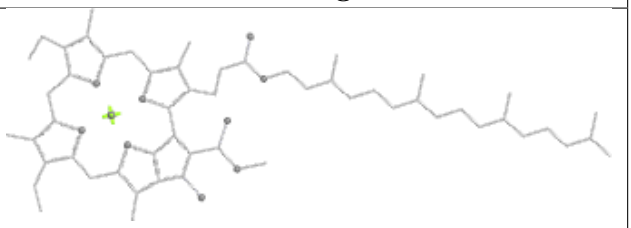
Bond angles

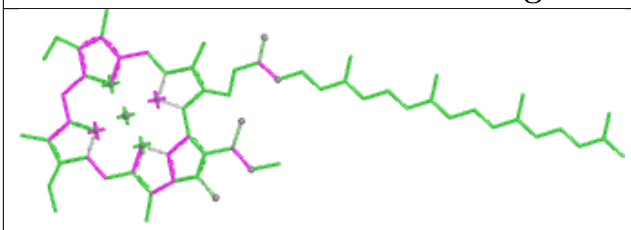
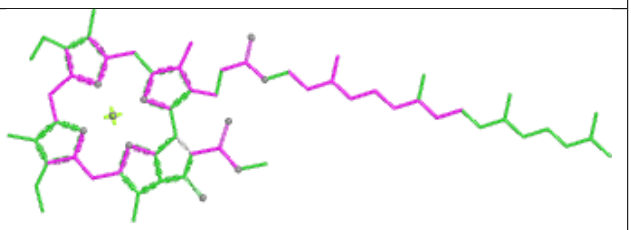
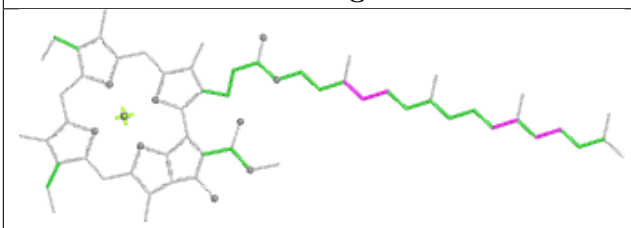
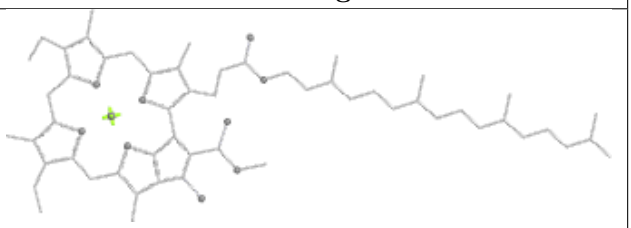


Torsions

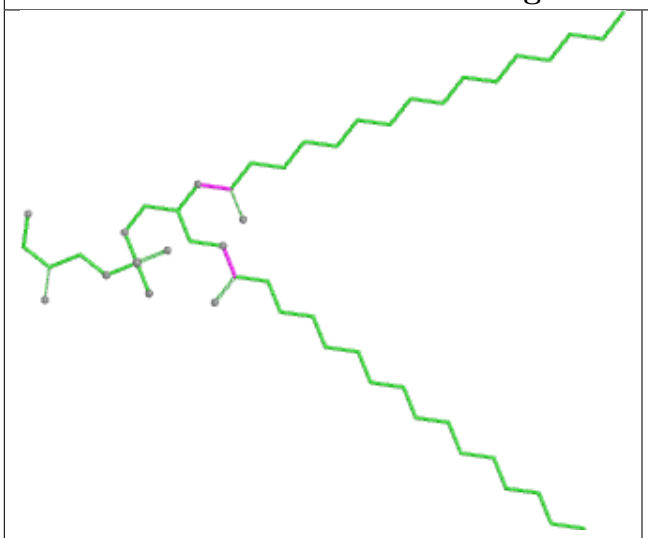


Rings

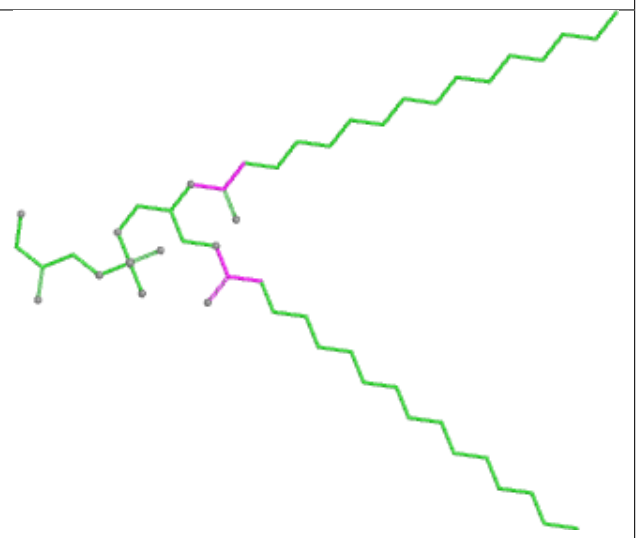
Ligand CLA C 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

