



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2026 – 05:56 AM JST

PDB ID : 8HQ8 / pdb_00008hq8
Title : Bry-LHCII homotrimer of Bryopsis corticulans
Authors : Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on : 2022-12-13
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

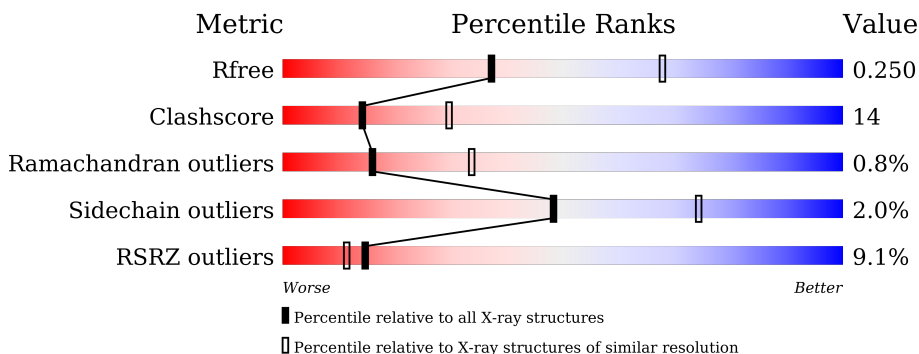
1 Overall quality at a glance

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 $\leq 5\%$. 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	249	9%	69%	20%	10%
1	B	249	7%	70%	19%	10%
1	C	249	5%	72%	17%	11%
1	D	249	7%	72%	17%	10%
1	E	249	12%	65%	23%	10%
1	F	249	8%	71%	18%	10%

2 Entry composition [i](#)

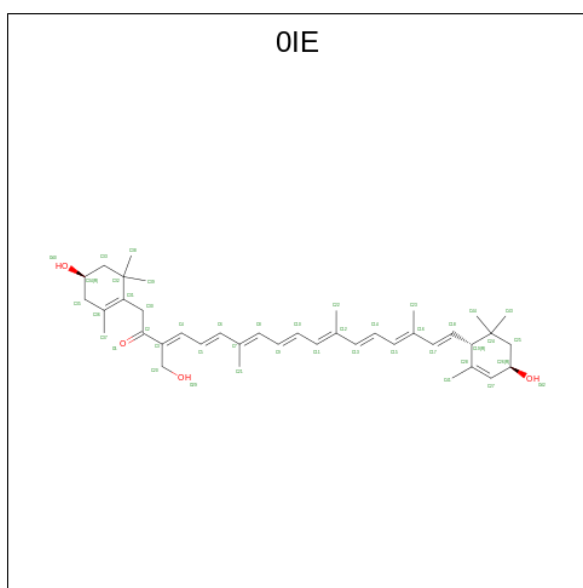
There are 12 unique types of molecules in this entry. The entry contains 16480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1.

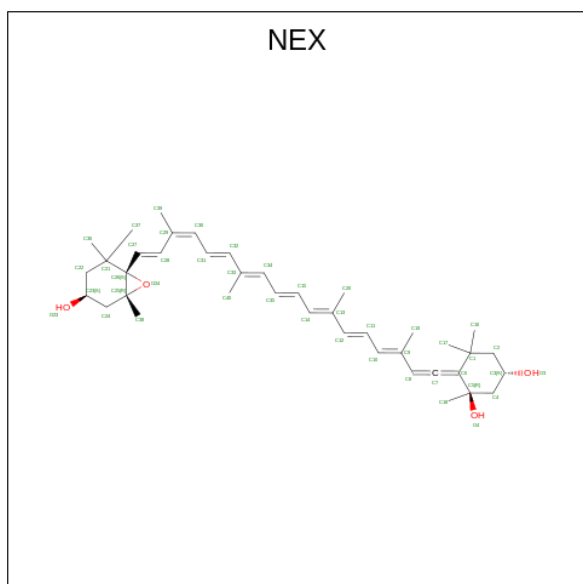
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1672	1083	265	314	10			
1	B	223	Total	C	N	O	S	0	0	0
			1669	1083	266	310	10			
1	C	222	Total	C	N	O	S	0	0	0
			1659	1075	264	310	10			
1	D	223	Total	C	N	O	S	0	0	0
			1682	1090	267	315	10			
1	E	223	Total	C	N	O	S	0	0	0
			1684	1095	267	312	10			
1	F	223	Total	C	N	O	S	0	0	0
			1685	1094	267	314	10			

- Molecule 2 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



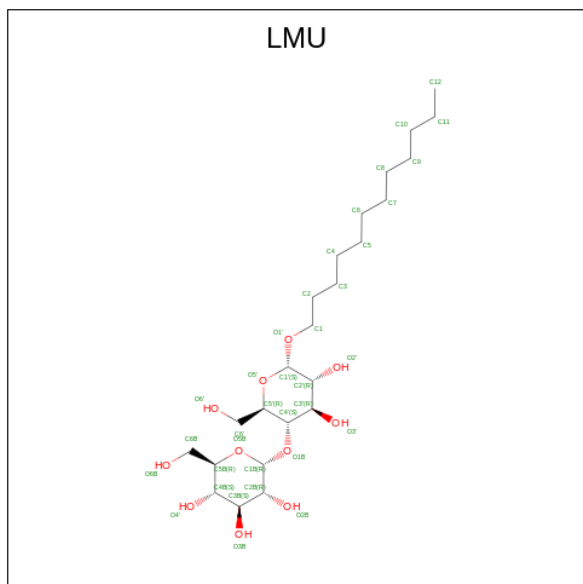
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 44 40 4	0	0
2	A	1	Total C O 44 40 4	0	0
2	B	1	Total C O 44 40 4	0	0
2	C	1	Total C O 44 40 4	0	0
2	C	1	Total C O 44 40 4	0	0
2	D	1	Total C O 44 40 4	0	0
2	D	1	Total C O 44 40 4	0	0
2	E	1	Total C O 44 40 4	0	0
2	E	1	Total C O 44 40 4	0	0
2	F	1	Total C O 44 40 4	0	0
2	F	1	Total C O 44 40 4	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: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



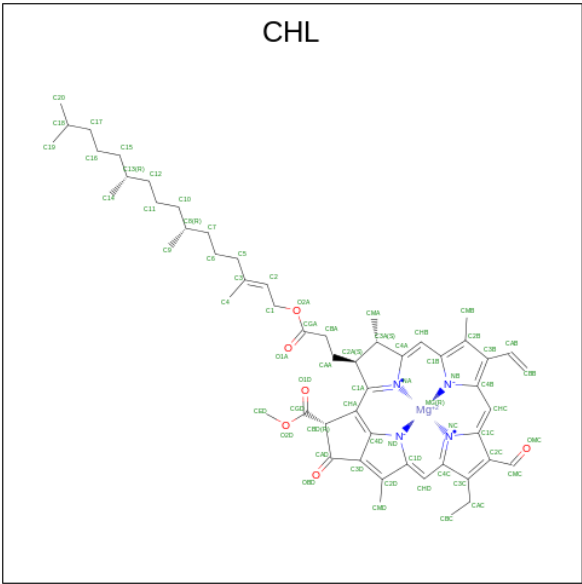
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		
3	D	1	Total	C	O	0	0
			44	40	4		
3	E	1	Total	C	O	0	0
			44	40	4		
3	F	1	Total	C	O	0	0
			44	40	4		

- Molecule 4 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			33	23	10		
4	B	1	Total	C	O	0	0
			35	24	11		
4	D	1	Total	C	O	0	0
			35	24	11		
4	E	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			64	53	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

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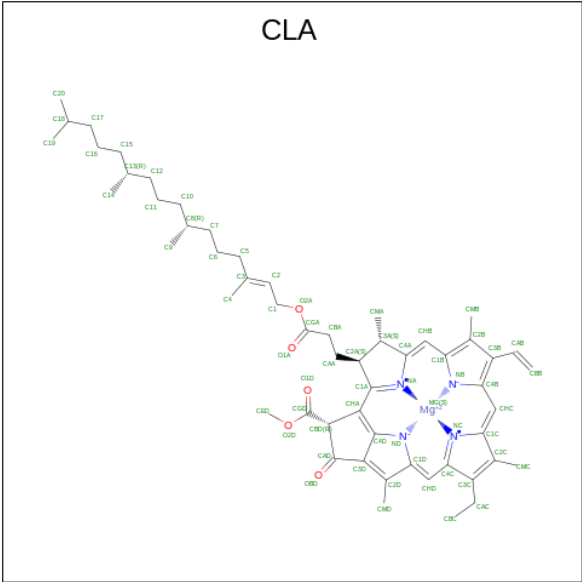
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Mg	N	O	0	0
			62	51	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			57	46	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	C	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
5	C	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			44	35	1	4	4		
5	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			65	54	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	D	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
5	D	1	Total	C	Mg	N	O	0	0
			62	51	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			57	46	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	D	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	Mg	N	O	0	0
			64	53	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			41	32	1	4	4		
5	E	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
5	E	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	E	1	Total	C	Mg	N	O	0	0
			41	32	1	4	4		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	F	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
5	F	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	F	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

- Molecule 6 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			63	53	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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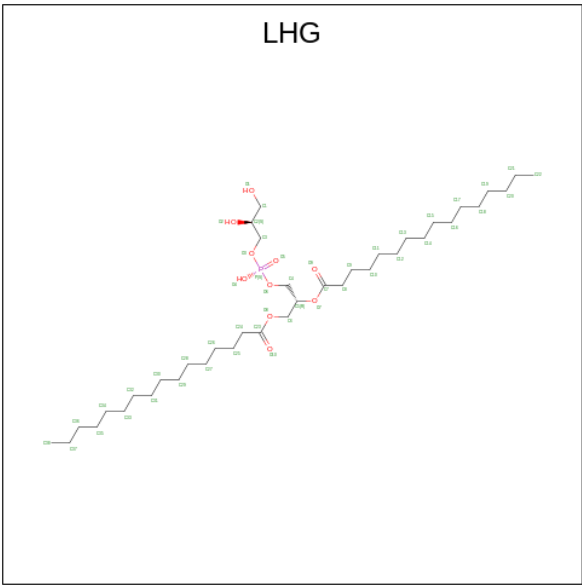
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			63	53	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
6	E	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
6	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).

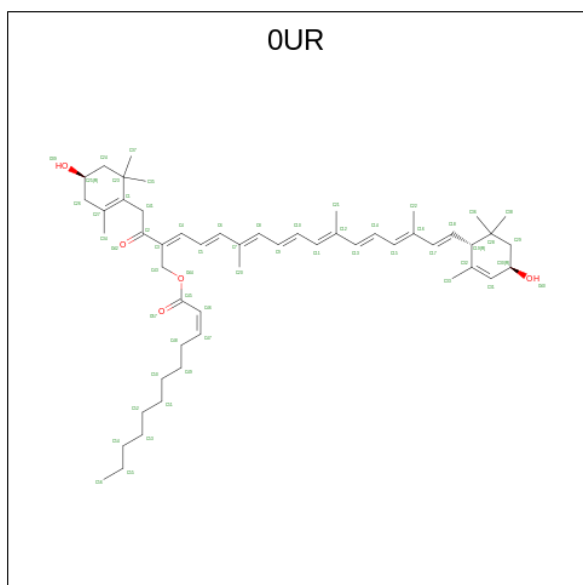


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			47	36	10	1		
7	B	1	Total	C	O	P	0	0
			46	35	10	1		
7	B	1	Total	C	O	P	0	0
			31	20	10	1		
7	C	1	Total	C	O	P	0	0
			25	14	10	1		
7	C	1	Total	C	O	P	0	0
			45	34	10	1		
7	D	1	Total	C	O	P	0	0
			46	35	10	1		
7	E	1	Total	C	O	P	0	0
			41	30	10	1		
7	F	1	Total	C	O	P	0	0
			45	34	10	1		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

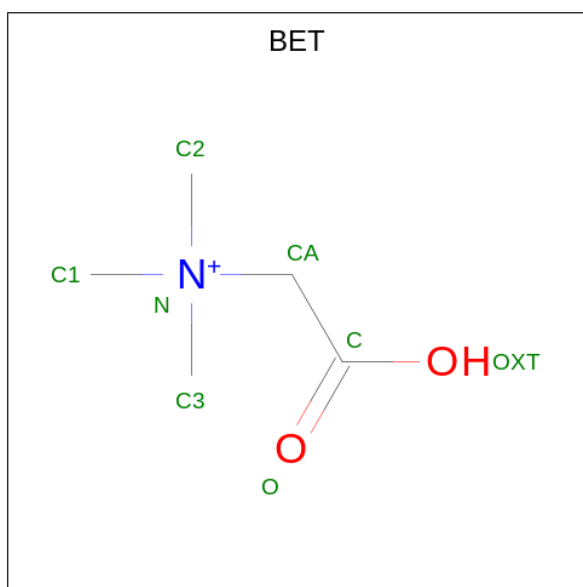
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Mg 2 2	0	0
8	D	1	Total Mg 1 1	0	0

- Molecule 9 is Siphonein (CCD ID: 0UR) (formula: C₅₂H₇₆O₅) (labeled as "Ligand of Interest" by depositor).



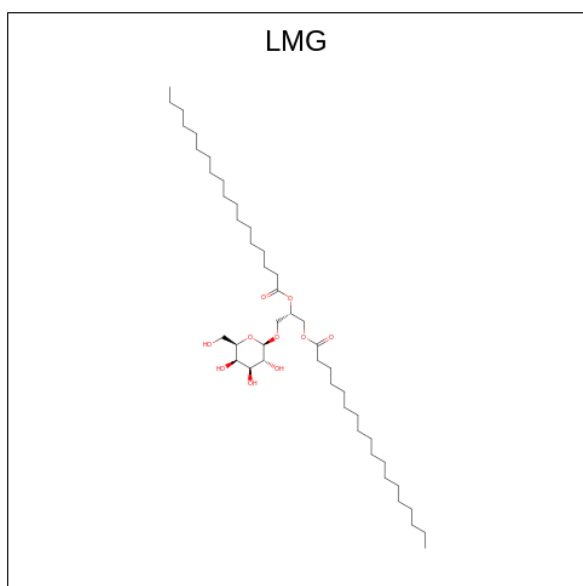
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 52 47 5	0	0
9	B	1	Total C O 50 45 5	0	0
9	B	1	Total C O 52 47 5	0	0
9	C	1	Total C O 52 47 5	0	0
9	D	1	Total C O 52 47 5	0	0
9	E	1	Total C O 52 47 5	0	0
9	F	1	Total C O 52 47 5	0	0

- Molecule 10 is TRIMETHYL GLYCINE (CCD ID: BET) (formula: C₅H₁₂NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			8	5	1	2		
10	B	1	Total	C	N	O	0	0
			8	5	1	2		
10	C	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			30	20	10		
11	F	1	Total	C	O	0	0
			30	20	10		

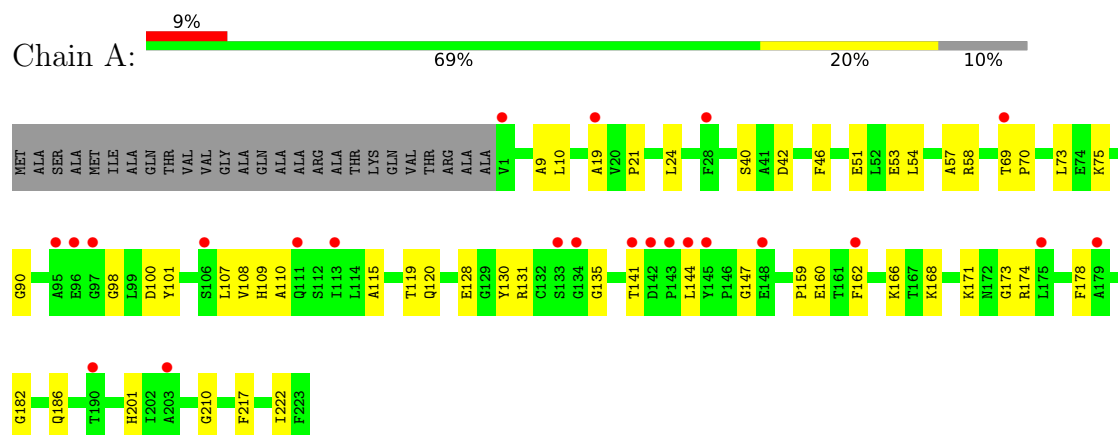
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	8	Total	O	0	0
			8	8		
12	B	7	Total	O	0	0
			7	7		
12	C	8	Total	O	0	0
			8	8		
12	D	4	Total	O	0	0
			4	4		
12	E	6	Total	O	0	0
			6	6		
12	F	8	Total	O	0	0
			8	8		

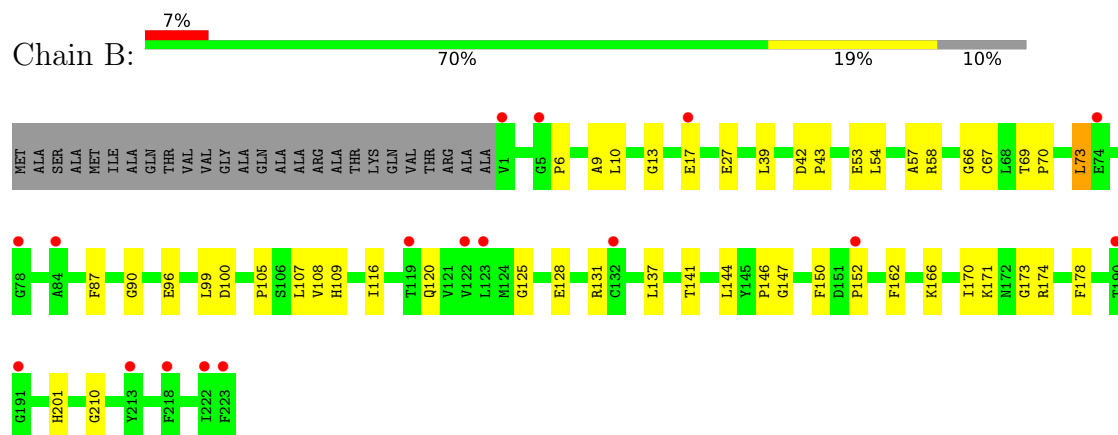
3 Residue-property plots [i](#)

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.

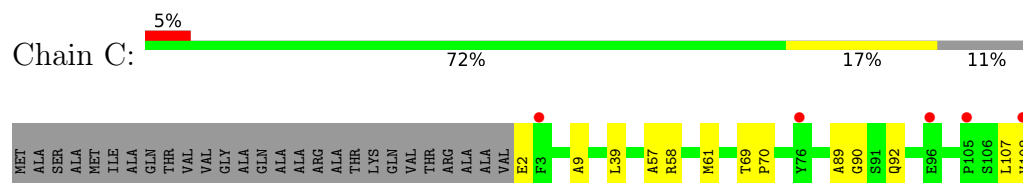
- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

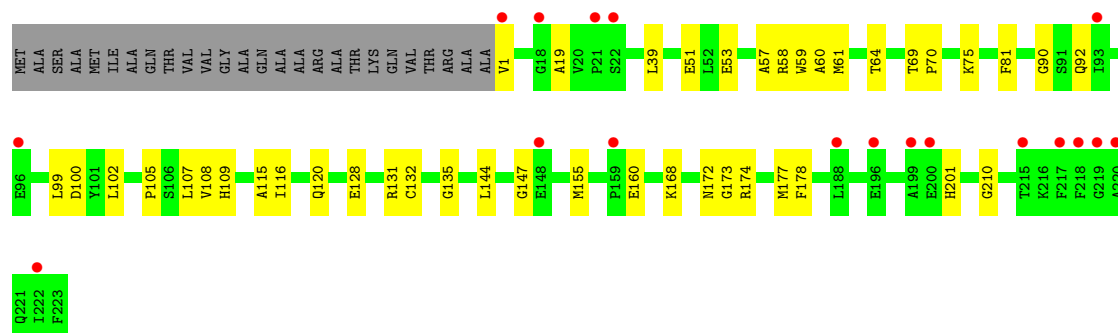
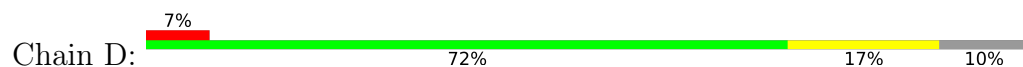


- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1

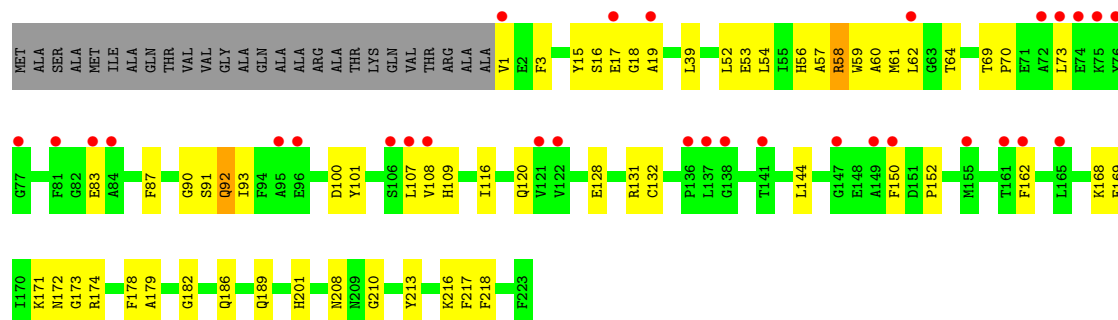




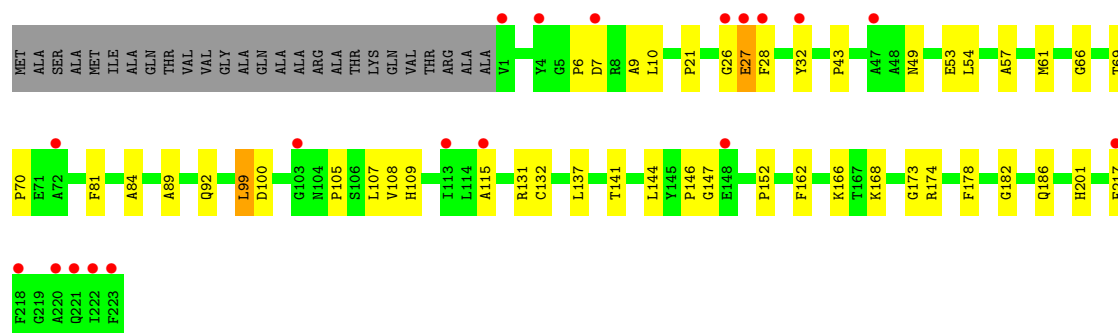
- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



- Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.72Å 91.61Å 169.22Å 90.00° 103.52° 90.00°	Depositor
Resolution (Å)	39.90 – 2.60 39.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	66.2 (39.90-2.60) 66.2 (39.90-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.18_3861: ???)	Depositor
R, R_{free}	0.207 , 0.249 0.216 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	75.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16480	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, NEX, LMG, LMU, OIE, LHG, OUR, CHL, CLA, BET

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	0.18	0/1725	0.38	0/2350
1	B	0.18	0/1722	0.37	0/2345
1	C	0.19	0/1712	0.35	0/2332
1	D	0.17	0/1735	0.37	0/2361
1	E	0.16	0/1737	0.36	0/2364
1	F	0.20	0/1738	0.40	0/2366
All	All	0.18	0/10369	0.37	0/14118

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1672	0	1547	42	0
1	B	1669	0	1552	44	0
1	C	1659	0	1523	43	0
1	D	1682	0	1572	36	0
1	E	1684	0	1581	52	0
1	F	1685	0	1579	41	0
2	A	88	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	0	1	0
2	C	88	0	0	2	0
2	D	88	0	0	0	0
2	E	88	0	0	1	0
2	F	88	0	0	0	0
3	A	44	0	56	3	0
3	B	44	0	54	4	0
3	C	44	0	55	4	0
3	D	44	0	55	4	0
3	E	44	0	55	3	0
3	F	44	0	53	1	0
4	A	35	0	46	4	0
4	B	68	0	85	3	0
4	D	35	0	46	3	0
4	E	35	0	46	3	0
5	A	449	0	397	25	0
5	B	457	0	407	35	0
5	C	445	0	403	35	0
5	D	449	0	402	34	0
5	E	438	0	384	29	0
5	F	445	0	397	29	0
6	A	333	0	305	22	0
6	B	344	0	337	22	0
6	C	330	0	306	25	0
6	D	344	0	337	22	0
6	E	333	0	305	19	0
6	F	325	0	293	23	0
7	A	47	0	67	3	0
7	B	77	0	97	13	0
7	C	70	0	83	4	0
7	D	46	0	65	4	0
7	E	41	0	52	7	0
7	F	45	0	63	8	0
8	A	2	0	0	0	0
8	D	1	0	0	0	0
9	A	52	0	0	0	0
9	B	102	0	0	5	0
9	C	52	0	0	4	0
9	D	52	0	0	0	0
9	E	52	0	0	4	0
9	F	52	0	0	3	0
10	B	16	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	8	0	11	0	0
11	B	30	0	30	0	0
11	F	30	0	30	1	0
12	A	8	0	0	0	0
12	B	7	0	0	1	0
12	C	8	0	0	1	0
12	D	4	0	0	1	0
12	E	6	0	0	0	0
12	F	8	0	0	2	0
All	All	16480	0	14698	441	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 14.

The worst 5 of 441 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)
1:E:83:GLU:H	1:E:92:GLN:HE21	1.12	0.94
6:F:313:CLA:H43	6:F:315:CLA:HBA1	1.50	0.89
3:D:303:NEX:H42	4:D:304:LMU:H6'2	1.56	0.88
5:D:311:CHL:H62	5:D:313:CHL:H193	1.61	0.81
1:B:150:PHE:HD1	5:B:313:CHL:H2	1.47	0.79

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	221/249 (89%)	213 (96%)	7 (3%)	1 (0%)	24	46
1	B	221/249 (89%)	213 (96%)	6 (3%)	2 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	220/249 (88%)	212 (96%)	7 (3%)	1 (0%)	24	46
1	D	221/249 (89%)	214 (97%)	6 (3%)	1 (0%)	24	46
1	E	221/249 (89%)	211 (96%)	7 (3%)	3 (1%)	9	19
1	F	221/249 (89%)	214 (97%)	5 (2%)	2 (1%)	14	30
All	All	1325/1494 (89%)	1277 (96%)	38 (3%)	10 (1%)	16	34

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	GLU
1	F	27	GLU
1	B	17	GLU
1	C	108	VAL
1	E	92	GLN

5.3.2 Protein sidechains ⓘ

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	160/184 (87%)	155 (97%)	5 (3%)	35	63
1	B	159/184 (86%)	154 (97%)	5 (3%)	35	63
1	C	156/184 (85%)	155 (99%)	1 (1%)	78	91
1	D	163/184 (89%)	161 (99%)	2 (1%)	63	83
1	E	162/184 (88%)	160 (99%)	2 (1%)	63	83
1	F	163/184 (89%)	159 (98%)	4 (2%)	42	69
All	All	963/1104 (87%)	944 (98%)	19 (2%)	48	74

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	73	LEU
1	F	99	LEU

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Mol	Chain	Res	Type
1	F	141	THR
1	F	10	LEU
1	B	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	B	186	GLN
1	E	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 3 are monoatomic - leaving 126 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	$\# Z > 2$
4	LMU	A	304	-	36,36,36	0.40	0	47,47,47	0.91	1 (2%)
5	CHL	A	318	1	46,50,74	3.29	22 (47%)	51,85,114	3.41	28 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHL	E	312	1	70,74,74	2.49	23 (32%)	80,114,114	3.08	33 (41%)
2	OIE	D	301	-	42,45,45	1.43	5 (11%)	49,63,63	1.86	10 (20%)
4	LMU	B	305	-	36,36,36	0.38	0	47,47,47	1.09	5 (10%)
6	CLA	A	307	1	69,73,73	1.27	8 (11%)	83,113,113	1.32	7 (8%)
6	CLA	C	307	1	69,73,73	1.26	7 (10%)	83,113,113	1.42	8 (9%)
9	OUR	F	320	-	50,53,58	1.09	3 (6%)	58,72,77	1.89	16 (27%)
6	CLA	A	314	1	59,63,73	1.43	11 (18%)	71,101,113	1.55	15 (21%)
6	CLA	C	317	-	60,64,73	1.41	9 (15%)	72,102,113	1.43	9 (12%)
5	CHL	B	312	12	66,70,74	2.84	21 (31%)	75,109,114	2.97	33 (44%)
5	CHL	C	318	1	48,52,74	3.16	22 (45%)	53,87,114	4.05	27 (50%)
6	CLA	A	315	7	67,71,73	1.29	7 (10%)	80,110,113	1.32	7 (8%)
6	CLA	C	315	7	69,73,73	1.26	6 (8%)	83,113,113	1.27	7 (8%)
5	CHL	C	306	1	70,74,74	2.34	21 (30%)	80,114,114	2.86	33 (41%)
4	LMU	D	304	-	36,36,36	0.50	0	47,47,47	1.19	4 (8%)
6	CLA	C	314	1	57,61,73	1.38	6 (10%)	68,98,113	1.41	10 (14%)
10	BET	B	322	-	7,7,7	1.02	0	10,10,10	0.87	1 (10%)
2	OIE	B	301	-	42,45,45	1.41	6 (14%)	49,63,63	1.70	9 (18%)
2	OIE	C	301	-	42,45,45	1.47	6 (14%)	49,63,63	1.71	9 (18%)
5	CHL	A	310	-	55,59,74	3.11	21 (38%)	62,96,114	3.39	30 (48%)
5	CHL	C	312	12	60,64,74	2.97	22 (36%)	68,102,114	2.96	30 (44%)
5	CHL	B	310	1	47,51,74	3.12	21 (44%)	52,86,114	3.67	26 (50%)
5	CHL	F	304	1	70,74,74	2.53	22 (31%)	80,114,114	3.45	35 (43%)
3	NEX	D	303	-	38,46,46	0.95	2 (5%)	50,70,70	5.96	20 (40%)
9	OUR	A	322	-	50,53,58	1.01	2 (4%)	58,72,77	2.10	21 (36%)
5	CHL	F	312	1	70,74,74	2.26	20 (28%)	80,114,114	2.53	32 (40%)
5	CHL	F	311	12	60,64,74	2.55	23 (38%)	68,102,114	3.80	32 (47%)
6	CLA	A	308	12	54,58,73	1.43	7 (12%)	65,95,113	1.42	7 (10%)
5	CHL	B	306	1	70,74,74	2.73	23 (32%)	80,114,114	3.66	32 (40%)
5	CHL	F	308	1	46,50,74	3.18	22 (47%)	51,85,114	4.04	30 (58%)
7	LHG	C	319	6	44,44,48	0.73	1 (2%)	47,50,54	1.30	7 (14%)
5	CHL	B	319	1	51,55,74	3.15	23 (45%)	57,91,114	4.16	28 (49%)
6	CLA	B	308	1	69,73,73	1.26	8 (11%)	83,113,113	1.39	7 (8%)
5	CHL	D	305	1	70,74,74	2.92	23 (32%)	80,114,114	2.90	30 (37%)
6	CLA	E	313	1	59,63,73	1.36	6 (10%)	71,101,113	1.31	9 (12%)
5	CHL	F	310	12	65,69,74	2.77	25 (38%)	74,108,114	3.27	29 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHL	B	313	12	61,65,74	2.69	23 (37%)	69,103,114	3.50	30 (43%)
5	CHL	A	313	1	70,74,74	2.44	22 (31%)	80,114,114	2.57	26 (32%)
5	CHL	B	314	1	70,74,74	2.26	22 (31%)	80,114,114	2.73	29 (36%)
6	CLA	D	308	12	50,54,73	1.48	8 (16%)	60,90,113	1.41	7 (11%)
5	CHL	D	311	-	66,70,74	2.78	20 (30%)	75,109,114	2.92	34 (45%)
6	CLA	D	315	7	69,73,73	1.26	8 (11%)	83,113,113	1.26	8 (9%)
7	LHG	B	320	6	45,45,48	0.67	1 (2%)	48,51,54	1.30	6 (12%)
7	LHG	F	318	6	44,44,48	0.67	1 (2%)	47,50,54	1.33	8 (17%)
6	CLA	D	314	1	62,66,73	1.39	10 (16%)	74,104,113	1.41	13 (17%)
6	CLA	C	308	12	50,54,73	1.47	8 (16%)	60,90,113	1.39	7 (11%)
10	BET	C	320	-	7,7,7	1.01	0	10,10,10	0.75	0
11	LMG	B	323	-	30,30,55	1.05	0	38,38,63	1.12	5 (13%)
6	CLA	B	309	12	50,54,73	1.50	9 (18%)	60,90,113	1.41	7 (11%)
9	OUR	B	325	-	50,53,58	1.01	2 (4%)	58,72,77	2.09	18 (31%)
6	CLA	E	315	1	49,53,73	1.48	8 (16%)	59,89,113	1.45	5 (8%)
6	CLA	D	317	1	69,73,73	1.27	8 (11%)	83,113,113	1.28	6 (7%)
5	CHL	D	309	1	46,50,74	3.20	22 (47%)	51,85,114	5.51	31 (60%)
6	CLA	F	306	1	69,73,73	1.27	8 (11%)	83,113,113	1.34	6 (7%)
6	CLA	E	306	1	69,73,73	1.28	7 (10%)	83,113,113	1.32	8 (9%)
6	CLA	F	315	1	49,53,73	1.49	8 (16%)	59,89,113	1.49	7 (11%)
11	LMG	F	319	-	30,30,55	0.93	0	38,38,63	1.21	3 (7%)
5	CHL	E	311	12	60,64,74	2.81	24 (40%)	68,102,114	3.00	31 (45%)
5	CHL	C	310	-	48,52,74	3.10	22 (45%)	53,87,114	3.36	24 (45%)
3	NEX	F	303	-	38,46,46	0.96	1 (2%)	50,70,70	6.25	22 (44%)
5	CHL	C	311	12	65,69,74	3.11	22 (33%)	74,108,114	3.03	31 (41%)
6	CLA	E	314	7	67,71,73	1.30	6 (8%)	80,110,113	1.28	6 (7%)
2	OIE	C	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.67	9 (18%)
6	CLA	D	316	1	49,53,73	1.50	9 (18%)	59,89,113	1.47	6 (10%)
10	BET	B	321	-	7,7,7	1.03	0	10,10,10	0.85	1 (10%)
5	CHL	E	304	1	70,74,74	2.41	23 (32%)	80,114,114	3.65	35 (43%)
5	CHL	E	309	-	47,51,74	3.18	20 (42%)	52,86,114	5.80	28 (53%)
7	LHG	C	304	-	24,24,48	0.87	0	27,30,54	1.22	2 (7%)
9	OUR	C	321	-	50,53,58	0.97	1 (2%)	58,72,77	1.98	16 (27%)
5	CHL	E	317	1	44,49,74	3.28	20 (45%)	49,83,114	5.17	26 (53%)
2	OIE	F	302	-	42,45,45	1.43	6 (14%)	49,63,63	1.71	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHL	F	305	1	70,74,74	2.13	19 (27%)	80,114,114	3.31	35 (43%)
7	LHG	D	319	6	45,45,48	0.69	1 (2%)	48,51,54	1.28	7 (14%)
2	OIE	E	301	-	42,45,45	1.46	5 (11%)	49,63,63	1.79	10 (20%)
2	OIE	F	301	-	42,45,45	1.44	6 (14%)	49,63,63	1.74	10 (20%)
5	CHL	D	312	12	61,65,74	2.69	24 (39%)	69,103,114	3.03	32 (46%)
4	LMU	E	319	-	36,36,36	0.38	0	47,47,47	0.91	1 (2%)
3	NEX	A	303	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)
6	CLA	C	316	1	49,53,73	1.49	8 (16%)	59,89,113	1.46	5 (8%)
5	CHL	C	313	1	70,74,74	2.46	22 (31%)	80,114,114	2.67	29 (36%)
4	LMU	B	304	-	34,34,36	0.39	0	42,44,47	1.07	3 (7%)
5	CHL	C	309	1	46,50,74	3.17	20 (43%)	51,85,114	3.59	28 (54%)
3	NEX	C	303	-	38,46,46	0.96	1 (2%)	50,70,70	6.57	19 (38%)
5	CHL	D	318	1	50,54,74	3.15	22 (44%)	56,90,114	3.29	27 (48%)
6	CLA	A	317	1	59,63,73	1.39	8 (13%)	70,100,113	1.36	9 (12%)
5	CHL	D	310	12	49,53,74	3.06	20 (40%)	53,88,114	3.42	24 (45%)
5	CHL	F	317	1	50,54,74	3.32	23 (46%)	56,90,114	3.76	30 (53%)
7	LHG	B	324	-	30,30,48	1.18	2 (6%)	33,36,54	1.40	4 (12%)
6	CLA	B	317	1	49,53,73	1.48	8 (16%)	59,89,113	1.45	7 (11%)
2	OIE	A	301	-	42,45,45	1.50	10 (23%)	49,63,63	2.07	13 (26%)
5	CHL	A	312	12	60,64,74	2.77	23 (38%)	68,102,114	3.16	32 (47%)
6	CLA	B	315	1	62,66,73	1.45	9 (14%)	74,104,113	1.61	12 (16%)
6	CLA	F	307	12	50,54,73	1.47	8 (16%)	60,90,113	1.43	4 (6%)
5	CHL	C	305	1	70,74,74	2.53	24 (34%)	80,114,114	2.88	30 (37%)
2	OIE	A	302	-	42,45,45	1.53	7 (16%)	49,63,63	2.04	10 (20%)
6	CLA	B	318	1	69,73,73	1.24	8 (11%)	83,113,113	1.29	7 (8%)
5	CHL	F	309	-	46,50,74	3.48	21 (45%)	51,85,114	3.64	31 (60%)
3	NEX	E	303	-	38,46,46	0.94	1 (2%)	50,70,70	6.17	19 (38%)
9	OUR	D	321	-	50,53,58	0.88	1 (2%)	58,72,77	1.92	14 (24%)
5	CHL	B	311	-	55,59,74	2.99	22 (40%)	62,96,114	5.09	33 (53%)
9	OUR	B	302	-	48,51,58	1.14	3 (6%)	56,70,77	2.80	19 (33%)
5	CHL	E	305	1	68,72,74	2.39	21 (30%)	77,111,114	2.55	31 (40%)
5	CHL	E	310	-	65,69,74	3.07	23 (35%)	73,107,114	2.95	32 (43%)
5	CHL	E	308	1	44,49,74	3.44	21 (47%)	49,83,114	3.36	23 (46%)
2	OIE	E	302	-	42,45,45	1.49	5 (11%)	49,63,63	1.76	9 (18%)
2	OIE	D	302	-	42,45,45	1.43	6 (14%)	49,63,63	1.68	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHL	A	305	1	70,74,74	2.72	23 (32%)	80,114,114	3.35	35 (43%)
5	CHL	A	306	1	68,72,74	2.34	20 (29%)	77,111,114	2.69	33 (42%)
6	CLA	F	313	1	62,66,73	1.42	10 (16%)	74,104,113	1.57	13 (17%)
6	CLA	E	316	1	59,63,73	1.34	8 (13%)	70,100,113	1.35	6 (8%)
3	NEX	B	303	-	38,46,46	0.94	2 (5%)	50,70,70	5.77	22 (44%)
6	CLA	F	314	7	59,63,73	1.39	7 (11%)	71,101,113	1.34	8 (11%)
7	LHG	A	319	6	46,46,48	0.64	1 (2%)	49,52,54	1.22	3 (6%)
5	CHL	D	313	1	70,74,74	2.60	20 (28%)	80,114,114	2.78	31 (38%)
5	CHL	A	311	12	65,69,74	2.86	23 (35%)	73,107,114	3.83	33 (45%)
5	CHL	B	307	1	69,73,74	2.22	20 (28%)	78,112,114	3.07	32 (41%)
6	CLA	E	307	-	54,58,73	1.42	8 (14%)	65,95,113	1.47	9 (13%)
6	CLA	A	316	1	49,53,73	1.51	8 (16%)	59,89,113	1.49	5 (8%)
6	CLA	D	307	1	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
7	LHG	E	318	6	40,40,48	0.67	1 (2%)	43,46,54	1.30	6 (13%)
5	CHL	A	309	1	47,51,74	3.17	22 (46%)	52,86,114	3.78	28 (53%)
5	CHL	D	306	1	69,73,74	2.29	20 (28%)	78,112,114	2.91	34 (43%)
6	CLA	B	316	7	69,73,73	1.28	7 (10%)	83,113,113	1.33	7 (8%)
6	CLA	F	316	-	60,64,73	1.35	9 (15%)	72,102,113	1.36	7 (9%)
9	OUR	E	320	-	50,53,58	0.99	1 (2%)	58,72,77	2.05	19 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMU	A	304	-	-	14/21/61/61	0/2/2/2
5	CHL	A	318	1	-	6/12/88/117	-
5	CHL	E	312	1	-	9/41/117/117	-
2	OIE	D	301	-	-	14/33/72/72	0/2/2/2
4	LMU	B	305	-	-	14/21/61/61	0/2/2/2
6	CLA	A	307	1	-	15/39/115/115	-
6	CLA	C	307	1	-	9/39/115/115	-
9	OUR	F	320	-	-	7/42/81/86	0/2/2/2
6	CLA	A	314	1	-	6/27/103/115	-
6	CLA	C	317	-	-	7/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	B	312	12	-	11/37/113/117	-
5	CHL	C	318	1	-	4/15/91/117	-
6	CLA	A	315	7	-	11/37/113/115	-
6	CLA	C	315	7	-	15/39/115/115	-
5	CHL	C	306	1	-	18/41/117/117	-
4	LMU	D	304	-	-	14/21/61/61	0/2/2/2
6	CLA	C	314	1	-	5/25/101/115	-
10	BET	B	322	-	-	5/5/5/5	-
2	0IE	B	301	-	-	11/33/72/72	0/2/2/2
2	0IE	C	301	-	-	9/33/72/72	0/2/2/2
5	CHL	A	310	-	-	6/23/99/117	-
5	CHL	C	312	12	-	13/29/105/117	-
5	CHL	B	310	1	-	6/14/90/117	-
5	CHL	F	304	1	-	16/41/117/117	-
3	NEX	D	303	-	-	6/27/83/83	0/3/3/3
9	0UR	A	322	-	-	8/42/81/86	0/2/2/2
5	CHL	F	312	1	-	16/41/117/117	-
5	CHL	F	311	12	-	14/29/105/117	-
6	CLA	A	308	12	-	6/21/97/115	-
5	CHL	B	306	1	-	16/41/117/117	-
5	CHL	F	308	1	-	6/12/88/117	-
7	LHG	C	319	6	-	18/49/49/53	-
5	CHL	B	319	1	-	7/19/95/117	-
6	CLA	B	308	1	-	16/39/115/115	-
5	CHL	D	305	1	-	20/41/117/117	-
6	CLA	E	313	1	-	4/27/103/115	-
5	CHL	F	310	12	-	19/35/111/117	-
5	CHL	B	313	12	-	9/31/107/117	-
5	CHL	A	313	1	-	14/41/117/117	-
5	CHL	B	314	1	-	19/41/117/117	-
6	CLA	D	308	12	-	6/17/93/115	-
5	CHL	D	311	-	-	17/37/113/117	-
6	CLA	D	315	7	-	9/39/115/115	-
7	LHG	B	320	6	-	24/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LHG	F	318	6	-	23/49/49/53	-
6	CLA	D	314	1	-	9/31/107/115	-
6	CLA	C	308	12	-	7/17/93/115	-
10	BET	C	320	-	-	5/5/5/5	-
11	LMG	B	323	-	-	9/25/45/70	0/1/1/1
6	CLA	B	309	12	-	4/17/93/115	-
9	OUR	B	325	-	-	7/42/81/86	0/2/2/2
6	CLA	E	315	1	-	8/15/91/115	-
6	CLA	D	317	1	-	10/39/115/115	-
5	CHL	D	309	1	-	4/12/88/117	-
6	CLA	F	306	1	-	17/39/115/115	-
6	CLA	E	306	1	-	12/39/115/115	-
6	CLA	F	315	1	-	4/15/91/115	-
11	LMG	F	319	-	-	11/25/45/70	0/1/1/1
5	CHL	E	311	12	-	10/29/105/117	-
5	CHL	C	310	-	-	9/15/91/117	-
3	NEX	F	303	-	-	3/27/83/83	0/3/3/3
5	CHL	C	311	12	-	17/35/111/117	-
6	CLA	E	314	7	-	11/37/113/115	-
2	OIE	C	302	-	-	14/33/72/72	0/2/2/2
6	CLA	D	316	1	-	2/15/91/115	-
10	BET	B	321	-	-	5/5/5/5	-
5	CHL	E	304	1	-	17/41/117/117	-
5	CHL	E	309	-	-	6/14/90/117	-
7	LHG	C	304	-	-	16/29/29/53	-
9	OUR	C	321	-	-	7/42/81/86	0/2/2/2
5	CHL	E	317	1	-	3/12/84/117	-
2	OIE	F	302	-	-	12/33/72/72	0/2/2/2
5	CHL	F	305	1	-	20/41/117/117	-
7	LHG	D	319	6	-	16/50/50/53	-
2	OIE	E	301	-	-	7/33/72/72	0/2/2/2
2	OIE	F	301	-	-	12/33/72/72	0/2/2/2
5	CHL	D	312	12	-	7/31/107/117	-
4	LMU	E	319	-	-	15/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NEX	A	303	-	-	5/27/83/83	0/3/3/3
6	CLA	C	316	1	-	4/15/91/115	-
5	CHL	C	313	1	-	13/41/117/117	-
4	LMU	B	304	-	-	9/20/56/61	1/2/2/2
5	CHL	C	309	1	-	6/12/88/117	-
3	NEX	C	303	-	-	2/27/83/83	0/3/3/3
5	CHL	D	318	1	-	4/17/93/117	-
6	CLA	A	317	1	-	10/27/103/115	-
5	CHL	D	310	12	-	4/15/92/117	-
5	CHL	F	317	1	-	7/17/93/117	-
7	LHG	B	324	-	-	24/35/35/53	-
6	CLA	B	317	1	-	3/15/91/115	-
2	OIE	A	301	-	-	10/33/72/72	0/2/2/2
5	CHL	A	312	12	-	9/29/105/117	-
6	CLA	B	315	1	-	6/31/107/115	-
6	CLA	F	307	12	-	4/17/93/115	-
5	CHL	C	305	1	-	24/41/117/117	-
2	OIE	A	302	-	-	11/33/72/72	0/2/2/2
6	CLA	B	318	1	-	18/39/115/115	-
5	CHL	F	309	-	-	5/12/88/117	-
3	NEX	E	303	-	-	4/27/83/83	0/3/3/3
9	OUR	D	321	-	-	7/42/81/86	0/2/2/2
5	CHL	B	311	-	-	7/23/99/117	-
9	OUR	B	302	-	-	16/40/79/86	0/2/2/2
5	CHL	E	305	1	-	12/39/115/117	-
5	CHL	E	310	-	-	16/35/111/117	-
5	CHL	E	308	1	-	4/12/84/117	-
2	OIE	E	302	-	-	12/33/72/72	0/2/2/2
2	OIE	D	302	-	-	16/33/72/72	0/2/2/2
5	CHL	A	305	1	-	23/41/117/117	-
5	CHL	A	306	1	-	17/39/115/117	-
6	CLA	F	313	1	-	12/31/107/115	-
6	CLA	E	316	1	-	9/27/103/115	-
3	NEX	B	303	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	F	314	7	-	4/27/103/115	-
7	LHG	A	319	6	-	18/51/51/53	-
5	CHL	D	313	1	-	18/41/117/117	-
5	CHL	A	311	12	-	16/35/111/117	-
5	CHL	B	307	1	-	15/40/116/117	-
6	CLA	E	307	-	-	2/21/97/115	-
6	CLA	A	316	1	-	6/15/91/115	-
6	CLA	D	307	1	-	12/39/115/115	-
7	LHG	E	318	6	-	15/45/45/53	-
5	CHL	A	309	1	-	7/14/90/117	-
5	CHL	D	306	1	-	20/40/116/117	-
6	CLA	B	316	7	-	8/39/115/115	-
6	CLA	F	316	-	-	7/29/105/115	-
9	OUR	E	320	-	-	6/42/81/86	0/2/2/2

The worst 5 of 1431 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	310	CHL	MG-ND	-13.99	1.78	2.05
5	C	311	CHL	MG-ND	-13.00	1.80	2.05
5	E	308	CHL	MG-NA	12.97	2.37	2.06
5	C	311	CHL	MG-NA	12.90	2.36	2.06
5	D	313	CHL	MG-NA	12.84	2.36	2.06

The worst 5 of 2153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	311	CHL	O2A-C1-C2	26.61	178.56	108.64
3	F	303	NEX	C15-C35-C34	26.60	177.96	123.47
3	E	303	NEX	C35-C15-C14	25.85	176.43	123.47
3	C	303	NEX	C15-C35-C34	24.82	174.32	123.47
5	E	309	CHL	CMD-C2D-C1D	24.02	167.04	124.71

There are no chirality outliers.

5 of 1327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	OIE	C5-C6-C7-C21

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Mol	Chain	Res	Type	Atoms
2	A	302	0IE	C5-C6-C7-C8
2	A	302	0IE	C3-C4-C5-C6
2	A	302	0IE	C15-C16-C17-C18
2	A	302	0IE	C23-C16-C17-C18

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	304	LMU	C1'-C2'-C3'-C4'-C5'-O5'

110 monomers are involved in 346 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	LMU	4	0
5	A	318	CHL	1	0
5	E	312	CHL	8	0
4	B	305	LMU	1	0
6	A	307	CLA	6	0
6	C	307	CLA	7	0
9	F	320	0UR	3	0
6	A	314	CLA	4	0
6	C	317	CLA	8	0
5	B	312	CHL	9	0
5	C	318	CHL	4	0
6	A	315	CLA	3	0
6	C	315	CLA	3	0
5	C	306	CHL	2	0
4	D	304	LMU	3	0
6	C	314	CLA	2	0
10	B	322	BET	2	0
2	B	301	0IE	1	0
5	A	310	CHL	2	0
5	C	312	CHL	3	0
5	B	310	CHL	1	0
5	F	304	CHL	8	0
3	D	303	NEX	4	0
5	F	312	CHL	3	0
5	F	311	CHL	2	0
6	A	308	CLA	3	0
5	B	306	CHL	3	0
5	F	308	CHL	1	0
7	C	319	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	319	CHL	2	0
6	B	308	CLA	5	0
5	D	305	CHL	2	0
6	E	313	CLA	3	0
5	F	310	CHL	5	0
5	B	313	CHL	6	0
5	A	313	CHL	5	0
5	B	314	CHL	9	0
6	D	308	CLA	2	0
5	D	311	CHL	9	0
6	D	315	CLA	4	0
7	B	320	LHG	5	0
7	F	318	LHG	8	0
6	D	314	CLA	4	0
6	C	308	CLA	3	0
6	B	309	CLA	1	0
9	B	325	OUR	5	0
6	E	315	CLA	3	0
6	D	317	CLA	8	0
5	D	309	CHL	2	0
6	F	306	CLA	5	0
6	E	306	CLA	2	0
6	F	315	CLA	5	0
11	F	319	LMG	1	0
5	E	311	CHL	5	0
5	C	310	CHL	5	0
3	F	303	NEX	1	0
5	C	311	CHL	2	0
6	E	314	CLA	3	0
2	C	302	OIE	2	0
6	D	316	CLA	4	0
5	E	304	CHL	4	0
5	E	309	CHL	3	0
9	C	321	OUR	4	0
5	E	317	CHL	2	0
5	F	305	CHL	8	0
7	D	319	LHG	4	0
5	D	312	CHL	2	0
4	E	319	LMU	3	0
3	A	303	NEX	3	0
6	C	316	CLA	4	0
5	C	313	CHL	10	0

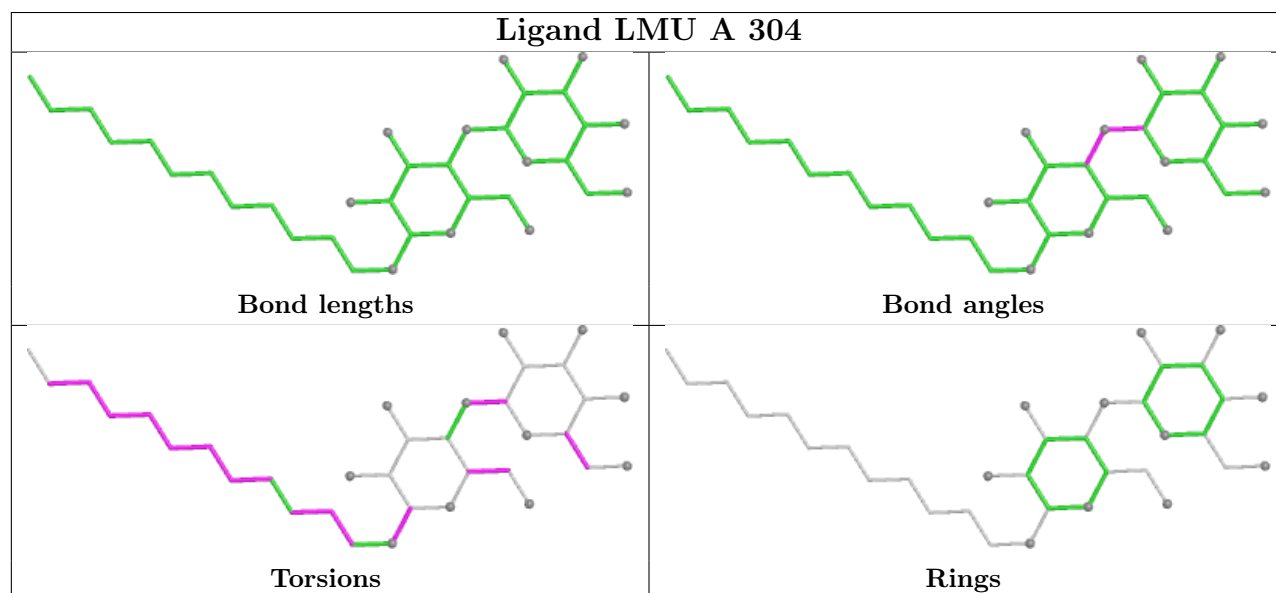
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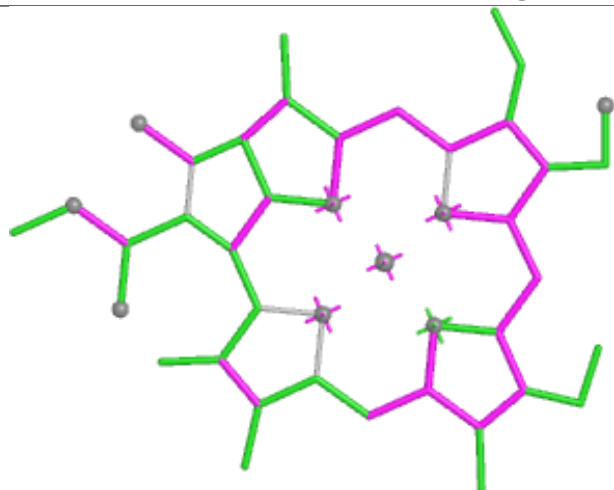
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	304	LMU	2	0
5	C	309	CHL	5	0
3	C	303	NEX	4	0
6	A	317	CLA	5	0
5	D	310	CHL	7	0
5	F	317	CHL	2	0
7	B	324	LHG	8	0
6	B	317	CLA	2	0
5	A	312	CHL	2	0
6	B	315	CLA	7	0
6	F	307	CLA	2	0
5	C	305	CHL	5	0
2	A	302	OIE	1	0
6	B	318	CLA	5	0
5	F	309	CHL	1	0
3	E	303	NEX	3	0
5	B	311	CHL	4	0
5	E	305	CHL	3	0
5	E	310	CHL	3	0
5	E	308	CHL	3	0
2	E	302	OIE	1	0
5	A	305	CHL	6	0
5	A	306	CHL	6	0
6	F	313	CLA	6	0
6	E	316	CLA	6	0
3	B	303	NEX	4	0
6	F	314	CLA	3	0
7	A	319	LHG	3	0
5	D	313	CHL	12	0
5	A	311	CHL	5	0
5	B	307	CHL	5	0
6	E	307	CLA	3	0
6	A	316	CLA	3	0
6	D	307	CLA	2	0
7	E	318	LHG	7	0
5	D	306	CHL	5	0
6	B	316	CLA	3	0
6	F	316	CLA	5	0
9	E	320	OUR	4	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

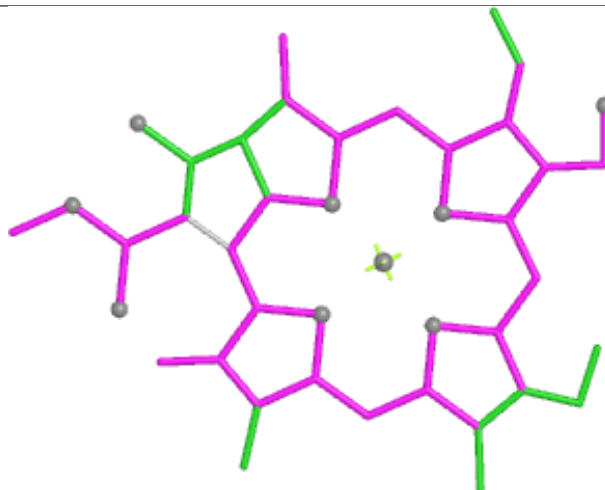
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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



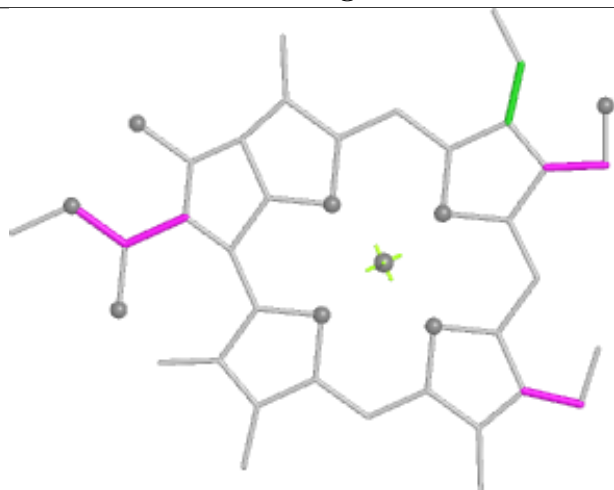
Ligand CHL A 318



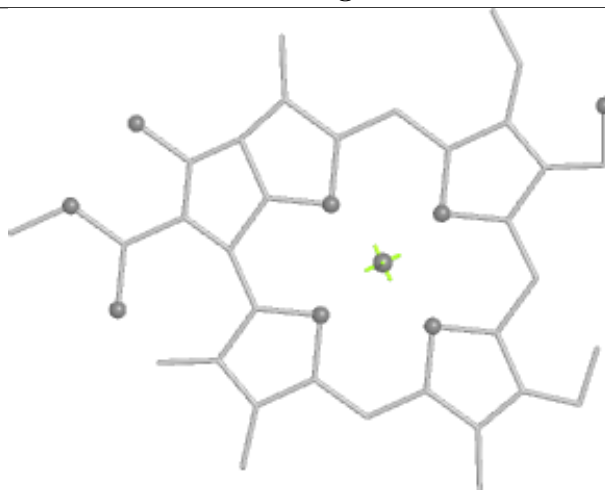
Bond lengths



Bond angles

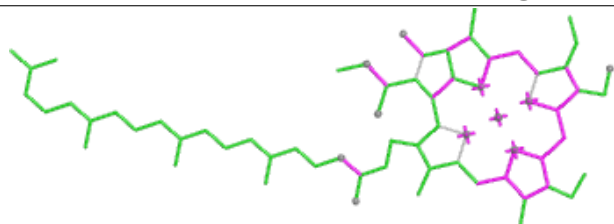


Torsions

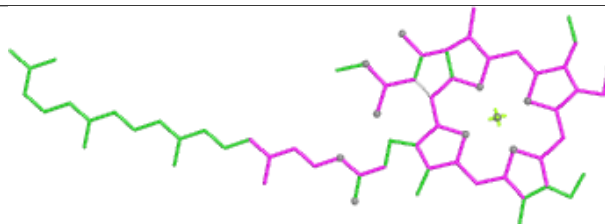


Rings

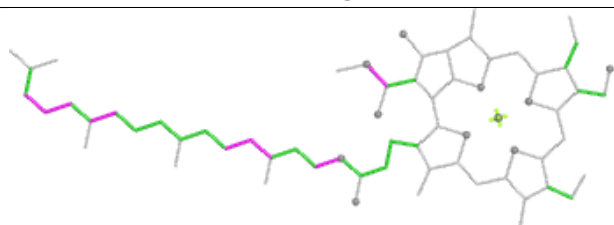
Ligand CHL E 312



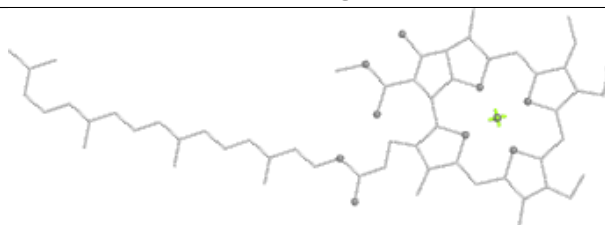
Bond lengths



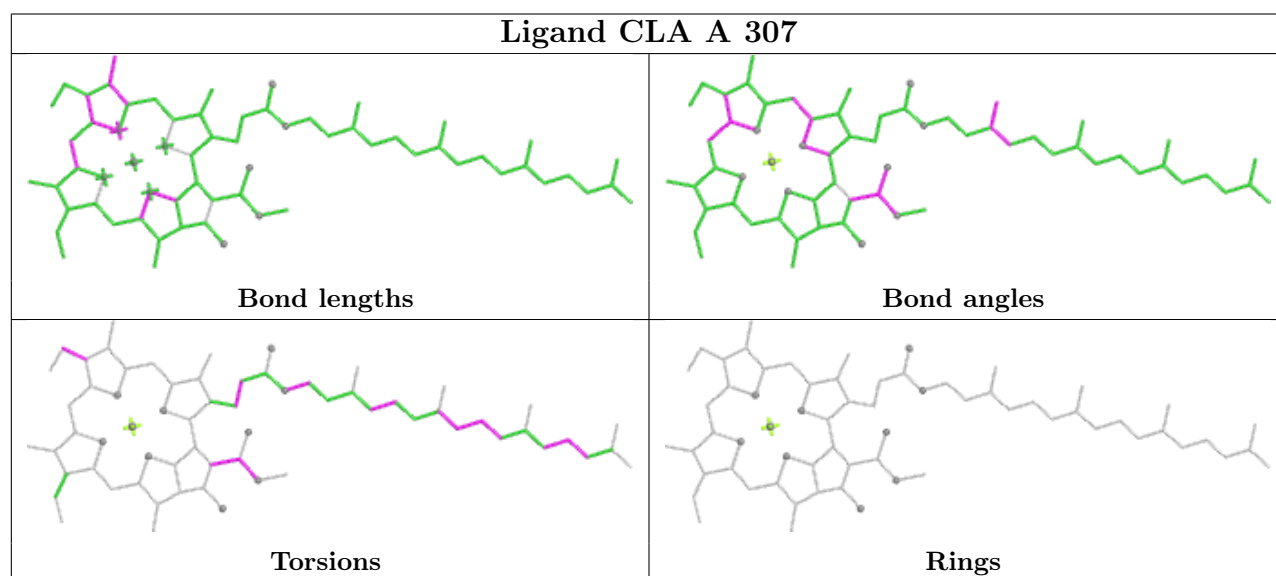
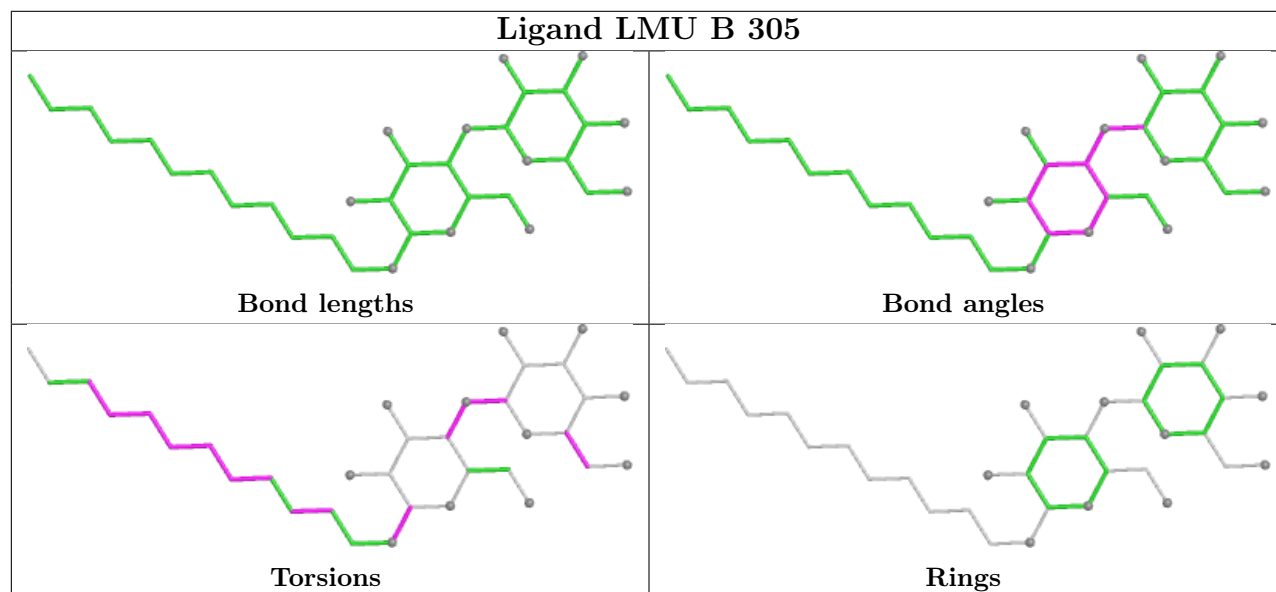
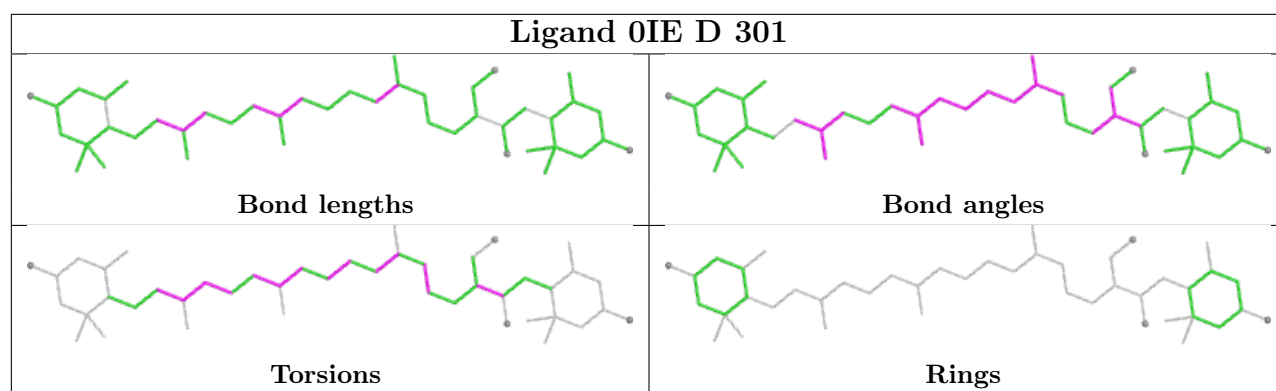
Bond angles

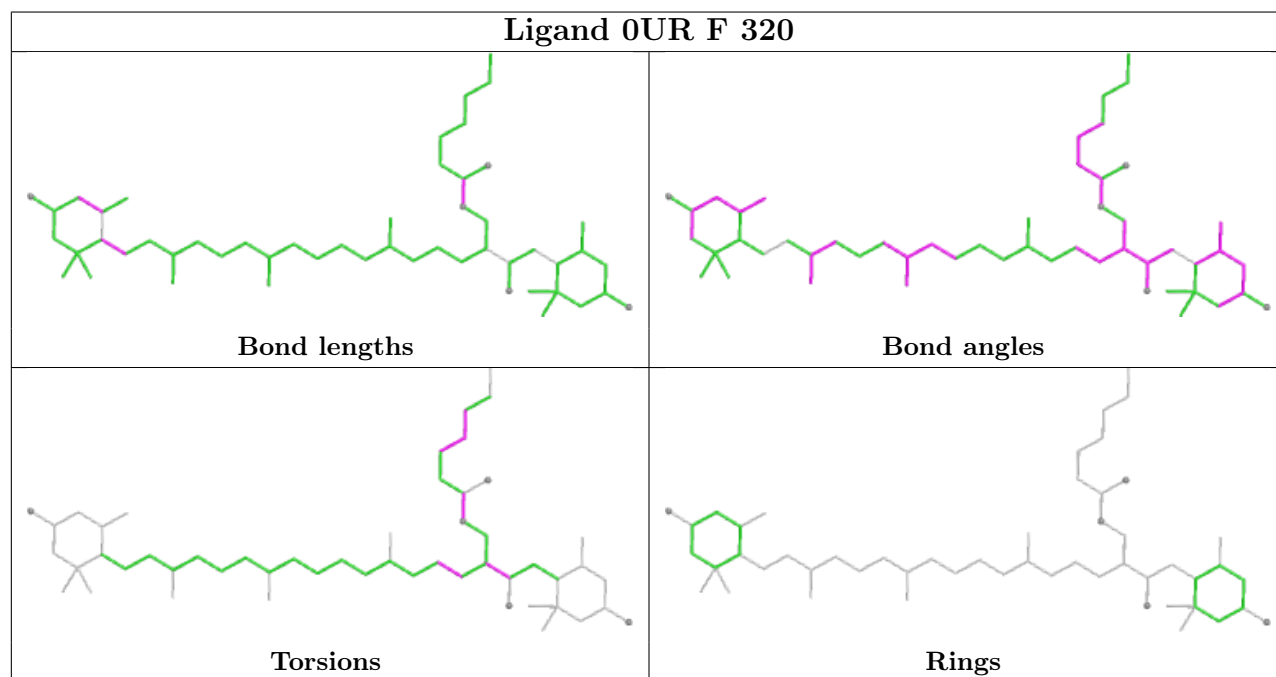
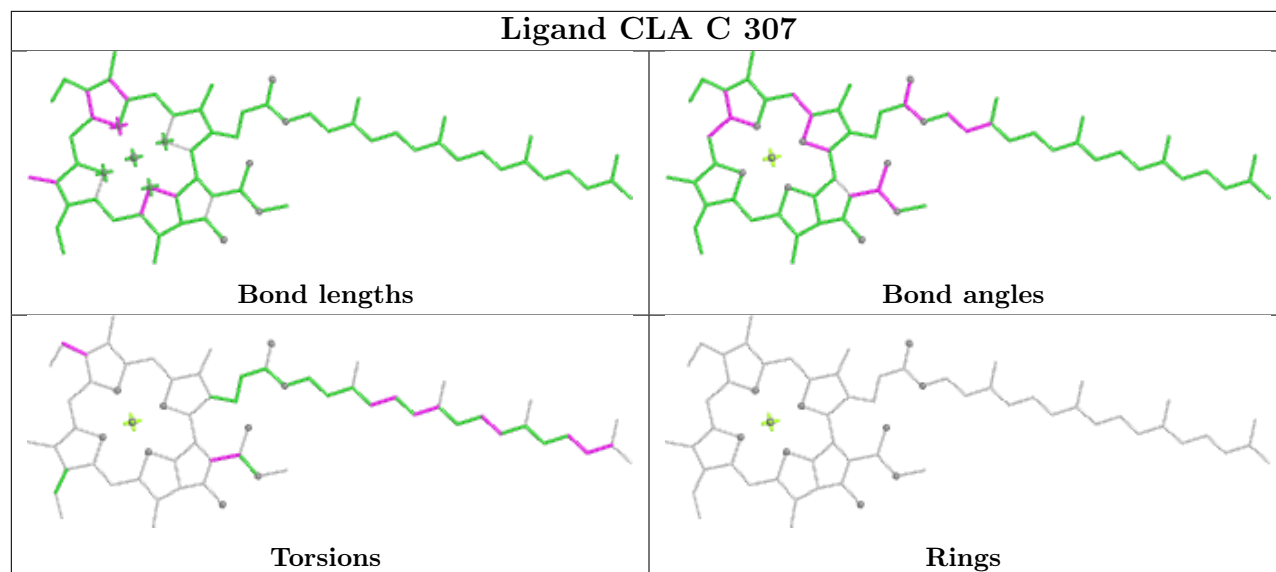


