



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 04:03 AM JST

PDB ID : 4XK8 / pdb_00004xk8
Title : Crystal structure of plant photosystem I-LHCI super-complex at 2.8 angstrom resolution
Authors : Suga, M.; Qin, X.; Kuang, T.; Shen, J.R.
Deposited on : 2015-01-10
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

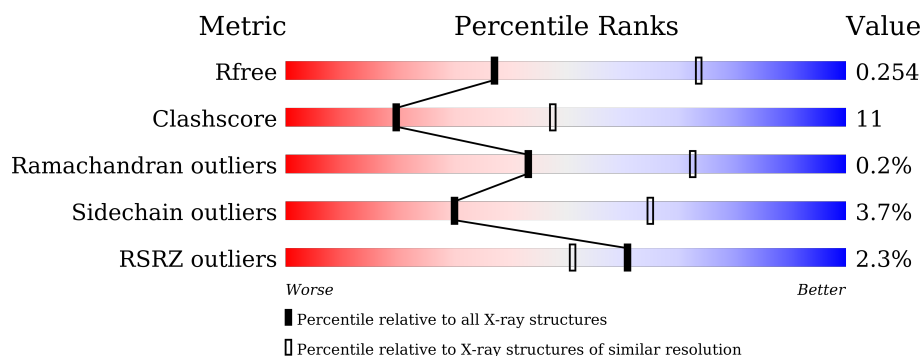
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	742	81%18%.
1	a	742	82%17%.
2	B	733	80%19%.
2	b	733	82%17%.
3	C	80	80%18%.
3	c	80	88%10%.

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Mol	Chain	Length	Quality of chain
4	D	141	
4	d	141	
5	E	64	
5	e	64	
6	F	151	
6	f	151	
7	G	95	
7	g	95	
8	H	90	
8	h	90	
9	I	30	
9	i	30	
10	J	39	
10	j	39	
11	K	84	
11	k	84	
12	L	153	
12	l	153	
13	1	195	
13	6	195	
14	2	206	
14	7	206	
15	3	218	
15	8	218	
16	4	196	

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Mol	Chain	Length	Quality of chain
16	9	196	

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
17	CLA	A	801	X	-	-	-
17	CLA	a	801	X	-	-	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 71157 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	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			
1	a	742	Total	C	N	O	S	0	0	0
			5846	3831	994	1003	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			
2	b	733	Total	C	N	O	S	0	0	0
			5863	3853	1002	994	14			

- 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
			611	379	107	114	11			
3	c	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	141	Total	C	N	O	S	0	0	0
			1114	716	193	202	3			
4	d	140	Total	C	N	O	S	0	0	0
			1107	712	192	200	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total	C	N	O	0	0	0
			507	321	90	96			
5	e	63	Total	C	N	O	0	0	0
			506	322	90	94			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			
6	f	151	Total	C	N	O	S	0	0	0
			1193	776	204	210	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			741	480	121	140			
7	g	95	Total	C	N	O	0	0	0
			737	478	121	138			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	90	Total	C	N	O	0	0	0
			678	439	110	129			
8	h	90	Total	C	N	O	0	0	0
			682	442	111	129			

- 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	33	34	1			
9	i	30	Total	C	N	O	S	0	0	0
			226	156	34	35	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
			311	211	48	51	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	j	39	Total	C	N	O	S	0	0	0
			311	211	48	51	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	45	Total	C	N	O	S	0	0	0
			311	204	48	56	3			
11	k	46	Total	C	N	O	S	0	0	0
			316	207	49	57	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	153	Total	C	N	O	S	0	0	0
			1136	746	183	206	1			
12	l	151	Total	C	N	O	S	0	0	0
			1122	738	180	203	1			

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	195	Total	C	N	O	S	0	0	0
			1491	969	249	268	5			
13	6	195	Total	C	N	O	S	0	0	0
			1483	963	247	268	5			

- Molecule 14 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			
14	7	206	Total	C	N	O	S	0	0	0
			1610	1055	263	288	4			

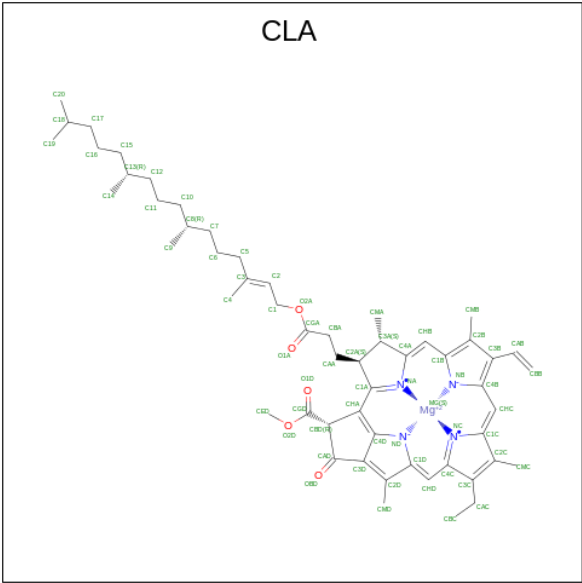
- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	218	Total	C	N	O	S	0	0	0
			1680	1100	273	302	5			
15	8	217	Total	C	N	O	S	0	0	0
			1672	1094	272	301	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	4	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			
16	9	196	Total	C	N	O	S	0	0	0
			1540	1009	251	277	3			

- Molecule 17 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	A	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	F	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	J	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	L	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	1	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	1	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
17	1	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	1	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	2	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	2	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	2	1	Total 60	C 50	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	2	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	3	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
17	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	a	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
17	a	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
17	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	a	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	a	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	a	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
17	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	b	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	f	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	f	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
17	g	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
17	g	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
17	g	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	j	1	Total 42	C 34	Mg 1	N 4	O 3	0	0
17	k	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
17	k	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	k	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
17	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
17	l	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	6	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	6	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	7	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	7	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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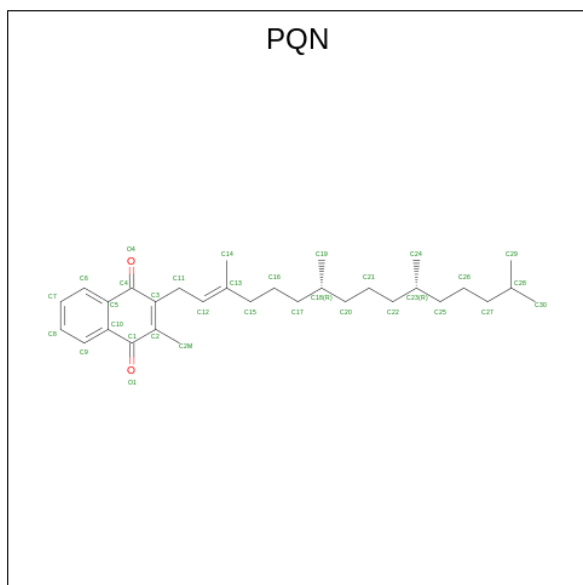
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	O	0	0
			43	35	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
17	8	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	8	1	Total	C	Mg	N		0	0
			25	20	1	4			
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
17	9	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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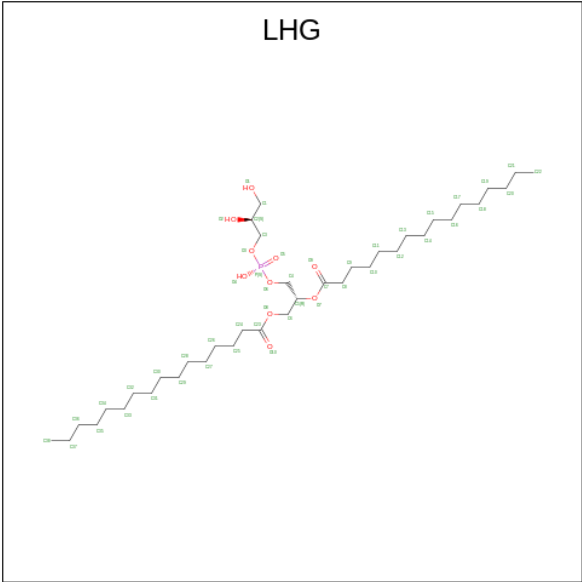
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	9	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
17	9	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



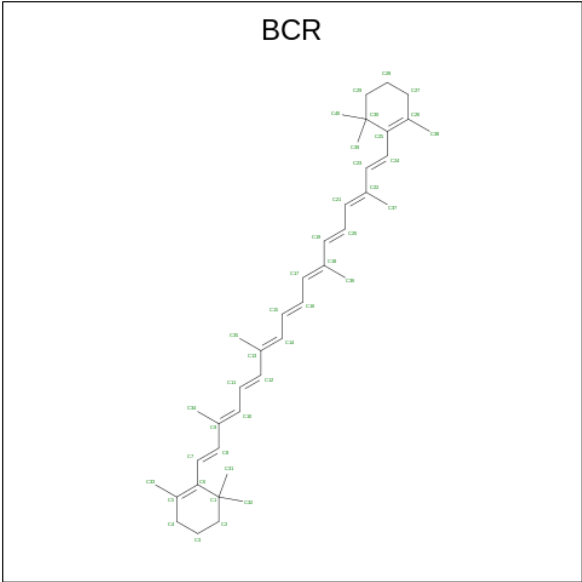
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			33	31	2		
18	B	1	Total	C	O	0	0
			33	31	2		
18	a	1	Total	C	O	0	0
			33	31	2		
18	b	1	Total	C	O	0	0
			33	31	2		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			49	38	10	1		
19	A	1	Total	C	O	P	0	0
			27	16	10	1		
19	1	1	Total	C	O	P	0	0
			23	12	10	1		
19	1	1	Total	C	O	P	0	0
			49	38	10	1		
19	2	1	Total	C	O	P	0	0
			37	26	10	1		
19	3	1	Total	C	O	P	0	0
			20	10	9	1		
19	a	1	Total	C	O	P	0	0
			49	38	10	1		
19	a	1	Total	C	O	P	0	0
			27	16	10	1		
19	6	1	Total	C	O	P	0	0
			23	12	10	1		
19	6	1	Total	C	O	P	0	0
			49	38	10	1		
19	7	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	A	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	B	1	Total C 40 40	0	0
20	F	1	Total C 40 40	0	0

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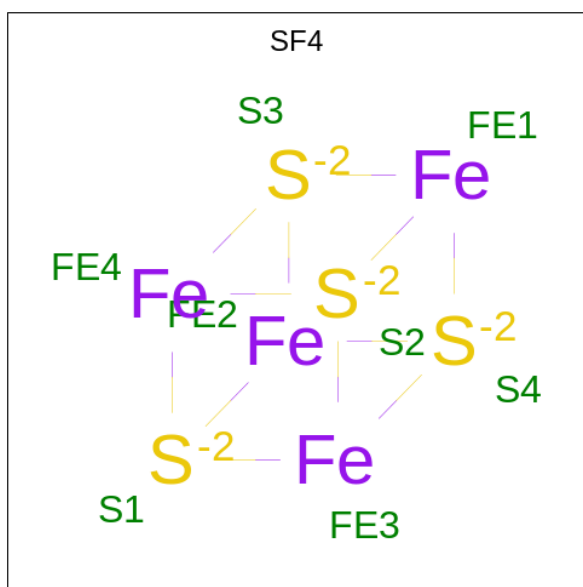
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	G	1	Total C 40 40	0	0
20	I	1	Total C 40 40	0	0
20	J	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	K	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	L	1	Total C 40 40	0	0
20	1	1	Total C 40 40	0	0
20	2	1	Total C 40 40	0	0
20	3	1	Total C 40 40	0	0
20	4	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	a	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0

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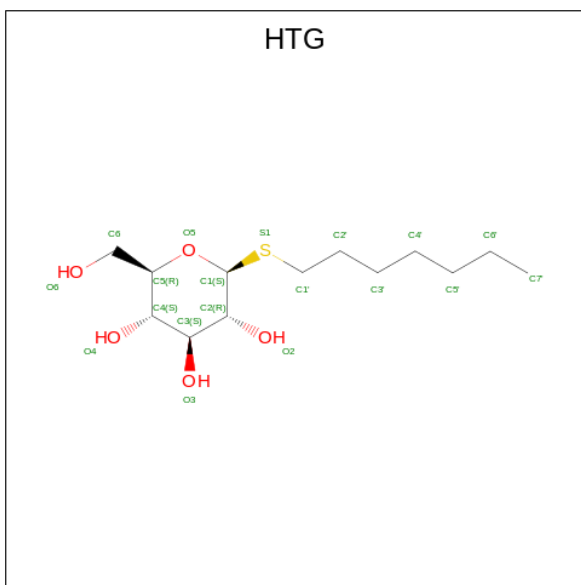
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	b	1	Total C 40 40	0	0
20	f	1	Total C 40 40	0	0
20	g	1	Total C 40 40	0	0
20	i	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	j	1	Total C 40 40	0	0
20	k	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	l	1	Total C 40 40	0	0
20	6	1	Total C 40 40	0	0
20	7	1	Total C 40 40	0	0
20	8	1	Total C 40 40	0	0
20	9	1	Total C 40 40	0	0

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



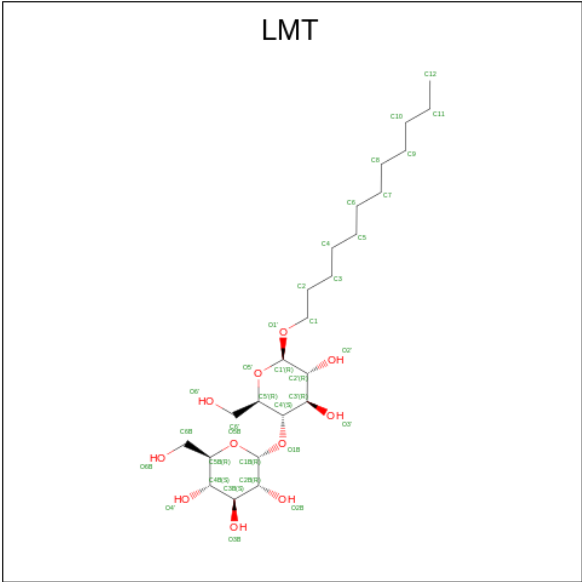
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	C	1	Total	Fe	S	0	0
			8	4	4		
21	a	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		
21	c	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 22 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



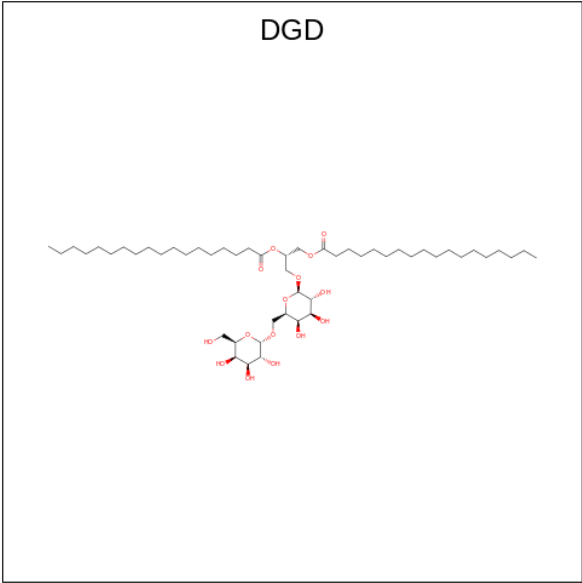
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	O	S	0	0
			19	13	5	1		
22	F	1	Total	C	O	S	0	0
			19	13	5	1		
22	J	1	Total	C	O	S	0	0
			19	13	5	1		
22	a	1	Total	C	O	S	0	0
			19	13	5	1		
22	f	1	Total	C	O	S	0	0
			19	13	5	1		
22	j	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



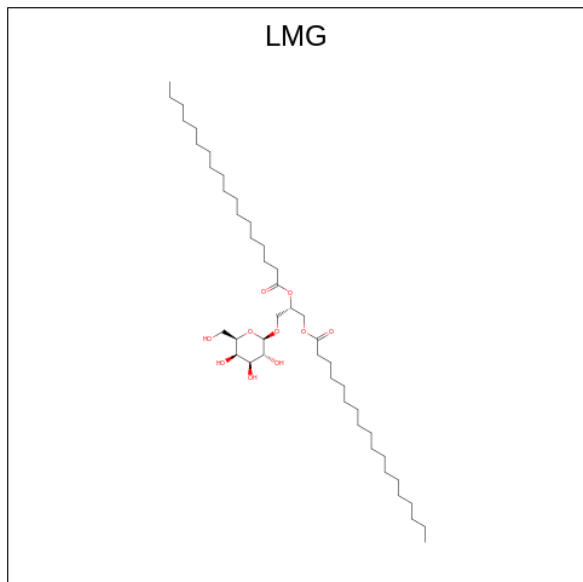
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



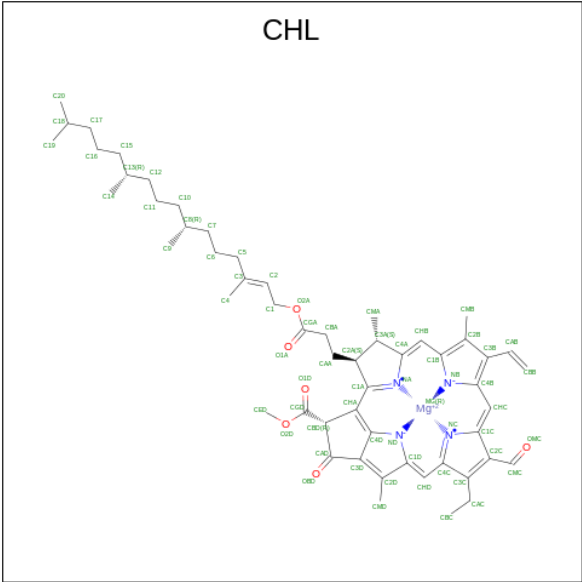
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			66	51	15		
24	b	1	Total	C	O	0	0
			66	51	15		

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	G	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	4	1	Total	C	O	0	0
			44	34	10		
25	6	1	Total	C	O	0	0
			40	30	10		
25	9	1	Total	C	O	0	0
			50	40	10		

- Molecule 26 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



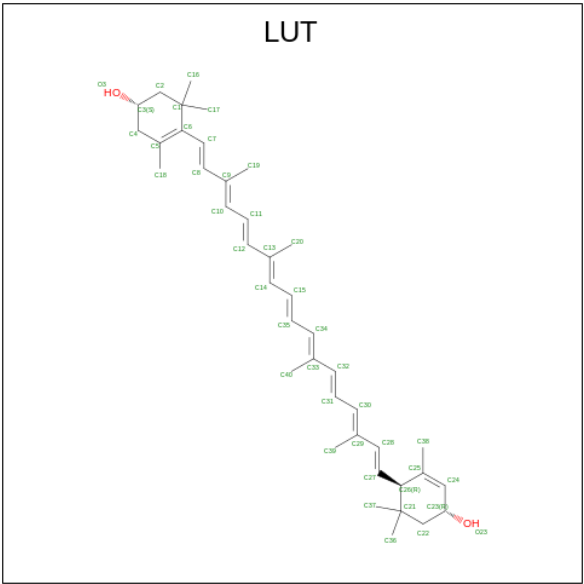
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	1	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	1	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	2	1	Total 48	C 37	Mg 1	N 4	O 6	0	0
26	2	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	2	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	3	1	Total 47	C 36	Mg 1	N 4	O 6	0	0
26	4	1	Total 56	C 45	Mg 1	N 4	O 6	0	0
26	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	4	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
26	4	1	Total 43	C 34	Mg 1	N 4	O 4	0	0
26	6	1	Total 61	C 50	Mg 1	N 4	O 6	0	0
26	6	1	Total 47	C 36	Mg 1	N 4	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	7	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	7	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	7	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
26	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
26	9	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



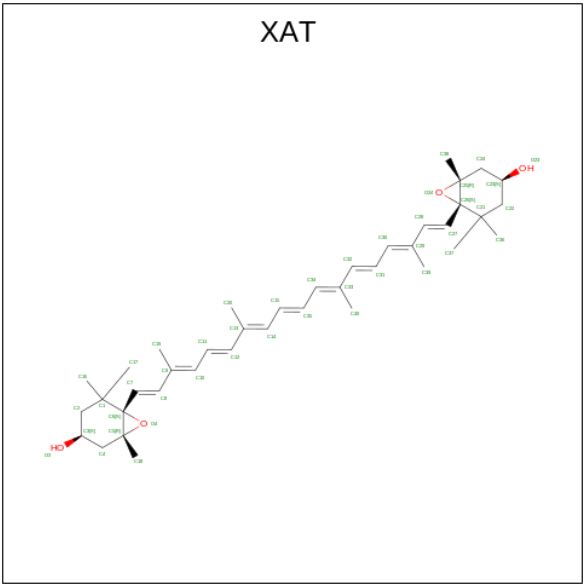
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	1	1	Total	C	O	0	0
			42	40	2		
27	2	1	Total	C	O	0	0
			42	40	2		
27	3	1	Total	C	O	0	0
			42	40	2		
27	4	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	6	1	Total	C	O	0	0
			42	40	2		
27	7	1	Total	C	O	0	0
			42	40	2		
27	8	1	Total	C	O	0	0
			42	40	2		
27	9	1	Total	C	O	0	0
			42	40	2		

- Molecule 28 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).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	1	1	Total	C	O	0	0
			44	40	4		
28	2	1	Total	C	O	0	0
			44	40	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	3	1	Total	C	O	0	0
			44	40	4		
28	4	1	Total	C	O	0	0
			44	40	4		
28	6	1	Total	C	O	0	0
			44	40	4		
28	7	1	Total	C	O	0	0
			44	40	4		
28	8	1	Total	C	O	0	0
			44	40	4		
28	9	1	Total	C	O	0	0
			44	40	4		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	29	Total	O	0	0
			29	29		
29	B	42	Total	O	0	0
			42	42		
29	C	1	Total	O	0	0
			1	1		
29	D	2	Total	O	0	0
			2	2		
29	F	5	Total	O	0	0
			5	5		
29	I	1	Total	O	0	0
			1	1		
29	L	1	Total	O	0	0
			1	1		
29	1	3	Total	O	0	0
			3	3		
29	2	4	Total	O	0	0
			4	4		
29	3	3	Total	O	0	0
			3	3		
29	4	6	Total	O	0	0
			6	6		
29	a	30	Total	O	0	0
			30	30		
29	b	32	Total	O	0	0
			32	32		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	d	1	Total 1	O 1	0	0
29	f	4	Total 4	O 4	0	0
29	h	1	Total 1	O 1	0	0
29	l	3	Total 3	O 3	0	0
29	6	3	Total 3	O 3	0	0
29	7	6	Total 6	O 6	0	0
29	8	3	Total 3	O 3	0	0
29	9	5	Total 5	O 5	0	0

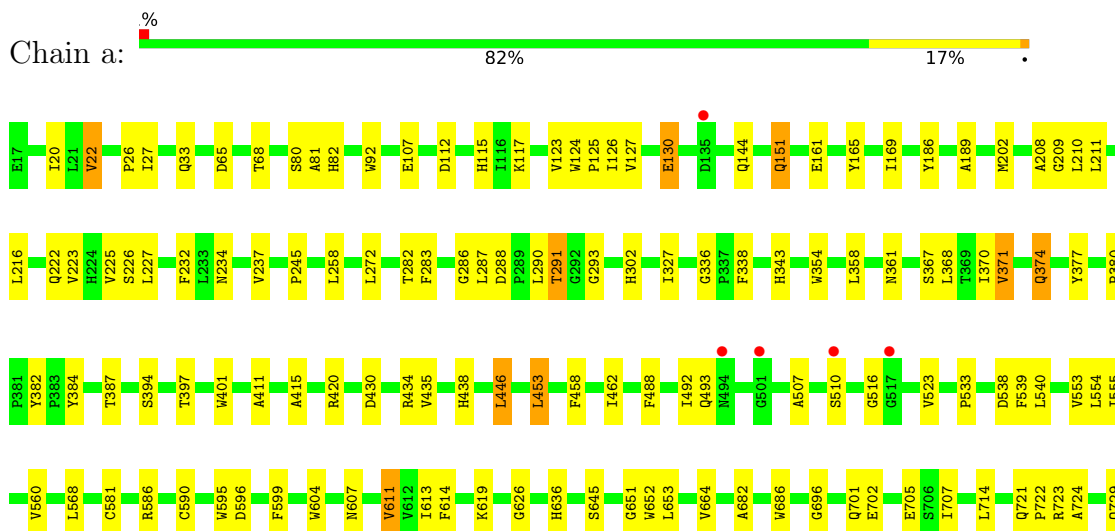
3 Residue-property plots

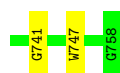
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

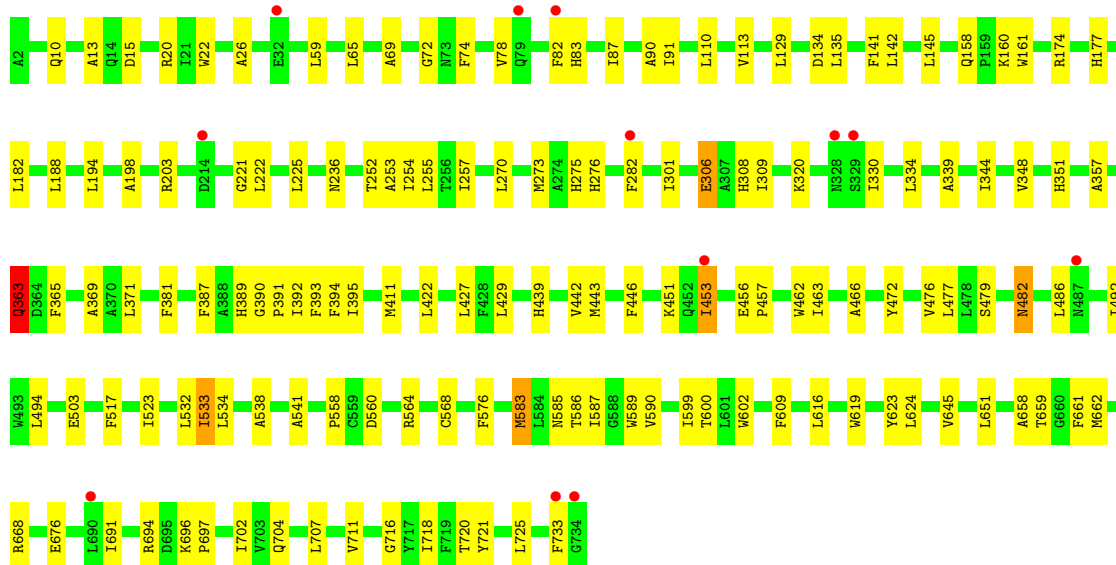
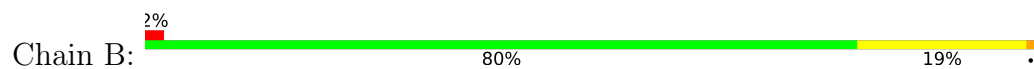


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

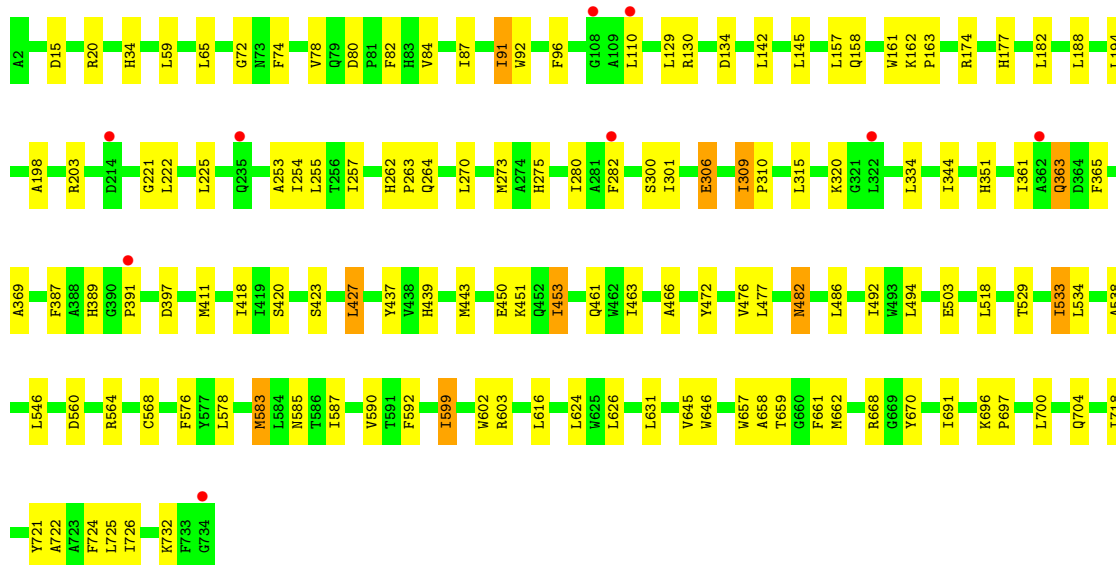
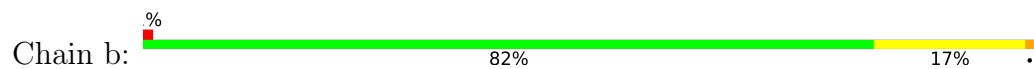




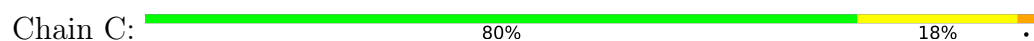
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 3: Photosystem I iron-sulfur center





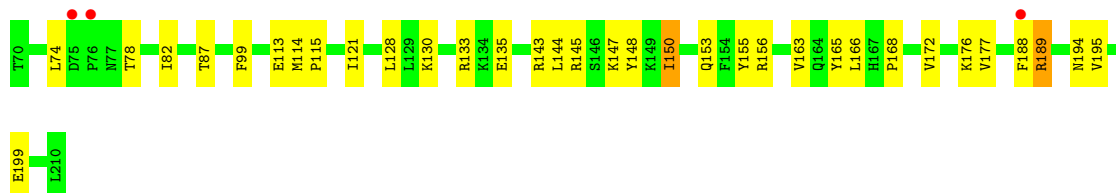
- Molecule 3: Photosystem I iron-sulfur center

Chain c: 88% 10% .



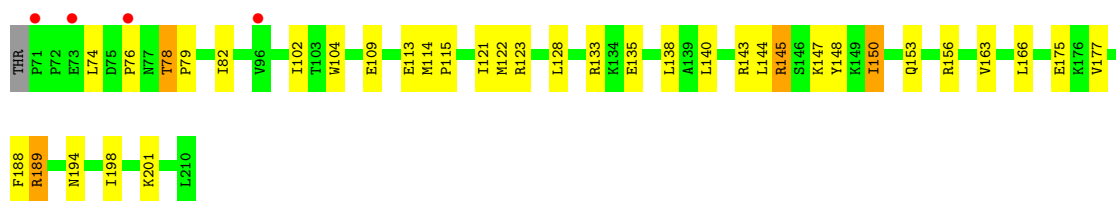
- Molecule 4: Uncharacterized protein

Chain D: 76% 23% .



- Molecule 4: Uncharacterized protein

Chain d: 74% 23% .



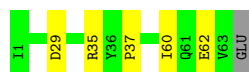
- Molecule 5: Putative uncharacterized protein

Chain E: 95% .



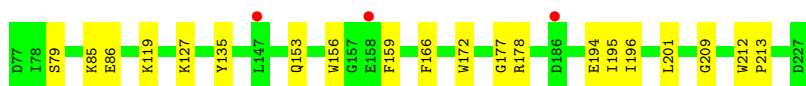
- Molecule 5: Putative uncharacterized protein

Chain e: 91% 8% .

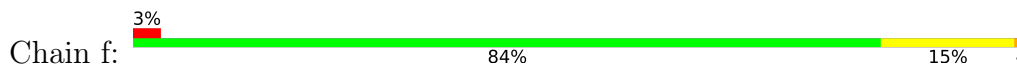


- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

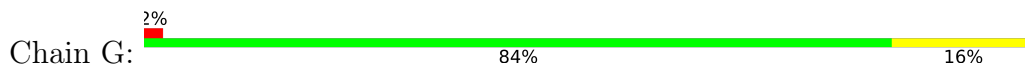
Chain F: 87% 13%



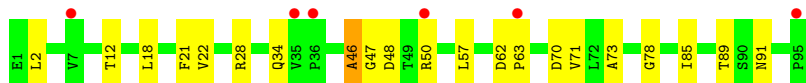
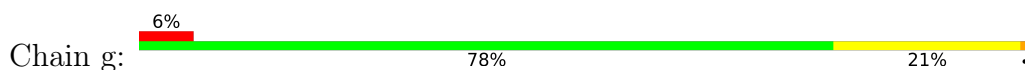
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



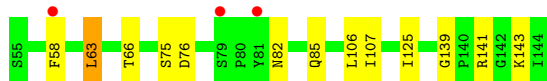
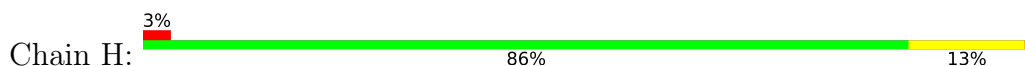
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



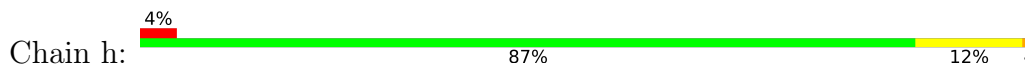
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



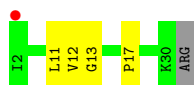
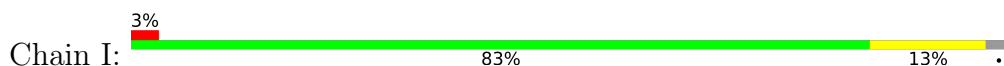
- Molecule 8: Putative uncharacterized protein



- Molecule 8: Putative uncharacterized protein



- Molecule 9: Photosystem I reaction center subunit VIII



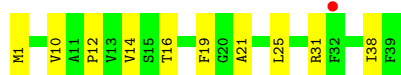
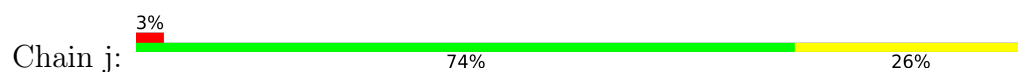
- Molecule 9: Photosystem I reaction center subunit VIII



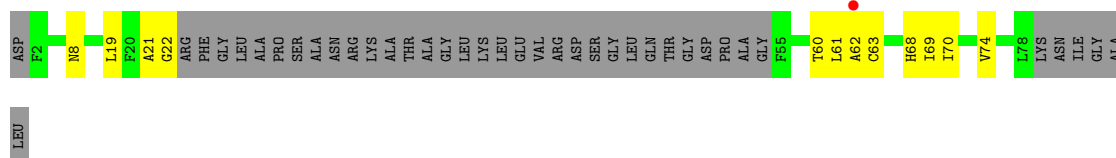
- Molecule 10: Photosystem I reaction center subunit IX



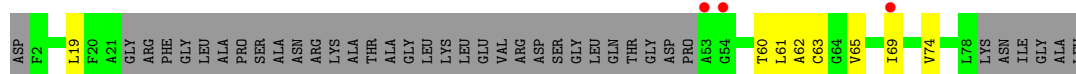
- Molecule 10: Photosystem I reaction center subunit IX



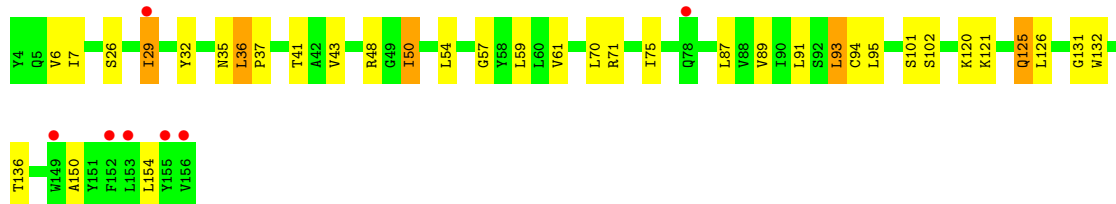
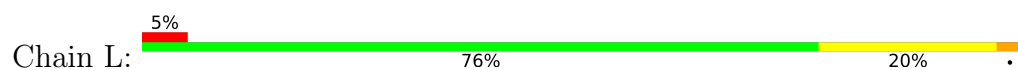
- Molecule 11: Photosystem I reaction center subunit X psaK



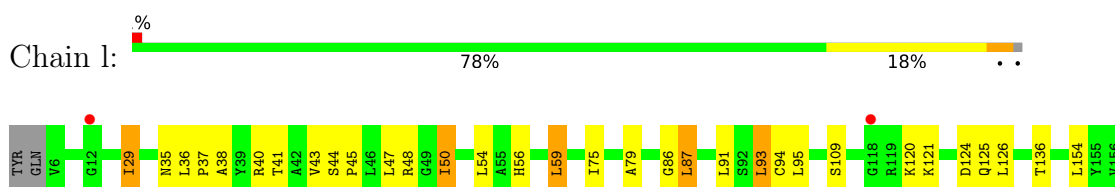
- Molecule 11: Photosystem I reaction center subunit X psaK



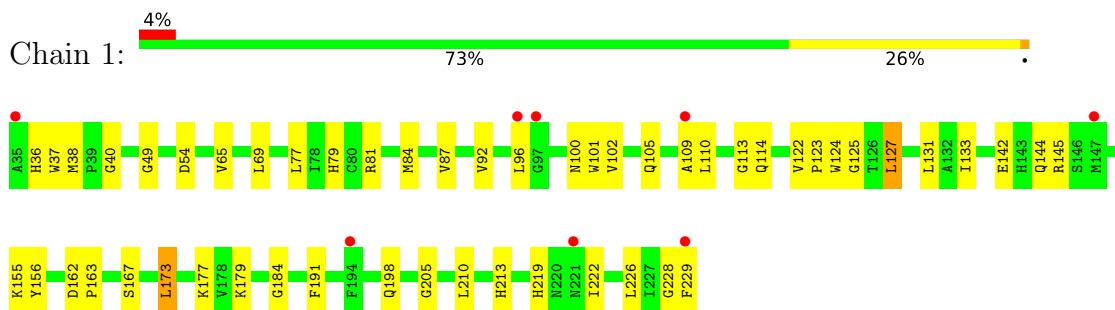
- Molecule 12: Putative uncharacterized protein



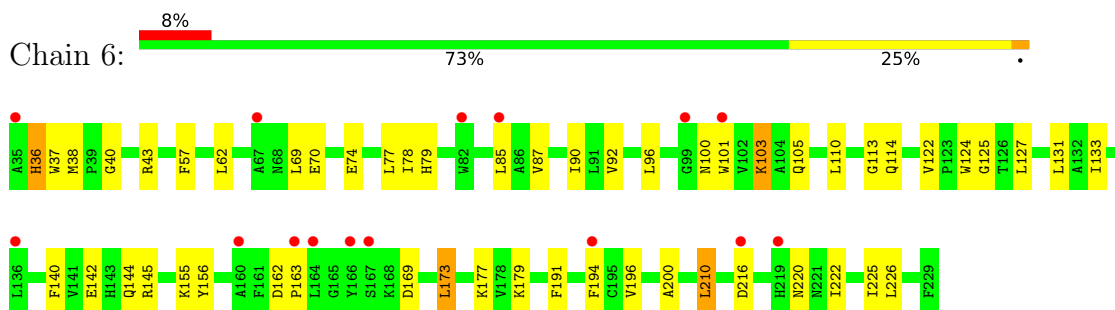
- Molecule 12: Putative uncharacterized protein



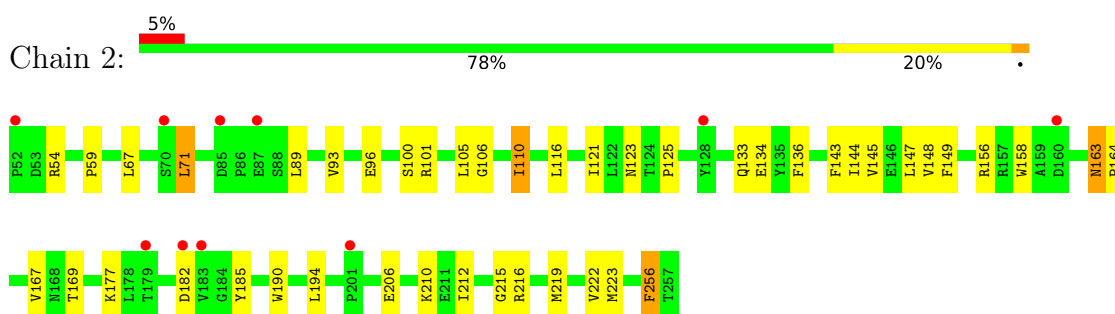
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



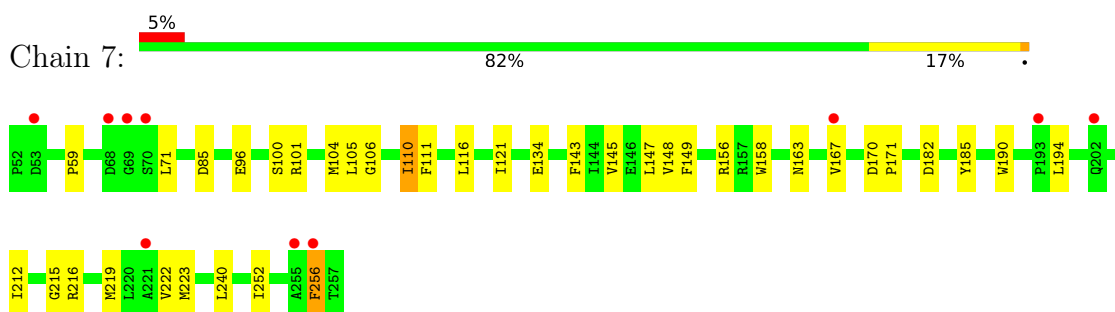
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



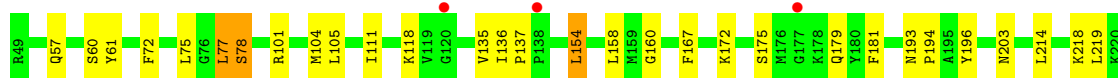
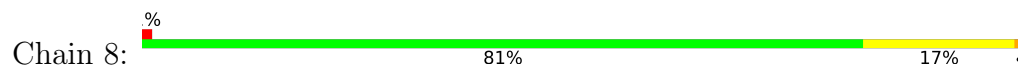
- Molecule 14: Type II chlorophyll a/b binding protein from photosystem I



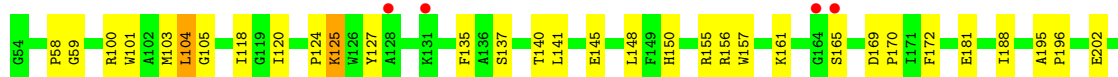
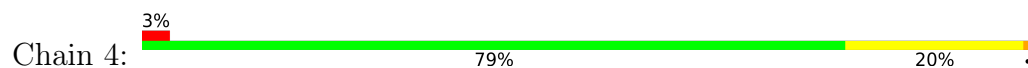
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



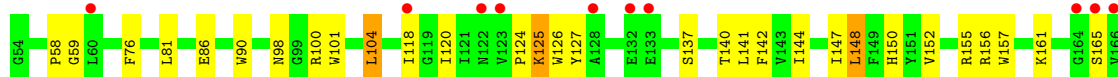
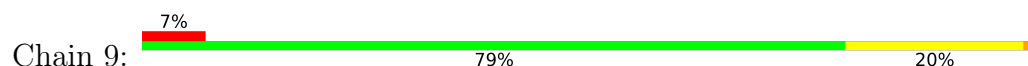
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	165.62Å 192.22Å 175.09Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	49.15 – 2.80 49.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.15-2.80) 99.8 (49.15-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.210 , 0.248 0.217 , 0.254	Depositor DCC
R_{free} test set	13503 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	71157	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: XAT, LHG, CHL, BCR, LUT, PQN, SF4, LMT, HTG, LMG, DGD, CLA

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	0.31	0/6043	0.72	3/8245 (0.0%)
1	a	0.32	0/6043	0.71	0/8245
2	B	0.31	0/6077	0.74	3/8299 (0.0%)
2	b	0.31	0/6077	0.75	4/8299 (0.0%)
3	C	0.29	0/624	0.72	0/846
3	c	0.30	0/624	0.74	0/846
4	D	0.30	0/1143	0.75	0/1545
4	d	0.31	0/1136	0.77	0/1534
5	E	0.26	0/517	0.70	0/701
5	e	0.27	0/516	0.68	0/700
6	F	0.31	0/1221	0.75	0/1648
6	f	0.31	0/1221	0.74	0/1648
7	G	0.30	0/759	0.75	1/1033 (0.1%)
7	g	0.29	0/755	0.78	3/1028 (0.3%)
8	H	0.31	0/697	0.78	2/950 (0.2%)
8	h	0.32	0/701	0.77	0/954
9	I	0.41	0/227	0.79	0/310
9	i	0.42	0/232	0.78	0/317
10	J	0.30	0/319	0.72	0/434
10	j	0.31	0/319	0.70	0/434
11	K	0.28	0/314	0.77	0/426
11	k	0.29	0/319	0.78	0/433
12	L	0.29	0/1167	0.77	0/1596
12	l	0.31	0/1153	0.77	0/1577
13	1	0.32	0/1539	0.79	2/2099 (0.1%)
13	6	0.31	0/1531	0.79	2/2091 (0.1%)
14	2	0.32	0/1670	0.78	2/2288 (0.1%)
14	7	0.32	0/1670	0.79	4/2288 (0.2%)
15	3	0.30	0/1732	0.75	1/2352 (0.0%)
15	8	0.30	0/1724	0.77	1/2341 (0.0%)
16	4	0.28	0/1589	0.74	0/2168
16	9	0.28	0/1589	0.75	0/2168

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.31	0/51248	0.75	28/69843 (0.0%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	668	ARG	N-CA-C	8.08	119.77	110.97
2	B	668	ARG	N-CA-C	8.07	119.70	111.07
7	g	46	ALA	N-CA-C	7.43	119.02	111.07
2	b	221	GLY	N-CA-C	7.13	119.70	111.36
7	G	46	ALA	N-CA-C	7.01	118.57	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5846	0	5708	109	0
1	a	5846	0	5708	102	0
2	B	5863	0	5654	117	0
2	b	5863	0	5654	107	0
3	C	611	0	591	9	0
3	c	611	0	591	5	0
4	D	1114	0	1119	19	0
4	d	1107	0	1113	22	0
5	E	507	0	504	1	0
5	e	506	0	512	3	0
6	F	1193	0	1219	15	0
6	f	1193	0	1219	16	0
7	G	741	0	728	11	0
7	g	737	0	724	16	0
8	H	678	0	670	14	0
8	h	682	0	681	10	0
9	I	221	0	240	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	i	226	0	242	1	0
10	J	311	0	326	11	0
10	j	311	0	326	11	0
11	K	311	0	324	11	0
11	k	316	0	329	7	0
12	L	1136	0	1147	24	0
12	l	1122	0	1137	21	0
13	1	1491	0	1456	38	0
13	6	1483	0	1434	44	0
14	2	1610	0	1547	34	0
14	7	1610	0	1547	30	0
15	3	1680	0	1643	32	0
15	8	1672	0	1632	29	0
16	4	1540	0	1502	31	0
16	9	1540	0	1502	37	0
17	1	683	0	659	37	0
17	2	501	0	478	27	0
17	3	650	0	494	34	0
17	4	570	0	477	25	0
17	6	648	0	593	29	0
17	7	487	0	447	25	0
17	8	567	0	436	30	0
17	9	553	0	453	29	0
17	A	2712	0	2791	174	0
17	B	2403	0	2449	145	0
17	F	165	0	154	12	0
17	G	141	0	105	6	0
17	J	42	0	31	1	0
17	K	91	0	66	5	0
17	L	180	0	183	11	0
17	a	2777	0	2862	162	0
17	b	2398	0	2439	158	0
17	f	100	0	82	6	0
17	g	137	0	101	2	0
17	j	42	0	31	1	0
17	k	137	0	99	7	0
17	l	180	0	183	7	0
18	A	33	0	46	5	0
18	B	33	0	46	2	0
18	a	33	0	46	3	0
18	b	33	0	46	1	0
19	1	72	0	90	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	37	0	44	3	0
19	3	20	0	14	1	0
19	6	72	0	90	5	0
19	7	37	0	44	2	0
19	A	76	0	98	5	0
19	a	76	0	98	5	0
20	1	40	0	56	4	0
20	2	40	0	56	11	0
20	3	40	0	56	2	0
20	4	40	0	56	8	0
20	6	40	0	56	7	0
20	7	40	0	56	13	0
20	8	40	0	56	5	0
20	9	40	0	56	6	0
20	A	240	0	336	25	0
20	B	280	0	392	34	0
20	F	40	0	56	6	0
20	G	40	0	56	5	0
20	I	40	0	56	4	0
20	J	40	0	56	3	0
20	K	80	0	112	6	0
20	L	120	0	168	9	0
20	a	240	0	336	20	0
20	b	280	0	392	29	0
20	f	40	0	56	5	0
20	g	40	0	56	3	0
20	i	40	0	56	2	0
20	j	80	0	112	9	0
20	k	40	0	56	3	0
20	l	120	0	168	11	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
21	a	8	0	0	0	0
21	c	16	0	0	0	0
22	A	19	0	26	0	0
22	F	19	0	26	2	0
22	J	19	0	26	0	0
22	a	19	0	26	0	0
22	f	19	0	26	2	0
22	j	19	0	26	0	0
23	B	35	0	46	1	0
24	B	66	0	96	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	b	66	0	96	5	0
25	4	88	0	122	8	0
25	6	40	0	53	3	0
25	9	50	0	73	2	0
25	G	44	0	61	2	0
26	1	109	0	90	11	0
26	2	246	0	185	13	0
26	3	47	0	31	0	0
26	4	201	0	150	9	0
26	6	108	0	88	7	0
26	7	246	0	185	14	0
26	8	47	0	31	1	0
26	9	201	0	150	10	0
27	1	84	0	112	11	0
27	2	42	0	56	5	0
27	3	42	0	56	6	0
27	4	42	0	56	5	0
27	6	84	0	112	14	0
27	7	42	0	56	9	0
27	8	42	0	56	7	0
27	9	42	0	56	5	0
28	1	44	0	56	6	0
28	2	44	0	56	5	0
28	3	44	0	56	4	0
28	4	44	0	56	4	0
28	6	44	0	56	8	0
28	7	44	0	56	5	0
28	8	44	0	56	7	0
28	9	44	0	56	7	0
29	1	3	0	0	0	0
29	2	4	0	0	0	0
29	3	3	0	0	0	0
29	4	6	0	0	0	0
29	6	3	0	0	0	0
29	7	6	0	0	0	0
29	8	3	0	0	0	0
29	9	5	0	0	0	0
29	A	29	0	0	1	0
29	B	42	0	0	0	0
29	C	1	0	0	0	0
29	D	2	0	0	0	0
29	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	I	1	0	0	0	0
29	L	1	0	0	0	0
29	a	30	0	0	2	0
29	b	32	0	0	0	0
29	d	1	0	0	0	0
29	f	4	0	0	0	0
29	h	1	0	0	0	0
29	l	3	0	0	0	0
All	All	71157	0	70537	1621	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 11.

The worst 5 of 1621 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)
17:4:609:CLA:HBB1	27:4:616:LUT:H32	1.51	0.92
17:2:609:CLA:HBB1	27:2:615:LUT:H32	1.53	0.88
2:B:334:LEU:HD11	17:B:829:CLA:HBB1	1.54	0.88
17:3:309:CLA:HBB1	27:3:316:LUT:H32	1.55	0.87
2:b:334:LEU:HD11	17:b:829:CLA:HBB1	1.57	0.86

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	740/742 (100%)	710 (96%)	28 (4%)	2 (0%)	36 66
1	a	740/742 (100%)	709 (96%)	29 (4%)	2 (0%)	36 66
2	B	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	48 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	731/733 (100%)	700 (96%)	30 (4%)	1 (0%)	48	77
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
3	c	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
4	d	138/141 (98%)	135 (98%)	3 (2%)	0	100	100
5	E	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
5	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
6	F	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	18	47
6	f	149/151 (99%)	147 (99%)	1 (1%)	1 (1%)	18	47
7	G	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
7	g	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
8	H	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
8	h	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
9	I	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
9	i	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
10	J	37/39 (95%)	37 (100%)	0	0	100	100
10	j	37/39 (95%)	37 (100%)	0	0	100	100
11	K	41/84 (49%)	41 (100%)	0	0	100	100
11	k	42/84 (50%)	42 (100%)	0	0	100	100
12	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
12	l	149/153 (97%)	143 (96%)	6 (4%)	0	100	100
13	1	193/195 (99%)	187 (97%)	6 (3%)	0	100	100
13	6	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
14	2	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
14	7	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
15	3	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
15	8	215/218 (99%)	204 (95%)	11 (5%)	0	100	100
16	4	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	24	55
16	9	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	24	55
All	All	6282/6434 (98%)	6041 (96%)	231 (4%)	10 (0%)	43	72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	159	PHE
6	f	159	PHE
1	A	581	CYS
16	9	137	SER
16	4	137	SER

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	602/602 (100%)	588 (98%)	14 (2%)	44	78
1	a	602/602 (100%)	585 (97%)	17 (3%)	38	73
2	B	597/597 (100%)	582 (98%)	15 (2%)	42	76
2	b	597/597 (100%)	580 (97%)	17 (3%)	38	73
3	C	69/69 (100%)	66 (96%)	3 (4%)	26	60
3	c	69/69 (100%)	66 (96%)	3 (4%)	26	60
4	D	119/120 (99%)	111 (93%)	8 (7%)	15	42
4	d	118/120 (98%)	110 (93%)	8 (7%)	14	42
5	E	55/56 (98%)	54 (98%)	1 (2%)	51	82
5	e	55/56 (98%)	54 (98%)	1 (2%)	51	82
6	F	123/125 (98%)	120 (98%)	3 (2%)	43	77
6	f	123/125 (98%)	121 (98%)	2 (2%)	55	83
7	G	81/81 (100%)	80 (99%)	1 (1%)	63	87
7	g	80/81 (99%)	79 (99%)	1 (1%)	61	86
8	H	72/73 (99%)	71 (99%)	1 (1%)	59	85
8	h	73/73 (100%)	71 (97%)	2 (3%)	39	74
9	I	25/26 (96%)	24 (96%)	1 (4%)	28	63
9	i	25/26 (96%)	24 (96%)	1 (4%)	28	63
10	J	33/33 (100%)	31 (94%)	2 (6%)	17	46
10	j	33/33 (100%)	31 (94%)	2 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	34/62 (55%)	34 (100%)	0	100	100
11	k	34/62 (55%)	34 (100%)	0	100	100
12	L	118/119 (99%)	106 (90%)	12 (10%)	7	23
12	l	117/119 (98%)	105 (90%)	12 (10%)	7	23
13	1	149/153 (97%)	141 (95%)	8 (5%)	20	51
13	6	147/153 (96%)	138 (94%)	9 (6%)	17	46
14	2	166/166 (100%)	157 (95%)	9 (5%)	20	51
14	7	166/166 (100%)	157 (95%)	9 (5%)	20	51
15	3	169/169 (100%)	163 (96%)	6 (4%)	31	66
15	8	168/169 (99%)	162 (96%)	6 (4%)	31	66
16	4	161/161 (100%)	154 (96%)	7 (4%)	26	60
16	9	161/161 (100%)	154 (96%)	7 (4%)	26	60
All	All	5141/5224 (98%)	4953 (96%)	188 (4%)	30	65

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	427	LEU
10	j	1	MET
2	b	533	ILE
4	d	147	LYS
12	l	75	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
13	6	105	GLN
13	6	209	ASN
16	9	168	GLN
12	L	125	GLN
12	L	5	GLN

5.3.3 RNA ⓘ

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](#)

414 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$
25	LMG	9	619	-	50,50,55	0.93	2 (4%)	58,58,63	0.98	3 (5%)
17	CLA	A	832	1	54,58,73	2.34	21 (38%)	65,95,113	3.11	29 (44%)
17	CLA	b	838	2	51,55,73	2.41	20 (39%)	61,91,113	3.22	26 (42%)
17	CLA	b	805	2	69,73,73	2.07	21 (30%)	83,113,113	2.80	30 (36%)
17	CLA	A	807	1	69,73,73	2.09	20 (28%)	83,113,113	2.79	30 (36%)
17	CLA	b	817	2	63,67,73	2.19	21 (33%)	75,105,113	2.91	32 (42%)
17	CLA	B	828	2	69,73,73	2.08	20 (28%)	83,113,113	2.80	28 (33%)
27	LUT	4	616	-	42,43,43	0.76	0	51,60,60	1.64	13 (25%)
17	CLA	F	301	29	69,73,73	2.08	20 (28%)	83,113,113	2.76	27 (32%)
17	CLA	6	310	13	69,73,73	2.08	20 (28%)	83,113,113	2.74	27 (32%)
17	CLA	A	837	1	49,53,73	2.49	21 (42%)	59,89,113	3.18	26 (44%)
17	CLA	B	826	2	69,73,73	2.06	20 (28%)	83,113,113	2.83	28 (33%)
17	CLA	a	802	-	69,73,73	2.07	19 (27%)	83,113,113	2.77	35 (42%)
17	CLA	a	804	1	69,73,73	2.07	21 (30%)	83,113,113	2.83	29 (34%)
17	CLA	b	832	2	69,73,73	2.06	21 (30%)	83,113,113	2.85	30 (36%)
26	CHL	3	307	29	51,55,74	2.30	21 (41%)	57,91,114	3.29	25 (43%)
17	CLA	g	103	7	50,54,73	2.45	21 (42%)	60,90,113	3.22	27 (45%)
17	CLA	A	809	1	69,73,73	2.09	20 (28%)	83,113,113	2.82	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	9	613	16	49,53,73	2.49	21 (42%)	59,89,113	3.25	27 (45%)
17	CLA	A	801	1	69,73,73	2.07	20 (28%)	83,113,113	2.81	35 (42%)
17	CLA	A	814	1	69,73,73	2.09	20 (28%)	83,113,113	2.80	28 (33%)
17	CLA	b	826	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	28 (33%)
20	BCR	B	801	-	41,41,41	1.06	1 (2%)	56,56,56	1.49	8 (14%)
17	CLA	4	604	29	54,58,73	2.36	21 (38%)	65,95,113	3.11	30 (46%)
22	HTG	A	855	-	19,19,19	1.03	2 (10%)	23,24,24	0.69	0
17	CLA	a	831	1	69,73,73	2.03	19 (27%)	83,113,113	2.76	29 (34%)
26	CHL	2	605	29	47,51,74	2.35	21 (44%)	52,86,114	3.49	24 (46%)
17	CLA	B	809	2	69,73,73	2.05	19 (27%)	83,113,113	2.74	27 (32%)
17	CLA	7	610	19	45,49,73	2.51	21 (46%)	54,84,113	3.40	26 (48%)
17	CLA	3	305	29	46,50,73	2.48	20 (43%)	55,85,113	3.30	26 (47%)
17	CLA	k	1402	11	50,54,73	2.44	21 (42%)	60,90,113	3.14	25 (41%)
17	CLA	a	815	1	49,53,73	2.47	21 (42%)	59,89,113	3.20	27 (45%)
17	CLA	3	309	15	54,58,73	2.36	20 (37%)	65,95,113	3.18	32 (49%)
17	CLA	a	818	1	69,73,73	2.08	21 (30%)	83,113,113	2.84	30 (36%)
17	CLA	8	307	15	54,58,73	2.35	20 (37%)	65,95,113	3.05	29 (44%)
28	XAT	8	315	-	39,47,47	0.88	0	54,74,74	2.71	21 (38%)
20	BCR	A	850	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	15 (26%)
17	CLA	A	813	1	58,62,73	2.28	21 (36%)	69,99,113	3.01	30 (43%)
20	BCR	a	850	-	41,41,41	1.01	1 (2%)	56,56,56	1.86	15 (26%)
17	CLA	b	824	29	69,73,73	2.09	20 (28%)	83,113,113	2.76	29 (34%)
17	CLA	6	309	29	50,54,73	2.45	21 (42%)	60,90,113	3.17	26 (43%)
17	CLA	l	202	12	69,73,73	2.09	20 (28%)	83,113,113	2.77	28 (33%)
20	BCR	F	305	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	16 (28%)
17	CLA	A	812	17,1	69,73,73	2.06	20 (28%)	83,113,113	2.84	30 (36%)
17	CLA	1	310	13	64,68,73	2.17	21 (32%)	77,107,113	2.91	31 (40%)
19	LHG	a	847	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
19	LHG	6	301	17	22,22,48	1.17	2 (9%)	25,28,54	1.22	2 (8%)
17	CLA	b	815	2	59,63,73	2.23	20 (33%)	71,101,113	2.98	30 (42%)
17	CLA	1	309	13	69,73,73	2.08	20 (28%)	83,113,113	2.77	28 (33%)
17	CLA	b	806	2	69,73,73	2.07	20 (28%)	83,113,113	2.81	28 (33%)
26	CHL	2	606	29	52,56,74	2.31	21 (40%)	58,92,114	3.37	25 (43%)
17	CLA	B	802	2	69,73,73	2.06	20 (28%)	83,113,113	2.86	31 (37%)
19	LHG	a	848	17	26,26,48	1.26	2 (7%)	29,32,54	1.32	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	843	29	69,73,73	2.07	20 (28%)	83,113,113	2.75	28 (33%)
22	HTG	F	302	-	19,19,19	1.01	2 (10%)	23,24,24	0.61	0
17	CLA	A	808	1	69,73,73	2.09	20 (28%)	83,113,113	2.80	29 (34%)
17	CLA	A	845	19	56,60,73	2.34	21 (37%)	67,97,113	3.11	26 (38%)
17	CLA	A	828	1	69,73,73	2.06	20 (28%)	83,113,113	2.82	28 (33%)
17	CLA	A	820	1	69,73,73	2.09	21 (30%)	83,113,113	2.81	29 (34%)
17	CLA	B	820	2	54,58,73	2.37	21 (38%)	65,95,113	3.09	29 (44%)
17	CLA	2	612	14	69,73,73	2.10	21 (30%)	83,113,113	2.78	29 (34%)
17	CLA	f	7003	6	59,63,73	2.28	21 (35%)	71,101,113	3.03	30 (42%)
17	CLA	1	312	13	56,60,73	2.30	20 (35%)	67,97,113	3.10	27 (40%)
26	CHL	7	605	29	47,51,74	2.34	20 (42%)	52,86,114	3.51	25 (48%)
17	CLA	6	311	13	64,68,73	2.17	21 (32%)	77,107,113	2.93	32 (41%)
17	CLA	b	827	2	69,73,73	2.07	20 (28%)	83,113,113	2.82	29 (34%)
17	CLA	A	811	1	69,73,73	2.09	21 (30%)	83,113,113	2.79	29 (34%)
17	CLA	b	822	2	59,63,73	2.26	21 (35%)	71,101,113	3.02	28 (39%)
25	LMG	4	619	-	44,44,55	1.01	2 (4%)	52,52,63	1.00	3 (5%)
26	CHL	8	306	29	51,55,74	2.30	20 (39%)	57,91,114	3.38	24 (42%)
17	CLA	9	611	16	56,60,73	2.32	21 (37%)	67,97,113	3.11	28 (41%)
17	CLA	b	835	29	49,53,73	2.48	21 (42%)	59,89,113	3.18	27 (45%)
17	CLA	b	831	2	53,57,73	2.36	21 (39%)	62,93,113	3.15	28 (45%)
17	CLA	A	821	1	49,53,73	2.45	20 (40%)	59,89,113	3.27	28 (47%)
17	CLA	a	834	1	69,73,73	2.08	21 (30%)	83,113,113	2.82	30 (36%)
19	LHG	7	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	4 (10%)
20	BCR	a	851	-	41,41,41	1.03	1 (2%)	56,56,56	1.72	14 (25%)
19	LHG	6	320	17	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
17	CLA	3	304	29	49,53,73	2.48	21 (42%)	59,89,113	3.22	26 (44%)
20	BCR	l	205	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	10 (17%)
20	BCR	1	318	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	16 (28%)
17	CLA	A	803	29	69,73,73	2.05	20 (28%)	83,113,113	2.82	31 (37%)
17	CLA	A	842	1	69,73,73	2.10	21 (30%)	83,113,113	2.82	30 (36%)
17	CLA	L	203	12	69,73,73	2.08	21 (30%)	83,113,113	2.88	30 (36%)
17	CLA	a	807	1	69,73,73	2.07	20 (28%)	83,113,113	2.87	31 (37%)
23	LMT	B	849	-	36,36,36	0.48	0	47,47,47	0.94	3 (6%)
17	CLA	b	809	2	69,73,73	2.03	19 (27%)	83,113,113	2.75	30 (36%)
17	CLA	B	829	2	69,73,73	2.06	20 (28%)	83,113,113	2.77	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	HTG	a	857	-	19,19,19	1.05	2 (10%)	23,24,24	0.55	0
22	HTG	f	7001	-	19,19,19	1.05	2 (10%)	23,24,24	0.58	0
17	CLA	9	604	29	54,58,73	2.37	21 (38%)	65,95,113	3.18	30 (46%)
17	CLA	2	611	14	56,60,73	2.32	20 (35%)	67,97,113	3.10	28 (41%)
17	CLA	k	1401	-	49,53,73	2.48	20 (40%)	59,89,113	3.23	25 (42%)
26	CHL	2	601	14	65,69,74	2.05	21 (32%)	74,108,114	3.06	27 (36%)
20	BCR	B	845	-	41,41,41	1.01	1 (2%)	56,56,56	2.01	18 (32%)
26	CHL	6	303	13	65,69,74	2.06	21 (32%)	74,108,114	3.03	28 (37%)
17	CLA	a	830	1	69,73,73	2.06	20 (28%)	83,113,113	2.77	28 (33%)
17	CLA	6	314	13	64,68,73	2.16	20 (31%)	77,107,113	2.84	28 (36%)
27	LUT	7	615	-	42,43,43	0.74	0	51,60,60	1.56	13 (25%)
17	CLA	2	613	14	47,51,73	2.46	20 (42%)	56,86,113	3.32	25 (44%)
27	LUT	3	316	-	42,43,43	0.74	0	51,60,60	1.63	14 (27%)
20	BCR	A	851	-	41,41,41	1.06	1 (2%)	56,56,56	2.02	14 (25%)
17	CLA	7	604	29	64,68,73	2.18	21 (32%)	77,107,113	2.87	30 (38%)
17	CLA	B	811	2	58,62,73	2.26	20 (34%)	73,100,113	3.02	32 (43%)
17	CLA	b	833	2	62,66,73	2.20	20 (32%)	74,104,113	3.00	30 (40%)
17	CLA	B	814	2	69,73,73	2.06	20 (28%)	83,113,113	2.84	31 (37%)
17	CLA	1	315	13	50,54,73	2.44	20 (40%)	60,90,113	3.18	25 (41%)
17	CLA	b	813	2	69,73,73	2.09	20 (28%)	83,113,113	2.76	27 (32%)
17	CLA	9	601	16	50,54,73	2.44	21 (42%)	60,90,113	3.18	28 (46%)
20	BCR	L	201	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	13 (23%)
17	CLA	4	613	16	49,53,73	2.48	21 (42%)	59,89,113	3.25	26 (44%)
17	CLA	3	311	-	56,60,73	2.33	21 (37%)	67,97,113	3.08	28 (41%)
17	CLA	1	308	29	69,73,73	2.09	21 (30%)	83,113,113	2.76	28 (33%)
20	BCR	J	3003	-	41,41,41	1.03	1 (2%)	56,56,56	1.76	14 (25%)
17	CLA	4	609	16	64,68,73	2.17	21 (32%)	77,107,113	2.94	32 (41%)
28	XAT	2	616	-	39,47,47	0.87	0	54,74,74	2.62	19 (35%)
17	CLA	7	608	14	54,58,73	2.37	21 (38%)	65,95,113	3.15	32 (49%)
17	CLA	A	805	17,1	59,63,73	2.23	20 (33%)	71,101,113	3.06	31 (43%)
17	CLA	B	838	2	51,55,73	2.38	20 (39%)	61,91,113	3.22	29 (47%)
26	CHL	7	601	14	65,69,74	2.07	21 (32%)	74,108,114	3.09	28 (37%)
17	CLA	b	828	2	69,73,73	2.07	20 (28%)	83,113,113	2.77	29 (34%)
17	CLA	A	802	-	69,73,73	2.08	20 (28%)	83,113,113	2.77	28 (33%)
17	CLA	a	819	1	69,73,73	2.11	20 (28%)	83,113,113	2.71	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	PQN	A	844	-	34,34,34	1.61	2 (5%)	42,45,45	1.21	4 (9%)
20	BCR	B	844	-	41,41,41	1.04	1 (2%)	56,56,56	1.97	13 (23%)
17	CLA	1	304	13	69,73,73	2.10	21 (30%)	83,113,113	2.77	28 (33%)
17	CLA	4	601	16	50,54,73	2.43	20 (40%)	60,90,113	3.21	26 (43%)
17	CLA	7	613	14	47,51,73	2.45	20 (42%)	56,86,113	3.30	26 (46%)
17	CLA	b	812	2	59,63,73	2.26	20 (33%)	71,101,113	2.95	28 (39%)
17	CLA	a	839	1	69,73,73	2.05	20 (28%)	83,113,113	2.82	28 (33%)
17	CLA	3	310	19	42,45,73	2.44	19 (45%)	50,78,113	3.39	25 (50%)
17	CLA	B	816	2	59,63,73	2.26	21 (35%)	71,101,113	3.05	31 (43%)
21	SF4	c	102	3	0,12,12	-	-	-	-	-
20	BCR	g	104	-	41,41,41	1.05	1 (2%)	56,56,56	1.89	16 (28%)
24	DGD	b	849	-	67,67,67	0.86	2 (2%)	81,81,81	1.00	4 (4%)
17	CLA	B	834	2	69,73,73	2.12	21 (30%)	83,113,113	2.75	29 (34%)
26	CHL	6	308	13	51,55,74	2.34	21 (41%)	57,91,114	3.33	24 (42%)
17	CLA	8	302	15	54,58,73	2.35	20 (37%)	65,95,113	3.20	30 (46%)
17	CLA	9	602	16	64,68,73	2.16	21 (32%)	77,107,113	2.93	32 (41%)
17	CLA	A	810	1	69,73,73	2.04	20 (28%)	83,113,113	2.77	30 (36%)
17	CLA	l	204	29	54,58,73	2.36	20 (37%)	65,95,113	3.13	30 (46%)
17	CLA	a	814	1	69,73,73	2.10	20 (28%)	83,113,113	2.79	27 (32%)
22	HTG	j	3001	-	19,19,19	1.11	2 (10%)	23,24,24	0.59	0
17	CLA	4	614	16	54,58,73	2.36	21 (38%)	65,95,113	3.18	29 (44%)
17	CLA	a	856	29	69,73,73	2.03	20 (28%)	83,113,113	2.95	32 (38%)
17	CLA	B	841	19	69,73,73	2.08	21 (30%)	83,113,113	2.86	29 (34%)
17	CLA	b	836	2	64,68,73	2.14	20 (31%)	77,107,113	2.92	26 (33%)
17	CLA	a	810	1	69,73,73	2.08	20 (28%)	83,113,113	2.78	29 (34%)
17	CLA	B	804	2	49,53,73	2.45	21 (42%)	59,89,113	3.25	28 (47%)
17	CLA	g	102	7	54,58,73	2.37	21 (38%)	65,95,113	3.15	29 (44%)
17	CLA	B	825	29	69,73,73	2.07	20 (28%)	83,113,113	2.83	32 (38%)
17	CLA	a	811	1	69,73,73	2.09	21 (30%)	83,113,113	2.80	29 (34%)
17	CLA	9	609	16	64,68,73	2.18	21 (32%)	77,107,113	2.88	32 (41%)
17	CLA	a	801	1	69,73,73	2.05	20 (28%)	83,113,113	2.83	33 (39%)
20	BCR	G	105	-	41,41,41	1.05	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	G	103	7	54,58,73	2.37	21 (38%)	65,95,113	3.14	28 (43%)
17	CLA	b	841	19	69,73,73	2.09	21 (30%)	83,113,113	2.86	29 (34%)
18	PQN	a	845	-	34,34,34	1.63	2 (5%)	42,45,45	1.09	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	b	804	2	49,53,73	2.43	20 (40%)	59,89,113	3.31	27 (45%)
24	DGD	B	850	-	67,67,67	0.86	2 (2%)	81,81,81	0.93	4 (4%)
26	CHL	4	605	29	60,64,74	2.14	22 (36%)	68,102,114	3.16	29 (42%)
20	BCR	K	4004	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
20	BCR	b	846	-	41,41,41	1.08	1 (2%)	56,56,56	1.66	13 (23%)
17	CLA	a	803	29	69,73,73	2.06	21 (30%)	83,113,113	2.77	29 (34%)
17	CLA	B	836	2	64,68,73	2.15	20 (31%)	77,107,113	2.92	26 (33%)
17	CLA	a	813	1	58,62,73	2.29	21 (36%)	69,99,113	3.03	27 (39%)
20	BCR	A	849	-	41,41,41	1.07	1 (2%)	56,56,56	1.65	13 (23%)
17	CLA	8	303	29	49,53,73	2.48	21 (42%)	59,89,113	3.22	26 (44%)
17	CLA	B	807	2	69,73,73	2.10	21 (30%)	83,113,113	2.82	31 (37%)
17	CLA	J	3002	10	46,50,73	2.50	20 (43%)	55,85,113	3.28	27 (49%)
17	CLA	A	806	1	69,73,73	2.07	20 (28%)	83,113,113	2.76	31 (37%)
17	CLA	k	1403	-	50,54,73	2.47	21 (42%)	60,90,113	3.22	28 (46%)
17	CLA	8	305	15	51,55,73	2.44	21 (41%)	61,91,113	3.16	26 (42%)
17	CLA	B	813	2	69,73,73	2.08	20 (28%)	83,113,113	2.78	29 (34%)
26	CHL	4	615	16	47,51,74	2.35	20 (42%)	52,86,114	3.50	22 (42%)
17	CLA	9	610	29	45,49,73	2.51	20 (44%)	54,84,113	3.35	26 (48%)
17	CLA	a	816	1	54,58,73	2.36	20 (37%)	65,95,113	3.10	29 (44%)
17	CLA	B	818	2	64,68,73	2.15	20 (31%)	77,107,113	2.87	28 (36%)
17	CLA	B	830	2	54,58,73	2.33	21 (38%)	65,95,113	3.13	28 (43%)
26	CHL	9	607	29	55,59,74	2.23	21 (38%)	62,96,114	3.24	27 (43%)
17	CLA	B	822	2	59,63,73	2.26	21 (35%)	71,101,113	2.96	30 (42%)
26	CHL	4	606	29	55,59,74	2.28	22 (40%)	62,96,114	3.28	24 (38%)
17	CLA	L	202	12	69,73,73	2.09	21 (30%)	83,113,113	2.76	28 (33%)
26	CHL	9	606	29	55,59,74	2.23	21 (38%)	62,96,114	3.31	27 (43%)
28	XAT	1	317	-	39,47,47	0.86	0	54,74,74	2.69	21 (38%)
17	CLA	A	826	29	69,73,73	2.06	20 (28%)	83,113,113	2.78	27 (32%)
17	CLA	A	839	1	69,73,73	2.04	20 (28%)	83,113,113	2.81	29 (34%)
17	CLA	a	833	1	69,73,73	2.09	21 (30%)	83,113,113	2.78	29 (34%)
20	BCR	9	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.81	16 (28%)
17	CLA	B	839	29	69,73,73	2.08	21 (30%)	83,113,113	2.77	27 (32%)
20	BCR	a	853	-	41,41,41	1.05	1 (2%)	56,56,56	1.93	14 (25%)
17	CLA	a	826	29	69,73,73	2.06	20 (28%)	83,113,113	2.83	28 (33%)
17	CLA	8	301	15	64,68,73	2.18	21 (32%)	77,107,113	2.91	31 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	315	-	26,32,73	3.08	16 (61%)	34,54,113	4.10	23 (67%)
26	CHL	2	614	-	47,51,74	2.35	20 (42%)	52,86,114	3.53	22 (42%)
17	CLA	a	808	1	69,73,73	2.08	20 (28%)	83,113,113	2.79	28 (33%)
17	CLA	2	610	19	45,49,73	2.52	21 (46%)	54,84,113	3.43	27 (50%)
17	CLA	A	854	29	69,73,73	2.03	20 (28%)	83,113,113	2.90	31 (37%)
17	CLA	4	611	16	56,60,73	2.30	20 (35%)	67,97,113	3.06	28 (41%)
17	CLA	A	829	1	69,73,73	2.04	20 (28%)	83,113,113	2.80	30 (36%)
17	CLA	a	843	1	69,73,73	2.05	20 (28%)	83,113,113	2.82	31 (37%)
17	CLA	8	311	15	49,53,73	2.49	21 (42%)	59,89,113	3.21	27 (45%)
17	CLA	F	303	29	49,53,73	2.46	20 (40%)	59,89,113	3.19	26 (44%)
17	CLA	a	805	17,1	59,63,73	2.24	21 (35%)	71,101,113	3.00	29 (40%)
20	BCR	k	1404	-	41,41,41	1.04	1 (2%)	56,56,56	1.78	12 (21%)
27	LUT	6	321	-	42,43,43	0.74	0	51,60,60	1.69	9 (17%)
20	BCR	b	847	-	41,41,41	1.05	1 (2%)	56,56,56	1.82	15 (26%)
28	XAT	6	318	-	39,47,47	0.89	0	54,74,74	2.62	19 (35%)
17	CLA	f	7002	29	49,53,73	2.44	20 (40%)	59,89,113	3.20	28 (47%)
17	CLA	A	835	1	69,73,73	2.09	21 (30%)	83,113,113	2.84	30 (36%)
17	CLA	A	831	1	69,73,73	2.07	19 (27%)	83,113,113	2.74	28 (33%)
17	CLA	b	811	2	58,62,73	2.24	19 (32%)	73,100,113	3.06	30 (41%)
17	CLA	B	823	2	64,68,73	2.15	20 (31%)	77,107,113	2.86	32 (41%)
26	CHL	4	607	29	55,59,74	2.21	21 (38%)	62,96,114	3.24	26 (41%)
26	CHL	9	605	29	60,64,74	2.15	22 (36%)	68,102,114	3.16	29 (42%)
17	CLA	a	846	19	56,60,73	2.35	21 (37%)	67,97,113	3.08	26 (38%)
20	BCR	b	801	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	6 (10%)
20	BCR	I	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.93	15 (26%)
20	BCR	b	844	-	41,41,41	1.03	1 (2%)	56,56,56	2.08	14 (25%)
17	CLA	a	812	17,1	69,73,73	2.09	21 (30%)	83,113,113	2.85	30 (36%)
17	CLA	a	838	1	55,59,73	2.32	19 (34%)	66,96,113	3.16	31 (46%)
17	CLA	a	840	1	69,73,73	2.08	20 (28%)	83,113,113	2.83	29 (34%)
17	CLA	a	817	29	49,53,73	2.47	21 (42%)	59,89,113	3.19	25 (42%)
27	LUT	6	317	-	42,43,43	0.75	0	51,60,60	1.66	14 (27%)
20	BCR	L	205	-	41,41,41	1.03	1 (2%)	56,56,56	1.66	11 (19%)
19	LHG	A	846	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
17	CLA	b	823	2	64,68,73	2.16	20 (31%)	77,107,113	2.82	28 (36%)
27	LUT	9	616	-	42,43,43	0.74	0	51,60,60	1.62	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	b	830	2	54,58,73	2.36	21 (38%)	65,95,113	3.17	31 (47%)
17	CLA	l	203	12	69,73,73	2.07	20 (28%)	83,113,113	2.85	31 (37%)
17	CLA	a	832	1	54,58,73	2.36	20 (37%)	65,95,113	3.10	29 (44%)
25	LMG	6	302	-	40,40,55	1.05	2 (5%)	48,48,63	1.10	3 (6%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
17	CLA	F	304	6	59,63,73	2.28	21 (35%)	71,101,113	2.96	31 (43%)
28	XAT	3	317	-	39,47,47	0.88	0	54,74,74	2.67	20 (37%)
26	CHL	7	614	-	47,51,74	2.35	20 (42%)	52,86,114	3.49	23 (44%)
20	BCR	j	3003	-	41,41,41	1.02	1 (2%)	56,56,56	1.71	13 (23%)
17	CLA	B	831	2	53,57,73	2.38	20 (37%)	62,93,113	3.13	29 (46%)
26	CHL	2	607	29	55,59,74	2.22	21 (38%)	62,96,114	3.24	26 (41%)
17	CLA	3	302	15	64,68,73	2.17	21 (32%)	77,107,113	2.90	31 (40%)
17	CLA	B	803	-	69,73,73	2.10	21 (30%)	83,113,113	2.77	31 (37%)
17	CLA	9	608	16	54,58,73	2.33	20 (37%)	65,95,113	3.07	29 (44%)
20	BCR	i	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	12 (21%)
17	CLA	2	609	14	64,68,73	2.19	21 (32%)	77,107,113	2.89	33 (42%)
27	LUT	1	320	-	42,43,43	0.74	0	51,60,60	1.65	11 (21%)
17	CLA	8	304	29	46,50,73	2.47	20 (43%)	55,85,113	3.29	26 (47%)
20	BCR	l	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.80	12 (21%)
17	CLA	A	833	1	69,73,73	2.09	21 (30%)	83,113,113	2.77	28 (33%)
28	XAT	4	617	-	39,47,47	0.88	0	54,74,74	2.59	18 (33%)
20	BCR	K	4001	-	41,41,41	1.05	1 (2%)	56,56,56	1.80	11 (19%)
17	CLA	A	830	1	69,73,73	2.07	20 (28%)	83,113,113	2.77	29 (34%)
20	BCR	A	848	-	41,41,41	1.02	1 (2%)	56,56,56	1.82	13 (23%)
17	CLA	3	306	15	51,55,73	2.44	20 (39%)	61,91,113	3.11	26 (42%)
26	CHL	1	302	13	65,69,74	2.05	21 (32%)	74,108,114	3.05	27 (36%)
17	CLA	A	840	1	69,73,73	2.09	20 (28%)	83,113,113	2.83	30 (36%)
19	LHG	A	847	17	26,26,48	1.28	2 (7%)	29,32,54	1.26	3 (10%)
17	CLA	b	839	29	69,73,73	2.08	20 (28%)	83,113,113	2.77	25 (30%)
17	CLA	A	824	1	55,59,73	2.34	21 (38%)	66,96,113	3.09	29 (43%)
17	CLA	a	821	1	49,53,73	2.43	20 (40%)	59,89,113	3.27	27 (45%)
20	BCR	B	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	12 (21%)
20	BCR	b	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.93	14 (25%)
20	BCR	a	849	-	41,41,41	1.06	1 (2%)	56,56,56	1.96	14 (25%)
17	CLA	B	835	29	49,53,73	2.47	21 (42%)	59,89,113	3.17	28 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	822	29	69,73,73	2.09	20 (28%)	83,113,113	2.69	29 (34%)
17	CLA	b	821	2	50,54,73	2.44	21 (42%)	60,90,113	3.19	26 (43%)
26	CHL	7	607	29	55,59,74	2.24	21 (38%)	62,96,114	3.24	24 (38%)
20	BCR	B	847	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	15 (26%)
17	CLA	7	609	14	64,68,73	2.18	20 (31%)	77,107,113	2.90	32 (41%)
17	CLA	b	829	2	69,73,73	2.04	19 (27%)	83,113,113	2.81	31 (37%)
17	CLA	B	832	2	69,73,73	2.06	20 (28%)	83,113,113	2.85	28 (33%)
17	CLA	B	833	2	62,66,73	2.19	20 (32%)	74,104,113	2.97	29 (39%)
17	CLA	2	603	14	69,73,73	2.08	21 (30%)	83,113,113	2.77	27 (32%)
17	CLA	7	612	14	69,73,73	2.09	21 (30%)	83,113,113	2.75	28 (33%)
17	CLA	j	3002	10	46,50,73	2.49	20 (43%)	55,85,113	3.32	27 (49%)
20	BCR	2	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.86	18 (32%)
26	CHL	7	606	29	52,56,74	2.30	21 (40%)	58,92,114	3.38	26 (44%)
17	CLA	6	306	29	55,59,73	2.35	21 (38%)	66,96,113	3.11	29 (43%)
28	XAT	9	617	-	39,47,47	0.86	1 (2%)	54,74,74	2.61	17 (31%)
20	BCR	f	7004	-	41,41,41	1.03	1 (2%)	56,56,56	1.75	18 (32%)
17	CLA	a	820	1	69,73,73	2.10	21 (30%)	83,113,113	2.75	28 (33%)
17	CLA	A	819	1	69,73,73	2.08	20 (28%)	83,113,113	2.78	29 (34%)
17	CLA	8	309	-	56,60,73	2.34	21 (37%)	67,97,113	3.09	27 (40%)
17	CLA	b	837	2	69,73,73	2.10	21 (30%)	83,113,113	2.81	31 (37%)
17	CLA	b	814	2	69,73,73	2.09	21 (30%)	83,113,113	2.85	28 (33%)
20	BCR	A	856	-	41,41,41	1.03	1 (2%)	56,56,56	2.03	16 (28%)
27	LUT	8	314	-	42,43,43	0.74	0	51,60,60	1.47	11 (21%)
17	CLA	K	4003	11	50,54,73	2.46	21 (42%)	60,90,113	3.19	26 (43%)
17	CLA	a	806	1	69,73,73	2.06	20 (28%)	83,113,113	2.82	31 (37%)
17	CLA	A	841	1	69,73,73	2.10	20 (28%)	83,113,113	2.80	26 (31%)
17	CLA	6	312	19	45,49,73	2.51	20 (44%)	54,84,113	3.39	27 (50%)
17	CLA	A	804	1	69,73,73	2.07	20 (28%)	83,113,113	2.84	30 (36%)
20	BCR	L	206	-	41,41,41	1.06	1 (2%)	56,56,56	1.84	12 (21%)
25	LMG	G	102	-	44,44,55	1.01	2 (4%)	52,52,63	0.98	3 (5%)
17	CLA	4	608	16	54,58,73	2.34	20 (37%)	65,95,113	3.07	29 (44%)
17	CLA	3	308	15	54,58,73	2.37	20 (37%)	65,95,113	3.12	29 (44%)
17	CLA	b	816	2	59,63,73	2.26	21 (35%)	71,101,113	3.03	31 (43%)
17	CLA	a	844	29	69,73,73	2.04	20 (28%)	83,113,113	2.77	28 (33%)
17	CLA	B	837	2	69,73,73	2.08	21 (30%)	83,113,113	2.82	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	BCR	a	852	-	41,41,41	1.04	1 (2%)	56,56,56	1.94	17 (30%)
17	CLA	3	313	15	49,53,73	2.50	21 (42%)	59,89,113	3.19	26 (44%)
17	CLA	8	313	-	26,32,73	3.08	16 (61%)	34,54,113	4.11	23 (67%)
17	CLA	a	842	29	69,73,73	2.08	20 (28%)	83,113,113	2.75	28 (33%)
17	CLA	A	818	1	69,73,73	2.08	20 (28%)	83,113,113	2.84	30 (36%)
17	CLA	B	806	2	69,73,73	2.08	21 (30%)	83,113,113	2.78	28 (33%)
20	BCR	l	201	-	41,41,41	1.04	1 (2%)	56,56,56	1.85	15 (26%)
17	CLA	G	101	29	49,53,73	2.46	21 (42%)	59,89,113	3.29	25 (42%)
17	CLA	B	812	2	59,63,73	2.26	21 (35%)	71,101,113	2.95	27 (38%)
19	LHG	1	301	17	22,22,48	1.18	2 (9%)	25,28,54	1.29	2 (8%)
17	CLA	7	611	14	56,60,73	2.31	20 (35%)	67,97,113	3.07	28 (41%)
19	LHG	2	618	17	36,36,48	1.08	2 (5%)	39,42,54	1.16	3 (7%)
20	BCR	3	318	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
20	BCR	b	845	-	41,41,41	1.05	1 (2%)	56,56,56	1.94	13 (23%)
17	CLA	a	827	29	69,73,73	2.08	20 (28%)	83,113,113	2.78	28 (33%)
17	CLA	b	820	2	54,58,73	2.35	20 (37%)	65,95,113	3.14	29 (44%)
17	CLA	6	315	13	59,63,73	2.26	21 (35%)	71,101,113	3.01	30 (42%)
17	CLA	7	603	14	55,59,73	2.33	20 (36%)	66,96,113	3.09	29 (43%)
20	BCR	7	617	-	41,41,41	1.09	1 (2%)	56,56,56	2.09	13 (23%)
17	CLA	1	306	-	56,60,73	2.32	21 (37%)	67,97,113	3.08	29 (43%)
17	CLA	6	313	13	56,60,73	2.32	20 (35%)	67,97,113	3.08	28 (41%)
17	CLA	4	610	29	59,63,73	2.25	20 (33%)	71,101,113	2.95	30 (42%)
27	LUT	1	316	-	42,43,43	0.74	0	51,60,60	1.55	12 (23%)
21	SF4	A	853	1,2	0,12,12	-	-	-	-	-
17	CLA	b	802	2	69,73,73	2.06	19 (27%)	83,113,113	2.83	33 (39%)
17	CLA	L	204	29	54,58,73	2.37	21 (38%)	65,95,113	3.16	29 (44%)
17	CLA	2	608	14	54,58,73	2.37	21 (38%)	65,95,113	3.14	31 (47%)
17	CLA	a	822	29	69,73,73	2.08	20 (28%)	83,113,113	2.74	30 (36%)
17	CLA	B	819	29	69,73,73	2.08	21 (30%)	83,113,113	2.73	31 (37%)
17	CLA	A	816	1	54,58,73	2.36	21 (38%)	65,95,113	3.17	28 (43%)
17	CLA	9	603	16	50,54,73	2.42	21 (42%)	60,90,113	3.28	28 (46%)
20	BCR	B	846	-	41,41,41	1.04	1 (2%)	56,56,56	1.76	18 (32%)
17	CLA	b	834	2	69,73,73	2.09	21 (30%)	83,113,113	2.80	29 (34%)
17	CLA	b	808	2	69,73,73	2.06	20 (28%)	83,113,113	2.86	32 (38%)
17	CLA	b	819	29	69,73,73	2.08	21 (30%)	83,113,113	2.71	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	303	15	54,58,73	2.36	21 (38%)	65,95,113	3.14	27 (41%)
17	CLA	g	101	-	45,49,73	2.49	21 (46%)	54,84,113	3.46	28 (51%)
18	PQN	b	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.07	3 (7%)
17	CLA	B	817	2	63,67,73	2.17	21 (33%)	75,105,113	2.92	31 (41%)
17	CLA	a	829	1	69,73,73	2.06	20 (28%)	83,113,113	2.79	28 (33%)
20	BCR	6	319	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	b	810	2	69,73,73	2.08	20 (28%)	83,113,113	2.78	28 (33%)
17	CLA	4	602	16	64,68,73	2.17	21 (32%)	77,107,113	2.90	32 (41%)
17	CLA	B	824	29	69,73,73	2.06	20 (28%)	83,113,113	2.77	28 (33%)
17	CLA	A	823	1	53,57,73	2.40	21 (39%)	62,93,113	3.18	28 (45%)
21	SF4	C	101	3	0,12,12	-	-	-		
21	SF4	a	855	1,2	0,12,12	-	-	-		
17	CLA	a	835	1	69,73,73	2.09	21 (30%)	83,113,113	2.84	32 (38%)
17	CLA	3	314	15	50,54,73	2.44	20 (40%)	60,90,113	3.23	25 (41%)
17	CLA	a	837	1	49,53,73	2.48	21 (42%)	59,89,113	3.20	27 (45%)
17	CLA	1	313	13	69,73,73	2.09	21 (30%)	83,113,113	2.78	29 (34%)
17	CLA	A	836	1	54,58,73	2.34	20 (37%)	65,95,113	3.05	31 (47%)
17	CLA	6	316	13	50,54,73	2.45	21 (42%)	60,90,113	3.20	26 (43%)
17	CLA	A	834	1	69,73,73	2.07	21 (30%)	83,113,113	2.81	29 (34%)
20	BCR	j	3004	-	41,41,41	1.05	1 (2%)	56,56,56	2.15	18 (32%)
26	CHL	9	615	16	47,51,74	2.35	21 (44%)	52,86,114	3.56	22 (42%)
17	CLA	4	603	16,25	50,54,73	2.38	20 (40%)	60,90,113	3.28	27 (45%)
17	CLA	3	312	15	59,63,73	2.26	20 (33%)	71,101,113	2.97	29 (40%)
19	LHG	1	319	17	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
17	CLA	1	314	13	59,63,73	2.26	21 (35%)	71,101,113	3.04	30 (42%)
17	CLA	a	836	1	54,58,73	2.33	20 (37%)	65,95,113	3.03	30 (46%)
17	CLA	8	308	15	54,58,73	2.39	21 (38%)	65,95,113	3.14	30 (46%)
17	CLA	A	815	1	49,53,73	2.47	21 (42%)	59,89,113	3.23	26 (44%)
17	CLA	b	803	-	69,73,73	2.06	20 (28%)	83,113,113	2.66	29 (34%)
17	CLA	6	307	-	46,50,73	2.47	20 (43%)	55,85,113	3.29	26 (47%)
17	CLA	B	810	2	69,73,73	2.08	21 (30%)	83,113,113	2.81	31 (37%)
17	CLA	2	602	14	69,73,73	2.11	21 (30%)	83,113,113	2.80	30 (36%)
17	CLA	a	809	1	69,73,73	2.07	19 (27%)	83,113,113	2.90	29 (34%)
17	CLA	b	807	2	69,73,73	2.10	21 (30%)	83,113,113	2.76	28 (33%)
17	CLA	1	303	13	69,73,73	2.09	21 (30%)	83,113,113	2.79	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	8	310	15	59,63,73	2.26	21 (35%)	71,101,113	2.96	29 (40%)
17	CLA	3	301	-	50,54,73	2.45	21 (42%)	60,90,113	3.20	27 (45%)
20	BCR	A	852	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	14 (25%)
17	CLA	B	827	2	69,73,73	2.08	20 (28%)	83,113,113	2.88	30 (36%)
28	XAT	7	616	-	39,47,47	0.85	0	54,74,74	2.60	19 (35%)
17	CLA	9	612	16	60,64,73	2.24	21 (35%)	72,102,113	2.95	28 (38%)
17	CLA	1	305	29	56,60,73	2.33	21 (37%)	67,97,113	3.13	30 (44%)
17	CLA	a	823	1	53,57,73	2.37	20 (37%)	62,93,113	3.15	27 (43%)
17	CLA	G	104	7	50,54,73	2.45	21 (42%)	60,90,113	3.20	26 (43%)
21	SF4	c	101	3	0,12,12	-	-	-	-	-
25	LMG	4	620	17	44,44,55	1.02	3 (6%)	52,52,63	1.18	4 (7%)
17	CLA	6	305	13	69,73,73	2.08	21 (30%)	83,113,113	2.78	28 (33%)
20	BCR	8	316	-	41,41,41	1.07	1 (2%)	56,56,56	1.92	17 (30%)
20	BCR	a	854	-	41,41,41	1.04	1 (2%)	56,56,56	1.74	12 (21%)
17	CLA	b	840	2	69,73,73	2.06	20 (28%)	83,113,113	2.82	30 (36%)
20	BCR	b	848	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	10 (17%)
20	BCR	B	843	-	41,41,41	1.06	1 (2%)	56,56,56	1.88	14 (25%)
17	CLA	a	828	1	69,73,73	2.05	20 (28%)	83,113,113	2.81	27 (32%)
17	CLA	K	4002	-	49,53,73	2.49	21 (42%)	59,89,113	3.24	25 (42%)
17	CLA	B	821	2	50,54,73	2.43	21 (42%)	60,90,113	3.21	25 (41%)
17	CLA	4	612	16	60,64,73	2.24	21 (35%)	72,102,113	2.97	28 (38%)
17	CLA	B	808	2	69,73,73	2.07	20 (28%)	83,113,113	2.80	32 (38%)
17	CLA	B	815	2	64,68,73	2.15	20 (31%)	77,107,113	2.85	29 (37%)
17	CLA	A	825	1	59,63,73	2.27	21 (35%)	71,101,113	2.93	30 (42%)
17	CLA	2	604	29	64,68,73	2.18	21 (32%)	77,107,113	2.86	30 (38%)
17	CLA	1	311	19	45,49,73	2.52	20 (44%)	54,84,113	3.37	26 (48%)
17	CLA	B	840	2	69,73,73	2.08	21 (30%)	83,113,113	2.81	28 (33%)
17	CLA	a	824	1	55,59,73	2.33	20 (36%)	66,96,113	3.13	27 (40%)
17	CLA	a	825	1	59,63,73	2.27	20 (33%)	71,101,113	2.94	29 (40%)
18	PQN	B	842	-	34,34,34	1.60	2 (5%)	42,45,45	1.12	3 (7%)
17	CLA	7	602	14	69,73,73	2.09	21 (30%)	83,113,113	2.83	30 (36%)
26	CHL	1	307	13	52,56,74	2.32	21 (40%)	58,92,114	3.32	24 (41%)
17	CLA	9	614	16	51,55,73	2.40	21 (41%)	61,91,113	3.24	26 (42%)
17	CLA	A	838	1	55,59,73	2.33	20 (36%)	66,96,113	3.19	30 (45%)
17	CLA	B	805	2	69,73,73	2.07	21 (30%)	83,113,113	2.83	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	817	29	49,53,73	2.48	21 (42%)	59,89,113	3.20	25 (42%)
17	CLA	A	827	29	69,73,73	2.09	21 (30%)	83,113,113	2.82	28 (33%)
19	LHG	3	319	17	19,19,48	1.10	1 (5%)	21,24,54	0.99	1 (4%)
20	BCR	4	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	15 (26%)
17	CLA	6	304	13	69,73,73	2.10	21 (30%)	83,113,113	2.80	30 (36%)
17	CLA	8	312	15	50,54,73	2.43	21 (42%)	60,90,113	3.22	27 (45%)
17	CLA	b	818	2	64,68,73	2.16	20 (31%)	77,107,113	2.85	29 (37%)
17	CLA	b	825	29	69,73,73	2.07	20 (28%)	83,113,113	2.81	30 (36%)
27	LUT	2	615	-	42,43,43	0.75	0	51,60,60	1.62	11 (21%)
22	HTG	J	3001	-	19,19,19	1.05	2 (10%)	23,24,24	0.53	0
17	CLA	a	841	1	69,73,73	2.09	20 (28%)	83,113,113	2.77	30 (36%)

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
25	LMG	9	619	-	-	10/45/65/70	0/1/1/1
17	CLA	A	832	1	-	4/21/97/115	-
17	CLA	b	838	2	-	2/18/94/115	-
17	CLA	b	805	2	-	19/39/115/115	-
17	CLA	A	807	1	-	12/39/115/115	-
17	CLA	b	817	2	-	11/32/108/115	-
17	CLA	B	828	2	-	5/39/115/115	-
27	LUT	4	616	-	-	2/29/67/67	0/2/2/2
17	CLA	F	301	29	-	8/39/115/115	-
17	CLA	6	310	13	-	7/39/115/115	-
17	CLA	A	837	1	-	5/15/91/115	-
17	CLA	B	826	2	-	10/39/115/115	-
17	CLA	a	802	-	-	18/39/115/115	-
17	CLA	a	804	1	-	16/39/115/115	-
17	CLA	b	832	2	-	13/39/115/115	-
26	CHL	3	307	29	-	2/19/95/117	-
17	CLA	g	103	7	-	2/17/93/115	-
17	CLA	A	809	1	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	9	613	16	-	0/15/91/115	-
17	CLA	A	801	1	1/1/15/20	7/39/115/115	-
17	CLA	A	814	1	-	16/39/115/115	-
17	CLA	b	826	2	-	9/39/115/115	-
20	BCR	B	801	-	-	1/29/63/63	0/2/2/2
17	CLA	4	604	29	-	5/21/97/115	-
22	HTG	A	855	-	-	1/10/30/30	0/1/1/1
17	CLA	a	831	1	-	18/39/115/115	-
26	CHL	2	605	29	-	0/14/90/117	-
17	CLA	B	809	2	-	9/39/115/115	-
17	CLA	7	610	19	-	0/10/86/115	-
17	CLA	3	305	29	-	3/12/88/115	-
17	CLA	k	1402	11	-	0/17/93/115	-
17	CLA	a	815	1	-	3/15/91/115	-
17	CLA	3	309	15	-	3/21/97/115	-
17	CLA	a	818	1	-	12/39/115/115	-
17	CLA	8	307	15	-	7/21/97/115	-
28	XAT	8	315	-	-	0/31/93/93	0/4/4/4
20	BCR	A	850	-	-	3/29/63/63	0/2/2/2
17	CLA	A	813	1	-	7/26/102/115	-
20	BCR	a	850	-	-	6/29/63/63	0/2/2/2
17	CLA	b	824	29	-	12/39/115/115	-
17	CLA	6	309	29	-	3/17/93/115	-
17	CLA	l	202	12	-	10/39/115/115	-
20	BCR	F	305	-	-	4/29/63/63	0/2/2/2
17	CLA	A	812	17,1	-	13/39/115/115	-
17	CLA	1	310	13	-	5/33/109/115	-
19	LHG	a	847	-	-	10/53/53/53	-
19	LHG	6	301	17	-	7/26/26/53	-
17	CLA	b	815	2	-	9/27/103/115	-
17	CLA	1	309	13	-	10/39/115/115	-
17	CLA	b	806	2	-	9/39/115/115	-
26	CHL	2	606	29	-	2/20/96/117	-
17	CLA	B	802	2	-	15/39/115/115	-
19	LHG	a	848	17	-	12/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	843	29	-	18/39/115/115	-
22	HTG	F	302	-	-	2/10/30/30	0/1/1/1
17	CLA	A	808	1	-	8/39/115/115	-
17	CLA	A	845	19	-	10/24/100/115	-
17	CLA	A	828	1	-	14/39/115/115	-
17	CLA	A	820	1	-	14/39/115/115	-
17	CLA	B	820	2	-	3/21/97/115	-
17	CLA	2	612	14	-	9/39/115/115	-
17	CLA	f	7003	6	-	9/27/103/115	-
17	CLA	1	312	13	-	8/24/100/115	-
26	CHL	7	605	29	-	4/14/90/117	-
17	CLA	6	311	13	-	11/33/109/115	-
17	CLA	b	827	2	-	14/39/115/115	-
17	CLA	A	811	1	-	9/39/115/115	-
17	CLA	b	822	2	-	12/27/103/115	-
25	LMG	4	619	-	-	9/39/59/70	0/1/1/1
26	CHL	8	306	29	-	3/19/95/117	-
17	CLA	9	611	16	-	6/24/100/115	-
17	CLA	b	835	29	-	4/15/91/115	-
17	CLA	b	831	2	-	7/20/96/115	-
17	CLA	A	821	1	-	2/15/91/115	-
17	CLA	a	834	1	-	12/39/115/115	-
19	LHG	7	618	17	-	10/41/41/53	-
20	BCR	a	851	-	-	1/29/63/63	0/2/2/2
19	LHG	6	320	17	-	14/53/53/53	-
17	CLA	3	304	29	-	3/15/91/115	-
20	BCR	l	205	-	-	6/29/63/63	0/2/2/2
20	BCR	1	318	-	-	6/29/63/63	0/2/2/2
17	CLA	A	803	29	-	2/39/115/115	-
17	CLA	A	842	1	-	13/39/115/115	-
17	CLA	L	203	12	-	7/39/115/115	-
17	CLA	a	807	1	-	14/39/115/115	-
23	LMT	B	849	-	-	3/21/61/61	0/2/2/2
17	CLA	b	809	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	829	2	-	11/39/115/115	-
22	HTG	a	857	-	-	0/10/30/30	0/1/1/1
22	HTG	f	7001	-	-	1/10/30/30	0/1/1/1
17	CLA	9	604	29	-	5/21/97/115	-
17	CLA	2	611	14	-	5/24/100/115	-
17	CLA	k	1401	-	-	5/15/91/115	-
26	CHL	2	601	14	-	11/35/111/117	-
20	BCR	B	845	-	-	6/29/63/63	0/2/2/2
26	CHL	6	303	13	-	17/35/111/117	-
17	CLA	a	830	1	-	11/39/115/115	-
17	CLA	6	314	13	-	6/33/109/115	-
27	LUT	7	615	-	-	1/29/67/67	0/2/2/2
17	CLA	2	613	14	-	6/13/89/115	-
27	LUT	3	316	-	-	2/29/67/67	0/2/2/2
20	BCR	A	851	-	-	5/29/63/63	0/2/2/2
17	CLA	7	604	29	-	13/33/109/115	-
17	CLA	B	811	2	-	4/25/101/115	-
17	CLA	b	833	2	-	8/31/107/115	-
17	CLA	B	814	2	-	12/39/115/115	-
17	CLA	1	315	13	-	1/17/93/115	-
17	CLA	b	813	2	-	13/39/115/115	-
17	CLA	9	601	16	-	5/17/93/115	-
20	BCR	L	201	-	-	8/29/63/63	0/2/2/2
17	CLA	4	613	16	-	2/15/91/115	-
17	CLA	3	311	-	-	6/24/100/115	-
17	CLA	1	308	29	-	5/39/115/115	-
20	BCR	J	3003	-	-	2/29/63/63	0/2/2/2
17	CLA	4	609	16	-	6/33/109/115	-
28	XAT	2	616	-	-	0/31/93/93	0/4/4/4
17	CLA	7	608	14	-	6/21/97/115	-
17	CLA	A	805	17,1	-	10/27/103/115	-
17	CLA	B	838	2	-	1/18/94/115	-
26	CHL	7	601	14	-	8/35/111/117	-
17	CLA	b	828	2	-	9/39/115/115	-
17	CLA	A	802	-	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	819	1	-	14/39/115/115	-
18	PQN	A	844	-	-	8/23/43/43	0/2/2/2
20	BCR	B	844	-	-	6/29/63/63	0/2/2/2
17	CLA	1	304	13	-	12/39/115/115	-
17	CLA	4	601	16	-	3/17/93/115	-
17	CLA	7	613	14	-	0/13/89/115	-
17	CLA	b	812	2	-	11/27/103/115	-
17	CLA	a	839	1	-	10/39/115/115	-
17	CLA	3	310	19	-	0/4/76/115	-
17	CLA	B	816	2	-	11/27/103/115	-
21	SF4	c	102	3	-	-	0/6/5/5
20	BCR	g	104	-	-	2/29/63/63	0/2/2/2
24	DGD	b	849	-	-	10/55/95/95	0/2/2/2
17	CLA	B	834	2	-	16/39/115/115	-
26	CHL	6	308	13	-	1/19/95/117	-
17	CLA	8	302	15	-	1/21/97/115	-
17	CLA	9	602	16	-	12/33/109/115	-
17	CLA	A	810	1	-	4/39/115/115	-
17	CLA	l	204	29	-	6/21/97/115	-
17	CLA	a	814	1	-	11/39/115/115	-
22	HTG	j	3001	-	-	1/10/30/30	0/1/1/1
17	CLA	4	614	16	-	2/21/97/115	-
17	CLA	a	856	29	-	11/39/115/115	-
17	CLA	B	841	19	-	10/39/115/115	-
17	CLA	b	836	2	-	5/33/109/115	-
17	CLA	a	810	1	-	2/39/115/115	-
17	CLA	B	804	2	-	10/15/91/115	-
17	CLA	g	102	7	-	1/21/97/115	-
17	CLA	B	825	29	-	9/39/115/115	-
17	CLA	a	811	1	-	9/39/115/115	-
17	CLA	9	609	16	-	6/33/109/115	-
17	CLA	a	801	1	1/1/15/20	10/39/115/115	-
20	BCR	G	105	-	-	3/29/63/63	0/2/2/2
17	CLA	G	103	7	-	1/21/97/115	-
17	CLA	b	841	19	-	6/39/115/115	-
18	PQN	a	845	-	-	5/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	804	2	-	6/15/91/115	-
24	DGD	B	850	-	-	12/55/95/95	0/2/2/2
26	CHL	4	605	29	-	10/29/105/117	-
20	BCR	K	4004	-	-	4/29/63/63	0/2/2/2
20	BCR	b	846	-	-	5/29/63/63	0/2/2/2
17	CLA	a	803	29	-	1/39/115/115	-
17	CLA	B	836	2	-	5/33/109/115	-
17	CLA	a	813	1	-	6/26/102/115	-
20	BCR	A	849	-	-	2/29/63/63	0/2/2/2
17	CLA	8	303	29	-	3/15/91/115	-
17	CLA	B	807	2	-	15/39/115/115	-
17	CLA	J	3002	10	-	4/12/88/115	-
17	CLA	A	806	1	-	21/39/115/115	-
17	CLA	k	1403	-	-	4/17/93/115	-
17	CLA	8	305	15	-	3/18/94/115	-
17	CLA	B	813	2	-	16/39/115/115	-
26	CHL	4	615	16	-	0/14/90/117	-
17	CLA	9	610	29	-	2/10/86/115	-
17	CLA	a	816	1	-	9/21/97/115	-
17	CLA	B	818	2	-	10/33/109/115	-
17	CLA	B	830	2	-	7/21/97/115	-
26	CHL	9	607	29	-	3/23/99/117	-
17	CLA	B	822	2	-	13/27/103/115	-
26	CHL	4	606	29	-	8/23/99/117	-
17	CLA	L	202	12	-	8/39/115/115	-
26	CHL	9	606	29	-	4/23/99/117	-
28	XAT	1	317	-	-	0/31/93/93	0/4/4/4
17	CLA	A	826	29	-	14/39/115/115	-
17	CLA	A	839	1	-	5/39/115/115	-
17	CLA	a	833	1	-	5/39/115/115	-
20	BCR	9	618	-	-	6/29/63/63	0/2/2/2
17	CLA	B	839	29	-	7/39/115/115	-
20	BCR	a	853	-	-	7/29/63/63	0/2/2/2
17	CLA	a	826	29	-	8/39/115/115	-
17	CLA	8	301	15	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	2	614	-	-	0/14/90/117	-
17	CLA	a	808	1	-	10/39/115/115	-
17	CLA	2	610	19	-	0/10/86/115	-
17	CLA	A	854	29	-	10/39/115/115	-
17	CLA	4	611	16	-	7/24/100/115	-
17	CLA	A	829	1	-	13/39/115/115	-
17	CLA	a	843	1	-	14/39/115/115	-
17	CLA	8	311	15	-	3/15/91/115	-
17	CLA	F	303	29	-	2/15/91/115	-
17	CLA	a	805	17,1	-	11/27/103/115	-
20	BCR	k	1404	-	-	6/29/63/63	0/2/2/2
27	LUT	6	321	-	-	2/29/67/67	0/2/2/2
20	BCR	b	847	-	-	3/29/63/63	0/2/2/2
28	XAT	6	318	-	-	1/31/93/93	0/4/4/4
17	CLA	f	7002	29	-	1/15/91/115	-
17	CLA	A	835	1	-	12/39/115/115	-
17	CLA	A	831	1	-	15/39/115/115	-
17	CLA	b	811	2	-	10/25/101/115	-
17	CLA	B	823	2	-	14/33/109/115	-
26	CHL	4	607	29	-	5/23/99/117	-
26	CHL	9	605	29	-	10/29/105/117	-
17	CLA	a	846	19	-	13/24/100/115	-
20	BCR	b	801	-	-	0/29/63/63	0/2/2/2
20	BCR	I	101	-	-	3/29/63/63	0/2/2/2
20	BCR	b	844	-	-	6/29/63/63	0/2/2/2
17	CLA	a	812	17,1	-	13/39/115/115	-
17	CLA	a	838	1	-	9/23/99/115	-
17	CLA	a	840	1	-	9/39/115/115	-
17	CLA	a	817	29	-	2/15/91/115	-
27	LUT	6	317	-	-	2/29/67/67	0/2/2/2
20	BCR	L	205	-	-	6/29/63/63	0/2/2/2
19	LHG	A	846	-	-	10/53/53/53	-
17	CLA	b	823	2	-	7/33/109/115	-
27	LUT	9	616	-	-	2/29/67/67	0/2/2/2
17	CLA	b	830	2	-	3/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	l	203	12	-	8/39/115/115	-
17	CLA	a	832	1	-	6/21/97/115	-
25	LMG	6	302	-	-	6/35/55/70	0/1/1/1
21	SF4	C	102	3	-	-	0/6/5/5
17	CLA	F	304	6	-	8/27/103/115	-
28	XAT	3	317	-	-	2/31/93/93	0/4/4/4
26	CHL	7	614	-	-	3/14/90/117	-
20	BCR	j	3003	-	-	6/29/63/63	0/2/2/2
17	CLA	B	831	2	-	8/20/96/115	-
26	CHL	2	607	29	-	7/23/99/117	-
17	CLA	3	302	15	-	9/33/109/115	-
17	CLA	B	803	-	-	7/39/115/115	-
17	CLA	9	608	16	-	4/21/97/115	-
20	BCR	i	101	-	-	1/29/63/63	0/2/2/2
17	CLA	2	609	14	-	10/33/109/115	-
27	LUT	1	320	-	-	2/29/67/67	0/2/2/2
17	CLA	8	304	29	-	0/12/88/115	-
20	BCR	l	206	-	-	0/29/63/63	0/2/2/2
17	CLA	A	833	1	-	7/39/115/115	-
28	XAT	4	617	-	-	0/31/93/93	0/4/4/4
20	BCR	K	4001	-	-	1/29/63/63	0/2/2/2
17	CLA	A	830	1	-	13/39/115/115	-
20	BCR	A	848	-	-	6/29/63/63	0/2/2/2
17	CLA	3	306	15	-	3/18/94/115	-
26	CHL	1	302	13	-	7/35/111/117	-
17	CLA	A	840	1	-	7/39/115/115	-
19	LHG	A	847	17	-	9/31/31/53	-
17	CLA	b	839	29	-	9/39/115/115	-
17	CLA	A	824	1	-	9/23/99/115	-
17	CLA	a	821	1	-	4/15/91/115	-
20	BCR	B	848	-	-	2/29/63/63	0/2/2/2
20	BCR	b	843	-	-	0/29/63/63	0/2/2/2
20	BCR	a	849	-	-	2/29/63/63	0/2/2/2
17	CLA	B	835	29	-	1/15/91/115	-
17	CLA	A	822	29	-	7/39/115/115	-
17	CLA	b	821	2	-	3/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CHL	7	607	29	-	4/23/99/117	-
20	BCR	B	847	-	-	5/29/63/63	0/2/2/2
17	CLA	7	609	14	-	9/33/109/115	-
17	CLA	b	829	2	-	8/39/115/115	-
17	CLA	B	832	2	-	14/39/115/115	-
17	CLA	B	833	2	-	9/31/107/115	-
17	CLA	2	603	14	-	13/39/115/115	-
17	CLA	7	612	14	-	8/39/115/115	-
17	CLA	j	3002	10	-	1/12/88/115	-
20	BCR	2	617	-	-	3/29/63/63	0/2/2/2
26	CHL	7	606	29	-	0/20/96/117	-
17	CLA	6	306	29	-	3/23/99/115	-
28	XAT	9	617	-	-	0/31/93/93	0/4/4/4
20	BCR	f	7004	-	-	4/29/63/63	0/2/2/2
17	CLA	a	820	1	-	13/39/115/115	-
17	CLA	A	819	1	-	13/39/115/115	-
17	CLA	8	309	-	-	5/24/100/115	-
17	CLA	b	837	2	-	11/39/115/115	-
17	CLA	b	814	2	-	12/39/115/115	-
20	BCR	A	856	-	-	4/29/63/63	0/2/2/2
27	LUT	8	314	-	-	2/29/67/67	0/2/2/2
17	CLA	K	4003	11	-	2/17/93/115	-
17	CLA	a	806	1	-	18/39/115/115	-
17	CLA	A	841	1	-	10/39/115/115	-
17	CLA	6	312	19	-	0/10/86/115	-
17	CLA	A	804	1	-	7/39/115/115	-
20	BCR	L	206	-	-	3/29/63/63	0/2/2/2
25	LMG	G	102	-	-	10/39/59/70	0/1/1/1
17	CLA	4	608	16	-	3/21/97/115	-
17	CLA	3	308	15	-	7/21/97/115	-
17	CLA	b	816	2	-	13/27/103/115	-
17	CLA	a	844	29	-	14/39/115/115	-
17	CLA	B	837	2	-	9/39/115/115	-
20	BCR	a	852	-	-	6/29/63/63	0/2/2/2
17	CLA	3	313	15	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	a	842	29	-	5/39/115/115	-
17	CLA	A	818	1	-	12/39/115/115	-
17	CLA	B	806	2	-	18/39/115/115	-
20	BCR	l	201	-	-	8/29/63/63	0/2/2/2
17	CLA	G	101	29	-	2/15/91/115	-
17	CLA	B	812	2	-	8/27/103/115	-
19	LHG	1	301	17	-	9/26/26/53	-
17	CLA	7	611	14	-	5/24/100/115	-
19	LHG	2	618	17	-	9/41/41/53	-
20	BCR	3	318	-	-	6/29/63/63	0/2/2/2
20	BCR	b	845	-	-	6/29/63/63	0/2/2/2
17	CLA	a	827	29	-	10/39/115/115	-
17	CLA	b	820	2	-	2/21/97/115	-
17	CLA	6	315	13	-	6/27/103/115	-
17	CLA	7	603	14	-	4/23/99/115	-
20	BCR	7	617	-	-	4/29/63/63	0/2/2/2
17	CLA	1	306	-	-	4/24/100/115	-
17	CLA	6	313	13	-	10/24/100/115	-
17	CLA	4	610	29	-	7/27/103/115	-
27	LUT	1	316	-	-	2/29/67/67	0/2/2/2
21	SF4	A	853	1,2	-	-	0/6/5/5
17	CLA	b	802	2	-	7/39/115/115	-
17	CLA	L	204	29	-	3/21/97/115	-
17	CLA	2	608	14	-	3/21/97/115	-
17	CLA	a	822	29	-	5/39/115/115	-
17	CLA	B	819	29	-	11/39/115/115	-
17	CLA	A	816	1	-	3/21/97/115	-
17	CLA	9	603	16	-	4/17/93/115	-
20	BCR	B	846	-	-	4/29/63/63	0/2/2/2
17	CLA	b	834	2	-	13/39/115/115	-
17	CLA	b	808	2	-	8/39/115/115	-
17	CLA	b	819	29	-	7/39/115/115	-
17	CLA	3	303	15	-	2/21/97/115	-
17	CLA	g	101	-	-	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	PQN	b	842	-	-	3/23/43/43	0/2/2/2
17	CLA	B	817	2	-	10/32/108/115	-
17	CLA	a	829	1	-	14/39/115/115	-
20	BCR	6	319	-	-	4/29/63/63	0/2/2/2
17	CLA	b	810	2	-	14/39/115/115	-
17	CLA	4	602	16	-	8/33/109/115	-
17	CLA	B	824	29	-	8/39/115/115	-
17	CLA	A	823	1	-	7/20/96/115	-
21	SF4	C	101	3	-	-	0/6/5/5
21	SF4	a	855	1,2	-	-	0/6/5/5
17	CLA	a	835	1	-	10/39/115/115	-
17	CLA	3	314	15	-	1/17/93/115	-
17	CLA	a	837	1	-	5/15/91/115	-
17	CLA	1	313	13	-	5/39/115/115	-
17	CLA	A	836	1	-	0/21/97/115	-
17	CLA	6	316	13	-	3/17/93/115	-
17	CLA	A	834	1	-	11/39/115/115	-
20	BCR	j	3004	-	-	9/29/63/63	0/2/2/2
26	CHL	9	615	16	-	0/14/90/117	-
17	CLA	4	603	16,25	-	2/17/93/115	-
17	CLA	3	312	15	-	9/27/103/115	-
19	LHG	1	319	17	-	10/53/53/53	-
17	CLA	1	314	13	-	4/27/103/115	-
17	CLA	a	836	1	-	2/21/97/115	-
17	CLA	8	308	15	-	3/21/97/115	-
17	CLA	A	815	1	-	3/15/91/115	-
17	CLA	b	803	-	-	8/39/115/115	-
17	CLA	6	307	-	-	4/12/88/115	-
17	CLA	B	810	2	-	10/39/115/115	-
17	CLA	2	602	14	-	15/39/115/115	-
17	CLA	a	809	1	-	13/39/115/115	-
17	CLA	b	807	2	-	6/39/115/115	-
17	CLA	1	303	13	-	11/39/115/115	-
17	CLA	8	310	15	-	8/27/103/115	-
17	CLA	3	301	-	-	2/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	BCR	A	852	-	-	6/29/63/63	0/2/2/2
17	CLA	B	827	2	-	8/39/115/115	-
28	XAT	7	616	-	-	1/31/93/93	0/4/4/4
17	CLA	9	612	16	-	10/29/105/115	-
17	CLA	1	305	29	-	7/24/100/115	-
17	CLA	a	823	1	-	7/20/96/115	-
17	CLA	G	104	7	-	2/17/93/115	-
25	LMG	4	620	17	-	11/39/59/70	0/1/1/1
21	SF4	c	101	3	-	-	0/6/5/5
17	CLA	6	305	13	-	10/39/115/115	-
20	BCR	8	316	-	-	4/29/63/63	0/2/2/2
20	BCR	a	854	-	-	4/29/63/63	0/2/2/2
17	CLA	b	840	2	-	5/39/115/115	-
20	BCR	b	848	-	-	2/29/63/63	0/2/2/2
20	BCR	B	843	-	-	0/29/63/63	0/2/2/2
17	CLA	a	828	1	-	10/39/115/115	-
17	CLA	K	4002	-	-	4/15/91/115	-
17	CLA	B	821	2	-	2/17/93/115	-
17	CLA	4	612	16	-	9/29/105/115	-
17	CLA	B	808	2	-	9/39/115/115	-
17	CLA	B	815	2	-	12/33/109/115	-
17	CLA	A	825	1	-	7/27/103/115	-
17	CLA	2	604	29	-	11/33/109/115	-
17	CLA	1	311	19	-	0/10/86/115	-
17	CLA	B	840	2	-	9/39/115/115	-
17	CLA	a	824	1	-	8/23/99/115	-
17	CLA	a	825	1	-	6/27/103/115	-
18	PQN	B	842	-	-	3/23/43/43	0/2/2/2
17	CLA	7	602	14	-	10/39/115/115	-
26	CHL	1	307	13	-	3/20/96/117	-
17	CLA	9	614	16	-	4/18/94/115	-
17	CLA	A	838	1	-	5/23/99/115	-
17	CLA	B	805	2	-	16/39/115/115	-
17	CLA	A	817	29	-	3/15/91/115	-
17	CLA	A	827	29	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	3	319	17	-	11/23/23/53	-
20	BCR	4	618	-	-	6/29/63/63	0/2/2/2
17	CLA	6	304	13	-	9/39/115/115	-
17	CLA	8	312	15	-	1/17/93/115	-
17	CLA	b	818	2	-	13/33/109/115	-
17	CLA	b	825	29	-	10/39/115/115	-
27	LUT	2	615	-	-	2/29/67/67	0/2/2/2
22	HTG	J	3001	-	-	4/10/30/30	0/1/1/1
17	CLA	a	841	1	-	12/39/115/115	-

The worst 5 of 6430 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	845	PQN	C3-C2	7.78	1.49	1.35
18	b	842	PQN	C3-C2	7.70	1.49	1.35
18	A	844	PQN	C3-C2	7.61	1.49	1.35
18	B	842	PQN	C3-C2	7.59	1.49	1.35
17	3	315	CLA	C3D-C2D	6.56	1.49	1.35

The worst 5 of 9844 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	832	CLA	C1D-ND-C4D	-10.07	99.18	106.33
26	4	607	CHL	C2D-C1D-ND	10.04	117.50	110.10
17	L	203	CLA	C1D-ND-C4D	-10.01	99.23	106.33
26	7	606	CHL	C2D-C1D-ND	9.96	117.44	110.10
26	1	302	CHL	C2D-C1D-ND	9.90	117.40	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CLA	CBD
17	a	801	CLA	CBD

5 of 2740 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	805	CLA	CHA-CBD-CGD-O1D
17	A	809	CLA	C3A-C2A-CAA-CBA
17	A	809	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
17	A	809	CLA	C4B-C3B-CAB-CBB
17	A	809	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

382 monomers are involved in 1170 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	9	619	LMG	2	0
17	A	832	CLA	1	0
17	b	838	CLA	2	0
17	b	805	CLA	4	0
17	A	807	CLA	6	0
17	b	817	CLA	5	0
17	B	828	CLA	2	0
27	4	616	LUT	5	0
17	F	301	CLA	5	0
17	6	310	CLA	2	0
17	A	837	CLA	2	0
17	B	826	CLA	2	0
17	a	802	CLA	5	0
17	a	804	CLA	6	0
17	b	832	CLA	8	0
17	g	103	CLA	1	0
17	A	809	CLA	10	0
17	9	613	CLA	2	0
17	A	801	CLA	6	0
17	A	814	CLA	3	0
17	b	826	CLA	2	0
20	B	801	BCR	5	0
17	4	604	CLA	4	0
17	a	831	CLA	6	0
26	2	605	CHL	1	0
17	B	809	CLA	2	0
17	3	305	CLA	1	0
17	k	1402	CLA	1	0
17	a	815	CLA	2	0
17	3	309	CLA	6	0
17	a	818	CLA	4	0
17	8	307	CLA	4	0
28	8	315	XAT	7	0
20	A	850	BCR	3	0
17	A	813	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	a	850	BCR	3	0
17	b	824	CLA	7	0
17	l	202	CLA	3	0
20	F	305	BCR	6	0
17	A	812	CLA	5	0
17	1	310	CLA	2	0
19	a	847	LHG	1	0
17	b	815	CLA	7	0
17	1	309	CLA	4	0
17	b	806	CLA	8	0
26	2	606	CHL	1	0
17	B	802	CLA	7	0
19	a	848	LHG	4	0
17	A	843	CLA	8	0
22	F	302	HTG	2	0
17	A	808	CLA	3	0
17	A	845	CLA	2	0
17	A	828	CLA	2	0
17	A	820	CLA	3	0
17	B	820	CLA	2	0
17	2	612	CLA	2	0
17	f	7003	CLA	2	0
17	1	312	CLA	2	0
26	7	605	CHL	4	0
17	6	311	CLA	4	0
17	b	827	CLA	6	0
17	A	811	CLA	5	0
17	b	822	CLA	2	0
25	4	619	LMG	4	0
26	8	306	CHL	1	0
17	9	611	CLA	4	0
17	b	835	CLA	1	0
17	b	831	CLA	5	0
17	A	821	CLA	3	0
17	a	834	CLA	5	0
19	7	618	LHG	2	0
20	a	851	BCR	4	0
19	6	320	LHG	5	0
17	3	304	CLA	5	0
20	l	205	BCR	4	0
20	1	318	BCR	4	0
17	A	803	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	842	CLA	7	0
17	L	203	CLA	3	0
17	a	807	CLA	5	0
23	B	849	LMT	1	0
17	b	809	CLA	3	0
17	B	829	CLA	8	0
22	f	7001	HTG	2	0
17	9	604	CLA	3	0
17	2	611	CLA	2	0
17	k	1401	CLA	4	0
26	2	601	CHL	5	0
20	B	845	BCR	5	0
26	6	303	CHL	7	0
17	a	830	CLA	4	0
17	6	314	CLA	4	0
27	7	615	LUT	9	0
17	2	613	CLA	2	0
27	3	316	LUT	6	0
20	A	851	BCR	5	0
17	7	604	CLA	6	0
17	B	811	CLA	2	0
17	b	833	CLA	4	0
17	B	814	CLA	3	0
17	1	315	CLA	2	0
17	b	813	CLA	9	0
17	9	601	CLA	3	0
20	L	201	BCR	4	0
17	4	613	CLA	3	0
17	3	311	CLA	2	0
17	1	308	CLA	4	0
20	J	3003	BCR	3	0
17	4	609	CLA	4	0
28	2	616	XAT	5	0
17	7	608	CLA	5	0
17	A	805	CLA	3	0
17	B	838	CLA	7	0
26	7	601	CHL	2	0
17	b	828	CLA	3	0
17	A	802	CLA	7	0
17	a	819	CLA	5	0
18	A	844	PQN	5	0
20	B	844	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	1	304	CLA	6	0
17	4	601	CLA	3	0
17	7	613	CLA	1	0
17	b	812	CLA	3	0
17	a	839	CLA	5	0
17	B	816	CLA	4	0
20	g	104	BCR	3	0
24	b	849	DGD	5	0
17	B	834	CLA	1	0
17	8	302	CLA	1	0
17	9	602	CLA	4	0
17	A	810	CLA	5	0
17	l	204	CLA	1	0
17	a	814	CLA	5	0
17	a	856	CLA	10	0
17	B	841	CLA	5	0
17	b	836	CLA	5	0
17	a	810	CLA	5	0
17	B	804	CLA	2	0
17	B	825	CLA	5	0
17	a	811	CLA	3	0
17	9	609	CLA	3	0
17	a	801	CLA	4	0
20	G	105	BCR	5	0
17	G	103	CLA	1	0
17	b	841	CLA	4	0
18	a	845	PQN	3	0
17	b	804	CLA	6	0
24	B	850	DGD	1	0
26	4	605	CHL	2	0
20	K	4004	BCR	2	0
20	b	846	BCR	7	0
17	a	803	CLA	7	0
17	B	836	CLA	6	0
17	a	813	CLA	4	0
20	A	849	BCR	4	0
17	8	303	CLA	3	0
17	B	807	CLA	3	0
17	J	3002	CLA	1	0
17	A	806	CLA	9	0
17	k	1403	CLA	2	0
17	8	305	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	813	CLA	6	0
26	4	615	CHL	1	0
17	9	610	CLA	1	0
17	a	816	CLA	4	0
17	B	818	CLA	3	0
17	B	830	CLA	4	0
26	9	607	CHL	3	0
17	B	822	CLA	3	0
26	4	606	CHL	4	0
17	L	202	CLA	6	0
26	9	606	CHL	3	0
28	1	317	XAT	6	0
17	A	826	CLA	3	0
17	A	839	CLA	7	0
17	a	833	CLA	3	0
20	9	618	BCR	6	0
17	B	839	CLA	9	0
20	a	853	BCR	2	0
17	a	826	CLA	3	0
17	8	301	CLA	6	0
26	2	614	CHL	3	0
17	a	808	CLA	2	0
17	A	854	CLA	7	0
17	4	611	CLA	1	0
17	A	829	CLA	11	0
17	a	843	CLA	8	0
17	8	311	CLA	1	0
17	F	303	CLA	3	0
17	a	805	CLA	3	0
20	k	1404	BCR	3	0
27	6	321	LUT	5	0
20	b	847	BCR	1	0
28	6	318	XAT	8	0
17	f	7002	CLA	4	0
17	A	835	CLA	5	0
17	A	831	CLA	8	0
17	b	811	CLA	3	0
17	B	823	CLA	2	0
26	4	607	CHL	2	0
26	9	605	CHL	3	0
17	a	846	CLA	1	0
20	b	801	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	I	101	BCR	4	0
20	b	844	BCR	4	0
17	a	812	CLA	4	0
17	a	838	CLA	4	0
17	a	840	CLA	2	0
17	a	817	CLA	1	0
27	6	317	LUT	9	0
20	L	205	BCR	3	0
19	A	846	LHG	3	0
17	b	823	CLA	3	0
27	9	616	LUT	5	0
17	b	830	CLA	2	0
17	l	203	CLA	3	0
17	a	832	CLA	1	0
25	6	302	LMG	3	0
17	F	304	CLA	4	0
28	3	317	XAT	4	0
26	7	614	CHL	3	0
20	j	3003	BCR	5	0
17	B	831	CLA	7	0
26	2	607	CHL	5	0
17	3	302	CLA	7	0
17	B	803	CLA	6	0
17	9	608	CLA	5	0
20	i	101	BCR	2	0
17	2	609	CLA	4	0
27	1	320	LUT	3	0
20	l	206	BCR	4	0
17	A	833	CLA	5	0
28	4	617	XAT	4	0
20	K	4001	BCR	4	0
17	A	830	CLA	2	0
20	A	848	BCR	4	0
17	3	306	CLA	4	0
26	1	302	CHL	11	0
17	A	840	CLA	3	0
19	A	847	LHG	2	0
17	b	839	CLA	5	0
17	A	824	CLA	1	0
17	a	821	CLA	2	0
20	B	848	BCR	4	0
20	b	843	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	a	849	BCR	4	0
17	A	822	CLA	4	0
17	b	821	CLA	2	0
26	7	607	CHL	4	0
20	B	847	BCR	5	0
17	7	609	CLA	6	0
17	b	829	CLA	8	0
17	B	832	CLA	4	0
17	B	833	CLA	4	0
17	2	603	CLA	2	0
17	7	612	CLA	3	0
17	j	3002	CLA	1	0
20	2	617	BCR	11	0
26	7	606	CHL	2	0
17	6	306	CLA	3	0
28	9	617	XAT	7	0
20	f	7004	BCR	5	0
17	a	820	CLA	4	0
17	A	819	CLA	6	0
17	8	309	CLA	4	0
17	b	837	CLA	5	0
17	b	814	CLA	2	0
20	A	856	BCR	5	0
27	8	314	LUT	7	0
17	K	4003	CLA	2	0
17	a	806	CLA	7	0
17	A	841	CLA	9	0
17	6	312	CLA	1	0
17	A	804	CLA	5	0
20	L	206	BCR	2	0
25	G	102	LMG	2	0
17	4	608	CLA	4	0
17	3	308	CLA	3	0
17	b	816	CLA	6	0
17	a	844	CLA	7	0
17	B	837	CLA	8	0
20	a	852	BCR	3	0
17	3	313	CLA	1	0
17	a	842	CLA	6	0
17	A	818	CLA	7	0
17	B	806	CLA	4	0
20	l	201	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	101	CLA	2	0
17	B	812	CLA	3	0
17	7	611	CLA	1	0
19	2	618	LHG	3	0
20	3	318	BCR	2	0
20	b	845	BCR	4	0
17	a	827	CLA	4	0
17	b	820	CLA	1	0
17	6	315	CLA	4	0
20	7	617	BCR	13	0
17	1	306	CLA	3	0
17	6	313	CLA	3	0
17	4	610	CLA	4	0
27	1	316	LUT	8	0
17	b	802	CLA	7	0
17	L	204	CLA	2	0
17	2	608	CLA	4	0
17	a	822	CLA	1	0
17	A	816	CLA	3	0
17	9	603	CLA	1	0
20	B	846	BCR	4	0
17	b	834	CLA	2	0
17	b	808	CLA	6	0
17	b	819	CLA	2	0
17	3	303	CLA	2	0
17	g	101	CLA	1	0
18	b	842	PQN	1	0
17	B	817	CLA	7	0
17	a	829	CLA	9	0
20	6	319	BCR	7	0
17	b	810	CLA	4	0
17	4	602	CLA	3	0
17	B	824	CLA	2	0
17	A	823	CLA	1	0
17	a	835	CLA	1	0
17	3	314	CLA	3	0
17	a	837	CLA	1	0
17	1	313	CLA	8	0
17	A	836	CLA	3	0
17	6	316	CLA	1	0
17	A	834	CLA	4	0
20	j	3004	BCR	4	0

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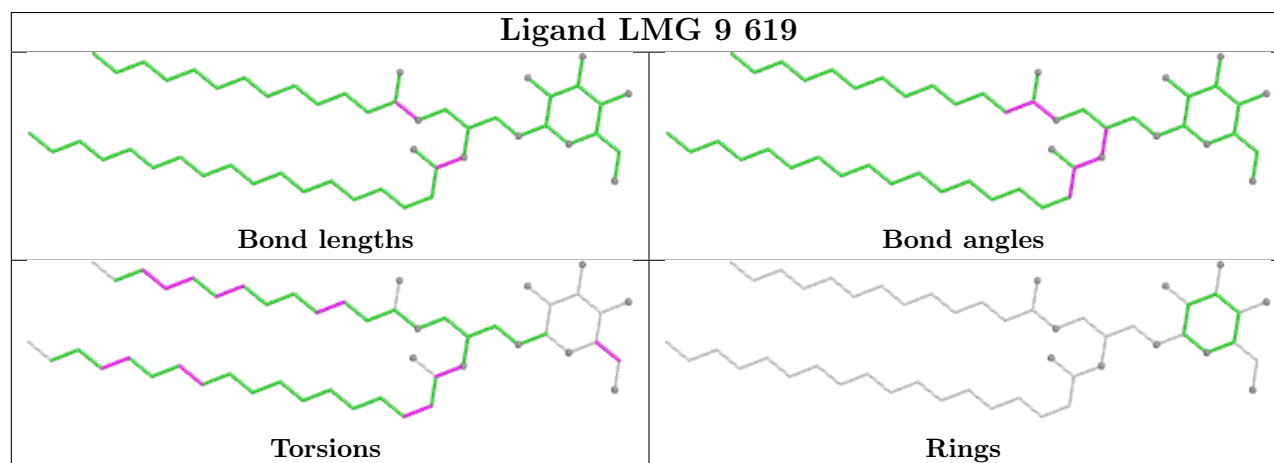
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	9	615	CHL	1	0
17	3	312	CLA	2	0
19	1	319	LHG	3	0
17	1	314	CLA	3	0
17	a	836	CLA	2	0
17	8	308	CLA	6	0
17	A	815	CLA	2	0
17	b	803	CLA	7	0
17	6	307	CLA	3	0
17	B	810	CLA	2	0
17	2	602	CLA	4	0
17	a	809	CLA	4	0
17	b	807	CLA	4	0
17	1	303	CLA	2	0
17	8	310	CLA	2	0
17	3	301	CLA	1	0
20	A	852	BCR	5	0
17	B	827	CLA	7	0
28	7	616	XAT	5	0
17	9	612	CLA	2	0
17	G	104	CLA	3	0
25	4	620	LMG	4	0
17	6	305	CLA	3	0
20	8	316	BCR	5	0
20	a	854	BCR	4	0
17	b	840	CLA	4	0
20	b	848	BCR	4	0
20	B	843	BCR	6	0
17	a	828	CLA	2	0
17	K	4002	CLA	3	0
17	B	821	CLA	2	0
17	B	808	CLA	4	0
17	B	815	CLA	7	0
17	A	825	CLA	5	0
17	2	604	CLA	7	0
17	1	311	CLA	2	0
17	B	840	CLA	4	0
17	a	824	CLA	4	0
17	a	825	CLA	1	0
18	B	842	PQN	2	0
17	7	602	CLA	3	0
17	9	614	CLA	2	0

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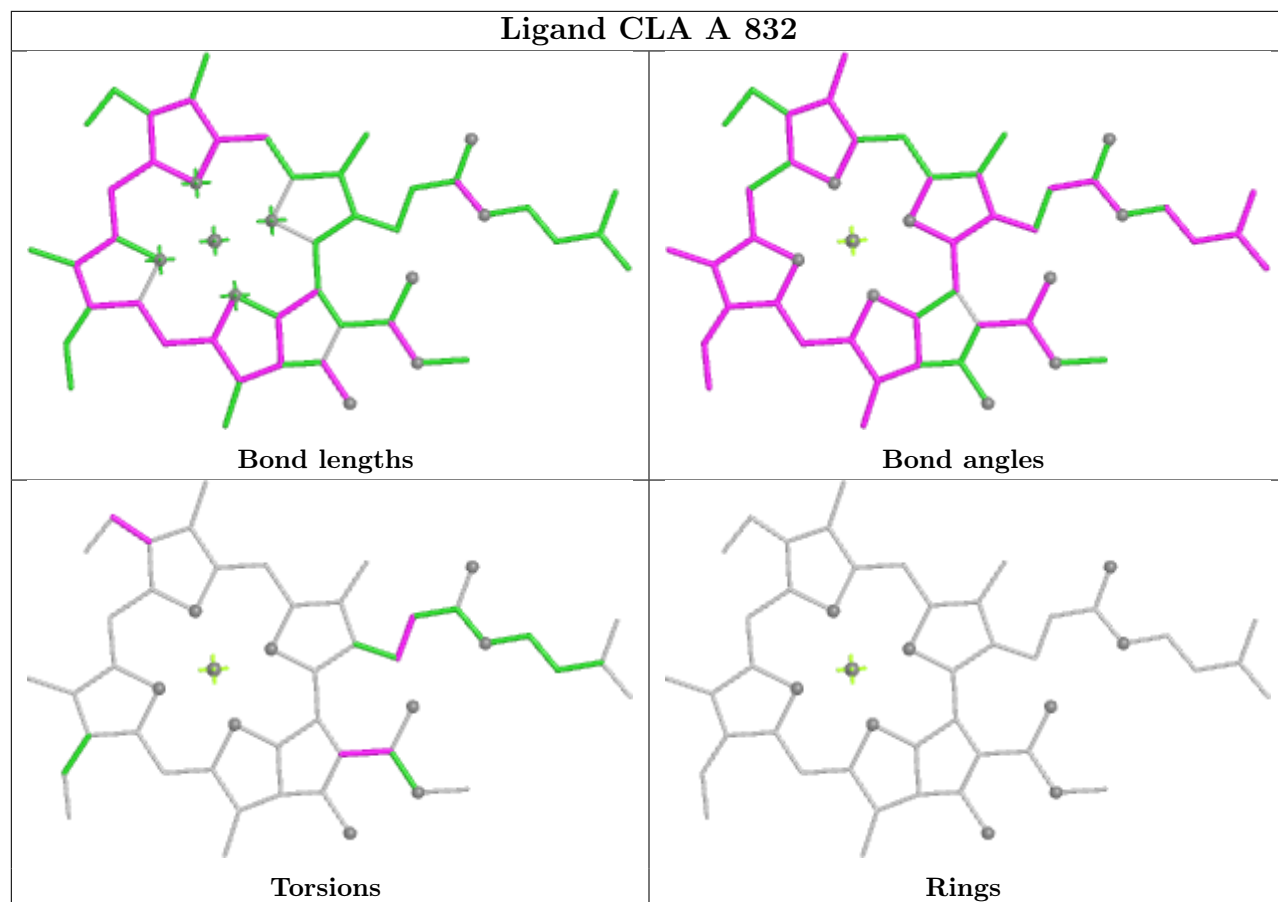
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	805	CLA	7	0
17	A	817	CLA	2	0
17	A	827	CLA	4	0
19	3	319	LHG	1	0
20	4	618	BCR	8	0
17	6	304	CLA	2	0
17	8	312	CLA	1	0
17	b	818	CLA	5	0
17	b	825	CLA	9	0
27	2	615	LUT	5	0
17	a	841	CLA	8	0

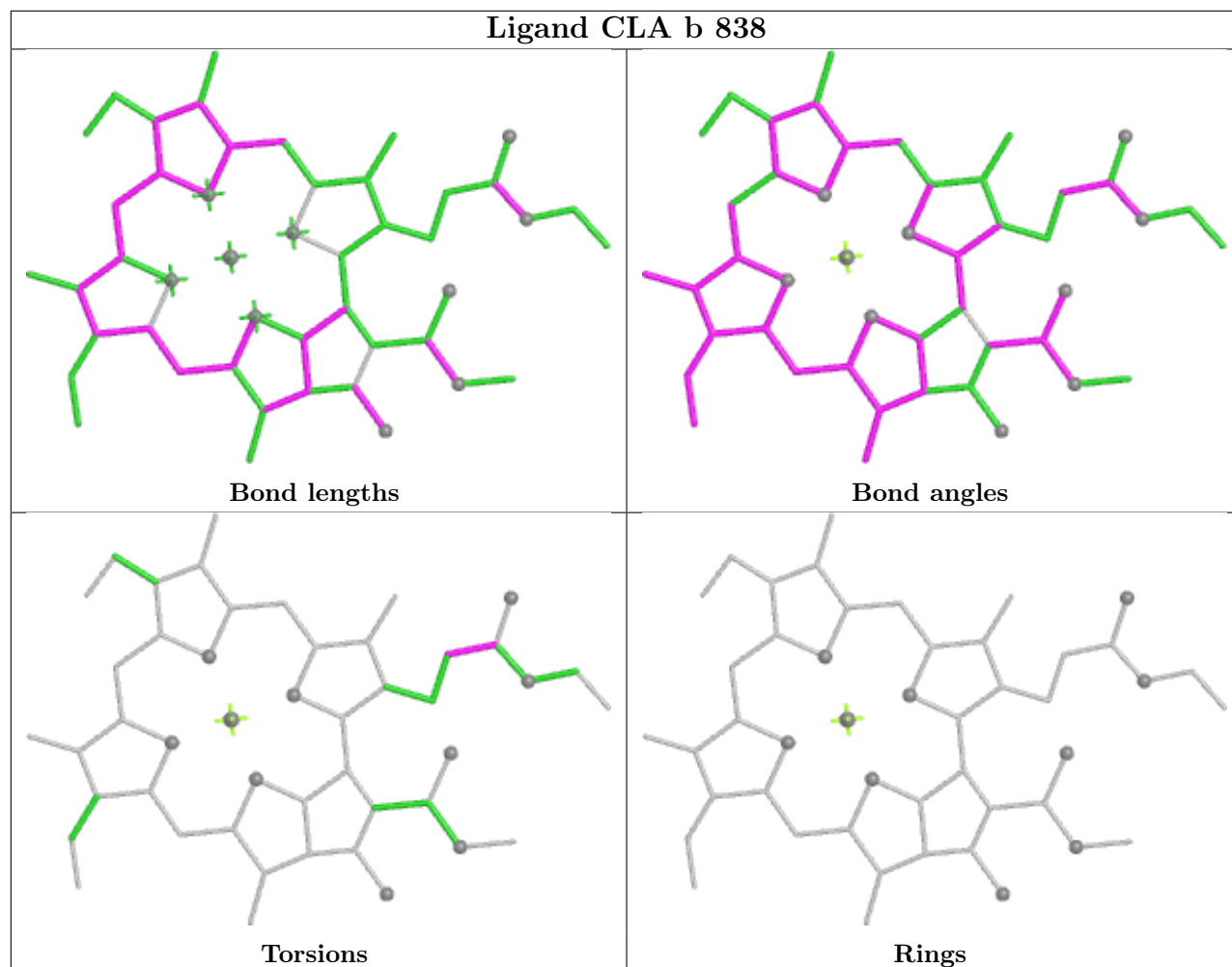
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



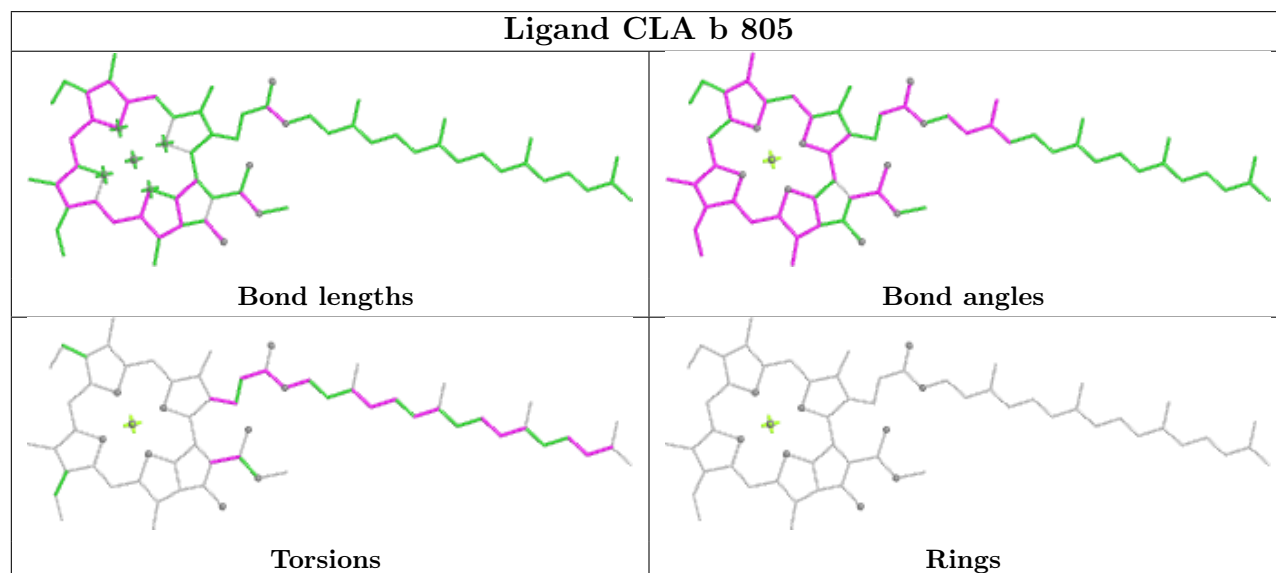
Ligand CLA A 832



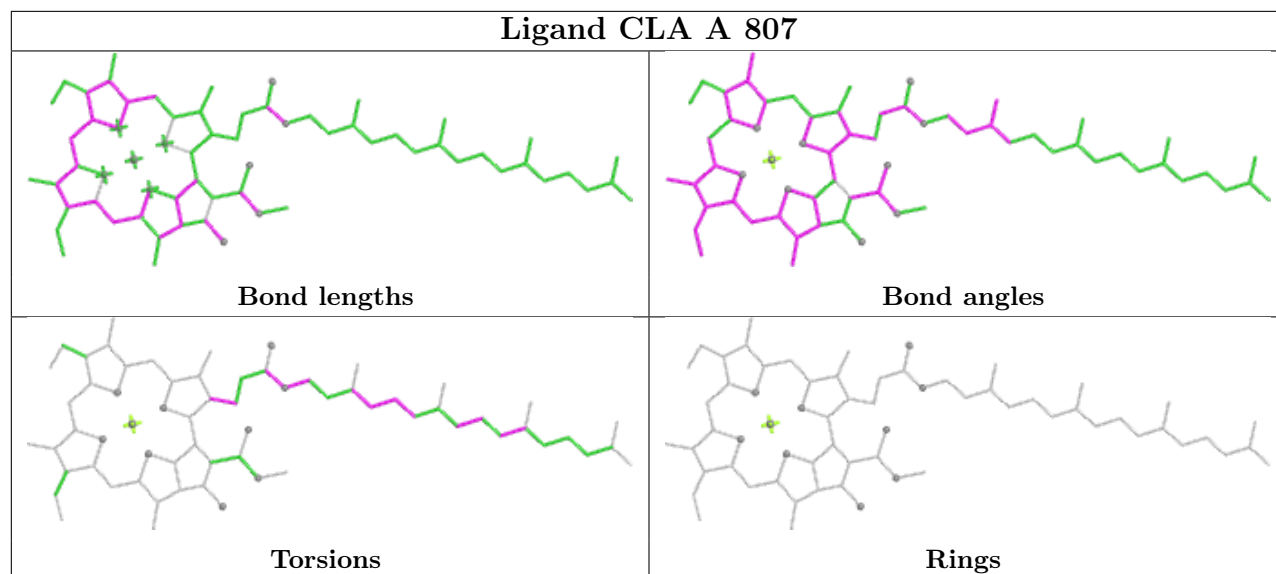
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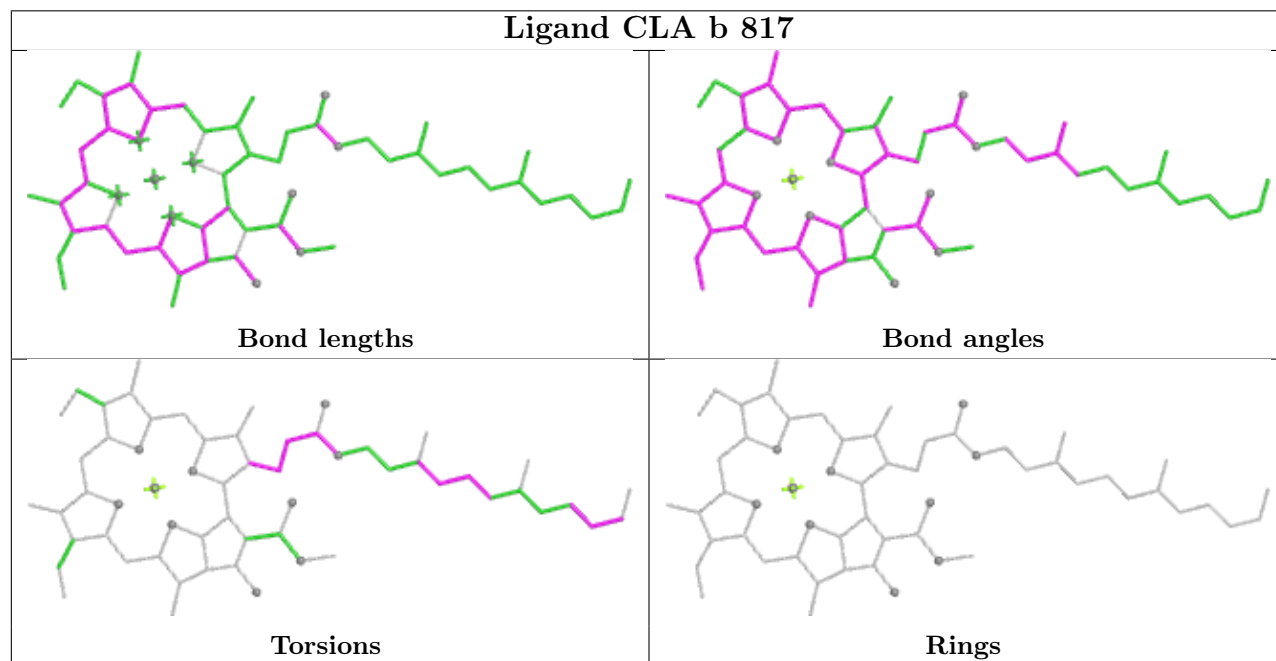
Ligand CLA b 805

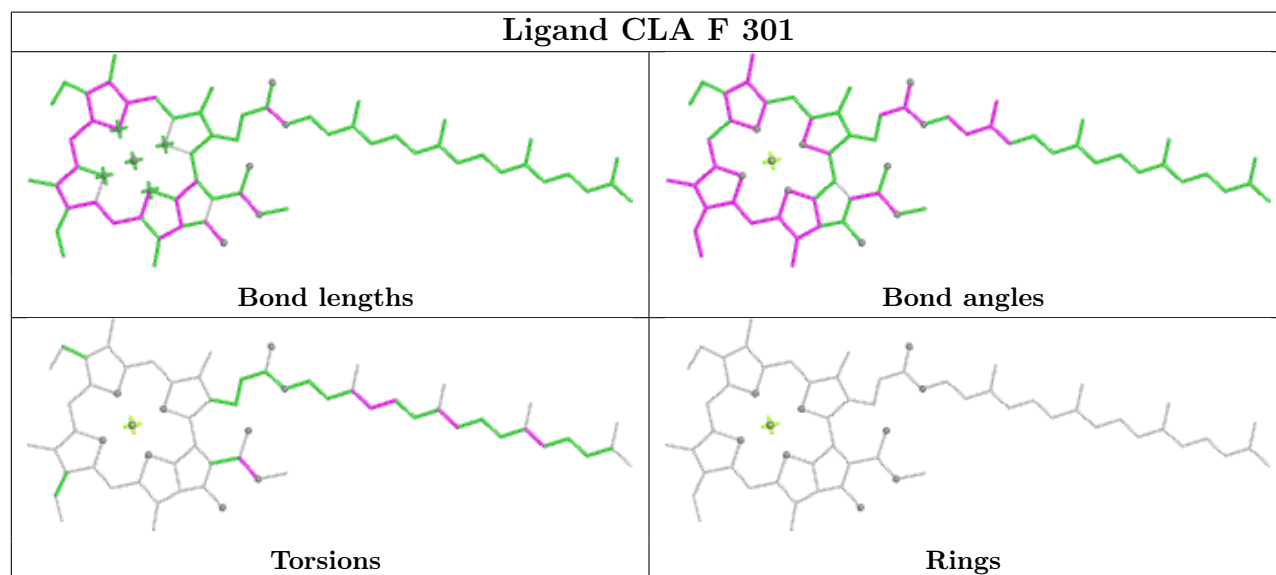
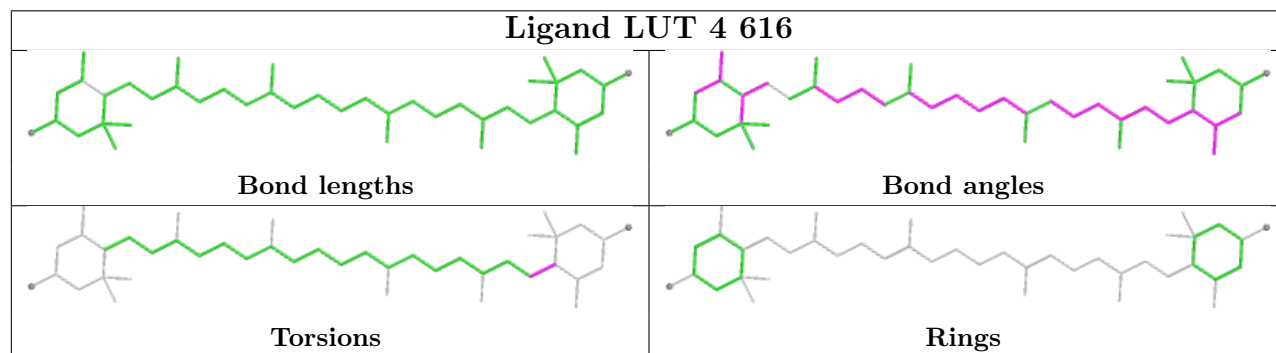
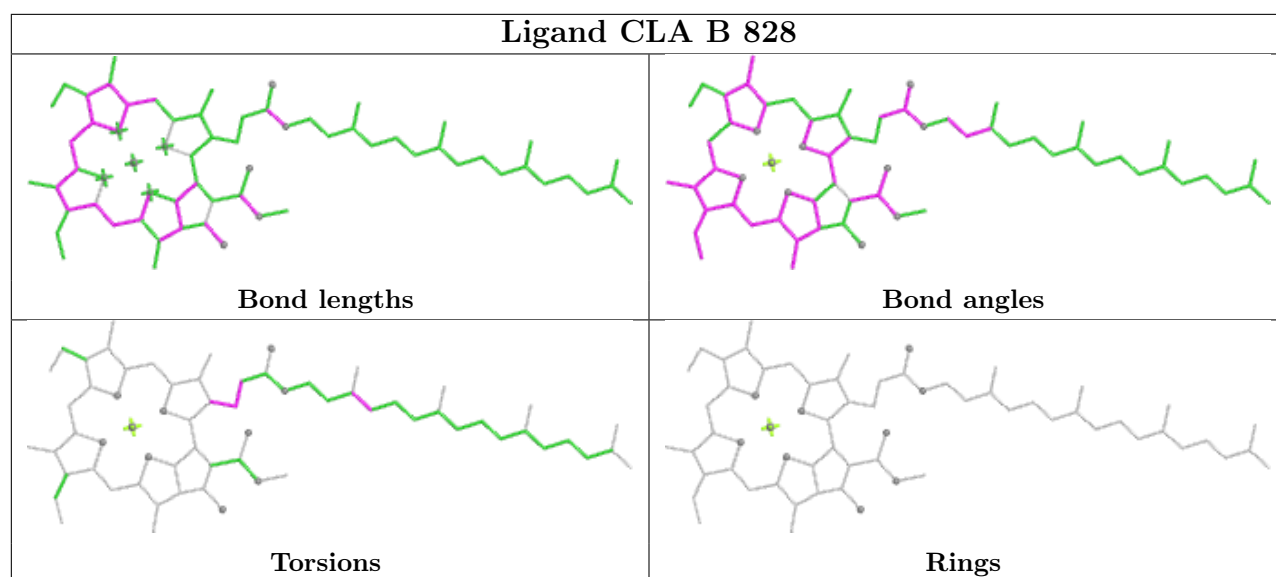


Ligand CLA A 807

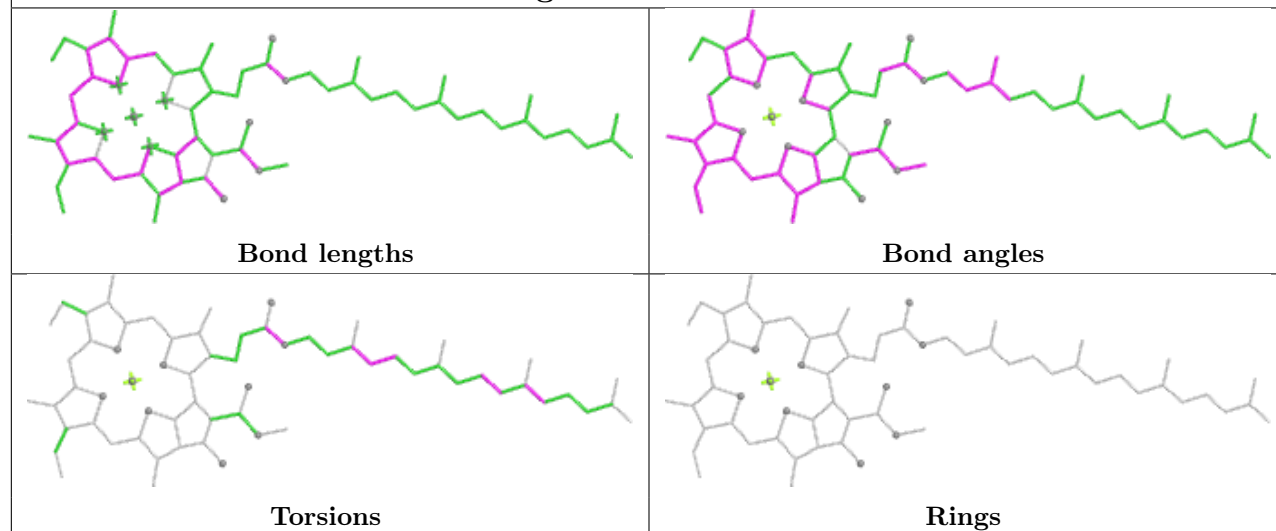


Ligand CLA b 817

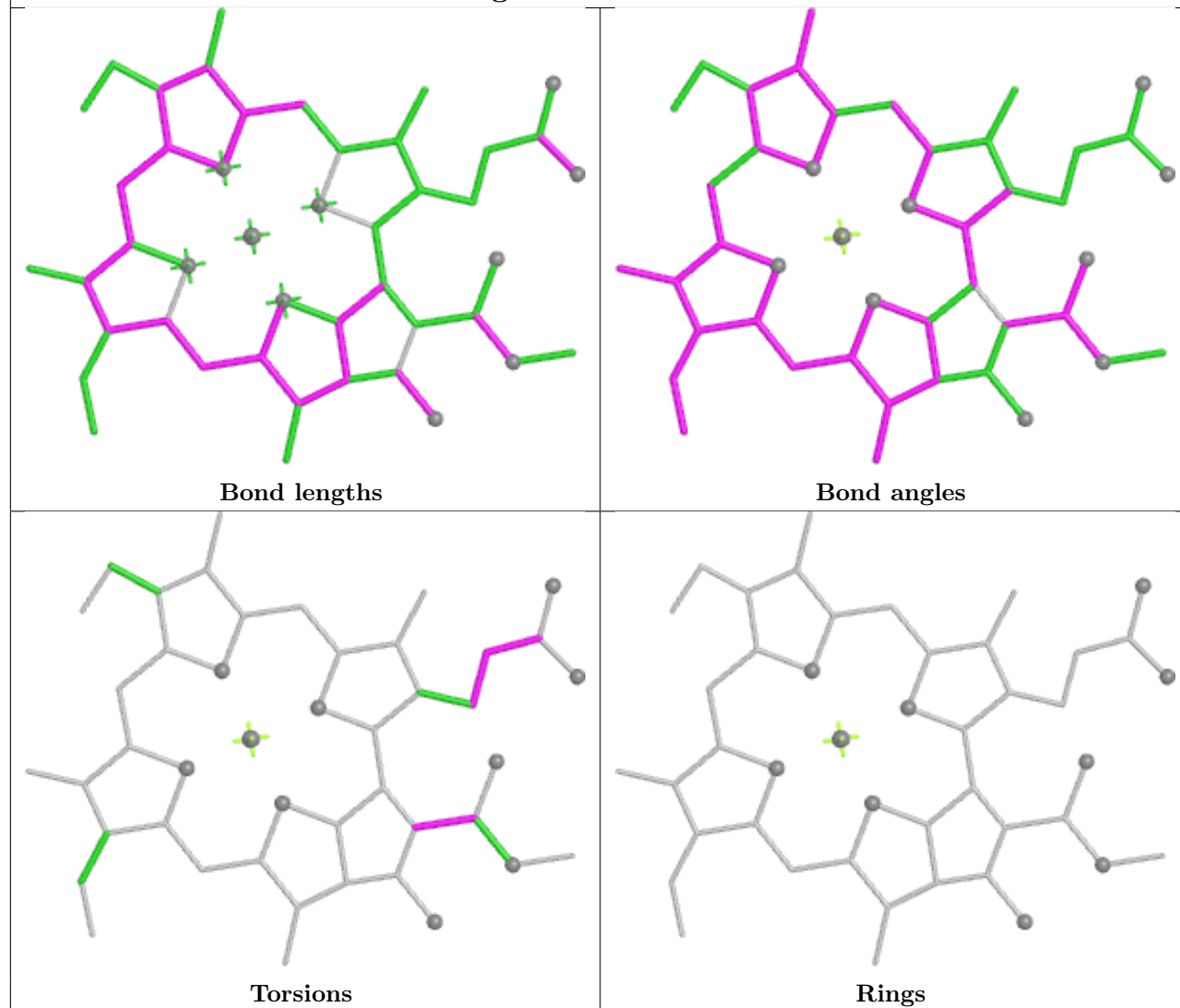


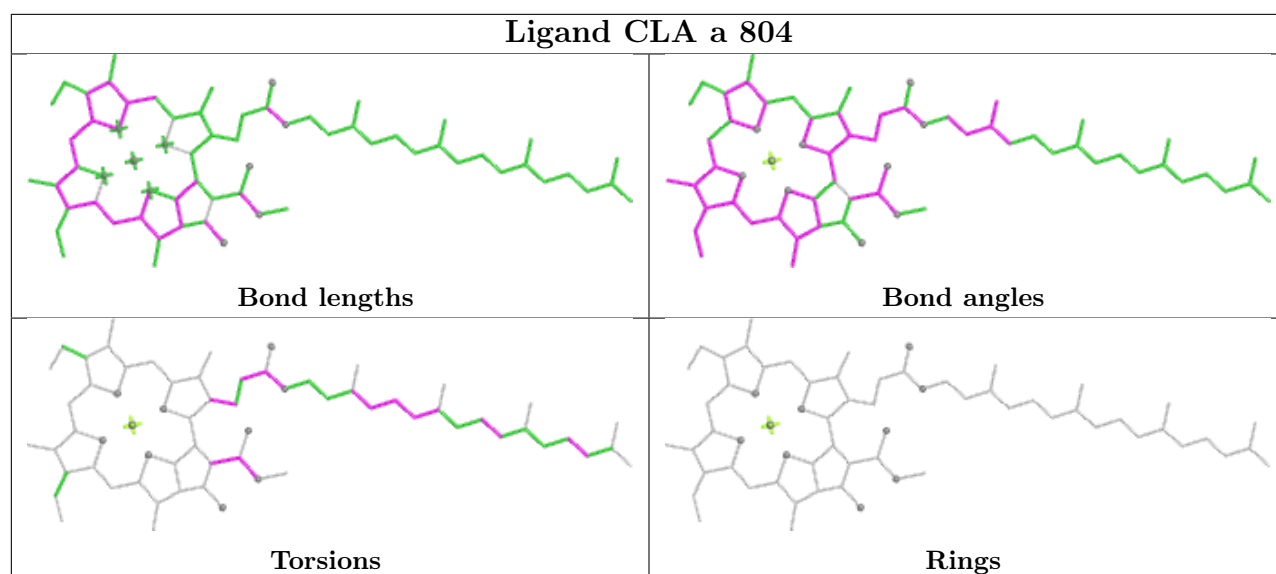
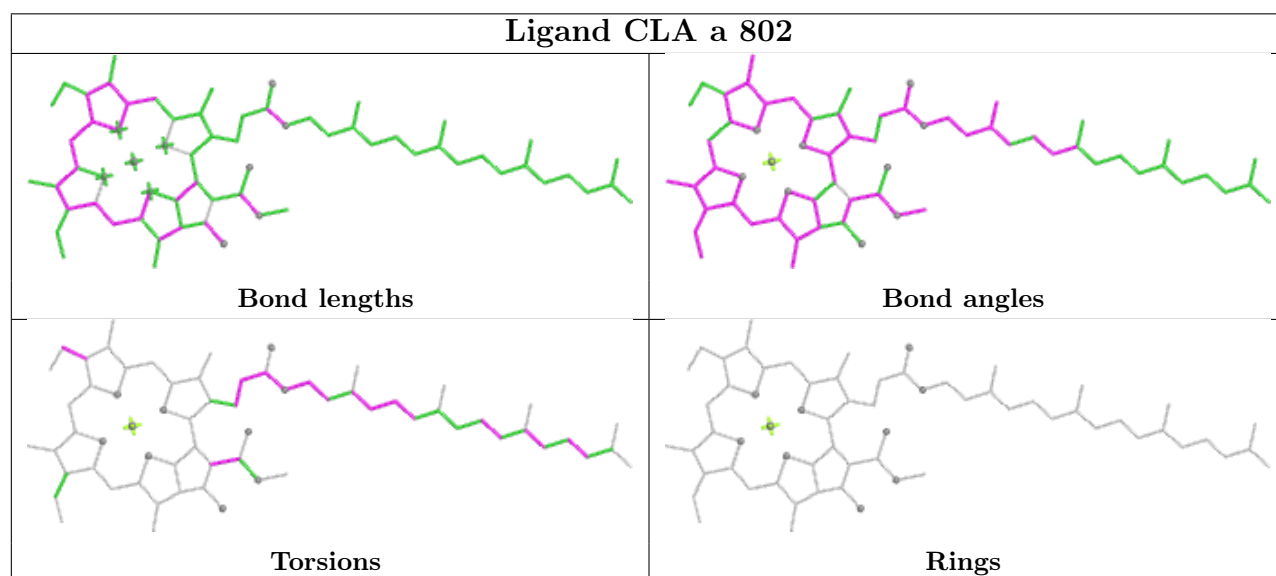
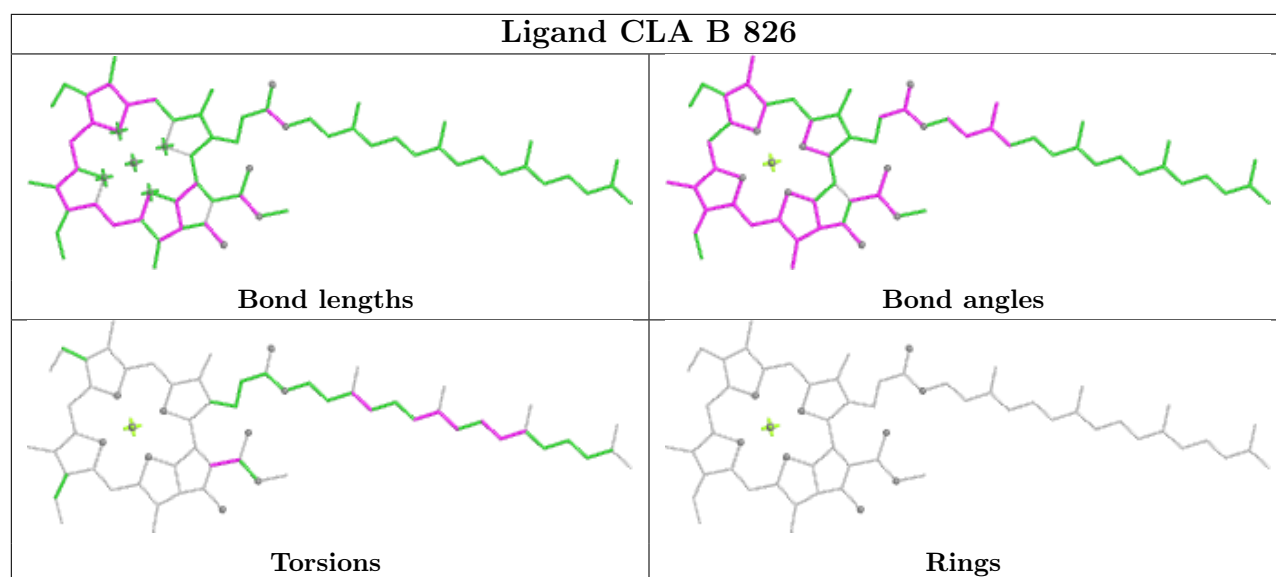