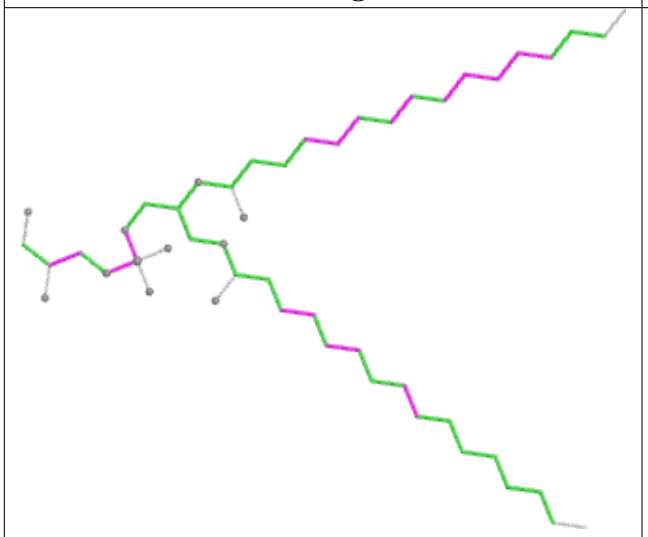
Ligand LHG B 304



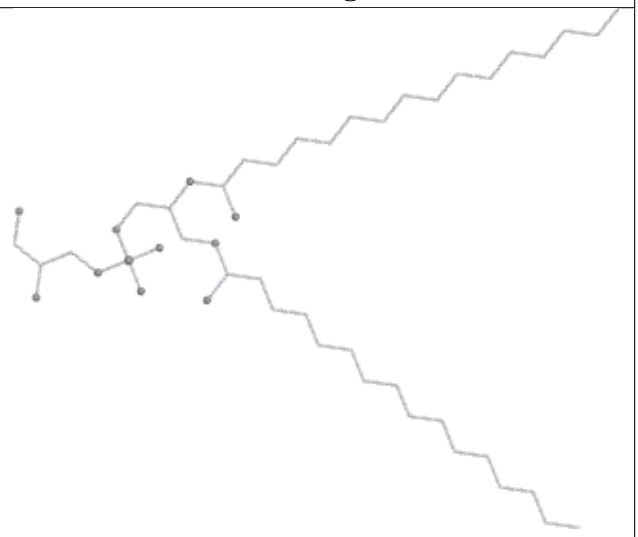
Bond lengths



Bond angles

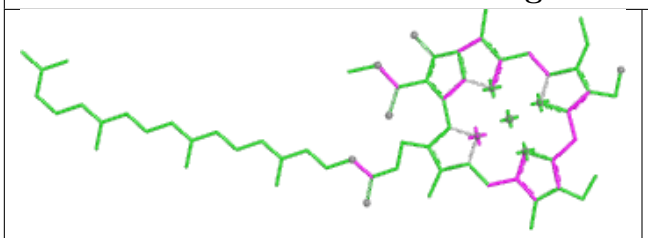


Torsions

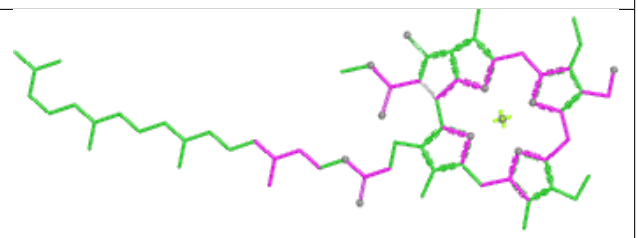


Rings

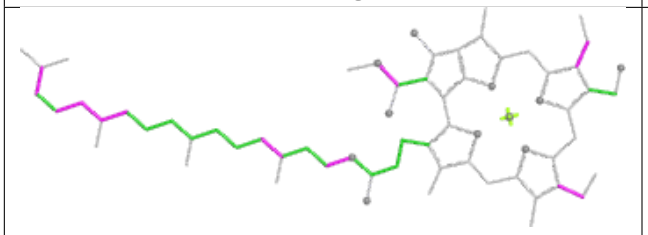
Ligand CHL B 313



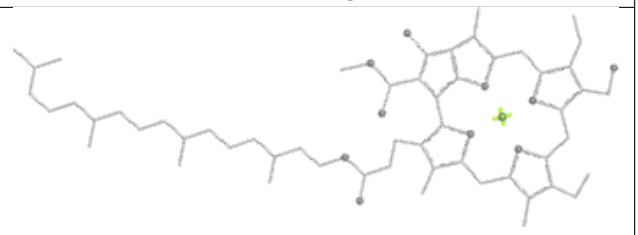
Bond lengths



Bond angles

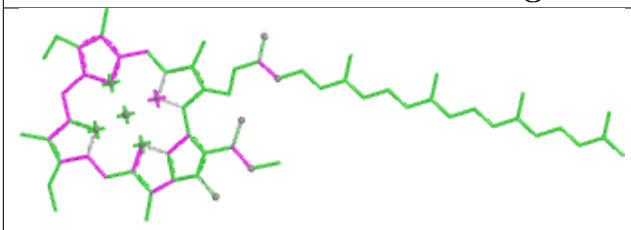


Torsions

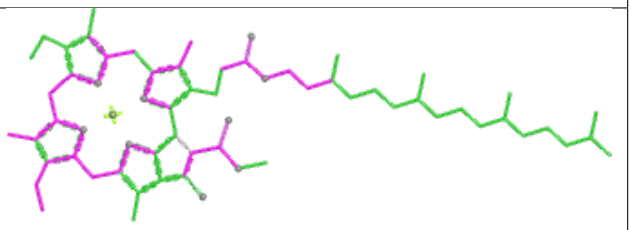


Rings

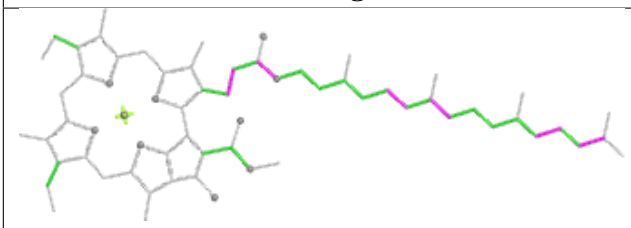
Ligand CLA C 314



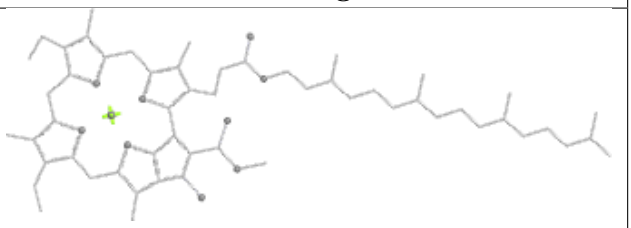
Bond lengths



Bond angles

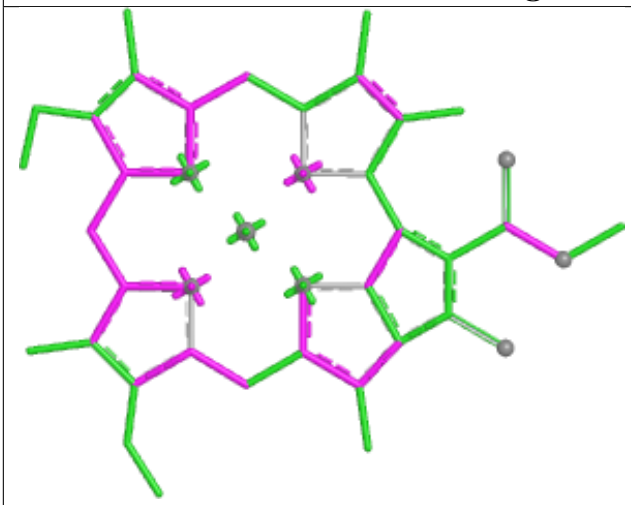


Torsions

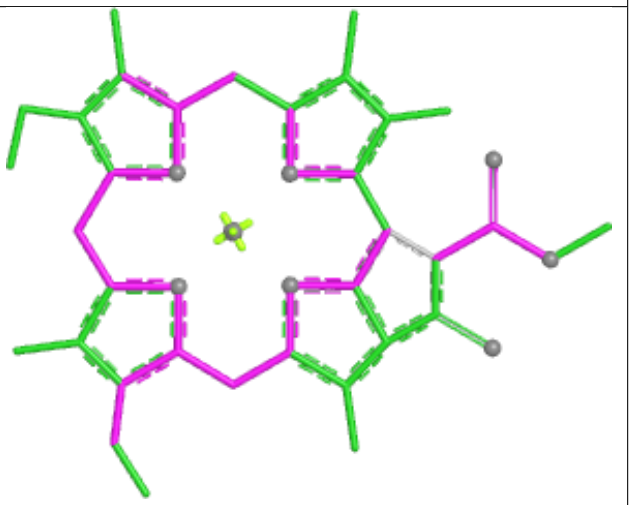


Rings

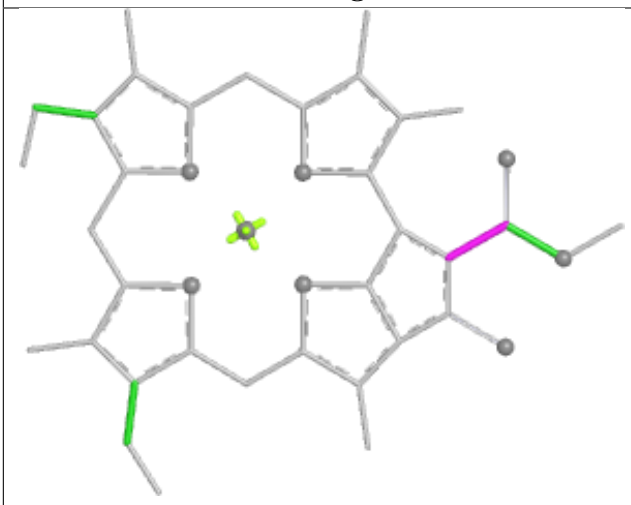
Ligand CLA B 318



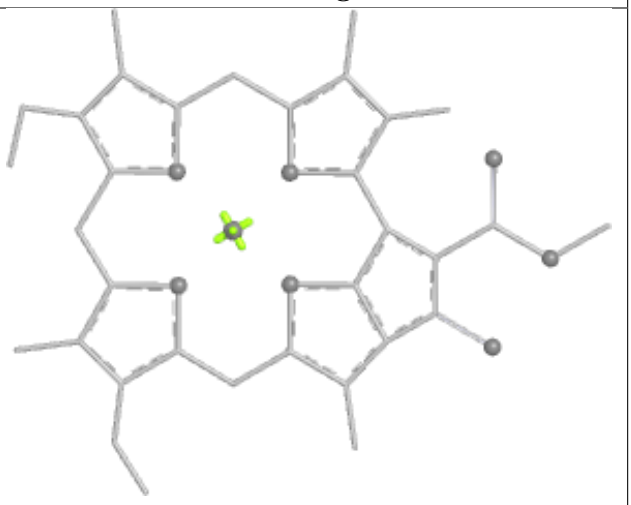
Bond lengths



Bond angles

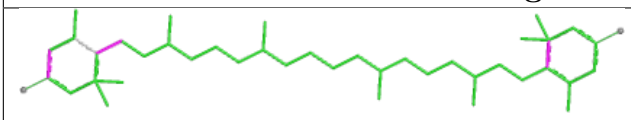


Torsions

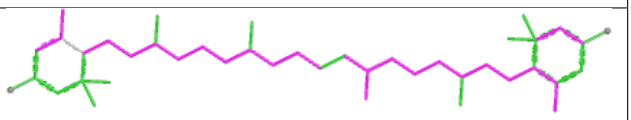


Rings

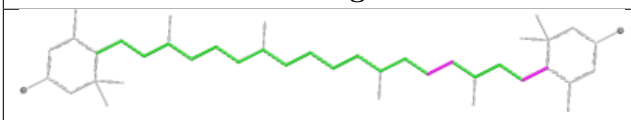
Ligand LUT B 302



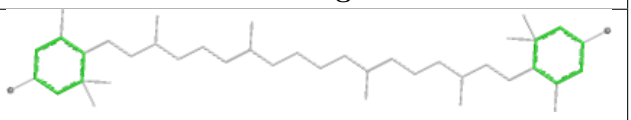
Bond lengths



Bond angles

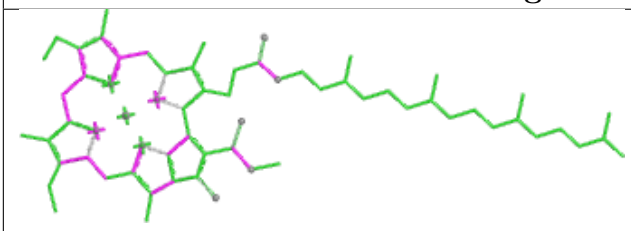


Torsions

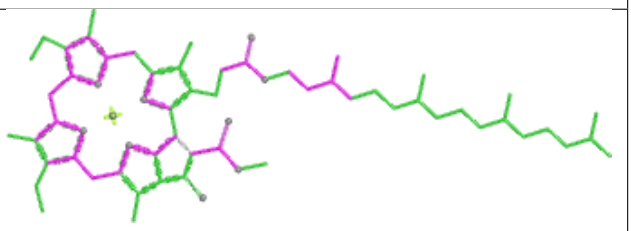


Rings

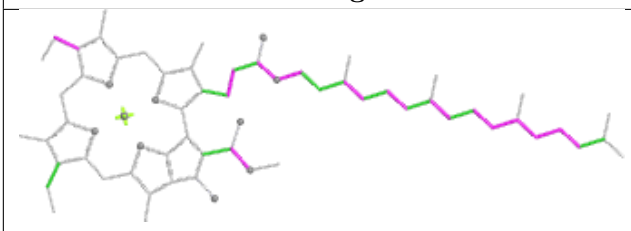
Ligand CLA B 317



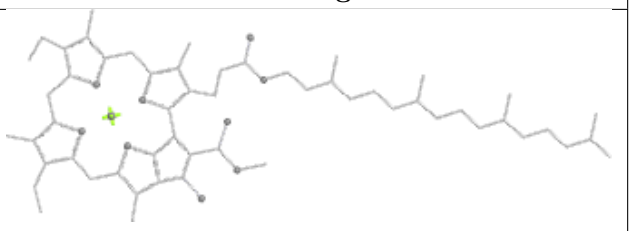
Bond lengths



Bond angles

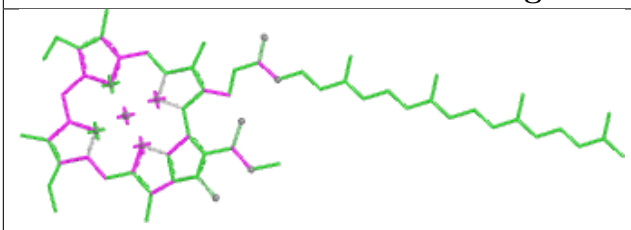


Torsions

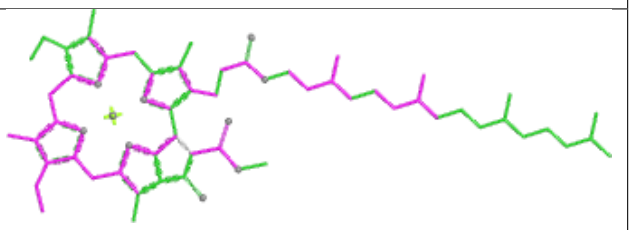


Rings

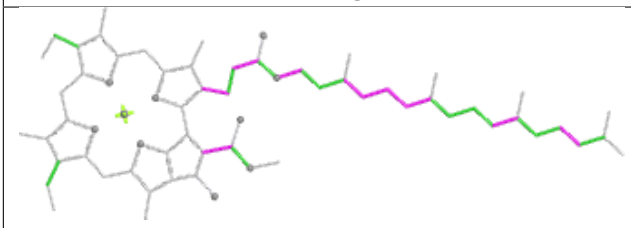
Ligand CLA C 307



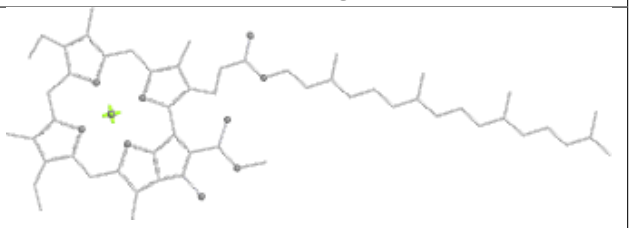
Bond lengths



Bond angles

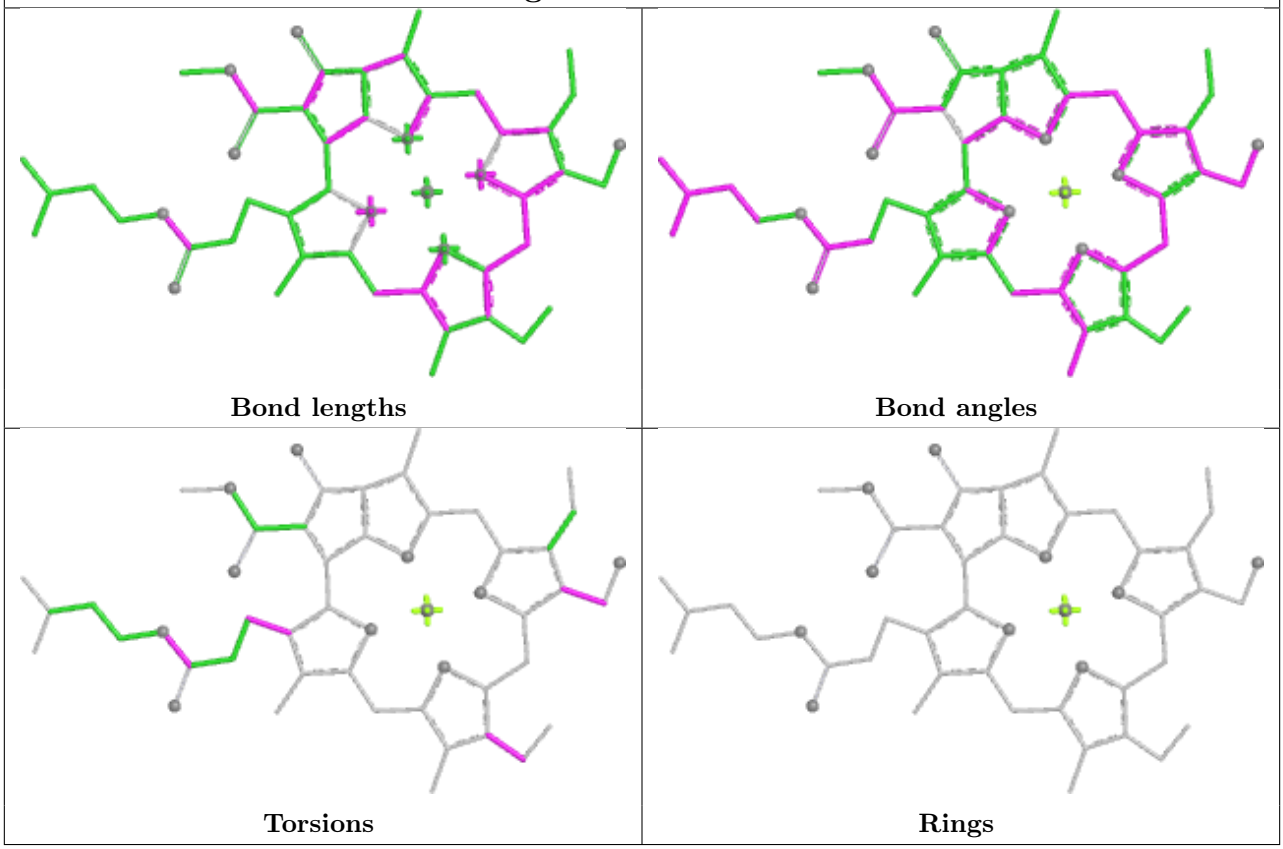


Torsions

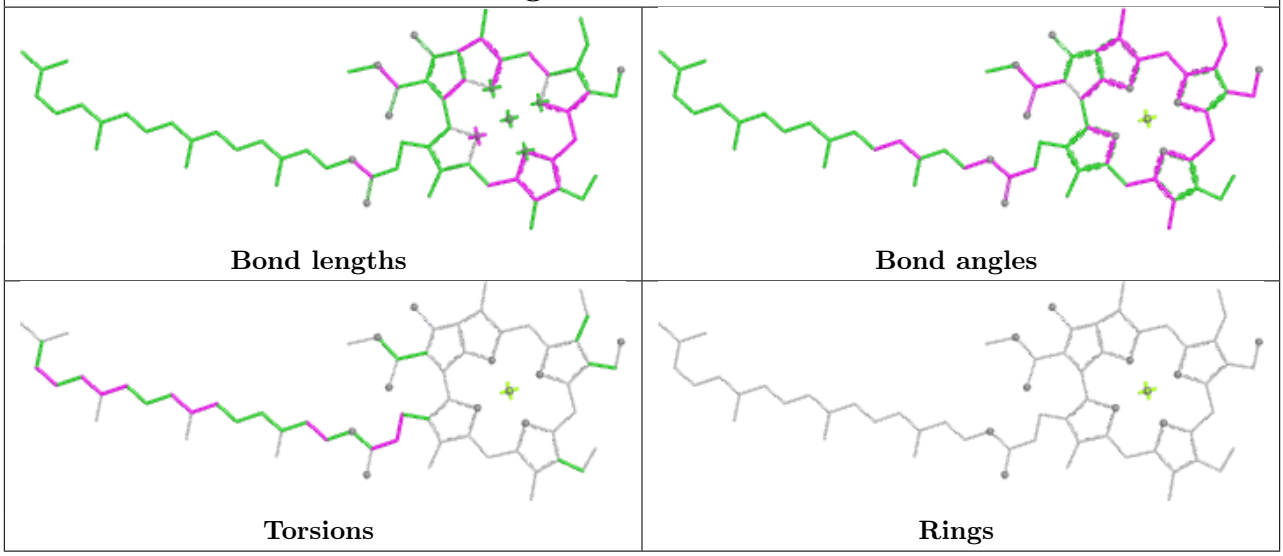


Rings

Ligand CHL C 310



Ligand CHL A 312



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	208/224 (92%)	0.36	17 (8%)	17	14	6, 39, 77, 97	0
1	B	208/224 (92%)	-0.04	2 (0%)	79	76	8, 34, 67, 94	0
1	C	208/224 (92%)	0.24	15 (7%)	21	17	6, 33, 69, 107	0
All	All	624/672 (92%)	0.19	34 (5%)	31	26	6, 35, 70, 107	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	VAL	7.0
1	A	217	VAL	5.4
1	A	151	VAL	4.5
1	C	91	LYS	4.4
1	C	31	GLU	4.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NA	C	322	1/1	0.48	0.20	80,80,80,80	1
9	NA	C	320	1/1	0.79	0.10	60,60,60,60	0
6	CLA	A	318	41/65	0.84	0.21	44,79,96,119	0
6	CLA	B	318	41/65	0.85	0.21	44,76,92,115	0
6	CLA	C	318	40/65	0.88	0.19	36,69,91,110	0
6	CLA	B	315	65/65	0.90	0.16	20,43,74,83	0
5	CHL	C	309	48/66	0.90	0.15	26,43,97,104	0
6	CLA	A	315	65/65	0.90	0.17	28,48,76,86	0
8	ZN	C	321	1/1	0.90	0.14	64,64,64,64	0
6	CLA	A	316	65/65	0.90	0.18	30,41,88,98	0
3	NEX	C	303	44/44	0.90	0.16	14,32,90,92	0
4	LHG	B	304	49/49	0.91	0.19	14,40,98,107	0
8	ZN	A	322	1/1	0.91	0.10	122,122,122,122	0
5	CHL	A	309	48/66	0.91	0.13	32,48,95,101	0
3	NEX	B	303	44/44	0.91	0.16	26,42,94,97	0
3	NEX	A	303	44/44	0.91	0.15	26,39,94,96	0
5	CHL	B	309	48/66	0.92	0.14	35,52,99,105	0
6	CLA	C	314	65/65	0.92	0.14	15,27,79,93	0
6	CLA	C	316	65/65	0.92	0.16	22,37,84,97	0
6	CLA	C	317	65/65	0.92	0.14	16,31,87,95	0
4	LHG	A	304	49/49	0.92	0.16	19,42,98,108	0
5	CHL	C	311	66/66	0.92	0.15	11,31,94,115	0
6	CLA	B	308	62/65	0.92	0.14	21,37,83,91	0
6	CLA	A	308	62/65	0.92	0.14	20,35,82,89	0
6	CLA	B	316	65/65	0.92	0.16	28,41,89,99	0
6	CLA	C	315	65/65	0.93	0.15	21,45,74,87	0
2	LUT	B	301	42/42	0.93	0.11	18,26,42,62	0
5	CHL	B	311	66/66	0.93	0.14	21,38,99,119	0
6	CLA	A	314	65/65	0.93	0.14	23,34,78,93	0
5	CHL	C	305	66/66	0.93	0.14	14,34,87,104	0
5	CHL	A	310	51/66	0.93	0.12	21,36,94,100	0
6	CLA	C	308	62/65	0.93	0.14	12,28,80,87	0
6	CLA	A	317	65/65	0.93	0.14	21,37,90,99	0
9	NA	C	323	1/1	0.93	0.13	68,68,68,68	0
6	CLA	B	314	65/65	0.94	0.13	24,31,80,96	0
5	CHL	A	305	66/66	0.94	0.13	17,32,86,104	0
5	CHL	A	311	66/66	0.94	0.14	19,37,99,119	0
6	CLA	B	317	65/65	0.94	0.14	14,30,85,94	0
5	CHL	A	312	66/66	0.94	0.12	19,36,68,81	0
5	CHL	B	305	66/66	0.94	0.13	8,26,81,100	0
5	CHL	C	312	66/66	0.94	0.13	9,32,66,79	0
4	LHG	C	304	49/49	0.94	0.17	16,42,96,107	0
5	CHL	B	310	51/66	0.95	0.10	20,32,92,97	0