Torsions

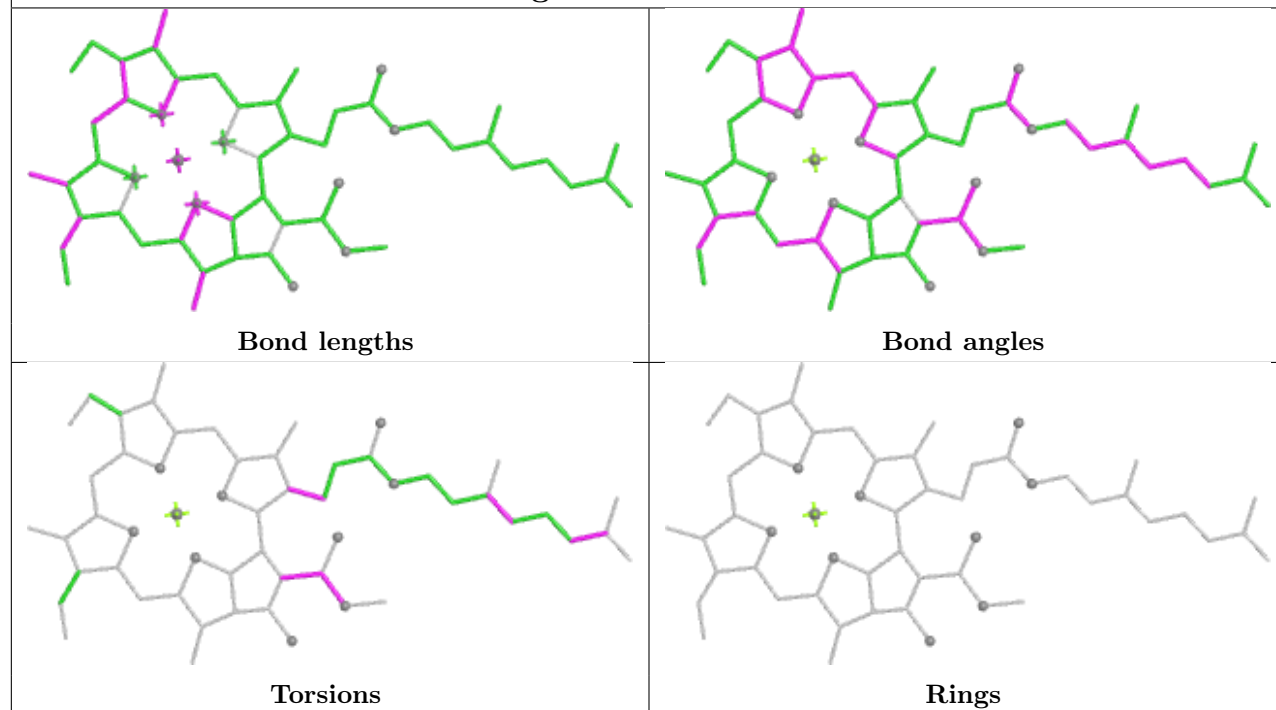


Rings

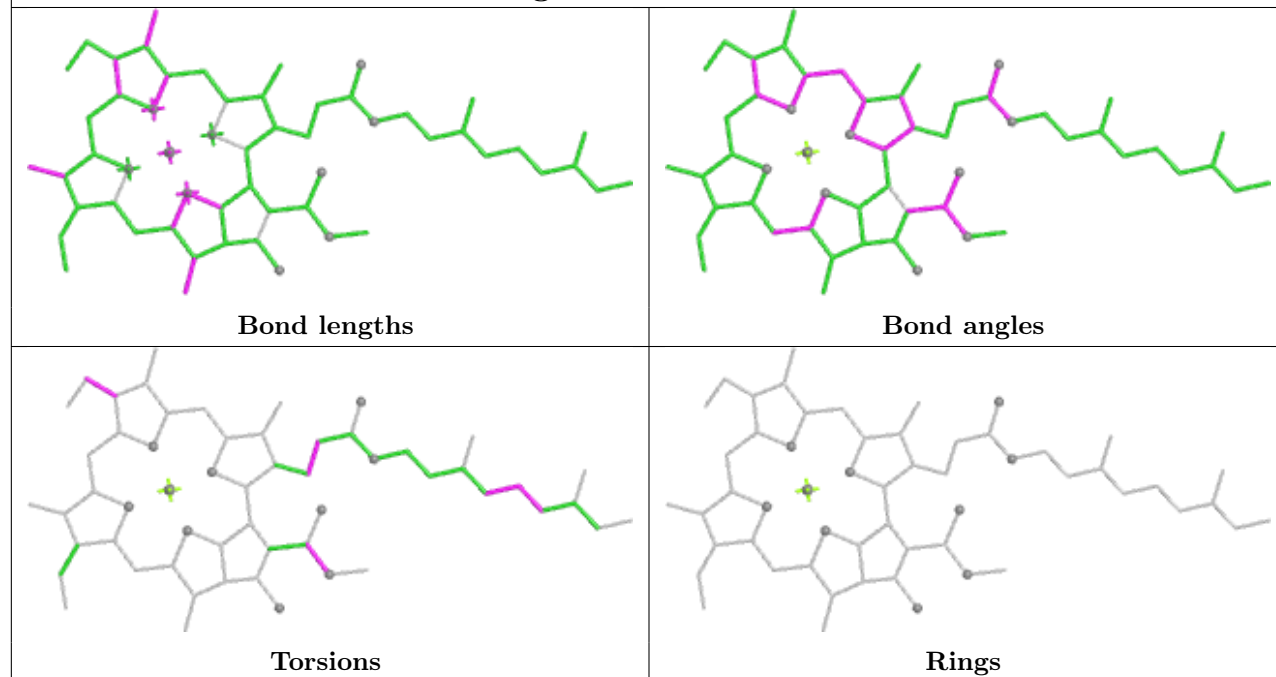


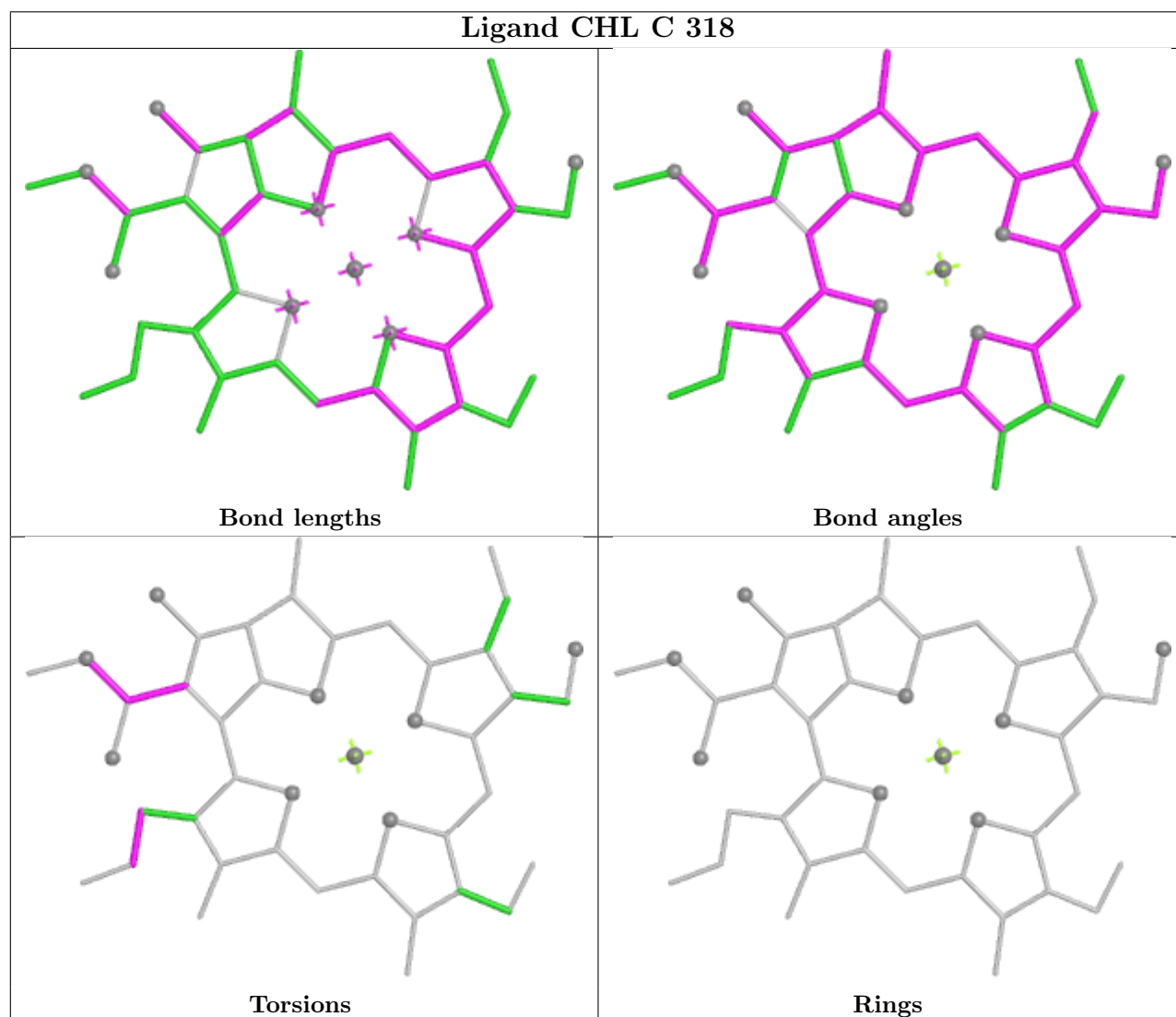
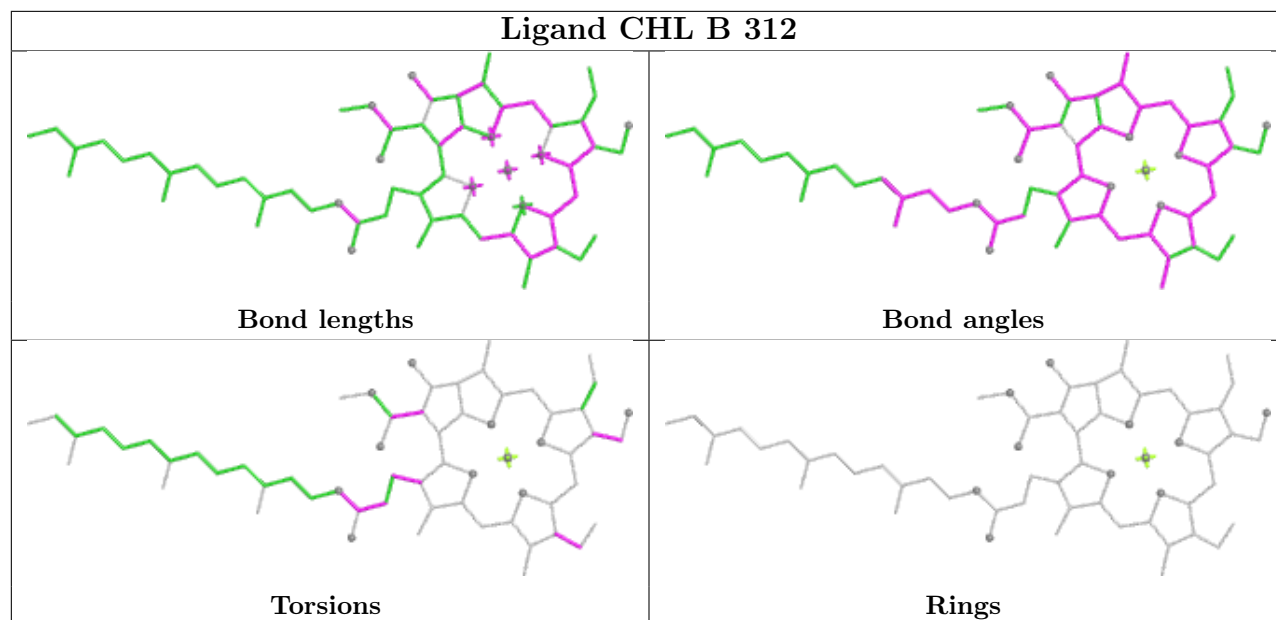


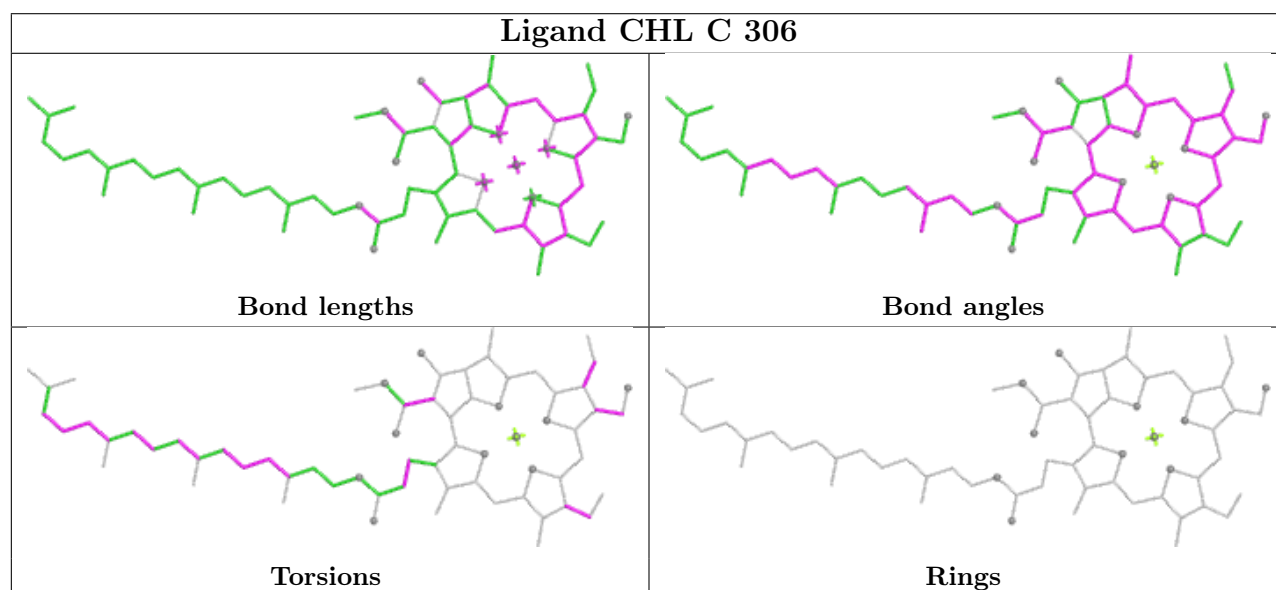
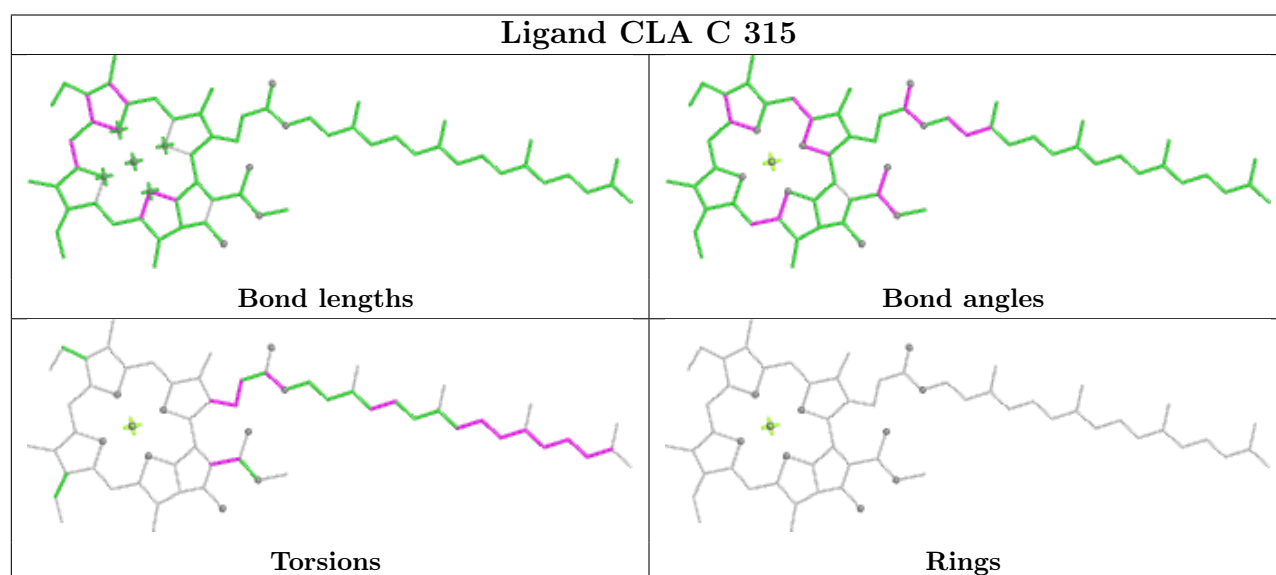
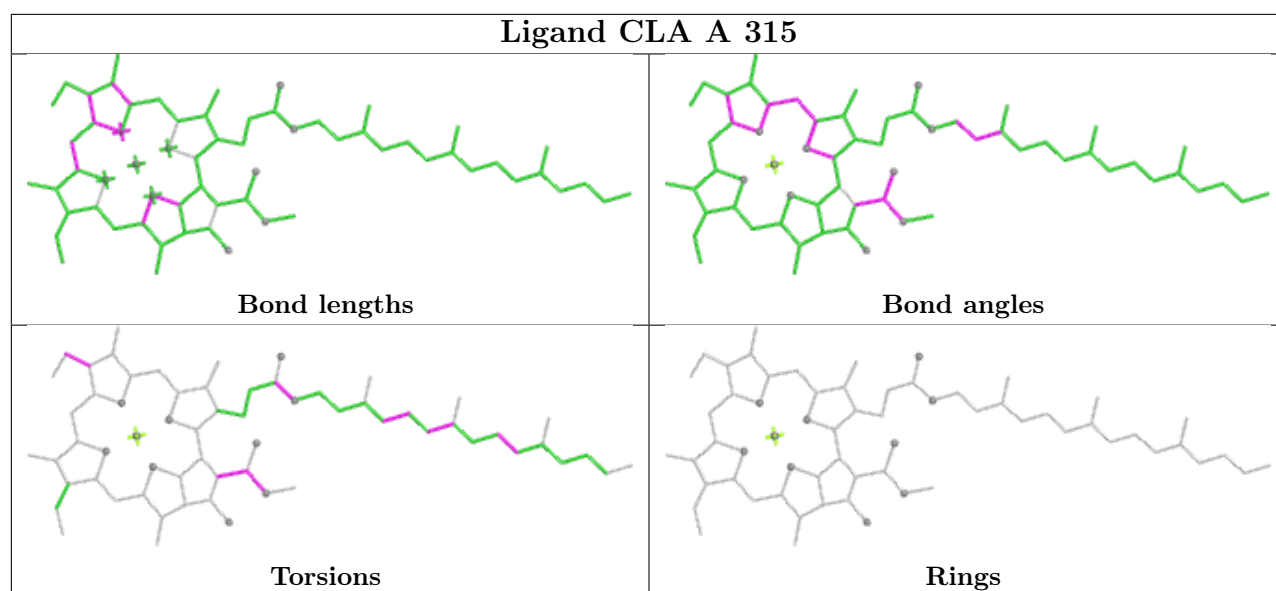
Ligand CLA A 314

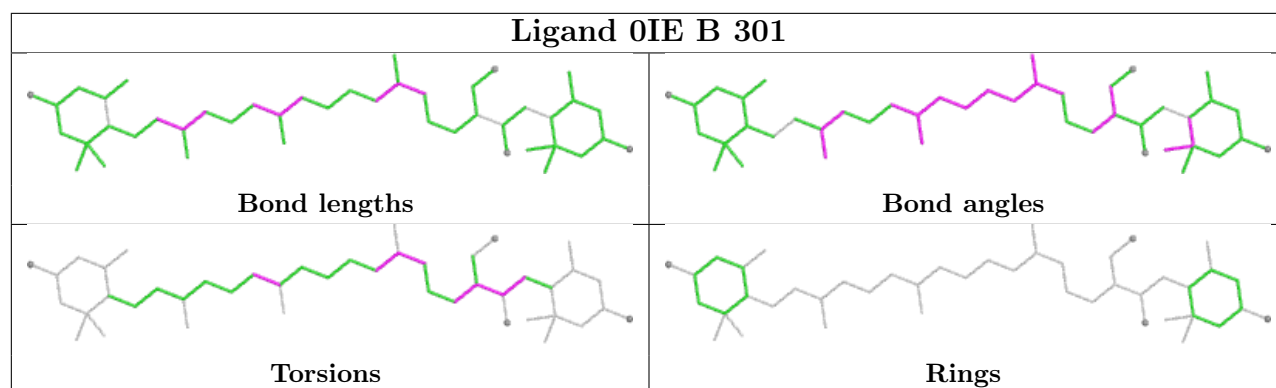
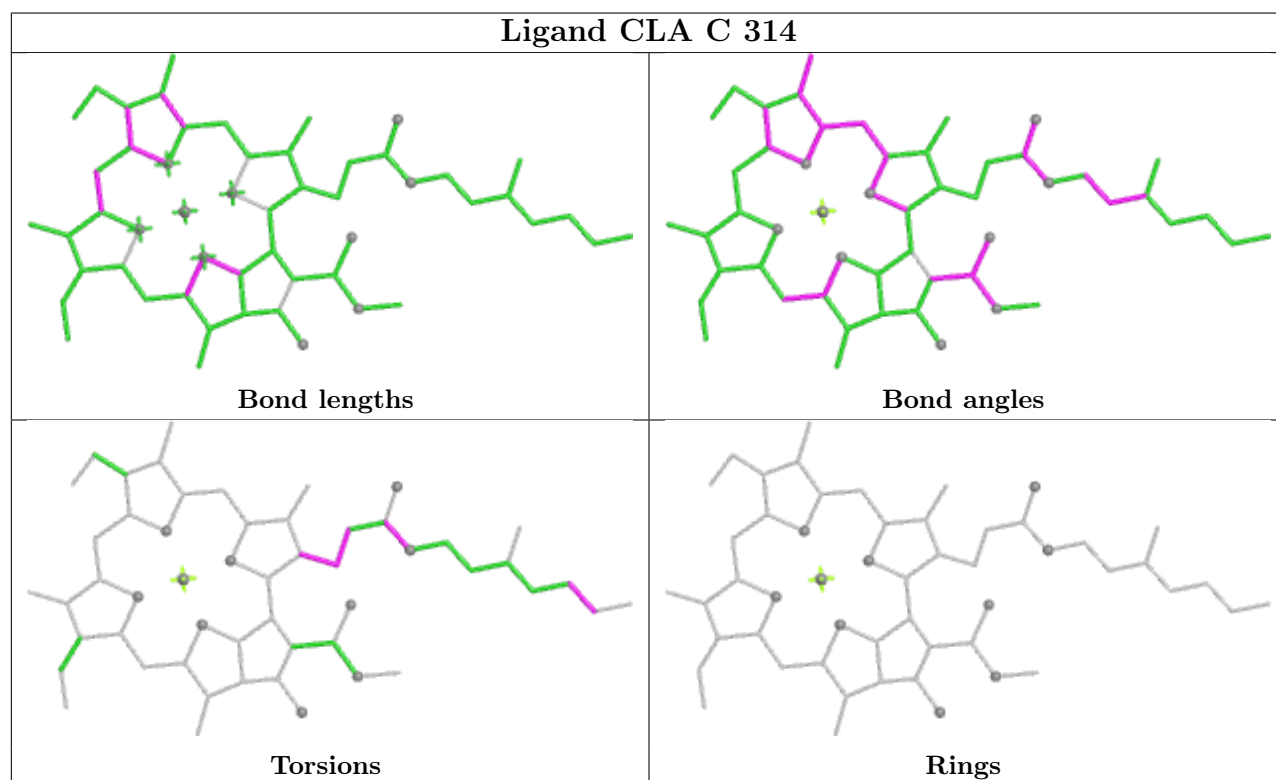
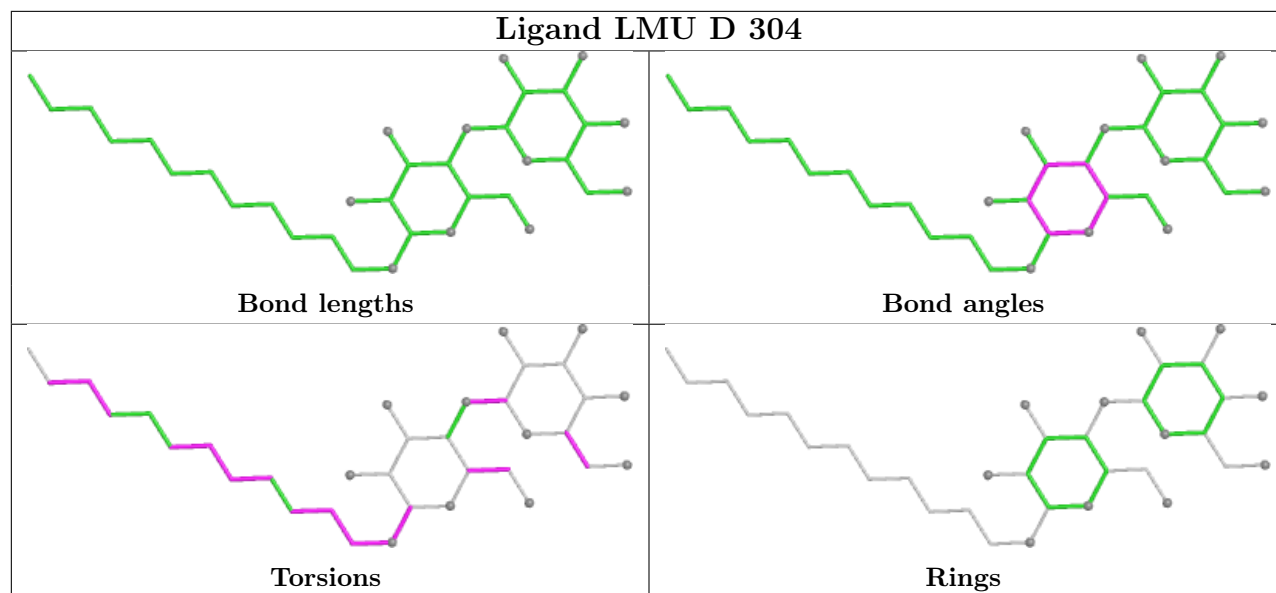


Ligand CLA C 317

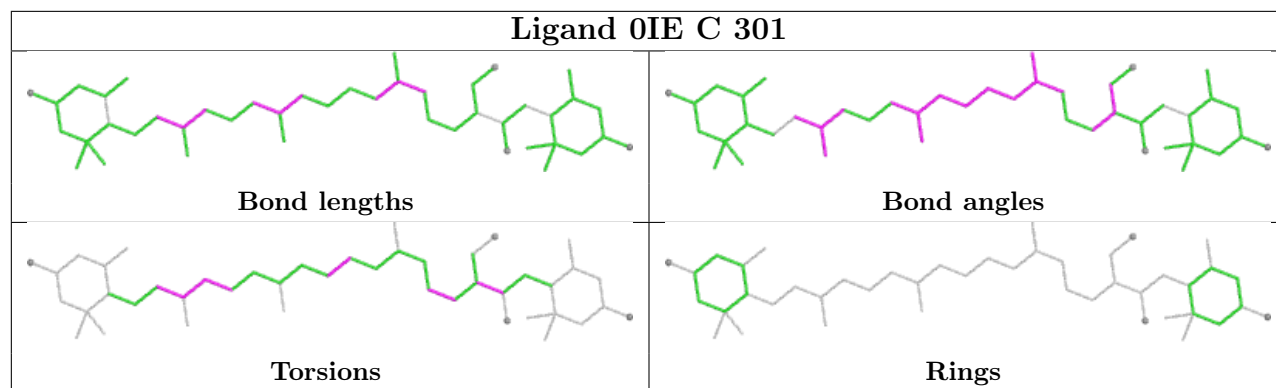




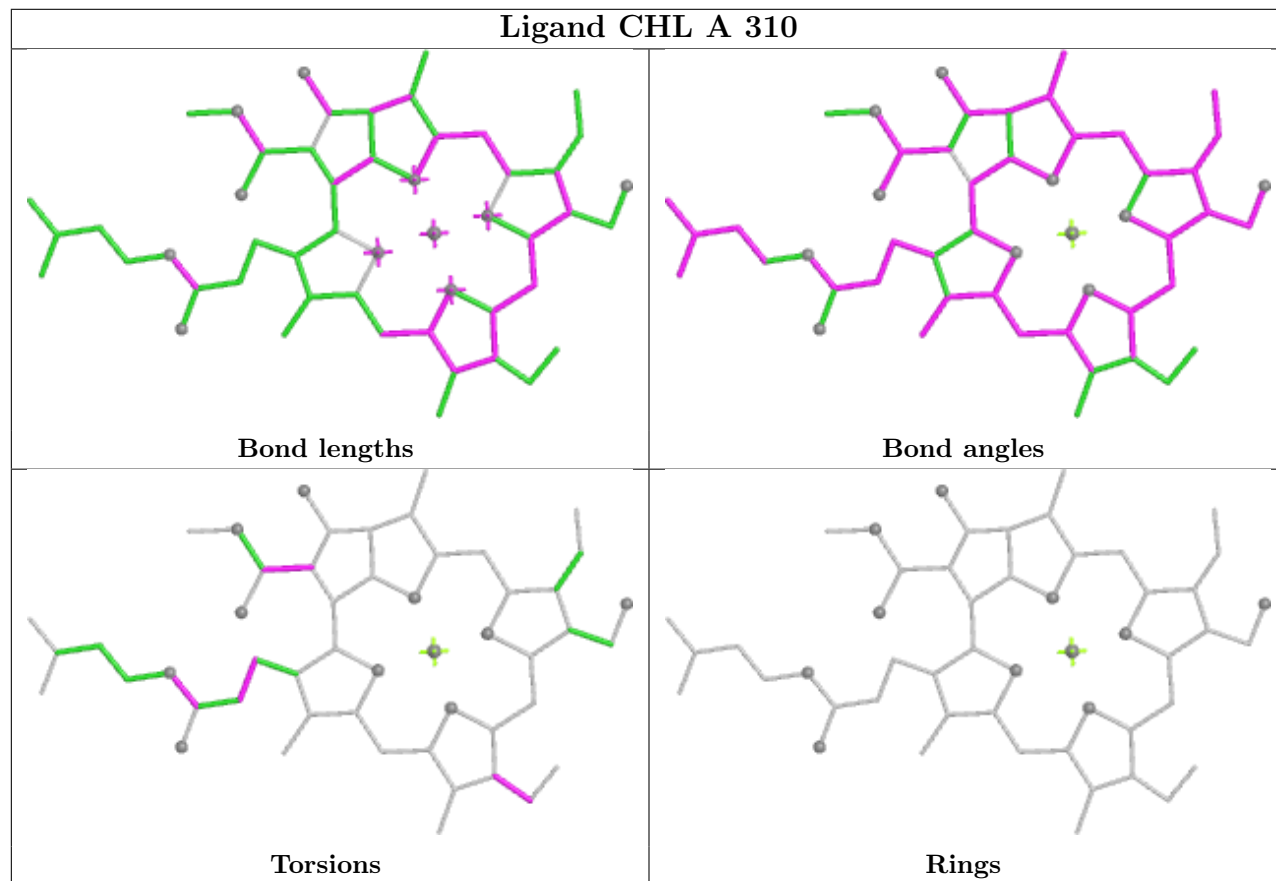


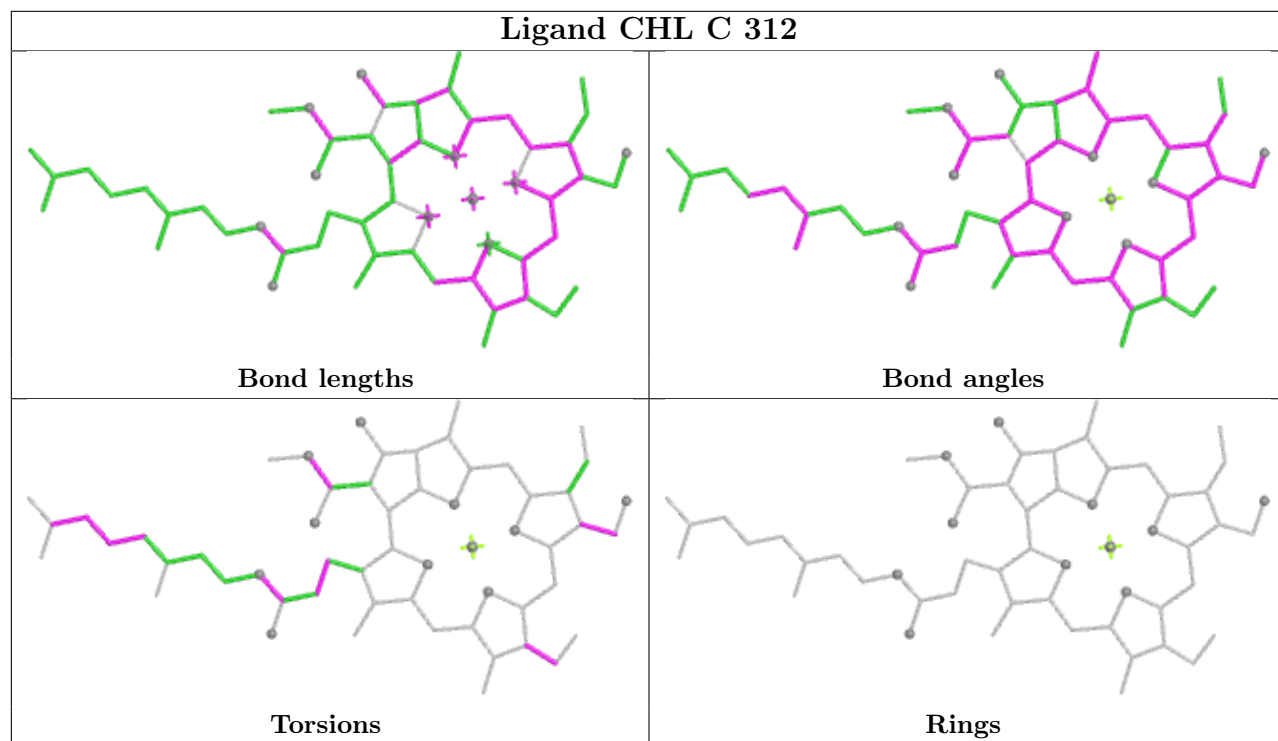


Ligand 0IE C 301

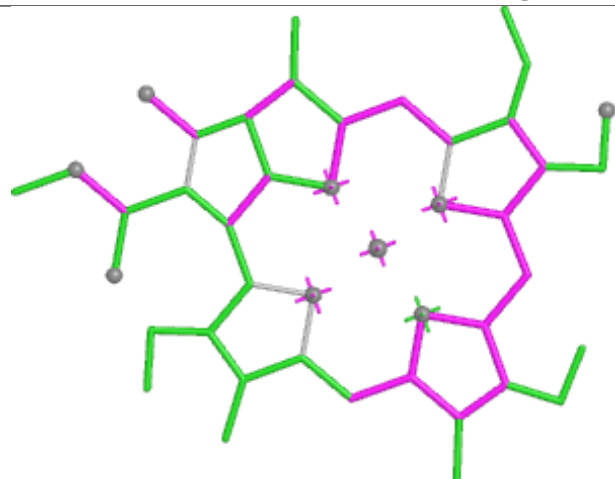


Ligand CHL A 310

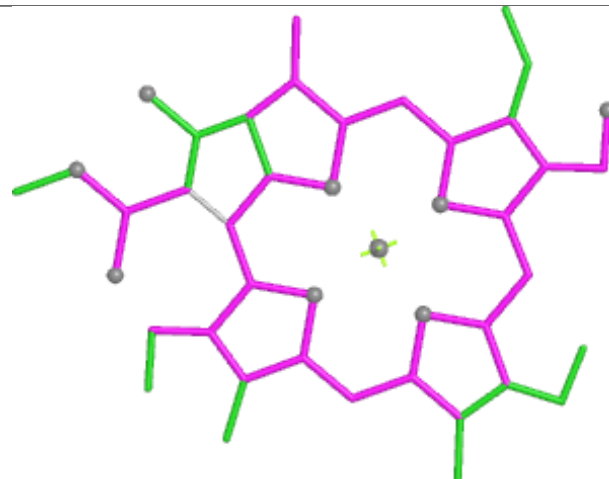




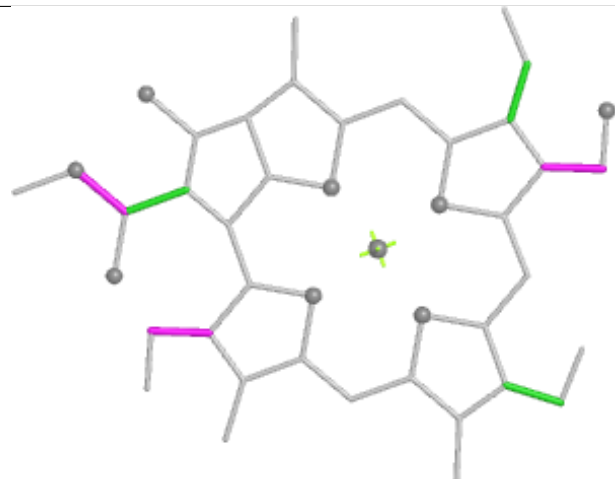
Ligand CHL B 310



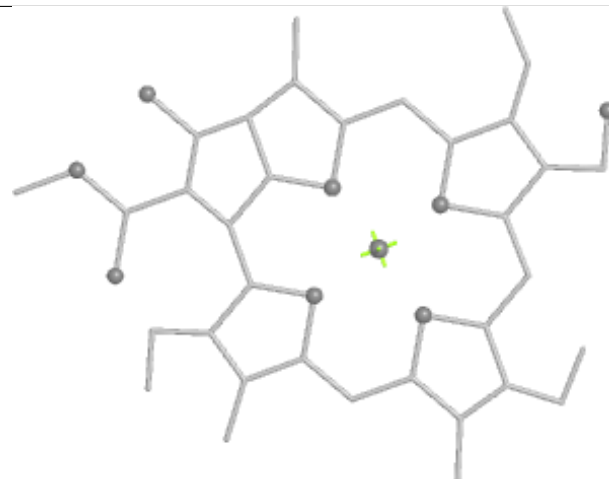
Bond lengths



Bond angles

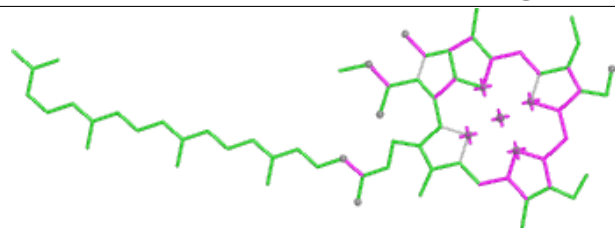


Torsions

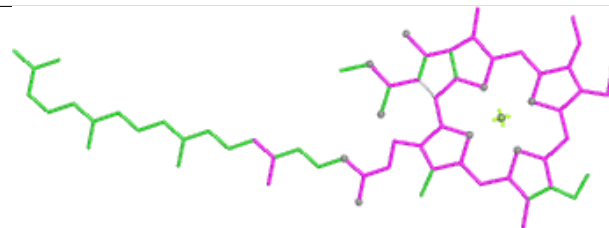


Rings

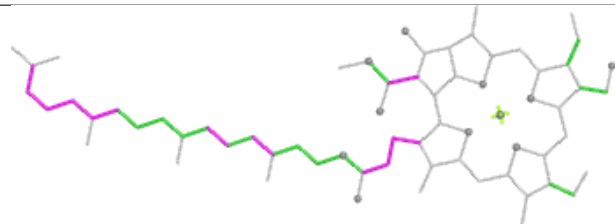
Ligand CHL F 304



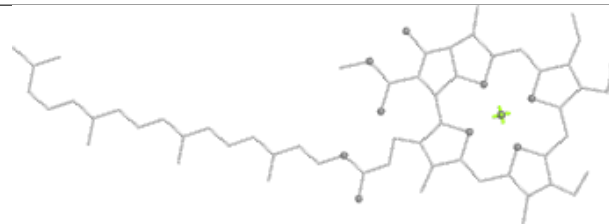
Bond lengths



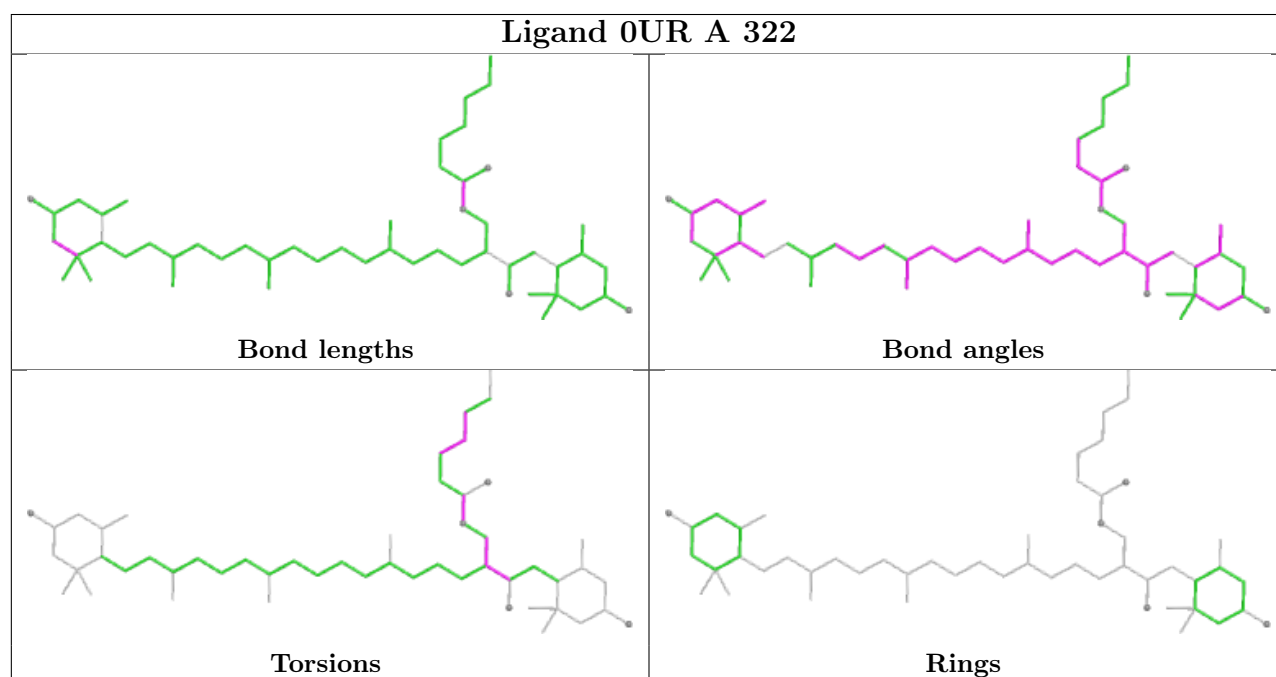
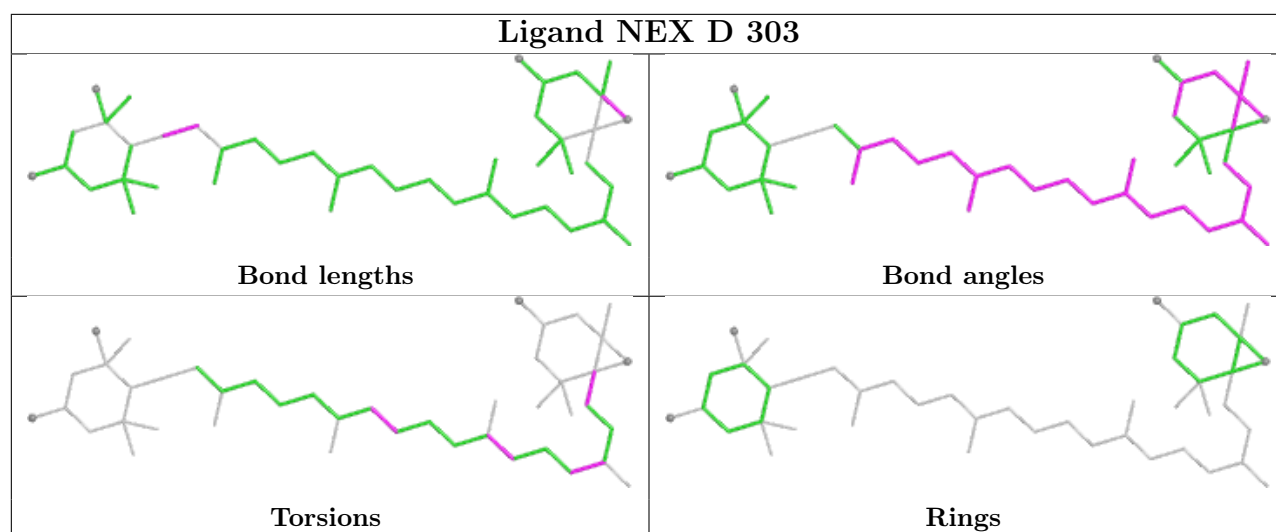
Bond angles

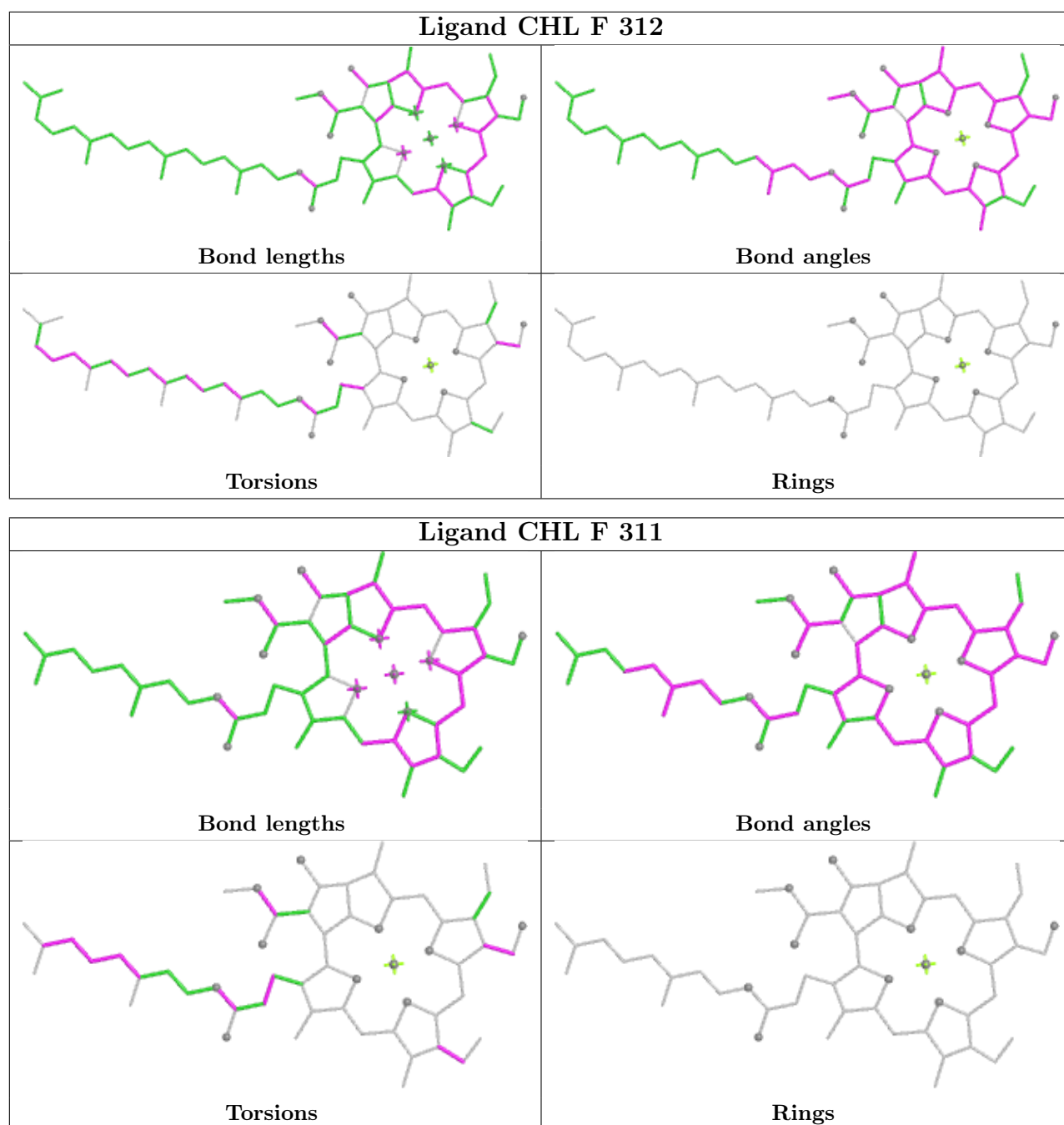


Torsions

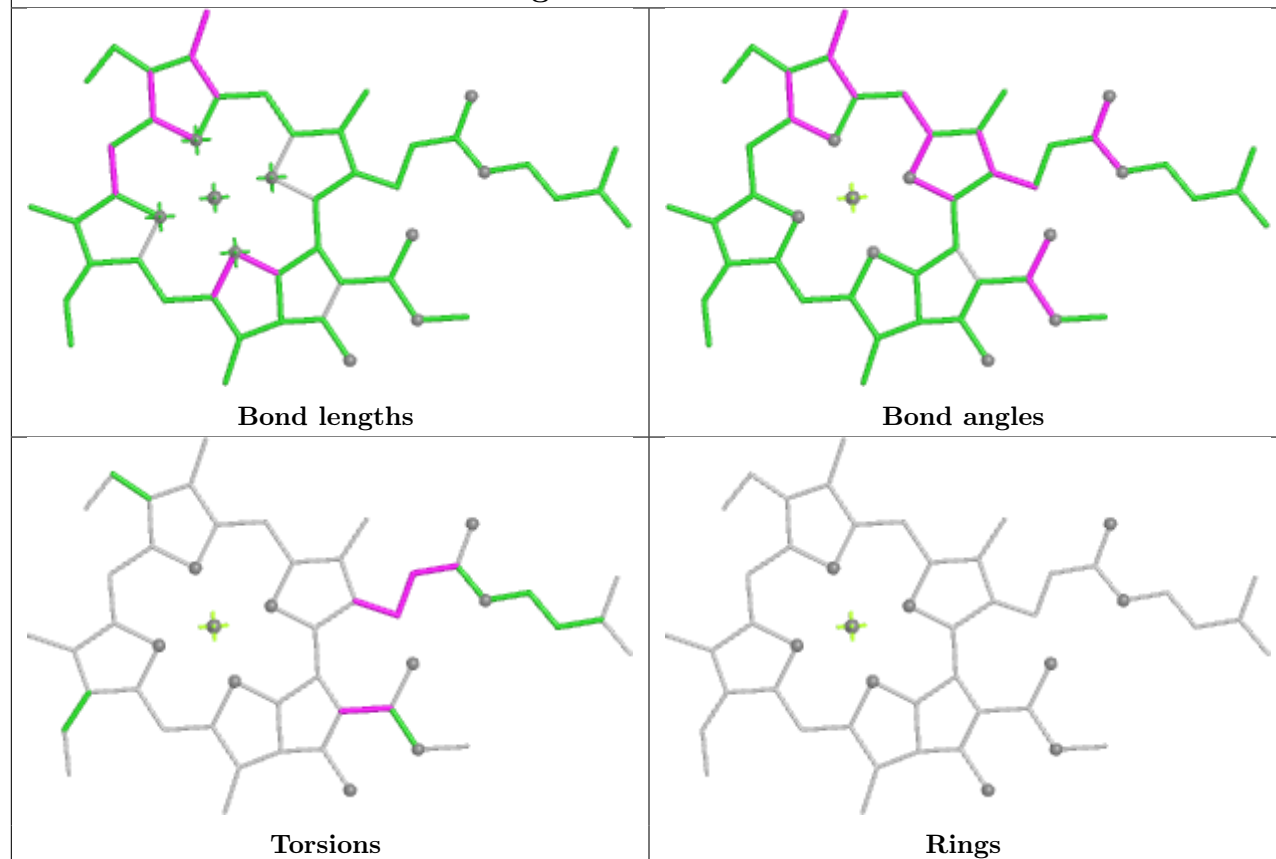


Rings

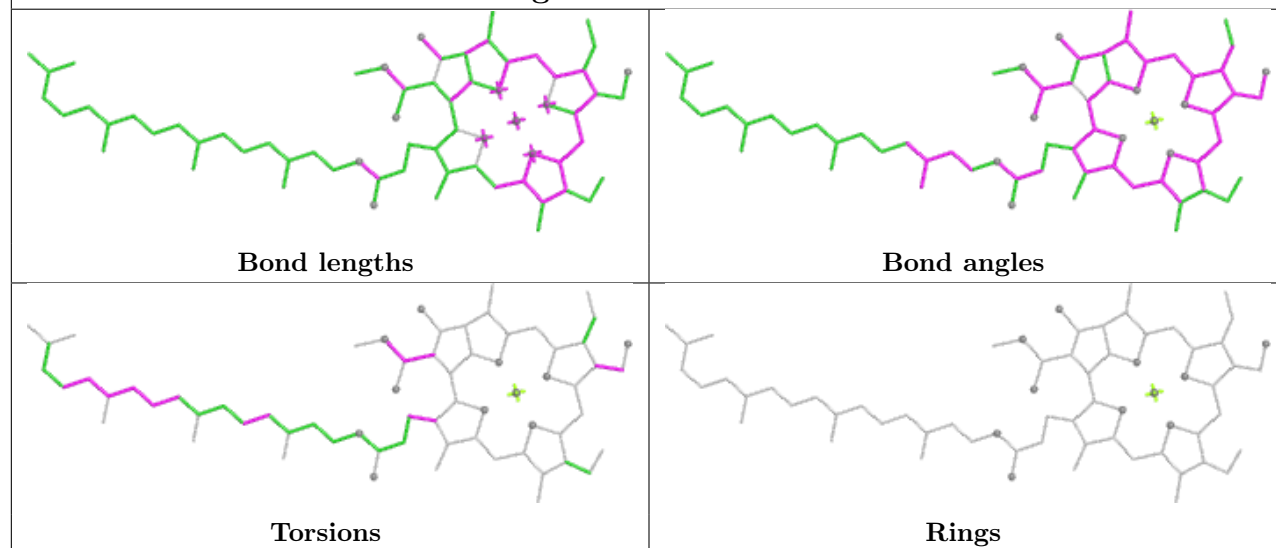




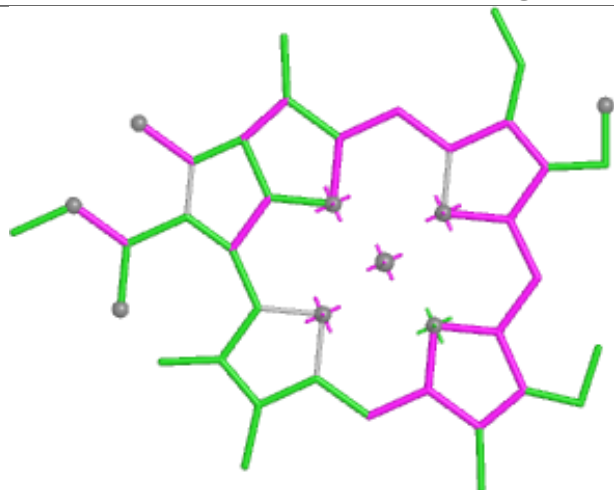
Ligand CLA A 308



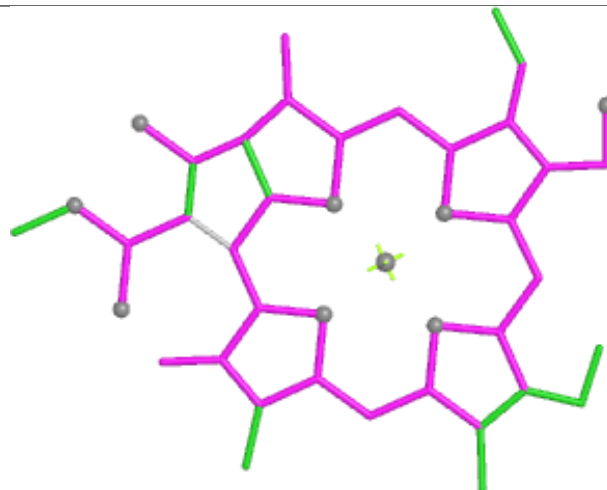
Ligand CHL B 306



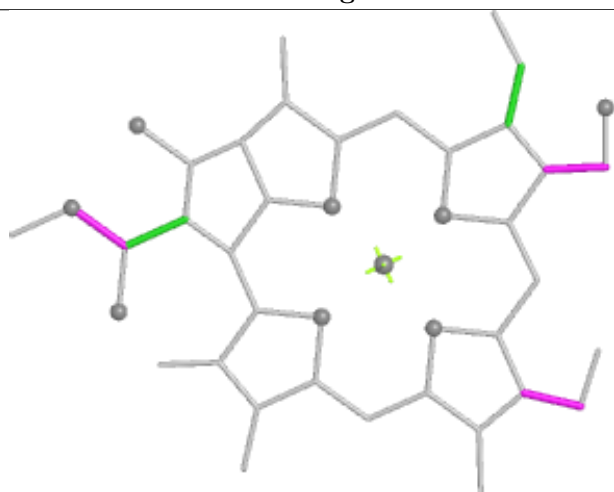
Ligand CHL F 308



Bond lengths



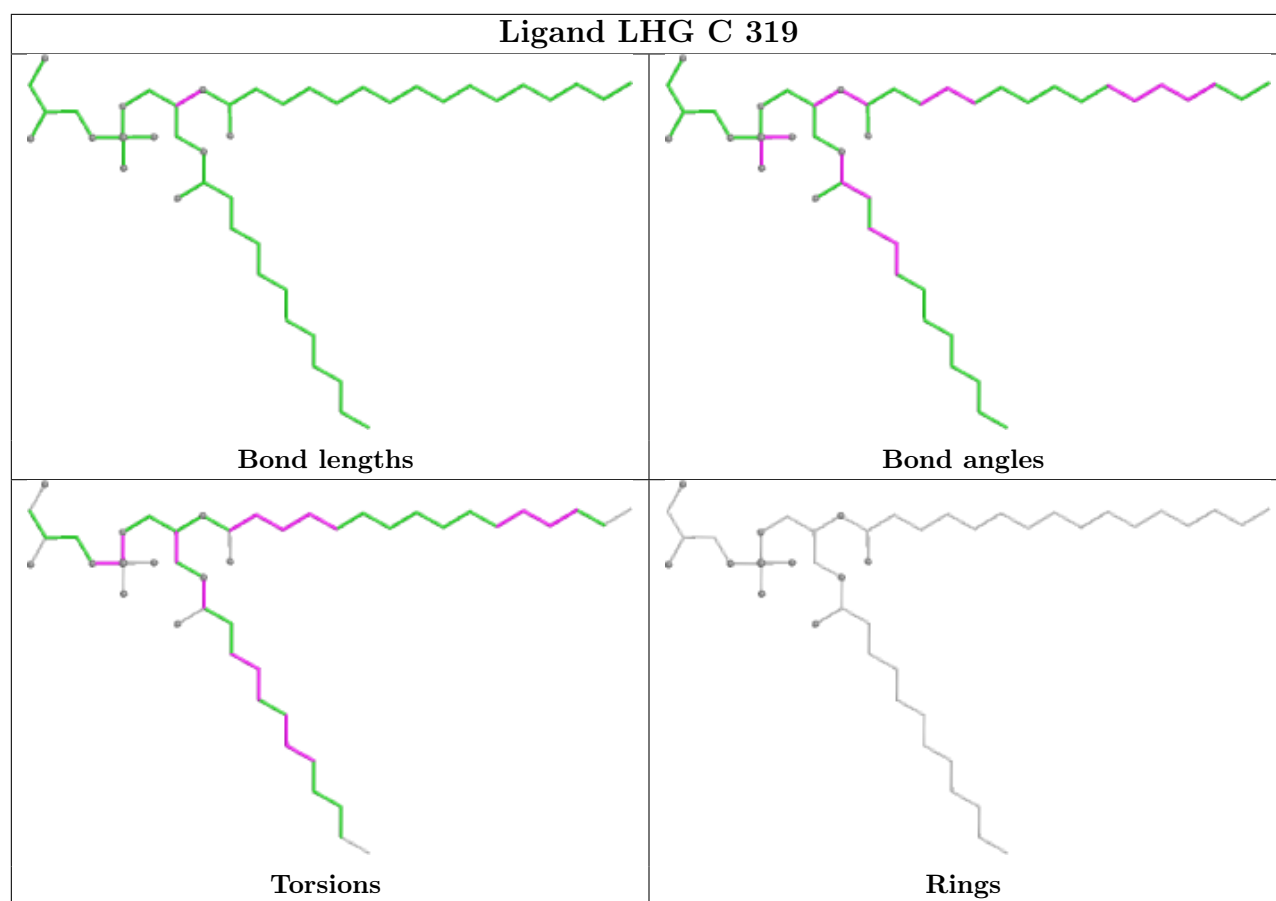
Bond angles



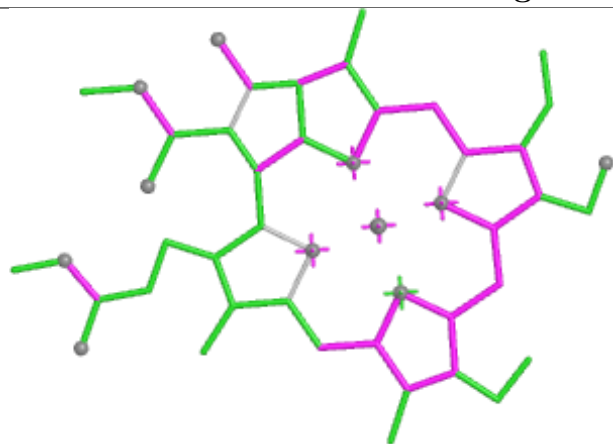
Torsions



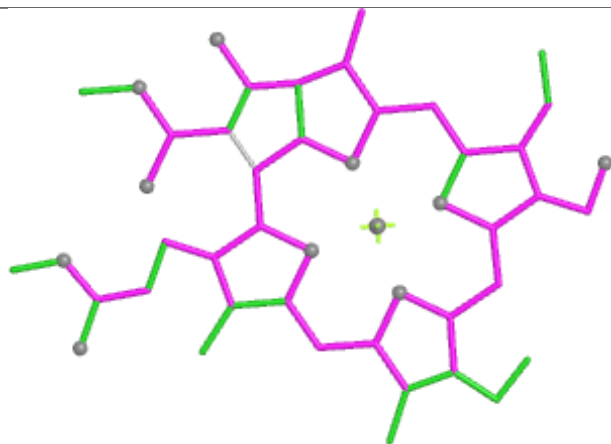
Rings



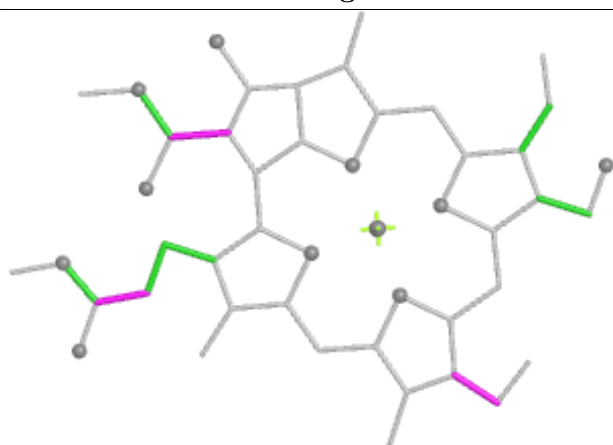
Ligand CHL B 319



Bond lengths



Bond angles

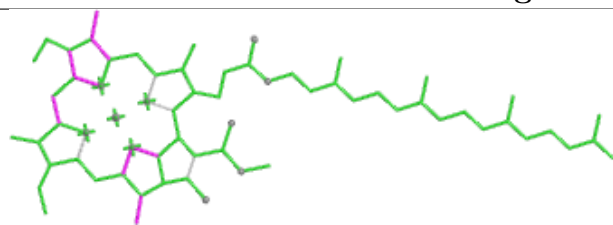


Torsions

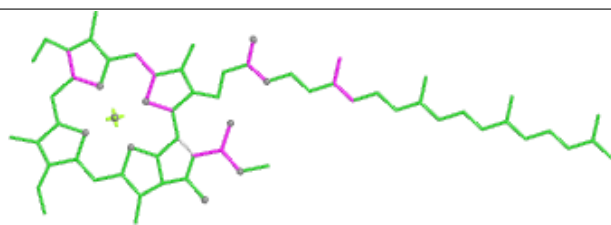


Rings

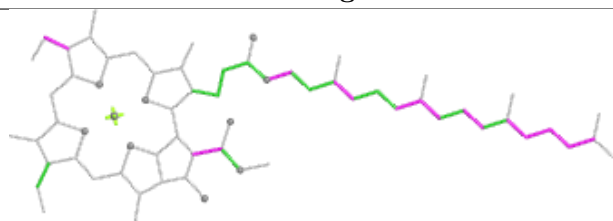
Ligand CLA B 308



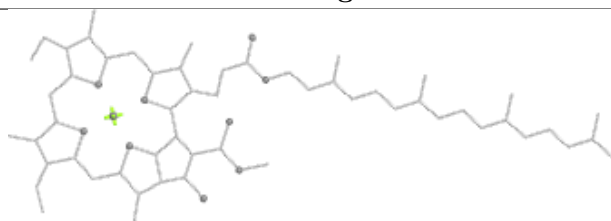
Bond lengths



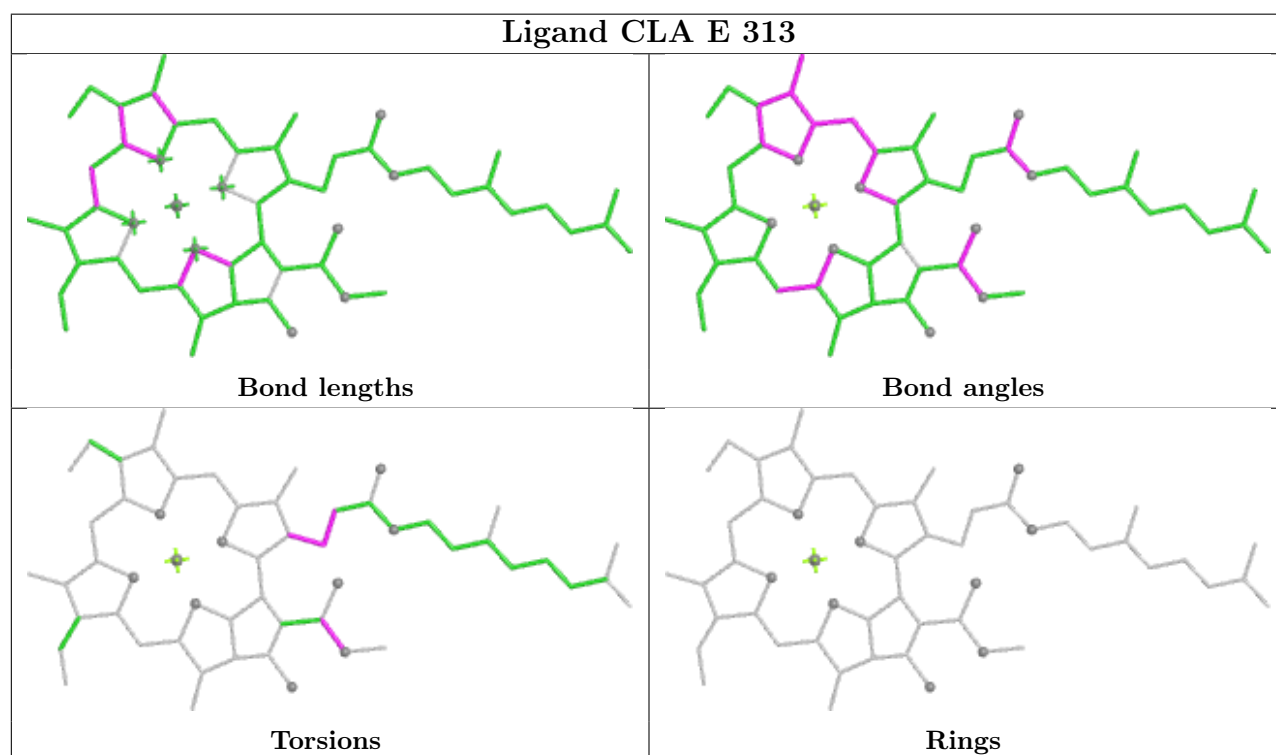
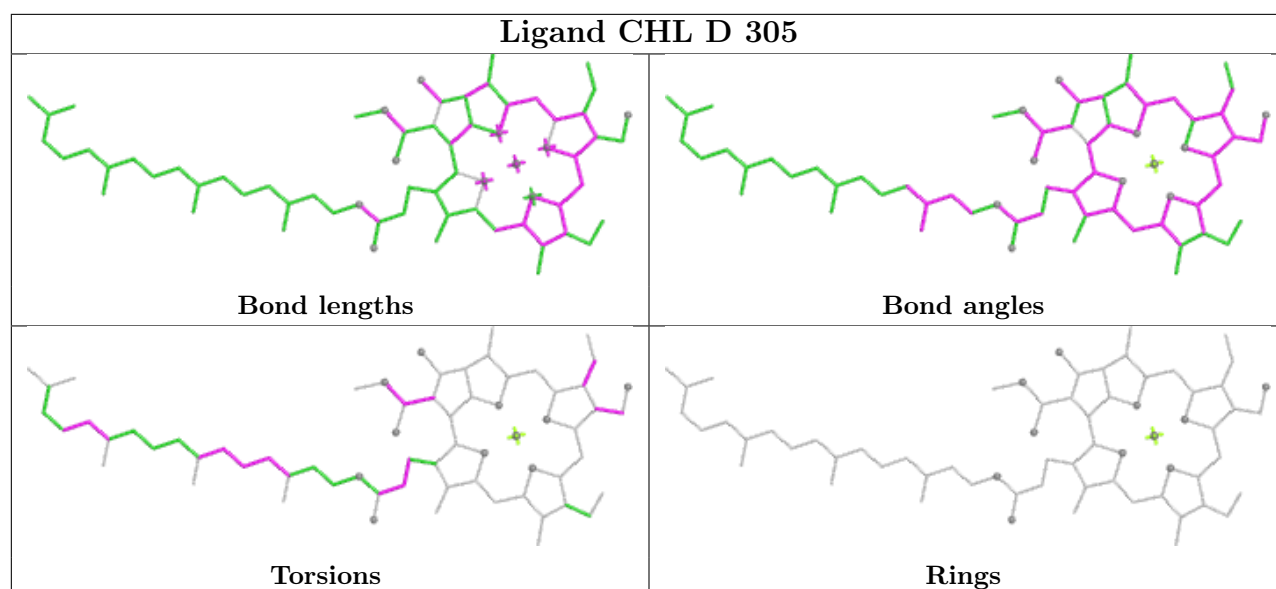
Bond angles

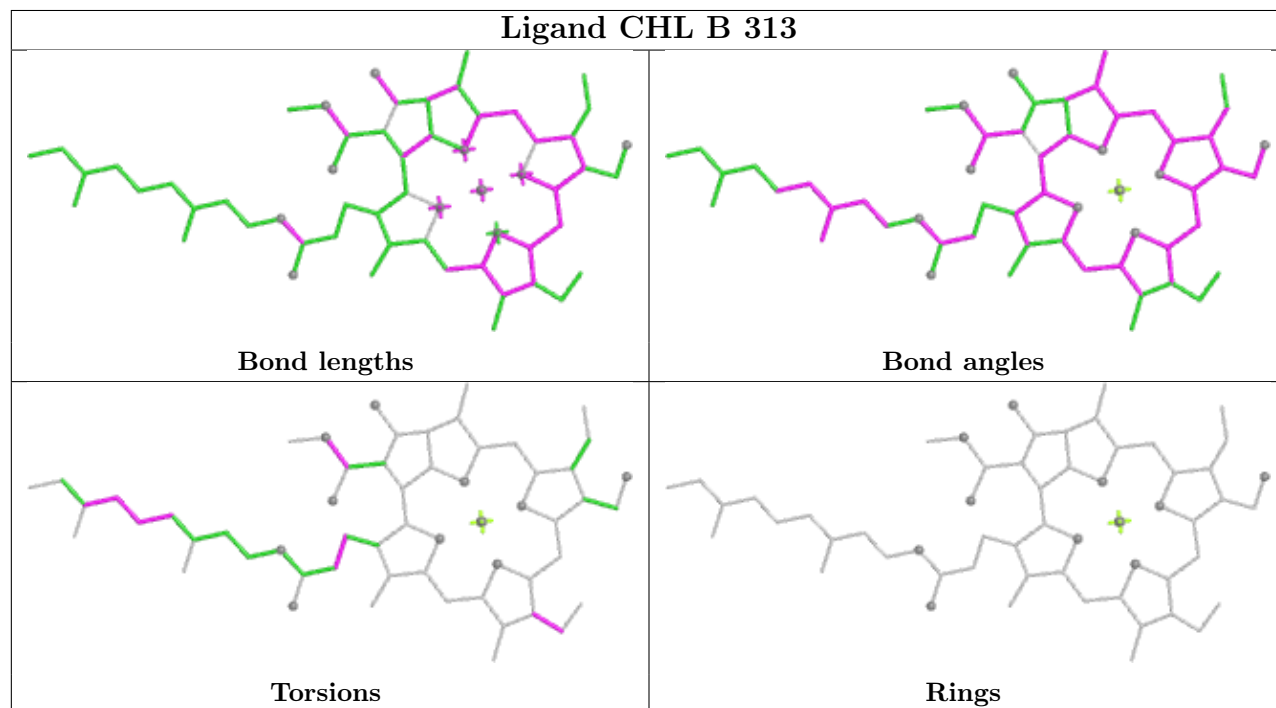
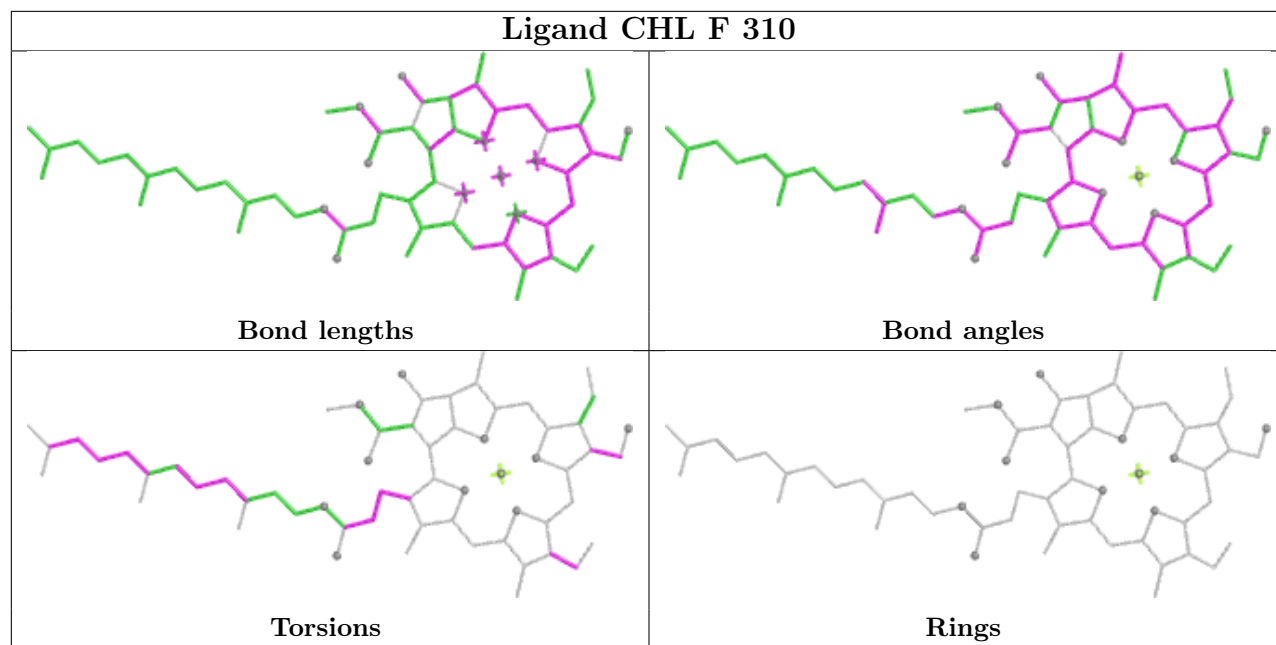