Ligand CLA 6 310

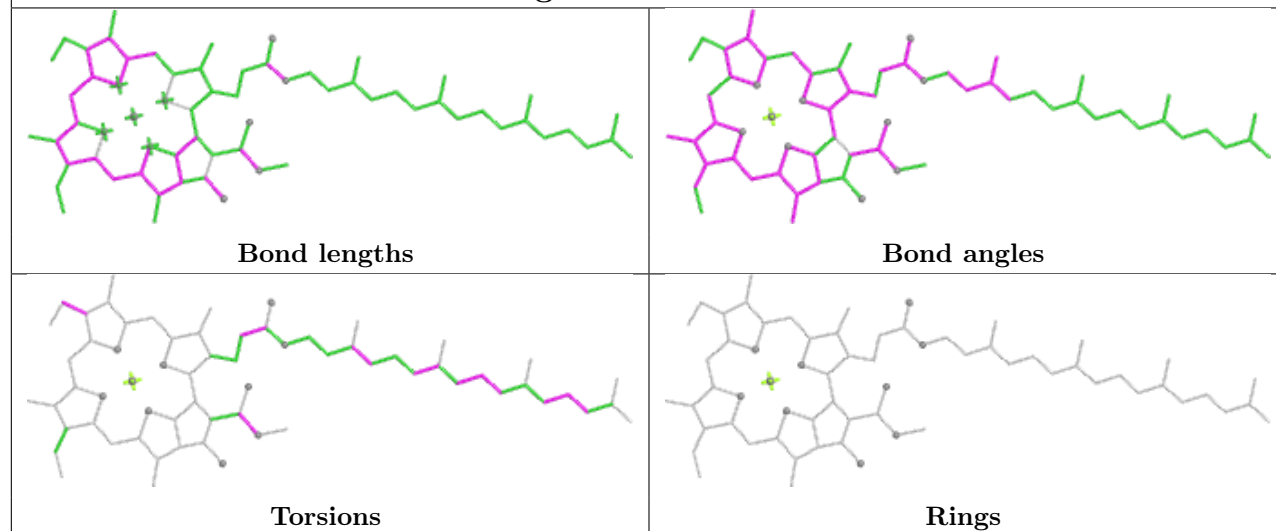


Ligand CLA A 837

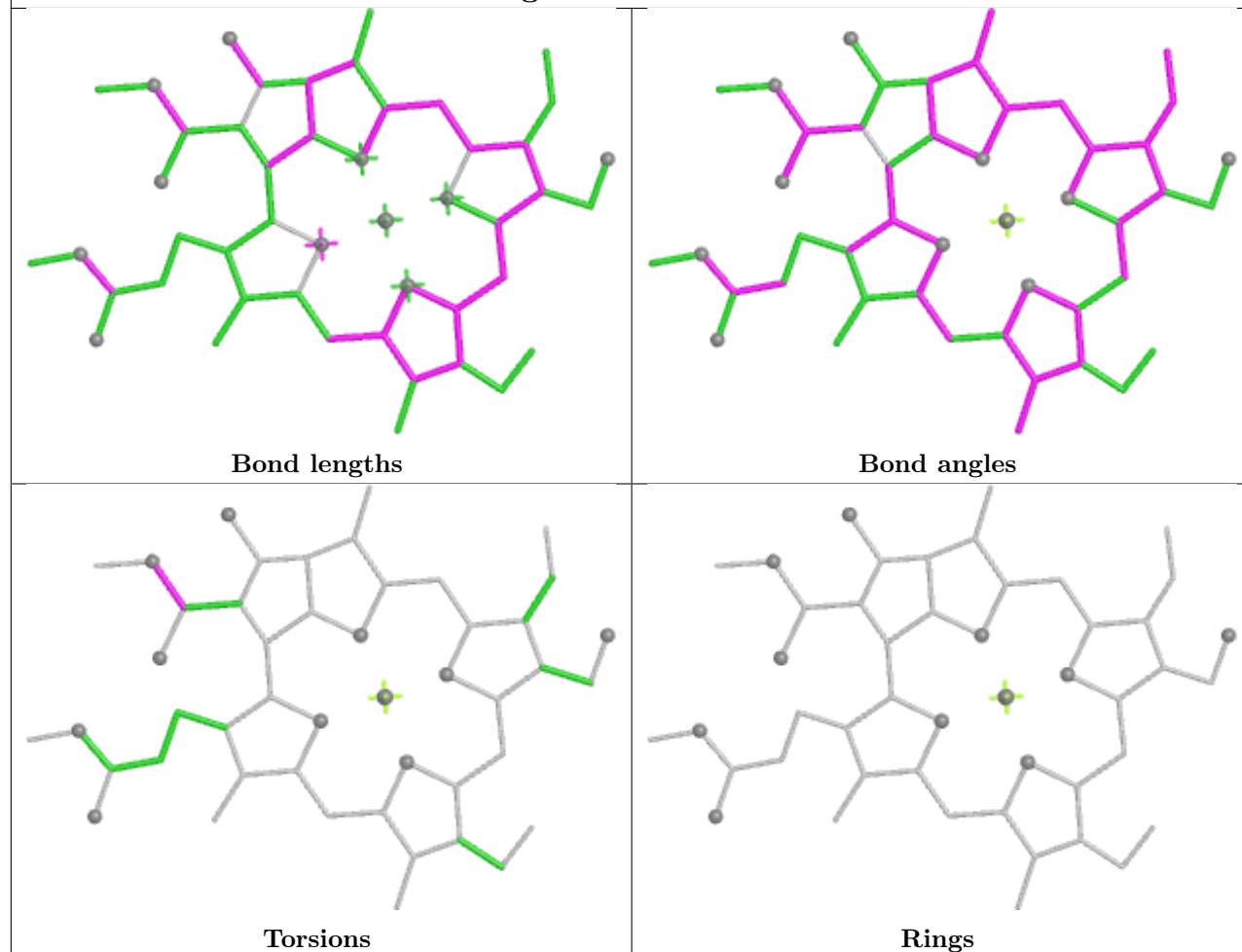




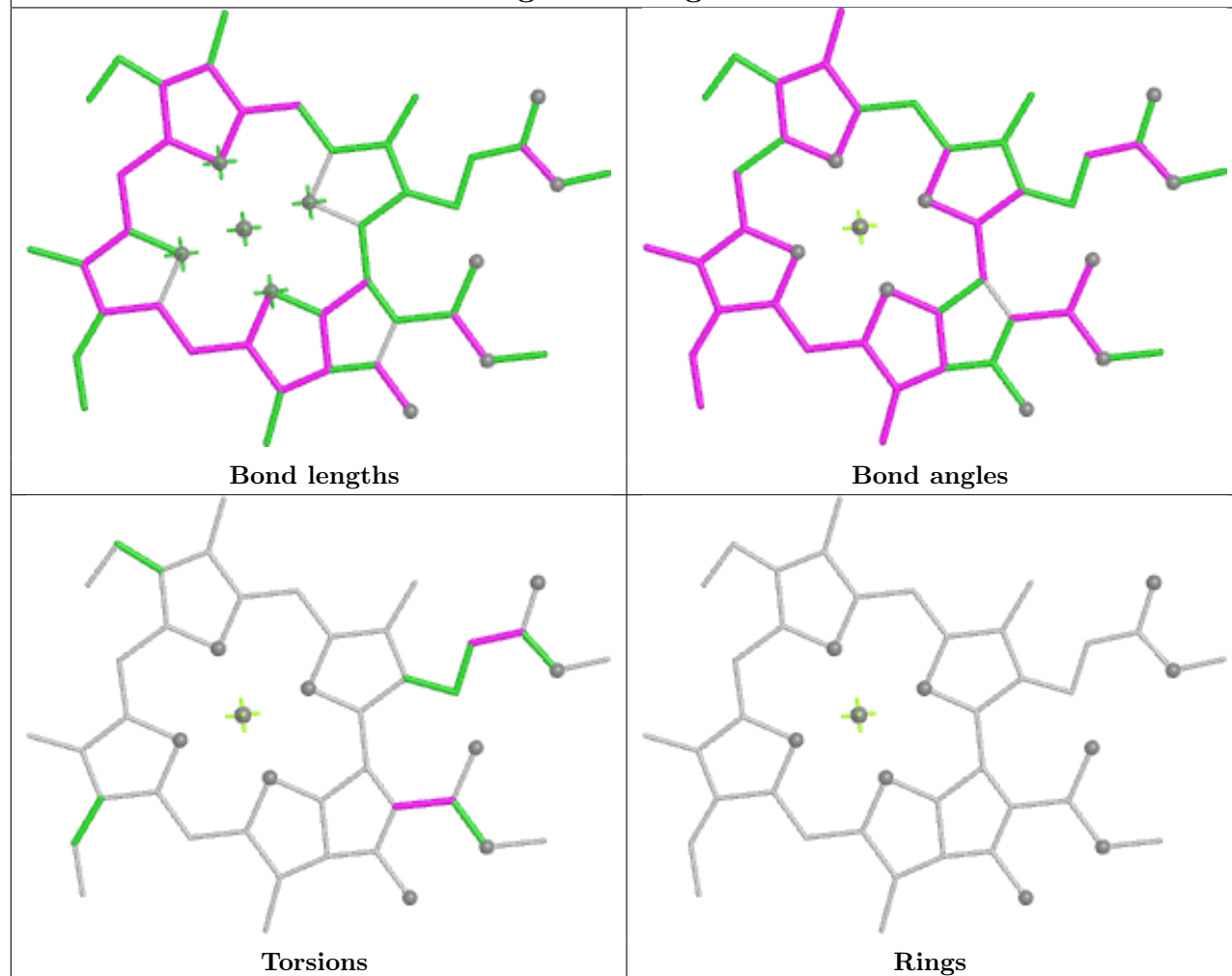
Ligand CLA b 832



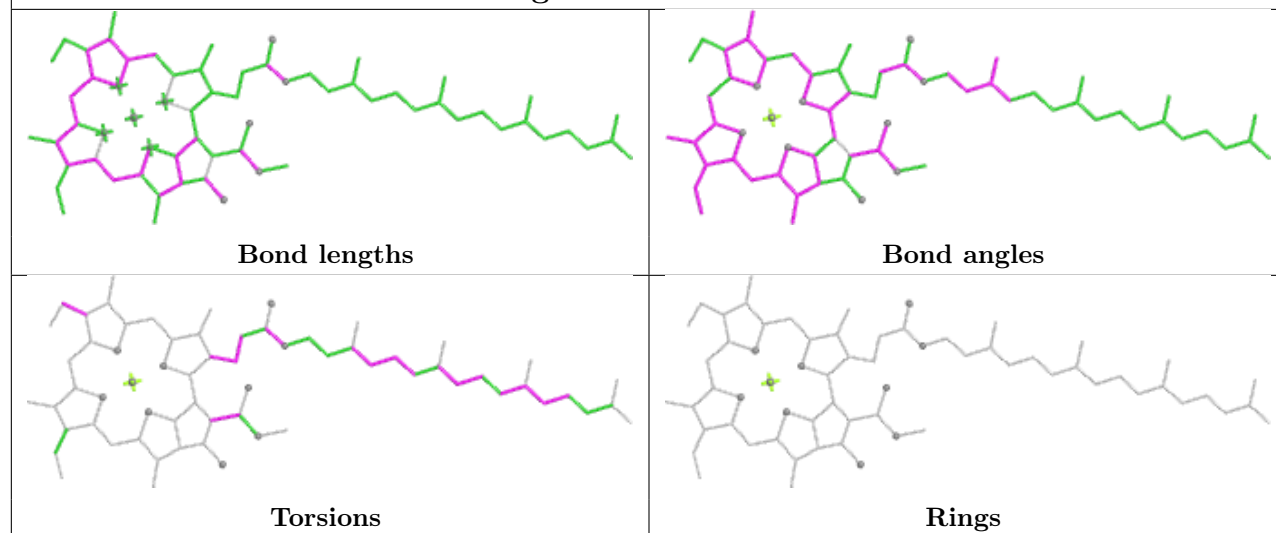
Ligand CHL 3 307



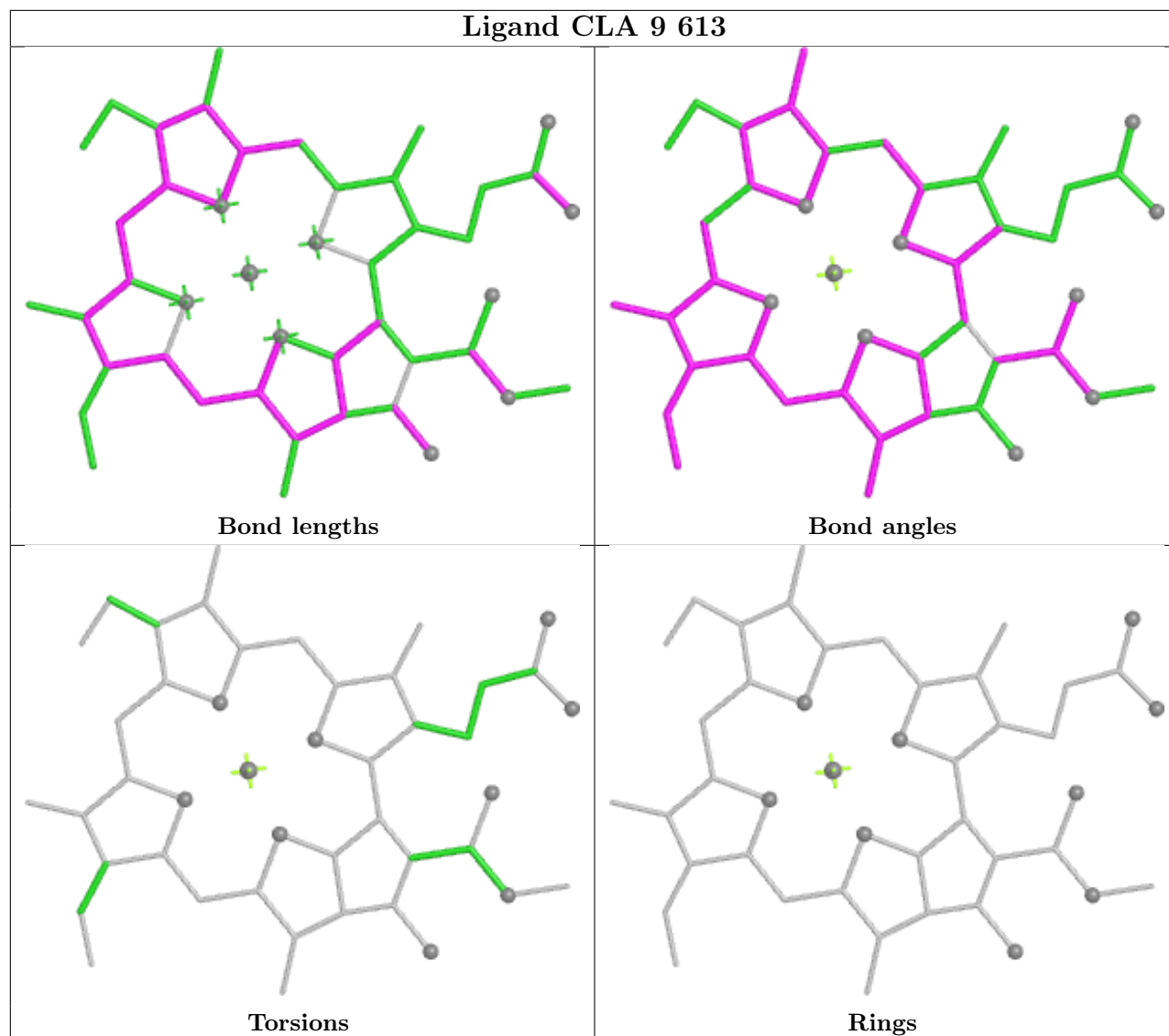
Ligand CLA g 103



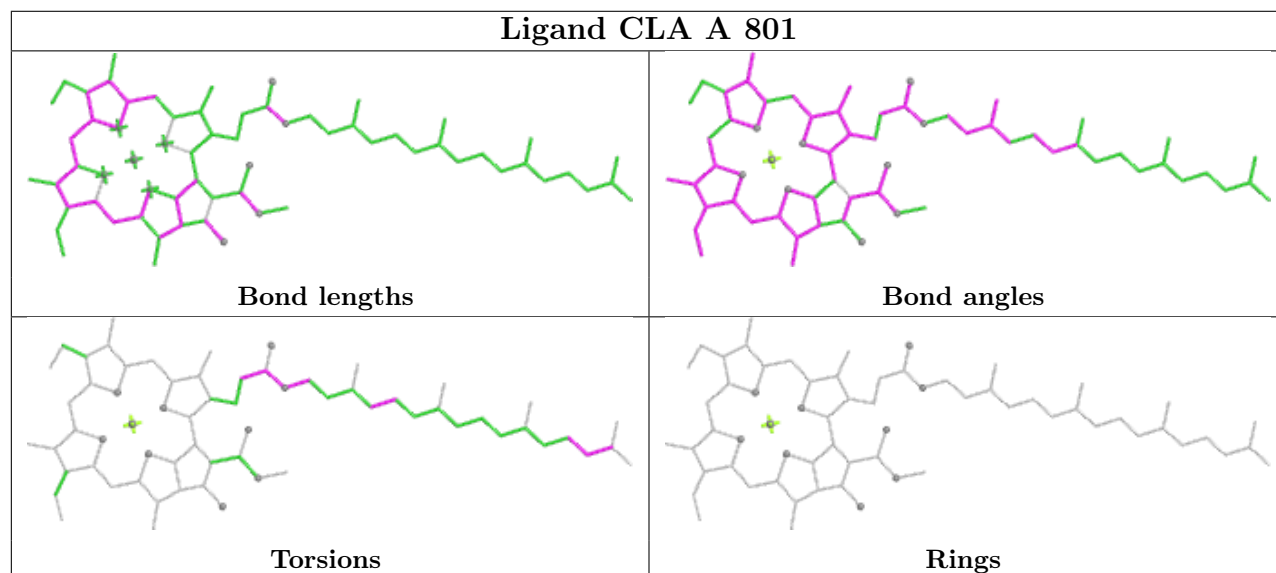
Ligand CLA A 809



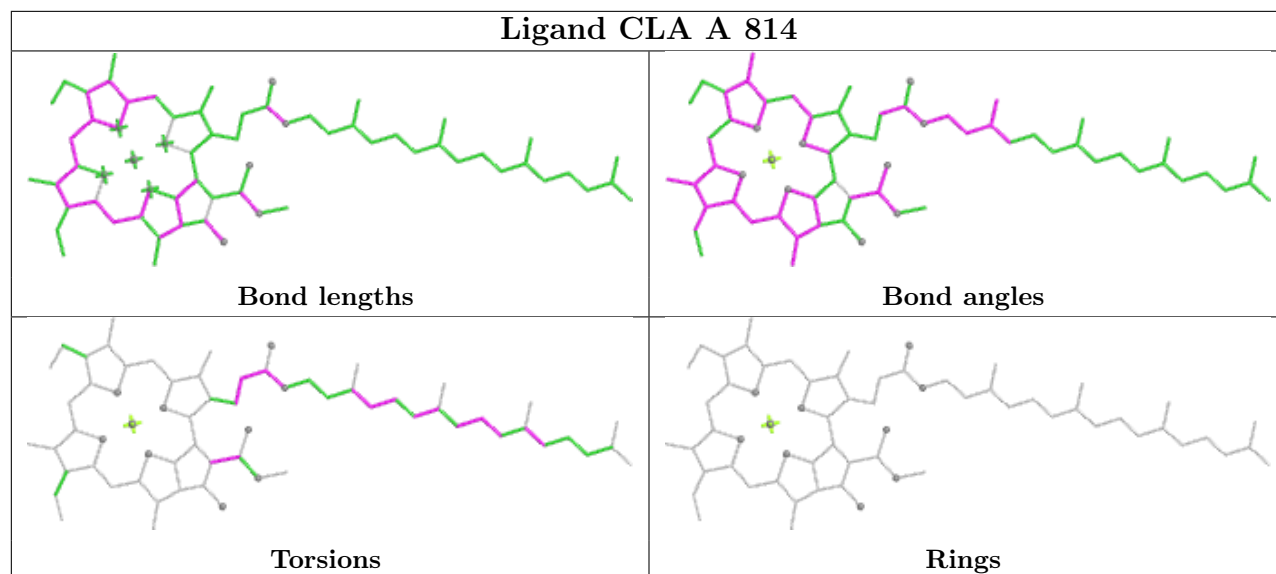
Ligand CLA 9 613



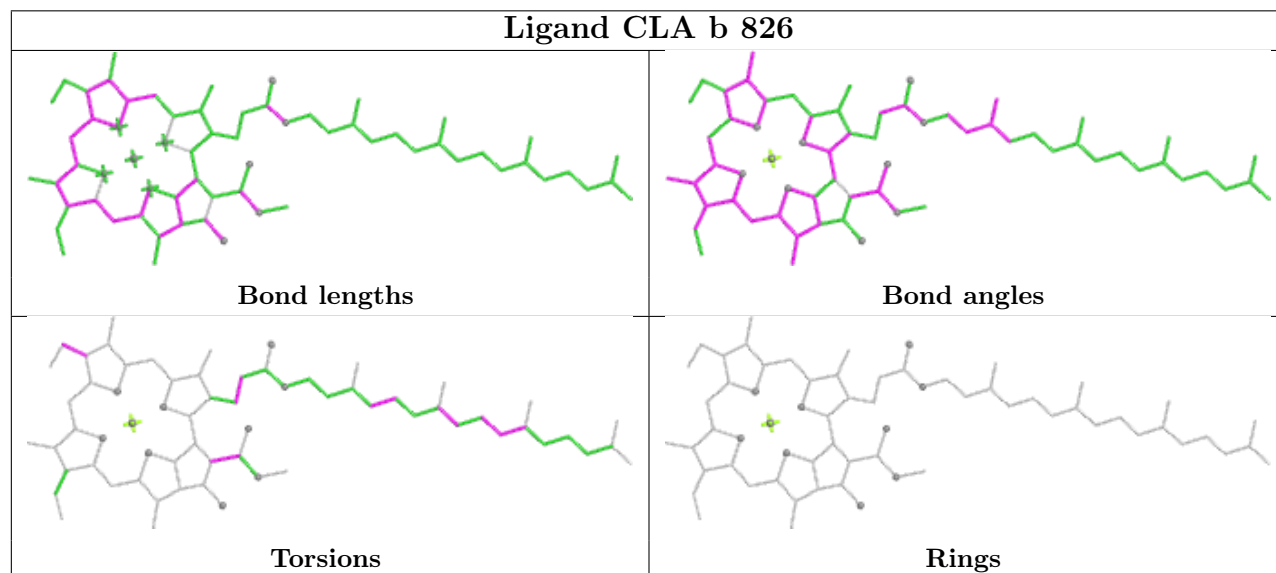
Ligand CLA A 801



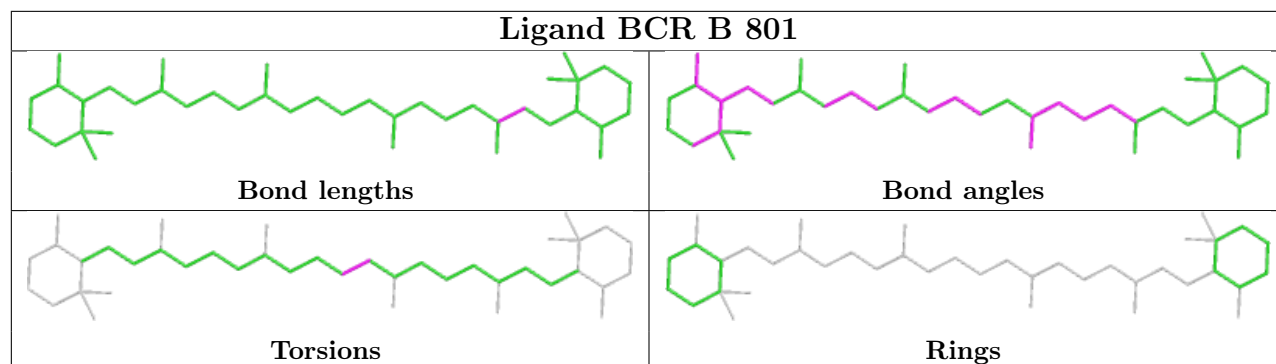
Ligand CLA A 814



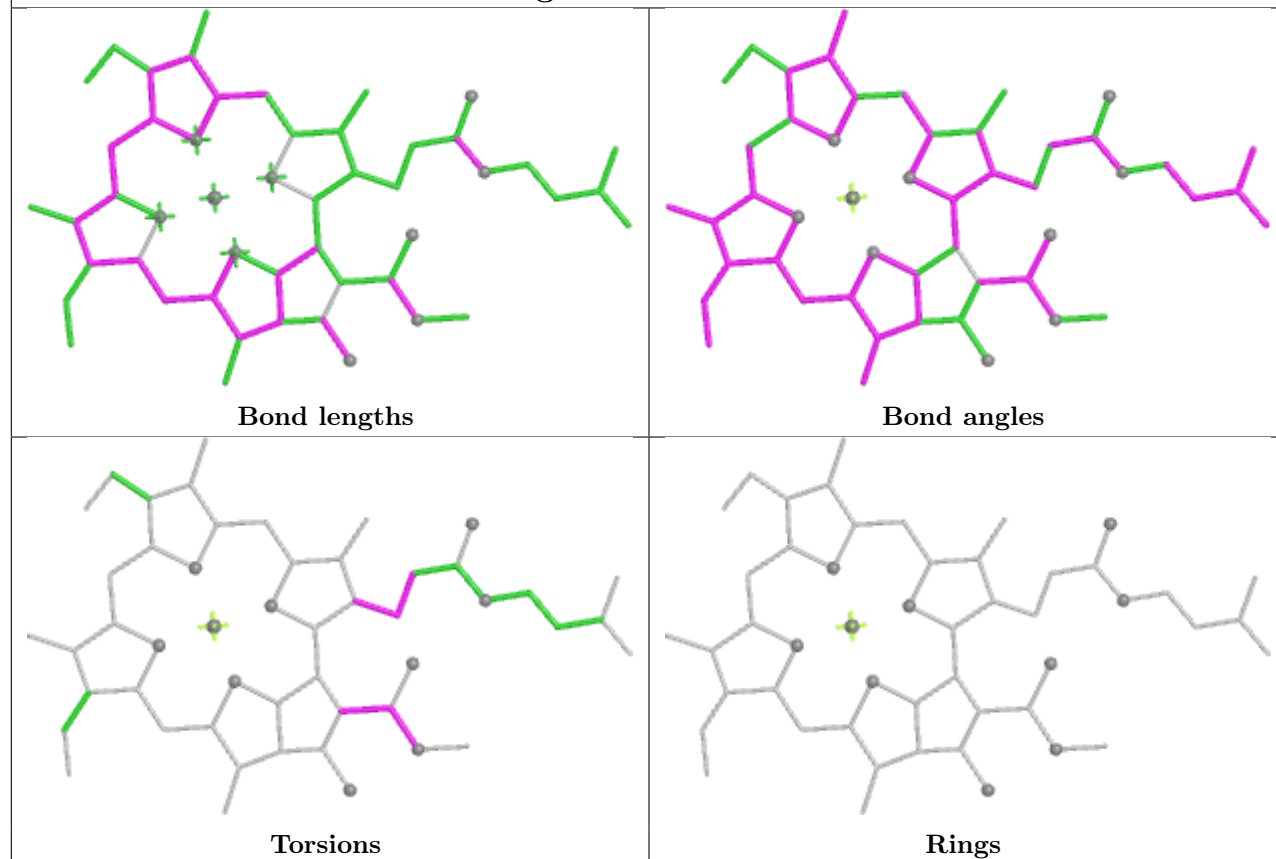
Ligand CLA b 826



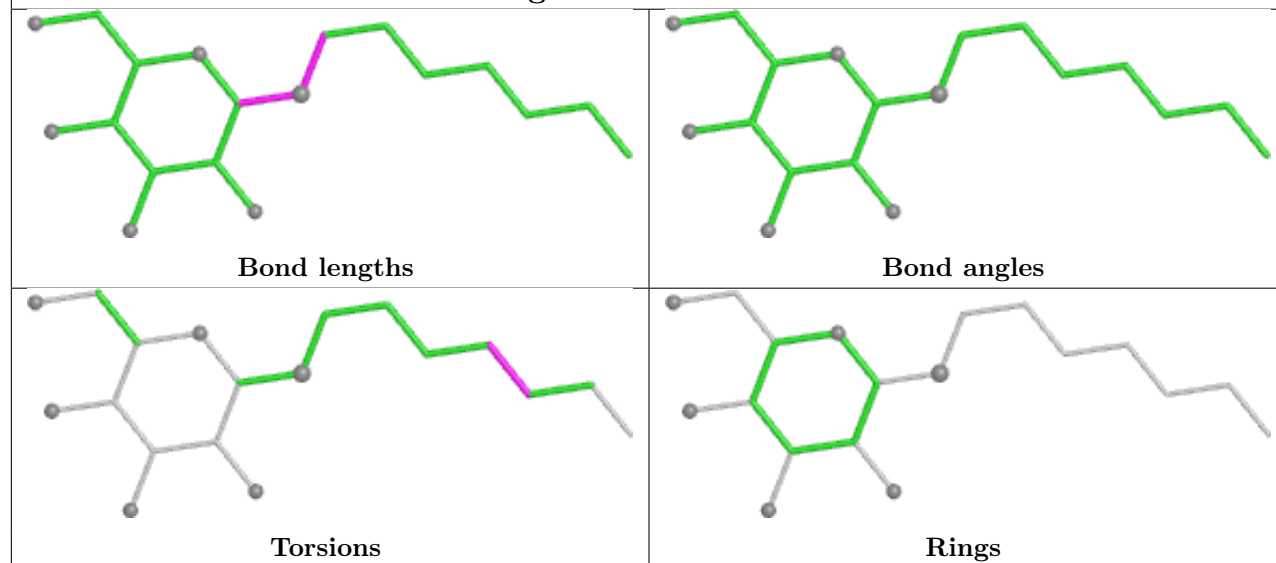
Ligand BCR B 801



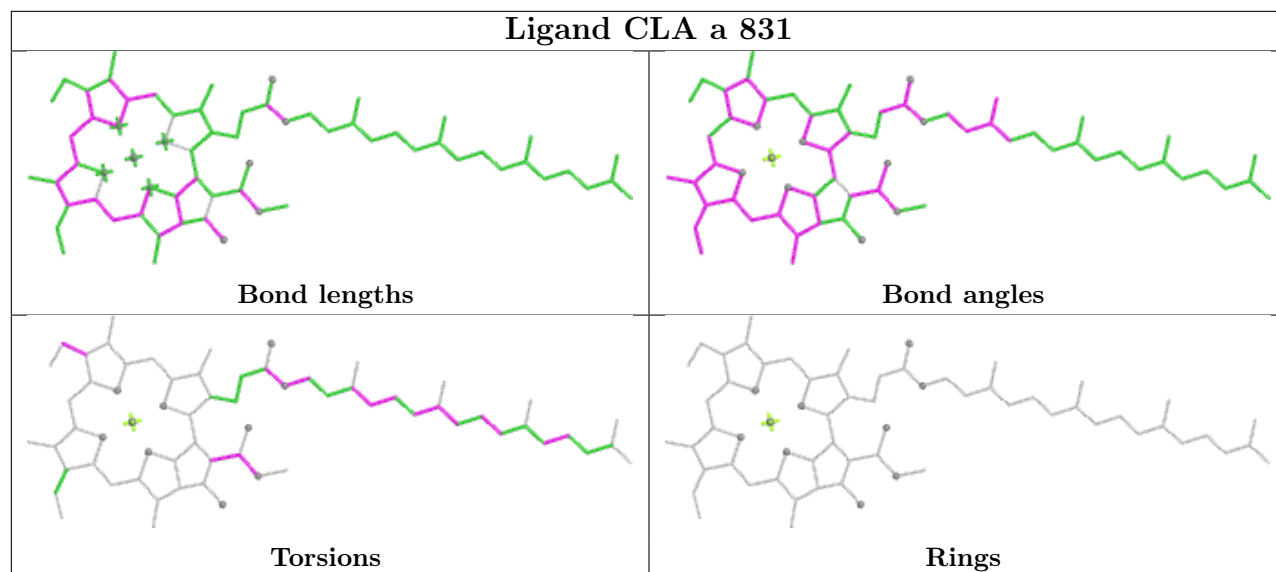
Ligand CLA 4 604



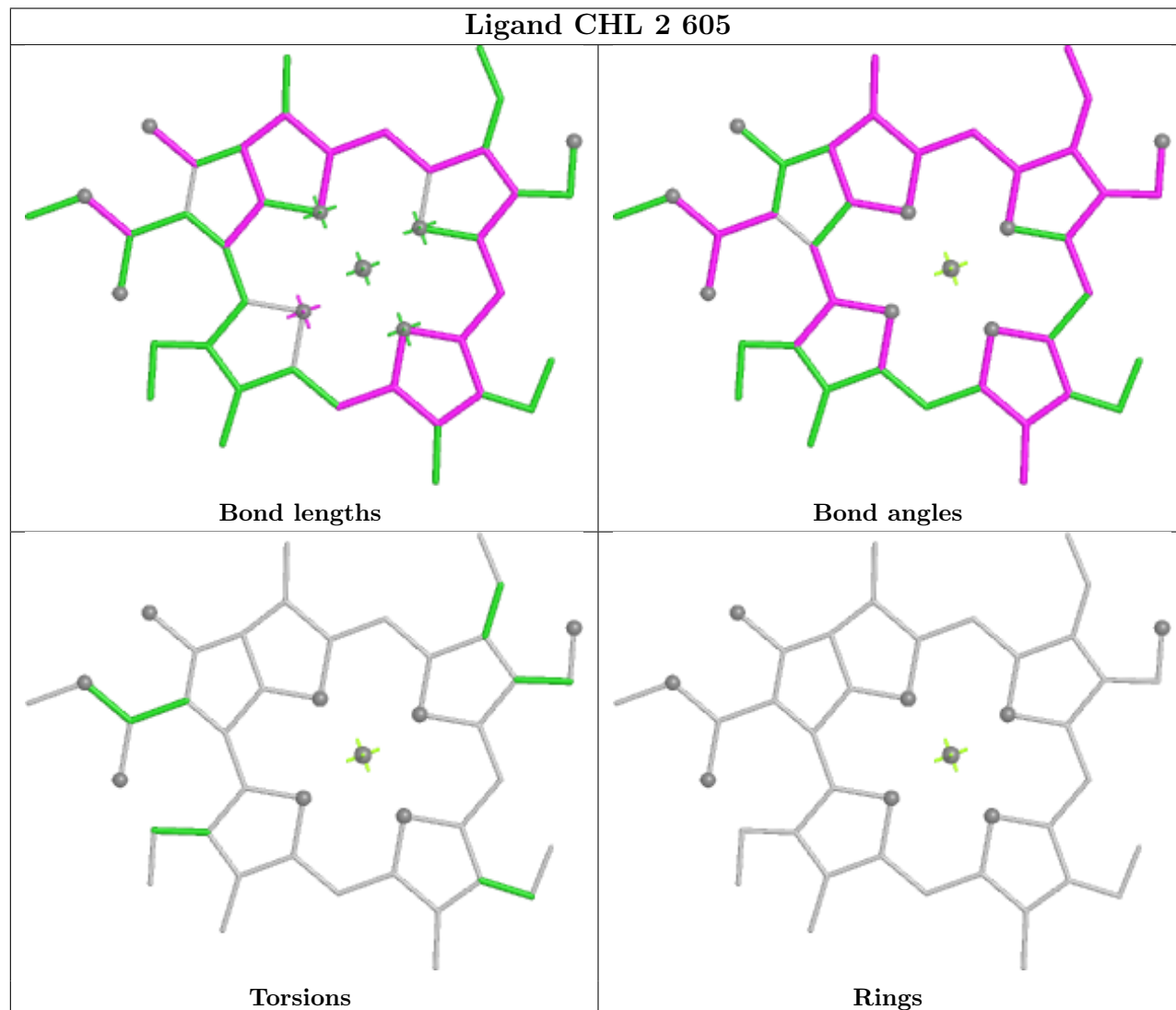
Ligand HTG A 855



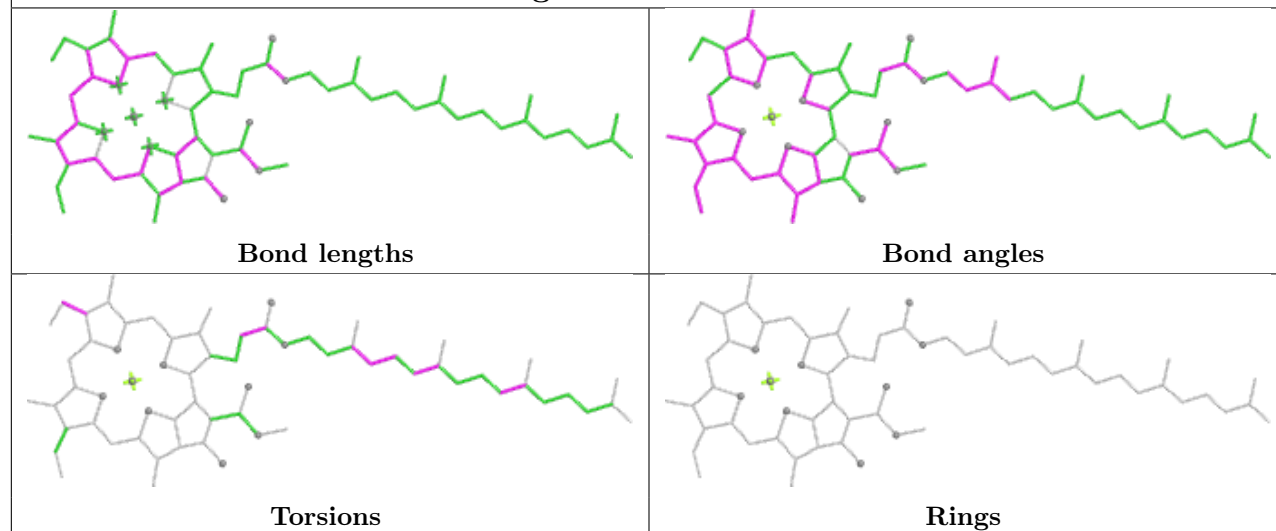
Ligand CLA a 831



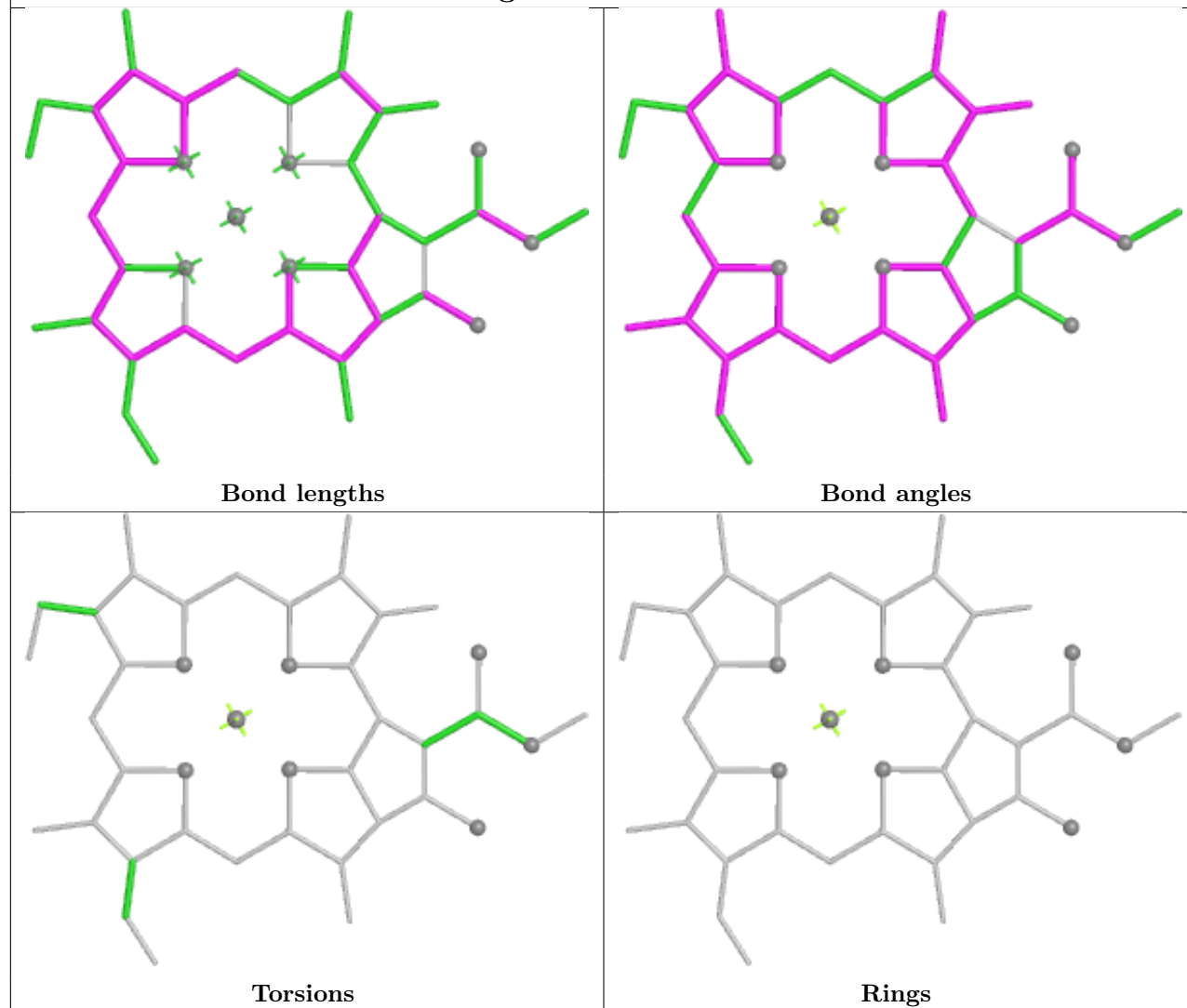
Ligand CHL 2 605



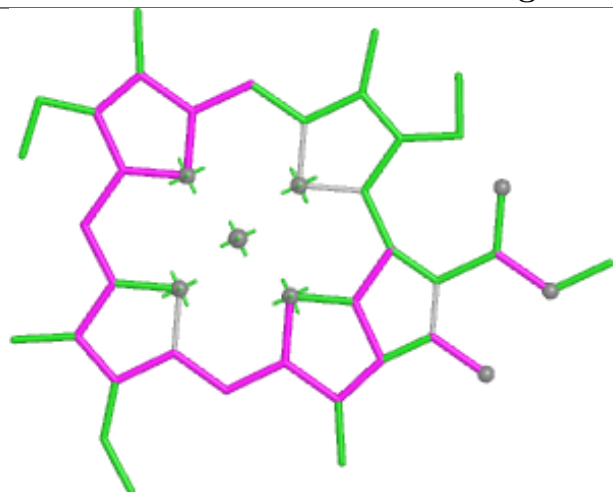
Ligand CLA B 809



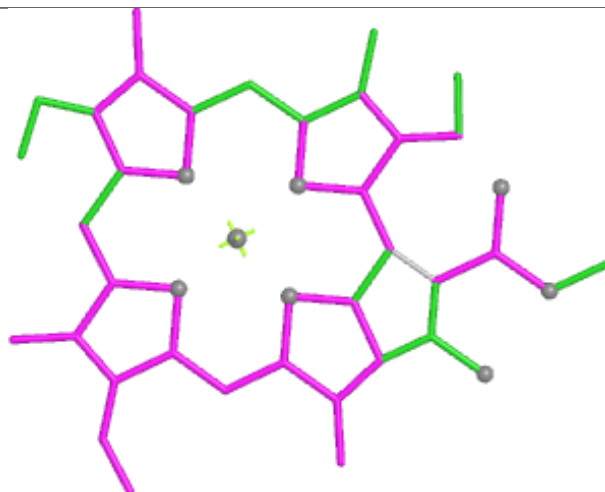
Ligand CLA 7 610



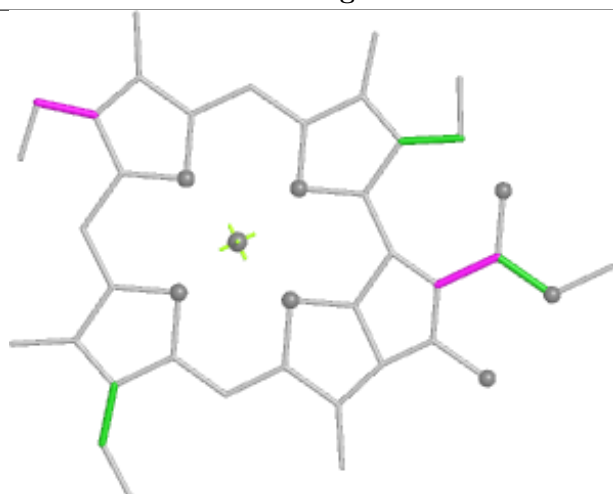
Ligand CLA 3 305



Bond lengths



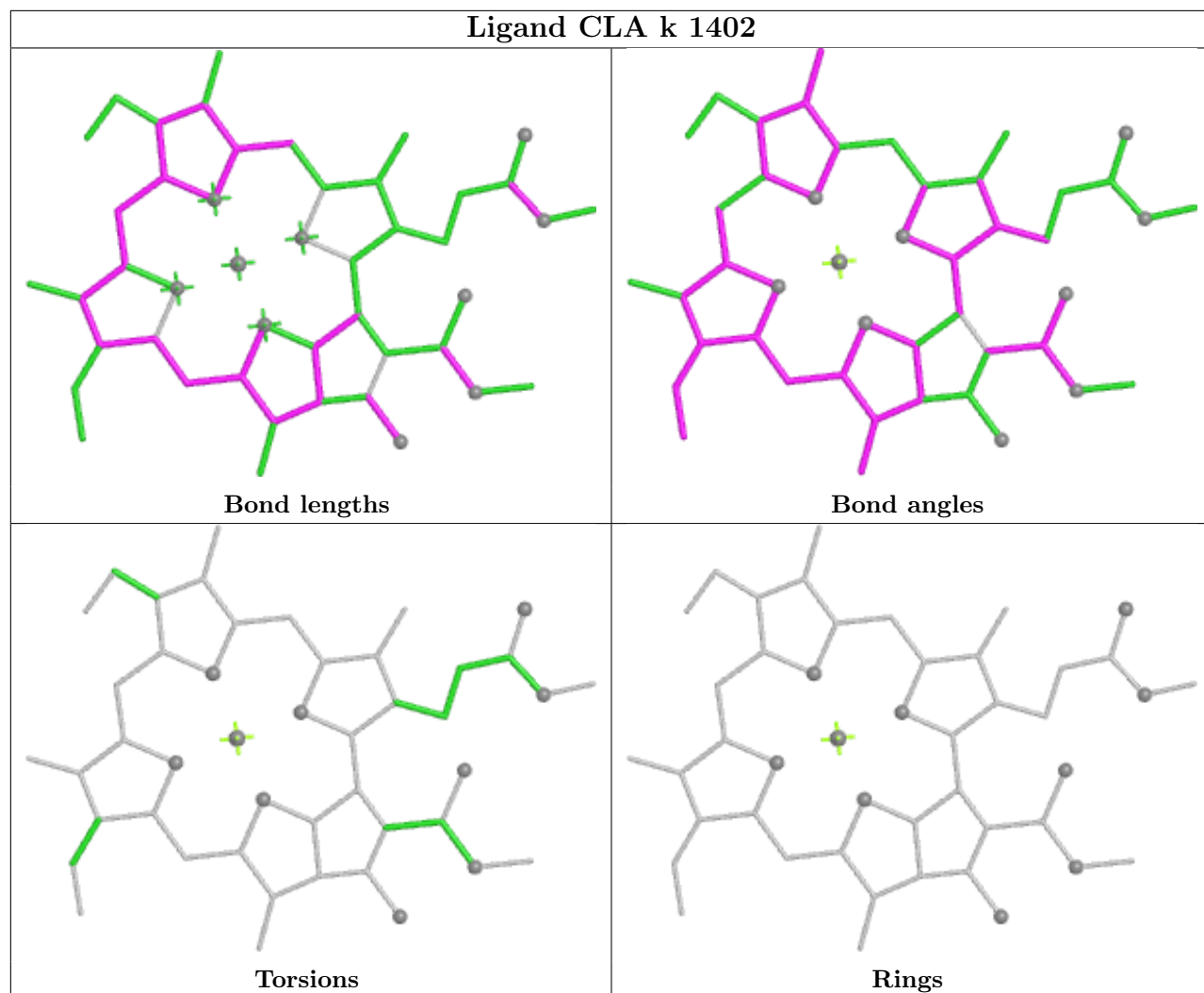
Bond angles



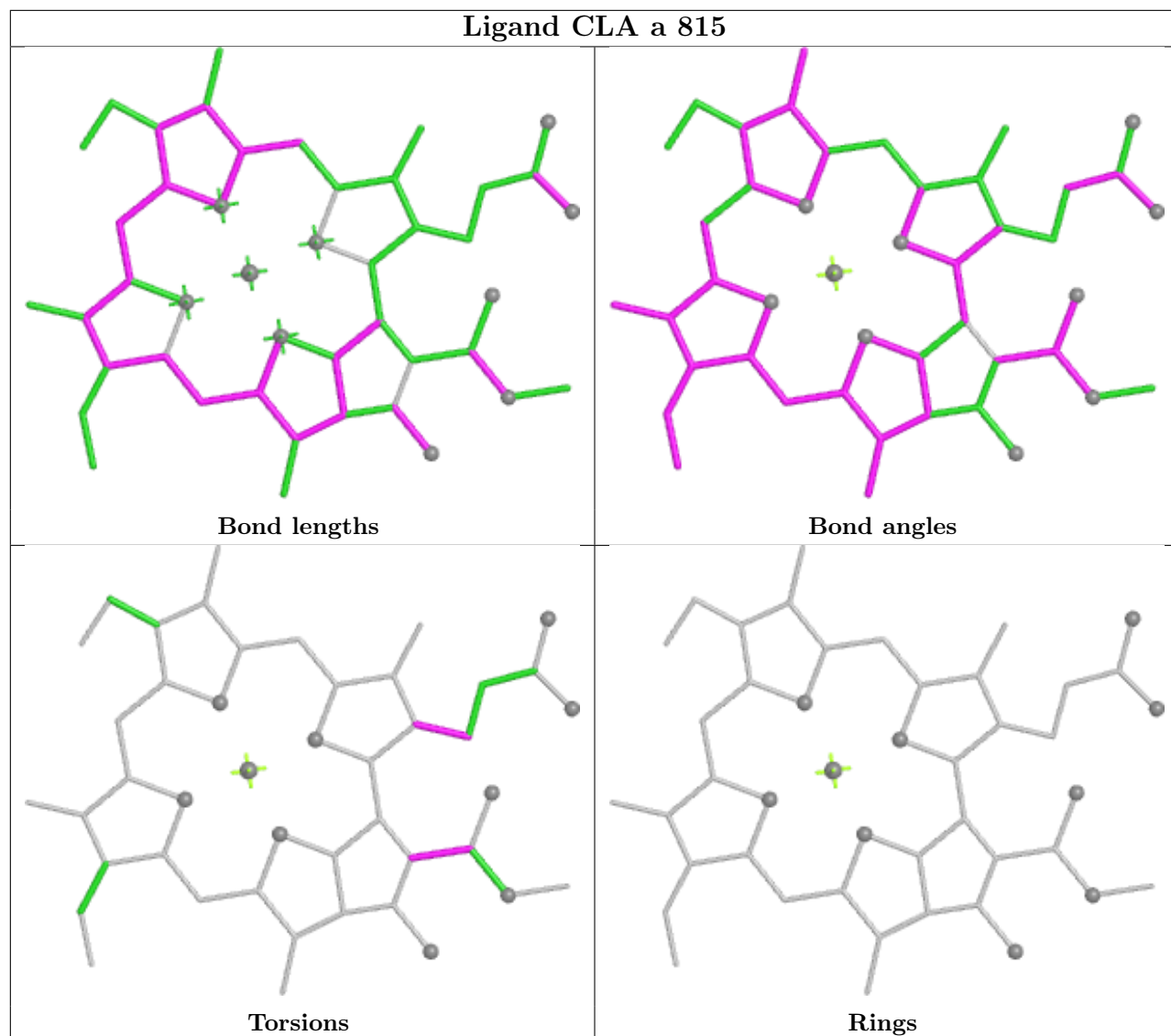
Torsions



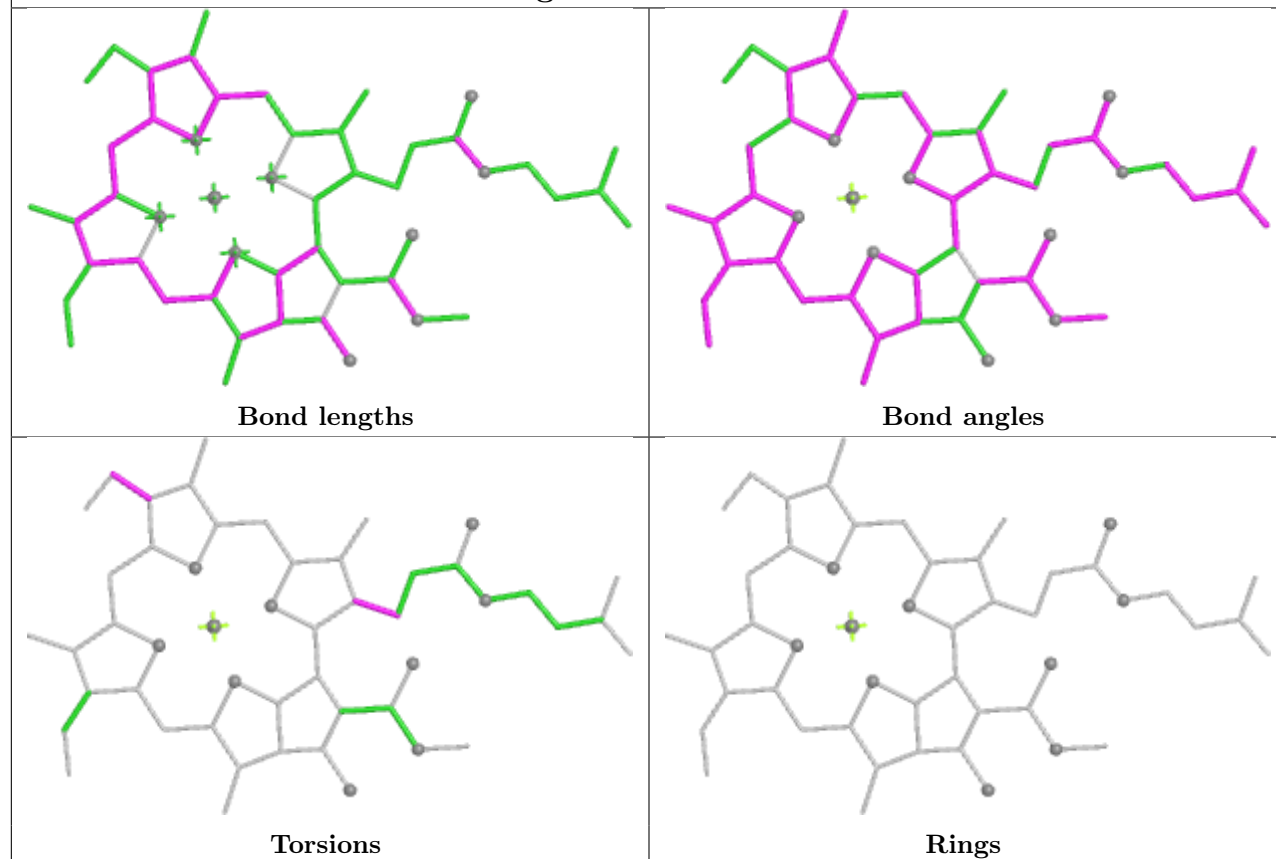
Rings



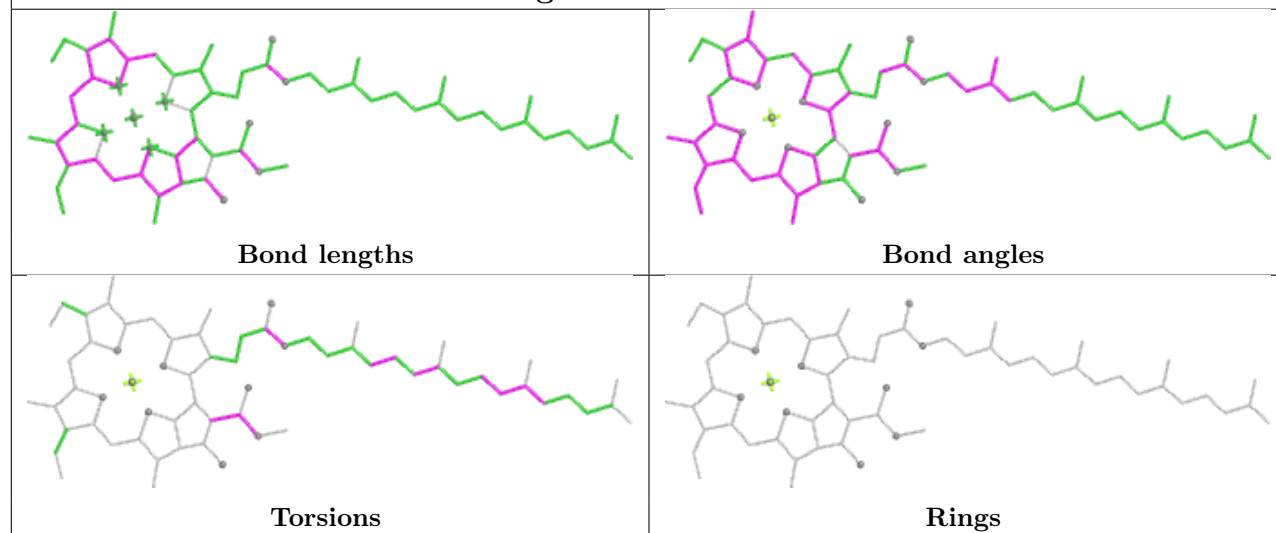
Ligand CLA a 815



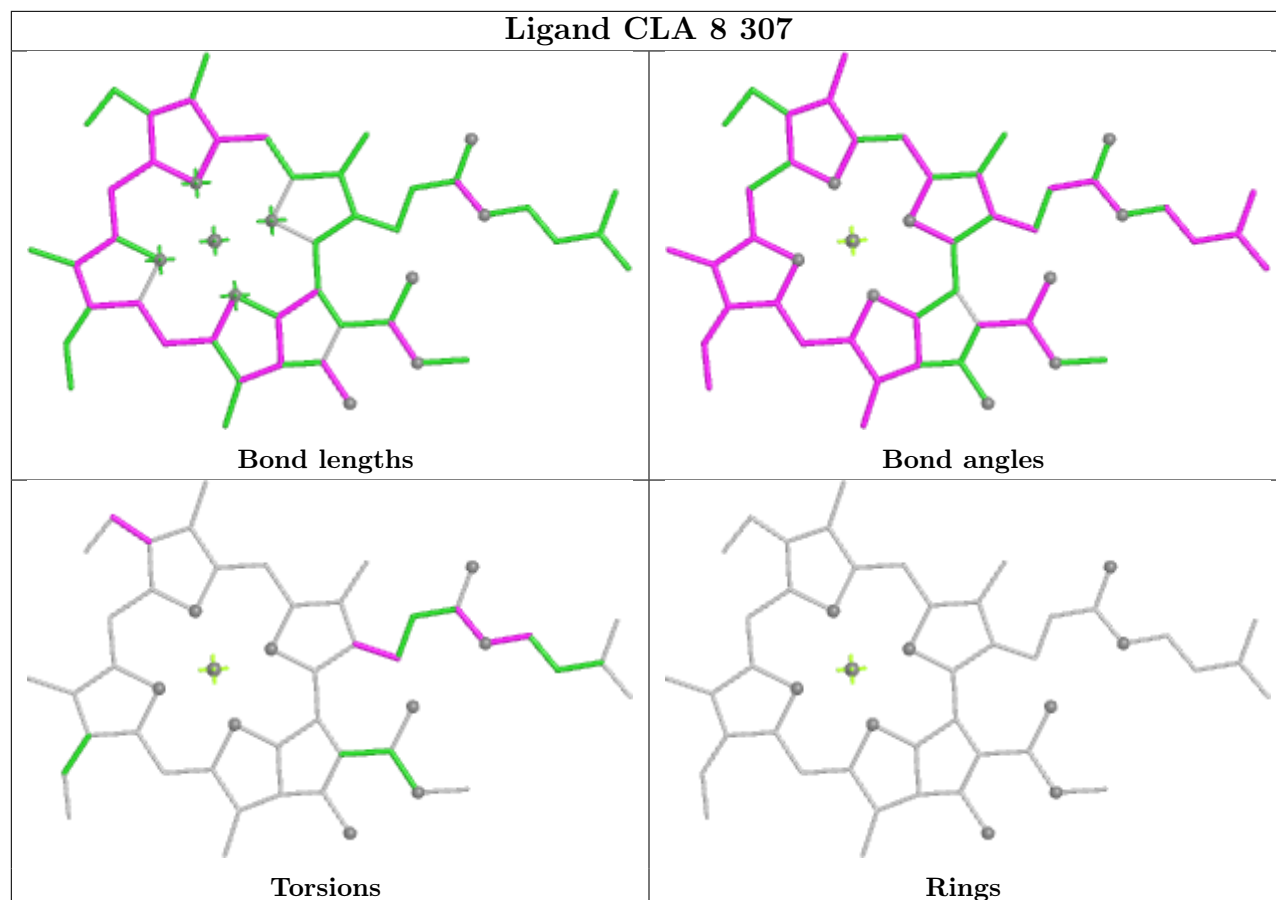
Ligand CLA 3 309



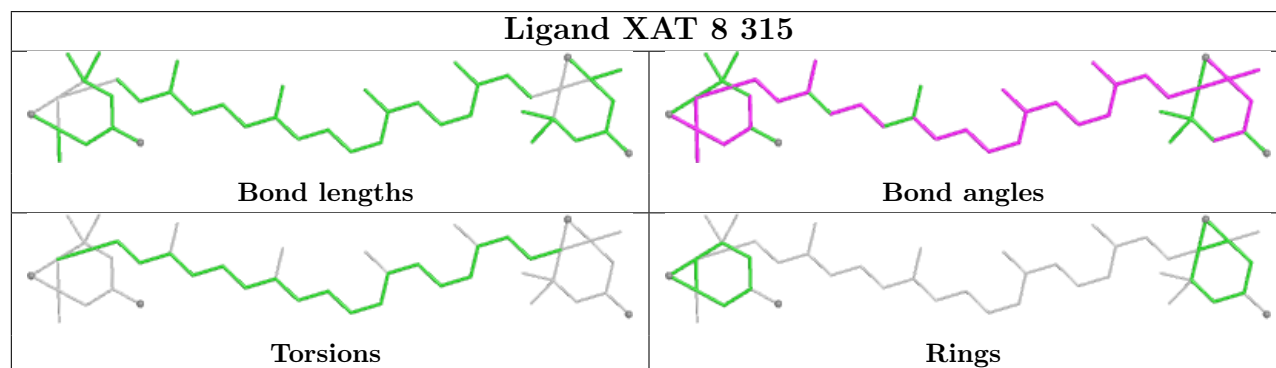
Ligand CLA a 818



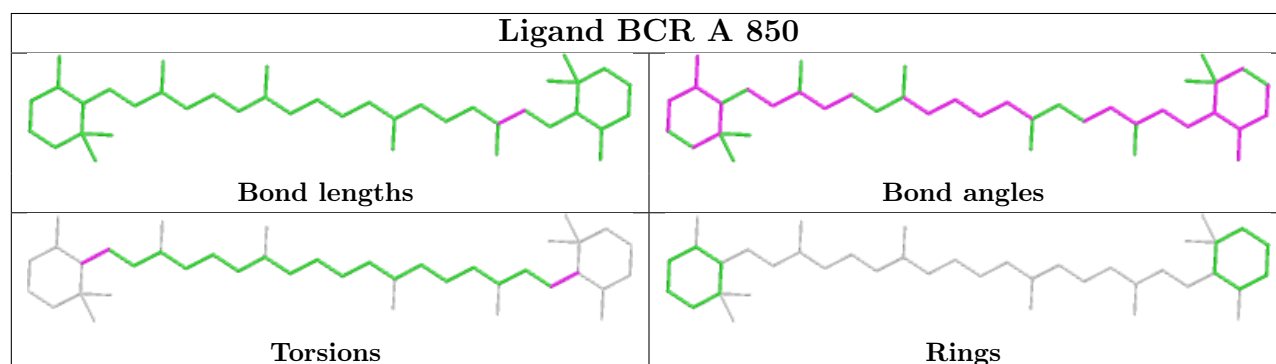
Ligand CLA 8 307

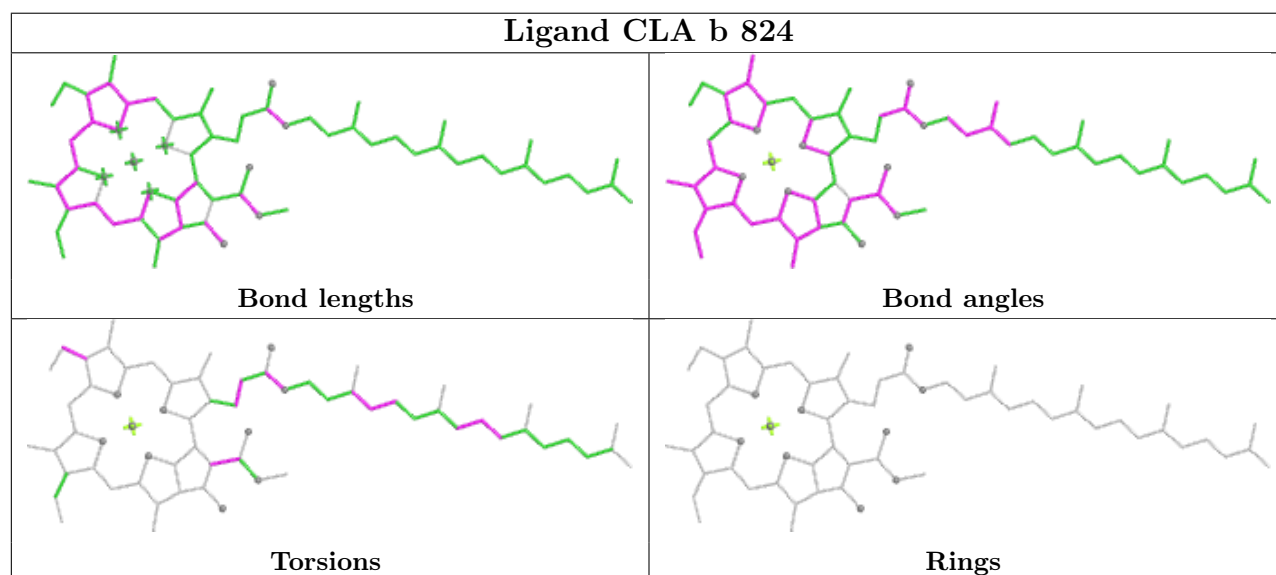
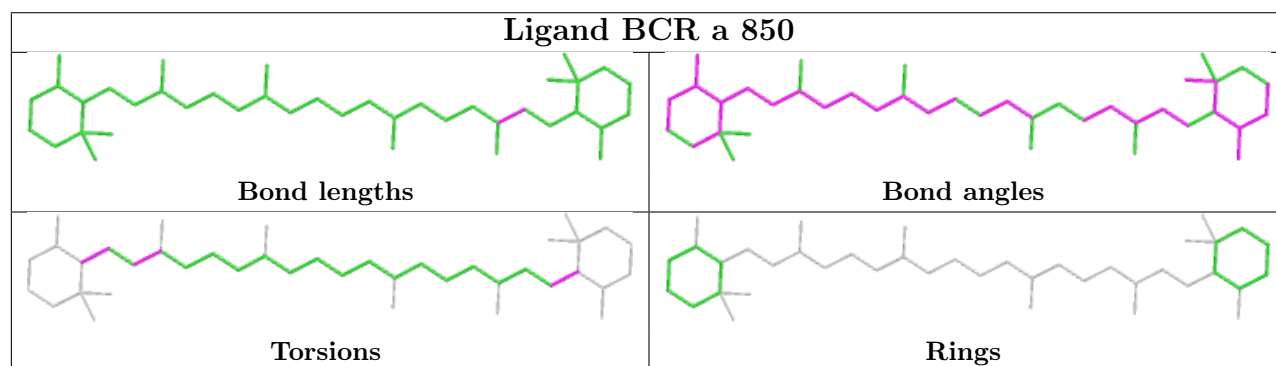
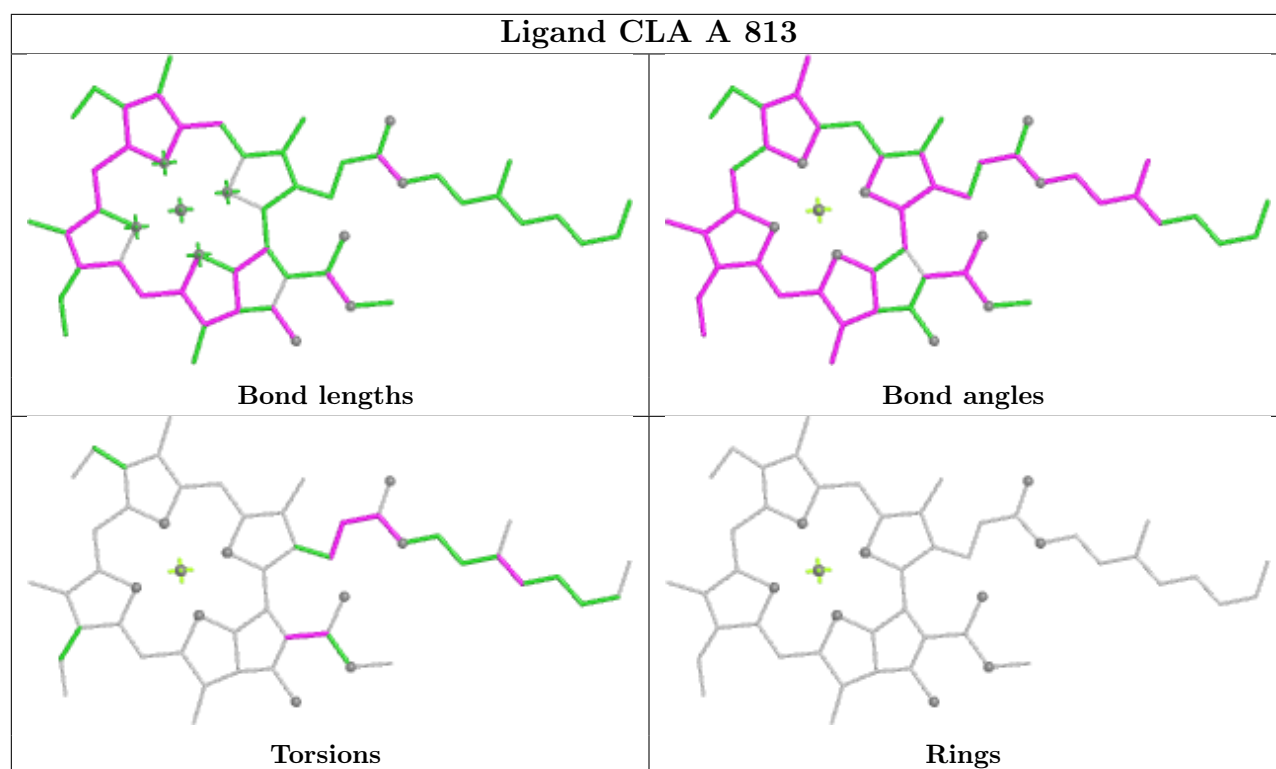


Ligand XAT 8 315

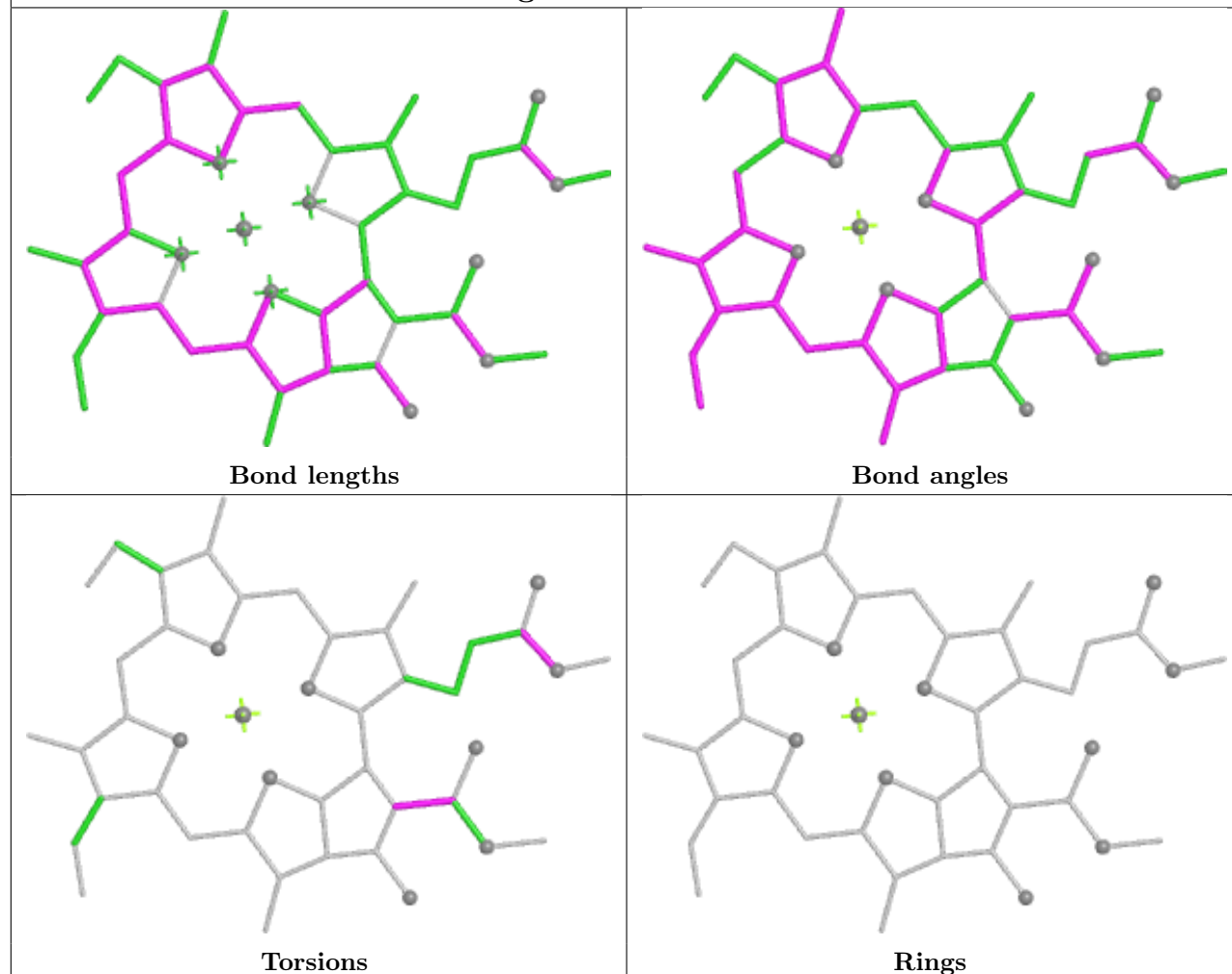


Ligand BCR A 850

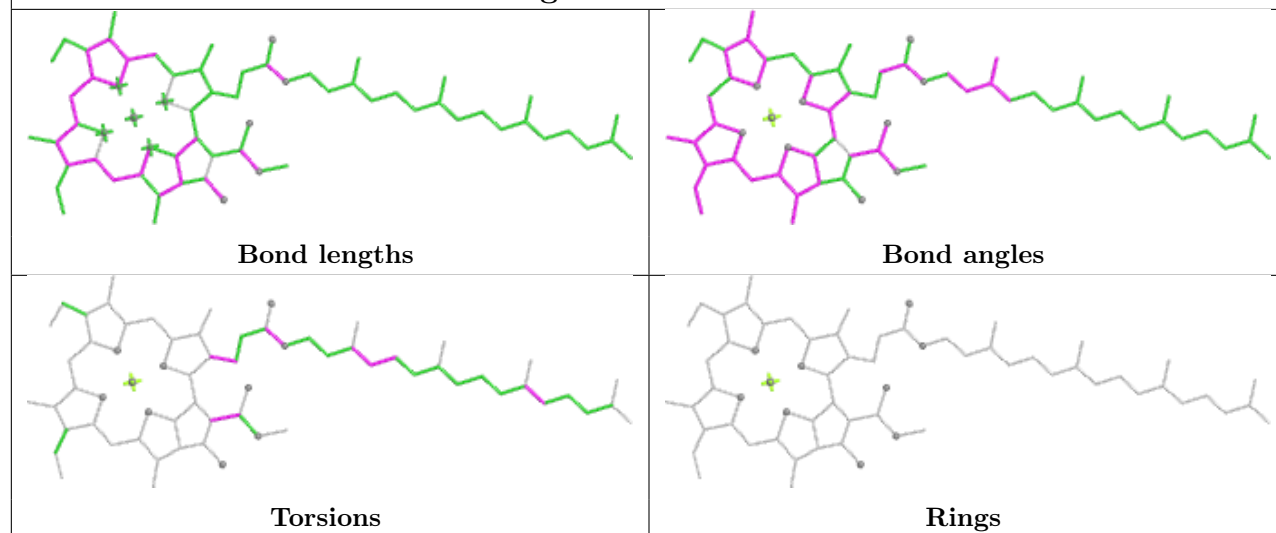


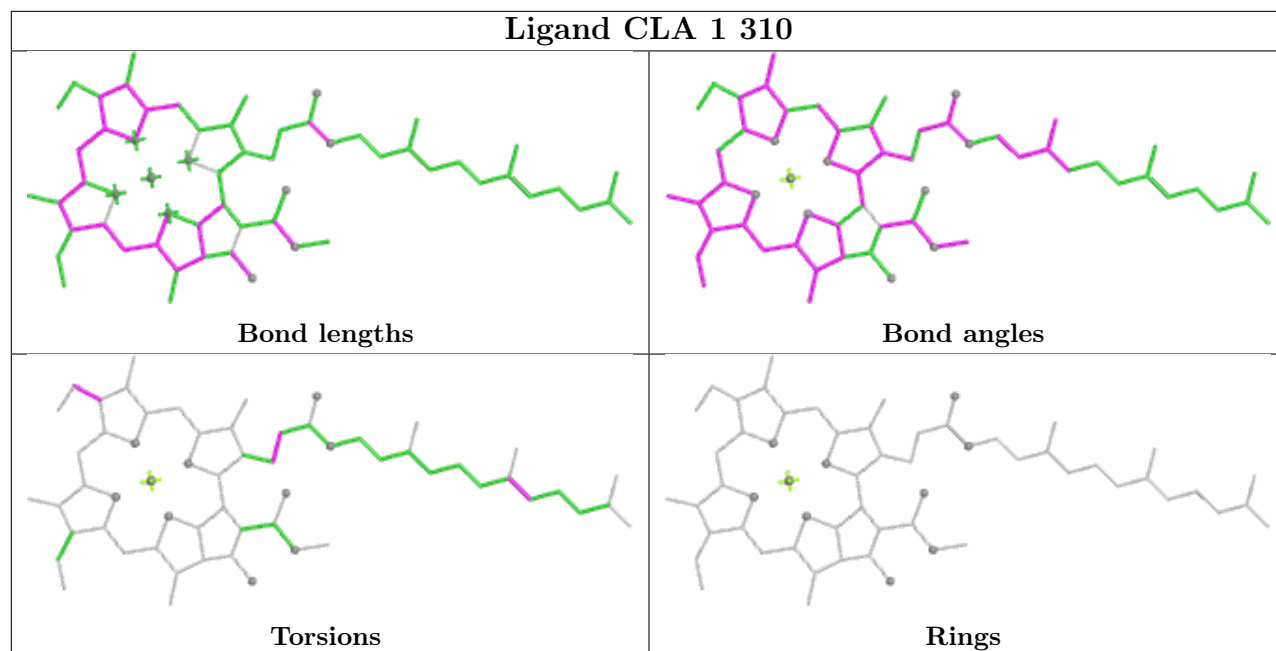
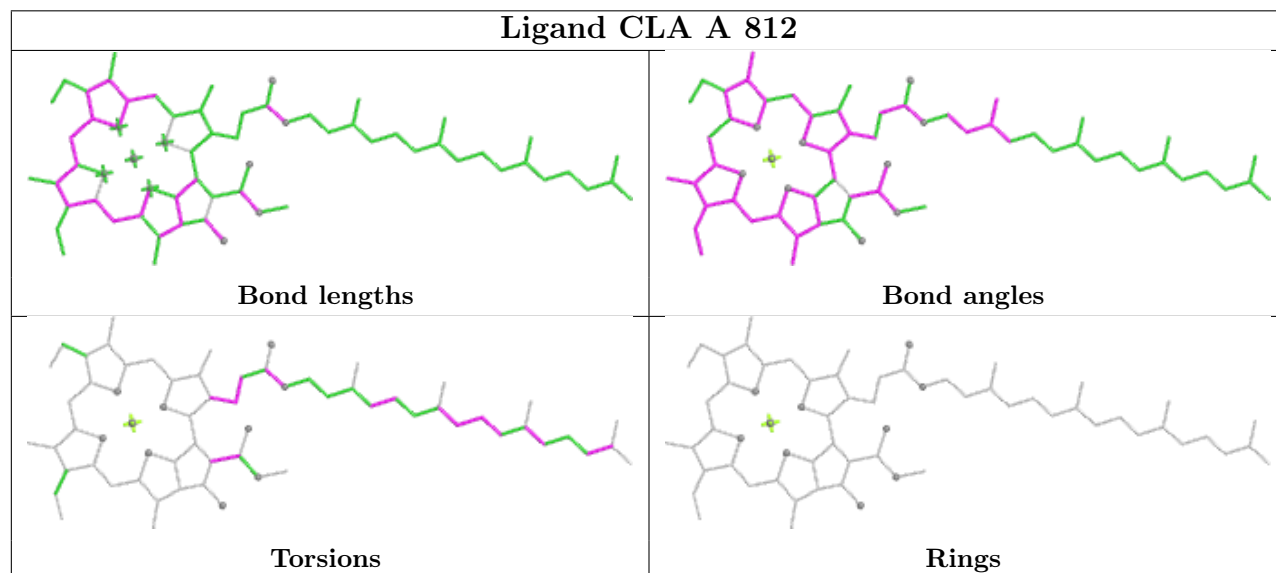
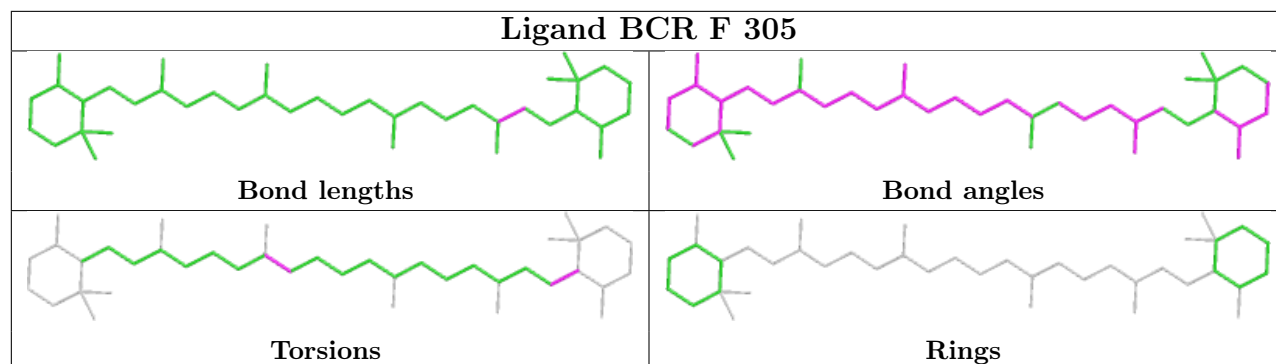


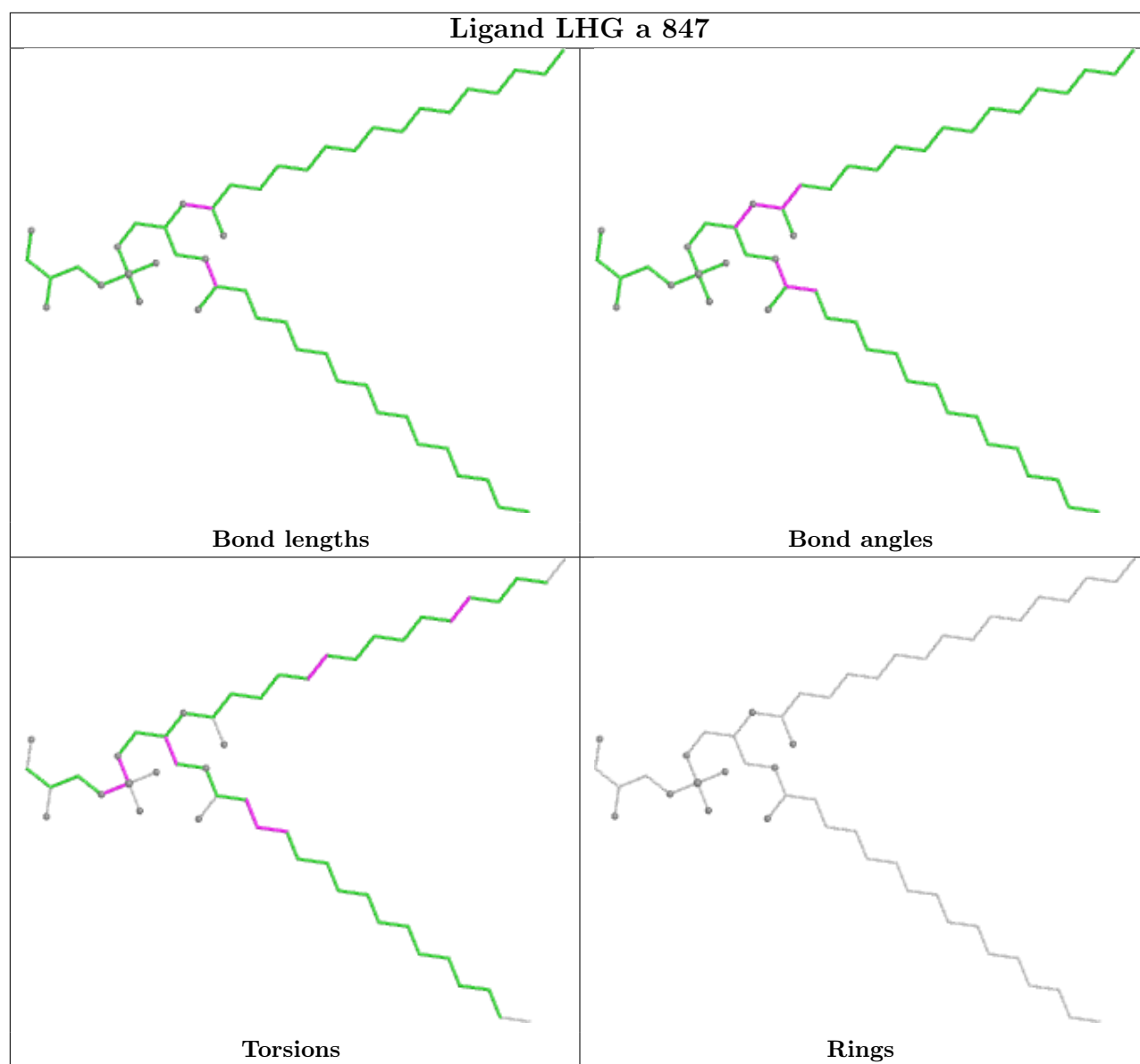
Ligand CLA 6 309



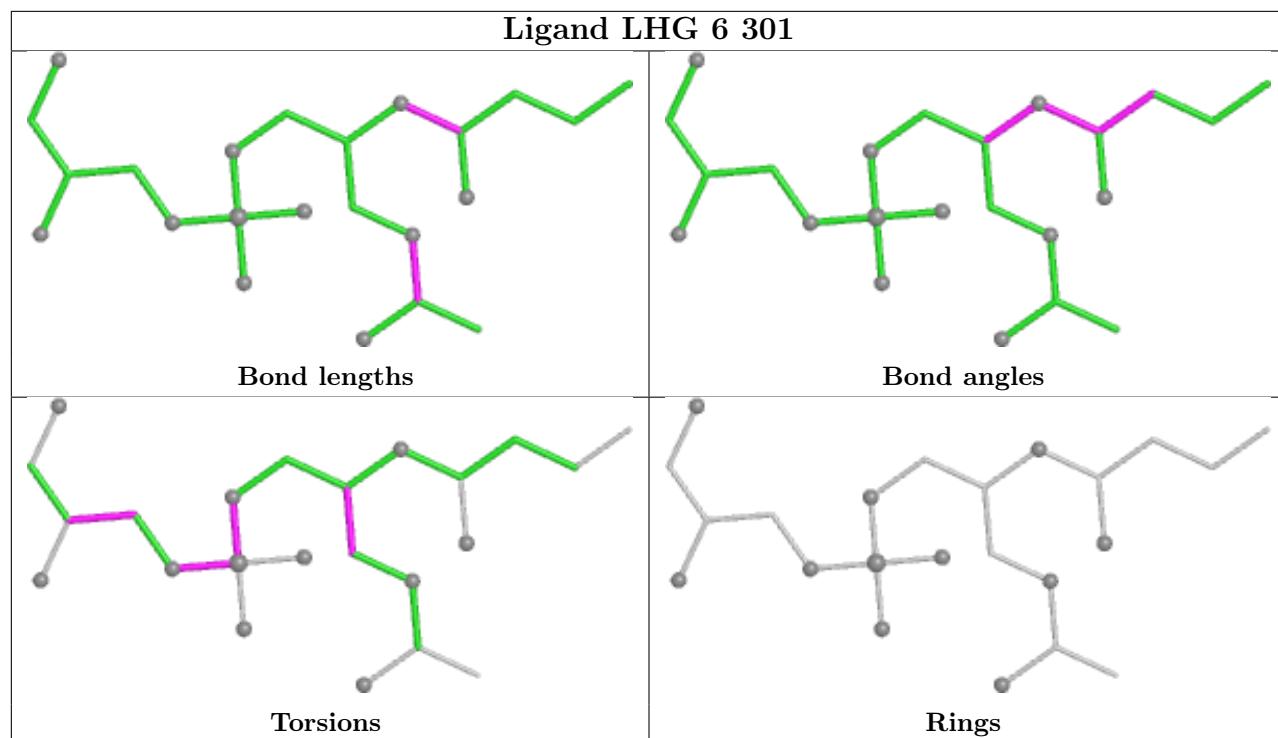
Ligand CLA 1 202



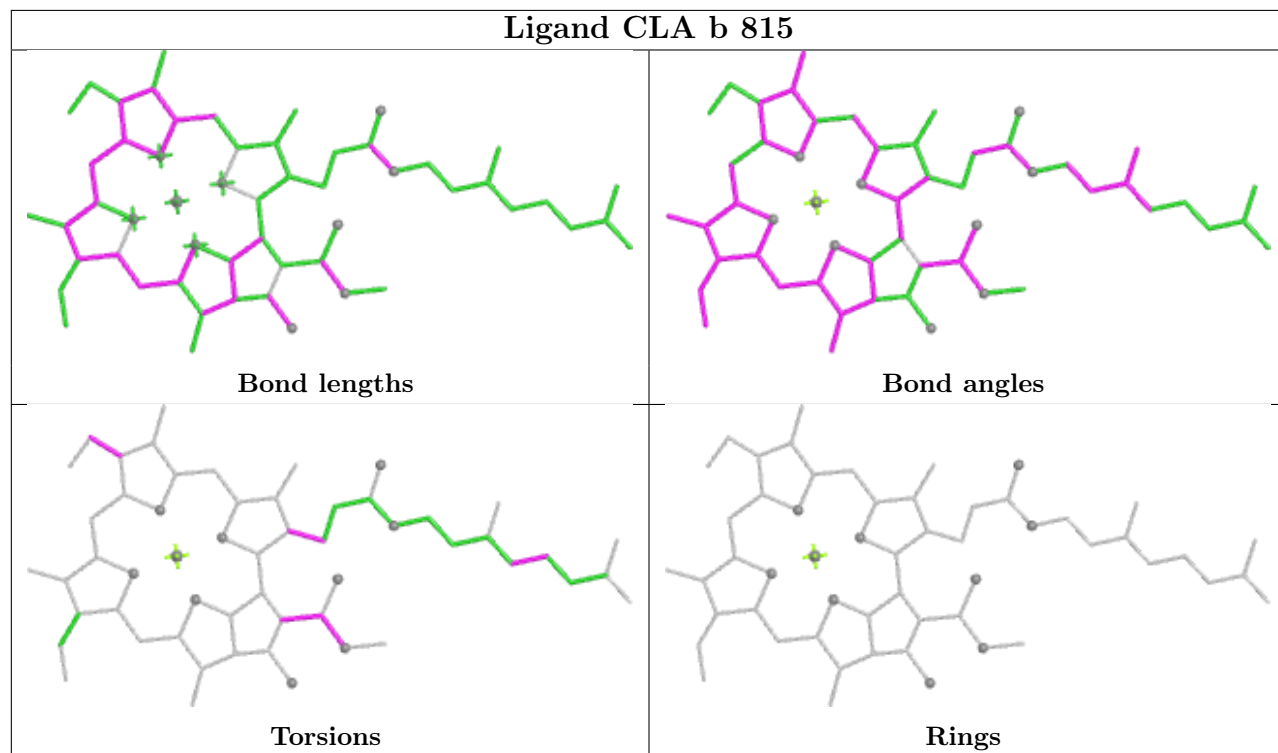


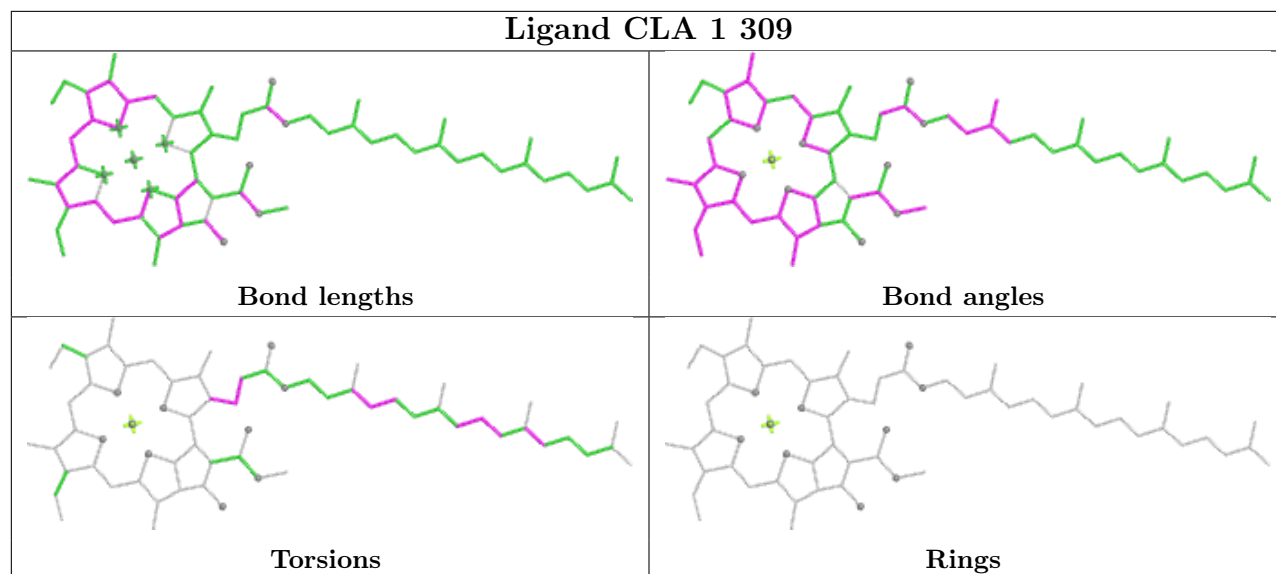
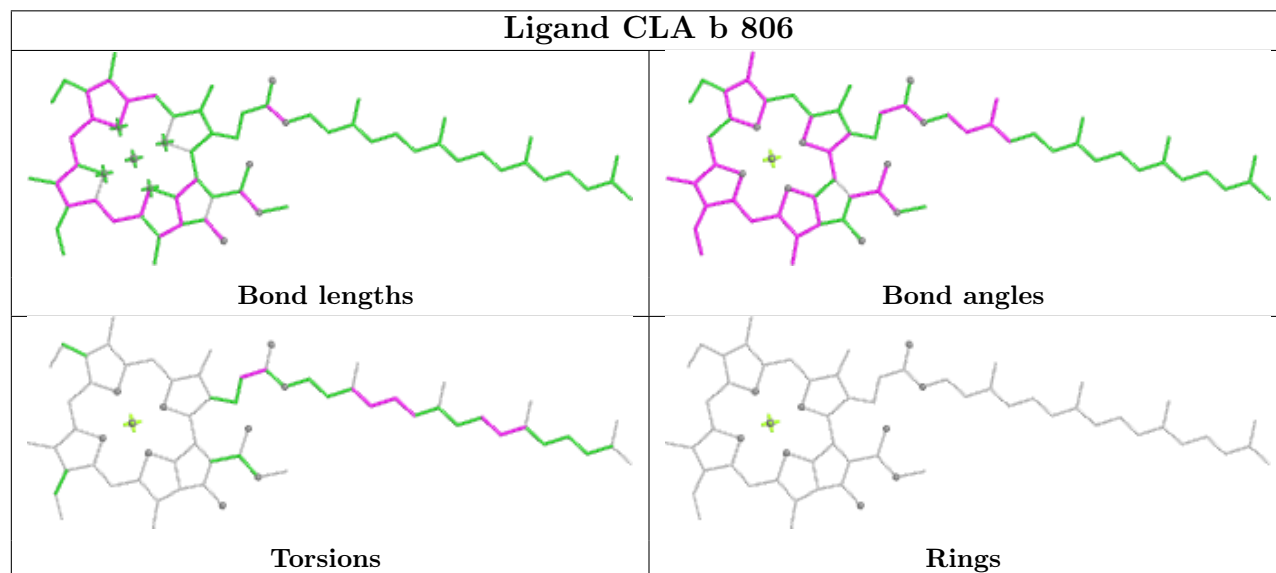


Ligand LHG 6 301

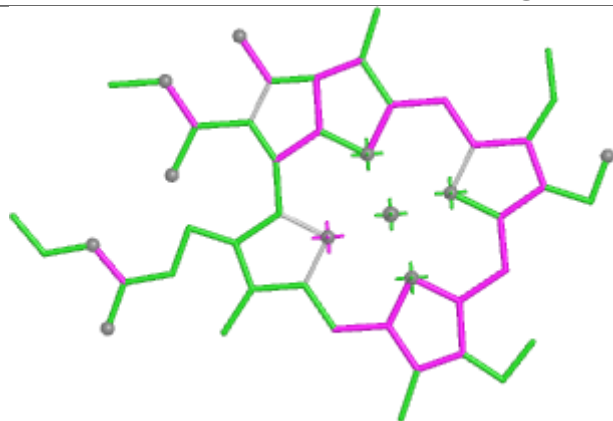


Ligand CLA b 815

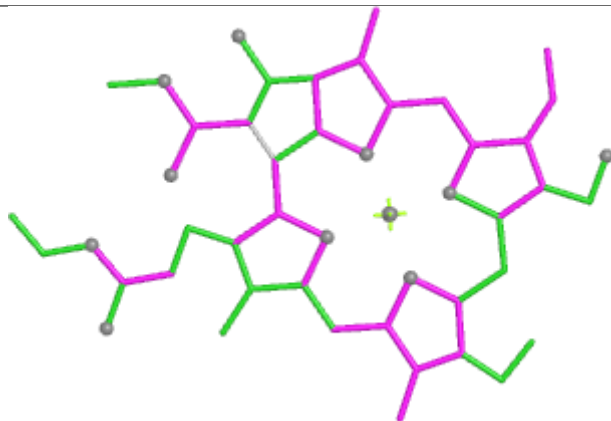


Ligand CLA 1 309**Ligand CLA b 806**

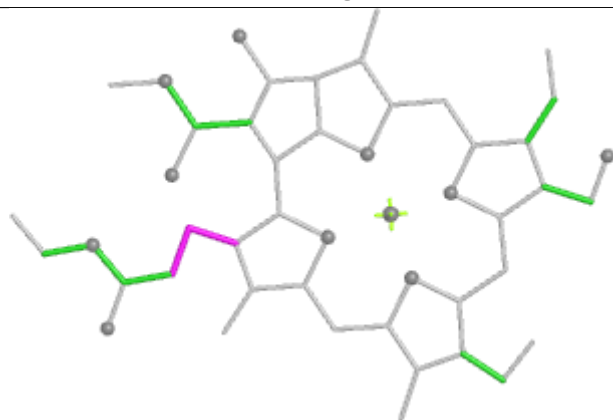
Ligand CHL 2 606



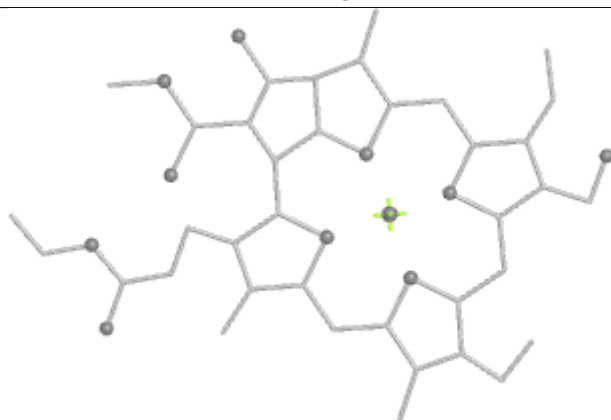
Bond lengths



Bond angles

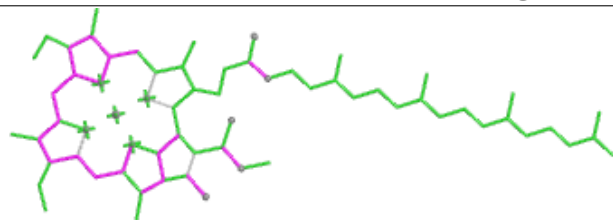


Torsions

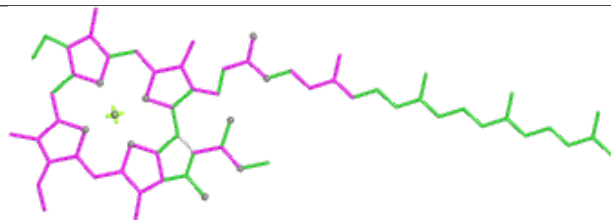


Rings

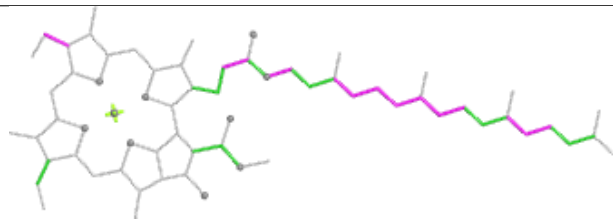
Ligand CLA B 802



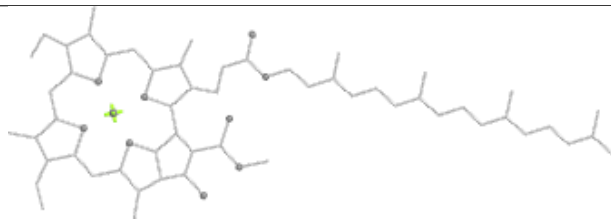
Bond lengths



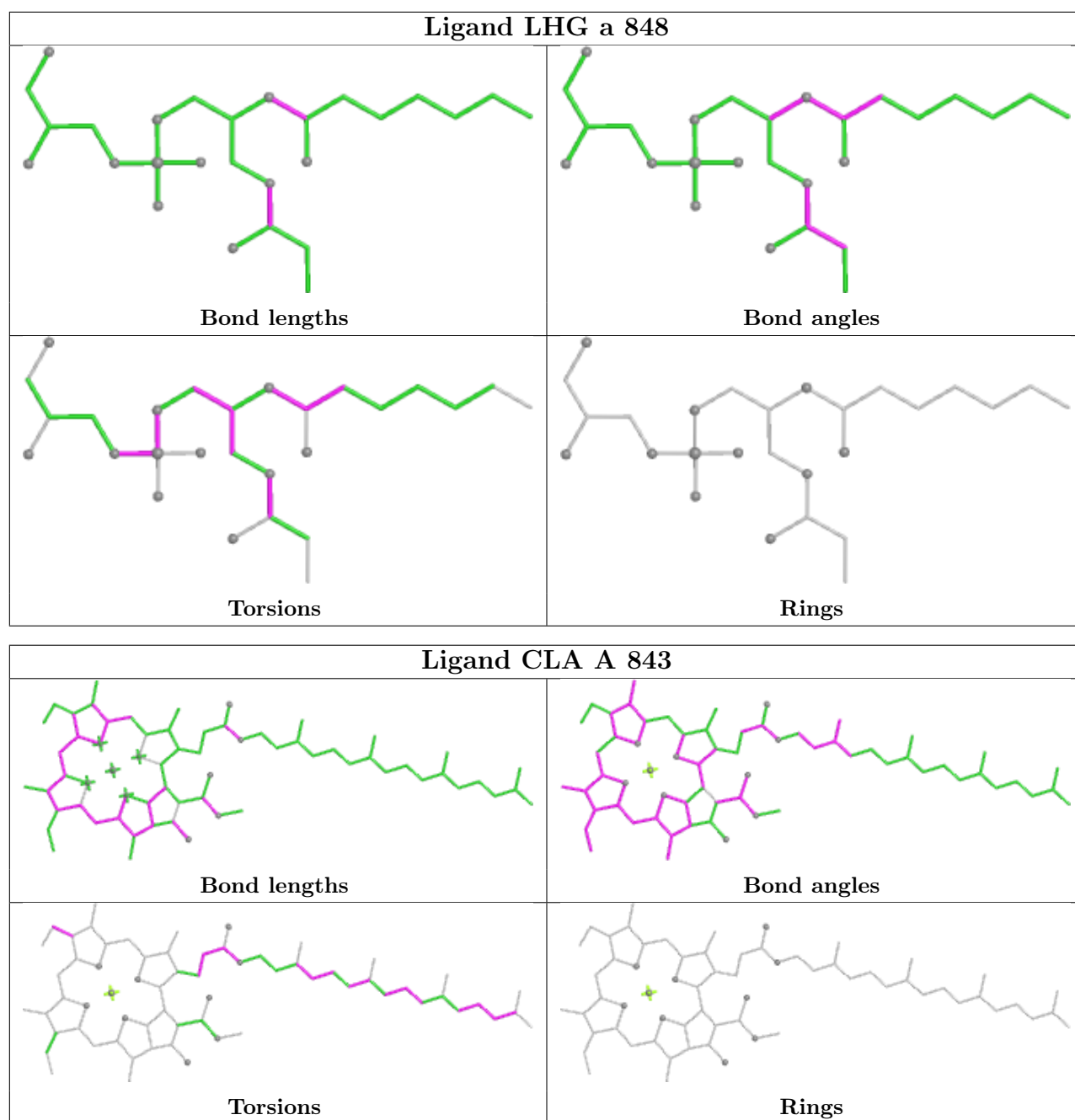
Bond angles

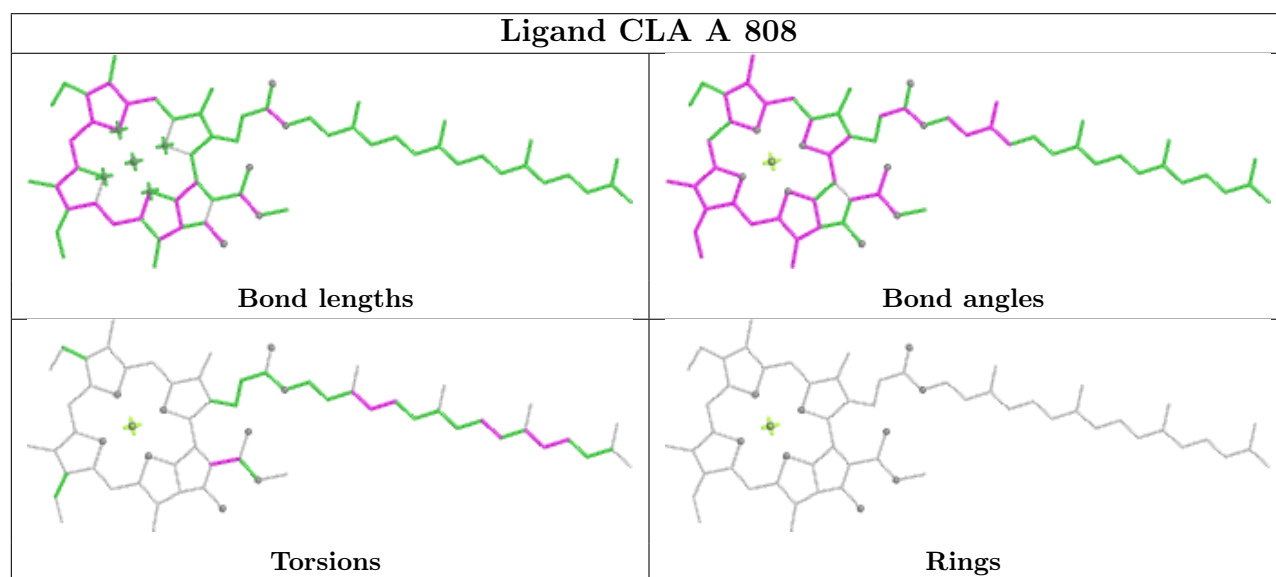
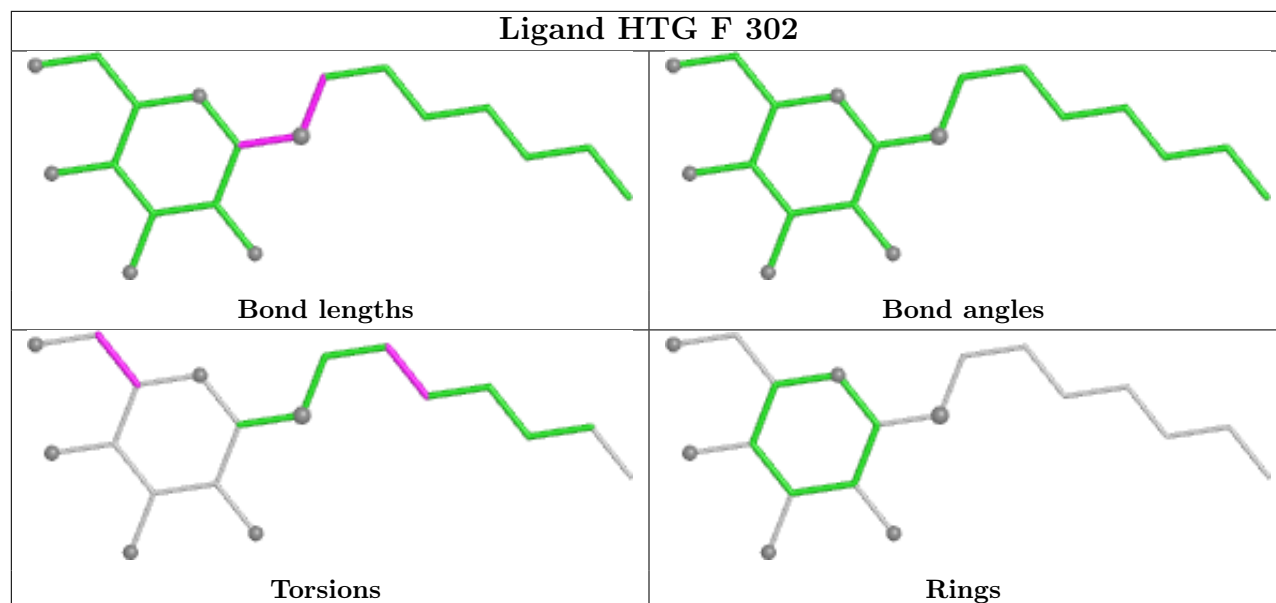


Torsions

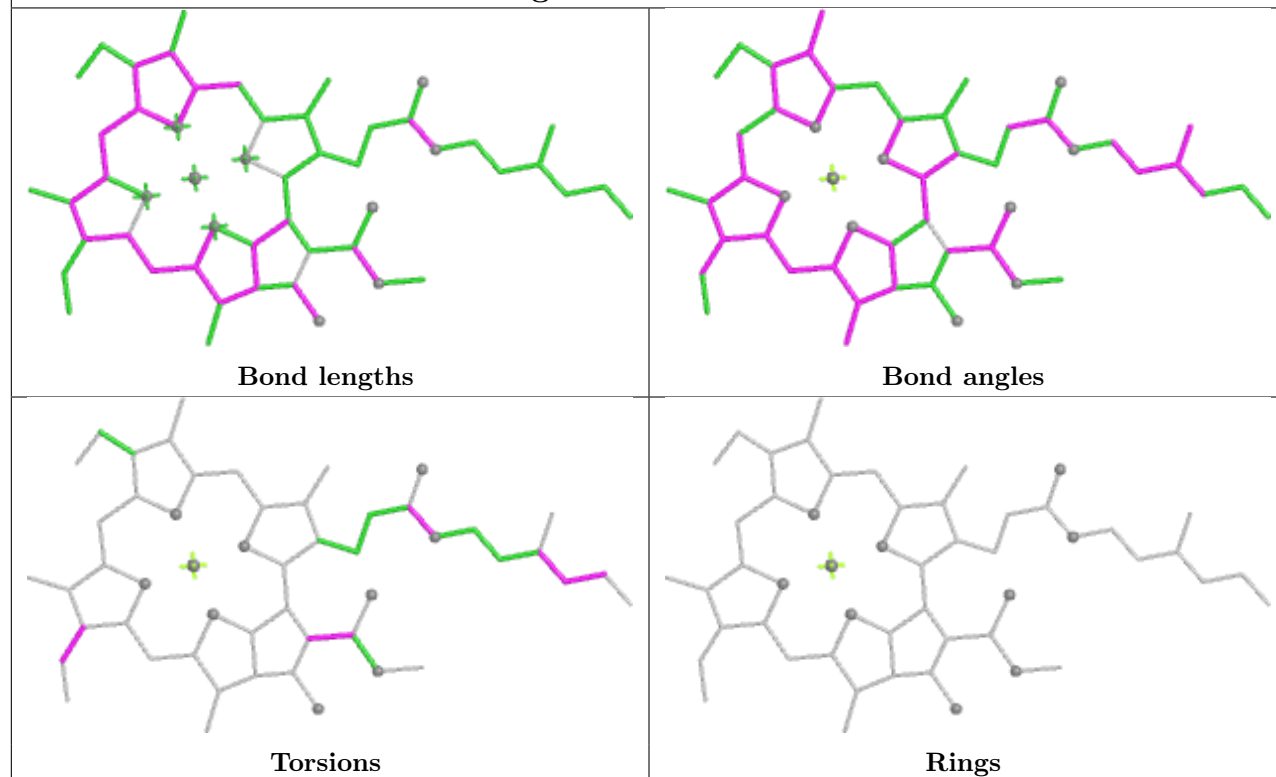


Rings

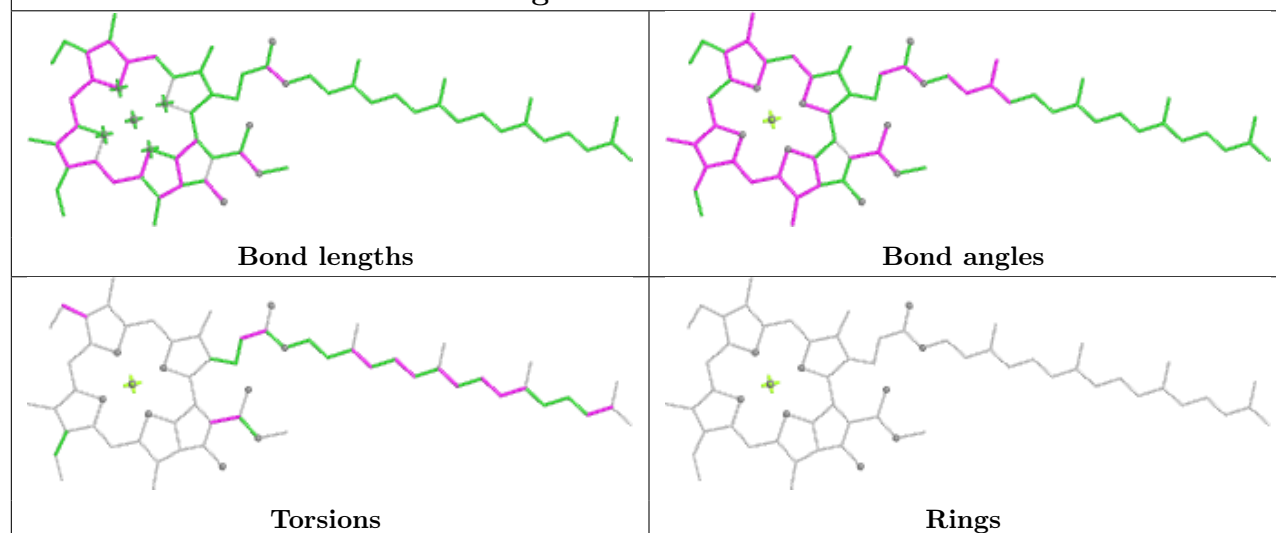




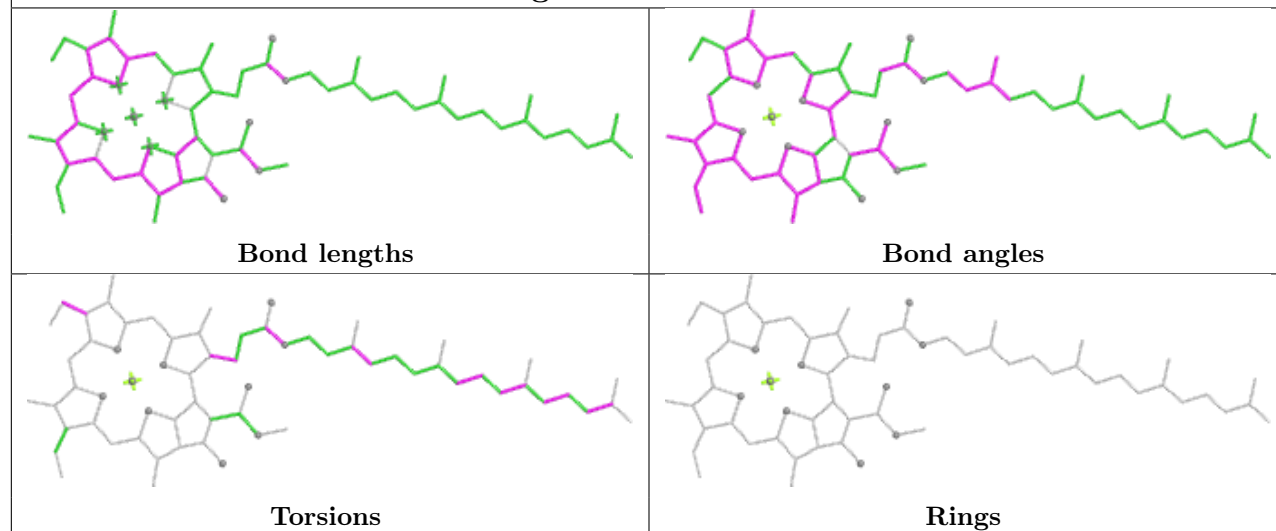
Ligand CLA A 845



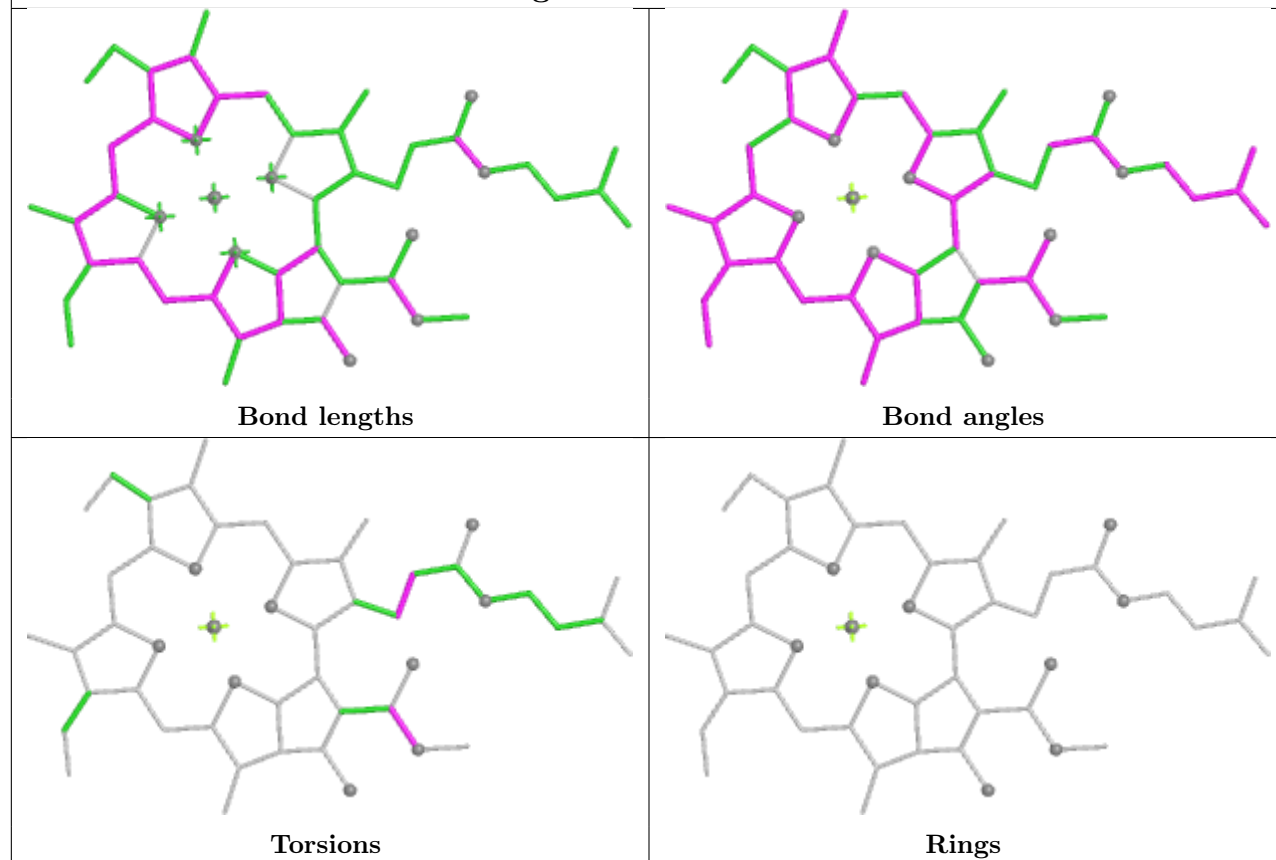
Ligand CLA A 828



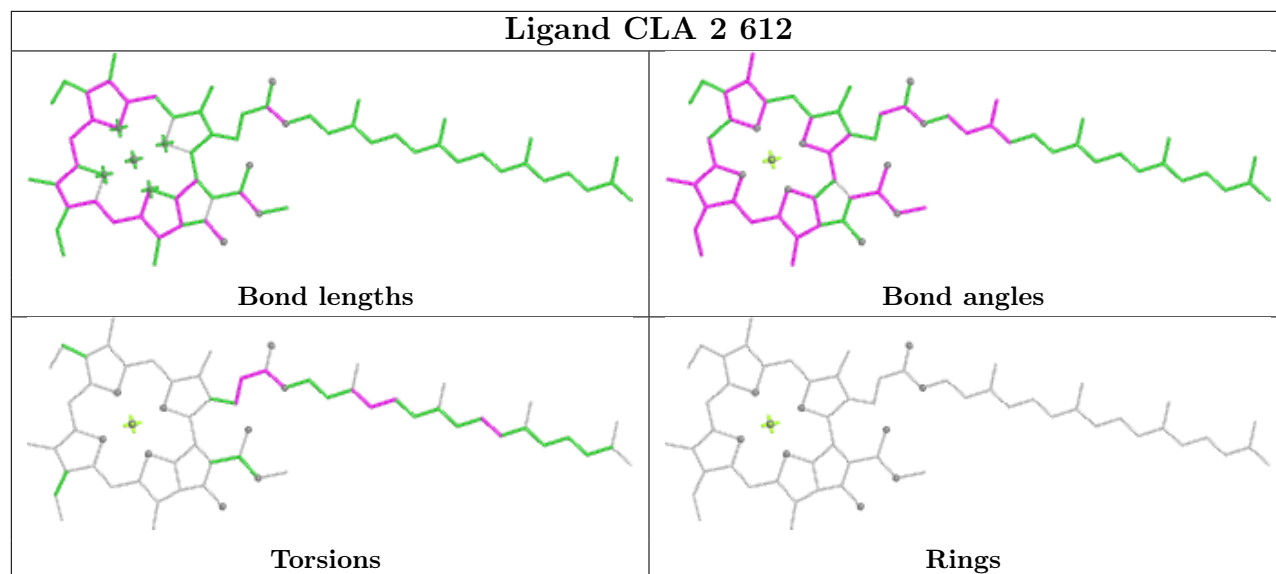
Ligand CLA A 820



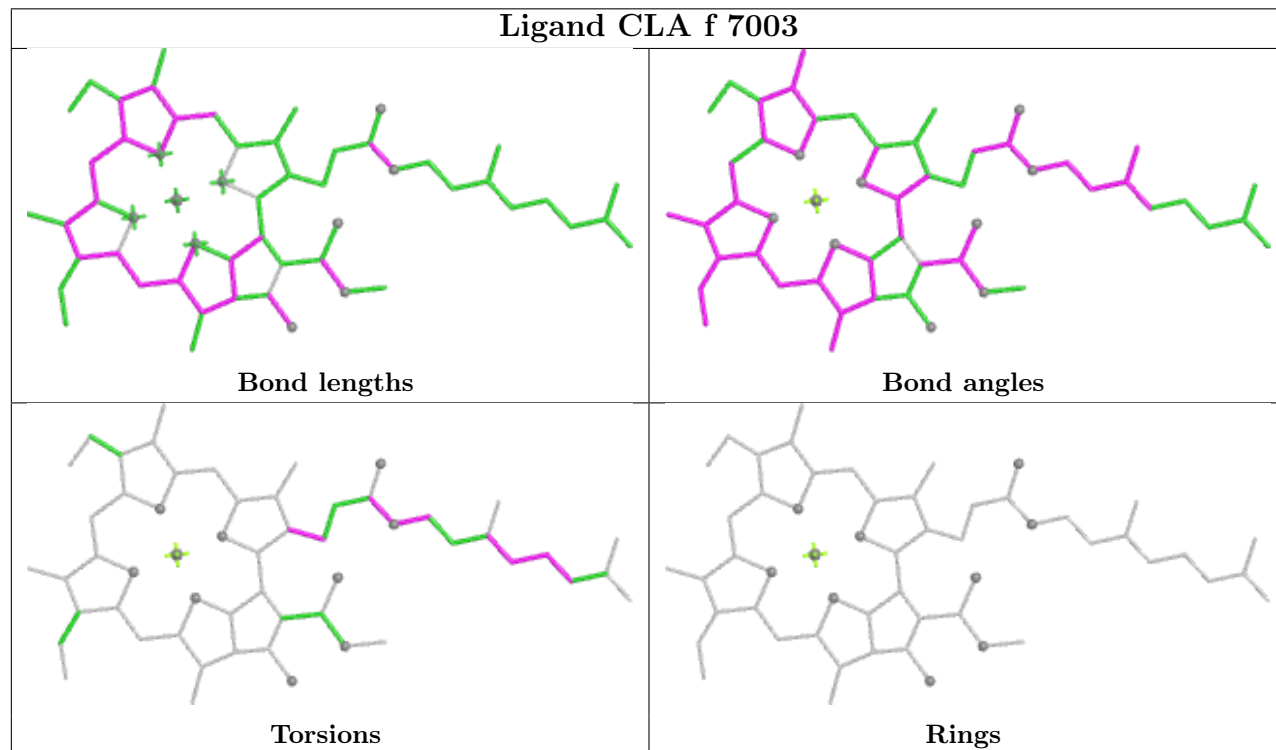
Ligand CLA B 820



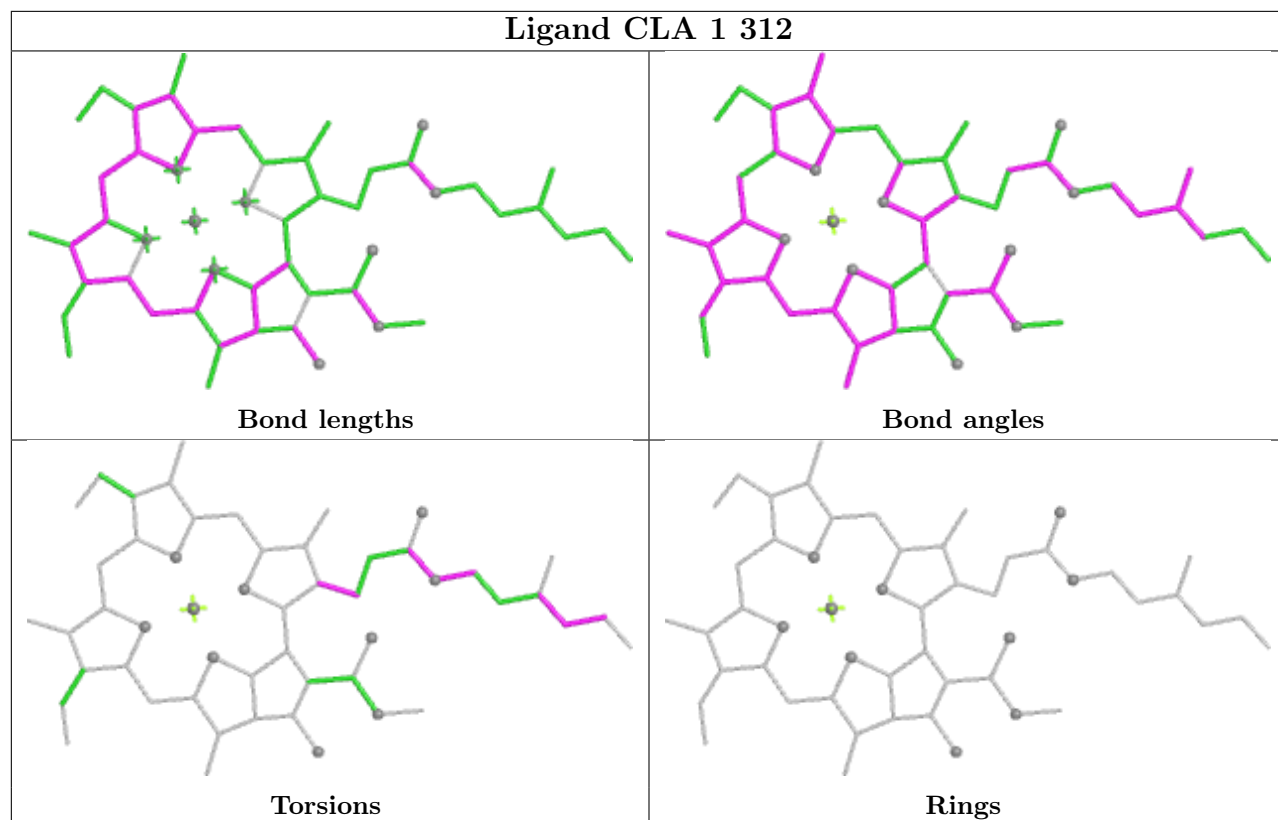
Ligand CLA 2 612



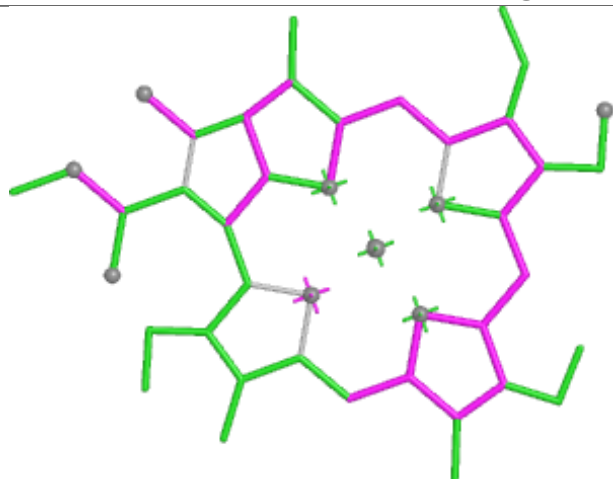
Ligand CLA f 7003



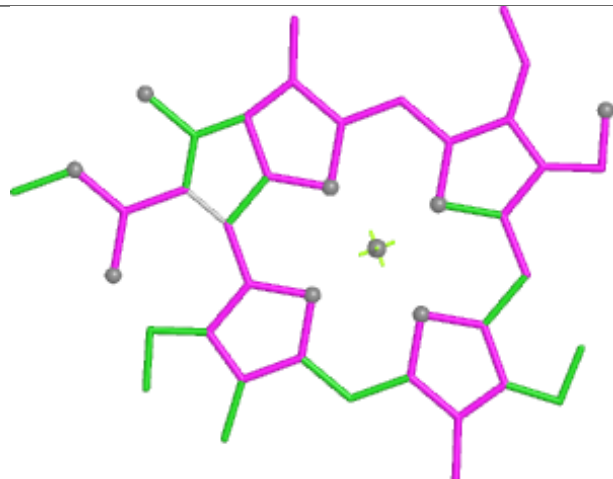
Ligand CLA 1 312



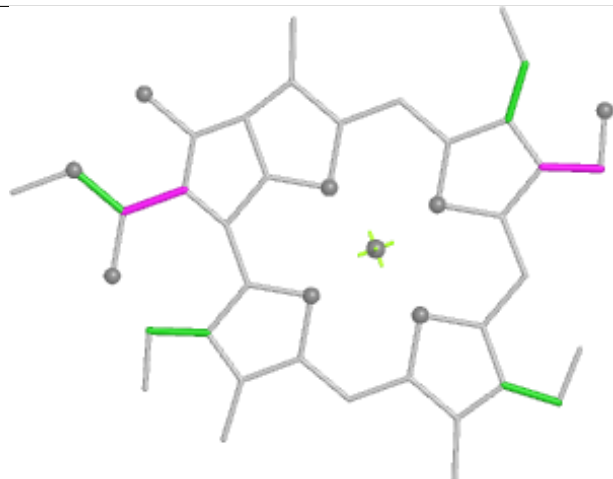
Ligand CHL 7 605



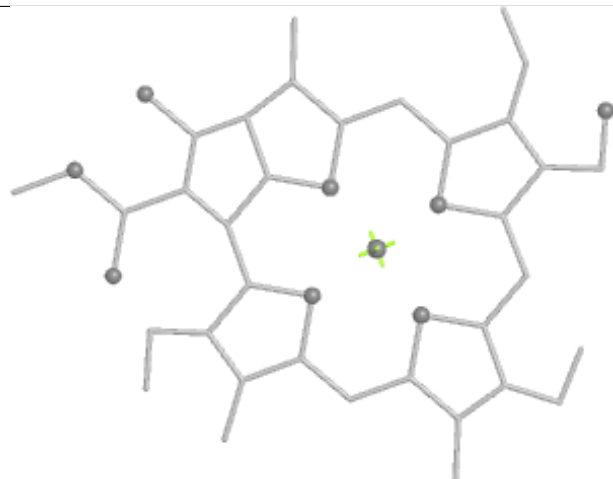
Bond lengths



Bond angles

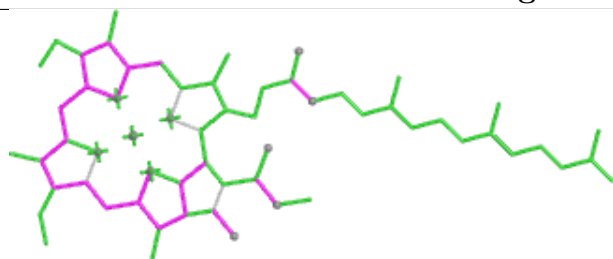


Torsions

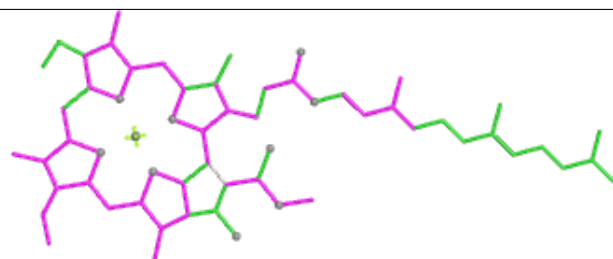


Rings

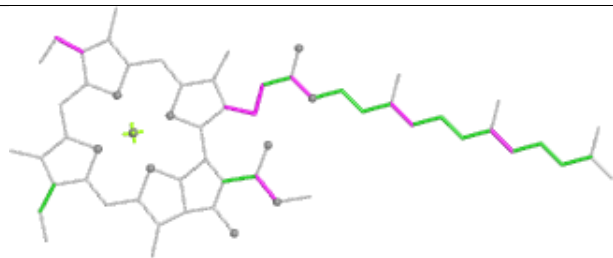
Ligand CLA 6 311



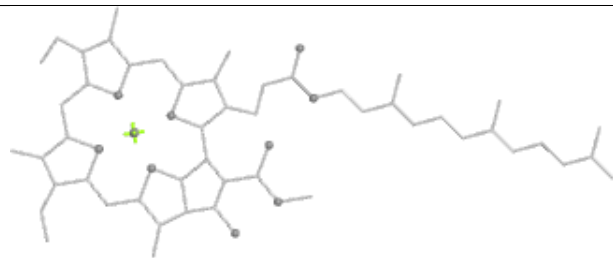
Bond lengths



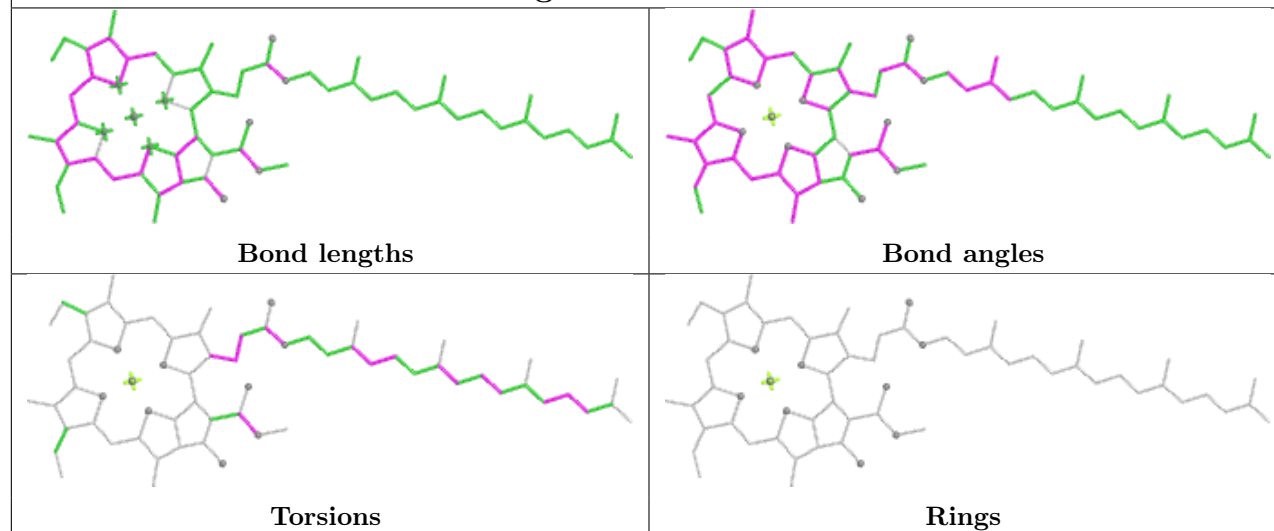
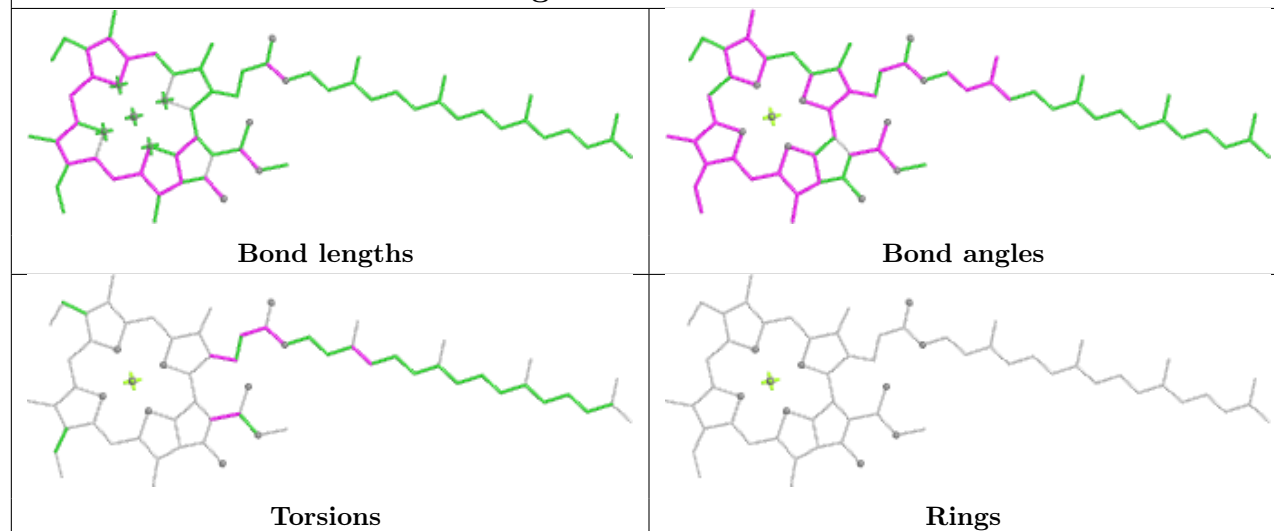
Bond angles

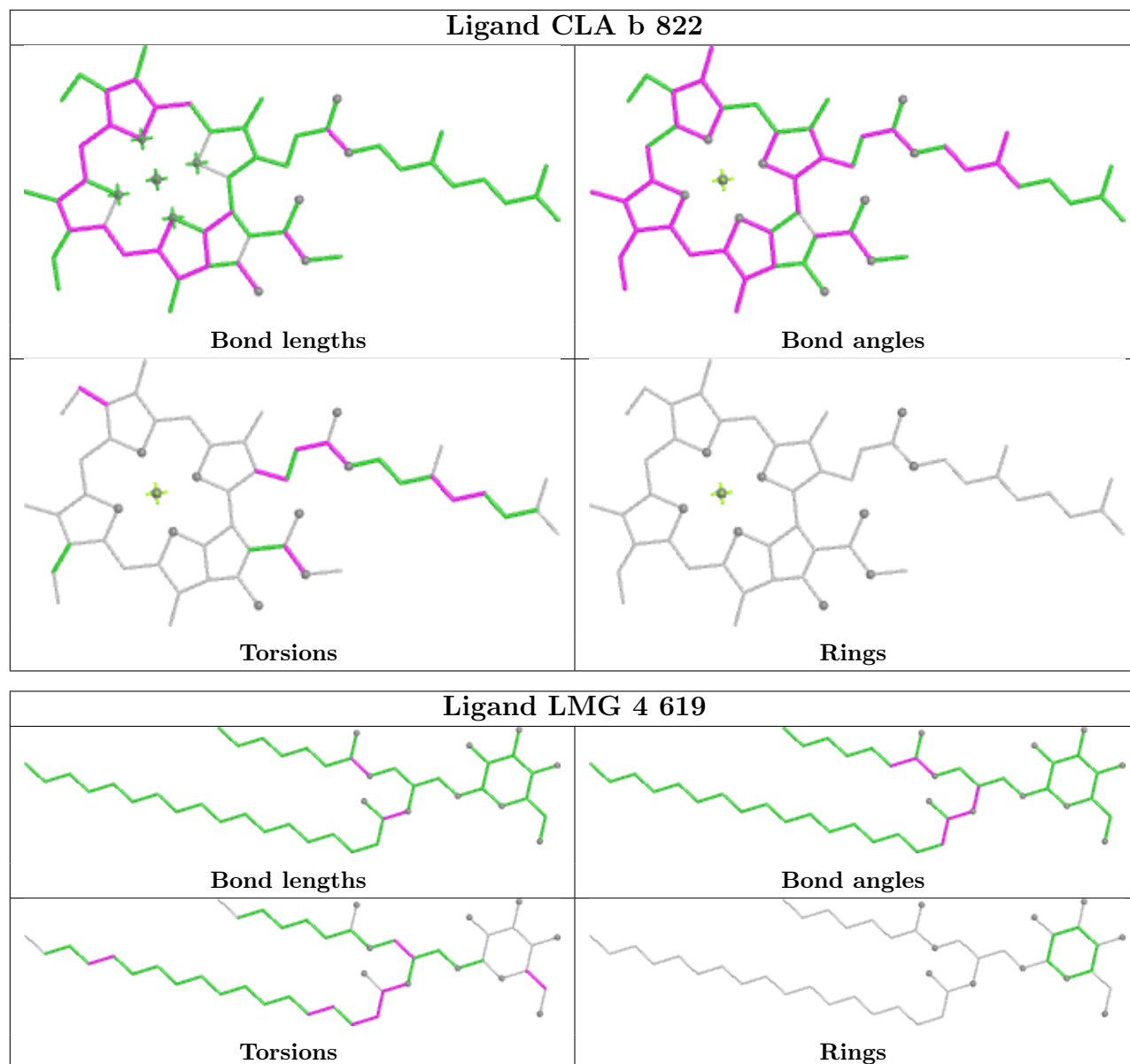


Torsions

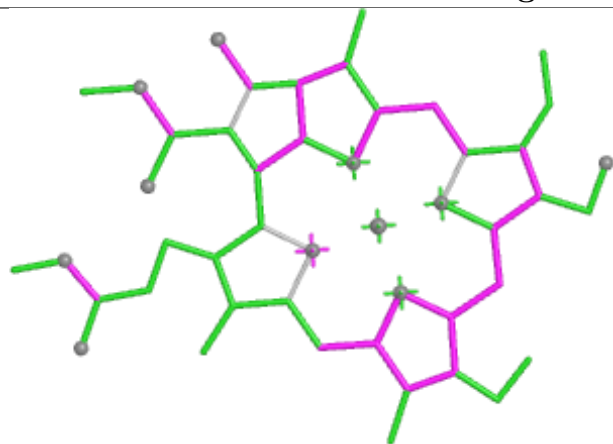


Rings

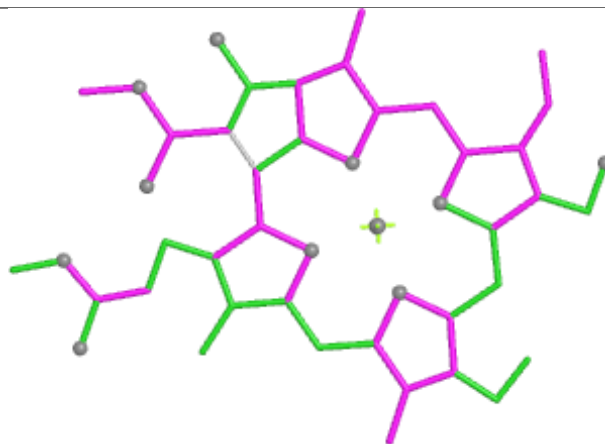
Ligand CLA b 827**Ligand CLA A 811**



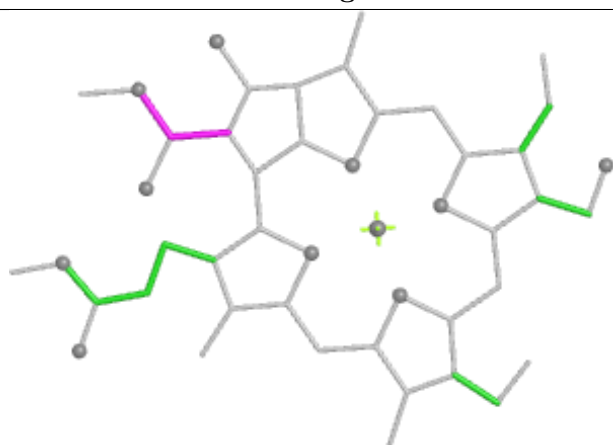
Ligand CHL 8 306



Bond lengths



Bond angles

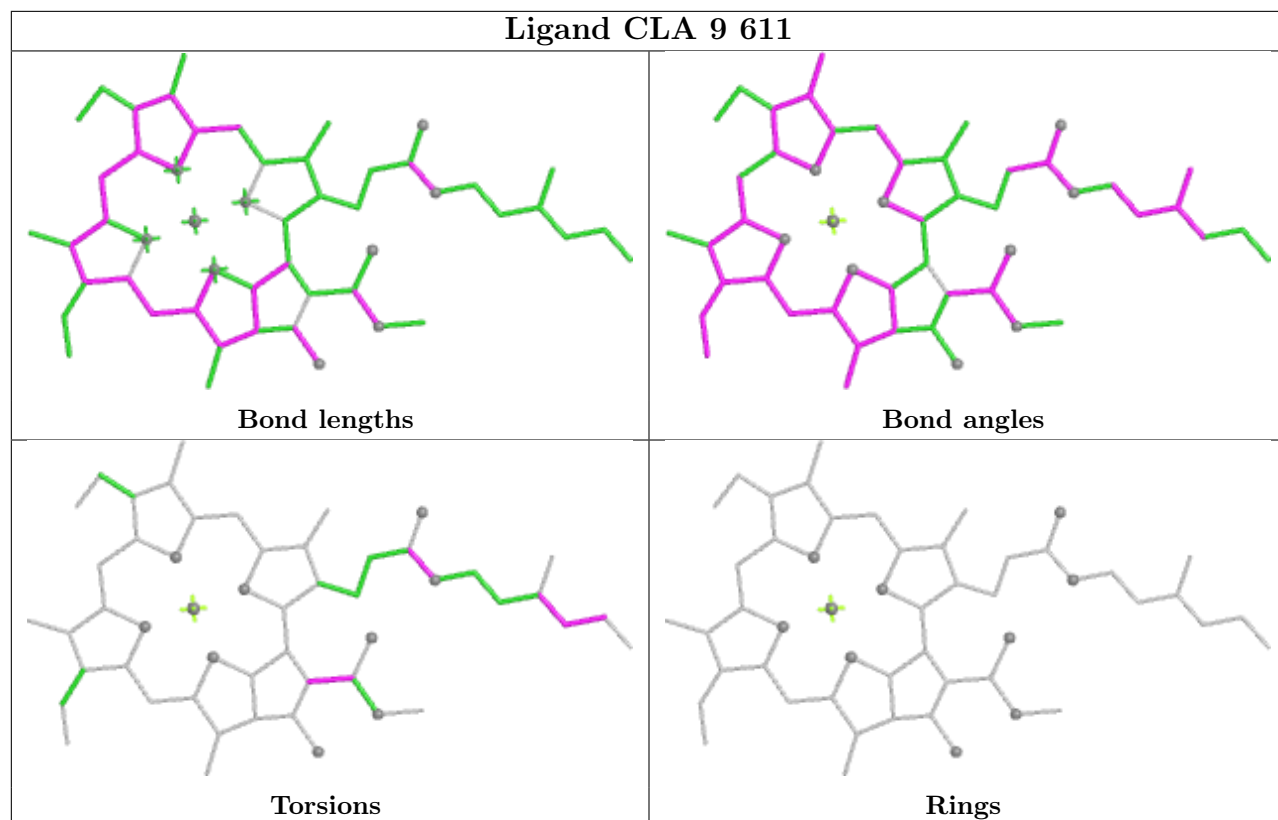


Torsions

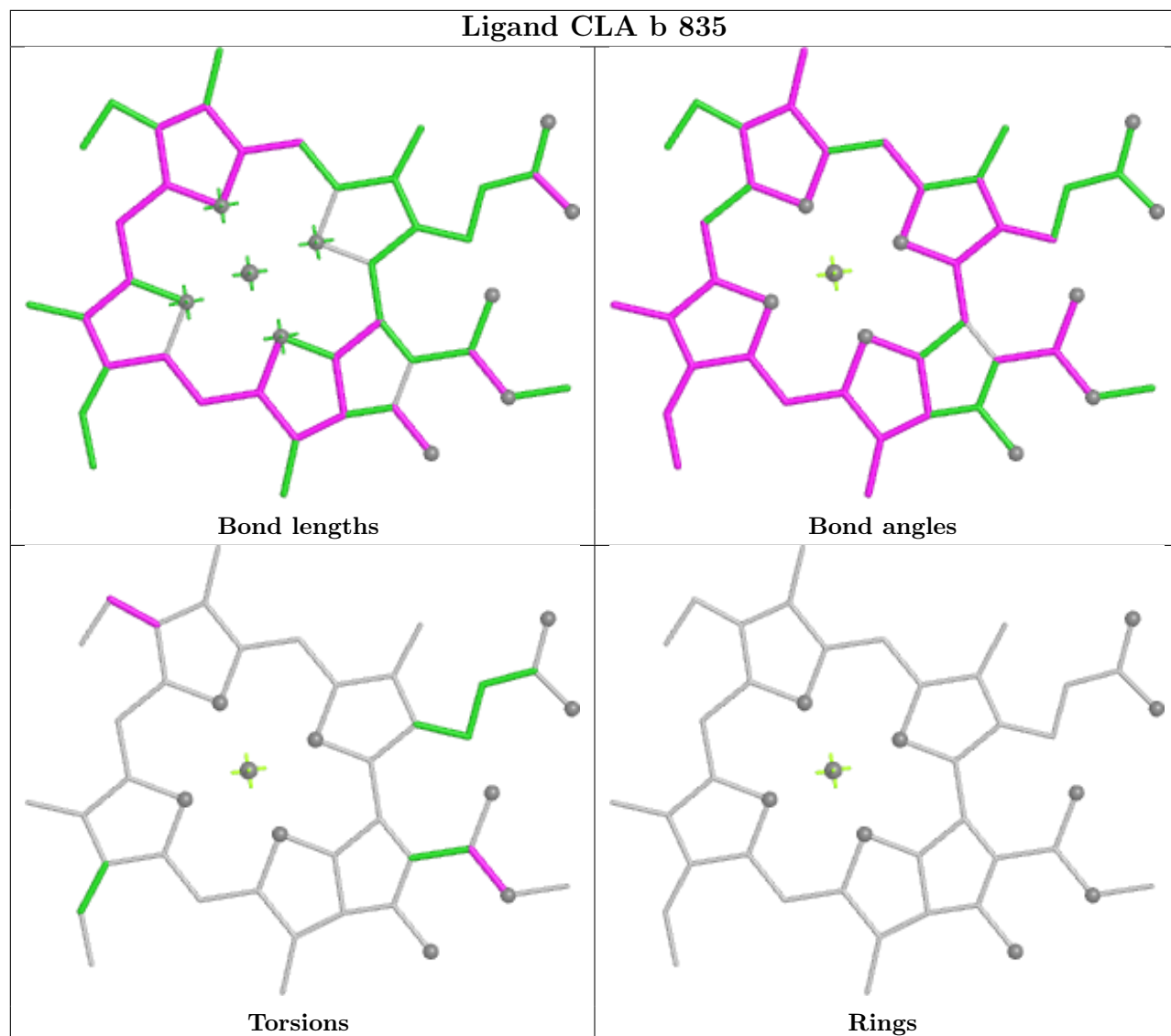


Rings

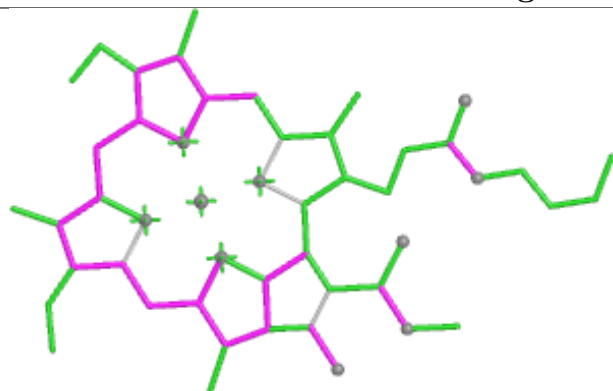
Ligand CLA 9 611



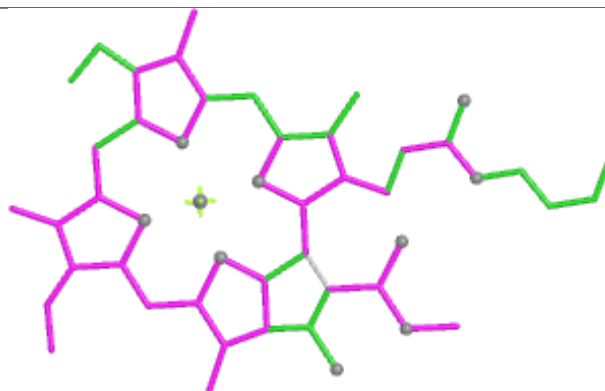
Ligand CLA b 835



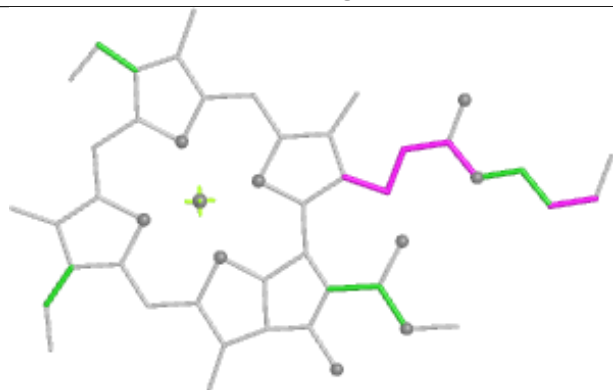
Ligand CLA b 831



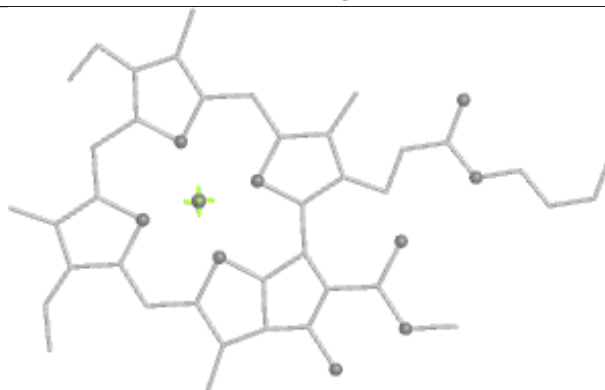
Bond lengths



Bond angles

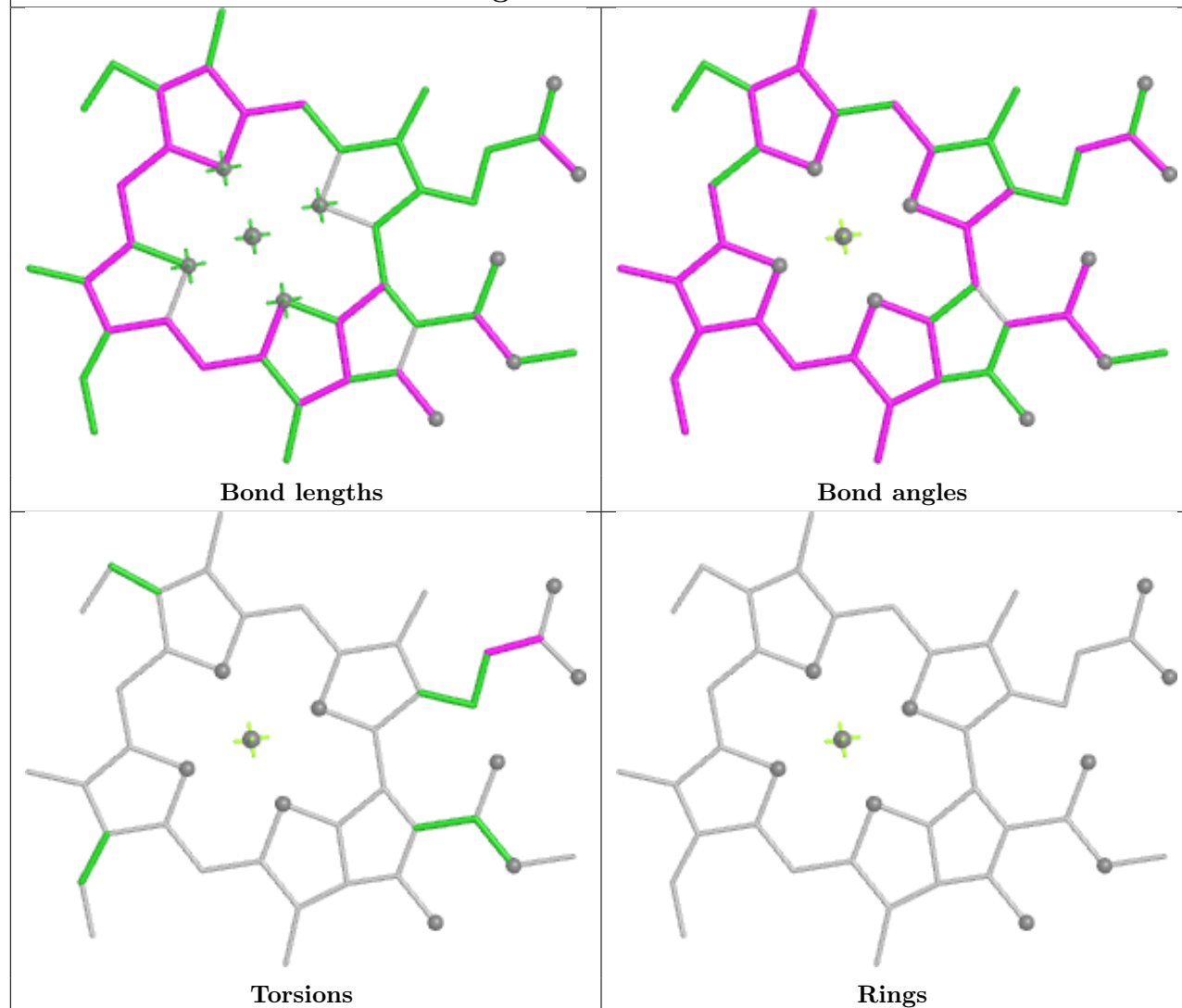


Torsions

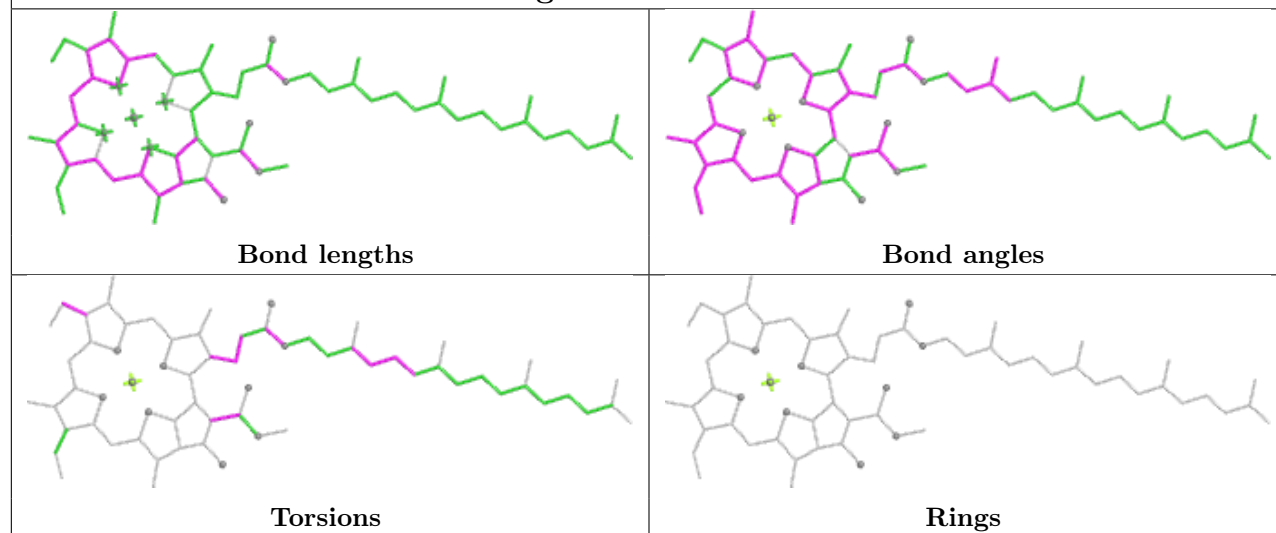


Rings

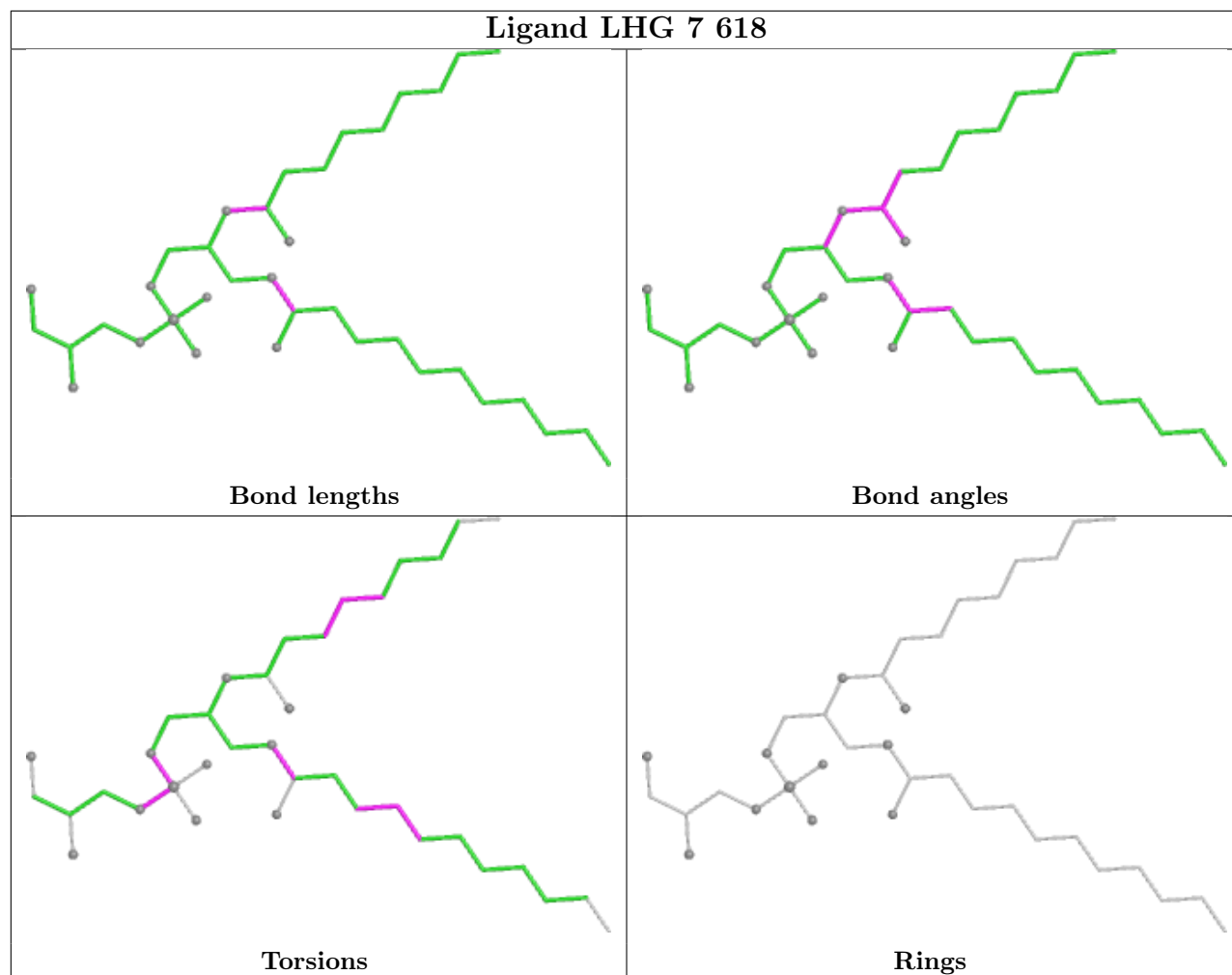
Ligand CLA A 821



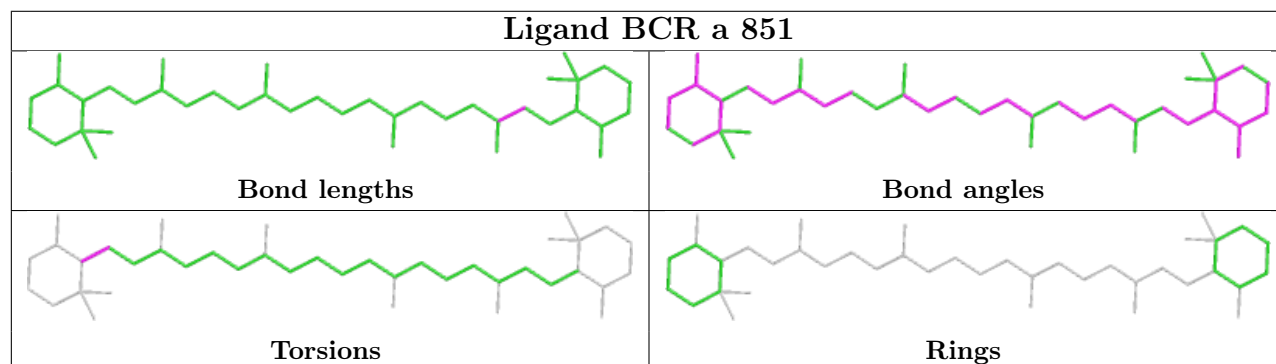
Ligand CLA a 834

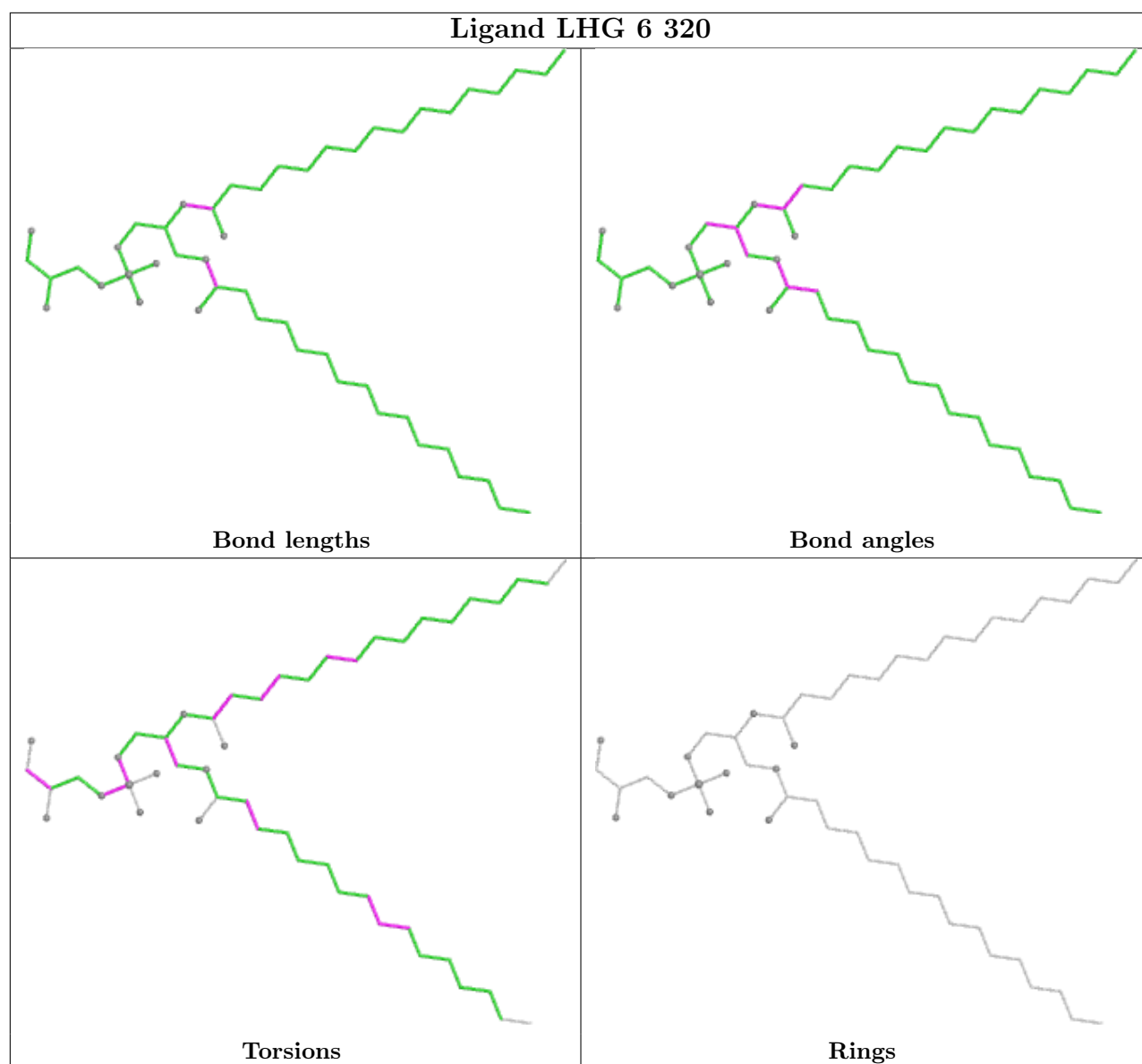


Ligand LHG 7 618

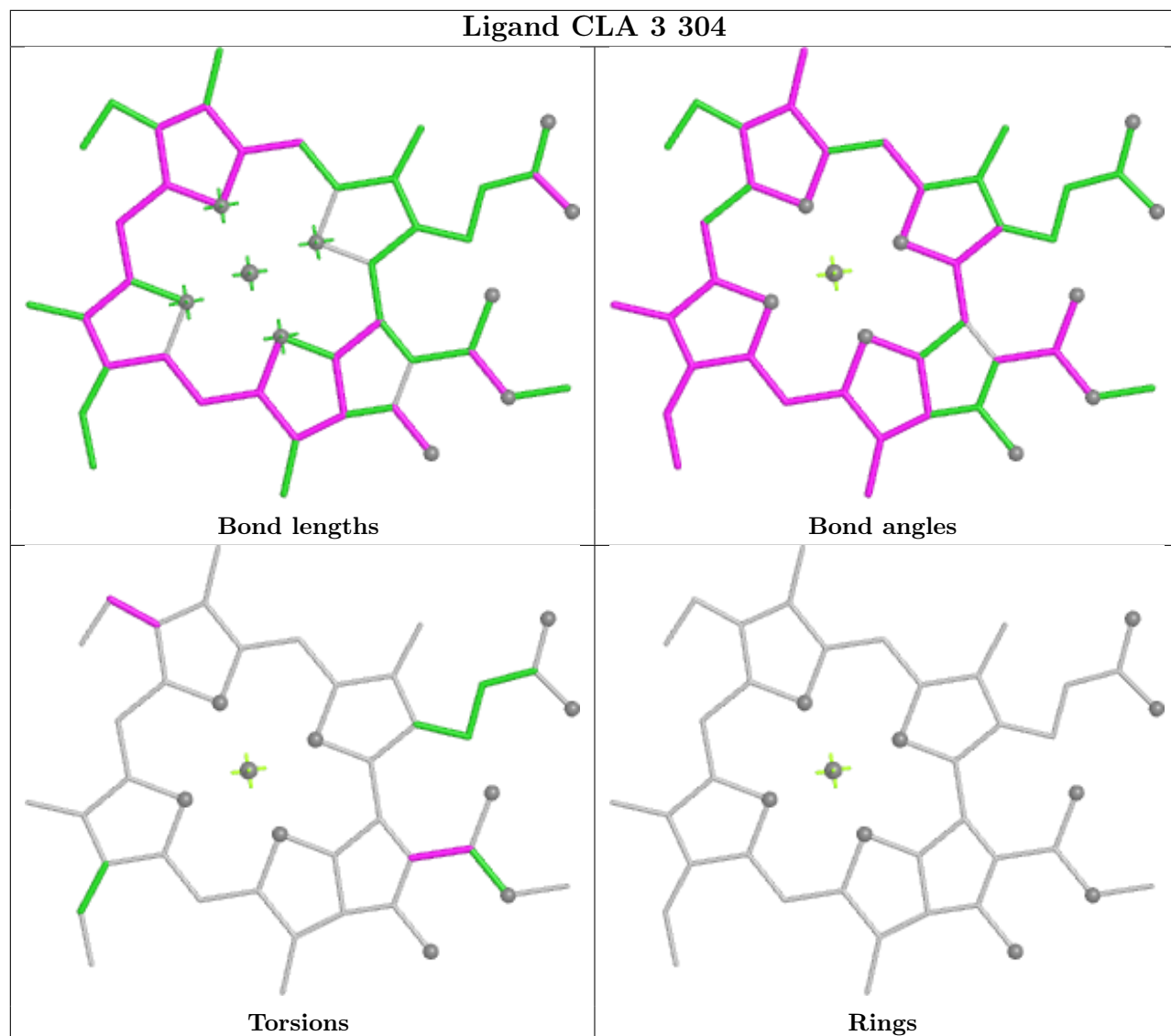


Ligand BCR a 851

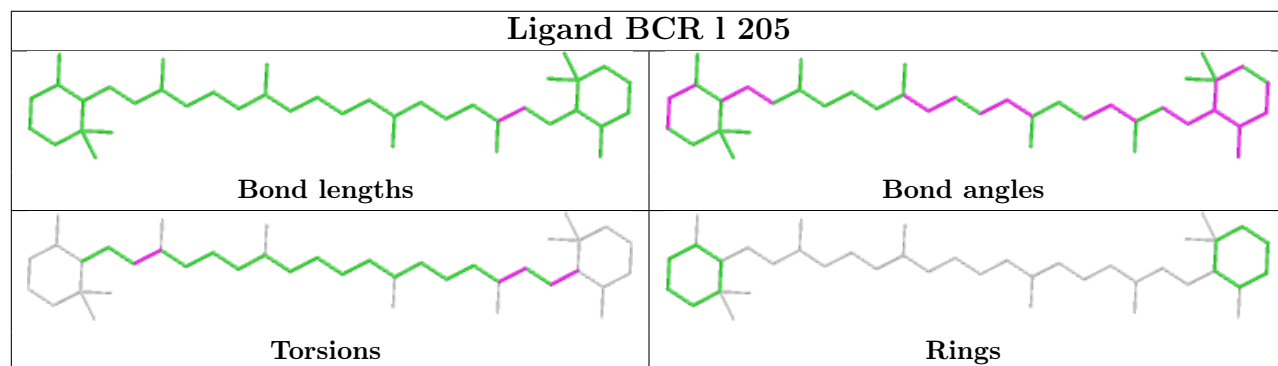


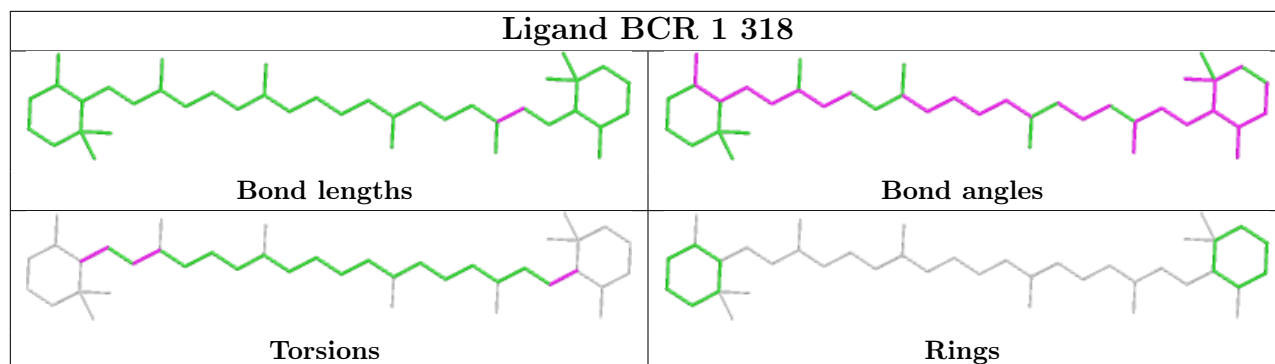
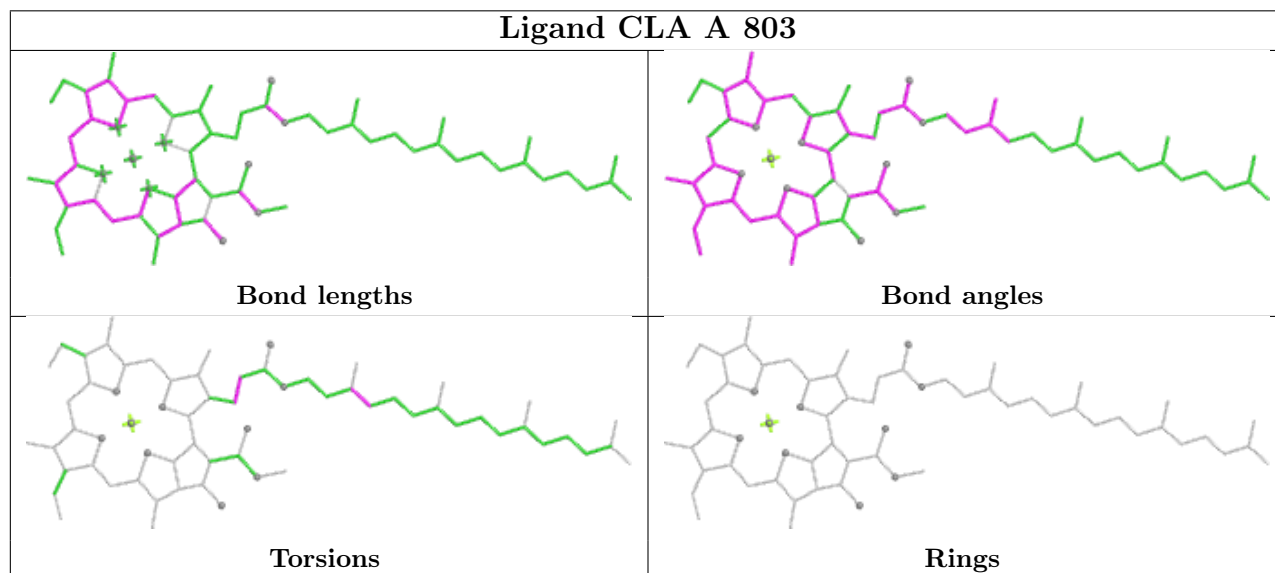
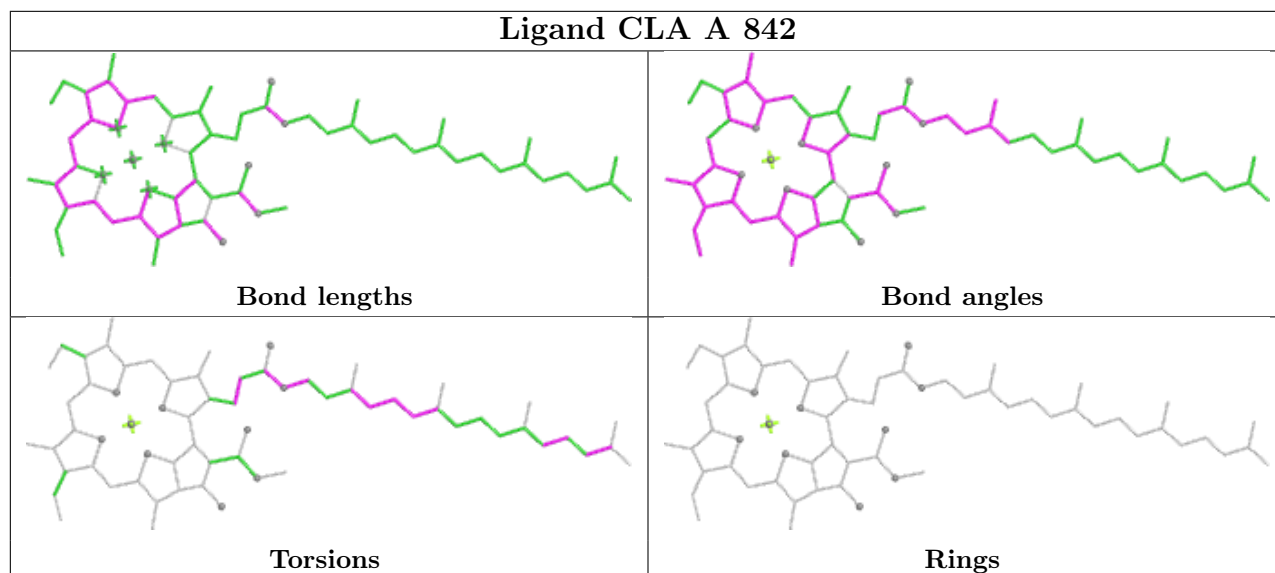