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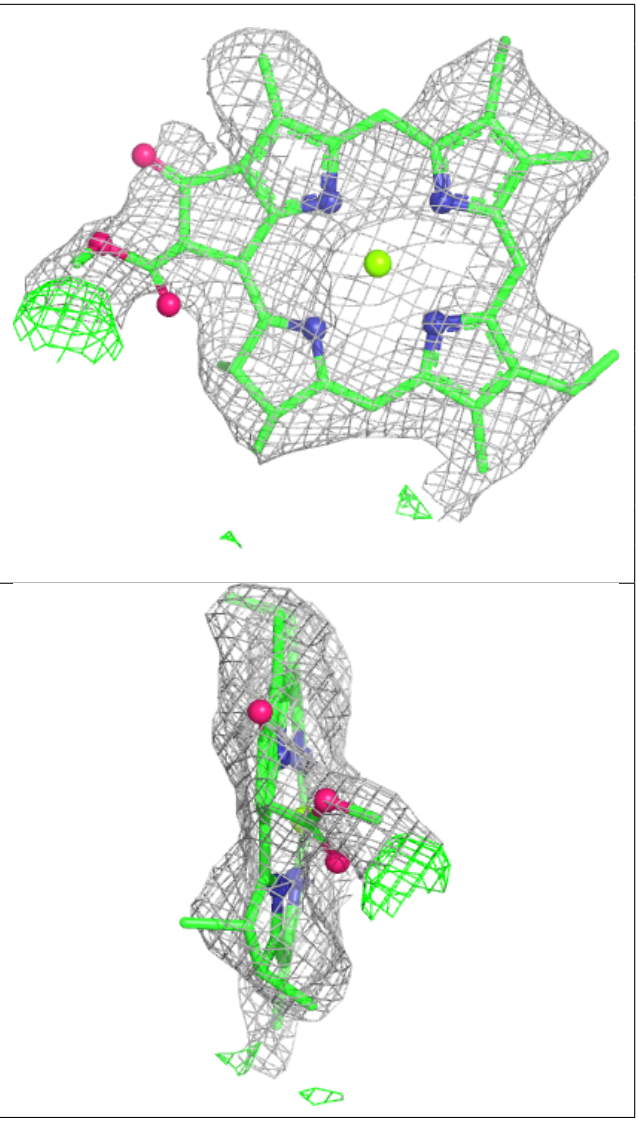
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CHL	C	313	66/66	0.95	0.10	5,21,66,80	0
2	LUT	A	301	42/42	0.95	0.10	20,25,39,61	0
5	CHL	B	312	66/66	0.95	0.12	22,40,71,83	0
2	LUT	B	302	42/42	0.95	0.09	6,19,32,35	0
8	ZN	B	321	1/1	0.95	0.09	66,66,66,66	0
2	LUT	C	301	42/42	0.95	0.10	15,22,35,57	0
9	NA	B	322	1/1	0.95	0.10	47,47,47,47	0
6	CLA	C	307	65/65	0.95	0.10	6,18,80,92	0
5	CHL	C	310	51/66	0.95	0.11	13,27,89,94	0
2	LUT	A	302	42/42	0.95	0.09	7,21,31,37	0
6	CLA	A	307	65/65	0.96	0.10	10,20,81,93	0
5	CHL	A	313	66/66	0.96	0.09	14,25,68,82	0
5	CHL	B	313	66/66	0.96	0.09	14,28,69,85	0
6	CLA	B	306	65/65	0.96	0.09	9,19,39,58	0
6	CLA	B	307	65/65	0.96	0.11	9,20,82,94	0
6	CLA	A	306	65/65	0.96	0.09	13,21,43,63	0
8	ZN	A	321	1/1	0.96	0.09	56,56,56,56	0
7	CAC	C	319	5/5	0.97	0.14	57,62,79,156	0
9	NA	B	320	1/1	0.97	0.06	42,42,42,42	0
8	ZN	A	320	1/1	0.97	0.07	98,98,98,98	0
6	CLA	C	306	65/65	0.97	0.08	7,19,41,60	0
2	LUT	C	302	42/42	0.97	0.07	6,16,30,35	0
7	CAC	A	319	5/5	0.97	0.13	57,59,68,81	0
7	CAC	B	319	5/5	0.98	0.12	59,62,68,97	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

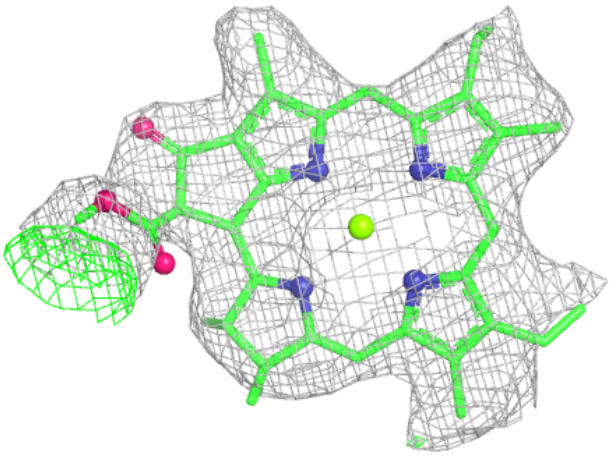
Electron density around CLA A 318:

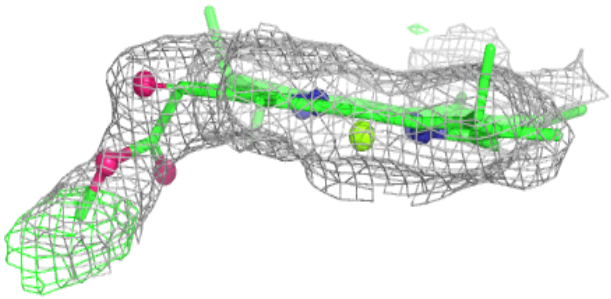
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

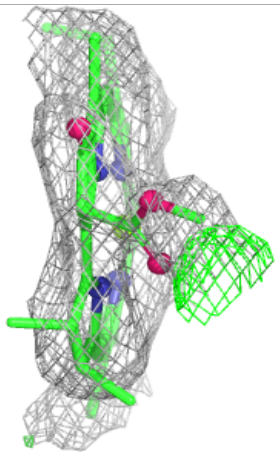


Electron density around CLA B 318:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

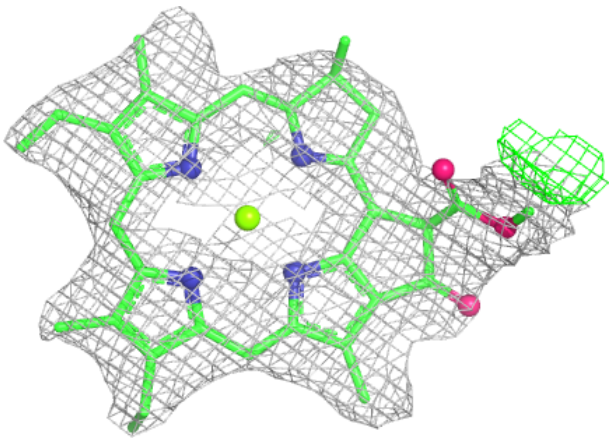


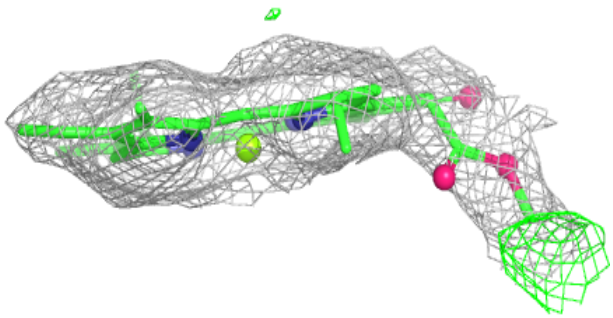


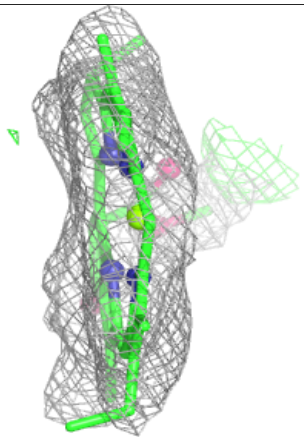


Electron density around CLA C 318:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

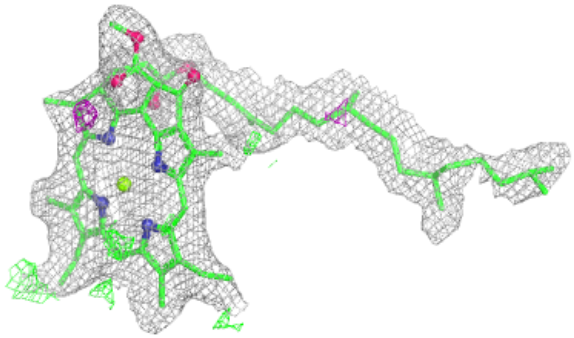


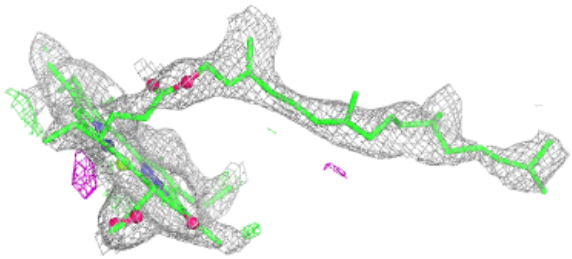


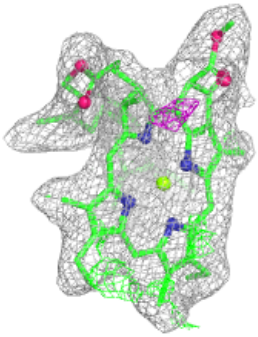


Electron density around CLA B 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

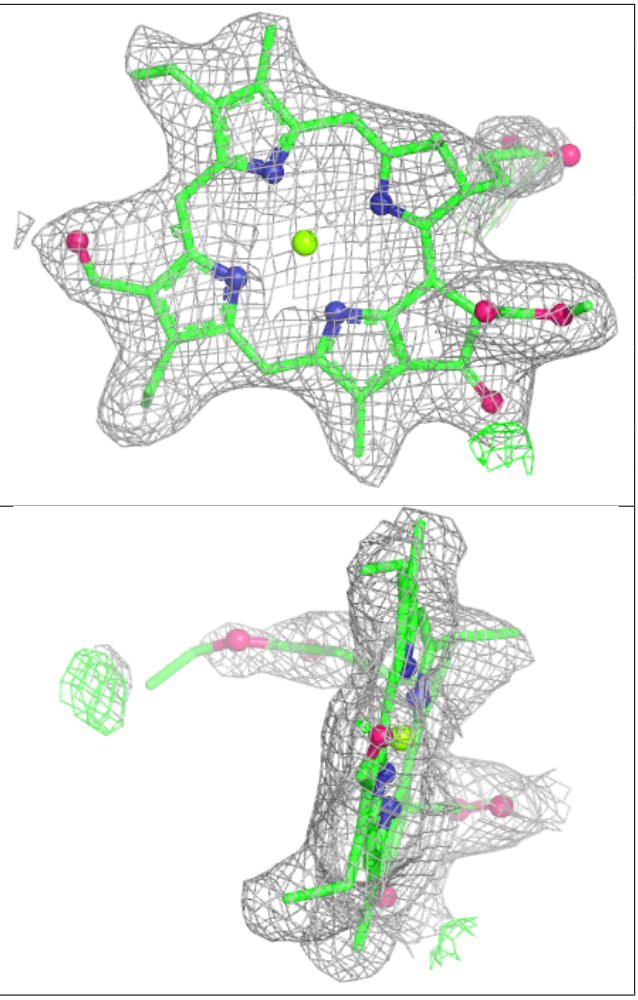






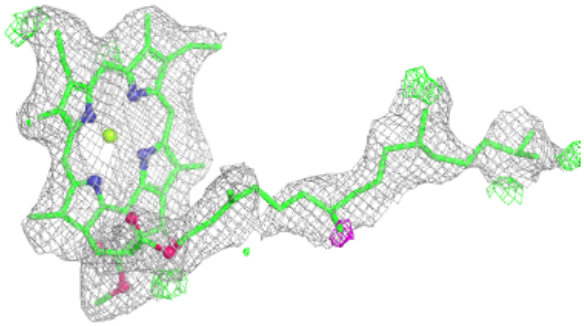
Electron density around CHL C 309:

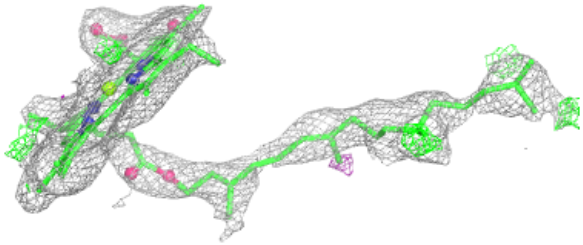
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

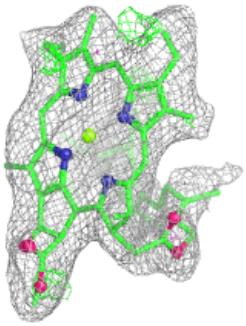


Electron density around CLA A 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

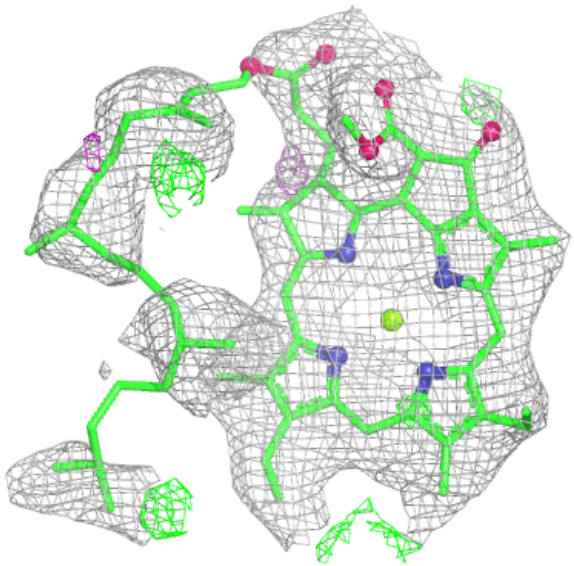


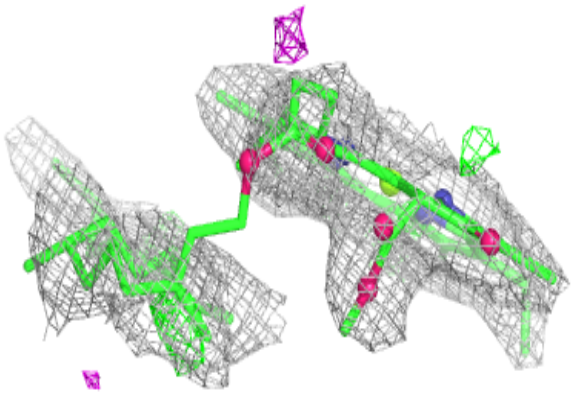


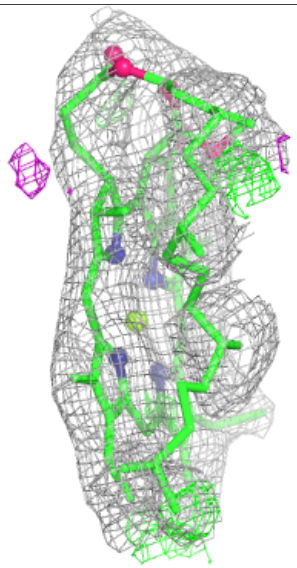


Electron density around CLA A 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

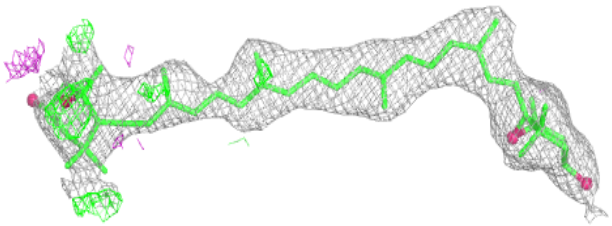


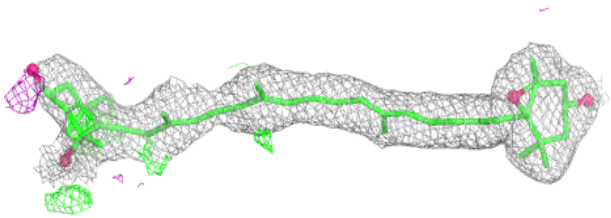


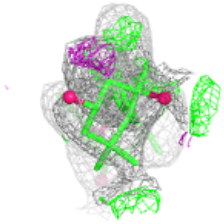


Electron density around NEX C 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