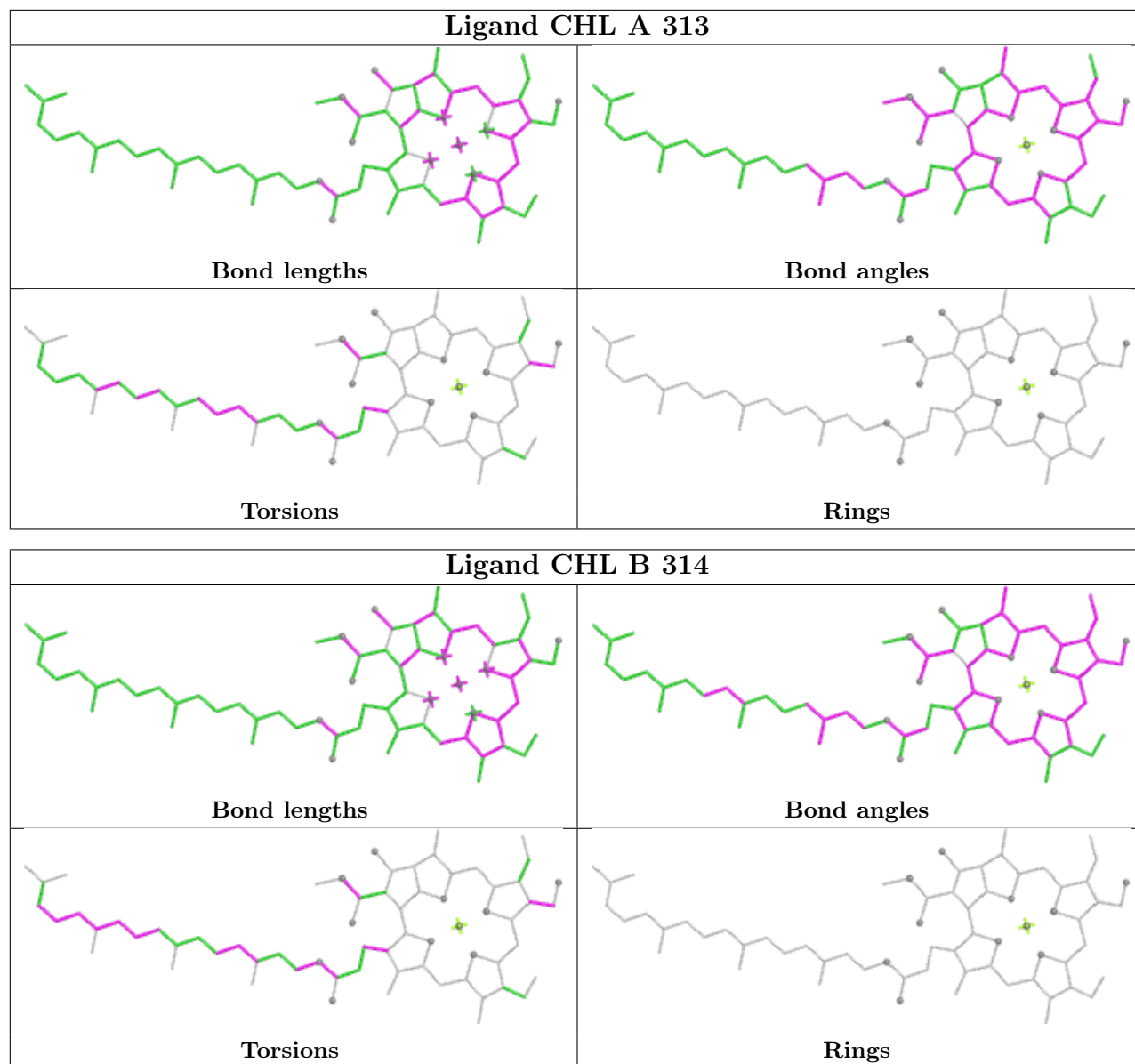
Torsions



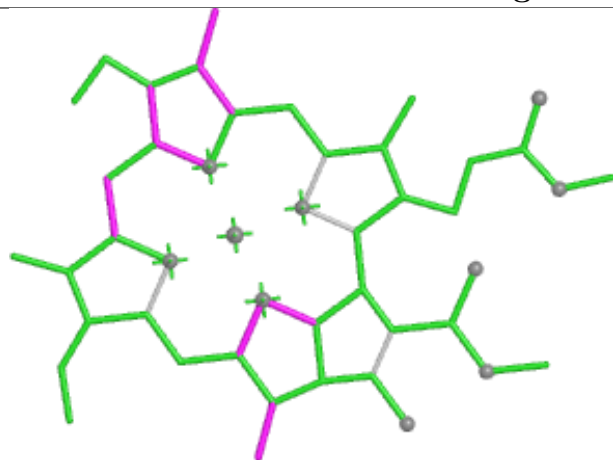
Rings



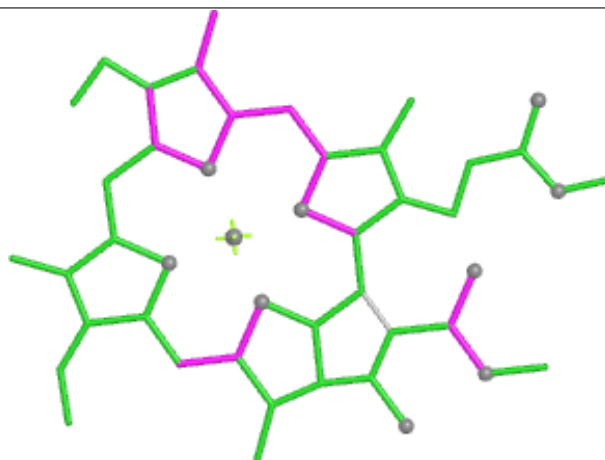




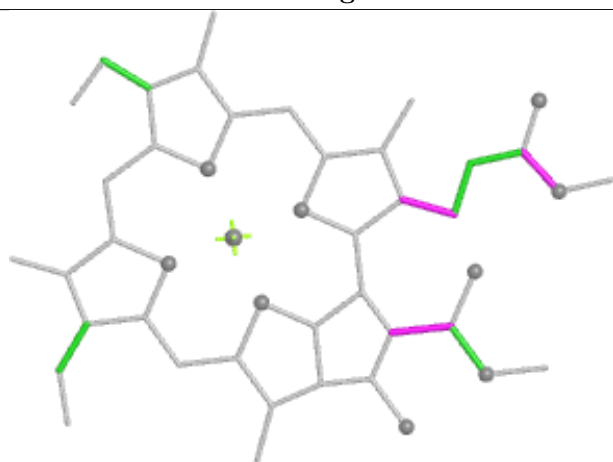
Ligand CLA D 308



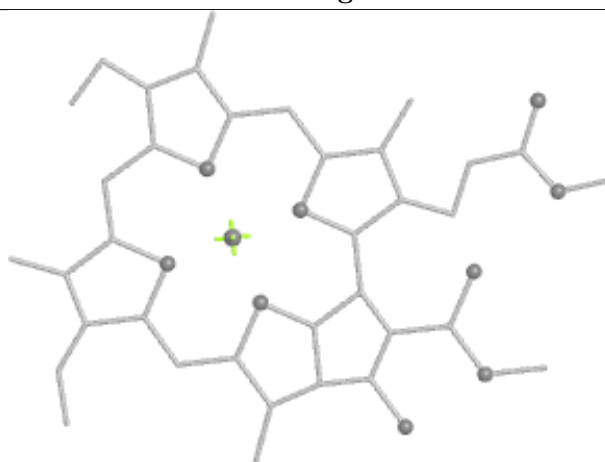
Bond lengths



Bond angles

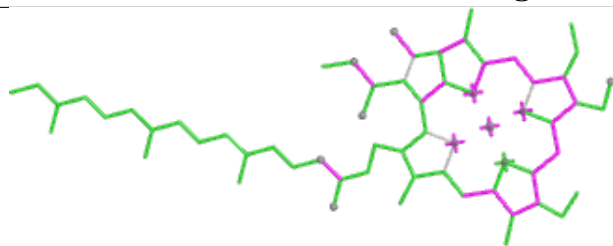


Torsions

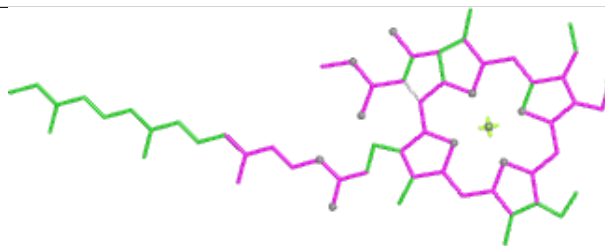


Rings

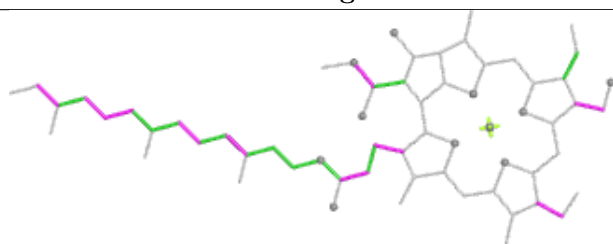
Ligand CHL D 311



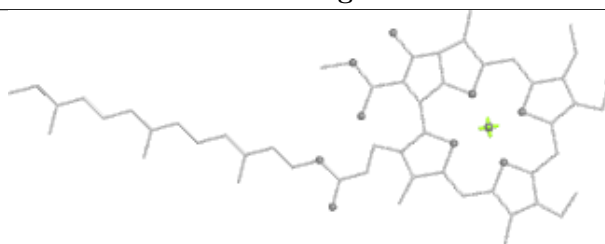
Bond lengths



Bond angles

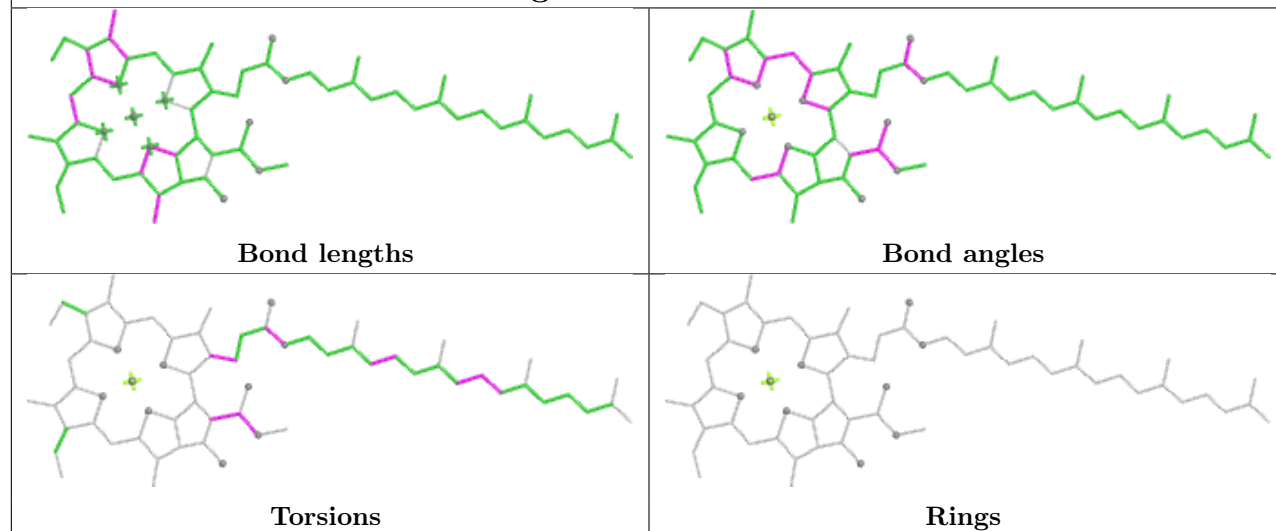


Torsions

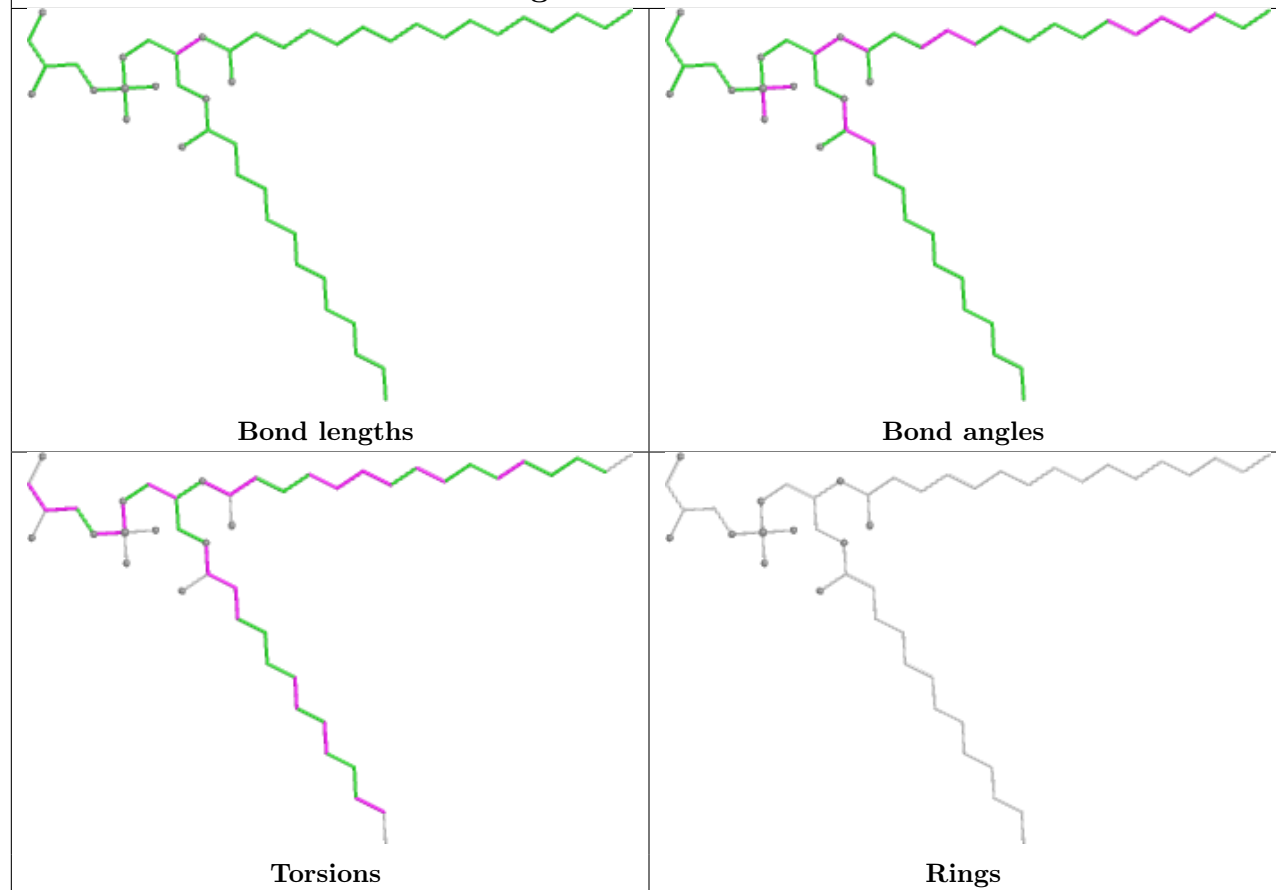


Rings

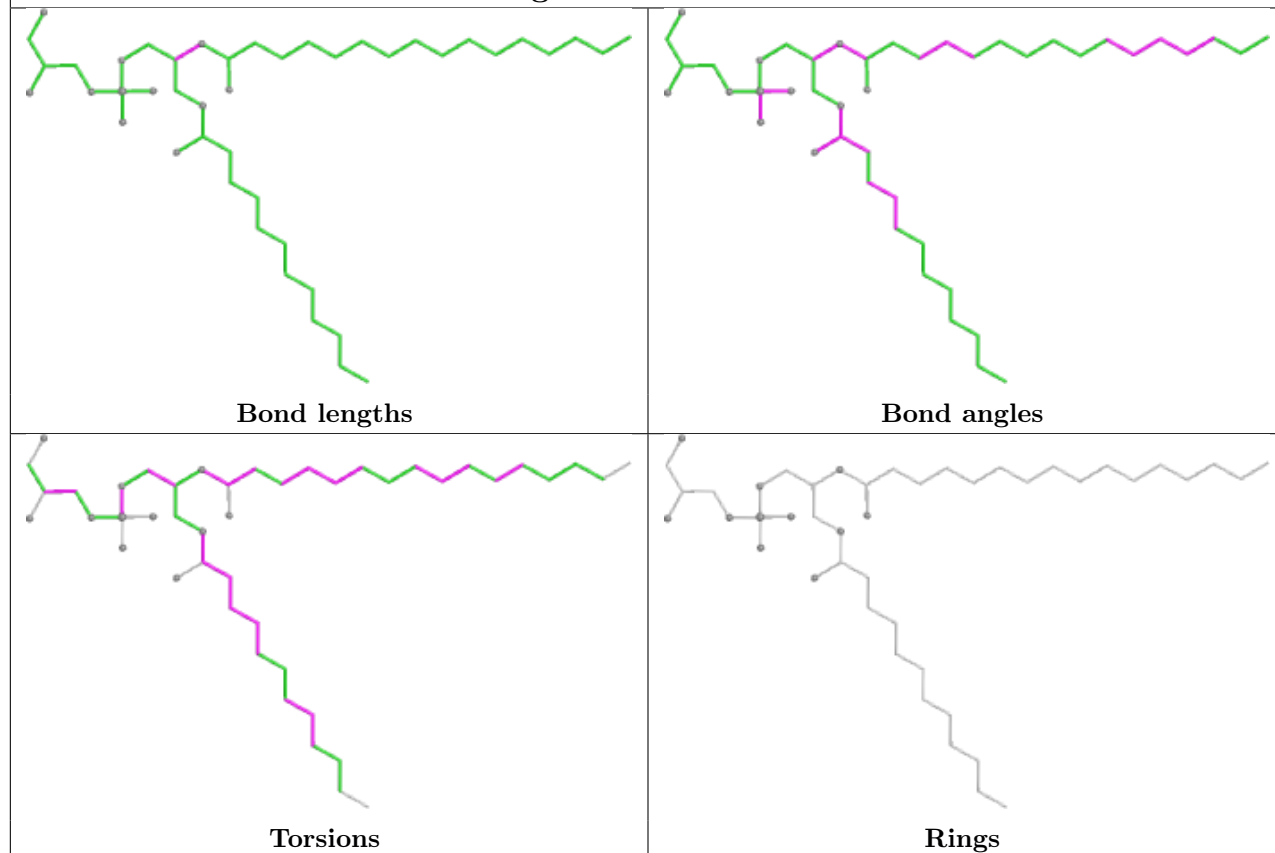
Ligand CLA D 315



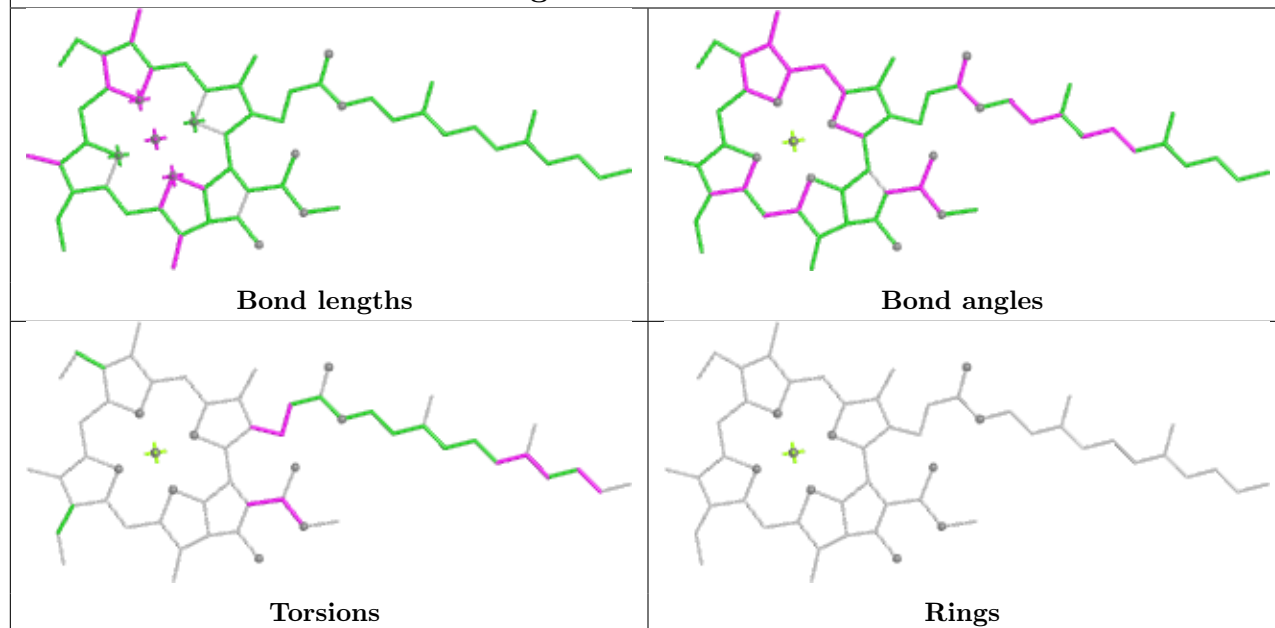
Ligand LHG B 320



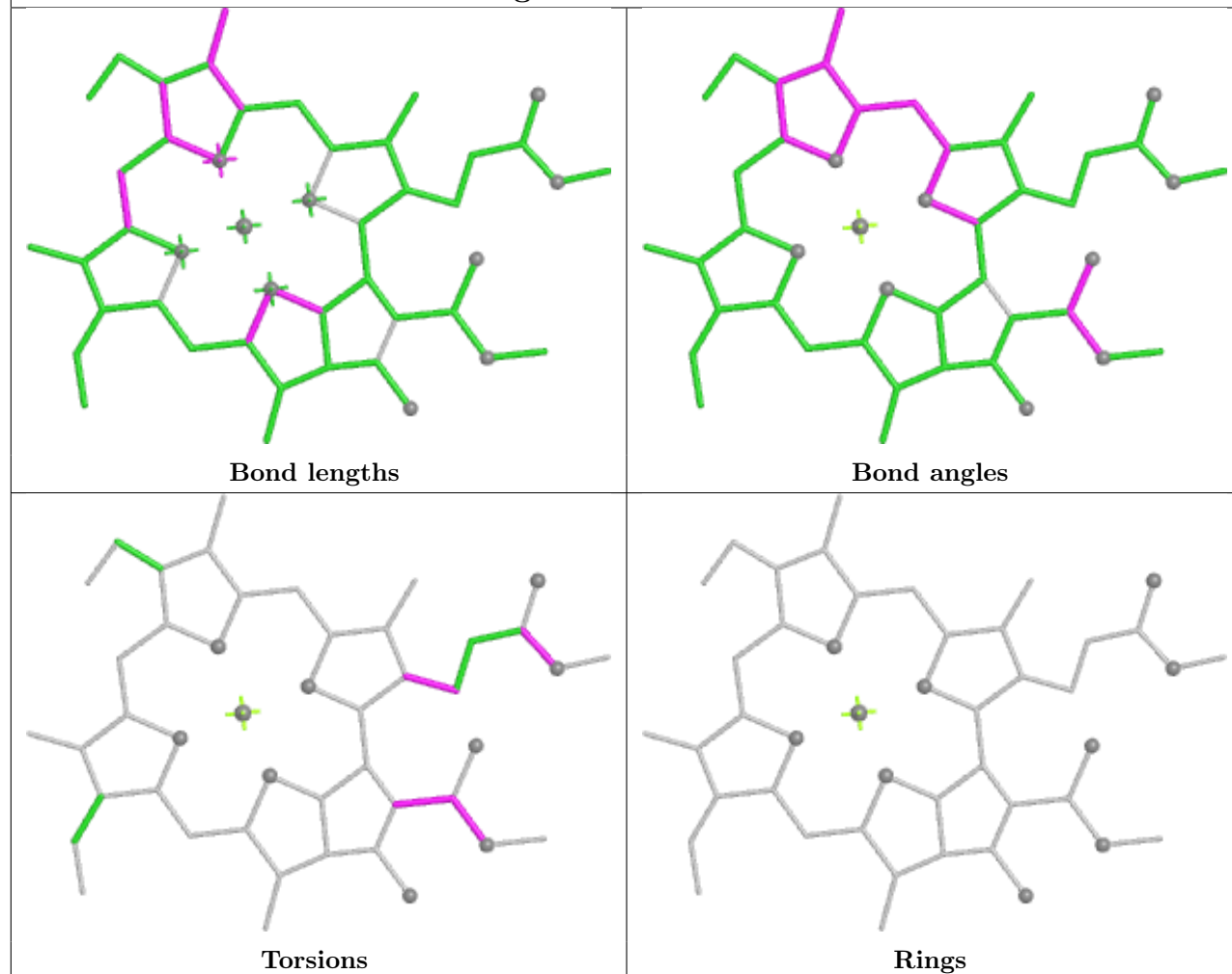
Ligand LHG F 318



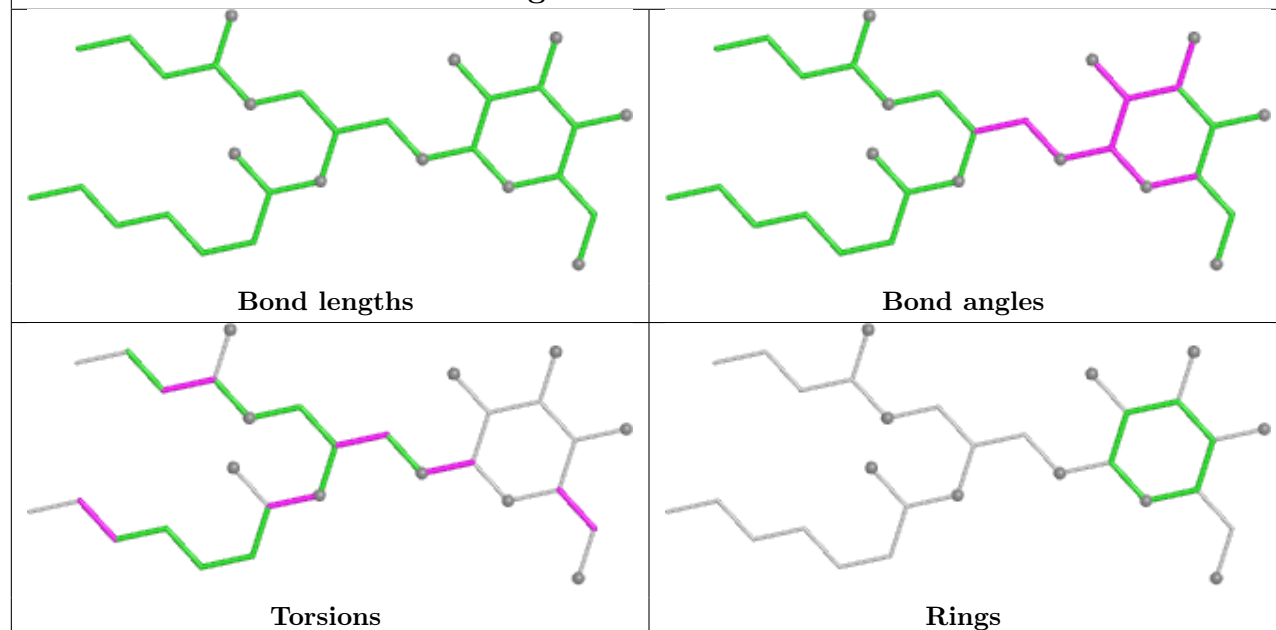
Ligand CLA D 314



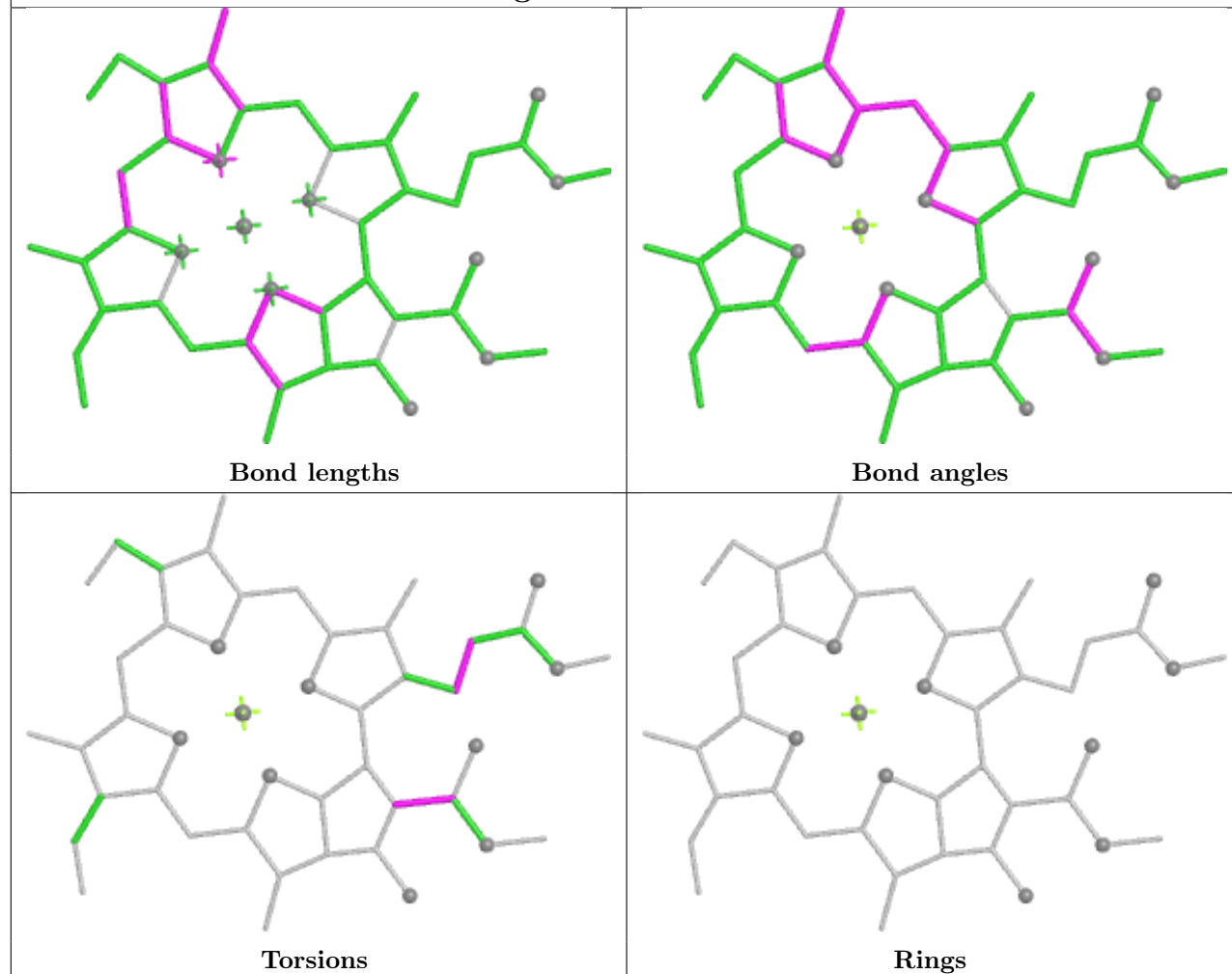
Ligand CLA C 308



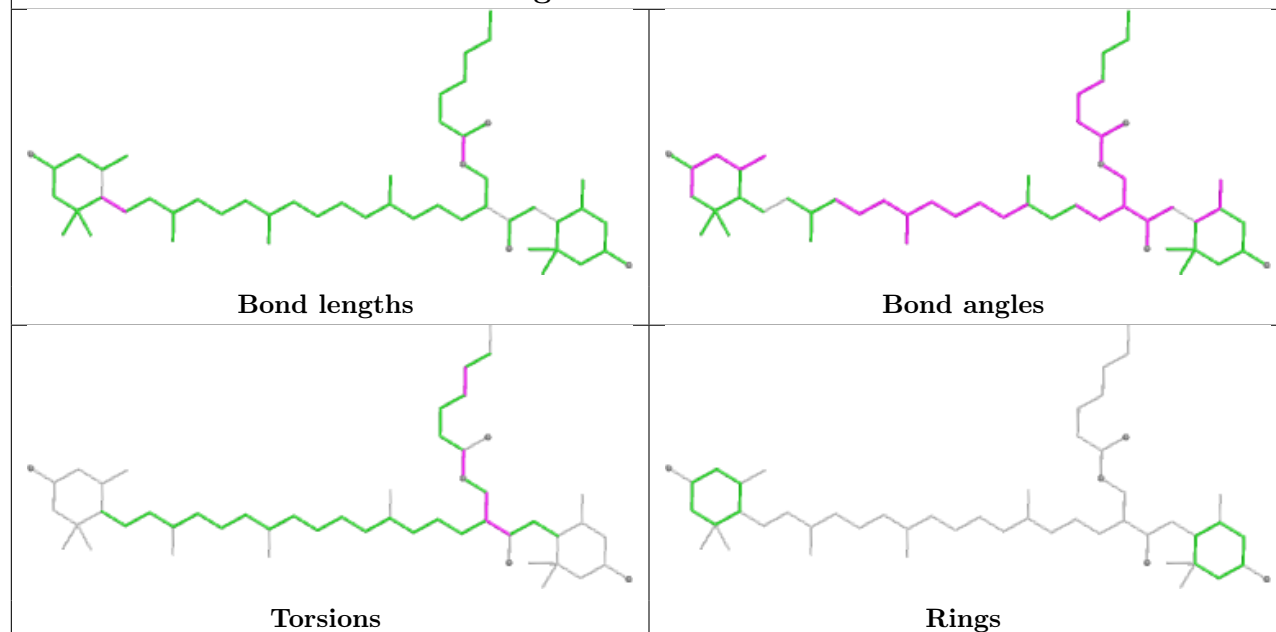
Ligand LMG B 323



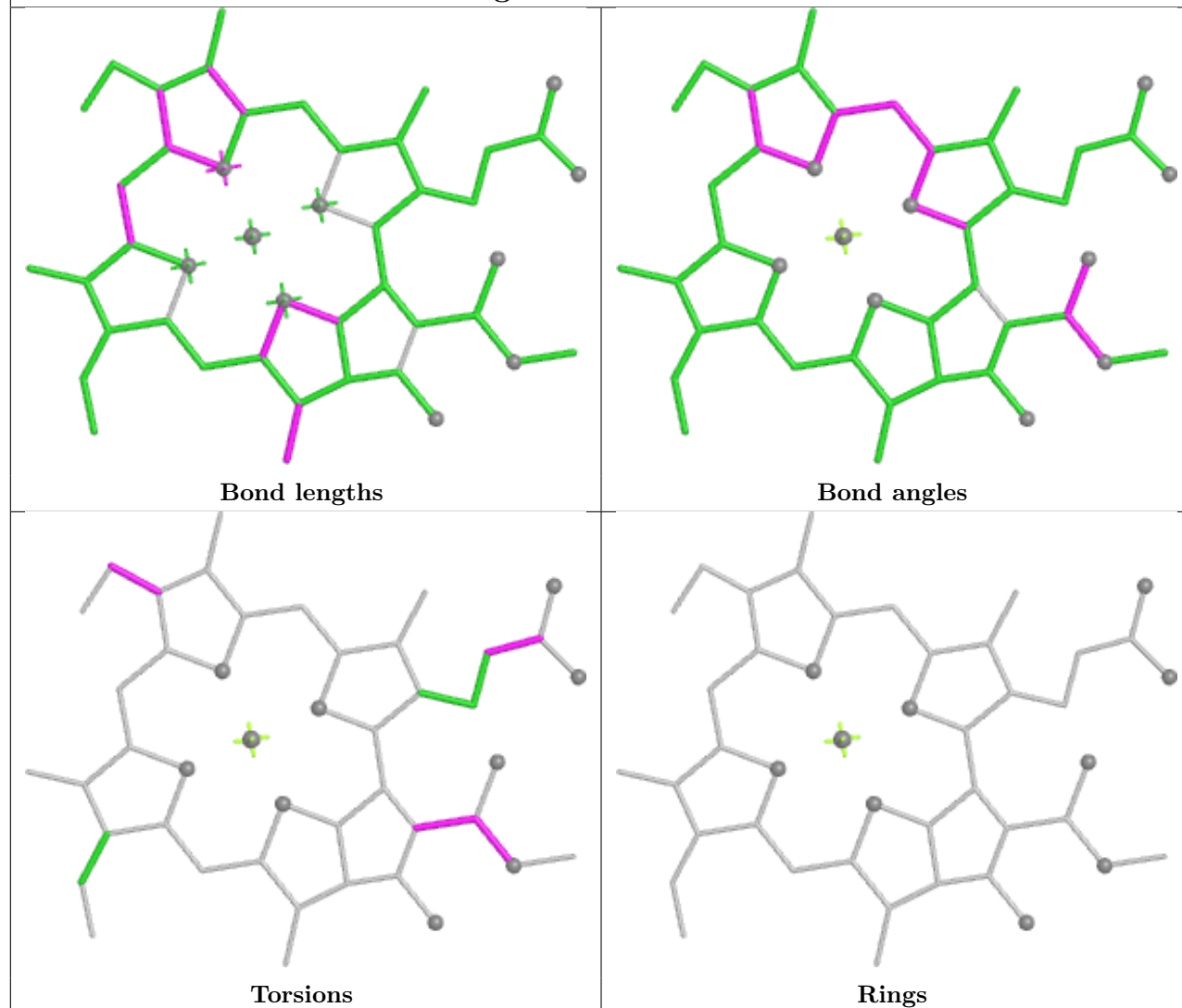
Ligand CLA B 309



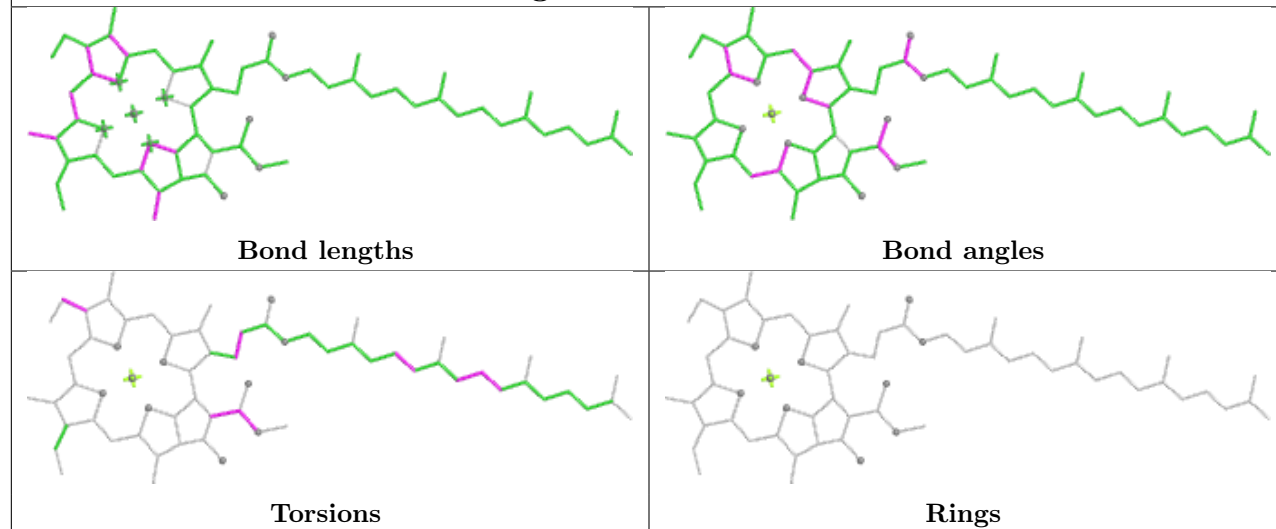
Ligand OUR B 325



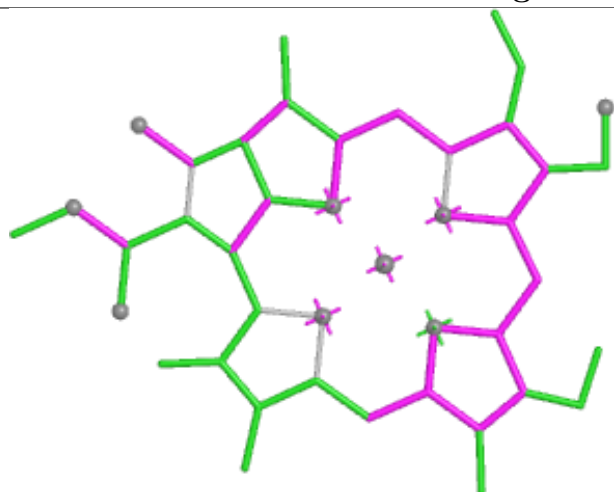
Ligand CLA E 315



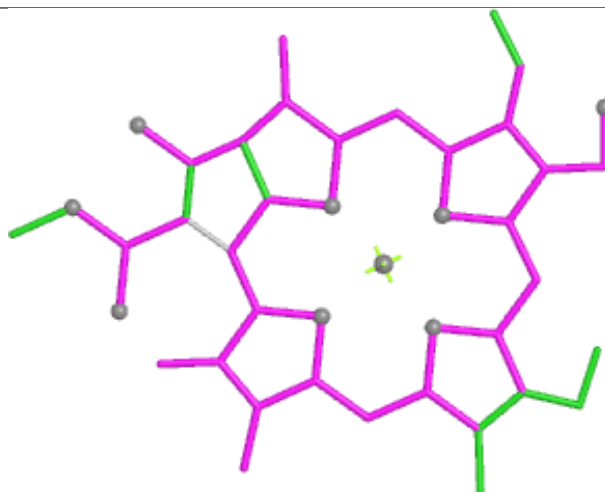
Ligand CLA D 317



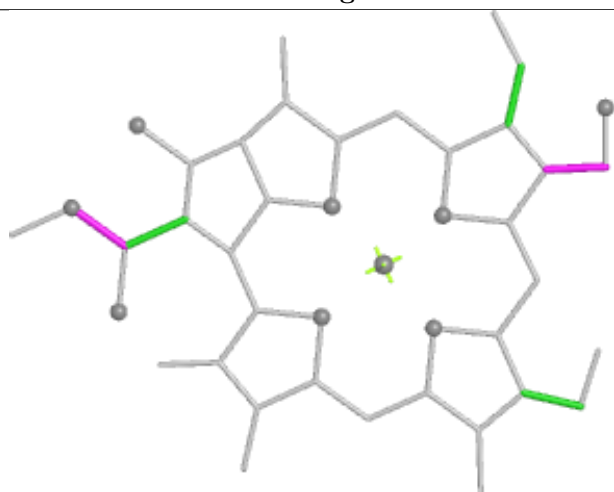
Ligand CHL D 309



Bond lengths



Bond angles

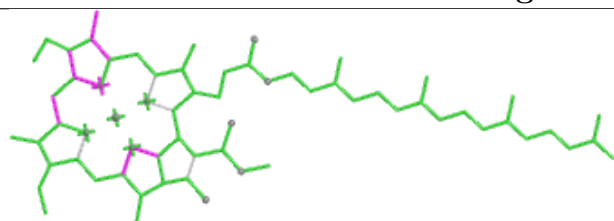


Torsions

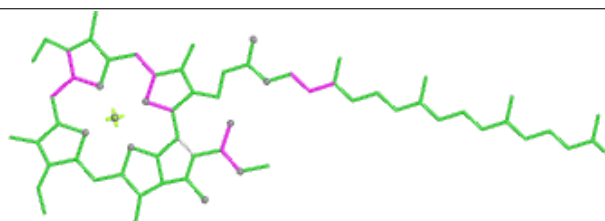


Rings

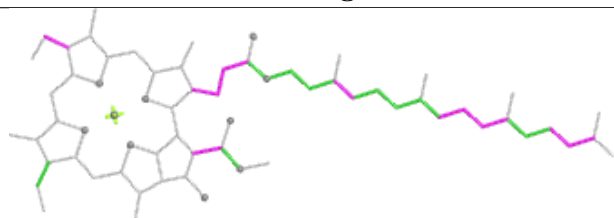
Ligand CLA F 306



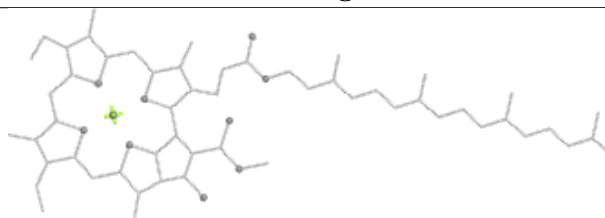
Bond lengths



Bond angles

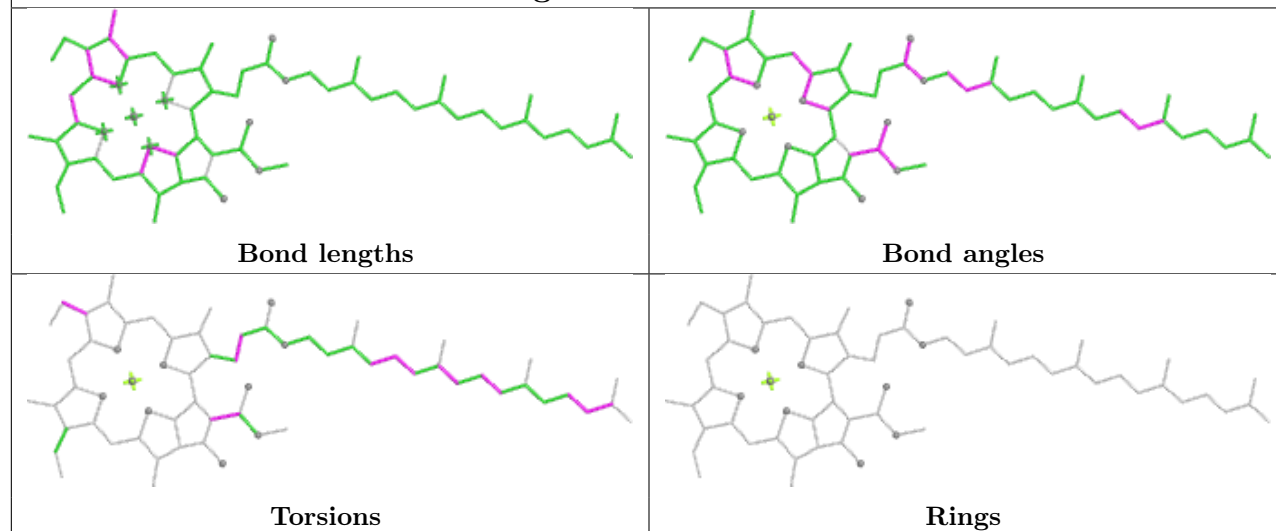


Torsions

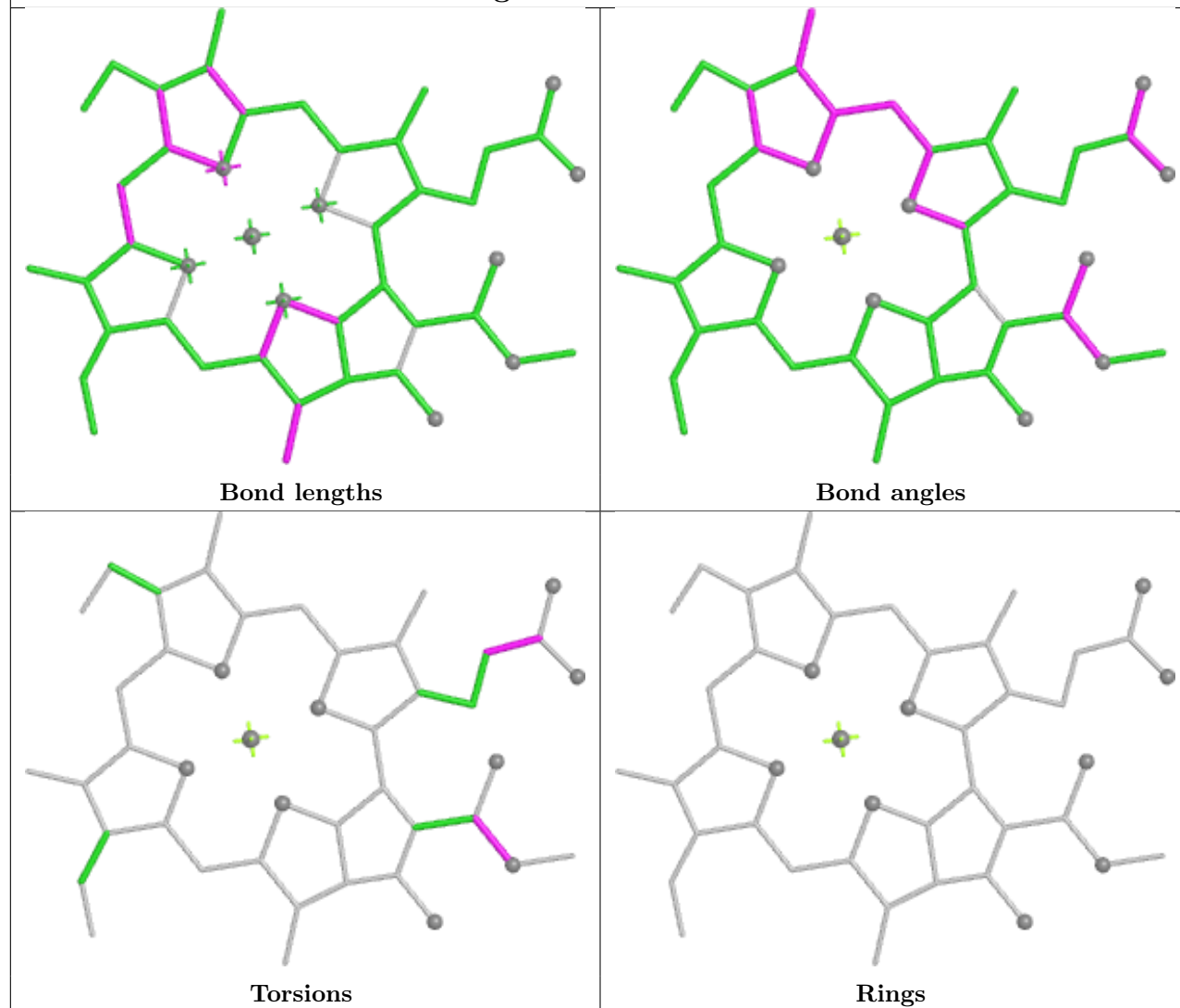


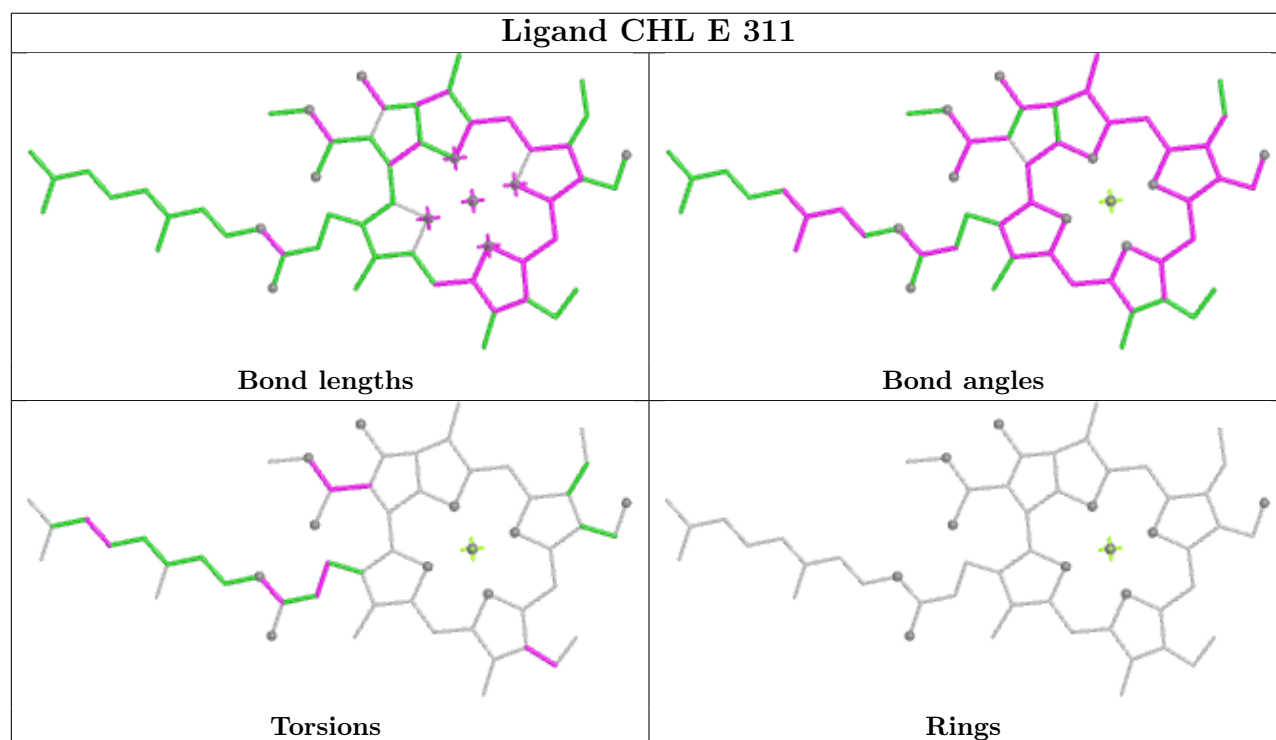
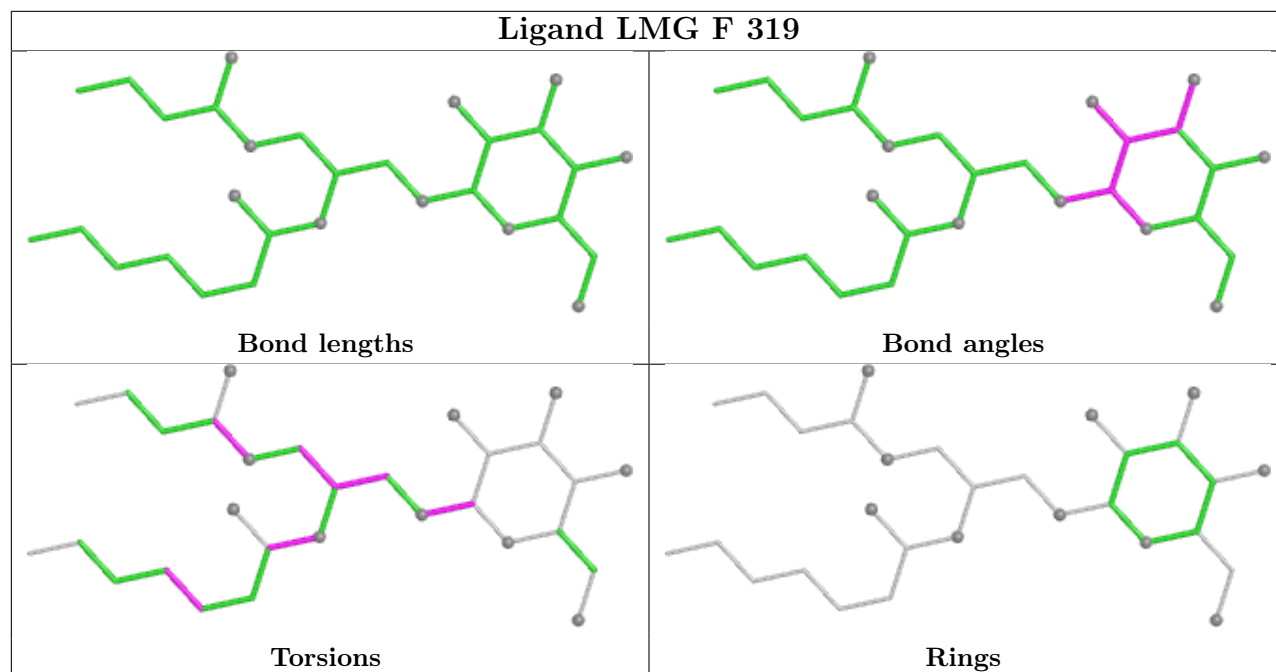
Rings

Ligand CLA E 306

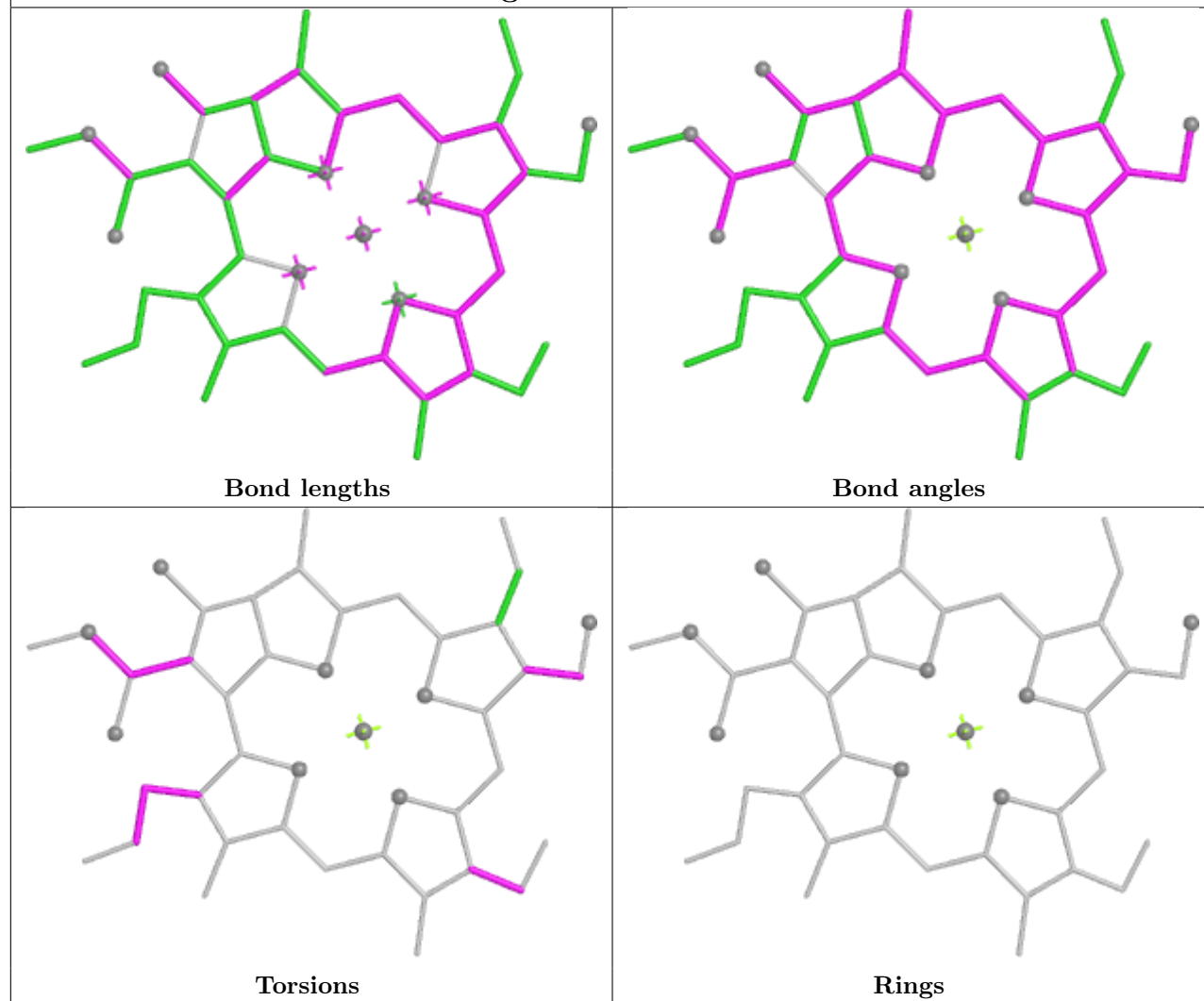


Ligand CLA F 315

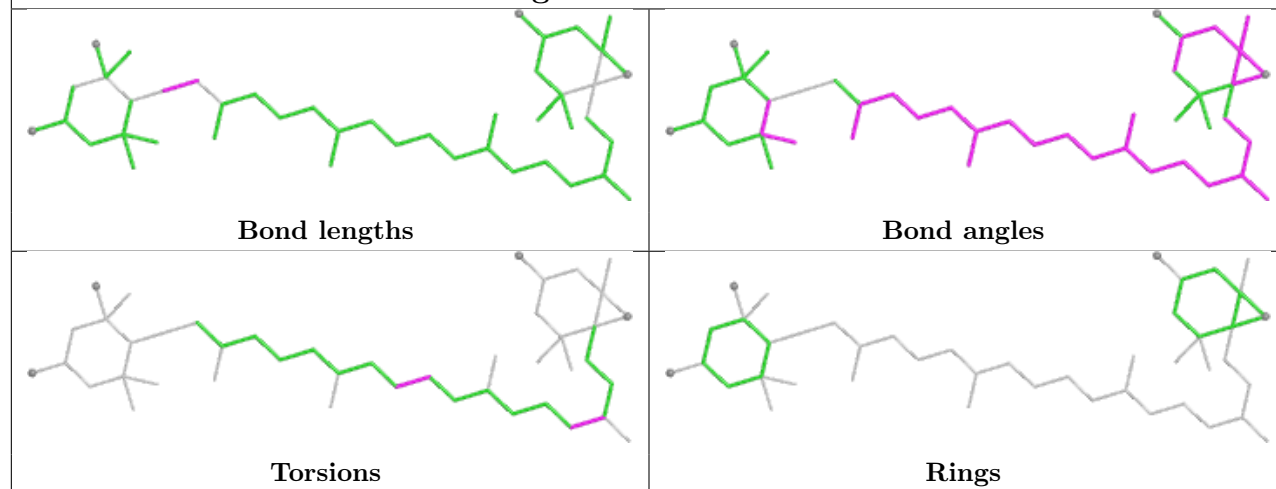


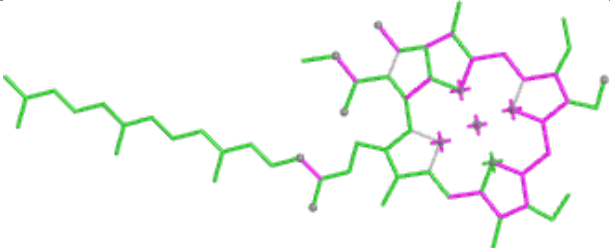
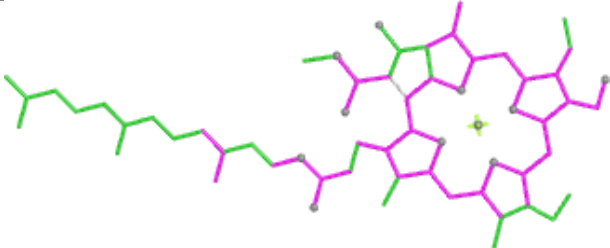
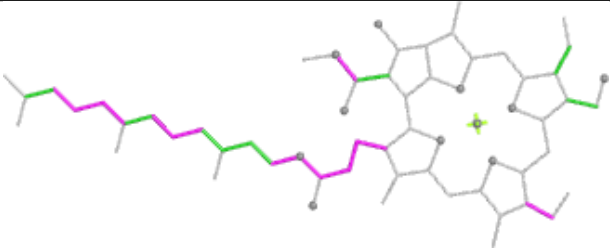
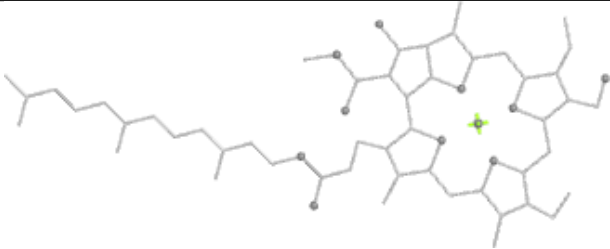
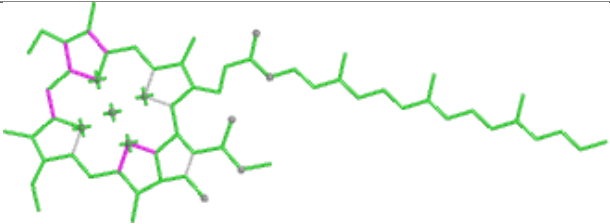
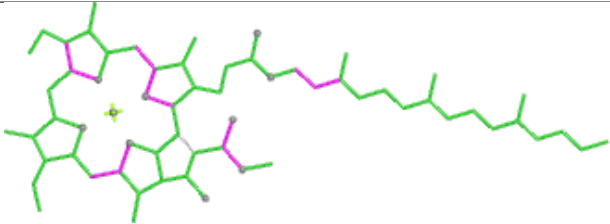
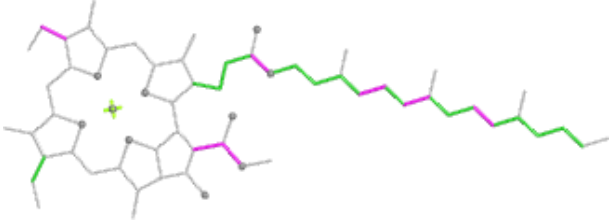
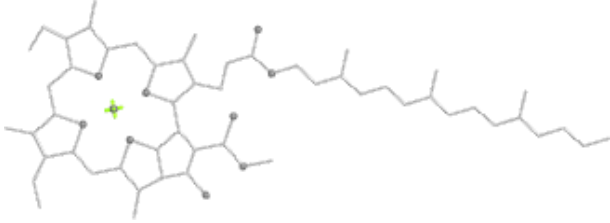
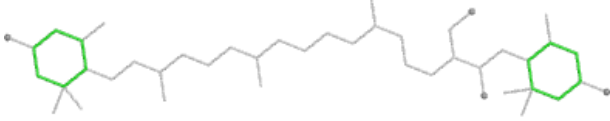


Ligand CHL C 310

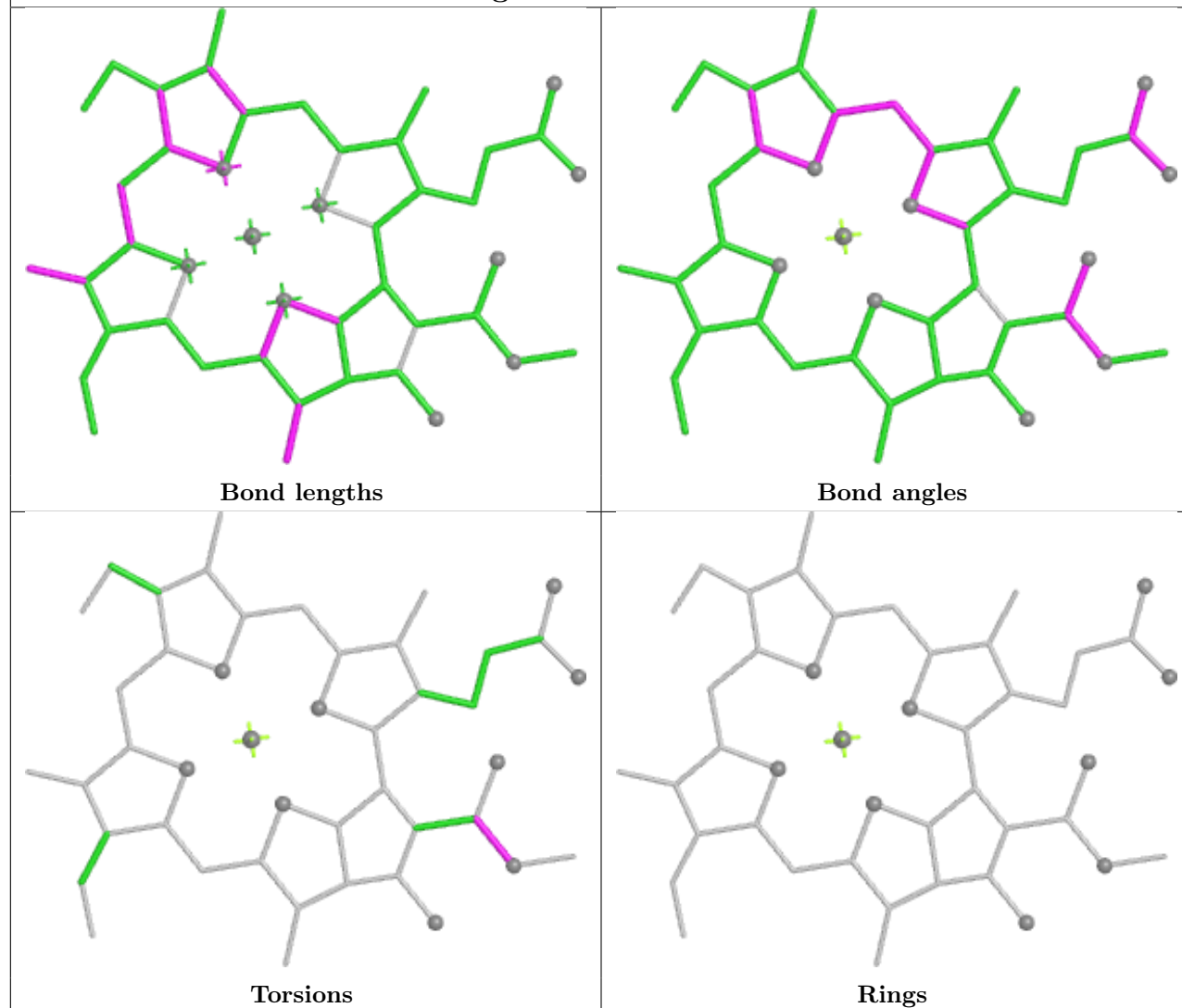


Ligand NEX F 303

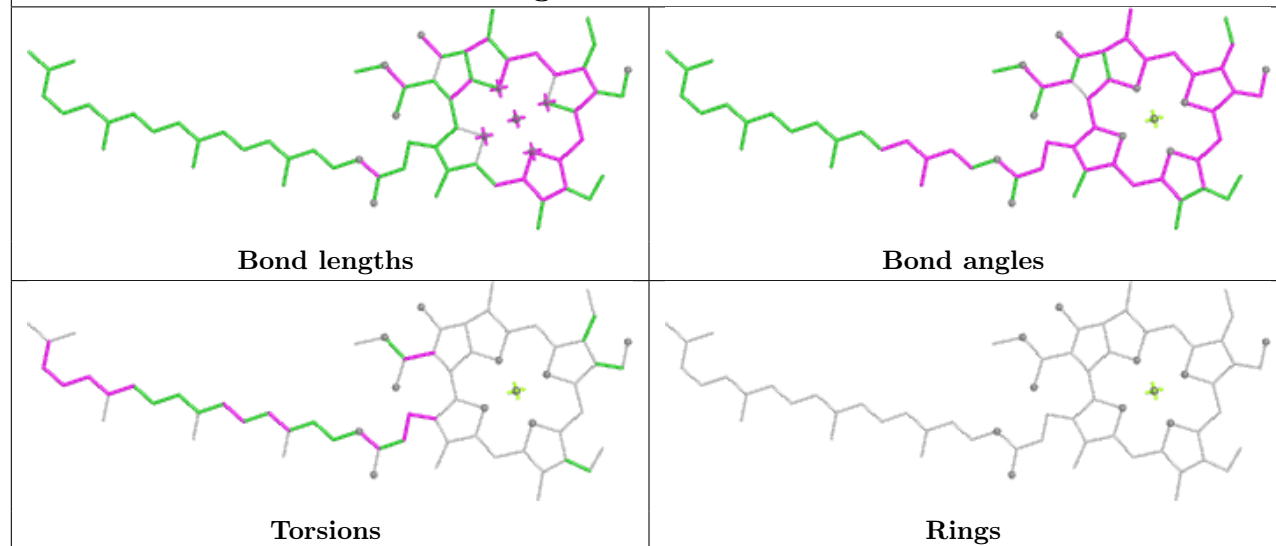


Ligand CHL C 311	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA E 314	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand OIE C 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

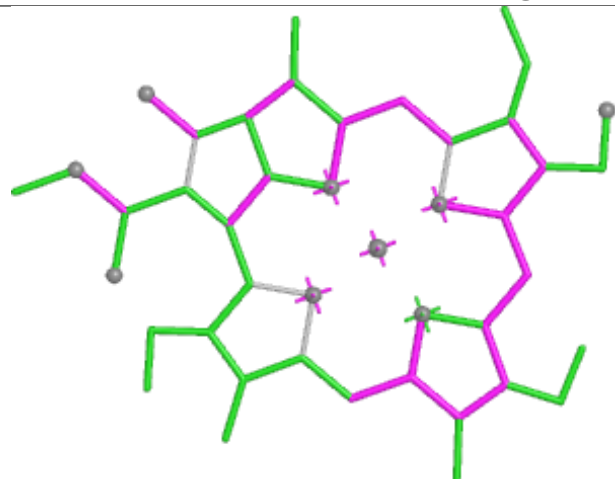
Ligand CLA D 316



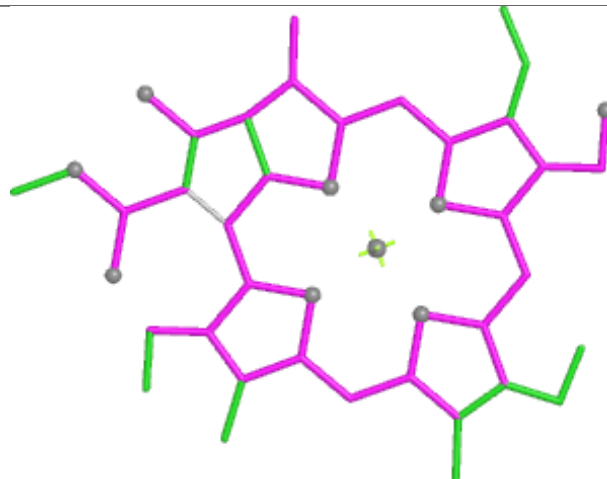
Ligand CHL E 304



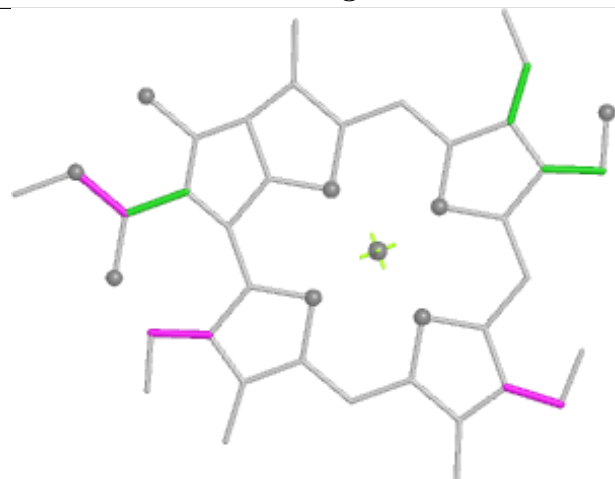
Ligand CHL E 309



Bond lengths



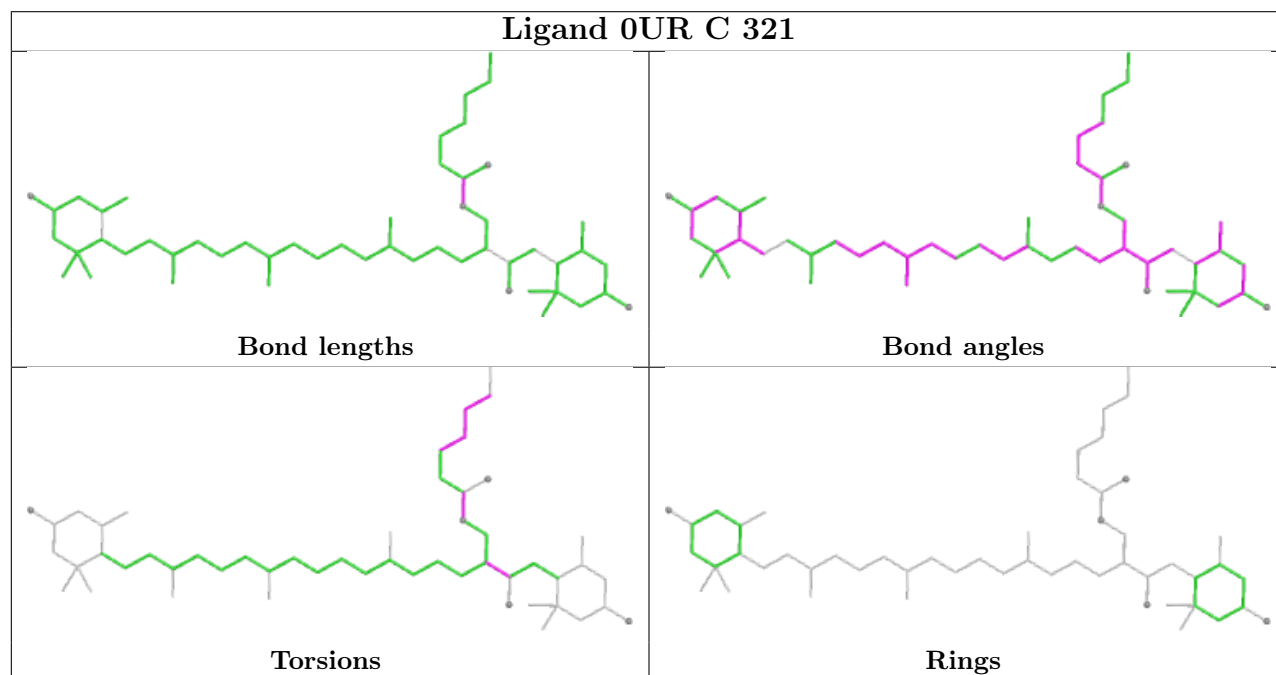
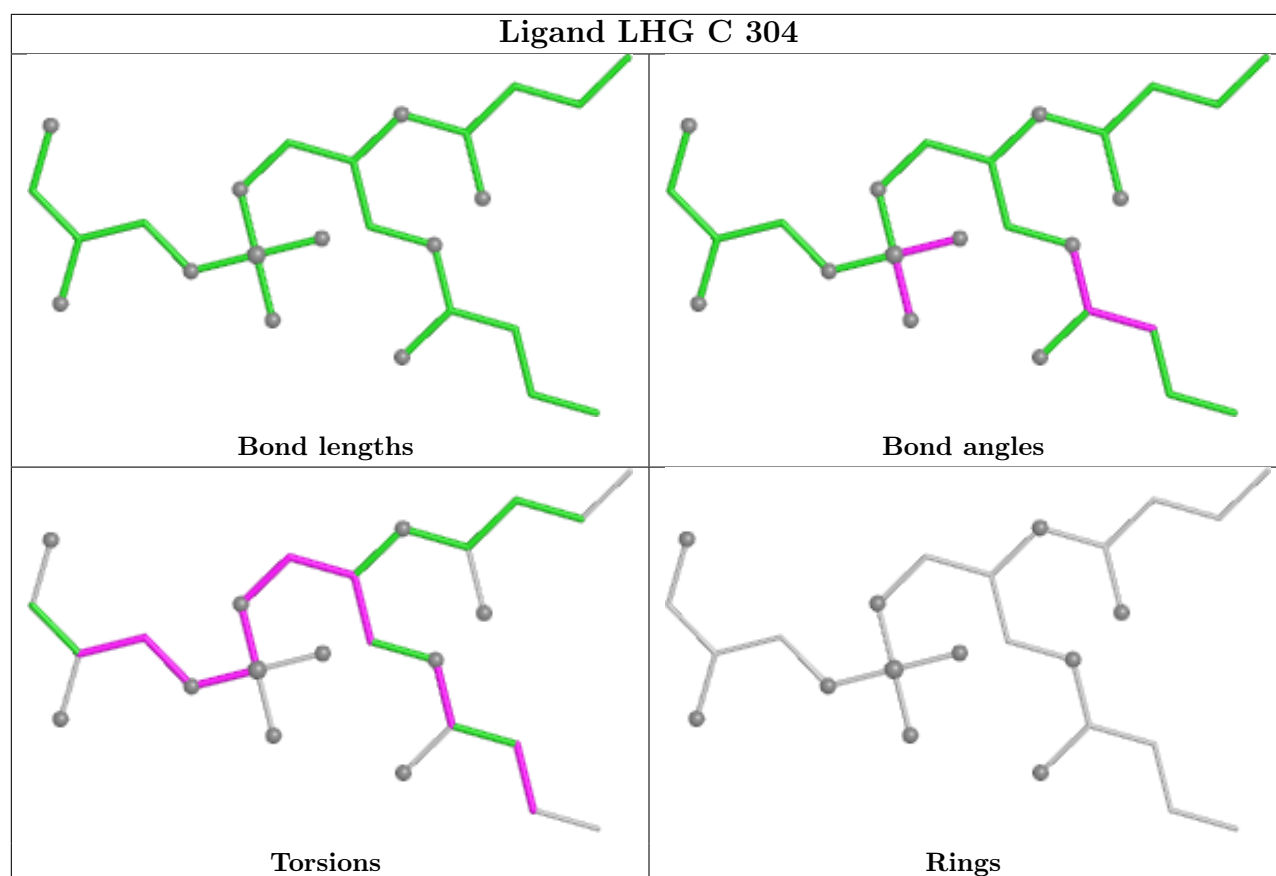
Bond angles



