



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:35 PM UTC

PDB ID : 8H2U / pdb_00008h2u
Title : X-ray Structure of photosystem I-LHCI super complex from *Chlamydomonas reinhardtii*.
Authors : Tanaka, H.; Kubota-Kawai, H.; Misumi, Y.; Kurisu, G.
Deposited on : 2022-10-07
Resolution : 3.40 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

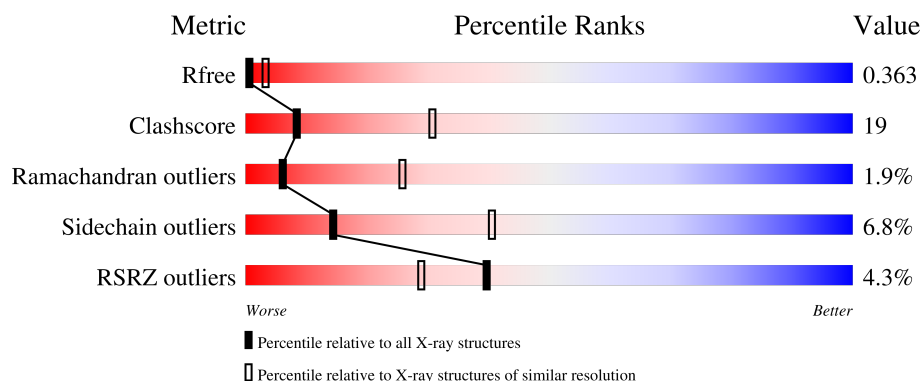
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	751	 4% 69% 26% ..
2	B	735	 4% 67% 28% ..
3	C	81	 9% 68% 28% ..
4	D	196	 2% 63% 8% . 28%
5	E	97	 54% 9% 37%

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Mol	Chain	Length	Quality of chain
6	F	227	
7	G	126	
8	H	130	
9	I	106	
10	J	41	
11	K	113	
12	L	196	
13	0	228	
13	1	228	
14	8	243	
15	7	241	
16	3	298	
17	4	264	
18	6	257	
19	5	257	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	0	301	X	-	-	-
20	CLA	0	305	X	-	-	-
20	CLA	0	306	X	-	-	-
20	CLA	0	307	X	-	-	-
20	CLA	0	308	X	-	-	-
20	CLA	0	309	X	-	-	-
20	CLA	0	310	X	-	-	-
20	CLA	0	311	X	-	-	-
20	CLA	0	312	X	-	-	-
20	CLA	0	313	X	-	-	-
20	CLA	0	316	X	-	-	-
20	CLA	1	1003	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	1004	X	-	-	-
20	CLA	1	1005	X	-	-	-
20	CLA	1	1006	X	-	-	-
20	CLA	1	1007	X	-	-	-
20	CLA	1	1008	X	-	-	-
20	CLA	1	1009	X	-	-	-
20	CLA	1	1010	X	-	-	-
20	CLA	1	1011	X	-	-	-
20	CLA	1	1014	X	-	-	-
20	CLA	1	1017	X	-	-	-
20	CLA	3	1005	X	-	-	-
20	CLA	3	1006	X	-	-	-
20	CLA	3	1007	X	-	-	-
20	CLA	3	1008	X	-	-	-
20	CLA	3	1009	X	-	-	-
20	CLA	3	1010	X	-	-	-
20	CLA	3	1011	X	-	-	-
20	CLA	3	1012	X	-	-	-
20	CLA	3	1013	X	-	-	-
20	CLA	3	1015	X	-	-	-
20	CLA	3	1016	X	-	-	-
20	CLA	3	1017	X	-	-	-
20	CLA	4	304	X	-	-	-
20	CLA	4	305	X	-	-	-
20	CLA	4	306	X	-	-	-
20	CLA	4	307	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	311	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	5	301	X	-	-	-
20	CLA	5	304	X	-	-	-
20	CLA	5	305	X	-	-	-
20	CLA	5	306	X	-	-	-
20	CLA	5	307	X	-	-	-
20	CLA	5	308	X	-	-	-
20	CLA	5	309	X	-	-	-
20	CLA	5	310	X	-	-	-
20	CLA	5	311	X	-	-	-
20	CLA	5	312	X	-	-	-
20	CLA	5	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	5	318	X	-	-	-
20	CLA	5	321	X	-	-	-
20	CLA	5	322	X	-	-	-
20	CLA	5	323	X	-	-	-
20	CLA	6	301	X	-	-	-
20	CLA	6	305	X	-	-	-
20	CLA	6	306	X	-	-	-
20	CLA	6	307	X	-	-	-
20	CLA	6	308	X	-	-	-
20	CLA	6	309	X	-	-	-
20	CLA	6	310	X	-	-	-
20	CLA	6	311	X	-	-	-
20	CLA	6	312	X	-	-	-
20	CLA	6	315	X	-	-	-
20	CLA	6	318	X	-	-	-
20	CLA	6	320	X	-	-	-
20	CLA	7	1004	X	-	-	-
20	CLA	7	1005	X	-	-	-
20	CLA	7	1006	X	-	-	-
20	CLA	7	1007	X	-	-	-
20	CLA	7	1008	X	-	-	-
20	CLA	7	1009	X	-	-	-
20	CLA	7	1010	X	-	-	-
20	CLA	7	1011	X	-	-	-
20	CLA	7	1014	X	-	-	-
20	CLA	8	305	X	-	-	-
20	CLA	8	306	X	-	-	-
20	CLA	8	307	X	-	-	-
20	CLA	8	308	X	-	-	-
20	CLA	8	309	X	-	-	-
20	CLA	8	310	X	-	-	-
20	CLA	8	311	X	-	-	-
20	CLA	8	312	X	-	-	-
20	CLA	8	313	X	-	-	-
20	CLA	8	316	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	852	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	B	840	X	-	-	-
20	CLA	B	841	X	-	-	-
20	CLA	B	850	X	-	-	-
20	CLA	F	302	X	-	-	-
20	CLA	F	303	X	-	-	-
20	CLA	F	305	X	-	-	-
20	CLA	G	201	X	-	-	-
20	CLA	G	202	X	-	-	-
20	CLA	G	203	X	-	-	-
20	CLA	J	102	X	-	-	-
20	CLA	K	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	K	202	X	-	-	-
20	CLA	L	201	X	-	-	-
20	CLA	L	202	X	-	-	-
20	CLA	L	203	X	-	-	-
20	CLA	L	204	X	-	-	-
21	SF4	C	1002	-	-	X	-
27	LMG	0	303	-	-	X	-
27	LMG	4	318	-	-	X	-
29	CHL	0	314	X	-	-	-
29	CHL	0	315	X	-	-	-
29	CHL	0	317	X	-	-	-
29	CHL	1	1012	X	-	-	-
29	CHL	1	1013	X	-	-	-
29	CHL	1	1015	X	-	-	-
29	CHL	3	1014	X	-	-	-
29	CHL	4	312	X	-	-	-
29	CHL	4	313	X	-	-	-
29	CHL	4	315	X	-	-	-
29	CHL	4	316	X	-	-	-
29	CHL	5	313	X	-	-	-
29	CHL	5	314	X	-	-	-
29	CHL	5	316	X	-	-	-
29	CHL	5	317	X	-	-	-
29	CHL	6	313	X	-	-	-
29	CHL	6	314	X	-	-	-
29	CHL	6	316	X	-	-	-
29	CHL	6	317	X	-	-	-
29	CHL	7	1012	X	-	-	-
29	CHL	7	1013	X	-	-	-
29	CHL	7	1015	X	-	-	-
29	CHL	7	1017	X	-	-	-
29	CHL	8	314	X	-	-	-
29	CHL	8	315	X	-	-	-
29	CHL	8	317	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 42070 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 Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5799	3792	989	996	22			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5786	3801	969	998	18			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	116	12			

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1101	703	196	195	7			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	61	Total	C	N	O	0	0	0
			480	306	85	89			

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	150	Total	C	N	O	S	0	0	0
			1150	745	192	210	3			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	85	Total	C	N	O	0	0	0
			620	398	108	114			

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	90	Total	C	N	O	S	0	0	0
			694	433	120	139	2			

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			221	153	31	36	1			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	39	Total	C	N	O	S	0	0	0
			320	219	45	55	1			

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	44	Total	C	N	O	S	0	0	0
			295	191	47	55	2			

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	150	Total	C	N	O	S	0	0	0
			1082	703	178	198	3			

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	0	182	Total	C	N	O	S	0	0	0
			1361	887	226	245	3			
13	1	182	Total	C	N	O	S	0	0	0
			1362	886	226	247	3			

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	8	193	Total	C	N	O	S	0	0	0
			1466	953	251	258	4			

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	7	209	Total	C	N	O	S	0	0	0
			1622	1051	271	294	6			

- Molecule 16 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	201	Total	C	N	O	S	0	0	0
			1542	1008	250	276	8			

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	202	Total	C	N	O	S	0	0	0
			1571	1031	254	281	5			

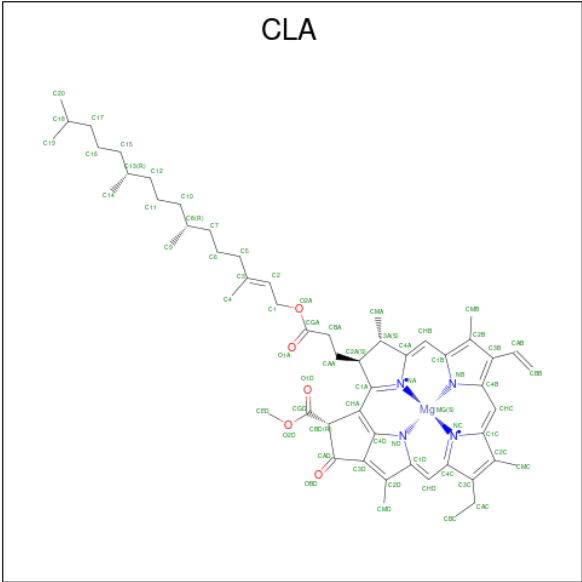
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	6	184	Total	C	N	O	S	0	0	0
			1431	945	235	247	4			

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	5	193	Total	C	N	O	S	0	0	0
			1510	984	255	264	7			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			40	32	1	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	A	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	A	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	A	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	A	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	A	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	A	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	B	1	Total 43	C 33	Mg 1	N 4	O 5	0	0
20	F	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	F	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	F	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	G	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	G	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	G	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	J	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	K	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	K	1	Total 27	C 22	Mg 1	N 4		0	0
20	L	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	L	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	L	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	L	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	O	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	O	1	Total 44	C 34	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	0	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	8	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	7	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 40	C 32	Mg 1	N 4	O 3	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	3	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	1	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	4	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0

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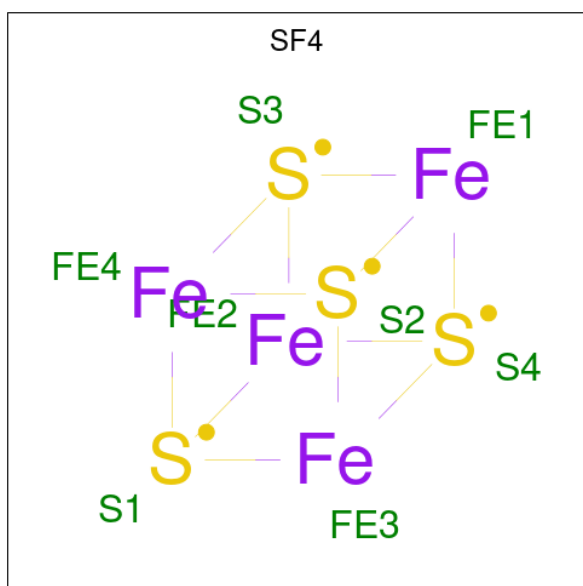
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	6	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0
20	5	1	Total 44	C 34	Mg 1	N 4	O 5	0	0

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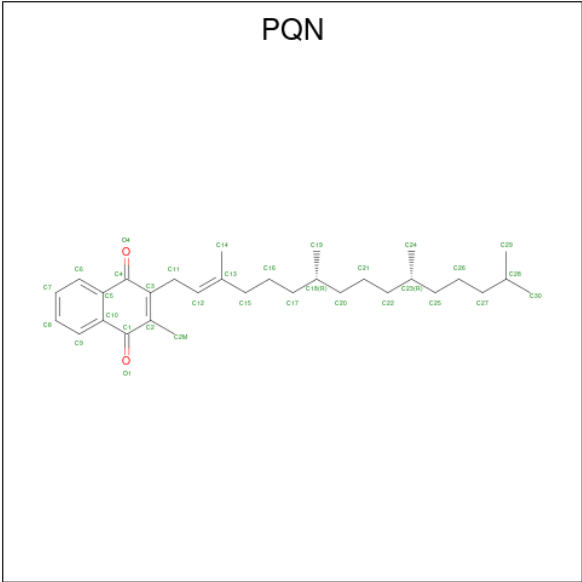
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
20	5	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



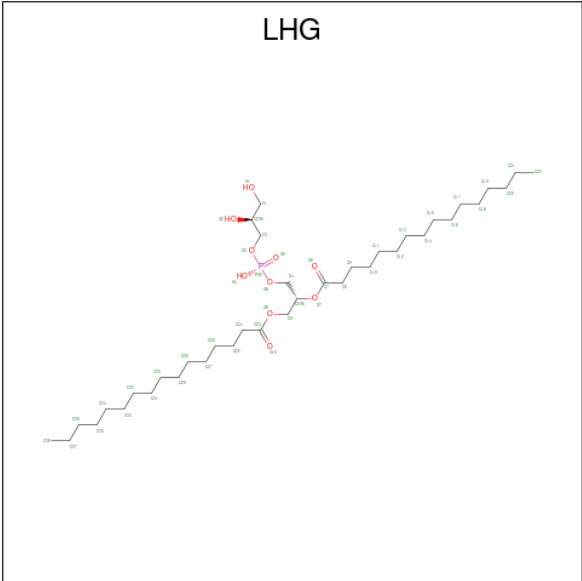
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $\text{C}_{31}\text{H}_{46}\text{O}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			33	31	2		
22	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



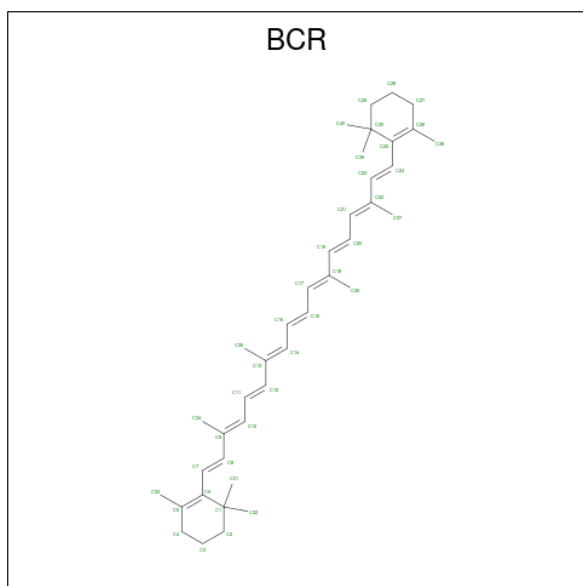
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	P	0	0
			40	29	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O	P	0	0
			49	38	10	1		
23	0	1	Total	C	O	P	0	0
			21	10	10	1		
23	8	1	Total	C	O	P	0	0
			49	38	10	1		
23	7	1	Total	C	O	P	0	0
			35	24	10	1		
23	3	1	Total	C	O	P	0	0
			20	10	9	1		
23	4	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		
24	A	1	Total	C	0	0
			40	40		

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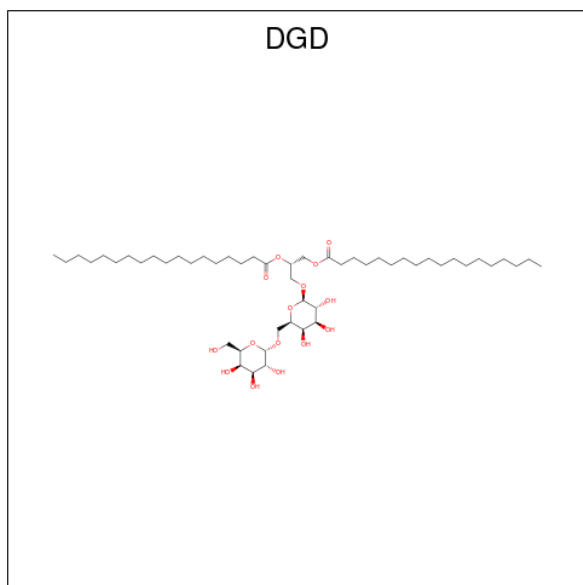
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	G	1	Total C 40 40	0	0
24	G	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	I	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	8	1	Total C 40 40	0	0
24	7	1	Total C 40 40	0	0
24	3	1	Total C 40 40	0	0
24	3	1	Total C 40 40	0	0
24	1	1	Total C 40 40	0	0
24	4	1	Total C 40 40	0	0
24	6	1	Total C 40 40	0	0

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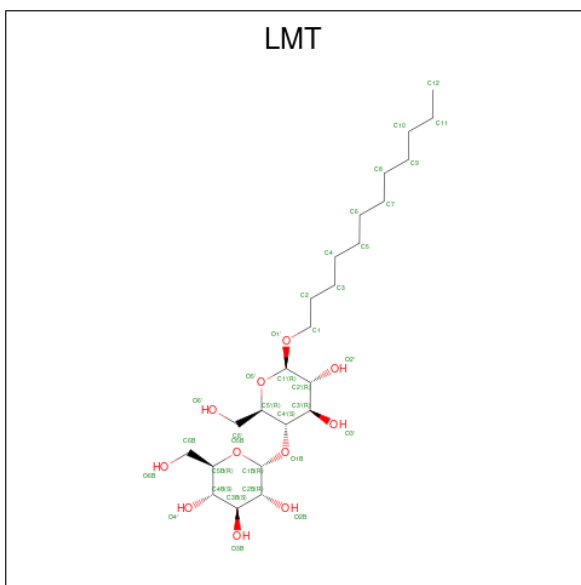
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	5	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



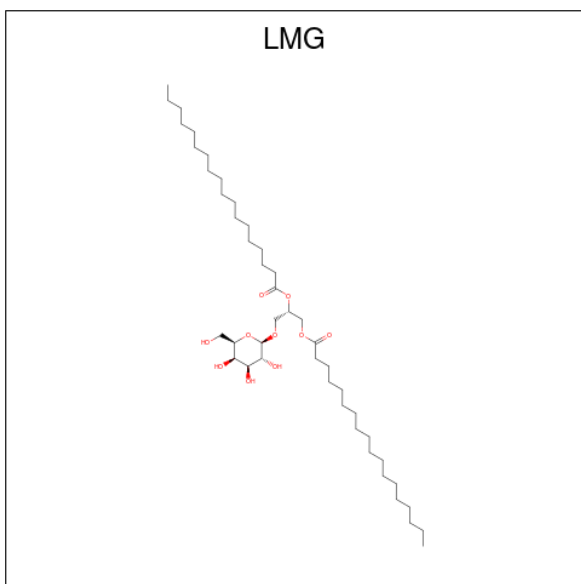
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 61 46 15	0	0
25	5	1	Total C O 51 36 15	0	0

- Molecule 26 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total 31	C 20	O 11	0	0
26	3	1	Total 31	C 20	O 11	0	0

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



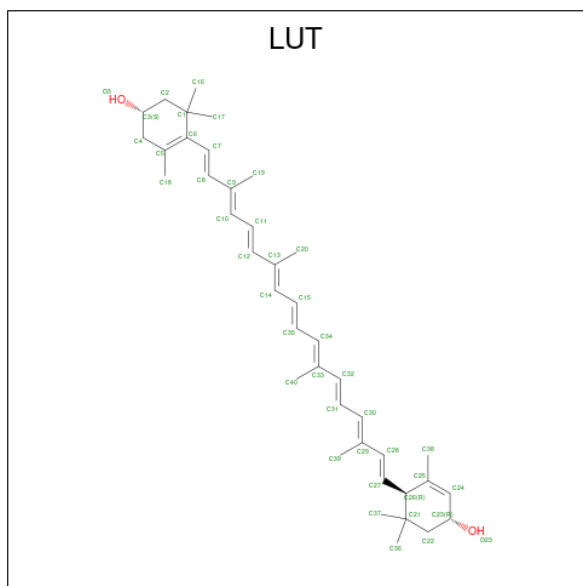
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	J	1	Total	C	O	0	0
			30	20	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	0	1	Total	C	O	0	0
			50	40	10		
27	8	1	Total	C	O	0	0
			28	18	10		
27	8	1	Total	C	O	0	0
			44	34	10		
27	4	1	Total	C	O	0	0
			34	24	10		
27	6	1	Total	C	O	0	0
			44	34	10		
27	5	1	Total	C	O	0	0
			45	35	10		

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



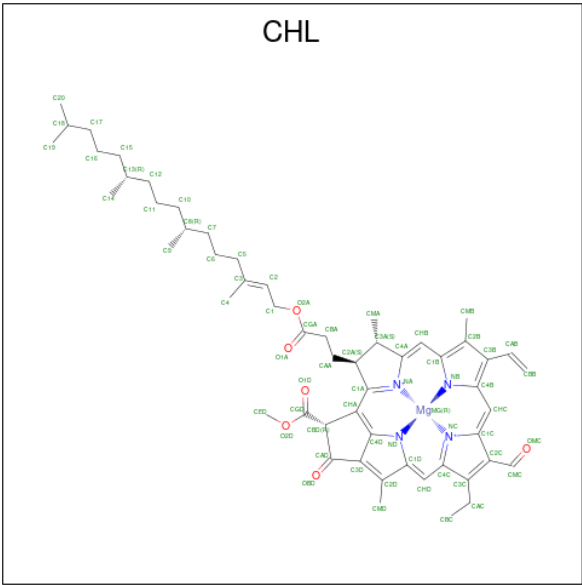
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	J	1	Total	C	O	0	0
			42	40	2		
28	0	1	Total	C	O	0	0
			42	40	2		
28	0	1	Total	C	O	0	0
			42	40	2		
28	8	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	7	1	Total	C	O	0	0
			42	40	2		
28	3	1	Total	C	O	0	0
			42	40	2		
28	3	1	Total	C	O	0	0
			42	40	2		
28	1	1	Total	C	O	0	0
			42	40	2		
28	1	1	Total	C	O	0	0
			42	40	2		
28	4	1	Total	C	O	0	0
			42	40	2		
28	6	1	Total	C	O	0	0
			42	40	2		
28	5	1	Total	C	O	0	0
			42	40	2		

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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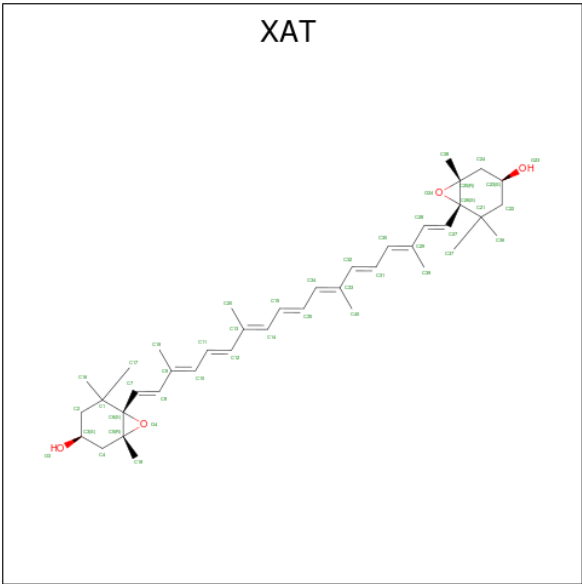
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	8	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	8	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
29	7	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
29	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
29	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	6	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
29	5	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
29	5	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

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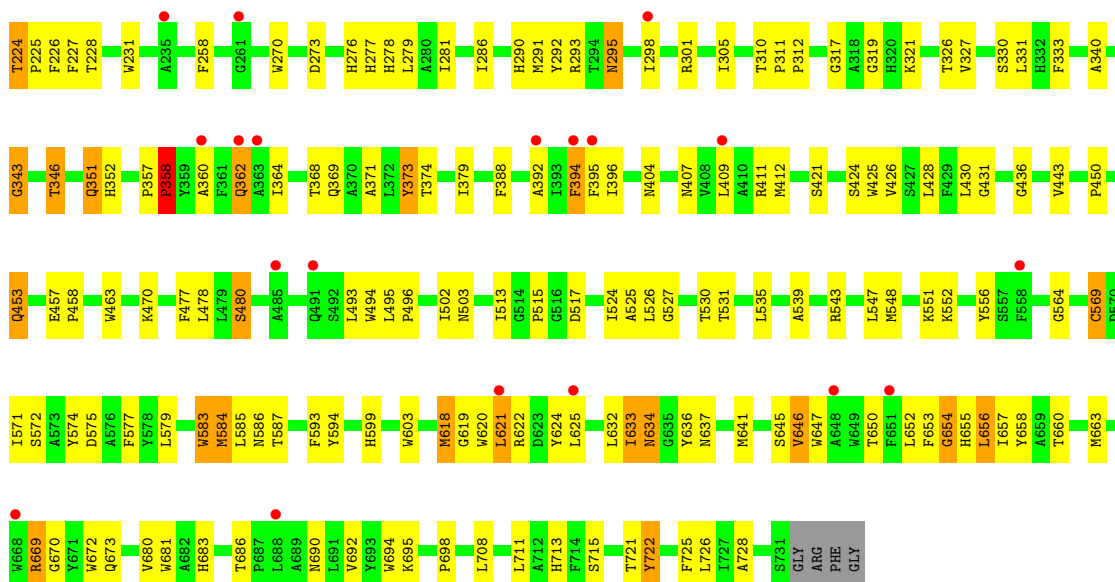
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	5	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
29	5	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

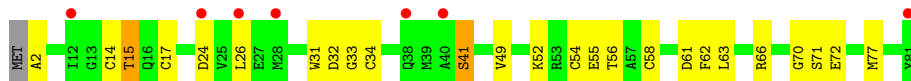
- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



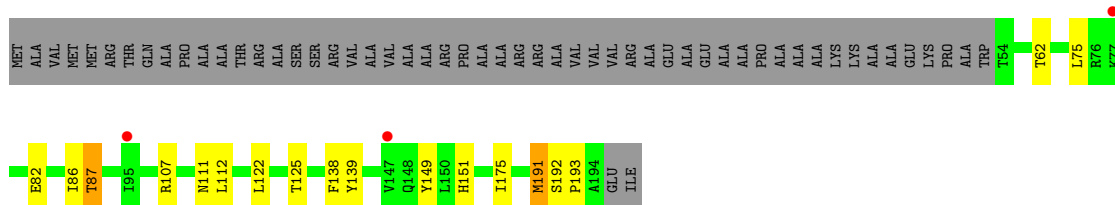
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	8	1	Total	C	O	0	0
			44	40	4		
30	7	1	Total	C	O	0	0
			44	40	4		
30	4	1	Total	C	O	0	0
			44	40	4		
30	6	1	Total	C	O	0	0
			44	40	4		
30	5	1	Total	C	O	0	0
			44	40	4		



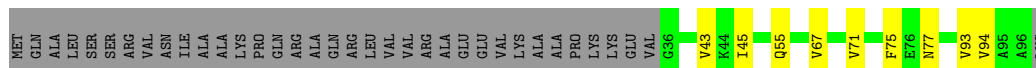
- Molecule 3: Photosystem I iron-sulfur center



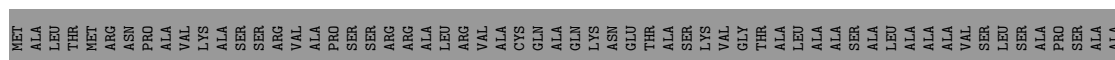
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

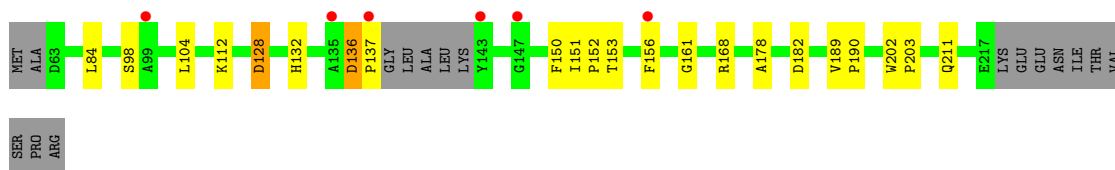


- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

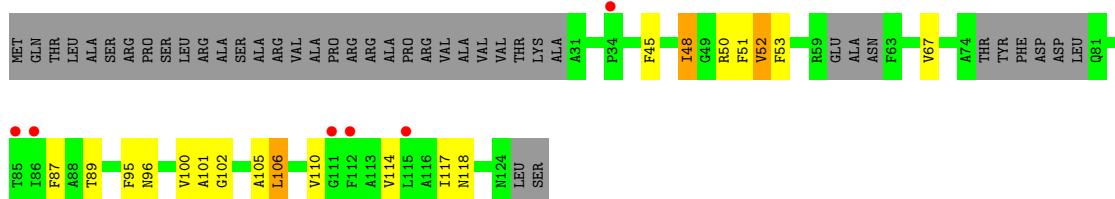


- Molecule 6: Photosystem I reaction center subunit III, chloroplactic

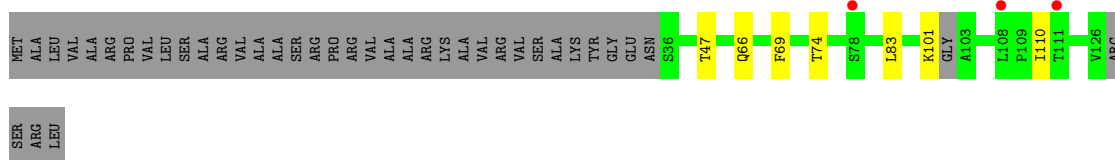




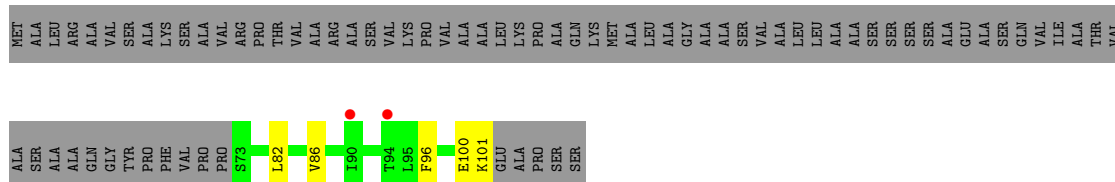
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



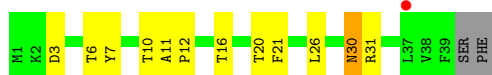
- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic



- Molecule 9: Photosystem I reaction center subunit VIII

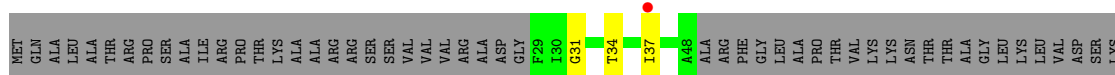


- Molecule 10: Photosystem I reaction center subunit IX

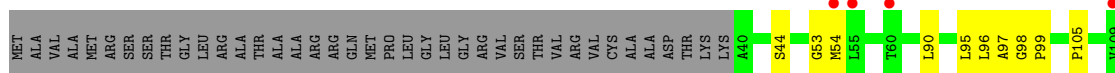


- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

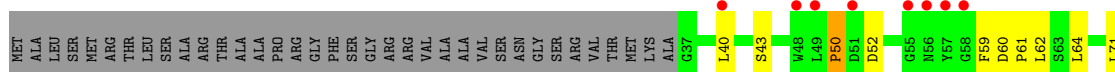




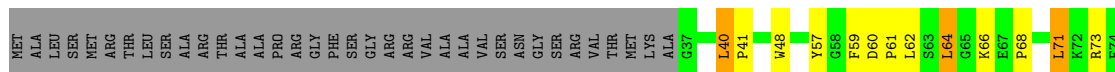
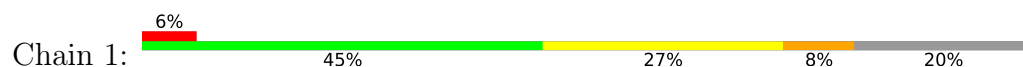
• Molecule 12: PSI subunit V



• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

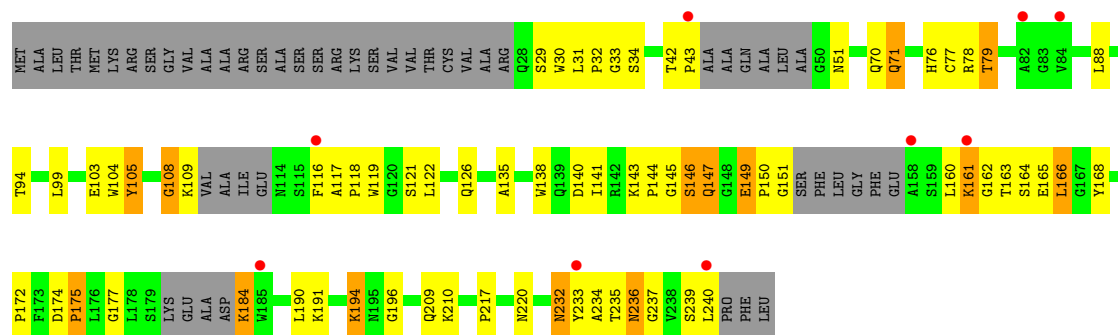


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

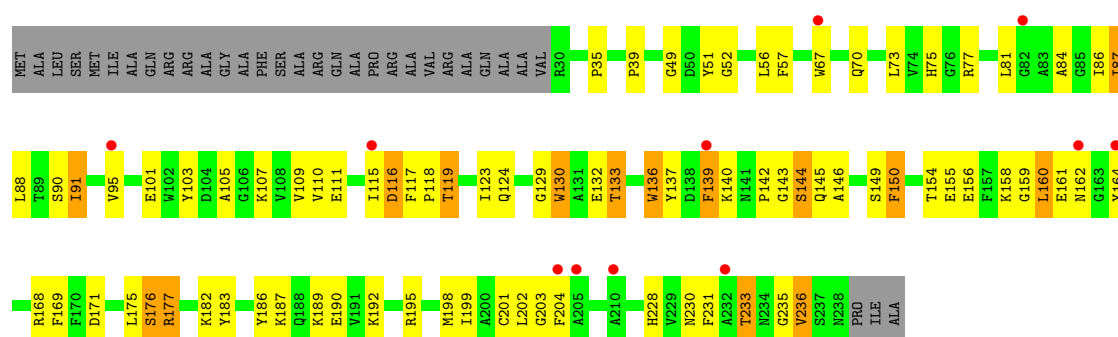


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

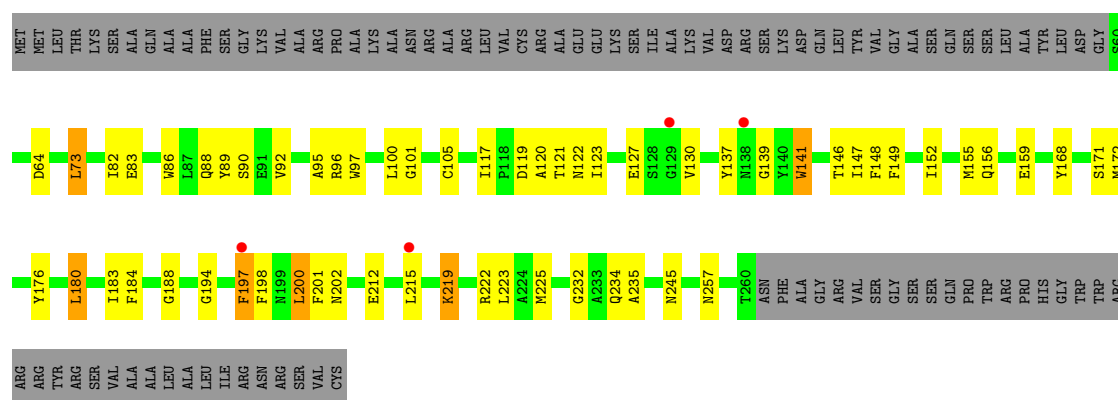




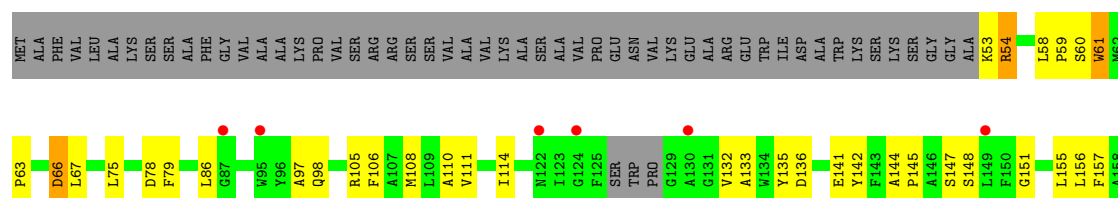
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



• Molecule 16: Lhca3



• Molecule 17: Chlorophyll a-b binding protein, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	194.57Å 98.12Å 210.13Å 90.00° 94.56° 90.00°	Depositor
Resolution (Å)	47.74 – 3.40 47.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.74-3.40) 99.1 (47.74-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.291 , 0.359 0.300 , 0.363	Depositor DCC
R_{free} test set	5416 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	108.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 121.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	42070	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, DGD, XAT, SF4, LMT, PQN, LUT, LHG, CHL, LMG, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.94	10/5995 (0.2%)	1.16	15/8175 (0.2%)
2	B	0.91	9/5997 (0.2%)	1.16	14/8190 (0.2%)
3	C	0.83	0/610	1.04	0/826
4	D	1.03	0/1127	1.33	0/1521
5	E	1.05	0/490	1.26	0/667
6	F	0.99	0/1174	1.53	2/1588 (0.1%)
7	G	1.04	0/631	1.55	2/855 (0.2%)
8	H	1.06	0/704	1.47	0/947
9	I	1.05	0/228	1.53	0/314
10	J	0.98	0/331	1.44	0/454
11	K	1.09	0/296	1.77	2/401 (0.5%)
12	L	1.08	0/1106	1.55	0/1512
13	0	1.00	0/1402	1.53	1/1906 (0.1%)
13	1	0.99	0/1403	1.47	0/1907
14	8	0.99	0/1509	1.51	4/2050 (0.2%)
15	7	1.00	0/1673	1.49	6/2270 (0.3%)
16	3	0.99	0/1587	1.52	0/2154
17	4	0.97	0/1621	1.47	2/2206 (0.1%)
18	6	0.98	0/1479	1.53	2/2012 (0.1%)
19	5	0.97	0/1553	1.41	2/2107 (0.1%)
All	All	0.97	19/30916 (0.1%)	1.36	52/42062 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
13	0	0	3
13	1	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
14	8	0	1
19	5	0	2
All	All	0	8

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TYR	C-O	7.60	1.32	1.24
1	A	652	ALA	C-O	7.22	1.32	1.24
2	B	583	TRP	C-O	-7.19	1.15	1.24
1	A	589	TRP	C-O	6.82	1.31	1.24
1	A	148	TRP	C-O	6.68	1.31	1.24

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	SER	N-CA-C	-8.48	101.07	111.33
2	B	152	PHE	N-CA-C	-8.25	100.95	111.02
2	B	191	TRP	N-CA-C	-7.78	102.49	110.97
14	8	88	LEU	CA-C-N	7.77	125.14	120.24
14	8	88	LEU	C-N-CA	7.77	125.14	120.24

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	0	125	PHE	Peptide
13	0	164	ALA	Peptide
13	0	198	THR	Peptide
14	8	232	ASN	Peptide
1	A	447	PHE	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5799	0	5646	194	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5786	0	5542	223	0
3	C	600	0	583	21	0
4	D	1101	0	1123	11	0
5	E	480	0	476	7	0
6	F	1150	0	1174	17	0
7	G	620	0	612	44	0
8	H	694	0	682	6	0
9	I	221	0	234	3	0
10	J	320	0	322	10	0
11	K	295	0	312	10	0
12	L	1082	0	1103	27	0
13	0	1361	0	1318	65	0
13	1	1362	0	1313	89	0
14	8	1466	0	1444	78	0
15	7	1622	0	1552	92	0
16	3	1542	0	1511	74	0
17	4	1571	0	1529	83	0
18	6	1431	0	1415	66	0
19	5	1510	0	1499	116	0
20	0	484	0	330	22	0
20	1	484	0	330	35	0
20	3	524	0	356	19	0
20	4	396	0	270	34	0
20	5	660	0	450	57	0
20	6	528	0	360	33	0
20	7	396	0	270	27	0
20	8	440	0	300	26	0
20	A	1844	0	1256	97	0
20	B	1803	0	1225	105	0
20	F	132	0	90	6	0
20	G	132	0	90	13	0
20	J	44	0	30	3	0
20	K	71	0	33	5	0
20	L	176	0	120	11	0
21	A	8	0	0	1	0
21	C	16	0	0	2	0
22	A	33	0	46	3	0
22	B	33	0	46	3	0
23	0	21	0	12	3	0
23	3	20	0	14	5	0
23	4	49	0	74	15	0
23	7	35	0	40	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	8	49	0	74	0	0
23	A	89	0	127	4	0
24	1	40	0	56	7	0
24	3	80	0	112	5	0
24	4	40	0	56	4	0
24	5	40	0	56	16	0
24	6	40	0	56	14	0
24	7	40	0	56	2	0
24	8	40	0	56	5	0
24	A	240	0	336	25	0
24	B	240	0	336	31	0
24	F	80	0	112	7	0
24	G	80	0	112	25	0
24	H	40	0	56	2	0
24	I	40	0	56	17	0
24	J	40	0	56	0	0
25	5	51	0	60	16	0
25	B	61	0	83	4	0
26	3	31	0	35	8	0
26	B	31	0	35	3	0
27	0	50	0	70	27	0
27	4	34	0	38	38	0
27	5	45	0	60	7	0
27	6	44	0	61	9	0
27	8	72	0	86	10	0
27	J	30	0	30	0	0
28	0	84	0	112	13	0
28	1	84	0	112	18	0
28	3	84	0	112	5	0
28	4	42	0	56	2	0
28	5	42	0	56	6	0
28	6	42	0	56	3	0
28	7	42	0	56	4	0
28	8	42	0	56	4	0
28	J	42	0	56	10	0
29	0	159	0	124	15	0
29	1	159	0	124	15	0
29	3	47	0	31	1	0
29	4	202	0	153	15	0
29	5	202	0	153	16	0
29	6	202	0	154	12	0
29	7	207	0	164	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	8	159	0	124	8	0
30	4	44	0	56	2	0
30	5	44	0	56	6	0
30	6	44	0	56	10	0
30	7	44	0	56	0	0
30	8	44	0	56	1	0
All	All	42070	0	39382	1552	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 19.

The worst 5 of 1552 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:A:738:THR:OG1	20:A:801:CLA:O2D	1.57	1.22
17:4:54:ARG:HB3	17:4:67:LEU:O	1.45	1.17
1:A:473:SER:O	1:A:477:ILE:O	1.64	1.14
20:1:1007:CLA:HBC1	20:1:1014:CLA:HBC2	1.26	1.14
20:4:307:CLA:HAC1	27:4:318:LMG:H151	1.22	1.14

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	736/751 (98%)	683 (93%)	51 (7%)	2 (0%)	36	65
2	B	726/735 (99%)	668 (92%)	54 (7%)	4 (1%)	21	50
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	139/196 (71%)	121 (87%)	18 (13%)	0	100	100
5	E	59/97 (61%)	52 (88%)	7 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	146/227 (64%)	128 (88%)	15 (10%)	3 (2%)	5	24
7	G	79/126 (63%)	69 (87%)	9 (11%)	1 (1%)	9	33
8	H	86/130 (66%)	74 (86%)	12 (14%)	0	100	100
9	I	27/106 (26%)	23 (85%)	4 (15%)	0	100	100
10	J	37/41 (90%)	34 (92%)	3 (8%)	0	100	100
11	K	40/113 (35%)	34 (85%)	5 (12%)	1 (2%)	4	21
12	L	146/196 (74%)	125 (86%)	19 (13%)	2 (1%)	9	31
13	0	176/228 (77%)	136 (77%)	28 (16%)	12 (7%)	1	6
13	1	176/228 (77%)	133 (76%)	37 (21%)	6 (3%)	3	17
14	8	183/243 (75%)	142 (78%)	34 (19%)	7 (4%)	2	15
15	7	207/241 (86%)	168 (81%)	31 (15%)	8 (4%)	2	15
16	3	199/298 (67%)	165 (83%)	32 (16%)	2 (1%)	12	40
17	4	196/264 (74%)	159 (81%)	35 (18%)	2 (1%)	12	40
18	6	178/257 (69%)	152 (85%)	14 (8%)	12 (7%)	1	6
19	5	187/257 (73%)	134 (72%)	42 (22%)	11 (6%)	1	8
All	All	3801/4815 (79%)	3276 (86%)	452 (12%)	73 (2%)	6	26

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	136	ASP
13	0	165	LYS
14	8	146	SER
15	7	150	PHE
13	1	165	LYS

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	599/610 (98%)	565 (94%)	34 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	593/597 (99%)	561 (95%)	32 (5%)	20	47
3	C	69/70 (99%)	65 (94%)	4 (6%)	18	45
4	D	118/152 (78%)	114 (97%)	4 (3%)	32	57
5	E	52/81 (64%)	51 (98%)	1 (2%)	50	66
6	F	114/169 (68%)	111 (97%)	3 (3%)	40	61
7	G	61/94 (65%)	59 (97%)	2 (3%)	33	57
8	H	73/102 (72%)	71 (97%)	2 (3%)	39	60
9	I	24/76 (32%)	24 (100%)	0	100	100
10	J	35/37 (95%)	34 (97%)	1 (3%)	37	60
11	K	30/80 (38%)	29 (97%)	1 (3%)	33	57
12	L	112/148 (76%)	108 (96%)	4 (4%)	31	56
13	0	130/162 (80%)	114 (88%)	16 (12%)	4	18
13	1	130/162 (80%)	111 (85%)	19 (15%)	3	12
14	8	146/183 (80%)	132 (90%)	14 (10%)	8	28
15	7	161/181 (89%)	142 (88%)	19 (12%)	5	20
16	3	154/230 (67%)	146 (95%)	8 (5%)	21	48
17	4	159/205 (78%)	148 (93%)	11 (7%)	14	40
18	6	146/203 (72%)	130 (89%)	16 (11%)	6	22
19	5	154/206 (75%)	136 (88%)	18 (12%)	5	20
All	All	3060/3748 (82%)	2851 (93%)	209 (7%)	14	40

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	8	194	LYS
16	3	200	LEU
19	5	127	ILE
15	7	88	LEU
15	7	144	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
14	8	232	ASN

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Mol	Chain	Res	Type
17	4	98	GLN
15	7	113	ASN
16	3	156	GLN
19	5	72	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](#)

278 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	CLA	5	311	-	47,52,73	2.15	8 (17%)	55,88,113	1.43	7 (12%)
20	CLA	B	802	-	47,52,73	1.94	10 (21%)	55,88,113	1.33	9 (16%)
20	CLA	8	311	-	47,52,73	1.92	8 (17%)	55,88,113	1.22	5 (9%)
24	BCR	J	103	-	41,41,41	0.33	0	56,56,56	0.42	0
28	LUT	4	317	-	42,43,43	0.35	0	51,60,60	0.54	1 (1%)
30	XAT	8	304	-	41,47,47	1.29	7 (17%)	54,74,74	1.62	11 (20%)
20	CLA	1	1004	13	47,52,73	2.00	8 (17%)	55,88,113	1.33	8 (14%)
20	CLA	B	834	-	47,52,73	1.90	11 (23%)	55,88,113	1.15	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	A	848	-	41,41,41	0.19	0	56,56,56	0.54	0
29	CHL	6	317	18	37,51,74	2.19	8 (21%)	30,86,114	1.46	4 (13%)
29	CHL	0	314	-	41,55,74	2.19	7 (17%)	35,91,114	1.40	5 (14%)
20	CLA	6	309	-	47,52,73	1.93	9 (19%)	55,88,113	1.34	8 (14%)
20	CLA	5	321	-	47,52,73	1.99	9 (19%)	55,88,113	1.33	7 (12%)
20	CLA	5	301	-	47,52,73	2.26	9 (19%)	55,88,113	1.51	13 (23%)
20	CLA	3	1009	-	47,52,73	1.97	10 (21%)	55,88,113	1.30	7 (12%)
20	CLA	8	307	14	47,52,73	1.89	8 (17%)	55,88,113	1.27	5 (9%)
20	CLA	A	829	-	47,52,73	1.92	10 (21%)	55,88,113	1.28	9 (16%)
20	CLA	B	821	-	47,52,73	1.97	9 (19%)	55,88,113	1.34	7 (12%)
20	CLA	B	838	-	47,52,73	1.93	9 (19%)	55,88,113	1.34	6 (10%)
20	CLA	5	322	-	47,52,73	1.91	9 (19%)	55,88,113	1.29	9 (16%)
29	CHL	7	1012	-	41,55,74	2.34	8 (19%)	35,91,114	1.37	4 (11%)
20	CLA	7	1007	15	47,52,73	2.10	10 (21%)	55,88,113	1.51	9 (16%)
20	CLA	A	804	-	47,52,73	1.97	10 (21%)	55,88,113	1.41	8 (14%)
20	CLA	A	826	-	47,52,73	2.06	9 (19%)	55,88,113	1.21	8 (14%)
20	CLA	7	1011	-	47,52,73	2.11	9 (19%)	55,88,113	1.24	8 (14%)
22	PQN	A	842	-	34,34,34	0.33	0	43,45,45	0.63	2 (4%)
28	LUT	1	1016	-	42,43,43	0.23	0	51,60,60	0.54	0
20	CLA	B	811	-	47,52,73	2.07	9 (19%)	55,88,113	1.29	6 (10%)
20	CLA	5	309	19	47,52,73	1.91	8 (17%)	55,88,113	1.46	8 (14%)
28	LUT	5	302	-	42,43,43	0.34	0	51,60,60	0.56	0
20	CLA	F	303	6	47,52,73	2.05	9 (19%)	55,88,113	1.29	8 (14%)
20	CLA	L	202	-	47,52,73	1.91	8 (17%)	55,88,113	1.26	7 (12%)
29	CHL	0	317	-	55,69,74	1.86	7 (12%)	52,108,114	1.24	8 (15%)
28	LUT	3	1002	-	42,43,43	0.41	0	51,60,60	0.79	2 (3%)
20	CLA	B	809	-	47,52,73	2.01	9 (19%)	55,88,113	1.28	7 (12%)
20	CLA	6	308	-	47,52,73	2.14	8 (17%)	55,88,113	1.42	11 (20%)
20	CLA	0	308	13	47,52,73	1.92	8 (17%)	55,88,113	1.29	7 (12%)
23	LHG	4	301	20	48,48,48	0.32	0	51,54,54	0.48	0
20	CLA	0	301	23	47,52,73	1.99	9 (19%)	55,88,113	1.27	6 (10%)
29	CHL	5	316	-	55,69,74	1.91	9 (16%)	52,108,114	1.35	7 (13%)
20	CLA	6	320	-	47,52,73	1.96	7 (14%)	55,88,113	1.49	12 (21%)
24	BCR	F	301	-	41,41,41	0.55	1 (2%)	56,56,56	0.65	1 (1%)
20	CLA	1	1008	-	47,52,73	1.95	9 (19%)	55,88,113	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	6	310	-	47,52,73	1.83	9 (19%)	55,88,113	1.37	8 (14%)
27	LMG	8	318	-	28,28,55	0.30	0	36,36,63	0.48	0
20	CLA	B	833	-	47,52,73	1.79	8 (17%)	55,88,113	1.28	8 (14%)
20	CLA	A	823	-	47,52,73	1.97	8 (17%)	55,88,113	1.32	8 (14%)
20	CLA	8	308	14	47,52,73	2.03	9 (19%)	55,88,113	1.45	11 (20%)
20	CLA	5	312	19	47,52,73	2.03	8 (17%)	55,88,113	1.42	11 (20%)
21	SF4	C	1002	3	0,12,12	-	-	-	-	-
20	CLA	8	309	27	47,52,73	2.05	9 (19%)	55,88,113	1.50	9 (16%)
20	CLA	8	312	-	47,52,73	1.92	10 (21%)	55,88,113	1.35	9 (16%)
20	CLA	B	837	-	47,52,73	2.04	8 (17%)	55,88,113	1.33	7 (12%)
20	CLA	6	318	-	47,52,73	2.05	10 (21%)	55,88,113	1.40	7 (12%)
20	CLA	A	803	20	47,52,73	1.88	9 (19%)	55,88,113	1.31	6 (10%)
27	LMG	6	319	-	44,44,55	0.38	0	52,52,63	0.61	1 (1%)
20	CLA	1	1014	-	47,52,73	2.03	8 (17%)	55,88,113	1.36	8 (14%)
20	CLA	B	818	-	47,52,73	1.92	8 (17%)	55,88,113	1.18	7 (12%)
20	CLA	B	823	-	47,52,73	2.00	9 (19%)	55,88,113	1.28	6 (10%)
28	LUT	J	104	-	42,43,43	0.49	0	51,60,60	0.90	2 (3%)
20	CLA	A	806	-	47,52,73	1.86	9 (19%)	55,88,113	1.38	8 (14%)
20	CLA	4	309	-	47,52,73	1.82	9 (19%)	55,88,113	1.31	6 (10%)
20	CLA	F	302	-	47,52,73	1.98	10 (21%)	55,88,113	1.29	8 (14%)
20	CLA	1	1011	13	47,52,73	1.98	8 (17%)	55,88,113	1.34	10 (18%)
29	CHL	8	317	-	55,69,74	1.89	6 (10%)	52,108,114	1.38	7 (13%)
20	CLA	5	306	-	47,52,73	1.96	9 (19%)	55,88,113	1.30	8 (14%)
20	CLA	A	835	-	47,52,73	1.92	9 (19%)	55,88,113	1.32	7 (12%)
20	CLA	B	816	-	47,52,73	1.95	10 (21%)	55,88,113	1.27	5 (9%)
20	CLA	A	830	-	47,52,73	1.97	9 (19%)	55,88,113	1.26	6 (10%)
20	CLA	A	812	-	47,52,73	1.91	9 (19%)	55,88,113	1.21	6 (10%)
20	CLA	A	834	-	47,52,73	2.04	9 (19%)	55,88,113	1.39	8 (14%)
30	XAT	5	303	-	41,47,47	0.26	0	54,74,74	1.08	4 (7%)
20	CLA	A	827	-	47,52,73	1.86	9 (19%)	55,88,113	1.28	7 (12%)
24	BCR	1	1001	-	41,41,41	0.53	1 (2%)	56,56,56	1.10	5 (8%)
20	CLA	8	316	14	47,52,73	1.83	8 (17%)	55,88,113	1.28	6 (10%)
20	CLA	3	1010	-	47,52,73	1.94	6 (12%)	55,88,113	1.26	8 (14%)
20	CLA	6	301	-	47,52,73	1.89	10 (21%)	55,88,113	1.27	8 (14%)
20	CLA	A	851	-	47,52,73	1.93	9 (19%)	55,88,113	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	4	313	-	45,59,74	2.10	10 (22%)	40,96,114	1.29	6 (15%)
20	CLA	B	832	-	47,52,73	1.92	10 (21%)	55,88,113	1.23	7 (12%)
20	CLA	3	1015	16	47,52,73	1.94	10 (21%)	55,88,113	1.23	8 (14%)
20	CLA	1	1006	13	47,52,73	2.02	7 (14%)	55,88,113	1.34	7 (12%)
20	CLA	B	830	-	47,52,73	1.77	8 (17%)	55,88,113	1.27	7 (12%)
20	CLA	A	819	-	47,52,73	1.98	9 (19%)	55,88,113	1.21	7 (12%)
20	CLA	B	827	-	47,52,73	2.02	10 (21%)	55,88,113	1.32	7 (12%)
20	CLA	7	1008	-	47,52,73	1.91	9 (19%)	55,88,113	1.24	7 (12%)
24	BCR	A	846	-	41,41,41	0.62	0	56,56,56	0.88	2 (3%)
21	SF4	C	1001	3	0,12,12	-	-	-	-	-
20	CLA	5	318	-	47,52,73	2.11	9 (19%)	55,88,113	1.35	10 (18%)
23	LHG	8	301	20	48,48,48	0.27	0	51,54,54	0.29	0
29	CHL	5	314	-	45,59,74	2.25	9 (20%)	40,96,114	1.34	6 (15%)
20	CLA	7	1005	15	47,52,73	2.10	10 (21%)	55,88,113	1.48	8 (14%)
20	CLA	0	305	-	47,52,73	1.95	10 (21%)	55,88,113	1.28	7 (12%)
29	CHL	8	314	-	41,55,74	2.16	10 (24%)	35,91,114	1.47	4 (11%)
28	LUT	6	303	-	42,43,43	0.30	0	51,60,60	0.59	0
20	CLA	B	819	-	47,52,73	1.95	10 (21%)	55,88,113	1.25	7 (12%)
20	CLA	1	1009	23	47,52,73	1.77	9 (19%)	55,88,113	1.14	6 (10%)
20	CLA	A	828	-	47,52,73	1.88	10 (21%)	55,88,113	1.32	8 (14%)
24	BCR	G	205	-	41,41,41	0.52	1 (2%)	56,56,56	1.23	4 (7%)
20	CLA	J	102	-	47,52,73	1.94	10 (21%)	55,88,113	1.18	7 (12%)
24	BCR	B	844	-	41,41,41	0.42	0	56,56,56	0.55	0
24	BCR	I	201	-	41,41,41	0.57	0	56,56,56	0.94	4 (7%)
26	LMT	3	1018	-	32,32,36	0.31	0	43,43,47	0.71	1 (2%)
20	CLA	A	837	-	47,52,73	1.93	10 (21%)	55,88,113	1.35	4 (7%)
29	CHL	1	1012	-	41,55,74	2.11	8 (19%)	35,91,114	1.44	7 (20%)
20	CLA	A	805	-	47,52,73	1.97	9 (19%)	55,88,113	1.23	7 (12%)
20	CLA	A	833	1	47,52,73	1.92	9 (19%)	55,88,113	1.39	5 (9%)
20	CLA	3	1016	-	47,52,73	2.03	8 (17%)	55,88,113	1.39	7 (12%)
29	CHL	7	1015	-	40,54,74	2.37	8 (20%)	34,90,114	1.61	5 (14%)
20	CLA	5	308	-	47,52,73	1.95	10 (21%)	55,88,113	1.41	10 (18%)
20	CLA	3	1011	23	43,48,73	2.09	10 (23%)	51,83,113	1.39	8 (15%)
20	CLA	5	310	-	47,52,73	1.87	10 (21%)	55,88,113	1.24	5 (9%)
29	CHL	4	316	17	37,51,74	2.21	8 (21%)	30,86,114	1.66	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	6	306	18	47,52,73	1.86	9 (19%)	55,88,113	1.29	8 (14%)
24	BCR	G	204	-	41,41,41	0.57	0	56,56,56	1.03	4 (7%)
24	BCR	3	1004	-	41,41,41	0.65	1 (2%)	56,56,56	1.05	3 (5%)
24	BCR	6	302	-	41,41,41	0.53	1 (2%)	56,56,56	1.25	3 (5%)
20	CLA	A	811	-	47,52,73	1.95	8 (17%)	55,88,113	1.36	8 (14%)
20	CLA	A	822	-	47,52,73	1.97	8 (17%)	55,88,113	1.30	8 (14%)
24	BCR	A	847	-	41,41,41	0.40	0	56,56,56	0.79	2 (3%)
29	CHL	8	315	-	45,59,74	2.35	9 (20%)	40,96,114	1.34	5 (12%)
27	LMG	J	101	-	30,30,55	0.24	0	38,38,63	0.24	0
24	BCR	4	302	-	41,41,41	0.51	1 (2%)	56,56,56	1.16	5 (8%)
20	CLA	A	816	-	47,52,73	1.98	9 (19%)	55,88,113	1.24	7 (12%)
23	LHG	A	843	-	39,39,48	0.28	0	42,45,54	0.26	0
29	CHL	0	315	-	45,59,74	2.03	9 (20%)	40,96,114	1.31	6 (15%)
20	CLA	A	802	-	47,52,73	1.97	10 (21%)	55,88,113	1.32	6 (10%)
20	CLA	B	803	-	47,52,73	2.00	9 (19%)	55,88,113	1.41	8 (14%)
20	CLA	L	204	-	47,52,73	1.99	9 (19%)	55,88,113	1.25	7 (12%)
20	CLA	6	312	18	47,52,73	1.93	8 (17%)	55,88,113	1.46	9 (16%)
20	CLA	0	309	-	47,52,73	2.00	9 (19%)	55,88,113	1.35	7 (12%)
24	BCR	B	847	-	41,41,41	0.17	0	56,56,56	0.63	0
20	CLA	L	201	-	47,52,73	1.88	9 (19%)	55,88,113	1.23	7 (12%)
20	CLA	7	1010	23	47,52,73	1.93	9 (19%)	55,88,113	1.17	6 (10%)
29	CHL	4	315	-	55,69,74	1.83	8 (14%)	52,108,114	1.35	6 (11%)
20	CLA	A	815	-	47,52,73	2.02	9 (19%)	55,88,113	1.36	7 (12%)
20	CLA	A	808	-	47,52,73	1.98	8 (17%)	55,88,113	1.29	7 (12%)
24	BCR	H	201	-	41,41,41	0.86	3 (7%)	56,56,56	1.22	6 (10%)
20	CLA	4	308	17	47,52,73	1.99	8 (17%)	55,88,113	1.38	8 (14%)
20	CLA	7	1009	-	47,52,73	1.91	8 (17%)	55,88,113	1.32	7 (12%)
20	CLA	B	828	-	47,52,73	1.90	10 (21%)	55,88,113	1.33	8 (14%)
20	CLA	5	304	19	47,52,73	2.05	9 (19%)	55,88,113	1.25	5 (9%)
20	CLA	5	323	-	47,52,73	1.98	8 (17%)	55,88,113	1.25	7 (12%)
24	BCR	7	1003	-	41,41,41	0.69	1 (2%)	56,56,56	1.59	6 (10%)
29	CHL	4	312	-	41,55,74	2.37	10 (24%)	35,91,114	1.47	6 (17%)
20	CLA	K	201	-	47,52,73	1.93	8 (17%)	55,88,113	1.24	6 (10%)
20	CLA	B	807	-	47,52,73	1.94	9 (19%)	55,88,113	1.25	6 (10%)
28	LUT	0	304	-	42,43,43	0.26	0	51,60,60	0.69	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	836	-	47,52,73	1.90	9 (19%)	55,88,113	1.33	8 (14%)
28	LUT	0	318	-	42,43,43	0.41	0	51,60,60	0.52	0
20	CLA	A	818	-	47,52,73	1.91	9 (19%)	55,88,113	1.26	7 (12%)
30	XAT	4	303	-	41,47,47	0.20	0	54,74,74	0.88	3 (5%)
27	LMG	0	303	-	50,50,55	0.31	0	58,58,63	0.53	1 (1%)
20	CLA	1	1017	-	47,52,73	1.97	8 (17%)	55,88,113	1.35	8 (14%)
20	CLA	6	315	18	47,52,73	1.89	8 (17%)	55,88,113	1.35	7 (12%)
20	CLA	7	1004	15	47,52,73	1.79	9 (19%)	55,88,113	1.33	9 (16%)
20	CLA	A	801	-	47,52,73	1.96	7 (14%)	55,88,113	1.45	10 (18%)
25	DGD	B	848	-	62,62,67	0.86	2 (3%)	76,76,81	1.13	6 (7%)
20	CLA	A	852	-	47,52,73	1.95	8 (17%)	55,88,113	1.28	8 (14%)
20	CLA	6	311	-	47,52,73	1.84	10 (21%)	55,88,113	1.13	4 (7%)
20	CLA	L	203	-	47,52,73	2.02	9 (19%)	55,88,113	1.26	7 (12%)
20	CLA	0	310	-	47,52,73	2.15	9 (19%)	55,88,113	1.29	6 (10%)
20	CLA	1	1007	-	47,52,73	1.98	10 (21%)	55,88,113	1.44	9 (16%)
24	BCR	A	844	-	41,41,41	0.34	0	56,56,56	0.55	0
20	CLA	A	838	-	47,52,73	1.98	8 (17%)	55,88,113	1.32	7 (12%)
20	CLA	B	822	-	47,52,73	1.99	10 (21%)	55,88,113	1.31	6 (10%)
28	LUT	8	303	-	42,43,43	0.31	0	51,60,60	0.50	0
20	CLA	G	201	-	47,52,73	1.95	8 (17%)	55,88,113	1.29	9 (16%)
20	CLA	8	305	14	47,52,73	1.83	7 (14%)	55,88,113	1.19	7 (12%)
29	CHL	1	1015	-	55,69,74	1.94	8 (14%)	52,108,114	1.25	9 (17%)
23	LHG	0	302	20	20,20,48	0.34	0	23,26,54	1.78	4 (17%)
20	CLA	B	814	-	47,52,73	1.96	9 (19%)	55,88,113	1.25	7 (12%)
20	CLA	8	313	14	47,52,73	2.00	7 (14%)	55,88,113	1.41	8 (14%)
20	CLA	5	315	19	47,52,73	1.87	9 (19%)	55,88,113	1.28	6 (10%)
28	LUT	7	1001	-	42,43,43	0.47	1 (2%)	51,60,60	0.86	4 (7%)
20	CLA	K	202	-	27,35,73	2.25	10 (37%)	32,60,113	2.39	11 (34%)
20	CLA	B	840	-	47,52,73	1.90	9 (19%)	55,88,113	1.23	7 (12%)
20	CLA	4	306	-	47,52,73	1.93	9 (19%)	55,88,113	1.23	6 (10%)
20	CLA	A	831	-	47,52,73	2.10	9 (19%)	55,88,113	1.24	4 (7%)
20	CLA	B	806	-	47,52,73	1.91	9 (19%)	55,88,113	1.21	6 (10%)
20	CLA	B	825	-	47,52,73	1.98	10 (21%)	55,88,113	1.29	9 (16%)
20	CLA	5	307	19	47,52,73	1.94	10 (21%)	55,88,113	1.46	7 (12%)
24	BCR	A	850	-	41,41,41	0.41	0	56,56,56	0.80	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LUT	3	1001	-	42,43,43	0.25	0	51,60,60	0.52	0
20	CLA	B	835	-	47,52,73	1.94	9 (19%)	55,88,113	1.31	7 (12%)
20	CLA	1	1003	-	47,52,73	1.94	9 (19%)	55,88,113	1.24	8 (14%)
20	CLA	4	305	17	47,52,73	2.11	10 (21%)	55,88,113	1.28	7 (12%)
20	CLA	0	311	23	47,52,73	1.93	9 (19%)	55,88,113	1.15	5 (9%)
20	CLA	B	812	2	47,52,73	1.95	8 (17%)	55,88,113	1.28	5 (9%)
20	CLA	B	815	-	47,52,73	2.07	9 (19%)	55,88,113	1.33	7 (12%)
24	BCR	B	846	-	41,41,41	0.34	0	56,56,56	0.47	0
20	CLA	B	805	-	47,52,73	1.97	7 (14%)	55,88,113	1.22	7 (12%)
20	CLA	A	824	-	47,52,73	2.03	9 (19%)	55,88,113	1.41	9 (16%)
20	CLA	B	831	-	47,52,73	2.07	9 (19%)	55,88,113	1.36	7 (12%)
20	CLA	A	820	-	47,52,73	1.98	10 (21%)	55,88,113	1.31	6 (10%)
20	CLA	3	1012	-	47,52,73	2.01	9 (19%)	55,88,113	1.22	8 (14%)
29	CHL	5	317	19	37,51,74	2.12	9 (24%)	30,86,114	1.49	5 (16%)
20	CLA	0	313	13	47,52,73	1.97	8 (17%)	55,88,113	1.25	10 (18%)
20	CLA	B	813	-	47,52,73	2.15	9 (19%)	55,88,113	1.38	8 (14%)
24	BCR	B	804	-	41,41,41	0.55	1 (2%)	56,56,56	1.88	13 (23%)
20	CLA	B	836	-	47,52,73	1.98	9 (19%)	55,88,113	1.28	9 (16%)
20	CLA	A	839	-	47,52,73	2.02	10 (21%)	55,88,113	1.20	6 (10%)
20	CLA	0	307	-	47,52,73	2.08	10 (21%)	55,88,113	1.25	7 (12%)
20	CLA	8	310	-	47,52,73	2.00	9 (19%)	55,88,113	1.27	5 (9%)
20	CLA	3	1008	16	47,52,73	2.02	9 (19%)	55,88,113	1.41	9 (16%)
20	CLA	6	305	18	47,52,73	1.93	10 (21%)	55,88,113	1.30	5 (9%)
21	SF4	A	841	1,2	0,12,12	-	-	-	-	-
20	CLA	1	1005	-	47,52,73	2.00	9 (19%)	55,88,113	1.26	6 (10%)
24	BCR	5	320	-	41,41,41	0.38	0	56,56,56	0.68	2 (3%)
20	CLA	B	820	-	47,52,73	1.98	9 (19%)	55,88,113	1.39	8 (14%)
20	CLA	B	839	-	47,52,73	1.91	9 (19%)	55,88,113	1.29	7 (12%)
20	CLA	3	1006	-	47,52,73	2.01	10 (21%)	55,88,113	1.41	8 (14%)
29	CHL	6	316	-	55,69,74	2.08	9 (16%)	52,108,114	1.16	6 (11%)
20	CLA	A	825	-	47,52,73	1.96	9 (19%)	55,88,113	1.29	6 (10%)
26	LMT	B	849	-	32,32,36	0.20	0	43,43,47	0.47	0
20	CLA	4	314	17	47,52,73	1.96	7 (14%)	55,88,113	1.27	8 (14%)
29	CHL	3	1014	-	41,55,74	2.31	9 (21%)	35,91,114	1.46	5 (14%)
20	CLA	4	311	17	47,52,73	1.89	8 (17%)	55,88,113	1.34	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	810	20	47,52,73	1.98	7 (14%)	55,88,113	1.32	7 (12%)
25	DGD	5	319	-	52,52,67	1.08	3 (5%)	66,66,81	1.45	7 (10%)
20	CLA	4	310	-	47,52,73	2.02	7 (14%)	55,88,113	1.32	6 (10%)
20	CLA	A	807	-	47,52,73	1.90	10 (21%)	55,88,113	1.30	7 (12%)
24	BCR	A	845	-	41,41,41	0.65	2 (4%)	56,56,56	1.62	10 (17%)
20	CLA	B	824	-	47,52,73	1.95	9 (19%)	55,88,113	1.37	8 (14%)
20	CLA	A	817	-	47,52,73	1.97	7 (14%)	55,88,113	1.35	8 (14%)
20	CLA	1	1010	-	47,52,73	1.92	9 (19%)	55,88,113	1.29	7 (12%)
20	CLA	7	1014	15	47,52,73	1.92	10 (21%)	55,88,113	1.33	8 (14%)
29	CHL	1	1013	-	45,59,74	2.08	9 (20%)	40,96,114	1.37	5 (12%)
20	CLA	B	841	-	47,52,73	2.00	8 (17%)	55,88,113	1.36	8 (14%)
28	LUT	1	1002	-	42,43,43	0.37	0	51,60,60	0.61	0
20	CLA	A	840	-	47,52,73	1.90	7 (14%)	55,88,113	1.28	6 (10%)
20	CLA	B	850	-	44,49,73	3.87	9 (20%)	42,80,113	1.38	6 (14%)
30	XAT	6	304	-	41,47,47	0.32	0	54,74,74	1.00	3 (5%)
27	LMG	5	324	-	45,45,55	0.46	0	53,53,63	0.63	1 (1%)
20	CLA	3	1007	-	47,52,73	1.96	10 (21%)	55,88,113	1.32	7 (12%)
24	BCR	F	304	-	41,41,41	0.32	0	56,56,56	0.65	0
20	CLA	3	1005	16	47,52,73	1.86	9 (19%)	55,88,113	1.19	6 (10%)
22	PQN	B	842	-	34,34,34	0.33	0	43,45,45	0.50	1 (2%)
20	CLA	A	813	-	47,52,73	2.01	8 (17%)	55,88,113	1.32	8 (14%)
20	CLA	B	826	-	47,52,73	1.99	9 (19%)	55,88,113	1.36	7 (12%)
20	CLA	4	304	17	47,52,73	1.83	9 (19%)	55,88,113	1.30	9 (16%)
20	CLA	B	817	-	47,52,73	1.96	8 (17%)	55,88,113	1.32	8 (14%)
20	CLA	A	832	-	47,52,73	1.85	9 (19%)	55,88,113	1.25	8 (14%)
20	CLA	4	307	17	47,52,73	2.14	9 (19%)	55,88,113	1.84	10 (18%)
27	LMG	8	319	20	44,44,55	0.28	0	52,52,63	0.78	1 (1%)
29	CHL	7	1017	15	60,74,74	1.92	8 (13%)	58,114,114	1.20	5 (8%)
30	XAT	7	1002	-	41,47,47	1.31	8 (19%)	54,74,74	1.70	12 (22%)
29	CHL	6	313	-	41,55,74	2.26	10 (24%)	35,91,114	1.31	4 (11%)
20	CLA	0	312	-	47,52,73	2.00	7 (14%)	55,88,113	1.34	8 (14%)
20	CLA	8	306	14	47,52,73	2.00	11 (23%)	55,88,113	1.42	5 (9%)
20	CLA	A	814	-	43,48,73	2.13	10 (23%)	51,83,113	1.43	9 (17%)
24	BCR	B	843	-	41,41,41	0.99	3 (7%)	56,56,56	1.48	10 (17%)
24	BCR	8	302	-	41,41,41	0.52	0	56,56,56	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	7	1013	-	42,56,74	2.56	8 (19%)	36,92,114	1.52	5 (13%)
20	CLA	3	1013	16	47,52,73	1.96	8 (17%)	55,88,113	1.37	8 (14%)
20	CLA	G	202	-	47,52,73	1.97	9 (19%)	55,88,113	1.28	8 (14%)
20	CLA	7	1006	-	47,52,73	1.81	7 (14%)	55,88,113	1.33	7 (12%)
20	CLA	B	829	-	47,52,73	1.94	9 (19%)	55,88,113	1.32	8 (14%)
20	CLA	6	307	-	47,52,73	2.02	7 (14%)	55,88,113	1.31	6 (10%)
29	CHL	5	313	-	41,55,74	2.34	8 (19%)	35,91,114	1.32	4 (11%)
23	LHG	7	1016	20	34,34,48	0.42	0	37,40,54	0.52	0
20	CLA	B	801	-	47,52,73	1.89	9 (19%)	55,88,113	1.27	7 (12%)
20	CLA	5	305	19	47,52,73	2.07	8 (17%)	55,88,113	1.29	7 (12%)
20	CLA	F	305	-	47,52,73	2.01	9 (19%)	55,88,113	1.28	7 (12%)
20	CLA	A	809	-	47,52,73	1.90	10 (21%)	55,88,113	1.18	7 (12%)
20	CLA	G	203	-	47,52,73	1.96	9 (19%)	55,88,113	1.19	7 (12%)
20	CLA	0	306	13	47,52,73	1.87	8 (17%)	55,88,113	1.35	8 (14%)
20	CLA	3	1017	-	47,52,73	2.01	10 (21%)	55,88,113	1.28	8 (14%)
23	LHG	A	849	-	48,48,48	0.24	0	51,54,54	0.34	0
27	LMG	4	318	-	34,34,55	0.32	0	42,42,63	0.95	3 (7%)
29	CHL	6	314	-	45,59,74	2.46	9 (20%)	40,96,114	1.40	7 (17%)
23	LHG	3	1019	20	19,19,48	0.71	1 (5%)	21,24,54	0.52	0
20	CLA	B	808	-	47,52,73	1.97	8 (17%)	55,88,113	1.31	7 (12%)
20	CLA	A	821	-	47,52,73	2.07	10 (21%)	55,88,113	1.44	9 (16%)
20	CLA	B	810	-	47,52,73	1.90	9 (19%)	55,88,113	1.36	8 (14%)
24	BCR	3	1003	-	41,41,41	0.61	0	56,56,56	0.92	2 (3%)
20	CLA	0	316	-	47,52,73	1.94	8 (17%)	55,88,113	1.35	7 (12%)
24	BCR	B	845	-	41,41,41	0.52	0	56,56,56	0.97	3 (5%)

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
20	CLA	5	311	-	1/1/11/20	5/13/89/115	-
20	CLA	B	802	-	1/1/11/20	3/13/89/115	-
20	CLA	8	311	-	1/1/11/20	6/13/89/115	-
24	BCR	J	103	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	4	317	-	-	0/29/67/67	0/2/2/2
30	XAT	8	304	-	-	12/31/93/93	0/4/4/4
20	CLA	1	1004	13	1/1/11/20	3/13/89/115	-
20	CLA	B	834	-	1/1/11/20	2/13/89/115	-
24	BCR	A	848	-	-	8/29/63/63	0/2/2/2
29	CHL	6	317	18	3/3/15/26	2/12/110/137	-
29	CHL	0	314	-	3/3/16/26	3/17/115/137	-
20	CLA	6	309	-	1/1/11/20	7/13/89/115	-
20	CLA	5	321	-	1/1/11/20	4/13/89/115	-
20	CLA	5	301	-	1/1/11/20	9/13/89/115	-
20	CLA	3	1009	-	1/1/11/20	9/13/89/115	-
20	CLA	8	307	14	1/1/11/20	3/13/89/115	-
20	CLA	A	829	-	1/1/11/20	4/13/89/115	-
20	CLA	B	821	-	1/1/11/20	3/13/89/115	-
20	CLA	B	838	-	1/1/11/20	6/13/89/115	-
20	CLA	5	322	-	1/1/11/20	3/13/89/115	-
29	CHL	7	1012	-	3/3/16/26	5/17/115/137	-
20	CLA	7	1007	15	1/1/11/20	2/13/89/115	-
20	CLA	A	804	-	1/1/11/20	3/13/89/115	-
20	CLA	A	826	-	1/1/11/20	0/13/89/115	-
20	CLA	7	1011	-	1/1/11/20	7/13/89/115	-
22	PQN	A	842	-	-	6/23/43/43	0/2/2/2
28	LUT	1	1016	-	-	0/29/67/67	0/2/2/2
20	CLA	B	811	-	1/1/11/20	1/13/89/115	-
20	CLA	5	309	19	1/1/11/20	9/13/89/115	-
28	LUT	5	302	-	-	2/29/67/67	0/2/2/2
20	CLA	F	303	6	1/1/11/20	4/13/89/115	-
20	CLA	L	202	-	1/1/11/20	4/13/89/115	-
29	CHL	0	317	-	3/3/19/26	14/33/131/137	-
28	LUT	3	1002	-	-	8/29/67/67	0/2/2/2
20	CLA	B	809	-	1/1/11/20	4/13/89/115	-
20	CLA	6	308	-	1/1/11/20	1/13/89/115	-
20	CLA	0	308	13	1/1/11/20	3/13/89/115	-
23	LHG	4	301	20	-	21/53/53/53	-
20	CLA	0	301	23	1/1/11/20	1/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	5	316	-	3/3/19/26	14/33/131/137	-
20	CLA	6	320	-	1/1/11/20	2/13/89/115	-
24	BCR	F	301	-	-	5/29/63/63	0/2/2/2
20	CLA	1	1008	-	1/1/11/20	9/13/89/115	-
20	CLA	6	310	-	1/1/11/20	7/13/89/115	-
27	LMG	8	318	-	-	5/22/42/70	0/1/1/1
20	CLA	B	833	-	1/1/11/20	3/13/89/115	-
20	CLA	A	823	-	1/1/11/20	3/13/89/115	-
20	CLA	8	308	14	1/1/11/20	2/13/89/115	-
20	CLA	5	312	19	1/1/11/20	1/13/89/115	-
21	SF4	C	1002	3	-	-	0/6/5/5
20	CLA	8	309	27	1/1/11/20	6/13/89/115	-
20	CLA	8	312	-	1/1/11/20	5/13/89/115	-
20	CLA	B	837	-	1/1/11/20	5/13/89/115	-
20	CLA	6	318	-	1/1/11/20	5/13/89/115	-
20	CLA	A	803	20	1/1/11/20	8/13/89/115	-
27	LMG	6	319	-	-	11/39/59/70	0/1/1/1
20	CLA	1	1014	-	1/1/11/20	3/13/89/115	-
20	CLA	B	818	-	1/1/11/20	4/13/89/115	-
20	CLA	B	823	-	1/1/11/20	4/13/89/115	-
28	LUT	J	104	-	-	7/29/67/67	0/2/2/2
20	CLA	A	806	-	1/1/11/20	5/13/89/115	-
20	CLA	4	309	-	1/1/11/20	10/13/89/115	-
20	CLA	F	302	-	1/1/11/20	2/13/89/115	-
20	CLA	1	1011	13	1/1/11/20	3/13/89/115	-
29	CHL	8	317	-	3/3/19/26	17/33/131/137	-
20	CLA	5	306	-	1/1/11/20	5/13/89/115	-
20	CLA	A	835	-	1/1/11/20	2/13/89/115	-
20	CLA	B	816	-	1/1/11/20	7/13/89/115	-
20	CLA	A	830	-	1/1/11/20	3/13/89/115	-
20	CLA	A	812	-	1/1/11/20	6/13/89/115	-
20	CLA	A	834	-	1/1/11/20	1/13/89/115	-
30	XAT	5	303	-	-	2/31/93/93	0/4/4/4
20	CLA	A	827	-	1/1/11/20	4/13/89/115	-
24	BCR	1	1001	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	8	316	14	1/1/11/20	3/13/89/115	-
20	CLA	3	1010	-	1/1/11/20	5/13/89/115	-
20	CLA	6	301	-	1/1/11/20	7/13/89/115	-
20	CLA	A	851	-	1/1/11/20	2/13/89/115	-
29	CHL	4	313	-	3/3/17/26	3/21/119/137	-
20	CLA	B	832	-	1/1/11/20	1/13/89/115	-
20	CLA	3	1015	16	1/1/11/20	2/13/89/115	-
20	CLA	1	1006	13	1/1/11/20	2/13/89/115	-
20	CLA	B	830	-	1/1/11/20	3/13/89/115	-
20	CLA	A	819	-	1/1/11/20	6/13/89/115	-
20	CLA	B	827	-	1/1/11/20	3/13/89/115	-
20	CLA	7	1008	-	1/1/11/20	4/13/89/115	-
24	BCR	A	846	-	-	6/29/63/63	0/2/2/2
21	SF4	C	1001	3	-	-	0/6/5/5
20	CLA	5	318	-	1/1/11/20	2/13/89/115	-
23	LHG	8	301	20	-	16/53/53/53	-
29	CHL	5	314	-	3/3/17/26	3/21/119/137	-
20	CLA	7	1005	15	1/1/11/20	1/13/89/115	-
20	CLA	0	305	-	1/1/11/20	3/13/89/115	-
29	CHL	8	314	-	3/3/16/26	6/17/115/137	-
28	LUT	6	303	-	-	2/29/67/67	0/2/2/2
20	CLA	B	819	-	1/1/11/20	4/13/89/115	-
20	CLA	1	1009	23	1/1/11/20	4/13/89/115	-
20	CLA	A	828	-	1/1/11/20	5/13/89/115	-
24	BCR	G	205	-	-	7/29/63/63	0/2/2/2
20	CLA	J	102	-	1/1/11/20	6/13/89/115	-
24	BCR	B	844	-	-	8/29/63/63	0/2/2/2
24	BCR	I	201	-	-	10/29/63/63	0/2/2/2
26	LMT	3	1018	-	-	4/17/57/61	0/2/2/2
20	CLA	A	837	-	1/1/11/20	4/13/89/115	-
29	CHL	1	1012	-	3/3/16/26	7/17/115/137	-
20	CLA	A	805	-	1/1/11/20	6/13/89/115	-
20	CLA	A	833	1	1/1/11/20	3/13/89/115	-
20	CLA	3	1016	-	1/1/11/20	11/13/89/115	-
29	CHL	7	1015	-	3/3/16/26	6/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	5	308	-	1/1/11/20	3/13/89/115	-
20	CLA	3	1011	23	1/1/10/20	2/8/84/115	-
20	CLA	5	310	-	1/1/11/20	7/13/89/115	-
29	CHL	4	316	17	3/3/15/26	4/12/110/137	-
20	CLA	6	306	18	1/1/11/20	4/13/89/115	-
24	BCR	G	204	-	-	2/29/63/63	0/2/2/2
24	BCR	3	1004	-	-	8/29/63/63	0/2/2/2
24	BCR	6	302	-	-	7/29/63/63	0/2/2/2
20	CLA	A	811	-	1/1/11/20	6/13/89/115	-
20	CLA	A	822	-	1/1/11/20	4/13/89/115	-
29	CHL	8	315	-	3/3/17/26	1/21/119/137	-
24	BCR	A	847	-	-	7/29/63/63	0/2/2/2
27	LMG	J	101	-	-	6/25/45/70	0/1/1/1
24	BCR	4	302	-	-	7/29/63/63	0/2/2/2
20	CLA	A	816	-	1/1/11/20	0/13/89/115	-
23	LHG	A	843	-	-	20/44/44/53	-
29	CHL	0	315	-	3/3/17/26	5/21/119/137	-
20	CLA	A	802	-	1/1/11/20	3/13/89/115	-
20	CLA	B	803	-	1/1/11/20	5/13/89/115	-
20	CLA	L	204	-	1/1/11/20	3/13/89/115	-
20	CLA	6	312	18	1/1/11/20	2/13/89/115	-
20	CLA	0	309	-	1/1/11/20	4/13/89/115	-
24	BCR	B	847	-	-	5/29/63/63	0/2/2/2
20	CLA	L	201	-	1/1/11/20	3/13/89/115	-
20	CLA	7	1010	23	1/1/11/20	0/13/89/115	-
29	CHL	4	315	-	3/3/19/26	16/33/131/137	-
20	CLA	A	815	-	1/1/11/20	5/13/89/115	-
20	CLA	A	808	-	1/1/11/20	3/13/89/115	-
24	BCR	H	201	-	-	12/29/63/63	0/2/2/2
20	CLA	4	308	17	1/1/11/20	5/13/89/115	-
20	CLA	7	1009	-	1/1/11/20	5/13/89/115	-
20	CLA	B	828	-	1/1/11/20	3/13/89/115	-
20	CLA	5	304	19	1/1/11/20	2/13/89/115	-
20	CLA	5	323	-	1/1/11/20	6/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	7	1003	-	-	16/29/63/63	0/2/2/2
29	CHL	4	312	-	3/3/16/26	4/17/115/137	-
20	CLA	K	201	-	1/1/11/20	6/13/89/115	-
20	CLA	B	807	-	1/1/11/20	4/13/89/115	-
28	LUT	0	304	-	-	6/29/67/67	0/2/2/2
20	CLA	A	836	-	1/1/11/20	6/13/89/115	-
28	LUT	0	318	-	-	2/29/67/67	0/2/2/2
20	CLA	A	818	-	1/1/11/20	5/13/89/115	-
30	XAT	4	303	-	-	2/31/93/93	0/4/4/4
27	LMG	0	303	-	-	21/45/65/70	0/1/1/1
20	CLA	1	1017	-	1/1/11/20	2/13/89/115	-
20	CLA	6	315	18	1/1/11/20	1/13/89/115	-
20	CLA	7	1004	15	1/1/11/20	6/13/89/115	-
20	CLA	A	801	-	1/1/11/20	1/13/89/115	-
25	DGD	B	848	-	-	18/50/90/95	0/2/2/2
20	CLA	A	852	-	1/1/11/20	2/13/89/115	-
20	CLA	6	311	-	1/1/11/20	5/13/89/115	-
20	CLA	L	203	-	1/1/11/20	3/13/89/115	-
20	CLA	0	310	-	1/1/11/20	6/13/89/115	-
20	CLA	1	1007	-	1/1/11/20	5/13/89/115	-
24	BCR	A	844	-	-	2/29/63/63	0/2/2/2
20	CLA	A	838	-	1/1/11/20	2/13/89/115	-
20	CLA	B	822	-	1/1/11/20	3/13/89/115	-
28	LUT	8	303	-	-	2/29/67/67	0/2/2/2
20	CLA	G	201	-	1/1/11/20	3/13/89/115	-
20	CLA	8	305	14	1/1/11/20	4/13/89/115	-
29	CHL	1	1015	-	3/3/19/26	12/33/131/137	-
23	LHG	0	302	20	-	8/23/23/53	-
20	CLA	B	814	-	1/1/11/20	0/13/89/115	-
20	CLA	8	313	14	1/1/11/20	4/13/89/115	-
20	CLA	5	315	19	1/1/11/20	0/13/89/115	-
28	LUT	7	1001	-	-	5/29/67/67	0/2/2/2
20	CLA	K	202	-	1/1/5/20	-	-
20	CLA	B	840	-	1/1/11/20	7/13/89/115	-
20	CLA	4	306	-	1/1/11/20	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	831	-	1/1/11/20	3/13/89/115	-
20	CLA	B	806	-	1/1/11/20	2/13/89/115	-
20	CLA	B	825	-	1/1/11/20	6/13/89/115	-
20	CLA	5	307	19	1/1/11/20	1/13/89/115	-
24	BCR	A	850	-	-	7/29/63/63	0/2/2/2
28	LUT	3	1001	-	-	2/29/67/67	0/2/2/2
20	CLA	B	835	-	1/1/11/20	0/13/89/115	-
20	CLA	1	1003	-	1/1/11/20	4/13/89/115	-
20	CLA	4	305	17	1/1/11/20	4/13/89/115	-
20	CLA	0	311	23	1/1/11/20	4/13/89/115	-
20	CLA	B	812	2	1/1/11/20	2/13/89/115	-
20	CLA	B	815	-	1/1/11/20	2/13/89/115	-
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
20	CLA	B	805	-	1/1/11/20	2/13/89/115	-
20	CLA	A	824	-	1/1/11/20	5/13/89/115	-
20	CLA	B	831	-	1/1/11/20	1/13/89/115	-
20	CLA	A	820	-	1/1/11/20	5/13/89/115	-
20	CLA	3	1012	-	1/1/11/20	5/13/89/115	-
29	CHL	5	317	19	3/3/15/26	4/12/110/137	-
20	CLA	0	313	13	1/1/11/20	3/13/89/115	-
20	CLA	B	813	-	1/1/11/20	2/13/89/115	-
24	BCR	B	804	-	-	6/29/63/63	0/2/2/2
20	CLA	B	836	-	1/1/11/20	0/13/89/115	-
20	CLA	A	839	-	1/1/11/20	4/13/89/115	-
20	CLA	0	307	-	1/1/11/20	3/13/89/115	-
20	CLA	8	310	-	1/1/11/20	4/13/89/115	-
20	CLA	3	1008	16	1/1/11/20	4/13/89/115	-
20	CLA	6	305	18	1/1/11/20	2/13/89/115	-
21	SF4	A	841	1,2	-	-	0/6/5/5
20	CLA	1	1005	-	1/1/11/20	3/13/89/115	-
24	BCR	5	320	-	-	5/29/63/63	0/2/2/2
20	CLA	B	820	-	1/1/11/20	4/13/89/115	-
20	CLA	B	839	-	1/1/11/20	5/13/89/115	-
20	CLA	3	1006	-	1/1/11/20	4/13/89/115	-
29	CHL	6	316	-	3/3/19/26	13/33/131/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	825	-	1/1/11/20	0/13/89/115	-
26	LMT	B	849	-	-	5/17/57/61	0/2/2/2
20	CLA	4	314	17	1/1/11/20	4/13/89/115	-
29	CHL	3	1014	-	3/3/16/26	5/17/115/137	-
20	CLA	4	311	17	1/1/11/20	3/13/89/115	-
20	CLA	A	810	20	1/1/11/20	7/13/89/115	-
29	CHL	1	1013	-	3/3/17/26	1/21/119/137	-
20	CLA	4	310	-	1/1/11/20	8/13/89/115	-
20	CLA	A	807	-	1/1/11/20	5/13/89/115	-
24	BCR	A	845	-	-	9/29/63/63	0/2/2/2
20	CLA	B	824	-	1/1/11/20	1/13/89/115	-
20	CLA	A	817	-	1/1/11/20	5/13/89/115	-
20	CLA	1	1010	-	1/1/11/20	7/13/89/115	-
20	CLA	7	1014	15	1/1/11/20	0/13/89/115	-
25	DGD	5	319	-	-	19/40/80/95	0/2/2/2
20	CLA	B	841	-	1/1/11/20	8/13/89/115	-
28	LUT	1	1002	-	-	5/29/67/67	0/2/2/2
20	CLA	A	840	-	1/1/11/20	3/13/89/115	-
20	CLA	B	850	-	1/1/11/20	6/13/86/115	-
30	XAT	6	304	-	-	5/31/93/93	0/4/4/4
27	LMG	5	324	-	-	26/40/60/70	0/1/1/1
20	CLA	3	1007	-	1/1/11/20	5/13/89/115	-
24	BCR	F	304	-	-	4/29/63/63	0/2/2/2
20	CLA	3	1005	16	1/1/11/20	8/13/89/115	-
22	PQN	B	842	-	-	7/23/43/43	0/2/2/2
20	CLA	A	813	-	1/1/11/20	4/13/89/115	-
20	CLA	B	826	-	1/1/11/20	5/13/89/115	-
20	CLA	4	304	17	1/1/11/20	3/13/89/115	-
20	CLA	B	817	-	1/1/11/20	2/13/89/115	-
20	CLA	A	832	-	1/1/11/20	2/13/89/115	-
20	CLA	4	307	17	1/1/11/20	3/13/89/115	-
29	CHL	7	1017	15	3/3/20/26	9/39/137/137	-
27	LMG	8	319	20	-	13/39/59/70	0/1/1/1
30	XAT	7	1002	-	-	6/31/93/93	0/4/4/4
29	CHL	6	313	-	3/3/16/26	2/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	0	312	-	1/1/11/20	4/13/89/115	-
20	CLA	8	306	14	1/1/11/20	3/13/89/115	-
20	CLA	A	814	-	1/1/10/20	4/8/84/115	-
24	BCR	B	843	-	-	8/29/63/63	0/2/2/2
24	BCR	8	302	-	-	7/29/63/63	0/2/2/2
29	CHL	7	1013	-	3/3/16/26	3/18/116/137	-
20	CLA	3	1013	16	1/1/11/20	4/13/89/115	-
20	CLA	G	202	-	1/1/11/20	4/13/89/115	-
20	CLA	7	1006	-	1/1/11/20	6/13/89/115	-
20	CLA	B	829	-	1/1/11/20	7/13/89/115	-
20	CLA	6	307	-	1/1/11/20	3/13/89/115	-
29	CHL	5	313	-	3/3/16/26	7/17/115/137	-
23	LHG	7	1016	20	-	12/39/39/53	-
20	CLA	B	801	-	1/1/11/20	3/13/89/115	-
20	CLA	5	305	19	1/1/11/20	6/13/89/115	-
20	CLA	F	305	-	1/1/11/20	0/13/89/115	-
20	CLA	A	809	-	1/1/11/20	2/13/89/115	-
20	CLA	G	203	-	1/1/11/20	9/13/89/115	-
20	CLA	0	306	13	1/1/11/20	3/13/89/115	-
20	CLA	3	1017	-	1/1/11/20	5/13/89/115	-
23	LHG	A	849	-	-	19/53/53/53	-
27	LMG	4	318	-	-	10/29/49/70	0/1/1/1
29	CHL	6	314	-	3/3/17/26	5/21/119/137	-
23	LHG	3	1019	20	-	11/23/23/53	-
20	CLA	B	808	-	1/1/11/20	4/13/89/115	-
20	CLA	A	821	-	1/1/11/20	2/13/89/115	-
20	CLA	B	810	-	1/1/11/20	3/13/89/115	-
24	BCR	3	1003	-	-	10/29/63/63	0/2/2/2
20	CLA	0	316	-	1/1/11/20	4/13/89/115	-
24	BCR	B	845	-	-	10/29/63/63	0/2/2/2

The worst 5 of 1898 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	850	CLA	C4C-NC	21.89	1.46	1.30
29	6	314	CHL	C3A-C2A	-9.91	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	5	301	CLA	C4B-NB	9.61	1.50	1.37
20	6	308	CLA	C4B-NB	9.41	1.50	1.37
20	B	837	CLA	C4B-NB	9.32	1.50	1.37

The worst 5 of 1676 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	202	CLA	C1C-NC-C4C	-8.76	102.68	106.68
24	6	302	BCR	C16-C15-C14	7.48	138.82	123.52
24	8	302	BCR	C16-C15-C14	6.96	137.76	123.52
24	7	1003	BCR	C16-C15-C14	6.76	137.36	123.52
24	B	804	BCR	C16-C15-C14	6.62	137.07	123.52

5 of 263 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	801	CLA	ND
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND
20	A	805	CLA	ND

5 of 1398 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	803	CLA	C1A-C2A-CAA-CBA
20	A	805	CLA	CAD-CBD-CGD-O2D
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	809	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

243 monomers are involved in 819 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	802	CLA	1	0
20	8	311	CLA	8	0
28	4	317	LUT	2	0
30	8	304	XAT	1	0
20	B	834	CLA	4	0
24	A	848	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	6	317	CHL	4	0
29	0	314	CHL	9	0
20	6	309	CLA	2	0
20	5	321	CLA	1	0
20	5	301	CLA	3	0
20	3	1009	CLA	1	0
20	8	307	CLA	2	0
20	A	829	CLA	1	0
20	B	821	CLA	5	0
20	B	838	CLA	2	0
29	7	1012	CHL	5	0
20	7	1007	CLA	2	0
20	A	804	CLA	3	0
20	A	826	CLA	2	0
20	7	1011	CLA	1	0
22	A	842	PQN	3	0
28	1	1016	LUT	2	0
20	B	811	CLA	2	0
20	5	309	CLA	5	0
28	5	302	LUT	6	0
20	F	303	CLA	1	0
20	L	202	CLA	1	0
29	0	317	CHL	5	0
28	3	1002	LUT	2	0
20	6	308	CLA	6	0
23	4	301	LHG	15	0
20	0	301	CLA	5	0
29	5	316	CHL	4	0
20	6	320	CLA	2	0
24	F	301	BCR	6	0
20	1	1008	CLA	6	0
20	6	310	CLA	6	0
27	8	318	LMG	4	0
20	B	833	CLA	2	0
20	A	823	CLA	3	0
20	8	308	CLA	2	0
20	5	312	CLA	15	0
21	C	1002	SF4	2	0
20	8	309	CLA	4	0
20	8	312	CLA	2	0
20	B	837	CLA	1	0
27	6	319	LMG	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	1014	CLA	5	0
20	B	818	CLA	5	0
20	B	823	CLA	3	0
28	J	104	LUT	10	0
20	4	309	CLA	1	0
20	F	302	CLA	4	0
20	1	1011	CLA	5	0
29	8	317	CHL	2	0
20	5	306	CLA	2	0
20	A	835	CLA	4	0
20	B	816	CLA	4	0
20	A	830	CLA	1	0
20	A	812	CLA	2	0
20	A	834	CLA	1	0
30	5	303	XAT	6	0
20	A	827	CLA	3	0
24	1	1001	BCR	7	0
20	8	316	CLA	1	0
20	A	851	CLA	3	0
29	4	313	CHL	1	0
20	3	1015	CLA	2	0
20	1	1006	CLA	5	0
20	B	830	CLA	3	0
20	A	819	CLA	2	0
20	B	827	CLA	2	0
20	7	1008	CLA	1	0
24	A	846	BCR	5	0
20	5	318	CLA	2	0
29	5	314	CHL	2	0
20	7	1005	CLA	2	0
20	0	305	CLA	3	0
29	8	314	CHL	3	0
28	6	303	LUT	3	0
20	B	819	CLA	3	0
20	1	1009	CLA	1	0
20	A	828	CLA	2	0
24	G	205	BCR	18	0
20	J	102	CLA	3	0
24	B	844	BCR	2	0
24	I	201	BCR	17	0
26	3	1018	LMT	8	0
20	A	837	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1	1012	CHL	4	0
20	A	833	CLA	6	0
20	3	1016	CLA	4	0
29	7	1015	CHL	1	0
20	5	308	CLA	5	0
20	3	1011	CLA	1	0
20	5	310	CLA	7	0
29	4	316	CHL	4	0
24	G	204	BCR	7	0
24	3	1004	BCR	3	0
24	6	302	BCR	14	0
20	A	811	CLA	1	0
24	A	847	BCR	7	0
29	8	315	CHL	3	0
24	4	302	BCR	4	0
20	A	816	CLA	1	0
23	A	843	LHG	2	0
29	0	315	CHL	2	0
20	A	802	CLA	5	0
20	B	803	CLA	1	0
20	L	204	CLA	3	0
20	6	312	CLA	12	0
20	0	309	CLA	4	0
24	B	847	BCR	3	0
20	L	201	CLA	6	0
20	7	1010	CLA	6	0
29	4	315	CHL	13	0
20	A	815	CLA	8	0
20	A	808	CLA	1	0
24	H	201	BCR	2	0
20	B	828	CLA	1	0
20	5	304	CLA	5	0
20	5	323	CLA	7	0
24	7	1003	BCR	2	0
29	4	312	CHL	1	0
20	K	201	CLA	5	0
28	0	304	LUT	10	0
20	A	836	CLA	1	0
28	0	318	LUT	3	0
20	A	818	CLA	1	0
30	4	303	XAT	2	0
27	0	303	LMG	27	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	1	1017	CLA	8	0
20	6	315	CLA	2	0
20	7	1004	CLA	10	0
20	A	801	CLA	8	0
25	B	848	DGD	4	0
20	A	852	CLA	5	0
20	6	311	CLA	2	0
20	L	203	CLA	1	0
20	0	310	CLA	3	0
20	1	1007	CLA	6	0
24	A	844	BCR	7	0
20	A	838	CLA	4	0
20	B	822	CLA	2	0
28	8	303	LUT	4	0
20	G	201	CLA	3	0
20	8	305	CLA	2	0
29	1	1015	CHL	12	0
23	0	302	LHG	3	0
20	8	313	CLA	3	0
20	5	315	CLA	7	0
28	7	1001	LUT	4	0
20	B	840	CLA	3	0
20	4	306	CLA	3	0
20	A	831	CLA	6	0
20	B	825	CLA	3	0
20	5	307	CLA	2	0
24	A	850	BCR	6	0
28	3	1001	LUT	3	0
20	B	835	CLA	2	0
20	1	1003	CLA	4	0
20	0	311	CLA	3	0
20	B	812	CLA	3	0
24	B	846	BCR	1	0
20	B	805	CLA	1	0
20	A	824	CLA	5	0
20	B	831	CLA	6	0
20	A	820	CLA	2	0
29	5	317	CHL	9	0
20	0	313	CLA	3	0
20	B	813	CLA	9	0
24	B	804	BCR	5	0
20	B	836	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	839	CLA	2	0
20	0	307	CLA	1	0
20	8	310	CLA	1	0
20	3	1008	CLA	2	0
20	6	305	CLA	2	0
21	A	841	SF4	1	0
20	1	1005	CLA	1	0
24	5	320	BCR	16	0
20	B	820	CLA	3	0
20	B	839	CLA	1	0
20	3	1006	CLA	2	0
29	6	316	CHL	3	0
20	A	825	CLA	2	0
26	B	849	LMT	3	0
29	3	1014	CHL	1	0
20	4	311	CLA	7	0
25	5	319	DGD	16	0
20	4	310	CLA	5	0
20	A	807	CLA	1	0
24	A	845	BCR	3	0
20	B	824	CLA	3	0
20	A	817	CLA	5	0
20	7	1014	CLA	3	0
29	1	1013	CHL	2	0
28	1	1002	LUT	16	0
20	A	840	CLA	9	0
20	B	850	CLA	8	0
30	6	304	XAT	10	0
27	5	324	LMG	7	0
20	3	1007	CLA	2	0
24	F	304	BCR	1	0
20	3	1005	CLA	4	0
22	B	842	PQN	3	0
20	A	813	CLA	5	0
20	B	826	CLA	1	0
20	4	304	CLA	1	0
20	B	817	CLA	9	0
20	4	307	CLA	17	0
27	8	319	LMG	6	0
29	7	1017	CHL	7	0
29	6	313	CHL	2	0
20	8	306	CLA	3	0

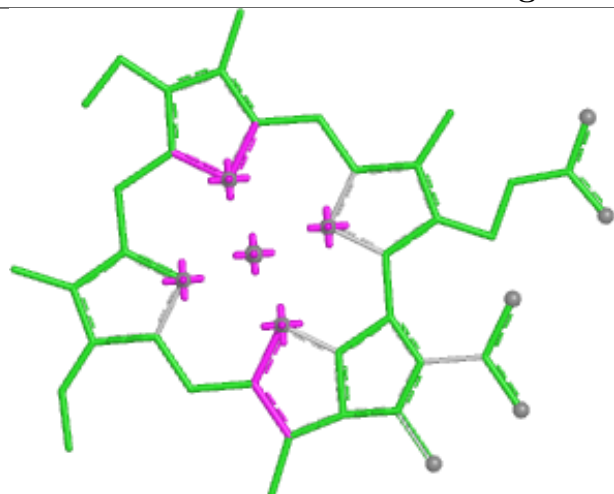
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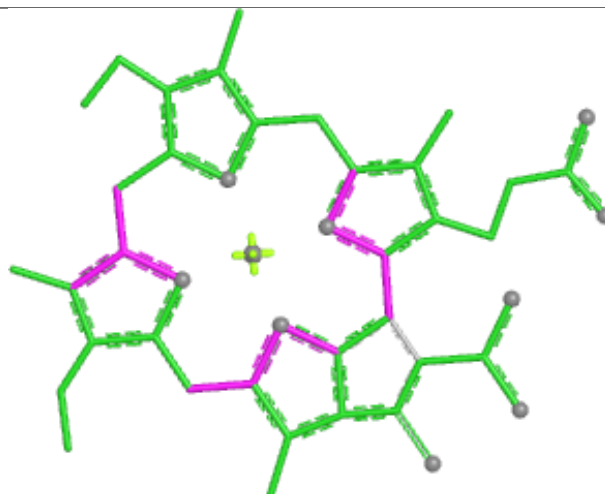
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	814	CLA	1	0
24	B	843	BCR	12	0
24	8	302	BCR	5	0
29	7	1013	CHL	3	0
20	3	1013	CLA	2	0
20	G	202	CLA	2	0
20	7	1006	CLA	2	0
20	B	829	CLA	5	0
20	6	307	CLA	1	0
29	5	313	CHL	4	0
23	7	1016	LHG	6	0
20	B	801	CLA	4	0
20	5	305	CLA	1	0
20	F	305	CLA	1	0
20	A	809	CLA	1	0
20	G	203	CLA	8	0
20	3	1017	CLA	1	0
23	A	849	LHG	2	0
27	4	318	LMG	38	0
29	6	314	CHL	4	0
23	3	1019	LHG	5	0
20	B	808	CLA	7	0
20	A	821	CLA	3	0
20	B	810	CLA	2	0
24	3	1003	BCR	2	0
20	0	316	CLA	4	0
24	B	845	BCR	8	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.

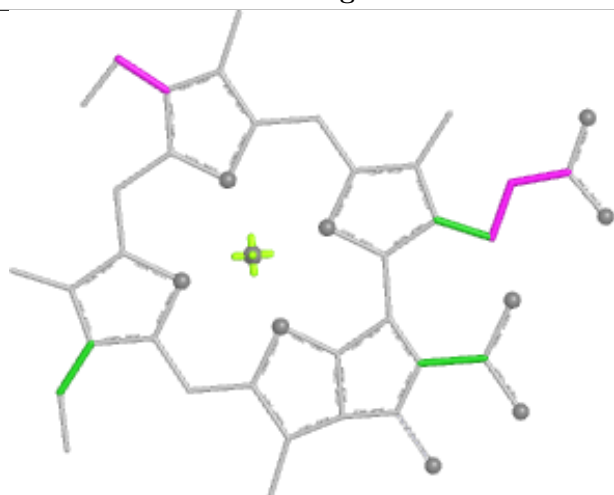
Ligand CLA 5 311



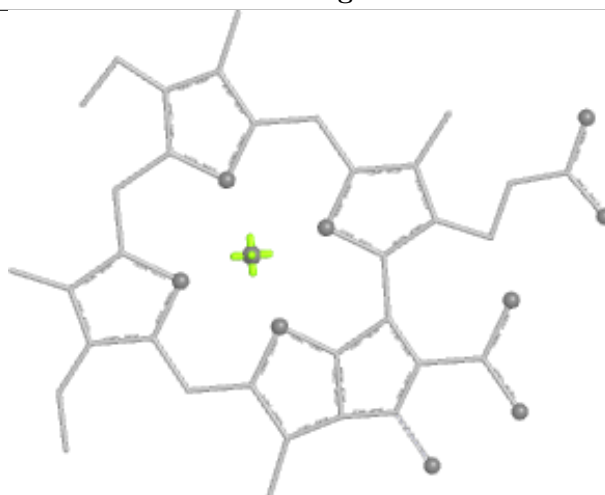
Bond lengths



Bond angles

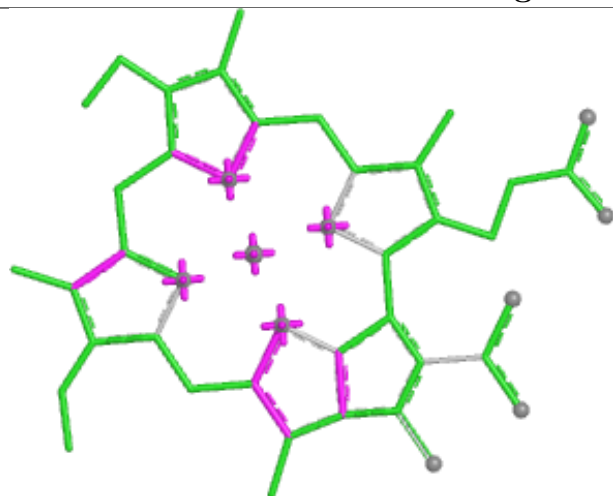


Torsions

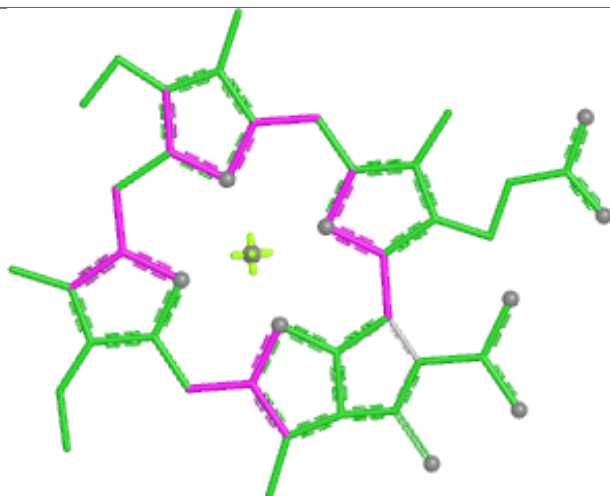


Rings

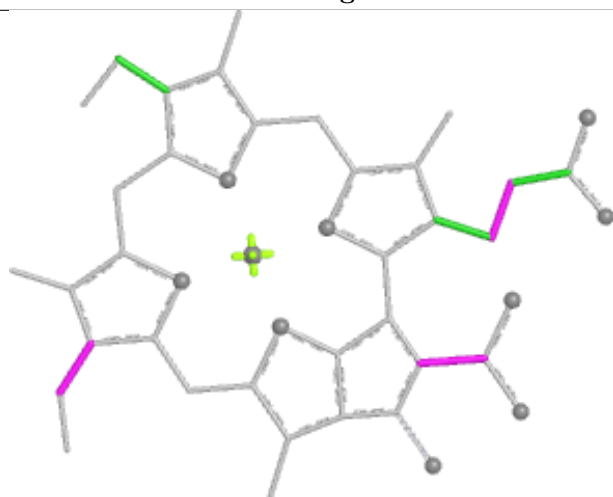
Ligand CLA B 802



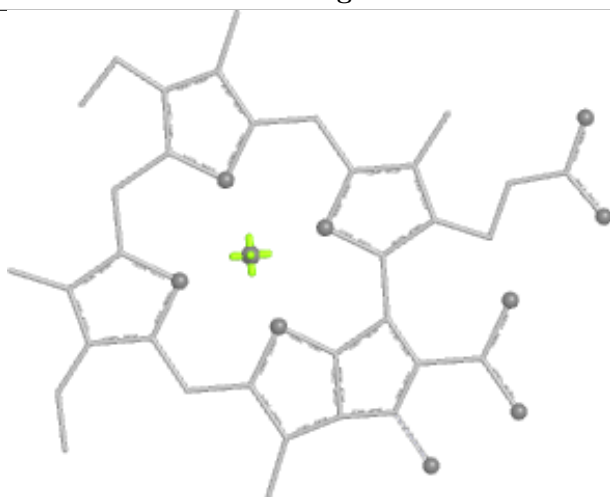
Bond lengths



Bond angles

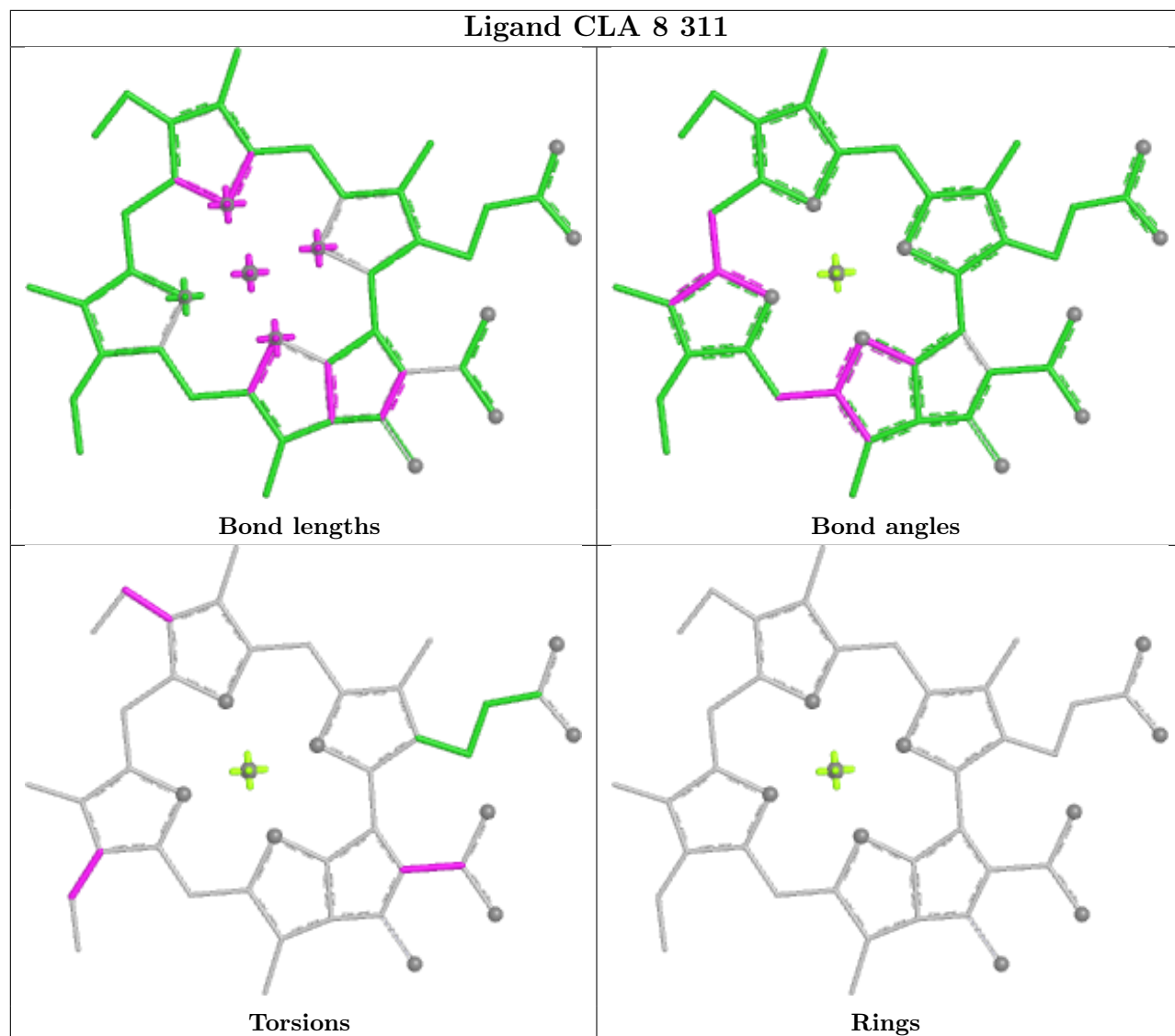


Torsions

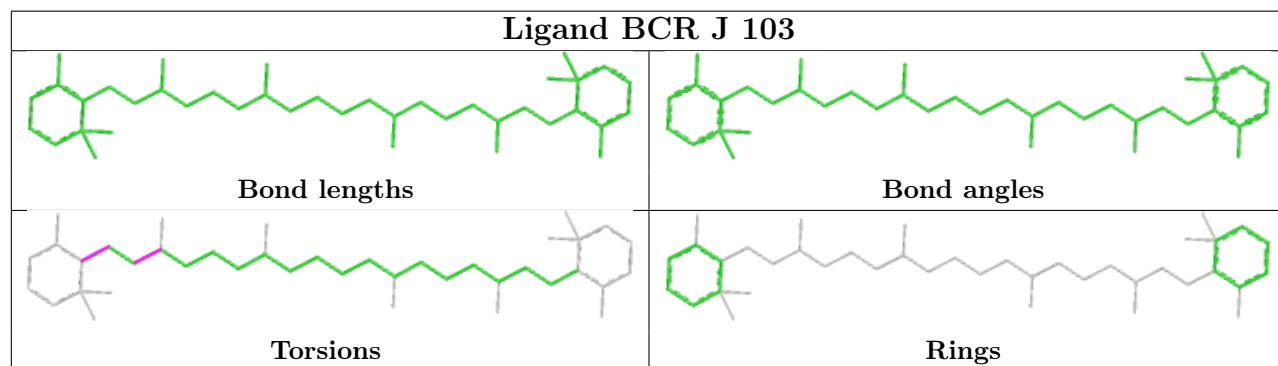


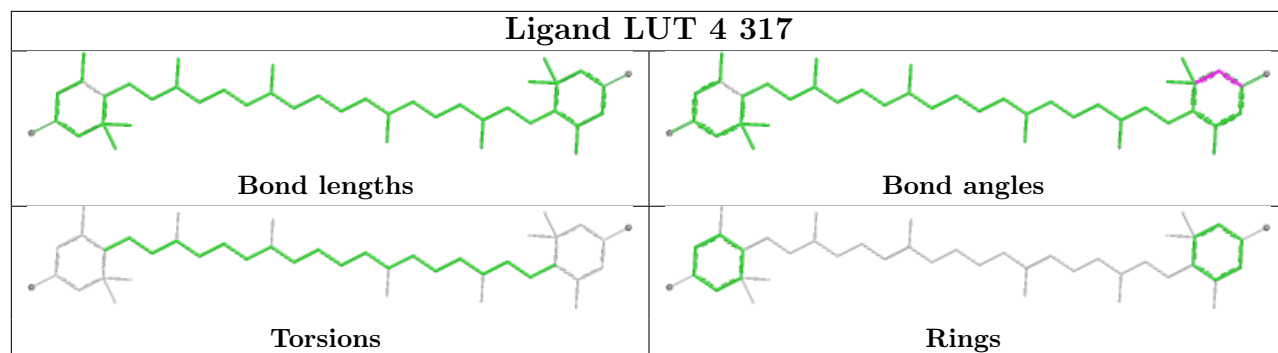
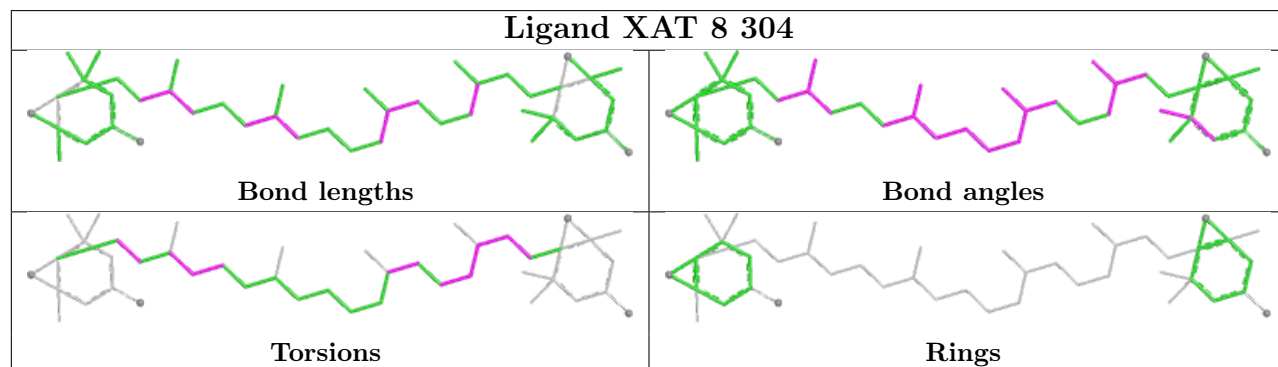
Rings

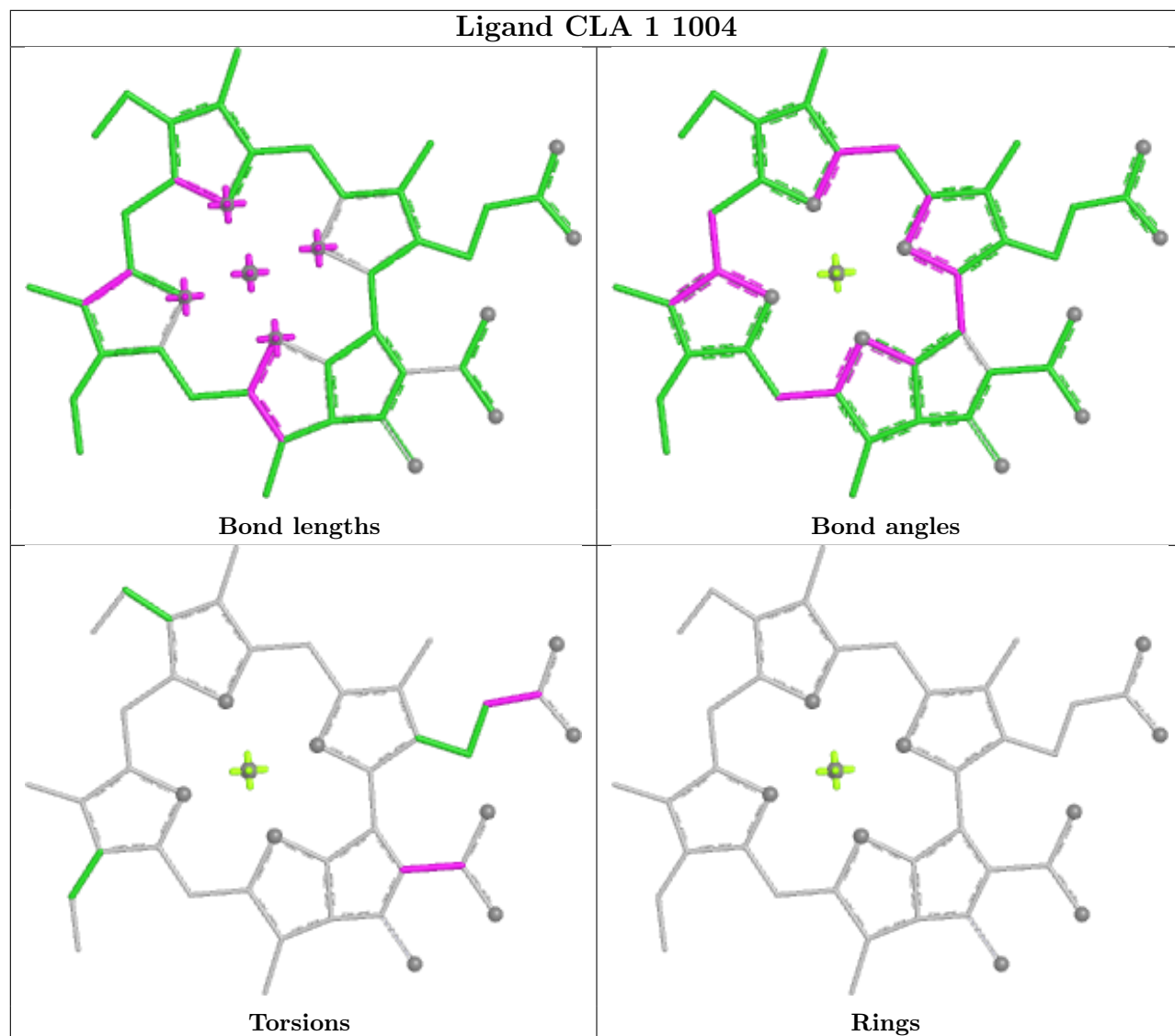
Ligand CLA 8 311



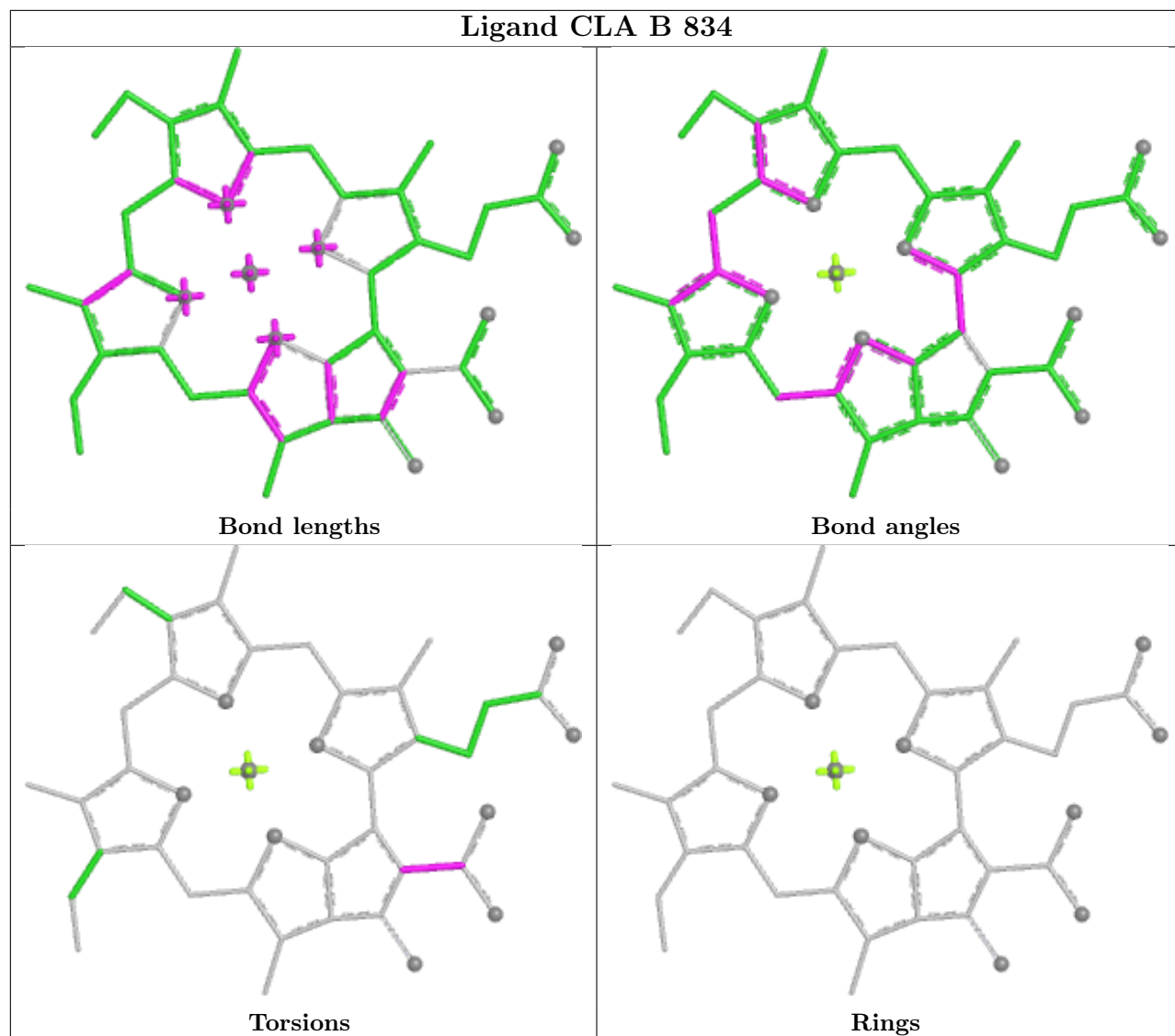
Ligand BCR J 103



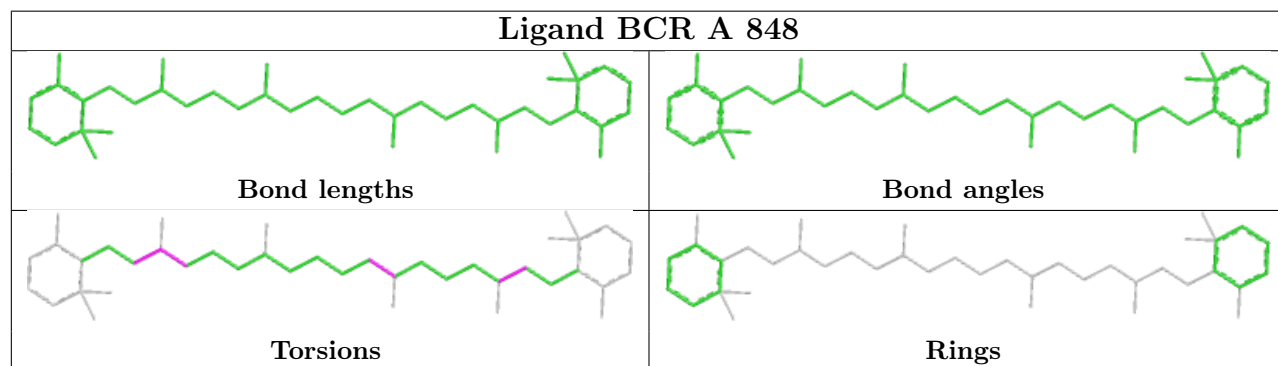
Ligand LUT 4 317**Ligand XAT 8 304**



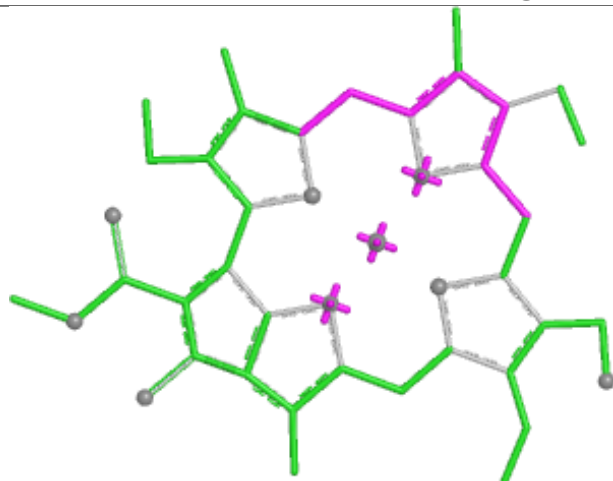
Ligand CLA B 834



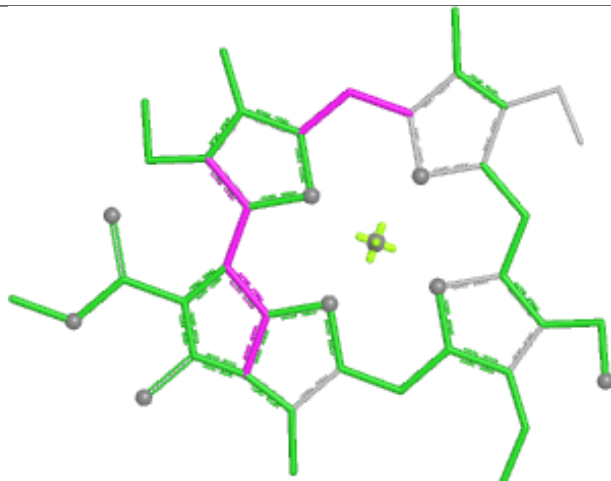
Ligand BCR A 848



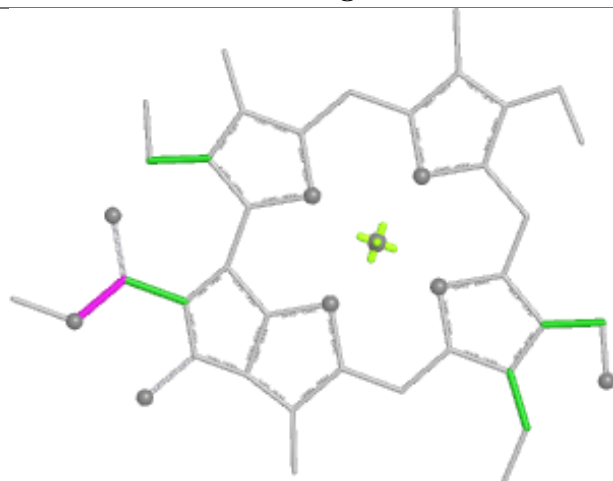
Ligand CHL 6 317



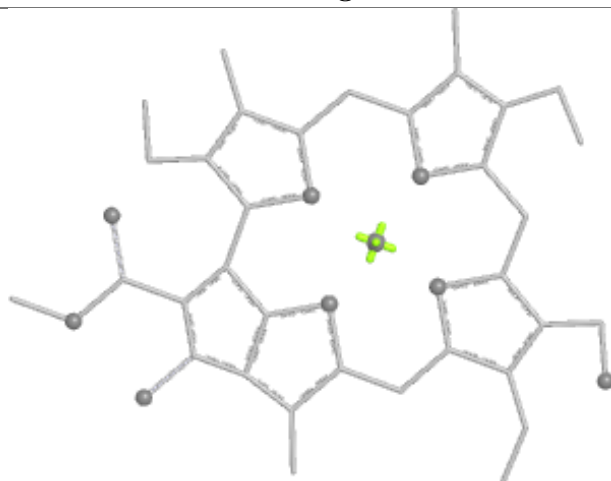
Bond lengths



Bond angles

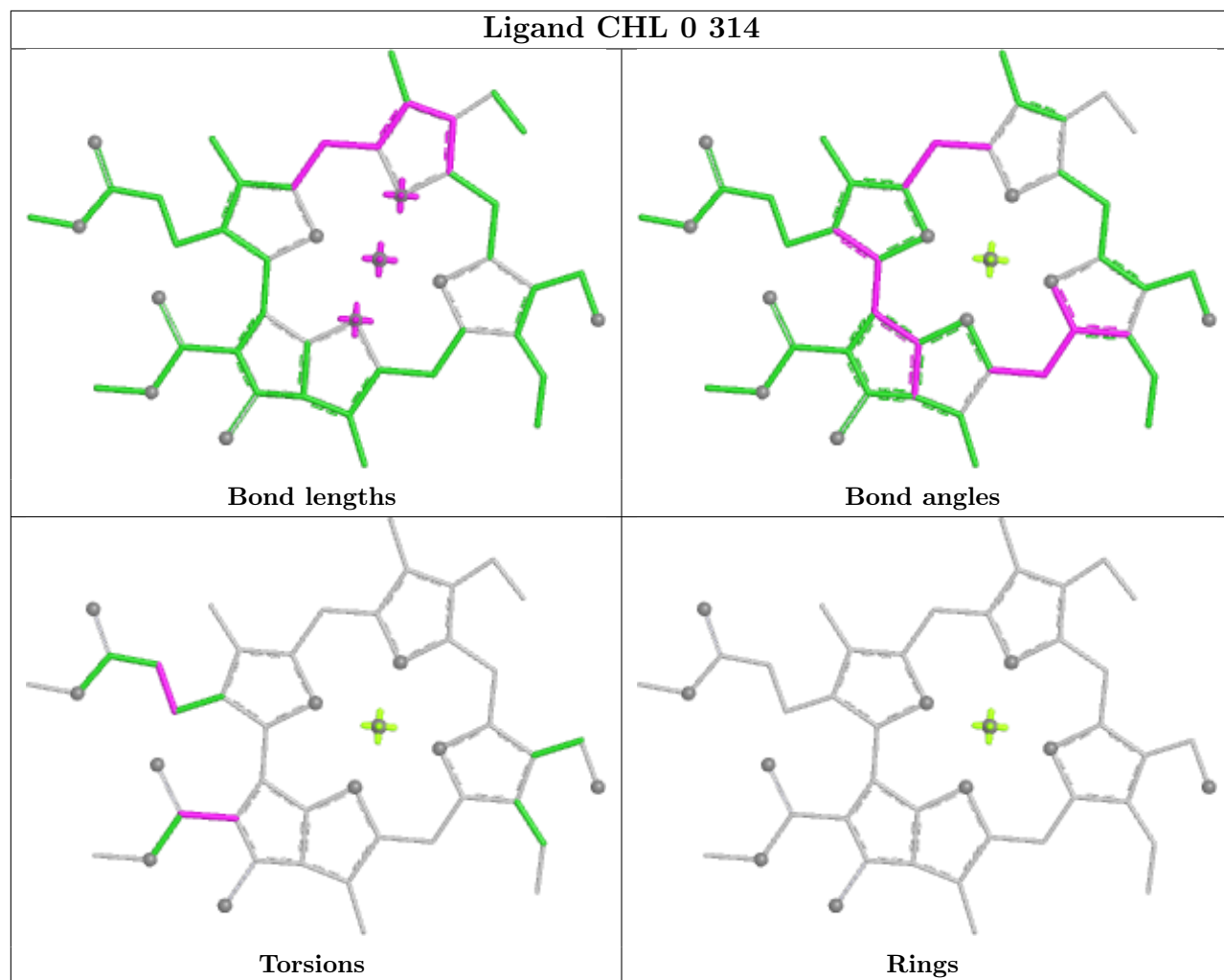


Torsions

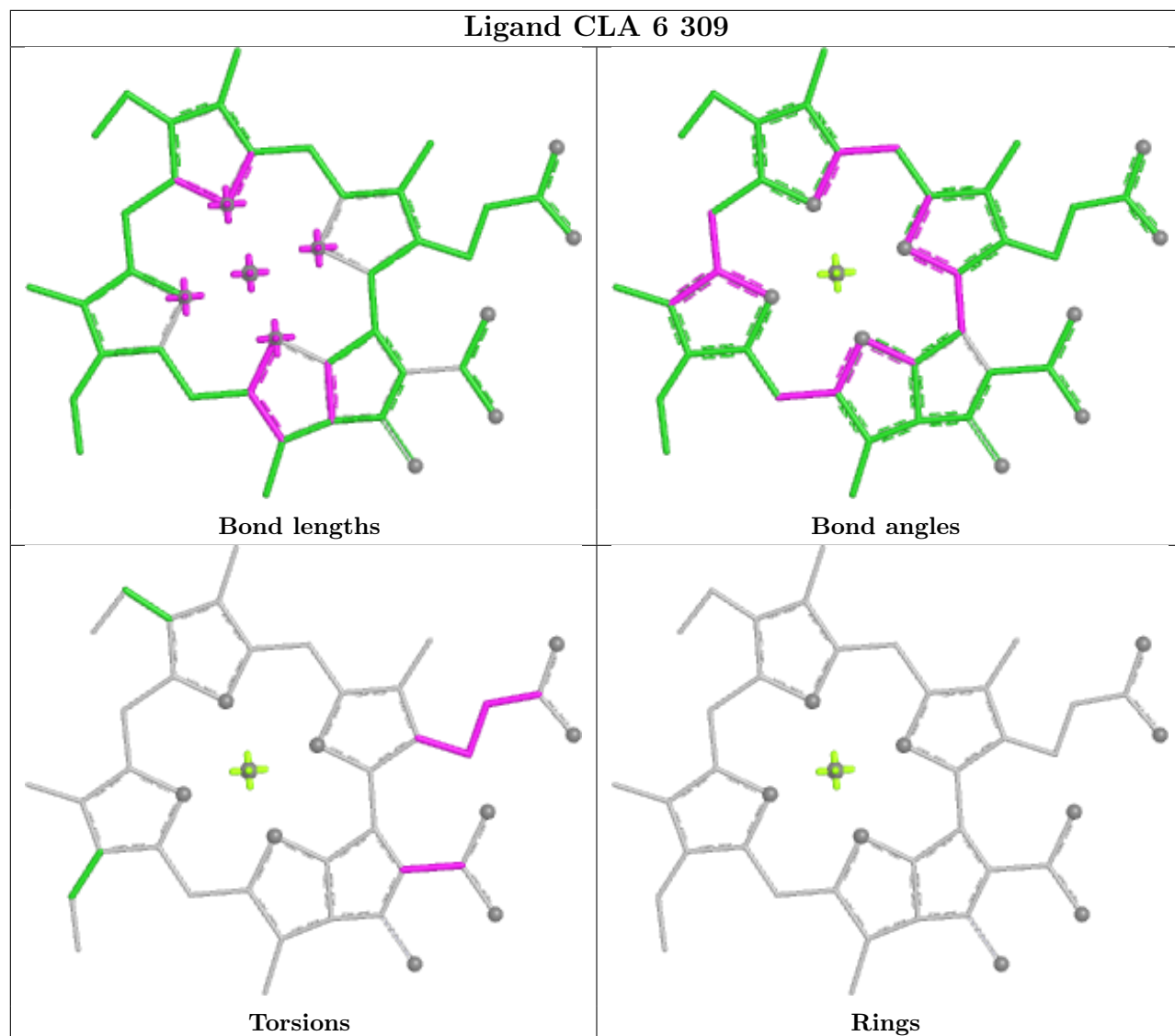


Rings

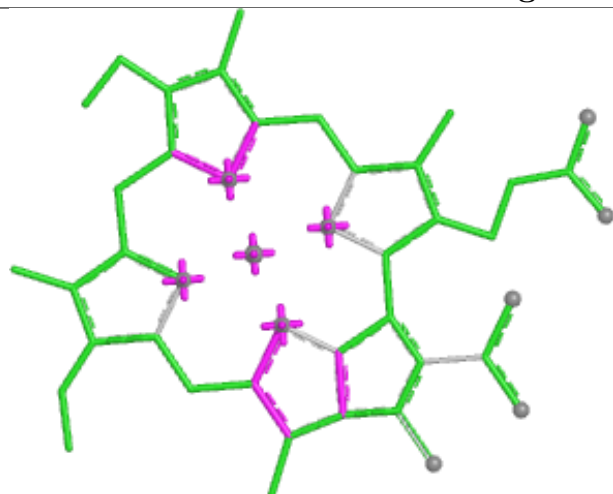
Ligand CHL 0 314



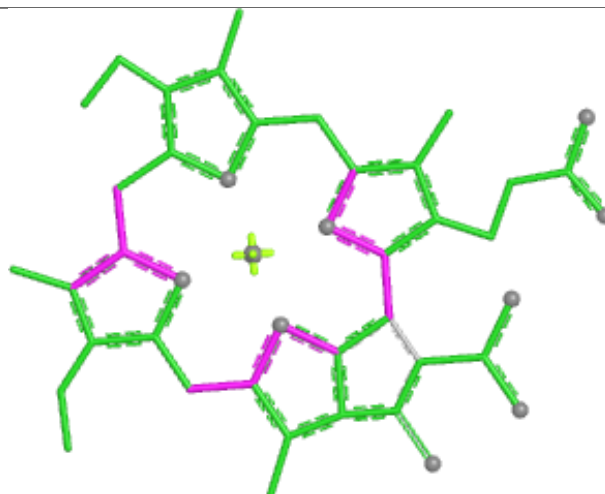
Ligand CLA 6 309



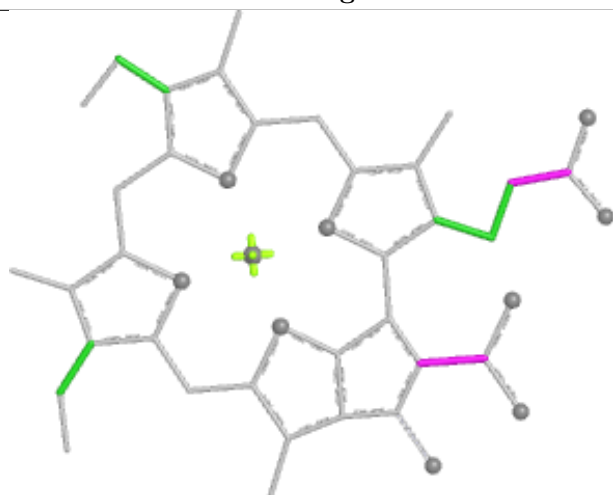
Ligand CLA 5 321



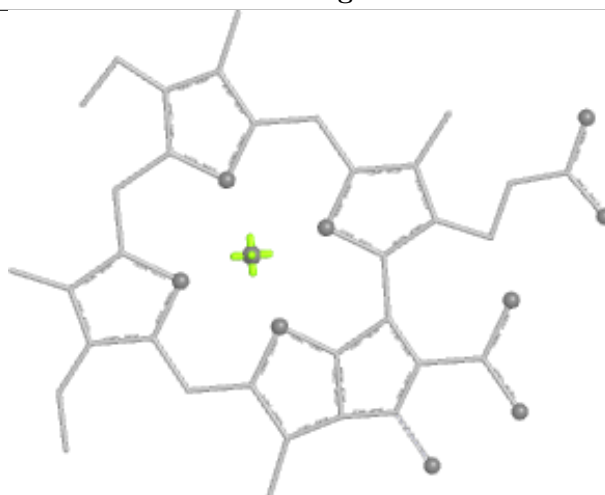
Bond lengths



Bond angles

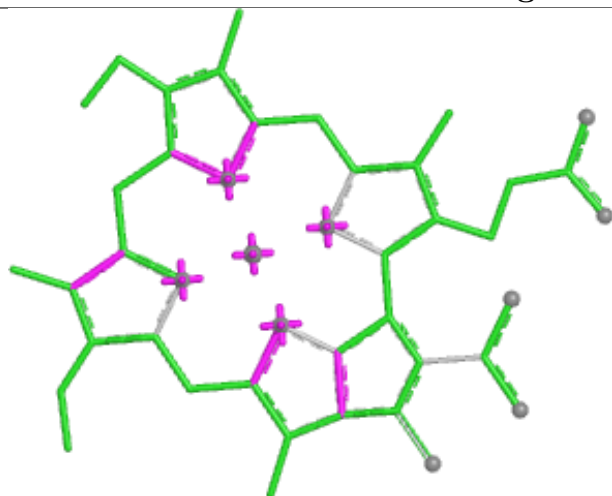


Torsions

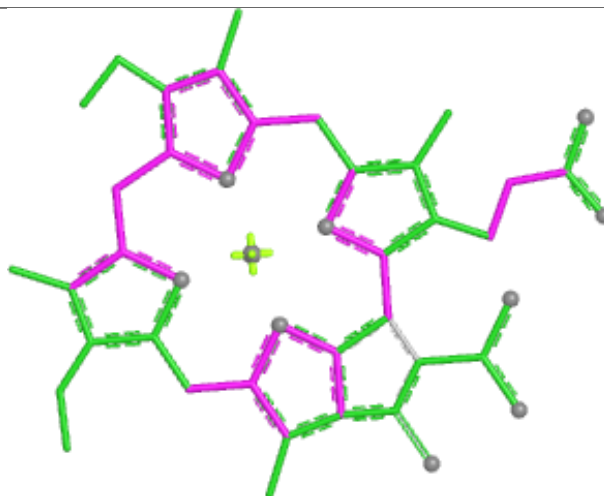


Rings

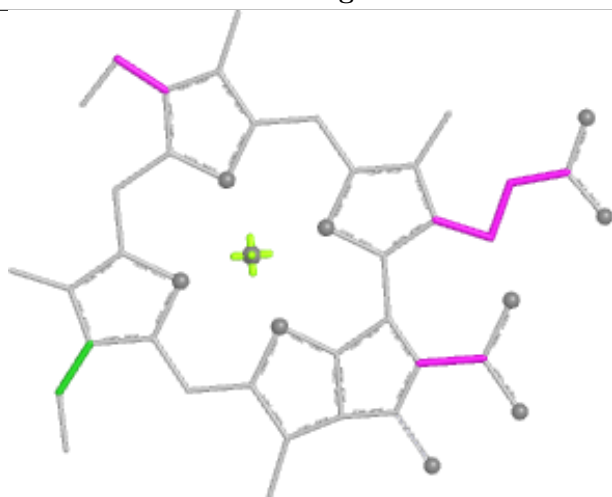
Ligand CLA 5 301



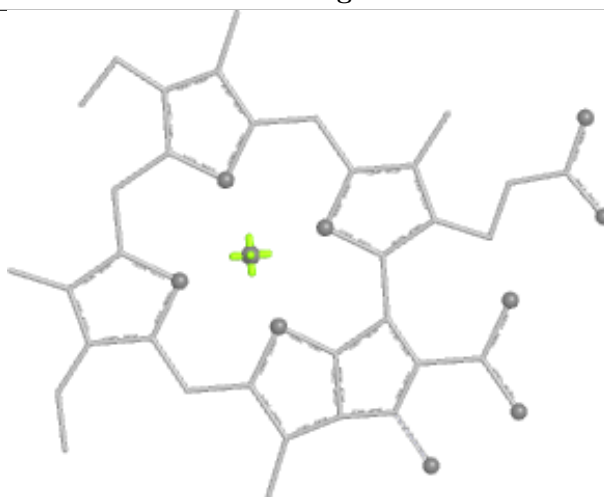
Bond lengths



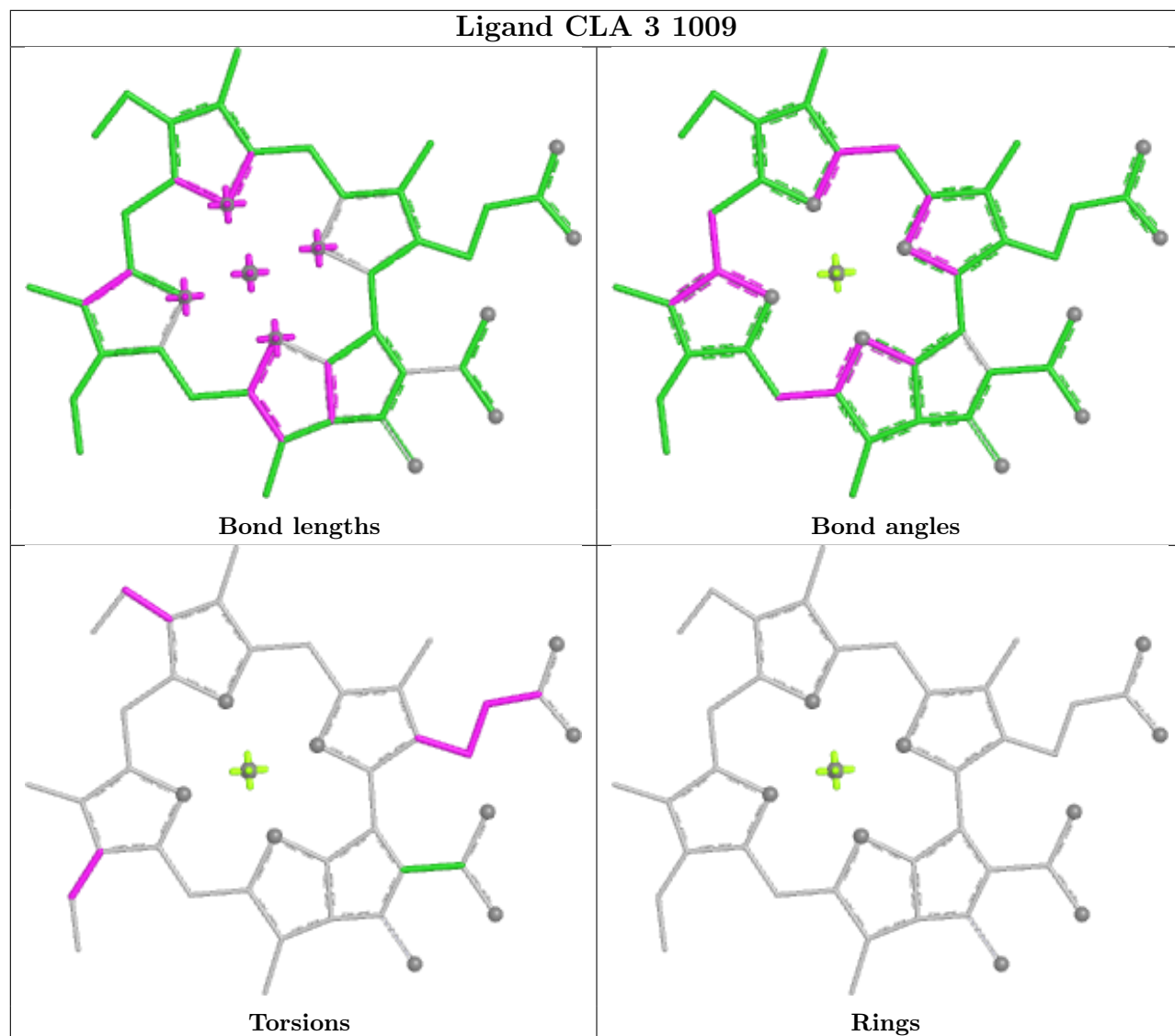
Bond angles



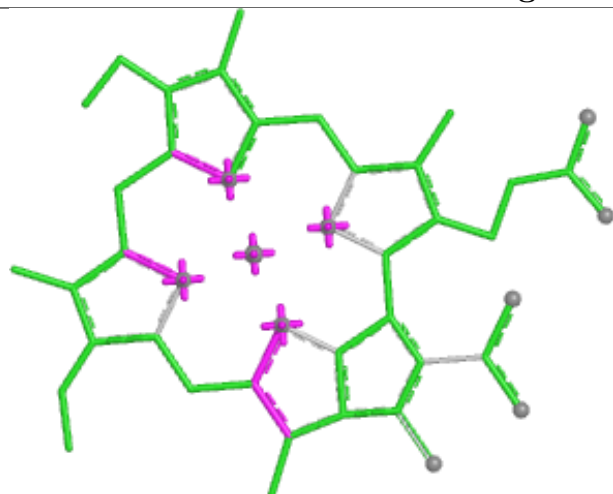
Torsions



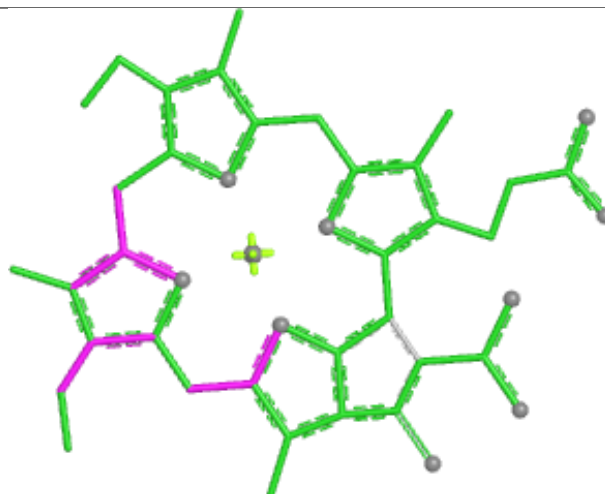
Rings



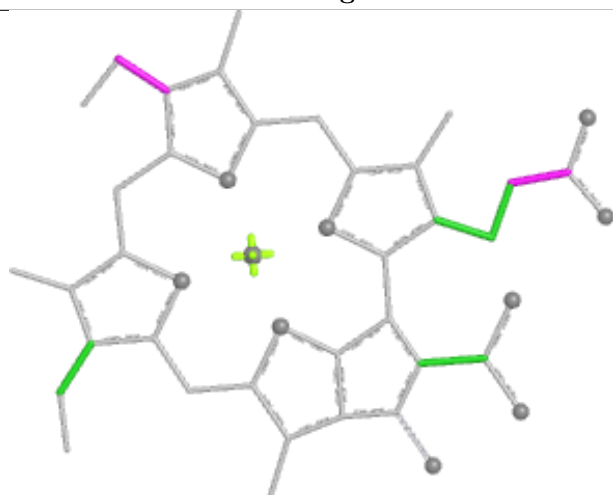
Ligand CLA 8 307



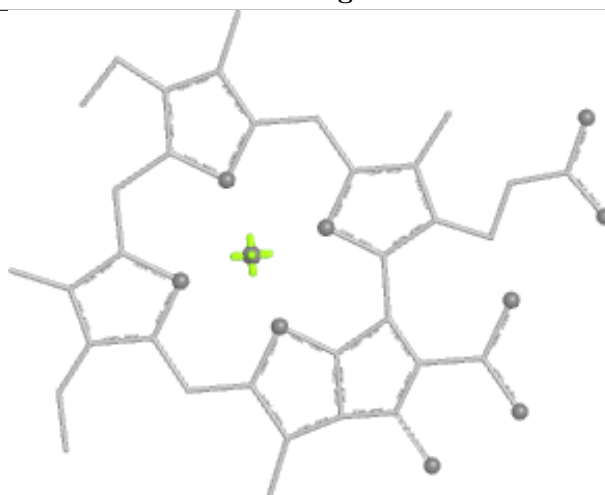
Bond lengths



Bond angles

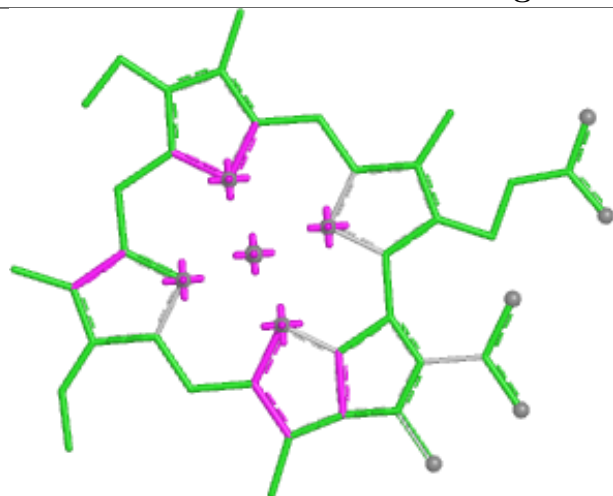


Torsions

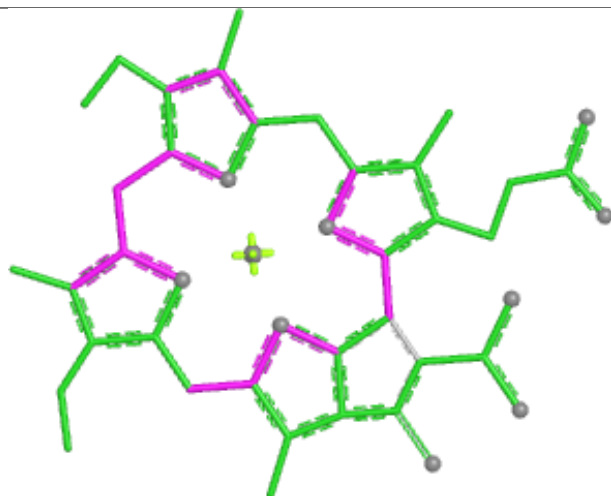


Rings

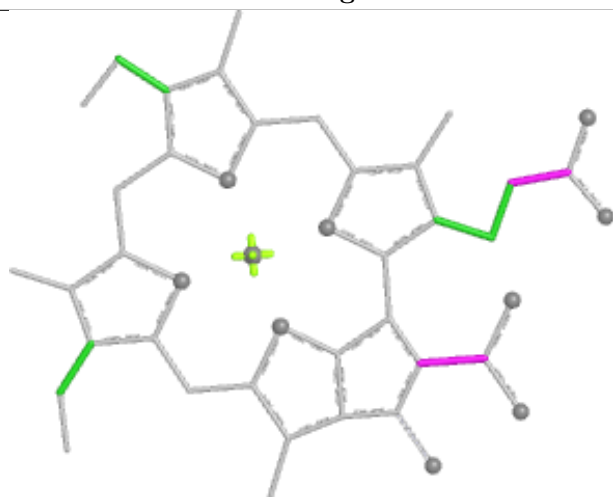
Ligand CLA A 829



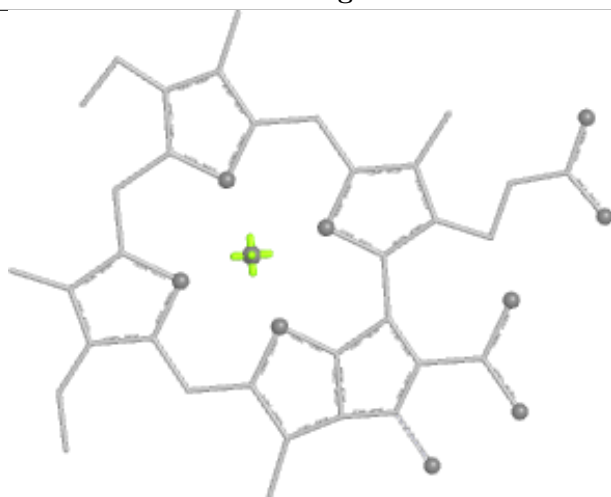
Bond lengths



Bond angles

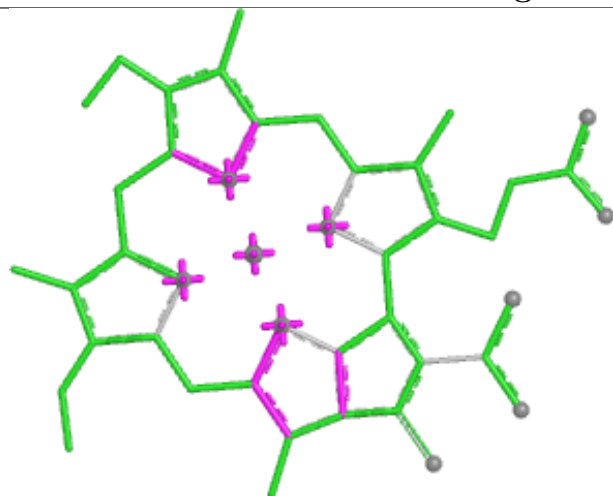


Torsions

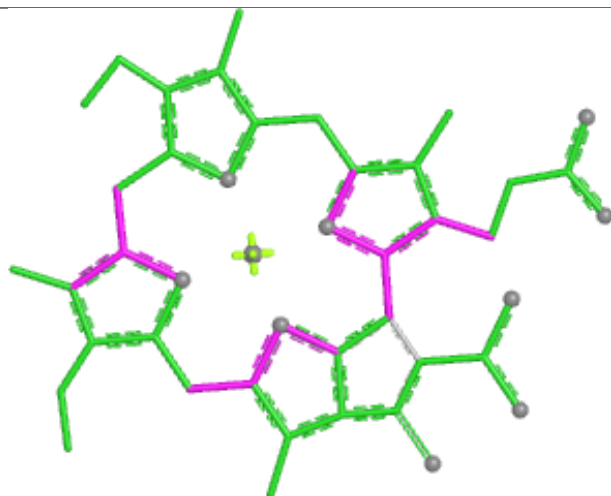


Rings

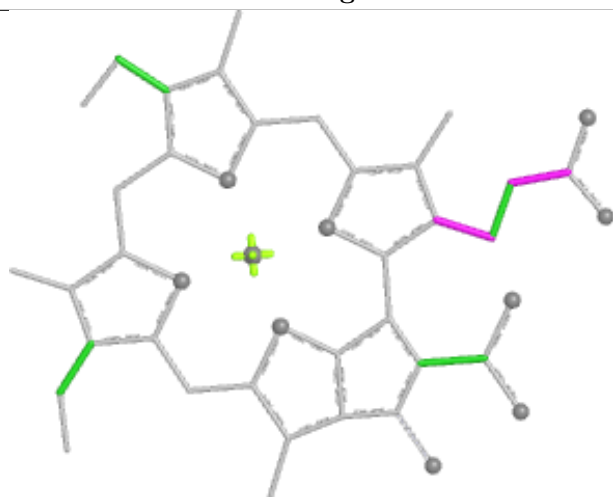
Ligand CLA B 821



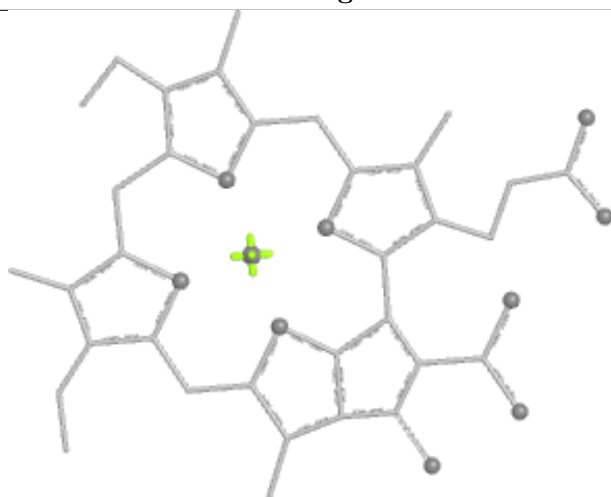
Bond lengths



Bond angles

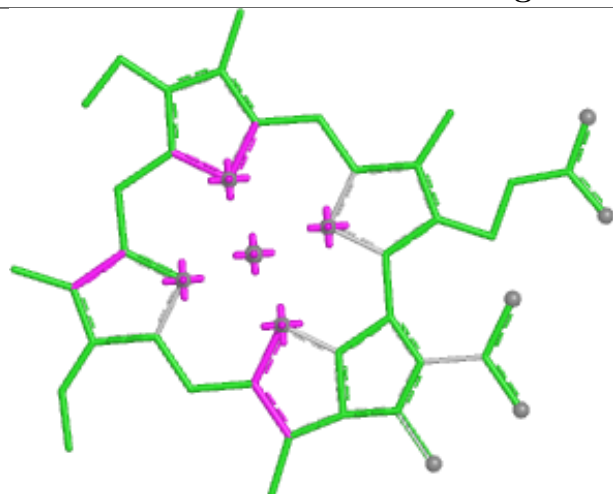


Torsions

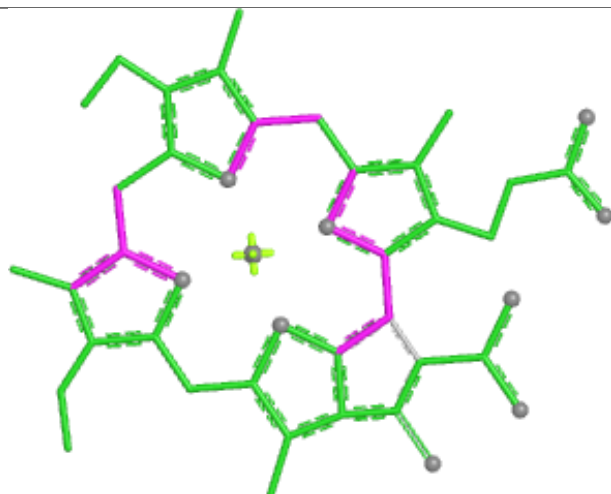


Rings

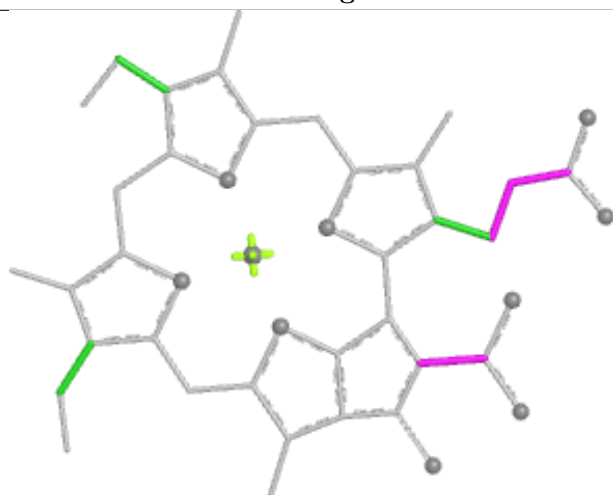
Ligand CLA B 838



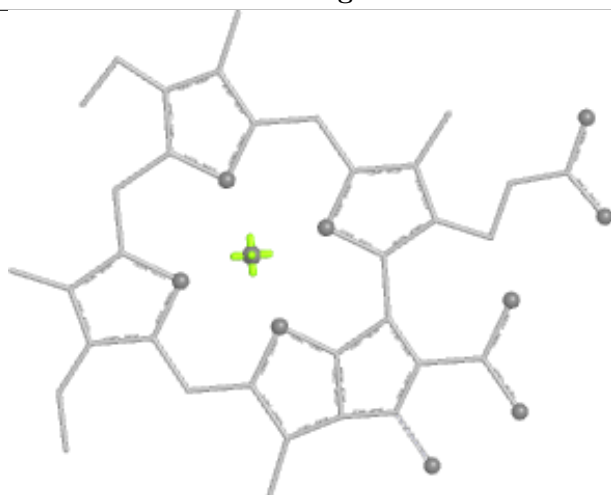
Bond lengths



Bond angles

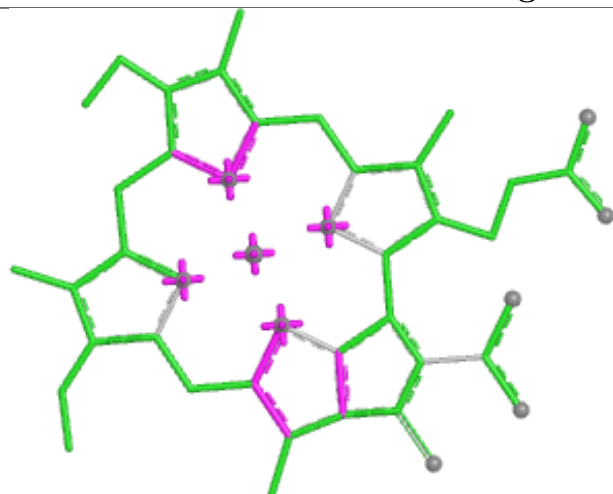


Torsions

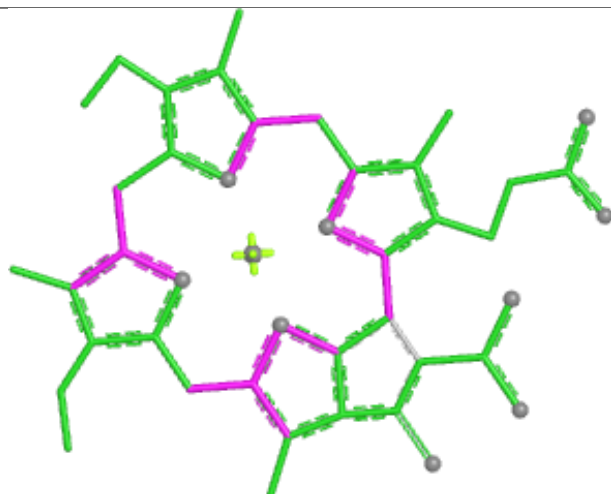


Rings

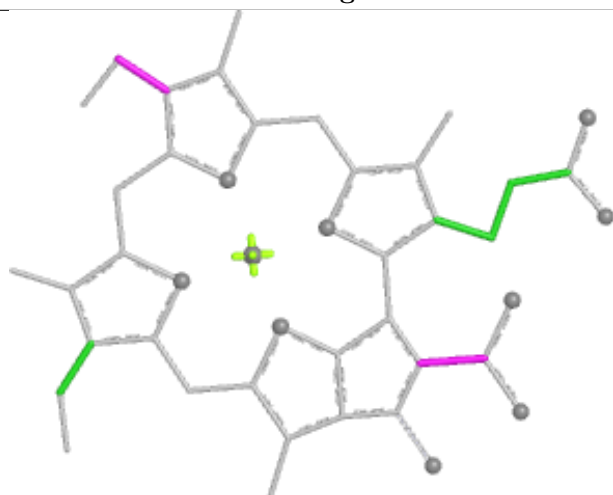
Ligand CLA 5 322



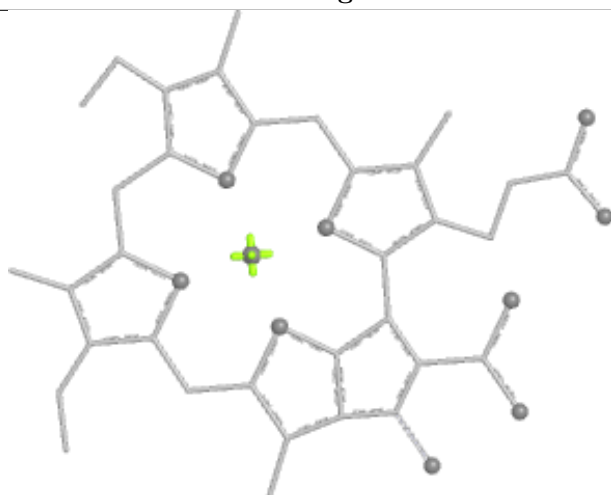
Bond lengths



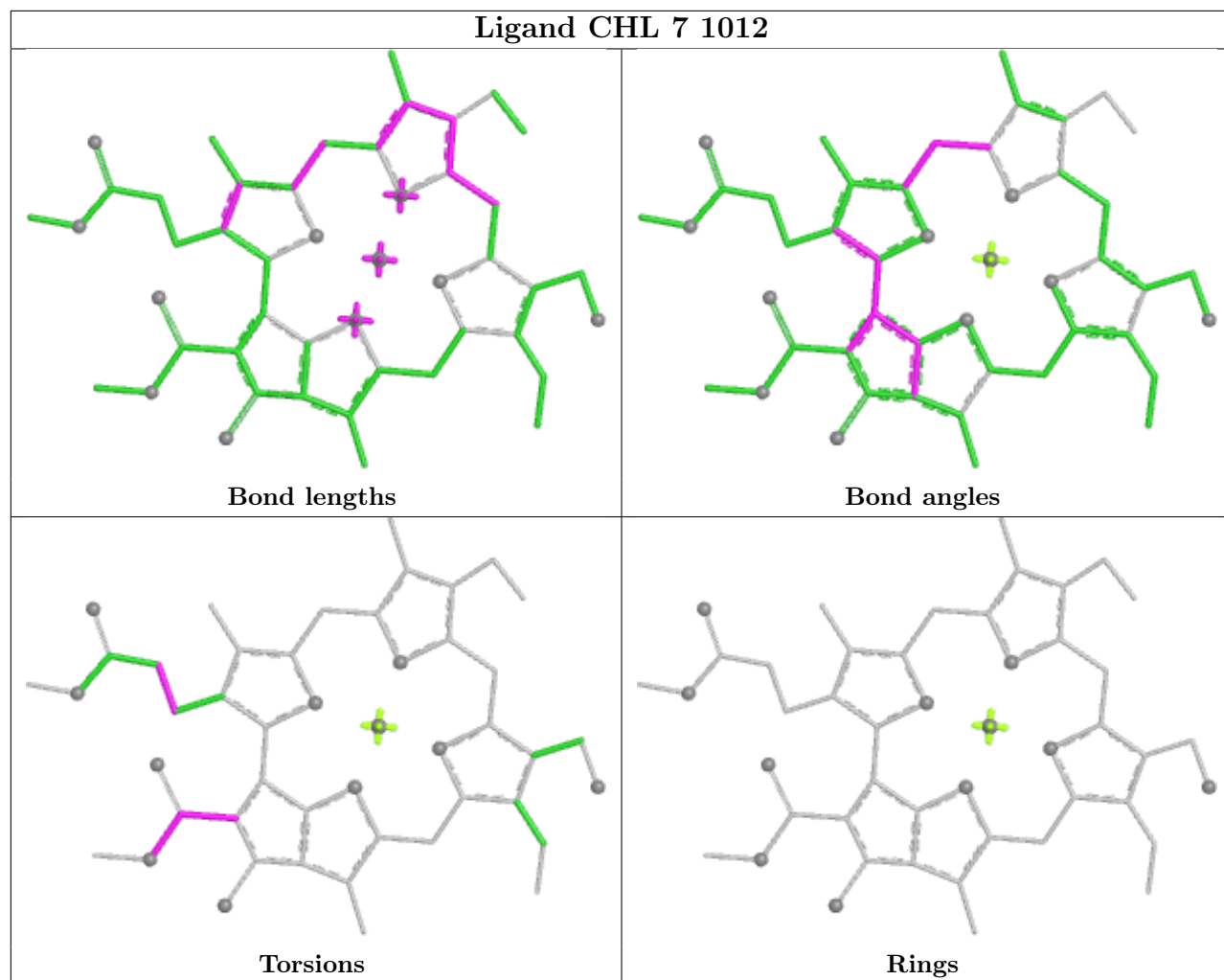
Bond angles

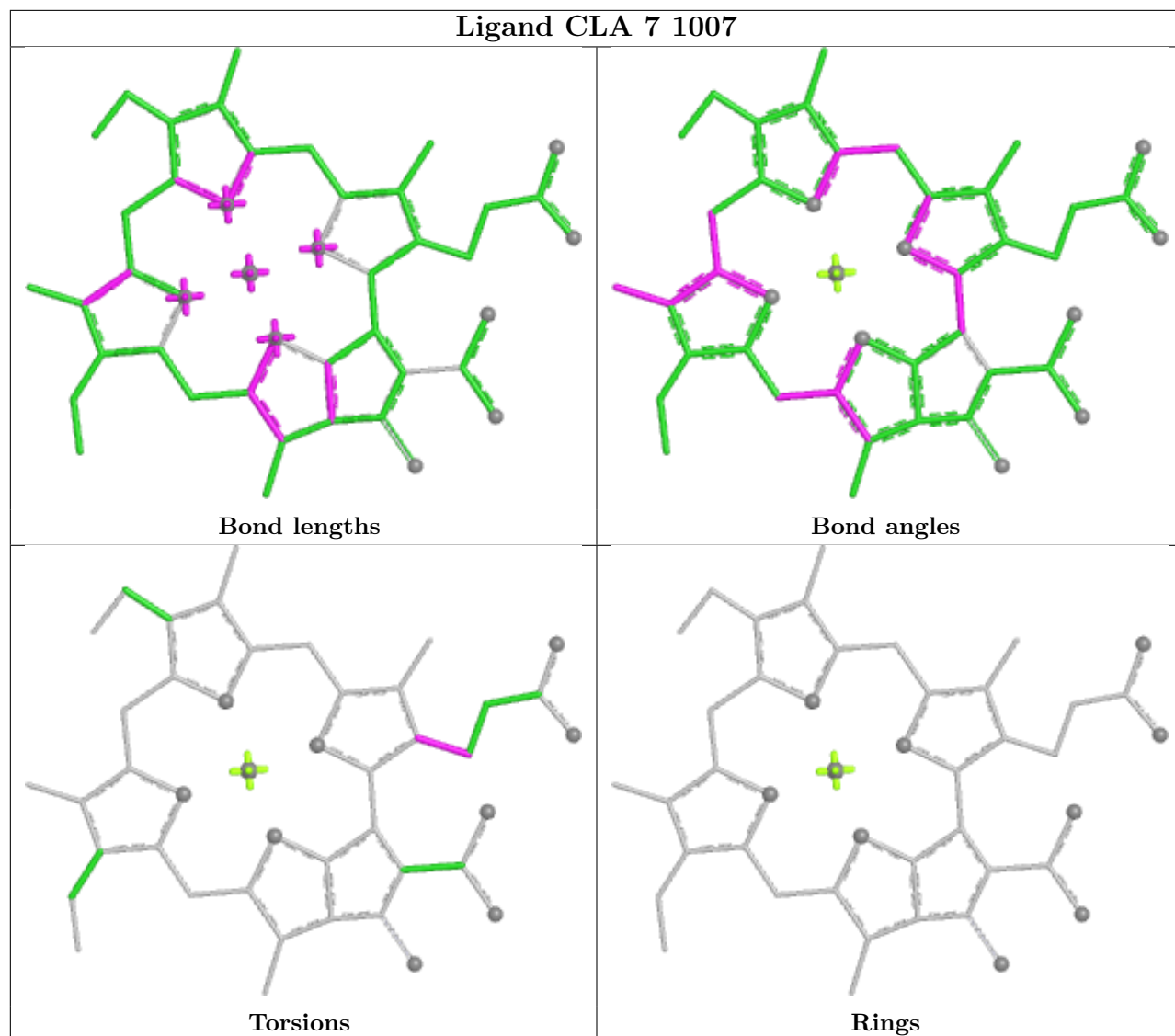


Torsions

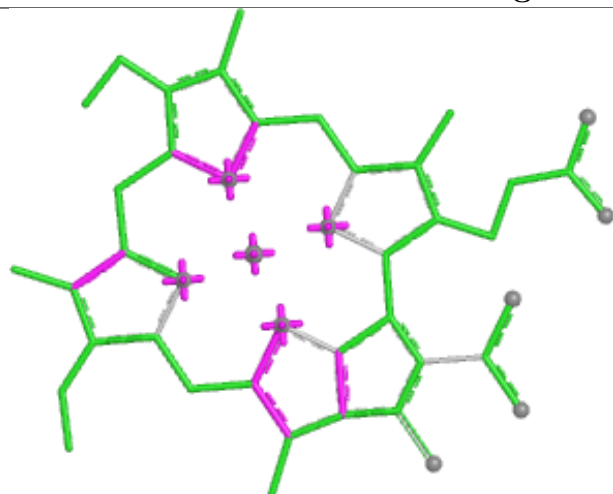


Rings

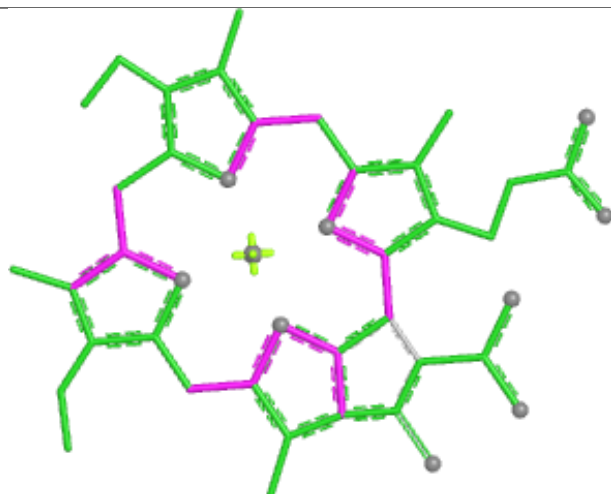




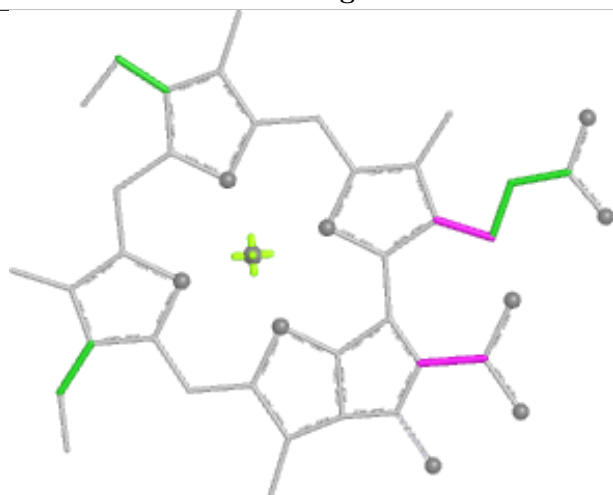
Ligand CLA A 804



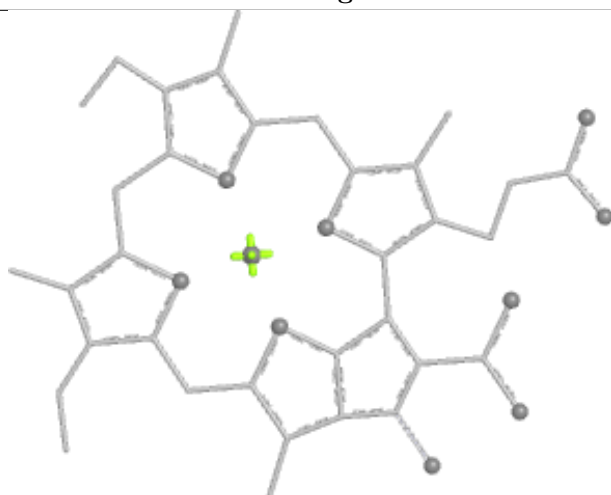
Bond lengths



Bond angles

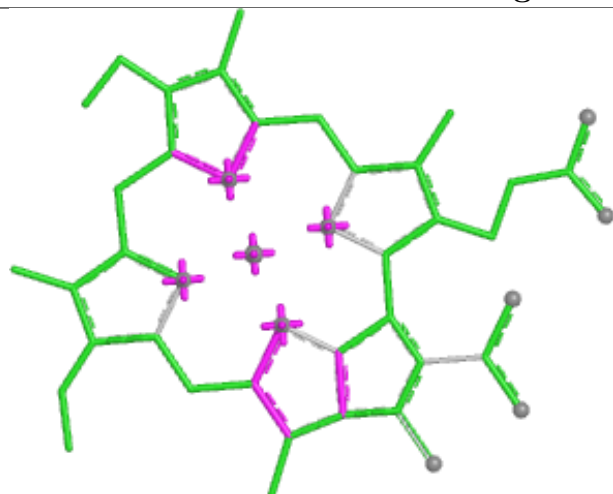


Torsions

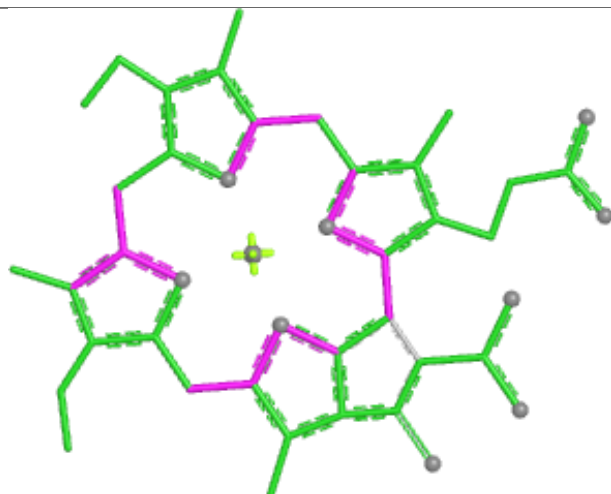


Rings

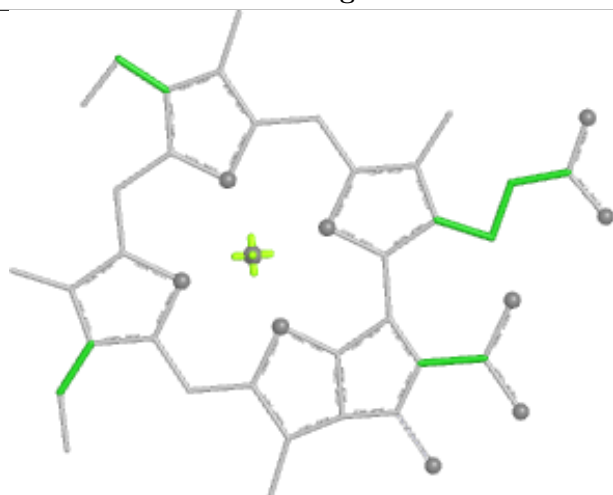
Ligand CLA A 826



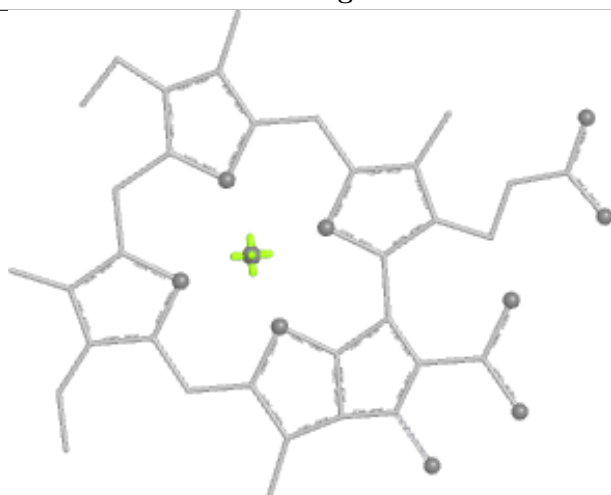
Bond lengths



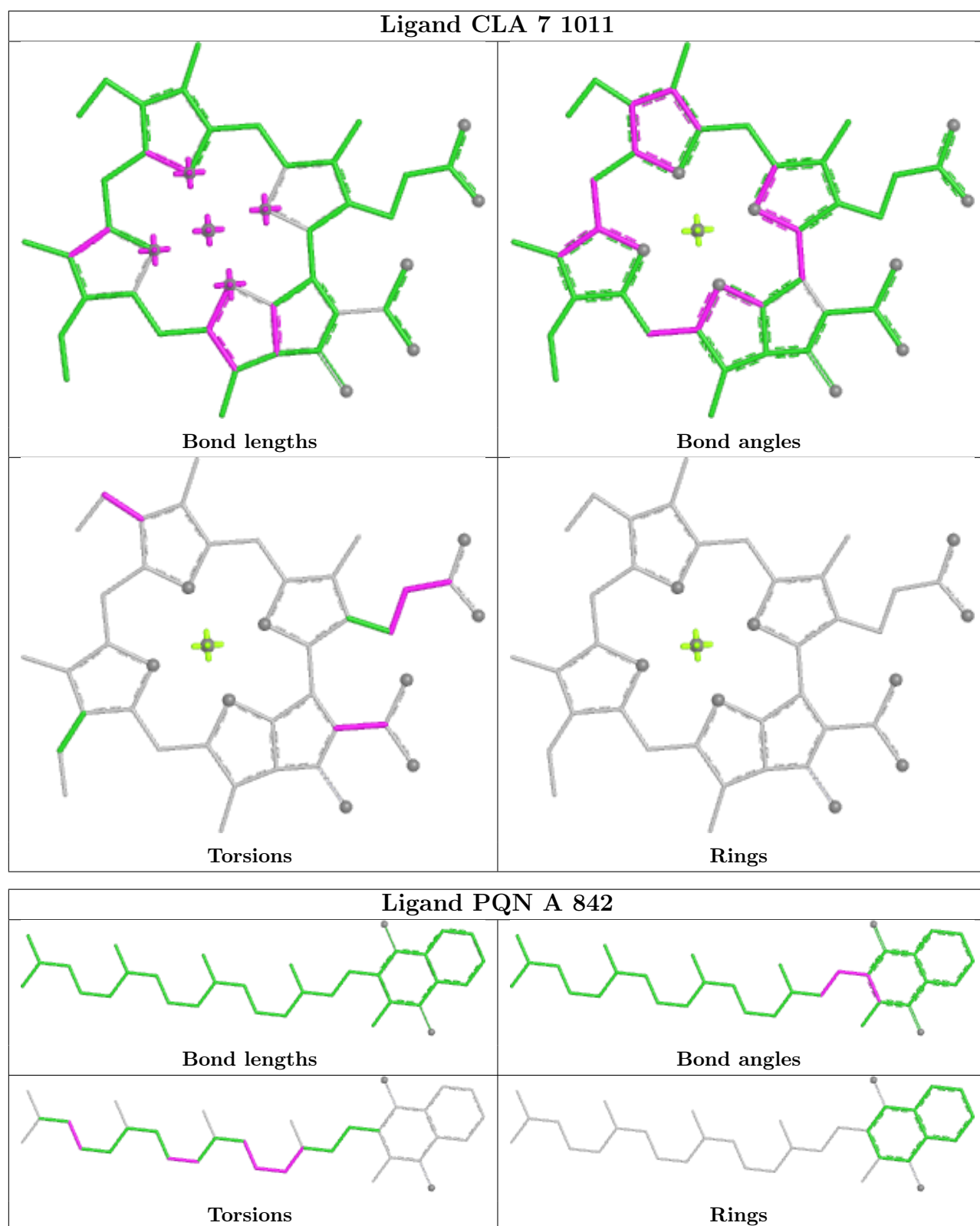
Bond angles

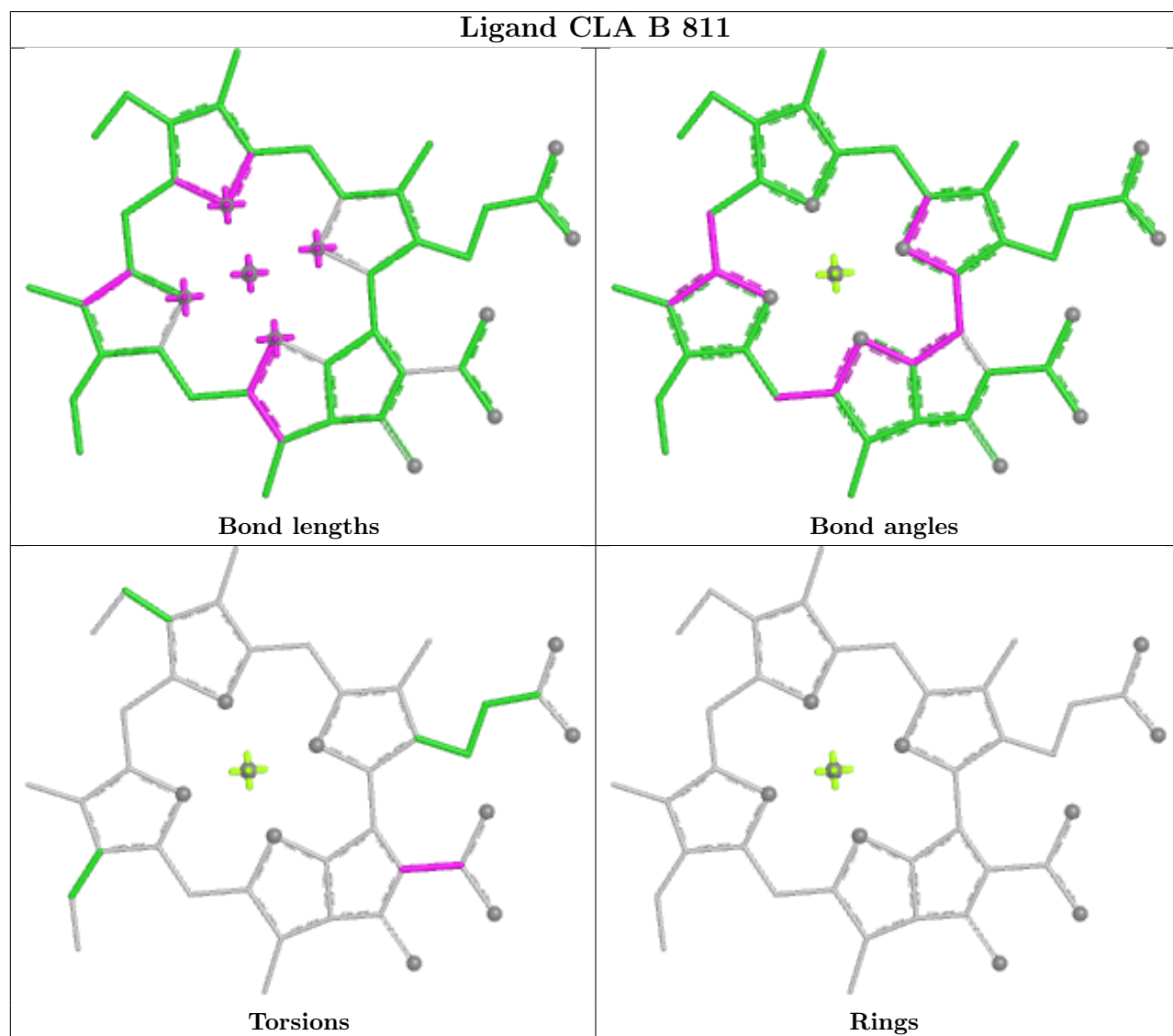
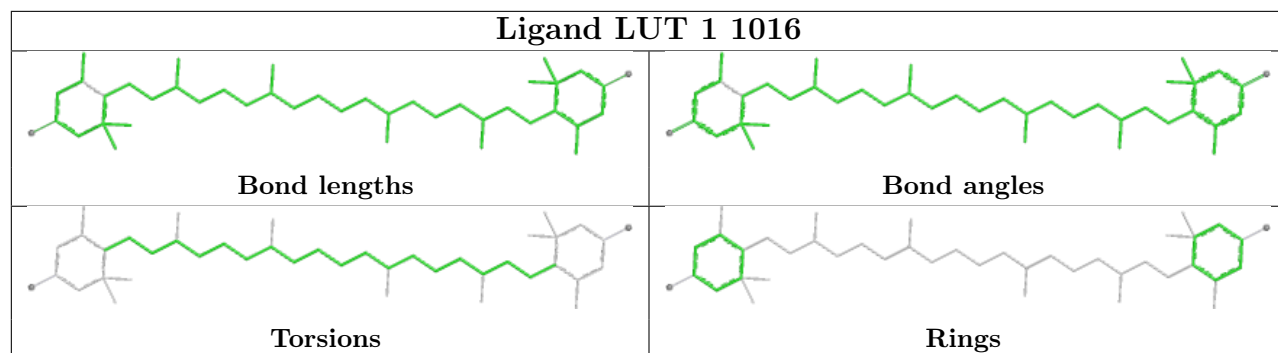