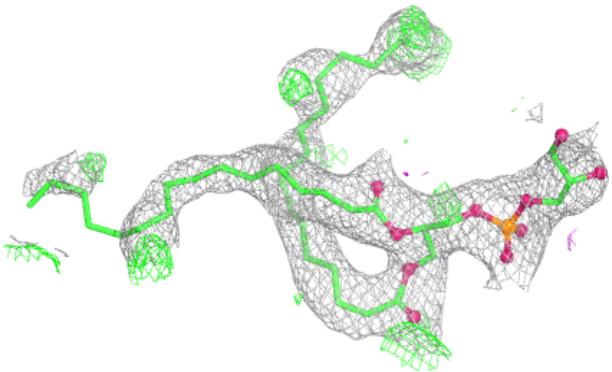


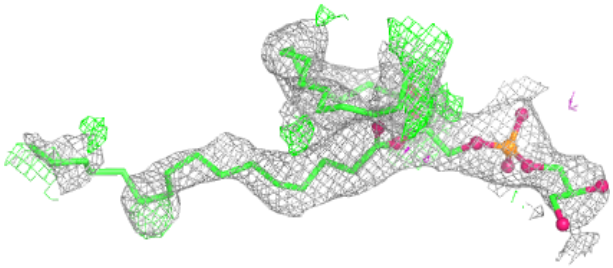


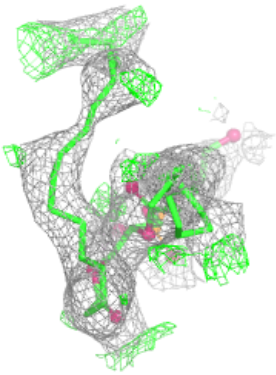


Electron density around LHG B 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

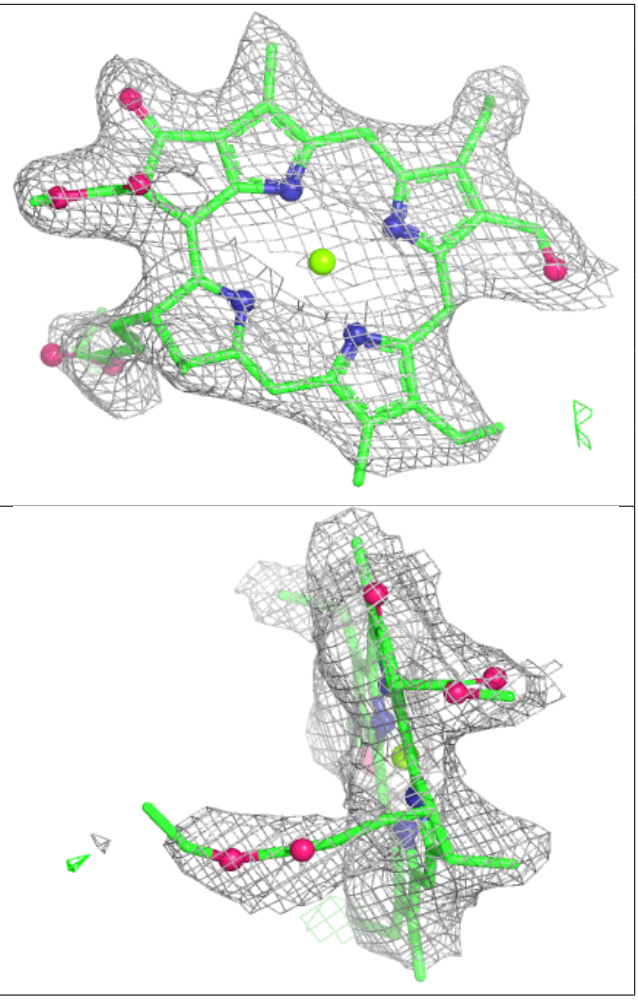






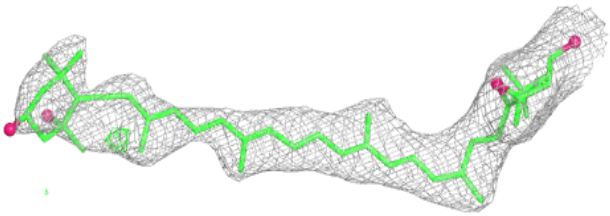
Electron density around CHL A 309:

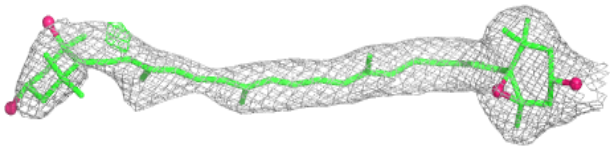
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

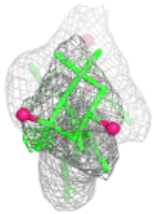


Electron density around NEX B 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

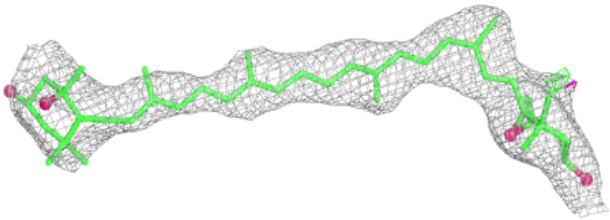


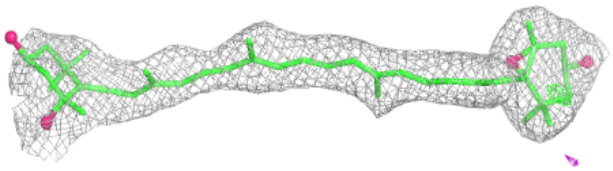


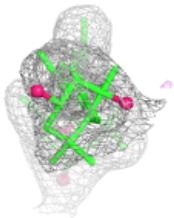


Electron density around NEX A 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

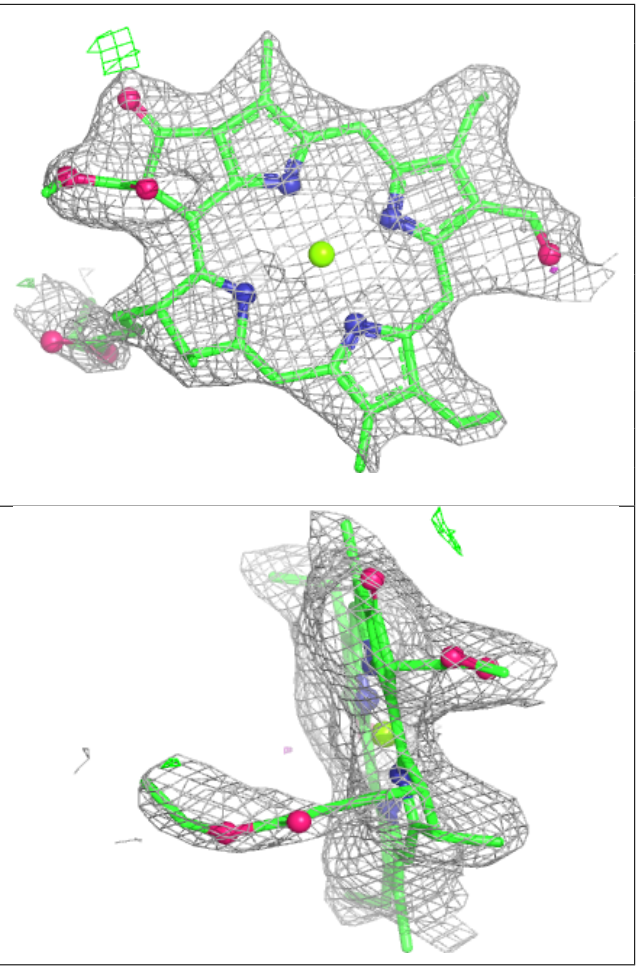






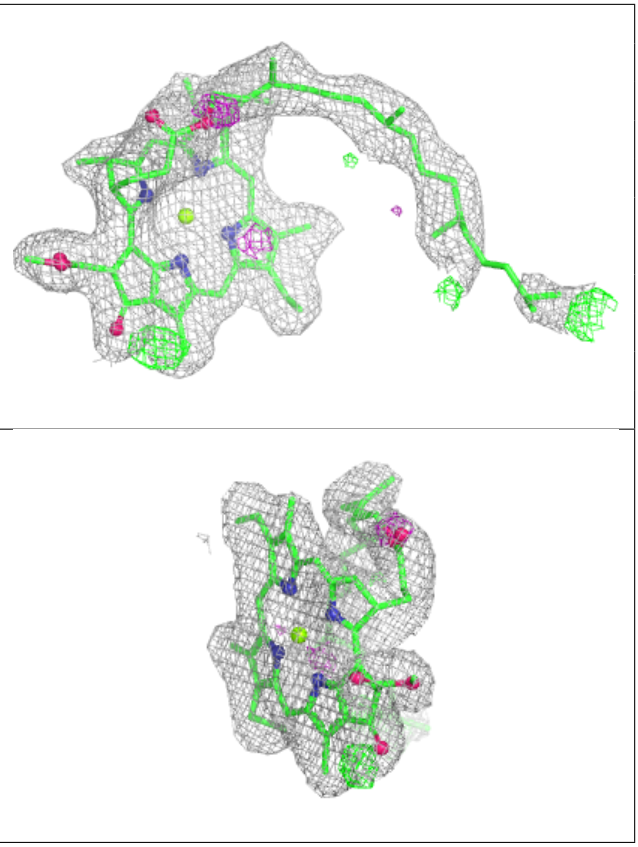
Electron density around CHL B 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



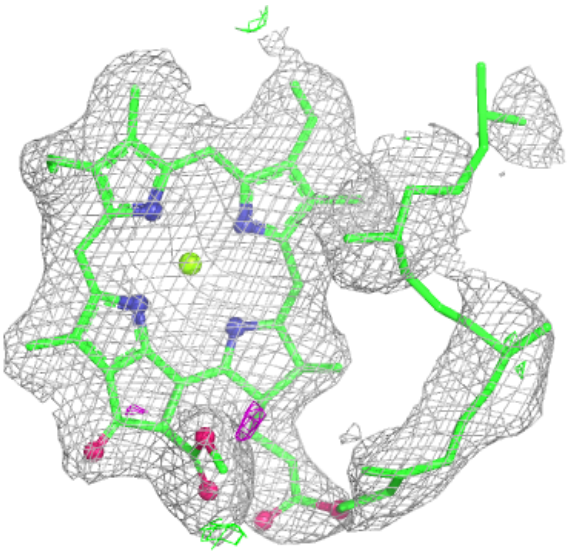
Electron density around CLA C 314:

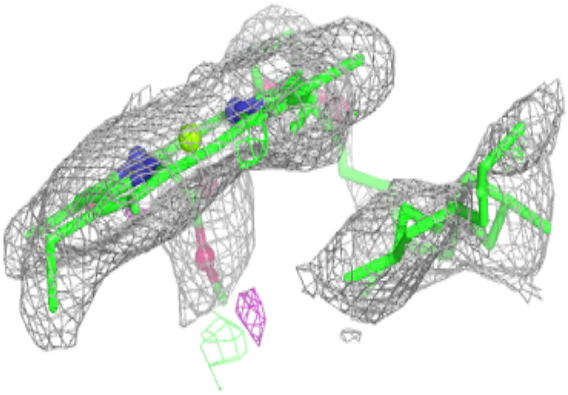
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

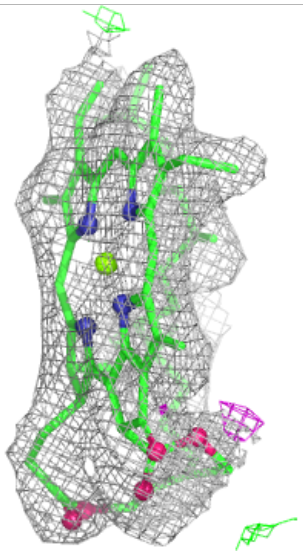


Electron density around CLA C 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

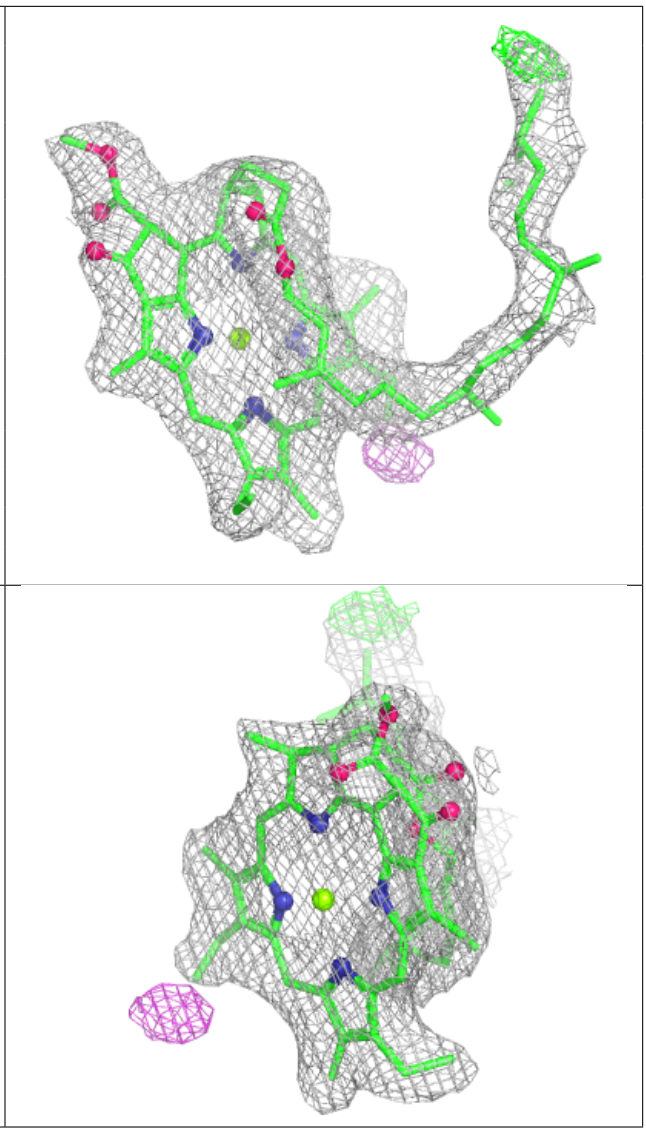






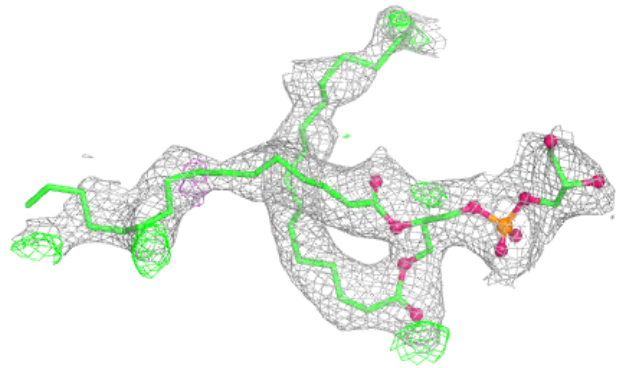
Electron density around CLA C 317:

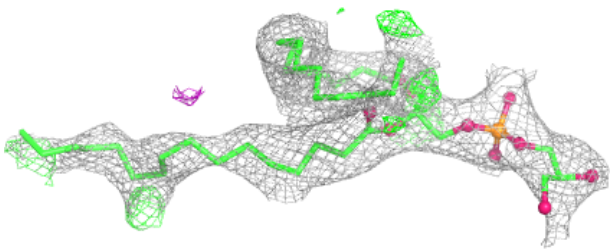
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

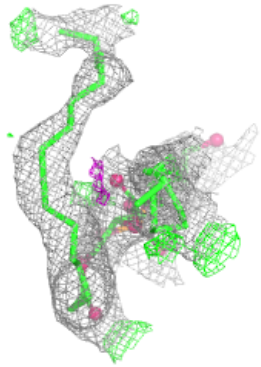


Electron density around LHG A 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