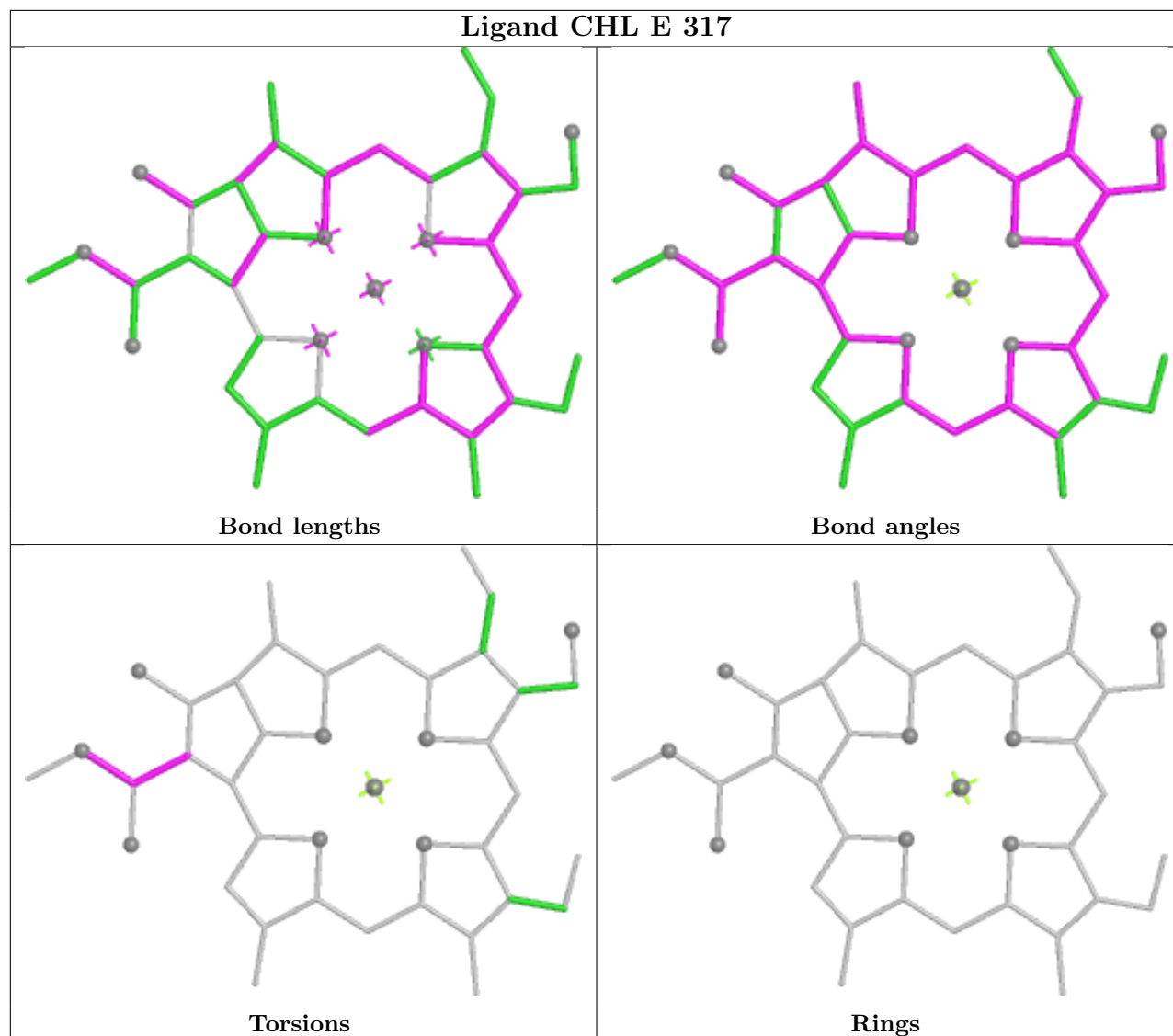
Torsions



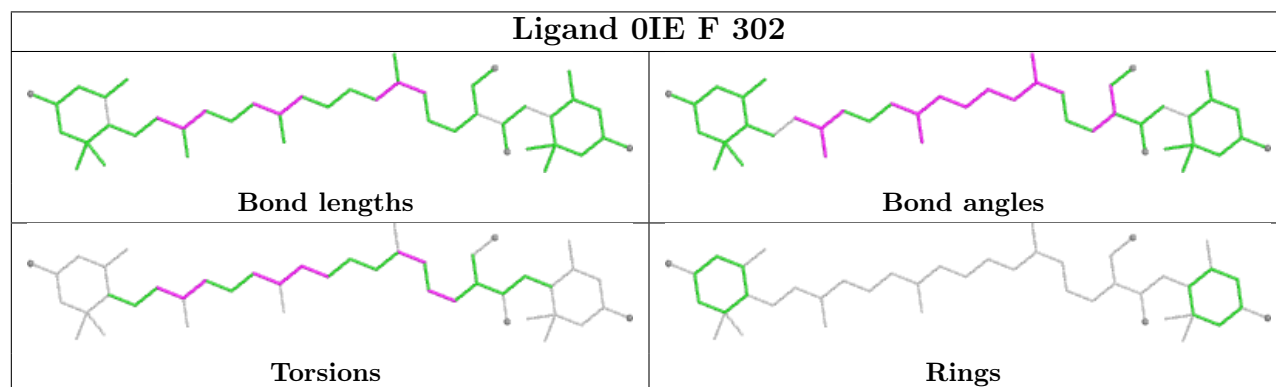
Rings

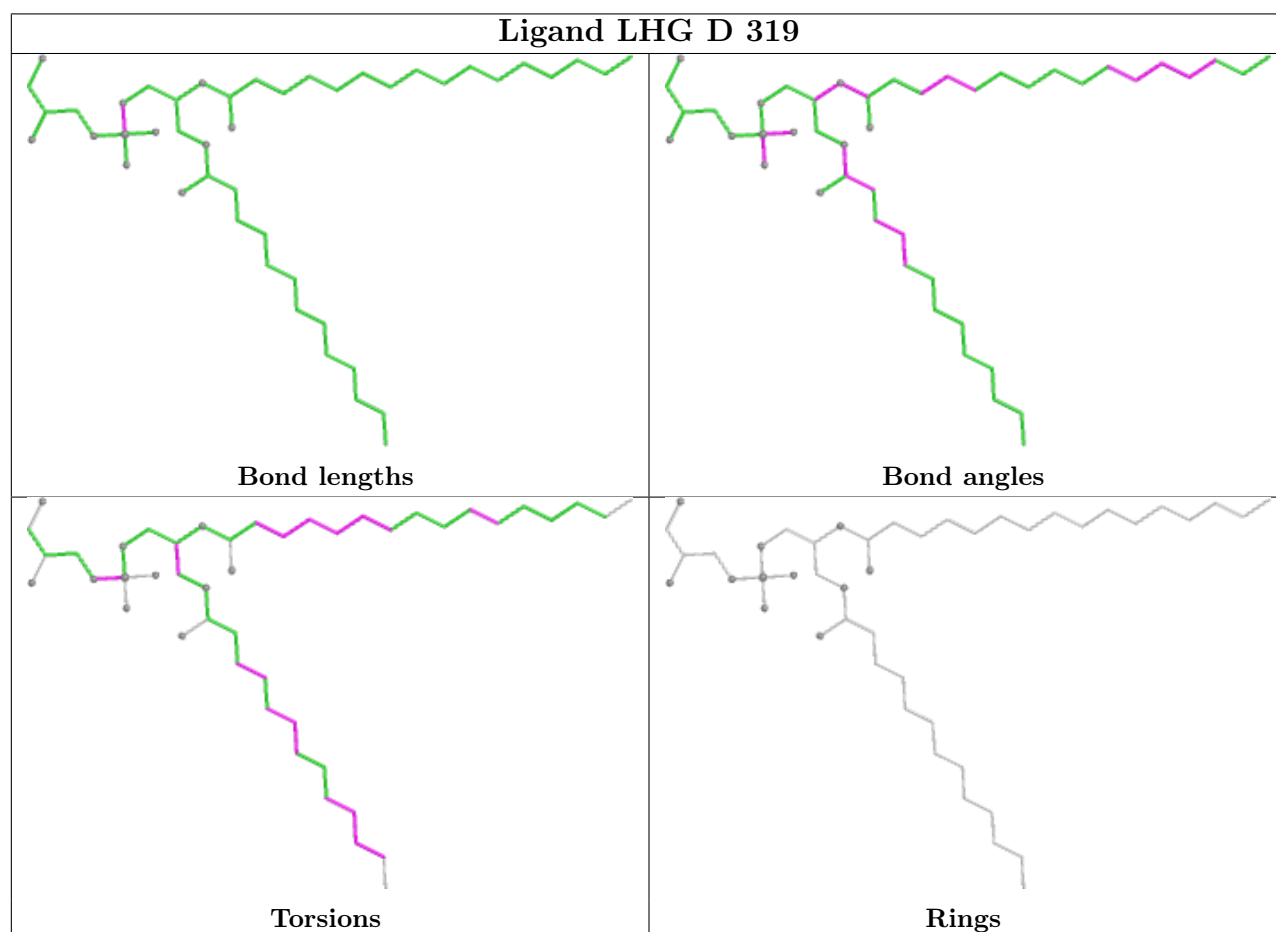
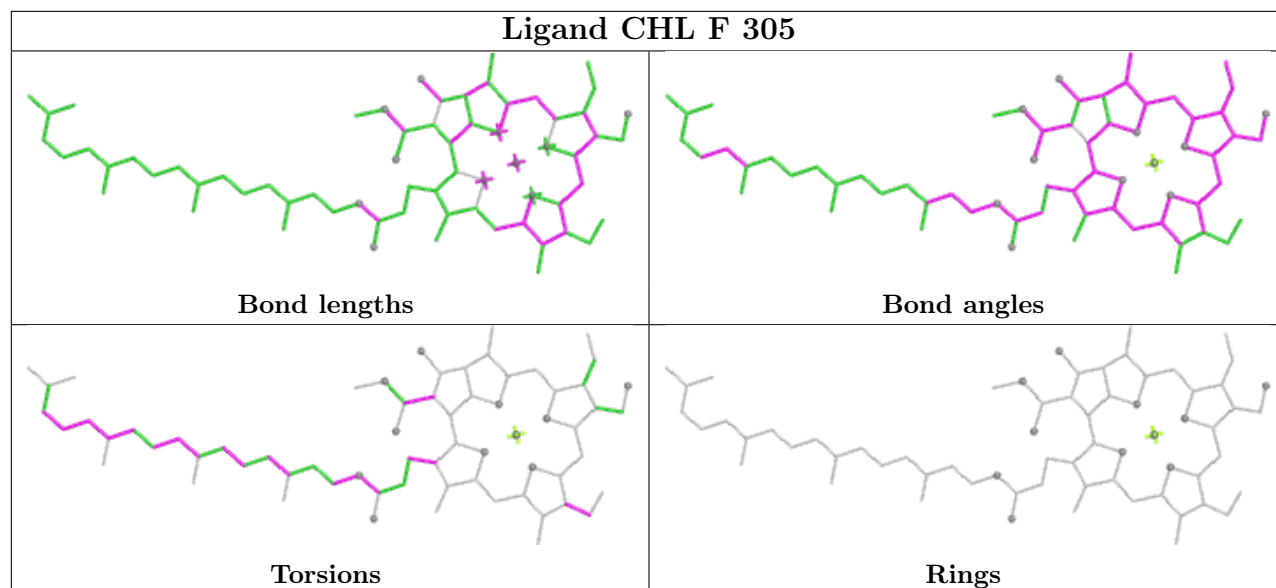


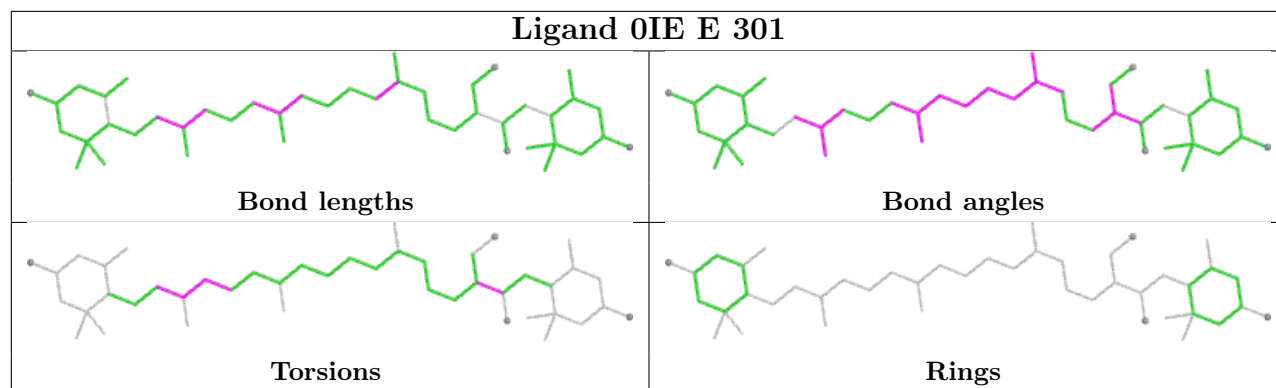
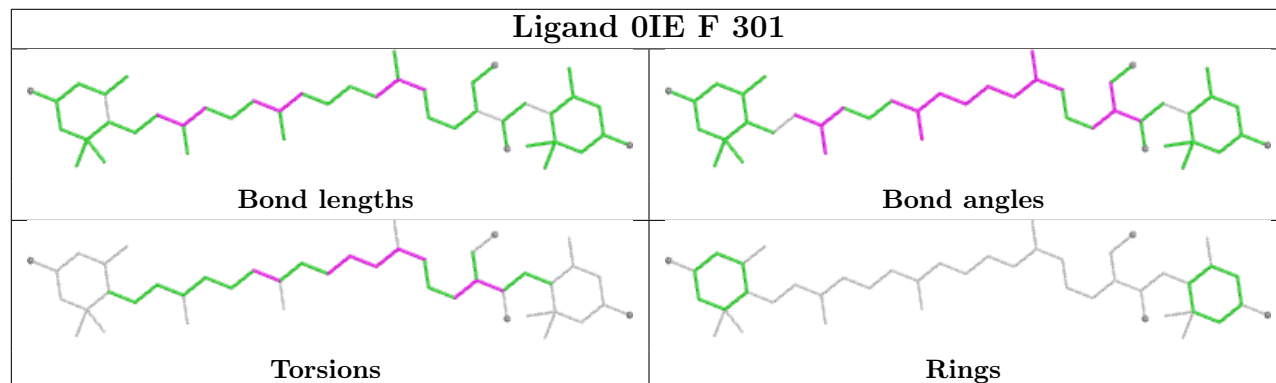
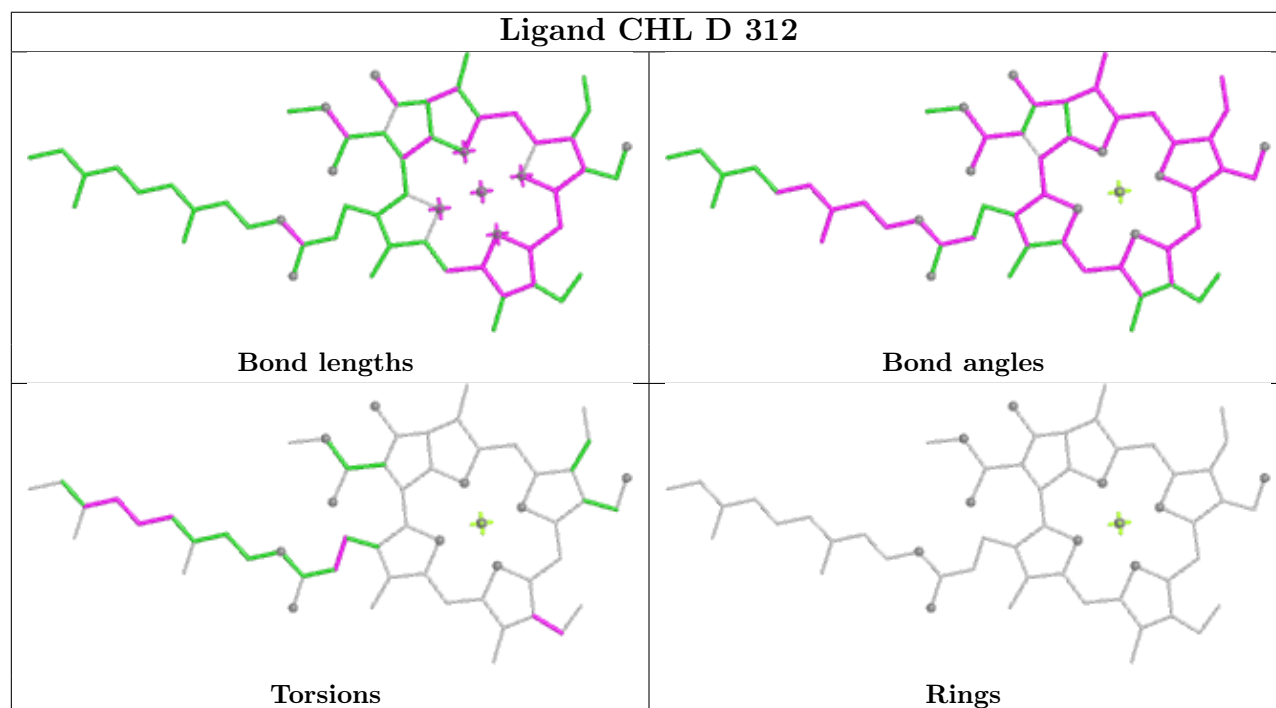
Ligand CHL E 317

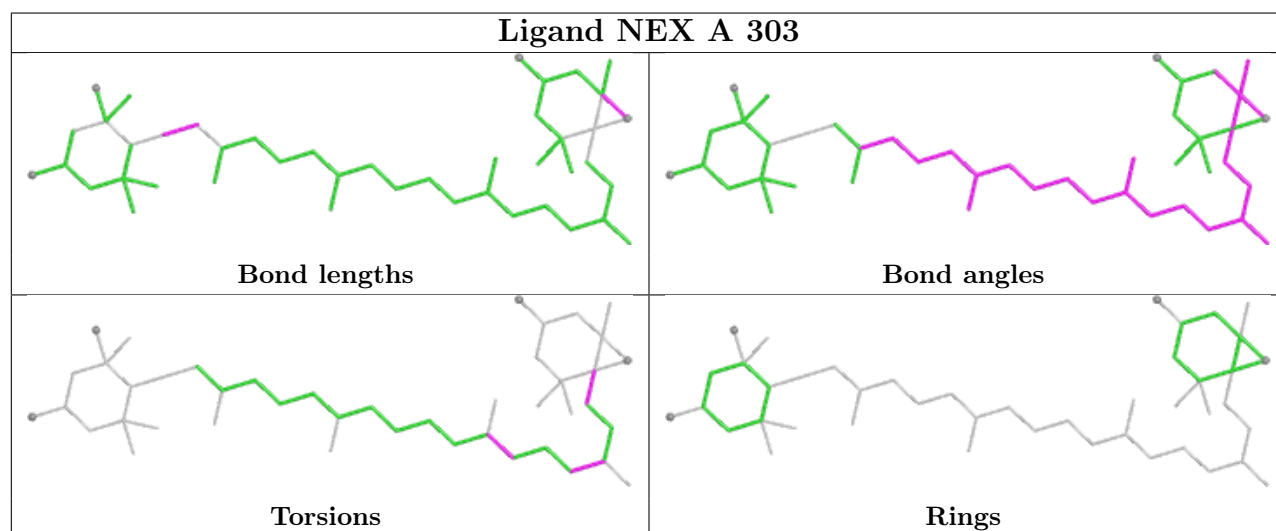
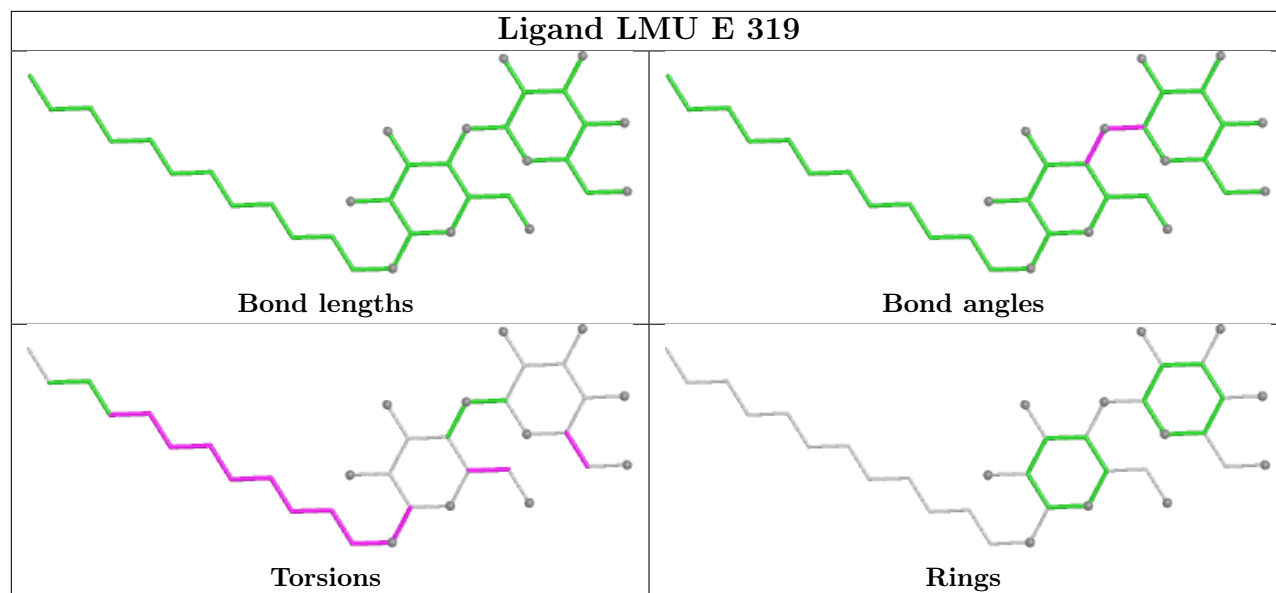


Ligand OIE F 302

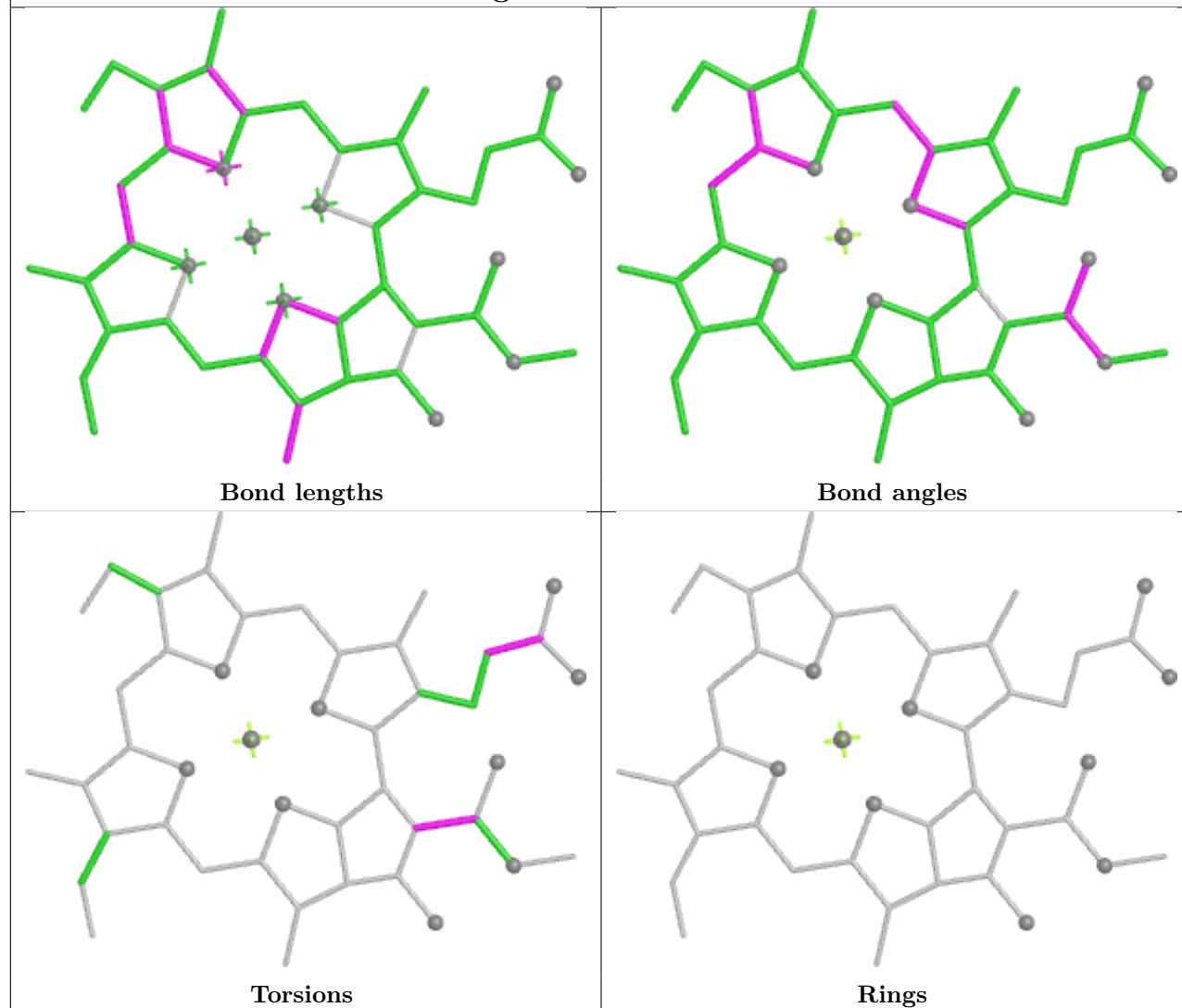




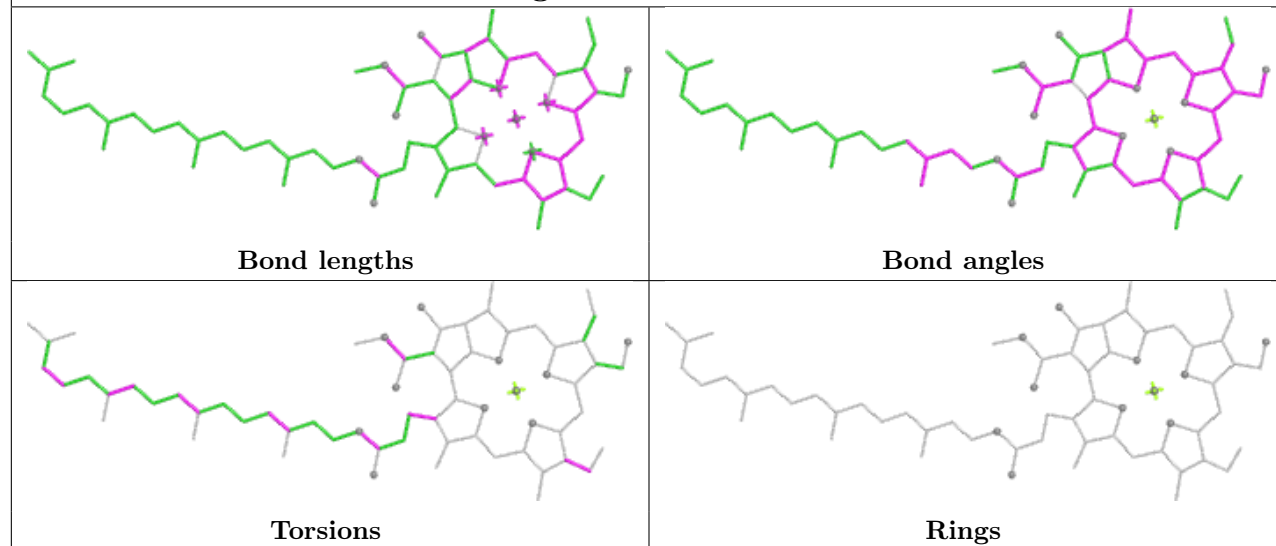
Ligand OIE E 301**Ligand OIE F 301****Ligand CHL D 312**

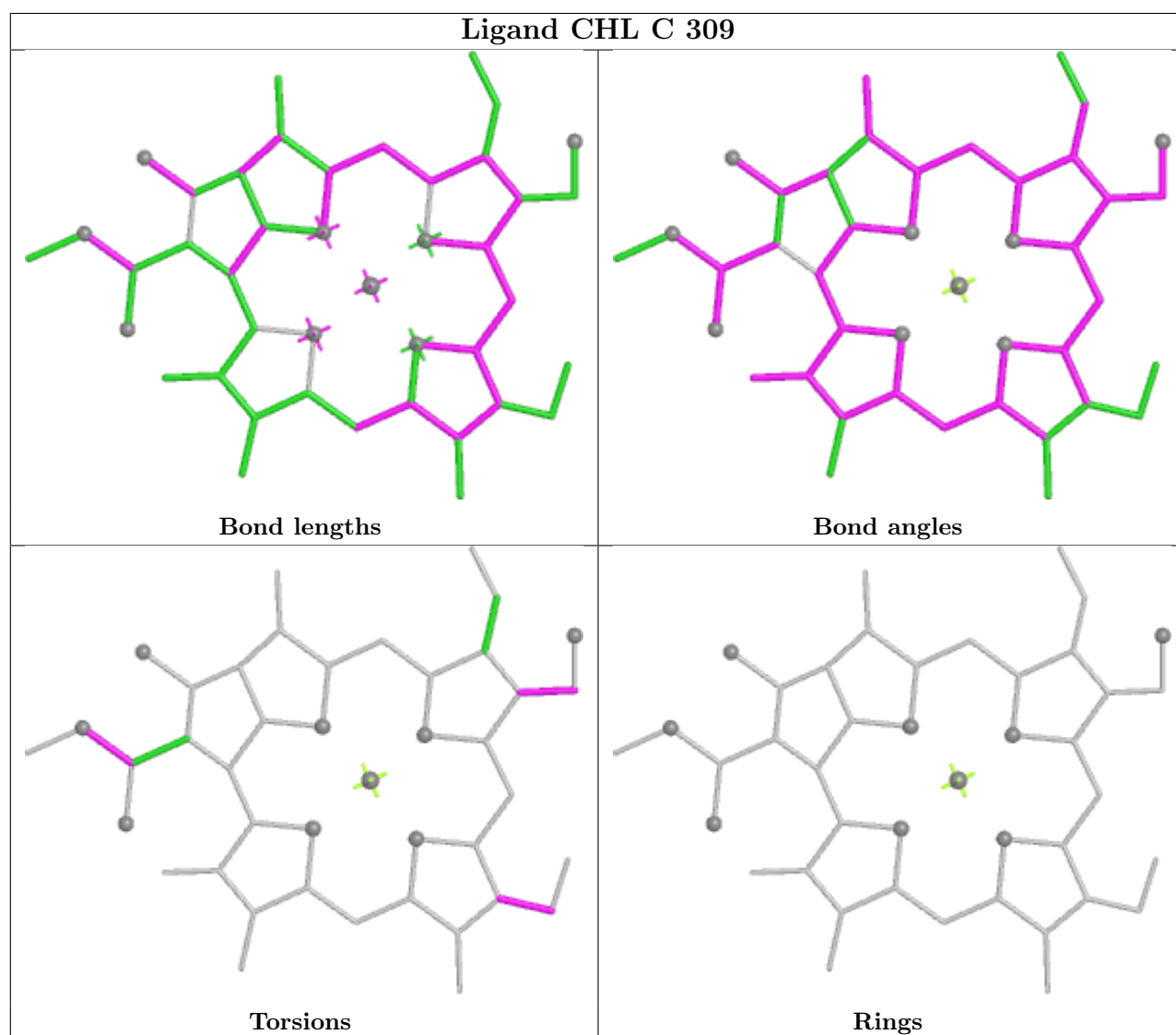
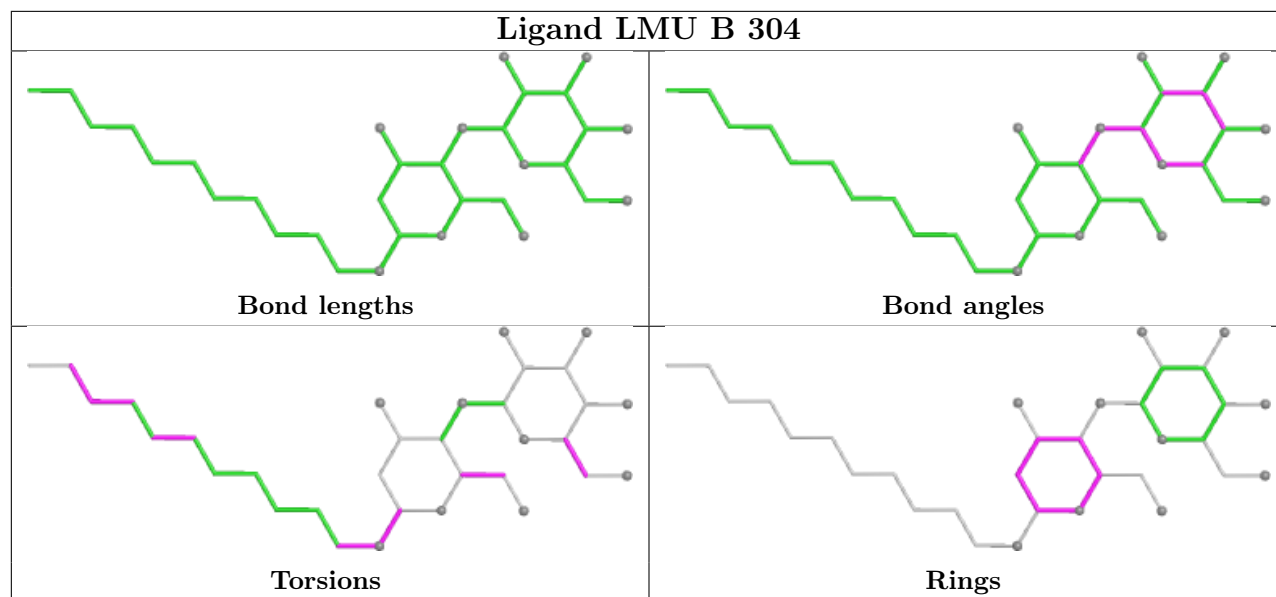


Ligand CLA C 316

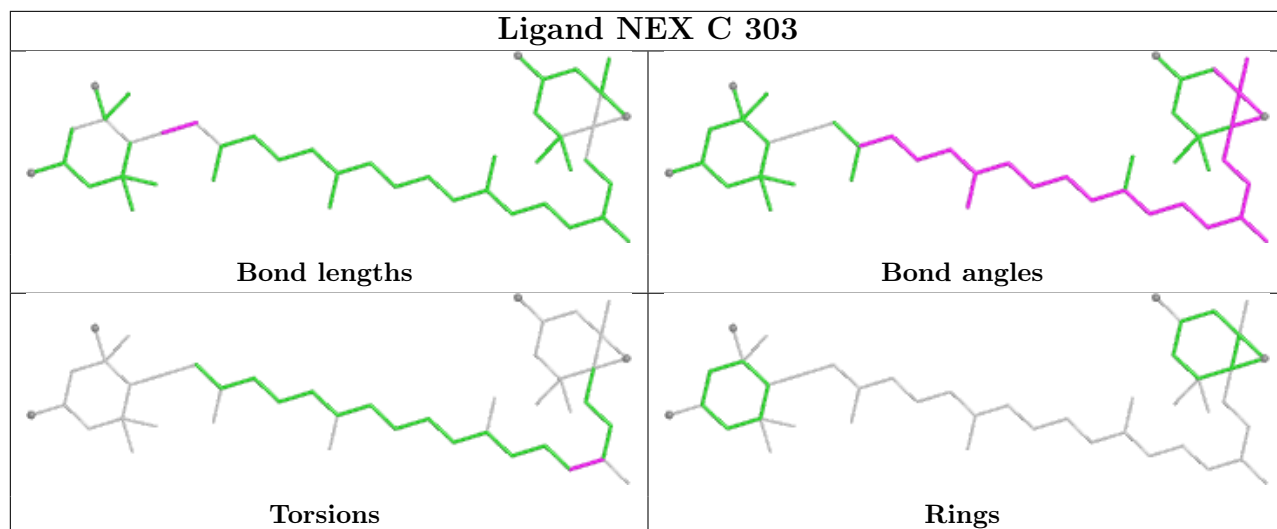


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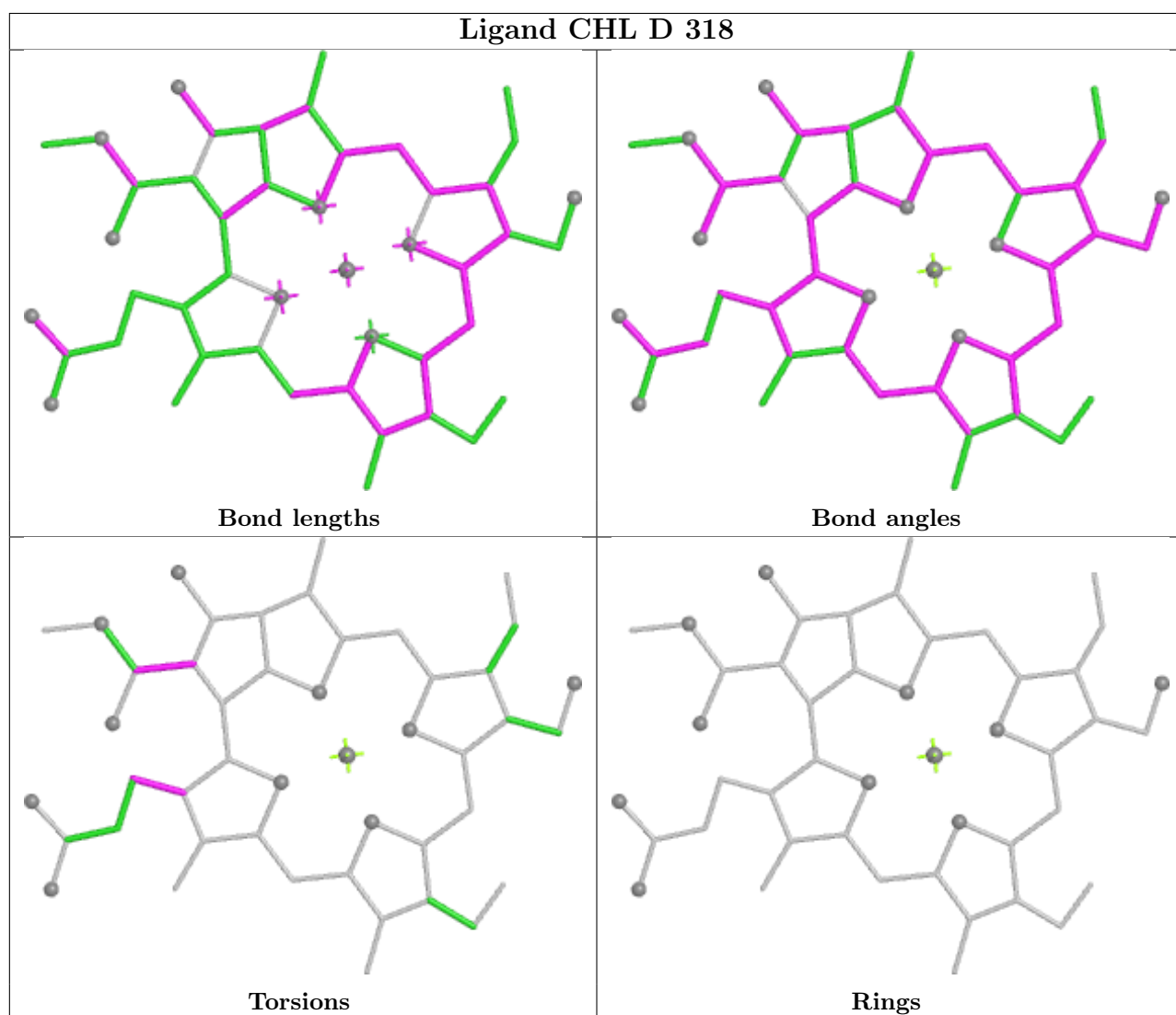


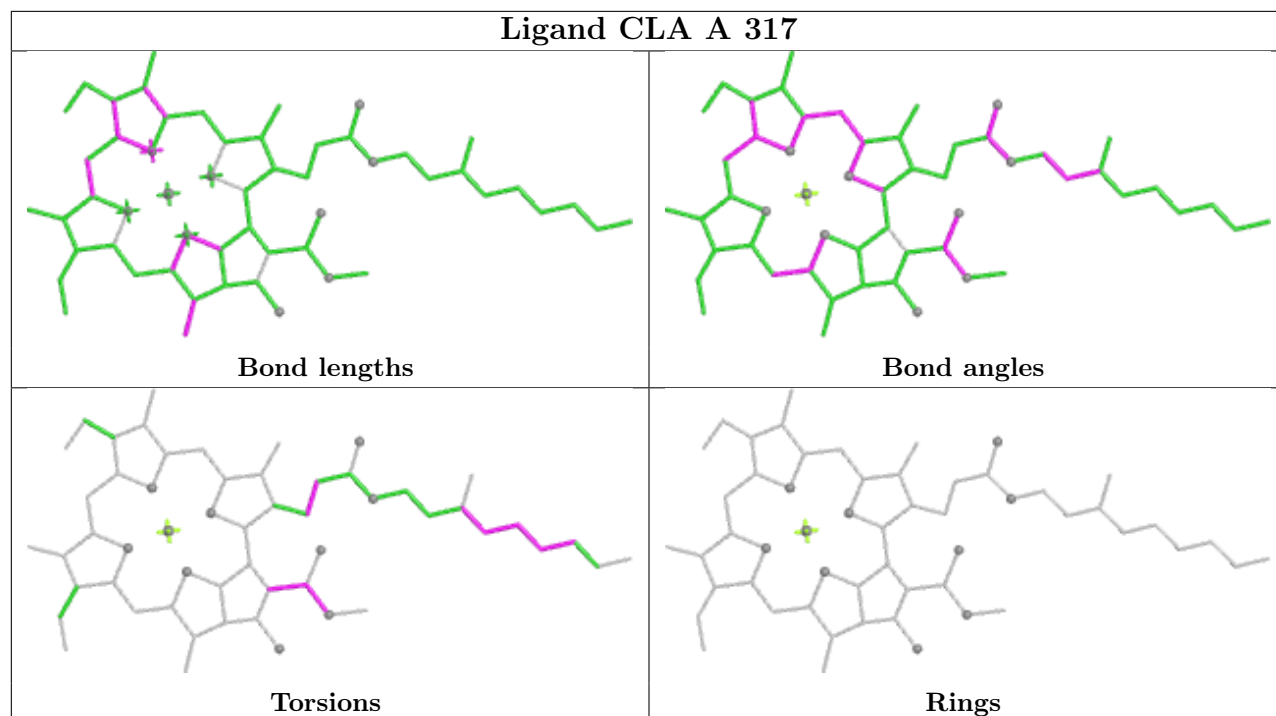


Ligand NEX C 303

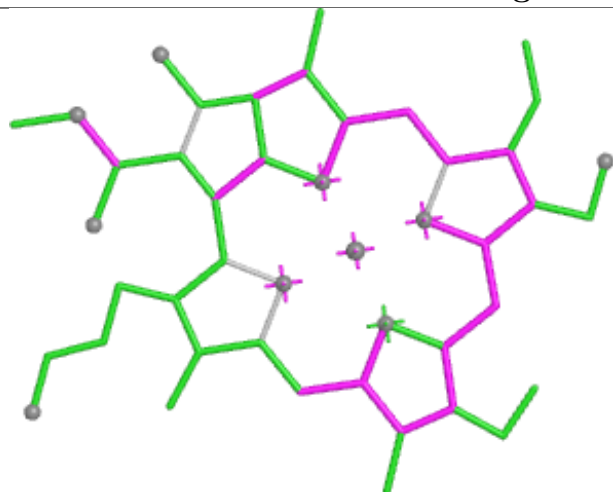


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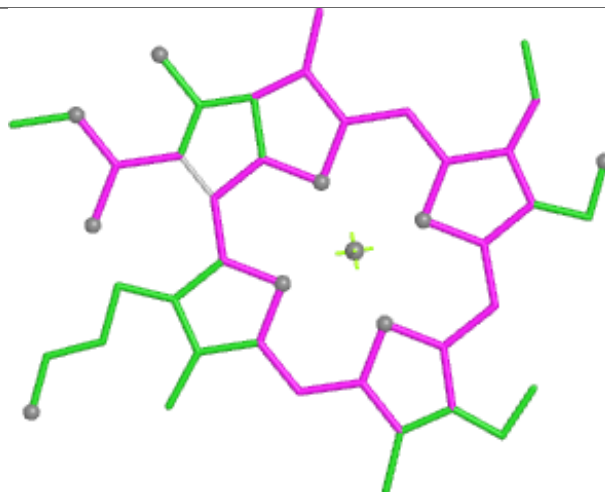




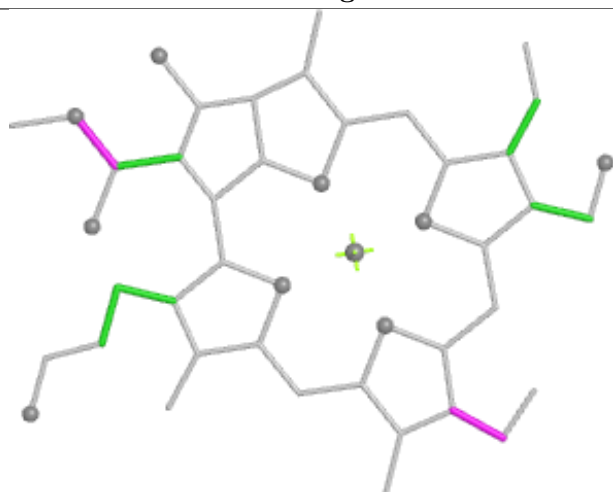
Ligand CHL D 310



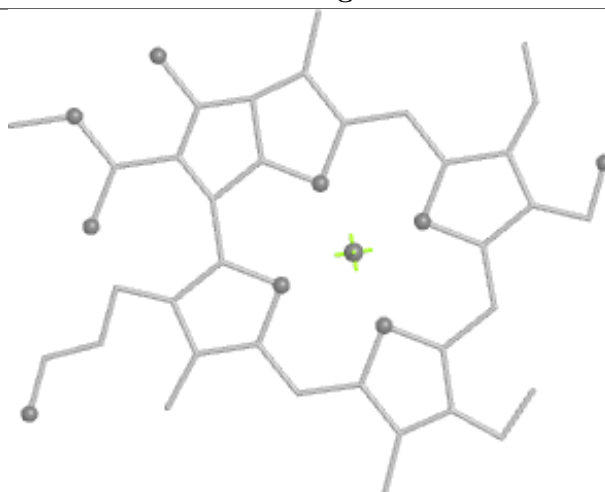
Bond lengths



Bond angles

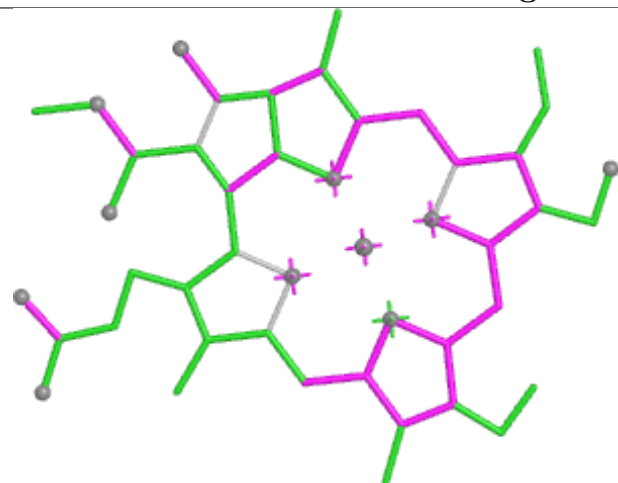


Torsions

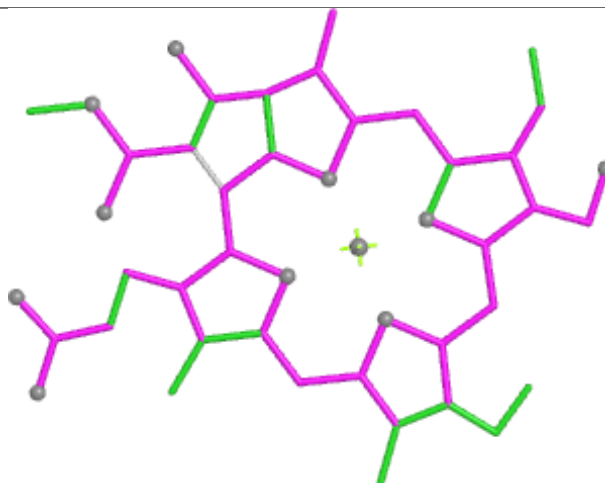


Rings

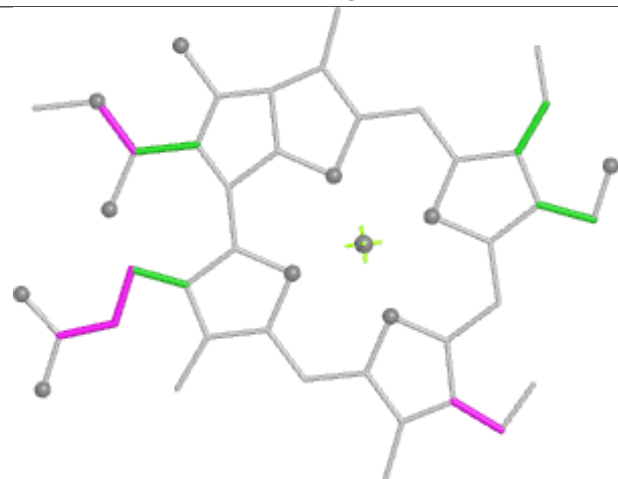
Ligand CHL F 317



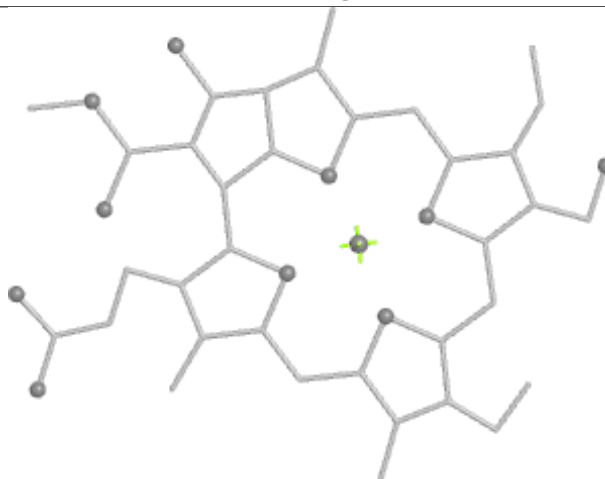
Bond lengths



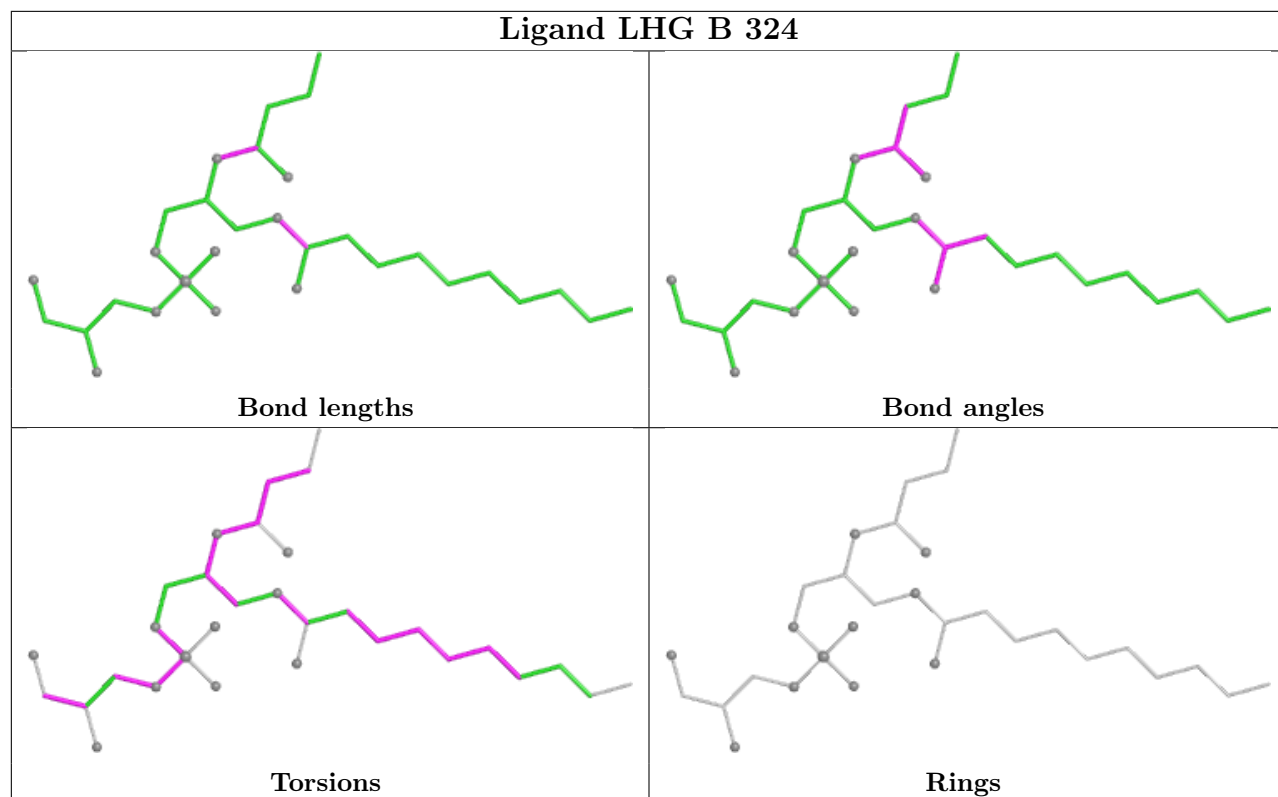
Bond angles



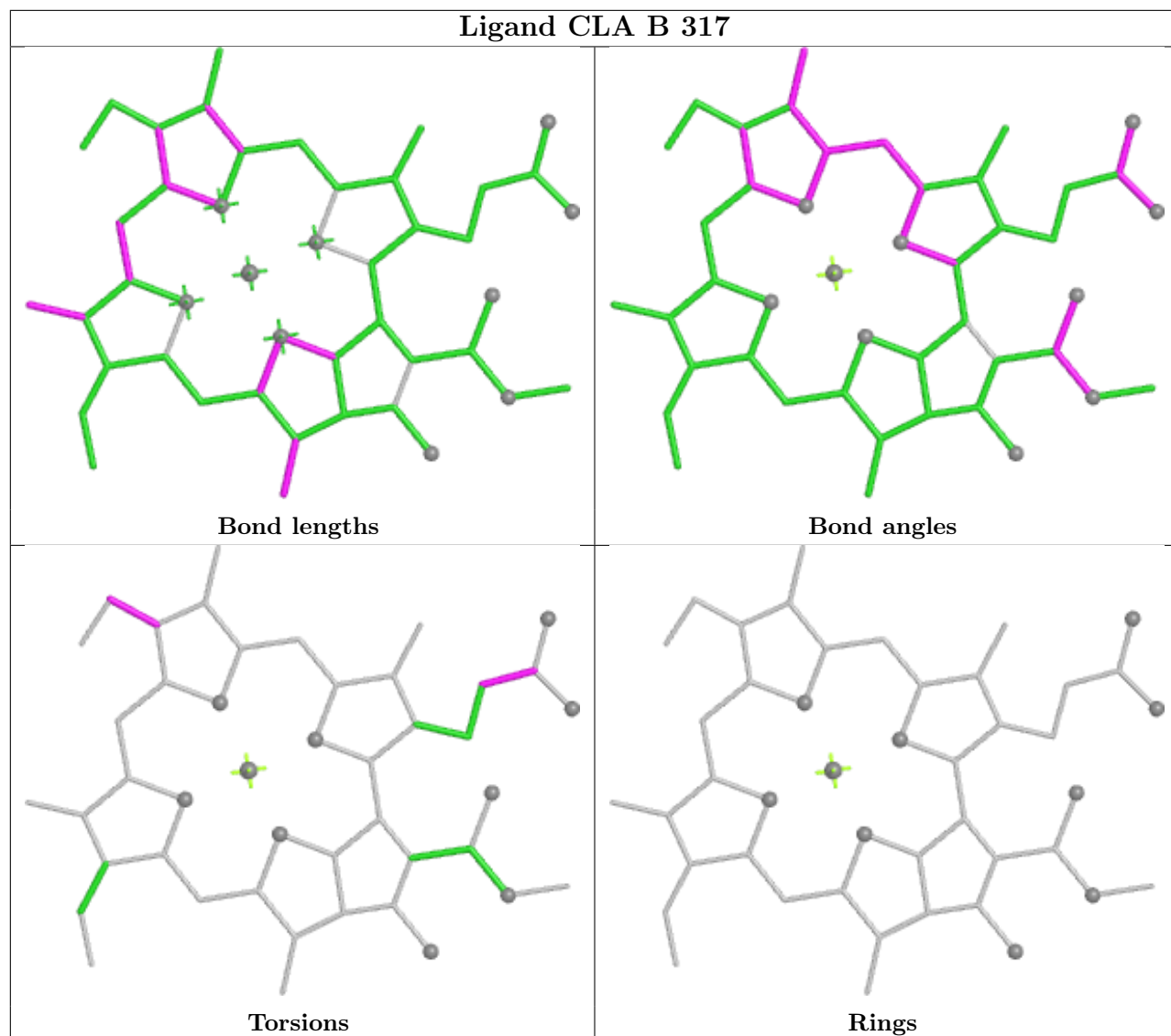
Torsions



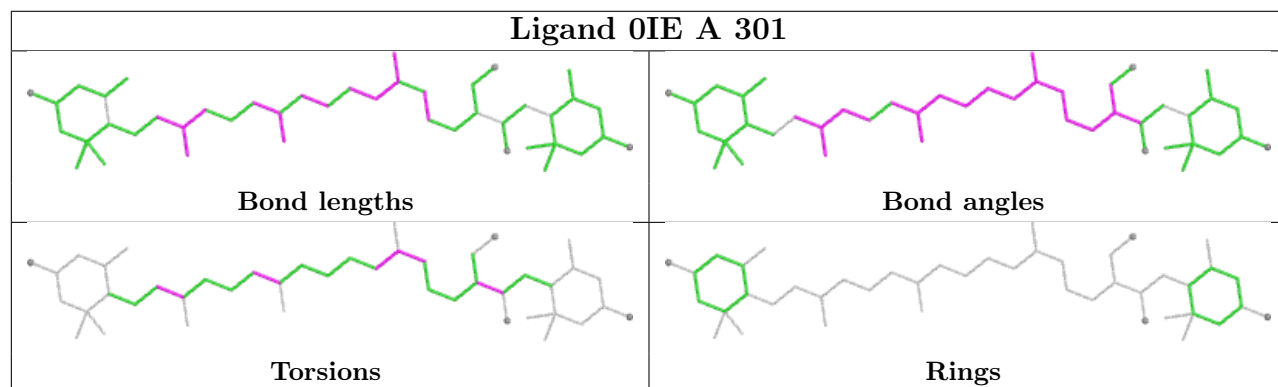
Rings



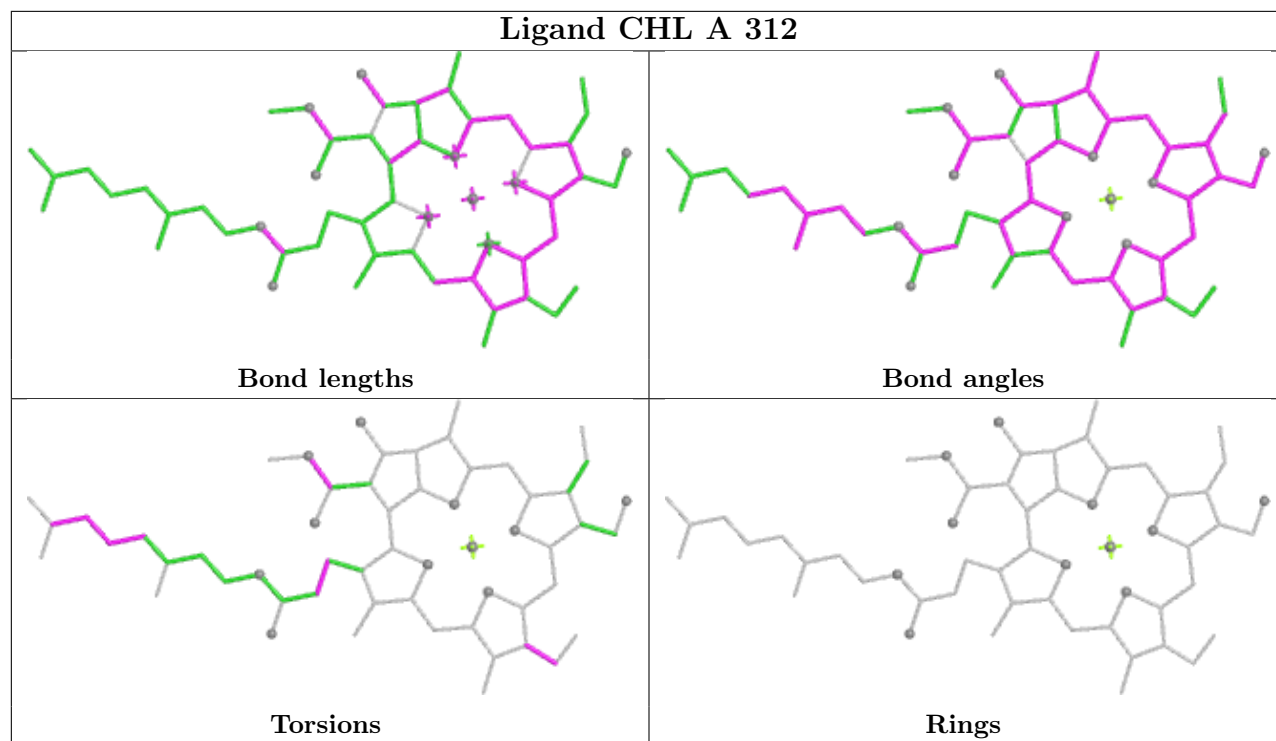
Ligand CLA B 317



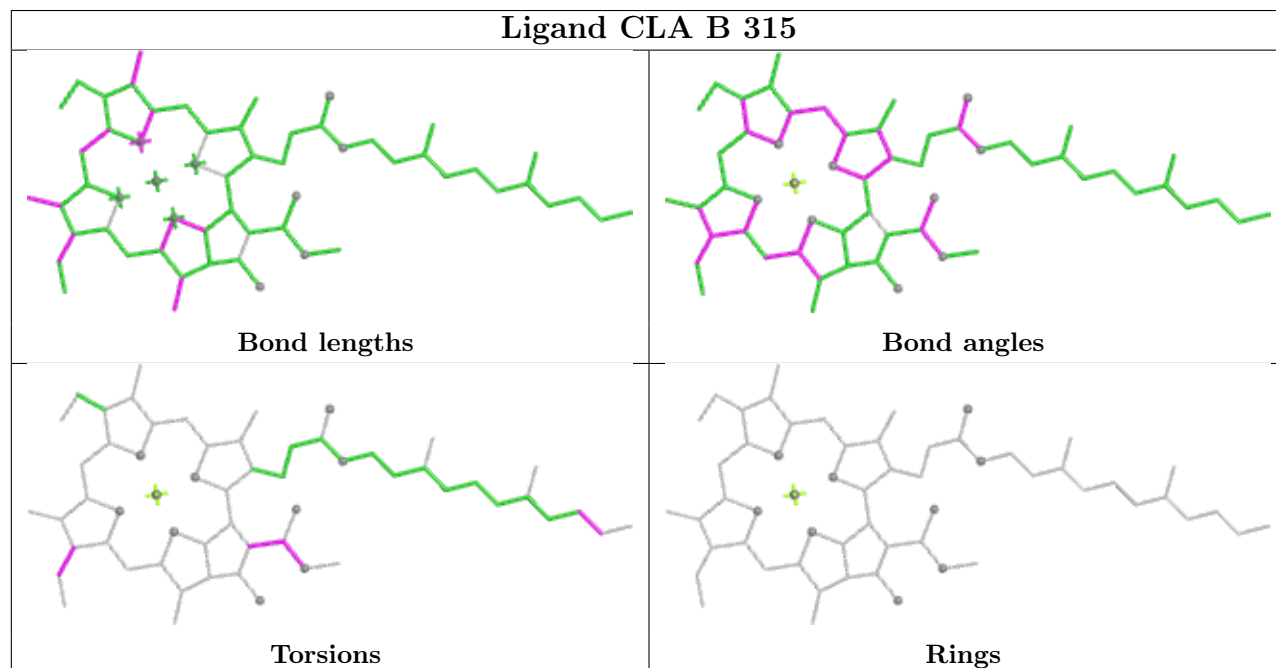
Ligand OIE A 301



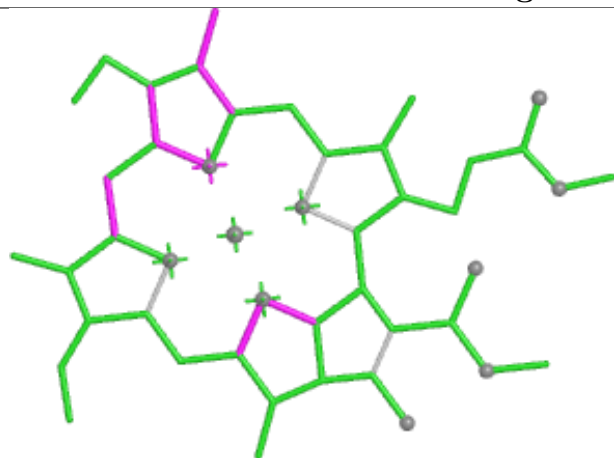
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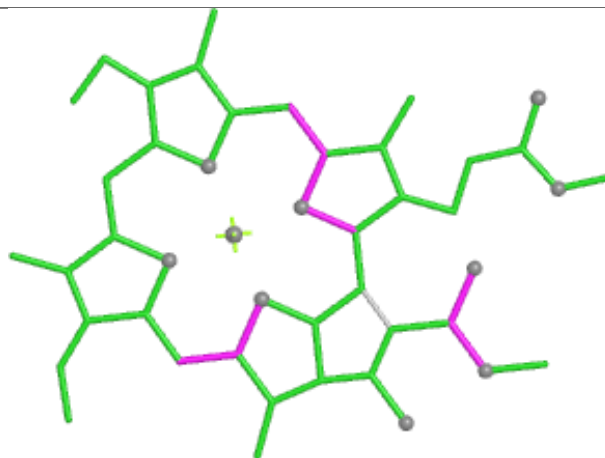
Ligand CLA B 315



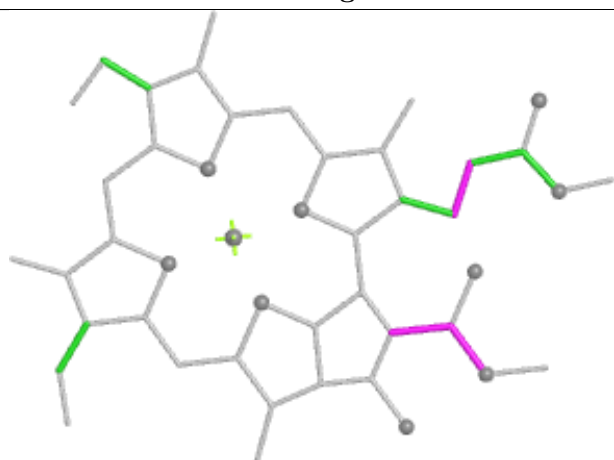
Ligand CLA F 307



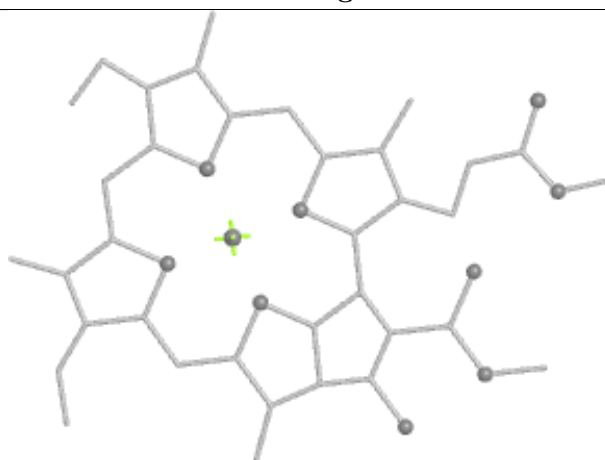
Bond lengths



Bond angles

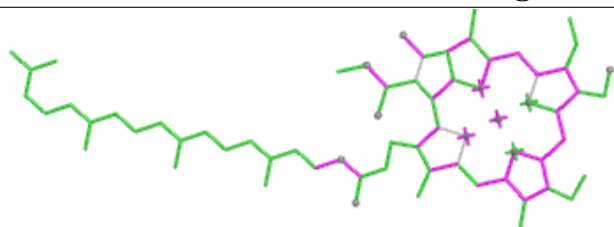


Torsions

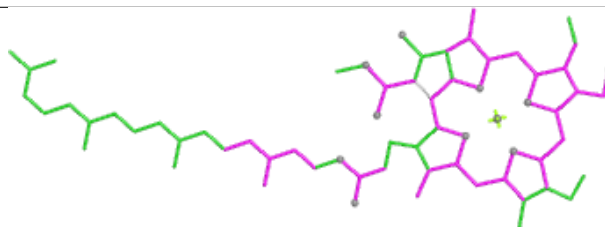


Rings

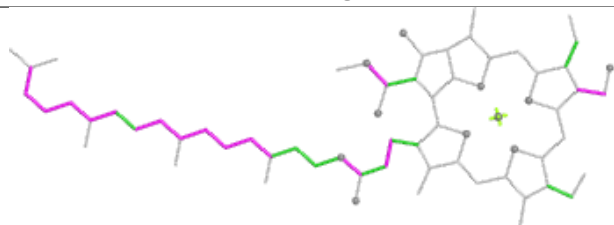
Ligand CHL C 305



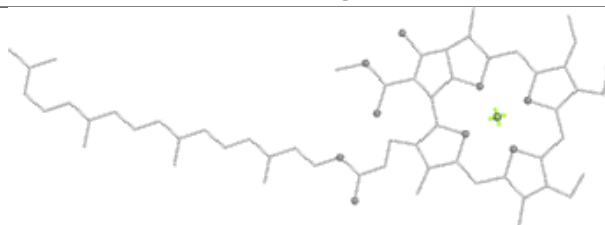
Bond lengths



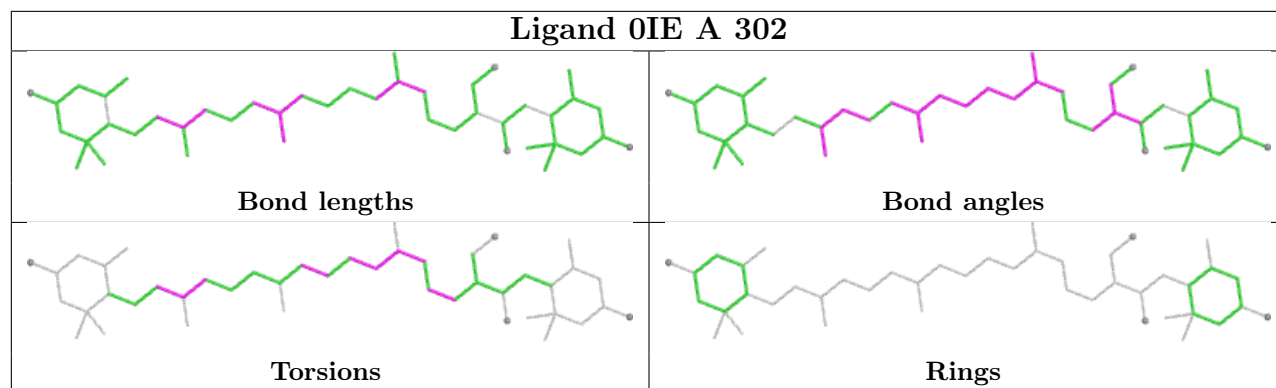
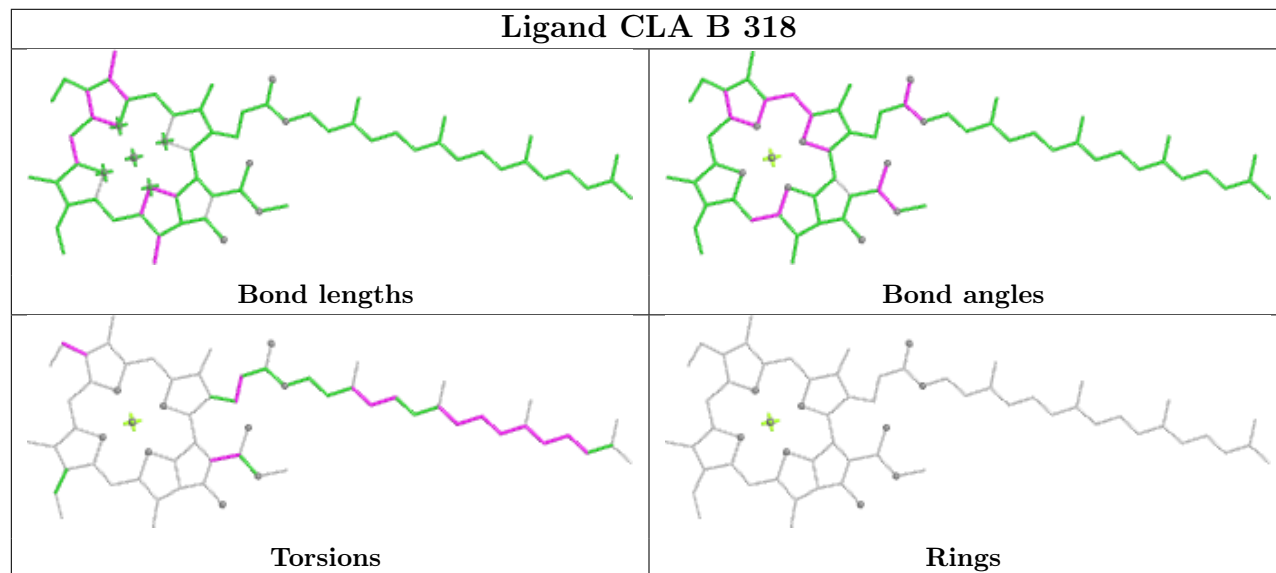
Bond angles