Ligand CLA 3 304

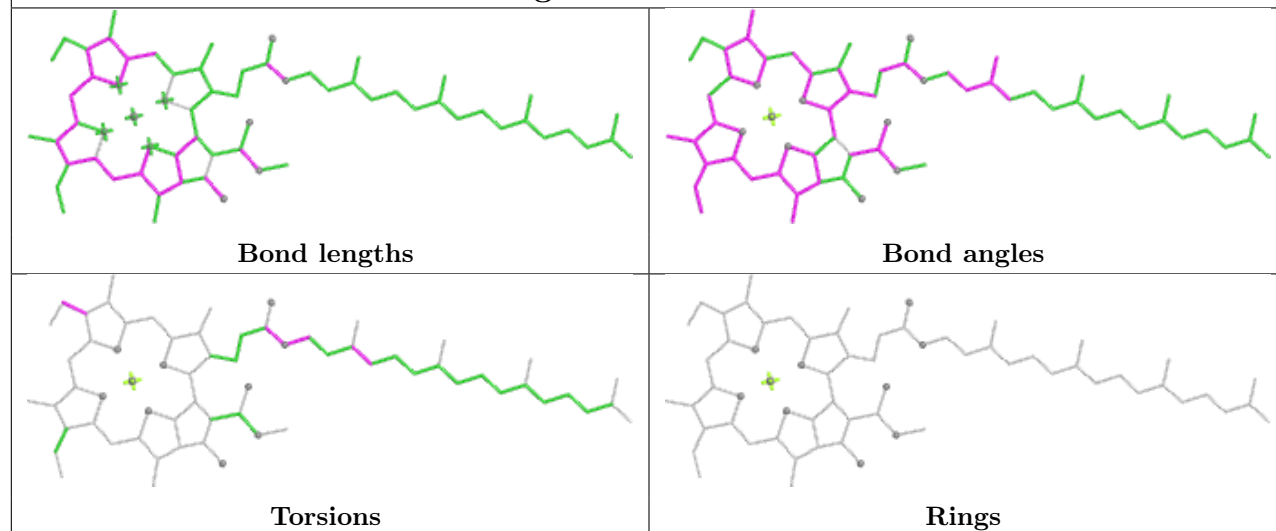


Ligand BCR 1 205

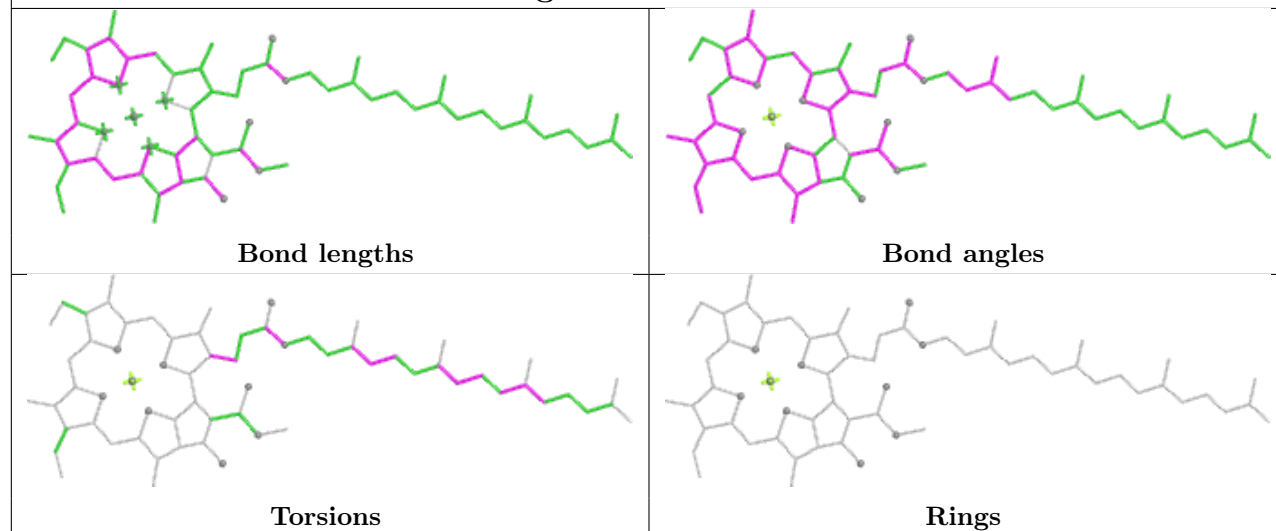


Ligand BCR 1 318**Ligand CLA A 803****Ligand CLA A 842**

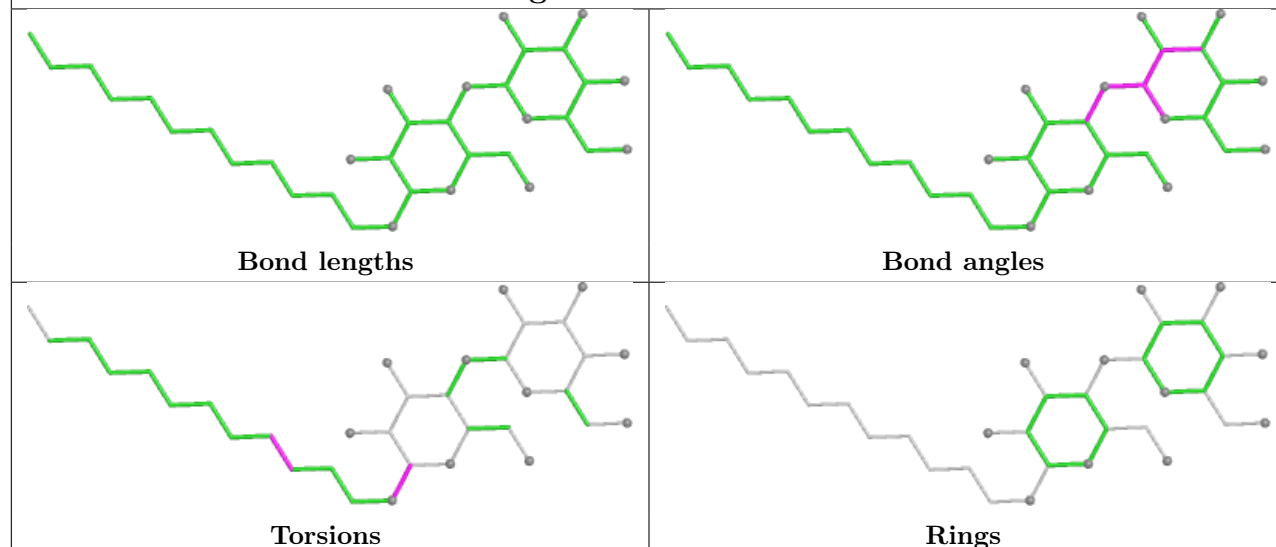
Ligand CLA L 203



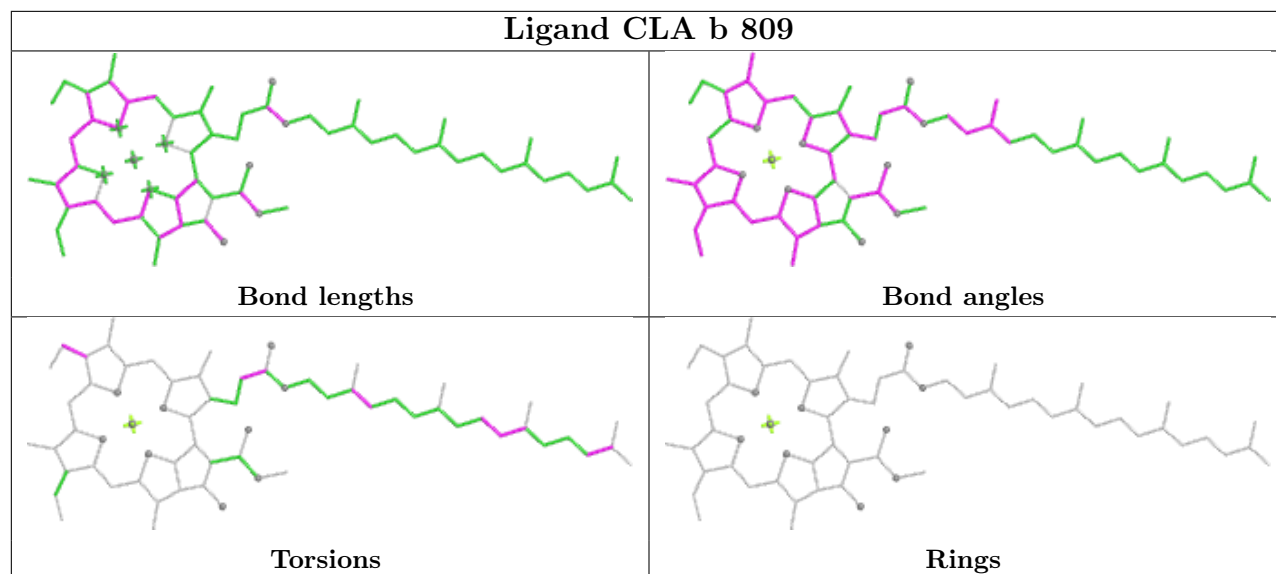
Ligand CLA a 807



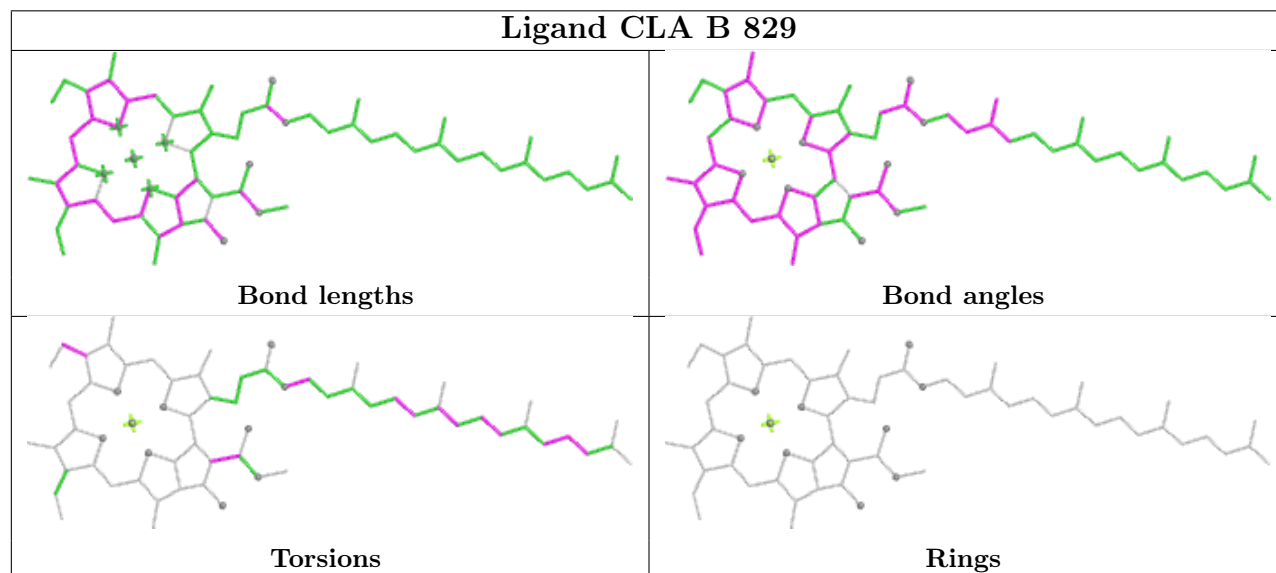
Ligand LMT B 849



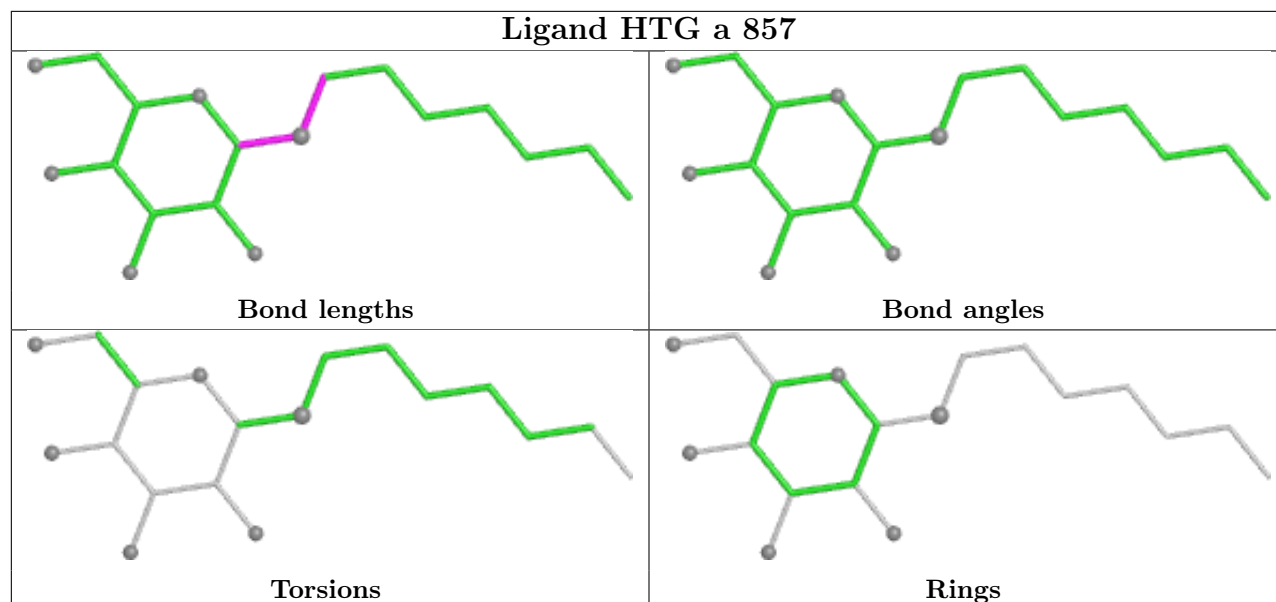
Ligand CLA b 809

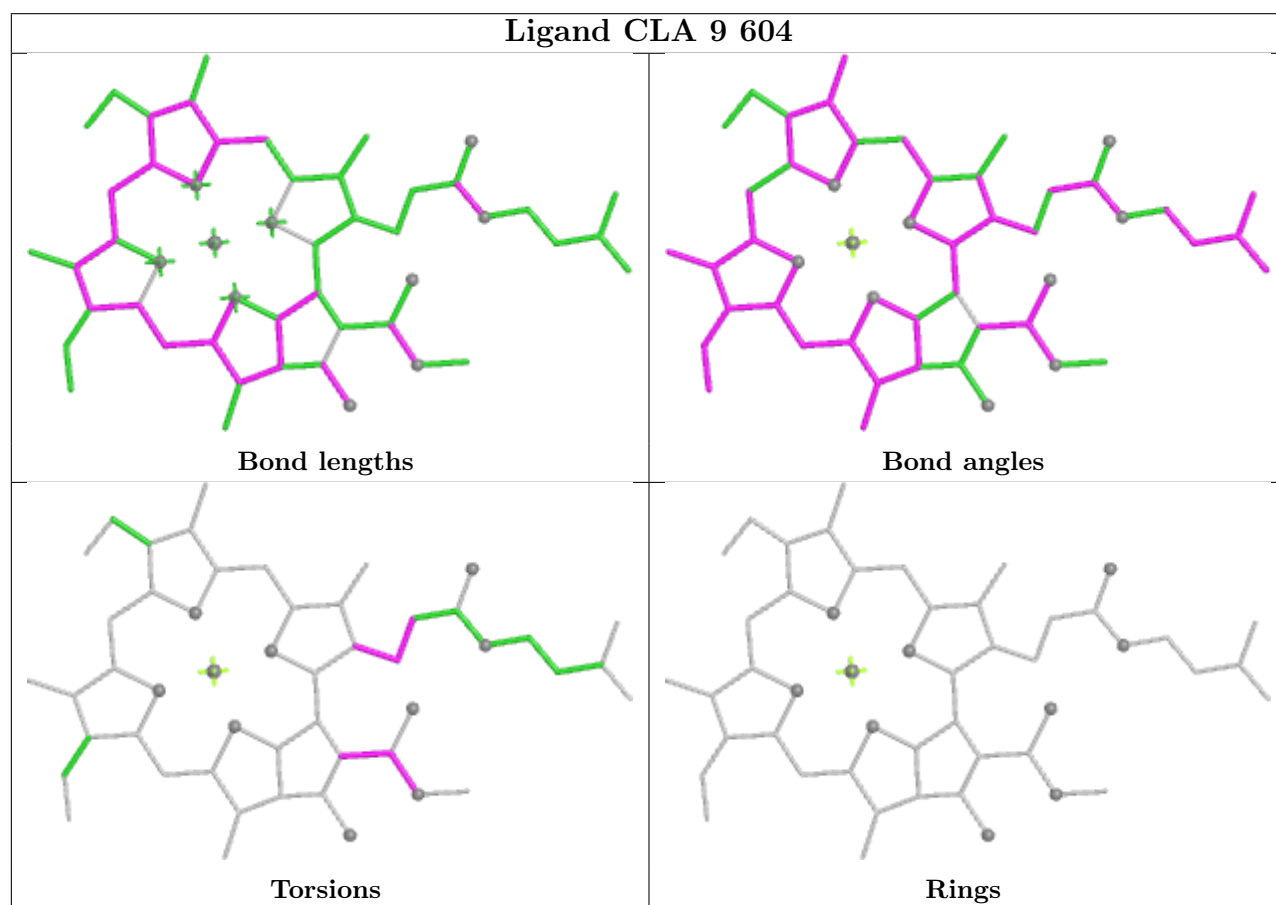
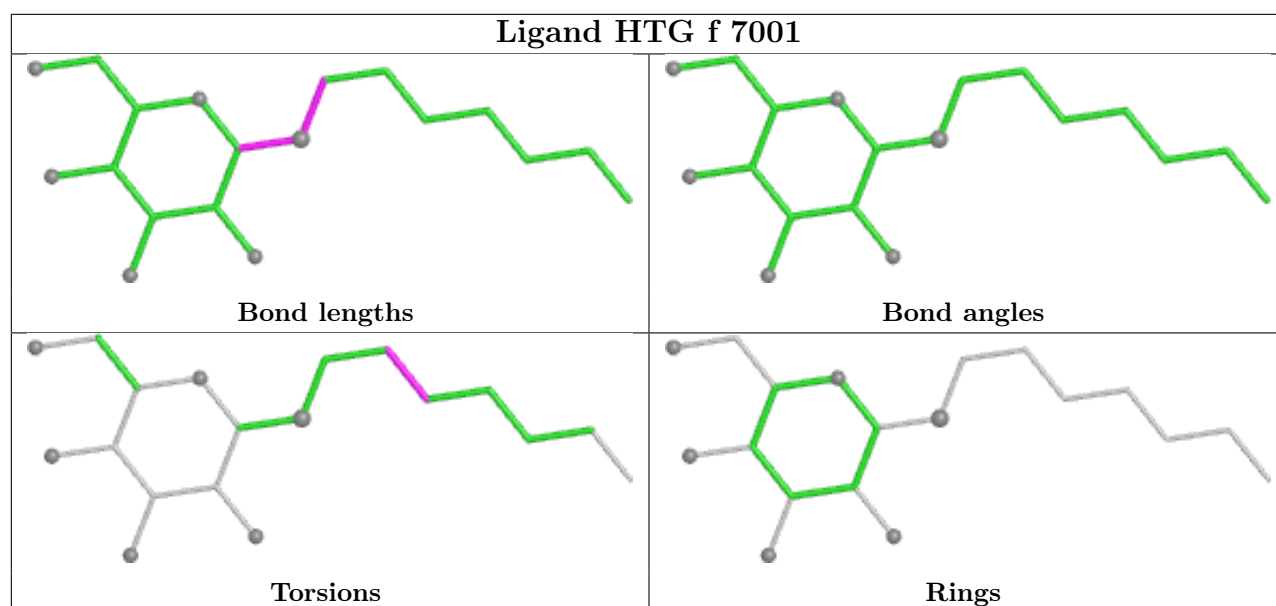


Ligand CLA B 829

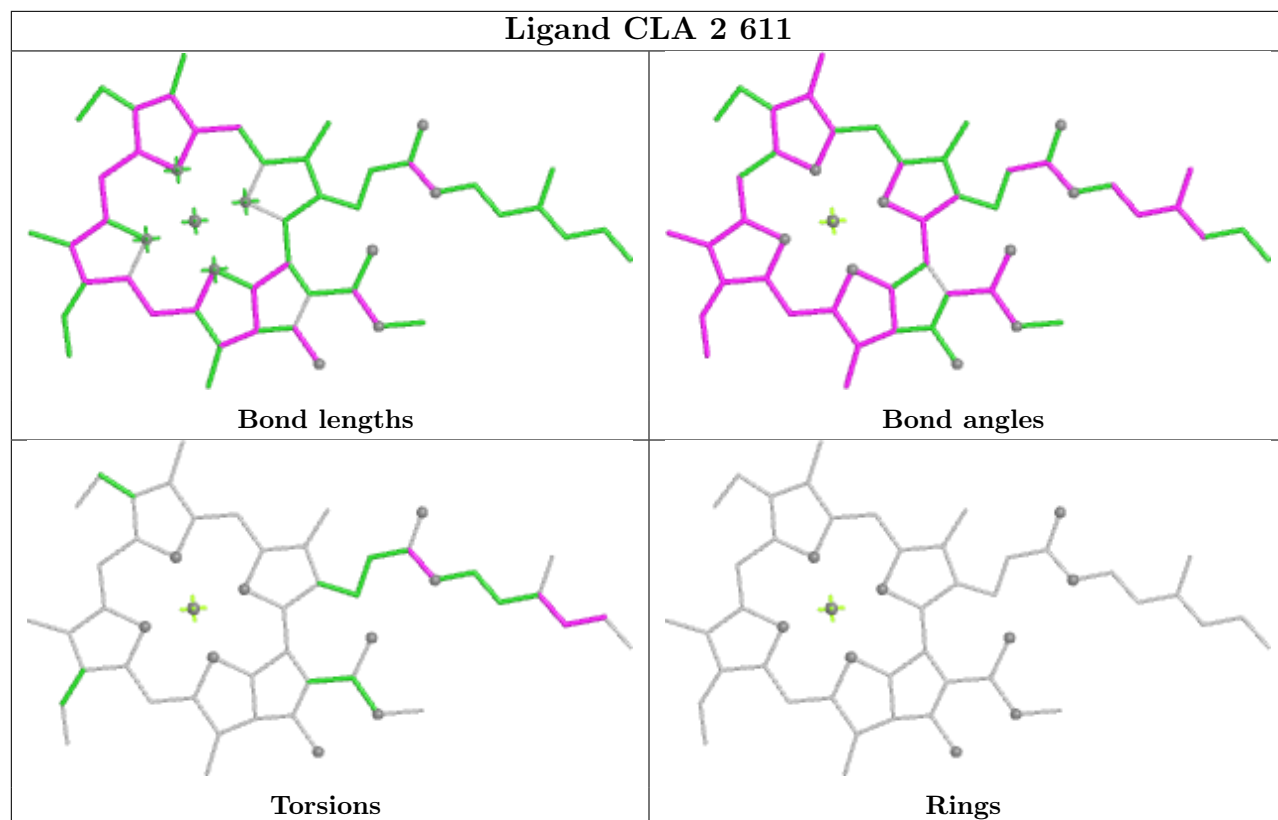


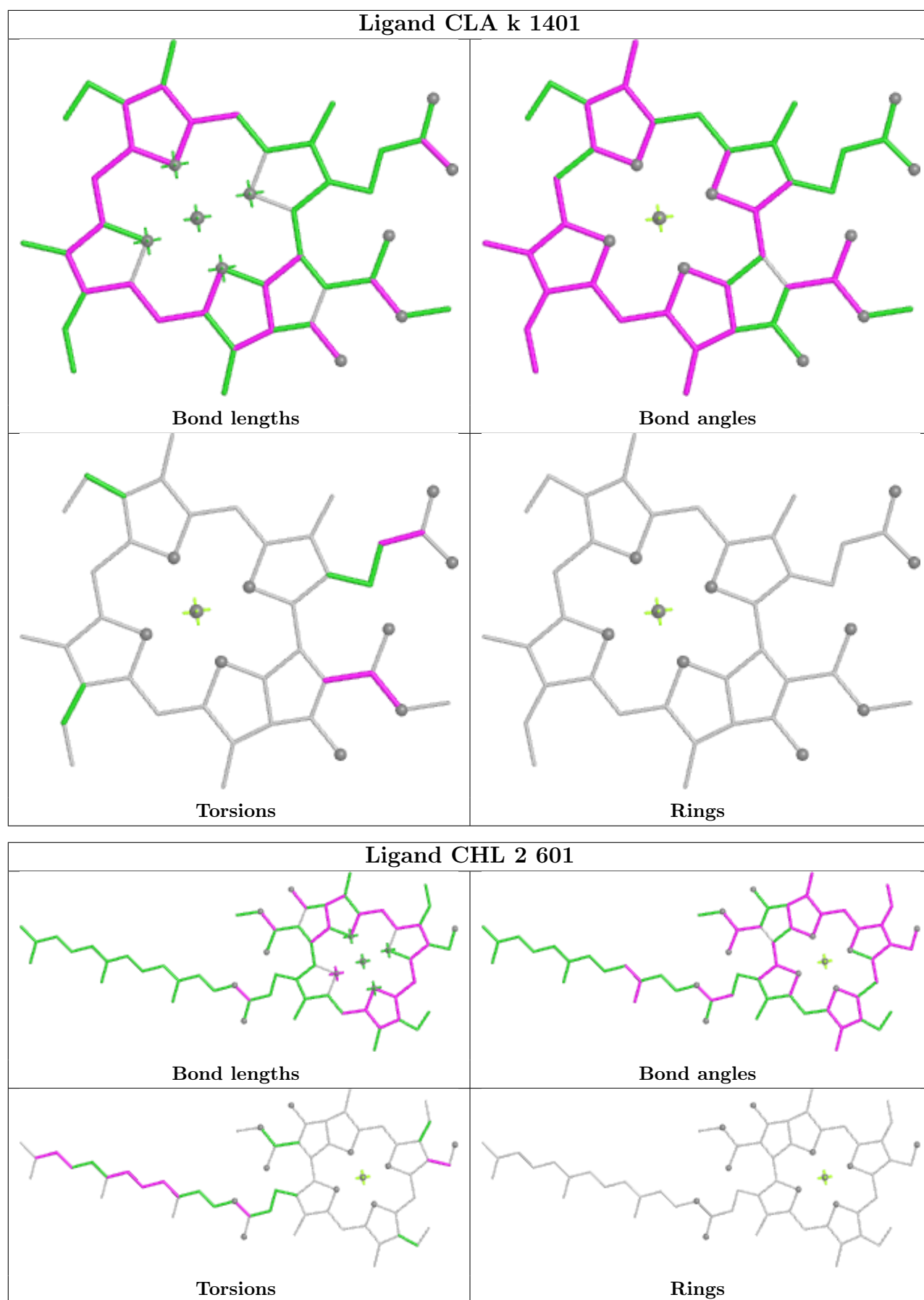
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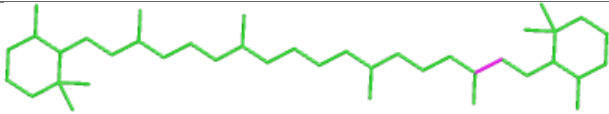
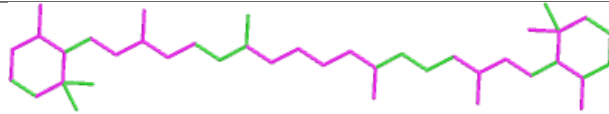
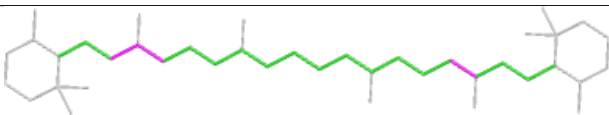
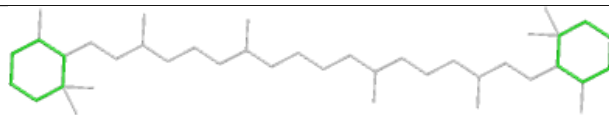


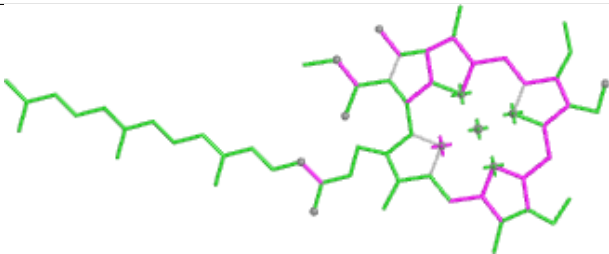
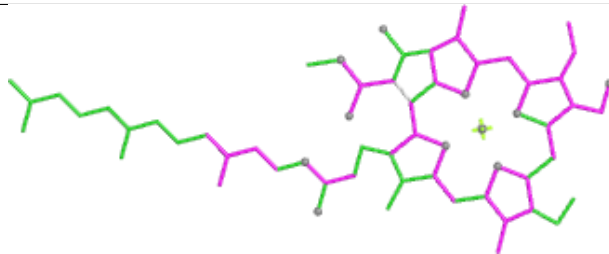
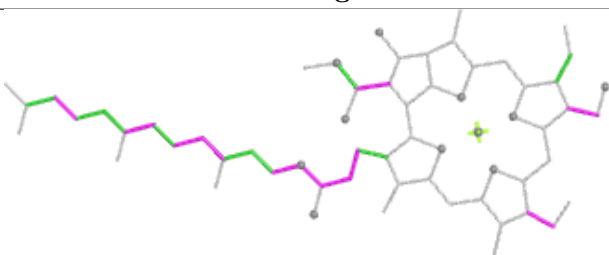
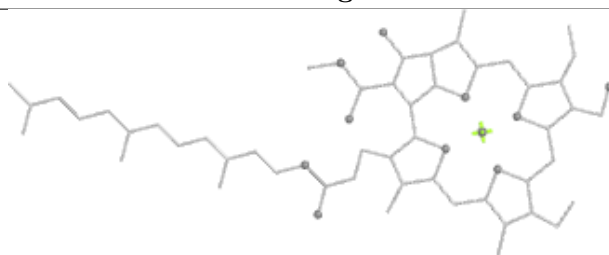


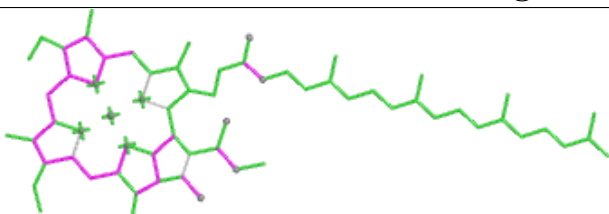
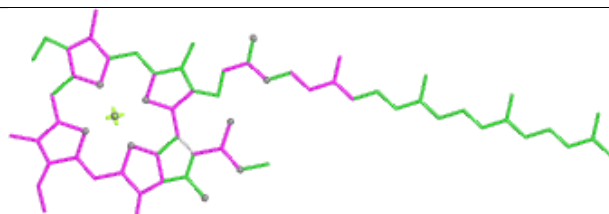
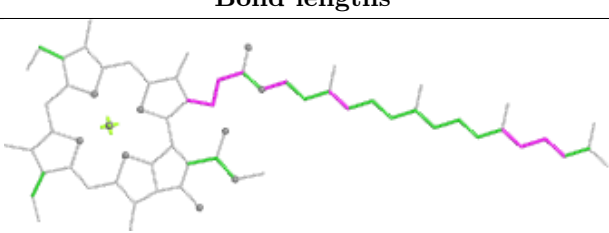
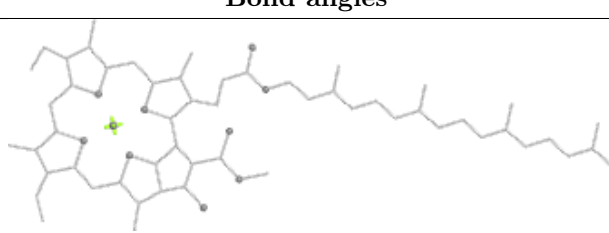
Ligand CLA 2 611

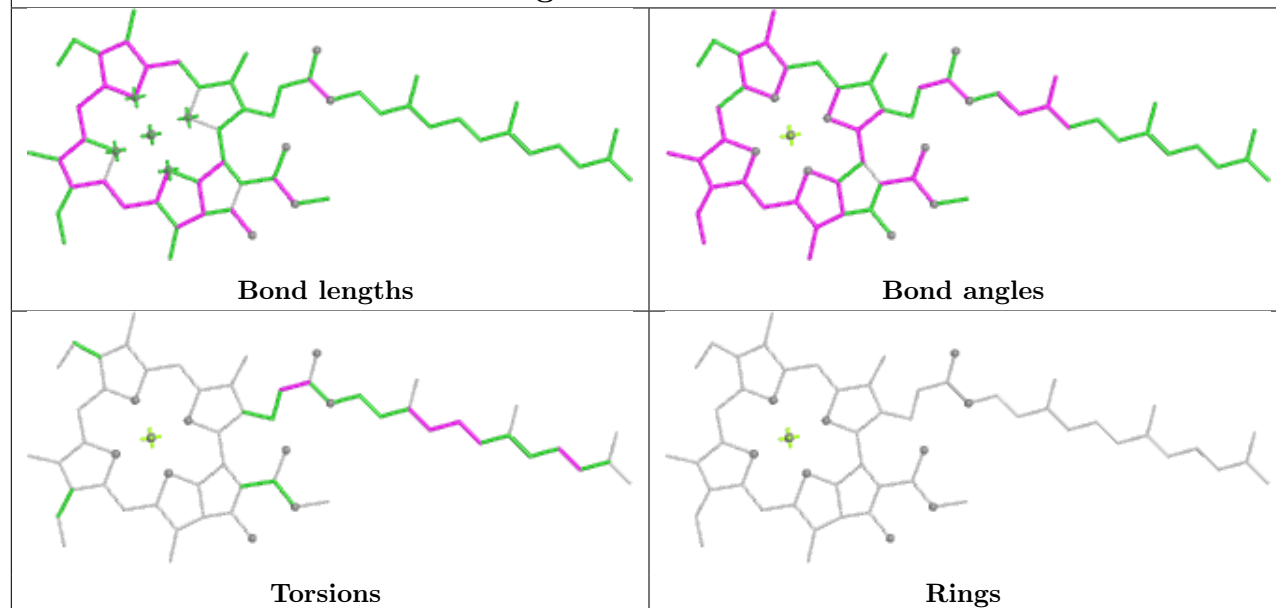
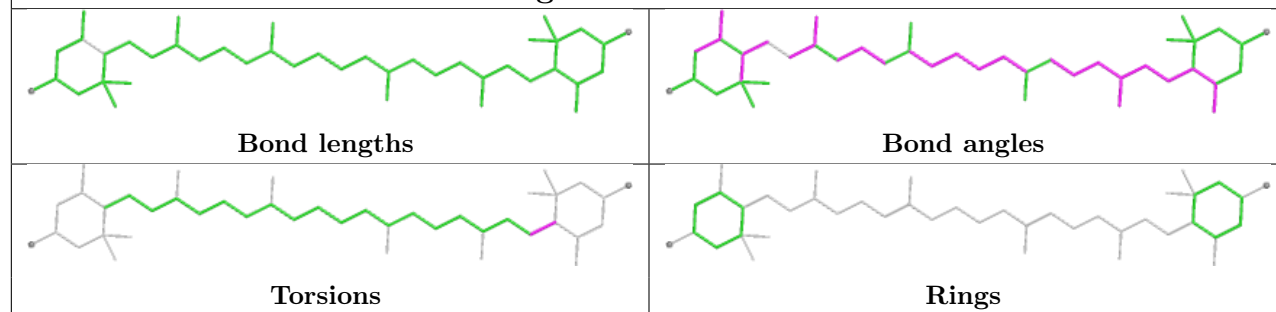




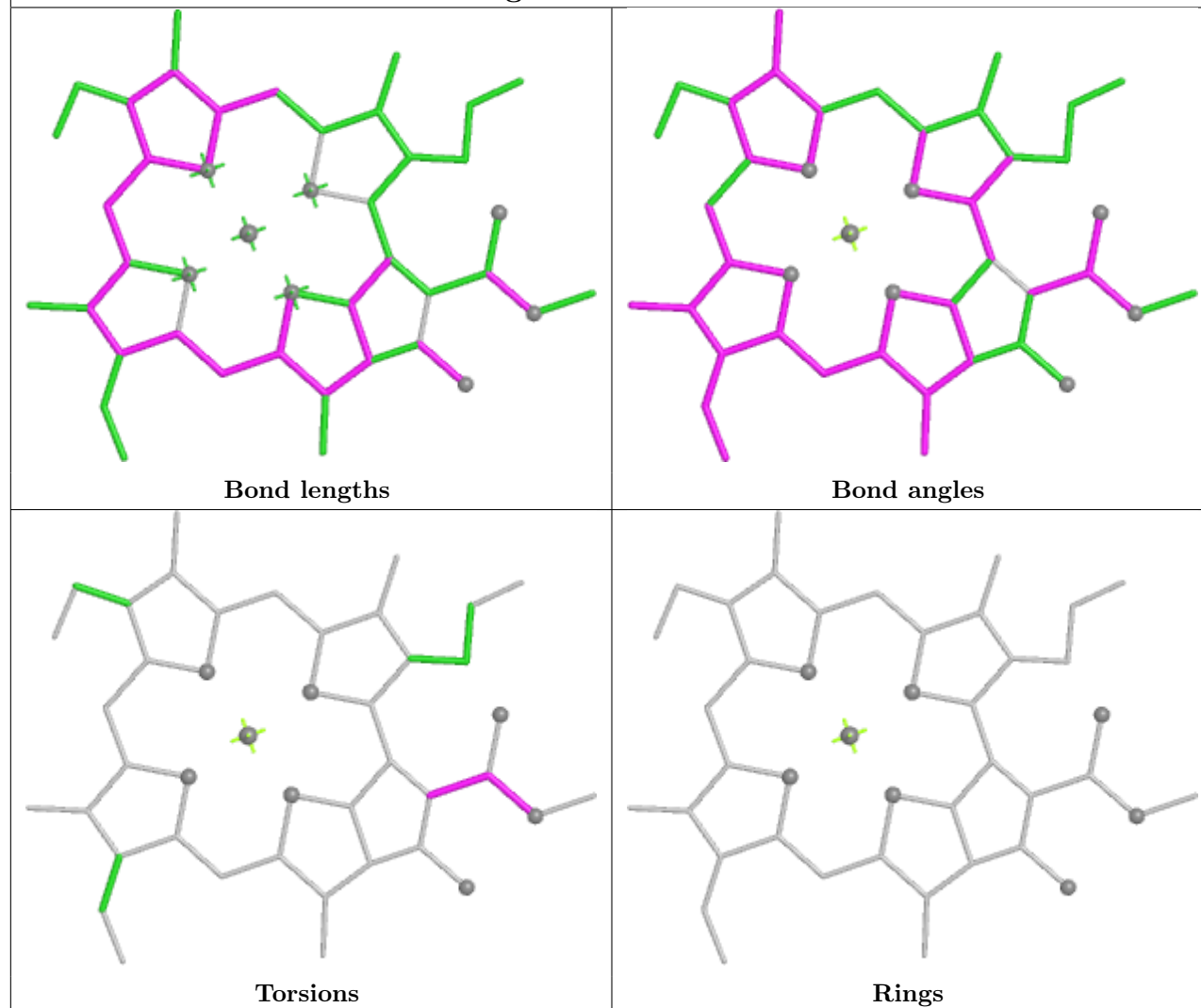
Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 6 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

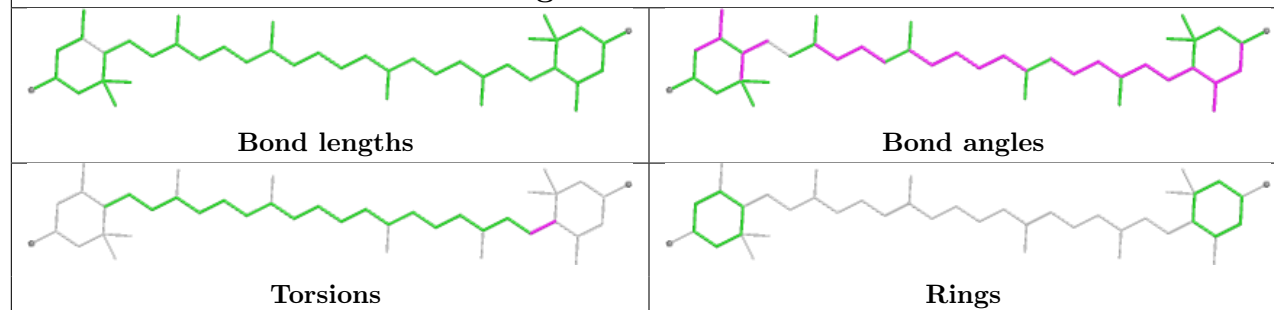
Ligand CLA a 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

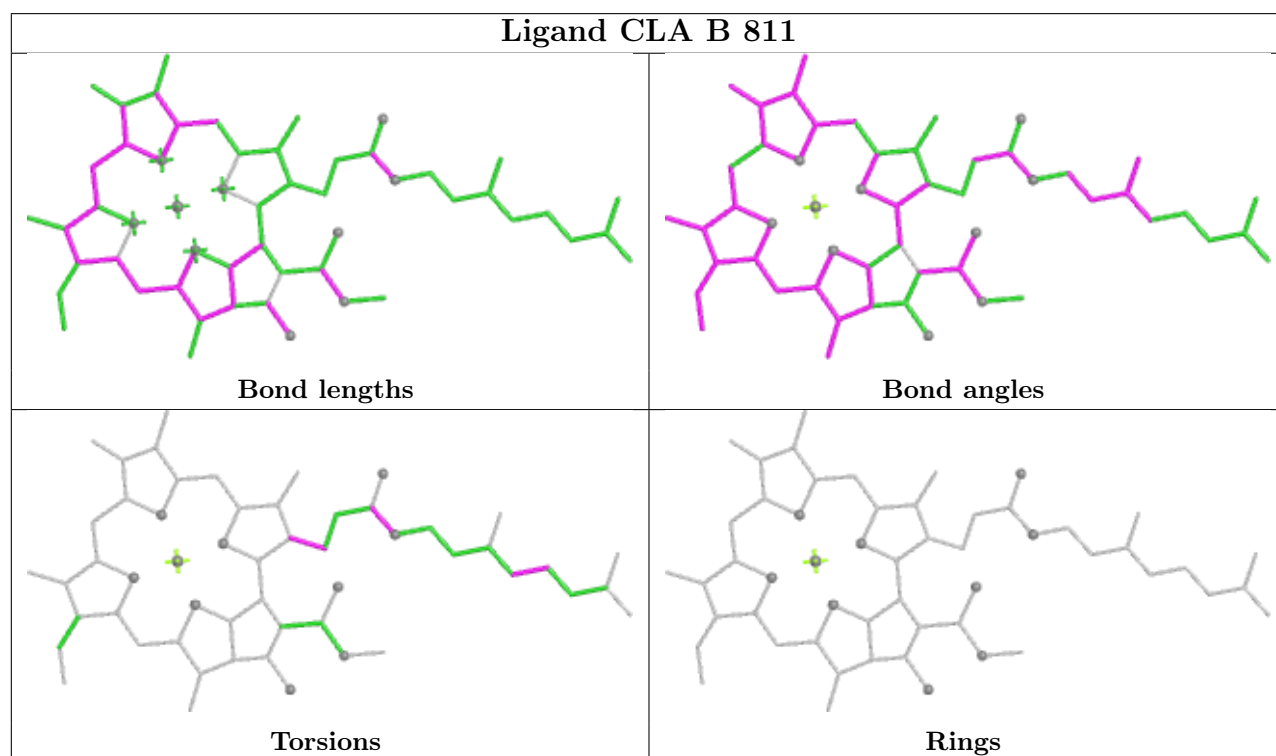
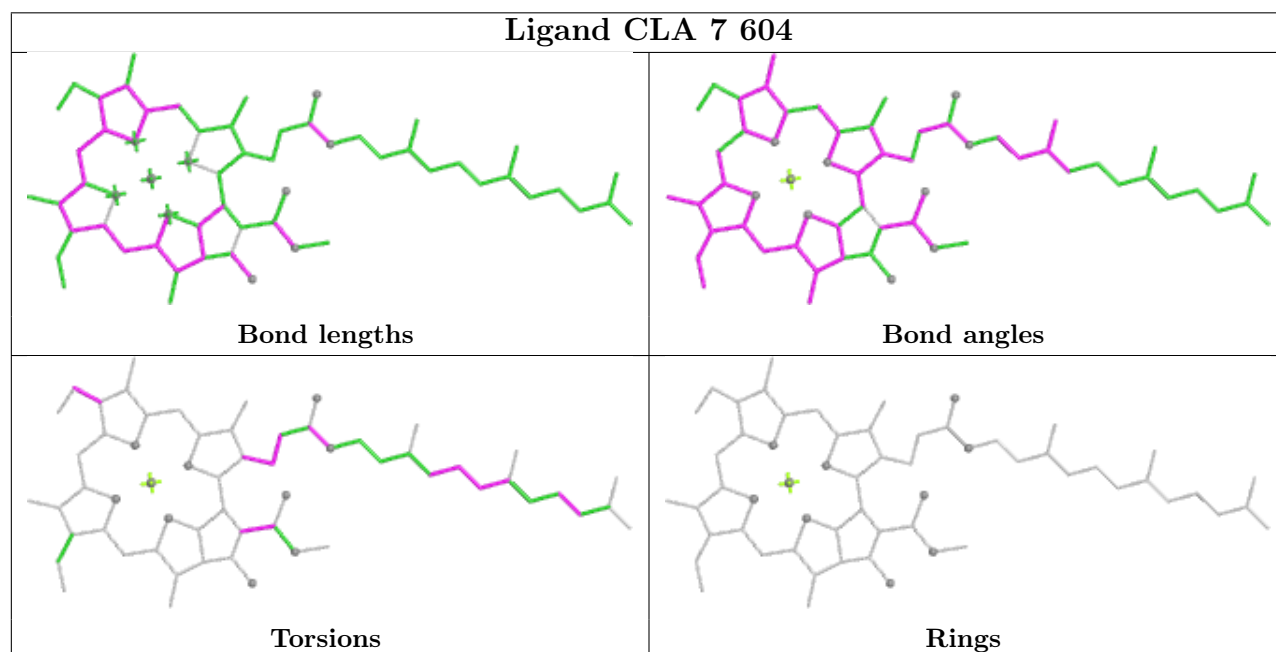
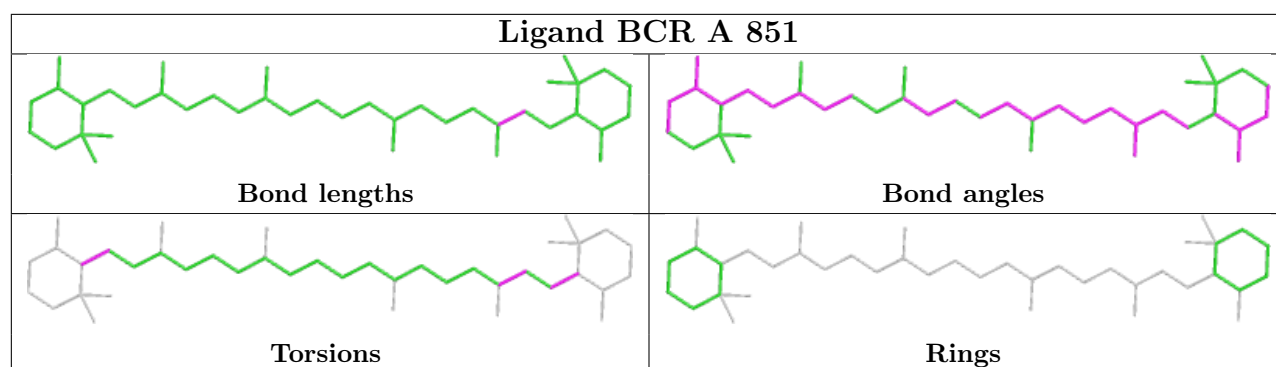
Ligand CLA 6 314**Ligand LUT 7 615**

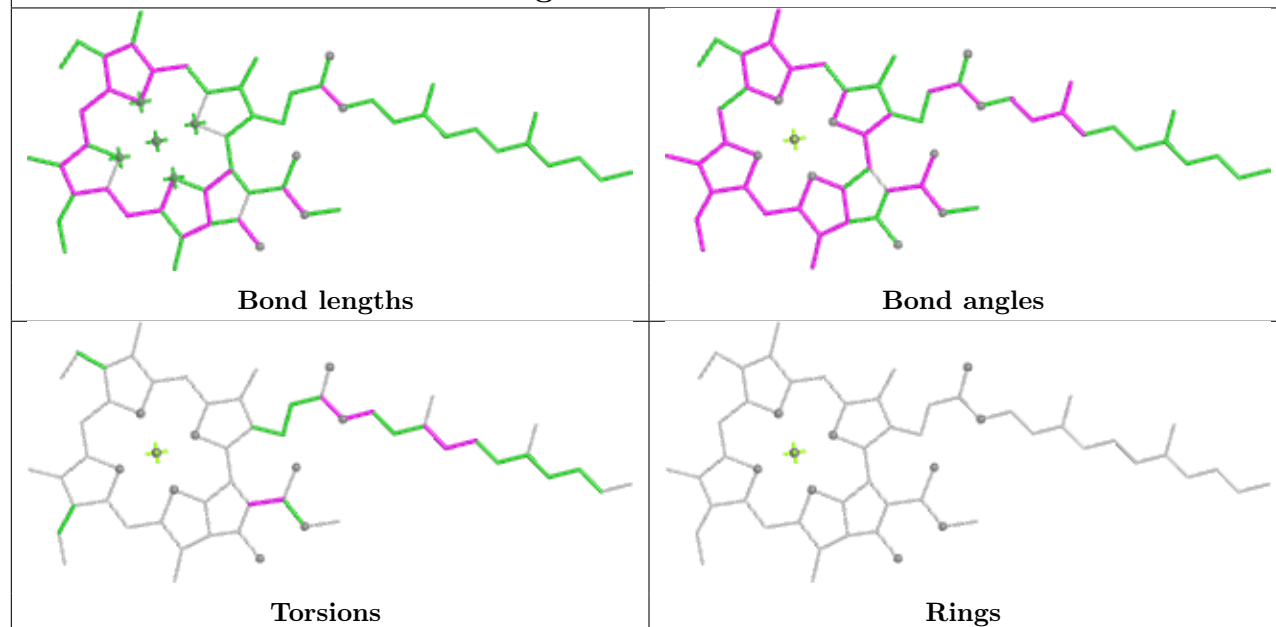
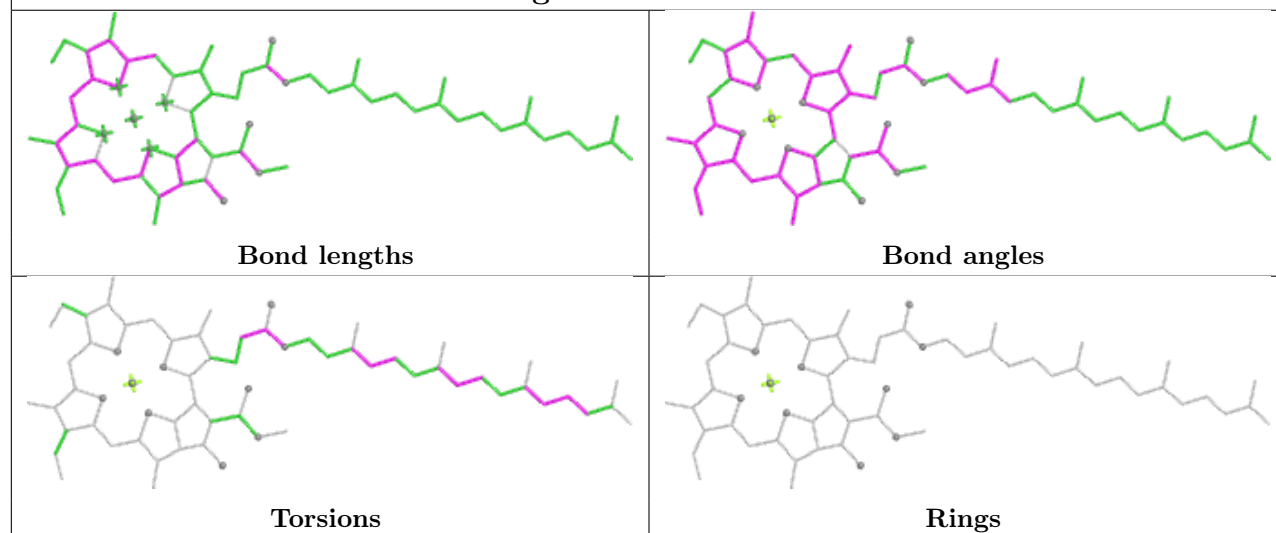
Ligand CLA 2 613



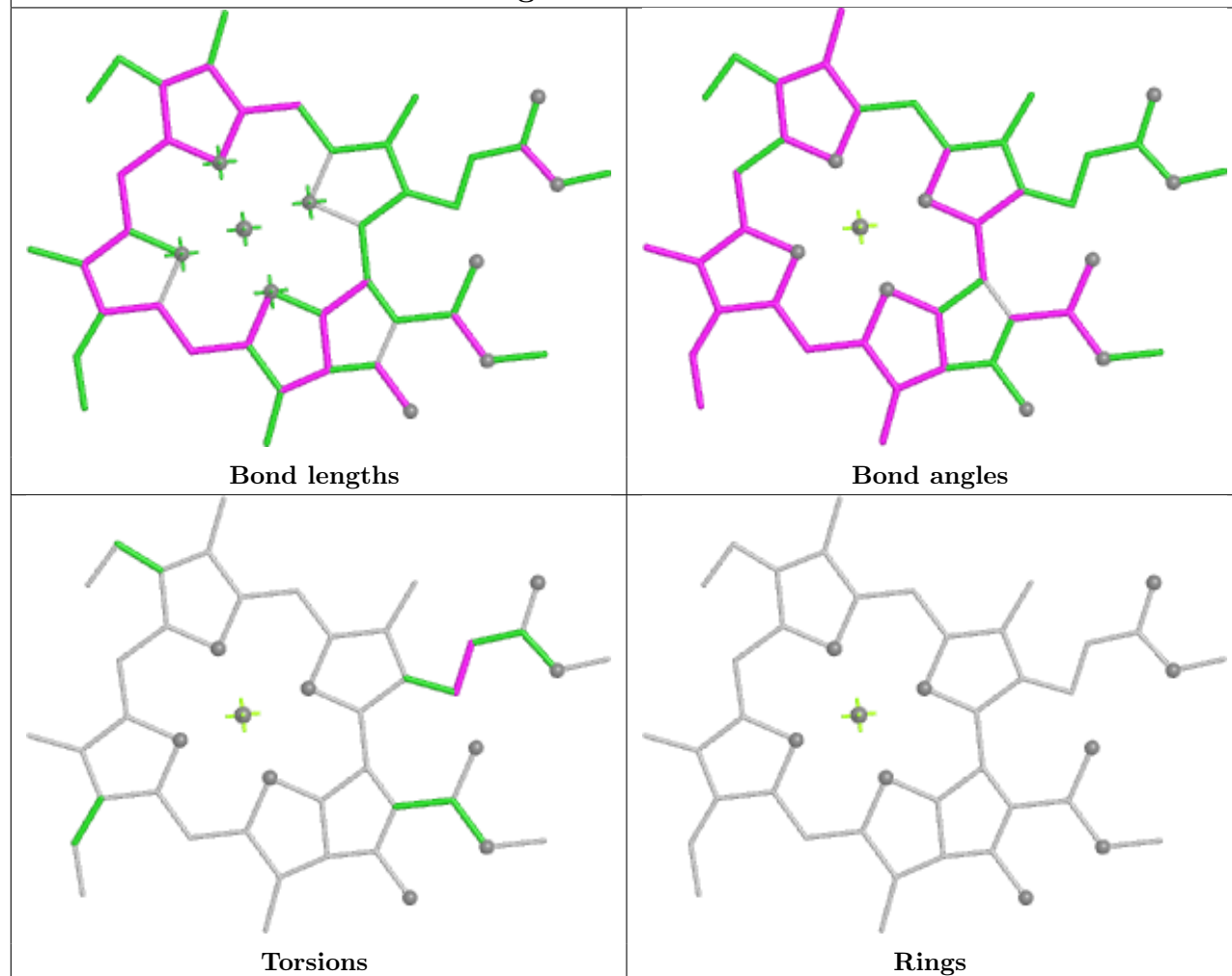
Ligand LUT 3 316



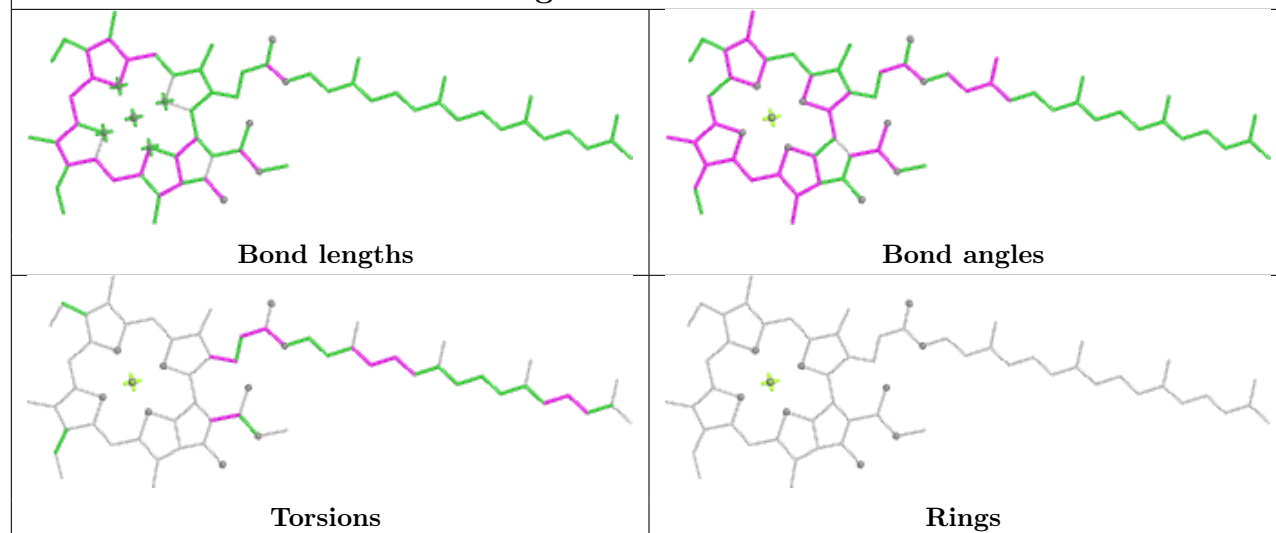


Ligand CLA b 833**Ligand CLA B 814**

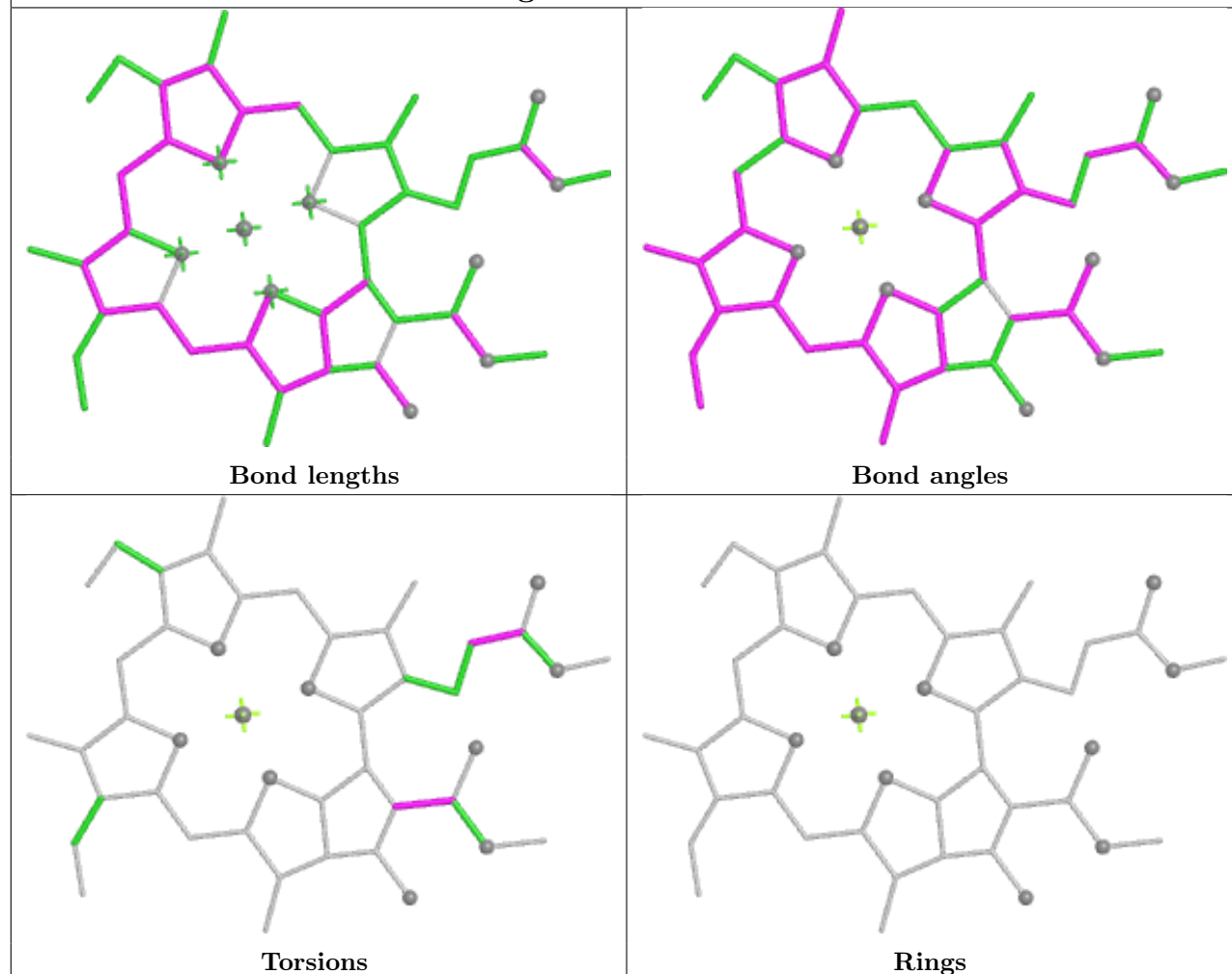
Ligand CLA 1 315



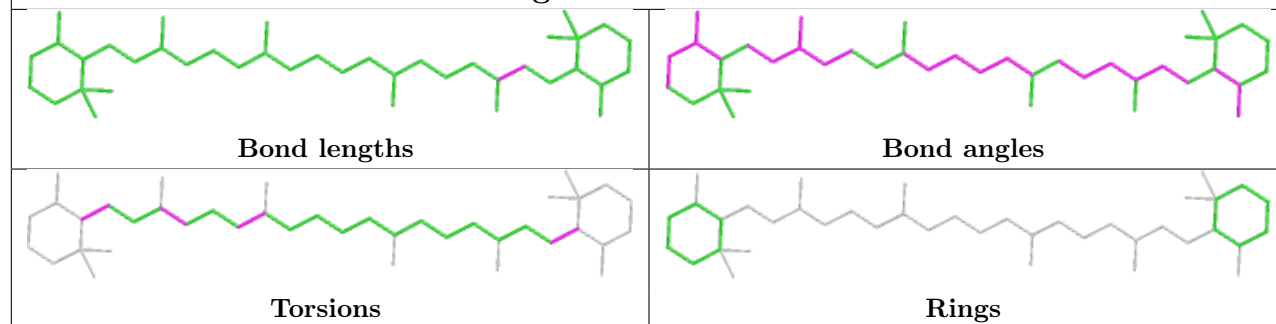
Ligand CLA b 813



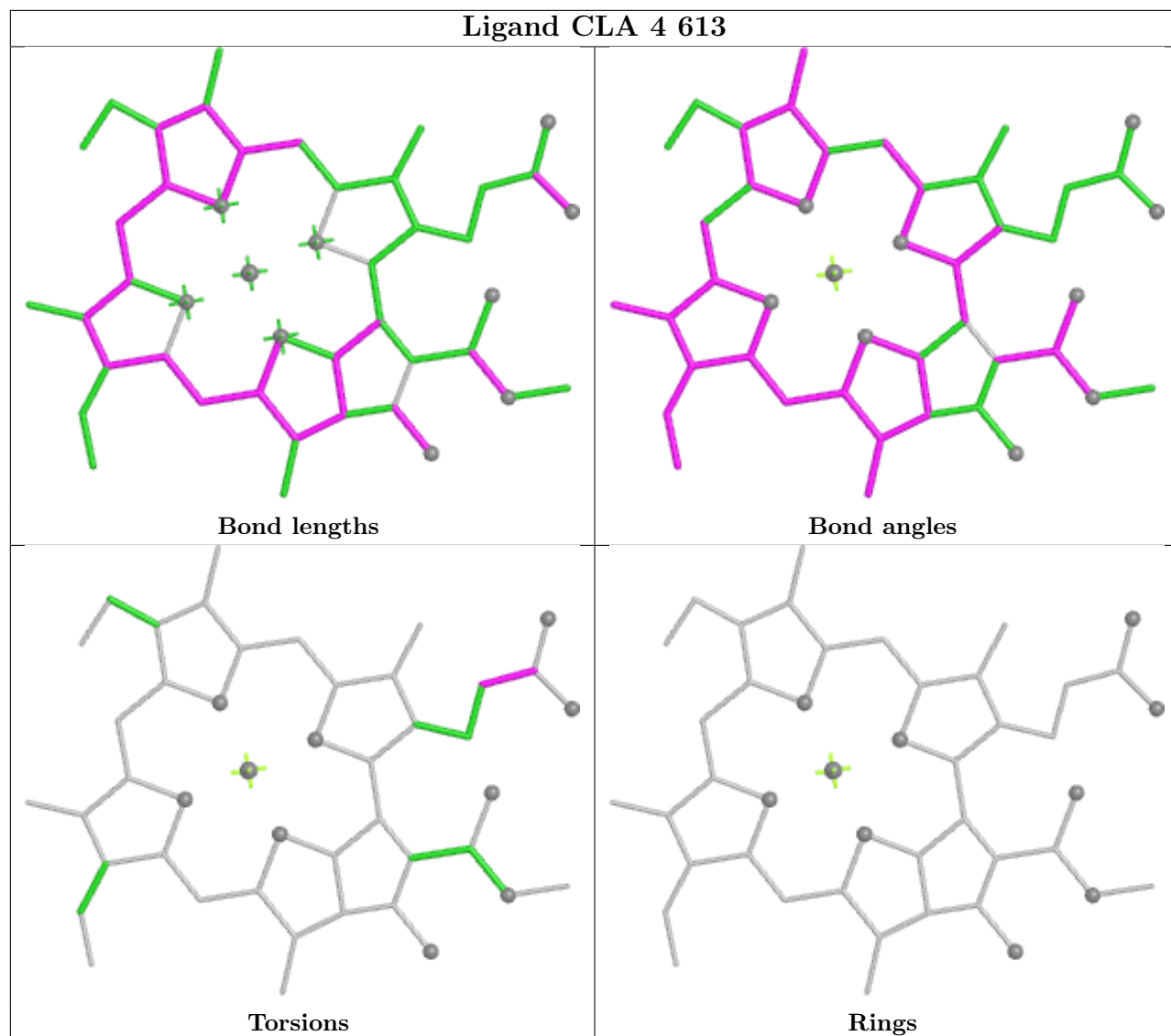
Ligand CLA 9 601



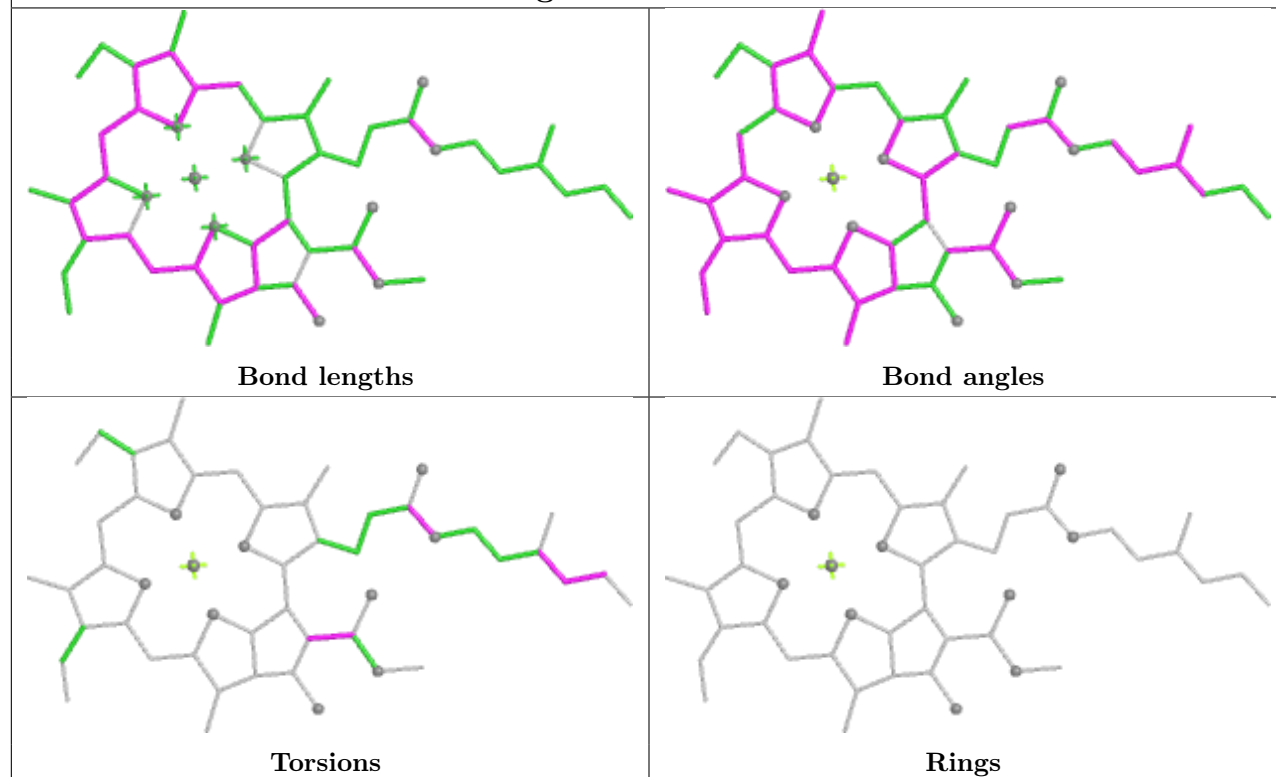
Ligand BCR L 201



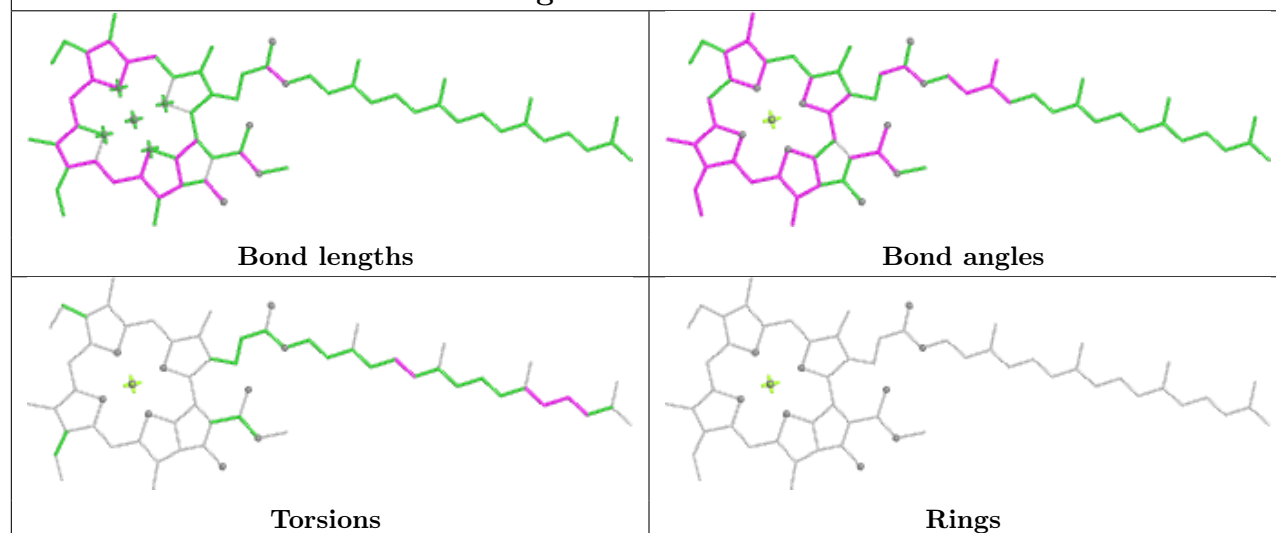
Ligand CLA 4 613



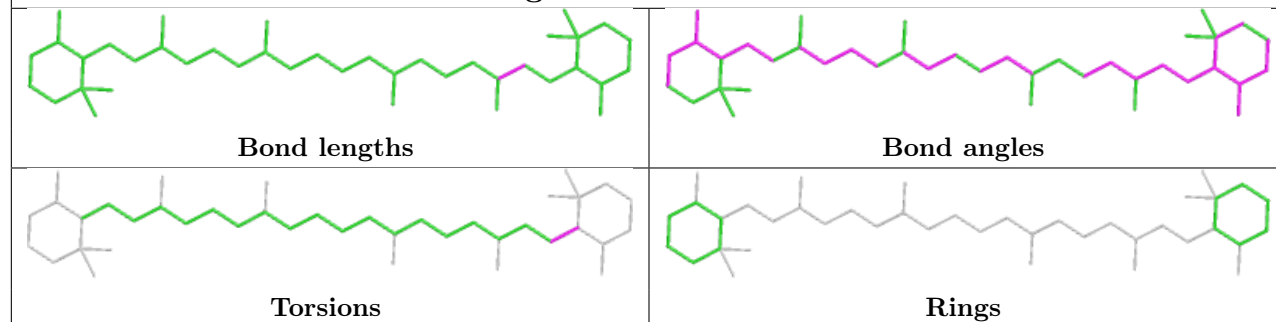
Ligand CLA 3 311

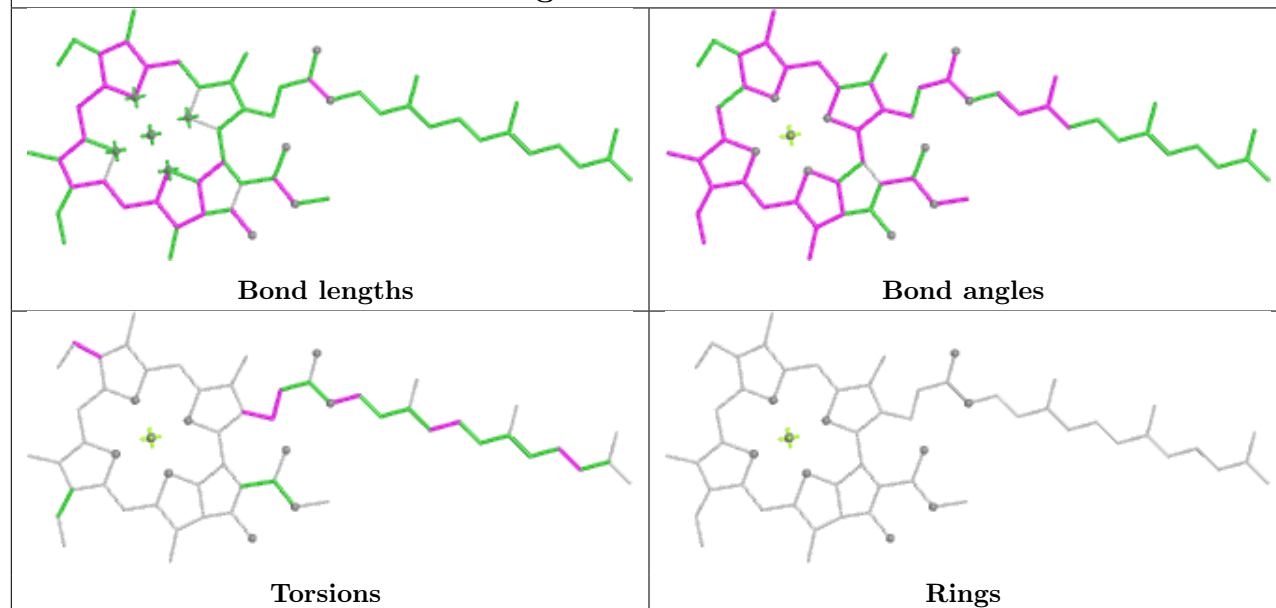
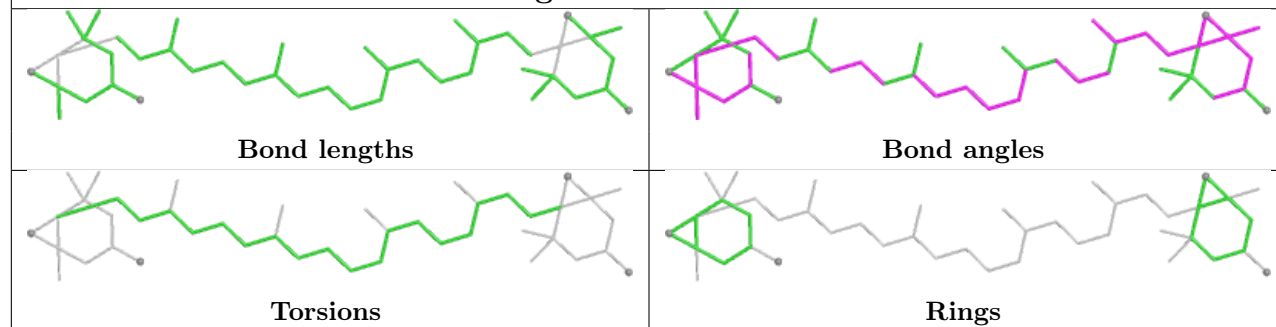


Ligand CLA 1 308

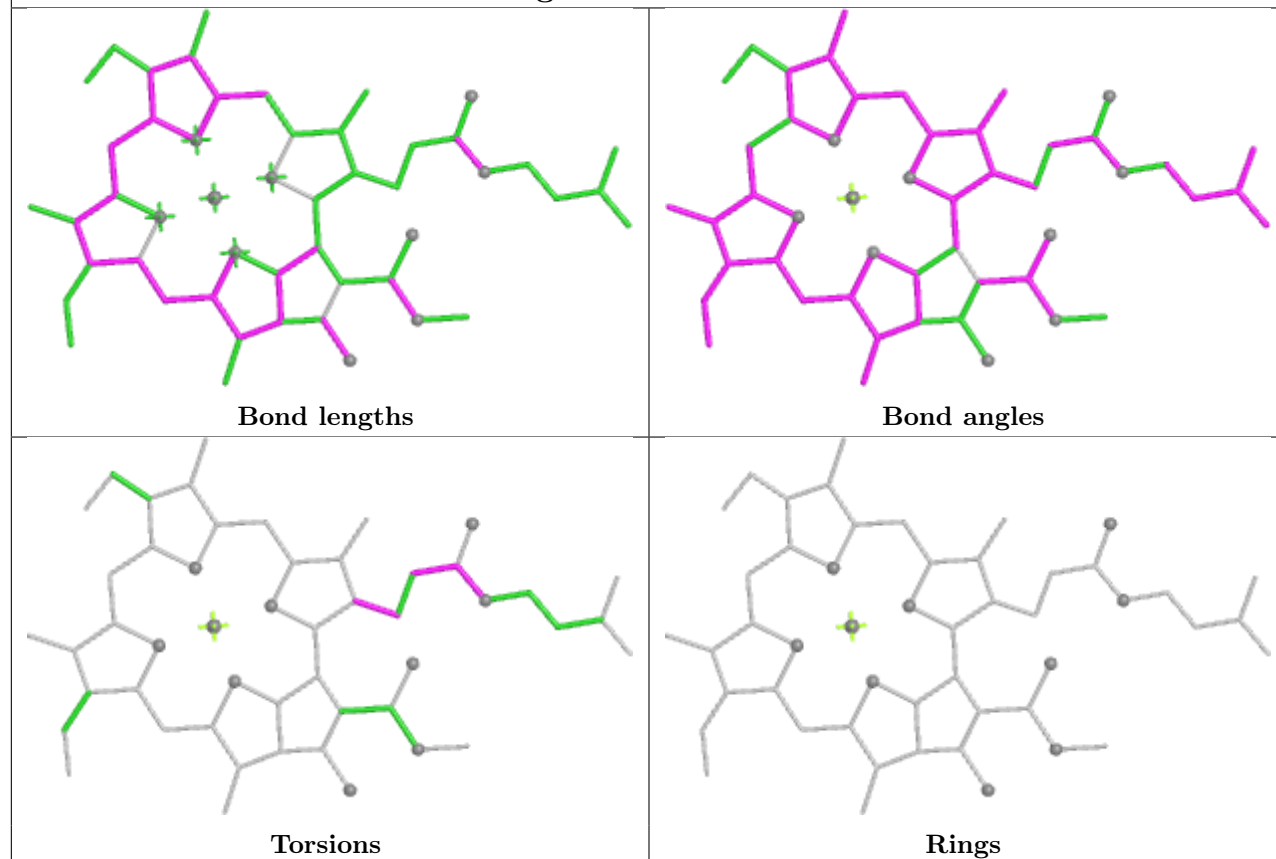


Ligand BCR J 3003

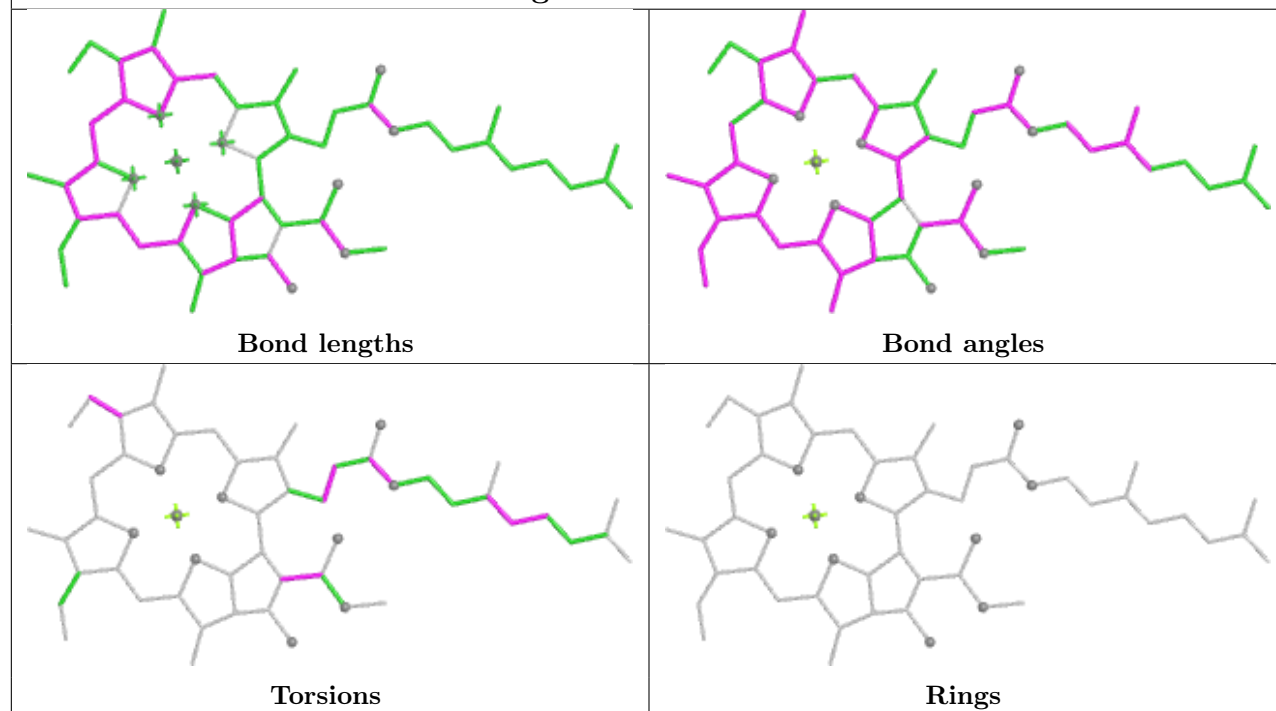


Ligand CLA 4 609**Ligand XAT 2 616**

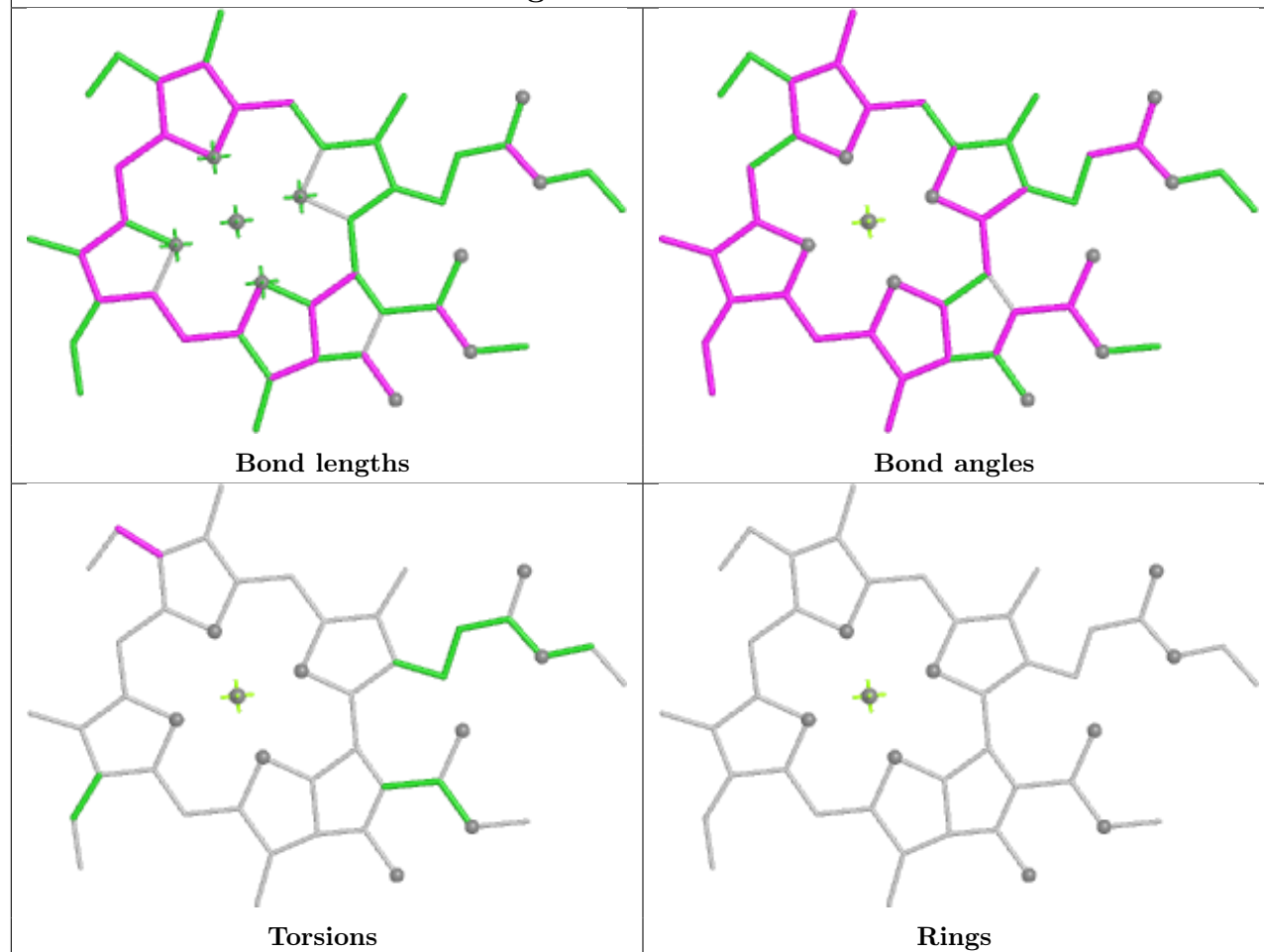
Ligand CLA 7 608



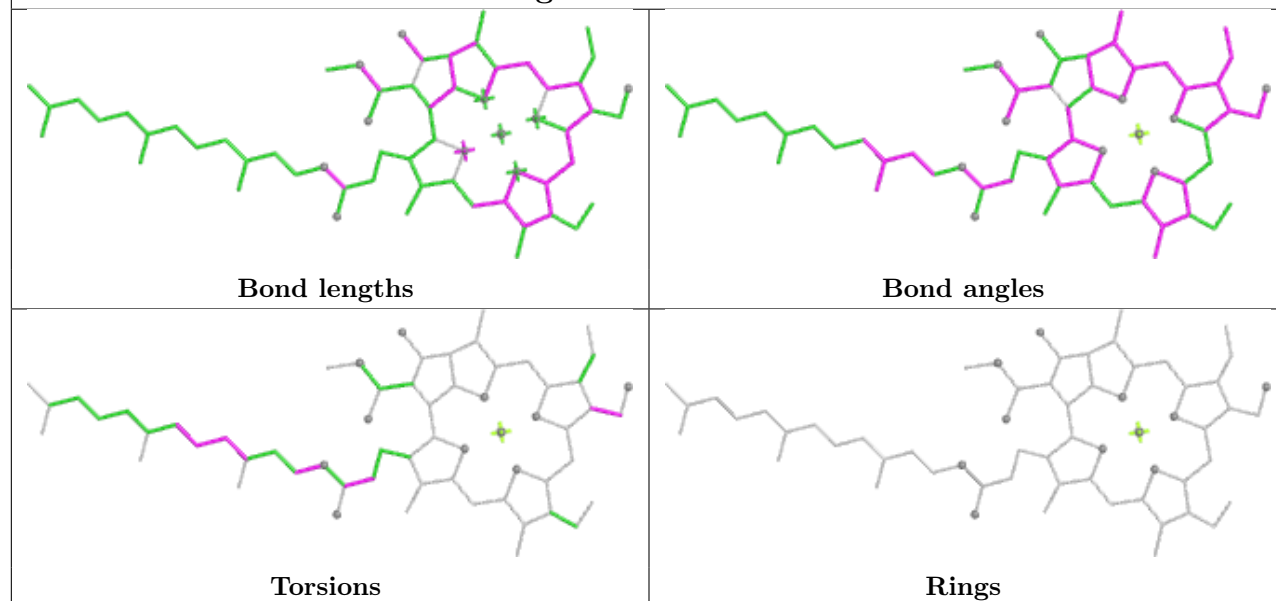
Ligand CLA A 805



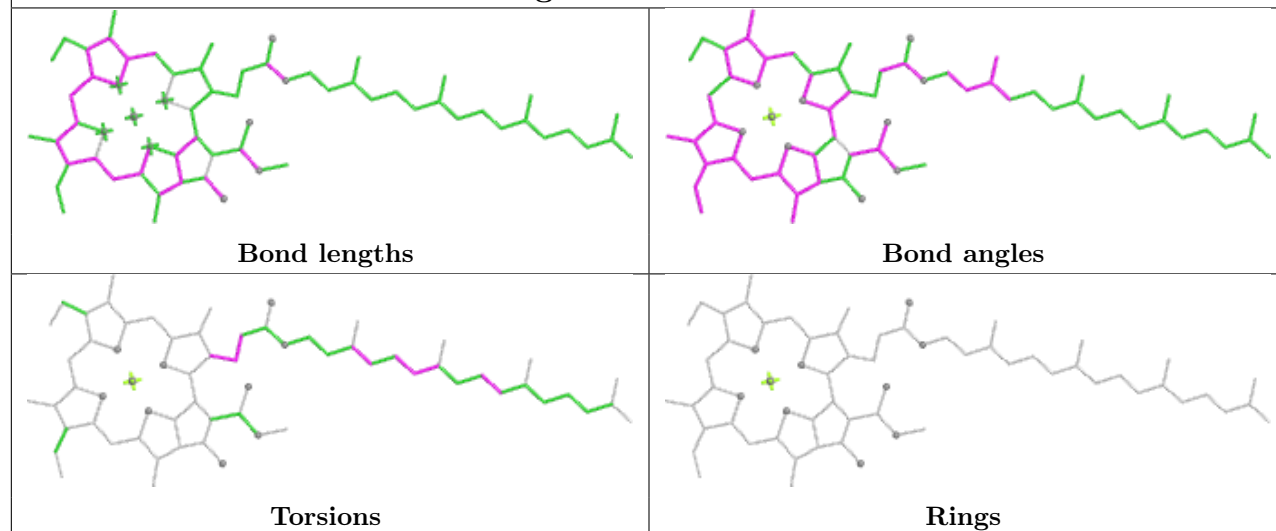
Ligand CLA B 838



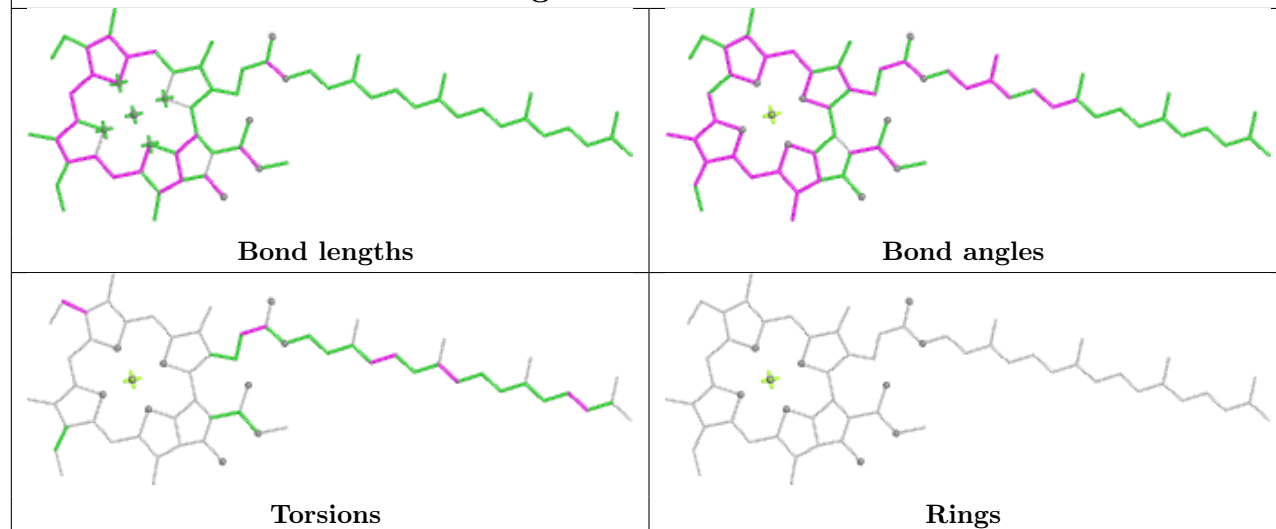
Ligand CHL 7 601



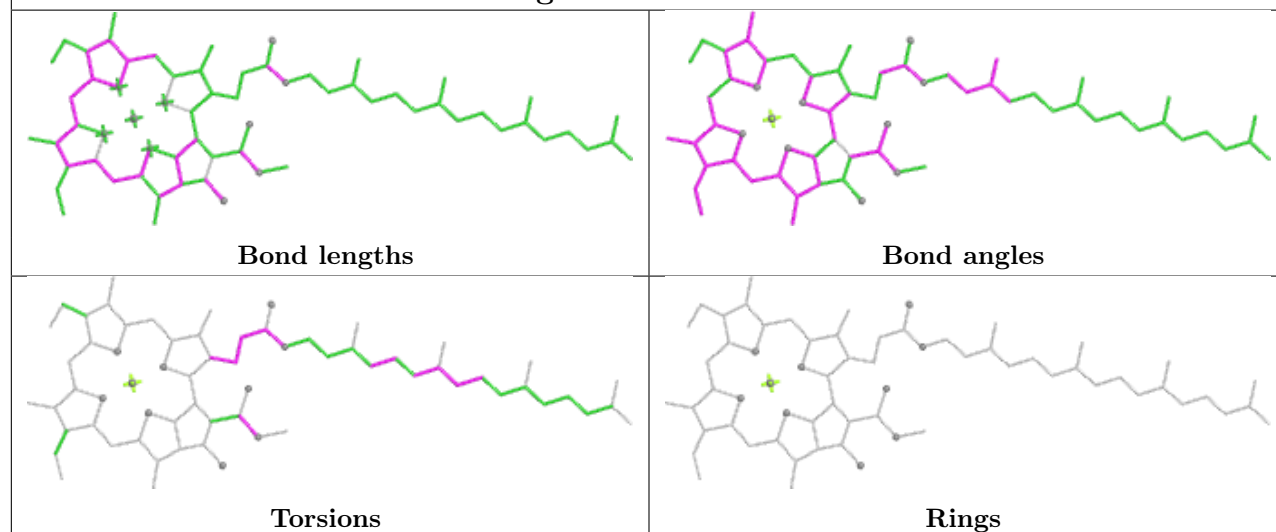
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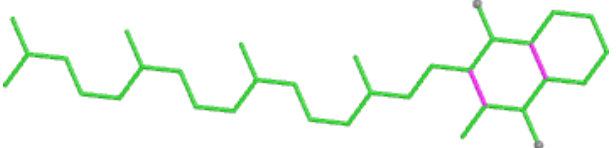
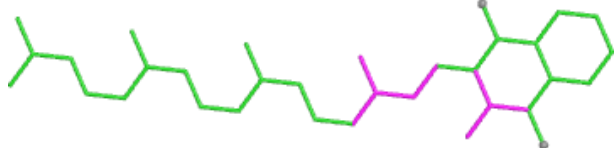
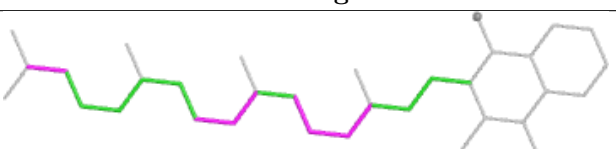
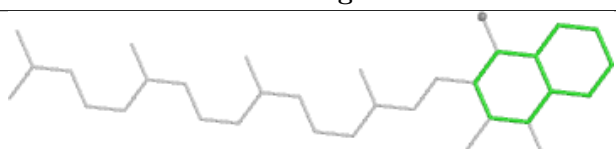
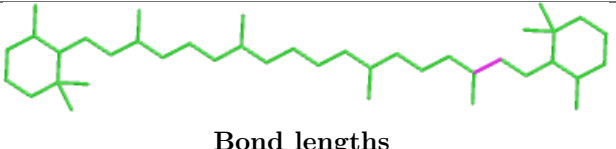
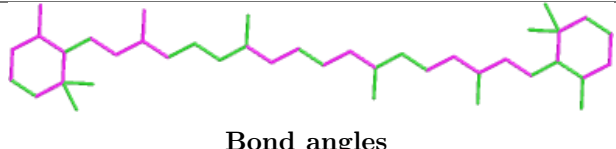
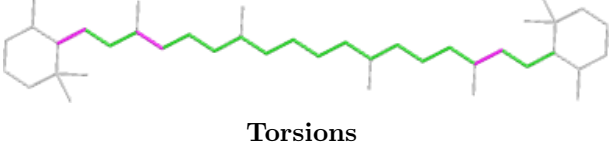
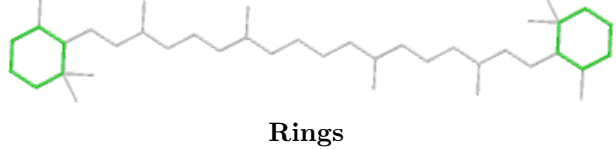
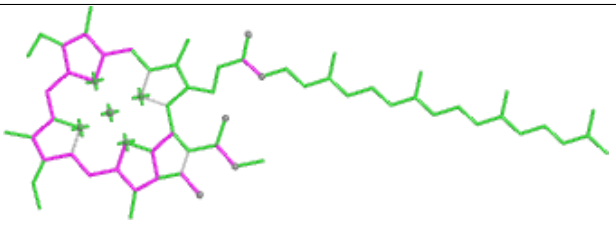
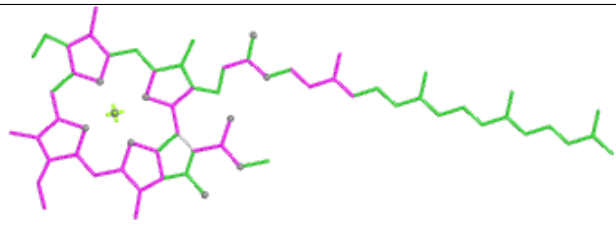
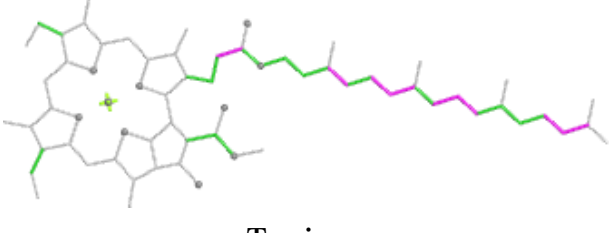
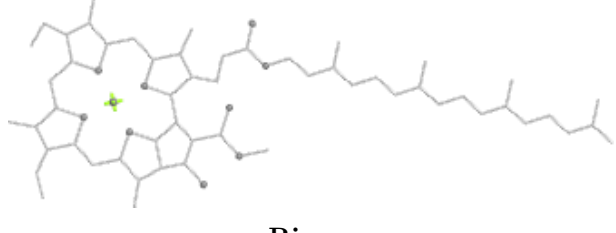


Ligand CLA A 802

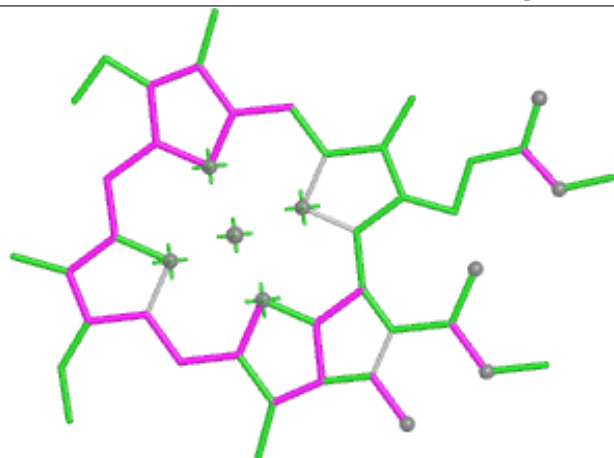


Ligand CLA a 819

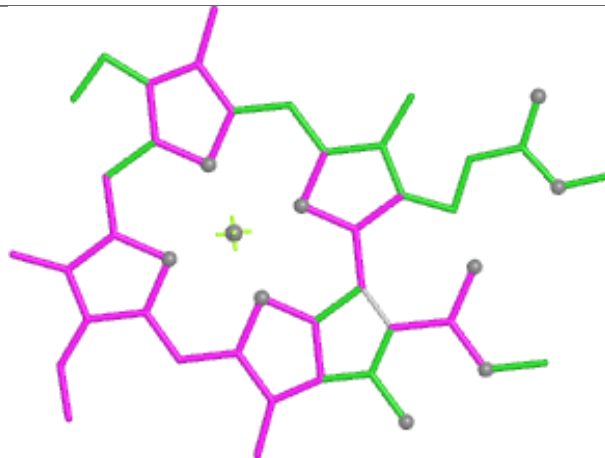


Ligand PQN A 844	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 1 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

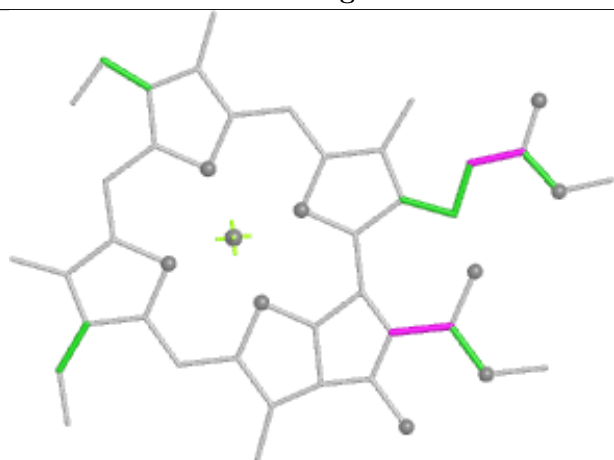
Ligand CLA 4 601



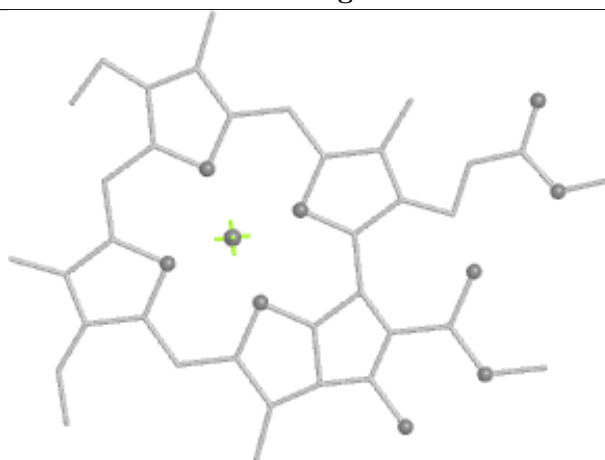
Bond lengths



Bond angles

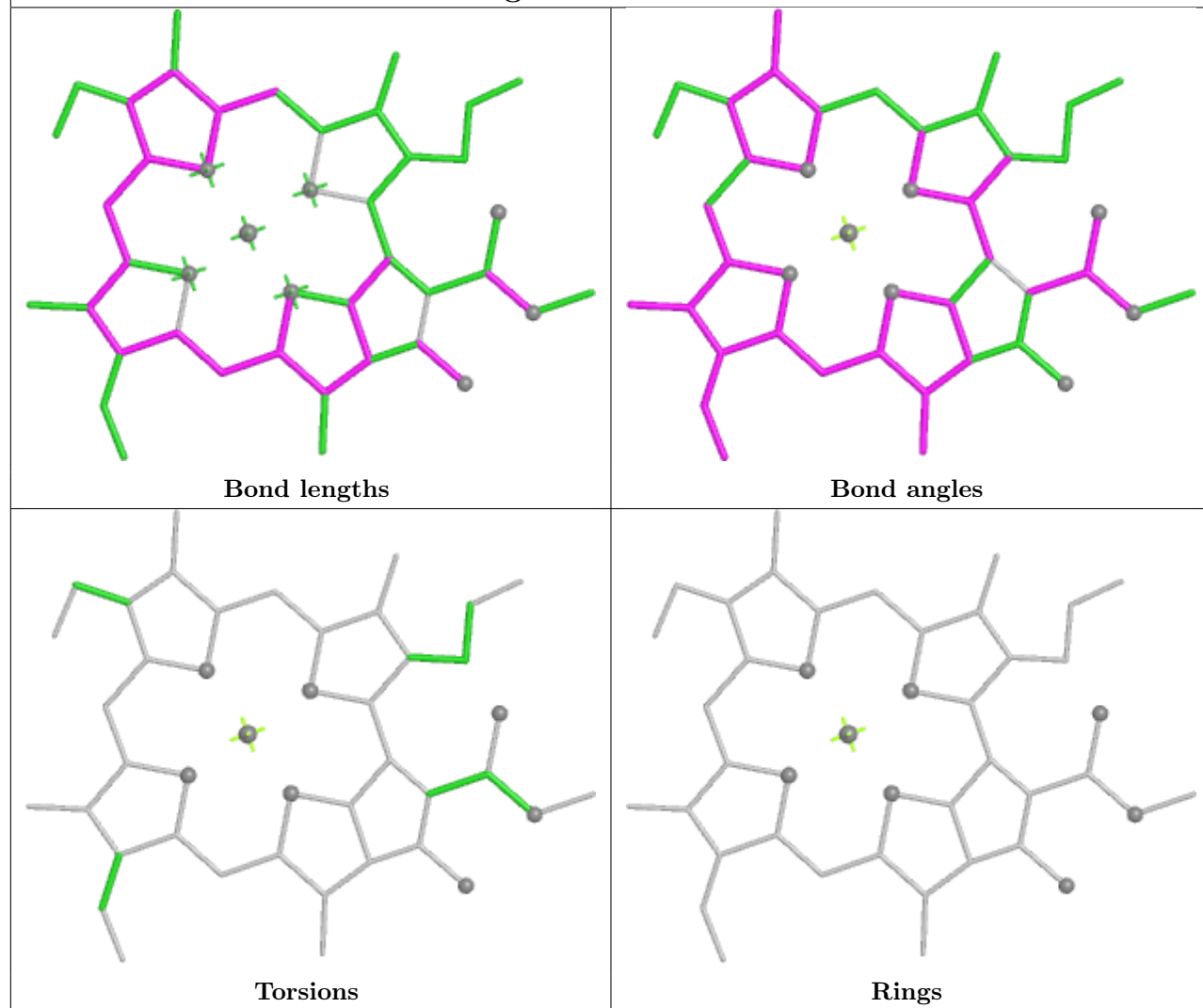


Torsions

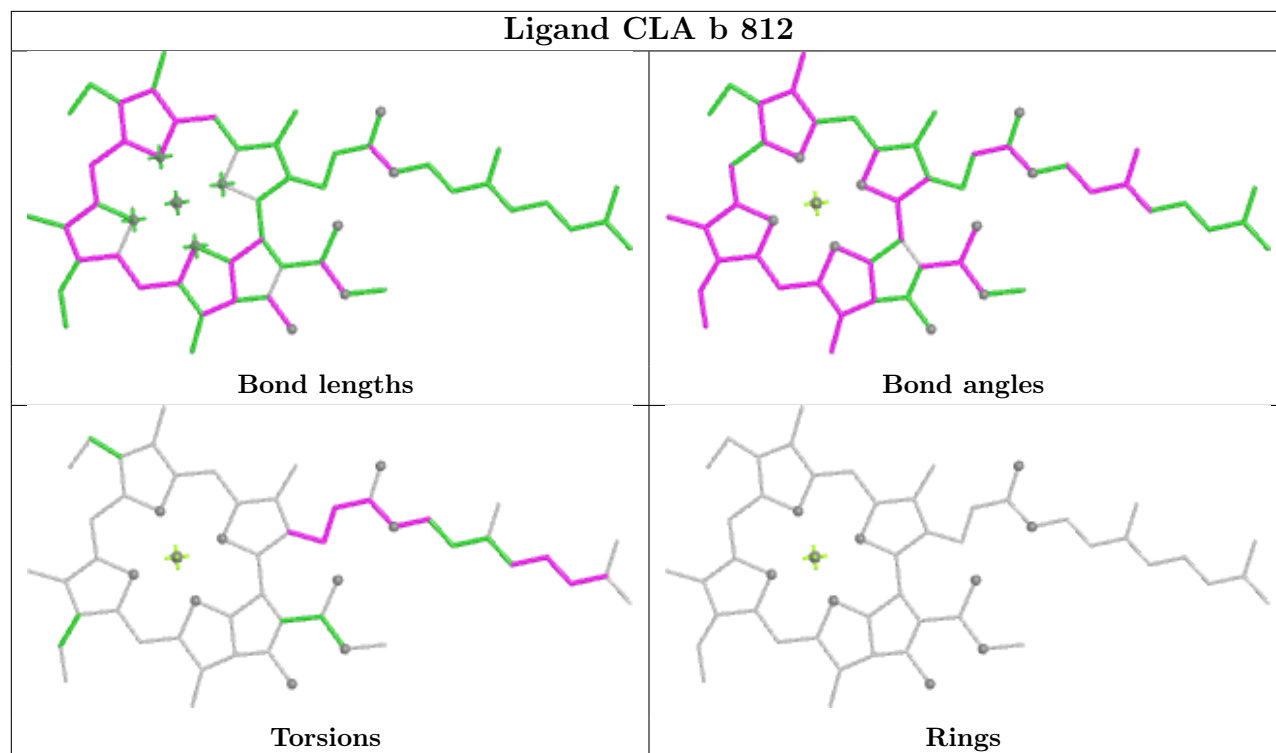


Rings

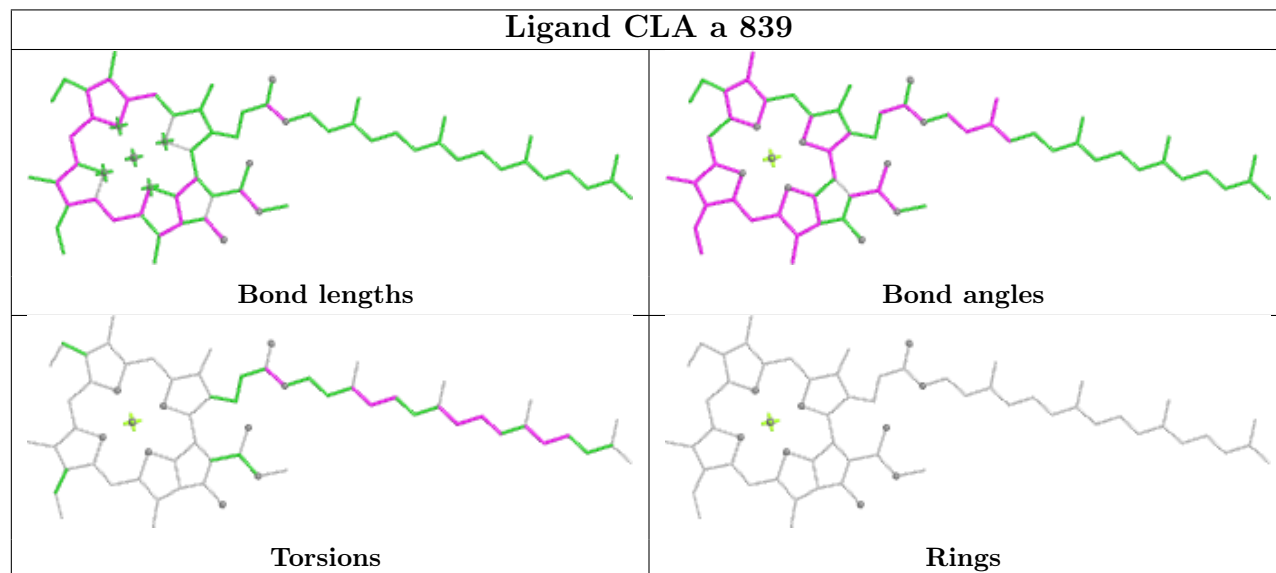
Ligand CLA 7 613



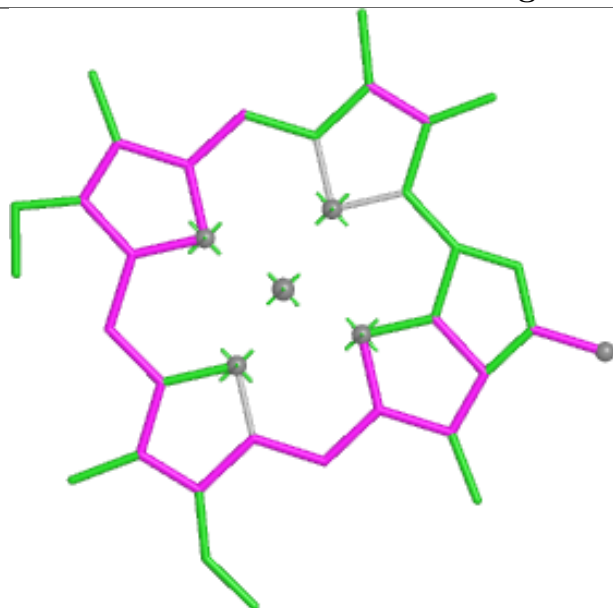
Ligand CLA b 812



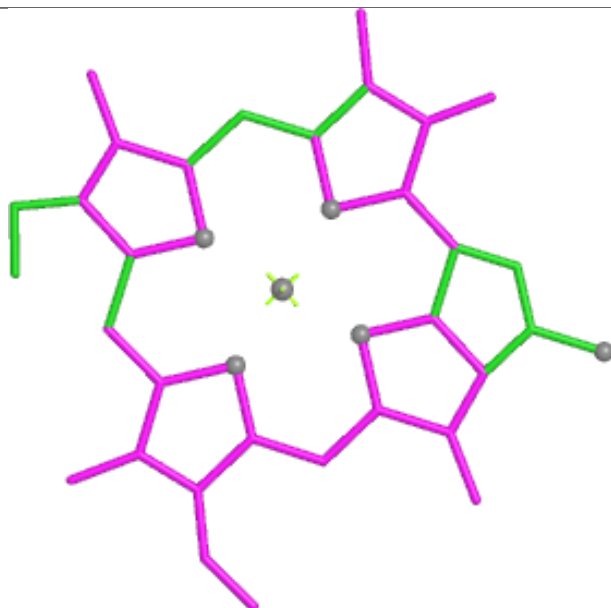
Ligand CLA a 839



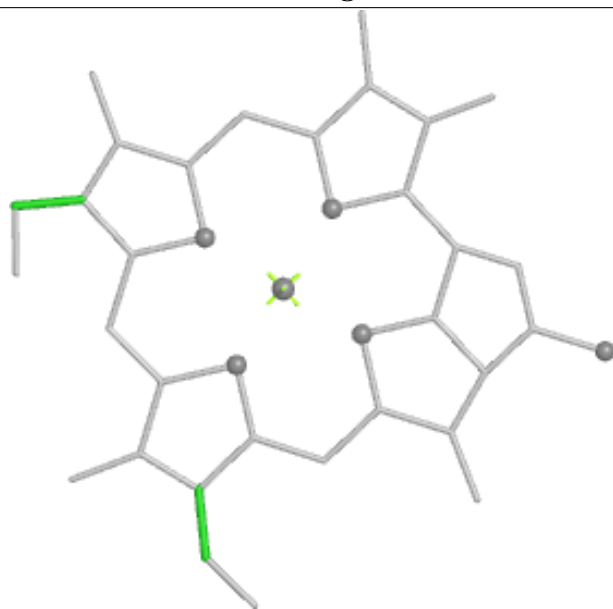
Ligand CLA 3 310



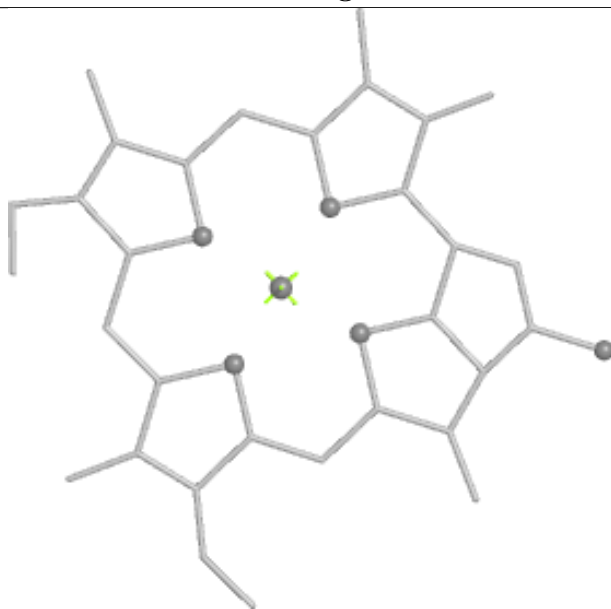
Bond lengths



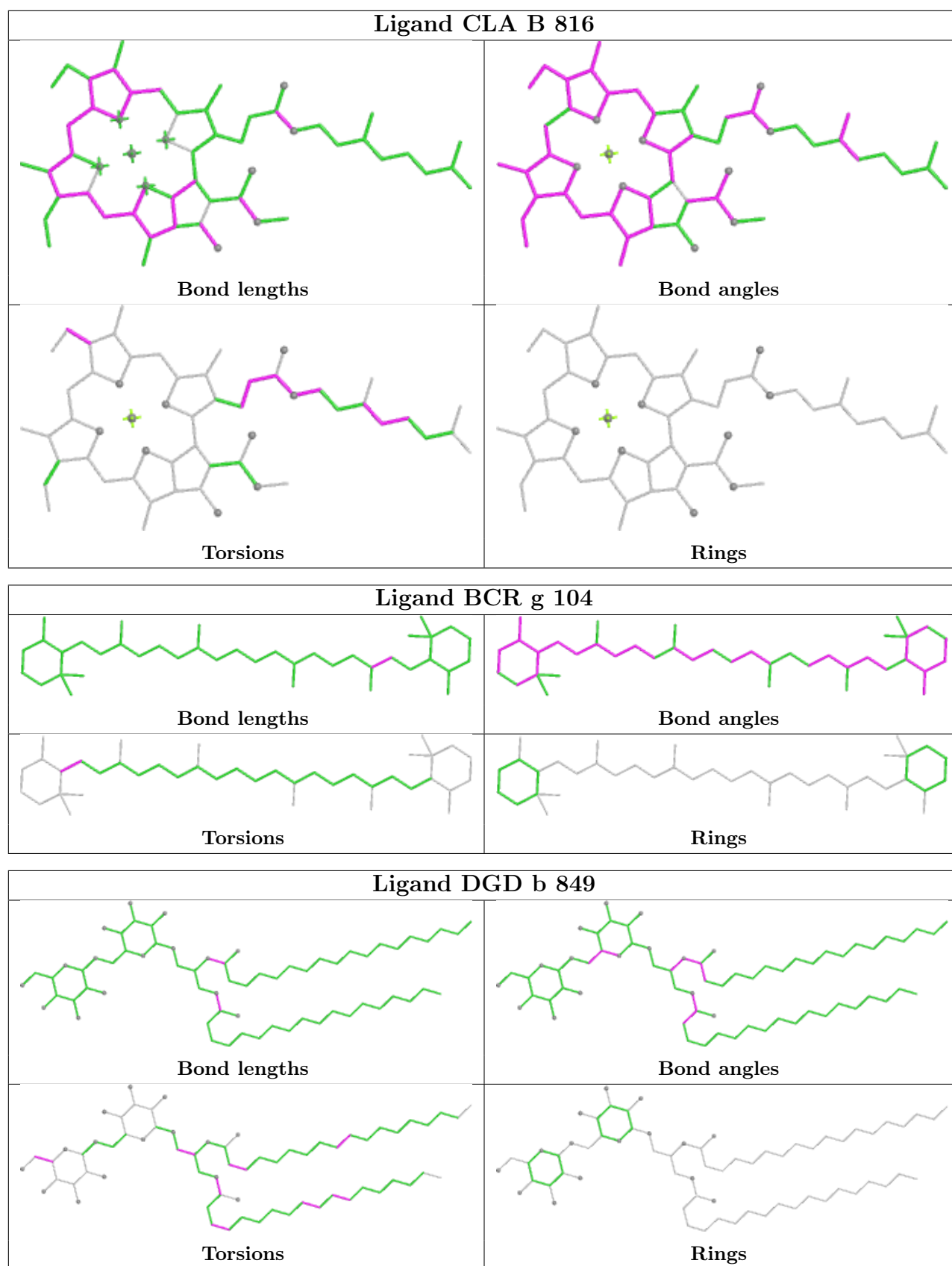
Bond angles



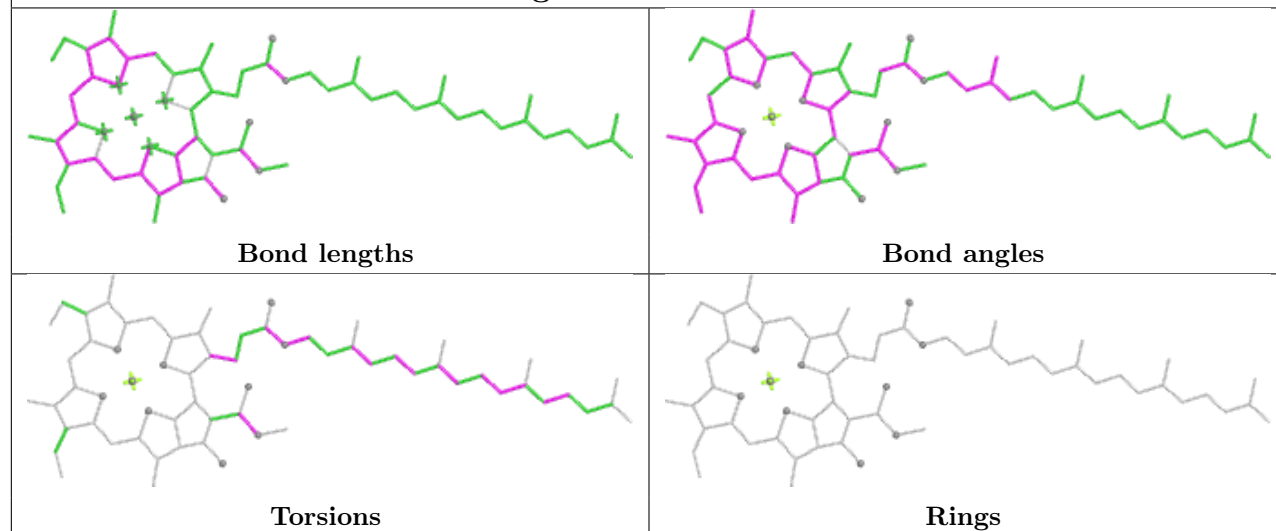
Torsions



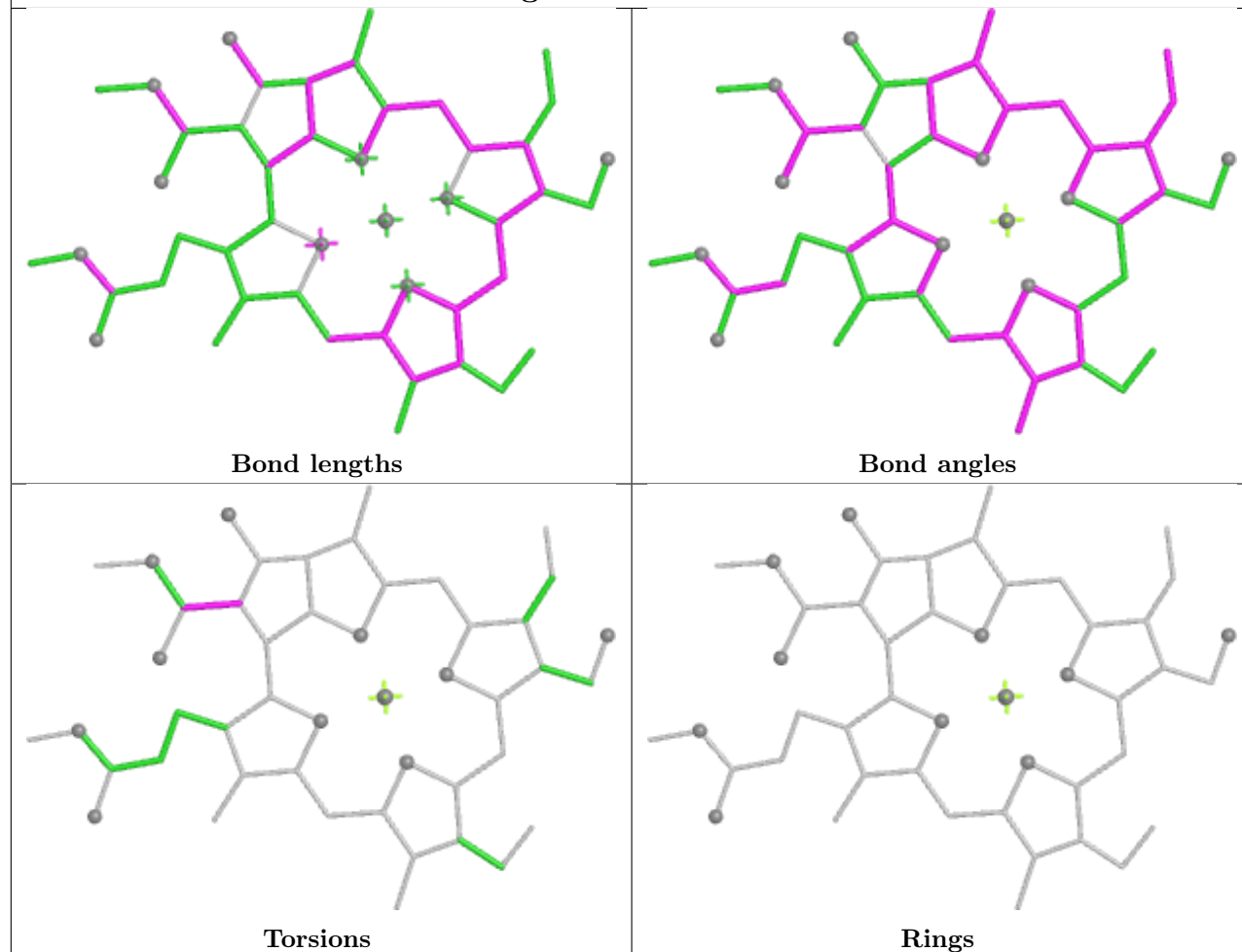
Rings



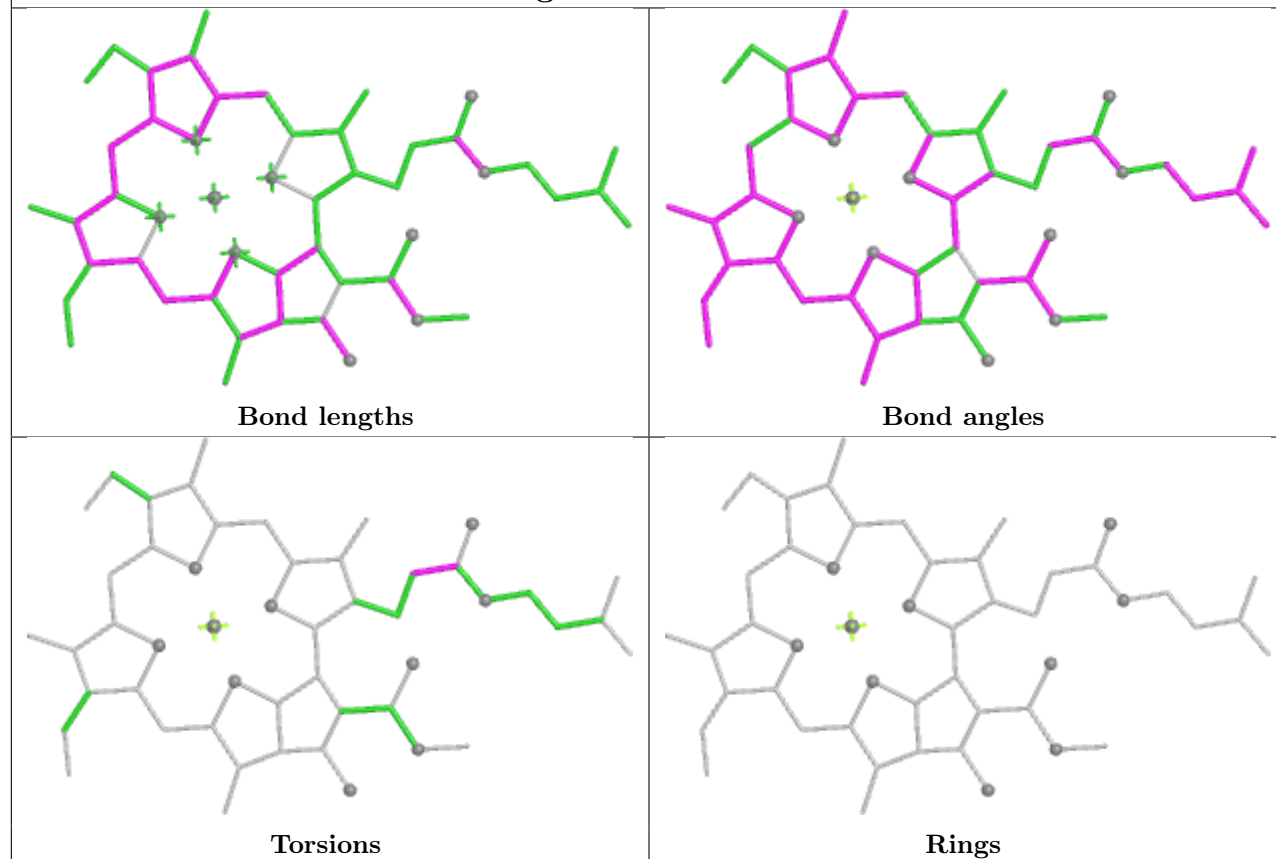
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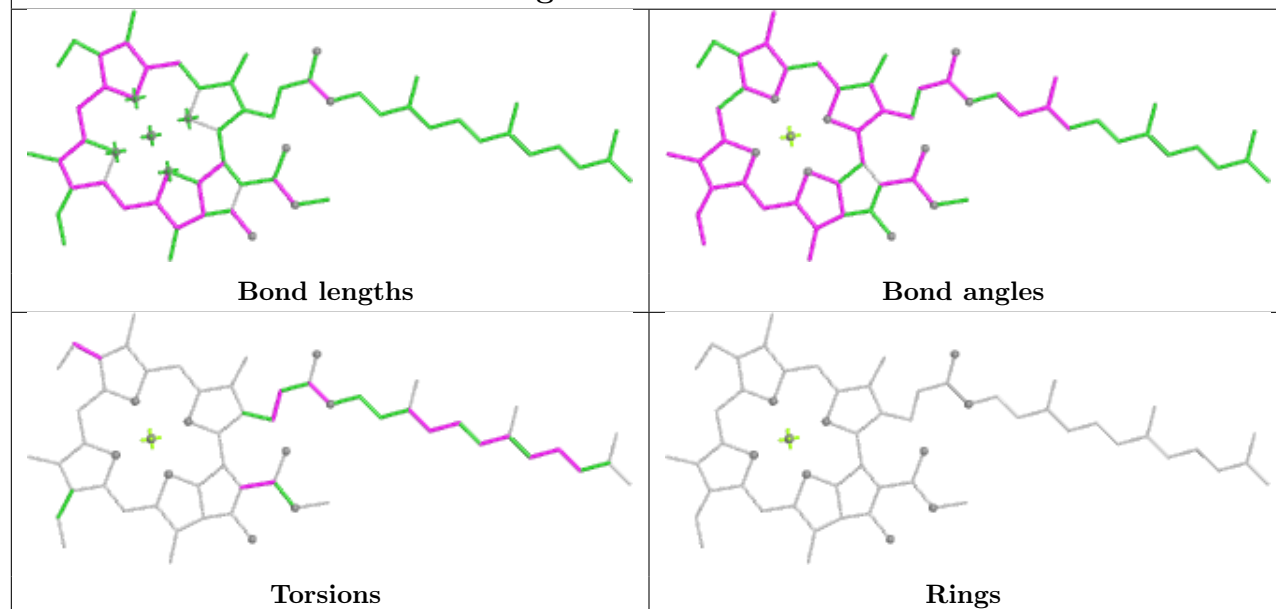
Ligand CHL 6 308



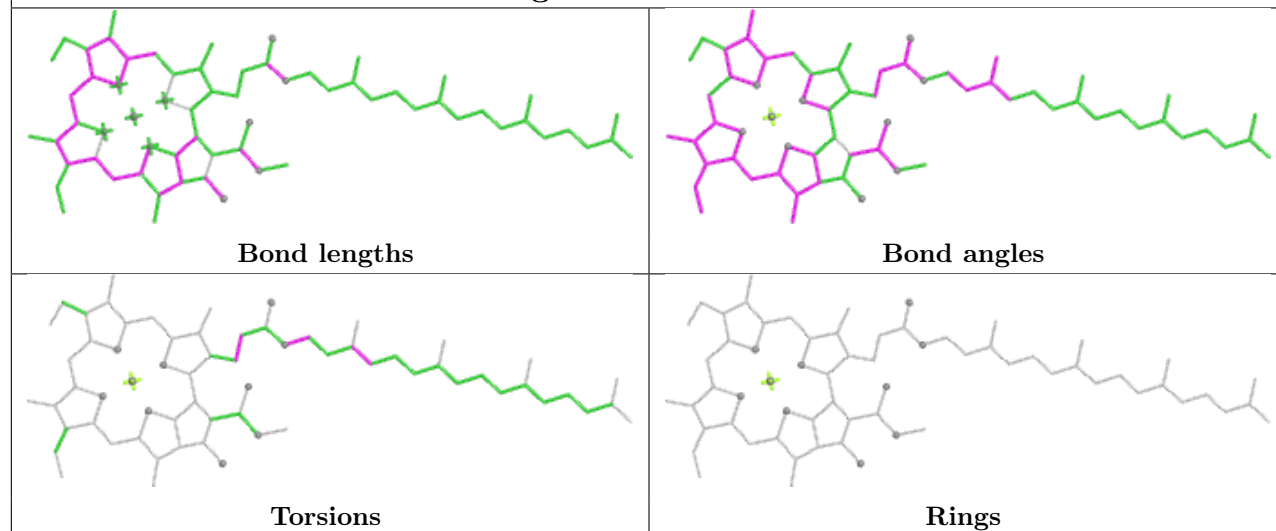
Ligand CLA 8 302



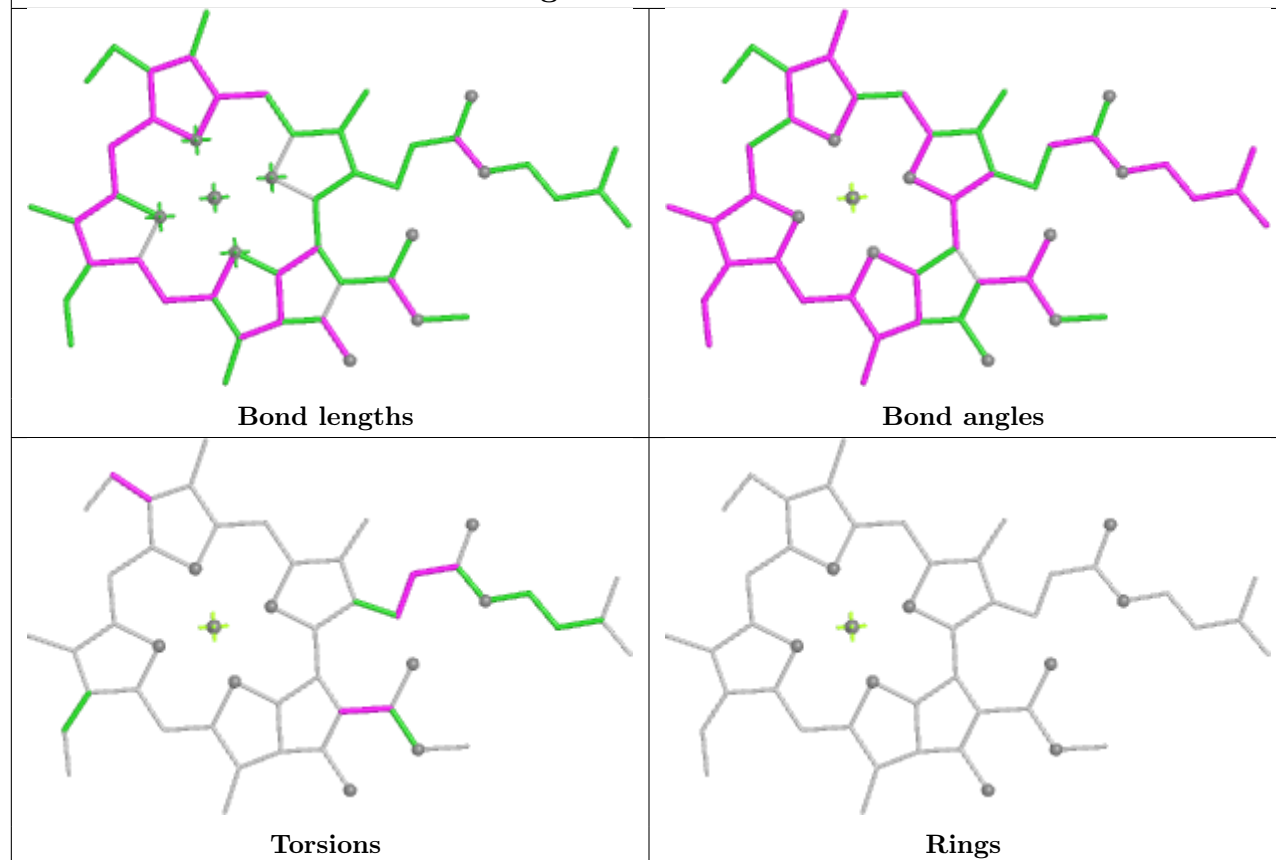
Ligand CLA 9 602



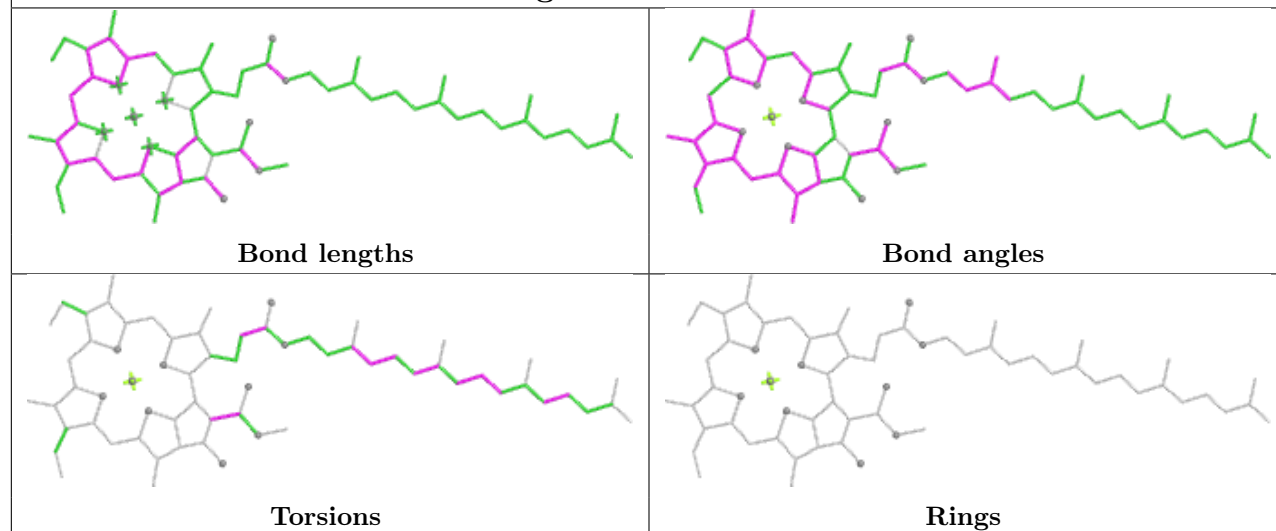
Ligand CLA A 810



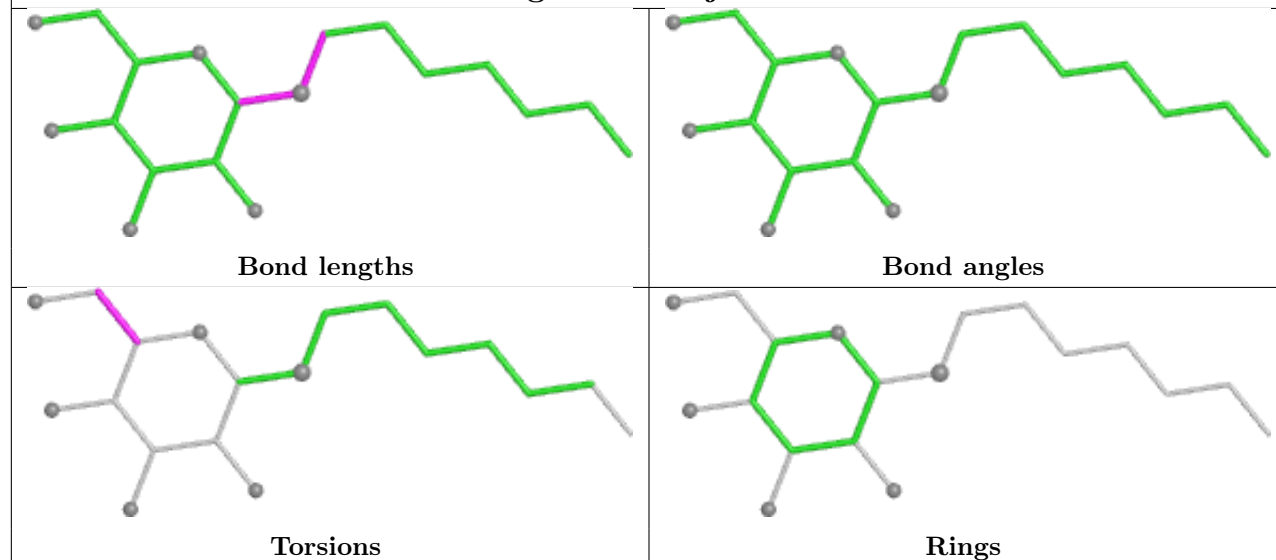
Ligand CLA I 204



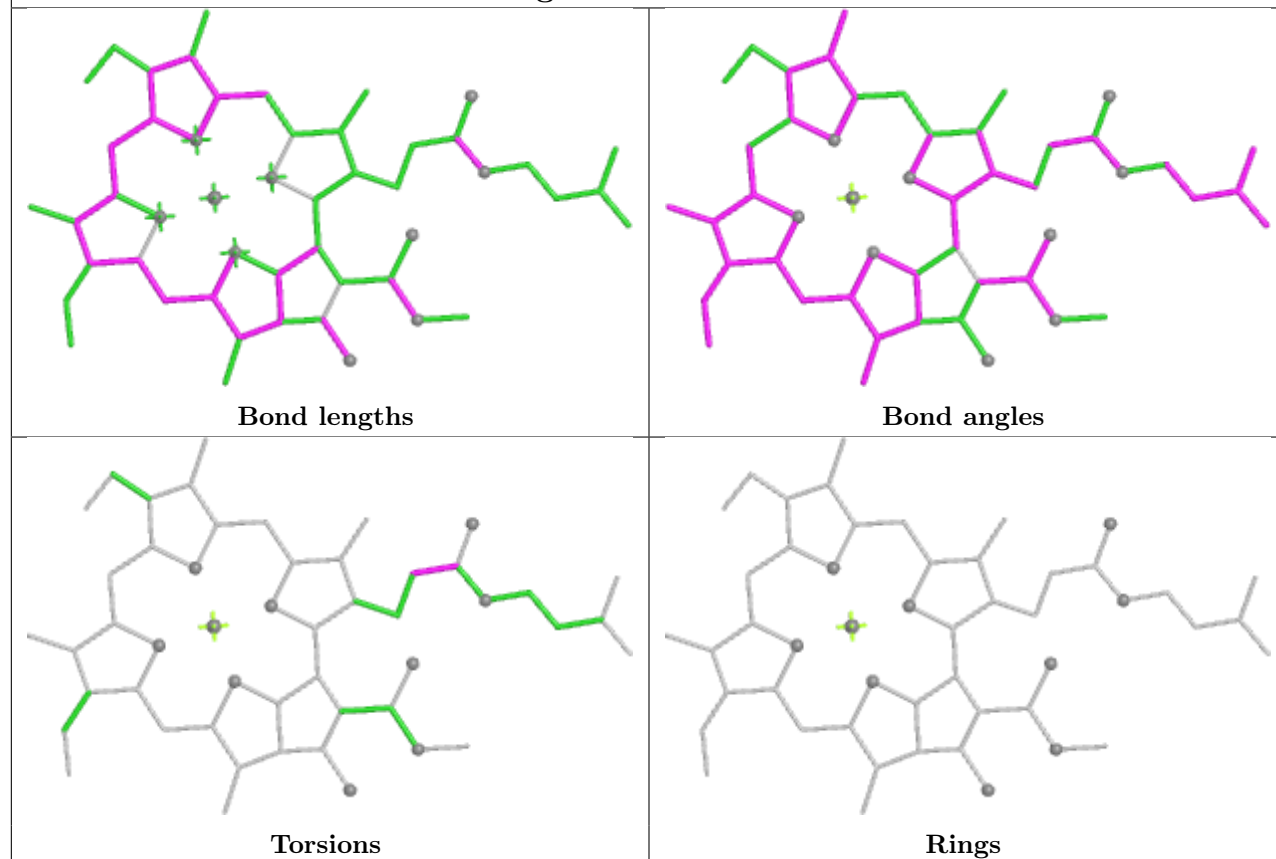
Ligand CLA a 814



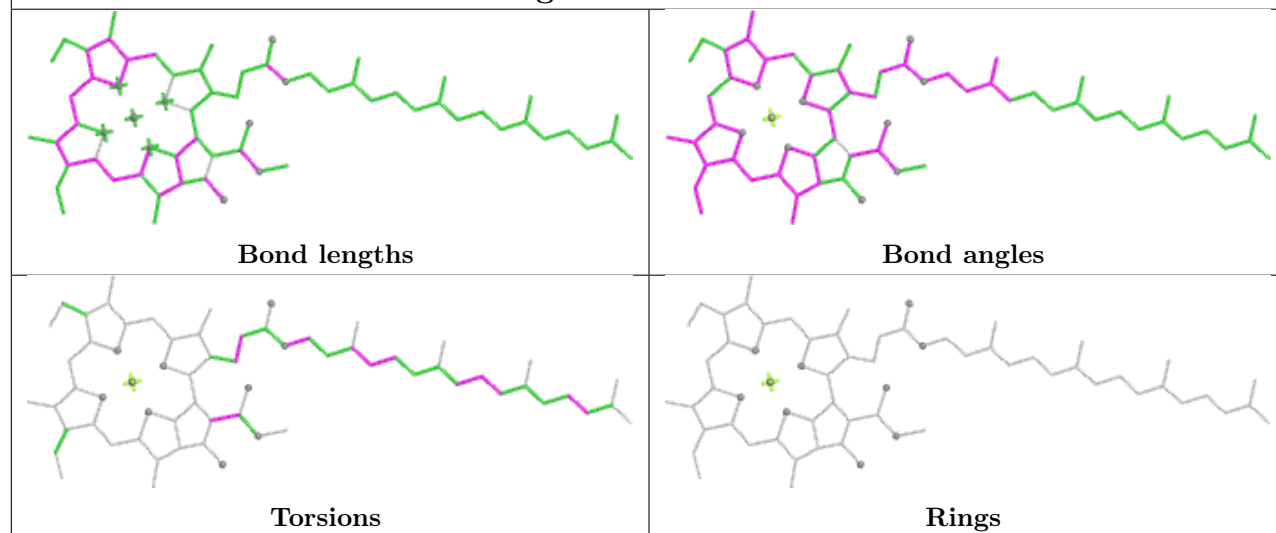
Ligand HTG j 3001

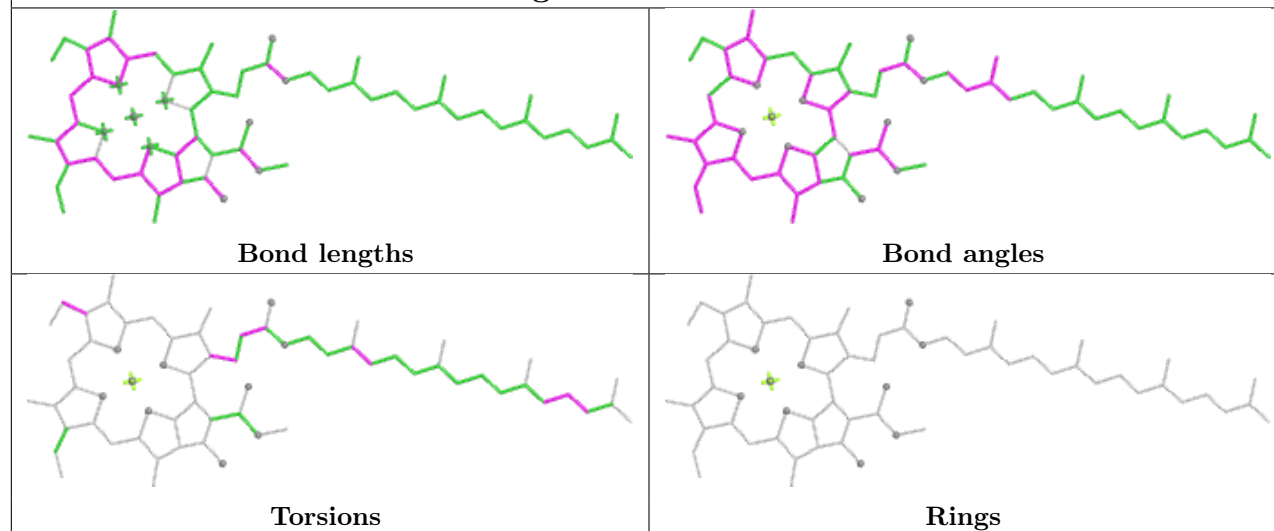
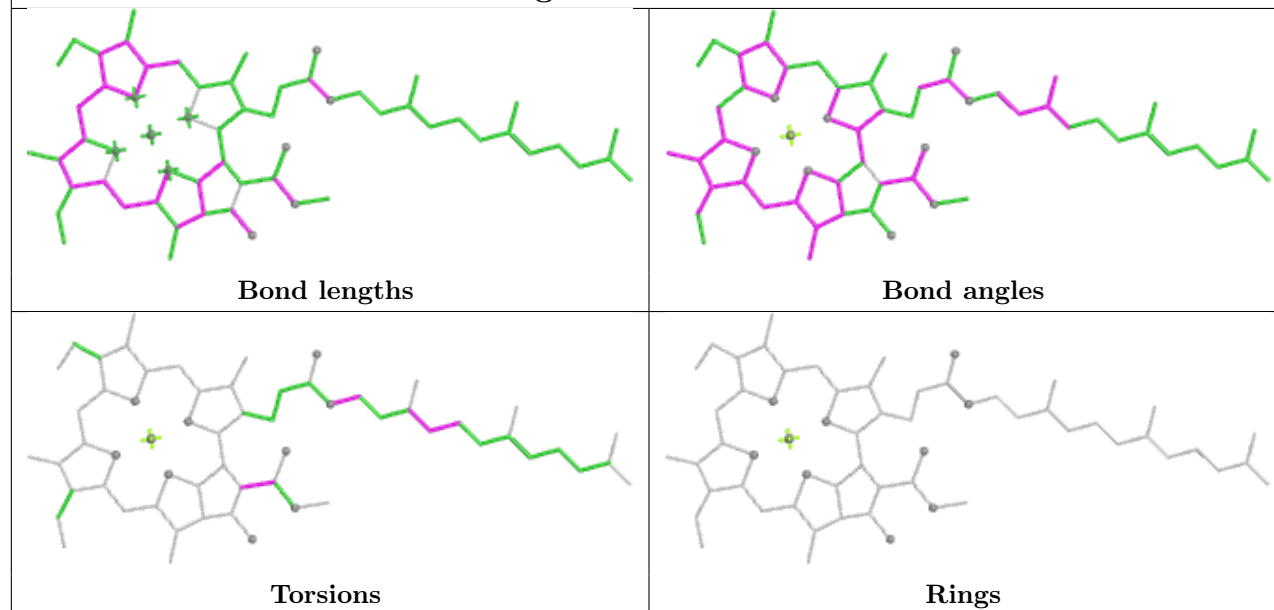


Ligand CLA 4 614

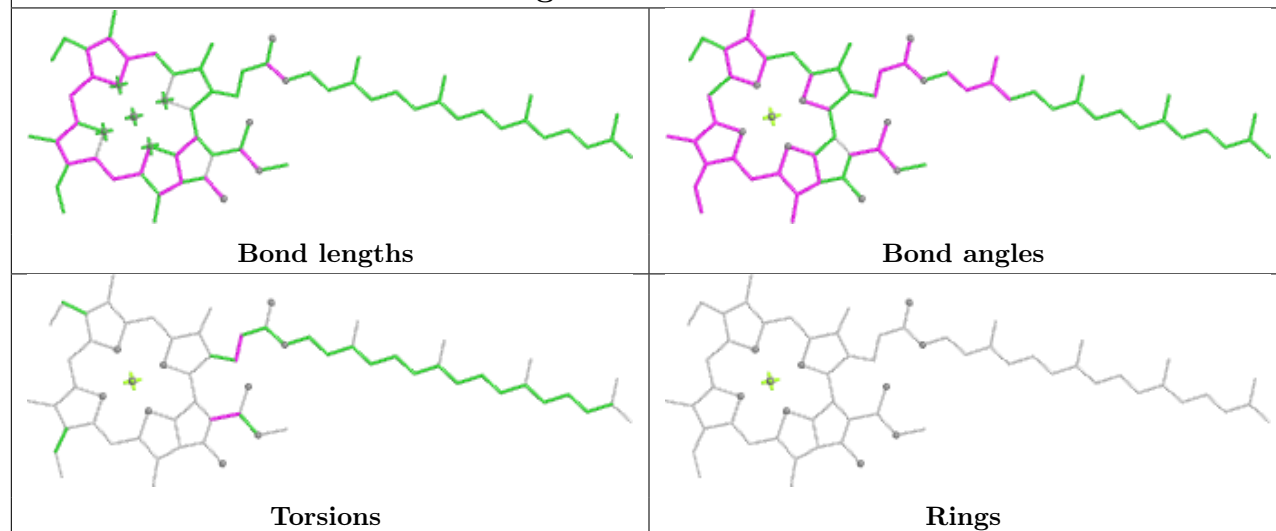


Ligand CLA a 856

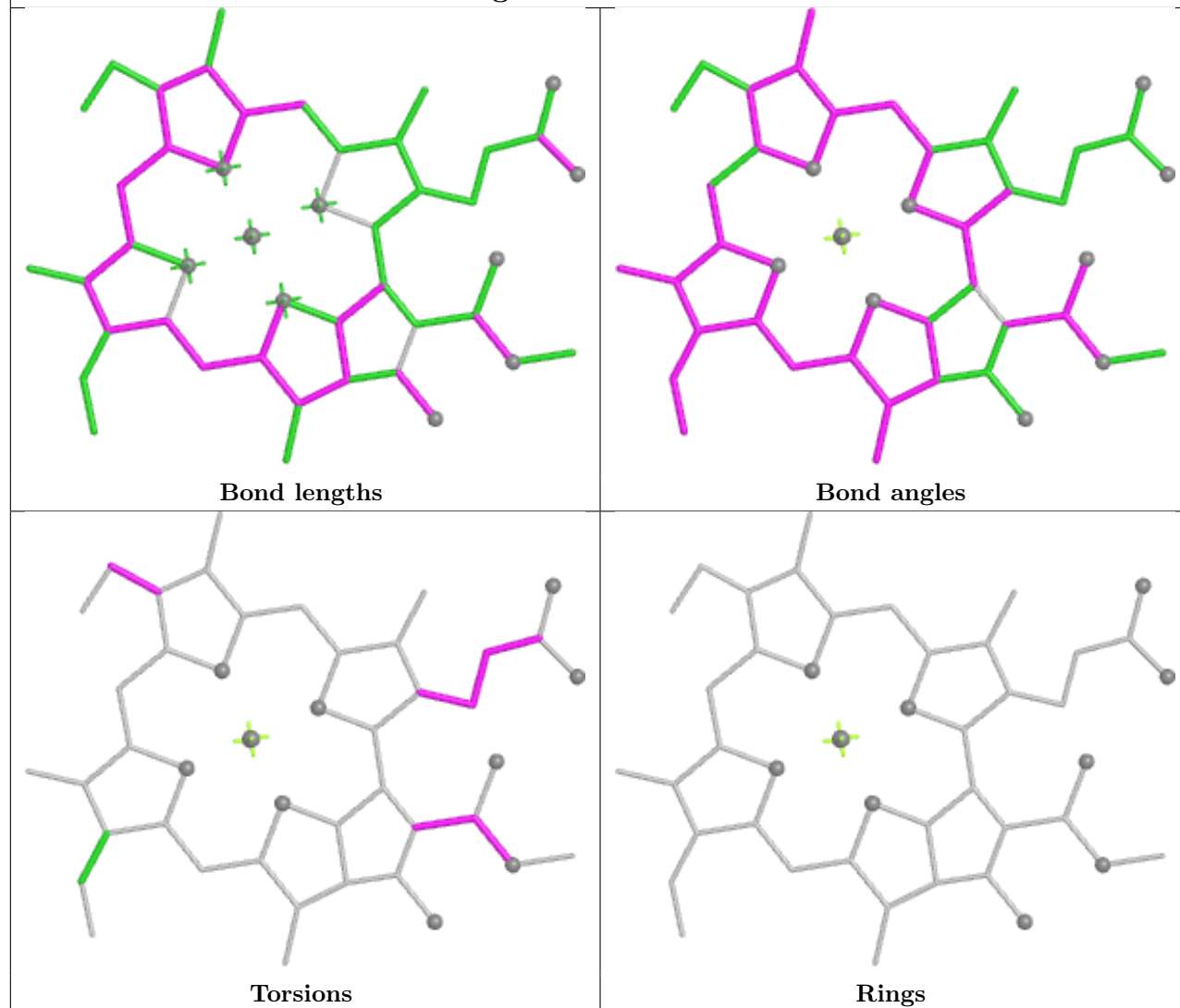


Ligand CLA B 841**Ligand CLA b 836**

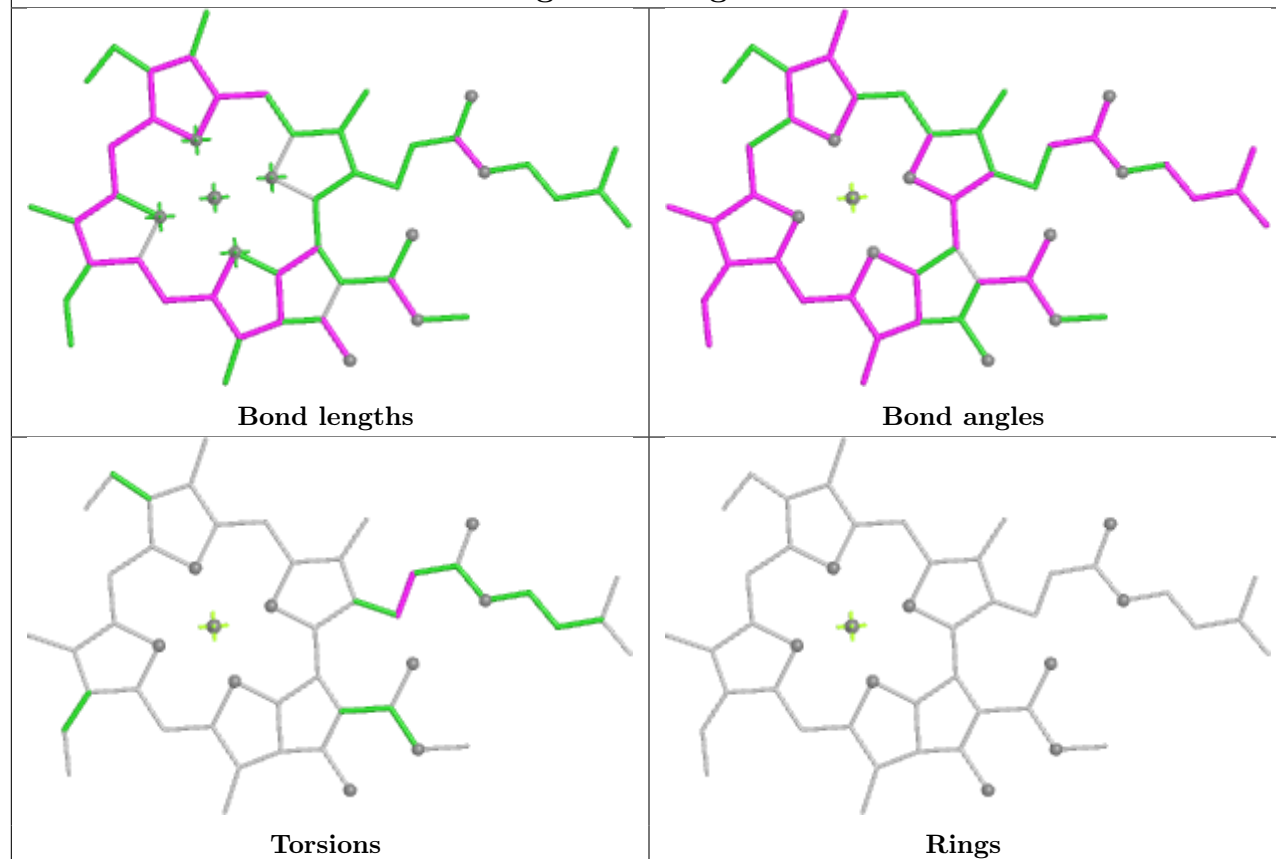
Ligand CLA a 810



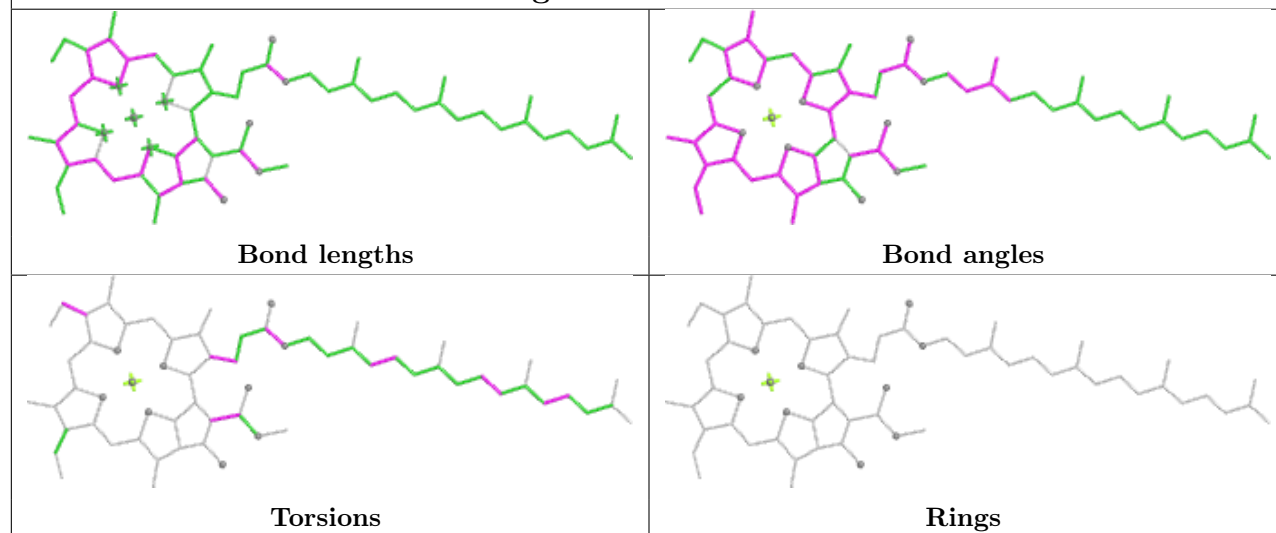
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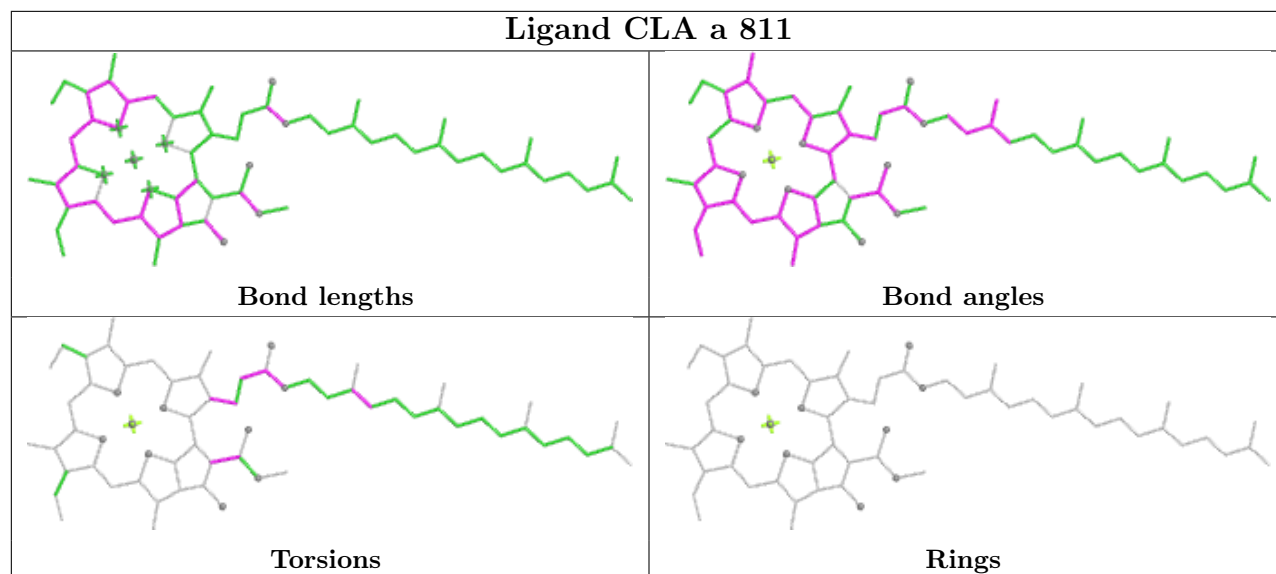
Ligand CLA g 102