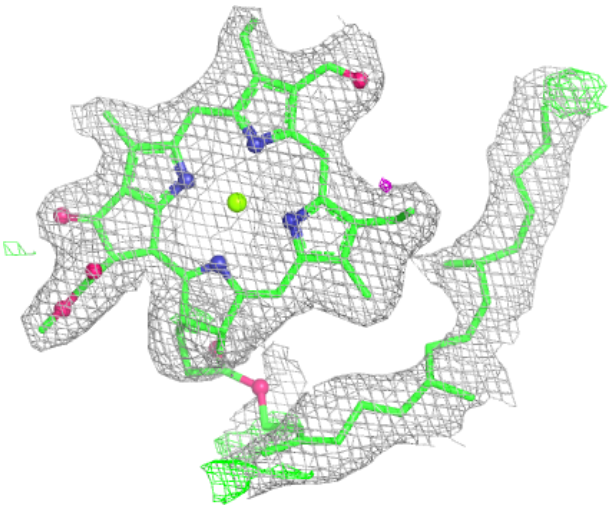


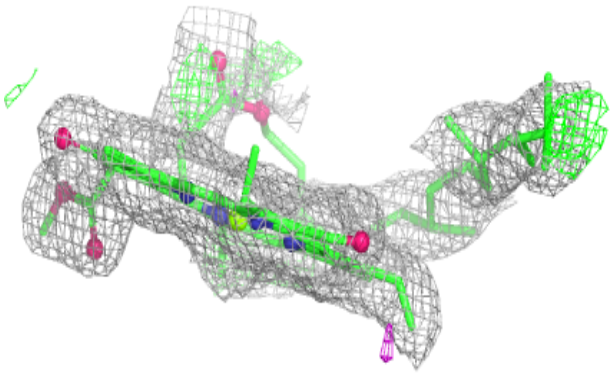


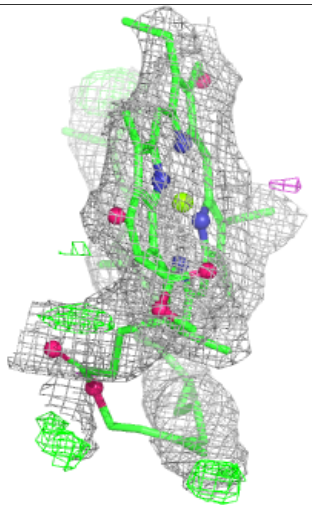


Electron density around CHL C 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

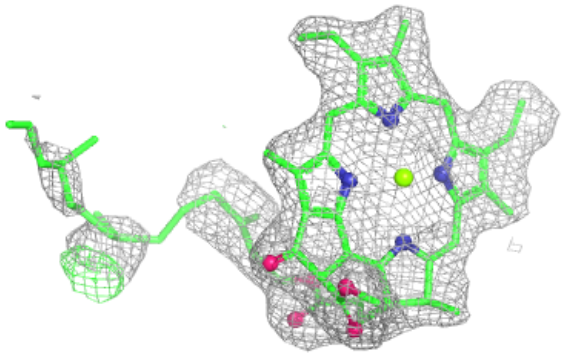


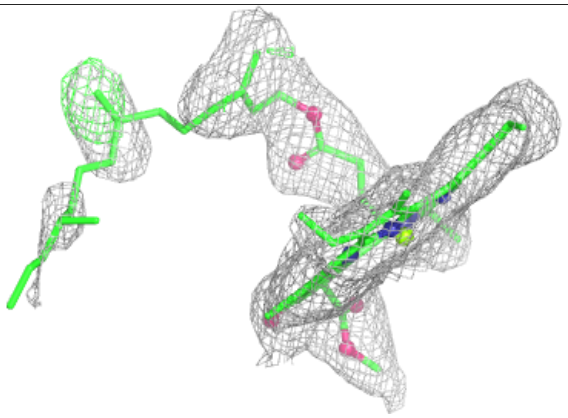


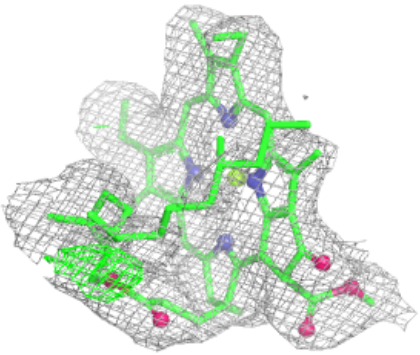


Electron density around CLA B 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

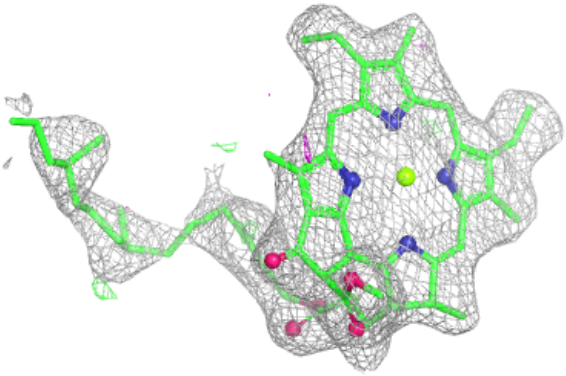


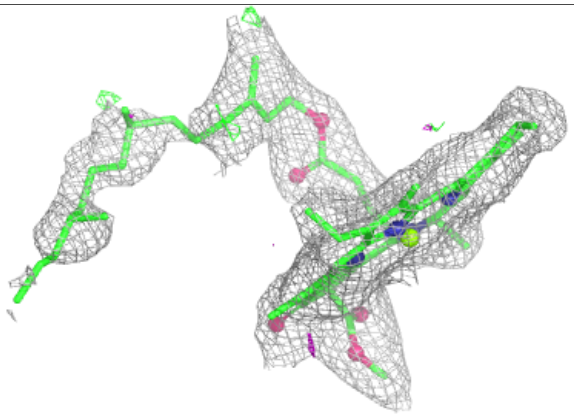


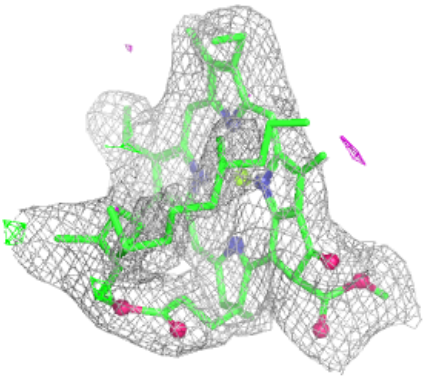


Electron density around CLA A 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

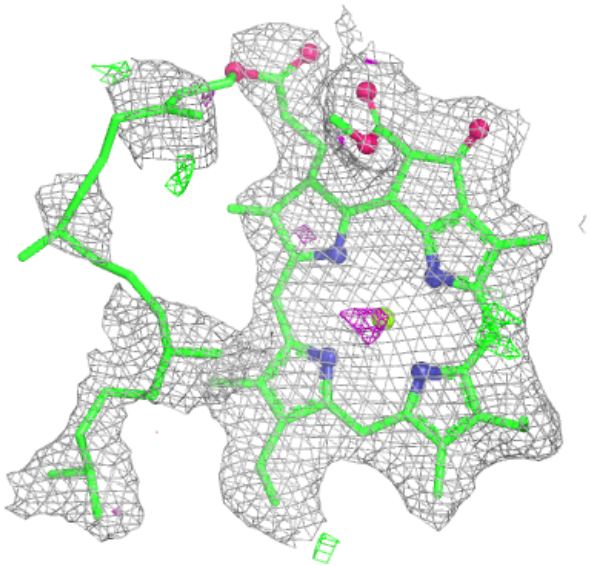


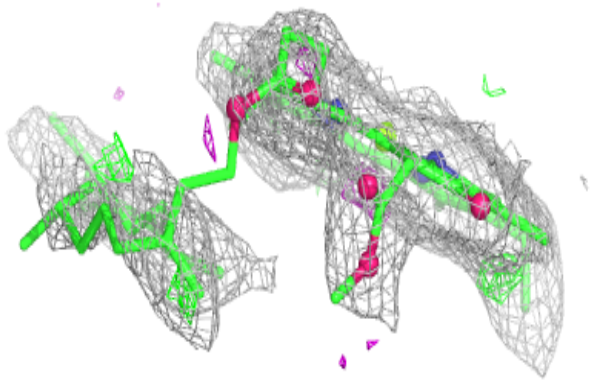




Electron density around CLA B 316:

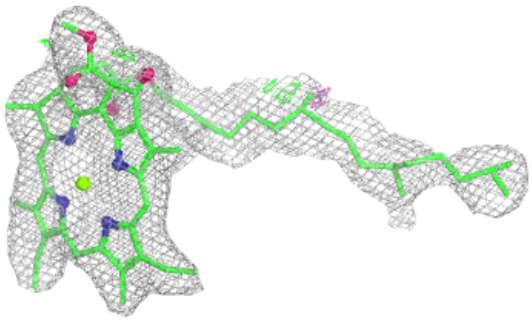
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

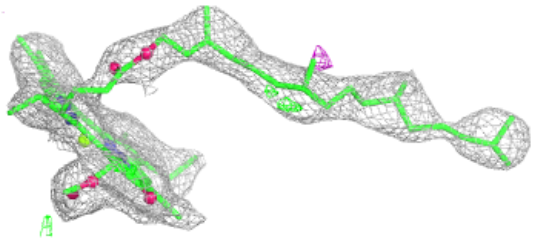


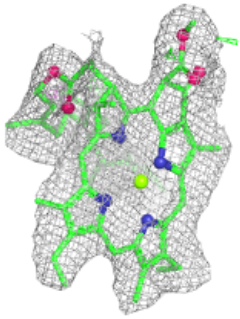


Electron density around CLA C 315:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

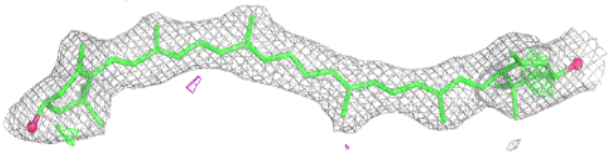


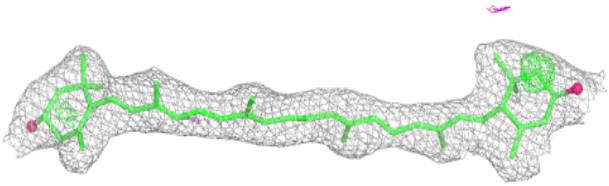


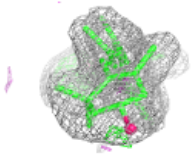


Electron density around LUT B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

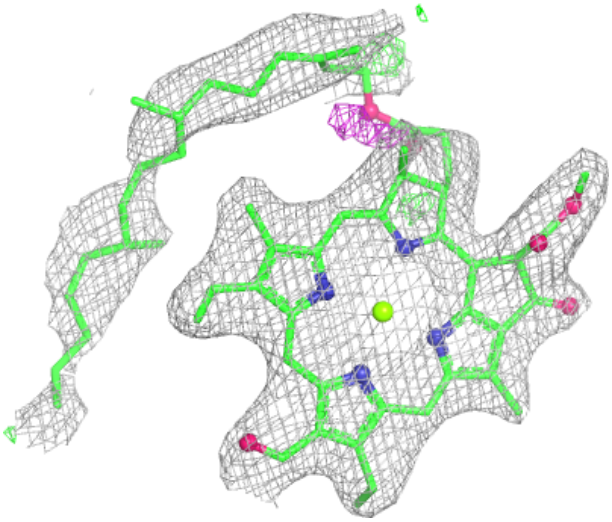


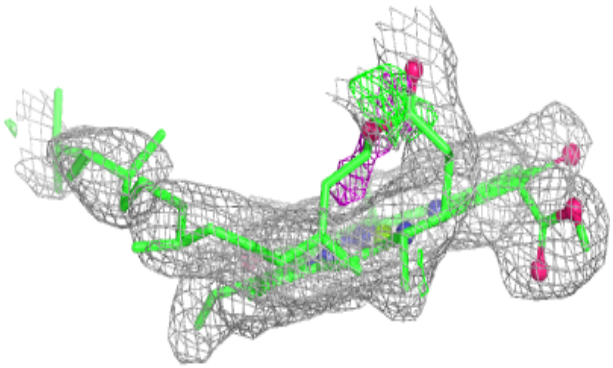




Electron density around CHL B 311:

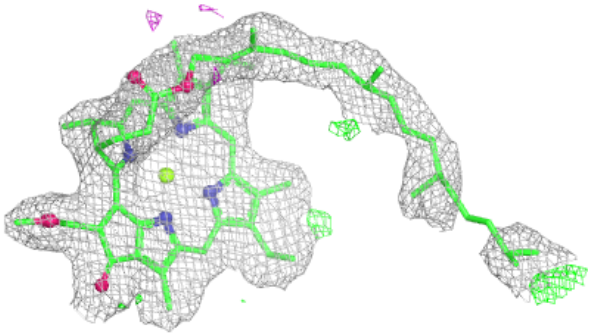
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

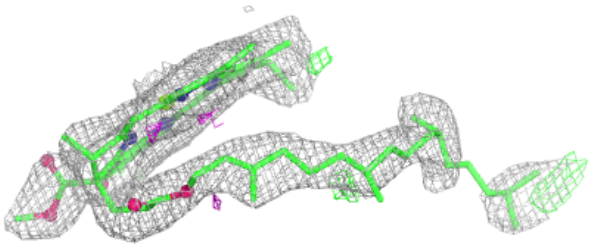


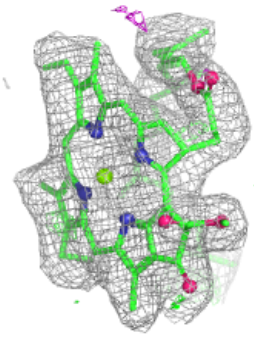


Electron density around CLA A 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

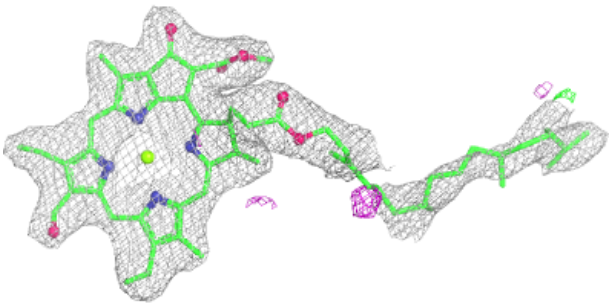


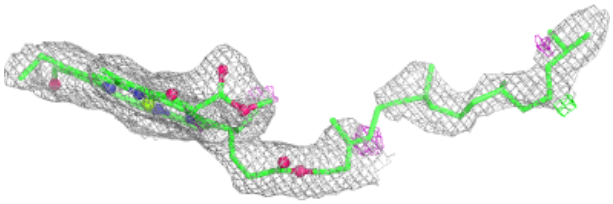




Electron density around CHL C 305:

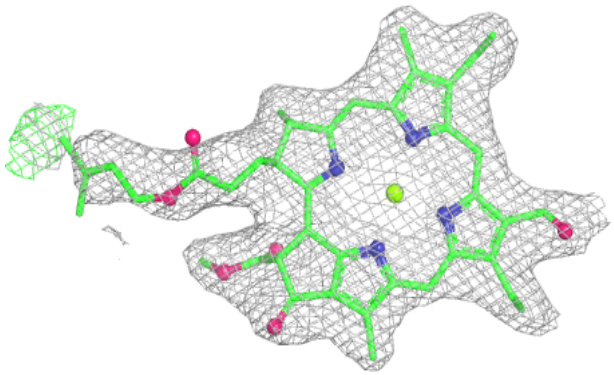
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

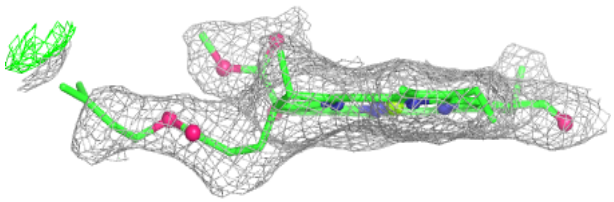


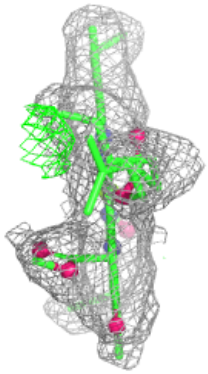


Electron density around CHL A 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