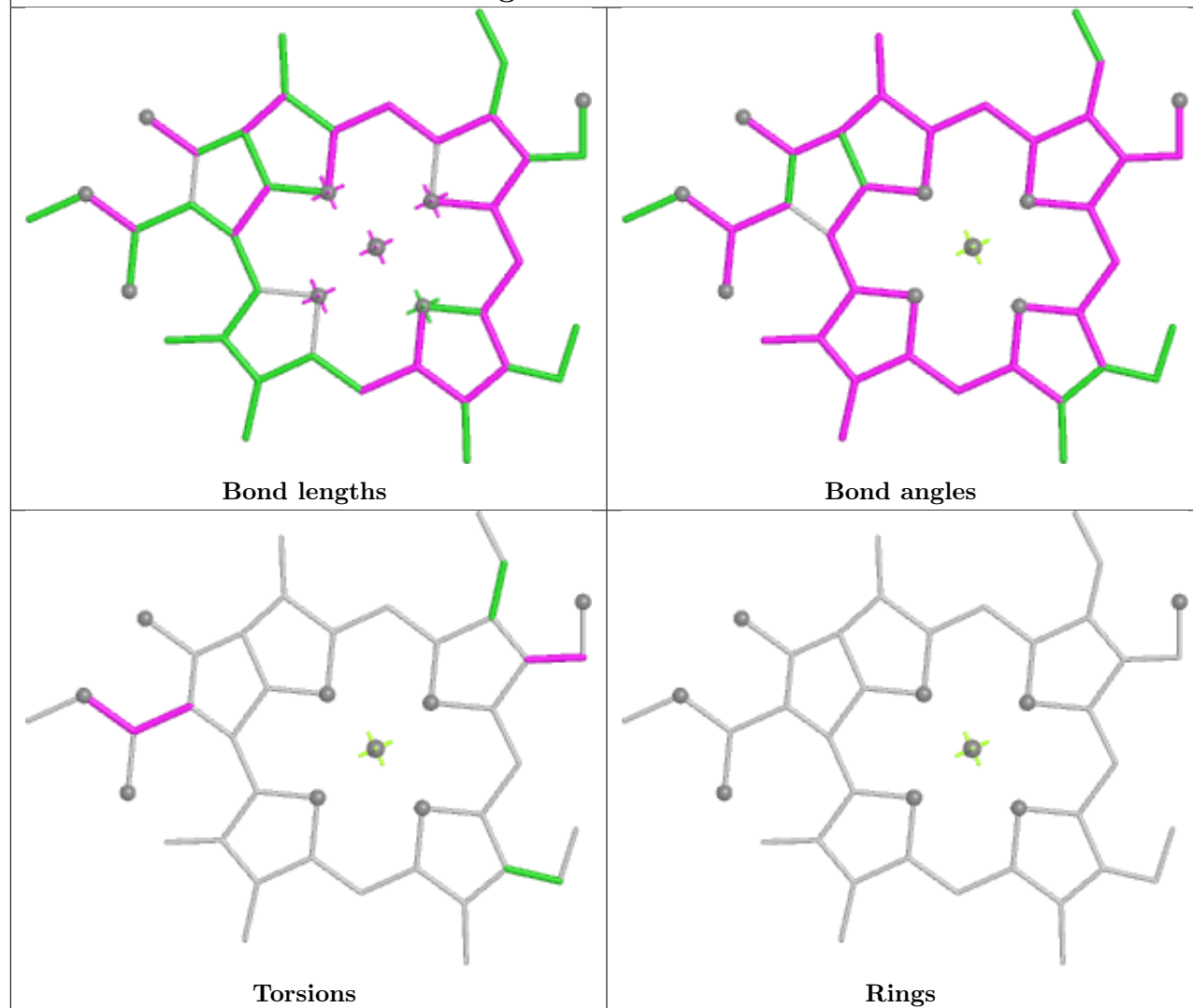
Torsions



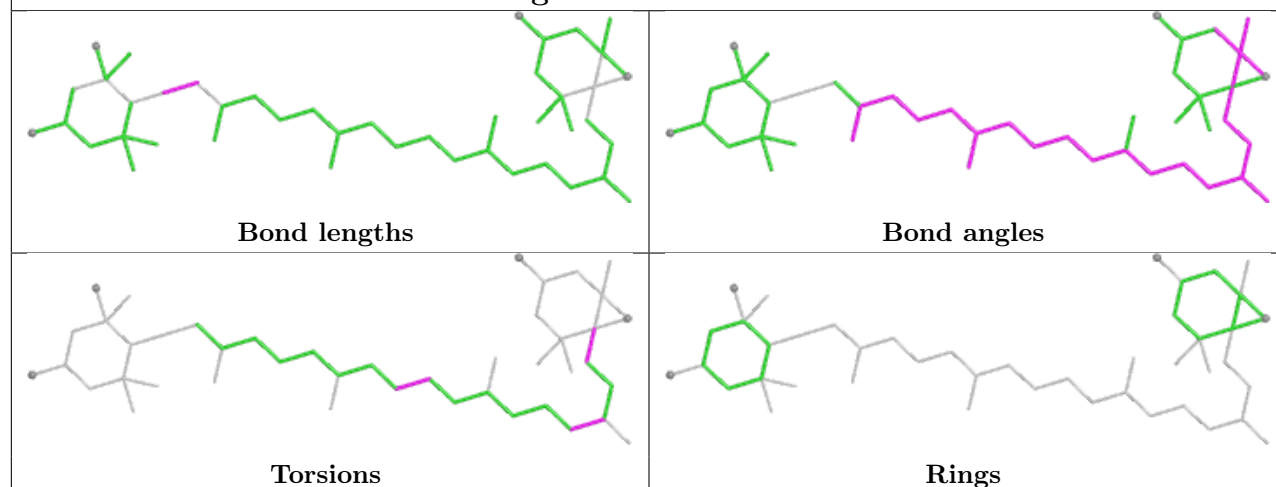
Rings

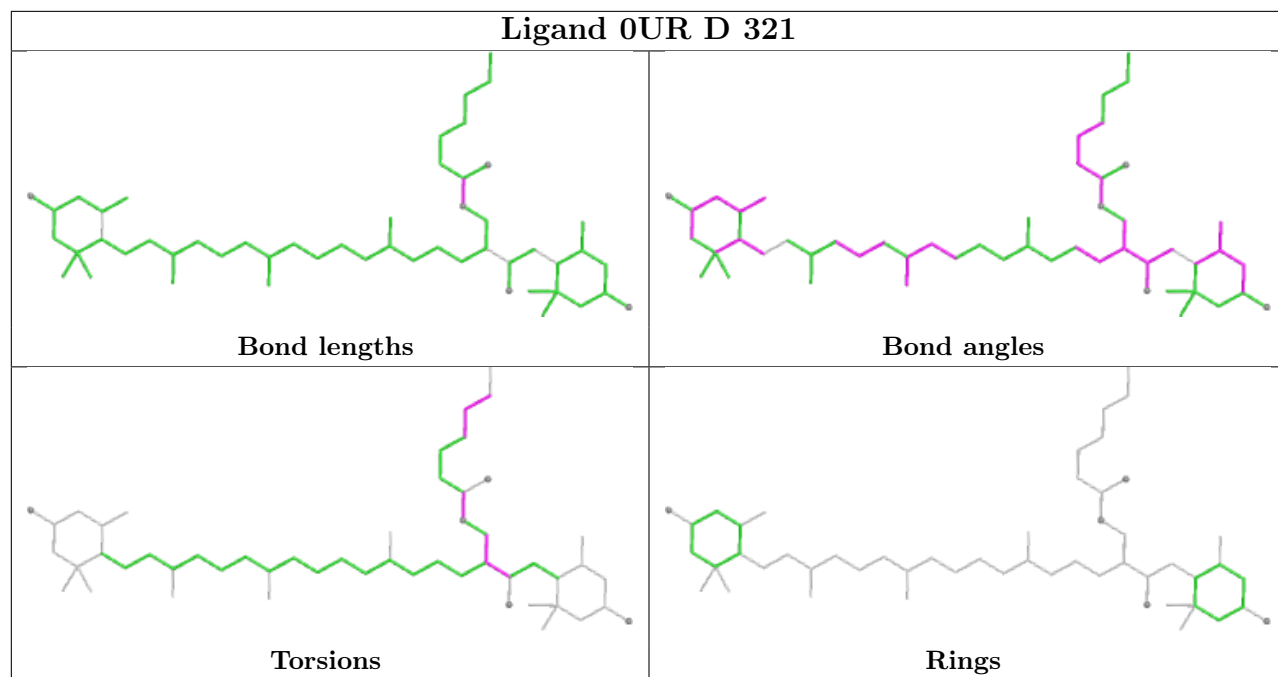
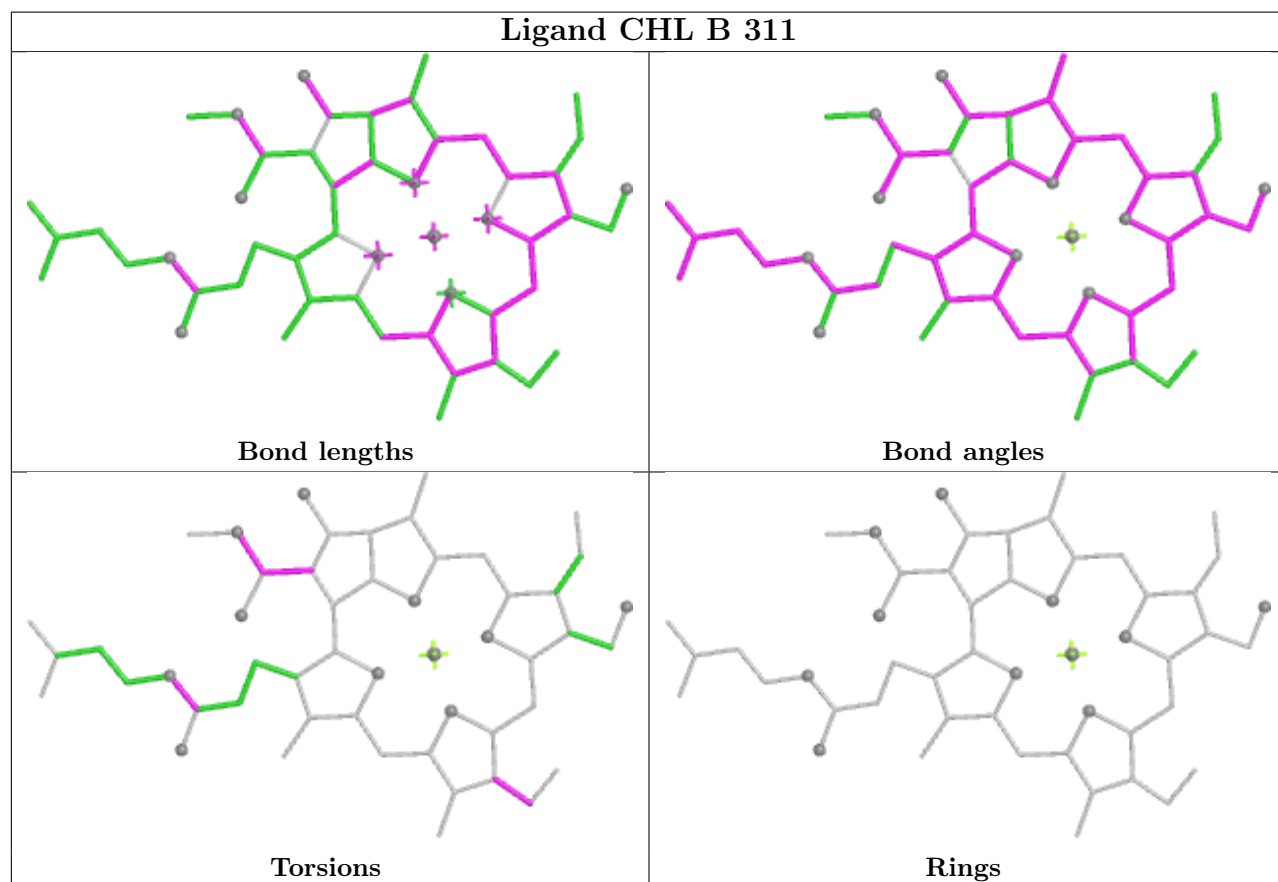
Ligand 0IE A 302**Ligand CLA B 318**

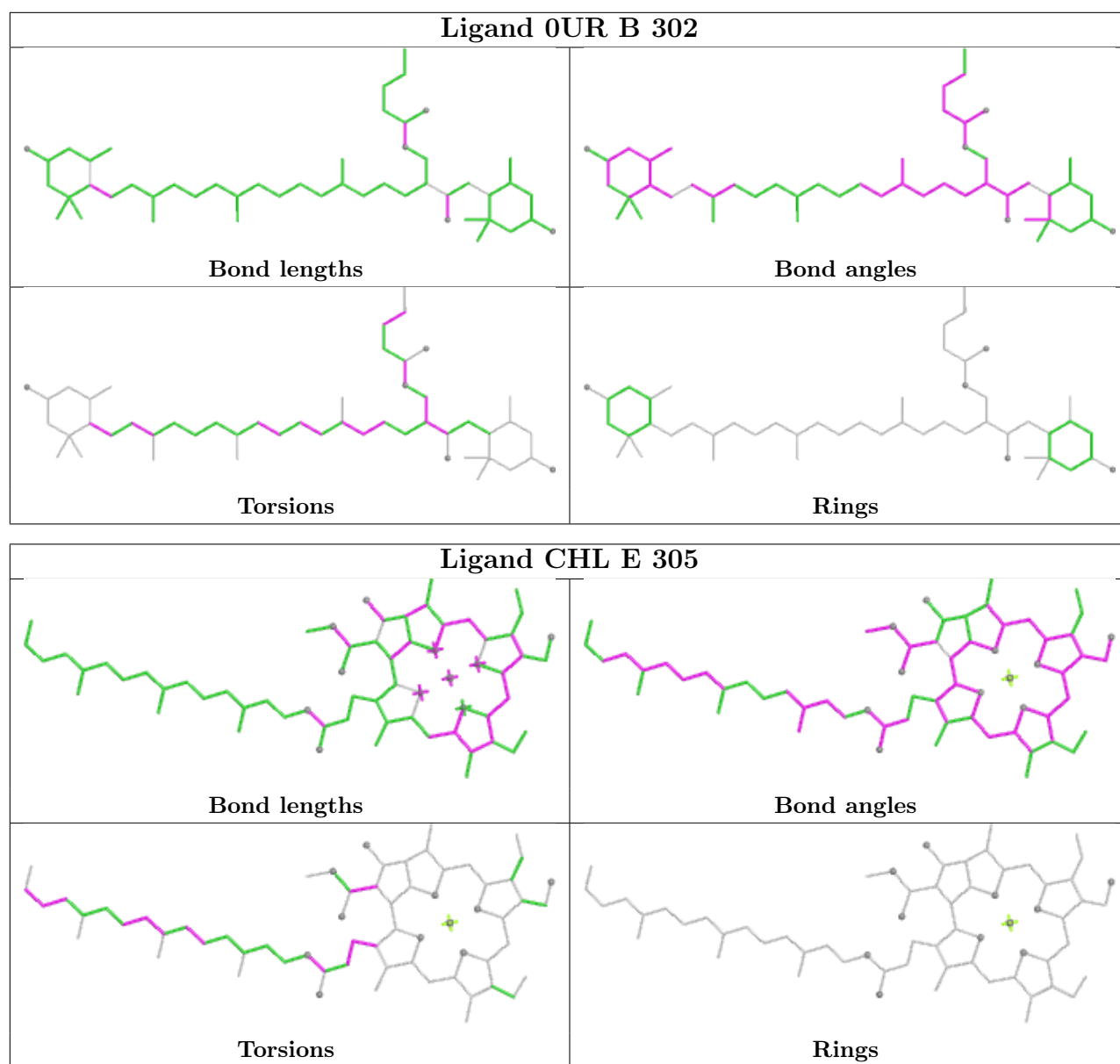
Ligand CHL F 309

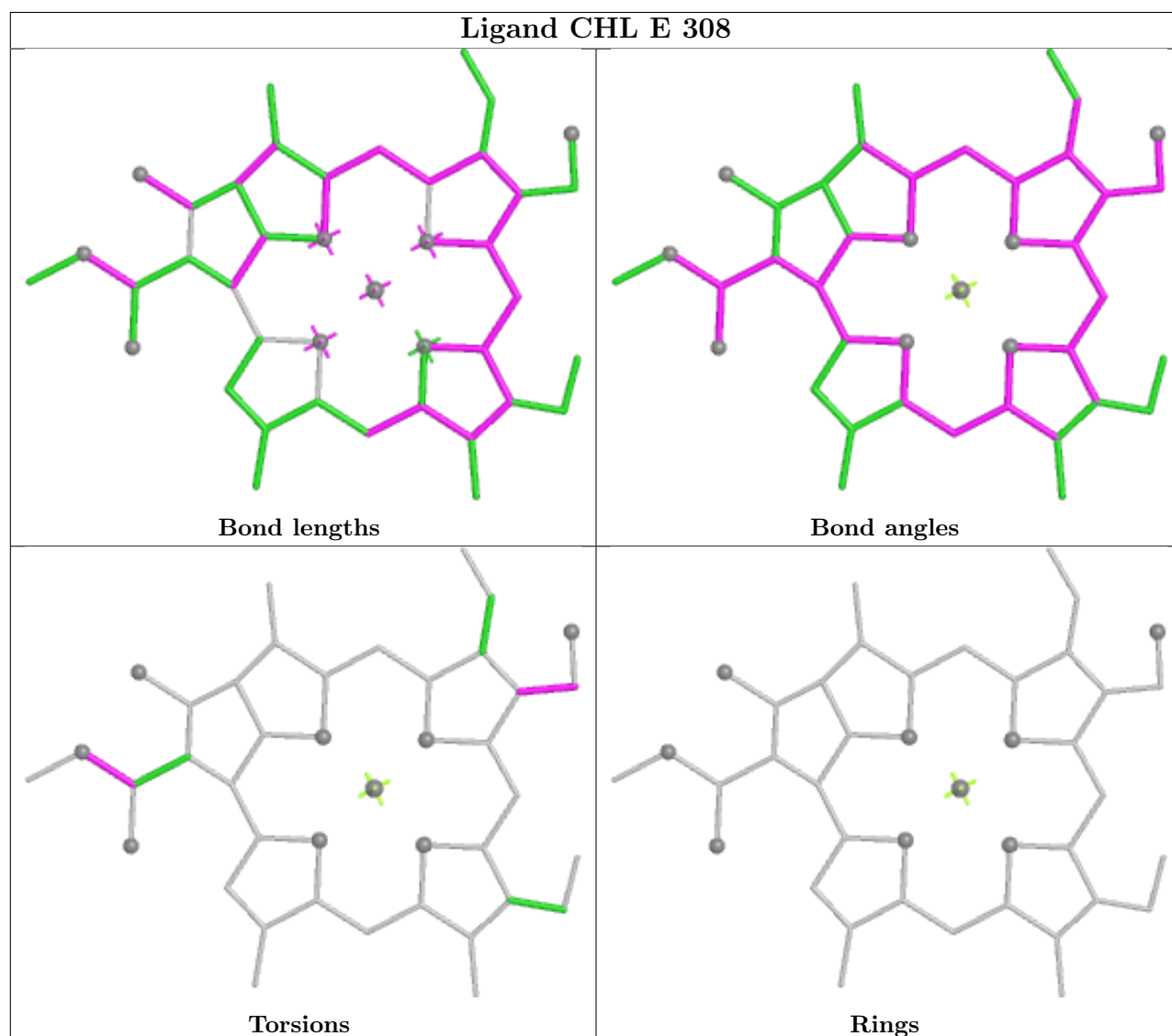
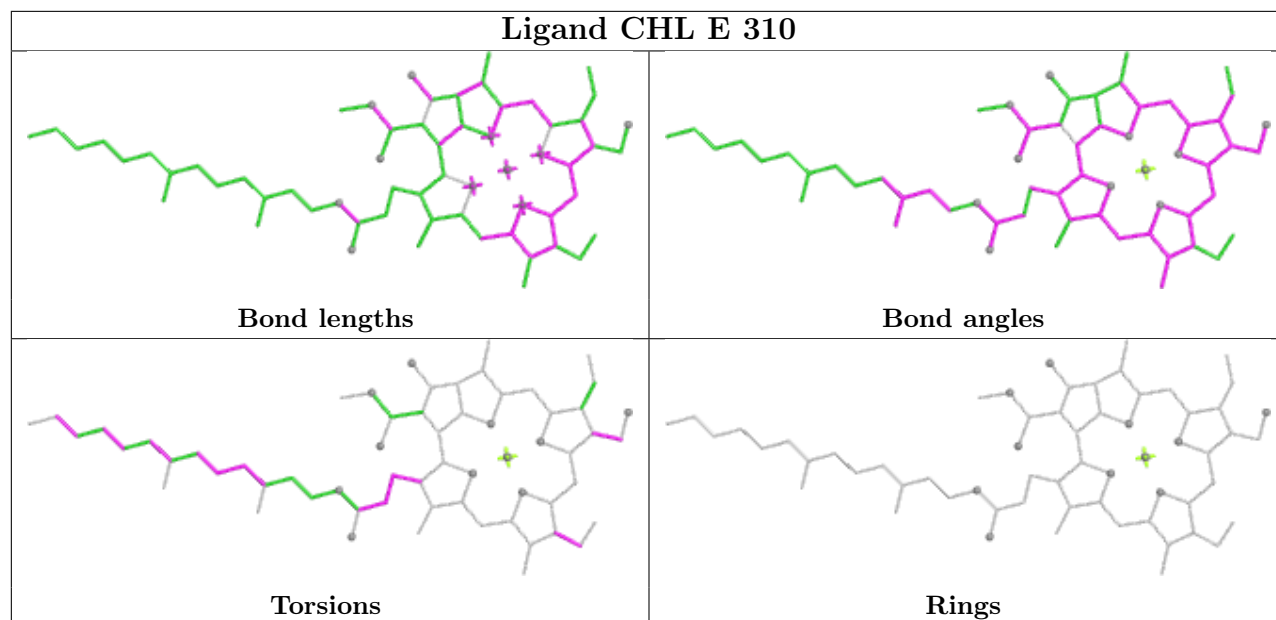


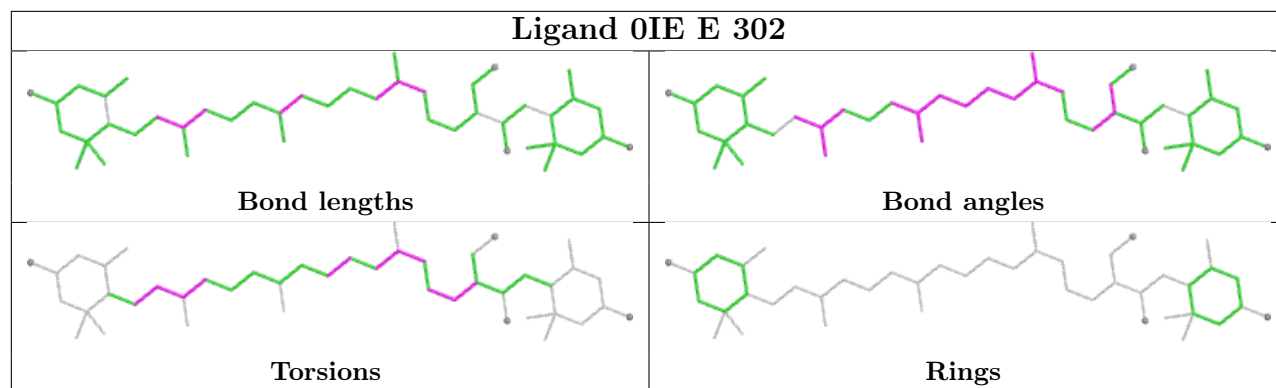
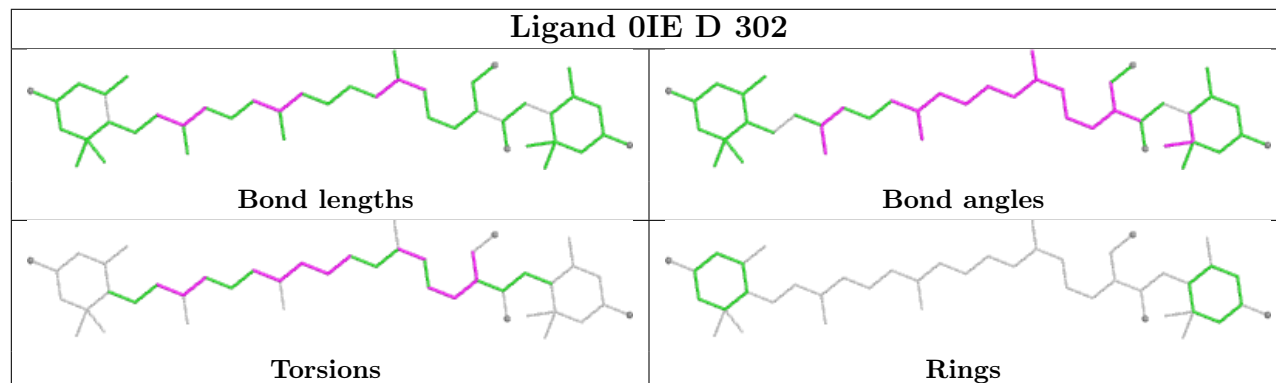
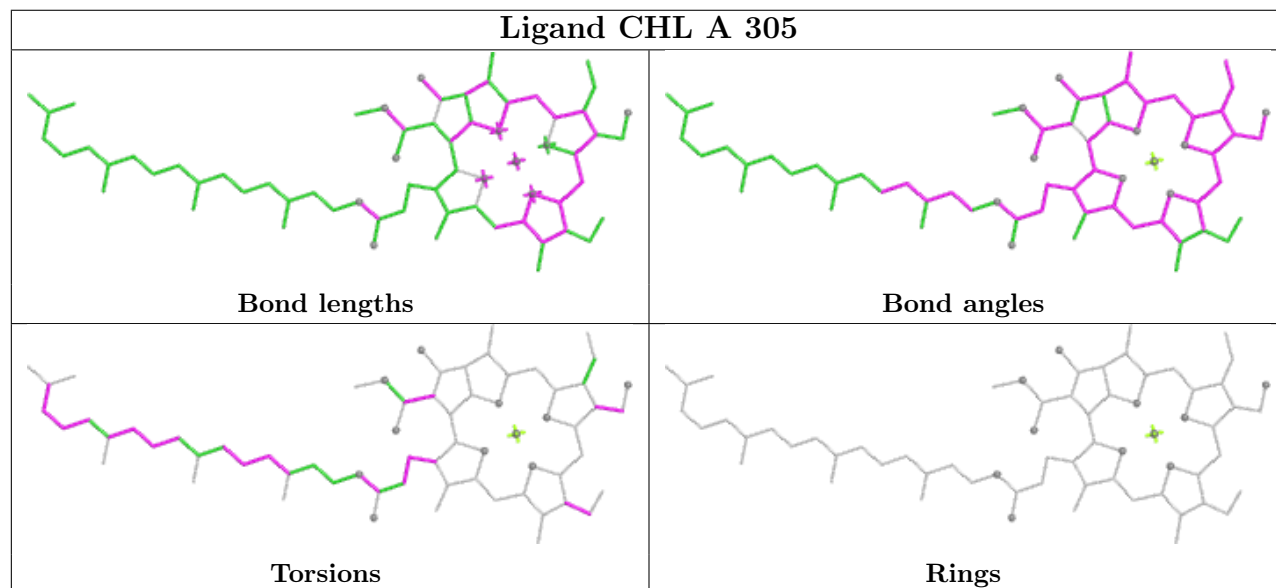
Ligand NEX E 303

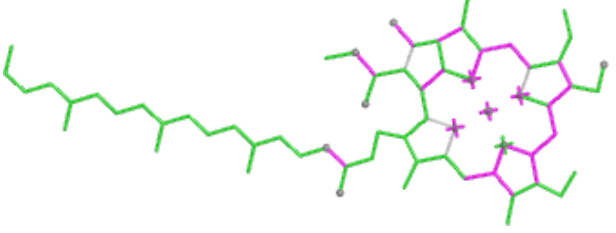
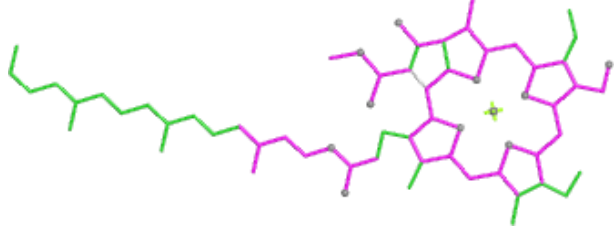
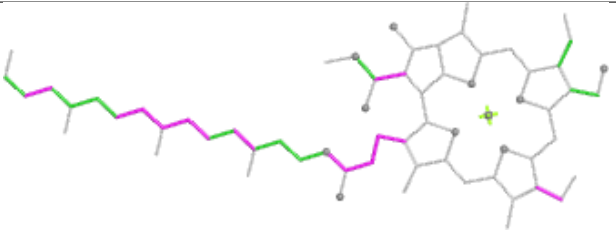
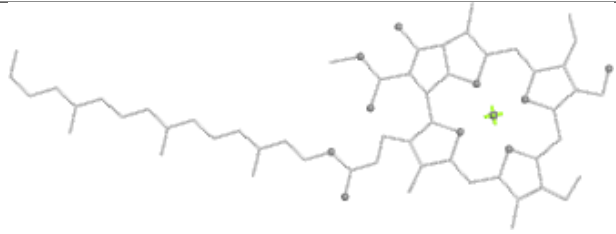
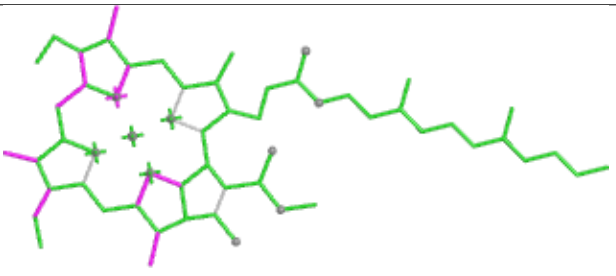
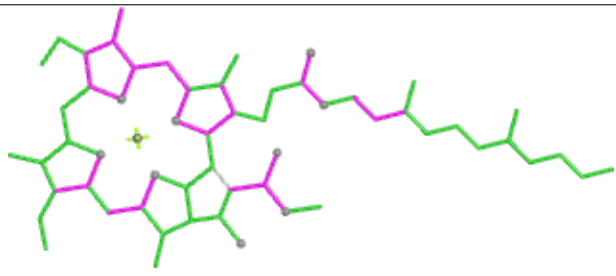
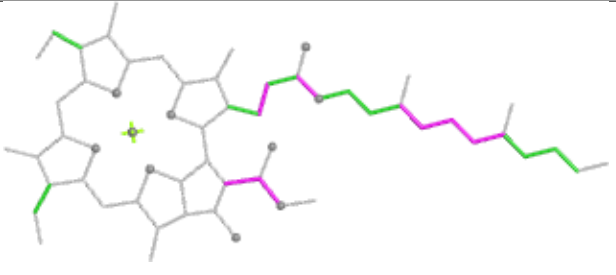
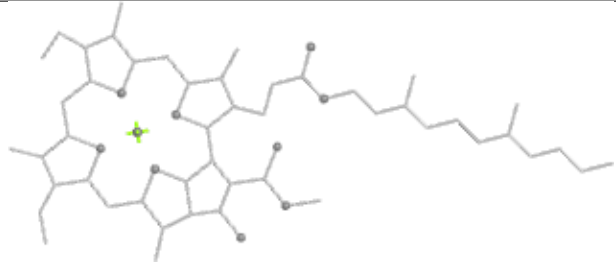


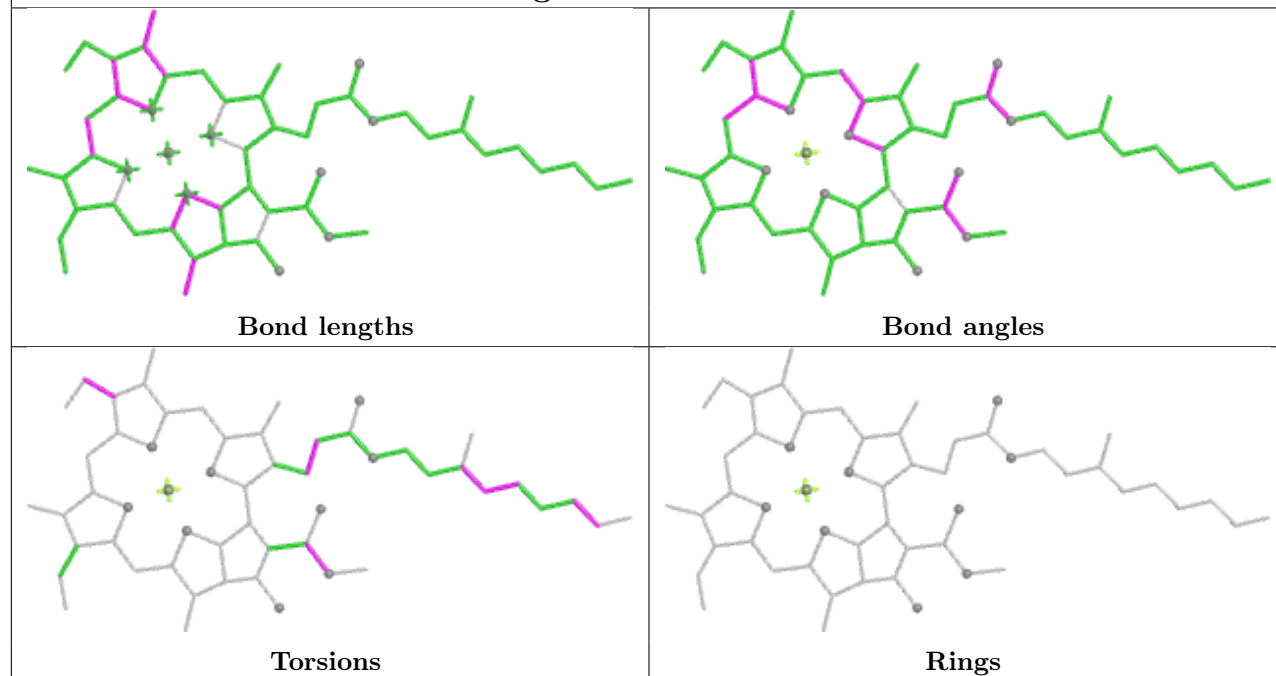
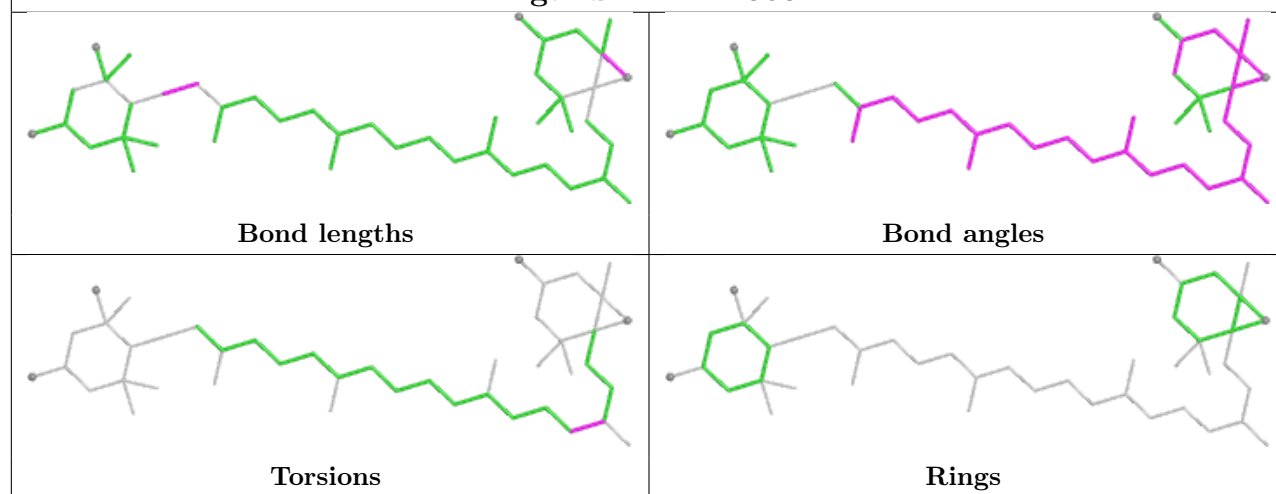
Ligand OUR D 321**Ligand CHL B 311**

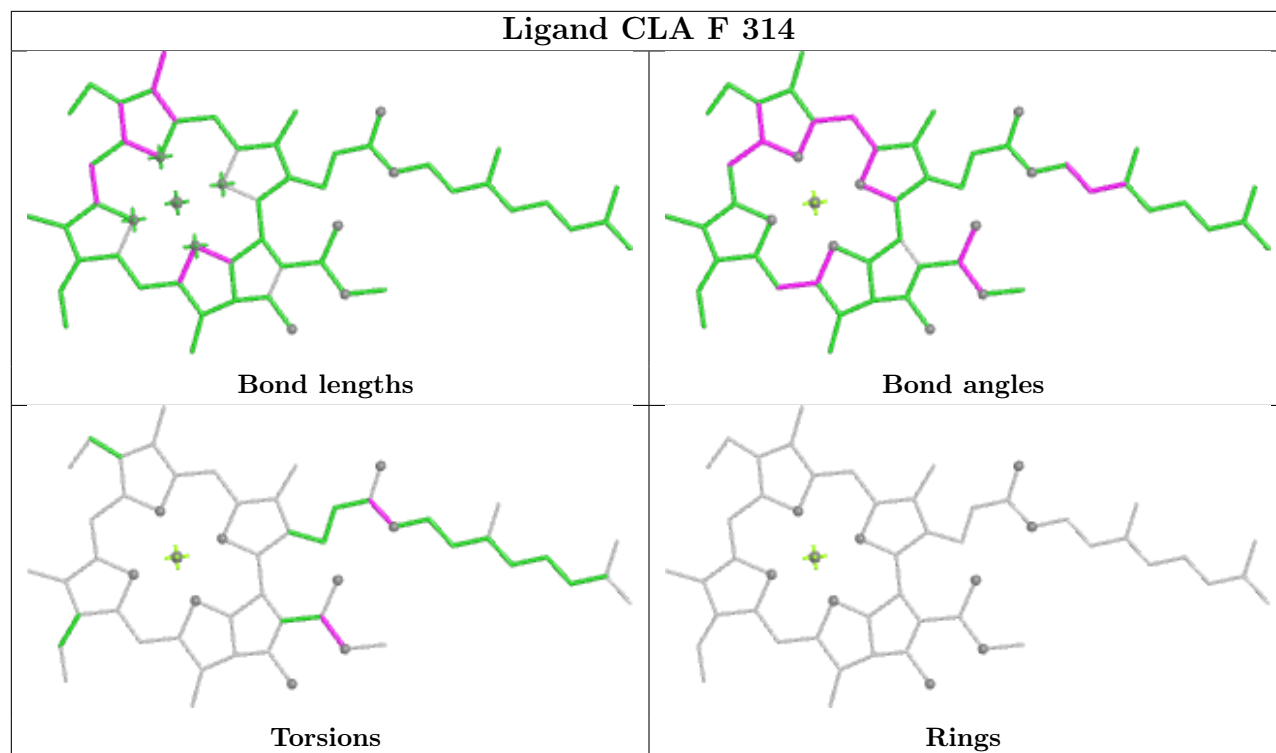


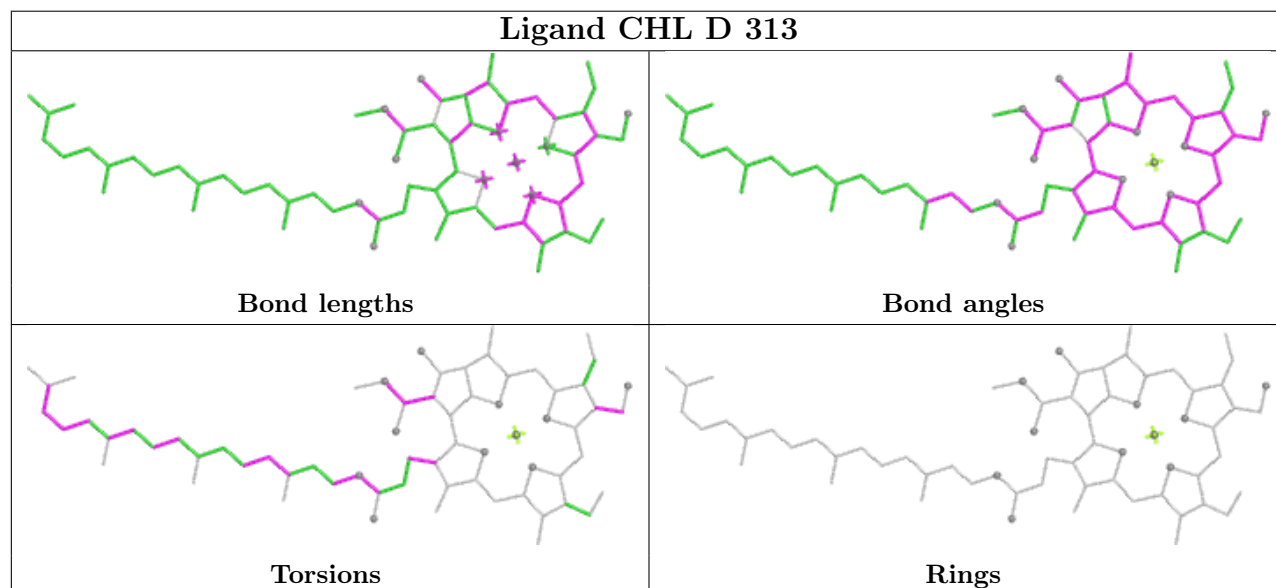
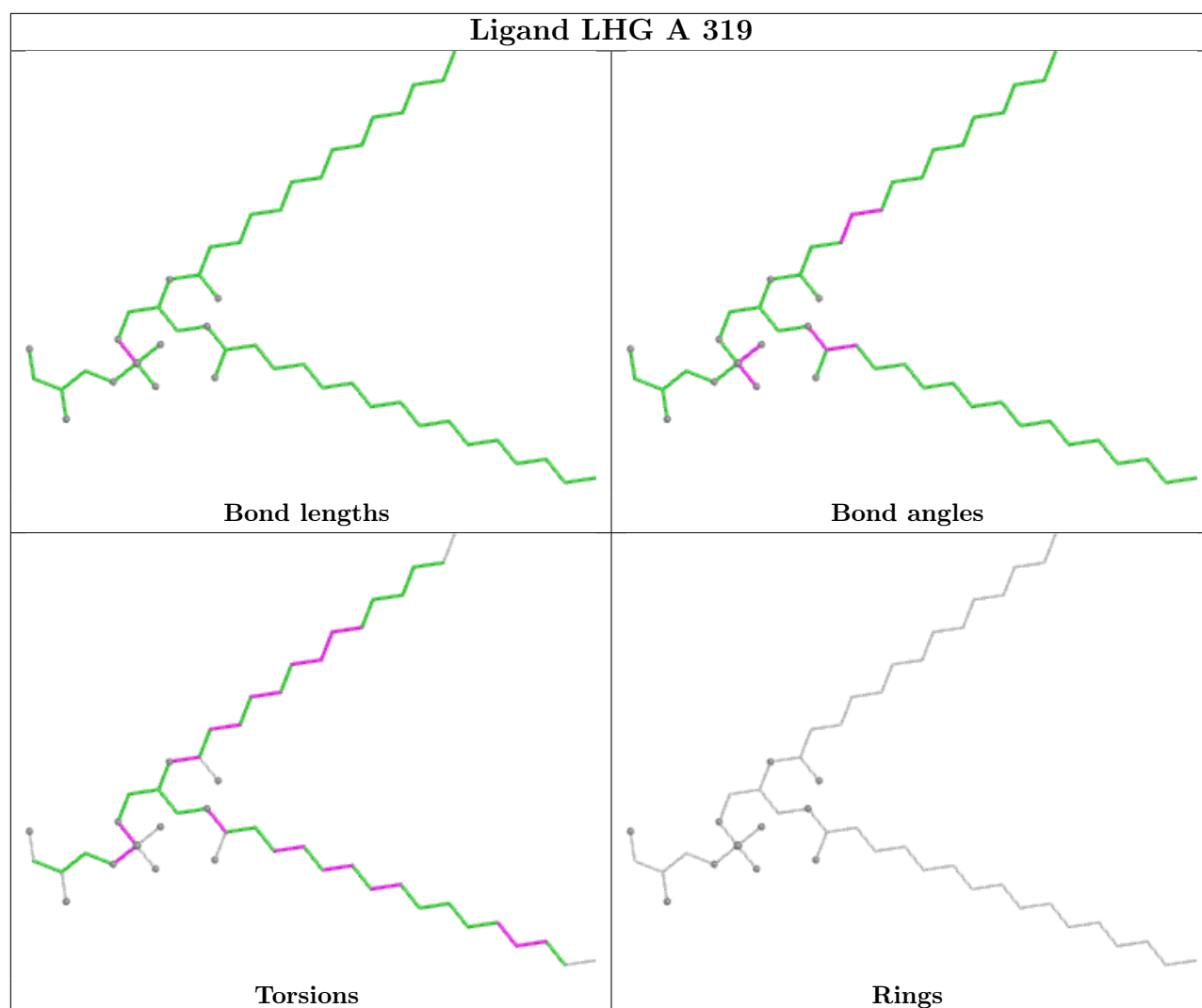


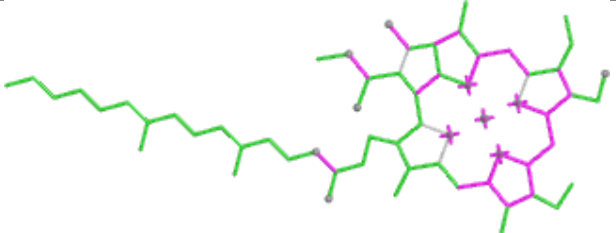
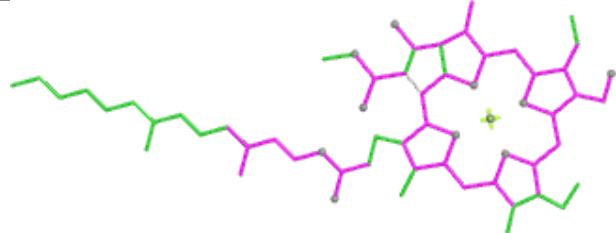
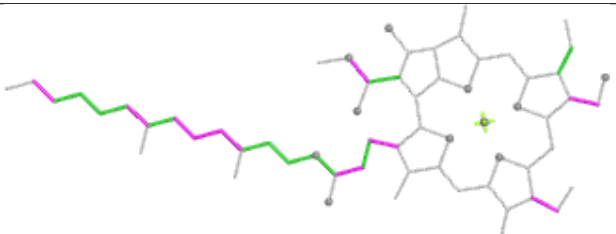
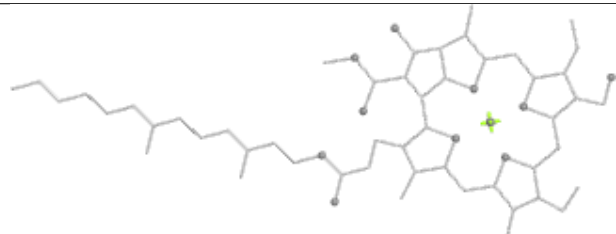
Ligand 01E E 302**Ligand 01E D 302****Ligand CHL A 305**

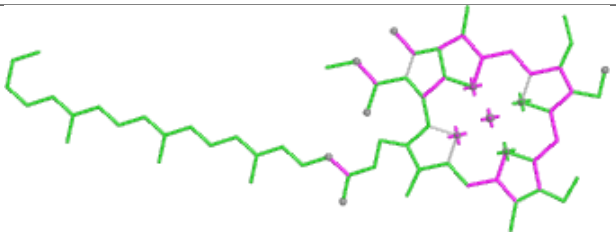
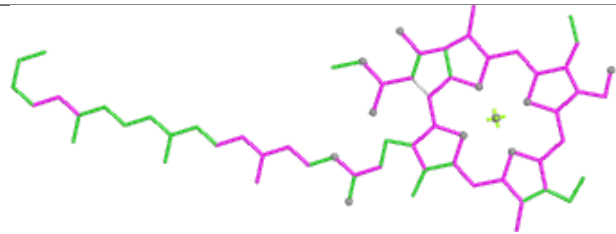
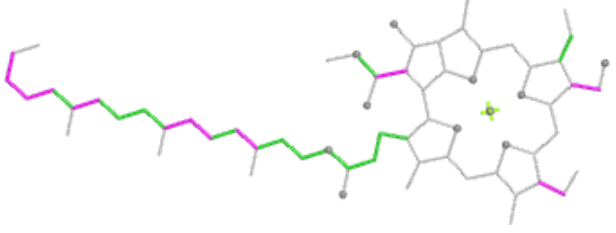
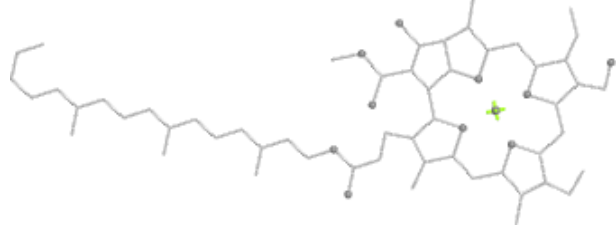
Ligand CHL A 306	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA F 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA E 316**Ligand NEX B 303**

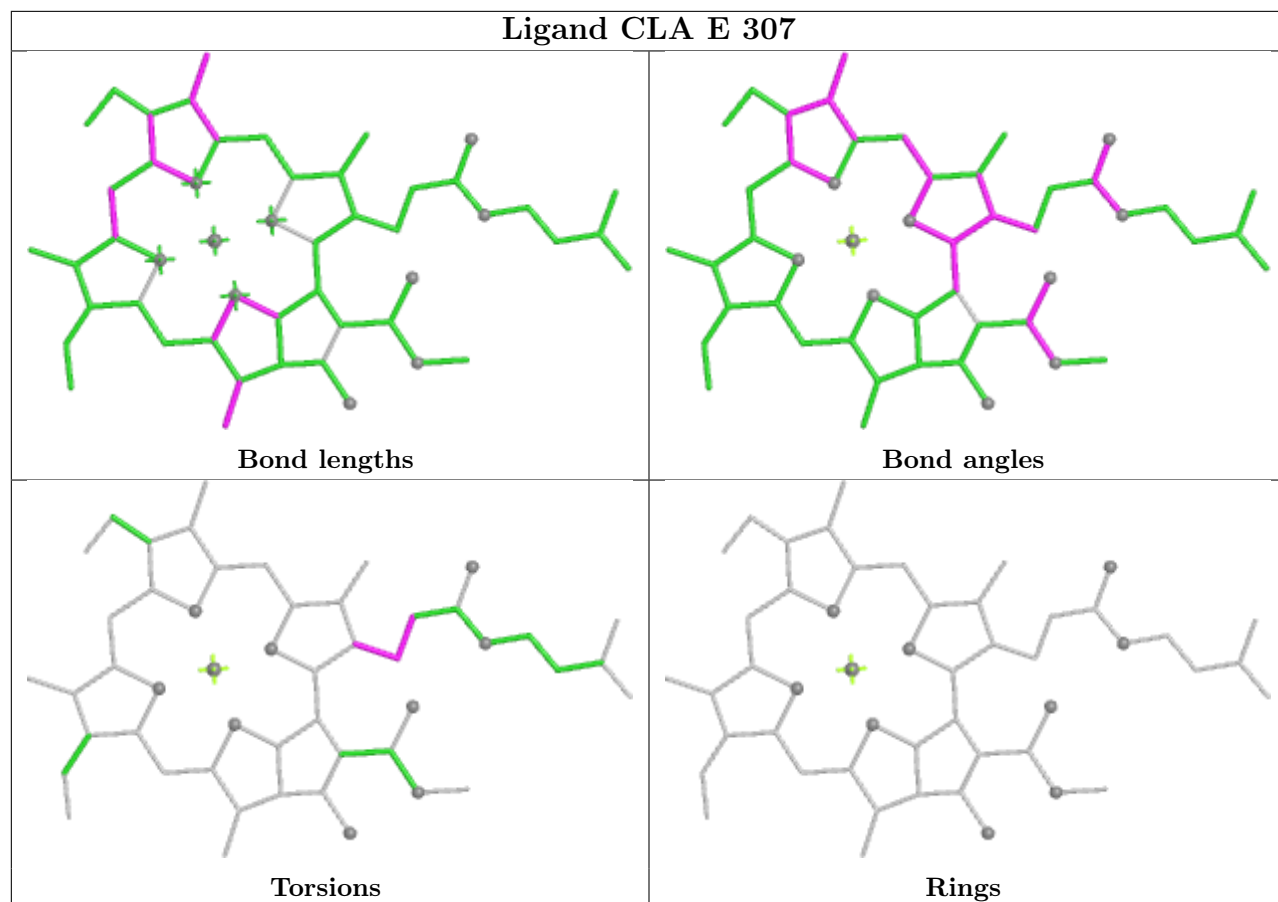




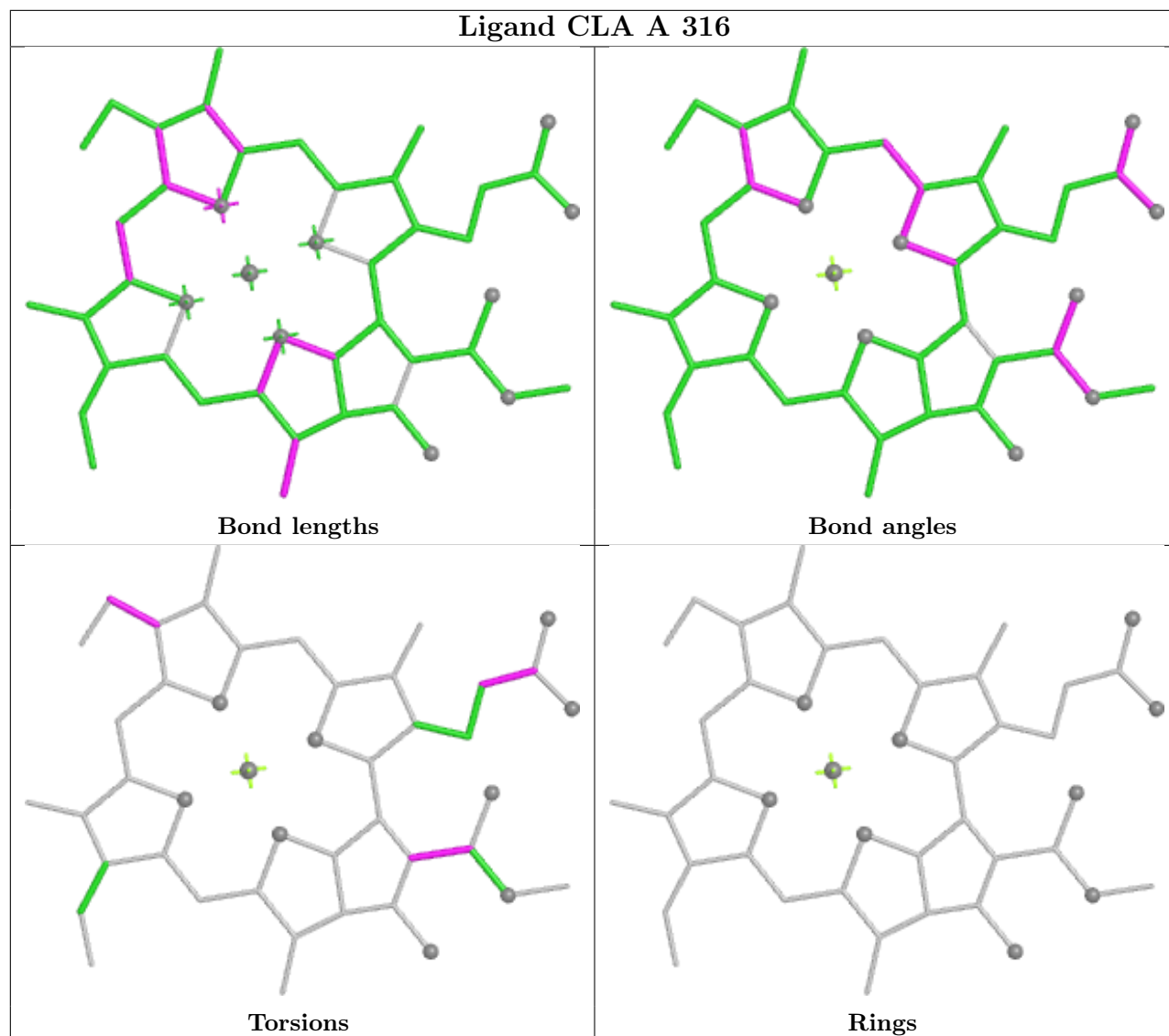
Ligand CHL A 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL B 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

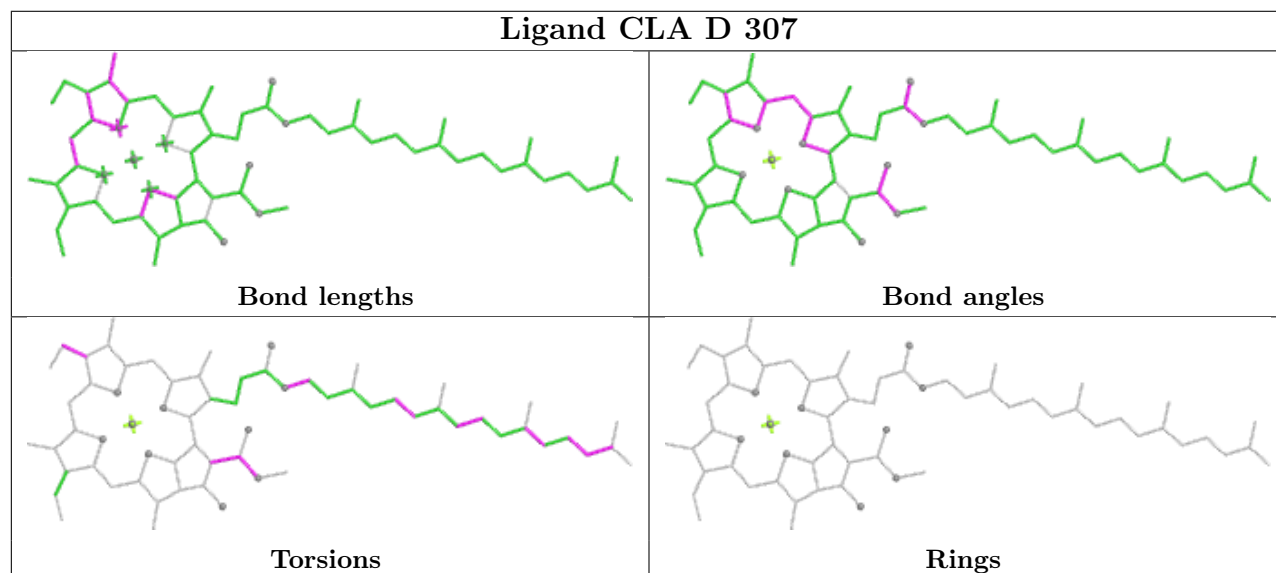
Ligand CLA E 307

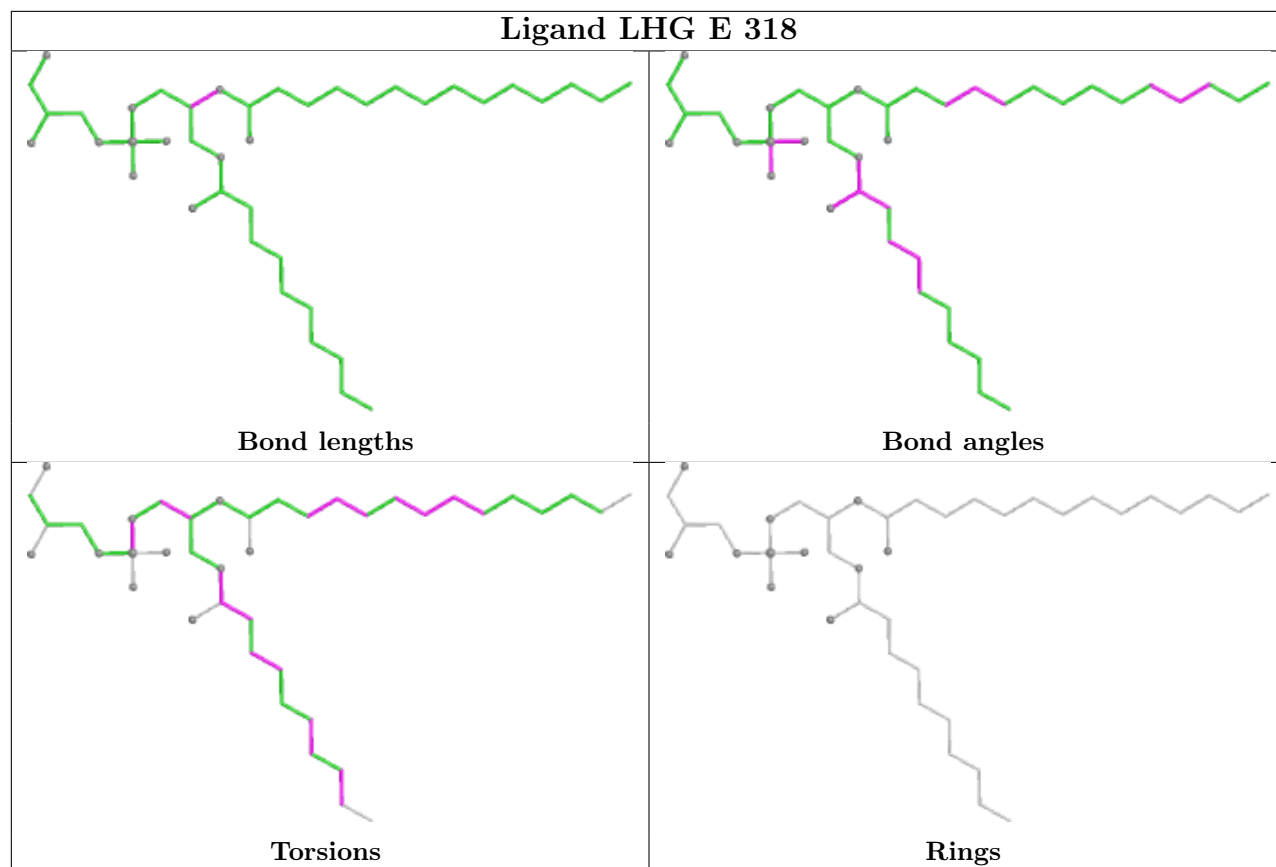


Ligand CLA A 316

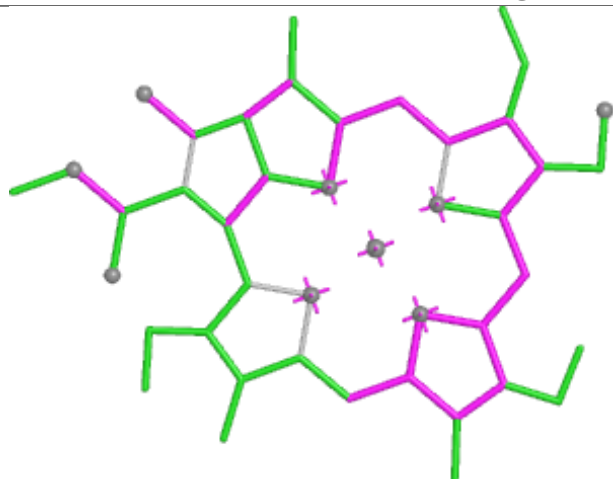


Ligand CLA D 307

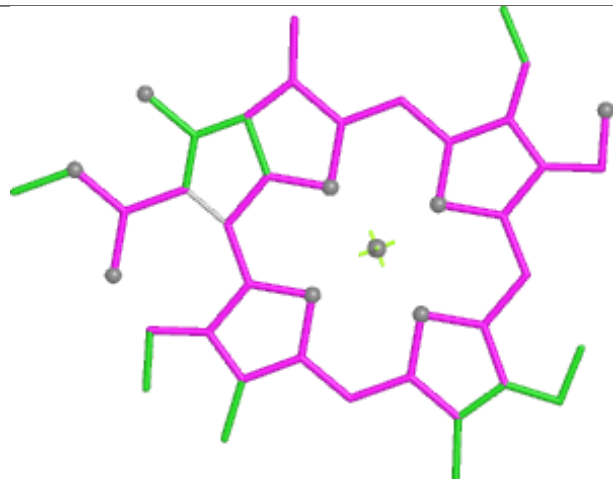




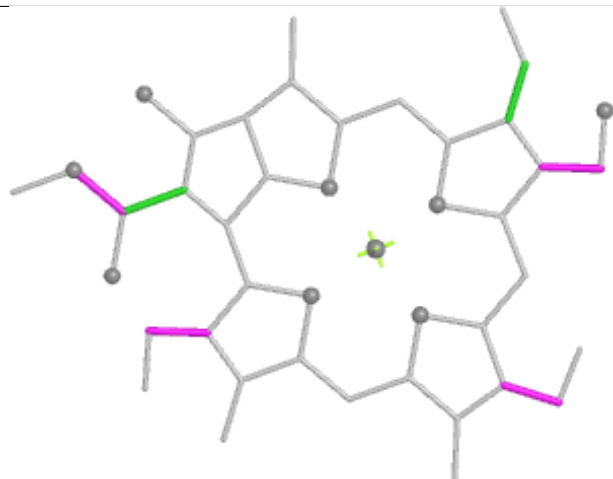
Ligand CHL A 309



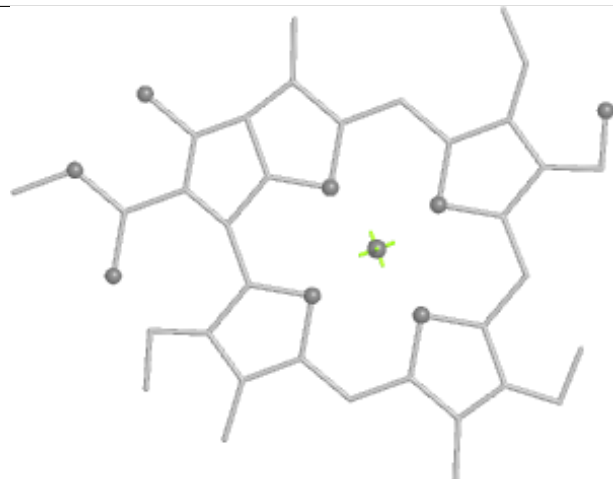
Bond lengths



Bond angles

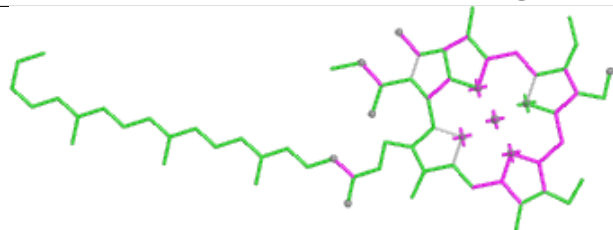


Torsions

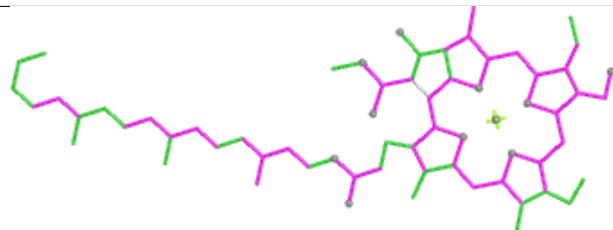


Rings

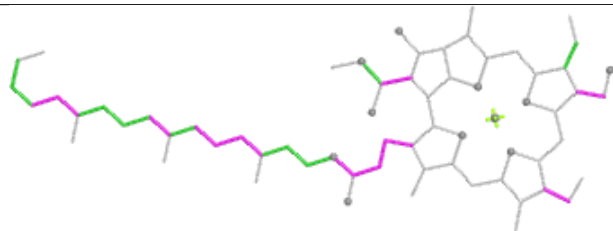
Ligand CHL D 306



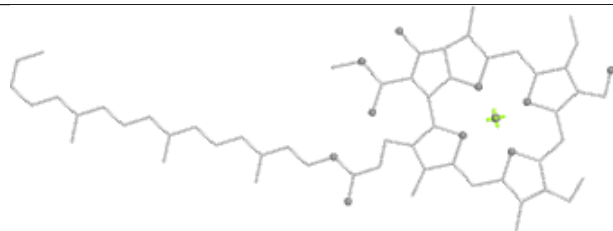
Bond lengths



Bond angles

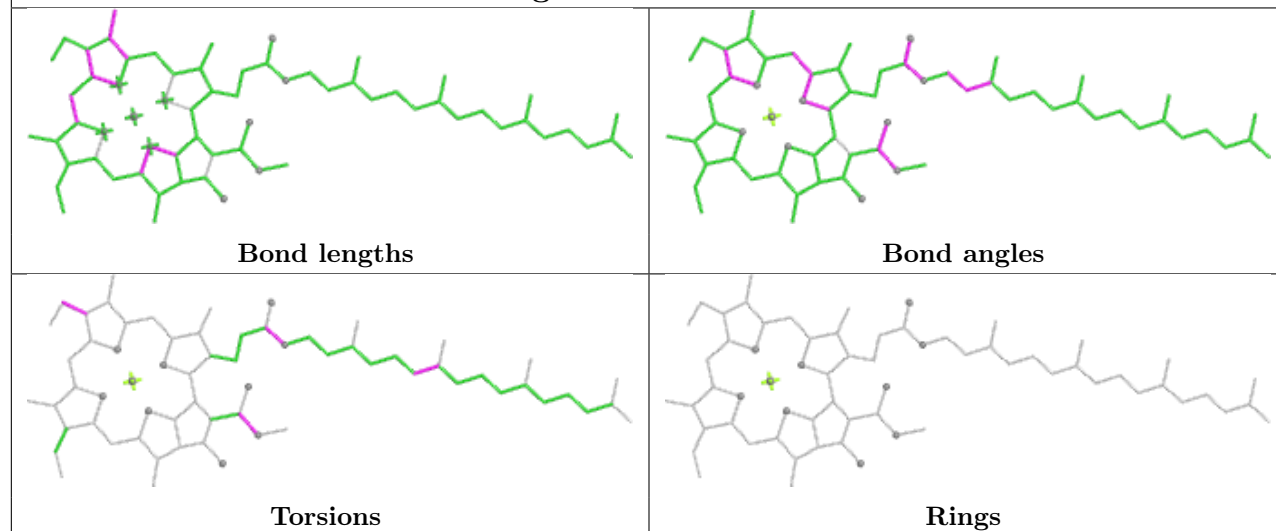


Torsions

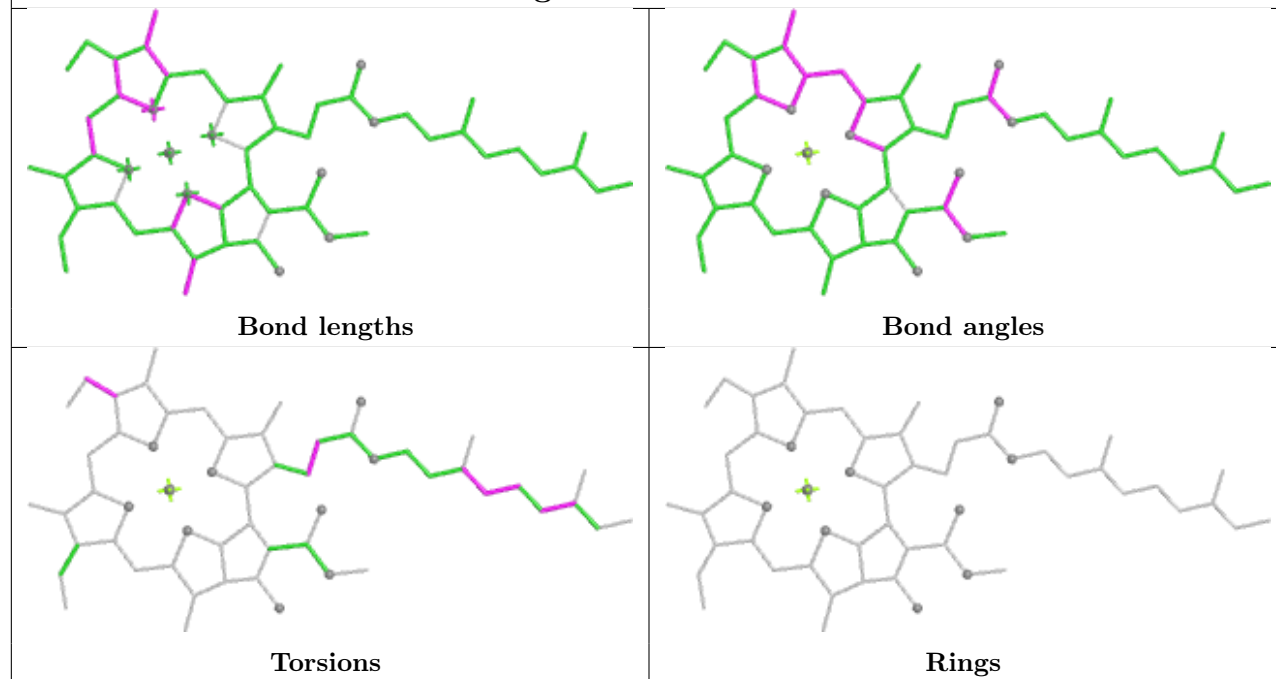


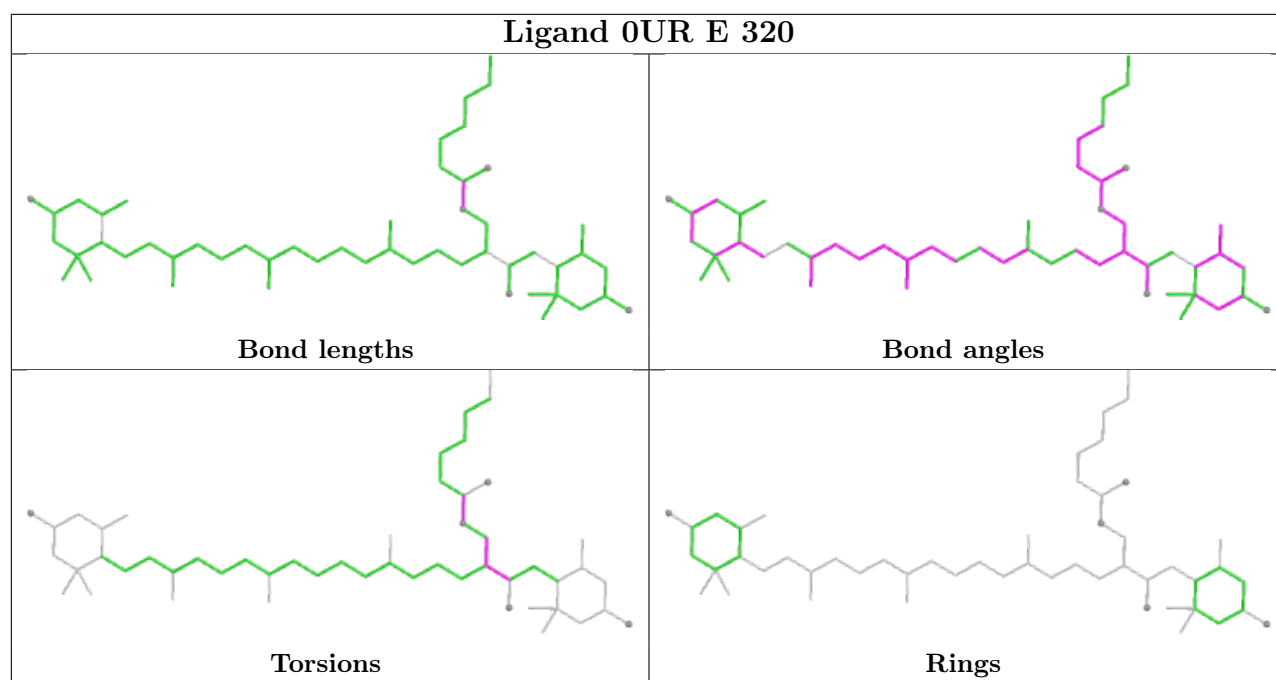
Rings

Ligand CLA B 316



Ligand CLA F 316





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	223/249 (89%)	0.55	23 (10%) 12 9	37, 79, 118, 154	0
1	B	223/249 (89%)	0.52	17 (7%) 20 16	38, 79, 117, 137	0
1	C	222/249 (89%)	0.41	13 (5%) 28 23	39, 84, 122, 158	0
1	D	223/249 (89%)	0.49	18 (8%) 18 14	43, 80, 120, 151	0
1	E	223/249 (89%)	0.78	31 (13%) 6 5	46, 100, 145, 161	0
1	F	223/249 (89%)	0.44	19 (8%) 16 13	34, 76, 109, 126	0
All	All	1337/1494 (89%)	0.53	121 (9%) 15 11	34, 83, 127, 161	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	VAL	11.1
1	F	1	VAL	7.0
1	E	74	GLU	7.0
1	E	84	ALA	6.2
1	D	219	GLY	6.1