Torsions

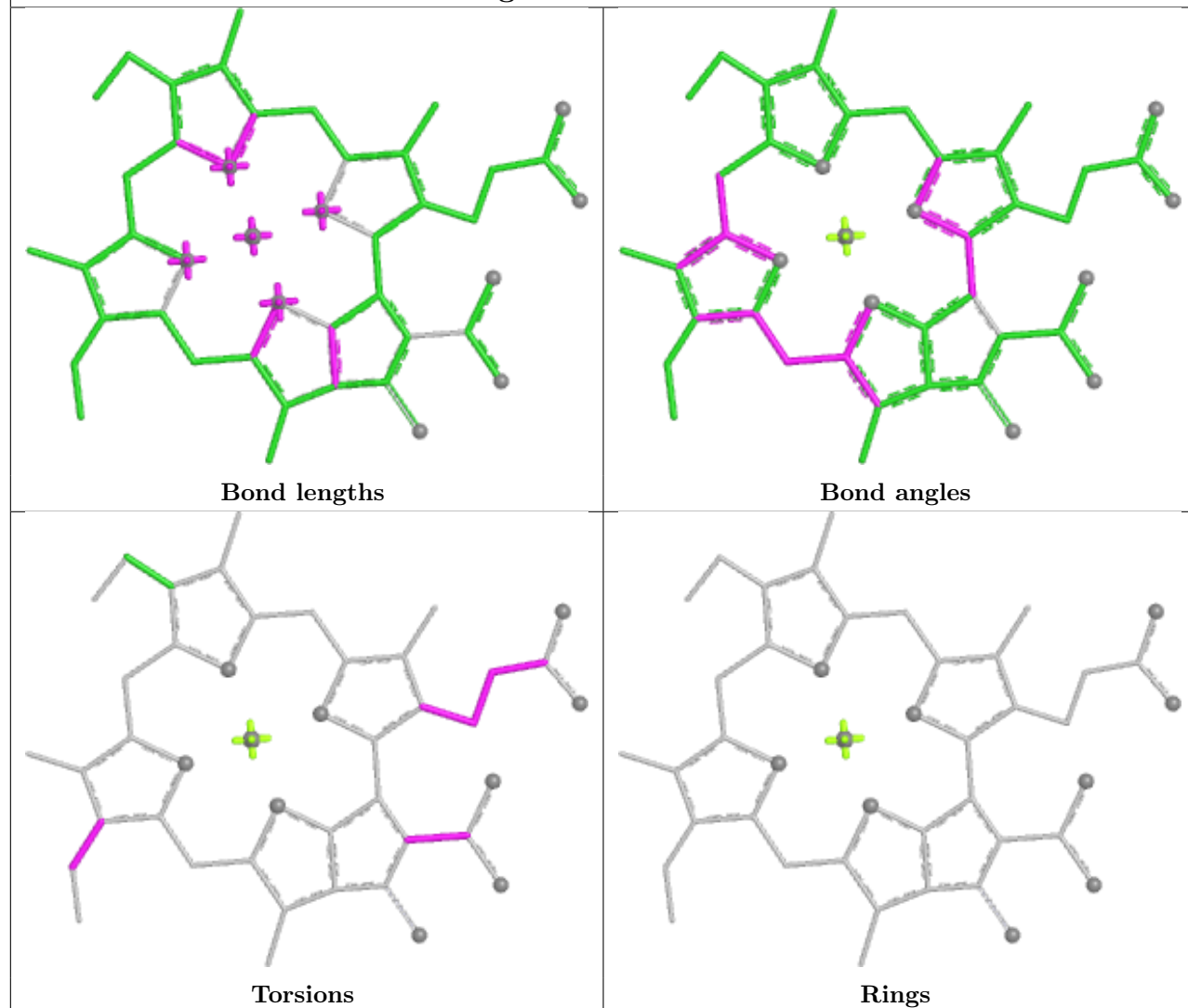


Rings

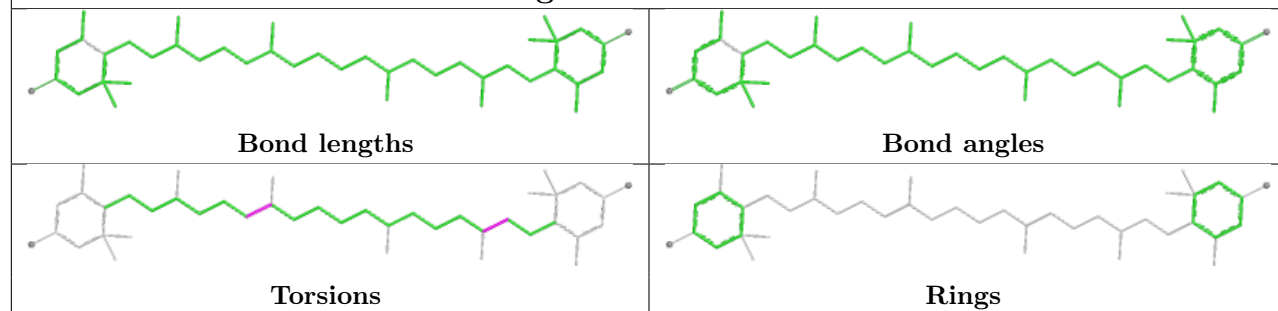




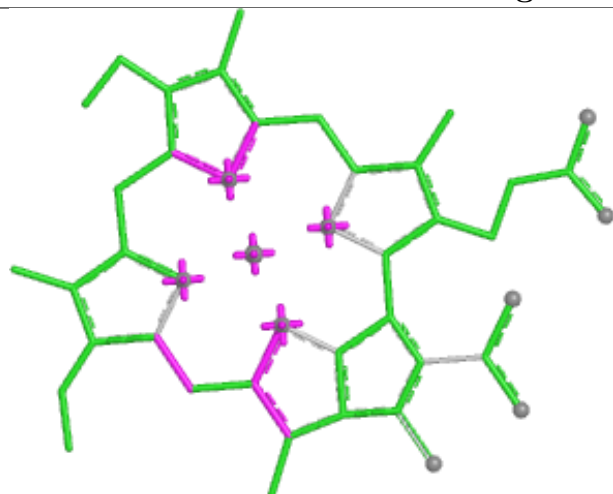
Ligand CLA 5 309



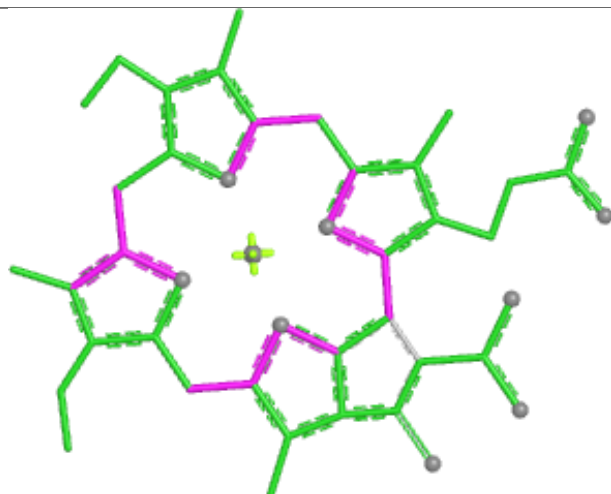
Ligand LUT 5 302



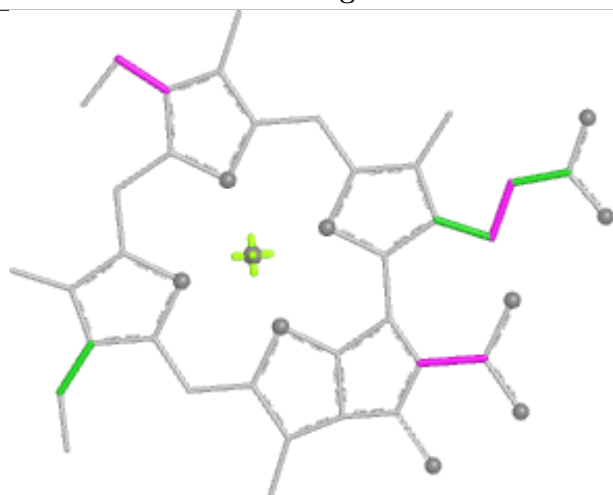
Ligand CLA F 303



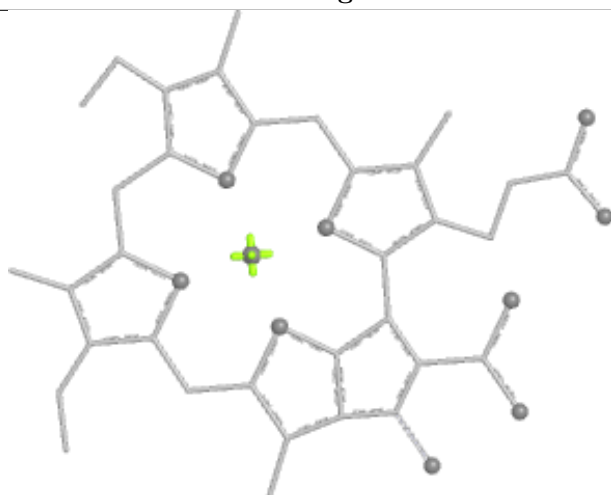
Bond lengths



Bond angles

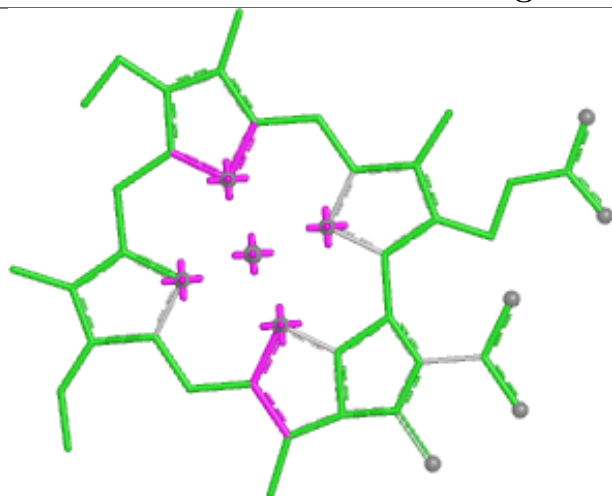


Torsions

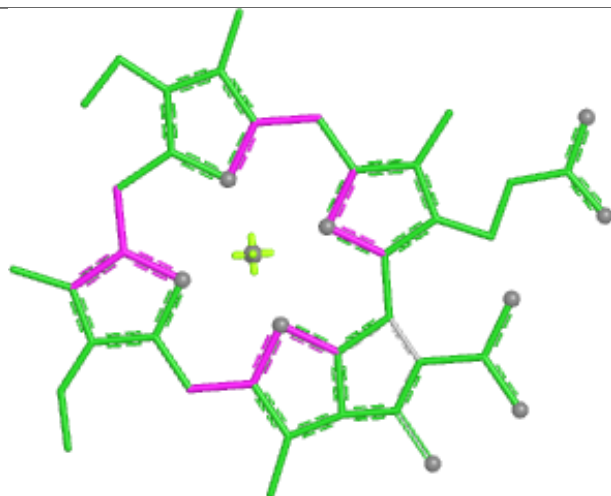


Rings

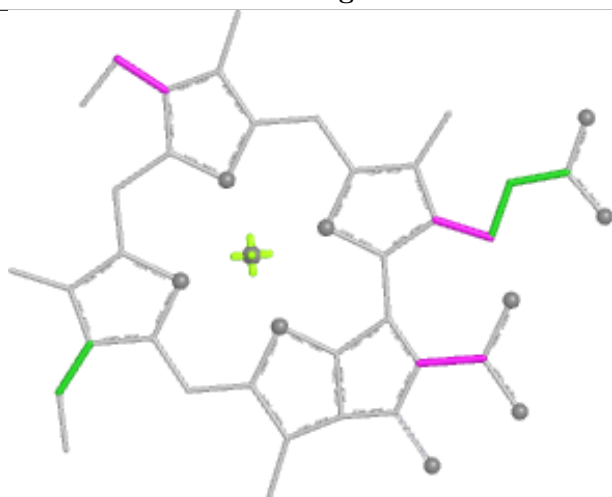
Ligand CLA L 202



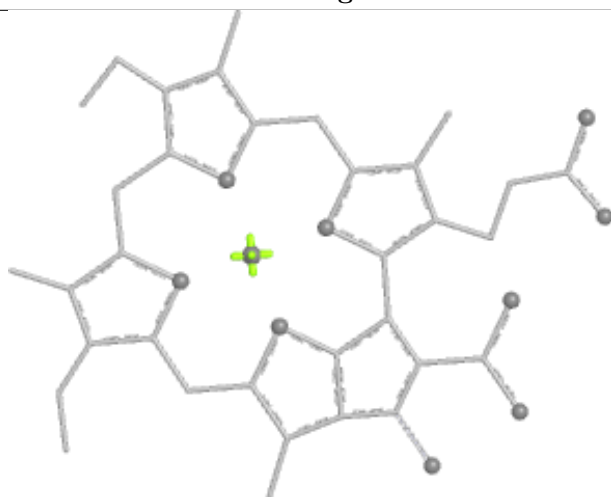
Bond lengths



Bond angles

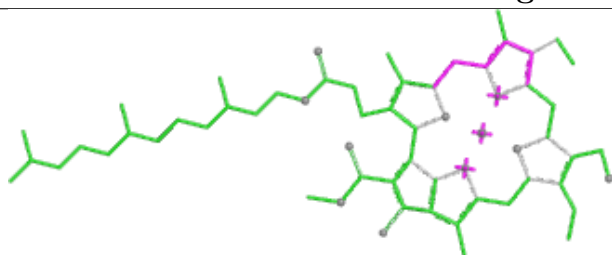


Torsions

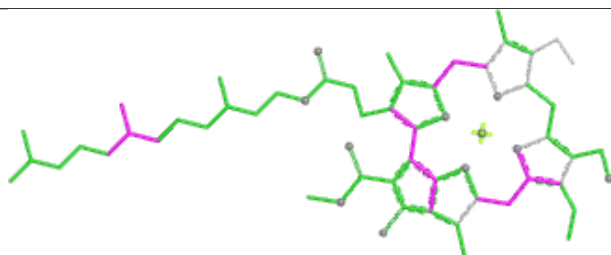


Rings

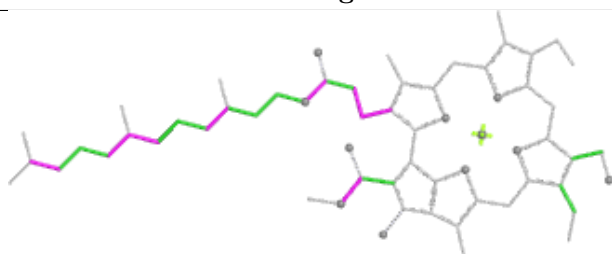
Ligand CHL 0 317



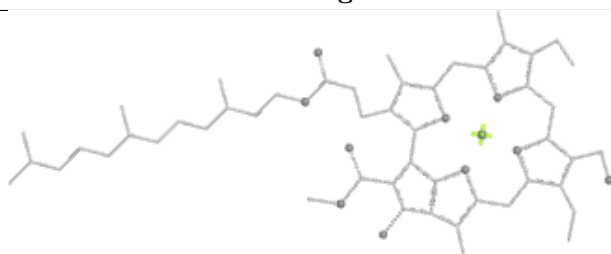
Bond lengths



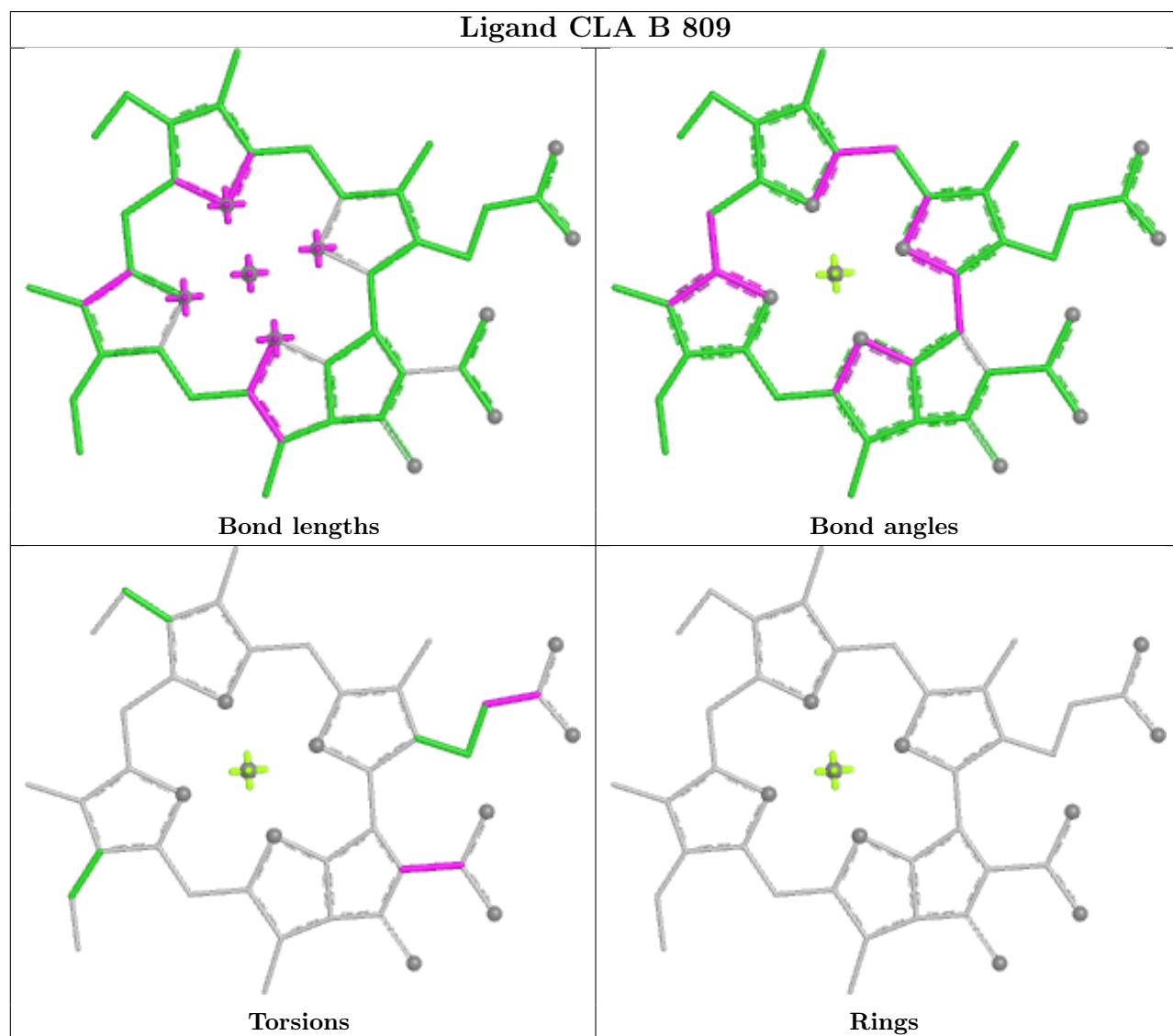
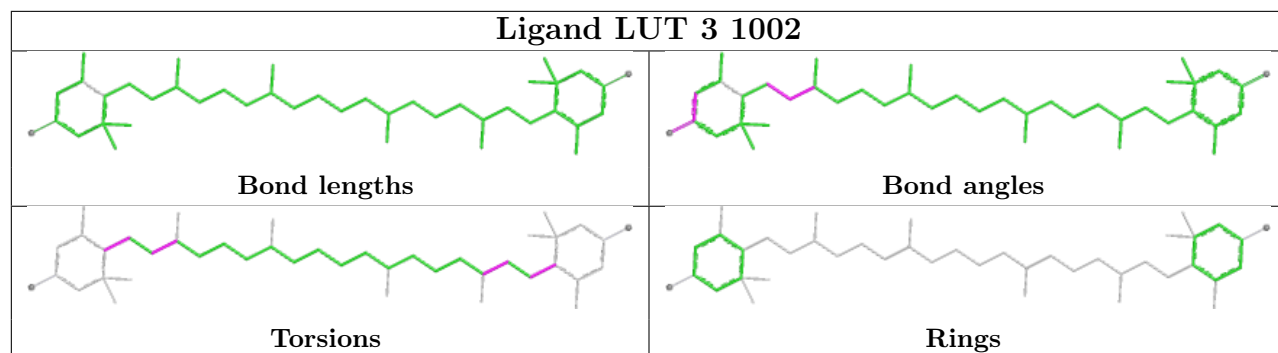
Bond angles



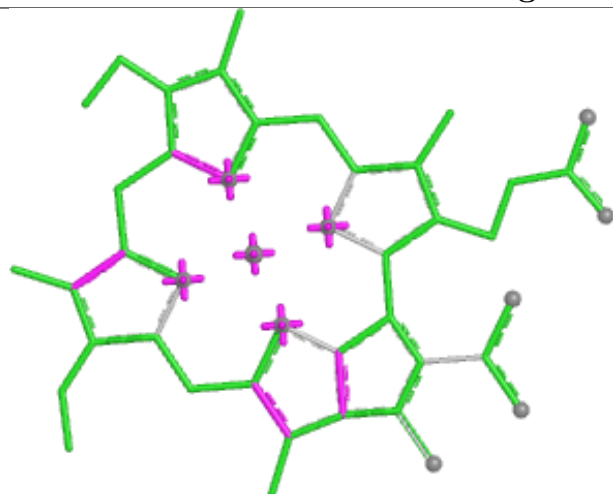
Torsions



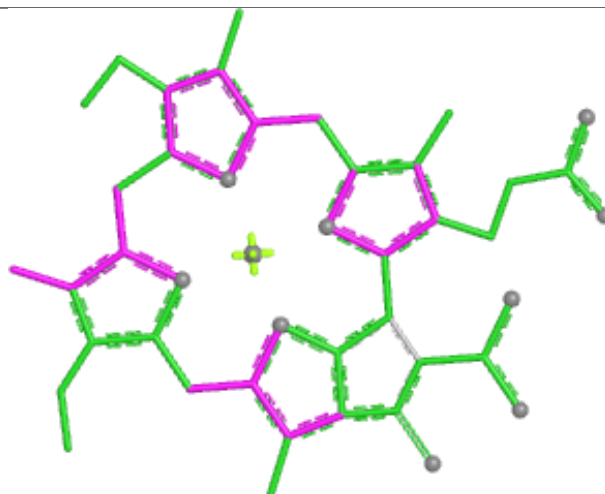
Rings



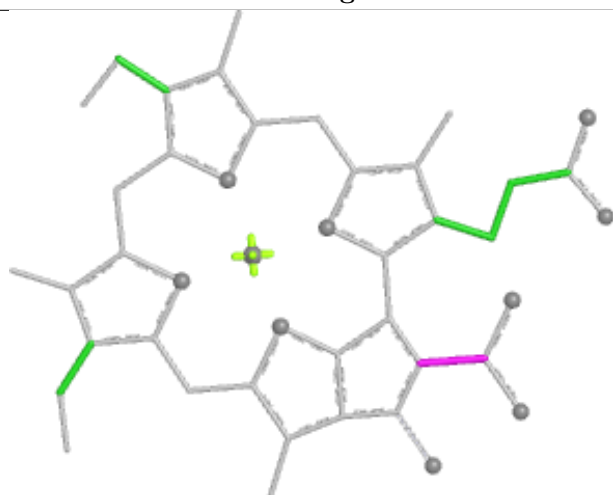
Ligand CLA 6 308



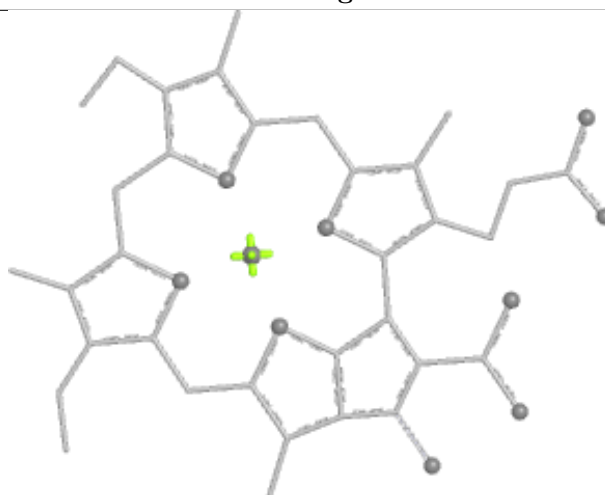
Bond lengths



Bond angles

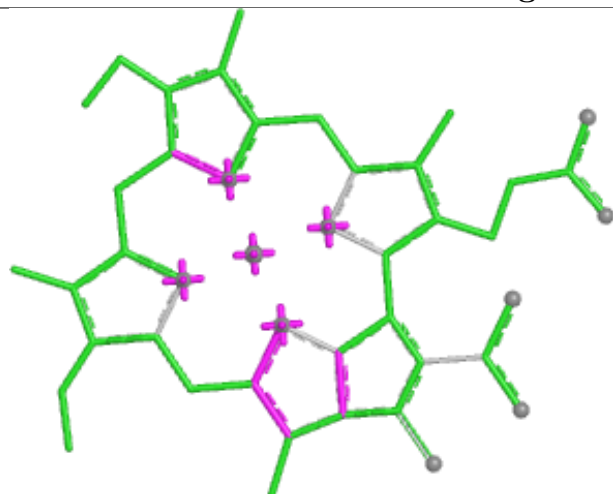


Torsions

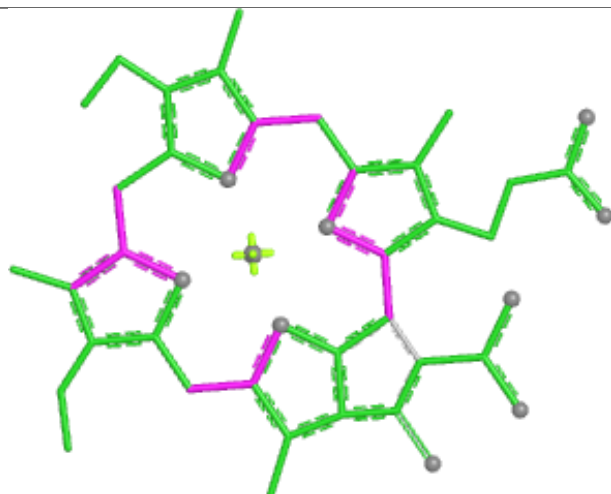


Rings

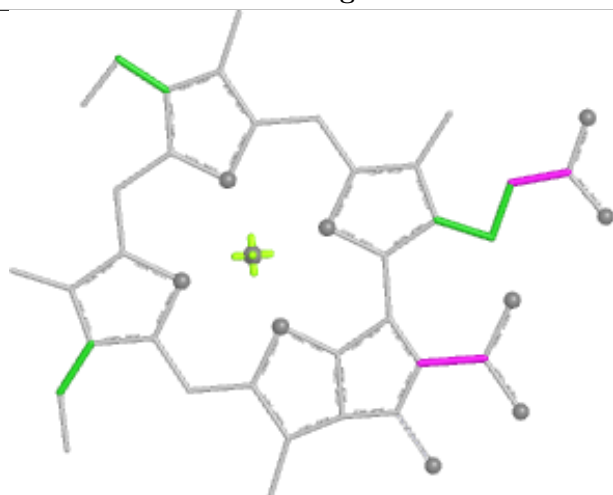
Ligand CLA 0 308



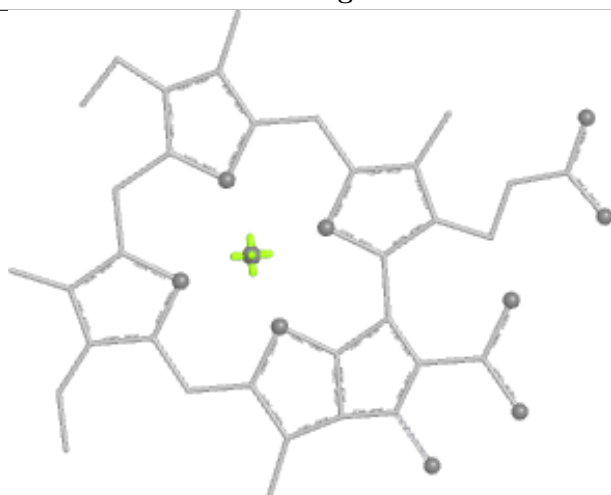
Bond lengths



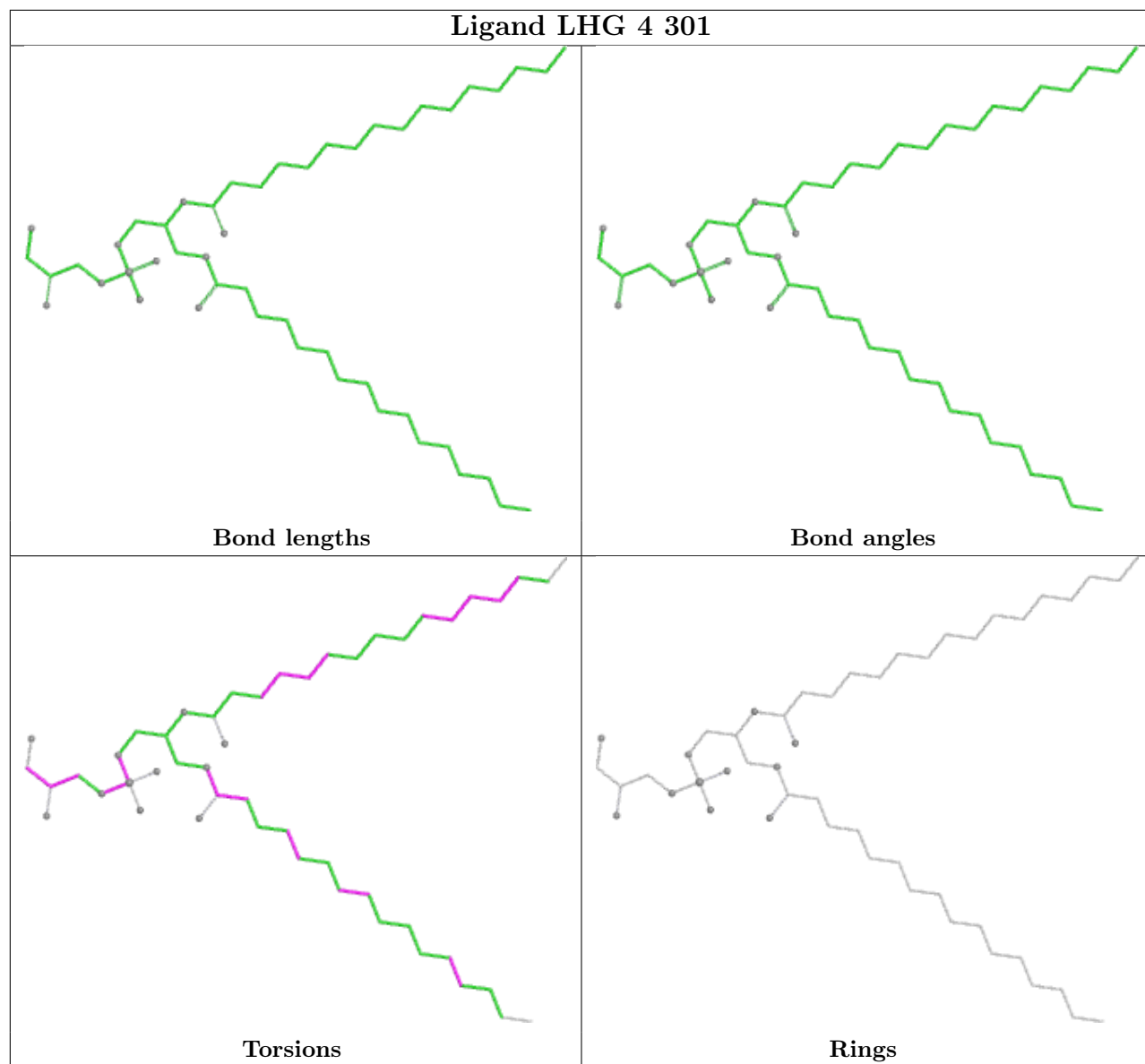
Bond angles



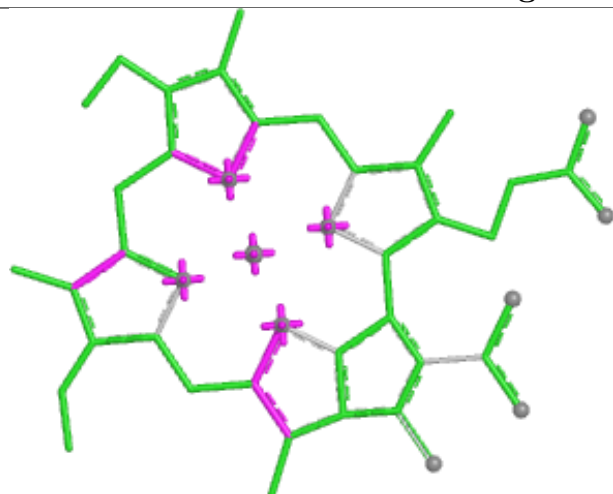
Torsions



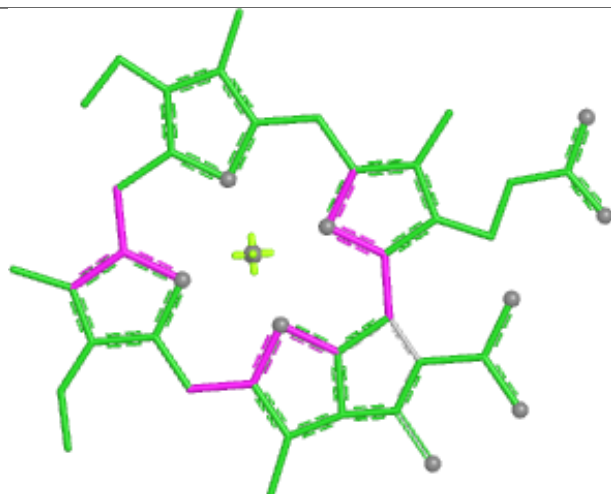
Rings



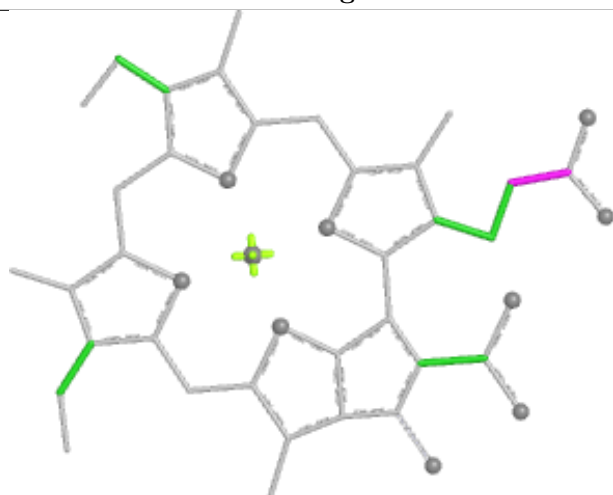
Ligand CLA 0 301



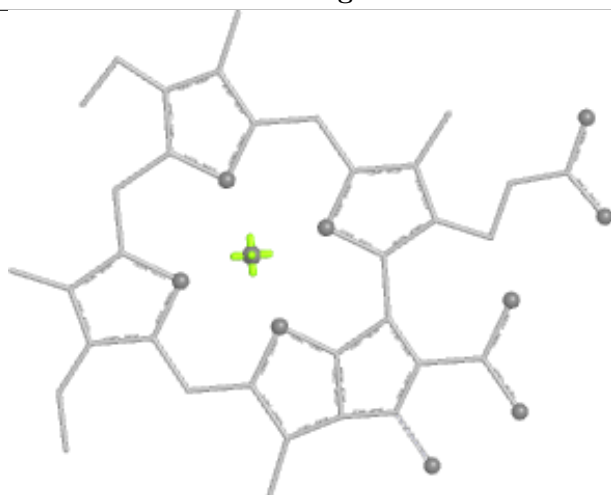
Bond lengths



Bond angles

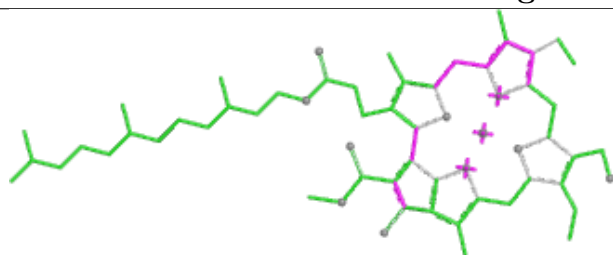


Torsions

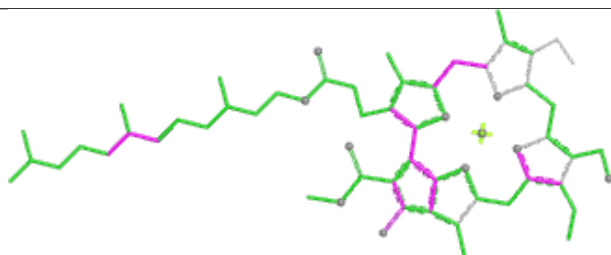


Rings

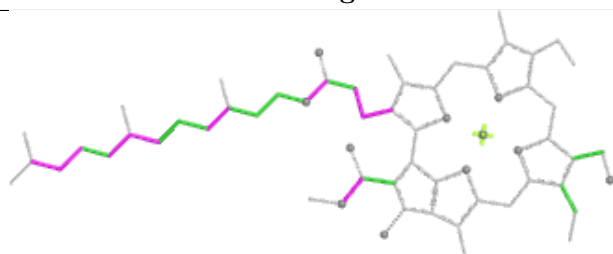
Ligand CHL 5 316



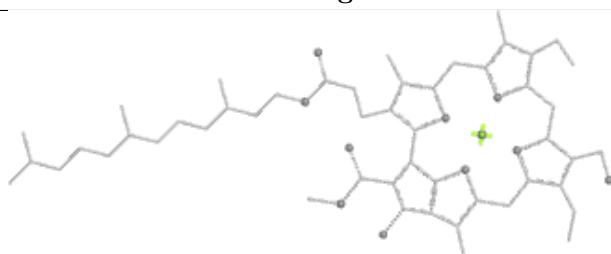
Bond lengths



Bond angles

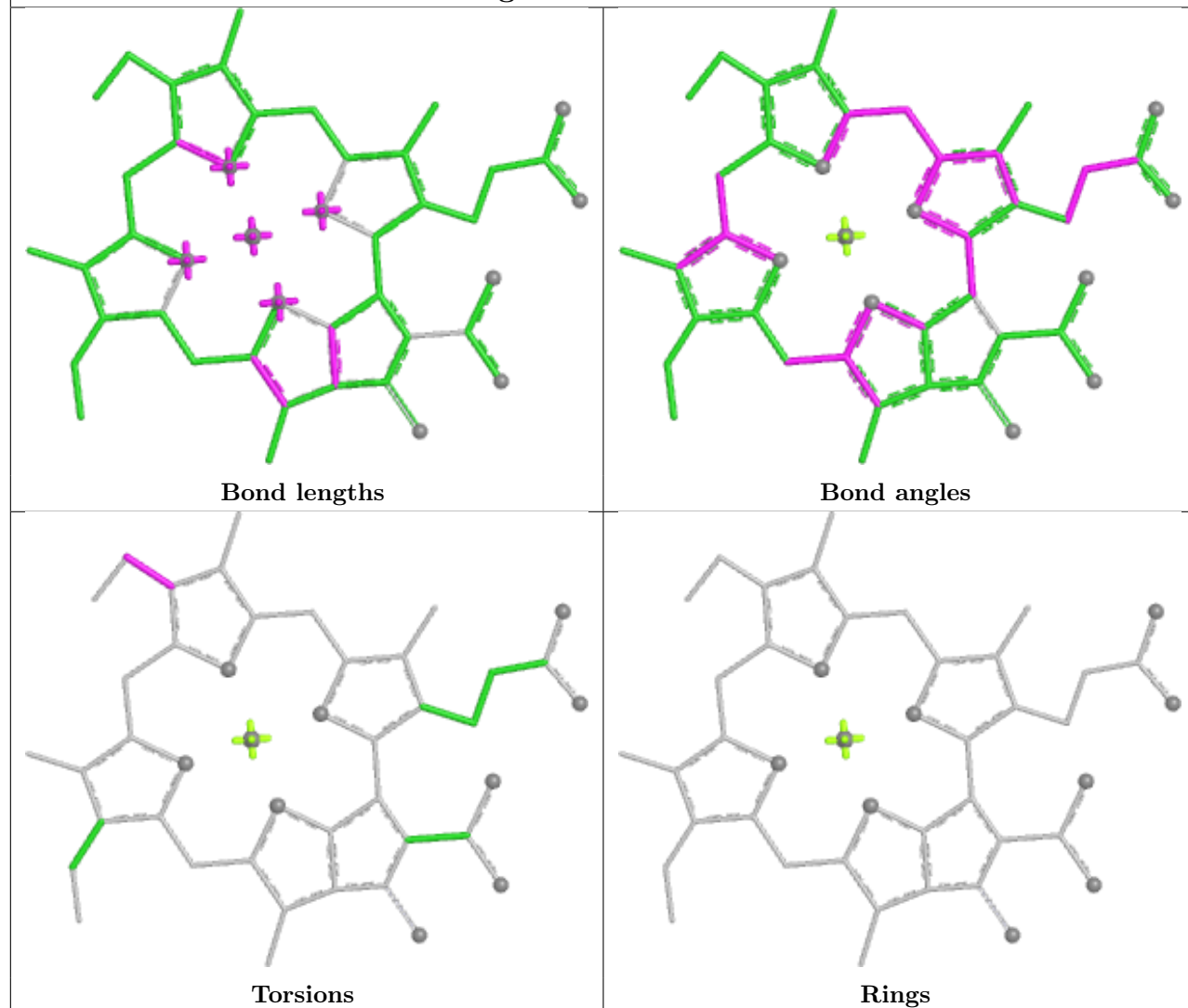


Torsions

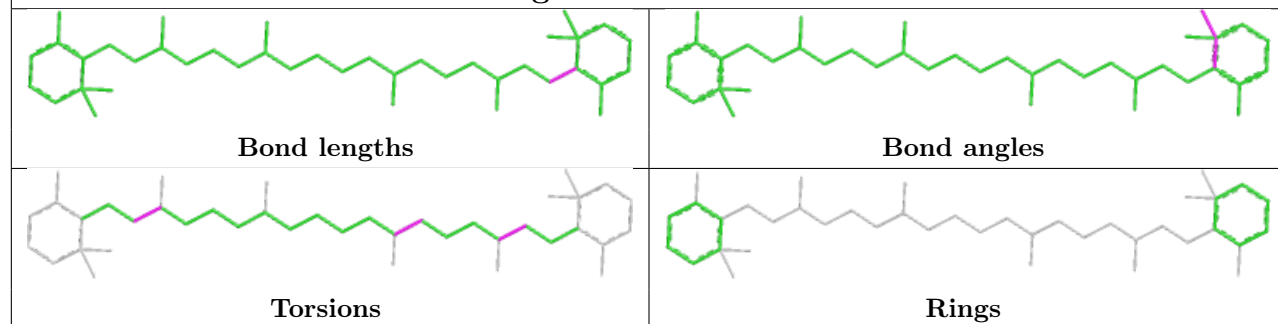


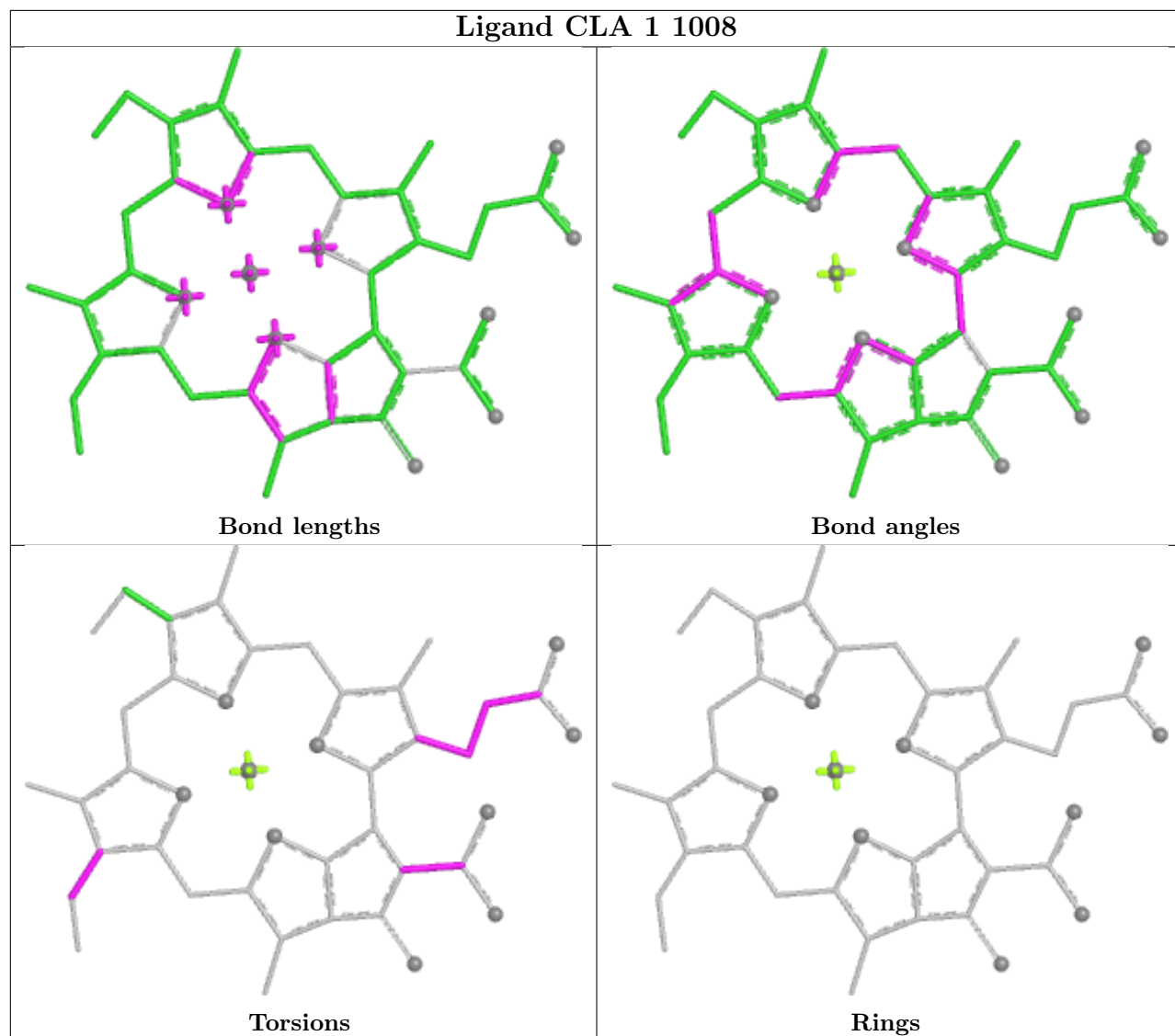
Rings

Ligand CLA 6 320

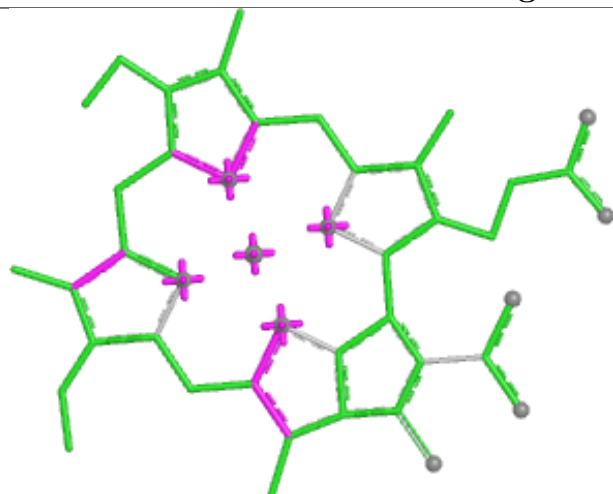


Ligand BCR F 301

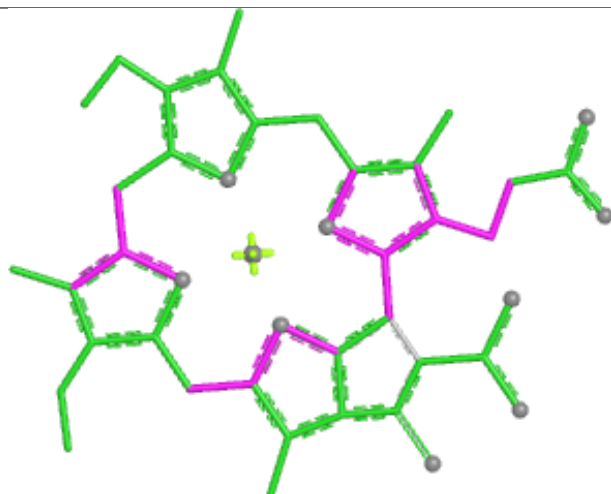




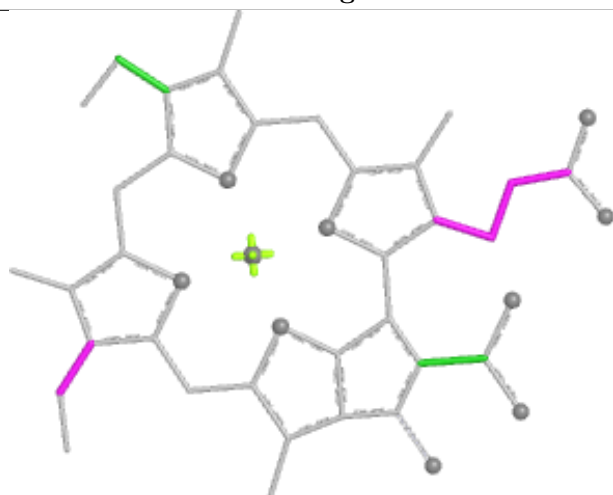
Ligand CLA 6 310



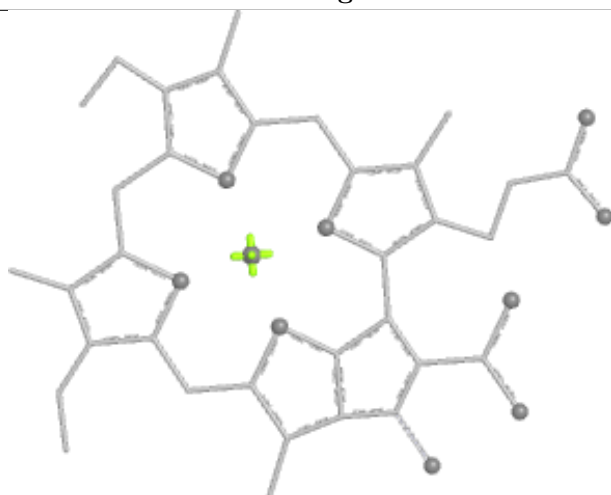
Bond lengths



Bond angles

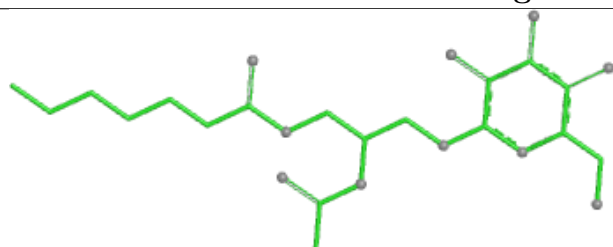


Torsions

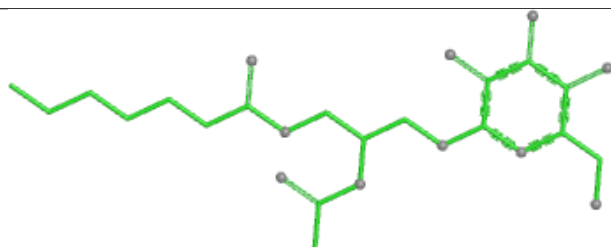


Rings

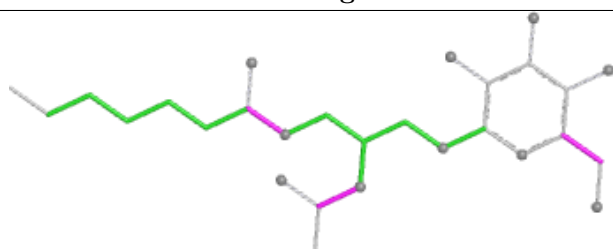
Ligand LMG 8 318



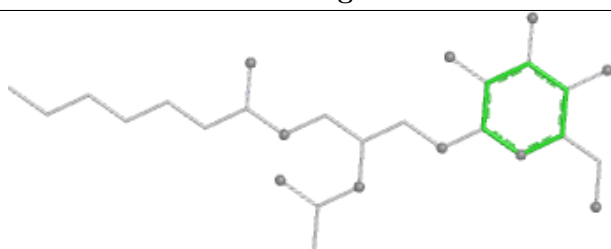
Bond lengths



Bond angles

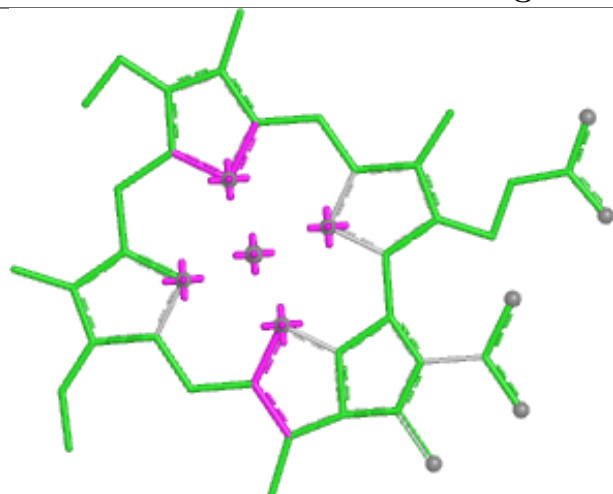


Torsions

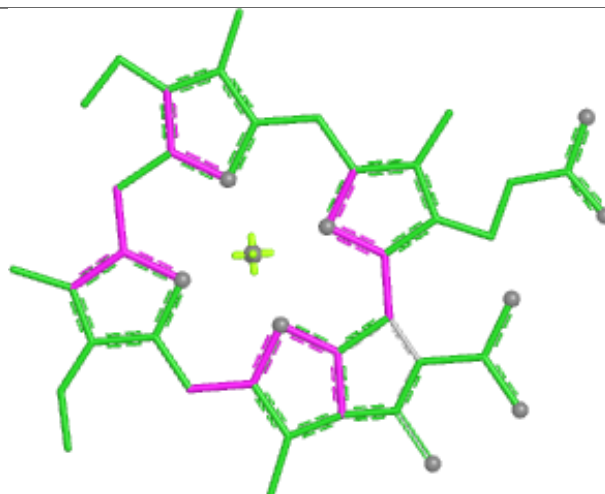


Rings

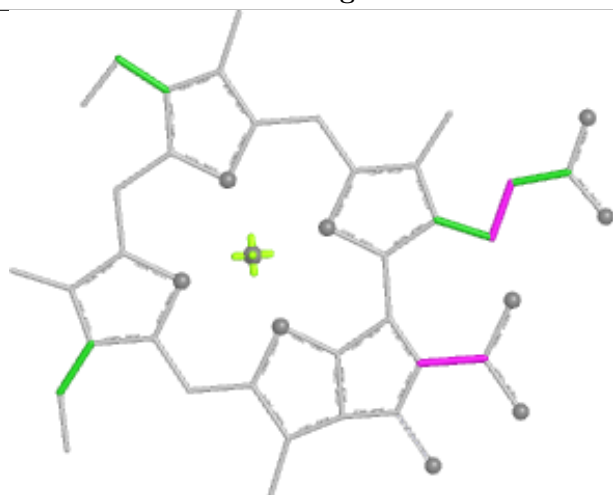
Ligand CLA B 833



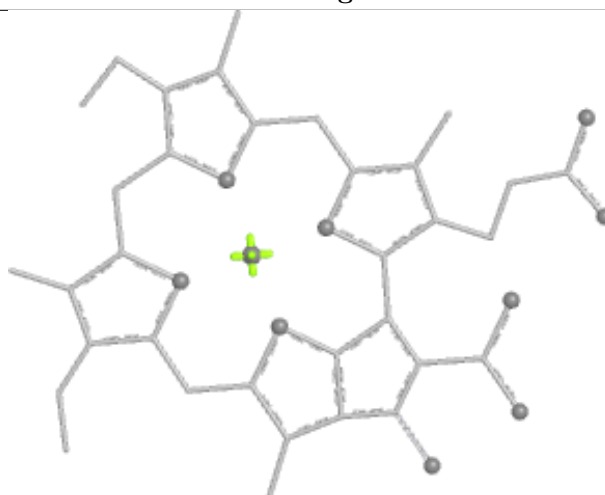
Bond lengths



Bond angles

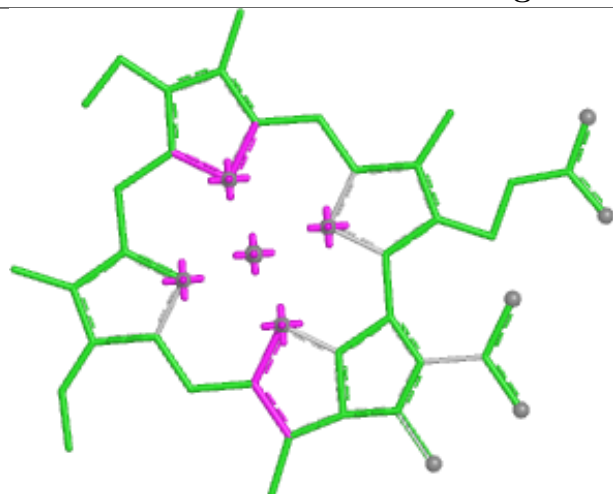


Torsions

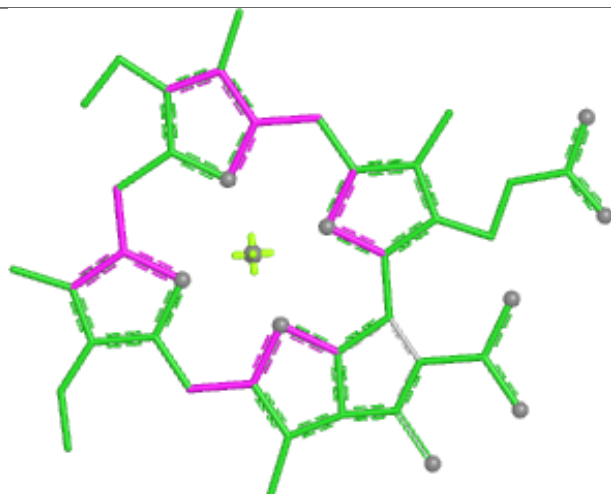


Rings

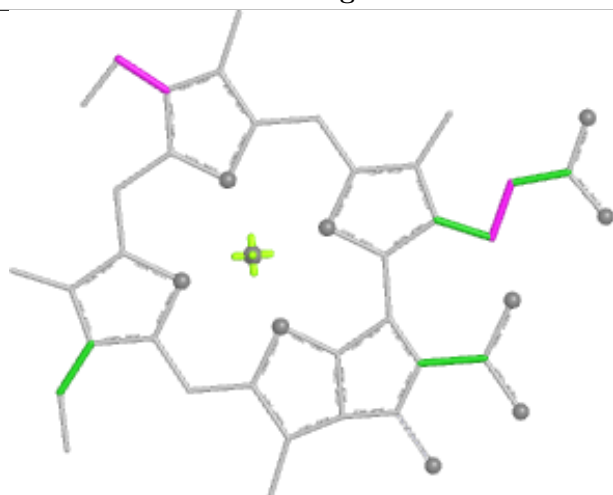
Ligand CLA A 823



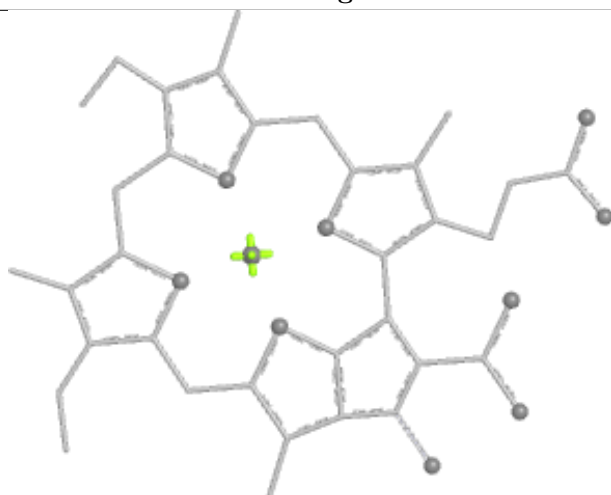
Bond lengths



Bond angles

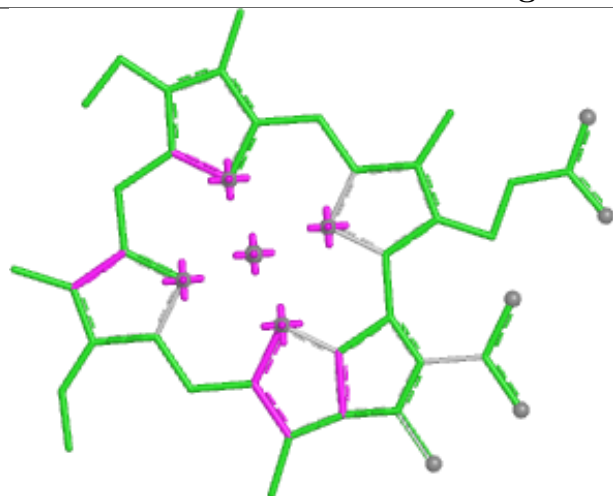


Torsions

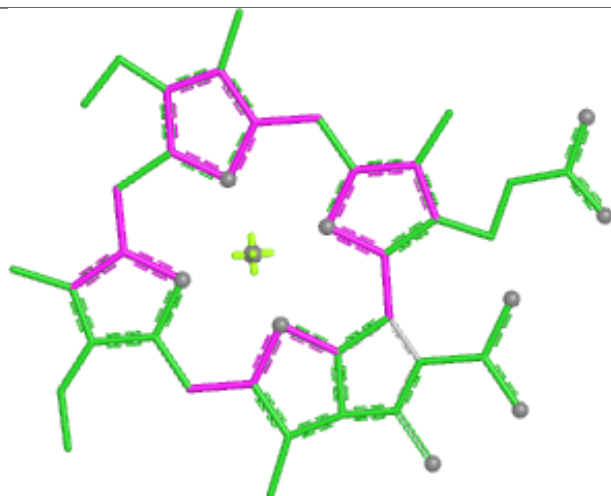


Rings

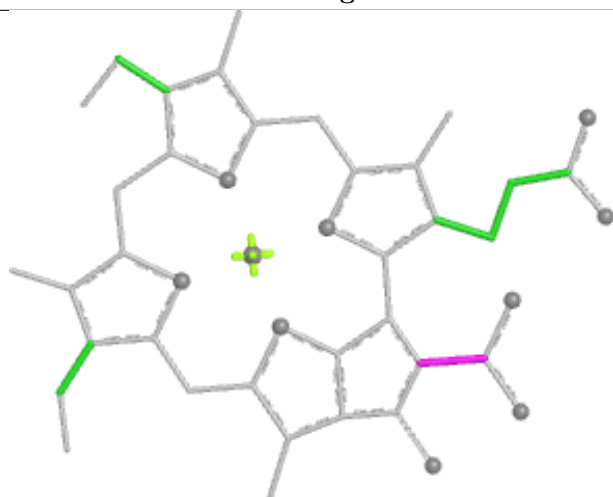
Ligand CLA 8 308



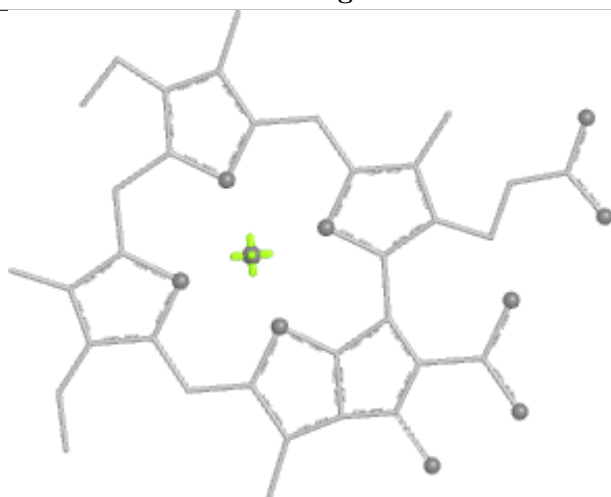
Bond lengths



Bond angles

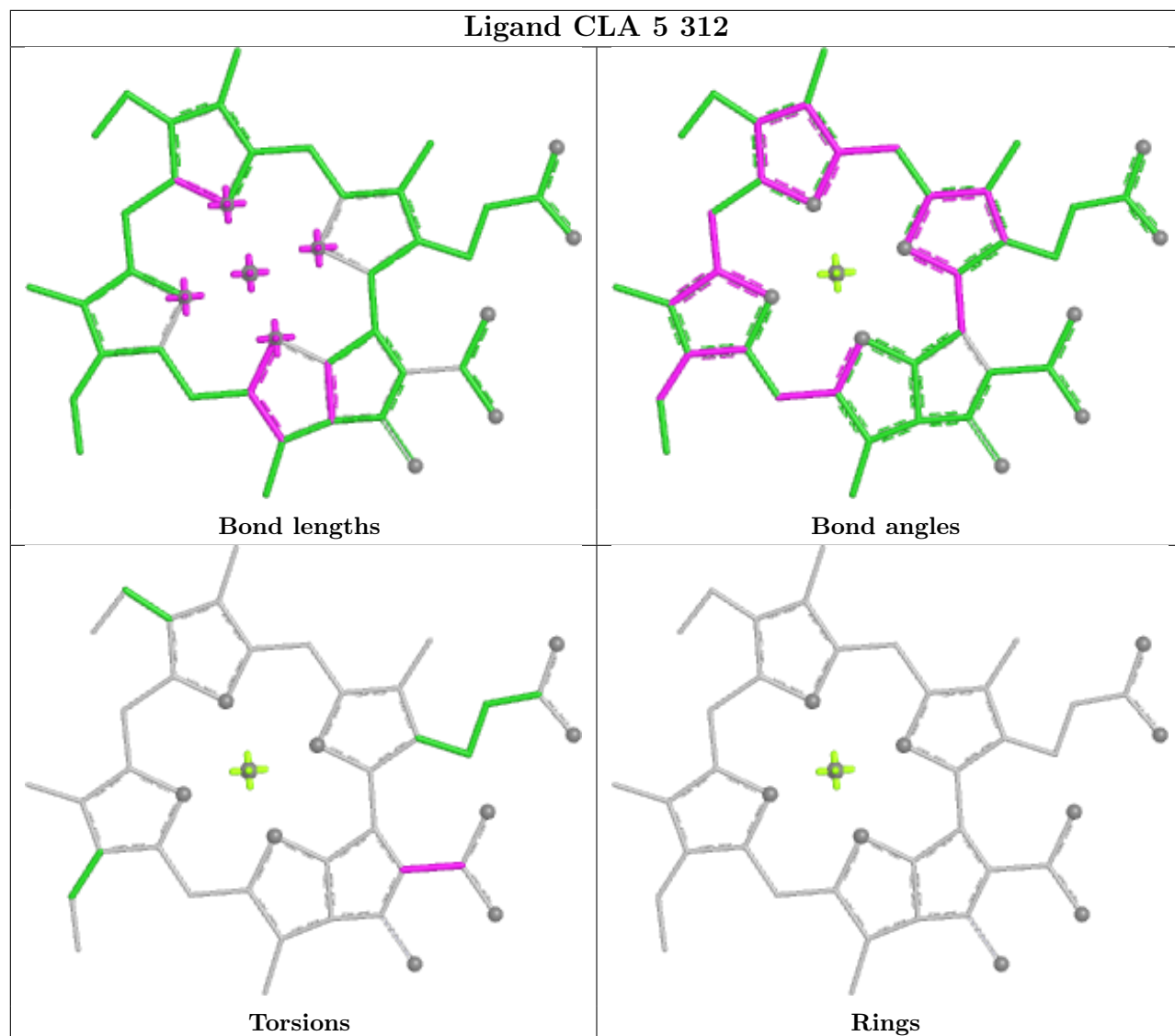


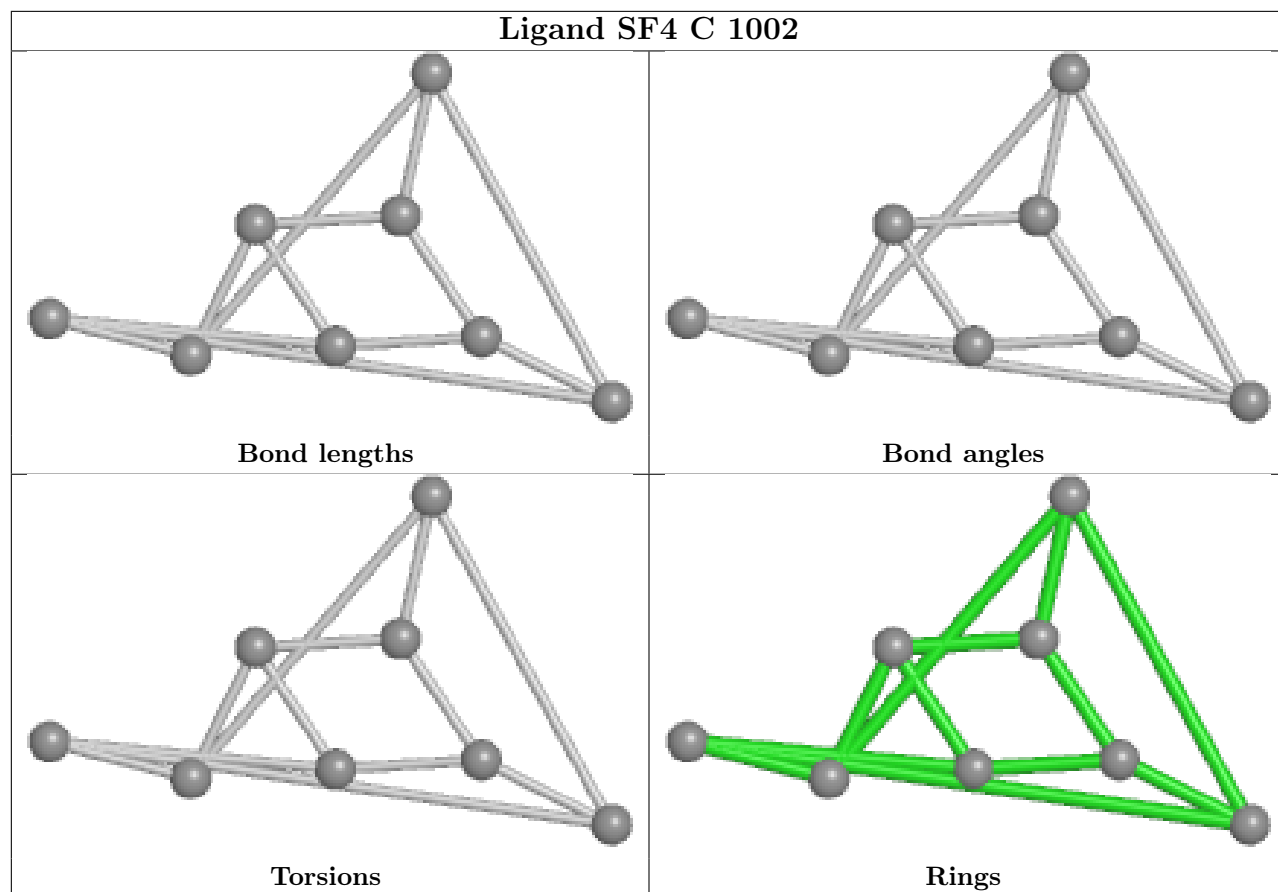
Torsions



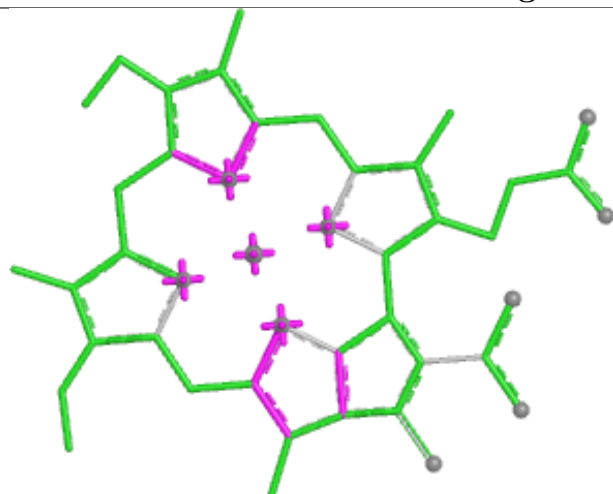
Rings

Ligand CLA 5 312

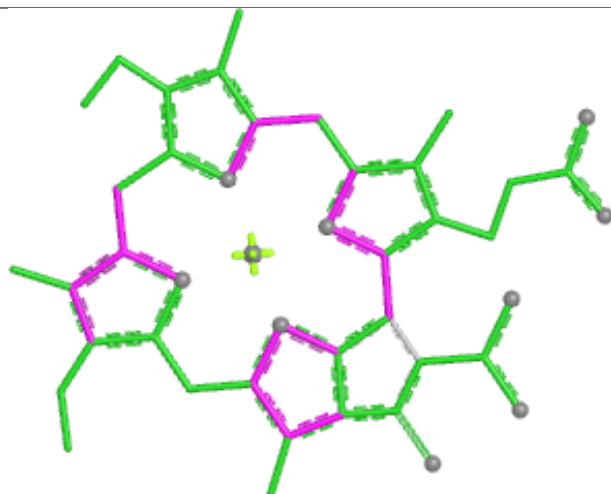




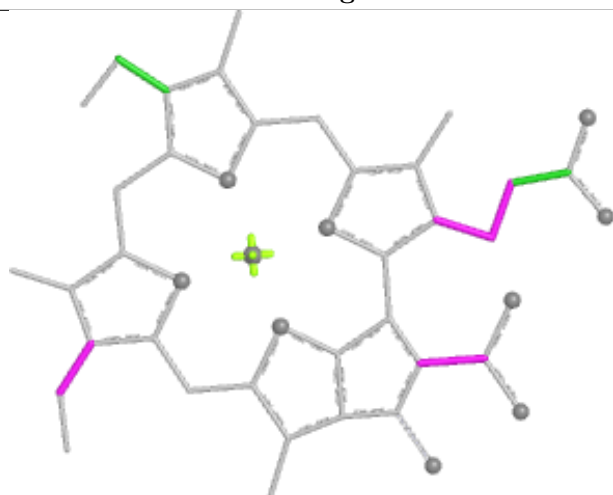
Ligand CLA 8 309



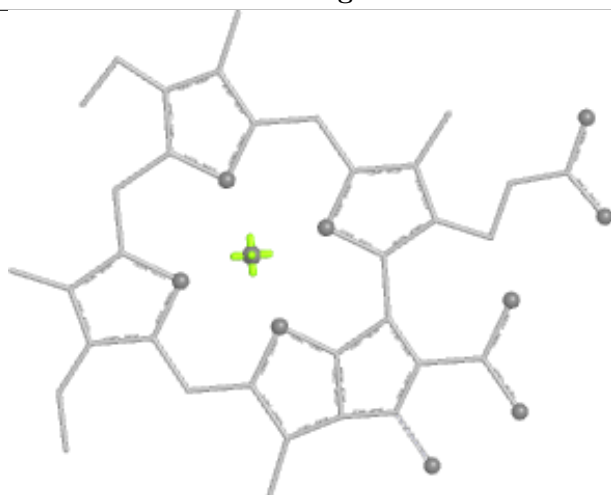
Bond lengths



Bond angles

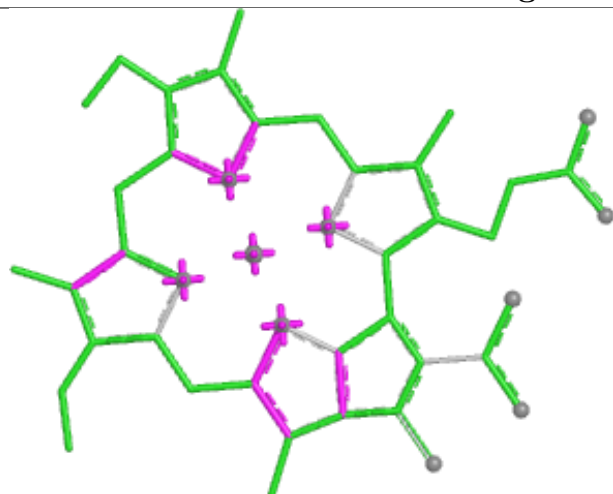


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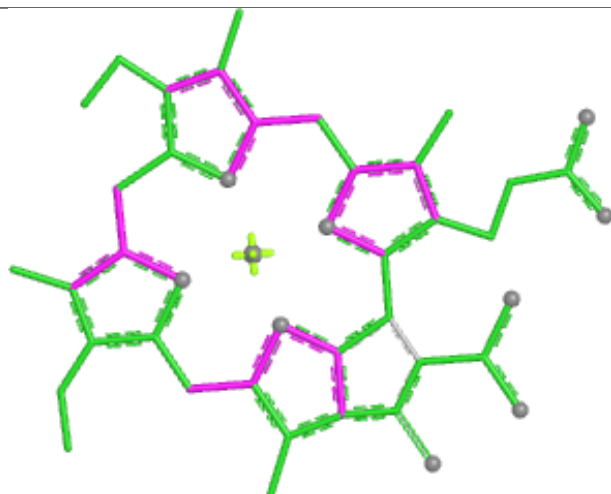


Rings

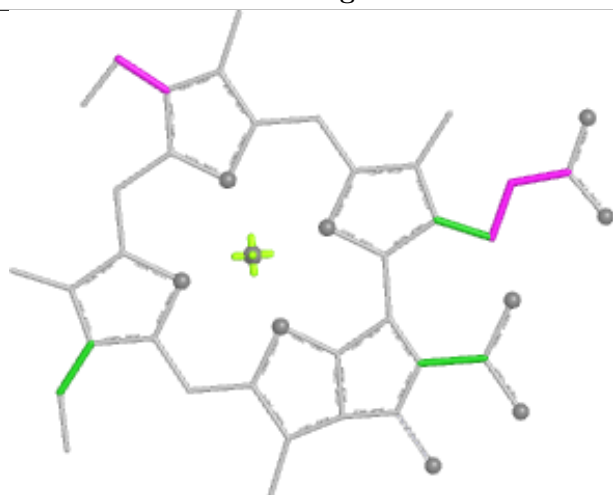
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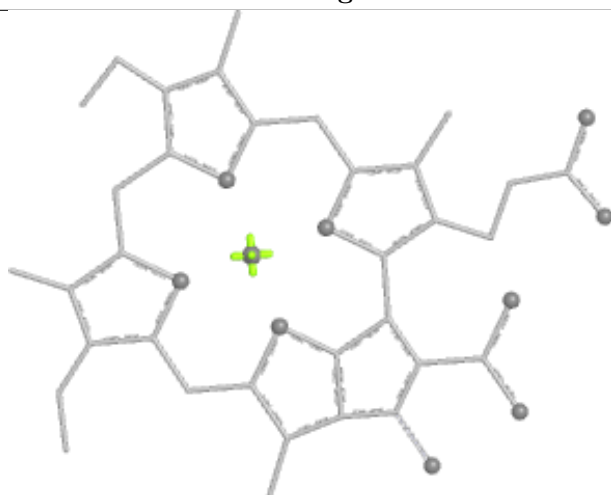
Bond lengths



Bond angles

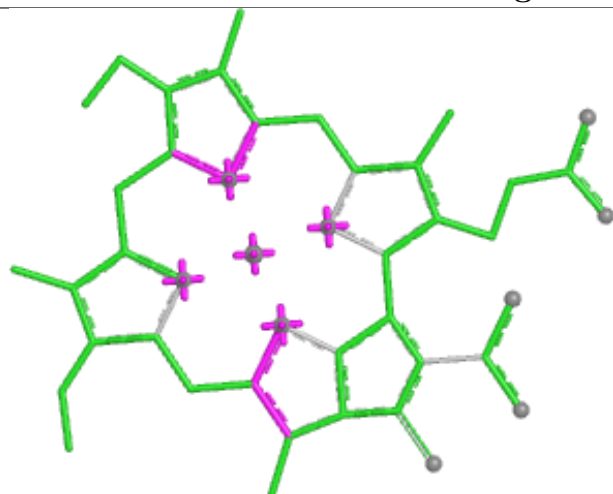


Torsions

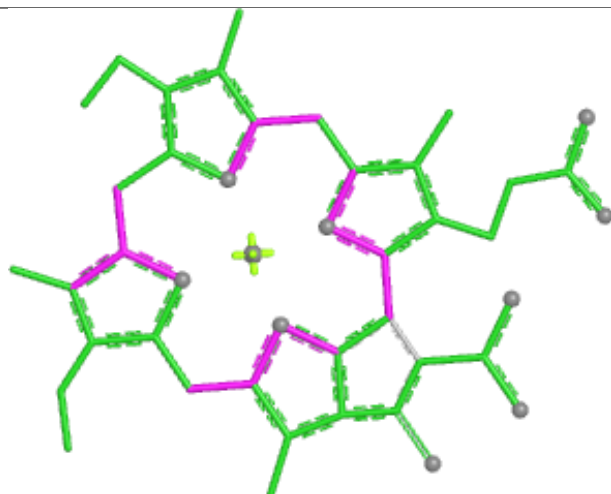


Rings

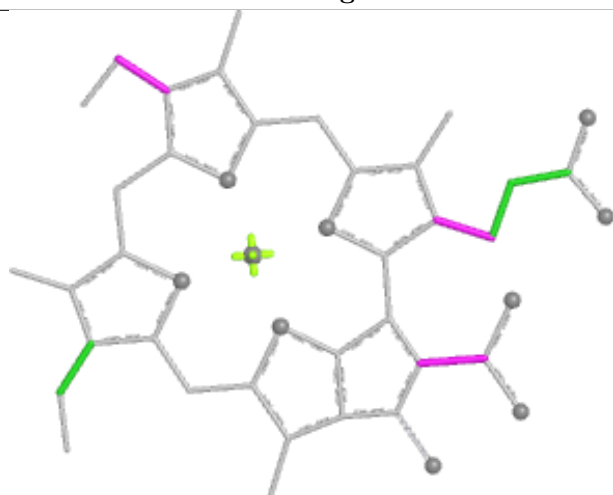
Ligand CLA B 837



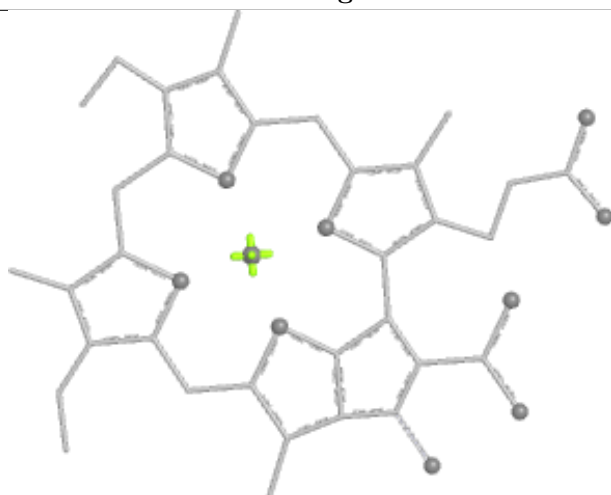
Bond lengths



Bond angles

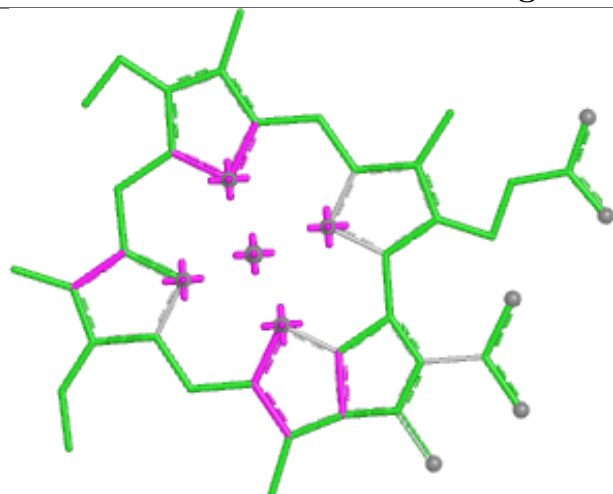


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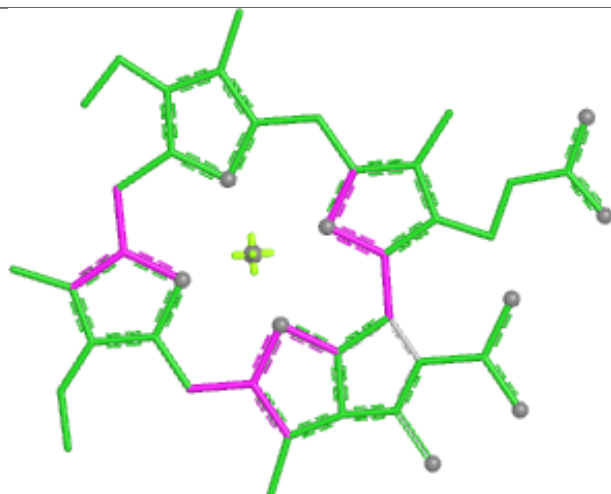


Rings

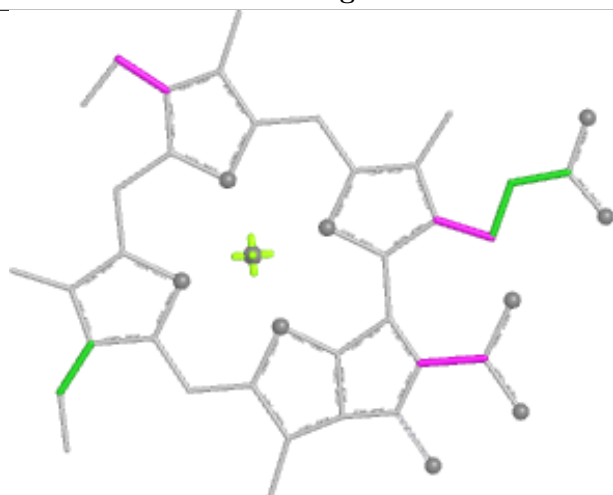
Ligand CLA 6 318



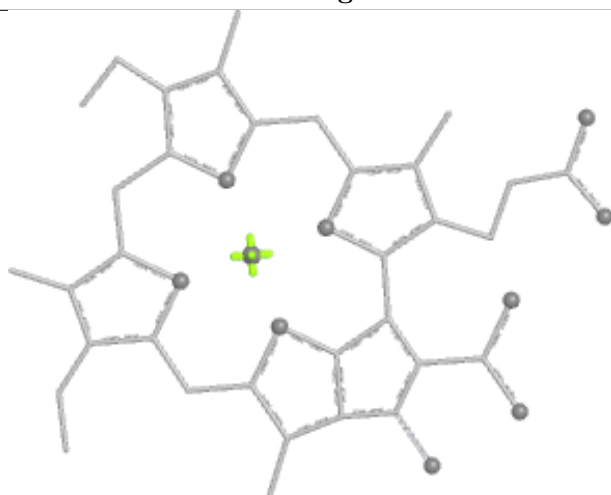
Bond lengths



Bond angles

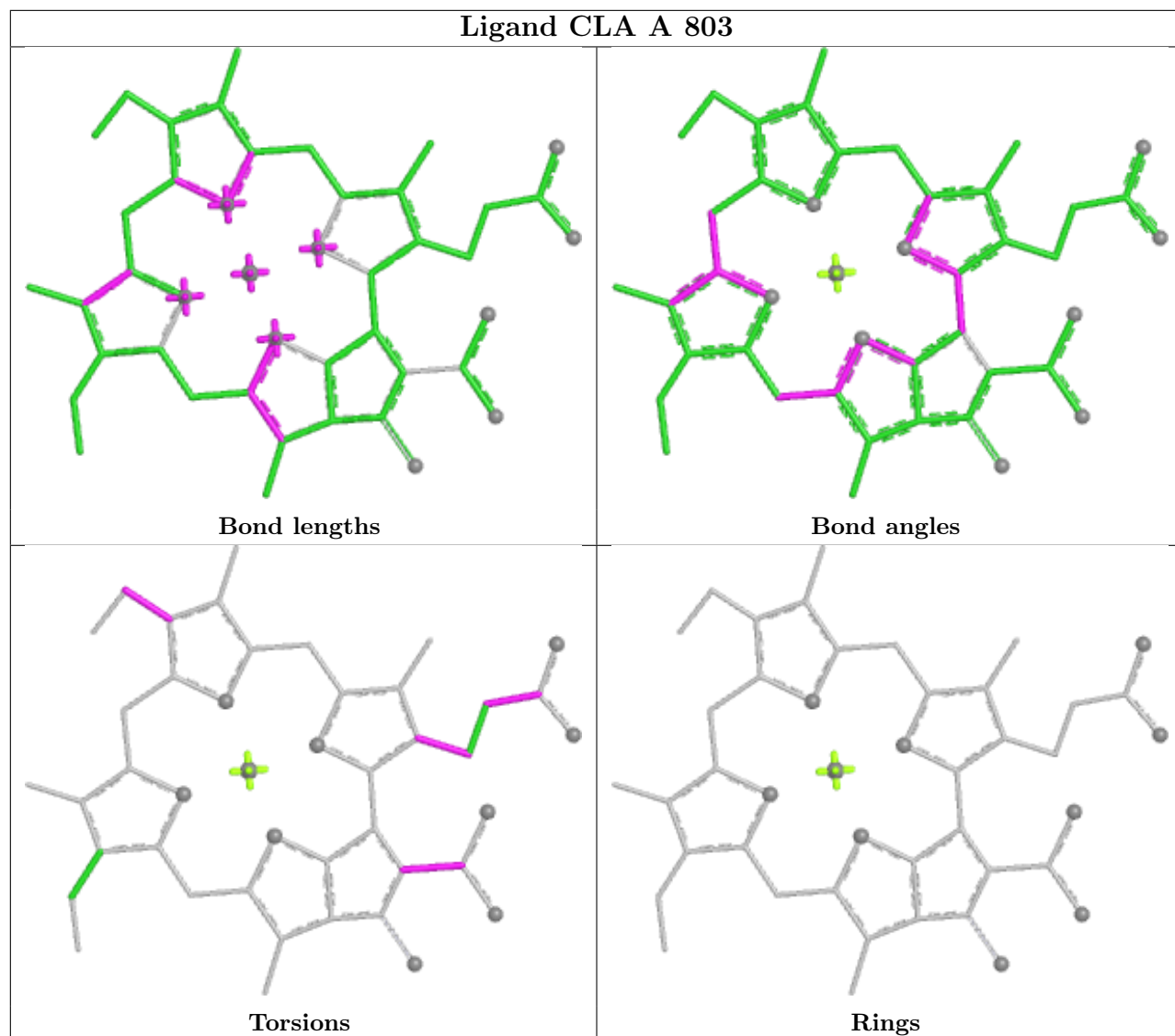


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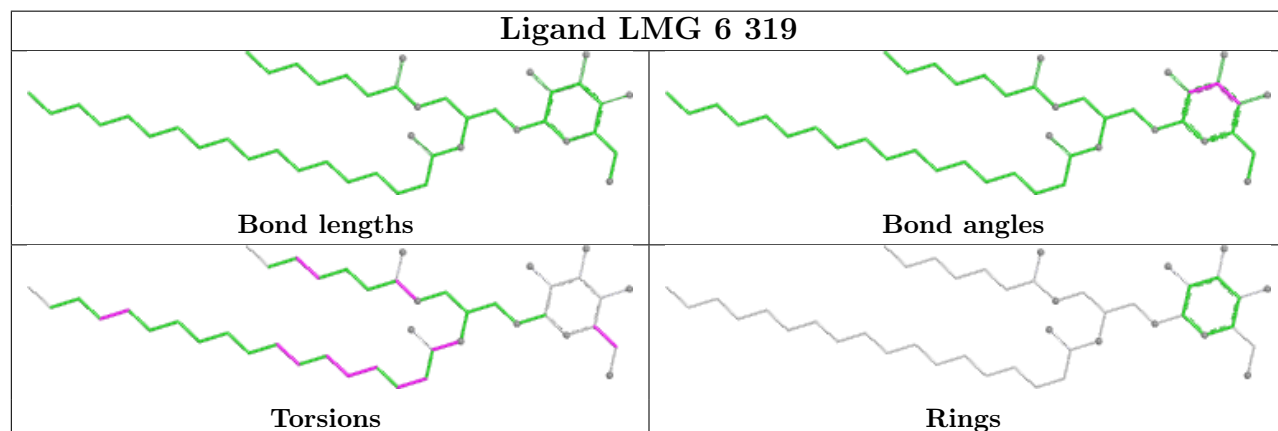


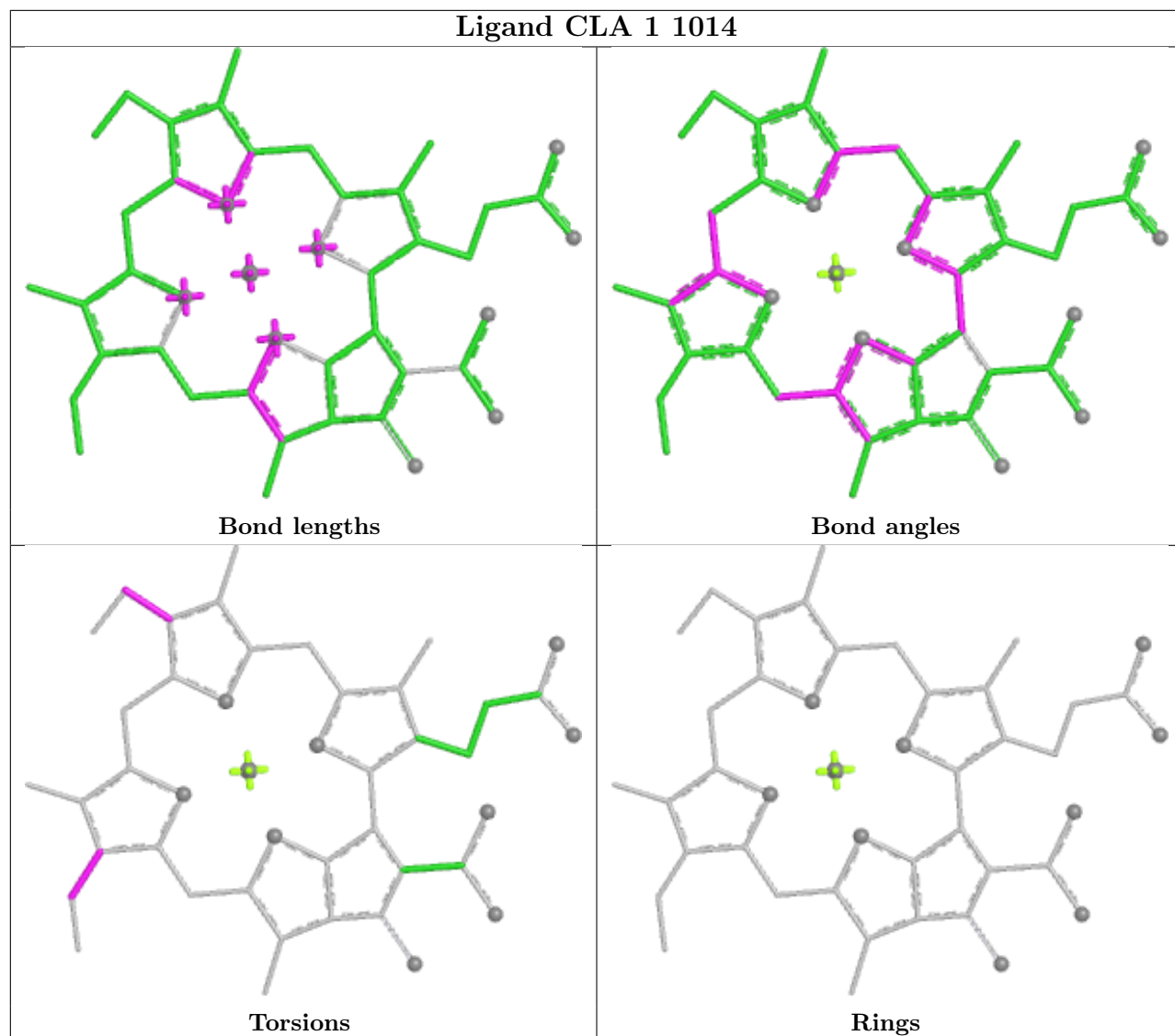
Rings

Ligand CLA A 803

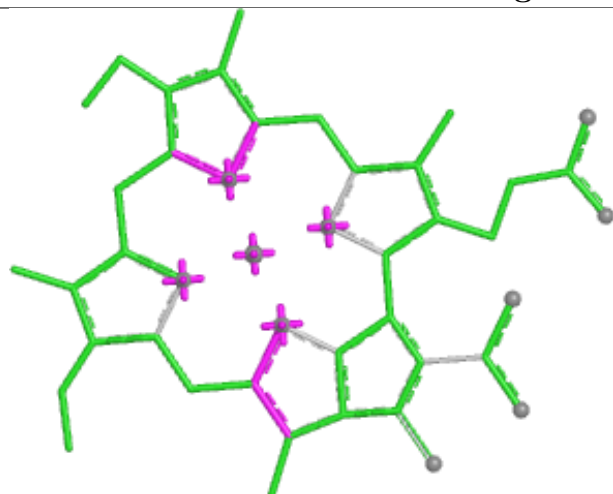


Ligand LMG 6 319

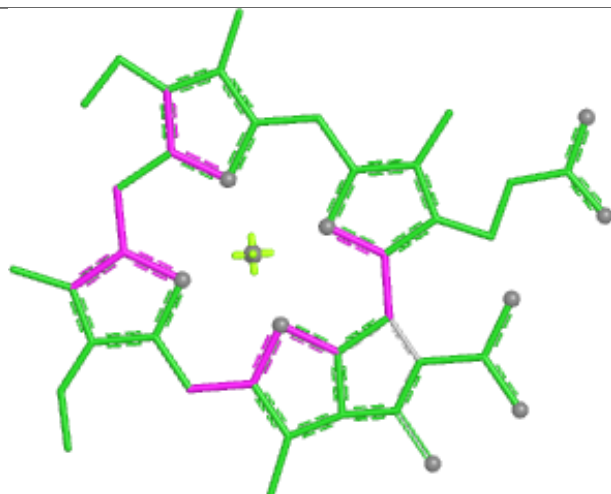




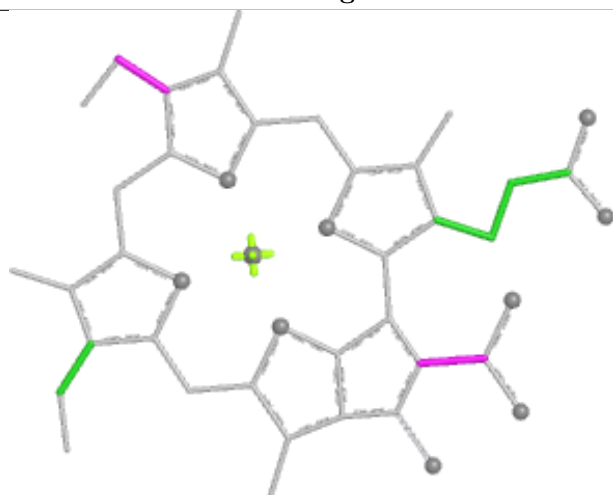
Ligand CLA B 818



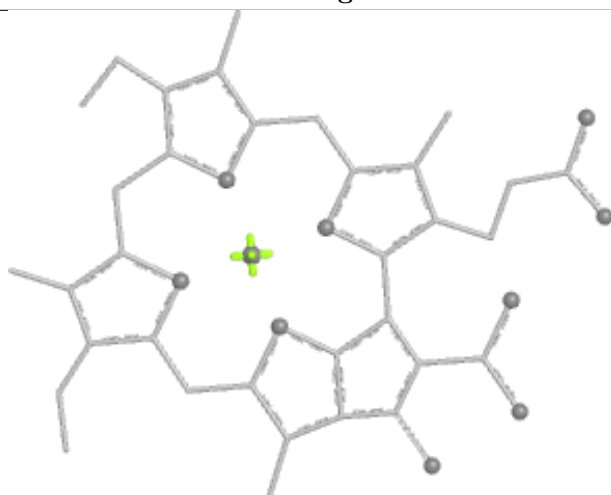
Bond lengths



Bond angles

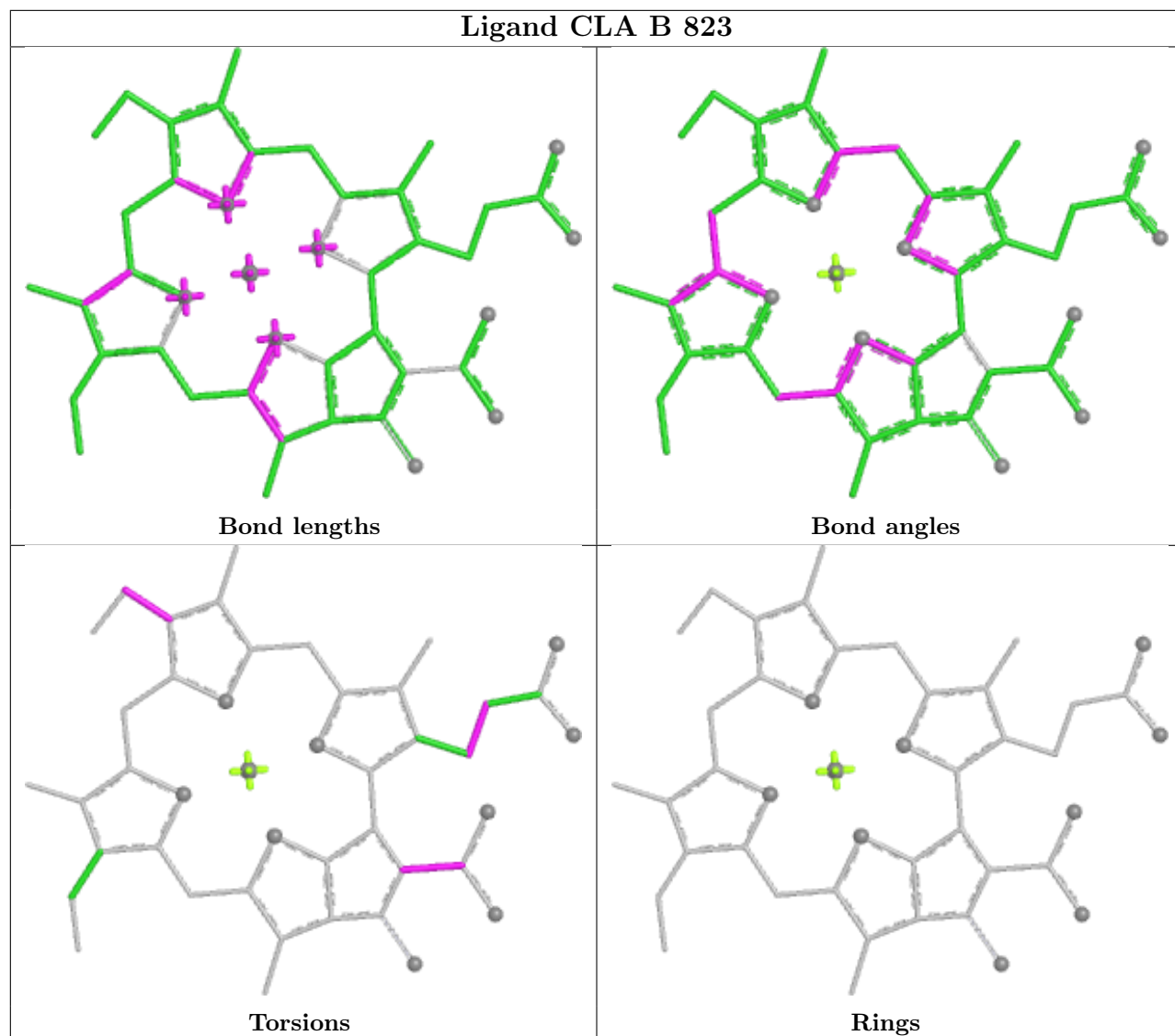


Torsions

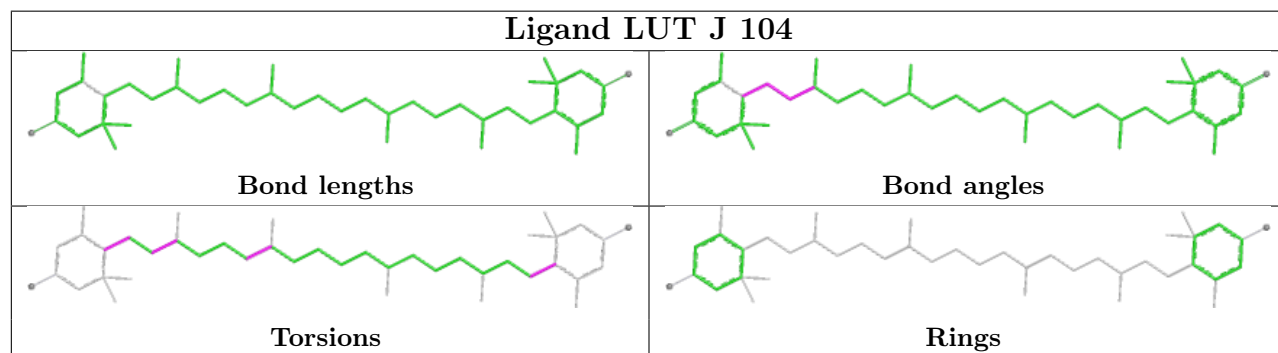


Rings

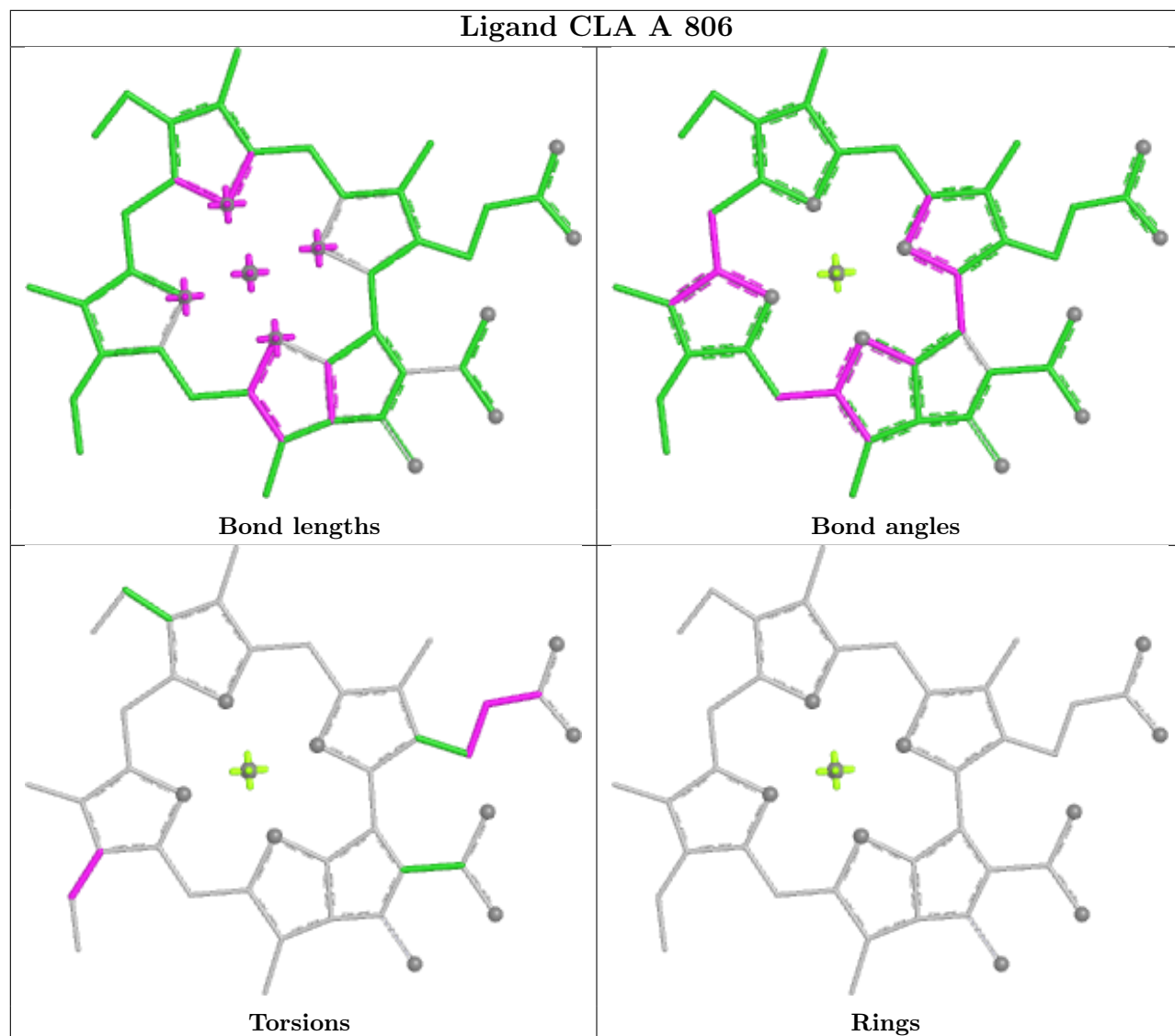
Ligand CLA B 823



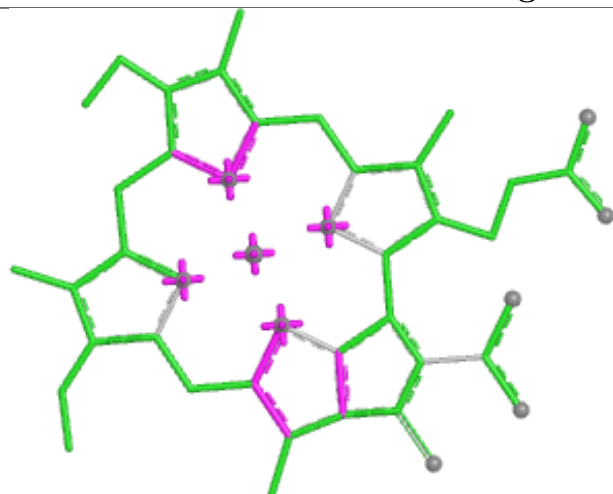
Ligand LUT J 104



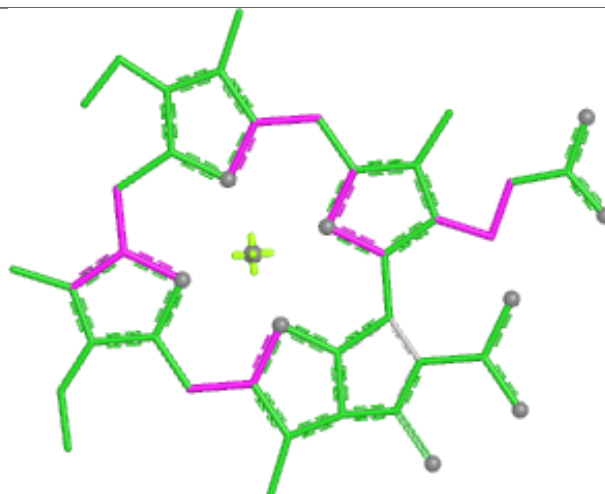
Ligand CLA A 806



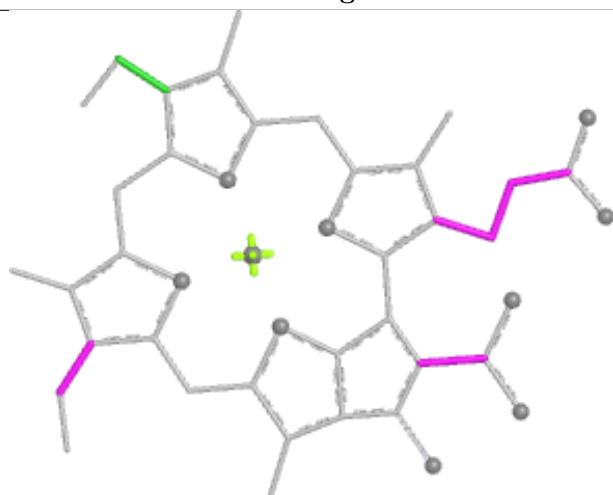
Ligand CLA 4 309



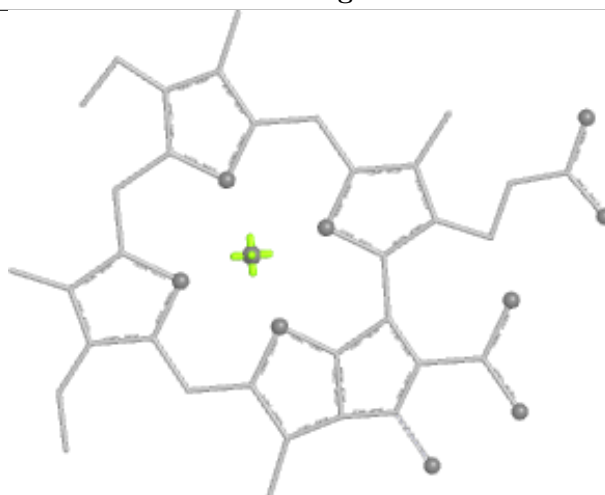
Bond lengths



Bond angles

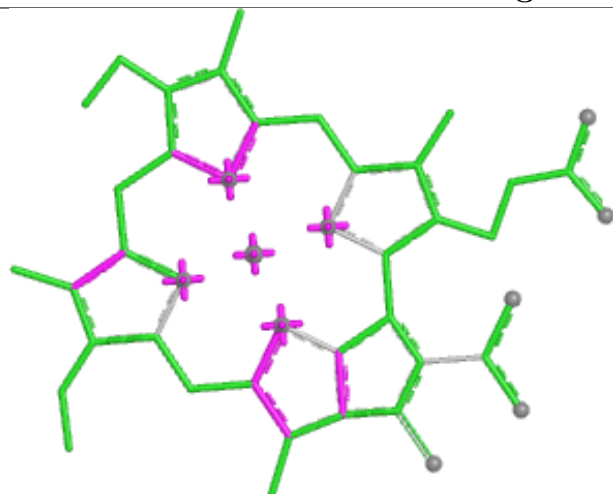


Torsions

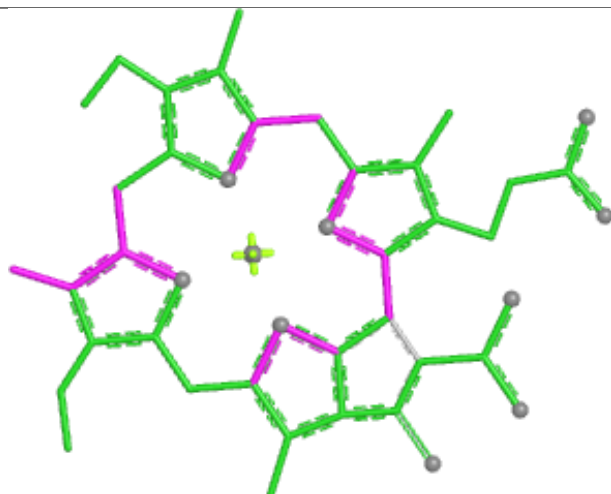


Rings

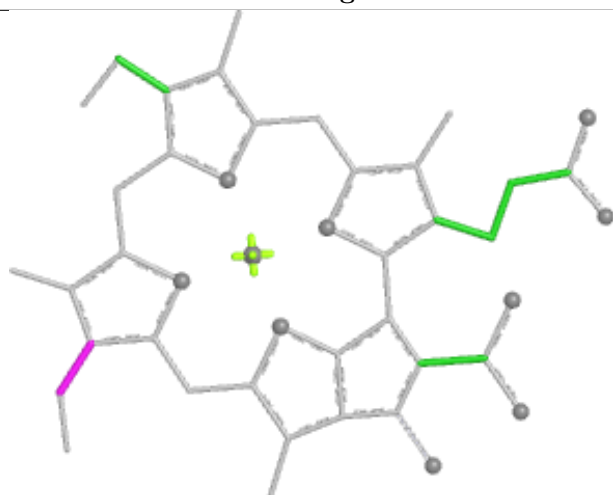
Ligand CLA F 302



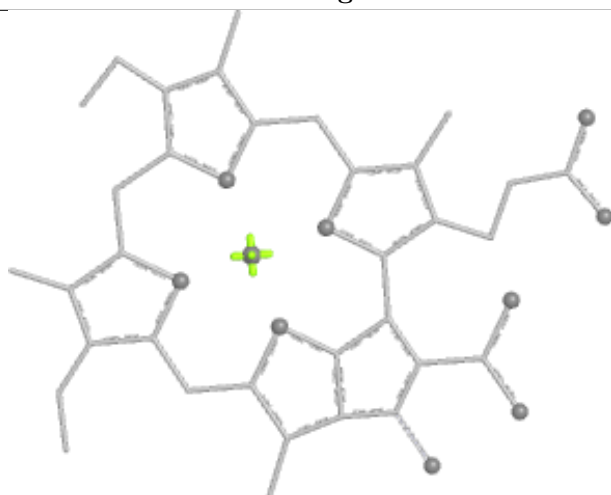
Bond lengths



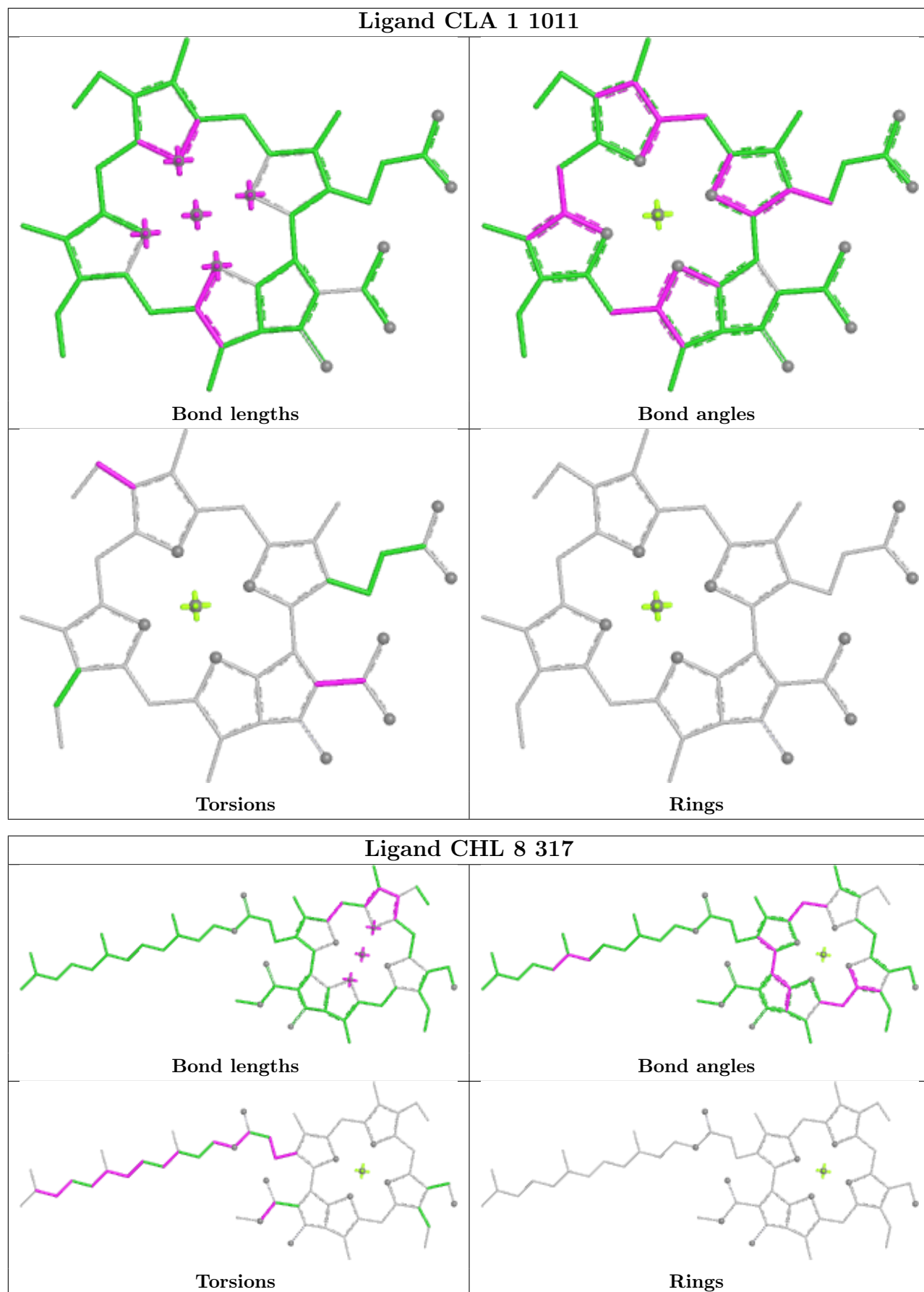
Bond angles



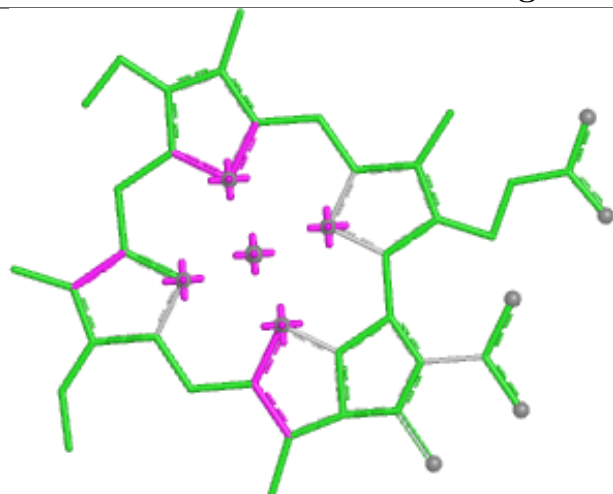
Torsions



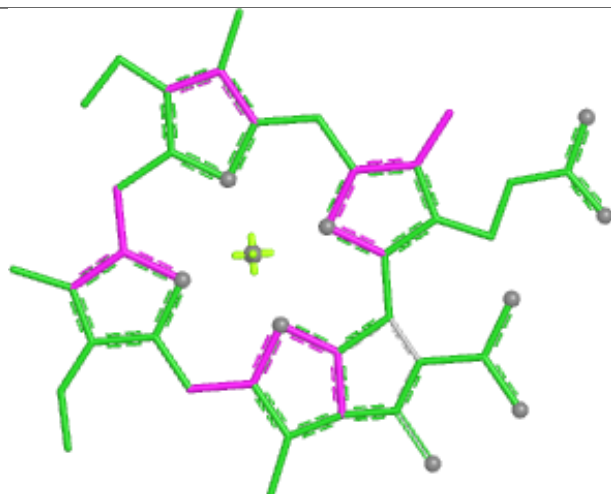
Rings



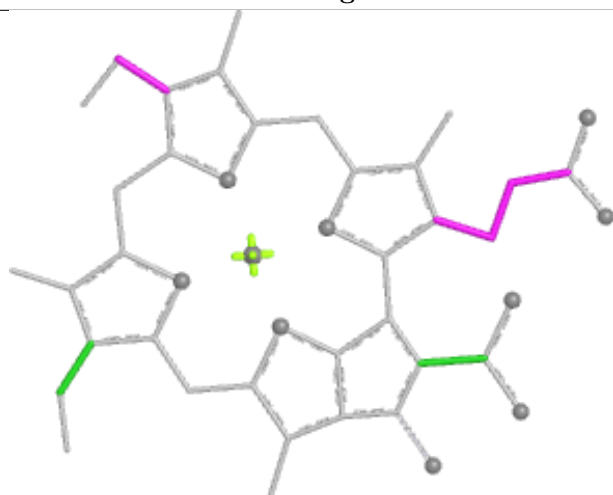
Ligand CLA 5 306



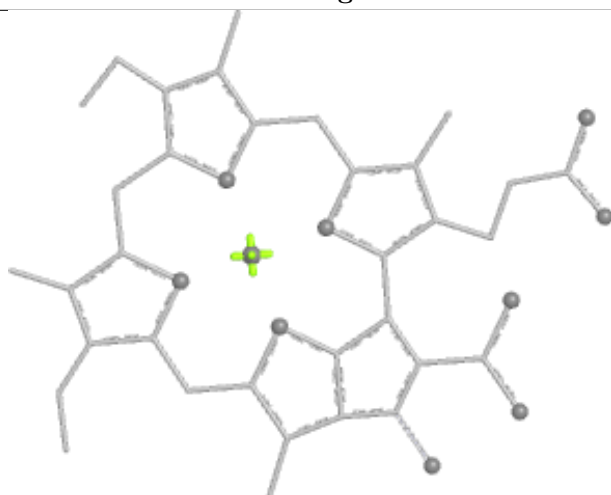
Bond lengths



Bond angles

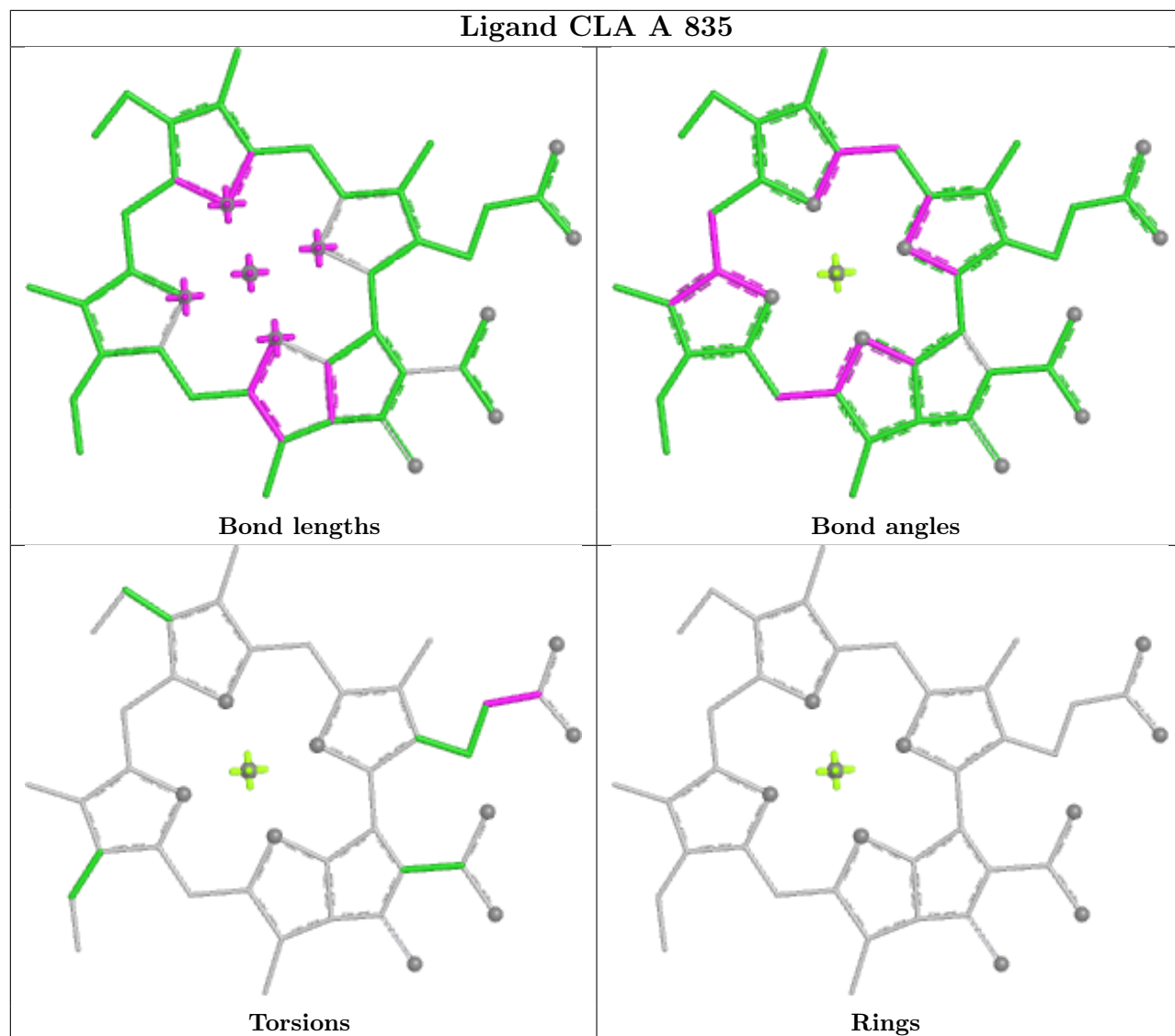


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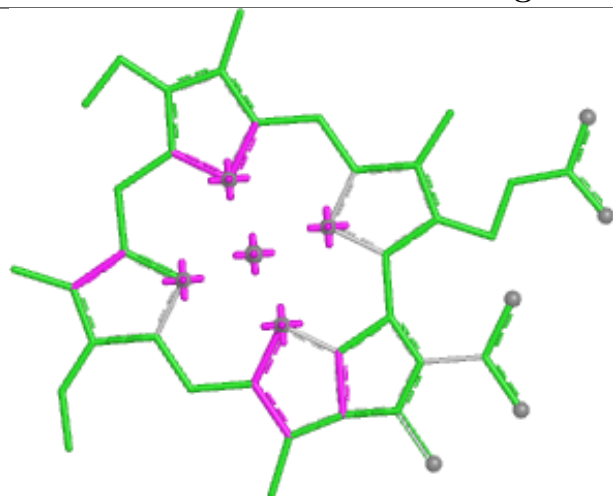