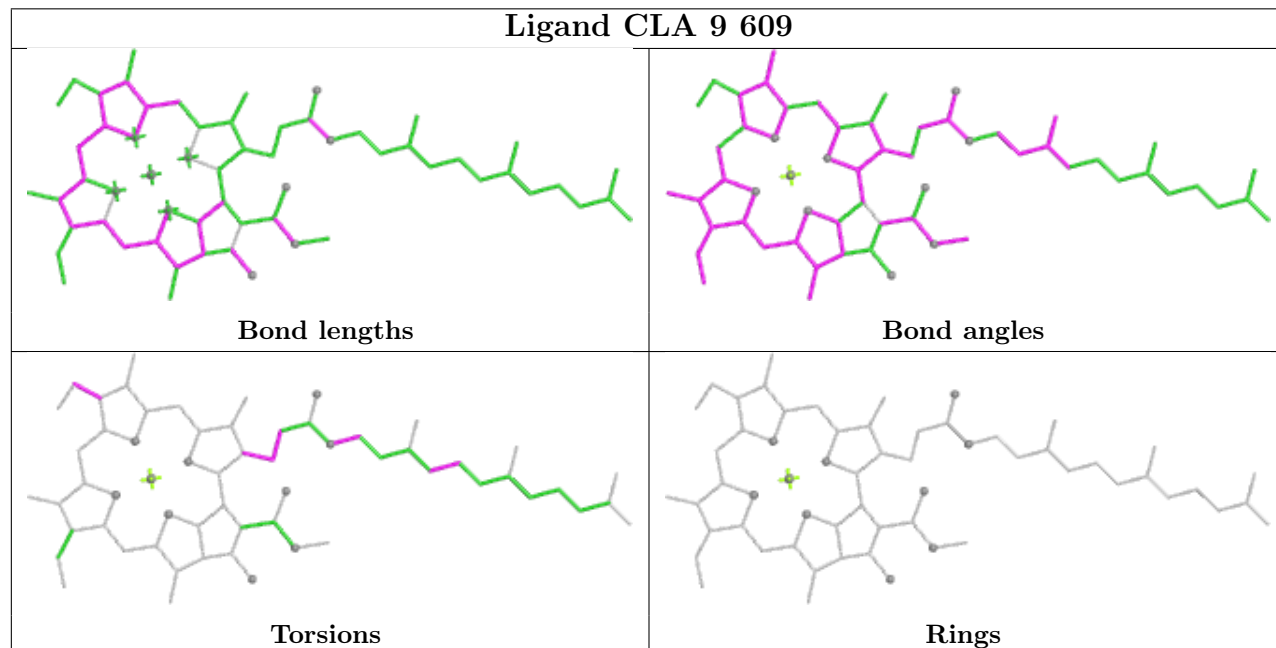
Ligand CLA B 825

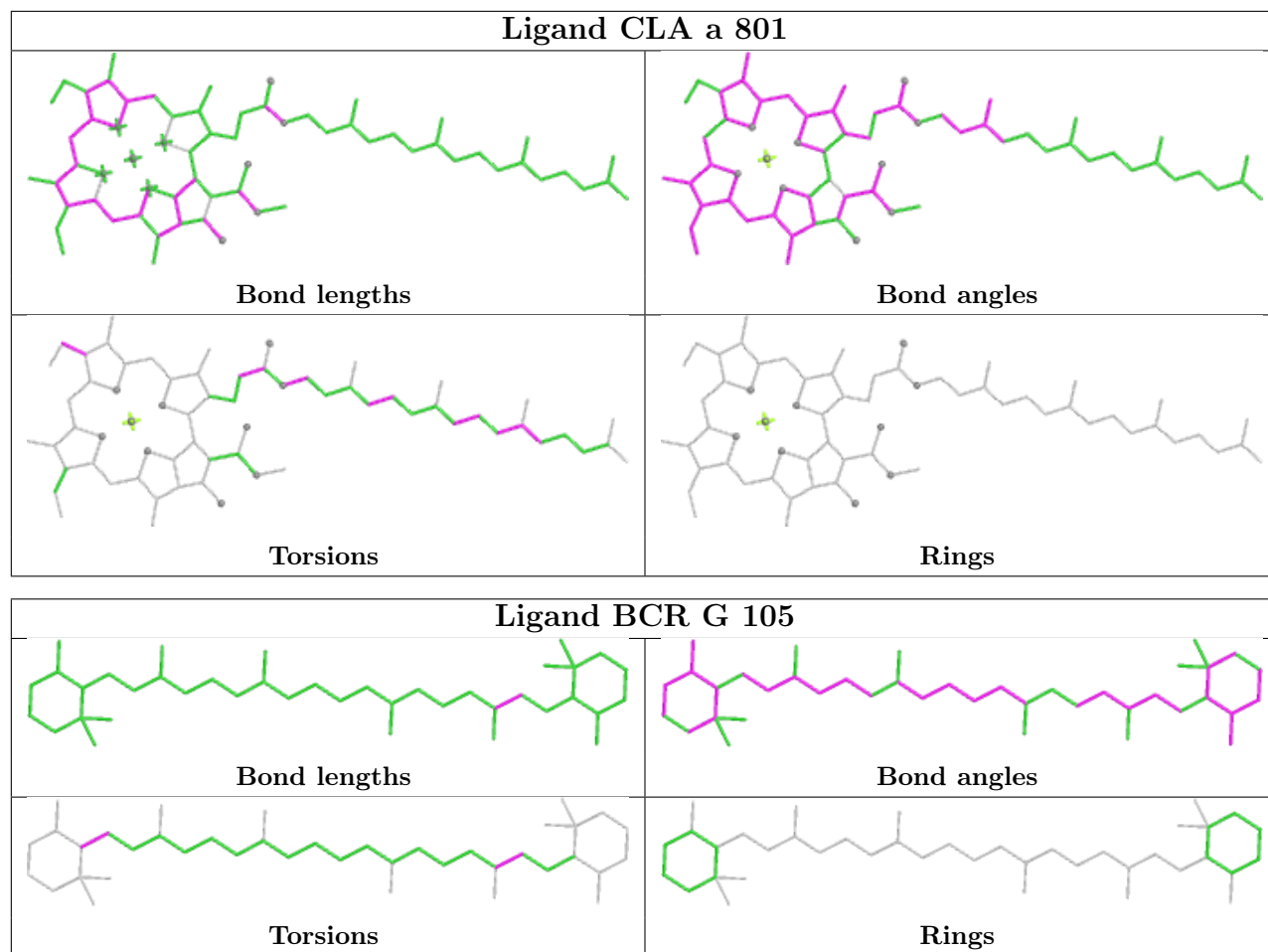


Ligand CLA a 811

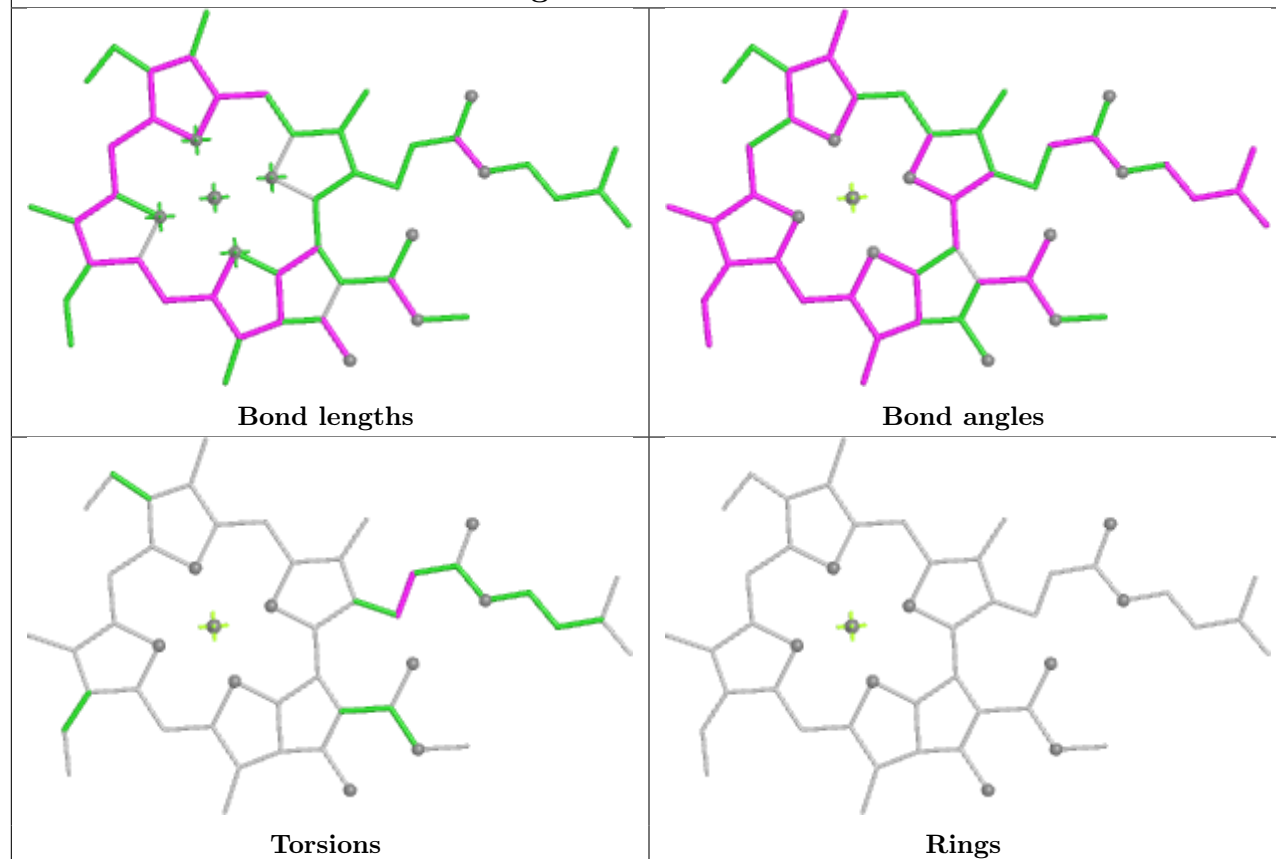


Ligand CLA 9 609

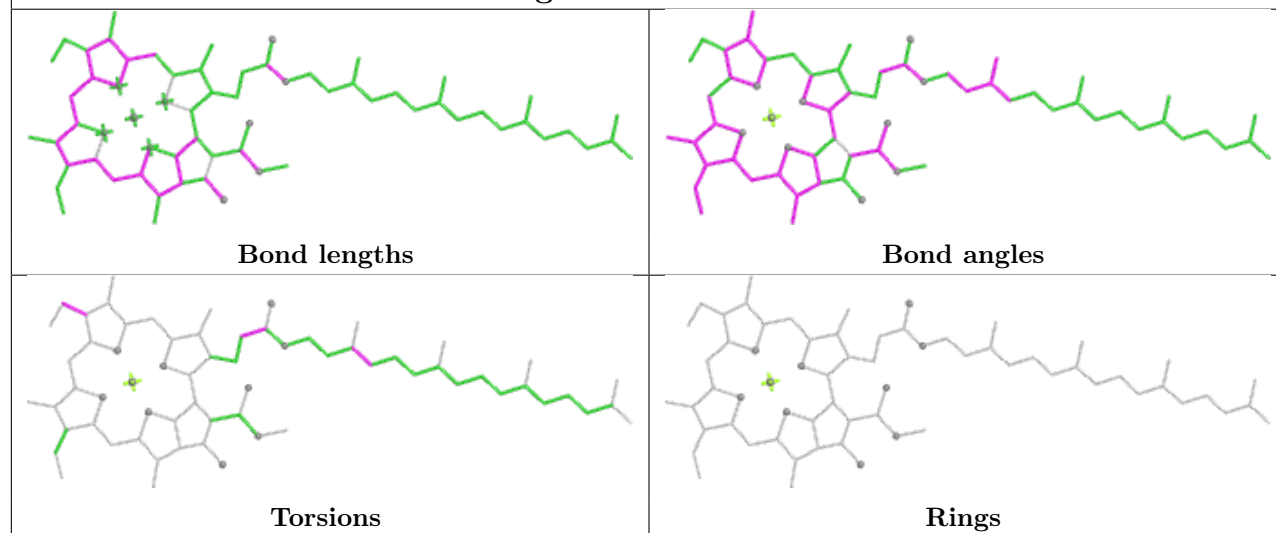


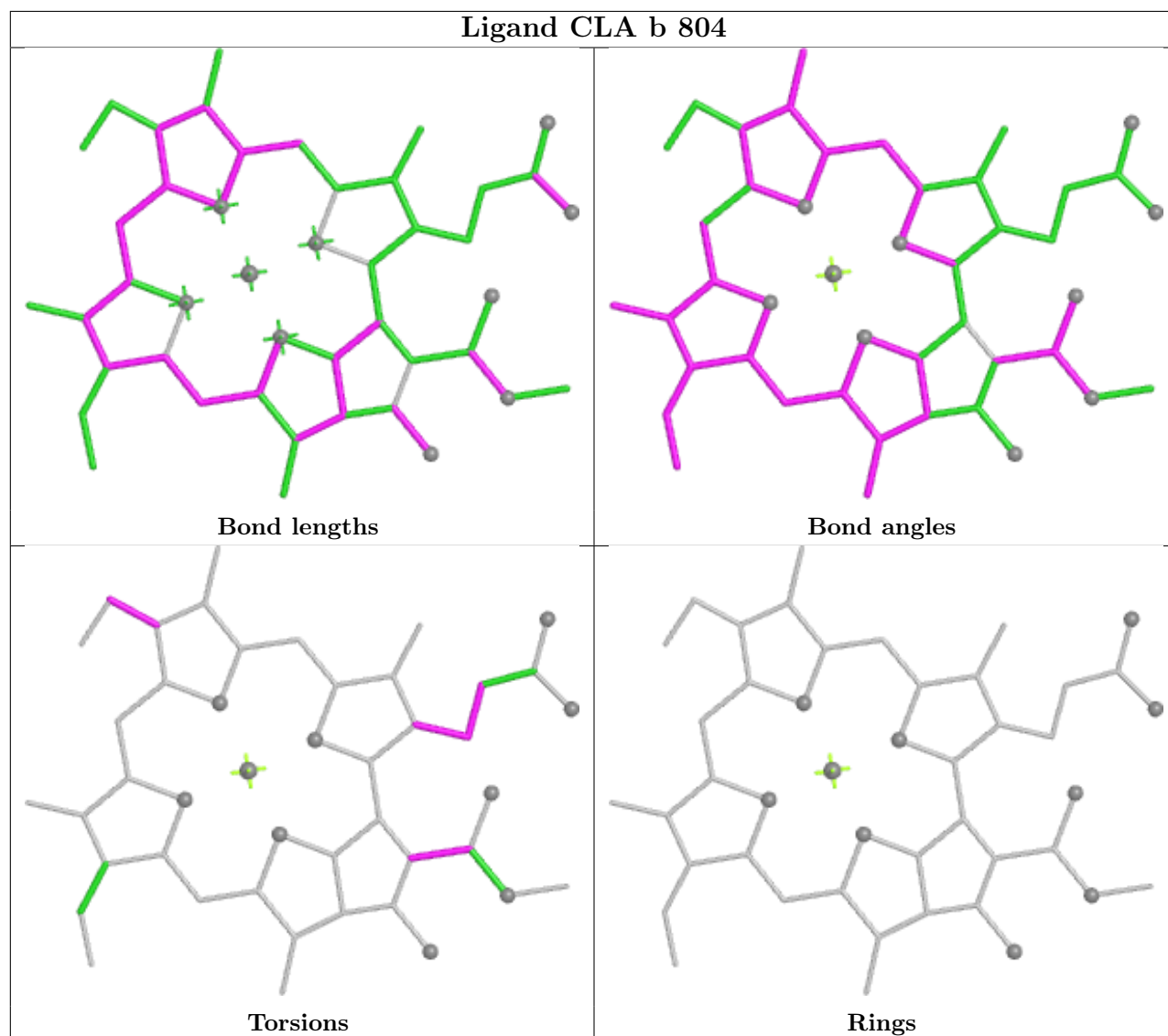
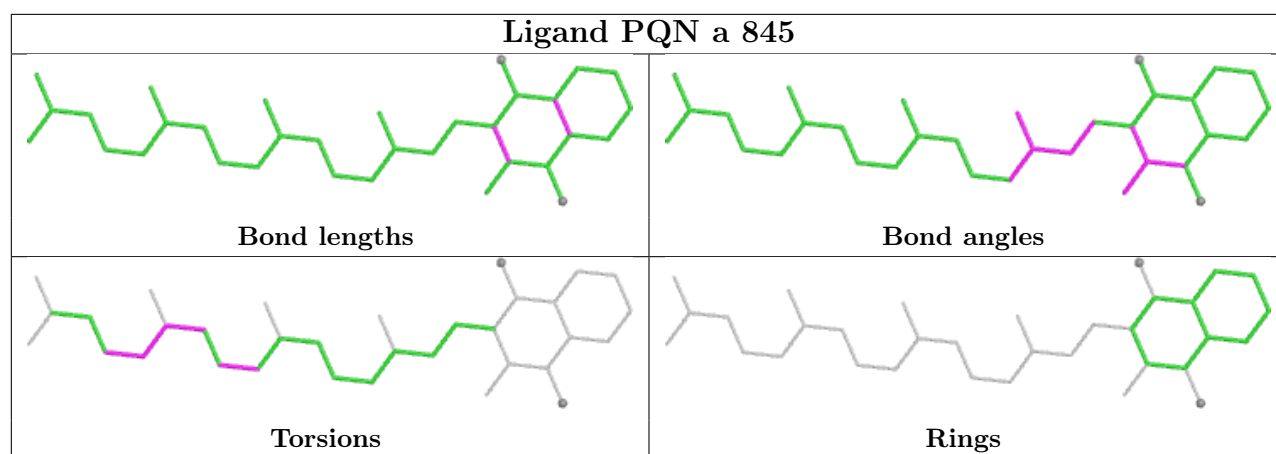


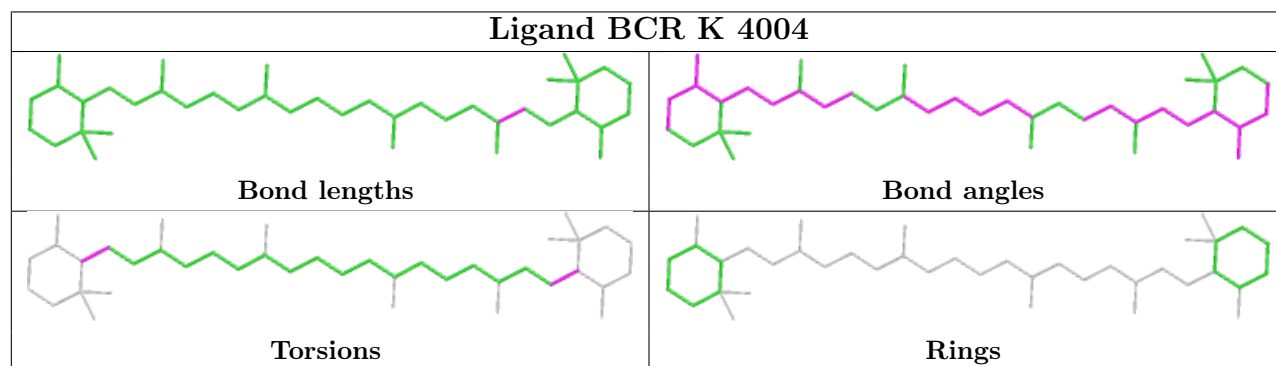
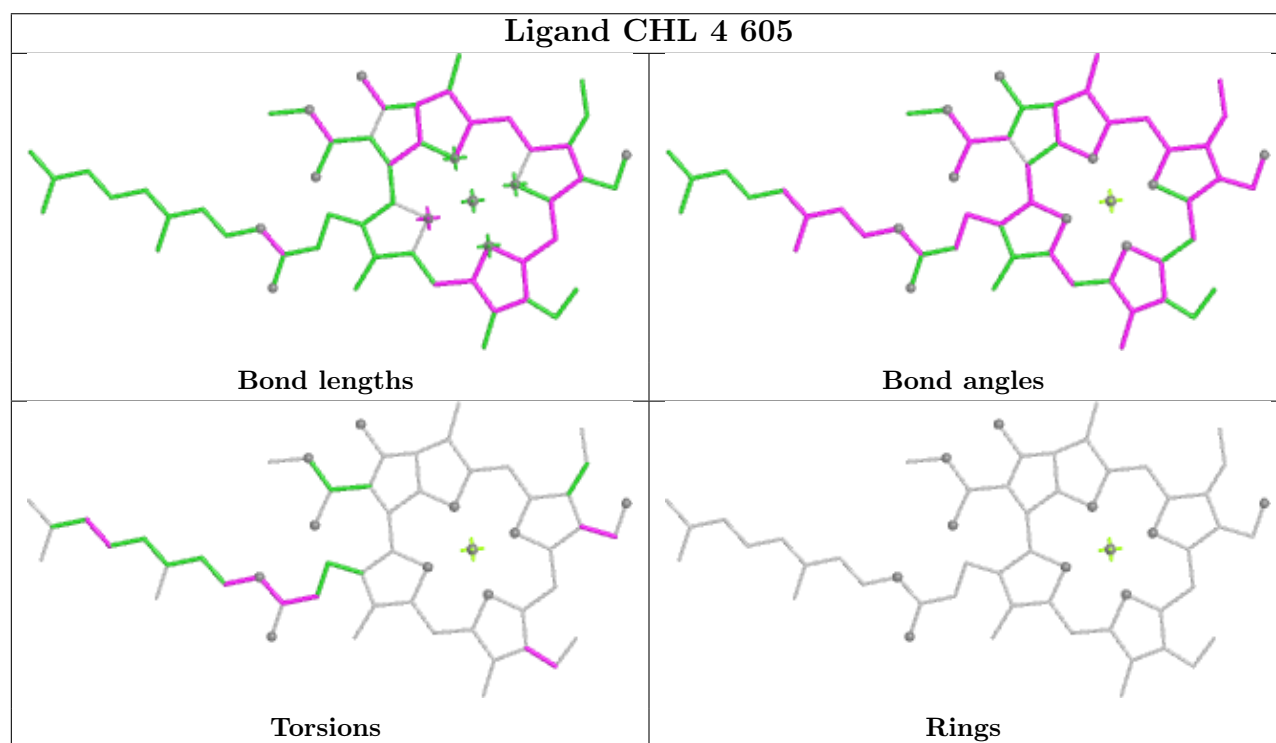
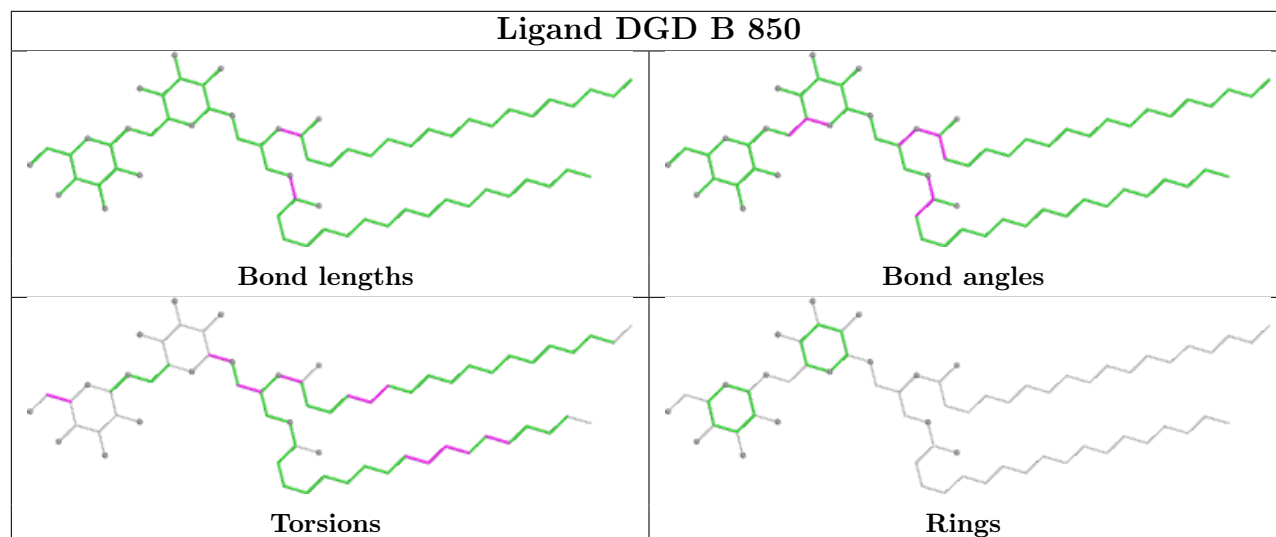
Ligand CLA G 103

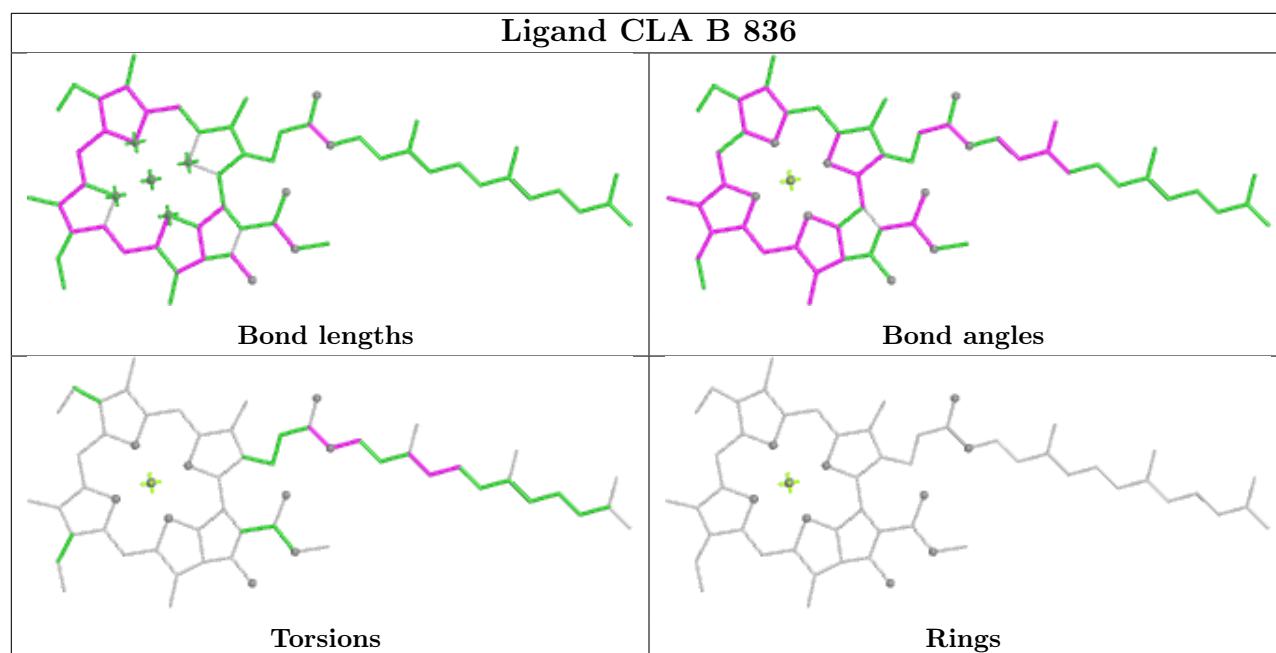
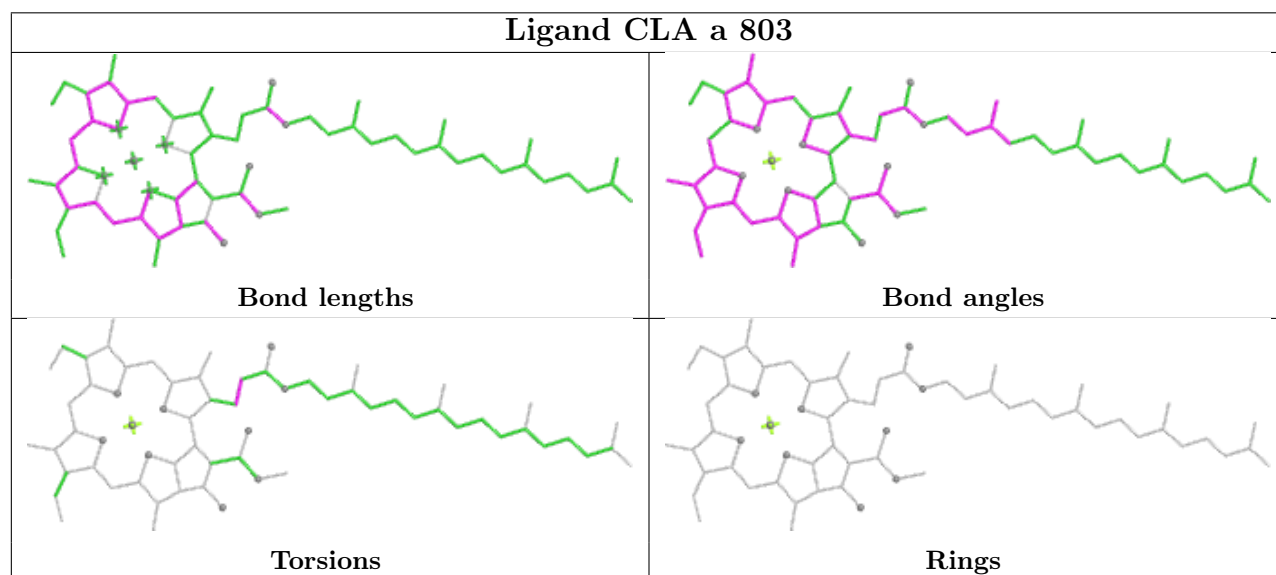
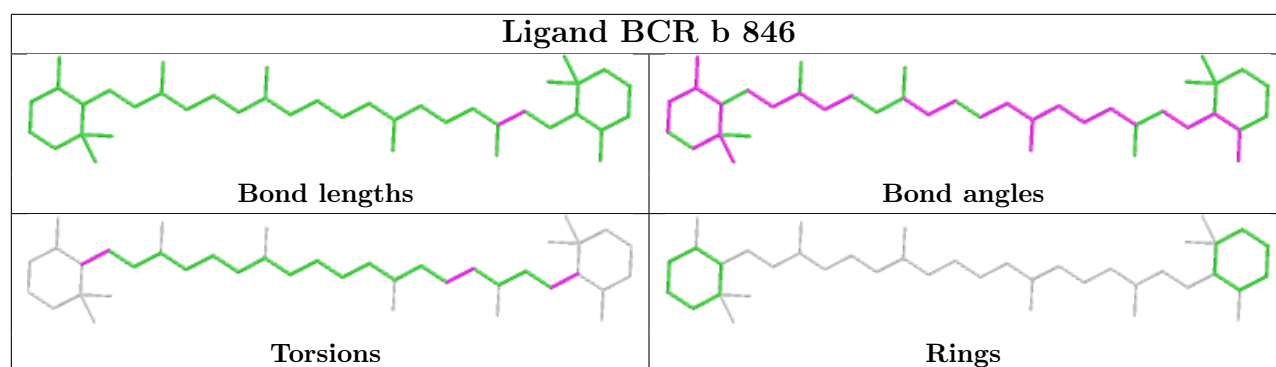


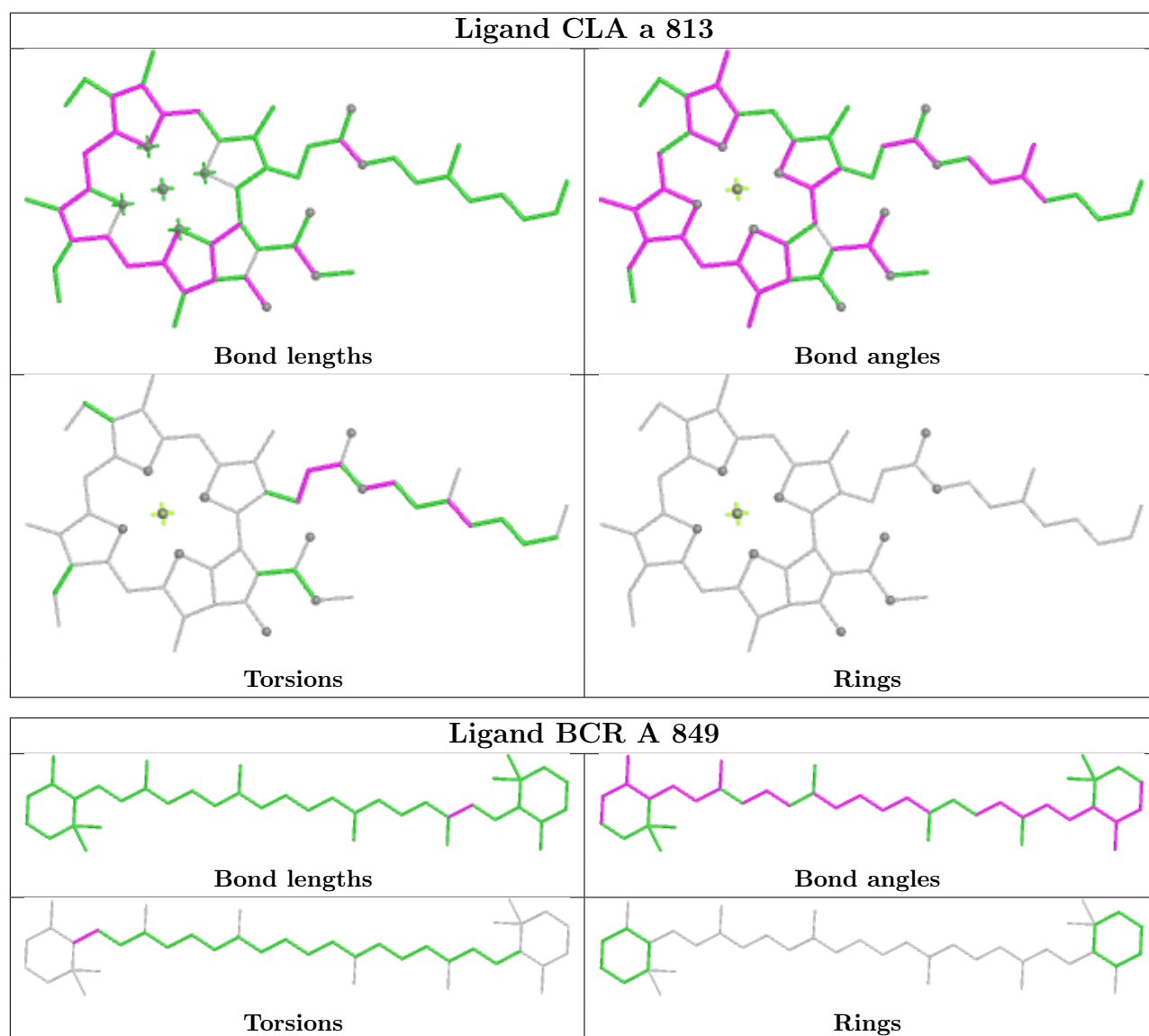
Ligand CLA b 841



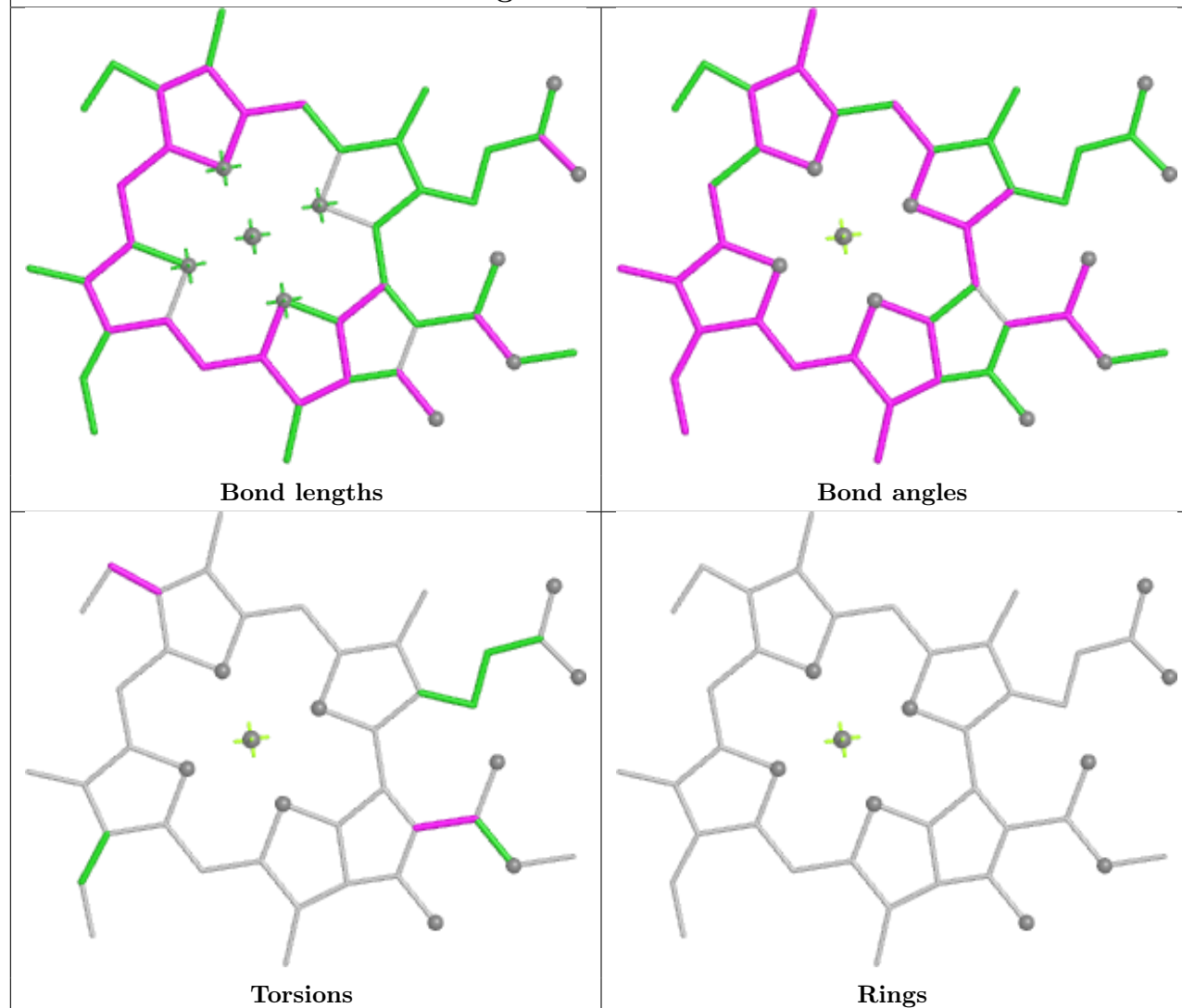




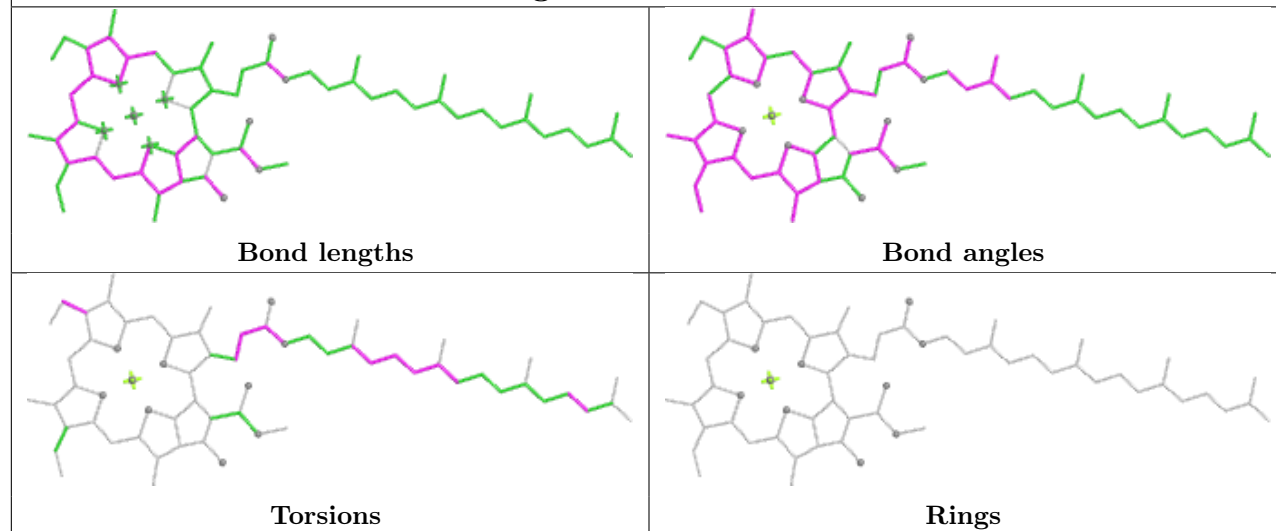


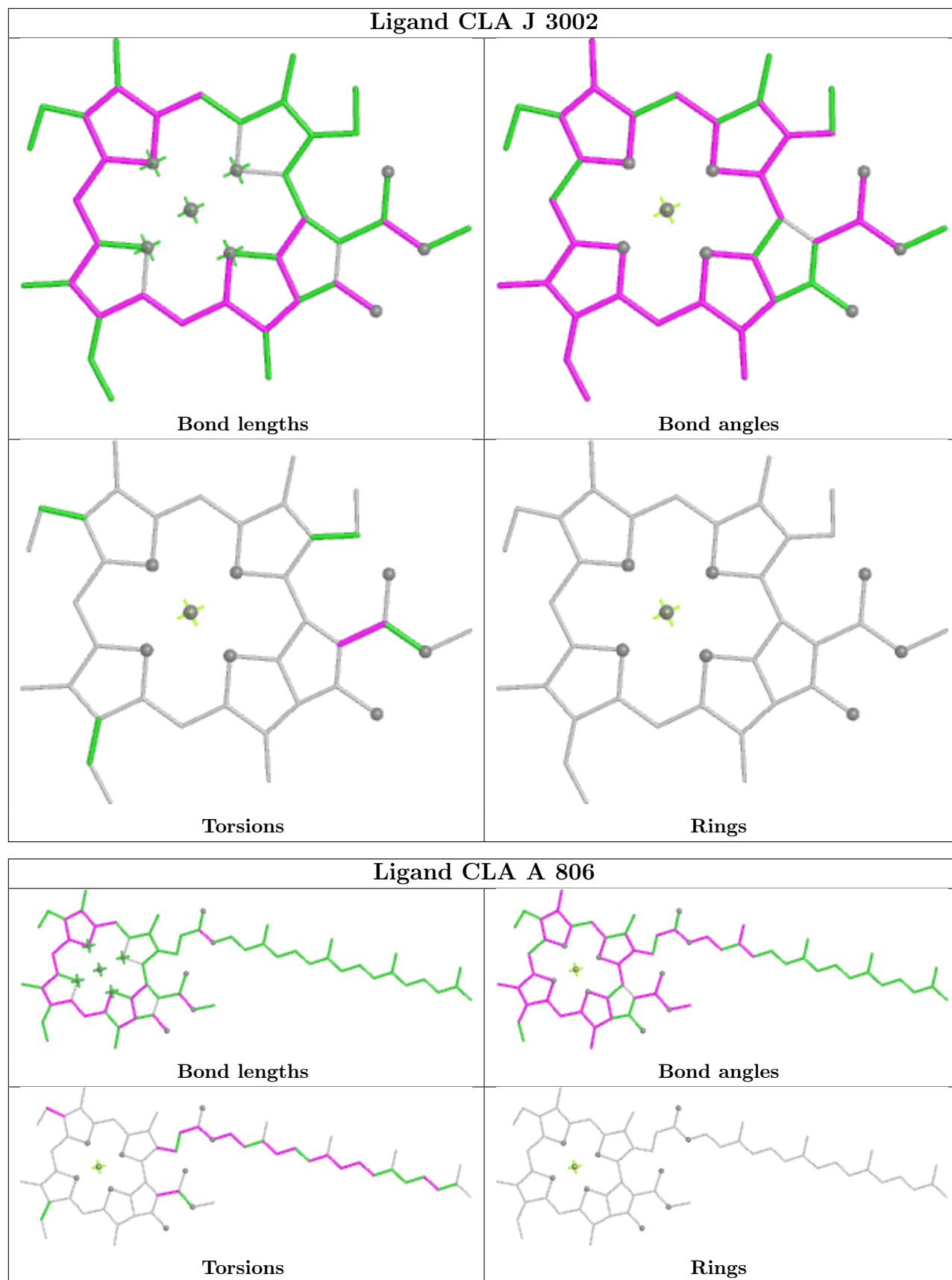


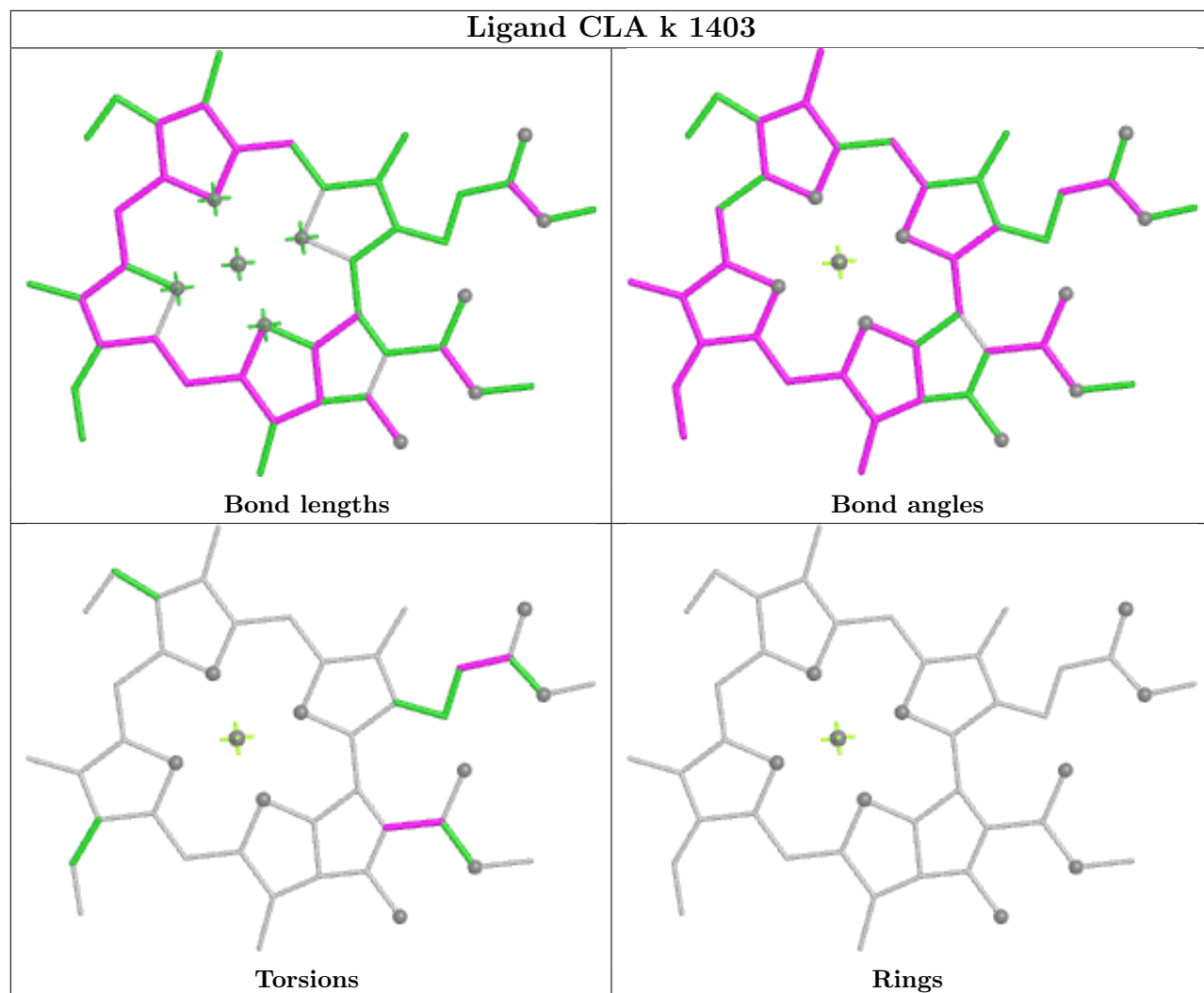
Ligand CLA 8 303



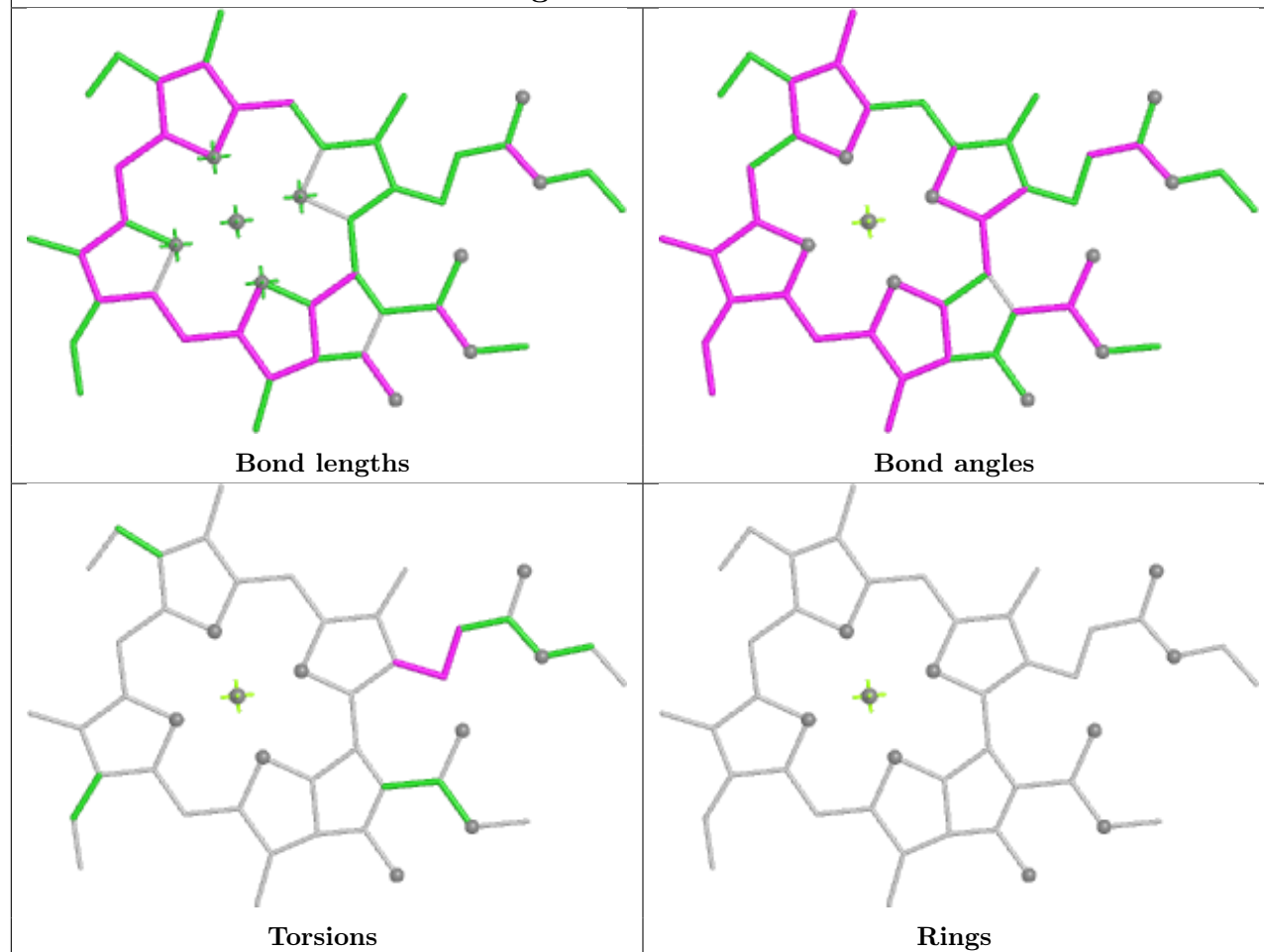
Ligand CLA B 807



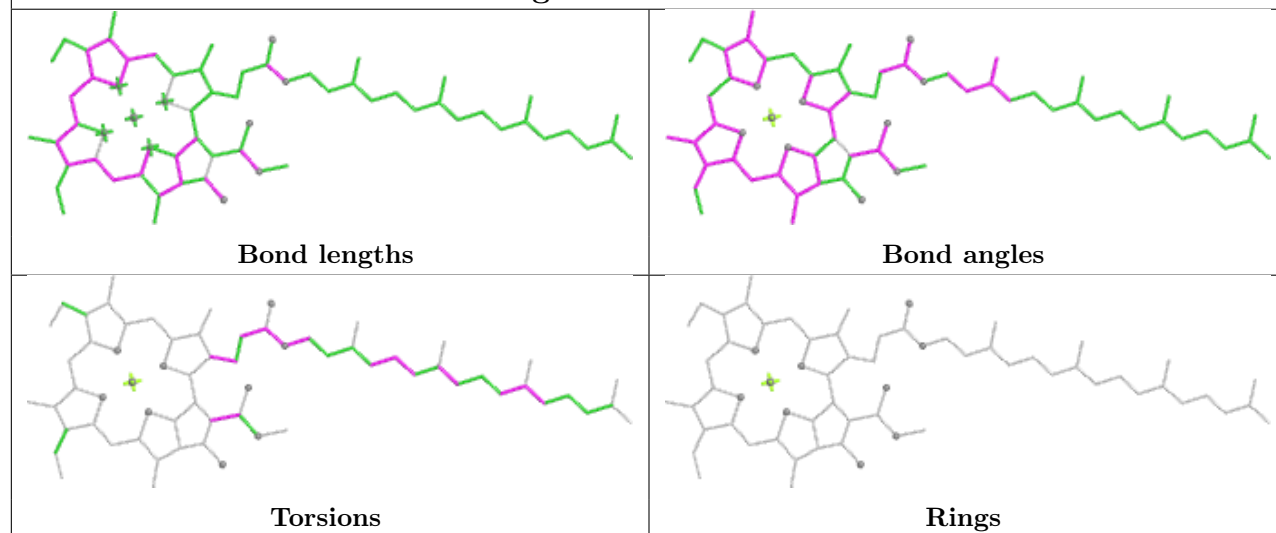




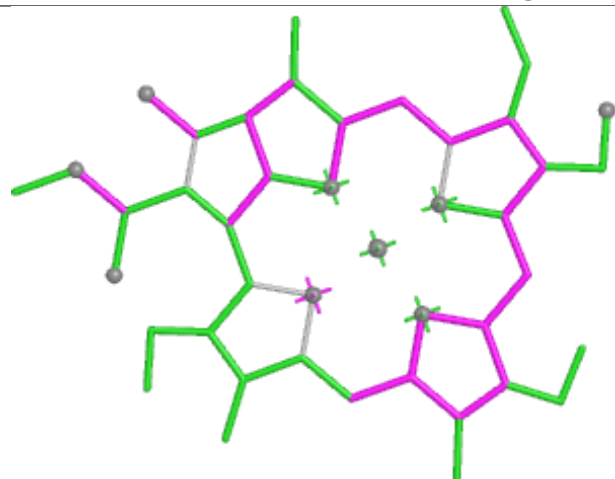
Ligand CLA 8 305



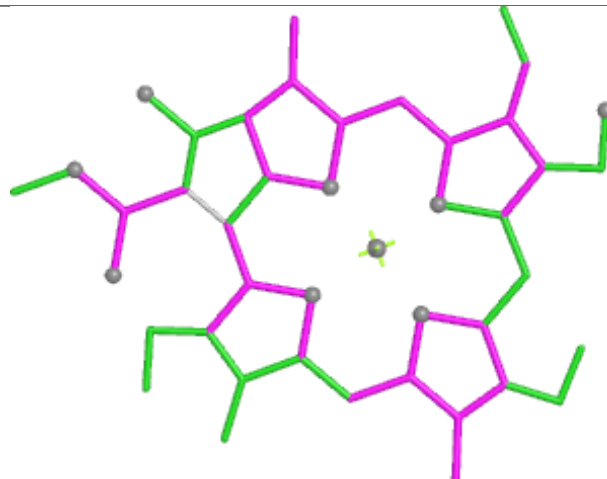
Ligand CLA B 813



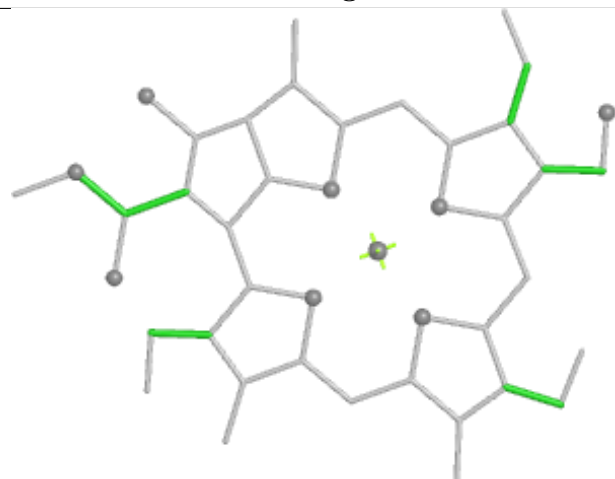
Ligand CHL 4 615



Bond lengths



Bond angles

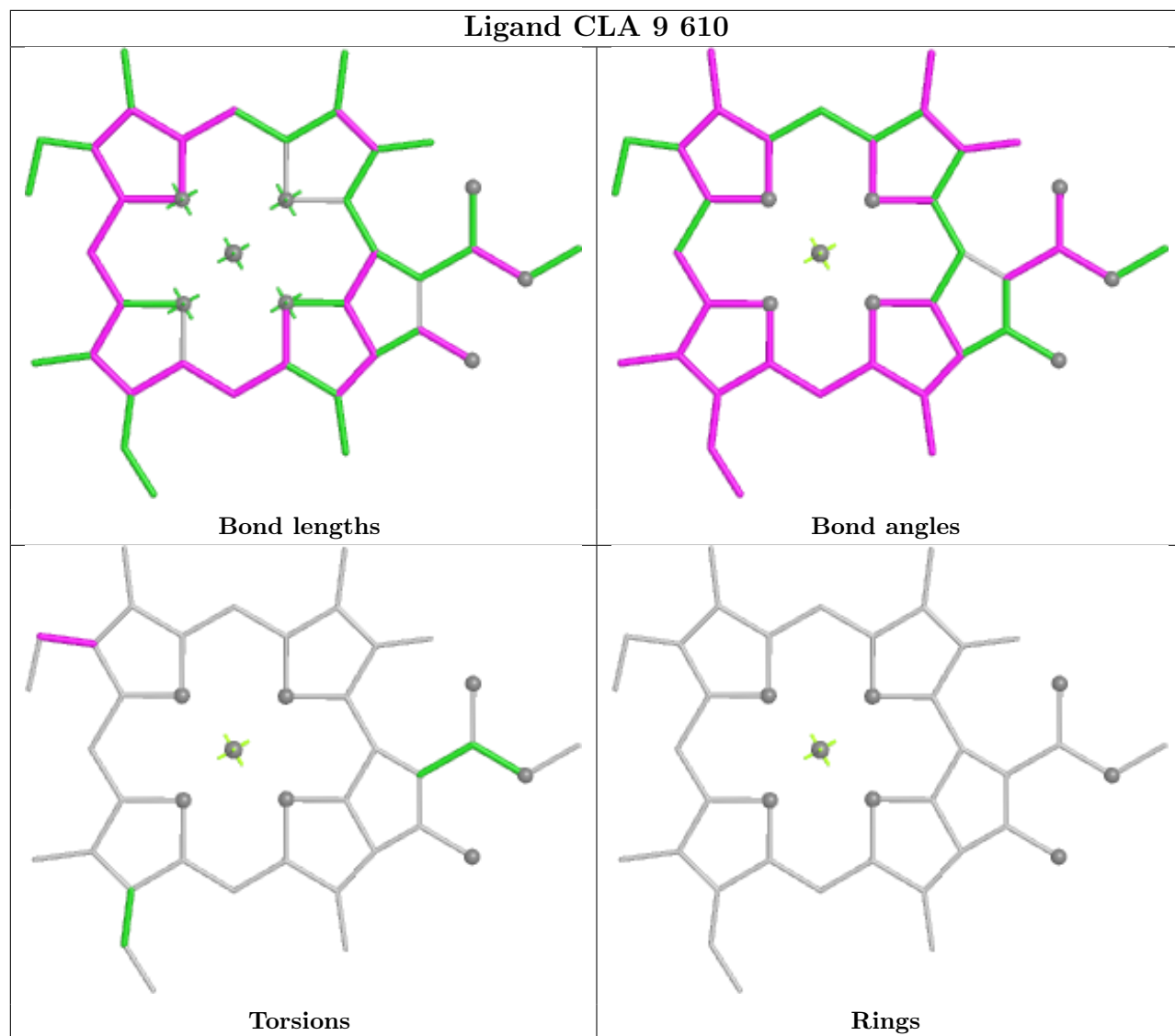


Torsions

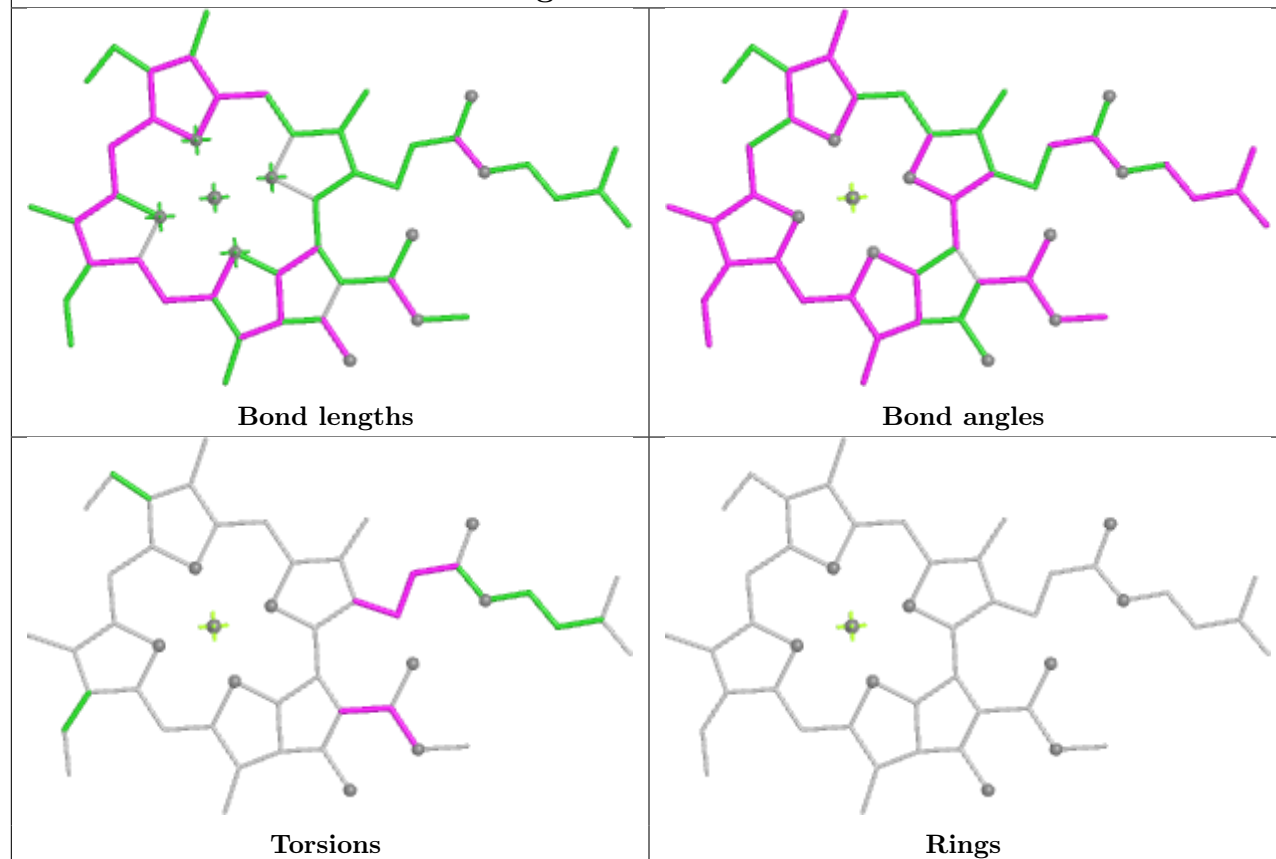


Rings

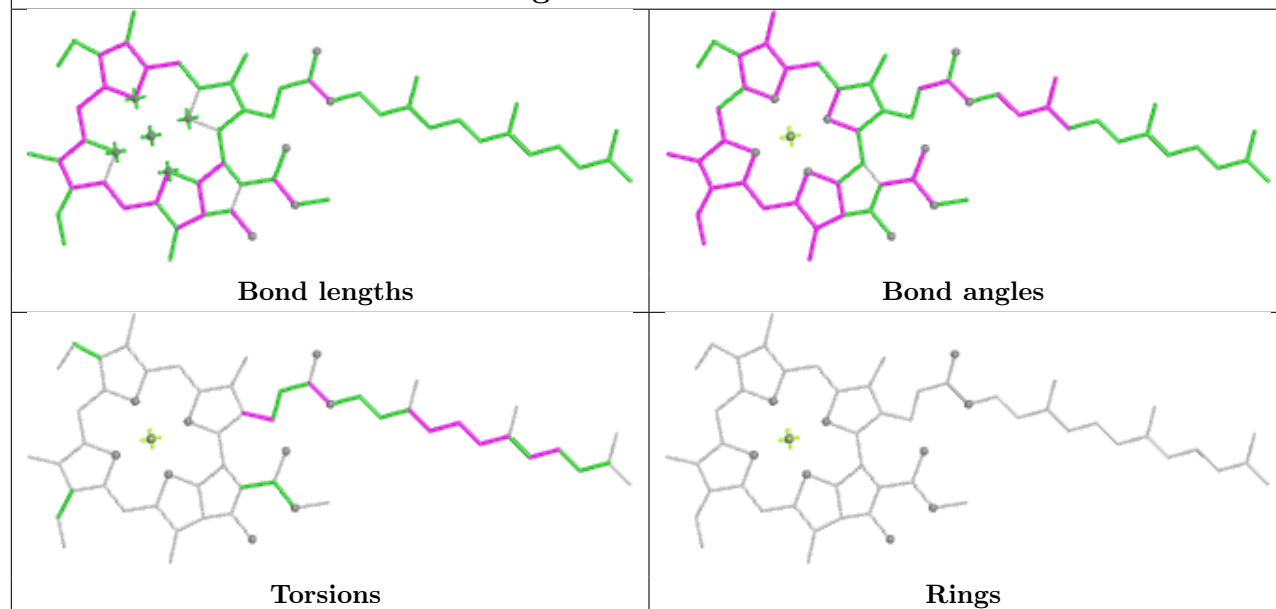
Ligand CLA 9 610



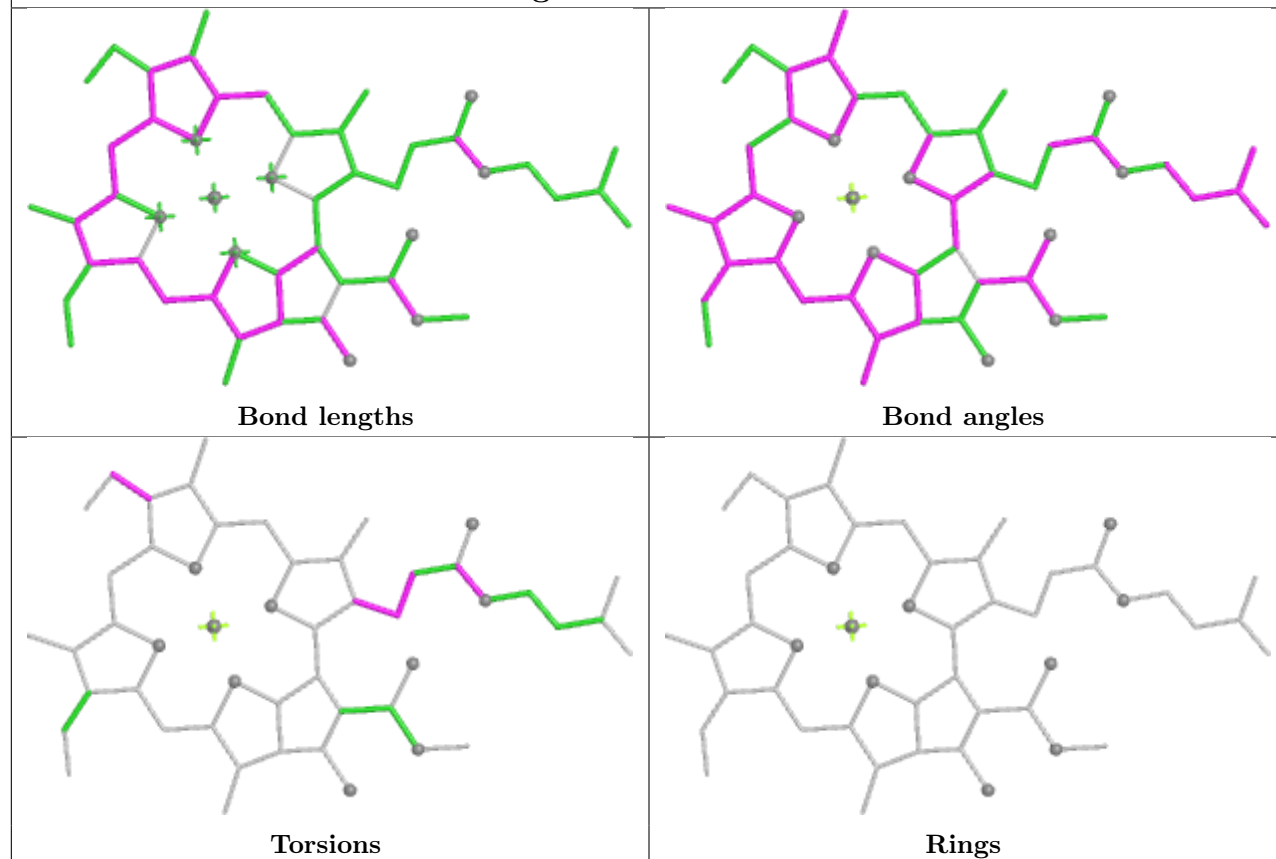
Ligand CLA a 816



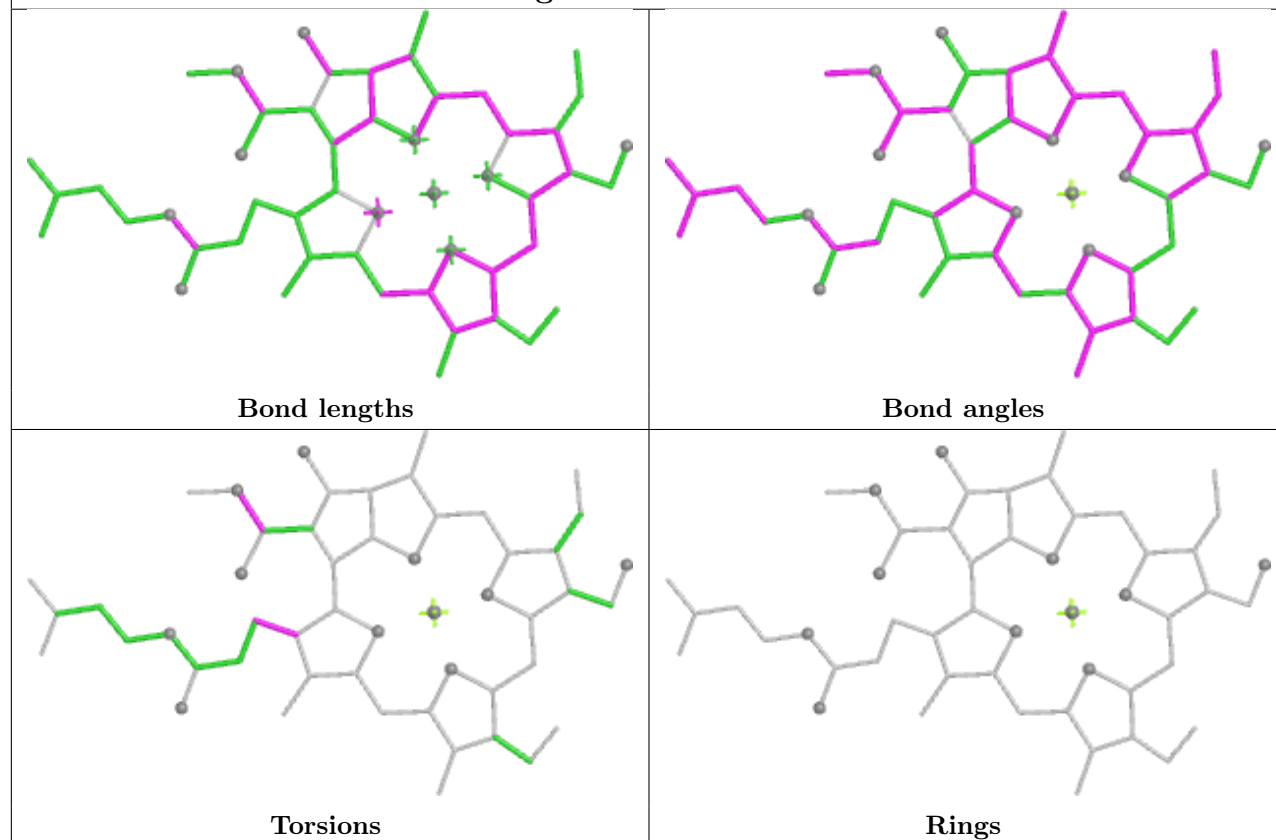
Ligand CLA B 818

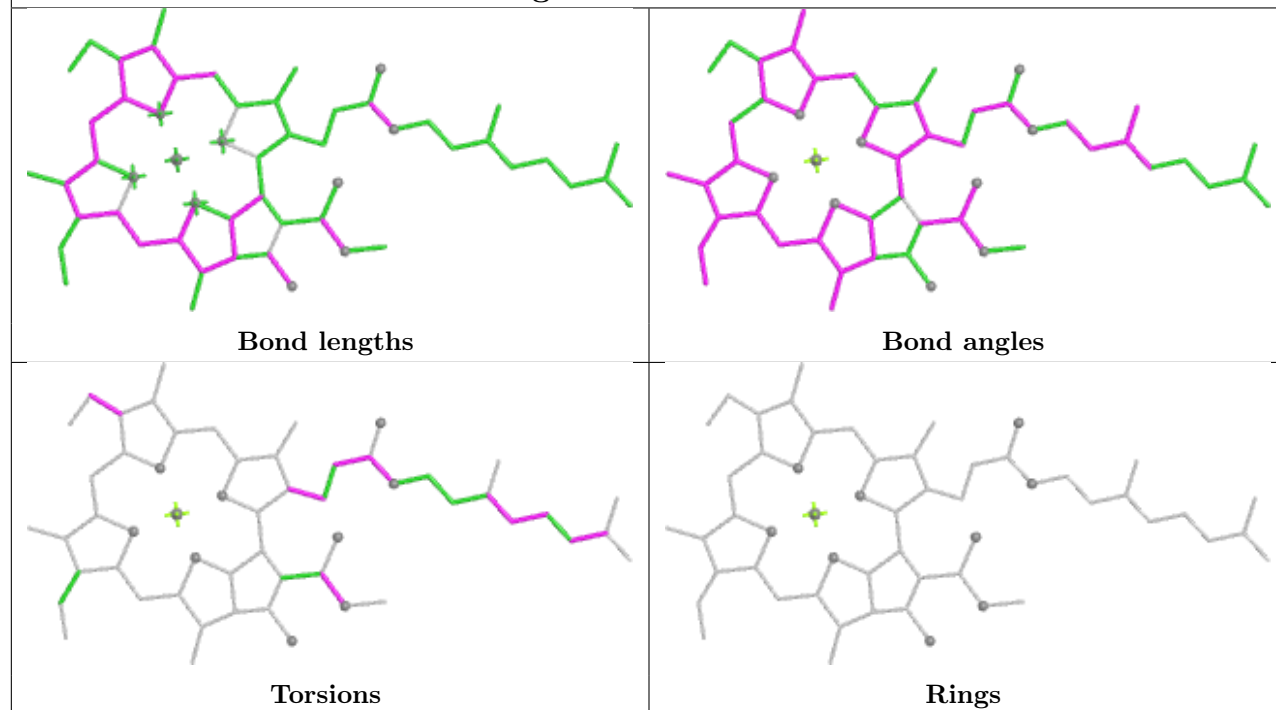
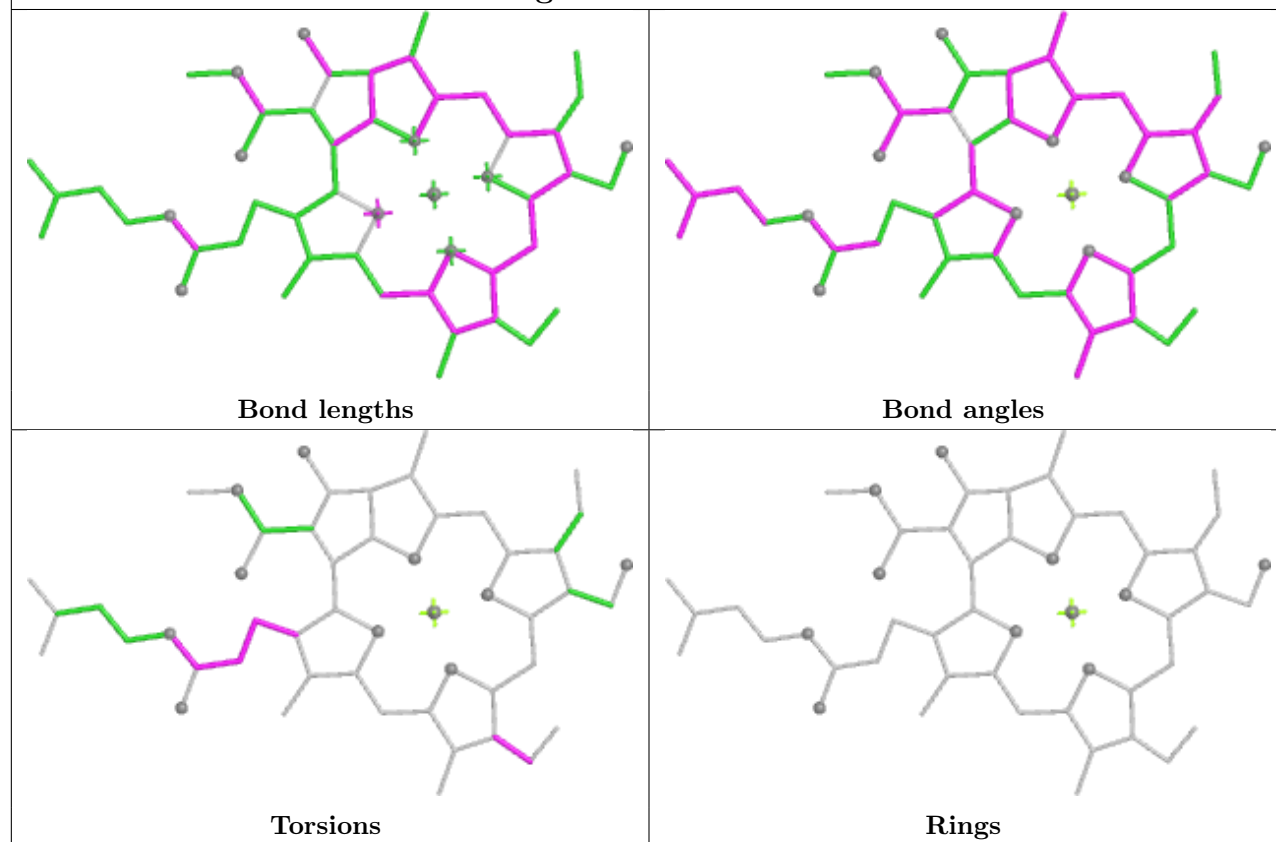


Ligand CLA B 830

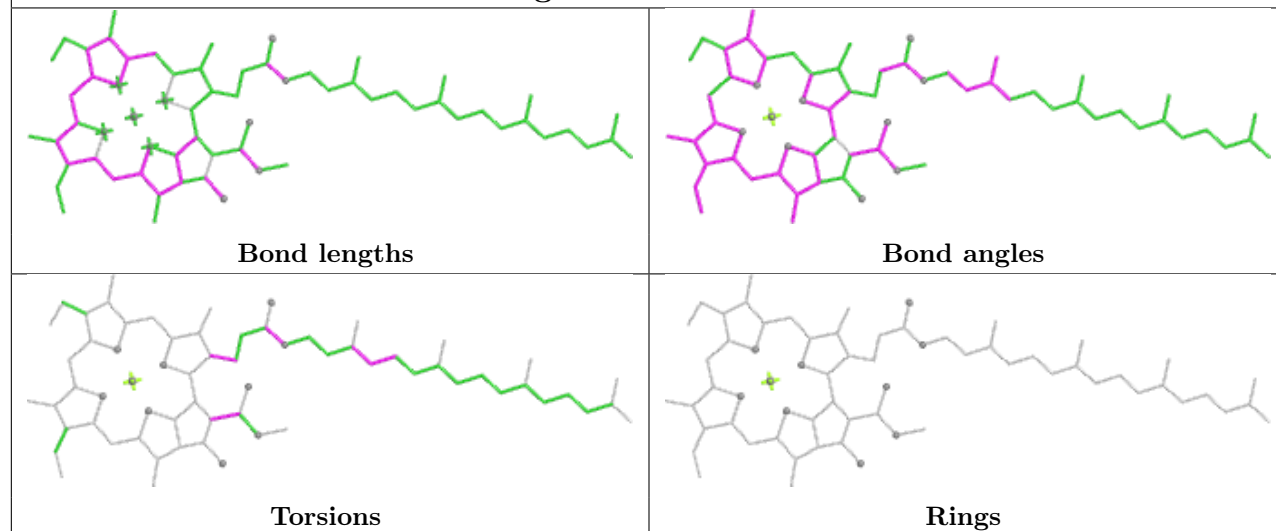


Ligand CHL 9 607

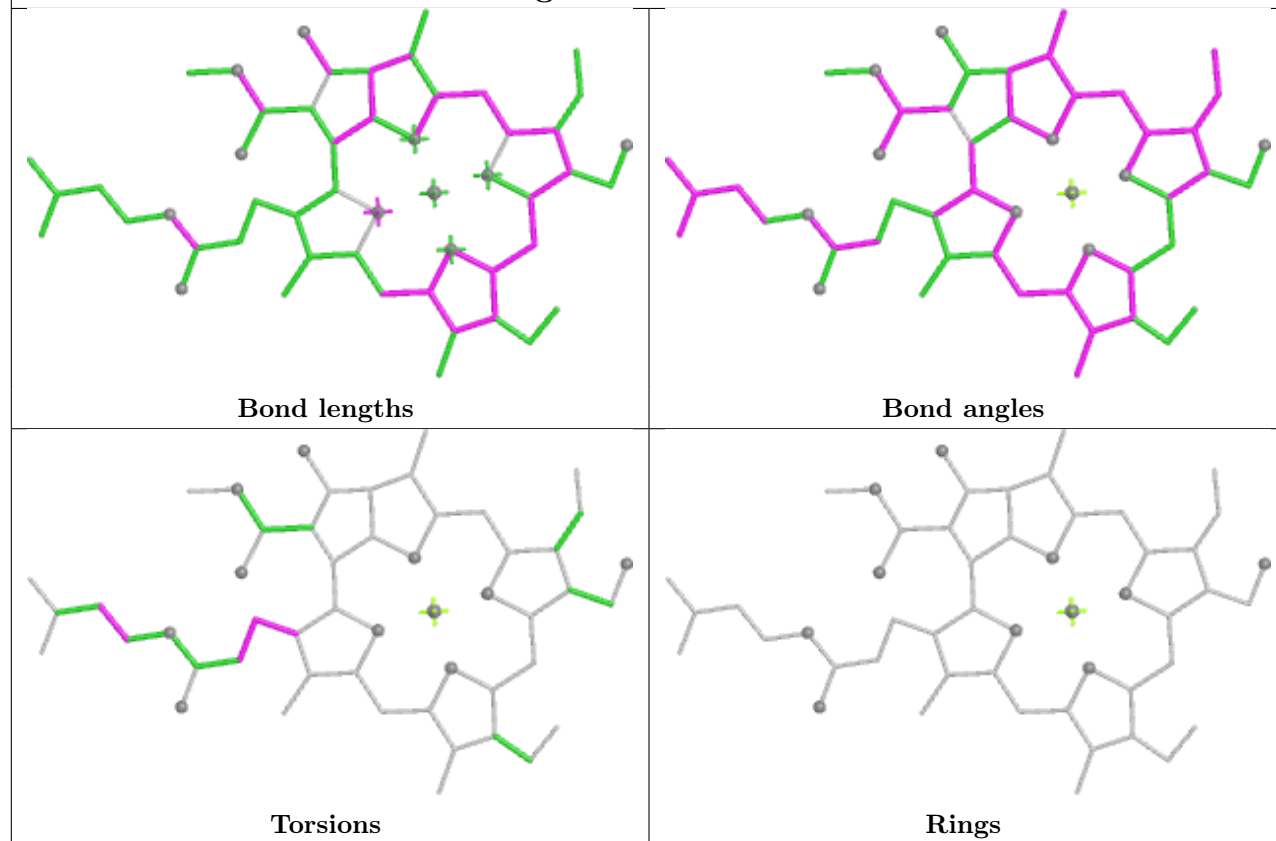


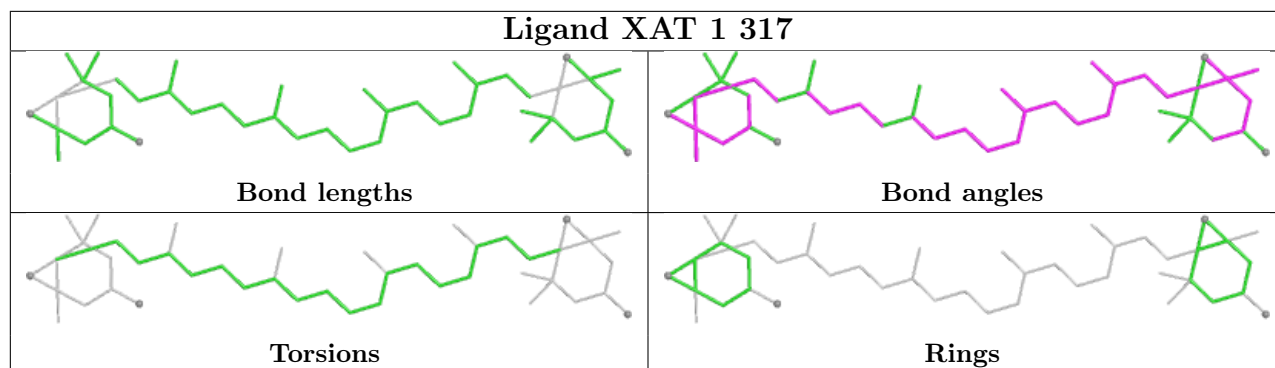
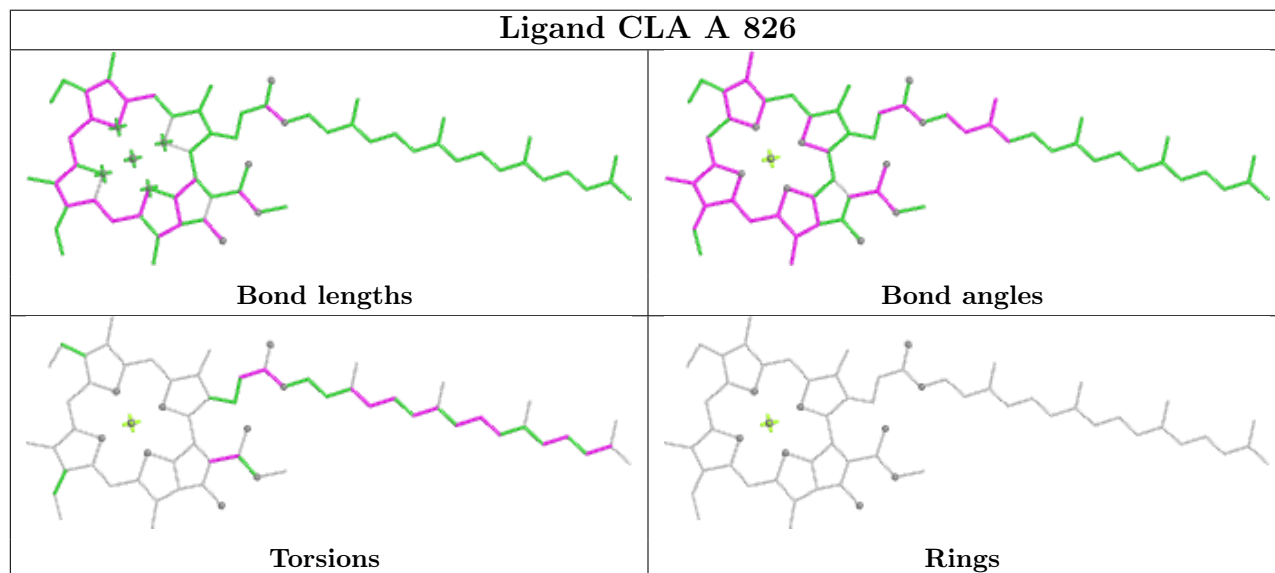
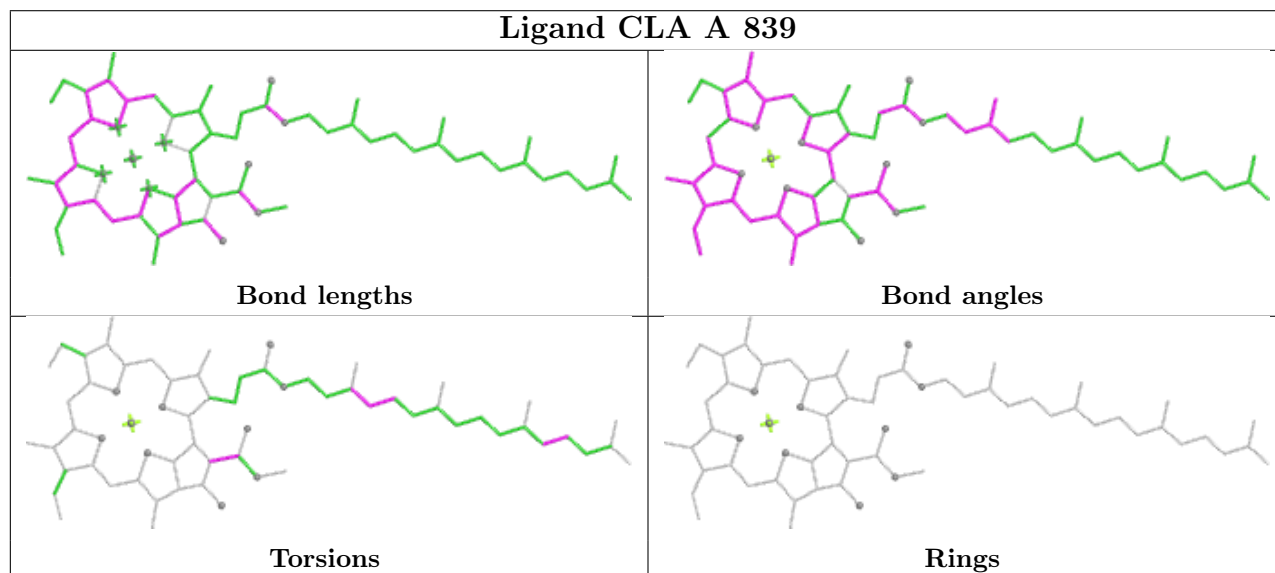
Ligand CLA B 822**Ligand CHL 4 606**

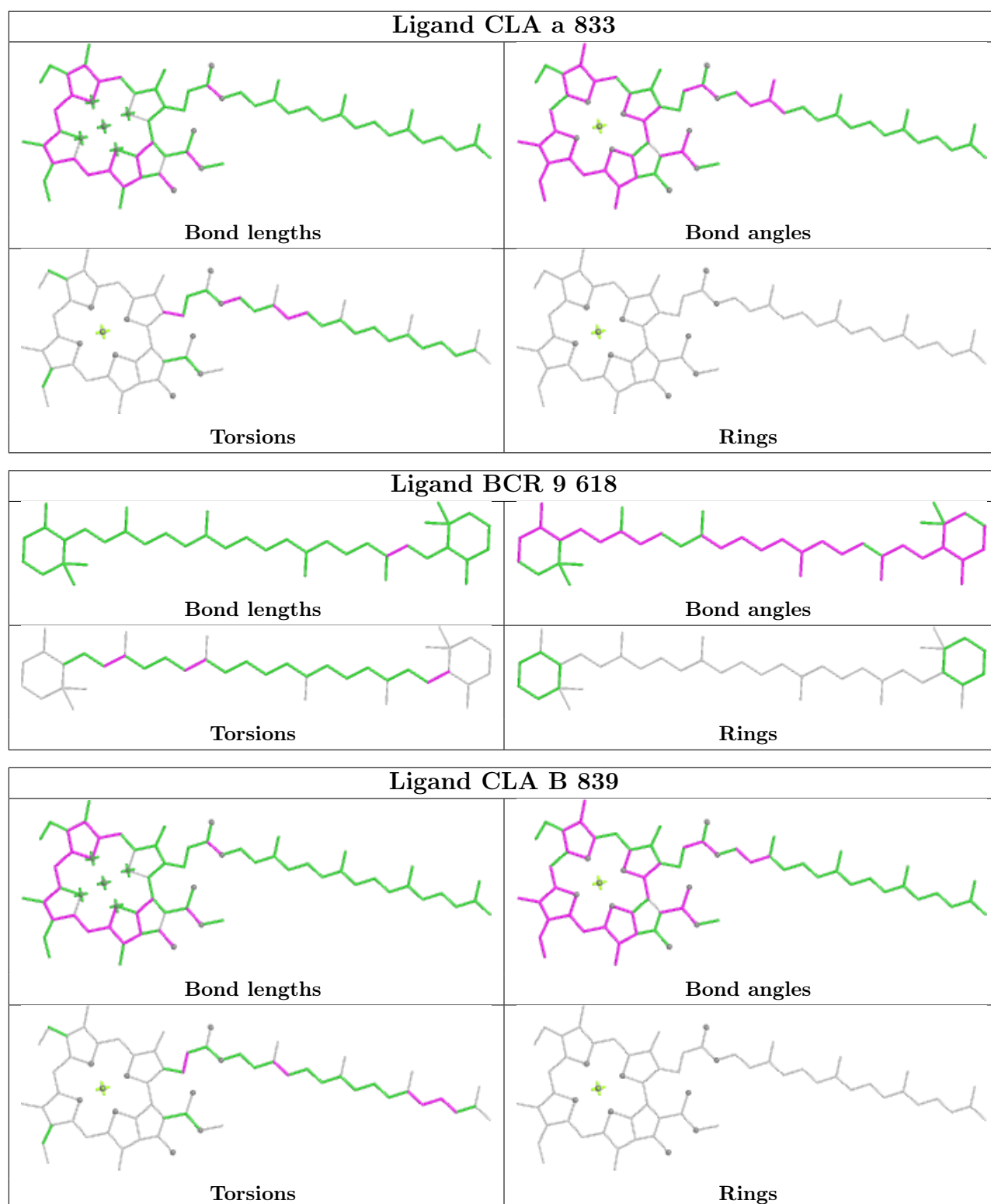
Ligand CLA L 202

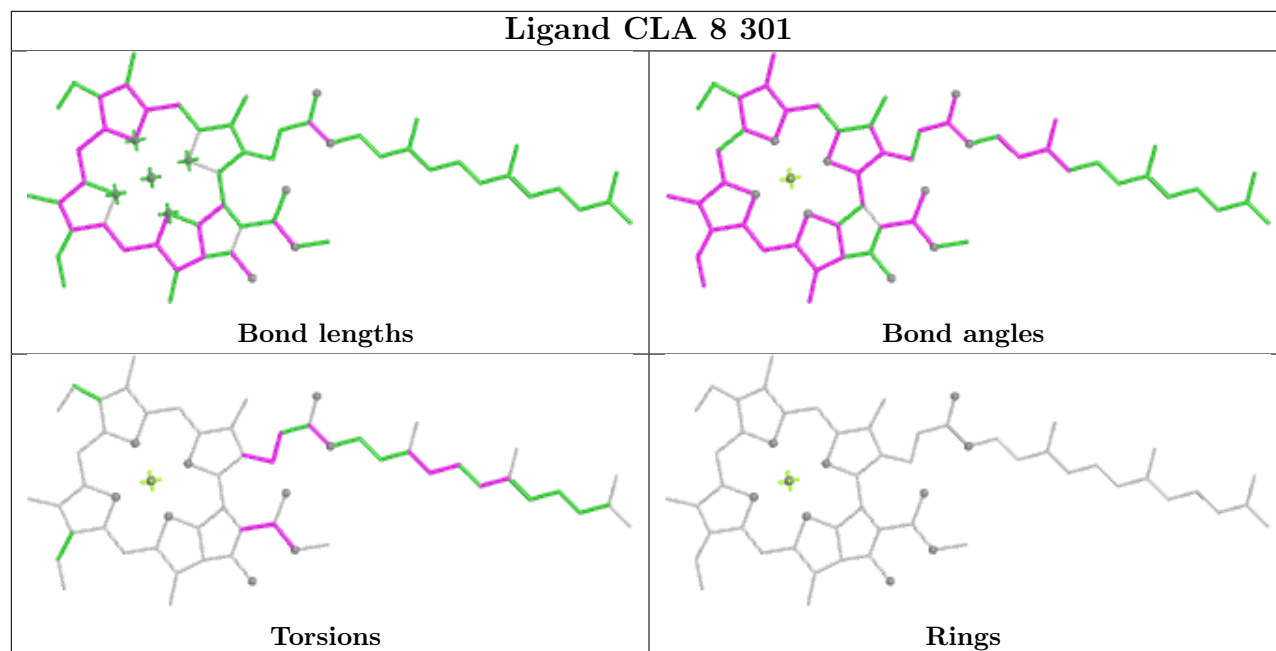
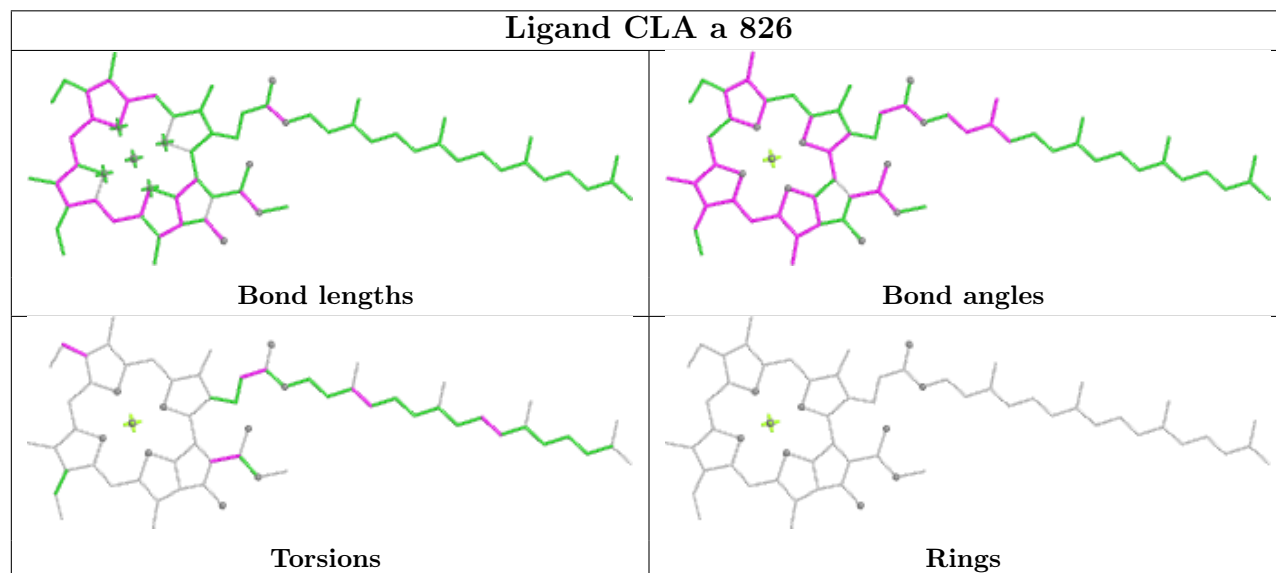
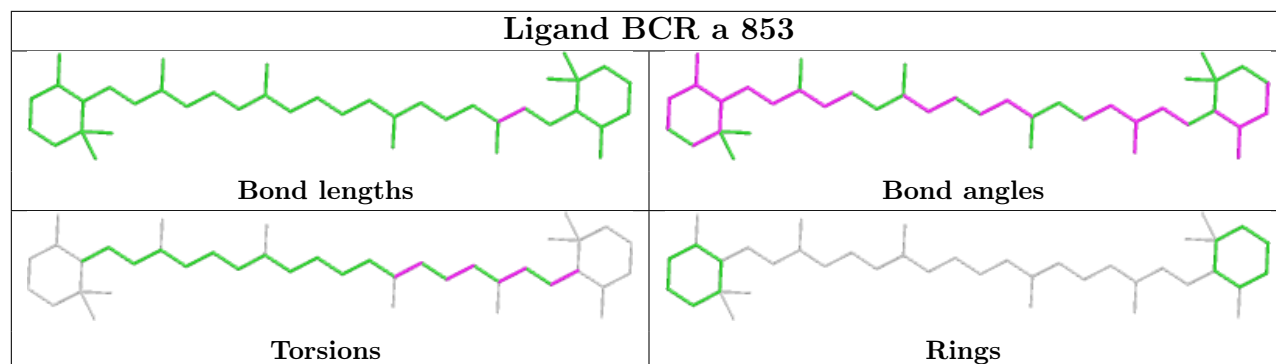


Ligand CHL 9 606

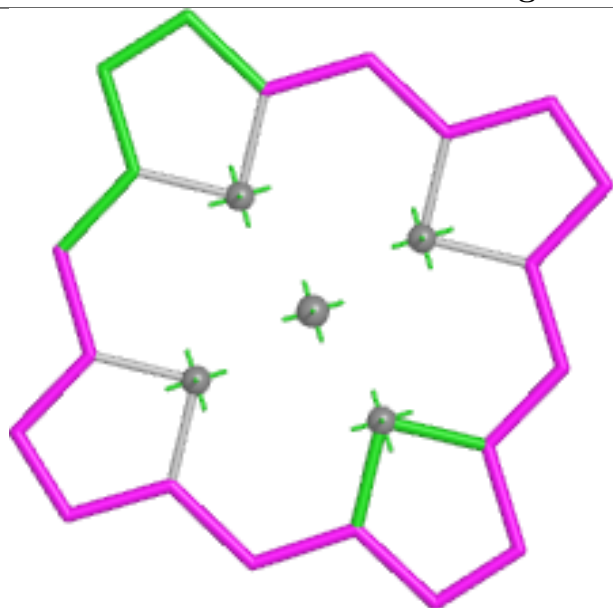


Ligand XAT 1 317**Ligand CLA A 826****Ligand CLA A 839**

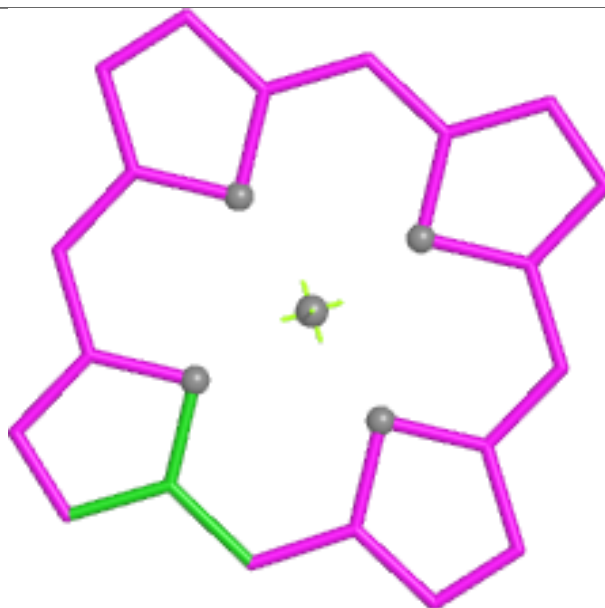




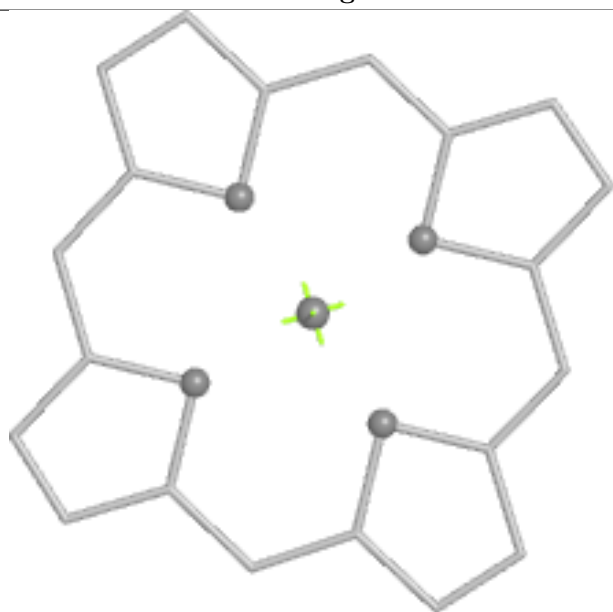
Ligand CLA 3 315



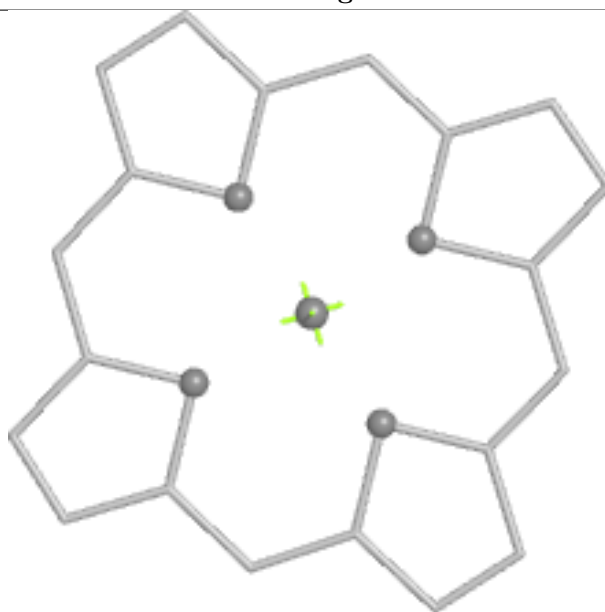
Bond lengths



Bond angles

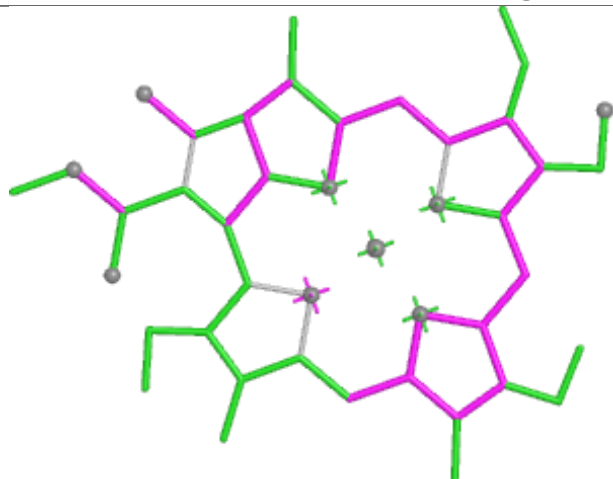


Torsions

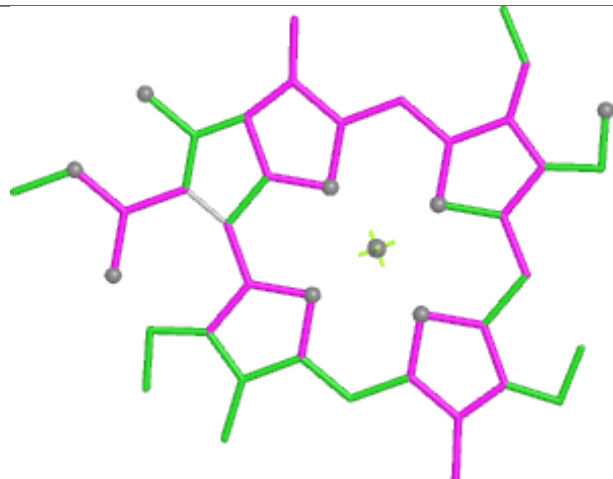


Rings

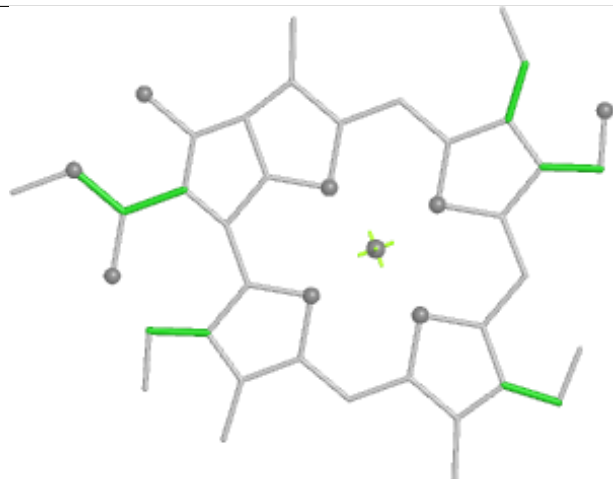
Ligand CHL 2 614



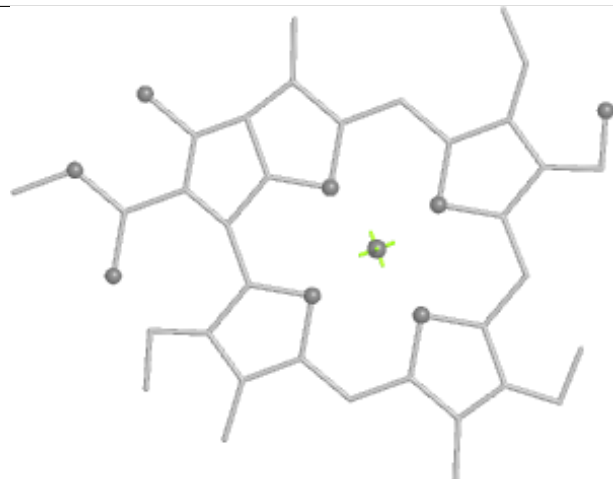
Bond lengths



Bond angles

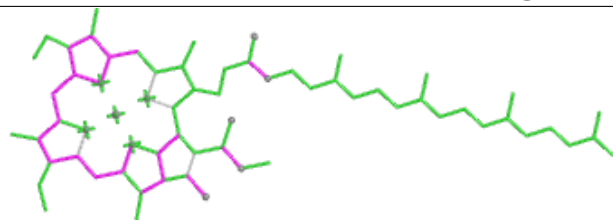


Torsions

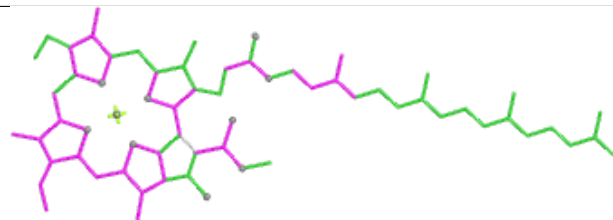


Rings

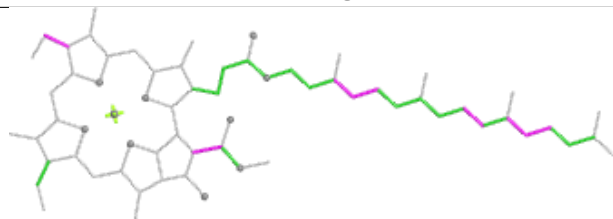
Ligand CLA a 808



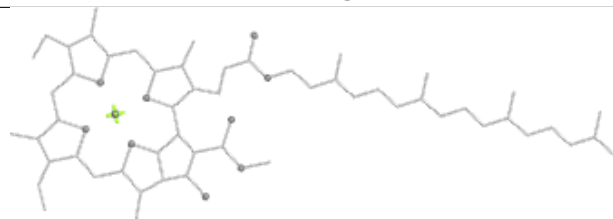
Bond lengths



Bond angles

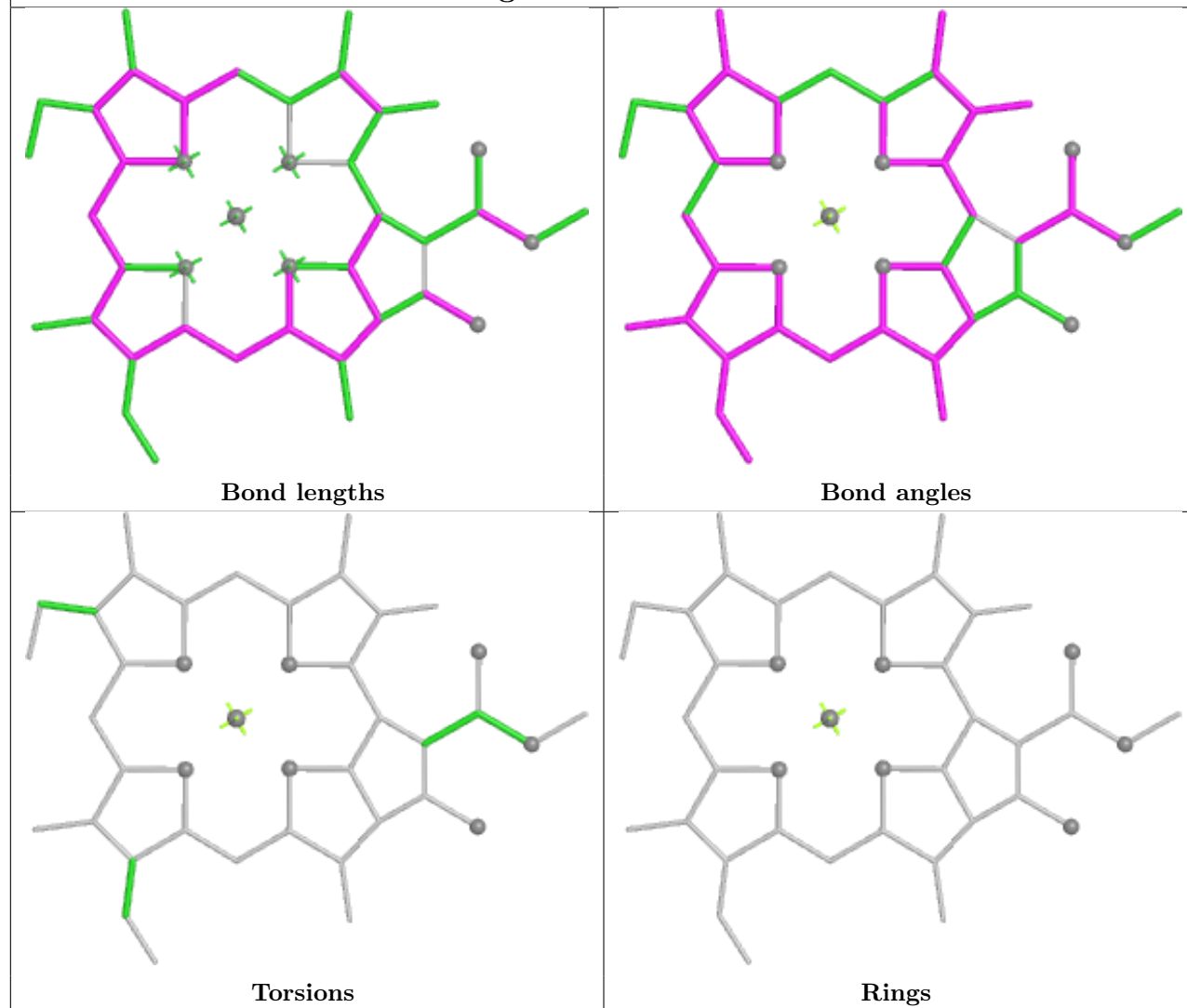


Torsions

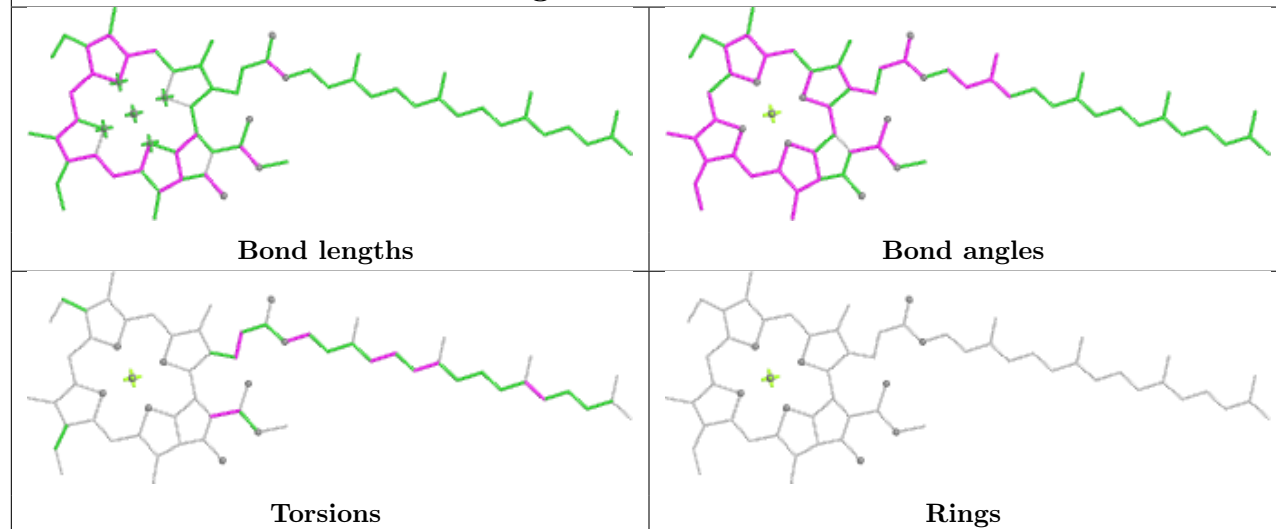


Rings

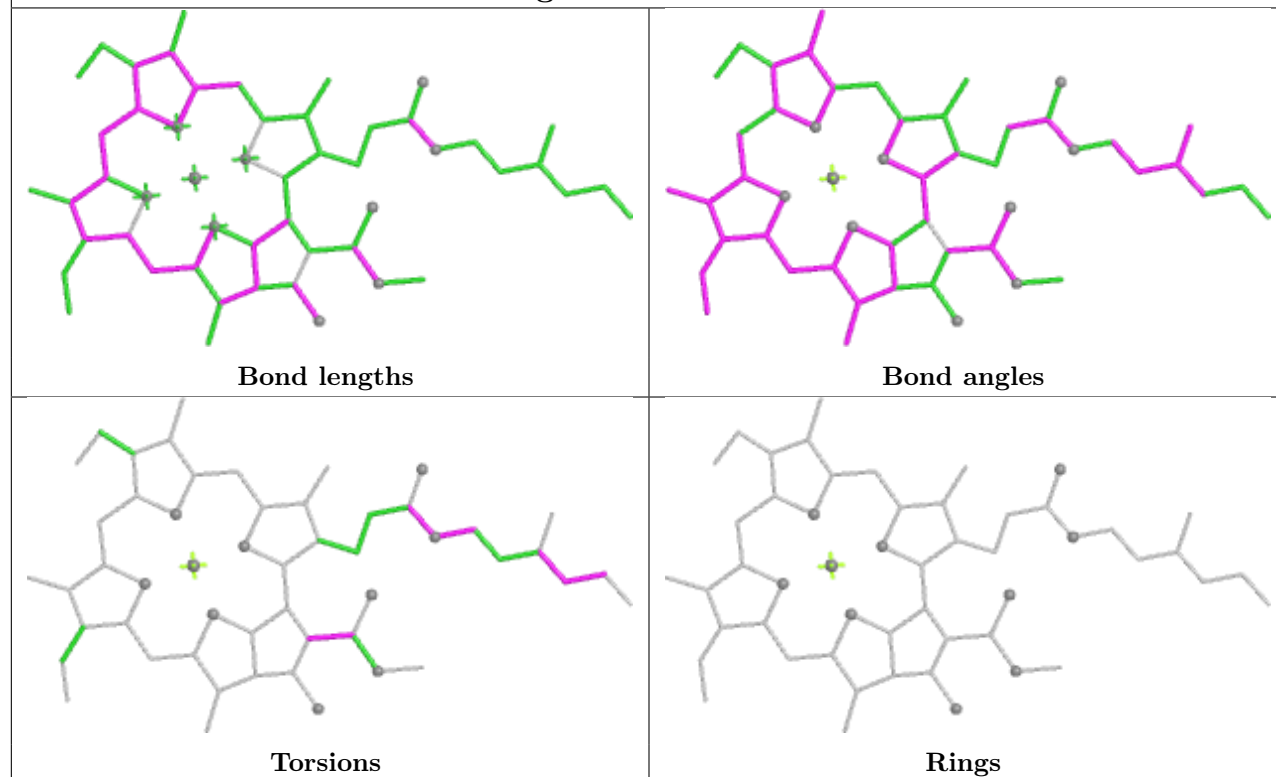
Ligand CLA 2 610



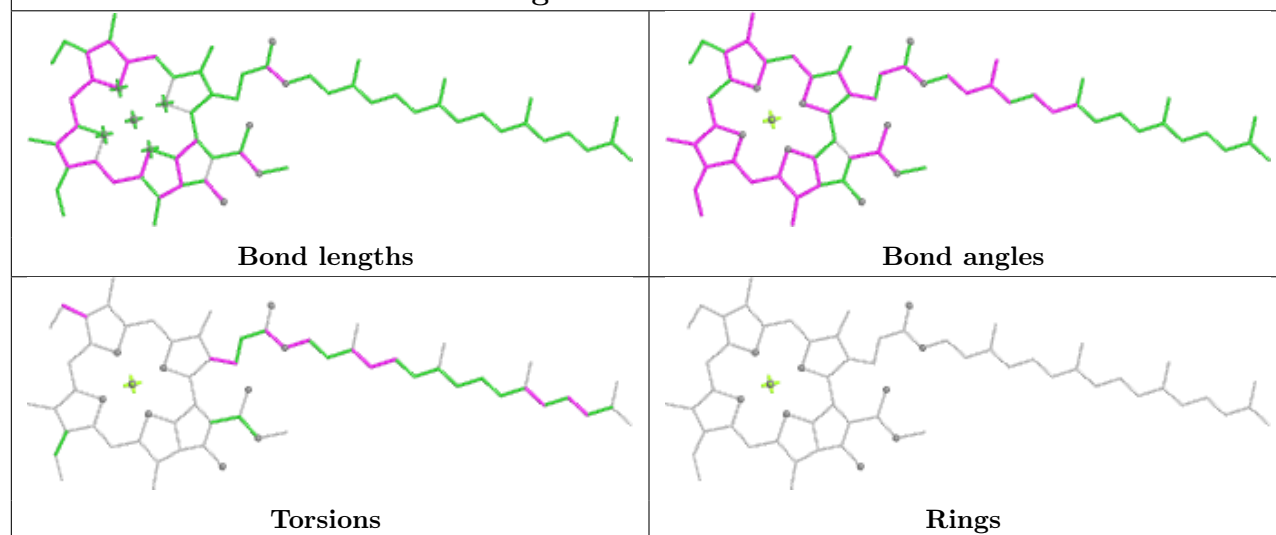
Ligand CLA A 854



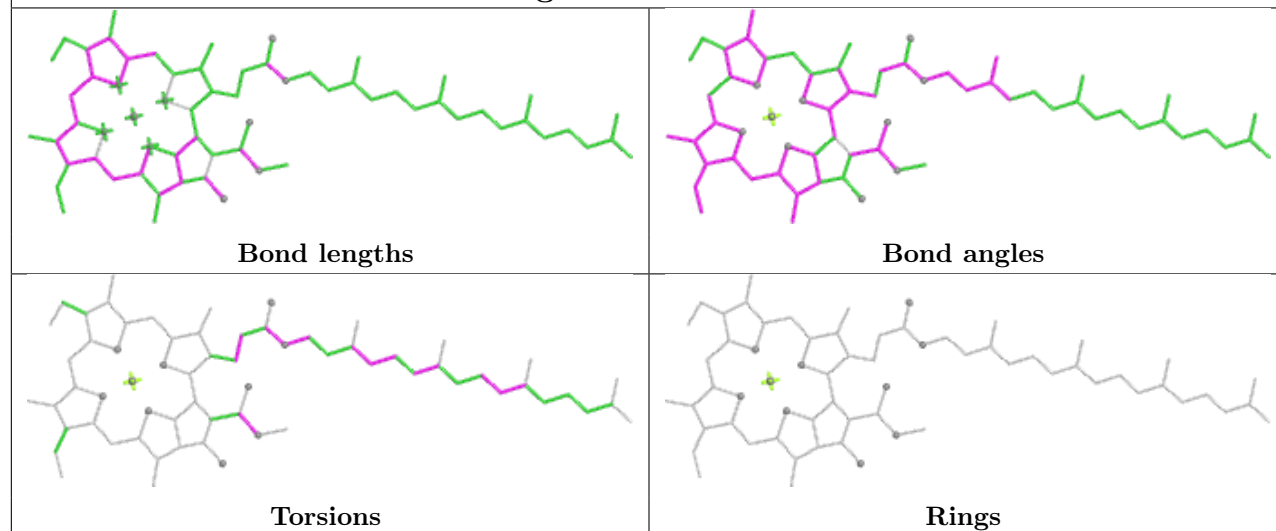
Ligand CLA 4 611



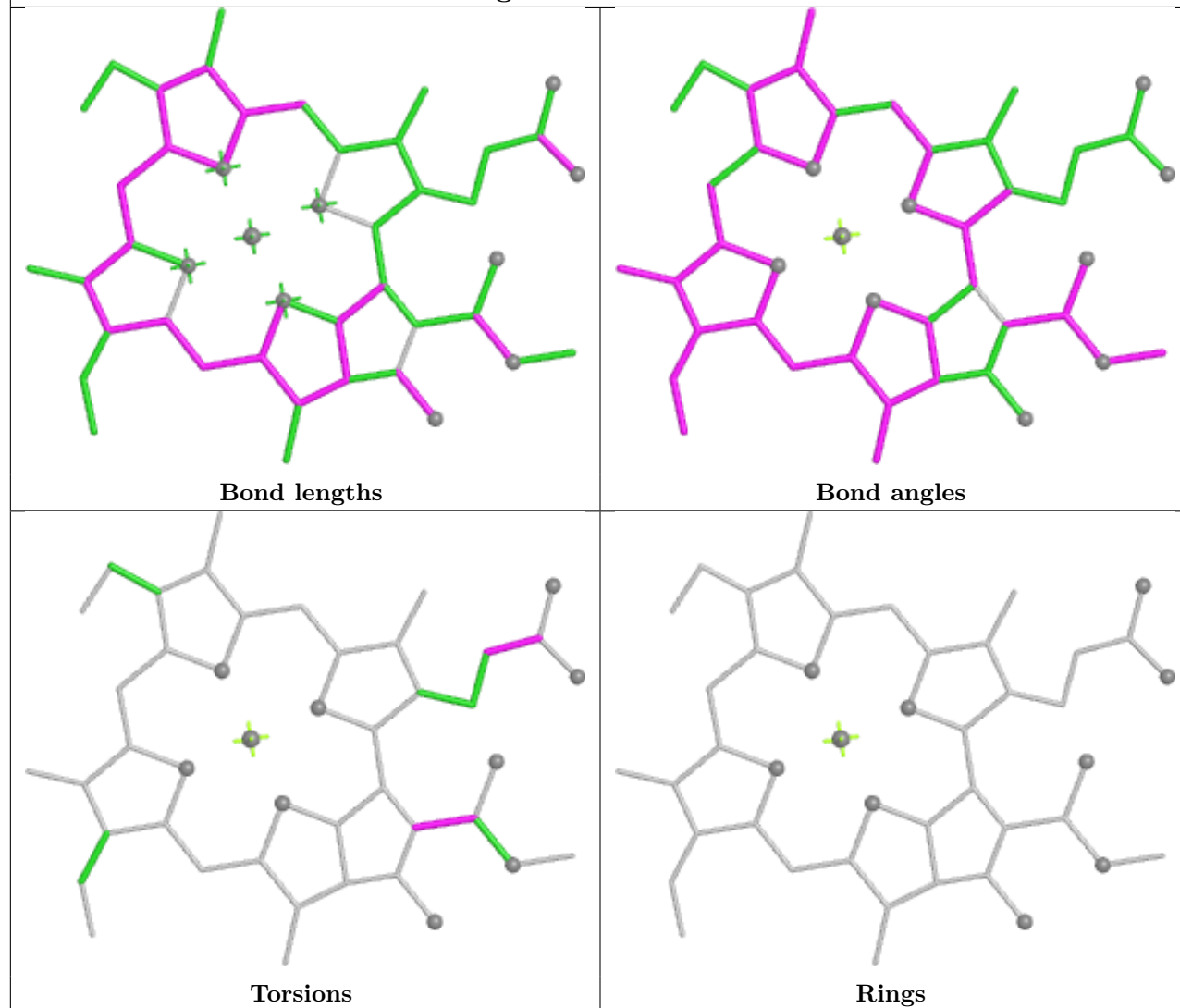
Ligand CLA A 829



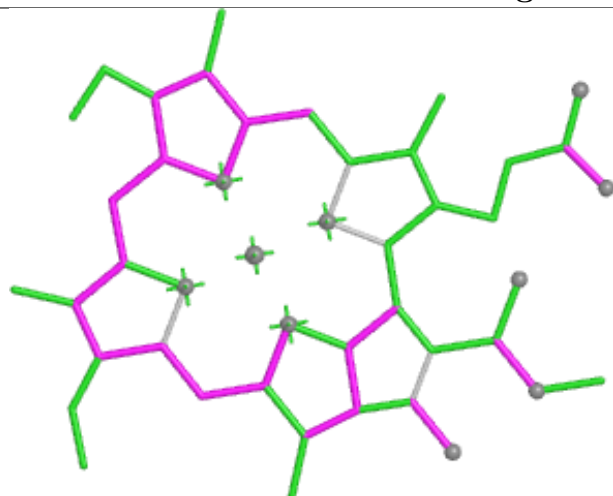
Ligand CLA a 843



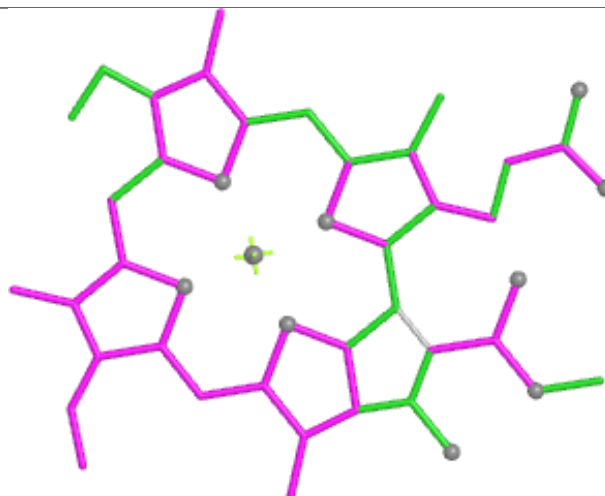
Ligand CLA 8 311



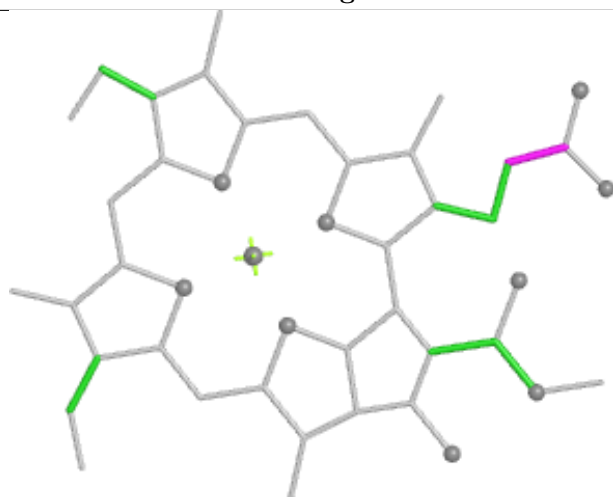
Ligand CLA F 303



Bond lengths



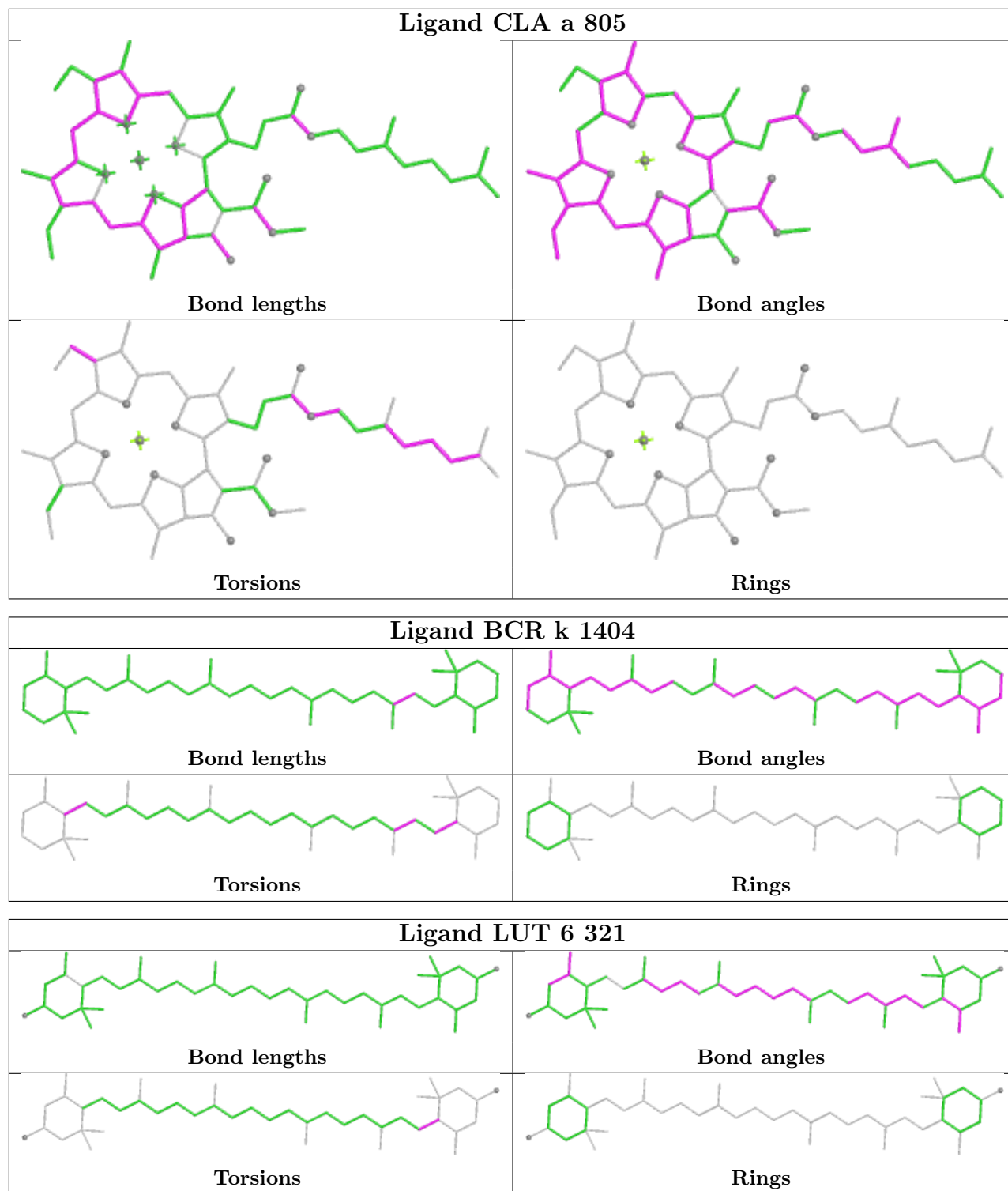
Bond angles

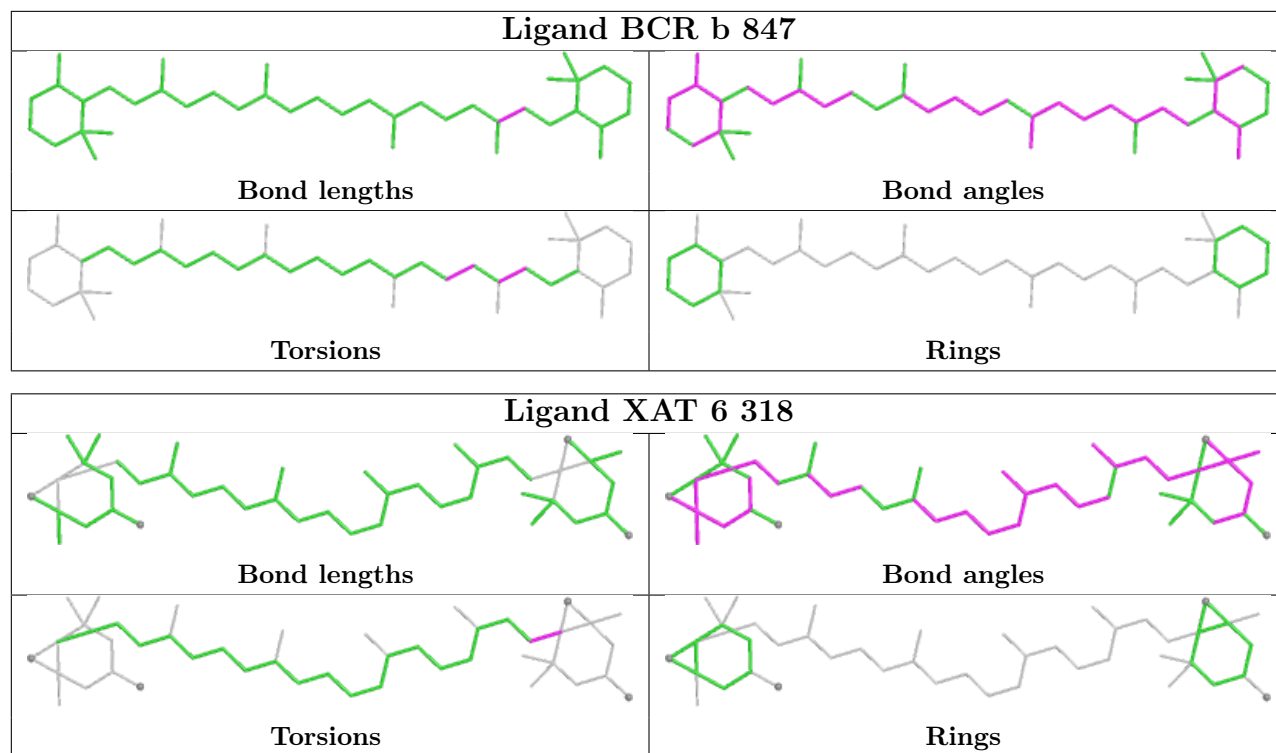


Torsions

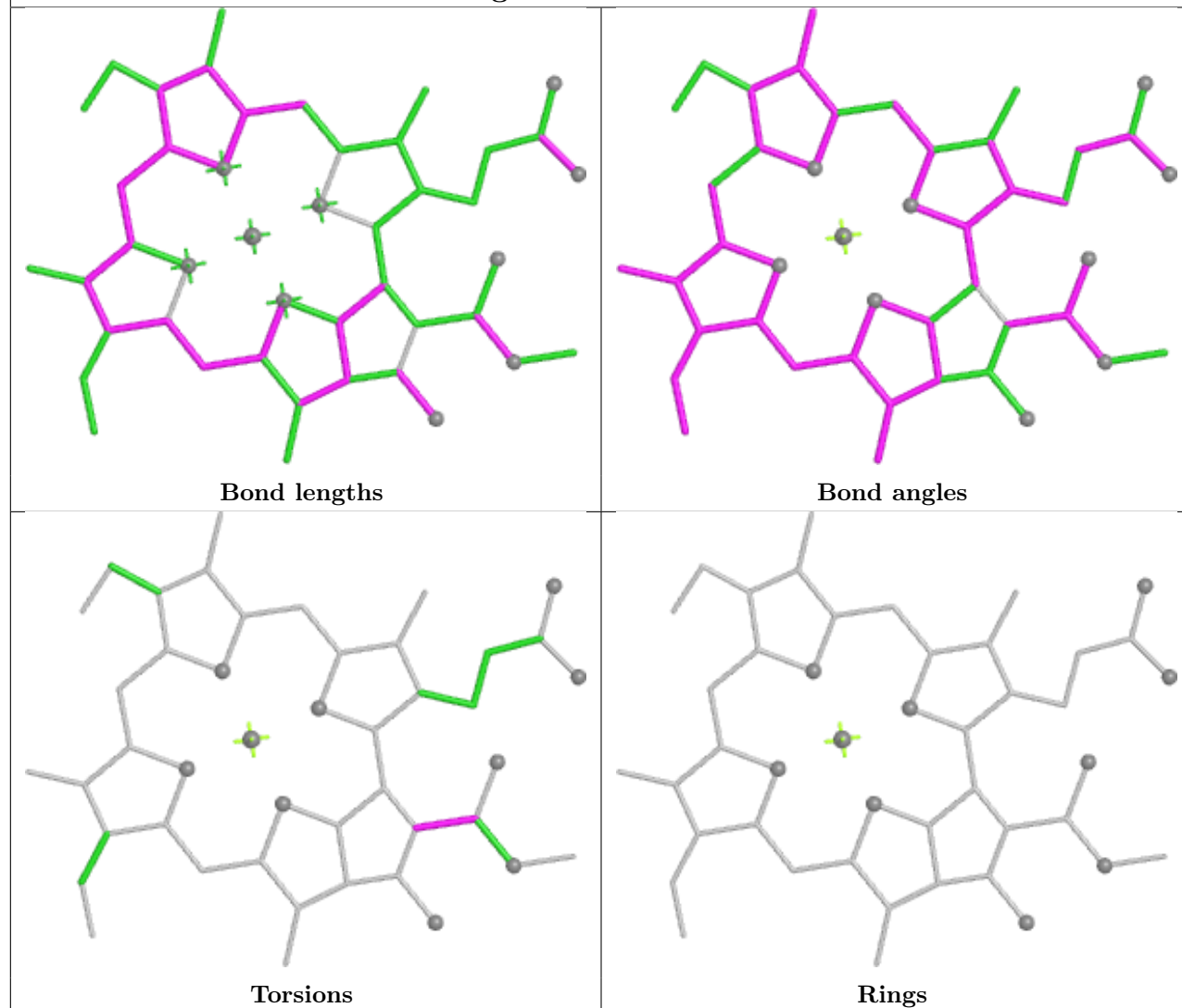


Rings

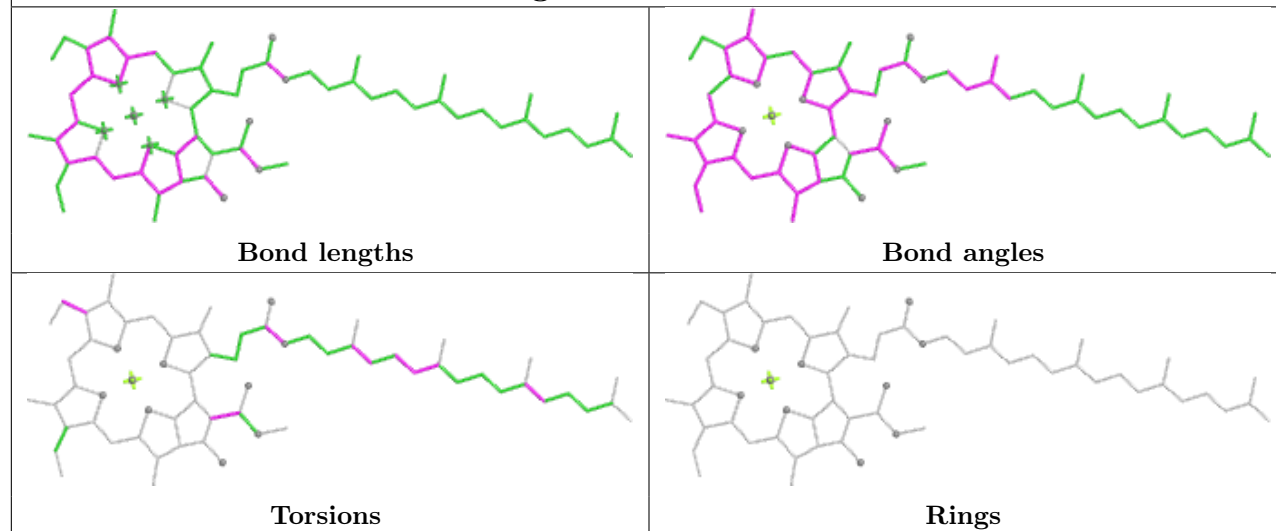




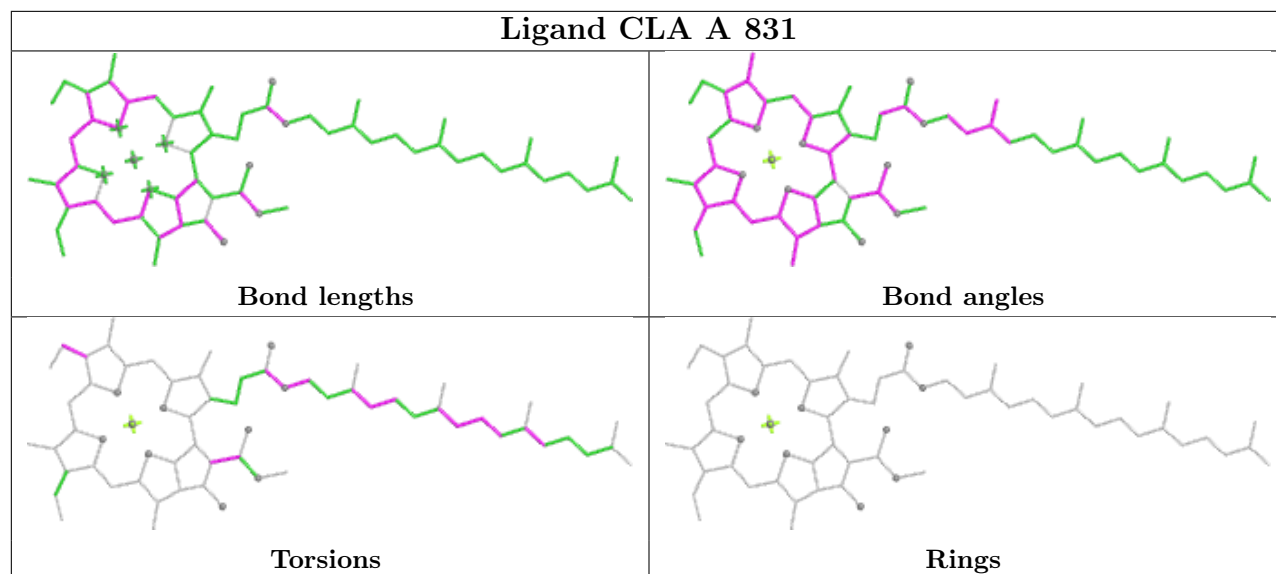
Ligand CLA f 7002



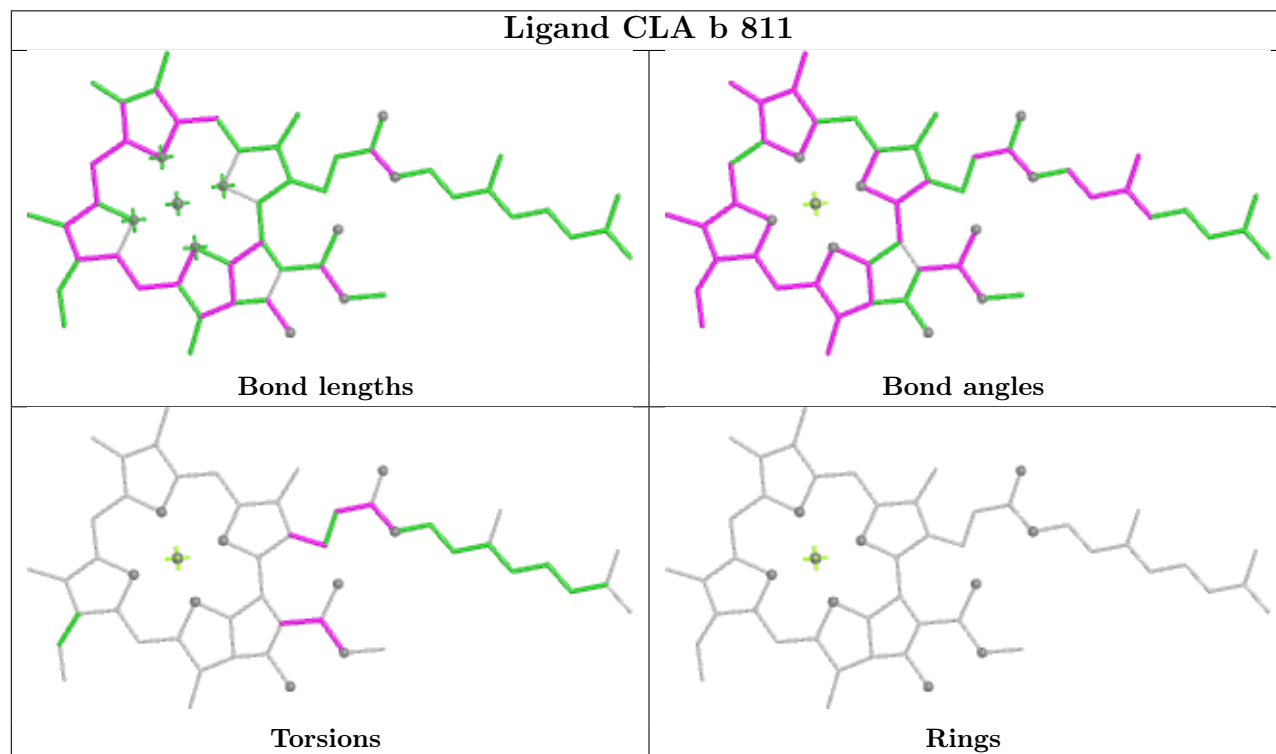
Ligand CLA A 835



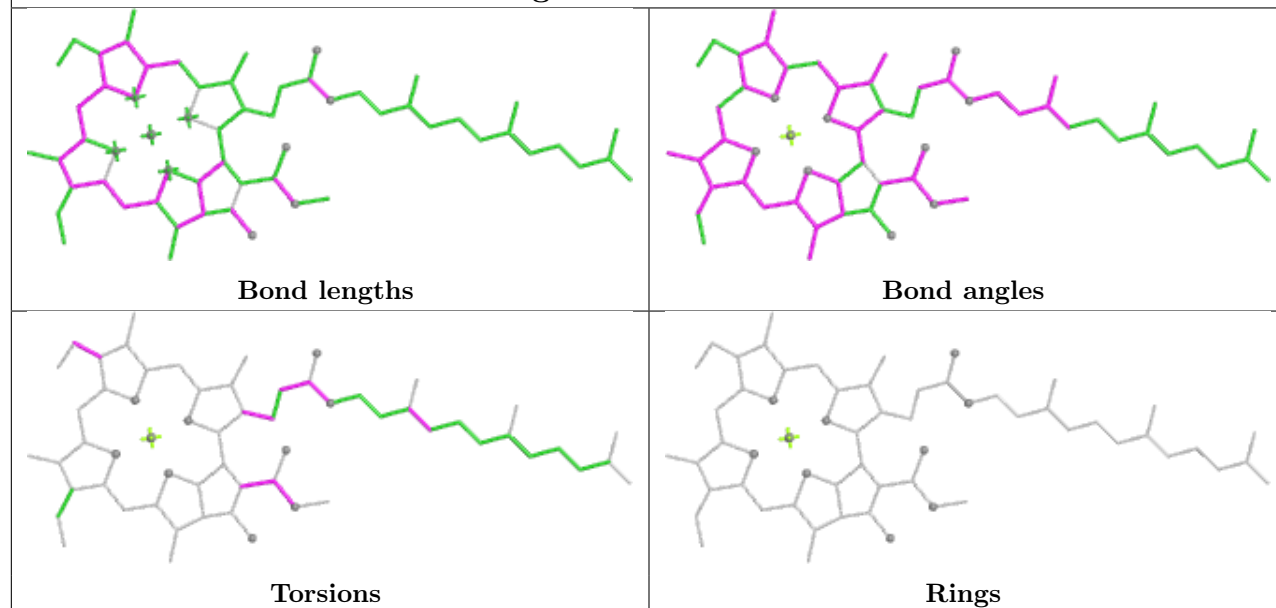
Ligand CLA A 831



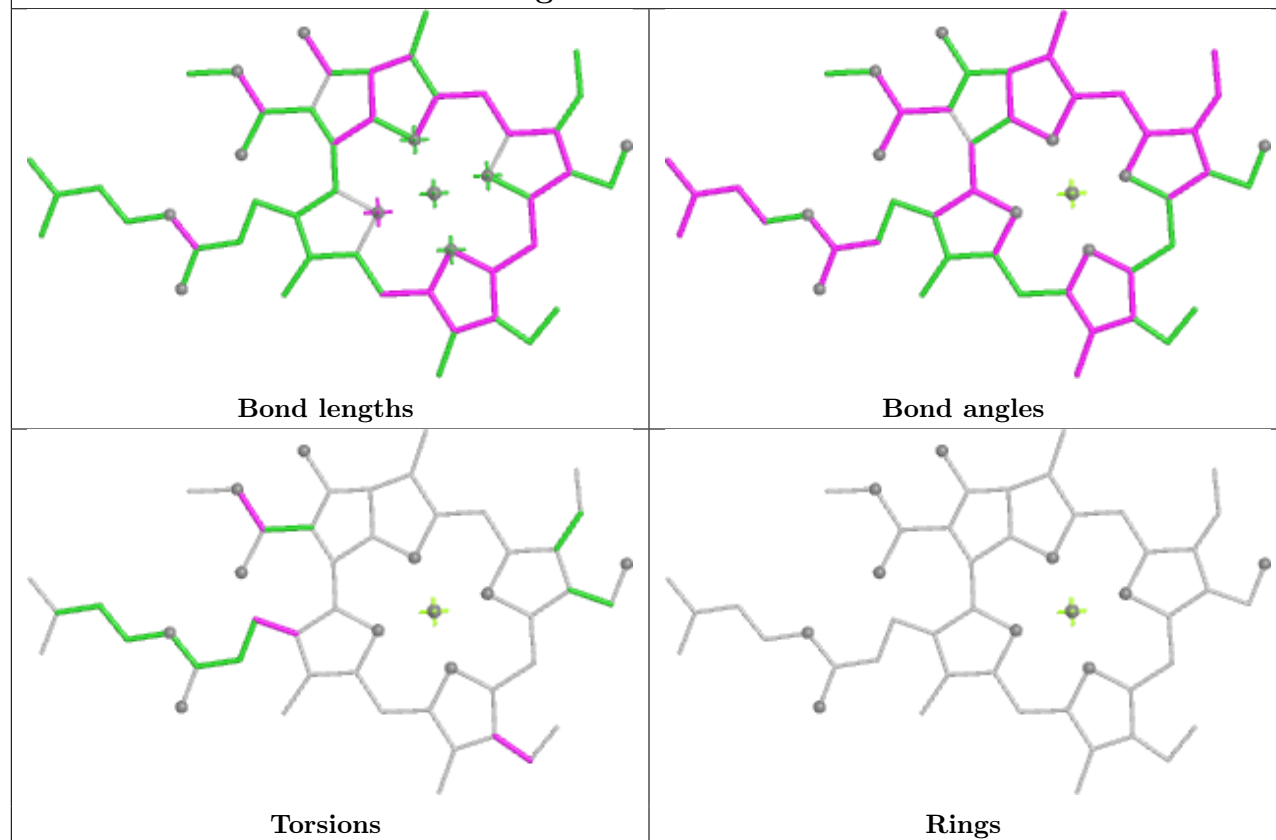
Ligand CLA b 811



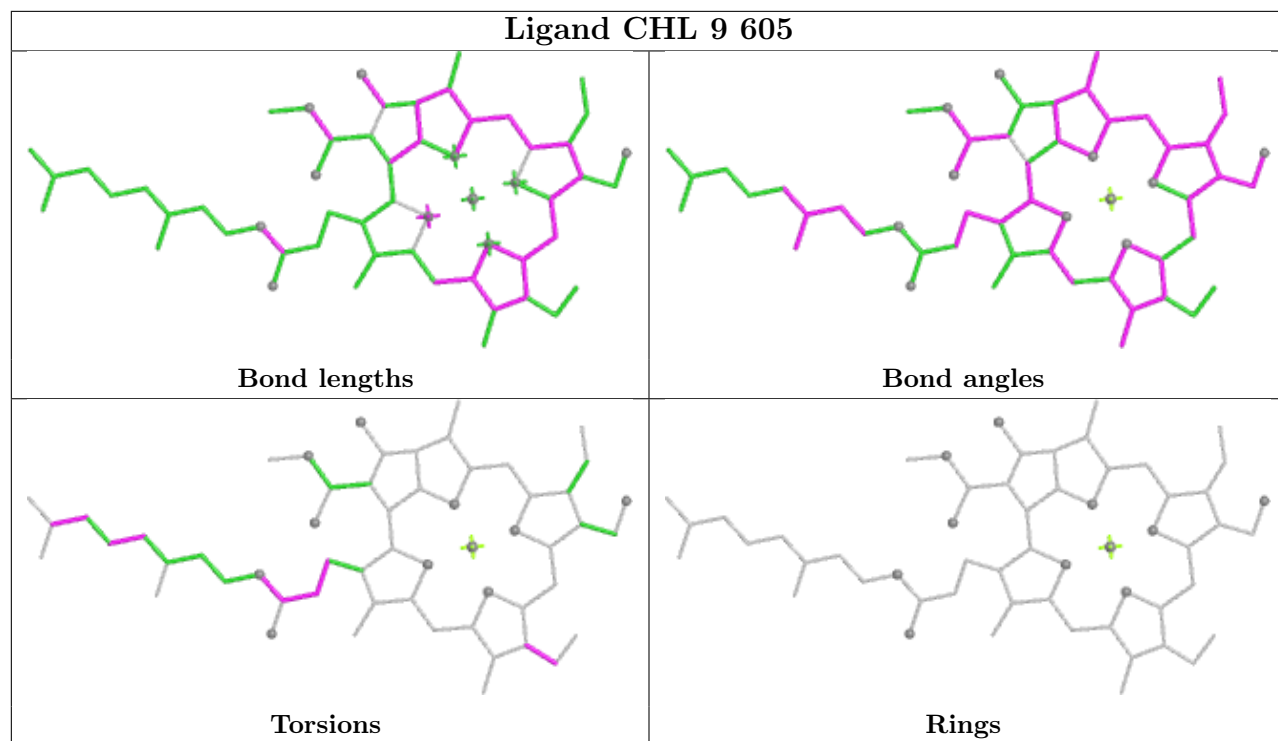
Ligand CLA B 823



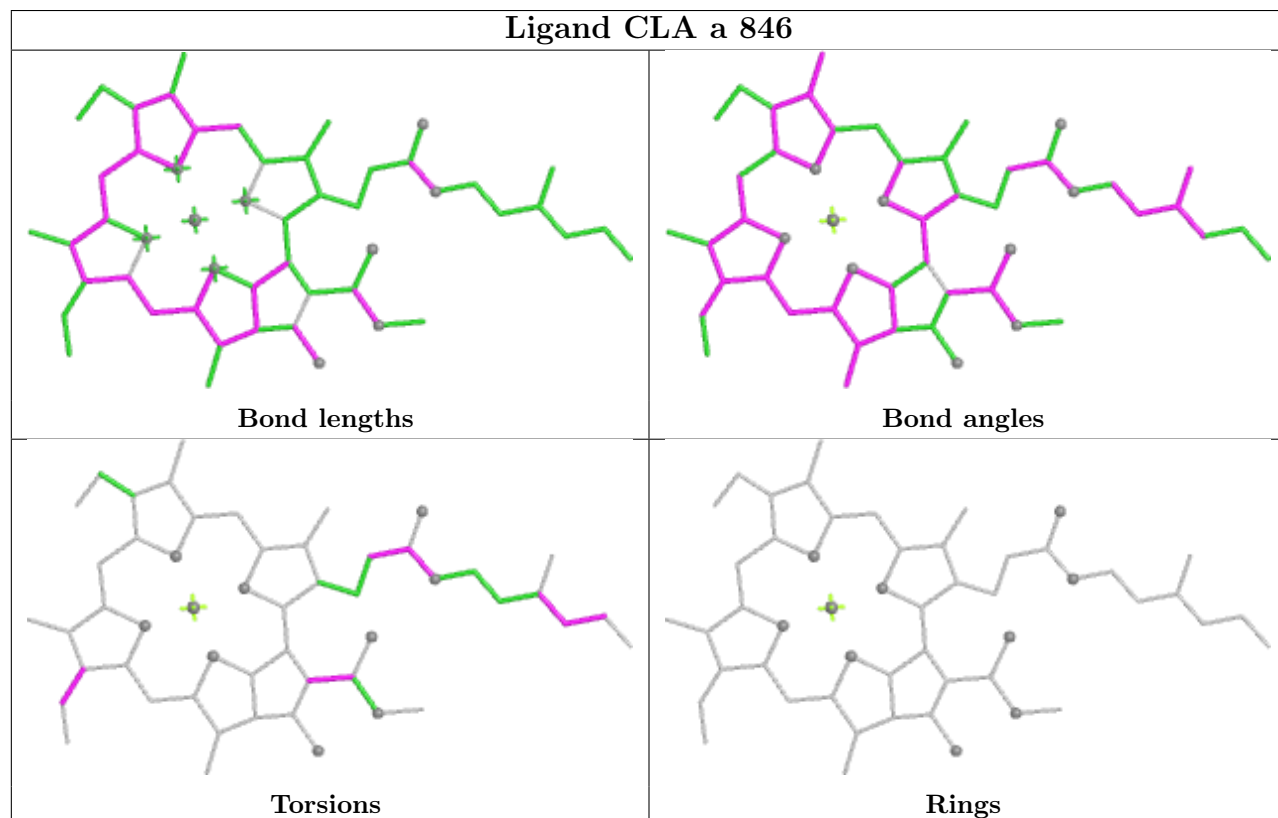
Ligand CHL 4 607

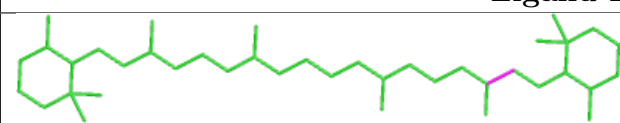
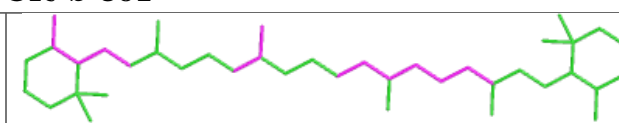
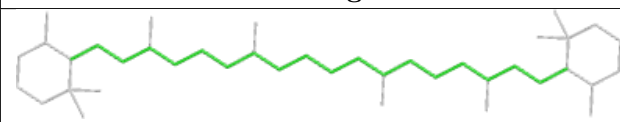
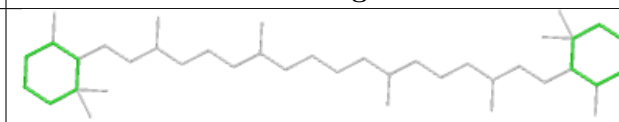


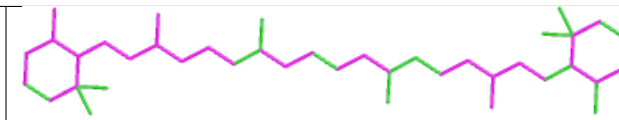
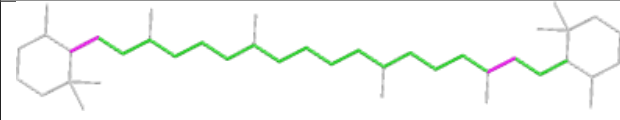
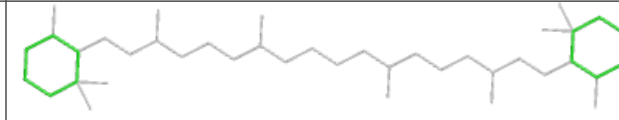
Ligand CHL 9 605

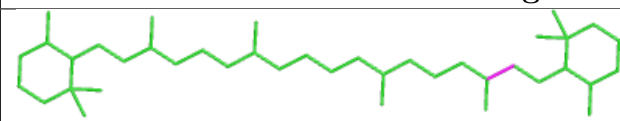
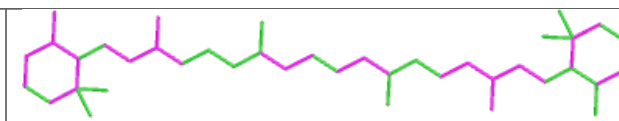
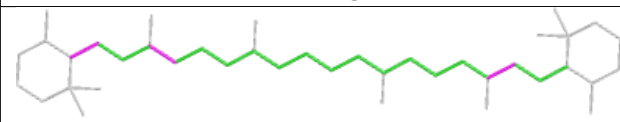
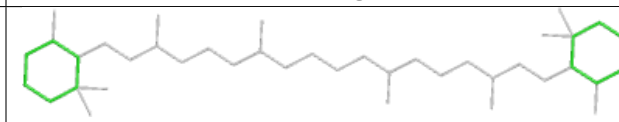


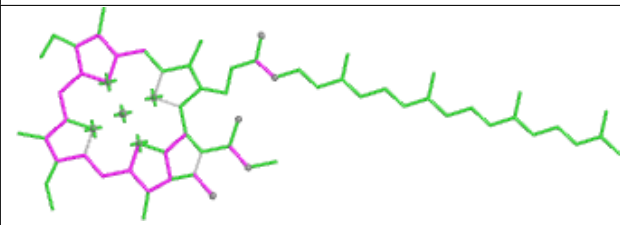
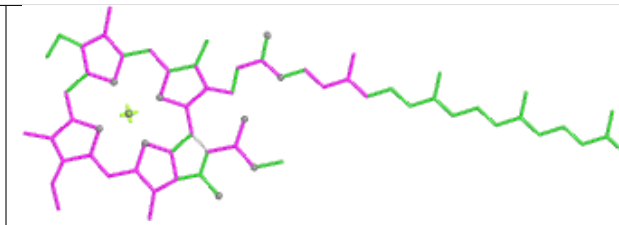
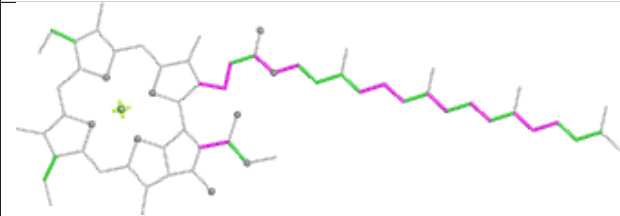
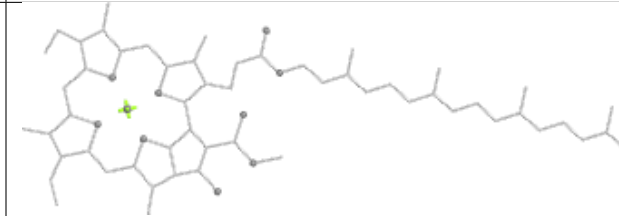
Ligand CLA a 846