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 ⓘ

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
11	LMG	F	319	30/55	0.23	0.19	127,171,183,186	0
7	LHG	C	304	25/49	0.31	0.19	132,176,208,243	0
4	LMU	A	304	35/35	0.56	0.19	115,156,181,187	0
4	LMU	E	319	35/35	0.56	0.19	117,171,194,195	0
4	LMU	D	304	35/35	0.58	0.23	86,132,160,170	0
10	BET	B	321	8/8	0.60	0.28	85,102,109,114	0
4	LMU	B	305	35/35	0.64	0.16	107,181,190,195	0
10	BET	C	320	8/8	0.68	0.25	112,121,126,133	0
10	BET	B	322	8/8	0.69	0.29	90,114,123,132	0
11	LMG	B	323	30/55	0.71	0.15	122,164,179,181	0
7	LHG	B	324	31/49	0.76	0.17	56,98,121,145	0
4	LMU	B	304	33/35	0.77	0.15	116,148,174,180	0
9	OUR	E	320	52/57	0.78	0.17	66,89,116,126	0
9	OUR	B	325	52/57	0.79	0.24	66,89,116,126	0
8	MG	A	321	1/1	0.82	0.28	74,74,74,74	0
9	OUR	D	321	52/57	0.84	0.21	66,89,116,126	0
3	NEX	E	303	44/44	0.85	0.19	101,120,167,186	0
9	OUR	C	321	52/57	0.85	0.18	66,89,116,126	0
3	NEX	F	303	44/44	0.85	0.15	71,92,168,179	0
6	CLA	C	315	65/65	0.86	0.13	72,104,124,139	0
5	CHL	A	309	43/66	0.86	0.12	103,123,135,140	0
9	OUR	A	322	52/57	0.86	0.21	66,89,116,126	0
9	OUR	B	302	50/57	0.87	0.18	67,87,107,123	0
3	NEX	C	303	44/44	0.87	0.14	75,94,147,175	0
5	CHL	E	310	61/66	0.87	0.15	62,79,92,98	0
3	NEX	A	303	44/44	0.87	0.15	78,96,144,152	0
7	LHG	A	319	47/49	0.87	0.17	49,74,99,106	0
5	CHL	E	308	41/66	0.88	0.12	119,142,157,160	0
5	CHL	E	309	43/66	0.88	0.16	89,105,127,130	0
2	OIE	D	302	44/44	0.88	0.16	74,87,104,108	0
5	CHL	F	308	42/66	0.88	0.13	93,110,123,128	0
5	CHL	B	310	43/66	0.88	0.14	95,121,136,143	0
6	CLA	E	314	63/65	0.88	0.12	89,121,136,151	0
5	CHL	C	309	42/66	0.88	0.11	92,113,122,129	0
7	LHG	C	319	45/49	0.89	0.15	59,84,108,139	0
2	OIE	C	302	44/44	0.89	0.15	57,77,101,107	0
6	CLA	D	317	65/65	0.89	0.16	66,85,110,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CHL	D	309	42/66	0.89	0.11	86,109,121,128	0
9	OUR	F	320	52/57	0.89	0.21	66,89,116,126	0
5	CHL	A	310	51/66	0.90	0.12	59,90,124,133	0
6	CLA	E	313	55/65	0.90	0.12	100,112,130,140	0
6	CLA	C	314	53/65	0.90	0.11	79,97,118,126	0
7	LHG	E	318	41/49	0.90	0.12	55,85,121,144	0
7	LHG	F	318	45/49	0.90	0.16	42,63,78,85	0
5	CHL	E	311	56/66	0.90	0.13	94,112,141,146	0
3	NEX	B	303	44/44	0.91	0.12	76,95,144,165	0
5	CHL	F	309	42/66	0.91	0.11	62,80,94,103	0
6	CLA	A	314	55/65	0.91	0.10	60,71,85,87	0
6	CLA	B	315	58/65	0.91	0.12	65,76,100,107	0
6	CLA	E	315	45/65	0.91	0.10	100,118,132,138	0
6	CLA	E	316	55/65	0.91	0.13	65,78,89,95	0
6	CLA	F	313	58/65	0.91	0.12	58,70,101,102	0
2	OIE	F	302	44/44	0.91	0.13	50,64,77,81	0
7	LHG	B	320	46/49	0.91	0.14	50,74,88,106	0
6	CLA	A	308	50/65	0.92	0.12	68,88,102,119	0
7	LHG	D	319	46/49	0.92	0.13	66,87,101,108	0
5	CHL	C	310	44/66	0.92	0.10	66,86,104,107	0
5	CHL	C	311	61/66	0.92	0.12	51,68,84,92	0
5	CHL	C	312	56/66	0.92	0.12	62,90,116,122	0
5	CHL	C	313	66/66	0.92	0.11	46,63,80,86	0
6	CLA	C	316	45/65	0.92	0.10	77,95,118,123	0
5	CHL	C	318	44/66	0.92	0.12	70,96,112,129	0
2	OIE	A	302	44/44	0.92	0.11	55,73,85,103	0
5	CHL	A	312	56/66	0.92	0.13	51,74,104,117	0
2	OIE	C	301	44/44	0.92	0.12	35,54,75,81	0
5	CHL	B	311	51/66	0.92	0.12	71,90,122,134	0
5	CHL	B	312	62/66	0.92	0.13	51,68,84,93	0
5	CHL	B	319	47/66	0.92	0.09	80,96,112,117	0
2	OIE	E	302	44/44	0.92	0.11	57,75,105,125	0
5	CHL	F	310	61/66	0.92	0.11	49,65,80,89	0
5	CHL	F	317	46/66	0.92	0.11	63,83,106,122	0
5	CHL	E	304	66/66	0.93	0.12	54,75,102,137	0
5	CHL	E	305	64/66	0.93	0.11	44,65,79,95	0
6	CLA	A	315	63/65	0.93	0.12	66,86,99,109	0
6	CLA	B	309	46/65	0.93	0.12	72,88,99,103	0
3	NEX	D	303	44/44	0.93	0.12	65,81,126,145	0
6	CLA	B	318	65/65	0.93	0.12	58,84,98,101	0
6	CLA	C	308	46/65	0.93	0.10	65,86,94,100	0
5	CHL	B	313	57/66	0.93	0.12	59,84,104,105	0

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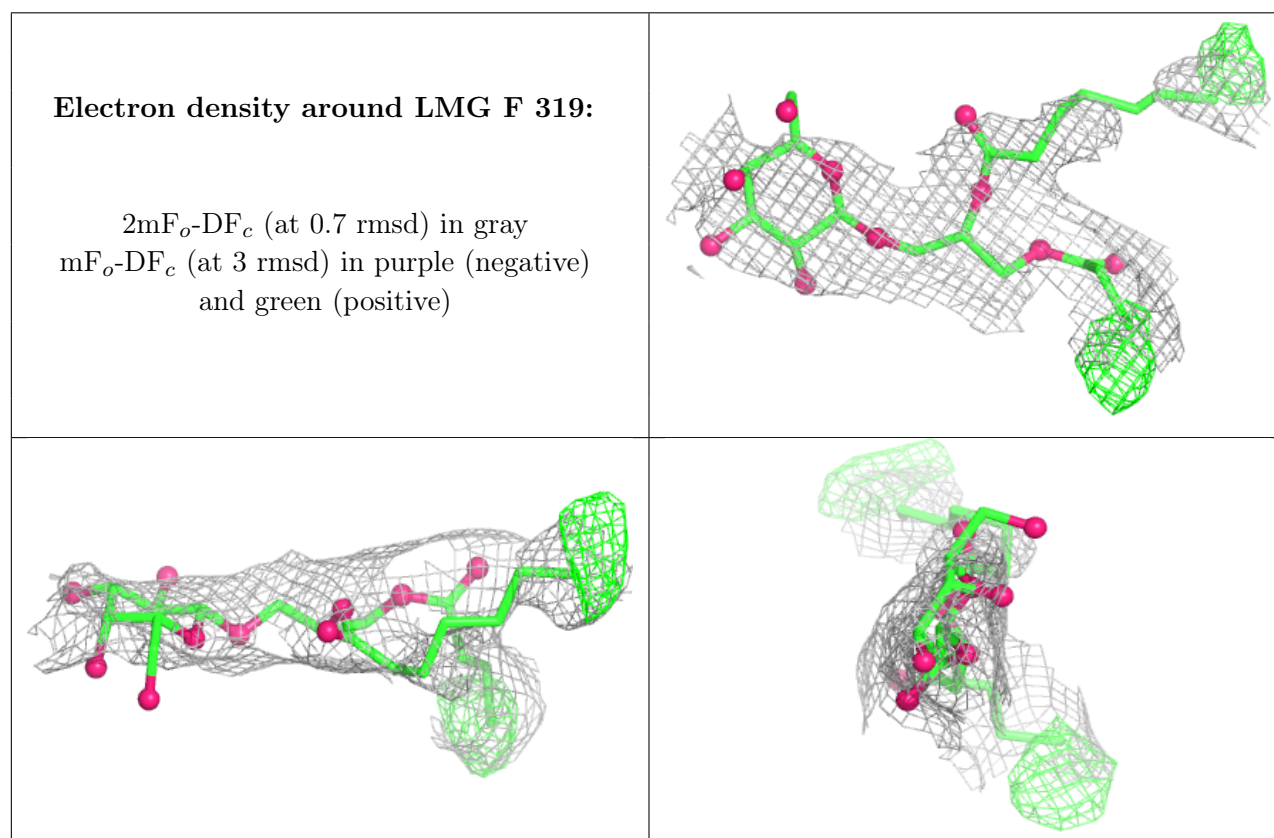
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CHL	A	318	42/66	0.93	0.12	66,89,100,101	0
5	CHL	A	305	66/66	0.93	0.12	45,73,91,106	0
6	CLA	D	308	46/65	0.93	0.08	68,84,96,104	0
6	CLA	D	314	58/65	0.93	0.12	60,76,97,101	0
5	CHL	E	312	66/66	0.93	0.12	46,76,90,100	0
6	CLA	E	307	50/65	0.93	0.12	89,108,130,132	0
5	CHL	E	317	41/66	0.93	0.11	83,96,113,116	0
5	CHL	D	306	65/66	0.93	0.12	42,58,76,89	0
5	CHL	A	311	61/66	0.93	0.10	51,70,82,97	0
5	CHL	D	310	45/66	0.93	0.08	52,77,90,91	0
6	CLA	F	307	46/65	0.93	0.09	61,79,91,96	0
5	CHL	D	311	62/66	0.93	0.12	40,72,88,94	0
6	CLA	F	315	45/65	0.93	0.09	58,74,92,100	0
5	CHL	B	306	66/66	0.94	0.12	45,63,77,93	0
5	CHL	D	305	66/66	0.94	0.12	59,85,100,108	0
6	CLA	B	316	65/65	0.94	0.11	63,79,109,139	0
5	CHL	C	305	66/66	0.94	0.11	51,71,86,102	0
6	CLA	C	307	65/65	0.94	0.09	33,51,75,92	0
5	CHL	C	306	66/66	0.94	0.12	34,58,71,87	0
2	OIE	B	301	44/44	0.94	0.10	33,46,75,79	0
5	CHL	F	304	66/66	0.94	0.11	41,58,70,84	0
5	CHL	F	305	66/66	0.94	0.10	29,43,59,71	0
6	CLA	C	317	56/65	0.94	0.11	57,75,89,96	0
2	OIE	F	301	44/44	0.94	0.11	29,43,65,81	0
8	MG	D	320	1/1	0.94	0.13	63,63,63,63	0
5	CHL	D	312	57/66	0.94	0.12	44,63,94,103	0
6	CLA	D	315	65/65	0.94	0.10	79,95,107,112	0
6	CLA	D	316	45/65	0.94	0.09	81,85,101,105	0
5	CHL	D	313	66/66	0.94	0.10	33,50,74,96	0
6	CLA	E	306	65/65	0.94	0.10	48,63,78,86	0
5	CHL	F	312	66/66	0.94	0.10	45,61,77,86	0
5	CHL	D	318	46/66	0.94	0.11	86,105,120,121	0
2	OIE	A	301	44/44	0.94	0.11	37,50,66,77	0
2	OIE	E	301	44/44	0.94	0.10	44,68,86,99	0
5	CHL	B	314	66/66	0.94	0.10	41,61,77,91	0
6	CLA	F	306	65/65	0.94	0.10	36,53,75,90	0
6	CLA	A	317	55/65	0.94	0.10	48,77,87,97	0
6	CLA	F	314	55/65	0.95	0.09	51,63,93,103	0
5	CHL	B	307	65/66	0.95	0.10	32,45,64,88	0
6	CLA	F	316	56/65	0.95	0.09	54,68,79,90	0
8	MG	A	320	1/1	0.95	0.09	83,83,83,83	0
6	CLA	A	316	45/65	0.95	0.08	74,80,98,116	0

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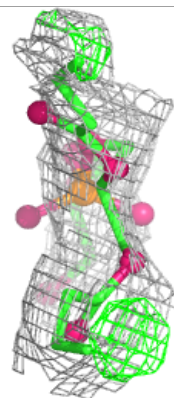
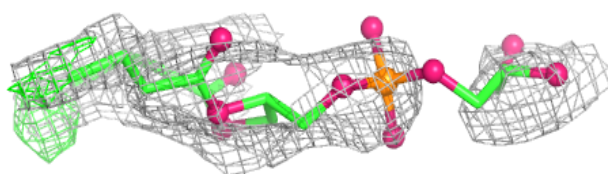
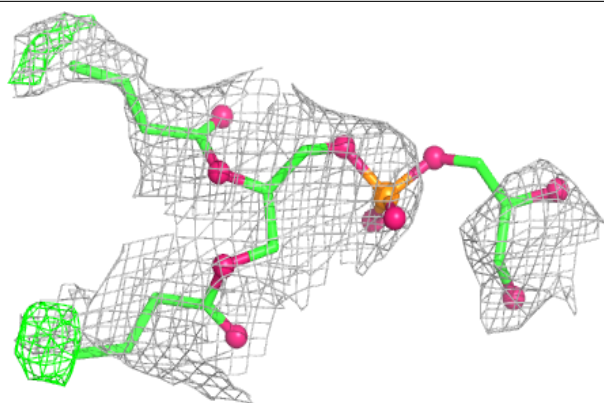
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OIE	D	301	44/44	0.95	0.10	44,58,74,85	0
6	CLA	D	307	65/65	0.95	0.10	34,51,81,90	0
5	CHL	A	313	66/66	0.95	0.10	43,58,76,95	0
5	CHL	F	311	56/66	0.95	0.11	55,83,110,118	0
6	CLA	A	307	65/65	0.96	0.10	31,47,79,85	0
5	CHL	A	306	64/66	0.96	0.09	30,51,64,82	0
6	CLA	B	308	65/65	0.96	0.09	35,49,75,84	0
6	CLA	B	317	45/65	0.96	0.09	74,82,99,112	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.

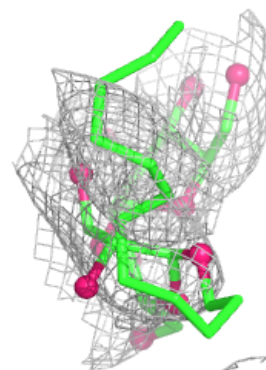
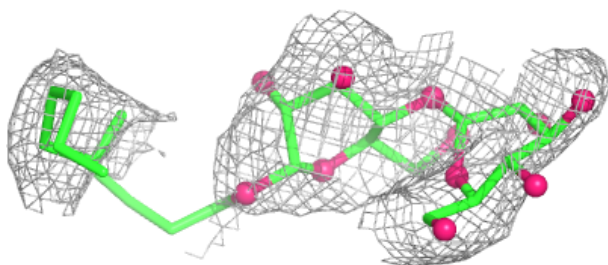
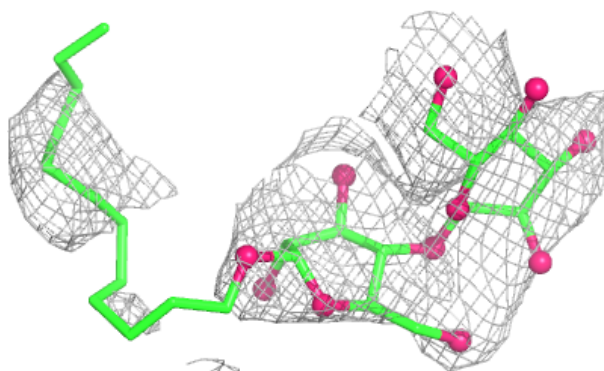


Electron density around LHG C 304:

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

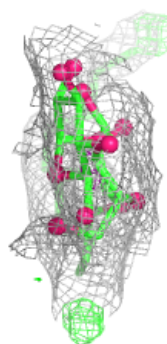
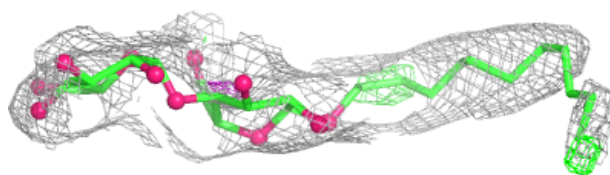
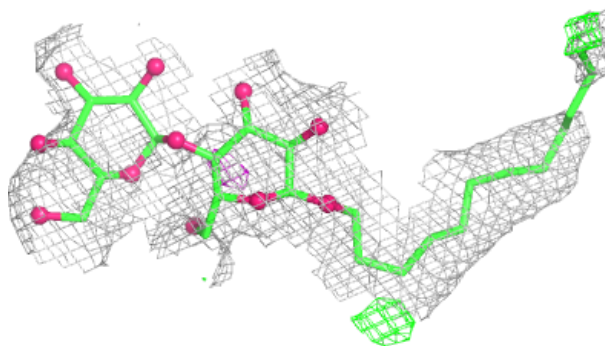
**Electron density around LMU A 304:**

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

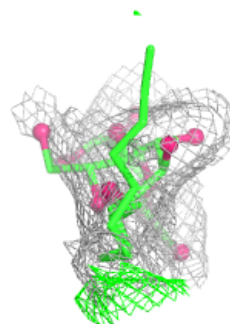
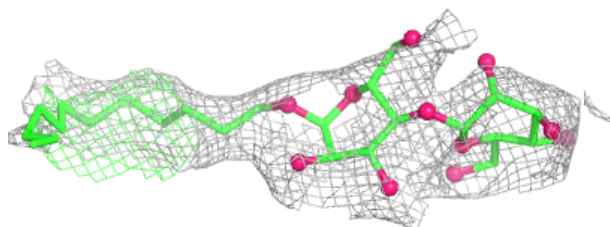
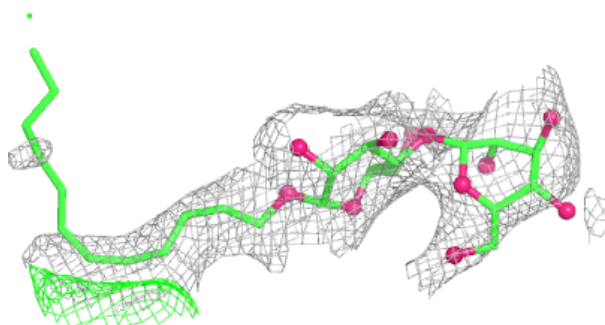


Electron density around LMU E 319:

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

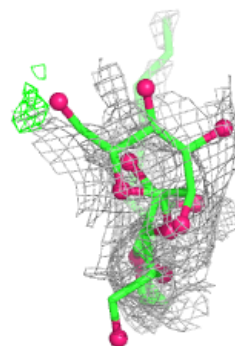
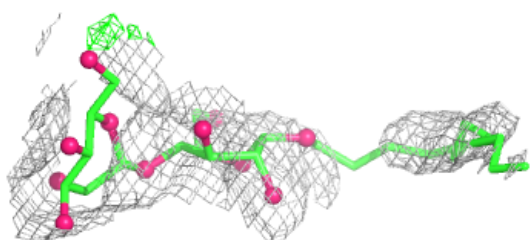
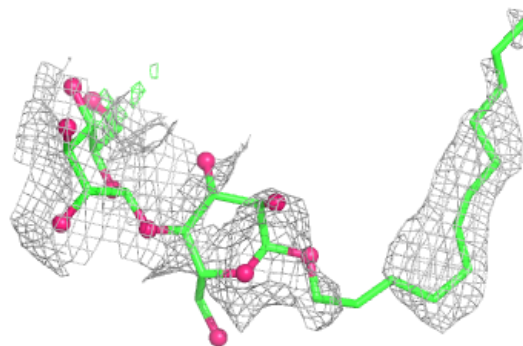
**Electron density around LMU D 304:**

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

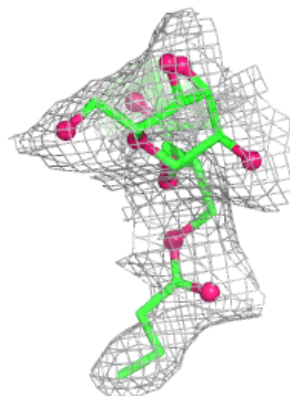
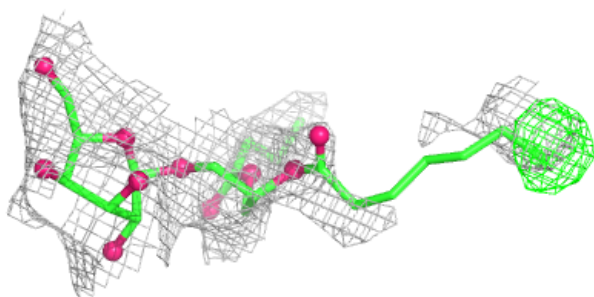
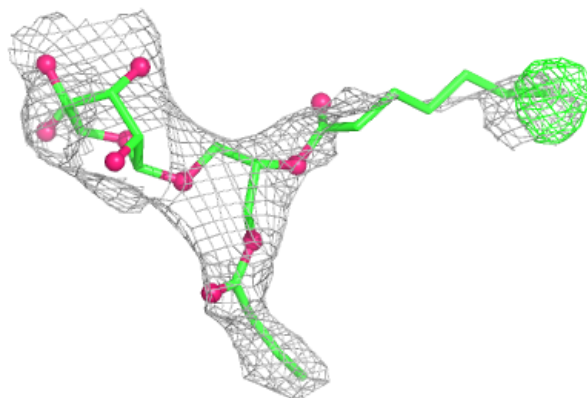


Electron density around LMU B 305:

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

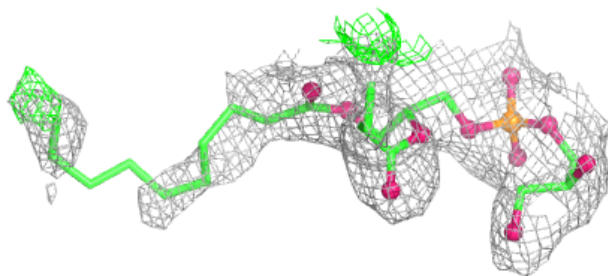
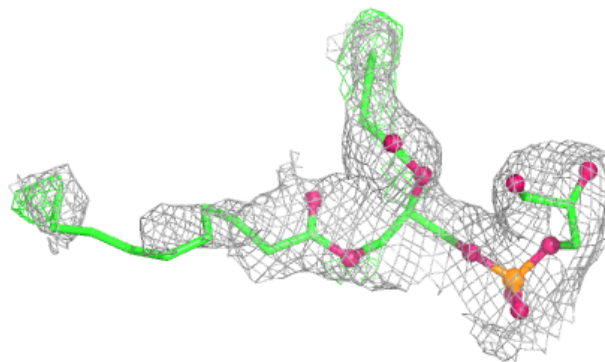
**Electron density around LMG B 323:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

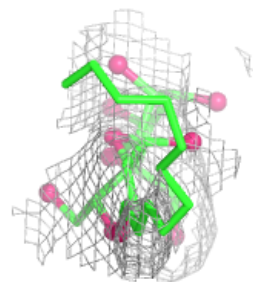
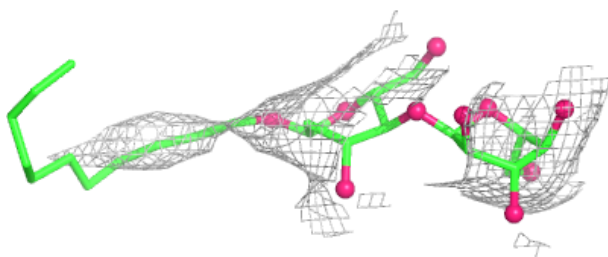


Electron density around LHG B 324:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

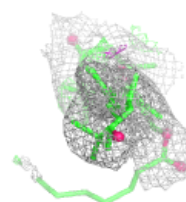
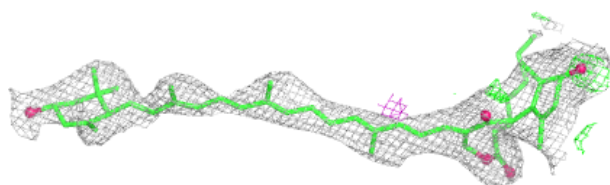
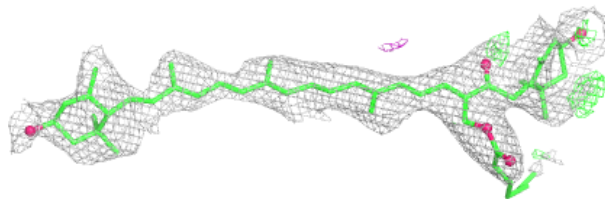
**Electron density around LMU B 304:**

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

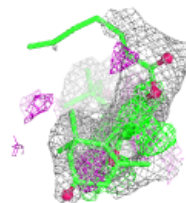
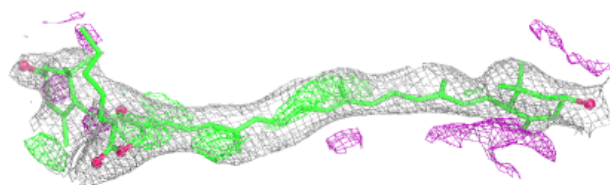
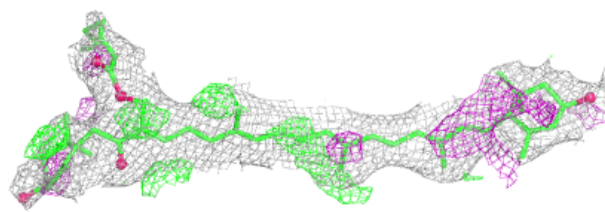


Electron density around 0UR E 320:

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

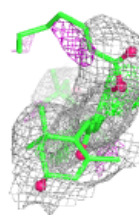
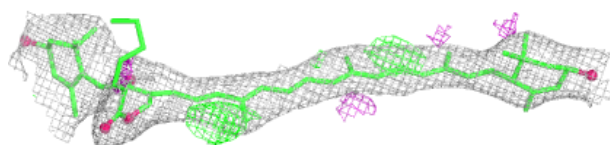
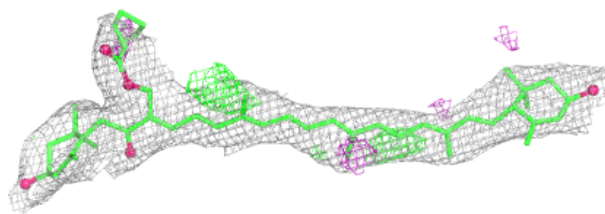
**Electron density around 0UR B 325:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

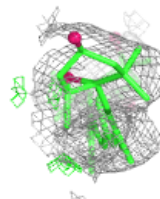
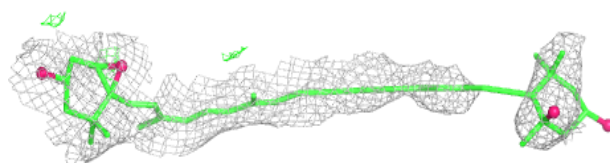
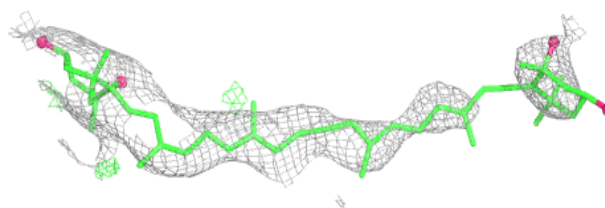


Electron density around 0UR D 321:

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

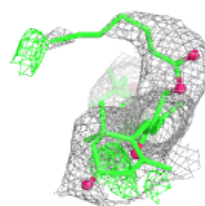
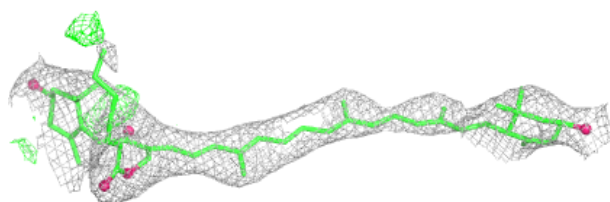
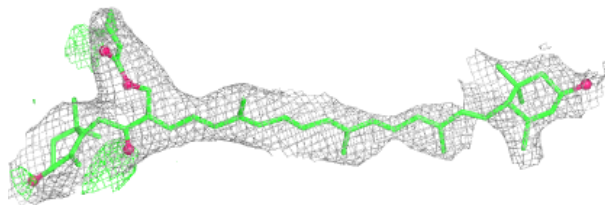
**Electron density around NEX E 303:**

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

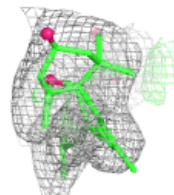
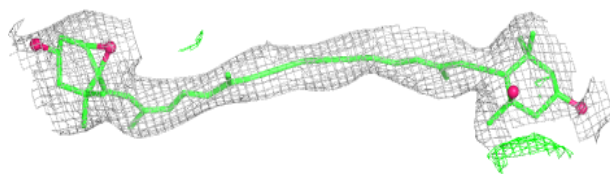
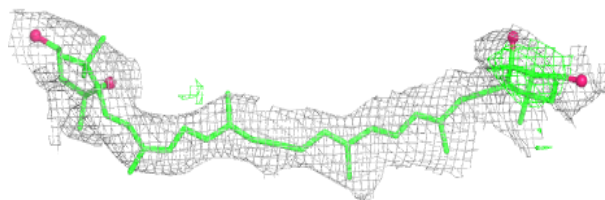


Electron density around 0UR C 321:

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

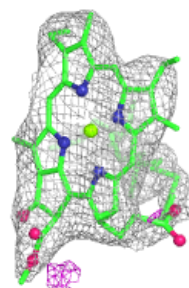
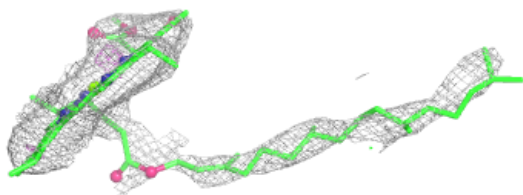
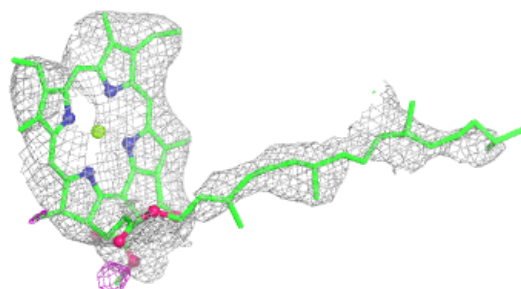
**Electron density around NEX F 303:**

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

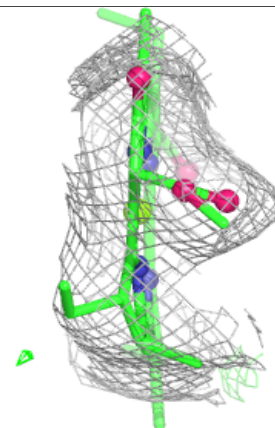
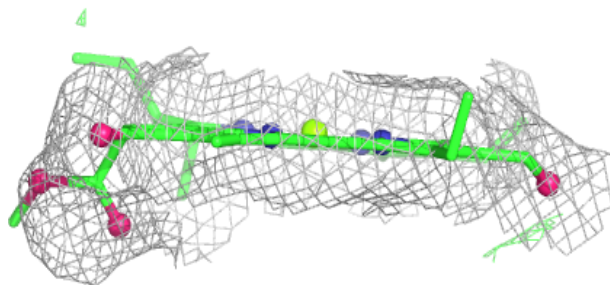
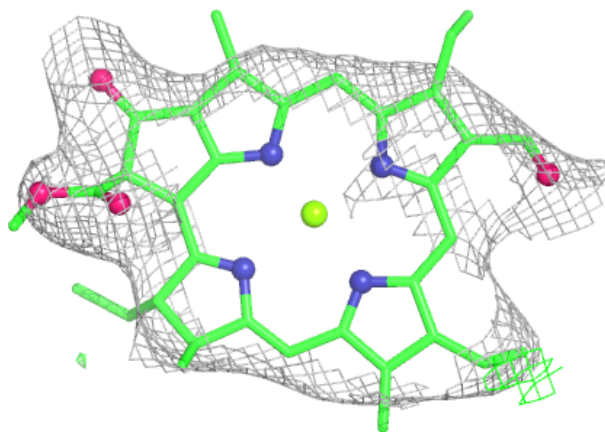


Electron density around CLA C 315:

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

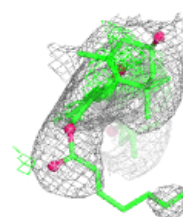
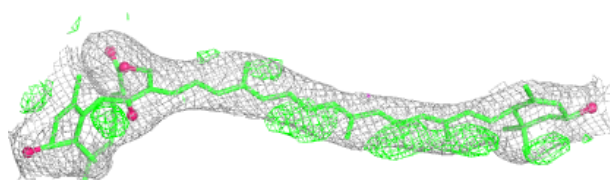
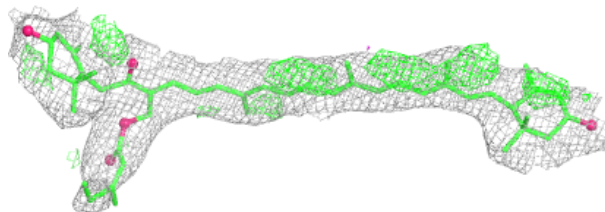
**Electron density around CHL A 309:**

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

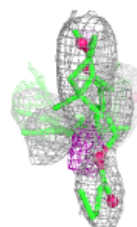
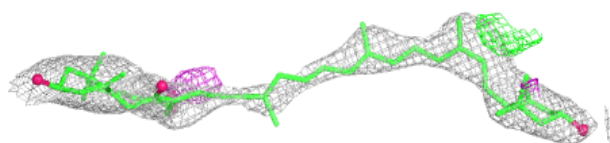
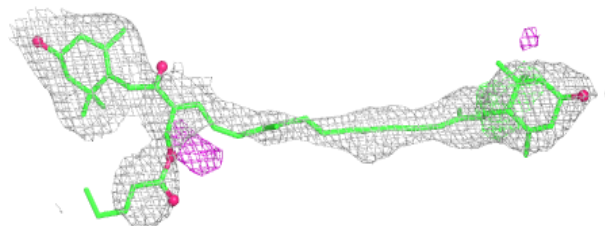


Electron density around 0UR A 322:

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

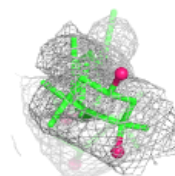
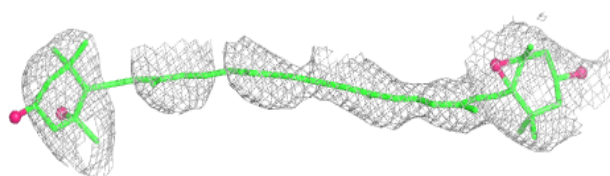
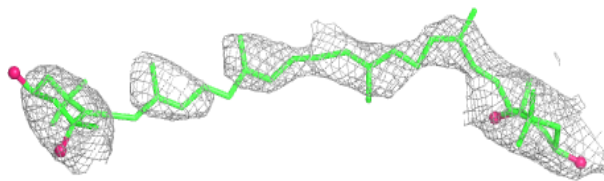
**Electron density around 0UR B 302:**

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



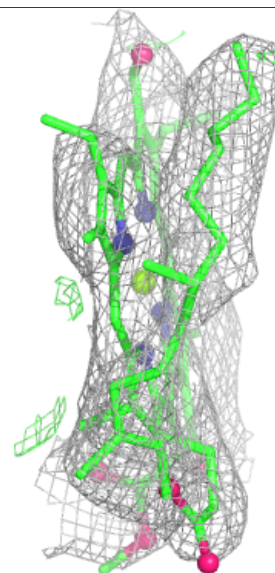
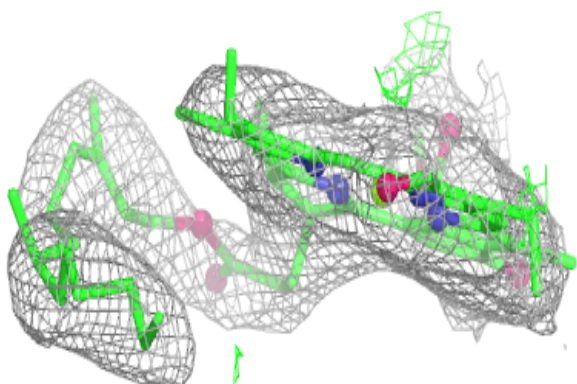
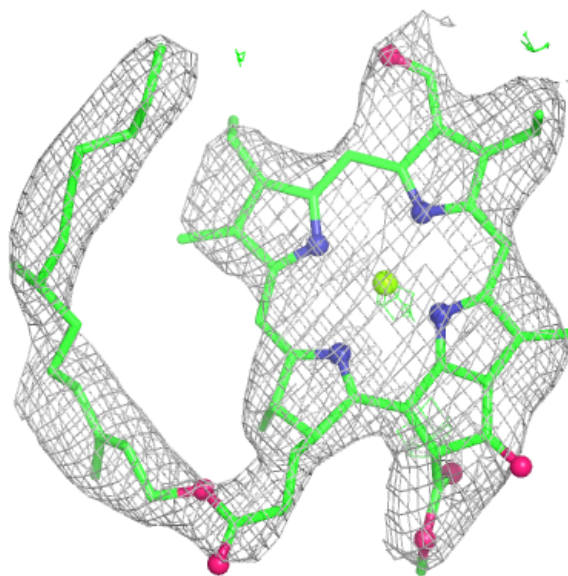
Electron density around NEX C 303:

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



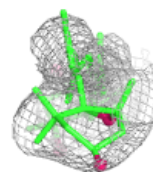
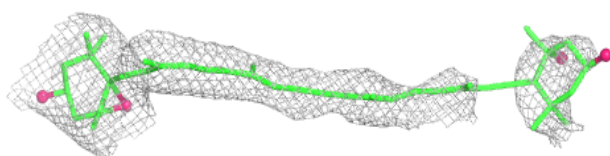
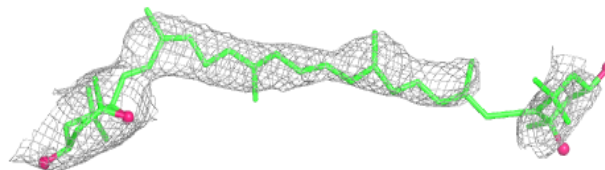
Electron density around CHL E 310:

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

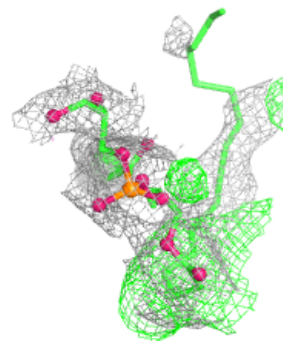
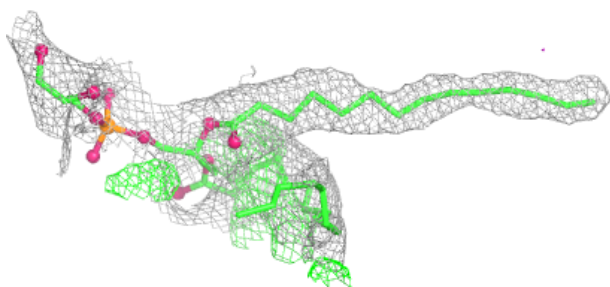
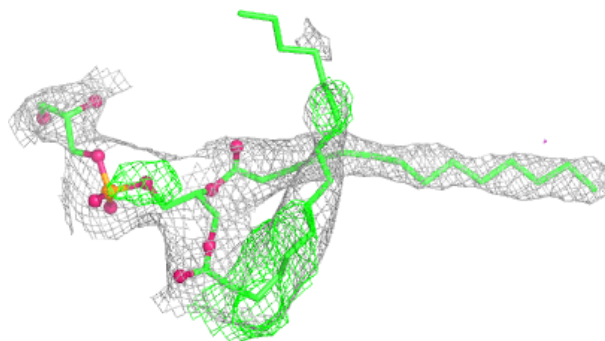


Electron density around NEX A 303:

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

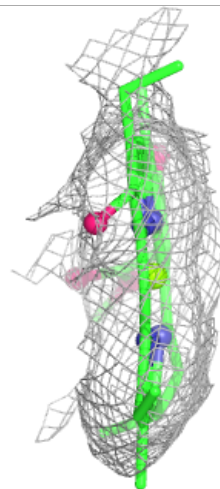
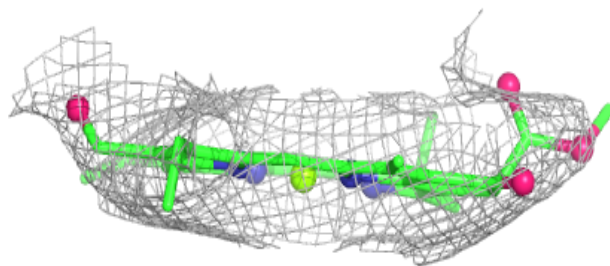
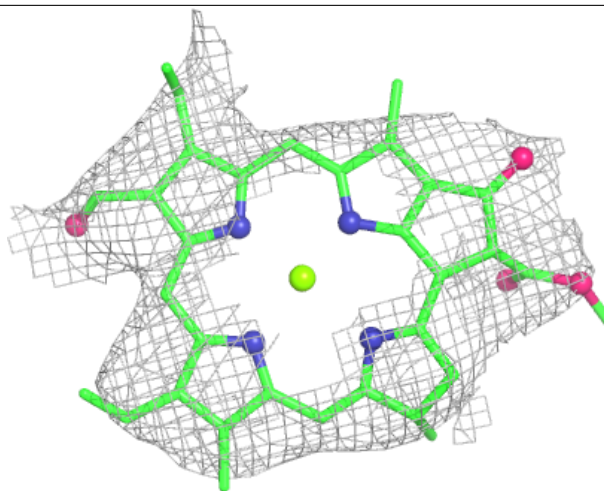
**Electron density around LHG A 319:**

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



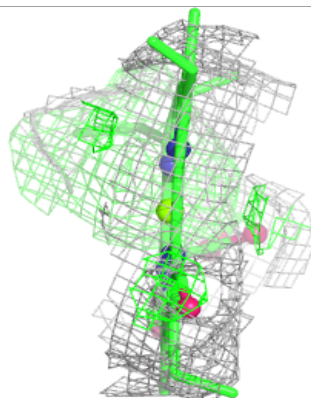
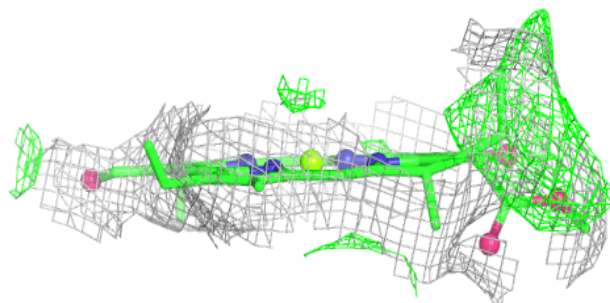
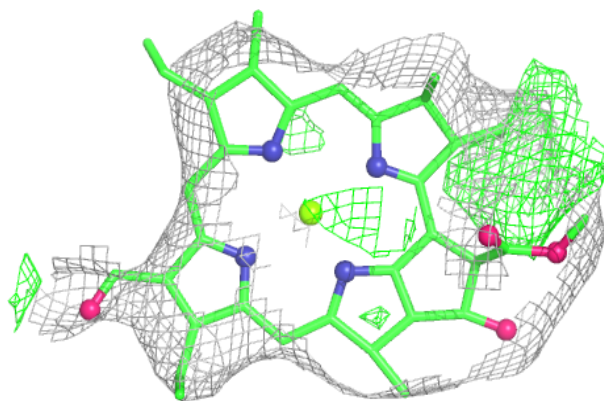
Electron density around CHL E 308:

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

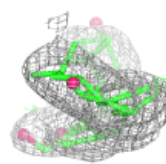
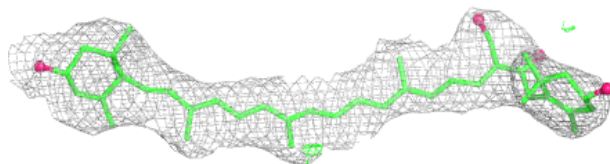
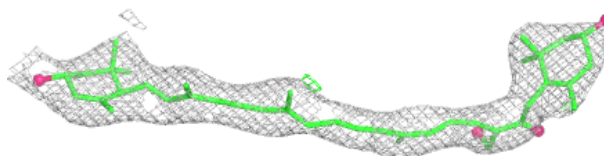


Electron density around CHL E 309:

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

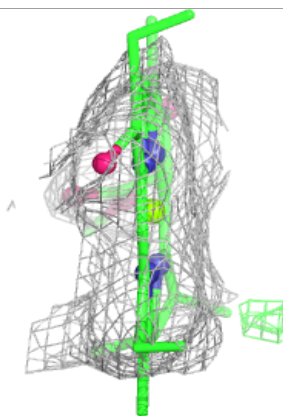
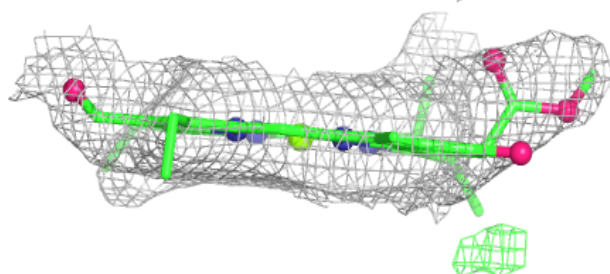
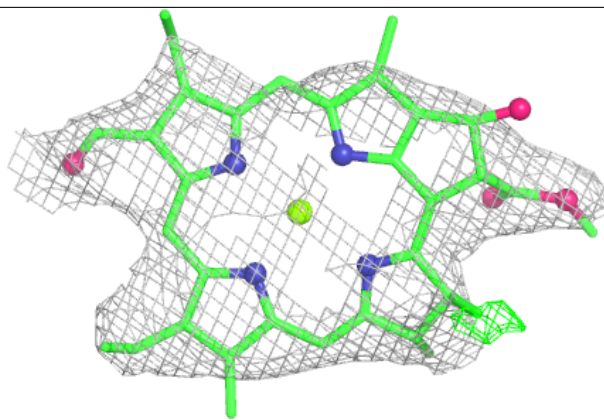
**Electron density around OIE D 302:**

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



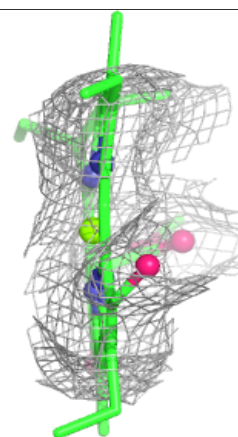
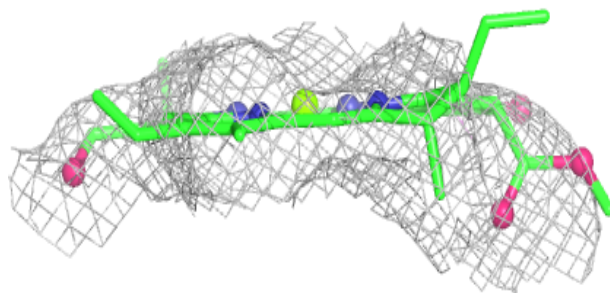
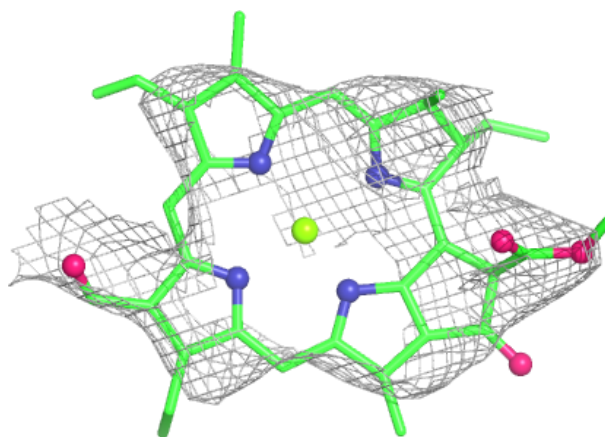
Electron density around CHL F 308:

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



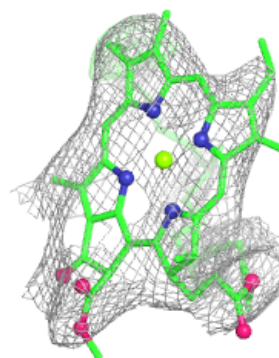
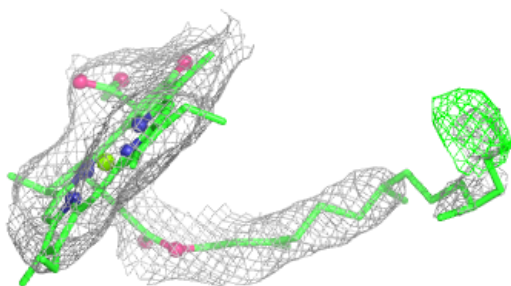
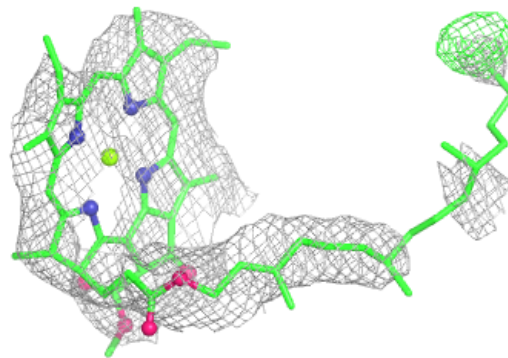
Electron density around CHL B 310:

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



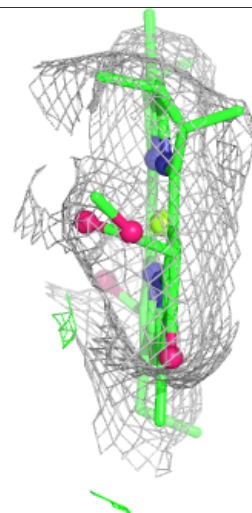
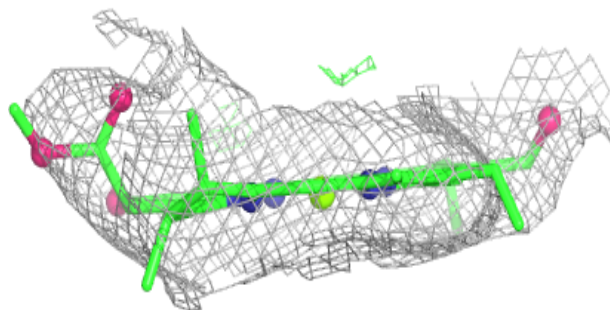
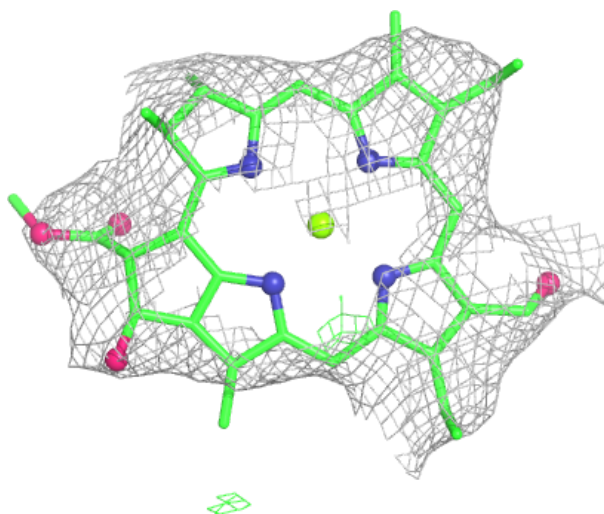
Electron density around CLA E 314:

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



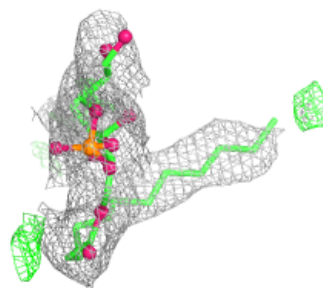
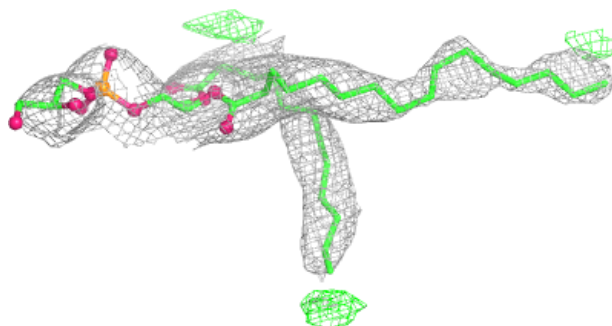
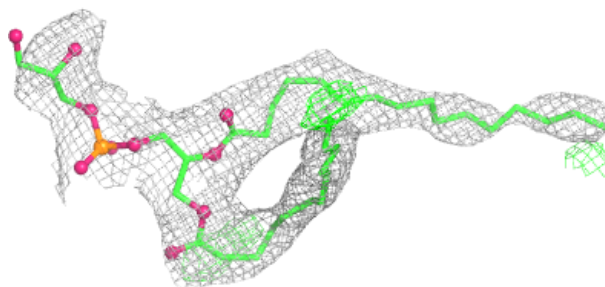
Electron density around CHL C 309:

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

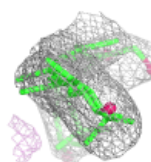
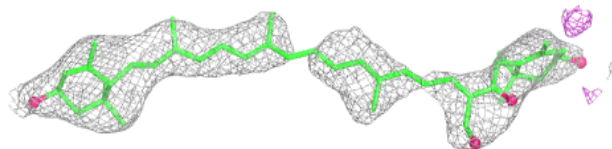
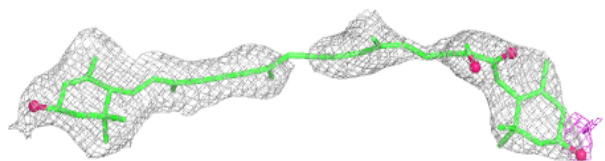


Electron density around LHG C 319:

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

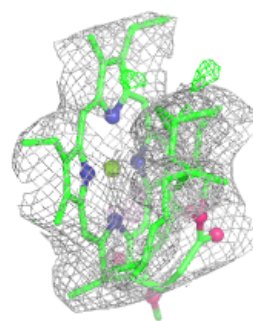
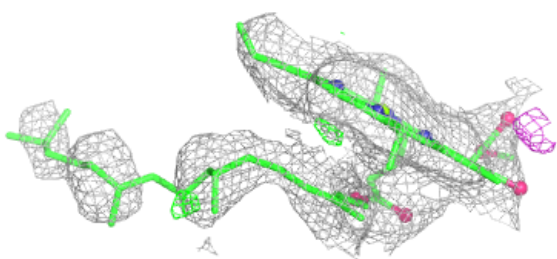
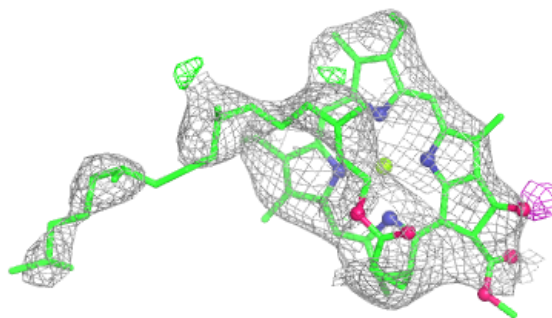
**Electron density around OIE C 302:**

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



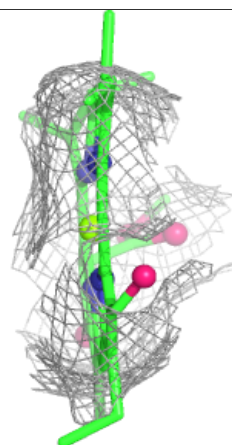
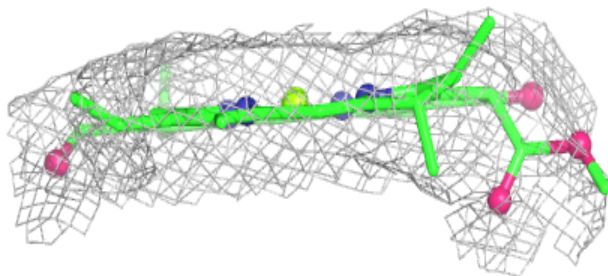
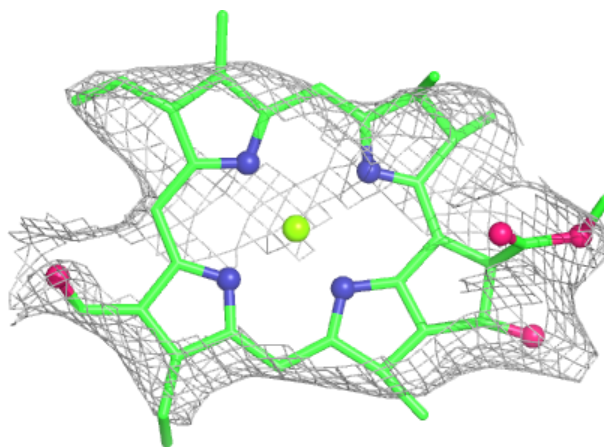
Electron density around CLA D 317:

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



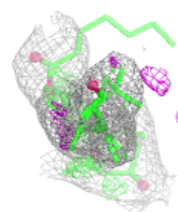
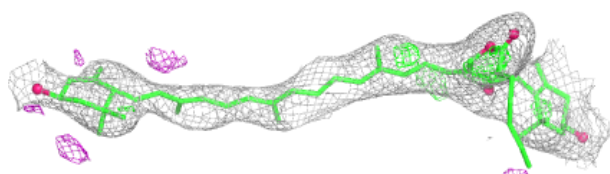
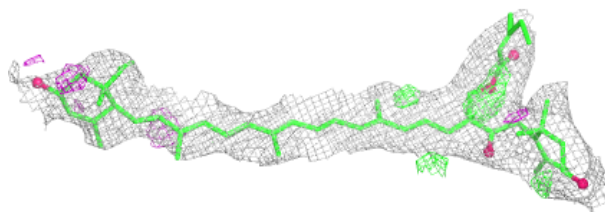
Electron density around CHL D 309:

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

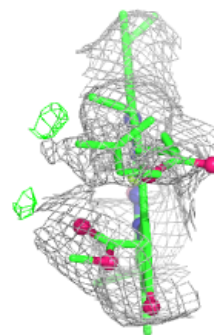
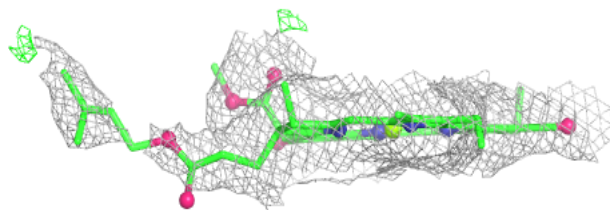
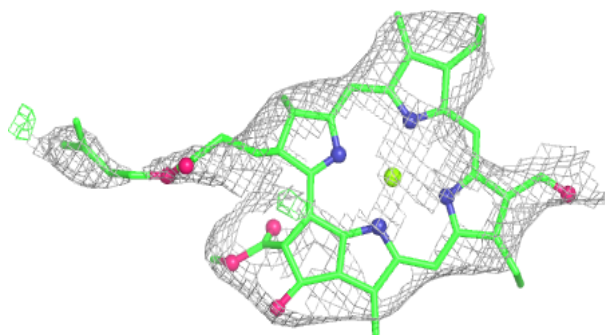


Electron density around 0UR F 320:

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

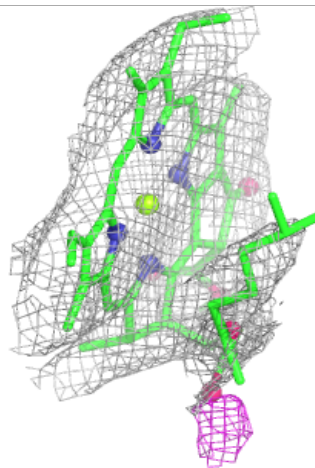
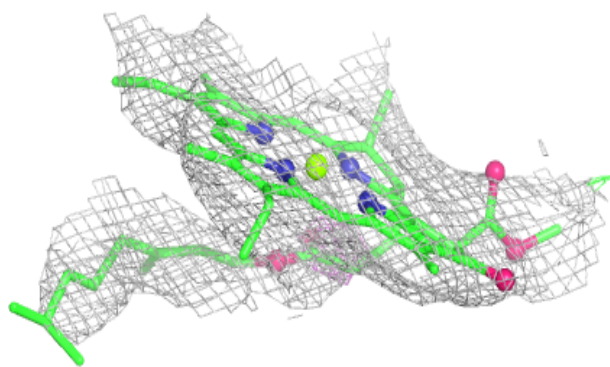
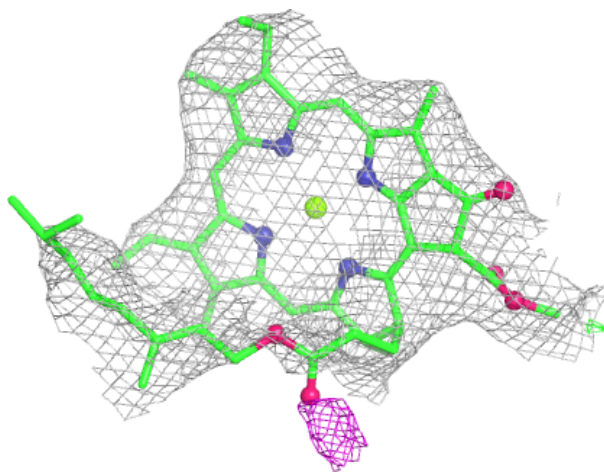
**Electron density around CHL A 310:**

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



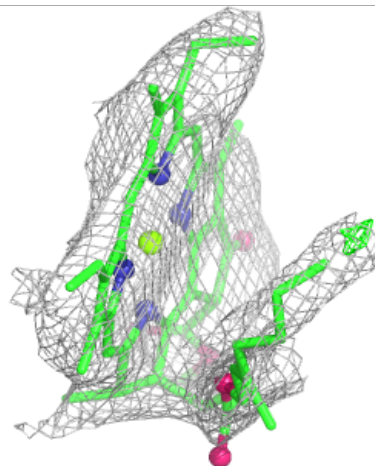
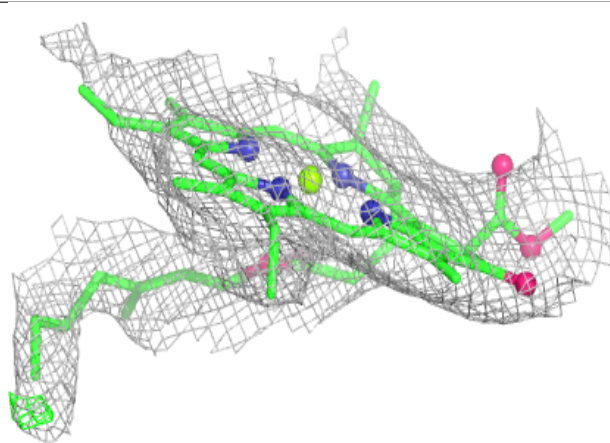
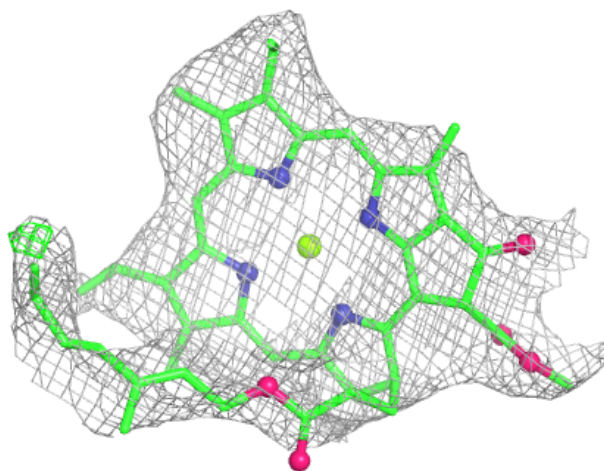
Electron density around CLA E 313:

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



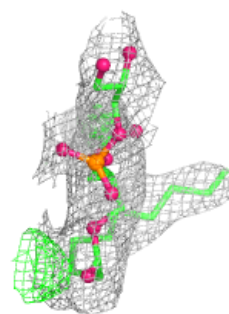
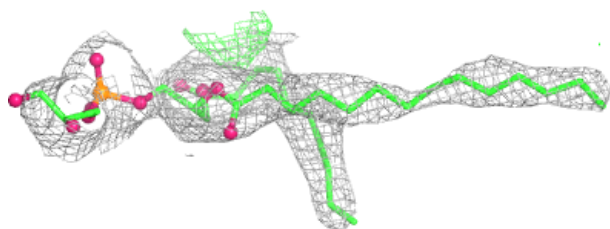
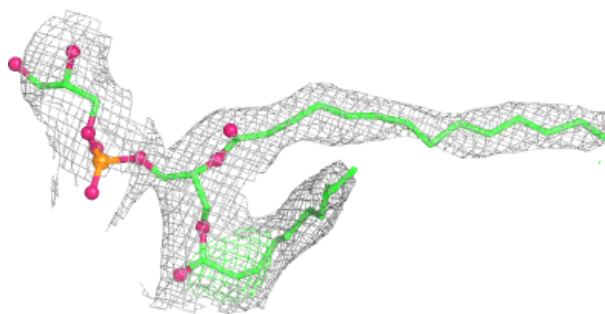
Electron density around CLA C 314:

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

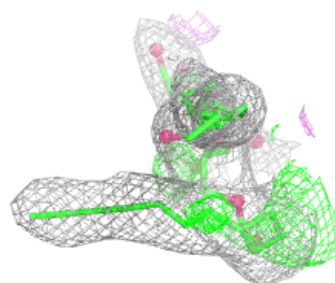
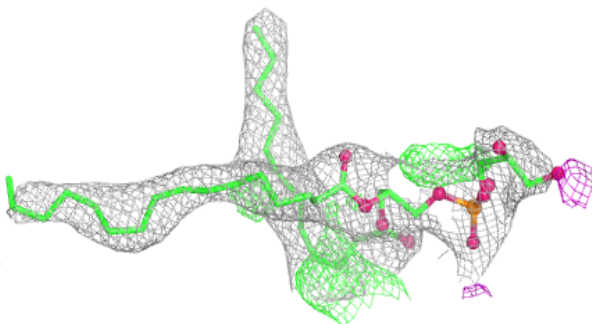
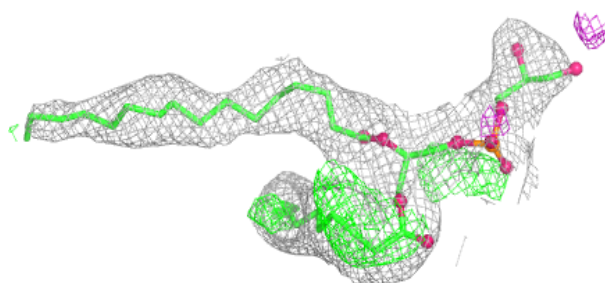


Electron density around LHG E 318:

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

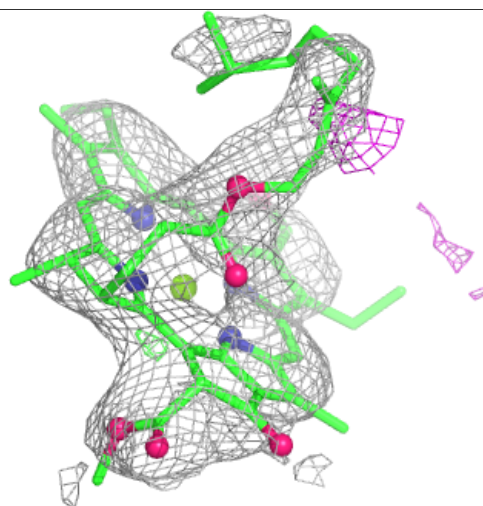
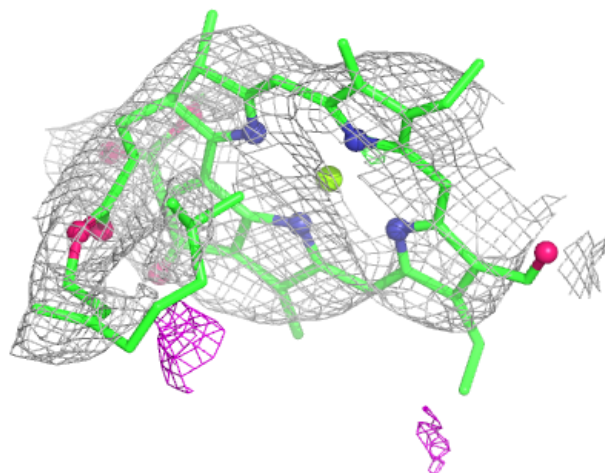
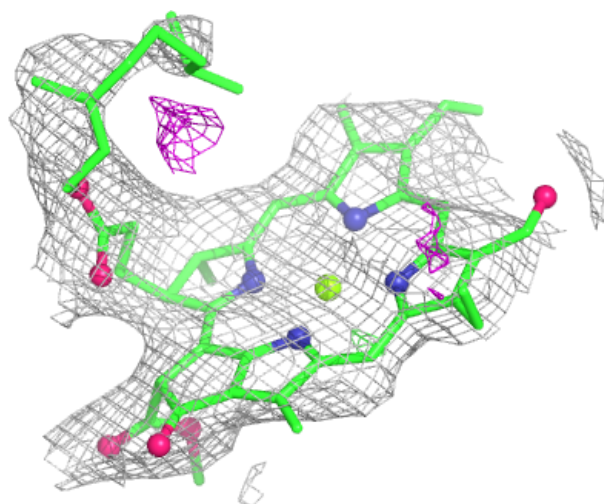
**Electron density around LHG F 318:**

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



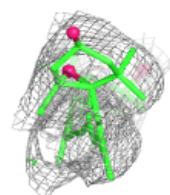
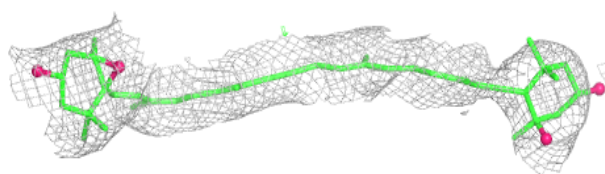
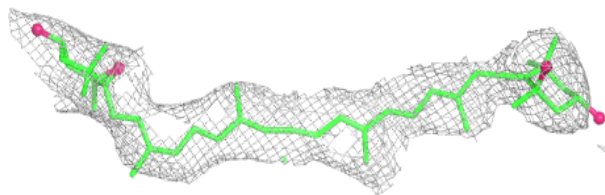
Electron density around CHL E 311:

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

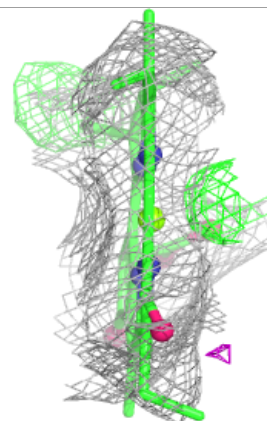
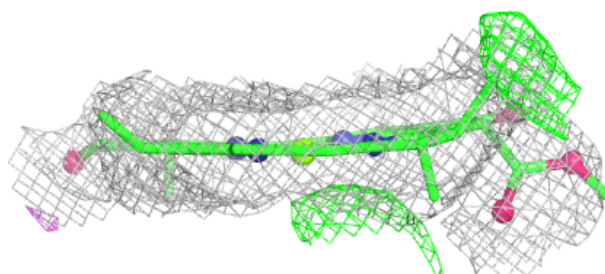
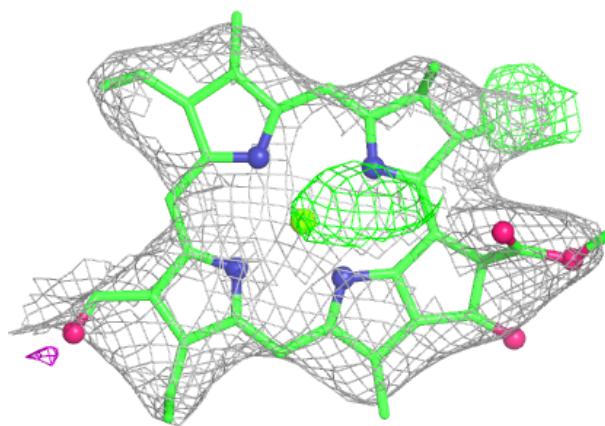


Electron density around NEX B 303:

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

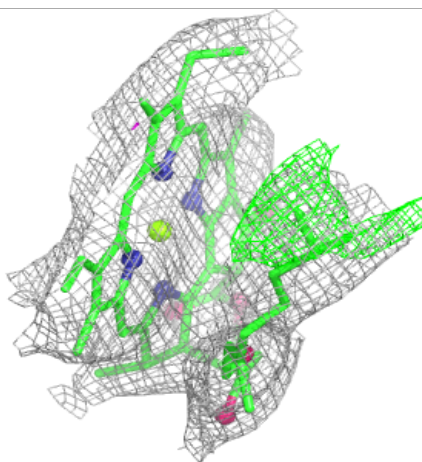
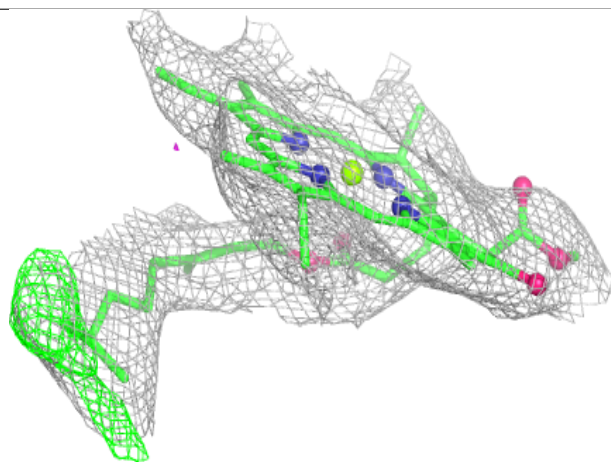
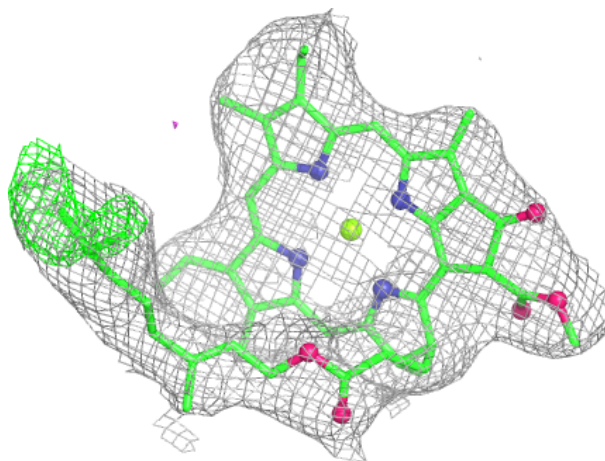
**Electron density around CHL F 309:**