Rings

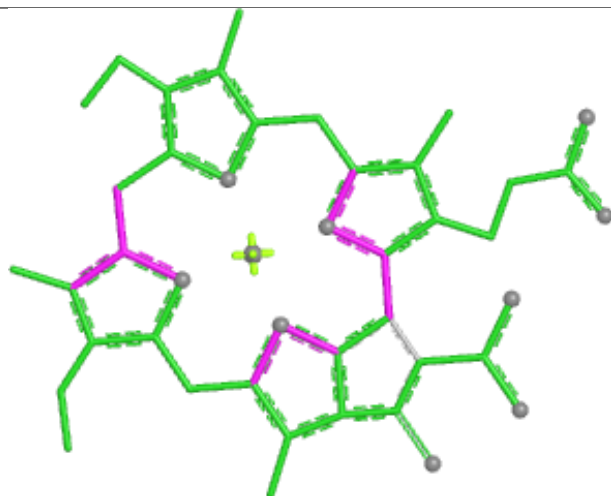
Ligand CLA A 835



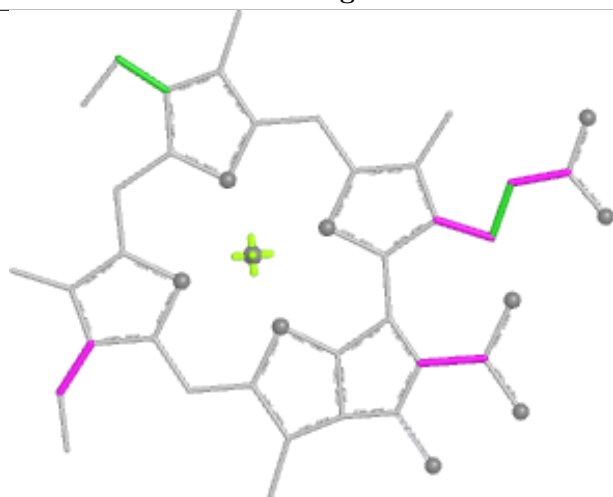
Ligand CLA B 816



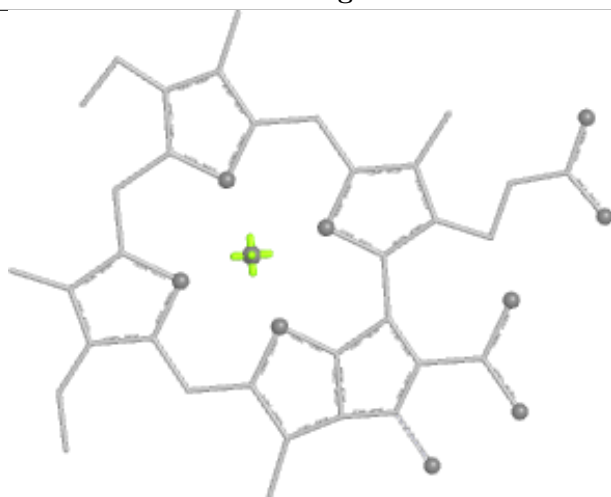
Bond lengths



Bond angles

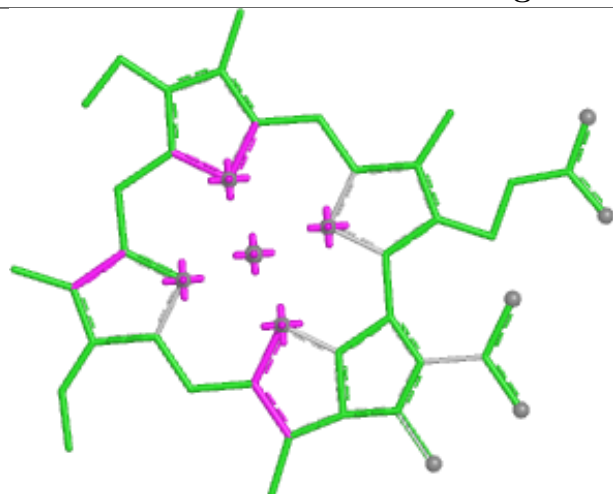


Torsions

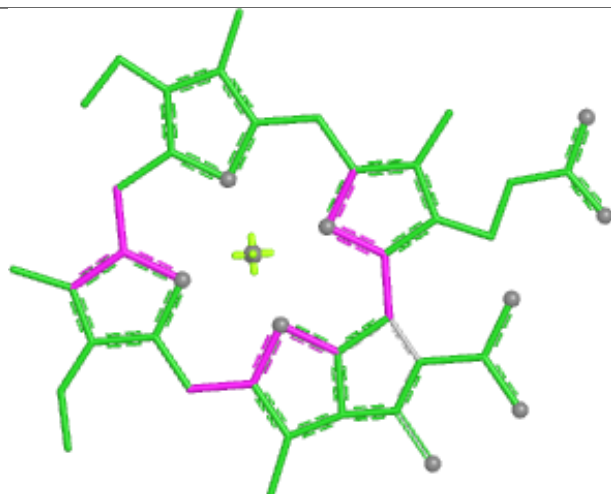


Rings

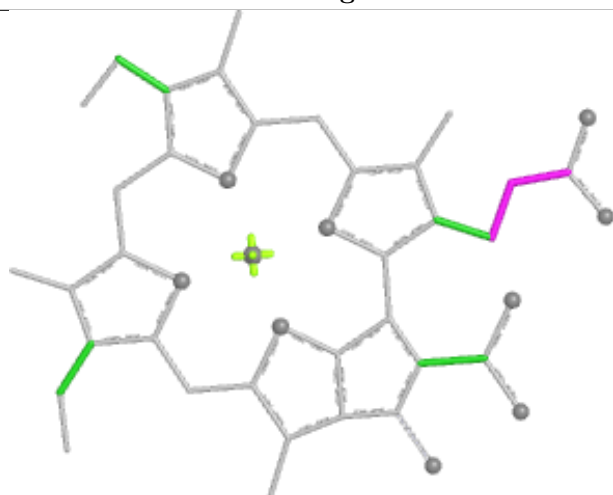
Ligand CLA A 830



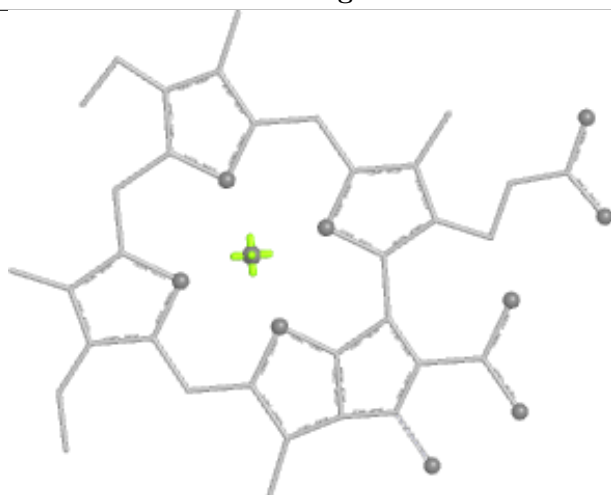
Bond lengths



Bond angles

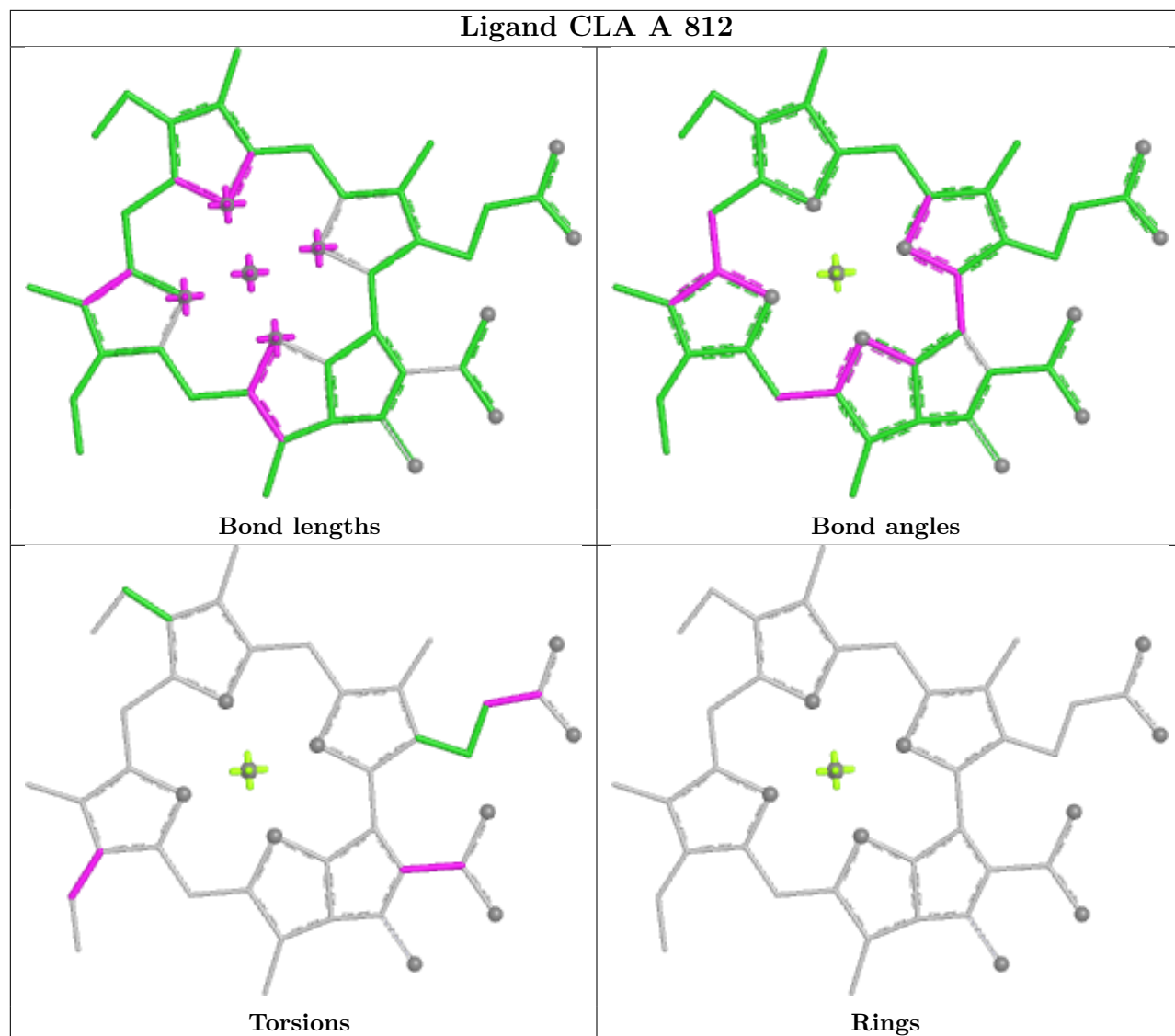


Torsions

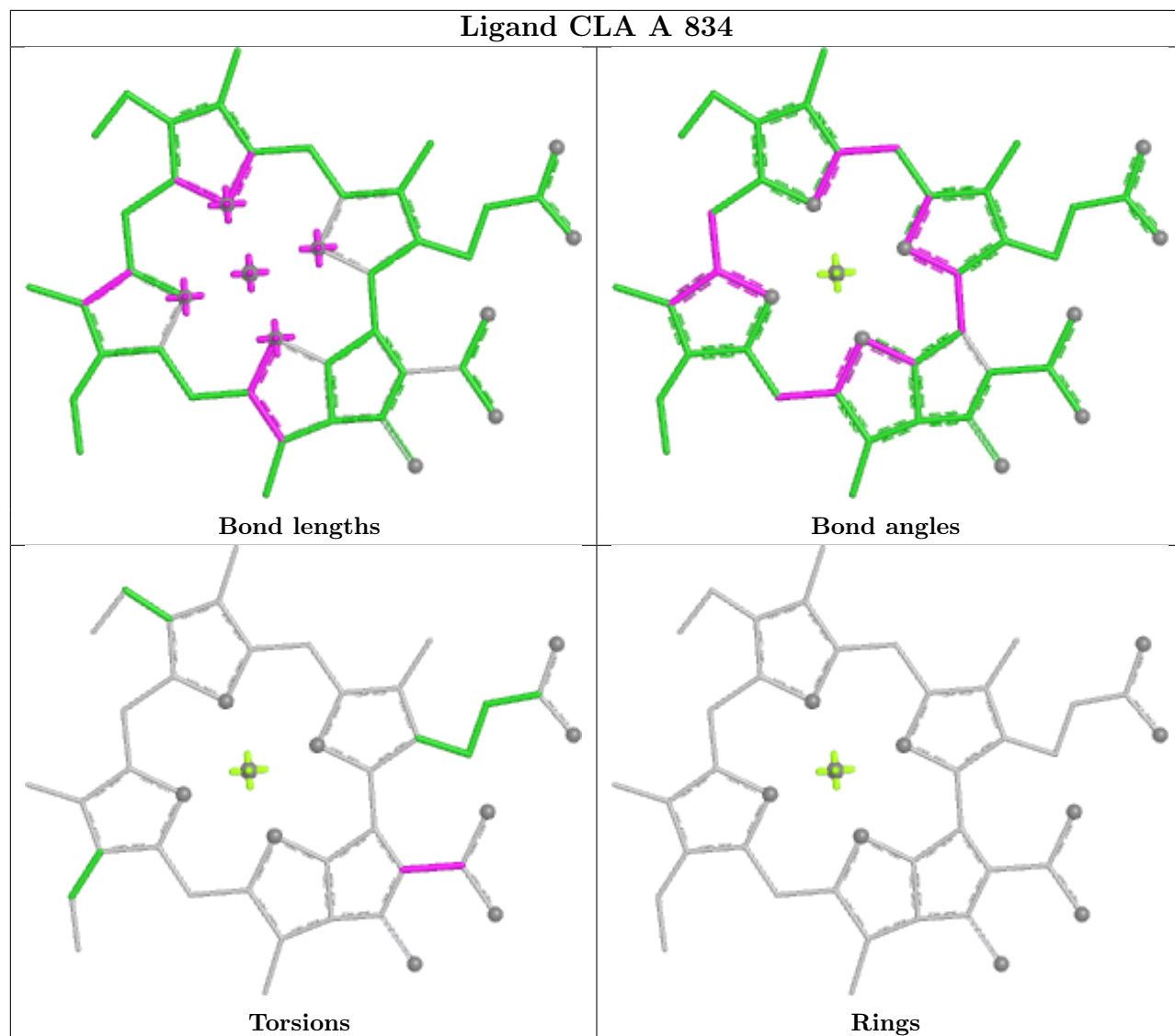


Rings

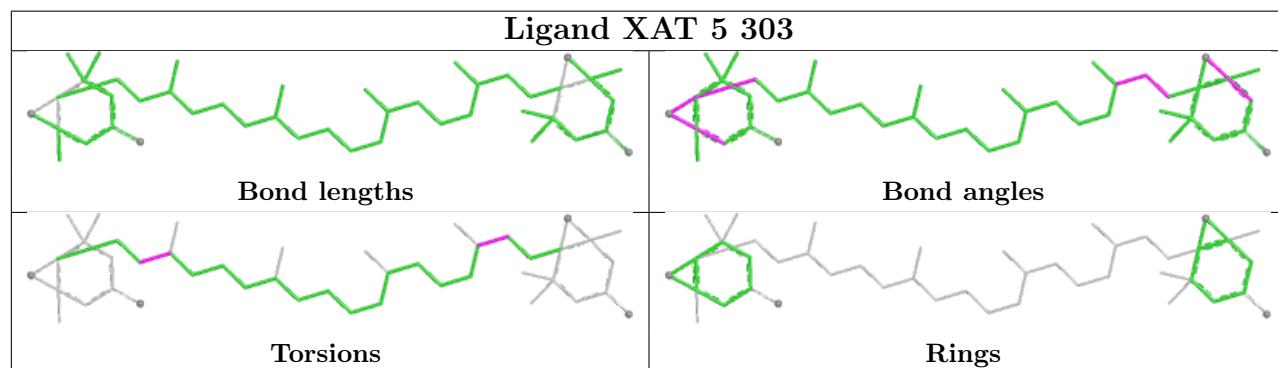
Ligand CLA A 812



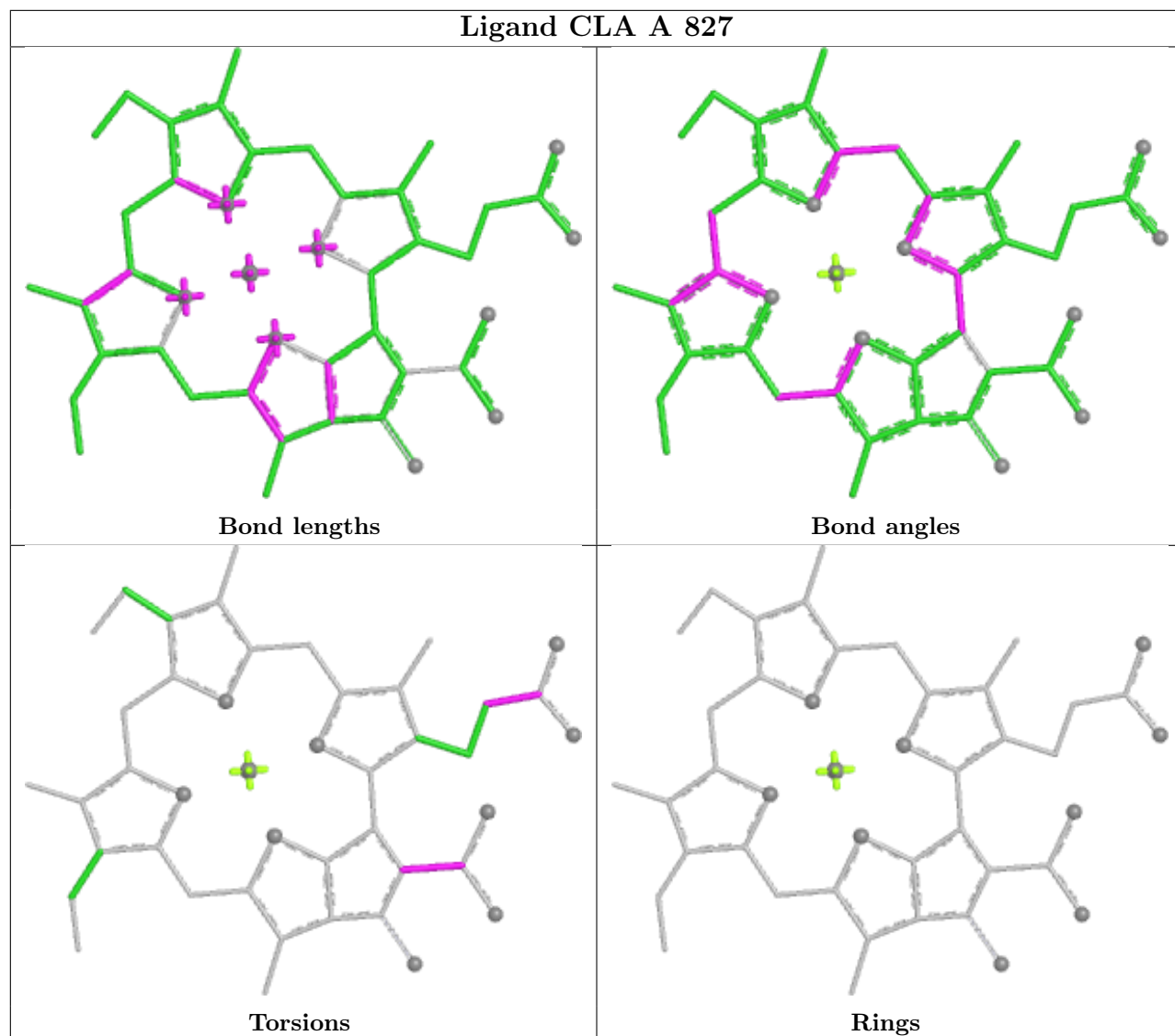
Ligand CLA A 834



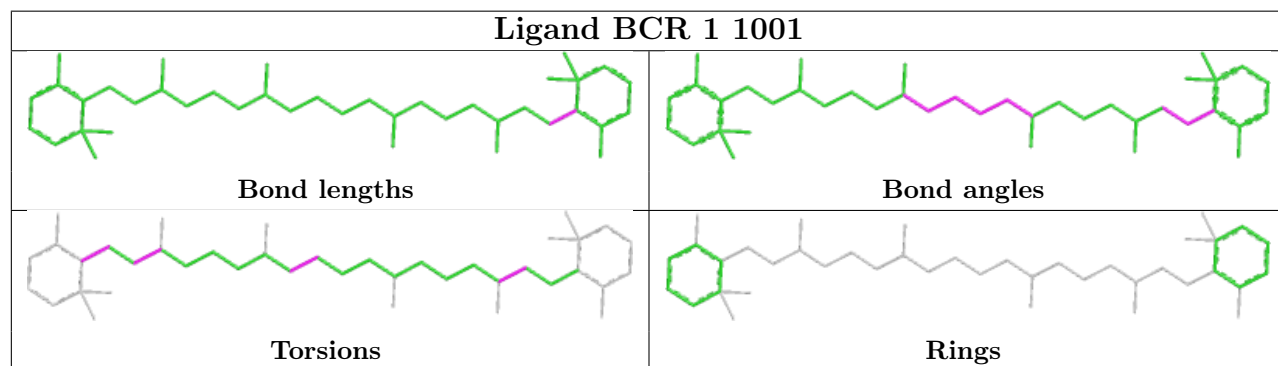
Ligand XAT 5 303



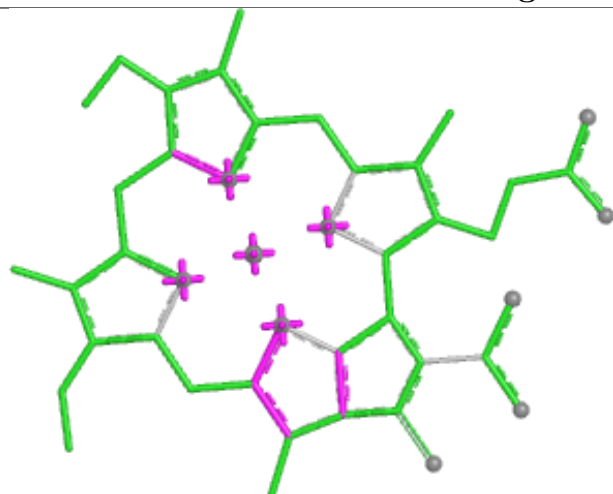
Ligand CLA A 827



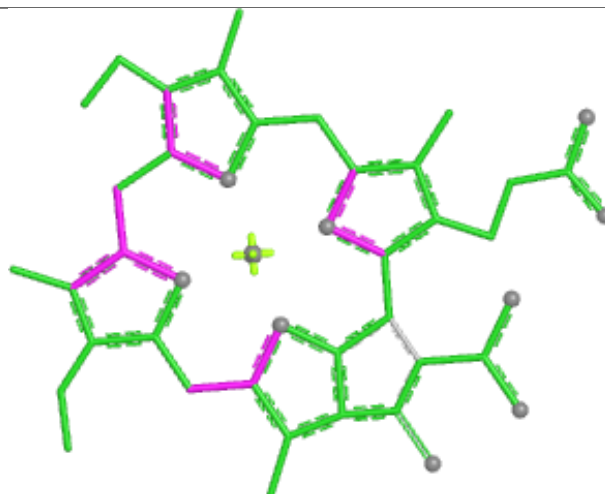
Ligand BCR 1 1001



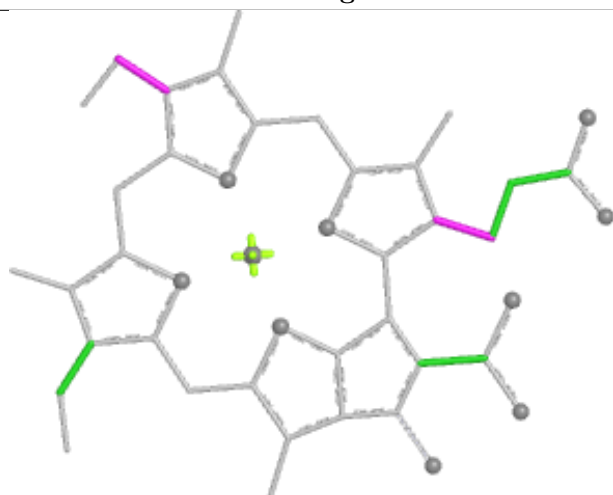
Ligand CLA 8 316



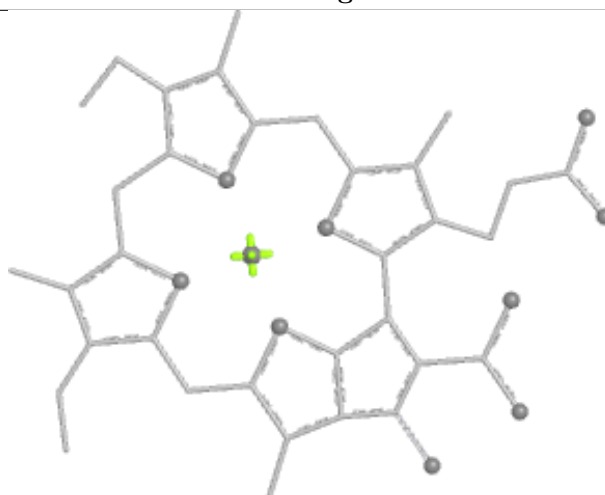
Bond lengths



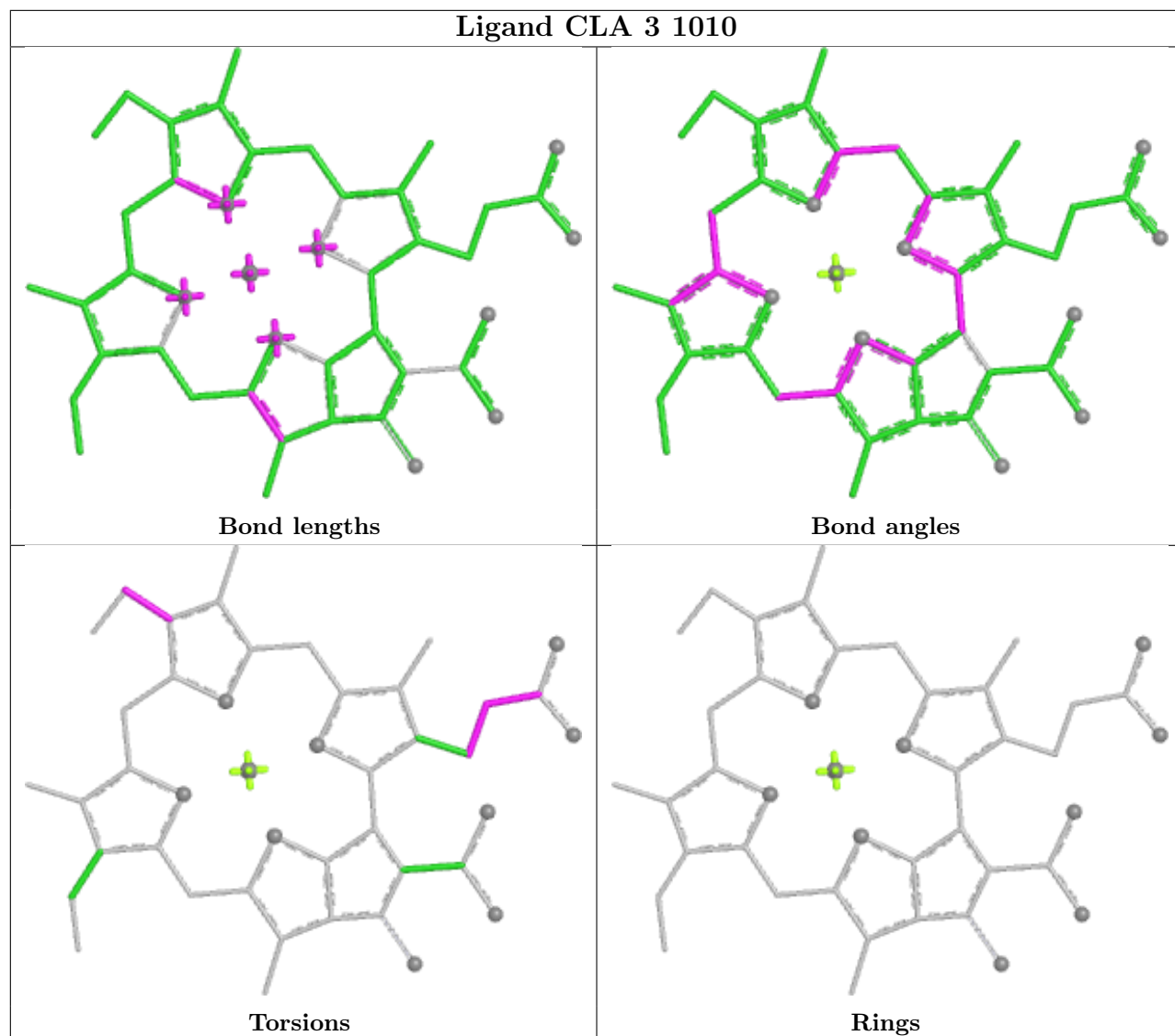
Bond angles



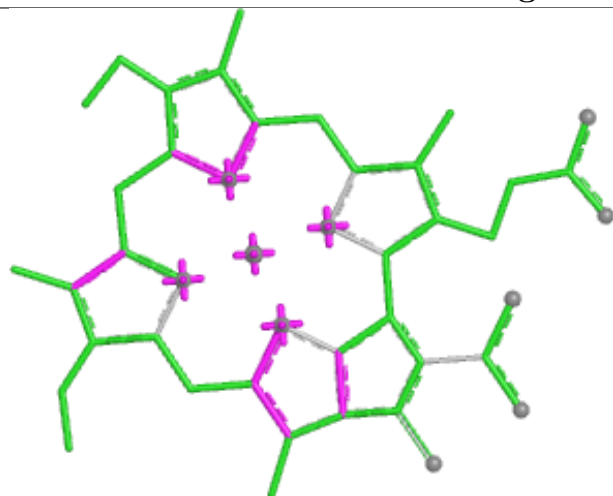
Torsions



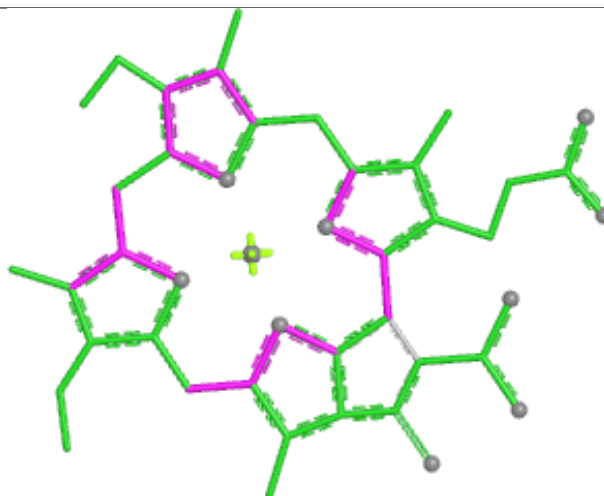
Rings



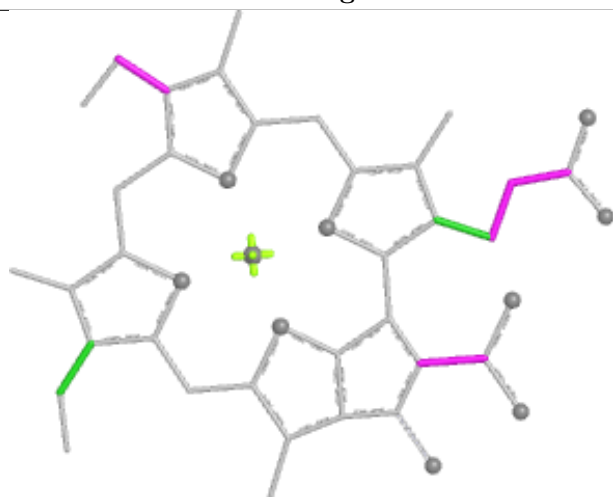
Ligand CLA 6 301



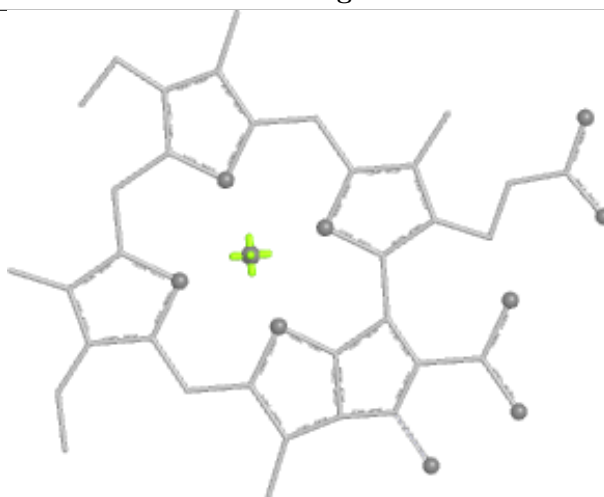
Bond lengths



Bond angles

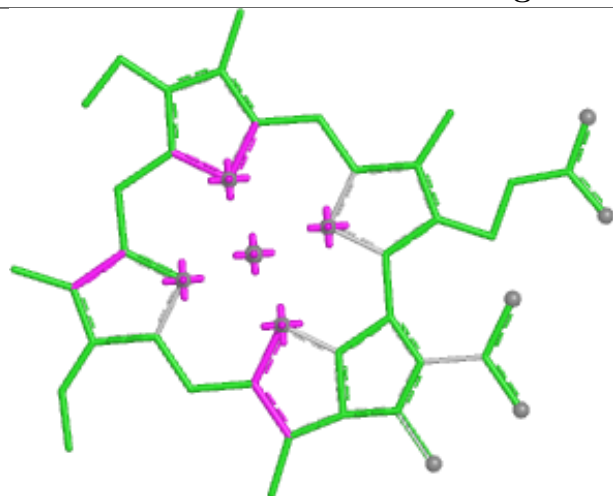


Torsions

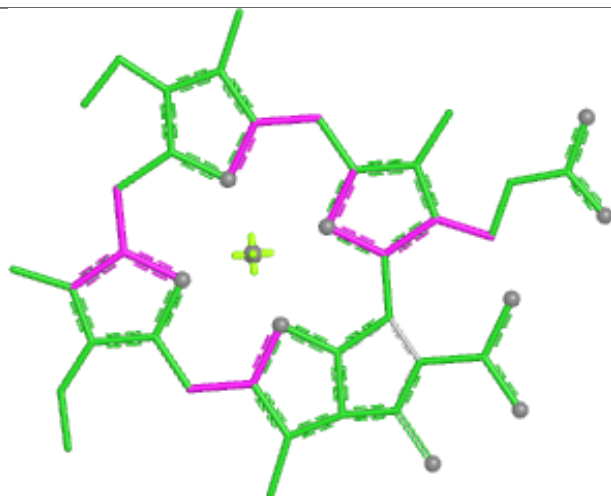


Rings

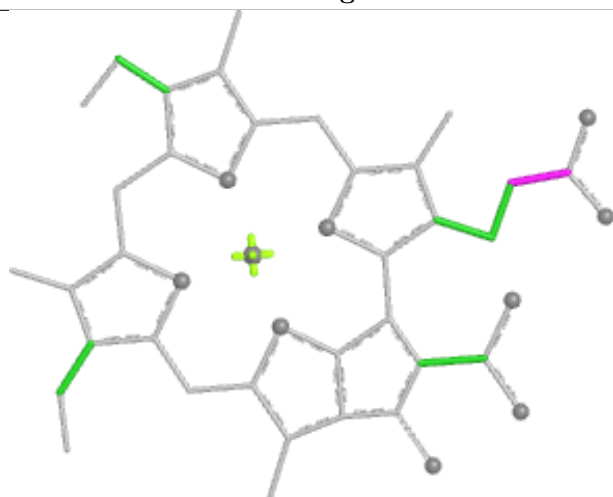
Ligand CLA A 851



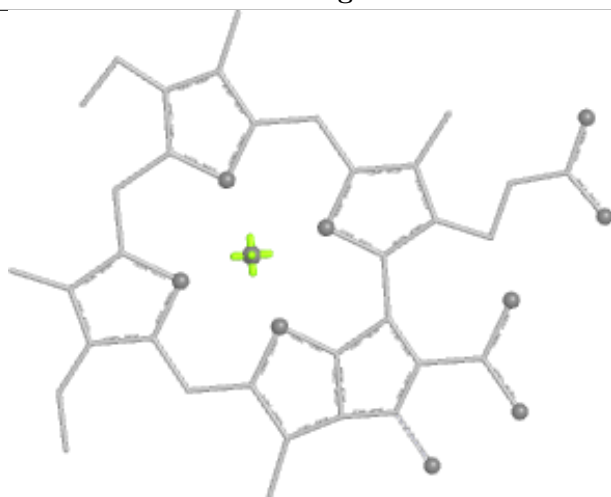
Bond lengths



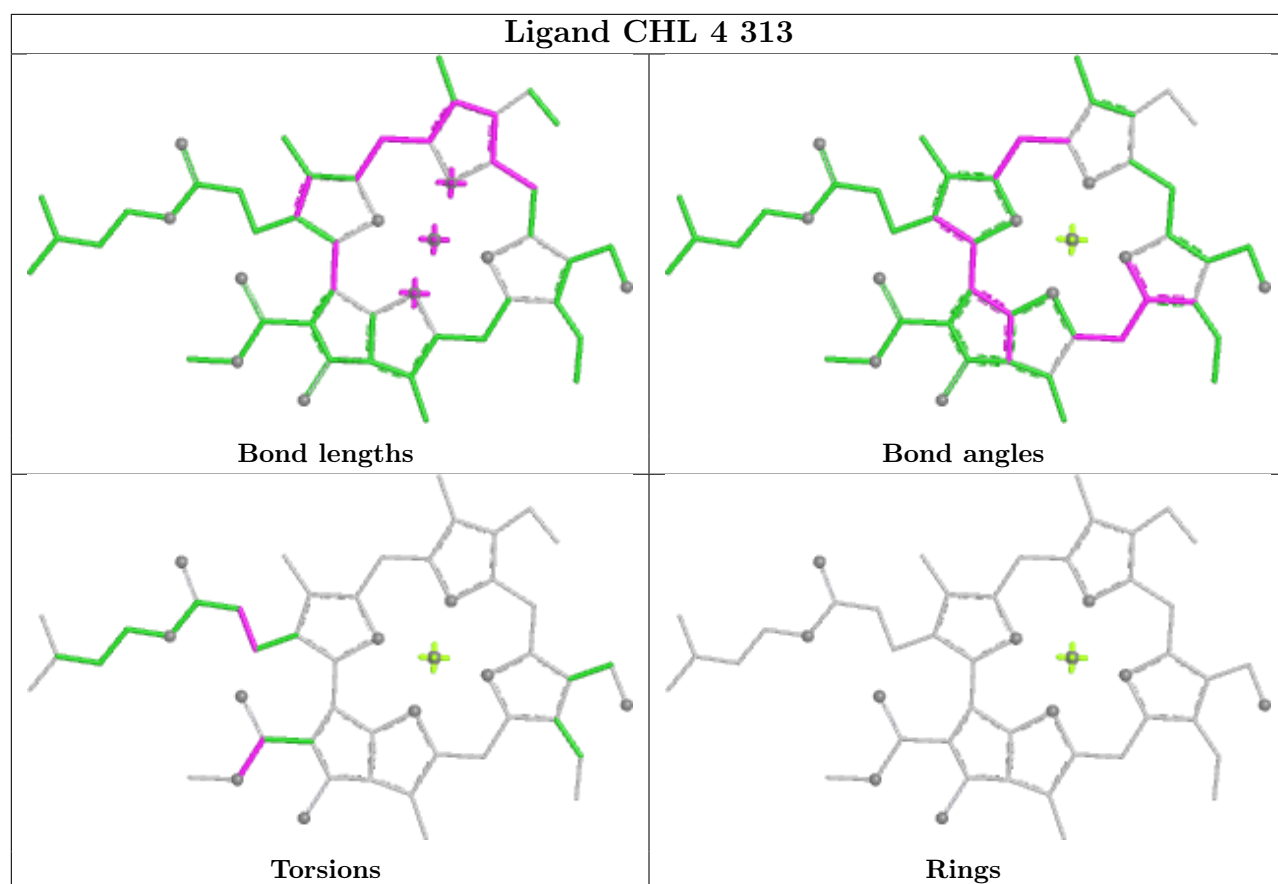
Bond angles



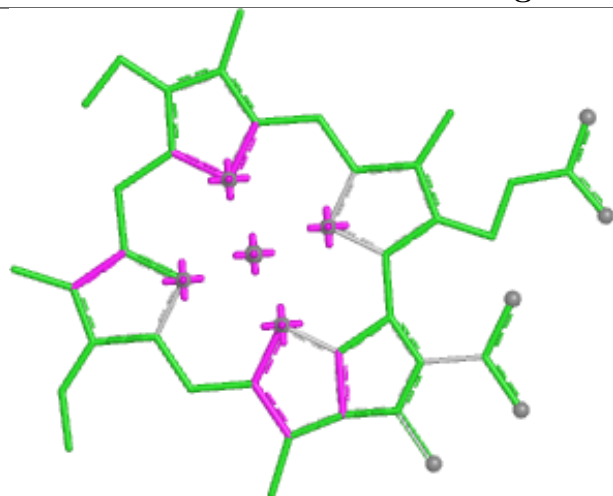
Torsions



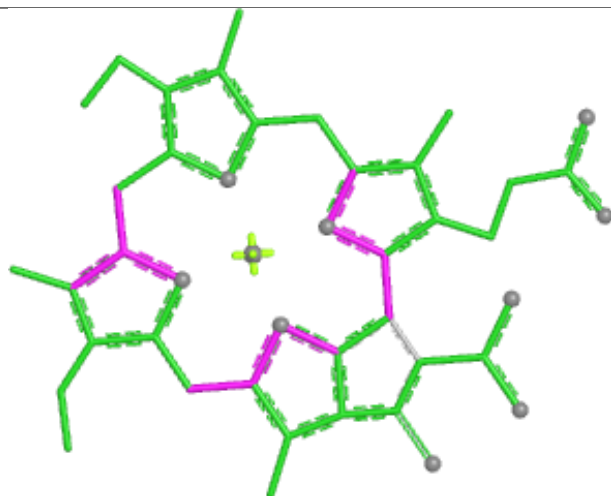
Rings



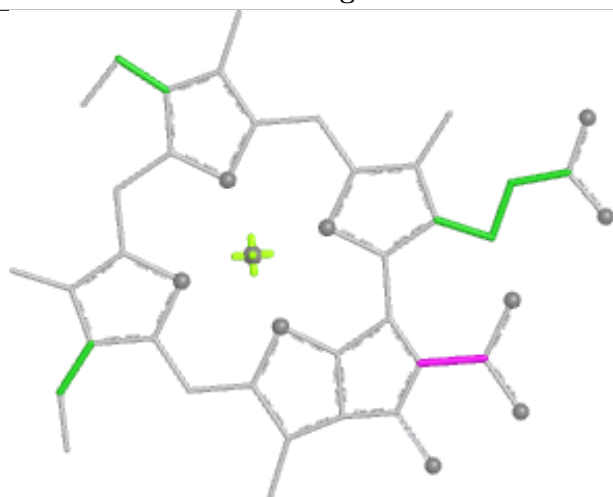
Ligand CLA B 832



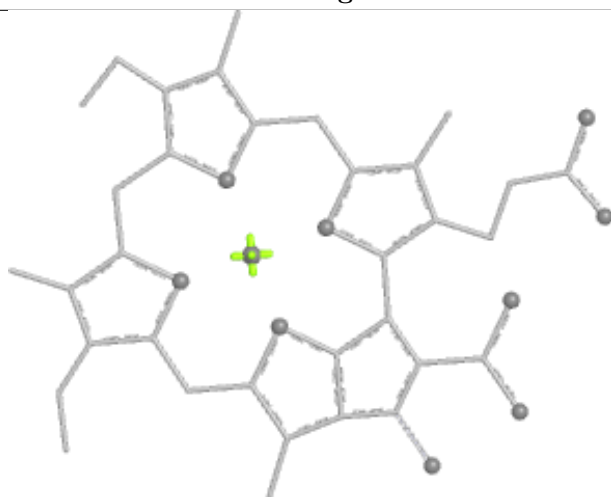
Bond lengths



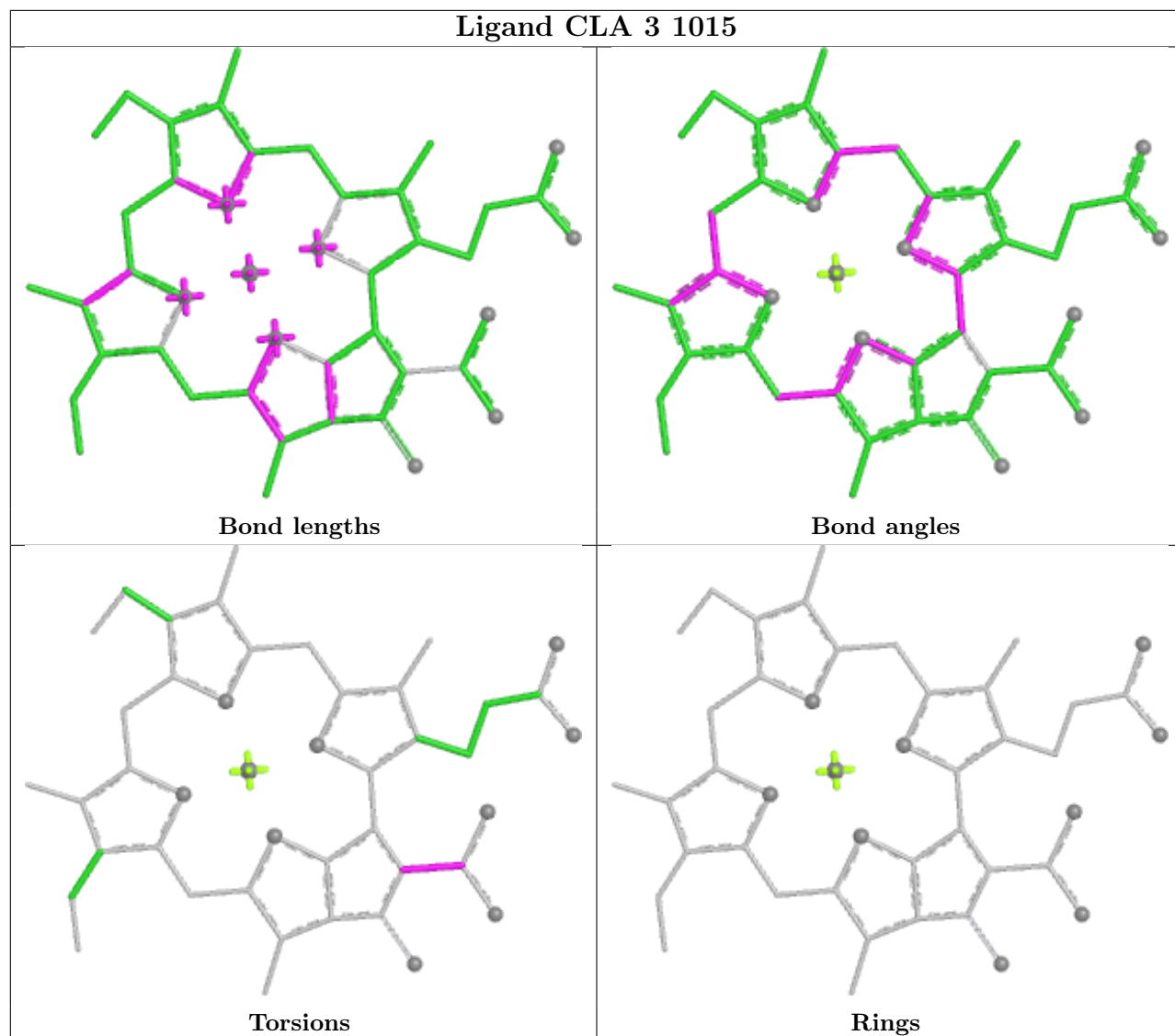
Bond angles

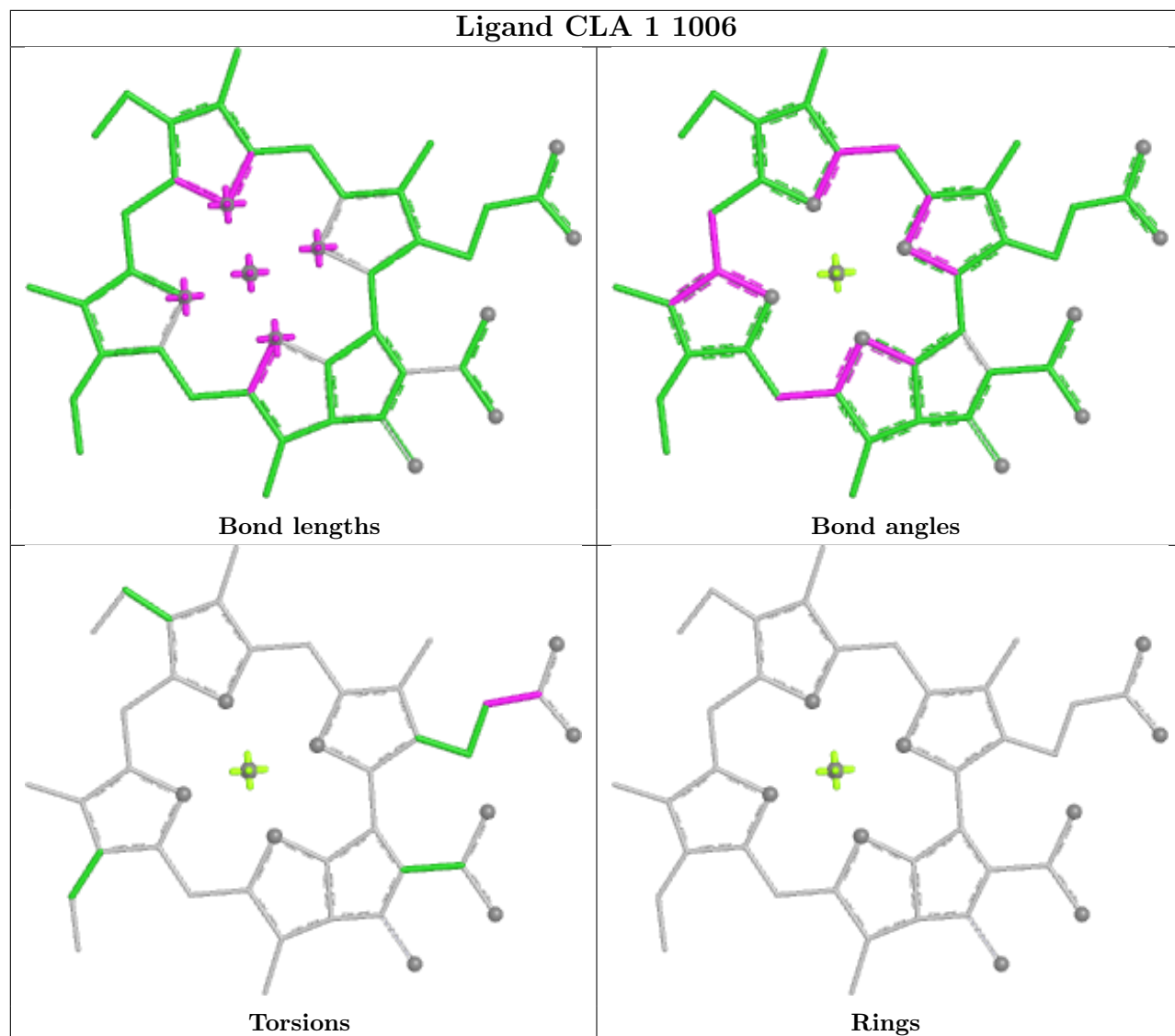


Torsions

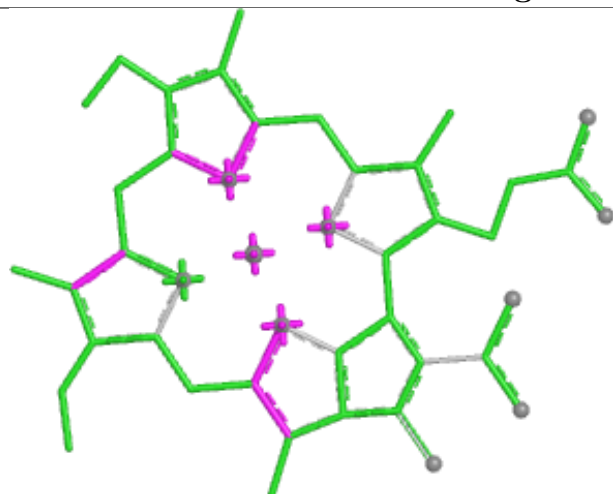


Rings

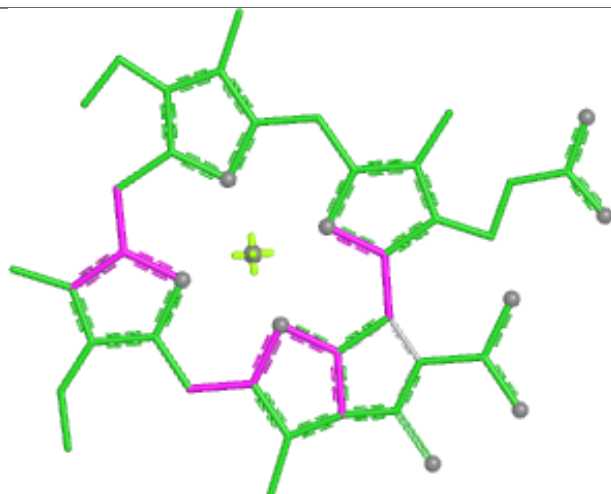




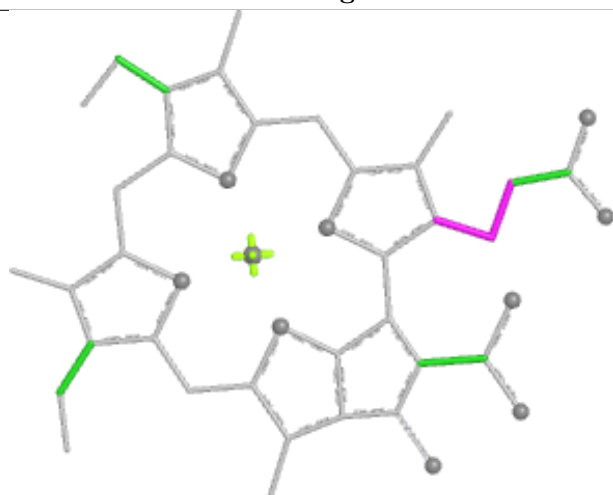
Ligand CLA B 830



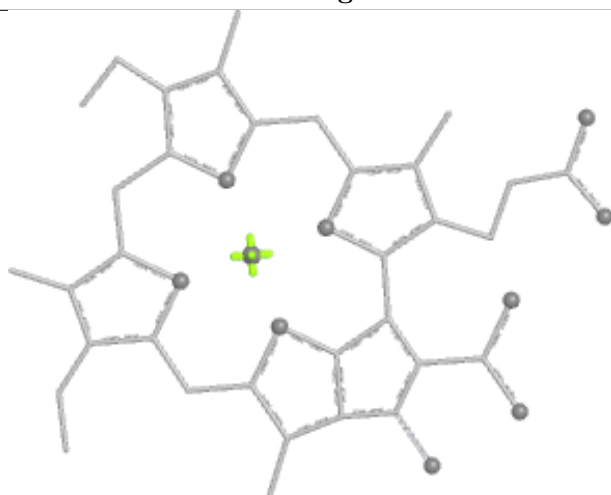
Bond lengths



Bond angles

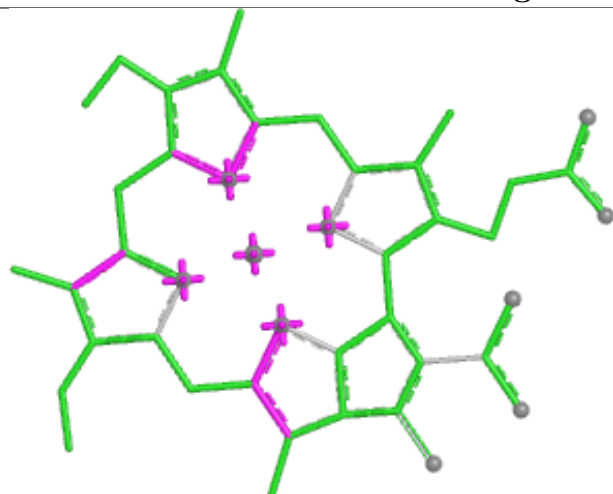


Torsions

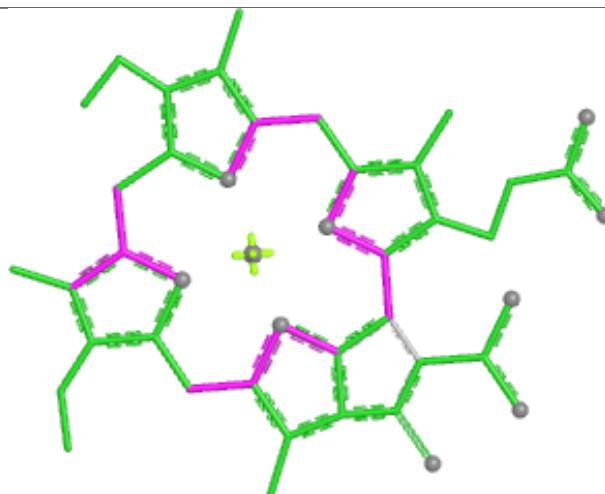


Rings

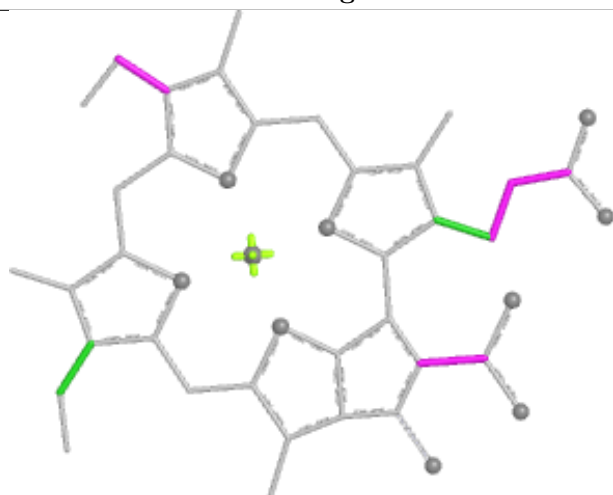
Ligand CLA A 819



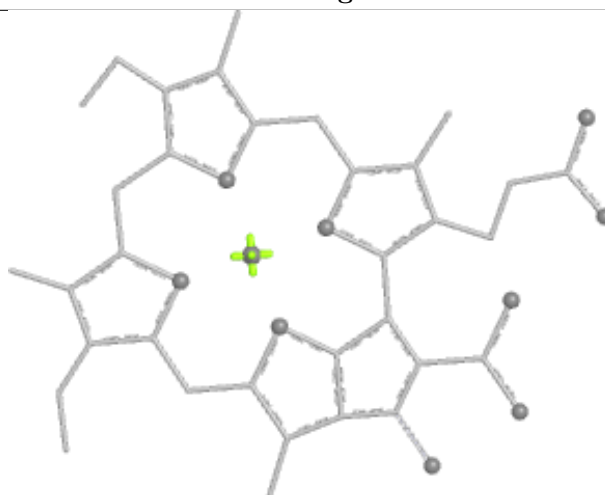
Bond lengths



Bond angles

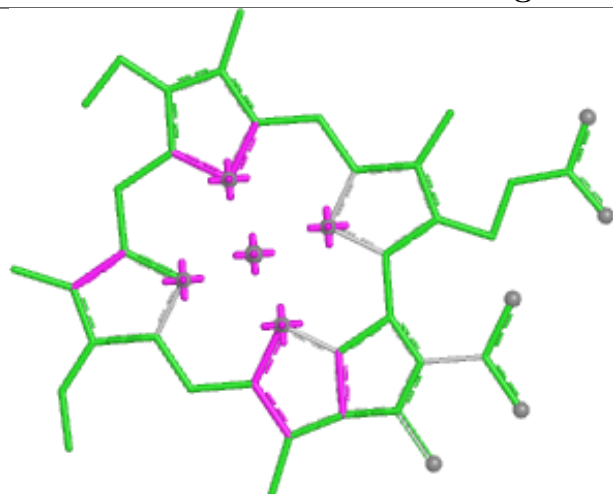


Torsions

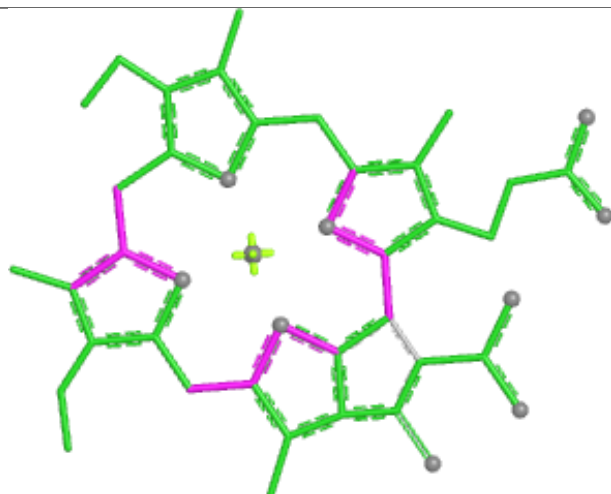


Rings

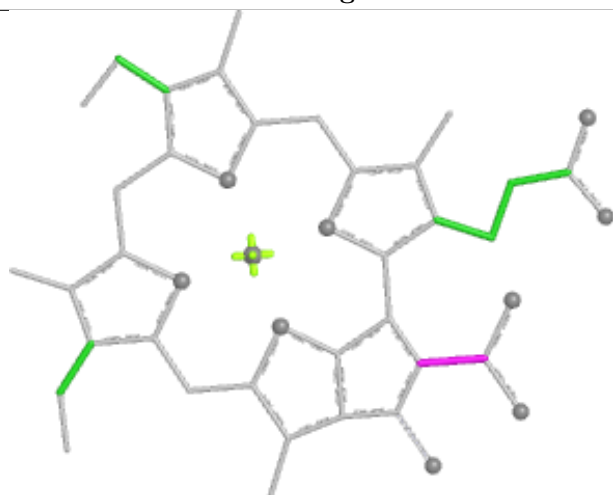
Ligand CLA B 827



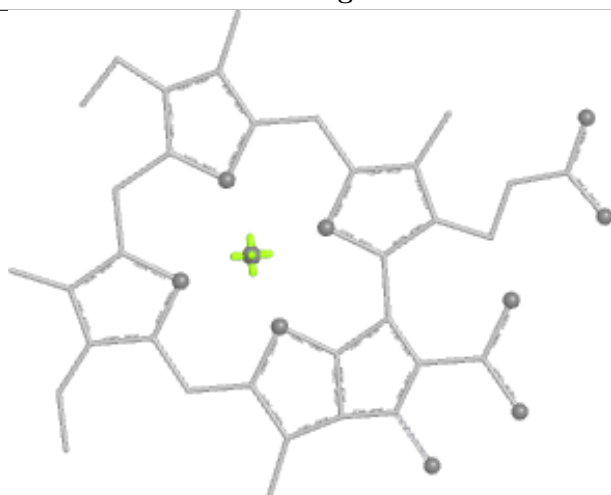
Bond lengths



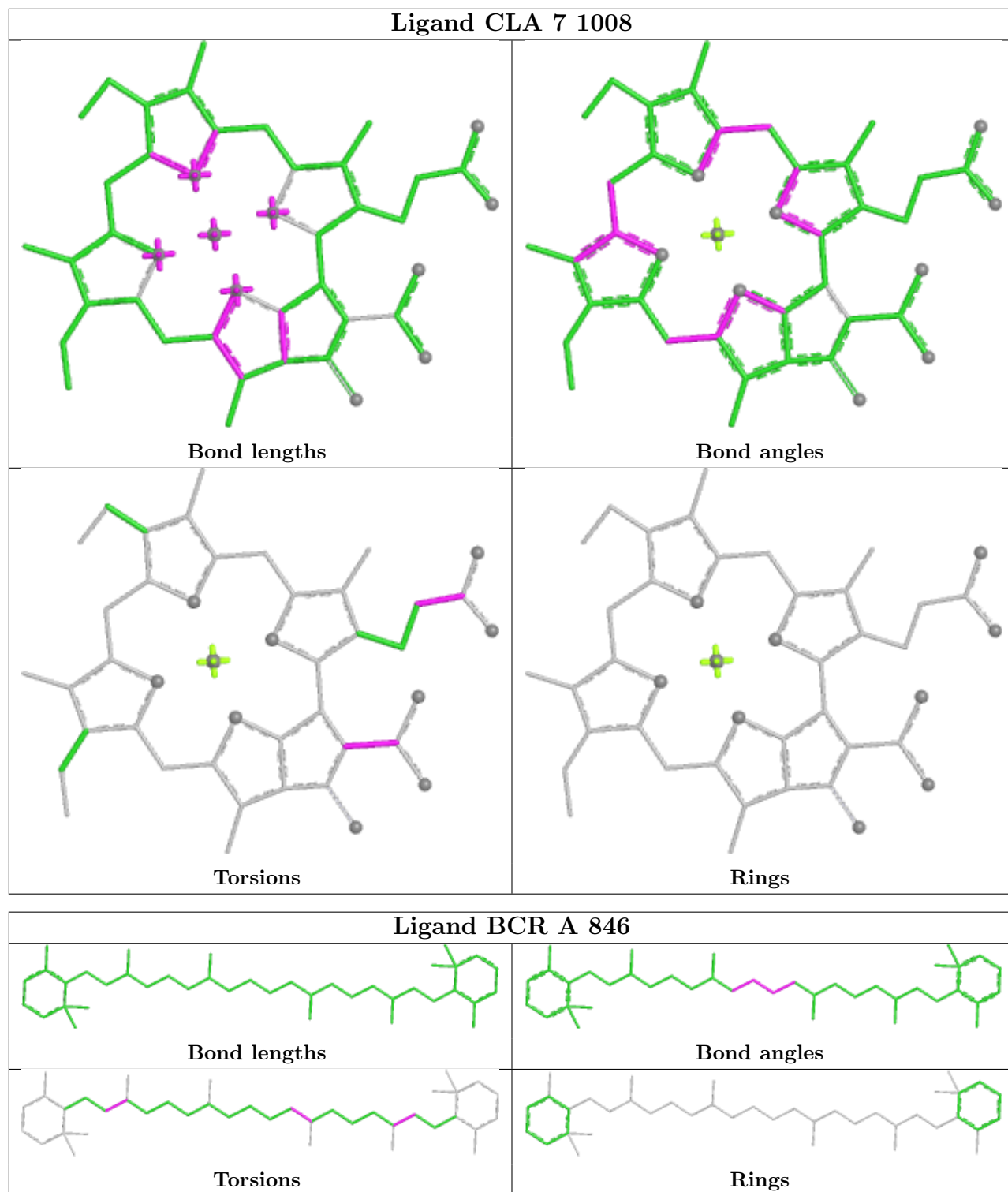
Bond angles

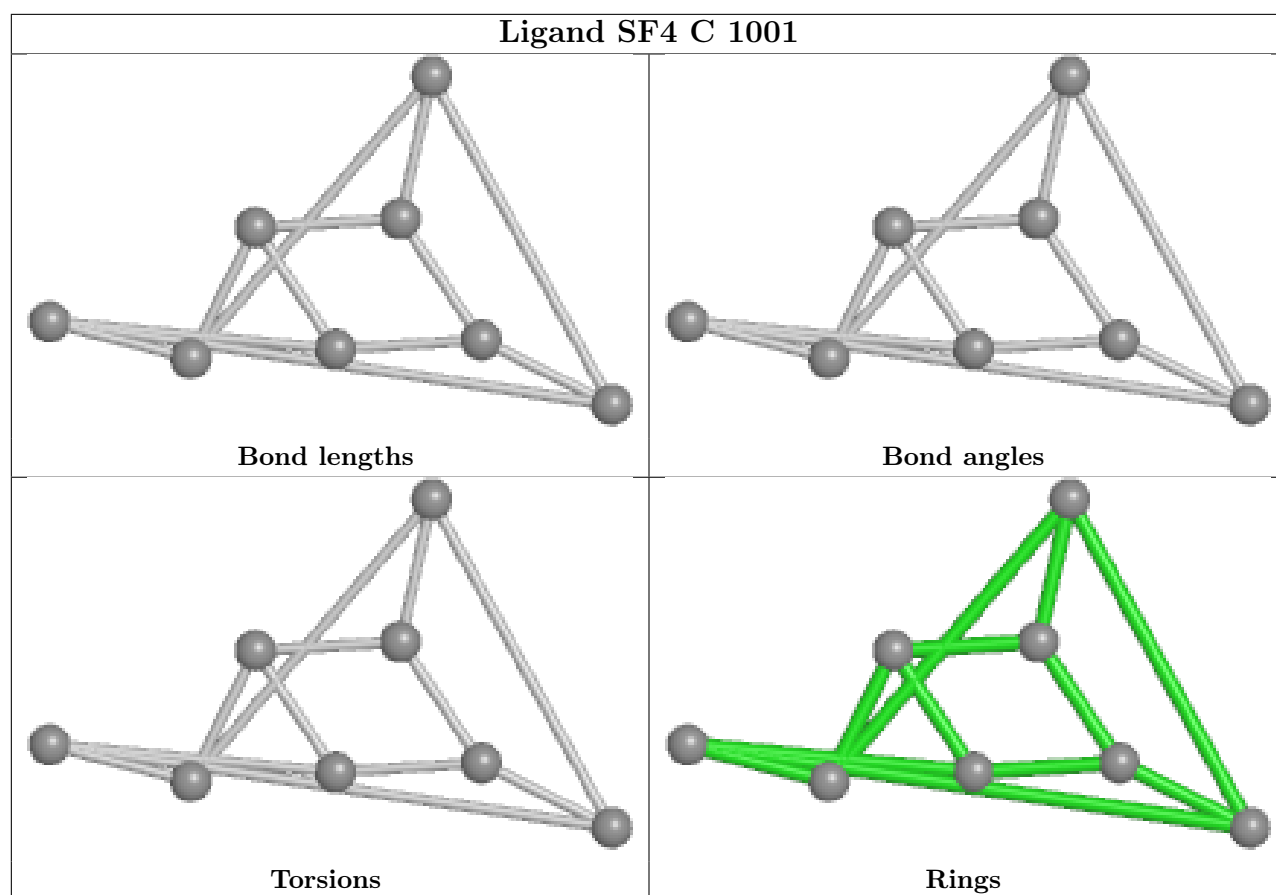


Torsions

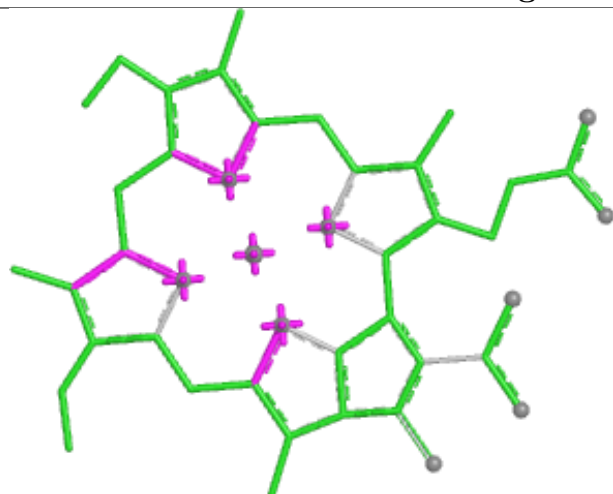


Rings

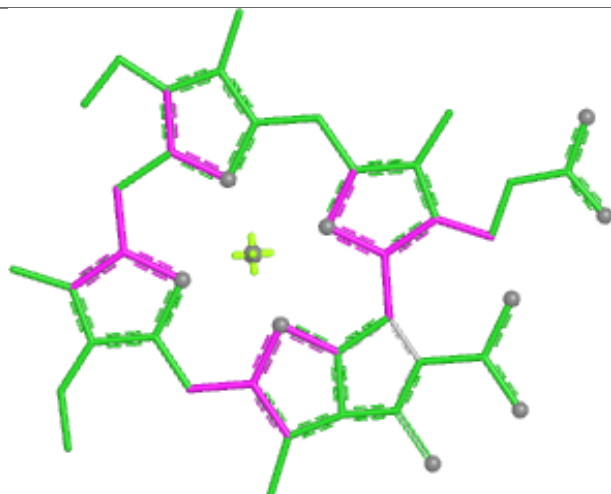




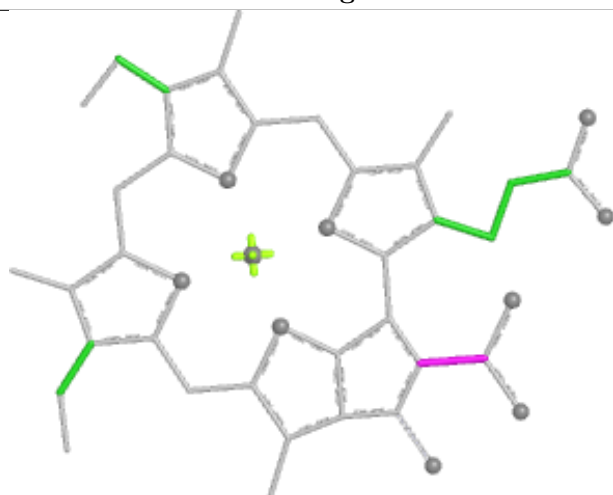
Ligand CLA 5 318



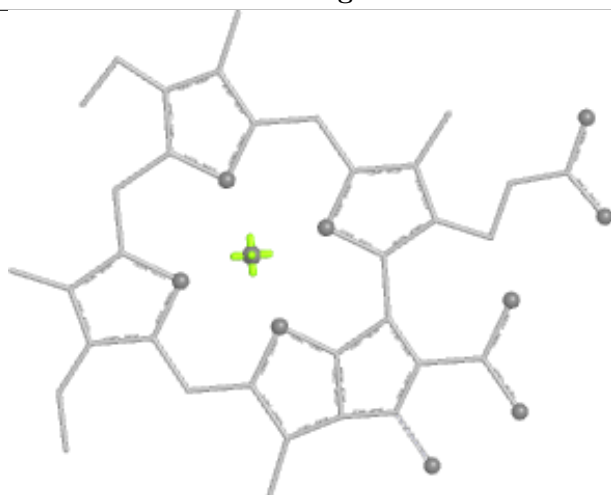
Bond lengths



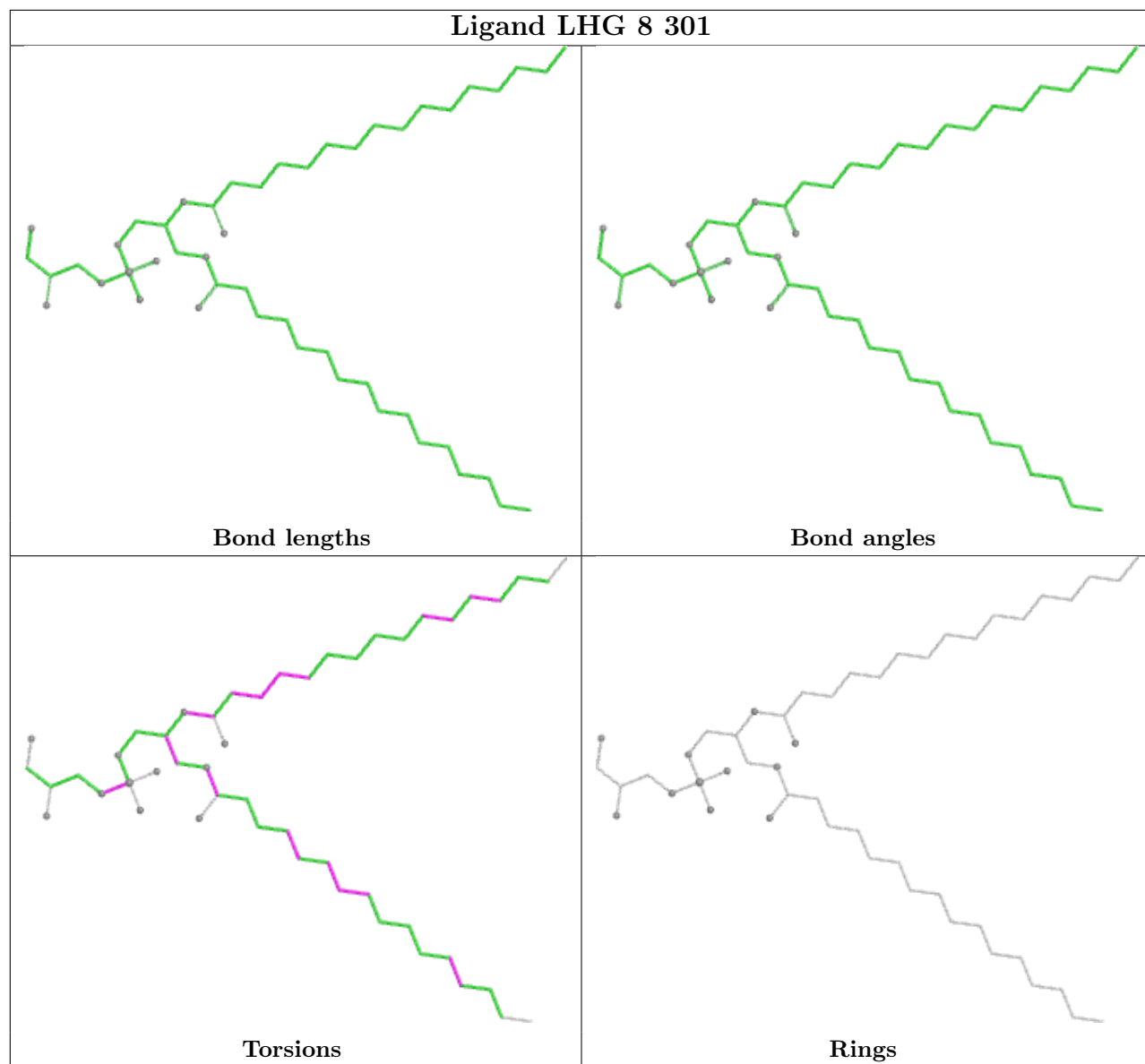
Bond angles

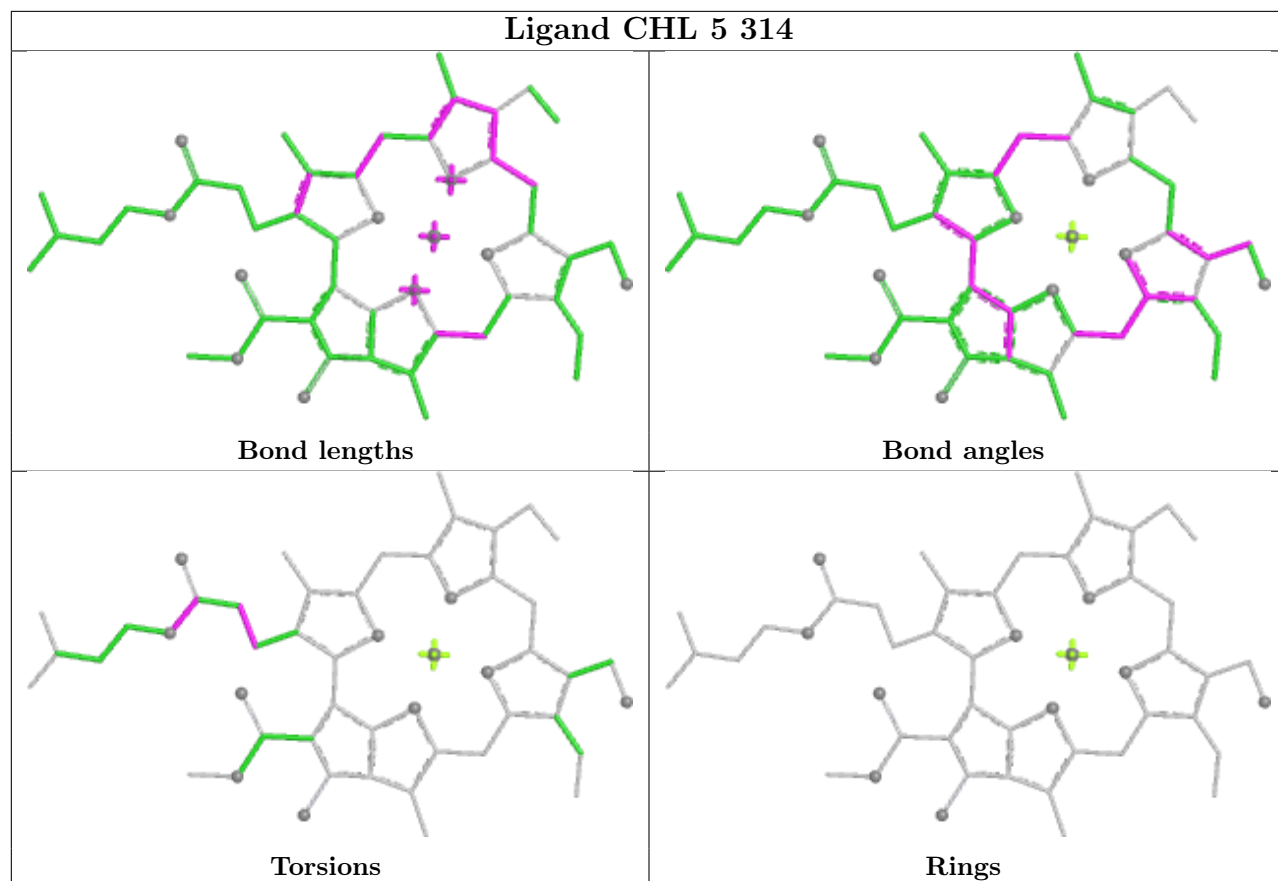


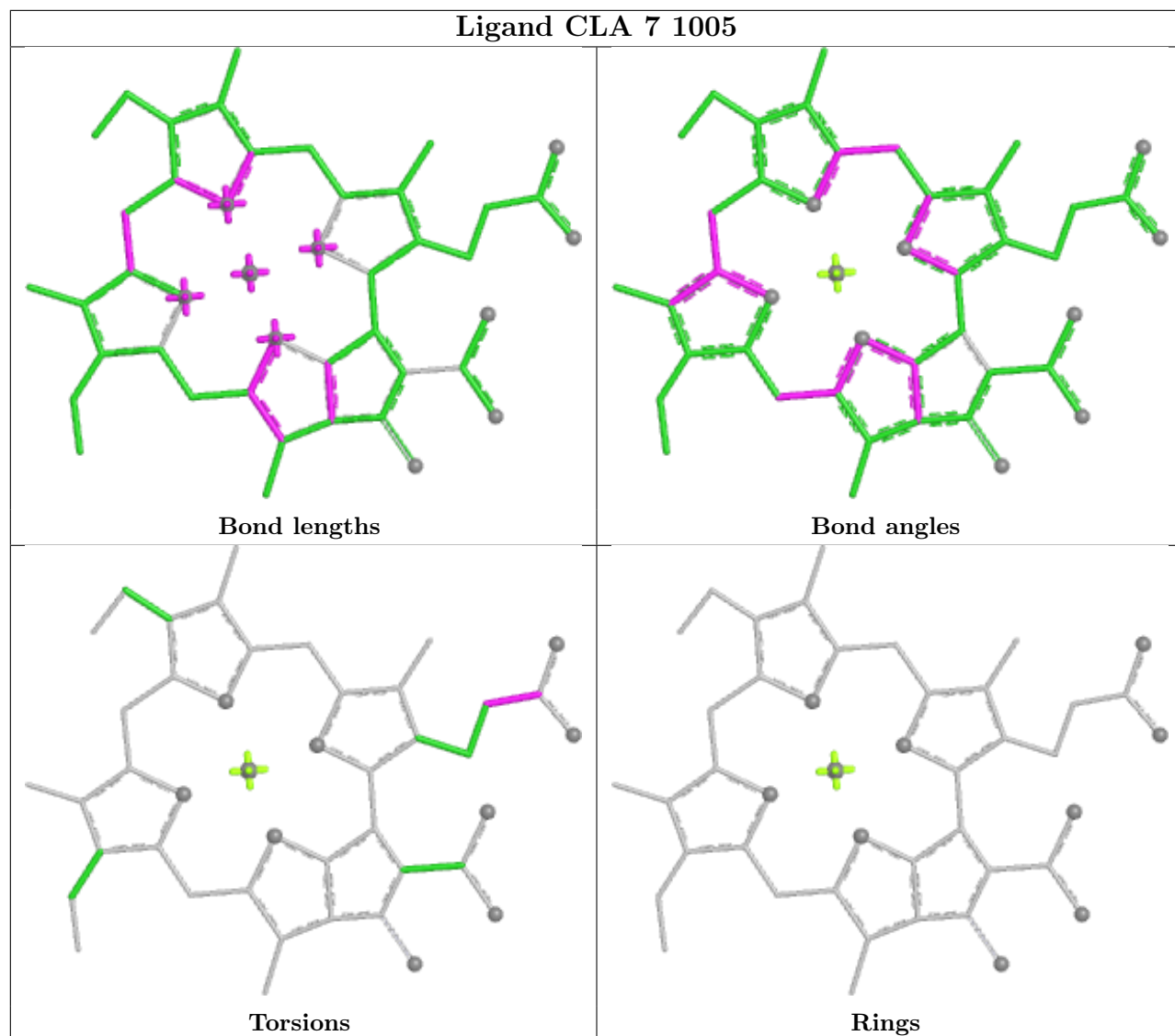
Torsions



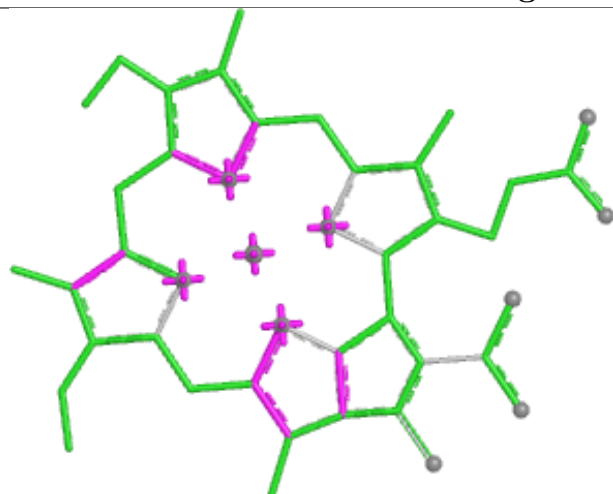
Rings



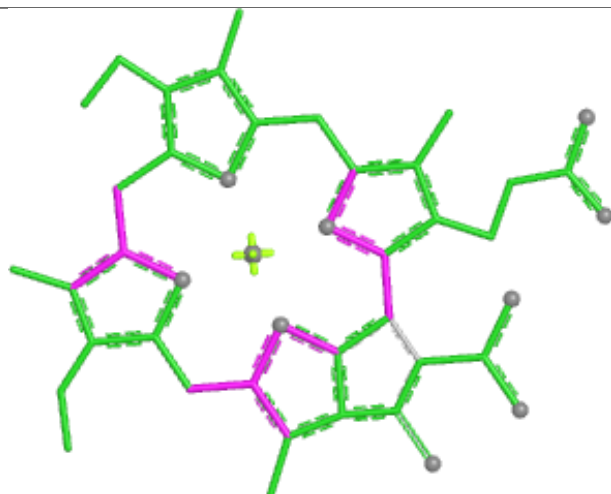




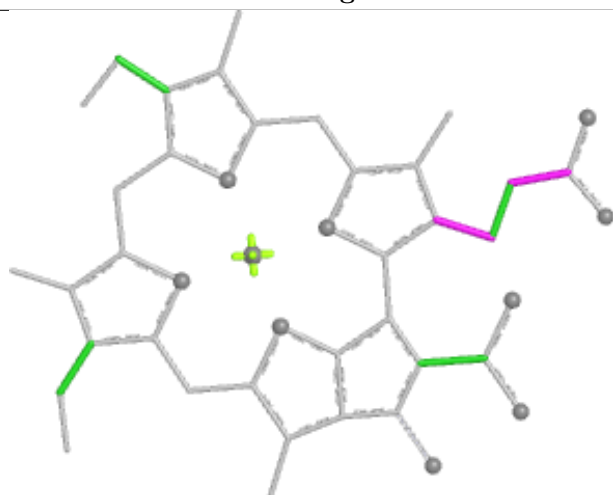
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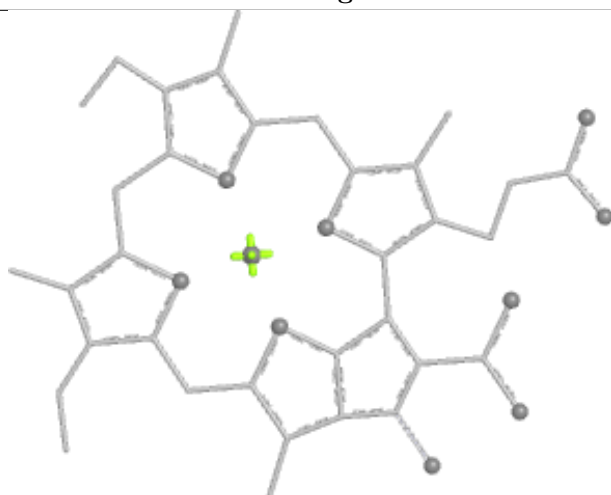
Bond lengths



Bond angles

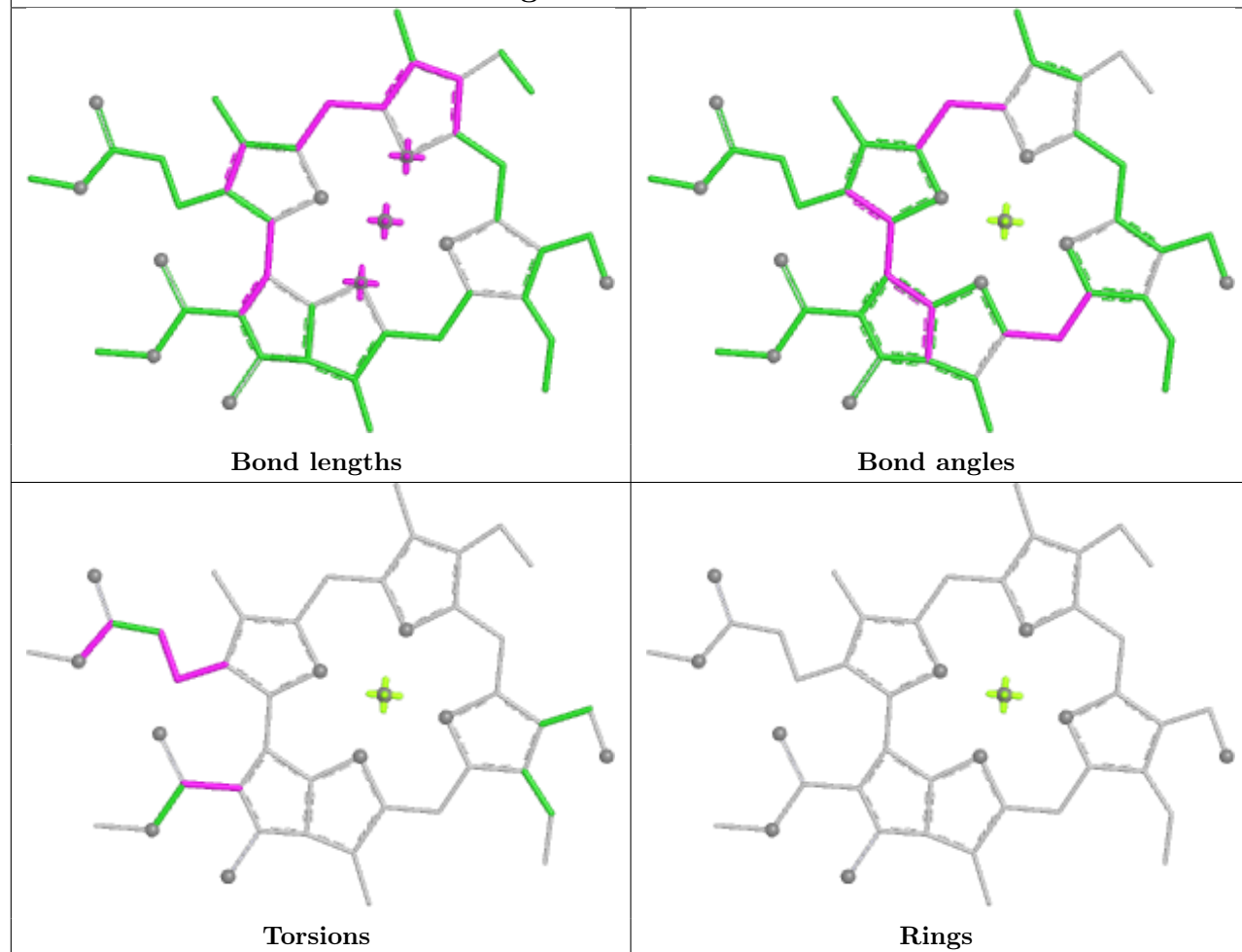


Torsions

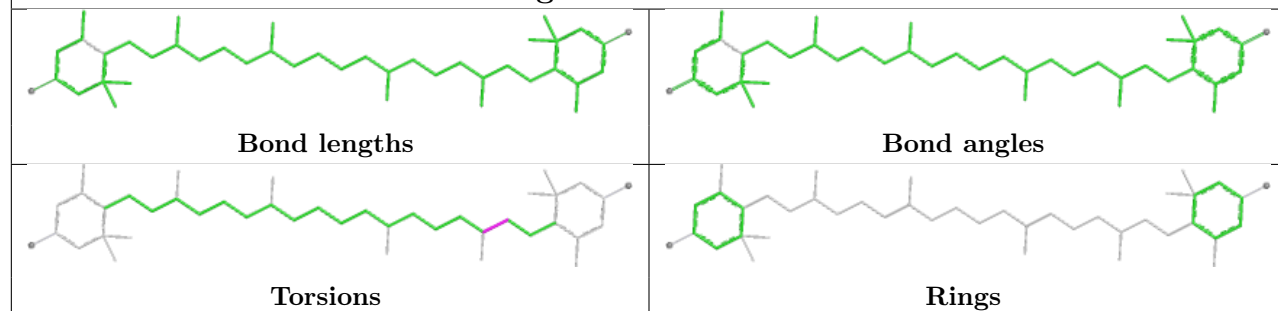


Rings

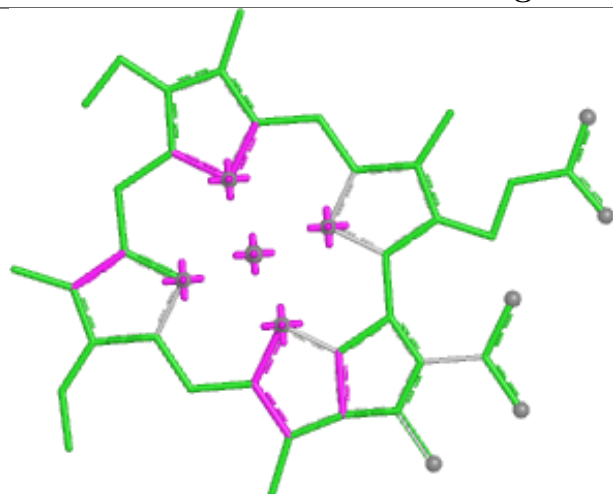
Ligand CHL 8 314



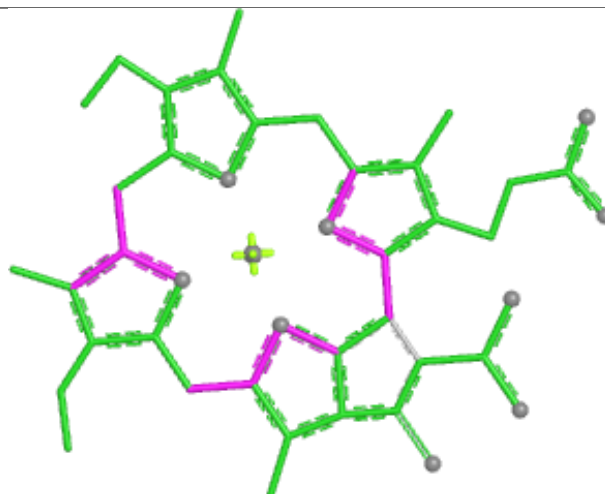
Ligand LUT 6 303



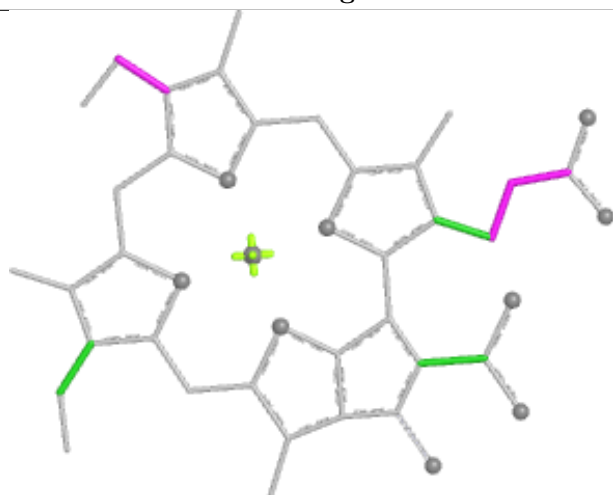
Ligand CLA B 819



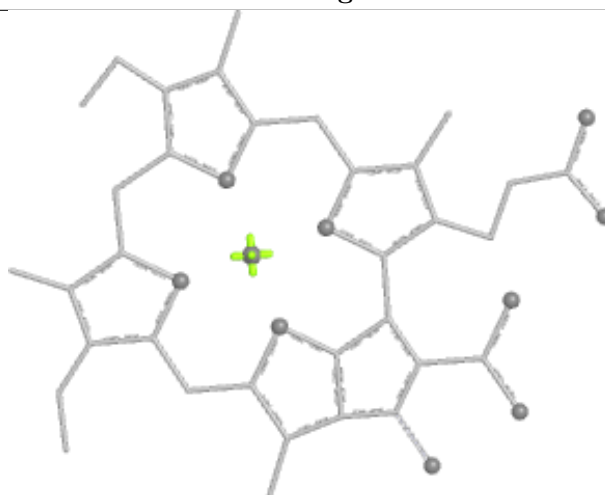
Bond lengths



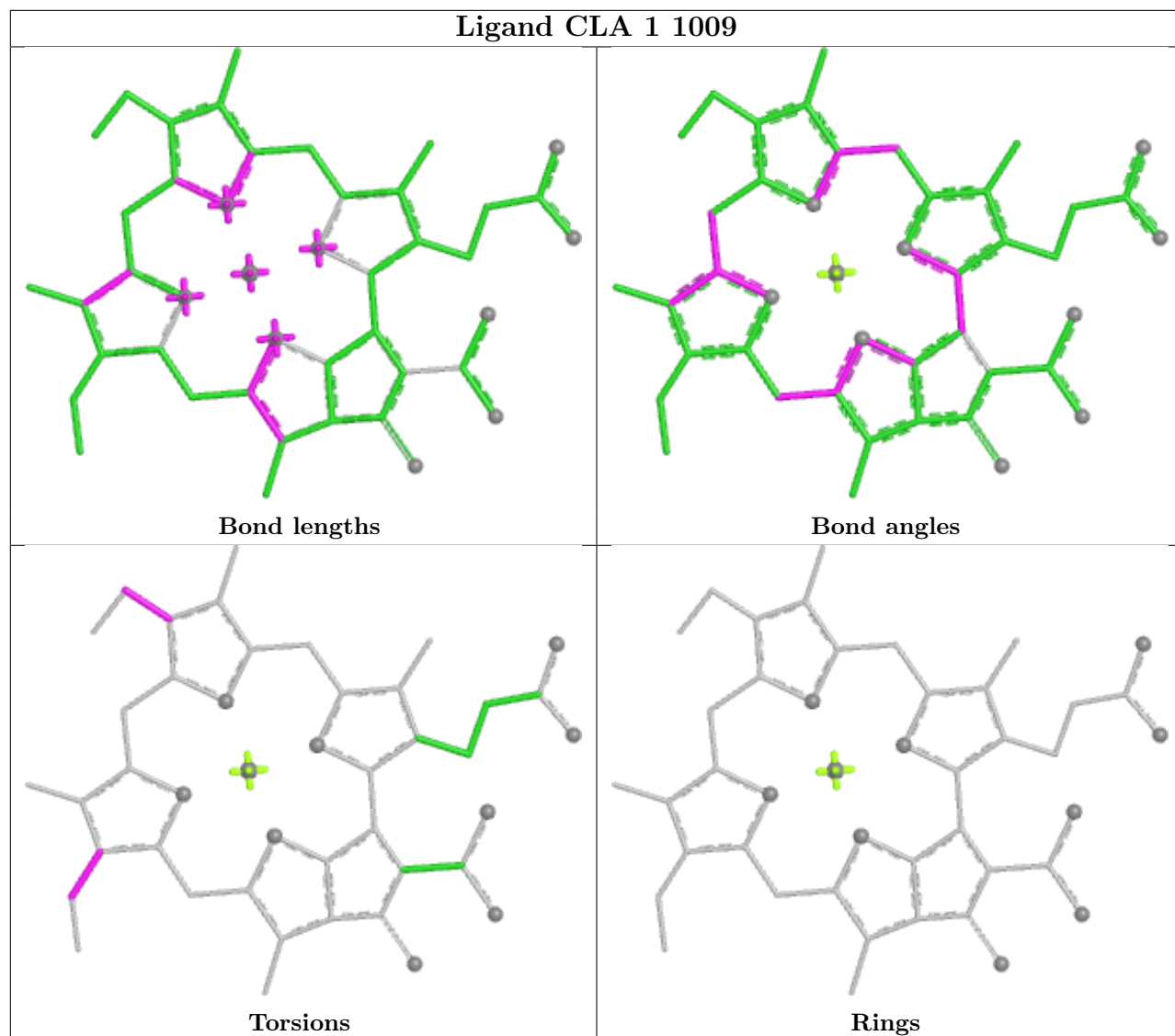
Bond angles



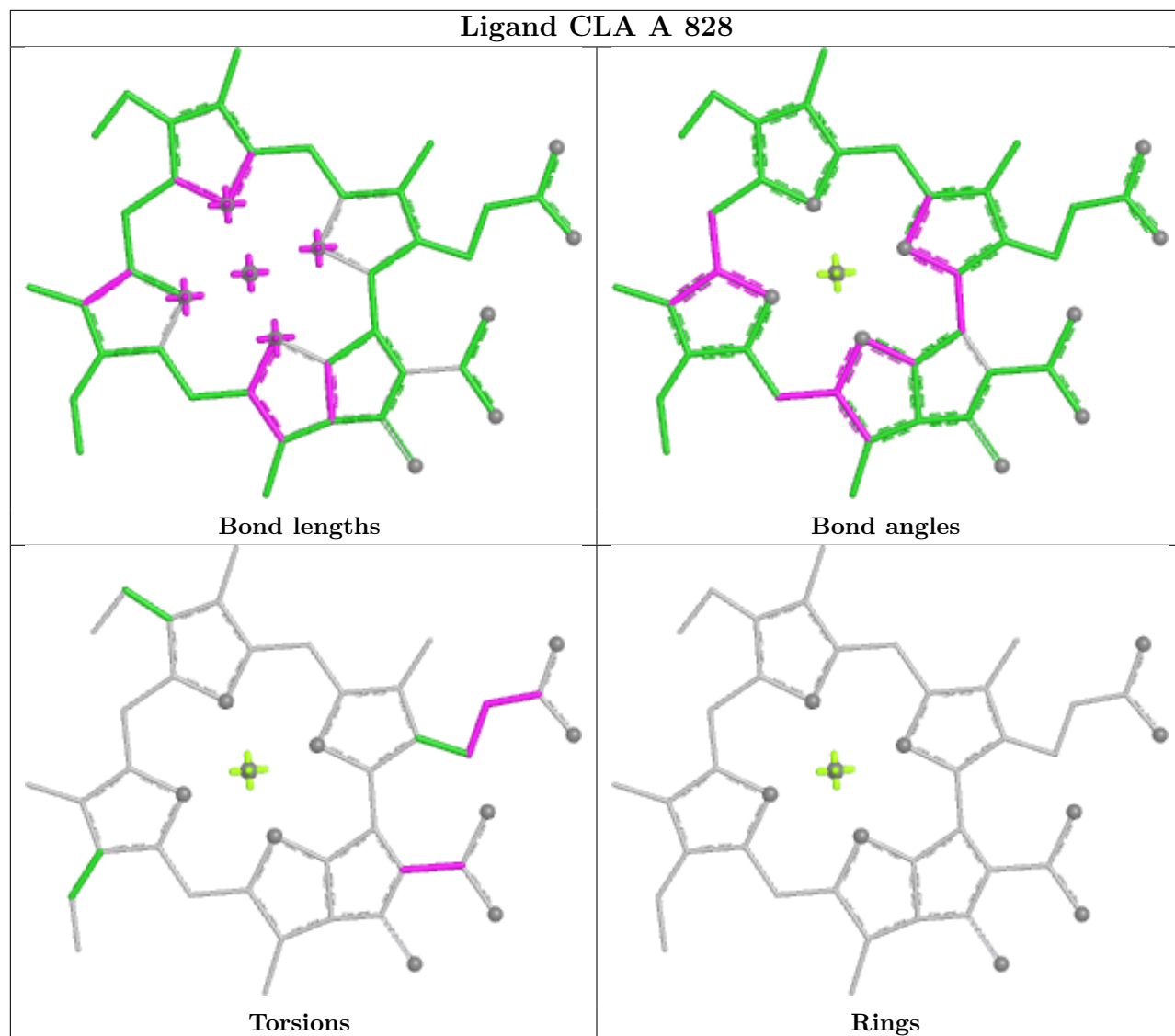
Torsions



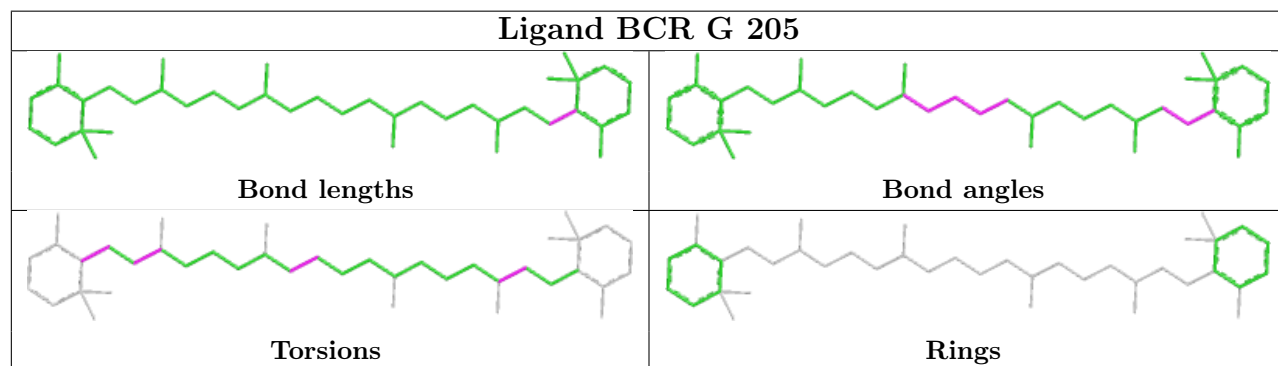
Rings



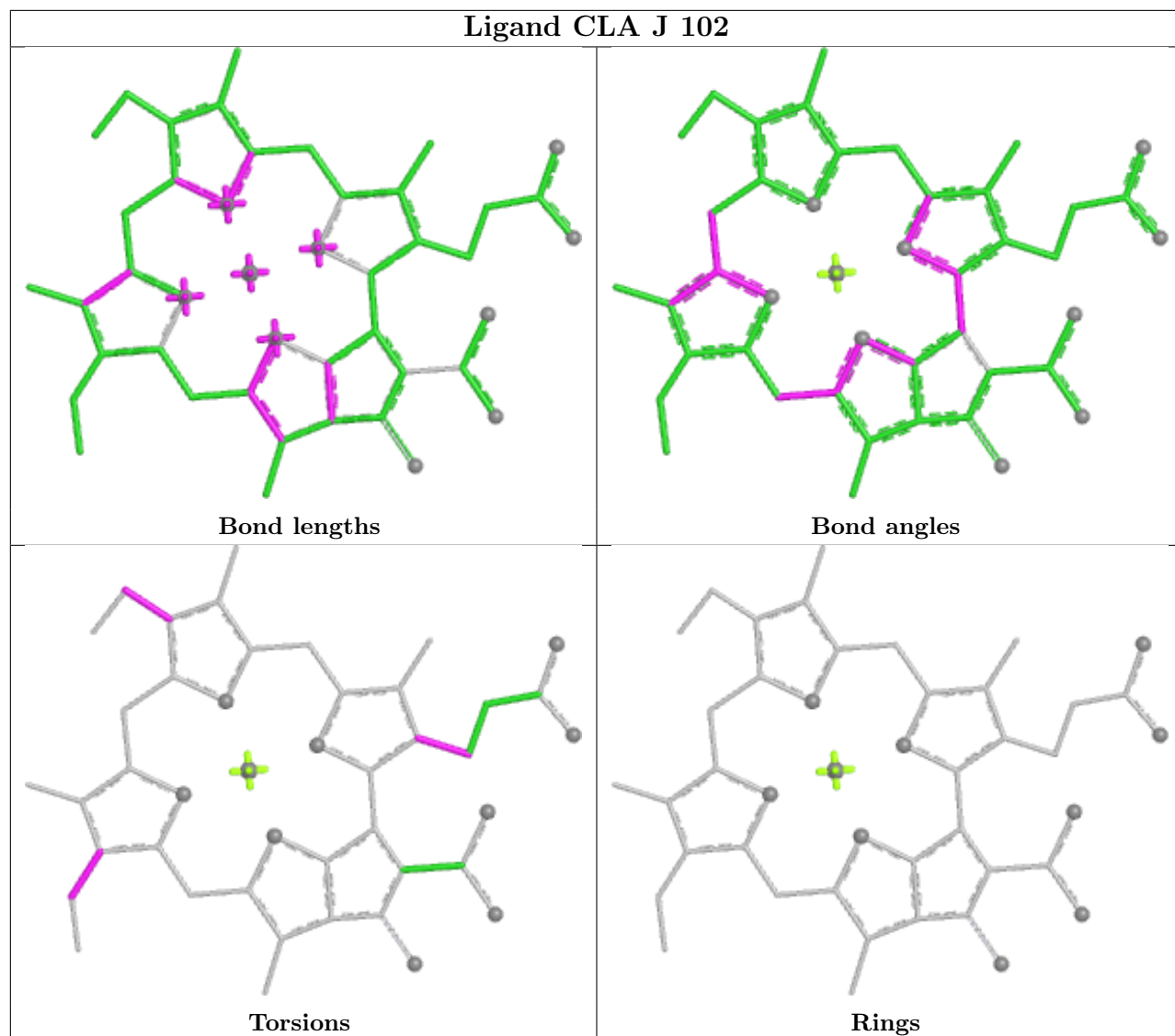
Ligand CLA A 828



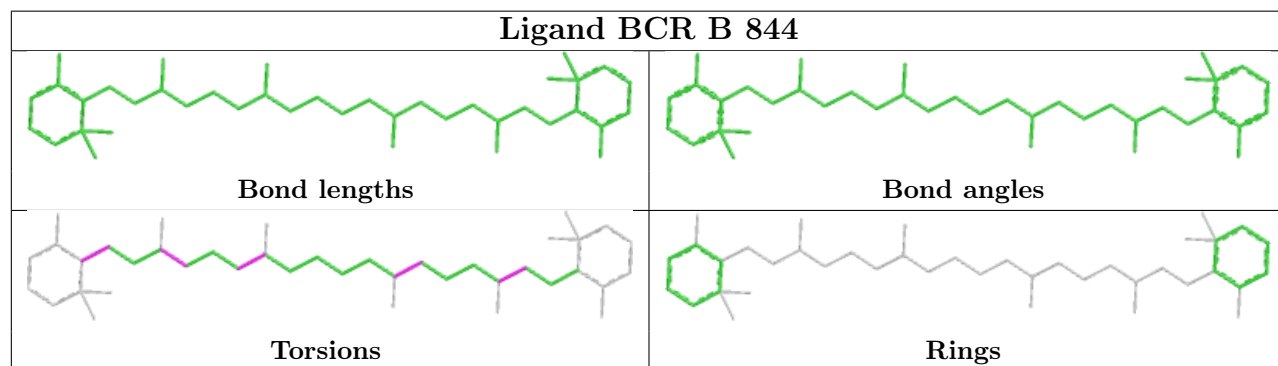
Ligand BCR G 205

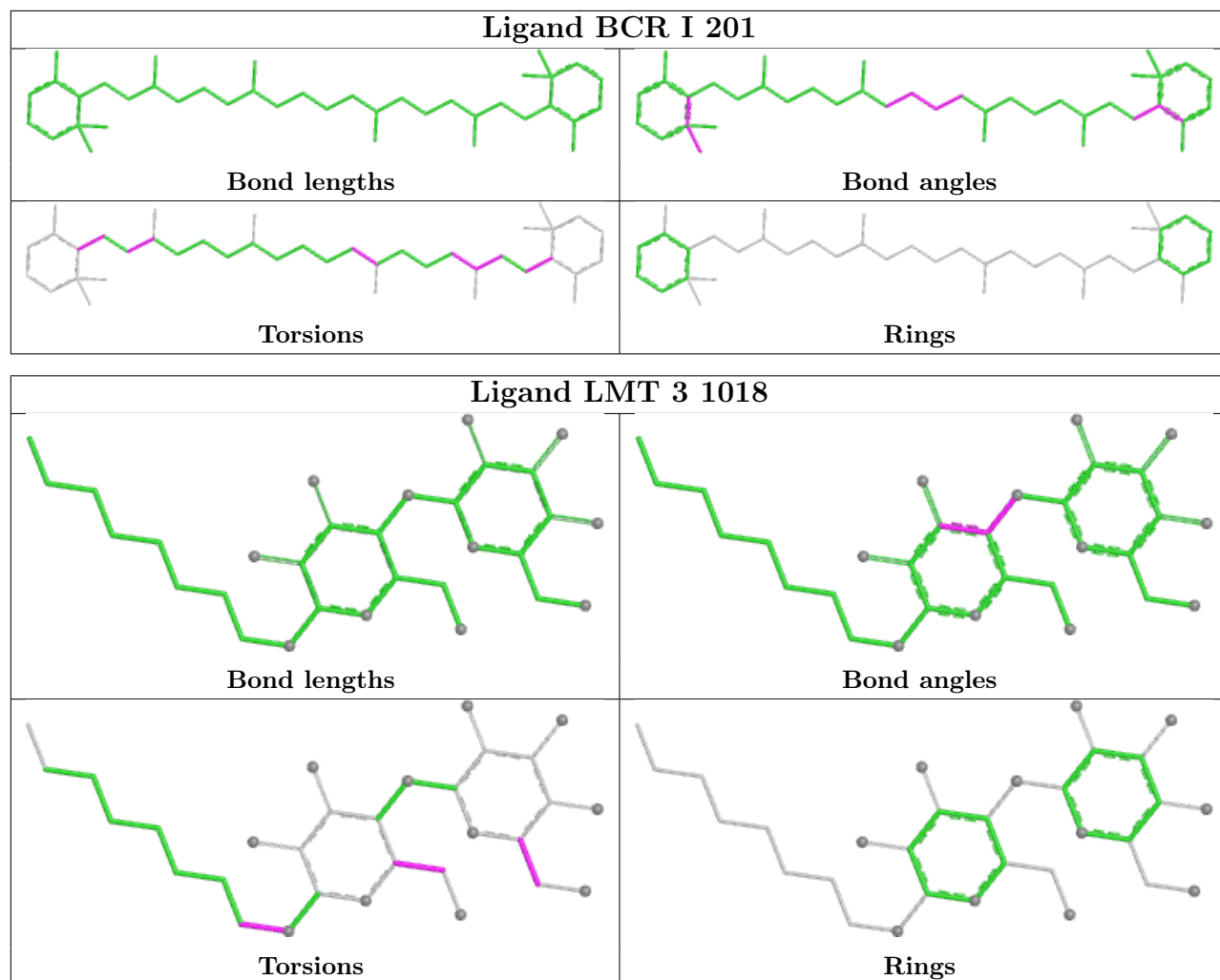


Ligand CLA J 102

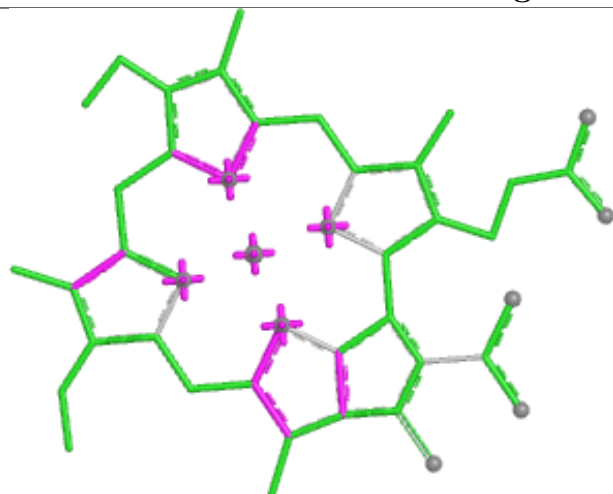


Ligand BCR B 844

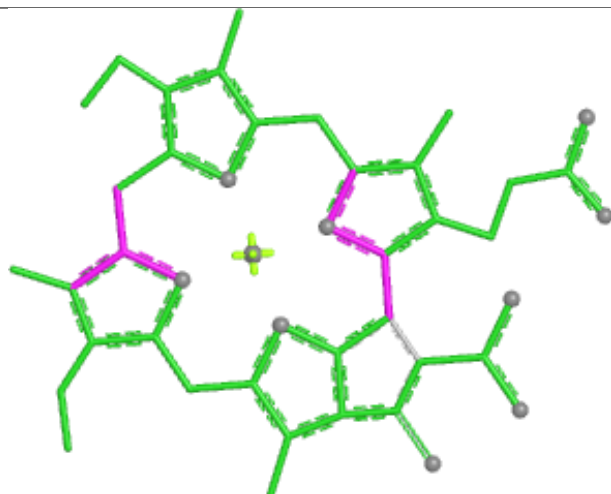




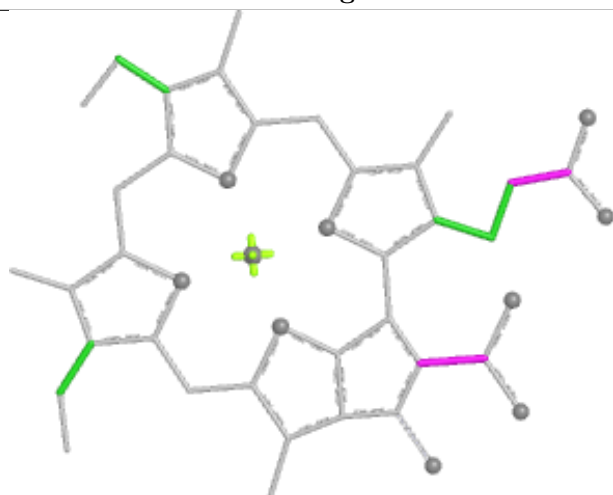
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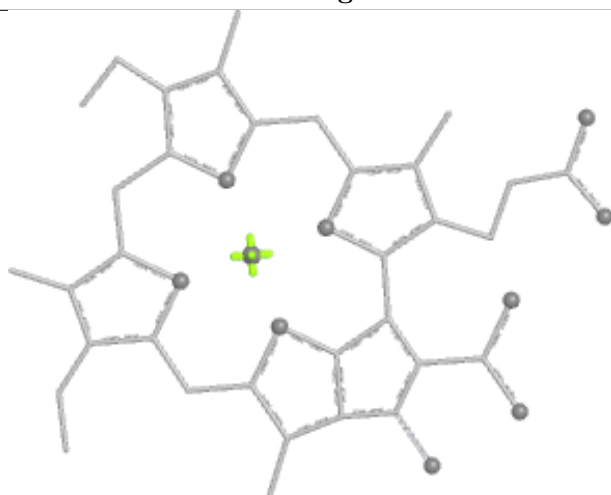
Bond lengths



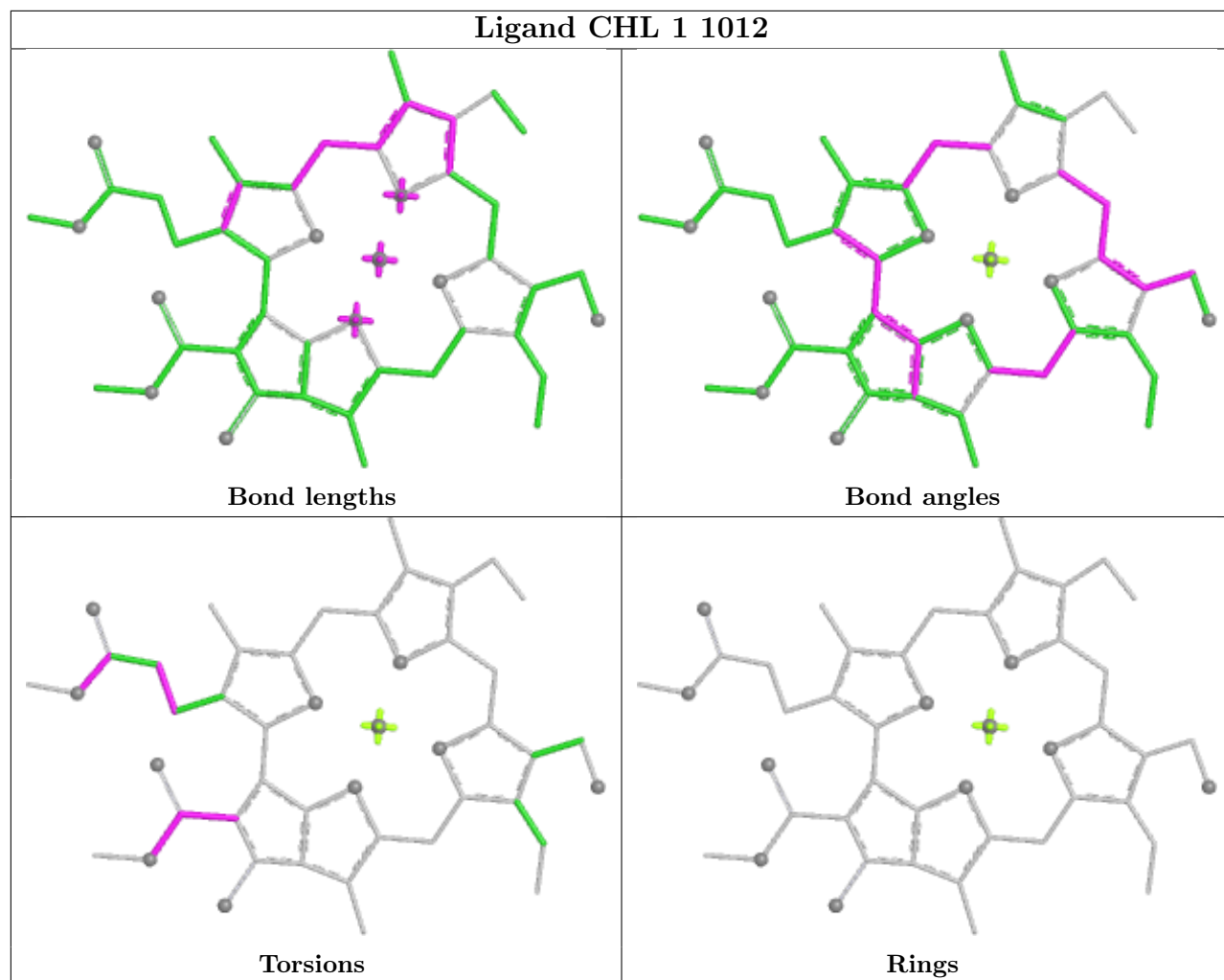
Bond angles



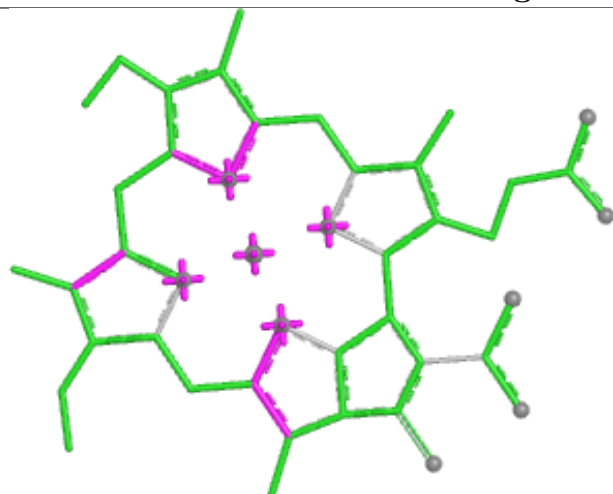
Torsions



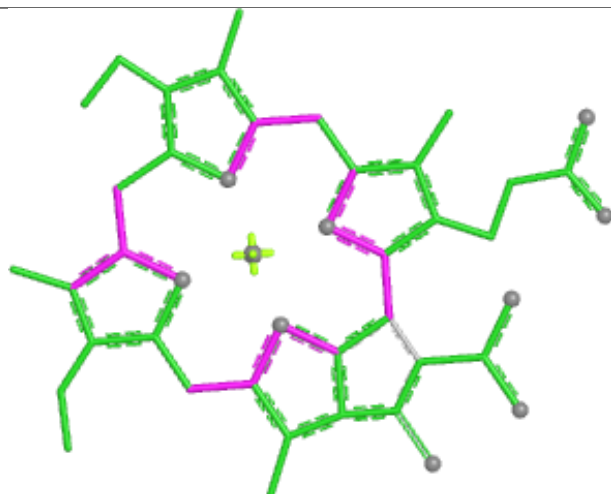
Rings



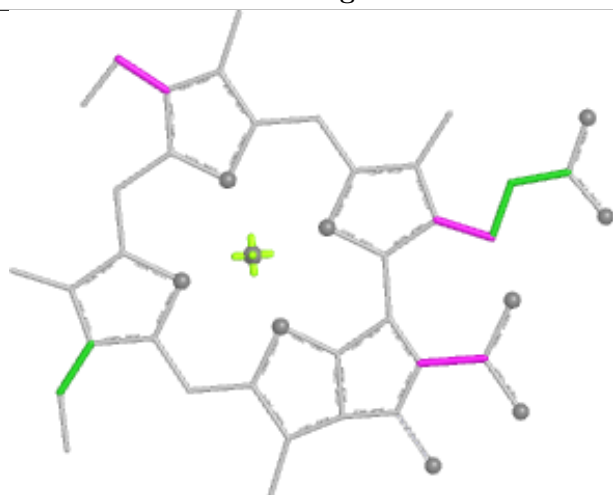
Ligand CLA A 805



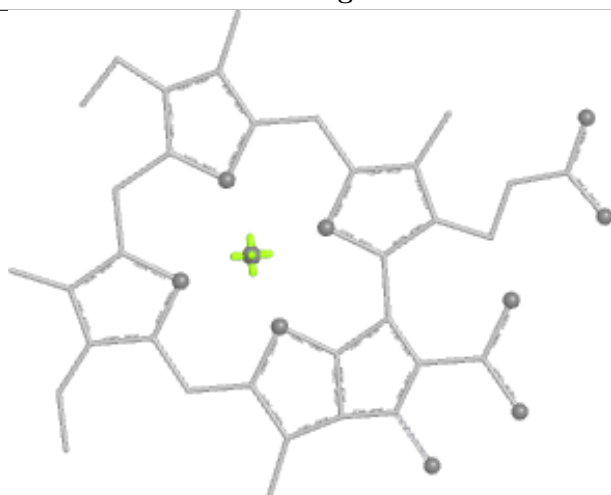
Bond lengths



Bond angles

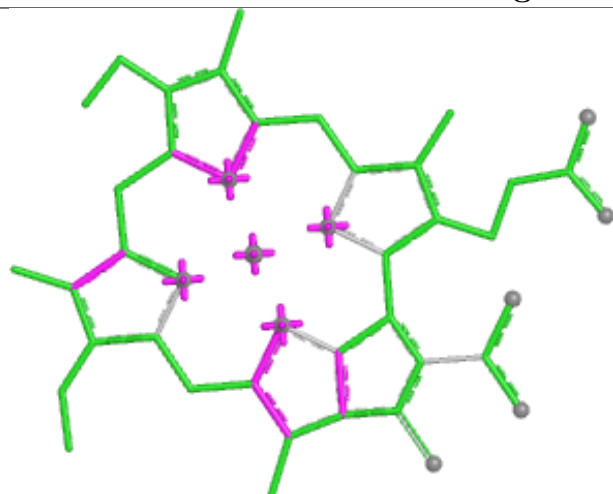


Torsions

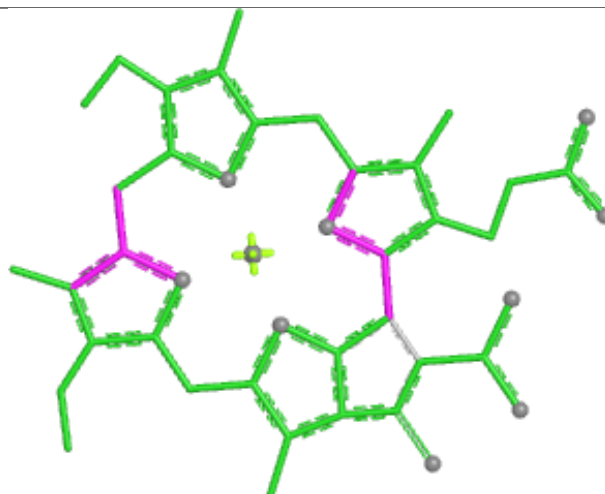


Rings

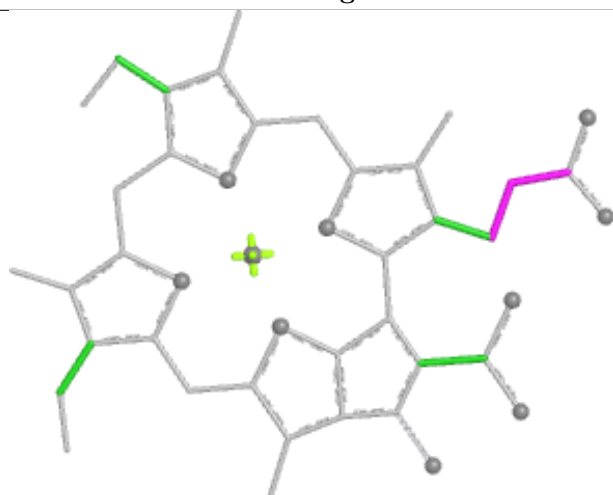
Ligand CLA A 833



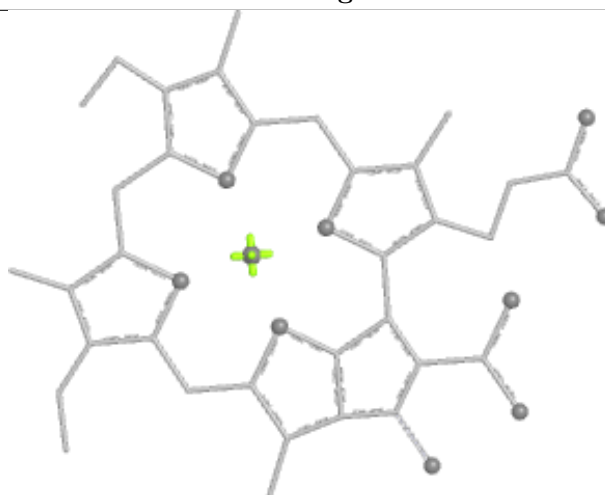
Bond lengths



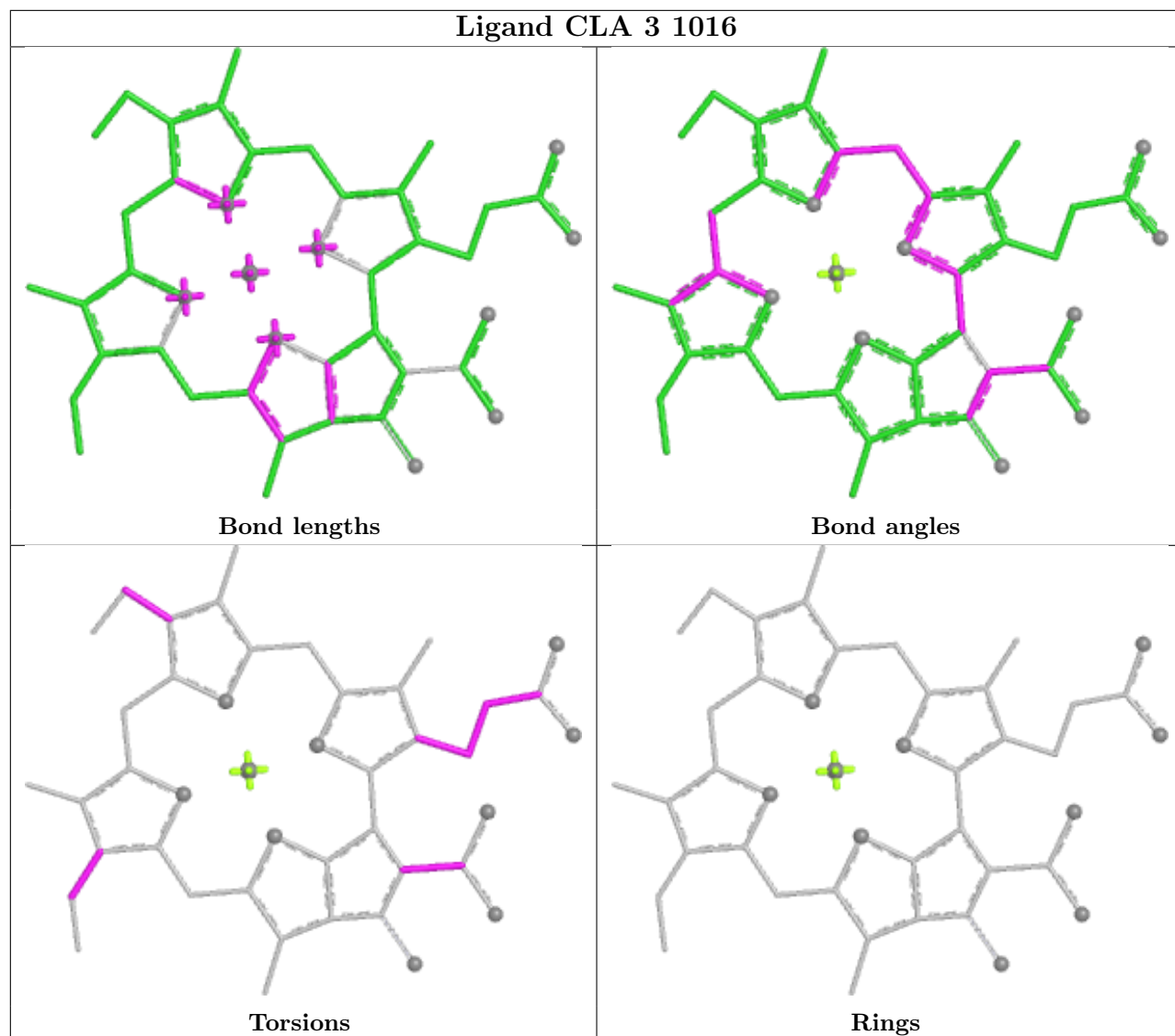
Bond angles

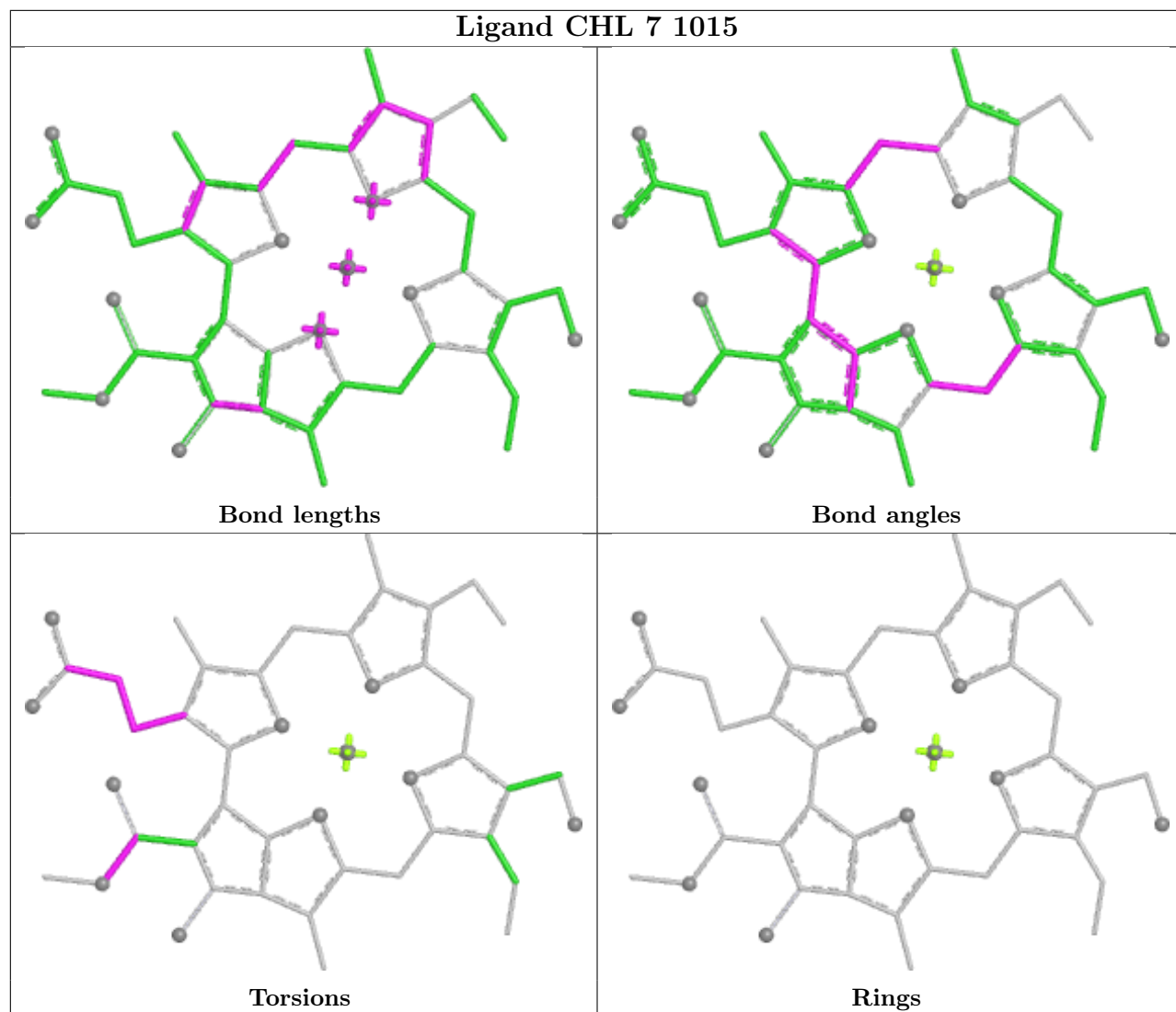


Torsions

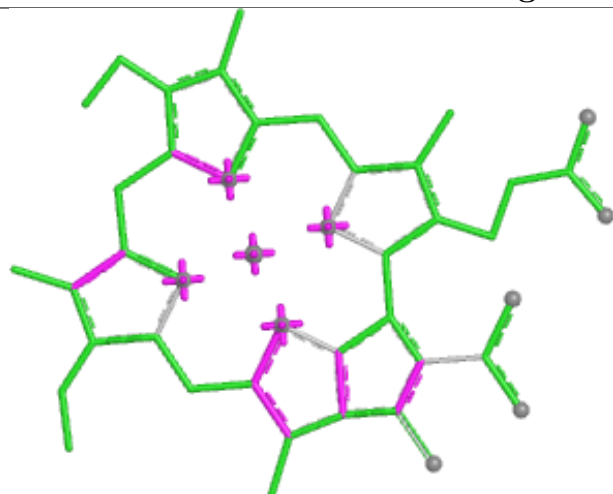


Rings

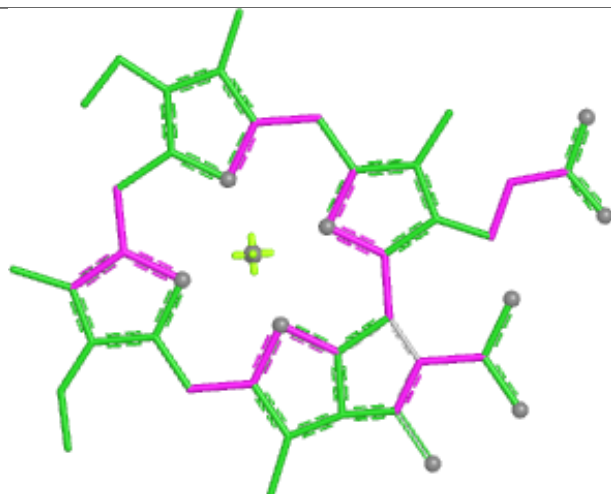




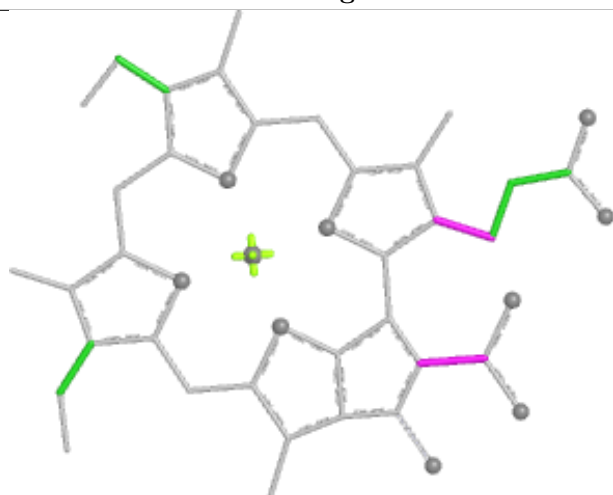
Ligand CLA 5 308



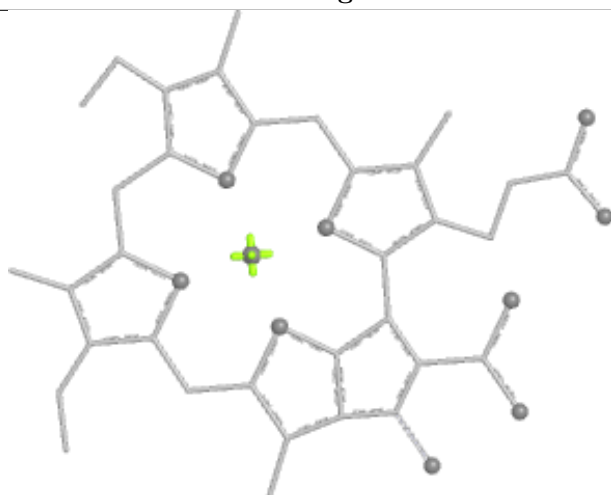
Bond lengths



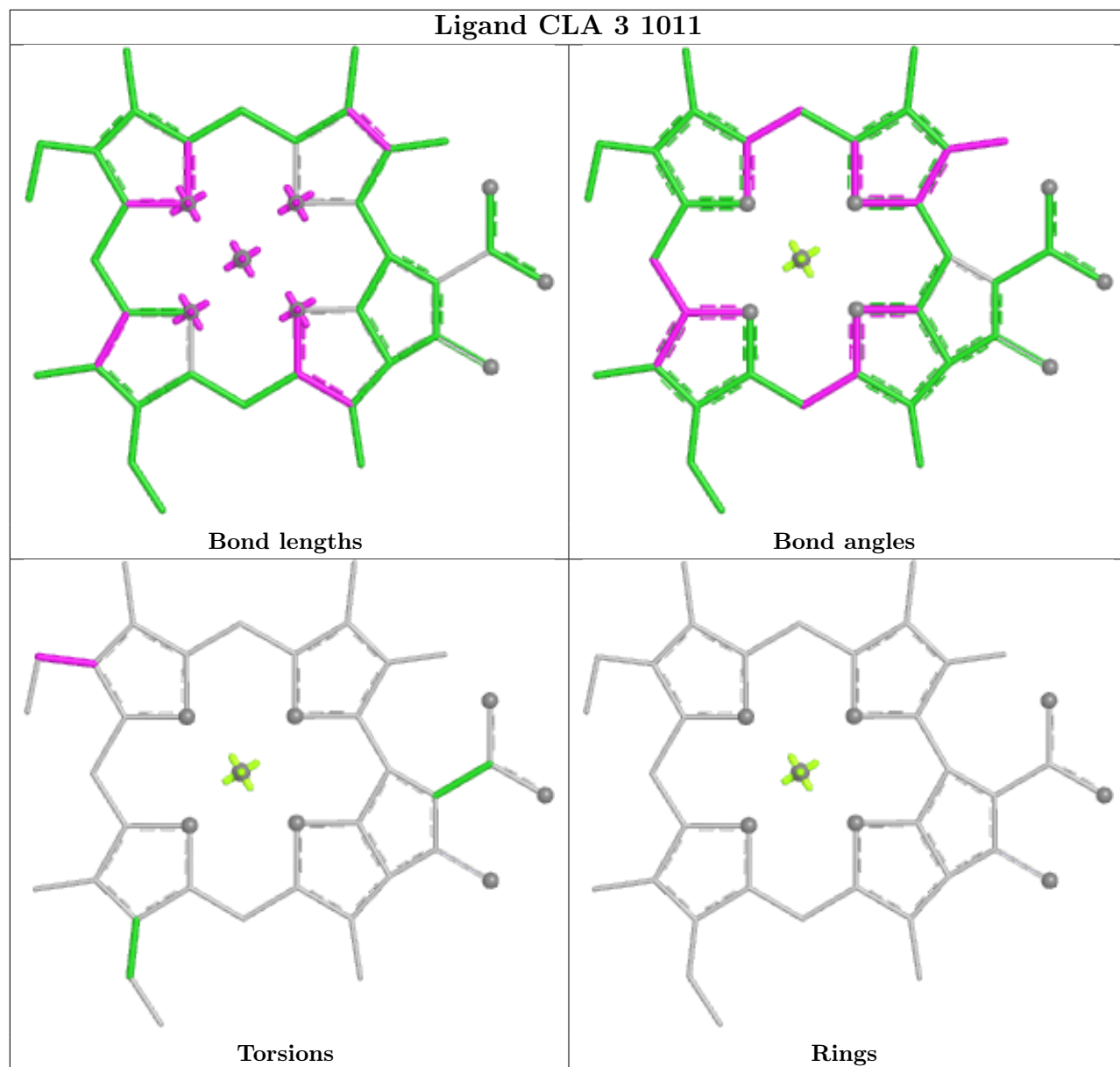
Bond angles



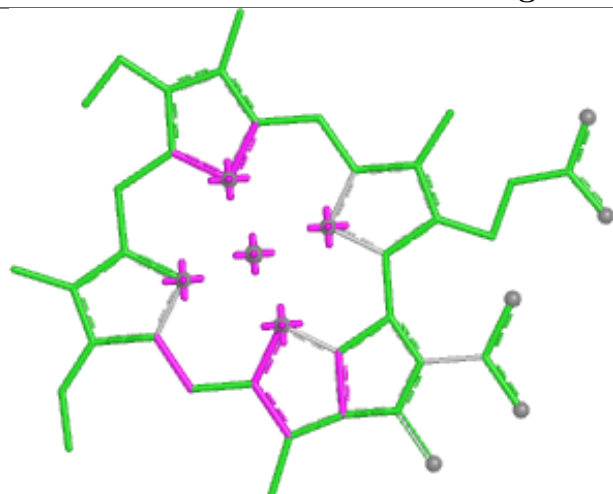
Torsions



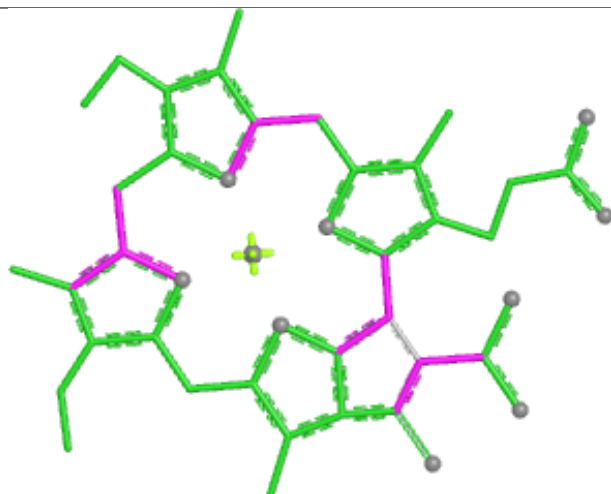
Rings



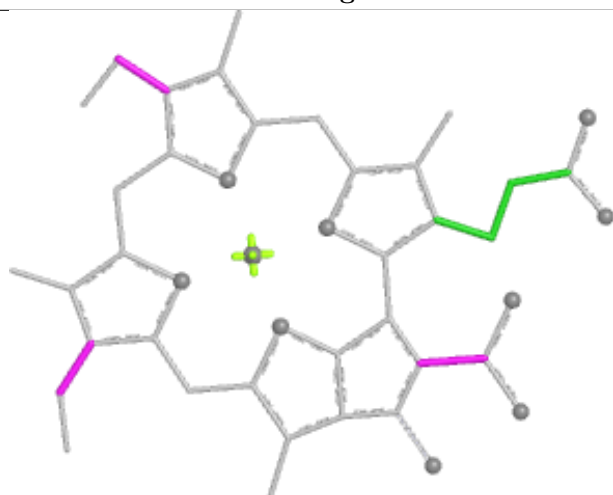
Ligand CLA 5 310



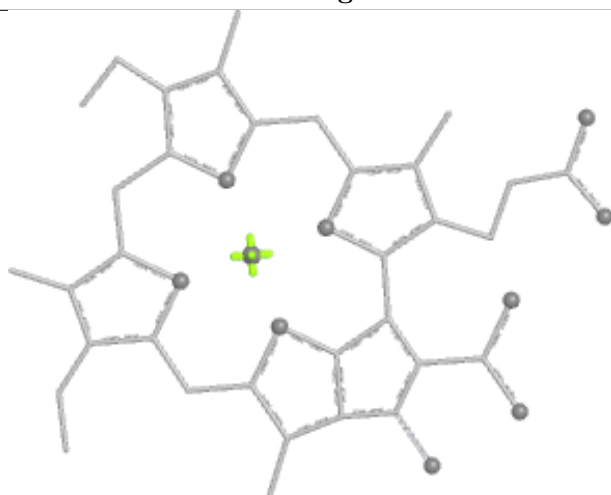
Bond lengths



Bond angles

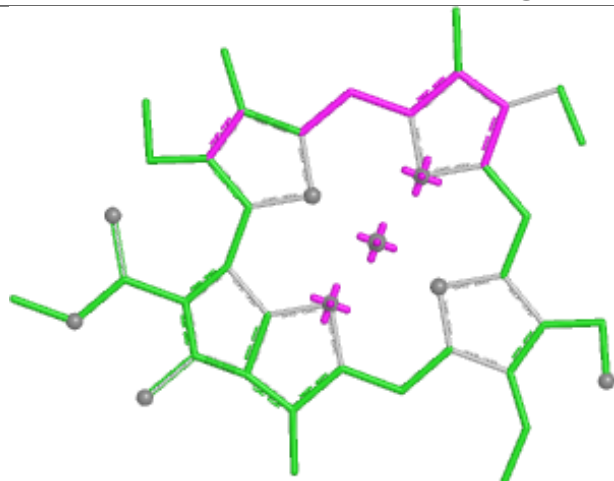


Torsions

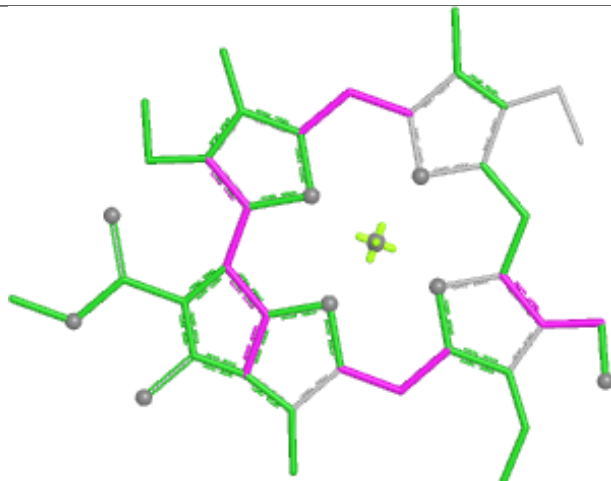


Rings

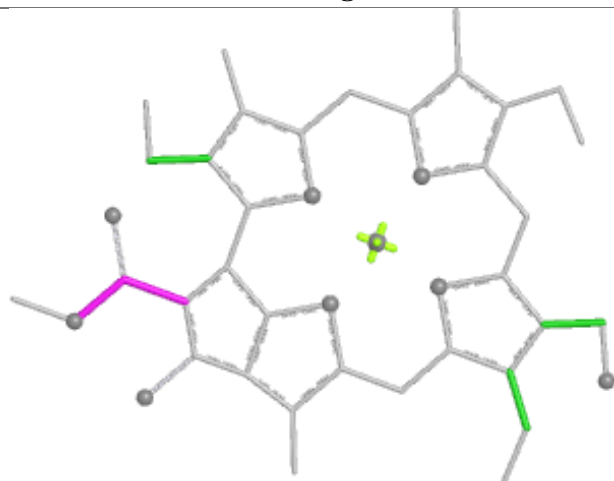
Ligand CHL 4 316



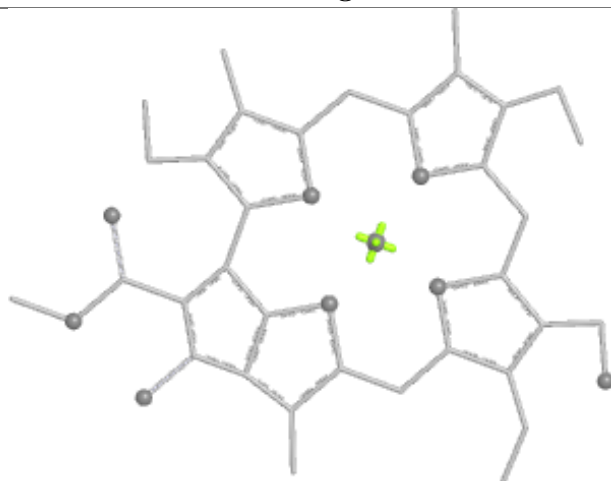
Bond lengths



Bond angles

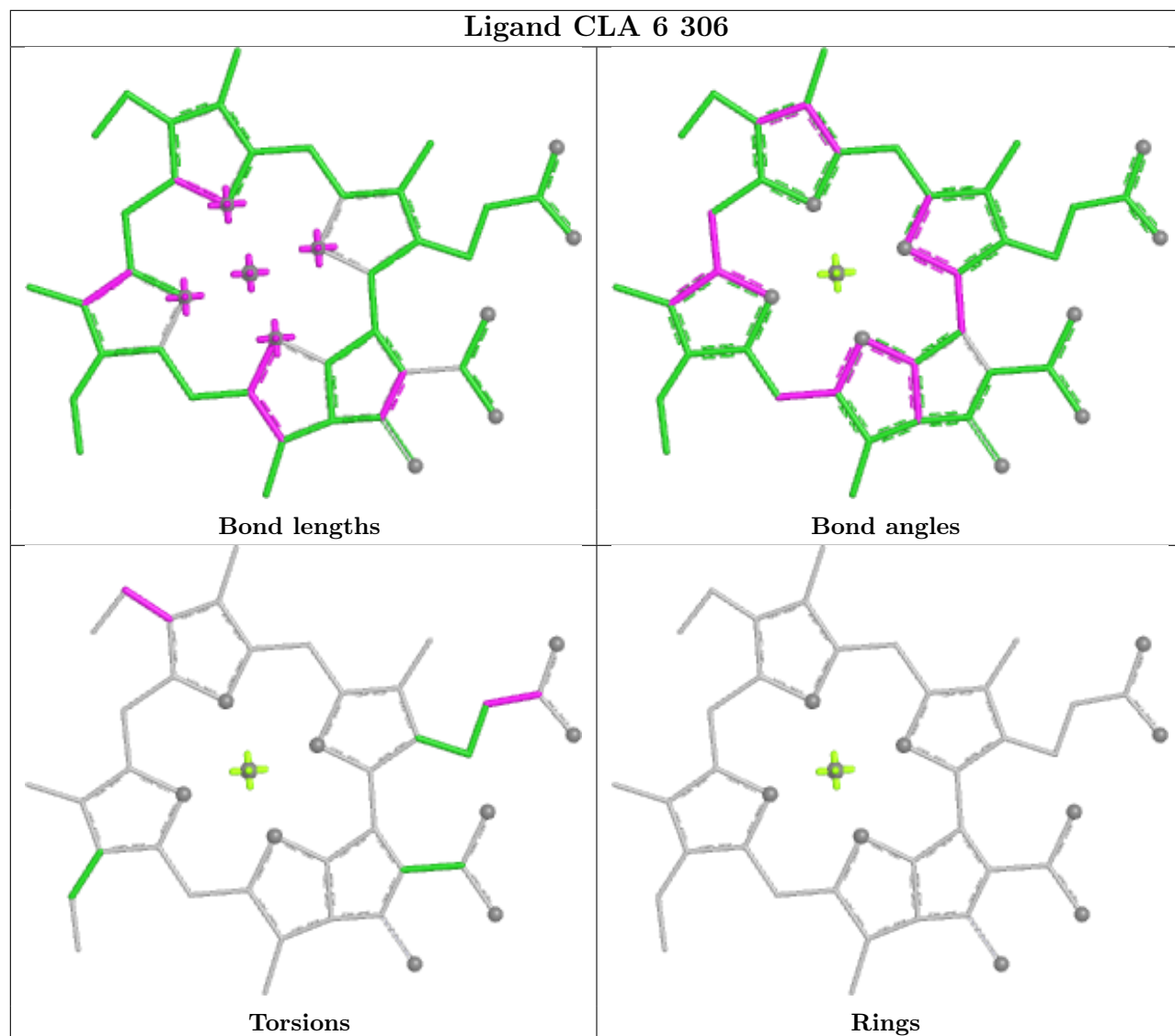


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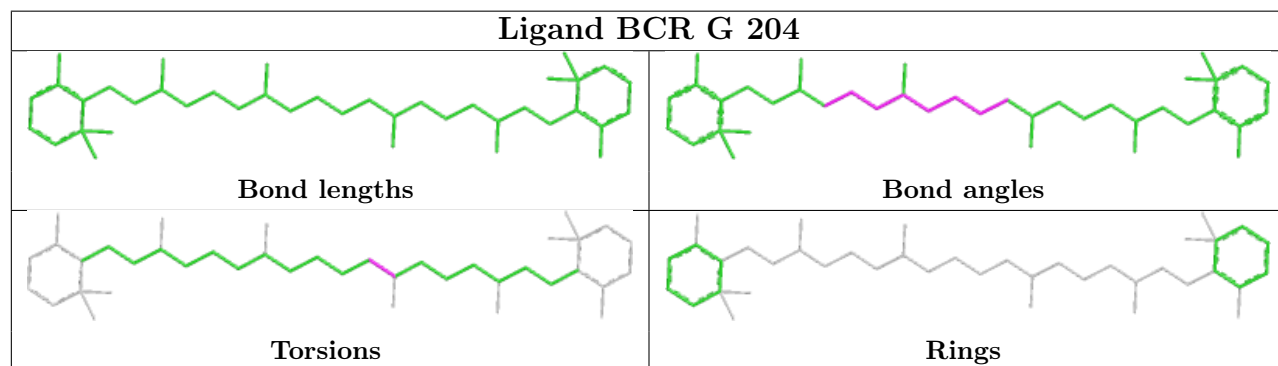


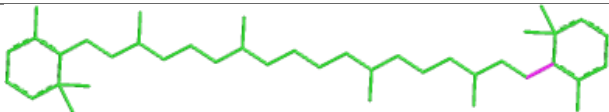
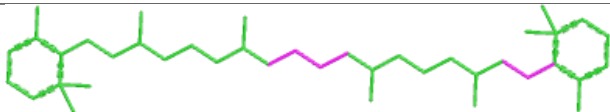
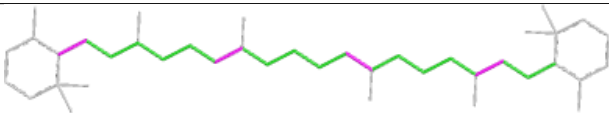
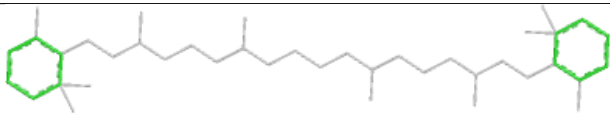
Rings

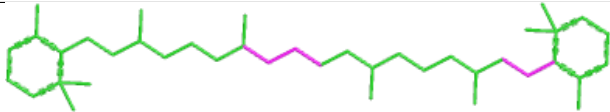
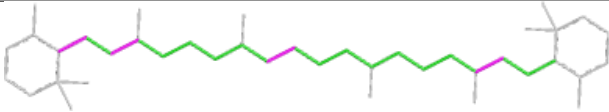
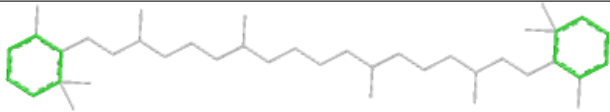
Ligand CLA 6 306



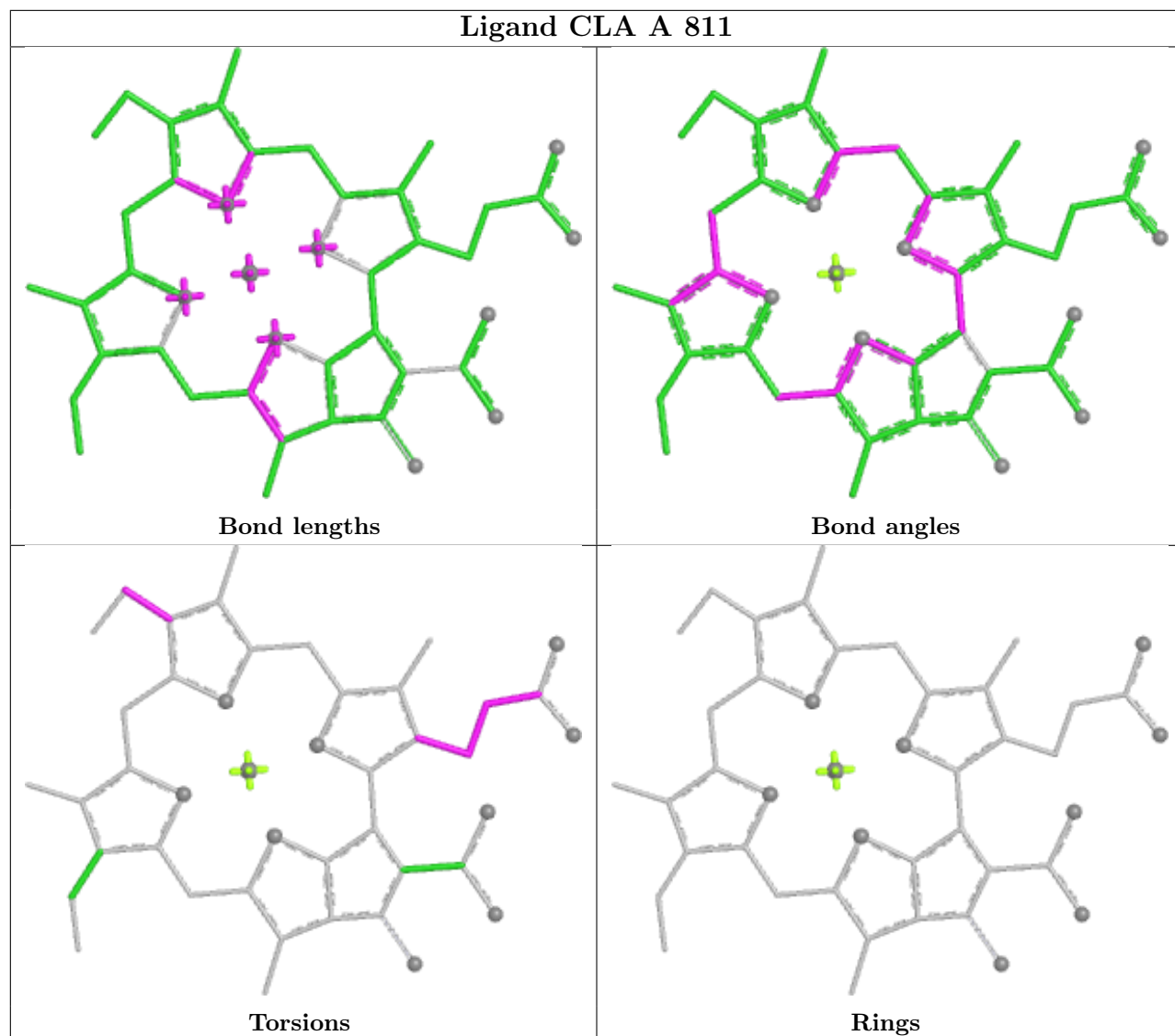
Ligand BCR G 204



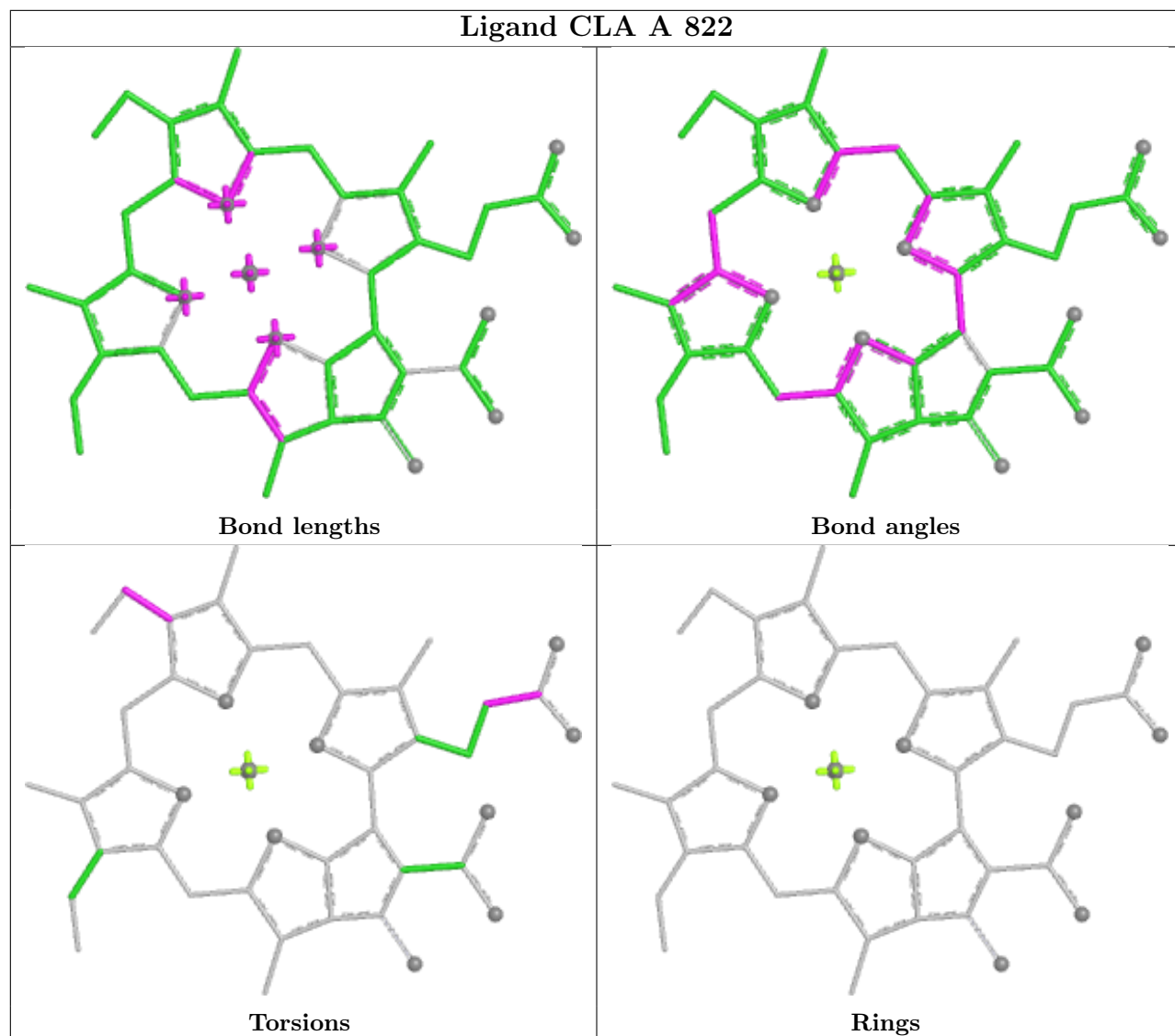
Ligand BCR 3 1004	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 6 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

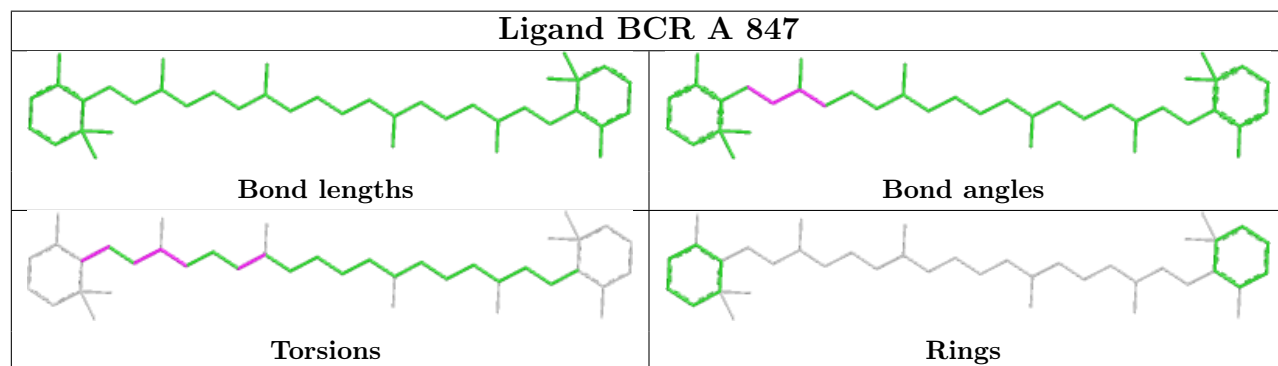
Ligand CLA A 811



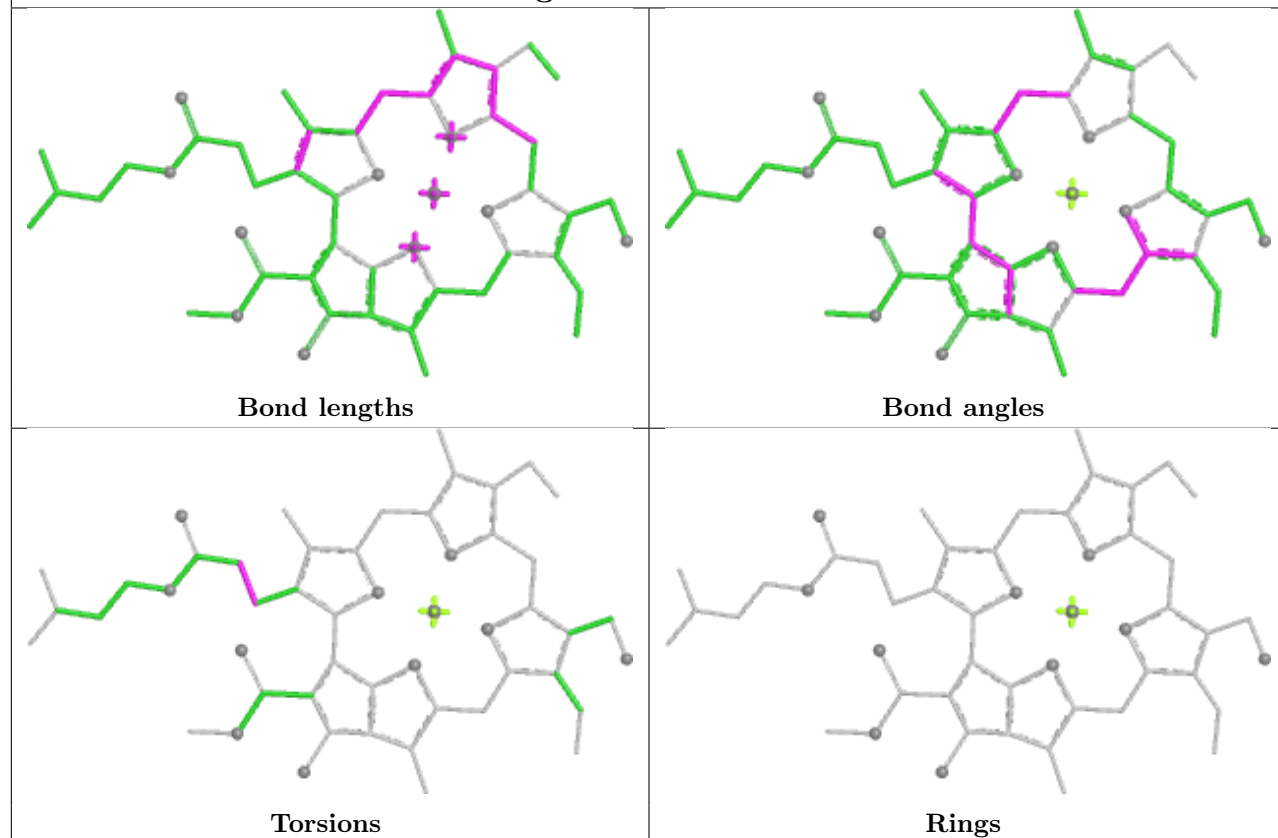
Ligand CLA A 822



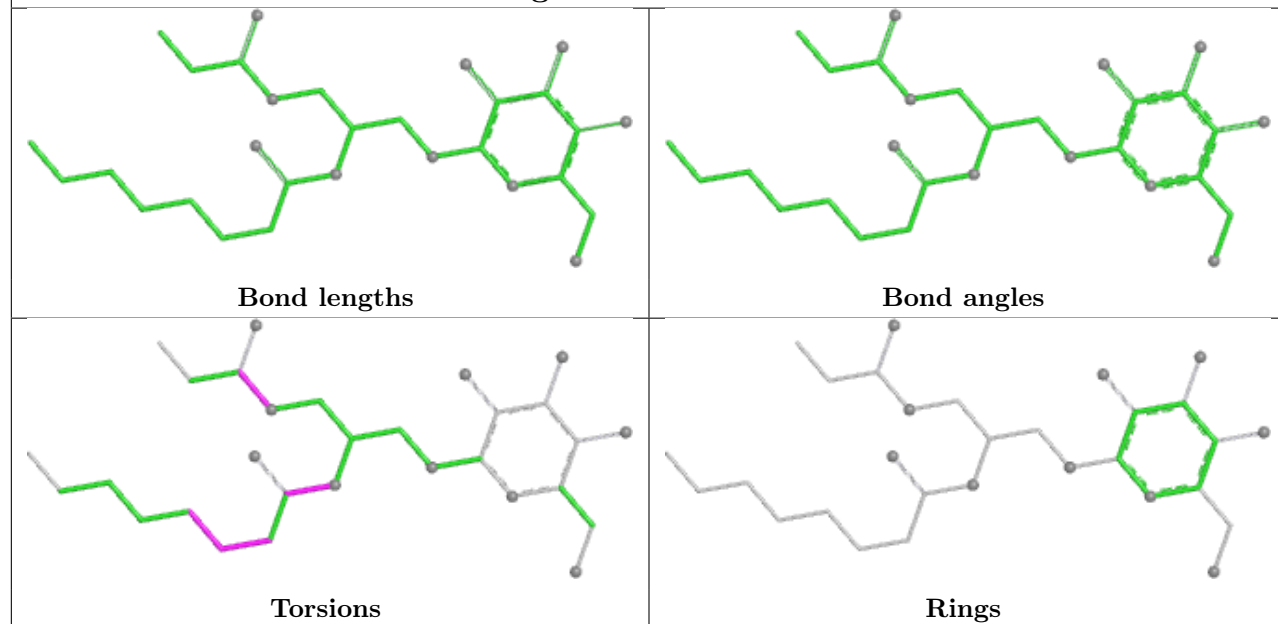
Ligand BCR A 847



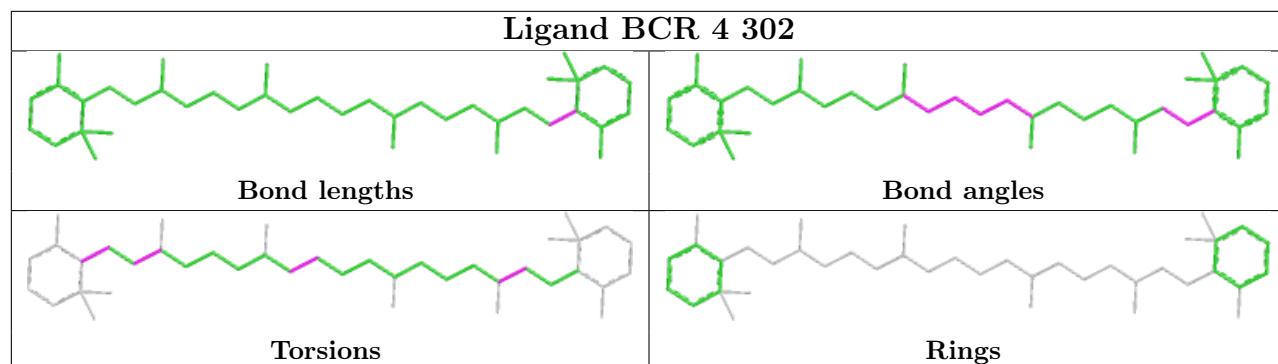
Ligand CHL 8 315



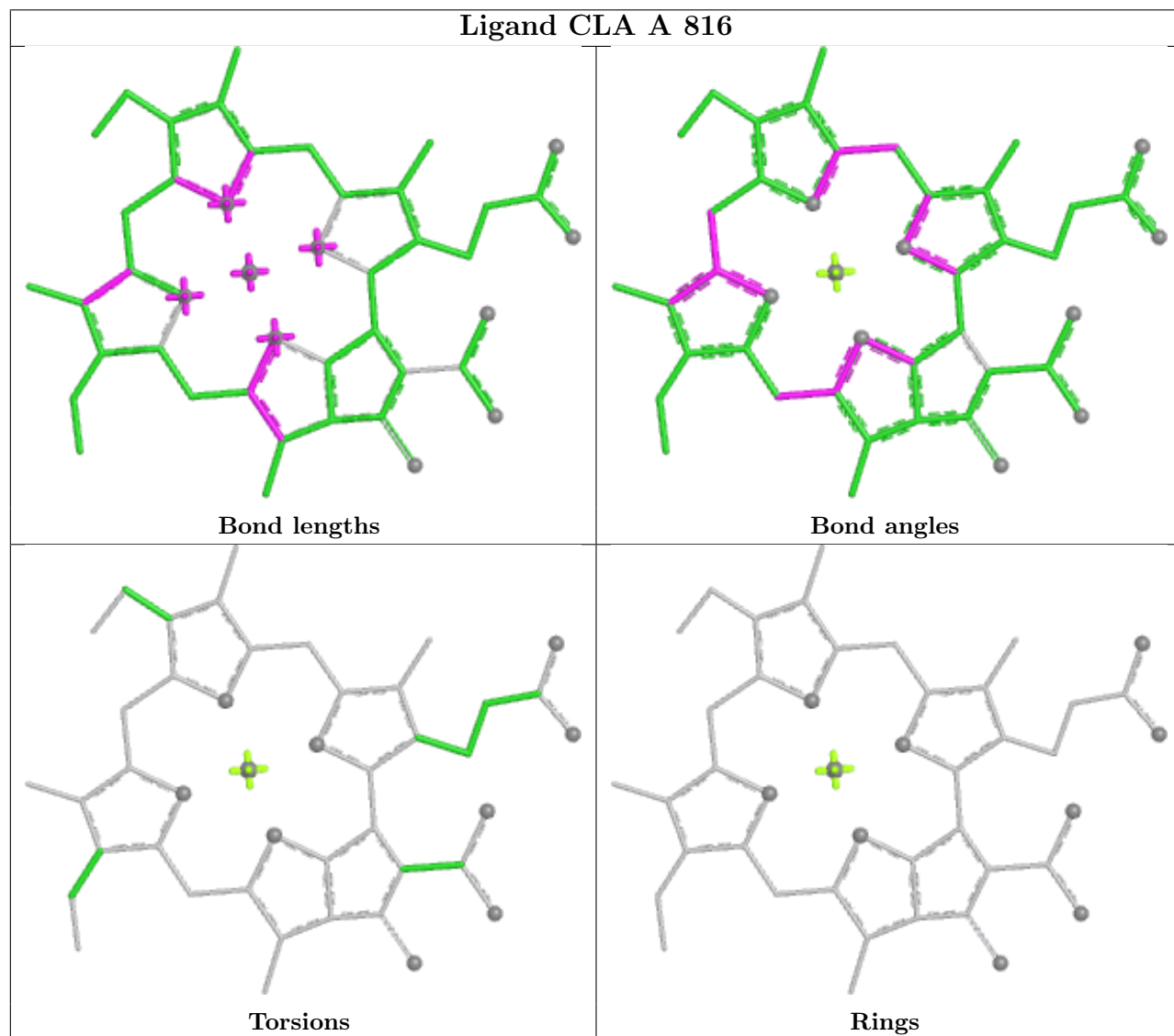
Ligand LMG J 101

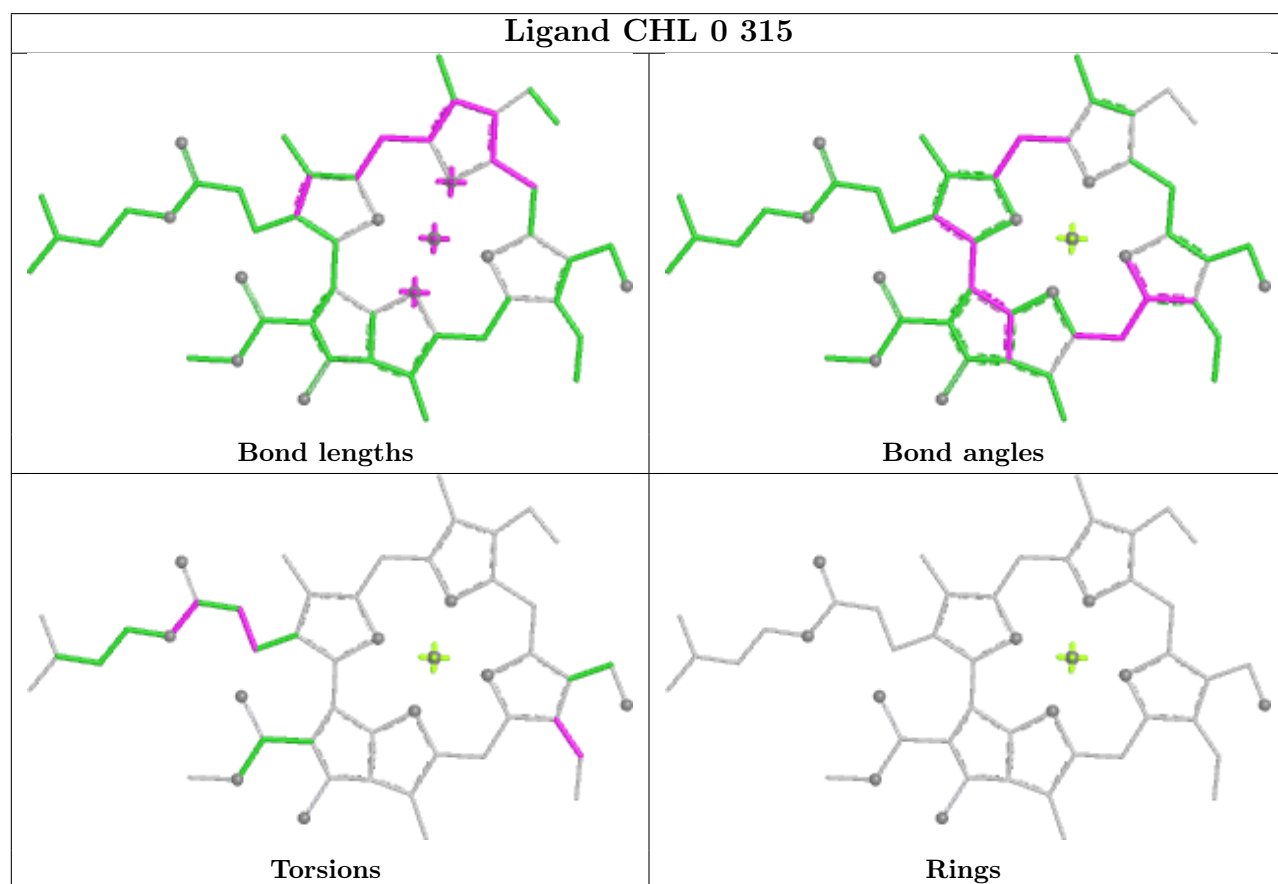
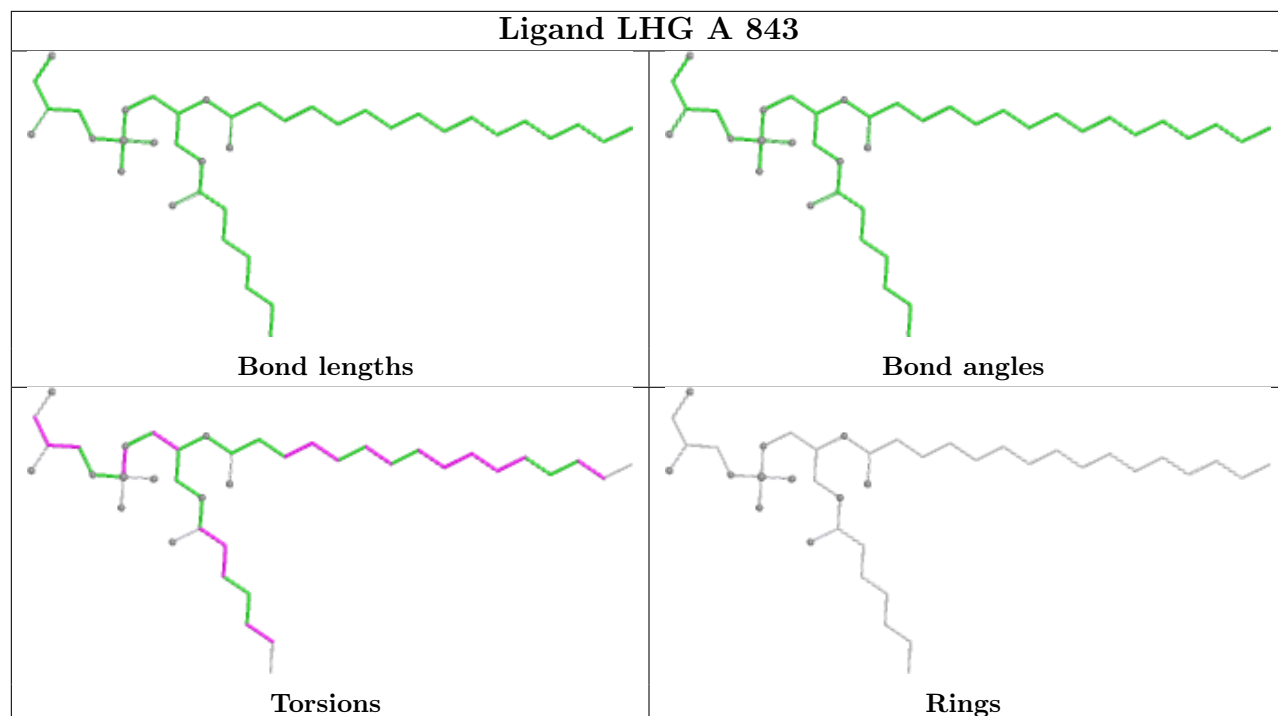


Ligand BCR 4 302

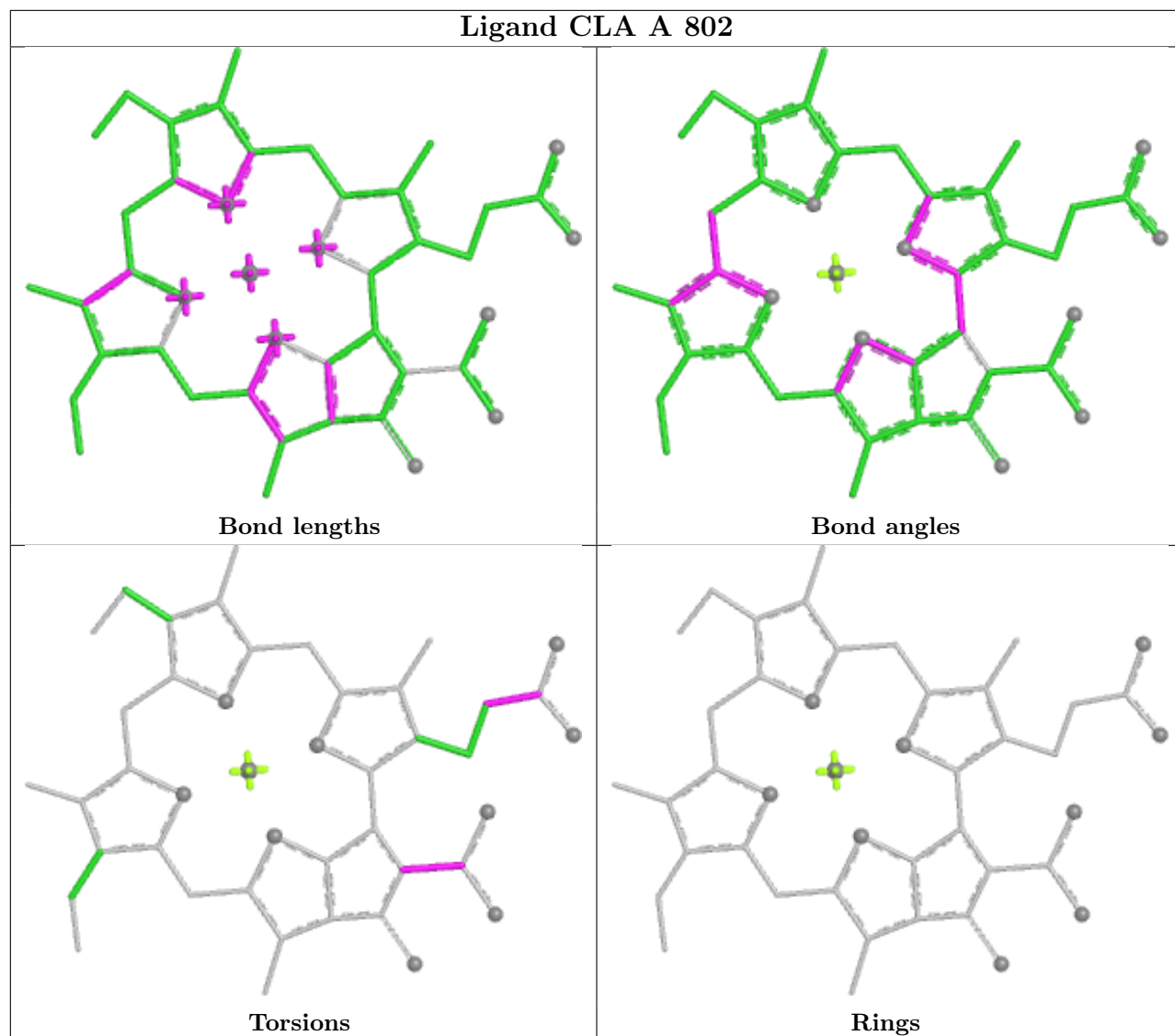


Ligand CLA A 816

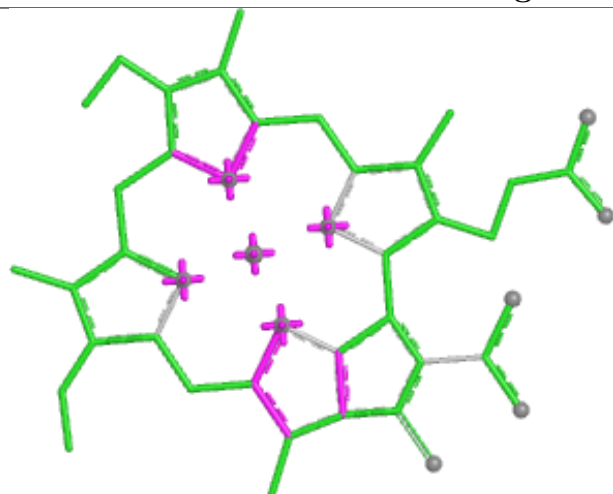




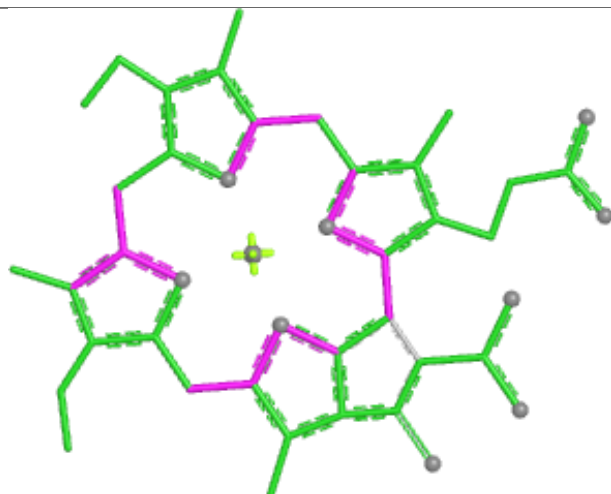
Ligand CLA A 802



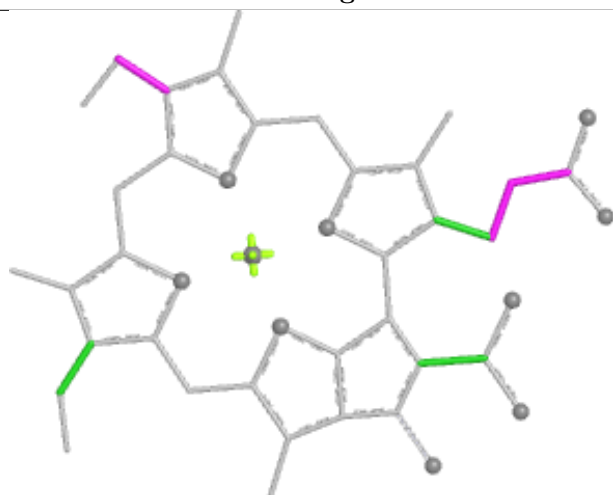
Ligand CLA B 803



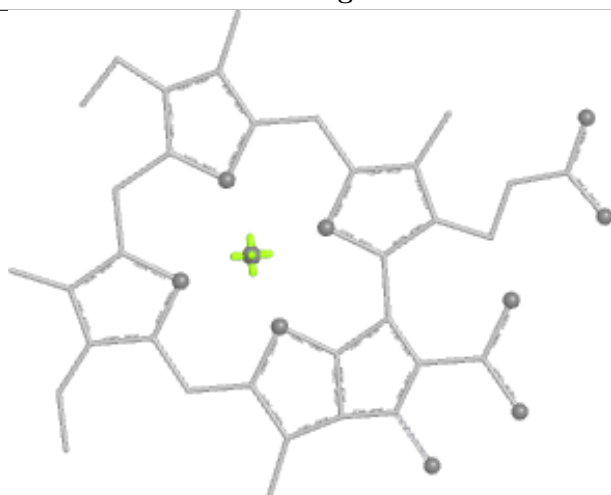
Bond lengths



Bond angles

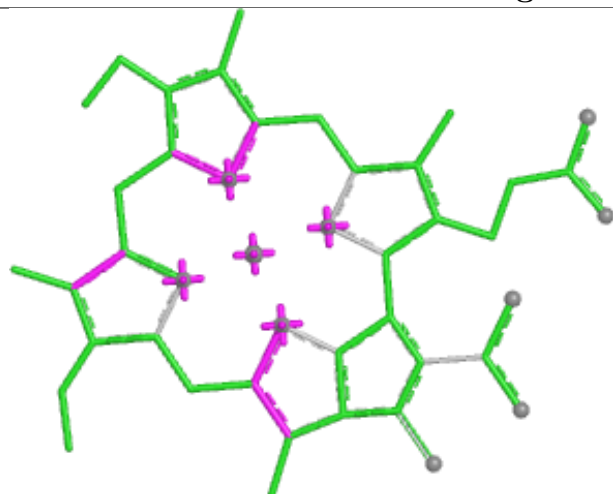


Torsions

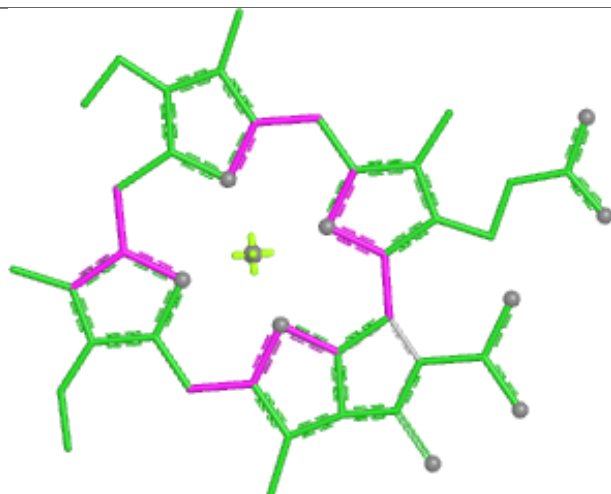


Rings

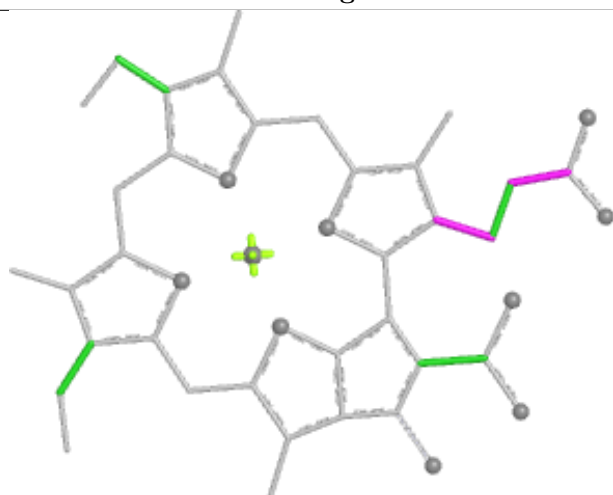
Ligand CLA L 204



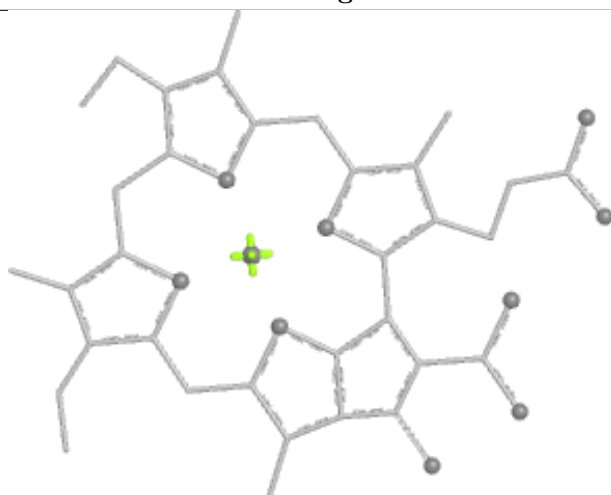
Bond lengths



Bond angles

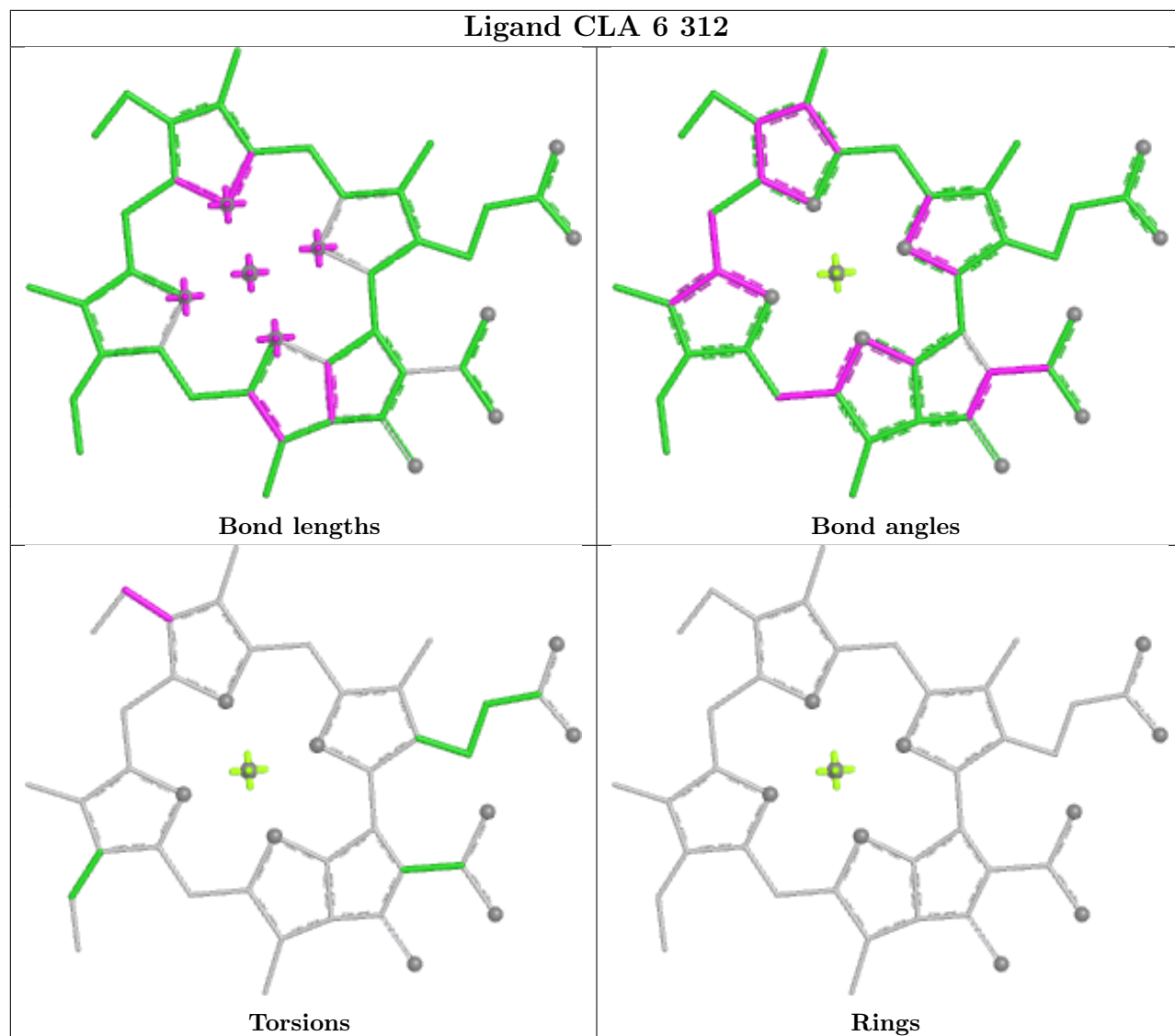


Torsions

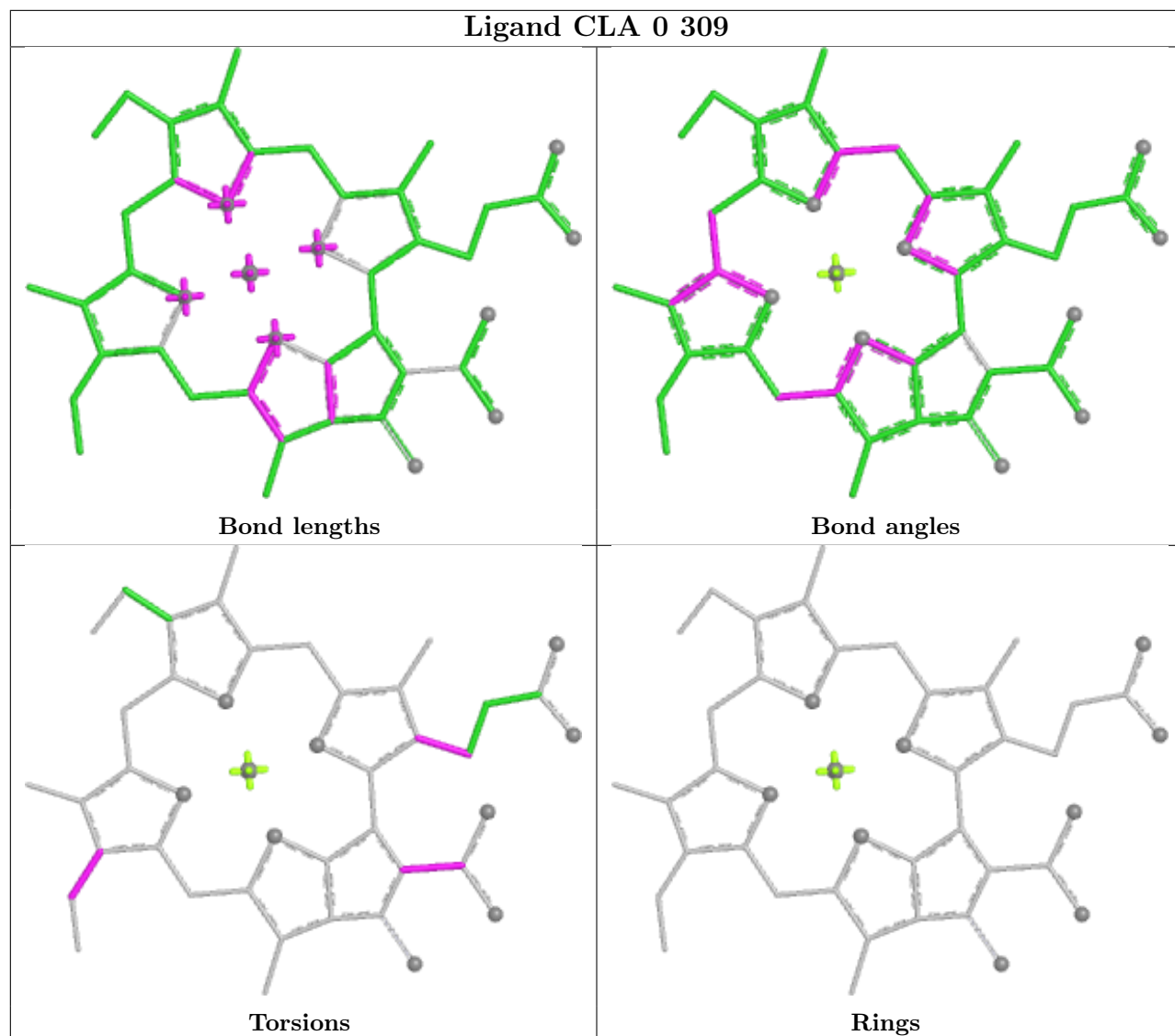


Rings

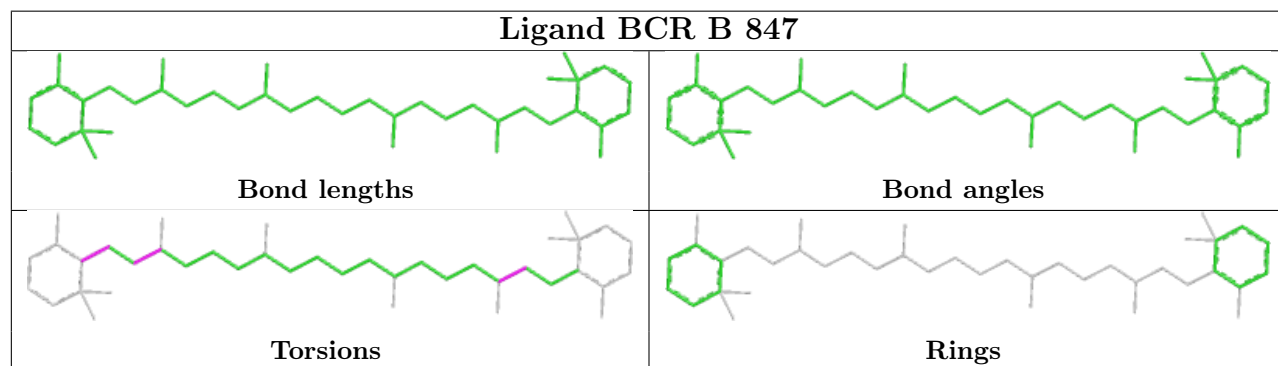
Ligand CLA 6 312



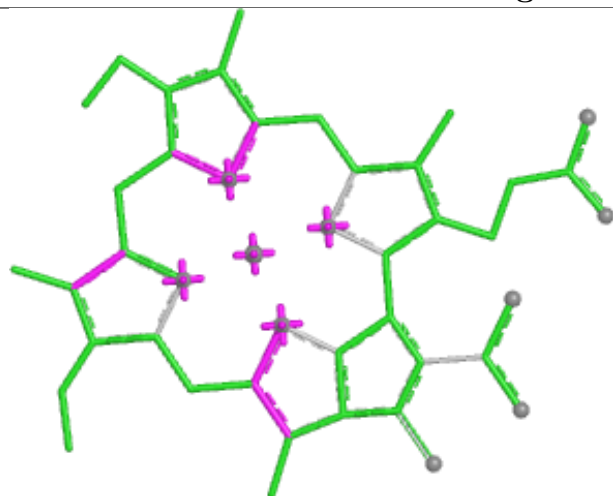
Ligand CLA 0 309



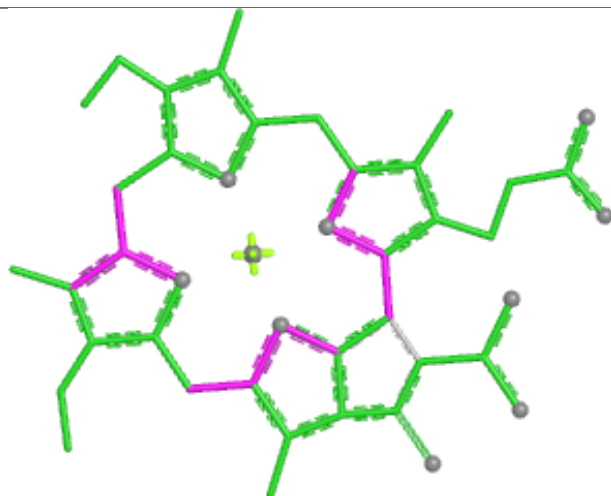
Ligand BCR B 847



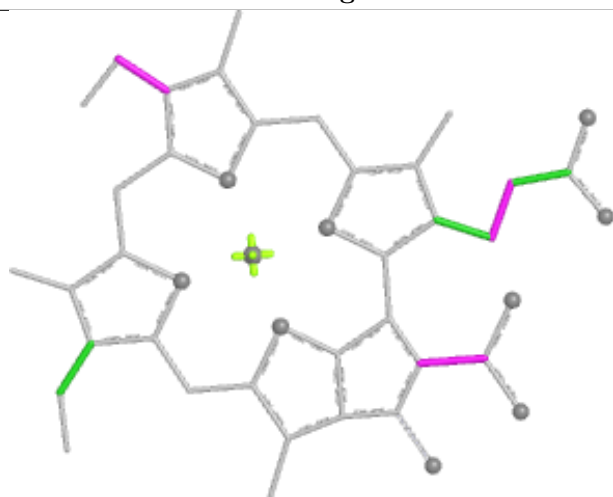
Ligand CLA L 201



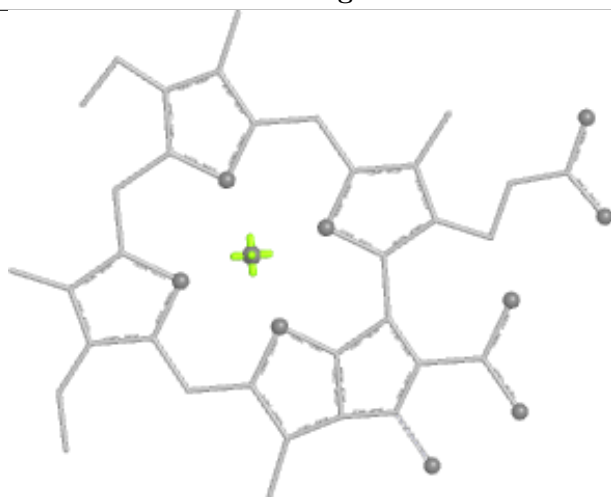
Bond lengths



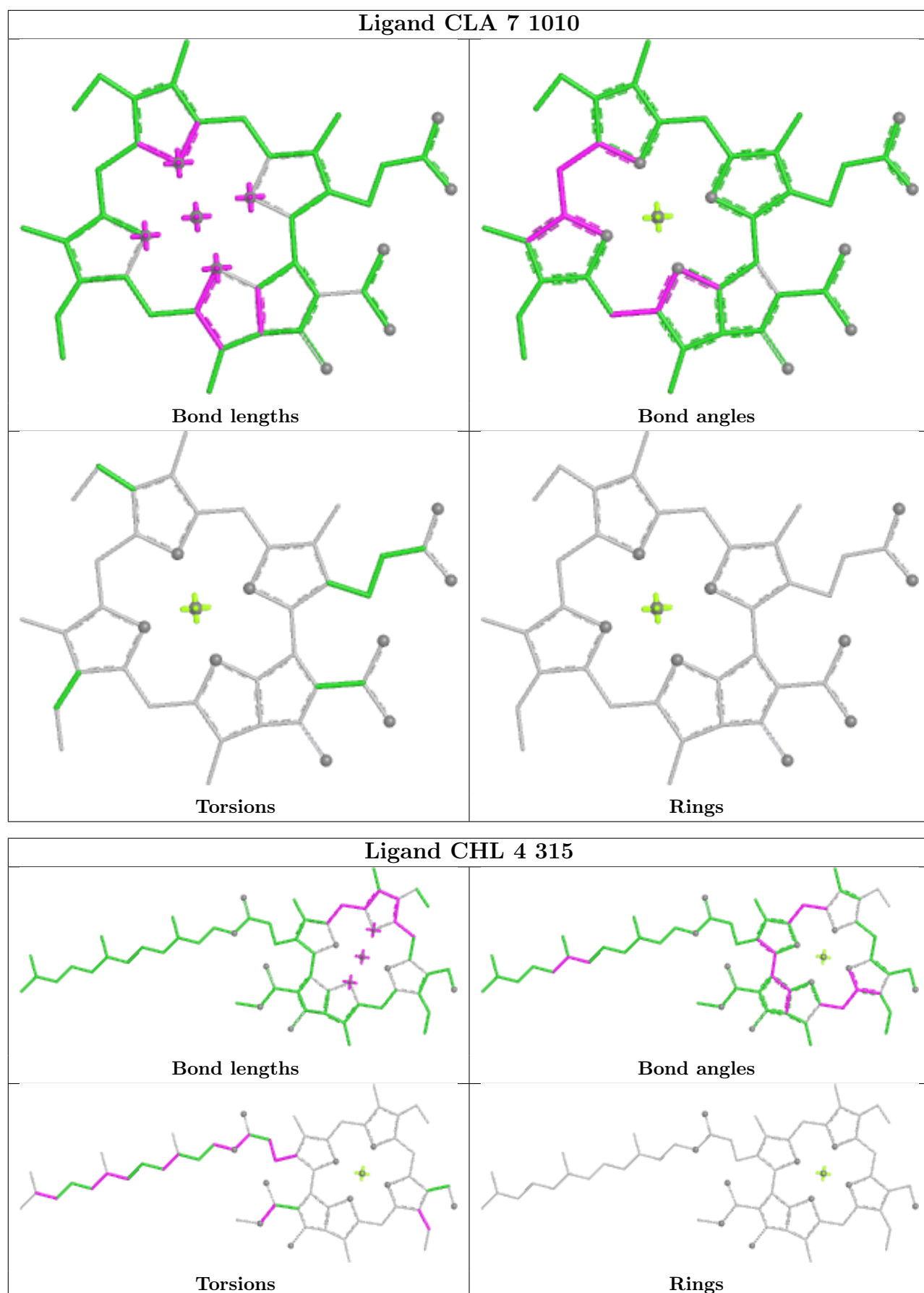
Bond angles



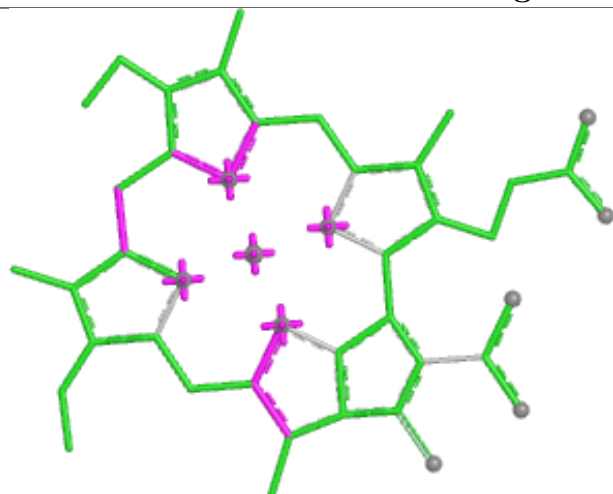
Torsions



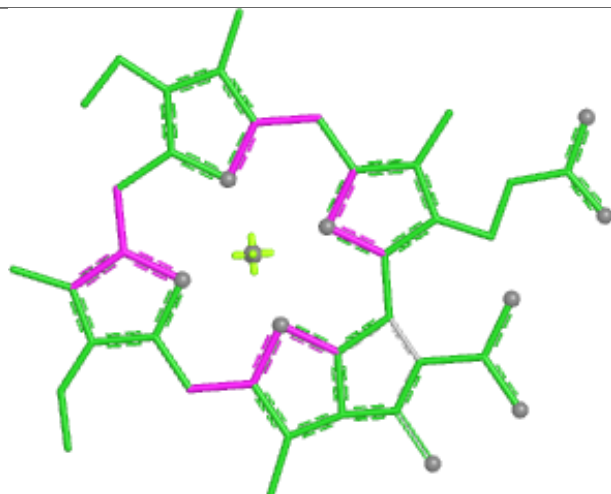
Rings



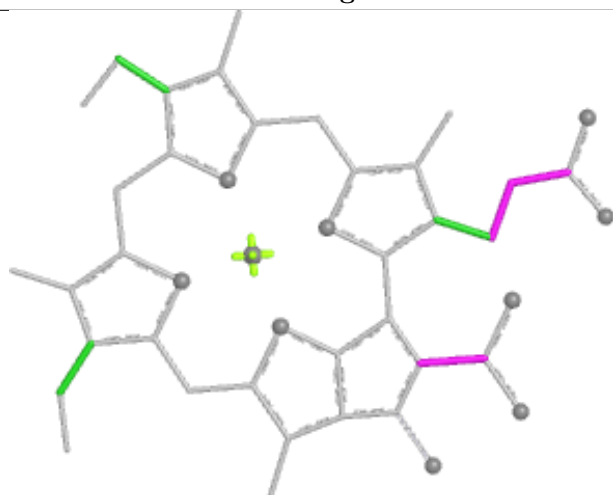
Ligand CLA A 815



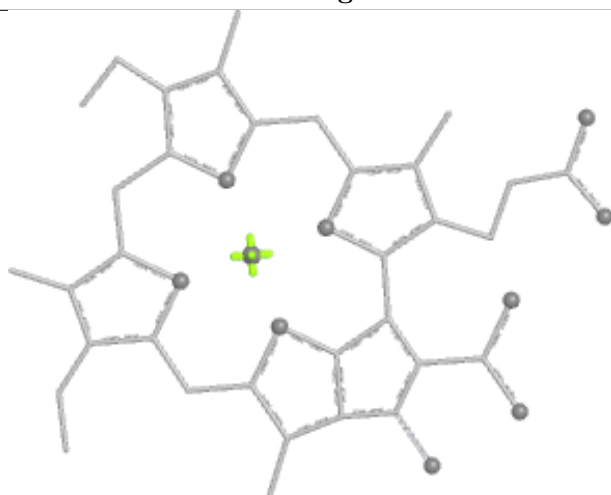
Bond lengths



Bond angles

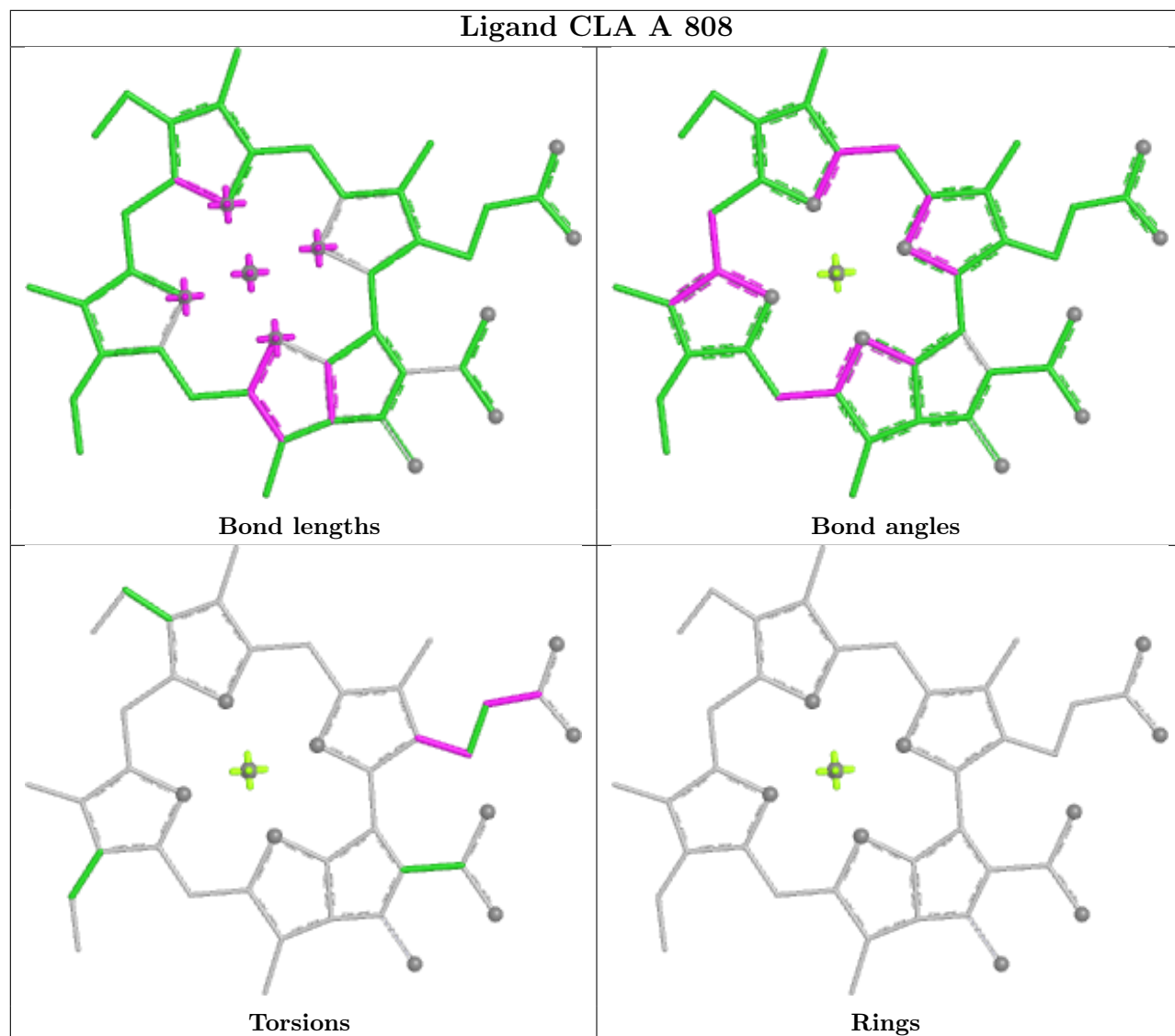


Torsions

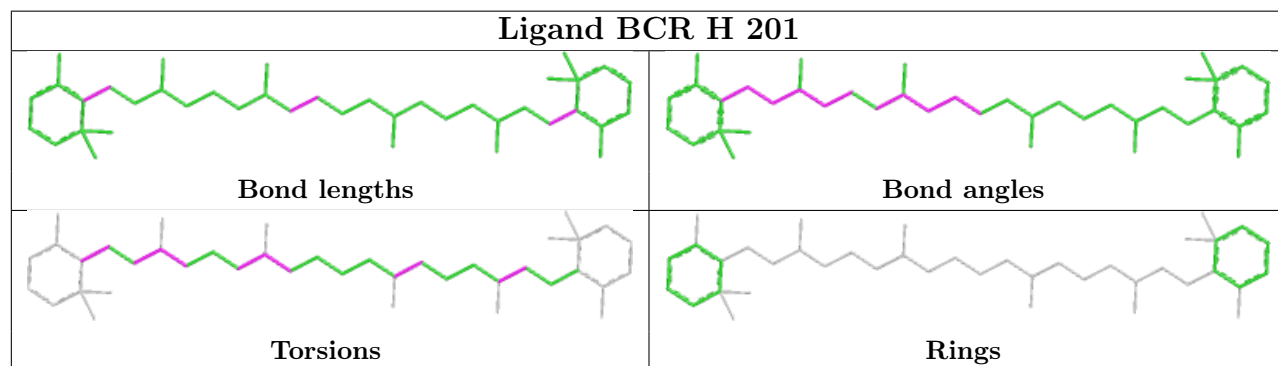


Rings

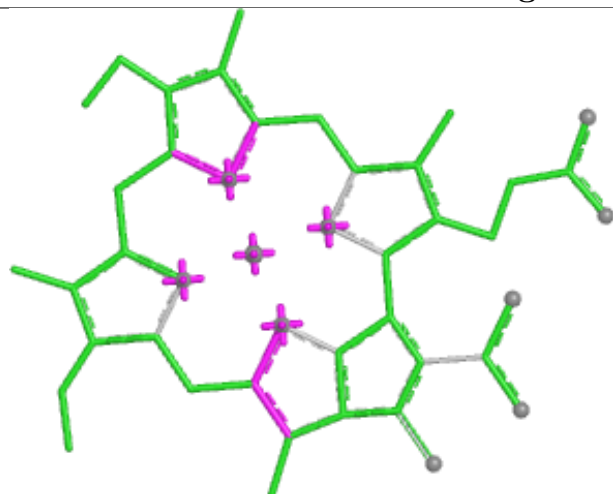
Ligand CLA A 808



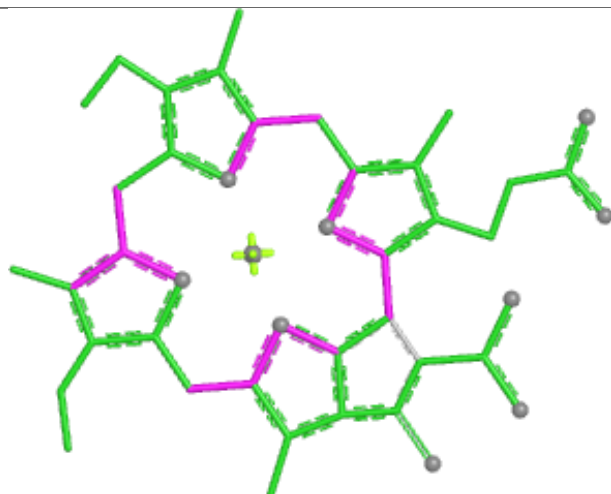
Ligand BCR H 201



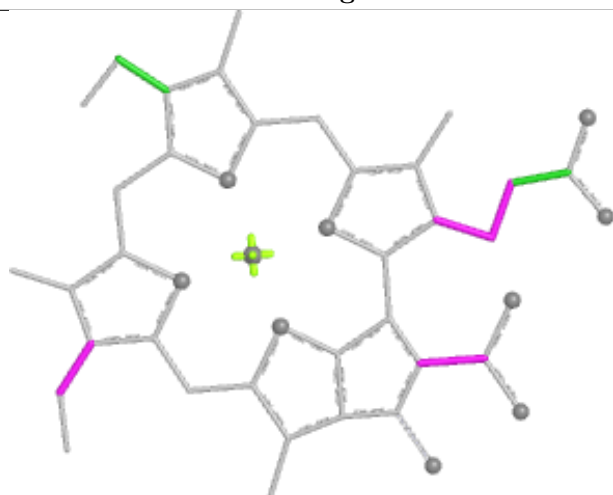
Ligand CLA 4 308



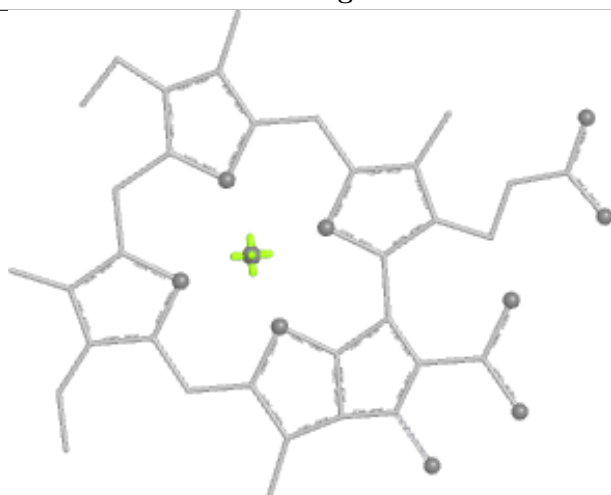
Bond lengths



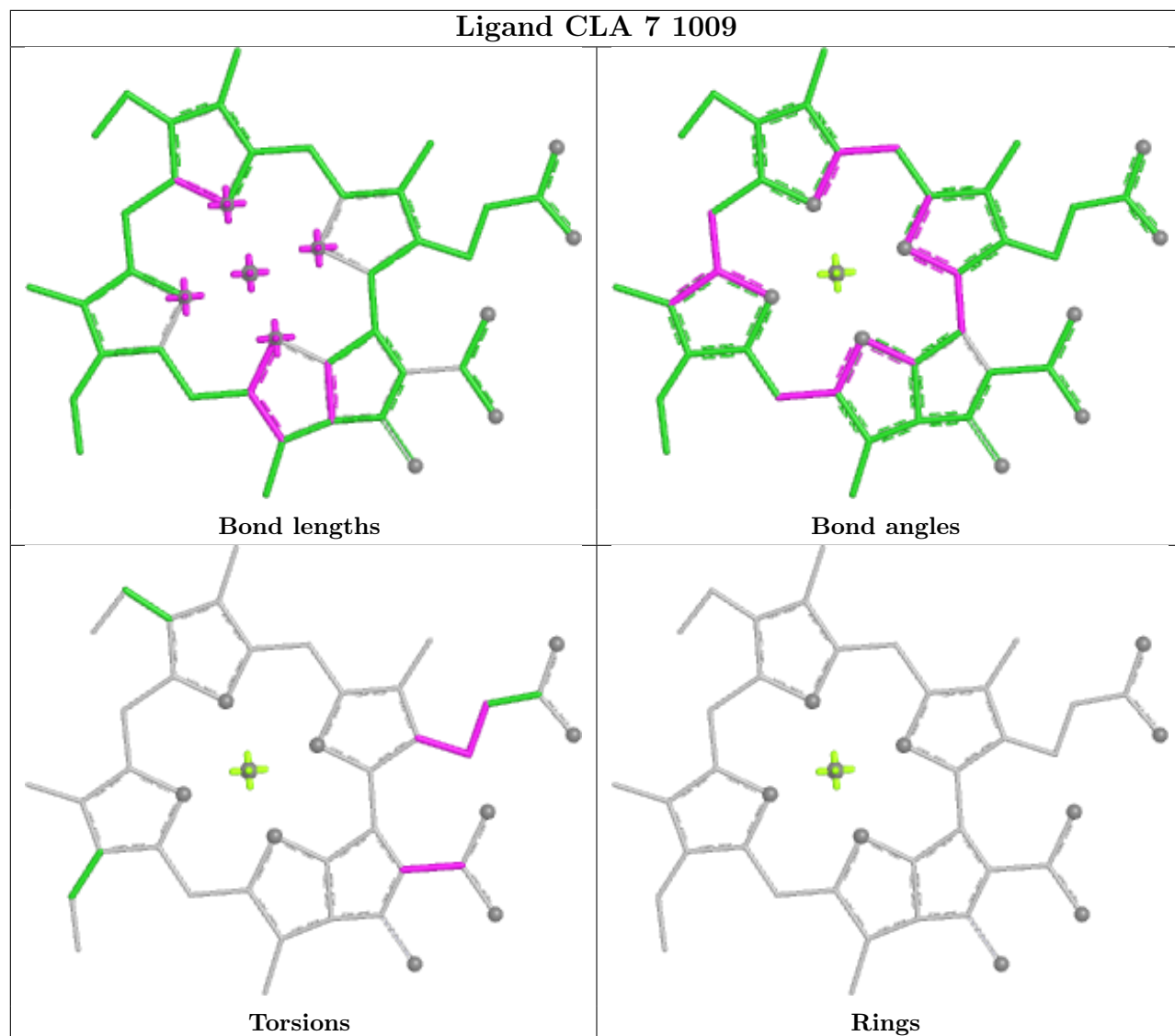
Bond angles



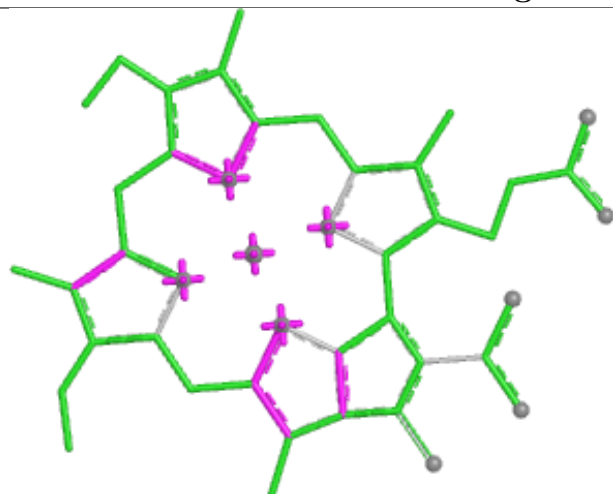
Torsions



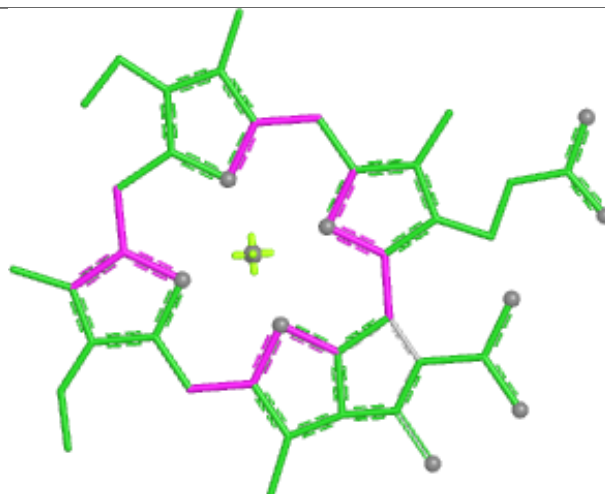
Rings



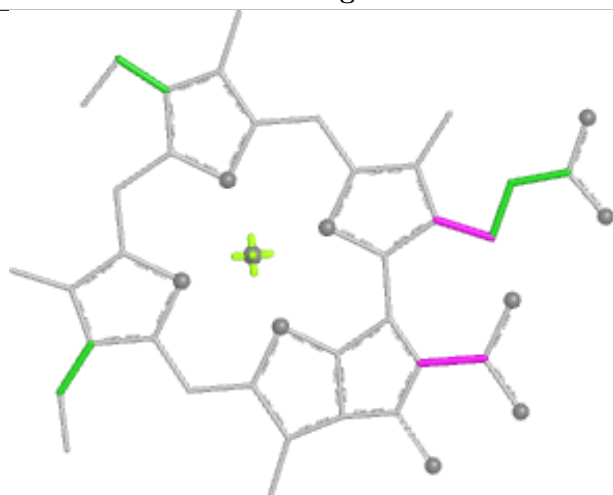
Ligand CLA B 828



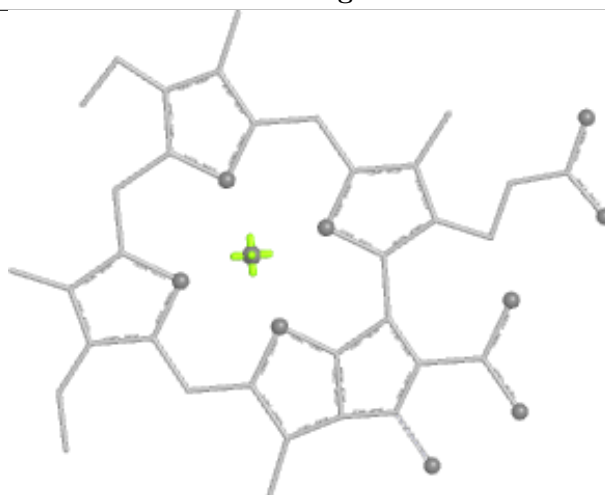
Bond lengths



Bond angles

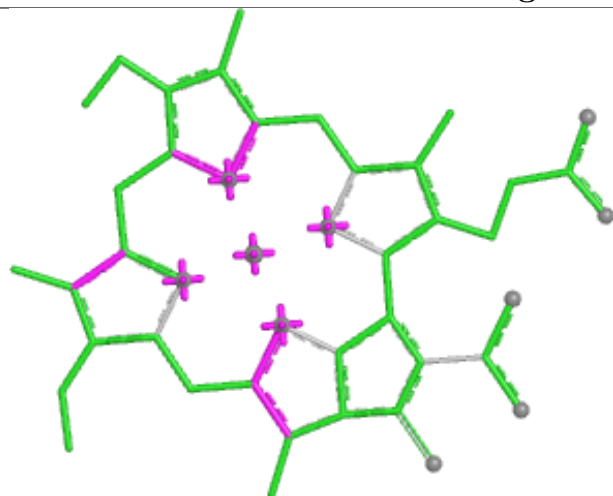


Torsions

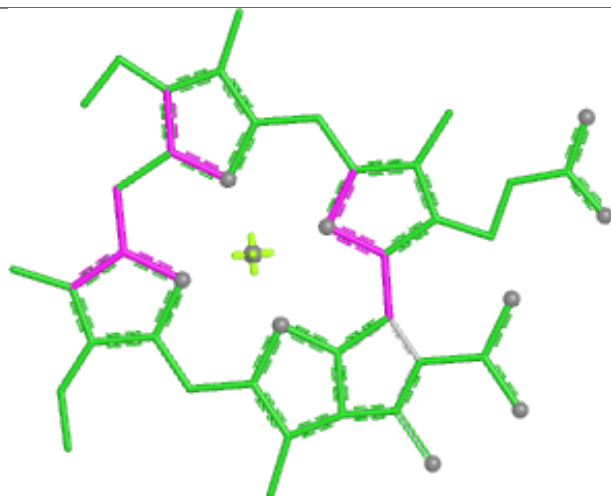


Rings

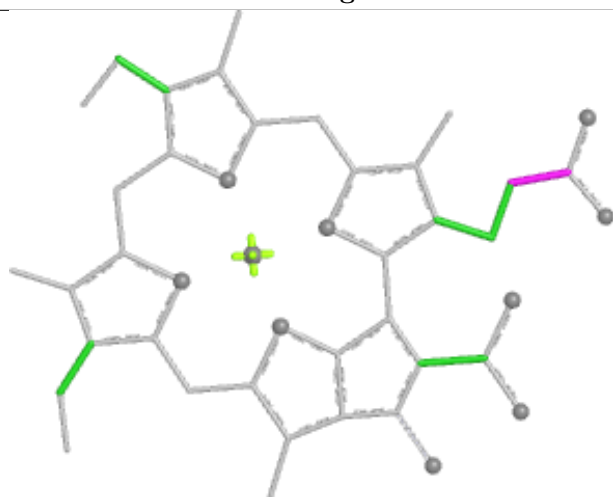
Ligand CLA 5 304



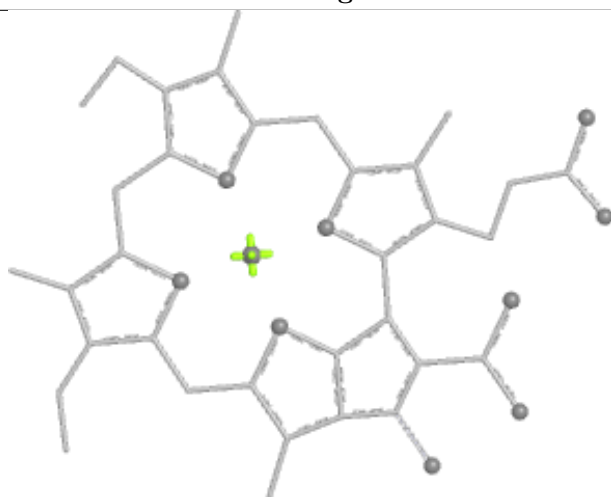
Bond lengths



Bond angles

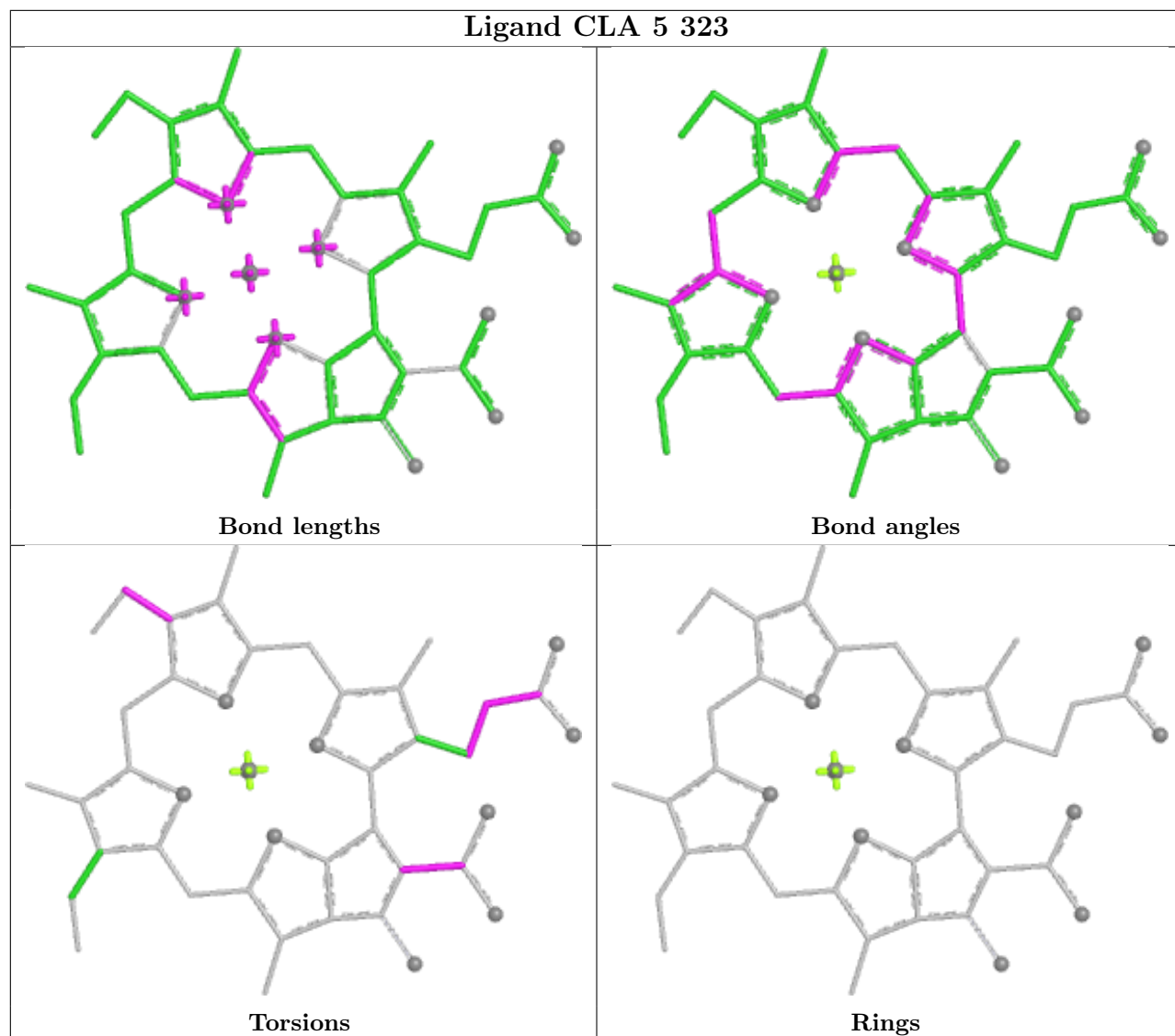


Torsions

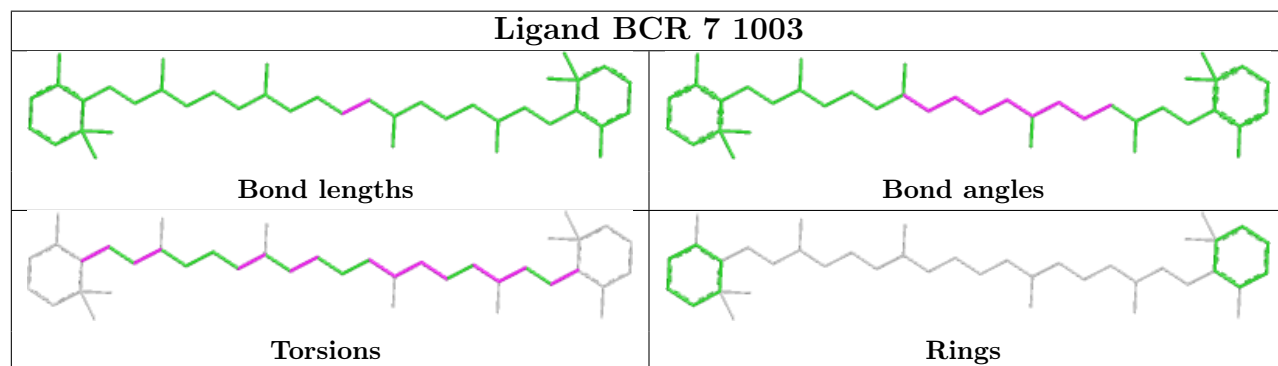


Rings

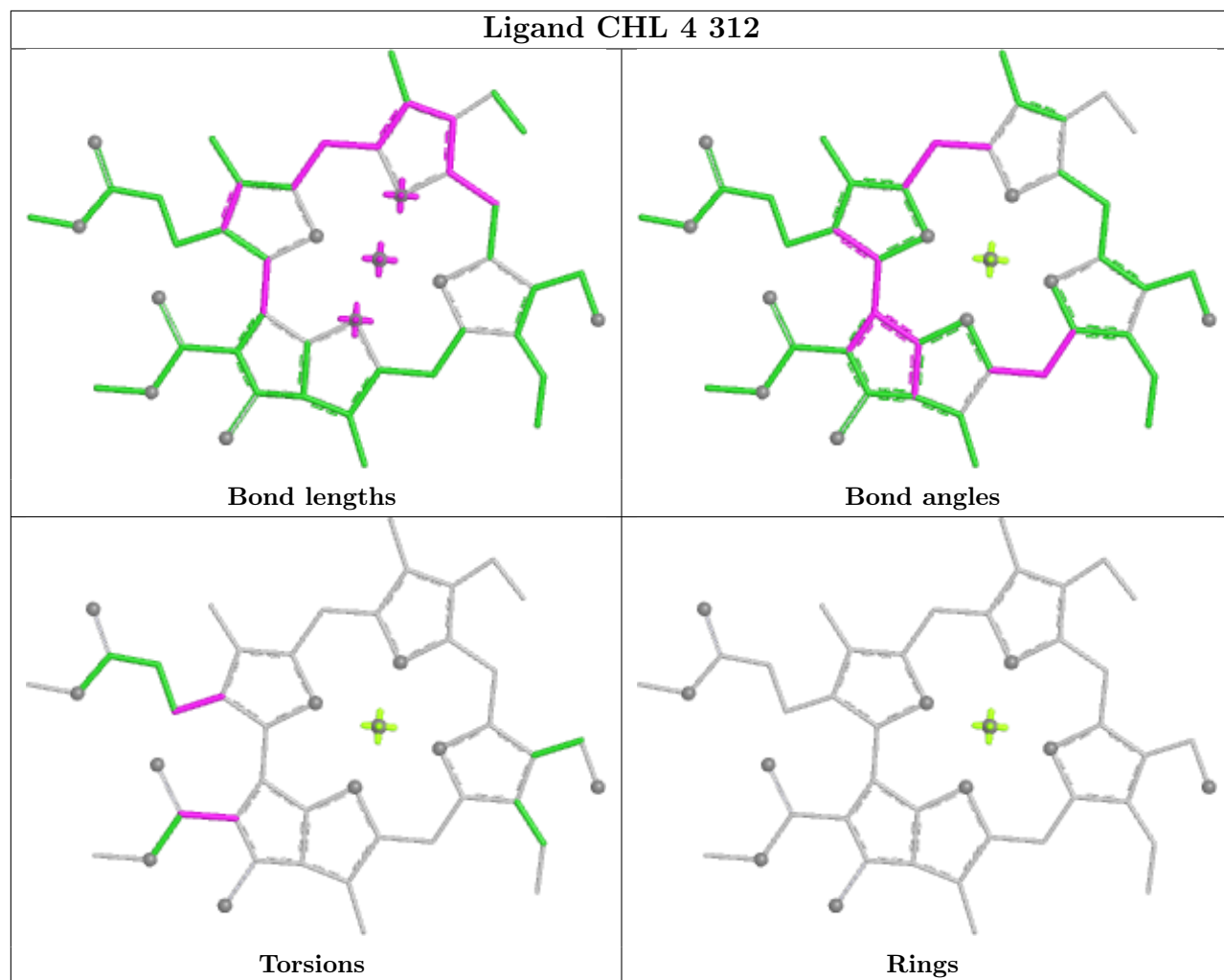
Ligand CLA 5 323



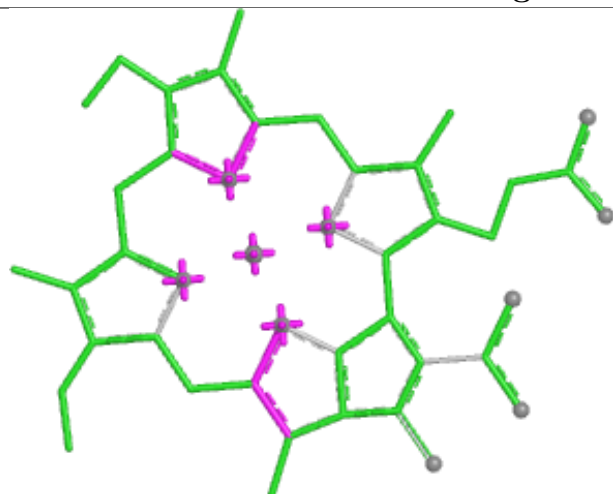
Ligand BCR 7 1003



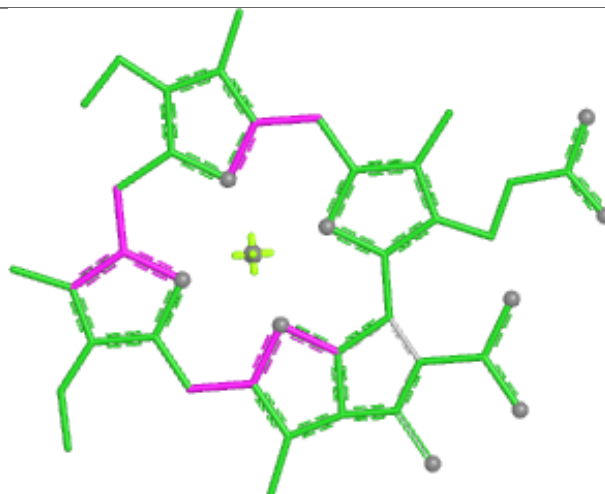
Ligand CHL 4 312



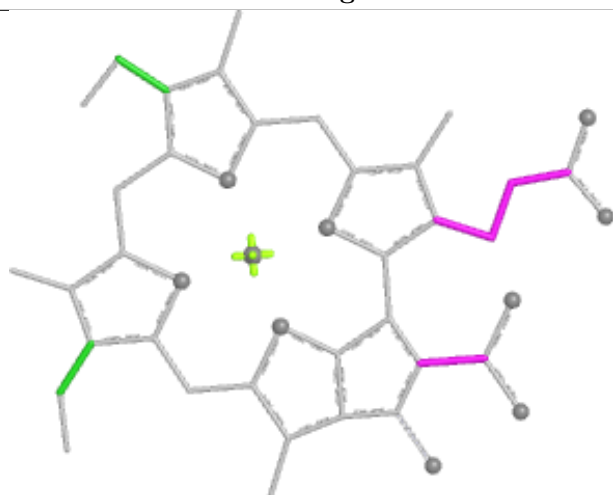
Ligand CLA K 201



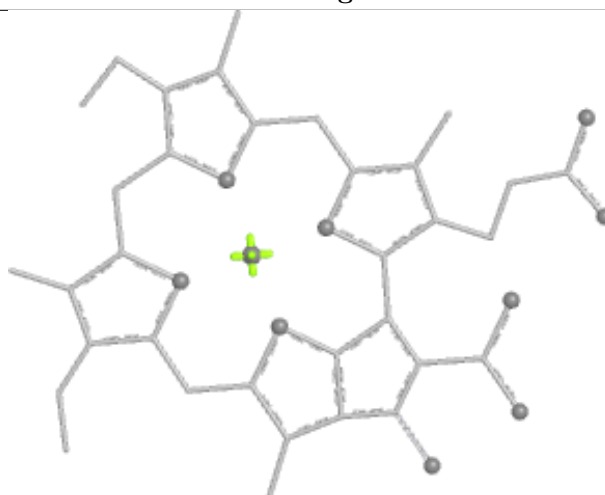
Bond lengths



Bond angles

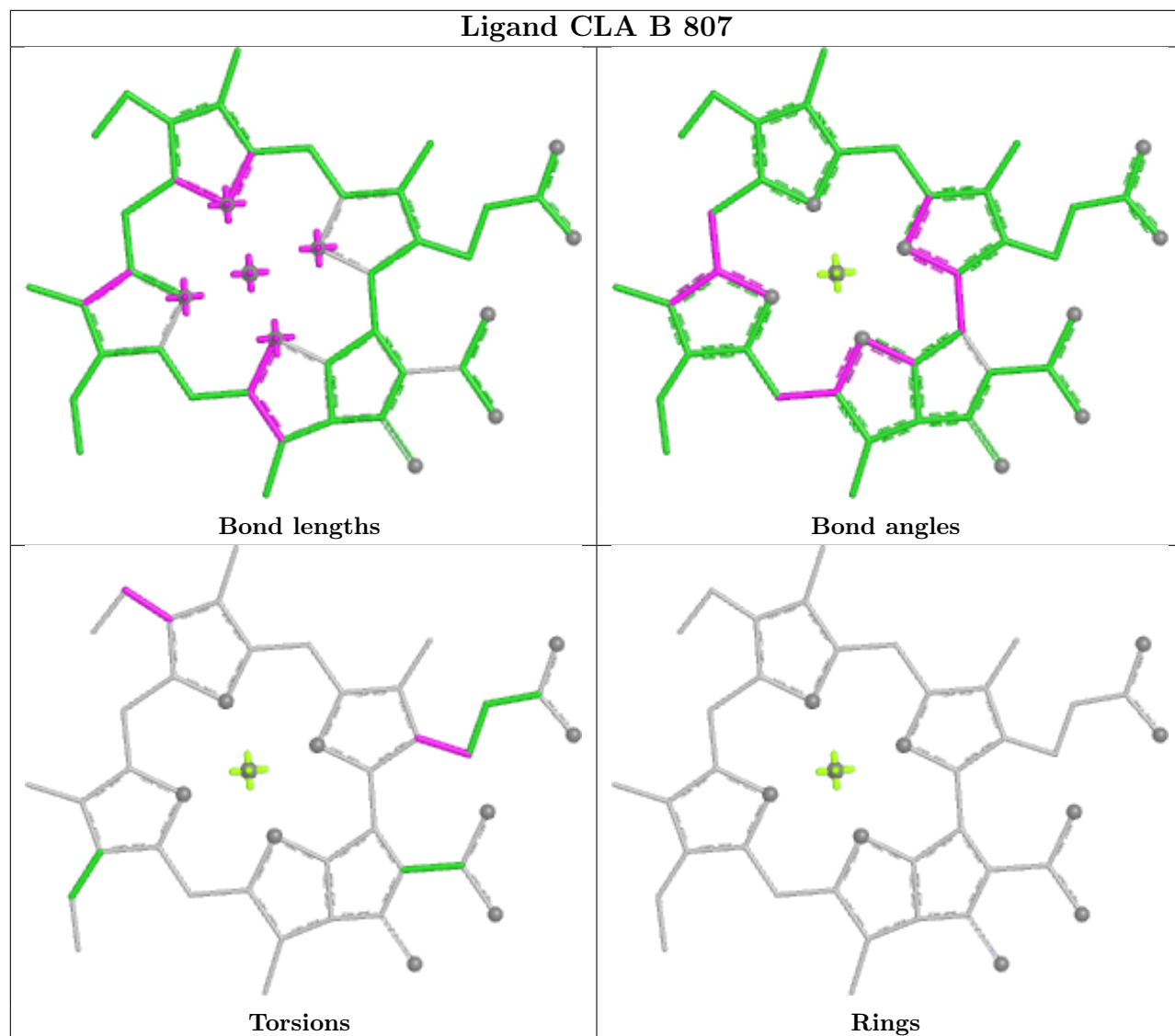


Torsions

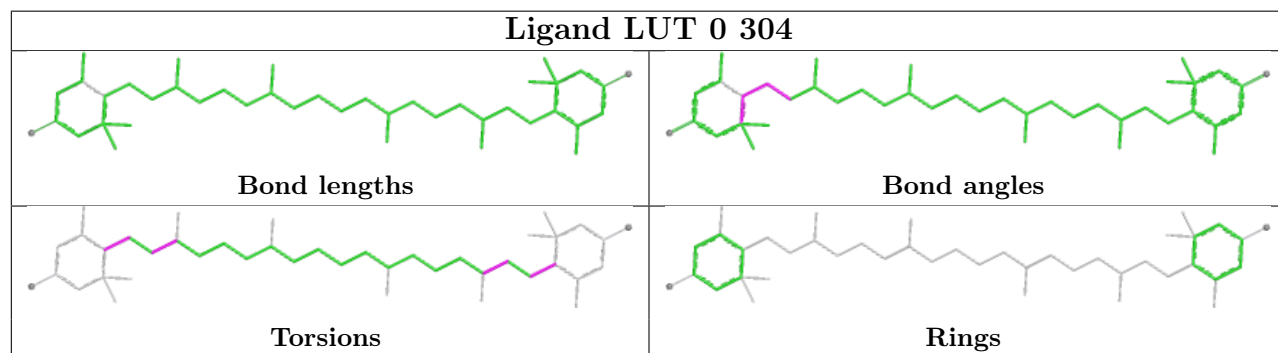


Rings

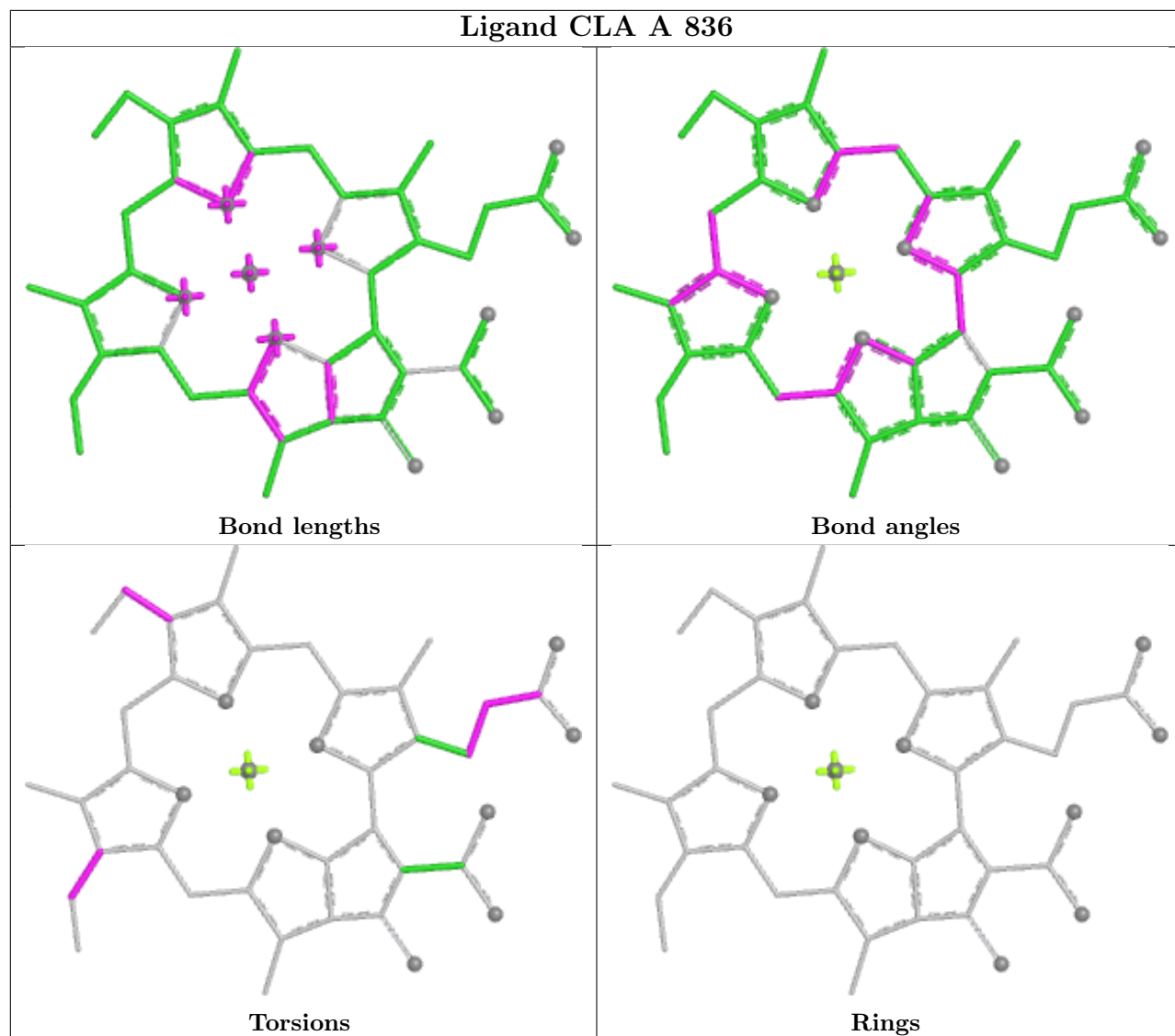
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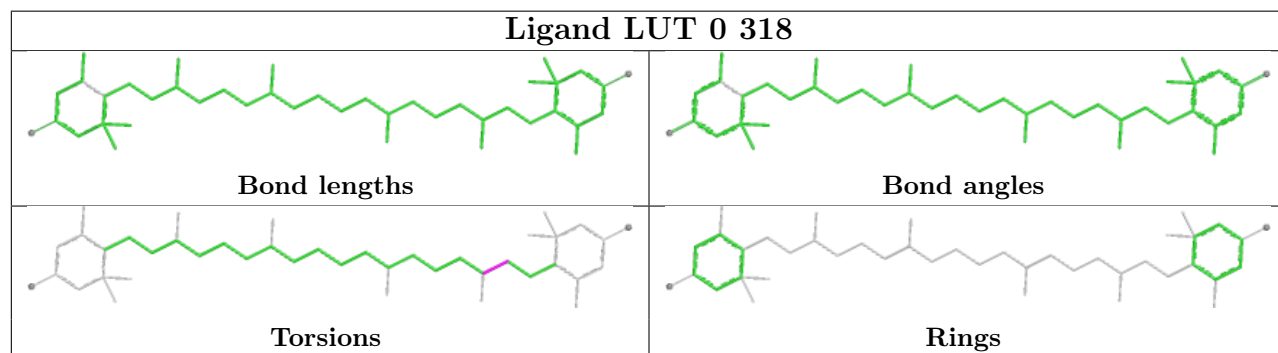
Ligand LUT 0 304