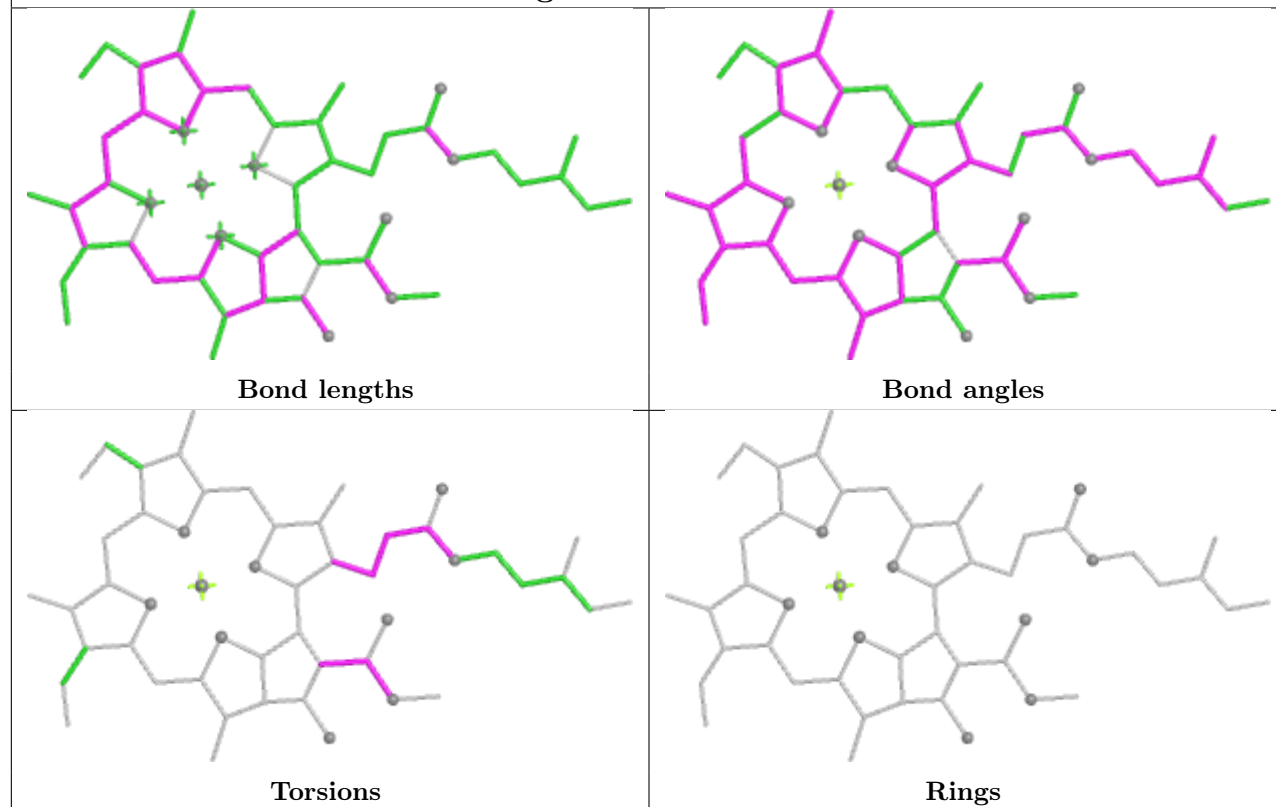
Ligand BCR b 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

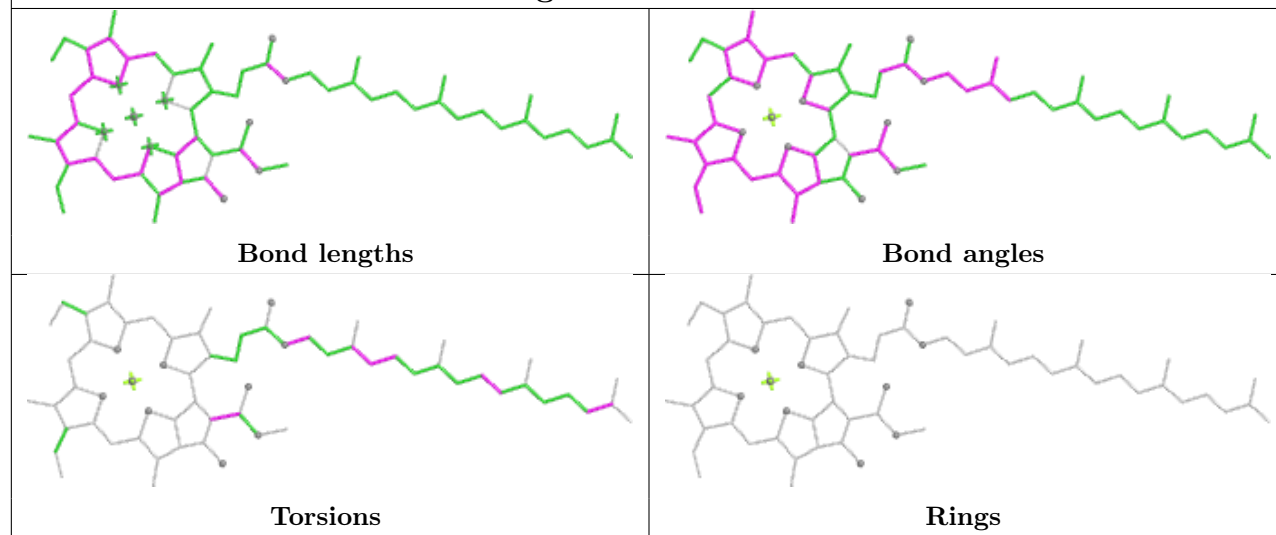
Ligand BCR b 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

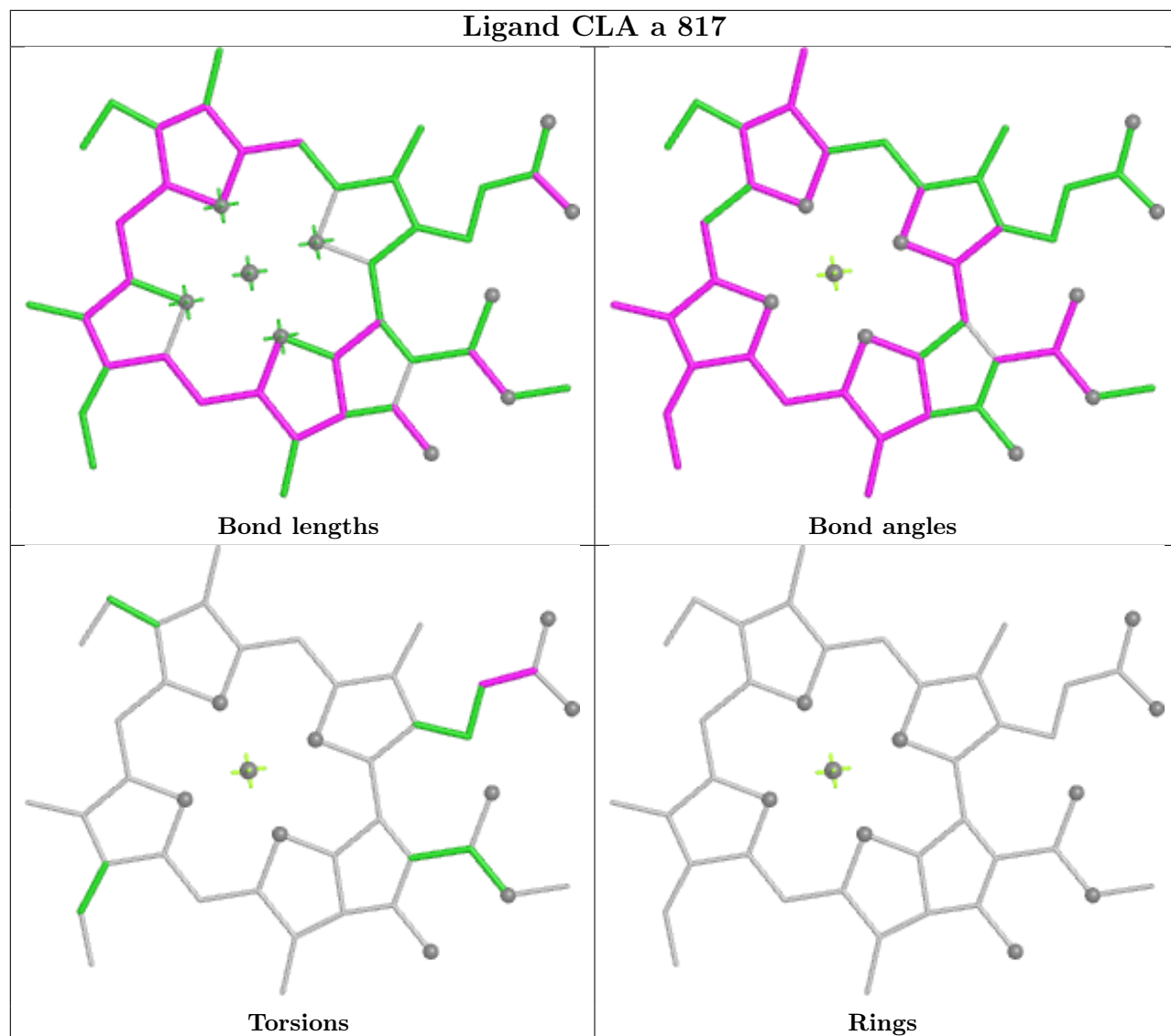
Ligand CLA a 838



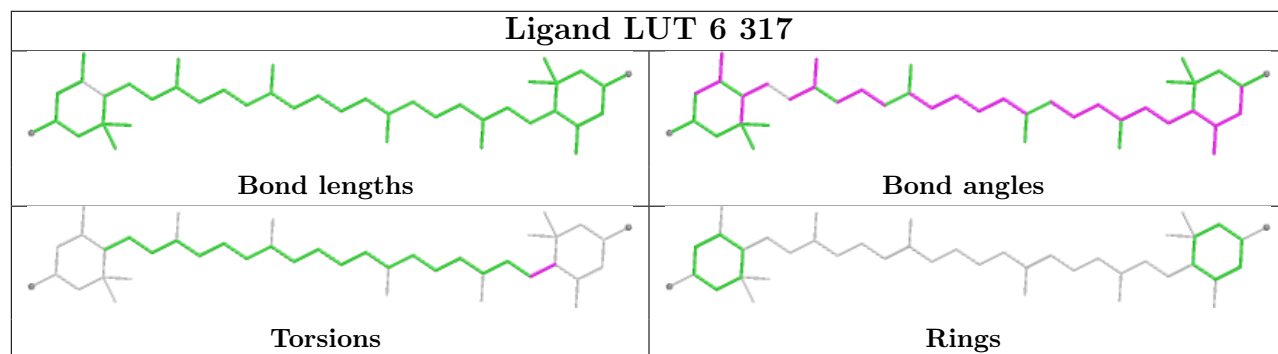
Ligand CLA a 840

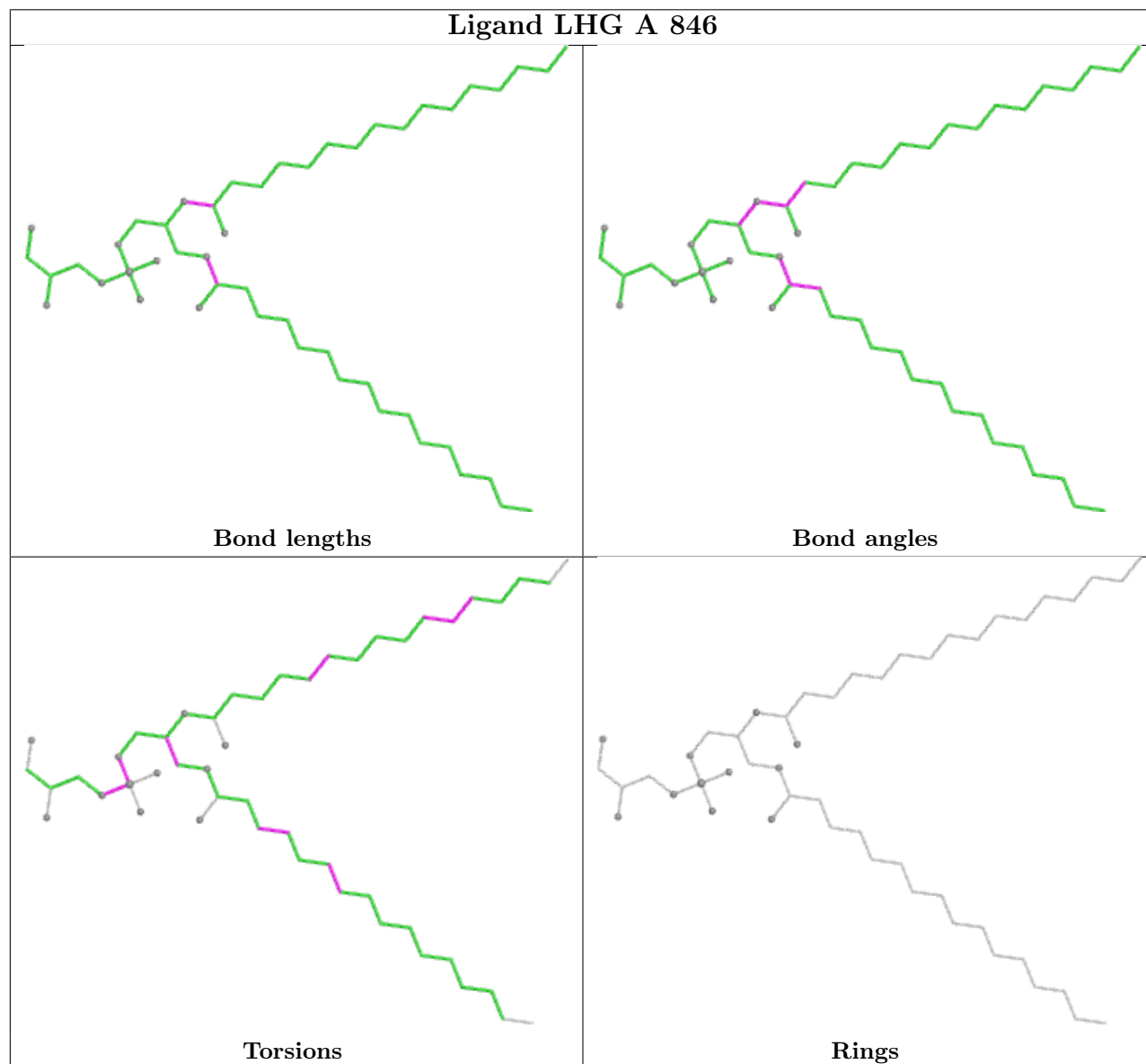
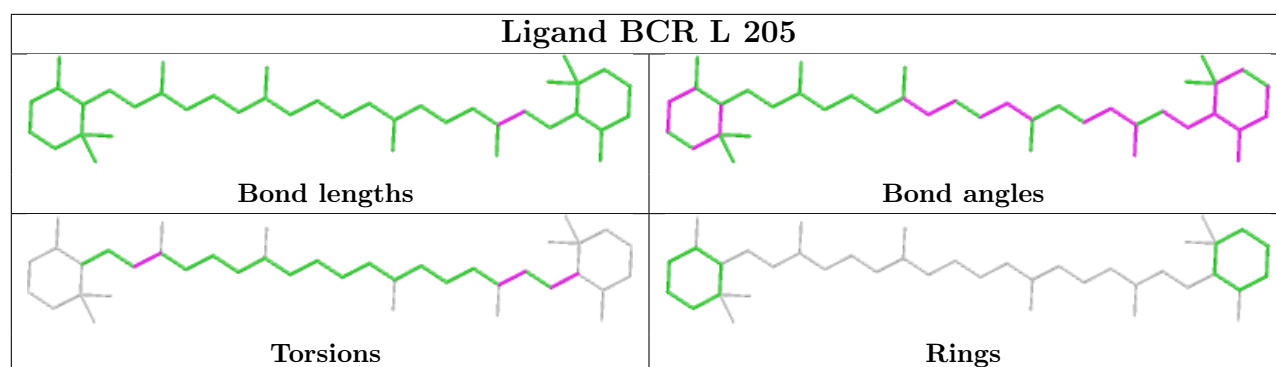


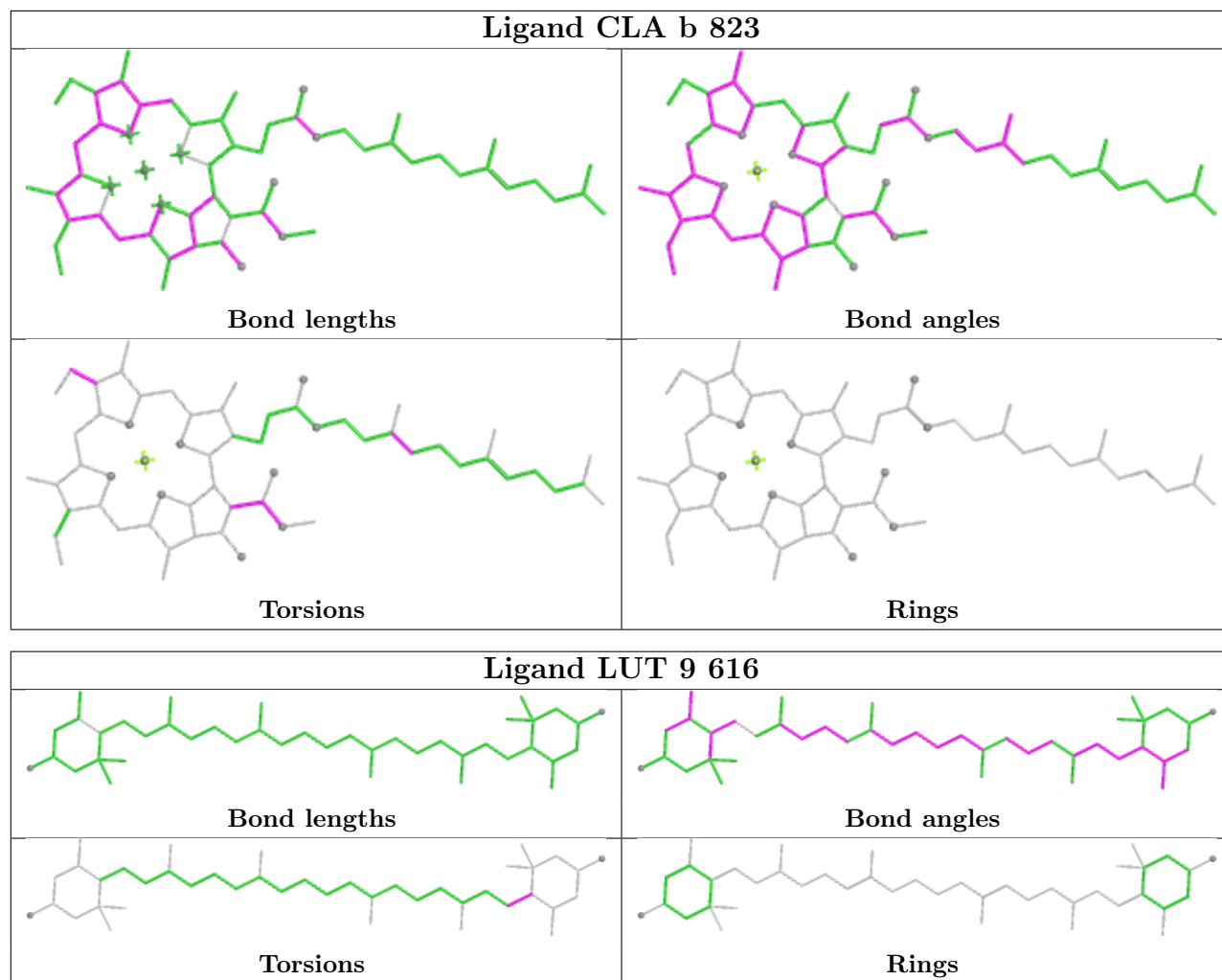
Ligand CLA a 817



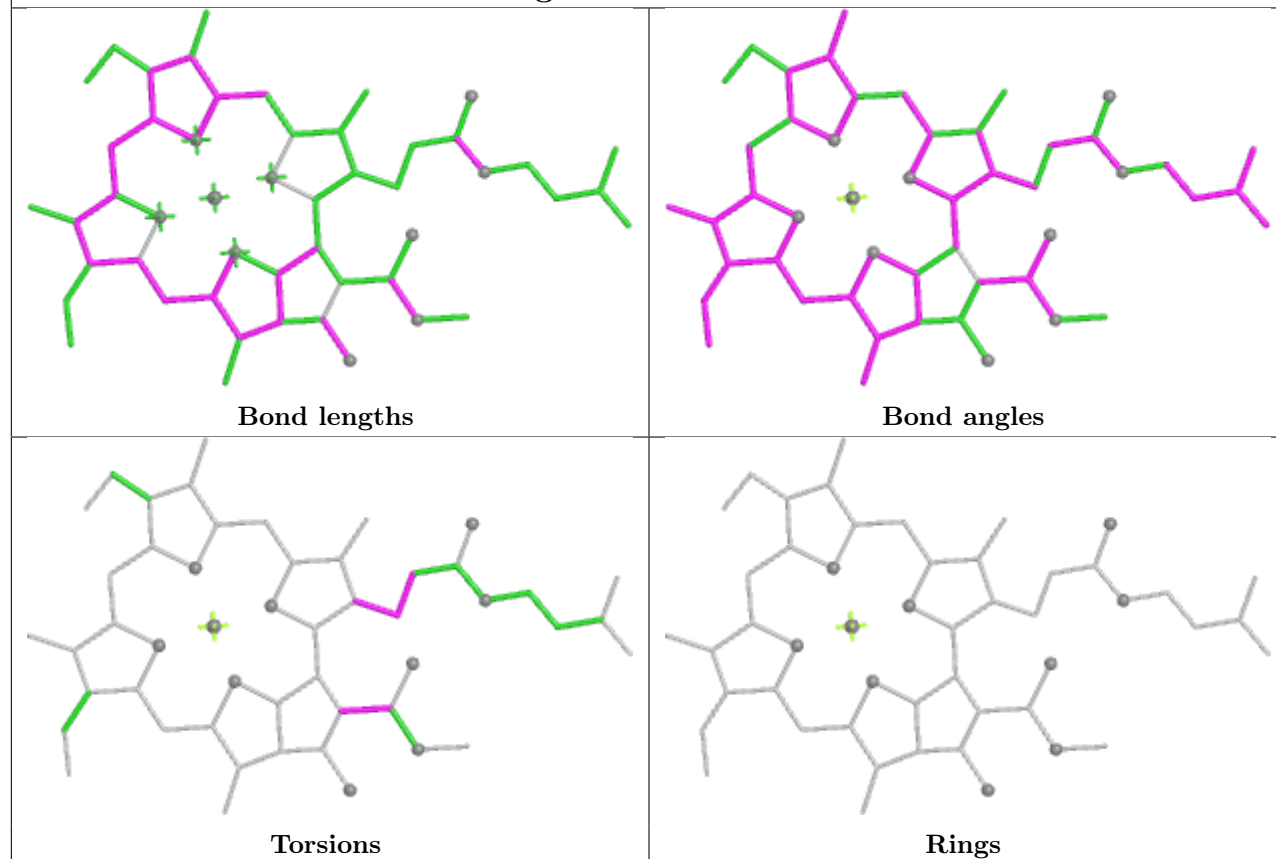
Ligand LUT 6 317



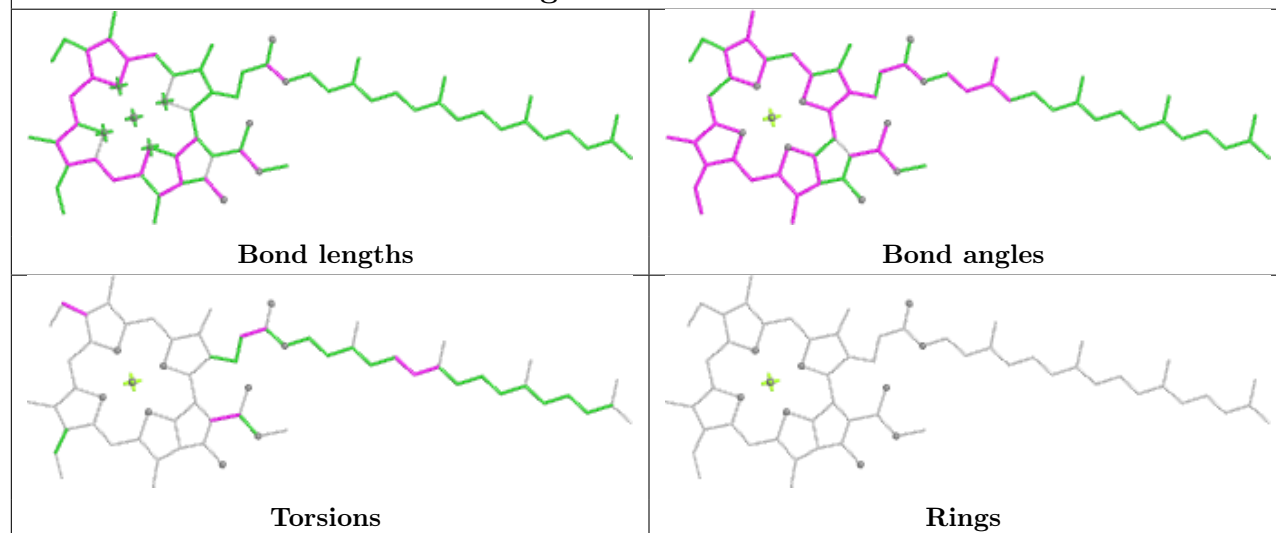




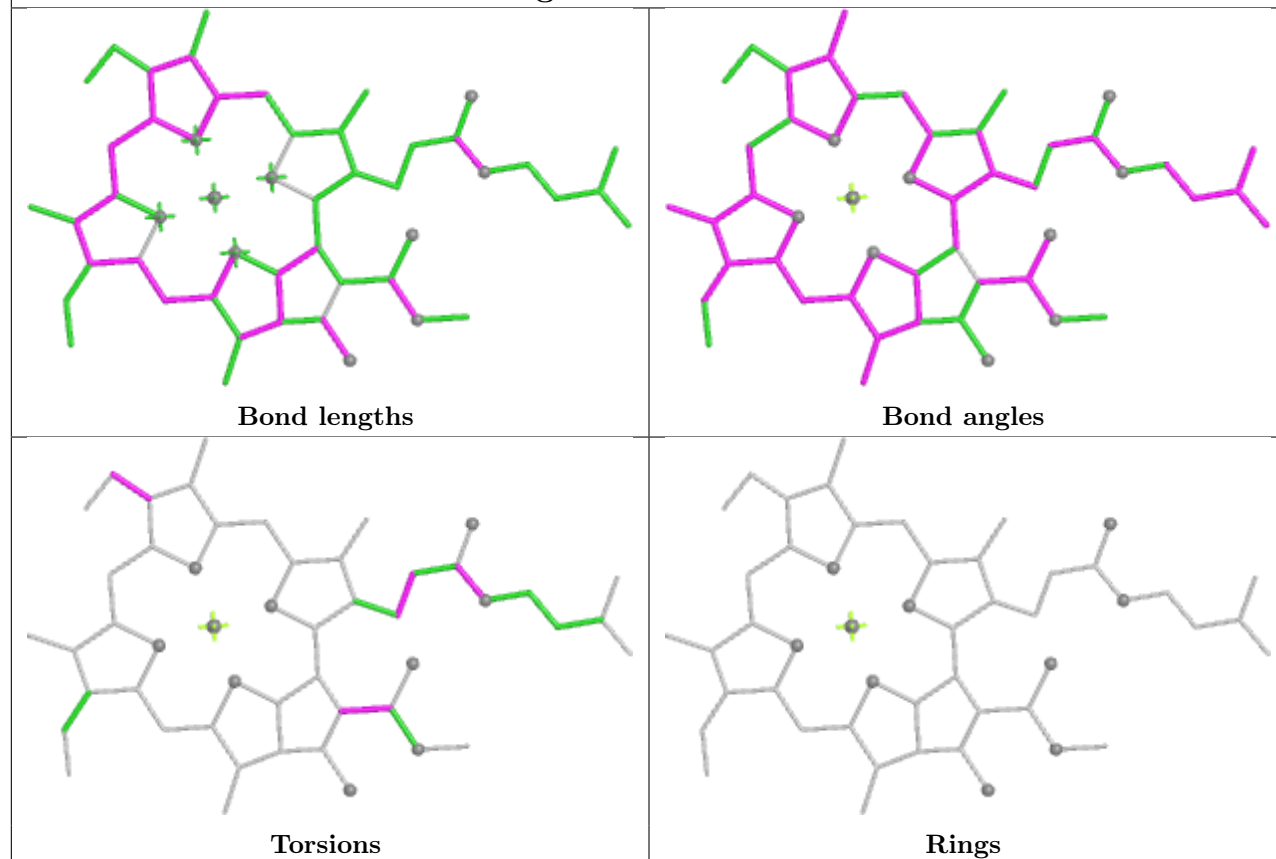
Ligand CLA b 830



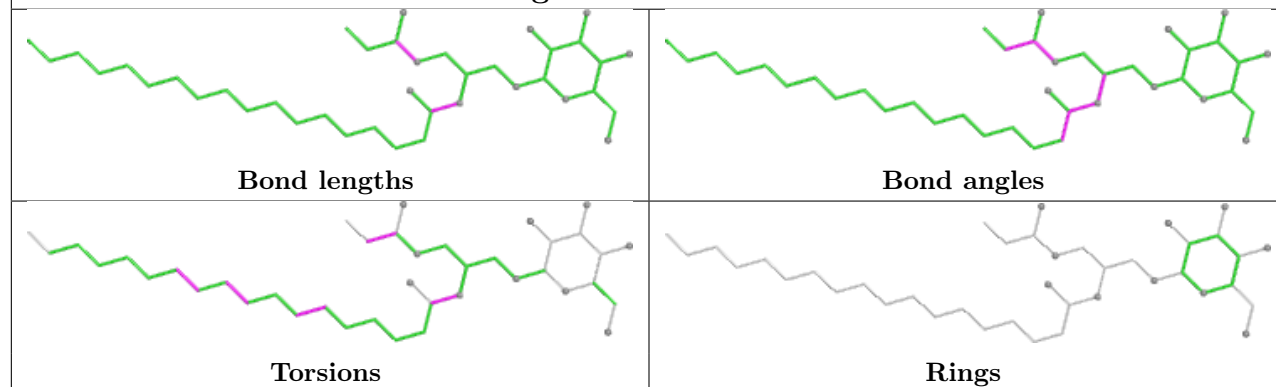
Ligand CLA l 203



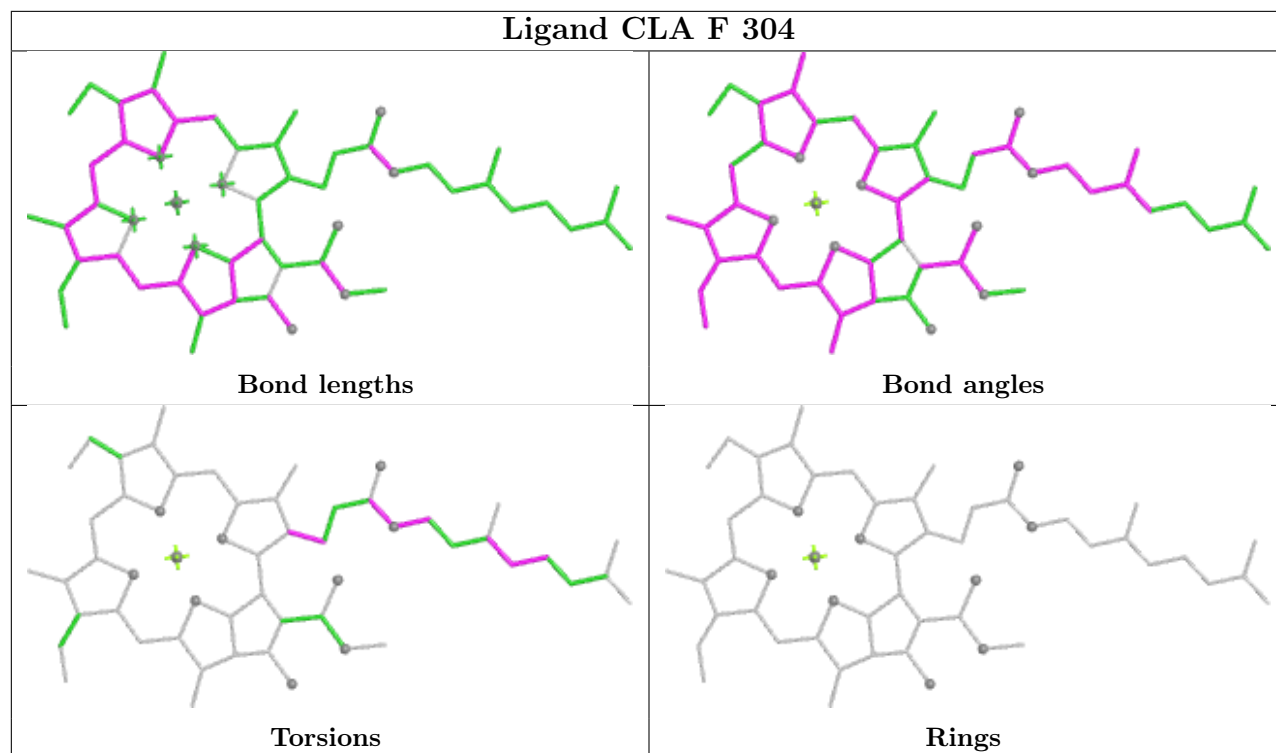
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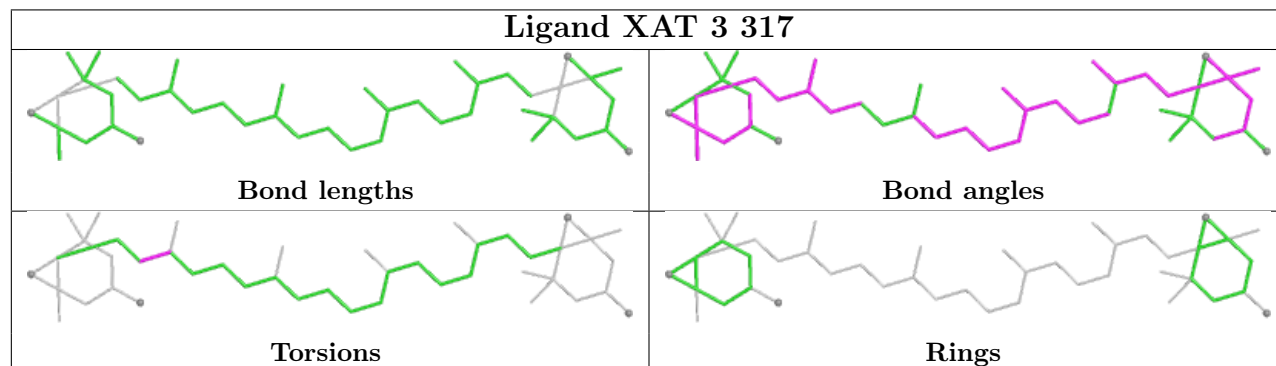
Ligand LMG 6 302



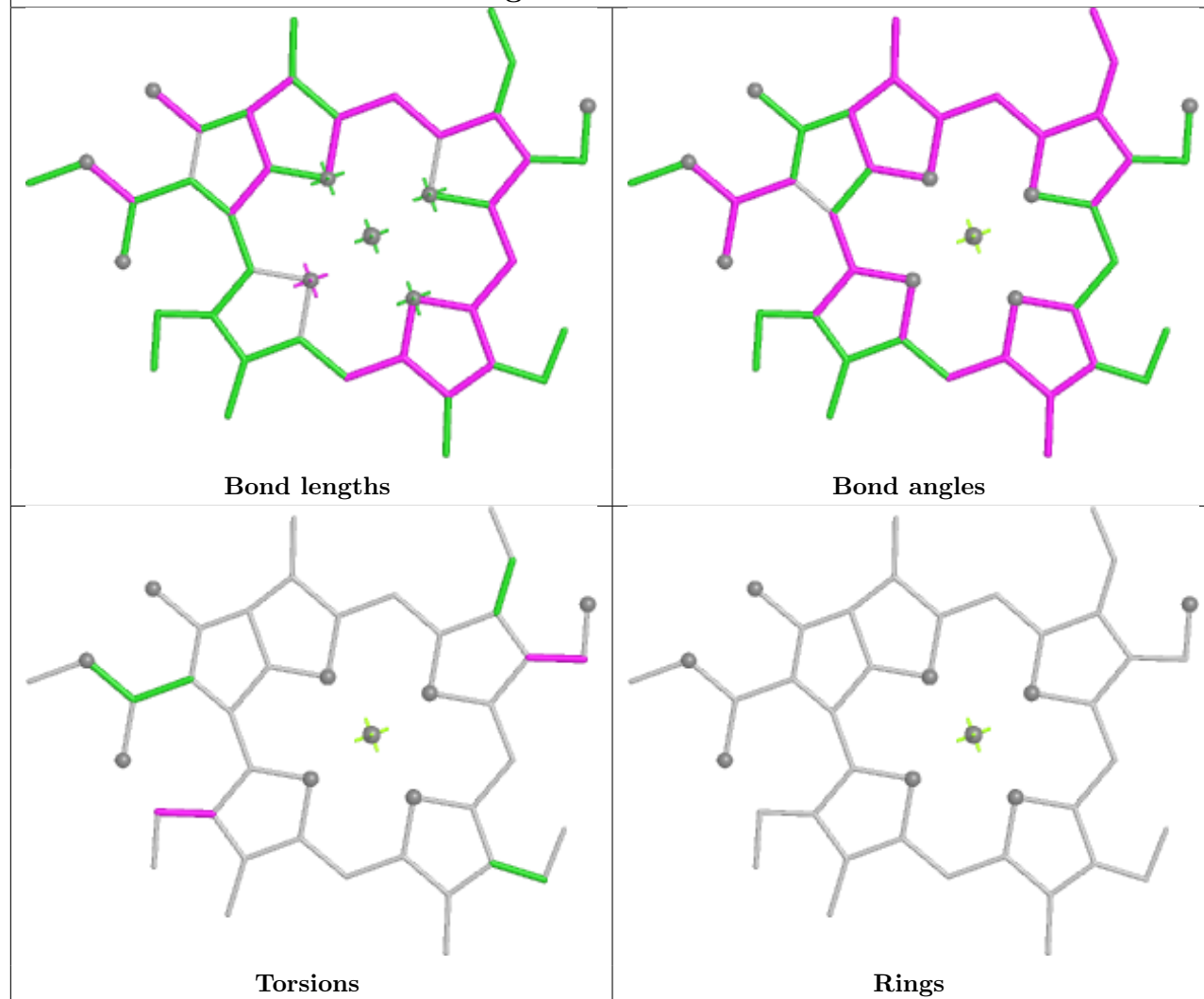
Ligand CLA F 304



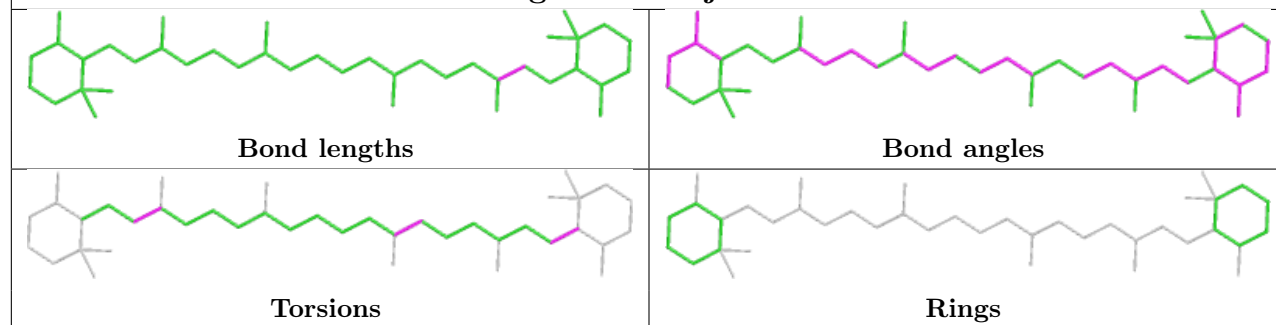
Ligand XAT 3 317



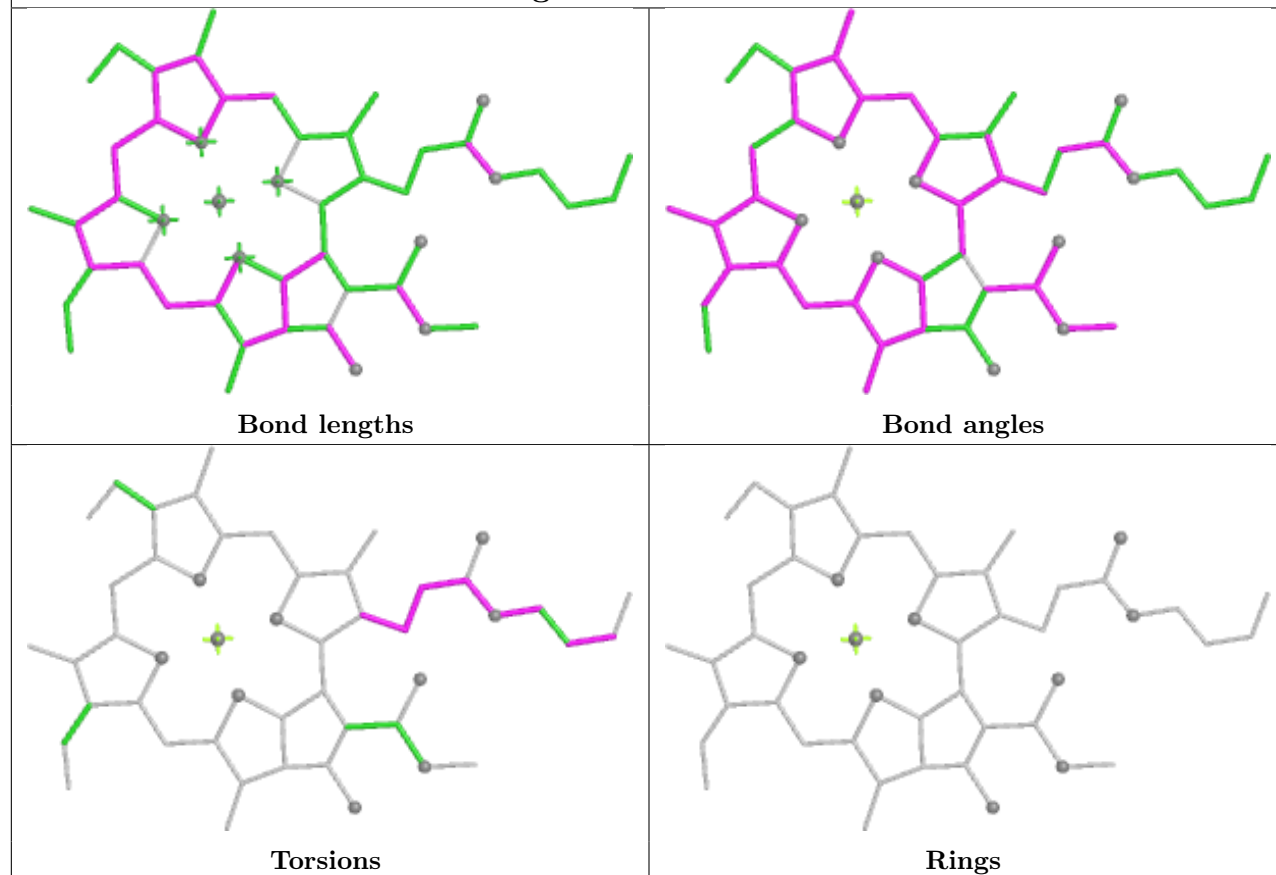
Ligand CHL 7 614



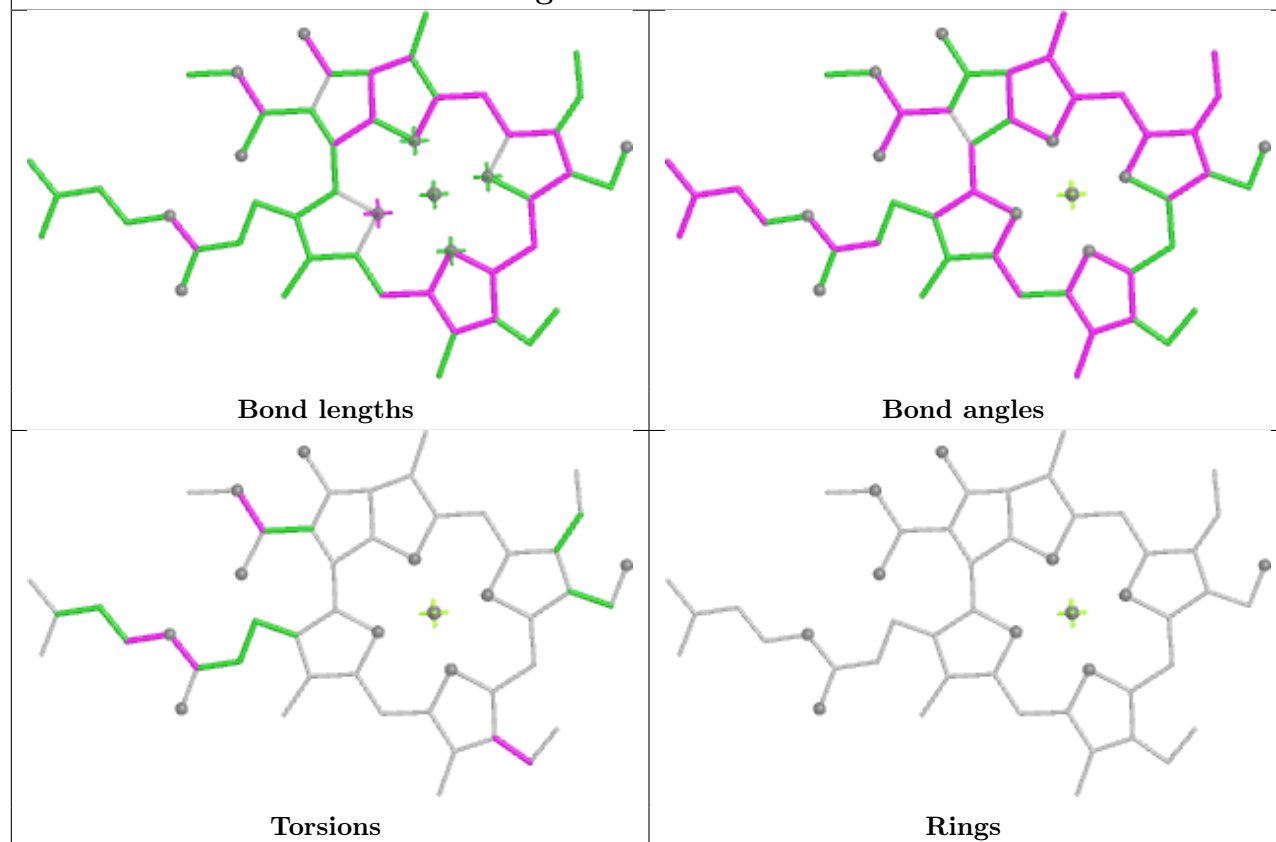
Ligand BCR j 3003

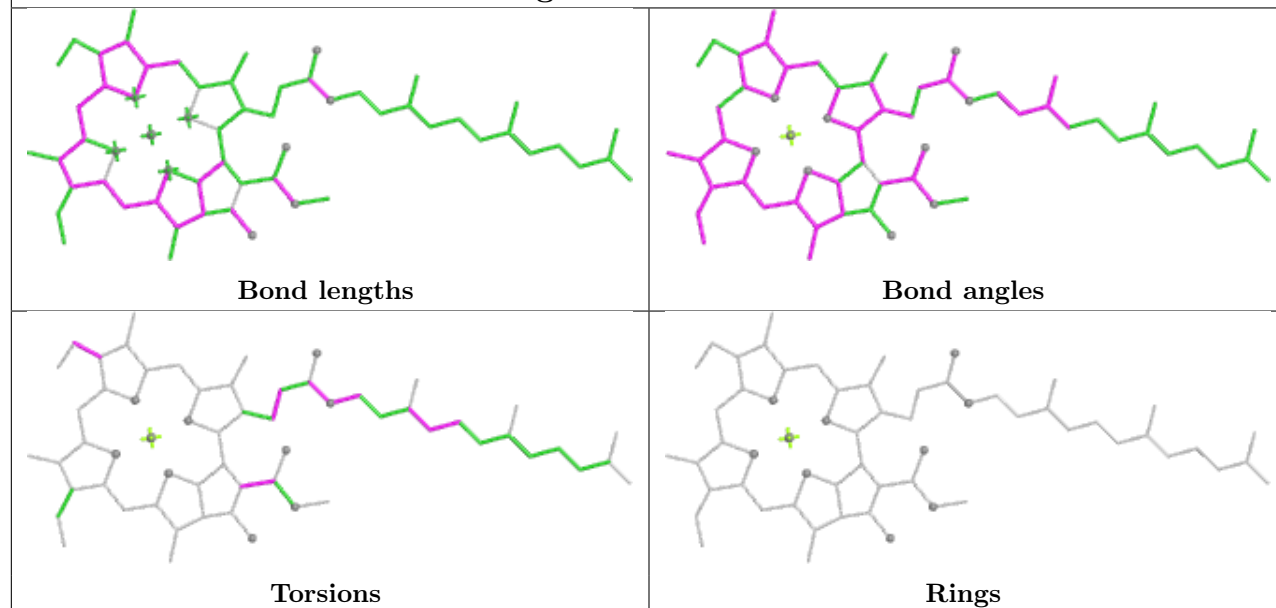
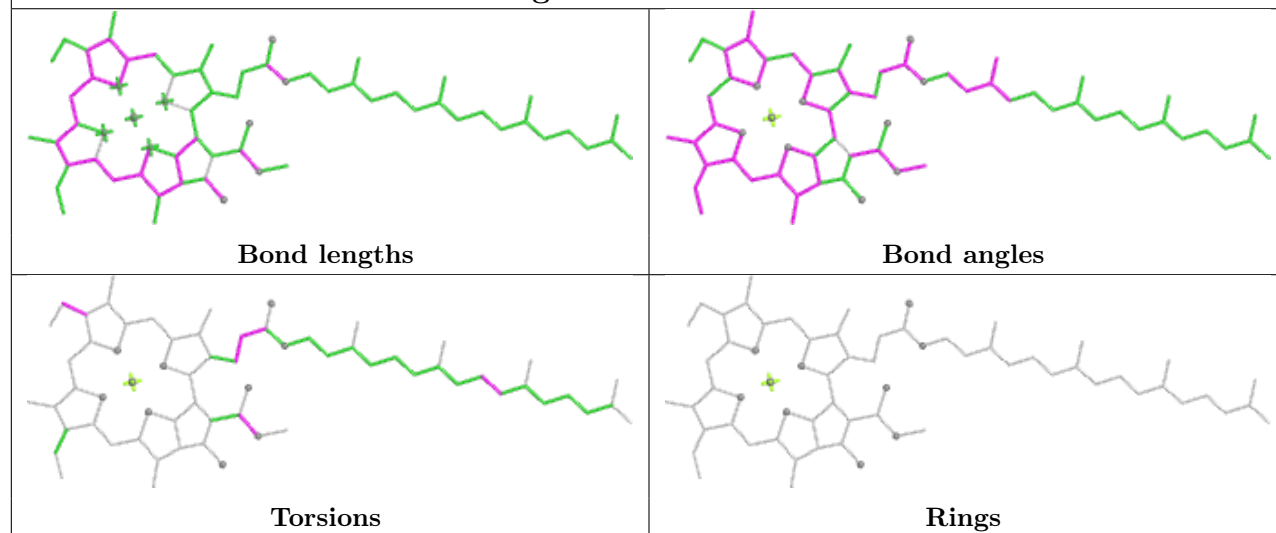


Ligand CLA B 831

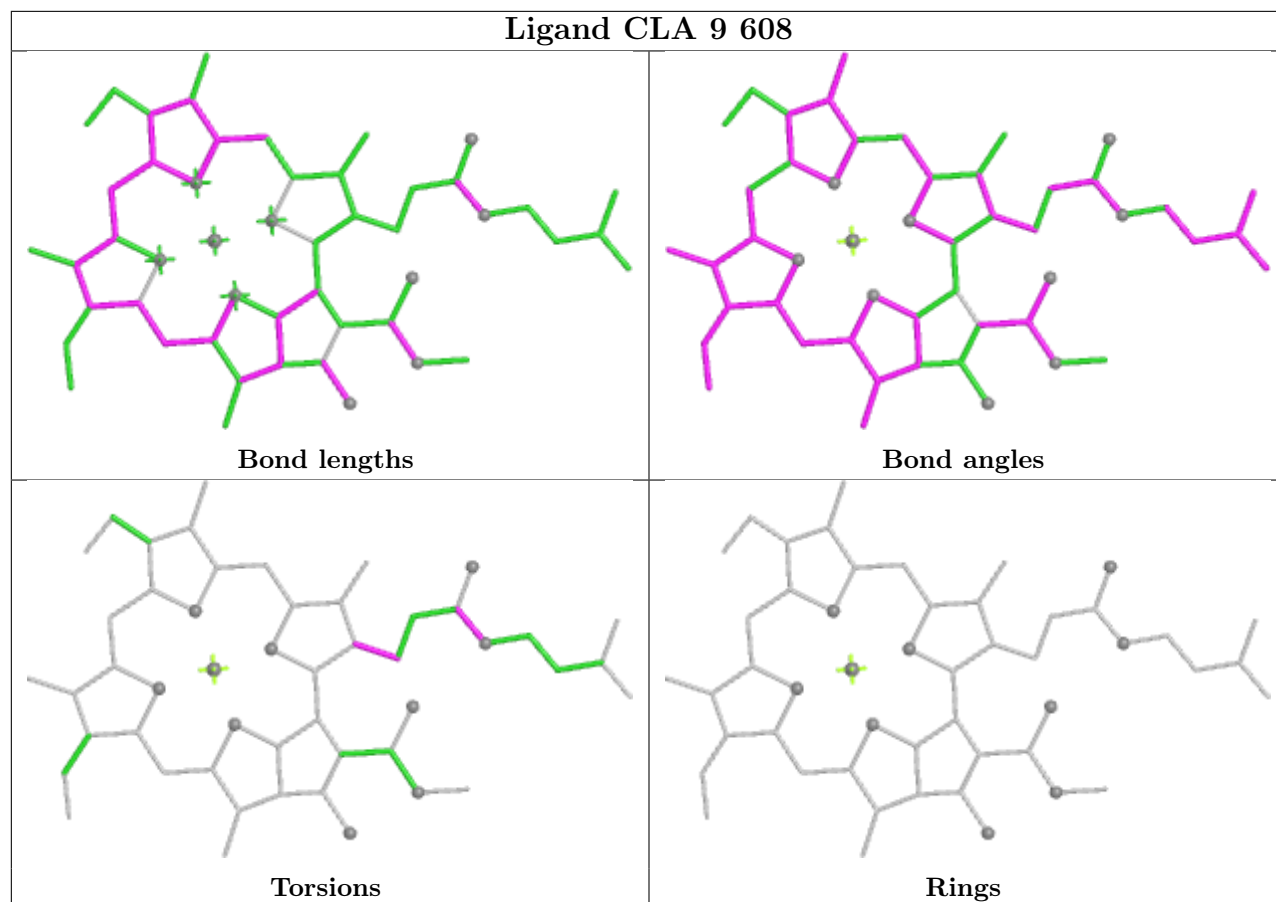


Ligand CHL 2 607

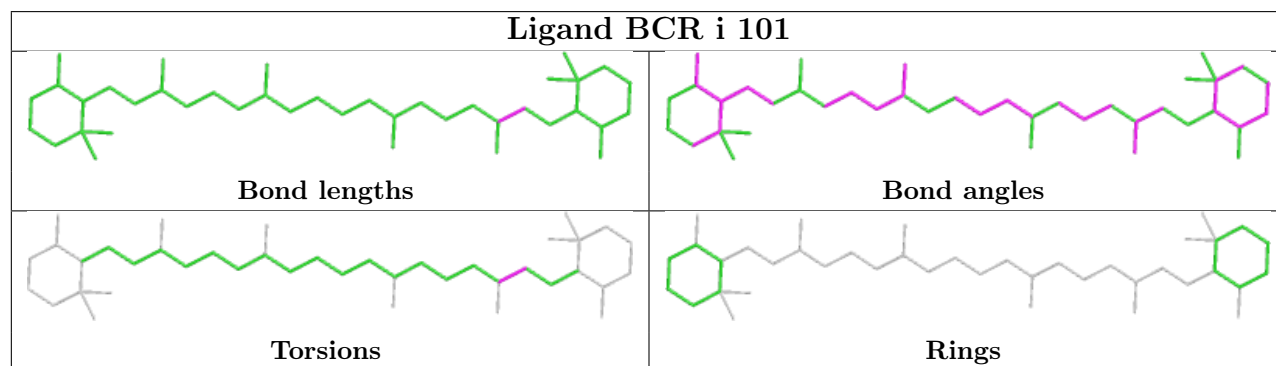


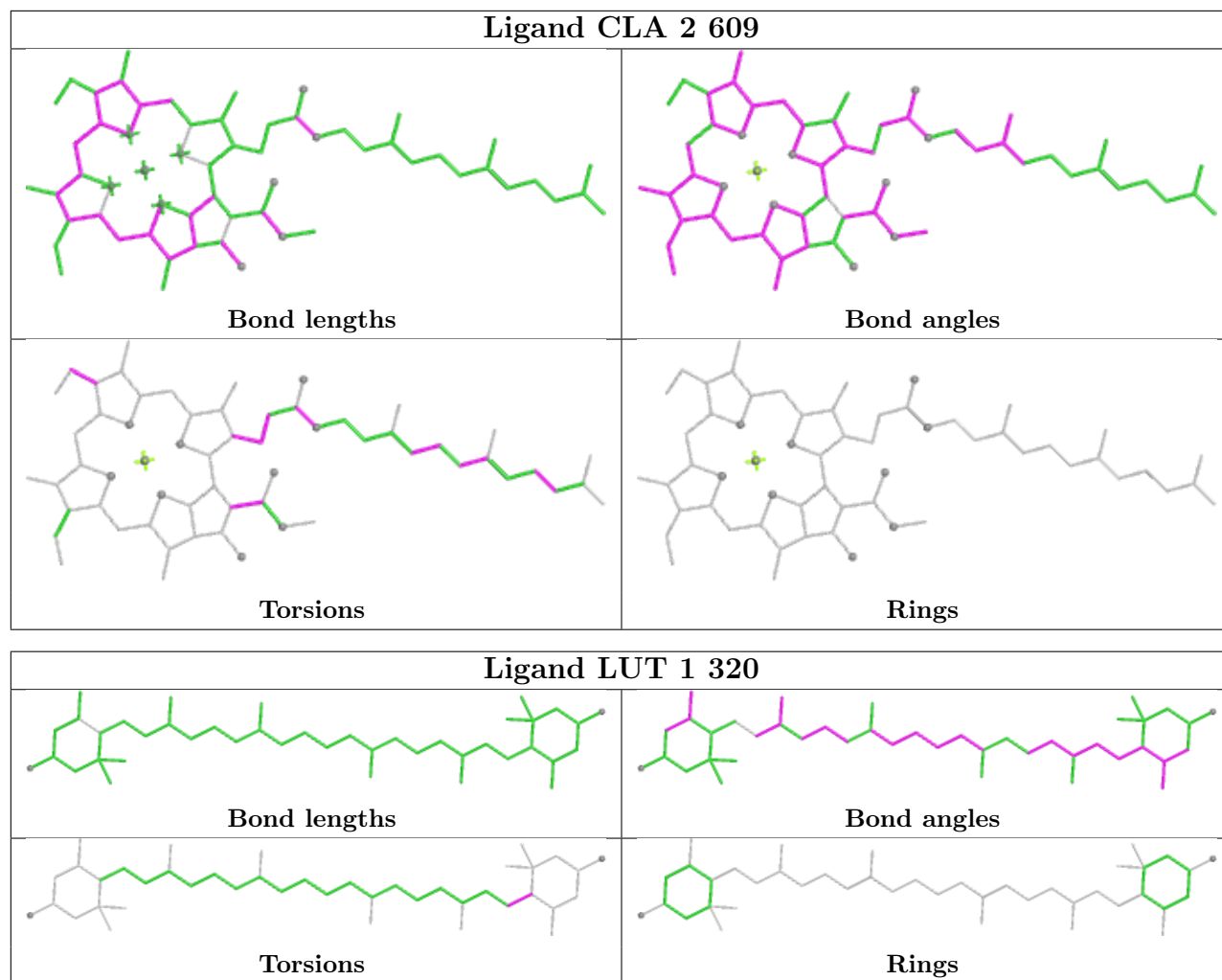
Ligand CLA 3 302**Ligand CLA B 803**

Ligand CLA 9 608

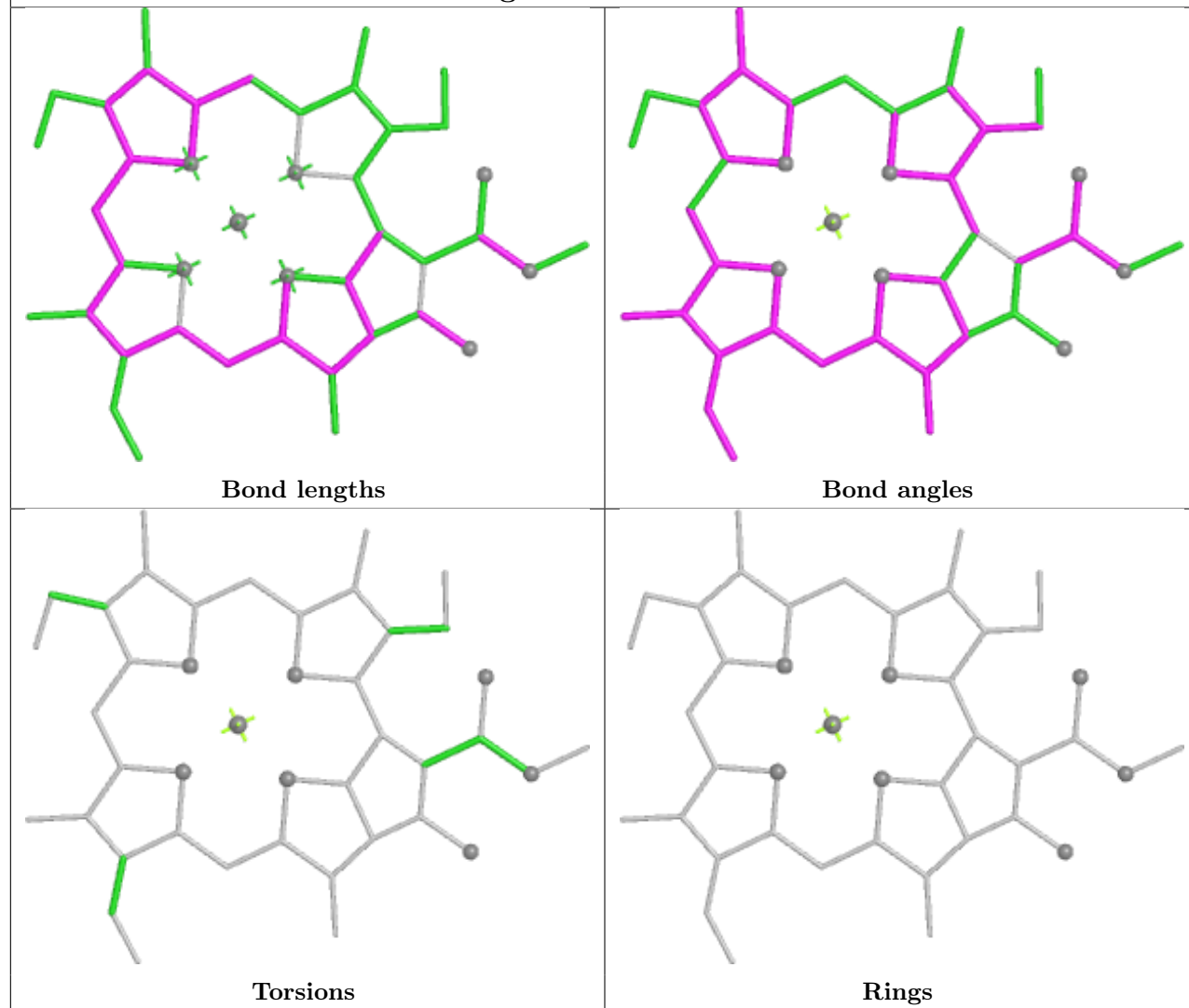


Ligand BCR i 101

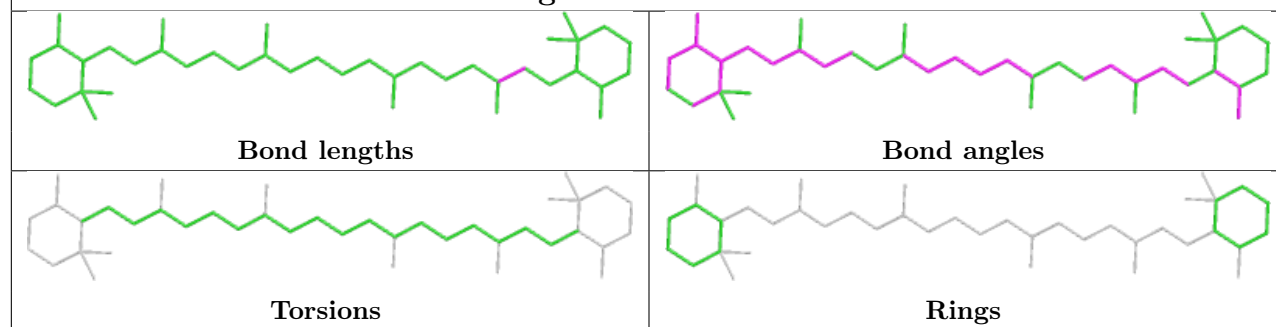


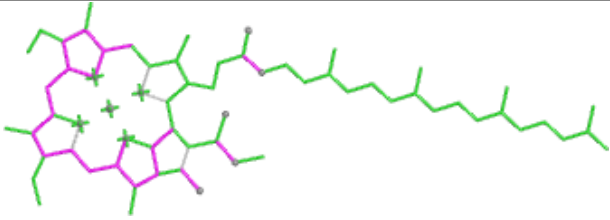
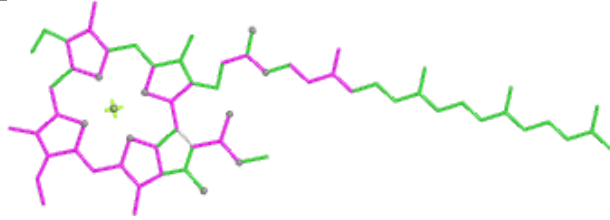
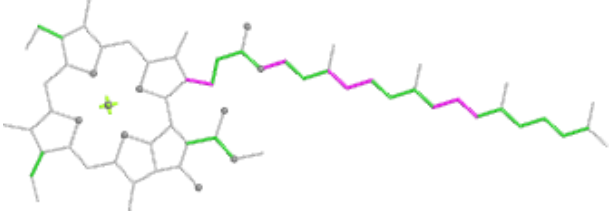
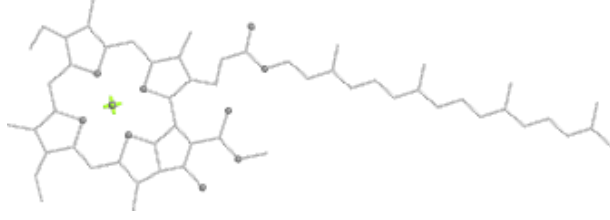
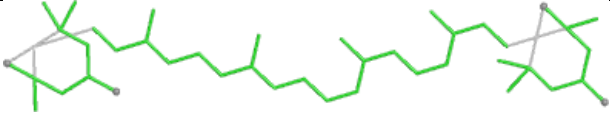
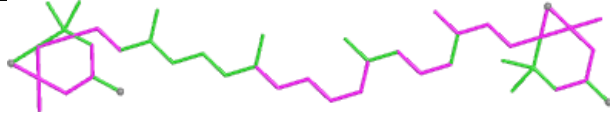
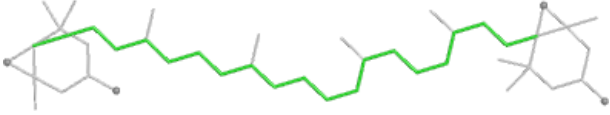
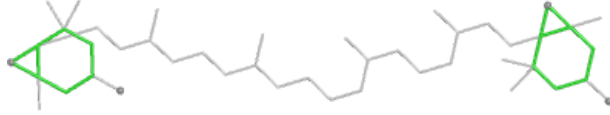
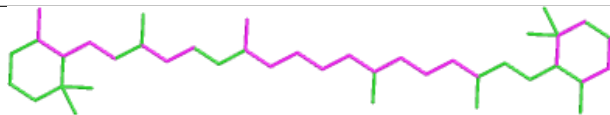
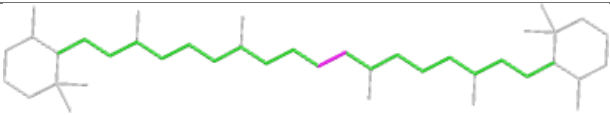
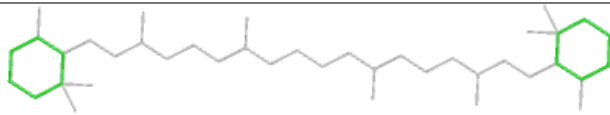


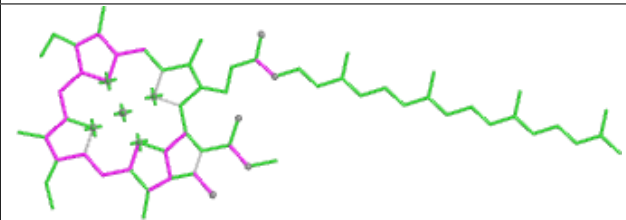
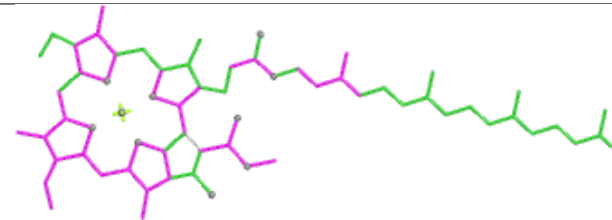
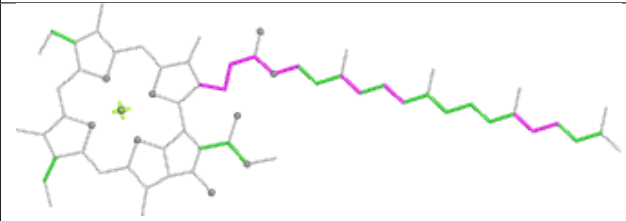
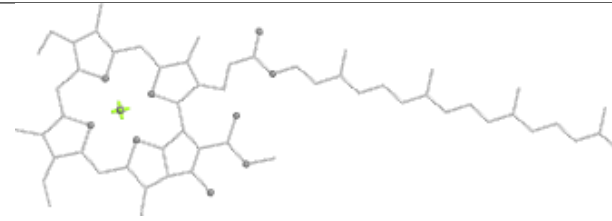
Ligand CLA 8 304

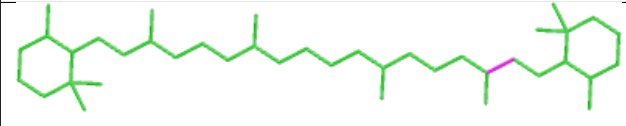
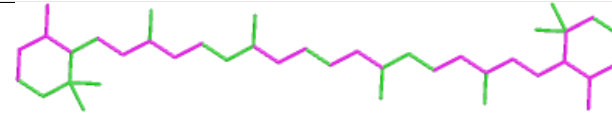
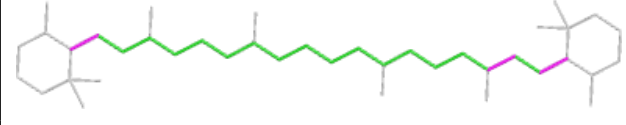
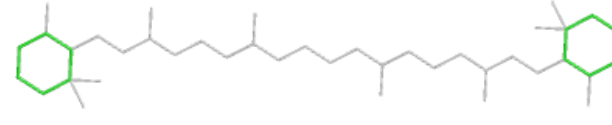


Ligand BCR 1 206

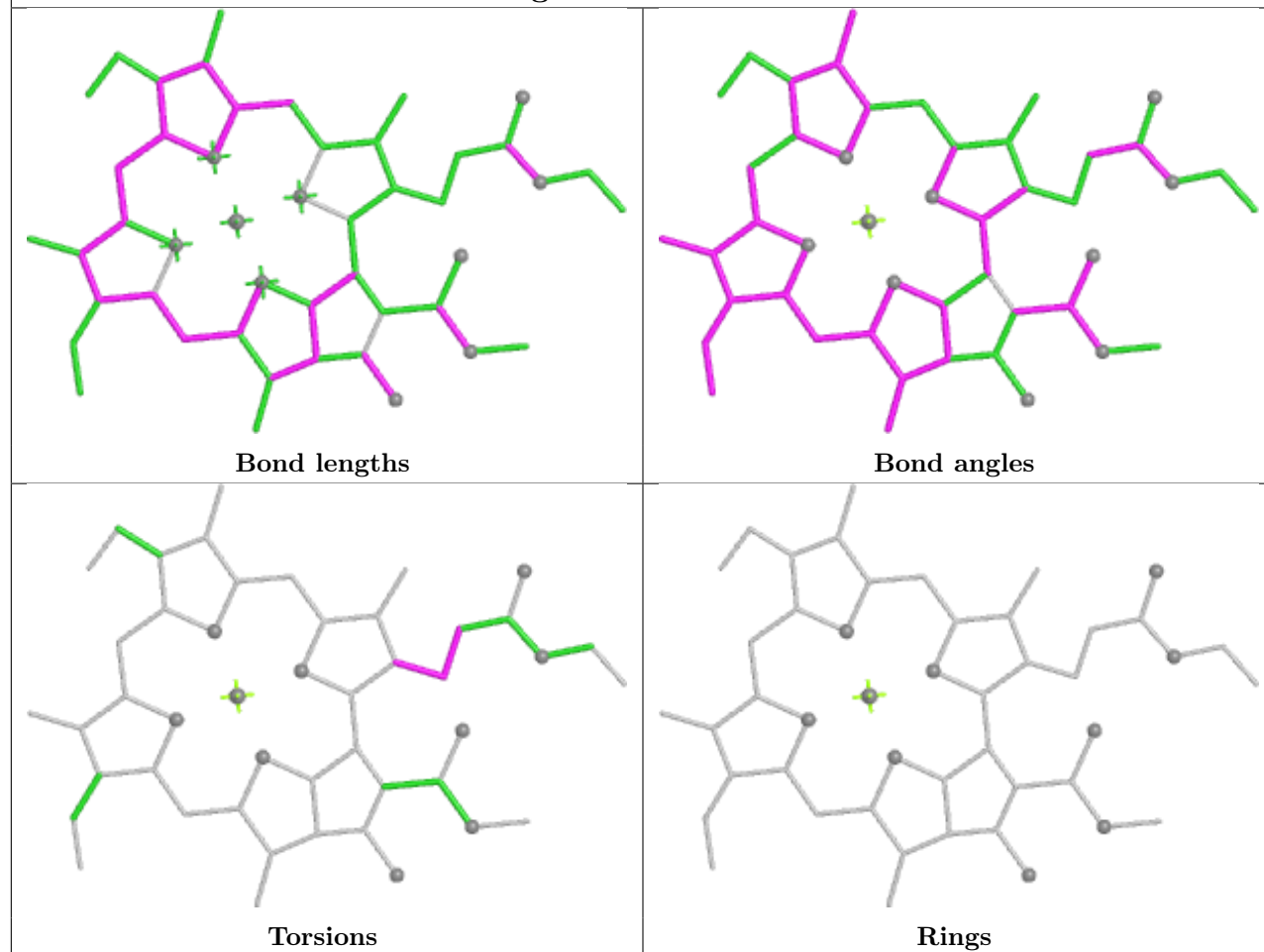


Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand XAT 4 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings

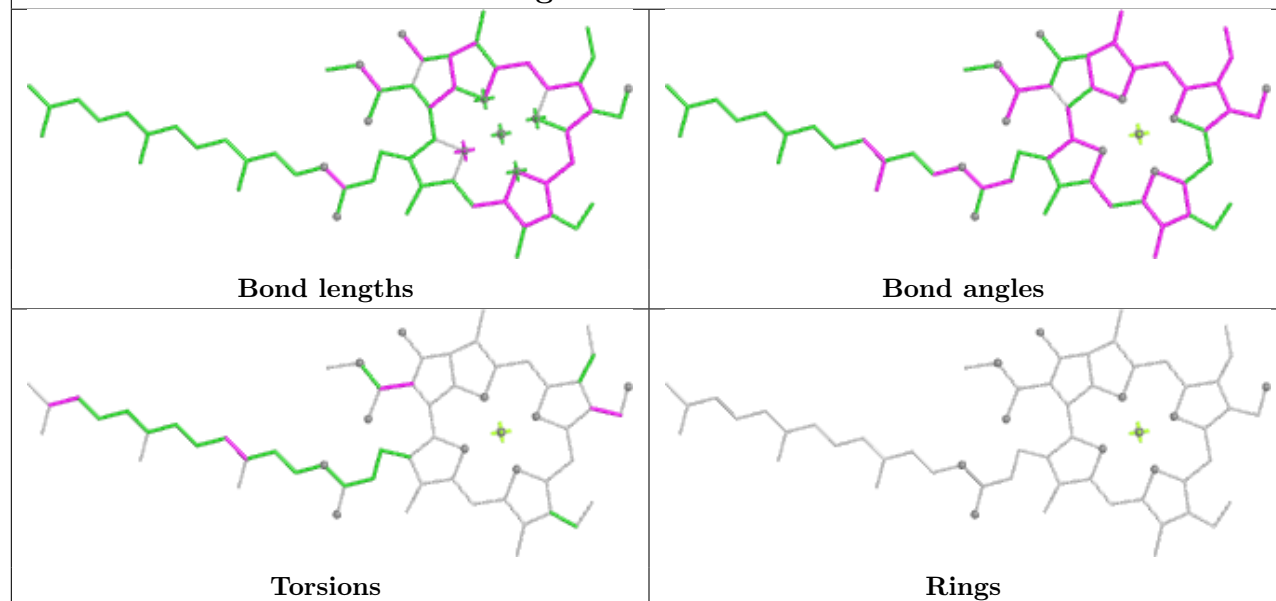
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

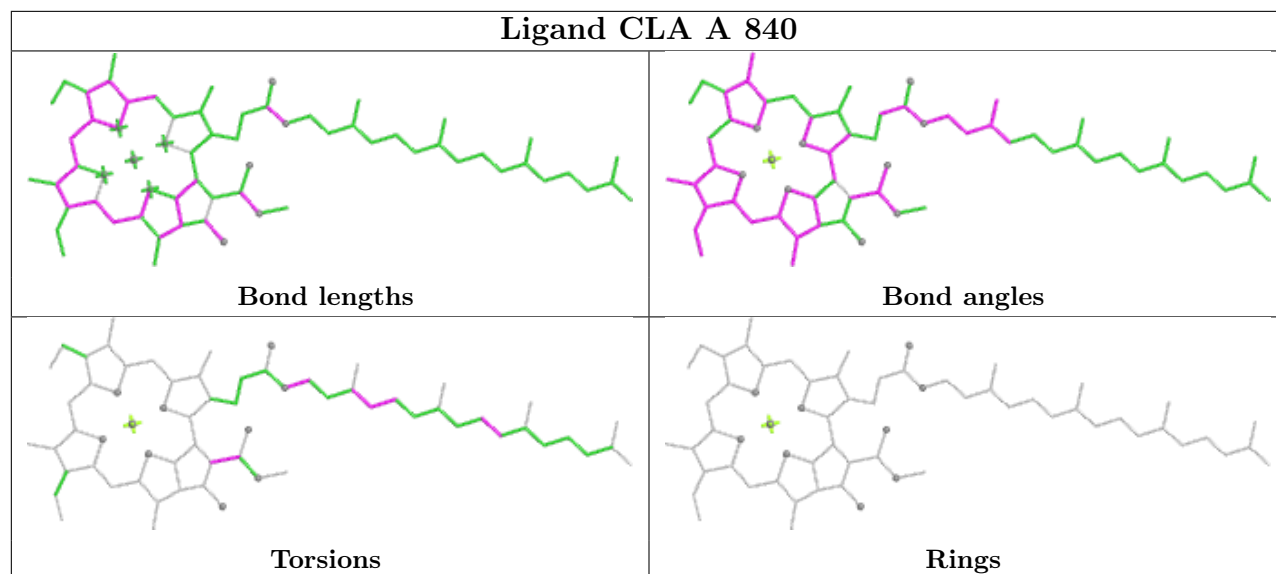
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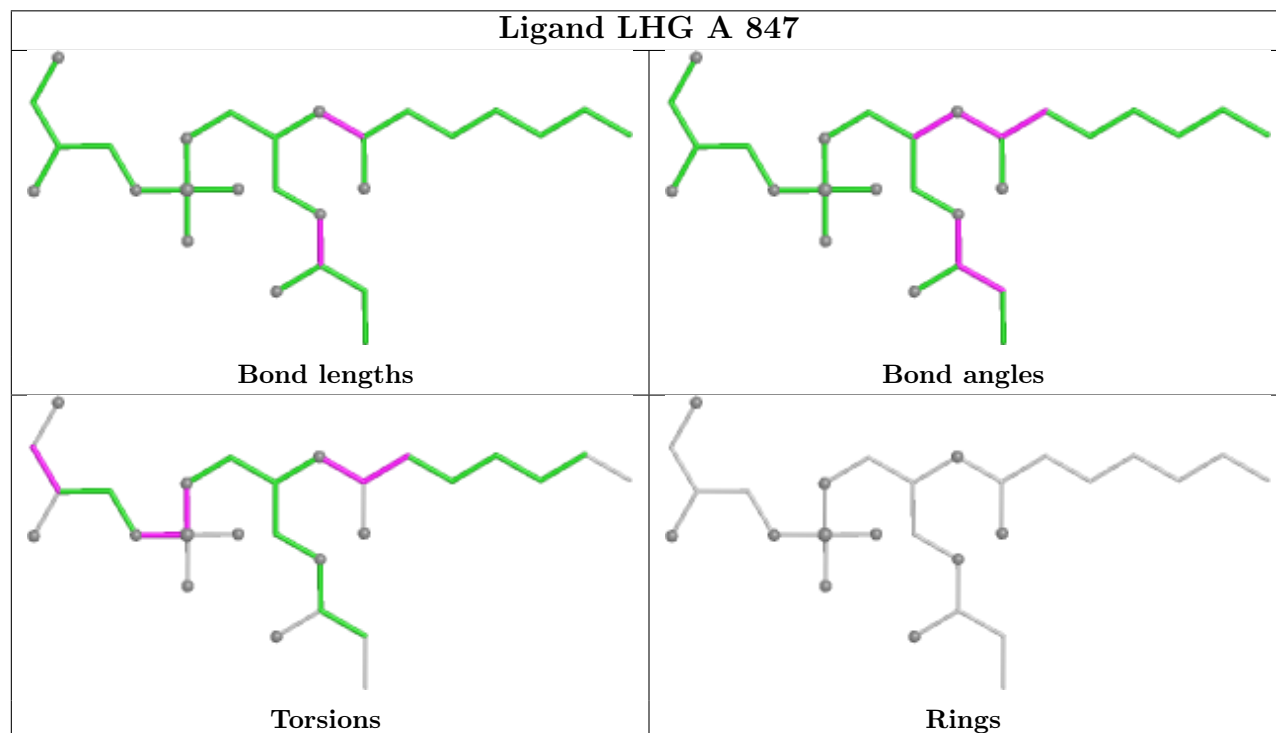
Ligand CHL 1 302



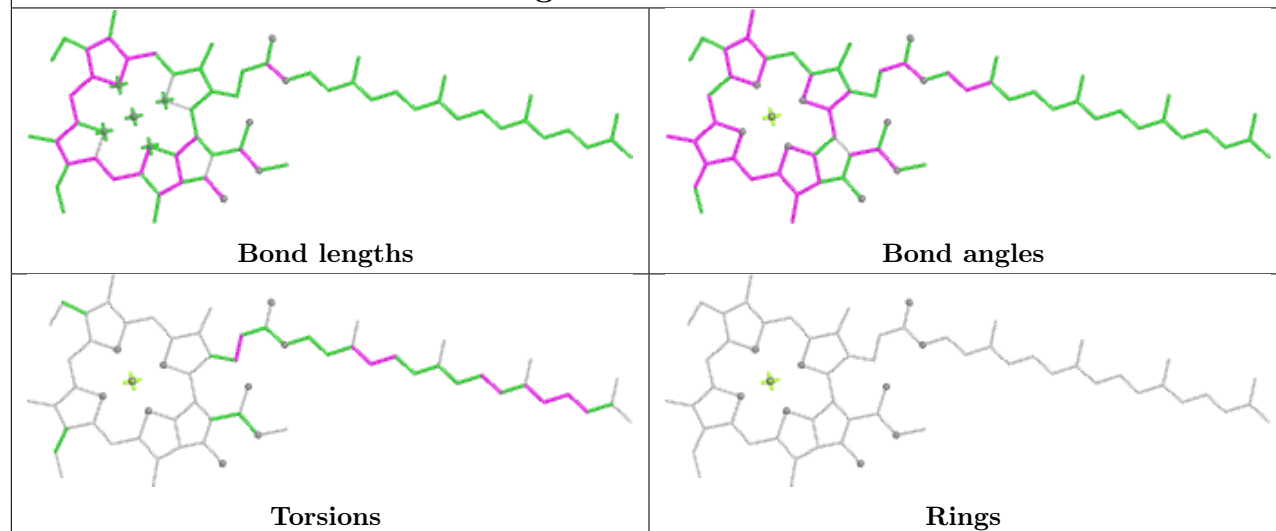
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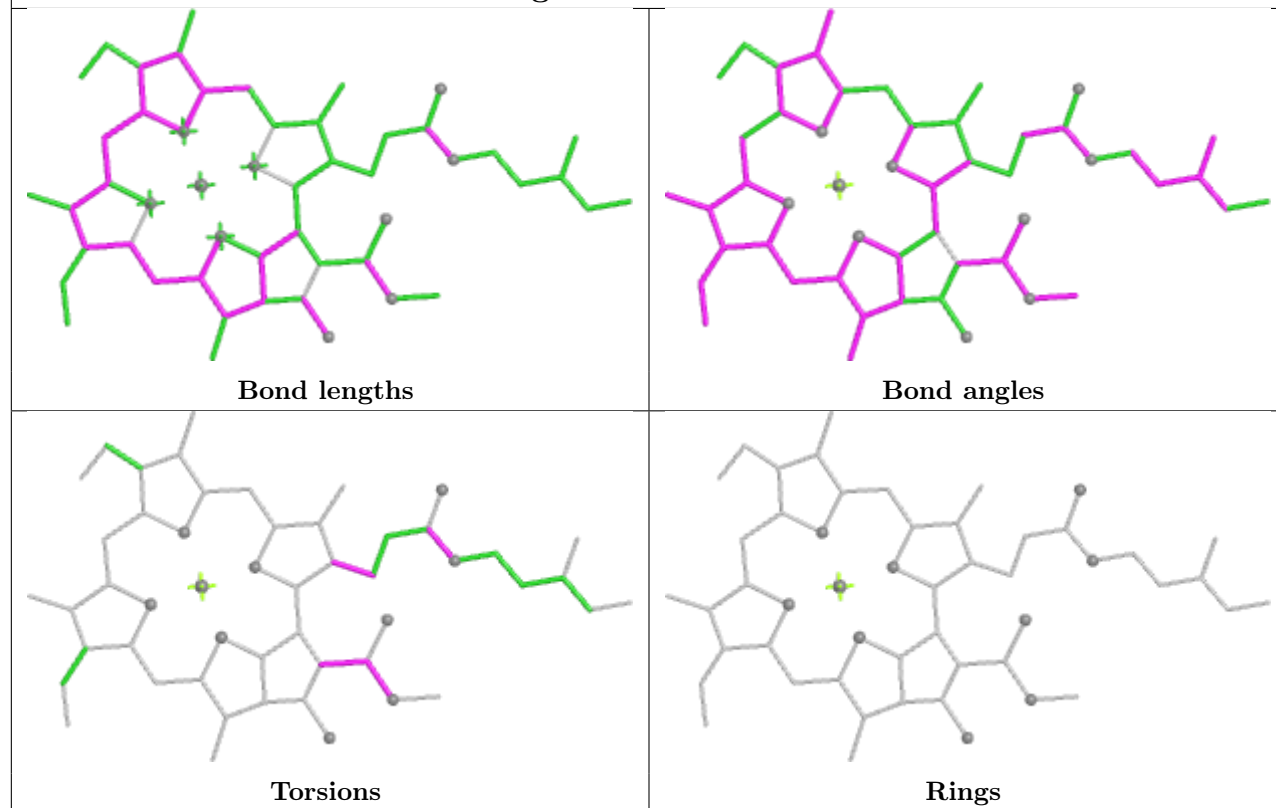
Ligand LHG A 847



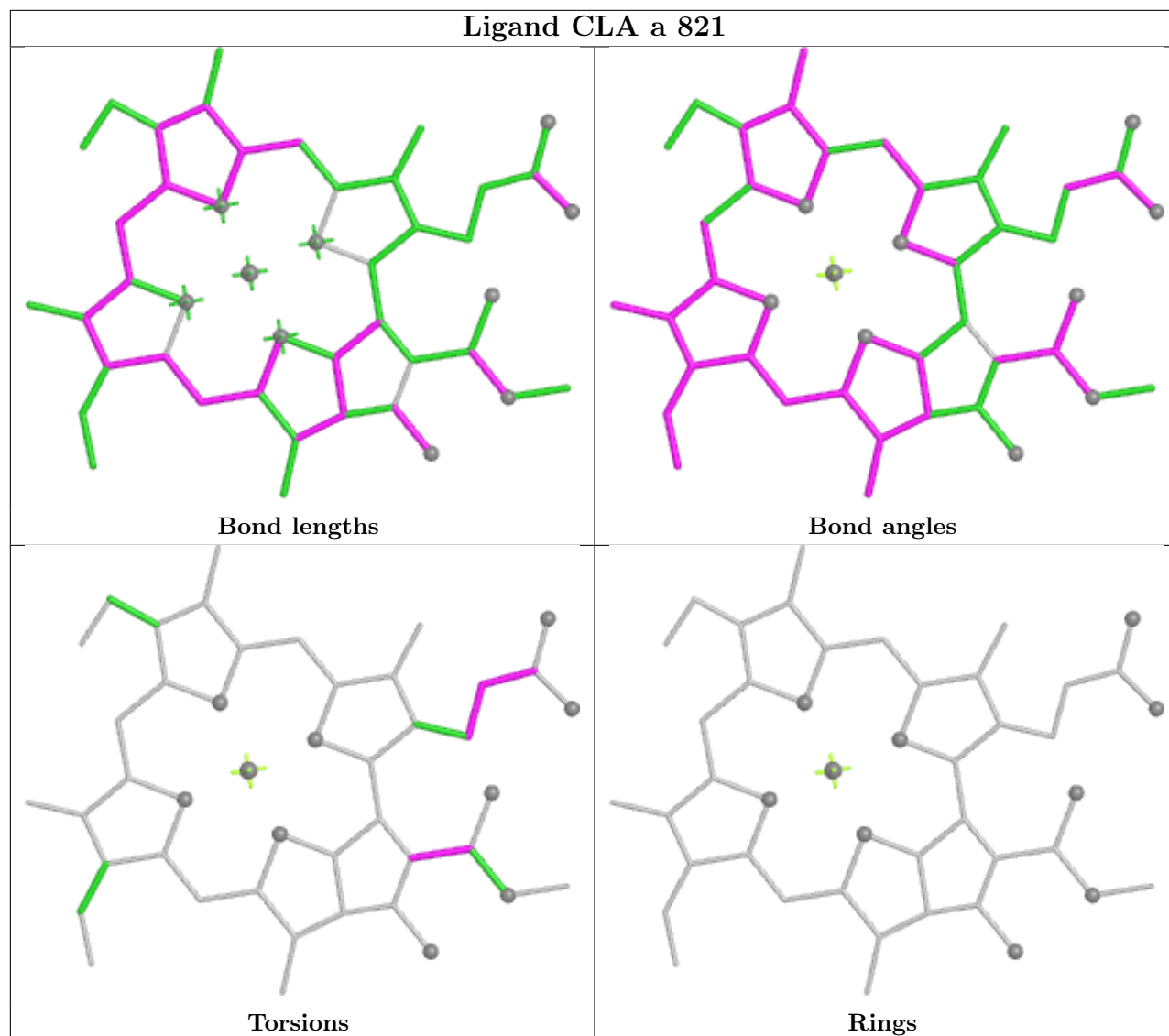
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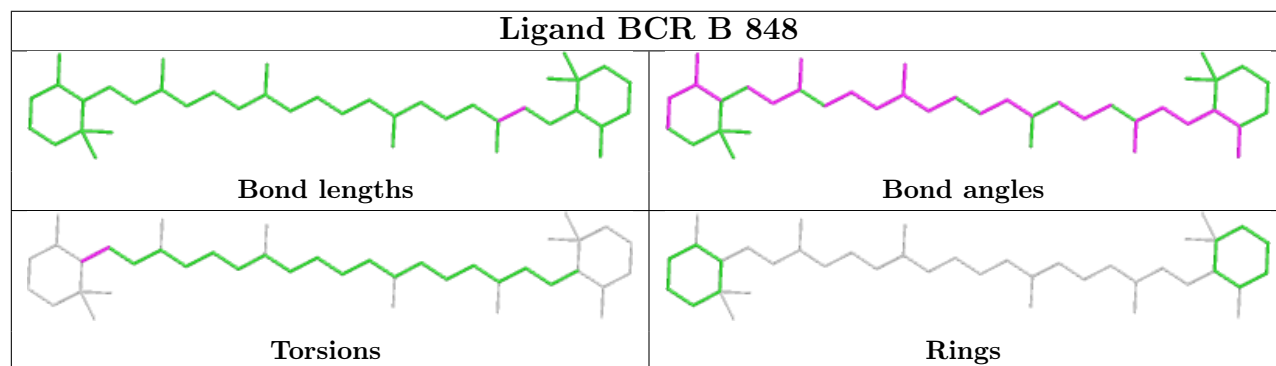
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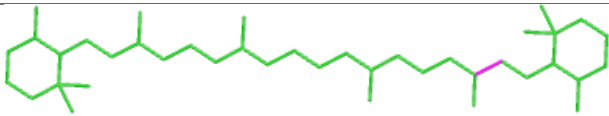
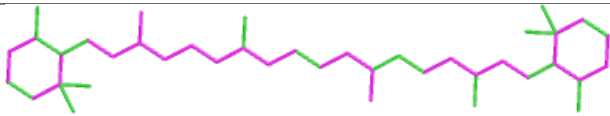
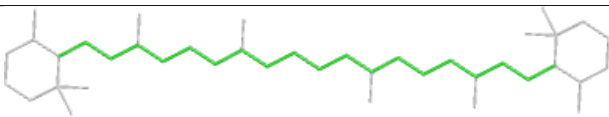
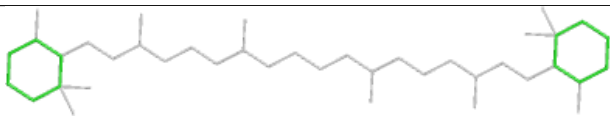
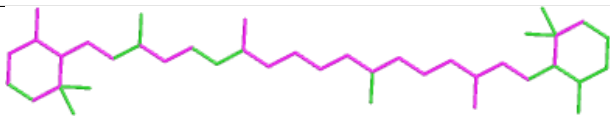
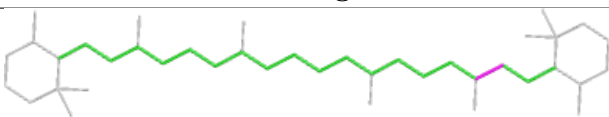
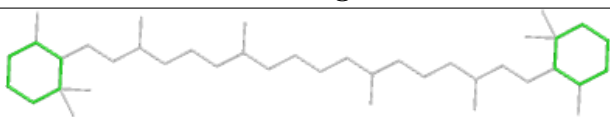


Ligand CLA a 821

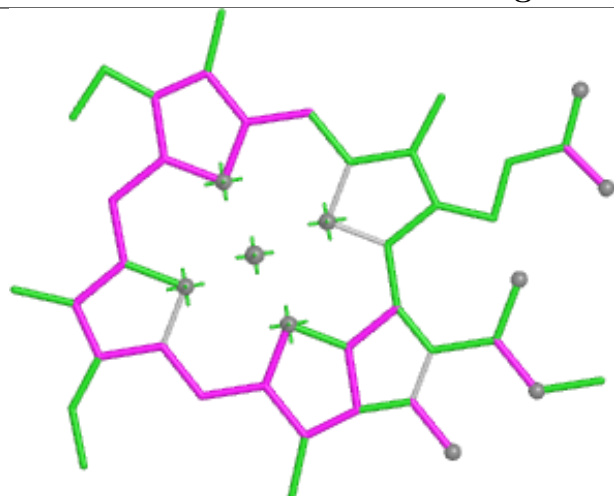


Ligand BCR B 848

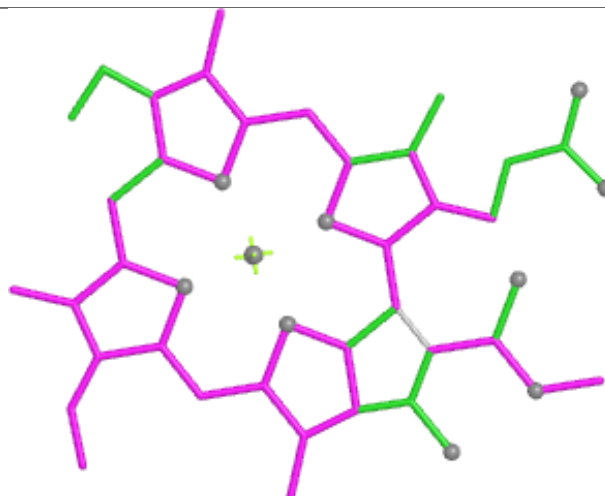


Ligand BCR b 843			
	Bond lengths		
	Torsions		
Ligand BCR a 849			
	Bond lengths		
	Torsions		

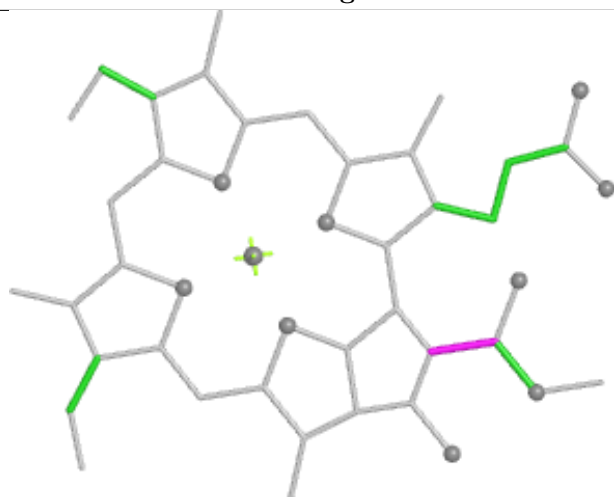
Ligand CLA B 835



Bond lengths



Bond angles

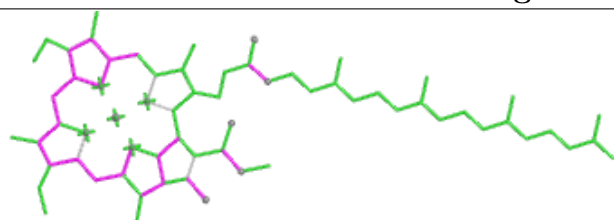


Torsions

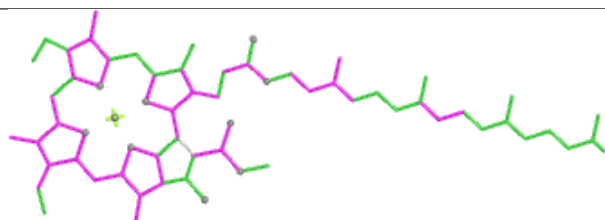


Rings

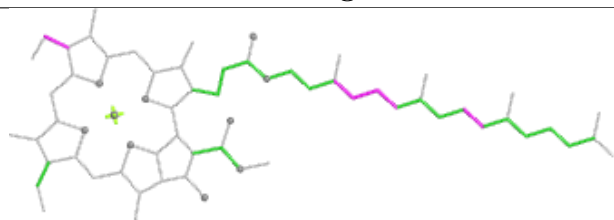
Ligand CLA A 822



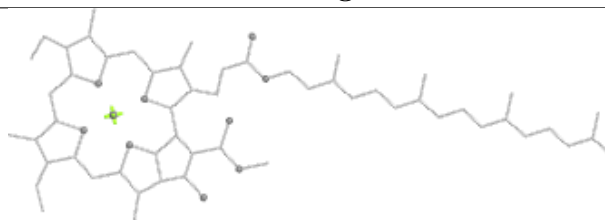
Bond lengths



Bond angles

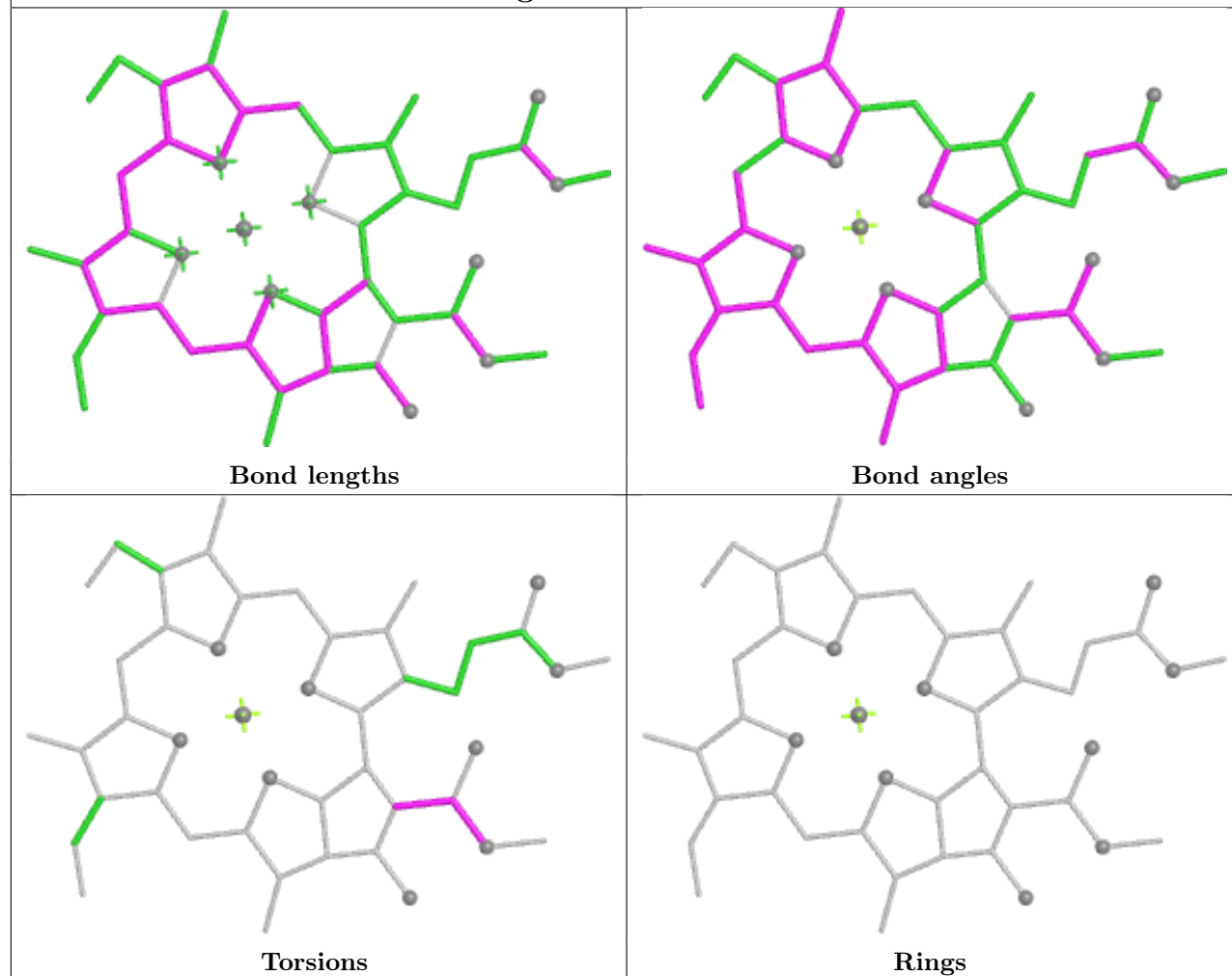


Torsions

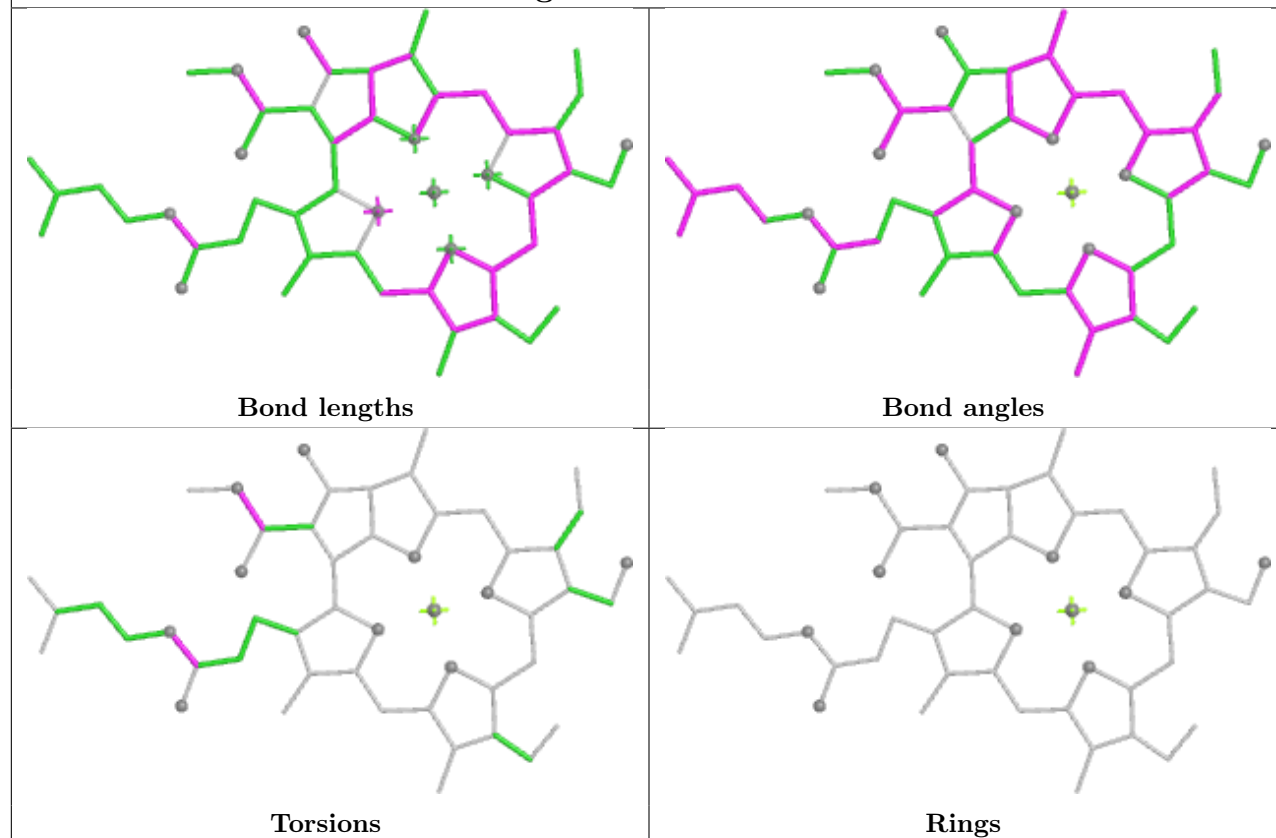


Rings

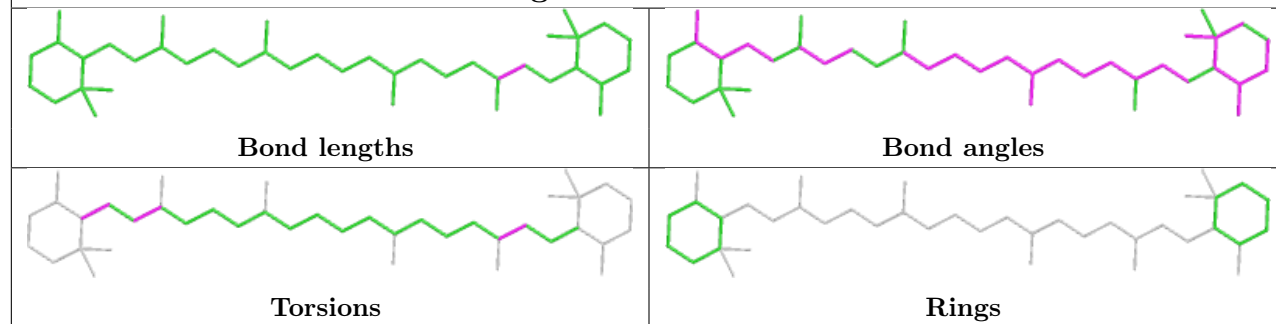
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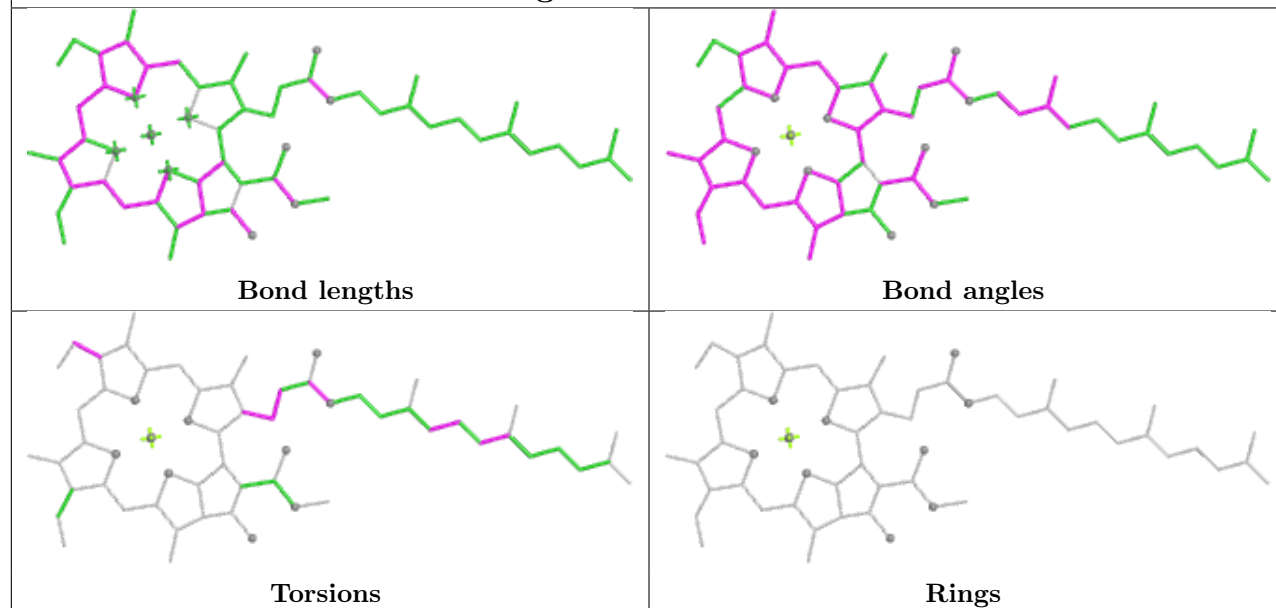
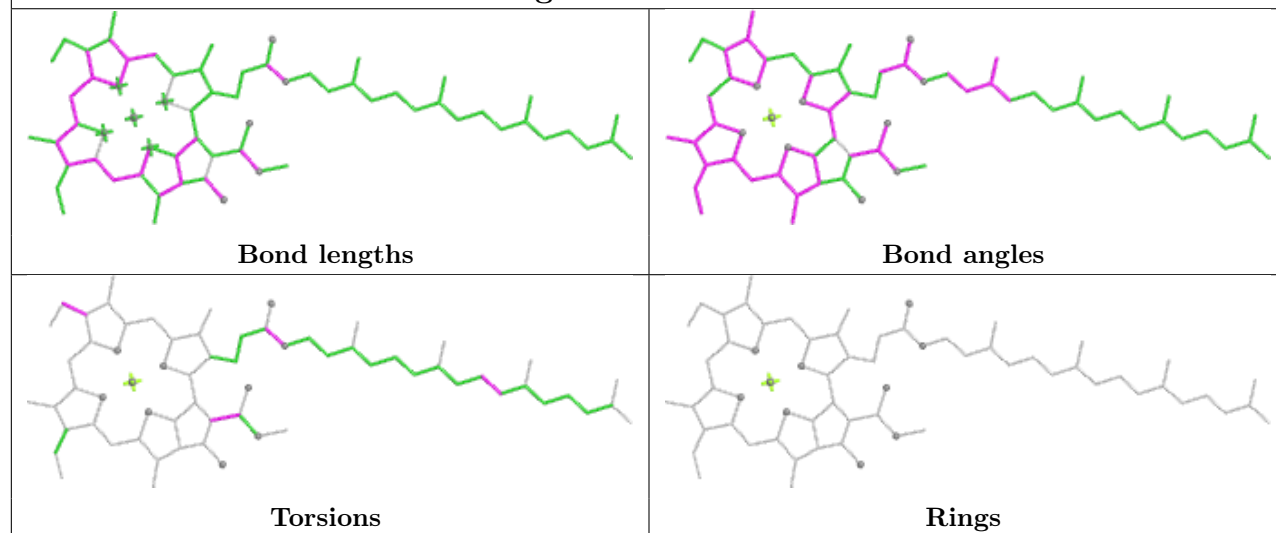


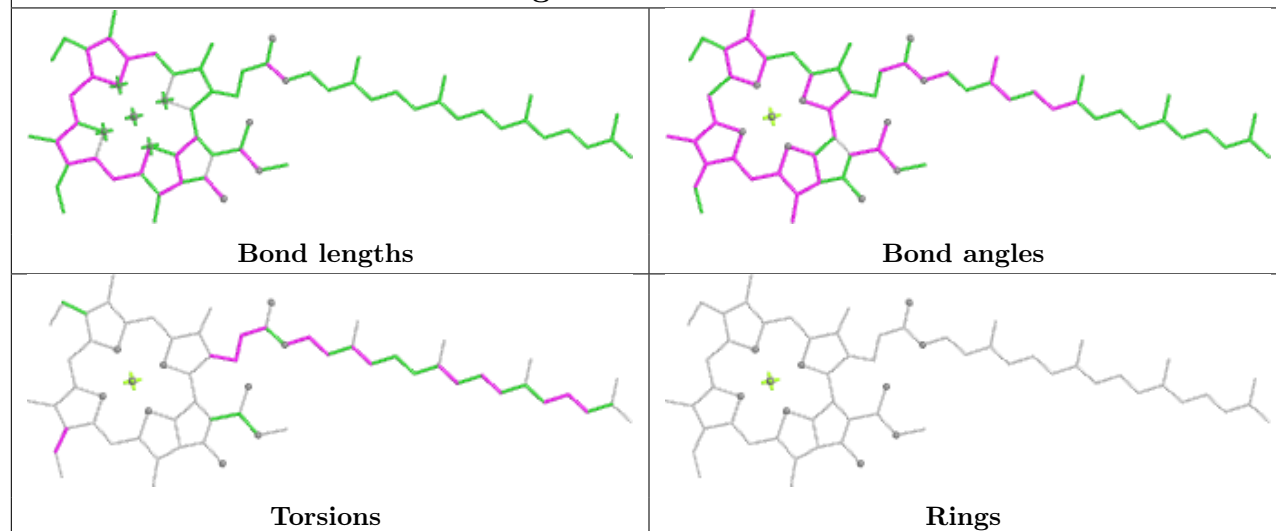
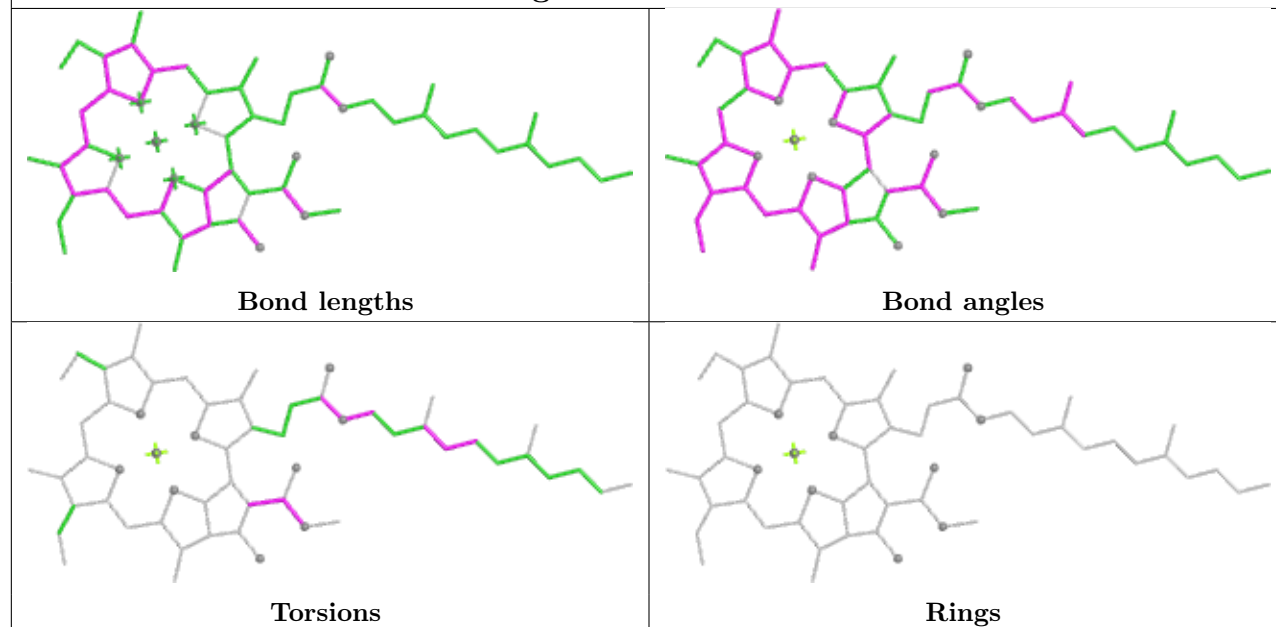
Ligand CHL 7 607

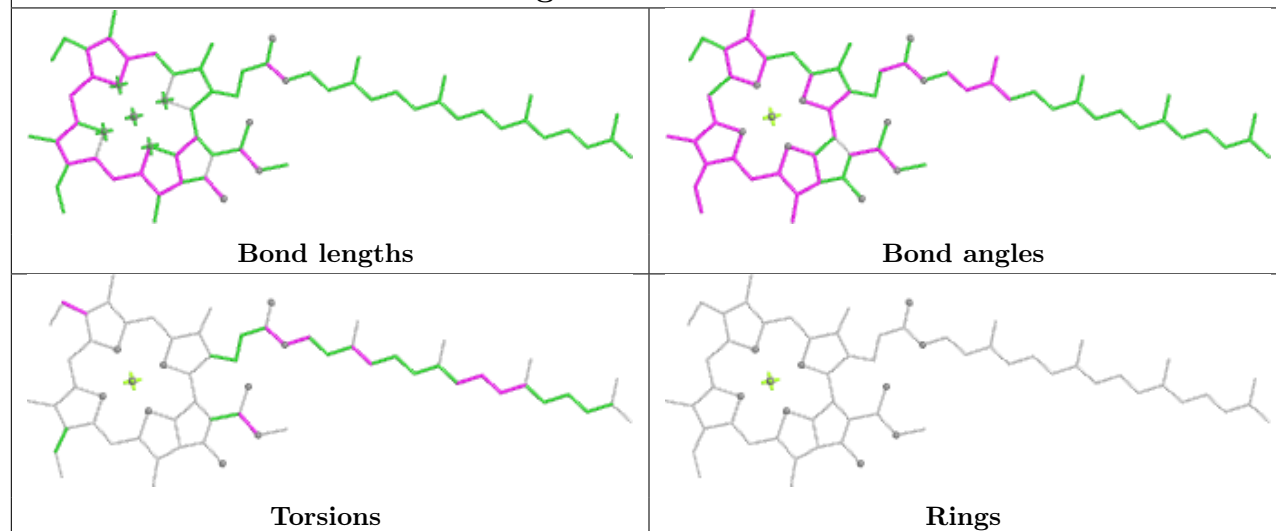
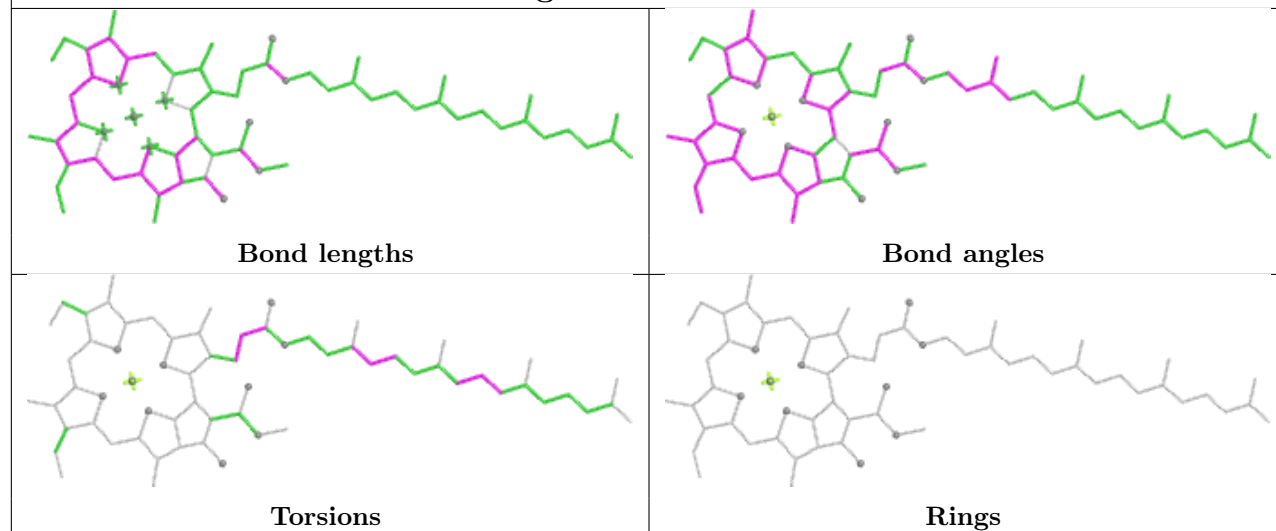


Ligand BCR B 847

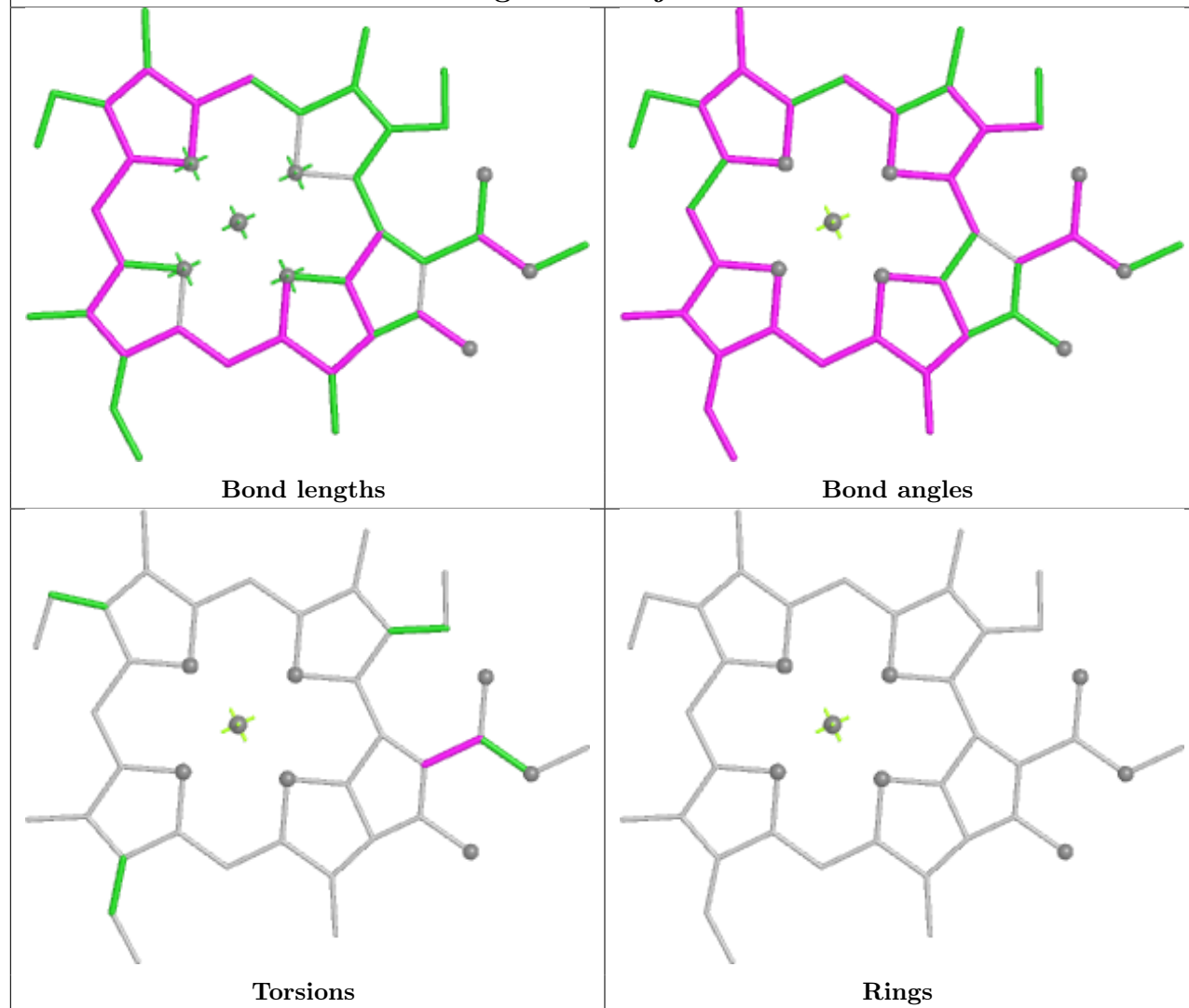


Ligand CLA 7 609**Ligand CLA b 829**

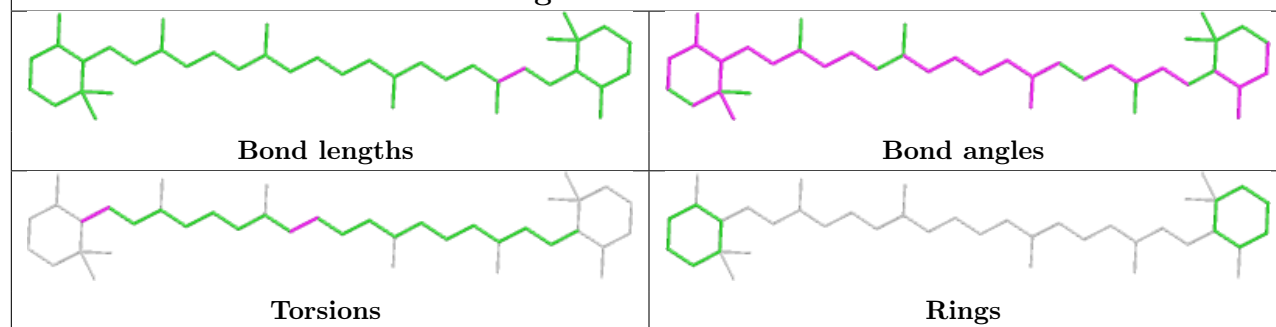
Ligand CLA B 832**Ligand CLA B 833**

Ligand CLA 2 603**Ligand CLA 7 612**

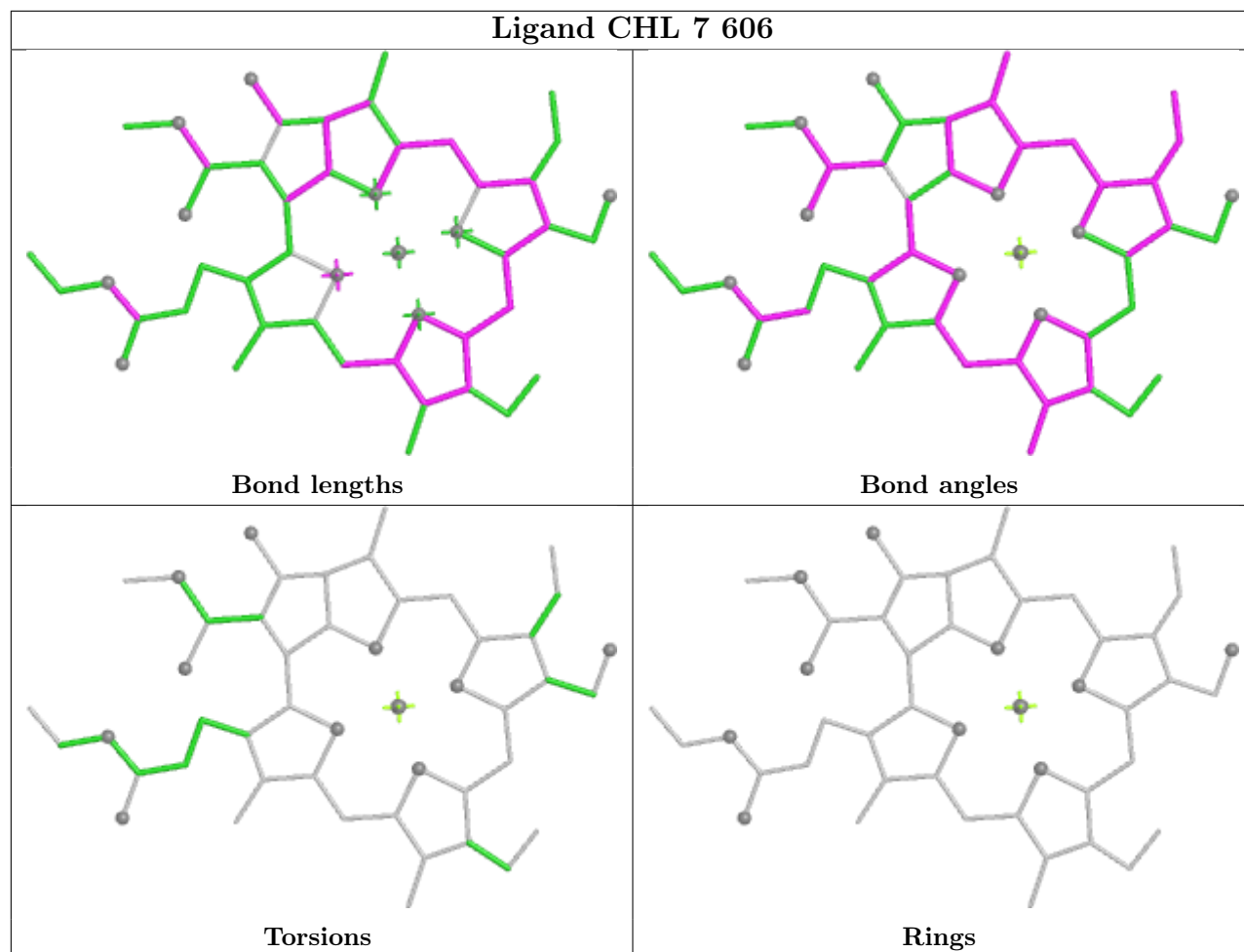
Ligand CLA j 3002

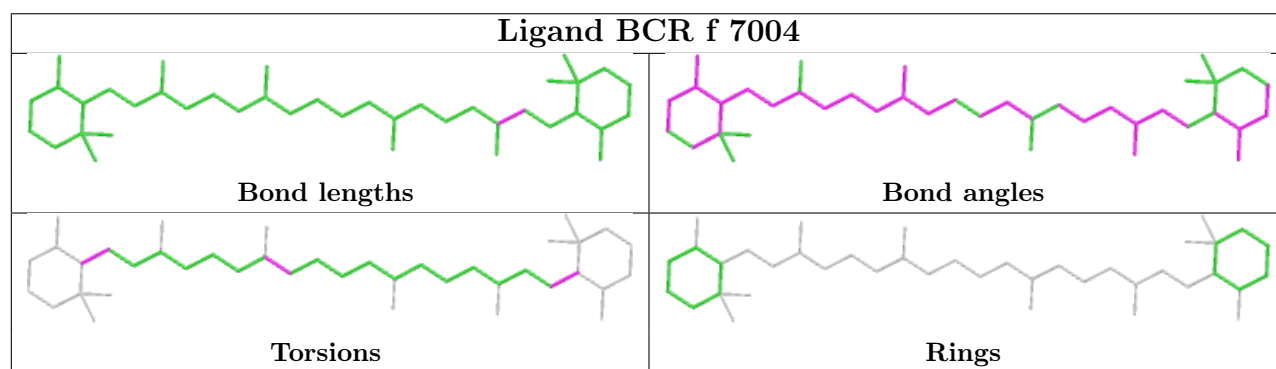
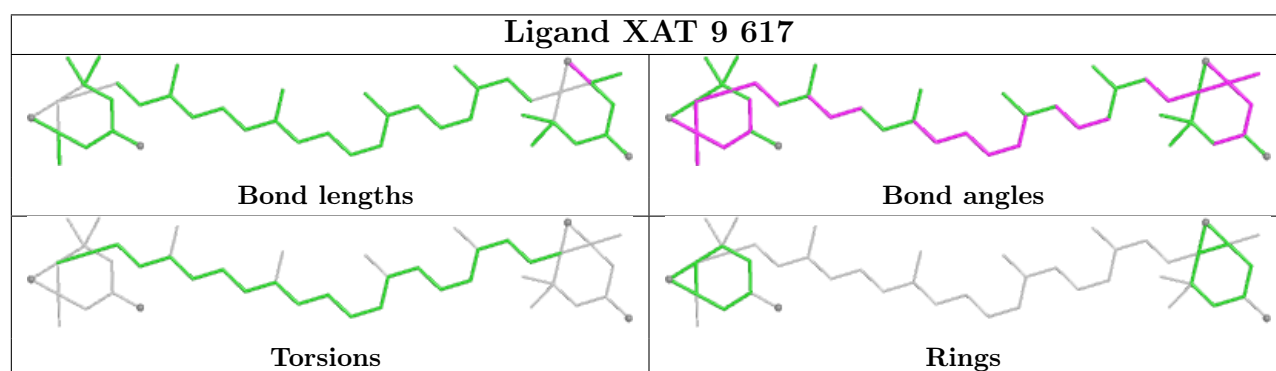
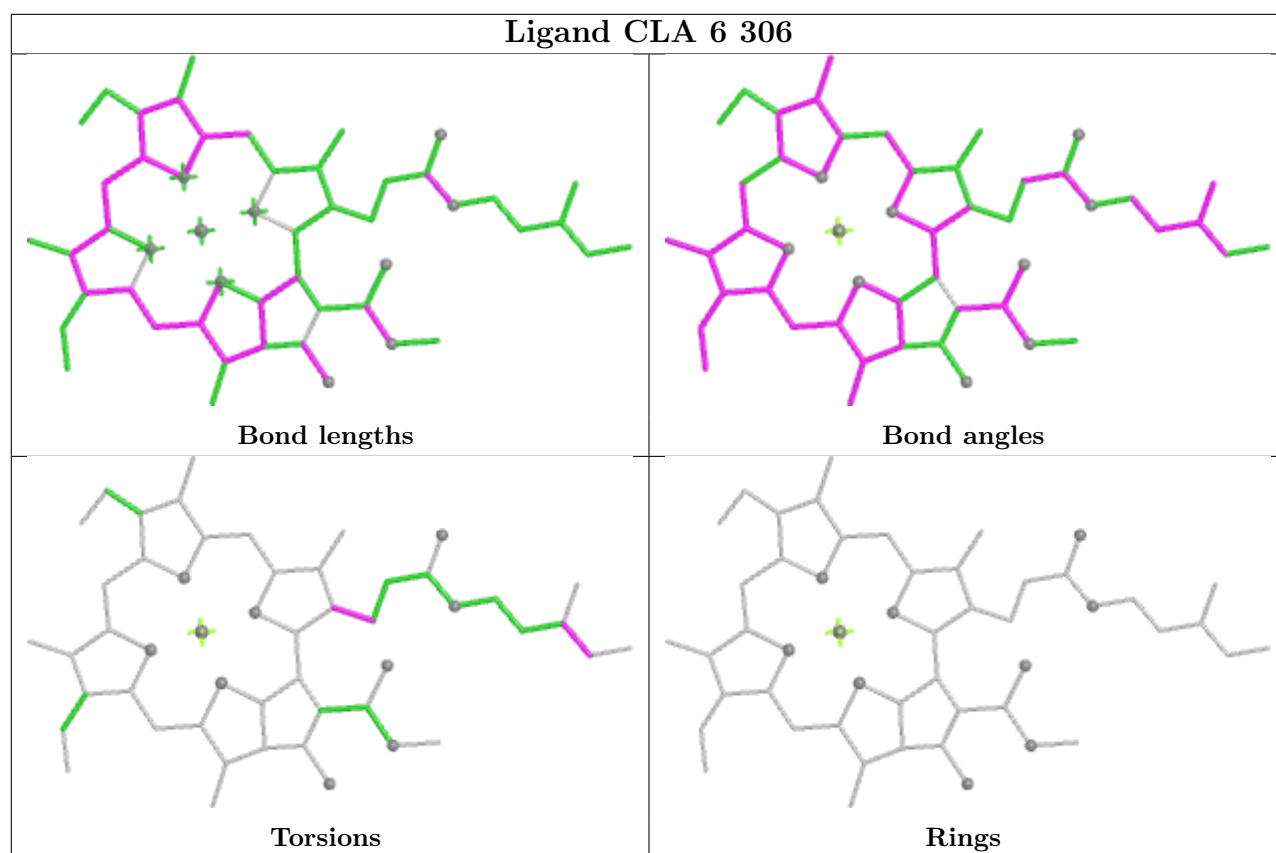


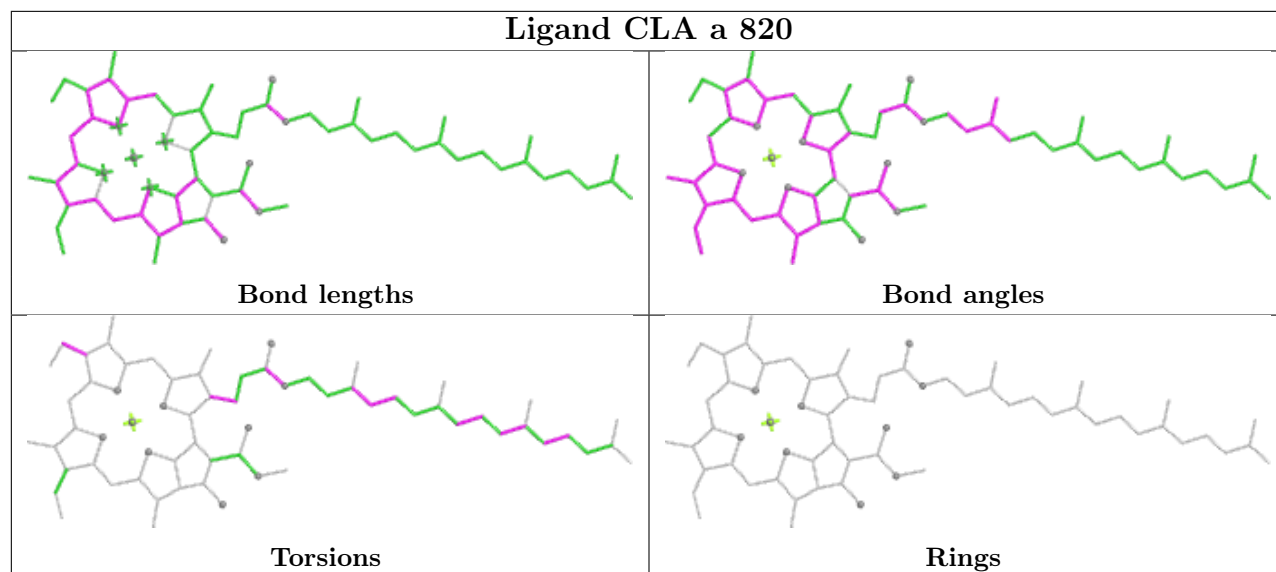
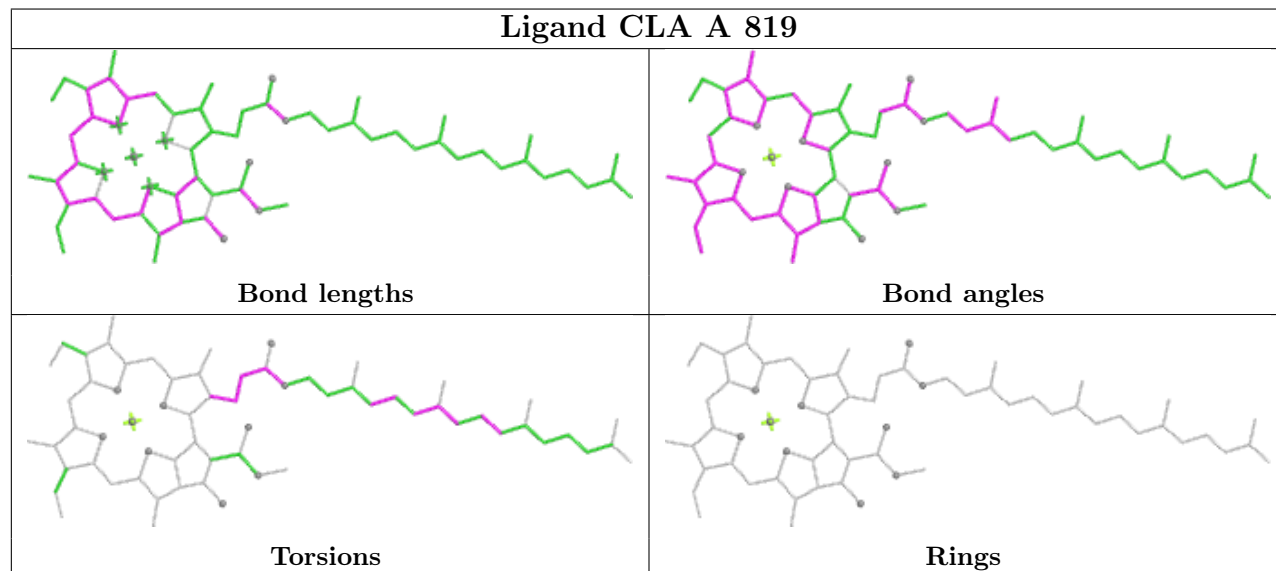
Ligand BCR 2 617



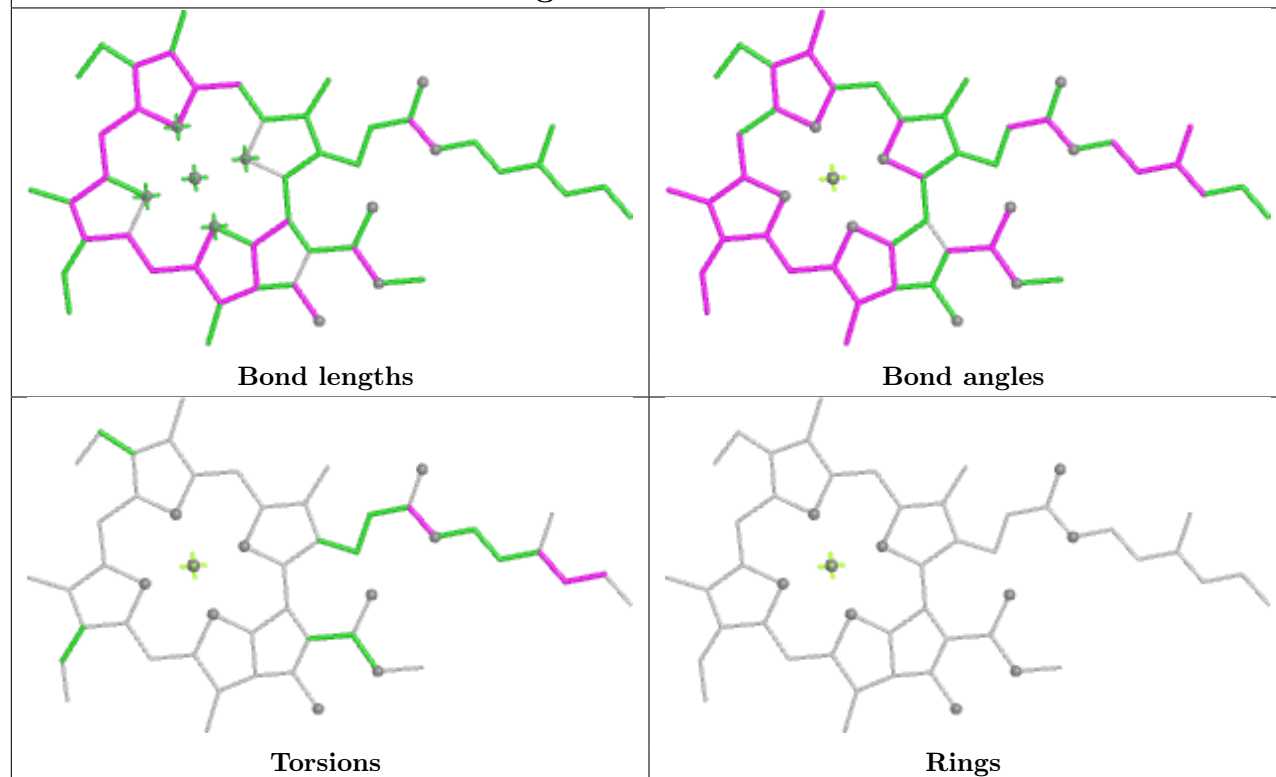
Ligand CHL 7 606



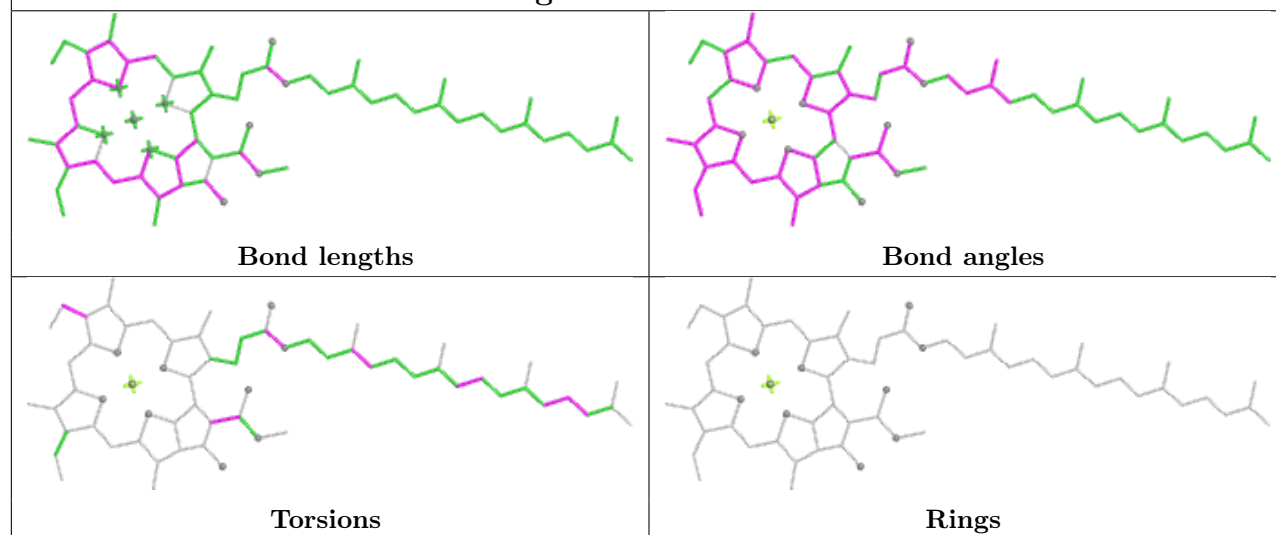


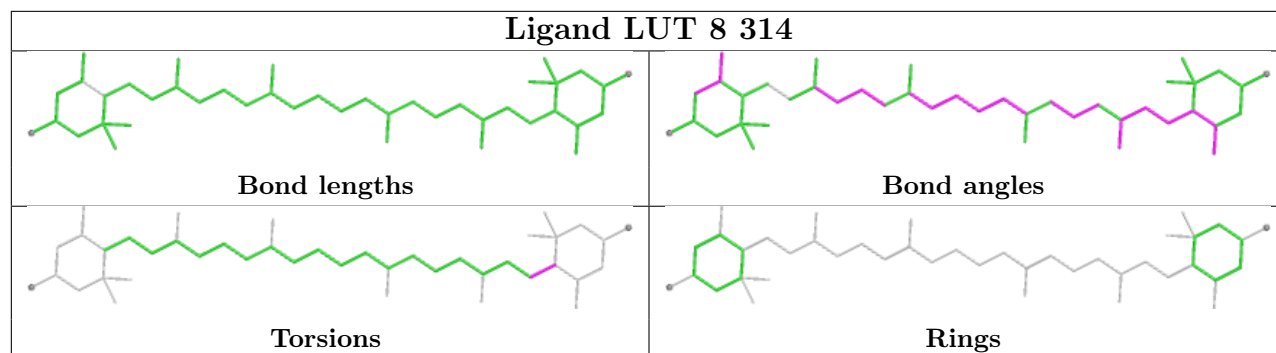
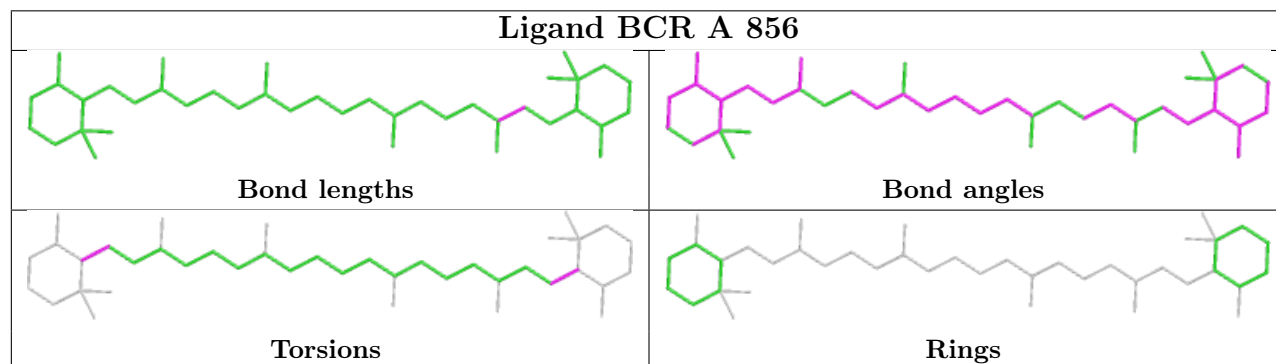
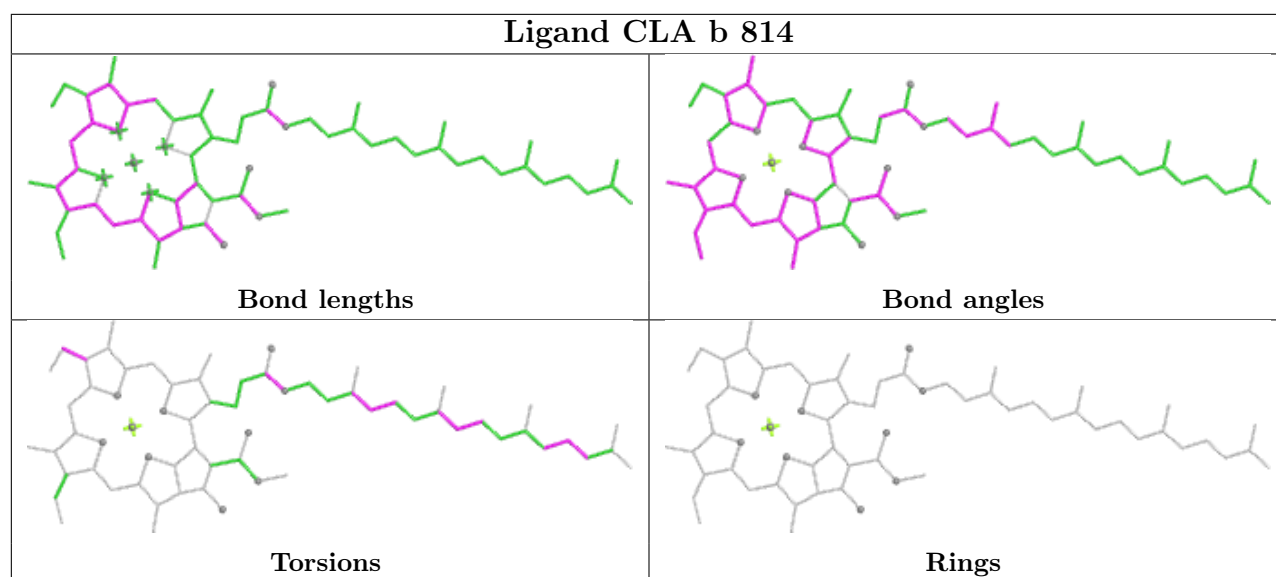
Ligand CLA a 820**Ligand CLA A 819**

Ligand CLA 8 309

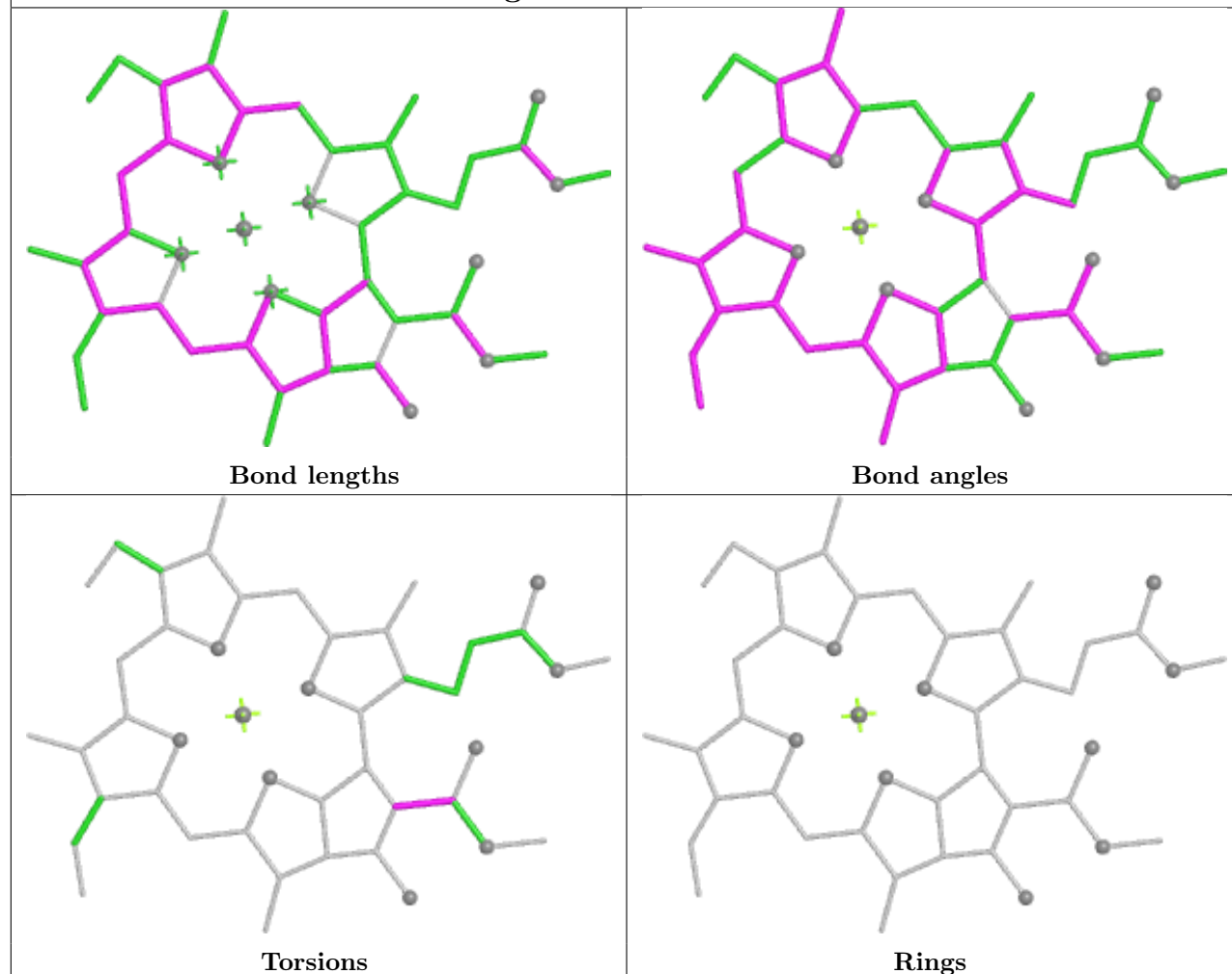


Ligand CLA b 837

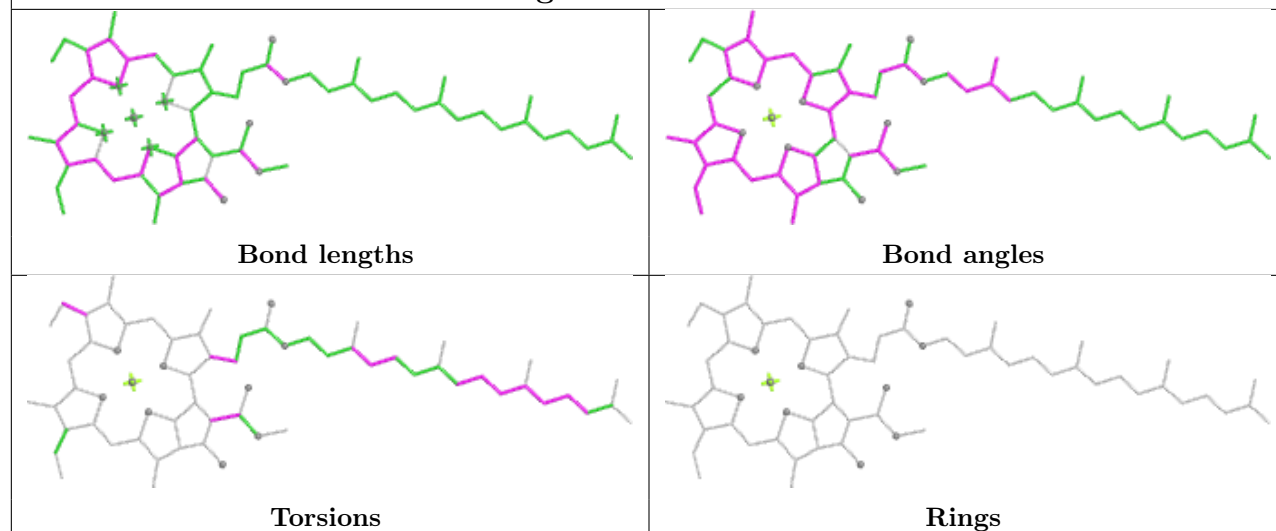




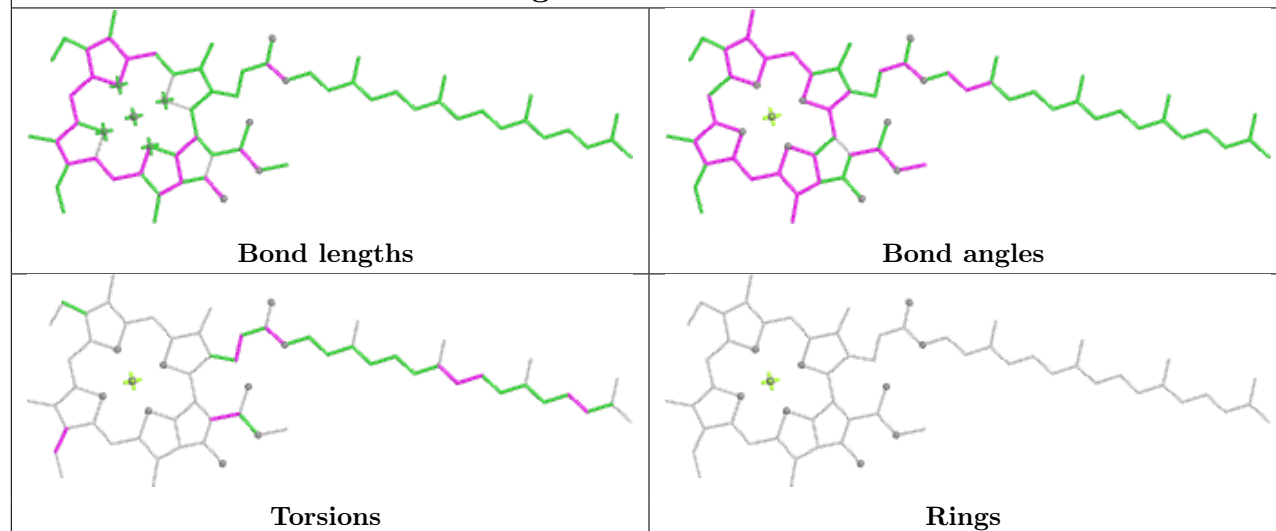
Ligand CLA K 4003



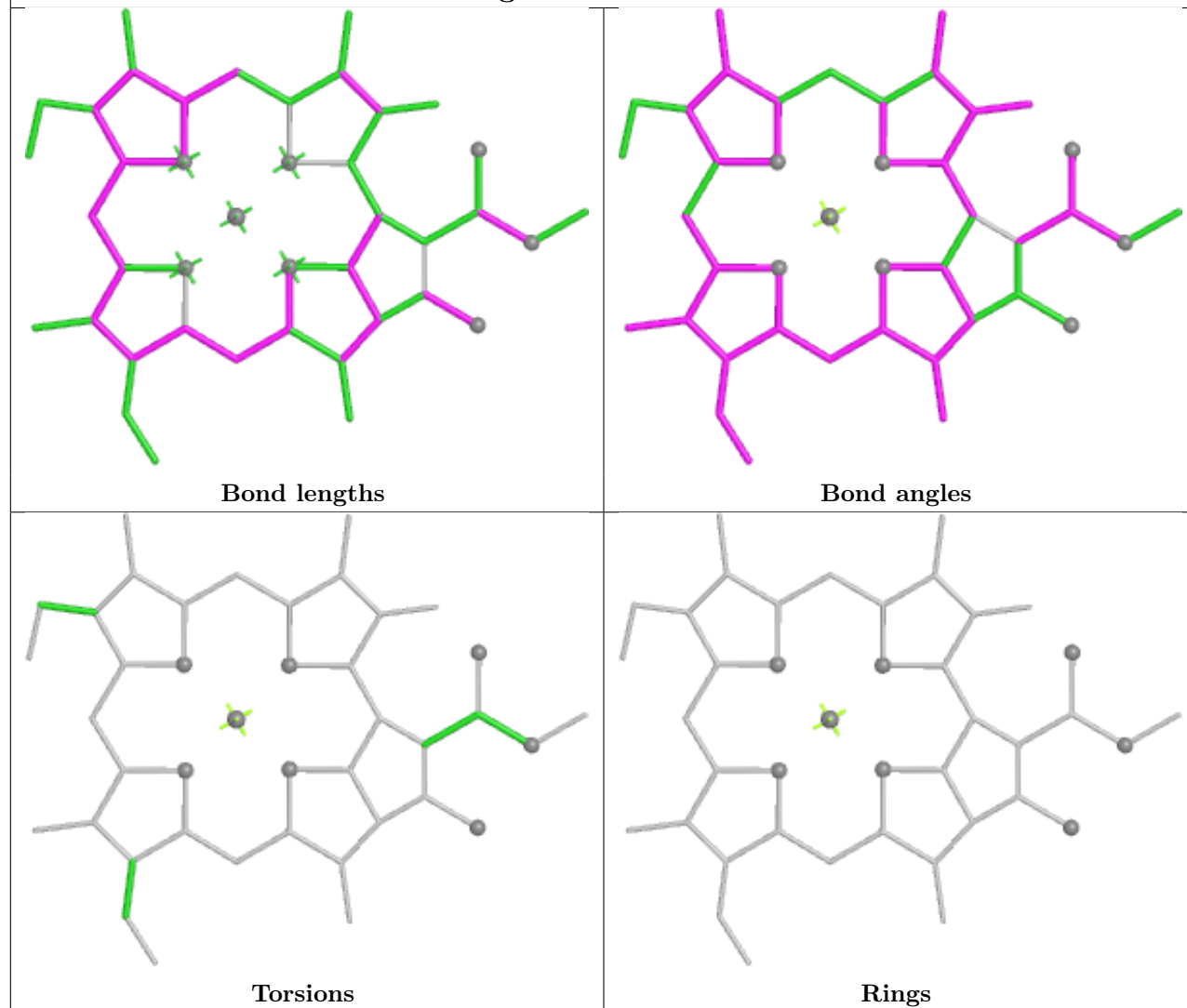
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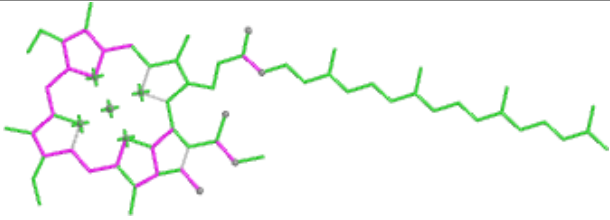
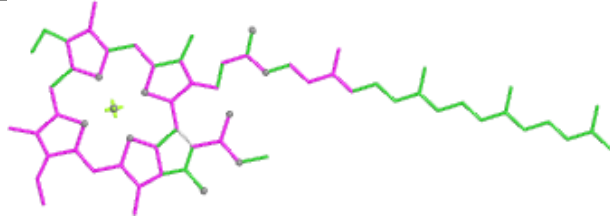
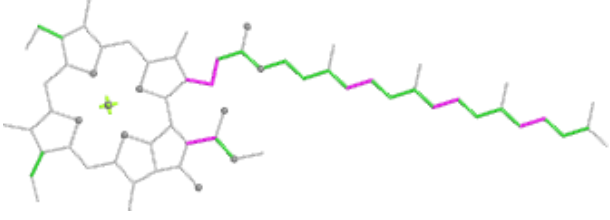
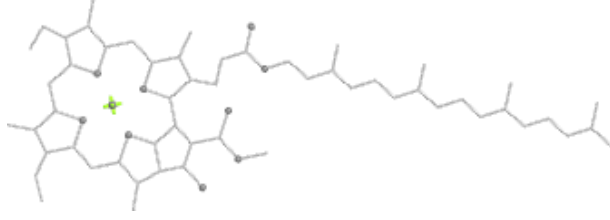
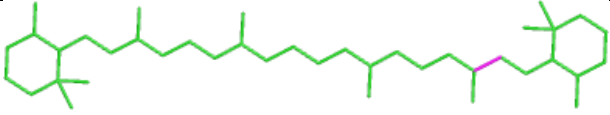
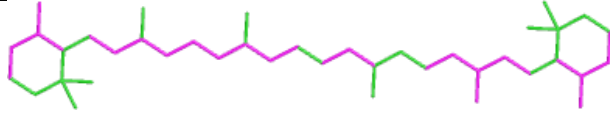
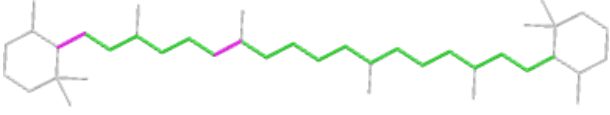
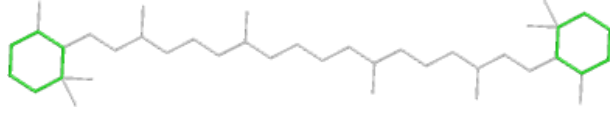
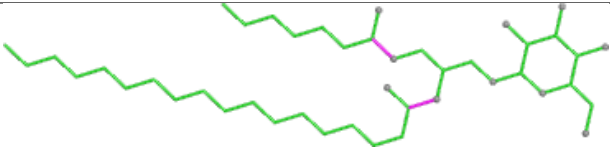
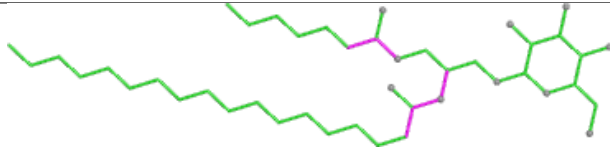