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



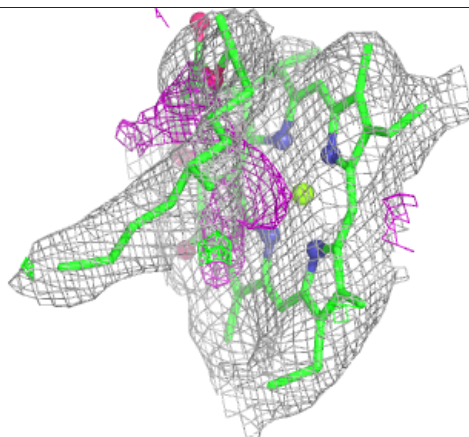
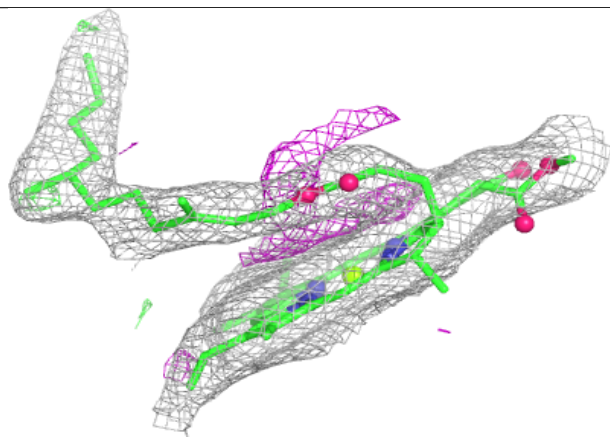
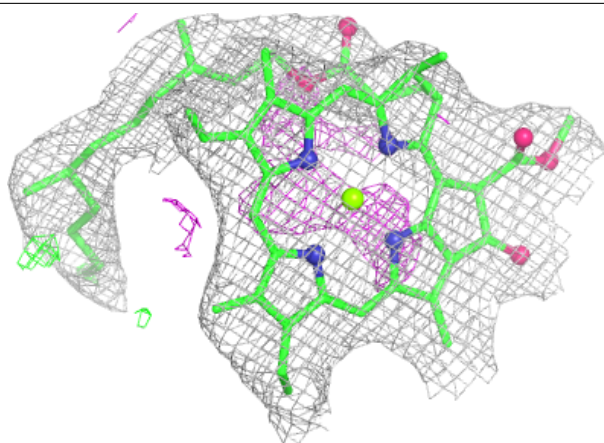
Electron density around CLA A 314:

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



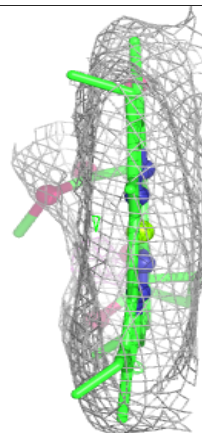
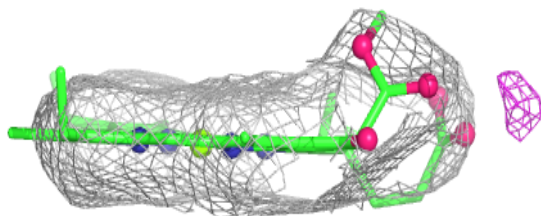
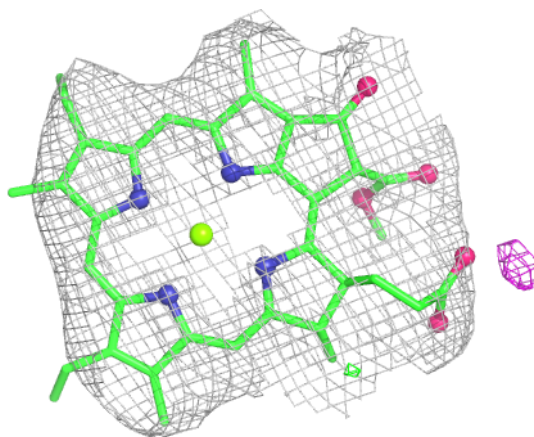
Electron density around CLA B 315:

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



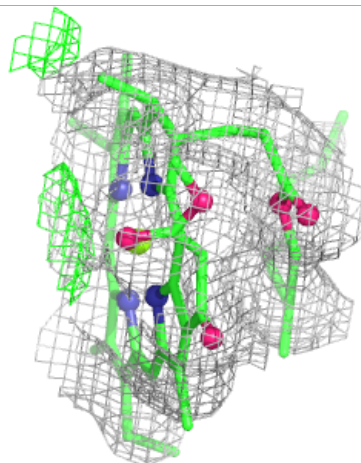
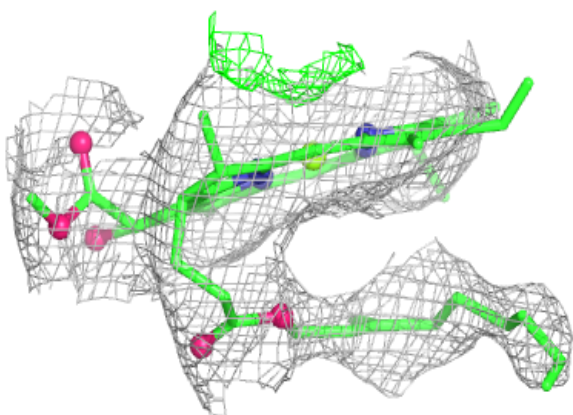
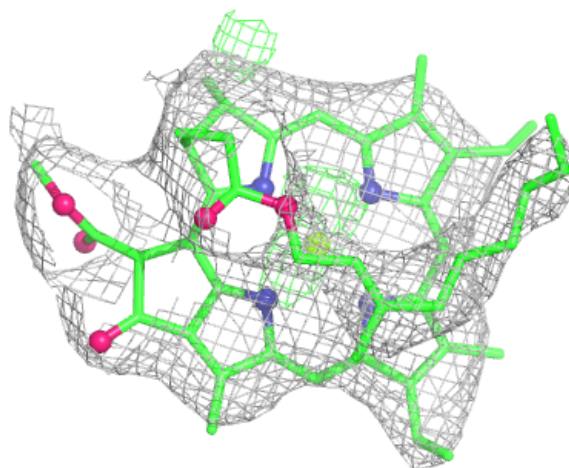
Electron density around CLA E 315:

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



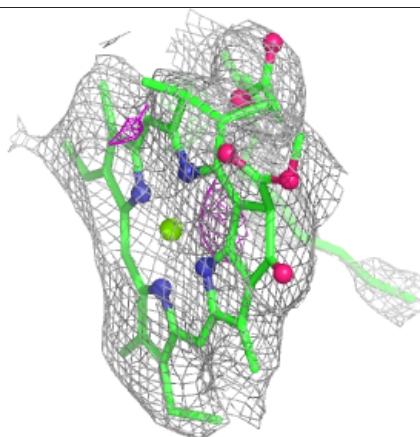
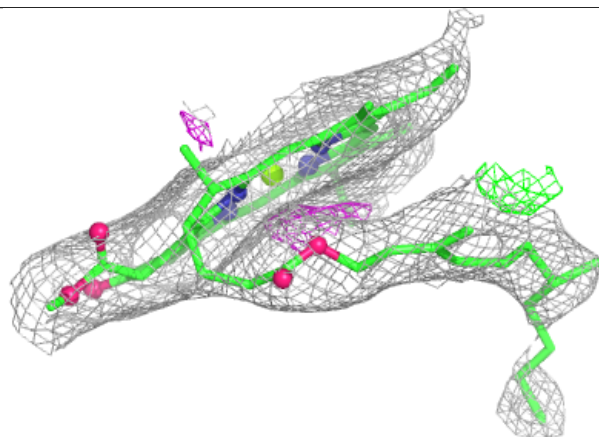
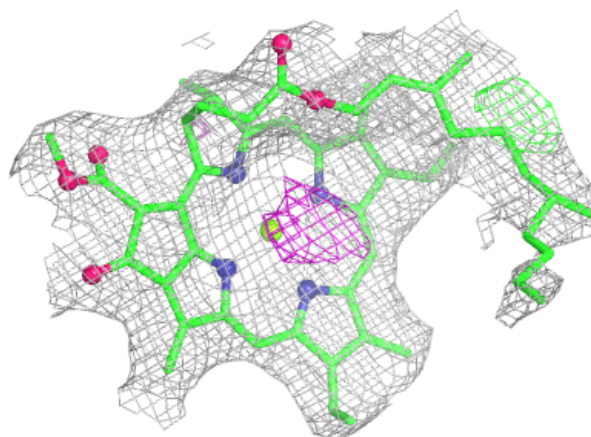
Electron density around CLA E 316:

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

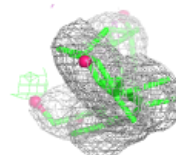
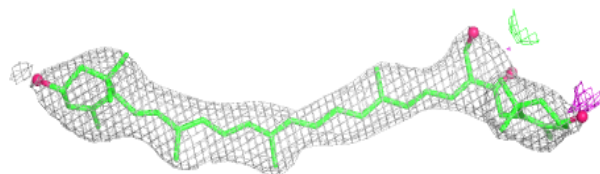


Electron density around CLA F 313:

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

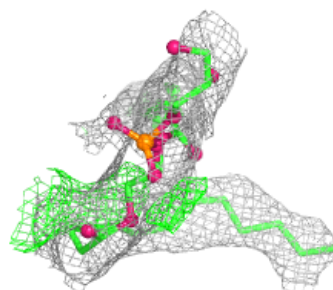
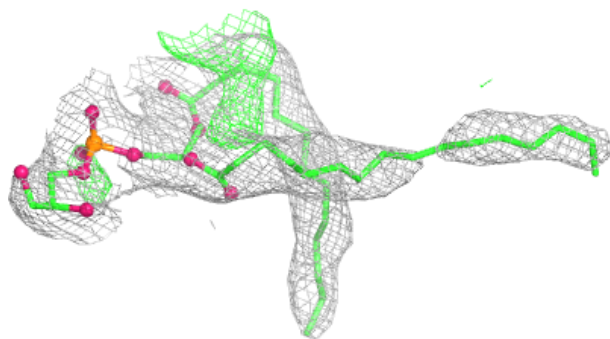
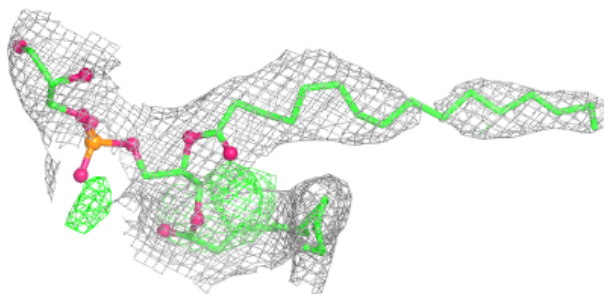
**Electron density around OIE F 302:**

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



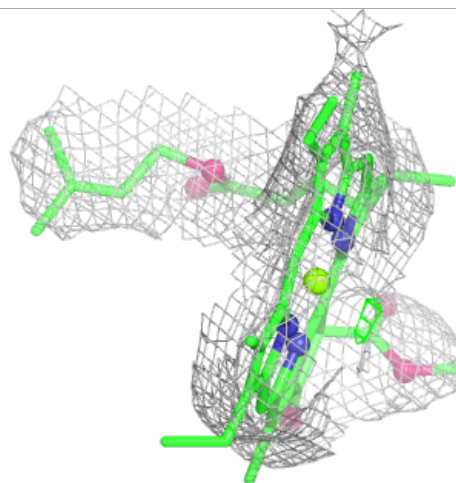
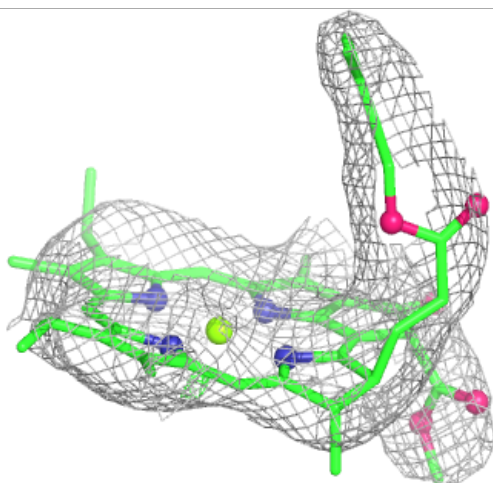
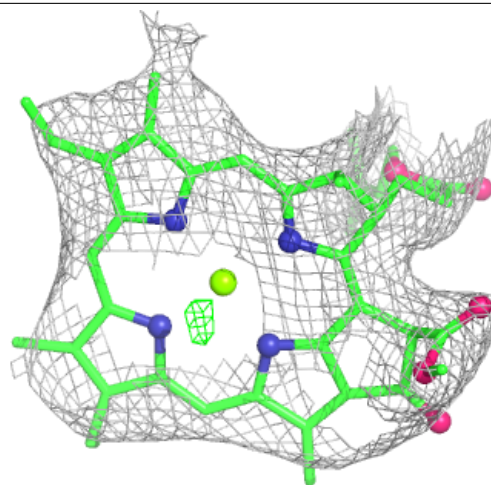
Electron density around LHG B 320:

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



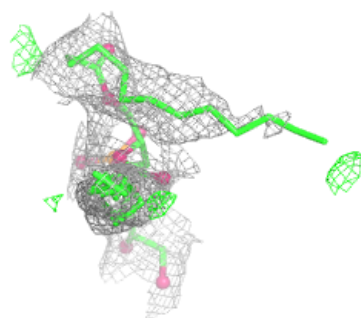
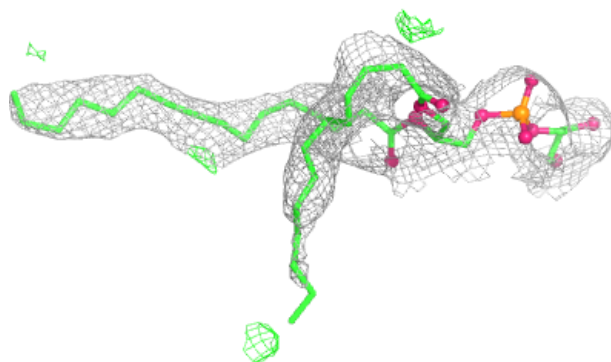
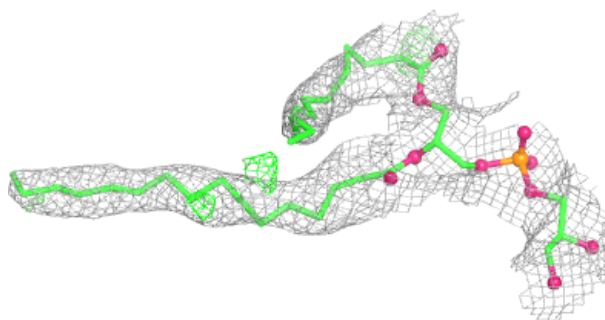
Electron density around CLA A 308:

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



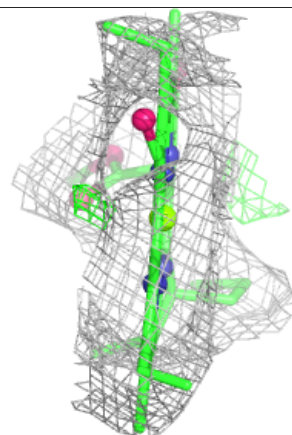
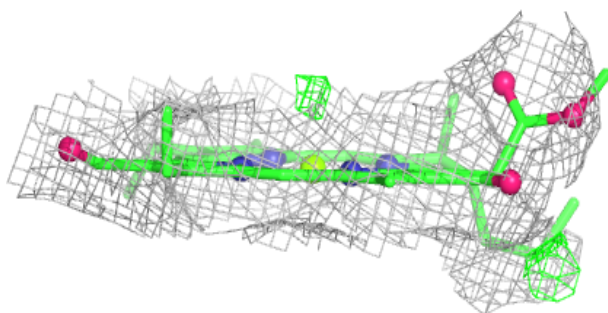
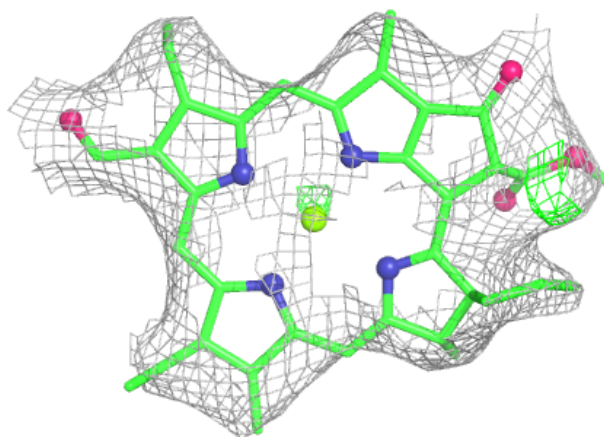
Electron density around LHG D 319:

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



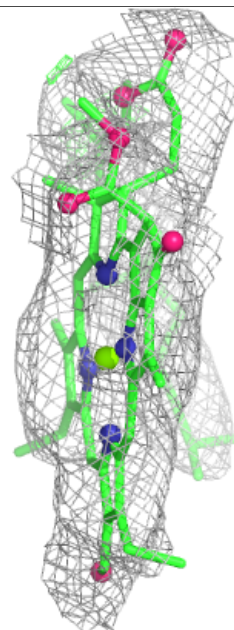
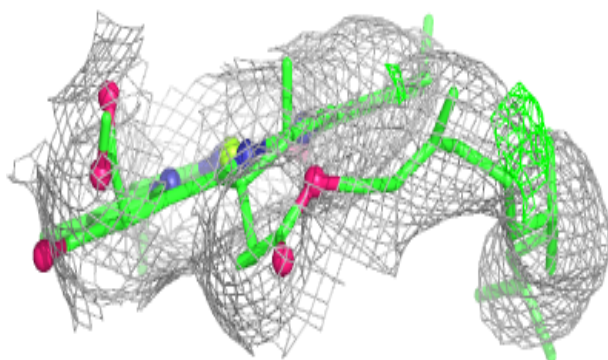
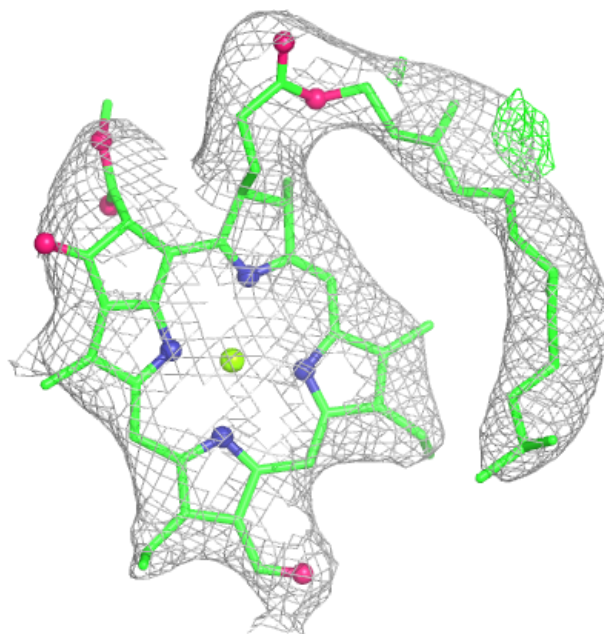
Electron density around CHL C 310:

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



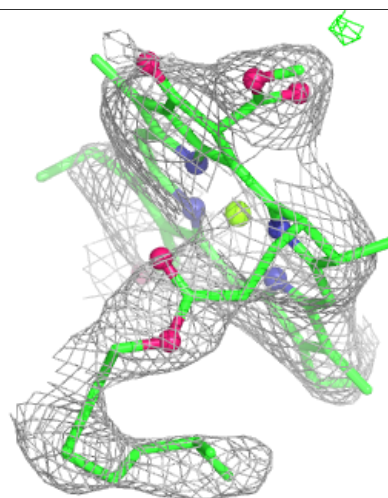
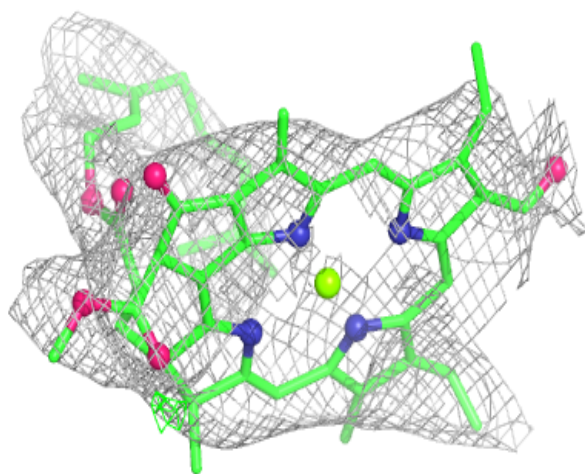
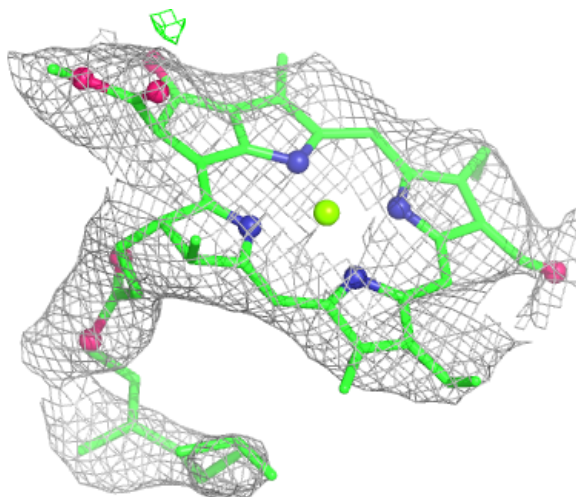
Electron density around CHL C 311:

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



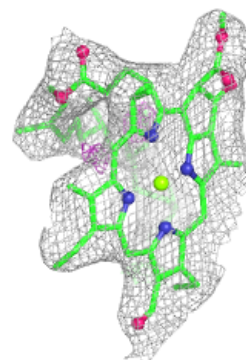
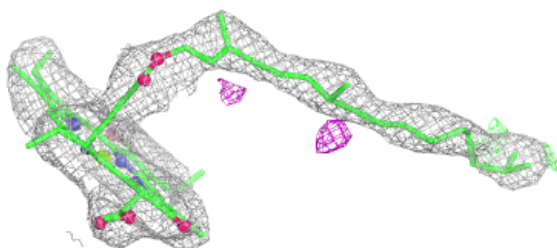
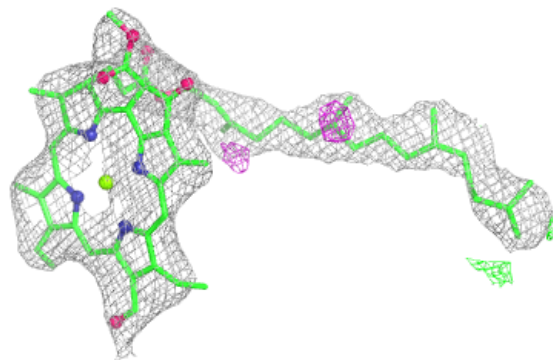
Electron density around CHL C 312:

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



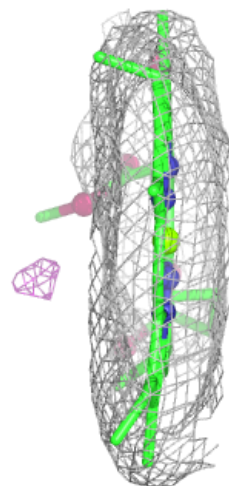
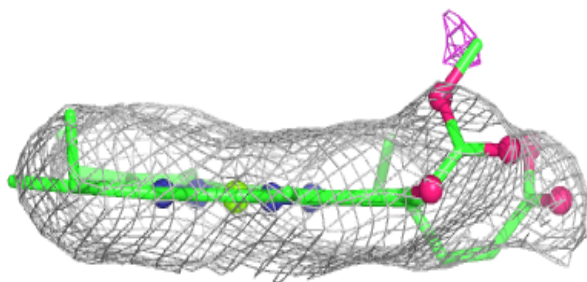
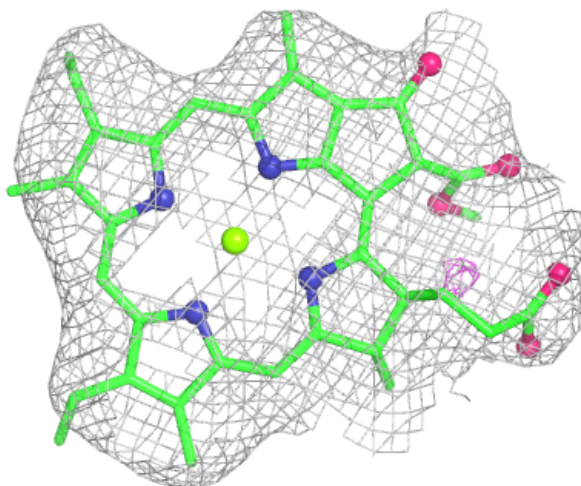
Electron density around CHL C 313:

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



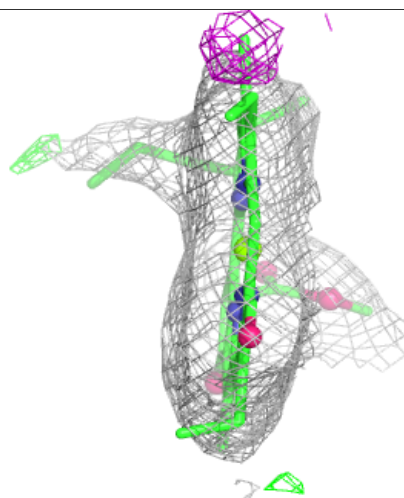
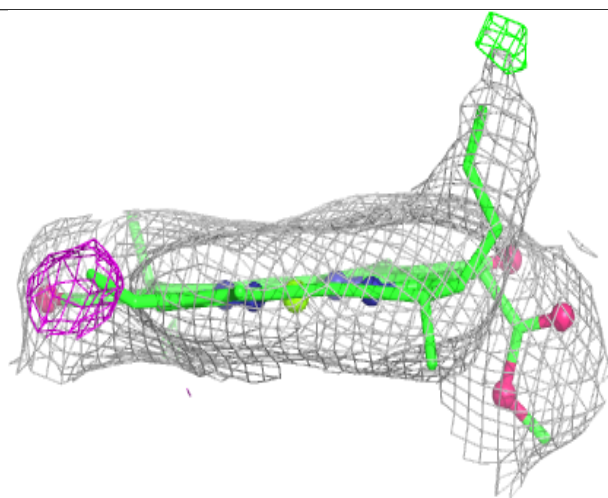
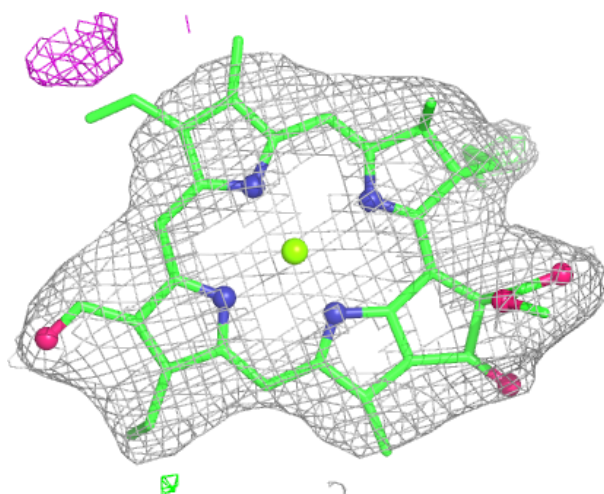
Electron density around CLA C 316:

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



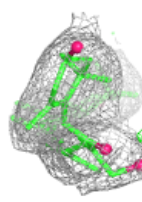
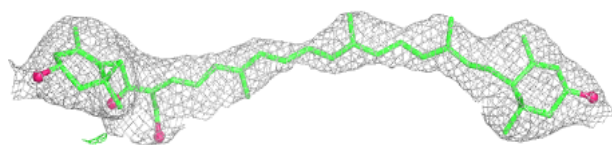
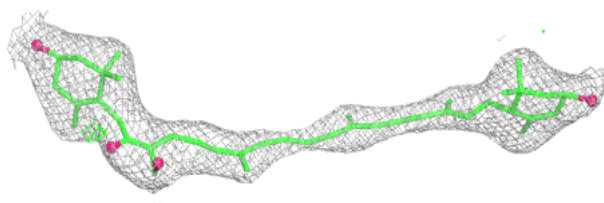
Electron density around CHL C 318:

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



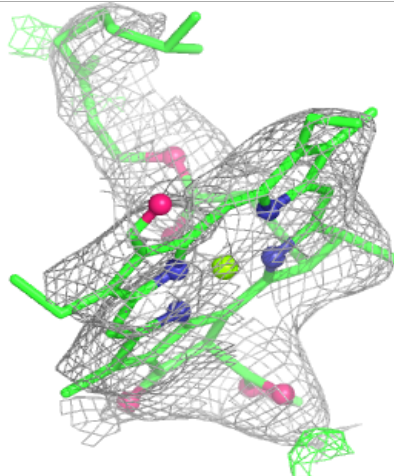
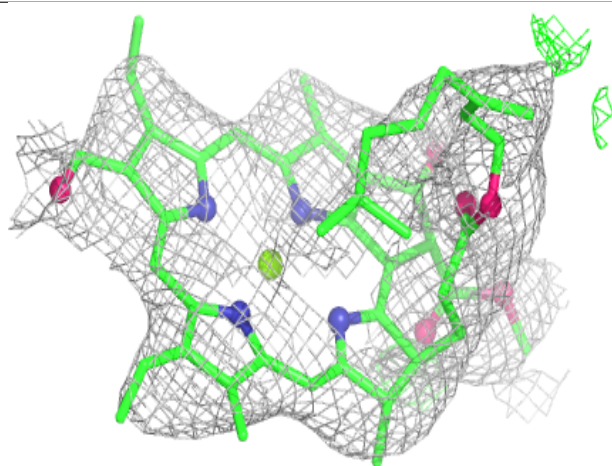
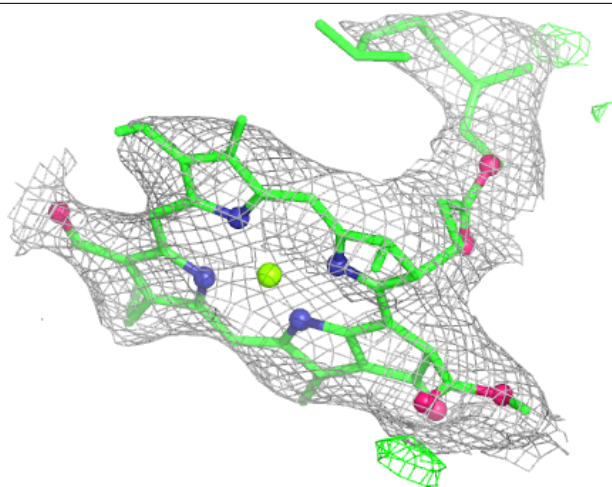
Electron density around OIE A 302:

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



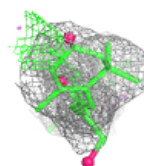
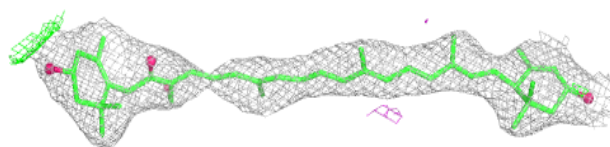
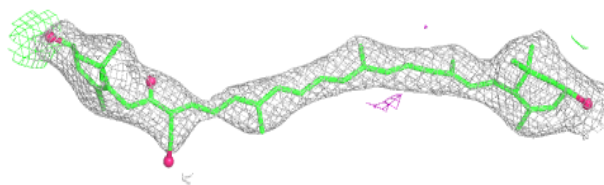
Electron density around CHL A 312:

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

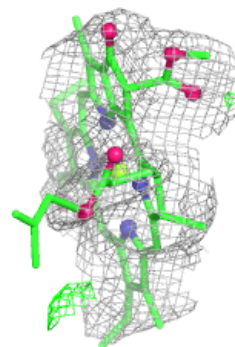
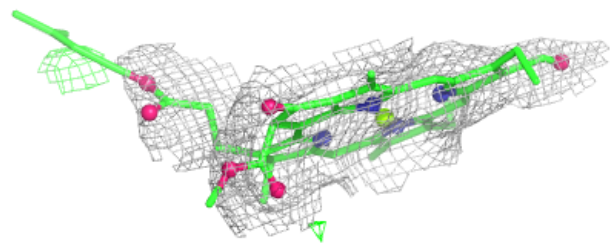
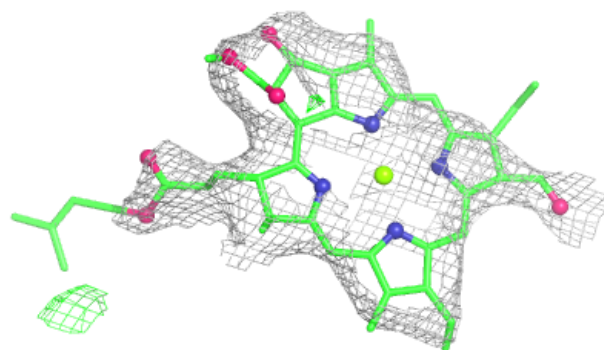


Electron density around OIE C 301:

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

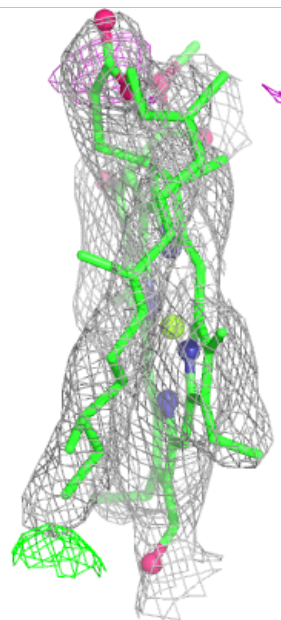
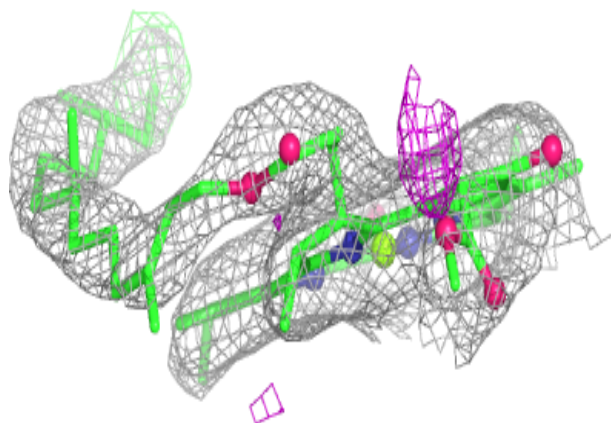
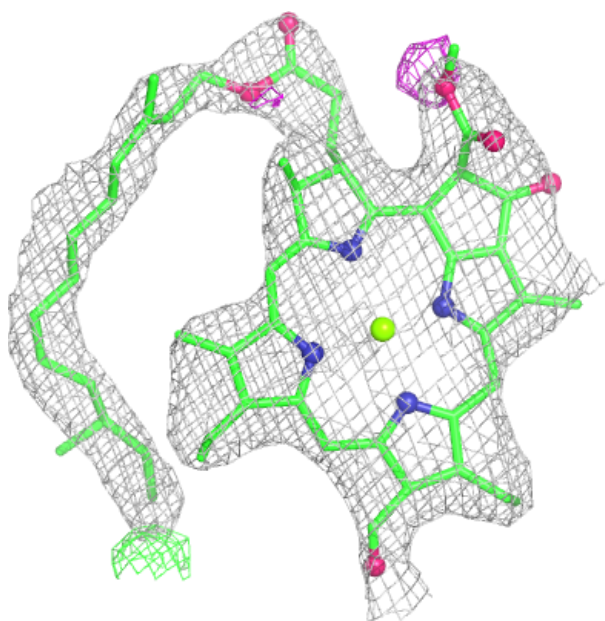
**Electron density around CHL B 311:**

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



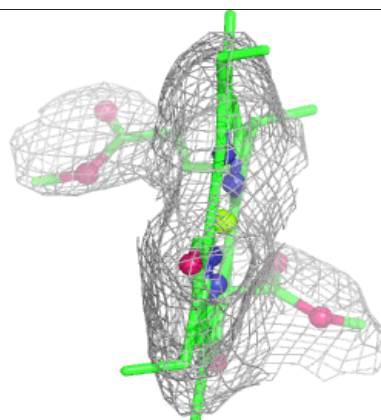
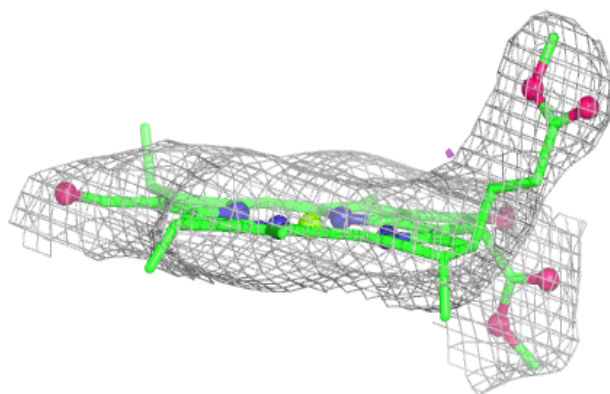
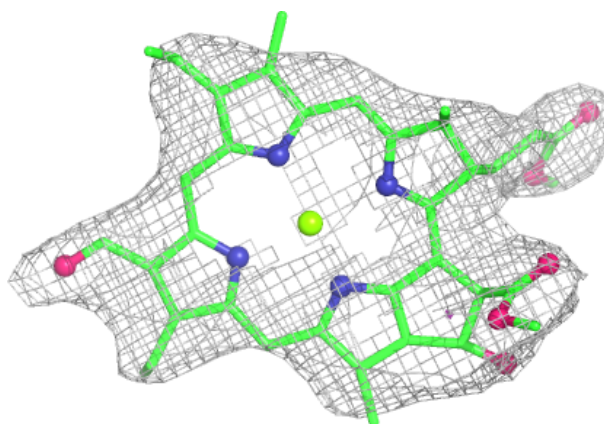
Electron density around CHL B 312:

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

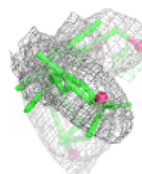
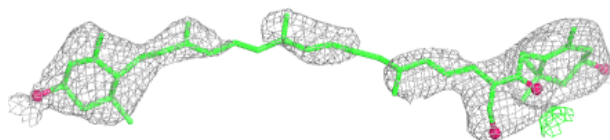
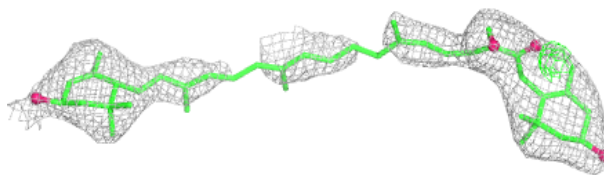


Electron density around CHL B 319:

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

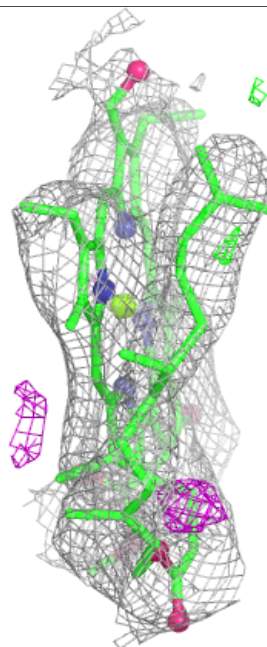
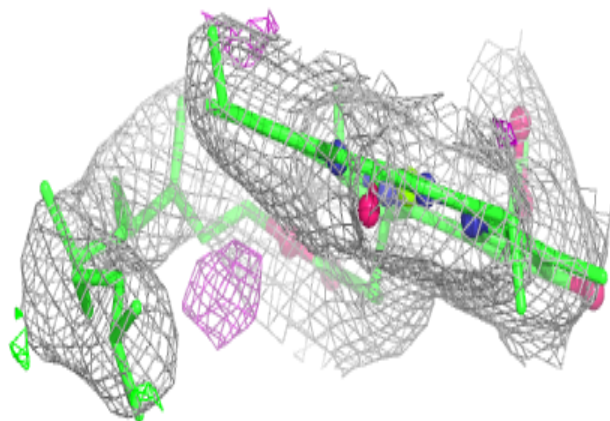
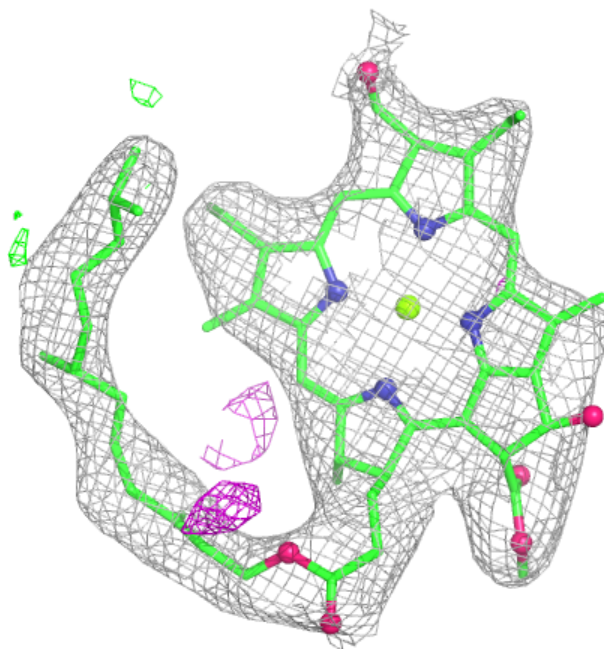
**Electron density around OIE E 302:**

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



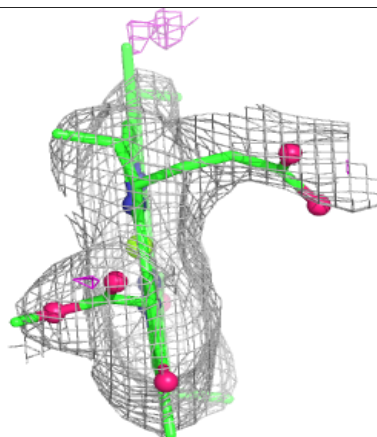
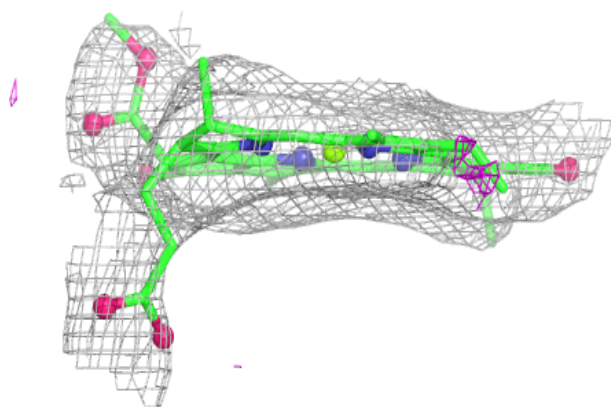
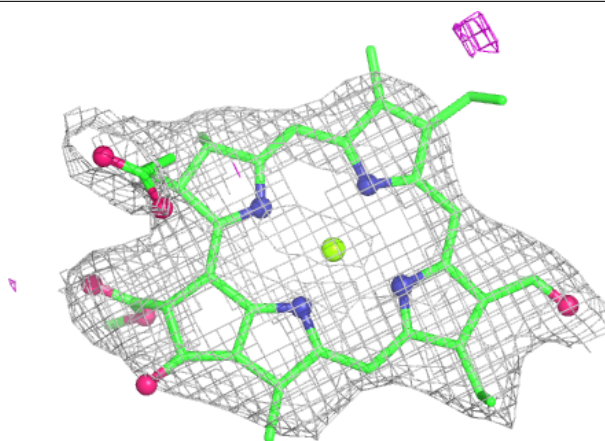
Electron density around CHL F 310:

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



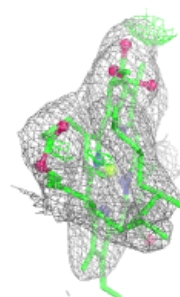
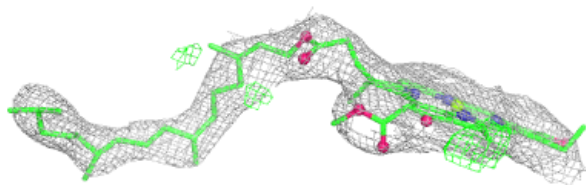
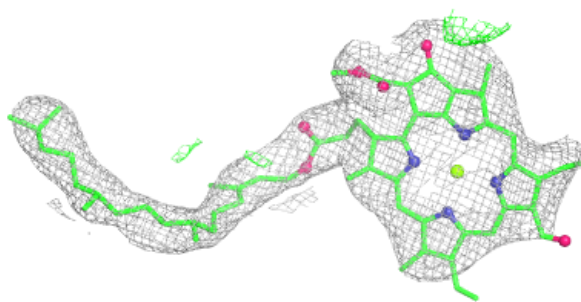
Electron density around CHL F 317:

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



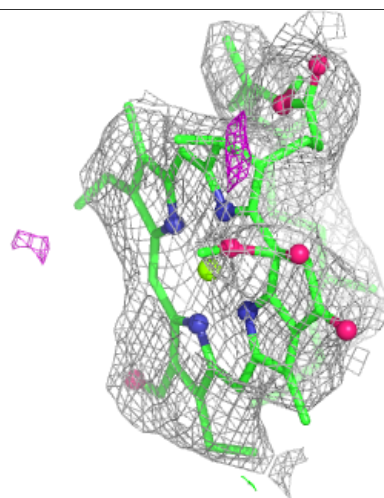
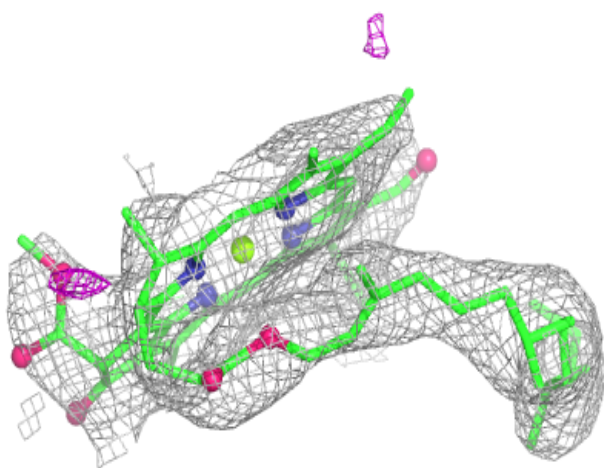
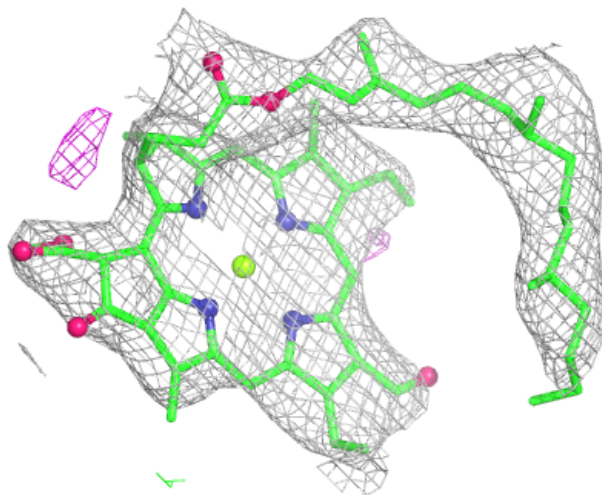
Electron density around CHL E 304:

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



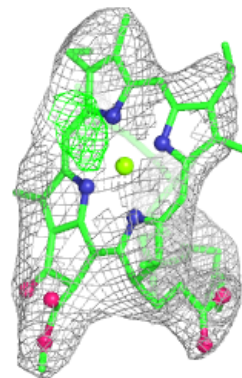
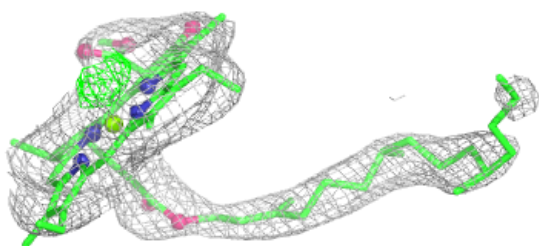
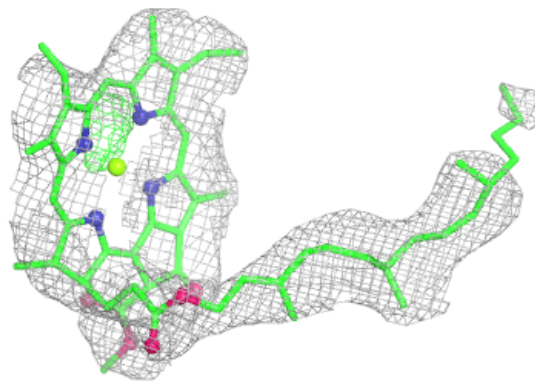
Electron density around CHL E 305:

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



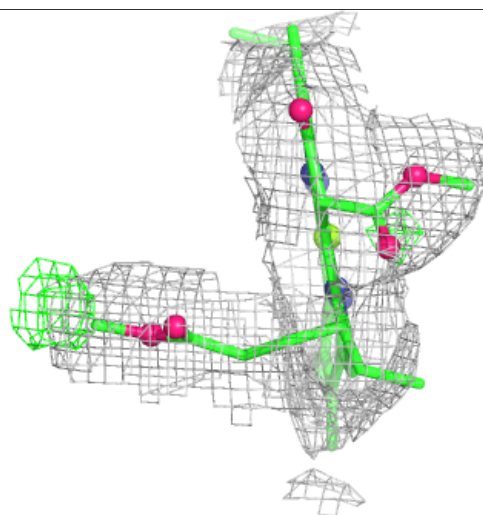
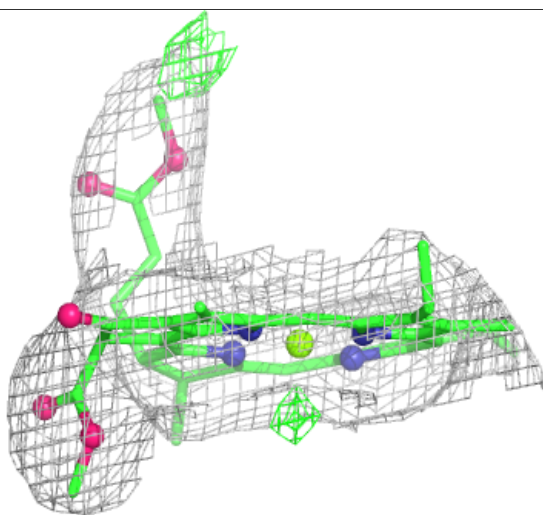
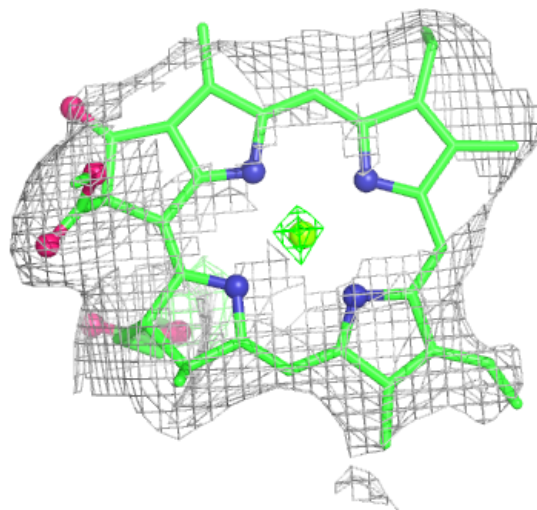
Electron density around CLA A 315:

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



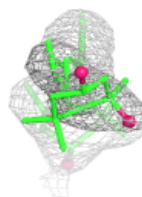
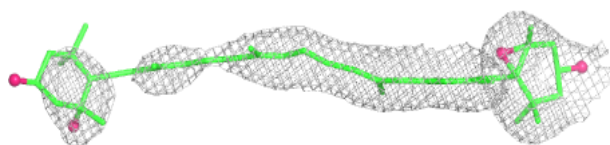
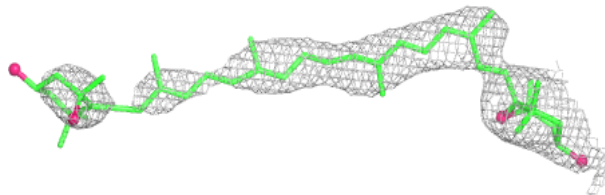
Electron density around CLA B 309:

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

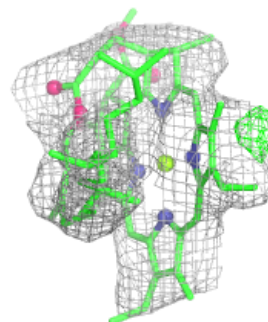
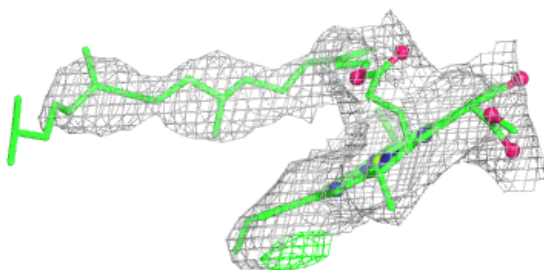
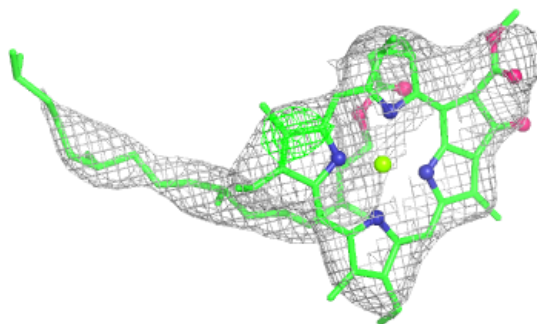


Electron density around NEX D 303:

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

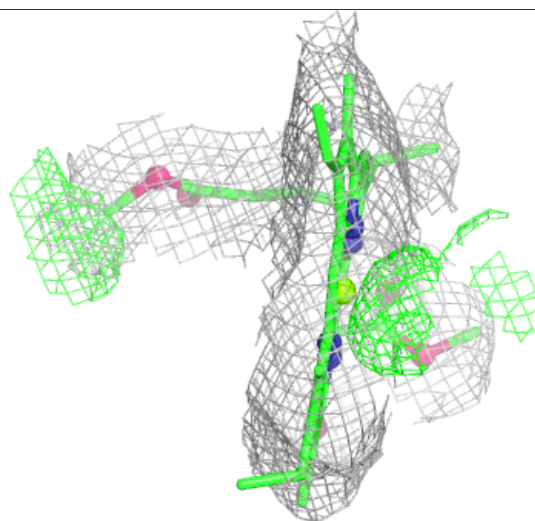
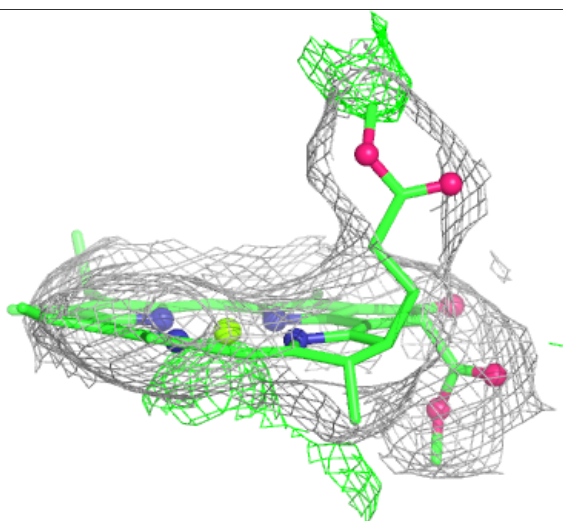
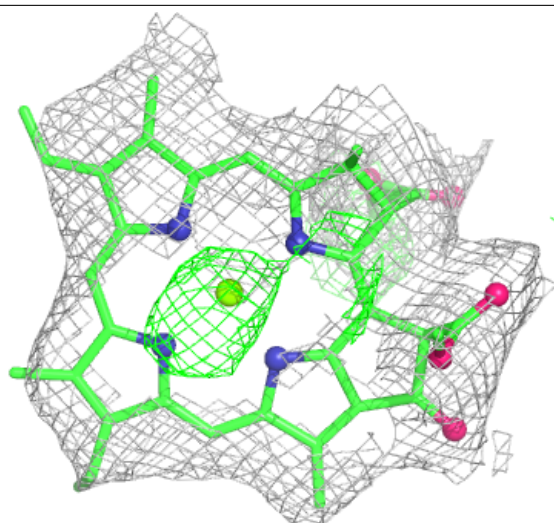
**Electron density around CLA B 318:**

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



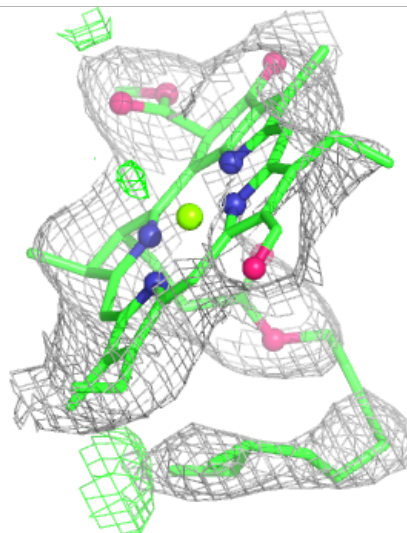
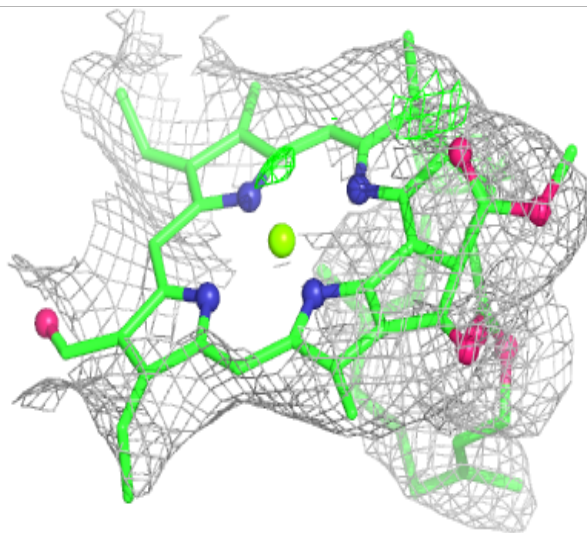
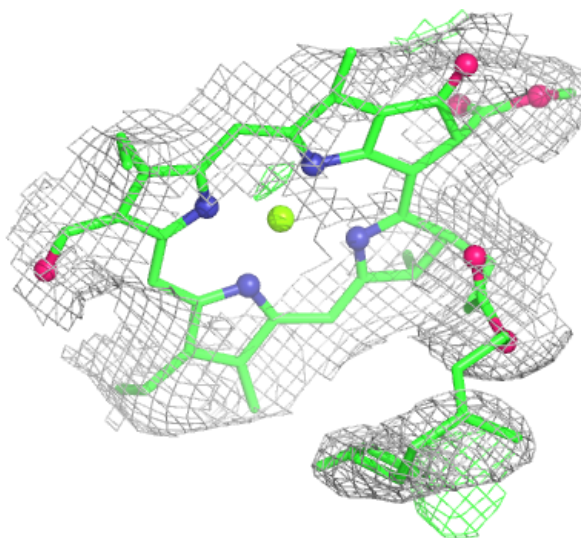
Electron density around CLA C 308:

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



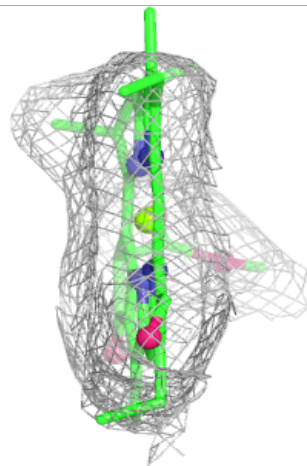
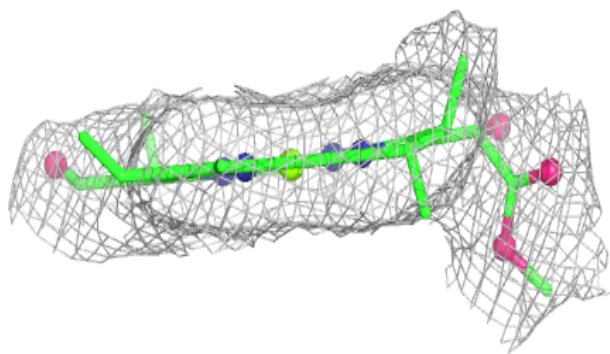
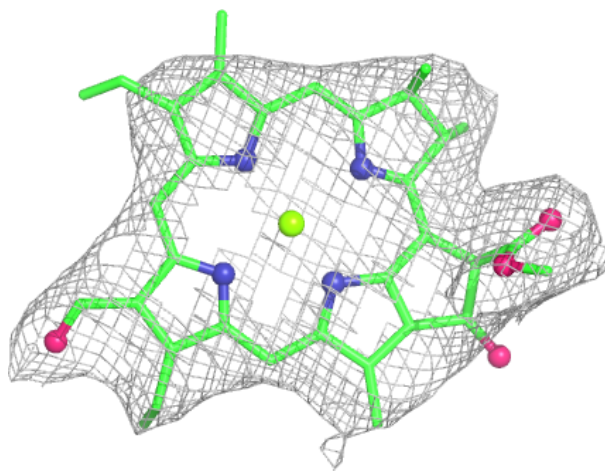
Electron density around CHL B 313:

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



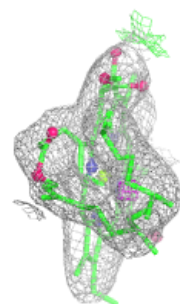
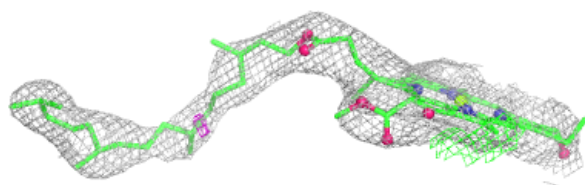
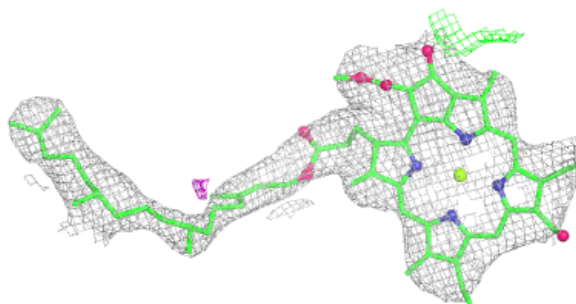
Electron density around CHL A 318:

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



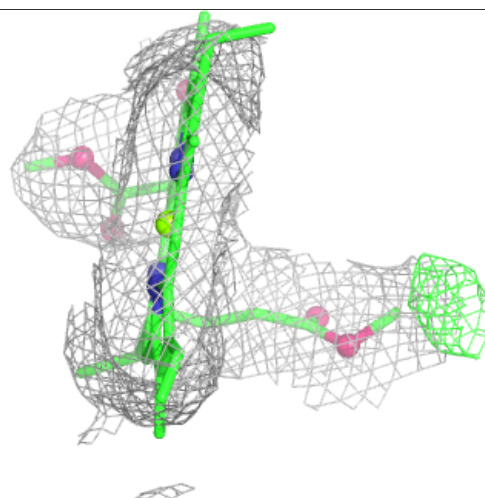
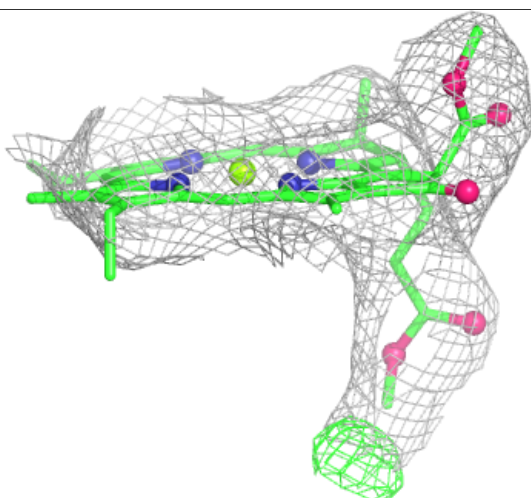
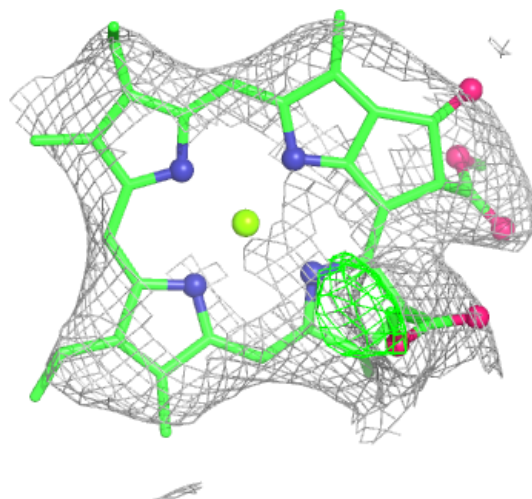
Electron density around CHL A 305:

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



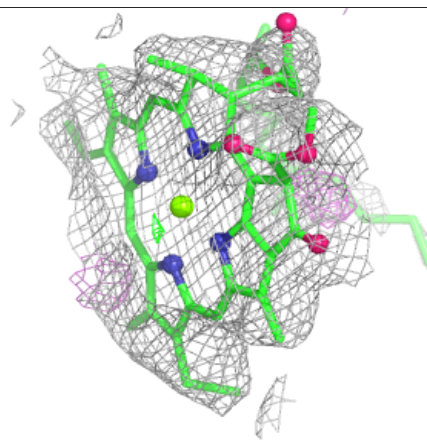
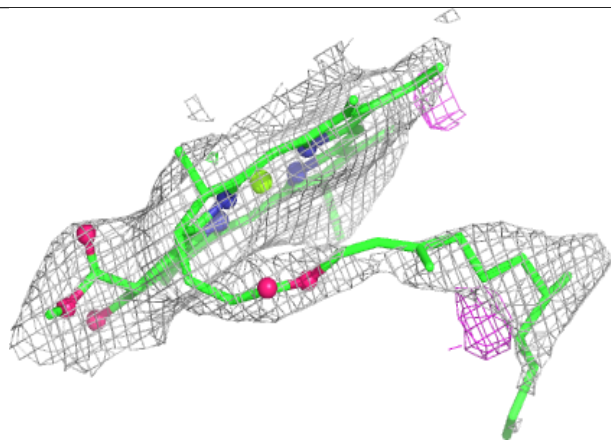
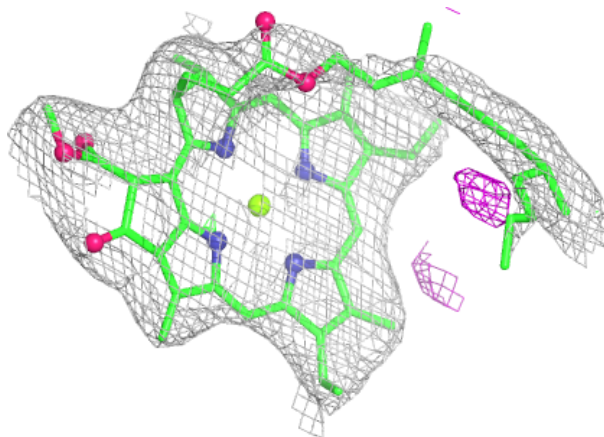
Electron density around CLA D 308:

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



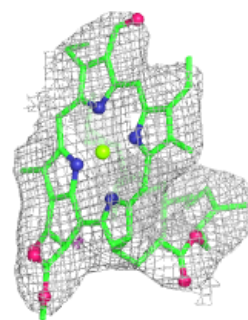
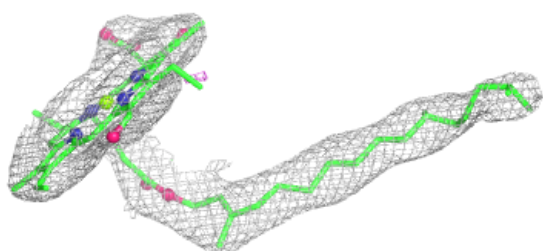
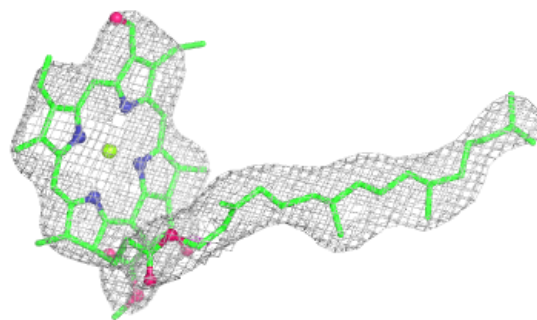
Electron density around CLA D 314:

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



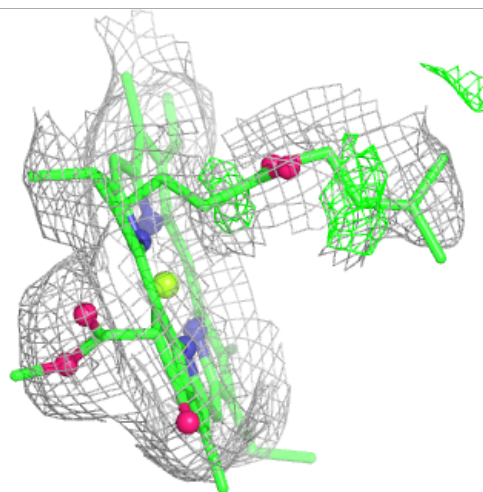
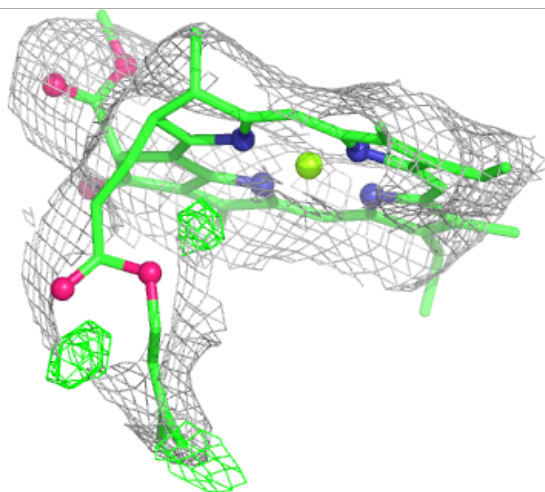
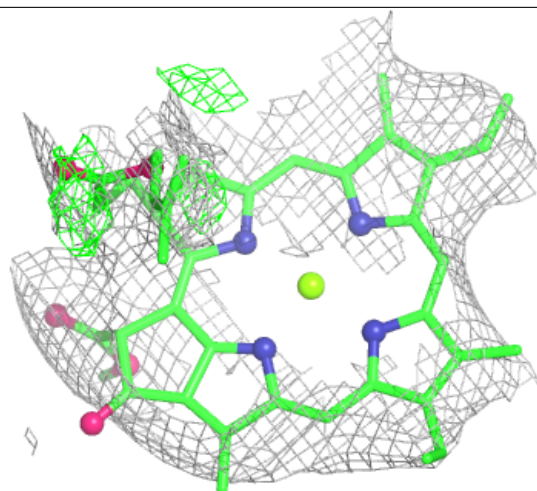
Electron density around CHL E 312:

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



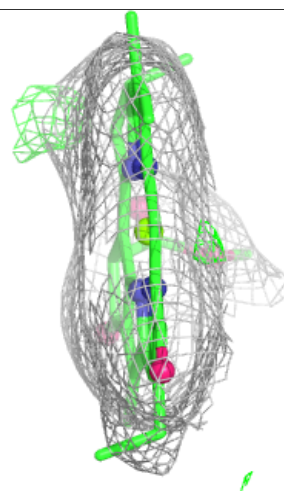
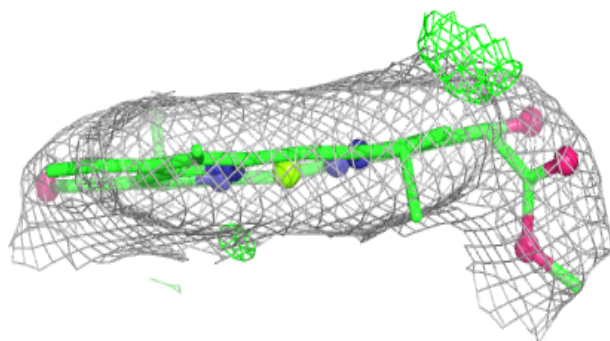
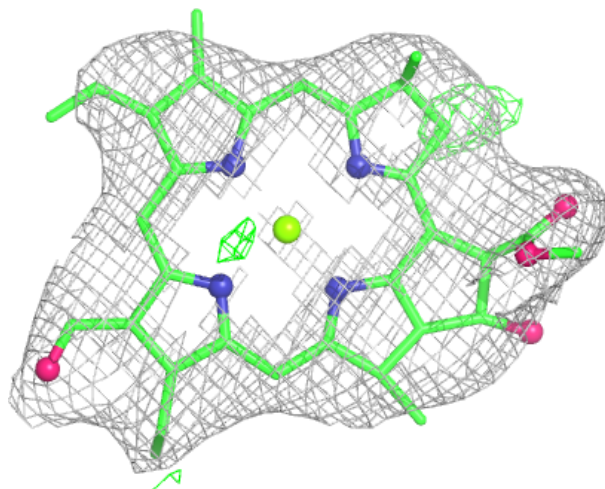
Electron density around CLA E 307:

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



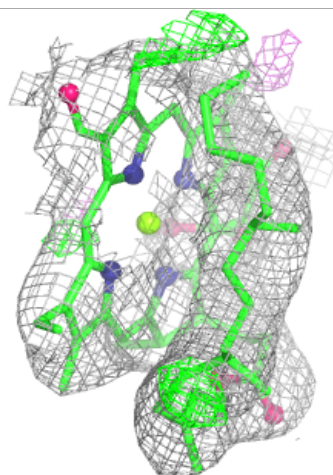
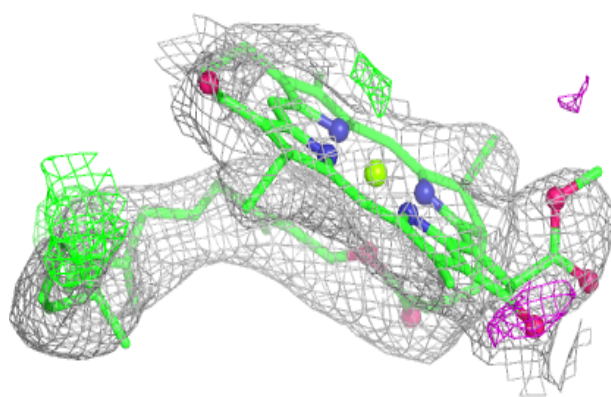
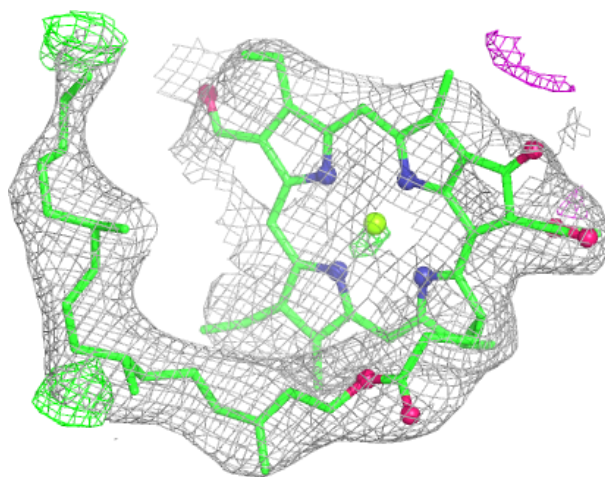
Electron density around CHL E 317:

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



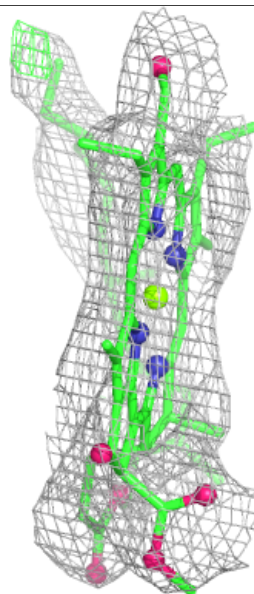
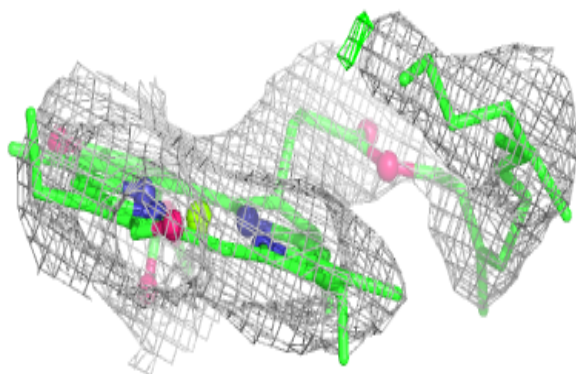
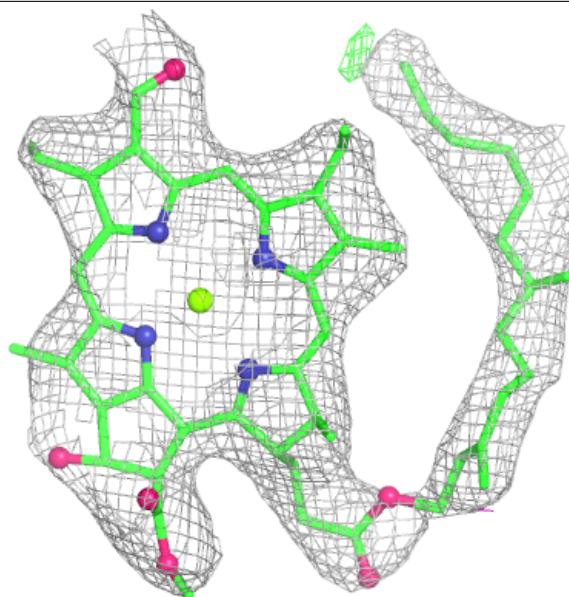
Electron density around CHL D 306:

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



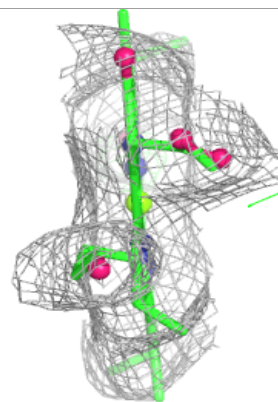
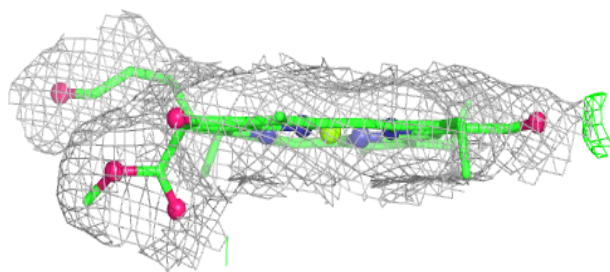
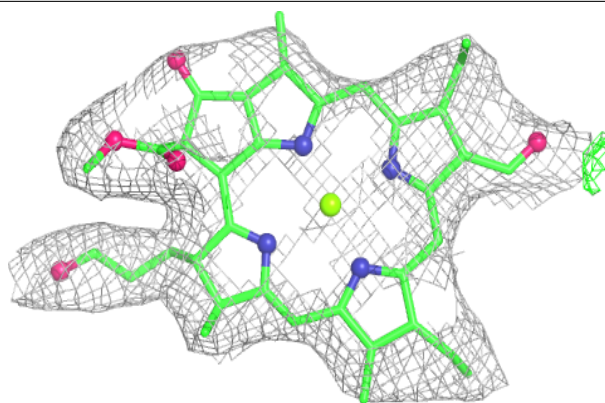
Electron density around CHL A 311:

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



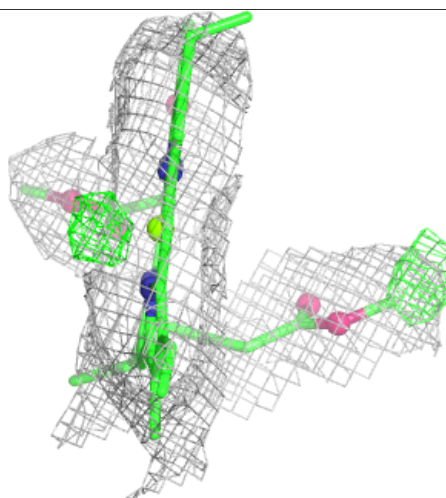
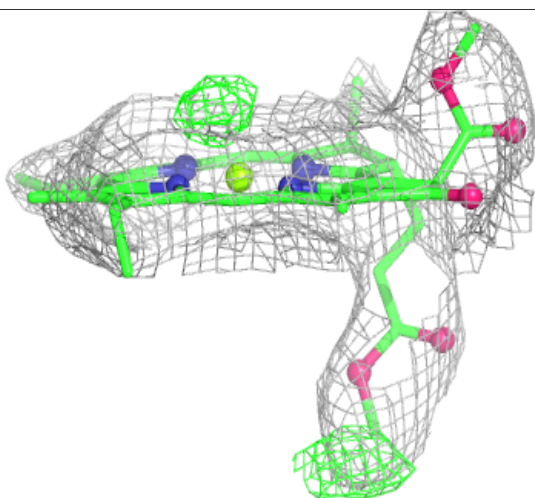
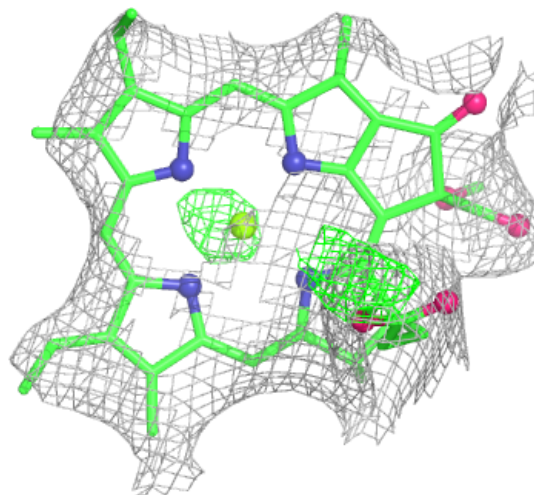
Electron density around CHL D 310:

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



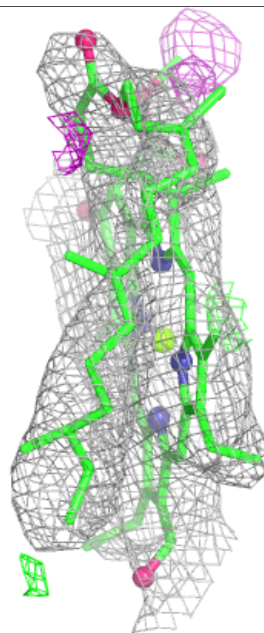
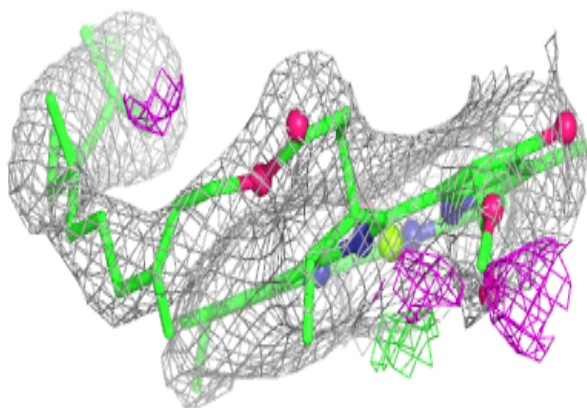
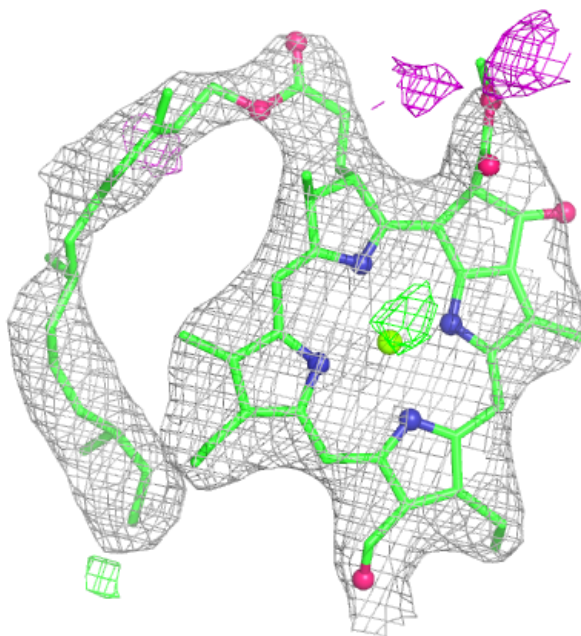
Electron density around CLA F 307:

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



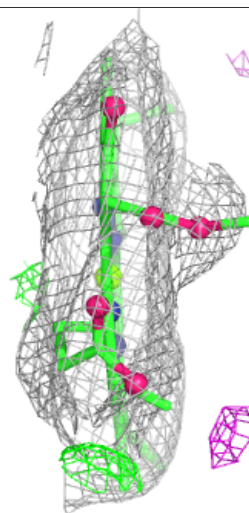
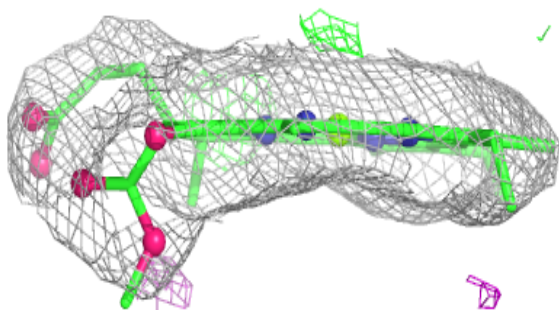
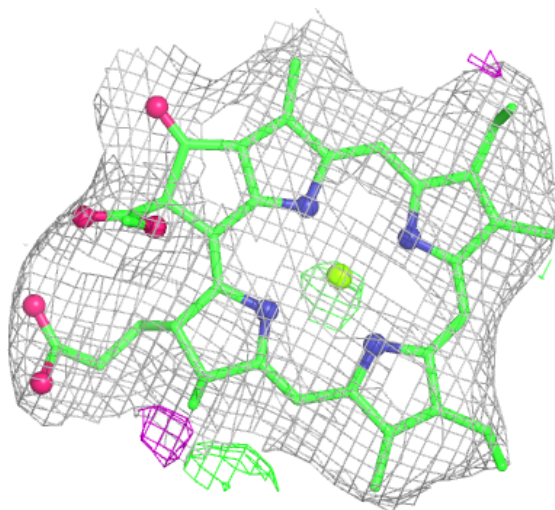
Electron density around CHL D 311:

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



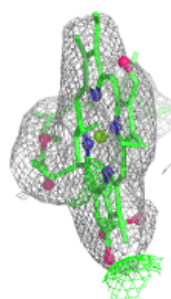
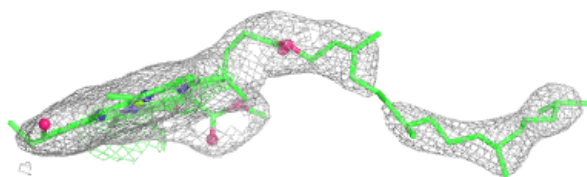
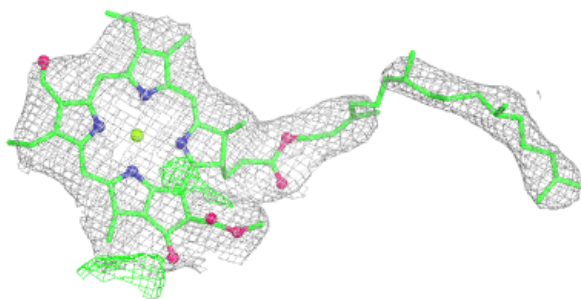
Electron density around CLA F 315:

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

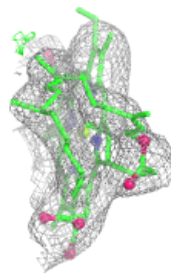
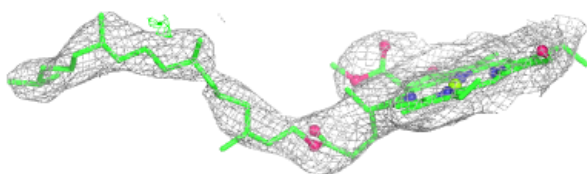
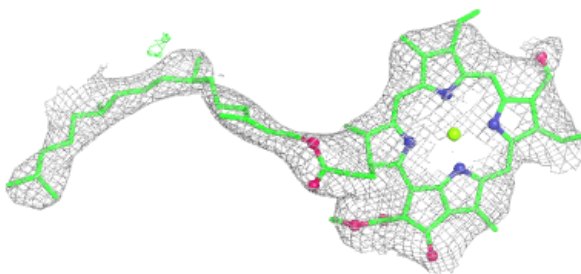


Electron density around CHL B 306:

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

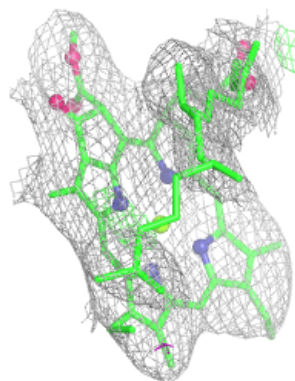
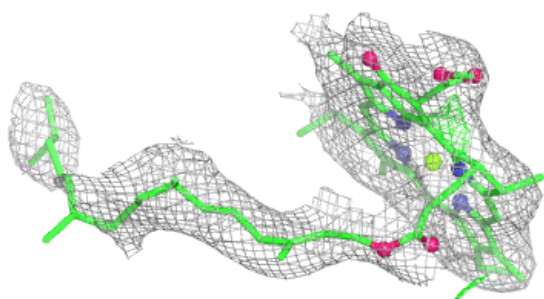
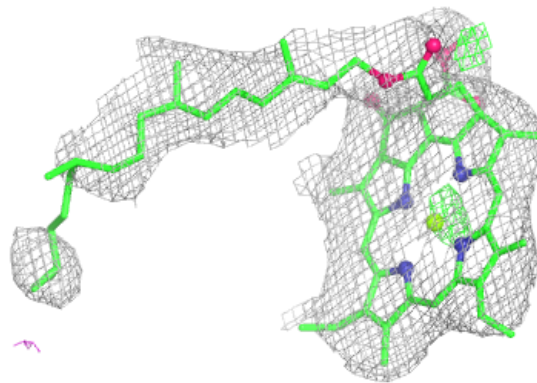
**Electron density around CHL D 305:**

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

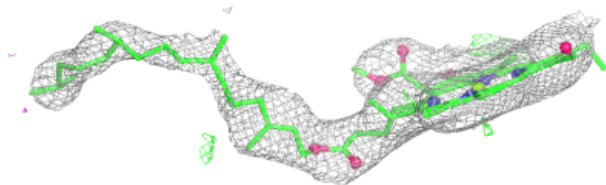
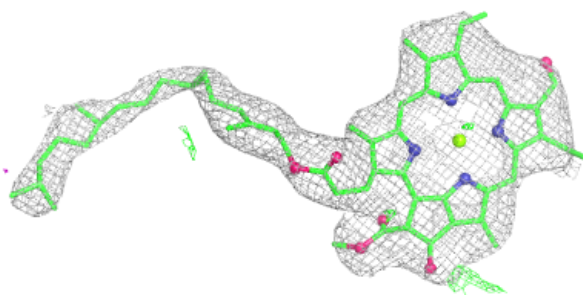


Electron density around CLA B 316:

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

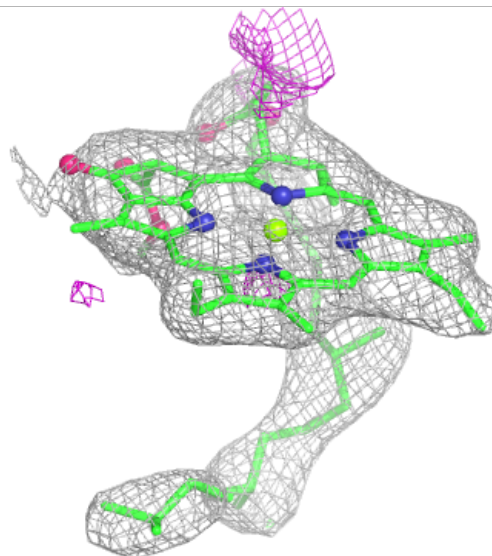
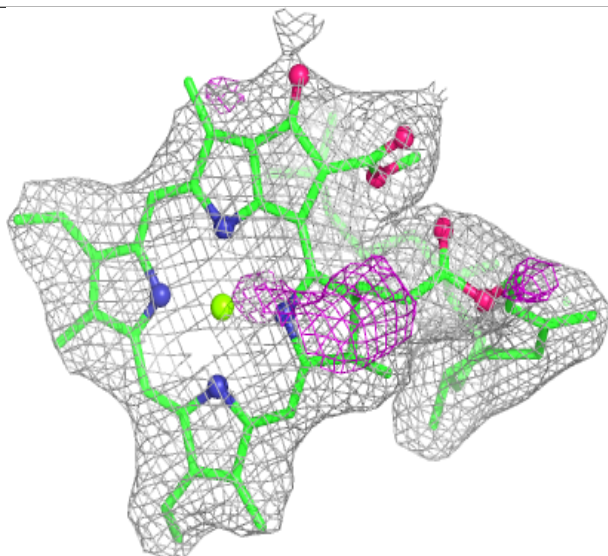
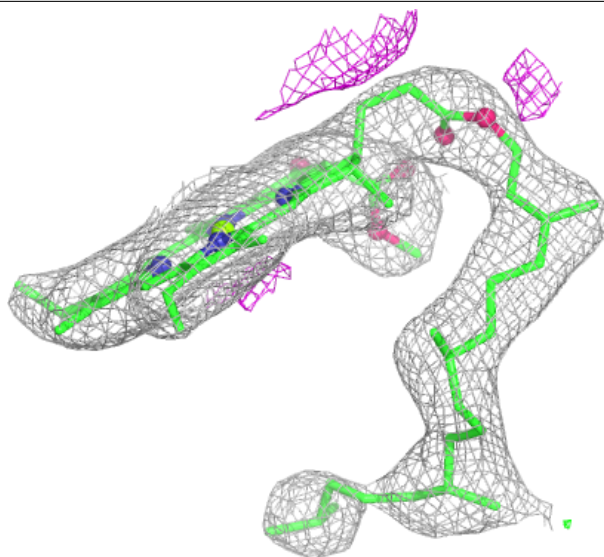
**Electron density around CHL C 305:**

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



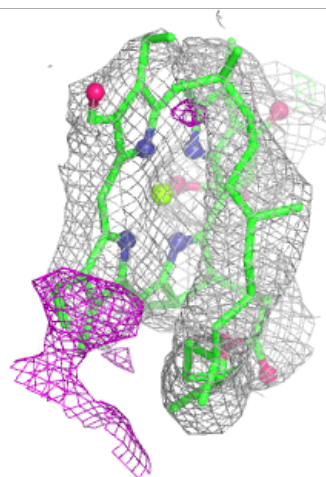
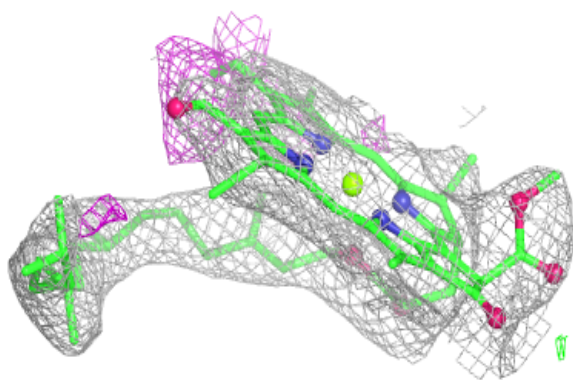
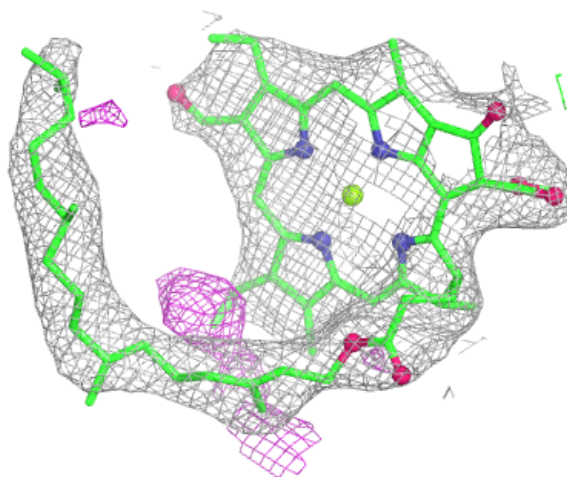
Electron density around CLA C 307:

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



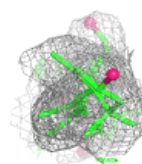
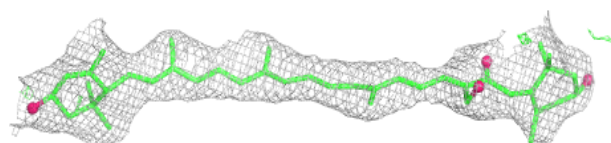
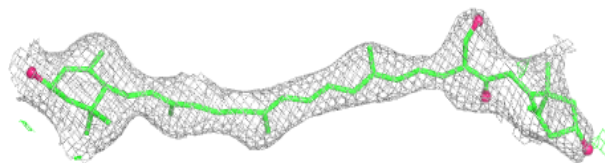
Electron density around CHL C 306:

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

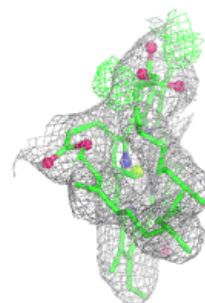
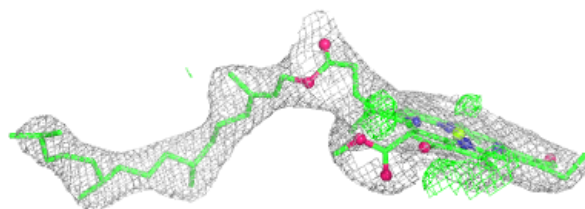
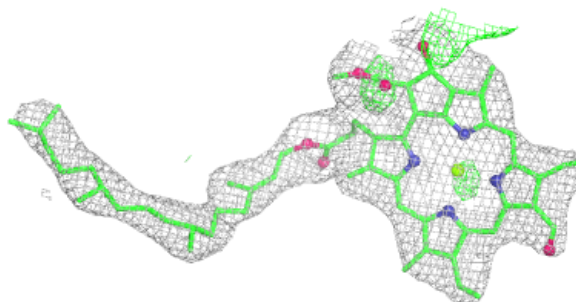


Electron density around OIE B 301:

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

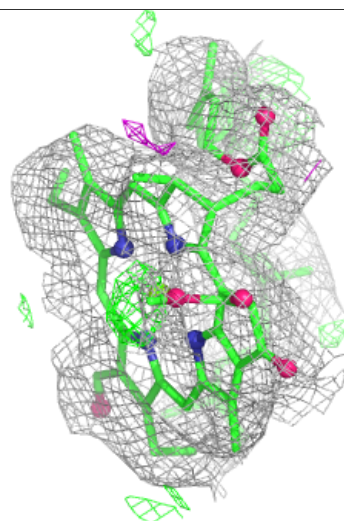
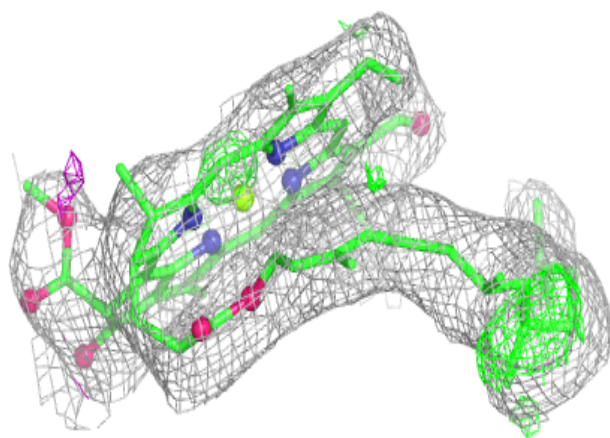
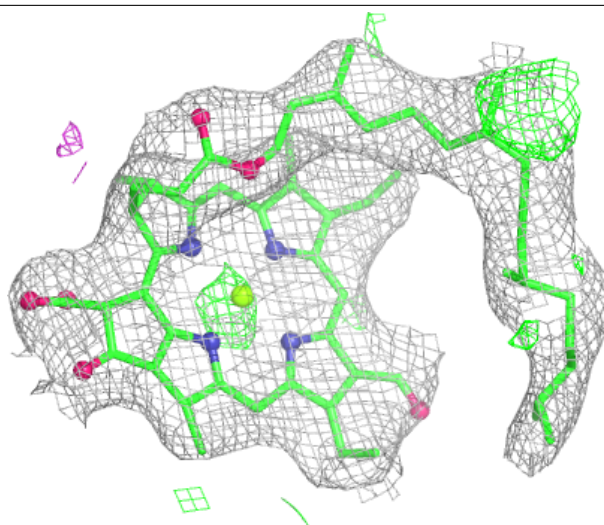
**Electron density around CHL F 304:**

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



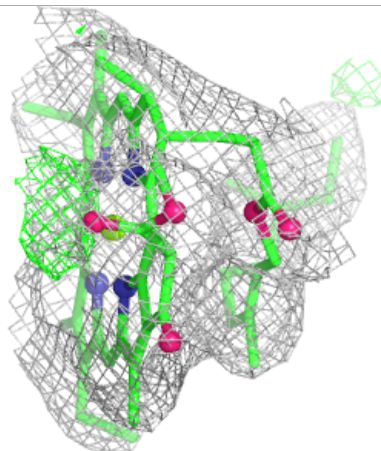
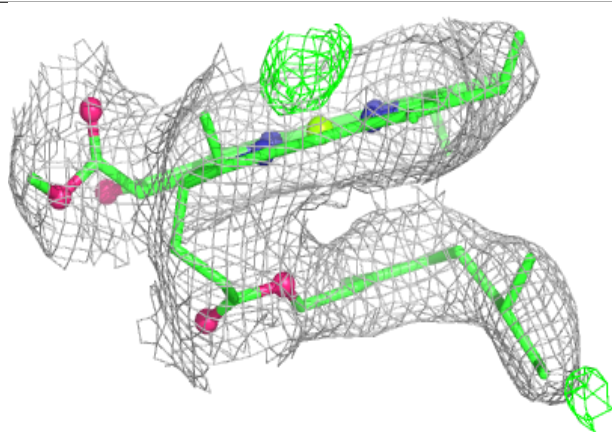
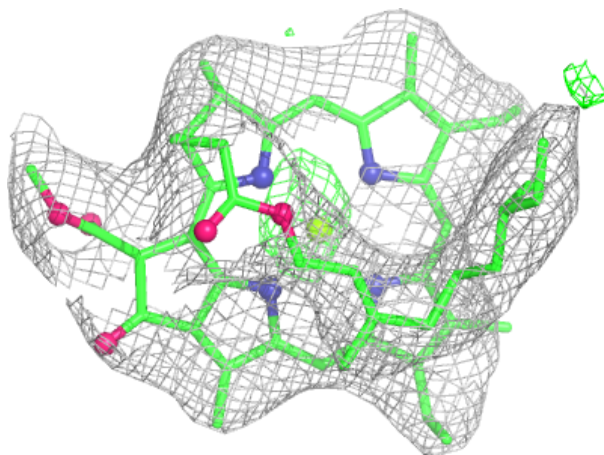
Electron density around CHL F 305:

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



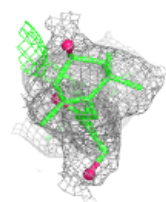
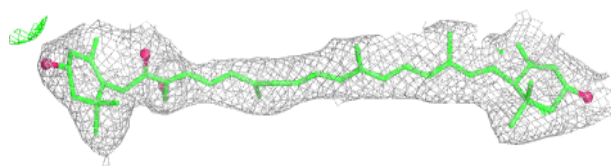
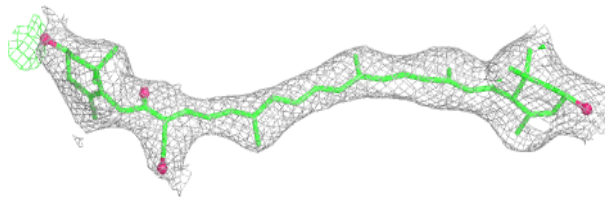
Electron density around CLA C 317:

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



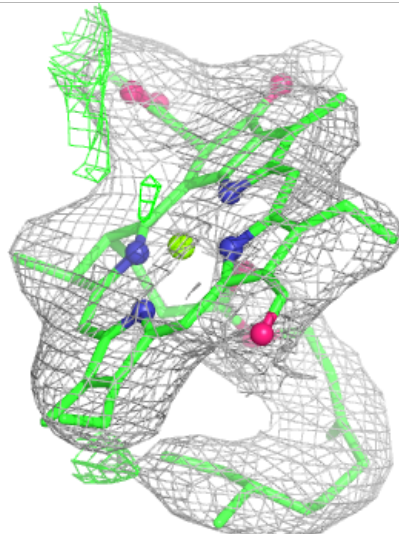
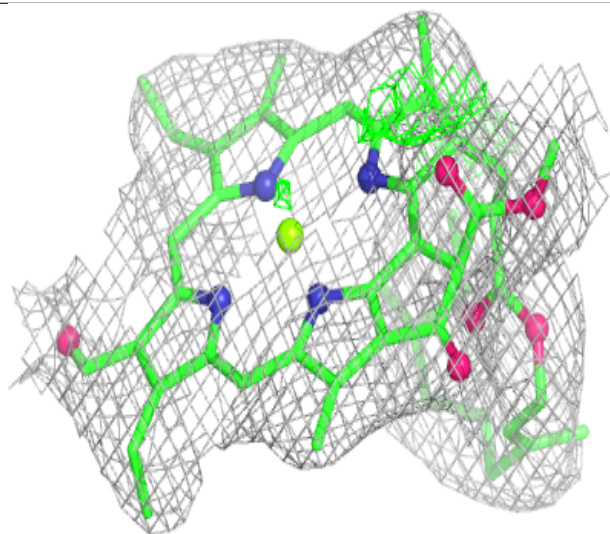
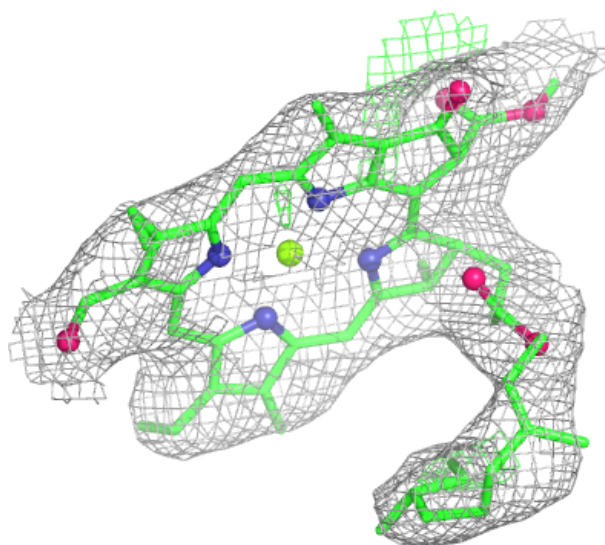
Electron density around OIE F 301:

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



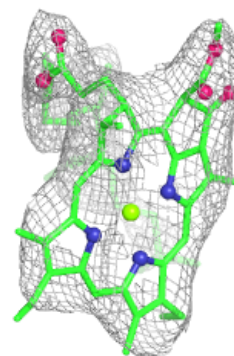
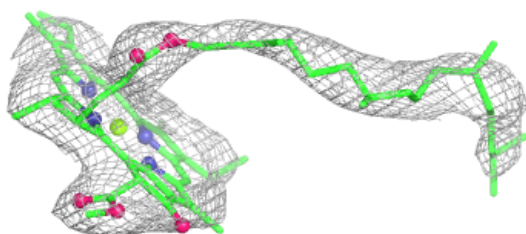
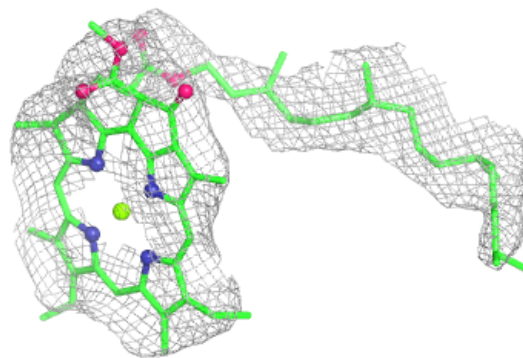
Electron density around CHL D 312:

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



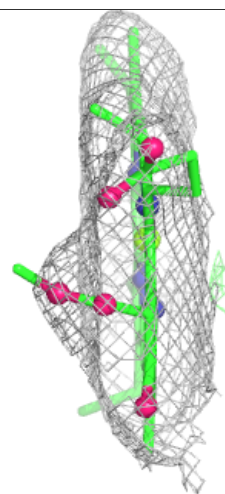
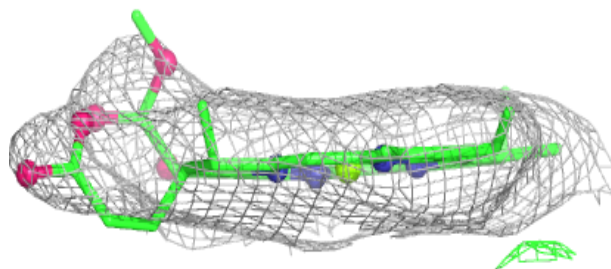
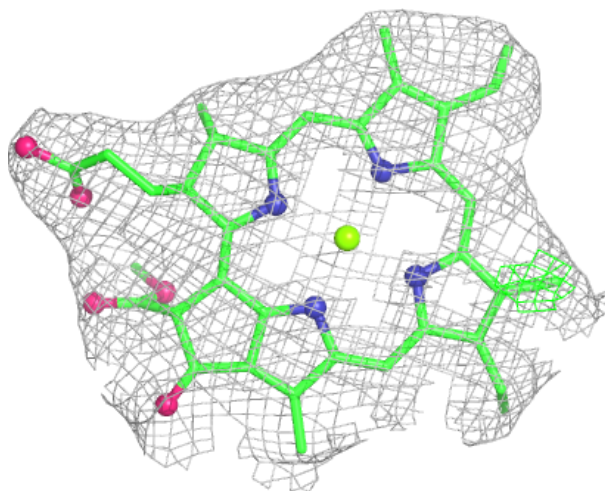
Electron density around CLA D 315:

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



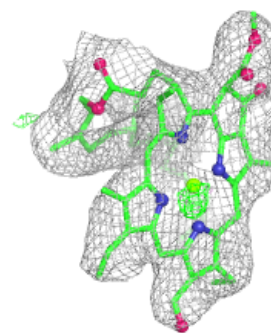
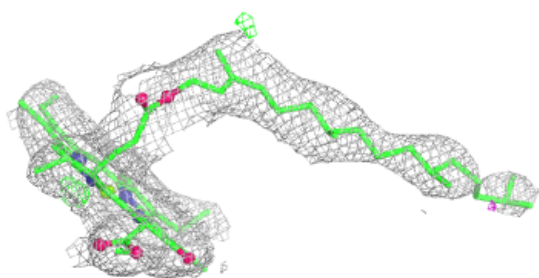
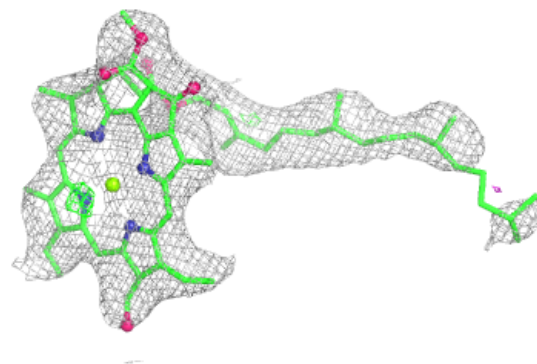
Electron density around CLA D 316:

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



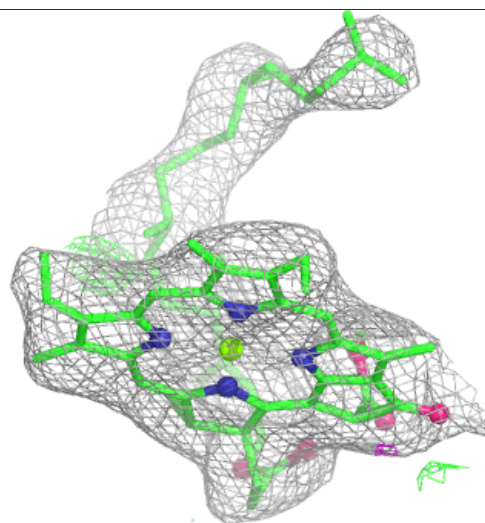
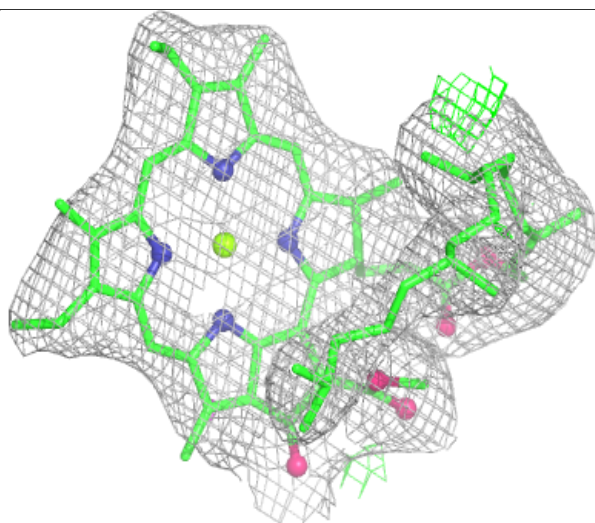
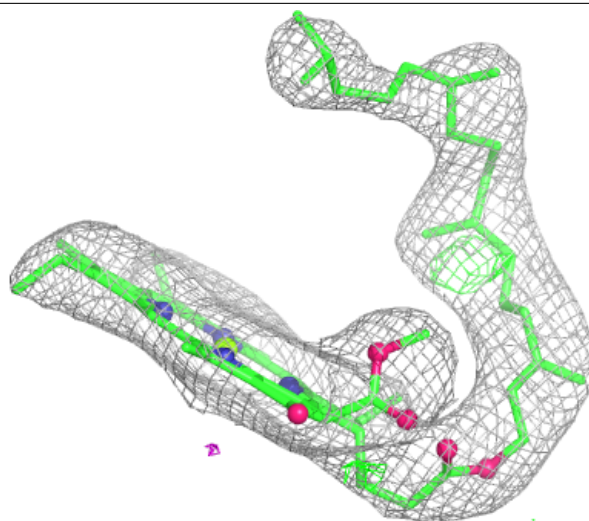
Electron density around CHL D 313:

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



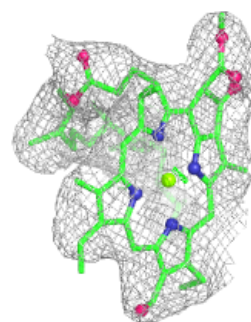
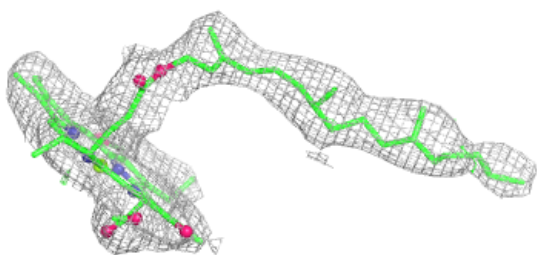
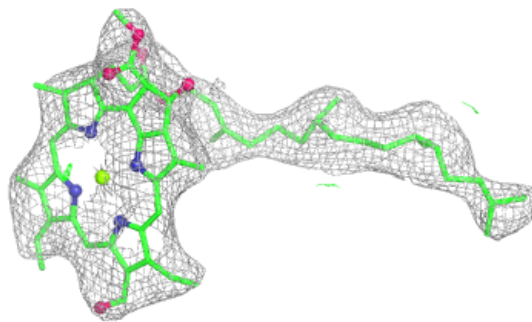
Electron density around CLA E 306:

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

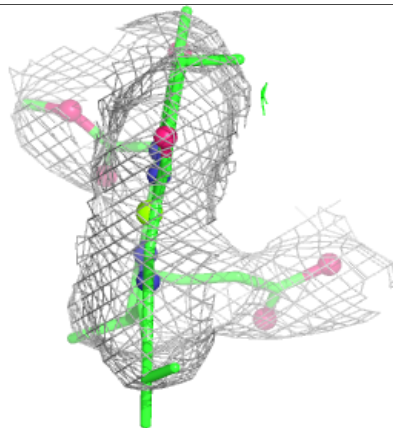
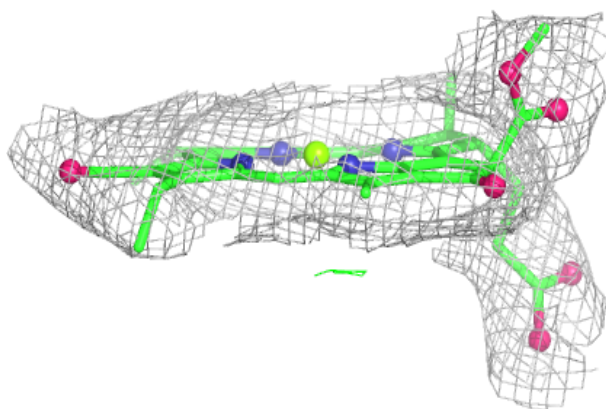
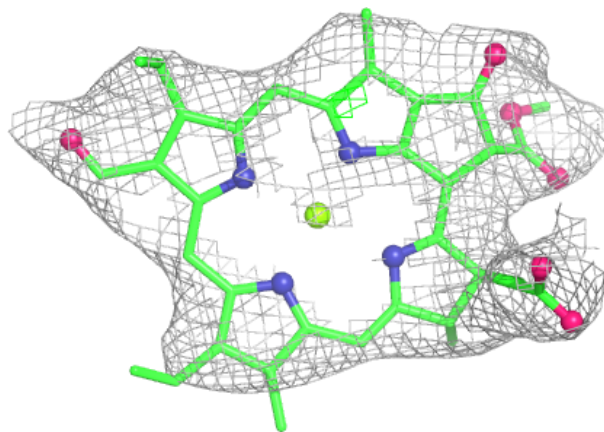


Electron density around CHL F 312:

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

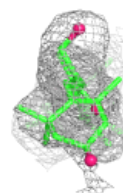
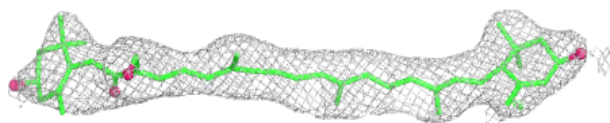
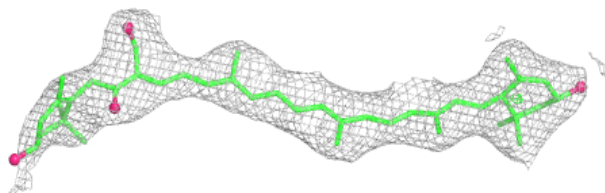
**Electron density around CHL D 318:**

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

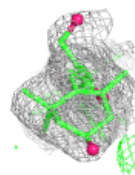
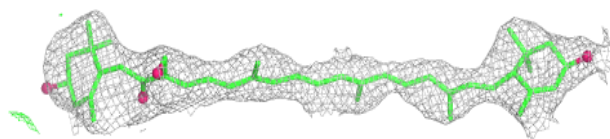
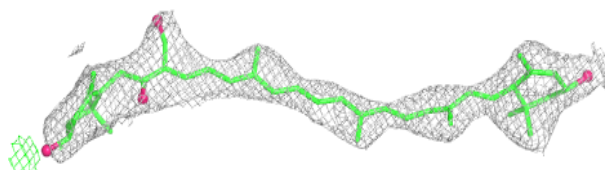


Electron density around OIE A 301:

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

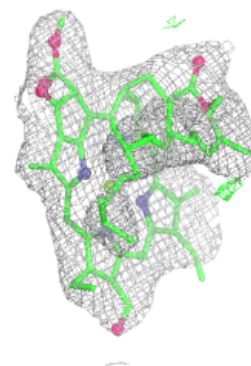
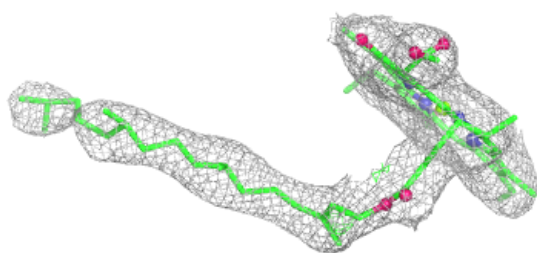
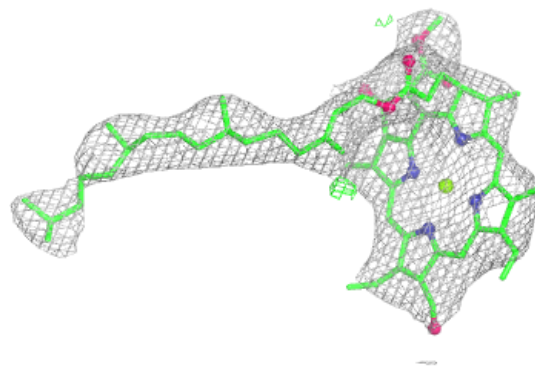
**Electron density around OIE E 301:**

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



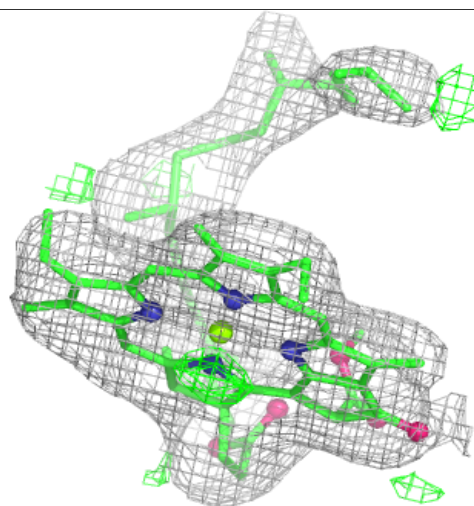
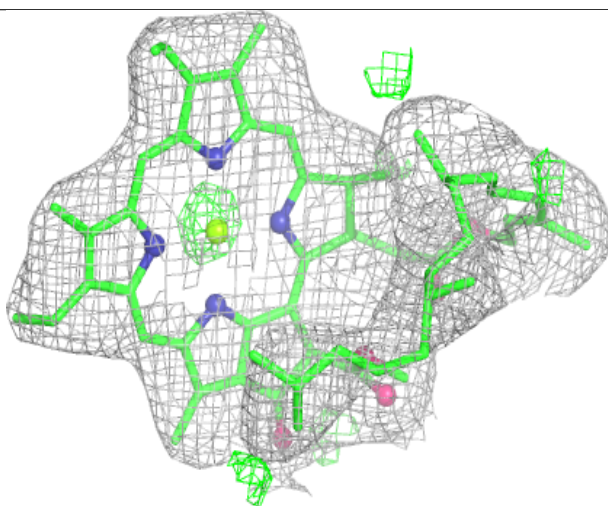
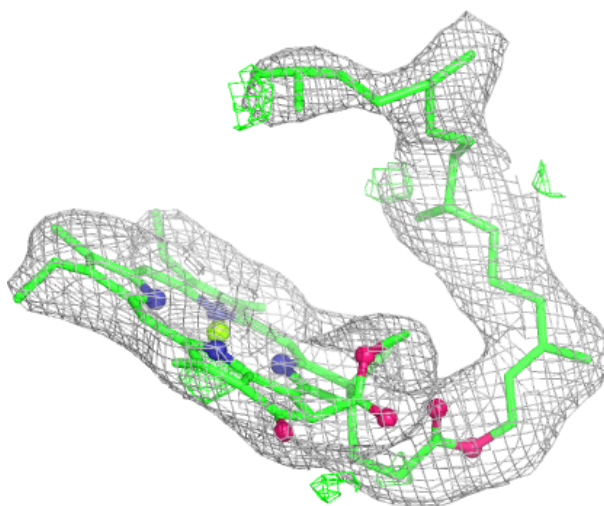
Electron density around CHL B 314:

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



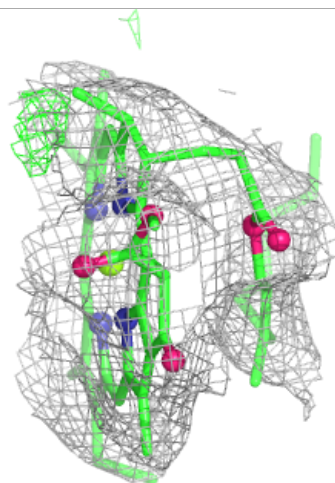
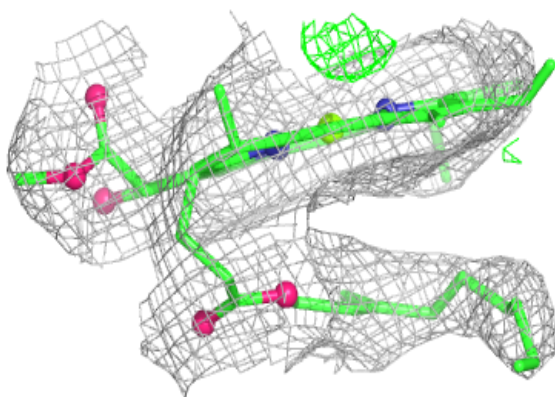
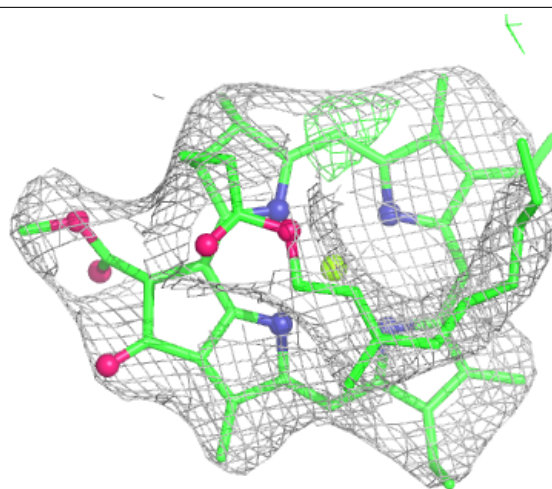
Electron density around CLA F 306:

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



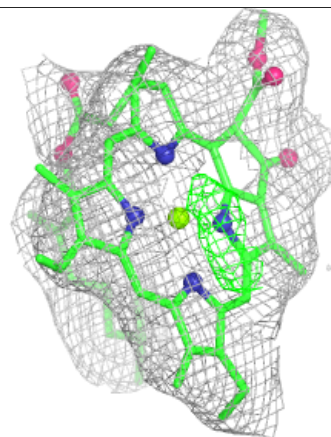
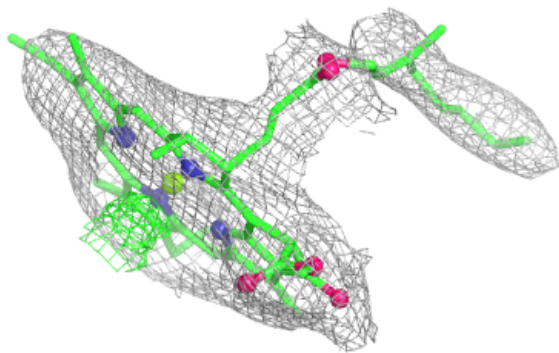
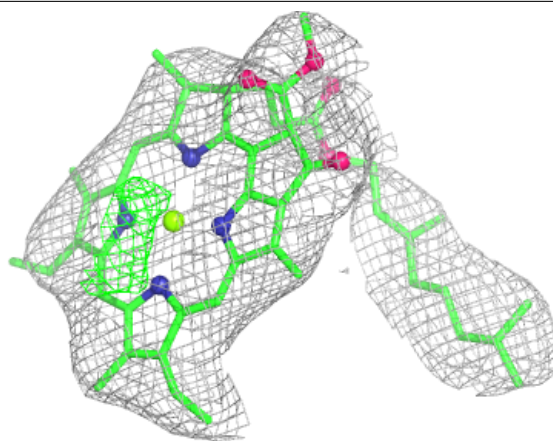
Electron density around CLA A 317:

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



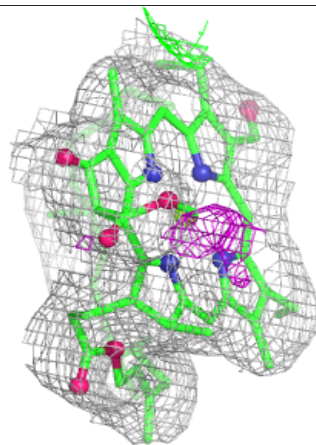
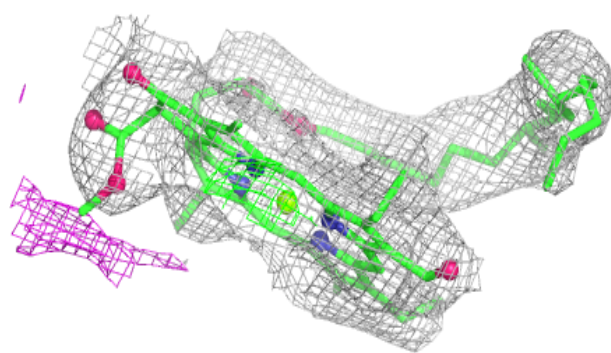
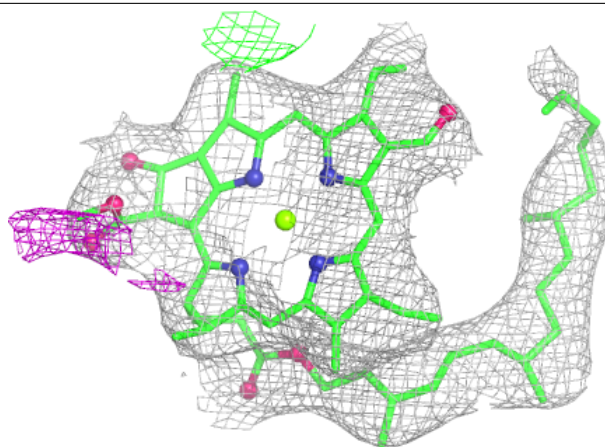
Electron density around CLA F 314:

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



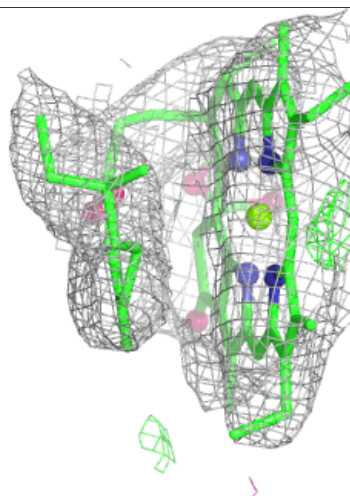
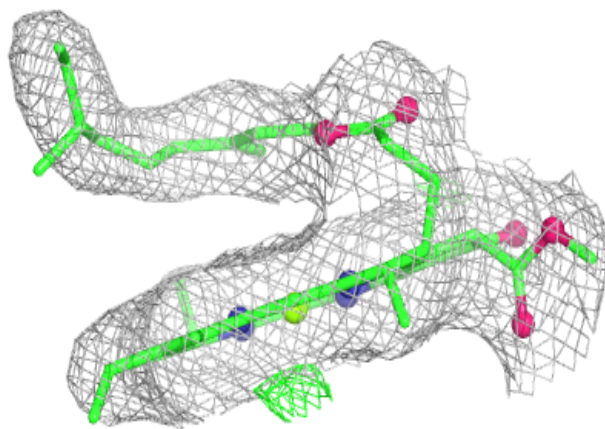
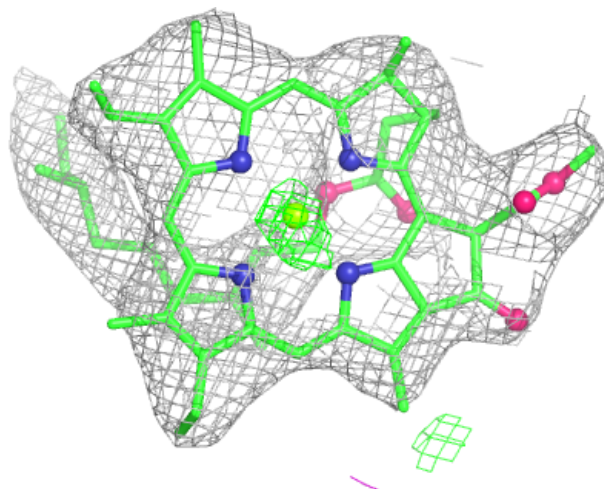
Electron density around CHL B 307:

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



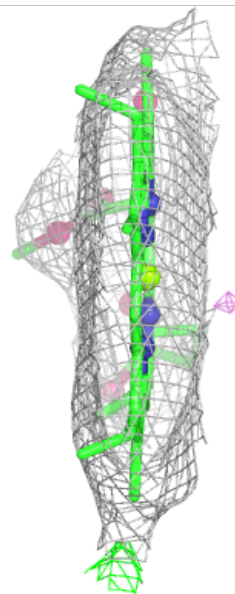
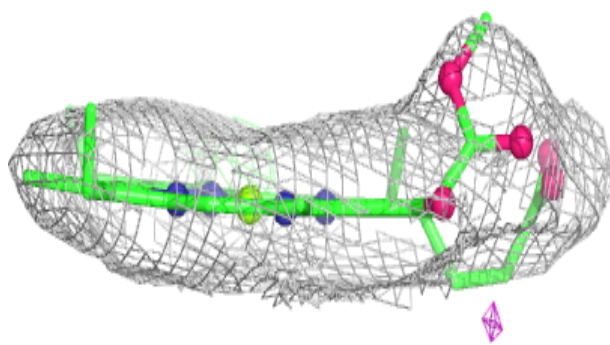
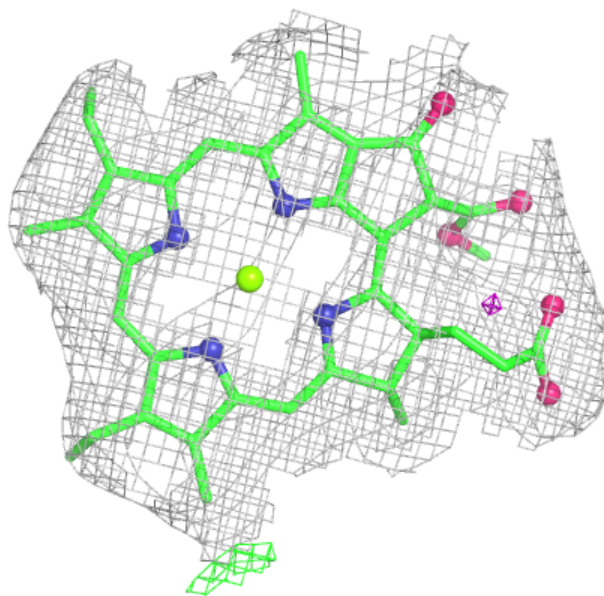
Electron density around CLA F 316:

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



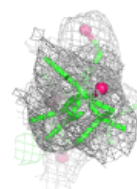
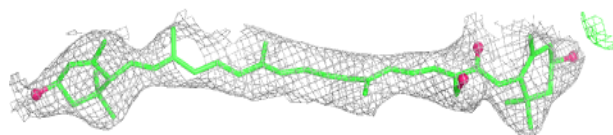
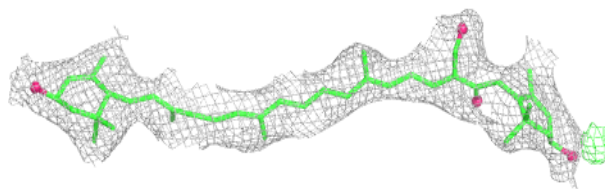
Electron density around CLA A 316:

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



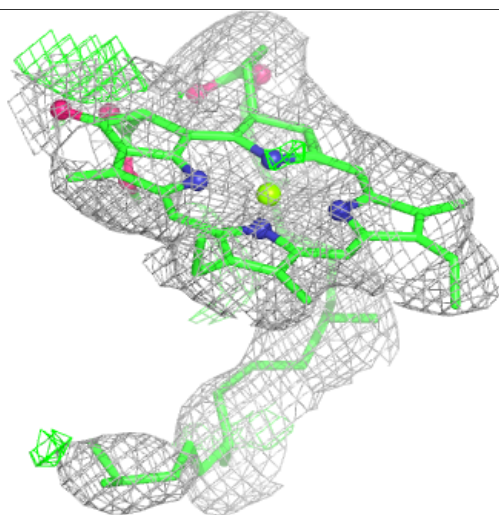
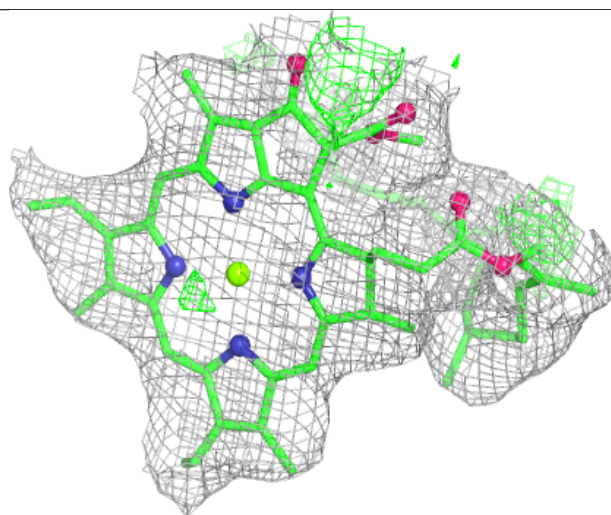
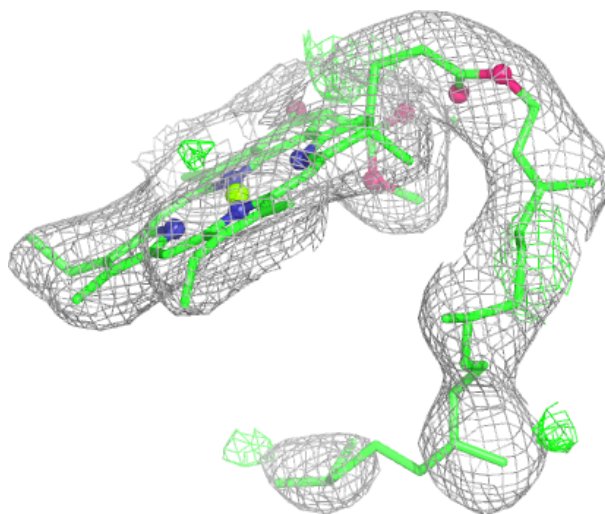
Electron density around OIE D 301:

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



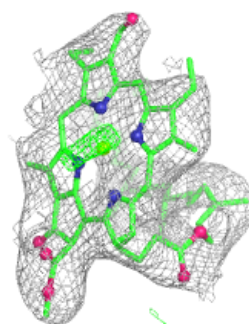
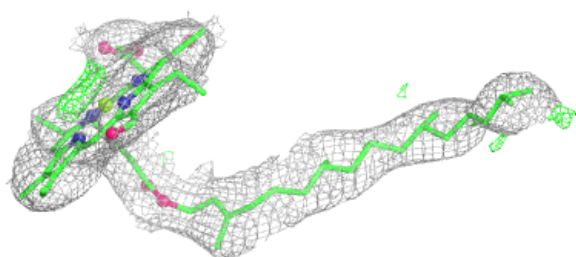
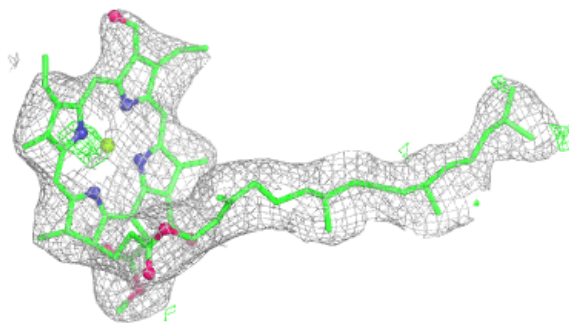
Electron density around CLA D 307:

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



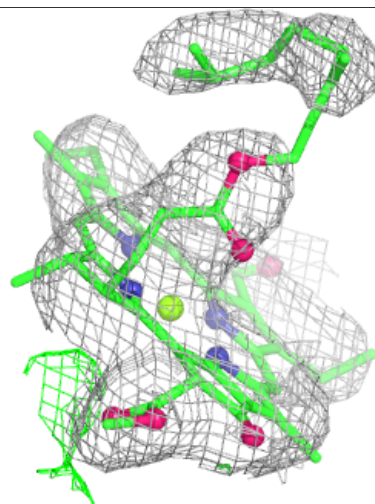
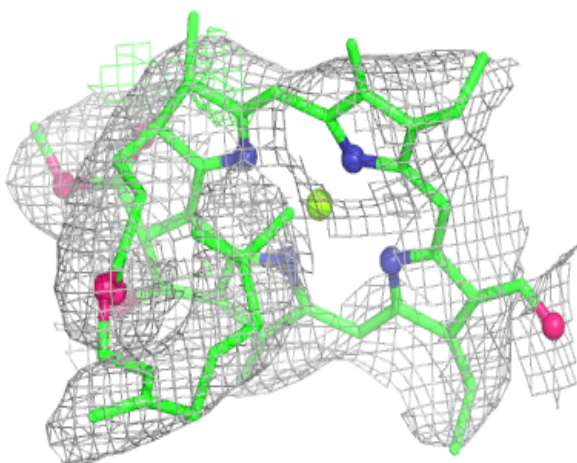
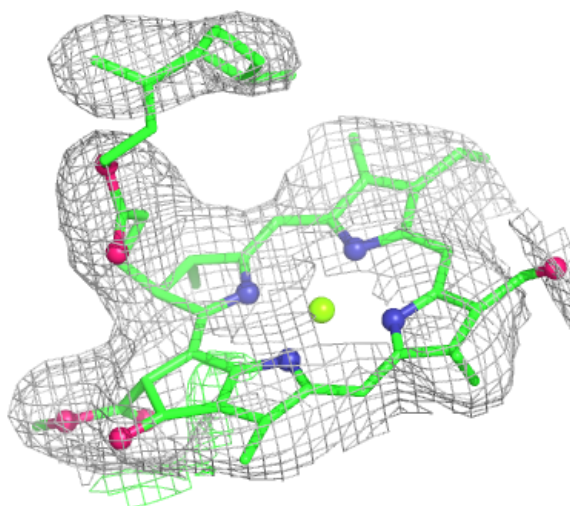
Electron density around CHL A 313:

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



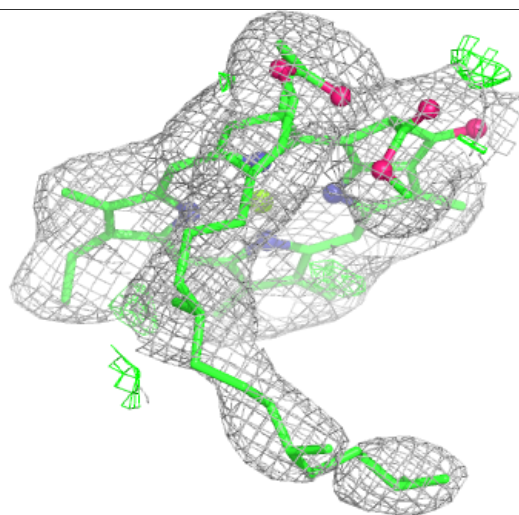
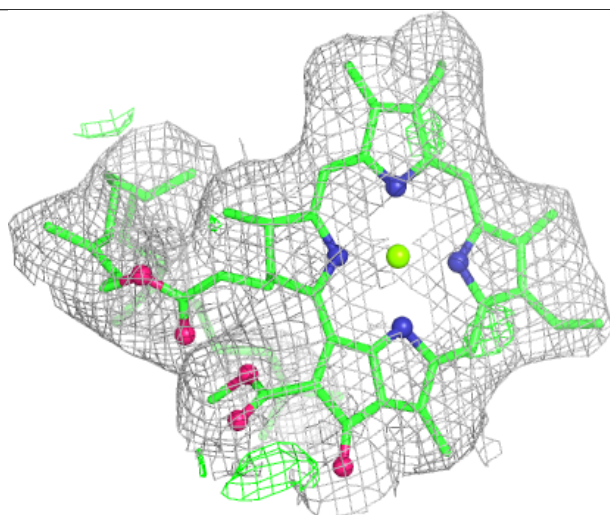
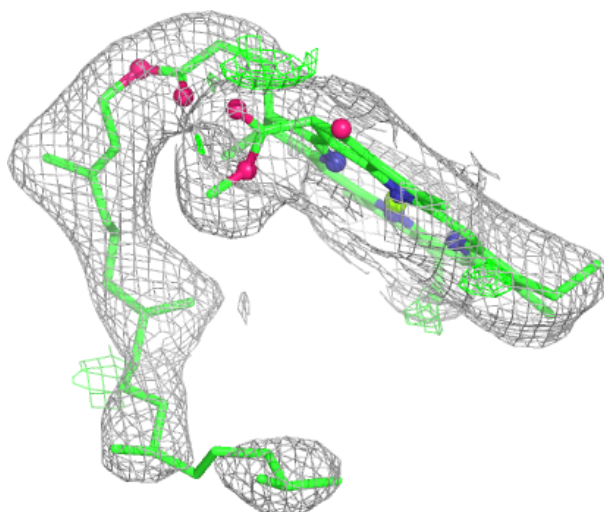
Electron density around CHL F 311:

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



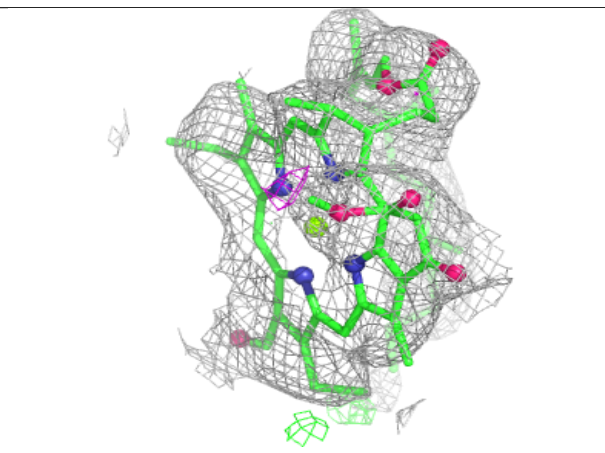
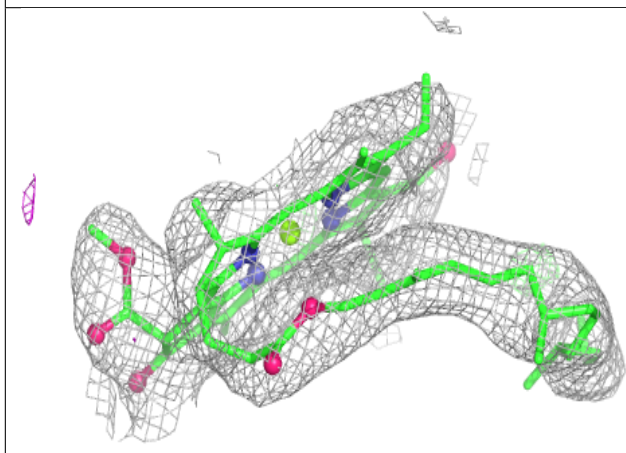
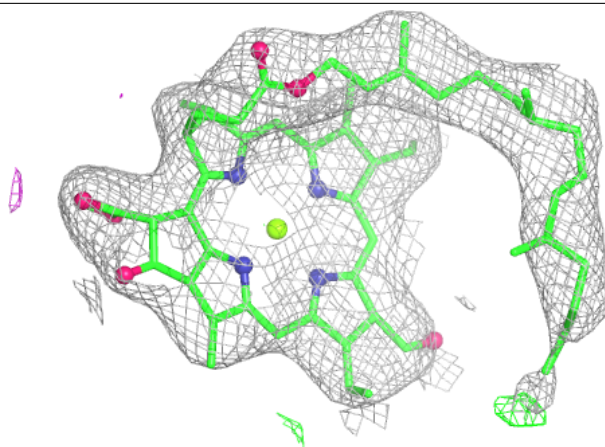
Electron density around CLA A 307:

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



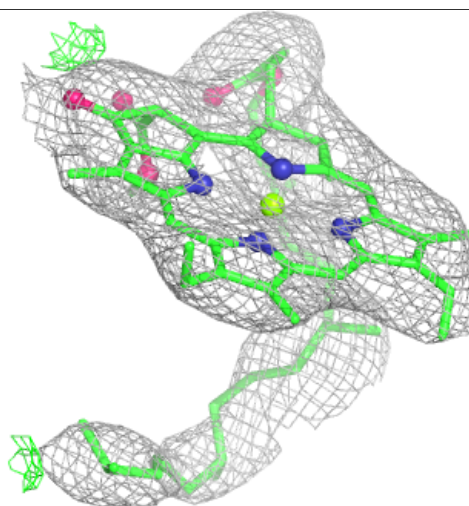
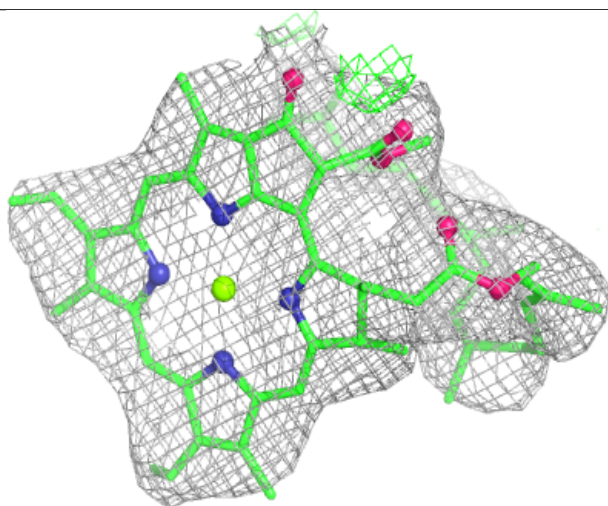
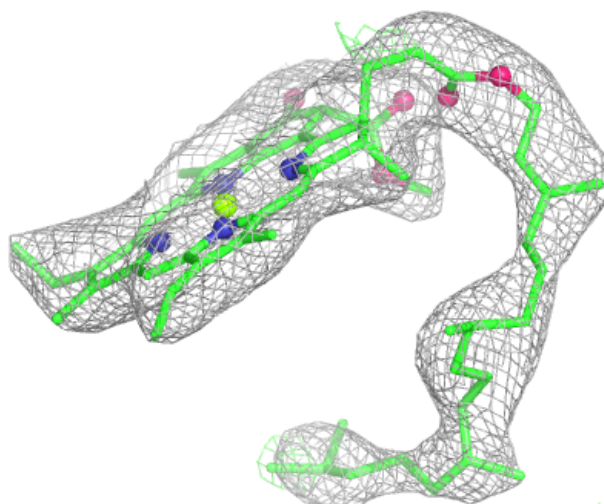
Electron density around CHL A 306:

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



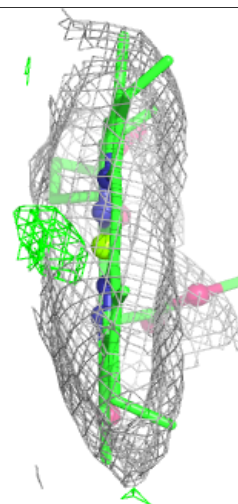
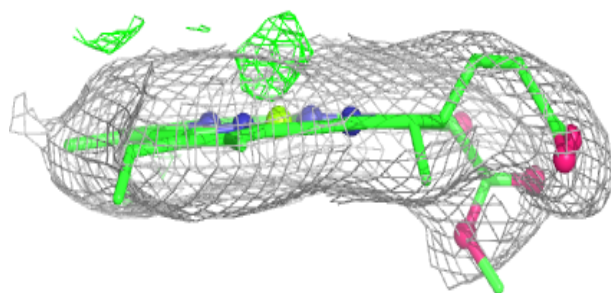
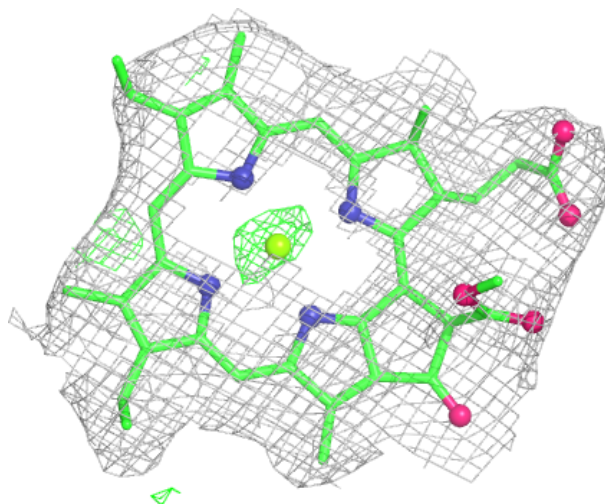
Electron density around CLA B 308:

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



Electron density around CLA B 317:

$2mF_o-DF_c$ (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.