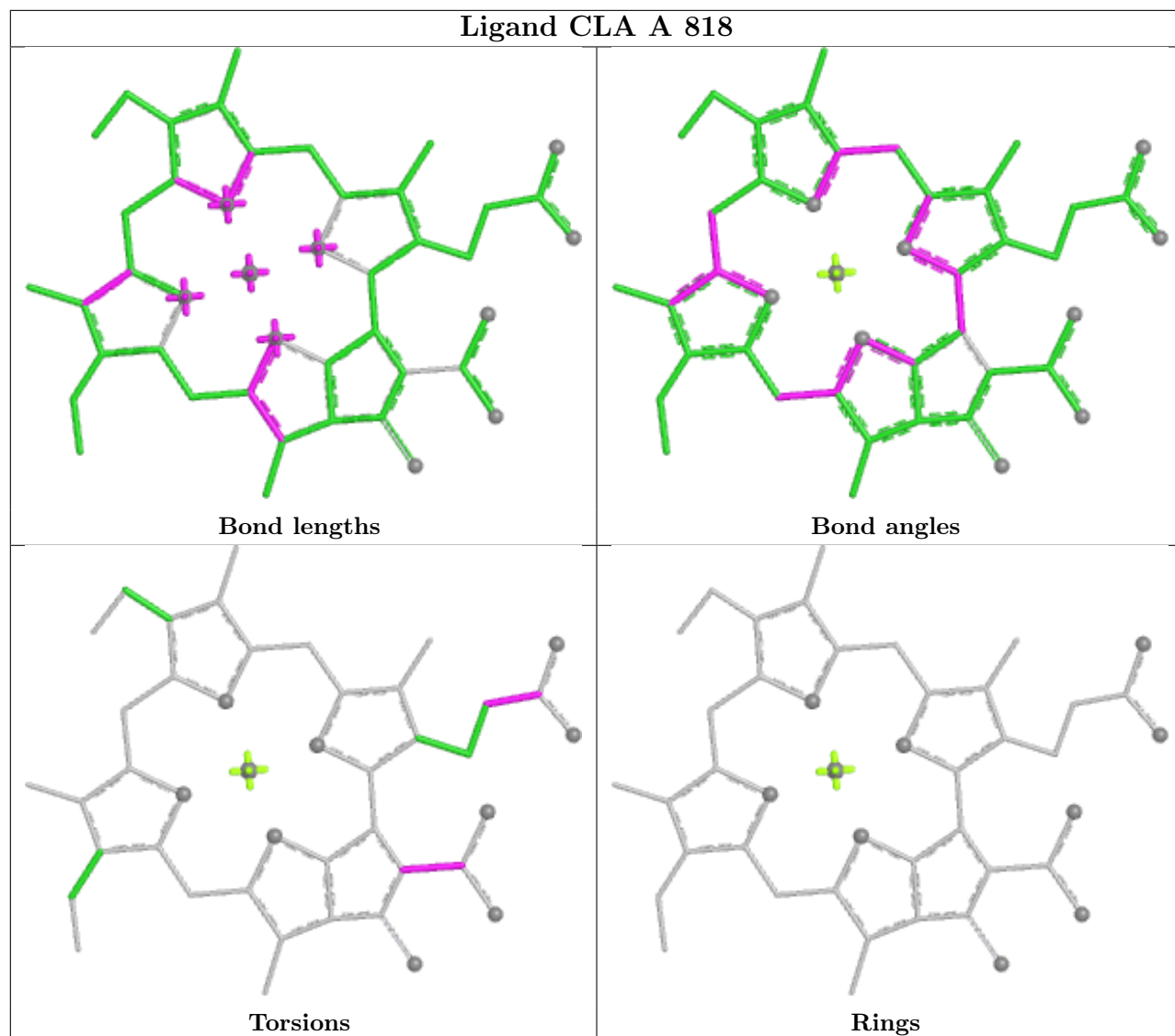
Ligand CLA A 836



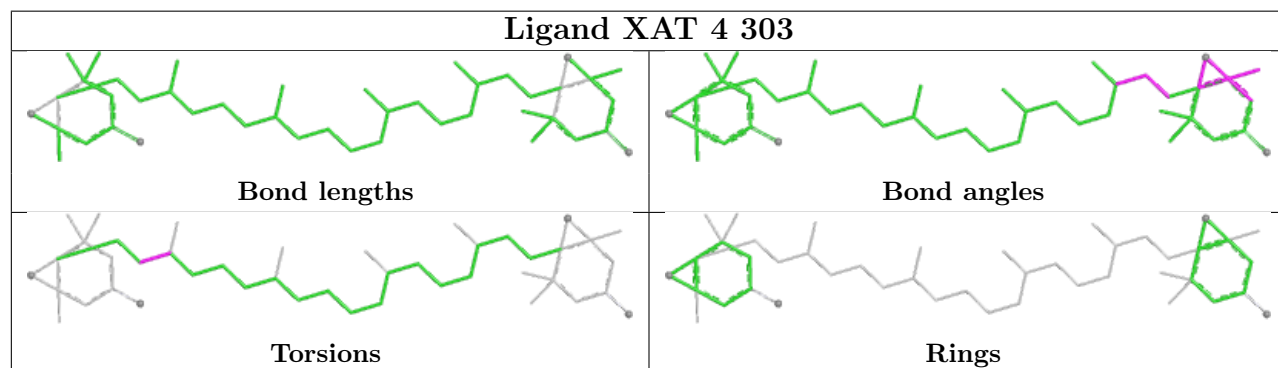
Ligand LUT 0 318

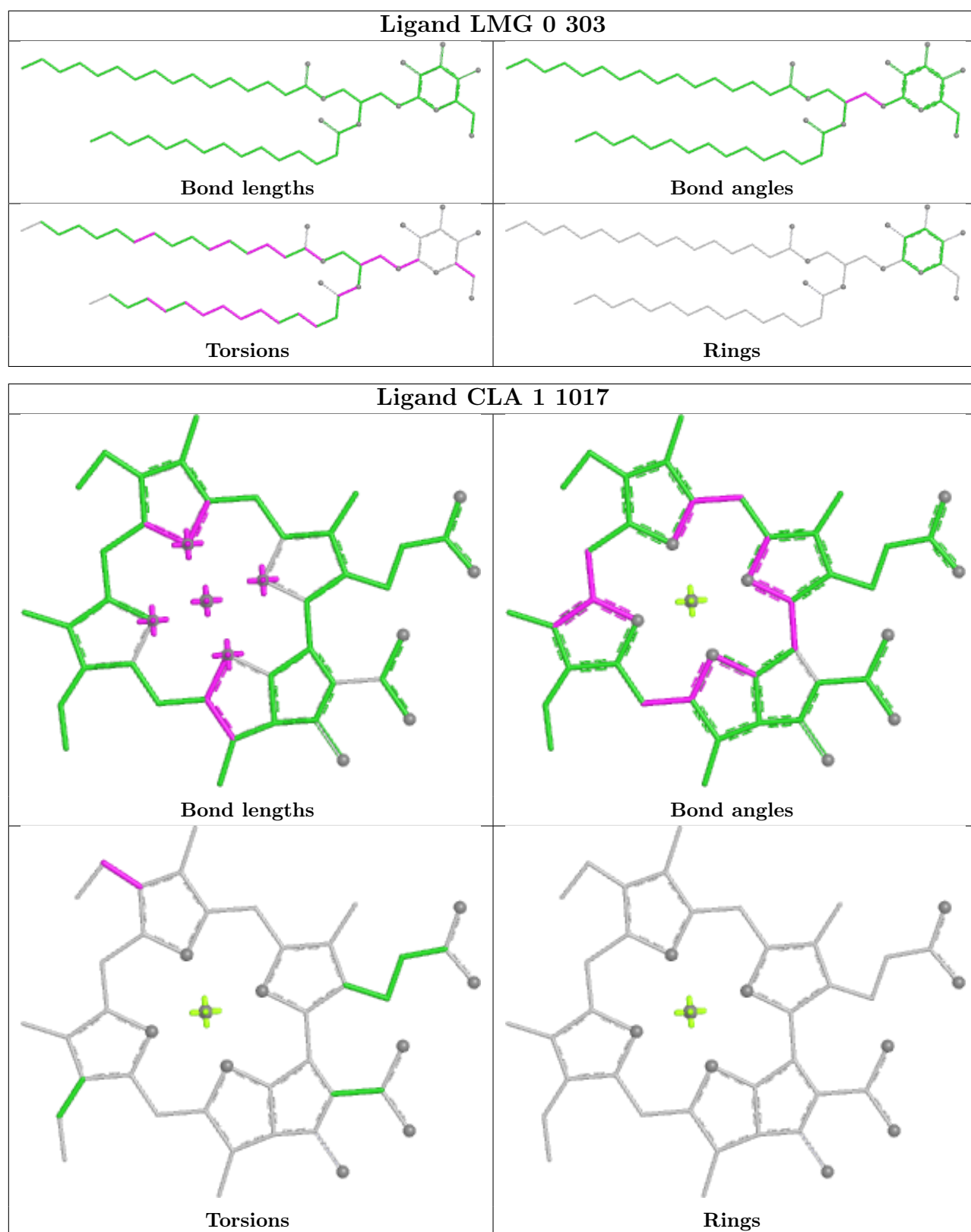


Ligand CLA A 818

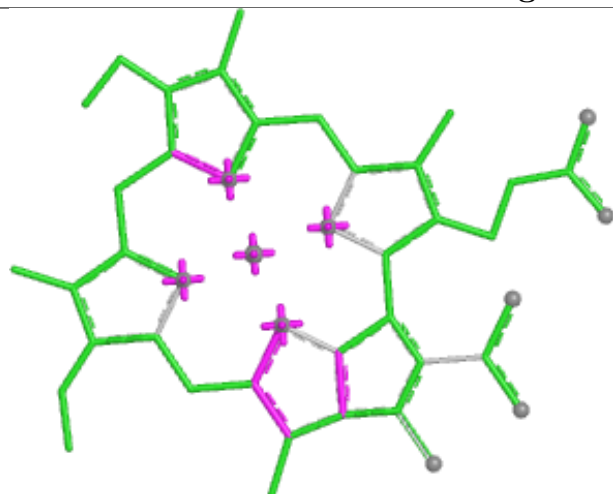


Ligand XAT 4 303

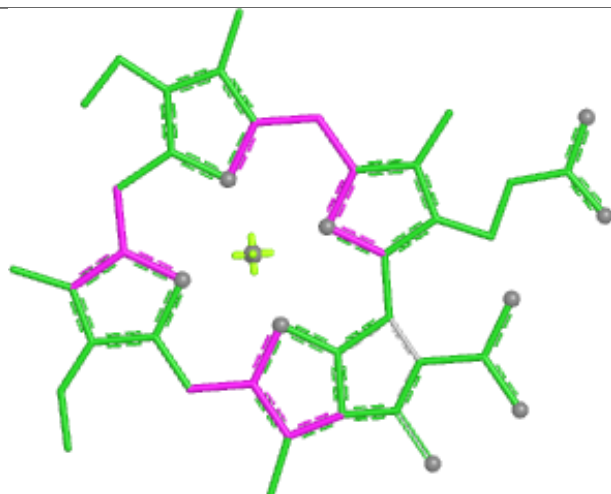




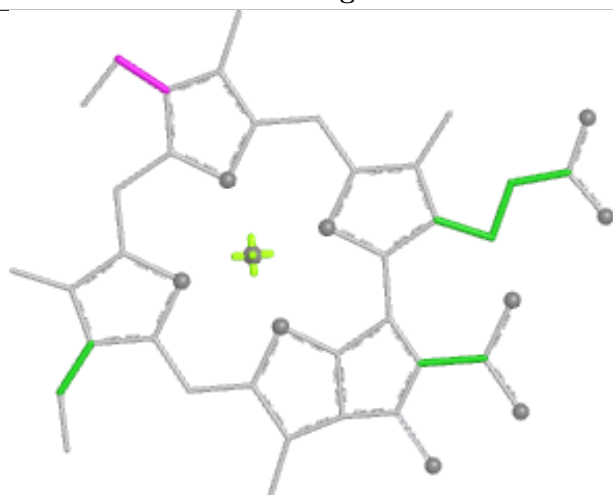
Ligand CLA 6 315



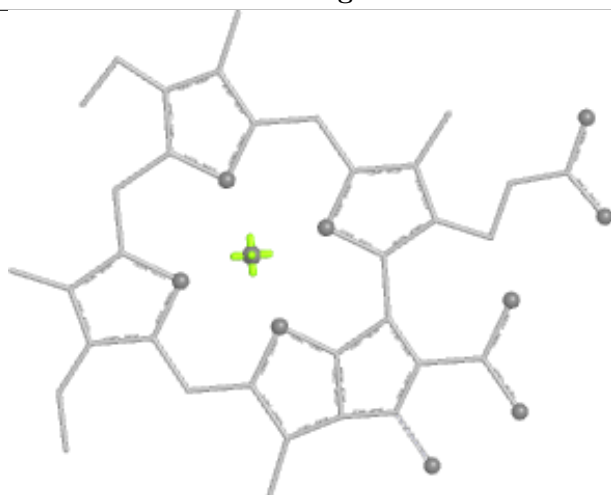
Bond lengths



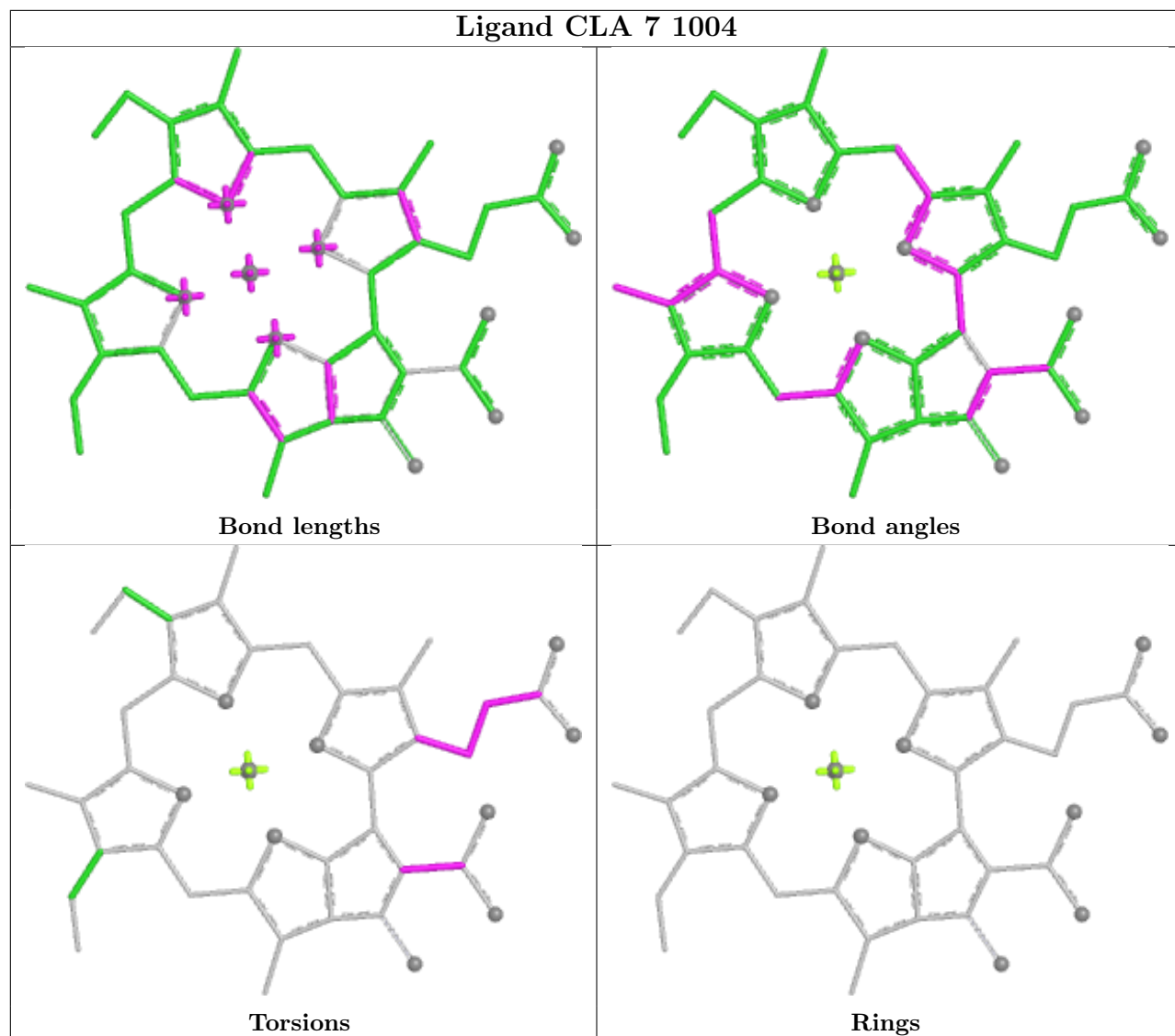
Bond angles



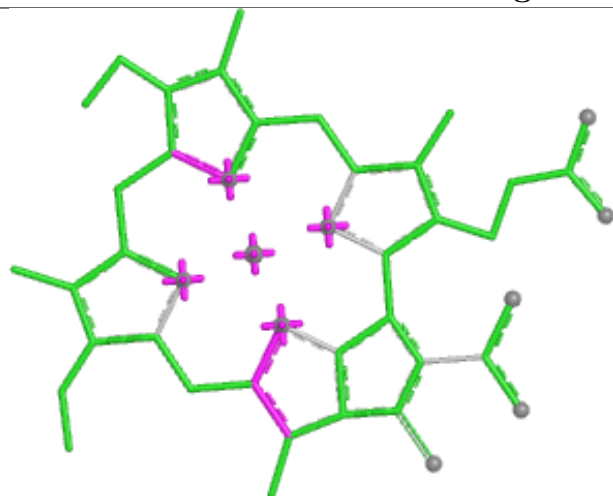
Torsions



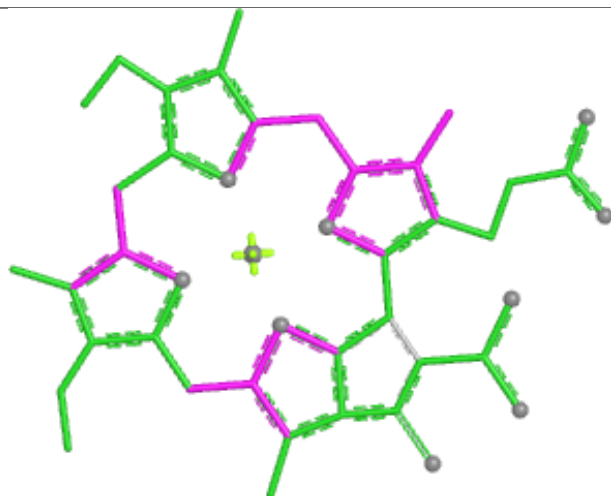
Rings



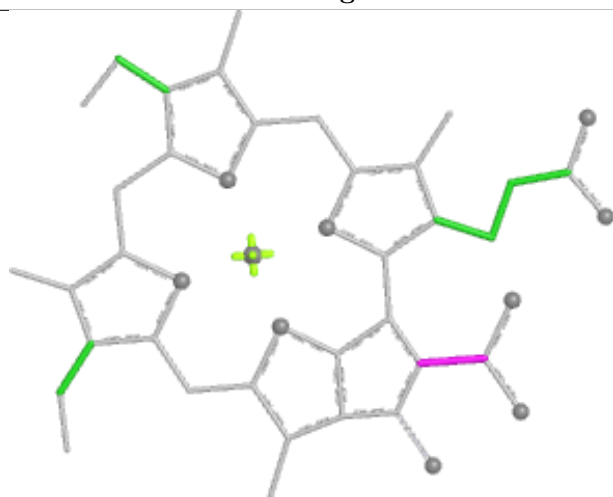
Ligand CLA A 801



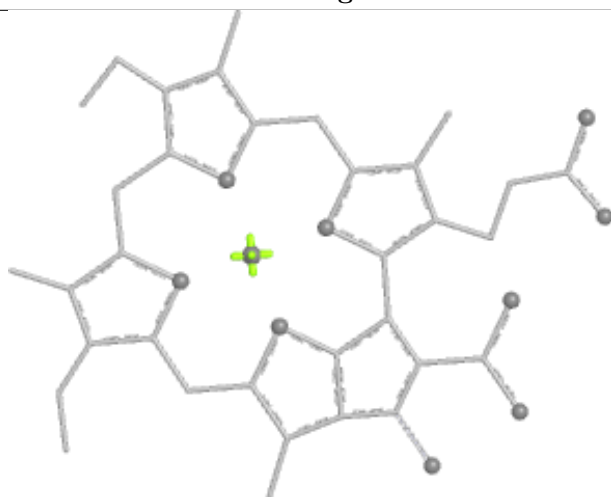
Bond lengths



Bond angles

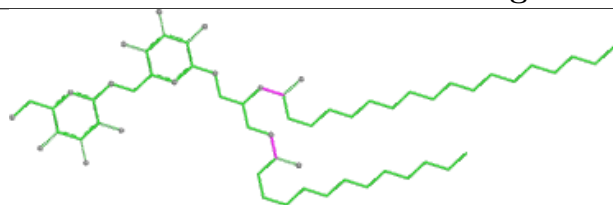


Torsions

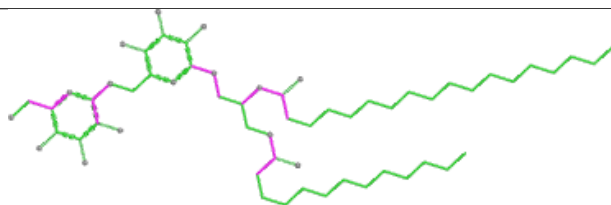


Rings

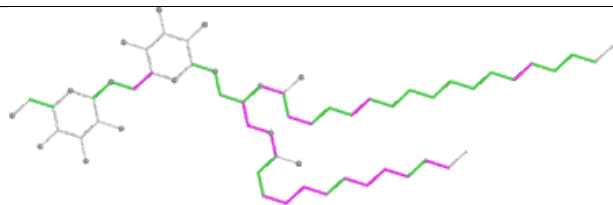
Ligand DGD B 848



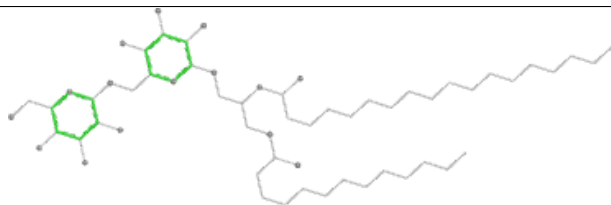
Bond lengths



Bond angles

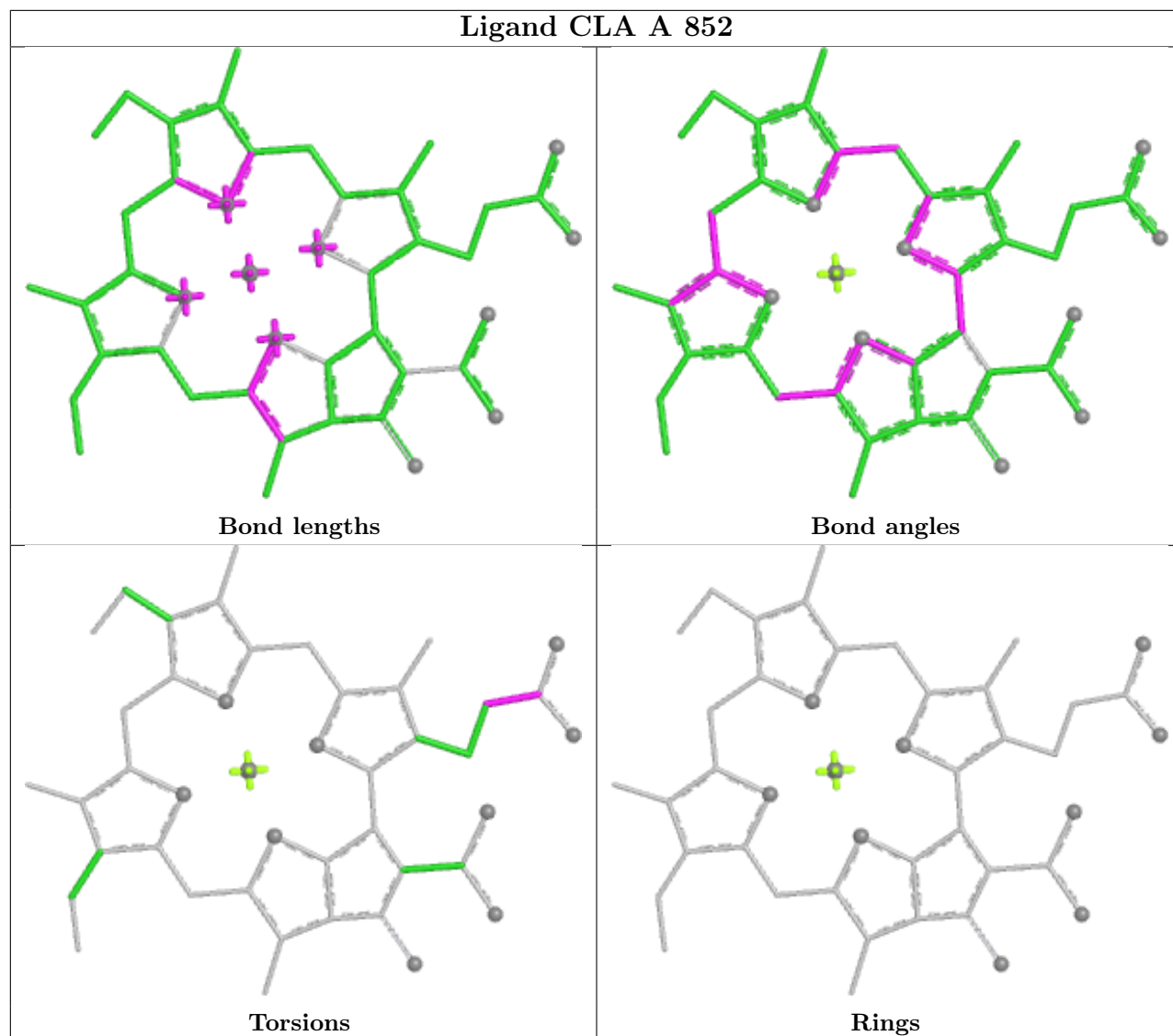


Torsions

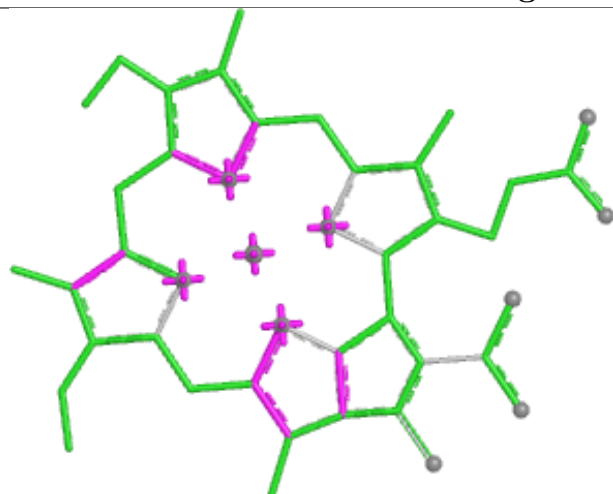


Rings

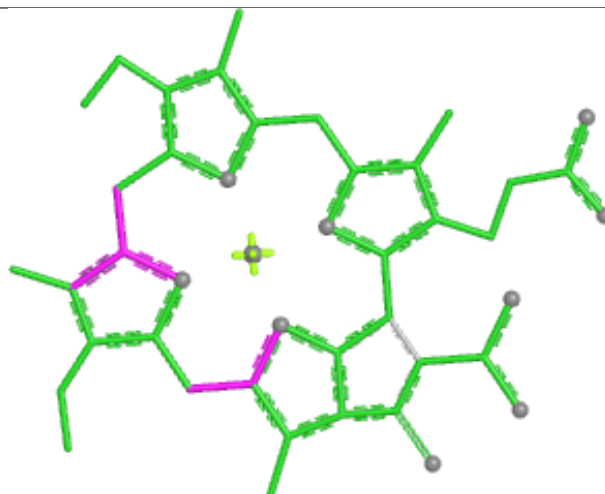
Ligand CLA A 852



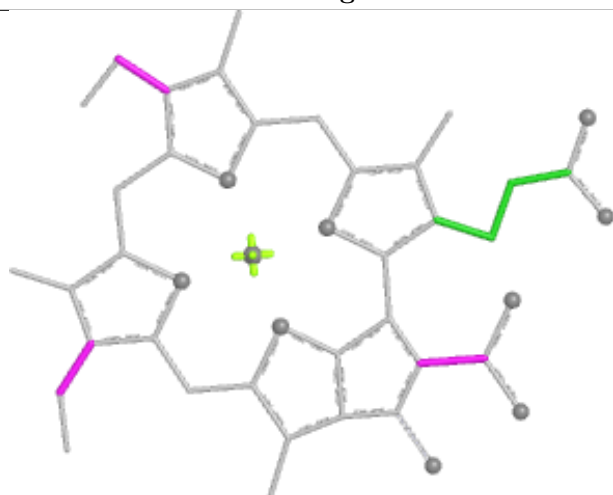
Ligand CLA 6 311



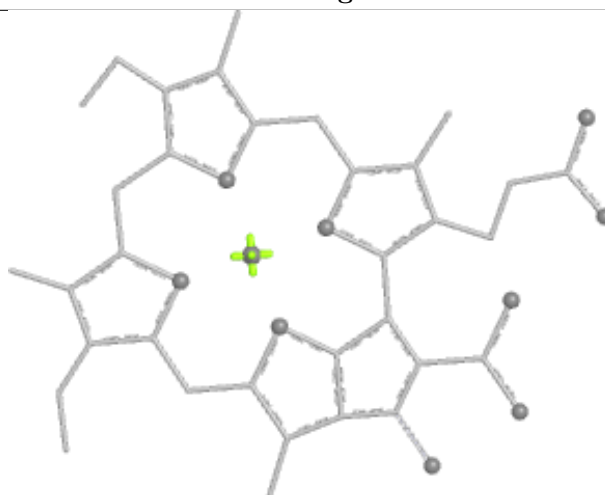
Bond lengths



Bond angles

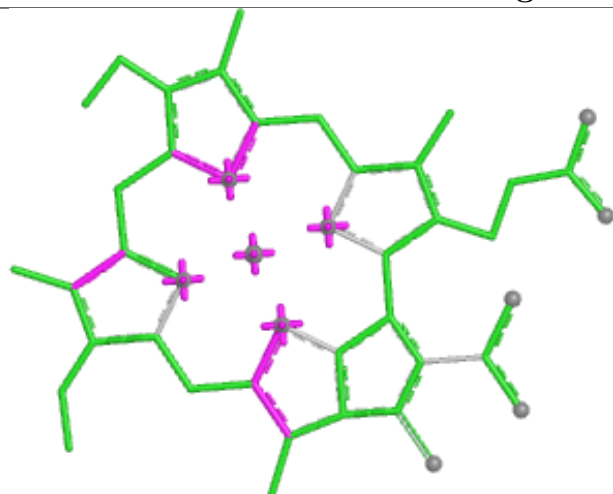


Torsions

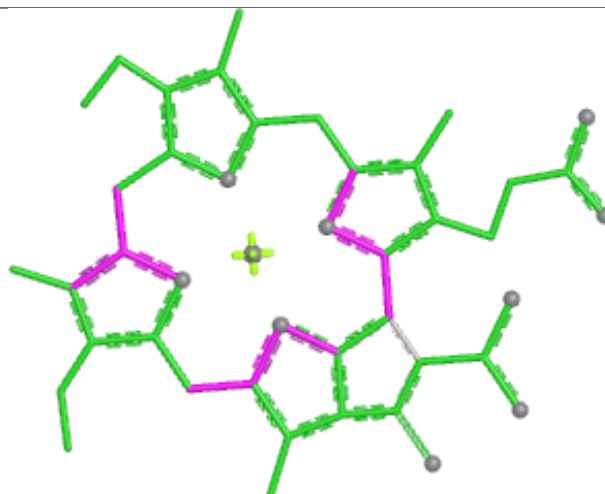


Rings

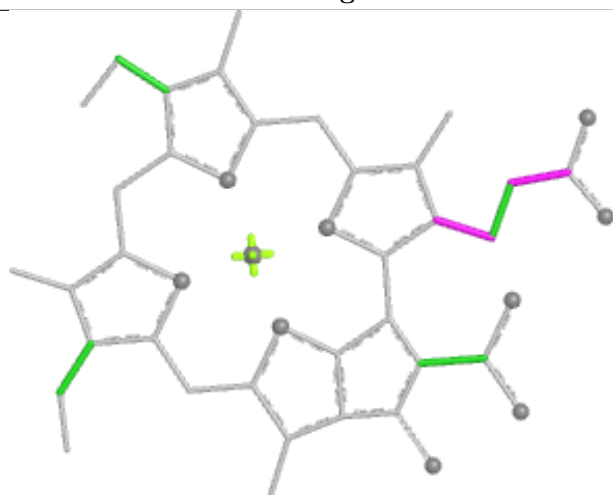
Ligand CLA L 203



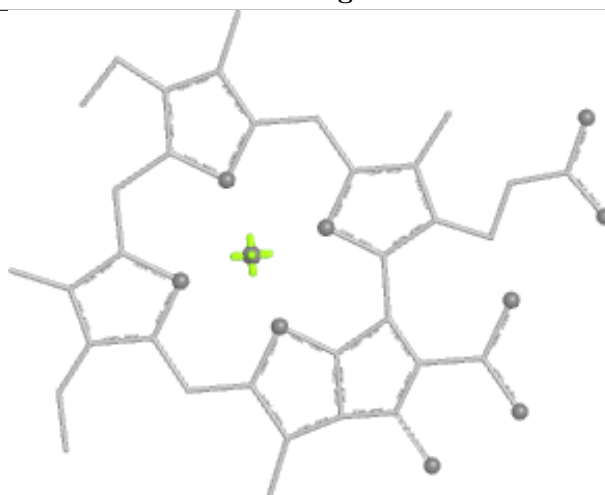
Bond lengths



Bond angles

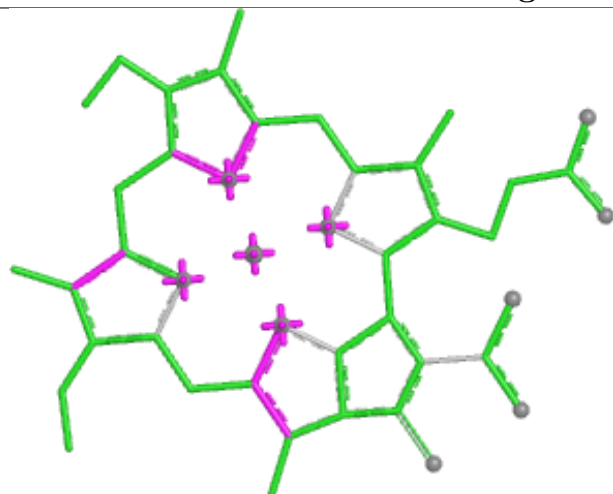


Torsions

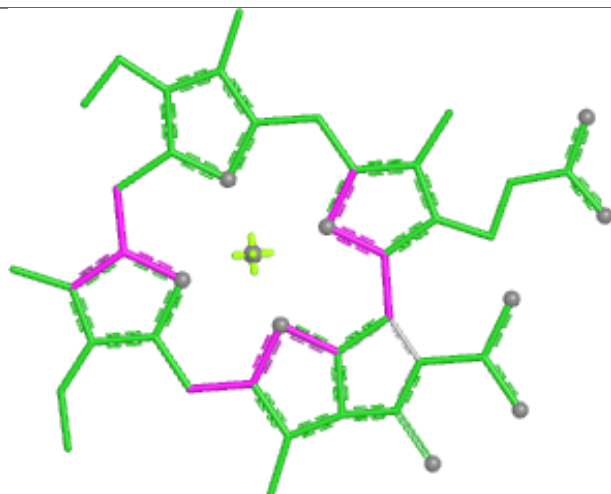


Rings

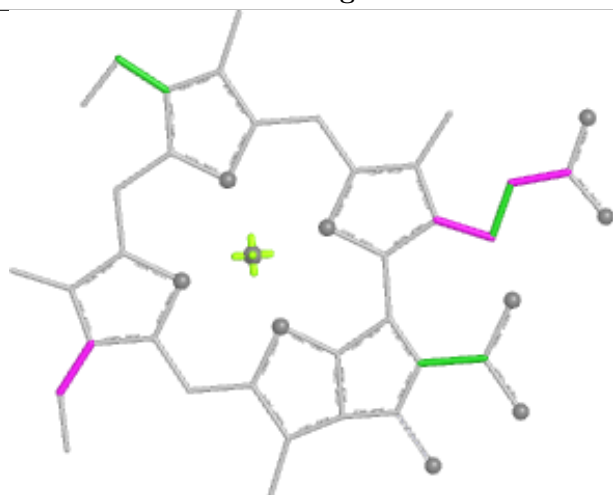
Ligand CLA 0 310



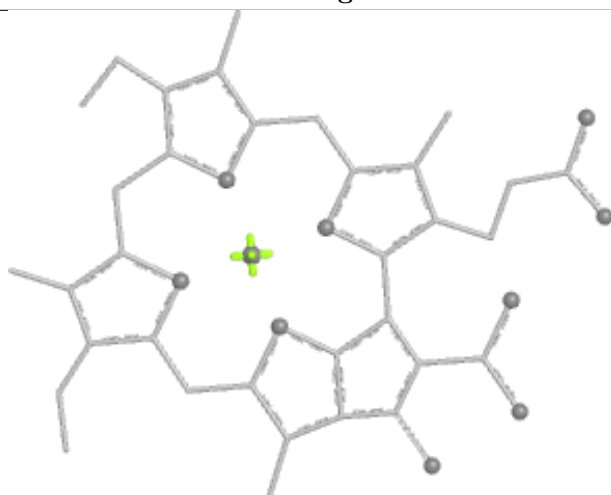
Bond lengths



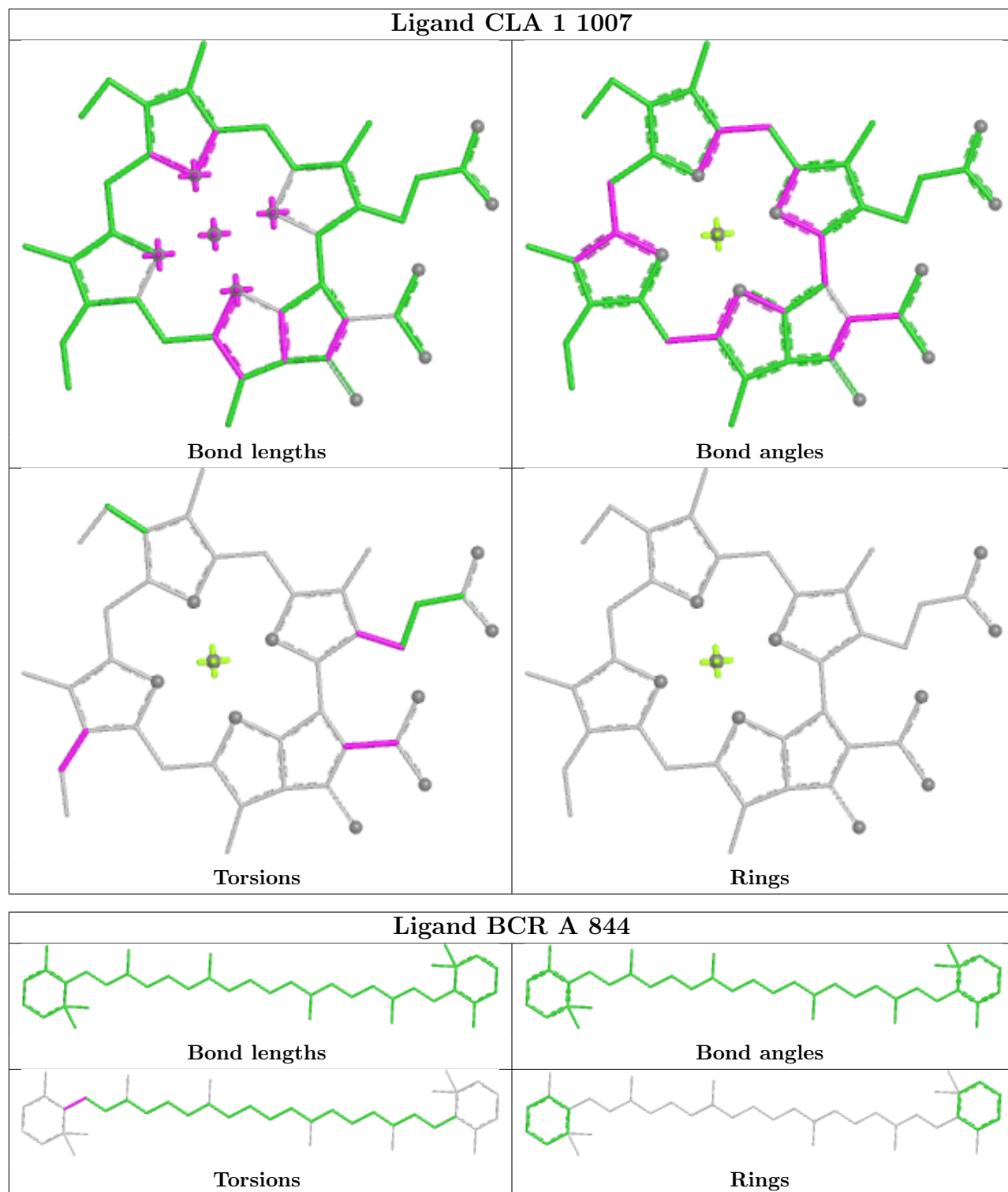
Bond angles



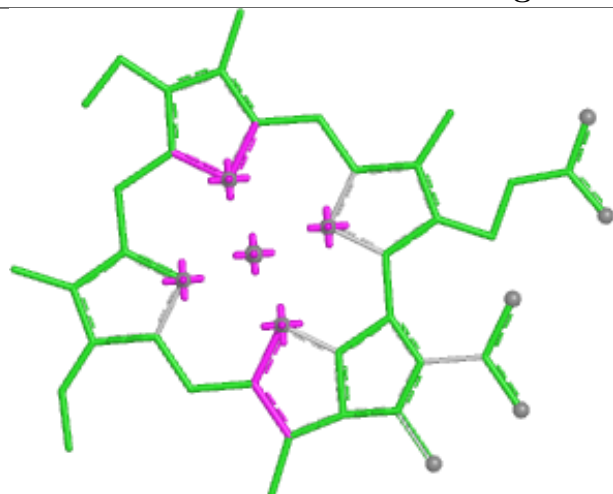
Torsions



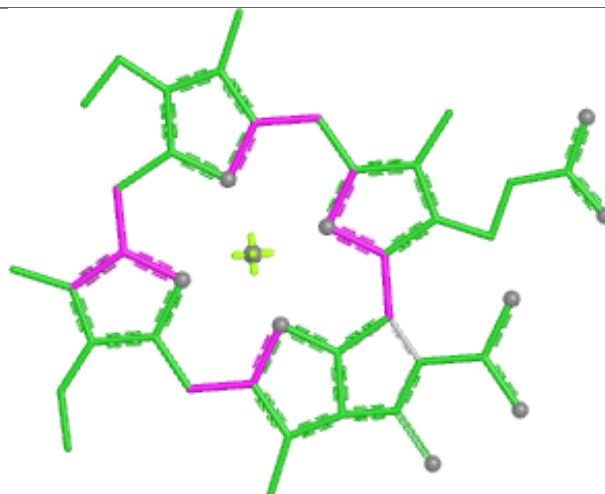
Rings



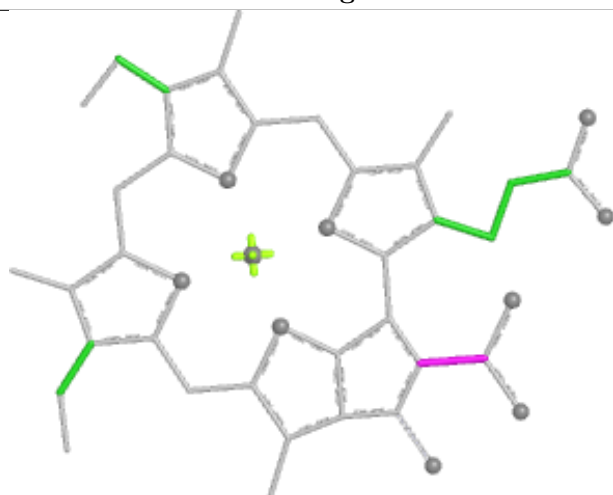
Ligand CLA A 838



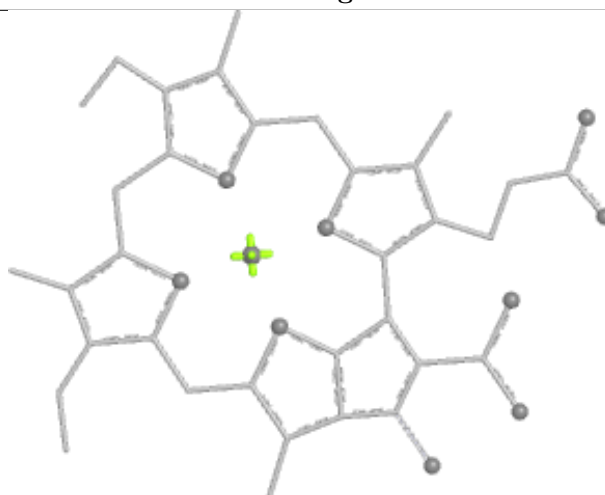
Bond lengths



Bond angles

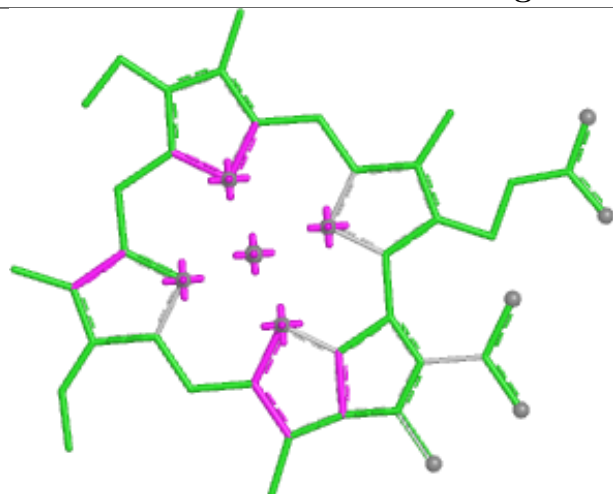


Torsions

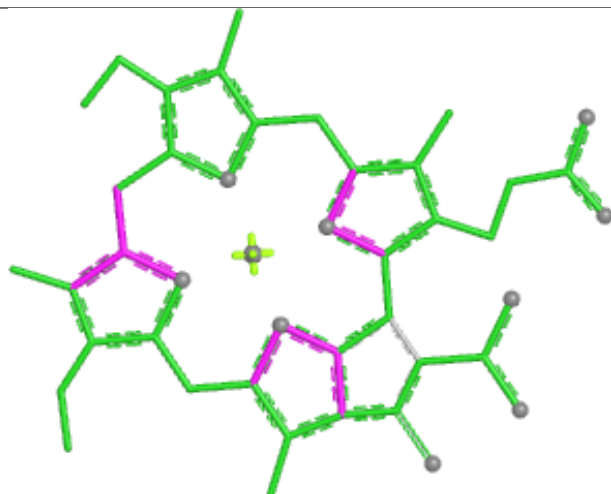


Rings

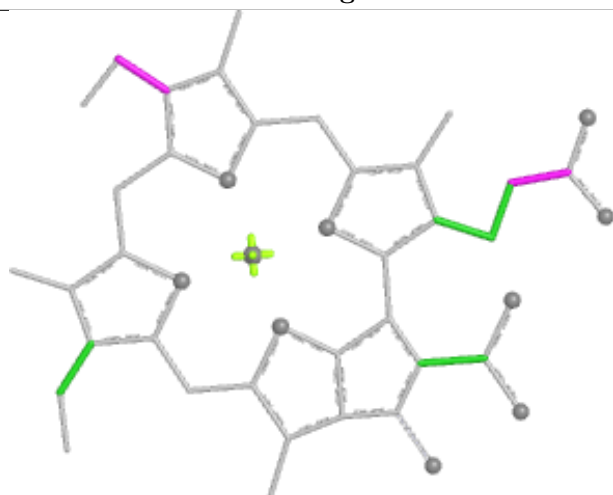
Ligand CLA B 822



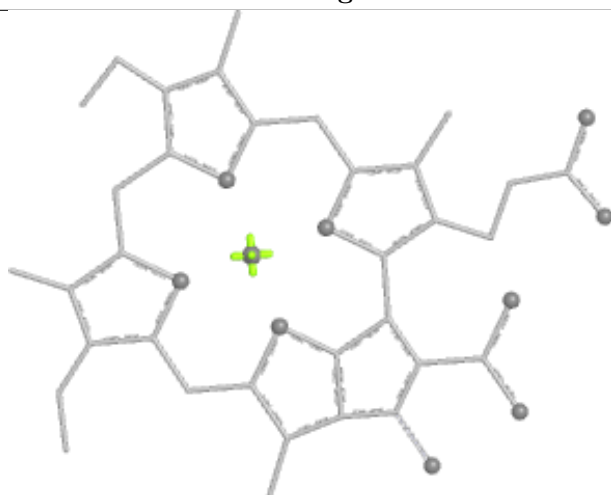
Bond lengths



Bond angles

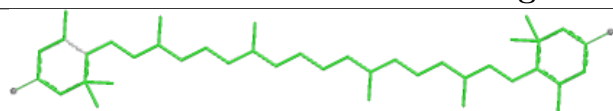


Torsions

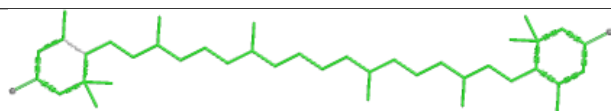


Rings

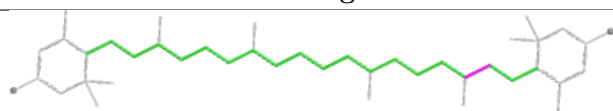
Ligand LUT 8 303



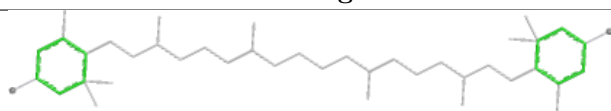
Bond lengths



Bond angles

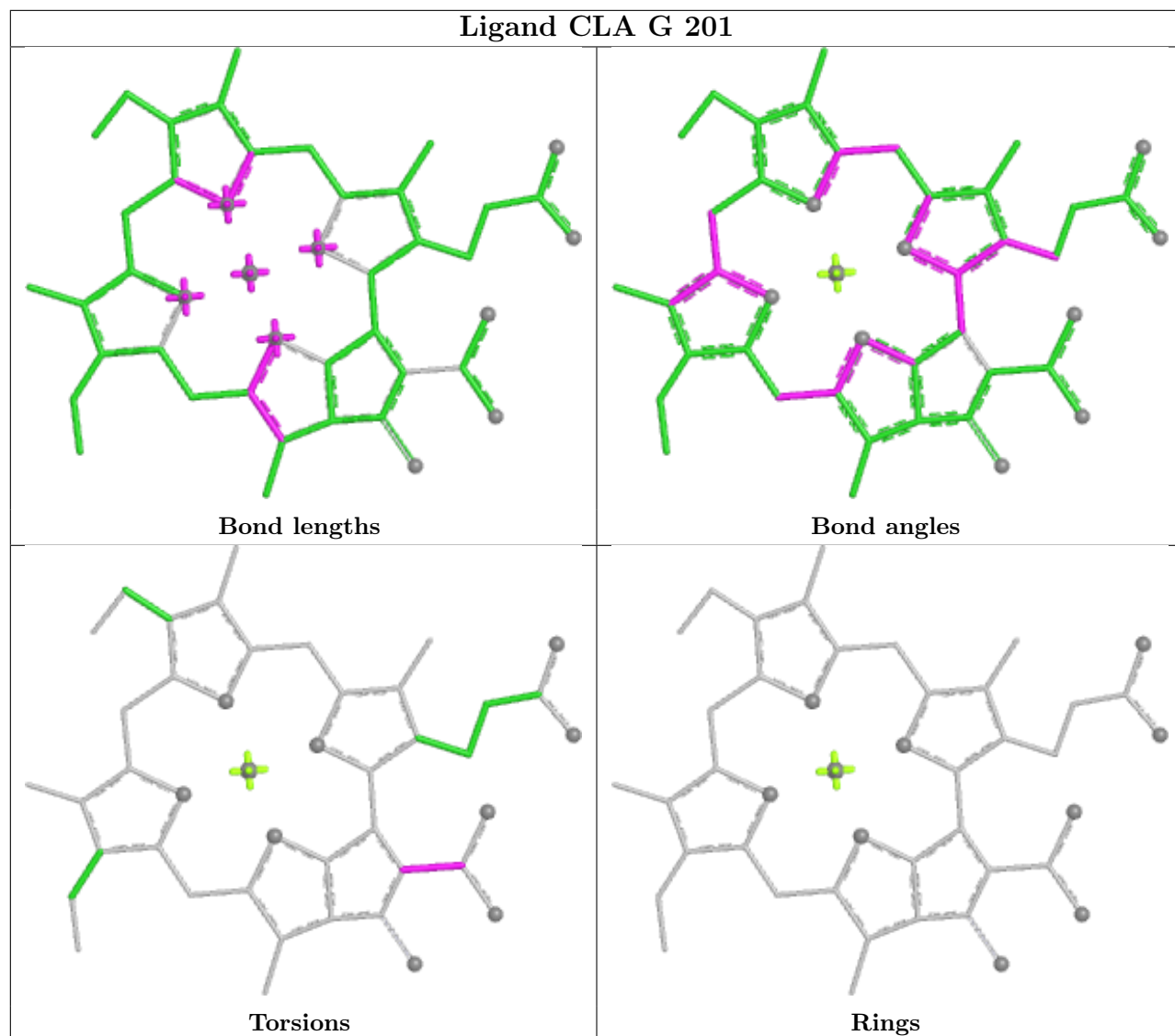


Torsions

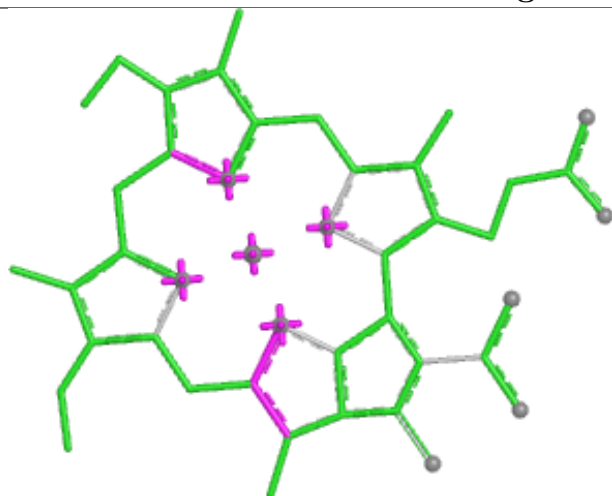


Rings

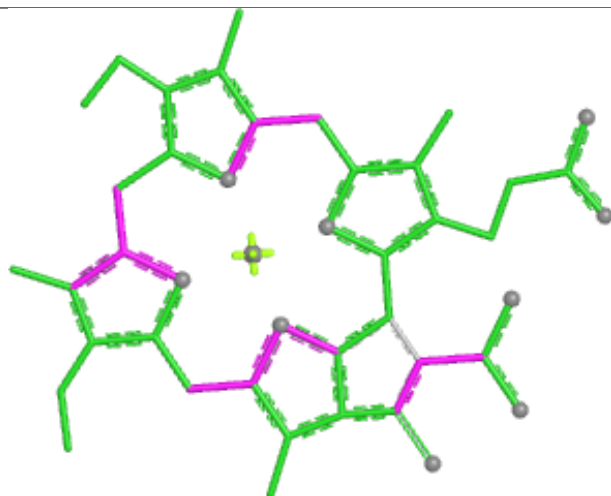
Ligand CLA G 201



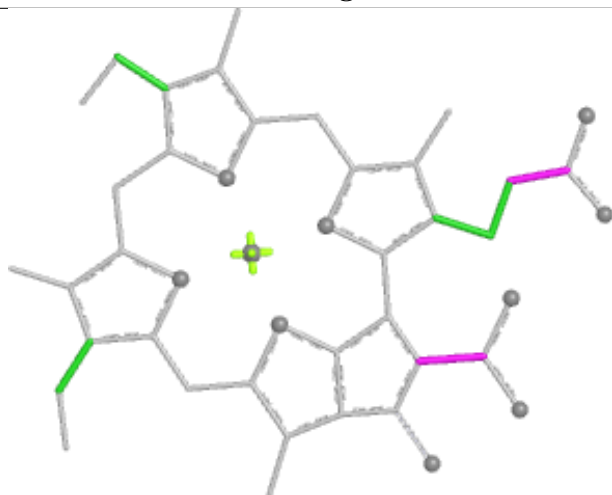
Ligand CLA 8 305



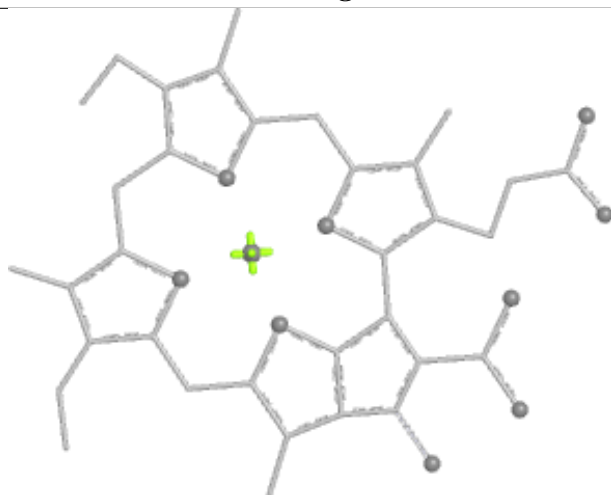
Bond lengths



Bond angles

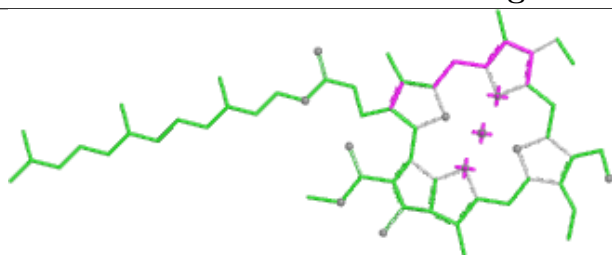


Torsions

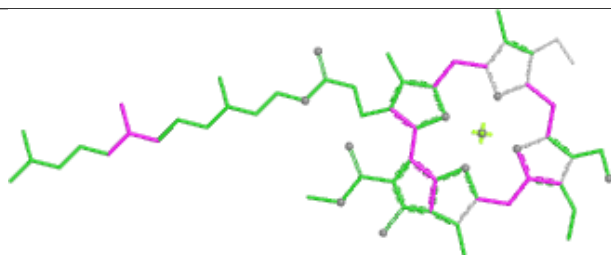


Rings

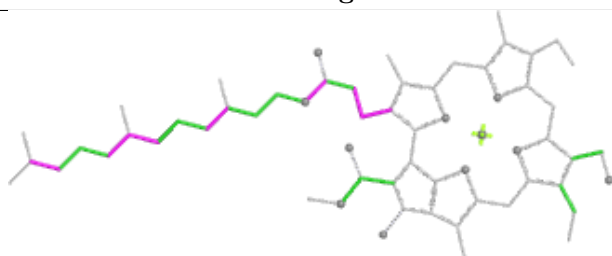
Ligand CHL 1 1015



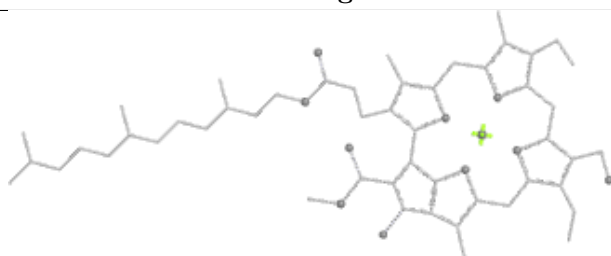
Bond lengths



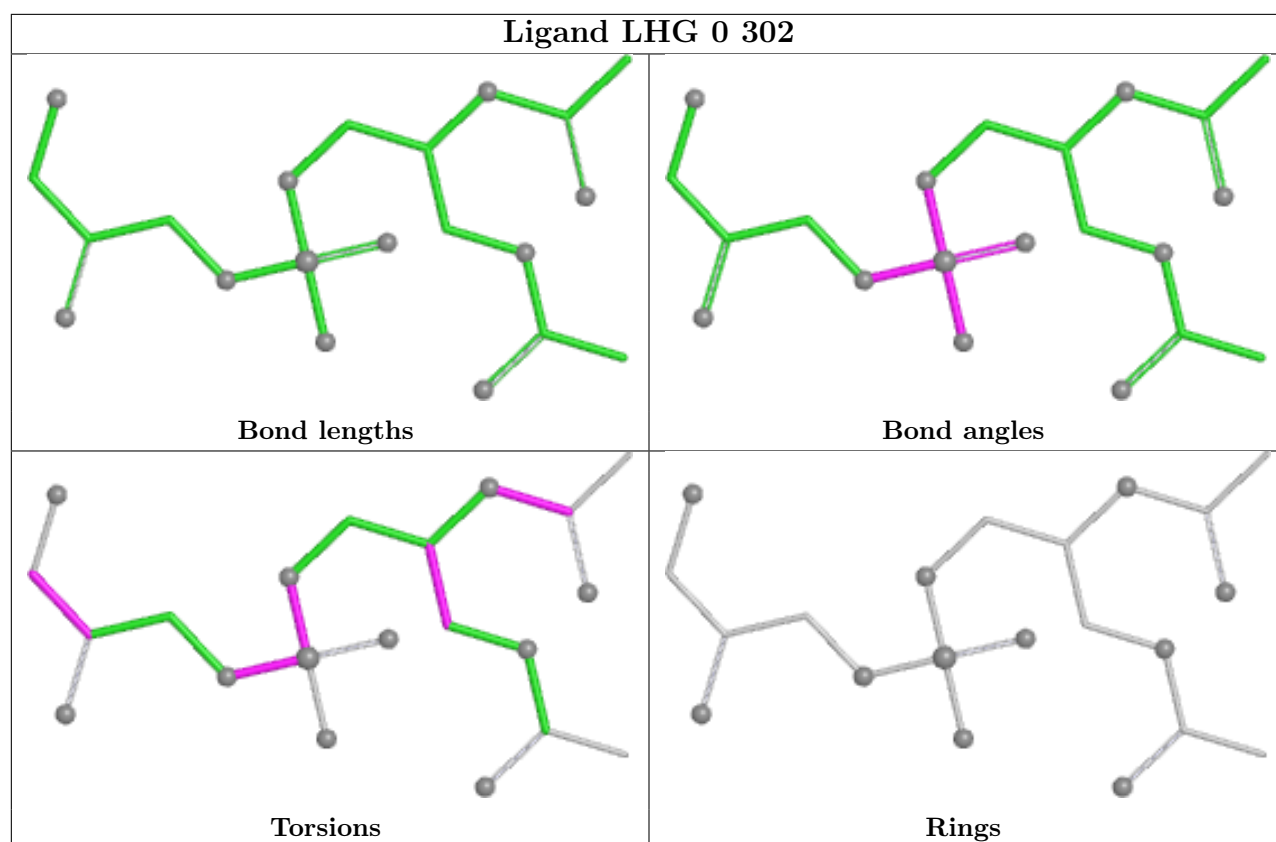
Bond angles



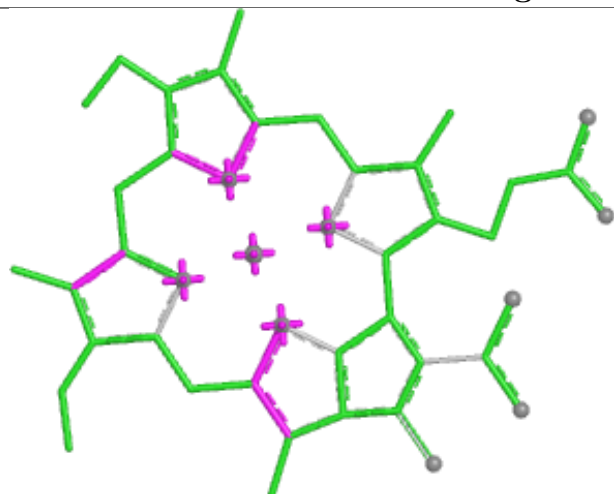
Torsions



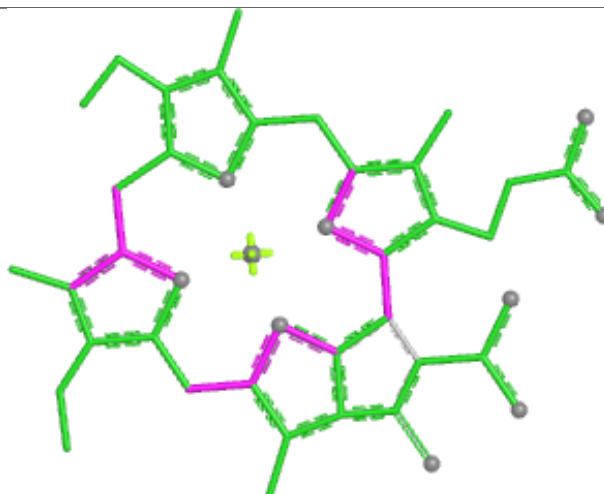
Rings



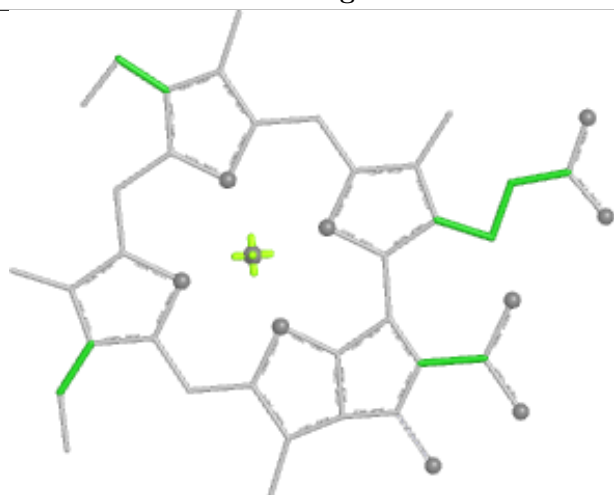
Ligand CLA B 814



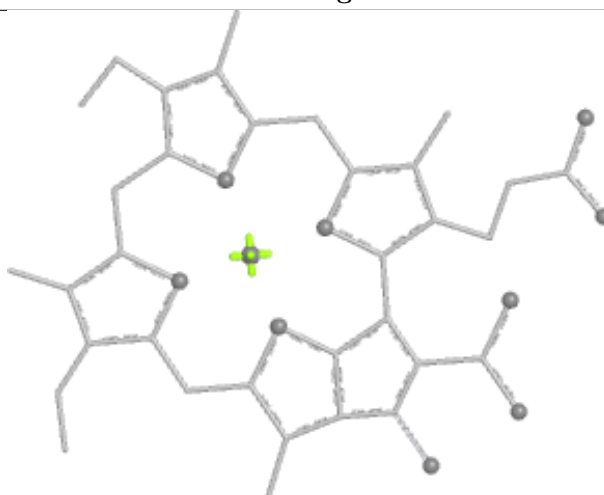
Bond lengths



Bond angles

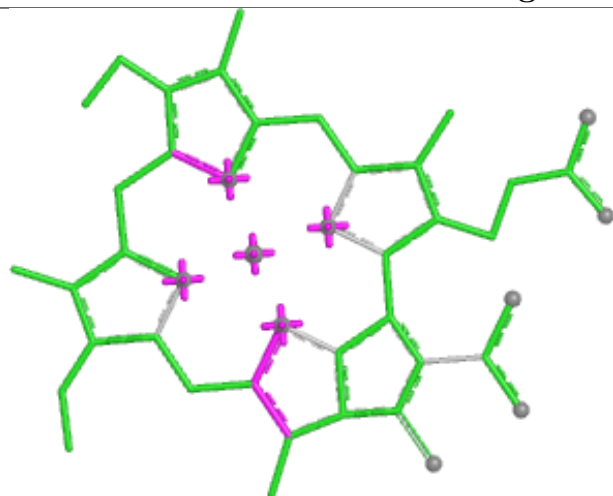


Torsions

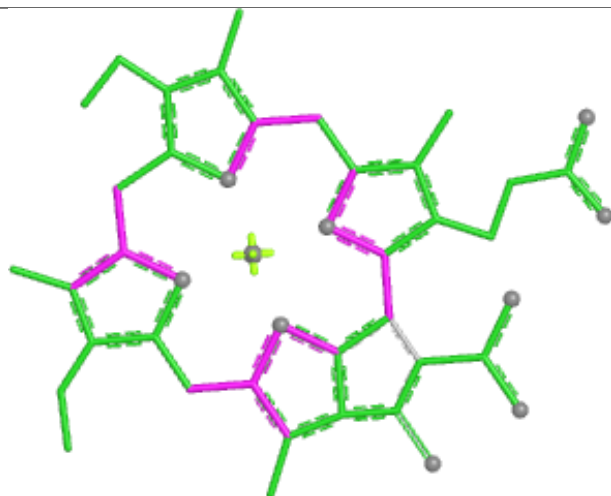


Rings

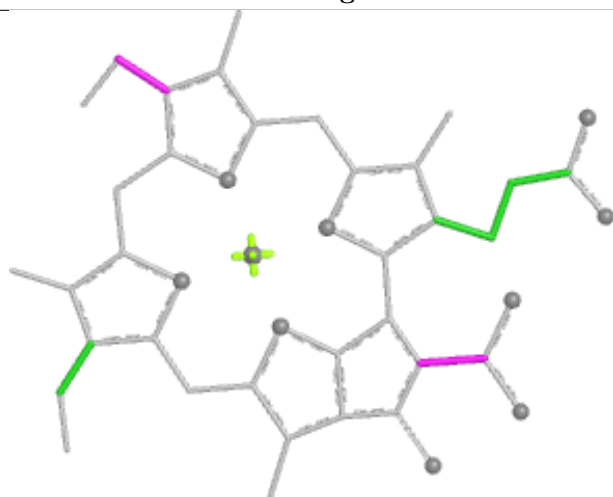
Ligand CLA 8 313



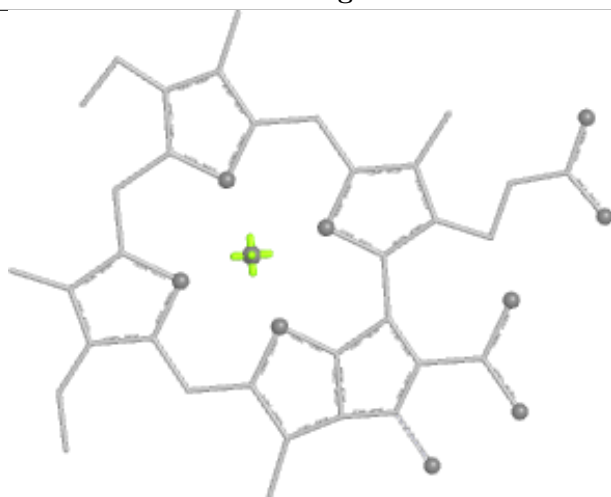
Bond lengths



Bond angles

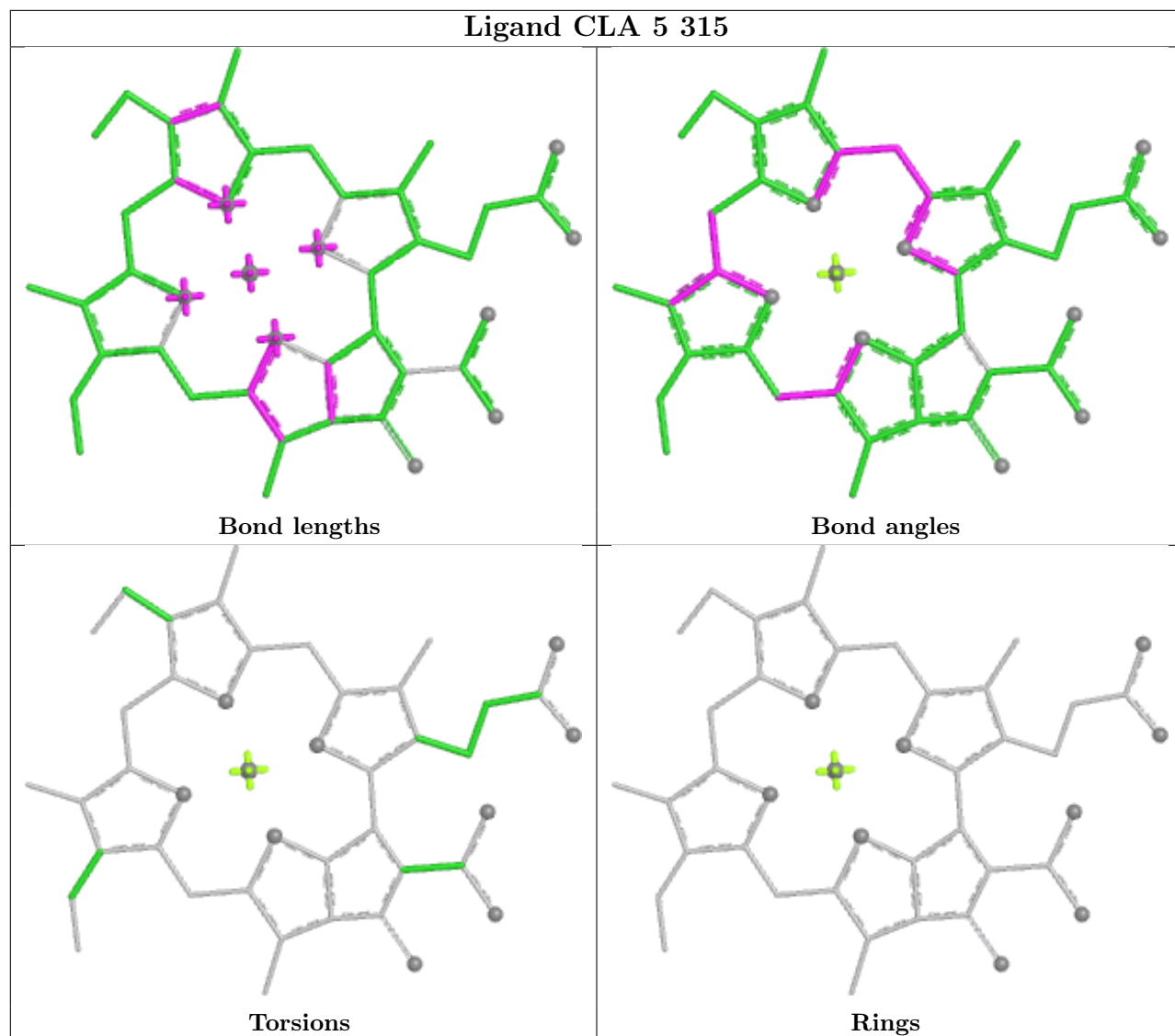


Torsions

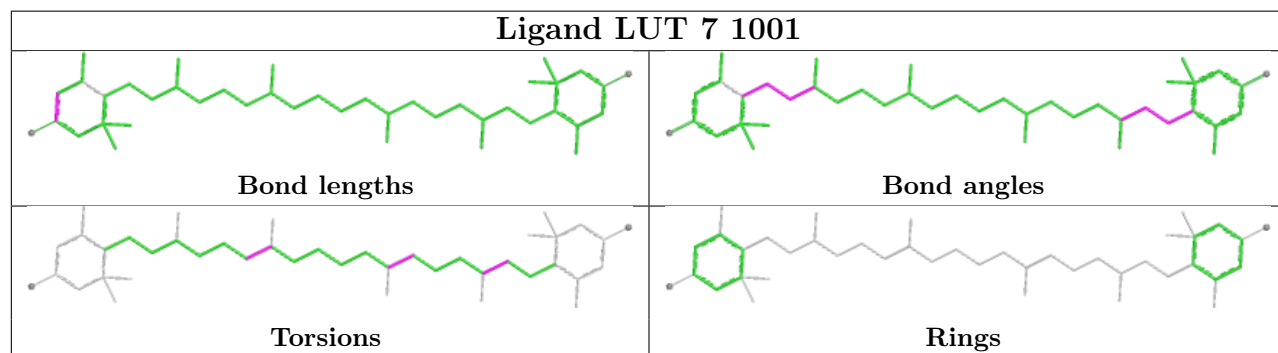


Rings

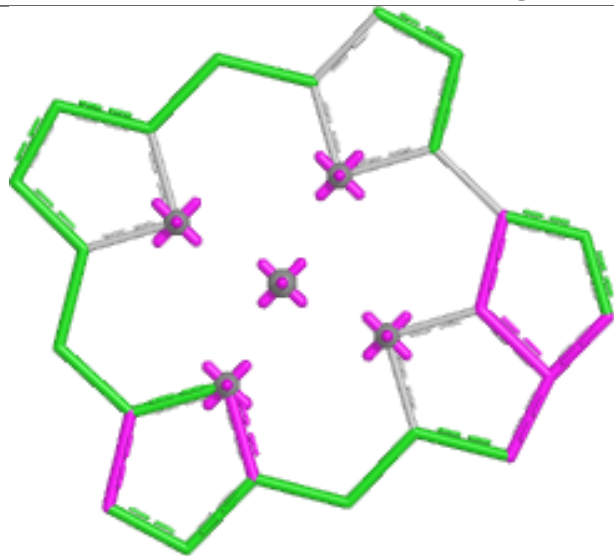
Ligand CLA 5 315



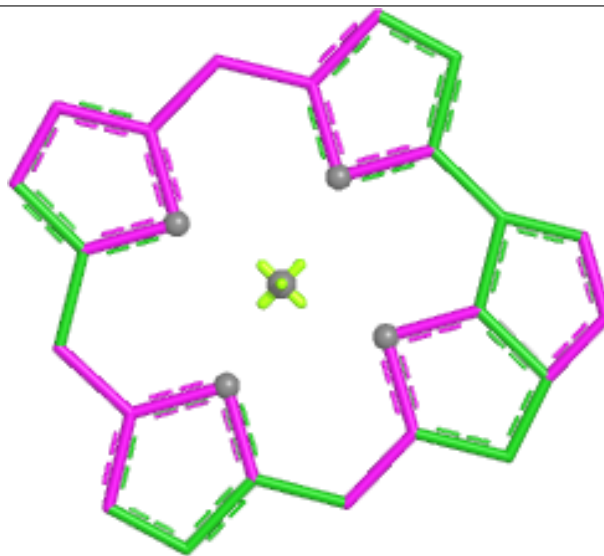
Ligand LUT 7 1001



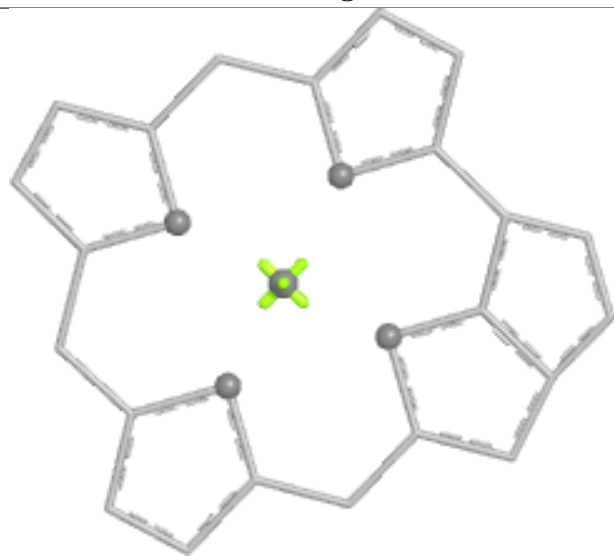
Ligand CLA K 202



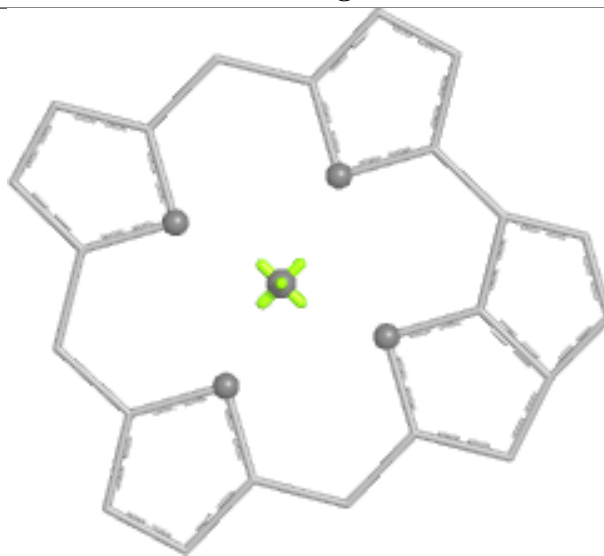
Bond lengths



Bond angles

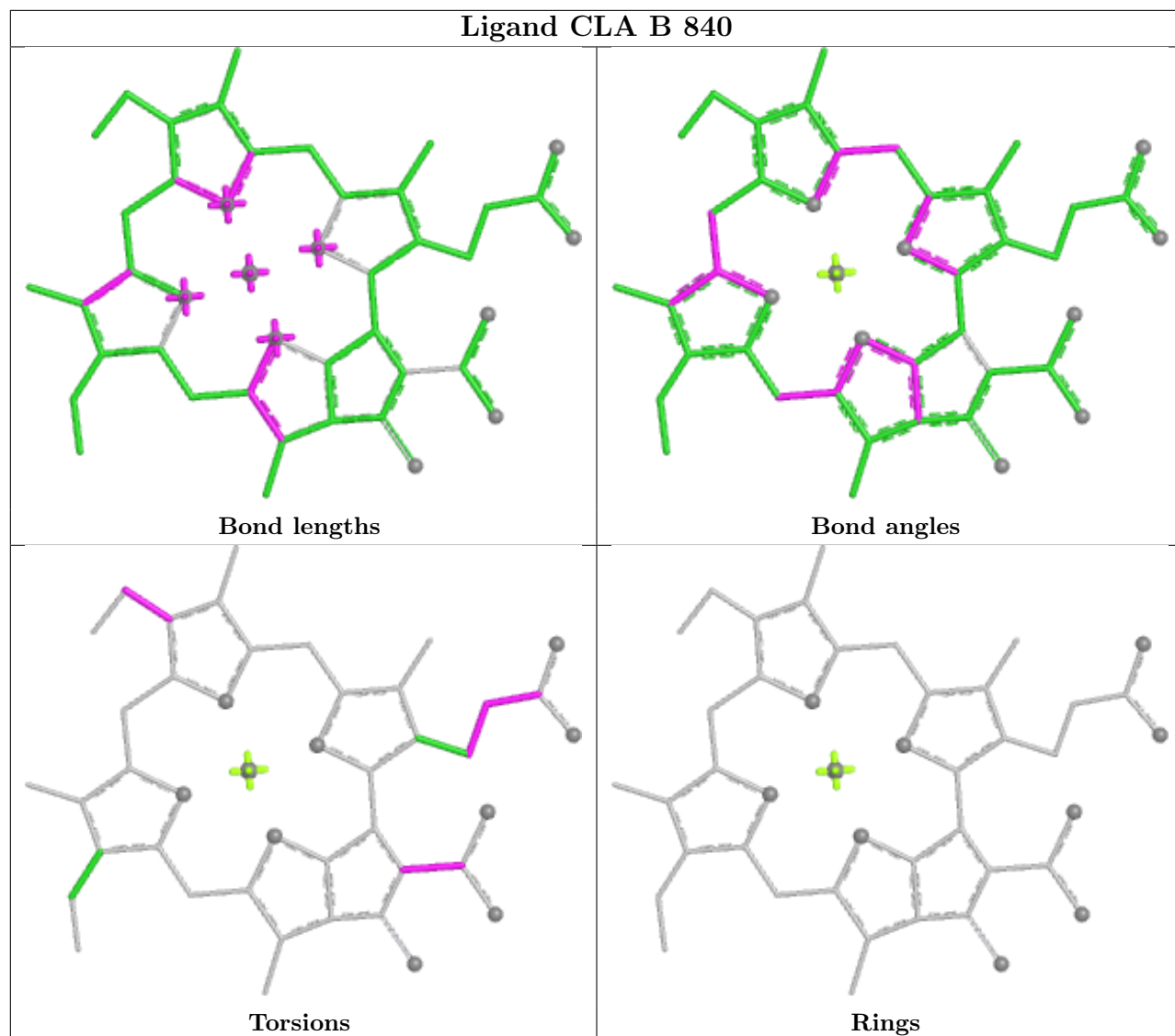


Torsions

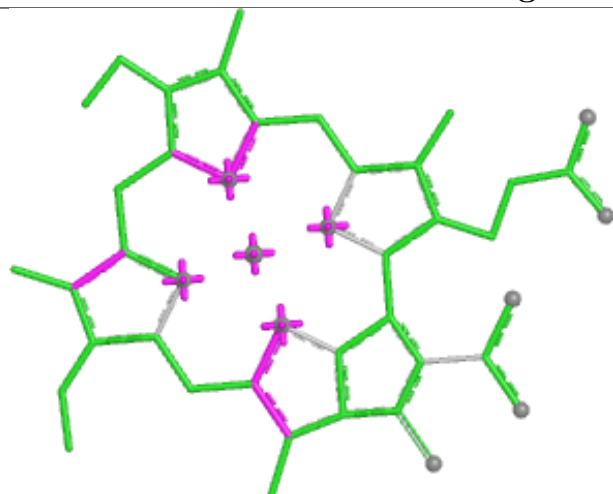


Rings

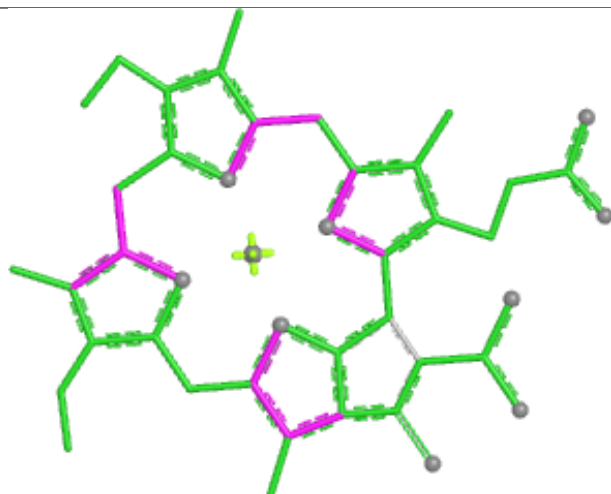
Ligand CLA B 840



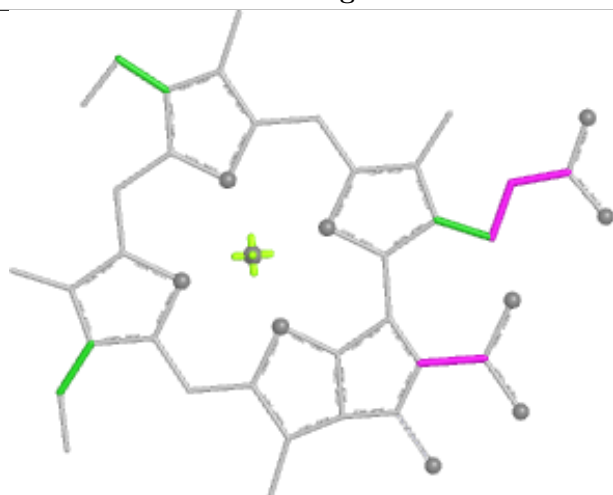
Ligand CLA 4 306



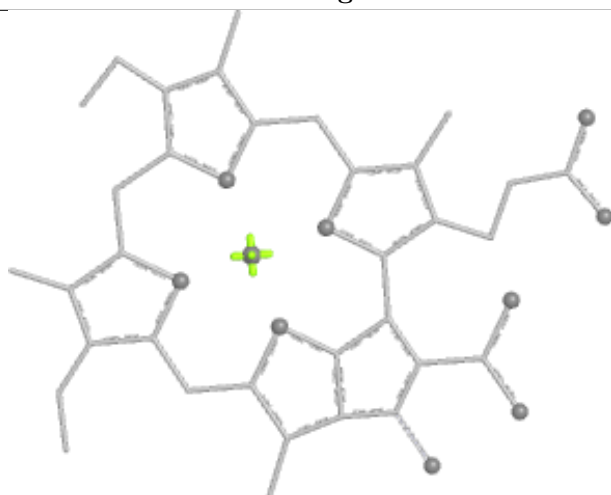
Bond lengths



Bond angles

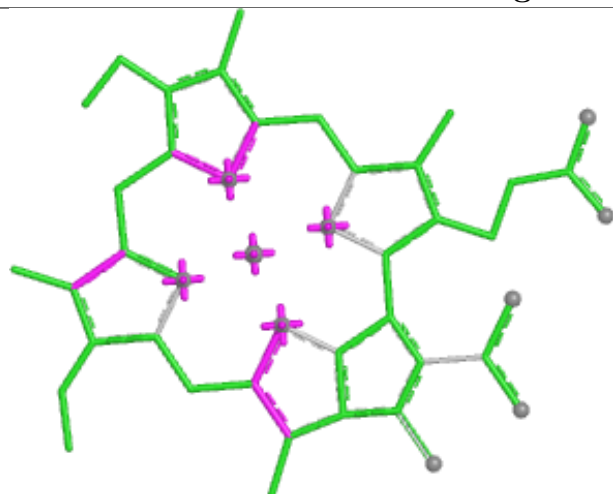


Torsions

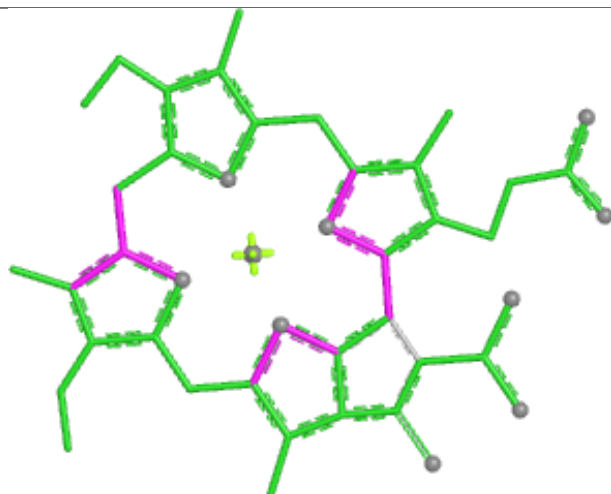


Rings

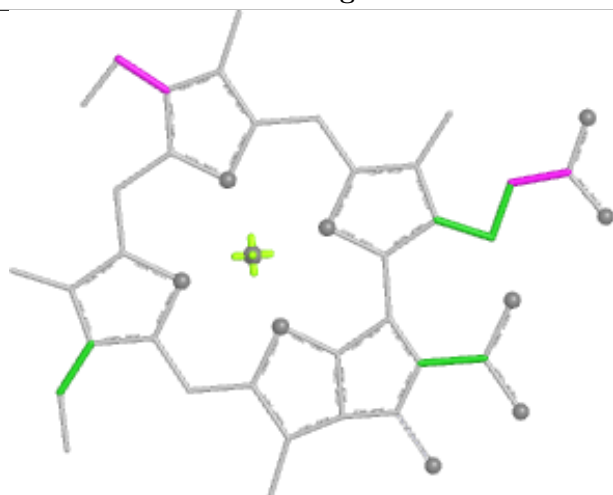
Ligand CLA A 831



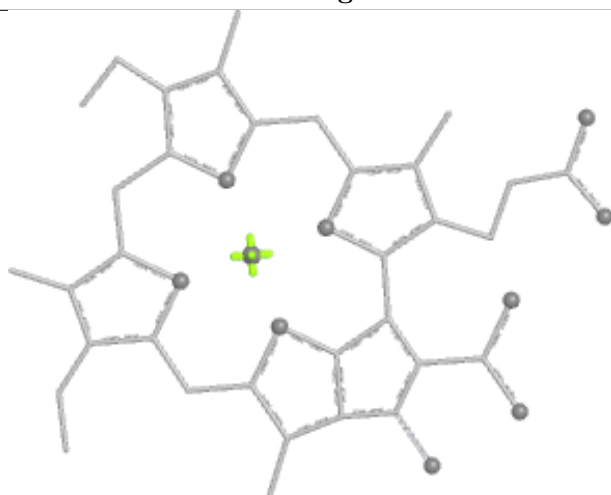
Bond lengths



Bond angles

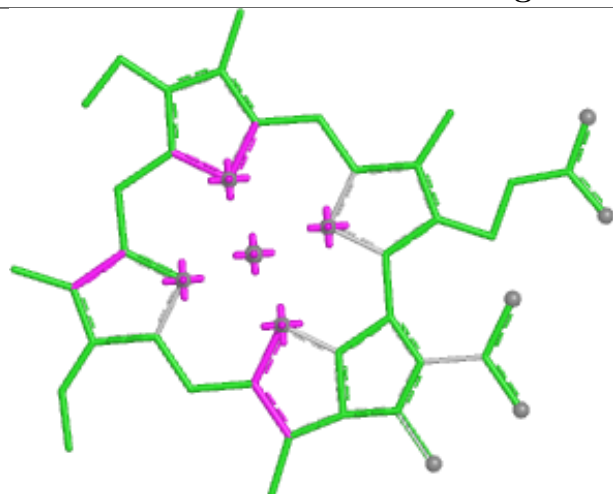


Torsions

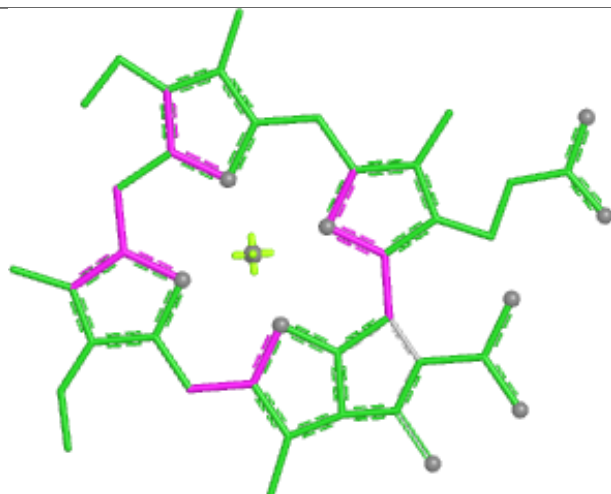


Rings

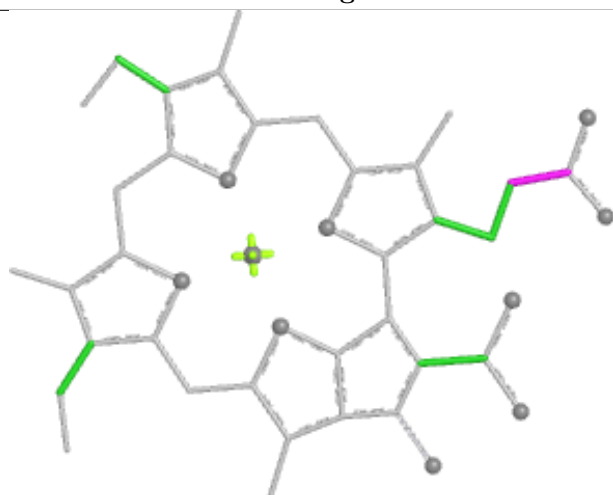
Ligand CLA B 806



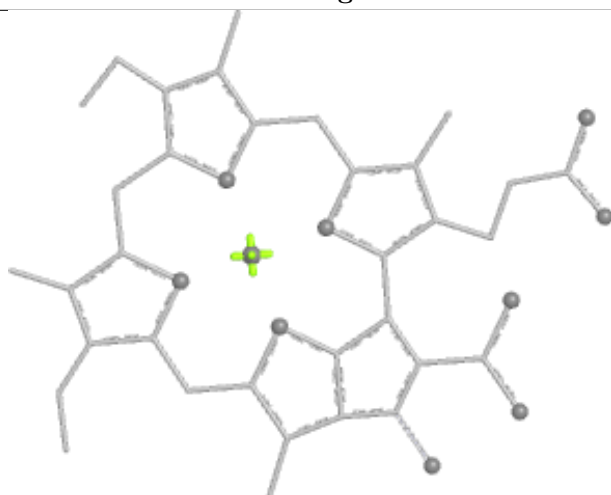
Bond lengths



Bond angles

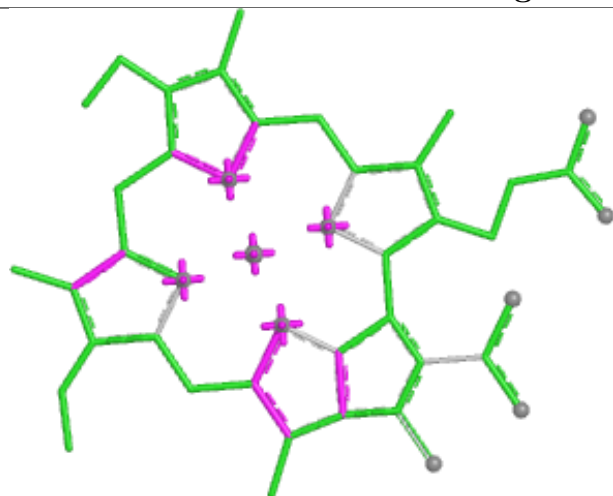


Torsions

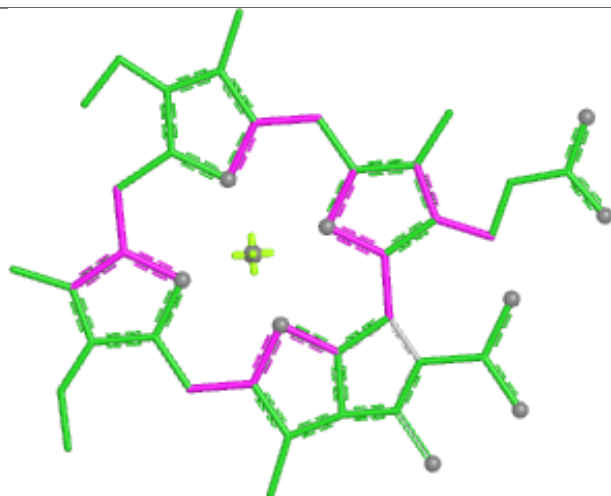


Rings

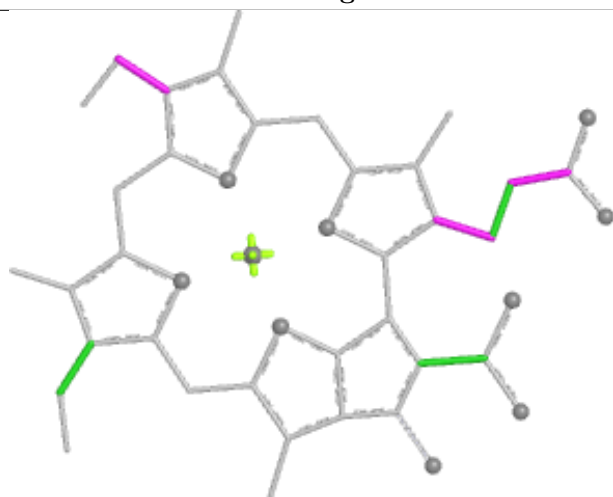
Ligand CLA B 825



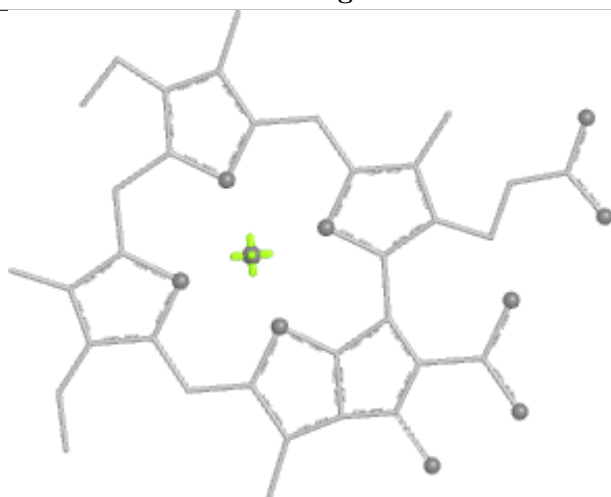
Bond lengths



Bond angles

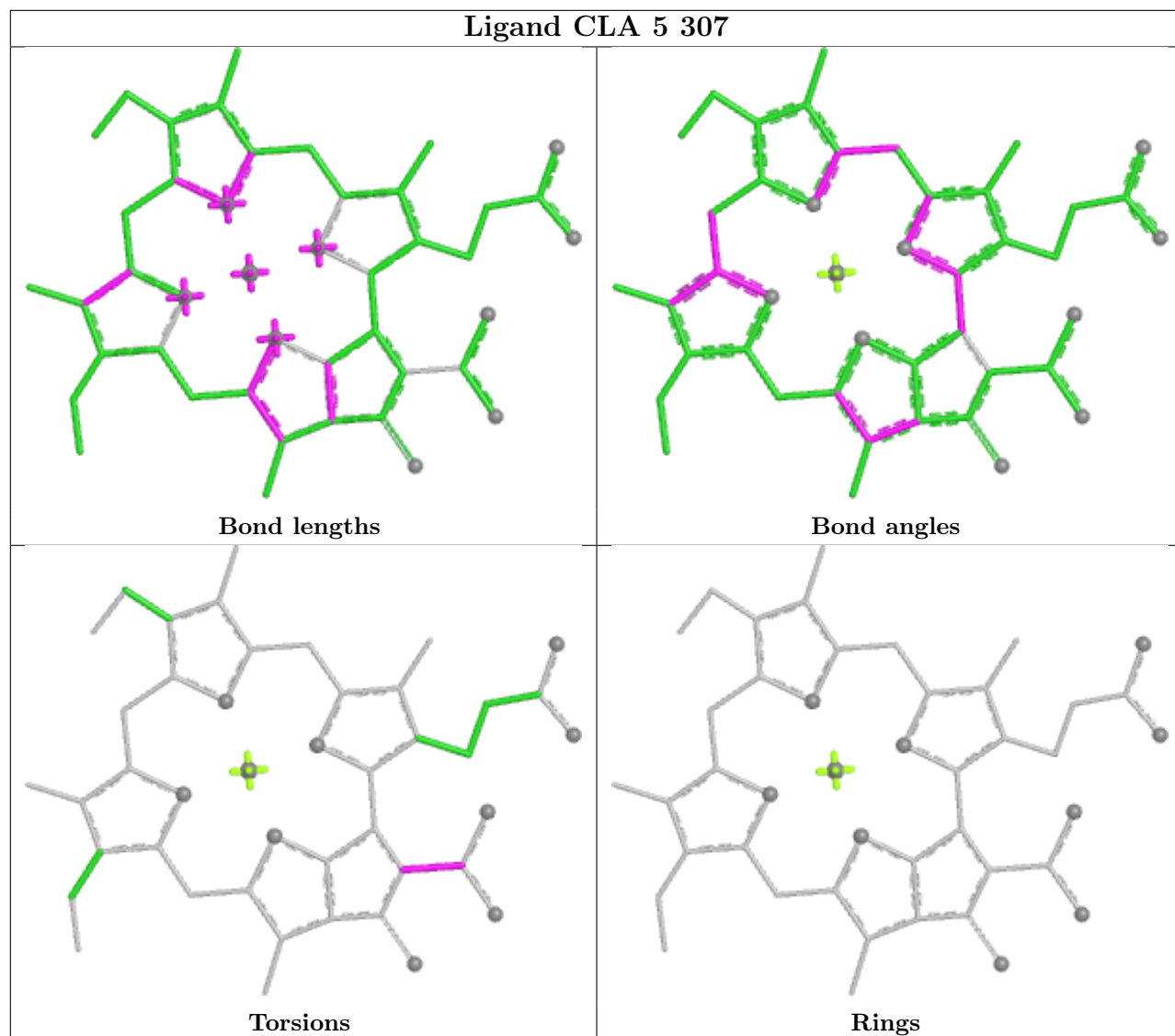


Torsions

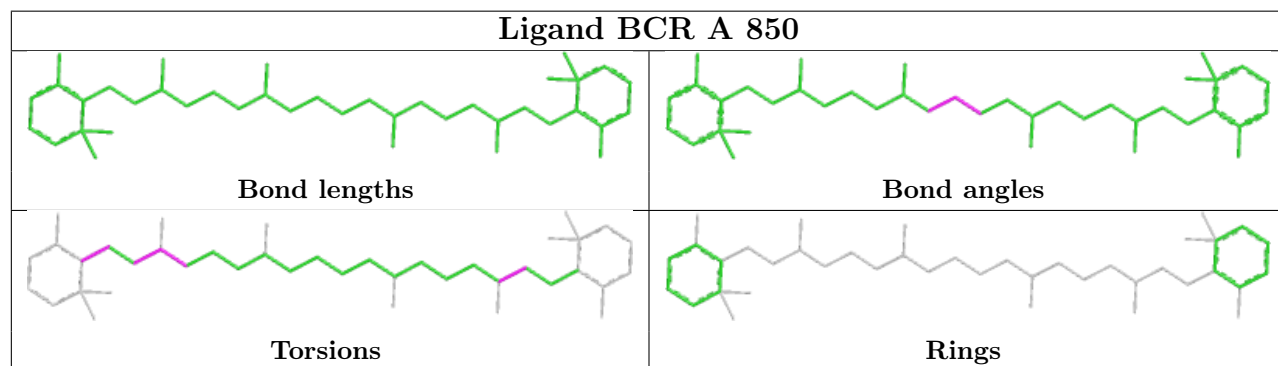


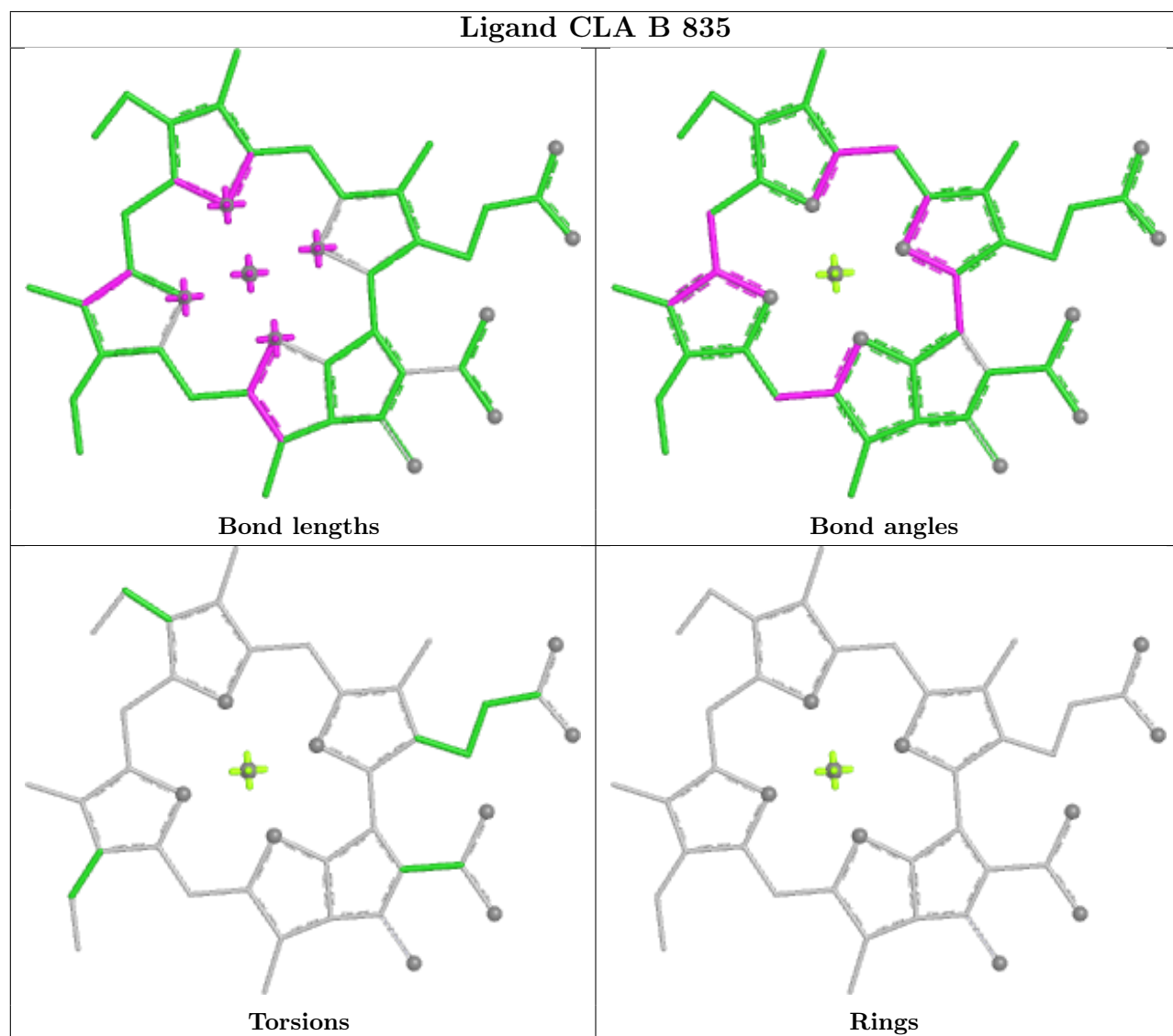
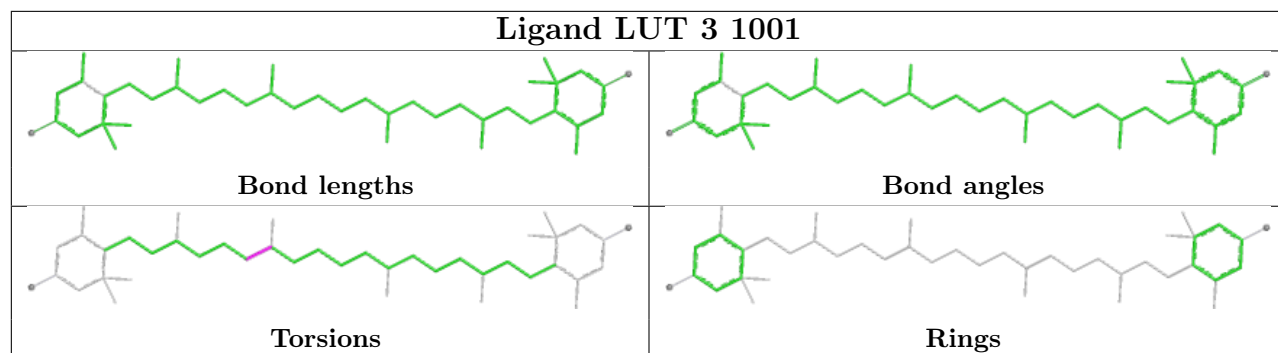
Rings

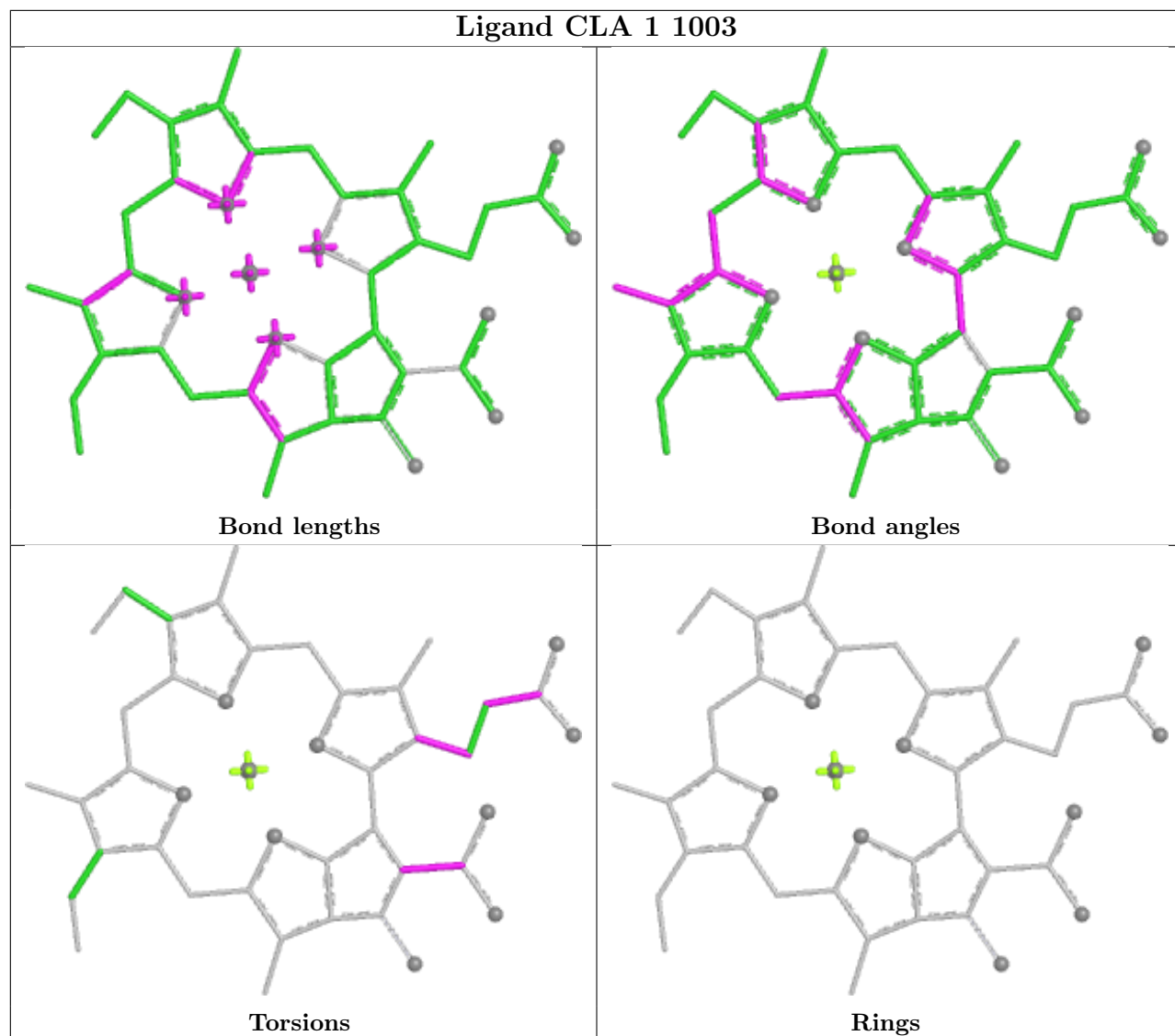
Ligand CLA 5 307



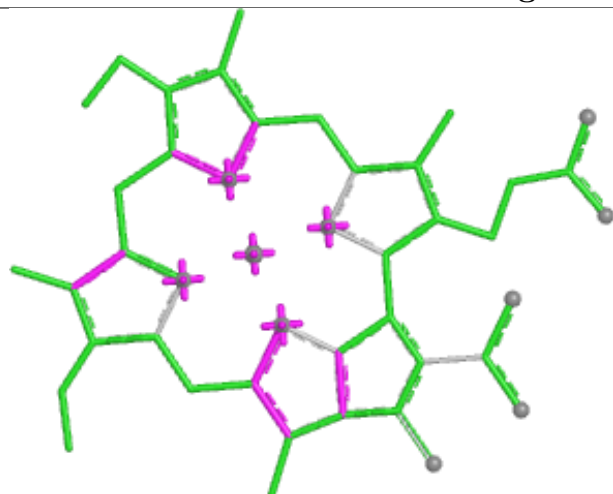
Ligand BCR A 850



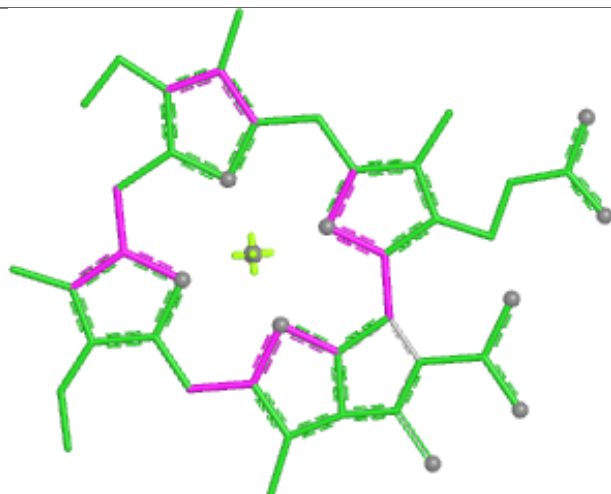




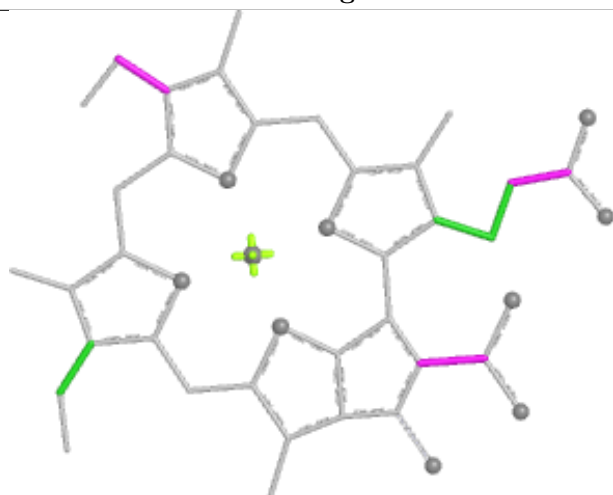
Ligand CLA 4 305



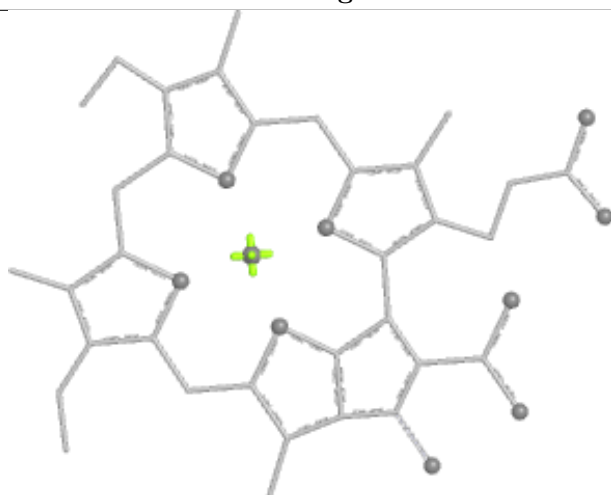
Bond lengths



Bond angles

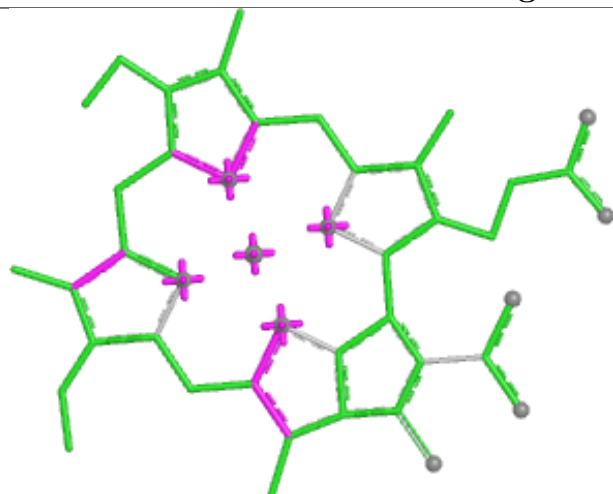


Torsions

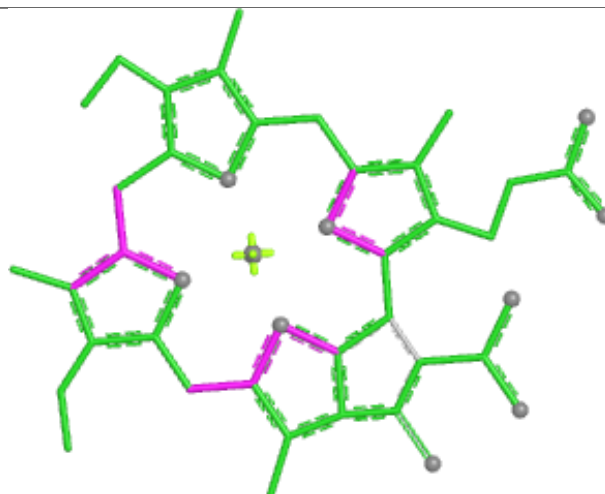


Rings

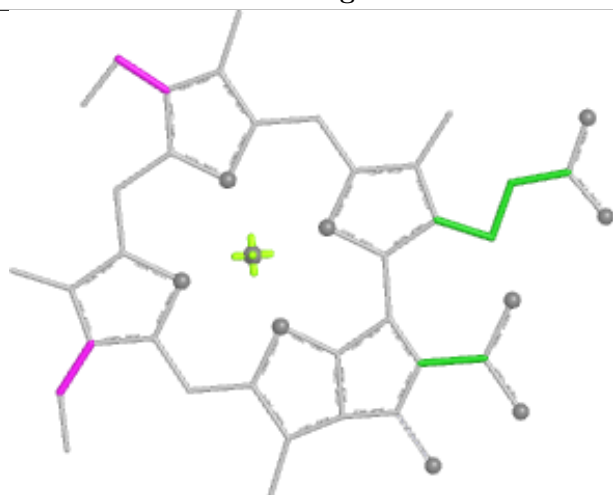
Ligand CLA 0 311



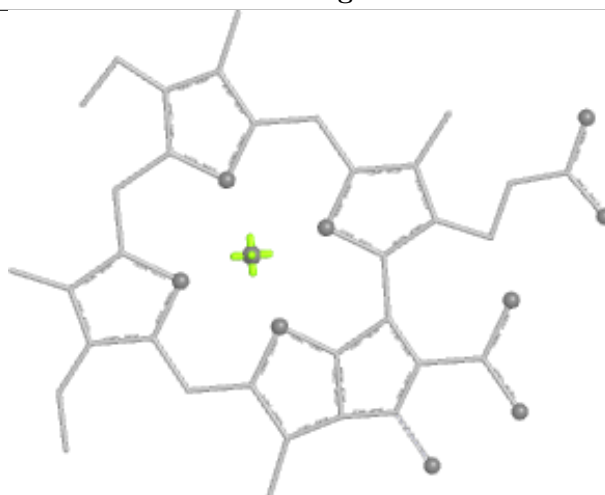
Bond lengths



Bond angles

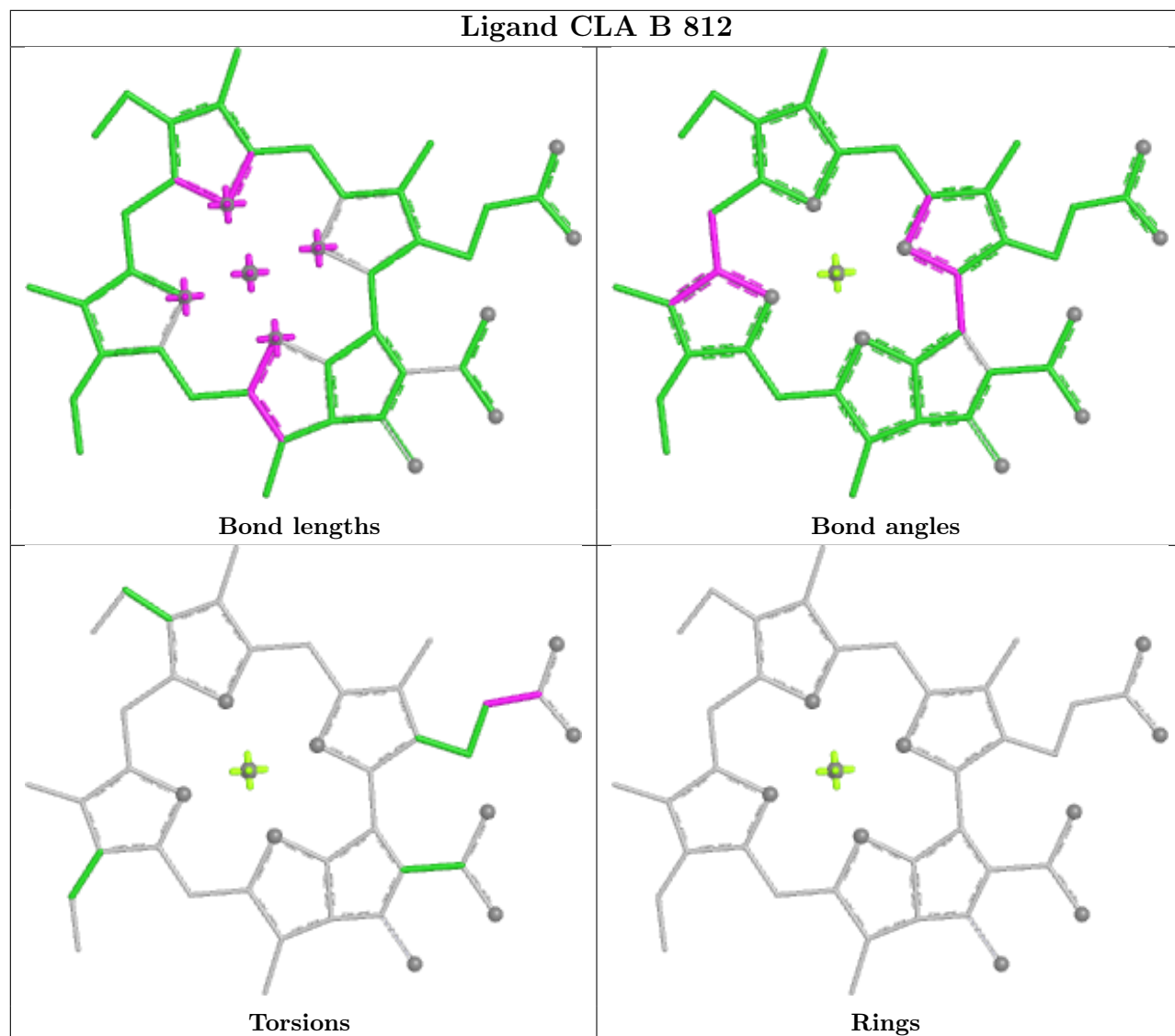


Torsions

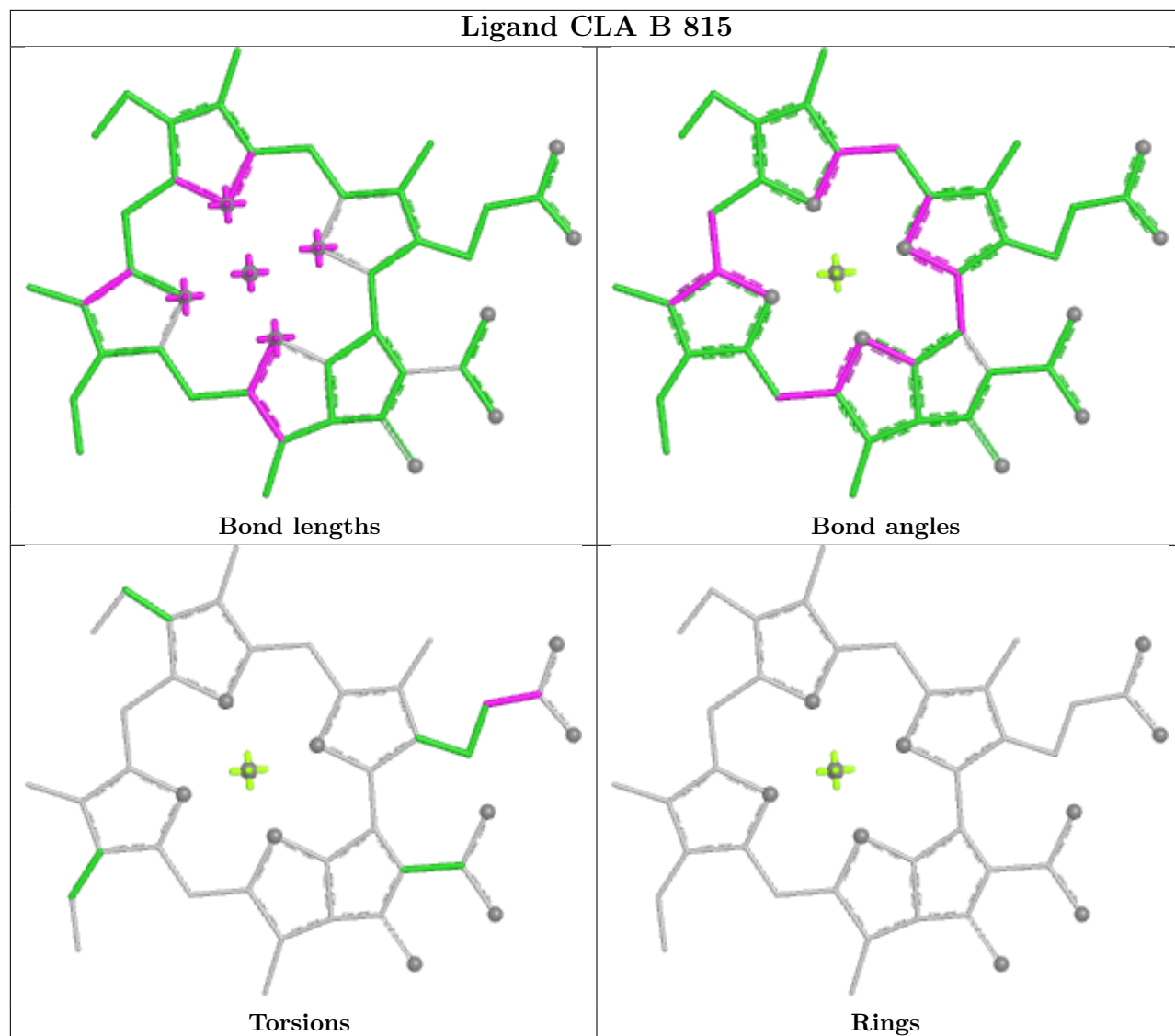


Rings

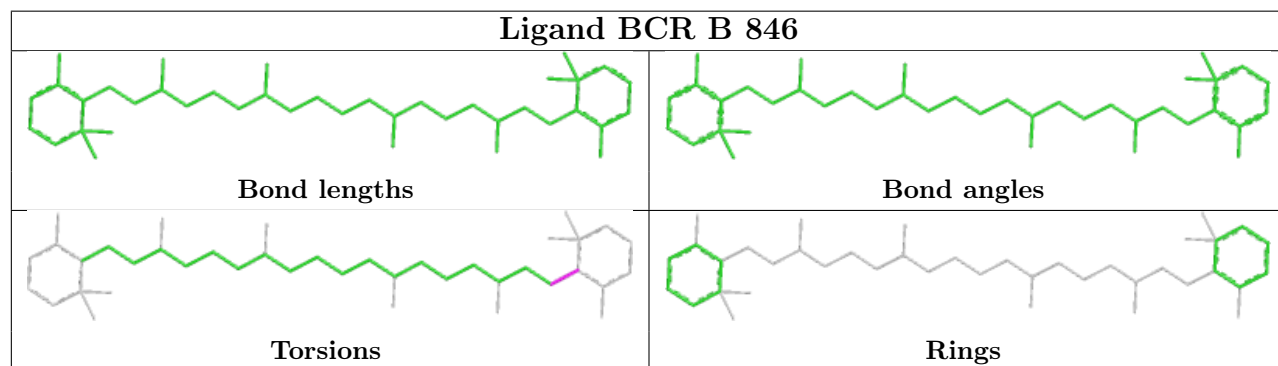
Ligand CLA B 812



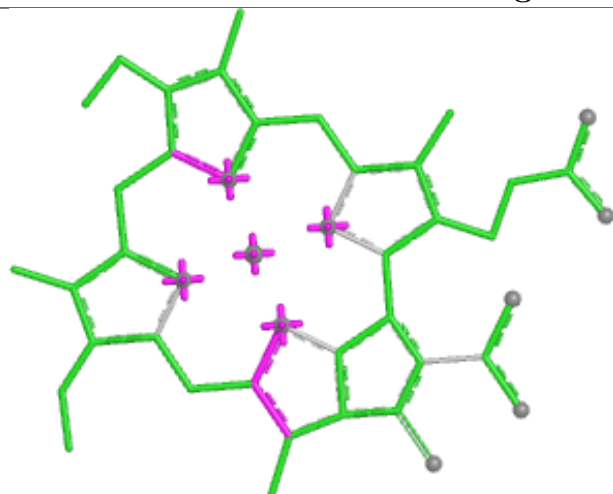
Ligand CLA B 815



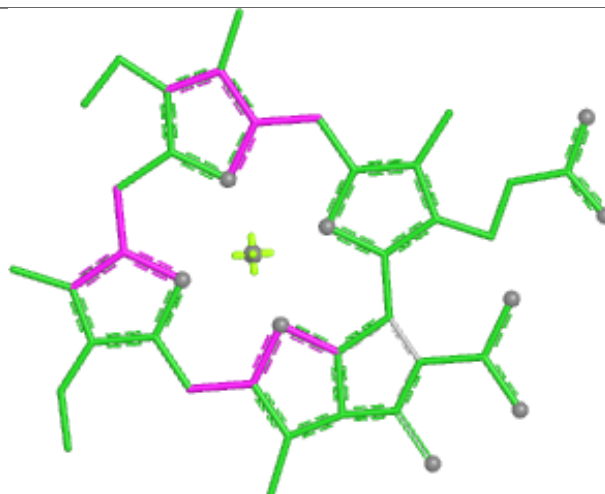
Ligand BCR B 846



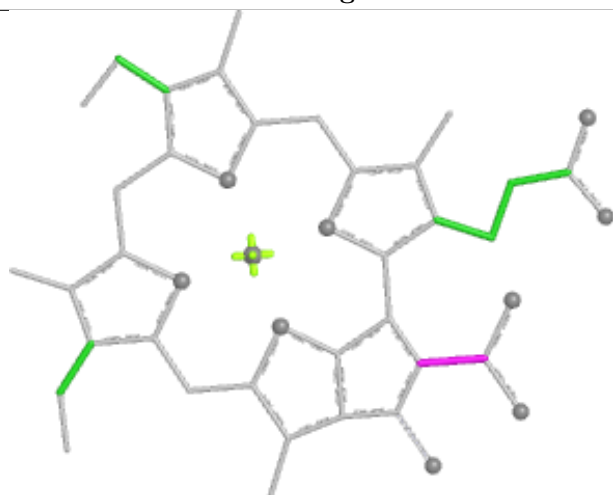
Ligand CLA B 805



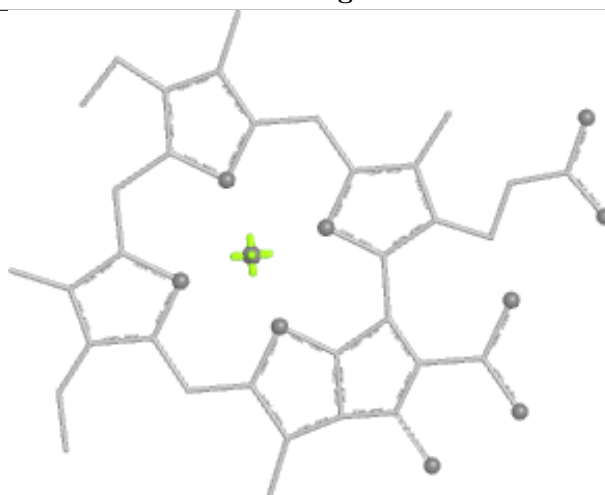
Bond lengths



Bond angles

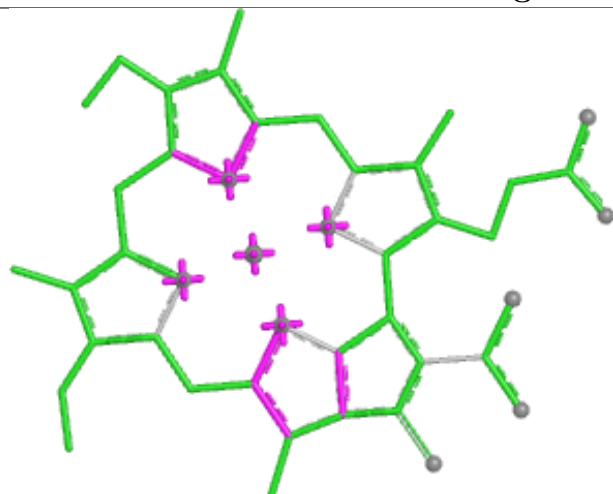


Torsions

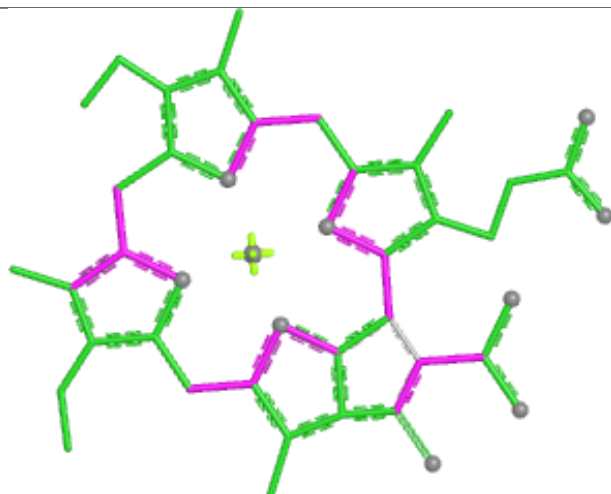


Rings

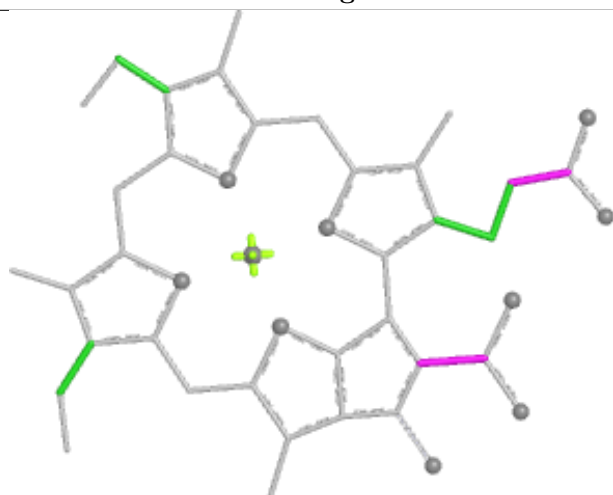
Ligand CLA A 824



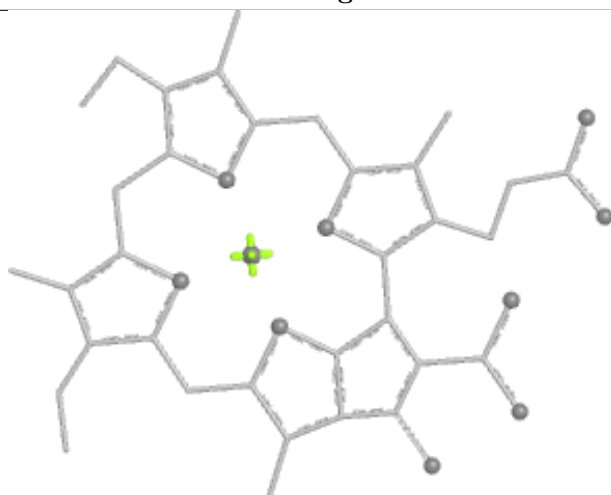
Bond lengths



Bond angles

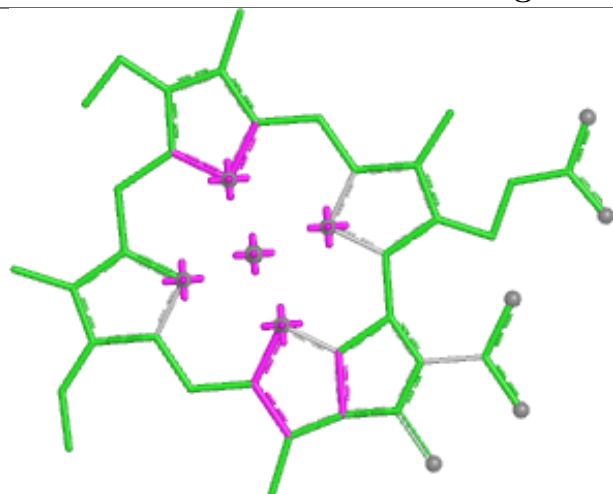


Torsions

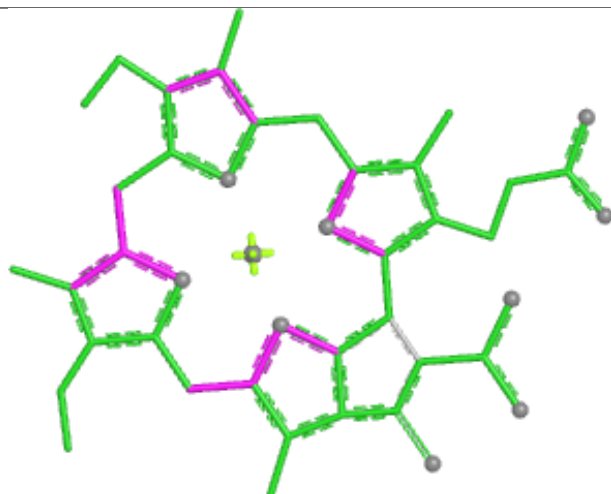


Rings

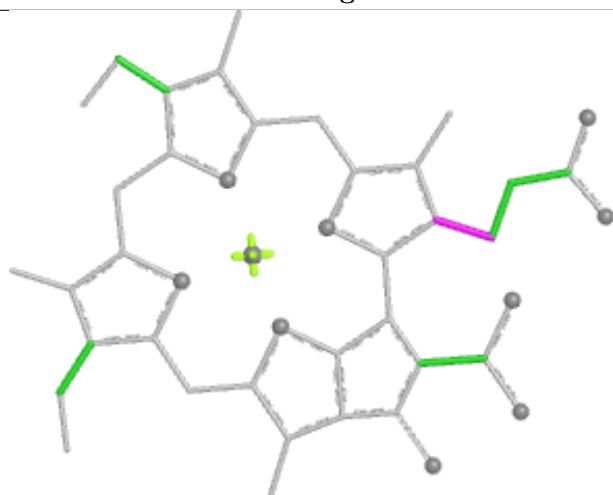
Ligand CLA B 831



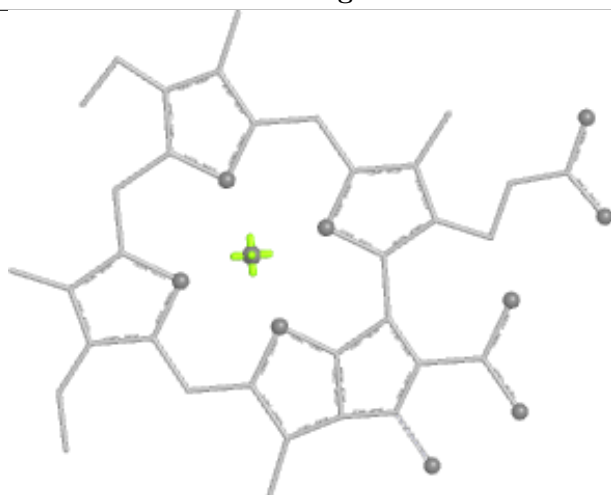
Bond lengths



Bond angles

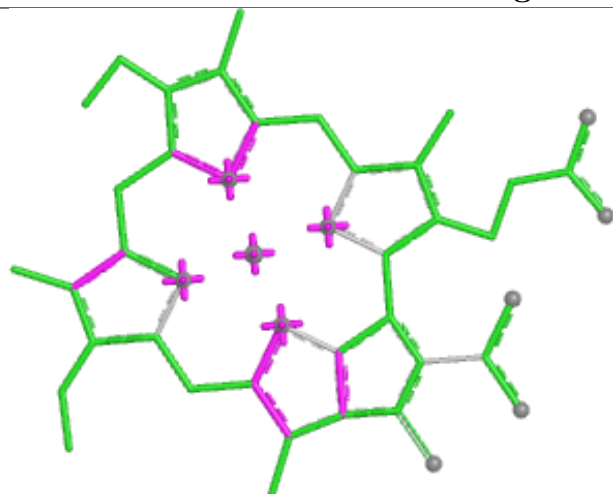


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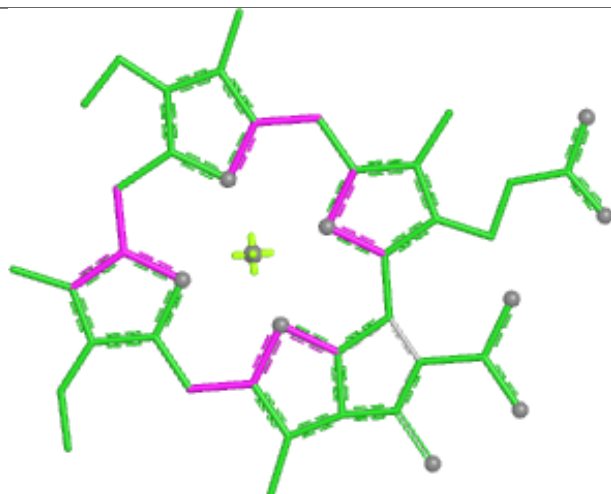


Rings

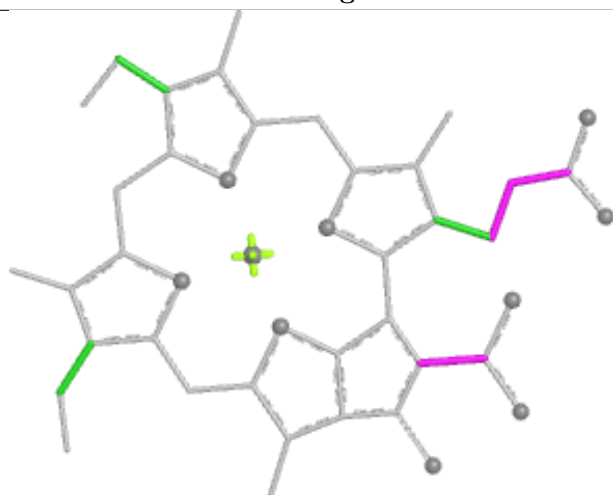
Ligand CLA A 820



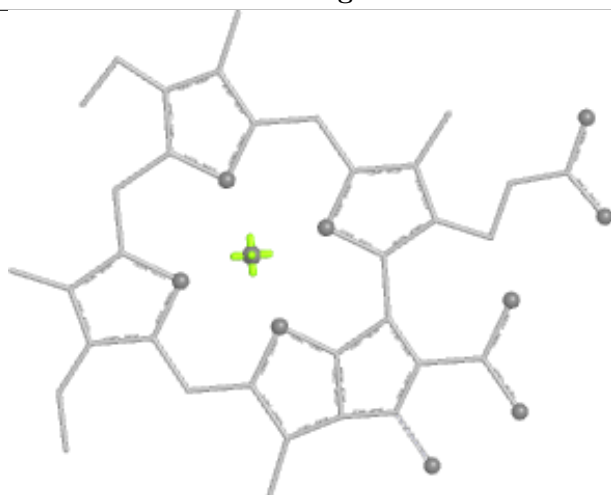
Bond lengths



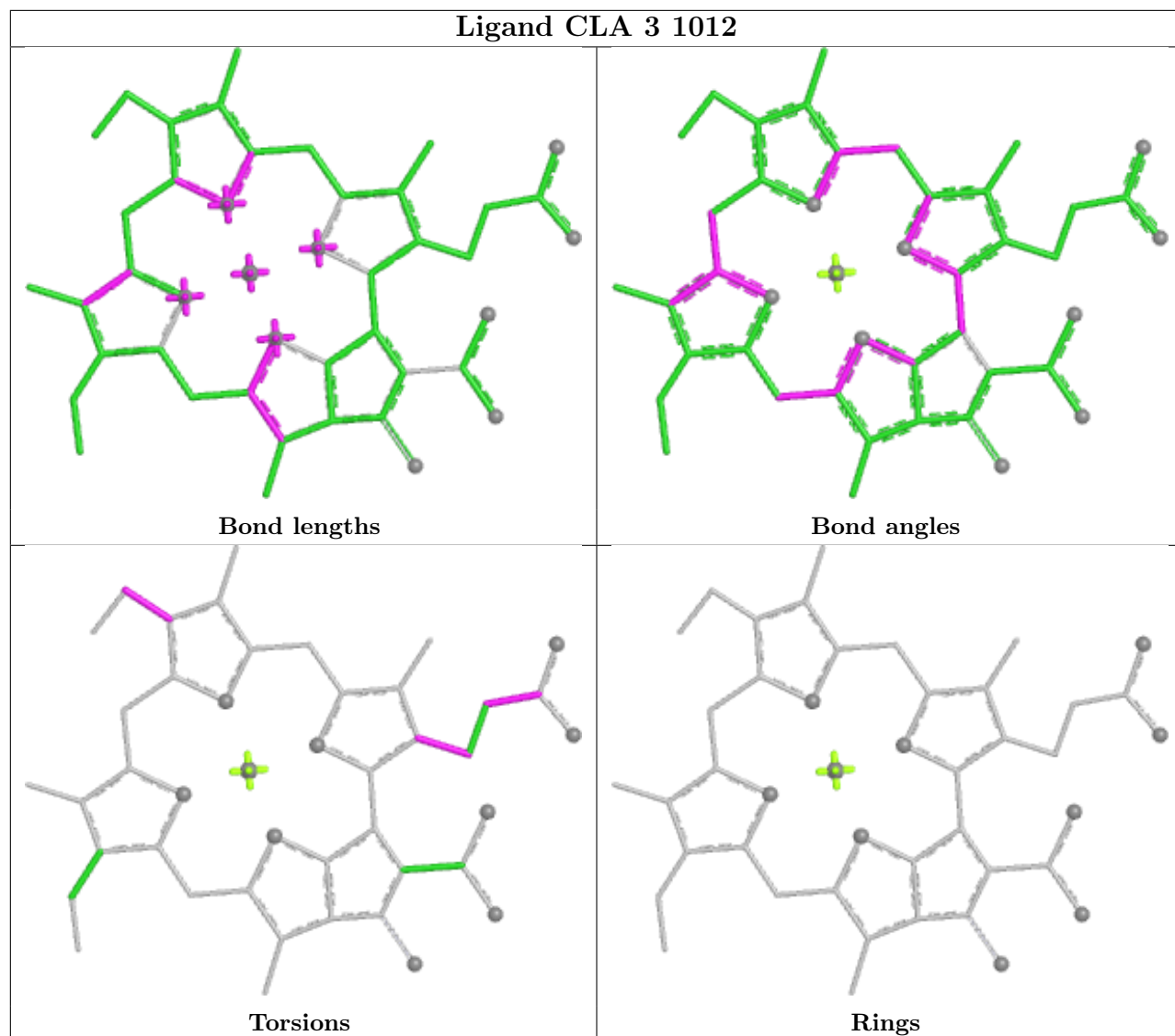
Bond angles



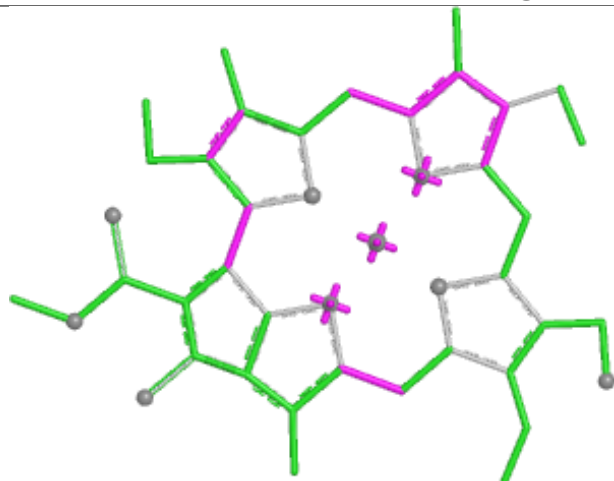
Torsions



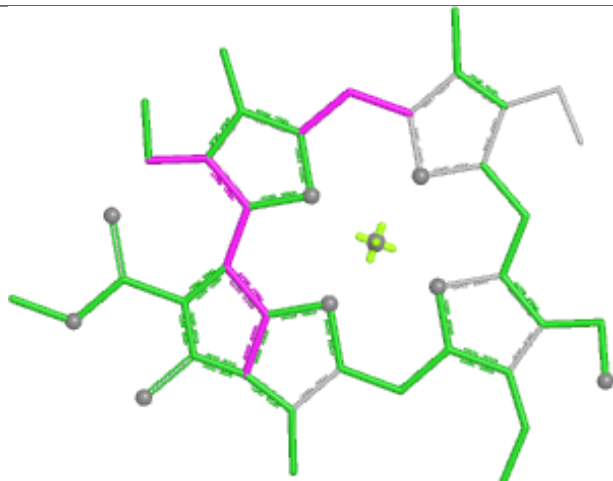
Rings



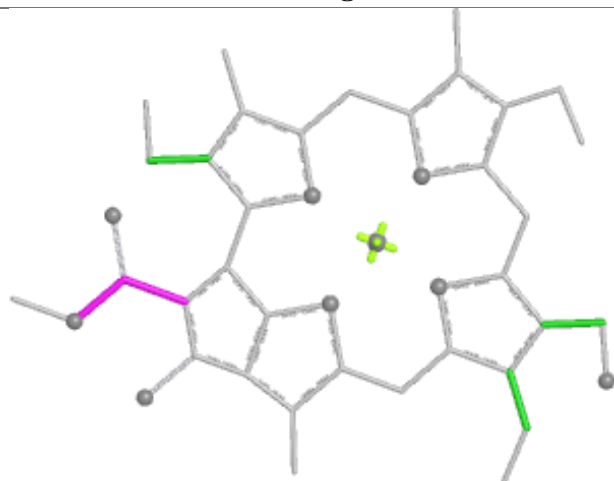
Ligand CHL 5 317



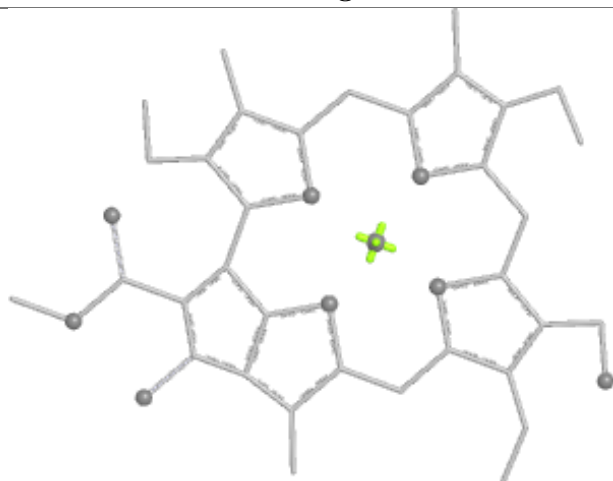
Bond lengths



Bond angles

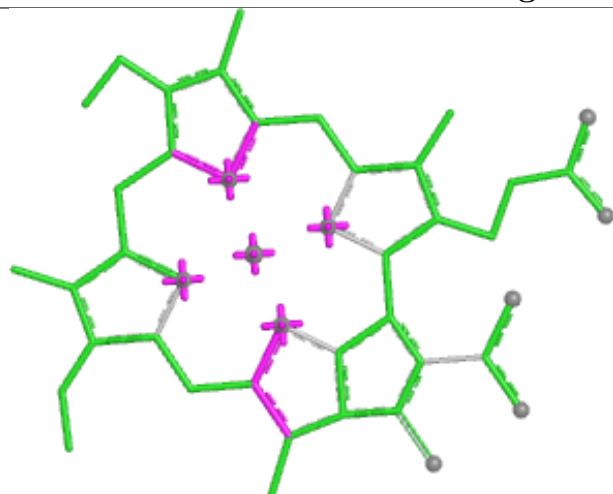


Torsions

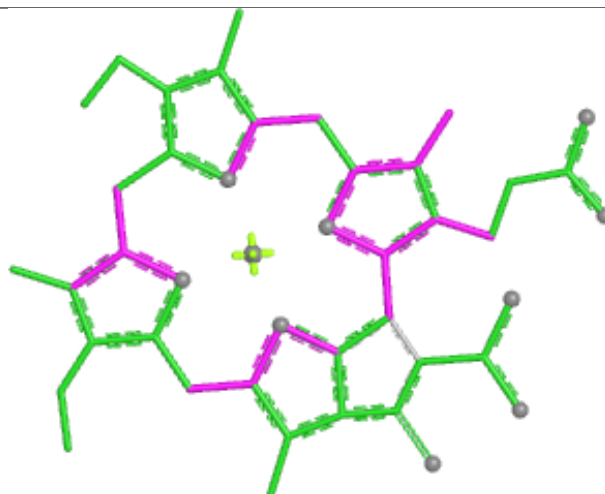


Rings

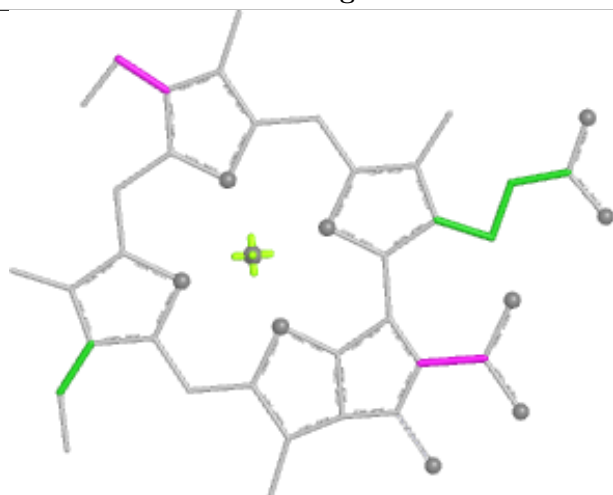
Ligand CLA 0 313



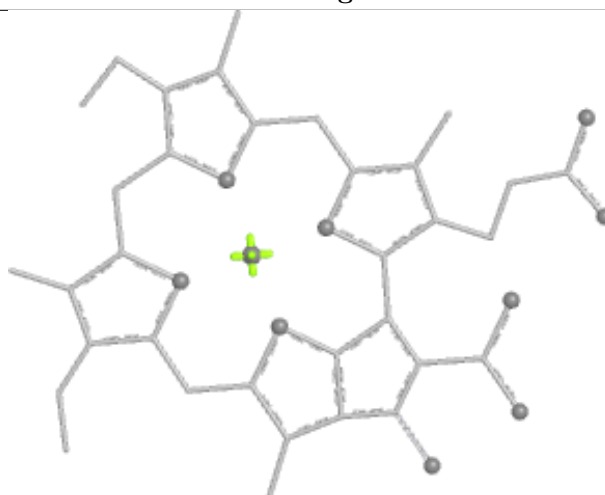
Bond lengths



Bond angles

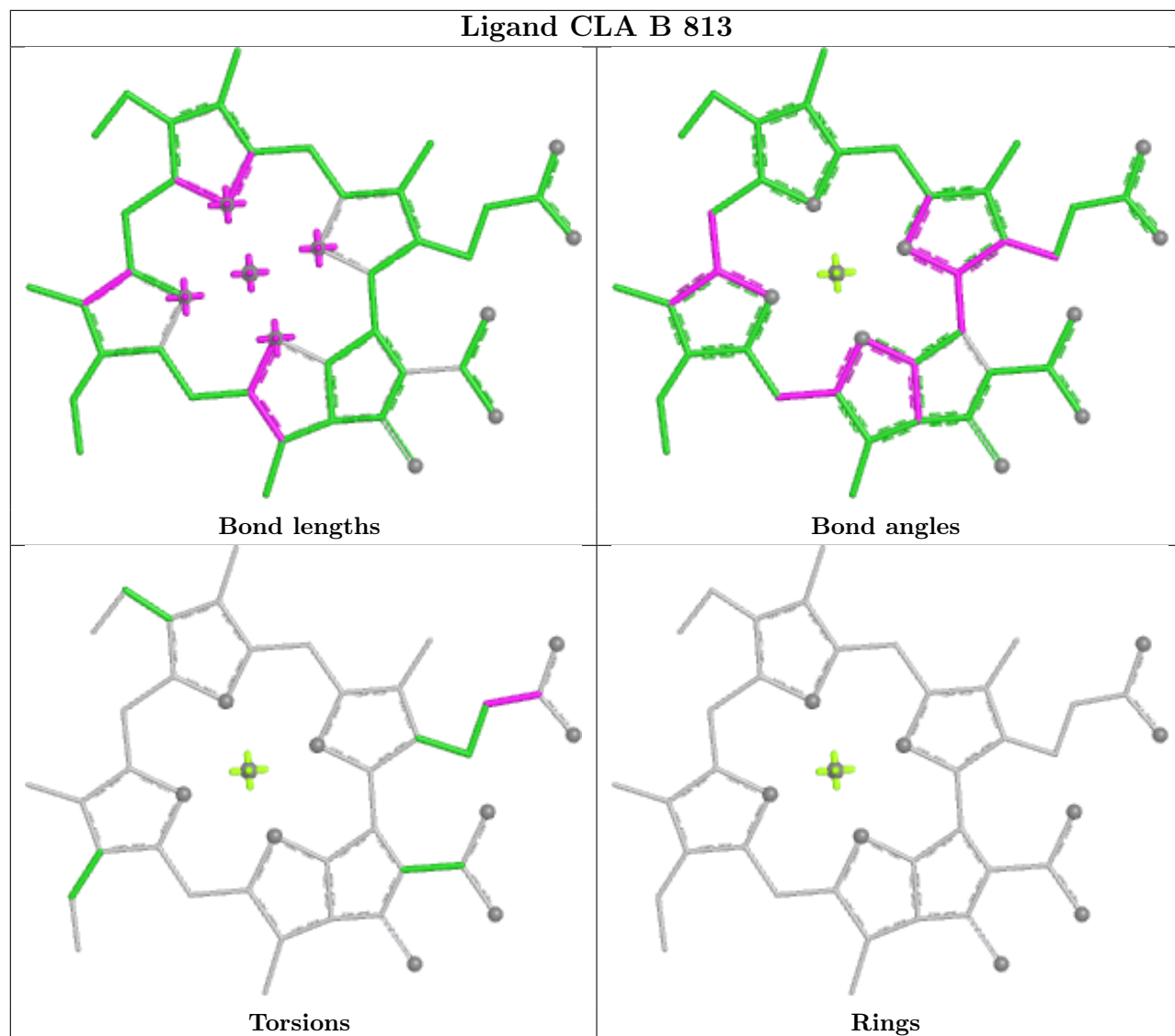


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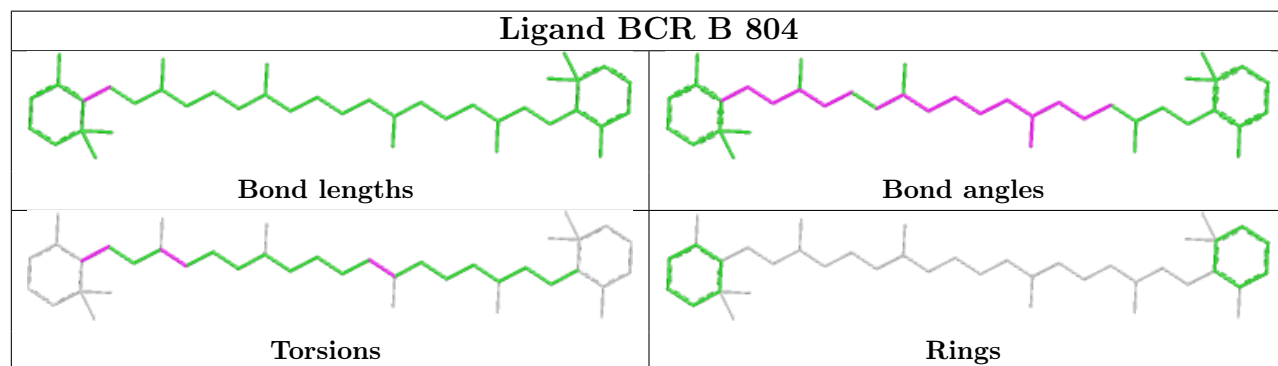