Ligand CLA A 841

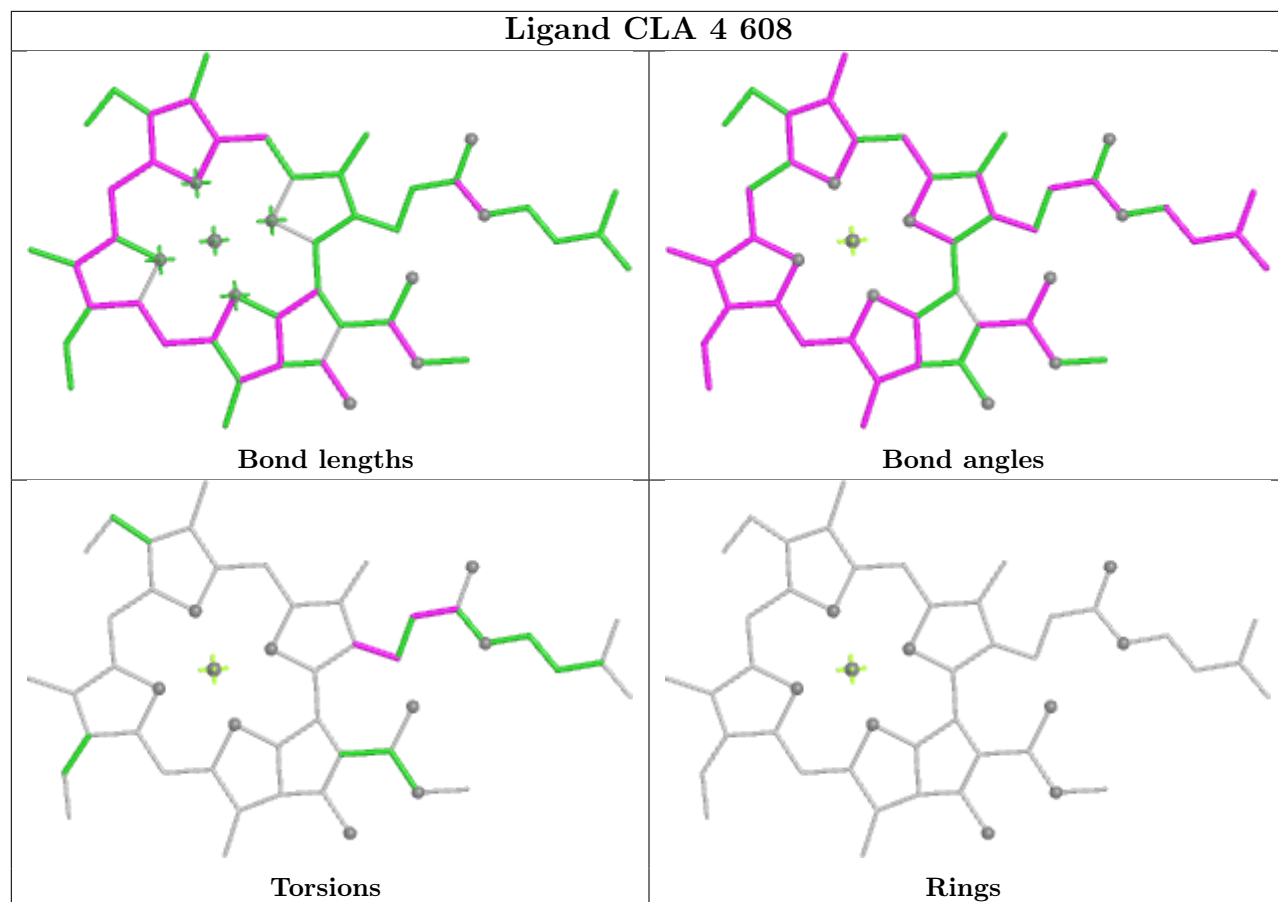


Ligand CLA 6 312

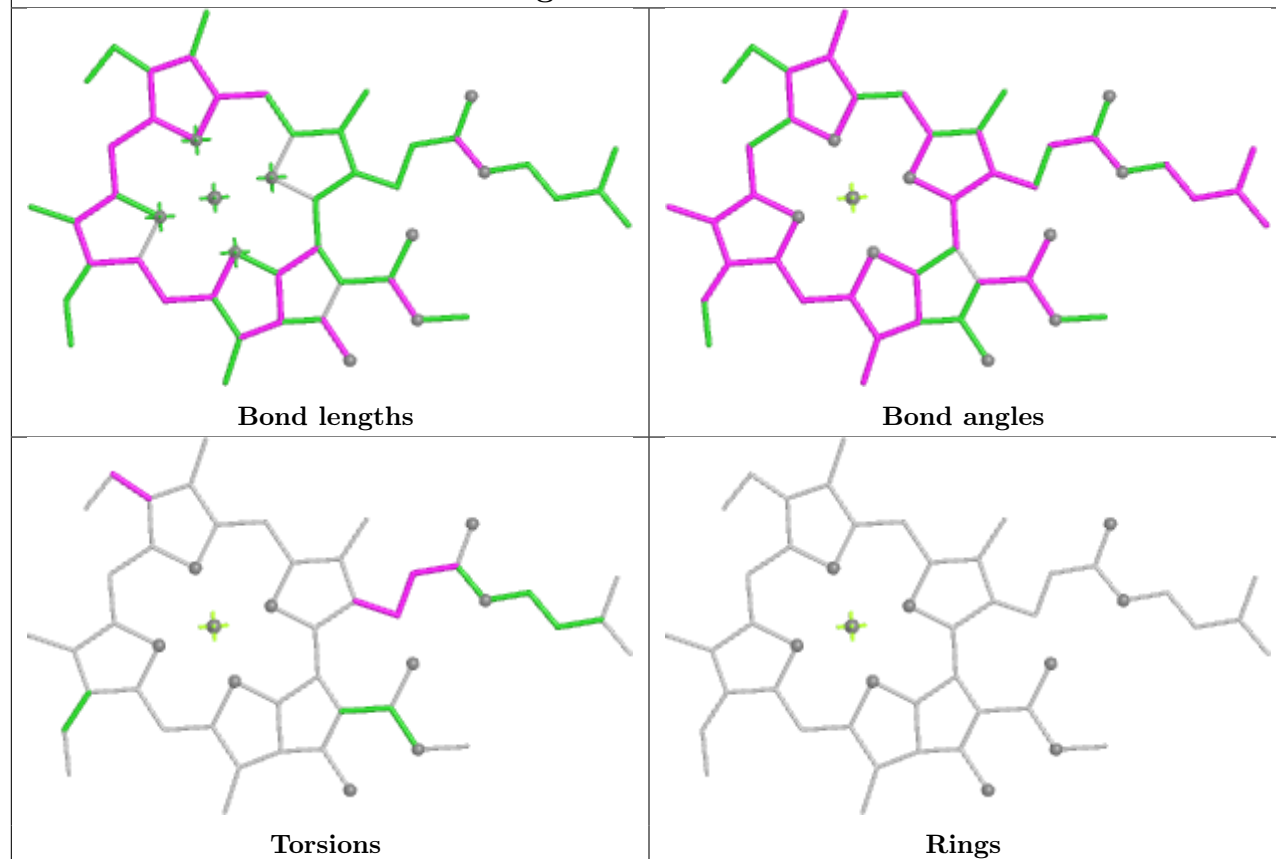


Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 206	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG G 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

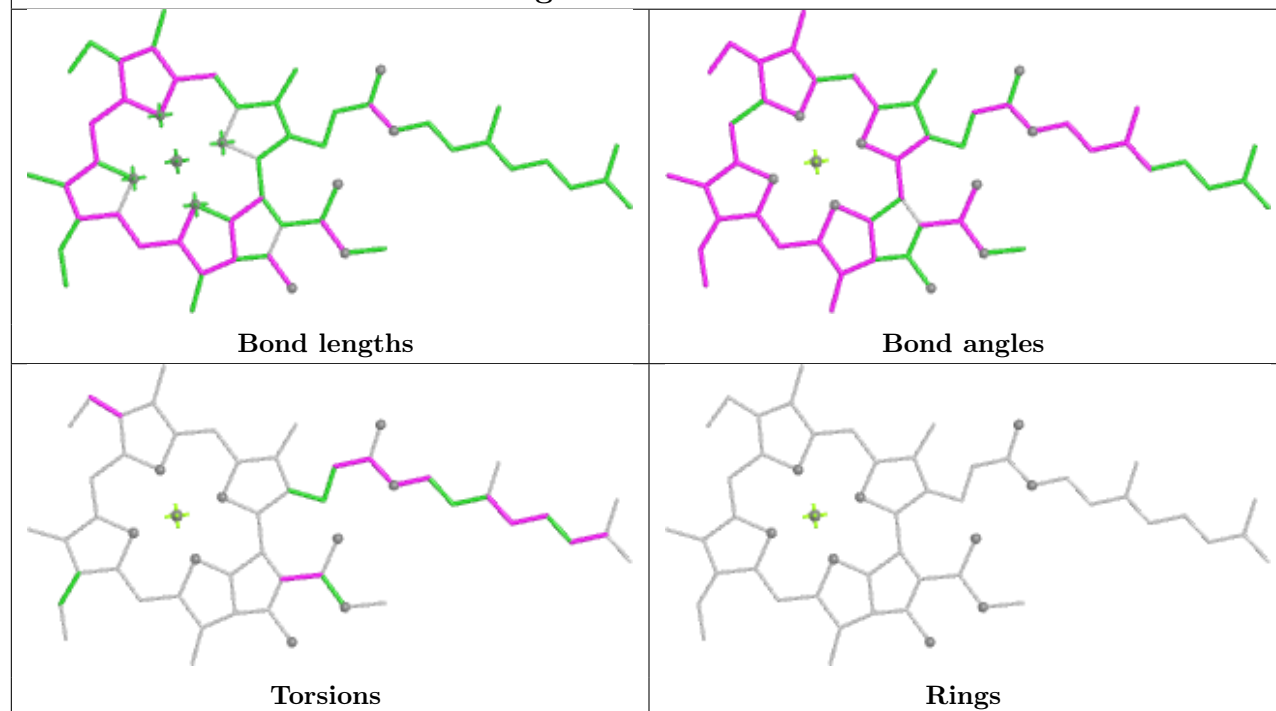
Ligand CLA 4 608

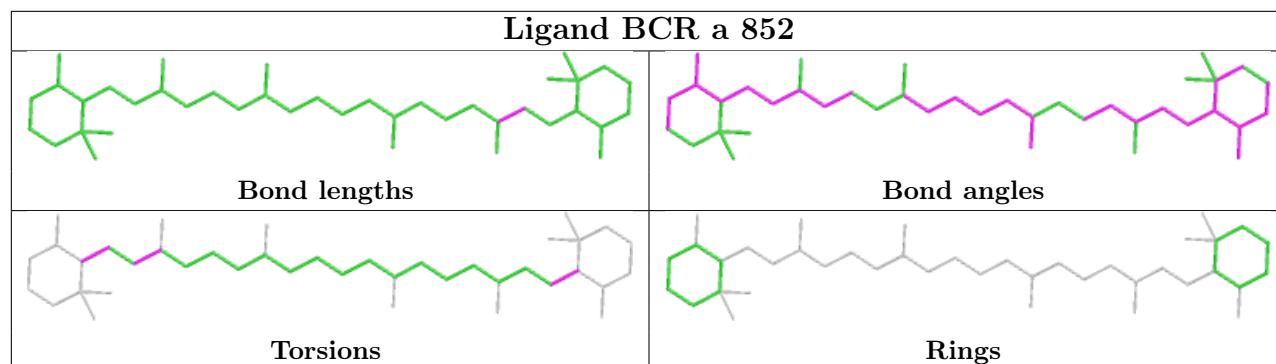
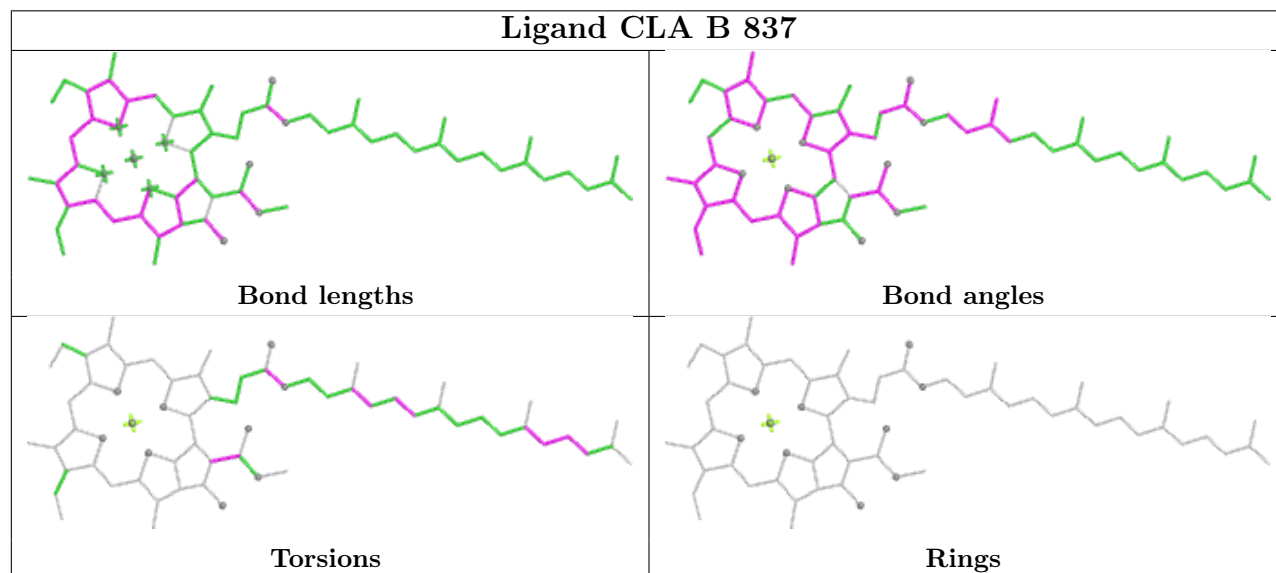
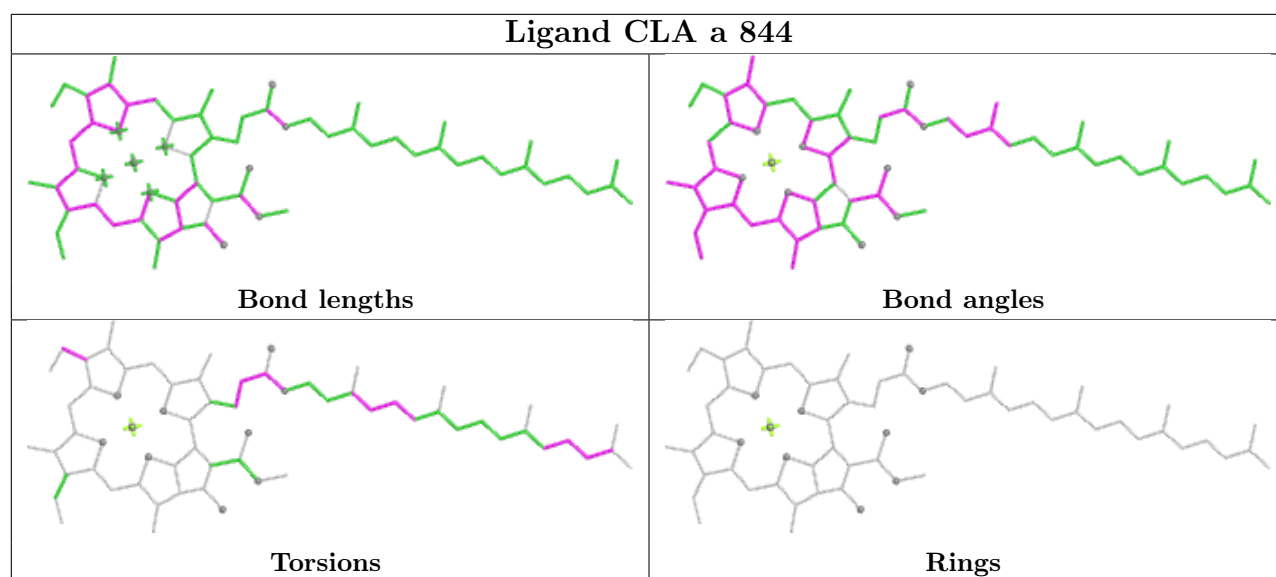


Ligand CLA 3 308

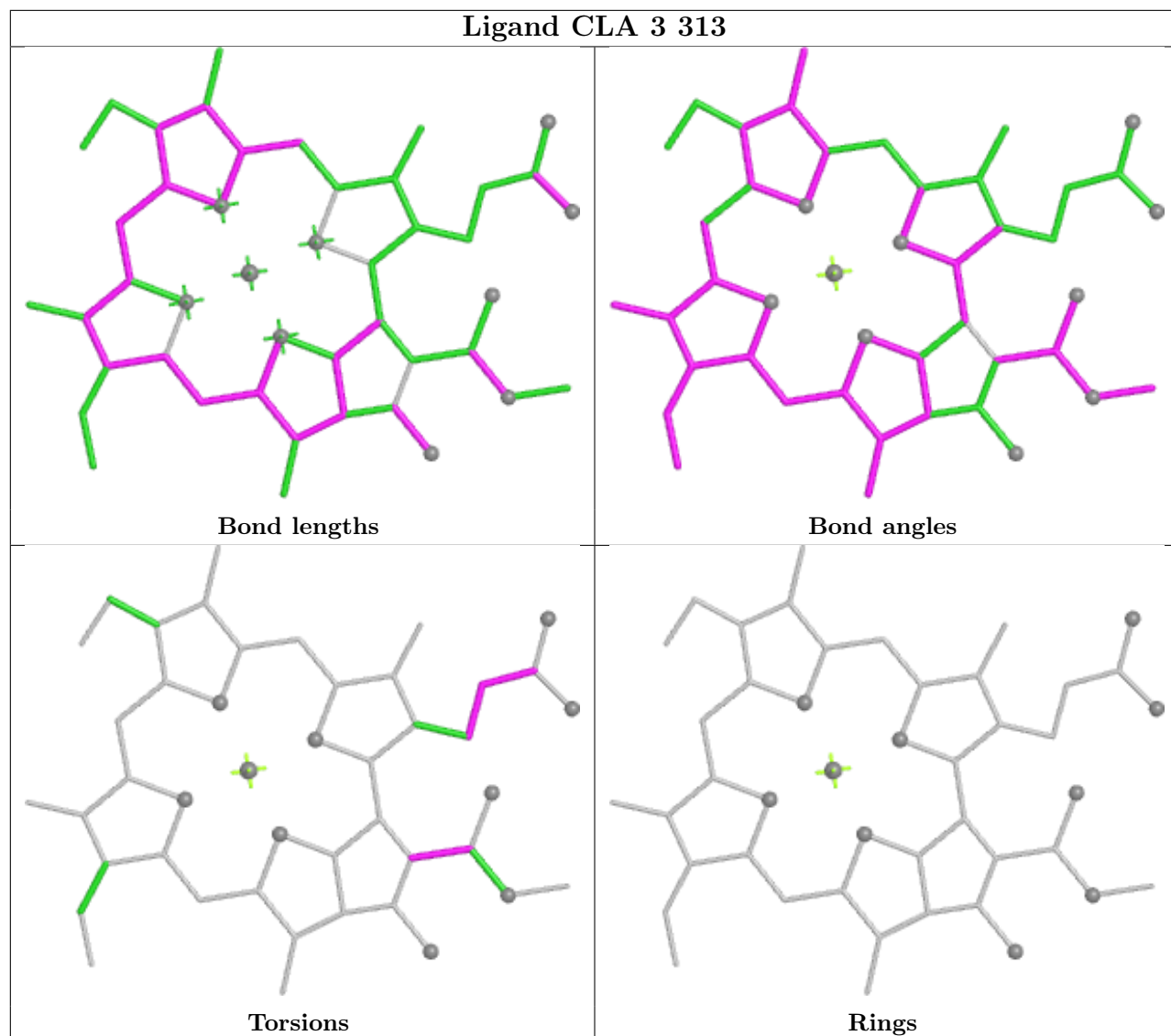


Ligand CLA b 816

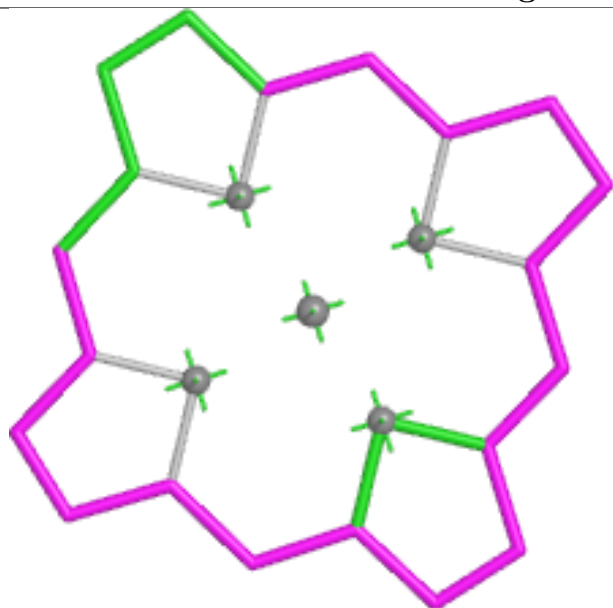




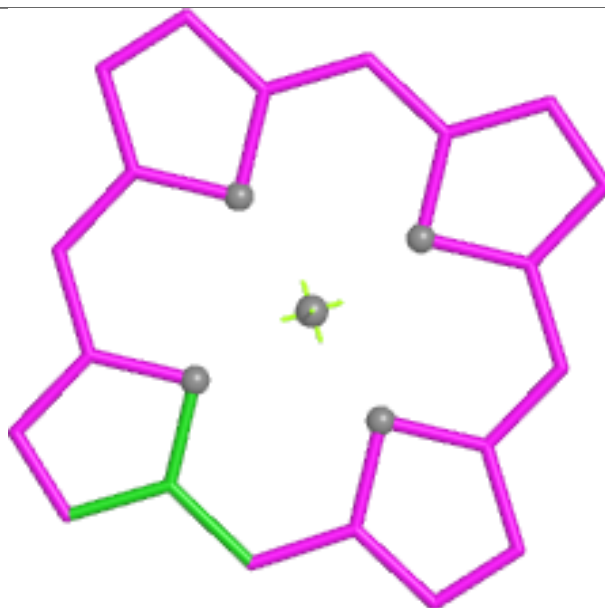
Ligand CLA 3 313



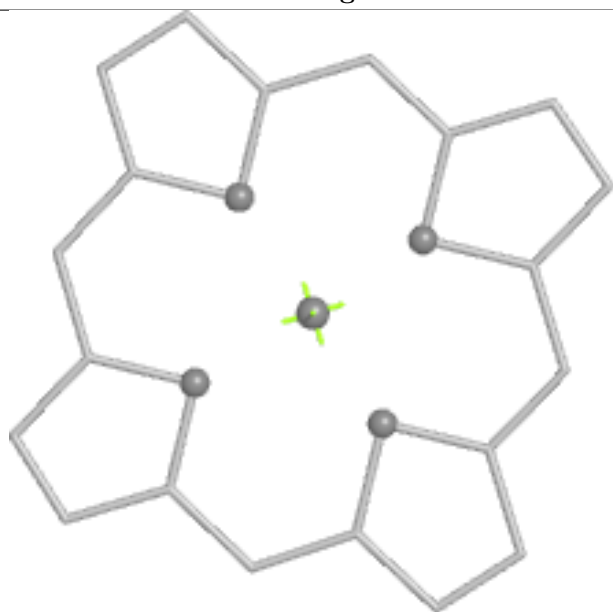
Ligand CLA 8 313



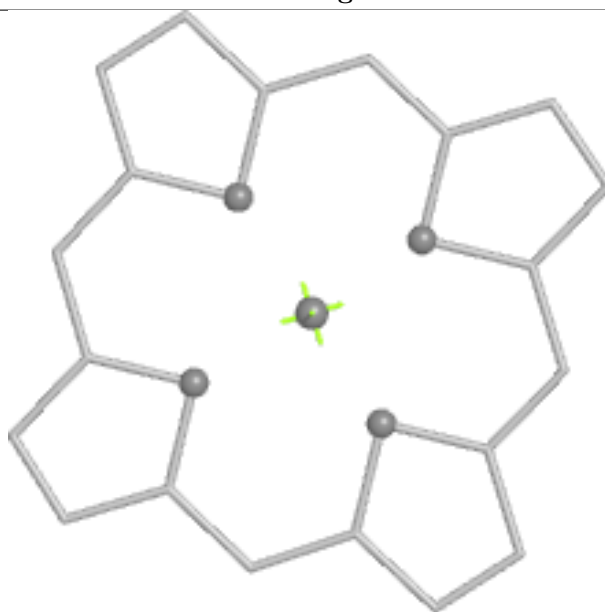
Bond lengths



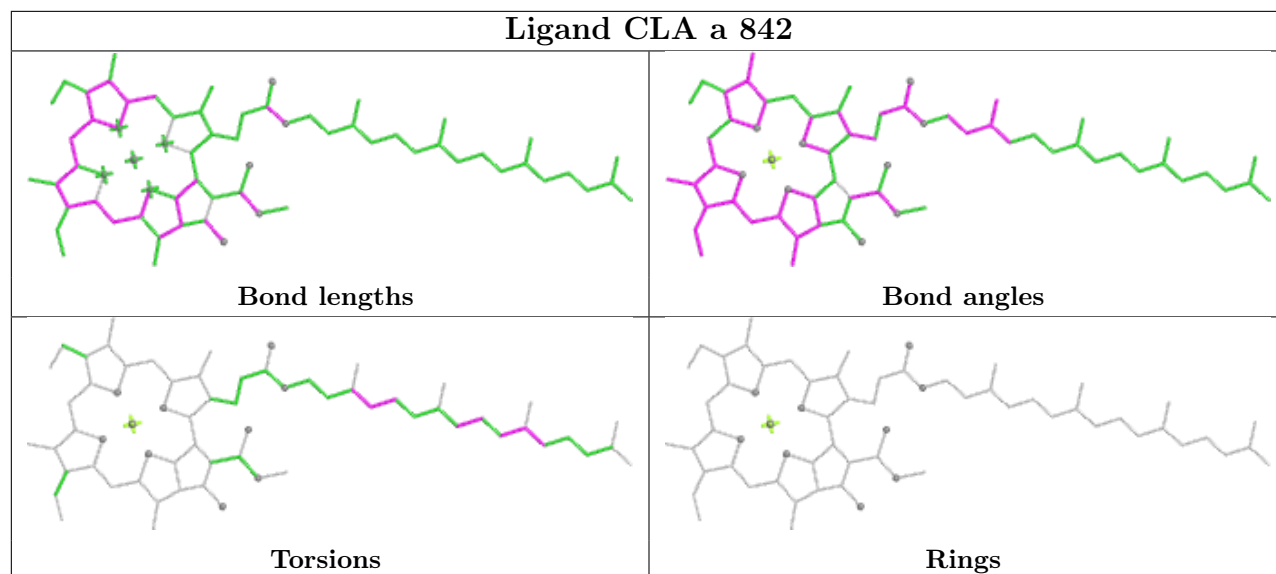
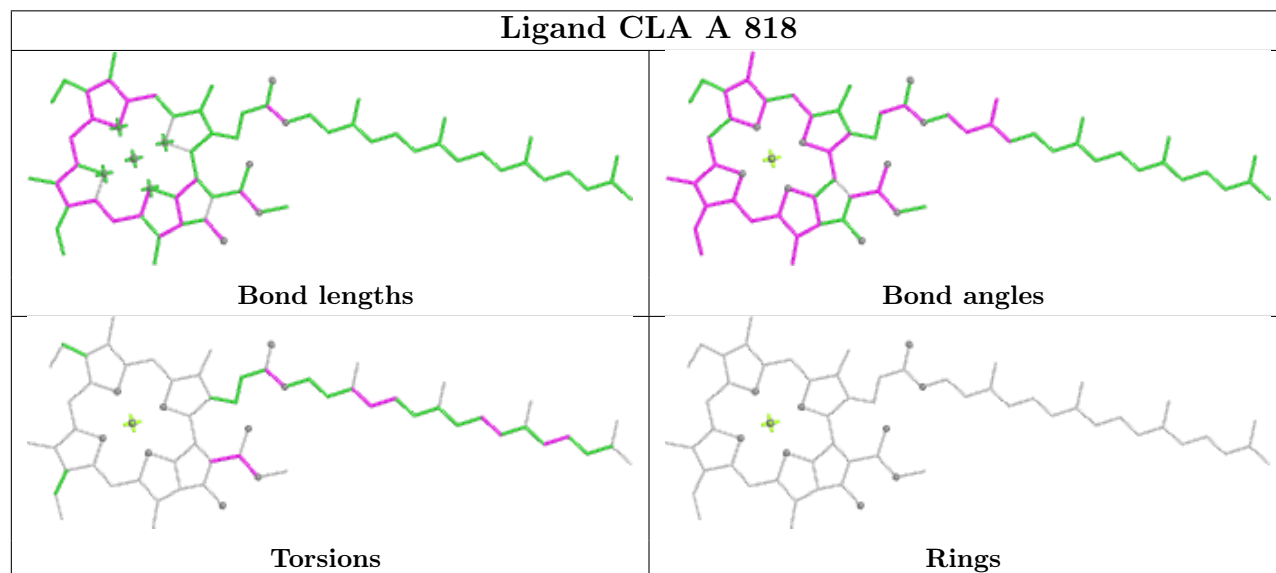
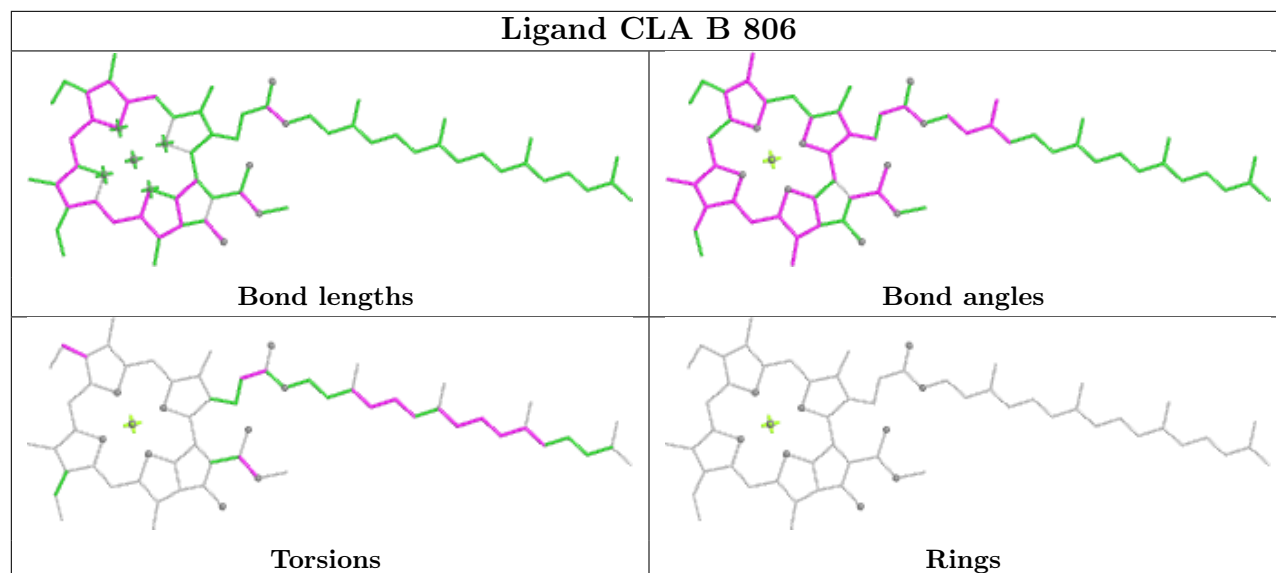
Bond angles

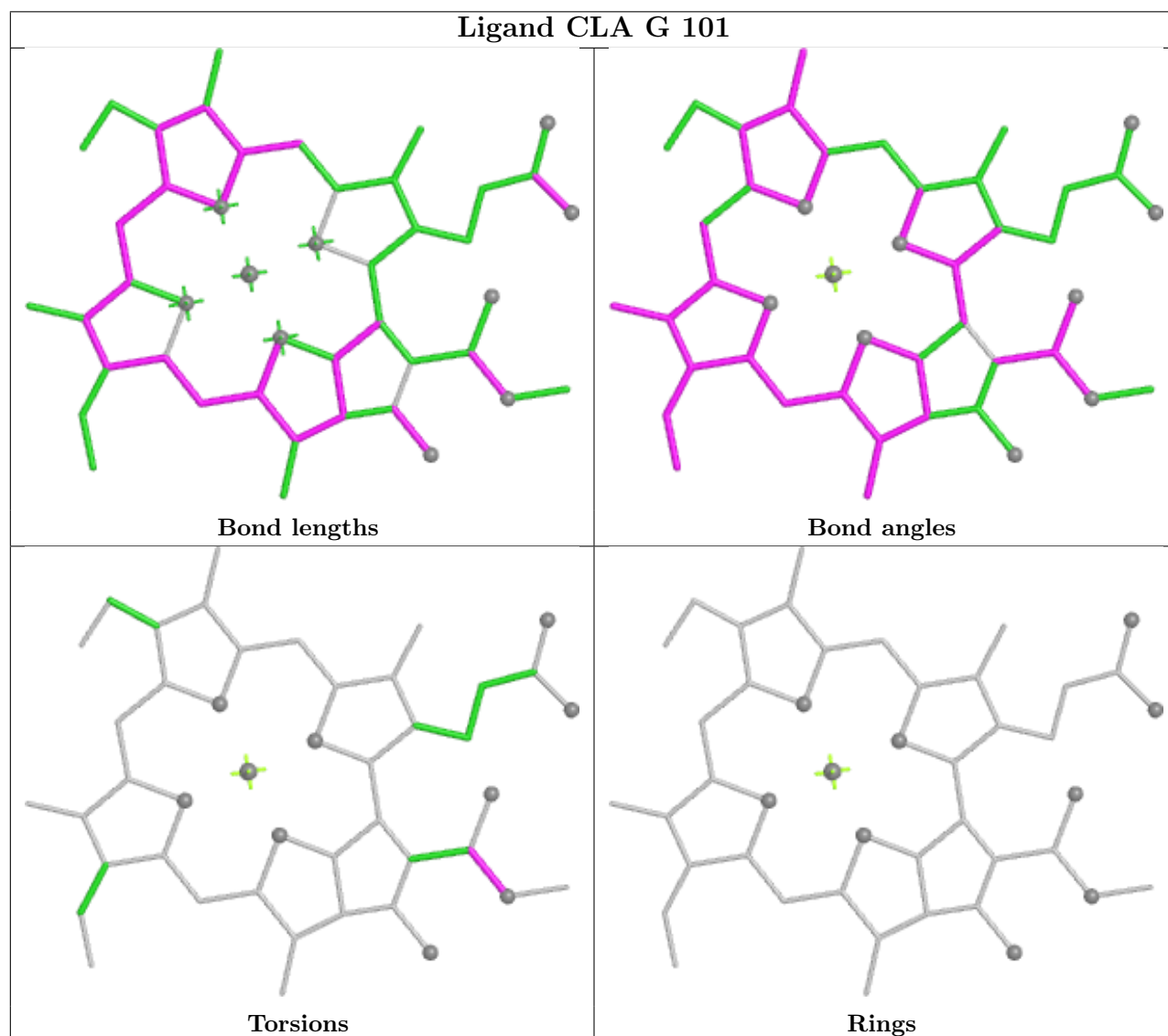
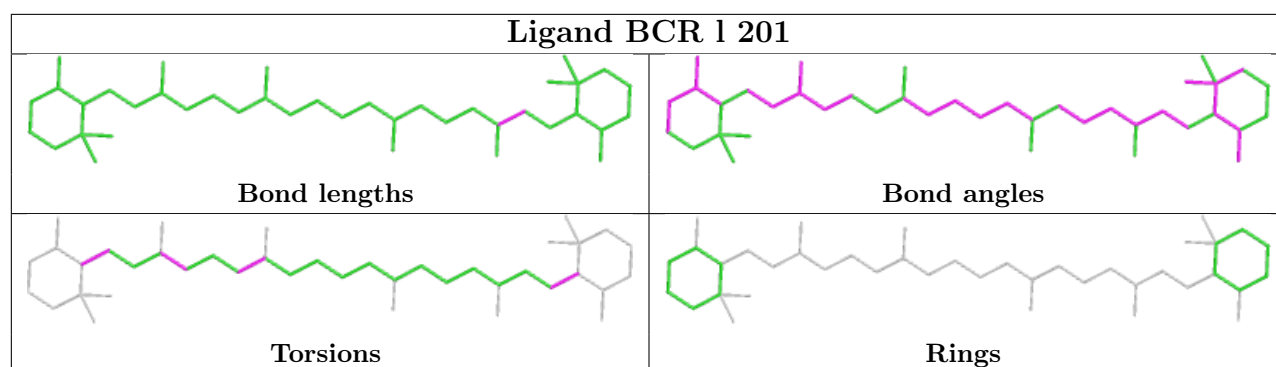


Torsions

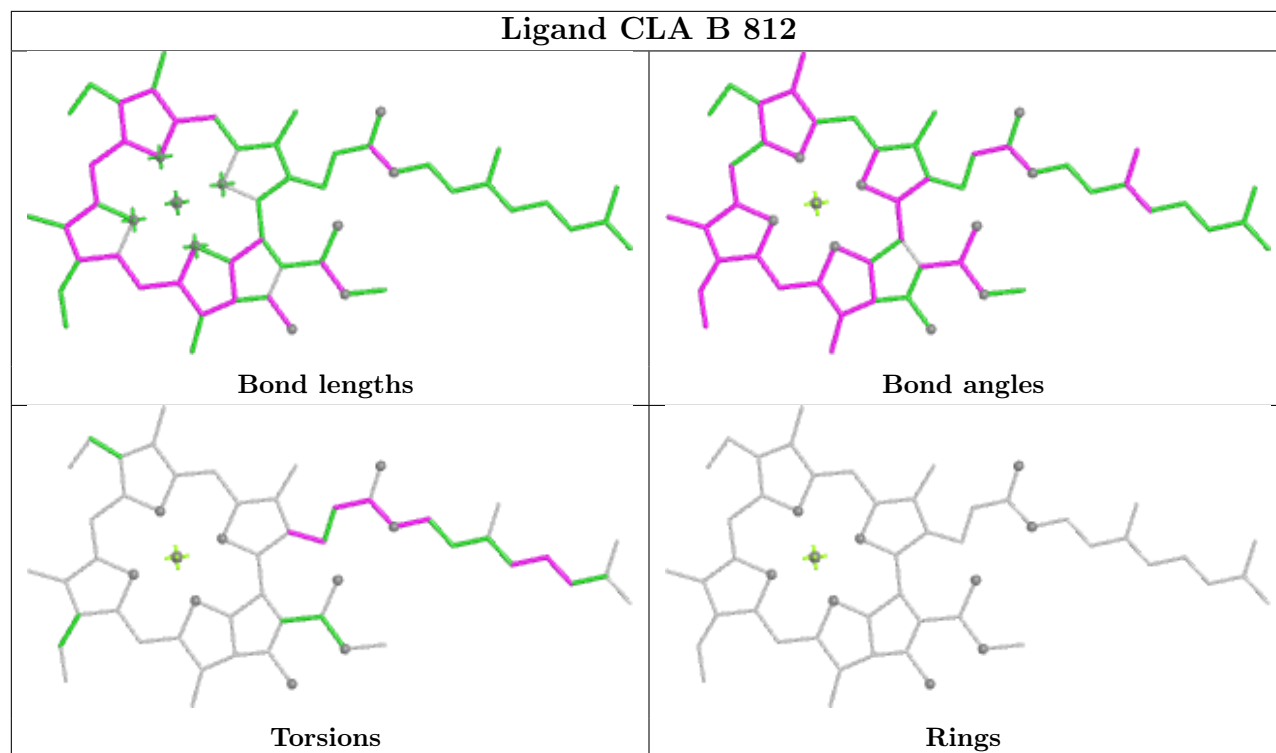


Rings

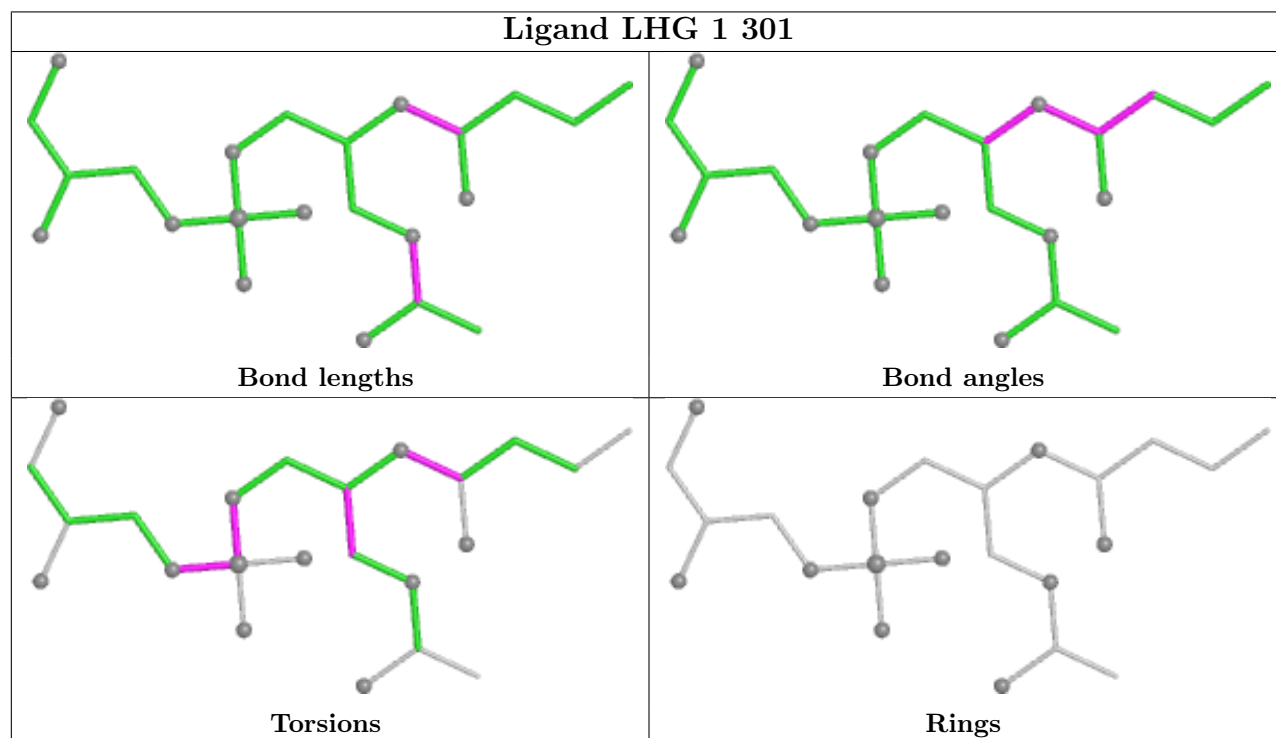
Ligand CLA a 842**Ligand CLA A 818****Ligand CLA B 806**



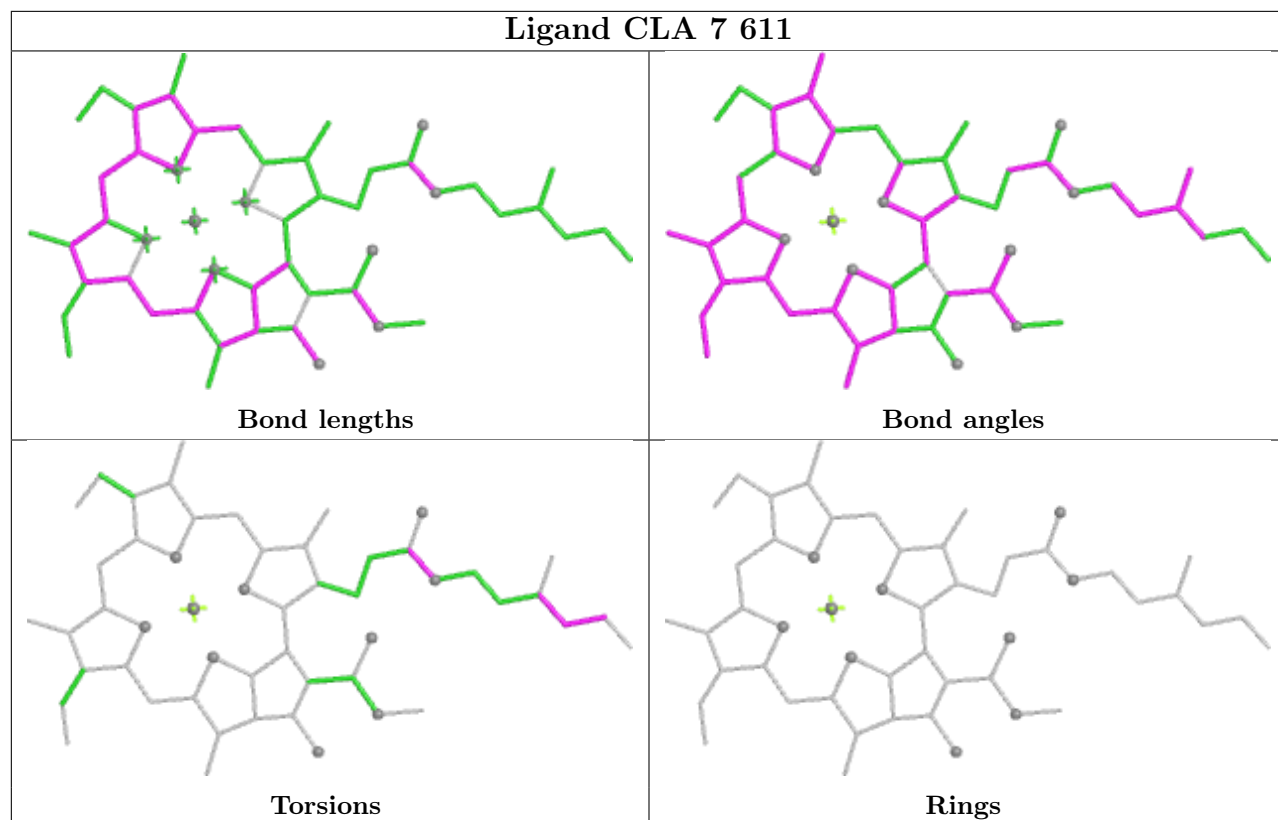
Ligand CLA B 812

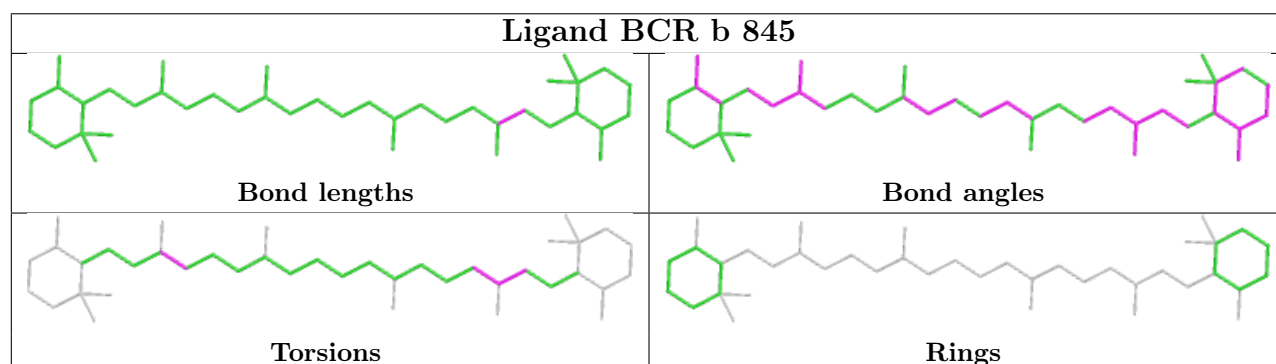
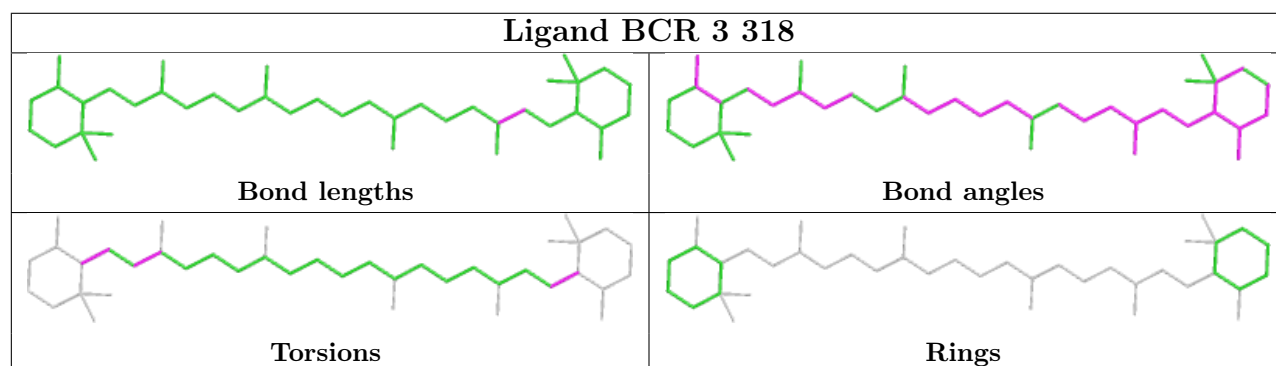
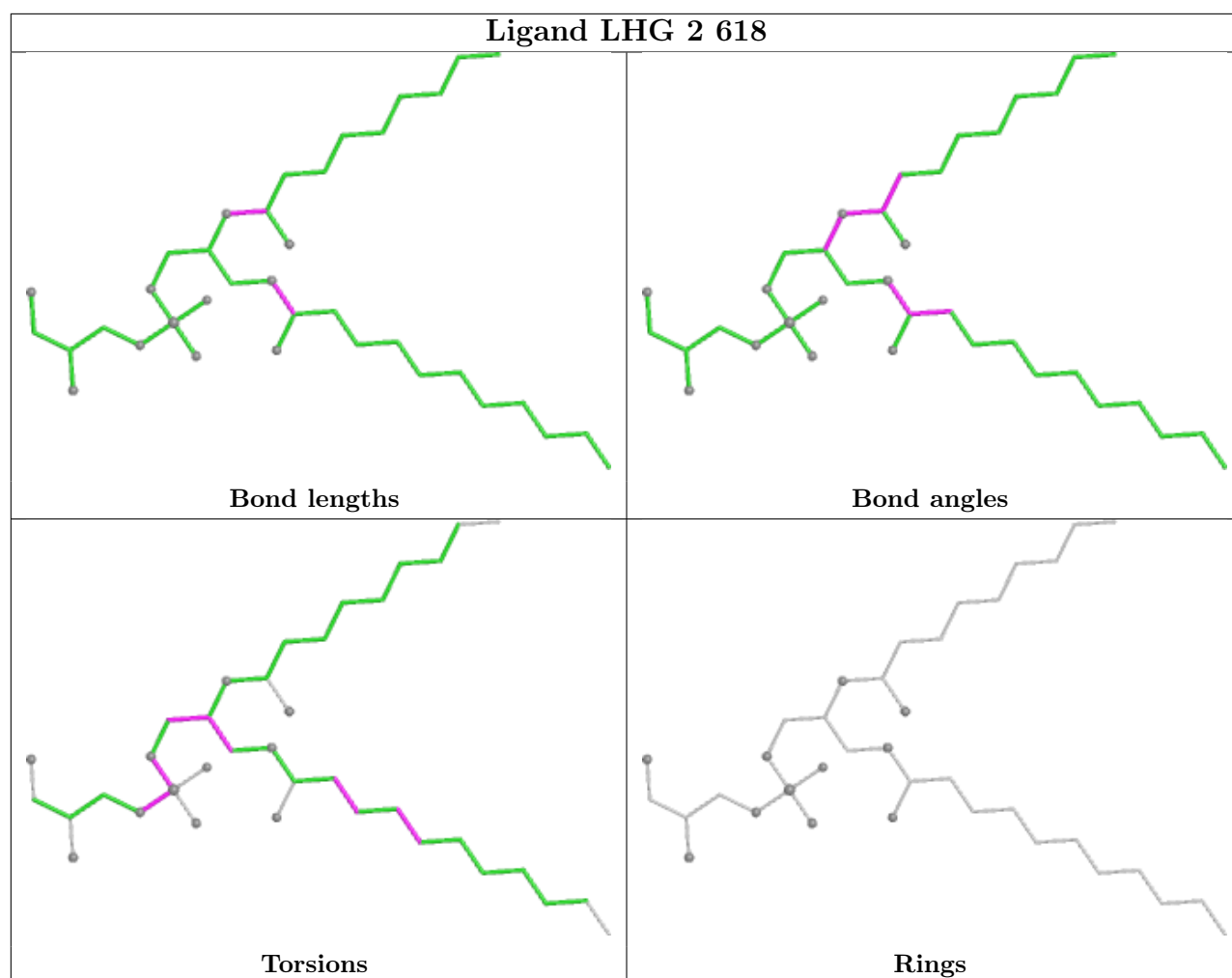


Ligand LHG 1 301

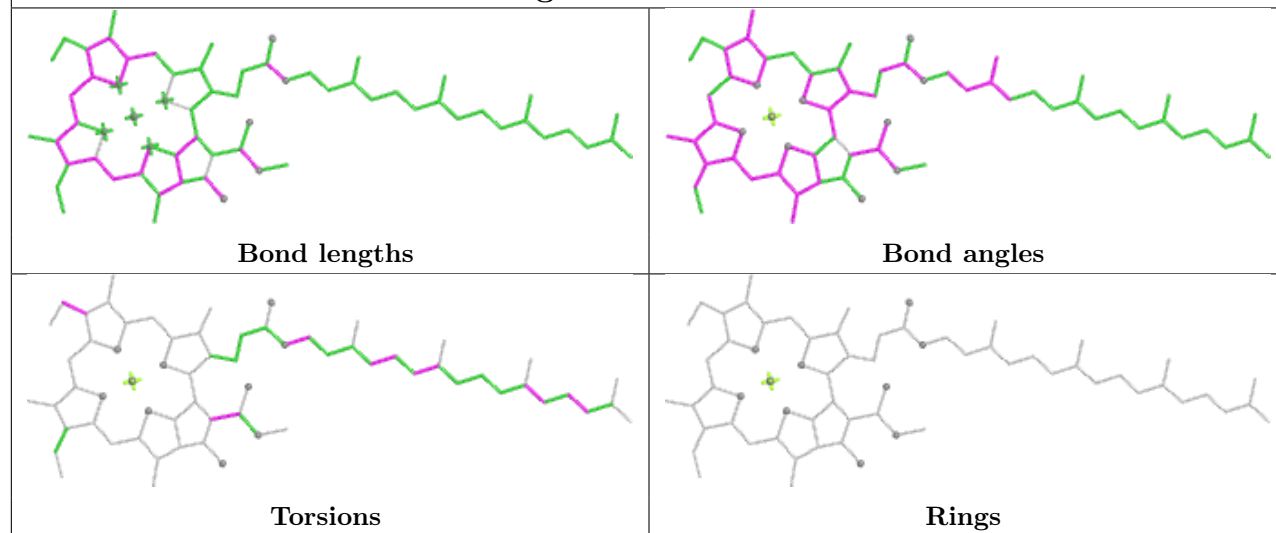


Ligand CLA 7 611

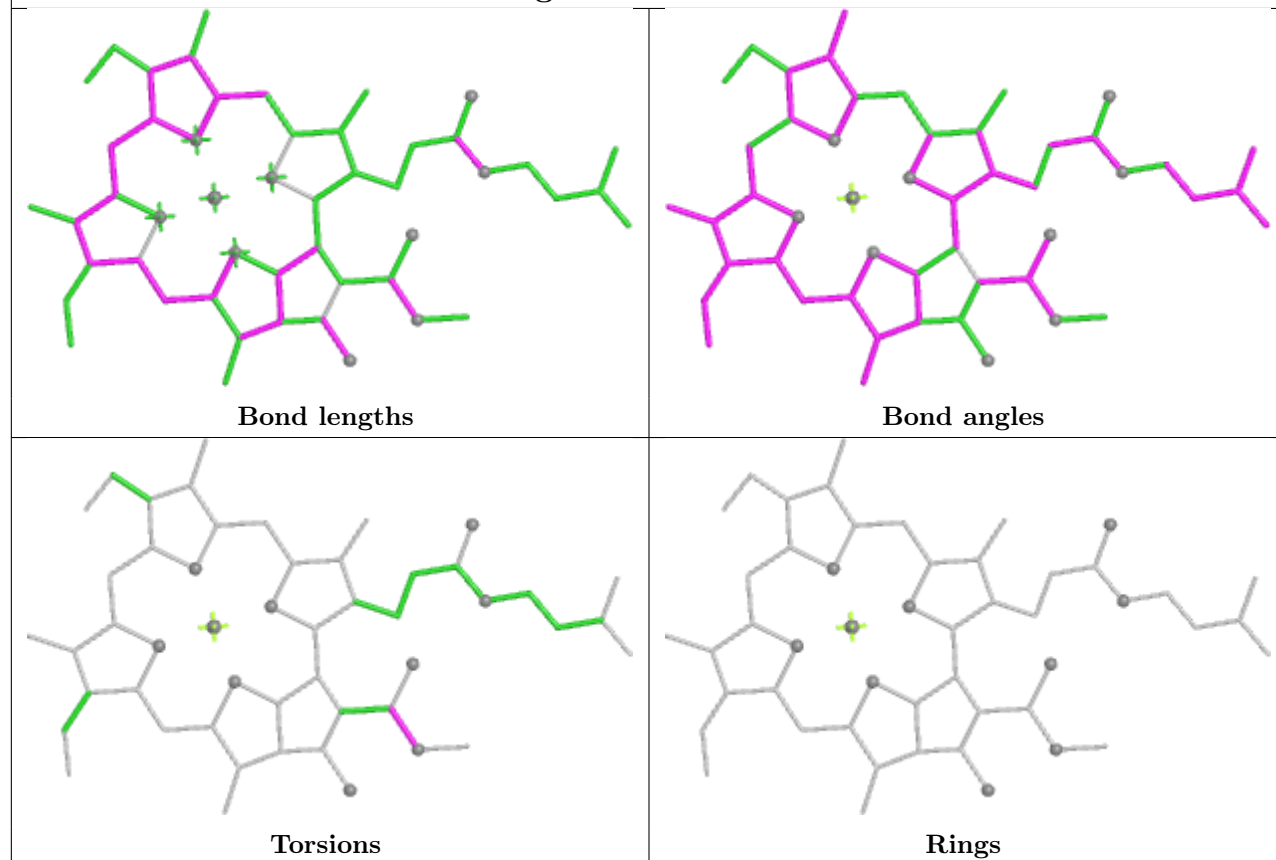




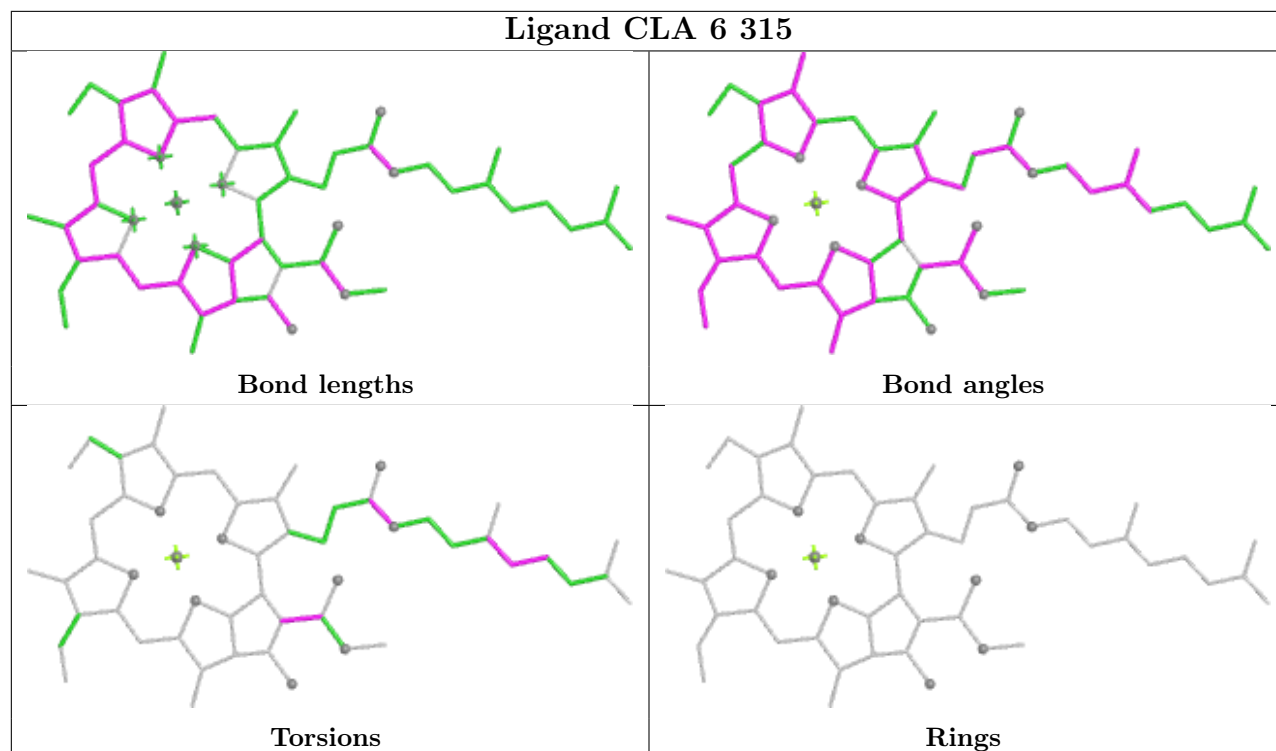
Ligand CLA a 827



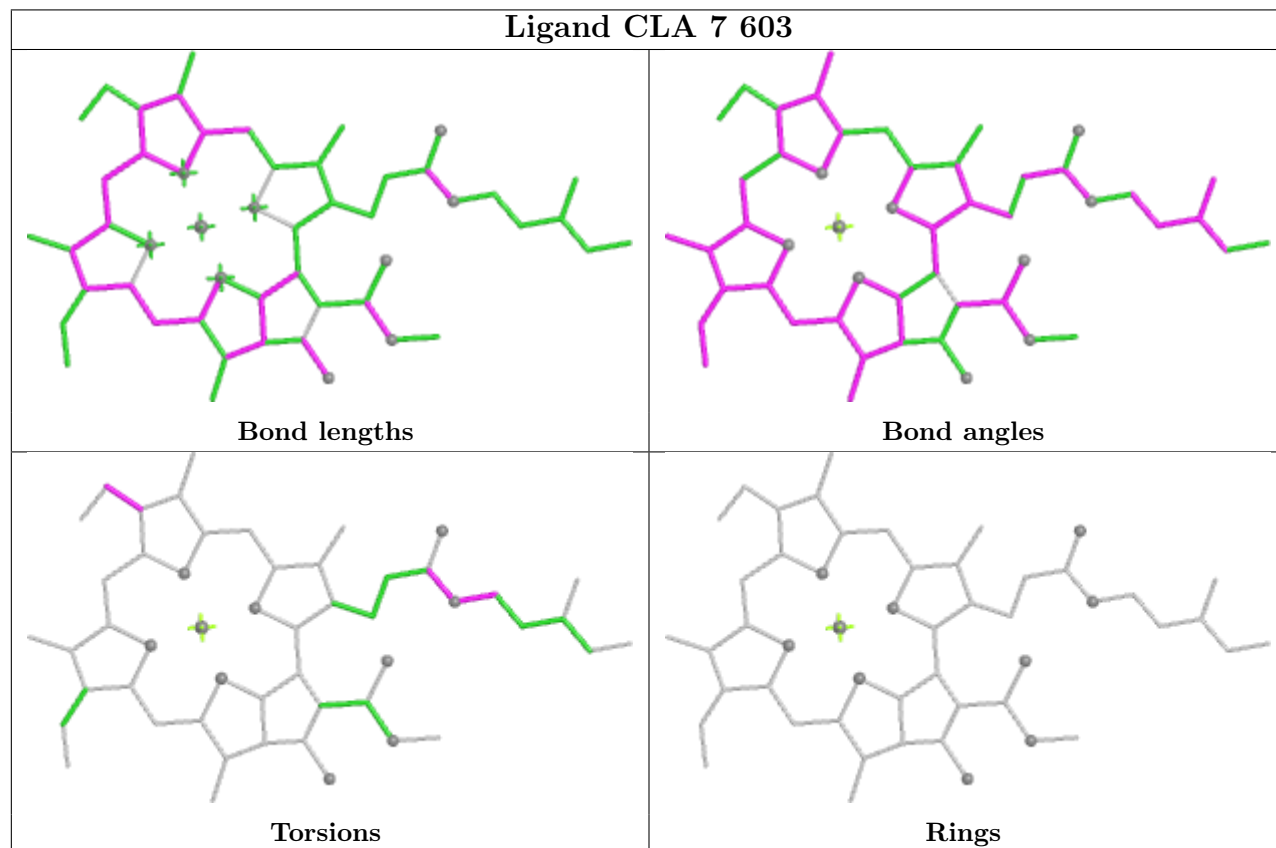
Ligand CLA b 820

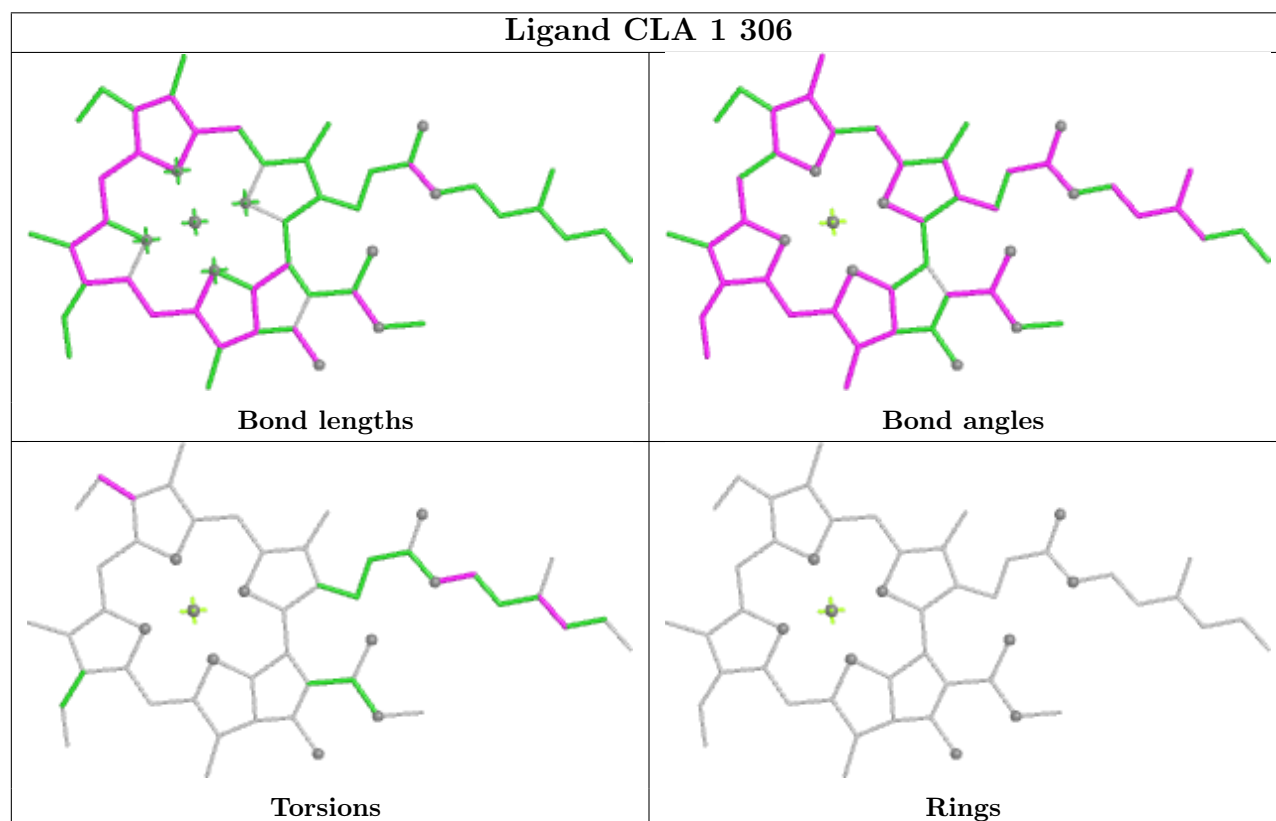
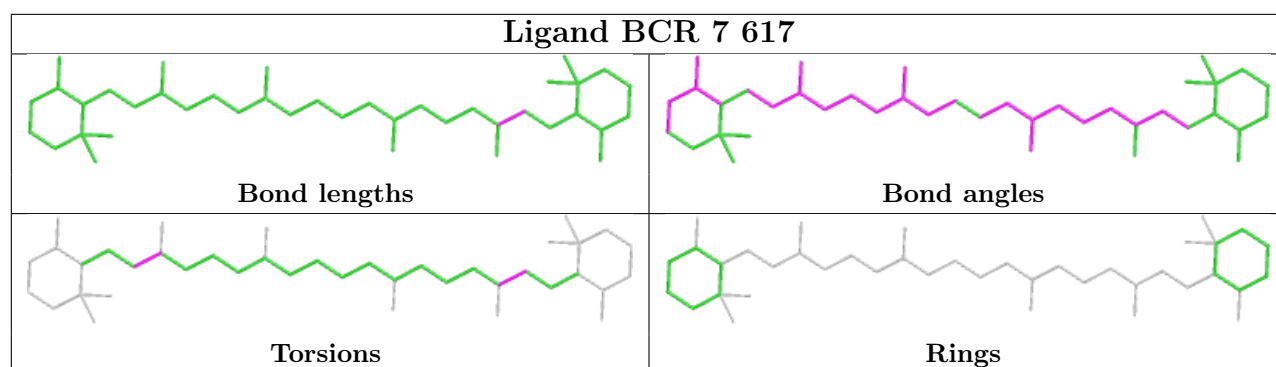


Ligand CLA 6 315

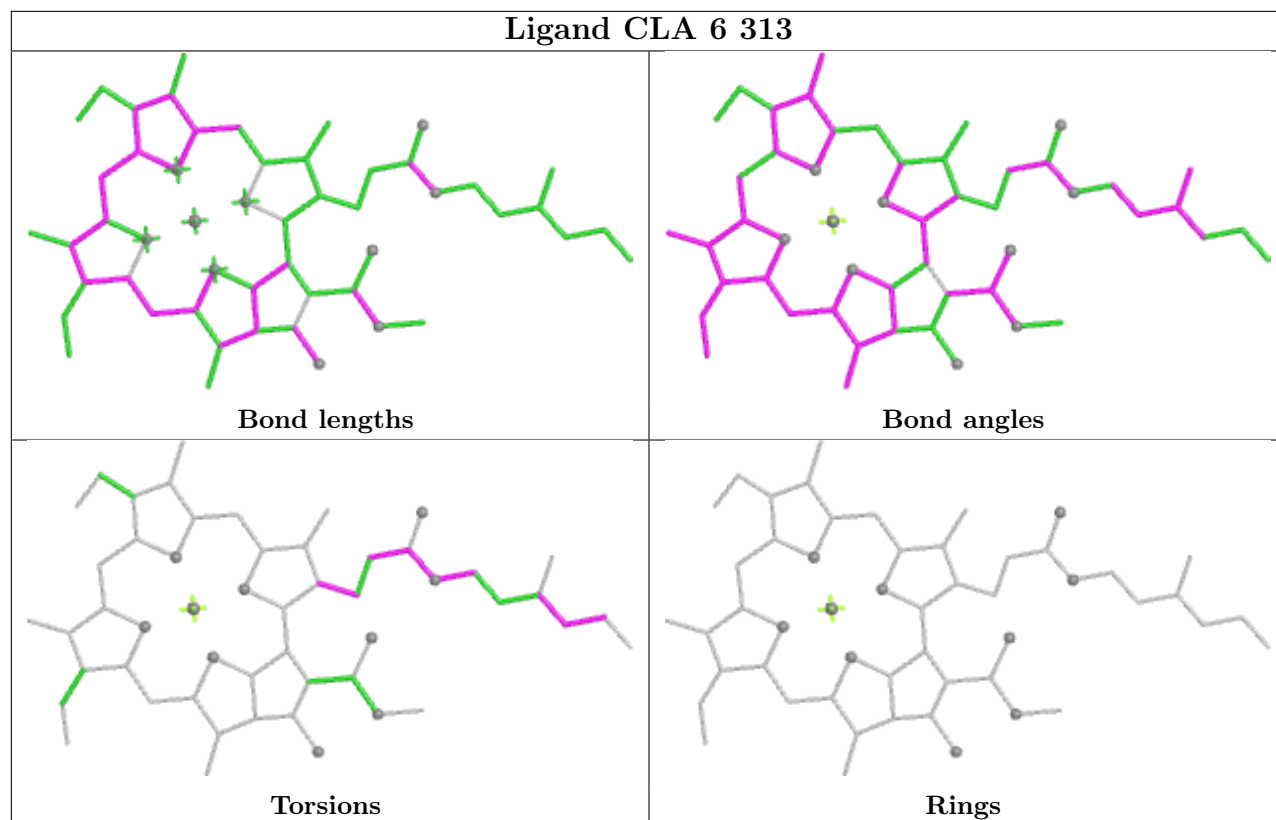


Ligand CLA 7 603

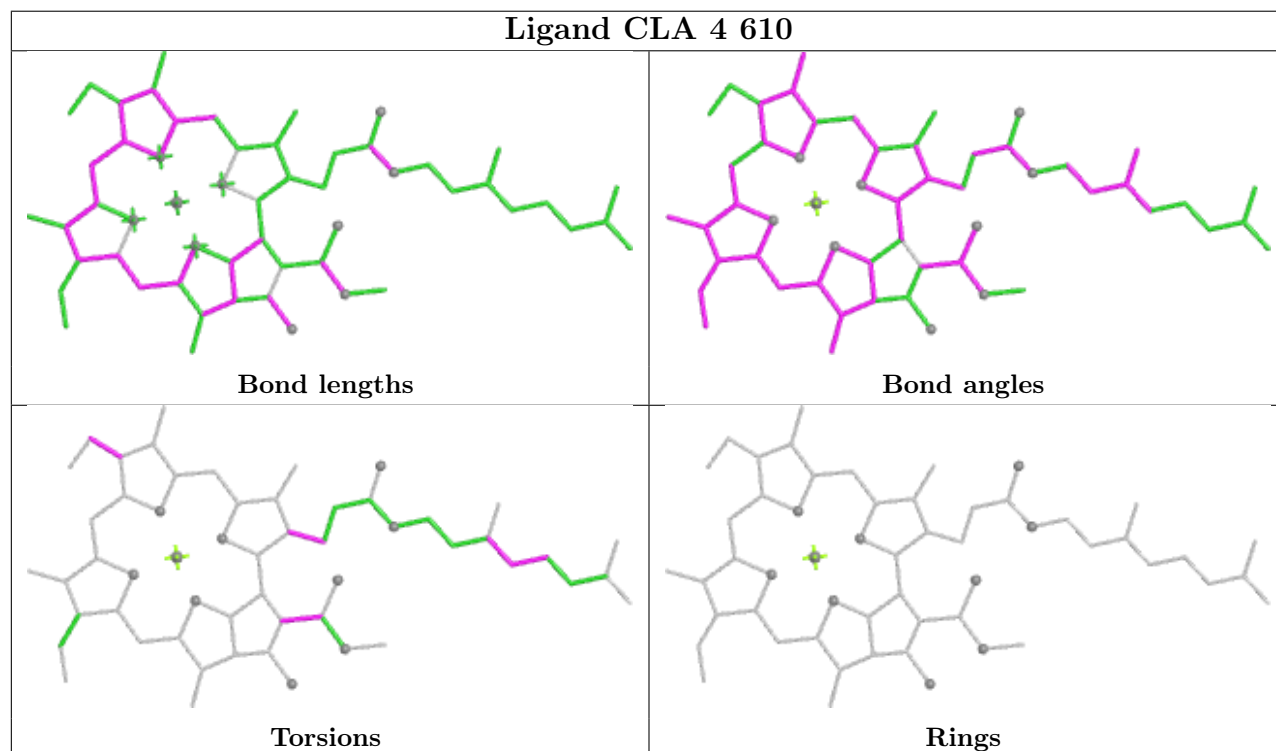


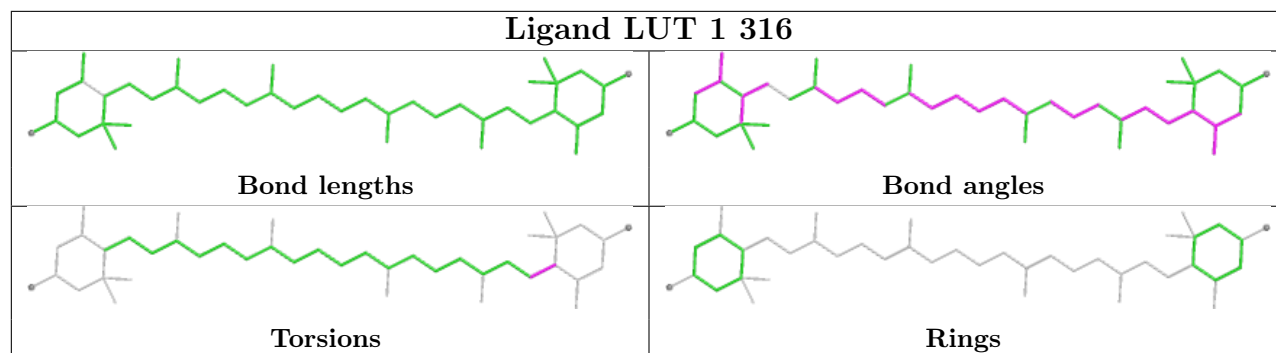
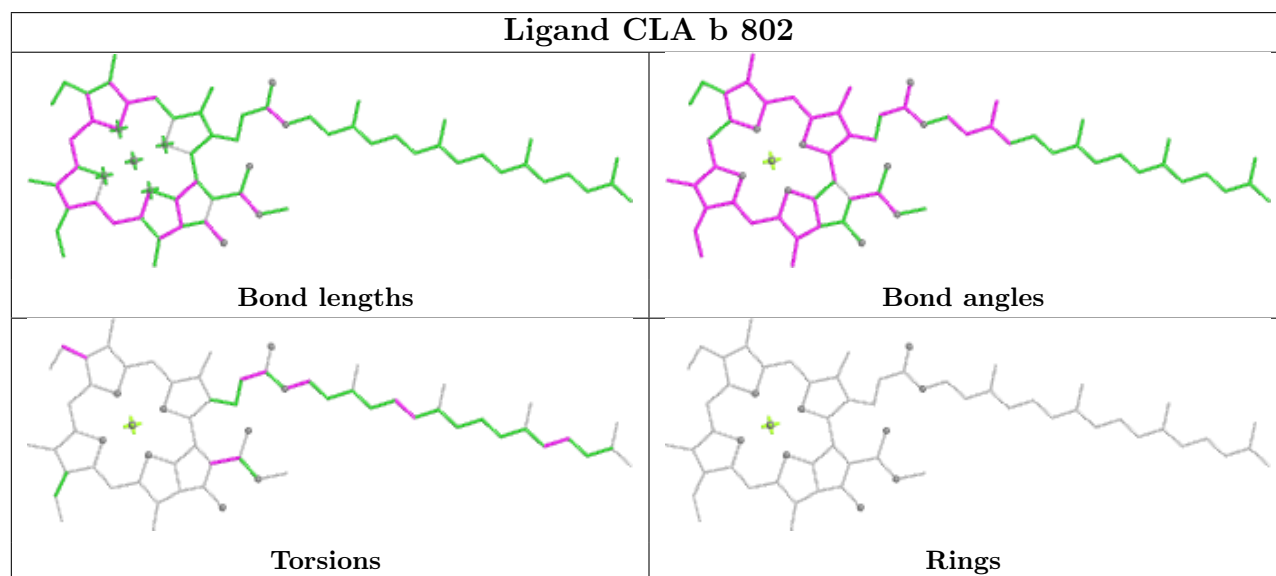


Ligand CLA 6 313

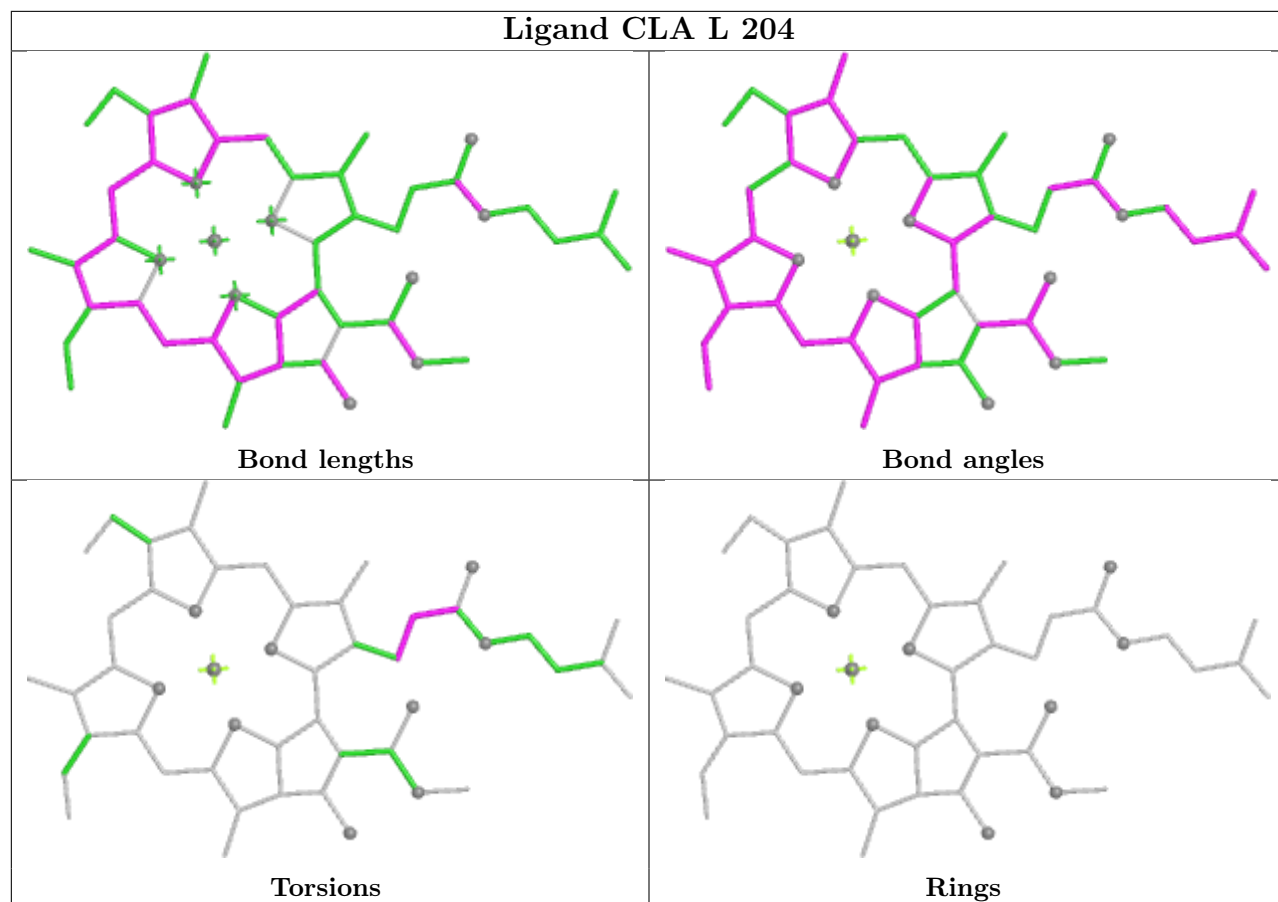


Ligand CLA 4 610

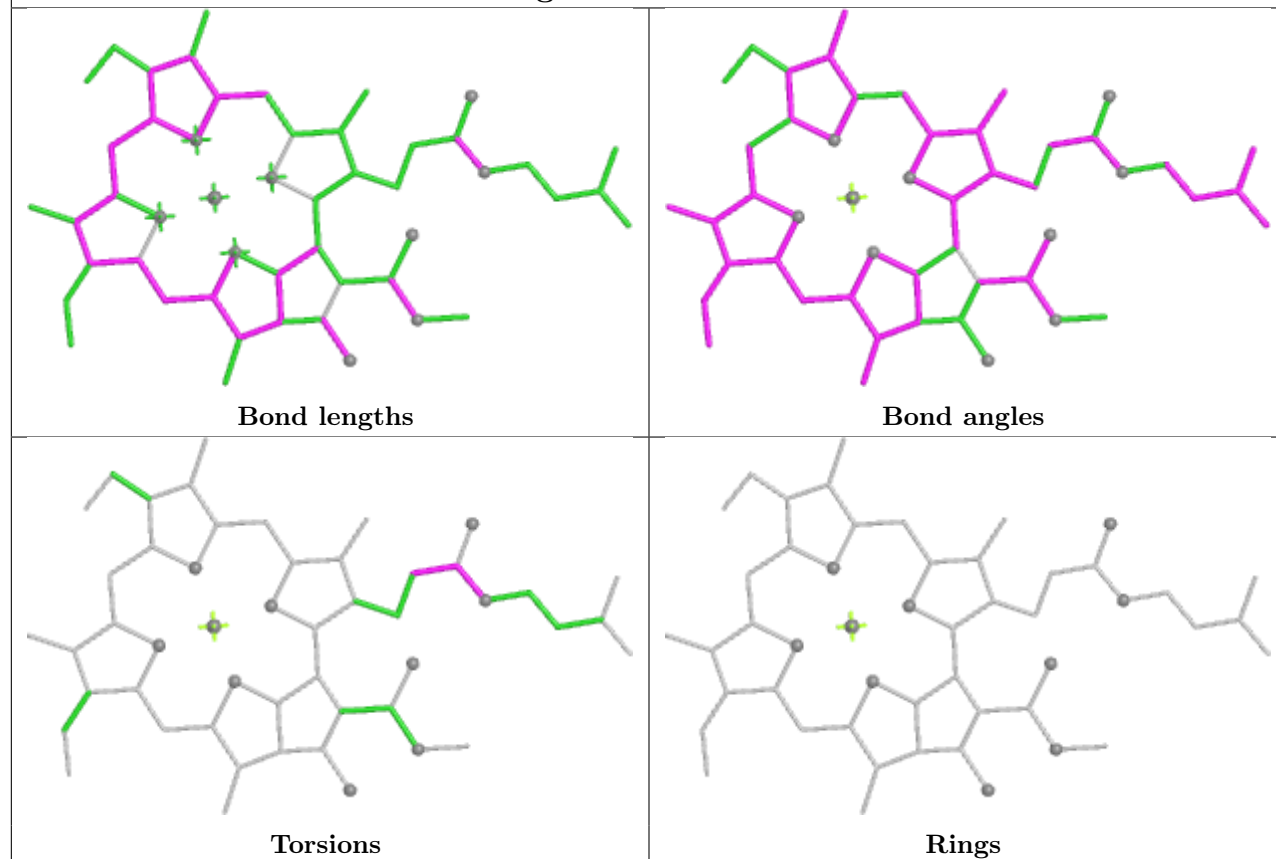


Ligand LUT 1 316**Ligand CLA b 802**

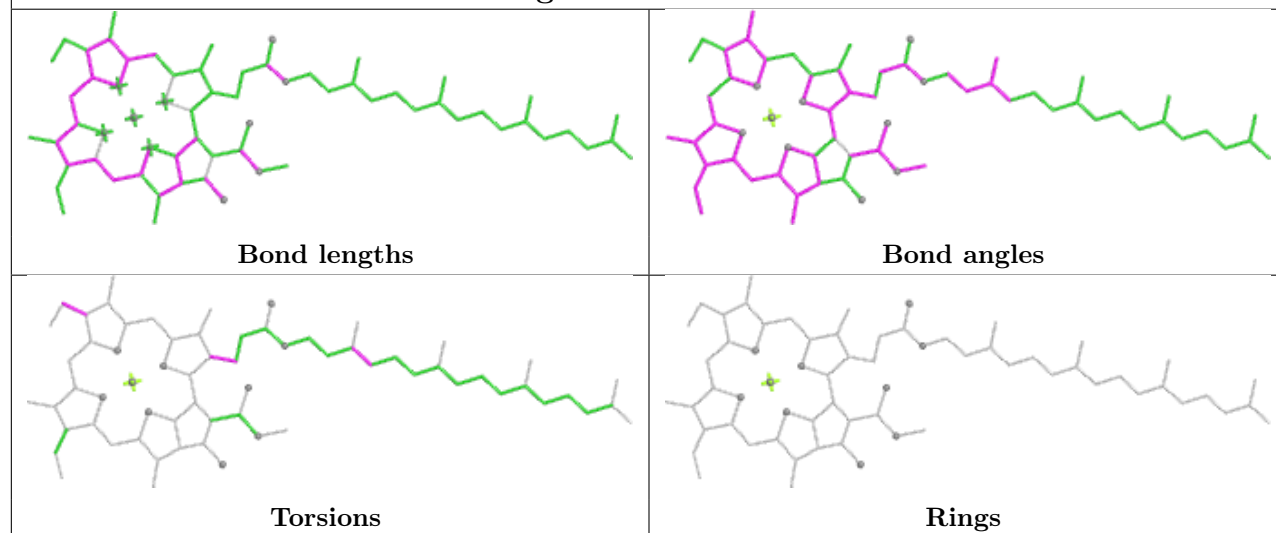
Ligand CLA L 204



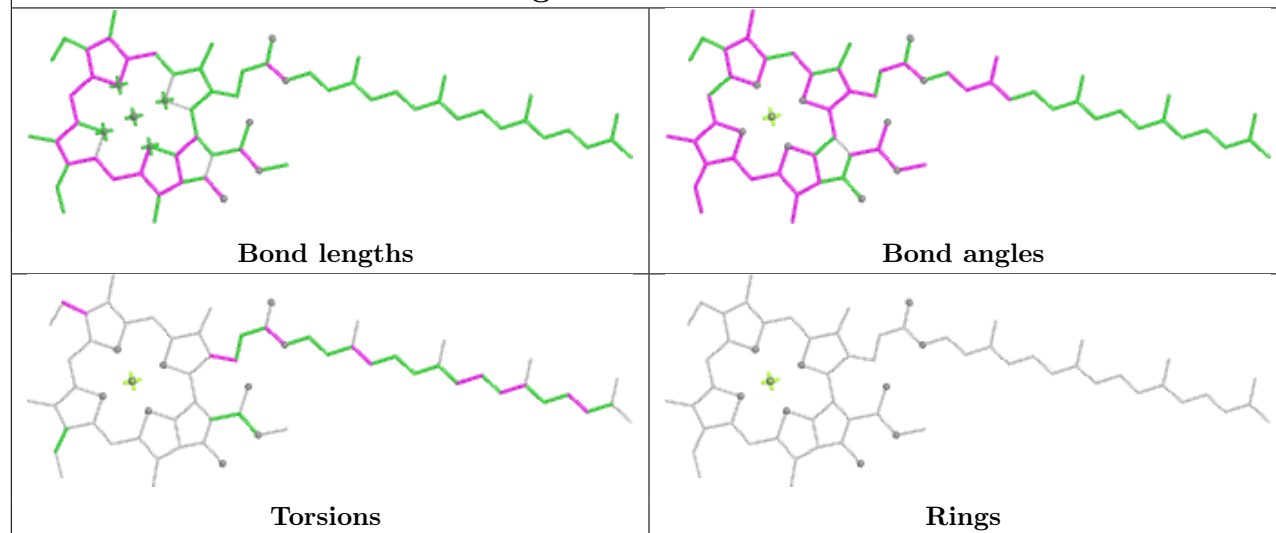
Ligand CLA 2 608



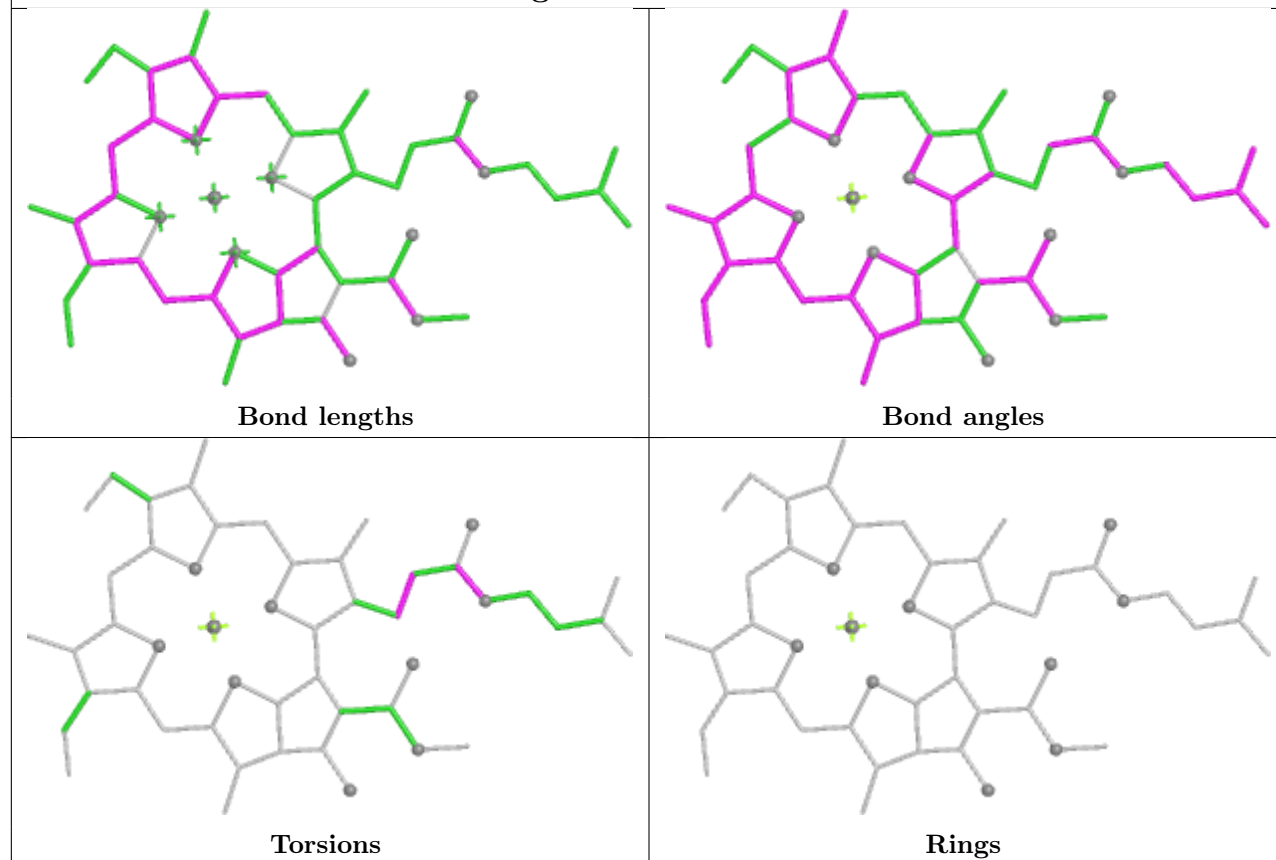
Ligand CLA a 822



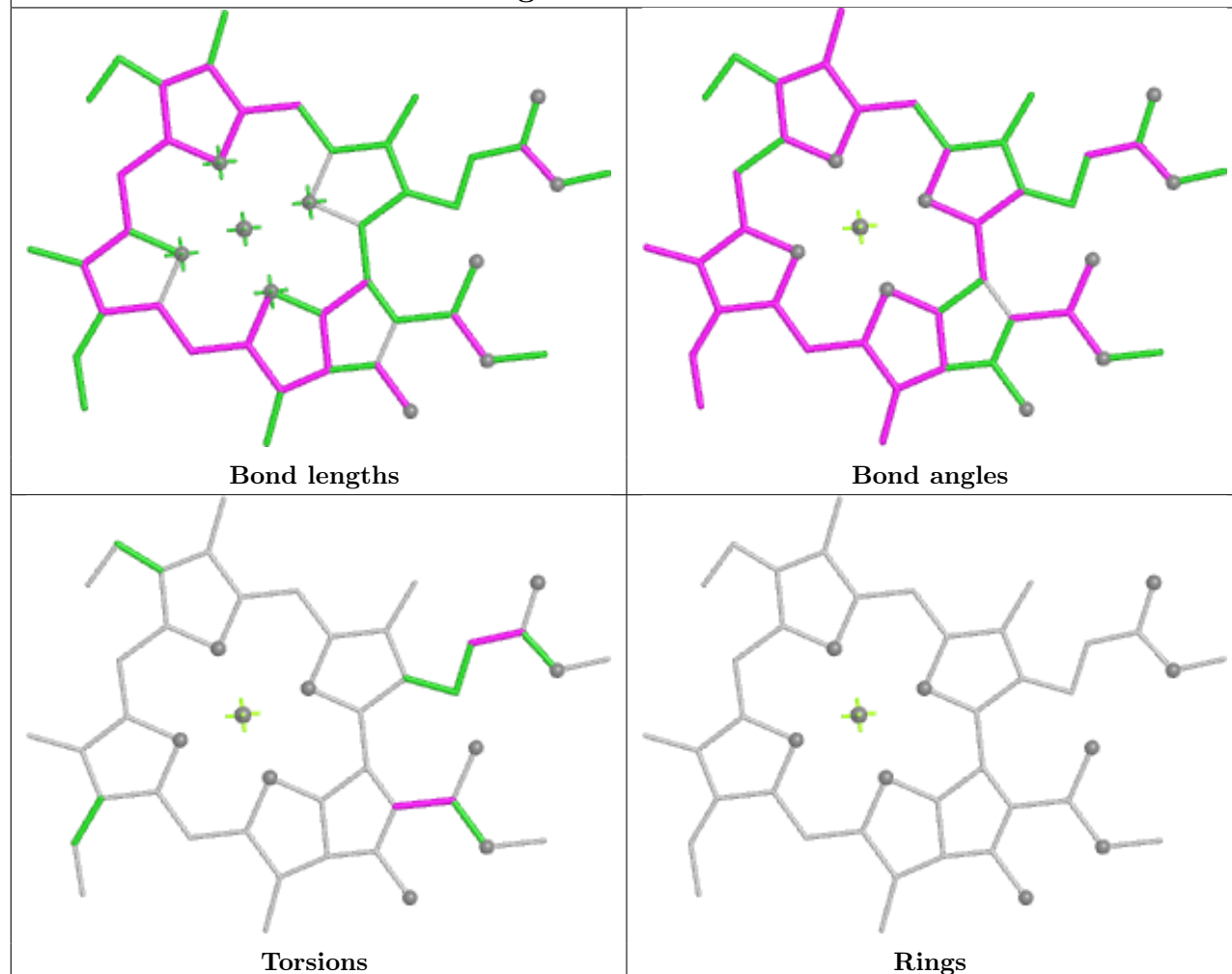
Ligand CLA B 819



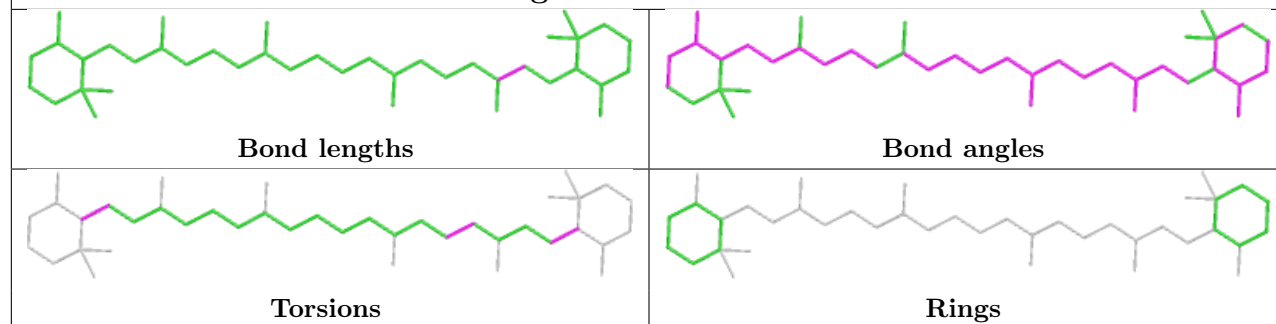
Ligand CLA A 816

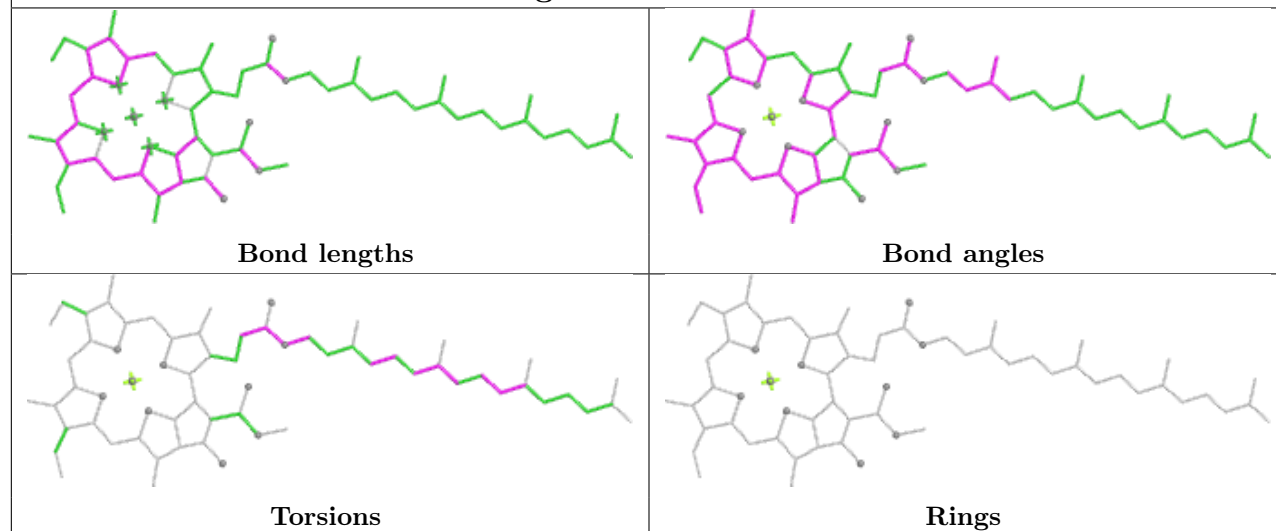
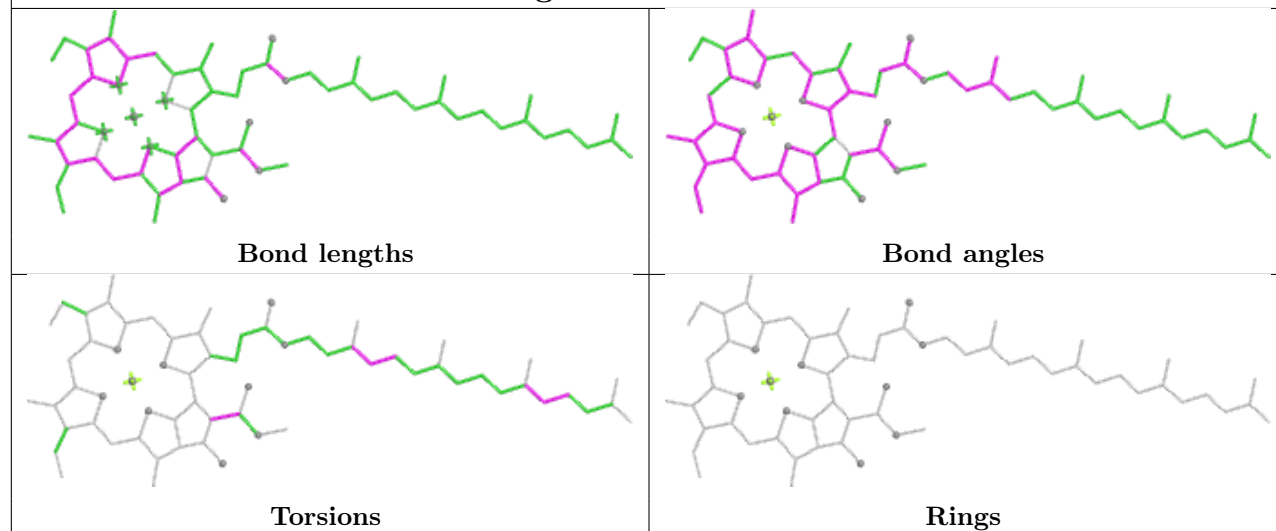
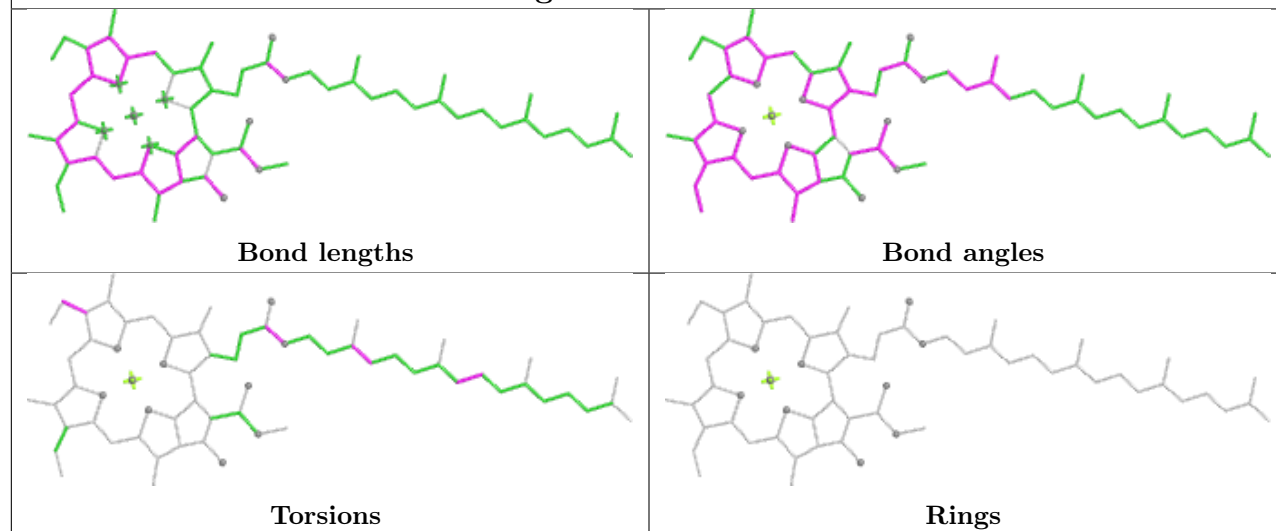


Ligand CLA 9 603

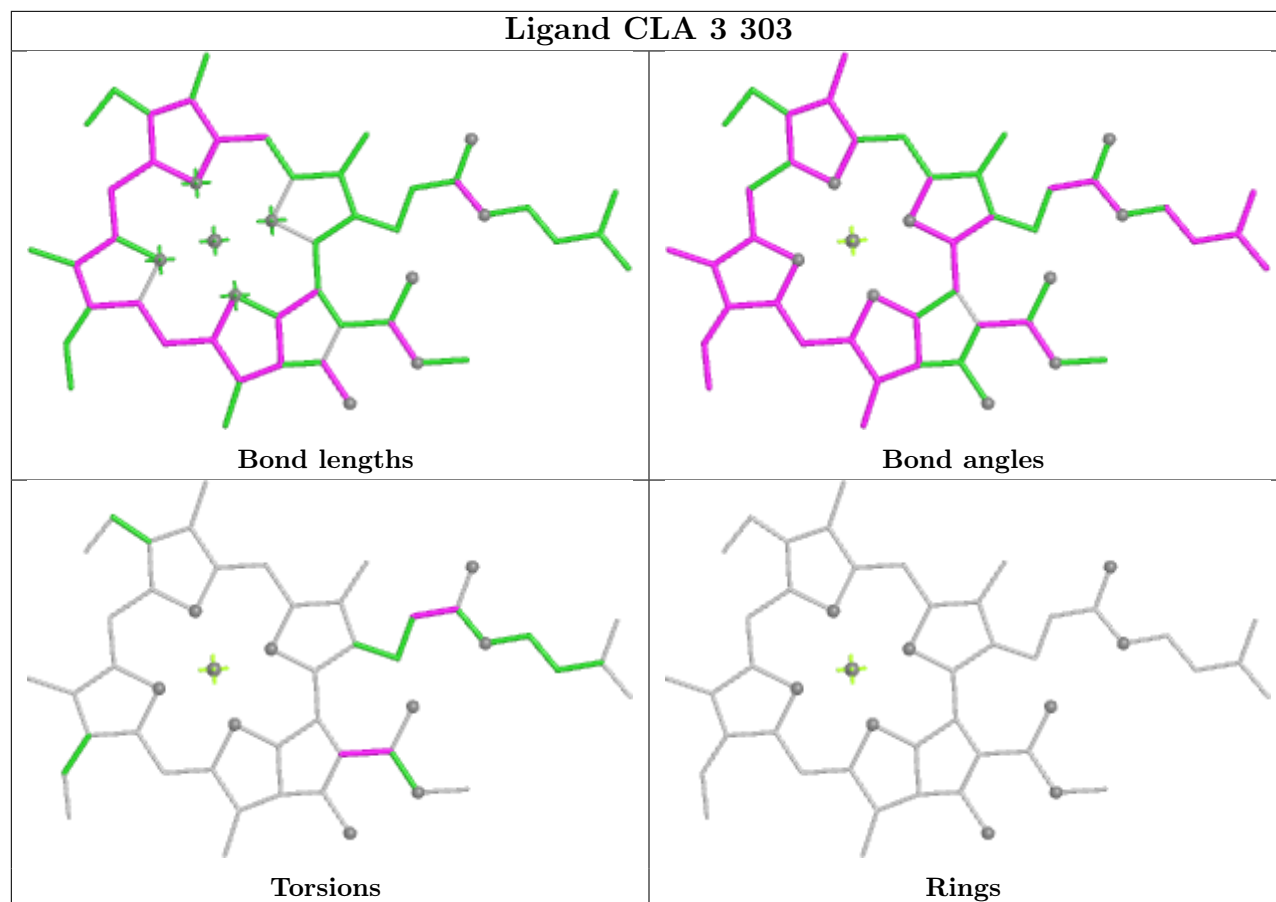


Ligand BCR B 846

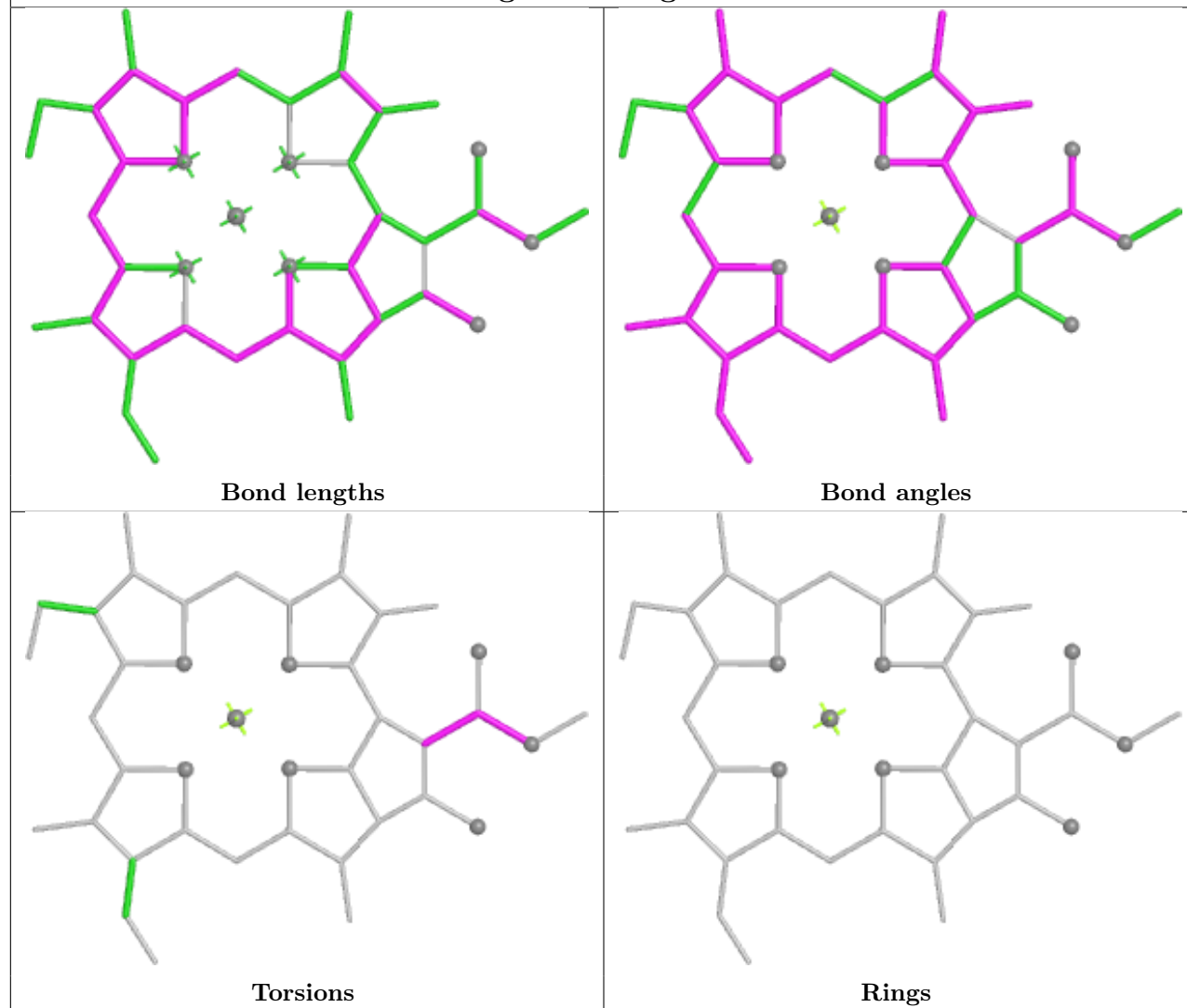


Ligand CLA b 834**Ligand CLA b 808****Ligand CLA b 819**

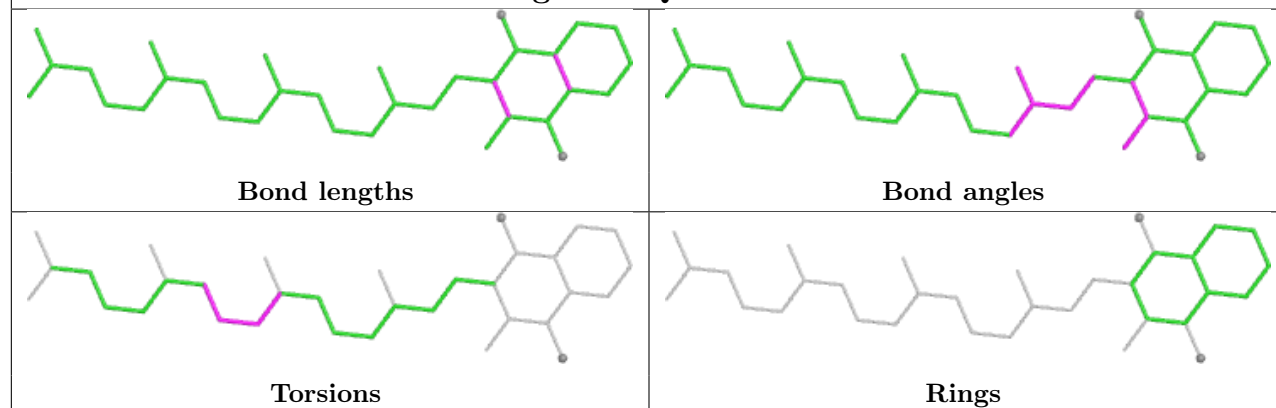
Ligand CLA 3 303



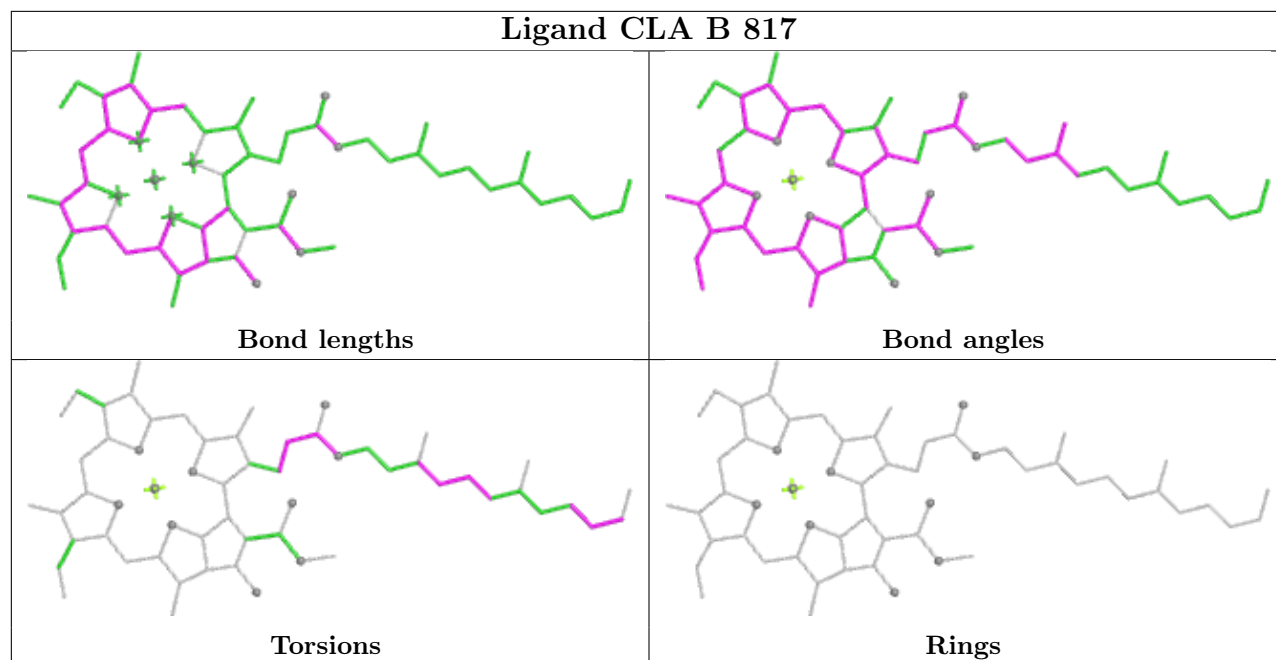
Ligand CLA g 101



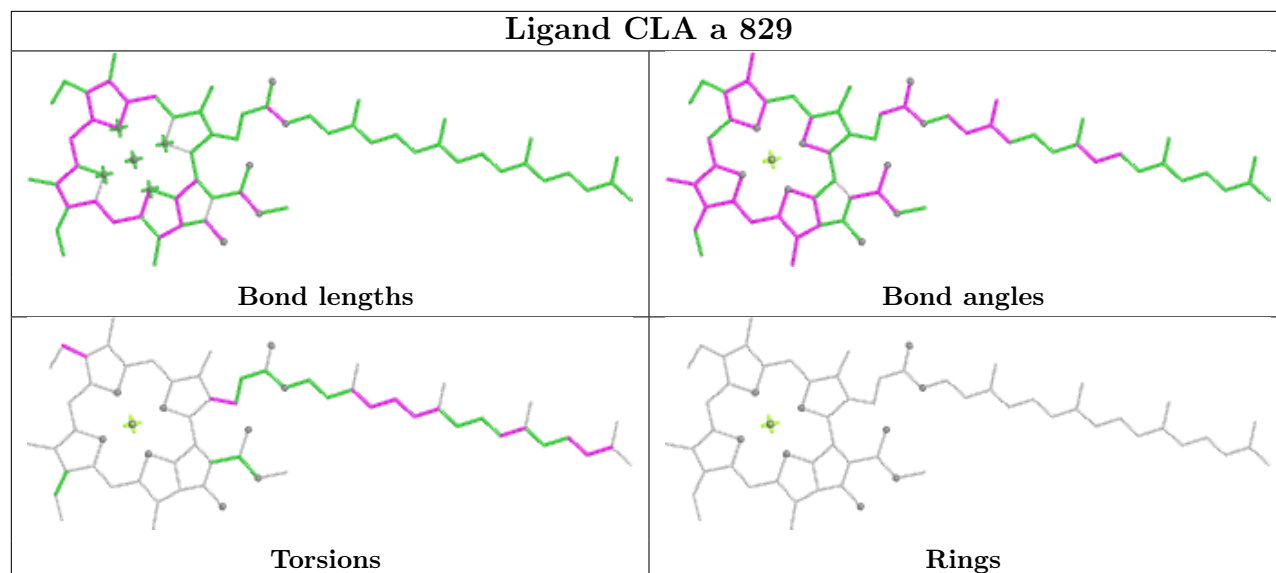
Ligand PQN b 842



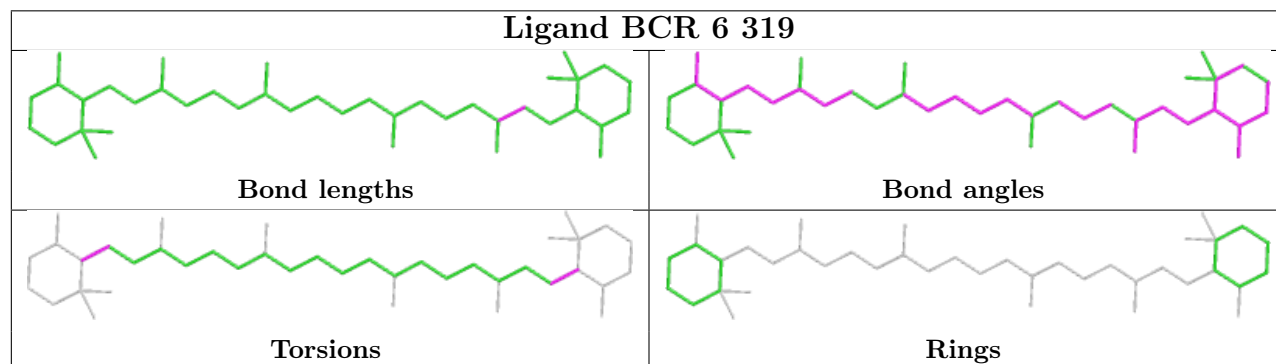
Ligand CLA B 817

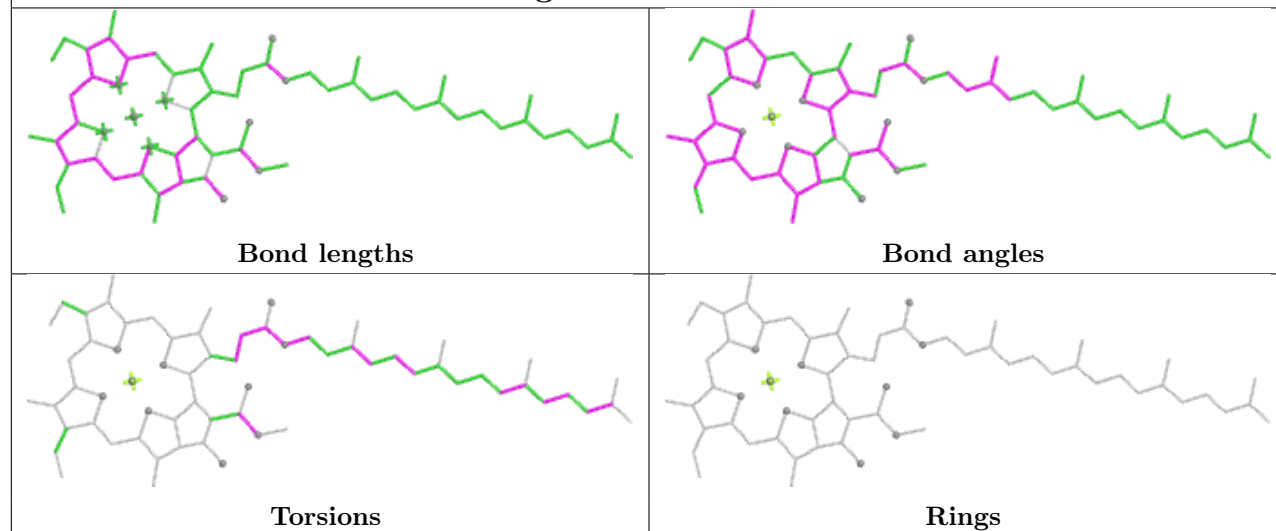
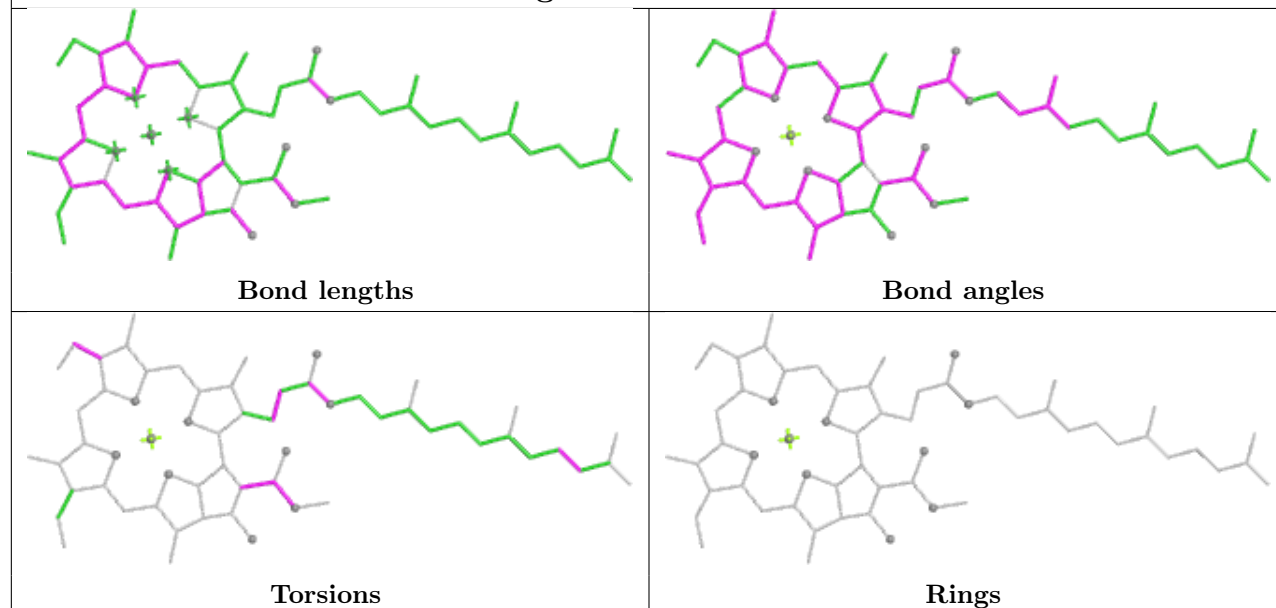


Ligand CLA a 829

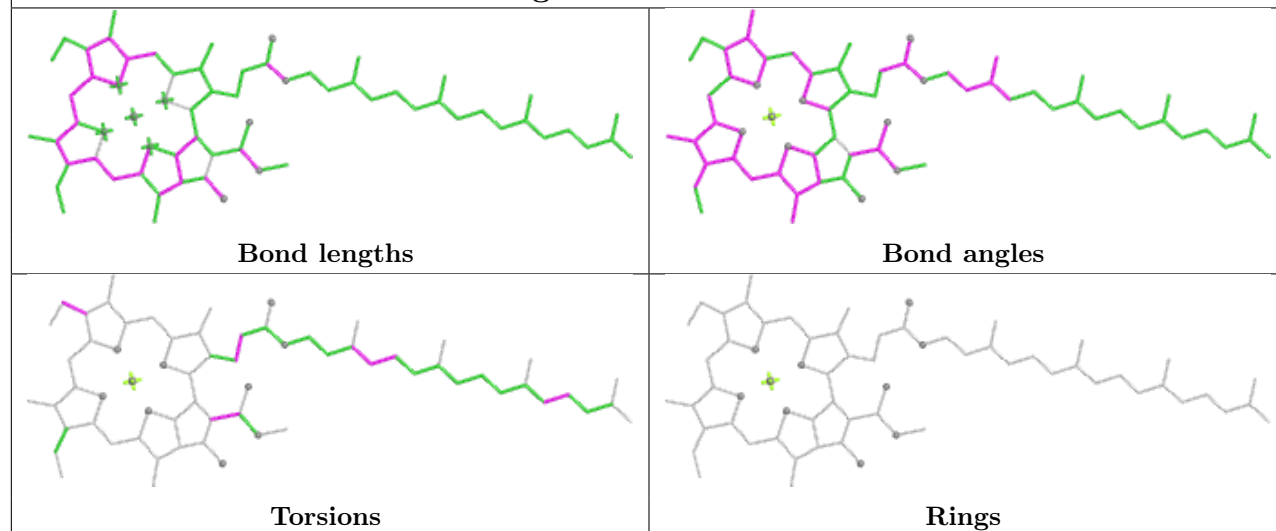


Ligand BCR 6 319

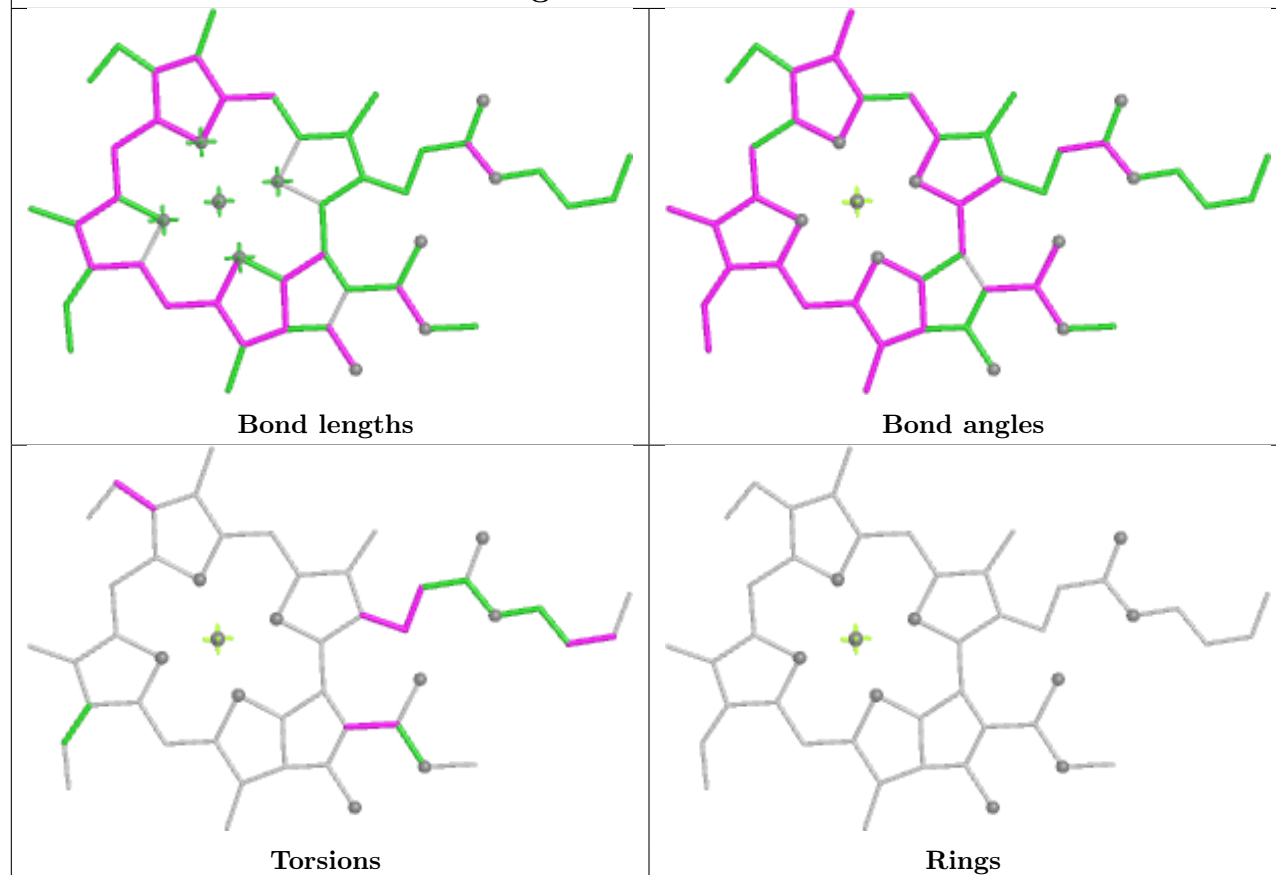


Ligand CLA b 810**Ligand CLA 4 602**

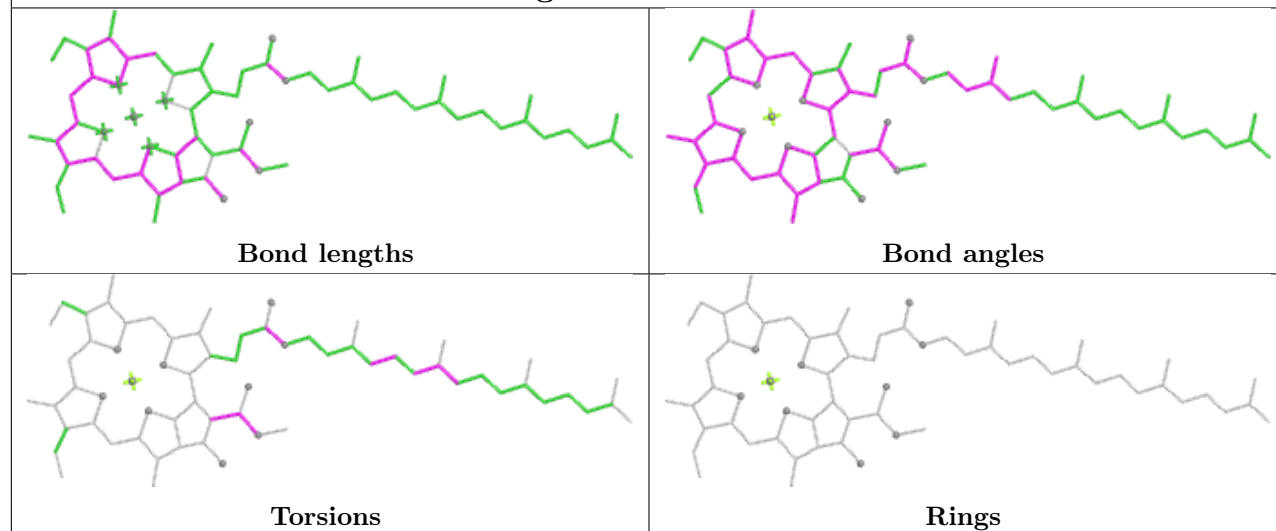
Ligand CLA B 824



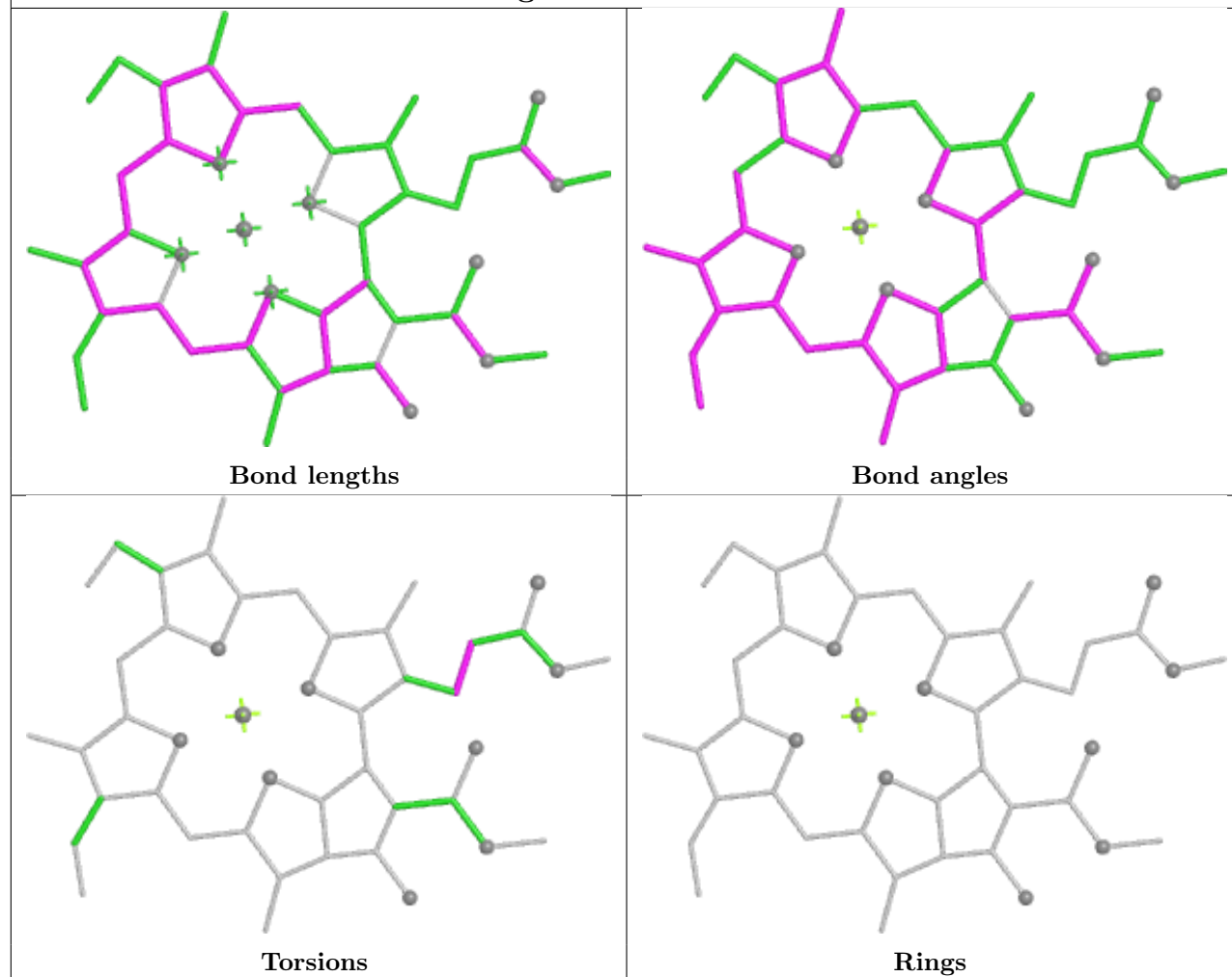
Ligand CLA A 823



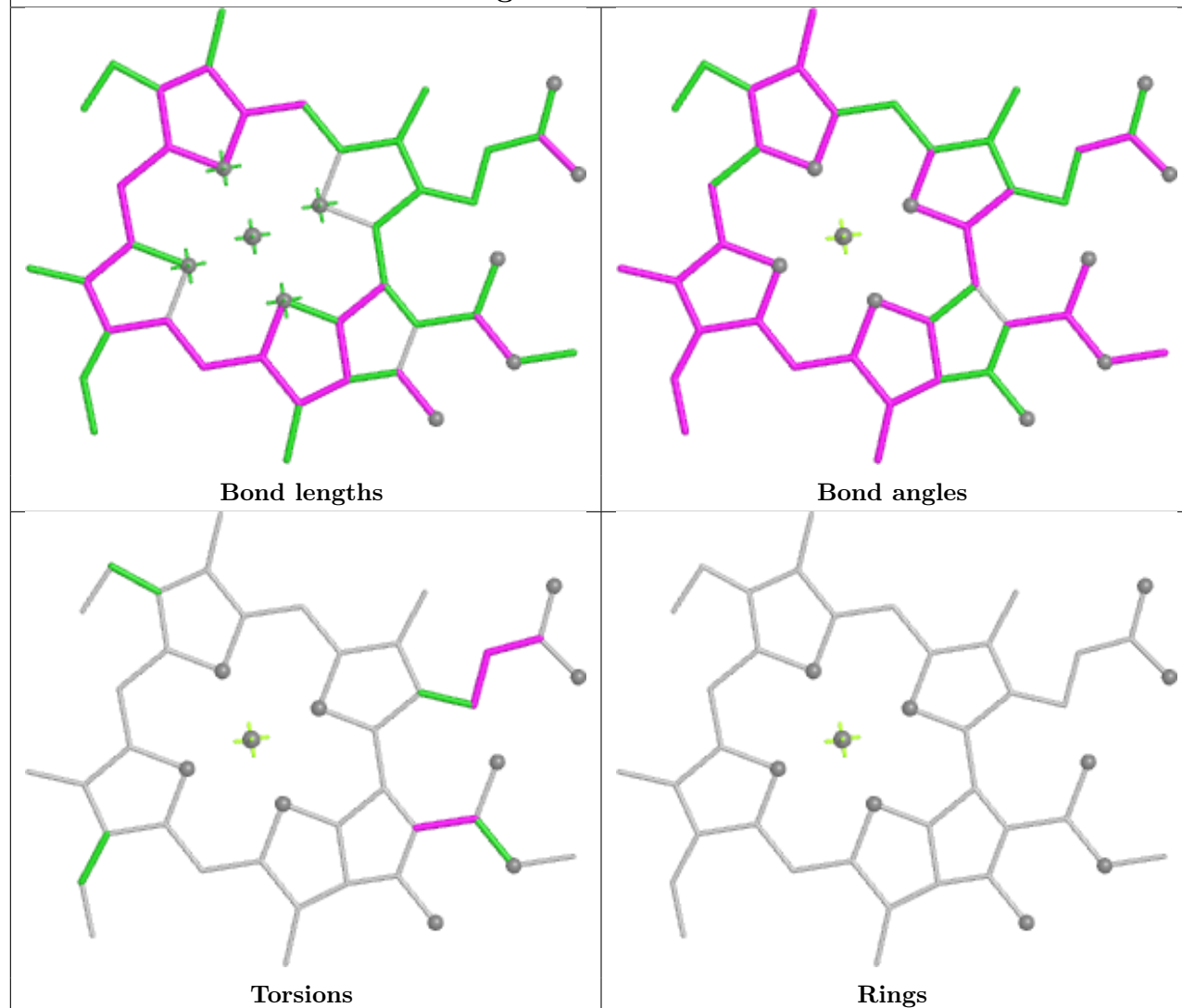
Ligand CLA a 835



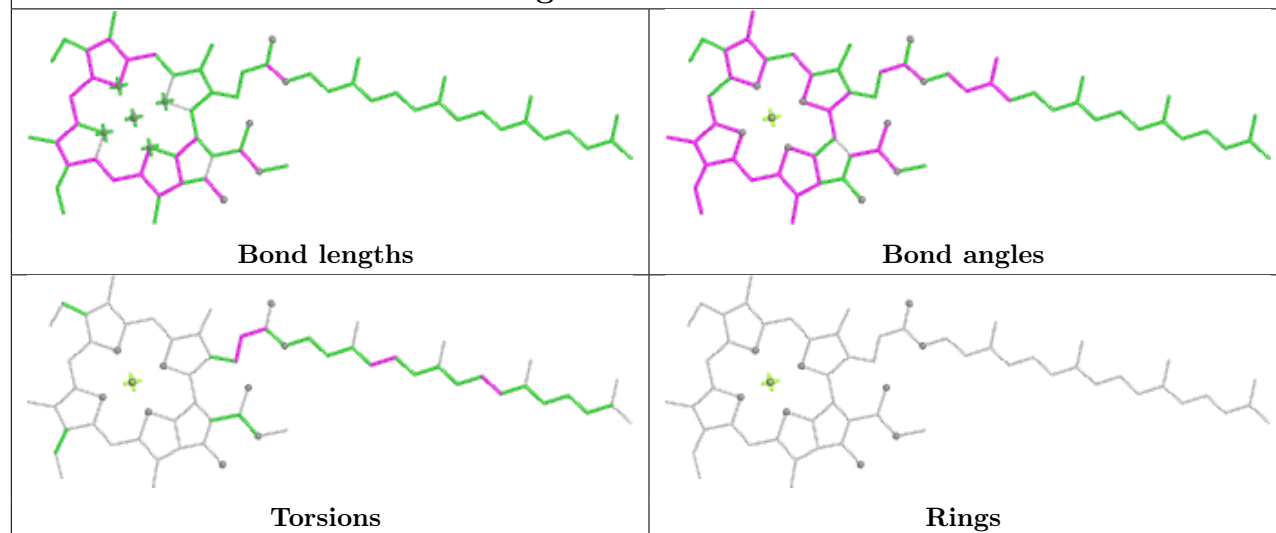
Ligand CLA 3 314



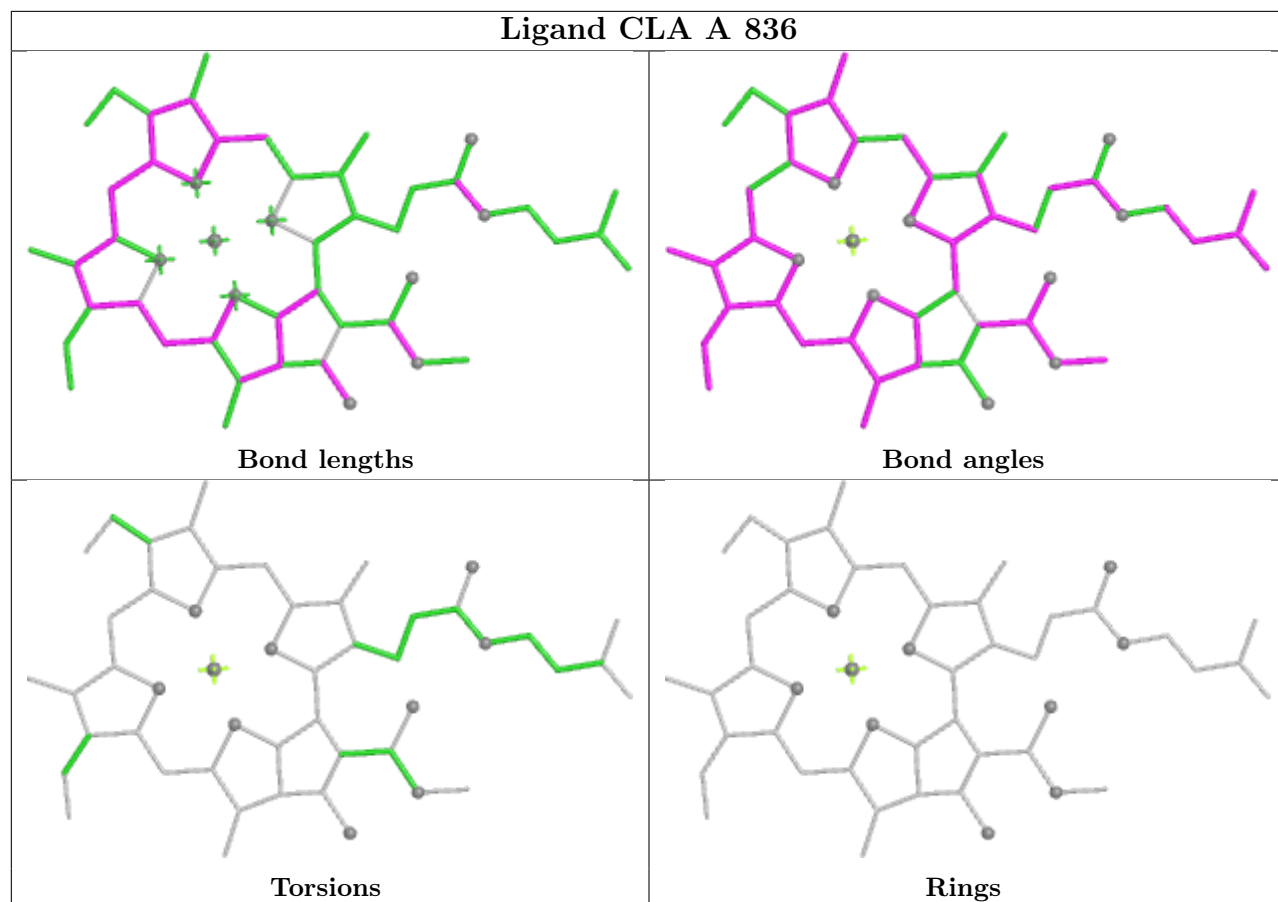
Ligand CLA a 837



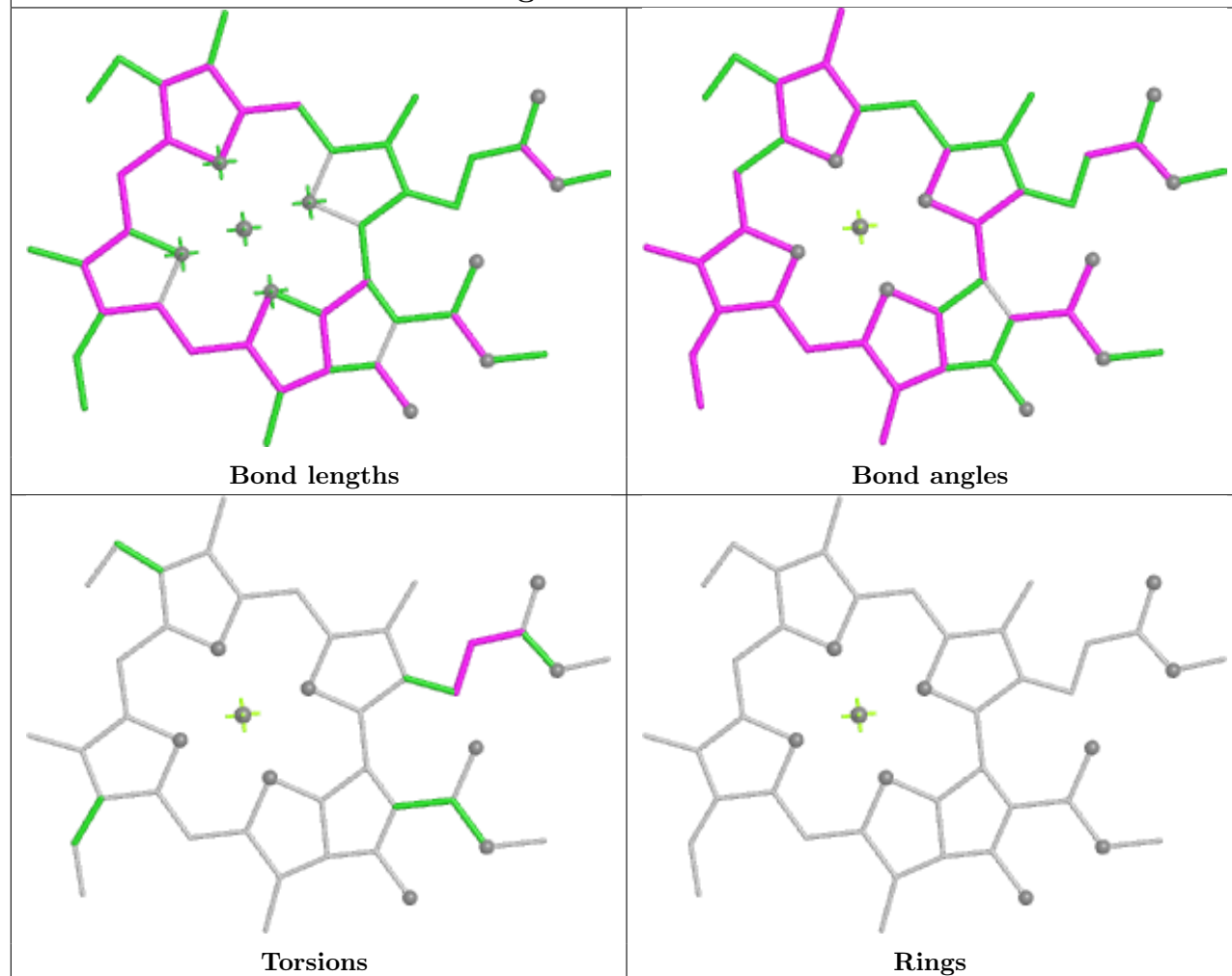
Ligand CLA 1 313



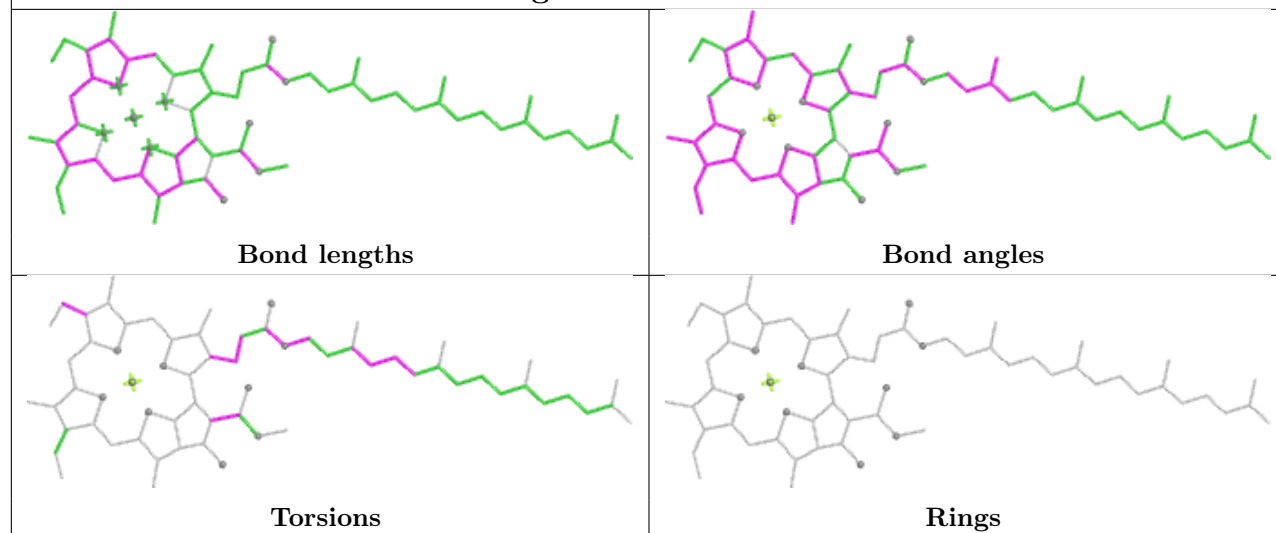
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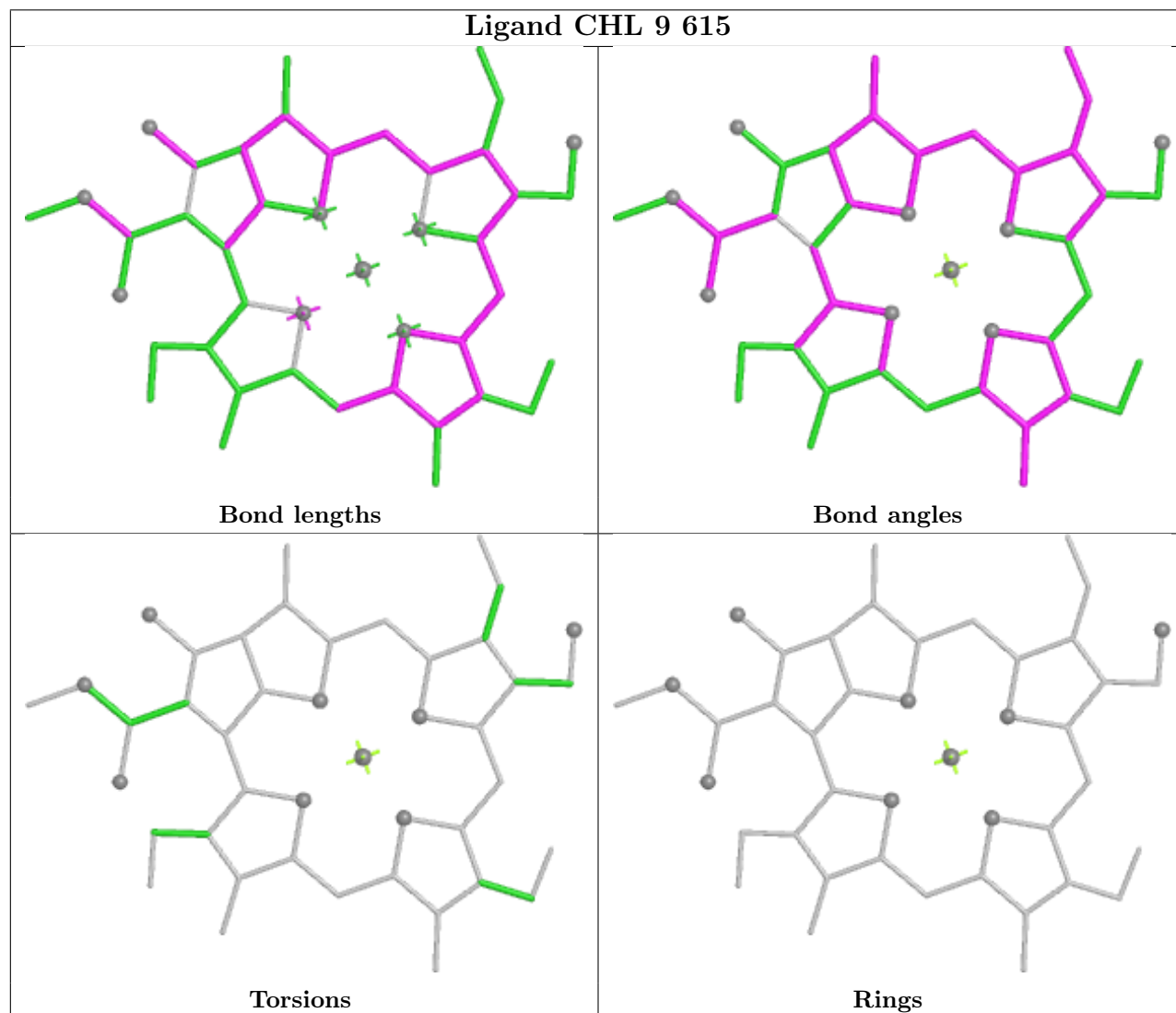
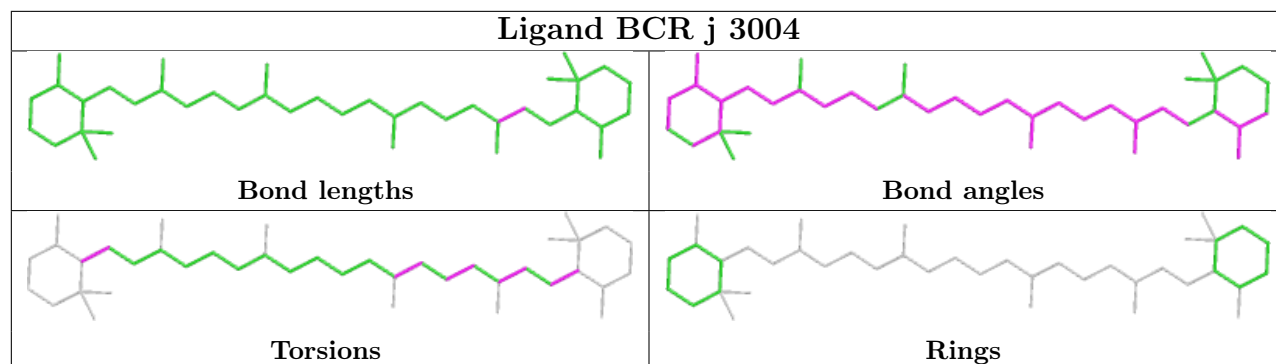


Ligand CLA 6 316

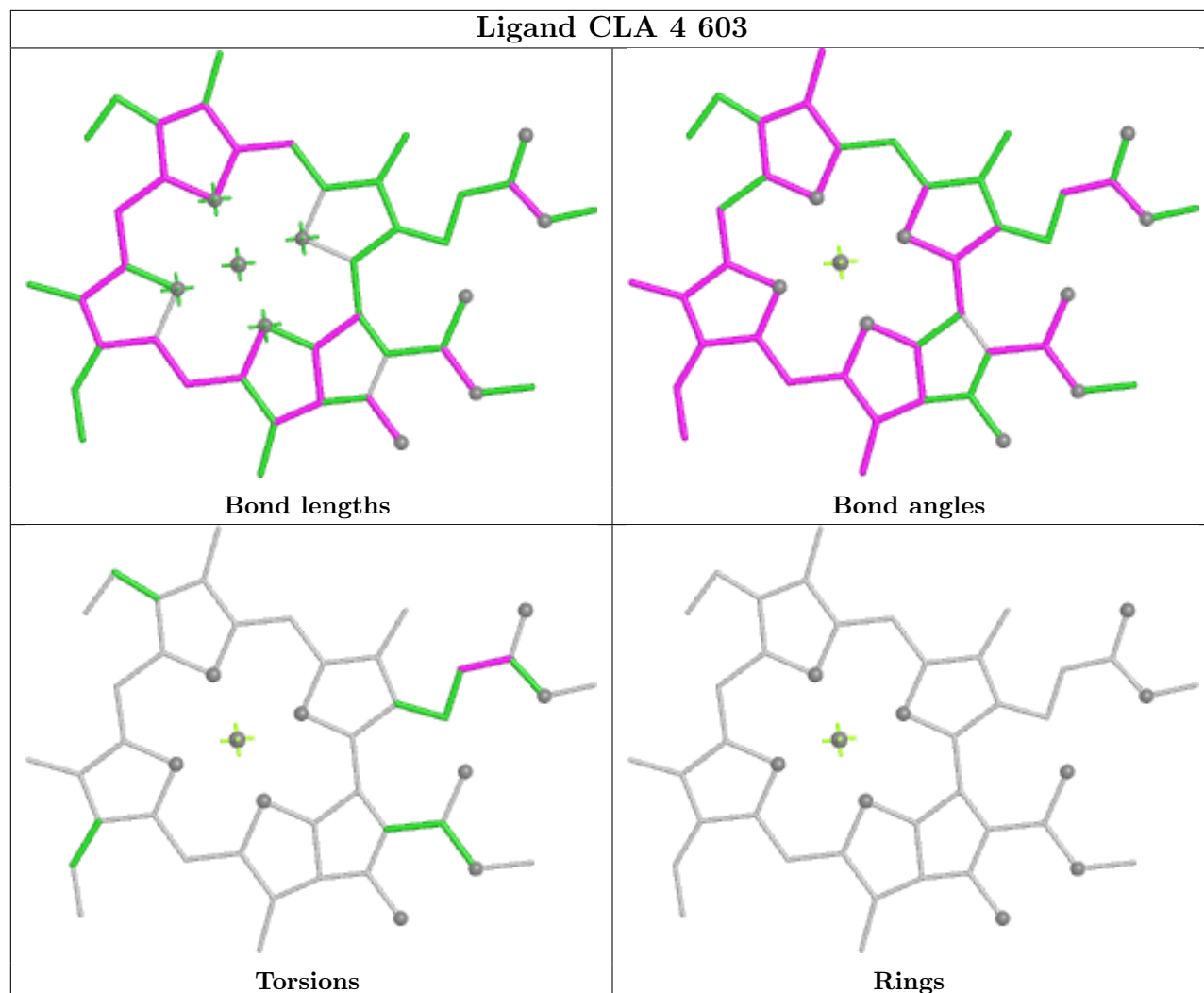


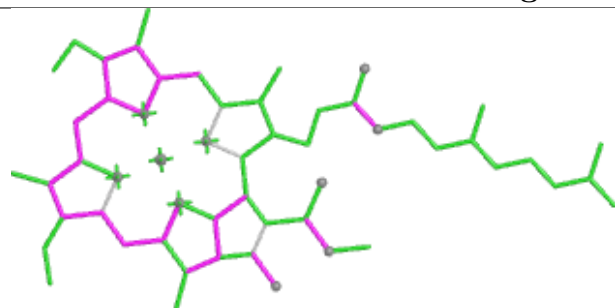
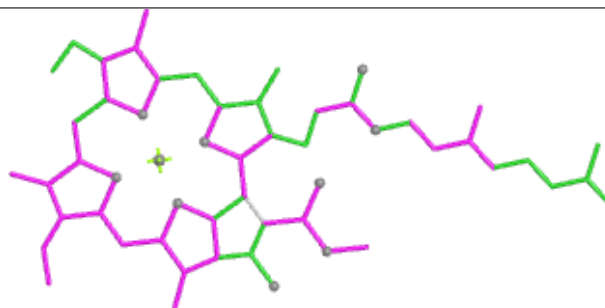
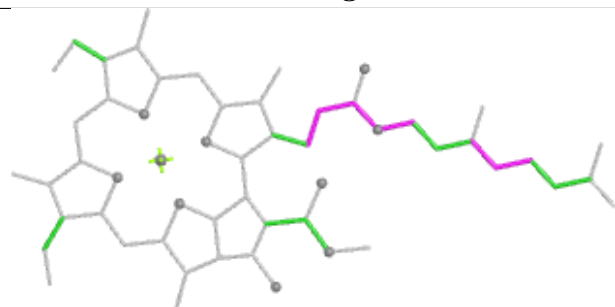
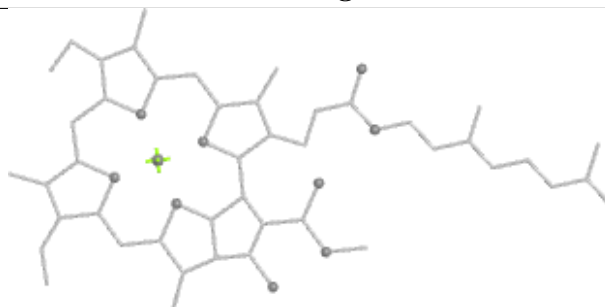
Ligand CLA A 834

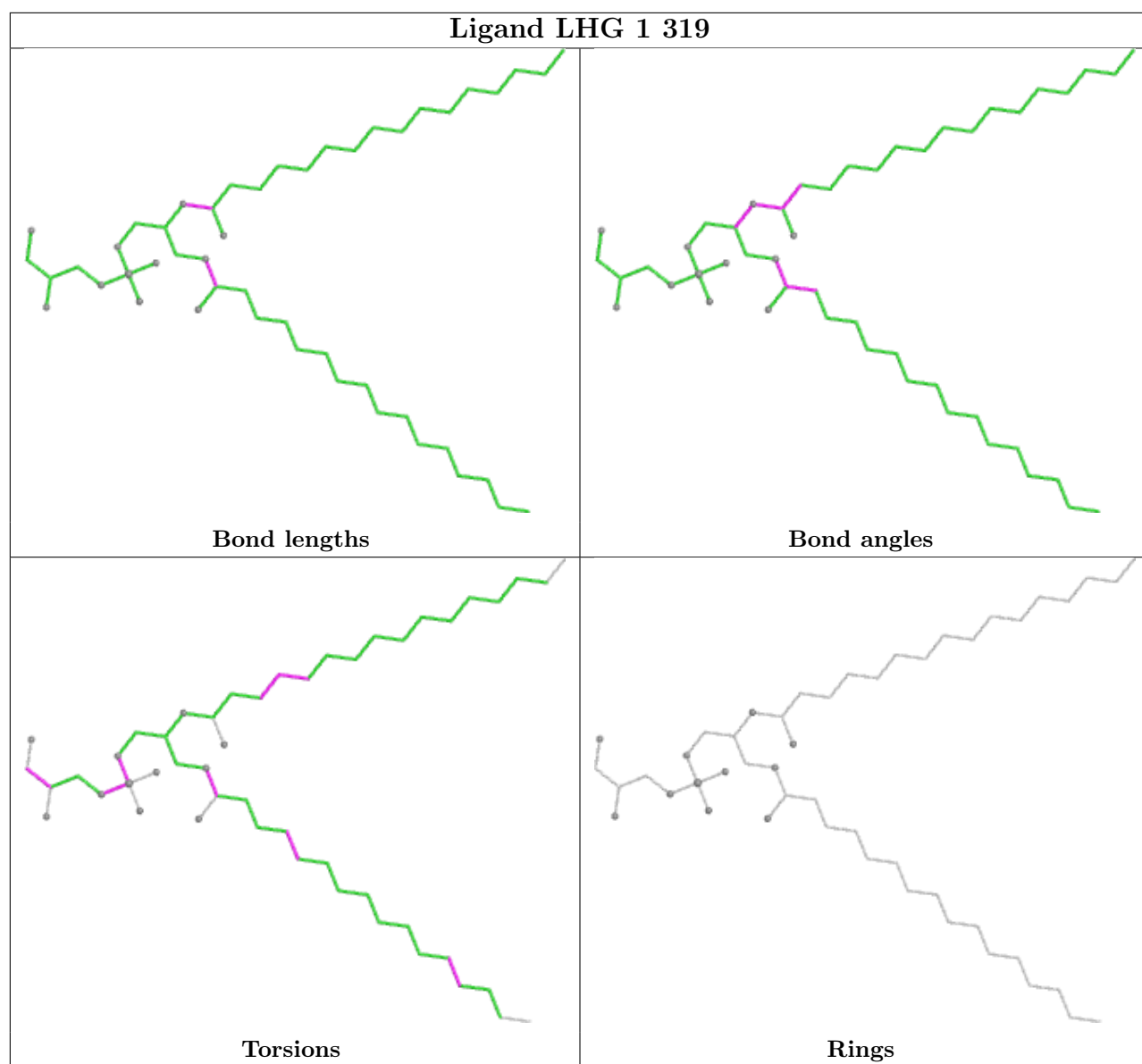




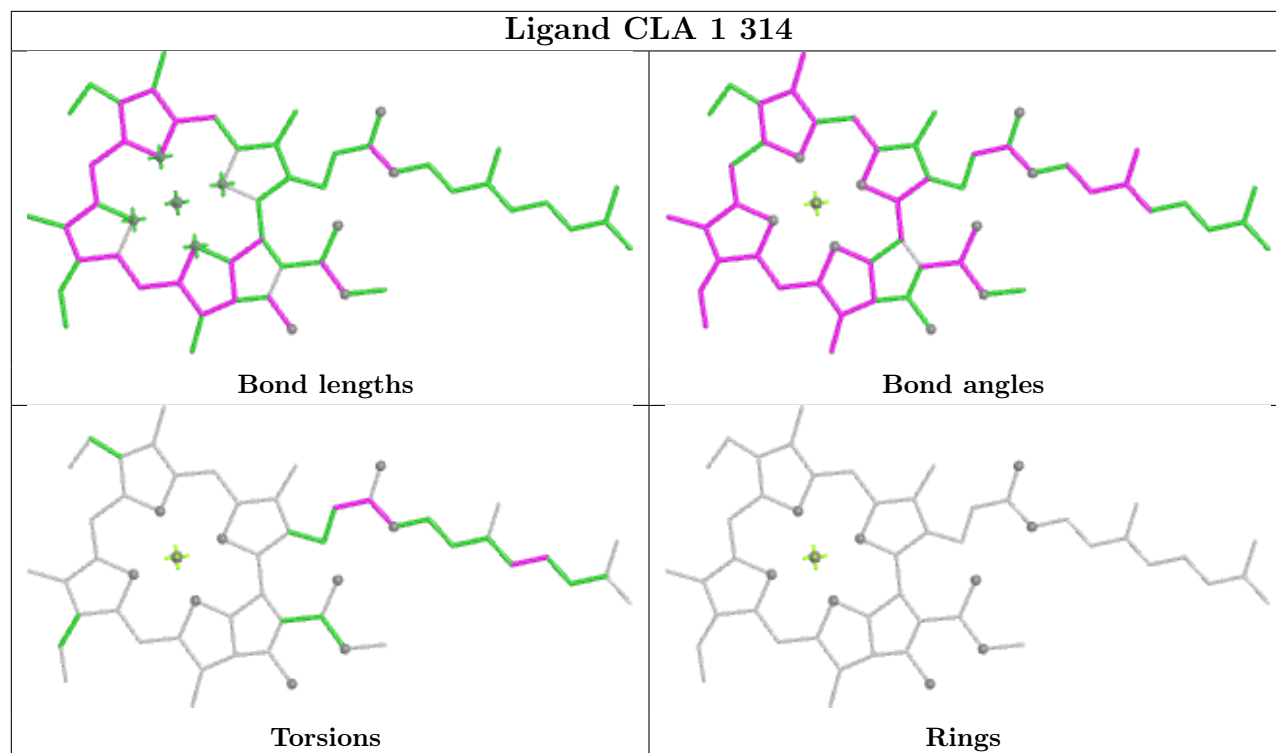
Ligand CLA 4 603



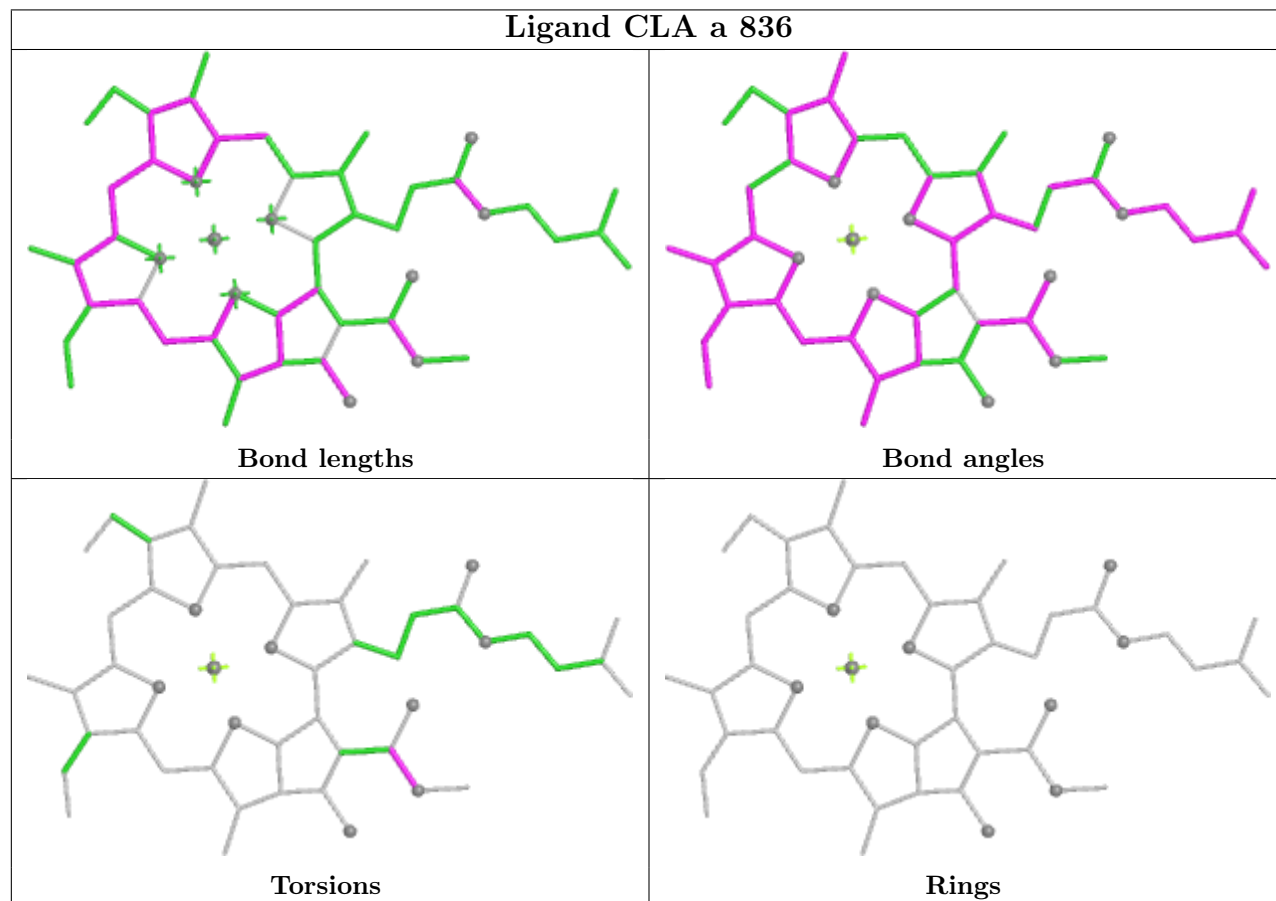
Ligand CLA 3 312**Bond lengths****Bond angles****Torsions****Rings**