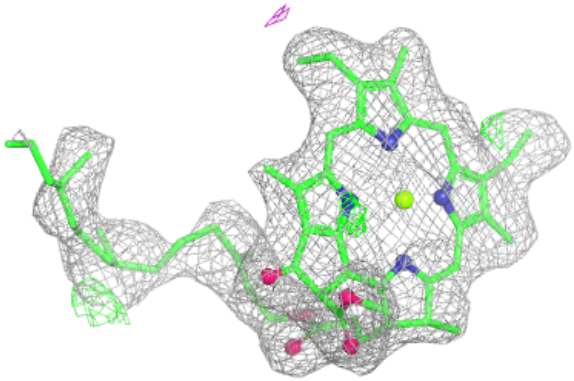


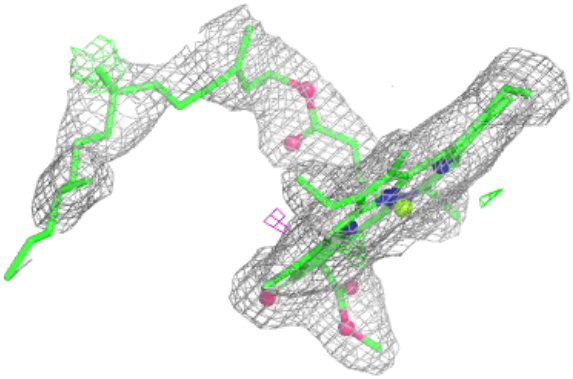


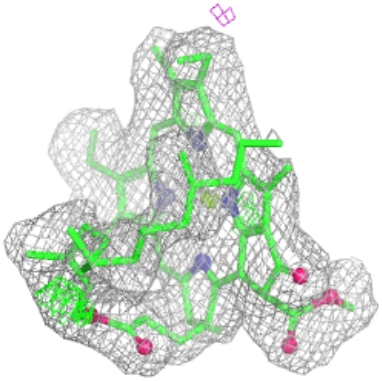


Electron density around CLA C 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

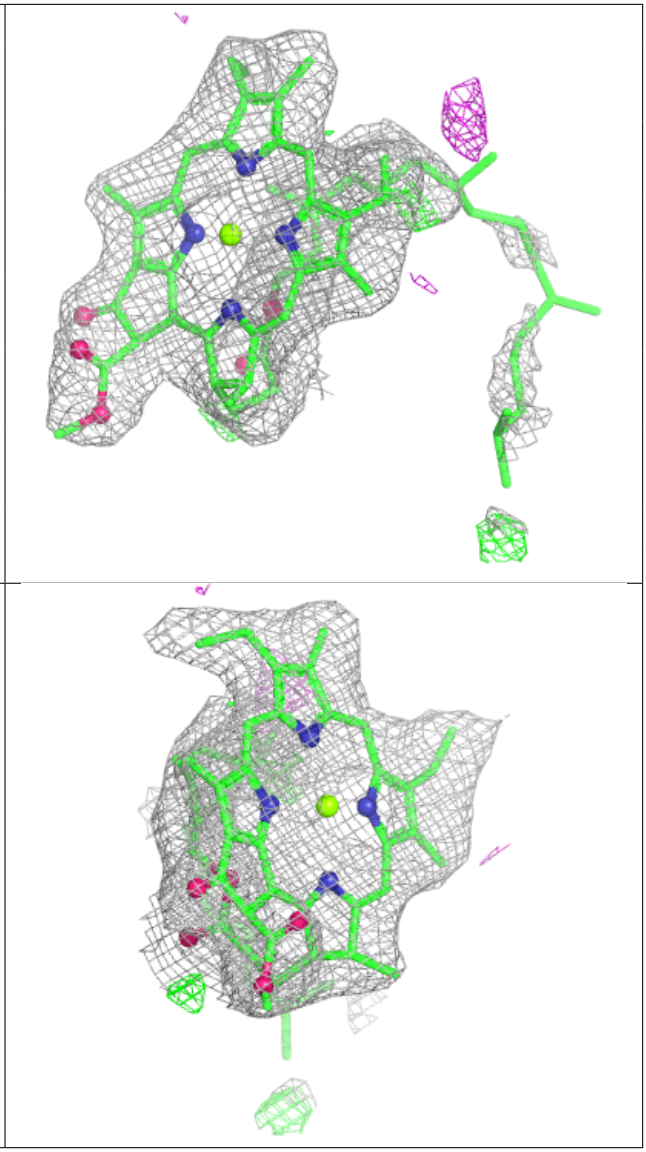






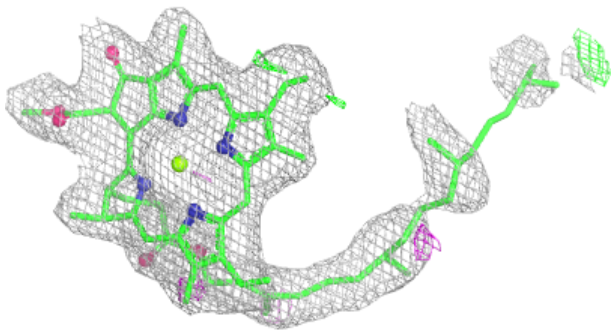
Electron density around CLA A 317:

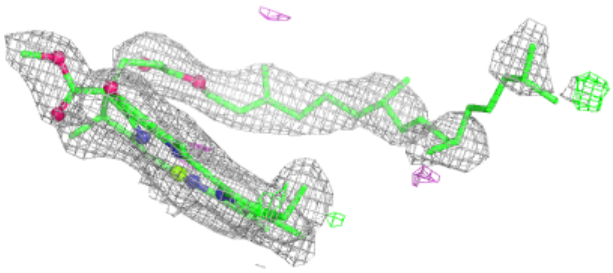
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

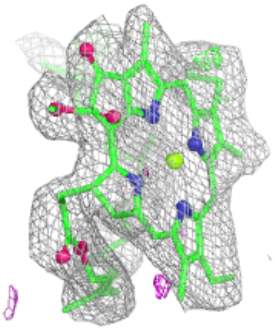


Electron density around CLA B 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

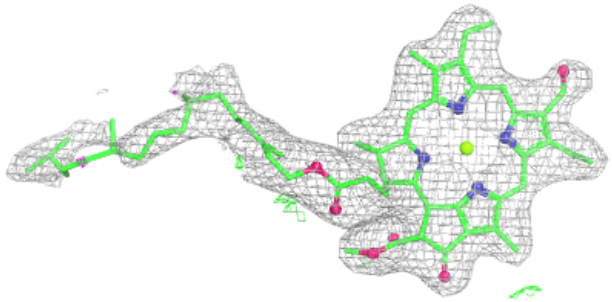


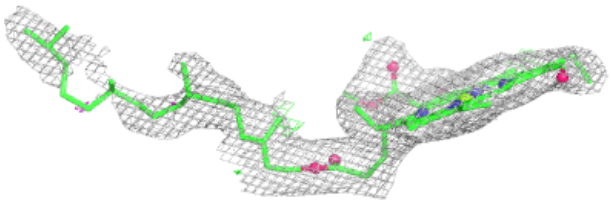


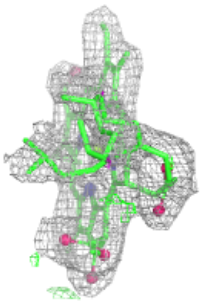


Electron density around CHL A 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

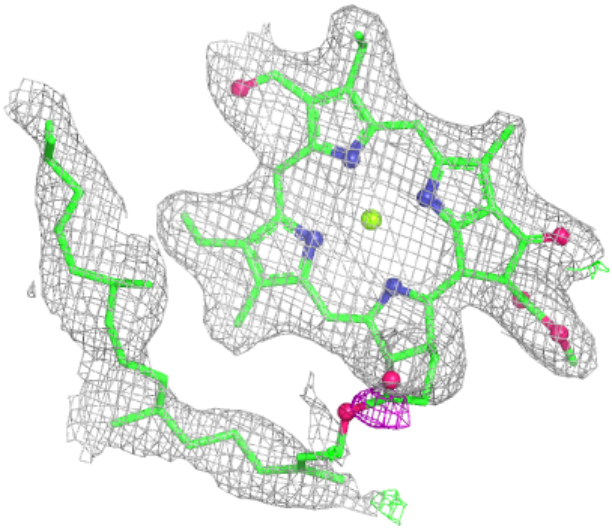


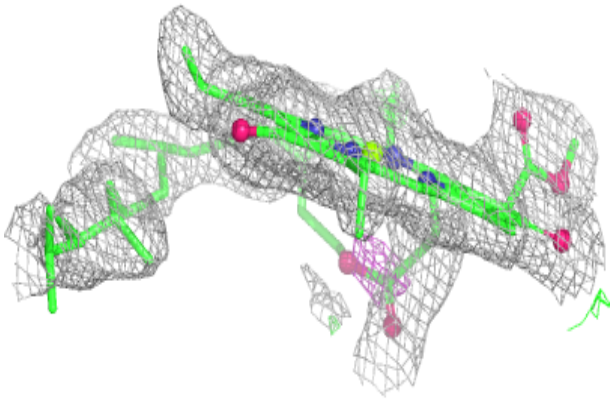


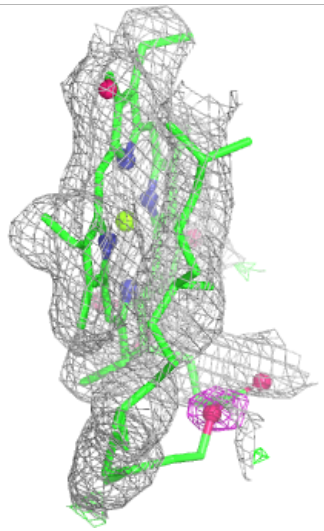


Electron density around CHL A 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

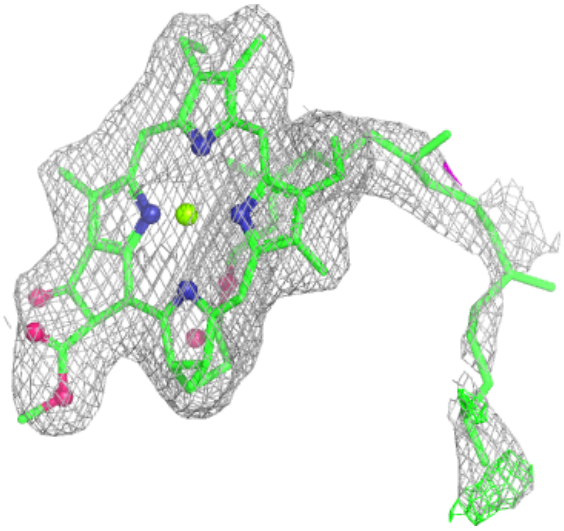


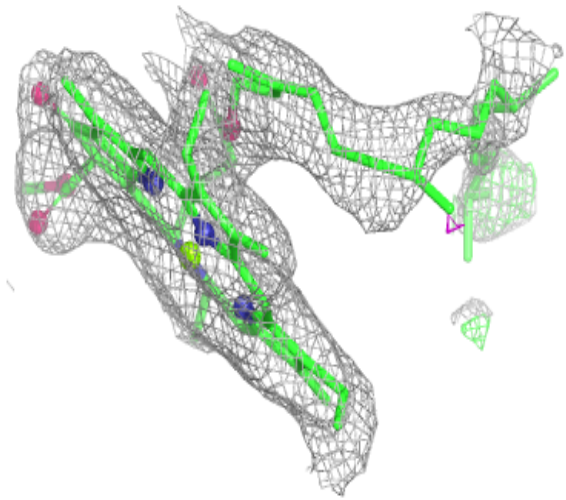


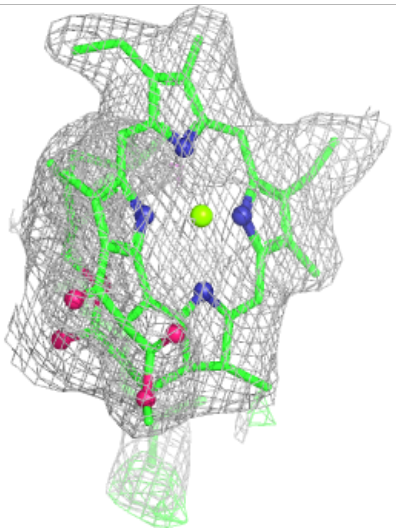


Electron density around CLA B 317:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

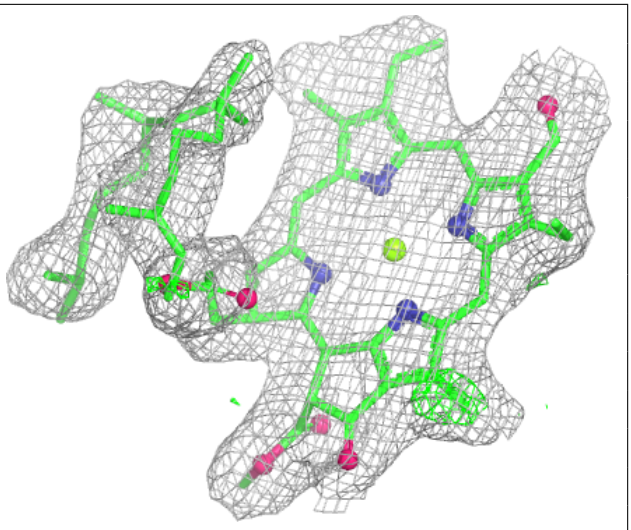


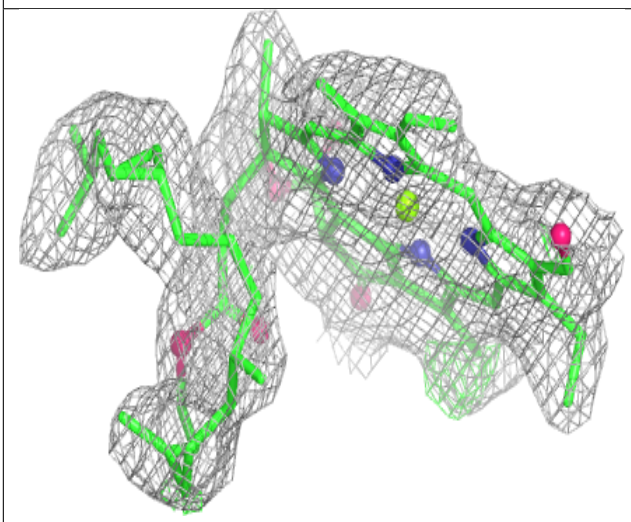


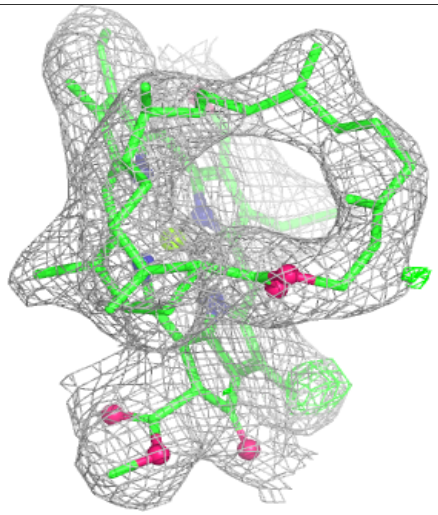


Electron density around CHL A 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

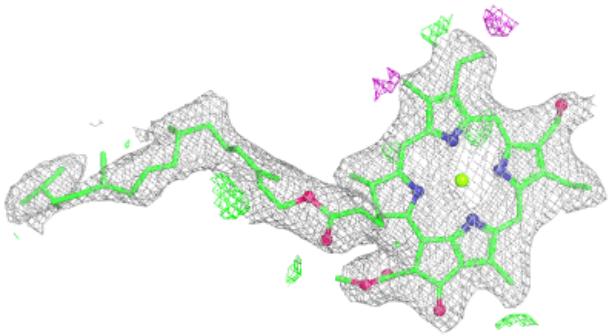


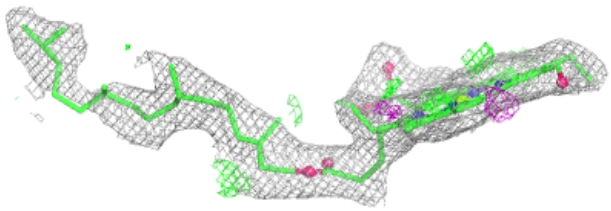


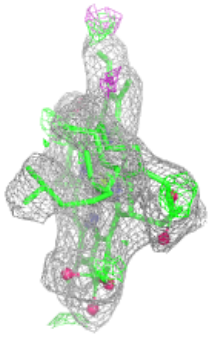


Electron density around CHL B 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