Rings

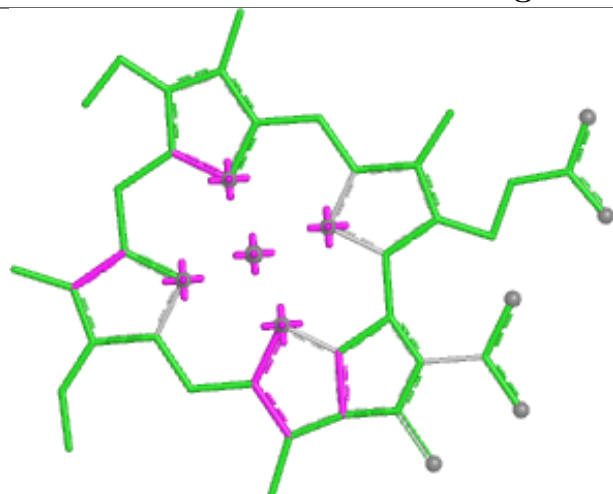
Ligand CLA B 813



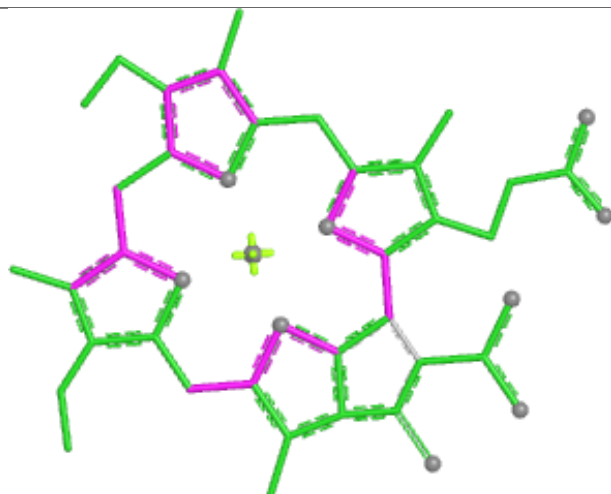
Ligand BCR B 804



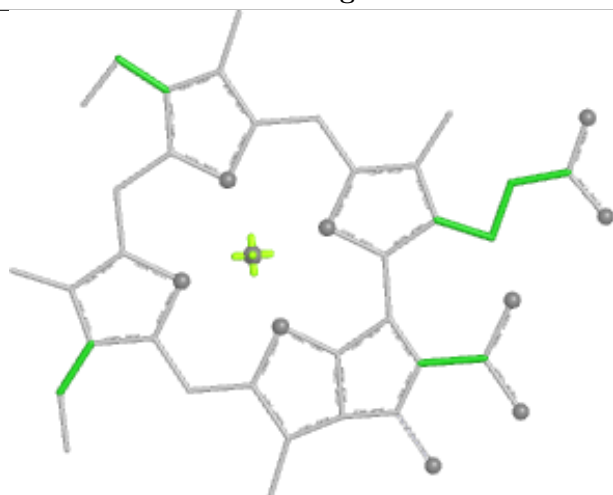
Ligand CLA B 836



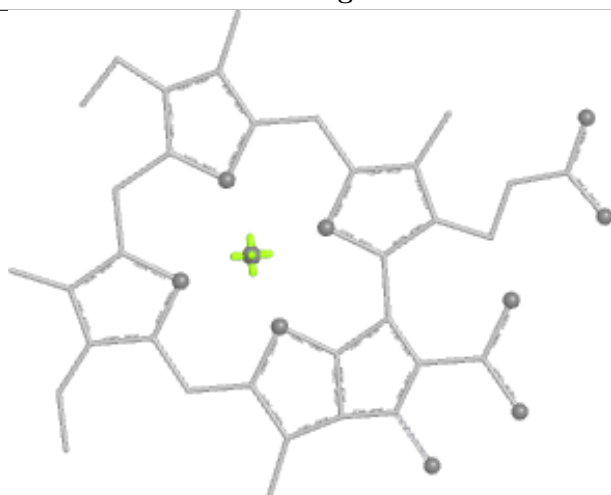
Bond lengths



Bond angles

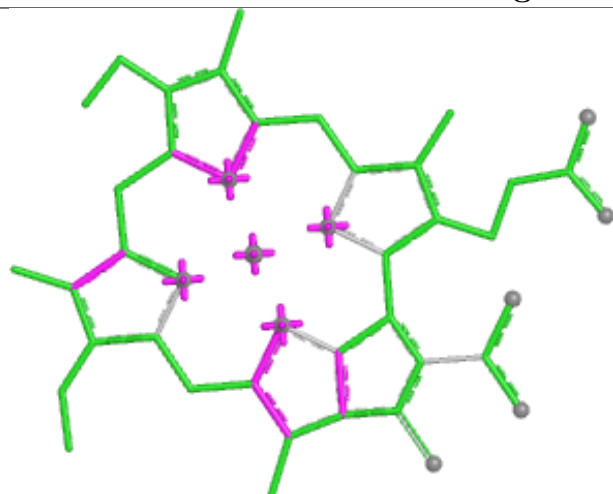


Torsions

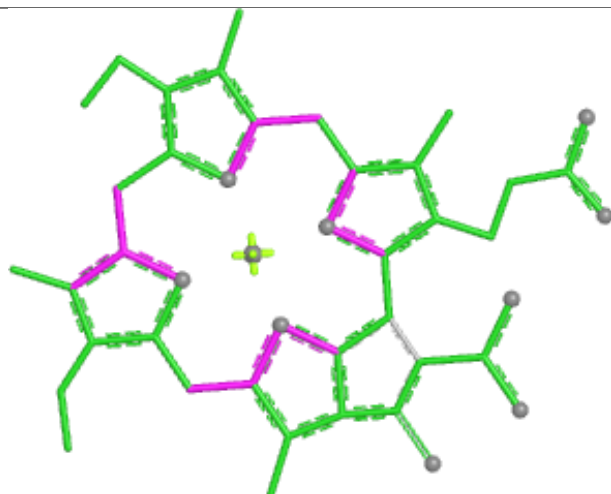


Rings

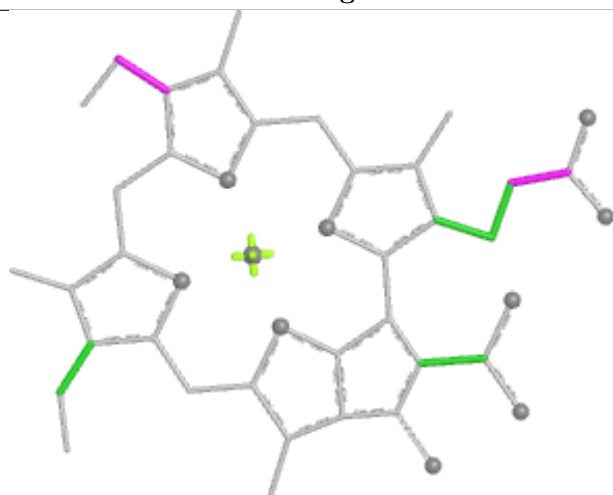
Ligand CLA A 839



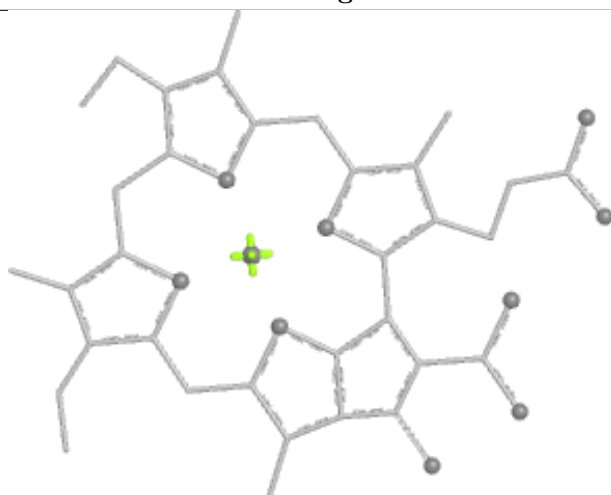
Bond lengths



Bond angles

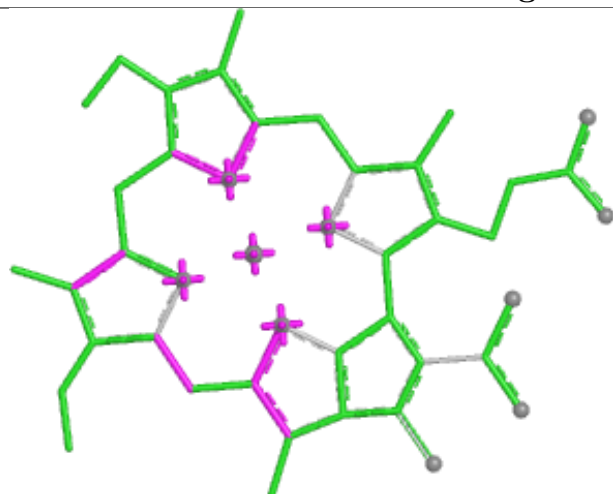


Torsions

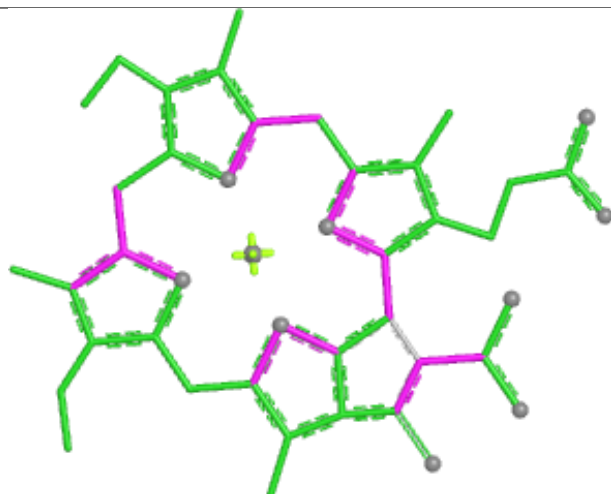


Rings

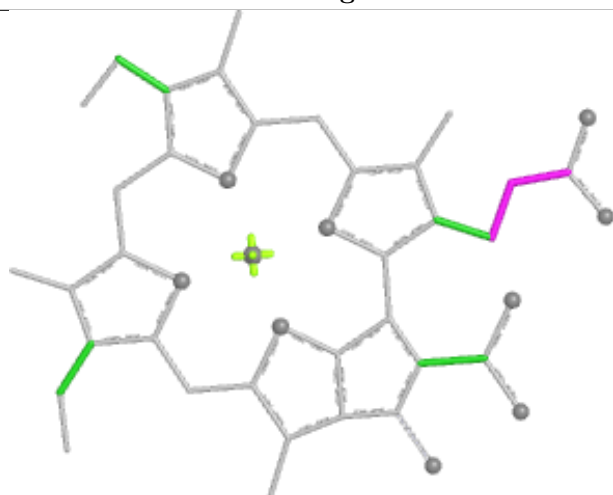
Ligand CLA 0 307



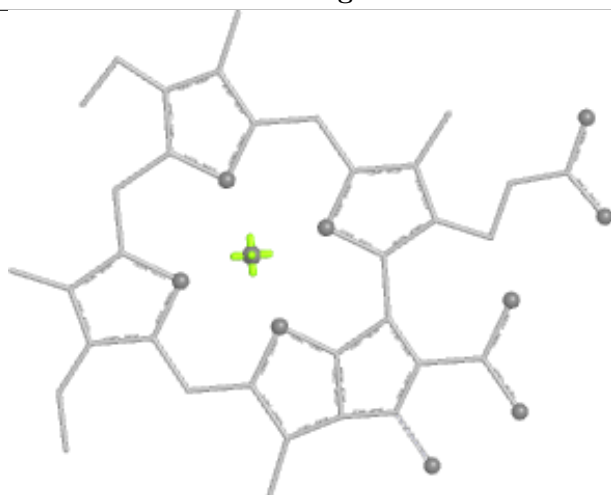
Bond lengths



Bond angles

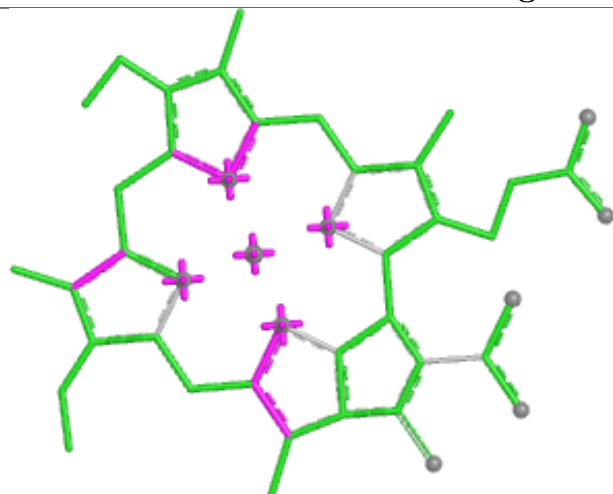


Torsions

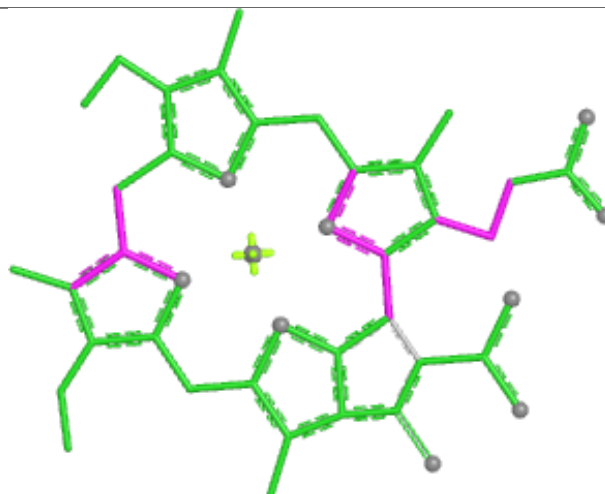


Rings

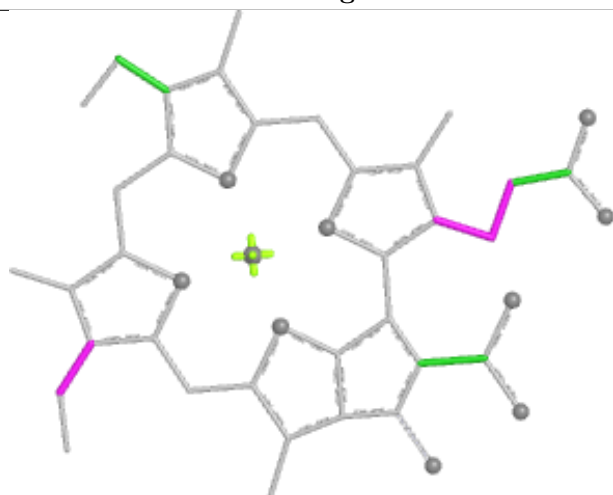
Ligand CLA 8 310



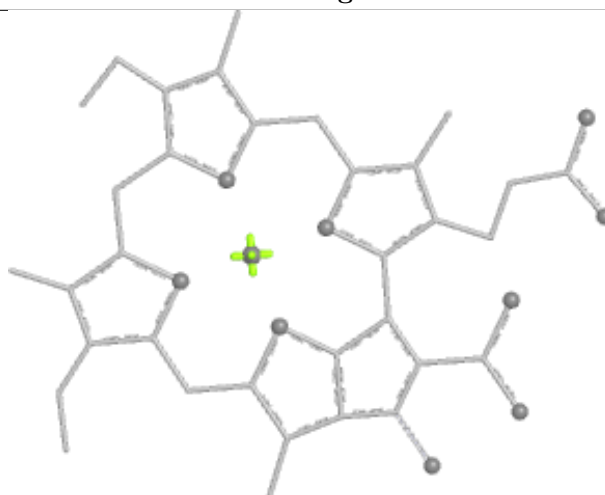
Bond lengths



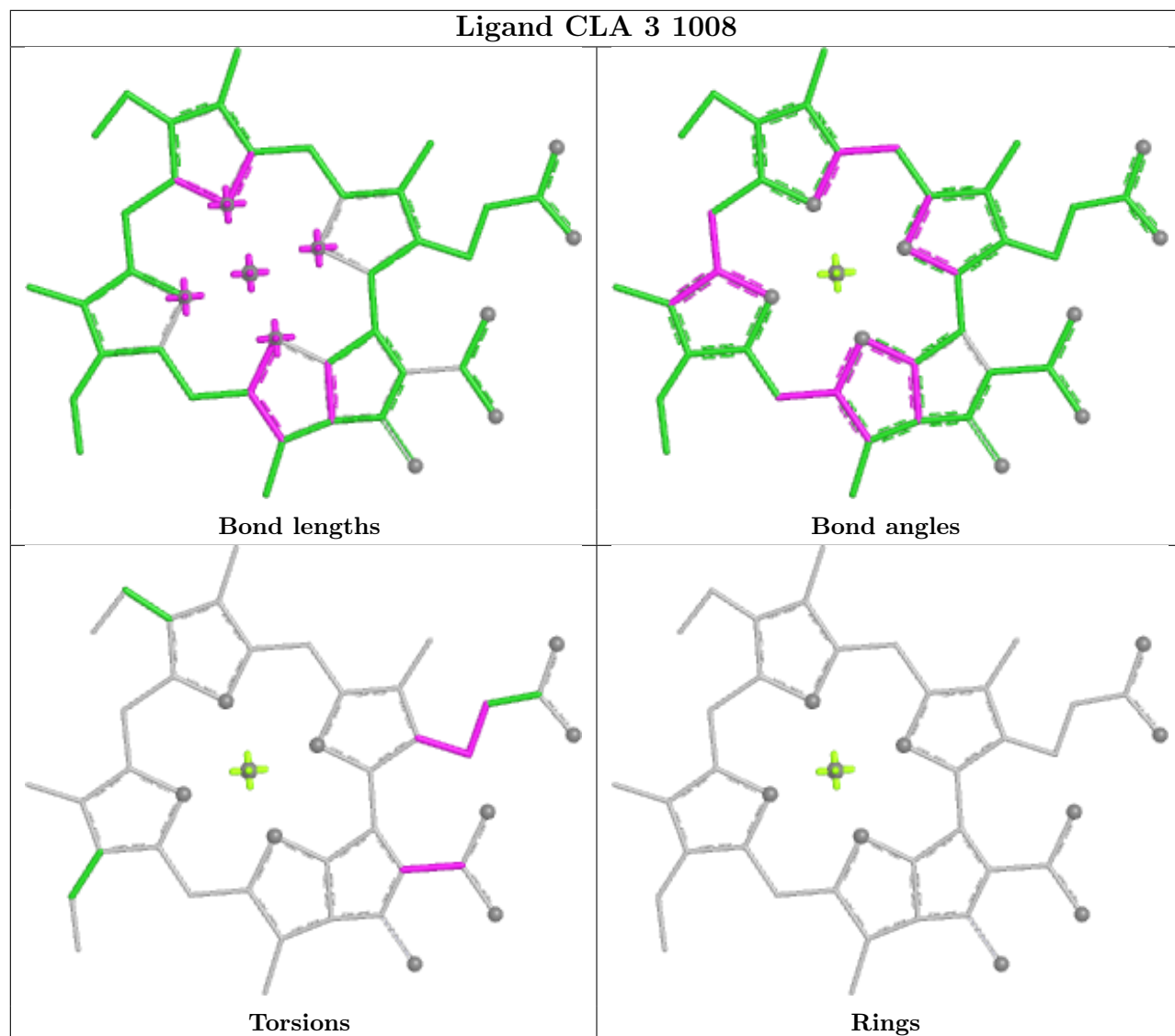
Bond angles



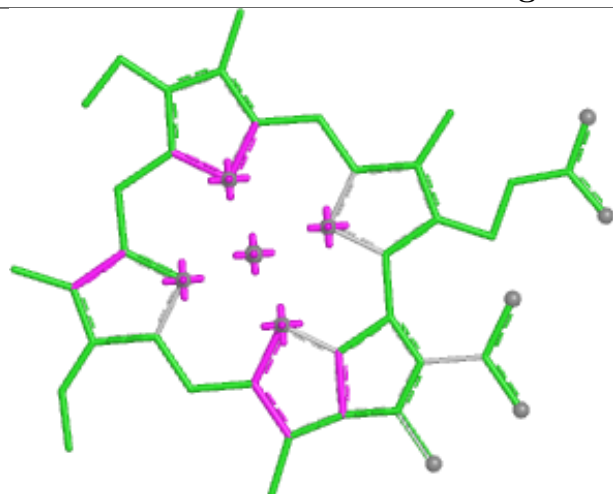
Torsions



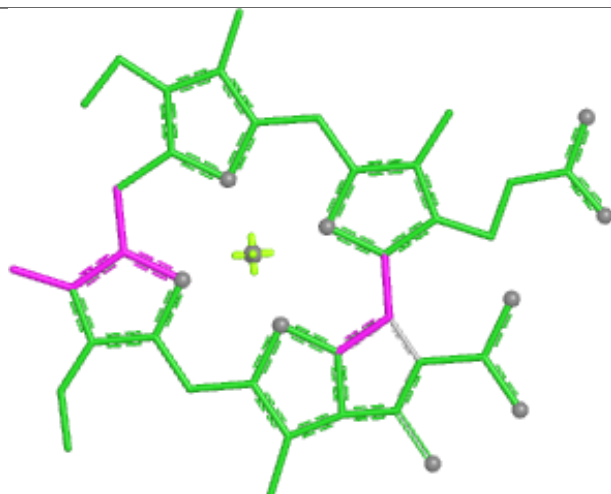
Rings



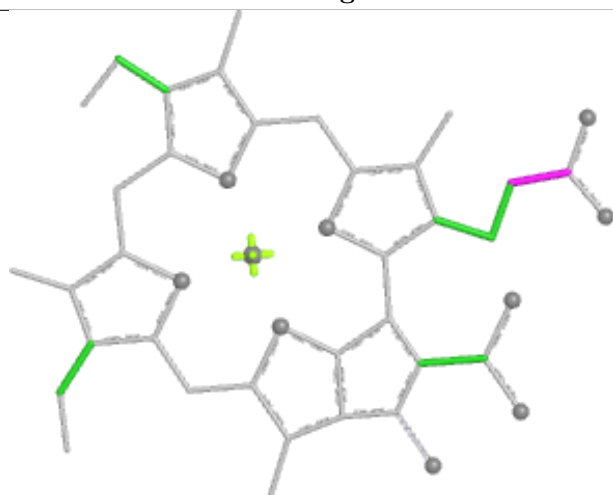
Ligand CLA 6 305



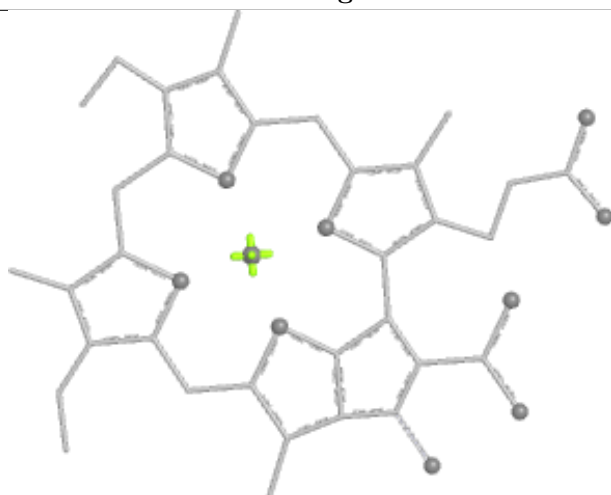
Bond lengths



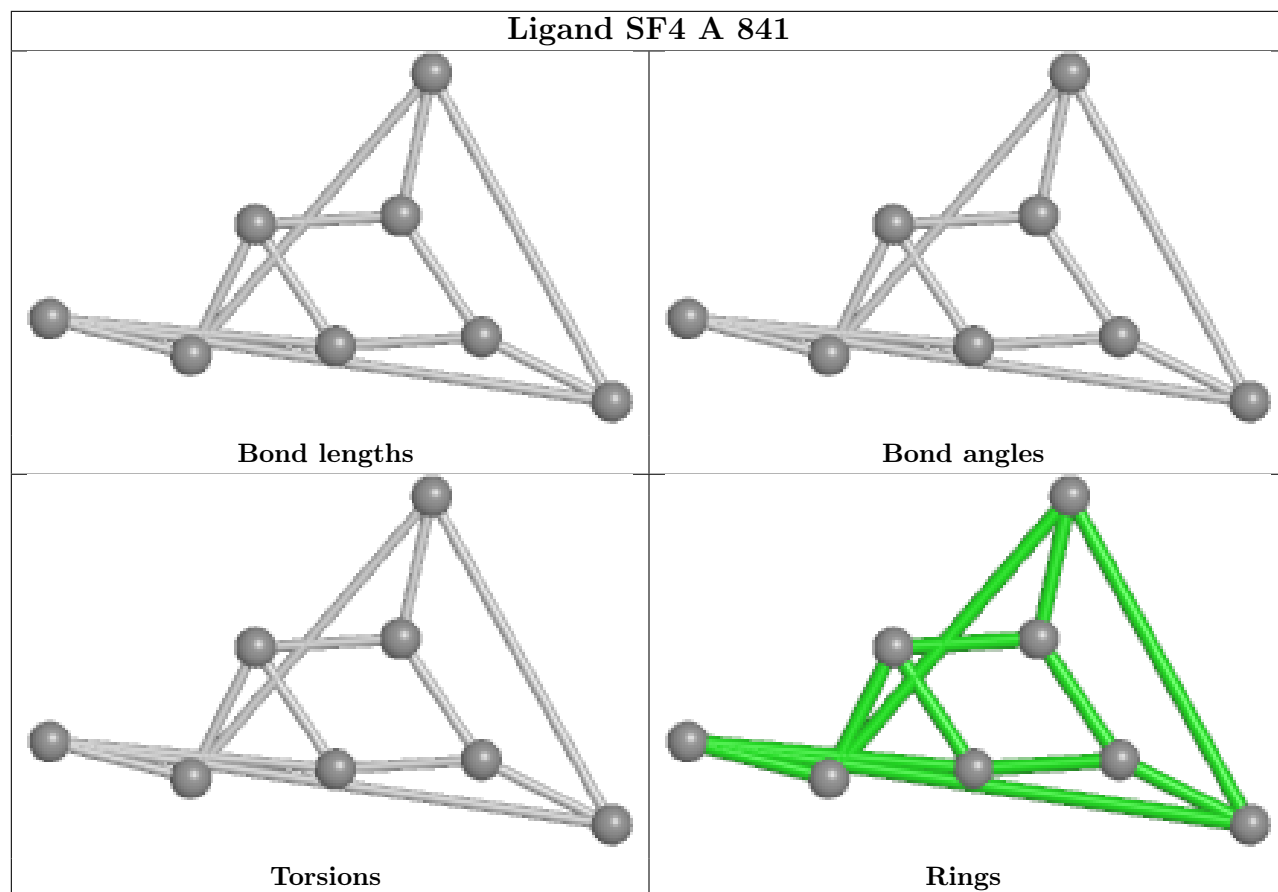
Bond angles

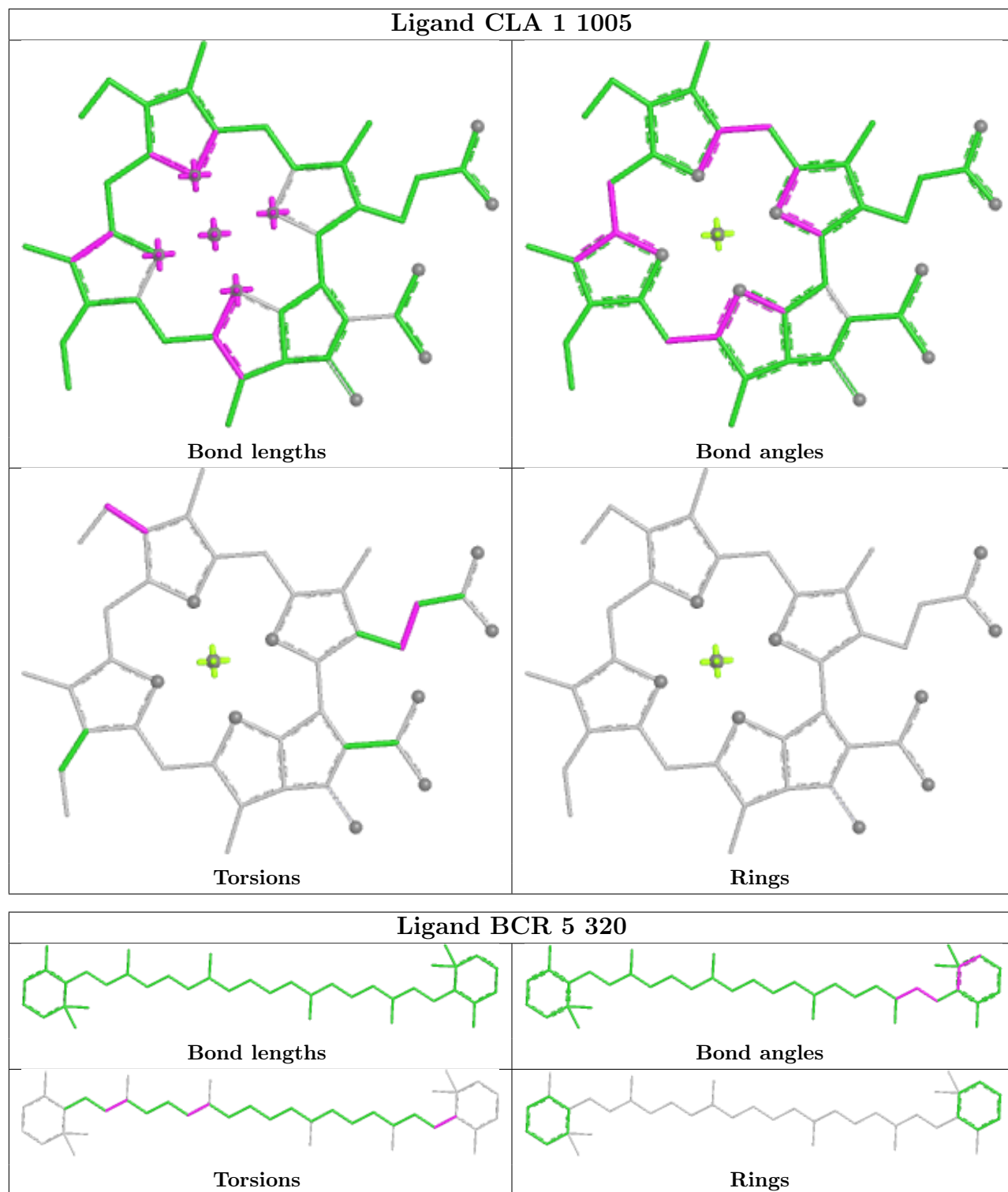


Torsions

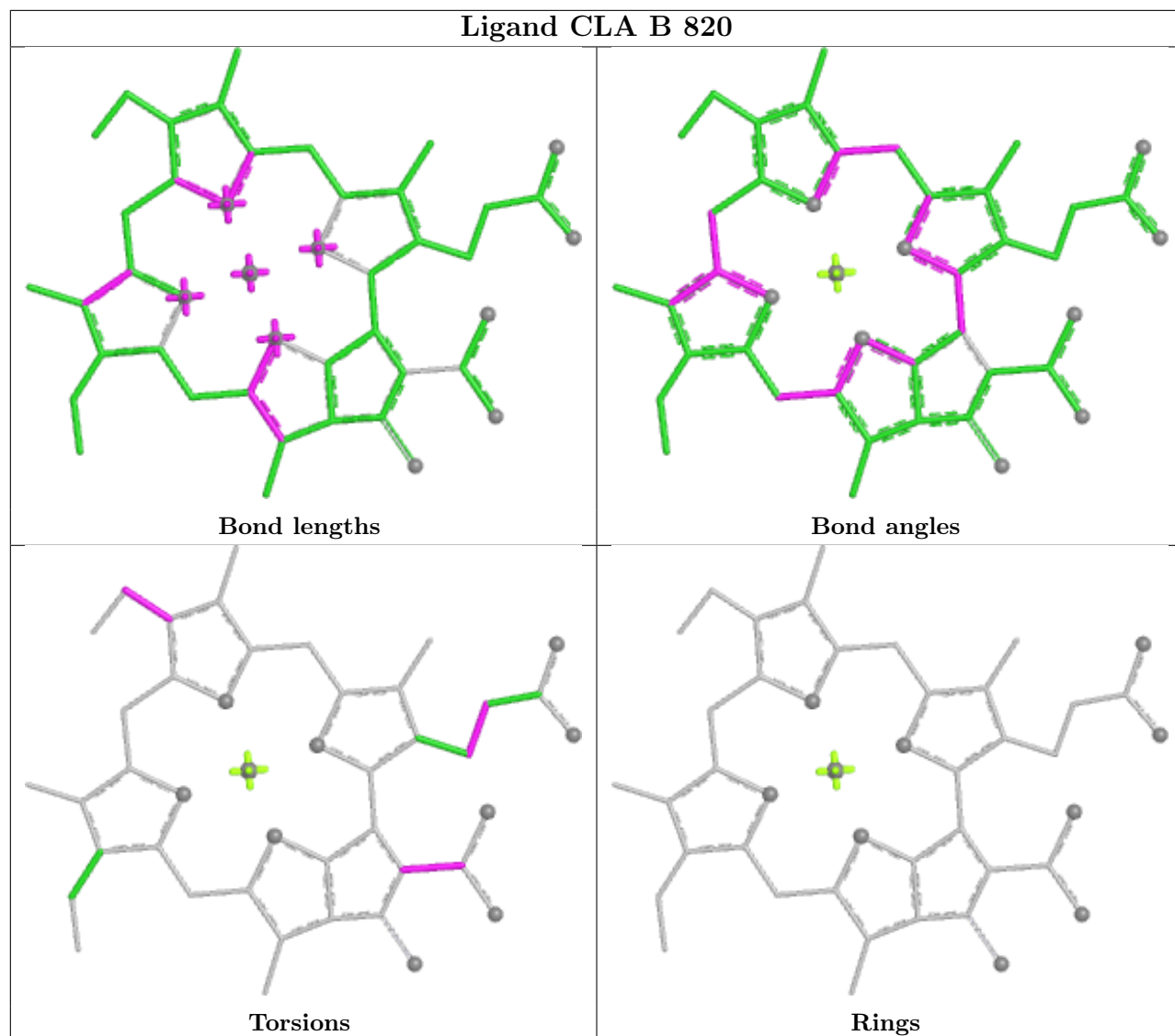


Rings

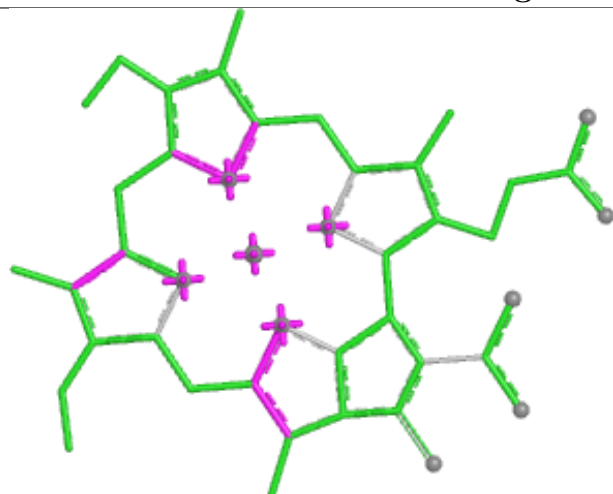




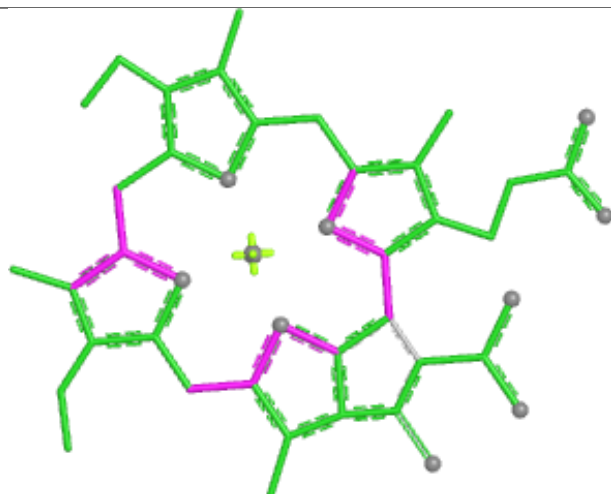
Ligand CLA B 820



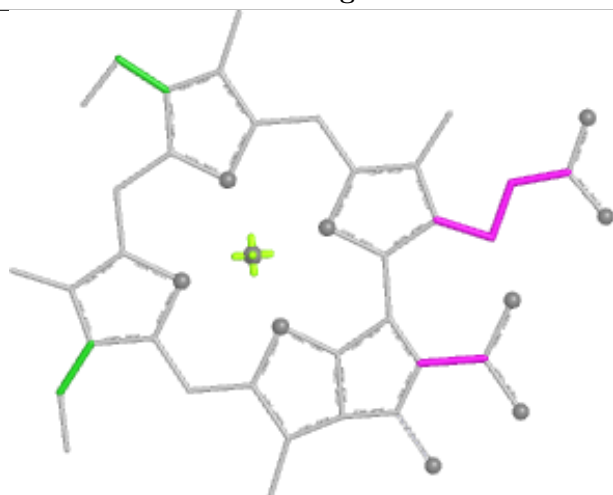
Ligand CLA B 839



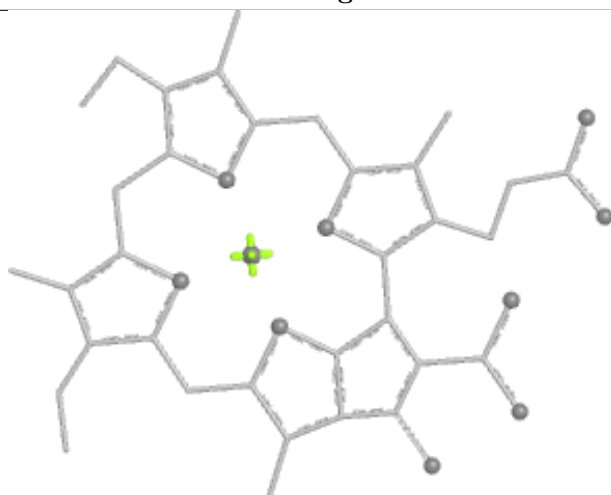
Bond lengths



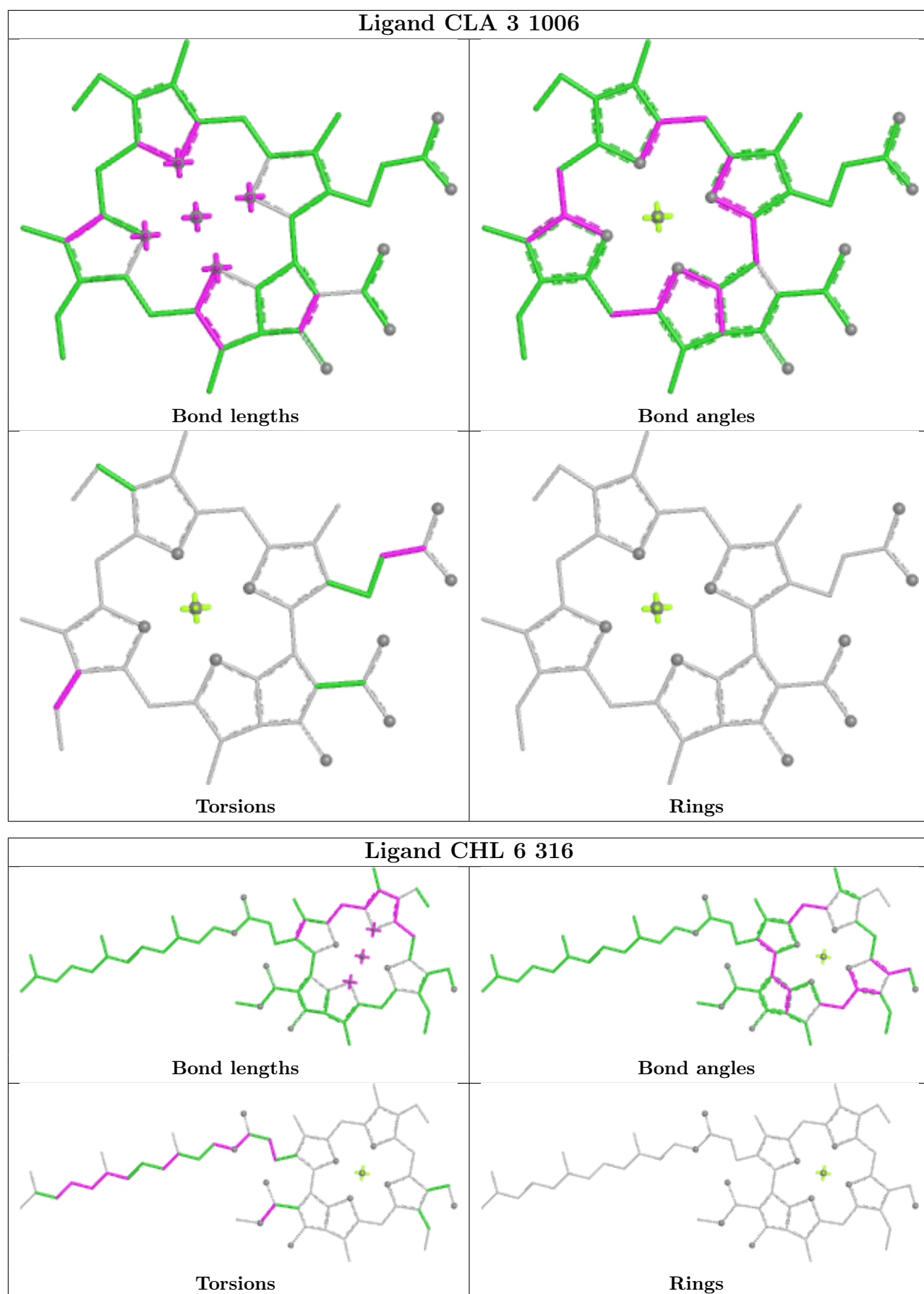
Bond angles



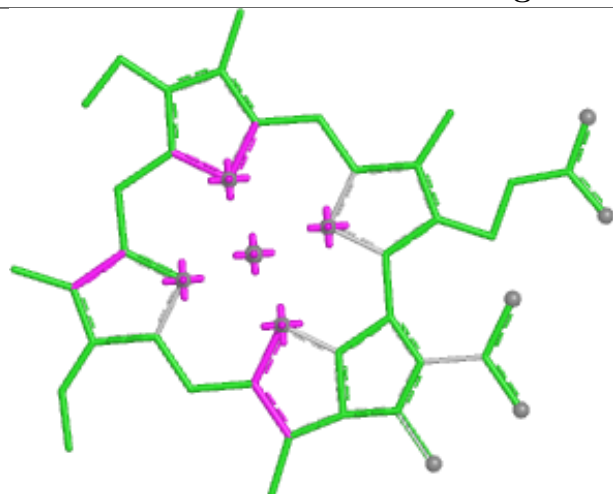
Torsions



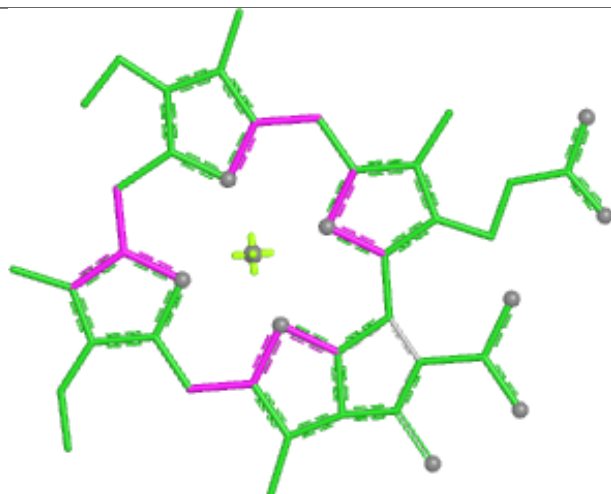
Rings



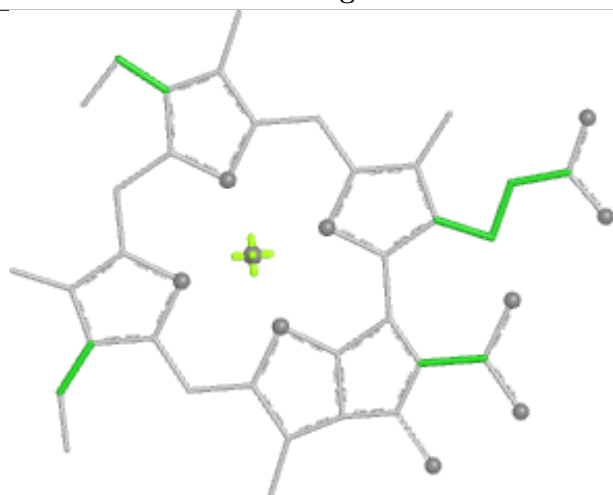
Ligand CLA A 825



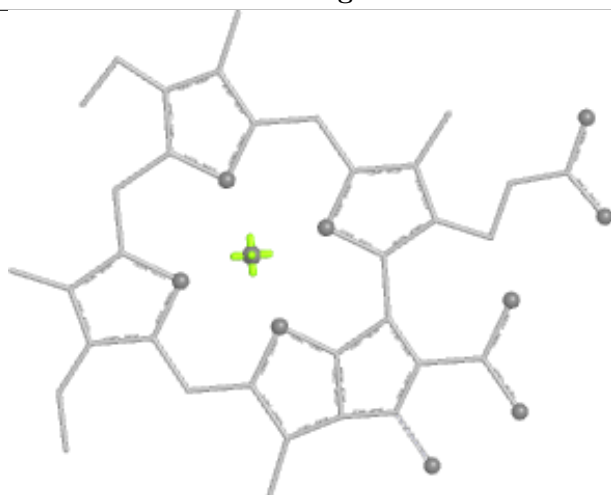
Bond lengths



Bond angles

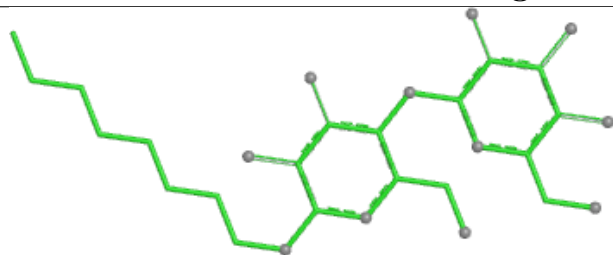


Torsions

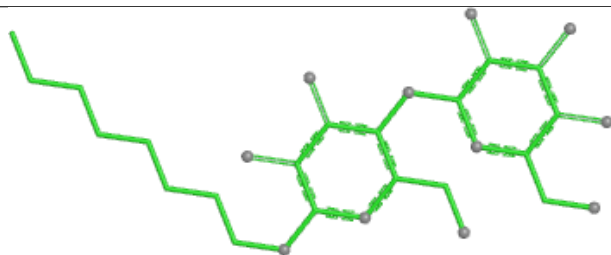


Rings

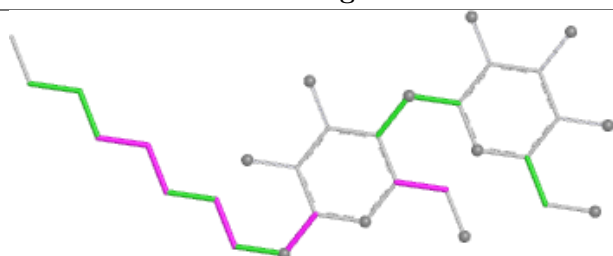
Ligand LMT B 849



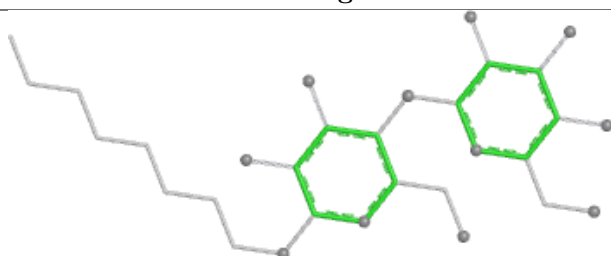
Bond lengths



Bond angles

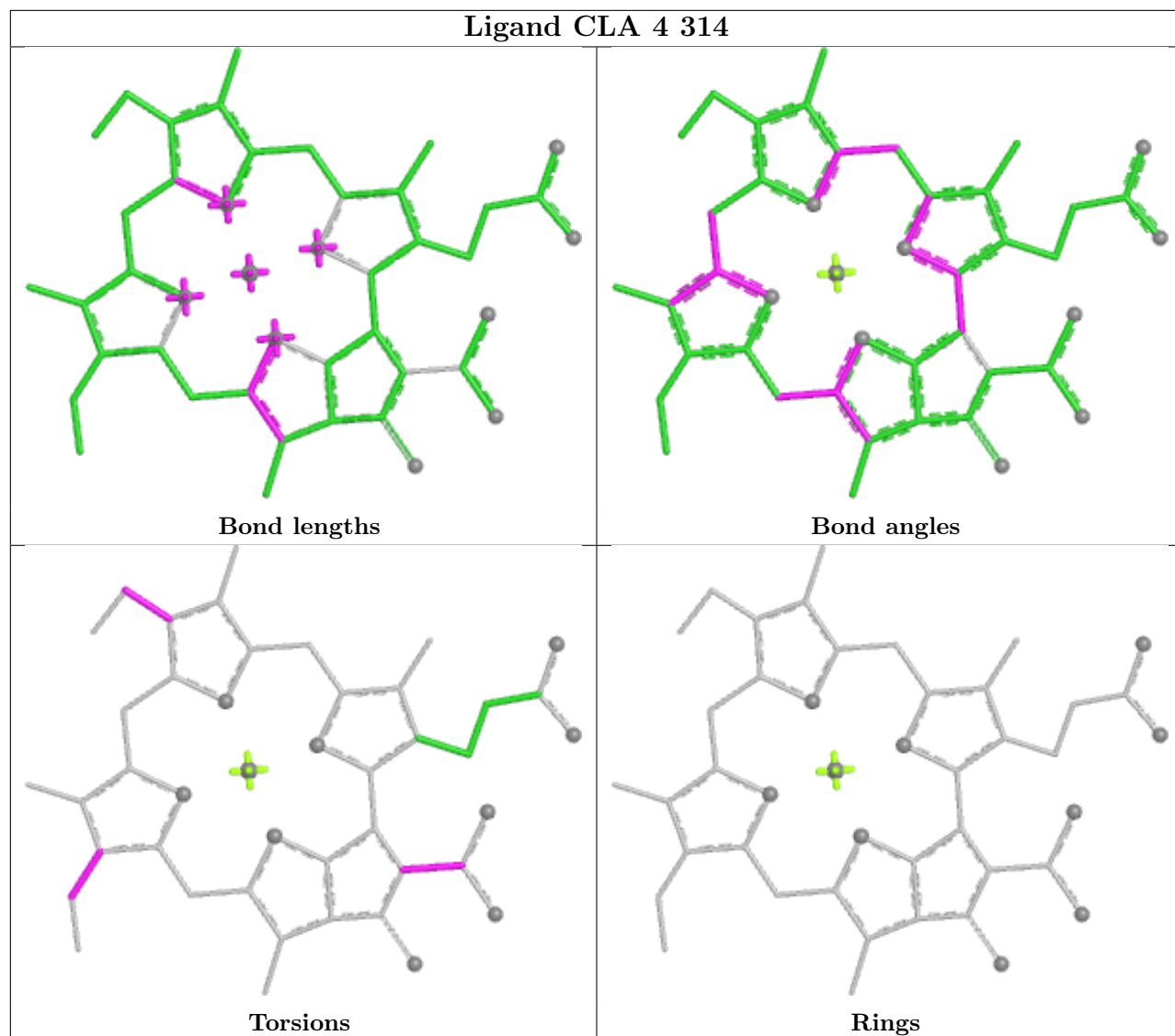


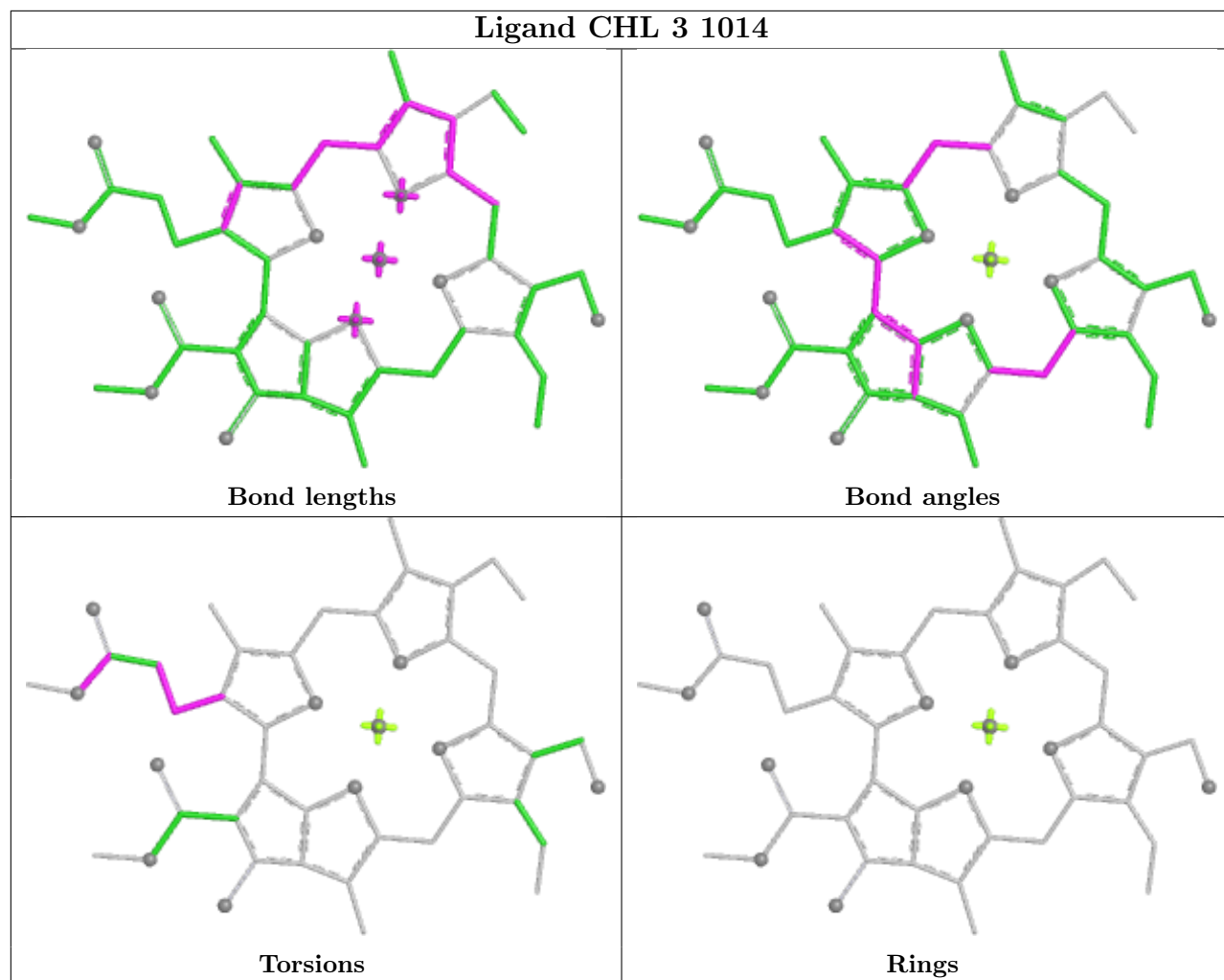
Torsions



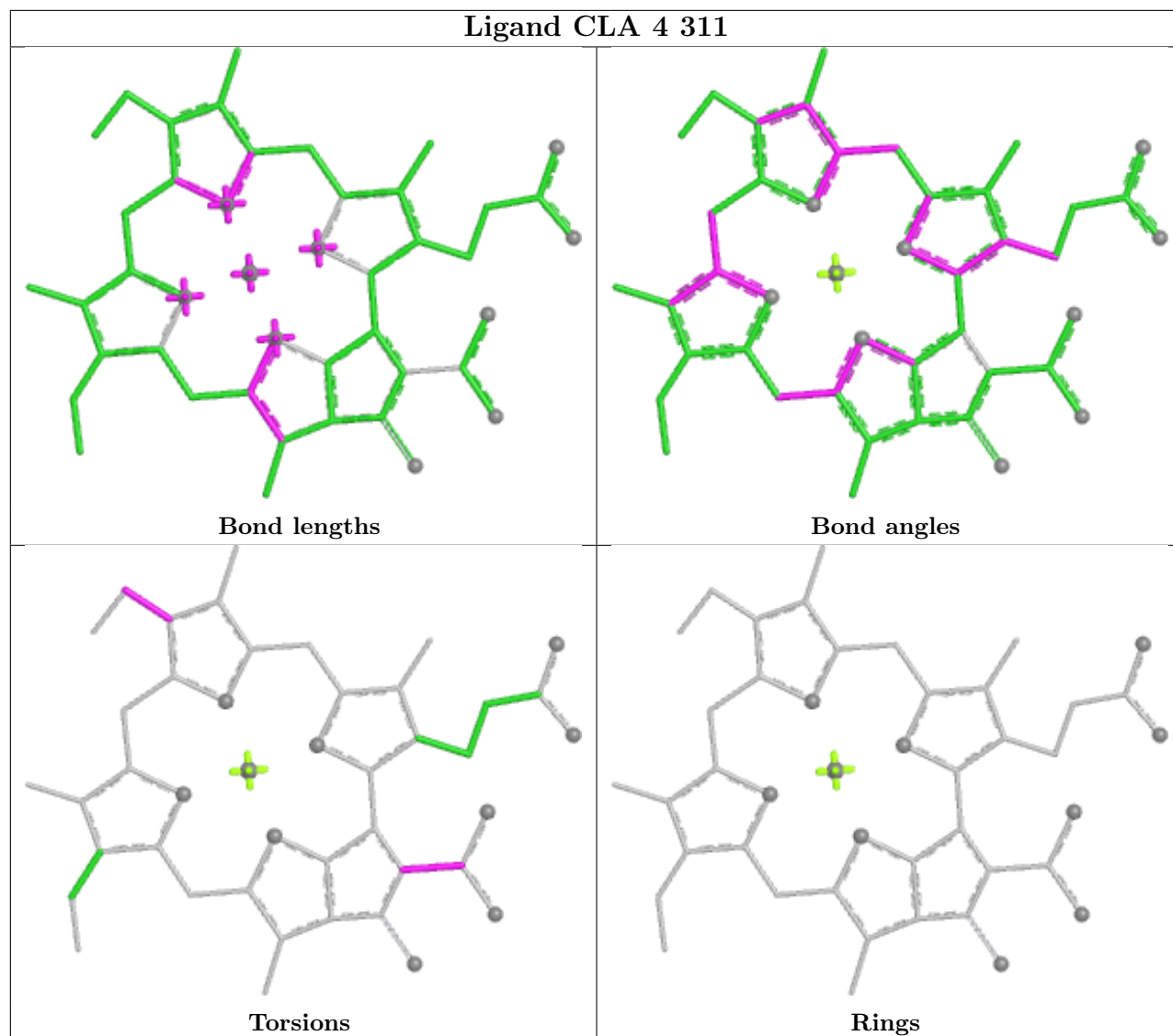
Rings

Ligand CLA 4 314

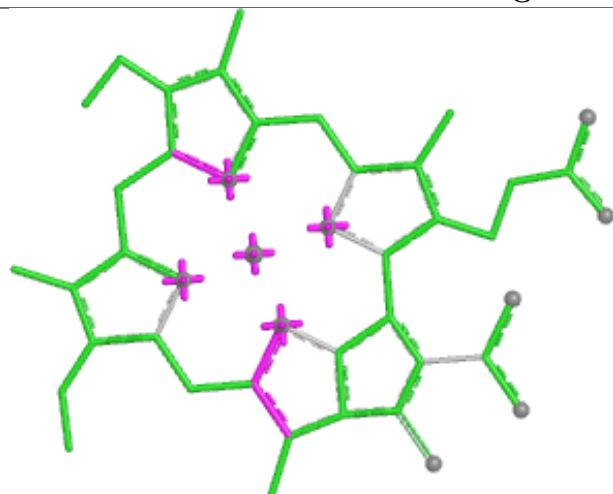




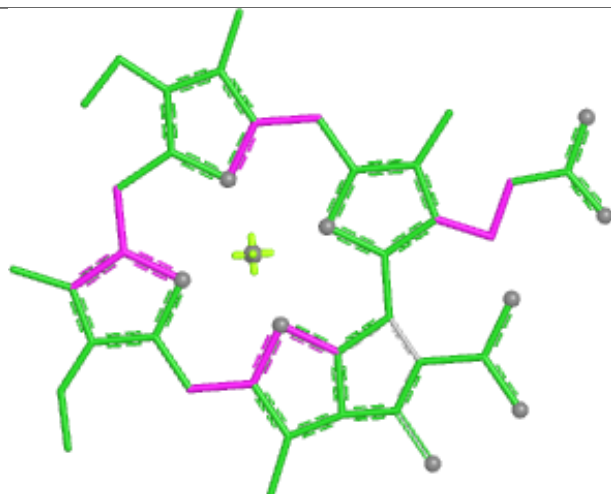
Ligand CLA 4 311



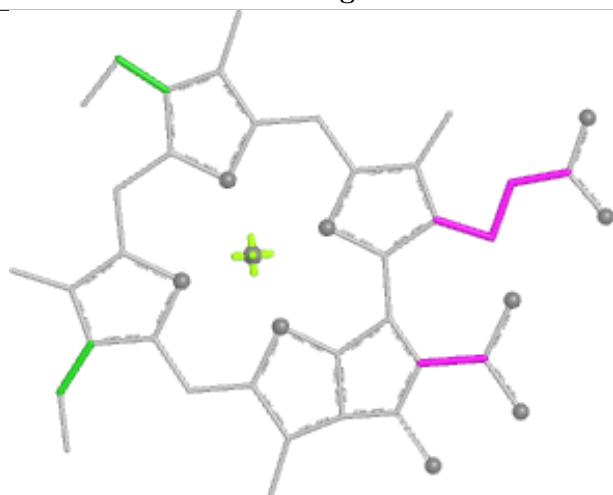
Ligand CLA A 810



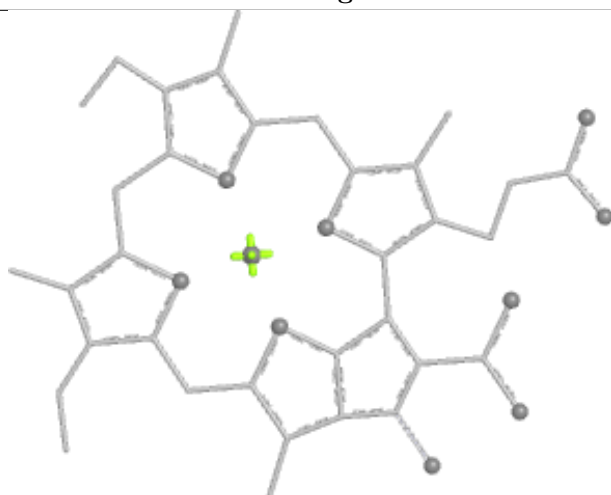
Bond lengths



Bond angles

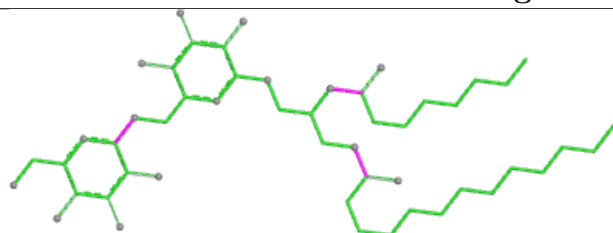


Torsions

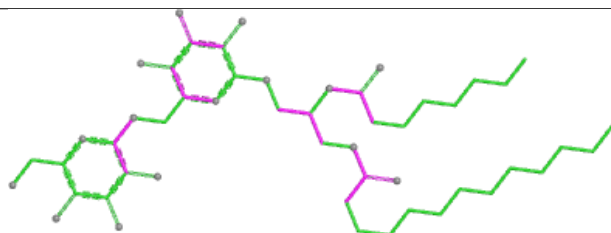


Rings

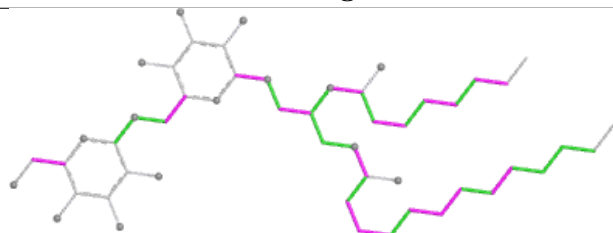
Ligand DGD 5 319



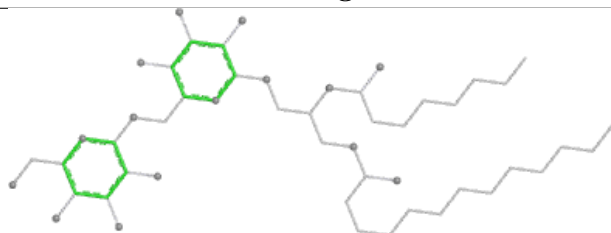
Bond lengths



Bond angles

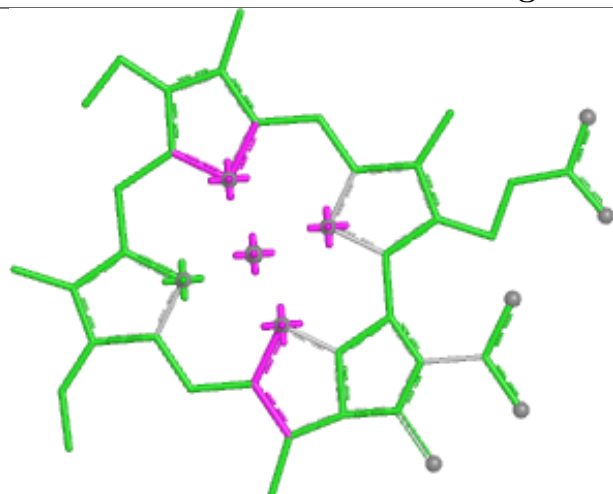


Torsions

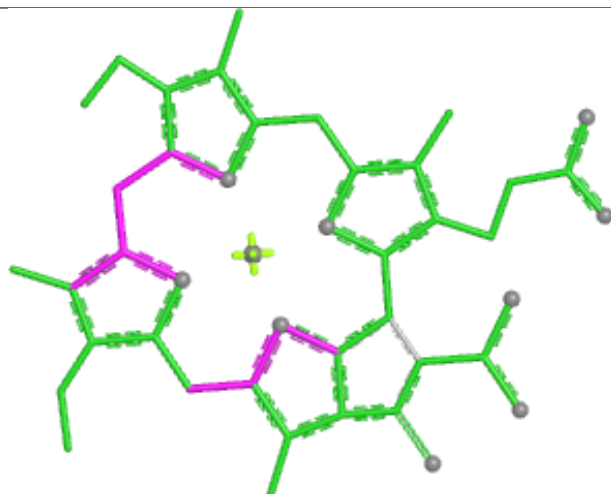


Rings

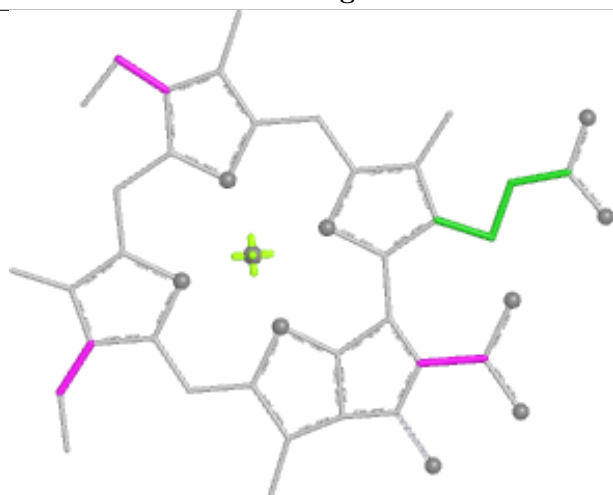
Ligand CLA 4 310



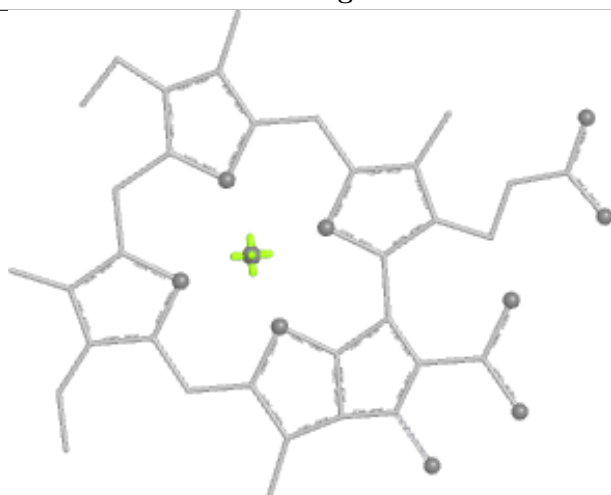
Bond lengths



Bond angles

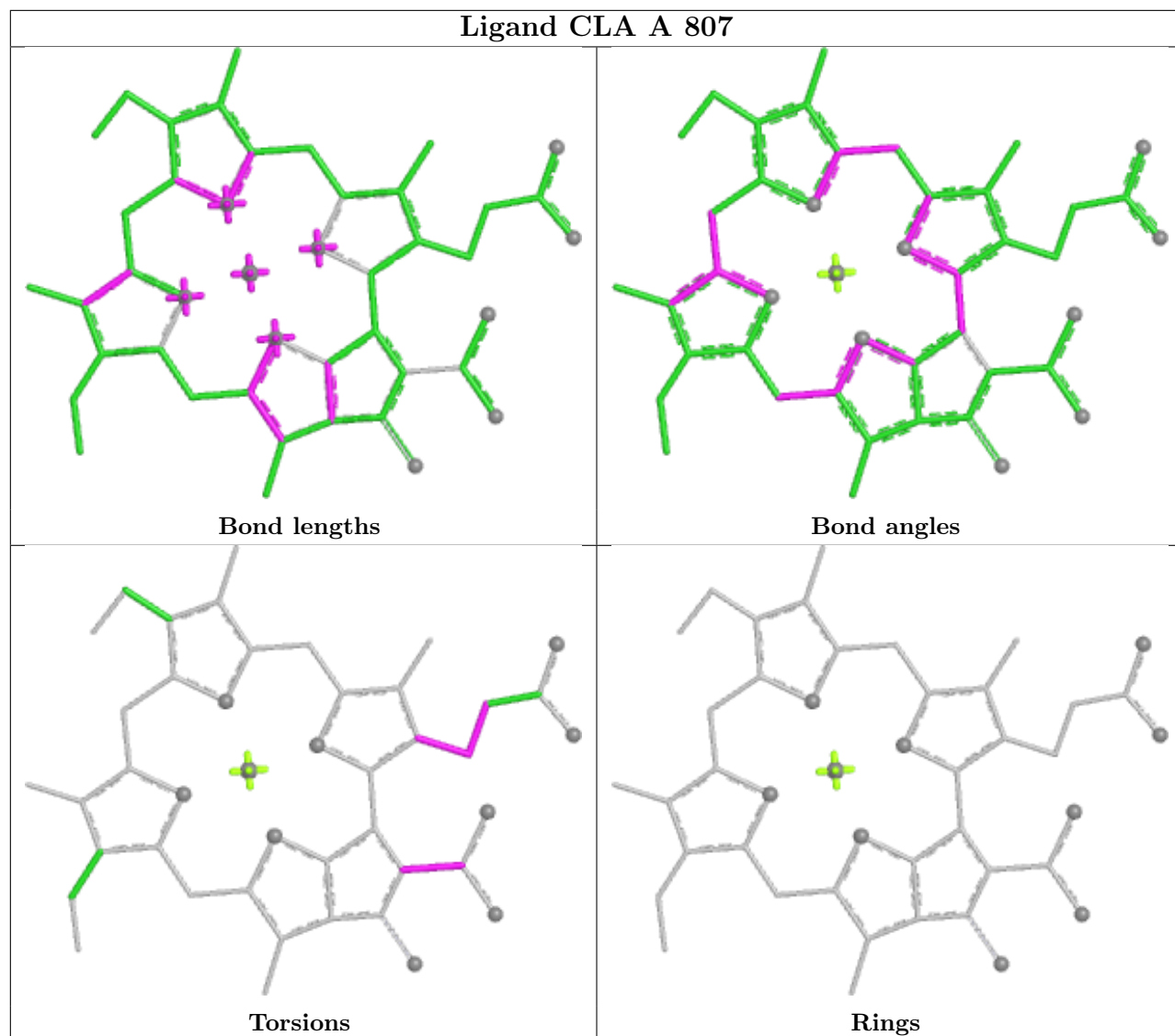


Torsions

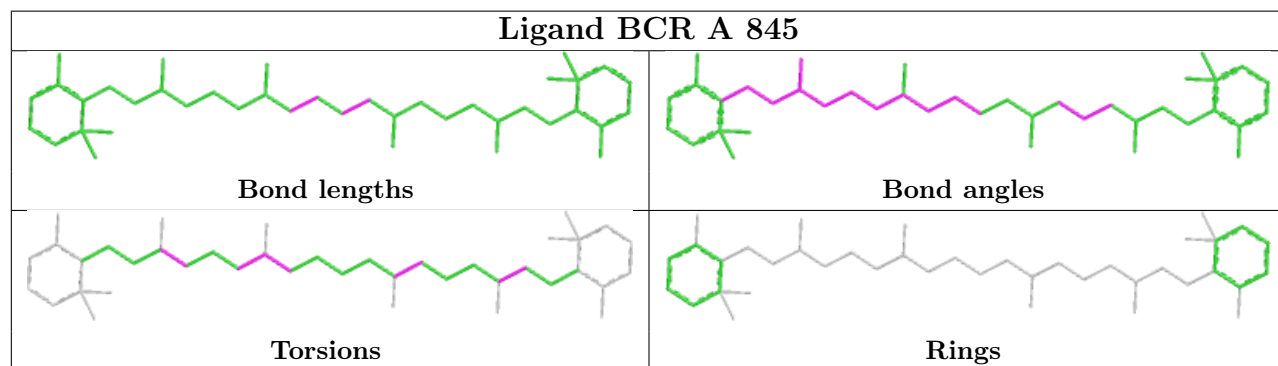


Rings

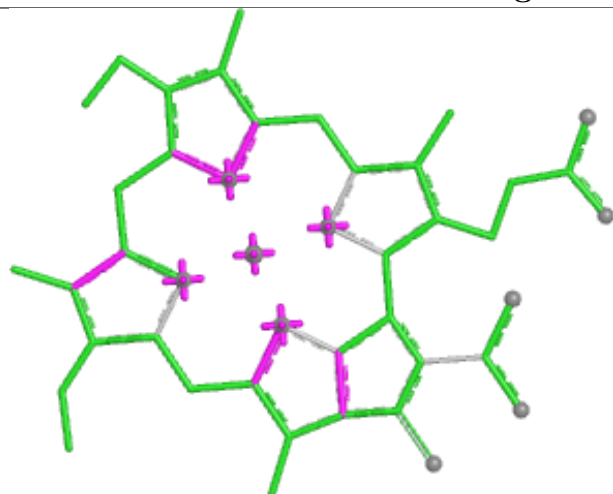
Ligand CLA A 807



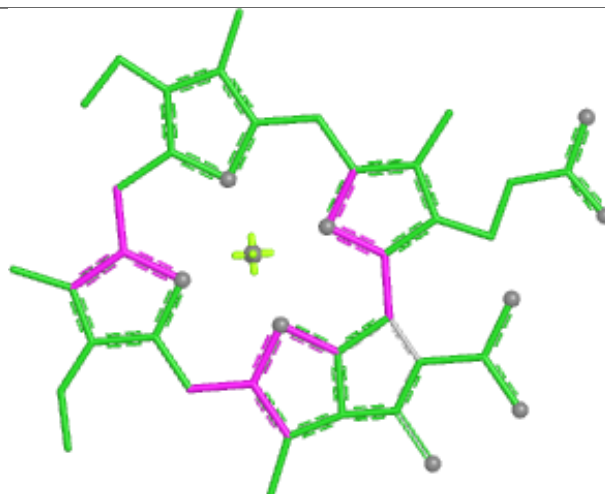
Ligand BCR A 845



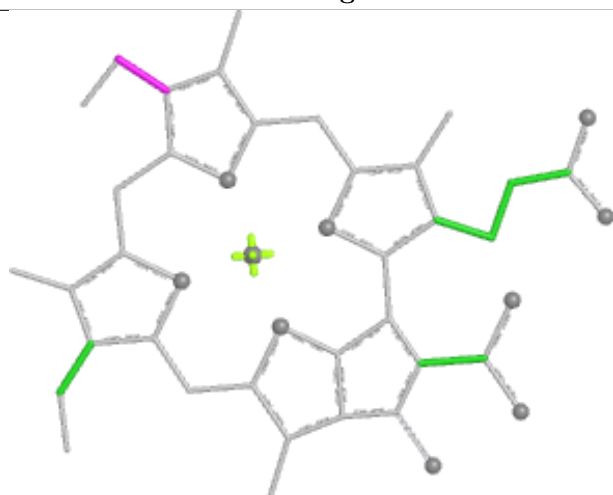
Ligand CLA B 824



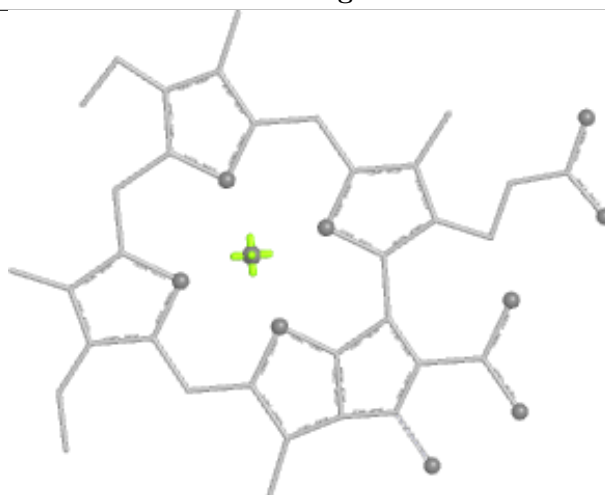
Bond lengths



Bond angles

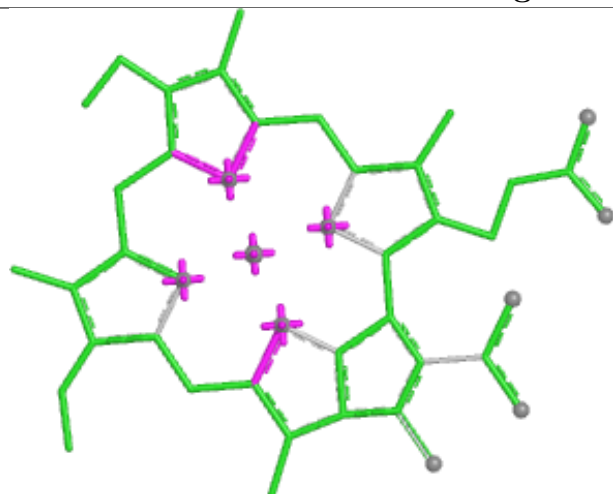


Torsions

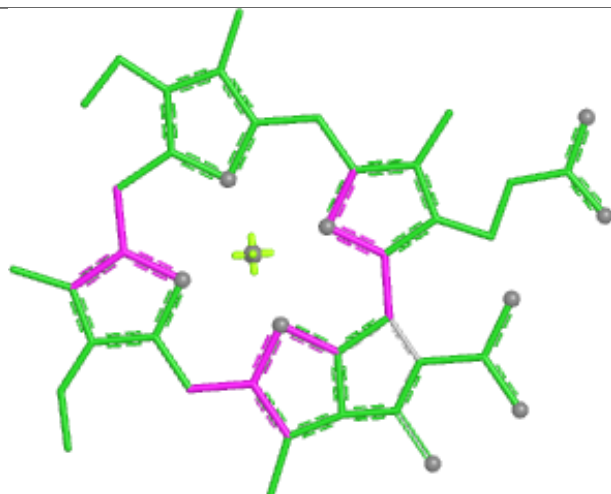


Rings

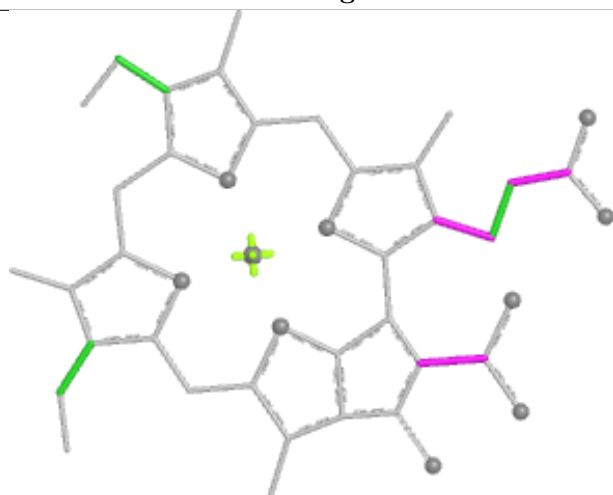
Ligand CLA A 817



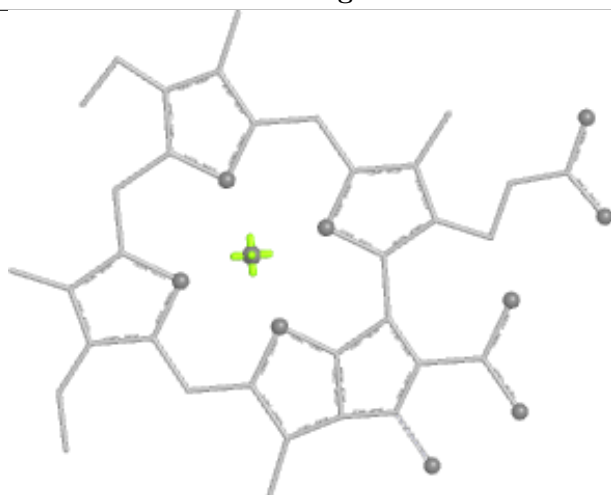
Bond lengths



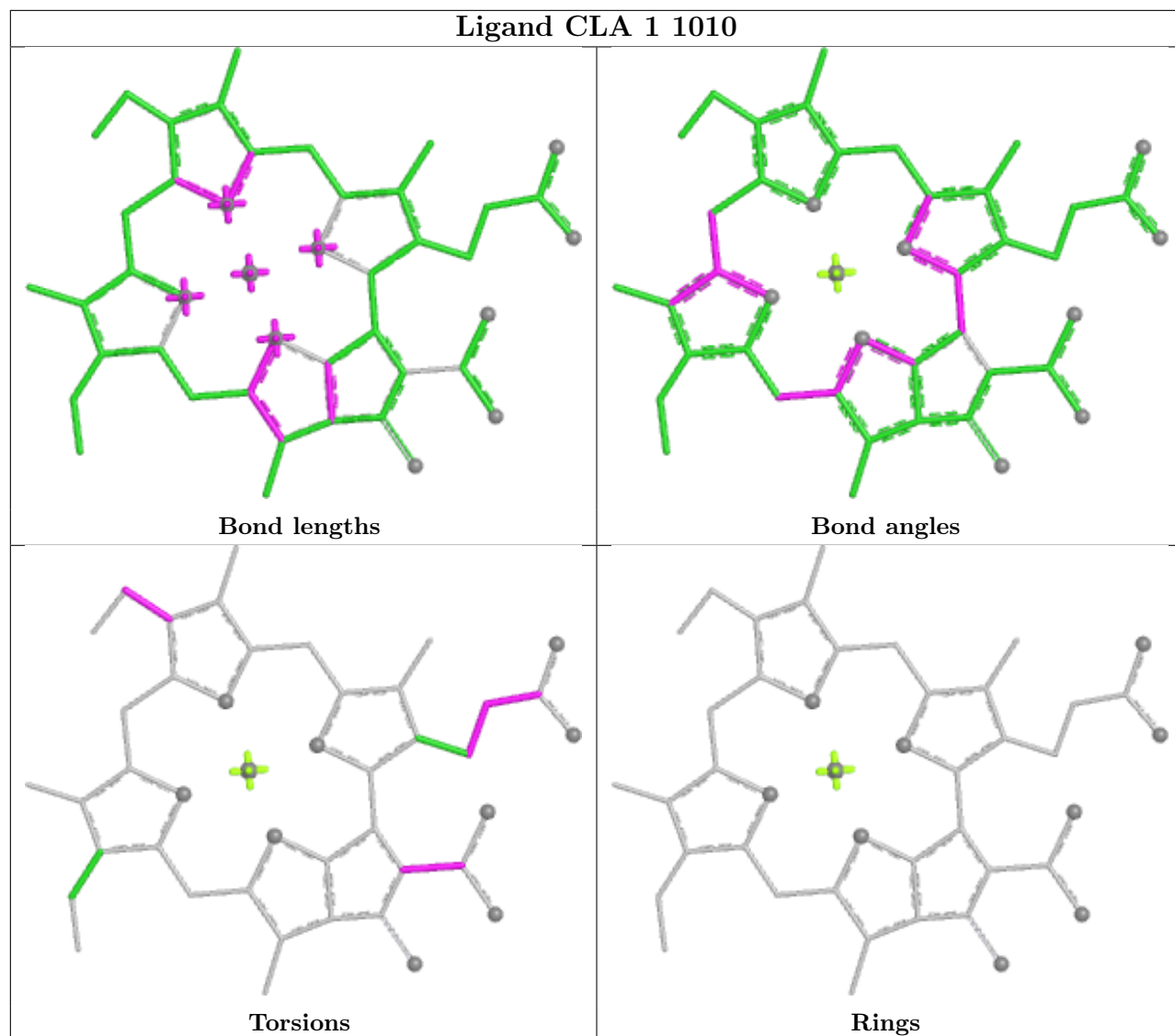
Bond angles

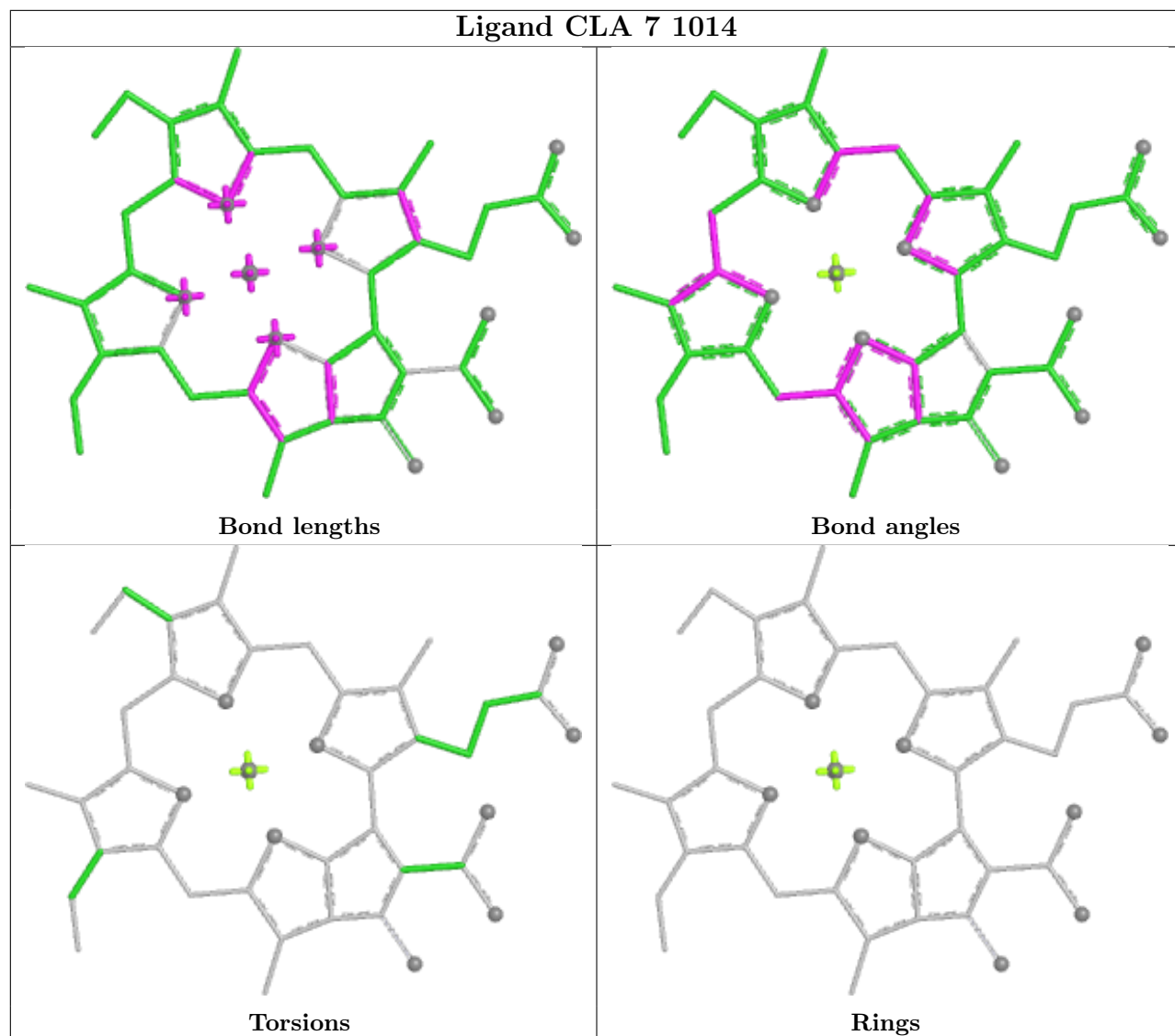


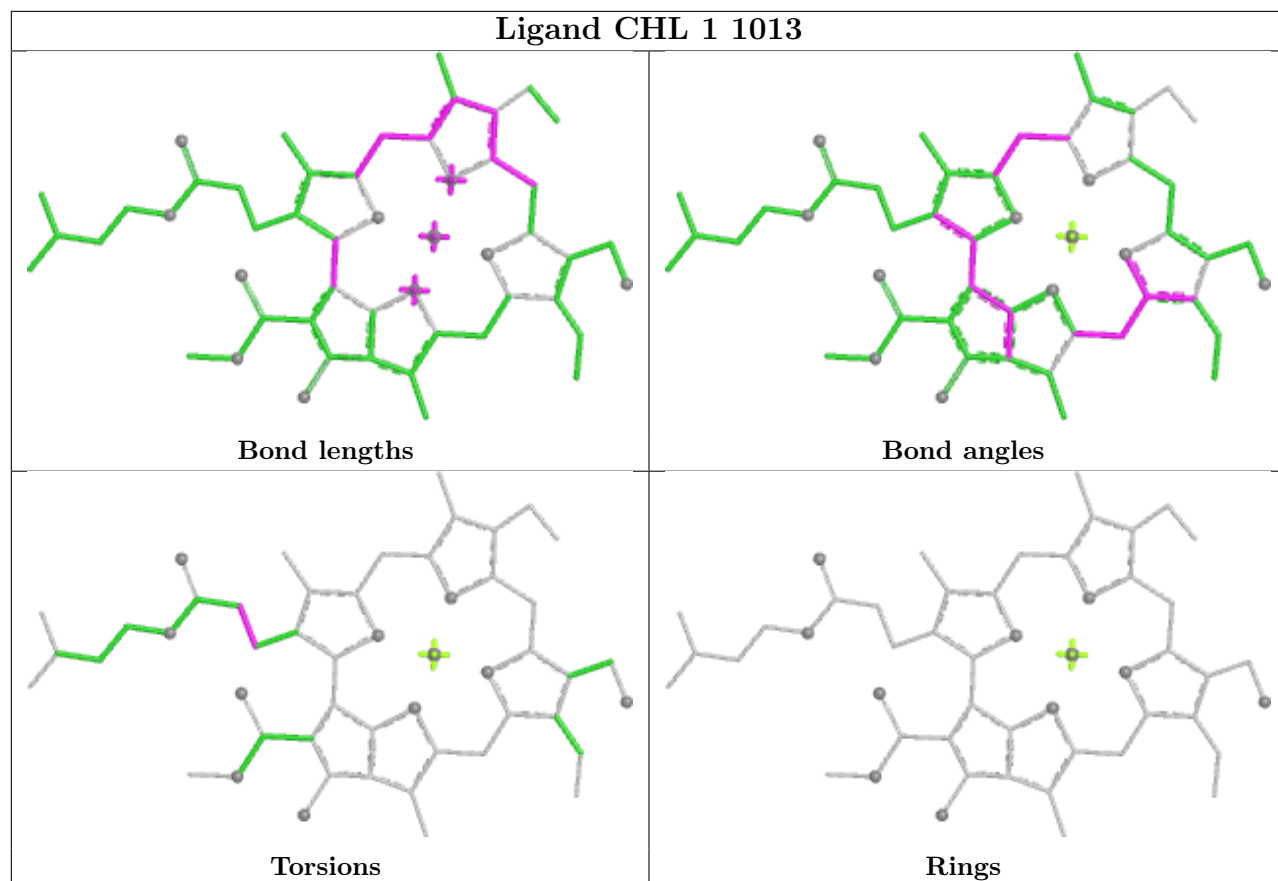
Torsions



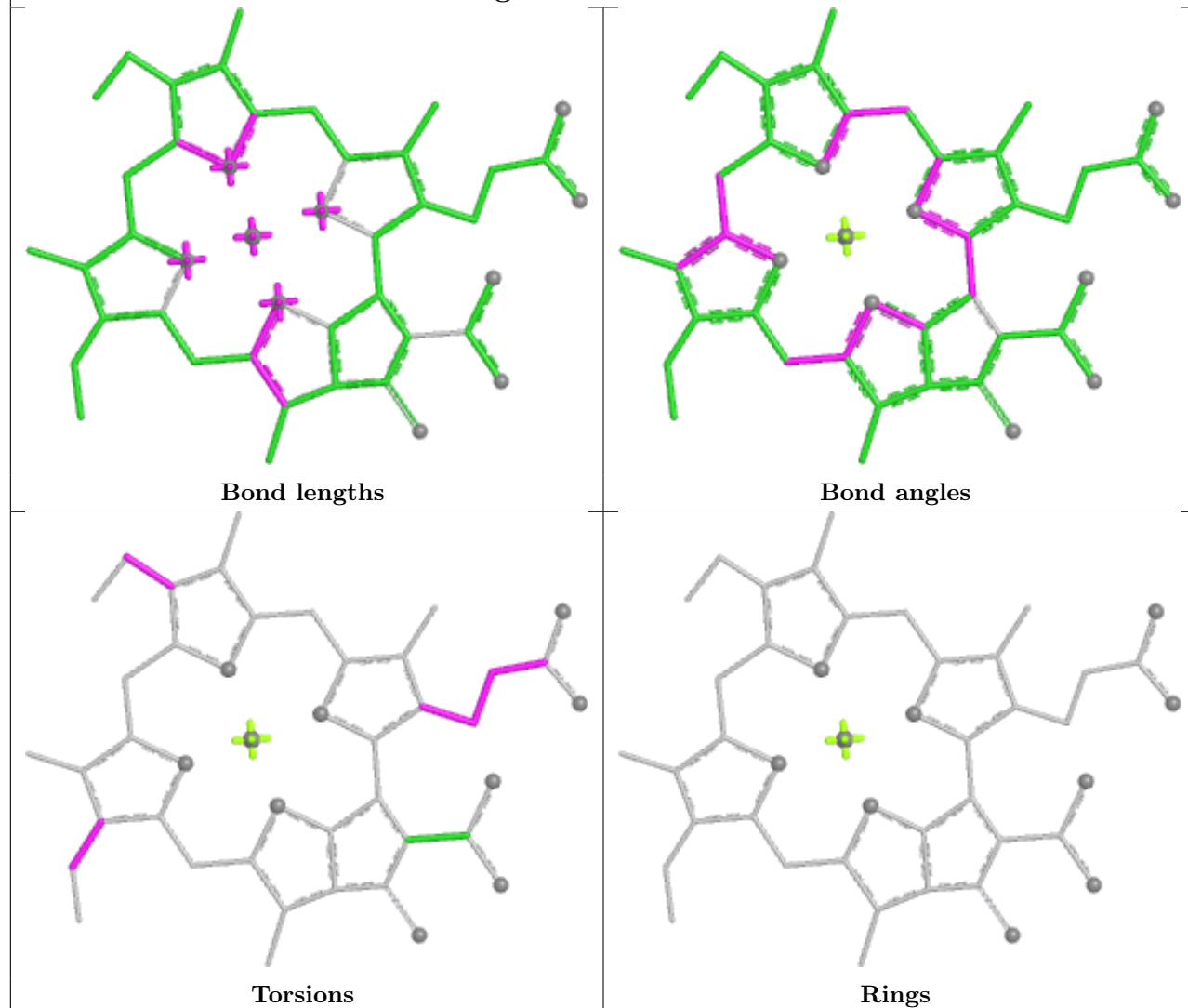
Rings



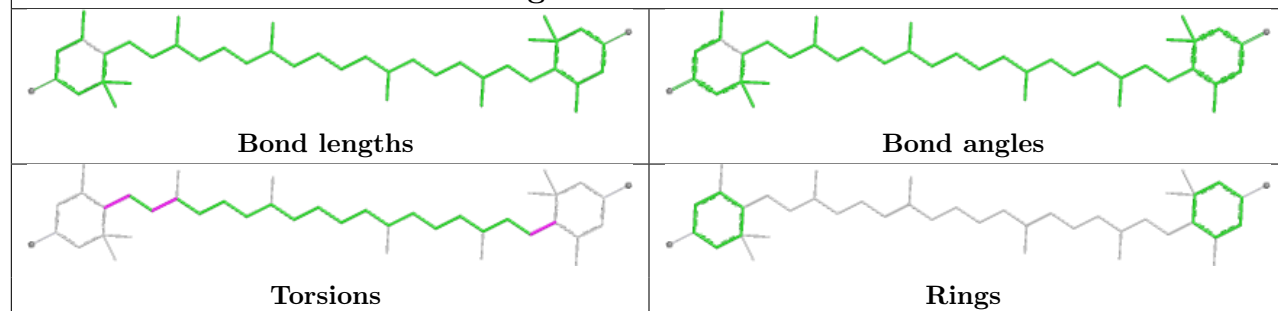




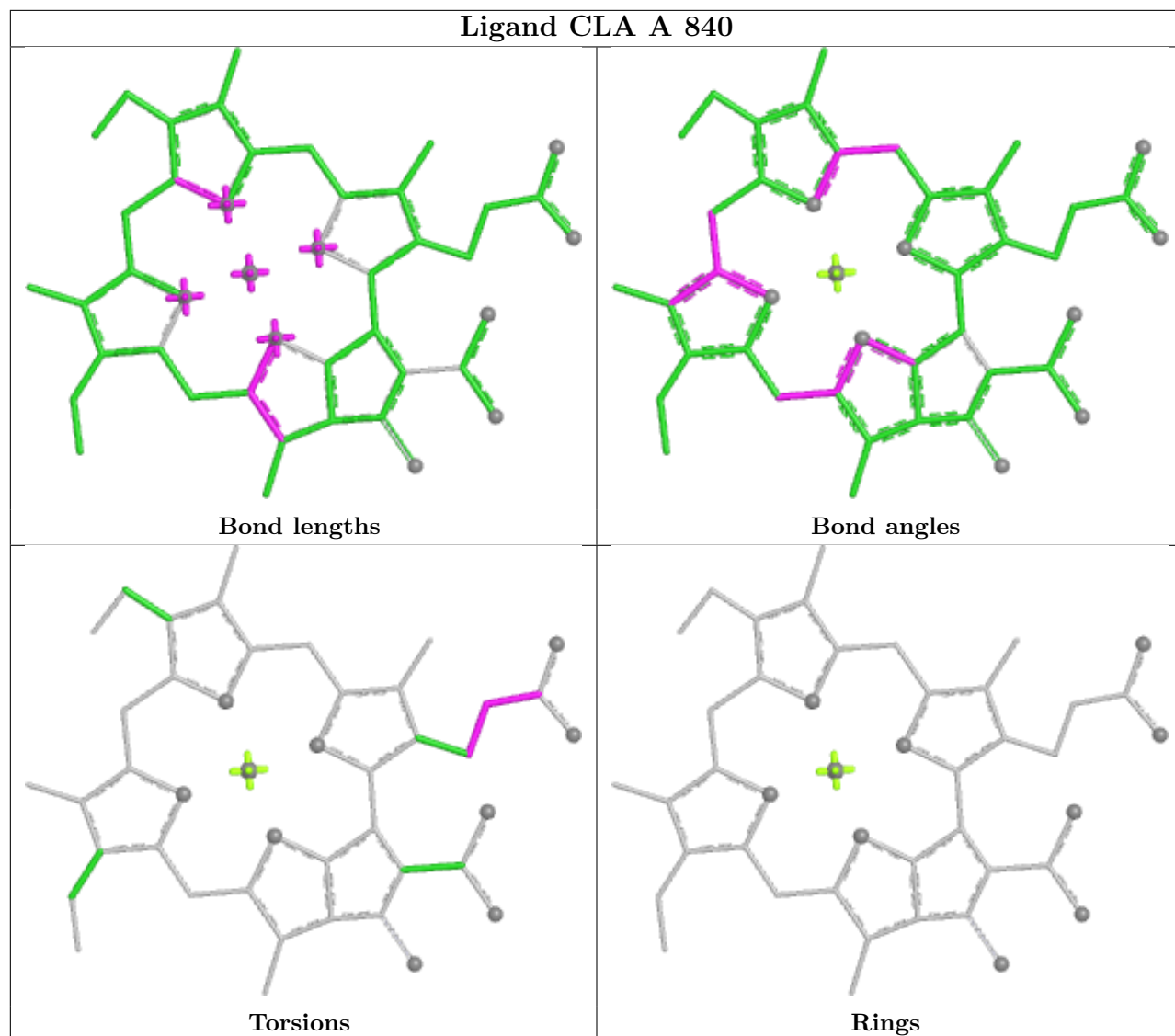
Ligand CLA B 841



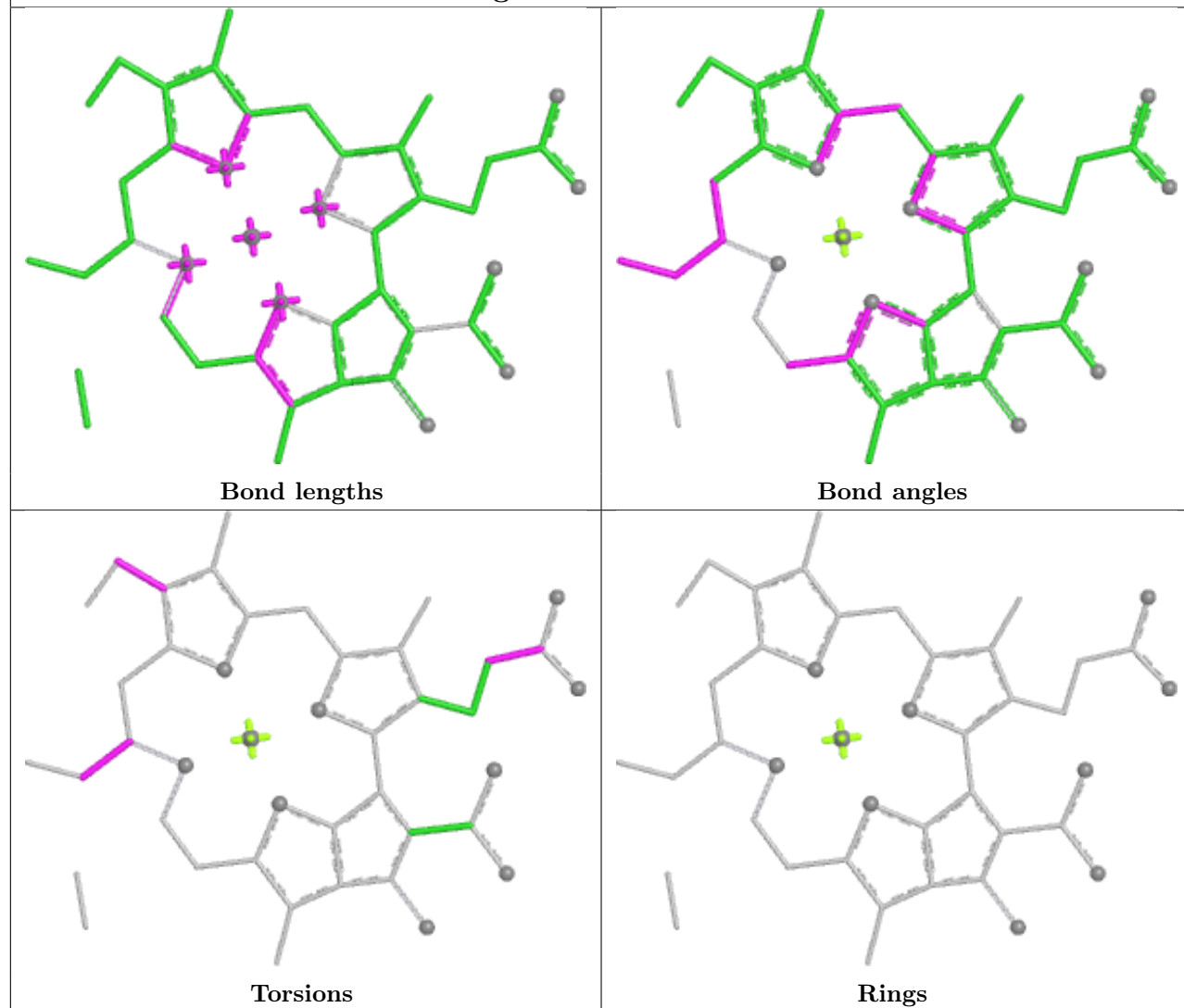
Ligand LUT 1 1002



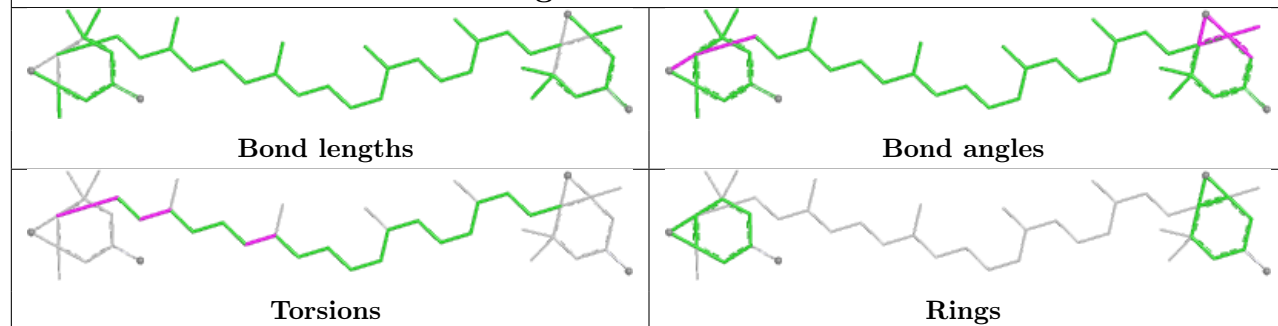
Ligand CLA A 840

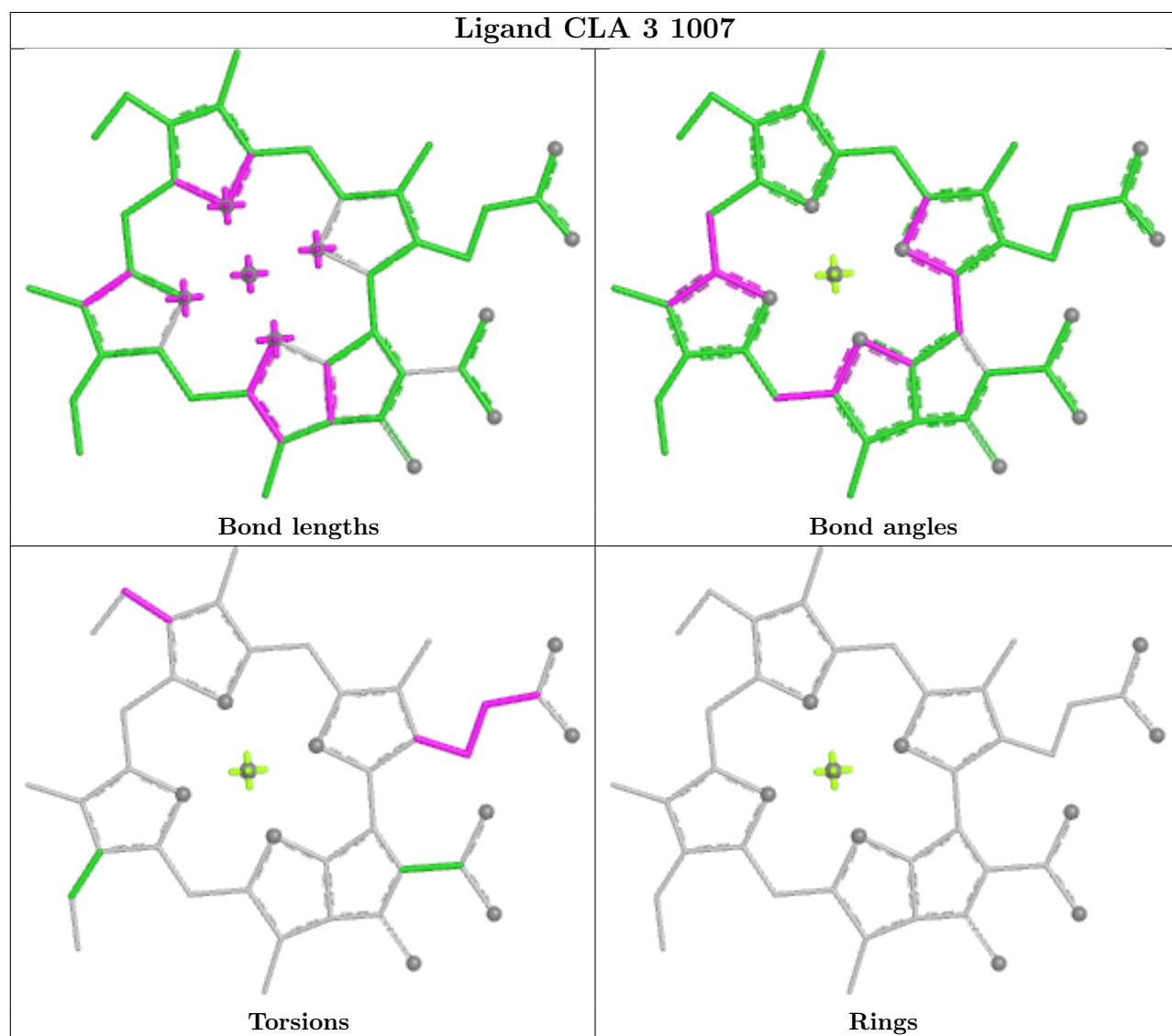
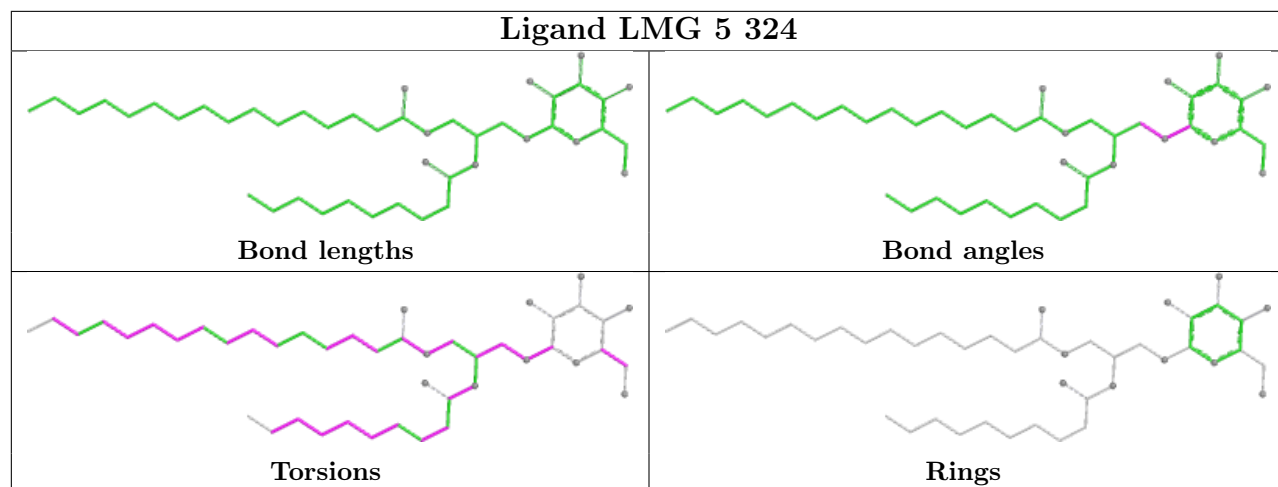


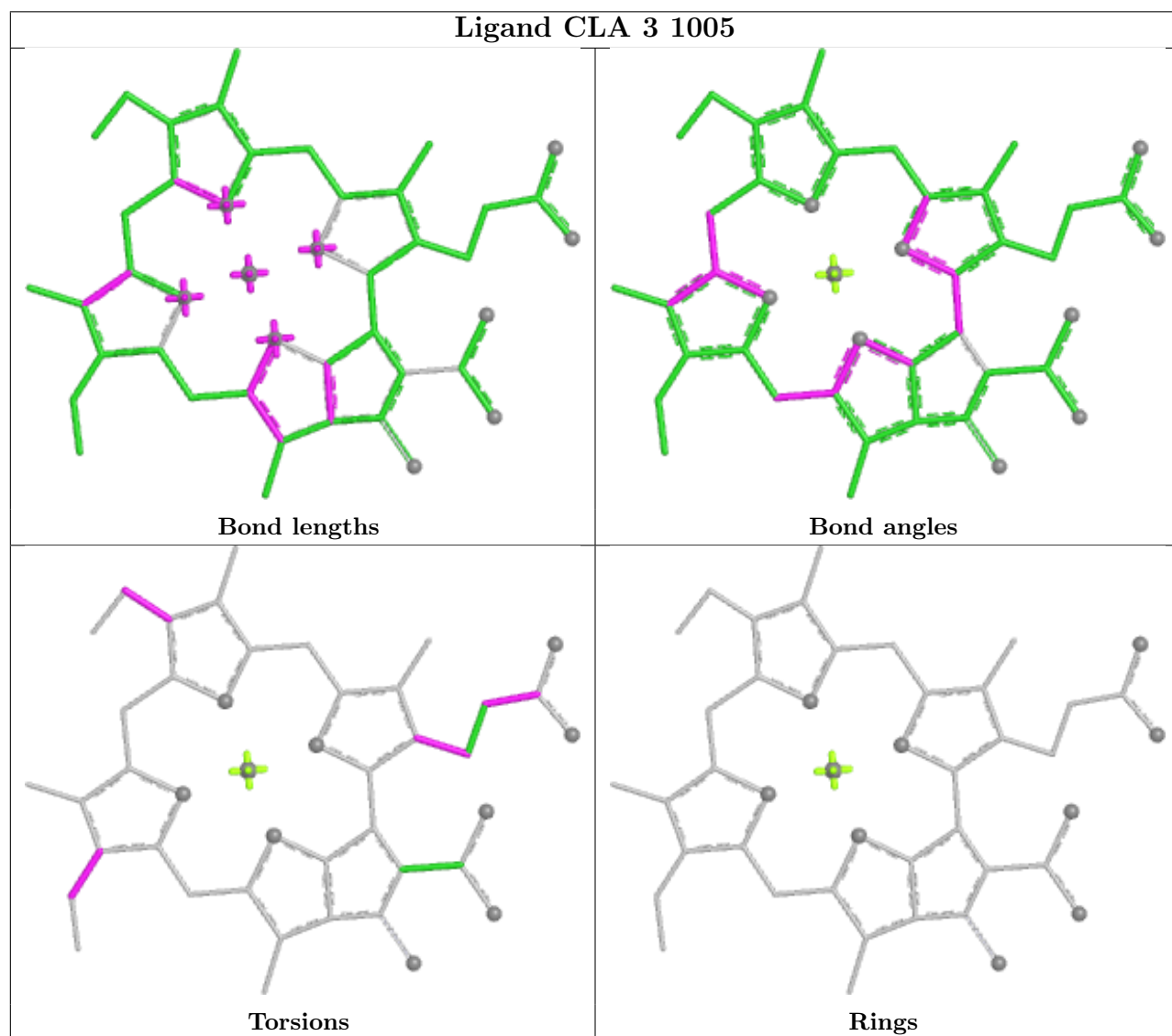
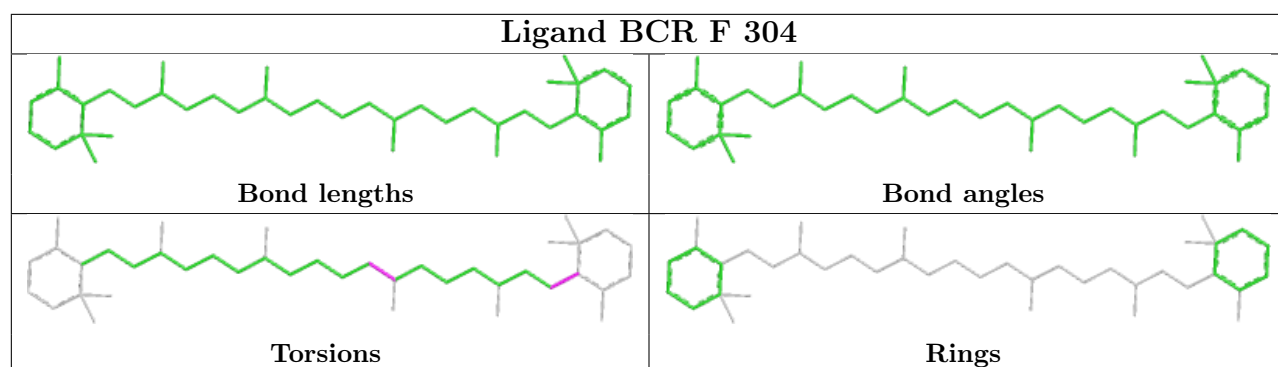
Ligand CLA B 850

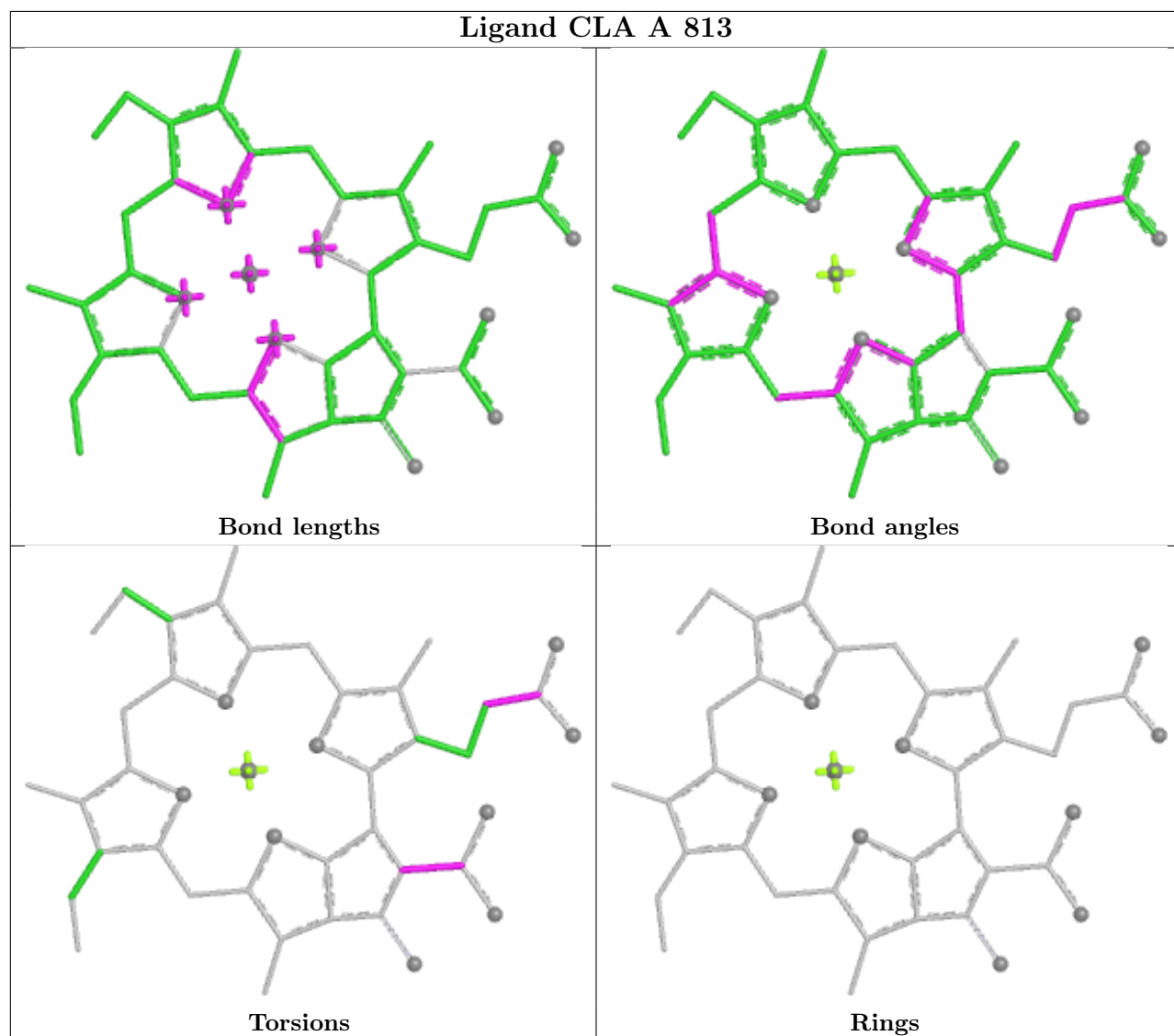
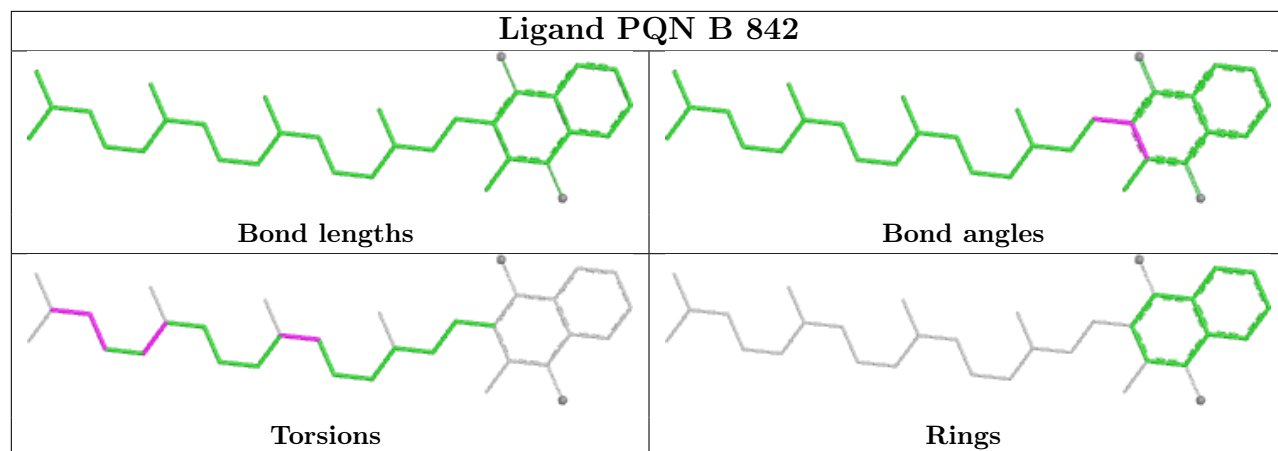


Ligand XAT 6 304

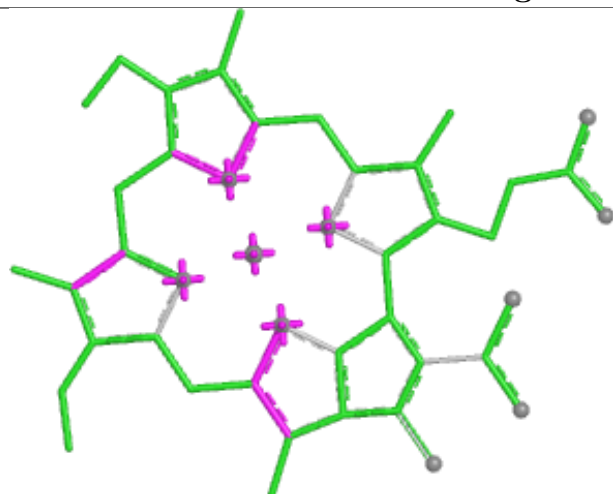




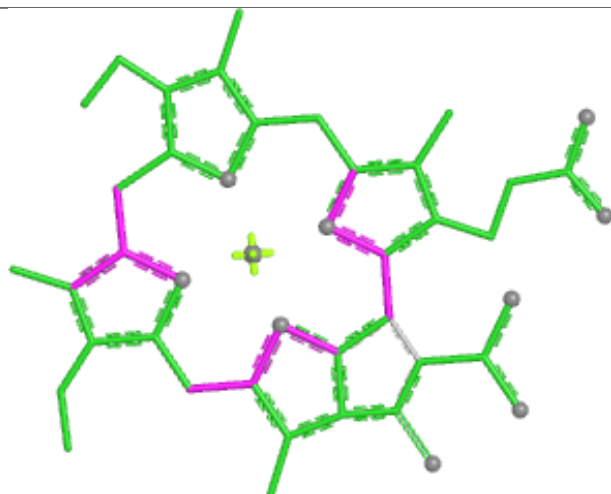




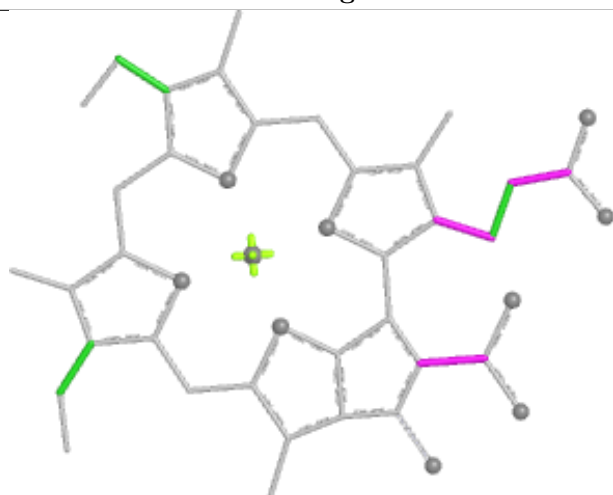
Ligand CLA B 826



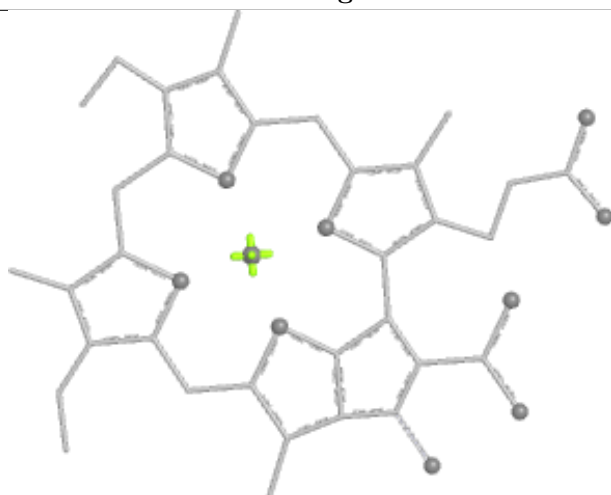
Bond lengths



Bond angles

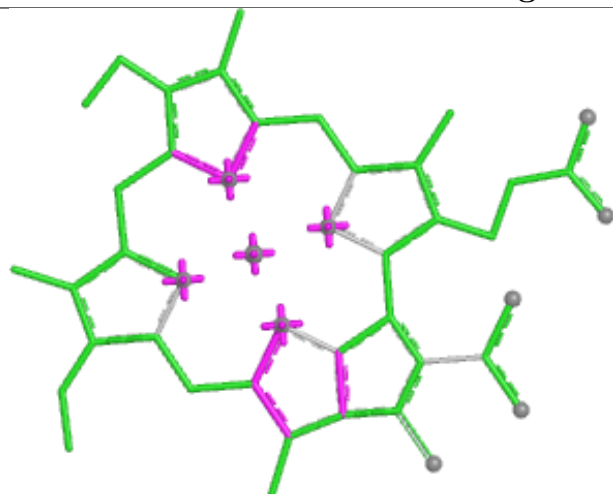


Torsions

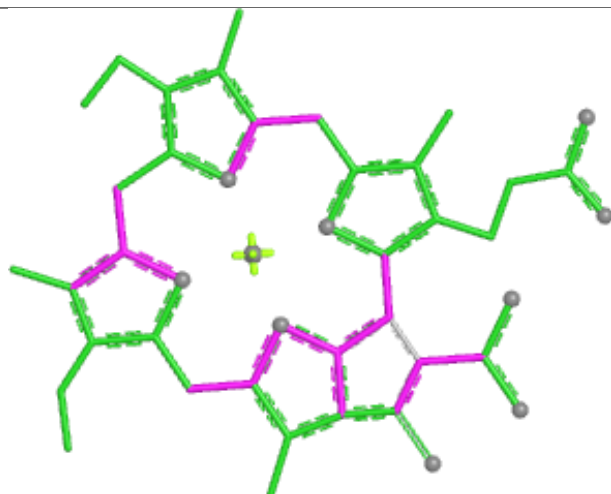


Rings

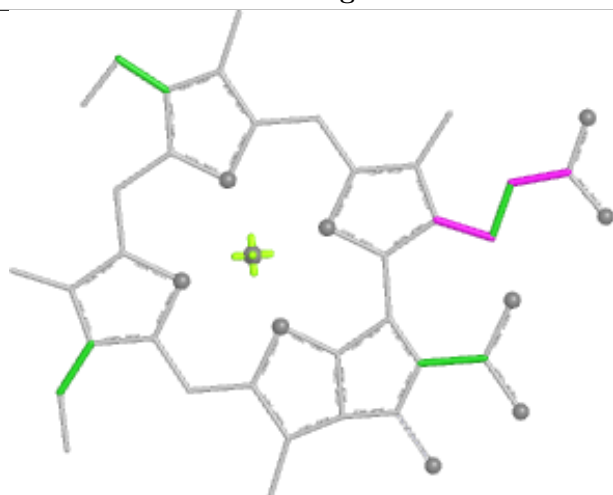
Ligand CLA 4 304



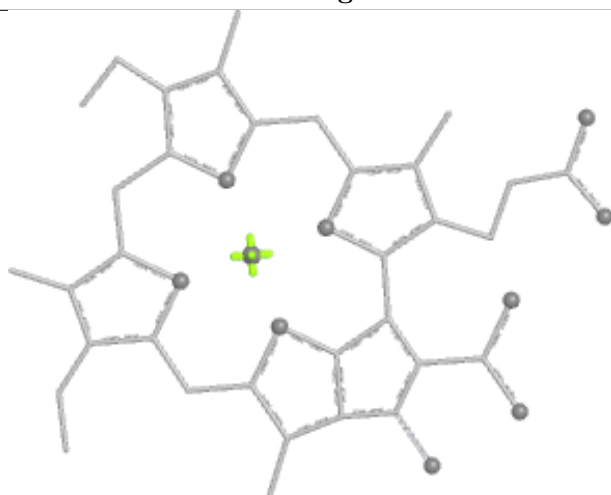
Bond lengths



Bond angles

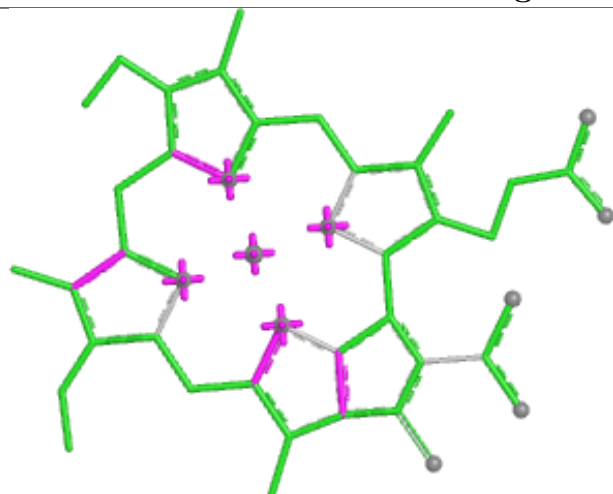


Torsions

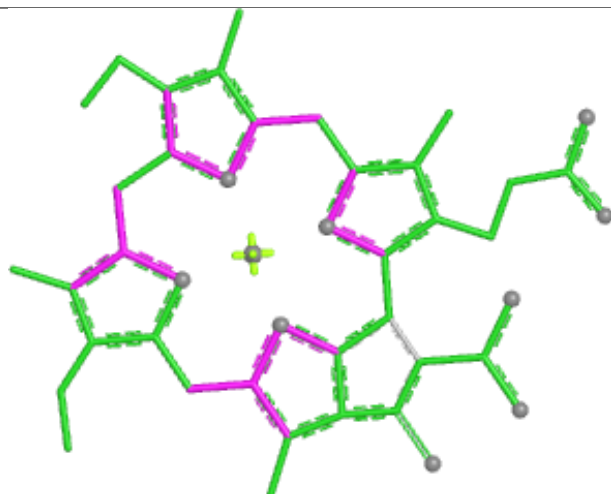


Rings

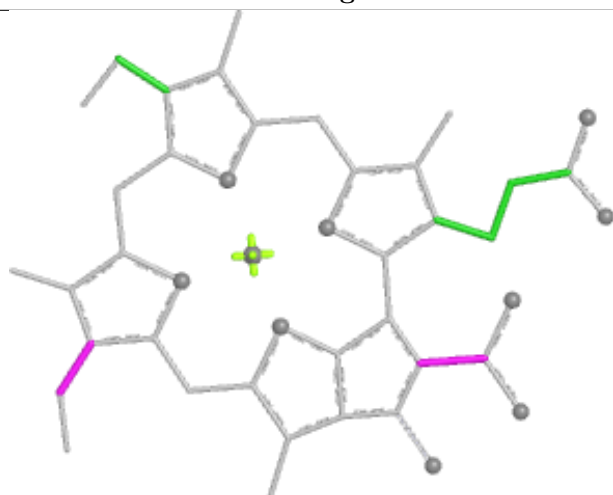
Ligand CLA B 817



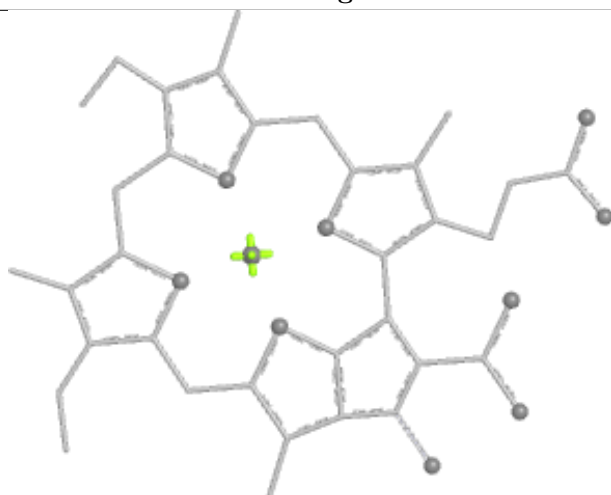
Bond lengths



Bond angles

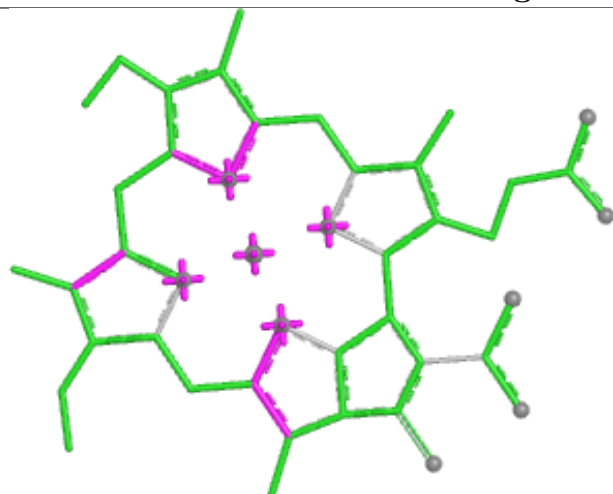


Torsions

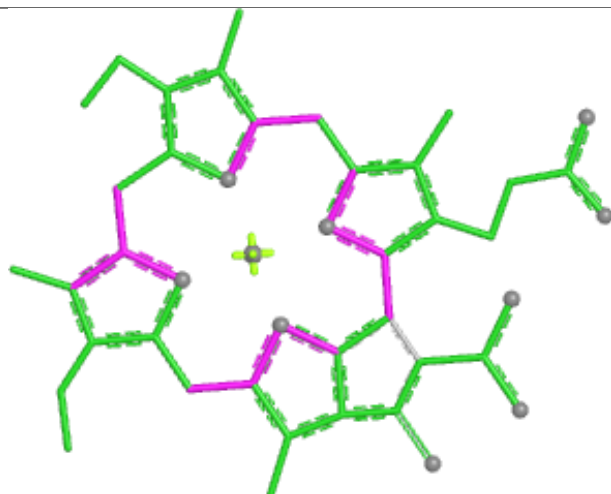


Rings

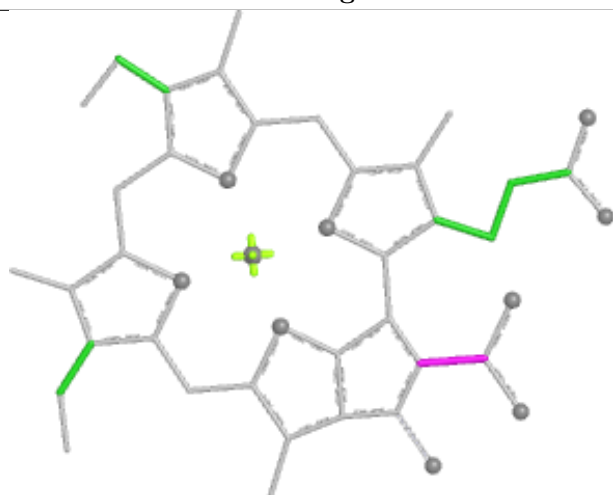
Ligand CLA A 832



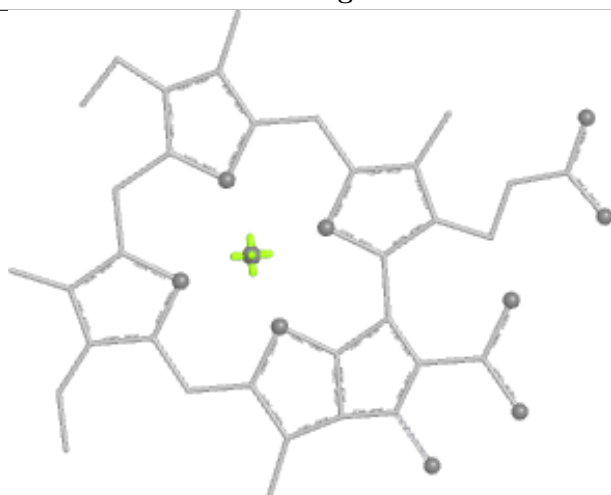
Bond lengths



Bond angles

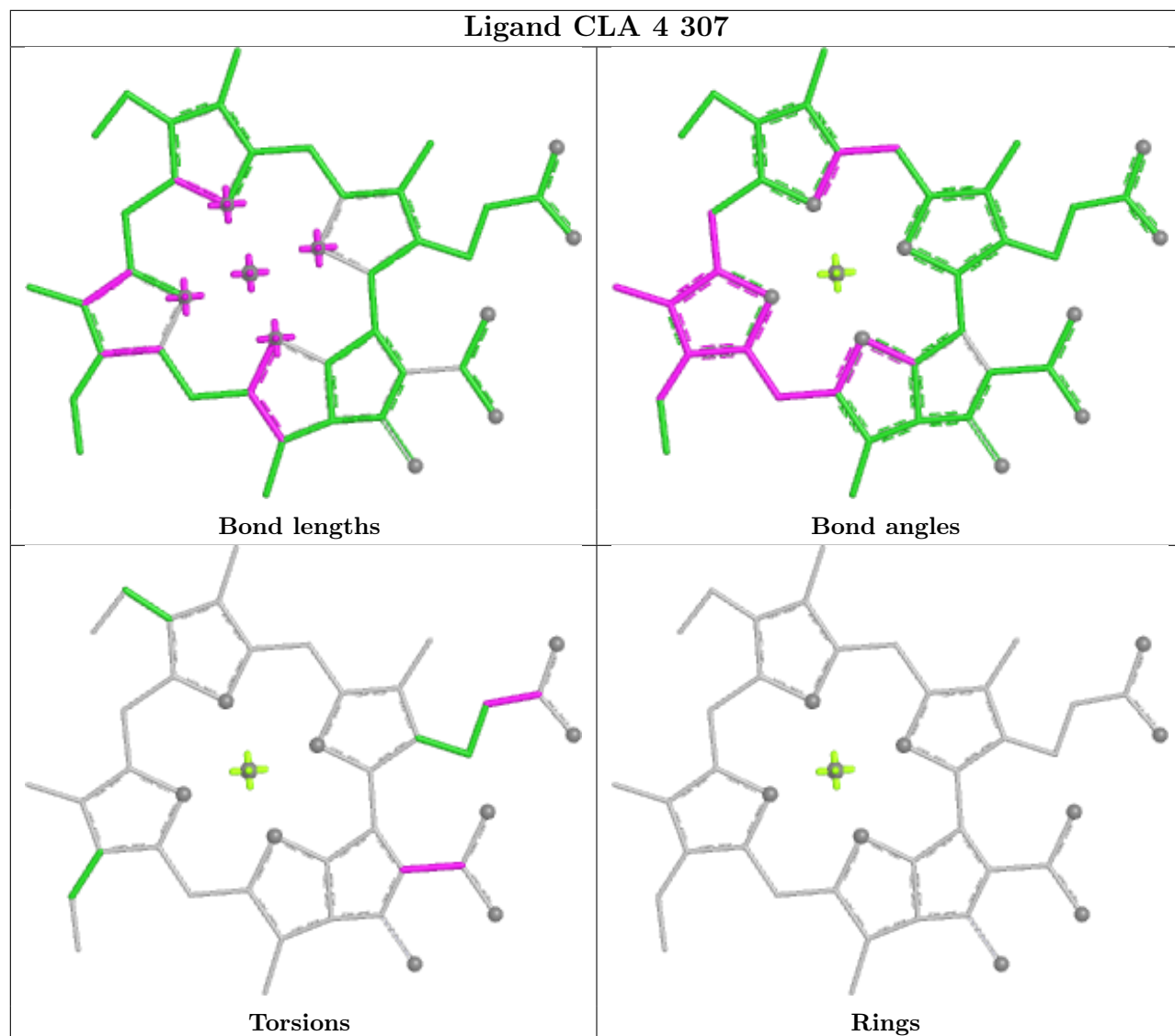


Torsions

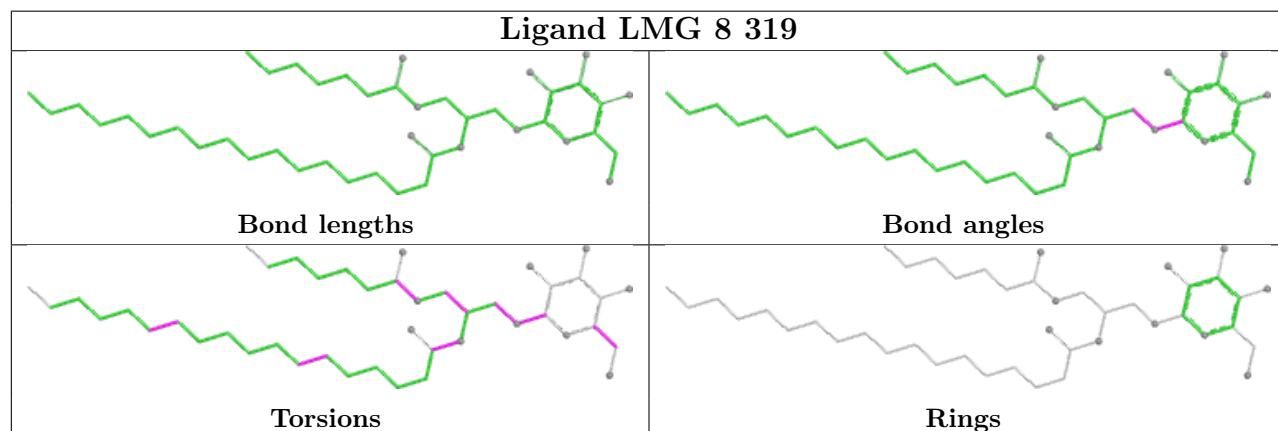


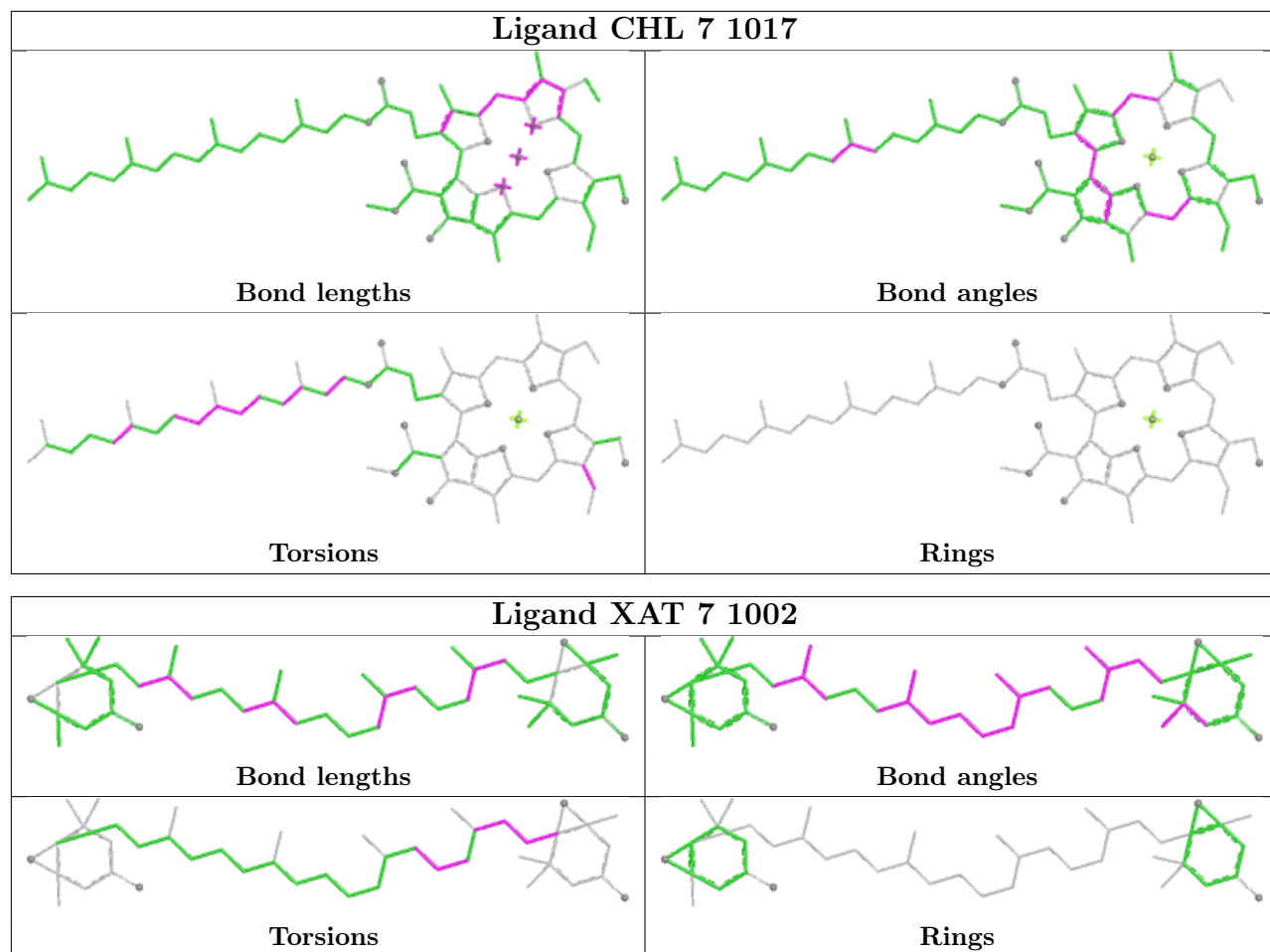
Rings

Ligand CLA 4 307

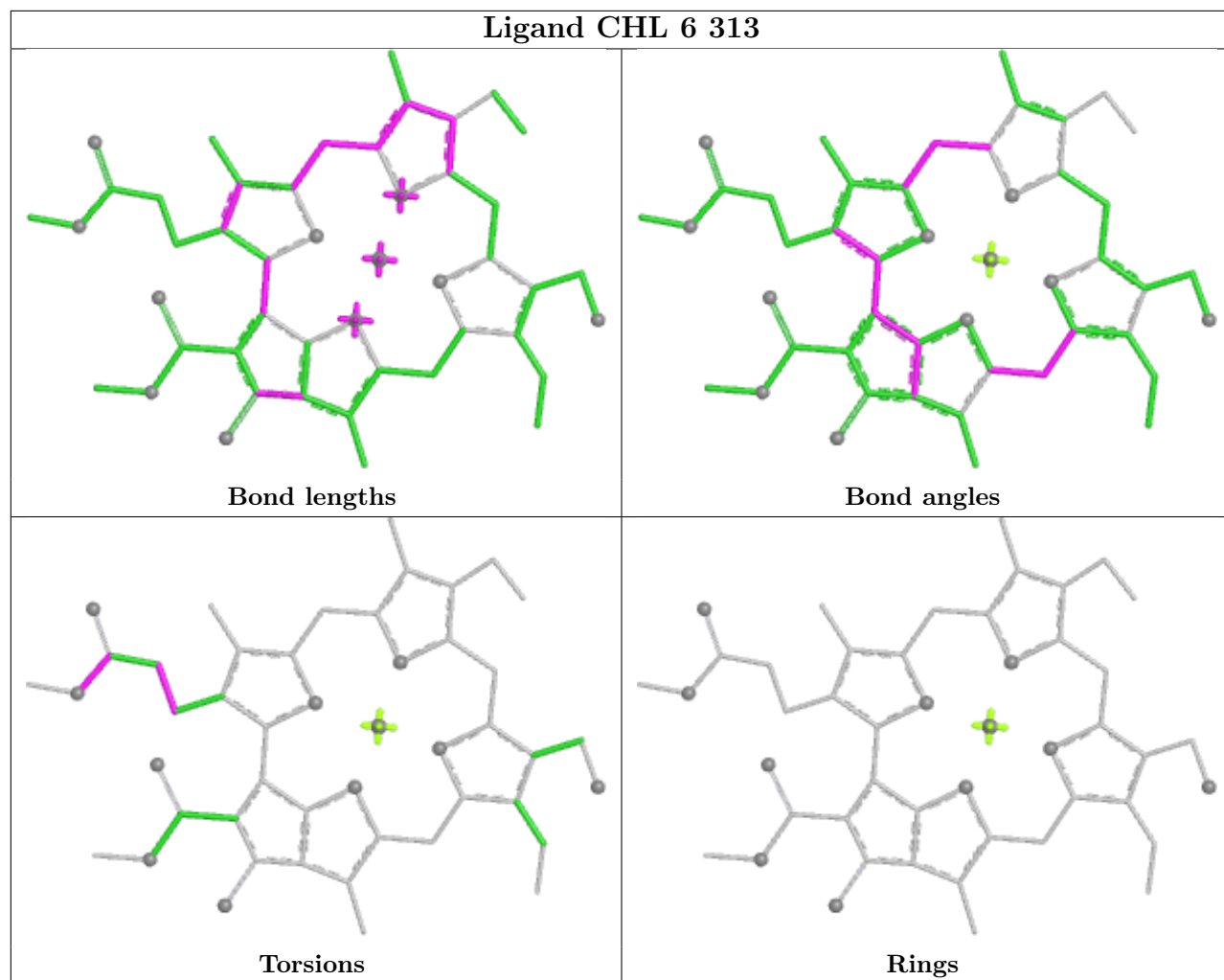


Ligand LMG 8 319

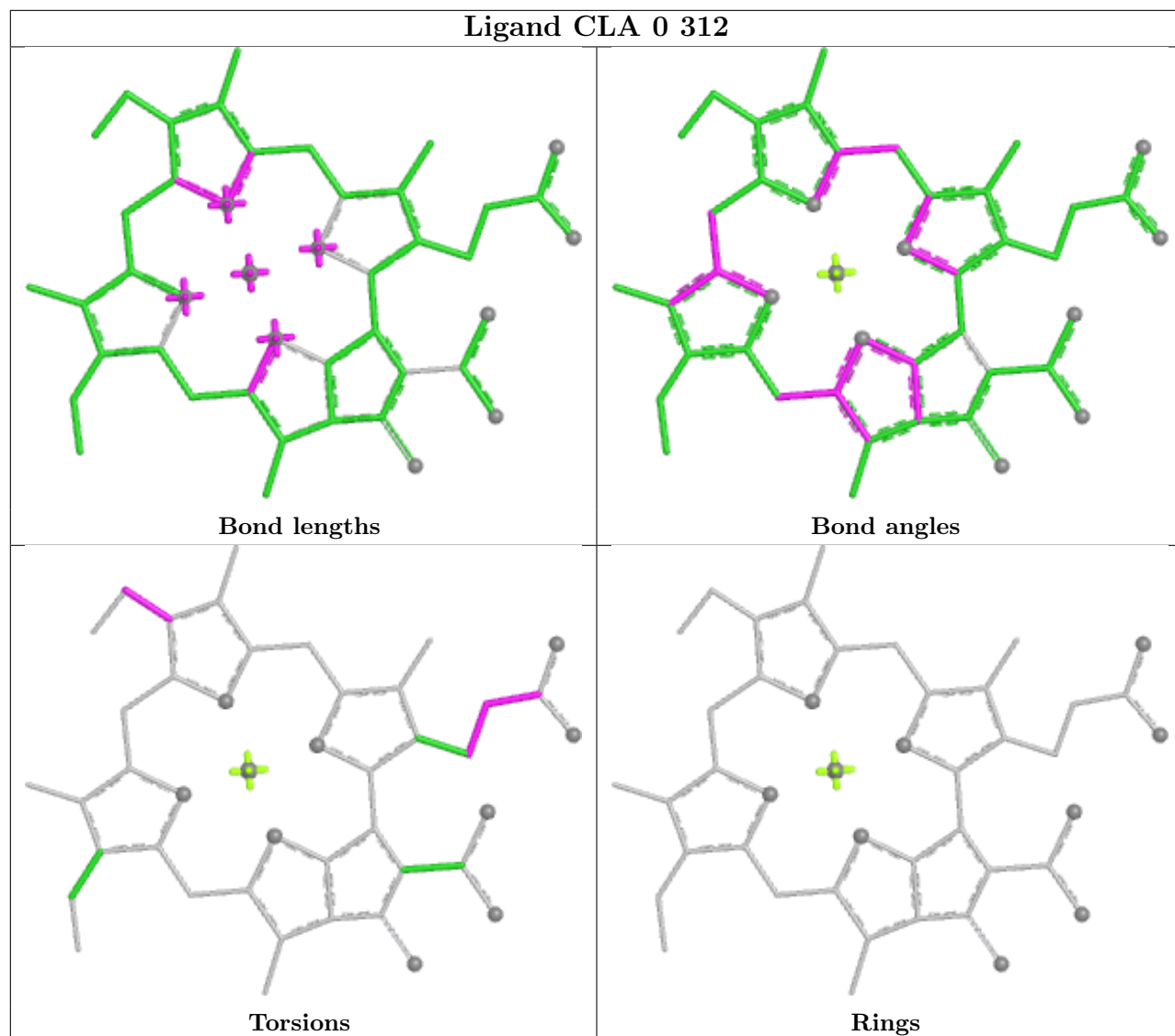




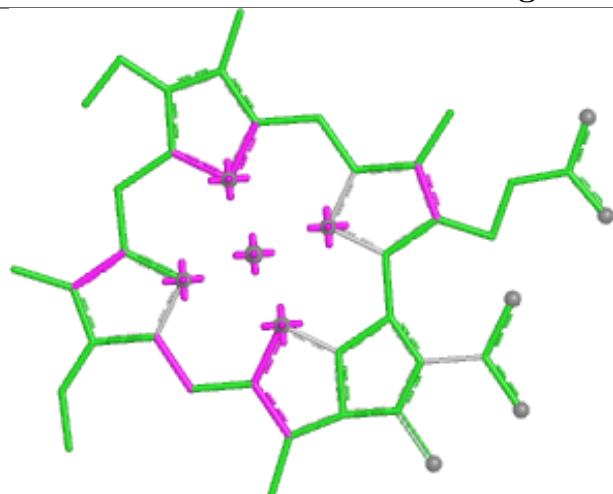
Ligand CHL 6 313



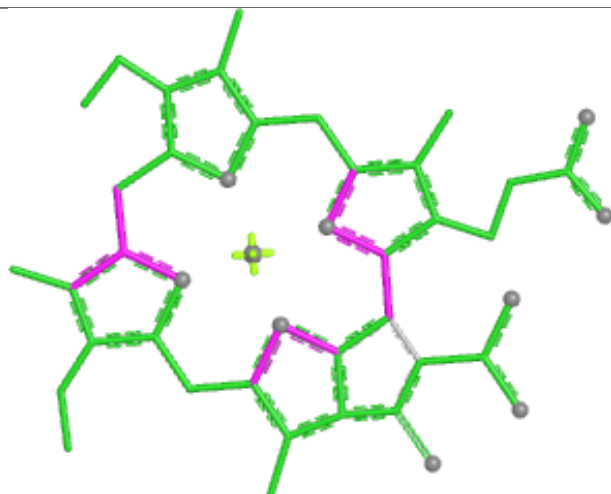
Ligand CLA 0 312



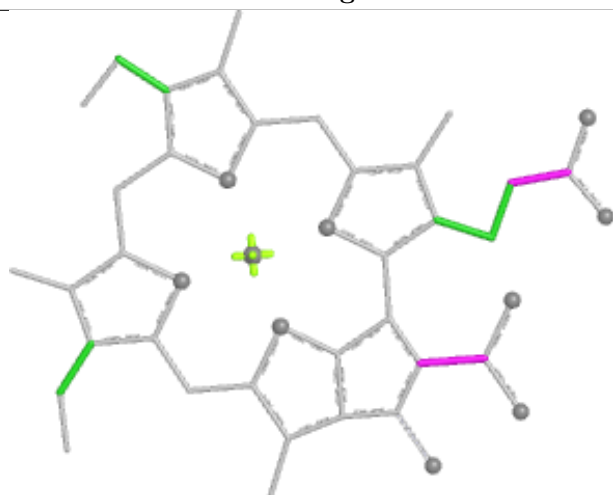
Ligand CLA 8 306



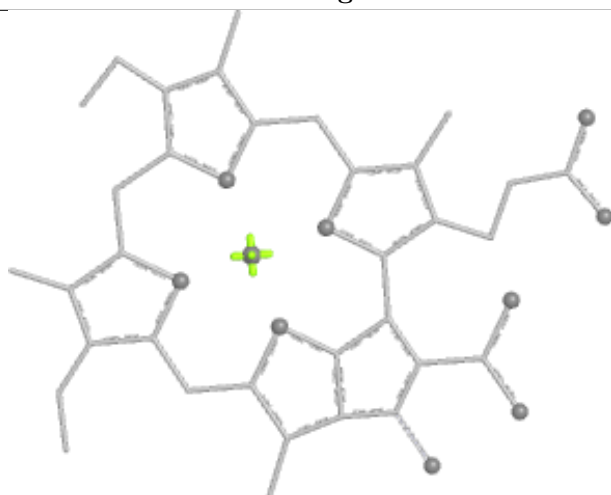
Bond lengths



Bond angles

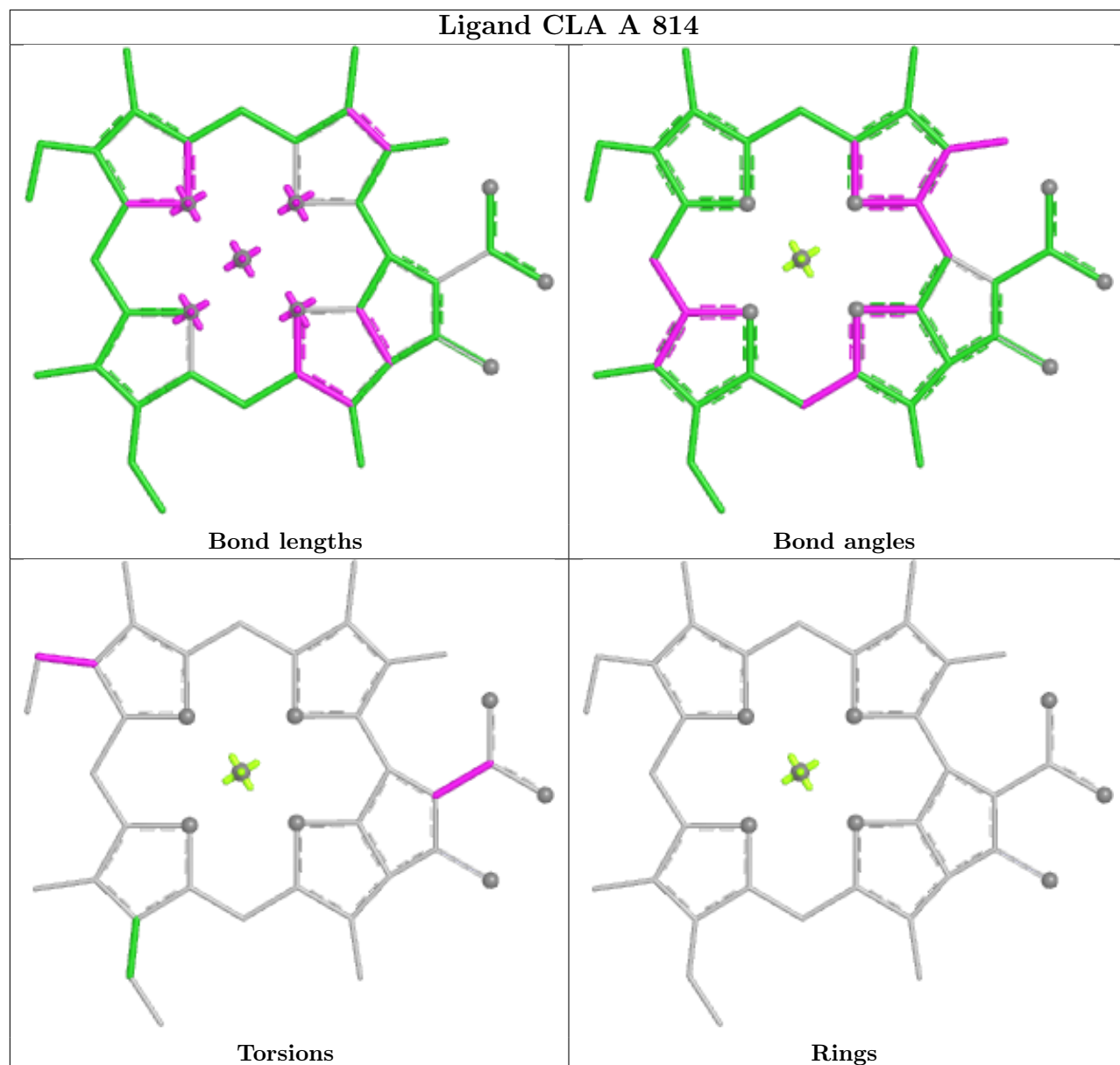


Torsions

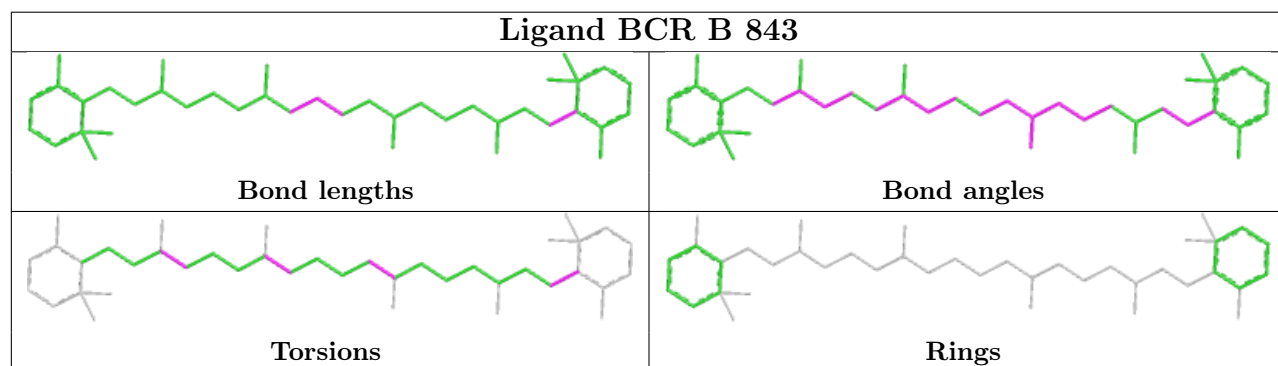


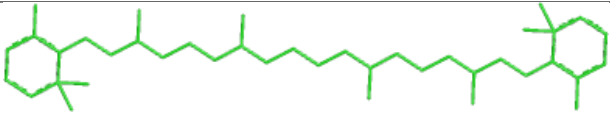
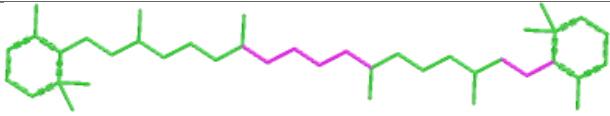
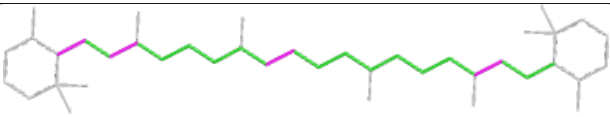
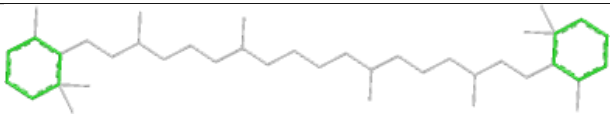
Rings

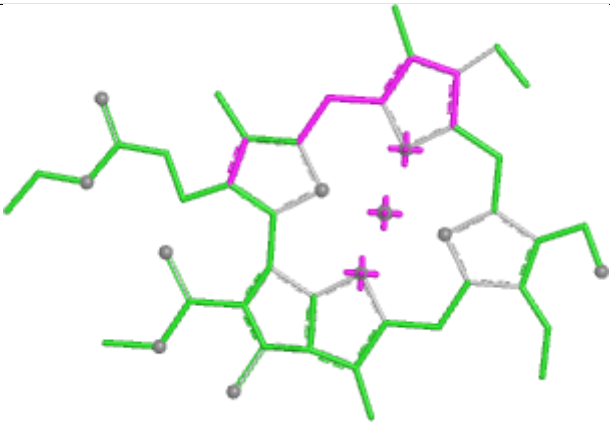
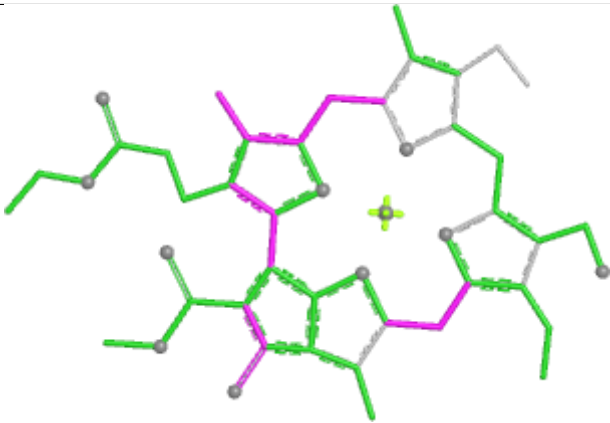
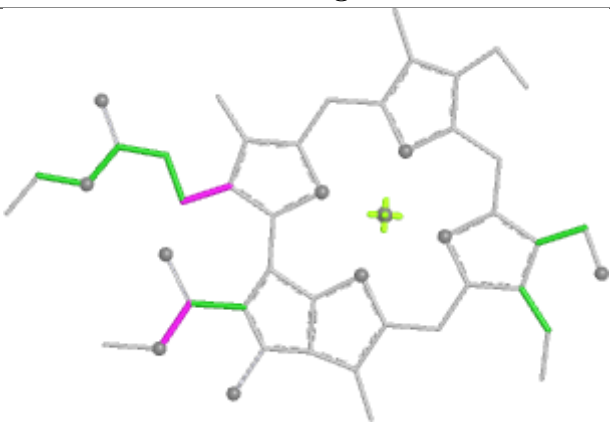
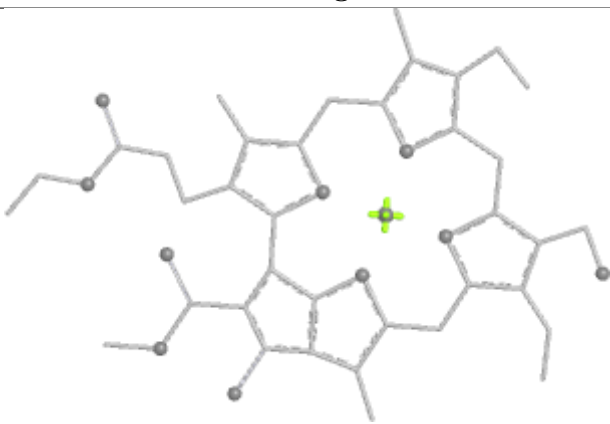
Ligand CLA A 814

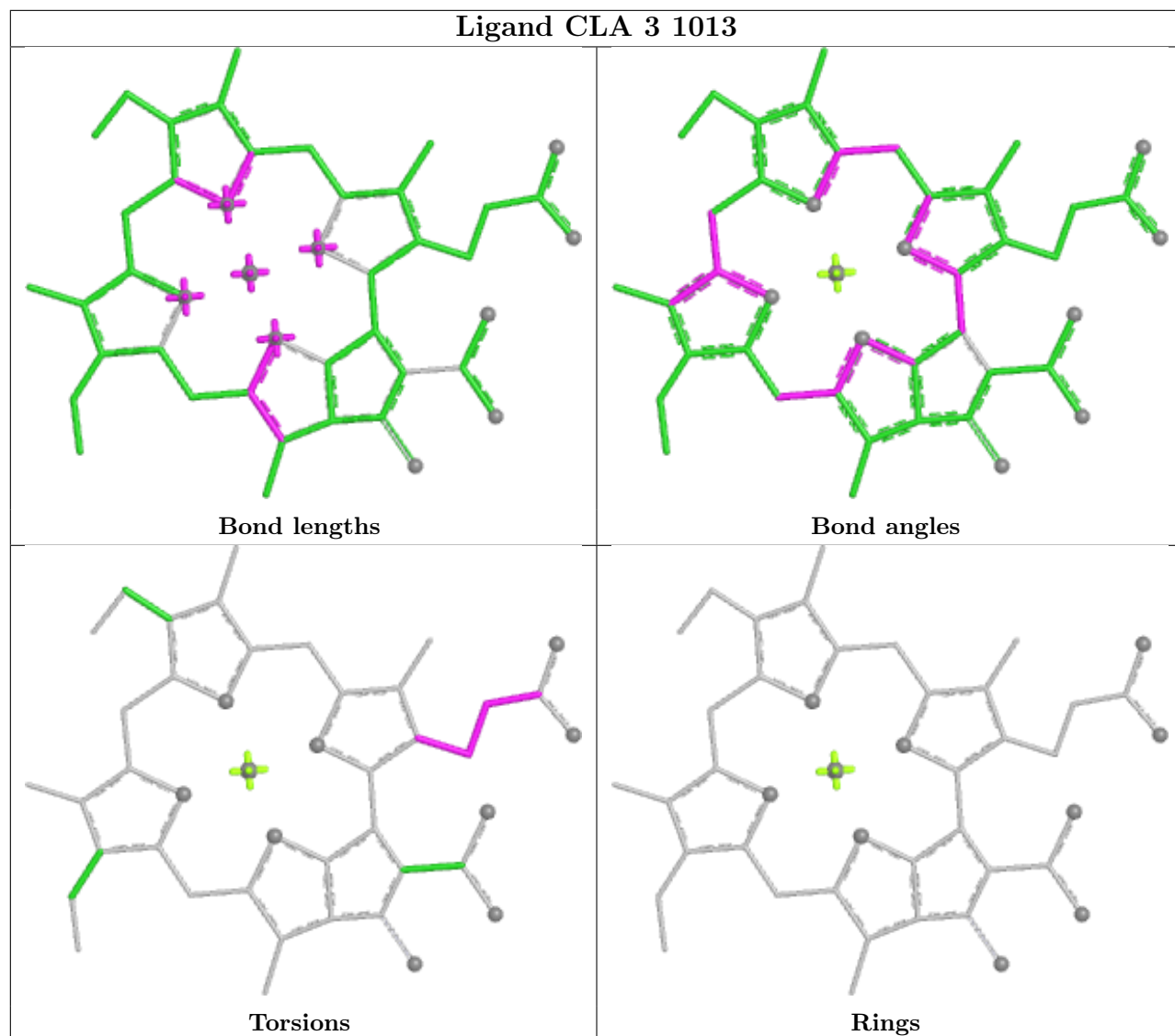


Ligand BCR B 843

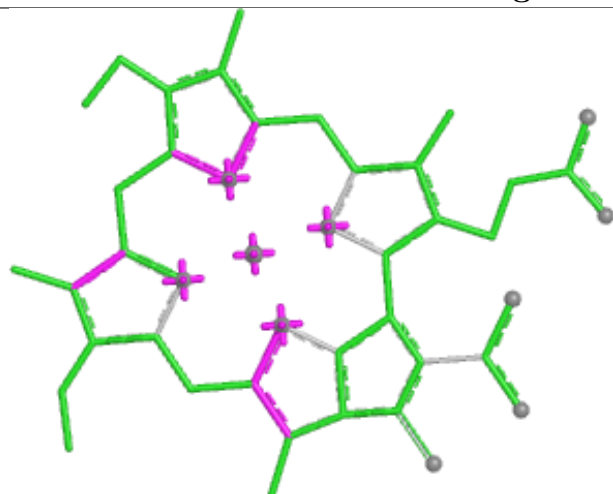


Ligand BCR 8 302			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

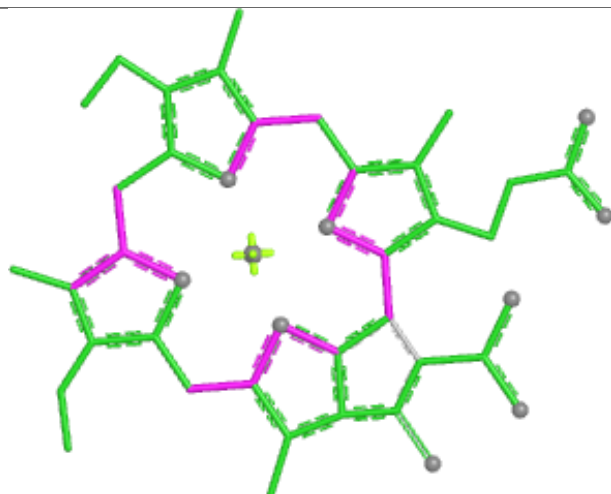
Ligand CHL 7 1013			
			
Bond lengths	Bond angles		
			
Torsions	Rings		



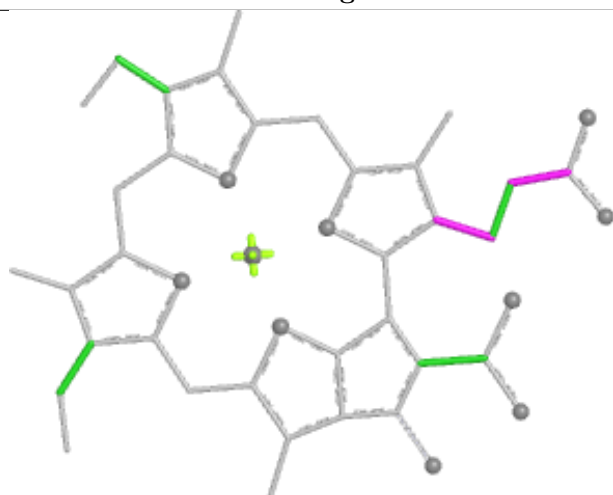
Ligand CLA G 202



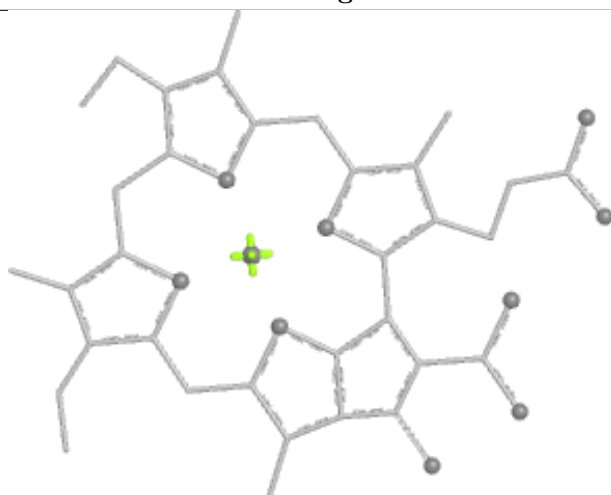
Bond lengths



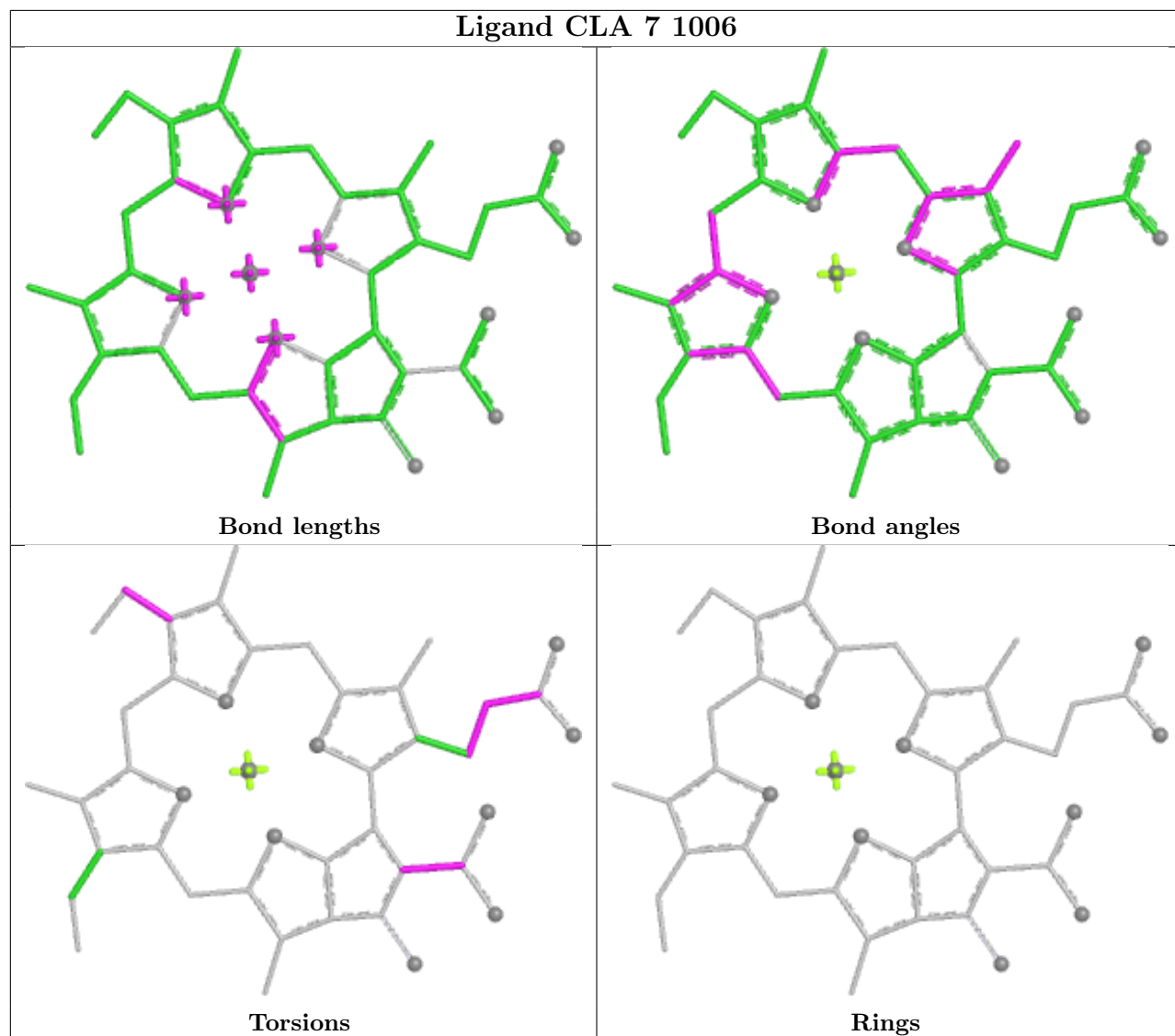
Bond angles



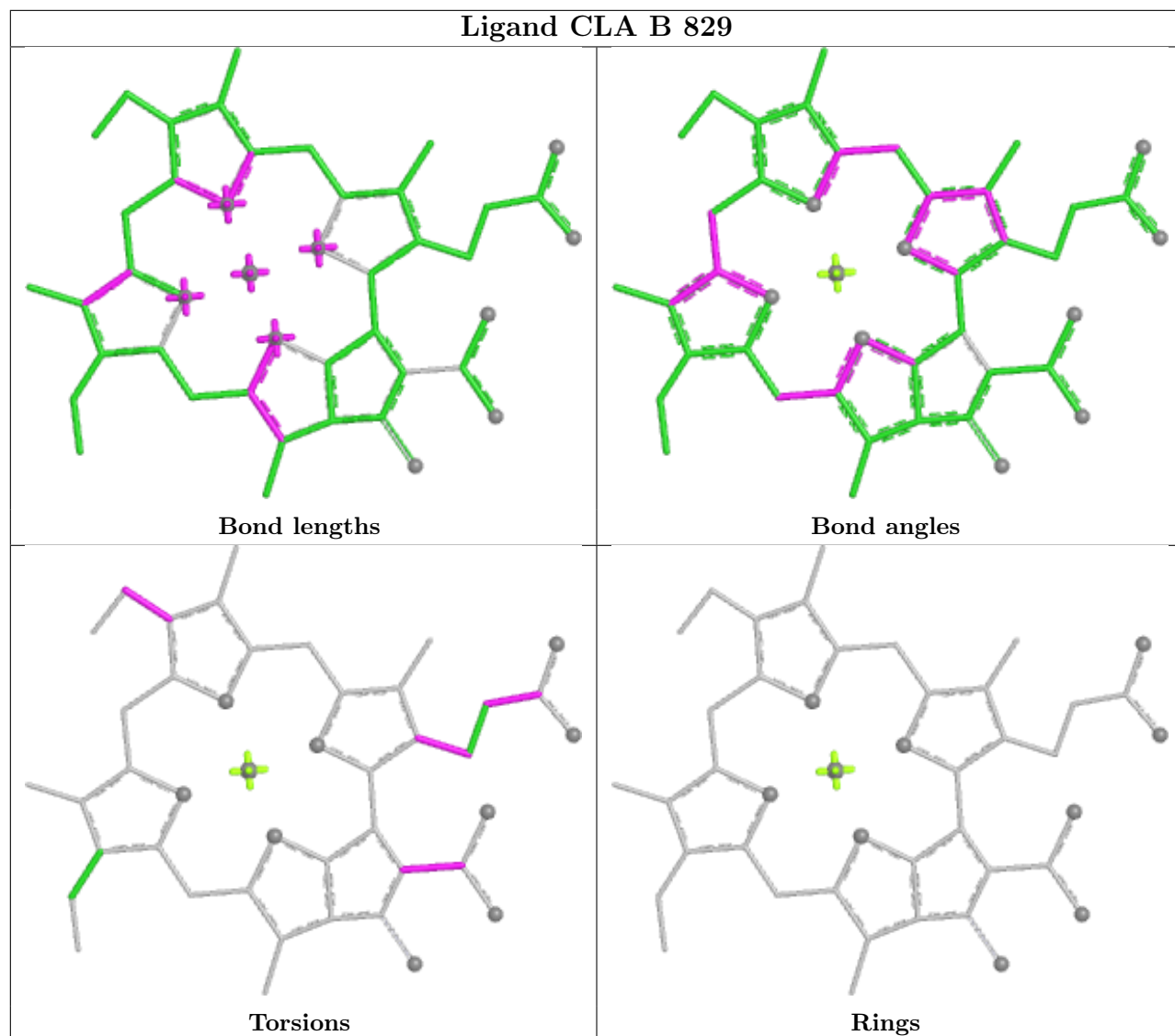
Torsions



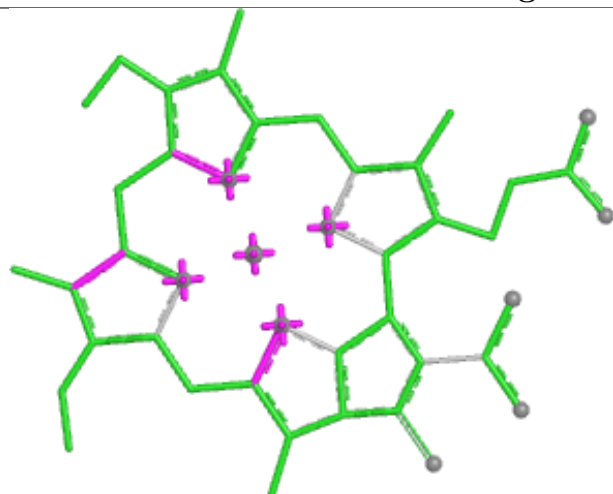
Rings



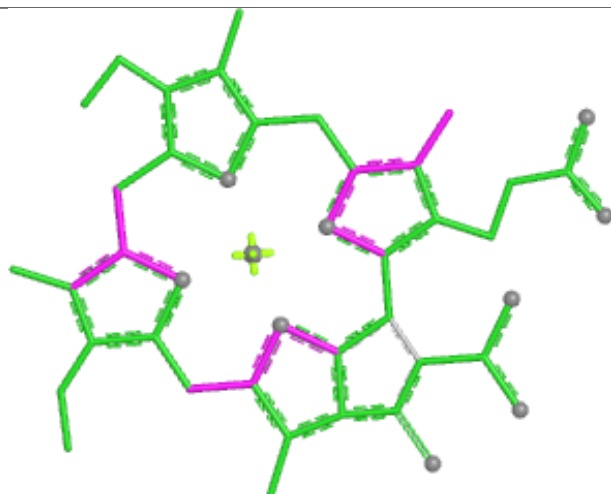
Ligand CLA B 829



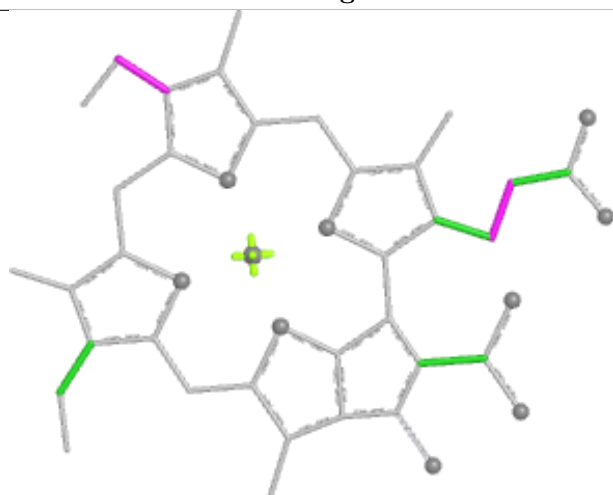
Ligand CLA 6 307



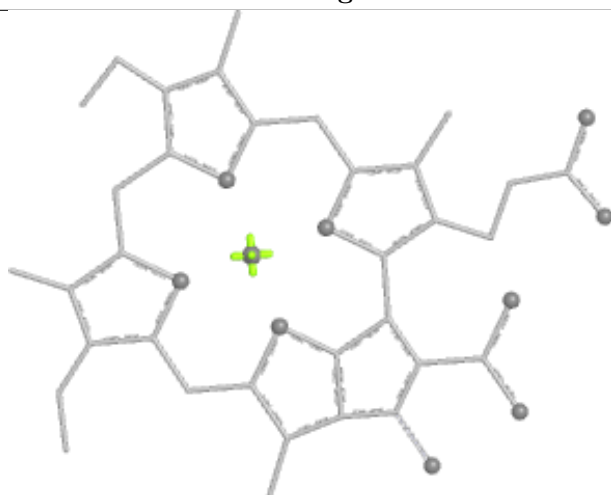
Bond lengths



Bond angles

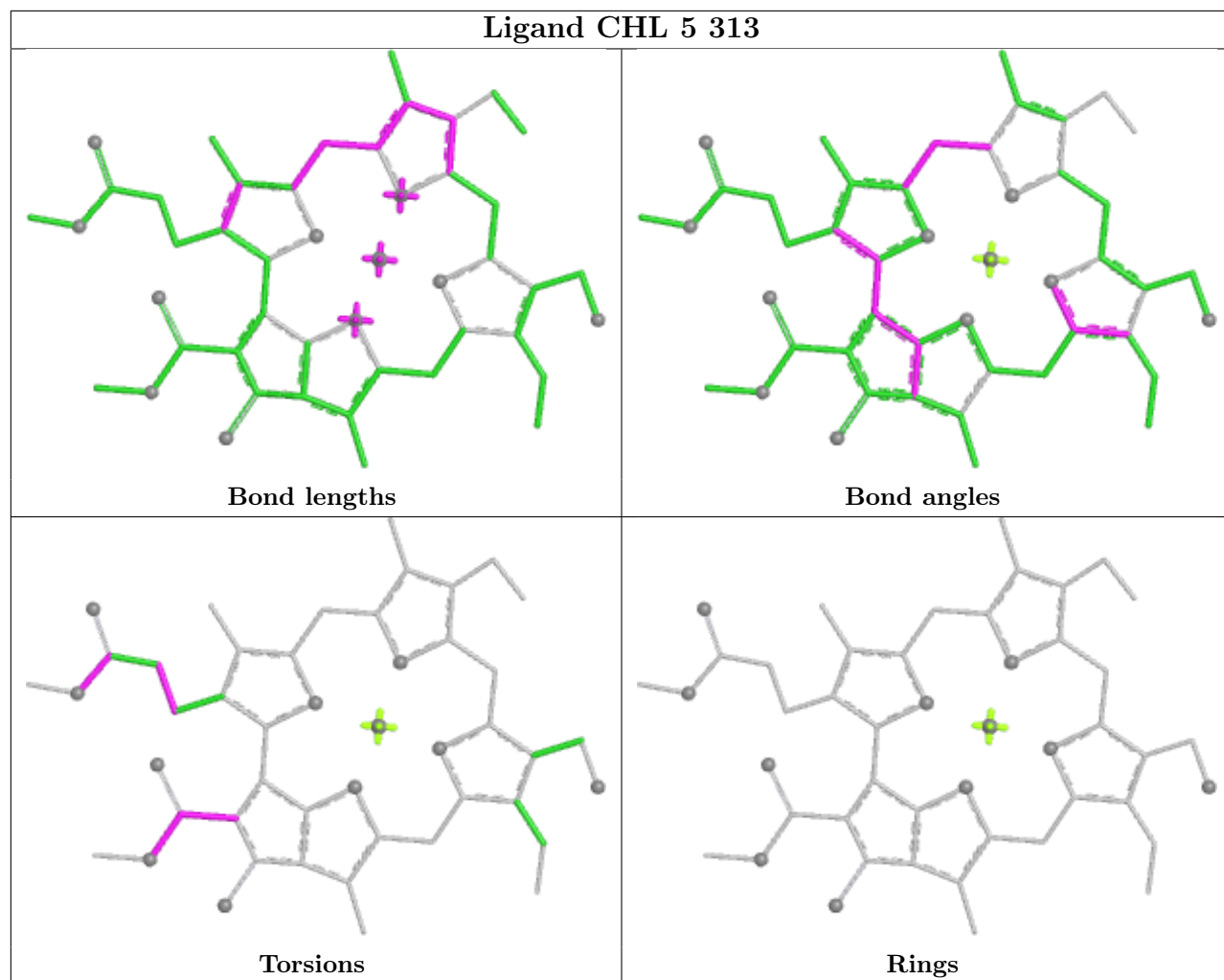


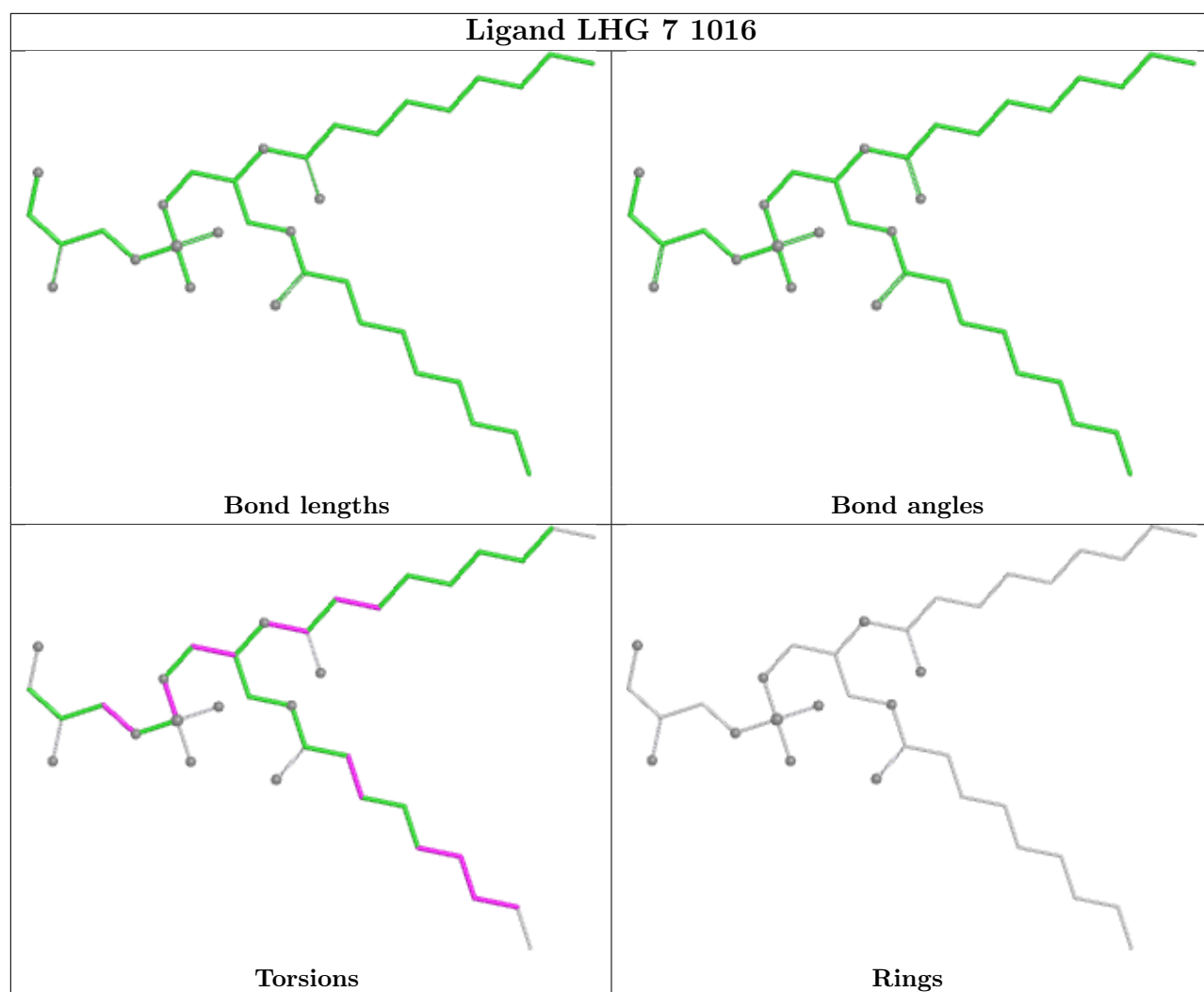
Torsions



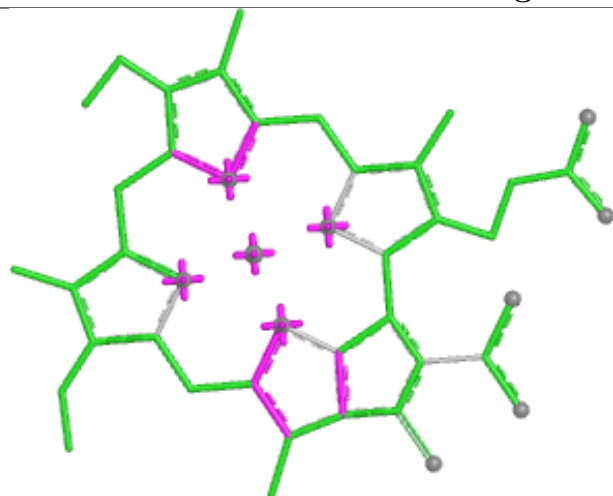
Rings

Ligand CHL 5 313

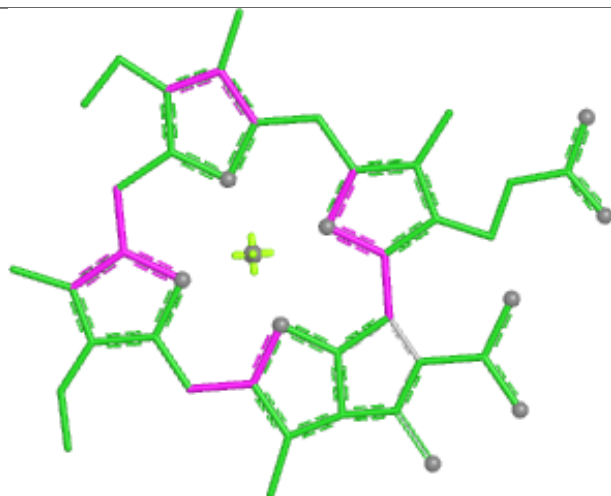




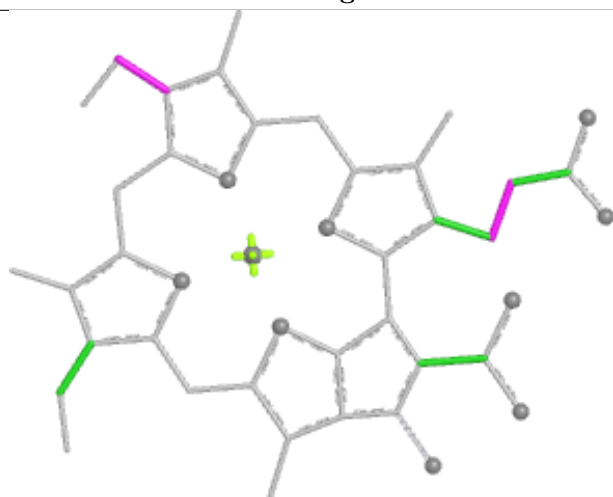
Ligand CLA B 801



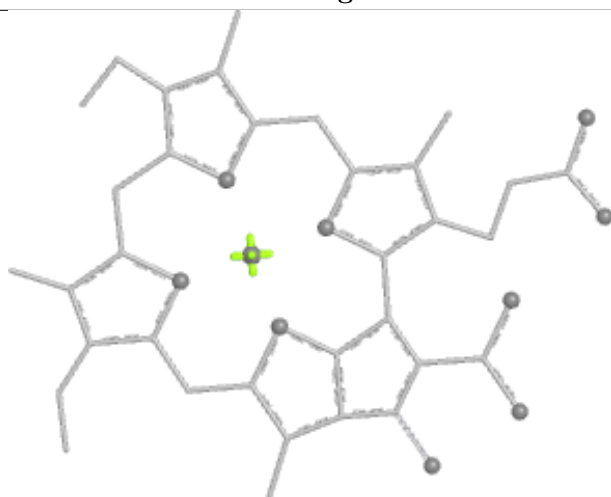
Bond lengths



Bond angles

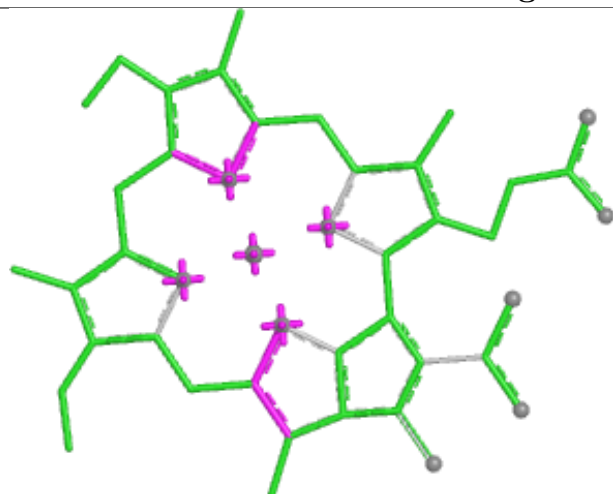


Torsions

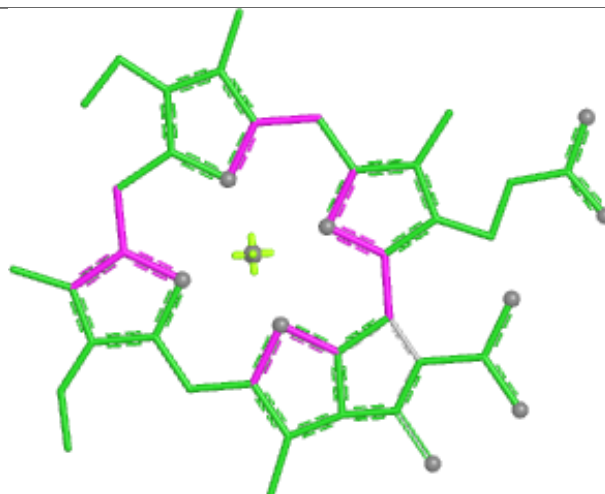


Rings

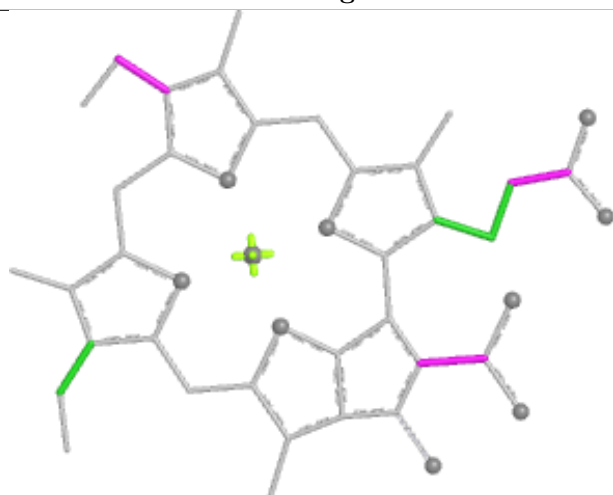
Ligand CLA 5 305



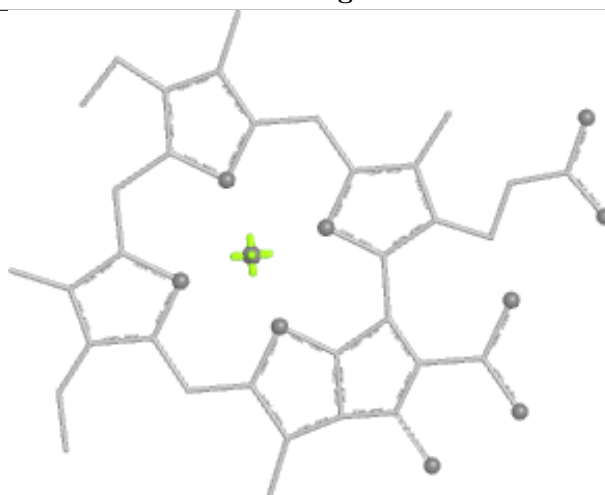
Bond lengths



Bond angles

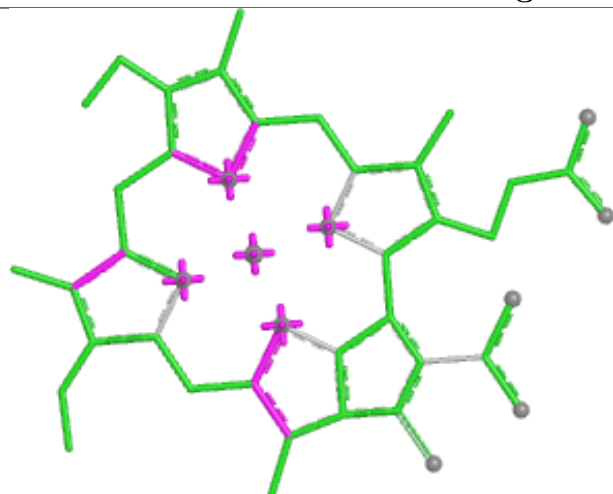


Torsions

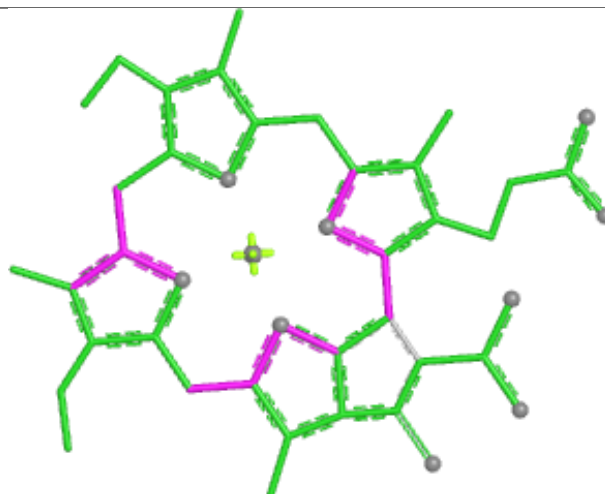


Rings

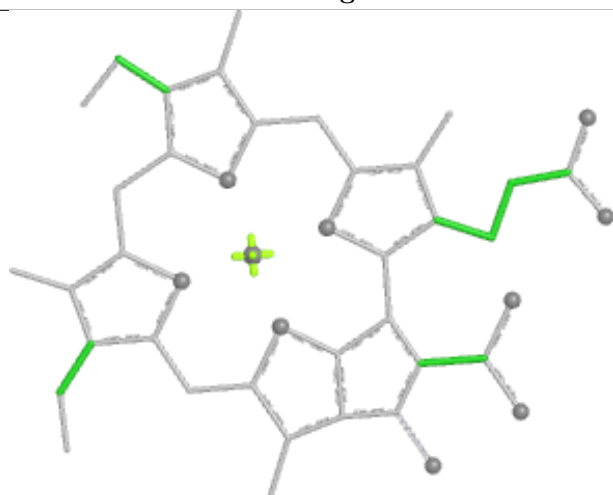
Ligand CLA F 305



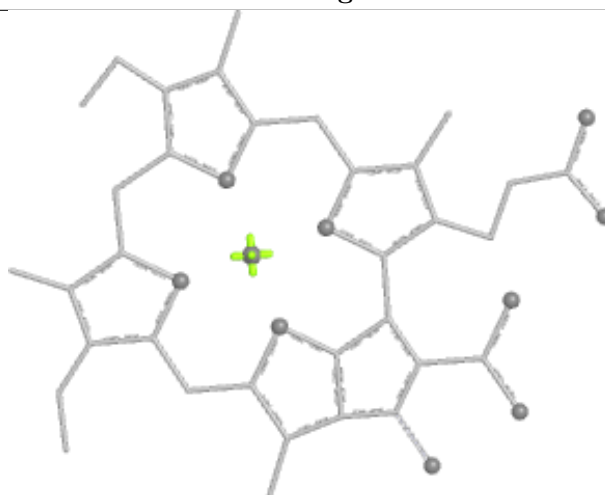
Bond lengths



Bond angles

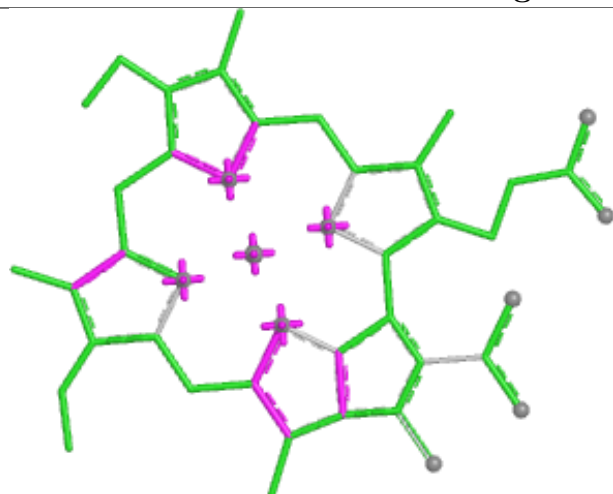


Torsions

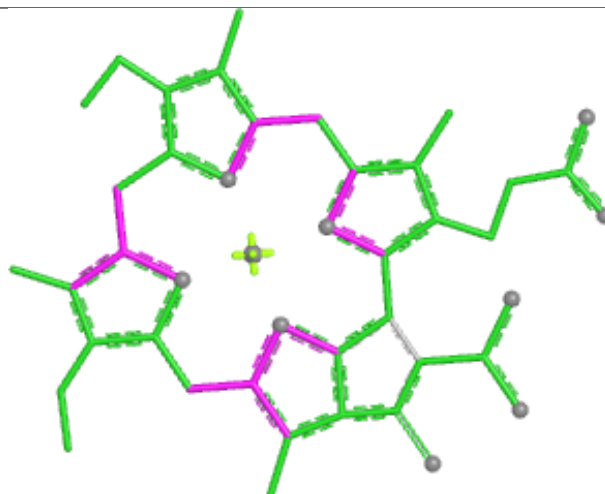


Rings

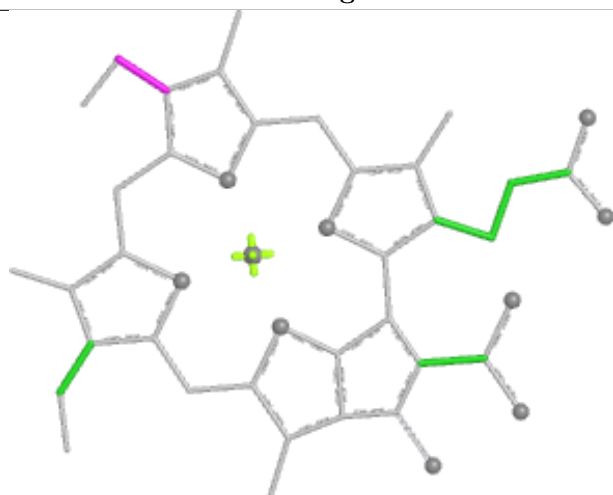
Ligand CLA A 809



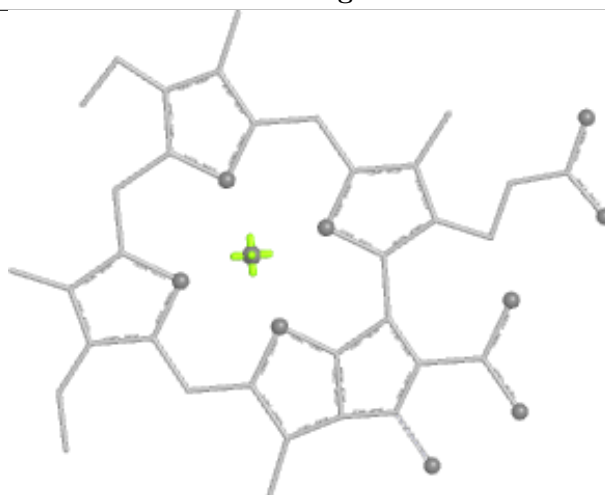
Bond lengths



Bond angles

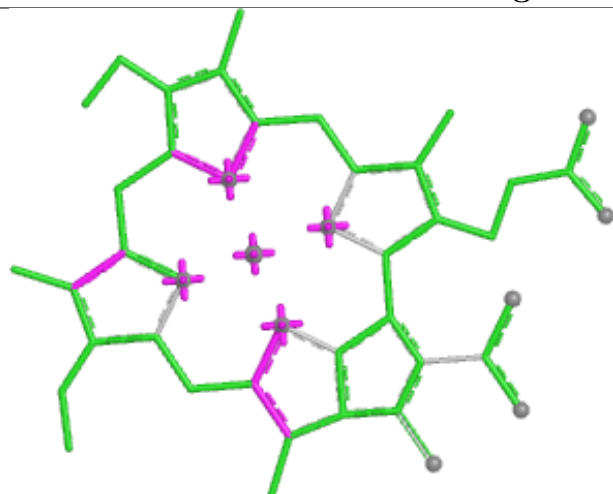


Torsions

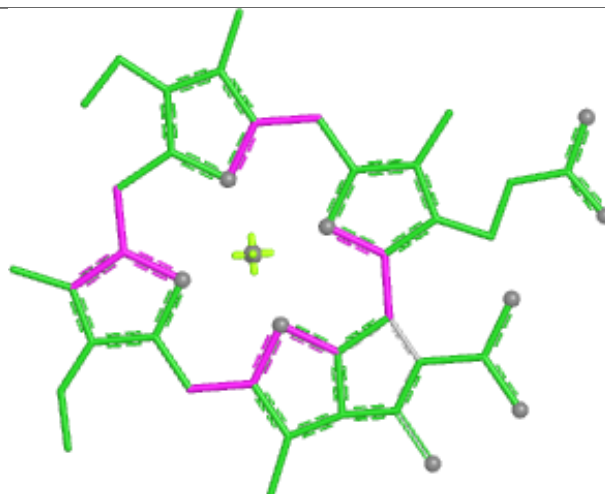


Rings

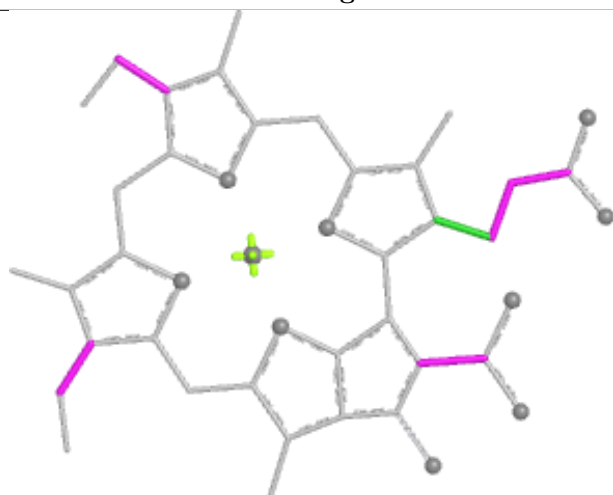
Ligand CLA G 203



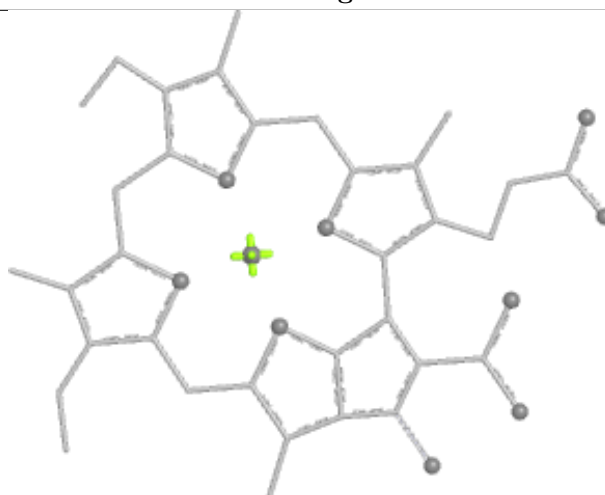
Bond lengths



Bond angles

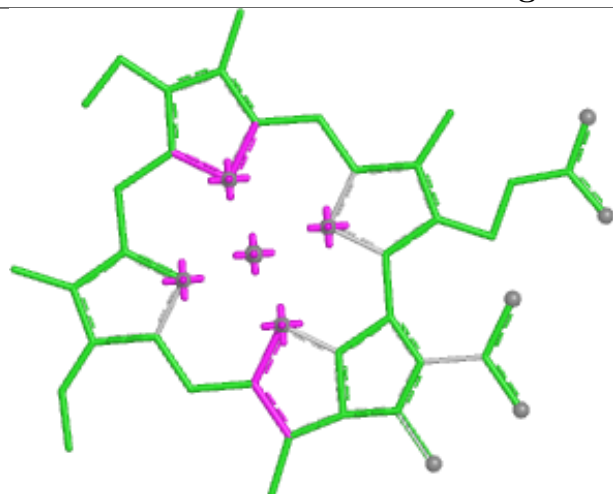


Torsions

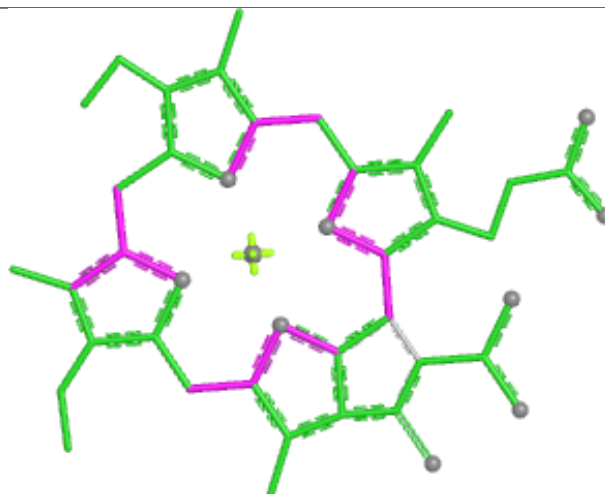


Rings

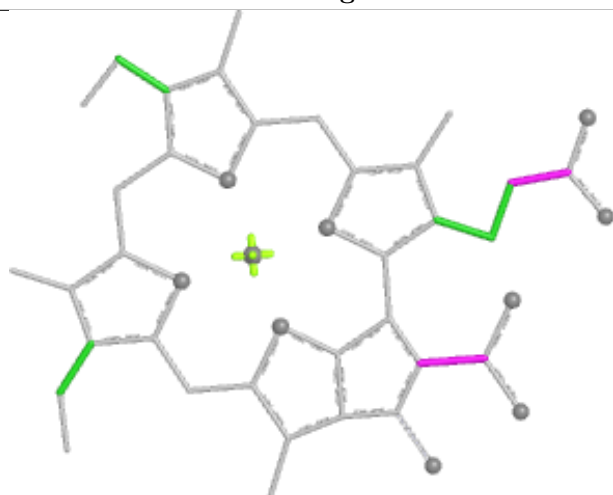
Ligand CLA 0 306



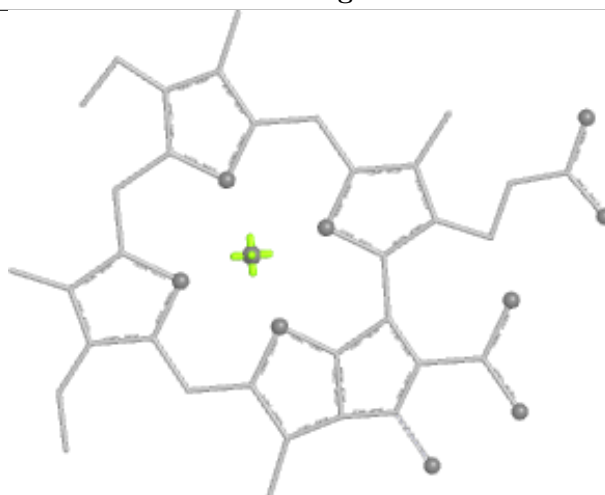
Bond lengths



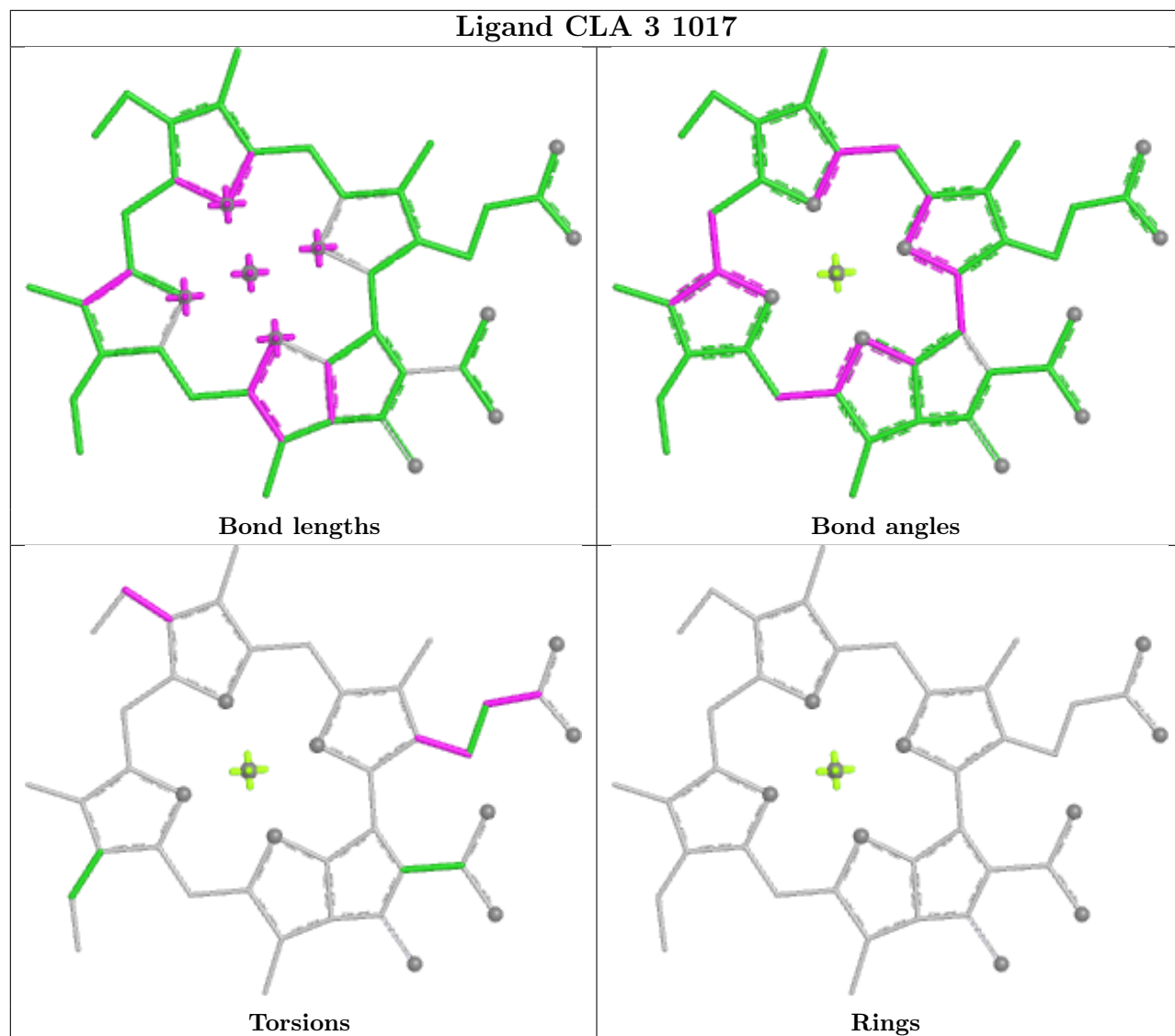
Bond angles

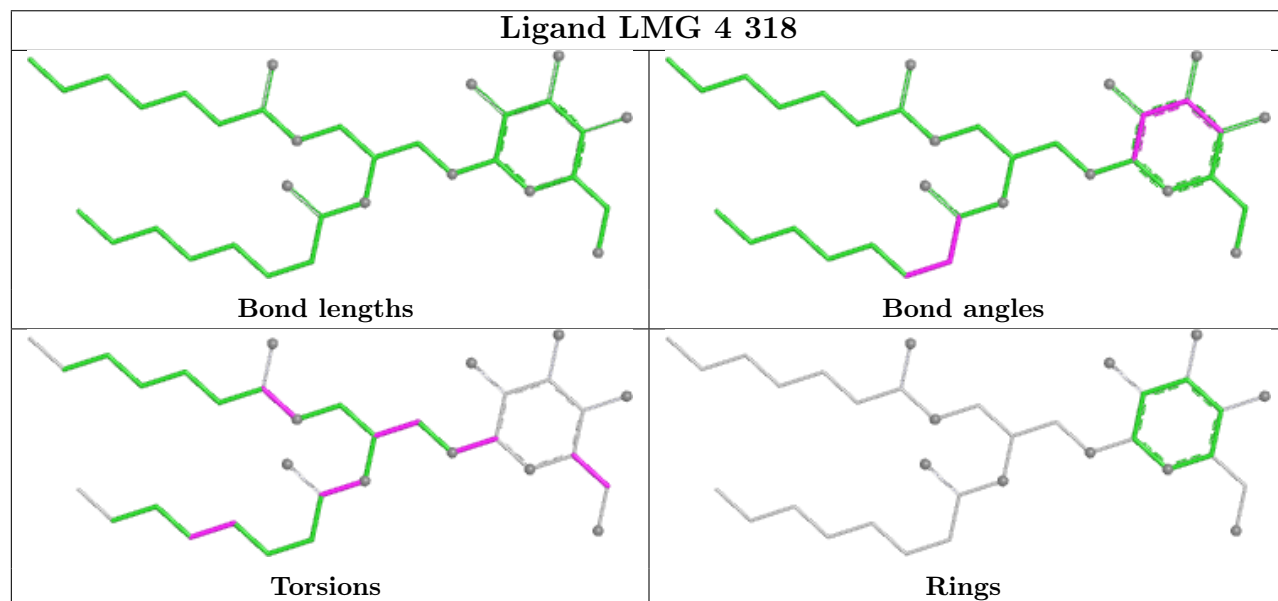
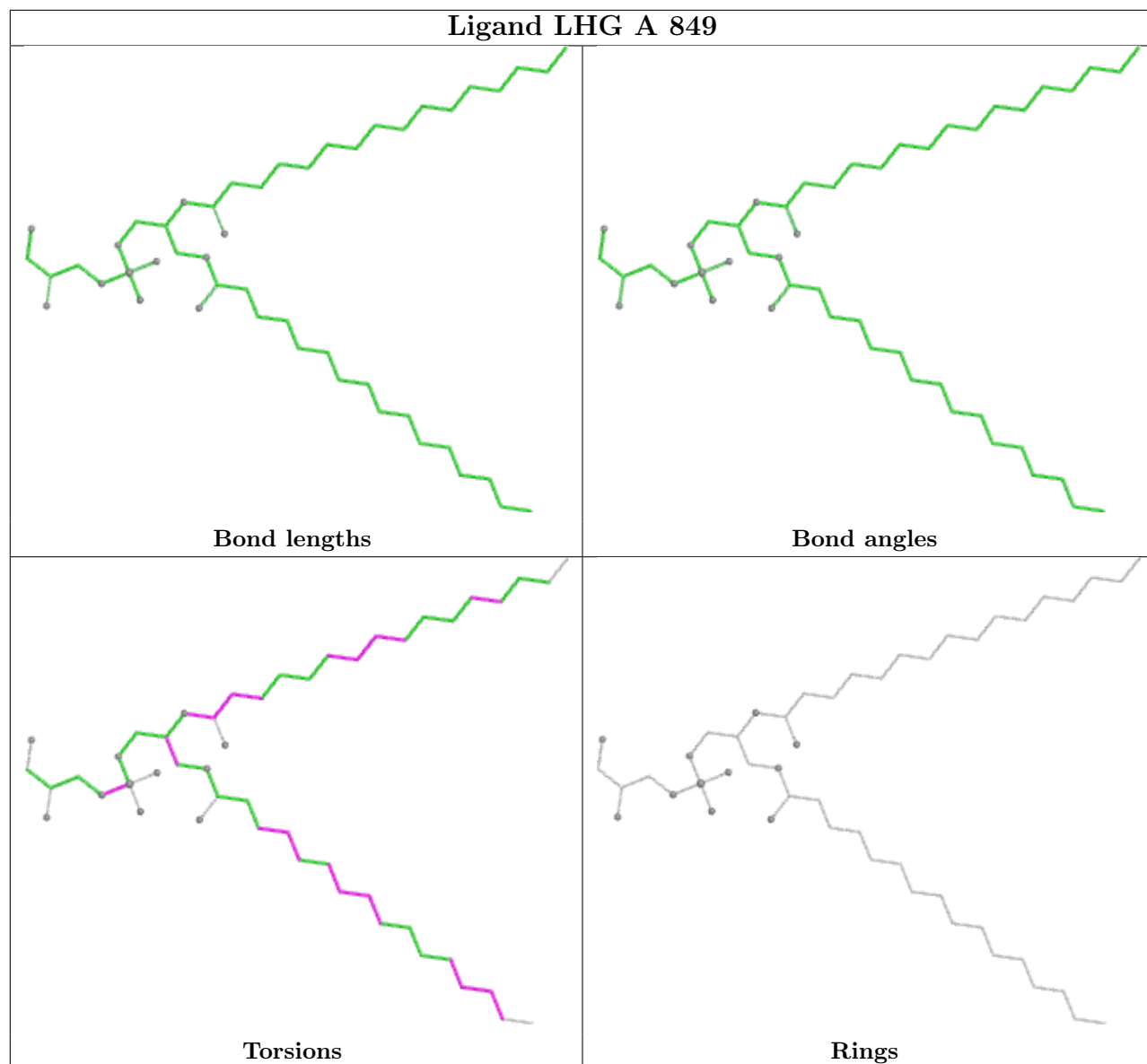