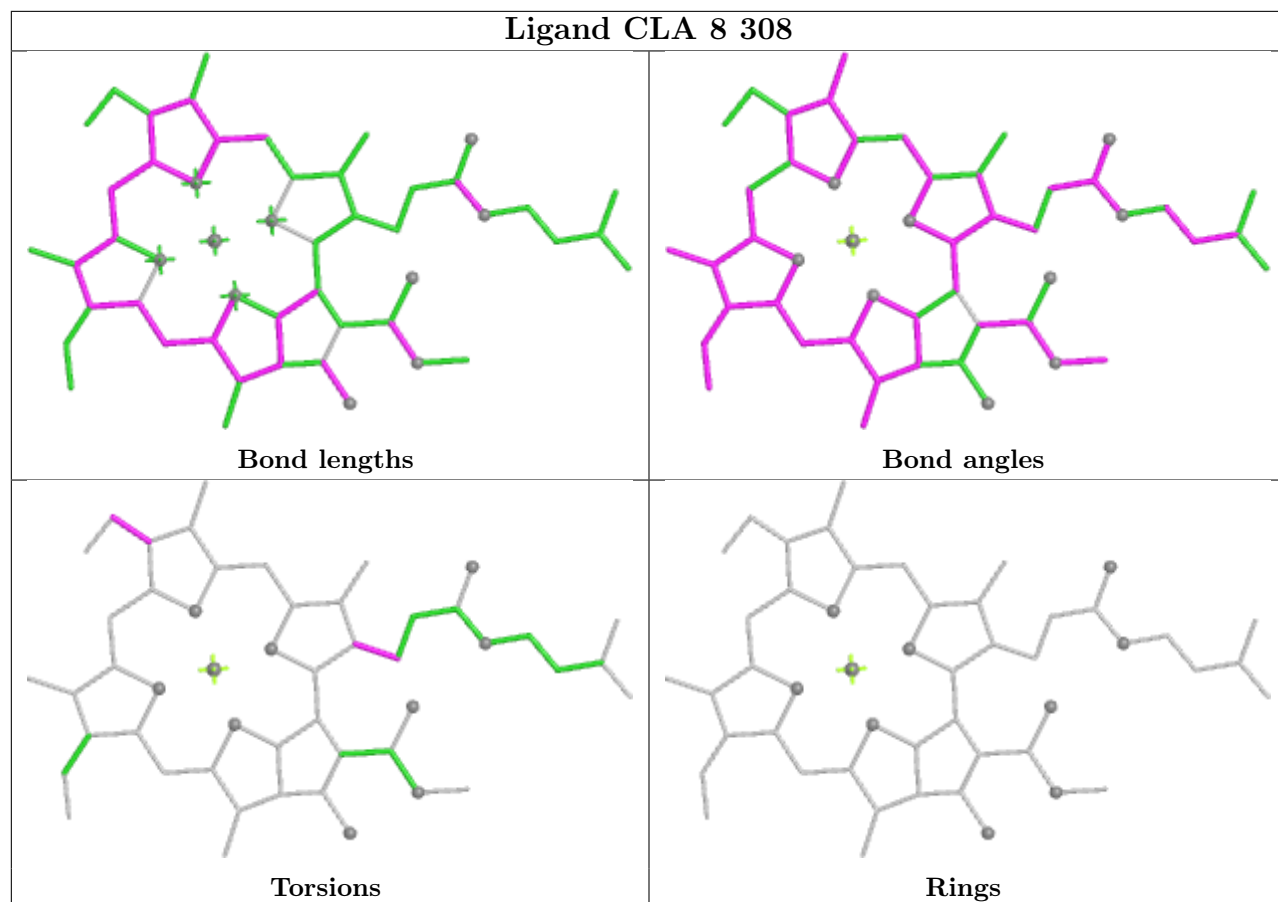
Ligand CLA 1 314



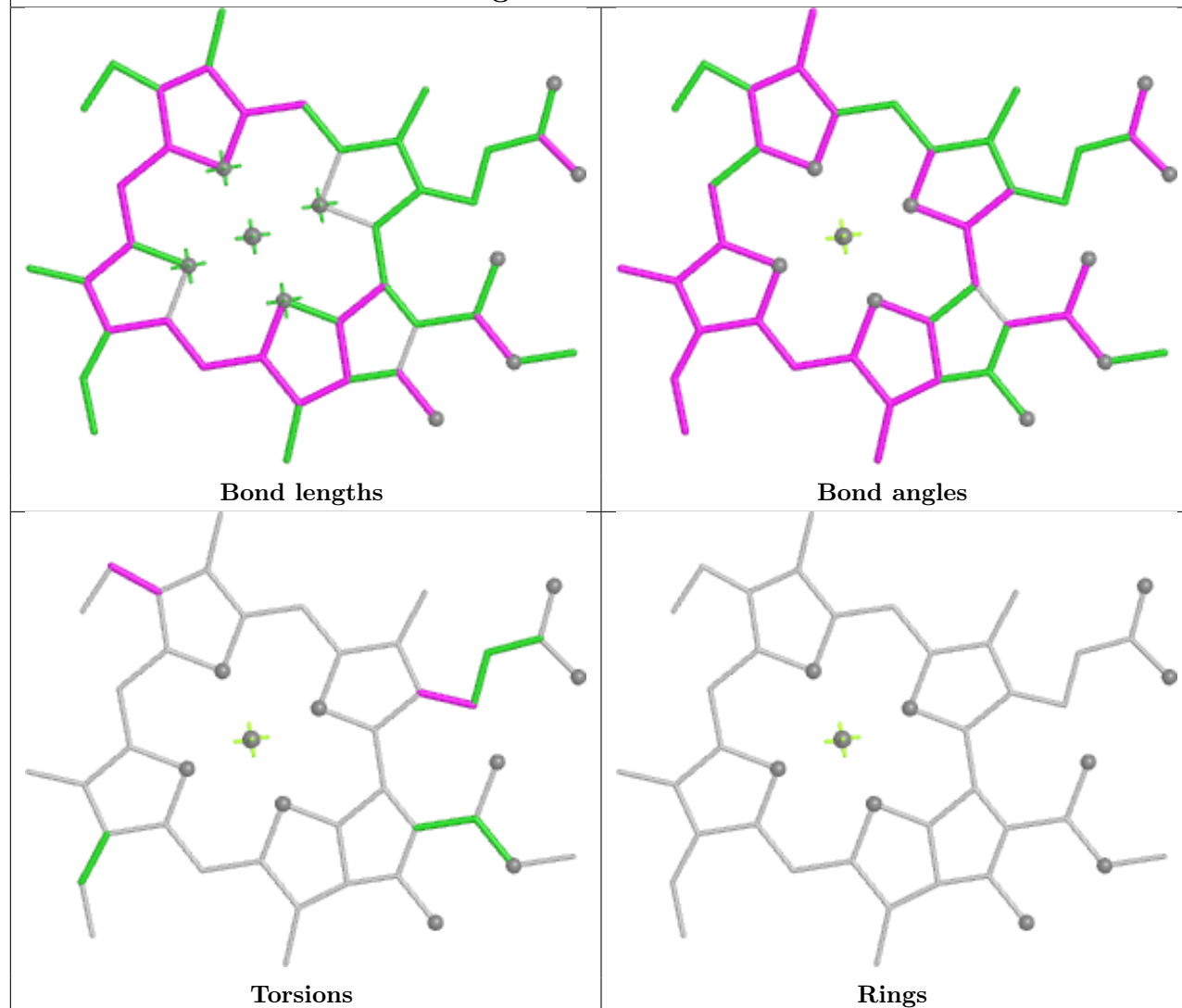
Ligand CLA a 836



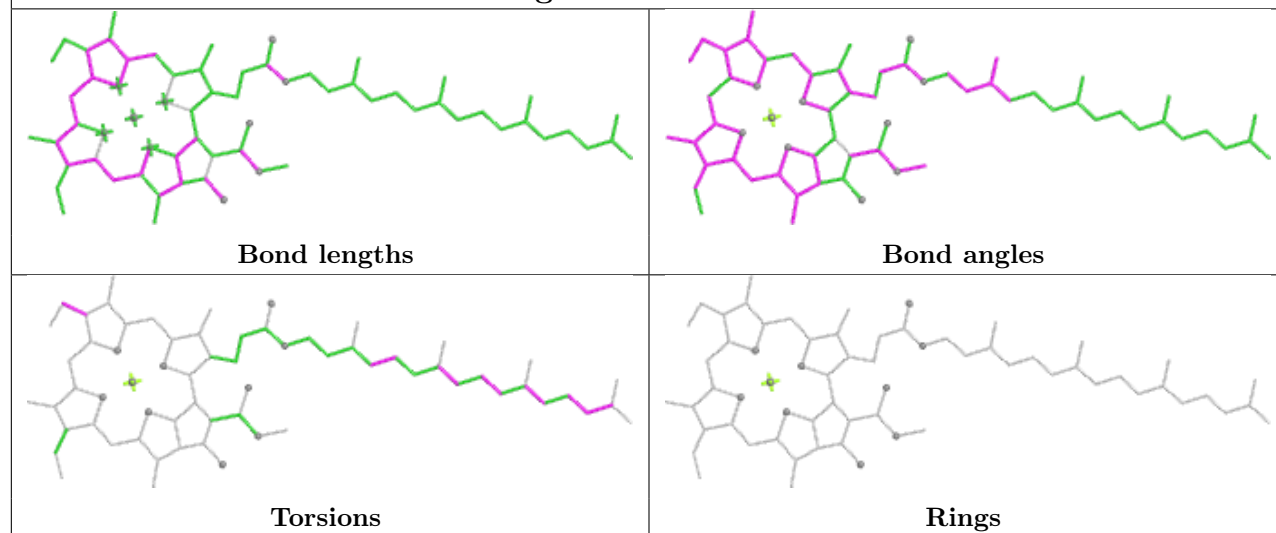
Ligand CLA 8 308



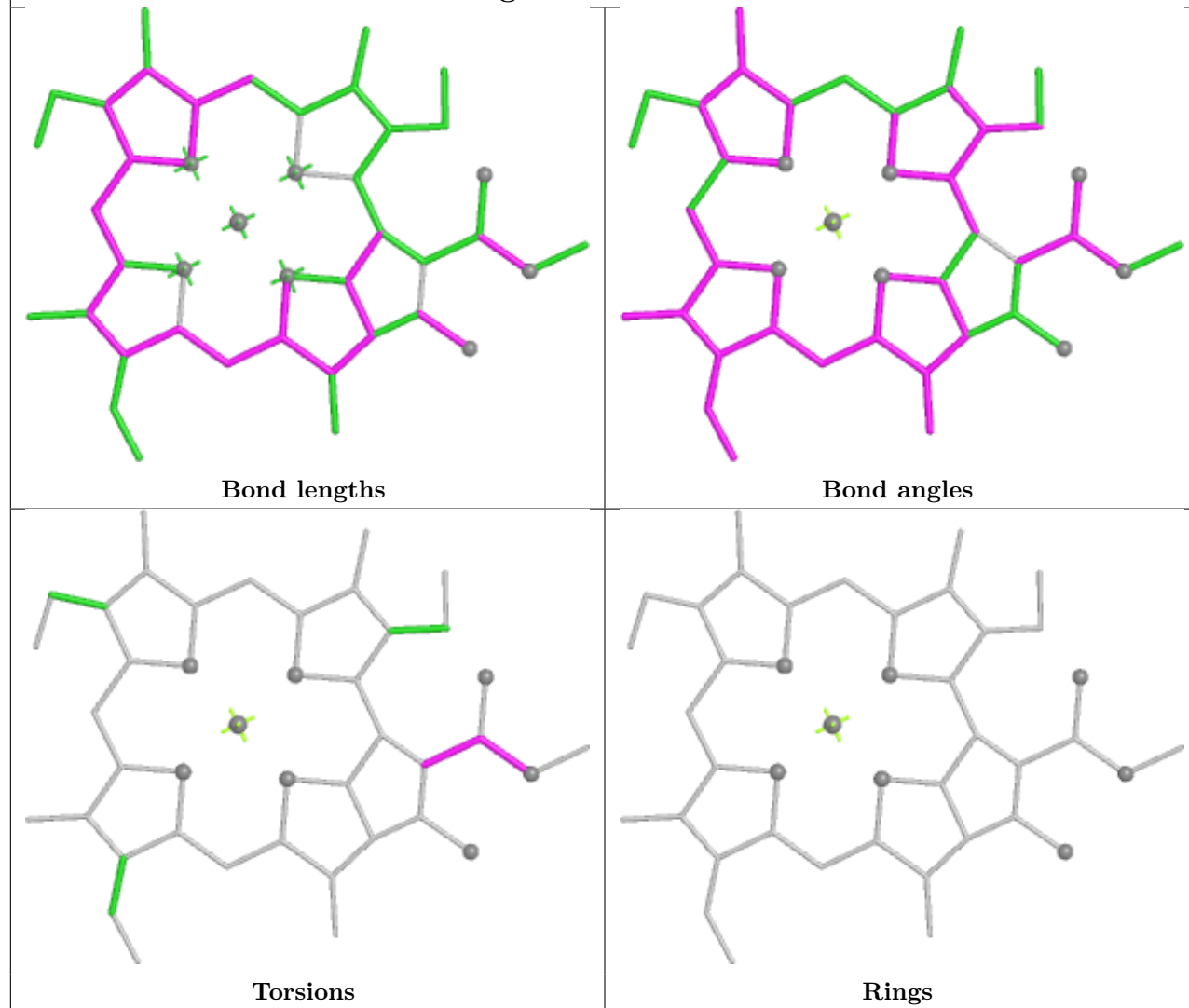
Ligand CLA A 815



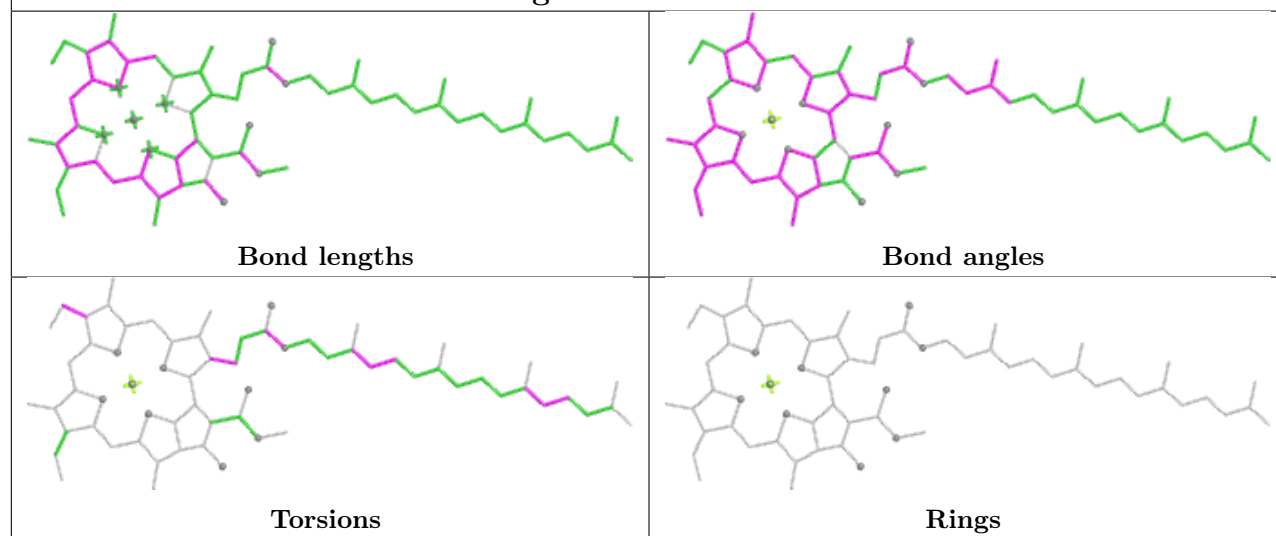
Ligand CLA b 803

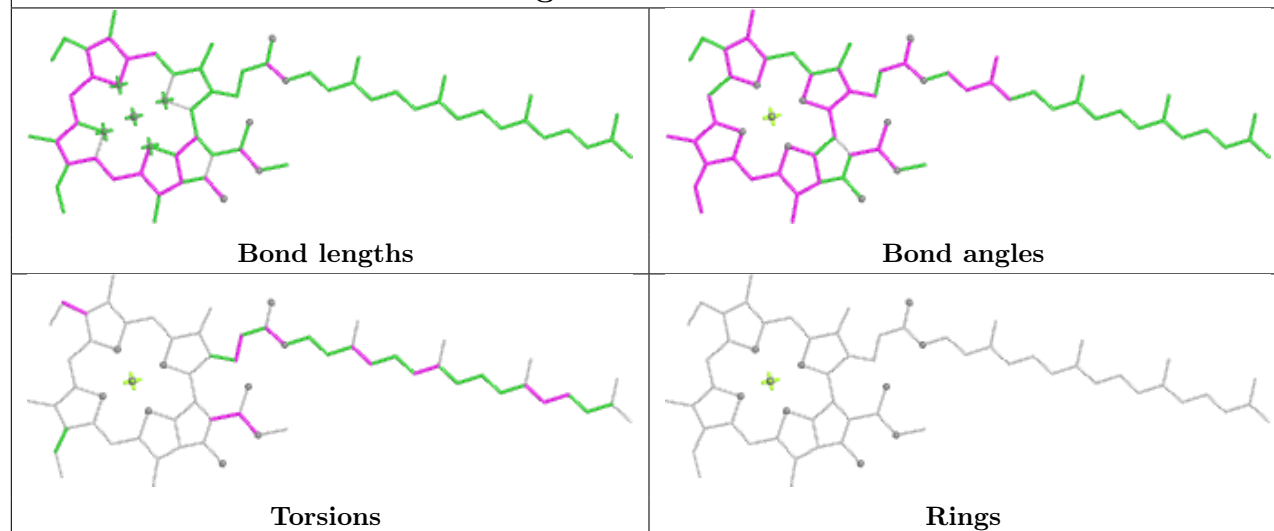
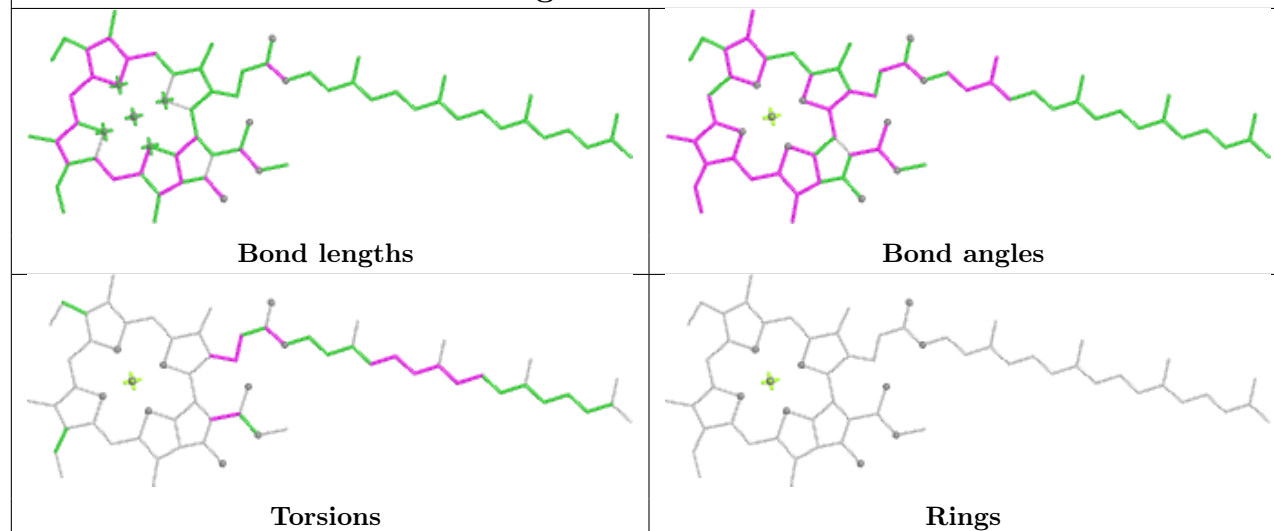
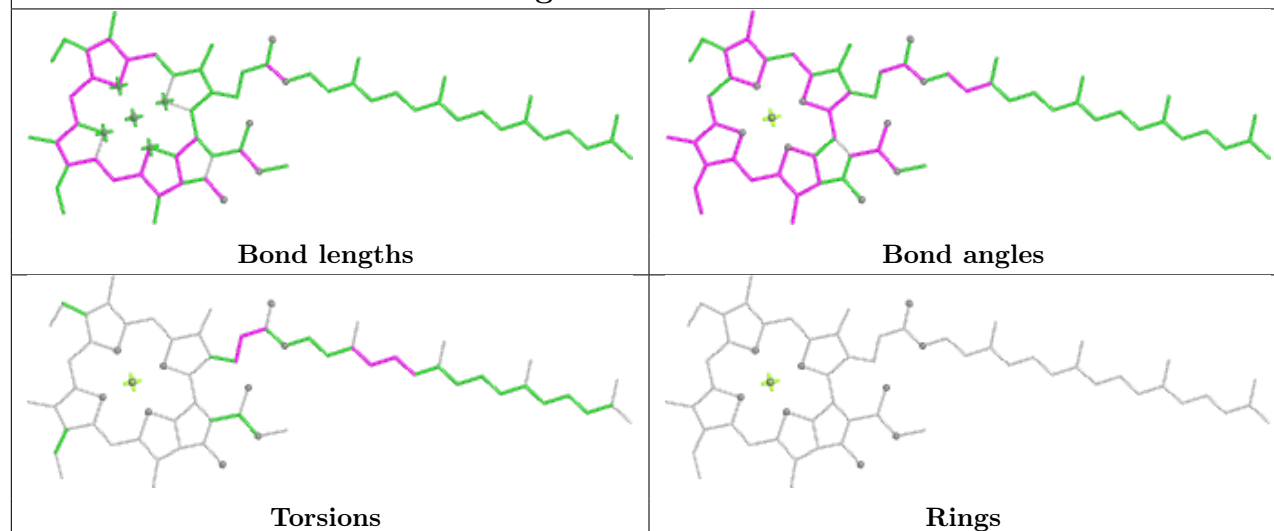


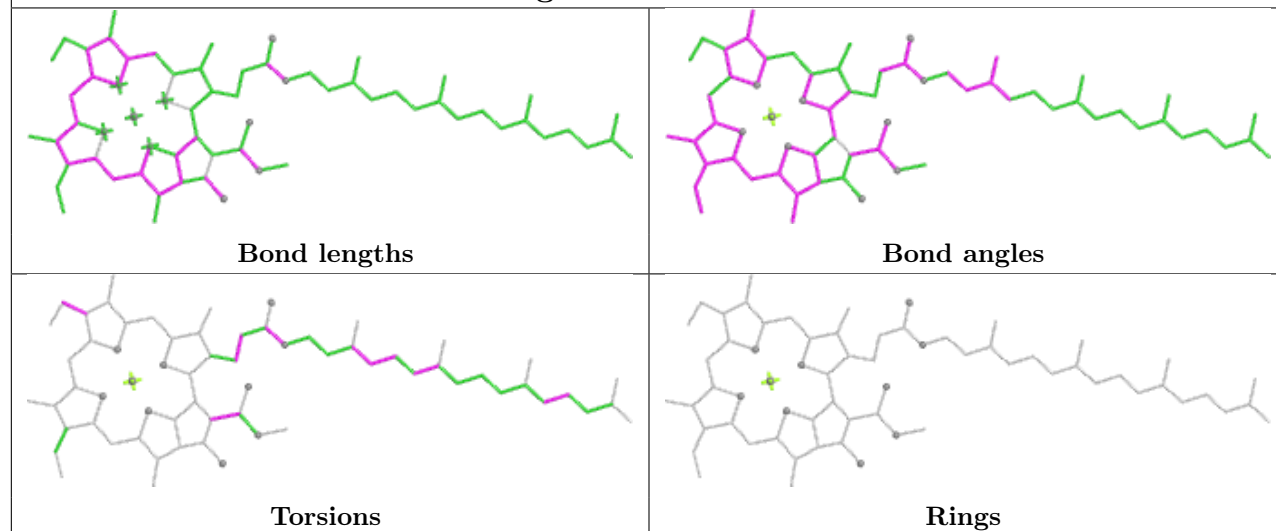
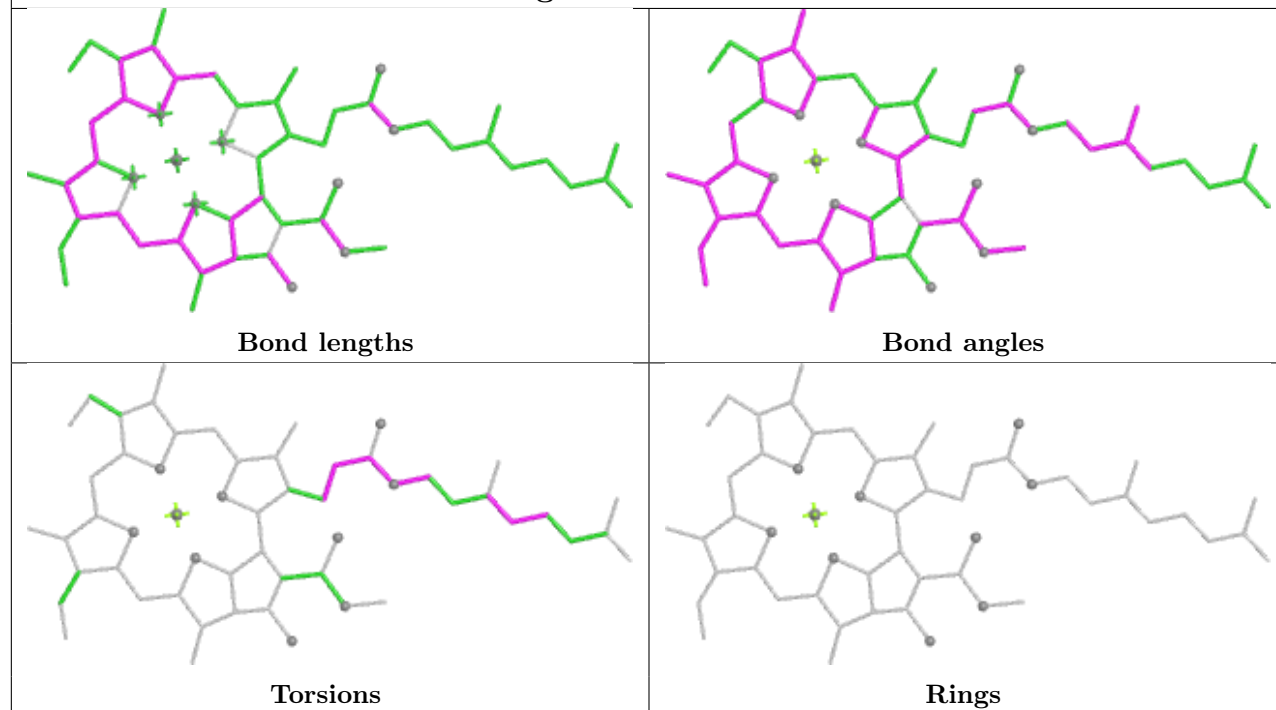
Ligand CLA 6 307



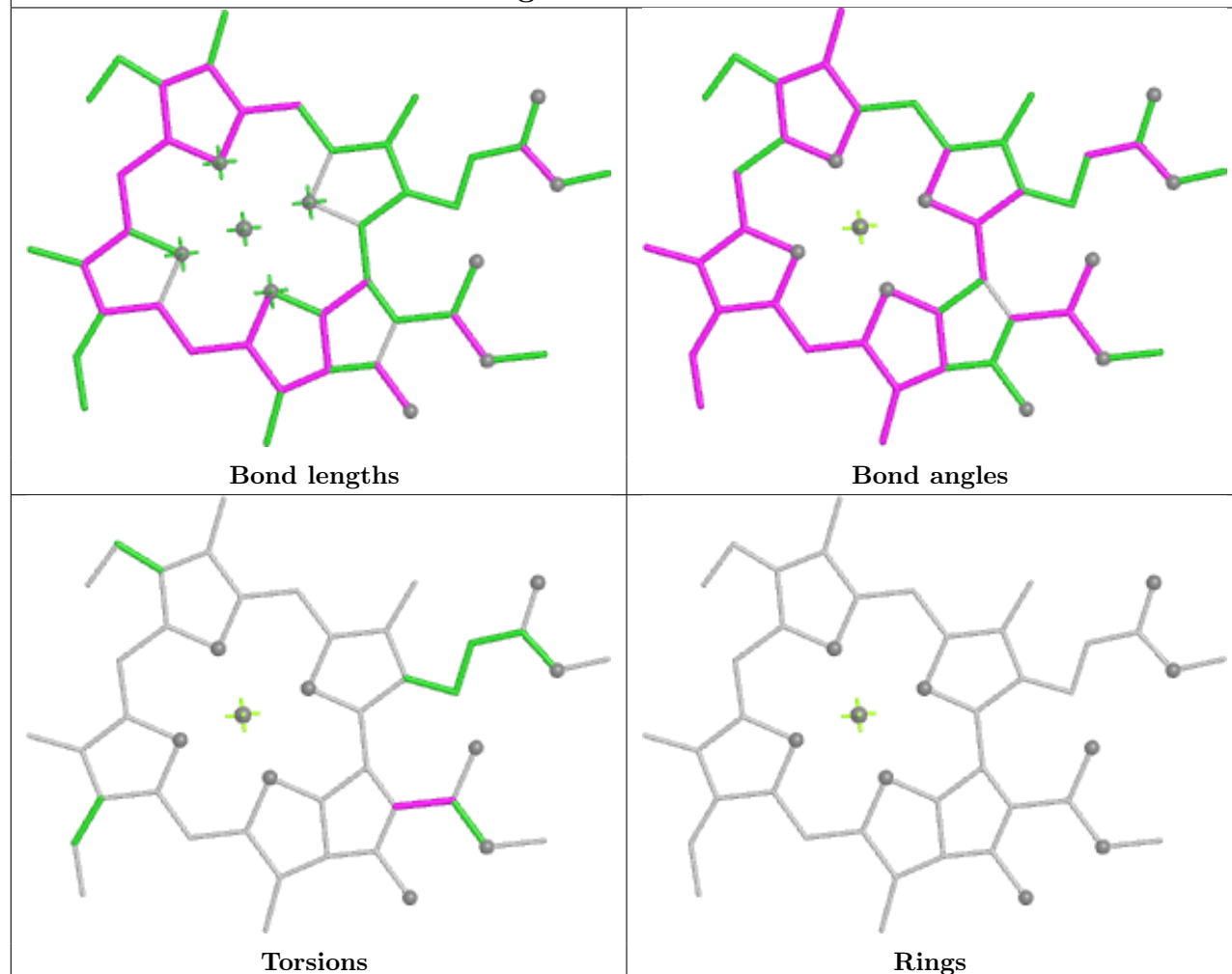
Ligand CLA B 810



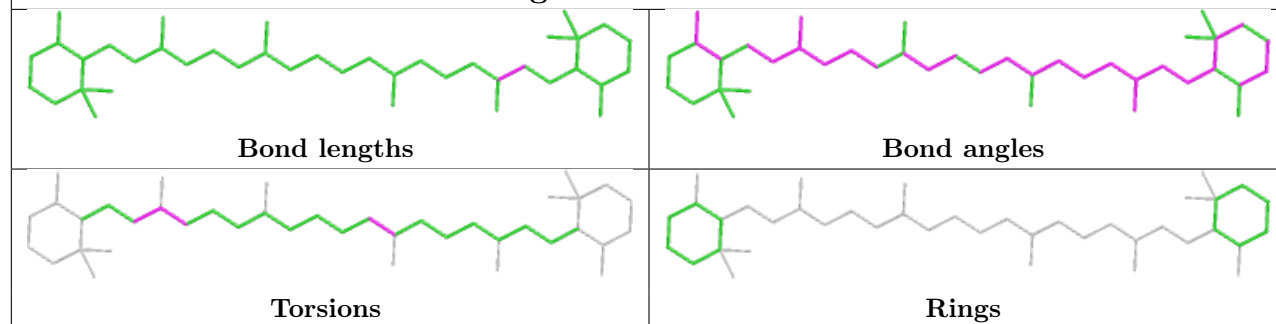
Ligand CLA 2 602**Ligand CLA a 809****Ligand CLA b 807**

Ligand CLA 1 303**Ligand CLA 8 310**

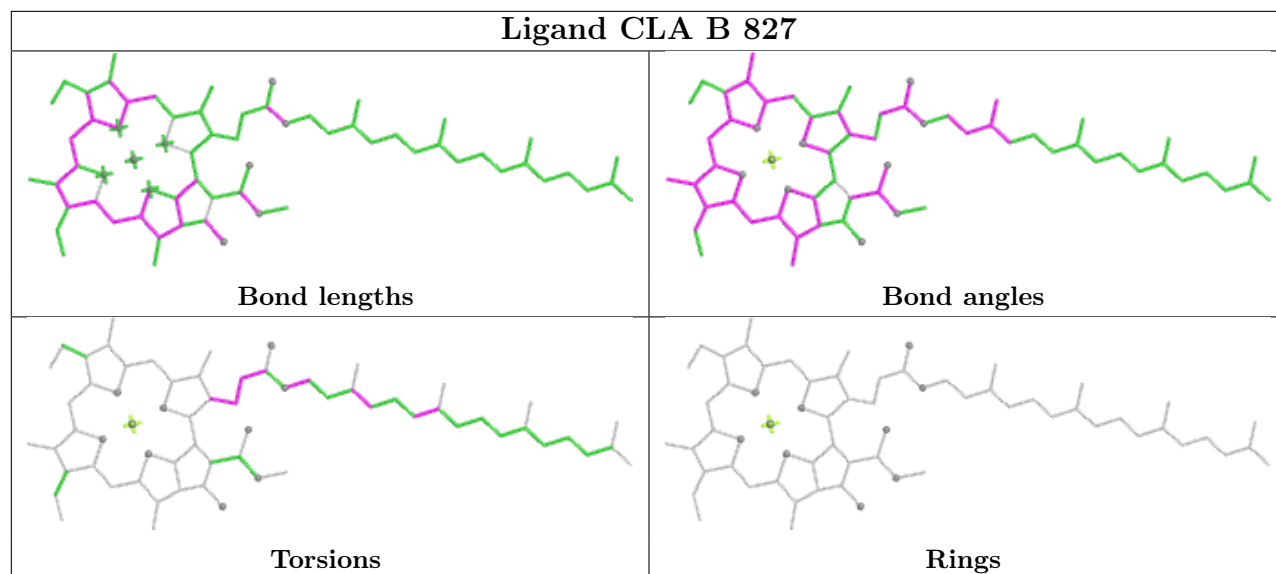
Ligand CLA 3 301



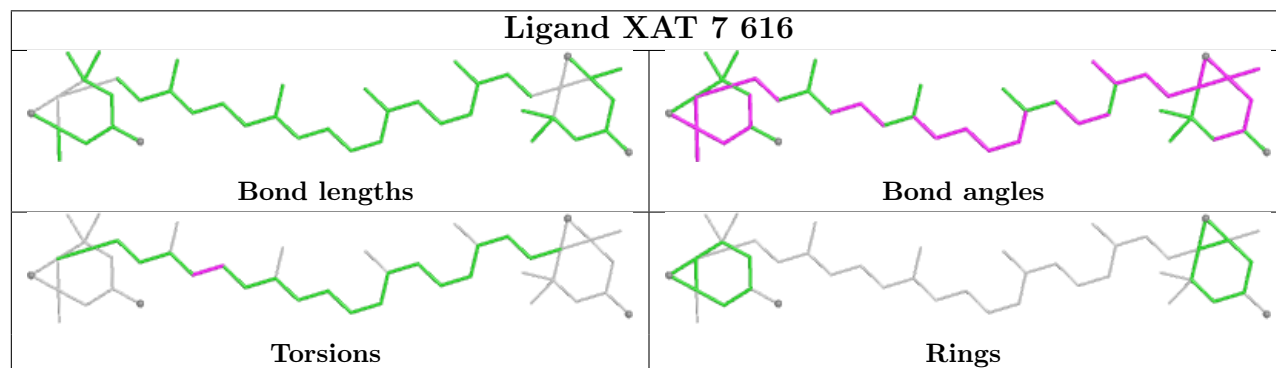
Ligand BCR A 852



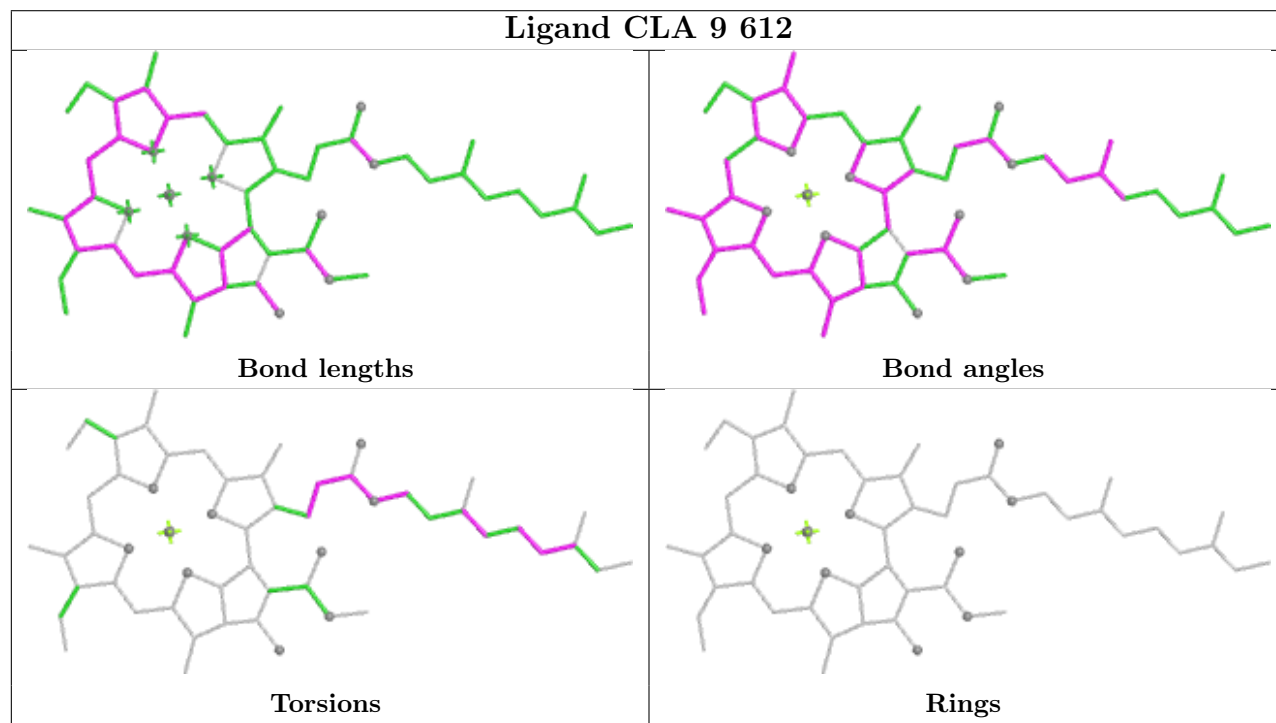
Ligand CLA B 827



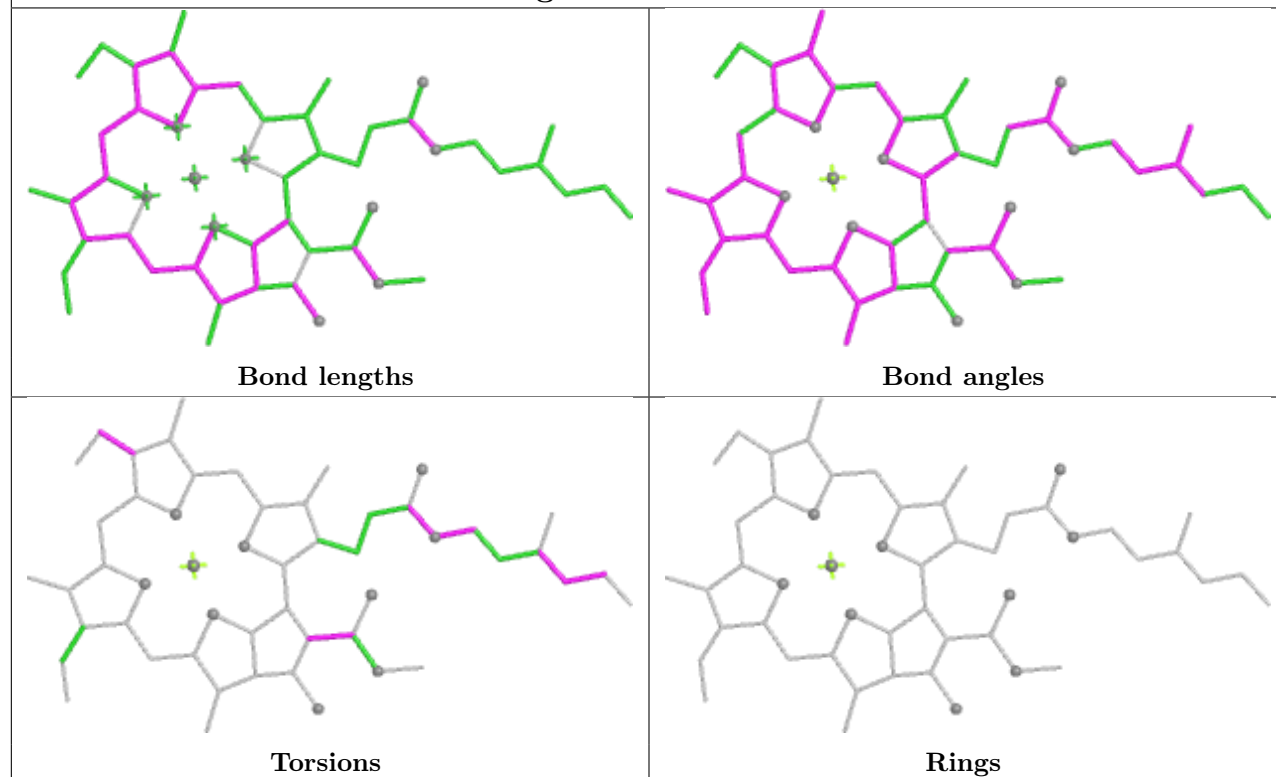
Ligand XAT 7 616



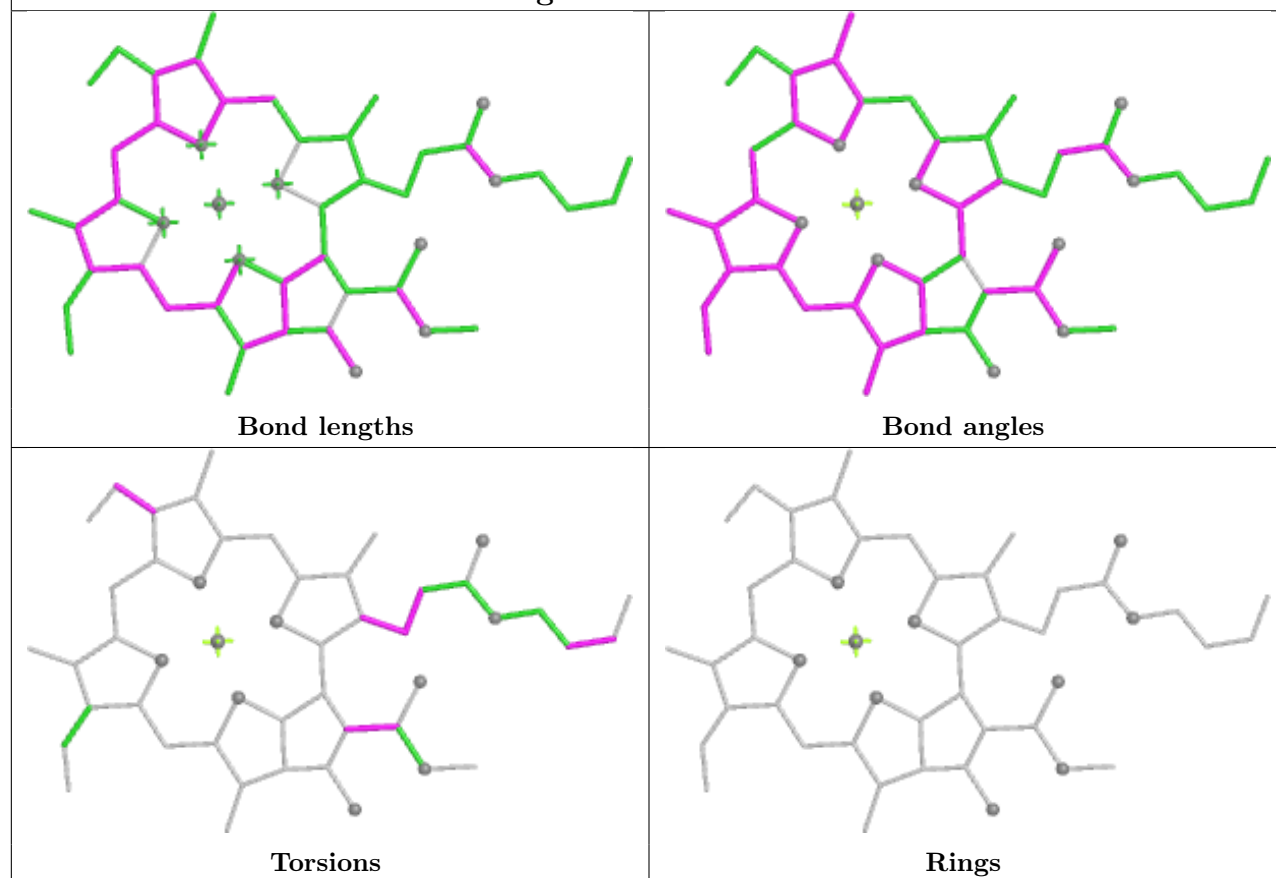
Ligand CLA 9 612

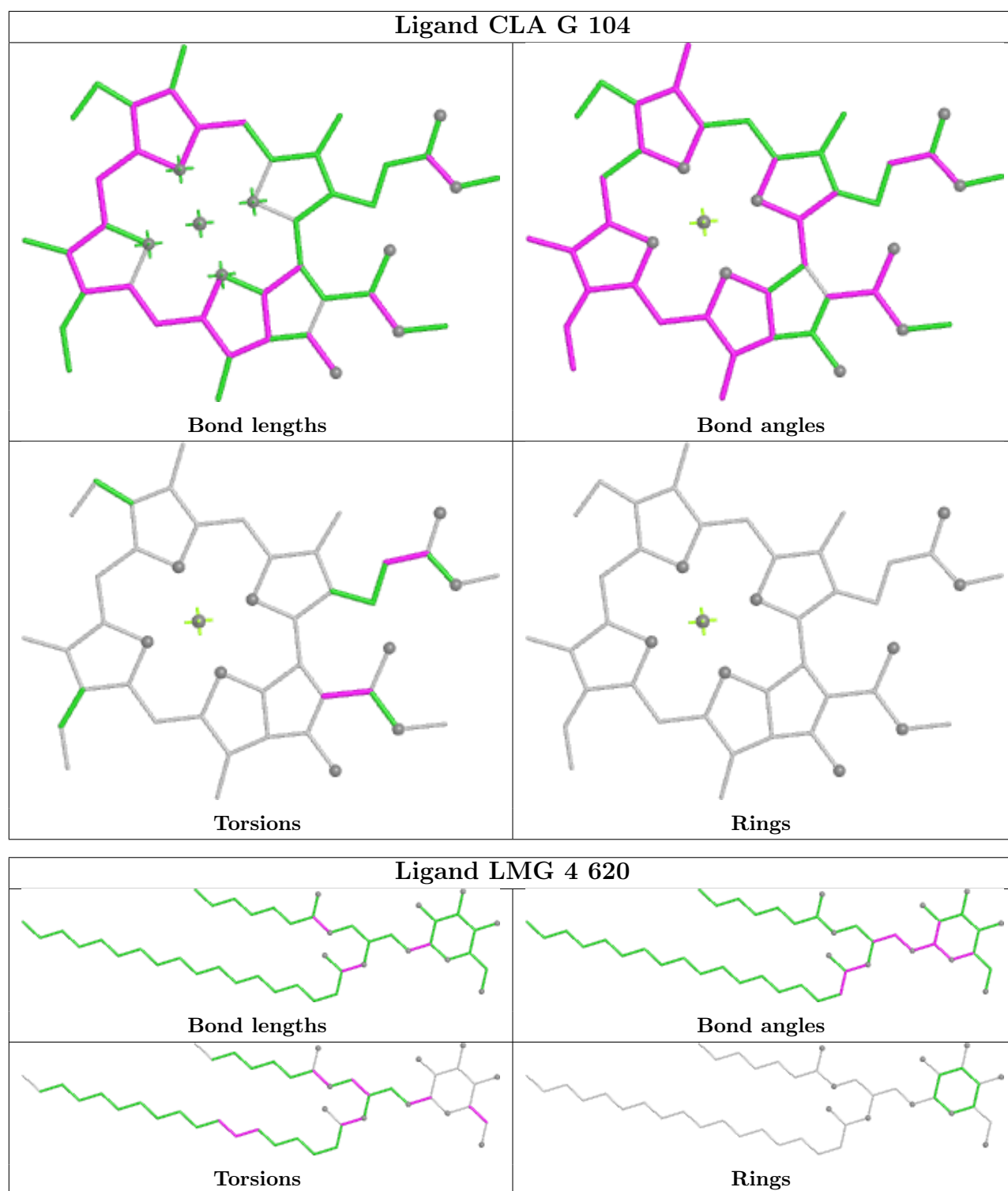


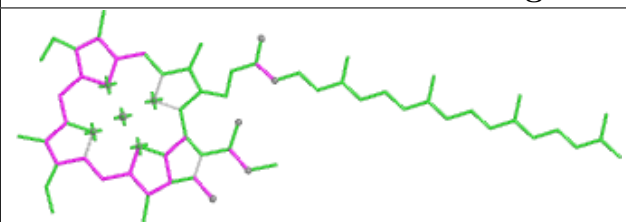
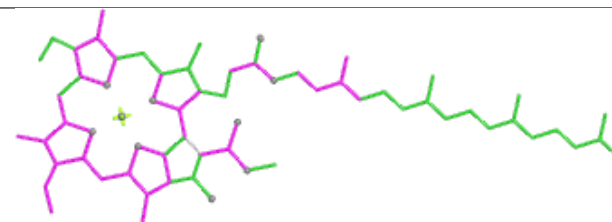
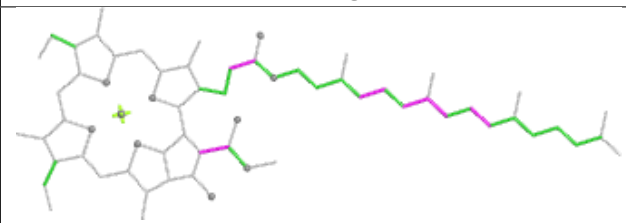
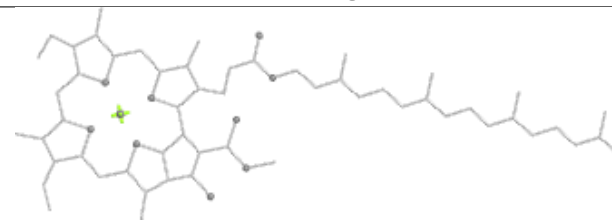
Ligand CLA 1 305

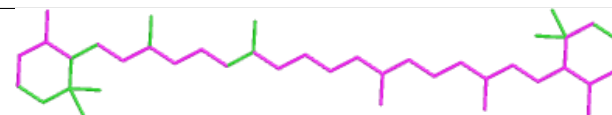
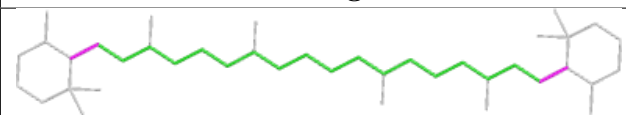
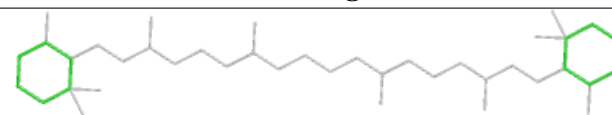


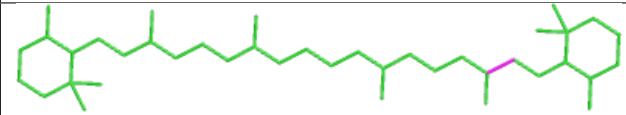
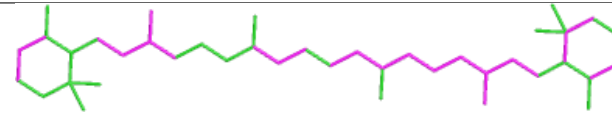
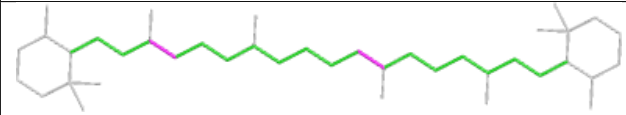
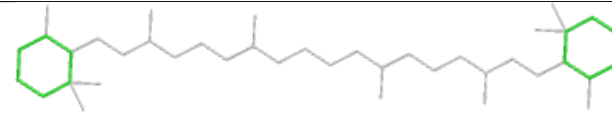
Ligand CLA a 823

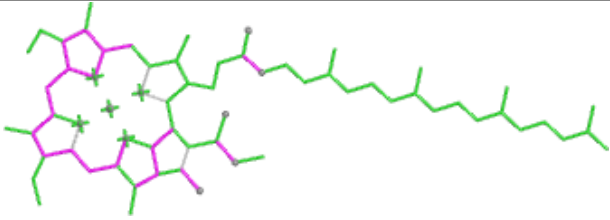
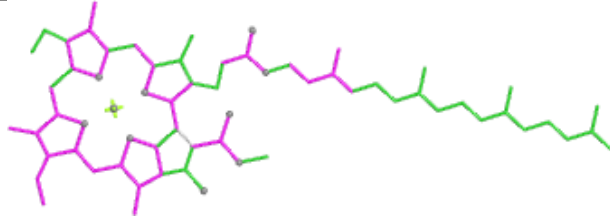
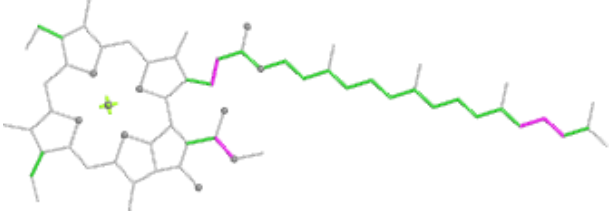
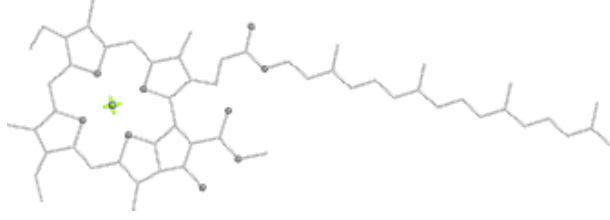
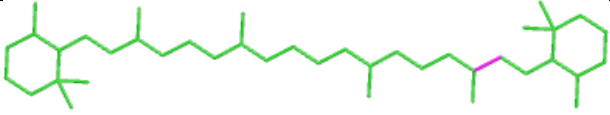
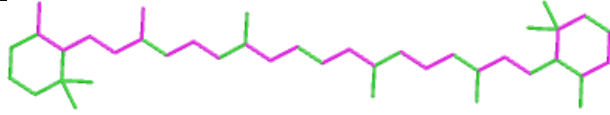
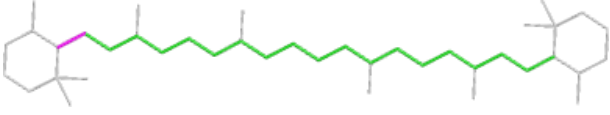
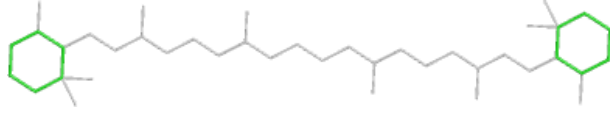
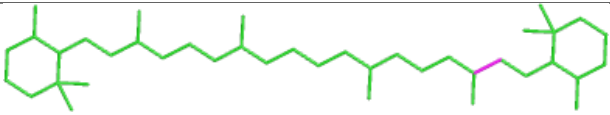
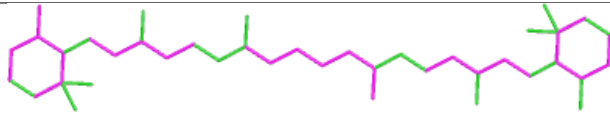
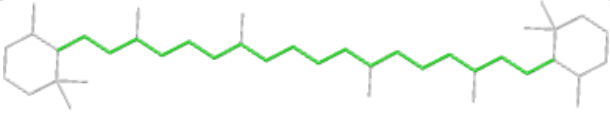
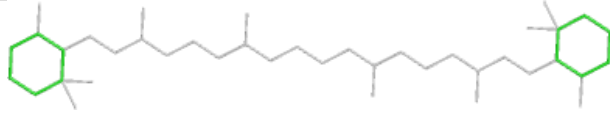




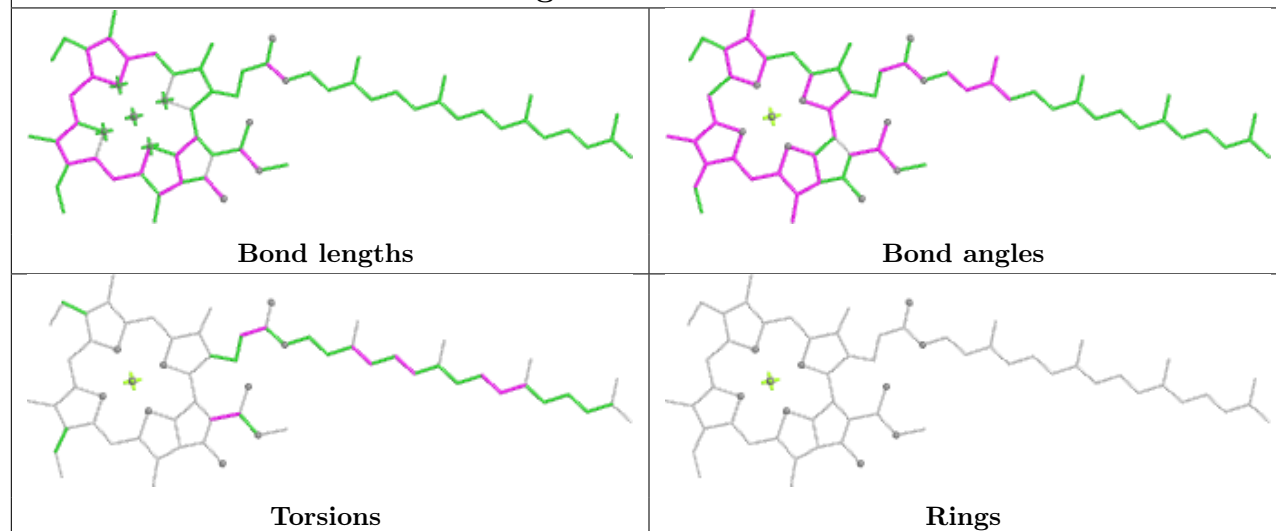
Ligand CLA 6 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 8 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

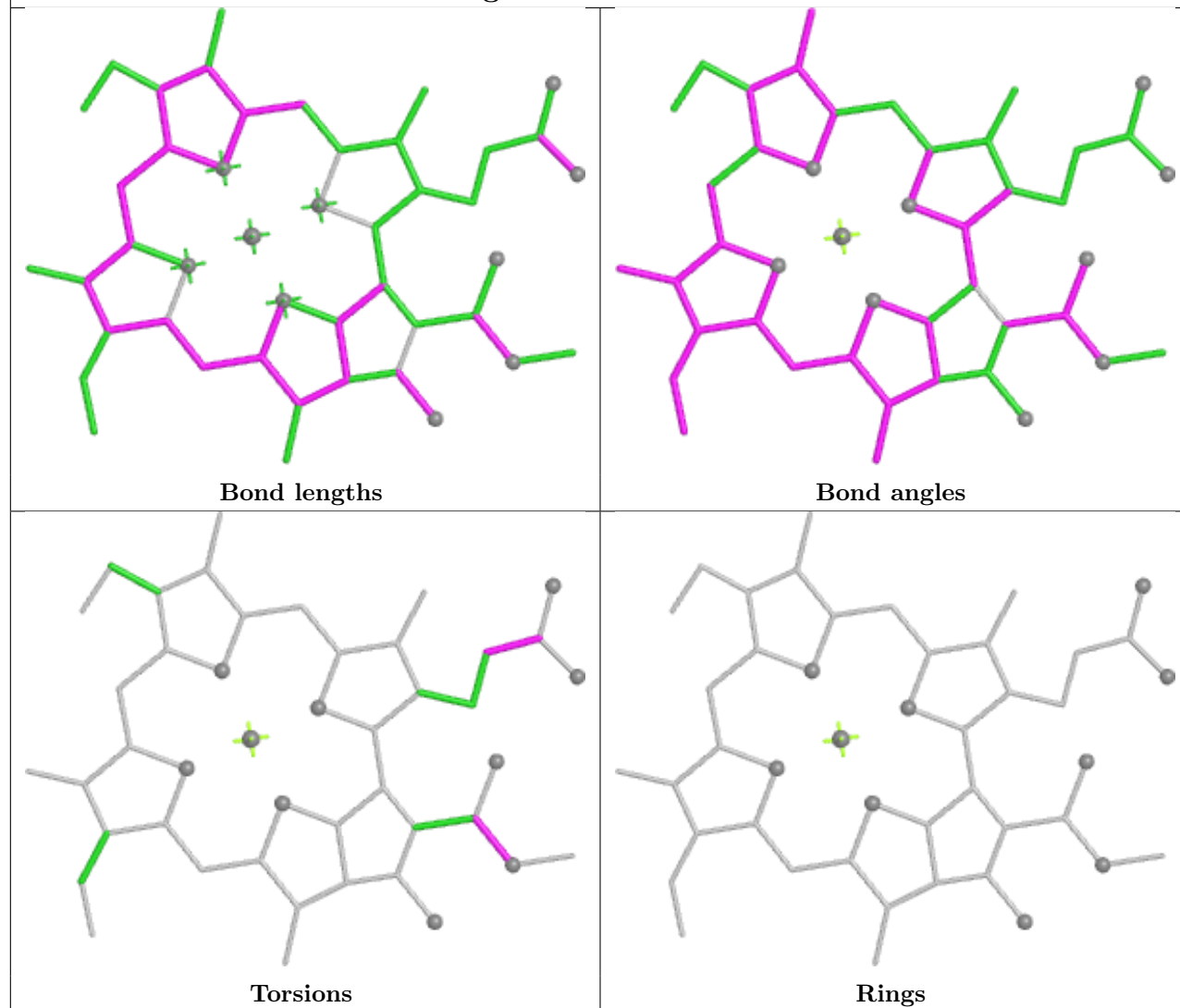
Ligand BCR a 854	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 840	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 848	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

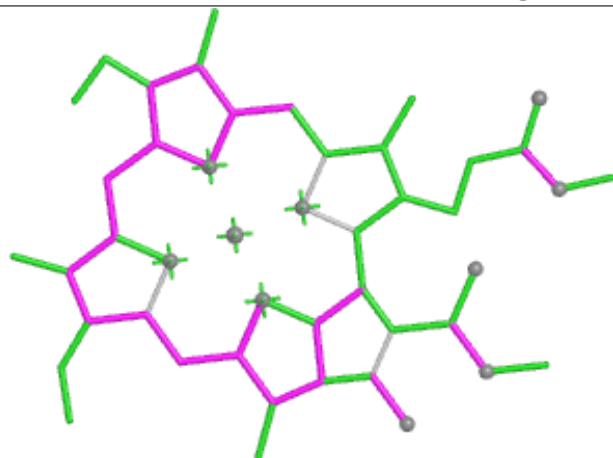
Ligand CLA a 828



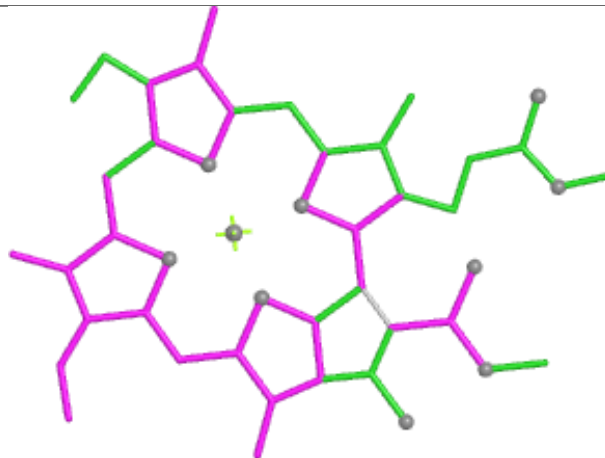
Ligand CLA K 4002



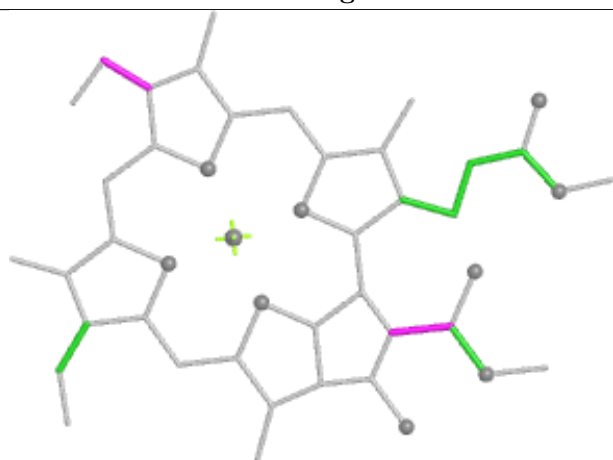
Ligand CLA B 821



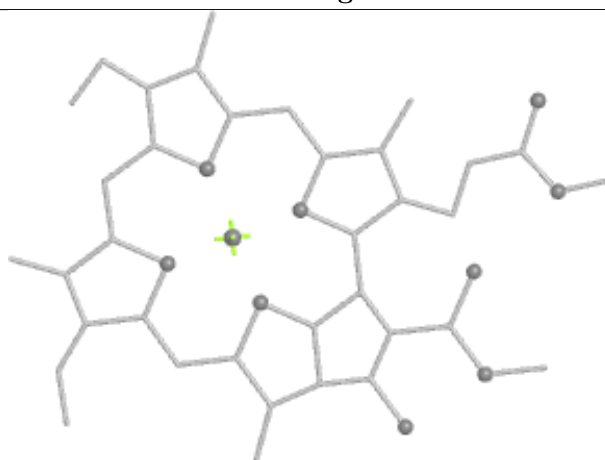
Bond lengths



Bond angles

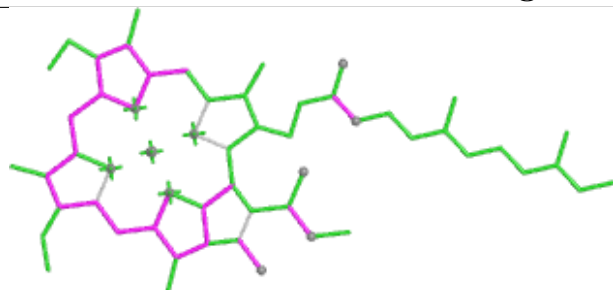


Torsions

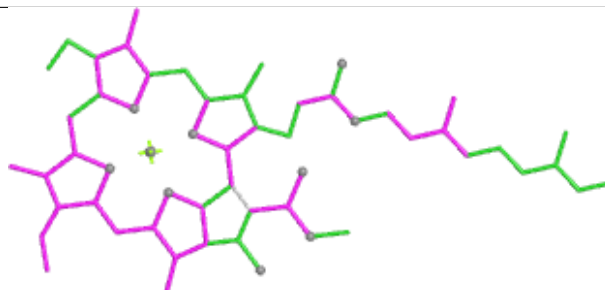


Rings

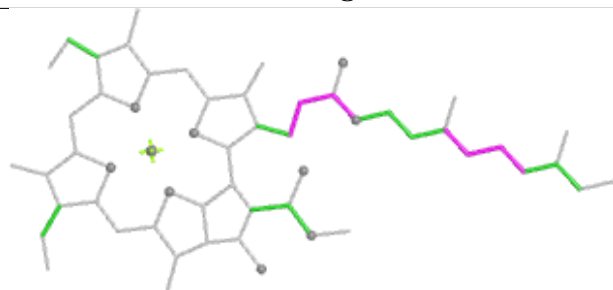
Ligand CLA 4 612



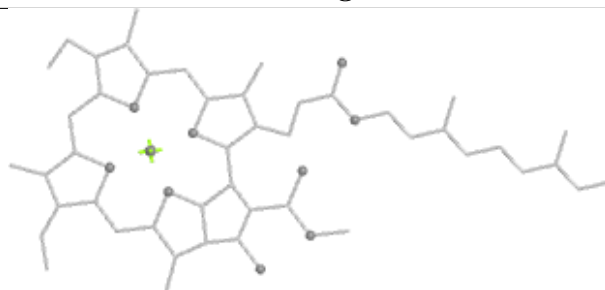
Bond lengths



Bond angles

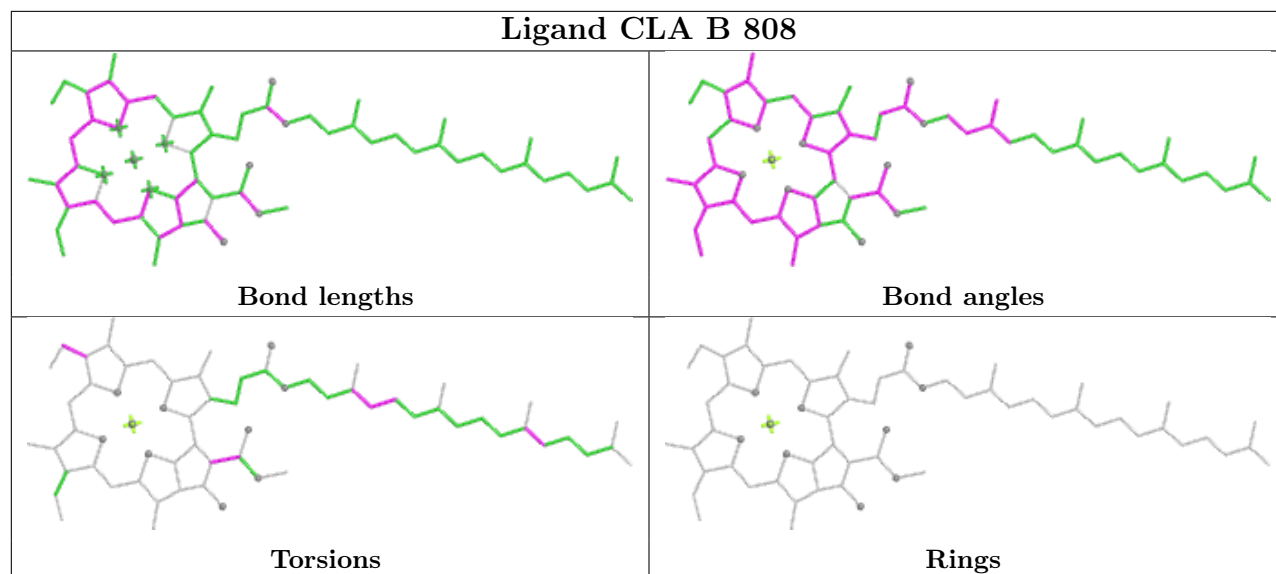


Torsions

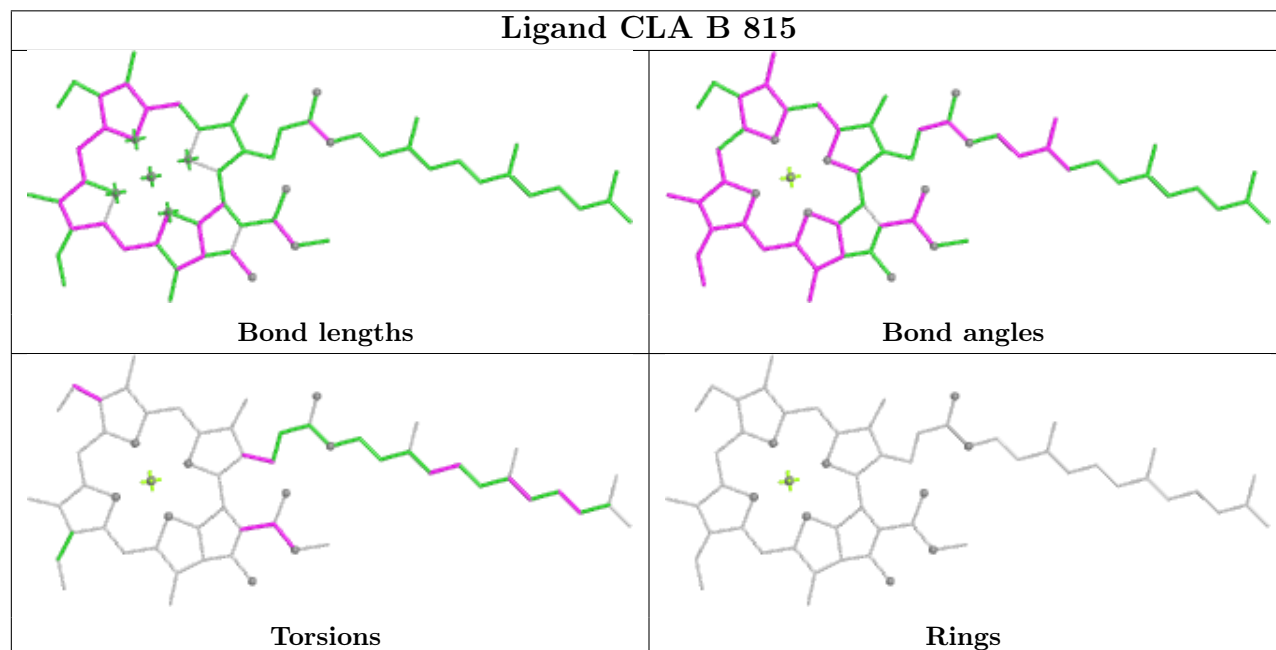


Rings

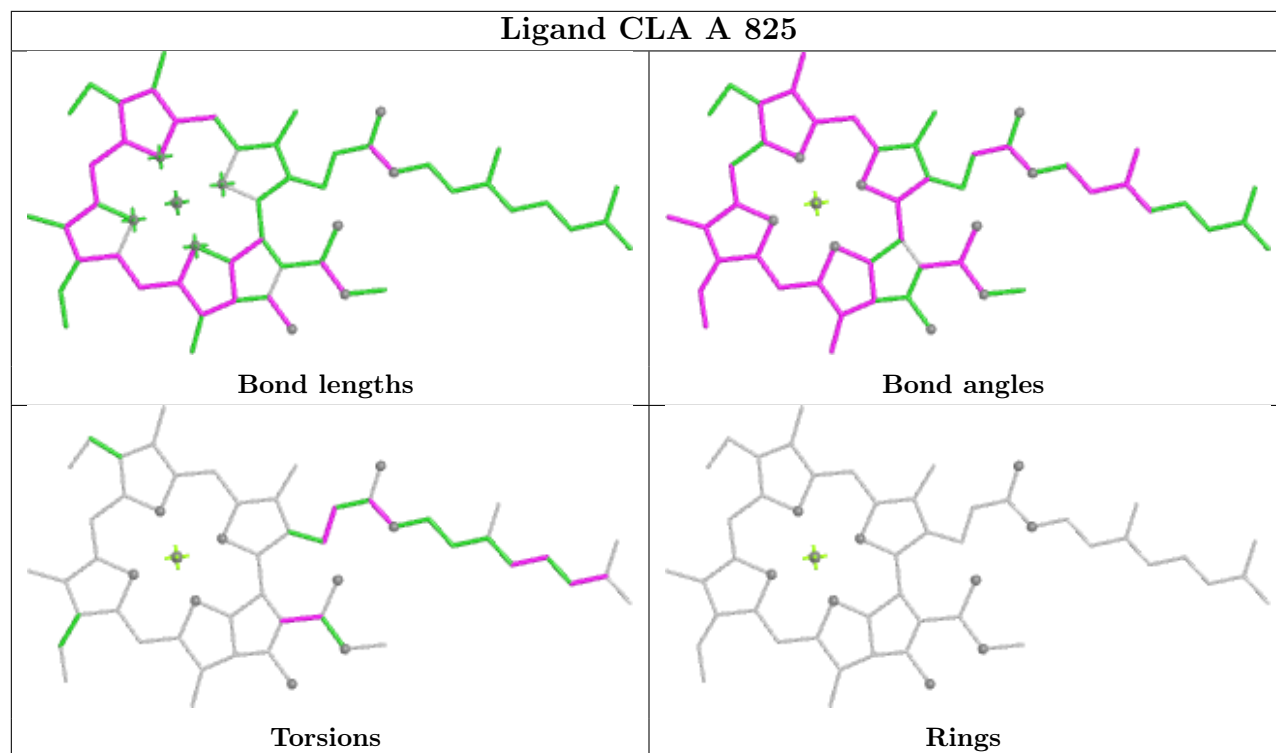
Ligand CLA B 808



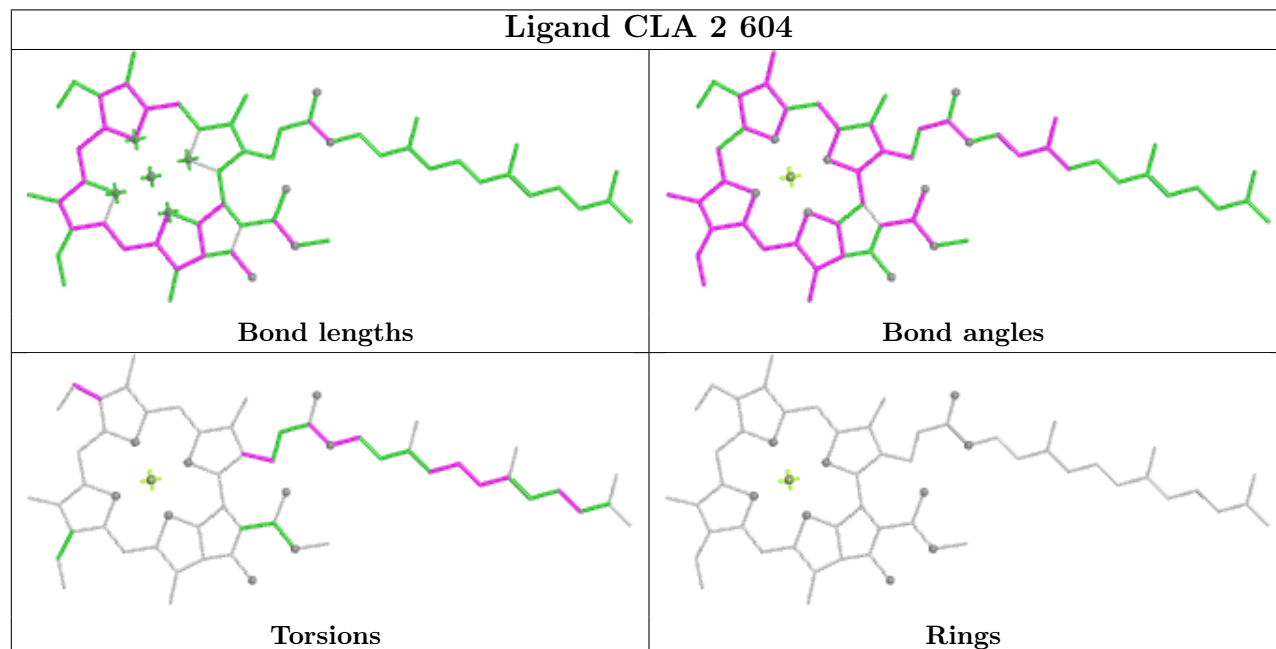
Ligand CLA B 815



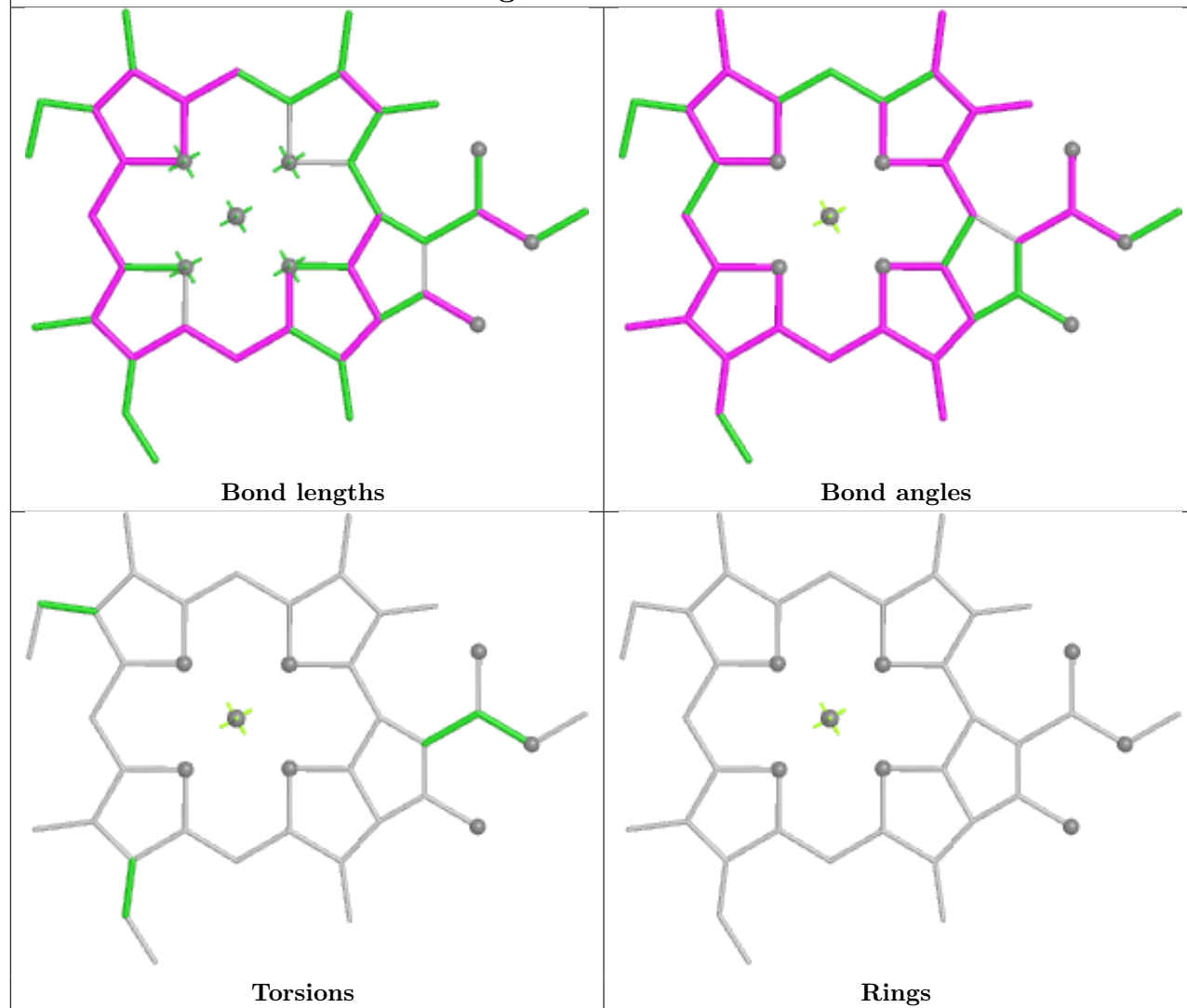
Ligand CLA A 825



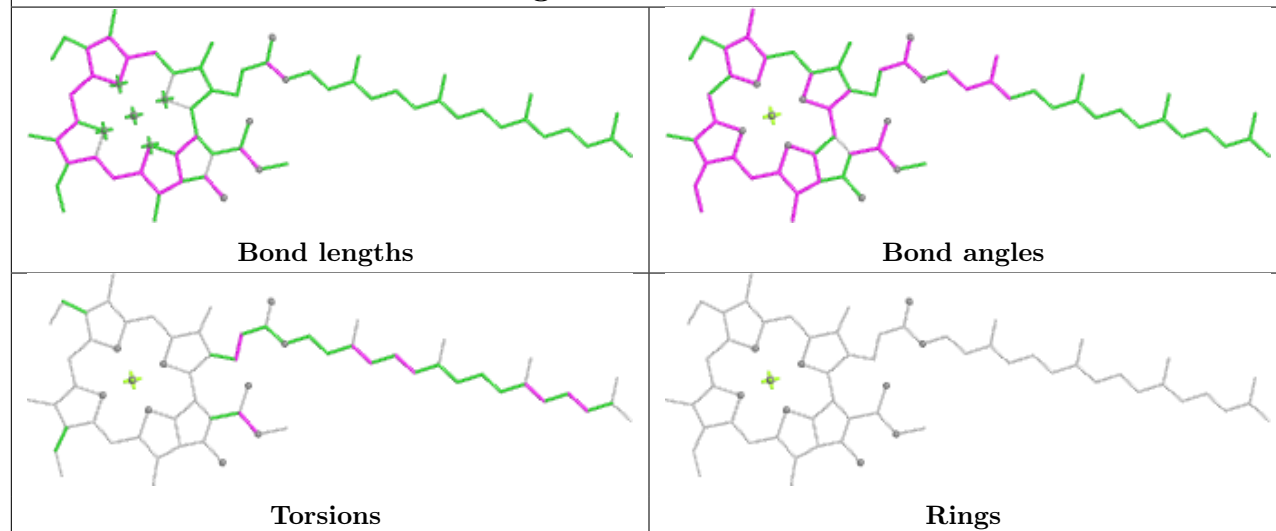
Ligand CLA 2 604



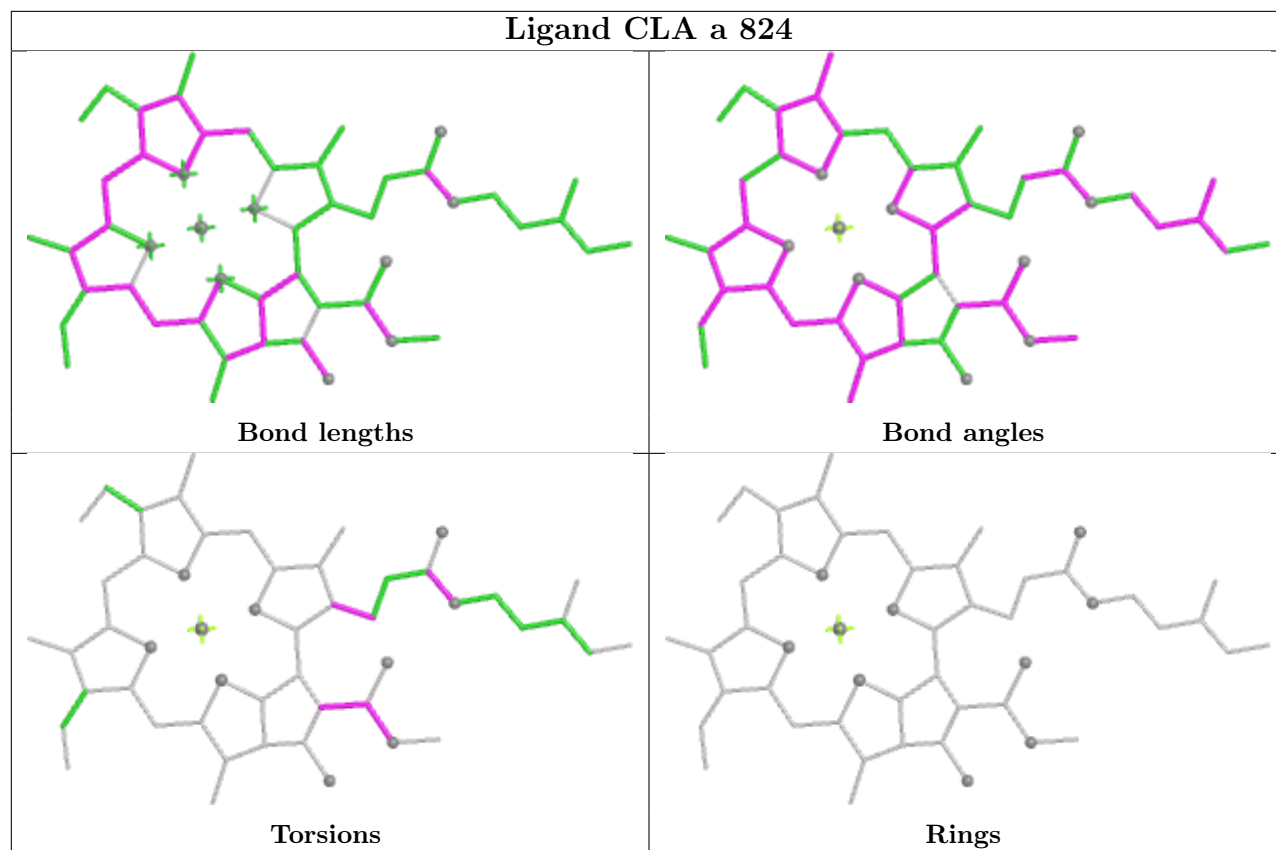
Ligand CLA 1 311



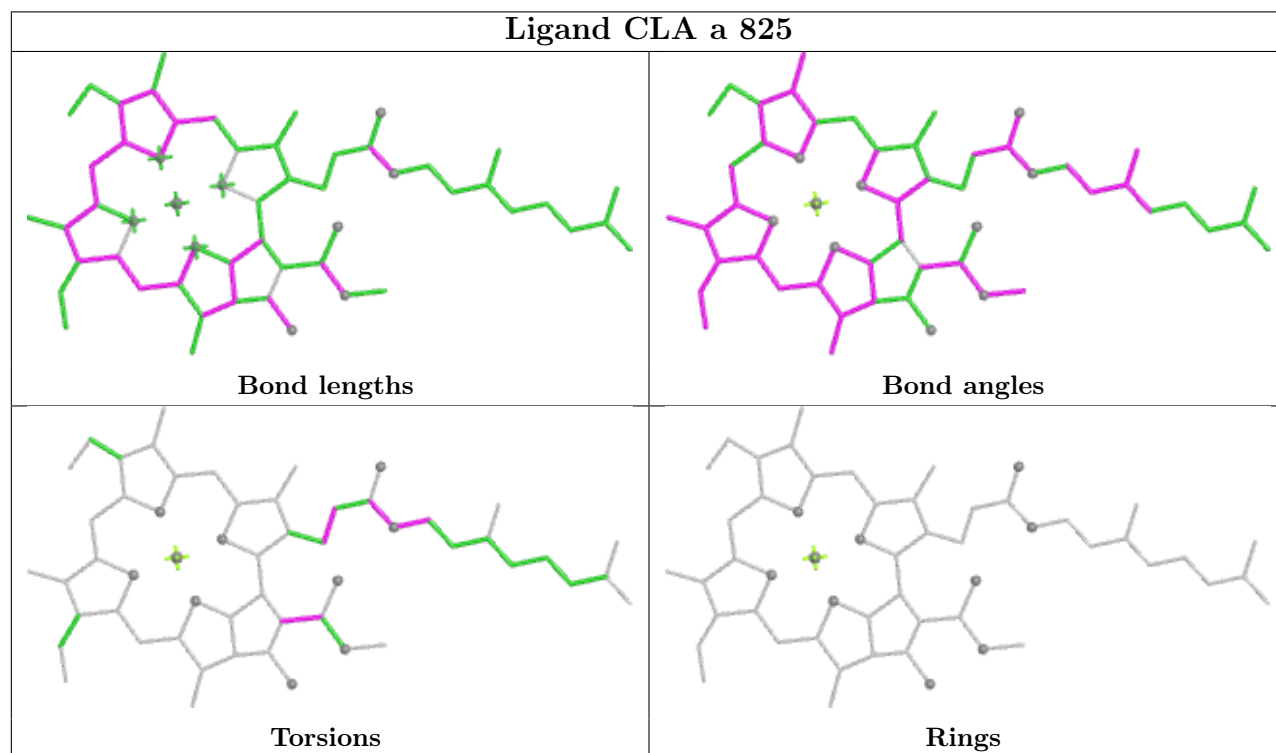
Ligand CLA B 840

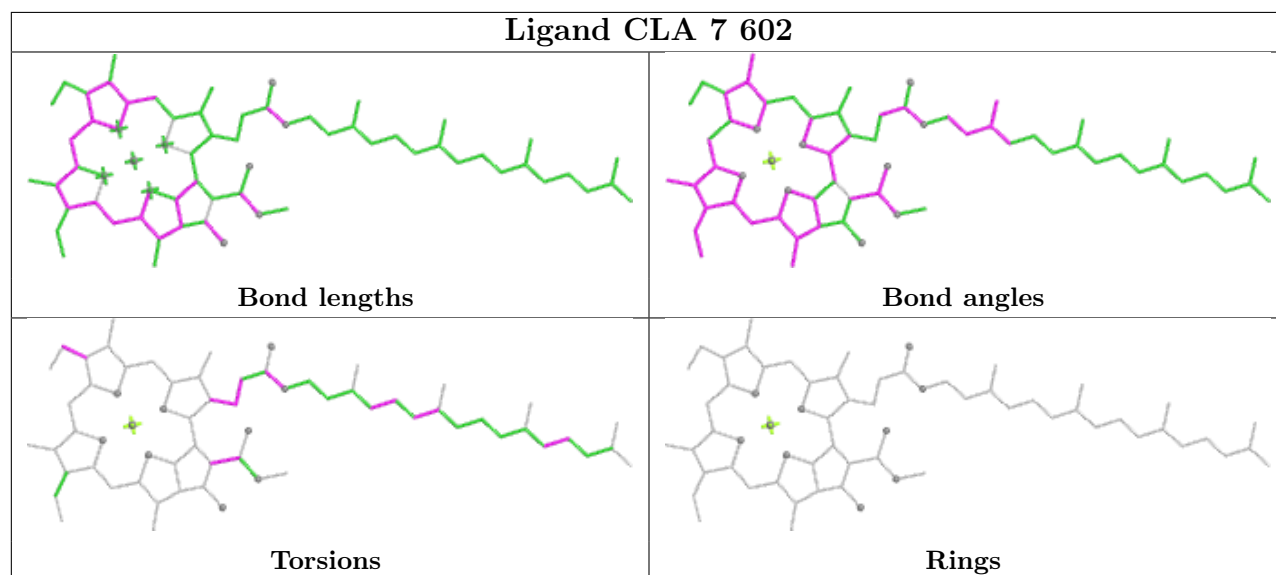
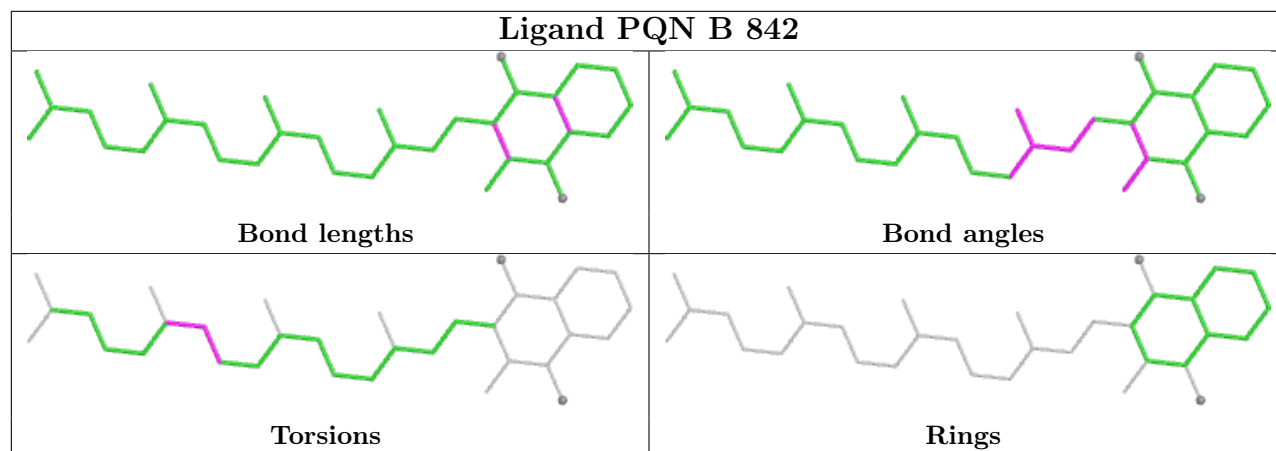


Ligand CLA a 824

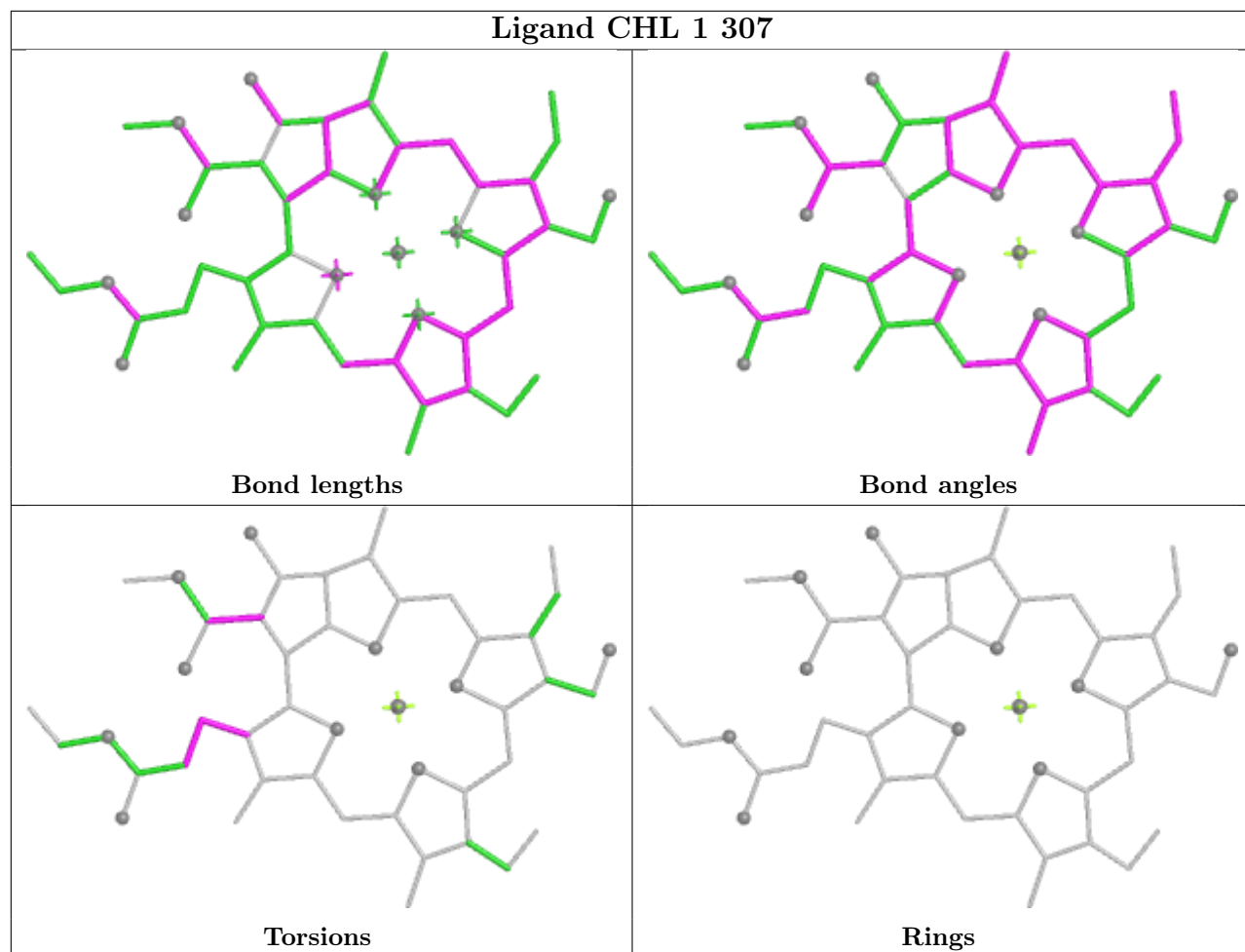


Ligand CLA a 825

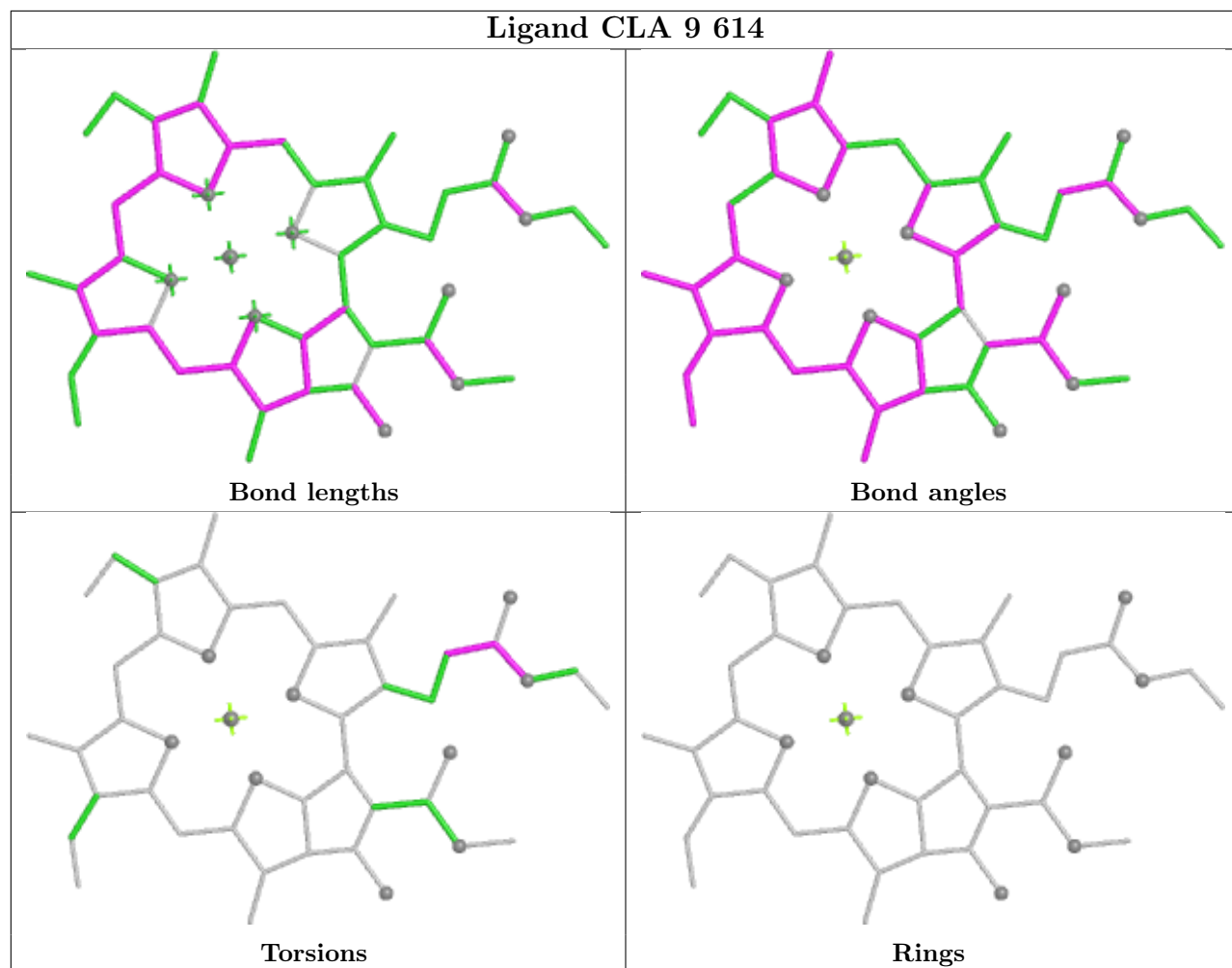




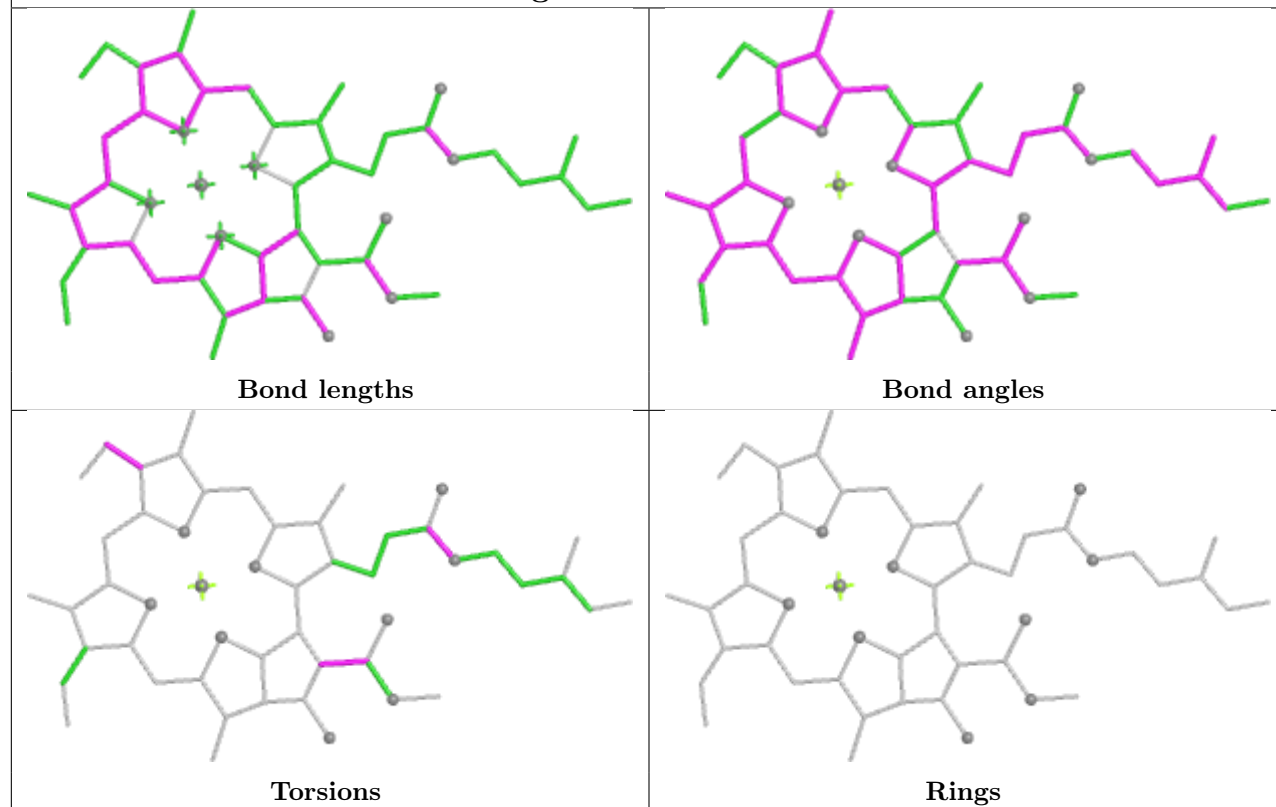
Ligand CHL 1 307



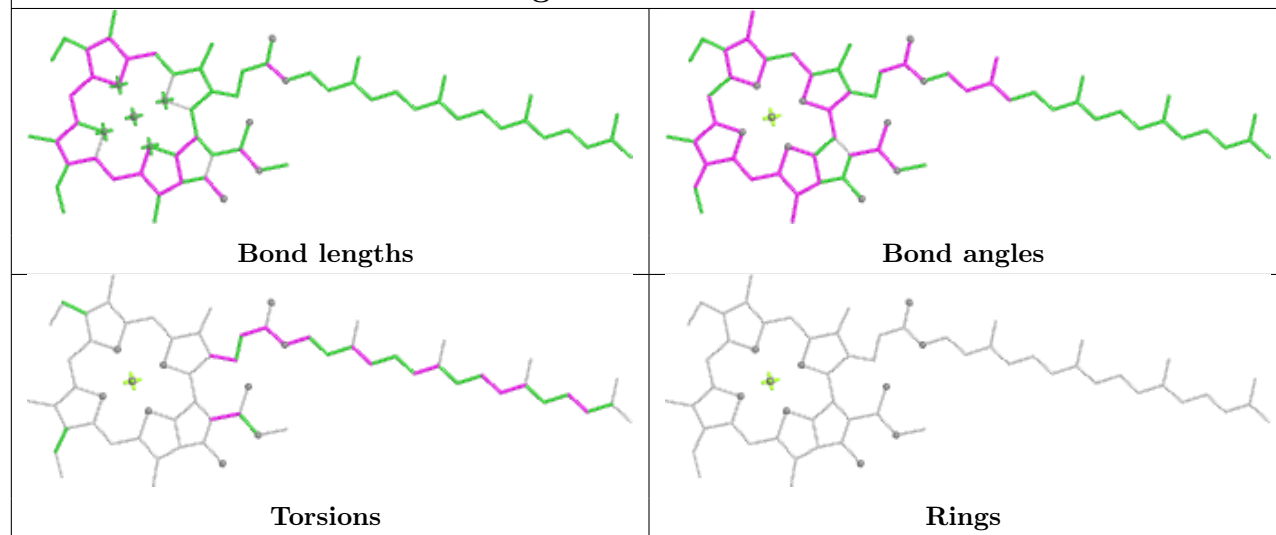
Ligand CLA 9 614



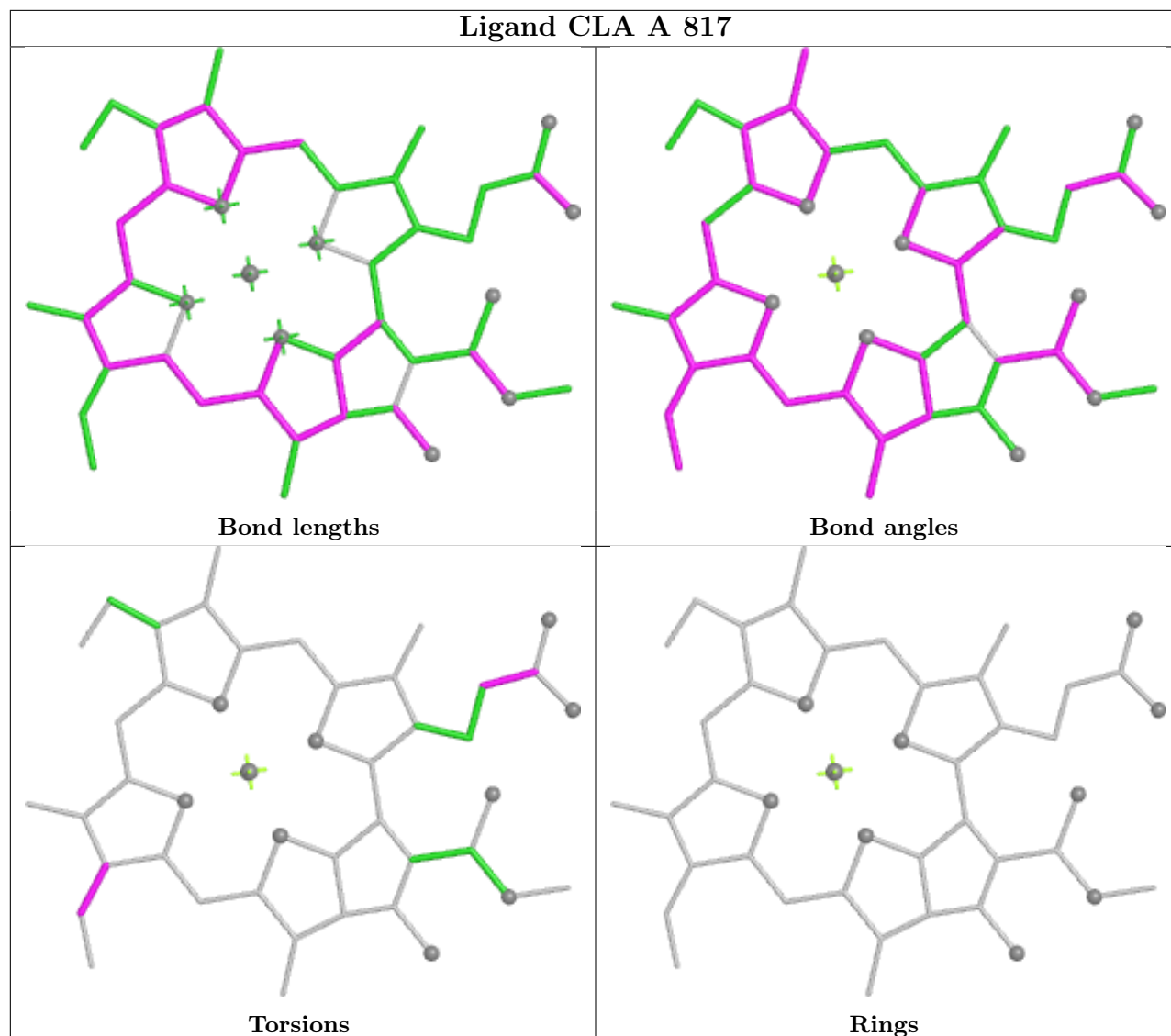
Ligand CLA A 838



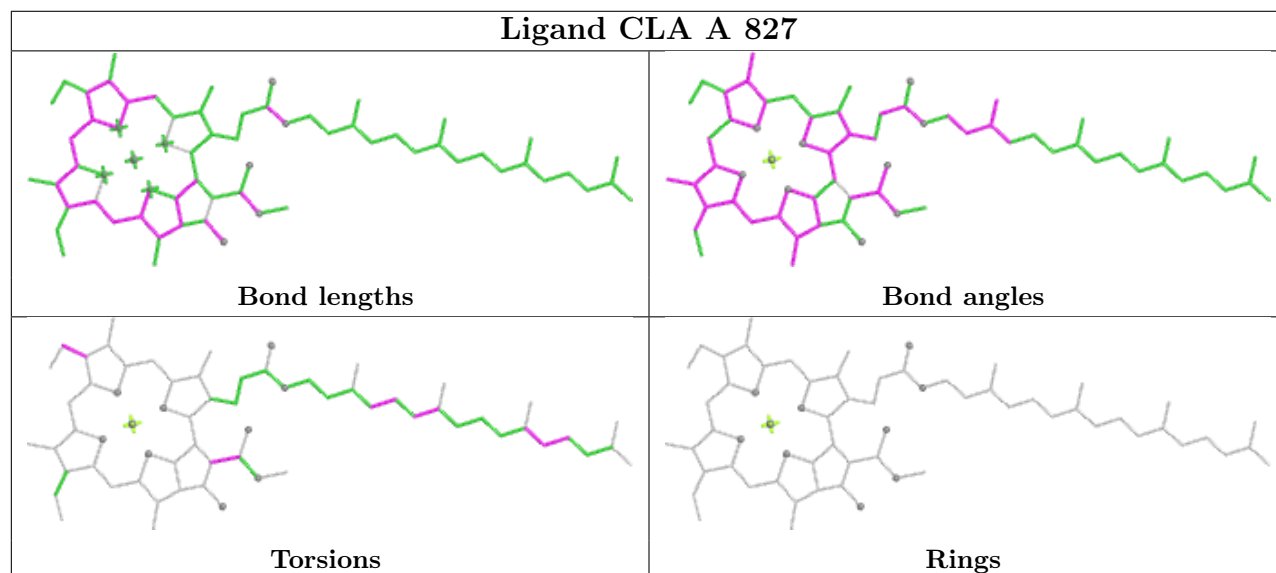
Ligand CLA B 805



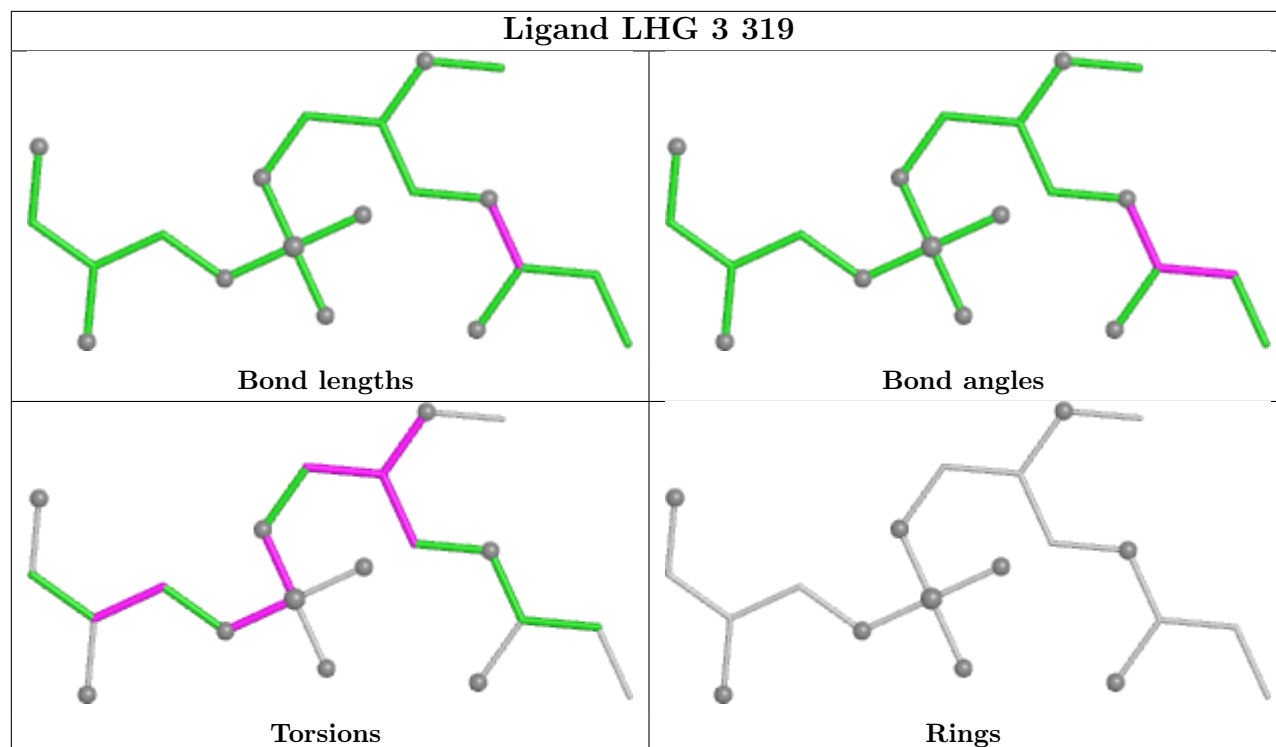
Ligand CLA A 817



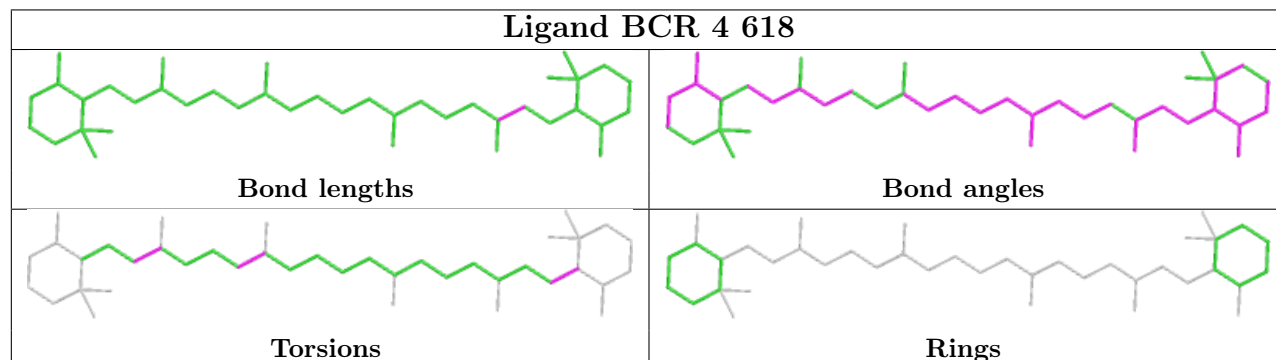
Ligand CLA A 827



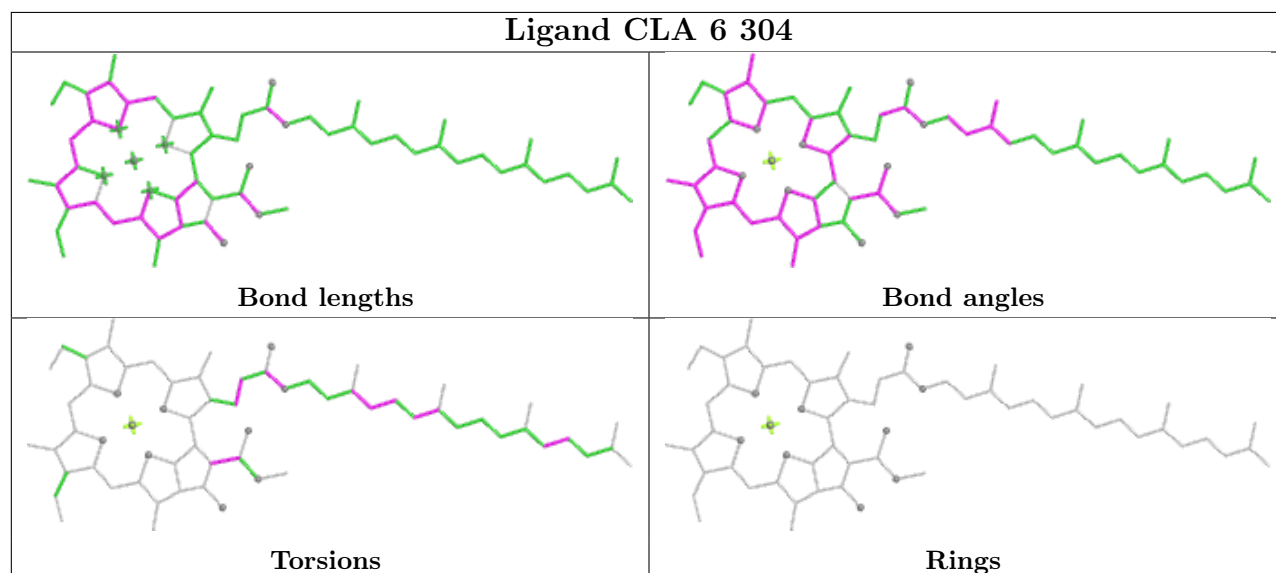
Ligand LHG 3 319



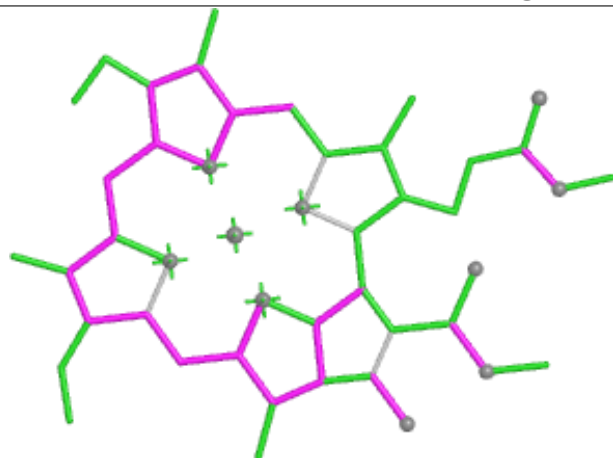
Ligand BCR 4 618



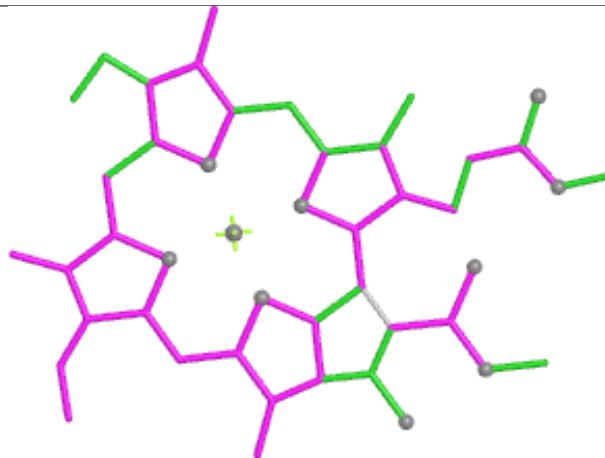
Ligand CLA 6 304



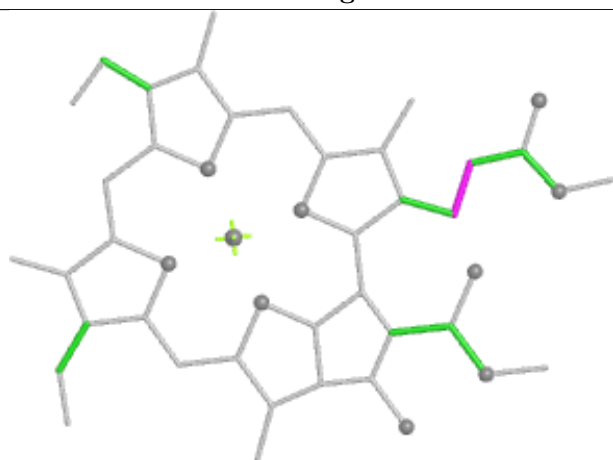
Ligand CLA 8 312



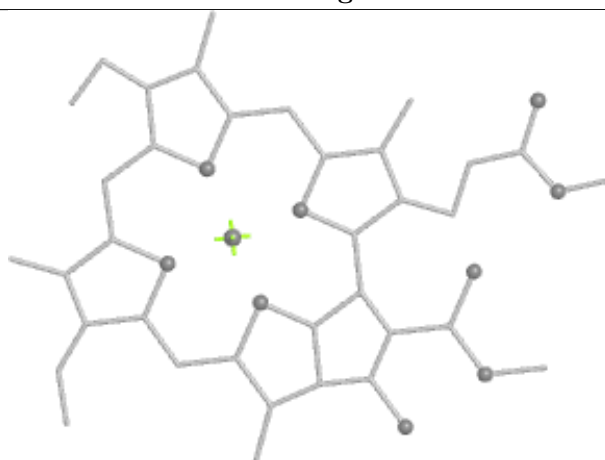
Bond lengths



Bond angles

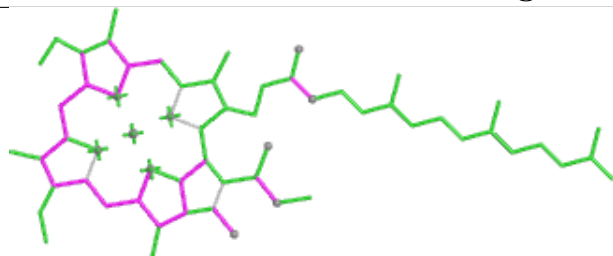


Torsions

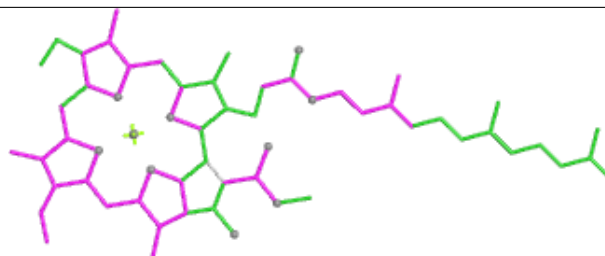


Rings

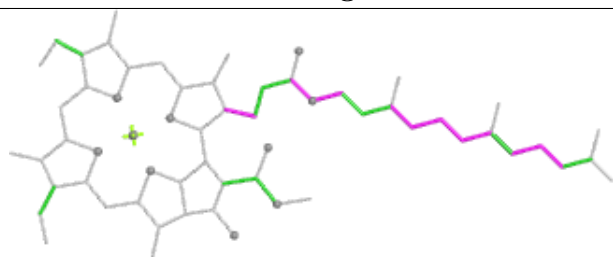
Ligand CLA b 818



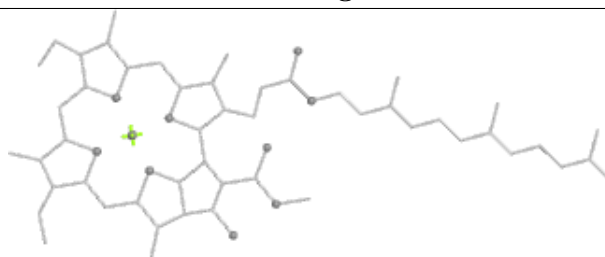
Bond lengths



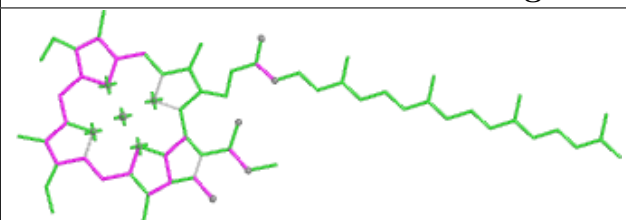
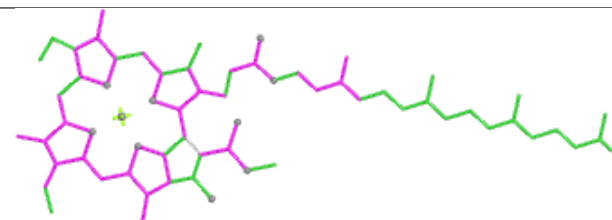
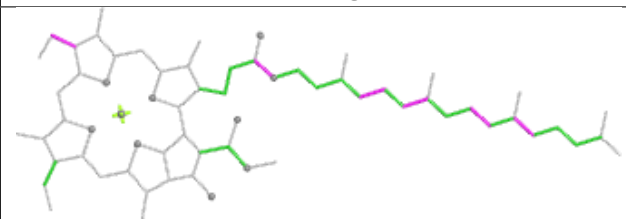
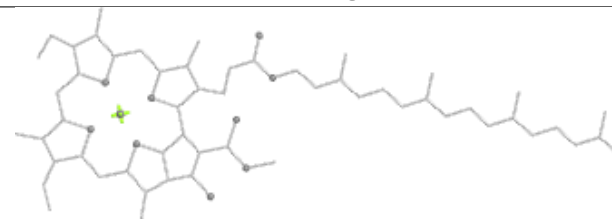
Bond angles

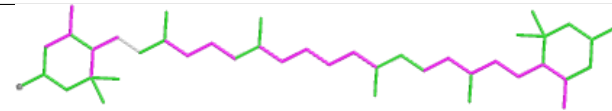
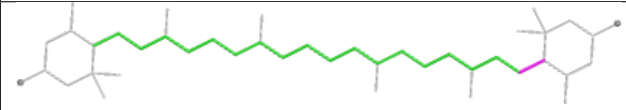
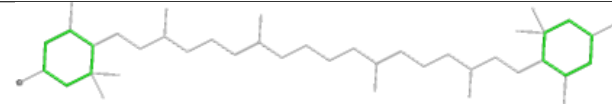


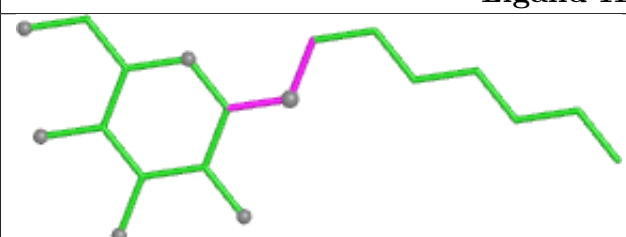
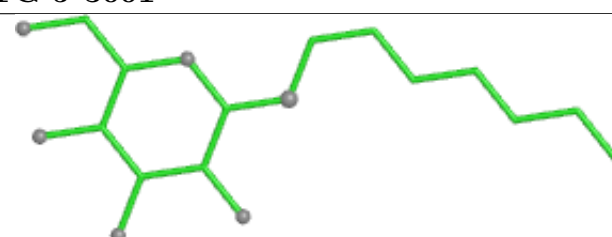
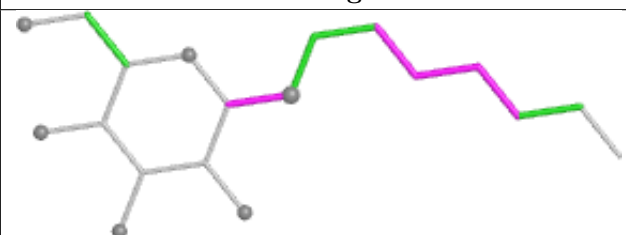
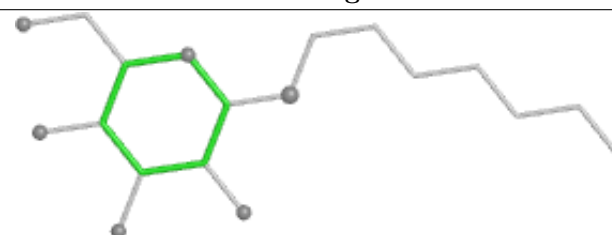
Torsions

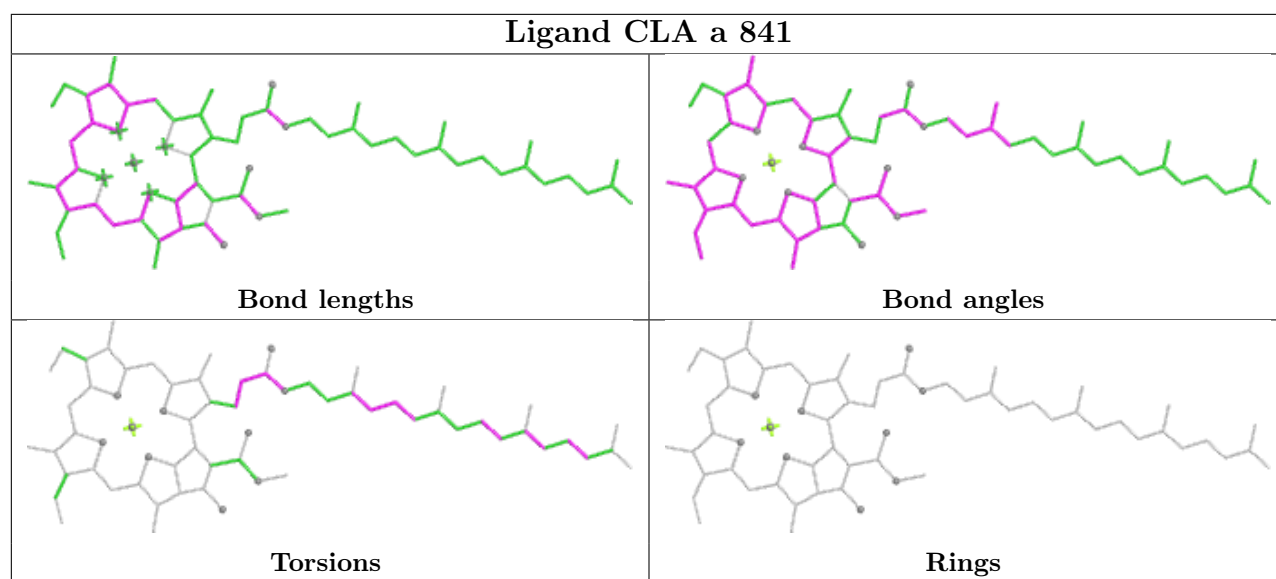


Rings

Ligand CLA b 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 2 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand HTG J 3001	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	742/742 (100%)	-0.07	7 (0%) 81 74	42, 58, 91, 169	0
1	a	742/742 (100%)	-0.27	5 (0%) 84 77	36, 48, 81, 140	0
2	B	733/733 (100%)	-0.07	12 (1%) 70 61	42, 56, 80, 121	0
2	b	733/733 (100%)	-0.09	9 (1%) 76 68	36, 55, 86, 139	0
3	C	80/80 (100%)	-0.06	0 100 100	50, 62, 77, 96	0
3	c	80/80 (100%)	0.03	0 100 100	44, 55, 72, 88	0
4	D	141/141 (100%)	0.12	3 (2%) 63 54	53, 71, 103, 163	0
4	d	140/141 (99%)	-0.01	4 (2%) 53 43	45, 61, 92, 132	0
5	E	63/64 (98%)	0.05	0 100 100	51, 77, 115, 127	0
5	e	63/64 (98%)	0.06	0 100 100	51, 78, 96, 119	0
6	F	151/151 (100%)	0.05	3 (1%) 65 56	50, 69, 98, 126	0
6	f	151/151 (100%)	0.08	4 (2%) 57 47	49, 73, 101, 132	0
7	G	95/95 (100%)	0.11	2 (2%) 63 54	60, 79, 103, 127	0
7	g	95/95 (100%)	0.45	6 (6%) 26 19	62, 83, 123, 171	0
8	H	90/90 (100%)	0.20	3 (3%) 49 39	61, 83, 116, 127	0
8	h	90/90 (100%)	0.16	4 (4%) 39 31	51, 70, 100, 111	0
9	I	29/30 (96%)	-0.04	1 (3%) 48 39	53, 65, 87, 117	0
9	i	30/30 (100%)	-0.24	2 (6%) 24 17	48, 56, 80, 129	0
10	J	39/39 (100%)	-0.16	1 (2%) 57 47	51, 62, 97, 100	0
10	j	39/39 (100%)	0.09	1 (2%) 57 47	48, 65, 94, 100	0
11	K	45/84 (53%)	0.47	1 (2%) 62 52	92, 111, 131, 142	0
11	k	46/84 (54%)	0.50	3 (6%) 25 18	68, 86, 126, 134	0
12	L	153/153 (100%)	0.46	7 (4%) 37 29	56, 80, 120, 143	0
12	l	151/153 (98%)	-0.00	2 (1%) 75 66	42, 60, 87, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	195/195 (100%)	0.31	8 (4%) 41 33	61, 87, 119, 136	0
13	6	195/195 (100%)	0.65	15 (7%) 19 14	74, 114, 164, 176	0
14	2	206/206 (100%)	0.51	10 (4%) 35 27	67, 97, 133, 188	0
14	7	206/206 (100%)	0.35	10 (4%) 35 27	61, 89, 122, 158	0
15	3	218/218 (100%)	0.34	4 (1%) 67 58	62, 96, 133, 154	0
15	8	217/218 (99%)	0.12	3 (1%) 73 64	56, 81, 112, 142	0
16	4	196/196 (100%)	0.43	6 (3%) 51 41	61, 85, 115, 160	0
16	9	196/196 (100%)	0.53	13 (6%) 24 18	65, 97, 134, 155	0
All	All	6350/6434 (98%)	0.08	149 (2%) 61 51	36, 68, 116, 188	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	2	87	GLU	6.3
16	9	164	GLY	5.6
16	9	122	ASN	5.3
7	g	35	VAL	4.7
7	G	35	VAL	4.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	CLA	8	309	52/65	0.50	0.24	155,164,169,259	0
17	CLA	a	846	52/65	0.59	0.17	86,102,115,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	LHG	3	319	20/49	0.62	0.17	152,157,193,194	0
17	CLA	3	310	37/65	0.67	0.17	179,186,191,221	0
27	LUT	6	321	42/42	0.68	0.19	107,113,133,134	0
20	BCR	L	206	40/40	0.69	0.26	146,151,156,156	0
23	LMT	B	849	35/35	0.70	0.15	80,97,102,103	0
17	CLA	A	845	52/65	0.70	0.16	90,115,146,149	0
17	CLA	6	316	46/65	0.72	0.17	152,162,171,203	0
17	CLA	8	311	45/65	0.72	0.14	100,110,122,161	0
17	CLA	3	301	46/65	0.74	0.14	142,149,154,175	0
17	CLA	K	4002	45/65	0.75	0.15	115,123,125,154	0
17	CLA	8	313	25/65	0.75	0.15	102,110,116,146	0
25	LMG	6	302	40/55	0.76	0.19	116,148,163,164	0
25	LMG	4	620	44/55	0.76	0.16	89,97,111,113	0
17	CLA	3	311	52/65	0.78	0.15	129,142,154,157	0
17	CLA	L	202	65/65	0.78	0.18	83,111,131,132	0
20	BCR	K	4004	40/40	0.80	0.17	94,115,138,138	0
17	CLA	k	1403	46/65	0.80	0.13	89,95,103,110	0
17	CLA	6	310	65/65	0.81	0.14	80,90,121,126	0
17	CLA	6	309	46/65	0.81	0.16	92,99,106,137	0
17	CLA	3	313	45/65	0.82	0.12	85,97,102,106	0
20	BCR	2	617	40/40	0.82	0.23	125,133,163,164	0
20	BCR	7	617	40/40	0.82	0.22	112,119,127,128	0
17	CLA	l	202	65/65	0.82	0.17	57,88,111,113	0
17	CLA	9	611	52/65	0.82	0.12	76,89,102,103	0
17	CLA	7	611	52/65	0.82	0.13	87,104,123,126	0
26	CHL	6	308	47/66	0.82	0.15	103,135,146,149	0
17	CLA	J	3002	42/65	0.82	0.12	92,105,119,148	0
17	CLA	j	3002	42/65	0.83	0.11	91,94,96,97	0
25	LMG	G	102	44/55	0.83	0.14	72,95,110,113	0
17	CLA	3	315	25/65	0.83	0.14	112,115,121,157	0
17	CLA	B	811	54/65	0.83	0.14	58,74,103,104	0
20	BCR	6	319	40/40	0.83	0.18	104,124,138,140	0
26	CHL	9	615	43/66	0.83	0.15	90,144,147,148	0
20	BCR	A	856	40/40	0.83	0.14	65,71,85,85	0
17	CLA	b	811	54/65	0.84	0.13	50,74,114,114	0
20	BCR	1	318	40/40	0.84	0.18	94,105,126,127	0
25	LMG	4	619	44/55	0.84	0.16	82,92,103,104	0
17	CLA	g	101	41/65	0.84	0.16	146,164,166,167	0
20	BCR	k	1404	40/40	0.84	0.14	49,89,103,104	0
26	CHL	2	606	48/66	0.84	0.12	89,97,105,107	0
20	BCR	l	206	40/40	0.84	0.16	77,82,93,93	0
17	CLA	1	309	65/65	0.84	0.15	71,79,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	CLA	2	604	60/65	0.84	0.14	100,111,118,119	0
17	CLA	2	613	43/65	0.85	0.12	80,88,94,95	0
17	CLA	A	837	45/65	0.85	0.12	84,95,103,165	0
17	CLA	6	312	41/65	0.85	0.14	90,102,109,129	0
17	CLA	6	313	52/65	0.85	0.14	83,94,119,120	0
20	BCR	b	844	40/40	0.85	0.15	52,67,91,93	0
25	LMG	9	619	50/55	0.85	0.15	68,88,96,98	0
26	CHL	2	605	43/66	0.85	0.11	77,89,100,106	0
17	CLA	A	824	51/65	0.85	0.14	77,89,118,118	0
20	BCR	A	848	40/40	0.85	0.15	50,59,95,95	0
17	CLA	2	608	50/65	0.85	0.13	65,69,108,111	0
27	LUT	4	616	42/42	0.85	0.16	71,90,94,95	0
27	LUT	6	317	42/42	0.85	0.16	86,93,118,120	0
20	BCR	K	4001	40/40	0.85	0.19	91,94,96,96	0
28	XAT	9	617	44/44	0.85	0.14	72,81,97,98	0
17	CLA	K	4003	46/65	0.86	0.14	81,119,128,130	0
17	CLA	k	1401	45/65	0.86	0.11	75,83,94,96	0
17	CLA	2	609	60/65	0.86	0.13	73,87,98,101	0
26	CHL	2	614	43/66	0.86	0.14	116,134,143,145	0
17	CLA	2	610	41/65	0.86	0.12	80,94,108,110	0
26	CHL	7	605	43/66	0.86	0.12	85,89,93,99	0
26	CHL	7	606	48/66	0.86	0.11	71,87,104,105	0
26	CHL	7	614	43/66	0.86	0.14	105,120,127,139	0
17	CLA	l	204	50/65	0.86	0.13	46,59,100,104	0
19	LHG	A	847	27/49	0.86	0.12	68,88,113,113	0
17	CLA	7	604	60/65	0.86	0.14	92,101,106,109	0
20	BCR	b	843	40/40	0.86	0.14	54,60,68,69	0
19	LHG	a	848	27/49	0.86	0.16	74,95,125,127	0
17	CLA	F	304	55/65	0.87	0.11	52,69,95,95	0
17	CLA	4	604	50/65	0.87	0.14	75,84,111,114	0
17	CLA	1	312	52/65	0.87	0.12	70,76,99,100	0
19	LHG	6	320	49/49	0.87	0.17	90,100,111,113	0
20	BCR	a	849	40/40	0.87	0.14	56,63,75,76	0
17	CLA	k	1402	46/65	0.87	0.12	62,78,100,106	0
27	LUT	1	320	42/42	0.87	0.12	71,79,90,91	0
17	CLA	1	315	46/65	0.87	0.09	76,87,93,132	0
20	BCR	j	3004	40/40	0.87	0.12	56,71,82,84	0
20	BCR	I	101	40/40	0.87	0.12	54,60,65,65	0
17	CLA	f	7003	55/65	0.87	0.12	68,87,121,122	0
17	CLA	8	308	50/65	0.88	0.11	75,81,87,88	0
17	CLA	g	102	50/65	0.88	0.12	92,107,123,124	0
17	CLA	g	103	46/65	0.88	0.11	87,99,103,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	L	204	50/65	0.88	0.13	76,84,109,109	0
26	CHL	4	615	43/66	0.88	0.10	61,74,87,89	0
26	CHL	6	303	61/66	0.88	0.13	78,91,102,103	0
20	BCR	4	618	40/40	0.88	0.17	79,86,89,90	0
20	BCR	8	316	40/40	0.88	0.16	66,71,88,90	0
22	HTG	J	3001	19/19	0.88	0.11	73,76,78,82	0
22	HTG	f	7001	19/19	0.88	0.14	49,104,107,108	0
17	CLA	9	604	50/65	0.88	0.13	105,116,125,126	0
24	DGD	b	849	66/66	0.88	0.13	41,64,90,91	0
20	BCR	a	852	40/40	0.88	0.12	40,62,120,120	0
17	CLA	4	610	55/65	0.88	0.11	72,88,94,122	0
17	CLA	B	821	46/65	0.88	0.12	51,60,72,80	0
20	BCR	g	104	40/40	0.88	0.14	57,102,117,118	0
20	BCR	b	846	40/40	0.89	0.11	48,56,76,77	0
26	CHL	2	601	61/66	0.89	0.14	68,99,113,115	0
17	CLA	3	305	42/65	0.89	0.09	67,78,84,90	0
17	CLA	1	314	55/65	0.89	0.12	78,93,105,110	0
20	BCR	B	845	40/40	0.89	0.12	47,63,102,102	0
26	CHL	4	605	56/66	0.89	0.12	69,88,96,102	0
20	BCR	B	846	40/40	0.89	0.12	49,53,70,70	0
17	CLA	G	104	46/65	0.89	0.10	70,93,100,111	0
17	CLA	b	817	59/65	0.89	0.12	56,59,67,68	0
17	CLA	6	315	55/65	0.89	0.12	105,114,131,131	0
17	CLA	2	611	52/65	0.89	0.11	68,83,119,128	0
17	CLA	9	613	45/65	0.89	0.12	87,105,115,137	0
26	CHL	9	606	51/66	0.89	0.13	86,106,118,119	0
17	CLA	9	614	47/65	0.89	0.10	62,75,97,99	0
17	CLA	1	310	60/65	0.89	0.12	63,80,90,92	0
17	CLA	7	610	41/65	0.89	0.10	74,82,94,99	0
17	CLA	A	816	50/65	0.89	0.11	52,70,108,108	0
17	CLA	7	613	43/65	0.89	0.10	73,78,82,86	0
27	LUT	7	615	42/42	0.89	0.13	72,83,97,98	0
19	LHG	7	618	37/49	0.89	0.15	83,95,102,104	0
22	HTG	F	302	19/19	0.90	0.16	43,98,105,107	0
17	CLA	B	812	55/65	0.90	0.11	53,62,106,107	0
17	CLA	B	817	59/65	0.90	0.11	46,53,59,64	0
22	HTG	j	3001	19/19	0.90	0.10	61,71,80,84	0
20	BCR	A	850	40/40	0.90	0.12	53,72,112,112	0
24	DGD	B	850	66/66	0.90	0.12	52,71,93,102	0
17	CLA	1	311	41/65	0.90	0.11	67,74,81,82	0
17	CLA	7	608	50/65	0.90	0.13	60,65,93,96	0
17	CLA	7	609	60/65	0.90	0.12	64,86,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	A	805	55/65	0.90	0.11	45,54,89,89	0
17	CLA	A	823	49/65	0.90	0.10	66,79,104,105	0
17	CLA	4	609	60/65	0.90	0.12	69,86,106,111	0
17	CLA	A	808	65/65	0.90	0.11	52,61,113,115	0
17	CLA	4	611	52/65	0.90	0.10	71,88,123,125	0
17	CLA	a	824	51/65	0.90	0.10	61,74,91,93	0
17	CLA	3	304	45/65	0.90	0.13	109,122,133,162	0
17	CLA	9	603	46/65	0.90	0.10	62,64,77,78	0
26	CHL	4	606	51/66	0.90	0.11	71,81,109,110	0
17	CLA	6	305	65/65	0.90	0.14	83,87,104,110	0
17	CLA	6	306	51/65	0.90	0.13	118,123,130,131	0
17	CLA	9	612	56/65	0.90	0.10	68,77,89,92	0
20	BCR	b	845	40/40	0.90	0.13	46,67,106,106	0
17	CLA	6	307	42/65	0.90	0.12	112,126,137,139	0
17	CLA	1	305	52/65	0.90	0.12	76,101,105,108	0
26	CHL	9	605	56/66	0.90	0.12	80,94,97,126	0
20	BCR	j	3003	40/40	0.90	0.11	42,52,59,61	0
26	CHL	9	607	51/66	0.90	0.12	67,77,98,99	0
17	CLA	3	309	50/65	0.90	0.12	76,95,104,107	0
19	LHG	1	301	23/49	0.90	0.14	63,84,93,94	0
27	LUT	3	316	42/42	0.90	0.11	74,78,97,99	0
19	LHG	1	319	49/49	0.90	0.14	77,84,109,109	0
17	CLA	6	311	60/65	0.90	0.13	81,99,115,116	0
17	CLA	b	821	46/65	0.90	0.11	58,69,90,118	0
17	CLA	b	835	45/65	0.90	0.10	86,92,94,96	0
27	LUT	8	314	42/42	0.90	0.12	57,73,82,84	0
27	LUT	9	616	42/42	0.90	0.13	68,79,103,104	0
28	XAT	8	315	44/44	0.90	0.12	64,69,80,83	0
20	BCR	9	618	40/40	0.90	0.13	86,92,100,101	0
17	CLA	1	308	65/65	0.91	0.14	57,92,120,121	0
17	CLA	G	101	45/65	0.91	0.10	74,79,85,89	0
17	CLA	4	613	45/65	0.91	0.12	92,103,108,160	0
22	HTG	A	855	19/19	0.91	0.09	68,72,74,75	0
17	CLA	a	816	50/65	0.91	0.11	43,52,94,96	0
19	LHG	2	618	37/49	0.91	0.13	80,91,127,130	0
22	HTG	a	857	19/19	0.91	0.08	53,70,79,81	0
17	CLA	a	817	45/65	0.91	0.10	64,73,78,79	0
17	CLA	a	823	49/65	0.91	0.10	60,67,102,104	0
19	LHG	6	301	23/49	0.91	0.12	67,101,110,111	0
17	CLA	A	822	65/65	0.91	0.12	49,67,76,79	0
17	CLA	3	303	50/65	0.91	0.10	60,67,75,76	0
17	CLA	b	807	65/65	0.91	0.12	42,51,102,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	B	816	55/65	0.91	0.12	60,67,73,91	0
20	BCR	A	851	40/40	0.91	0.12	43,66,78,79	0
17	CLA	b	812	55/65	0.91	0.12	59,70,103,104	0
20	BCR	B	801	40/40	0.91	0.12	43,46,54,55	0
26	CHL	1	307	48/66	0.91	0.12	75,95,109,110	0
20	BCR	B	843	40/40	0.91	0.13	54,64,72,72	0
20	BCR	B	844	40/40	0.91	0.13	50,53,85,87	0
17	CLA	b	814	65/65	0.91	0.10	47,55,69,71	0
26	CHL	2	607	51/66	0.91	0.12	66,75,117,118	0
17	CLA	b	815	55/65	0.91	0.11	62,78,93,94	0
20	BCR	G	105	40/40	0.91	0.12	63,71,83,83	0
17	CLA	b	816	55/65	0.91	0.10	57,65,72,75	0
17	CLA	A	832	50/65	0.91	0.11	52,70,98,99	0
17	CLA	b	820	50/65	0.91	0.12	65,72,77,82	0
17	CLA	B	818	60/65	0.91	0.10	45,50,57,61	0
17	CLA	b	834	65/65	0.91	0.10	61,74,105,106	0
17	CLA	8	303	45/65	0.91	0.12	75,92,99,133	0
20	BCR	3	318	40/40	0.91	0.13	77,83,105,108	0
17	CLA	8	304	42/65	0.91	0.10	59,72,78,80	0
17	CLA	B	807	65/65	0.91	0.13	51,66,113,117	0
17	CLA	2	603	65/65	0.91	0.11	64,72,106,108	0
17	CLA	8	310	55/65	0.91	0.10	74,88,99,104	0
27	LUT	1	316	42/42	0.91	0.12	69,74,100,101	0
17	CLA	3	312	55/65	0.91	0.12	86,107,114,117	0
27	LUT	2	615	42/42	0.91	0.12	77,84,89,89	0
17	CLA	B	835	45/65	0.91	0.09	57,66,70,72	0
17	CLA	3	314	46/65	0.91	0.10	73,78,101,103	0
17	CLA	1	304	65/65	0.91	0.12	63,70,95,97	0
20	BCR	i	101	40/40	0.91	0.10	36,45,49,50	0
17	CLA	9	609	60/65	0.91	0.12	72,93,107,108	0
17	CLA	9	610	41/65	0.91	0.11	99,103,113,114	0
17	CLA	4	603	46/65	0.91	0.11	54,62,69,72	0
28	XAT	3	317	44/44	0.91	0.14	61,74,100,101	0
28	XAT	4	617	44/44	0.91	0.12	63,72,87,88	0
28	XAT	6	318	44/44	0.91	0.12	71,81,94,95	0
28	XAT	7	616	44/44	0.91	0.13	57,64,73,74	0
17	CLA	A	835	65/65	0.91	0.13	58,67,75,81	0
17	CLA	1	306	52/65	0.91	0.10	90,99,109,111	0
20	BCR	A	849	40/40	0.92	0.10	54,62,83,84	0
17	CLA	B	814	65/65	0.92	0.10	50,57,80,82	0
17	CLA	b	810	65/65	0.92	0.10	39,49,59,62	0
17	CLA	1	303	65/65	0.92	0.12	60,67,83,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	B	815	60/65	0.92	0.11	60,72,100,102	0
17	CLA	3	308	50/65	0.92	0.11	76,86,93,104	0
17	CLA	A	834	65/65	0.92	0.10	49,60,71,75	0
17	CLA	A	818	65/65	0.92	0.11	58,71,95,97	0
17	CLA	A	836	50/65	0.92	0.10	60,73,80,86	0
20	BCR	B	848	40/40	0.92	0.10	40,45,51,52	0
20	BCR	F	305	40/40	0.92	0.10	46,51,58,60	0
17	CLA	b	818	60/65	0.92	0.10	44,47,53,56	0
26	CHL	1	302	61/66	0.92	0.11	64,74,101,105	0
17	CLA	A	810	65/65	0.92	0.10	43,51,85,89	0
20	BCR	J	3003	40/40	0.92	0.10	45,54,67,68	0
17	CLA	B	822	55/65	0.92	0.10	48,58,82,83	0
17	CLA	b	830	50/65	0.92	0.10	46,59,70,74	0
20	BCR	L	201	40/40	0.92	0.11	51,59,72,73	0
17	CLA	b	831	49/65	0.92	0.10	51,55,71,71	0
26	CHL	3	307	47/66	0.92	0.10	72,77,94,97	0
17	CLA	b	832	65/65	0.92	0.11	36,55,70,79	0
17	CLA	B	823	60/65	0.92	0.10	46,57,84,84	0
26	CHL	4	607	51/66	0.92	0.13	57,73,82,85	0
17	CLA	B	834	65/65	0.92	0.11	46,58,90,90	0
17	CLA	9	601	46/65	0.92	0.11	81,91,95,110	0
17	CLA	b	841	65/65	0.92	0.12	64,80,92,94	0
26	CHL	7	601	61/66	0.92	0.11	62,74,93,95	0
20	BCR	a	850	40/40	0.92	0.10	39,48,79,81	0
20	BCR	a	851	40/40	0.92	0.09	37,53,66,67	0
26	CHL	7	607	51/66	0.92	0.12	64,70,92,98	0
17	CLA	4	601	46/65	0.92	0.10	84,92,95,111	0
26	CHL	8	306	47/66	0.92	0.10	60,64,79,84	0
20	BCR	a	853	40/40	0.92	0.12	44,48,66,67	0
17	CLA	A	839	65/65	0.92	0.11	54,60,80,83	0
17	CLA	F	301	65/65	0.92	0.12	48,55,83,87	0
17	CLA	A	840	65/65	0.92	0.11	48,55,95,96	0
17	CLA	A	841	65/65	0.92	0.10	44,50,55,60	0
20	BCR	b	847	40/40	0.92	0.09	40,49,69,70	0
20	BCR	f	7004	40/40	0.92	0.10	55,62,66,66	0
17	CLA	A	813	54/65	0.92	0.10	60,68,77,95	0
17	CLA	A	804	65/65	0.92	0.10	46,58,70,71	0
17	CLA	4	614	50/65	0.92	0.10	60,68,90,91	0
17	CLA	a	804	65/65	0.92	0.10	36,52,71,73	0
17	CLA	a	809	65/65	0.92	0.10	36,39,53,57	0
20	BCR	l	205	40/40	0.92	0.10	39,46,52,54	0
17	CLA	B	810	65/65	0.92	0.12	59,77,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	XAT	2	616	44/44	0.92	0.12	69,79,86,87	0
17	CLA	A	817	45/65	0.92	0.10	66,75,86,92	0
17	CLA	a	819	65/65	0.92	0.12	38,54,96,99	0
17	CLA	2	612	65/65	0.92	0.12	70,93,113,118	0
17	CLA	A	833	65/65	0.92	0.10	54,61,101,102	0
17	CLA	a	843	65/65	0.92	0.10	35,39,60,65	0
17	CLA	L	203	65/65	0.92	0.12	64,74,87,89	0
17	CLA	B	833	58/65	0.93	0.10	43,52,79,80	0
17	CLA	A	812	65/65	0.93	0.10	49,63,74,82	0
17	CLA	7	602	65/65	0.93	0.11	62,70,88,93	0
17	CLA	7	603	51/65	0.93	0.10	52,60,97,98	0
20	BCR	B	847	40/40	0.93	0.10	44,49,52,53	0
17	CLA	4	608	50/65	0.93	0.10	56,66,76,86	0
17	CLA	A	819	65/65	0.93	0.12	54,65,117,120	0
17	CLA	B	836	60/65	0.93	0.11	43,46,97,97	0
17	CLA	B	803	65/65	0.93	0.10	39,50,61,68	0
17	CLA	4	612	56/65	0.93	0.10	63,78,87,88	0
17	CLA	3	302	60/65	0.93	0.10	67,79,85,95	0
17	CLA	8	302	50/65	0.93	0.09	46,54,73,74	0
17	CLA	b	822	55/65	0.93	0.08	46,60,80,83	0
20	BCR	L	205	40/40	0.93	0.11	51,61,70,71	0
17	CLA	b	823	60/65	0.93	0.10	50,60,92,94	0
17	CLA	b	829	65/65	0.93	0.10	39,54,67,69	0
17	CLA	A	825	55/65	0.93	0.09	58,67,74,78	0
17	CLA	a	802	65/65	0.93	0.10	35,42,56,62	0
17	CLA	B	809	65/65	0.93	0.11	41,50,81,82	0
17	CLA	8	312	46/65	0.93	0.09	57,66,99,103	0
17	CLA	b	833	58/65	0.93	0.11	48,63,77,78	0
17	CLA	a	808	65/65	0.93	0.10	54,63,86,87	0
17	CLA	9	602	60/65	0.93	0.10	60,67,74,86	0
17	CLA	G	103	50/65	0.93	0.10	61,80,91,93	0
17	CLA	b	836	60/65	0.93	0.10	43,53,106,107	0
17	CLA	9	608	50/65	0.93	0.11	72,78,103,105	0
17	CLA	a	810	65/65	0.93	0.10	44,59,94,95	0
17	CLA	a	812	65/65	0.93	0.11	47,59,70,77	0
17	CLA	3	306	47/65	0.93	0.09	67,79,90,91	0
20	BCR	b	848	40/40	0.93	0.10	37,42,45,47	0
17	CLA	A	828	65/65	0.93	0.10	49,61,79,84	0
17	CLA	1	313	65/65	0.93	0.12	81,88,108,112	0
17	CLA	a	821	45/65	0.93	0.09	51,62,70,87	0
17	CLA	a	822	65/65	0.93	0.09	42,46,53,57	0
17	CLA	A	821	45/65	0.93	0.09	69,74,88,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	A	811	65/65	0.93	0.10	54,69,89,90	0
20	BCR	l	201	40/40	0.93	0.10	38,46,54,54	0
17	CLA	a	827	65/65	0.93	0.10	35,41,82,85	0
17	CLA	l	203	65/65	0.93	0.09	40,51,71,73	0
17	CLA	a	837	45/65	0.93	0.08	57,65,74,77	0
17	CLA	6	304	65/65	0.93	0.13	66,79,104,106	0
17	CLA	a	838	51/65	0.93	0.10	36,40,63,68	0
28	XAT	1	317	44/44	0.93	0.11	63,68,93,96	0
17	CLA	a	839	65/65	0.93	0.11	36,43,65,69	0
17	CLA	a	842	65/65	0.93	0.12	47,59,96,98	0
17	CLA	2	602	65/65	0.93	0.11	66,73,80,83	0
17	CLA	B	825	65/65	0.93	0.12	42,50,83,88	0
17	CLA	B	827	65/65	0.93	0.12	49,61,78,80	0
17	CLA	B	829	65/65	0.93	0.11	42,50,76,77	0
17	CLA	B	832	65/65	0.93	0.11	43,48,73,76	0
17	CLA	A	814	65/65	0.94	0.10	50,59,67,68	0
17	CLA	A	854	65/65	0.94	0.11	40,44,57,59	0
17	CLA	B	802	65/65	0.94	0.10	40,44,50,52	0
17	CLA	8	305	47/65	0.94	0.09	61,71,78,79	0
17	CLA	A	815	45/65	0.94	0.09	54,59,65,70	0
17	CLA	4	602	60/65	0.94	0.10	54,67,73,74	0
17	CLA	B	804	45/65	0.94	0.08	44,50,68,77	0
17	CLA	a	828	65/65	0.94	0.10	37,44,67,72	0
17	CLA	b	837	65/65	0.94	0.09	46,57,69,70	0
17	CLA	a	829	65/65	0.94	0.09	35,41,56,58	0
17	CLA	a	833	65/65	0.94	0.10	39,46,98,102	0
17	CLA	a	834	65/65	0.94	0.08	37,44,48,50	0
17	CLA	a	836	50/65	0.94	0.08	42,54,73,74	0
17	CLA	B	824	65/65	0.94	0.10	48,53,70,74	0
17	CLA	B	806	65/65	0.94	0.09	43,52,60,64	0
17	CLA	A	820	65/65	0.94	0.09	46,50,57,58	0
17	CLA	A	826	65/65	0.94	0.10	47,57,65,66	0
17	CLA	B	830	50/65	0.94	0.09	45,56,75,75	0
20	BCR	b	801	40/40	0.94	0.09	36,43,52,55	0
17	CLA	B	831	49/65	0.94	0.09	45,53,62,65	0
17	CLA	b	806	65/65	0.94	0.09	39,43,52,65	0
17	CLA	A	827	65/65	0.94	0.11	40,60,97,98	0
18	PQN	A	844	33/33	0.94	0.10	42,45,57,58	0
18	PQN	B	842	33/33	0.94	0.10	46,56,63,63	0
18	PQN	a	845	33/33	0.94	0.10	35,48,54,58	0
17	CLA	b	809	65/65	0.94	0.10	39,50,72,75	0
17	CLA	A	802	65/65	0.94	0.11	41,45,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	A	829	65/65	0.94	0.09	42,46,55,58	0
17	CLA	A	809	65/65	0.94	0.09	44,51,63,65	0
17	CLA	b	813	65/65	0.94	0.10	44,57,67,69	0
17	CLA	A	842	65/65	0.94	0.09	42,45,56,65	0
17	CLA	B	838	47/65	0.94	0.09	43,48,65,68	0
17	CLA	B	839	65/65	0.94	0.10	53,60,69,72	0
17	CLA	a	811	65/65	0.94	0.11	42,59,94,96	0
17	CLA	6	314	60/65	0.94	0.12	66,109,124,125	0
17	CLA	B	841	65/65	0.94	0.10	49,56,63,68	0
17	CLA	b	819	65/65	0.94	0.09	50,57,92,95	0
17	CLA	a	813	54/65	0.94	0.09	43,51,60,70	0
20	BCR	A	852	40/40	0.94	0.09	42,44,49,50	0
17	CLA	a	815	45/65	0.94	0.08	41,54,63,63	0
17	CLA	A	843	65/65	0.94	0.10	48,64,79,81	0
17	CLA	F	303	45/65	0.94	0.08	51,60,71,76	0
17	CLA	b	825	65/65	0.94	0.11	38,55,82,83	0
17	CLA	b	826	65/65	0.94	0.10	48,55,59,62	0
17	CLA	b	828	65/65	0.94	0.10	41,47,56,56	0
17	CLA	7	612	65/65	0.94	0.09	56,66,87,89	0
17	CLA	a	818	65/65	0.94	0.11	45,53,81,83	0
19	LHG	A	846	49/49	0.95	0.10	44,49,58,59	0
17	CLA	a	841	65/65	0.95	0.10	55,62,65,67	0
17	CLA	A	806	65/65	0.95	0.08	46,51,59,59	0
20	BCR	a	854	40/40	0.95	0.07	35,40,47,47	0
17	CLA	B	826	65/65	0.95	0.09	44,50,56,64	0
17	CLA	a	844	65/65	0.95	0.09	38,49,59,64	0
17	CLA	B	840	65/65	0.95	0.09	41,50,72,78	0
19	LHG	a	847	49/49	0.95	0.09	35,41,47,48	0
17	CLA	a	856	65/65	0.95	0.09	36,41,56,59	0
17	CLA	b	804	45/65	0.95	0.07	42,52,68,75	0
17	CLA	A	838	51/65	0.95	0.09	45,60,67,68	0
17	CLA	b	838	47/65	0.95	0.07	38,44,54,64	0
17	CLA	b	839	65/65	0.95	0.08	38,44,50,53	0
17	CLA	8	301	60/65	0.95	0.09	56,64,68,72	0
17	CLA	b	840	65/65	0.95	0.08	36,41,59,67	0
17	CLA	B	828	65/65	0.95	0.09	43,48,58,61	0
17	CLA	b	808	65/65	0.95	0.09	39,47,53,59	0
17	CLA	B	808	65/65	0.95	0.09	41,45,70,73	0
17	CLA	8	307	50/65	0.95	0.10	52,65,91,93	0
17	CLA	A	807	65/65	0.95	0.09	44,47,58,69	0
17	CLA	B	819	65/65	0.95	0.08	46,53,80,83	0
17	CLA	a	805	55/65	0.95	0.09	38,43,76,78	0

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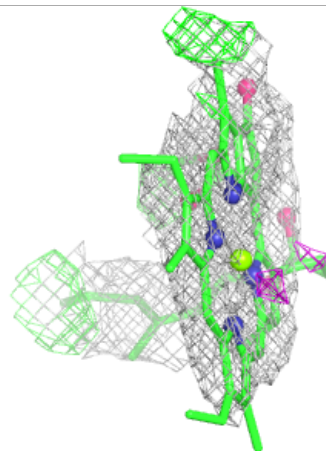
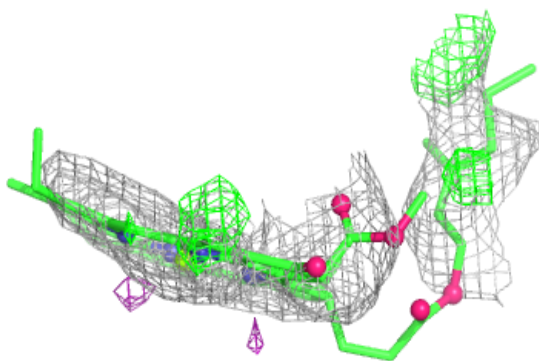
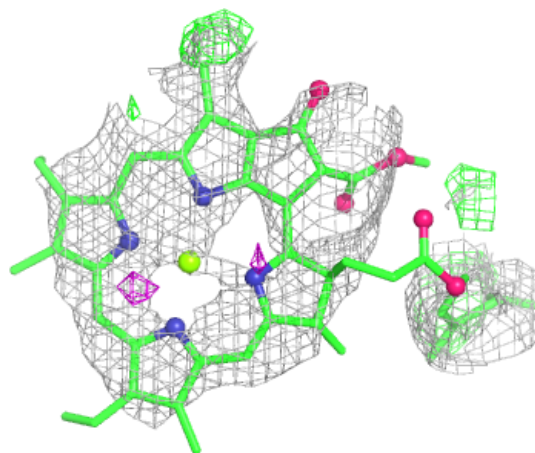
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	CLA	a	825	55/65	0.95	0.07	39,44,58,68	0
17	CLA	a	806	65/65	0.95	0.08	37,39,49,51	0
17	CLA	a	807	65/65	0.95	0.09	35,41,50,54	0
17	CLA	B	820	50/65	0.95	0.09	53,69,95,100	0
17	CLA	a	830	65/65	0.95	0.08	36,40,47,49	0
17	CLA	a	831	65/65	0.95	0.08	36,43,54,56	0
17	CLA	a	832	50/65	0.95	0.08	41,54,78,83	0
17	CLA	A	803	65/65	0.95	0.09	39,44,54,59	0
17	CLA	A	830	65/65	0.95	0.08	45,53,58,61	0
17	CLA	a	835	65/65	0.95	0.08	36,43,48,49	0
17	CLA	A	831	65/65	0.95	0.08	43,52,59,61	0
17	CLA	b	824	65/65	0.95	0.09	45,51,69,72	0
17	CLA	B	805	65/65	0.95	0.09	45,47,53,60	0
17	CLA	B	837	65/65	0.95	0.09	49,55,61,65	0
17	CLA	b	827	65/65	0.95	0.09	40,53,83,83	0
17	CLA	a	814	65/65	0.95	0.10	39,47,64,67	0
17	CLA	a	840	65/65	0.95	0.10	36,41,87,89	0
18	PQN	b	842	33/33	0.95	0.08	36,41,49,50	0
17	CLA	b	805	65/65	0.96	0.08	42,45,52,58	0
17	CLA	f	7002	45/65	0.96	0.07	54,59,76,77	0
17	CLA	a	803	65/65	0.96	0.07	35,38,50,53	0
17	CLA	a	820	65/65	0.96	0.08	38,43,48,50	0
17	CLA	a	826	65/65	0.96	0.08	39,43,48,56	0
17	CLA	B	813	65/65	0.96	0.08	47,51,54,55	0
17	CLA	a	801	65/65	0.96	0.08	35,39,44,46	0
17	CLA	b	802	65/65	0.96	0.09	36,41,45,52	0
17	CLA	b	803	65/65	0.96	0.07	35,40,47,49	0
17	CLA	A	801	65/65	0.96	0.09	40,44,49,53	0
21	SF4	C	102	8/8	0.99	0.05	51,62,72,84	0
21	SF4	a	855	8/8	0.99	0.04	37,37,43,43	0
21	SF4	c	101	8/8	0.99	0.06	41,46,54,56	0
21	SF4	c	102	8/8	0.99	0.04	41,50,62,77	0
21	SF4	A	853	8/8	0.99	0.05	43,44,48,51	0
21	SF4	C	101	8/8	0.99	0.06	47,49,53,57	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.