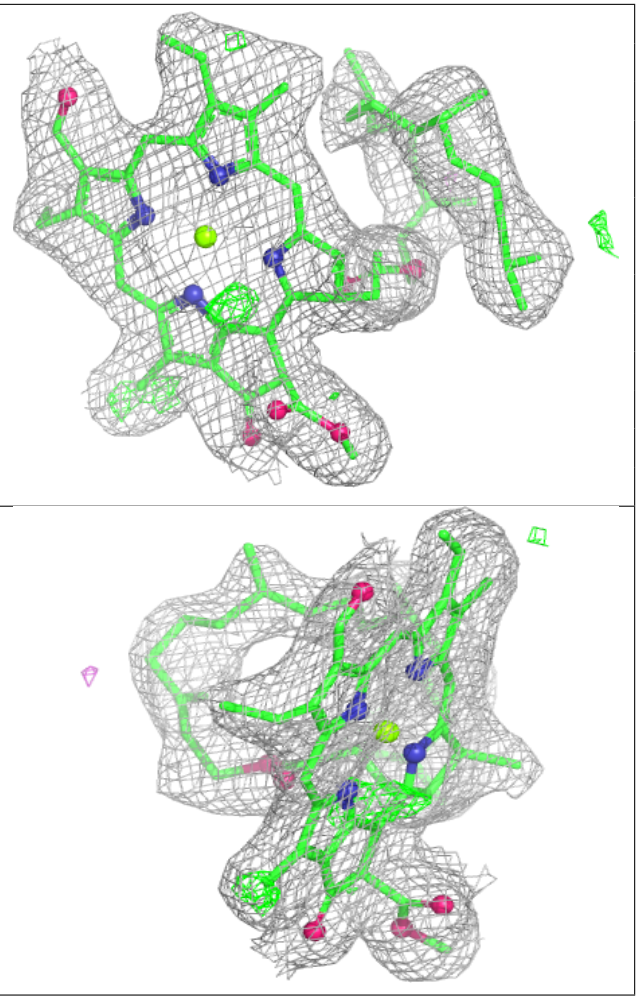






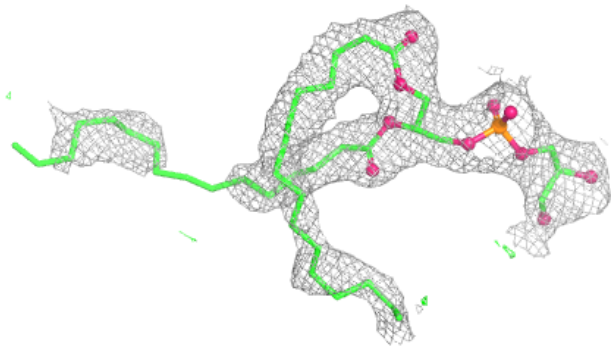
Electron density around CHL C 312:

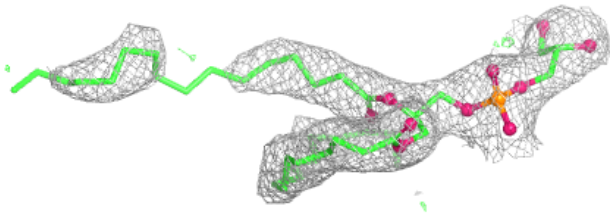
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

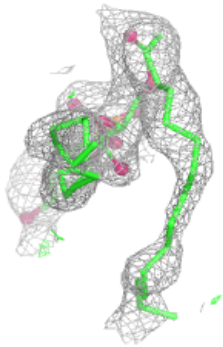


Electron density around LHG C 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

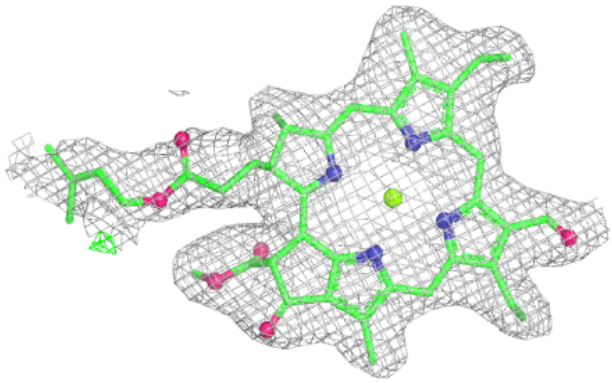


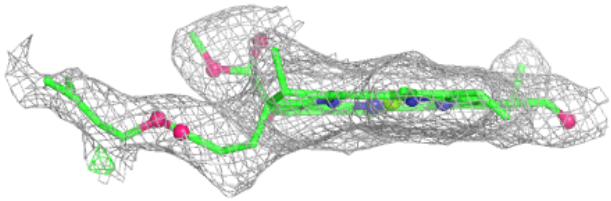


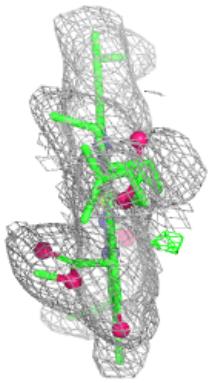


Electron density around CHL B 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

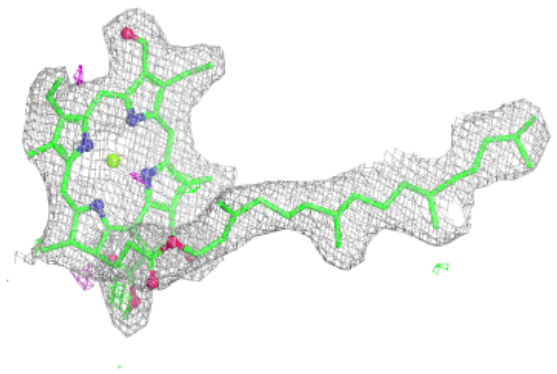


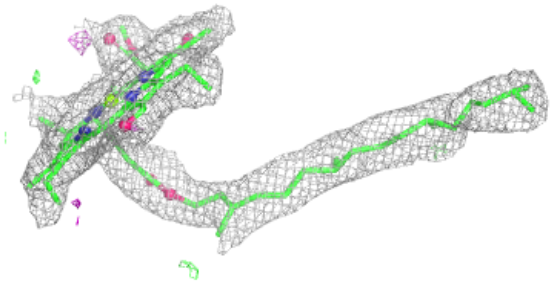


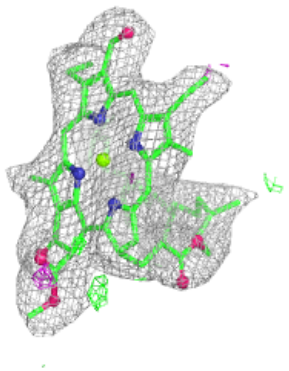


Electron density around CHL C 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

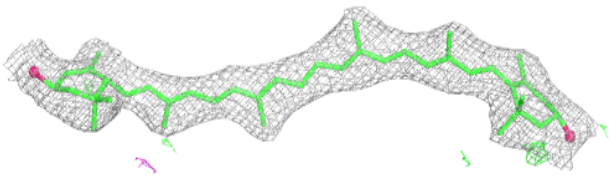


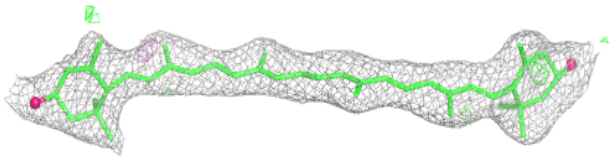


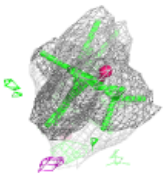


Electron density around LUT A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

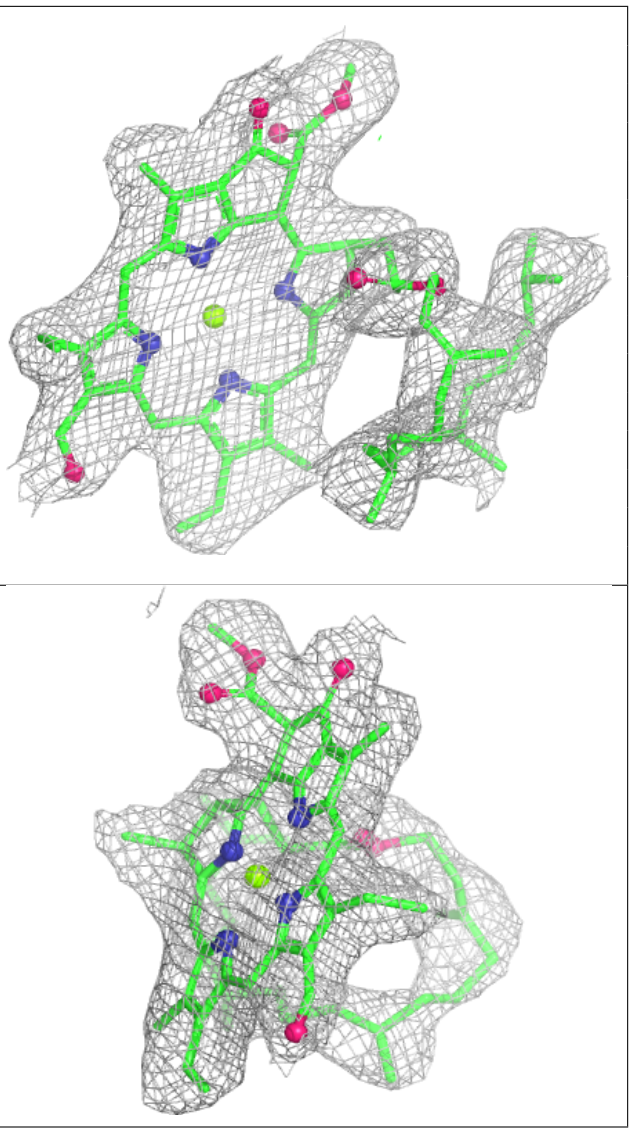






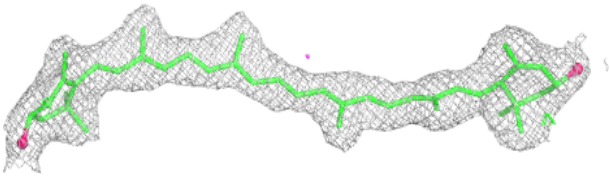
Electron density around CHL B 312:

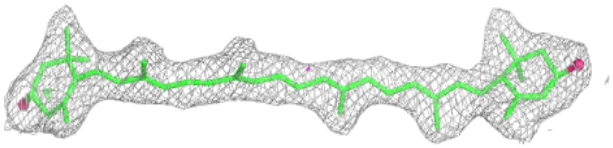
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

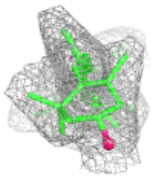


Electron density around LUT B 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

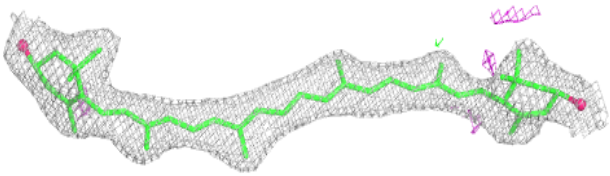


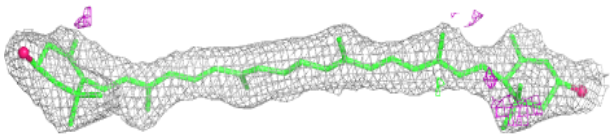


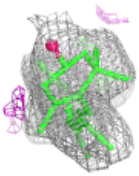


Electron density around LUT C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

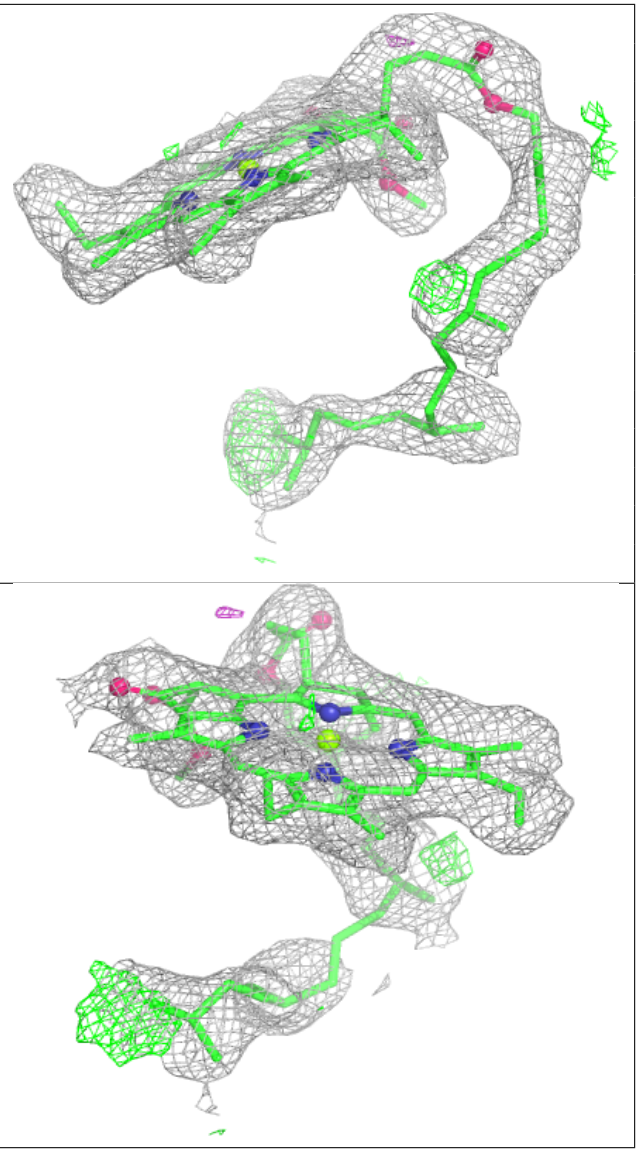






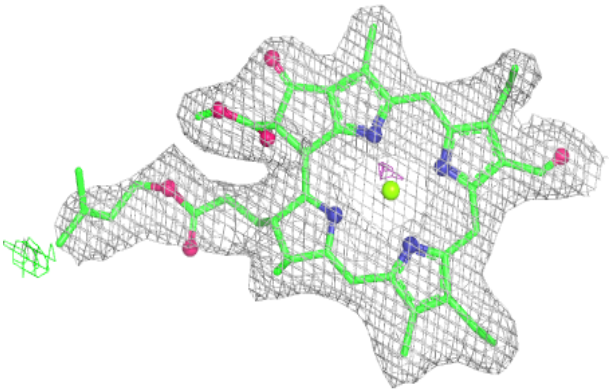
Electron density around CLA C 307:

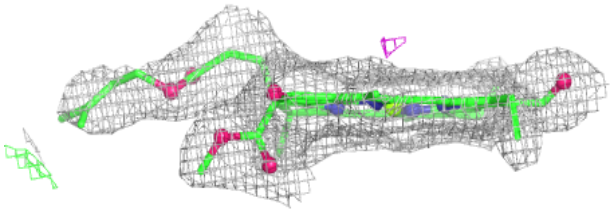
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

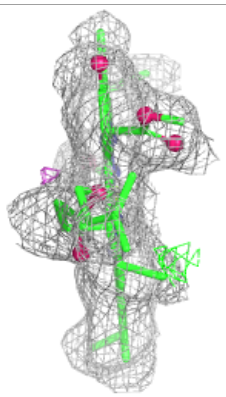


Electron density around CHL C 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

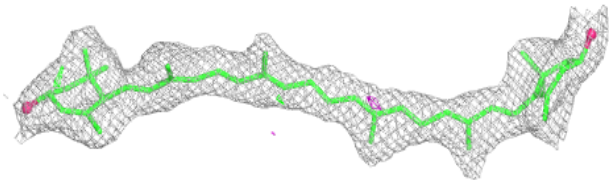


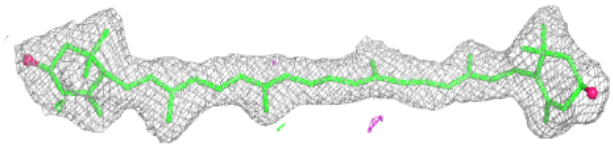


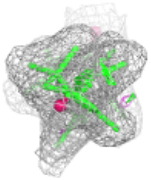


Electron density around LUT A 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