Torsions

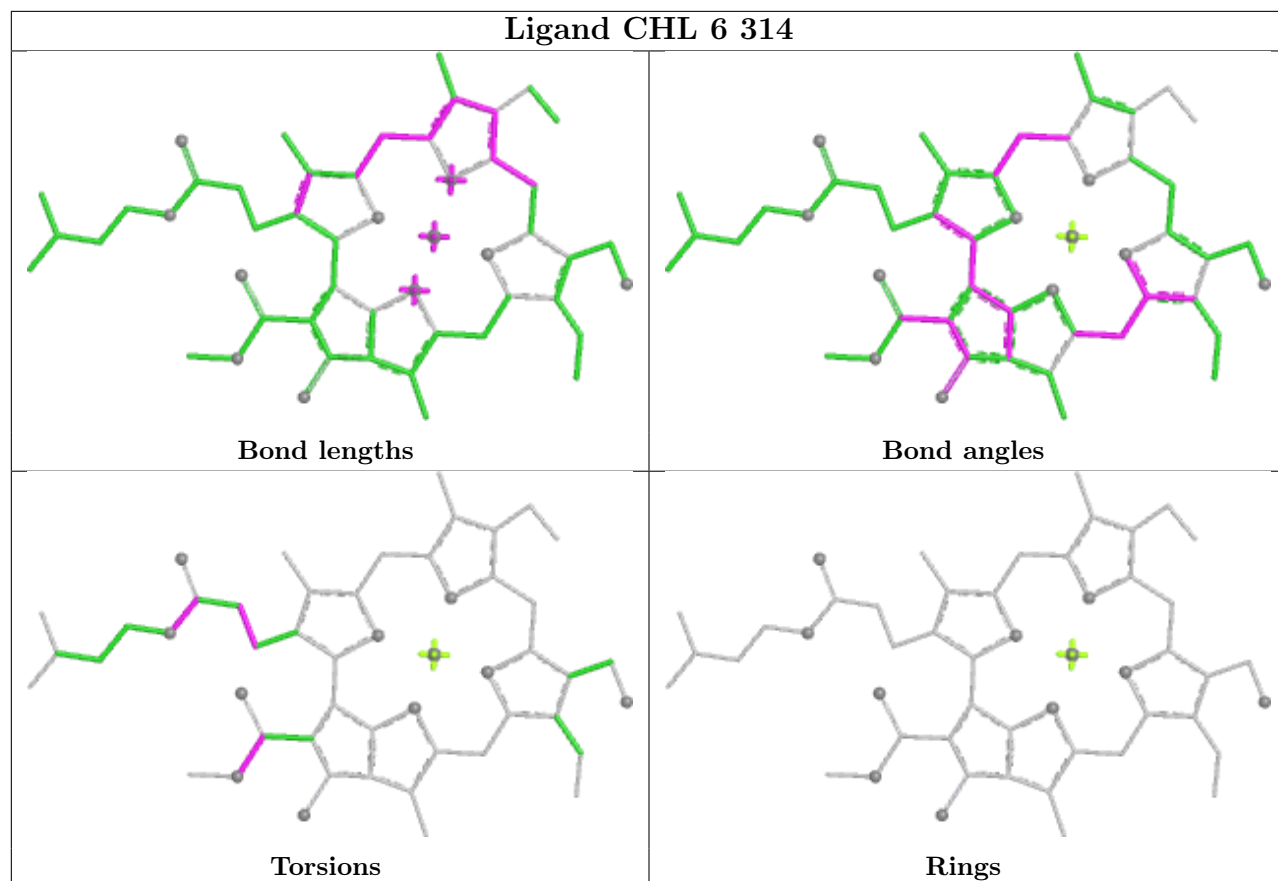


Rings

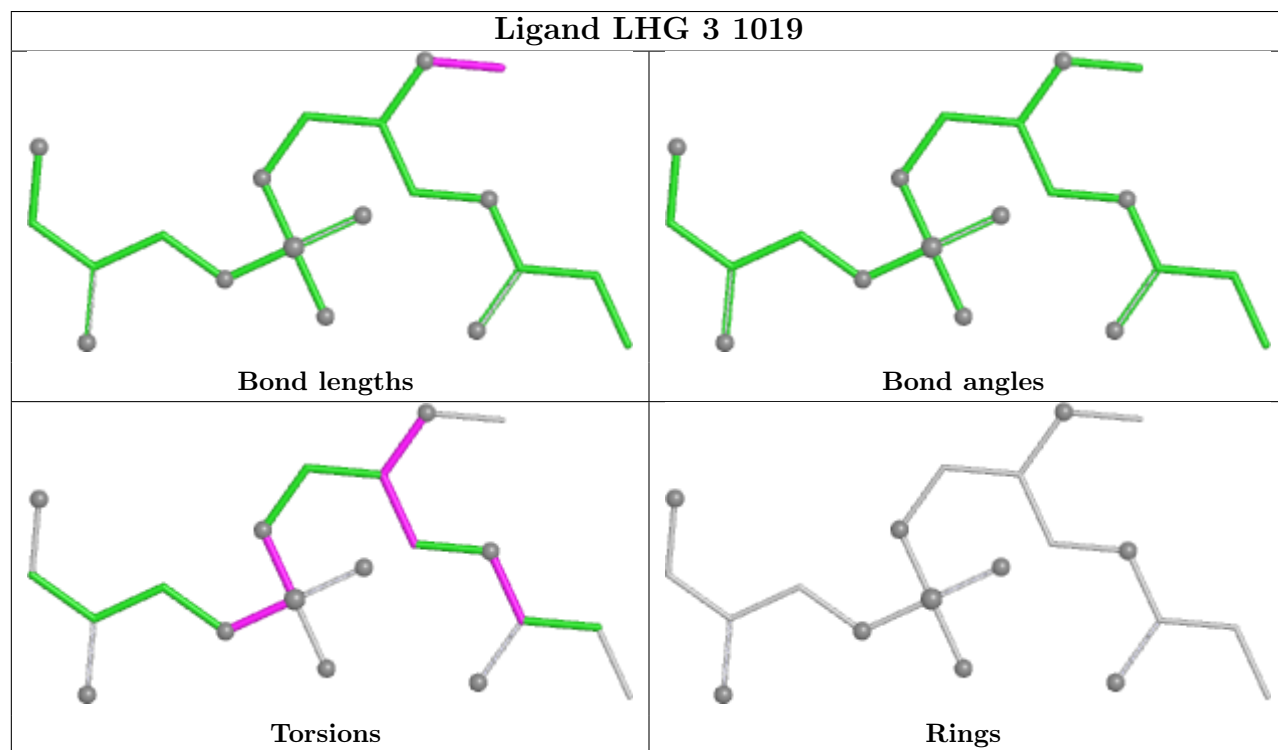




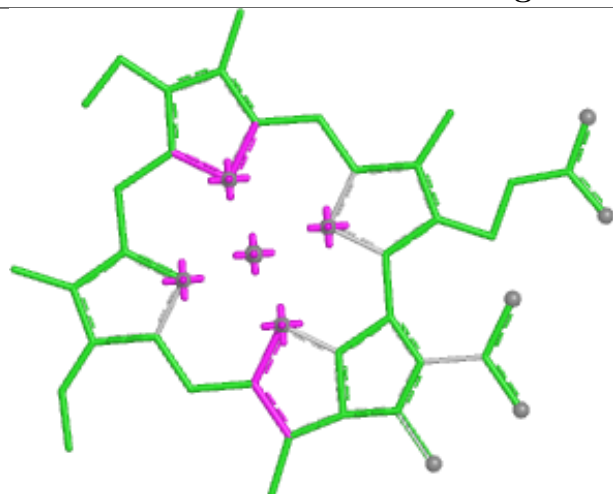
Ligand CHL 6 314



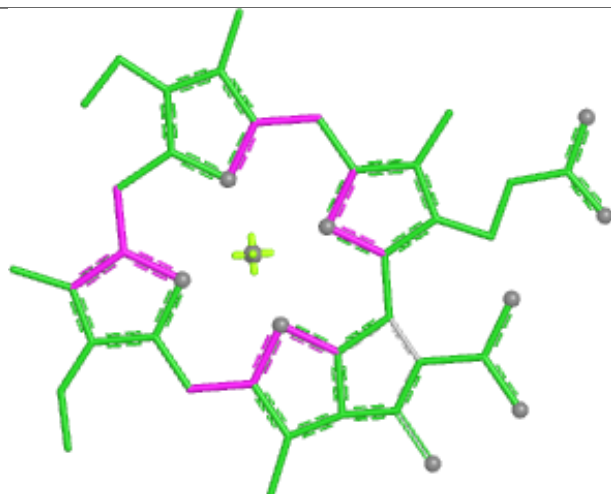
Ligand LHG 3 1019



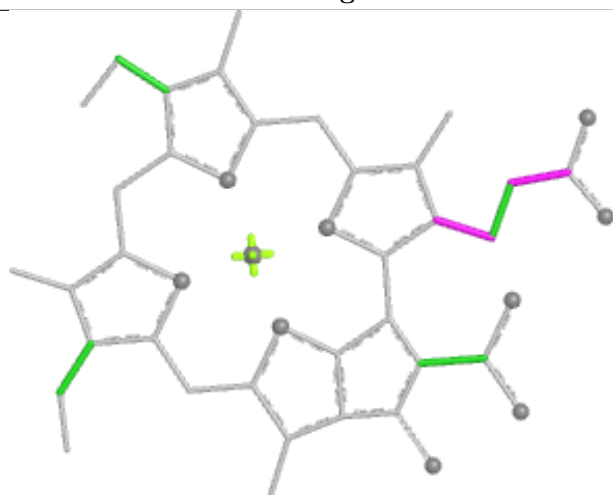
Ligand CLA B 808



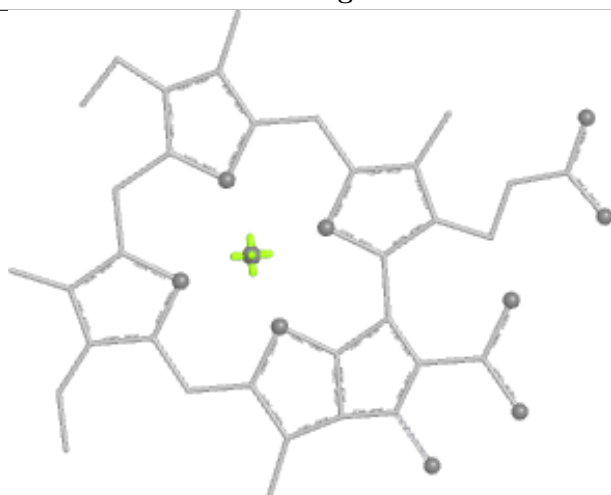
Bond lengths



Bond angles

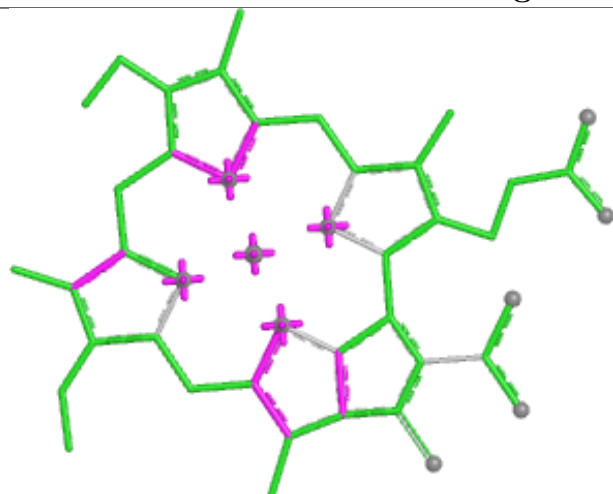


Torsions

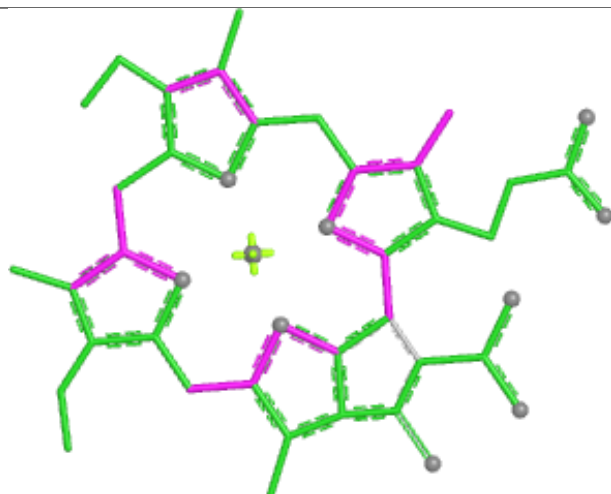


Rings

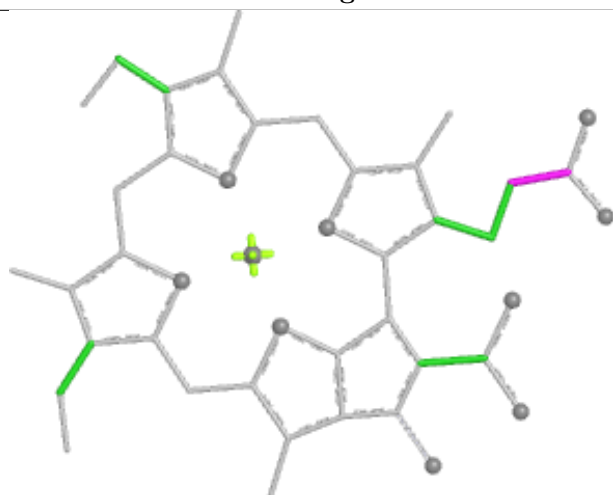
Ligand CLA A 821



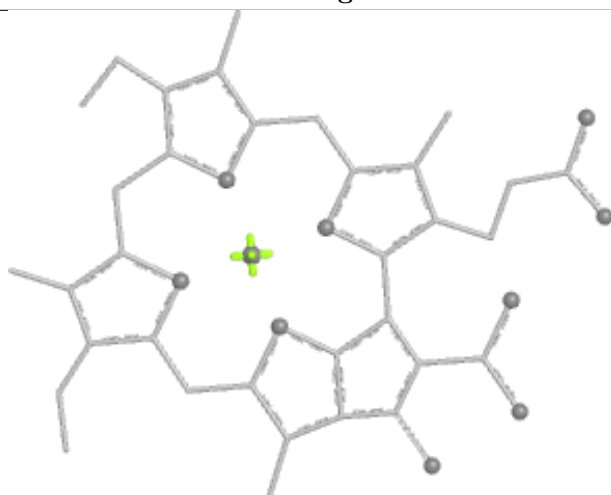
Bond lengths



Bond angles

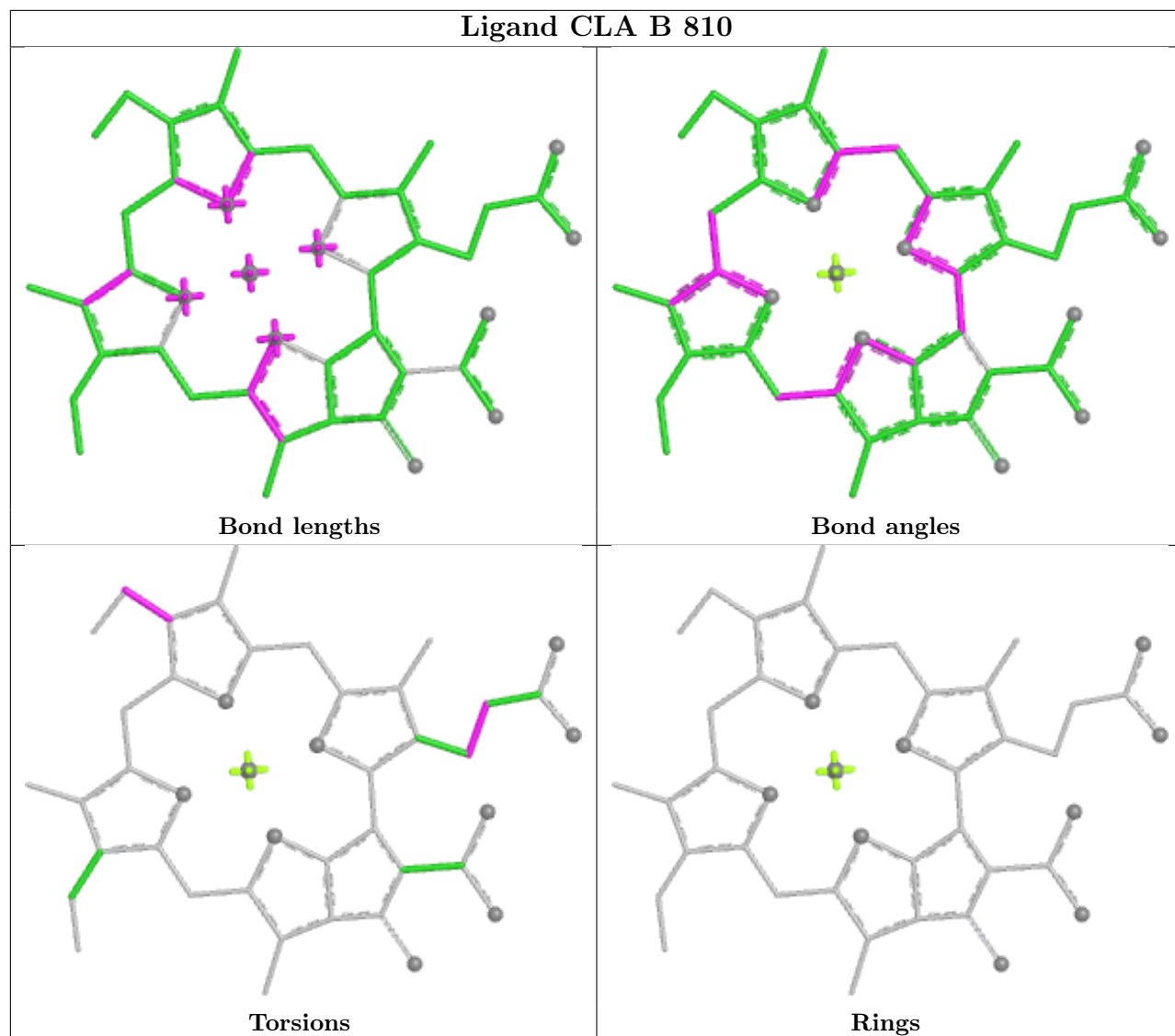


Torsions

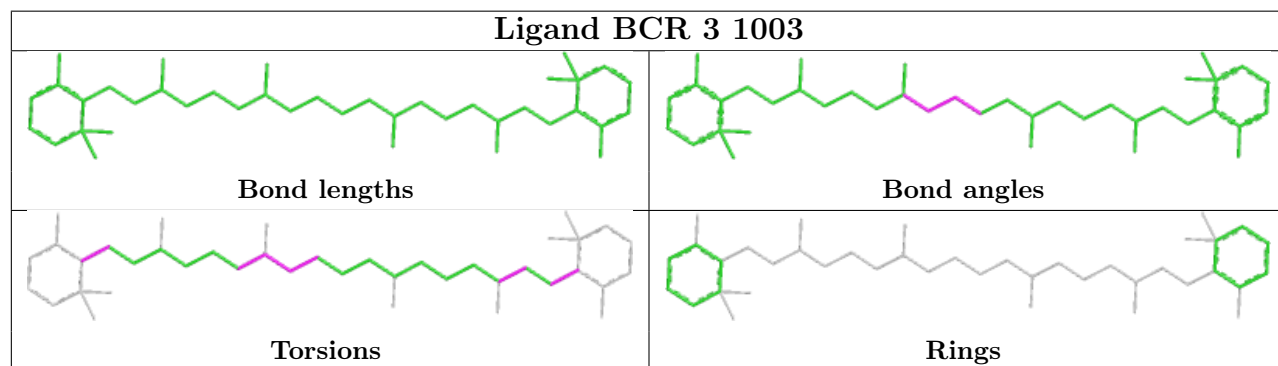


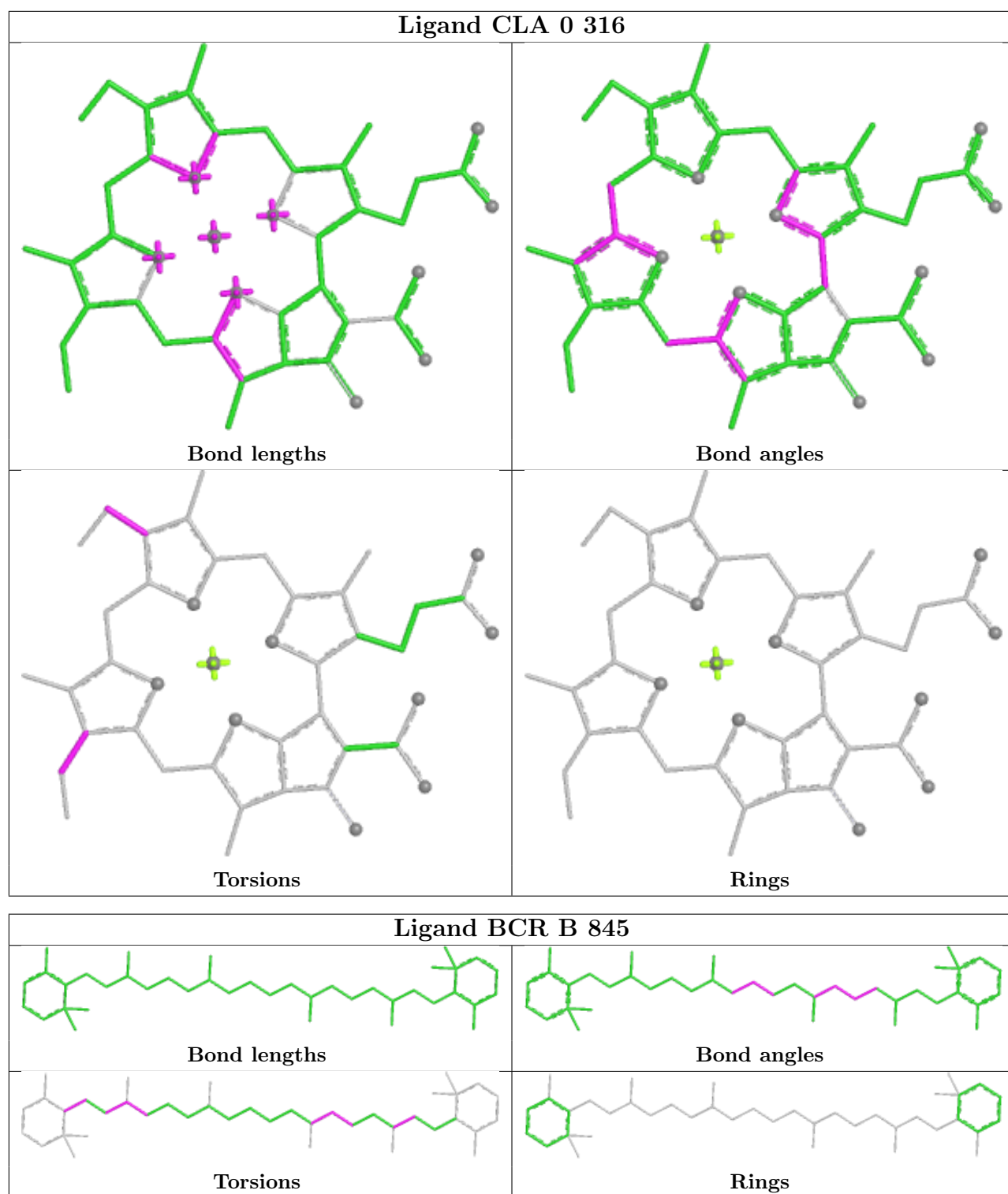
Rings

Ligand CLA B 810



Ligand BCR 3 1003





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	738/751 (98%)	0.39	31 (4%) 40 29	91, 155, 210, 250	0
2	B	728/735 (99%)	0.46	26 (3%) 46 33	106, 177, 229, 279	0
3	C	80/81 (98%)	0.58	7 (8%) 15 14	136, 172, 199, 219	0
4	D	141/196 (71%)	0.27	3 (2%) 63 48	132, 182, 217, 255	0
5	E	61/97 (62%)	0.36	0 100 100	111, 159, 184, 195	0
6	F	150/227 (66%)	0.17	6 (4%) 42 30	89, 138, 175, 204	0
7	G	85/126 (67%)	0.48	6 (7%) 22 18	175, 261, 344, 421	0
8	H	90/130 (69%)	0.55	3 (3%) 49 36	197, 283, 367, 430	0
9	I	29/106 (27%)	0.86	2 (6%) 23 18	204, 305, 350, 396	0
10	J	39/41 (95%)	0.12	1 (2%) 57 42	107, 131, 165, 179	0
11	K	44/113 (38%)	0.72	6 (13%) 7 8	195, 342, 432, 470	0
12	L	150/196 (76%)	0.74	7 (4%) 36 27	185, 331, 501, 579	0
13	0	182/228 (79%)	0.63	13 (7%) 22 18	101, 152, 203, 245	0
13	1	182/228 (79%)	0.48	13 (7%) 22 18	80, 119, 167, 195	0
14	8	193/243 (79%)	0.36	9 (4%) 36 27	61, 100, 129, 158	0
15	7	209/241 (86%)	0.48	11 (5%) 32 24	55, 89, 126, 164	0
16	3	201/298 (67%)	0.17	4 (1%) 65 49	73, 122, 160, 195	0
17	4	202/264 (76%)	0.31	7 (3%) 47 34	70, 106, 141, 170	0
18	6	184/257 (71%)	0.14	5 (2%) 56 42	43, 90, 128, 185	0
19	5	193/257 (75%)	0.33	8 (4%) 41 29	56, 95, 137, 166	0
All	All	3881/4815 (80%)	0.41	168 (4%) 40 29	43, 147, 298, 579	0

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	517	VAL	5.1
13	1	124	PRO	4.5
7	G	115	LEU	4.4
2	B	65	ASN	4.3
15	7	139	PHE	4.1

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	L	204	44/65	0.09	0.18	210,255,268,270	0
20	CLA	K	201	44/65	0.15	0.15	212,242,252,254	0
20	CLA	K	202	27/65	0.24	0.13	214,233,244,248	0
20	CLA	G	203	44/65	0.45	0.15	155,244,268,275	0
20	CLA	G	201	44/65	0.47	0.15	201,273,294,301	0
26	LMT	B	849	31/35	0.48	0.12	164,183,224,228	0
20	CLA	L	202	44/65	0.50	0.13	240,279,308,311	0
20	CLA	L	203	44/65	0.55	0.17	225,282,298,301	0
20	CLA	G	202	44/65	0.58	0.12	177,217,238,249	0
20	CLA	B	813	44/65	0.61	0.12	195,214,224,228	0
24	BCR	H	201	40/40	0.63	0.16	189,232,262,263	0
23	LHG	3	1019	20/49	0.64	0.15	202,256,264,269	0
20	CLA	B	815	44/65	0.65	0.13	128,158,232,249	0
20	CLA	A	840	44/65	0.66	0.14	173,213,233,245	0
24	BCR	I	201	40/40	0.68	0.17	194,224,242,243	0
24	BCR	A	850	40/40	0.68	0.20	177,223,310,313	0
27	LMG	5	324	45/55	0.68	0.16	46,97,156,183	0
24	BCR	G	204	40/40	0.69	0.14	206,227,250,259	0
24	BCR	G	205	40/40	0.69	0.18	119,205,273,275	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	LMG	8	319	44/55	0.70	0.21	151,179,216,229	0
29	CHL	0	317	61/66	0.70	0.17	186,220,246,264	0
29	CHL	1	1015	61/66	0.71	0.21	139,177,205,216	0
27	LMG	0	303	50/55	0.72	0.15	196,217,237,261	0
26	LMT	3	1018	31/35	0.73	0.19	111,185,218,227	0
20	CLA	A	822	44/65	0.74	0.15	170,196,205,216	0
24	BCR	1	1001	40/40	0.75	0.18	91,137,239,246	0
20	CLA	B	836	44/65	0.75	0.13	142,175,192,198	0
20	CLA	5	312	44/65	0.77	0.18	106,124,150,154	0
24	BCR	B	845	40/40	0.77	0.17	142,194,236,238	0
24	BCR	B	847	40/40	0.77	0.17	137,156,174,181	0
24	BCR	B	844	40/40	0.78	0.16	164,196,213,216	0
20	CLA	B	812	44/65	0.78	0.15	140,165,186,188	0
20	CLA	F	303	44/65	0.78	0.17	118,132,162,189	0
24	BCR	A	846	40/40	0.78	0.14	134,183,205,209	0
20	CLA	3	1011	40/65	0.78	0.13	180,202,216,218	0
27	LMG	8	318	28/55	0.79	0.22	72,118,150,161	0
29	CHL	0	314	47/66	0.79	0.19	164,201,252,295	0
20	CLA	3	1012	44/65	0.79	0.12	139,174,214,234	0
27	LMG	4	318	34/55	0.79	0.21	126,166,215,225	0
29	CHL	4	312	47/66	0.79	0.15	97,120,136,169	0
24	BCR	A	844	40/40	0.80	0.20	123,155,197,200	0
23	LHG	8	301	49/49	0.80	0.21	111,140,220,230	0
25	DGD	B	848	61/66	0.80	0.16	120,168,217,250	0
29	CHL	8	317	61/66	0.80	0.17	96,109,139,149	0
25	DGD	5	319	51/66	0.80	0.19	96,147,186,192	0
20	CLA	5	323	44/65	0.80	0.14	75,122,154,168	0
20	CLA	A	821	44/65	0.81	0.12	159,185,199,231	0
20	CLA	5	322	44/65	0.81	0.11	95,115,135,153	0
20	CLA	B	823	44/65	0.81	0.13	153,173,203,206	0
22	PQN	B	842	33/33	0.81	0.17	121,166,191,200	0
24	BCR	8	302	40/40	0.81	0.19	91,102,155,160	0
20	CLA	B	850	43/65	0.82	0.12	183,226,244,260	0
27	LMG	J	101	30/55	0.82	0.15	135,158,176,180	0
27	LMG	6	319	44/55	0.82	0.25	95,120,158,169	0
22	PQN	A	842	33/33	0.83	0.27	106,115,157,162	0
20	CLA	A	831	44/65	0.83	0.11	132,146,202,227	0
23	LHG	0	302	21/49	0.83	0.11	136,159,173,187	0
29	CHL	5	313	47/66	0.83	0.14	65,87,107,125	0
28	LUT	0	318	42/42	0.84	0.18	122,137,164,167	0
24	BCR	F	304	40/40	0.84	0.19	104,116,140,143	0
29	CHL	0	315	51/66	0.84	0.17	154,226,245,260	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	B	826	44/65	0.84	0.12	161,182,190,192	0
24	BCR	B	804	40/40	0.84	0.13	122,142,155,163	0
29	CHL	1	1012	47/66	0.84	0.11	102,132,156,174	0
20	CLA	B	803	44/65	0.84	0.14	170,200,215,220	0
24	BCR	A	845	40/40	0.84	0.18	102,120,156,172	0
20	CLA	B	824	44/65	0.84	0.16	148,171,185,200	0
20	CLA	0	306	44/65	0.85	0.10	123,146,154,163	0
20	CLA	0	311	44/65	0.85	0.12	113,128,159,183	0
20	CLA	0	313	44/65	0.85	0.14	90,114,149,162	0
20	CLA	A	819	44/65	0.85	0.13	147,180,190,194	0
20	CLA	B	816	44/65	0.85	0.12	174,190,199,205	0
20	CLA	5	311	44/65	0.85	0.12	88,107,161,222	0
20	CLA	A	820	44/65	0.85	0.11	135,178,186,193	0
20	CLA	A	815	44/65	0.85	0.15	120,138,154,165	0
28	LUT	0	304	42/42	0.85	0.23	128,147,202,207	0
20	CLA	1	1009	44/65	0.86	0.10	83,108,131,160	0
20	CLA	1	1017	44/65	0.86	0.14	92,114,125,136	0
20	CLA	B	840	44/65	0.86	0.12	158,197,210,214	0
24	BCR	J	103	40/40	0.86	0.15	113,134,148,157	0
20	CLA	J	102	44/65	0.86	0.10	121,142,156,168	0
24	BCR	A	847	40/40	0.86	0.11	120,138,183,185	0
24	BCR	4	302	40/40	0.86	0.18	99,130,160,164	0
20	CLA	0	307	44/65	0.86	0.12	90,104,125,144	0
20	CLA	A	812	44/65	0.86	0.12	95,111,124,135	0
29	CHL	8	314	47/66	0.86	0.15	102,134,169,185	0
20	CLA	B	801	44/65	0.86	0.13	118,166,178,191	0
20	CLA	A	833	44/65	0.86	0.12	181,193,207,213	0
23	LHG	A	849	49/49	0.86	0.18	121,149,179,196	0
20	CLA	B	810	44/65	0.86	0.12	160,186,210,222	0
20	CLA	1	1004	44/65	0.86	0.13	91,123,152,161	0
30	XAT	7	1002	44/44	0.86	0.19	69,83,91,97	0
28	LUT	1	1002	42/42	0.87	0.24	99,133,171,176	0
24	BCR	B	843	40/40	0.87	0.12	175,201,216,221	0
20	CLA	B	822	44/65	0.87	0.09	130,151,188,201	0
20	CLA	B	832	44/65	0.87	0.11	143,153,171,179	0
24	BCR	B	846	40/40	0.87	0.14	143,161,184,187	0
24	BCR	7	1003	40/40	0.87	0.25	92,124,149,156	0
20	CLA	B	835	44/65	0.87	0.14	127,158,171,189	0
29	CHL	1	1013	51/66	0.87	0.19	111,140,153,172	0
24	BCR	F	301	40/40	0.87	0.18	104,125,152,163	0
20	CLA	A	832	44/65	0.87	0.12	155,176,191,202	0
29	CHL	4	315	61/66	0.87	0.19	113,149,173,192	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	B	814	44/65	0.87	0.12	149,201,229,238	0
23	LHG	4	301	49/49	0.87	0.19	110,136,193,195	0
20	CLA	B	820	44/65	0.88	0.14	149,174,193,209	0
20	CLA	1	1014	44/65	0.88	0.12	86,113,129,136	0
20	CLA	A	823	44/65	0.88	0.13	155,173,187,192	0
20	CLA	4	310	44/65	0.88	0.11	85,107,115,129	0
20	CLA	6	310	44/65	0.88	0.13	84,99,108,121	0
20	CLA	A	830	44/65	0.88	0.14	161,200,217,226	0
24	BCR	A	848	40/40	0.88	0.15	102,125,154,157	0
28	LUT	1	1016	42/42	0.88	0.18	105,124,136,145	0
24	BCR	3	1004	40/40	0.88	0.15	111,134,161,169	0
20	CLA	0	310	44/65	0.88	0.12	98,110,151,172	0
20	CLA	B	841	44/65	0.88	0.10	84,105,159,184	0
24	BCR	6	302	40/40	0.88	0.18	98,133,141,150	0
24	BCR	5	320	40/40	0.88	0.17	81,107,129,134	0
20	CLA	A	809	44/65	0.88	0.15	98,121,134,143	0
20	CLA	0	316	44/65	0.88	0.13	145,186,199,209	0
20	CLA	L	201	44/65	0.88	0.12	149,200,218,235	0
23	LHG	A	843	40/49	0.88	0.13	166,193,211,225	0
20	CLA	A	852	44/65	0.88	0.10	141,151,167,187	0
29	CHL	6	316	61/66	0.88	0.15	95,112,152,159	0
20	CLA	B	819	44/65	0.88	0.14	171,196,246,285	0
20	CLA	1	1007	44/65	0.88	0.12	110,118,130,141	0
20	CLA	A	825	44/65	0.89	0.13	117,135,157,167	0
20	CLA	B	833	44/65	0.89	0.13	94,117,146,175	0
20	CLA	B	808	44/65	0.89	0.11	134,145,169,180	0
20	CLA	8	311	44/65	0.89	0.14	72,109,143,161	0
20	CLA	6	311	44/65	0.89	0.11	89,99,113,132	0
20	CLA	8	313	44/65	0.89	0.13	71,101,113,120	0
20	CLA	3	1007	44/65	0.89	0.11	118,139,154,166	0
20	CLA	A	826	44/65	0.89	0.10	104,122,141,146	0
20	CLA	B	811	44/65	0.89	0.09	130,155,170,179	0
20	CLA	A	816	44/65	0.89	0.12	131,154,200,217	0
20	CLA	1	1005	44/65	0.89	0.11	84,120,130,145	0
20	CLA	0	309	44/65	0.89	0.14	143,171,200,215	0
28	LUT	J	104	42/42	0.89	0.15	79,115,162,172	0
20	CLA	B	830	44/65	0.89	0.14	132,144,168,179	0
29	CHL	5	317	43/66	0.89	0.12	80,97,120,132	0
30	XAT	8	304	44/44	0.89	0.17	50,85,95,109	0
20	CLA	1	1010	44/65	0.89	0.14	95,135,156,184	0
20	CLA	8	316	44/65	0.90	0.14	77,101,116,126	0
20	CLA	3	1006	44/65	0.90	0.10	104,132,140,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	B	807	44/65	0.90	0.09	119,158,173,175	0
20	CLA	6	308	44/65	0.90	0.11	32,39,48,71	0
20	CLA	B	829	44/65	0.90	0.12	155,179,193,196	0
20	CLA	B	817	44/65	0.90	0.10	148,178,197,209	0
29	CHL	7	1012	47/66	0.90	0.13	98,115,161,176	0
29	CHL	7	1017	66/66	0.90	0.16	100,117,150,172	0
20	CLA	6	318	44/65	0.90	0.10	79,94,106,123	0
20	CLA	6	320	44/65	0.90	0.11	68,87,93,104	0
20	CLA	5	305	44/65	0.90	0.10	66,81,103,125	0
20	CLA	5	309	44/65	0.90	0.11	84,103,114,120	0
20	CLA	5	310	44/65	0.90	0.11	91,112,129,150	0
29	CHL	4	316	43/66	0.90	0.12	93,105,118,145	0
29	CHL	6	313	47/66	0.90	0.14	83,98,121,171	0
20	CLA	0	312	44/65	0.90	0.12	101,128,147,160	0
20	CLA	B	831	44/65	0.90	0.12	141,164,178,198	0
20	CLA	0	305	44/65	0.90	0.12	115,150,185,194	0
20	CLA	B	818	44/65	0.90	0.11	214,236,252,260	0
20	CLA	A	811	44/65	0.90	0.12	110,148,160,171	0
28	LUT	3	1001	42/42	0.91	0.15	89,116,145,156	0
20	CLA	A	803	44/65	0.91	0.11	80,90,114,117	0
20	CLA	6	312	44/65	0.91	0.14	59,98,130,141	0
28	LUT	4	317	42/42	0.91	0.14	75,98,117,123	0
28	LUT	6	303	42/42	0.91	0.15	64,81,96,113	0
28	LUT	5	302	42/42	0.91	0.15	68,88,99,105	0
20	CLA	A	835	44/65	0.91	0.11	138,164,192,219	0
20	CLA	3	1013	44/65	0.91	0.11	89,133,159,173	0
20	CLA	1	1003	44/65	0.91	0.12	68,85,114,138	0
20	CLA	5	308	44/65	0.91	0.12	81,90,105,119	0
20	CLA	A	836	44/65	0.91	0.12	143,180,192,207	0
20	CLA	F	302	44/65	0.91	0.11	91,99,108,109	0
20	CLA	A	810	44/65	0.91	0.12	101,123,131,139	0
20	CLA	1	1008	44/65	0.91	0.13	96,118,156,180	0
20	CLA	F	305	44/65	0.91	0.11	102,130,154,167	0
20	CLA	A	817	44/65	0.91	0.09	107,120,144,168	0
20	CLA	1	1011	44/65	0.91	0.13	99,108,125,138	0
29	CHL	4	313	51/66	0.91	0.15	86,105,120,132	0
20	CLA	A	814	40/65	0.91	0.12	147,160,199,217	0
20	CLA	7	1006	44/65	0.91	0.11	62,81,91,104	0
20	CLA	4	305	44/65	0.91	0.10	76,87,106,122	0
20	CLA	4	307	44/65	0.91	0.11	63,79,93,99	0
20	CLA	A	824	44/65	0.91	0.12	102,147,173,183	0
20	CLA	B	806	44/65	0.91	0.13	166,188,198,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	3	1010	44/65	0.91	0.12	99,114,127,142	0
28	LUT	7	1001	42/42	0.91	0.14	56,73,85,91	0
30	XAT	4	303	44/44	0.91	0.17	66,91,98,101	0
30	XAT	6	304	44/44	0.91	0.17	39,78,87,91	0
20	CLA	3	1009	44/65	0.92	0.10	87,120,129,132	0
20	CLA	4	308	44/65	0.92	0.10	65,82,94,100	0
20	CLA	4	309	44/65	0.92	0.09	69,79,107,136	0
24	BCR	3	1003	40/40	0.92	0.15	63,111,123,129	0
20	CLA	A	827	44/65	0.92	0.13	110,133,141,161	0
20	CLA	4	311	44/65	0.92	0.11	63,96,112,119	0
20	CLA	6	307	44/65	0.92	0.12	65,82,89,92	0
20	CLA	A	839	44/65	0.92	0.08	70,83,98,111	0
20	CLA	6	309	44/65	0.92	0.12	64,88,100,134	0
20	CLA	B	838	44/65	0.92	0.13	114,136,149,158	0
29	CHL	7	1015	46/66	0.92	0.12	70,81,108,131	0
20	CLA	A	801	44/65	0.92	0.12	93,116,157,224	0
20	CLA	3	1017	44/65	0.92	0.10	91,110,140,160	0
20	CLA	A	851	44/65	0.92	0.11	115,135,143,146	0
20	CLA	B	809	44/65	0.92	0.10	150,162,177,184	0
20	CLA	5	304	44/65	0.92	0.13	69,97,114,125	0
20	CLA	8	309	44/65	0.92	0.10	75,95,102,114	0
20	CLA	5	307	44/65	0.92	0.11	52,64,76,83	0
20	CLA	A	834	44/65	0.92	0.13	144,167,186,190	0
20	CLA	A	818	44/65	0.92	0.10	113,142,151,156	0
20	CLA	B	802	44/65	0.92	0.12	99,123,145,168	0
20	CLA	B	821	44/65	0.92	0.09	133,160,183,185	0
20	CLA	7	1007	44/65	0.92	0.12	52,60,67,75	0
20	CLA	5	321	44/65	0.92	0.09	60,71,80,82	0
20	CLA	7	1009	44/65	0.92	0.11	62,80,95,104	0
20	CLA	B	834	44/65	0.92	0.10	98,111,121,136	0
20	CLA	0	308	44/65	0.92	0.12	93,113,124,125	0
20	CLA	8	308	44/65	0.93	0.12	53,76,86,92	0
20	CLA	B	837	44/65	0.93	0.10	100,117,128,141	0
20	CLA	4	314	44/65	0.93	0.12	77,98,118,140	0
20	CLA	6	301	44/65	0.93	0.14	93,111,124,154	0
20	CLA	3	1015	44/65	0.93	0.11	99,108,120,132	0
29	CHL	7	1013	48/66	0.93	0.14	73,86,106,112	0
20	CLA	8	310	44/65	0.93	0.10	51,72,106,148	0
20	CLA	A	806	44/65	0.93	0.09	92,115,135,141	0
20	CLA	A	837	44/65	0.93	0.10	91,107,122,126	0
20	CLA	A	838	44/65	0.93	0.11	98,111,134,136	0
20	CLA	7	1005	44/65	0.93	0.08	64,79,92,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	A	829	44/65	0.93	0.10	90,109,125,128	0
20	CLA	A	813	44/65	0.93	0.12	112,132,149,155	0
28	LUT	8	303	42/42	0.93	0.12	60,74,91,96	0
20	CLA	7	1008	44/65	0.93	0.10	73,91,104,129	0
20	CLA	B	825	44/65	0.93	0.10	150,176,188,201	0
29	CHL	6	314	51/66	0.93	0.14	73,98,112,134	0
28	LUT	3	1002	42/42	0.93	0.16	97,117,129,142	0
20	CLA	7	1010	44/65	0.93	0.12	85,104,121,130	0
20	CLA	A	802	44/65	0.93	0.11	68,90,128,167	0
20	CLA	B	828	44/65	0.93	0.11	134,151,160,167	0
20	CLA	0	301	44/65	0.93	0.13	133,166,178,188	0
20	CLA	8	305	44/65	0.93	0.10	75,87,99,115	0
20	CLA	8	306	44/65	0.93	0.08	59,71,95,103	0
30	XAT	5	303	44/44	0.93	0.13	49,77,104,108	0
20	CLA	7	1011	44/65	0.94	0.11	73,87,129,156	0
20	CLA	8	312	44/65	0.94	0.10	78,90,106,124	0
20	CLA	A	804	44/65	0.94	0.12	124,142,150,157	0
20	CLA	1	1006	44/65	0.94	0.10	56,75,91,94	0
20	CLA	5	301	44/65	0.94	0.10	71,78,106,120	0
20	CLA	B	839	44/65	0.94	0.10	118,134,148,154	0
20	CLA	B	827	44/65	0.94	0.10	98,109,123,130	0
20	CLA	5	306	44/65	0.94	0.11	91,110,117,118	0
20	CLA	8	307	44/65	0.94	0.10	57,65,89,126	0
20	CLA	A	807	44/65	0.94	0.11	117,131,148,155	0
20	CLA	6	306	44/65	0.94	0.08	68,87,93,118	0
29	CHL	6	317	43/66	0.94	0.10	85,96,129,160	0
20	CLA	A	828	44/65	0.94	0.12	112,134,146,155	0
29	CHL	5	316	61/66	0.94	0.12	54,73,167,176	0
20	CLA	A	808	44/65	0.94	0.11	102,112,122,129	0
29	CHL	8	315	51/66	0.94	0.12	56,101,126,149	0
20	CLA	A	805	44/65	0.94	0.10	102,121,133,140	0
20	CLA	5	315	44/65	0.94	0.12	65,89,99,104	0
20	CLA	5	318	44/65	0.94	0.10	55,72,92,103	0
20	CLA	4	304	44/65	0.94	0.10	74,83,90,101	0
29	CHL	3	1014	47/66	0.95	0.12	83,110,124,131	0
23	LHG	7	1016	35/49	0.95	0.15	88,105,127,130	0
20	CLA	6	315	44/65	0.95	0.11	59,82,87,100	0
20	CLA	7	1014	44/65	0.95	0.09	73,91,97,111	0
20	CLA	3	1008	44/65	0.95	0.09	111,129,174,202	0
20	CLA	3	1005	44/65	0.95	0.10	78,106,124,128	0
20	CLA	7	1004	44/65	0.95	0.10	40,58,84,93	0
20	CLA	4	306	44/65	0.95	0.08	71,80,88,96	0

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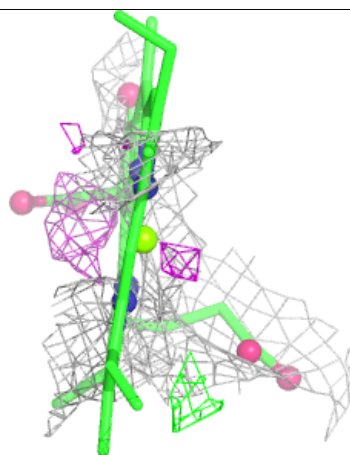
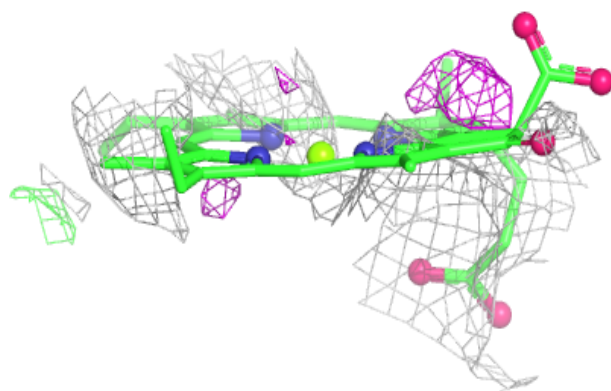
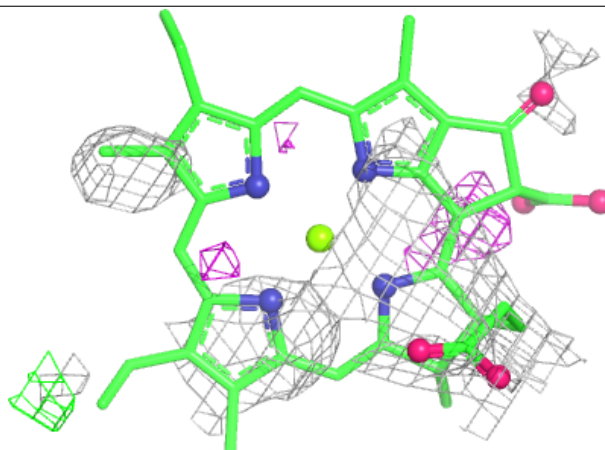
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	3	1016	44/65	0.95	0.10	66,74,123,169	0
20	CLA	6	305	44/65	0.95	0.08	44,58,76,90	0
29	CHL	5	314	51/66	0.96	0.10	64,82,117,121	0
20	CLA	B	805	44/65	0.96	0.08	87,109,132,149	0
21	SF4	A	841	8/8	0.98	0.03	110,119,124,131	0
21	SF4	C	1001	8/8	0.98	0.03	136,146,148,158	0
21	SF4	C	1002	8/8	0.99	0.03	143,149,158,161	0

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

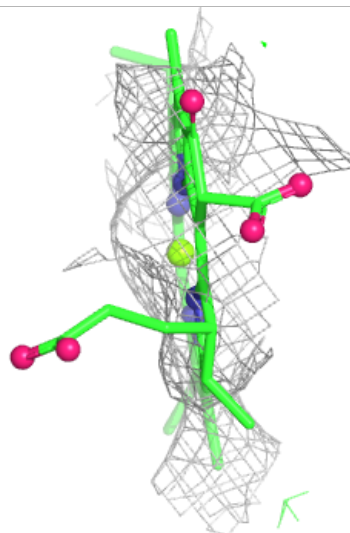
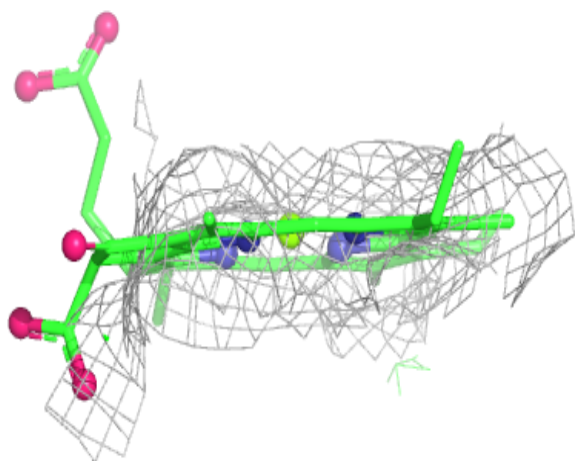
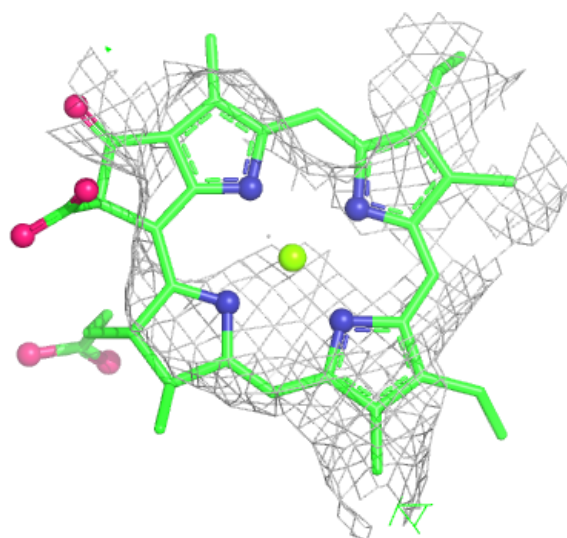
Electron density around CLA L 204:

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



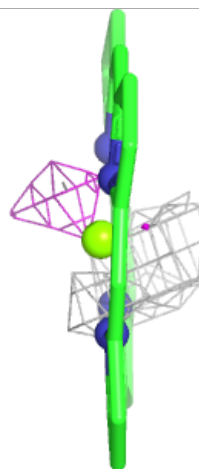
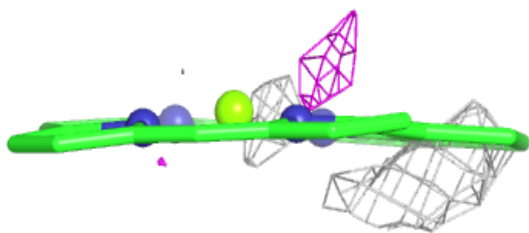
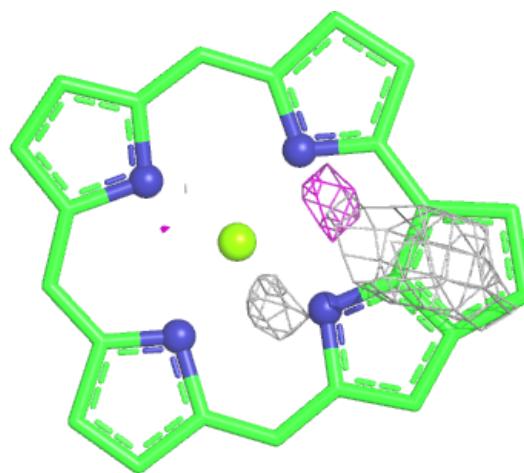
Electron density around CLA K 201:

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



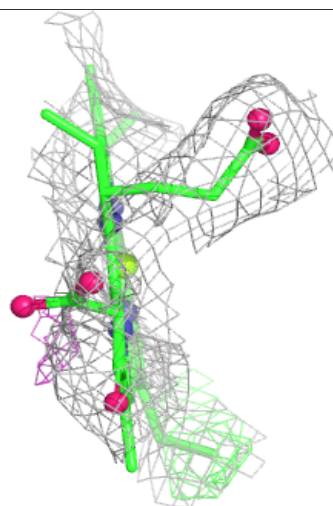
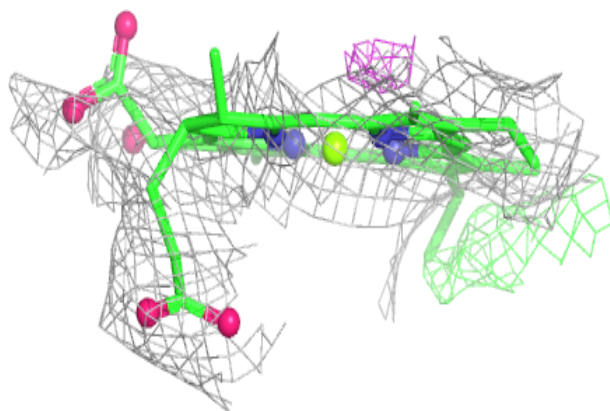
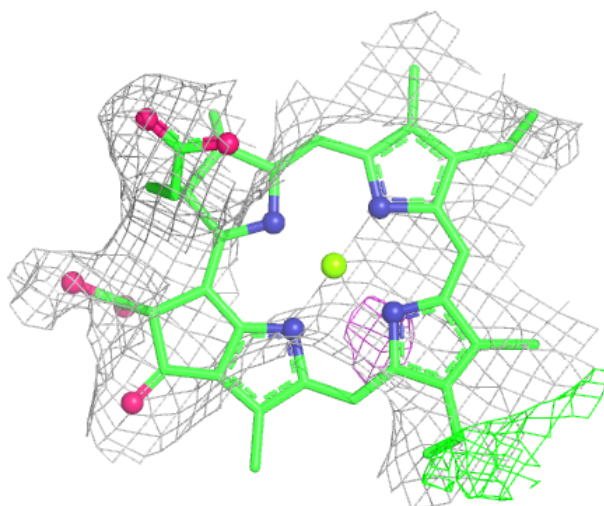
Electron density around CLA K 202:

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



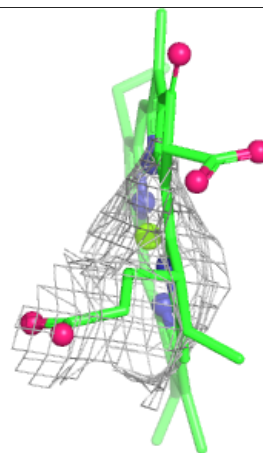
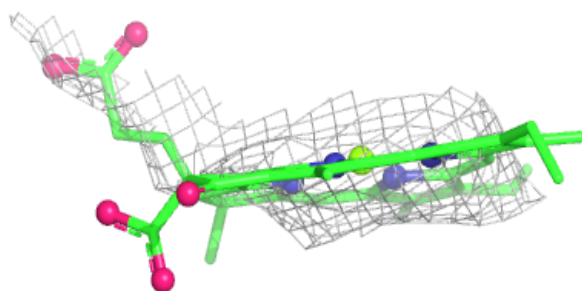
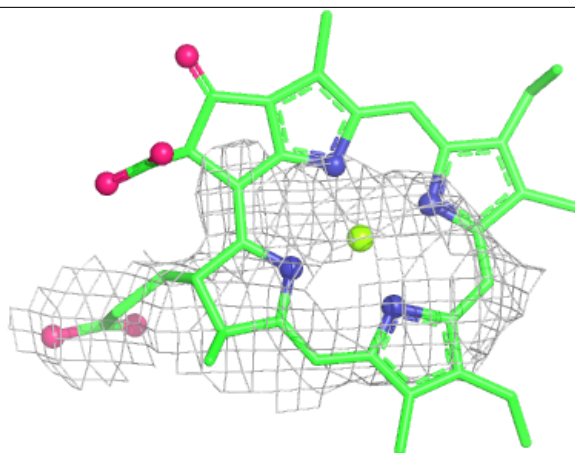
Electron density around CLA G 203:

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



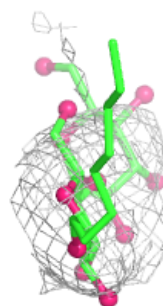
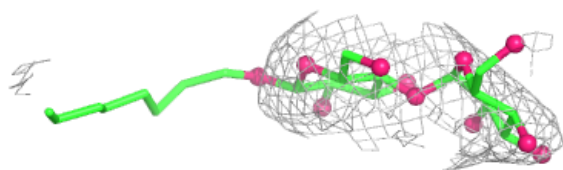
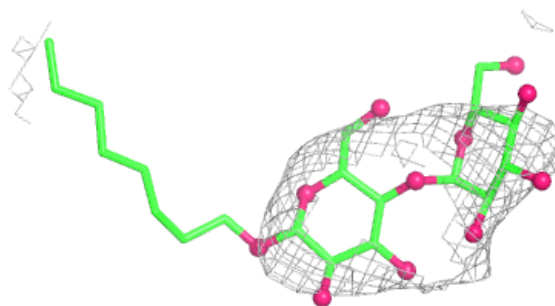
Electron density around CLA G 201:

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



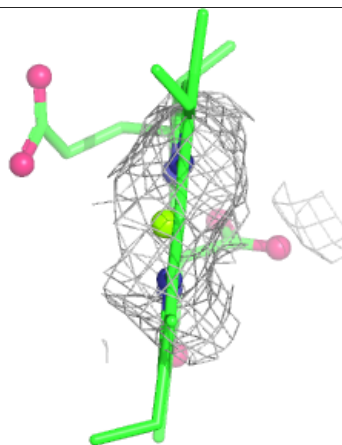
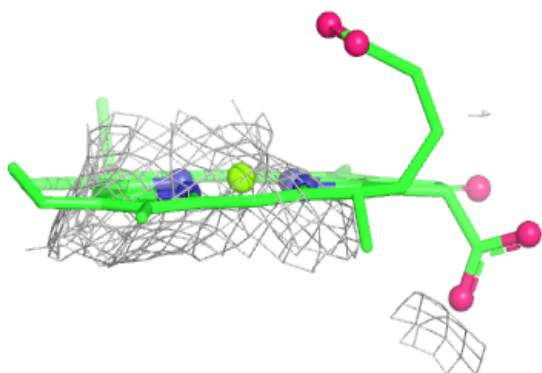
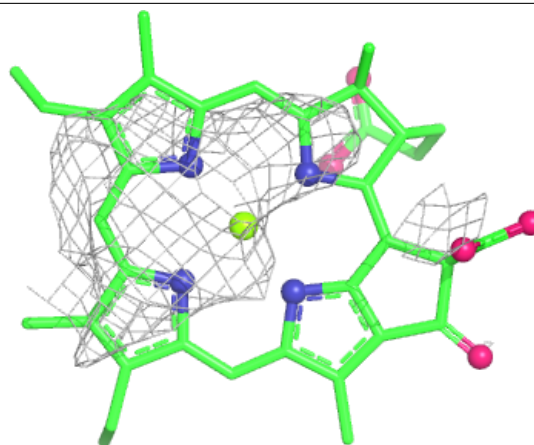
Electron density around LMT B 849:

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



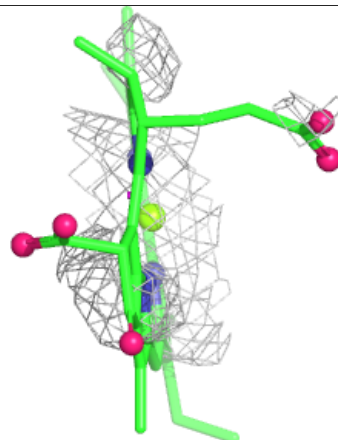
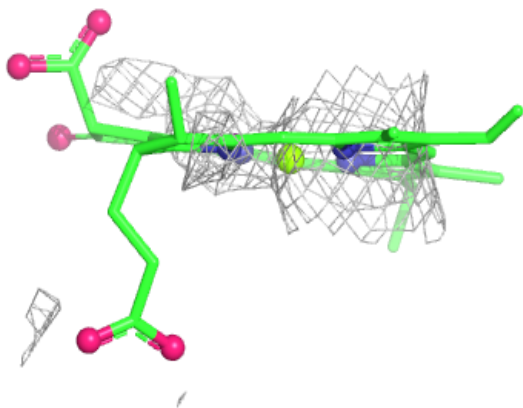
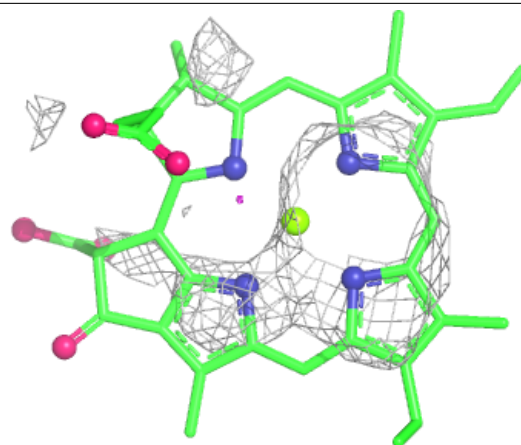
Electron density around CLA L 202:

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



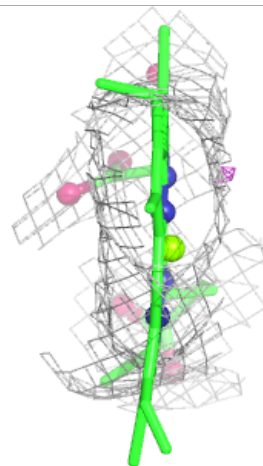
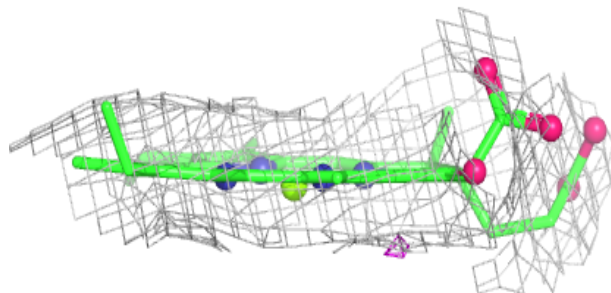
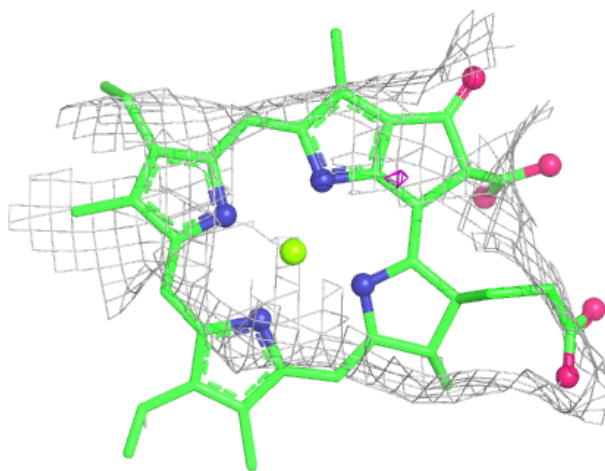
Electron density around CLA L 203:

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



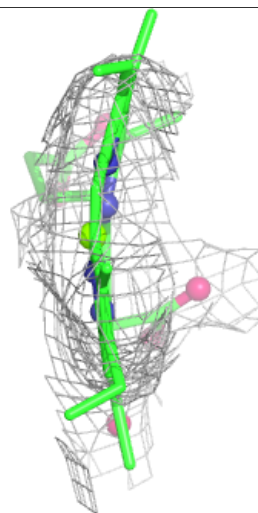
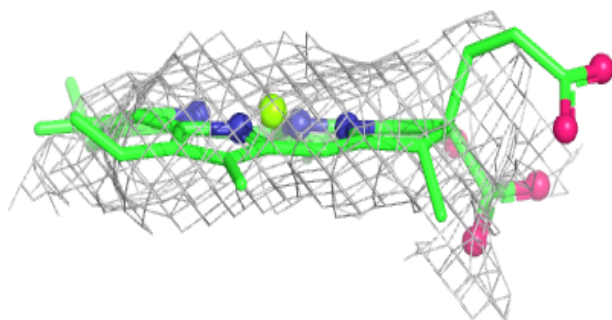
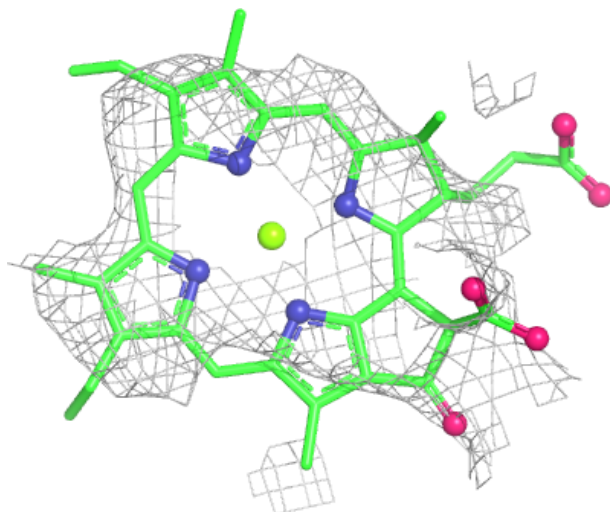
Electron density around CLA G 202:

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



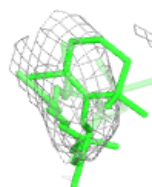
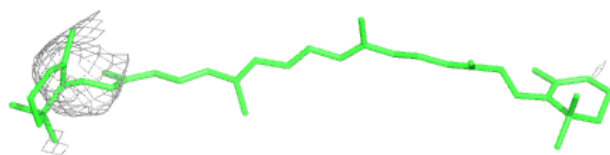
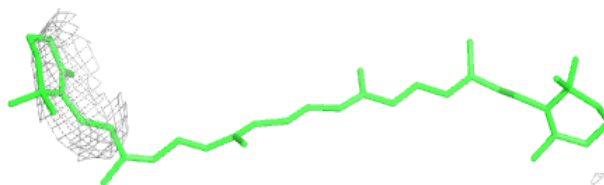
Electron density around CLA B 813:

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

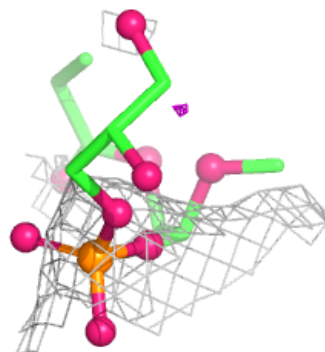
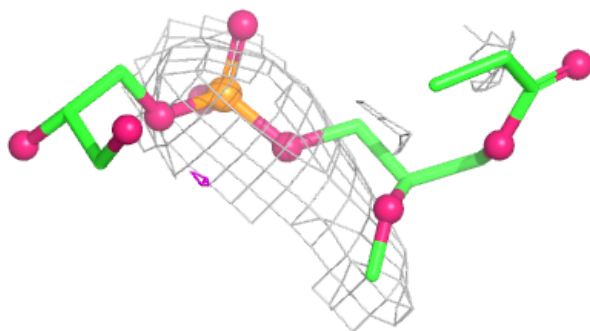
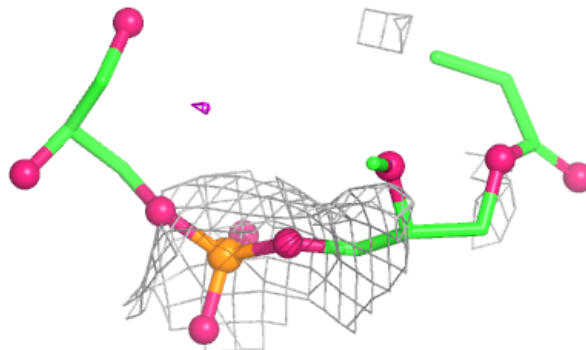


Electron density around BCR H 201:

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

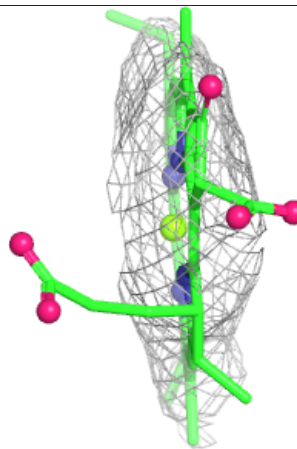
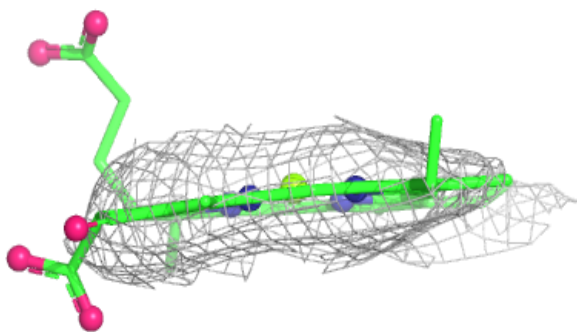
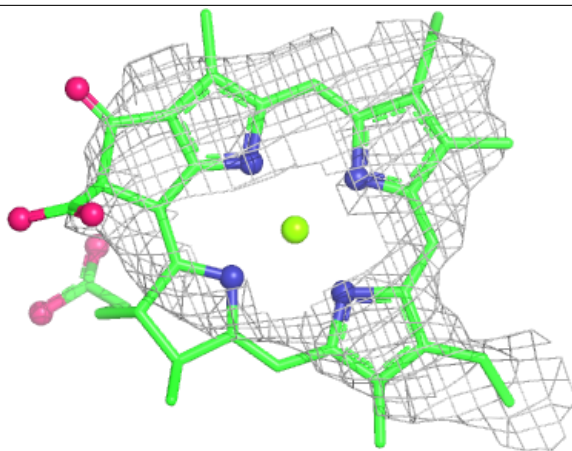
**Electron density around LHG 3 1019:**

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



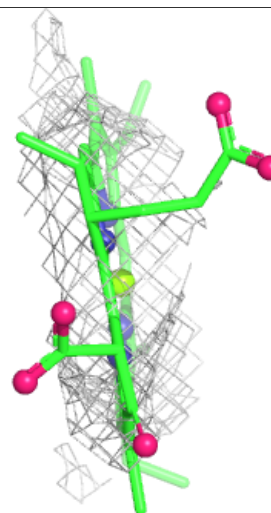
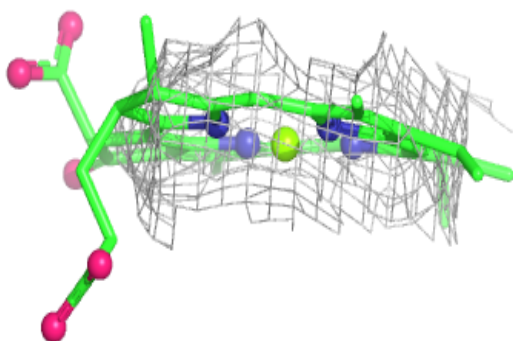
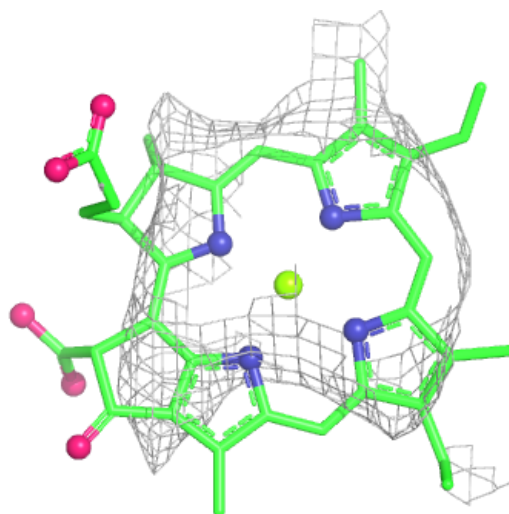
Electron density around CLA B 815:

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



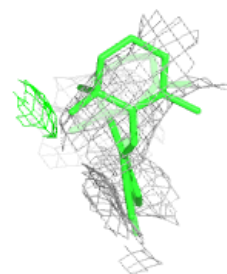
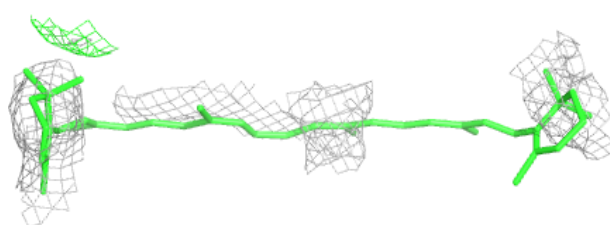
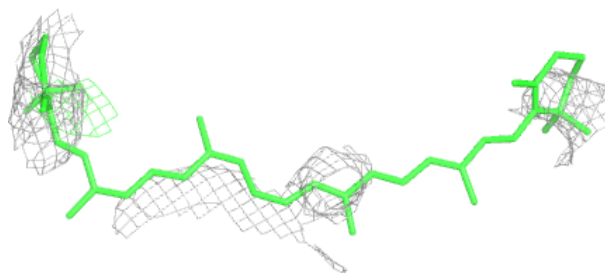
Electron density around CLA A 840:

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

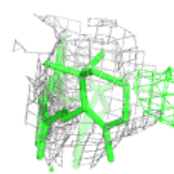
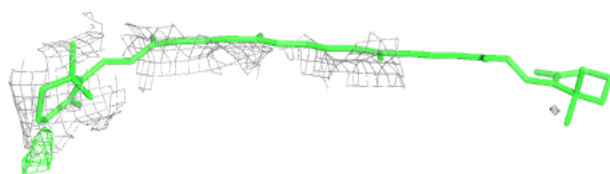
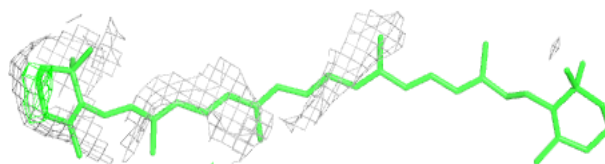


Electron density around BCR I 201:

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

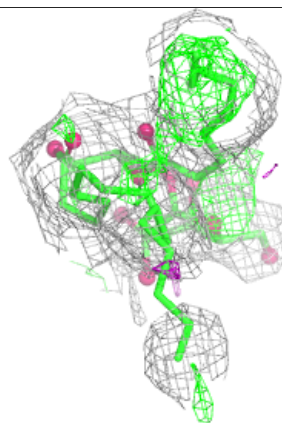
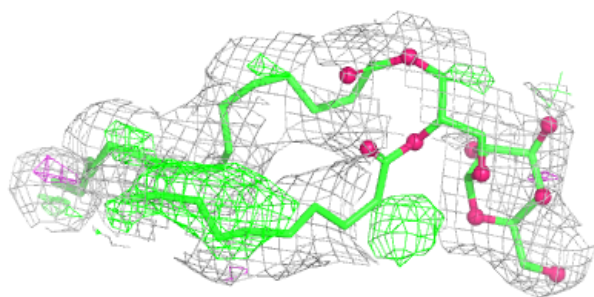
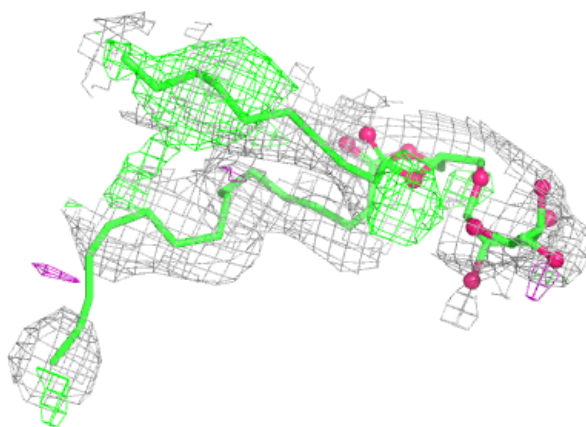
**Electron density around BCR A 850:**

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

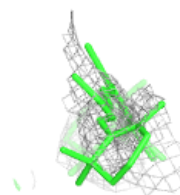
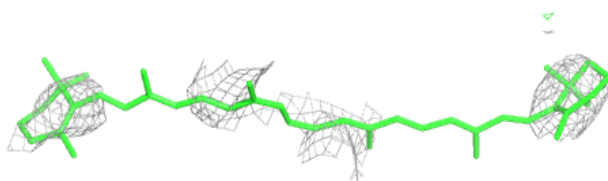
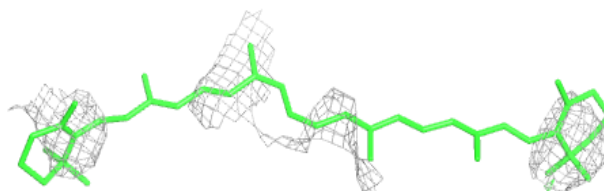


Electron density around LMG 5 324:

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

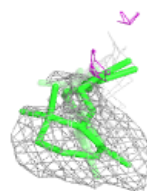
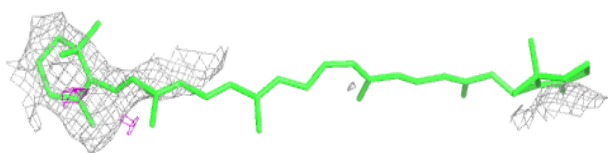
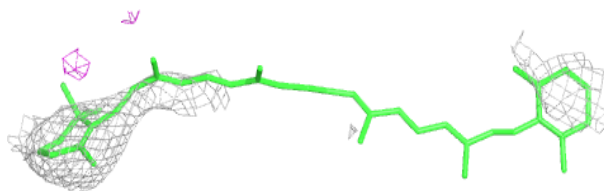
**Electron density around BCR G 204:**

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

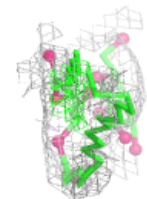
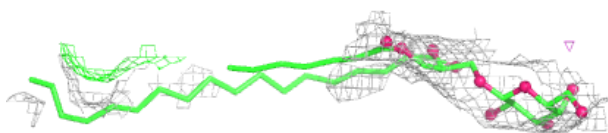
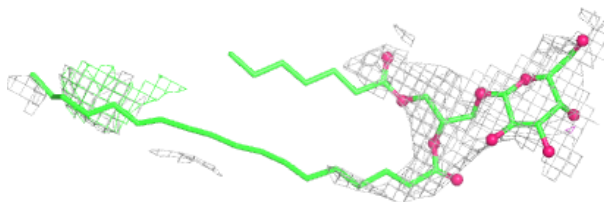


Electron density around BCR G 205:

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

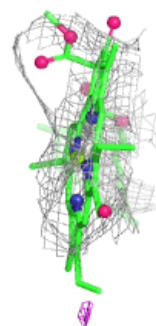
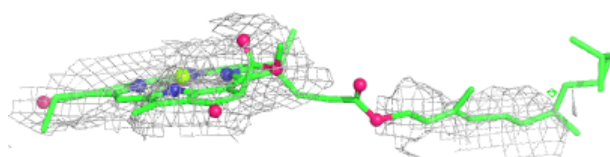
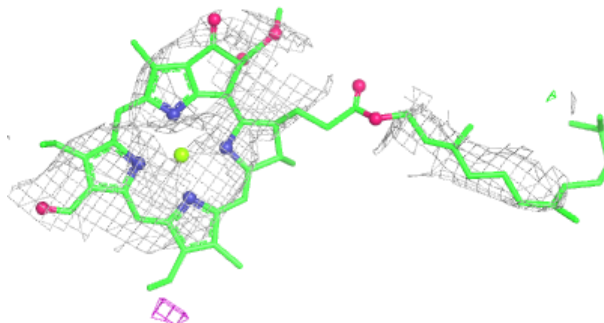
**Electron density around LMG 8 319:**

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

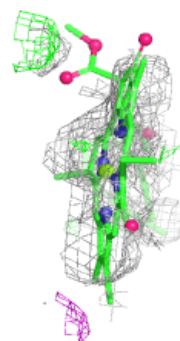
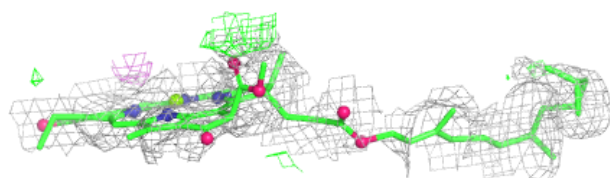
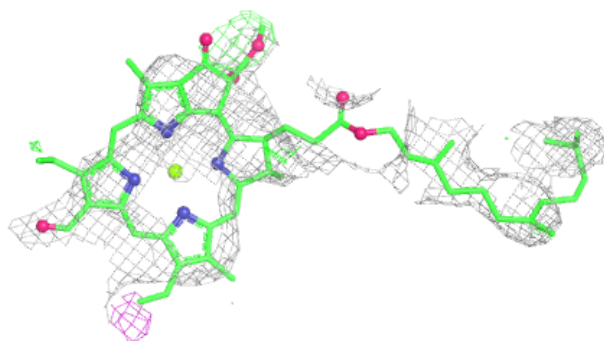


Electron density around CHL 0 317:

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

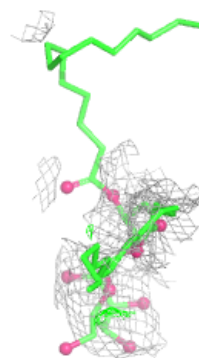
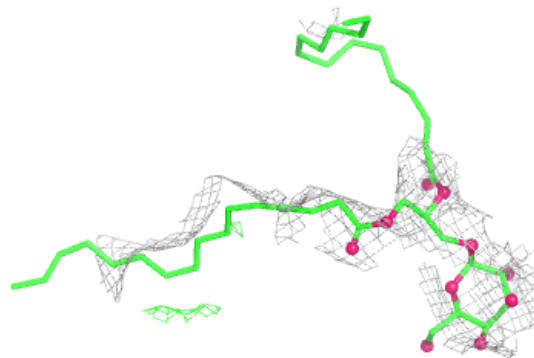
**Electron density around CHL 1 1015:**

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

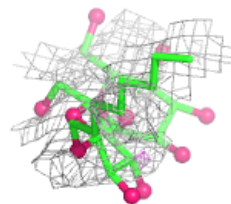
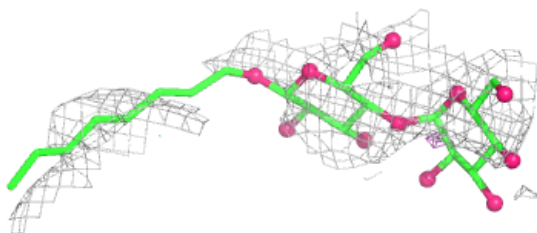
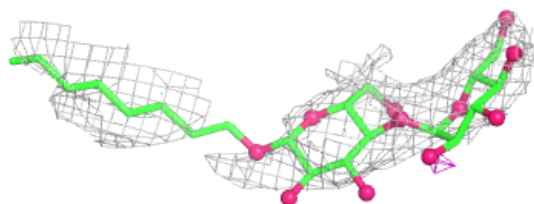


Electron density around LMG 0 303:

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

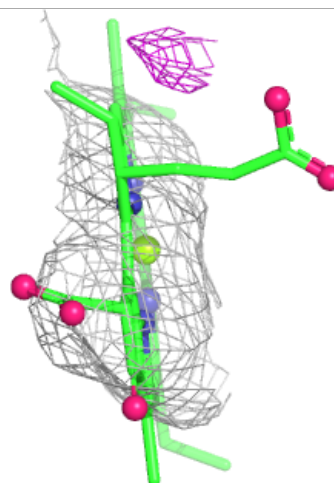
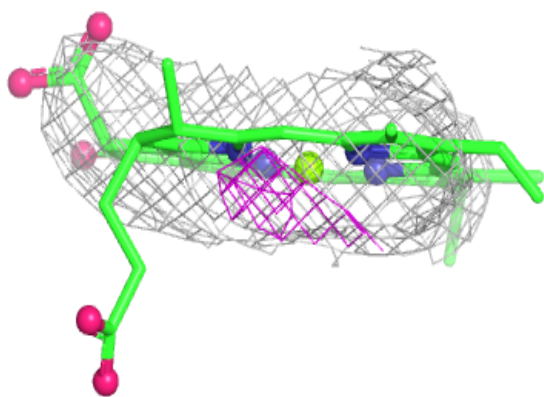
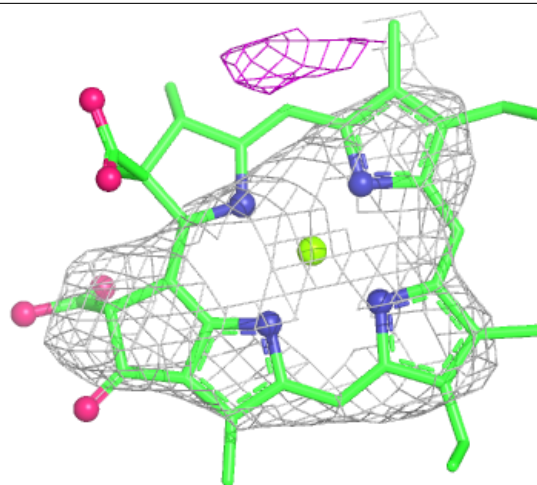
**Electron density around LMT 3 1018:**

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



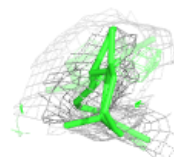
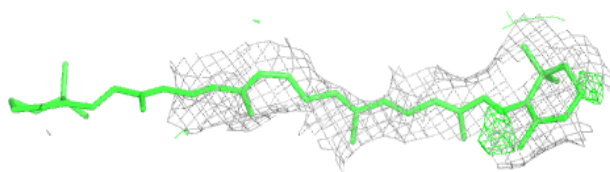
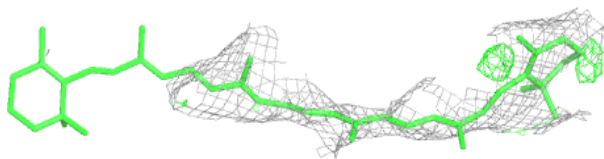
Electron density around CLA A 822:

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



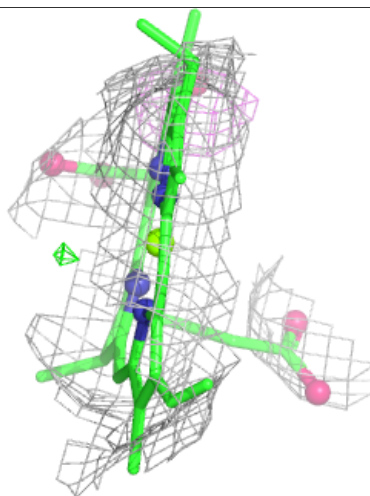
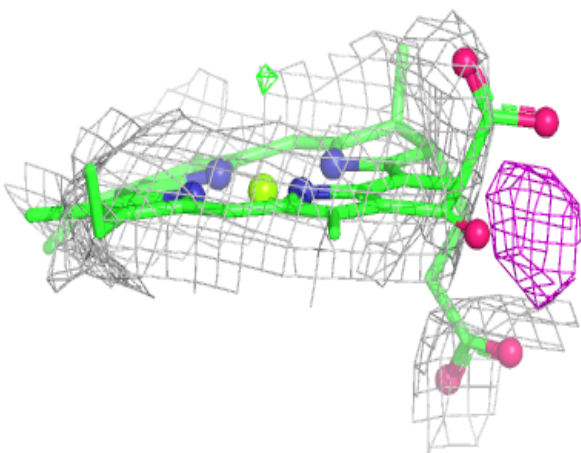
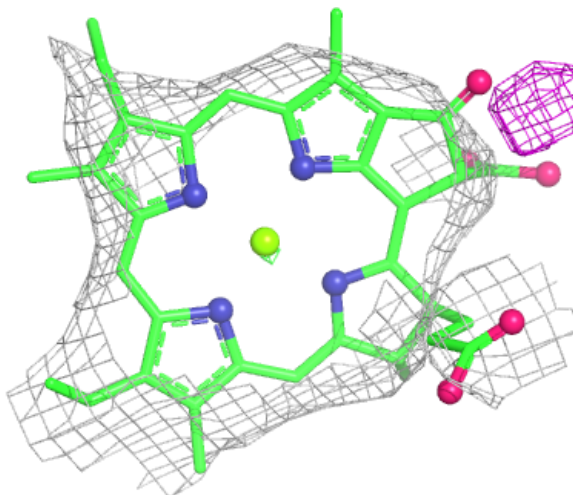
Electron density around BCR 1 1001:

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



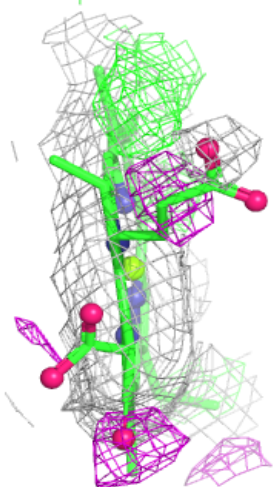
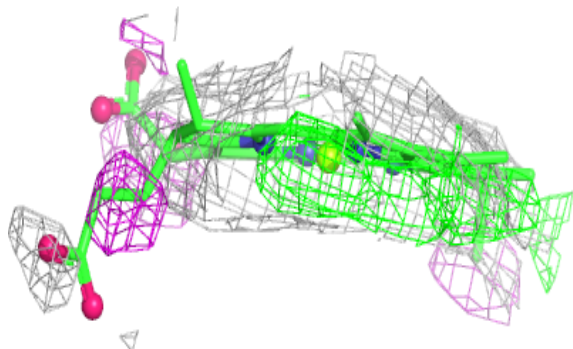
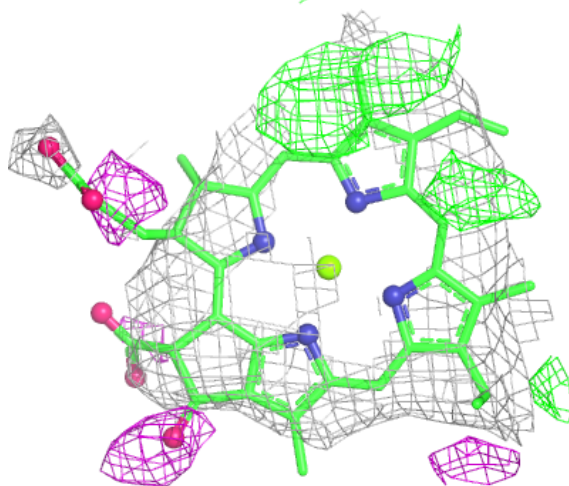
Electron density around CLA B 836:

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



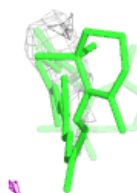
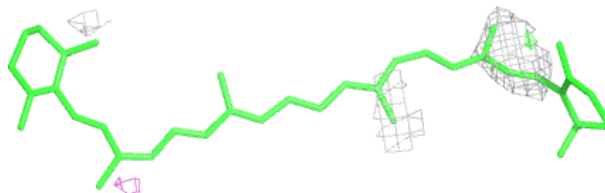
Electron density around CLA 5 312:

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

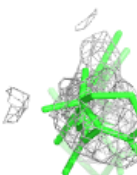
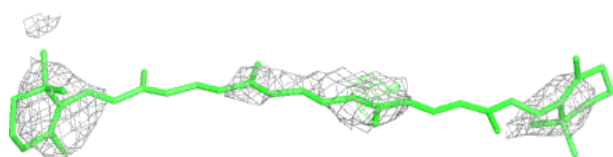
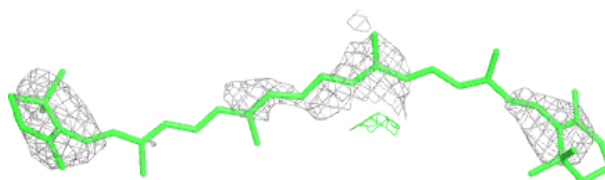


Electron density around BCR B 845:

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

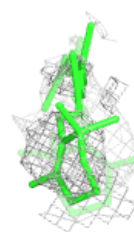
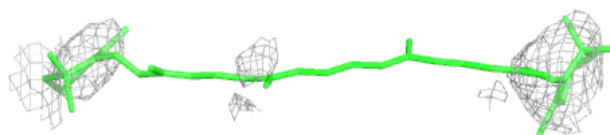
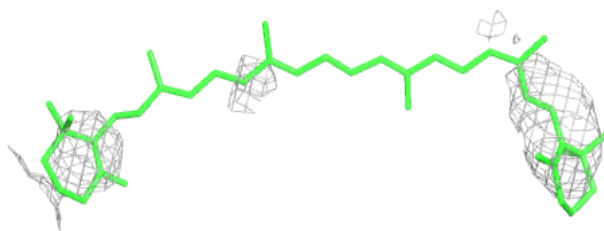
**Electron density around BCR B 847:**

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



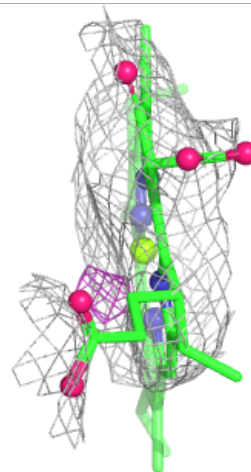
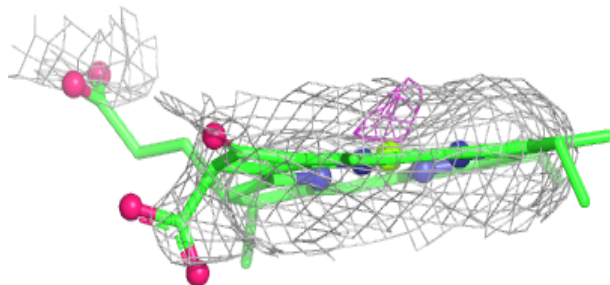
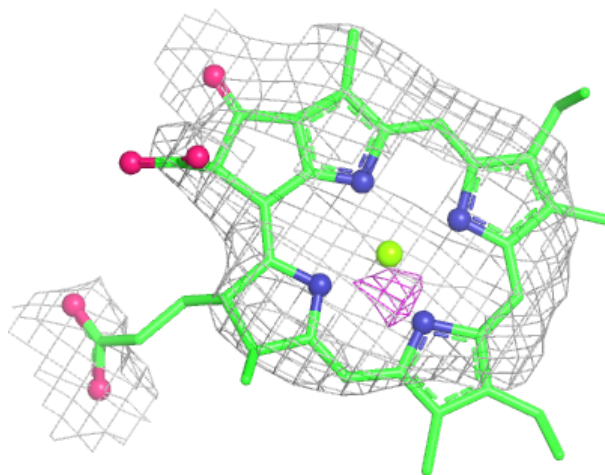
Electron density around BCR B 844:

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



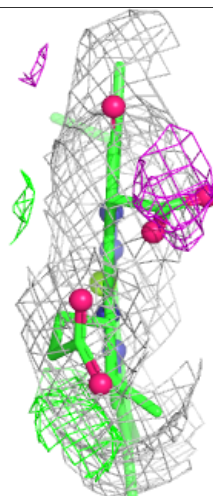
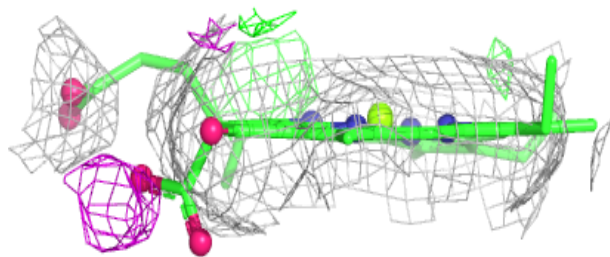
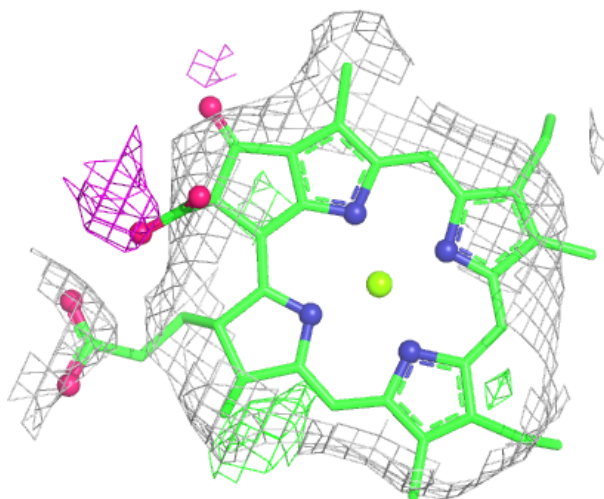
Electron density around CLA B 812:

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



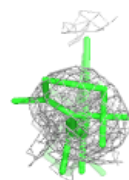
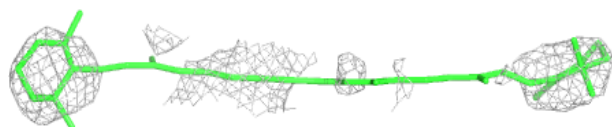
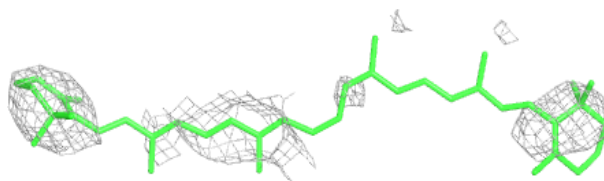
Electron density around CLA F 303:

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



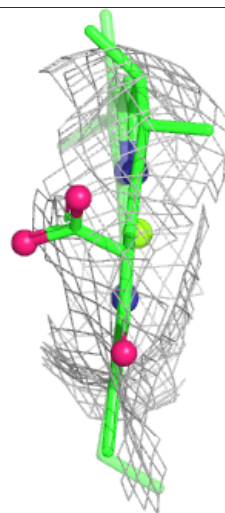
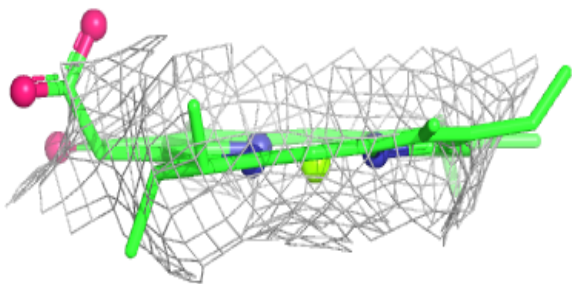
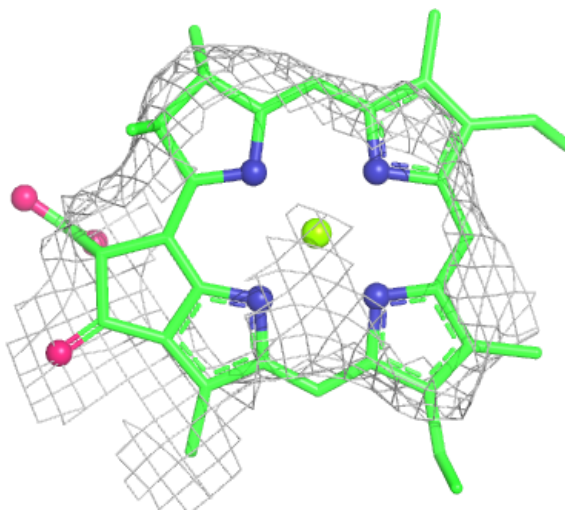
Electron density around BCR A 846:

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



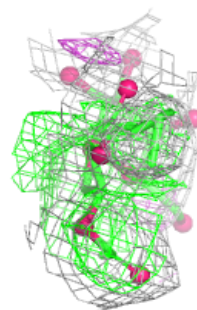
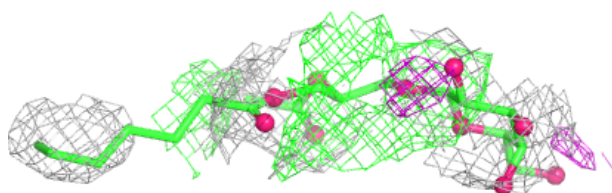
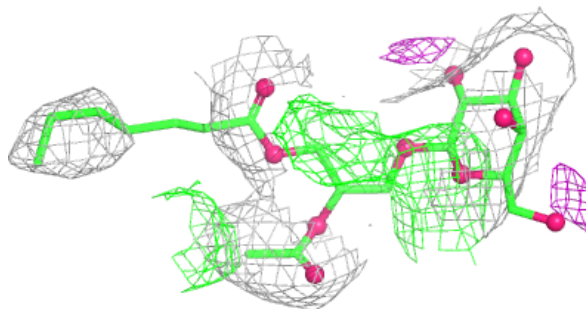
Electron density around CLA 3 1011:

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

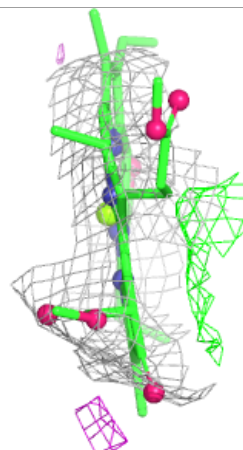
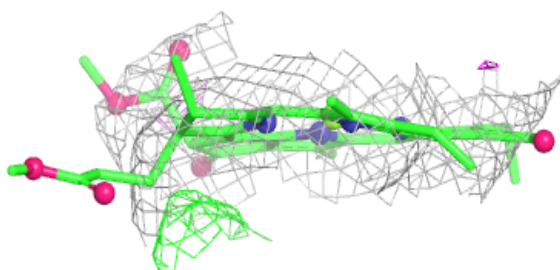
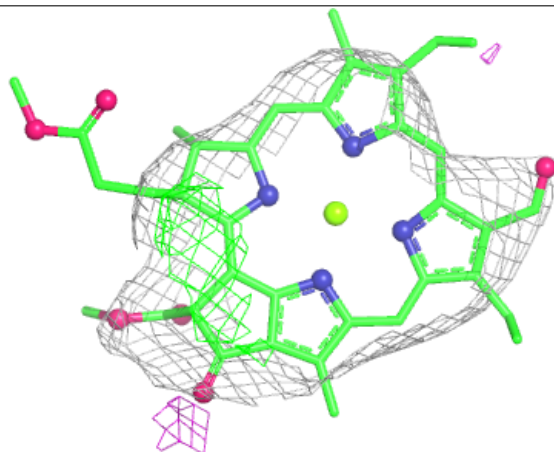


Electron density around LMG 8 318:

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

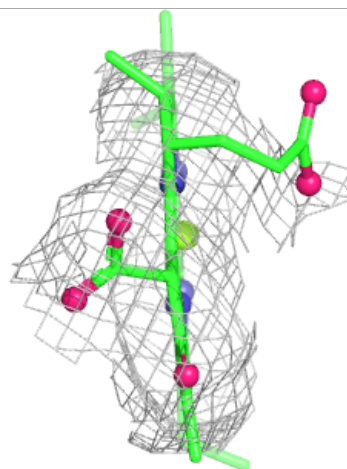
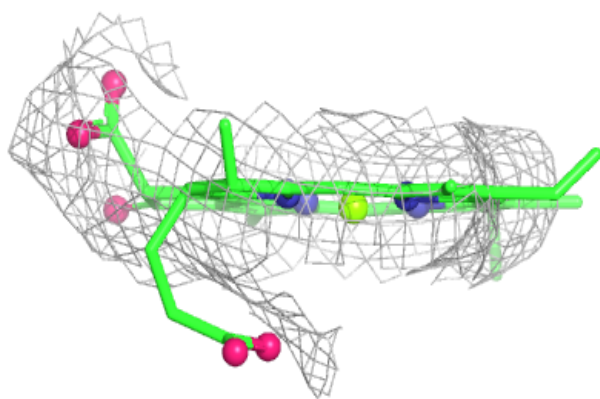
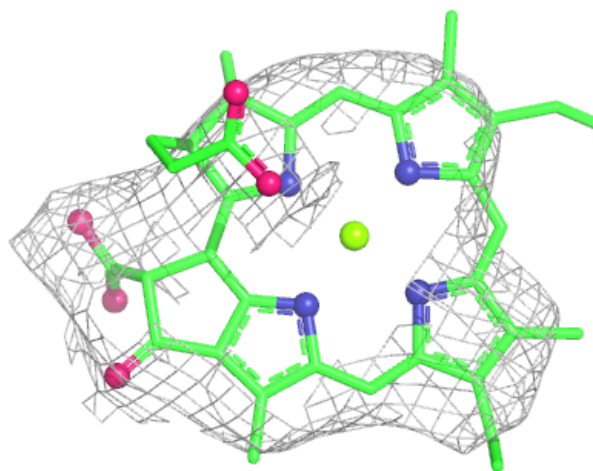
**Electron density around CHL 0 314:**

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



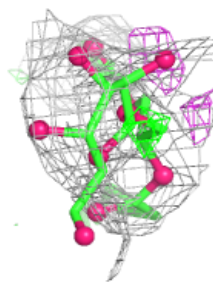
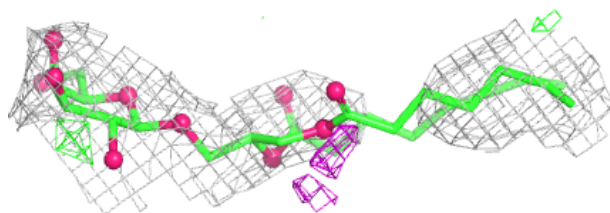
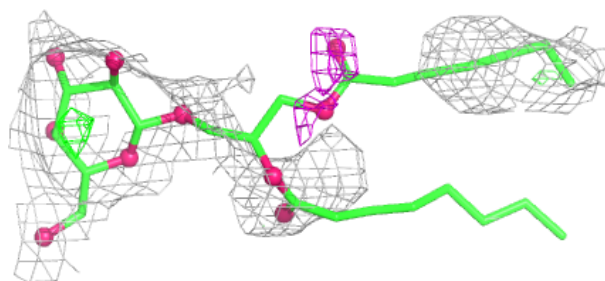
Electron density around CLA 3 1012:

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



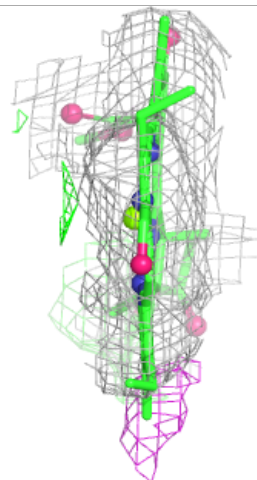
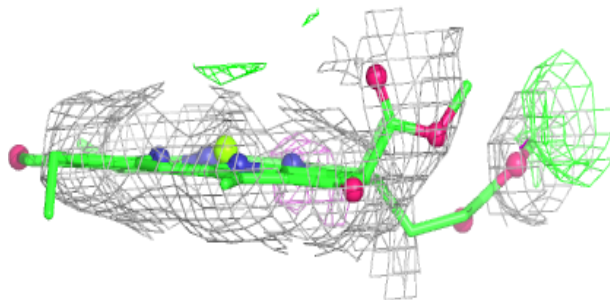
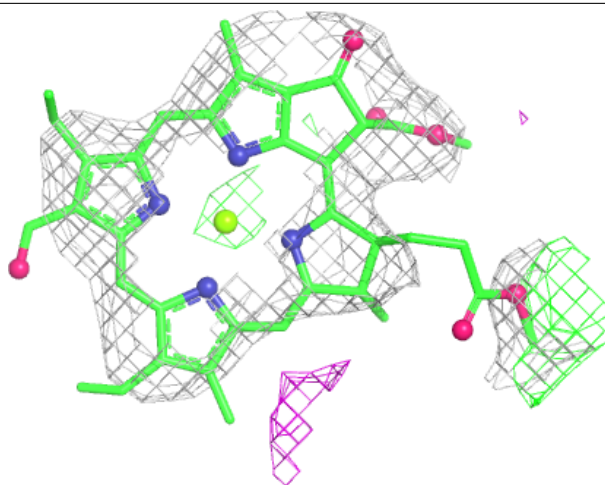
Electron density around LMG 4 318:

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



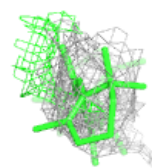
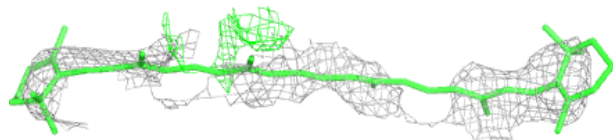
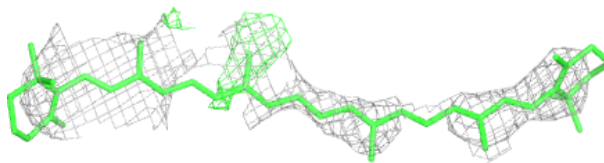
Electron density around CHL 4 312:

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

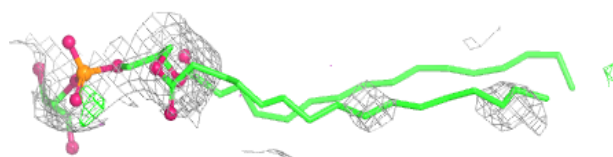
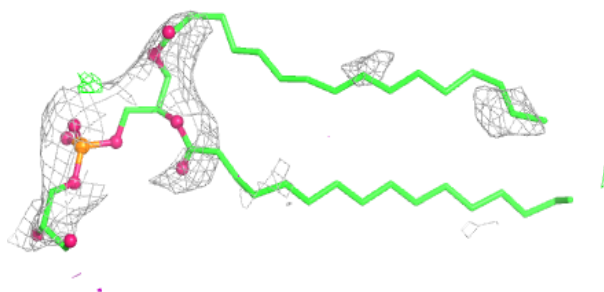


Electron density around BCR A 844:

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

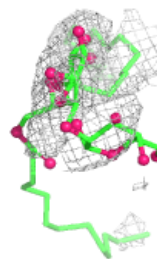
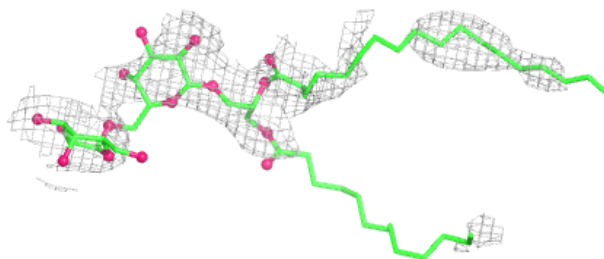
**Electron density around LHG 8 301:**

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

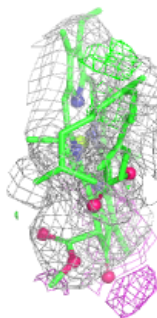
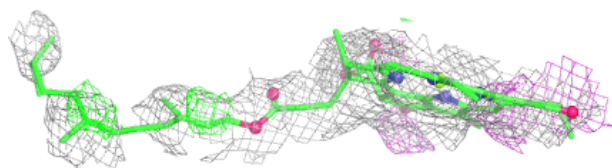
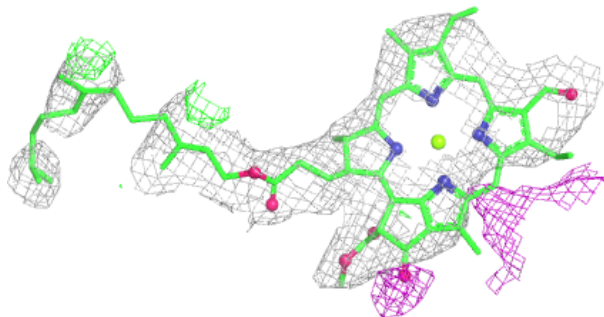


Electron density around DGD B 848:

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

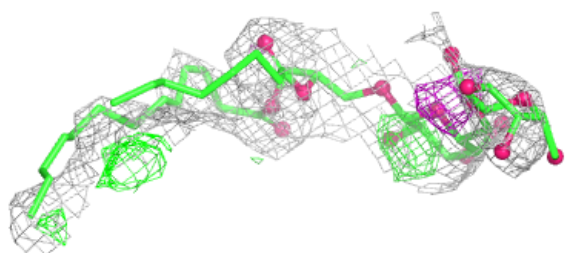
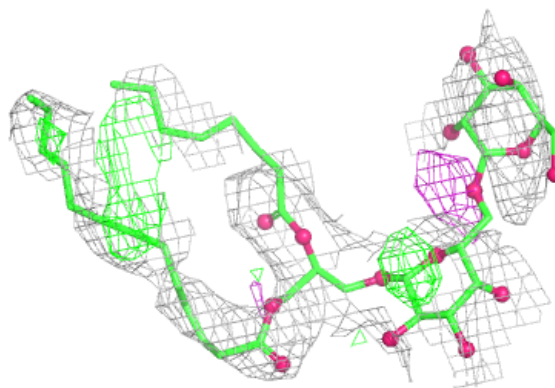
**Electron density around CHL 8 317:**

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



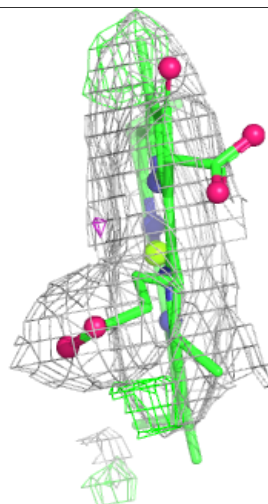
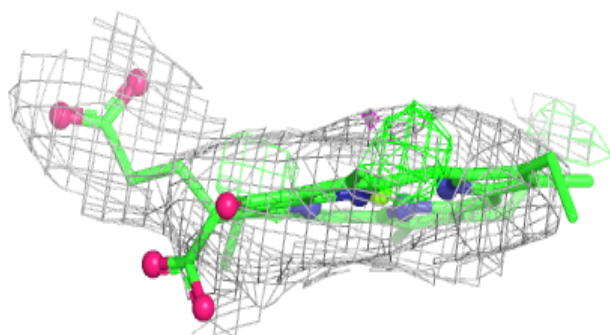
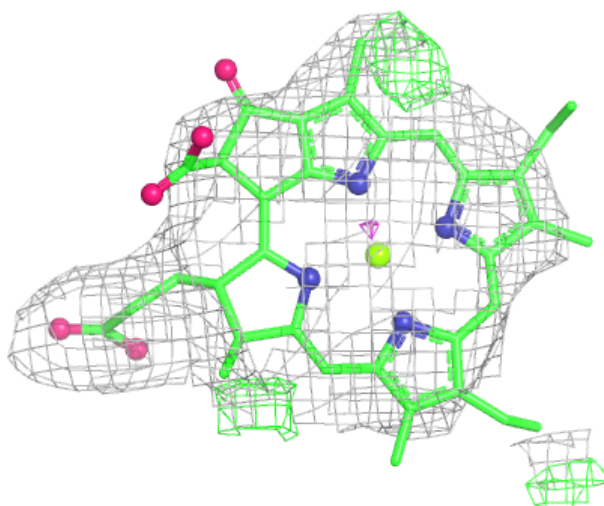
Electron density around DGD 5 319:

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



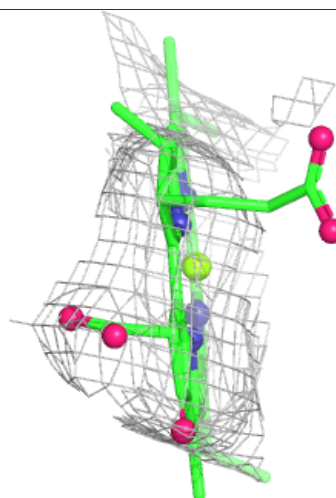
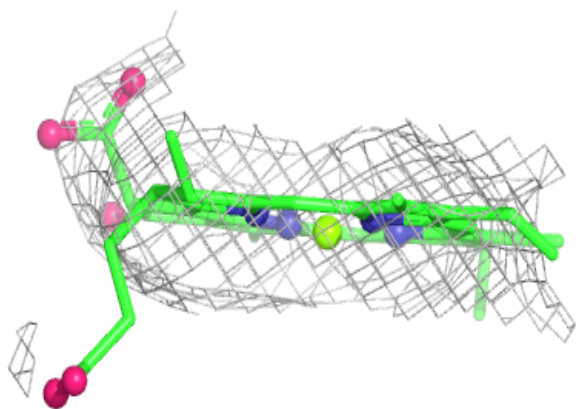
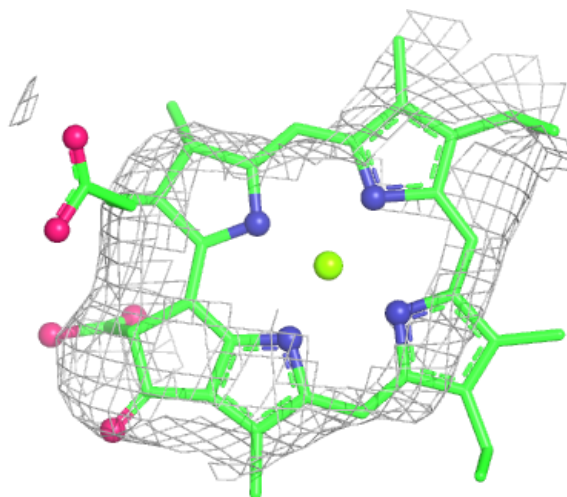
Electron density around CLA 5 323:

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



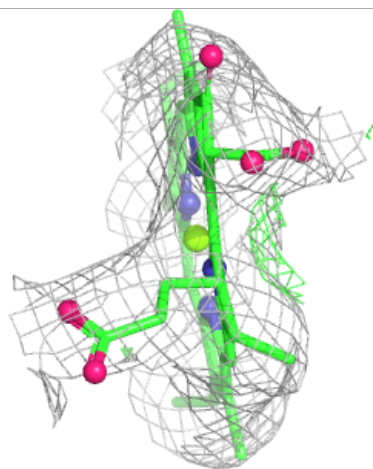
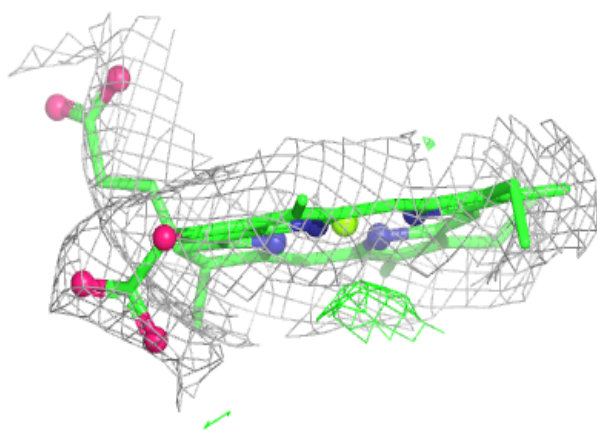
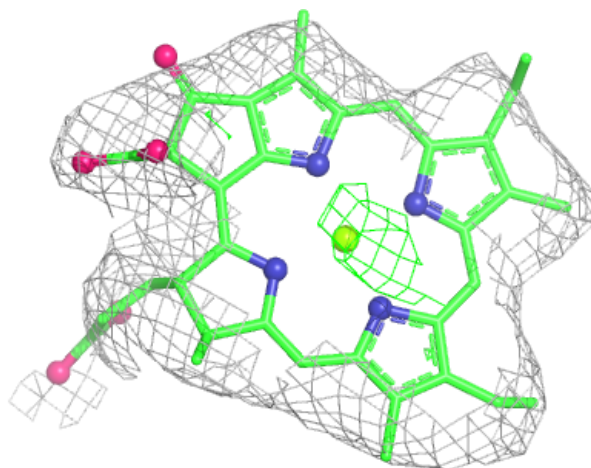
Electron density around CLA A 821:

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



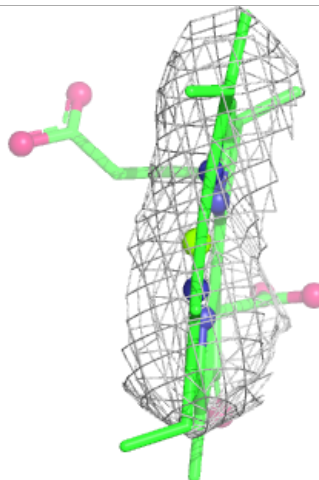
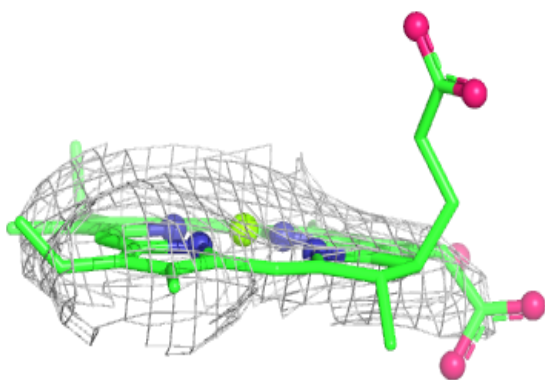
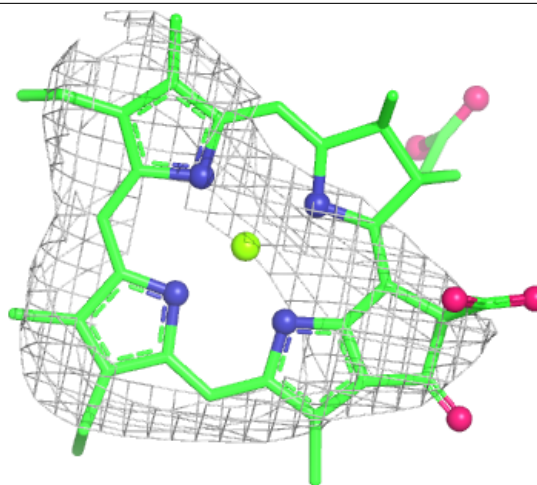
Electron density around CLA 5 322:

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



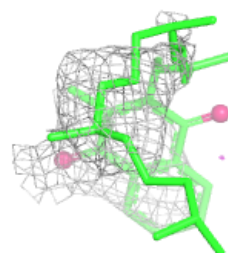
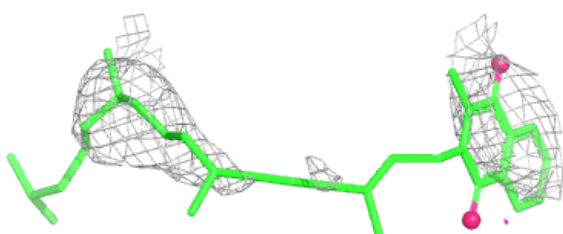
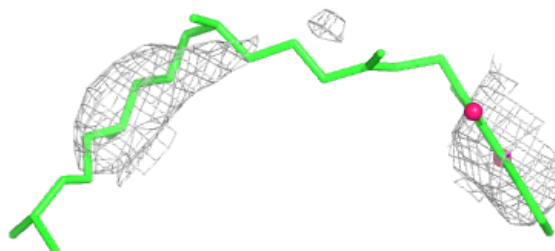
Electron density around CLA B 823:

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

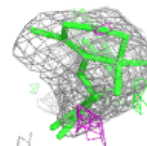
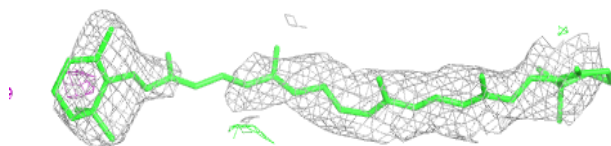
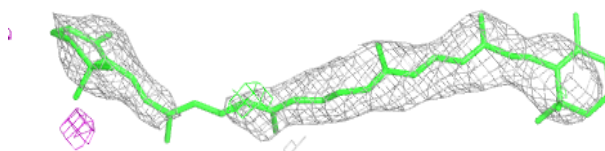


Electron density around PQN B 842:

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

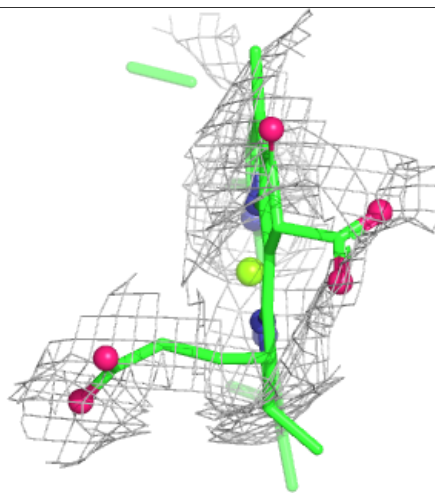
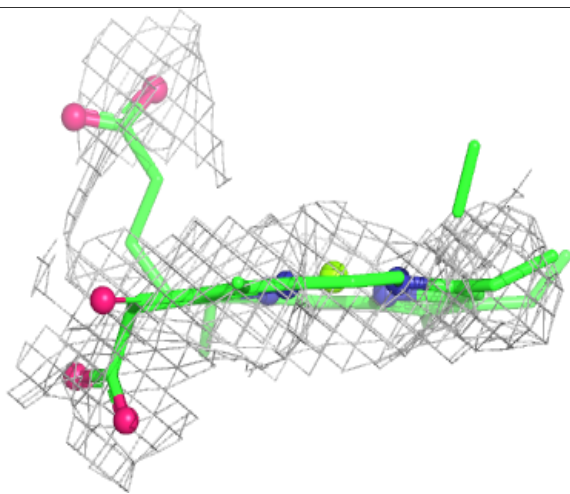
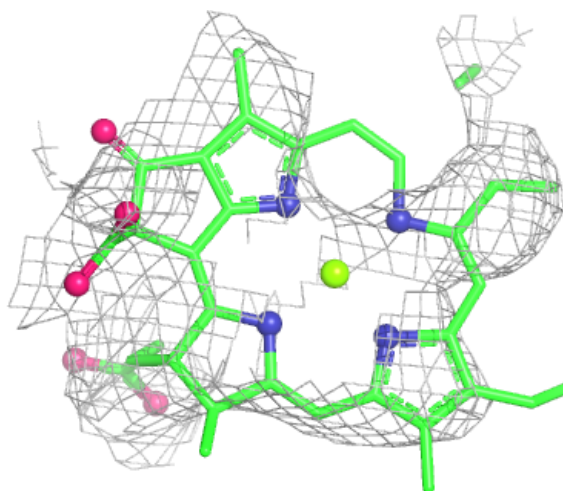
**Electron density around BCR 8 302:**

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



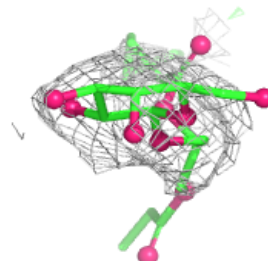
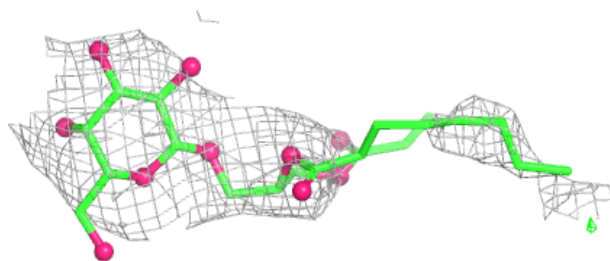
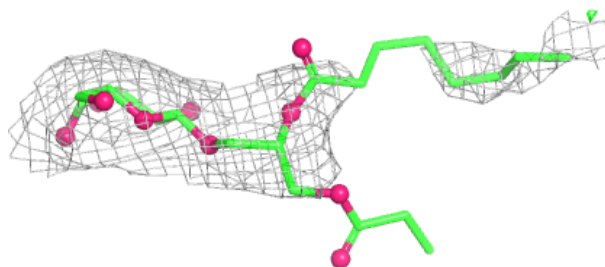
Electron density around CLA B 850:

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

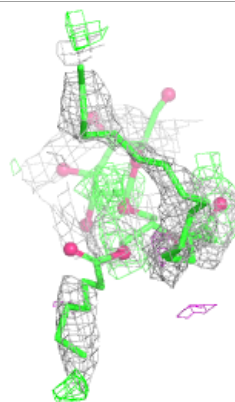
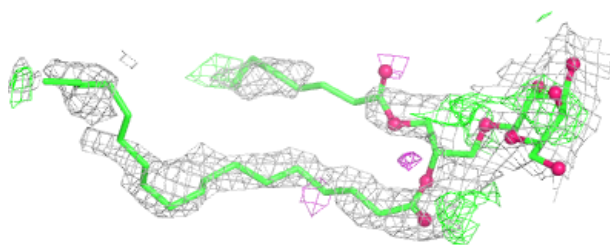
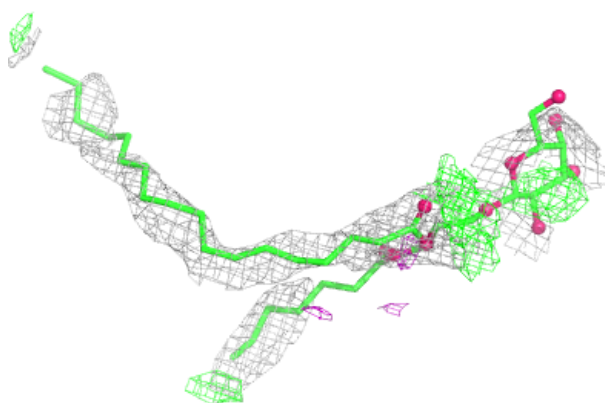


Electron density around LMG J 101:

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

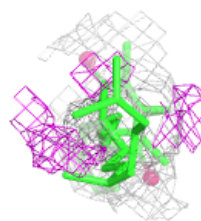
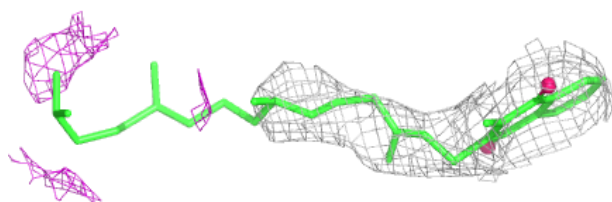
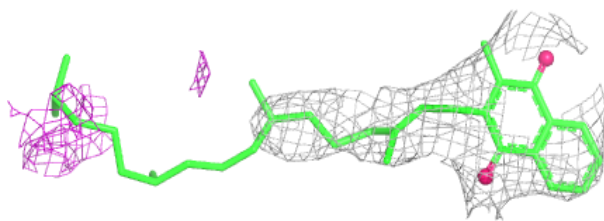
**Electron density around LMG 6 319:**

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



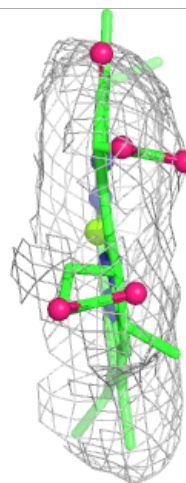
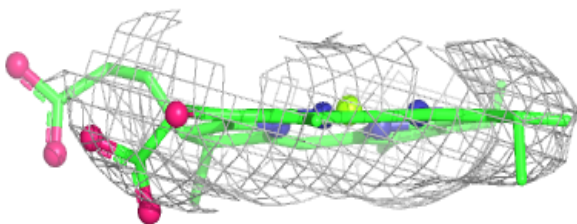
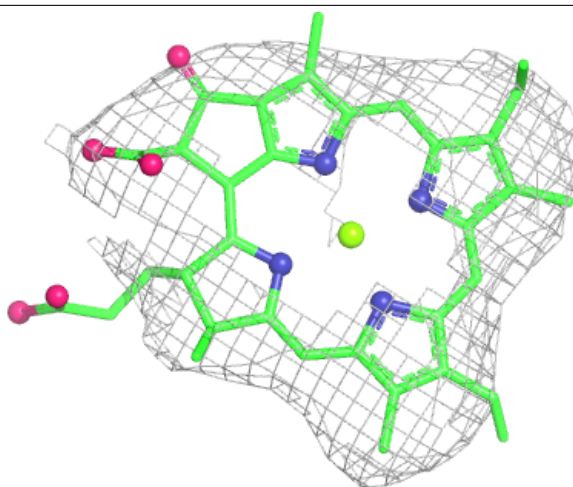
Electron density around PQN A 842:

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



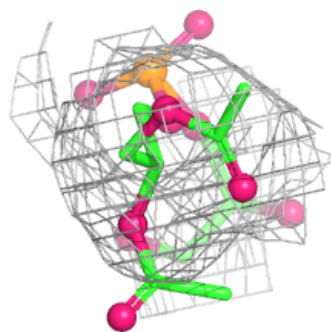
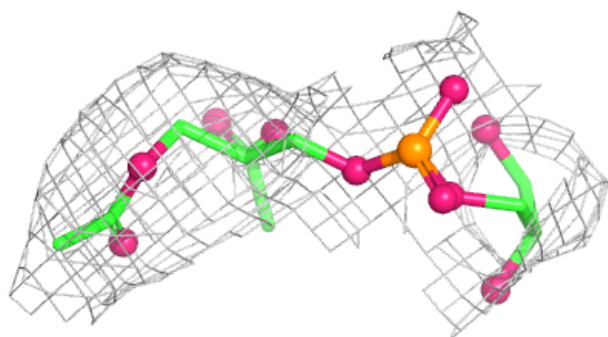
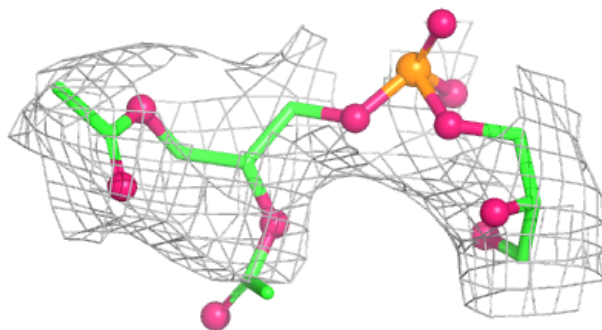
Electron density around CLA A 831:

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



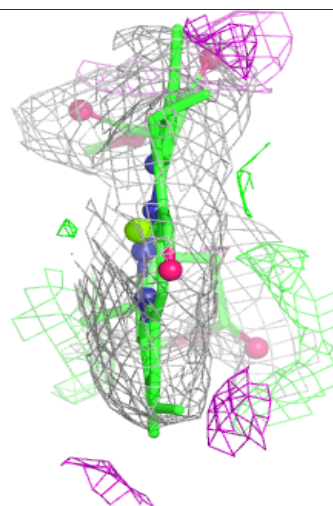
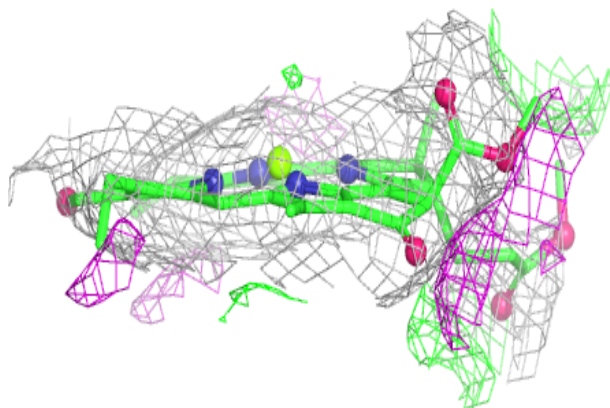
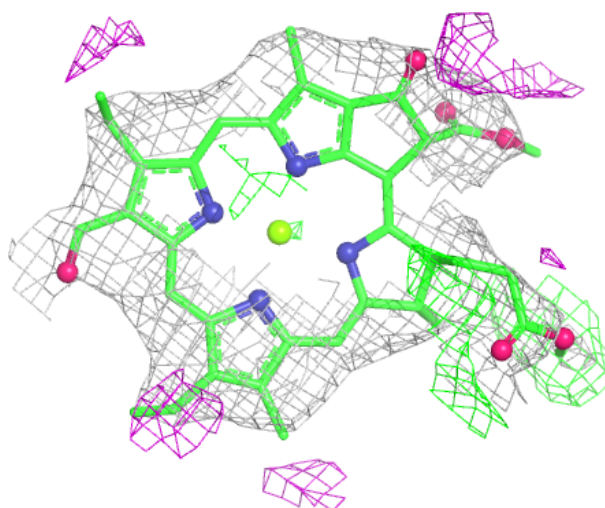
Electron density around LHG 0 302:

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



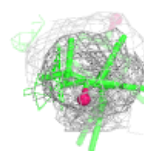
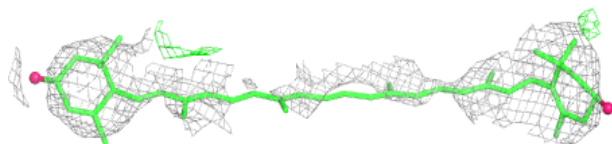
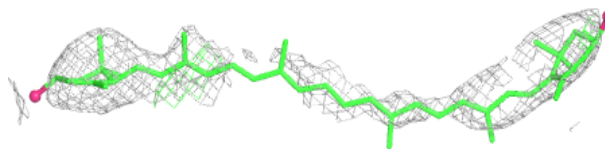
Electron density around CHL 5 313:

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

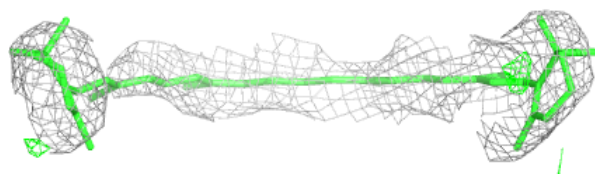
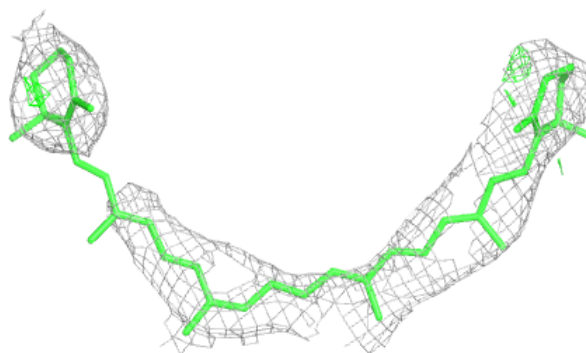


Electron density around LUT 0 318:

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

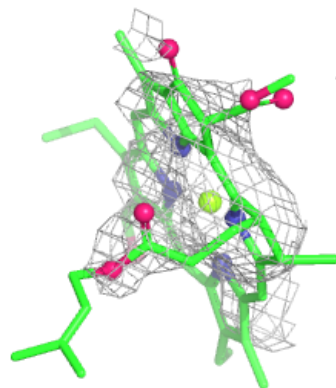
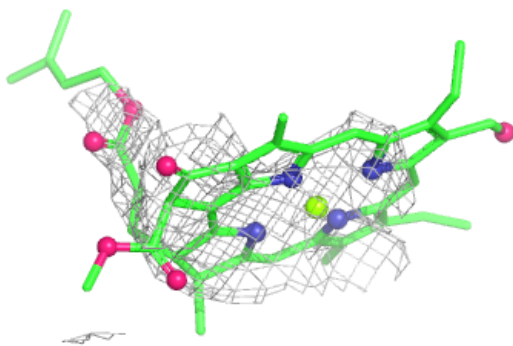
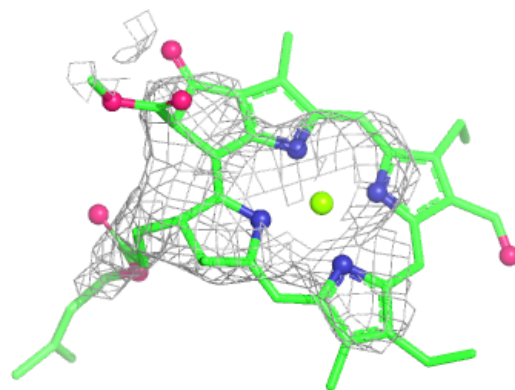
**Electron density around BCR F 304:**

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



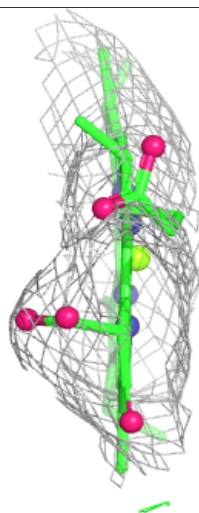
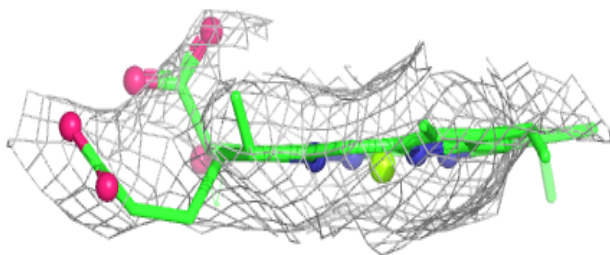
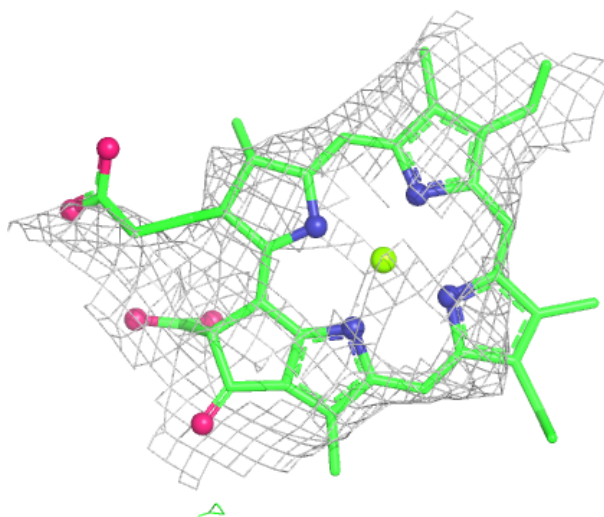
Electron density around CHL 0 315:

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



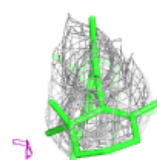
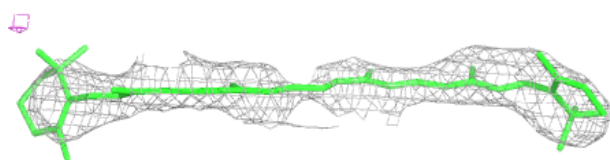
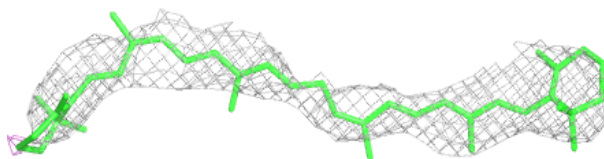
Electron density around CLA B 826:

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

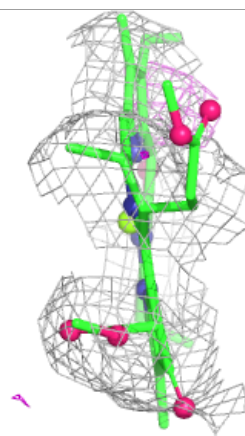
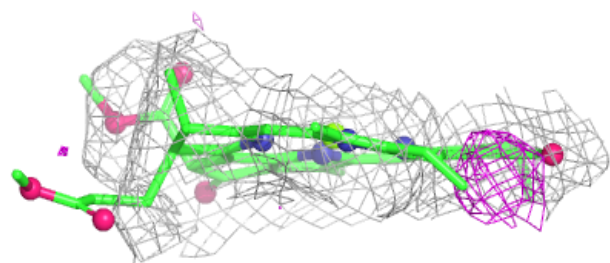
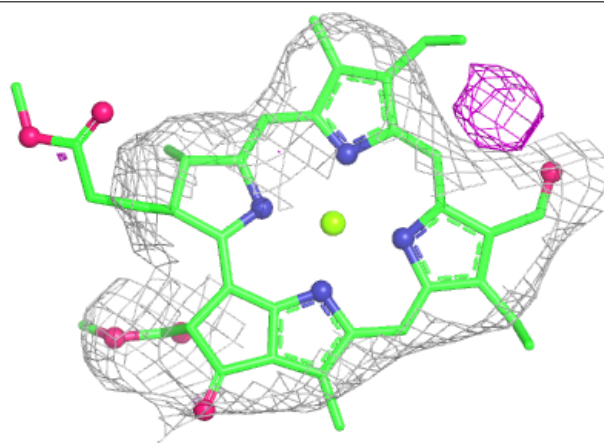


Electron density around BCR B 804:

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

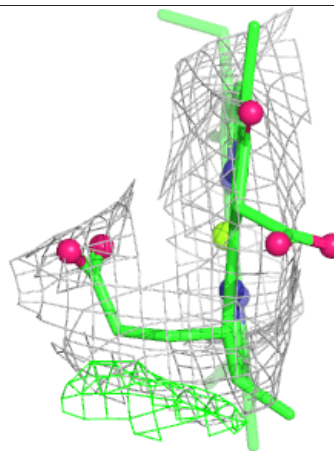
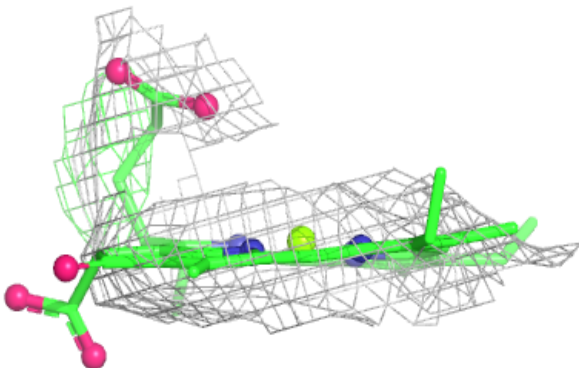
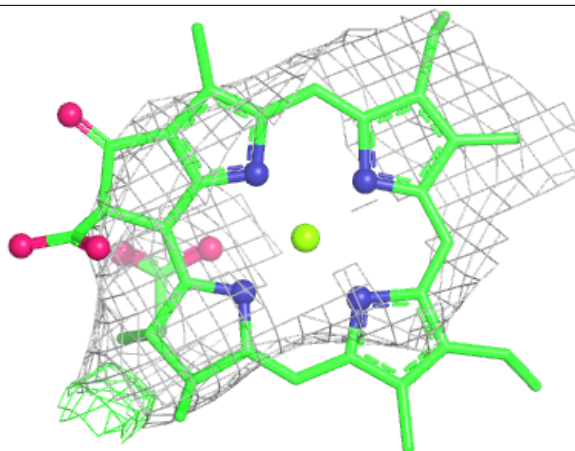
**Electron density around CHL 1 1012:**

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

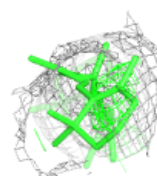
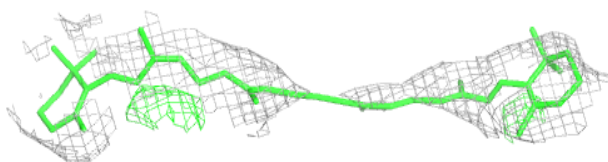


Electron density around CLA B 803:

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

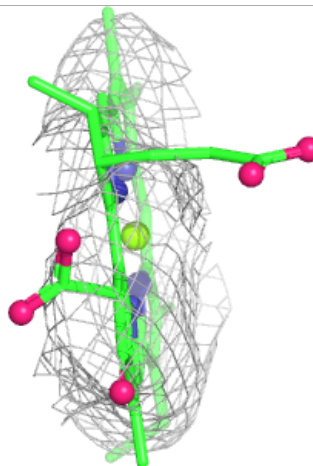
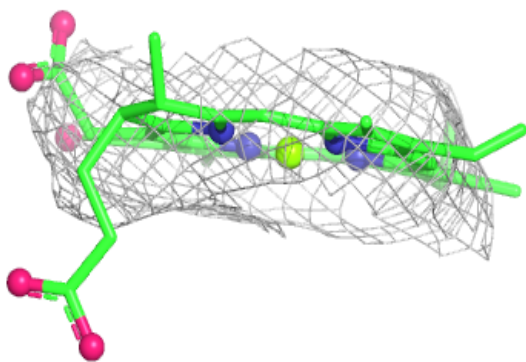
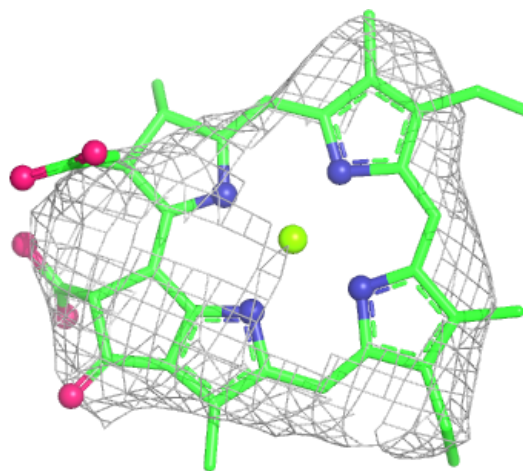
**Electron density around BCR A 845:**

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



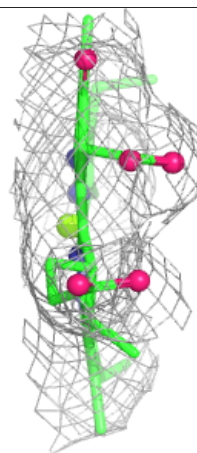
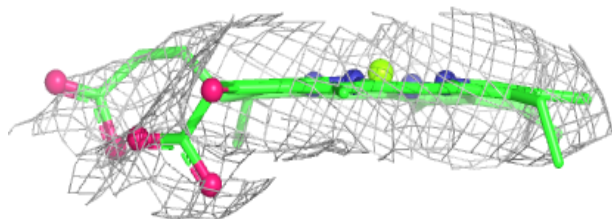
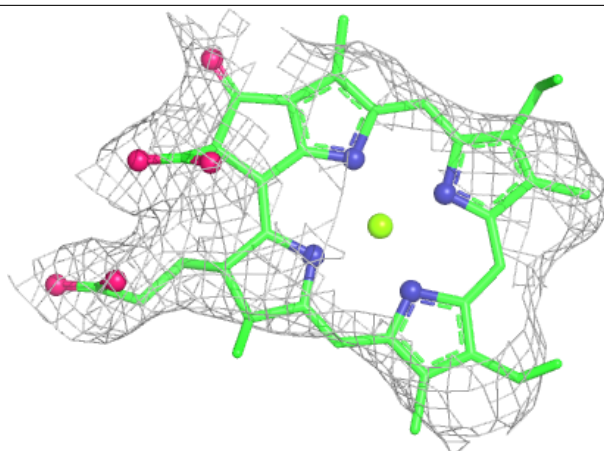
Electron density around CLA B 824:

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



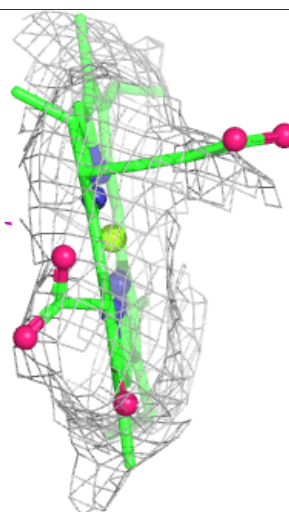
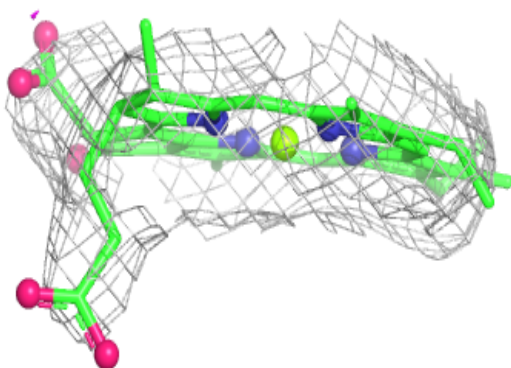
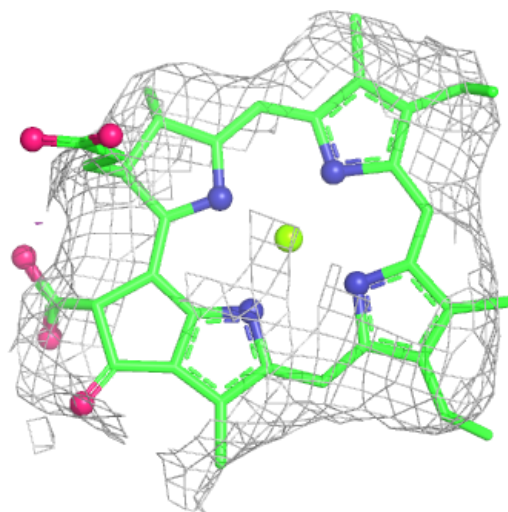
Electron density around CLA 0 306:

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



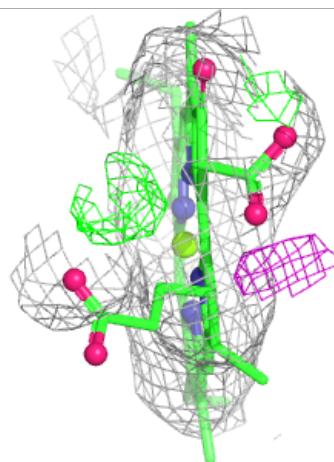
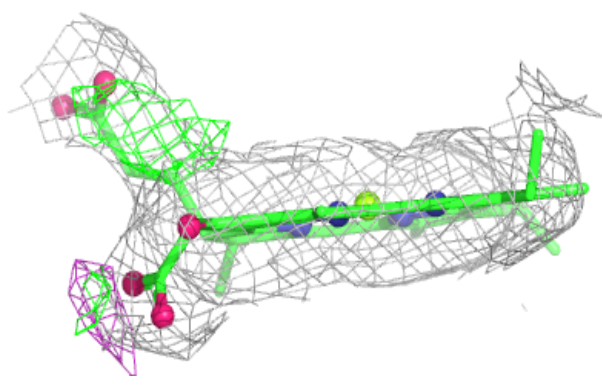
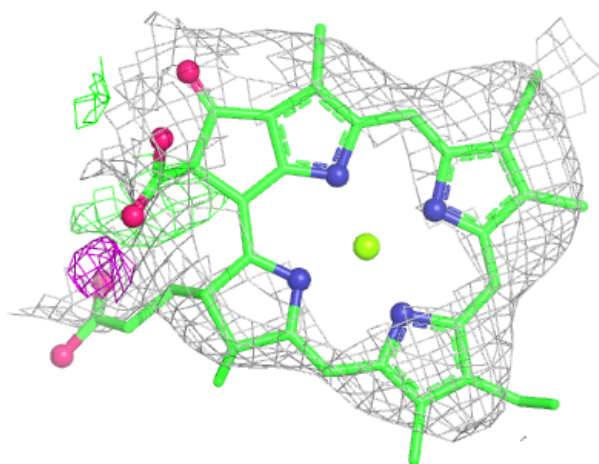
Electron density around CLA 0 311:

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



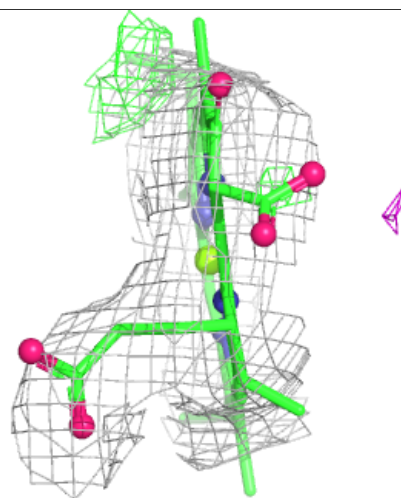
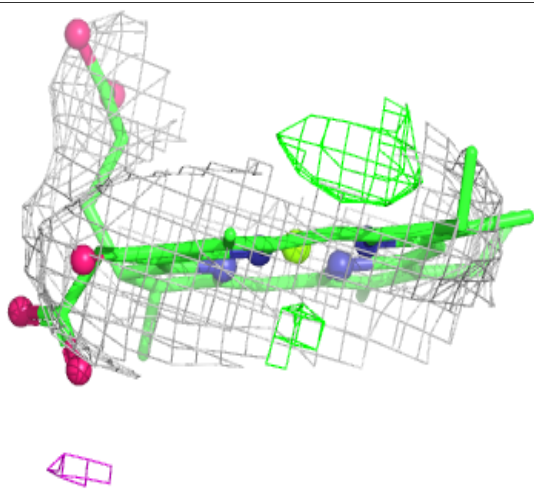
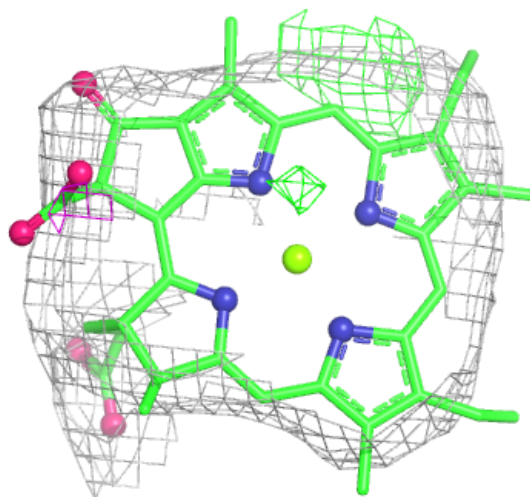
Electron density around CLA 0 313:

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



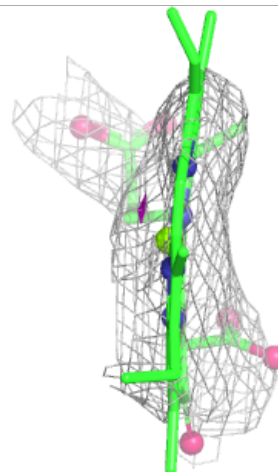
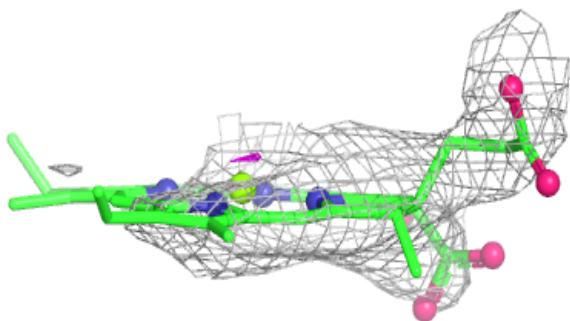
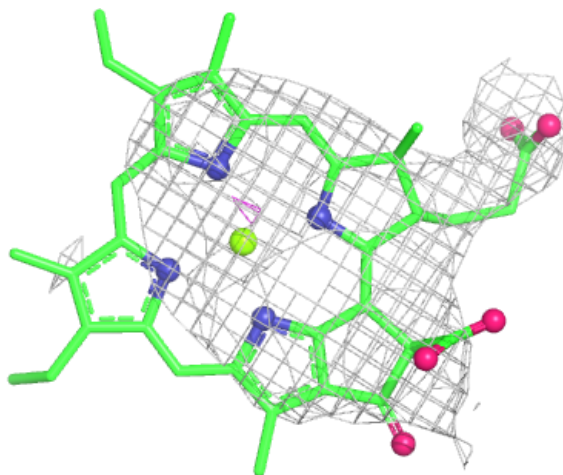
Electron density around CLA A 819:

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



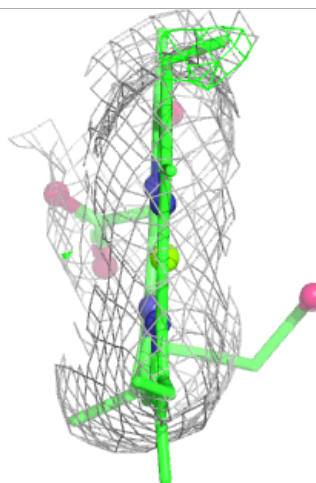
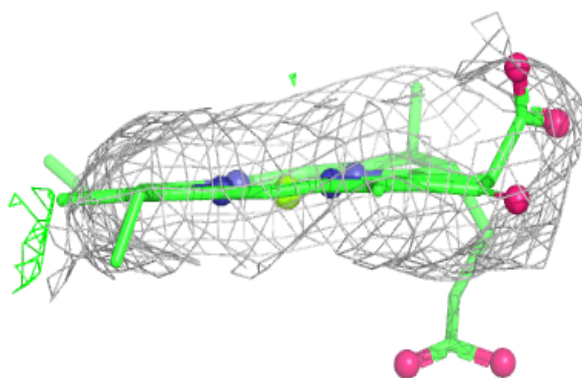
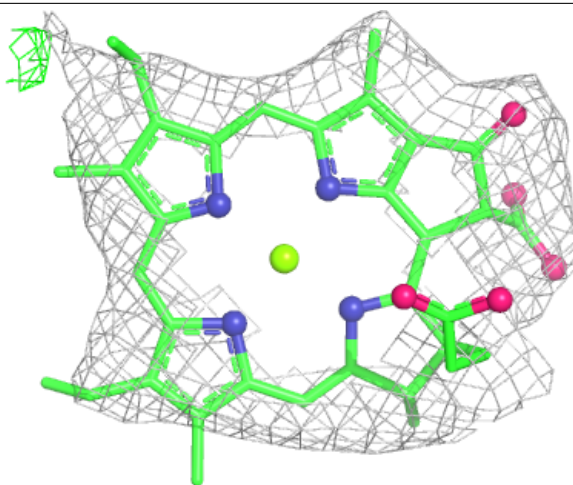
Electron density around CLA B 816:

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



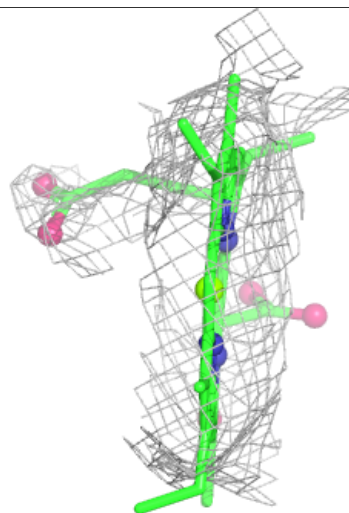
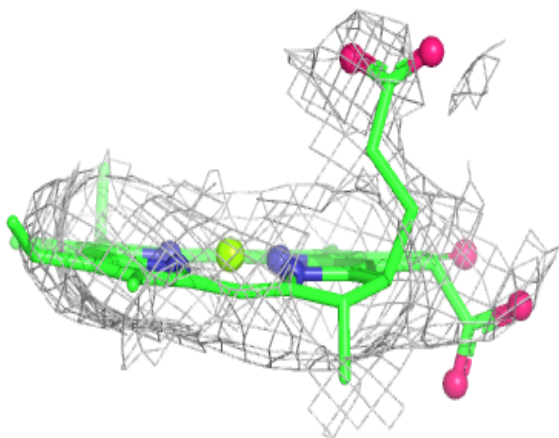
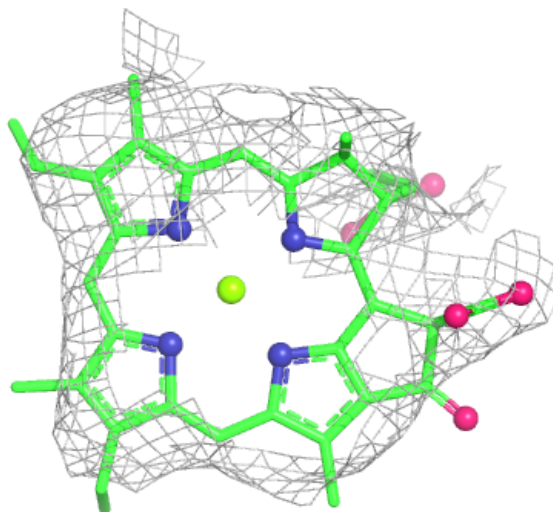
Electron density around CLA 5 311:

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



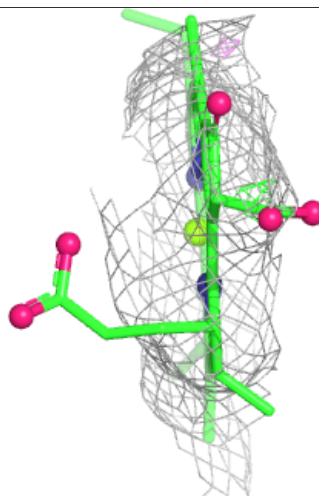
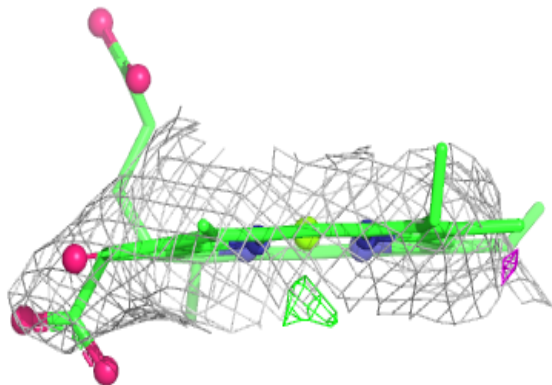
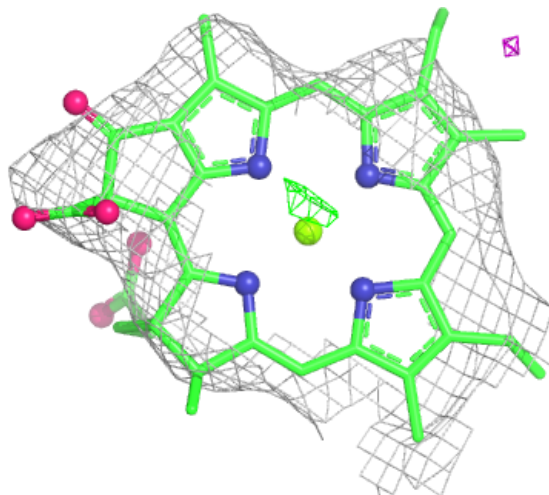
Electron density around CLA A 820:

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



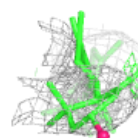
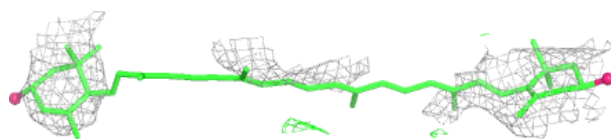
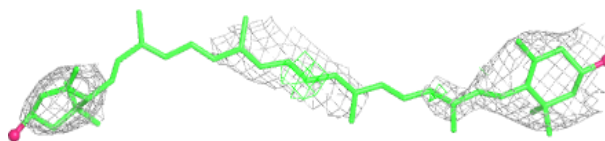
Electron density around CLA A 815:

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



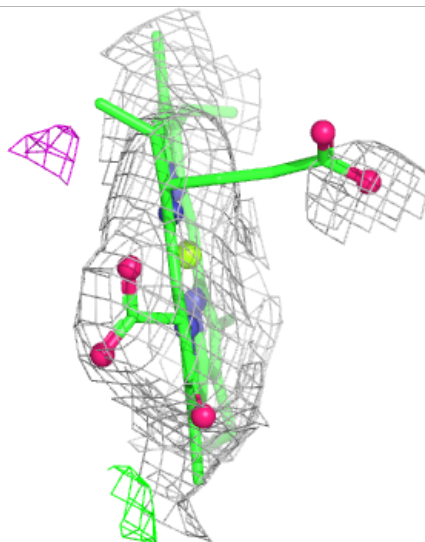
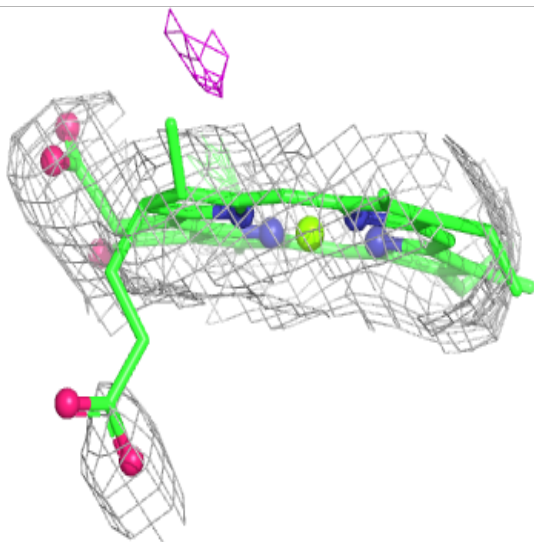
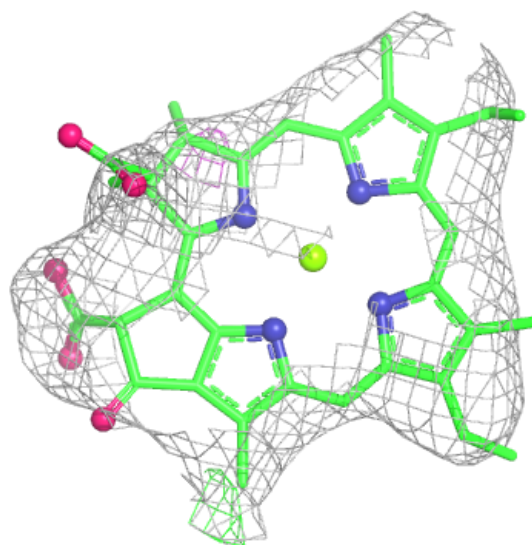
Electron density around LUT 0 304:

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



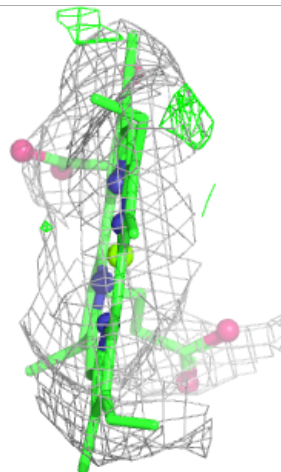
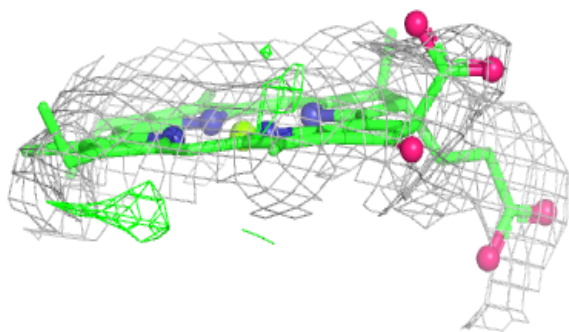
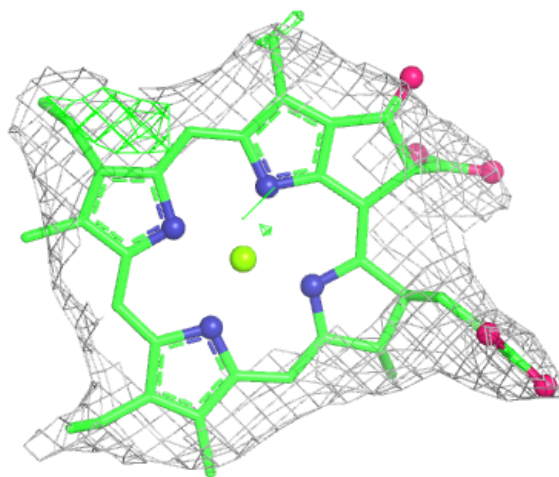
Electron density around CLA 1 1009:

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



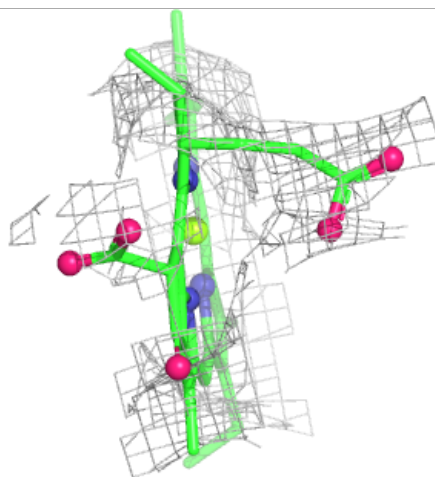
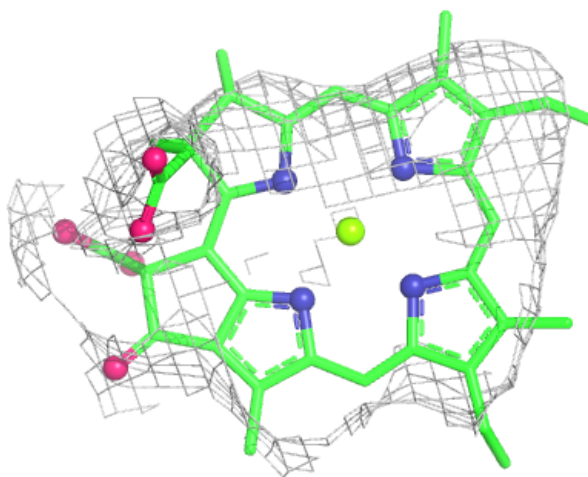
Electron density around CLA 1 1017:

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



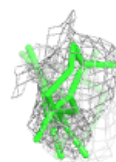
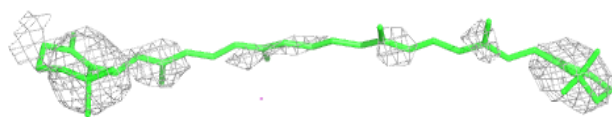
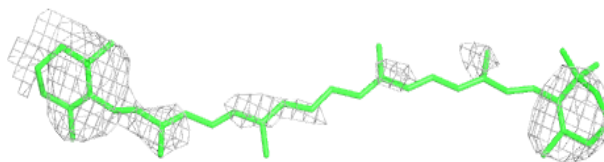
Electron density around CLA B 840:

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

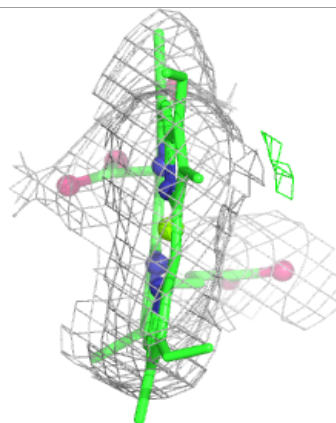
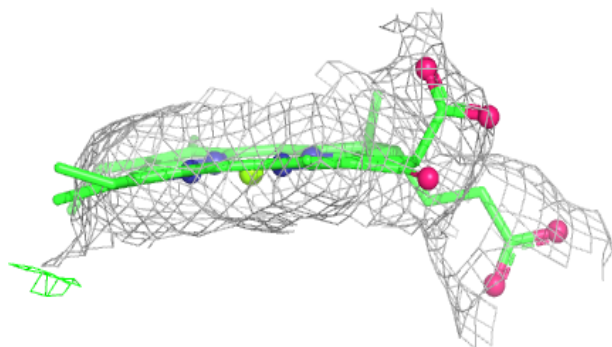
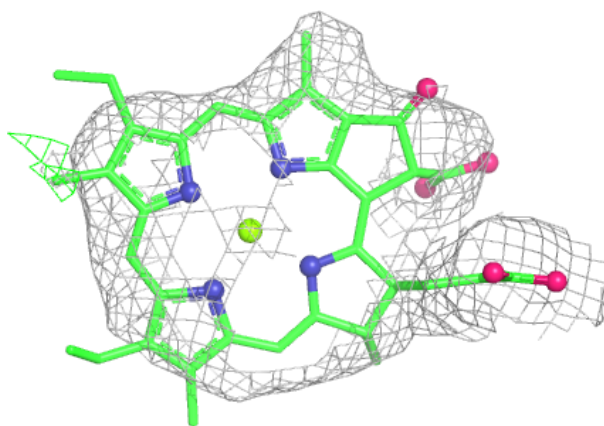


Electron density around BCR J 103:

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

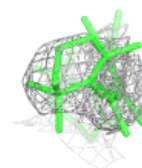
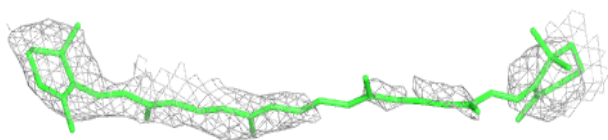
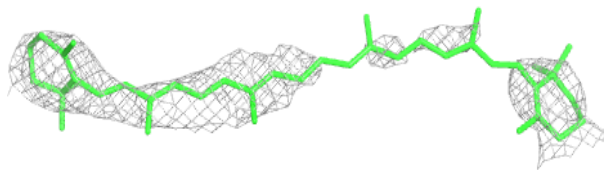
**Electron density around CLA J 102:**

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

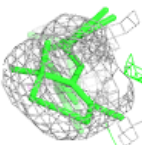
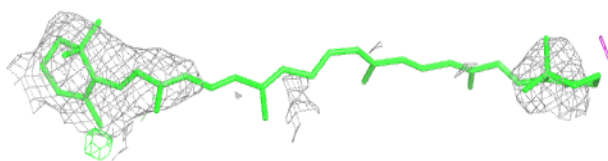
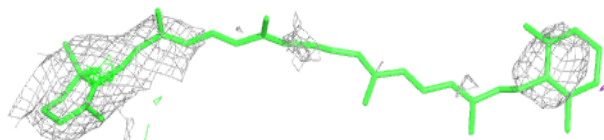


Electron density around BCR A 847:

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

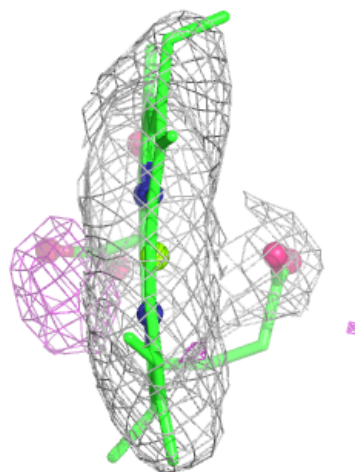
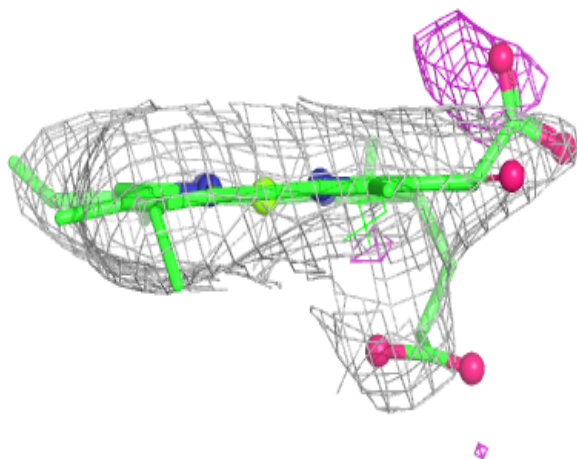
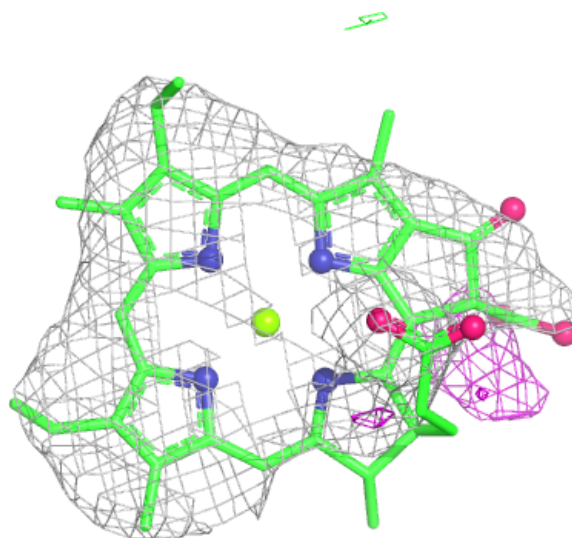
**Electron density around BCR 4 302:**

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



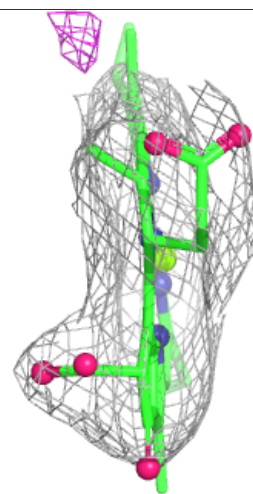
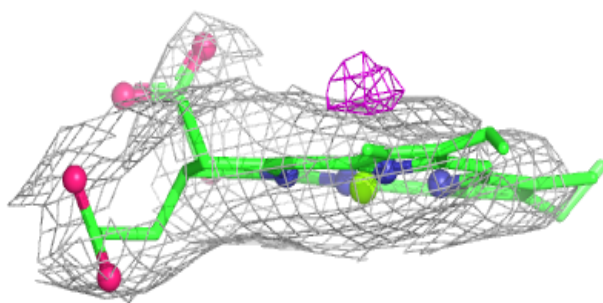
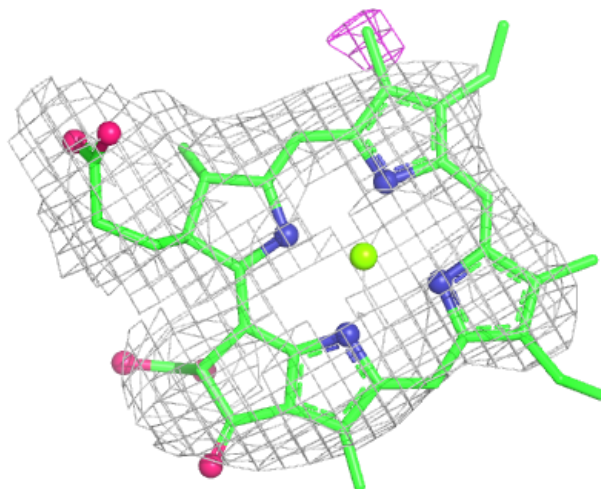
Electron density around CLA 0 307:

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



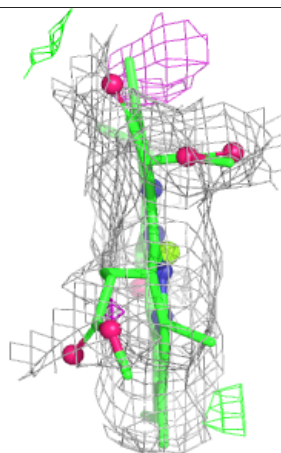
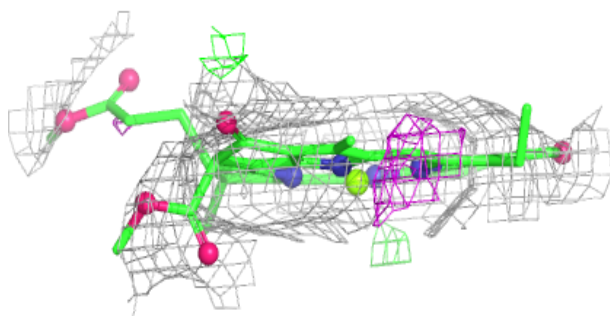
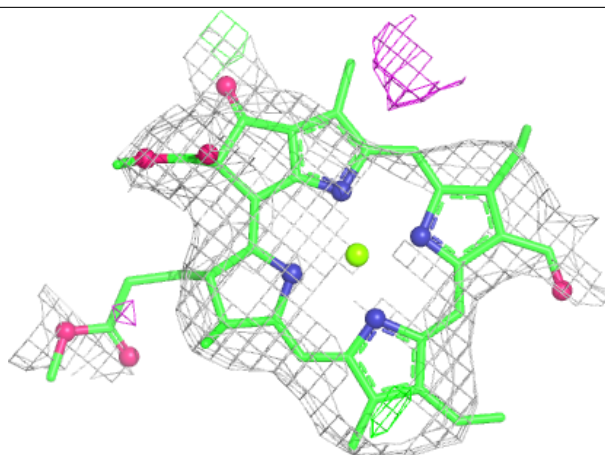
Electron density around CLA A 812:

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



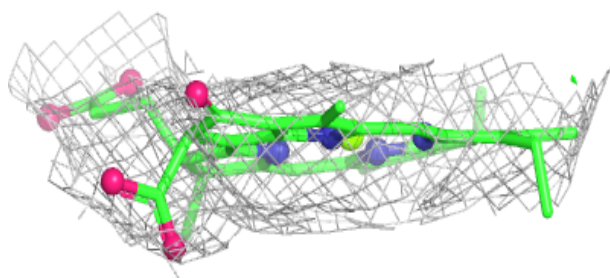
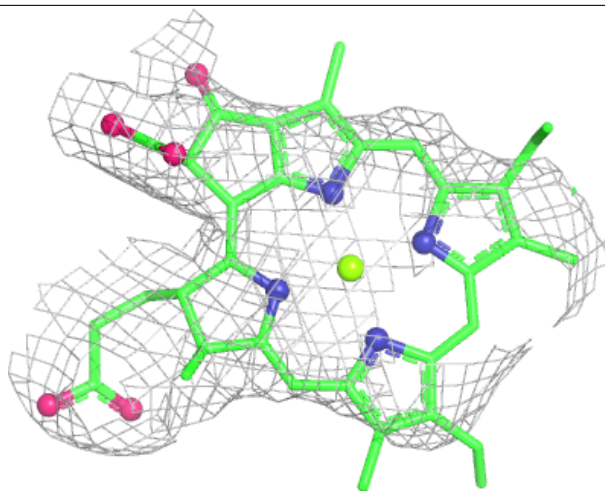
Electron density around CHL 8 314:

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



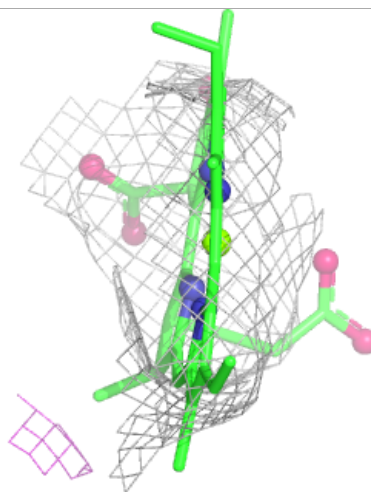
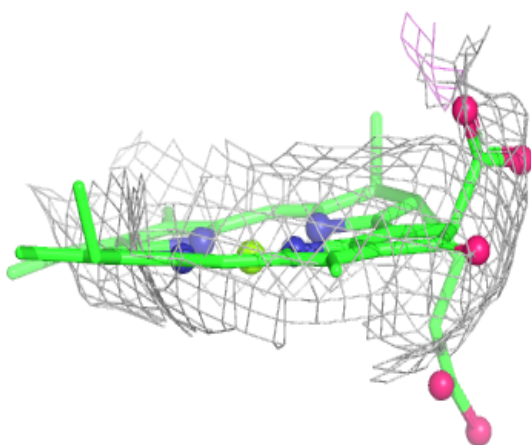
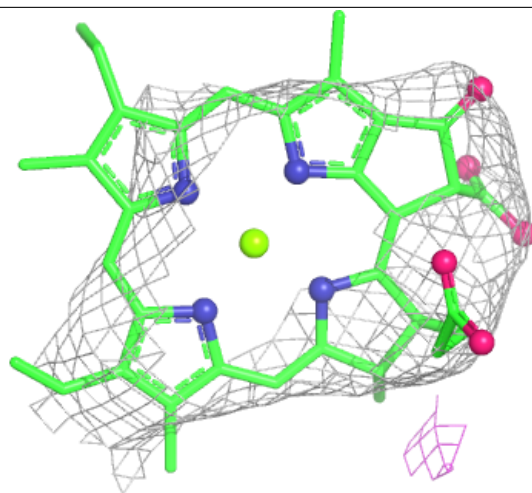
Electron density around CLA B 801:

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



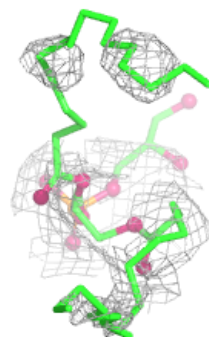
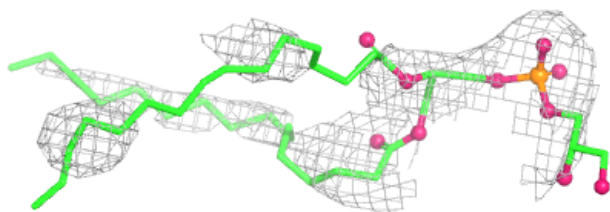
Electron density around CLA A 833:

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



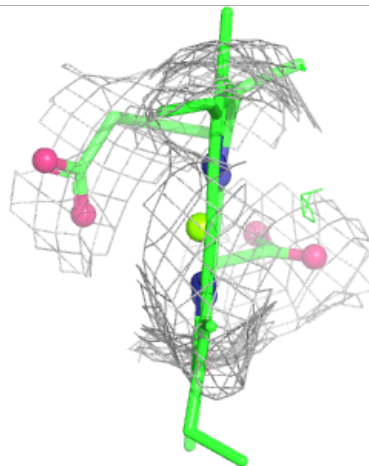
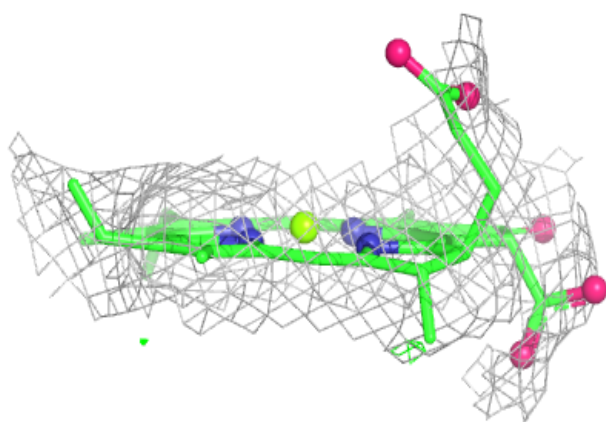
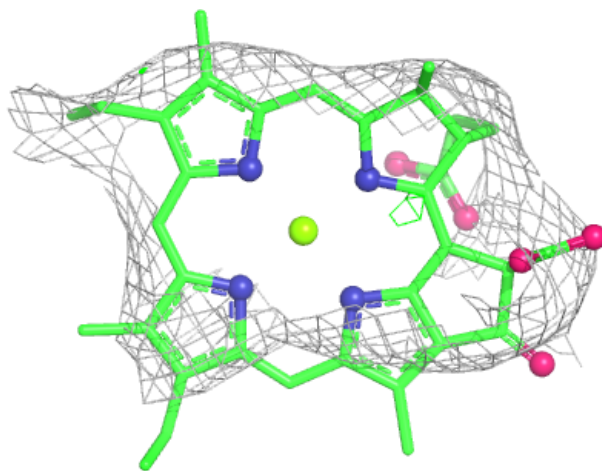
Electron density around LHG A 849:

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



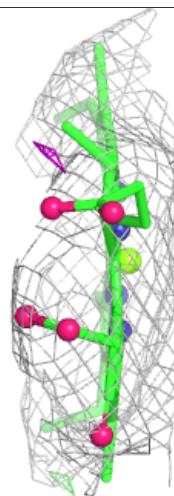
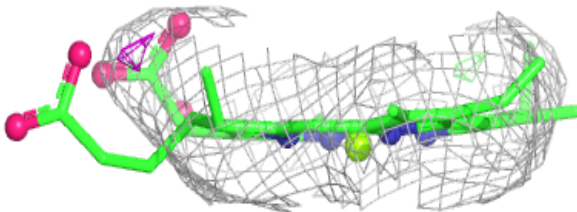
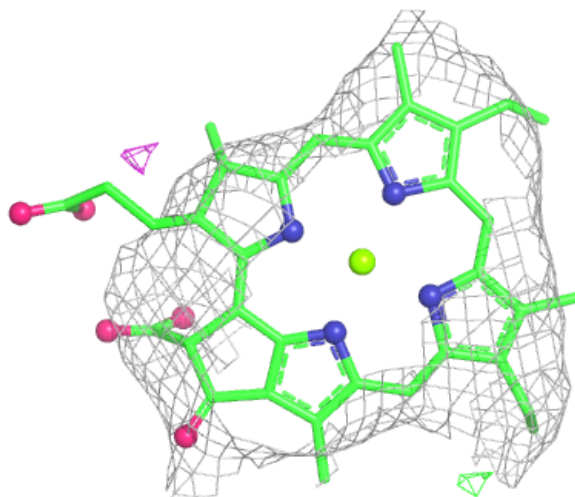
Electron density around CLA B 810:

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



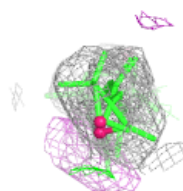
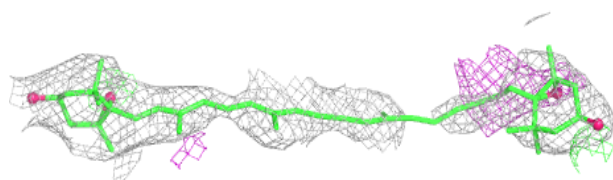
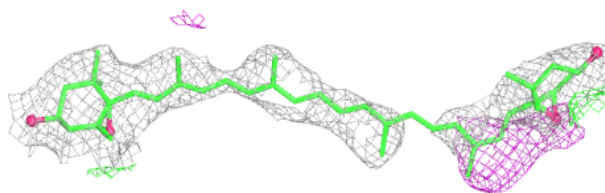
Electron density around CLA 1 1004:

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

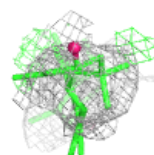
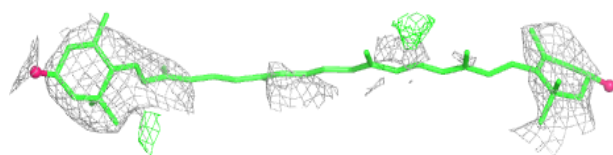
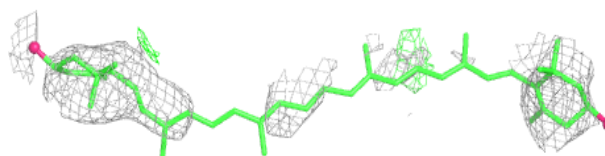


Electron density around XAT 7 1002:

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

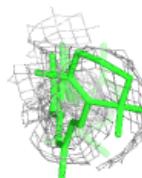
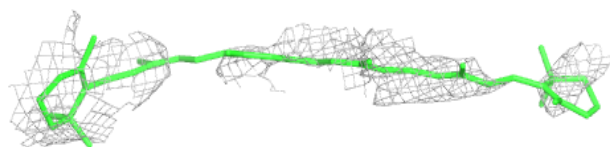
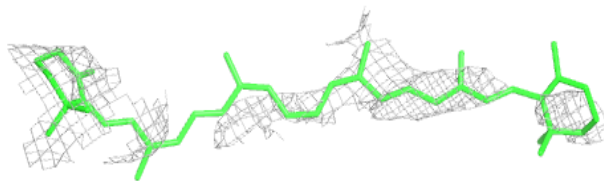
**Electron density around LUT 1 1002:**

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



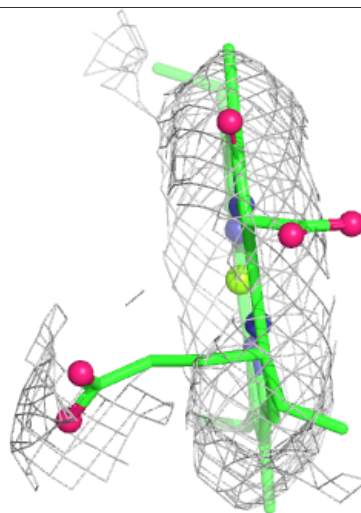
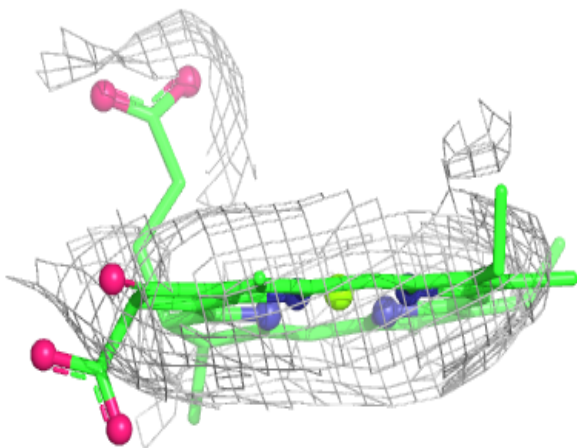
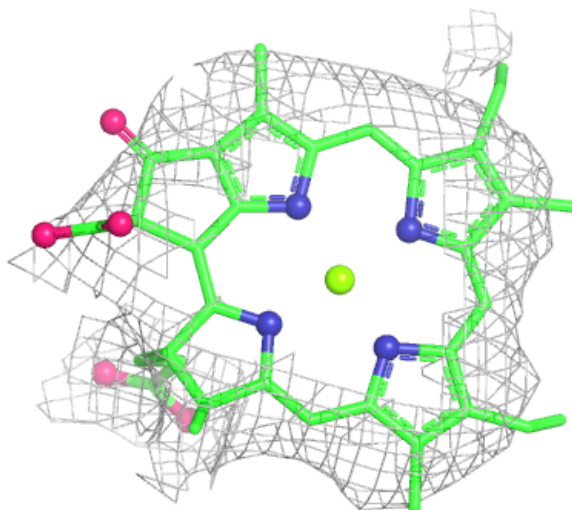
Electron density around BCR B 843:

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



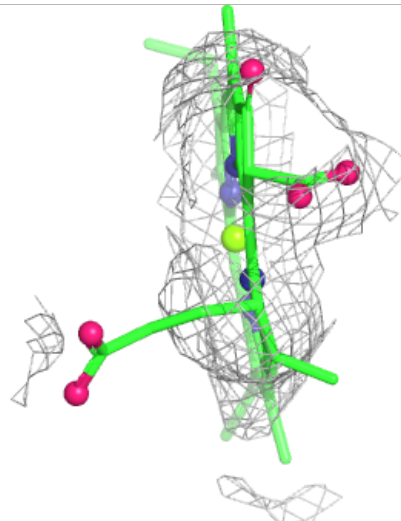
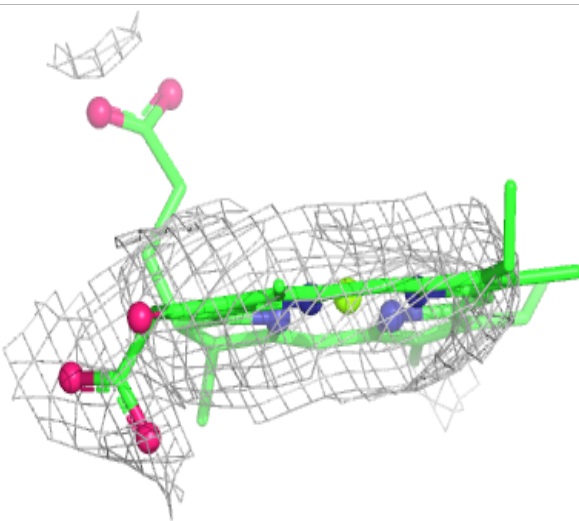
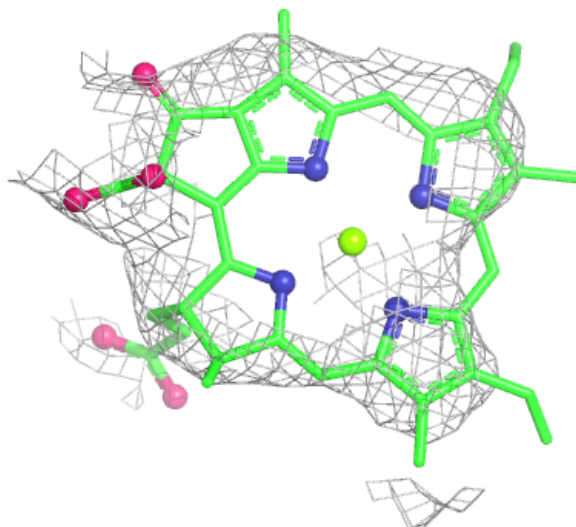
Electron density around CLA B 822:

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



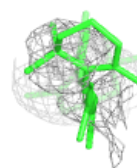
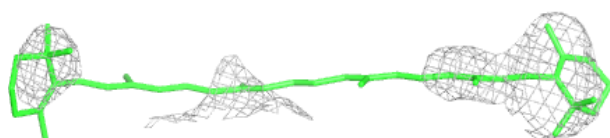
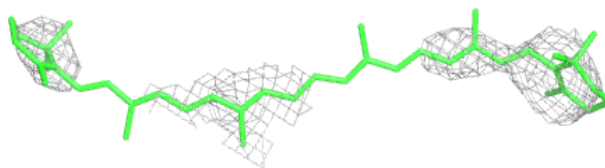
Electron density around CLA B 832:

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

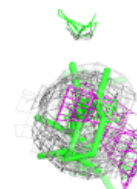
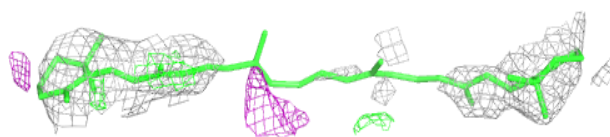
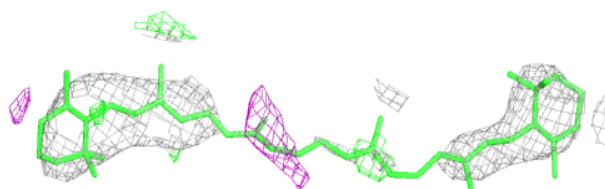


Electron density around BCR B 846:

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

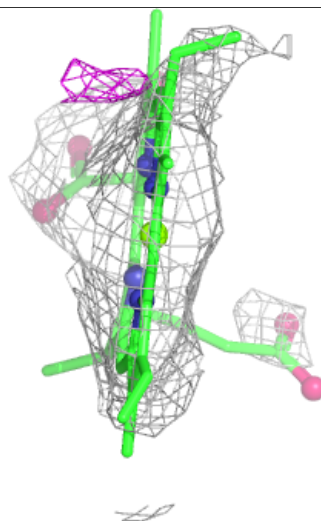
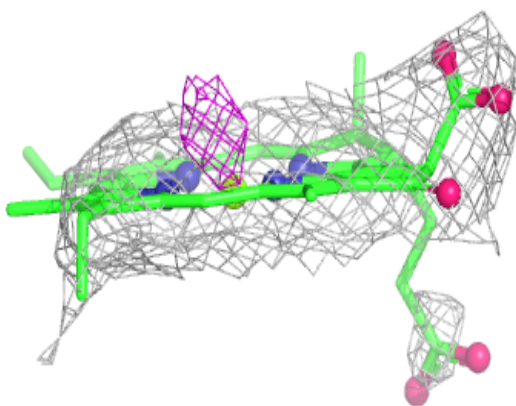
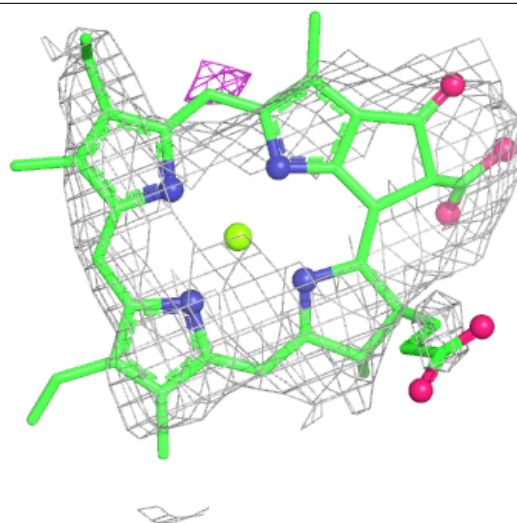
**Electron density around BCR 7 1003:**

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



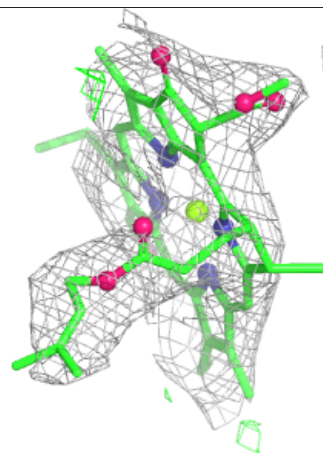
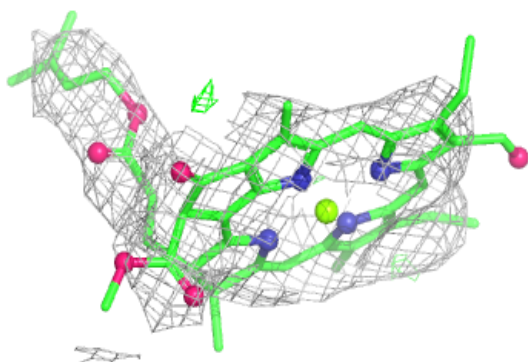
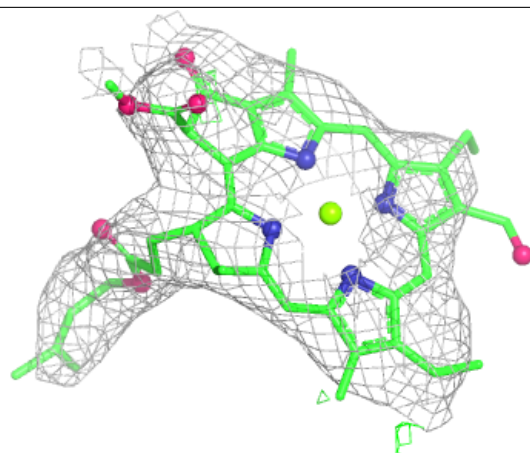
Electron density around CLA B 835:

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

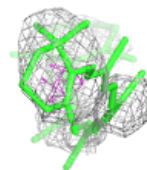
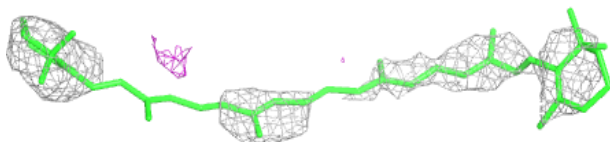
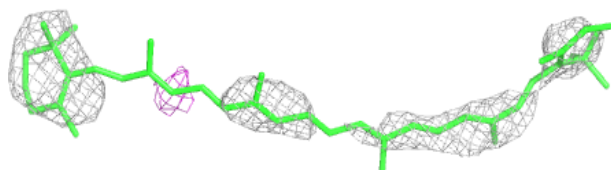


Electron density around CHL 1 1013:

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

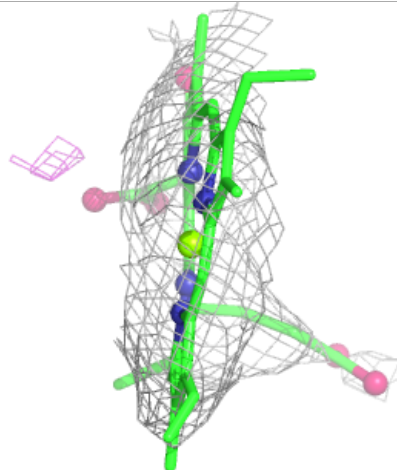
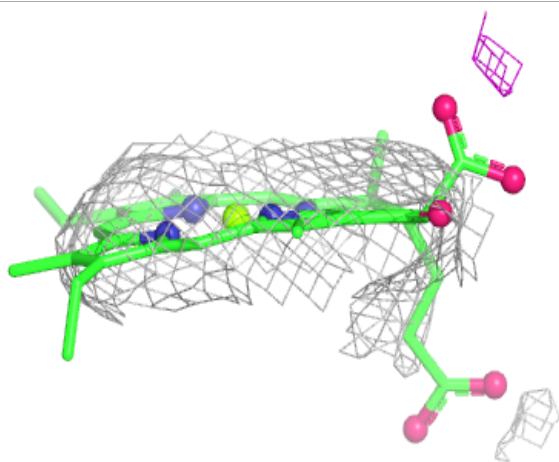
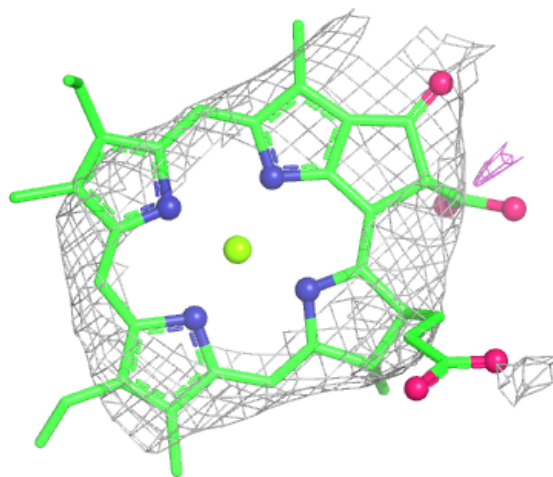
**Electron density around BCR F 301:**

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



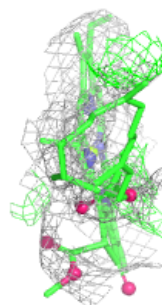
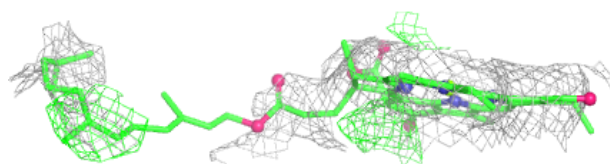
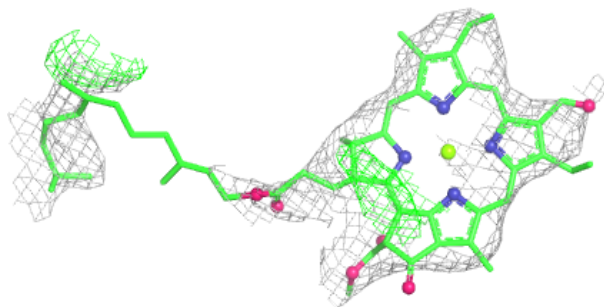
Electron density around CLA A 832:

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



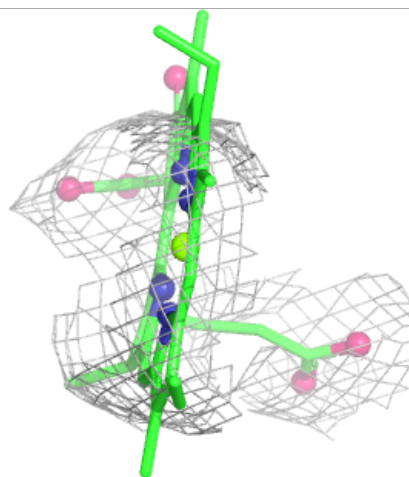
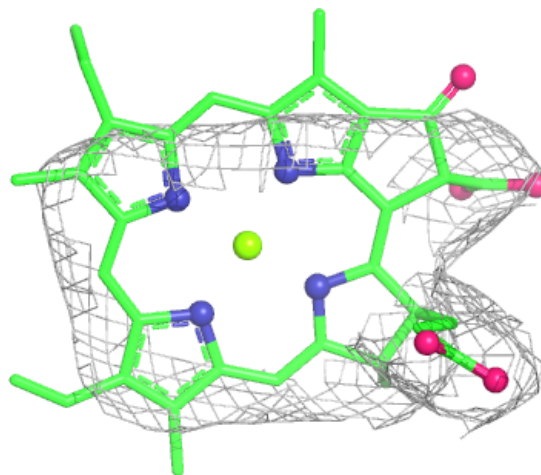
Electron density around CHL 4 315:

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



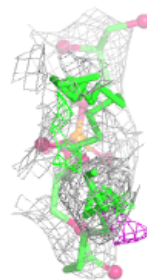
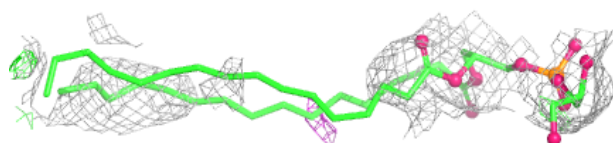
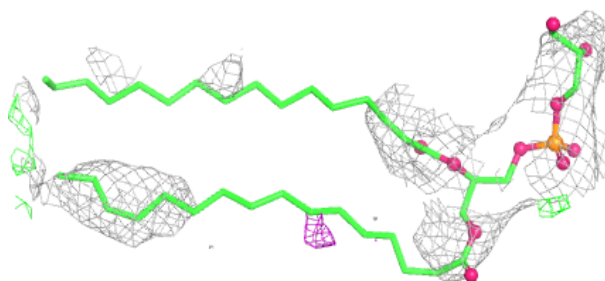
Electron density around CLA B 814:

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



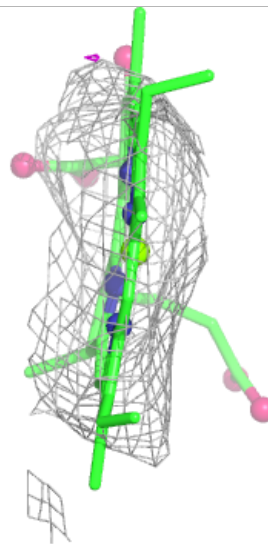
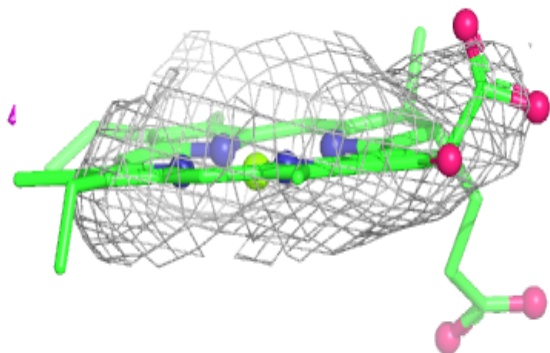
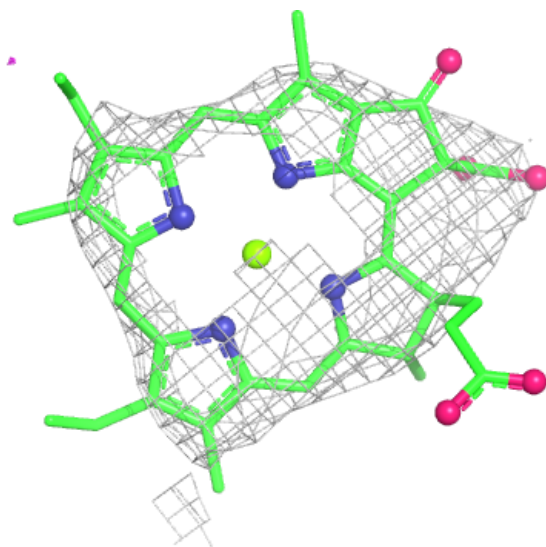
Electron density around LHG 4 301:

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



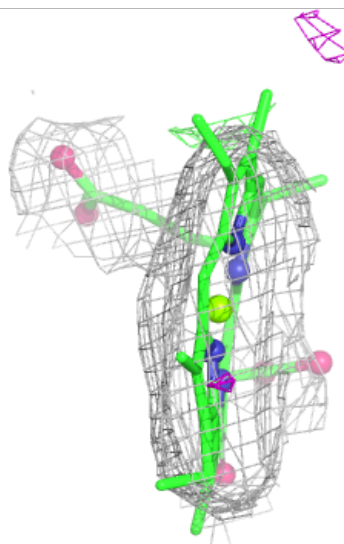
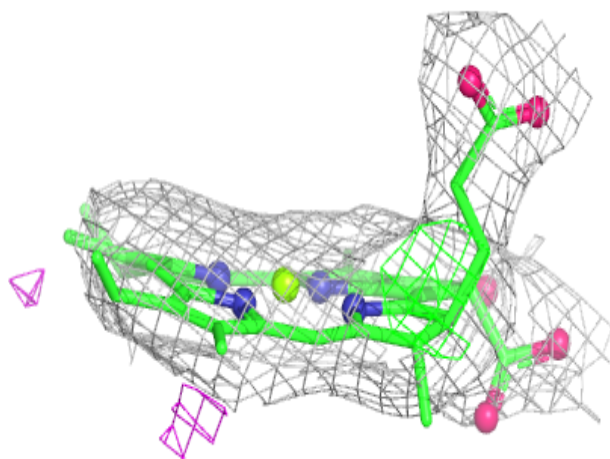
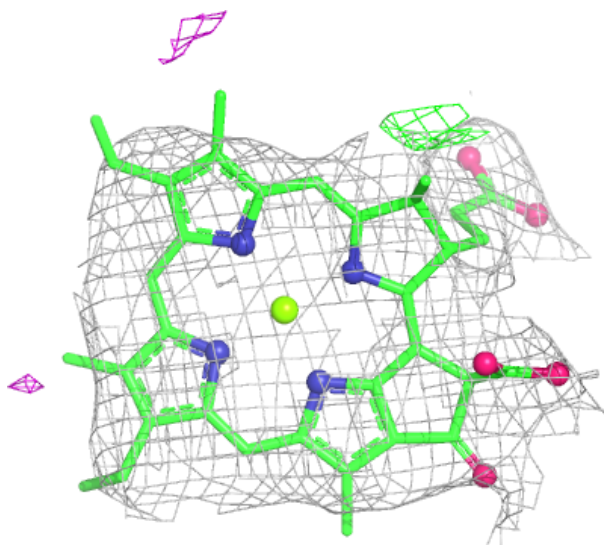
Electron density around CLA B 820:

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



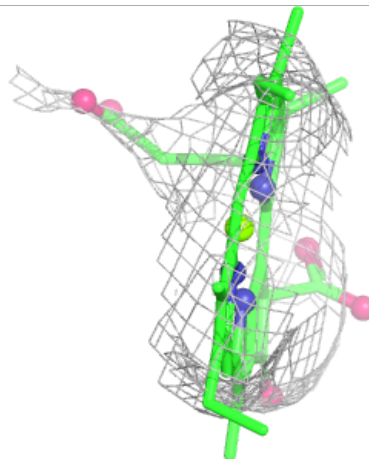
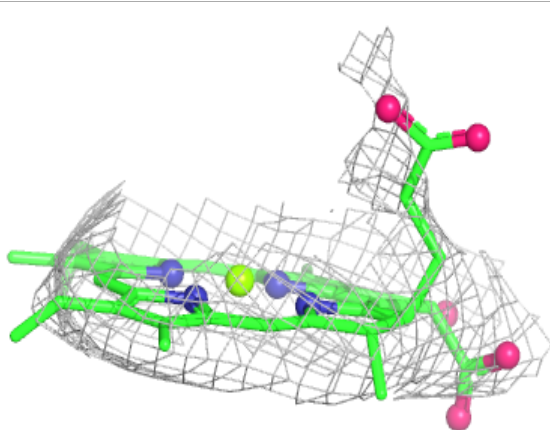
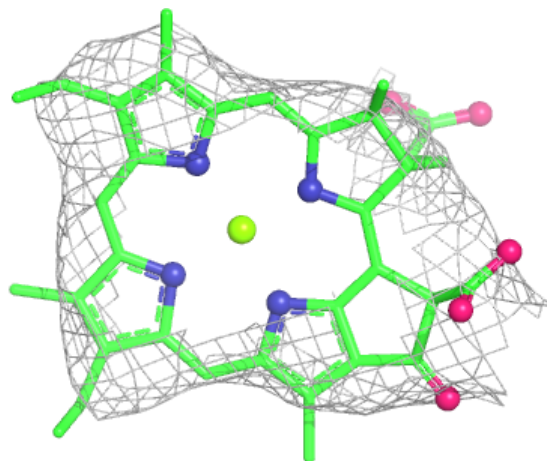
Electron density around CLA 1 1014:

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



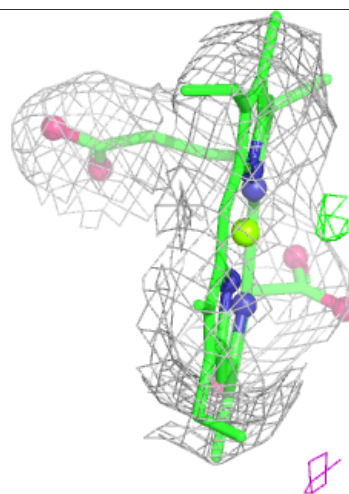
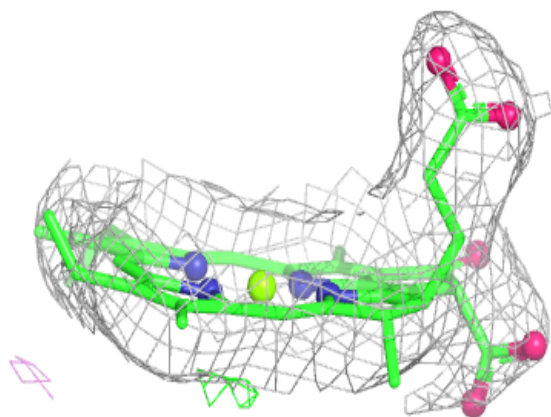
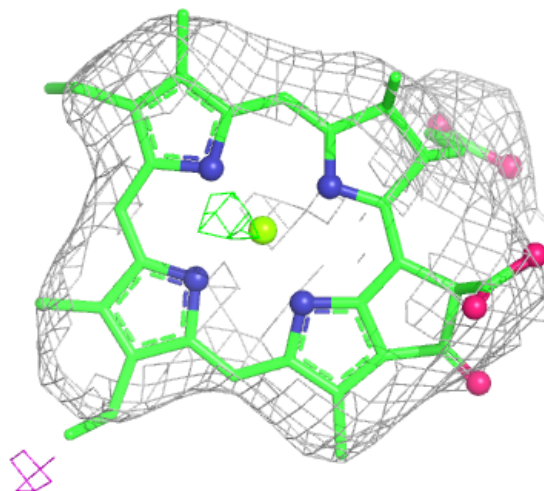
Electron density around CLA A 823:

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



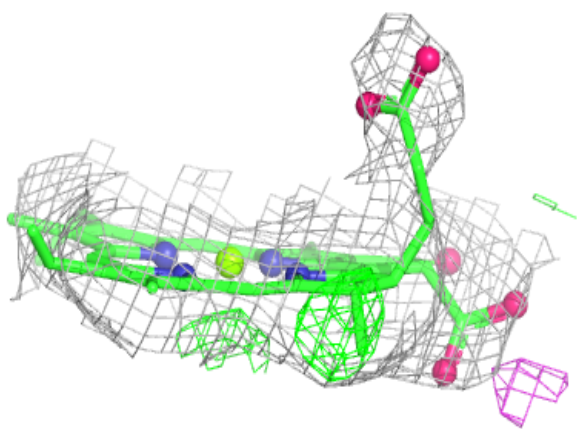
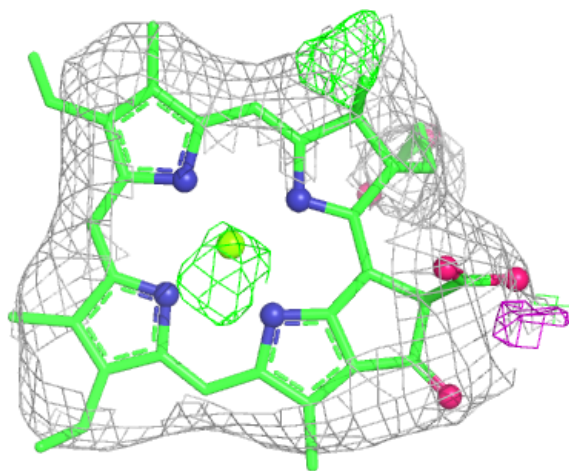
Electron density around CLA 4 310:

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



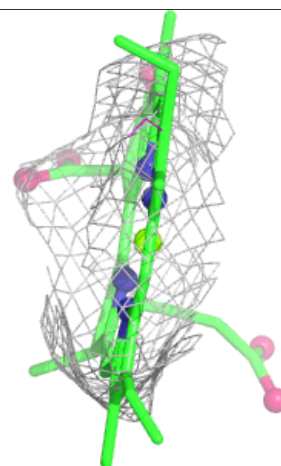
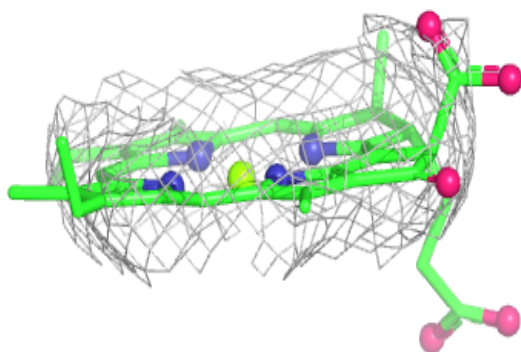
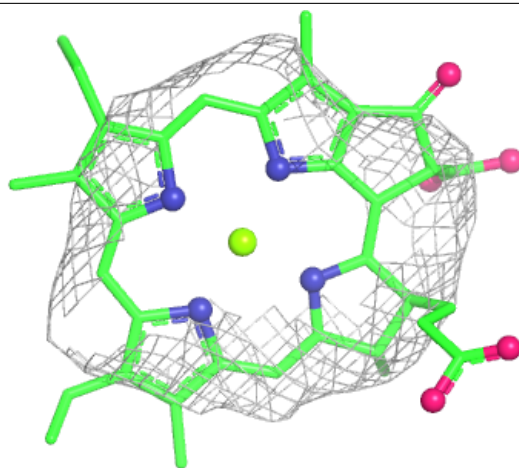
Electron density around CLA 6 310:

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



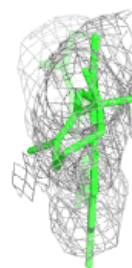
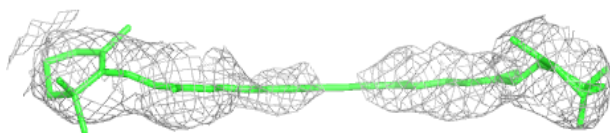
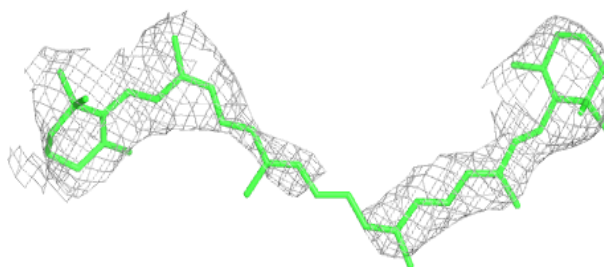
Electron density around CLA A 830:

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

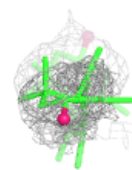
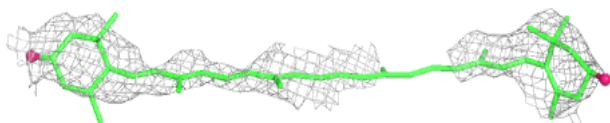
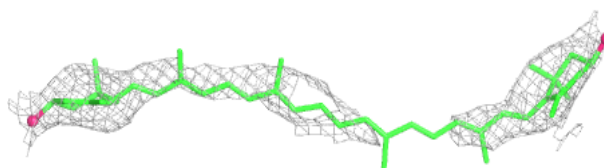


Electron density around BCR A 848:

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

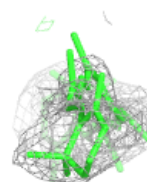
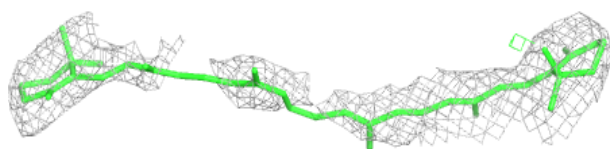
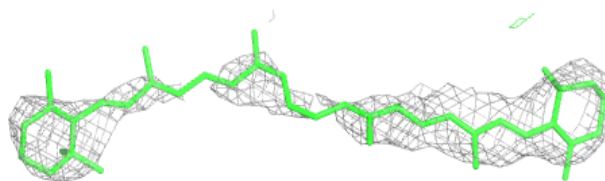
**Electron density around LUT 1 1016:**

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



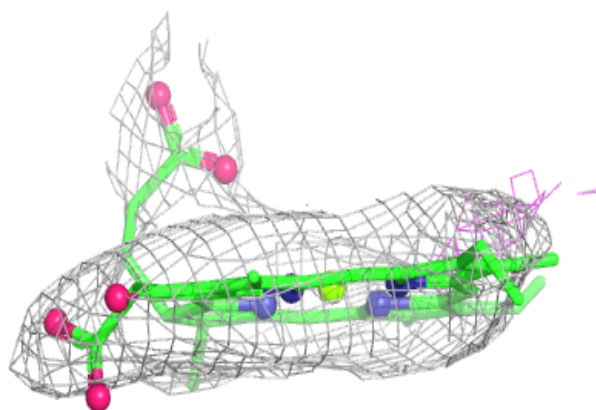
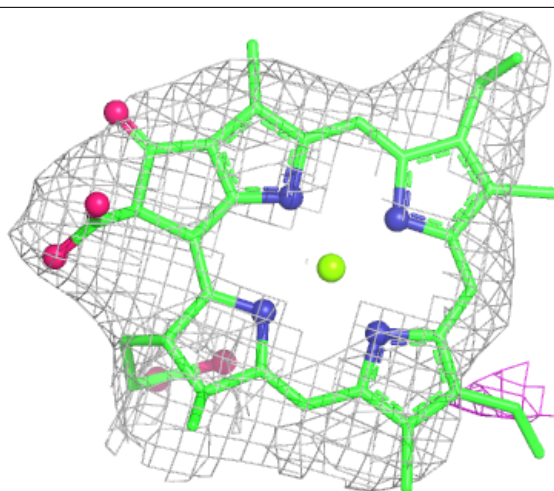
Electron density around BCR 3 1004:

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



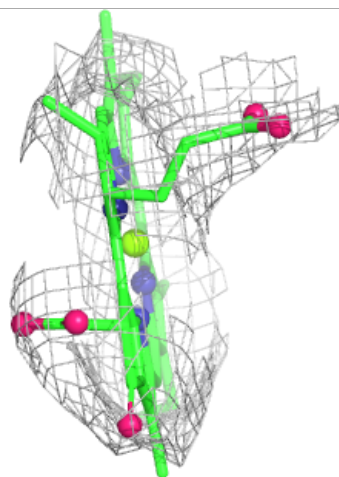
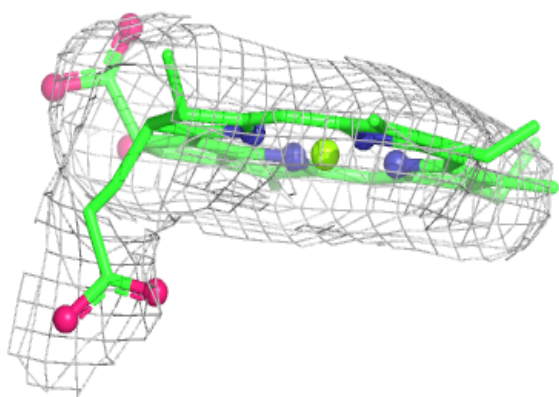
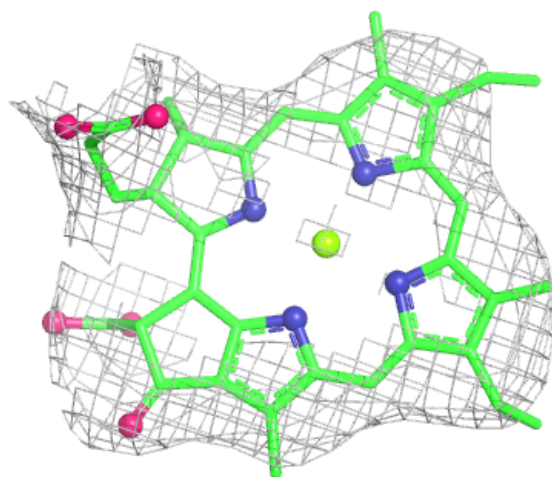
Electron density around CLA 0 310:

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



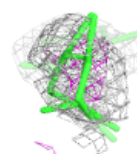
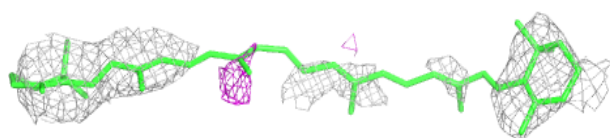
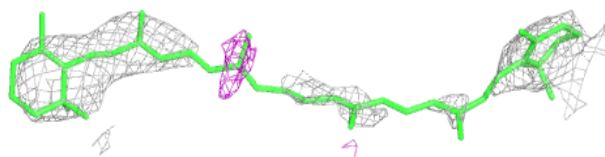
Electron density around CLA B 841:

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

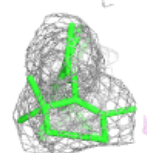
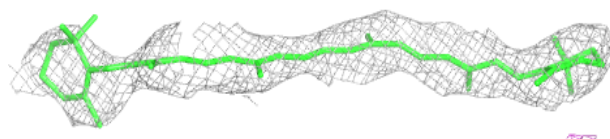
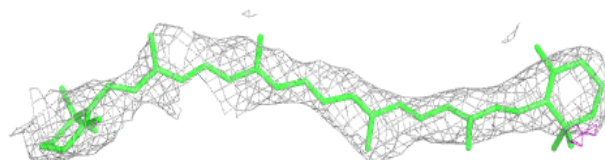


Electron density around BCR 6 302:

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

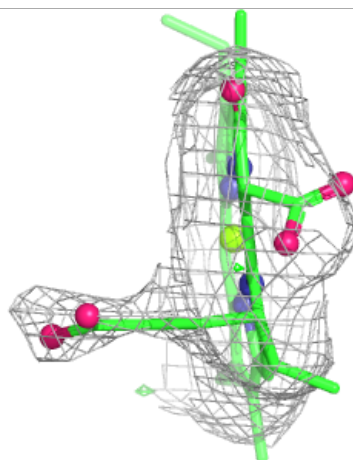
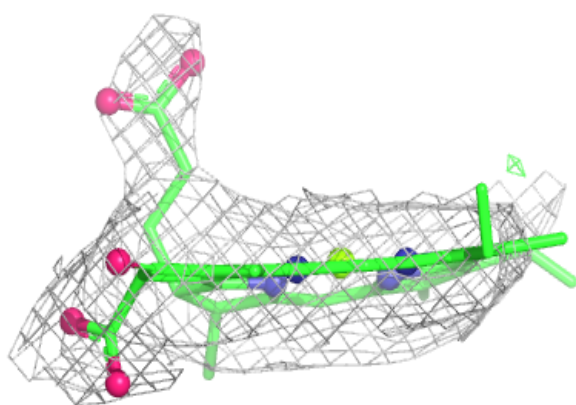
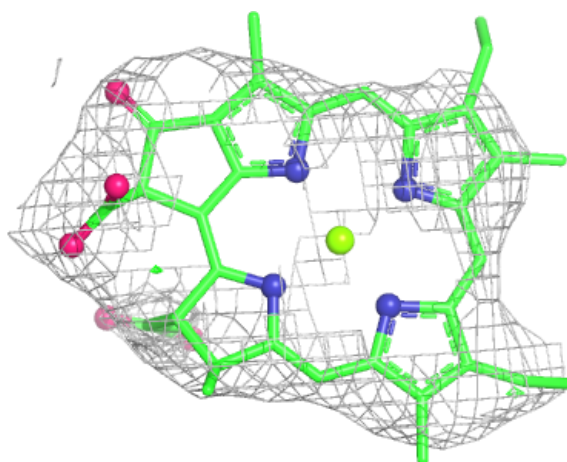
**Electron density around BCR 5 320:**

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



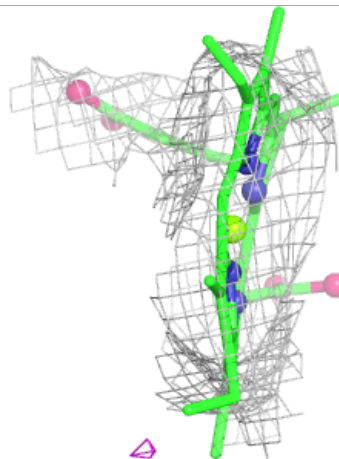
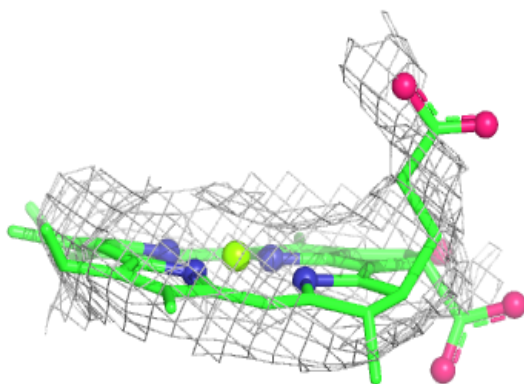
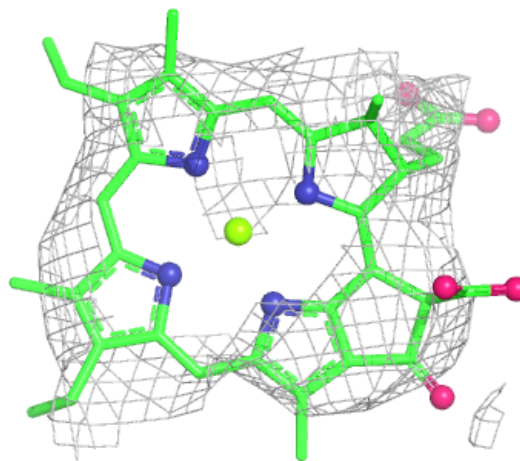
Electron density around CLA A 809:

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



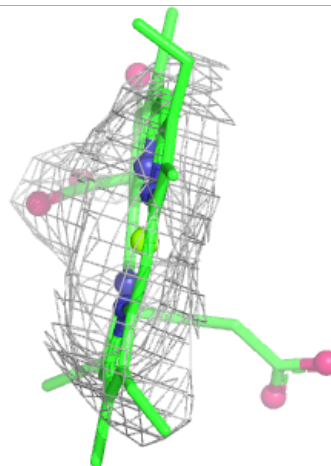
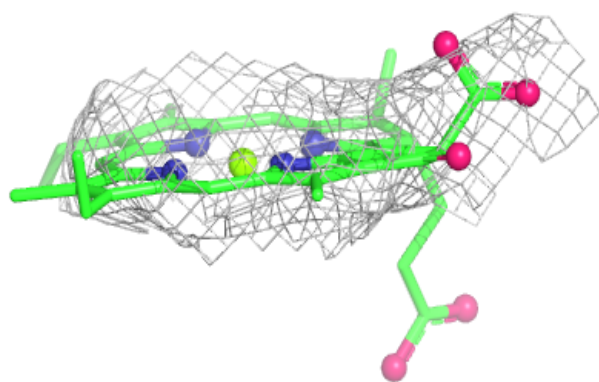
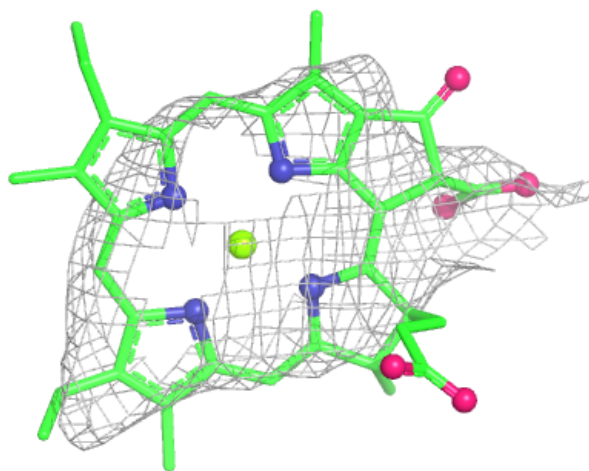
Electron density around CLA 0 316:

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



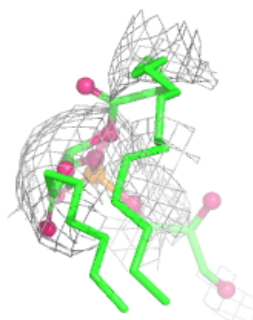
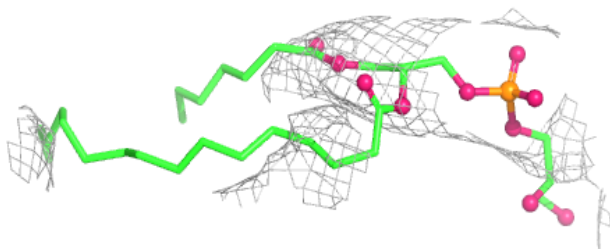
Electron density around CLA L 201:

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

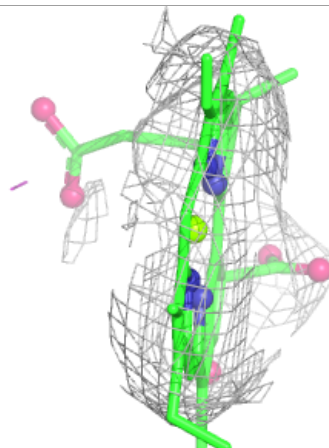
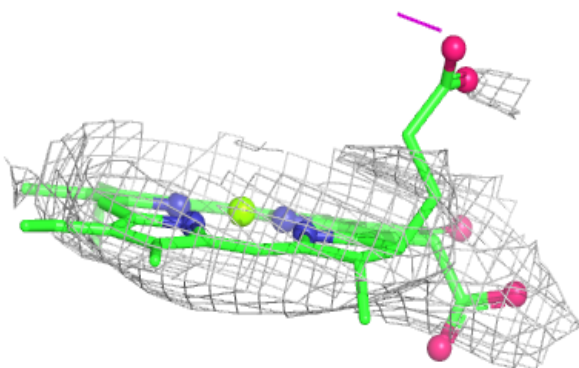
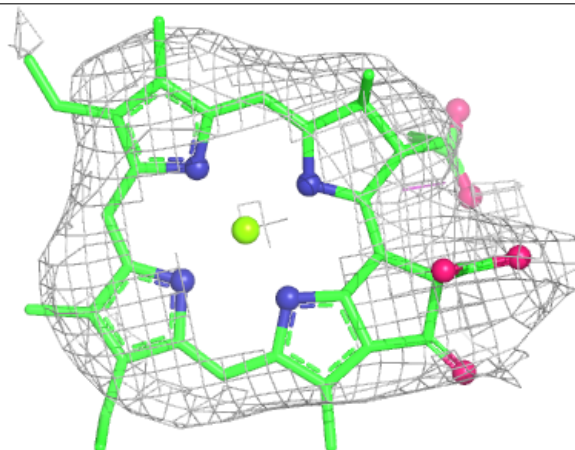


Electron density around LHG A 843:

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

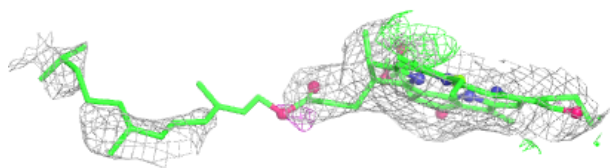
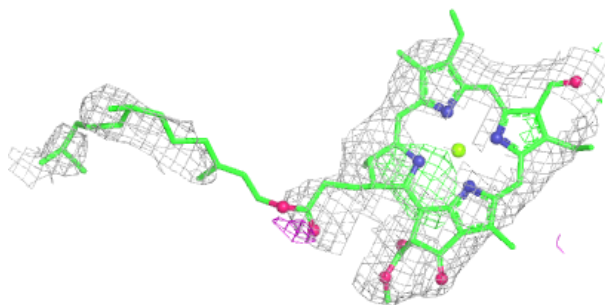
**Electron density around CLA A 852:**

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



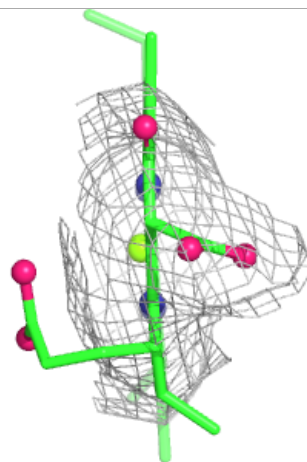
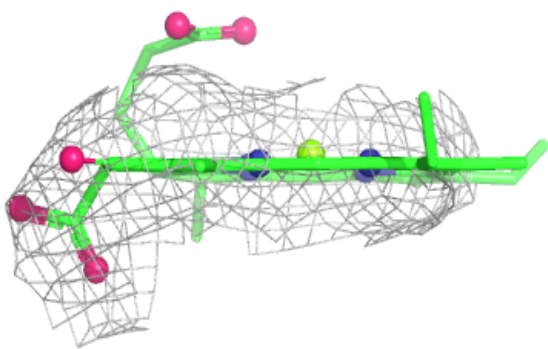
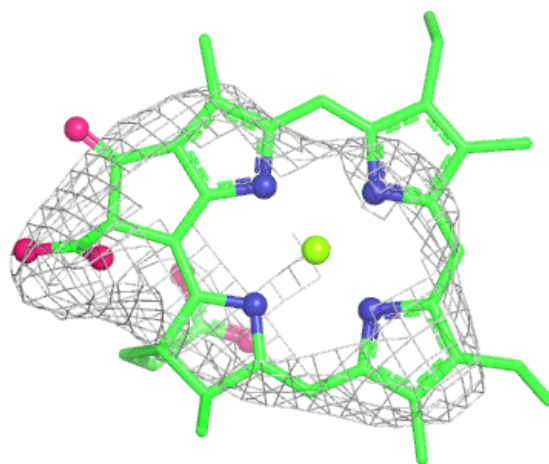
Electron density around CHL 6 316:

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



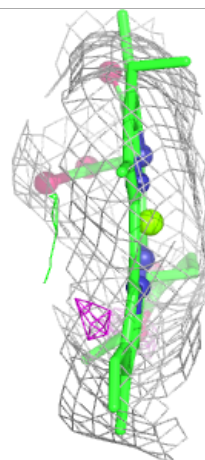
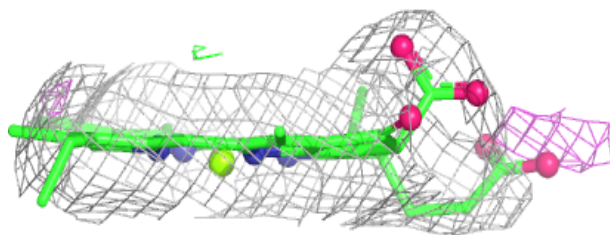
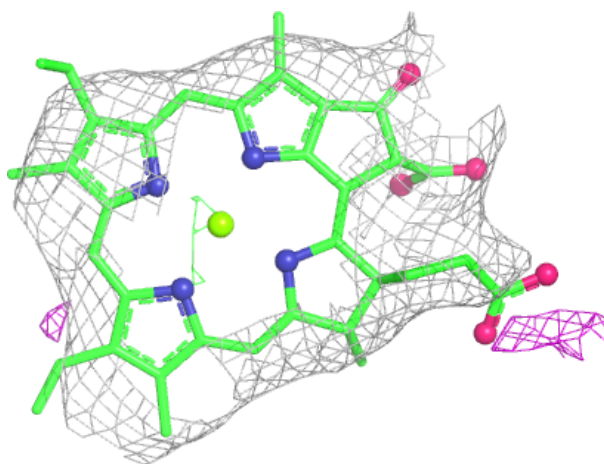
Electron density around CLA B 819:

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



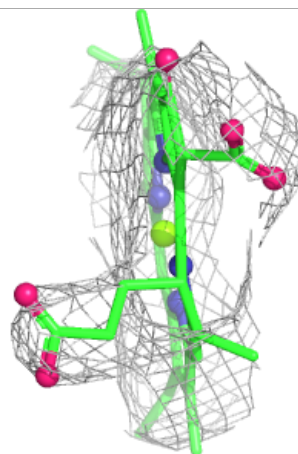
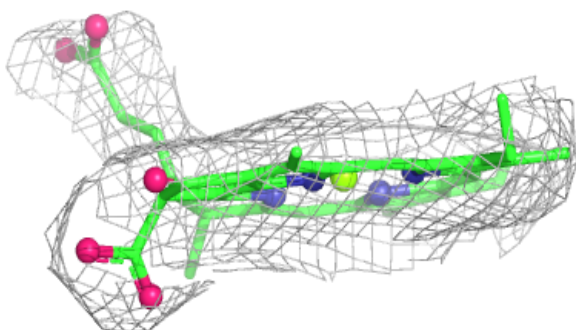
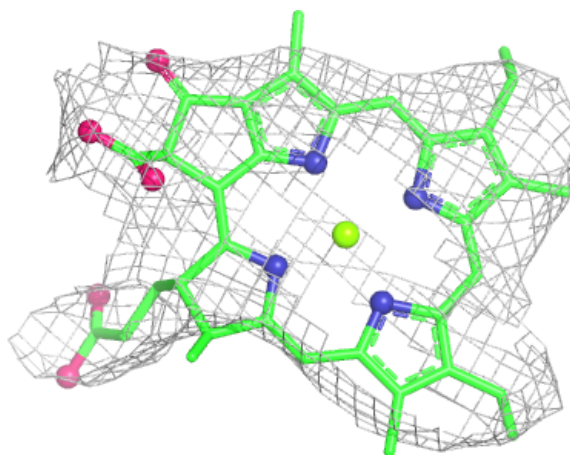
Electron density around CLA 1 1007:

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



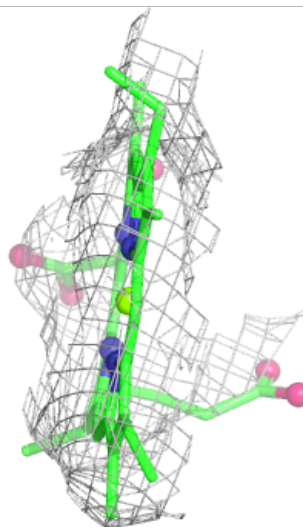
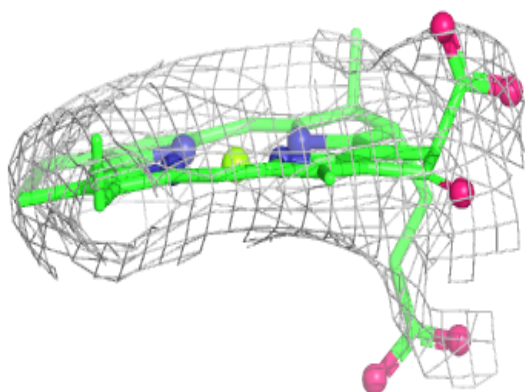
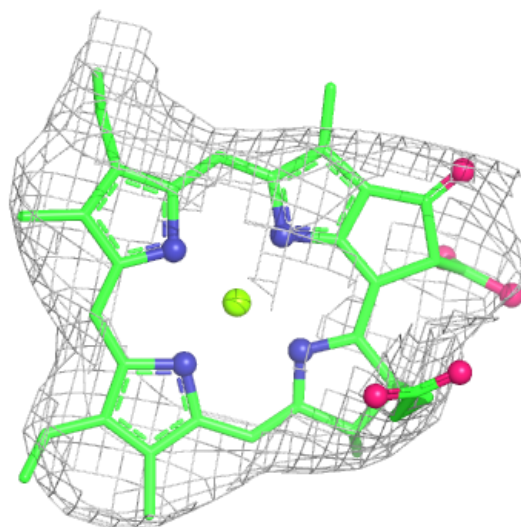
Electron density around CLA A 825:

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



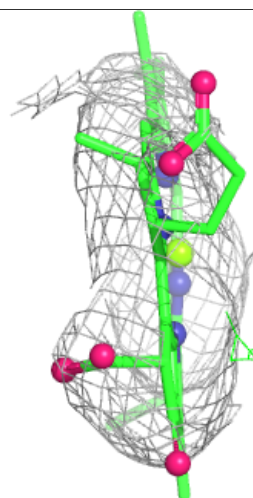
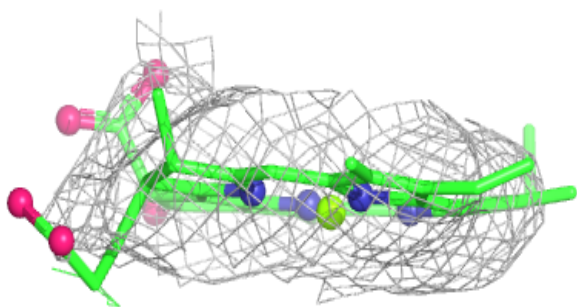
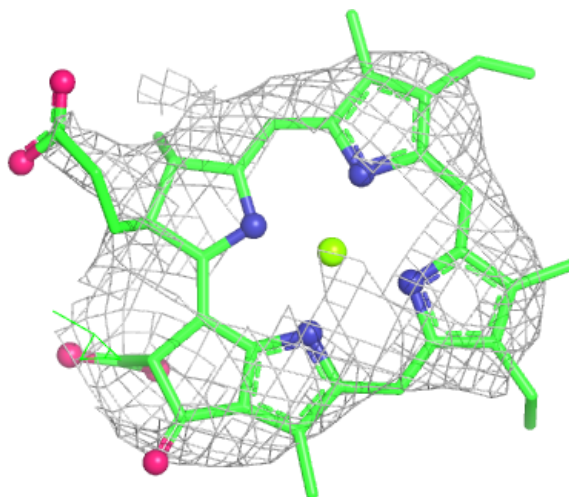
Electron density around CLA B 833:

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



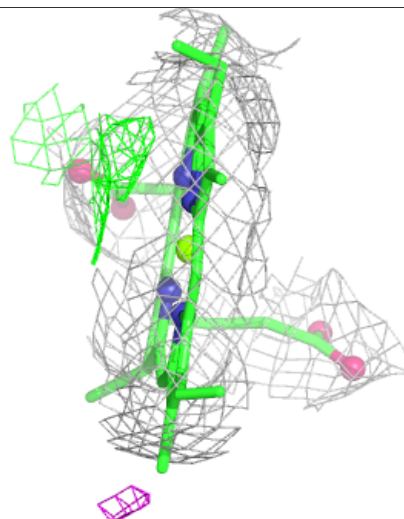
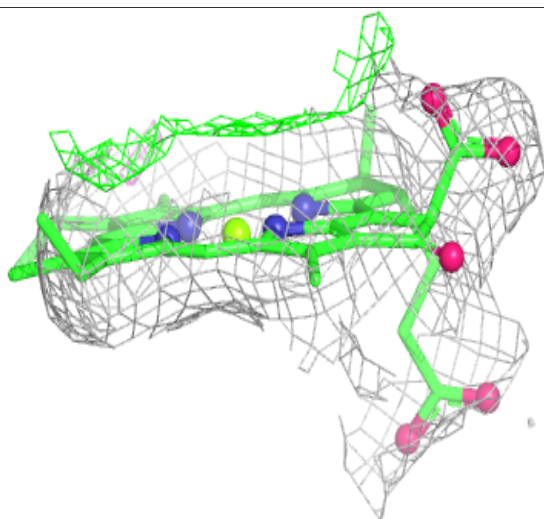
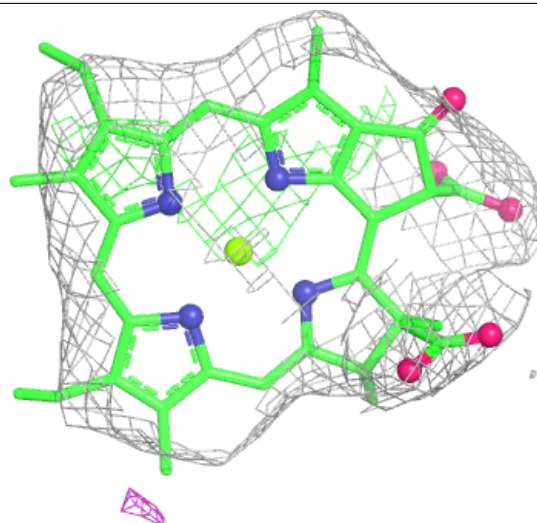
Electron density around CLA B 808:

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



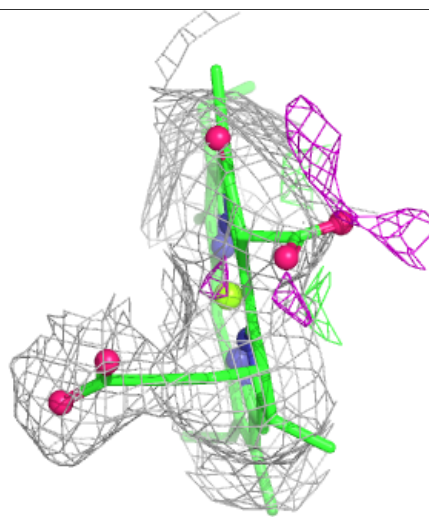
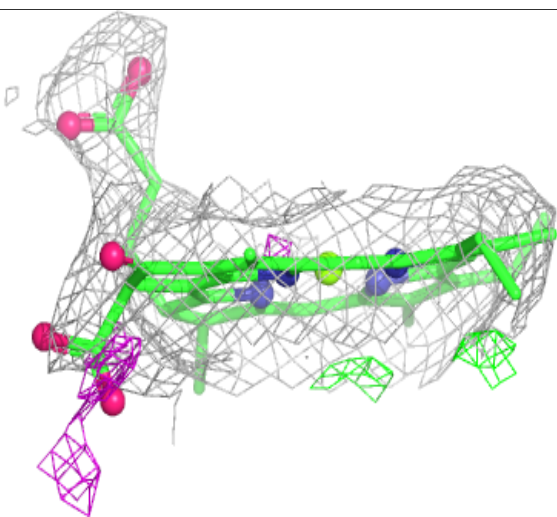
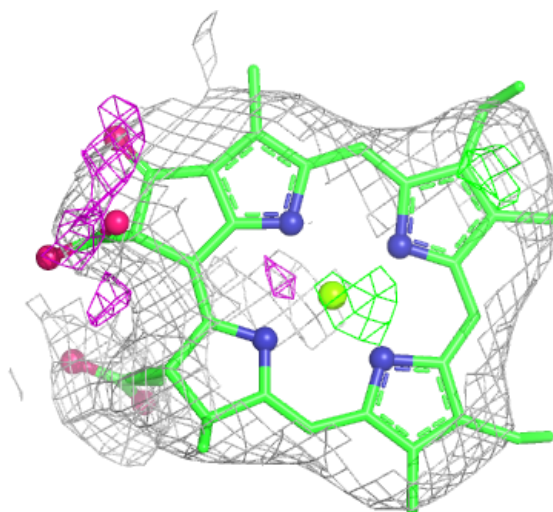
Electron density around CLA 8 311:

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



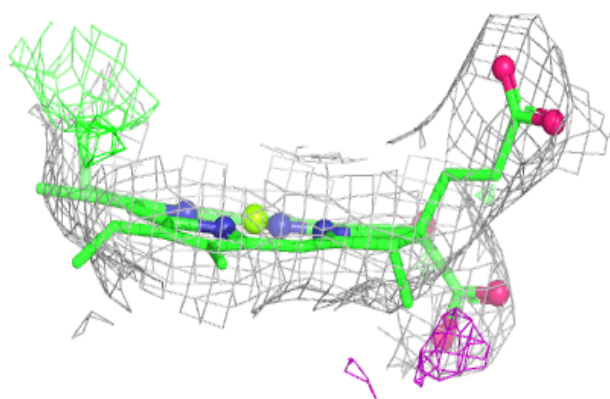
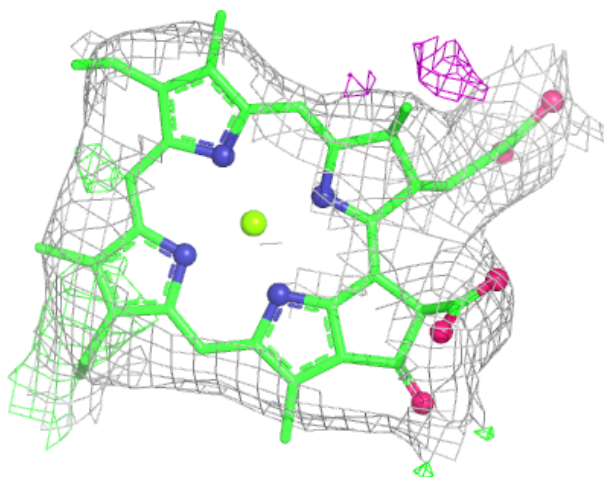
Electron density around CLA 6 311:

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



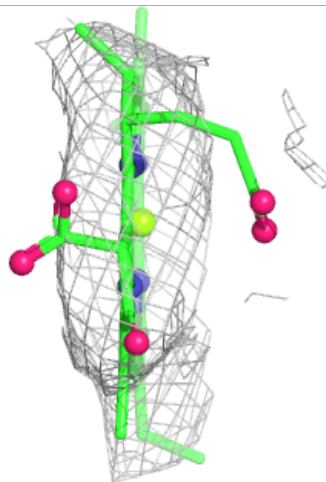
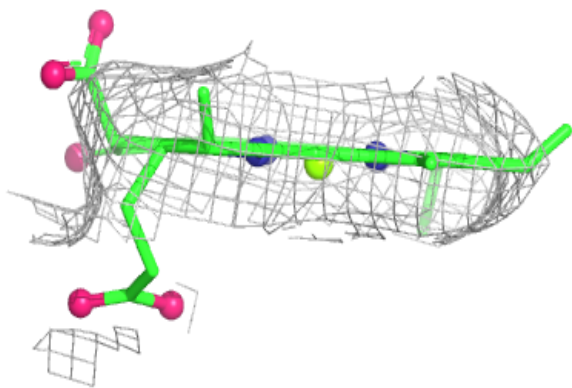
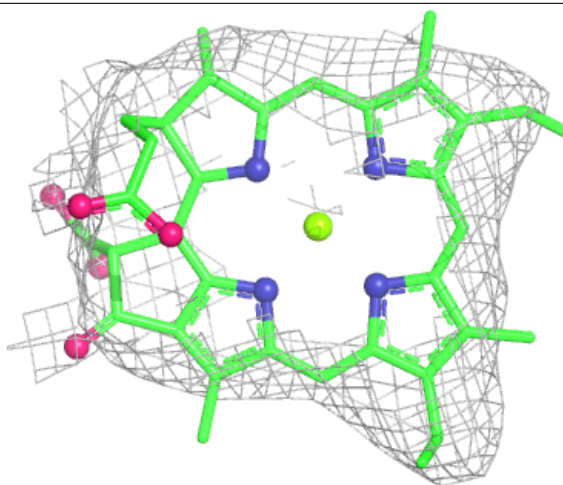
Electron density around CLA 8 313:

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



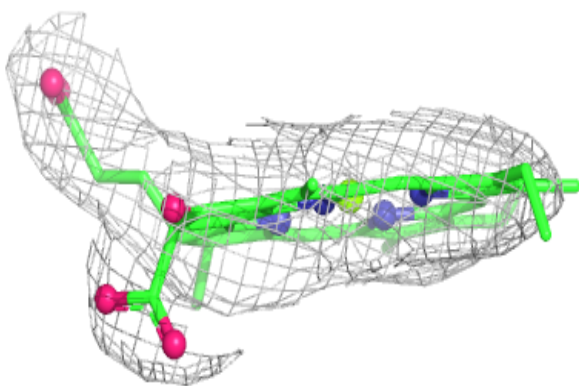
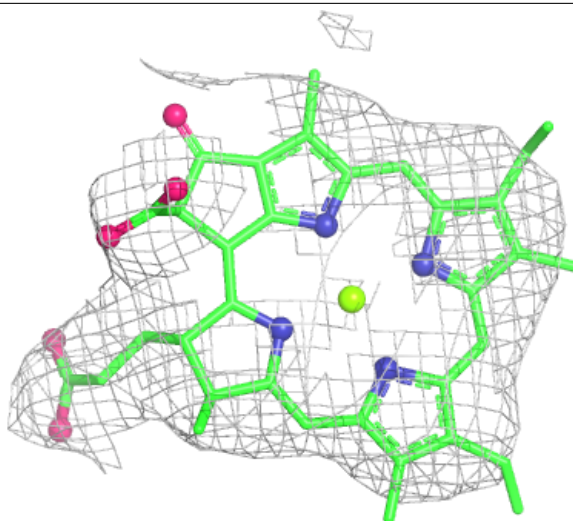
Electron density around CLA 3 1007:

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



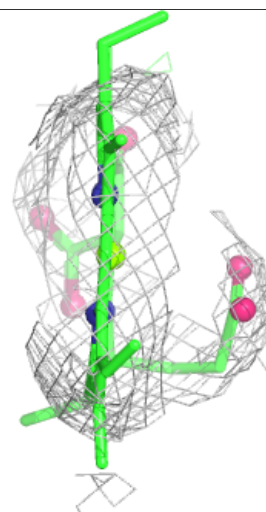
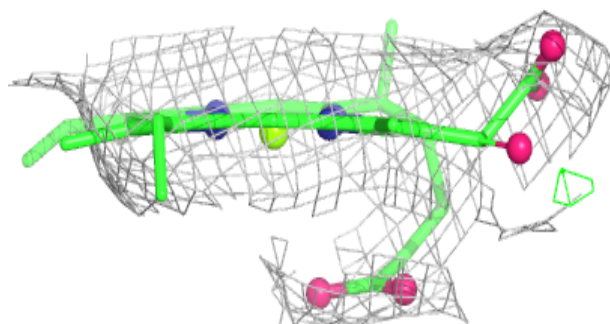
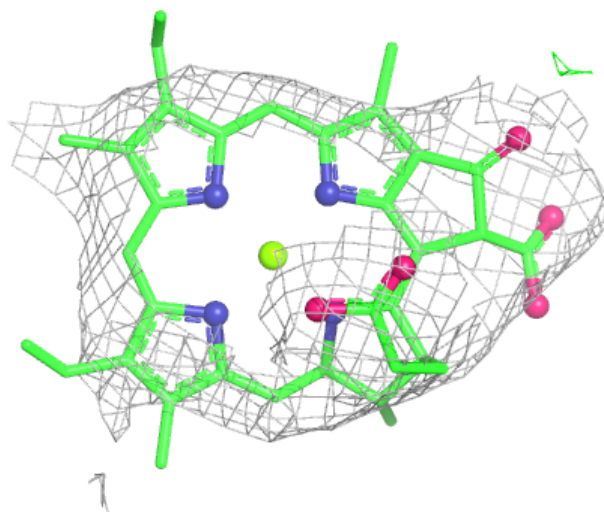
Electron density around CLA A 826:

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



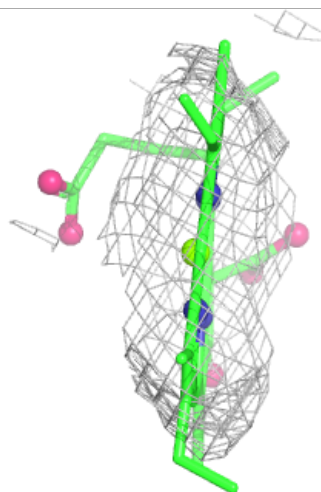
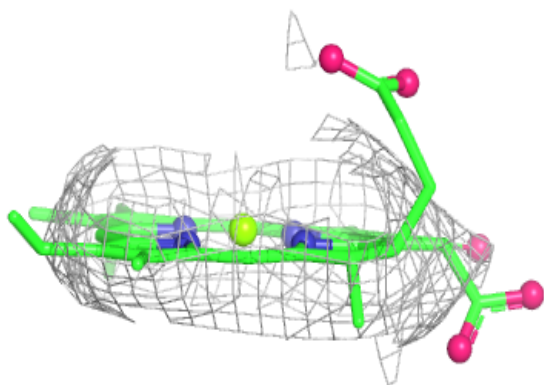
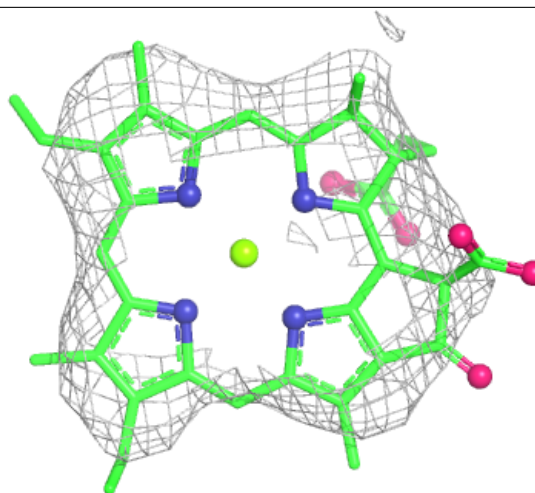
Electron density around CLA B 811:

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



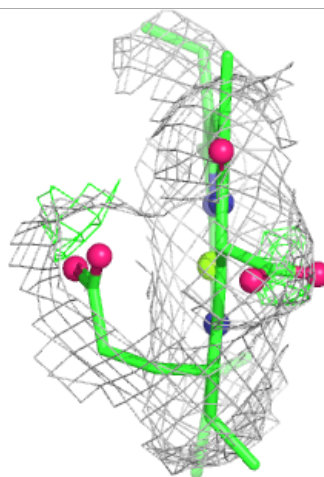
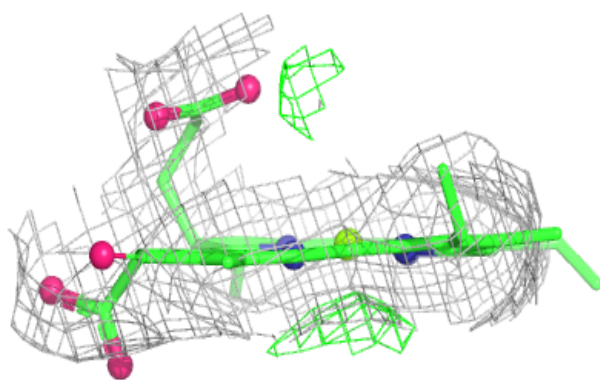
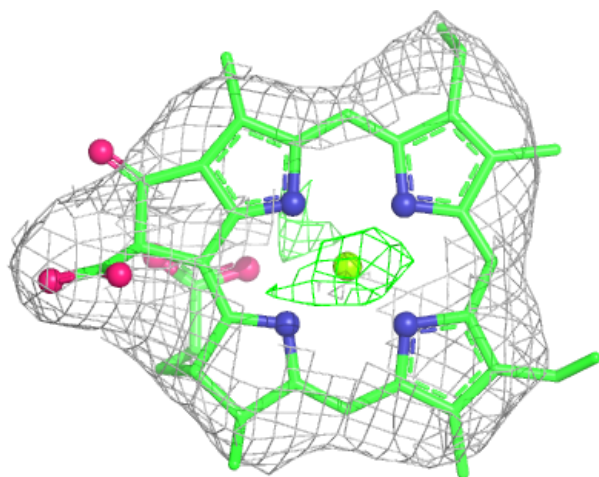
Electron density around CLA A 816:

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



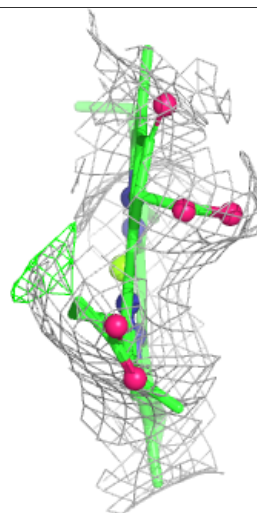
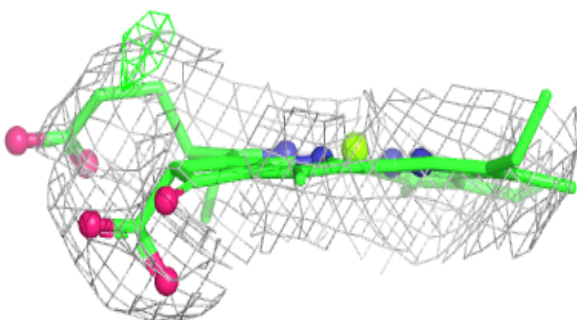
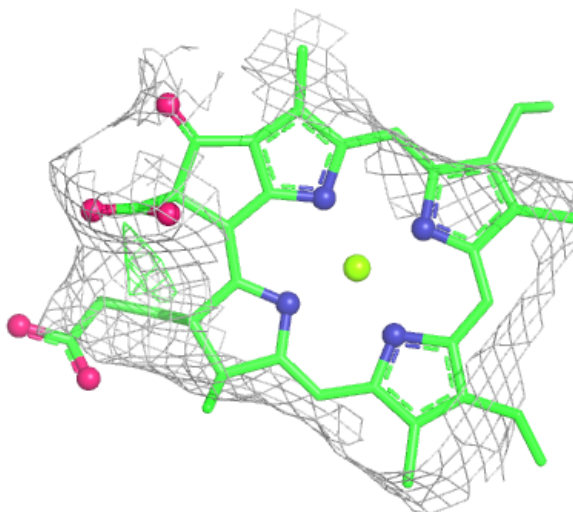
Electron density around CLA 1 1005:

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



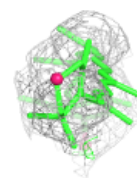
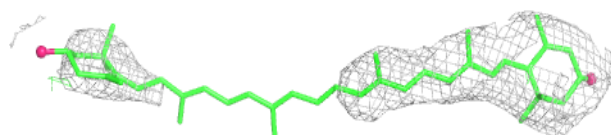
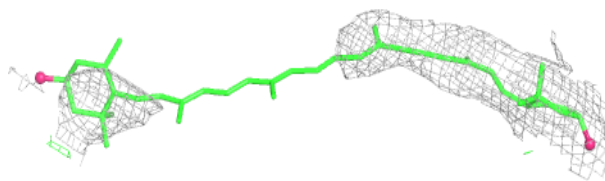
Electron density around CLA 0 309:

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



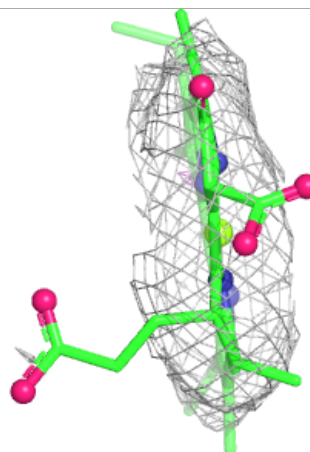
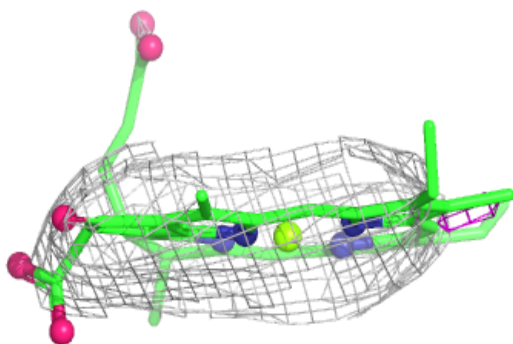
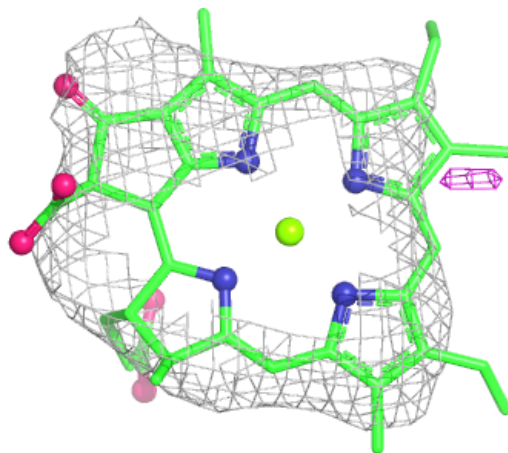
Electron density around LUT J 104:

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



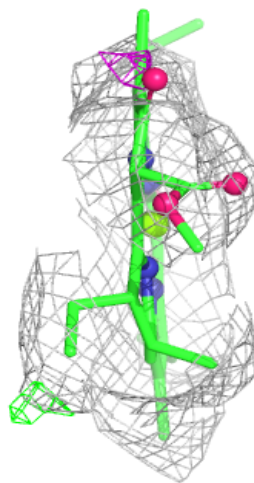
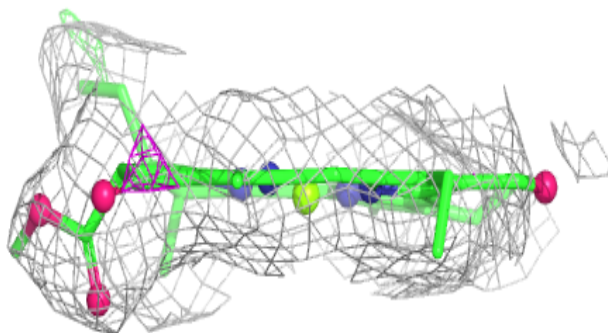
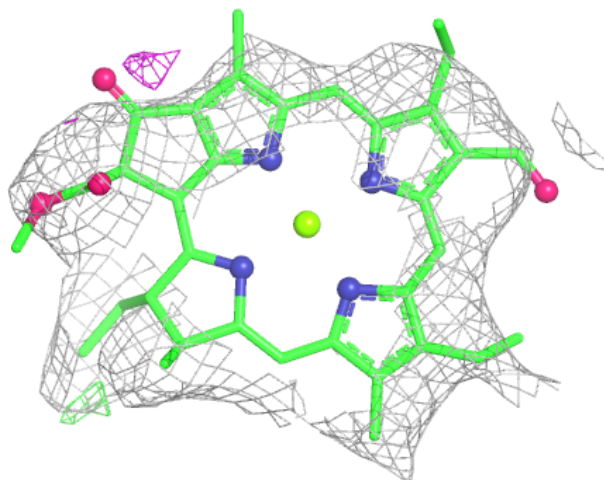
Electron density around CLA B 830:

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



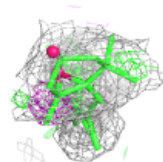
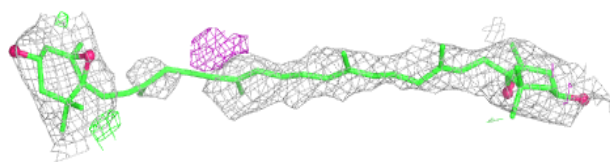
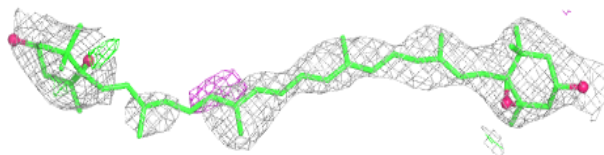
Electron density around CHL 5 317:

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



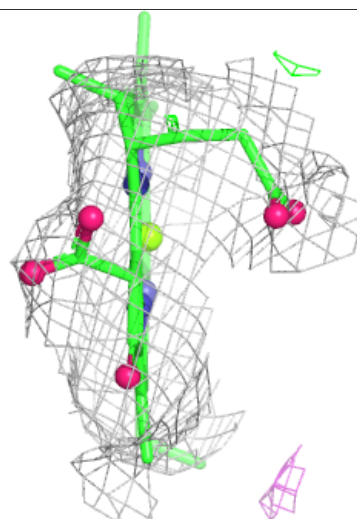
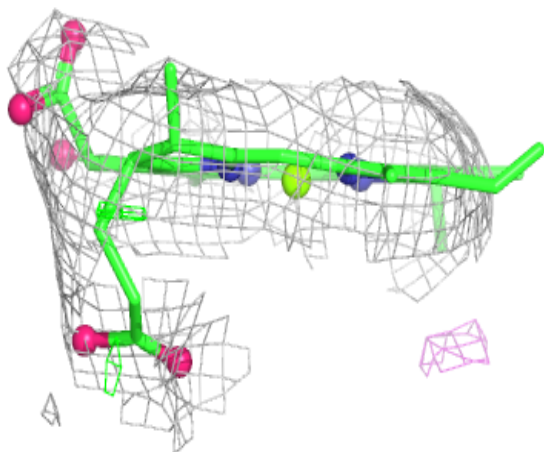
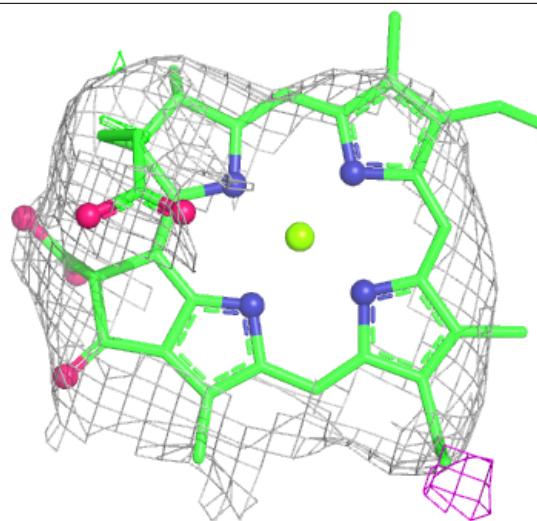
Electron density around XAT 8 304:

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



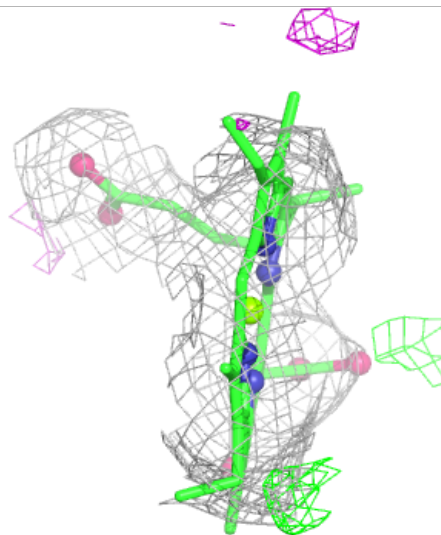
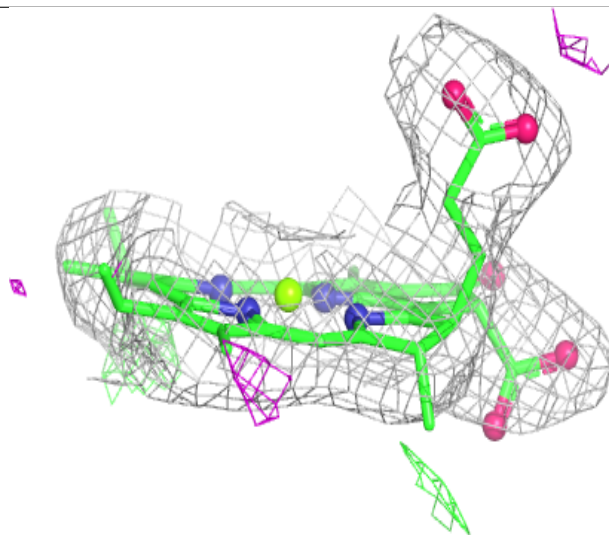
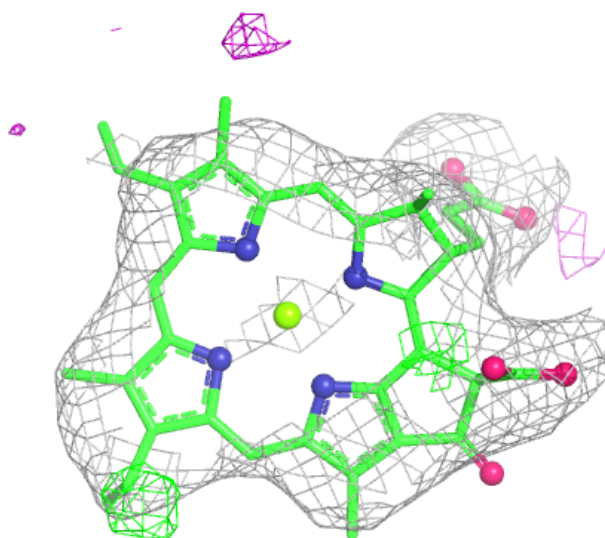
Electron density around CLA 1 1010:

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



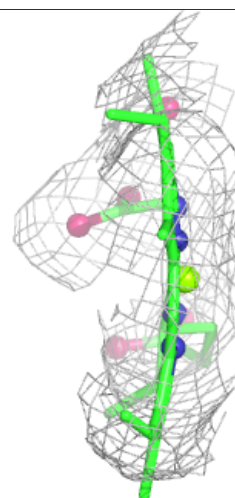
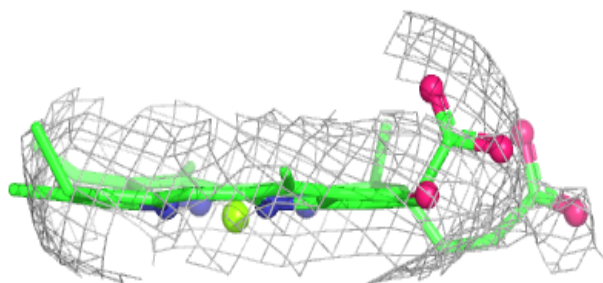
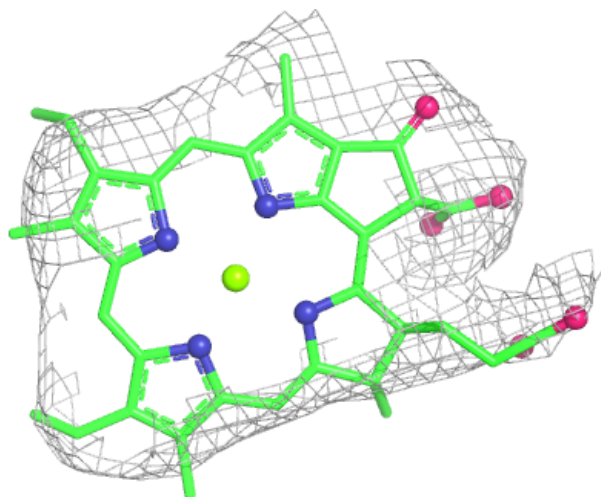
Electron density around CLA 8 316:

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



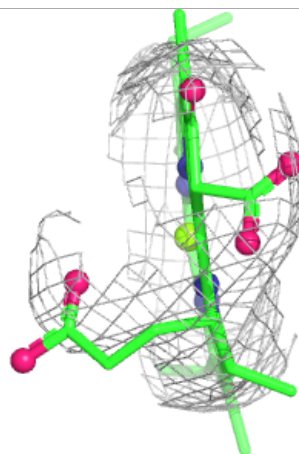
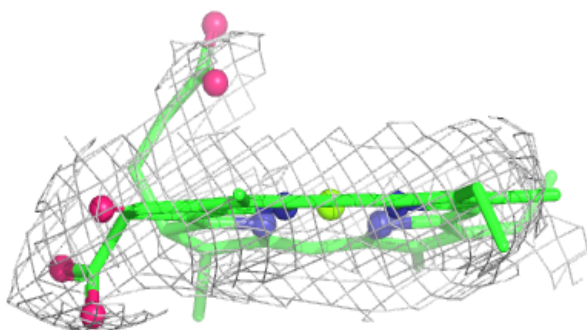
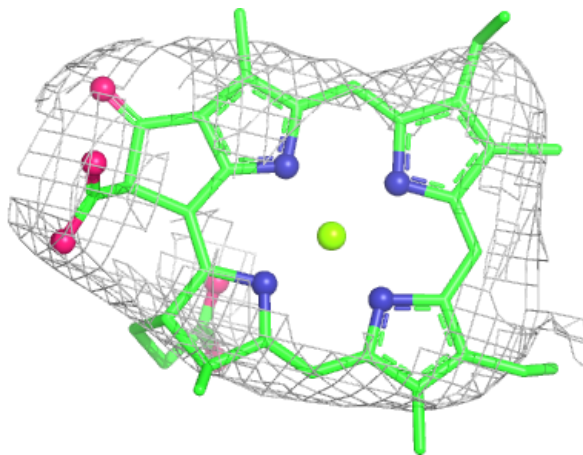
Electron density around CLA 3 1006:

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



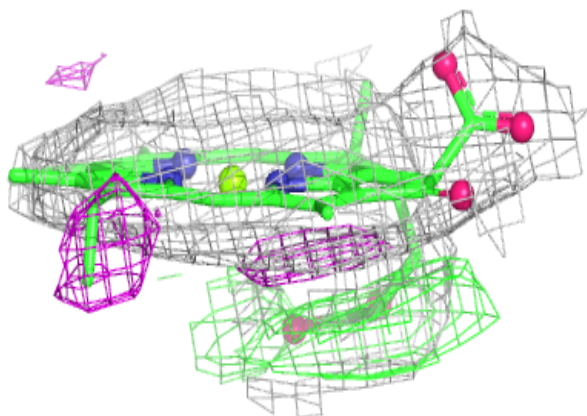
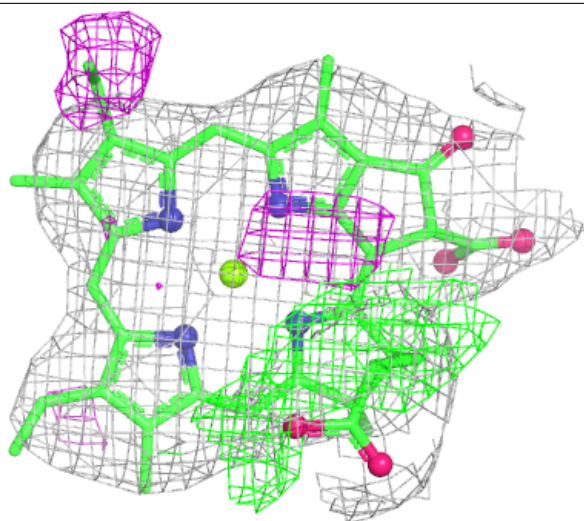
Electron density around CLA B 807:

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



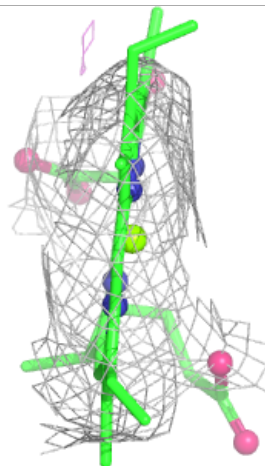
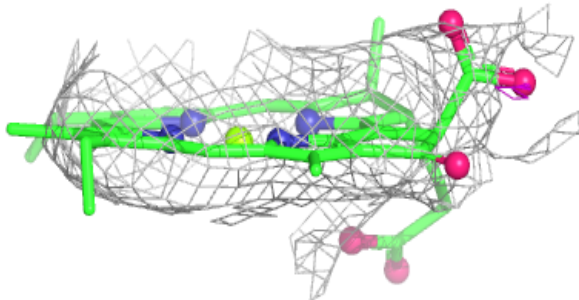
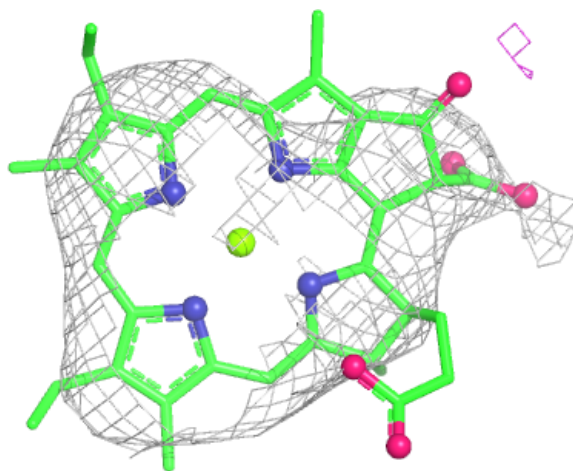
Electron density around CLA 6 308:

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



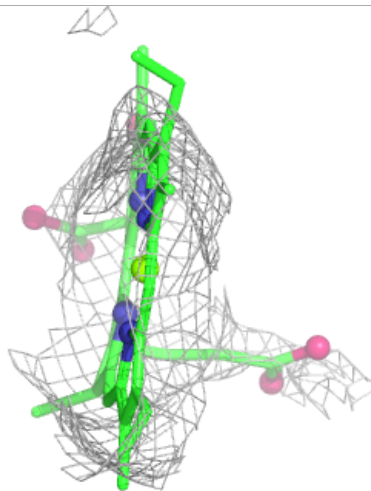
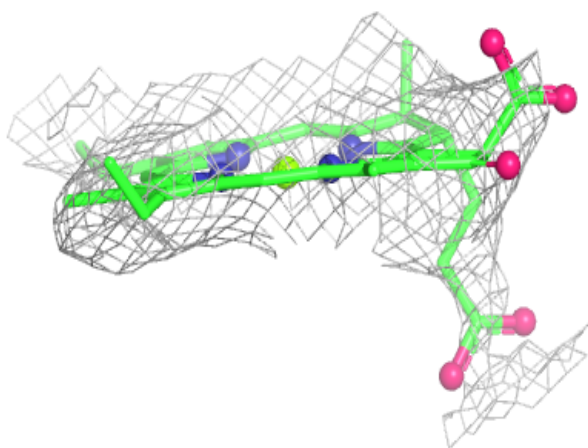
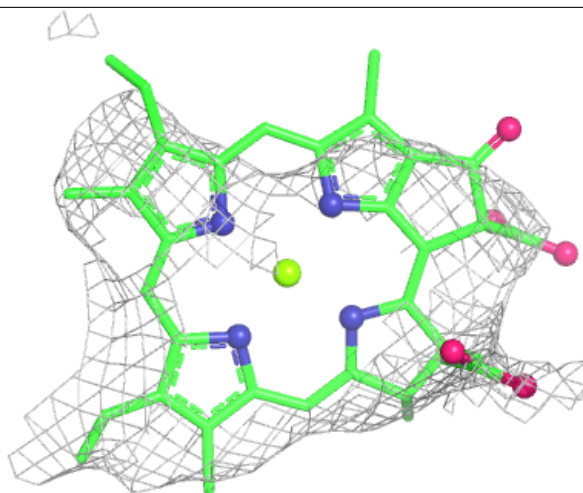
Electron density around CLA B 829:

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



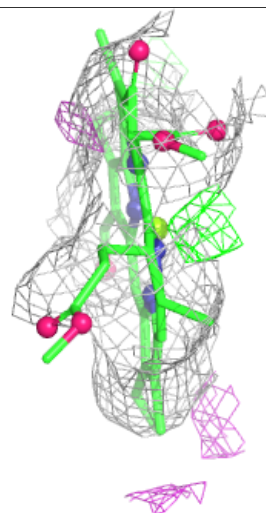
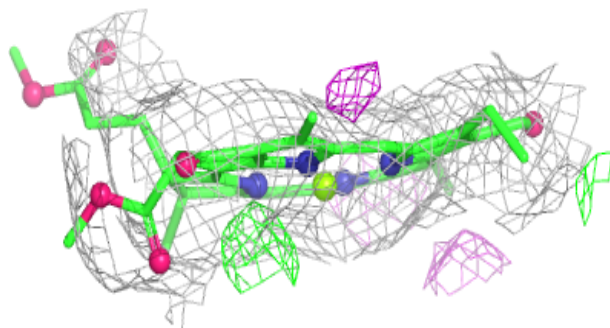
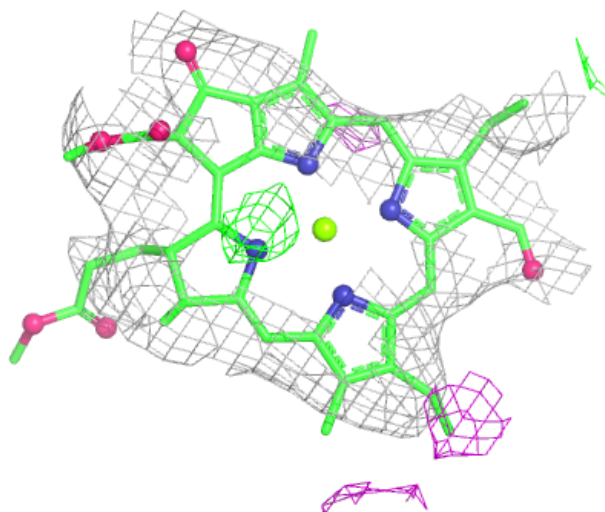
Electron density around CLA B 817:

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



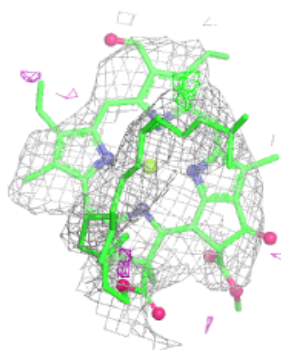
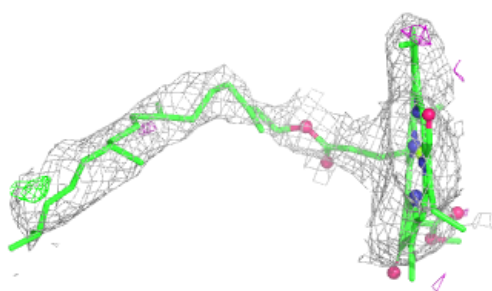
Electron density around CHL 7 1012:

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



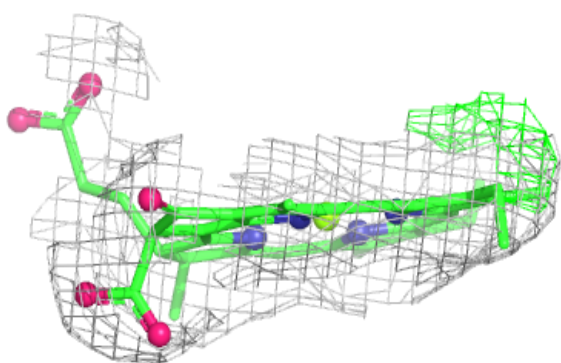
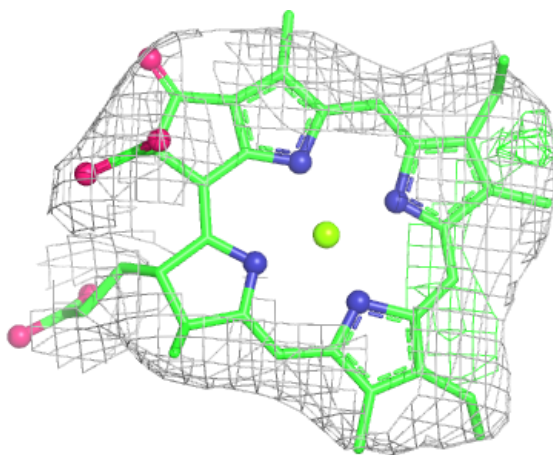
Electron density around CHL 7 1017:

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



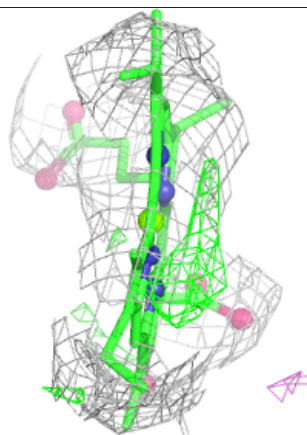
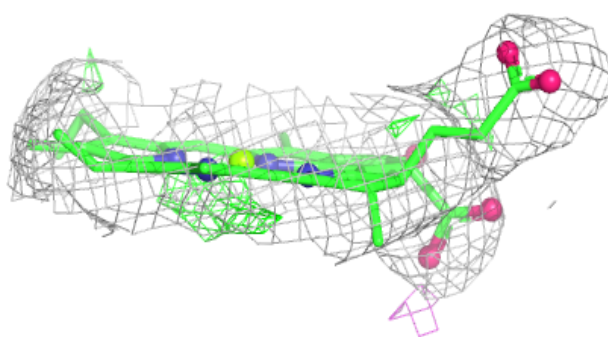
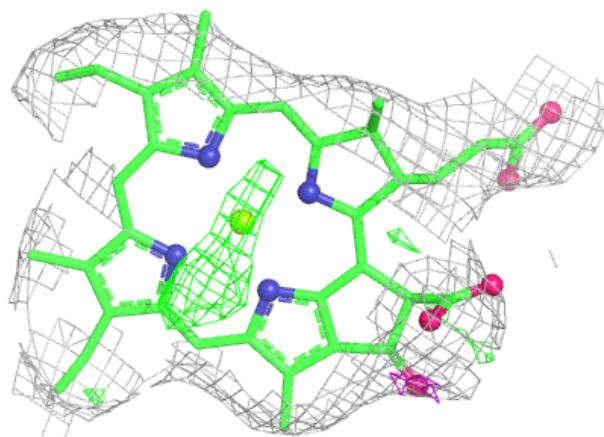
Electron density around CLA 6 318:

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



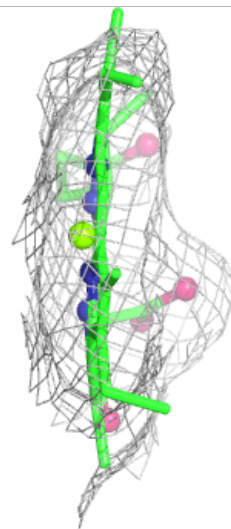
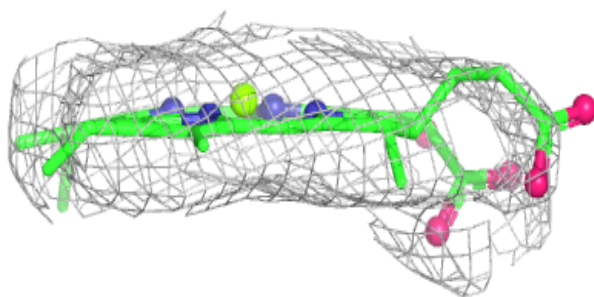
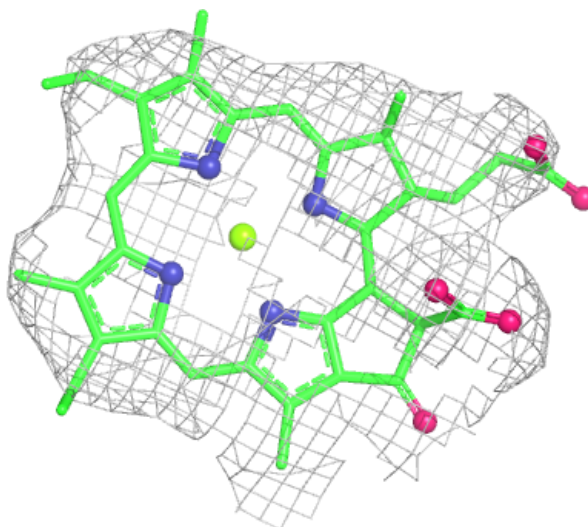
Electron density around CLA 6 320:

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



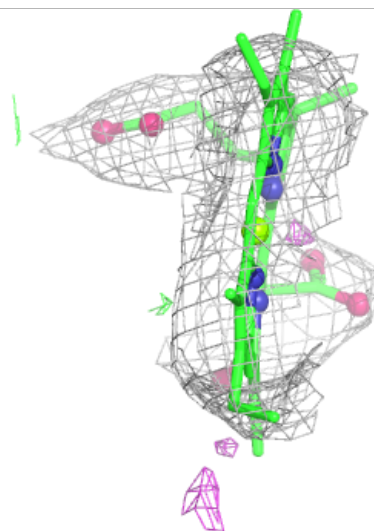
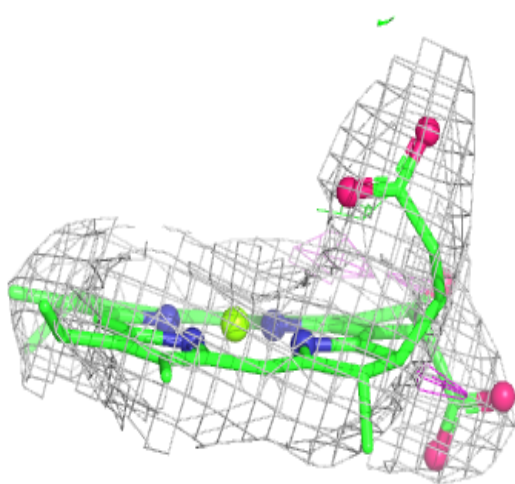
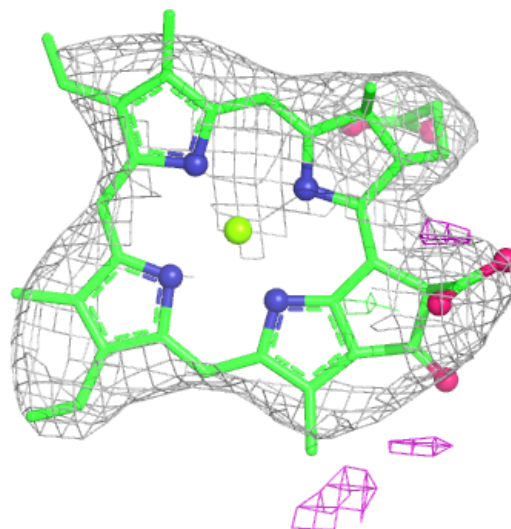
Electron density around CLA 5 305:

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



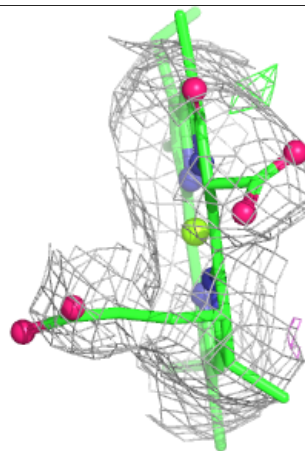
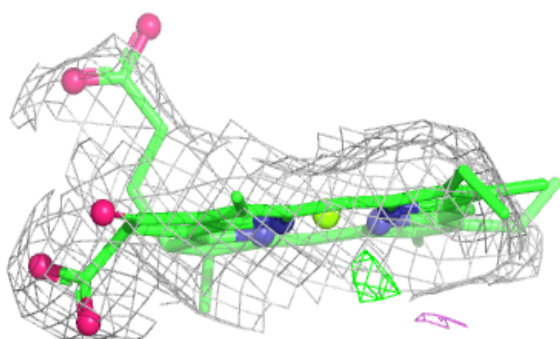
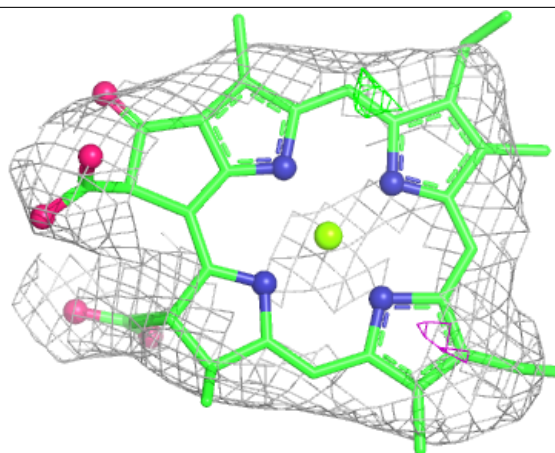
Electron density around CLA 5 309:

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



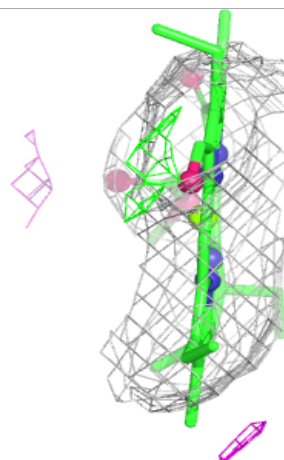
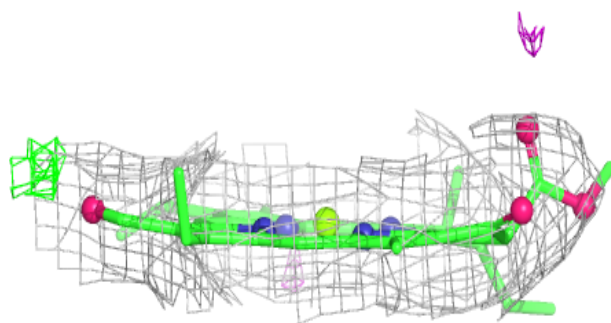
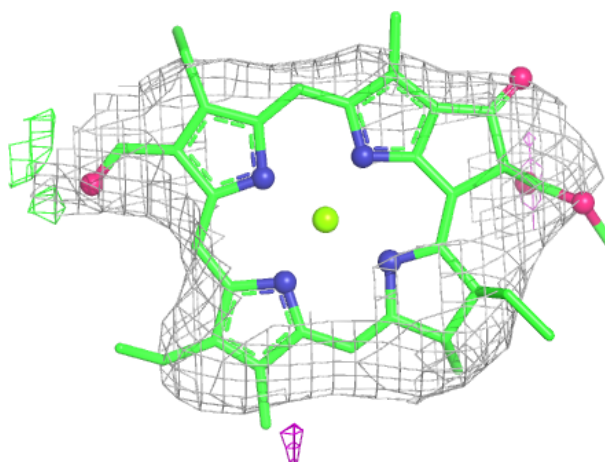
Electron density around CLA 5 310:

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



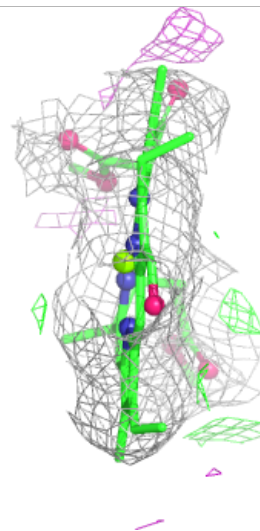
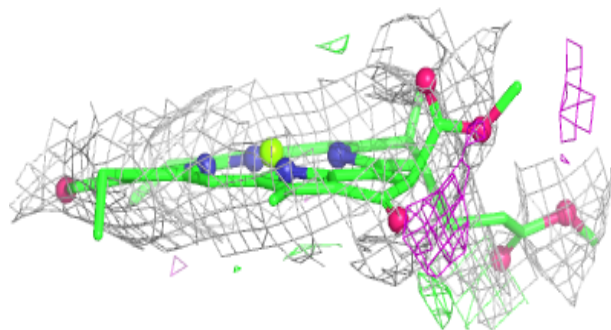
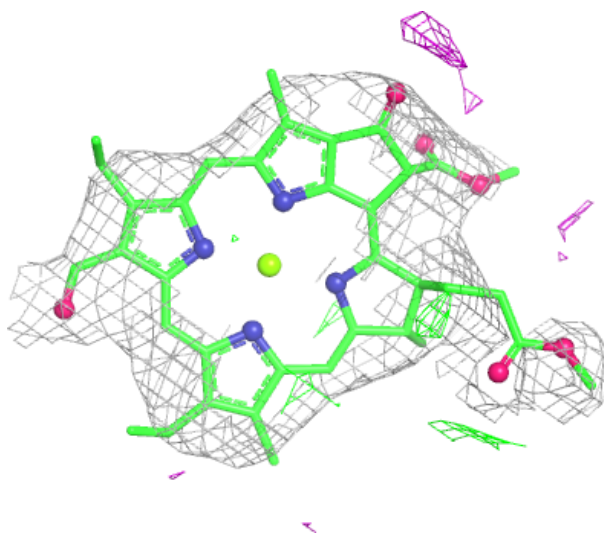
Electron density around CHL 4 316:

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



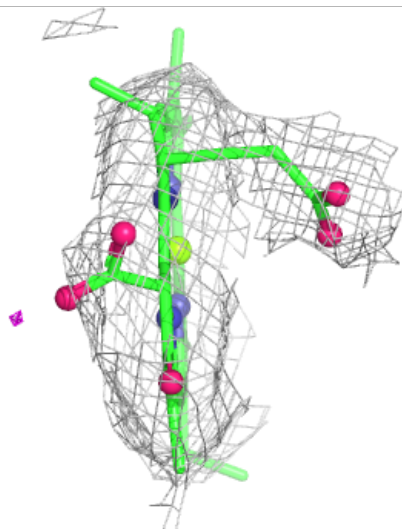
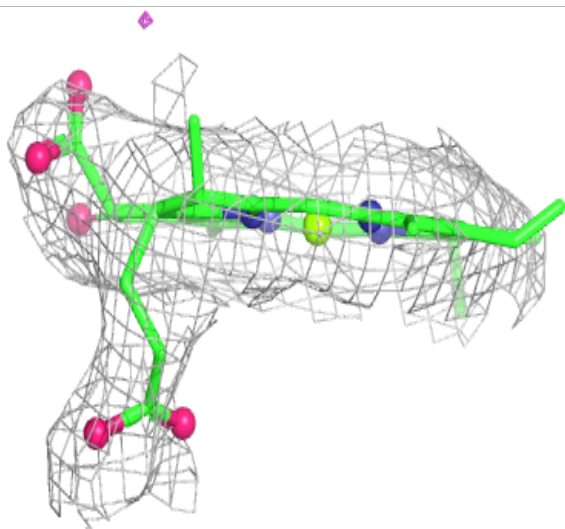
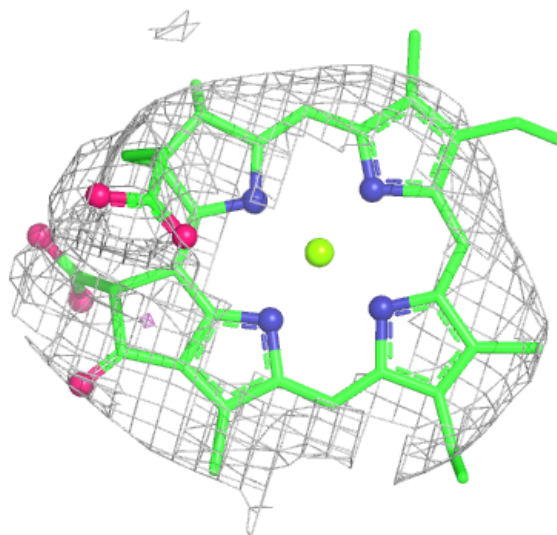
Electron density around CHL 6 313:

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



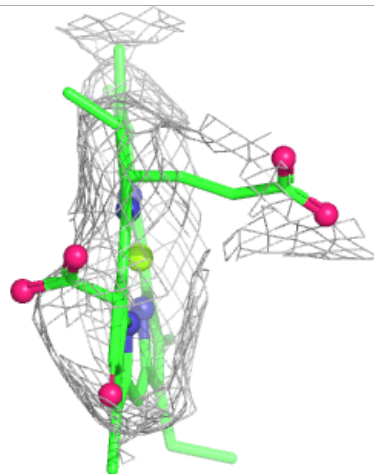
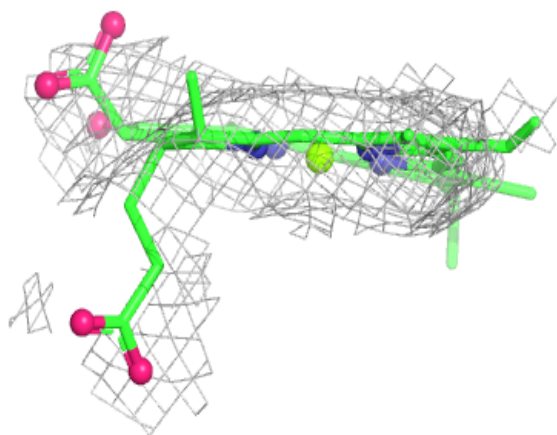
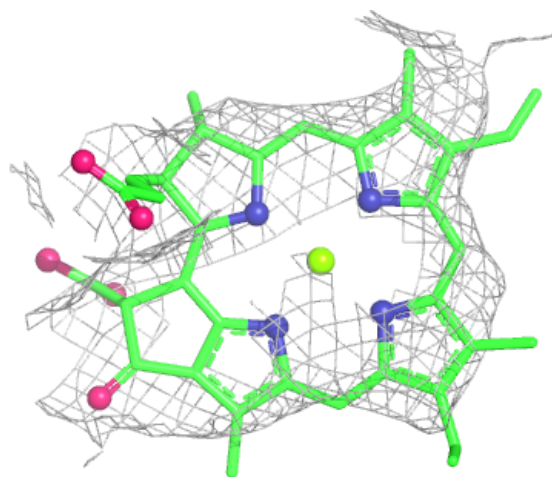
Electron density around CLA 0 312:

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



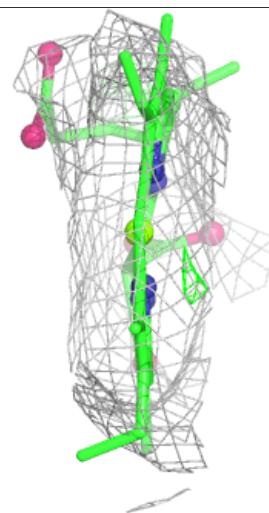
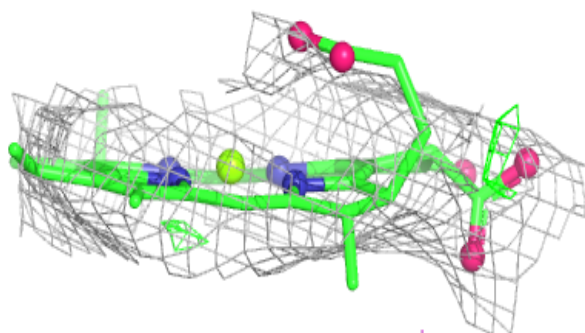
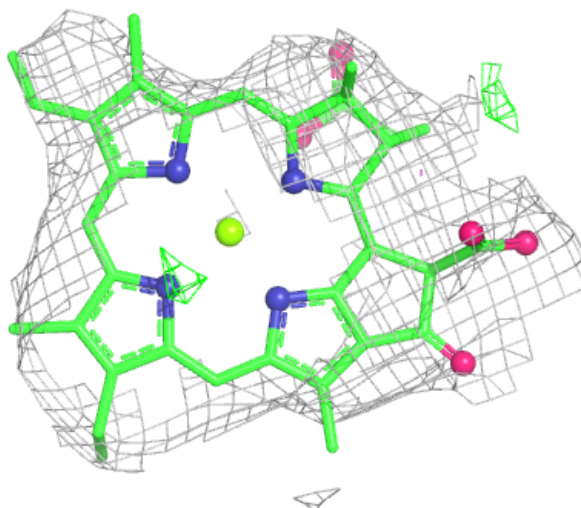
Electron density around CLA B 831:

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



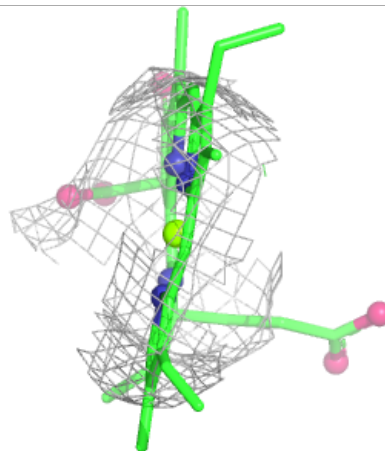
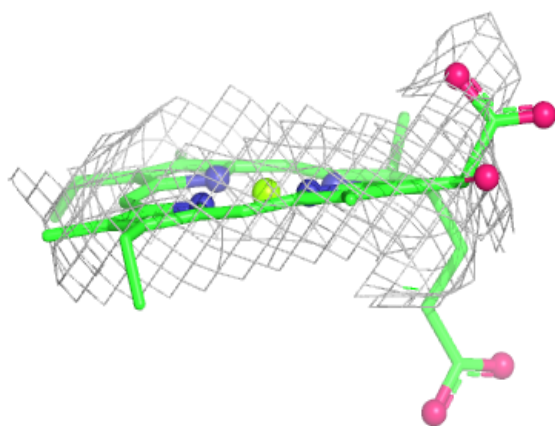
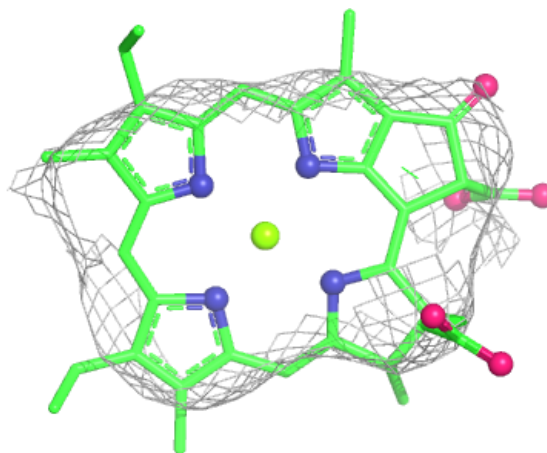
Electron density around CLA 0 305:

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



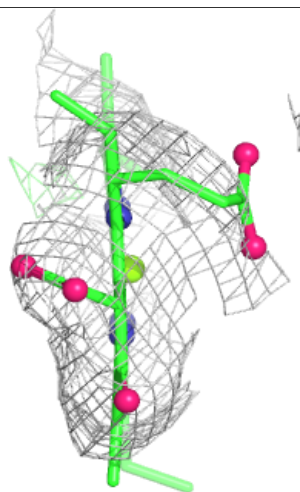
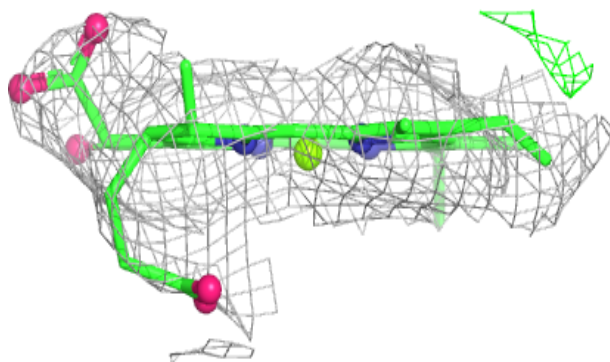
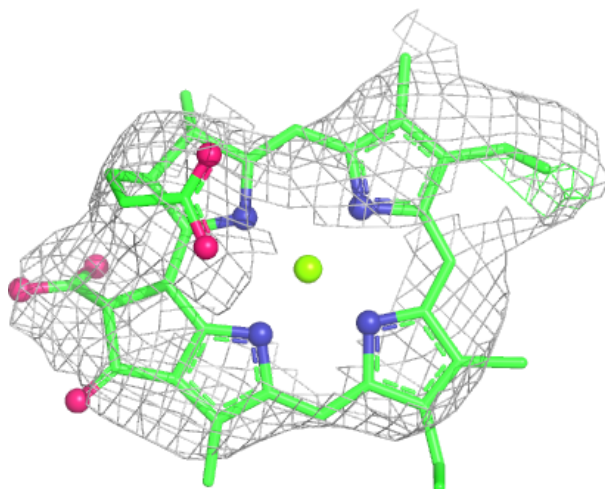
Electron density around CLA B 818:

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



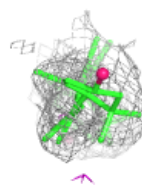
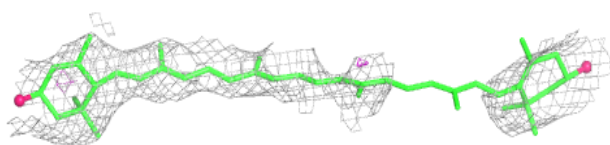
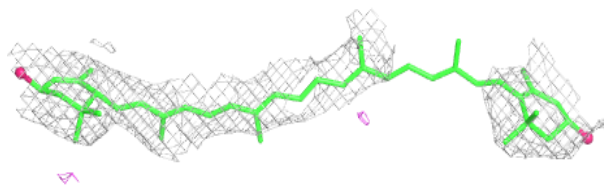
Electron density around CLA A 811:

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



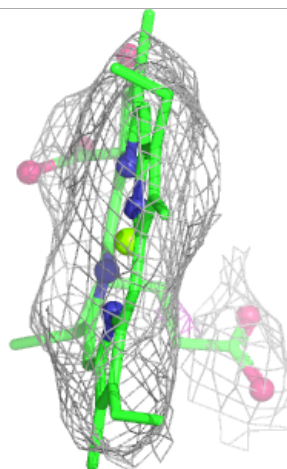
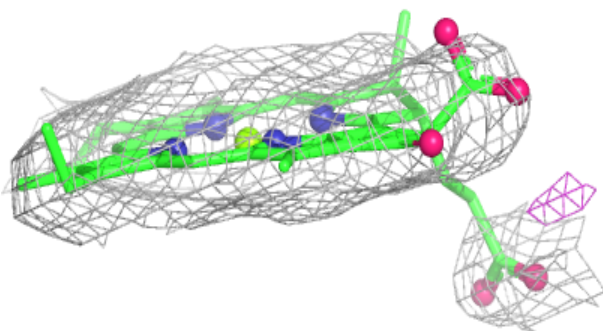
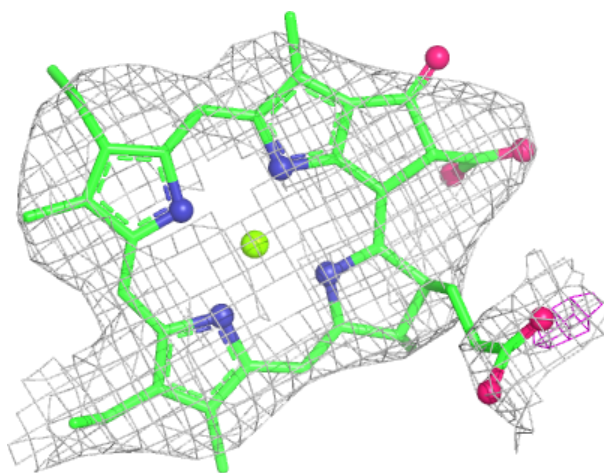
Electron density around LUT 3 1001:

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



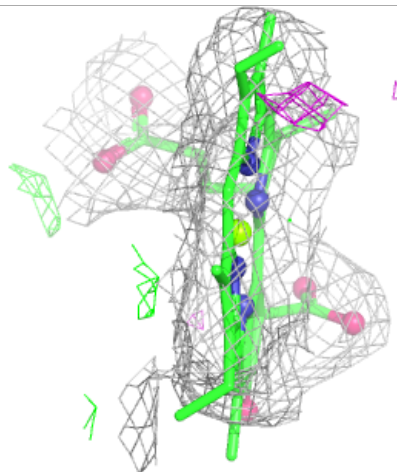
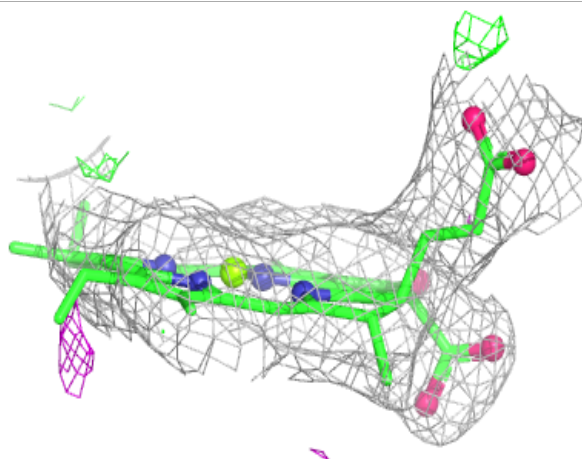
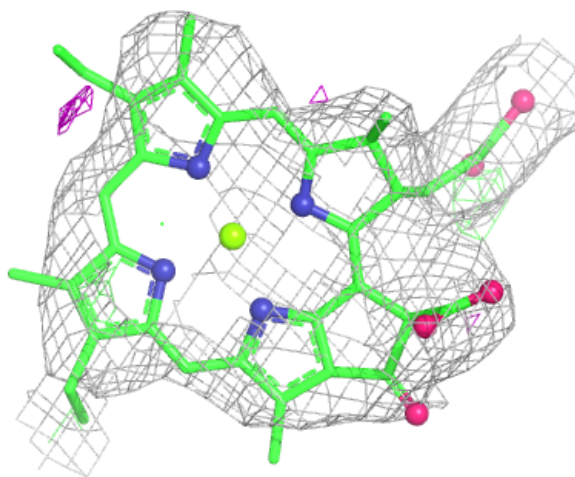
Electron density around CLA A 803:

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



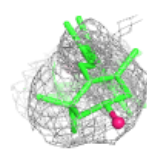
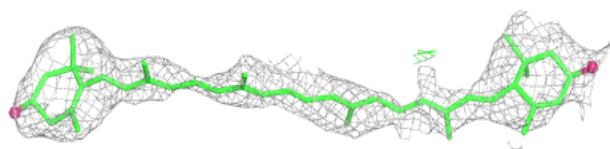
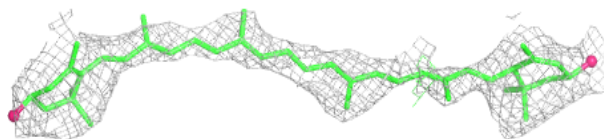
Electron density around CLA 6 312:

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

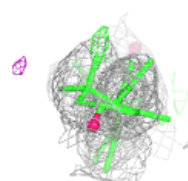
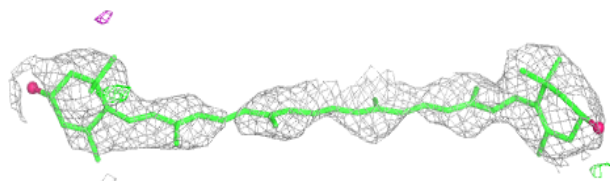
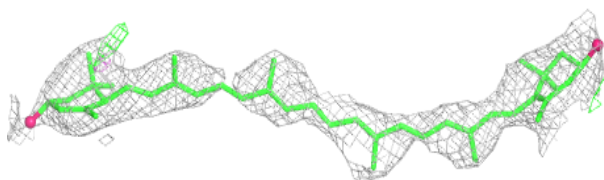


Electron density around LUT 4 317:

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

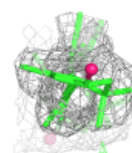
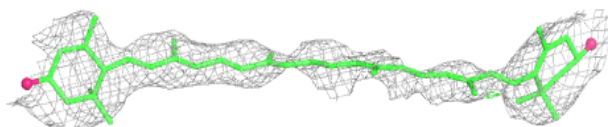
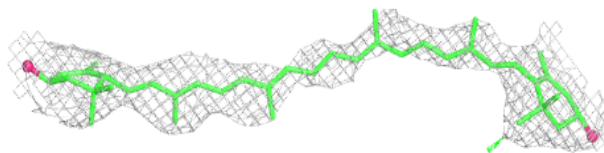
**Electron density around LUT 6 303:**

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



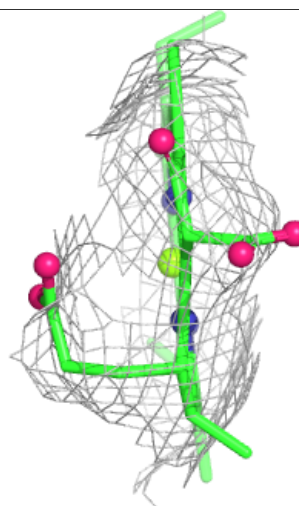
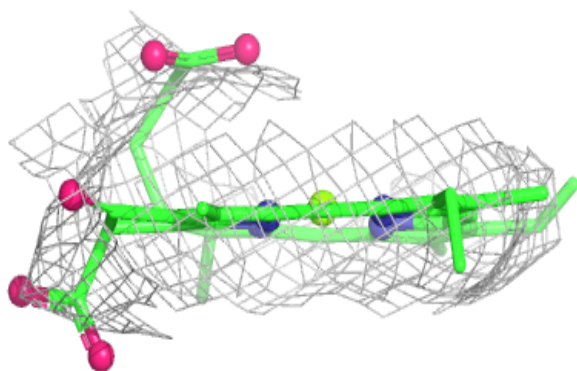
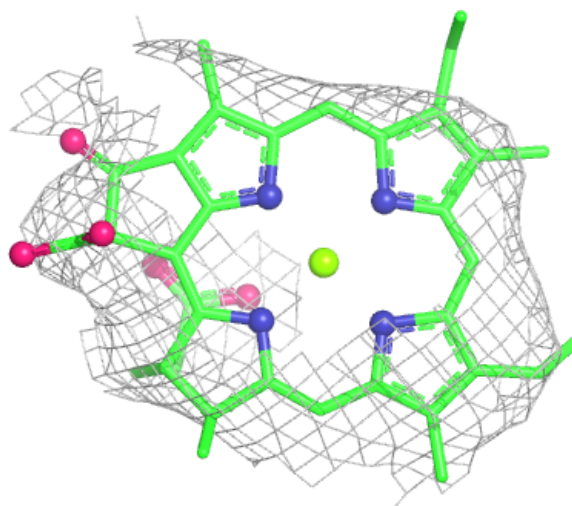
Electron density around LUT 5 302:

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



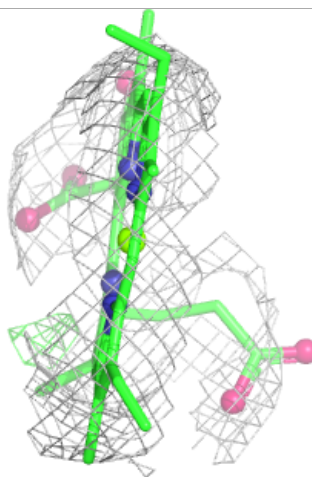
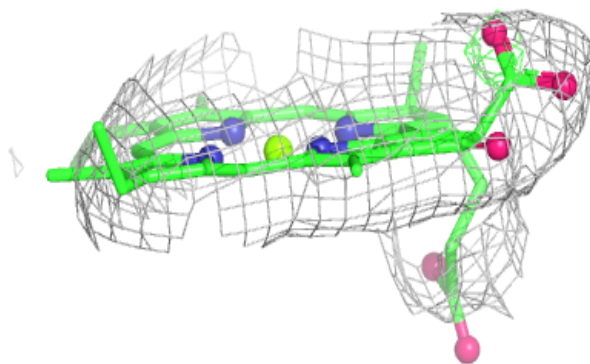
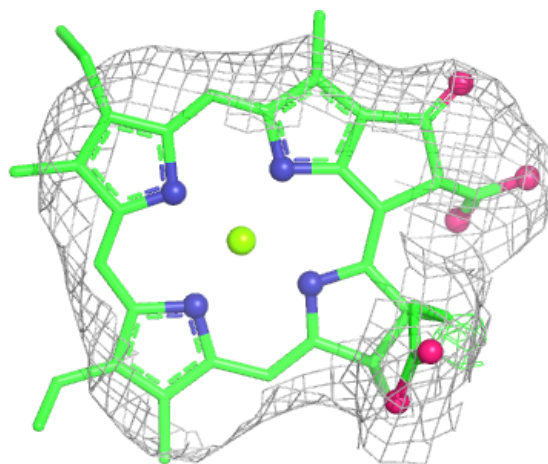
Electron density around CLA A 835:

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



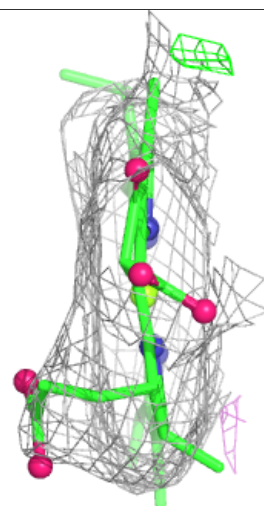
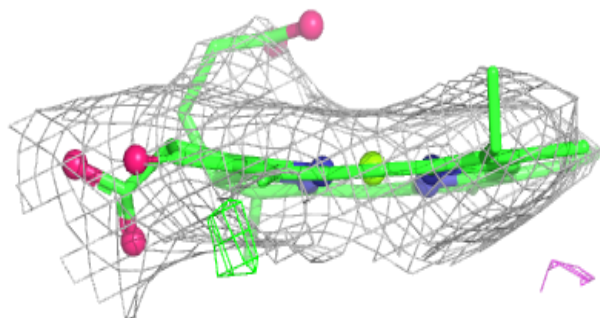
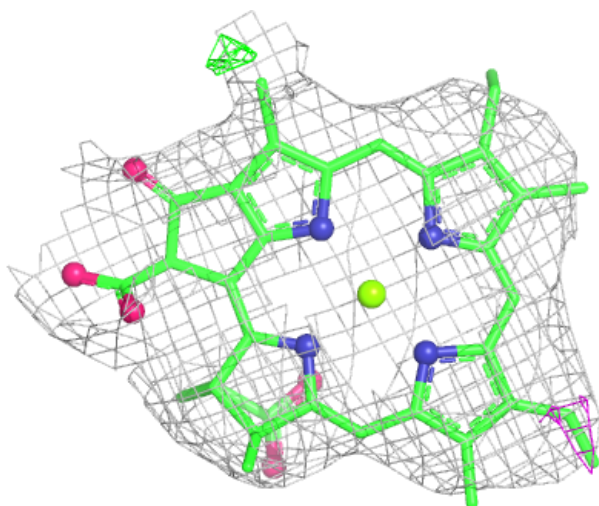
Electron density around CLA 3 1013:

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



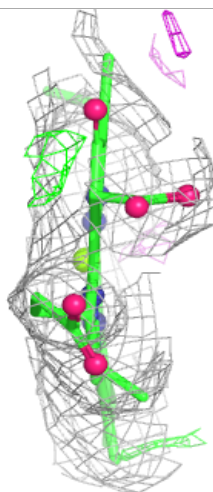
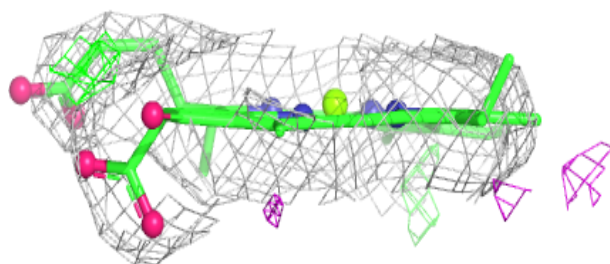
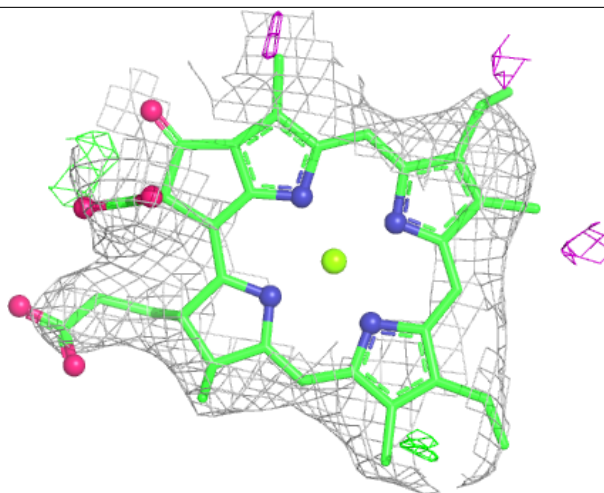
Electron density around CLA 1 1003:

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



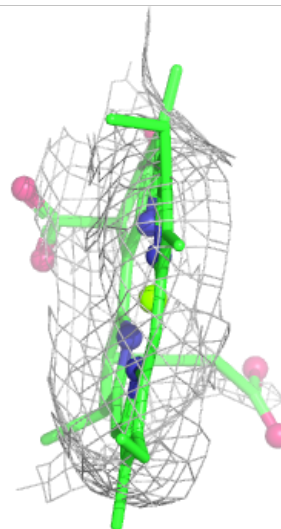
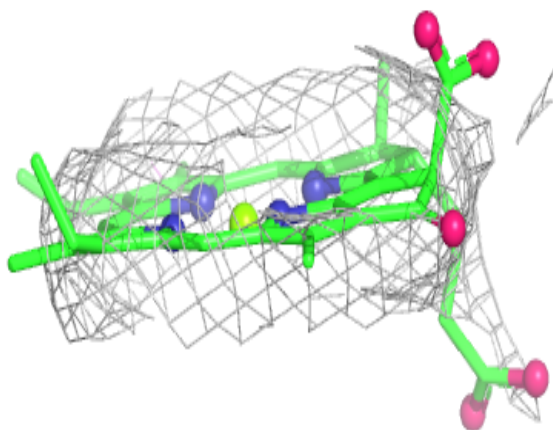
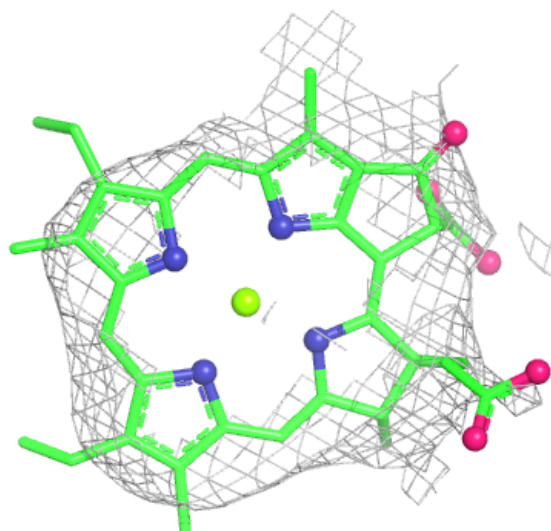
Electron density around CLA 5 308:

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



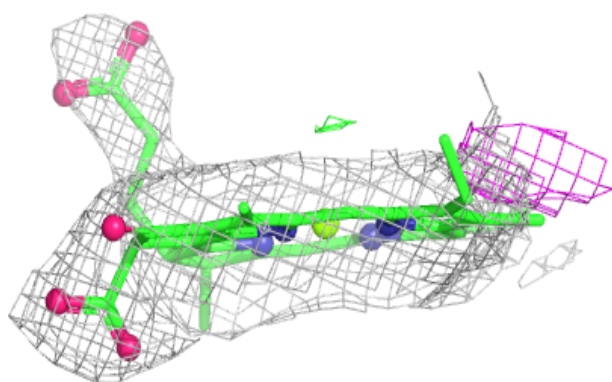
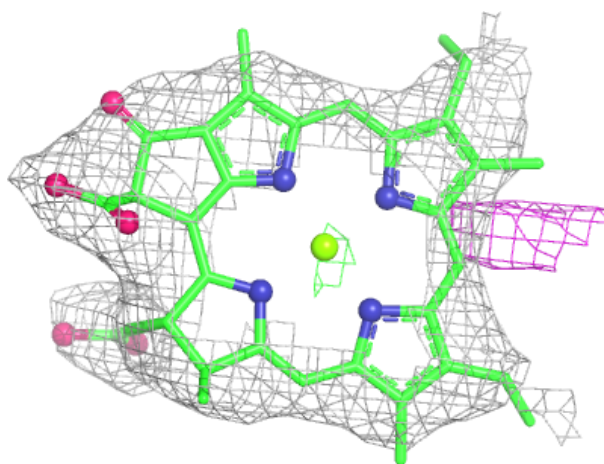
Electron density around CLA A 836:

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



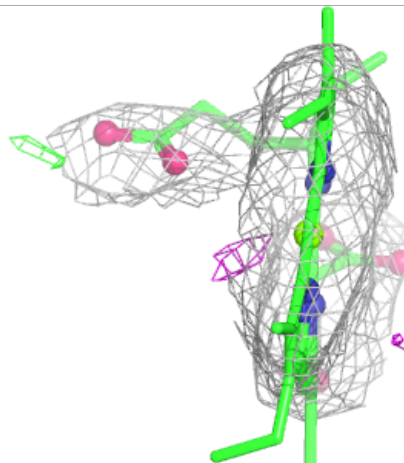
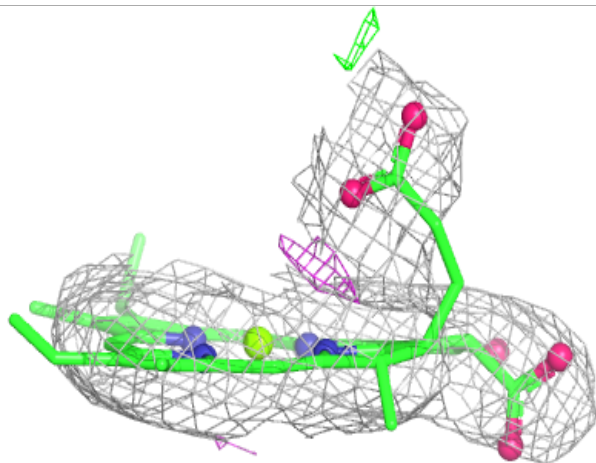
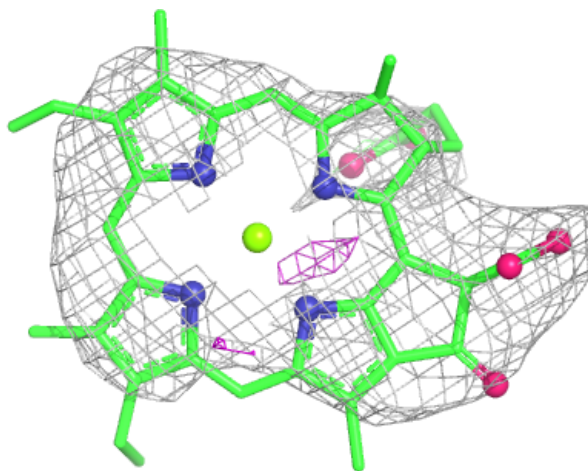
Electron density around CLA F 302:

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



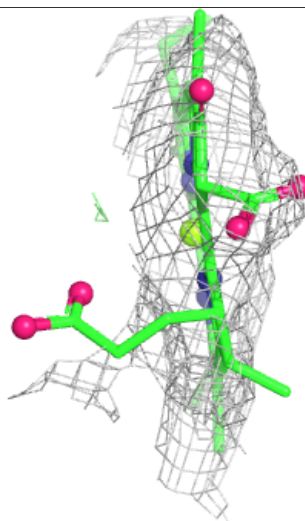
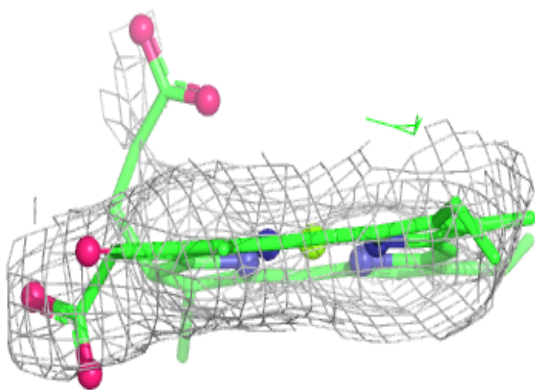
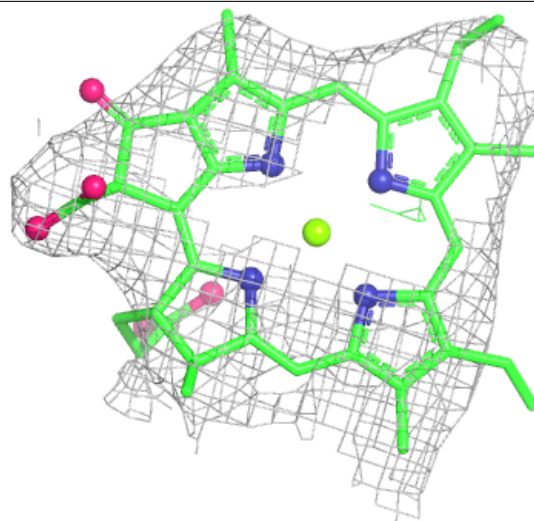
Electron density around CLA A 810:

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



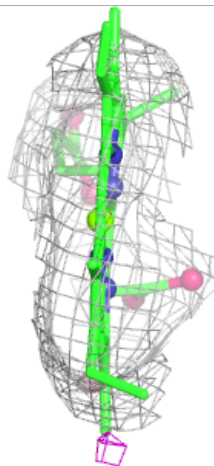
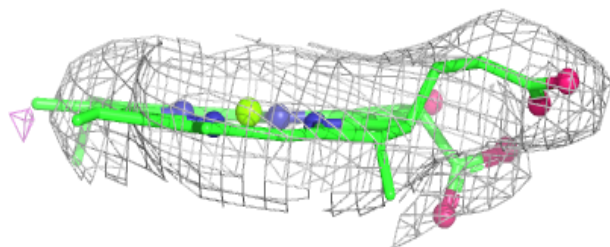
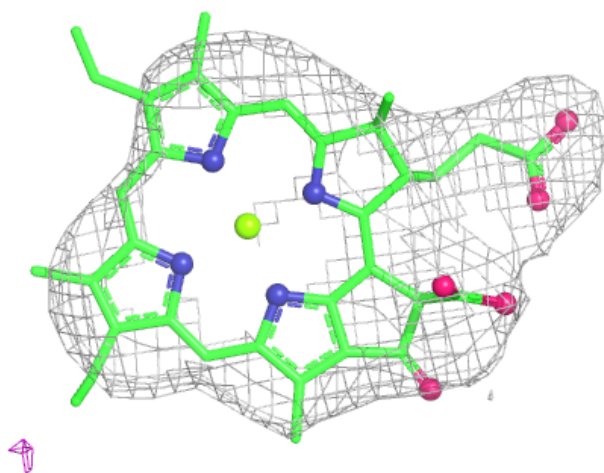
Electron density around CLA 1 1008:

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



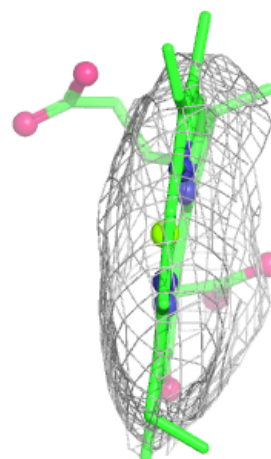
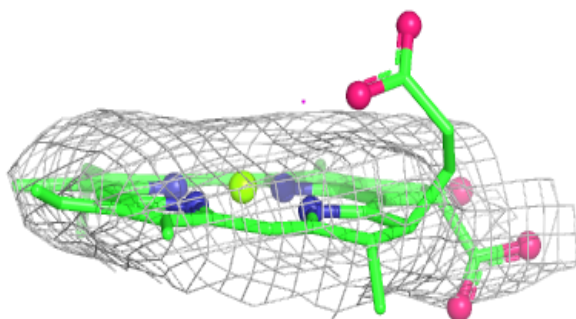
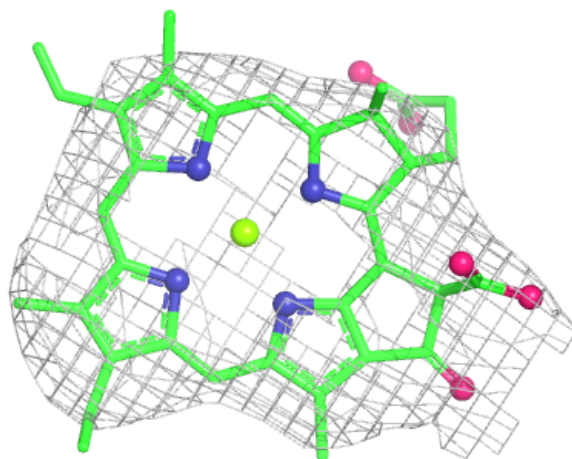
Electron density around CLA F 305:

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



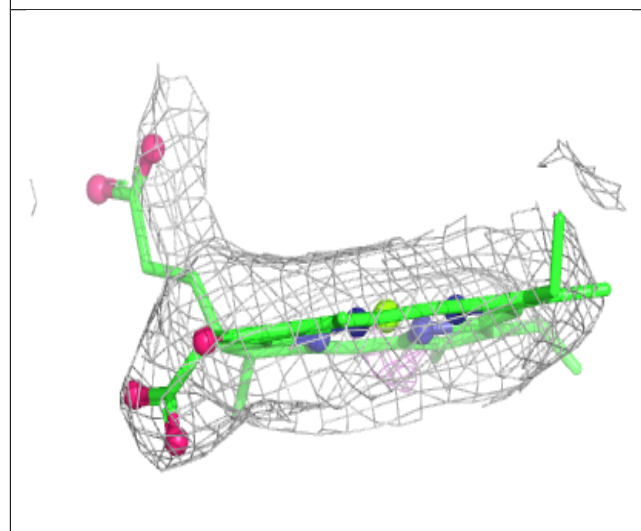
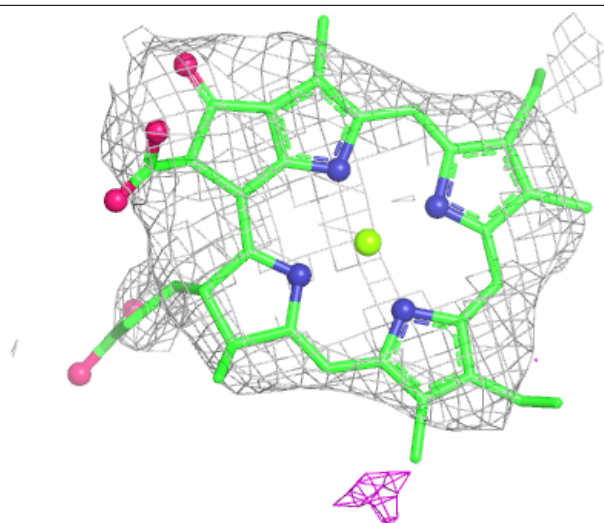
Electron density around CLA A 817:

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



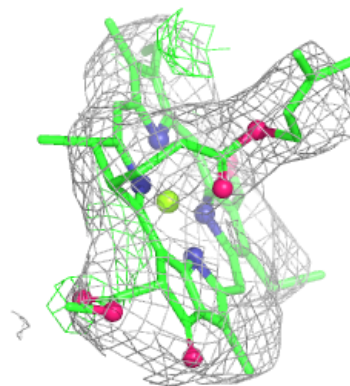
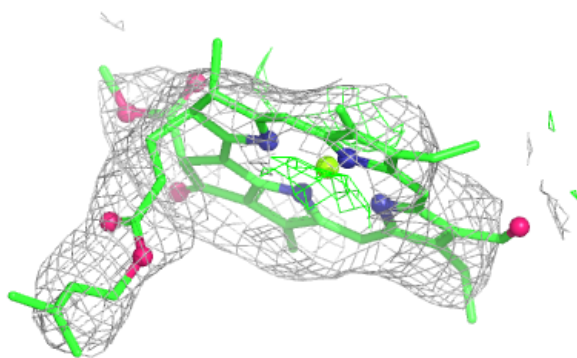
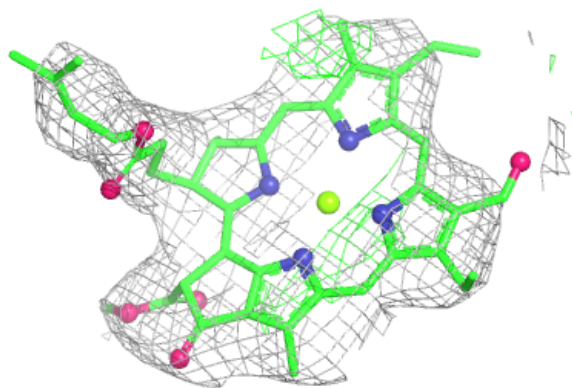
Electron density around CLA 1 1011:

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



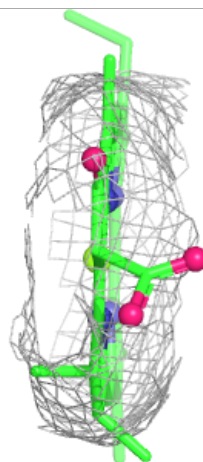
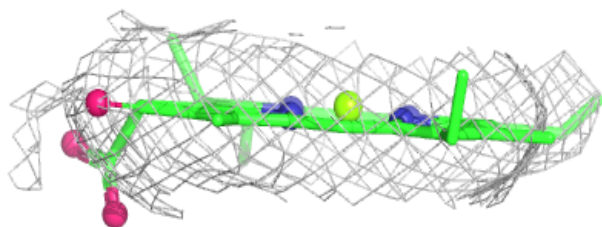
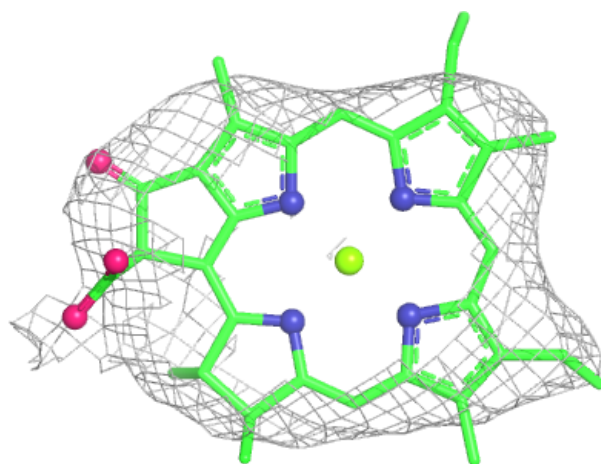
Electron density around CHL 4 313:

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



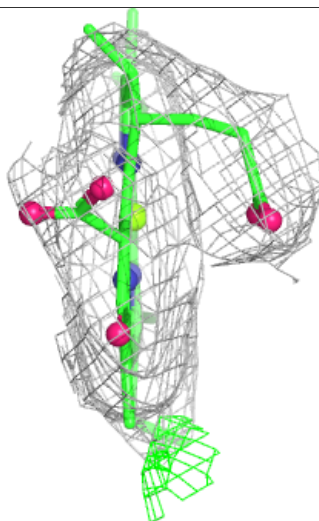
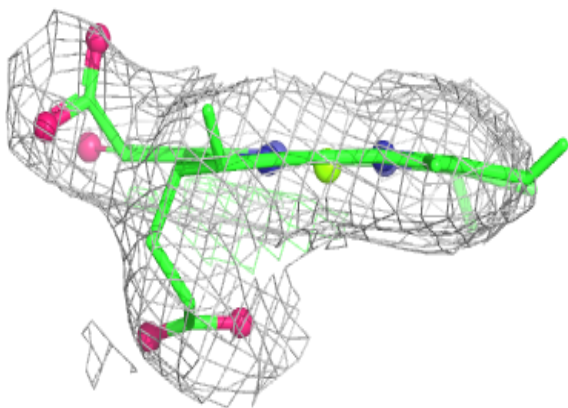
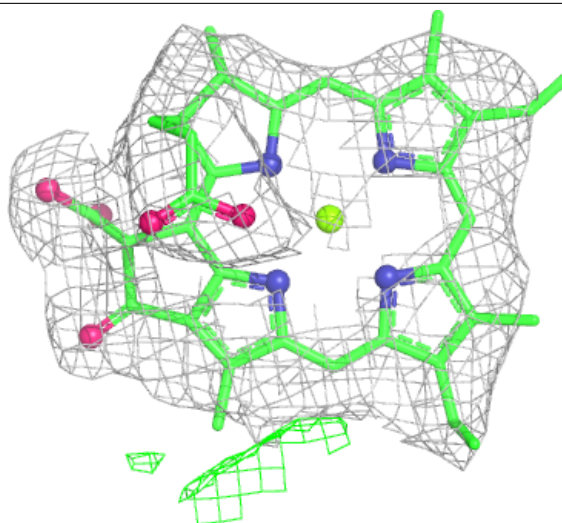
Electron density around CLA A 814:

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



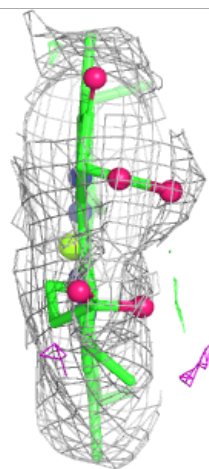
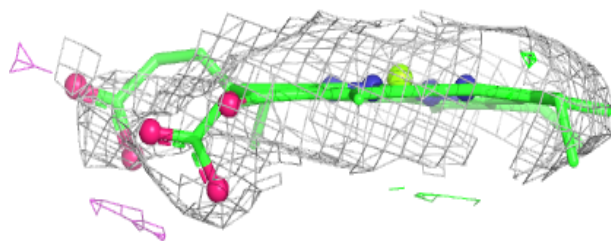
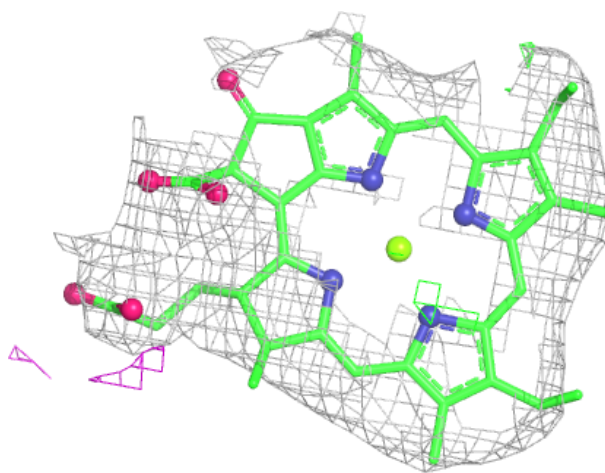
Electron density around CLA 7 1006:

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



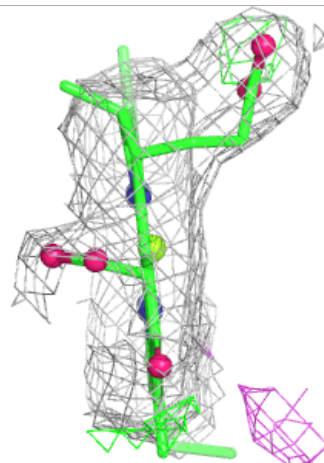
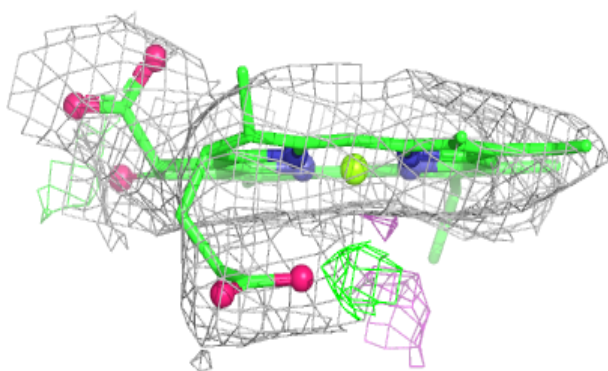
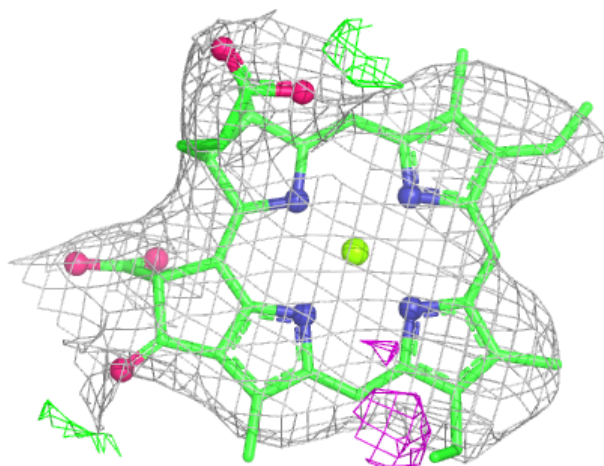
Electron density around CLA 4 305:

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



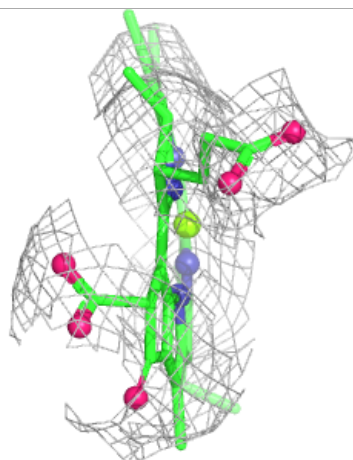
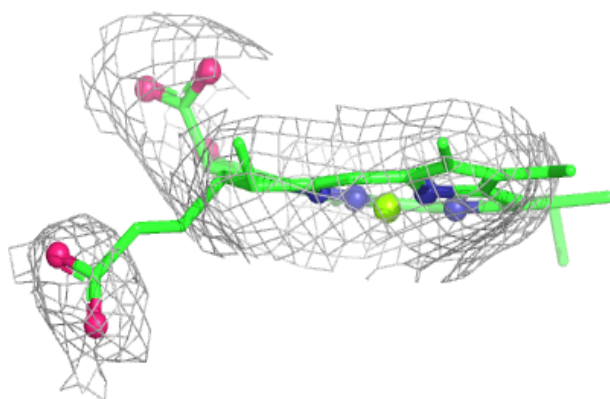
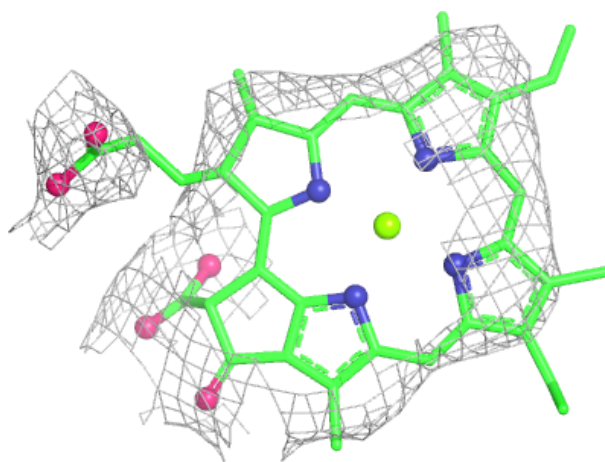
Electron density around CLA 4 307:

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



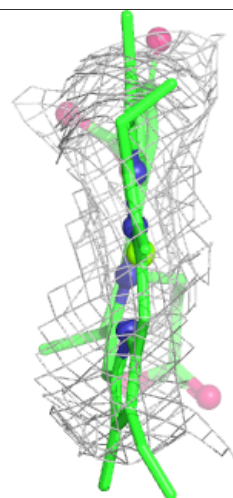
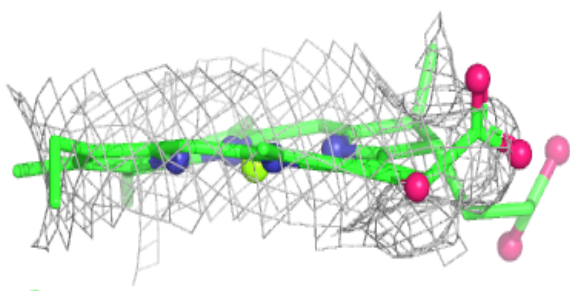
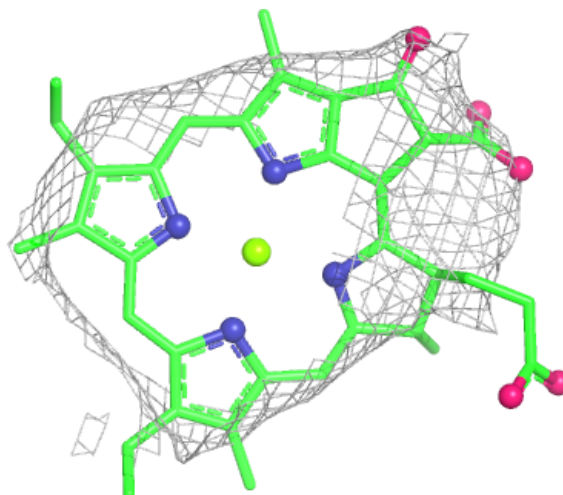
Electron density around CLA A 824:

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



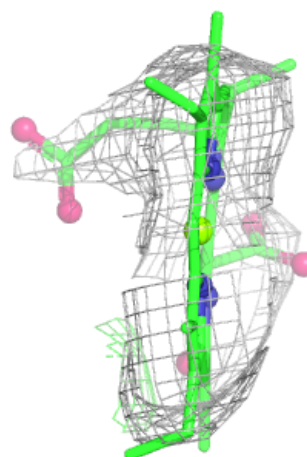
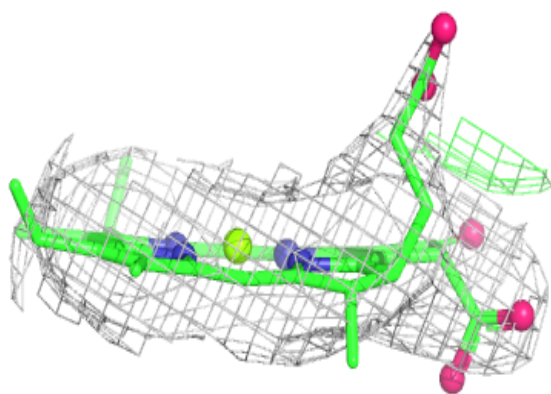
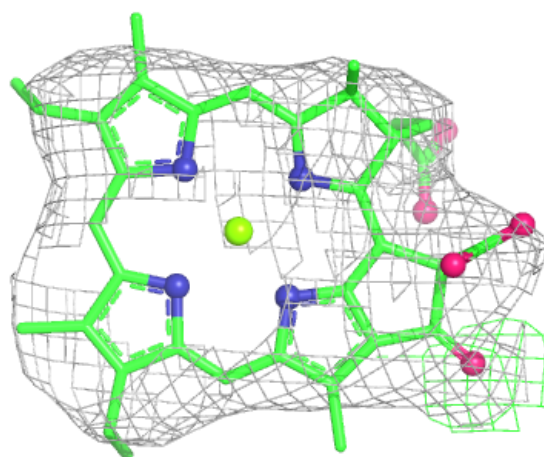
Electron density around CLA B 806:

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



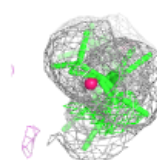
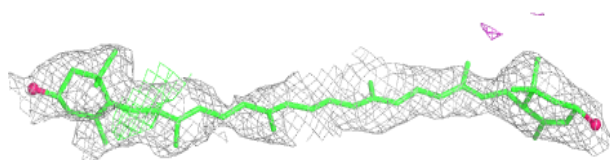
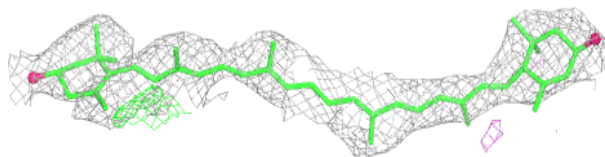
Electron density around CLA 3 1010:

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

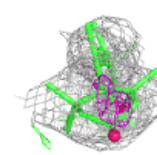
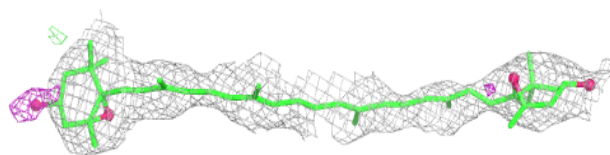
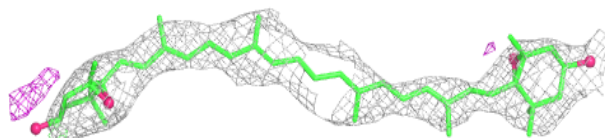


Electron density around LUT 7 1001:

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

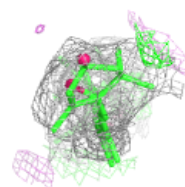
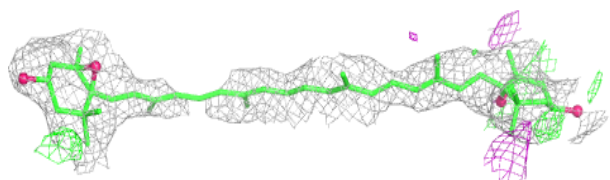
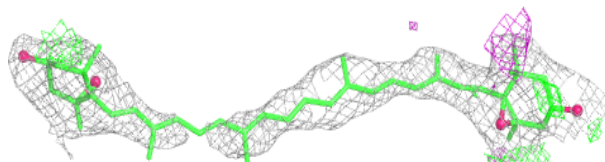
**Electron density around XAT 4 303:**

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



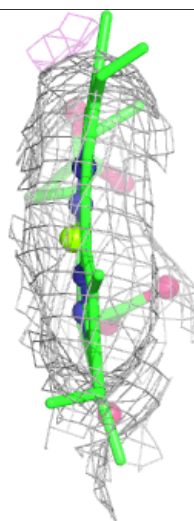
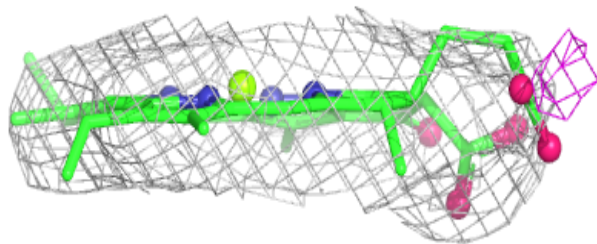
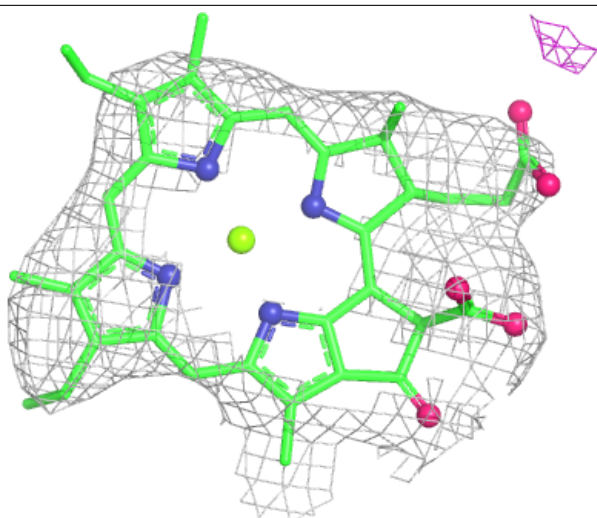
Electron density around XAT 6 304:

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



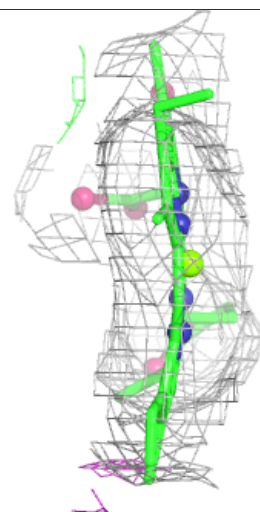
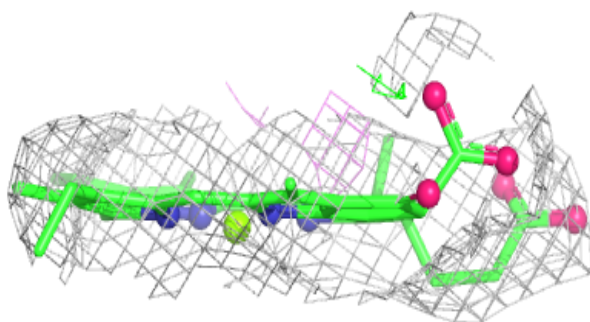
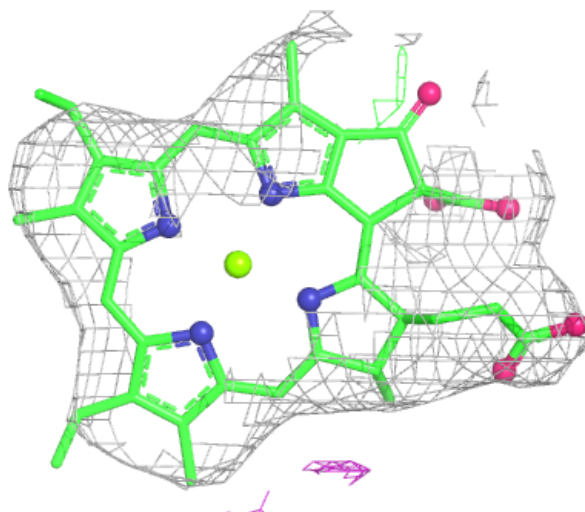
Electron density around CLA 3 1009:

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



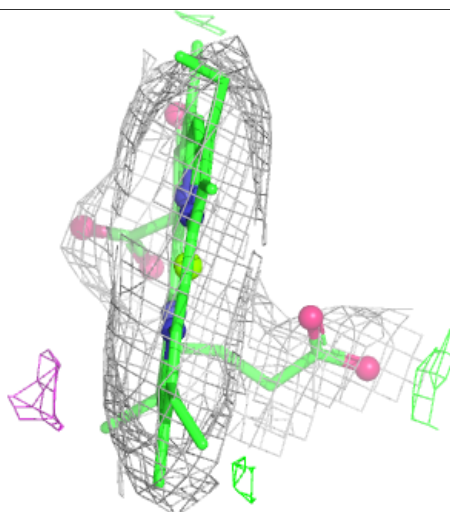
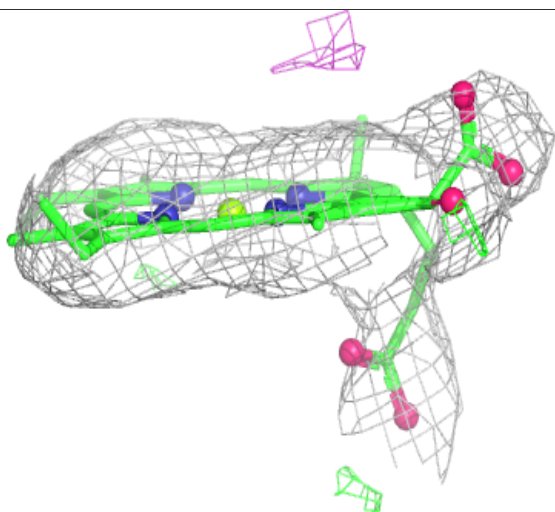
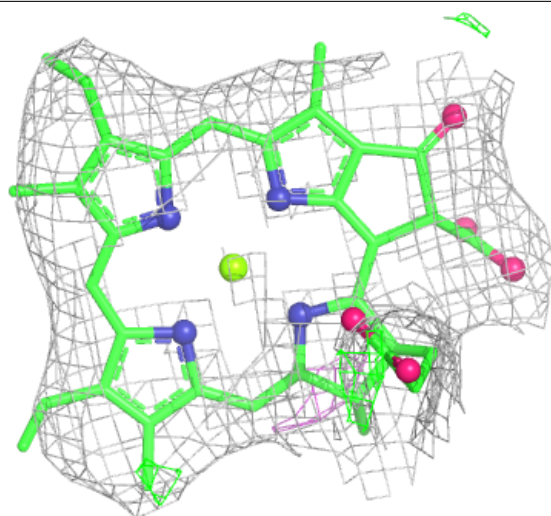
Electron density around CLA 4 308:

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



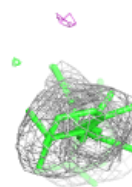
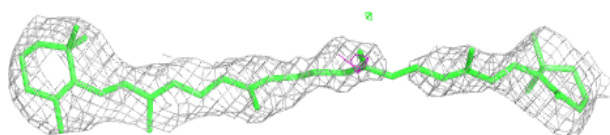
Electron density around CLA 4 309:

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



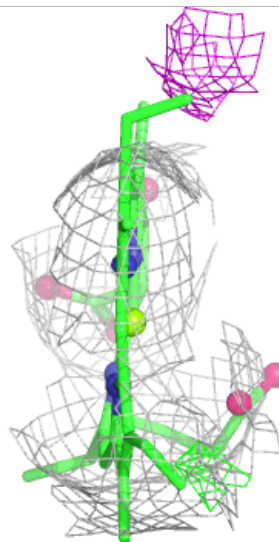
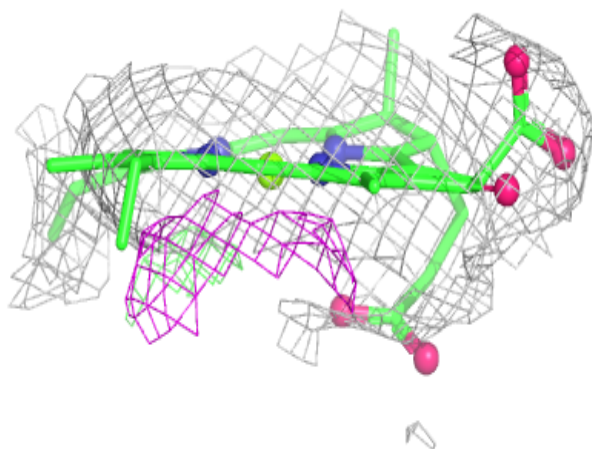
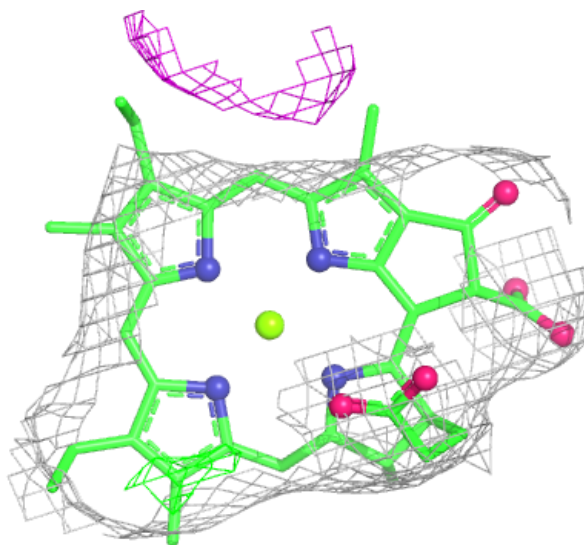
Electron density around BCR 3 1003:

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



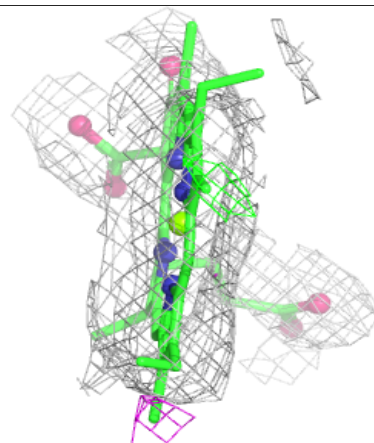
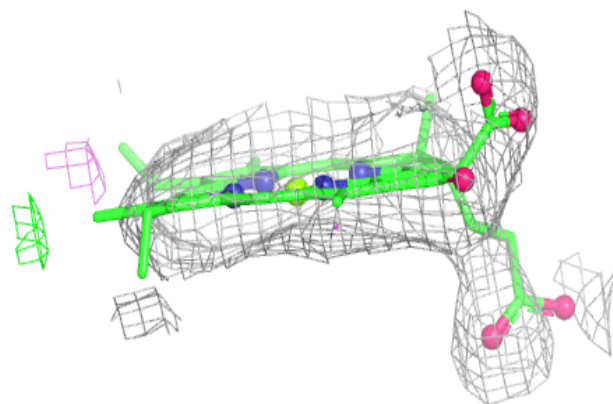
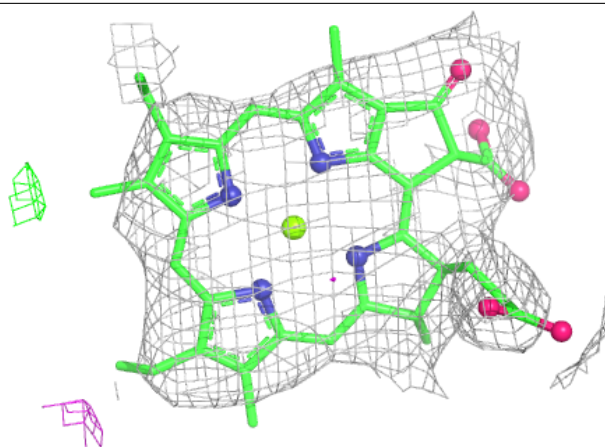
Electron density around CLA A 827:

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



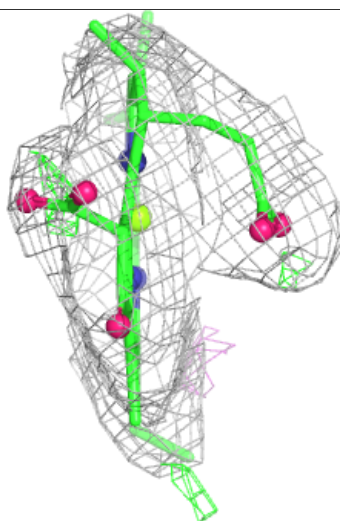
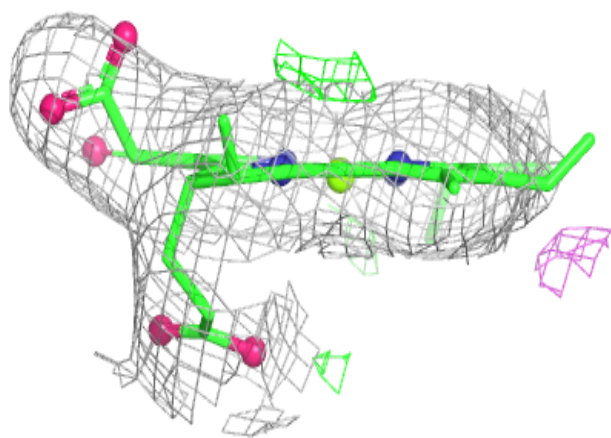
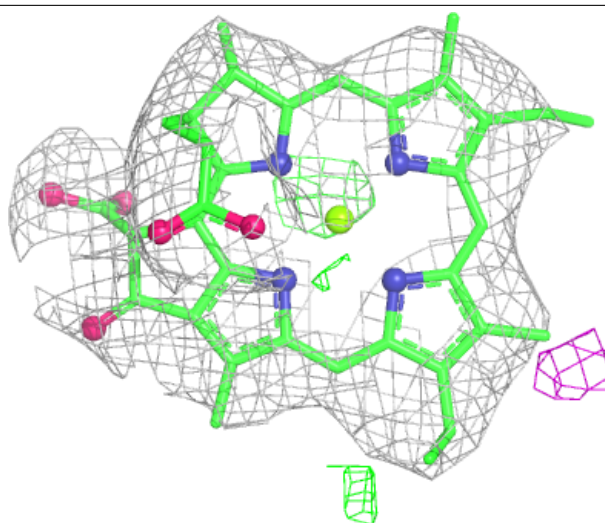
Electron density around CLA 4 311:

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



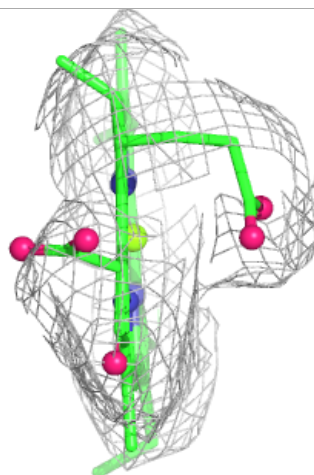
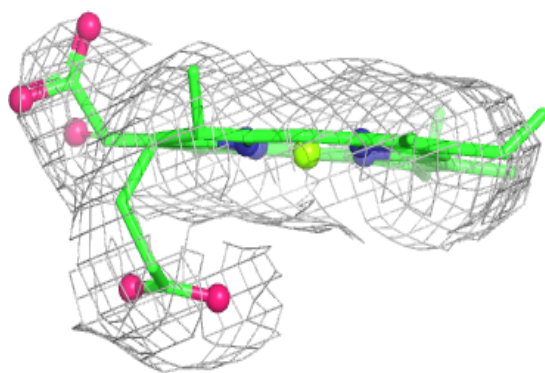
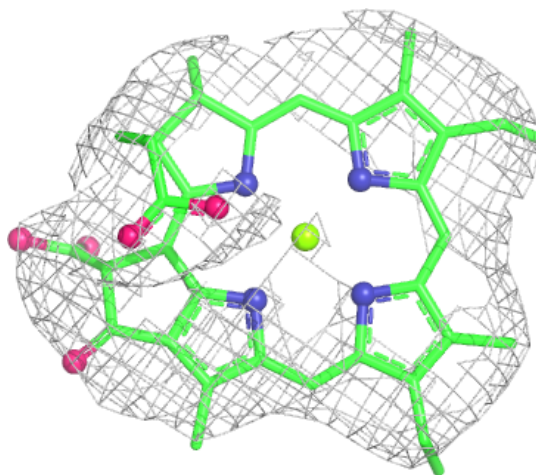
Electron density around CLA 6 307:

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



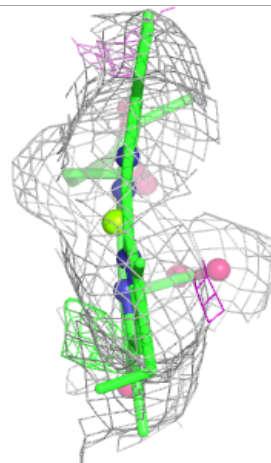
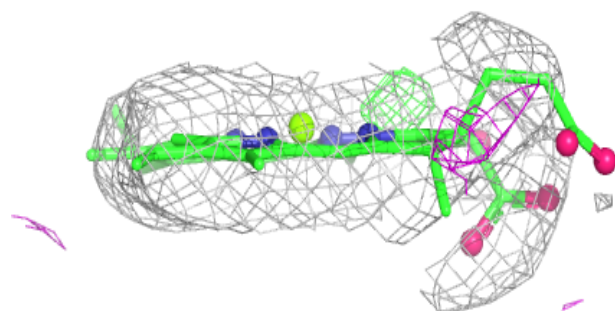
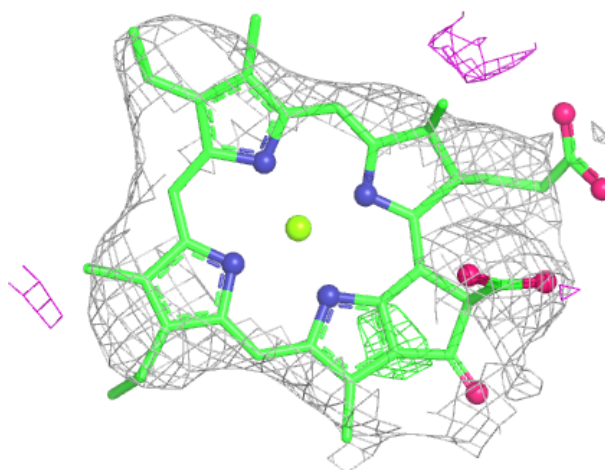
Electron density around CLA A 839:

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



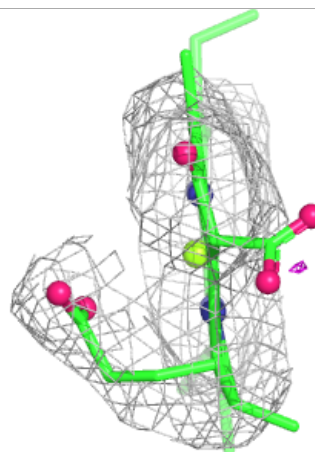
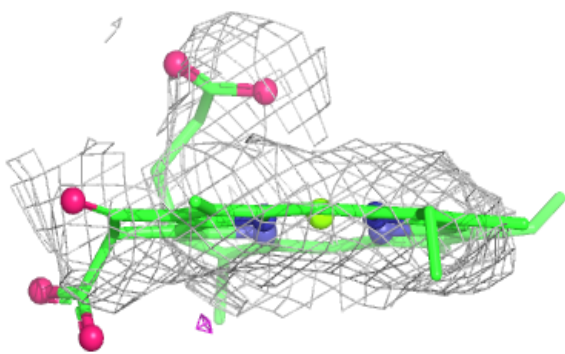
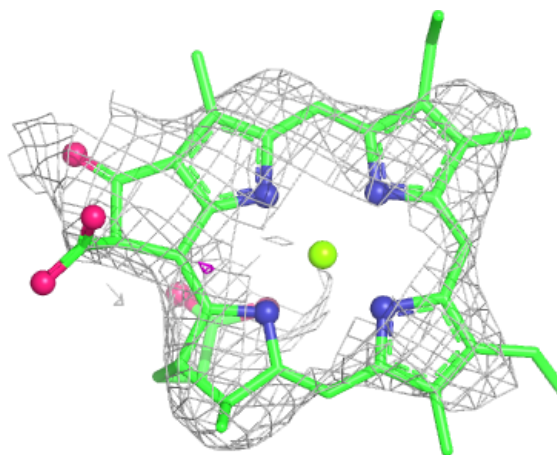
Electron density around CLA 6 309:

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



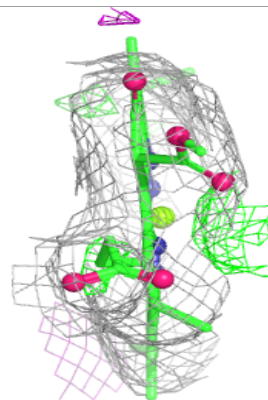
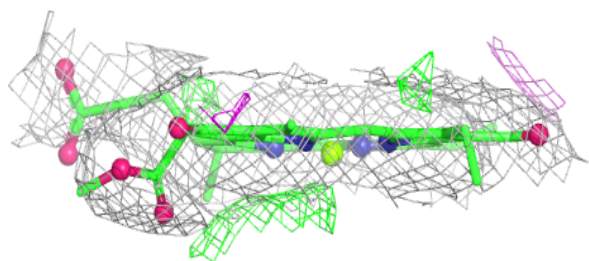
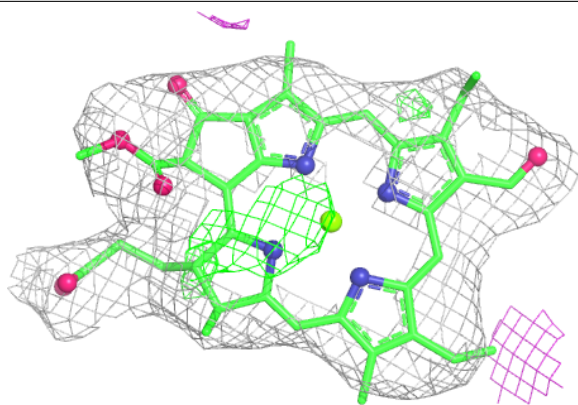
Electron density around CLA B 838:

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



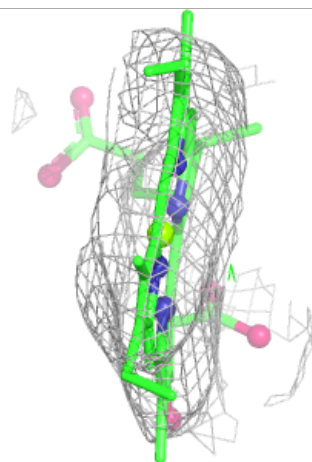
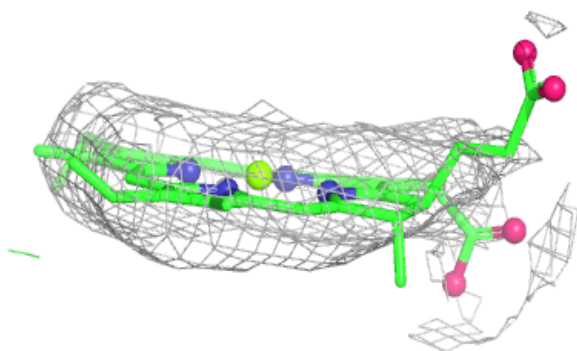
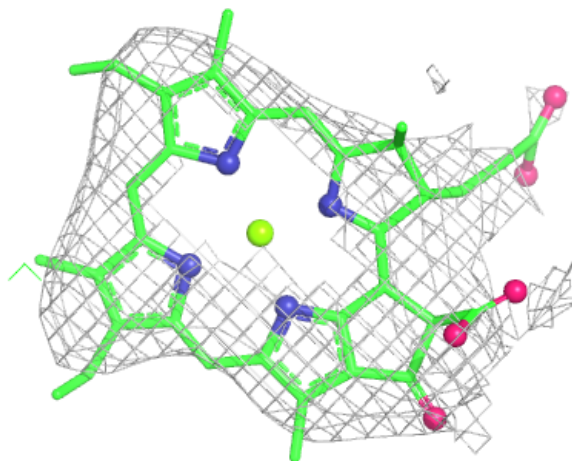
Electron density around CHL 7 1015:

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



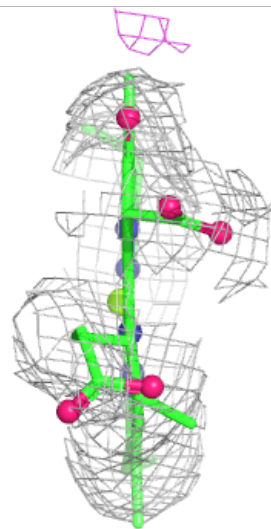
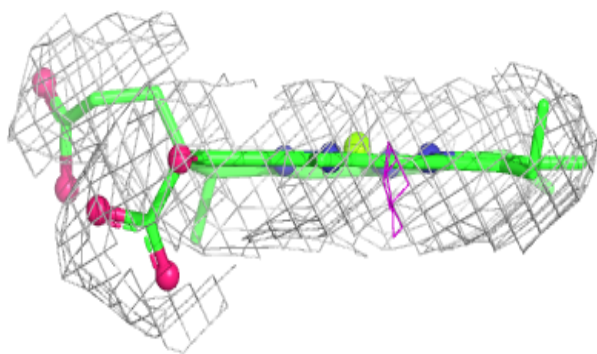
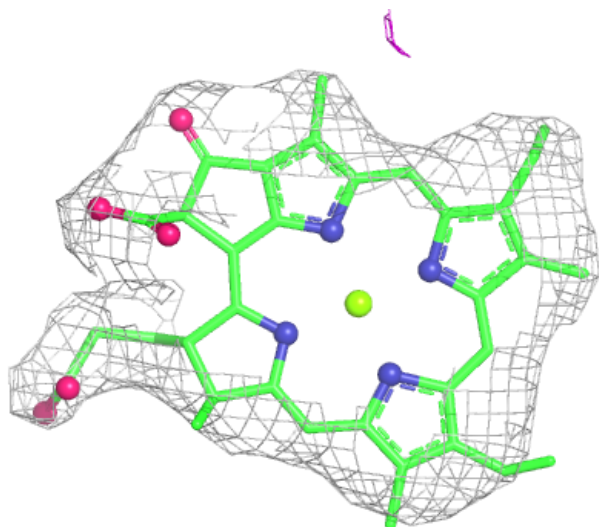
Electron density around CLA A 801:

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



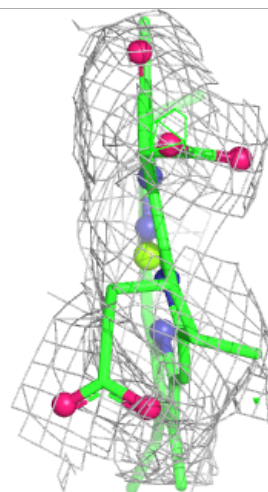
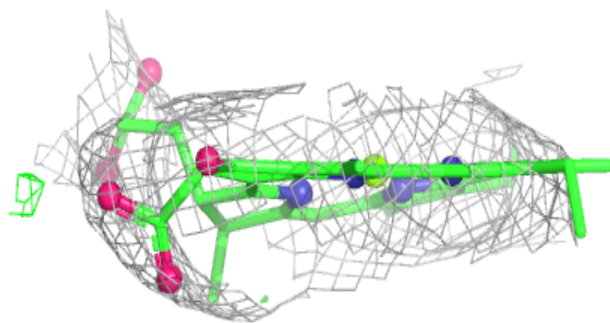
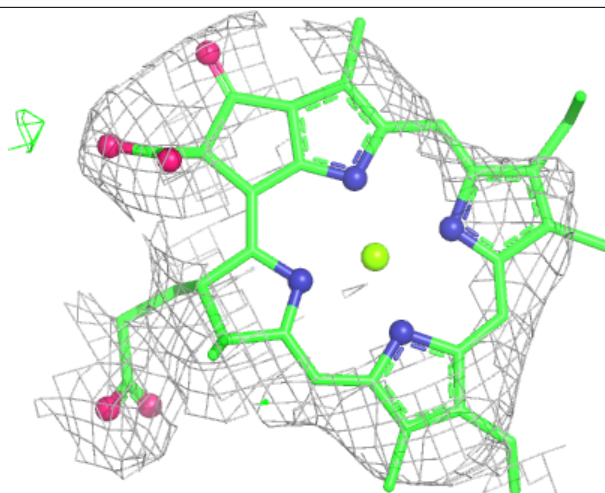
Electron density around CLA 3 1017:

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



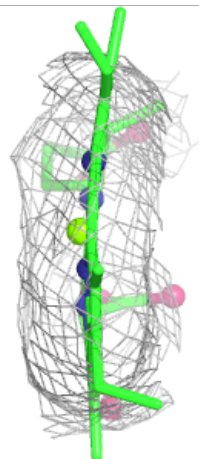
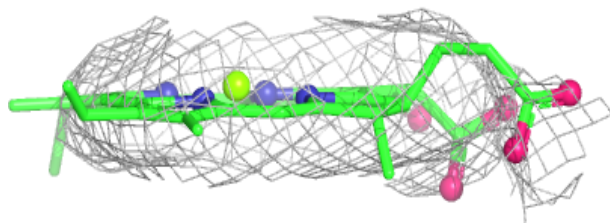
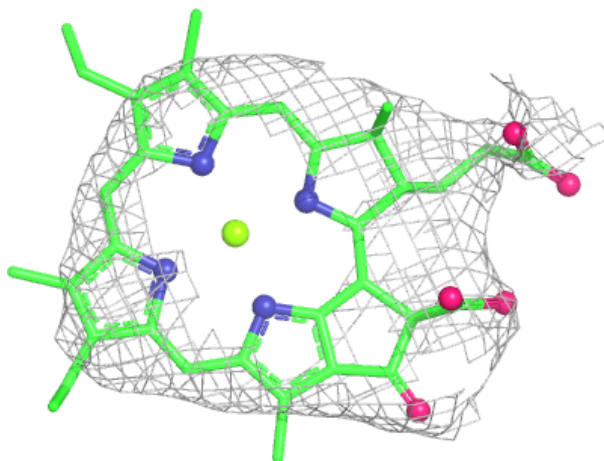
Electron density around CLA A 851:

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



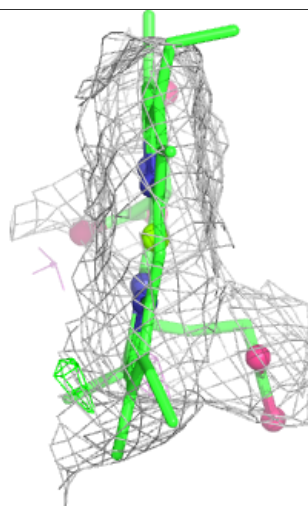
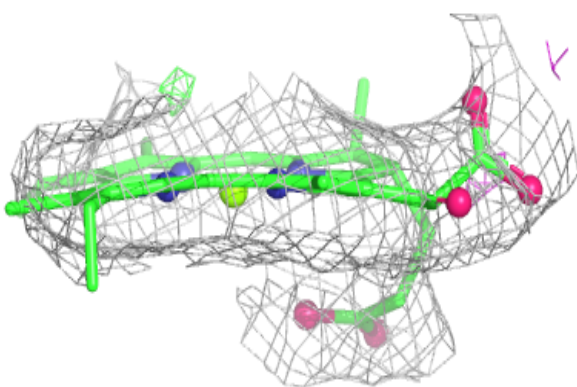
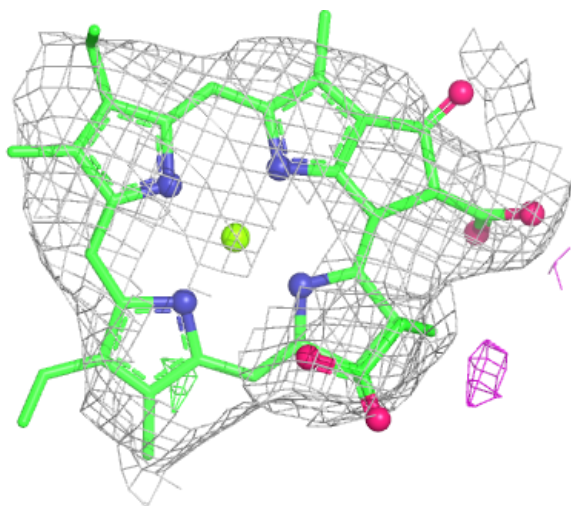
Electron density around CLA B 809:

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



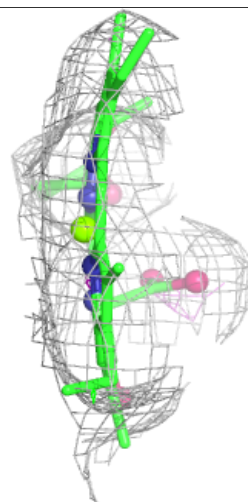
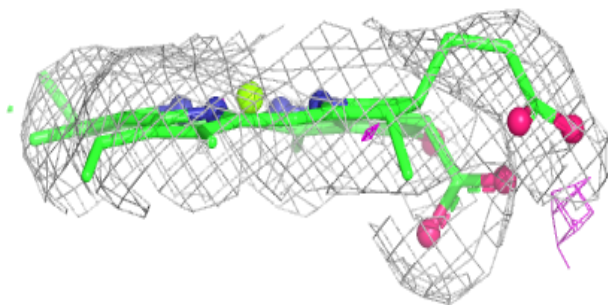
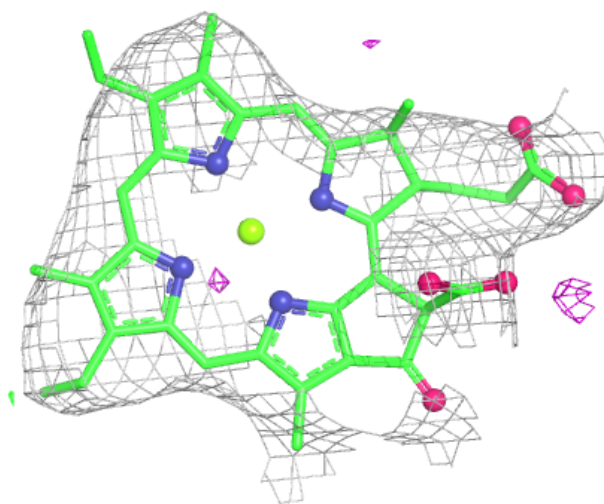
Electron density around CLA 5 304:

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



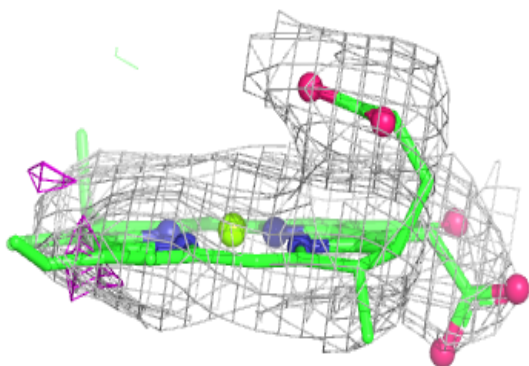
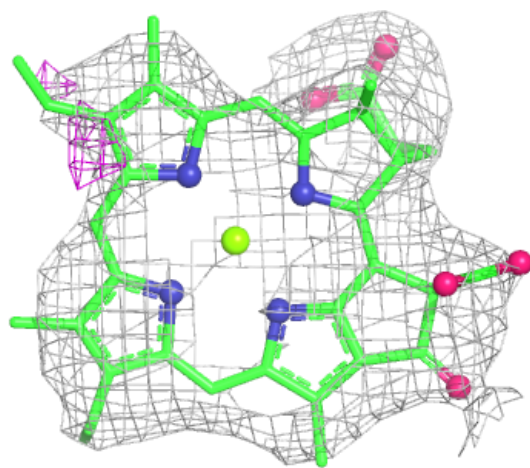
Electron density around CLA 8 309:

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



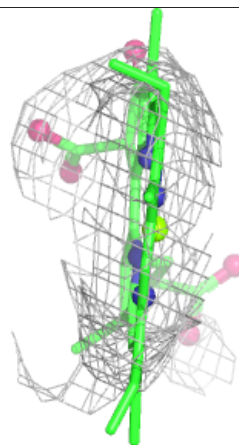
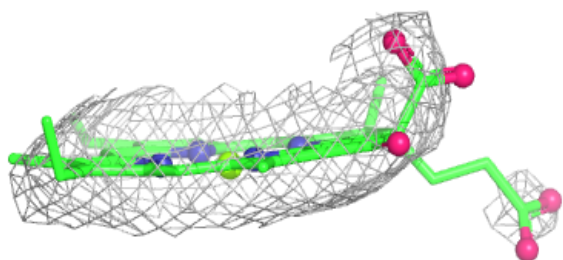
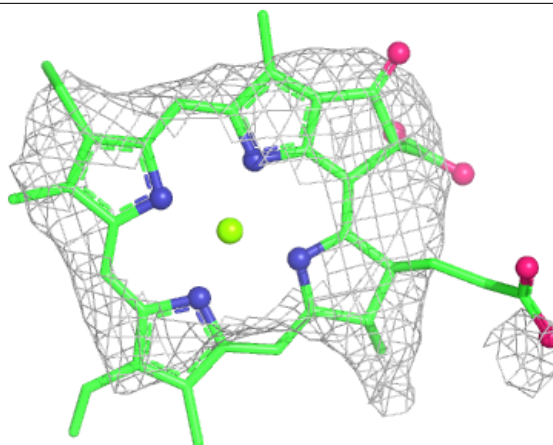
Electron density around CLA 5 307:

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



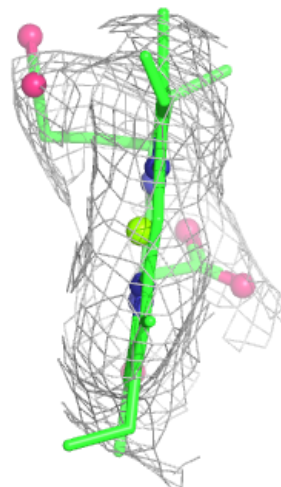
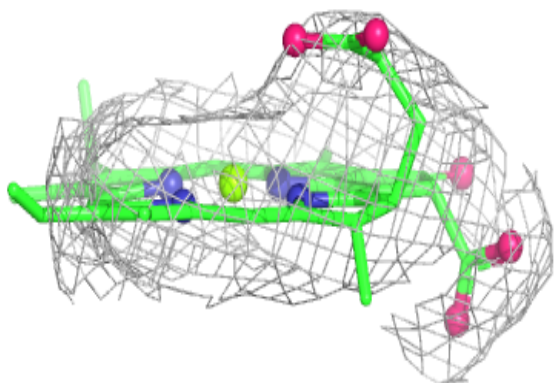
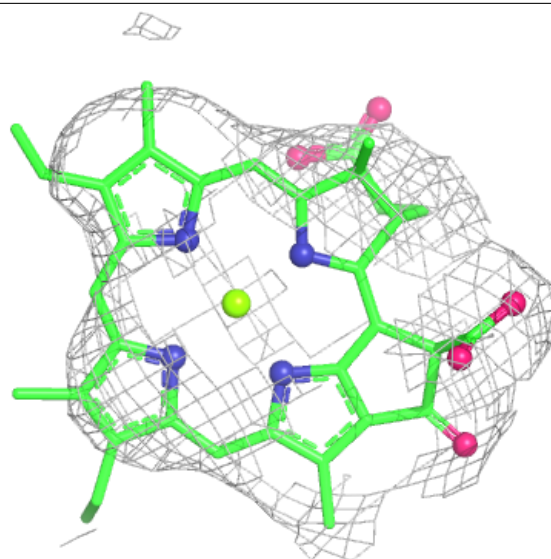
Electron density around CLA A 834:

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



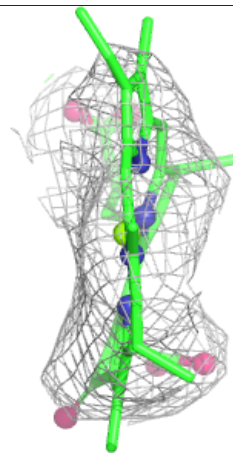
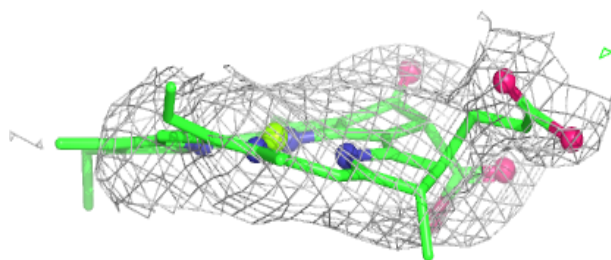
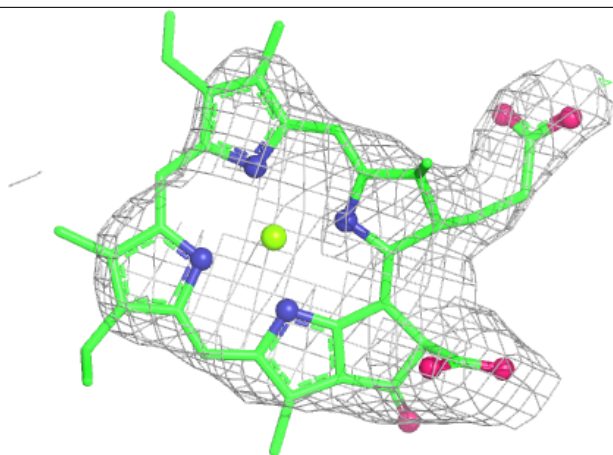
Electron density around CLA A 818:

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



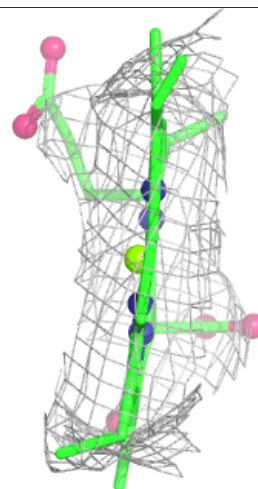
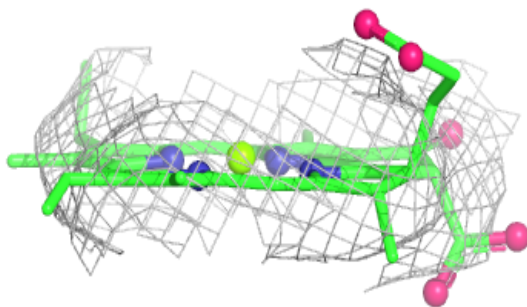
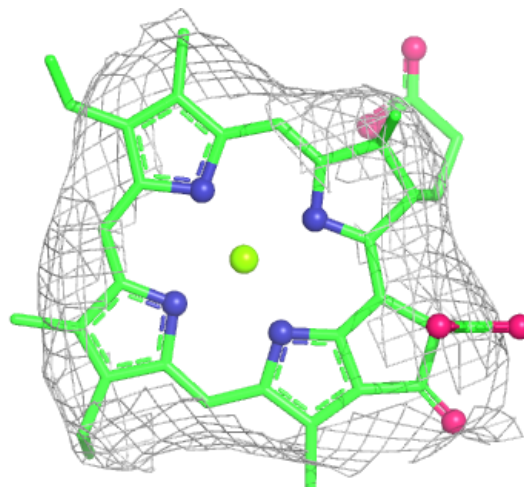
Electron density around CLA B 802:

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



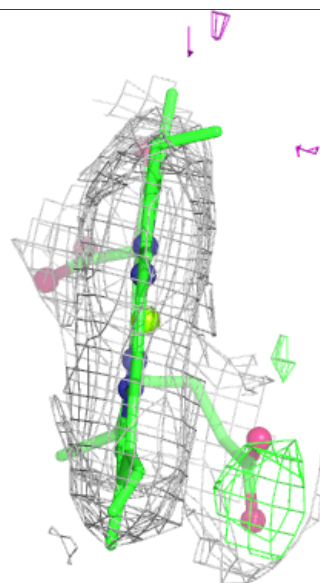
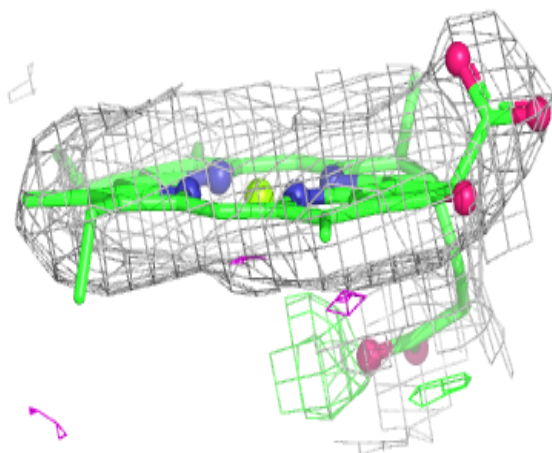
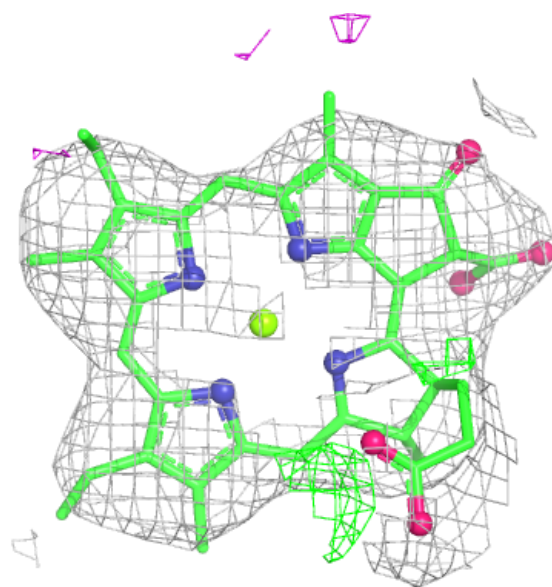
Electron density around CLA B 821:

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



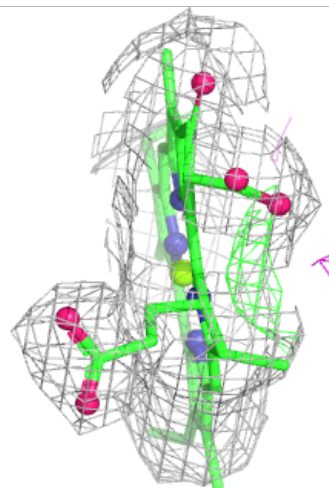
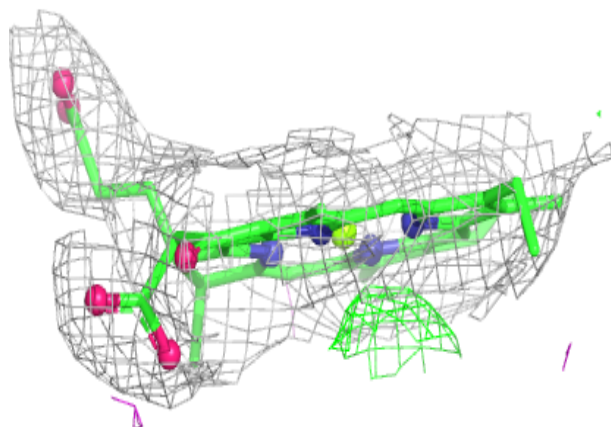
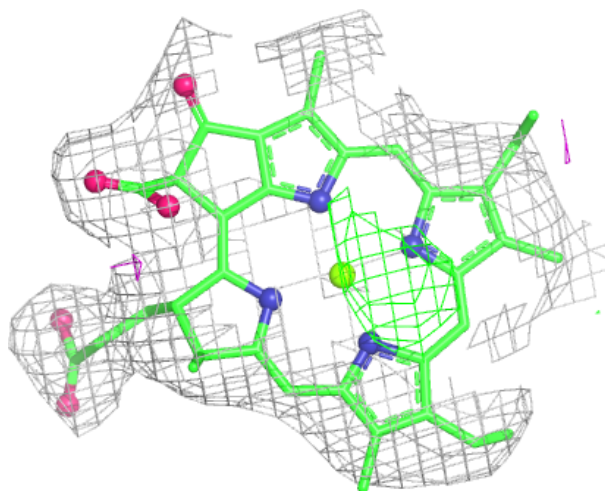
Electron density around CLA 7 1007:

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



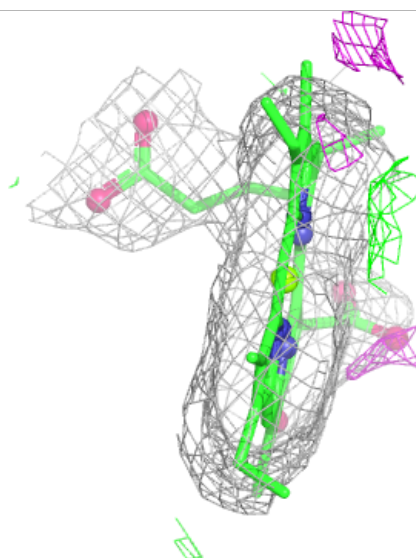
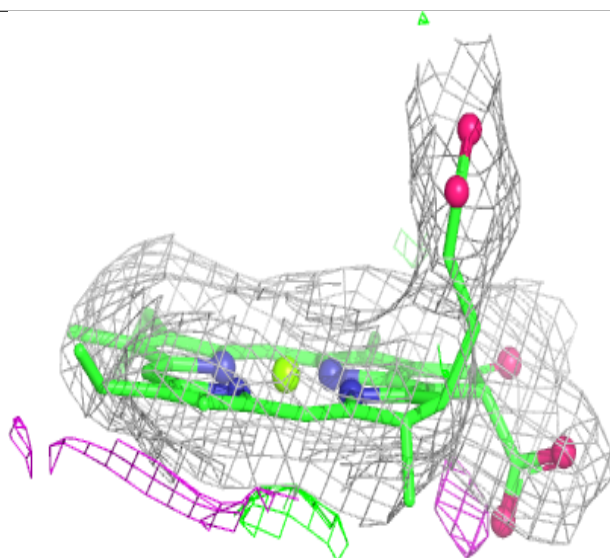
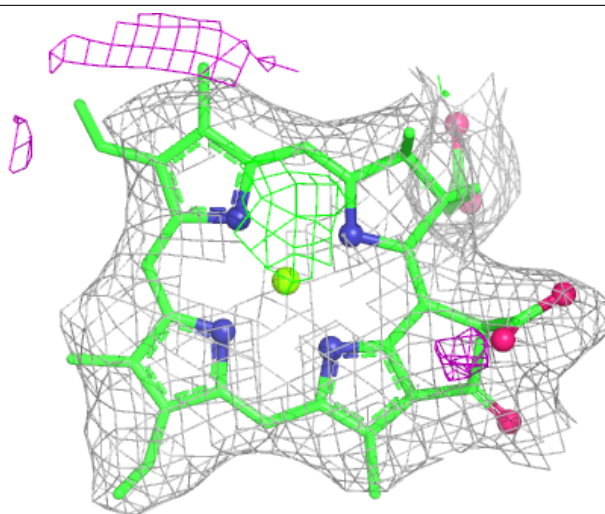
Electron density around CLA 5 321:

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



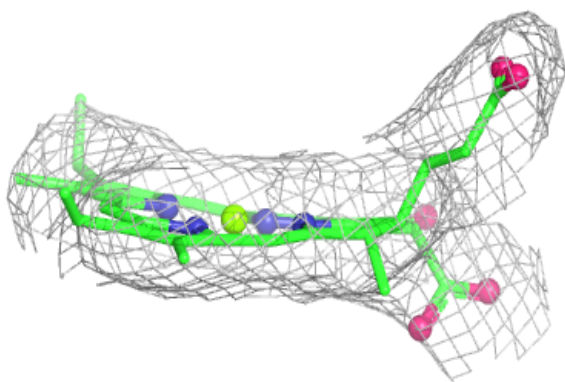
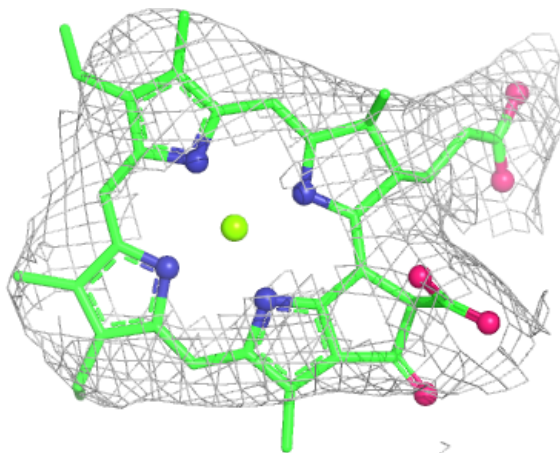
Electron density around CLA 7 1009:

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



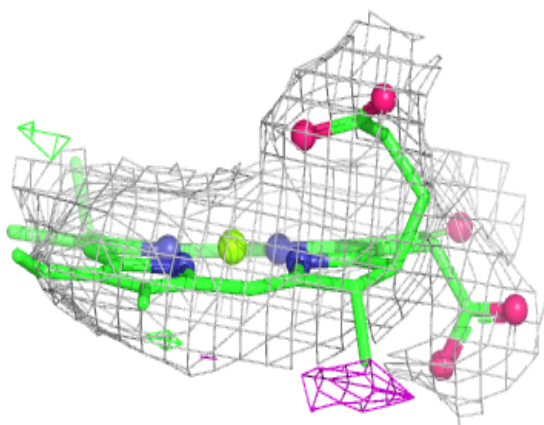
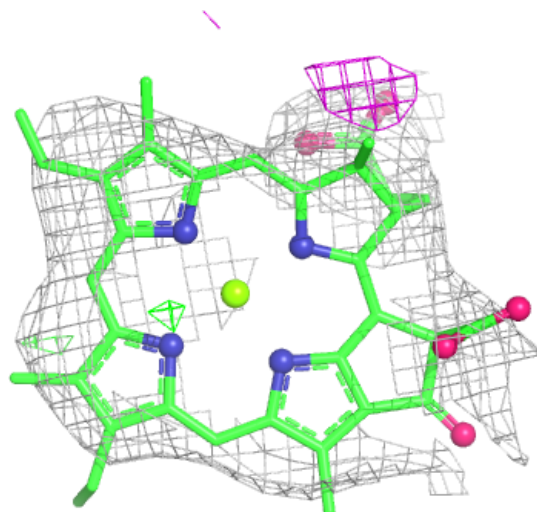
Electron density around CLA B 834:

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



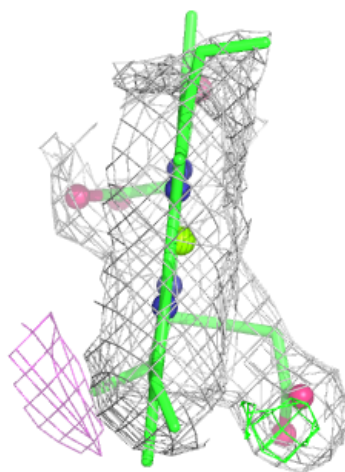
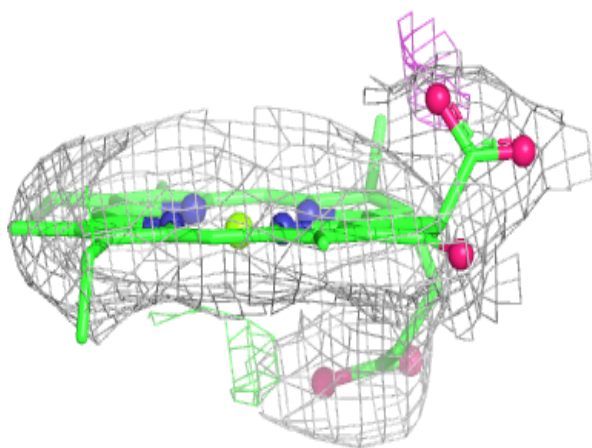
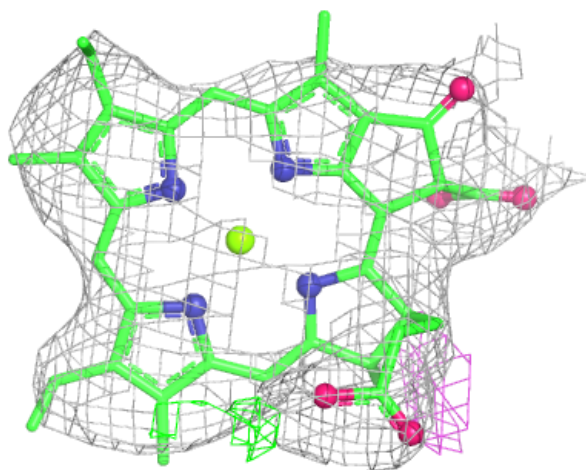
Electron density around CLA 0 308:

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



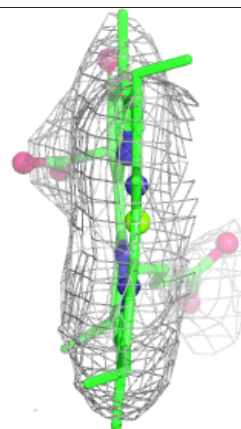
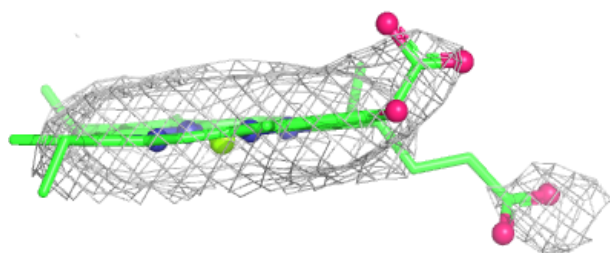
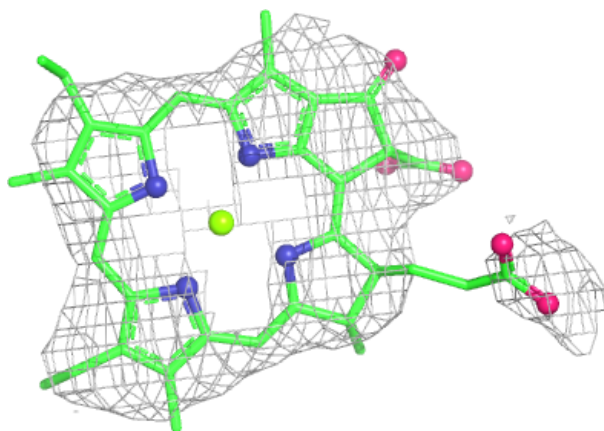
Electron density around CLA 8 308:

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



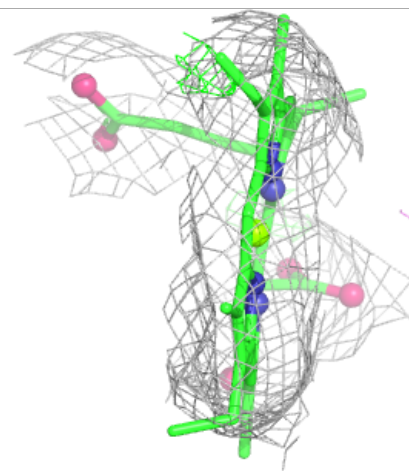
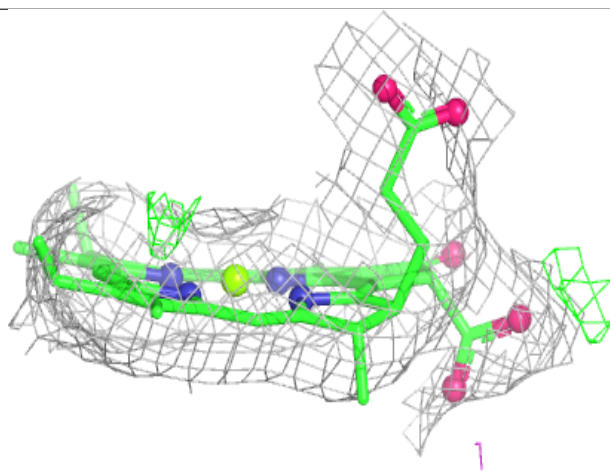
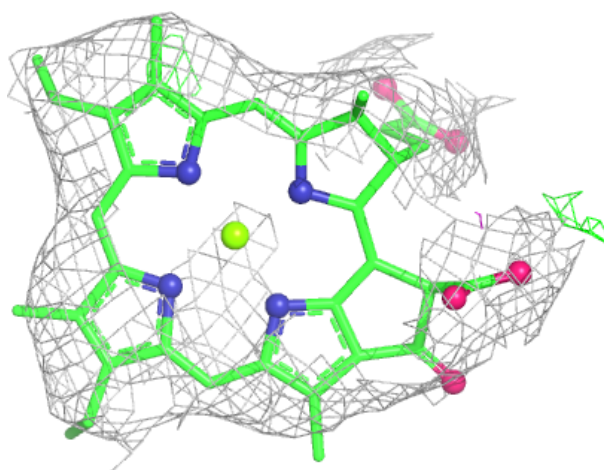
Electron density around CLA B 837:

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



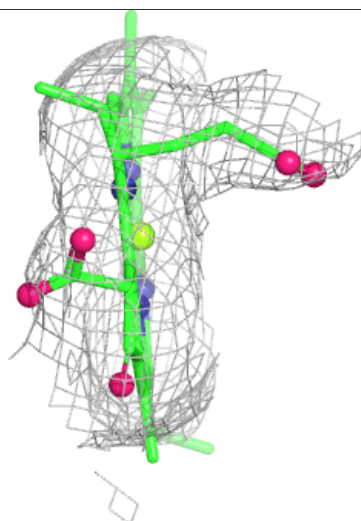
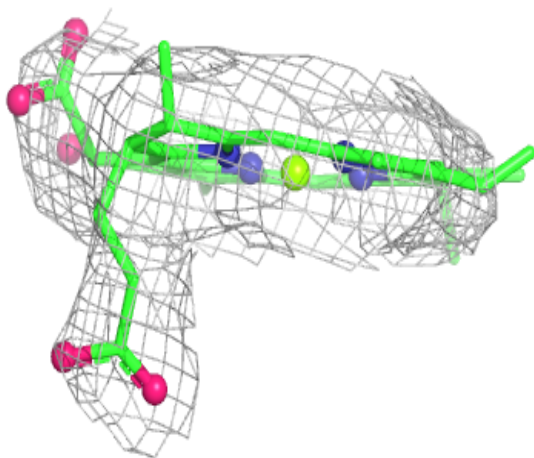
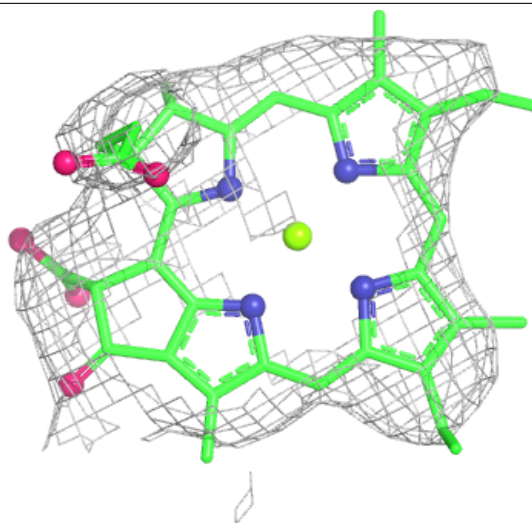
Electron density around CLA 4 314:

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



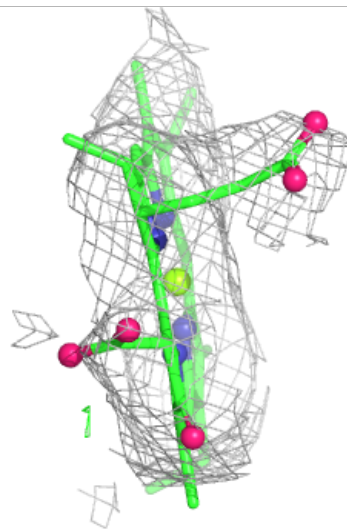
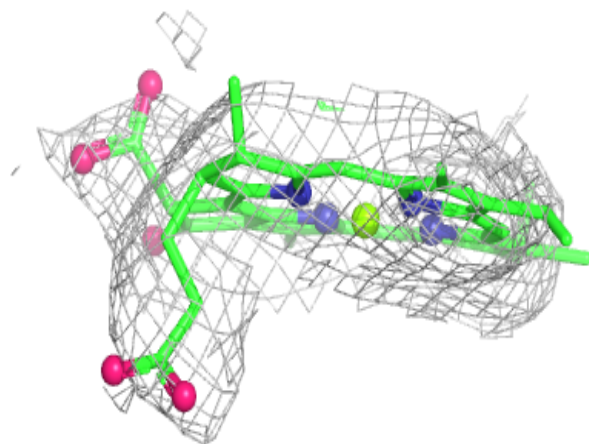
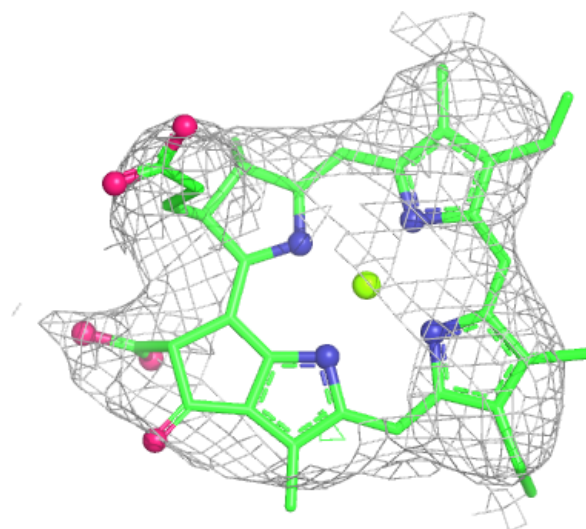
Electron density around CLA 6 301:

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



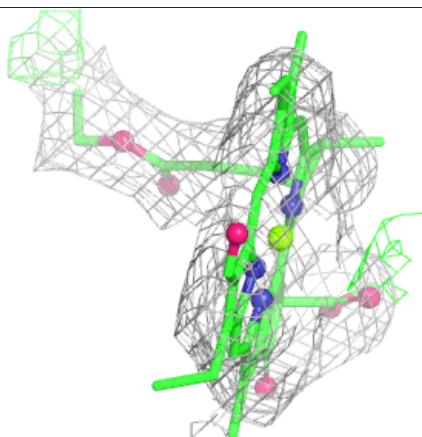
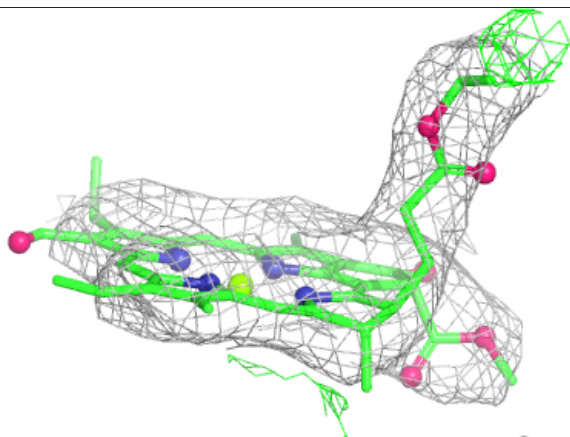
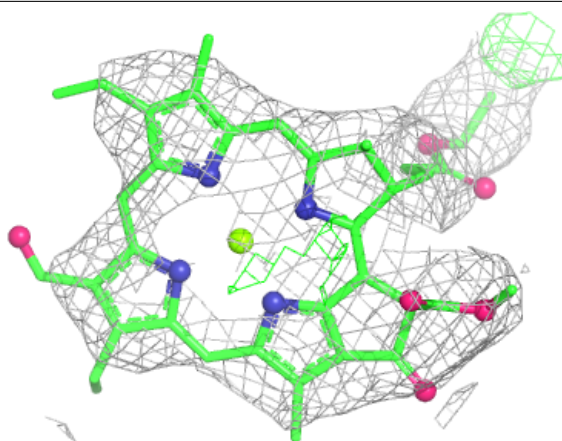
Electron density around CLA 3 1015:

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



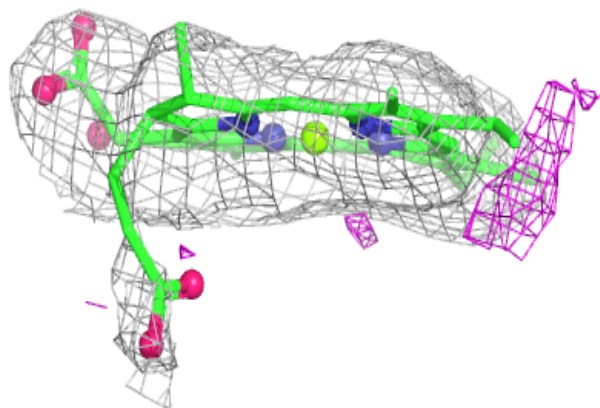
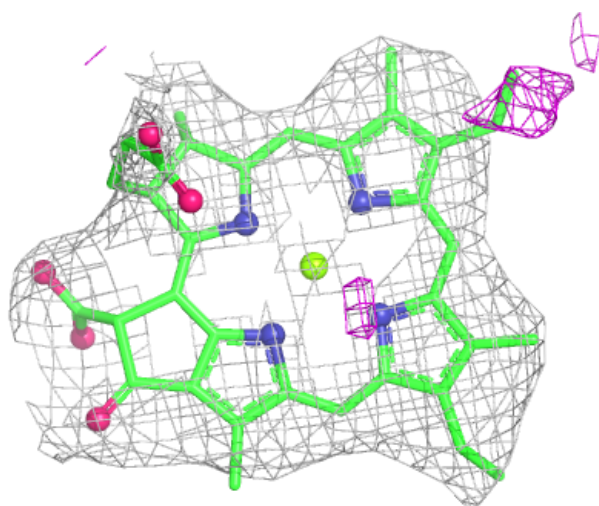
Electron density around CHL 7 1013:

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



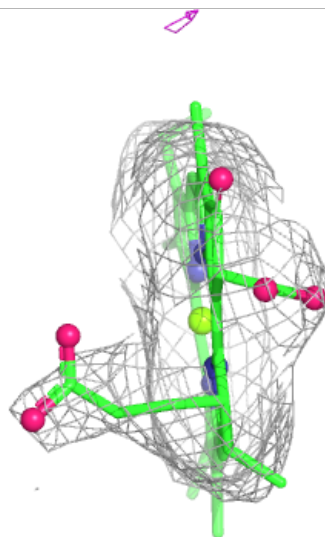
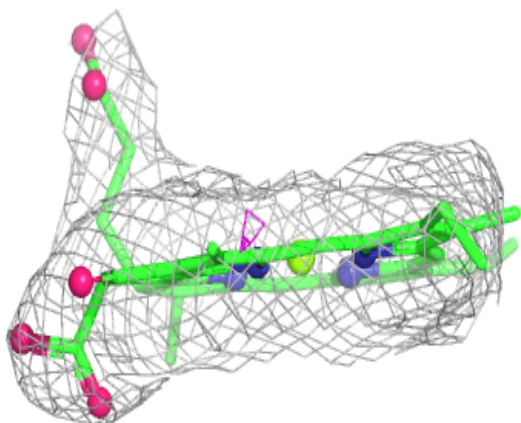
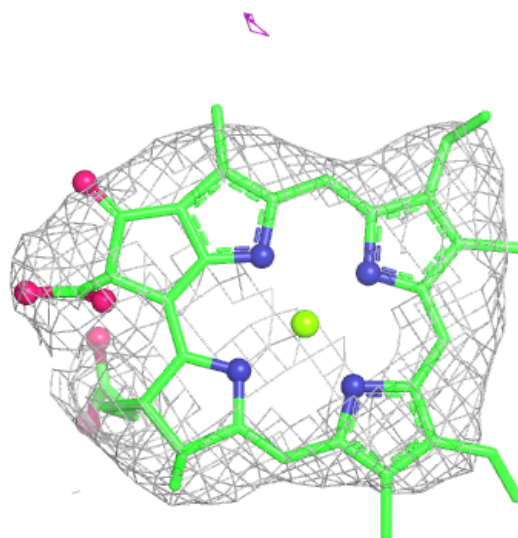
Electron density around CLA 8 310:

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



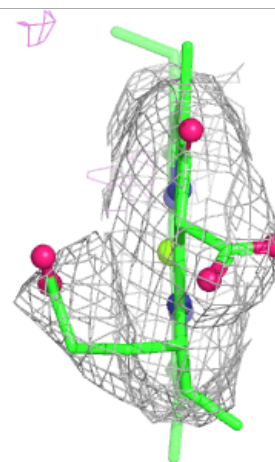
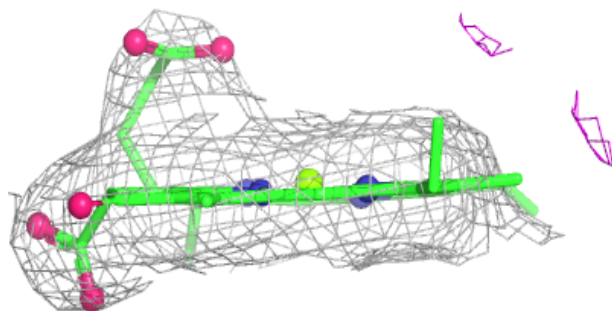
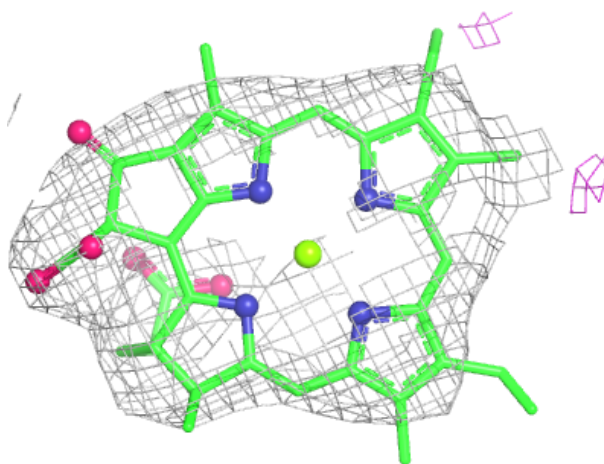
Electron density around CLA A 806:

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



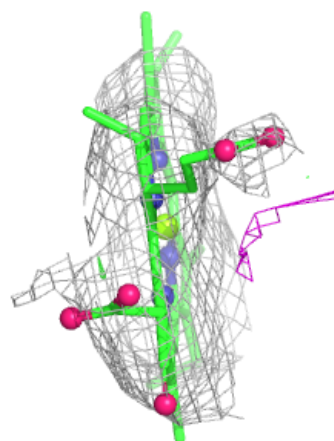
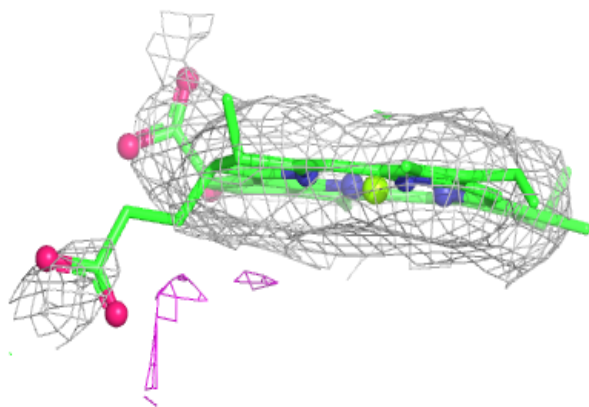
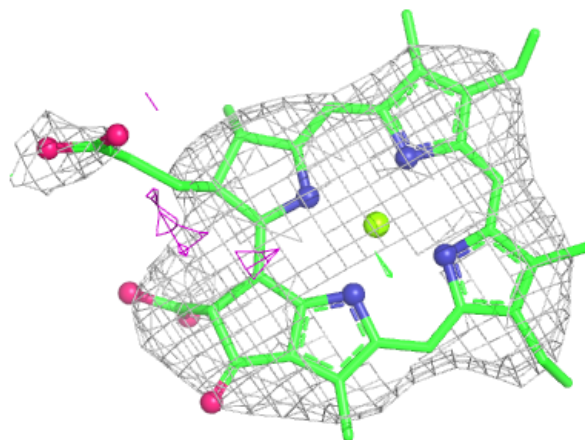
Electron density around CLA A 837:

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



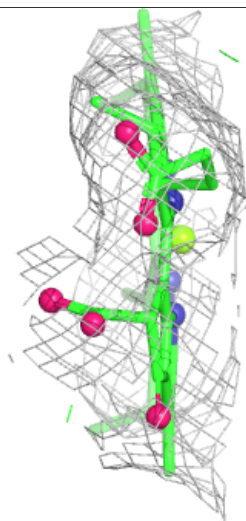
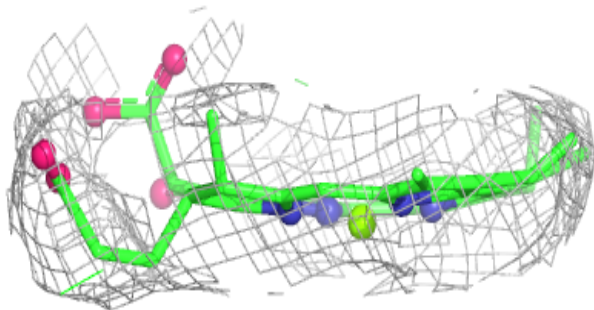
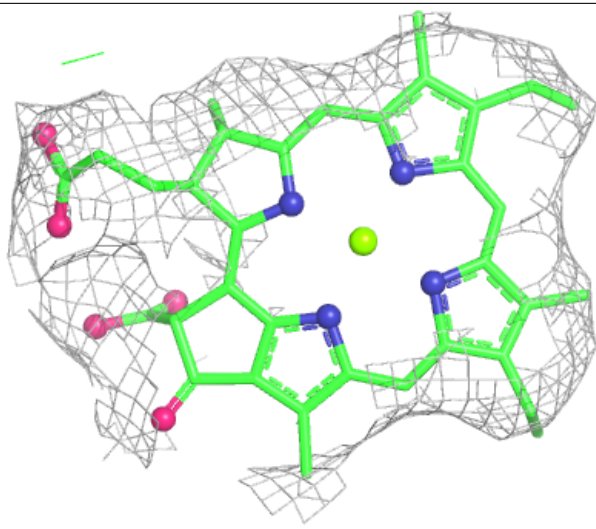
Electron density around CLA A 838:

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



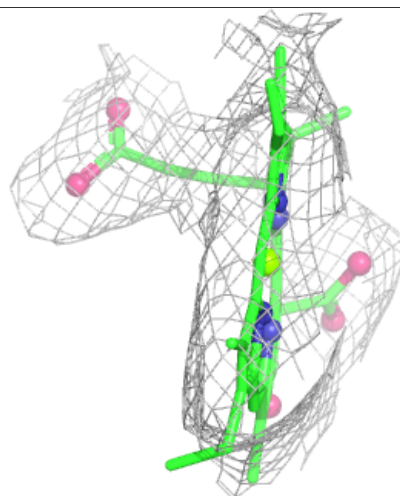
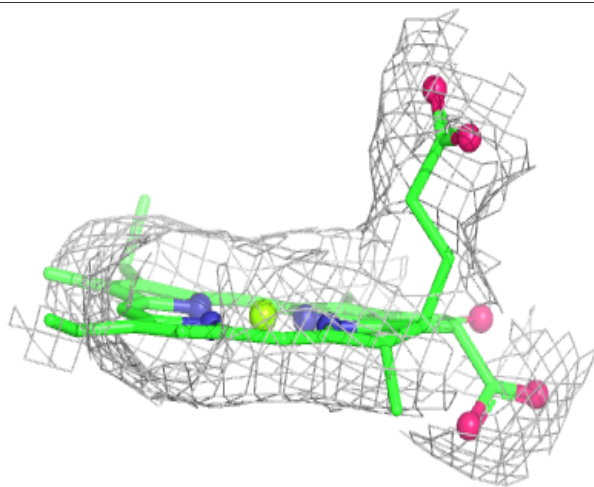
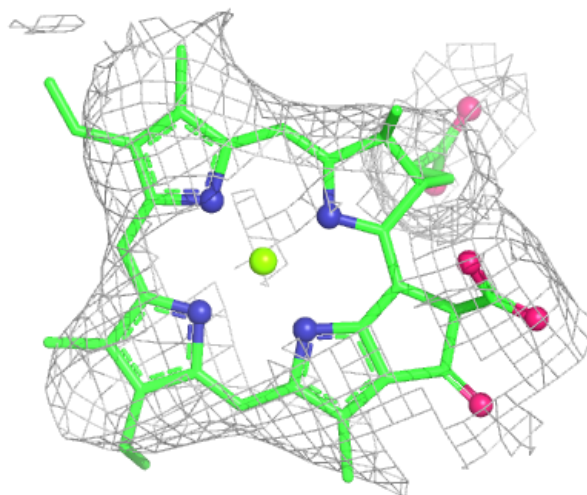
Electron density around CLA 7 1005:

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



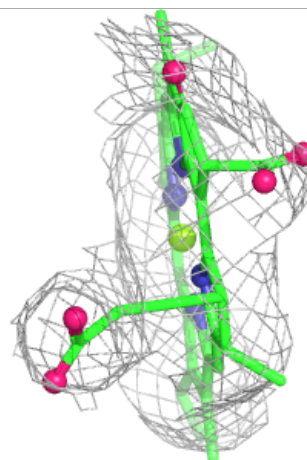
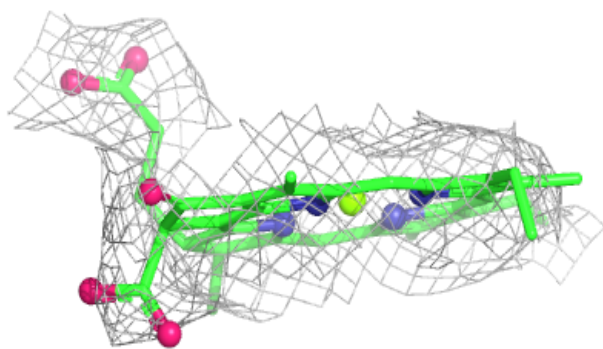
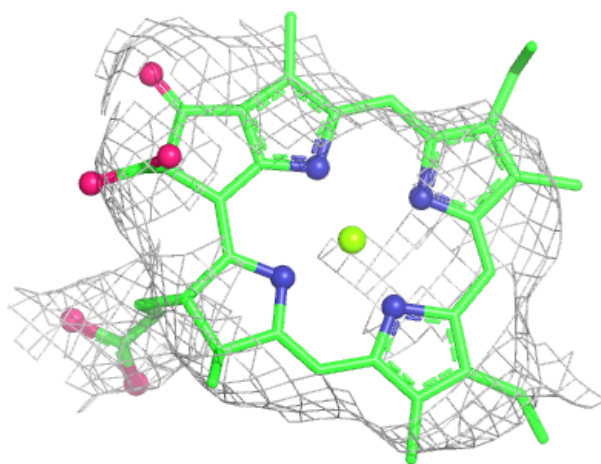
Electron density around CLA A 829:

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



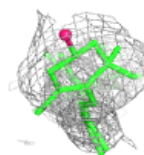
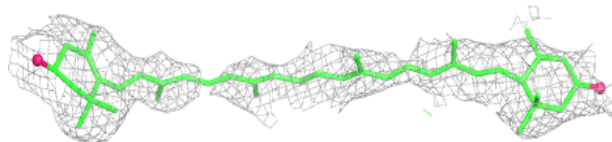
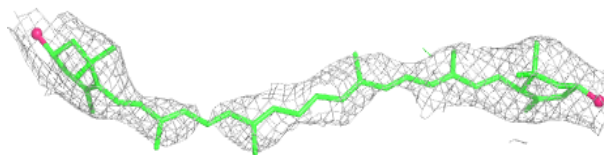
Electron density around CLA A 813:

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



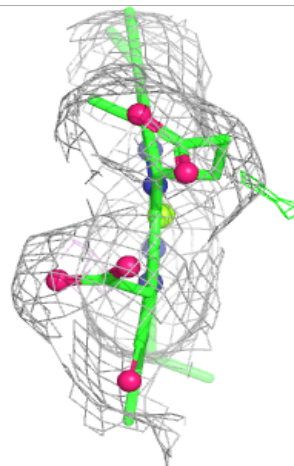
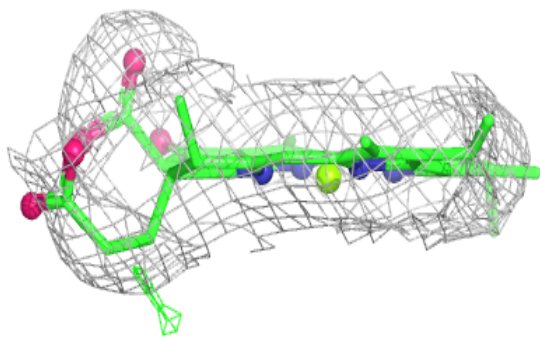
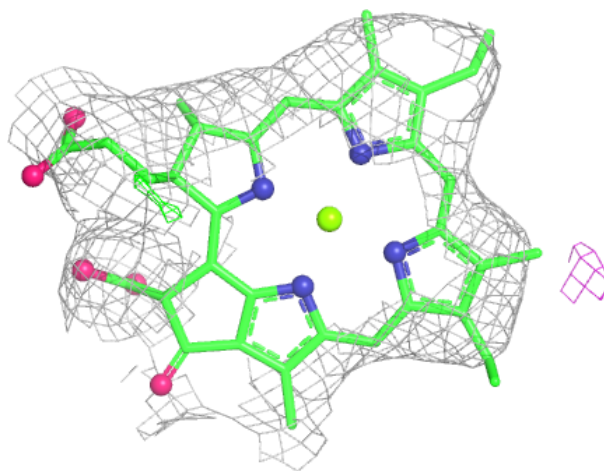
Electron density around LUT 8 303:

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



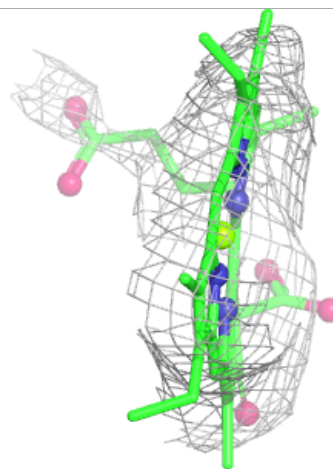
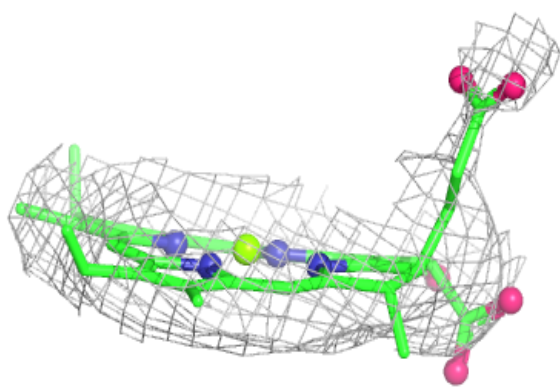
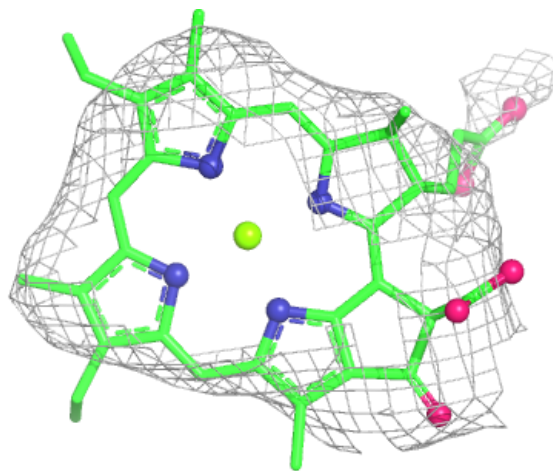
Electron density around CLA 7 1008:

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



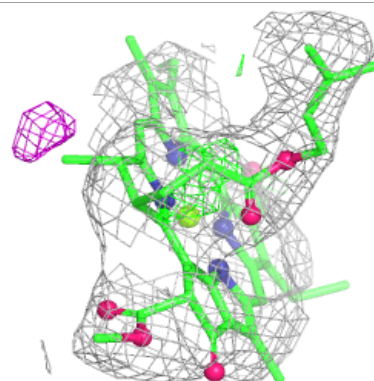
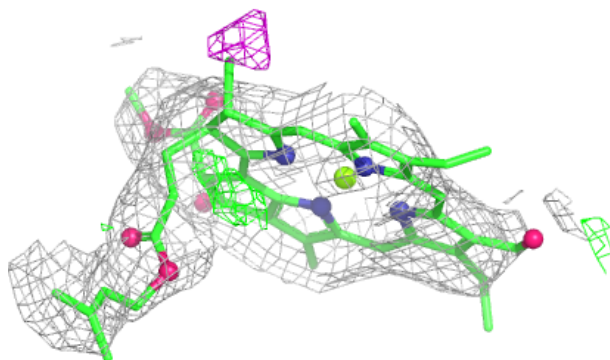
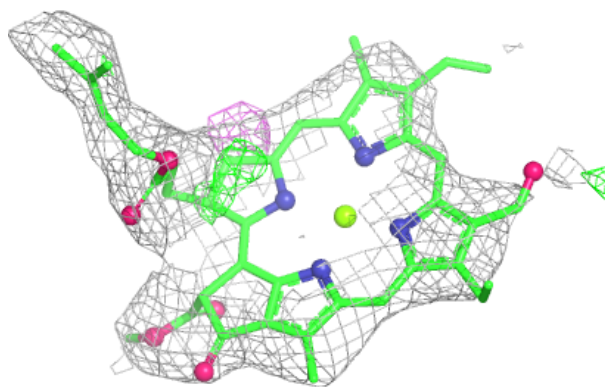
Electron density around CLA B 825:

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

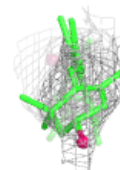
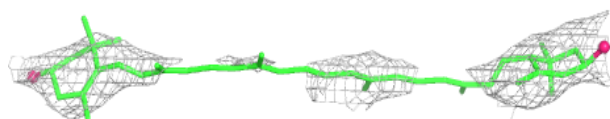
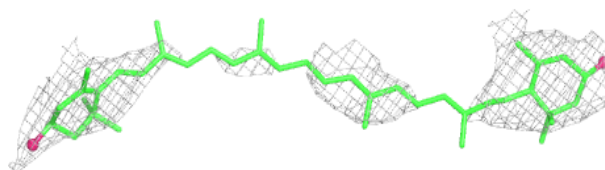


Electron density around CHL 6 314:

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

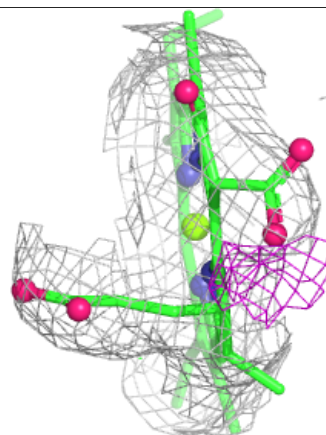
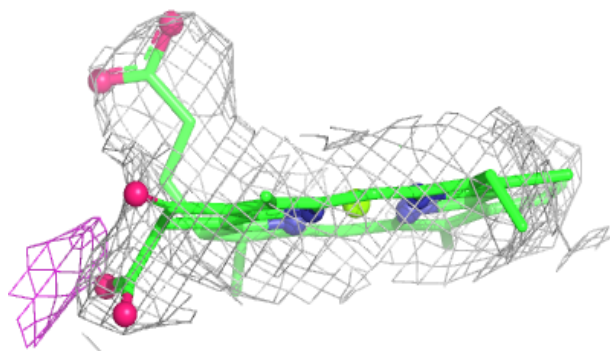
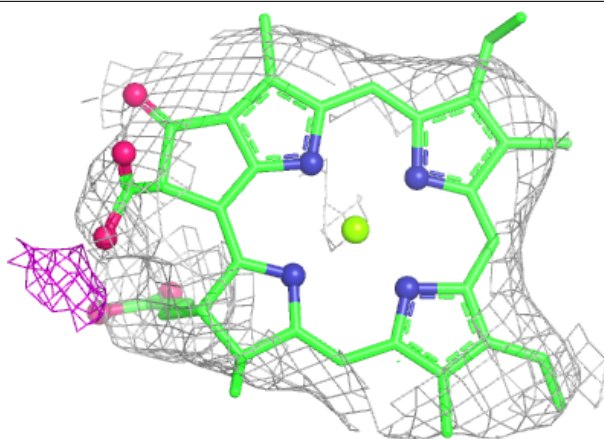
**Electron density around LUT 3 1002:**

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



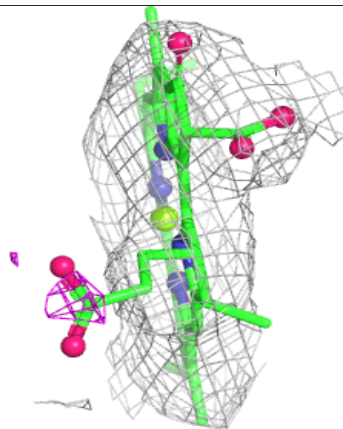
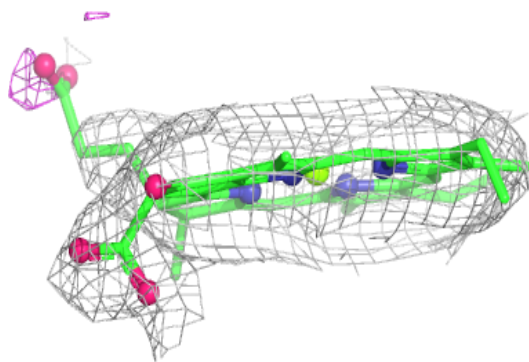
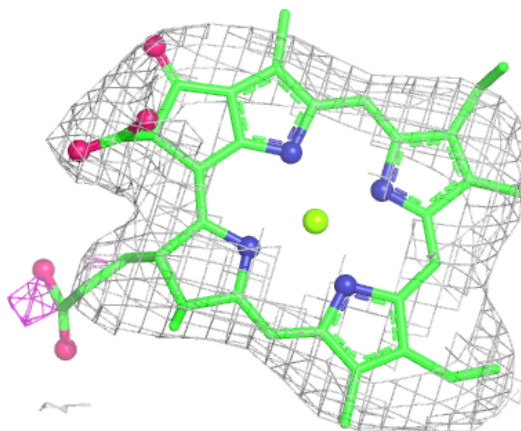
Electron density around CLA 7 1010:

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



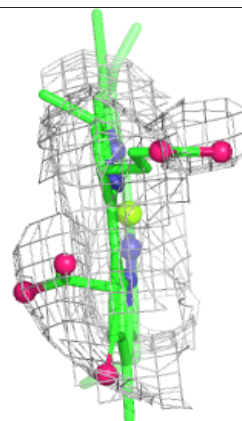
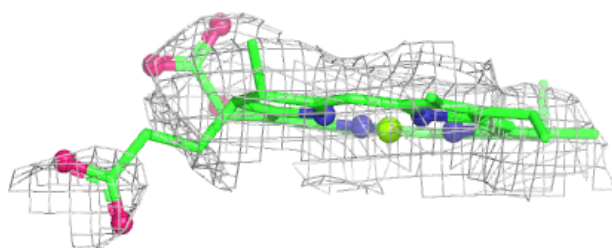
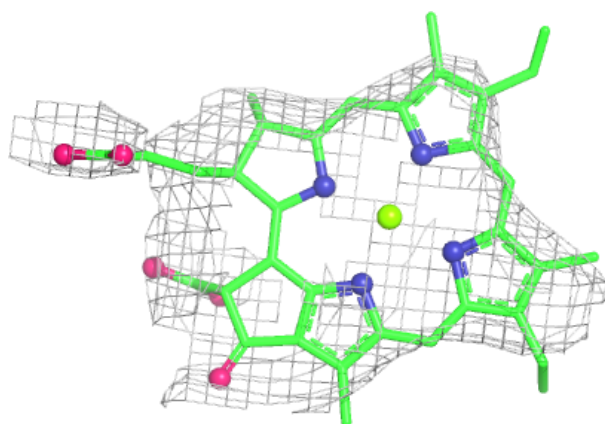
Electron density around CLA A 802:

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



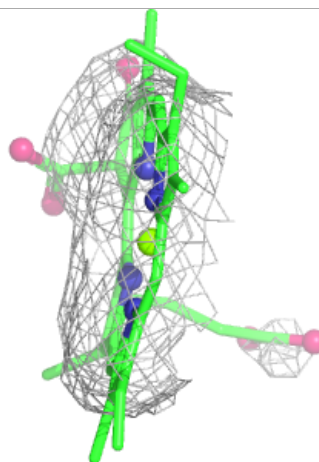
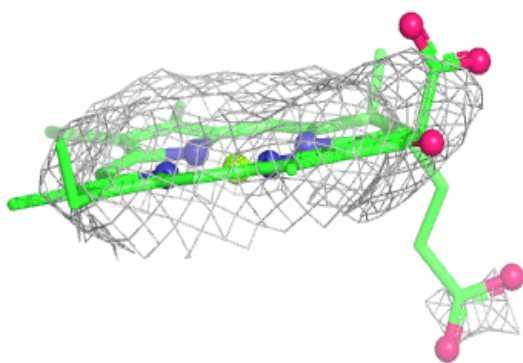
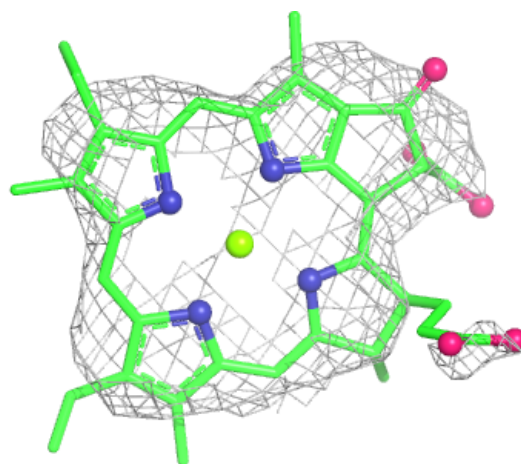
Electron density around CLA B 828:

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



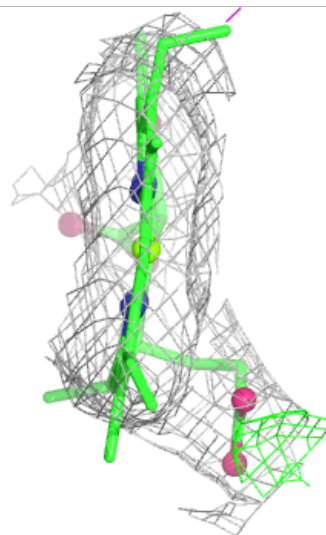
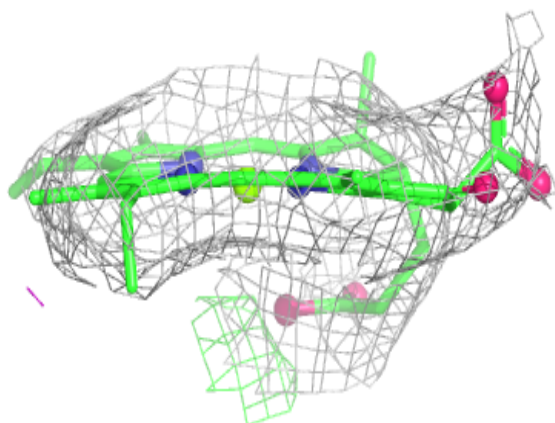
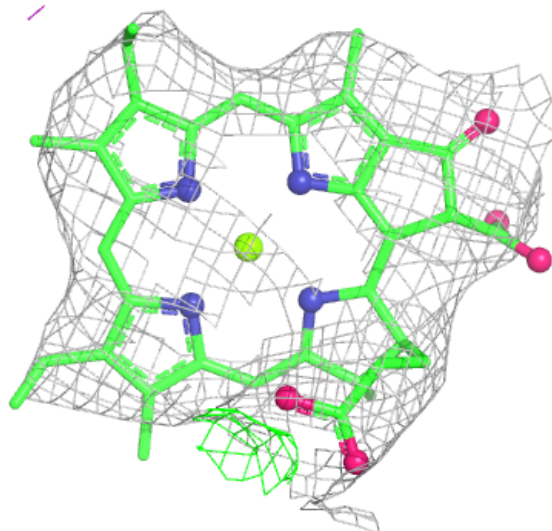
Electron density around CLA 0 301:

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



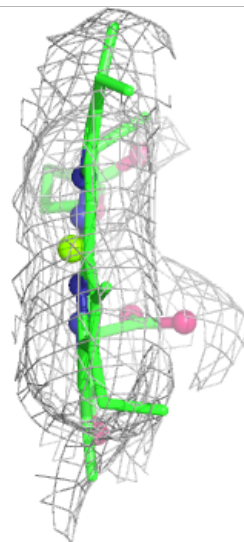
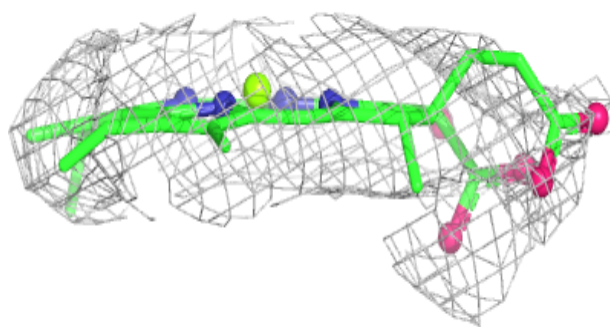
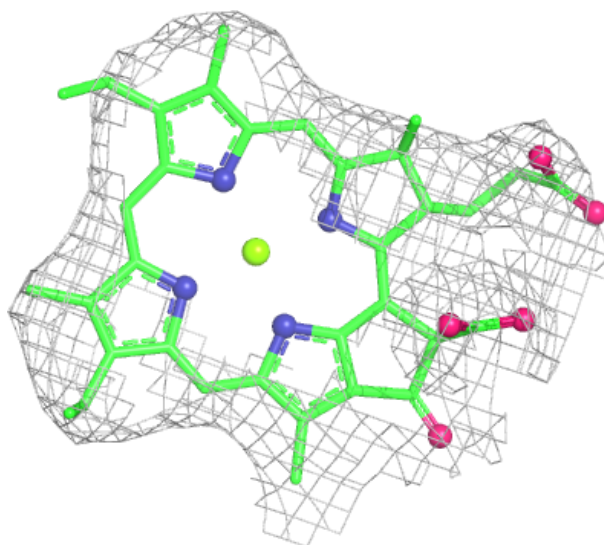
Electron density around CLA 8 305:

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



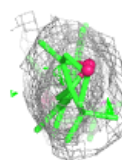
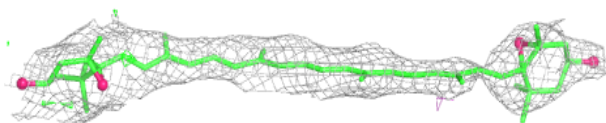
Electron density around CLA 8 306:

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



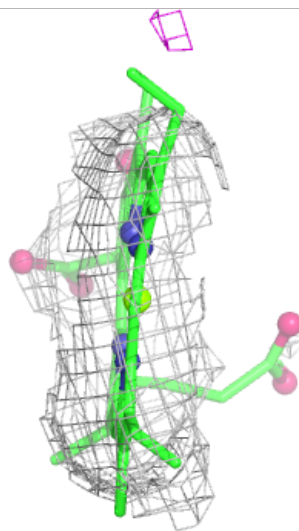
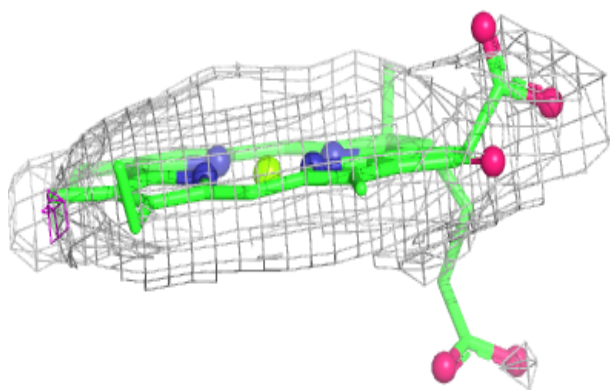
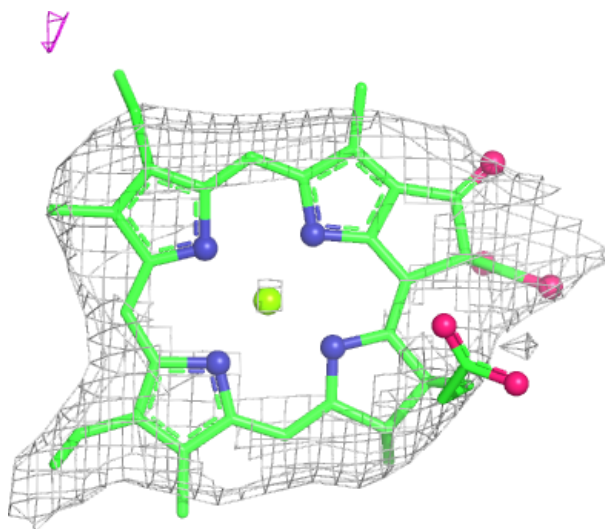
Electron density around XAT 5 303:

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



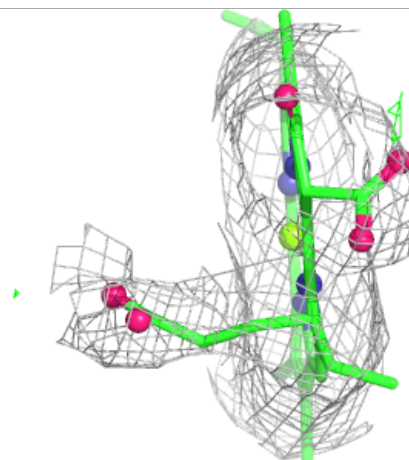
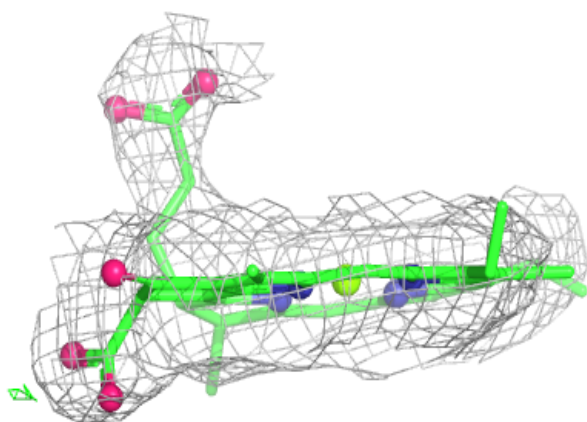
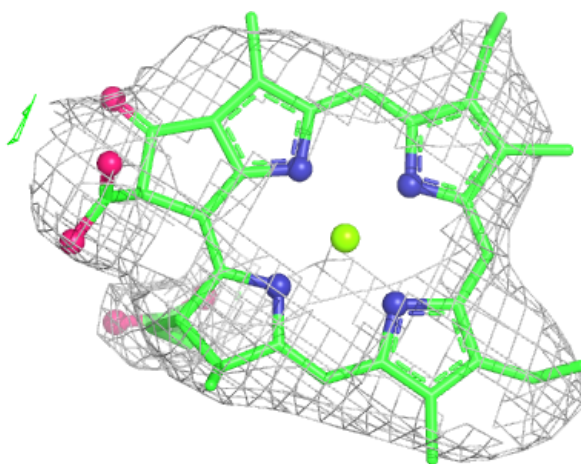
Electron density around CLA 7 1011:

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



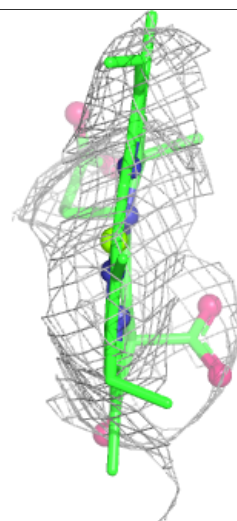
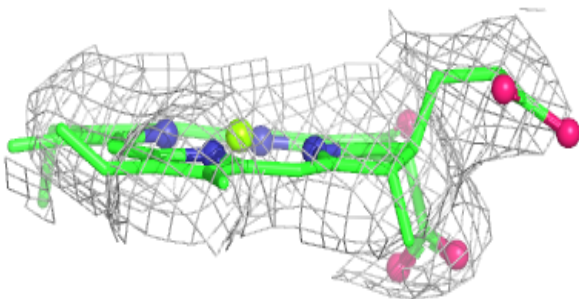
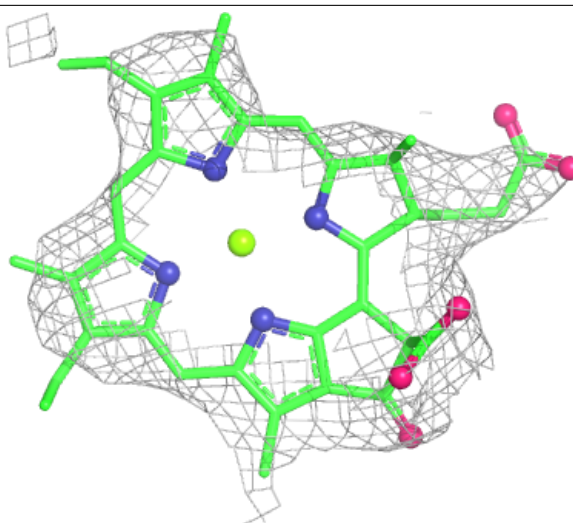
Electron density around CLA 8 312:

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



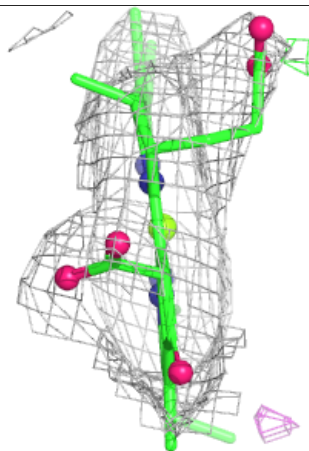
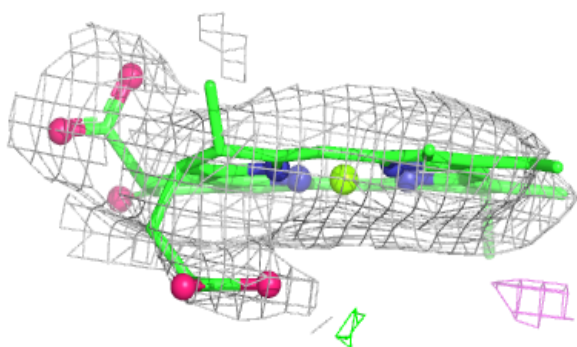
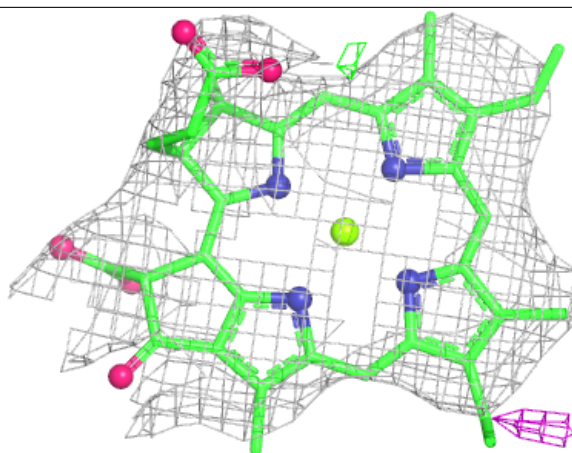
Electron density around CLA A 804:

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



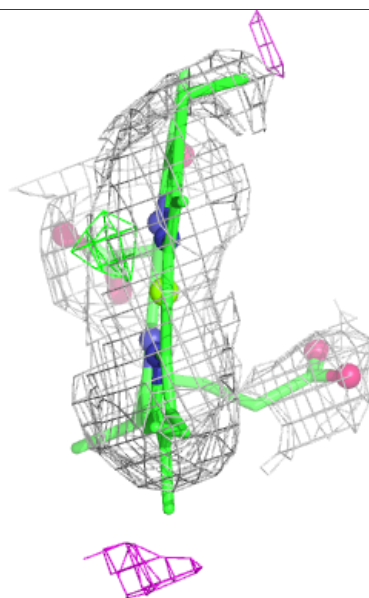
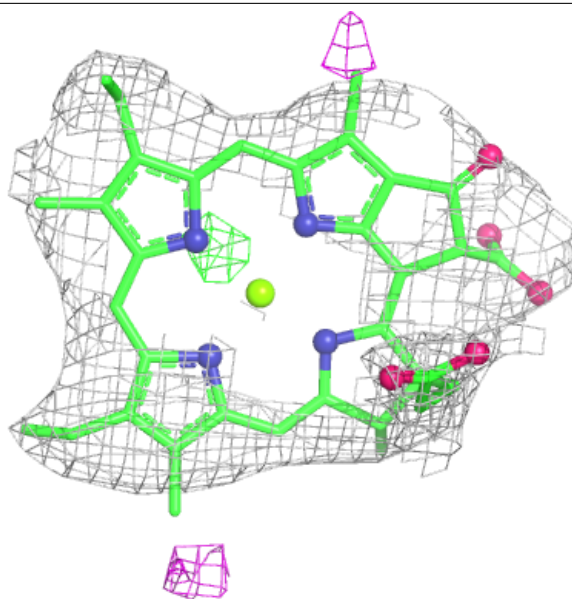
Electron density around CLA 1 1006:

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



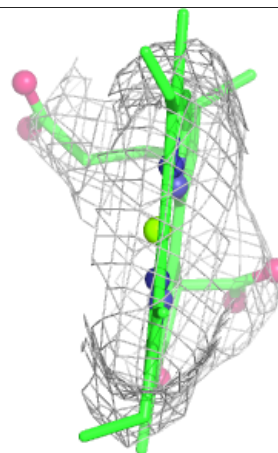
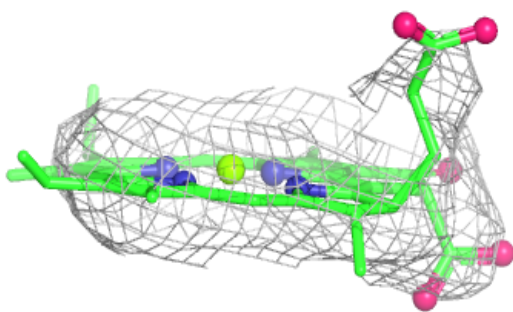
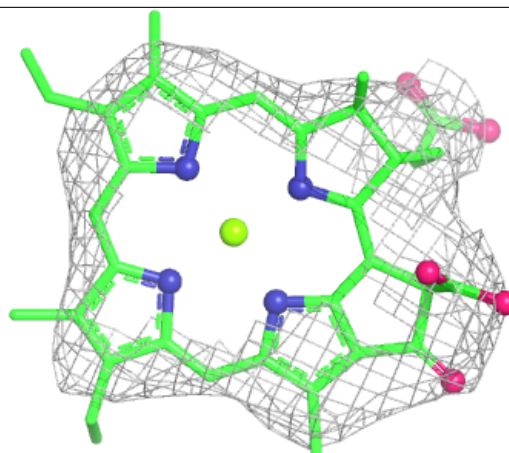
Electron density around CLA 5 301:

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



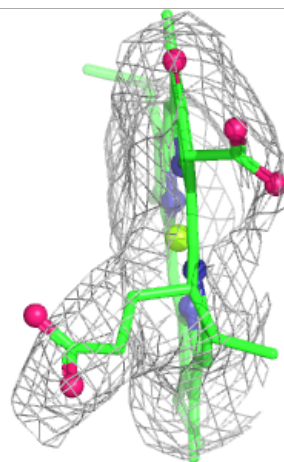
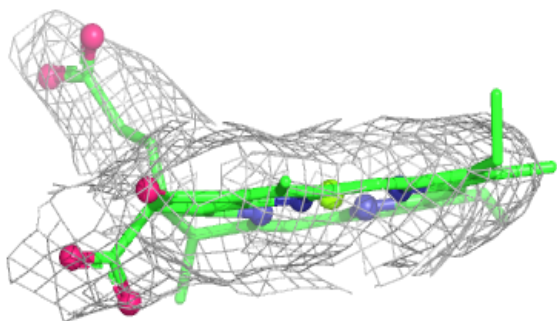
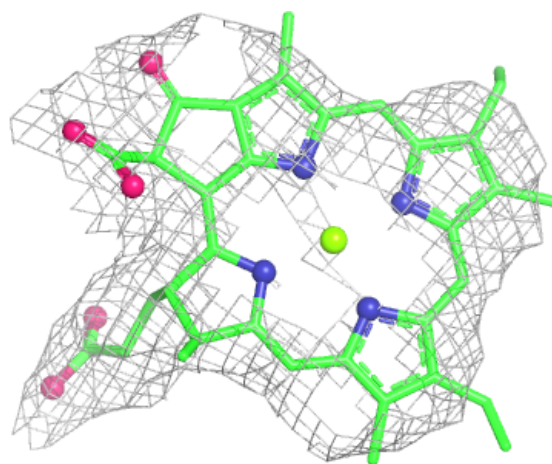
Electron density around CLA B 839:

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



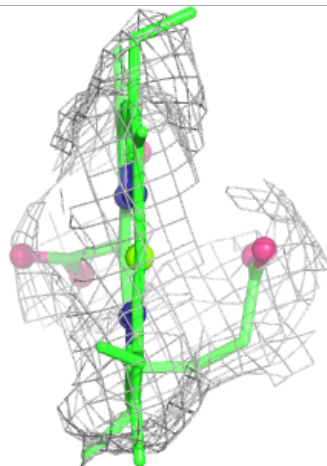
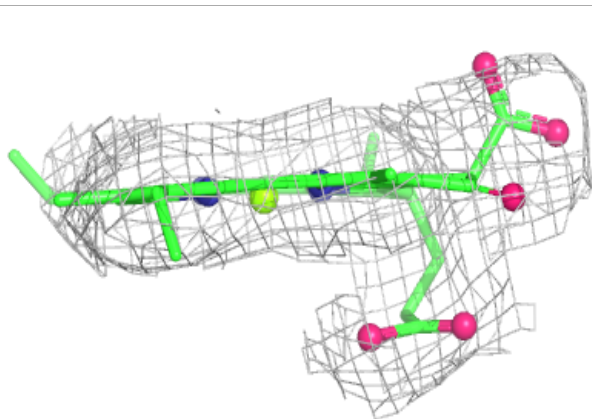
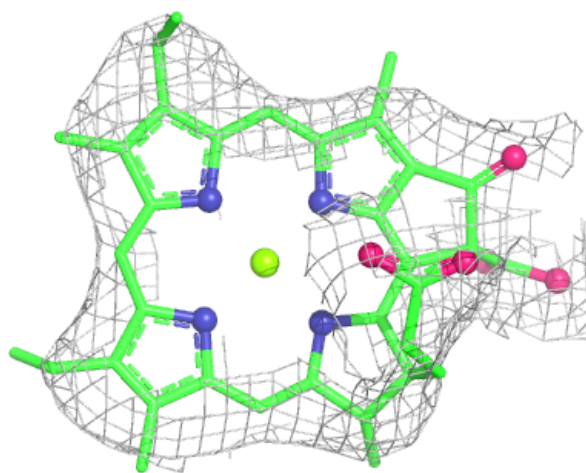
Electron density around CLA B 827:

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



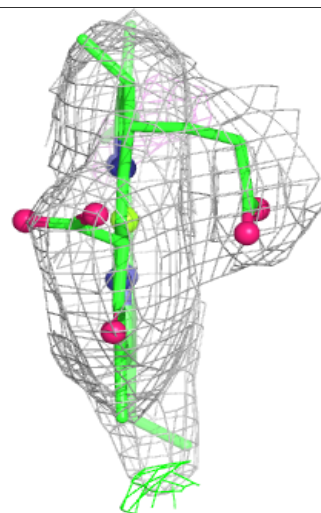
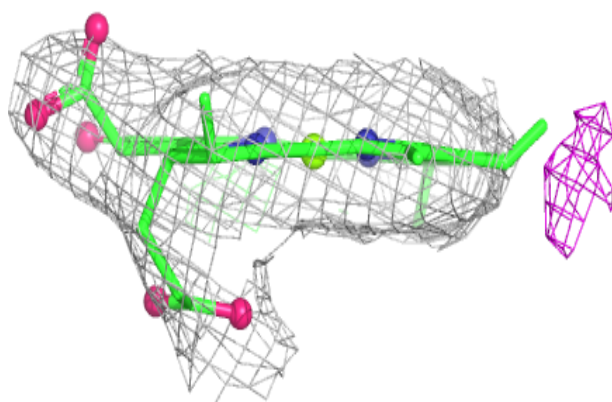
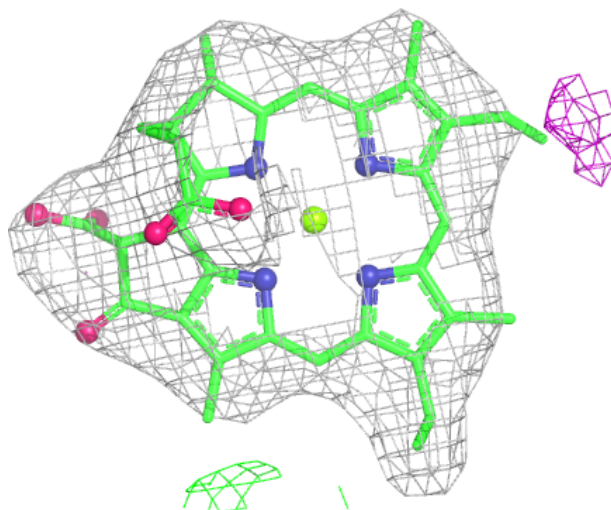
Electron density around CLA 5 306:

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



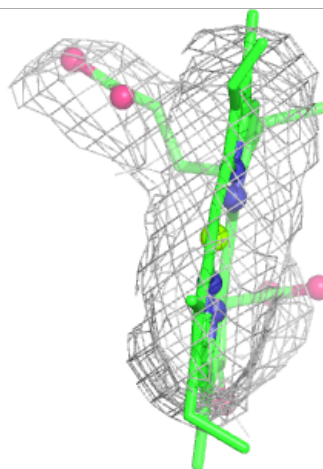
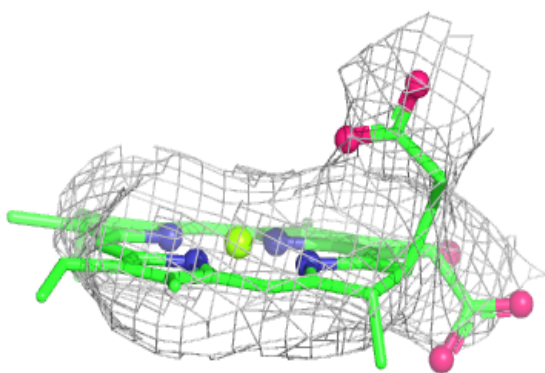
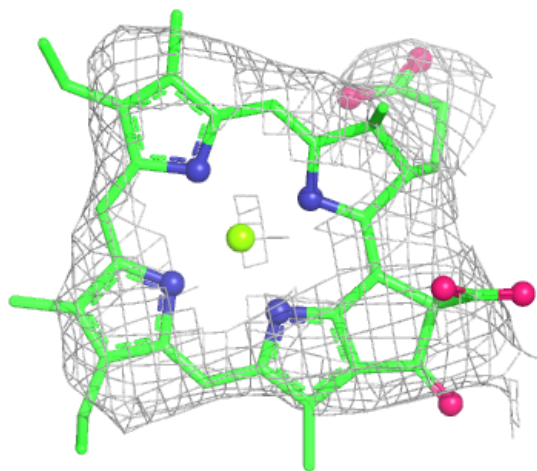
Electron density around CLA 8 307:

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



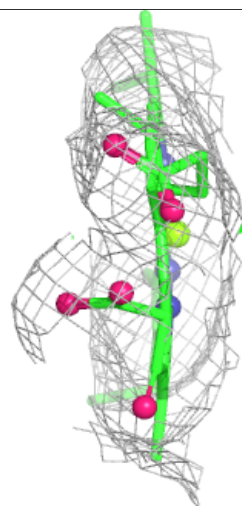
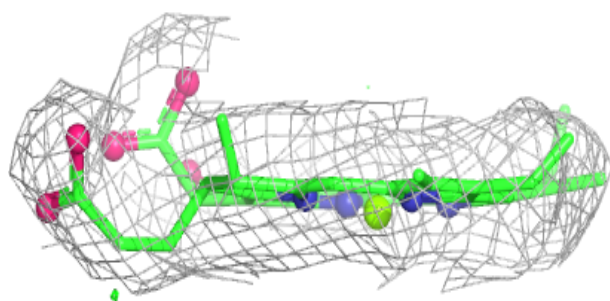
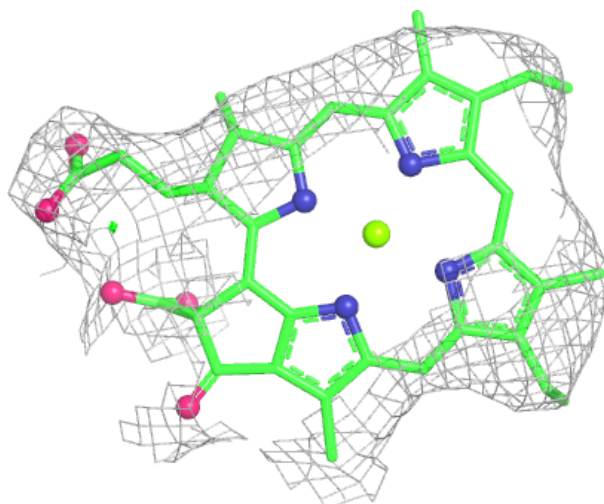
Electron density around CLA A 807:

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



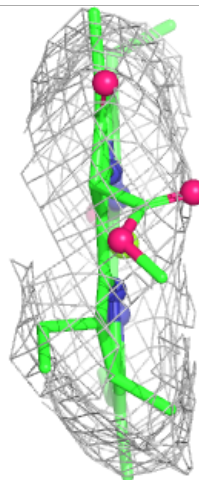
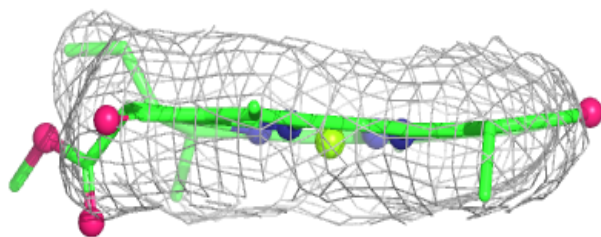
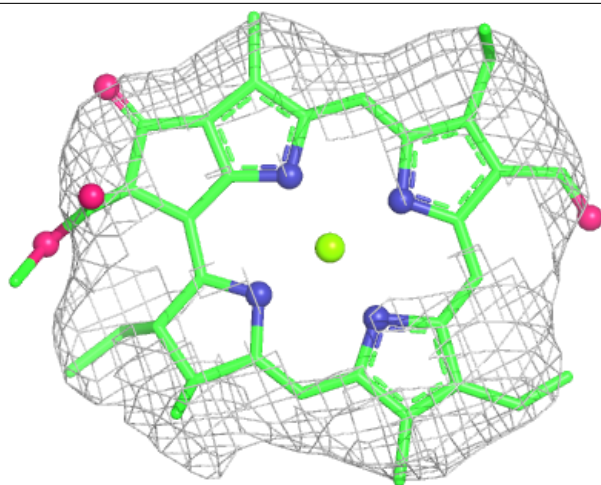
Electron density around CLA 6 306:

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



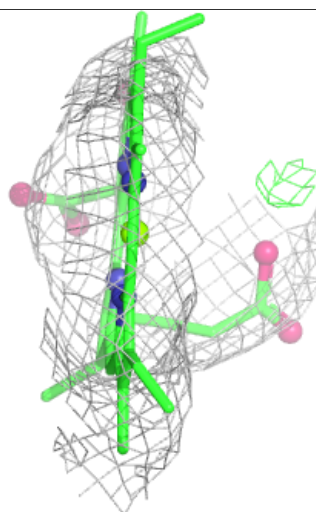
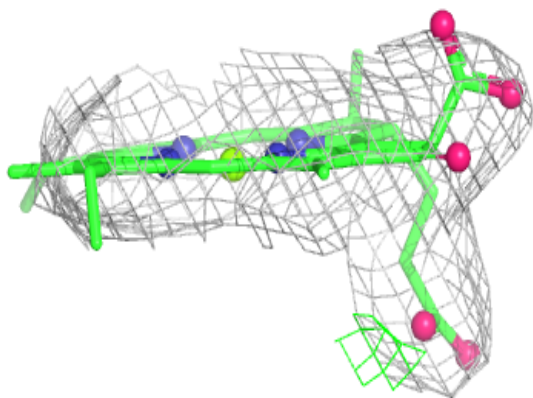
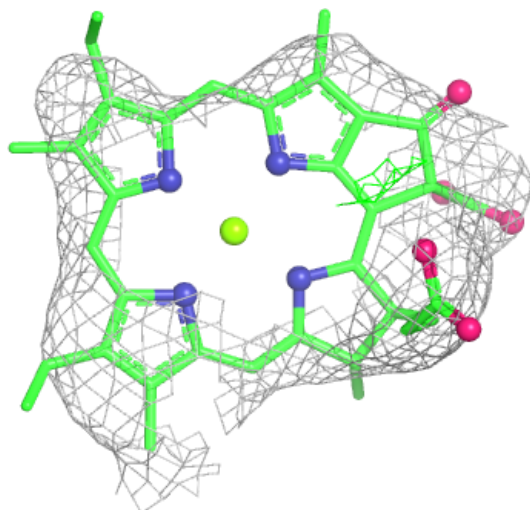
Electron density around CHL 6 317:

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



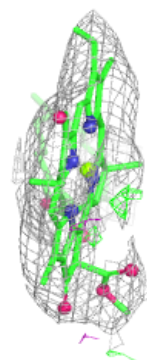
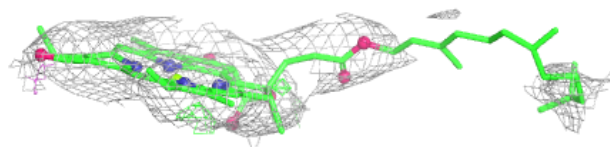
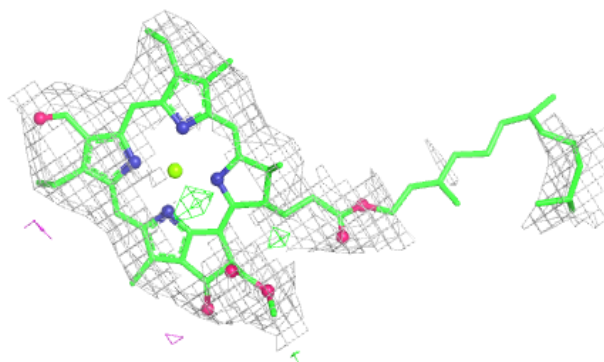
Electron density around CLA A 828:

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



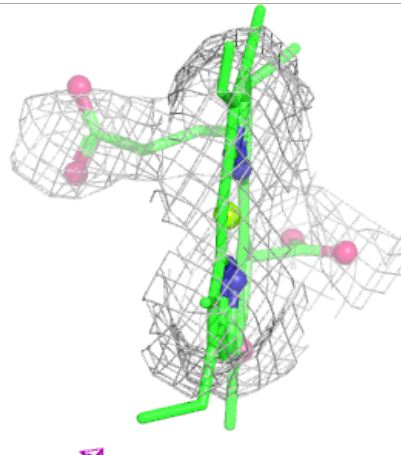
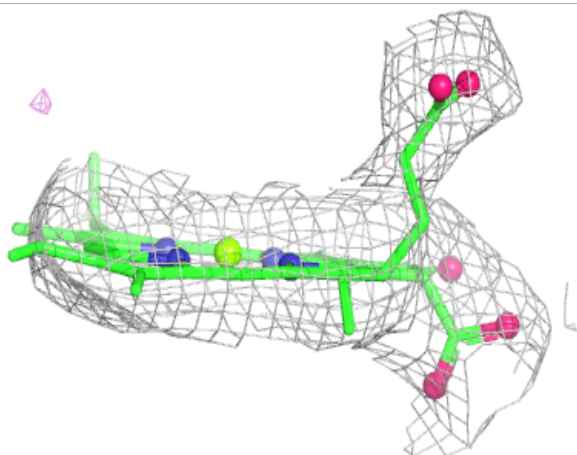
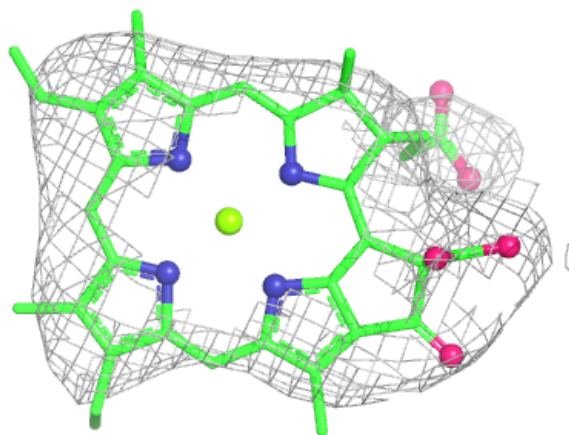
Electron density around CHL 5 316:

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



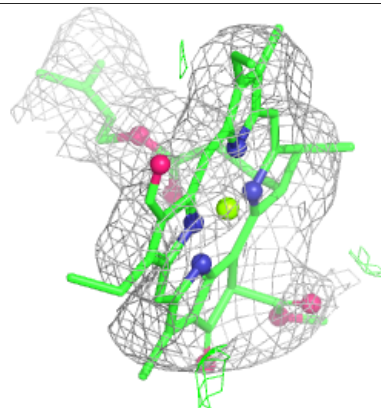
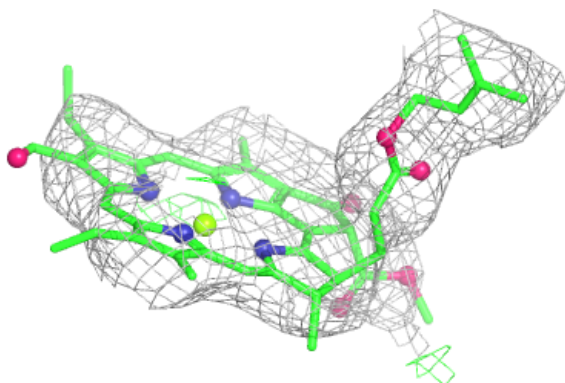
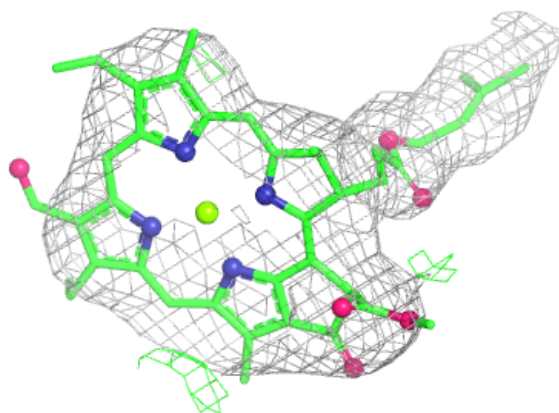
Electron density around CLA A 808:

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



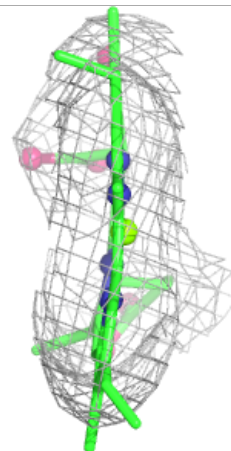
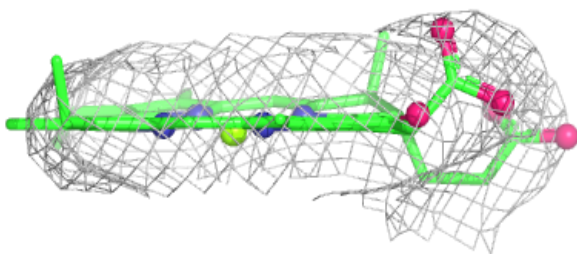
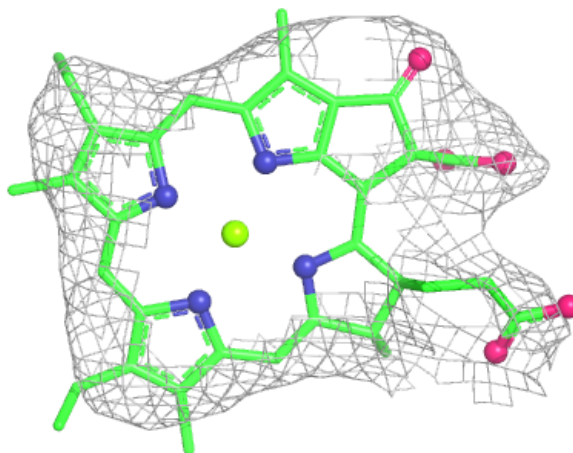
Electron density around CHL 8 315:

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



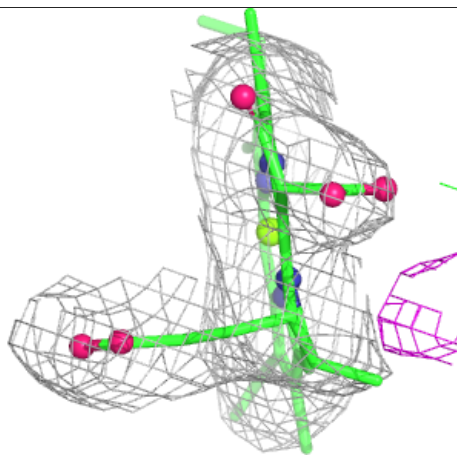
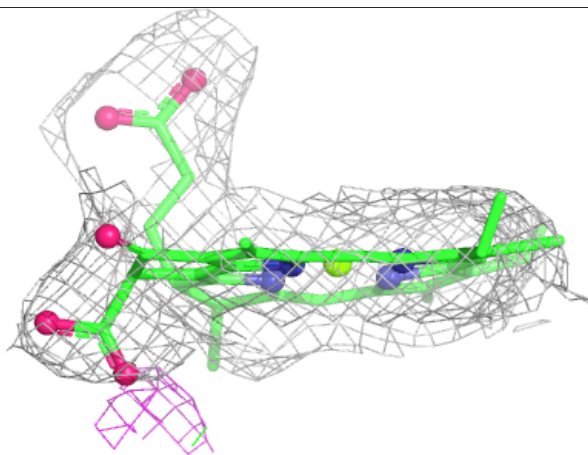
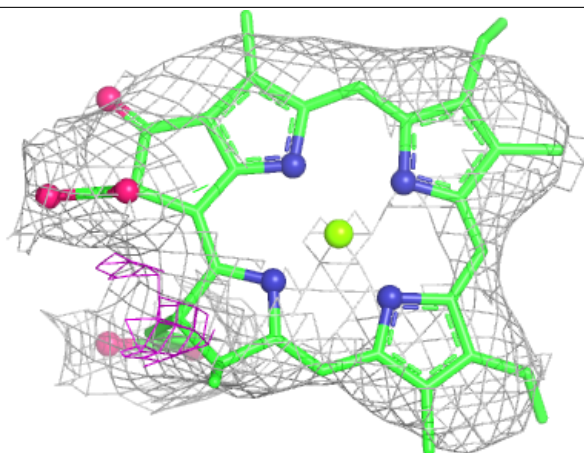
Electron density around CLA A 805:

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



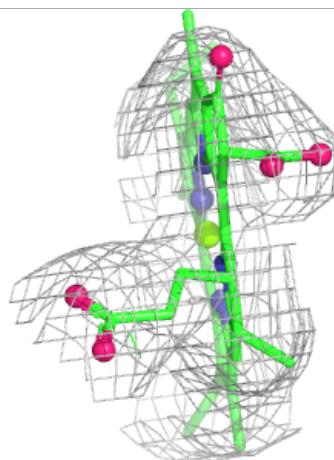
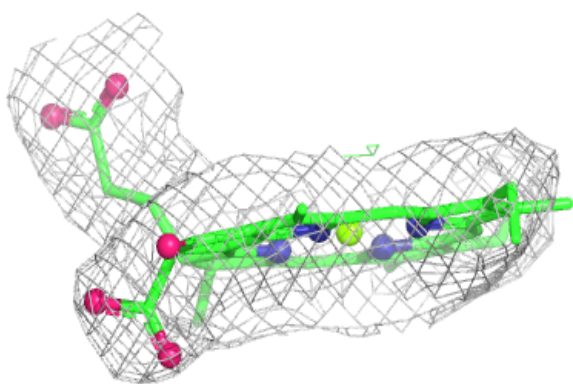
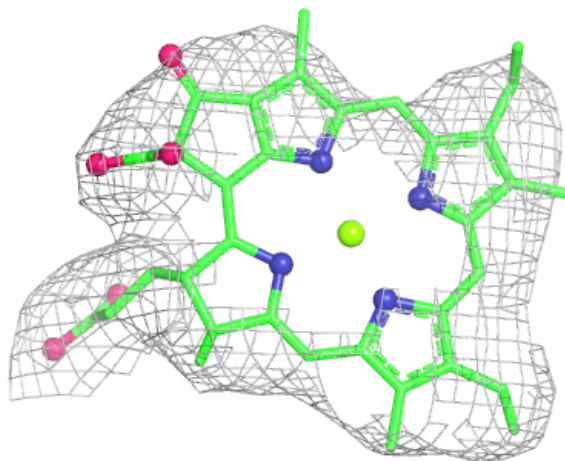
Electron density around CLA 5 315:

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



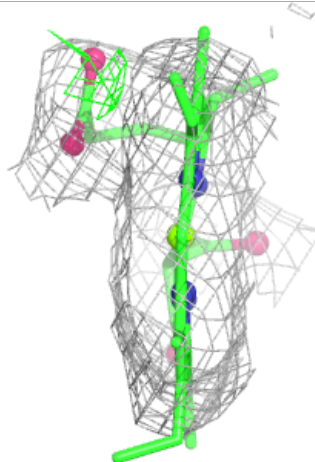
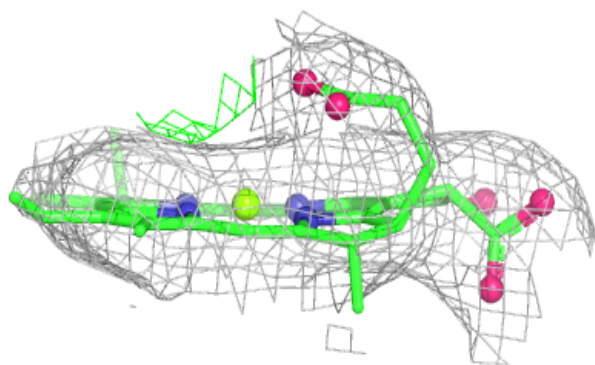
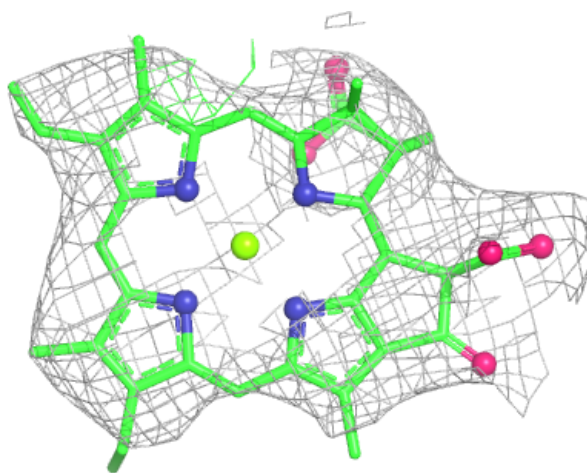
Electron density around CLA 5 318:

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



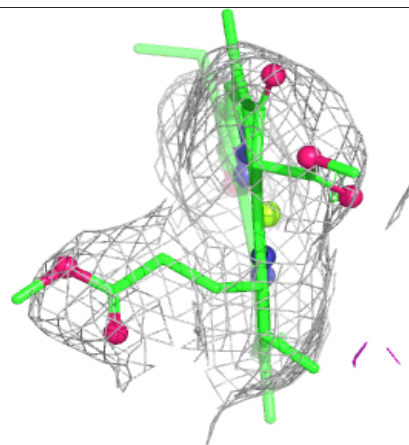
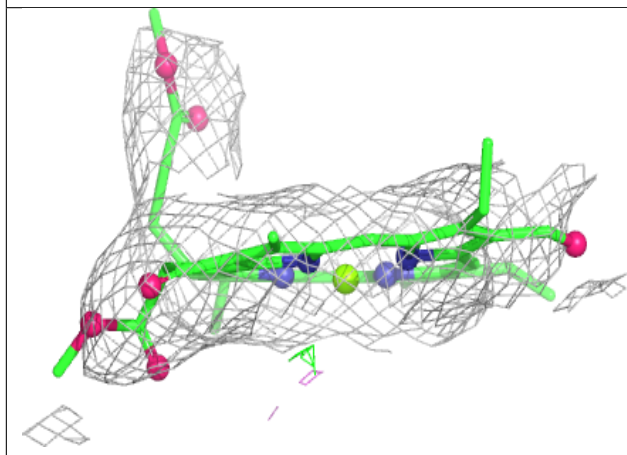
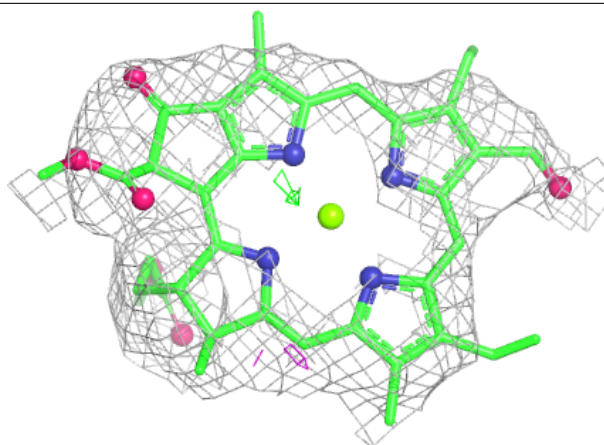
Electron density around CLA 4 304:

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



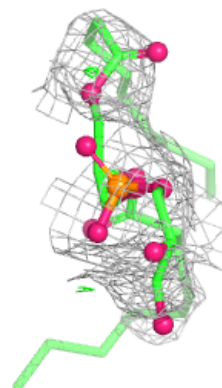
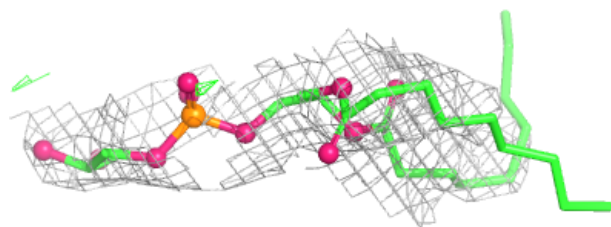
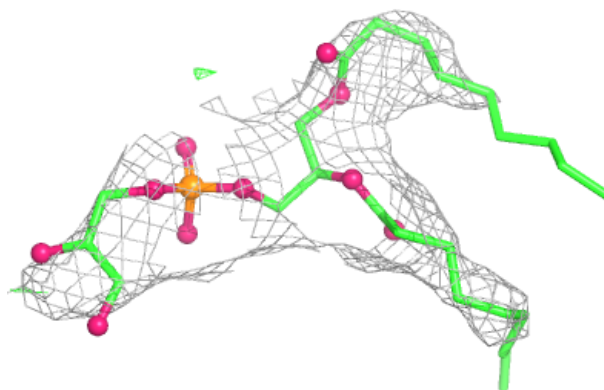
Electron density around CHL 3 1014:

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



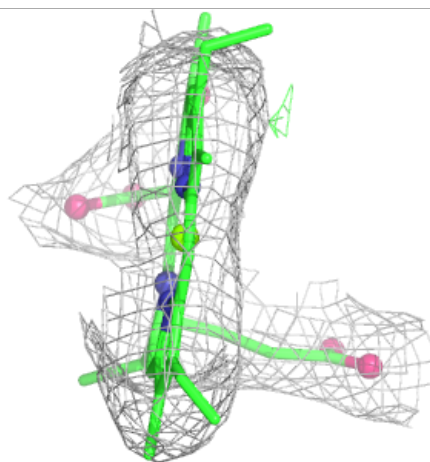
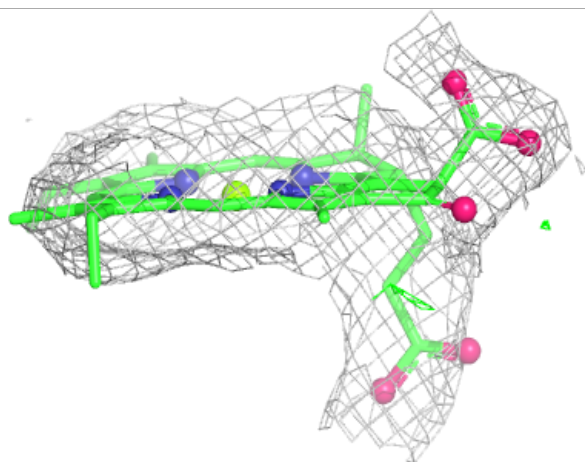
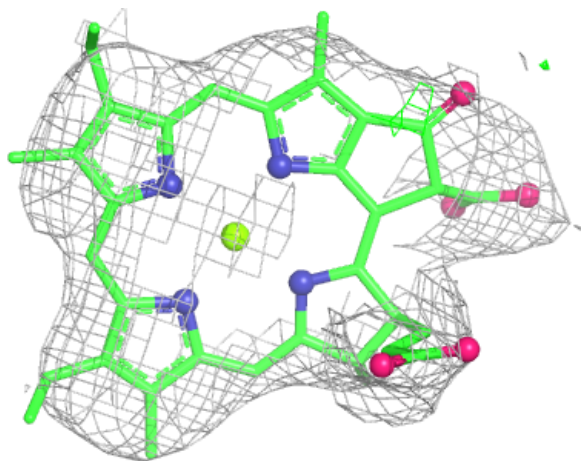
Electron density around LHG 7 1016:

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



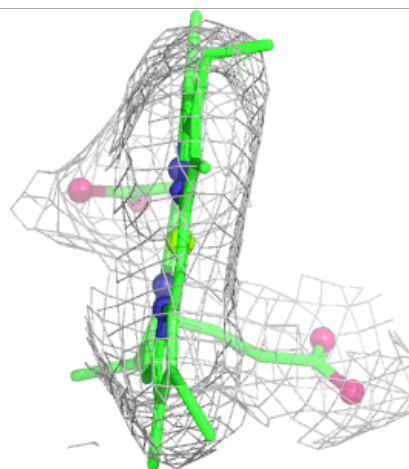
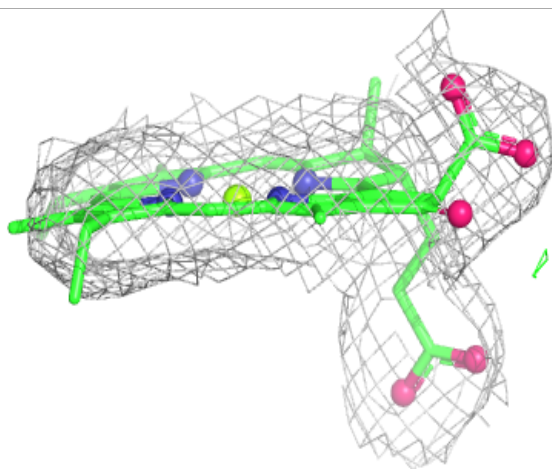
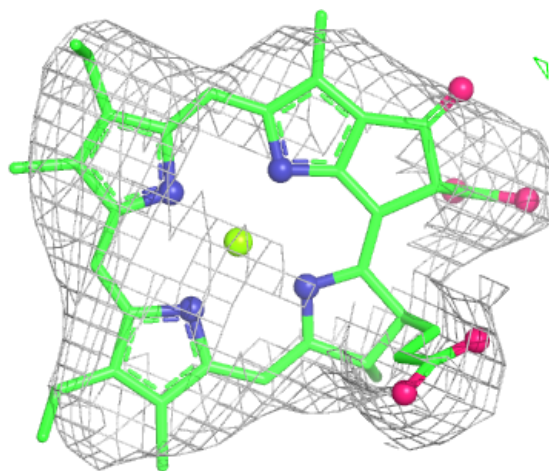
Electron density around CLA 6 315:

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



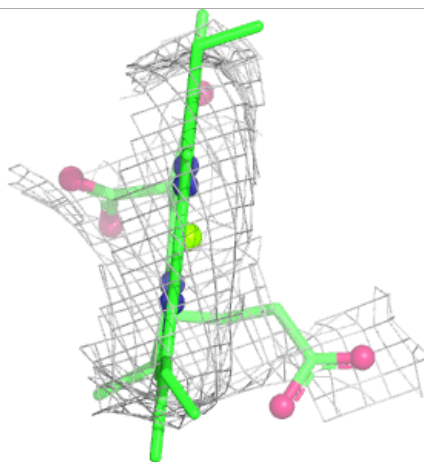
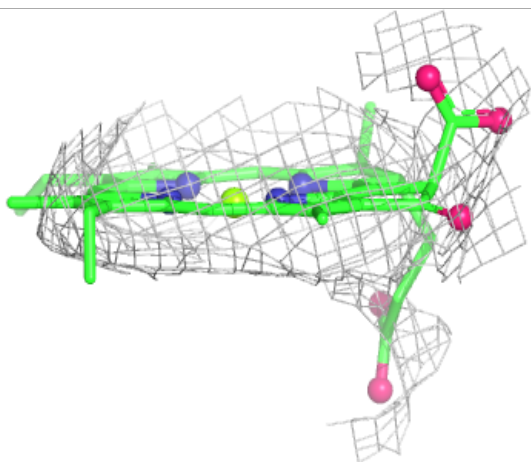
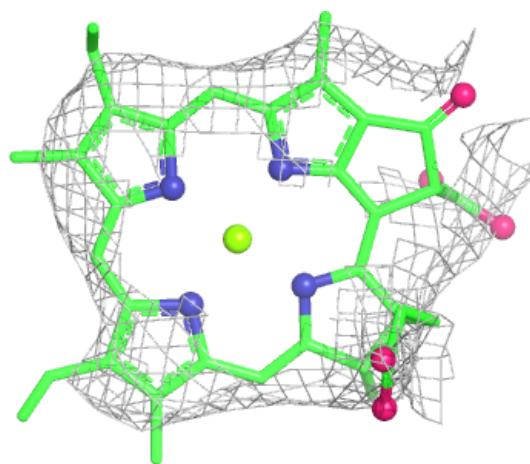
Electron density around CLA 7 1014:

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



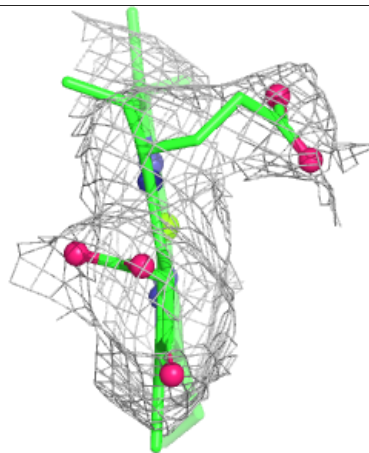
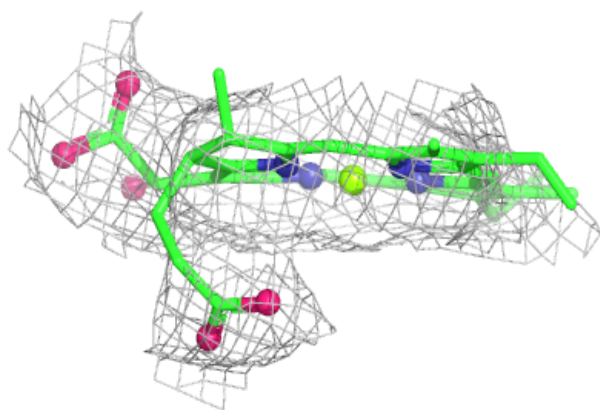
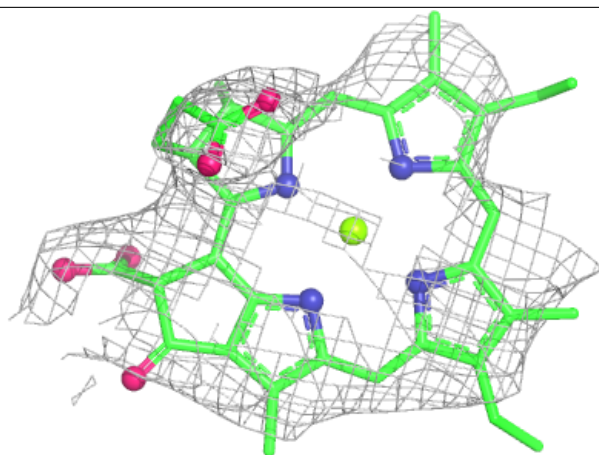
Electron density around CLA 3 1008:

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



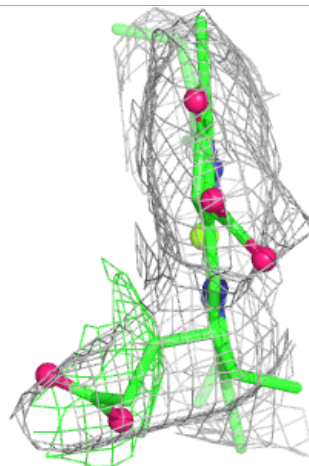
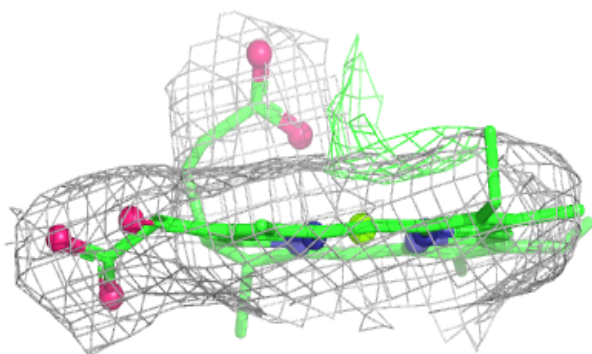
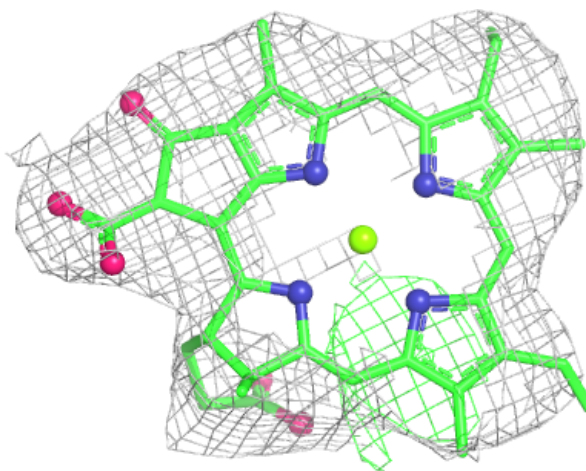
Electron density around CLA 3 1005:

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



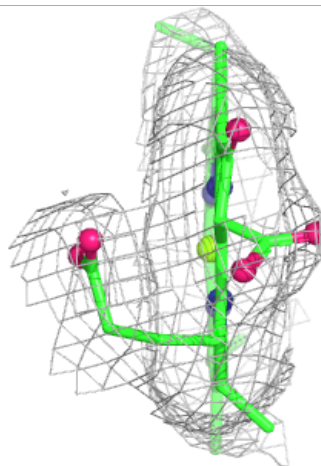
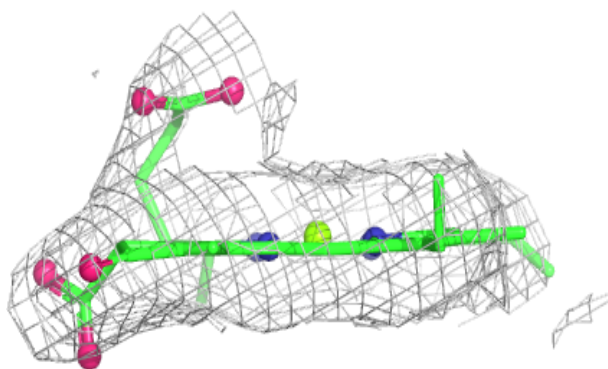
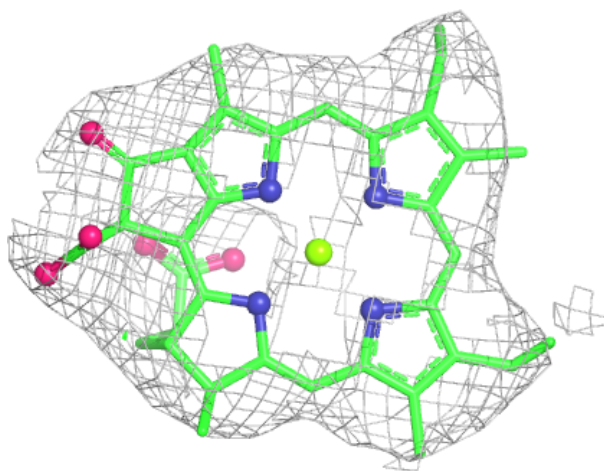
Electron density around CLA 7 1004:

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



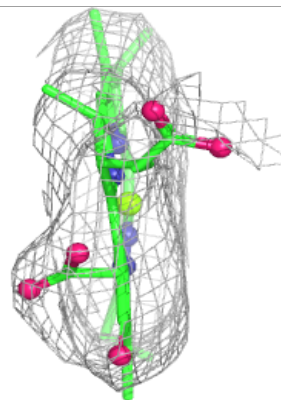
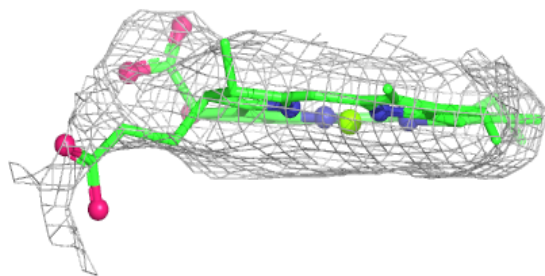
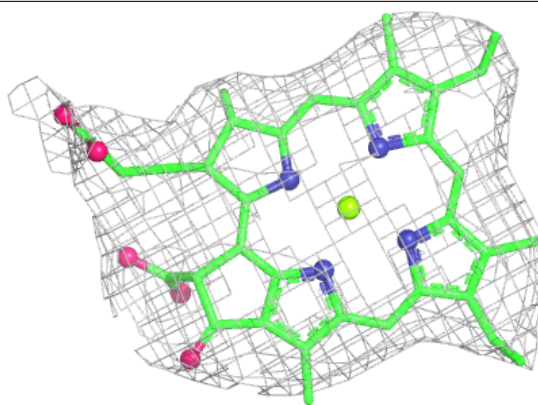
Electron density around CLA 4 306:

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



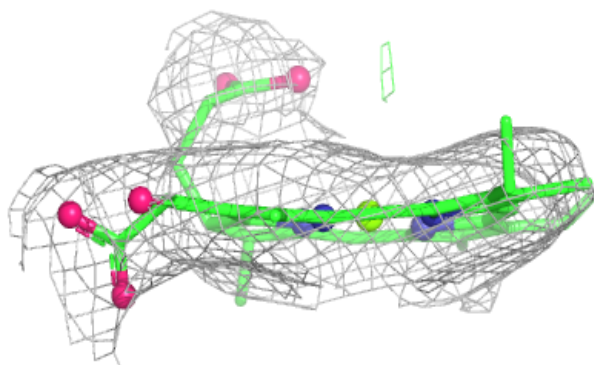
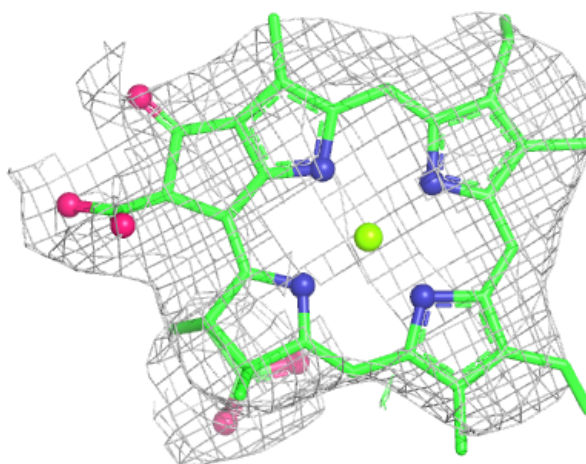
Electron density around CLA 3 1016:

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



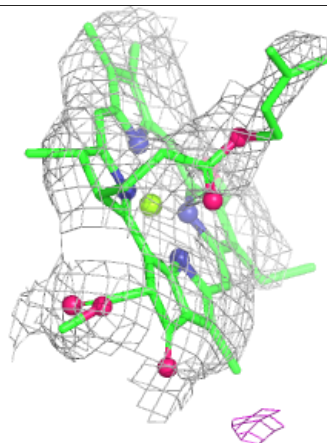
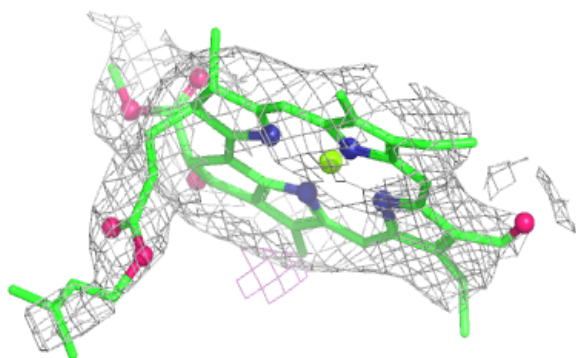
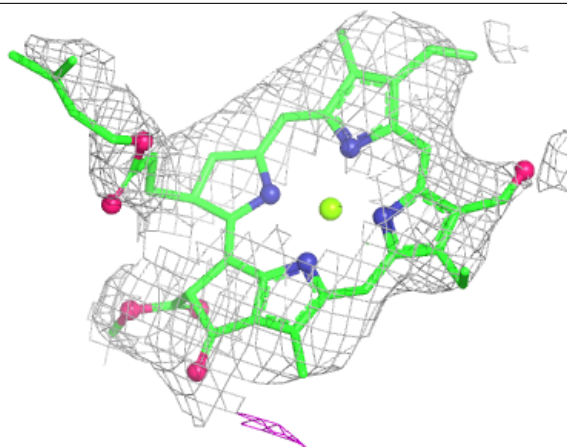
Electron density around CLA 6 305:

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



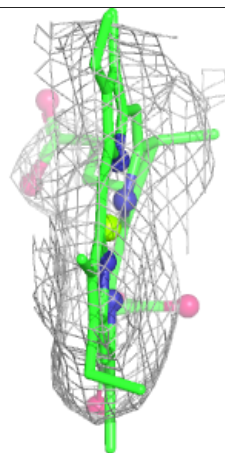
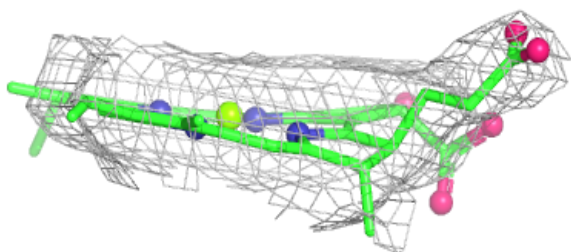
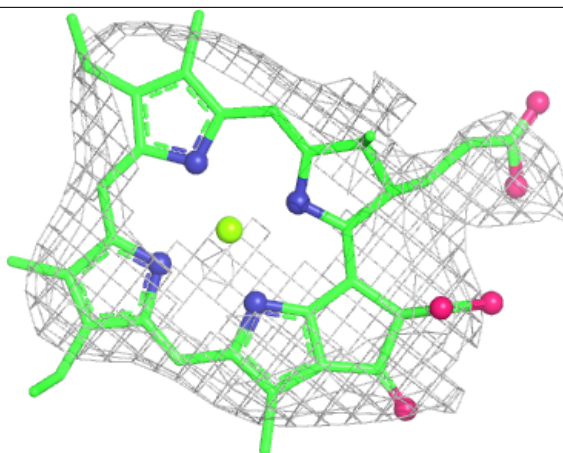
Electron density around CHL 5 314:

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



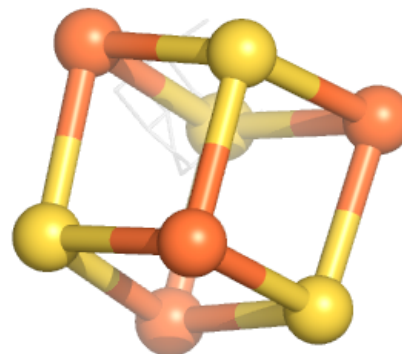
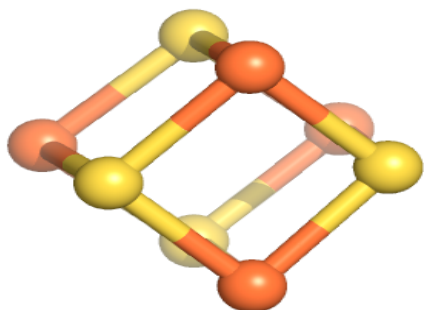
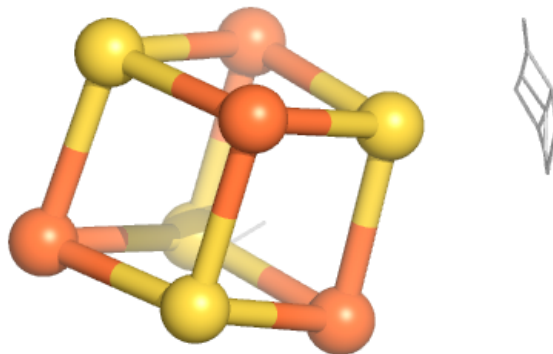
Electron density around CLA B 805:

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



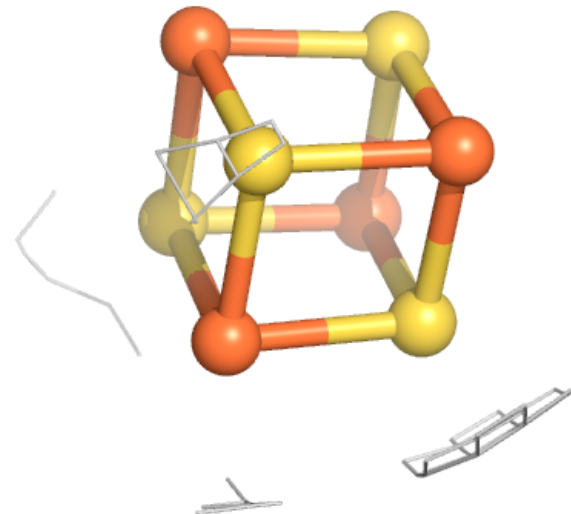
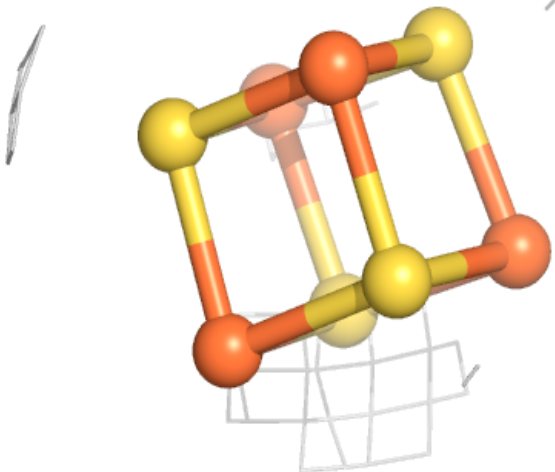
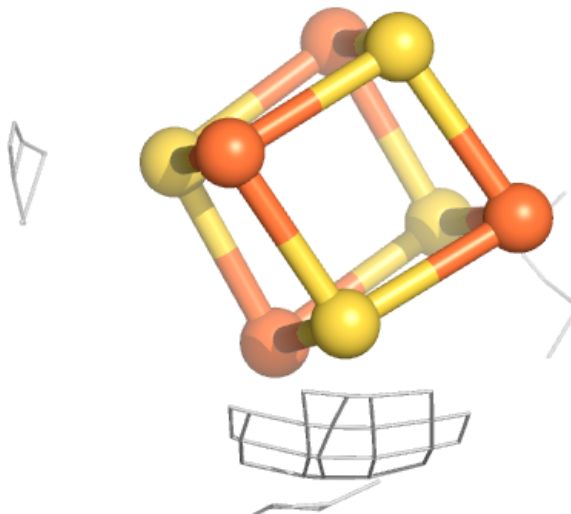
Electron density around SF4 A 841:

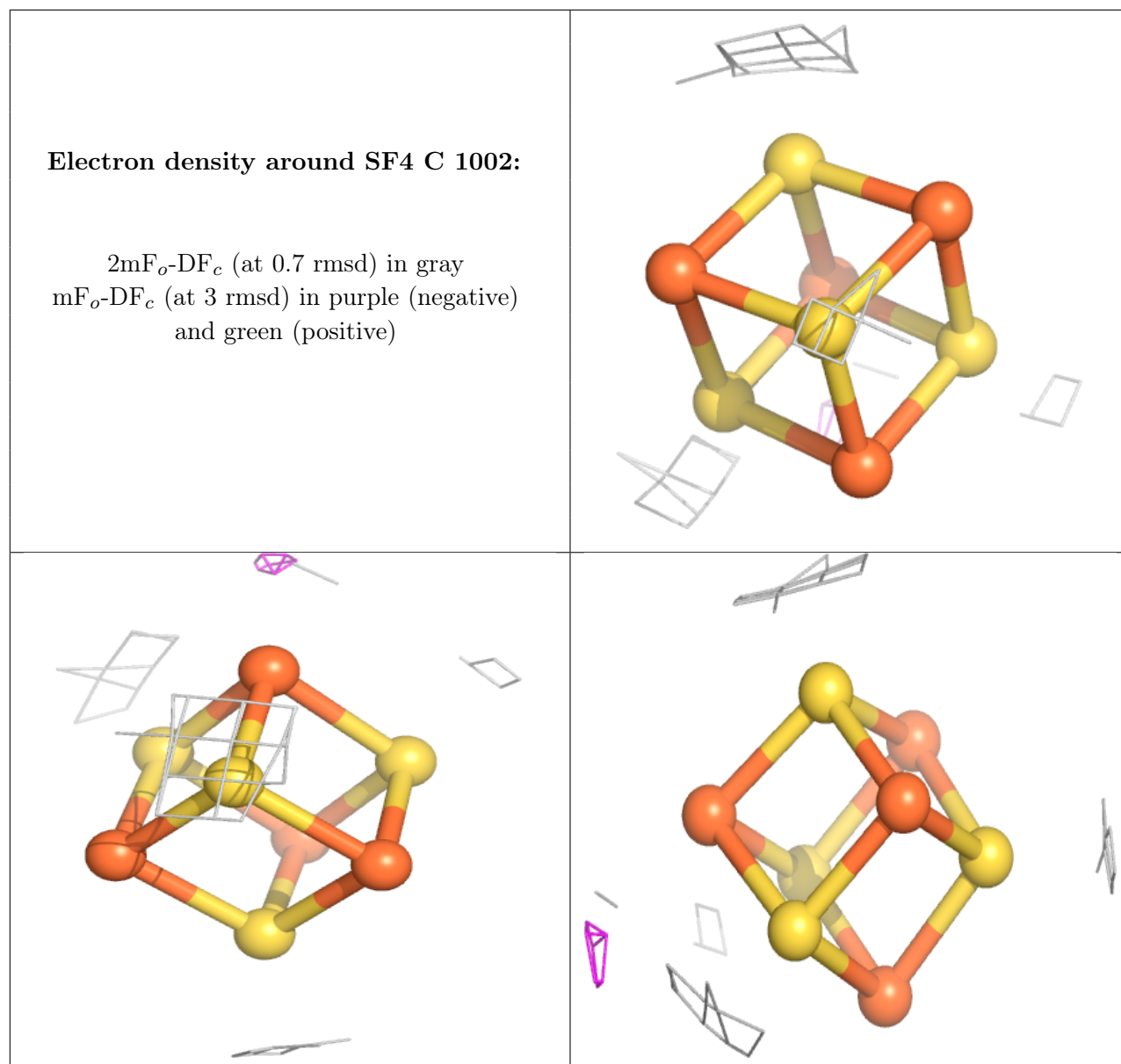
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SF4 C 1001:

$2mF_o-DF_c$ (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.