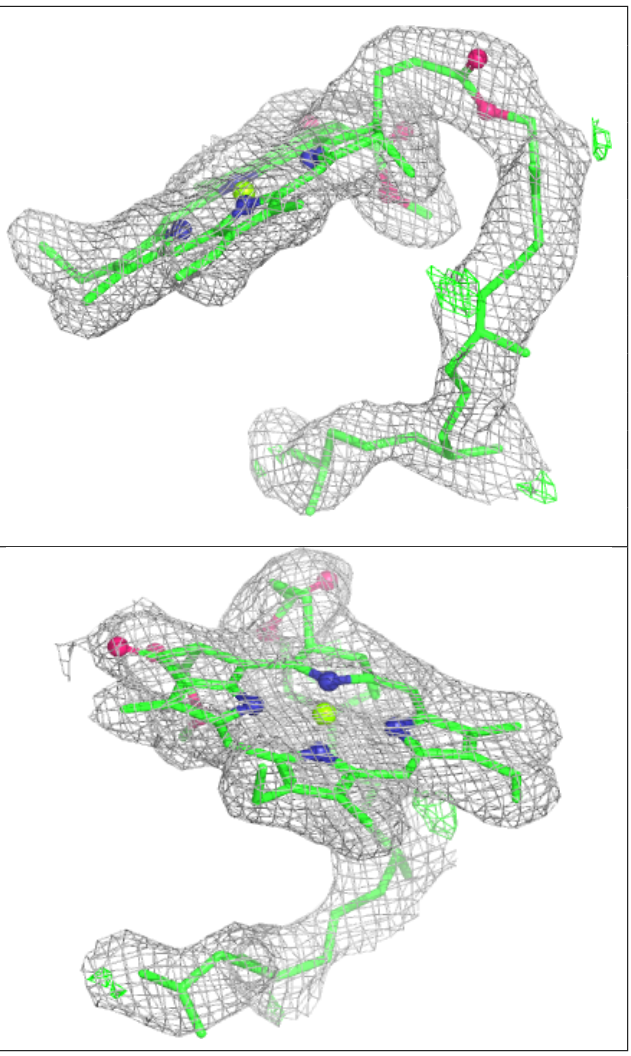






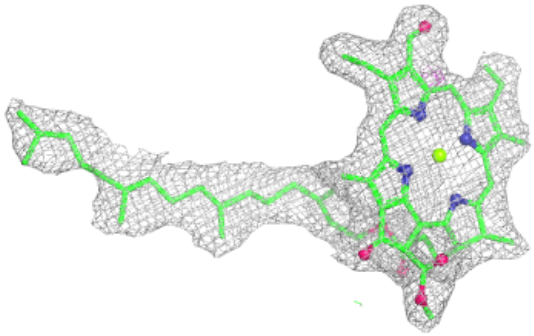
Electron density around CLA A 307:

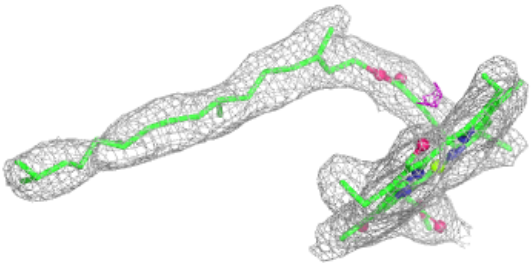
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

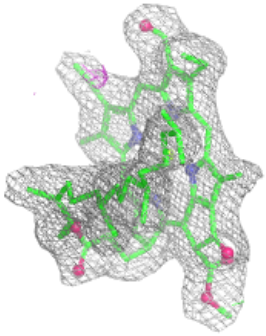


Electron density around CHL A 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

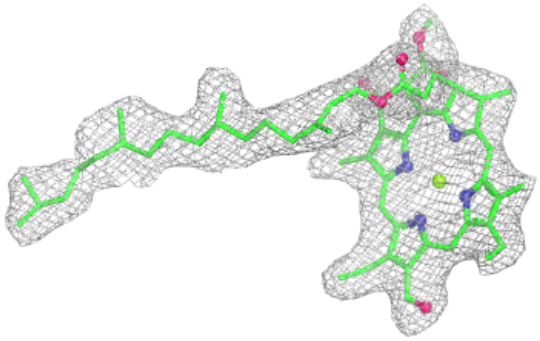


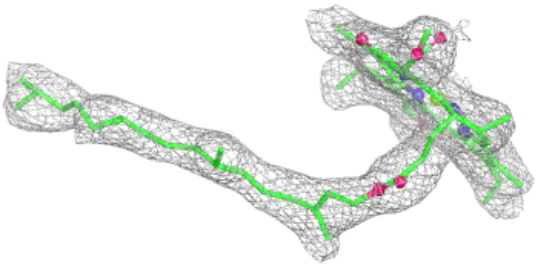


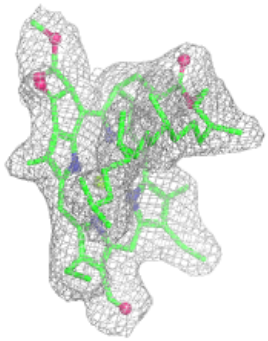


Electron density around CHL B 313:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

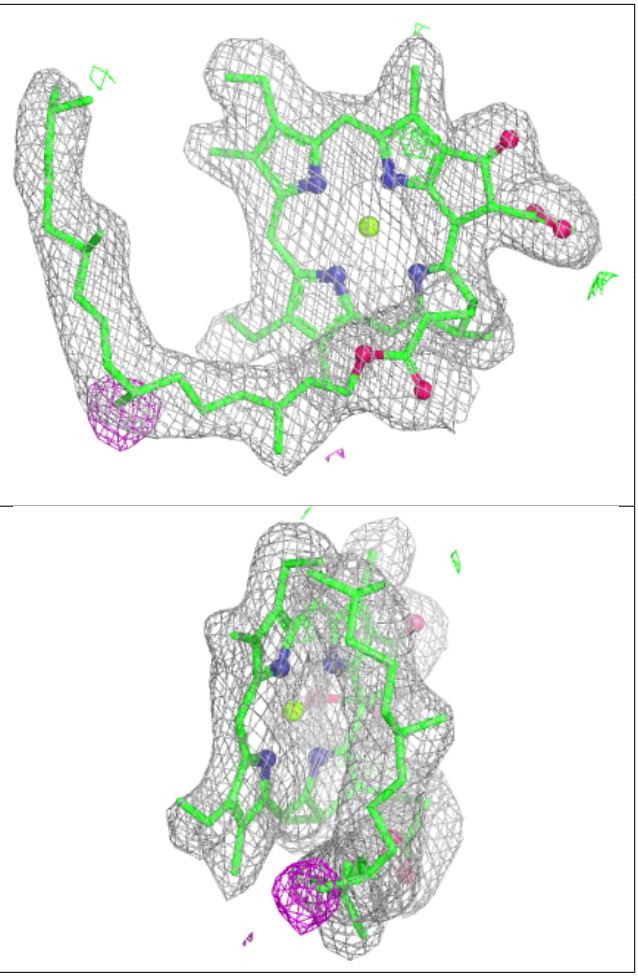






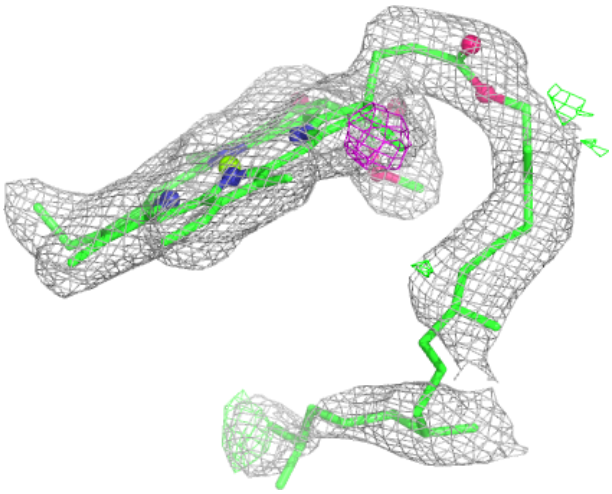
Electron density around CLA B 306:

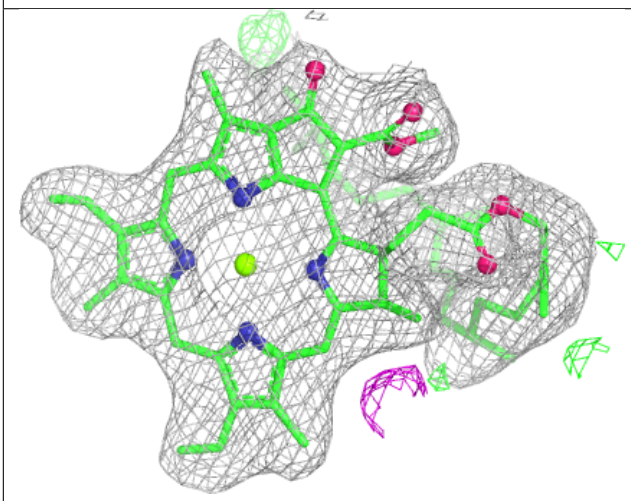
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

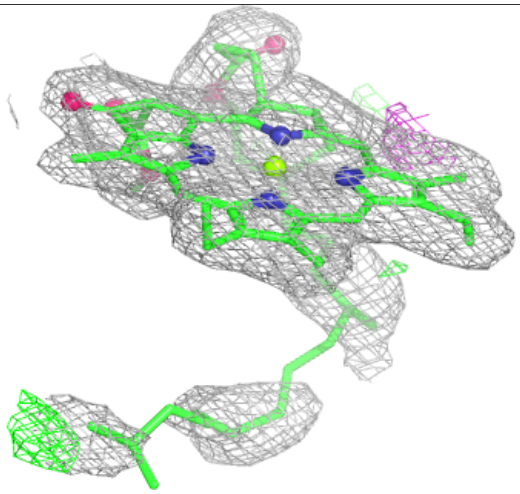


Electron density around CLA B 307:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

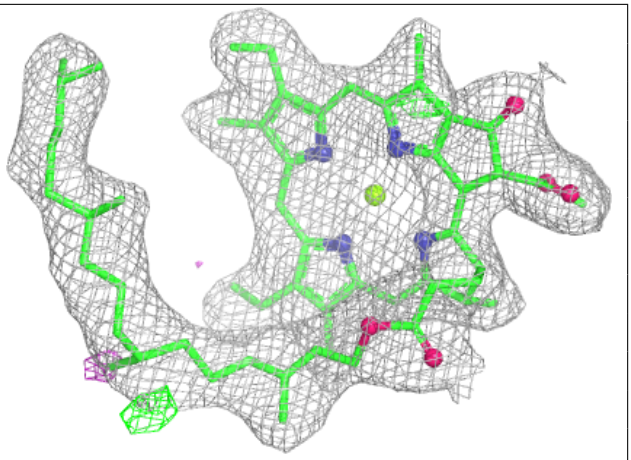


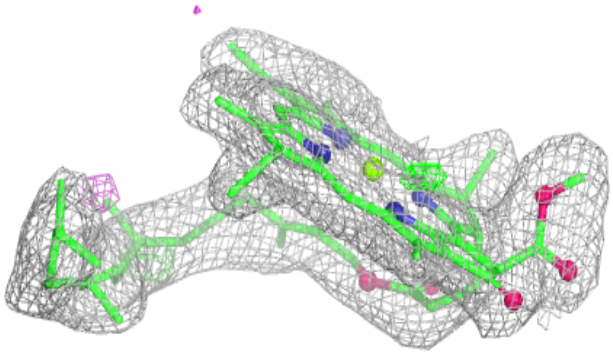


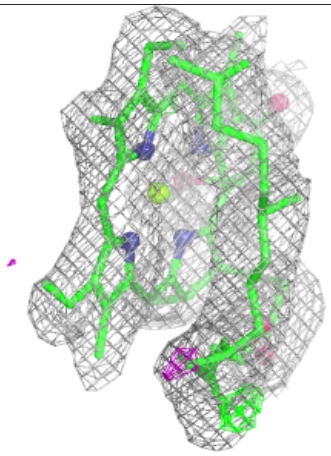


Electron density around CLA A 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

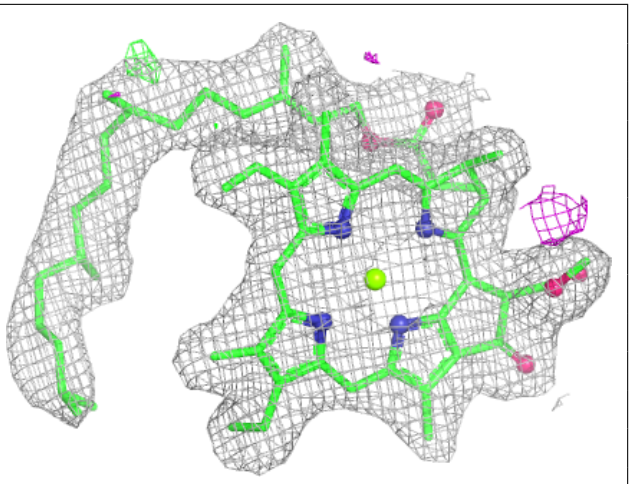


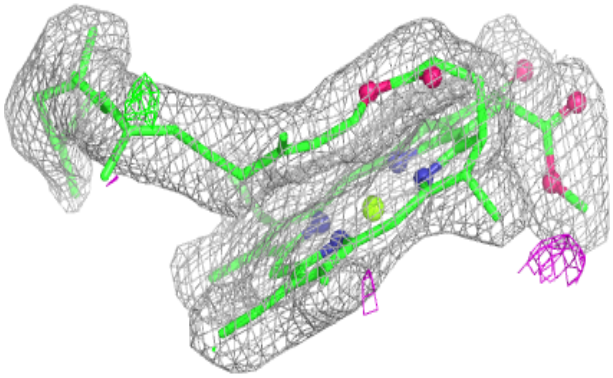


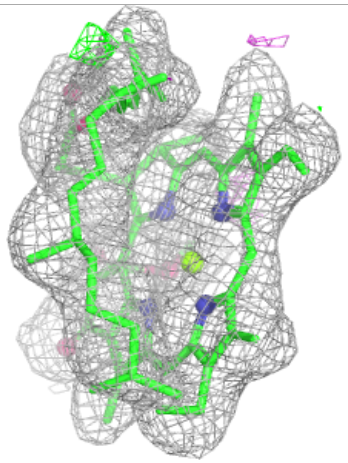


Electron density around CLA C 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

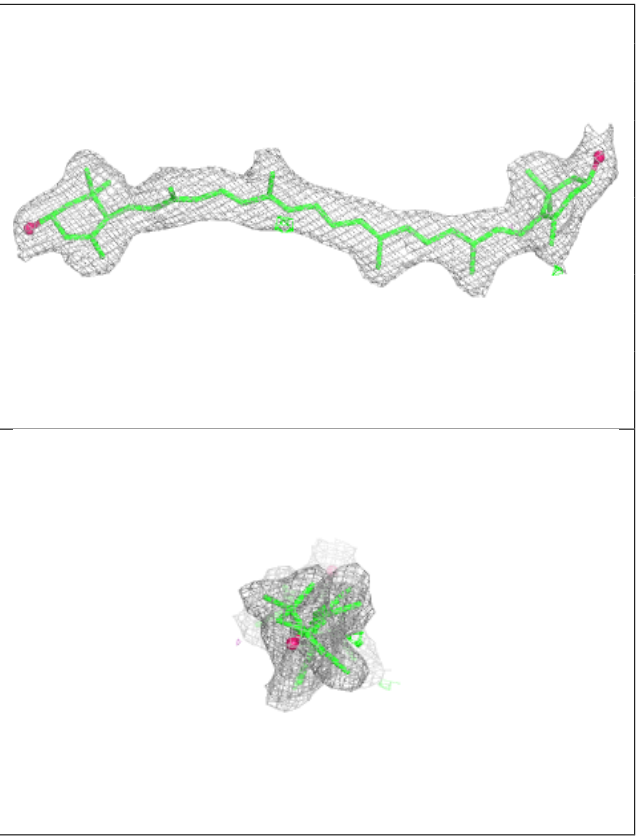






Electron density around LUT C 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.