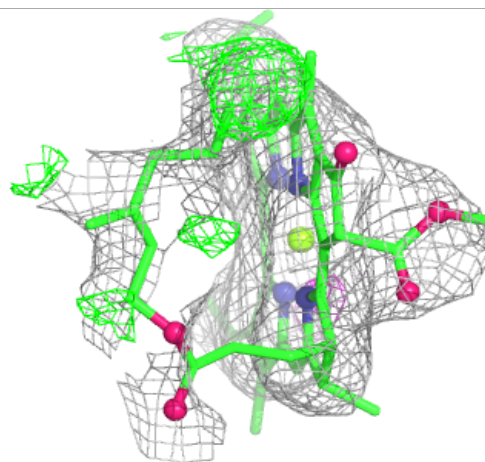
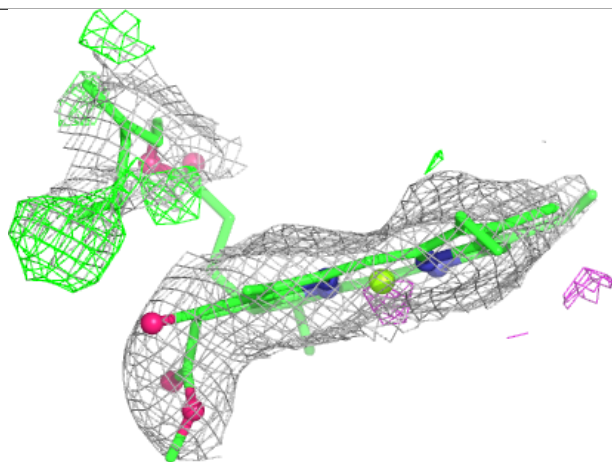
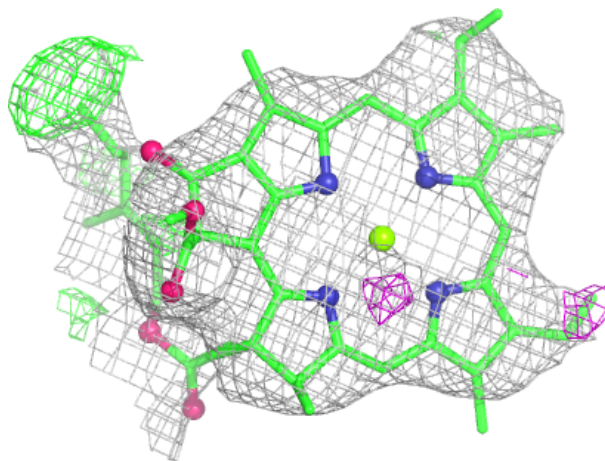
Electron density around CLA 8 309:

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



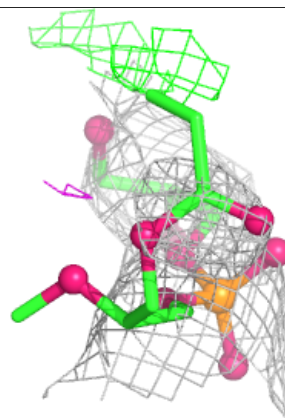
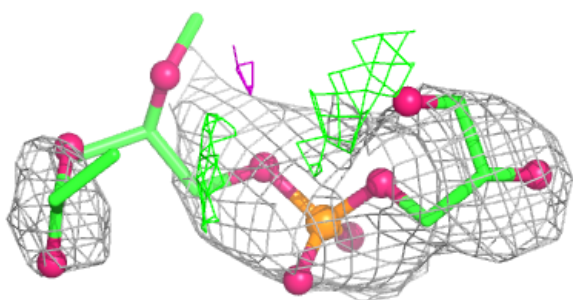
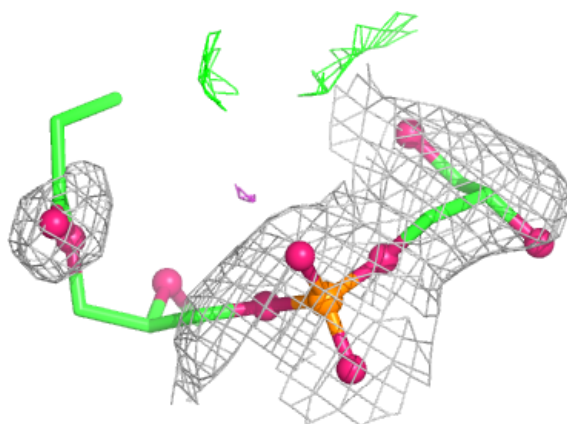
Electron density around CLA a 846:

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



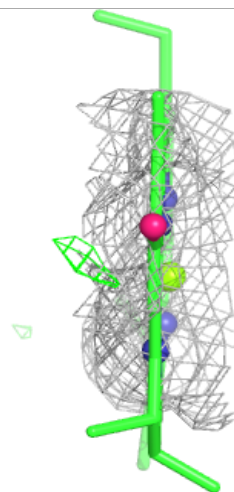
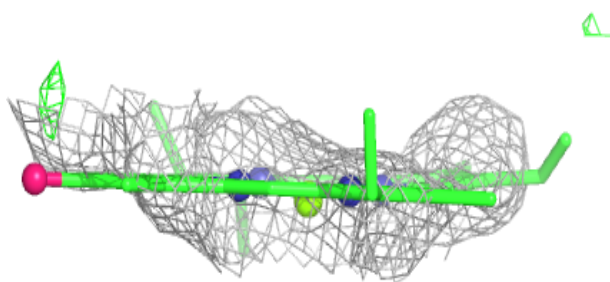
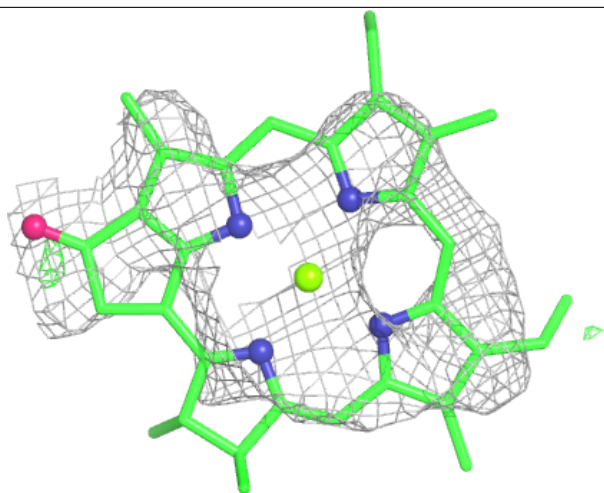
Electron density around LHG 3 319:

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



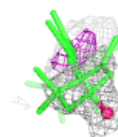
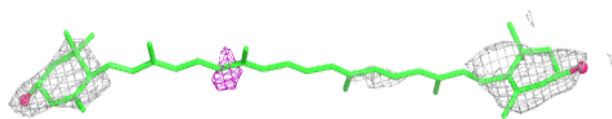
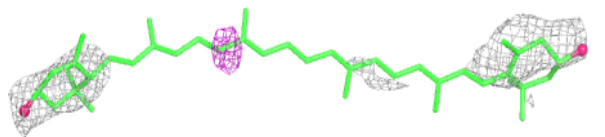
Electron density around CLA 3 310:

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

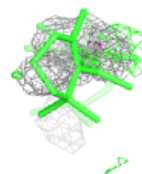
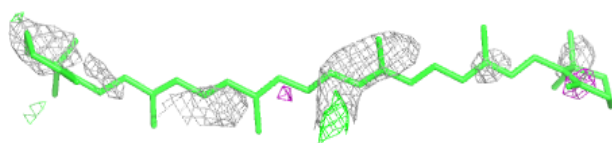
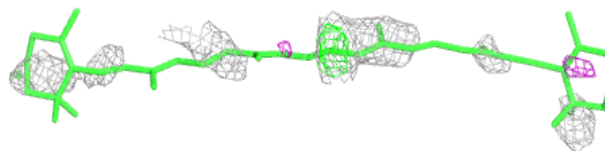


Electron density around LUT 6 321:

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

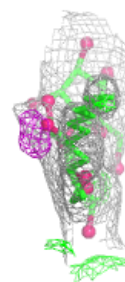
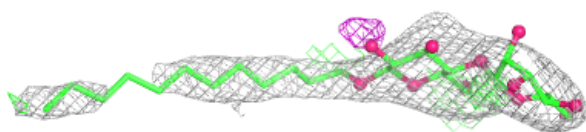
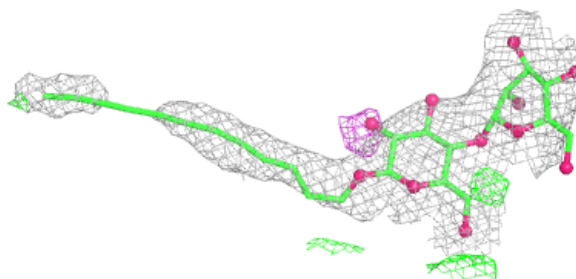
**Electron density around BCR L 206:**

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

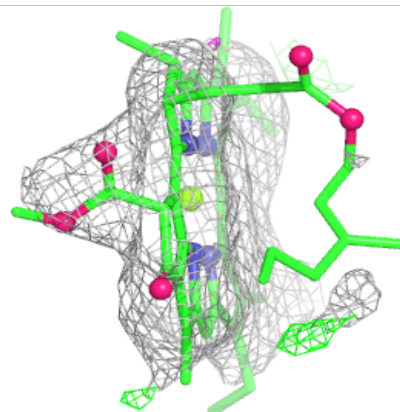
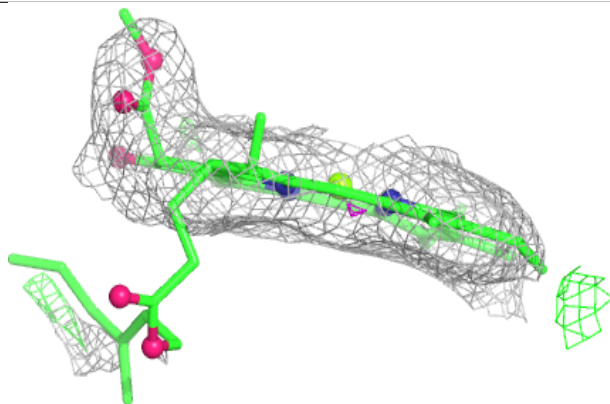
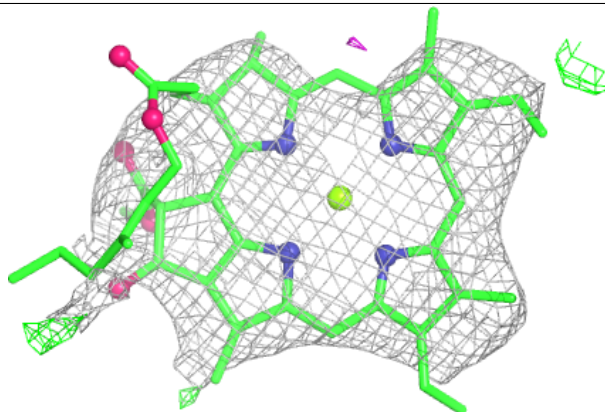


Electron density around LMT B 849:

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

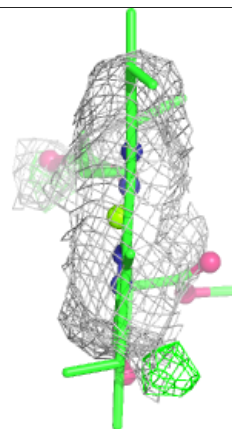
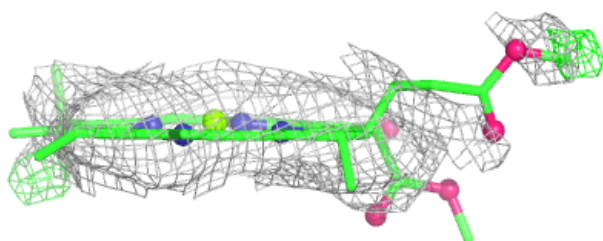
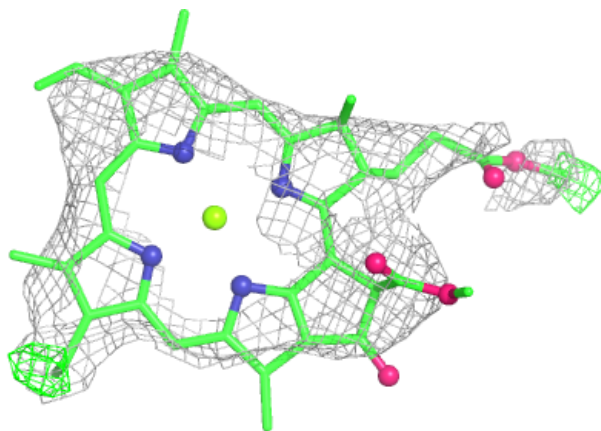
**Electron density around CLA A 845:**

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



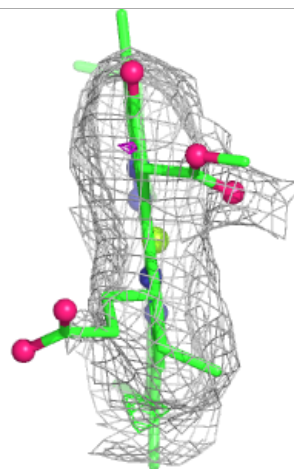
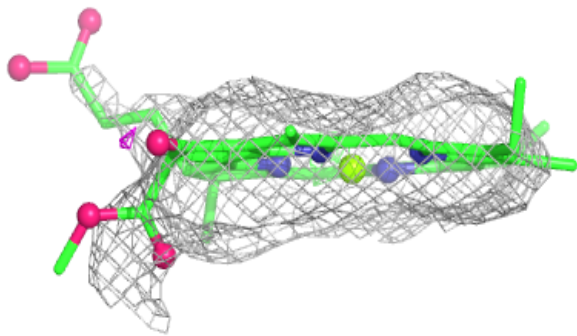
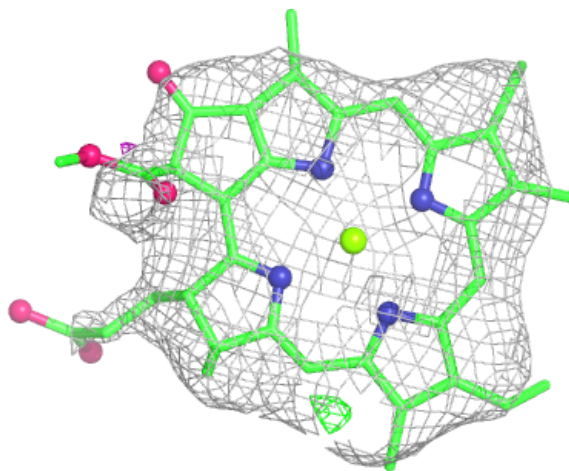
Electron density around CLA 6 316:

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



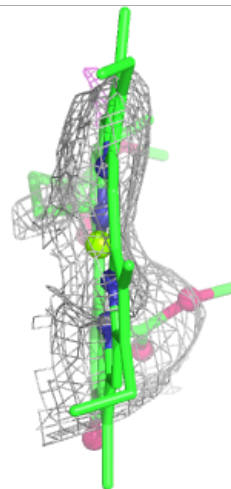
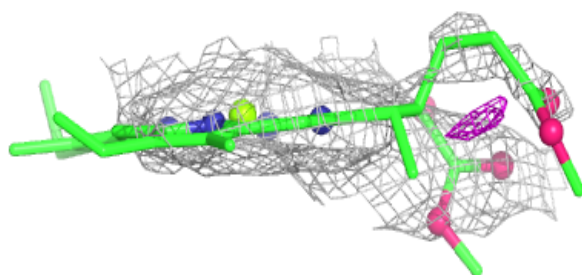
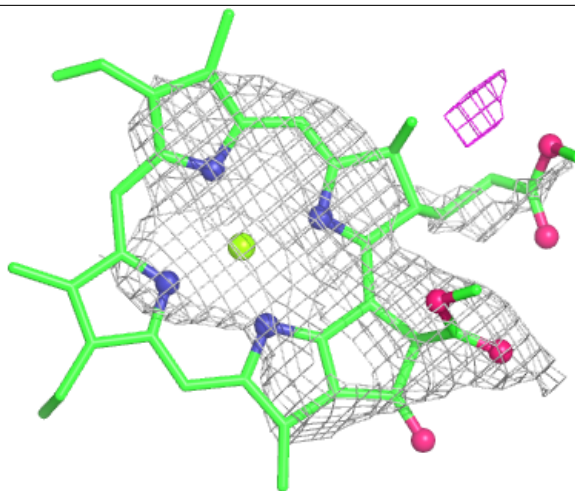
Electron density around CLA 8 311:

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



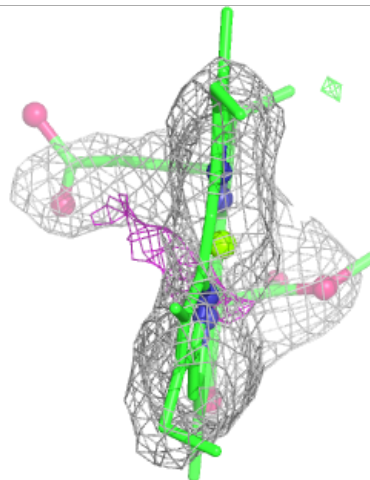
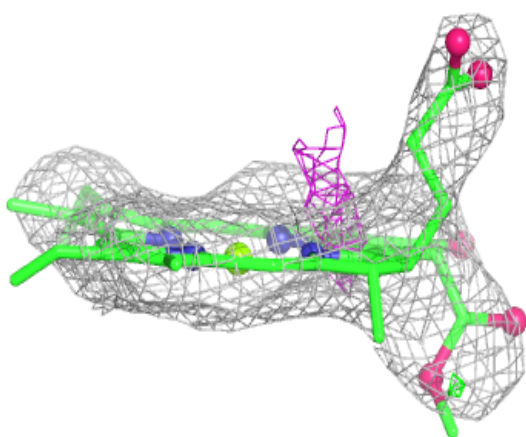
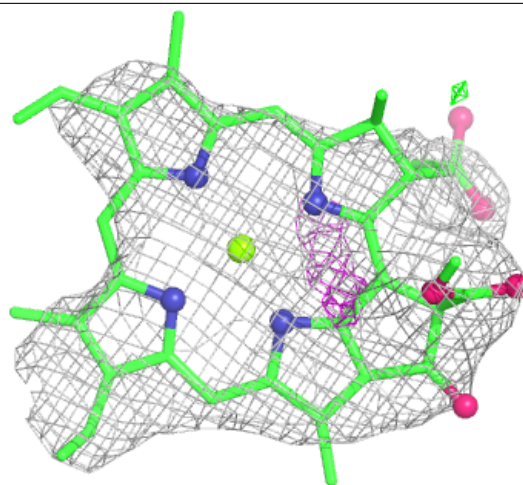
Electron density around CLA 3 301:

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



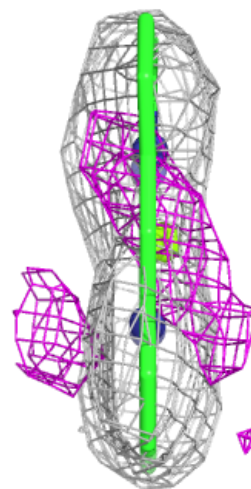
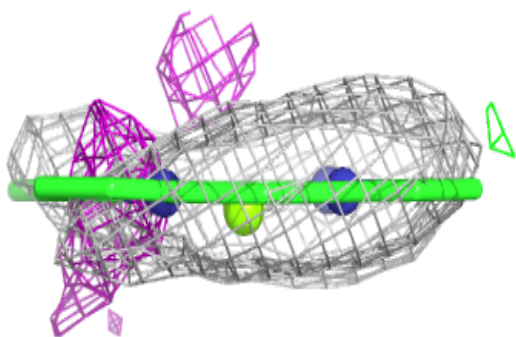
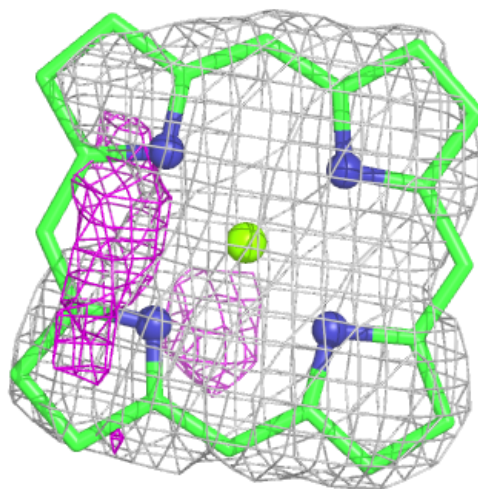
Electron density around CLA K 4002:

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



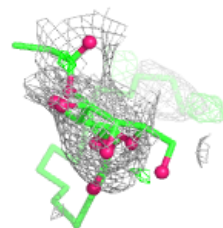
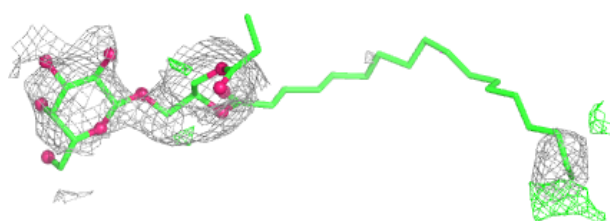
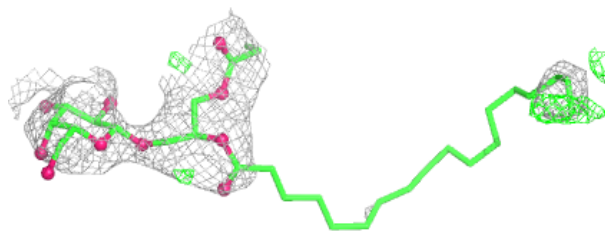
Electron density around CLA 8 313:

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

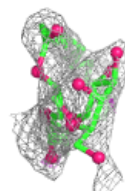
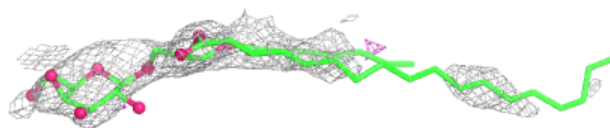
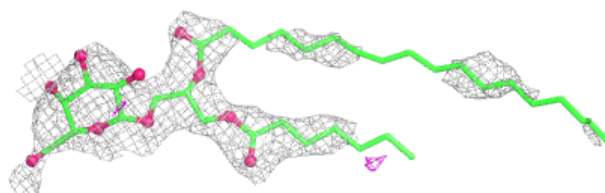


Electron density around LMG 6 302:

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

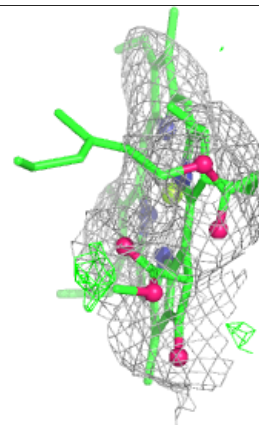
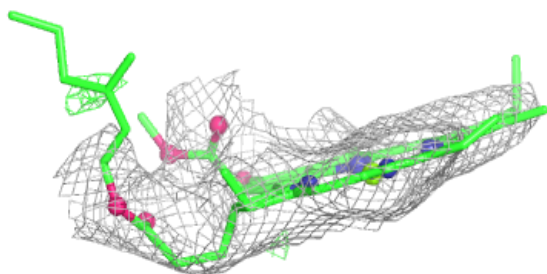
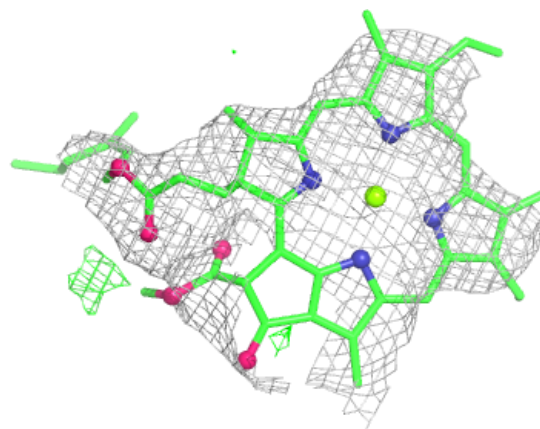
**Electron density around LMG 4 620:**

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



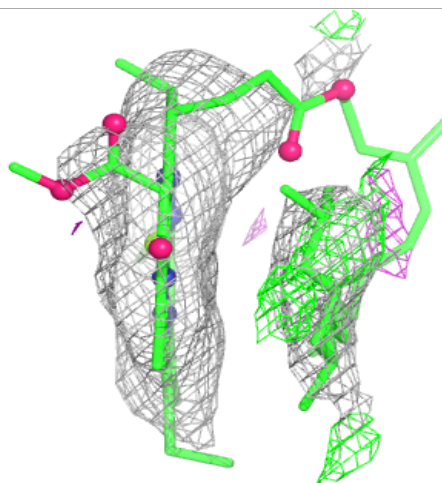
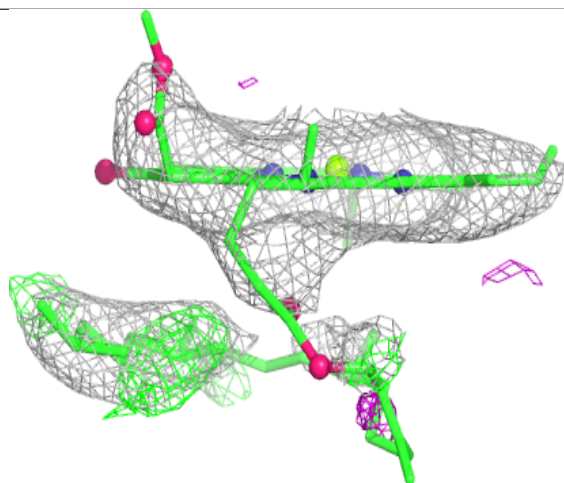
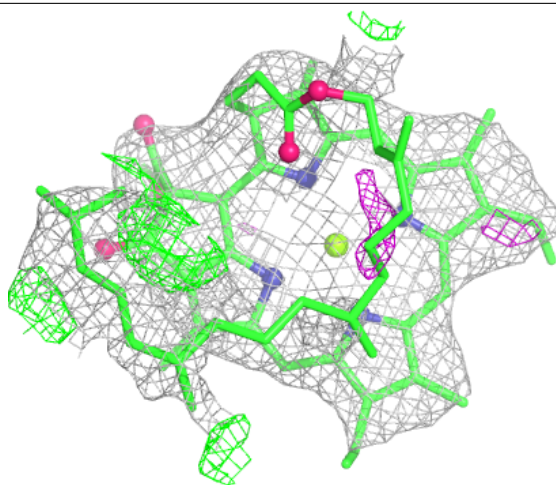
Electron density around CLA 3 311:

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



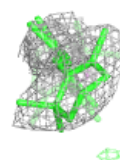
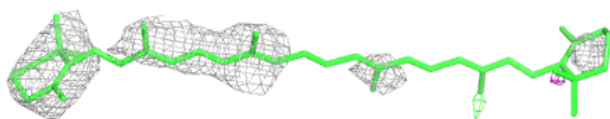
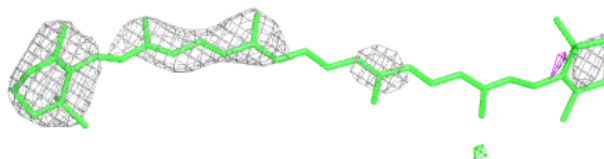
Electron density around CLA L 202:

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



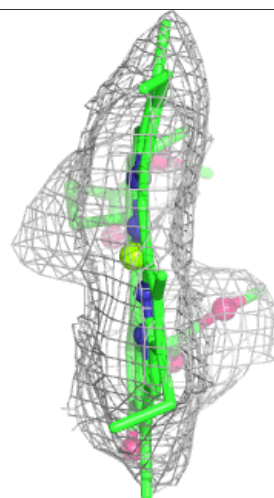
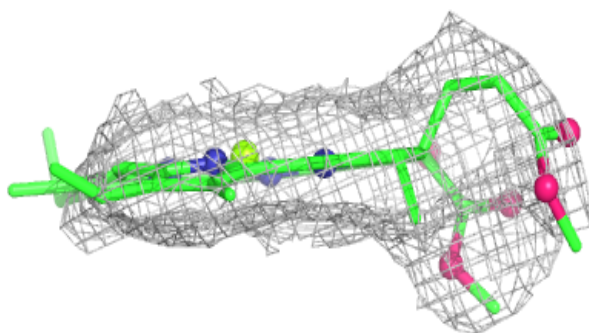
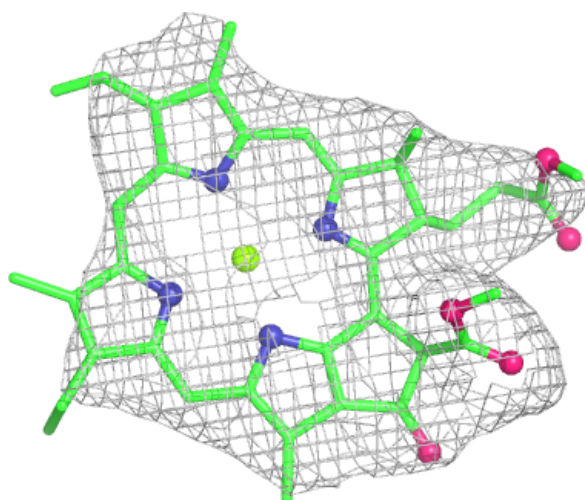
Electron density around BCR K 4004:

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



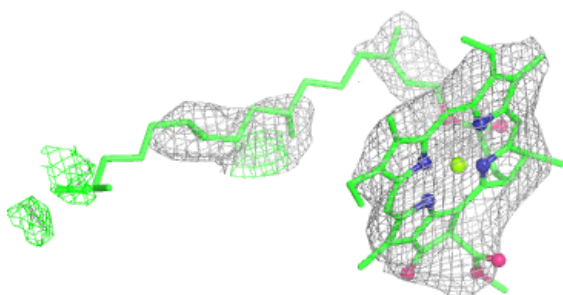
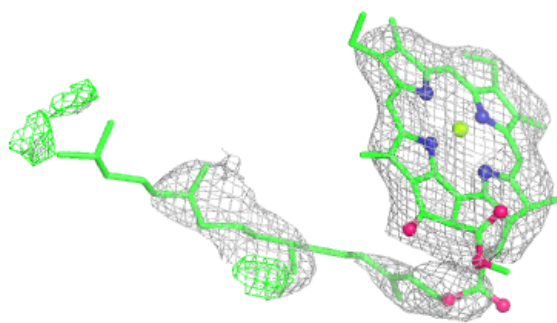
Electron density around CLA k 1403:

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



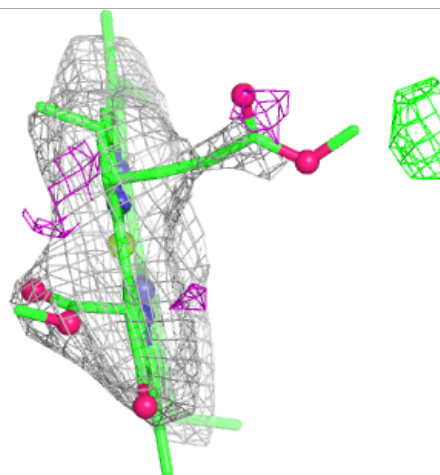
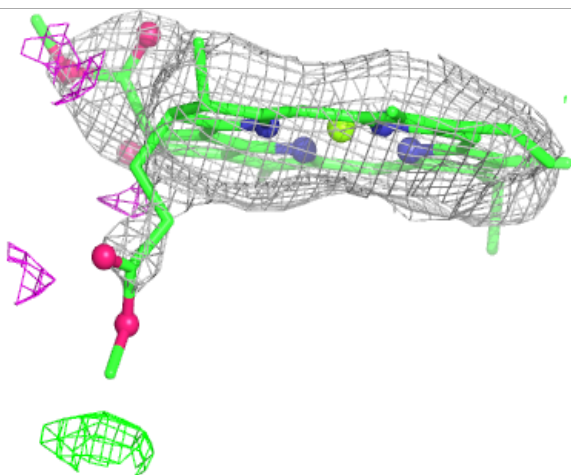
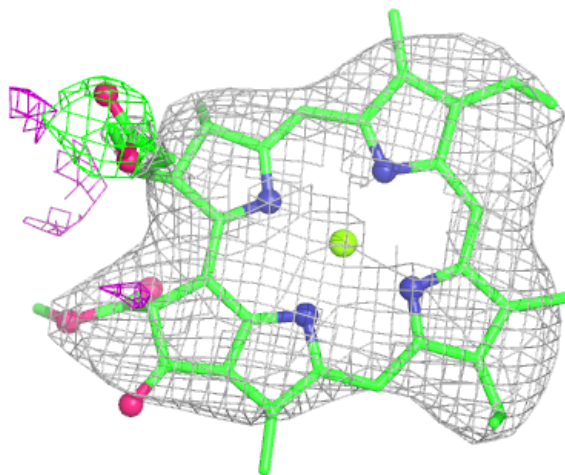
Electron density around CLA 6 310:

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



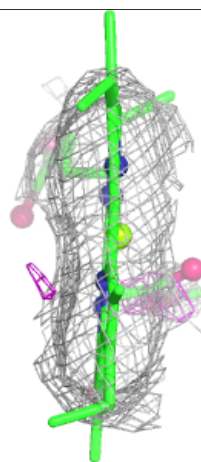
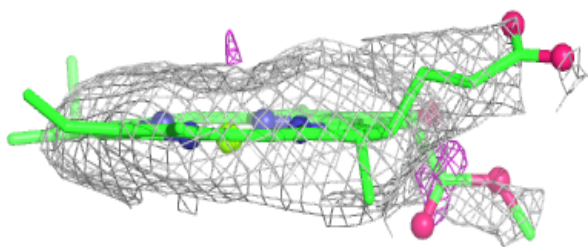
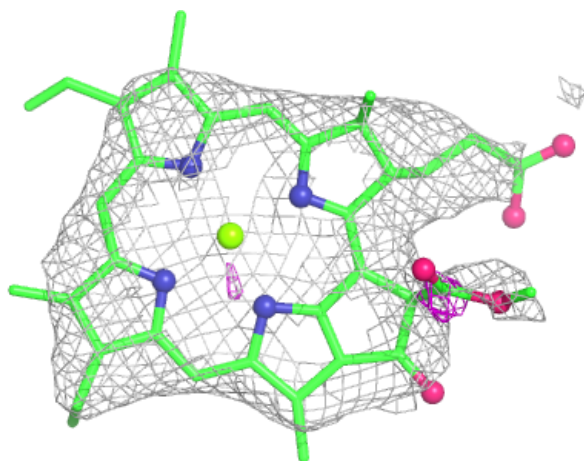
Electron density around CLA 6 309:

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



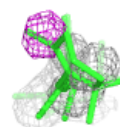
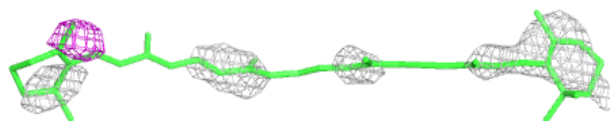
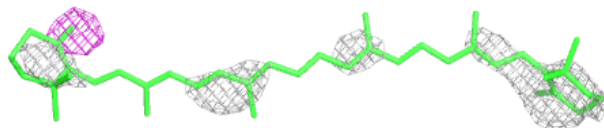
Electron density around CLA 3 313:

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

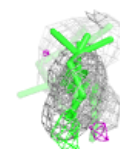
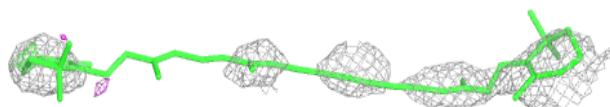
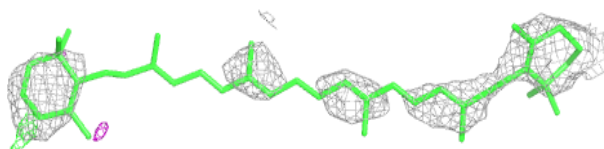


Electron density around BCR 2 617:

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

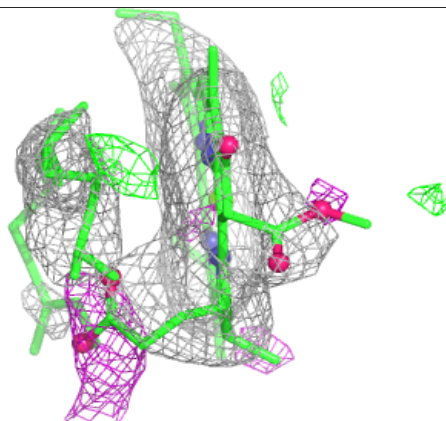
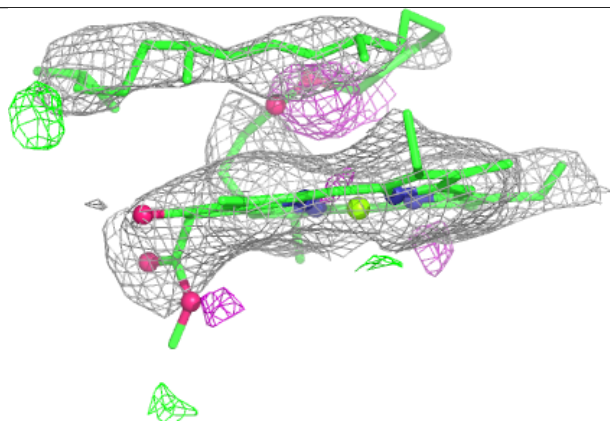
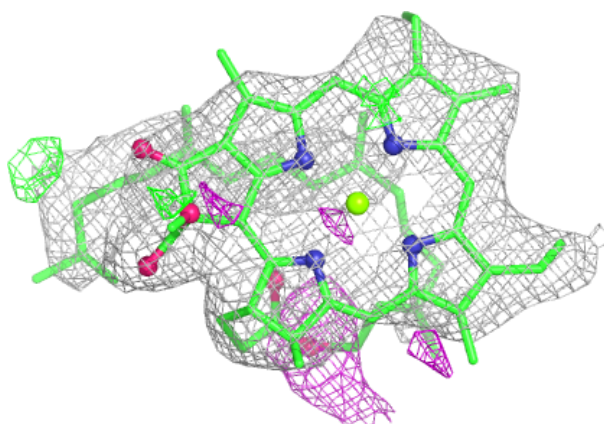
**Electron density around BCR 7 617:**

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

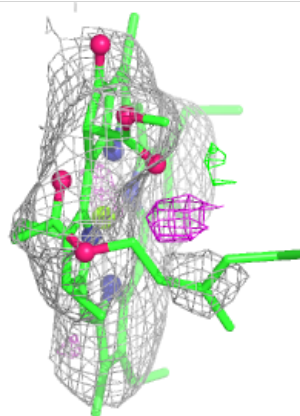
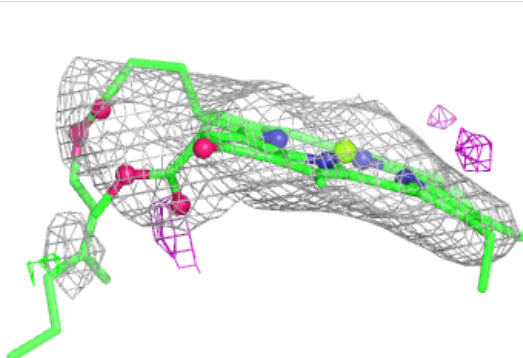
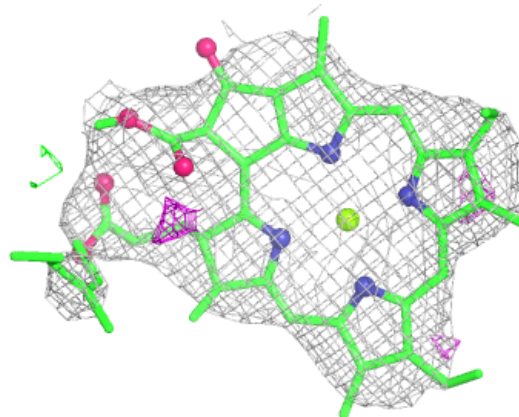


Electron density around CLA 1 202:

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

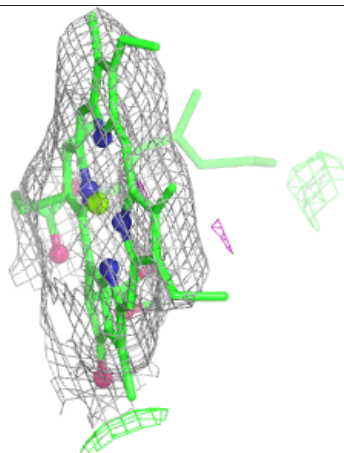
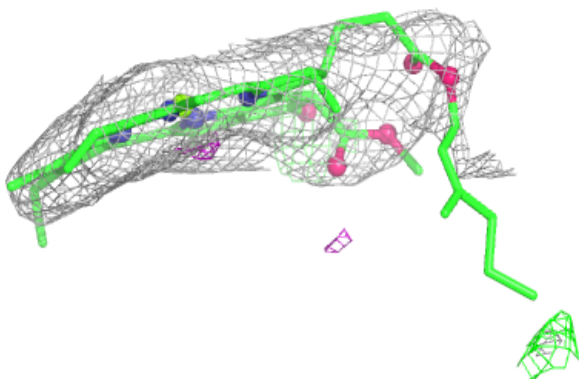
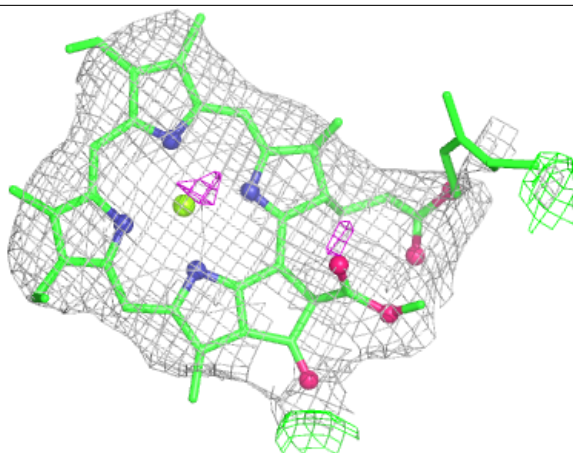
**Electron density around CLA 9 611:**

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



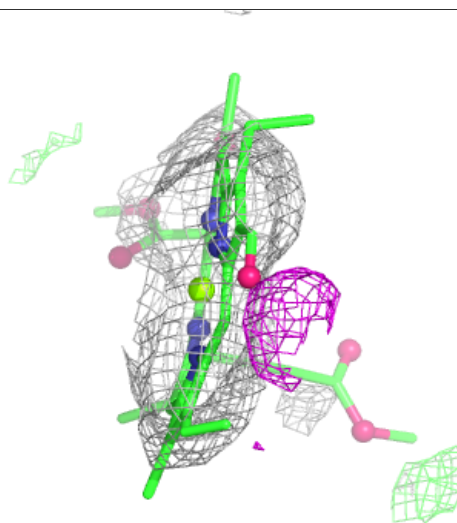
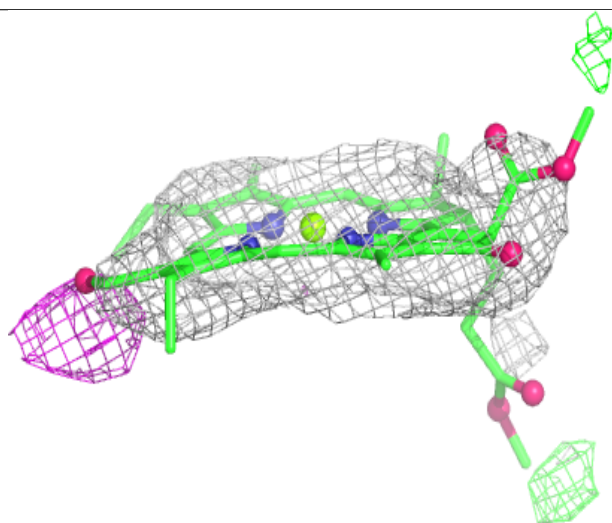
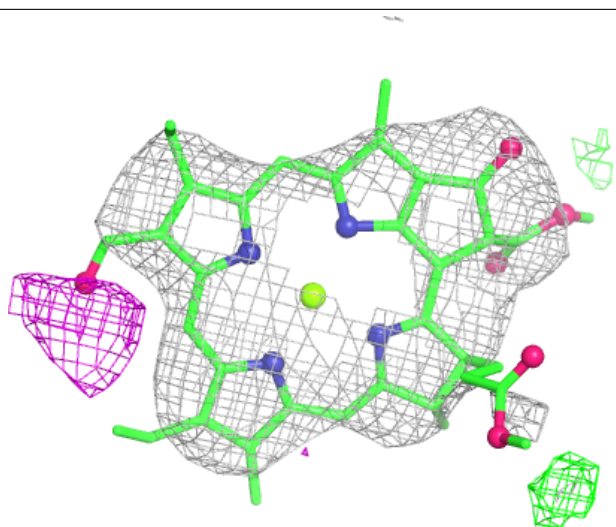
Electron density around CLA 7 611:

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



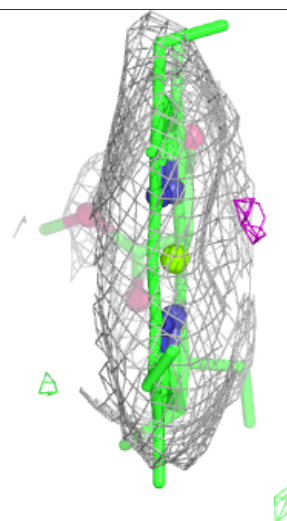
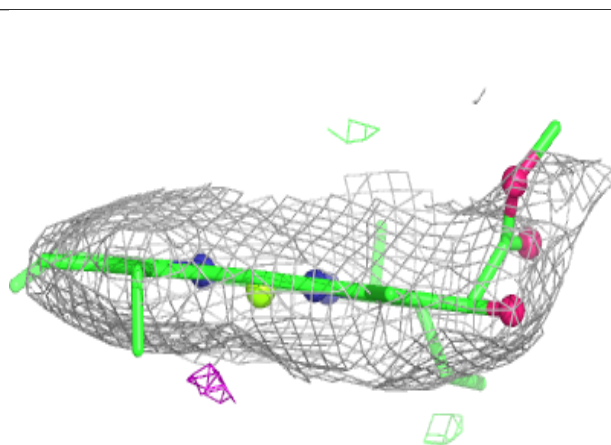
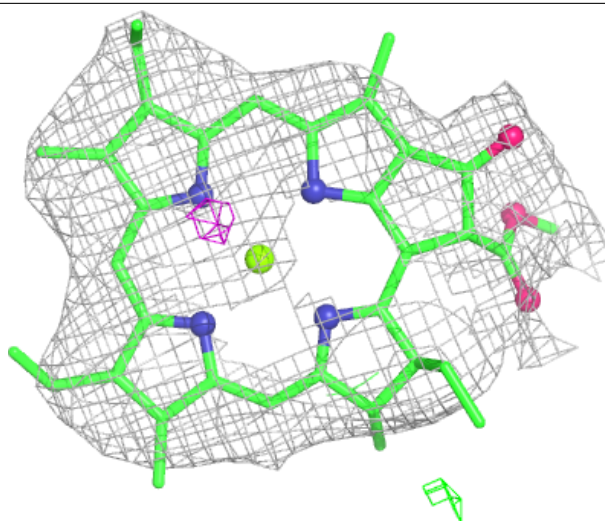
Electron density around CHL 6 308:

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



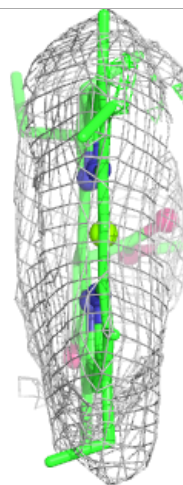
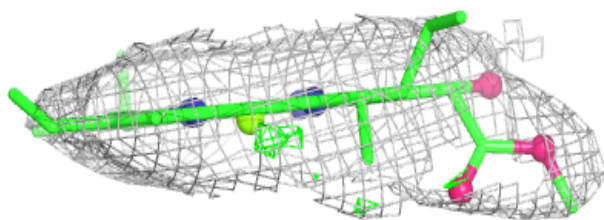
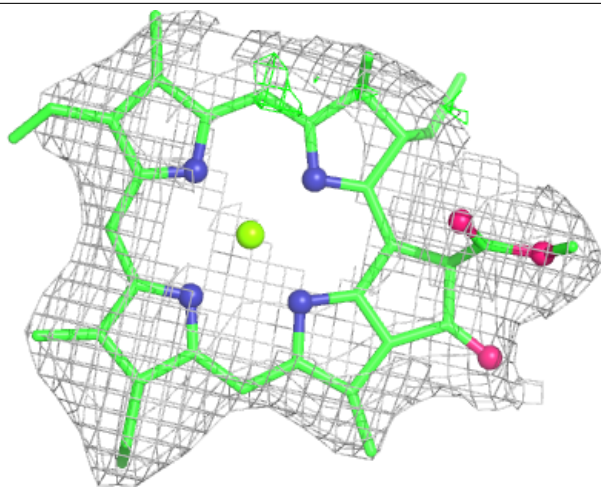
Electron density around CLA J 3002:

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



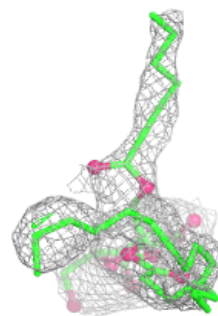
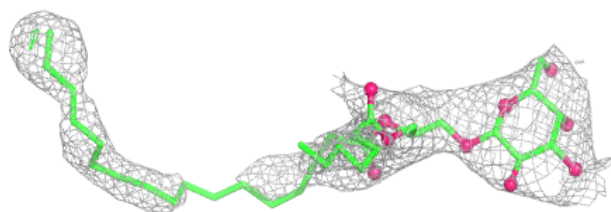
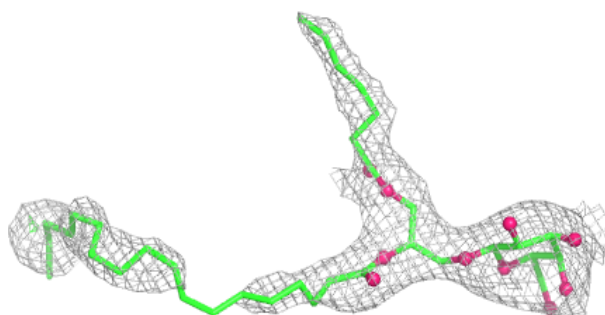
Electron density around CLA j 3002:

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



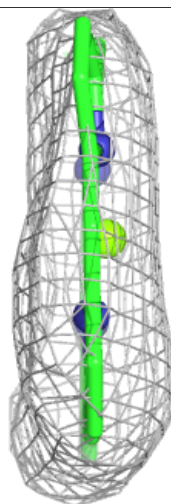
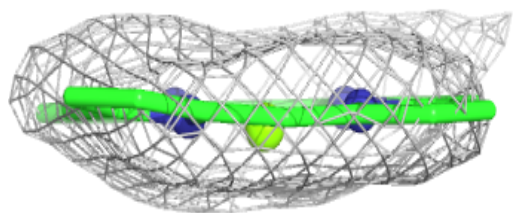
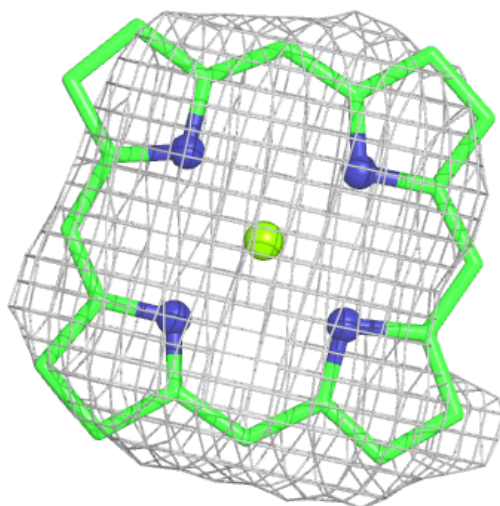
Electron density around LMG G 102:

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



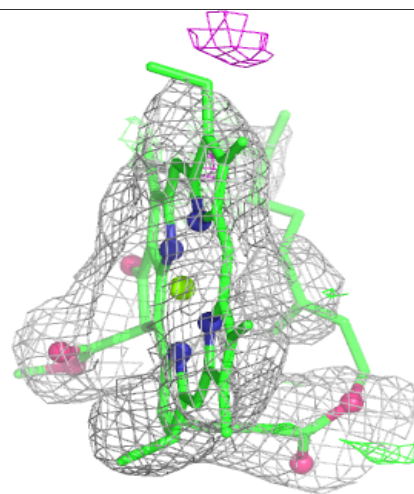
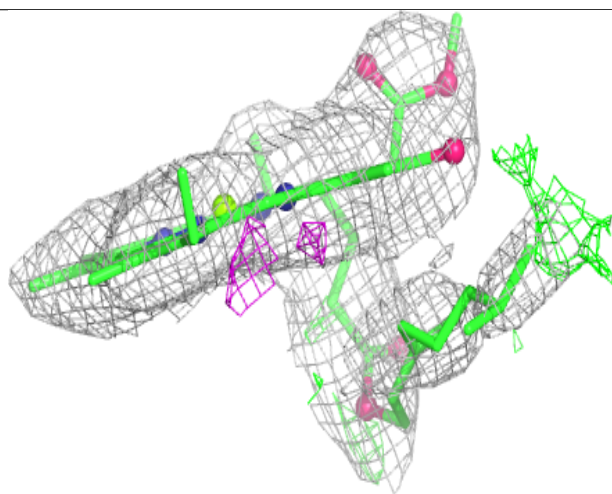
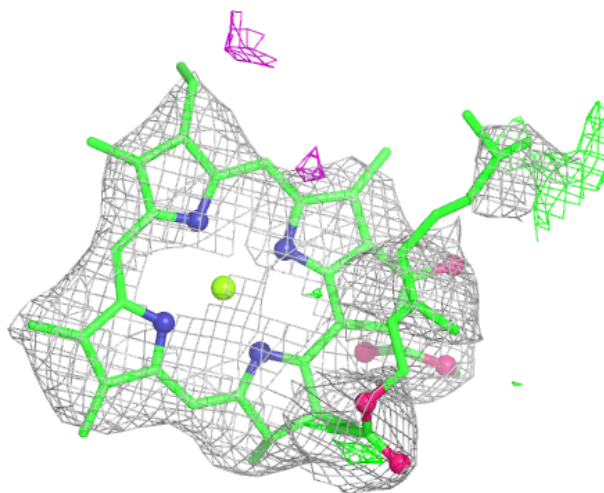
Electron density around CLA 3 315:

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



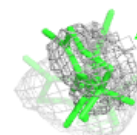
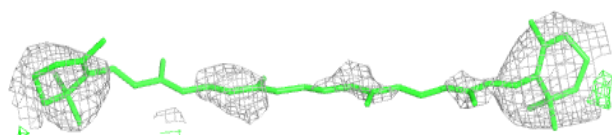
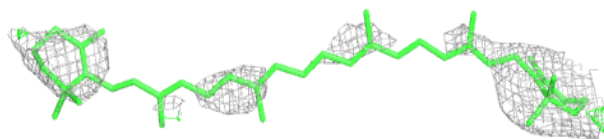
Electron density around CLA B 811:

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

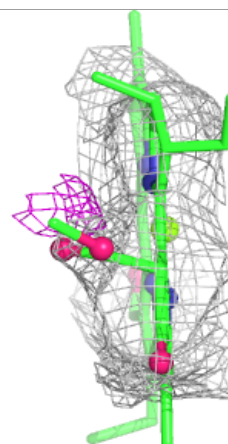
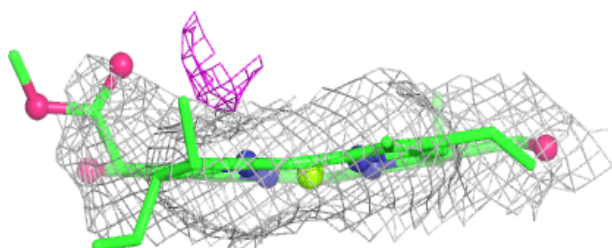
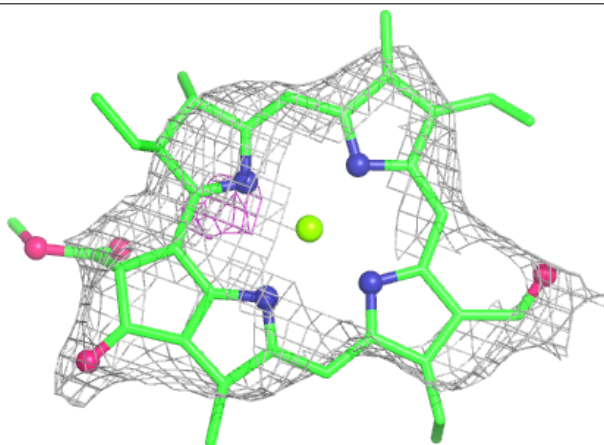


Electron density around BCR 6 319:

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

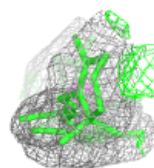
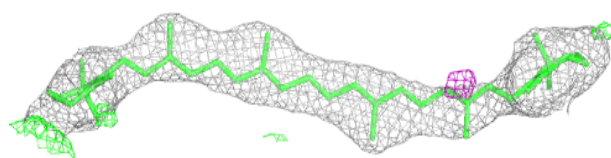
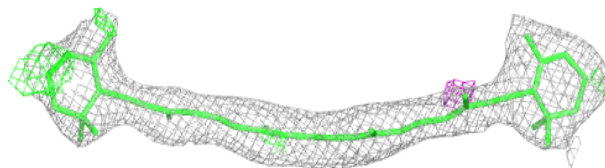
**Electron density around CHL 9 615:**

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



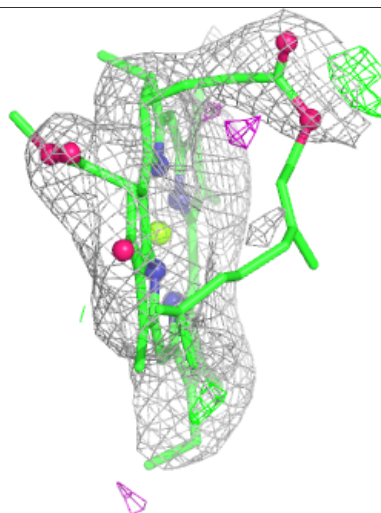
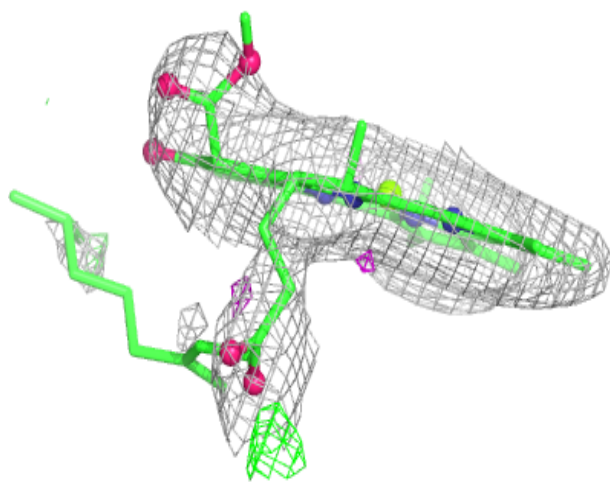
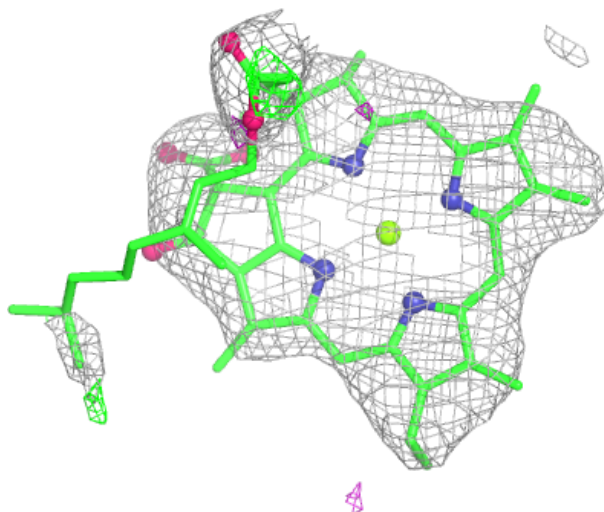
Electron density around BCR A 856:

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



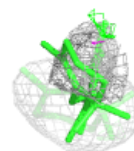
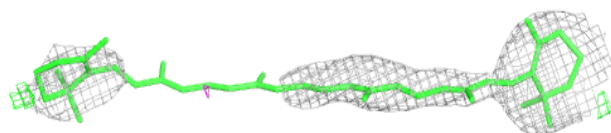
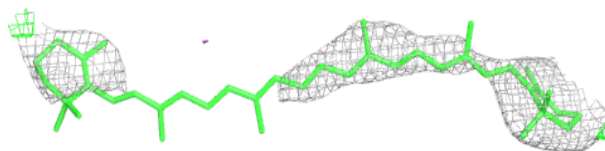
Electron density around CLA b 811:

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

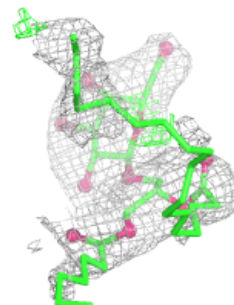
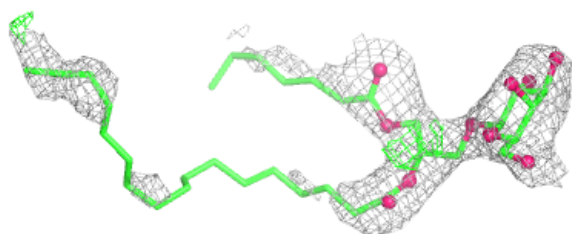


Electron density around BCR 1 318:

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

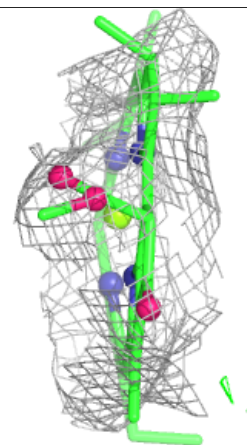
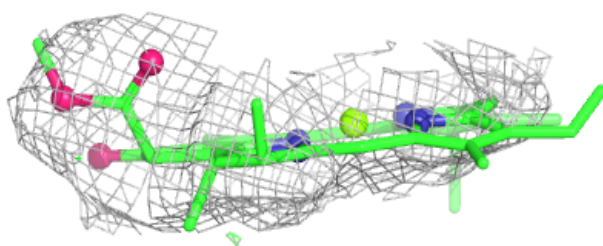
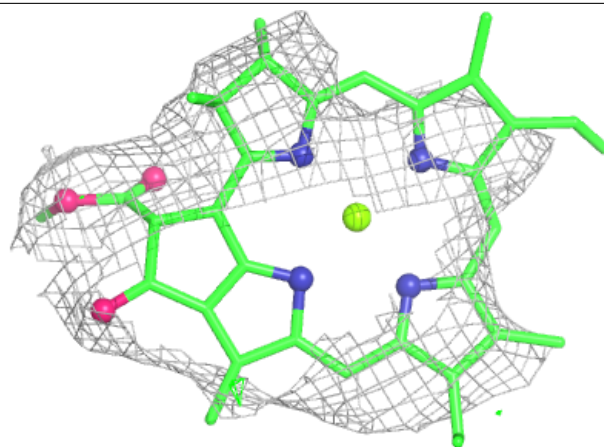
**Electron density around LMG 4 619:**

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

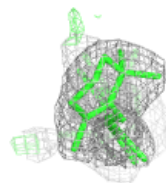
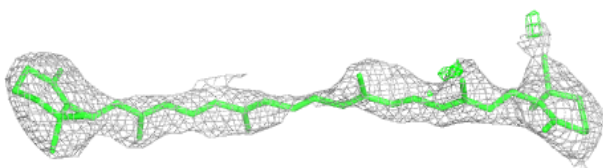
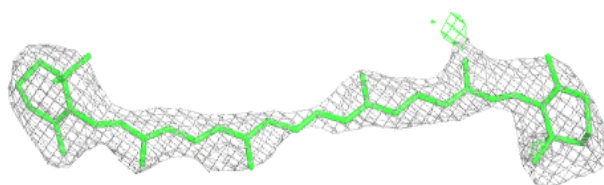


Electron density around CLA g 101:

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

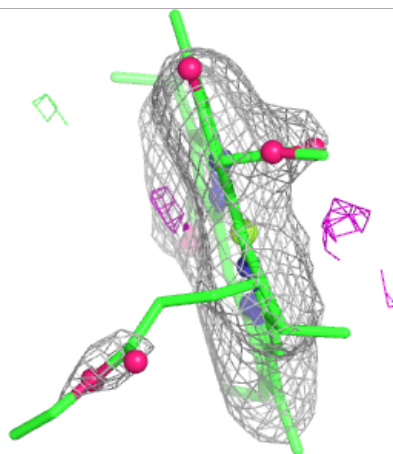
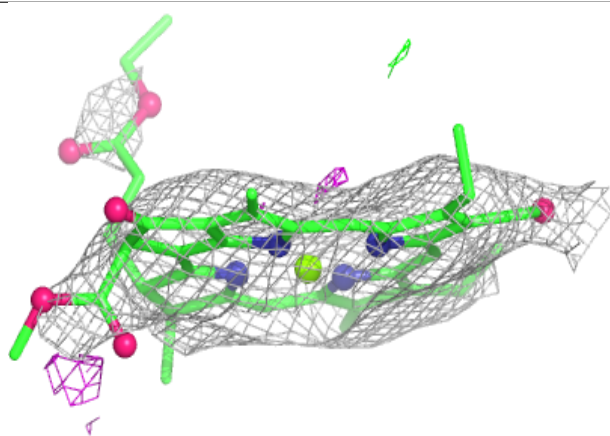
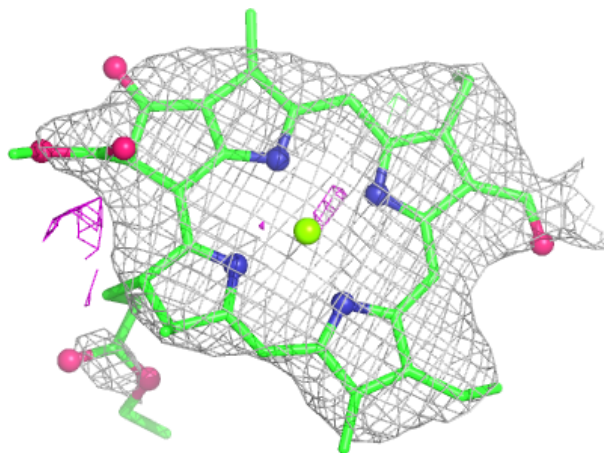
**Electron density around BCR k 1404:**

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



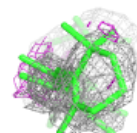
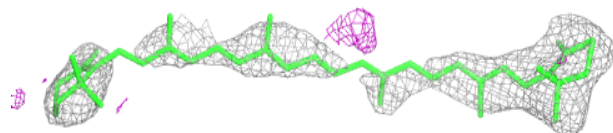
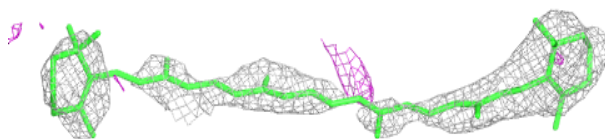
Electron density around CHL 2 606:

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

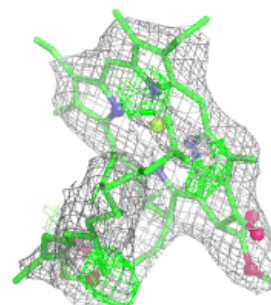
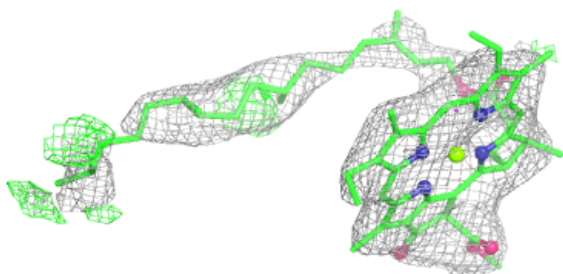
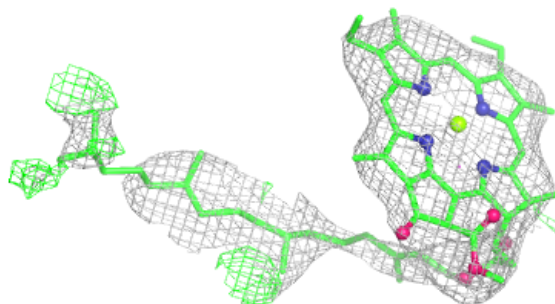


Electron density around BCR 1 206:

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

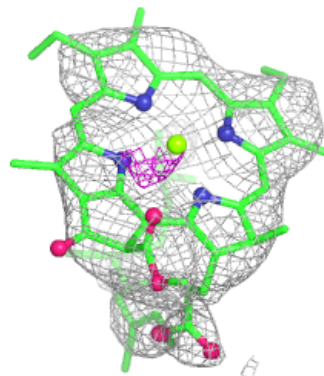
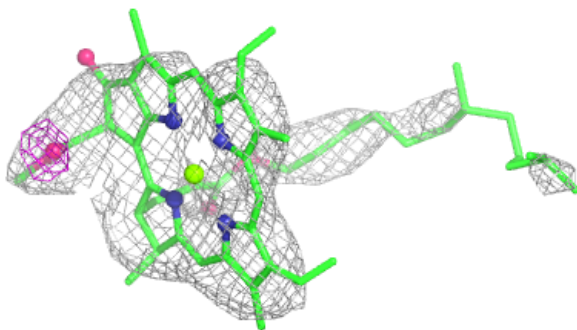
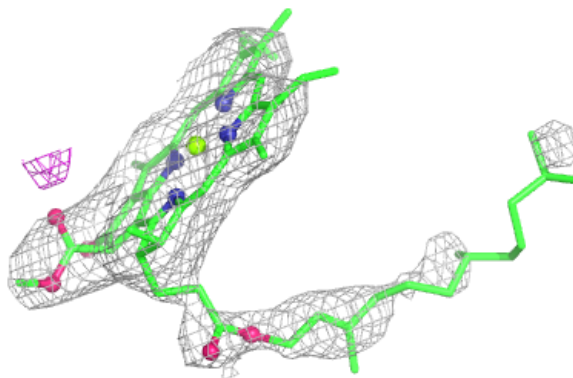
**Electron density around CLA 1 309:**

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



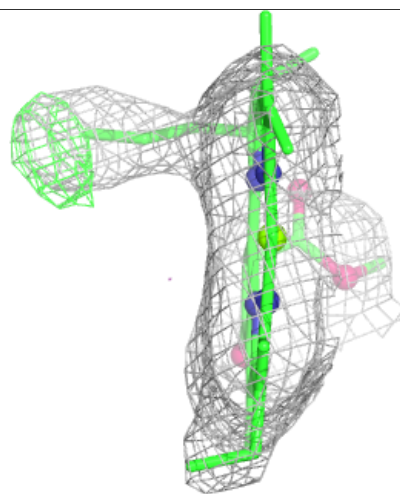
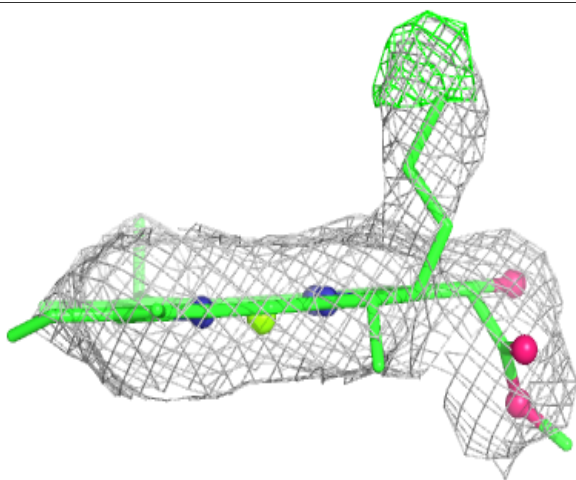
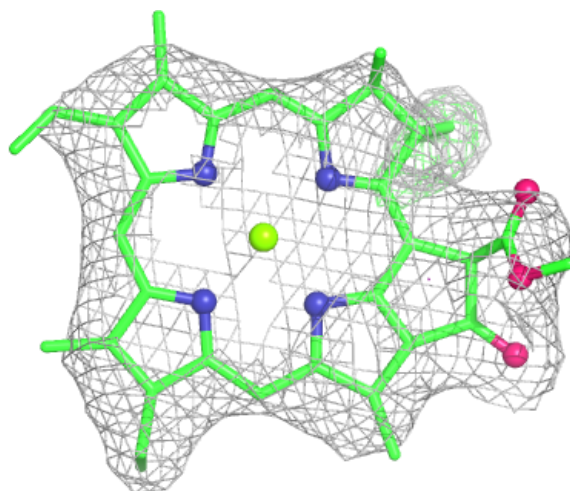
Electron density around CLA 2 604:

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



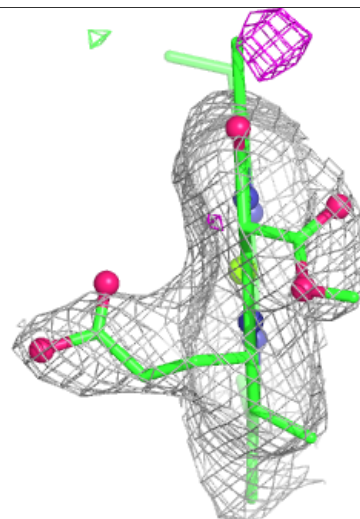
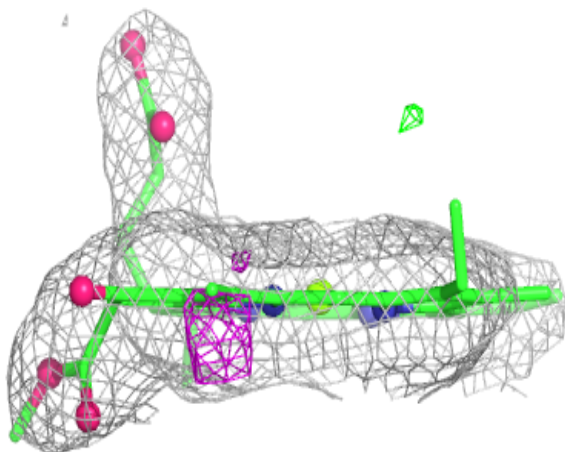
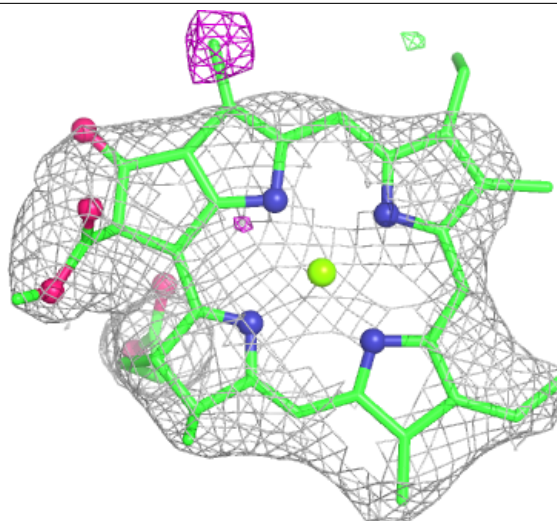
Electron density around CLA 2 613:

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



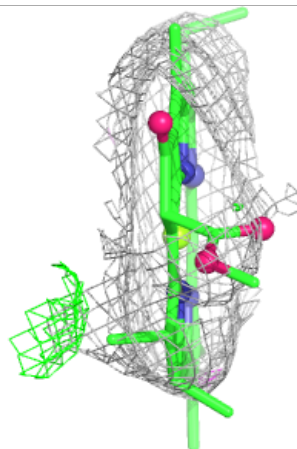
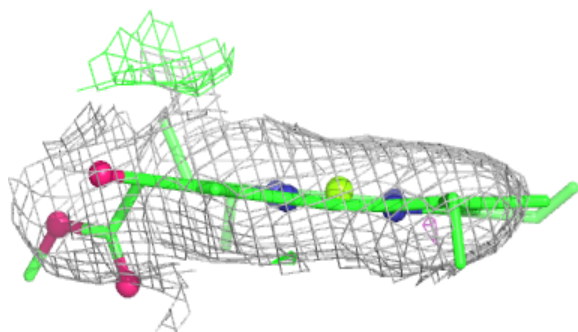
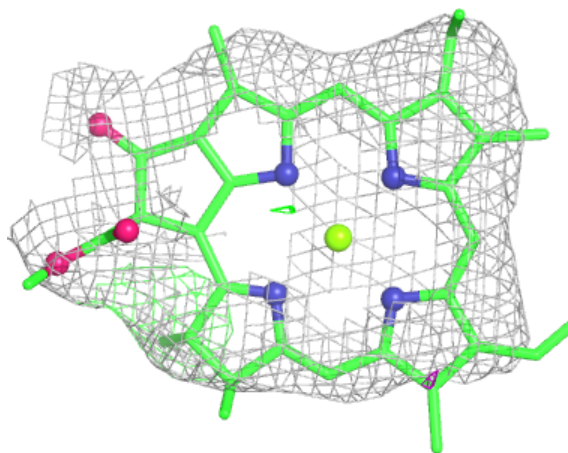
Electron density around CLA A 837:

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



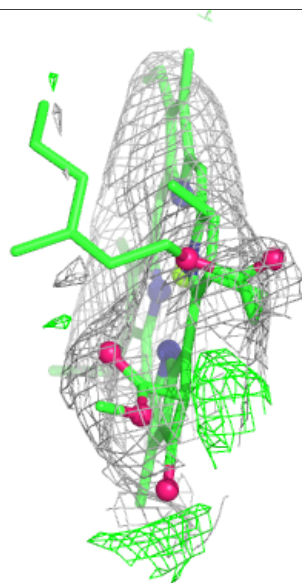
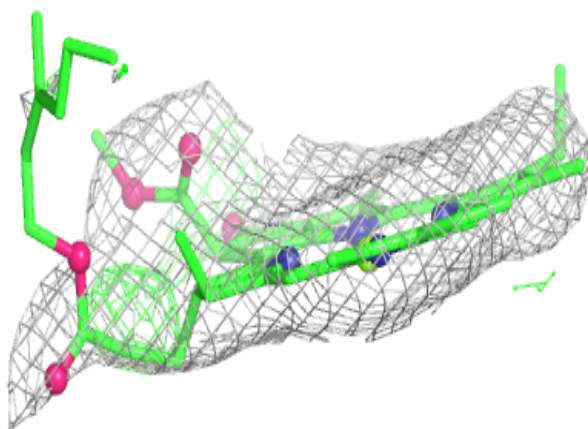
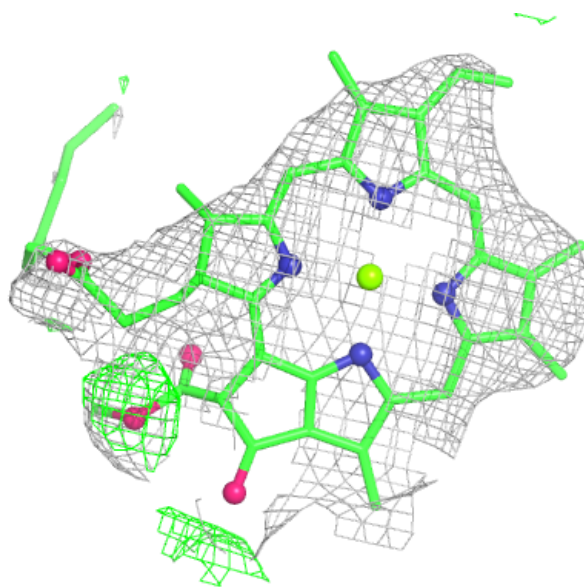
Electron density around CLA 6 312:

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



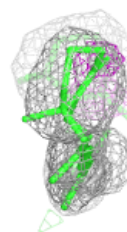
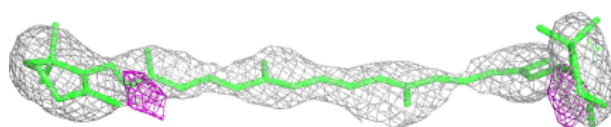
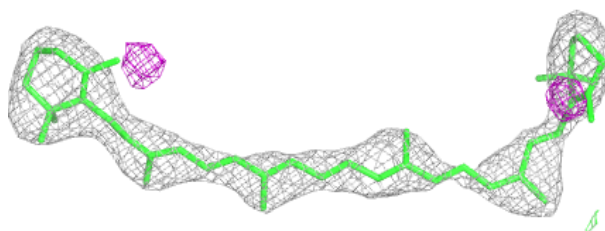
Electron density around CLA 6 313:

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

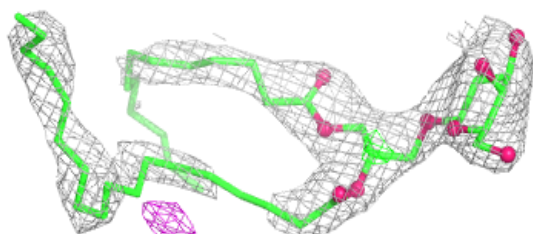
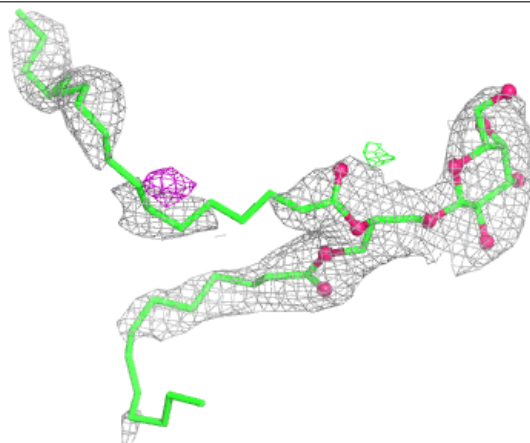


Electron density around BCR b 844:

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

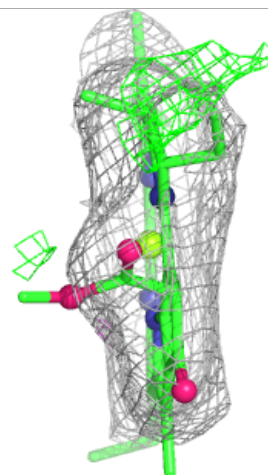
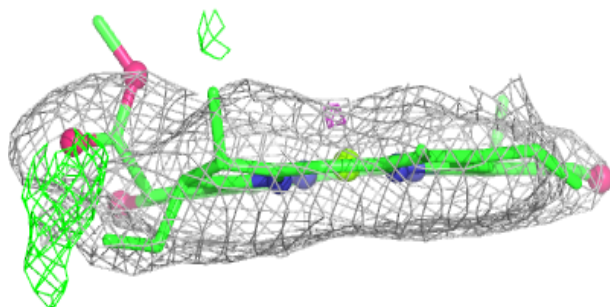
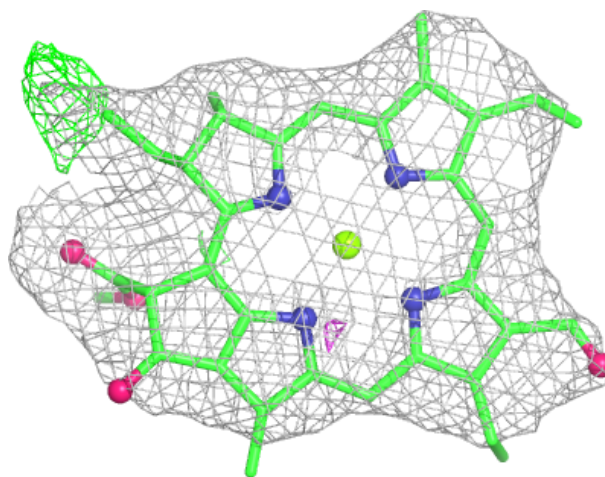
**Electron density around LMG 9 619:**

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



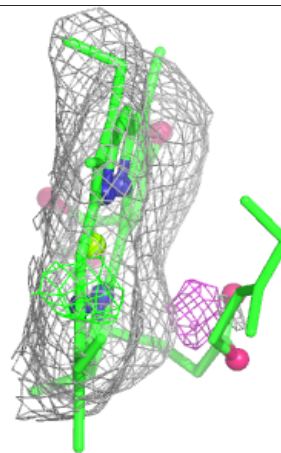
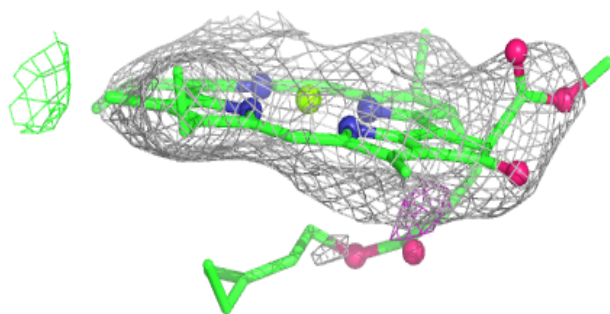
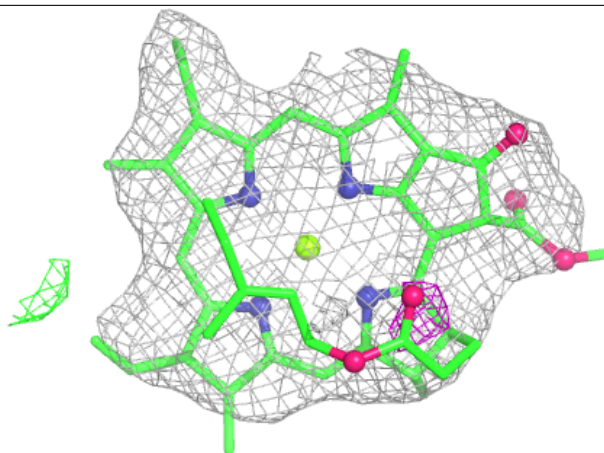
Electron density around CHL 2 605:

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

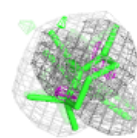
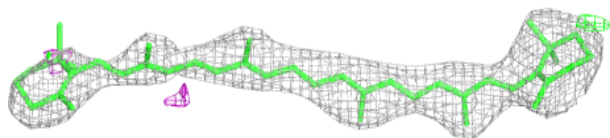
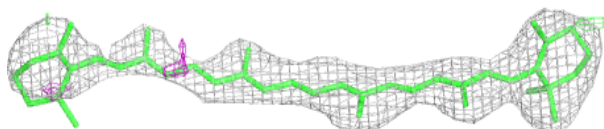


Electron density around CLA A 824:

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

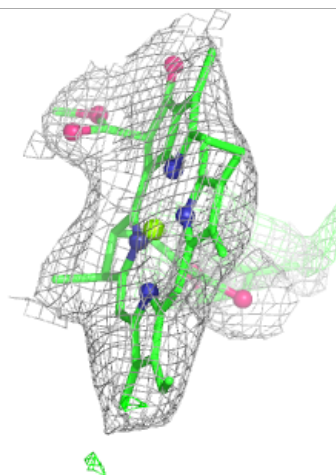
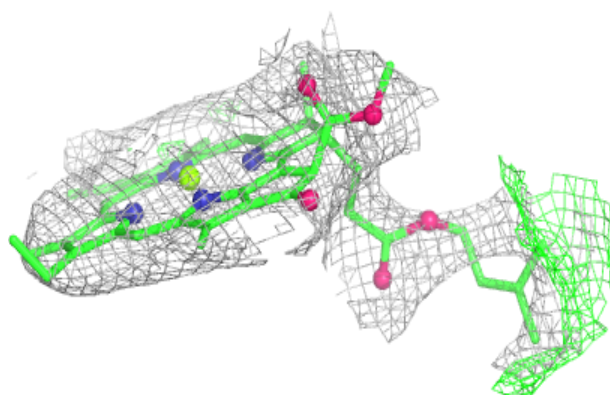
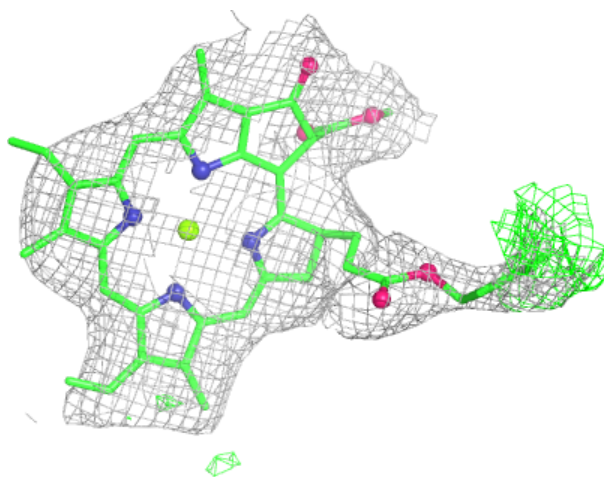
**Electron density around BCR A 848:**

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



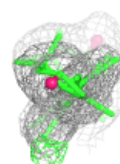
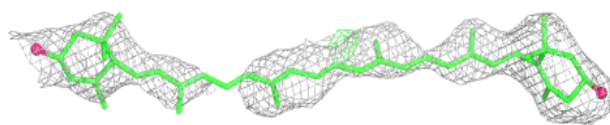
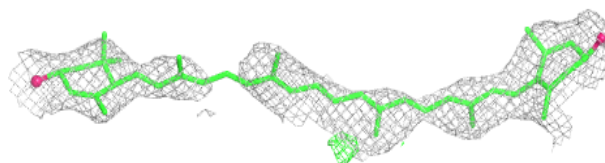
Electron density around CLA 2 608:

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

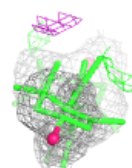
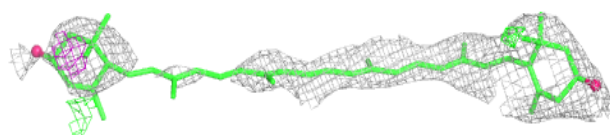
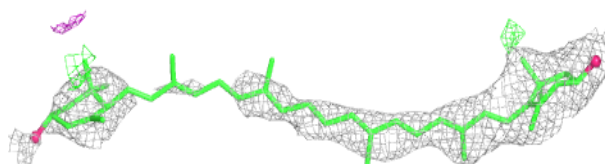


Electron density around LUT 4 616:

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

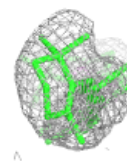
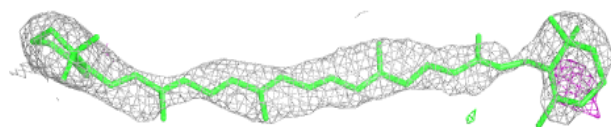
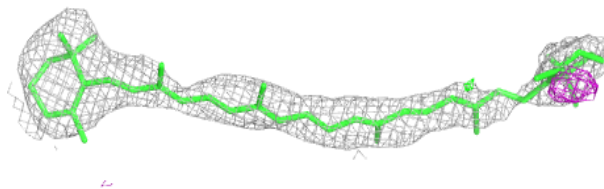
**Electron density around LUT 6 317:**

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

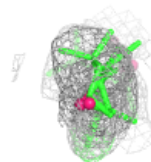
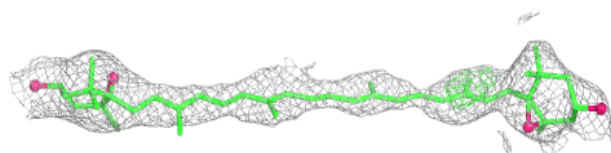
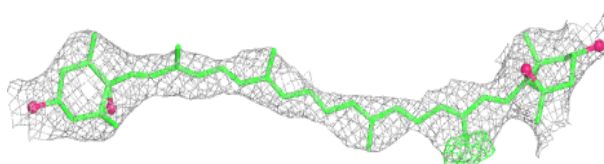


Electron density around BCR K 4001:

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

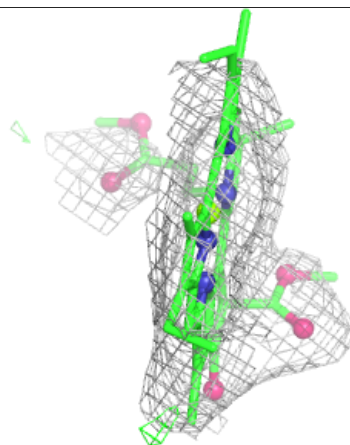
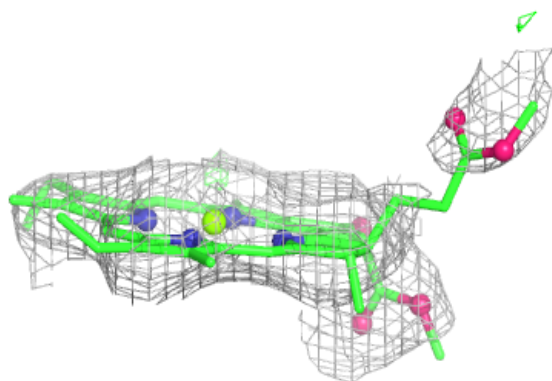
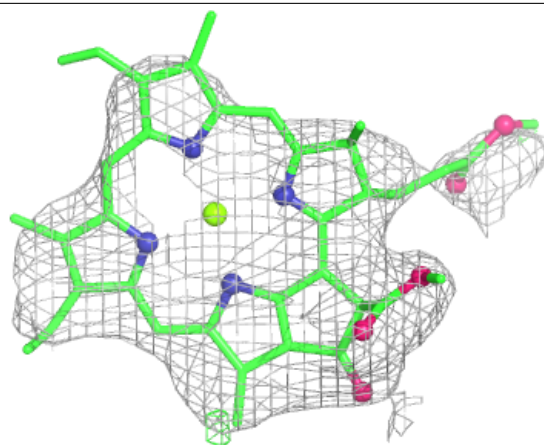
**Electron density around XAT 9 617:**

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



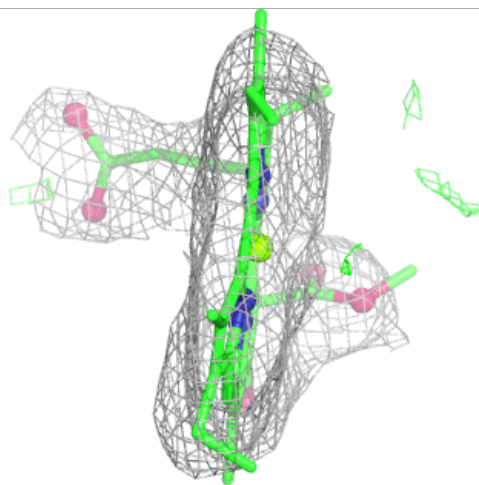
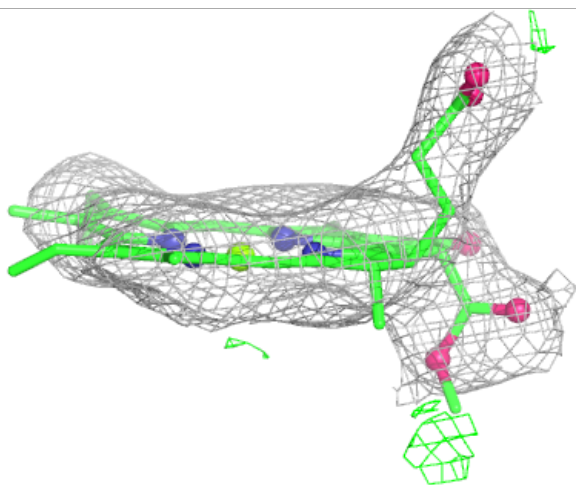
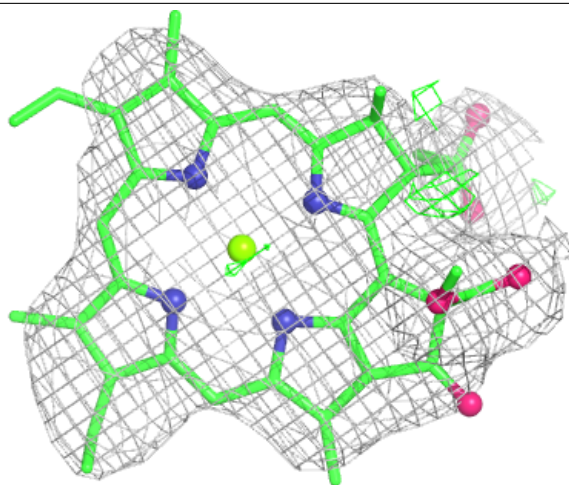
Electron density around CLA K 4003:

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



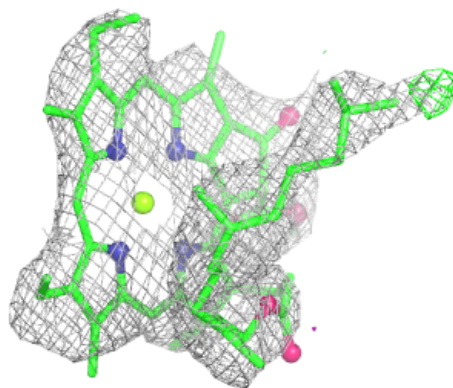
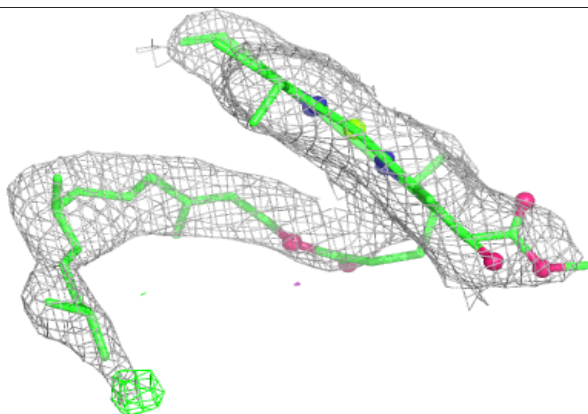
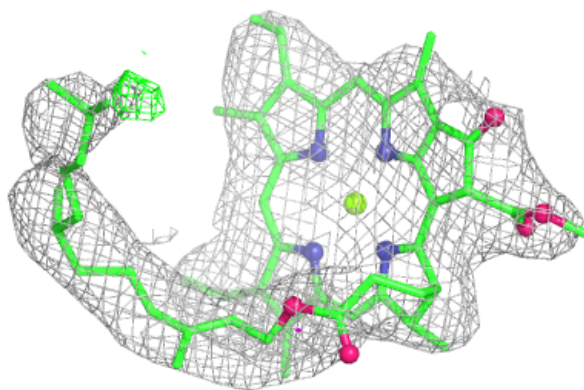
Electron density around CLA k 1401:

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



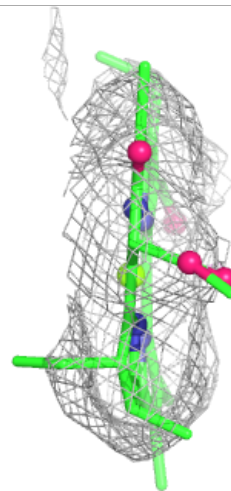
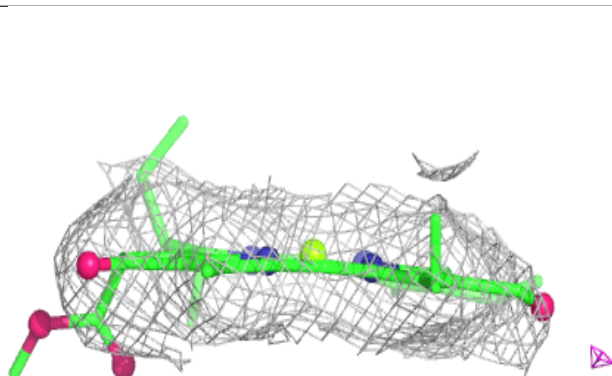
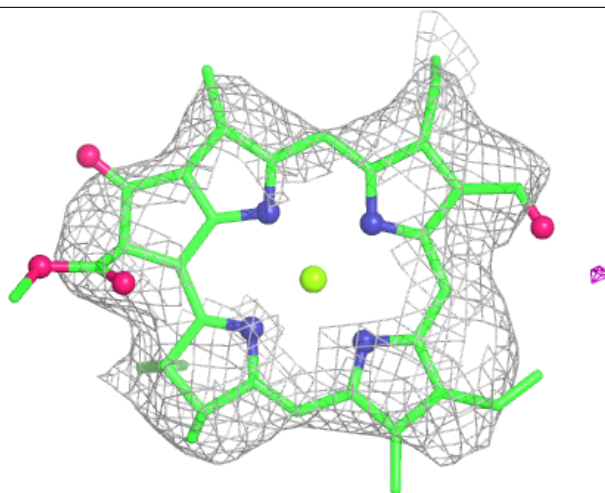
Electron density around CLA 2 609:

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



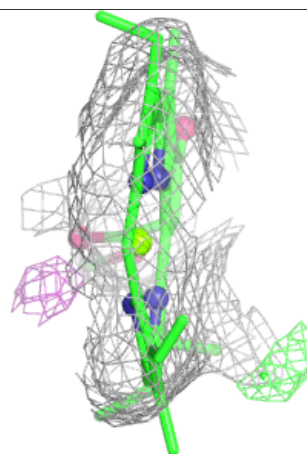
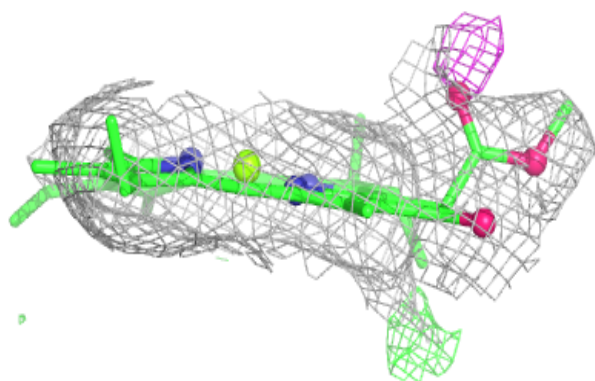
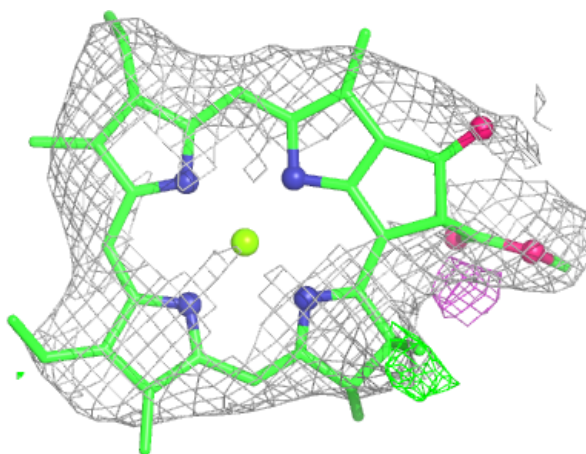
Electron density around CHL 2 614:

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



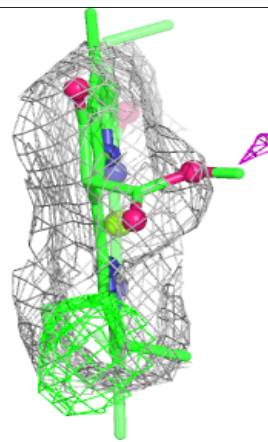
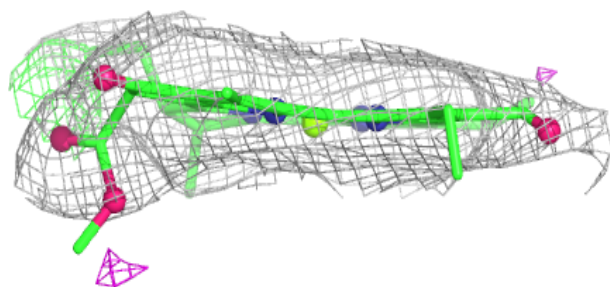
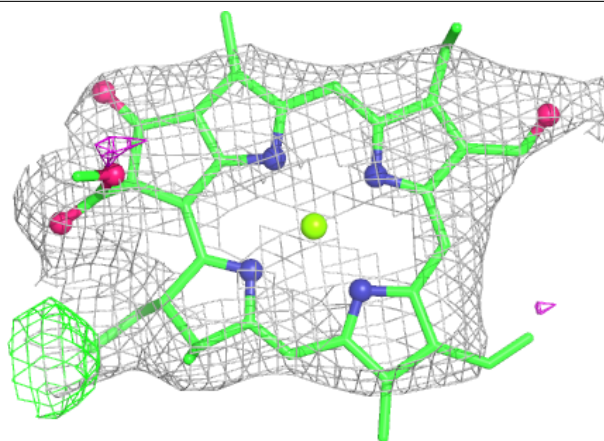
Electron density around CLA 2 610:

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



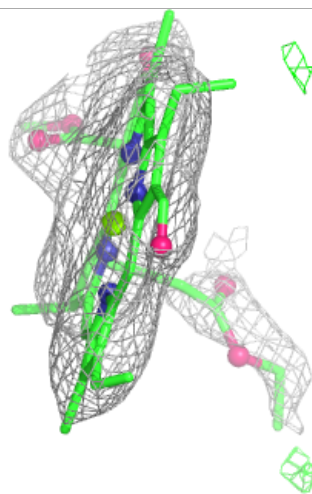
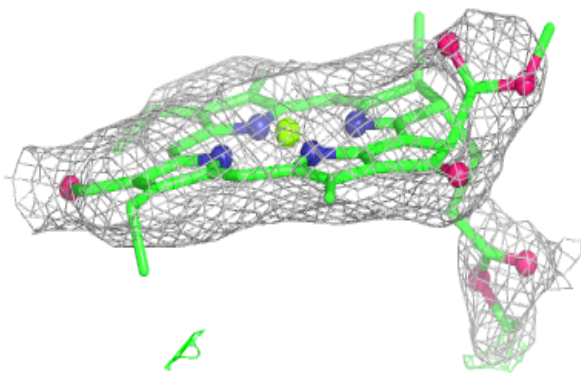
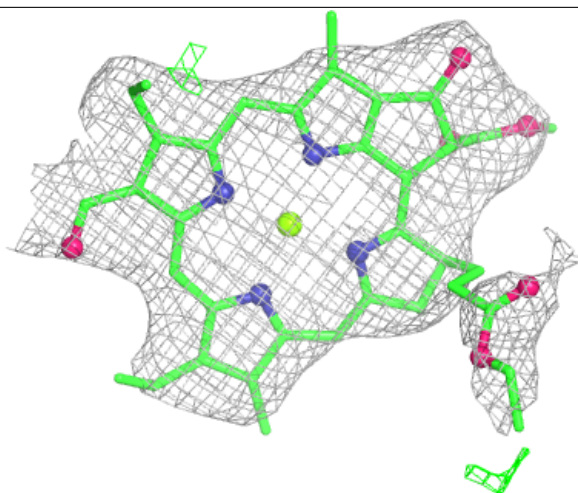
Electron density around CHL 7 605:

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



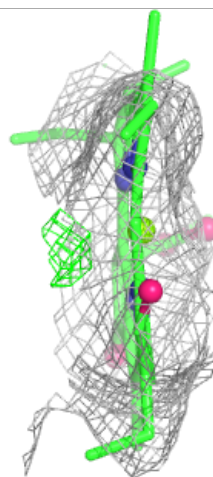
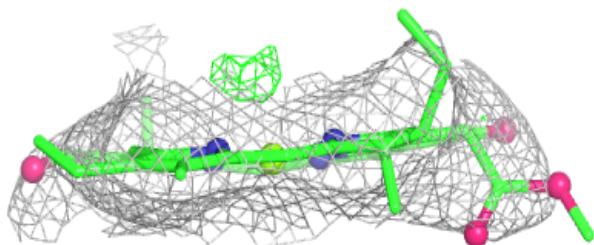
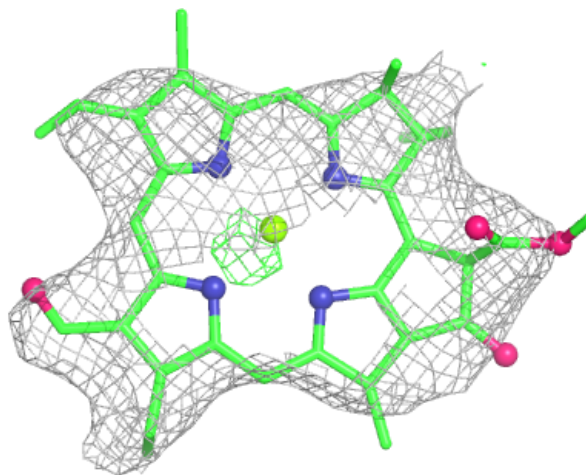
Electron density around CHL 7 606:

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



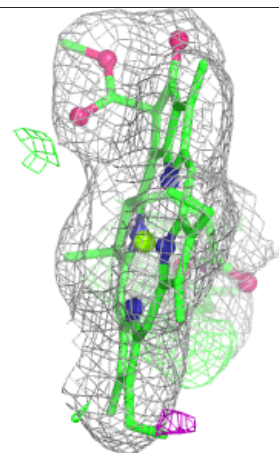
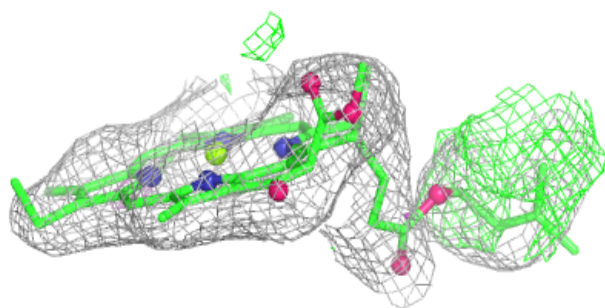
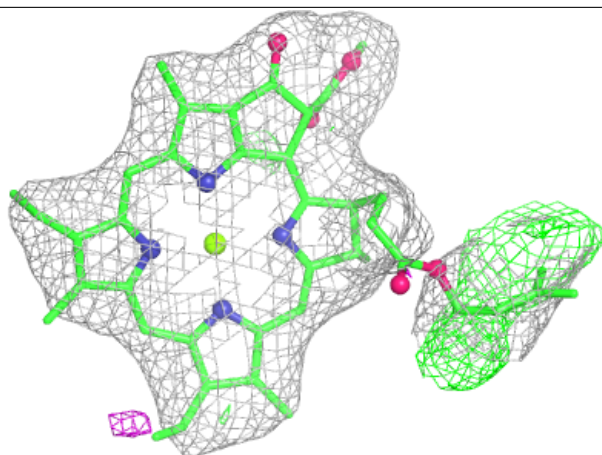
Electron density around CHL 7 614:

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

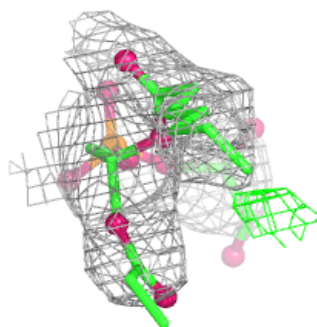
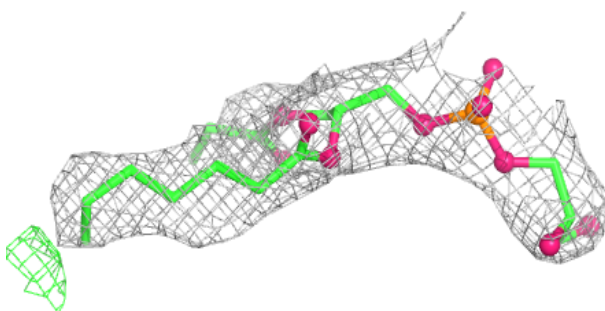
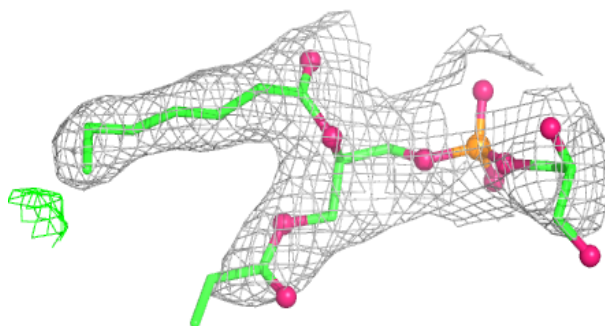


Electron density around CLA 1 204:

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

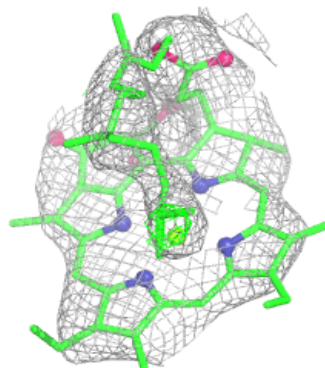
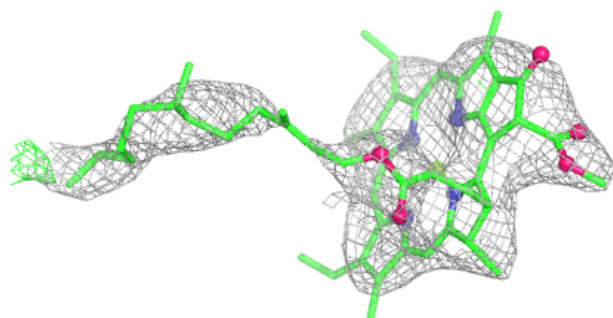
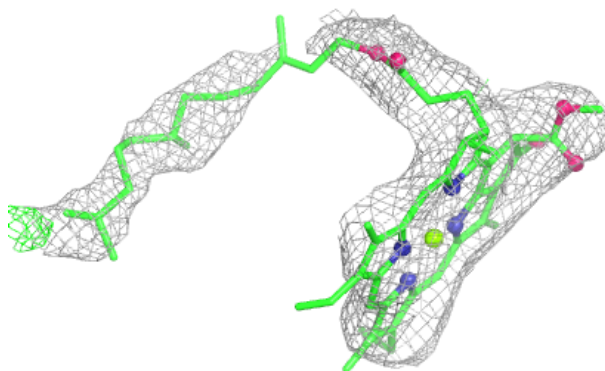
**Electron density around LHG A 847:**

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

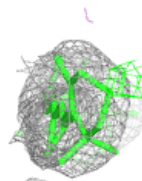
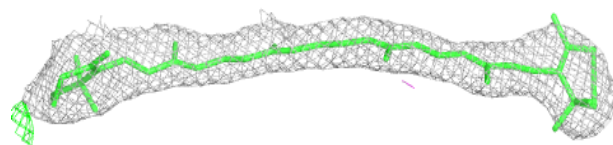
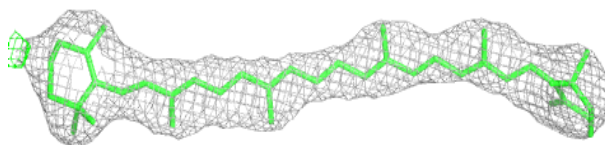


Electron density around CLA 7 604:

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

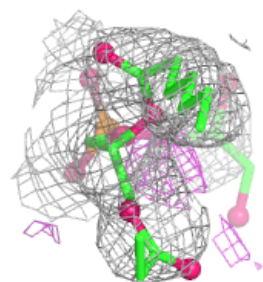
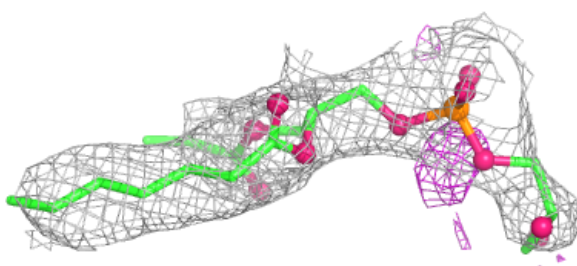
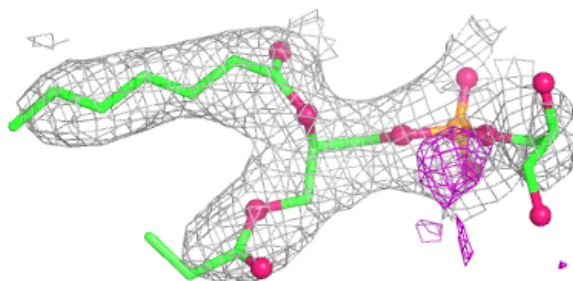
**Electron density around BCR b 843:**

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



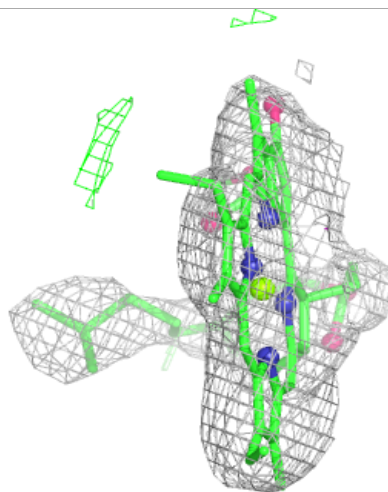
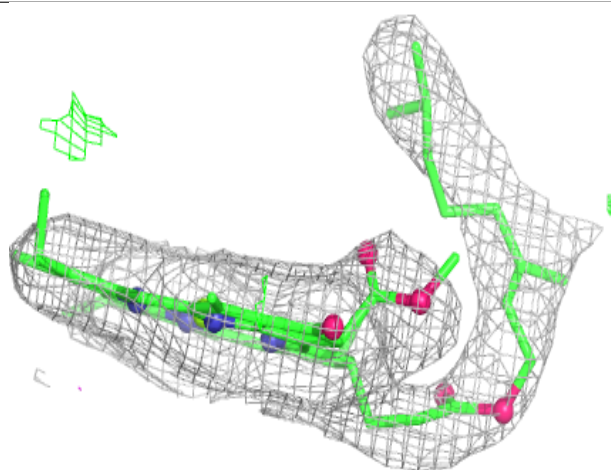
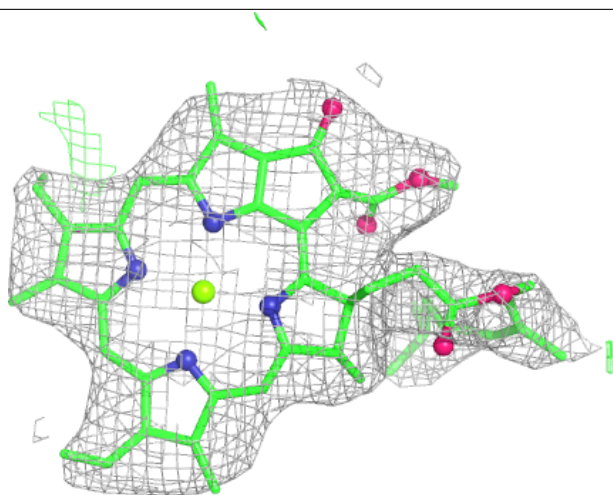
Electron density around LHG a 848:

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



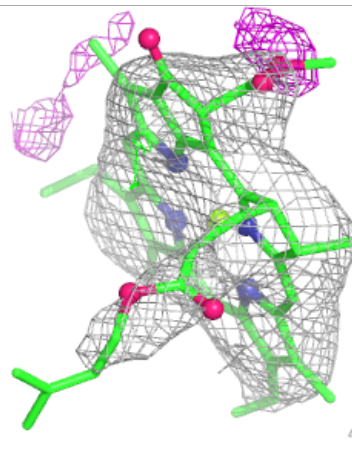
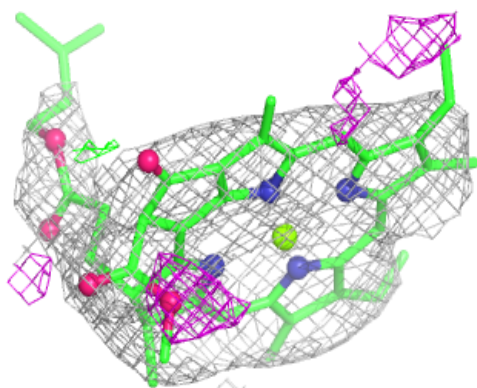
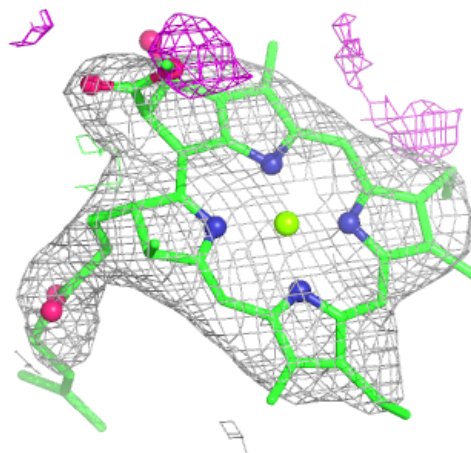
Electron density around CLA F 304:

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



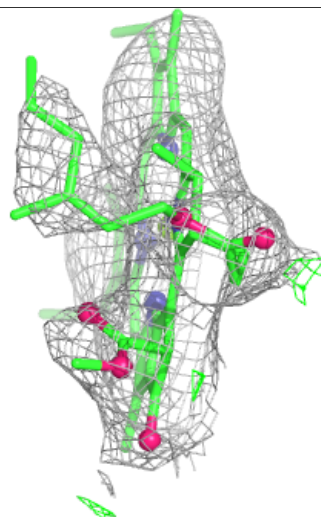
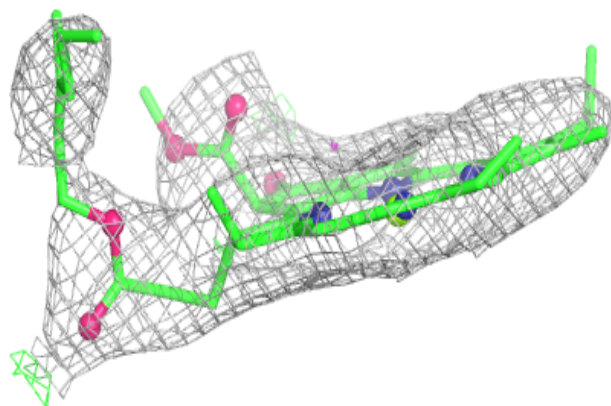
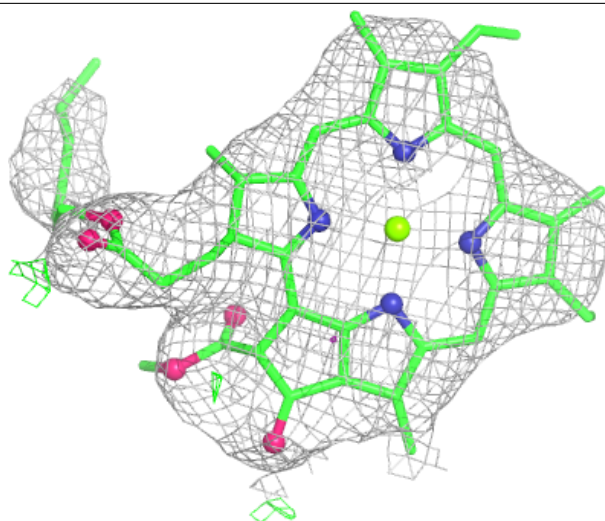
Electron density around CLA 4 604:

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



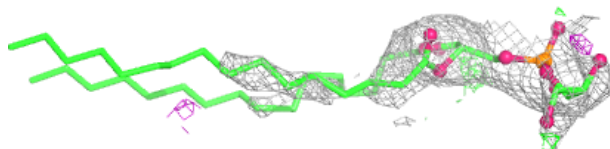
Electron density around CLA 1 312:

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

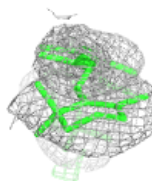
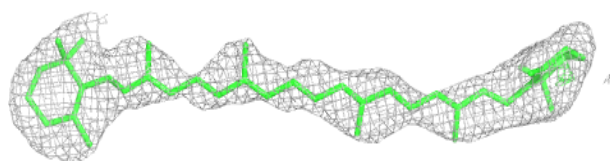
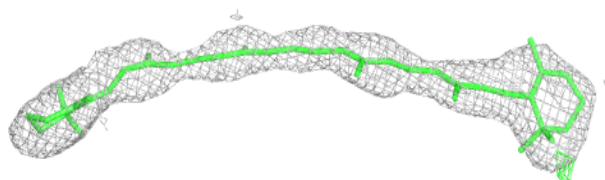


Electron density around LHG 6 320:

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

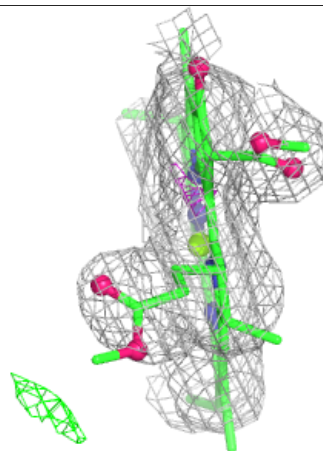
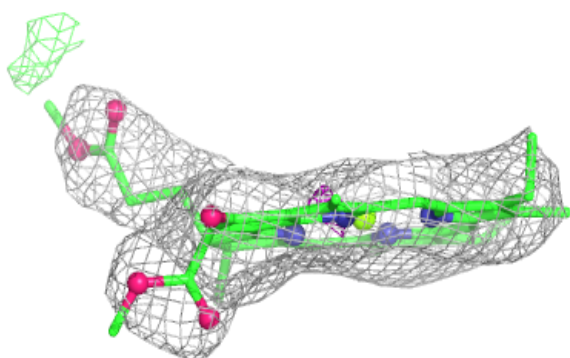
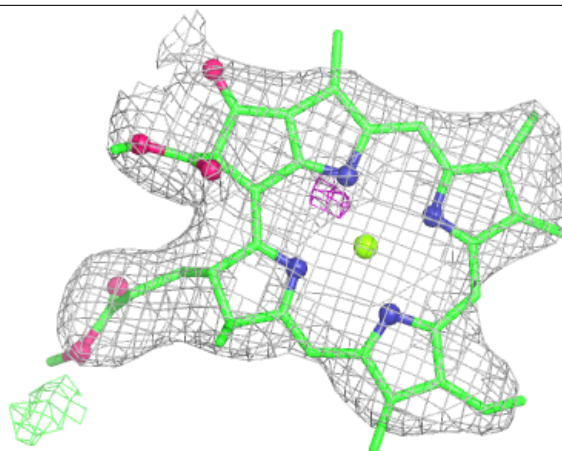
**Electron density around BCR a 849:**

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

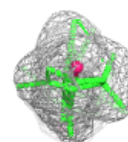
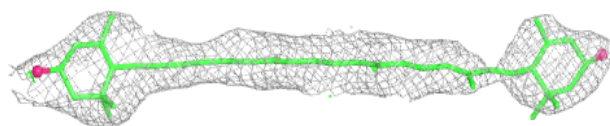
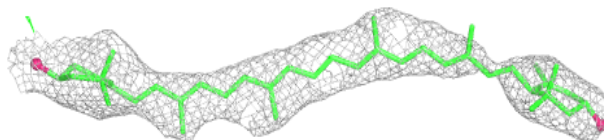


Electron density around CLA k 1402:

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

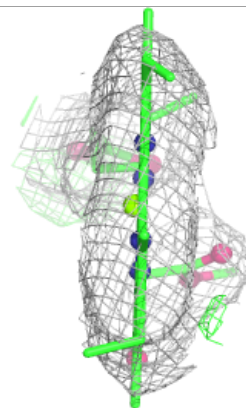
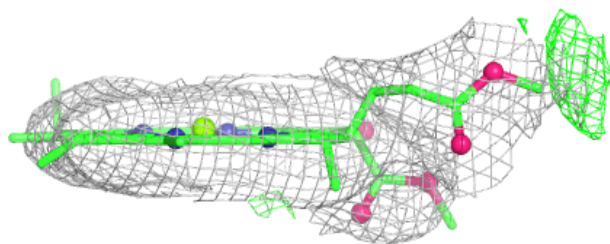
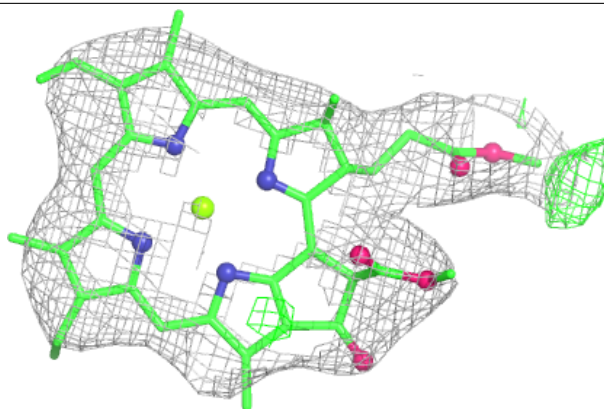
**Electron density around LUT 1 320:**

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

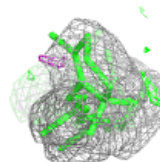
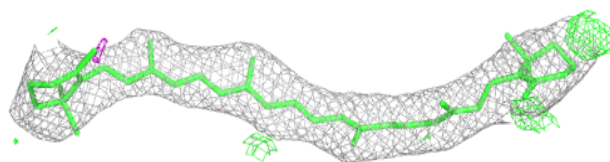
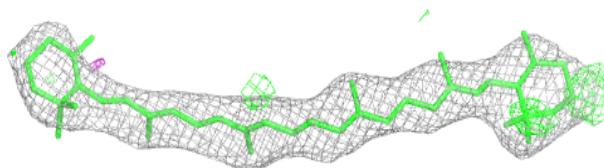


Electron density around CLA 1 315:

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

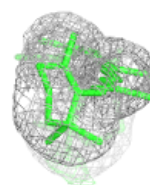
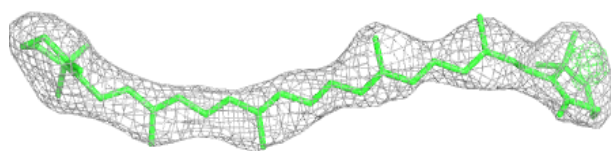
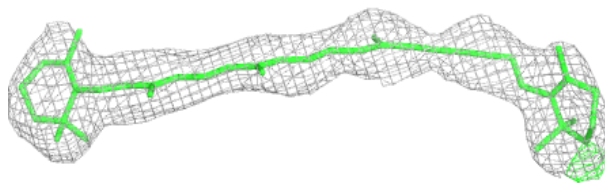
**Electron density around BCR j 3004:**

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



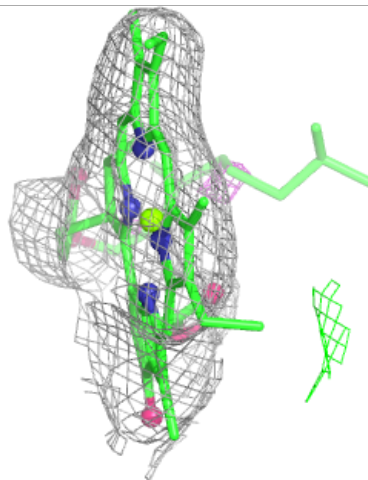
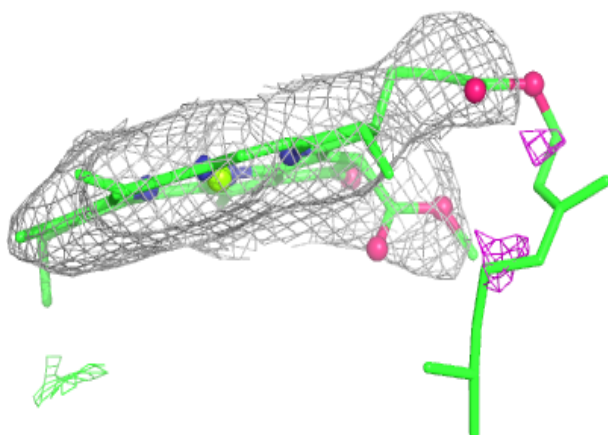
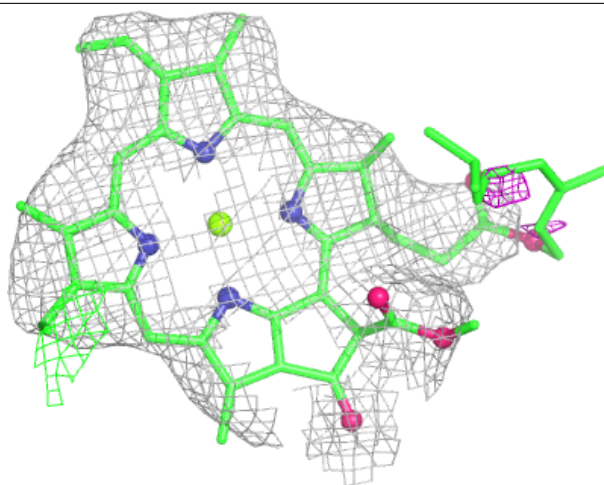
Electron density around BCR I 101:

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



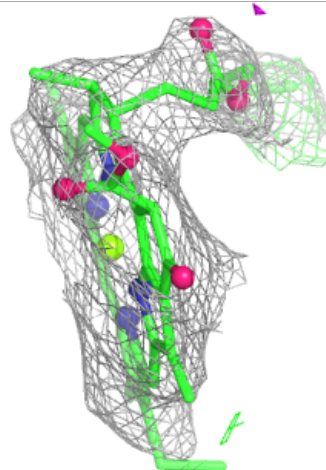
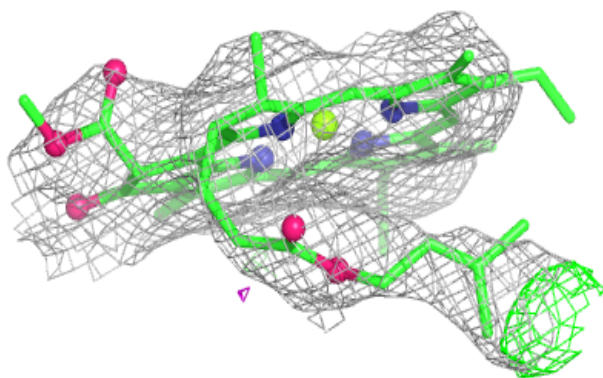
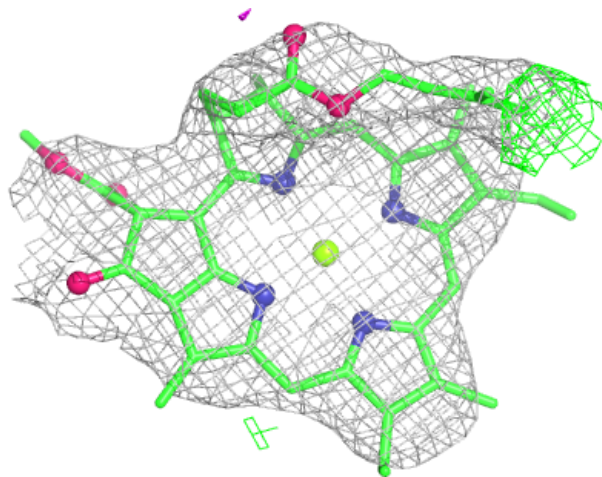
Electron density around CLA f 7003:

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



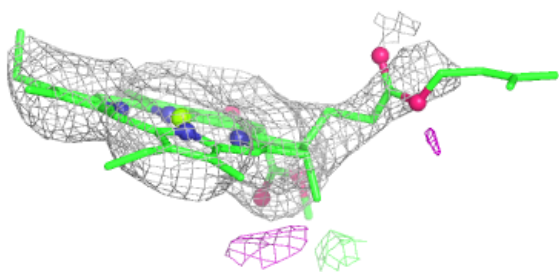
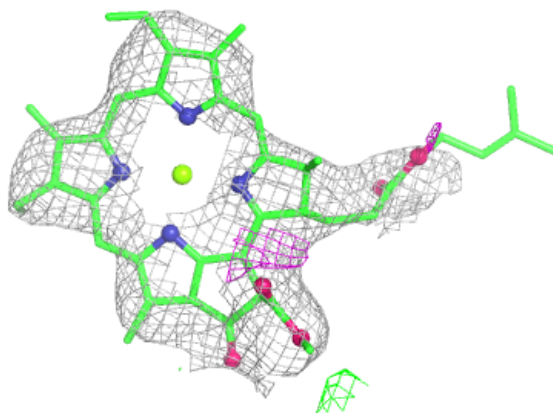
Electron density around CLA 8 308:

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



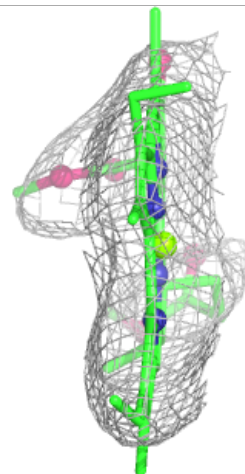
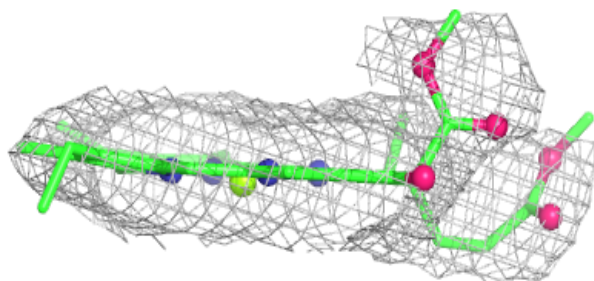
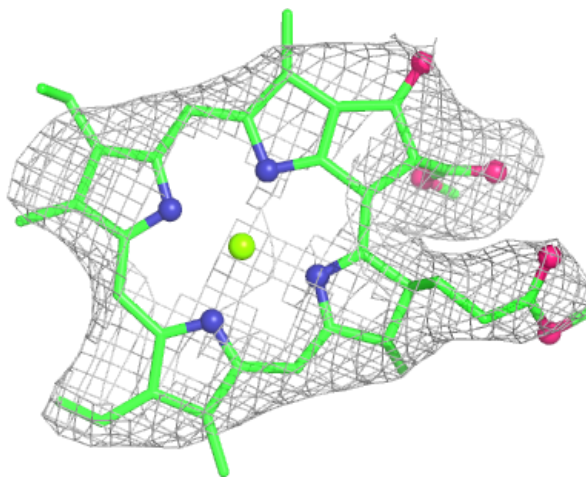
Electron density around CLA g 102:

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



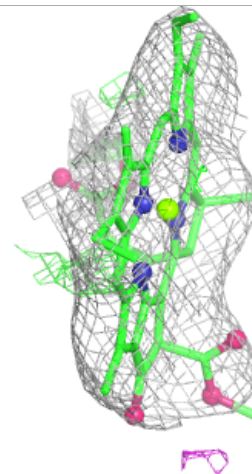
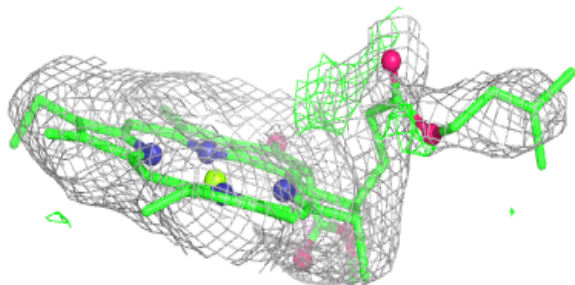
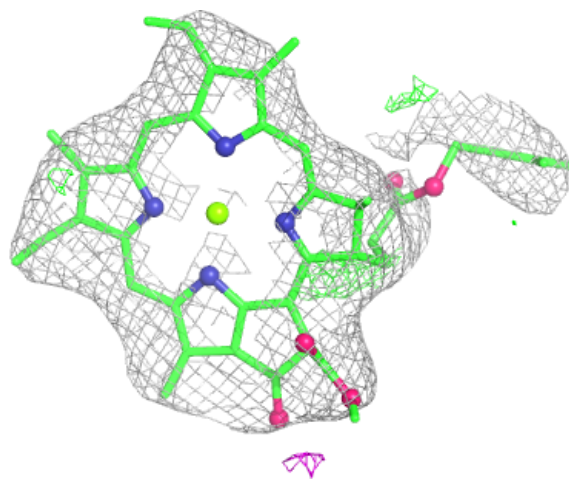
Electron density around CLA g 103:

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



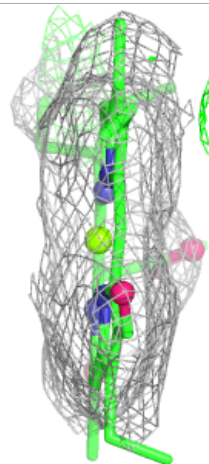
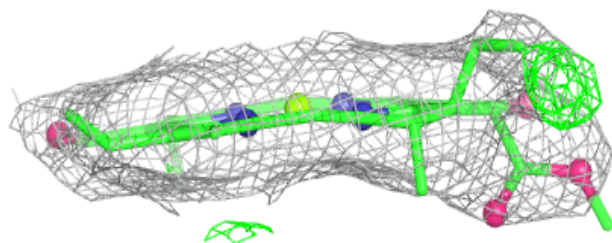
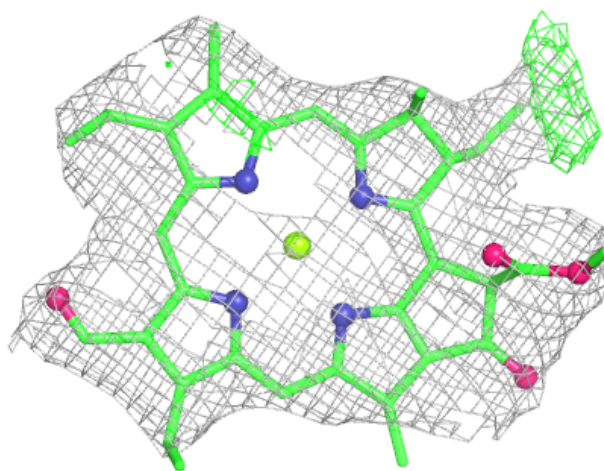
Electron density around CLA L 204:

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



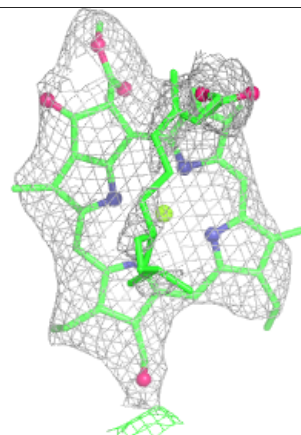
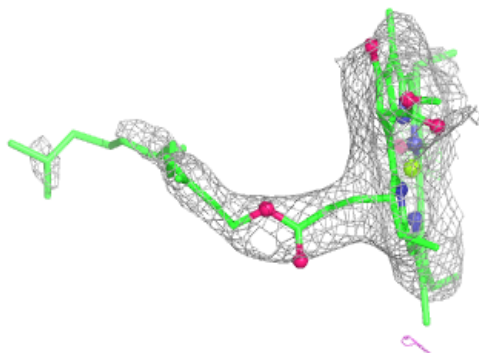
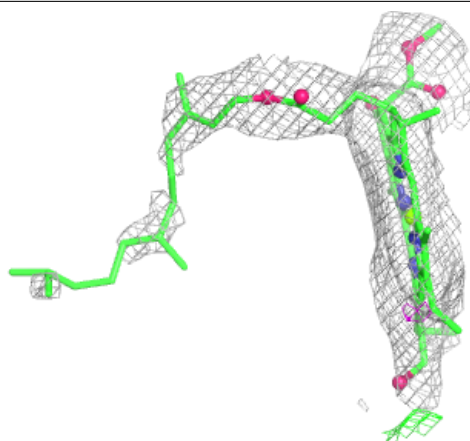
Electron density around CHL 4 615:

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

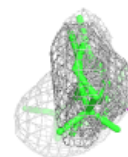
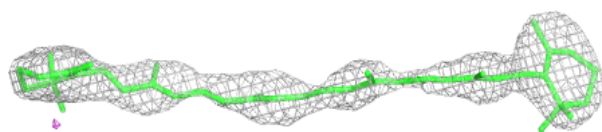
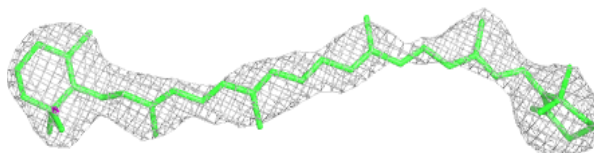


Electron density around CHL 6 303:

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

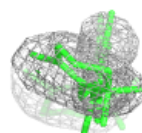
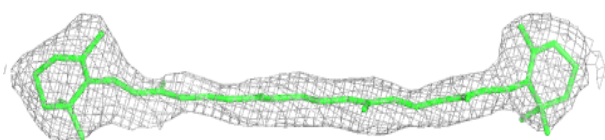
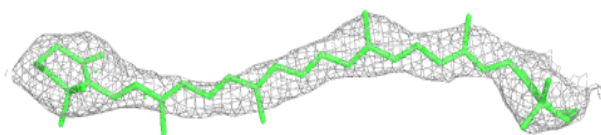
**Electron density around BCR 4 618:**

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

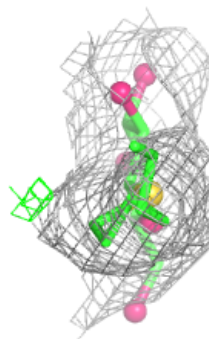
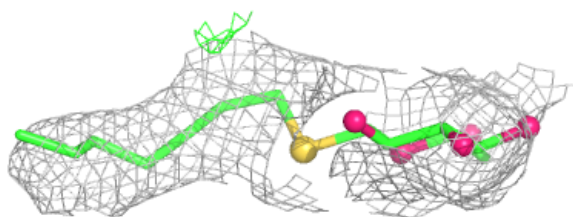
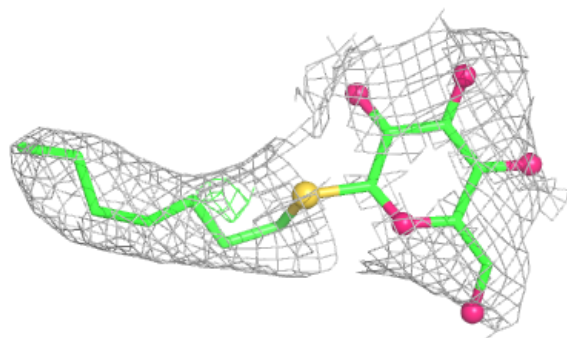


Electron density around BCR 8 316:

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

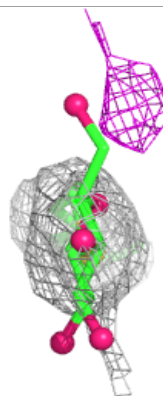
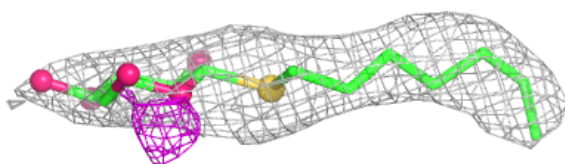
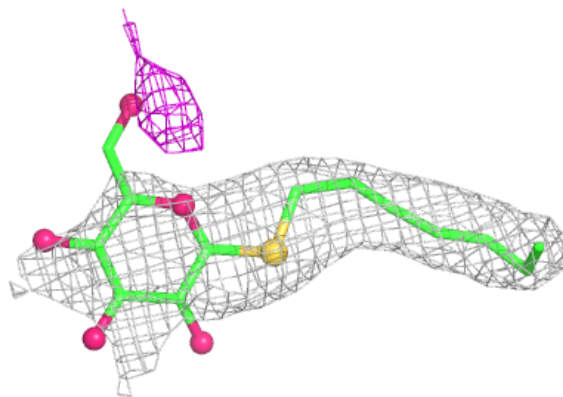
**Electron density around HTG J 3001:**

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



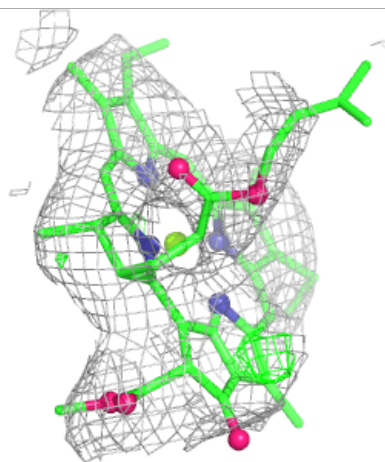
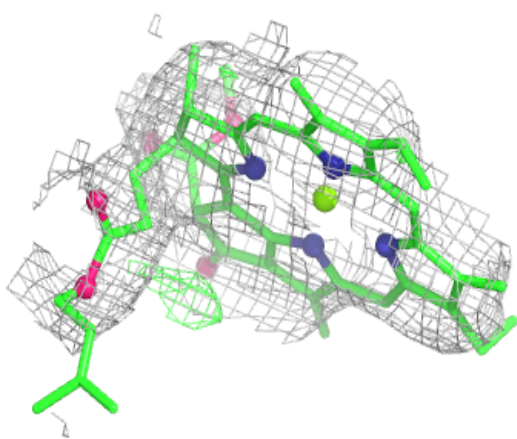
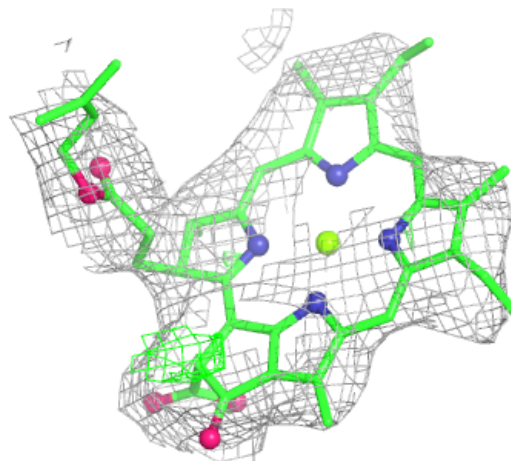
Electron density around HTG f 7001:

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



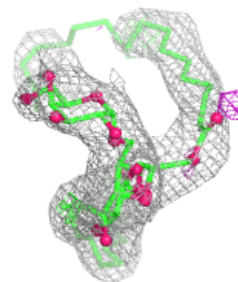
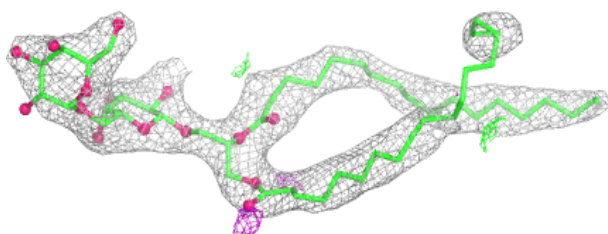
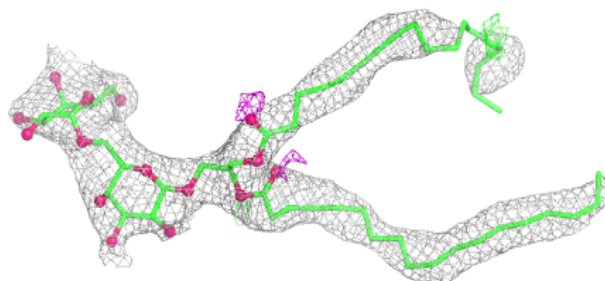
Electron density around CLA 9 604:

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

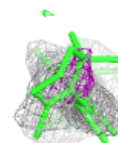
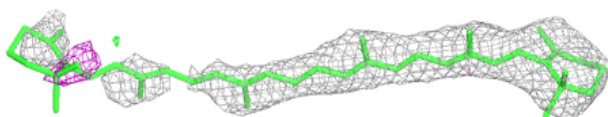
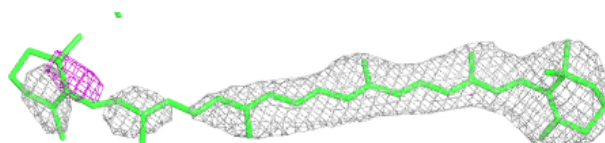


Electron density around DGD b 849:

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

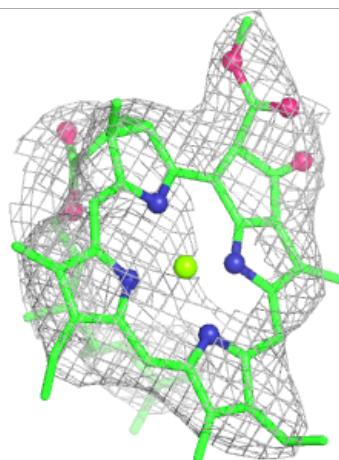
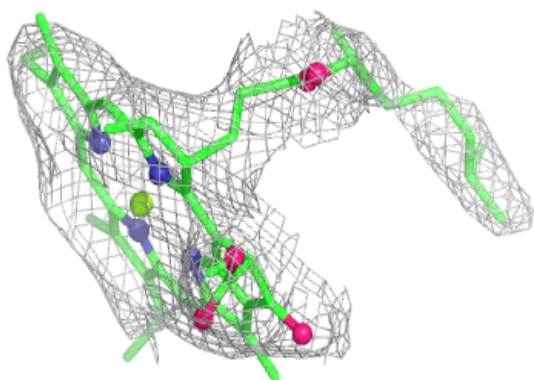
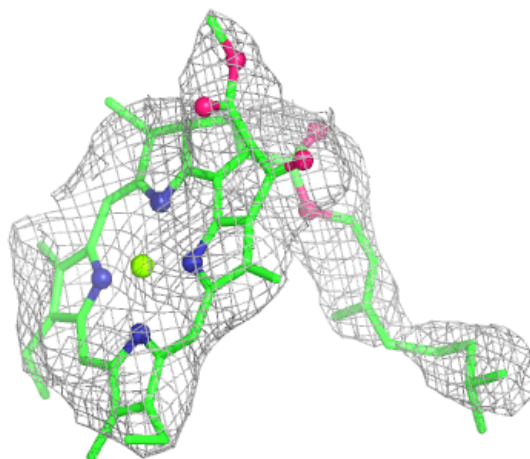
**Electron density around BCR a 852:**

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



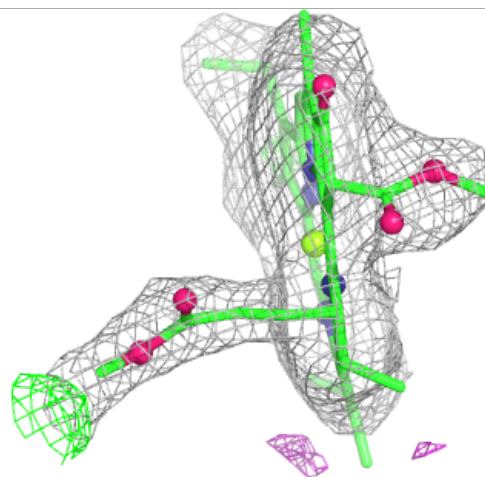
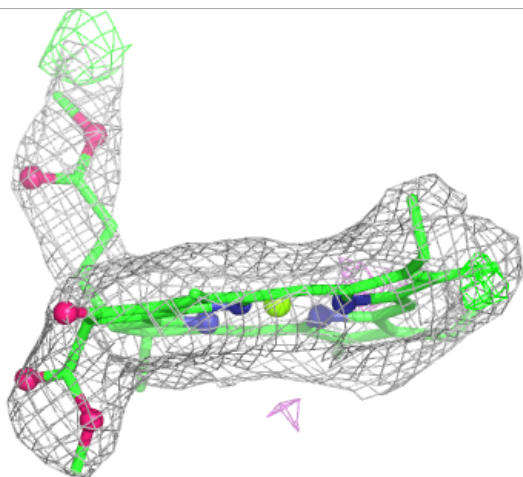
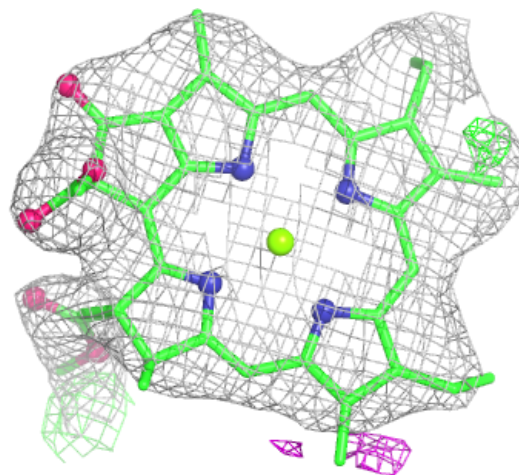
Electron density around CLA 4 610:

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



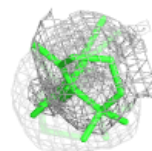
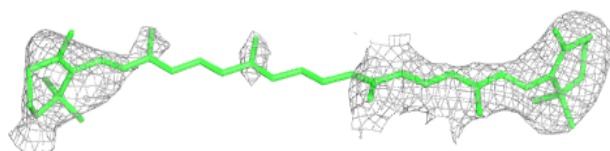
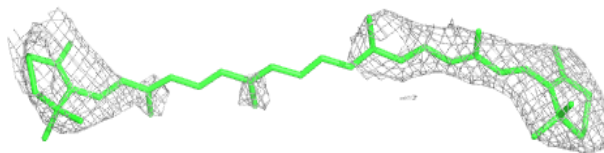
Electron density around CLA B 821:

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

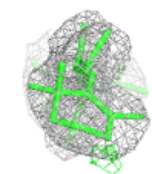
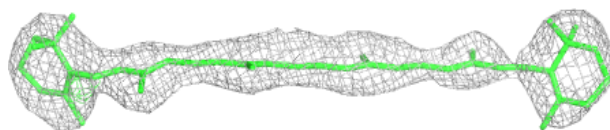
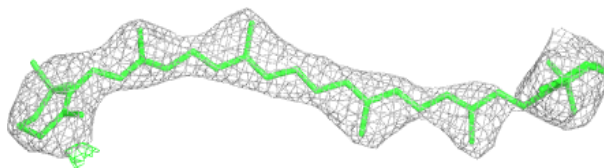


Electron density around BCR g 104:

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

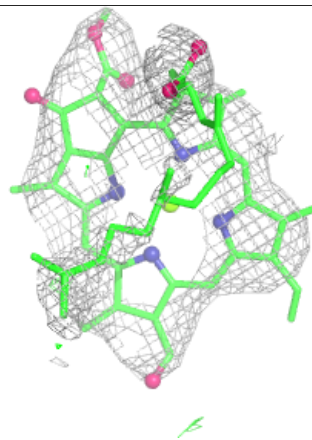
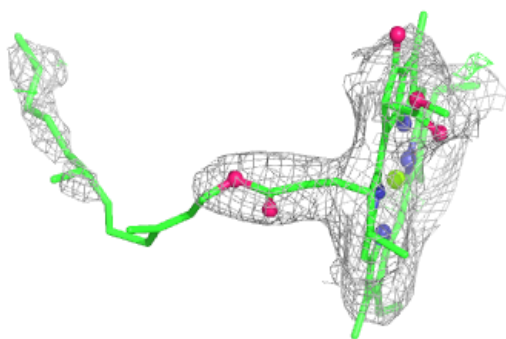
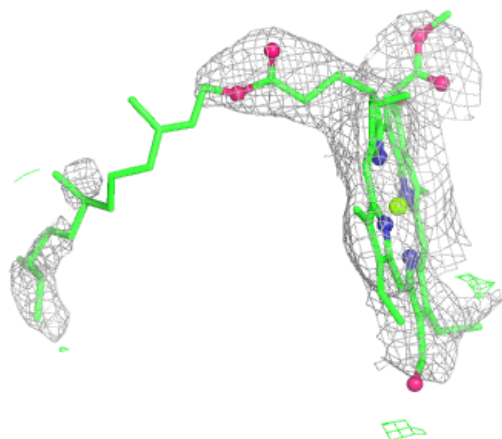
**Electron density around BCR b 846:**

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



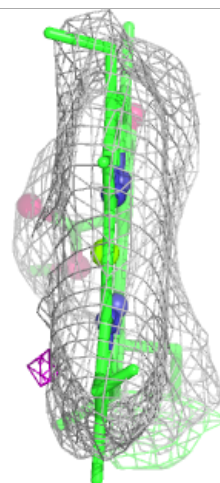
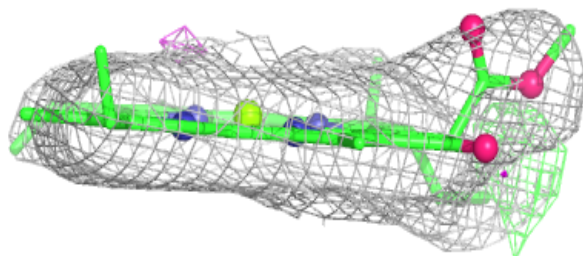
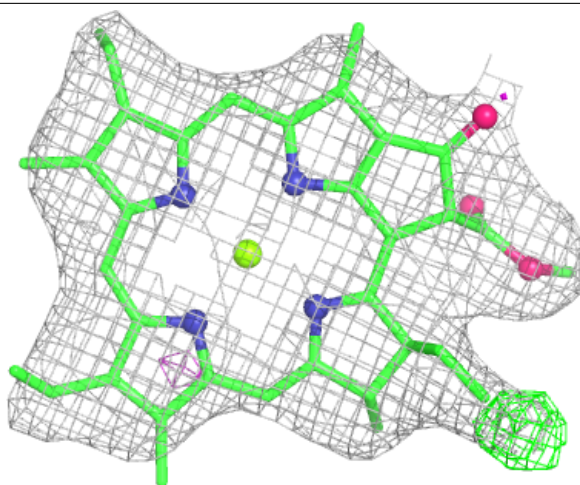
Electron density around CHL 2 601:

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



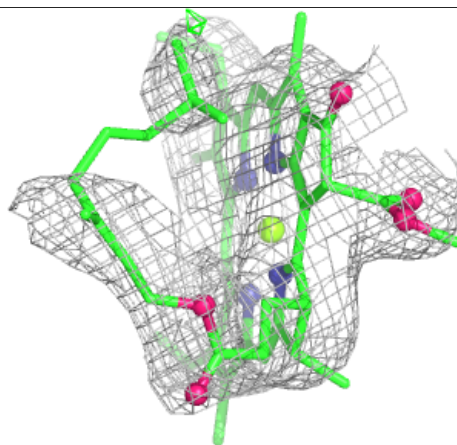
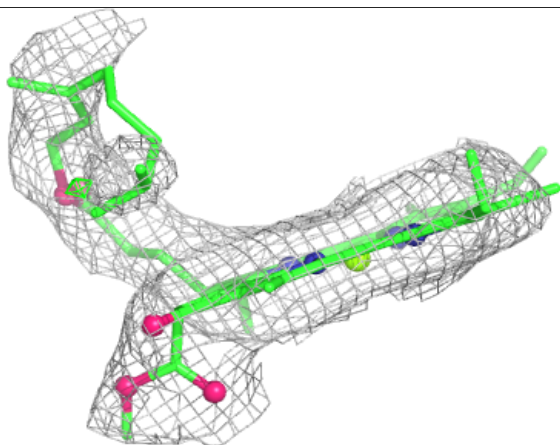
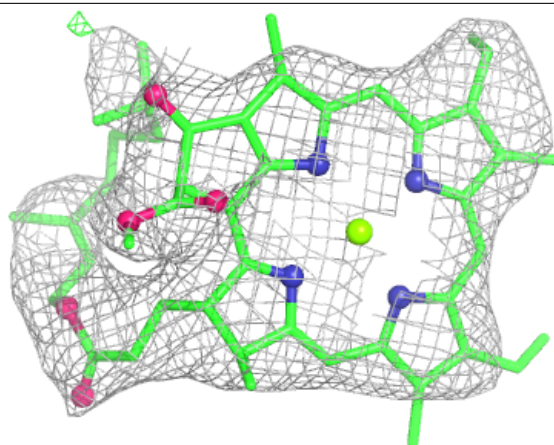
Electron density around CLA 3 305:

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

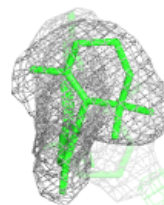
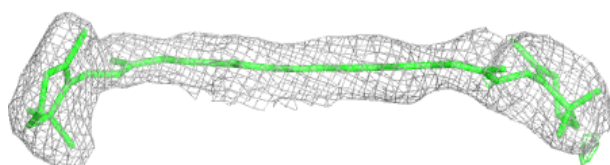
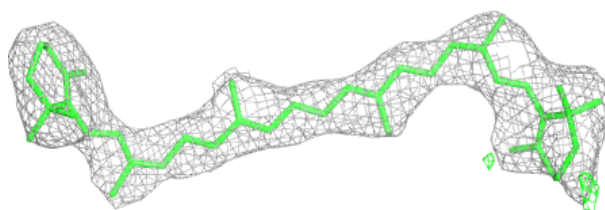


Electron density around CLA 1 314:

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

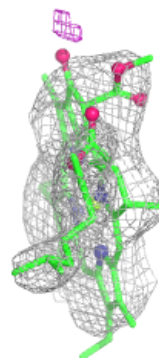
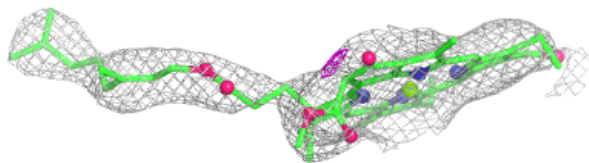
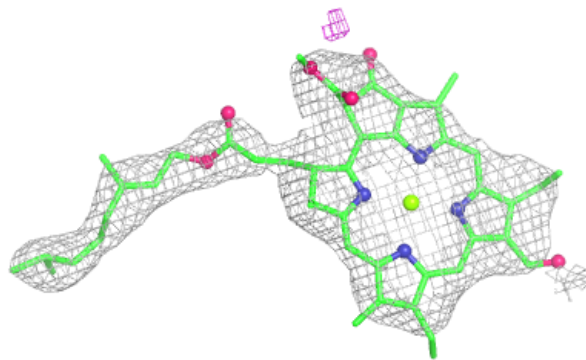
**Electron density around BCR B 845:**

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

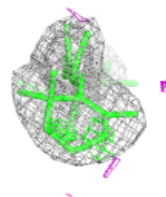
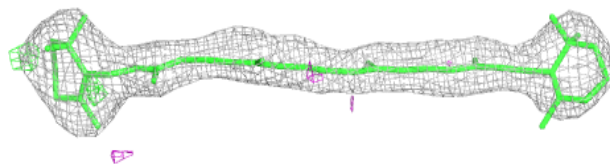
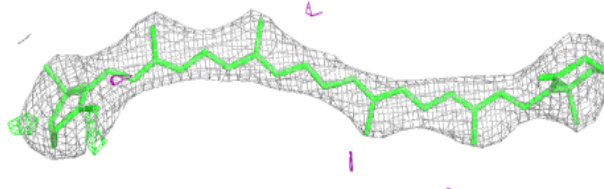


Electron density around CHL 4 605:

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

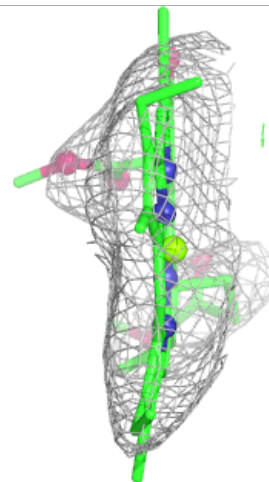
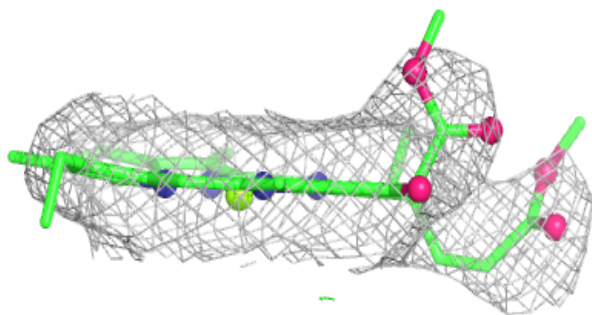
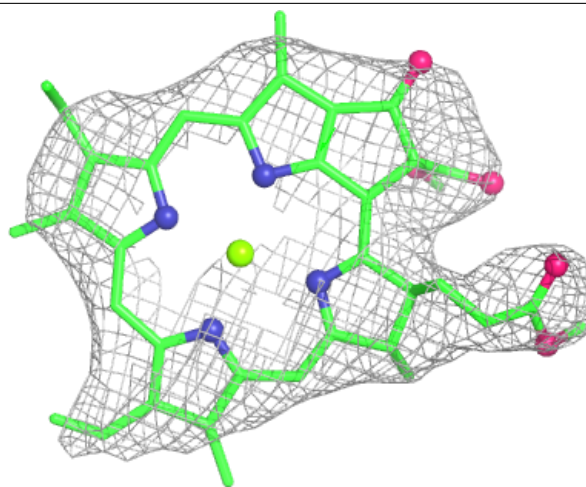
**Electron density around BCR B 846:**

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



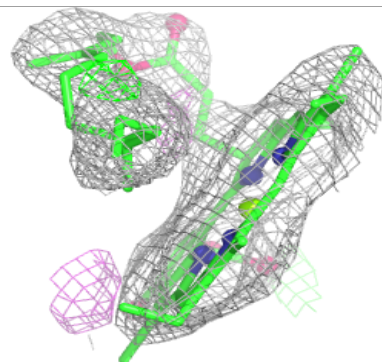
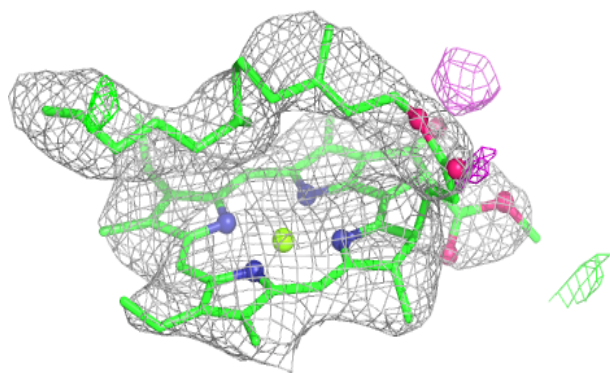
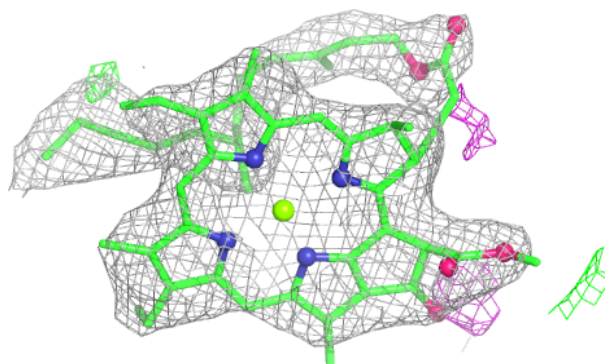
Electron density around CLA G 104:

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



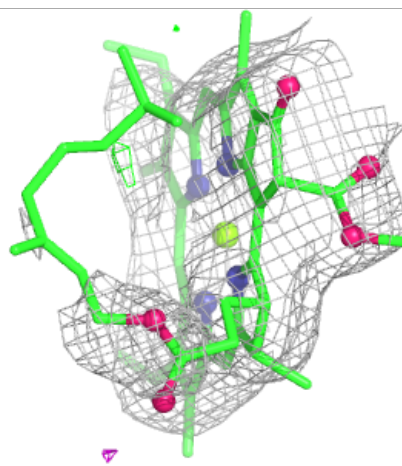
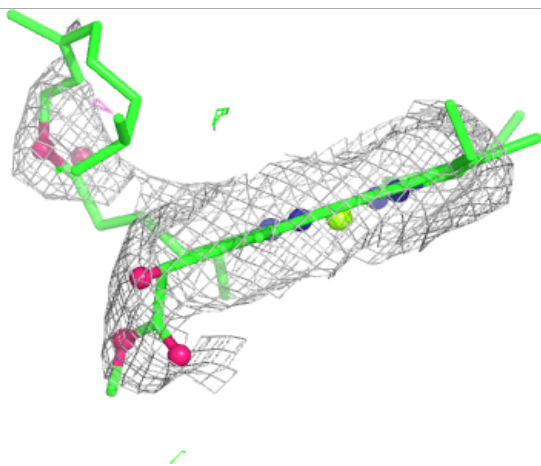
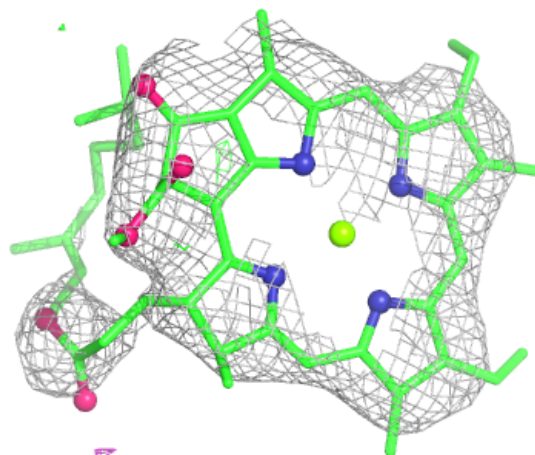
Electron density around CLA b 817:

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



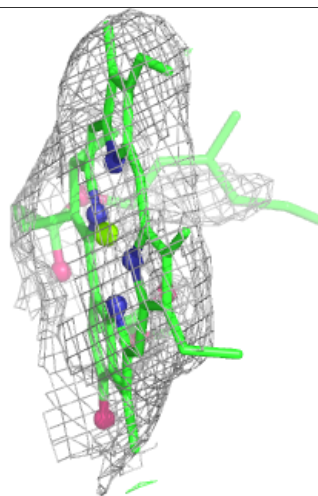
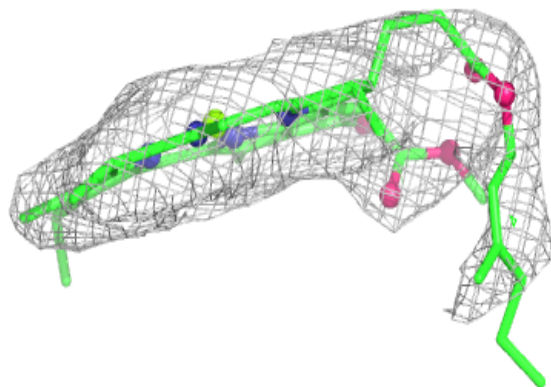
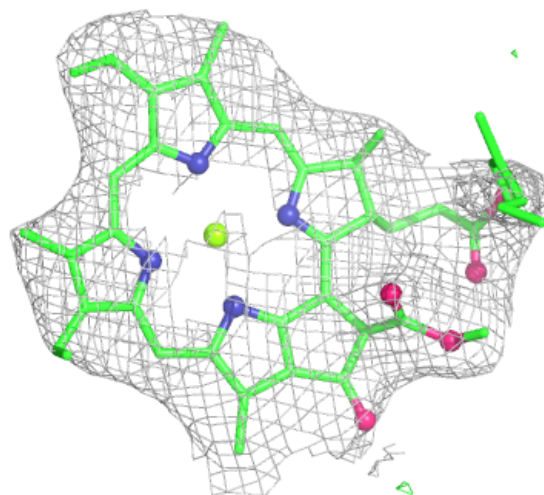
Electron density around CLA 6 315:

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



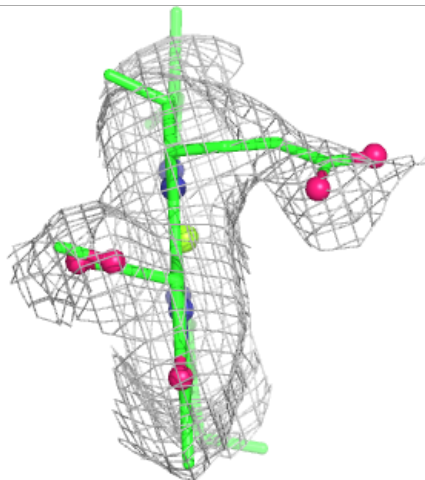
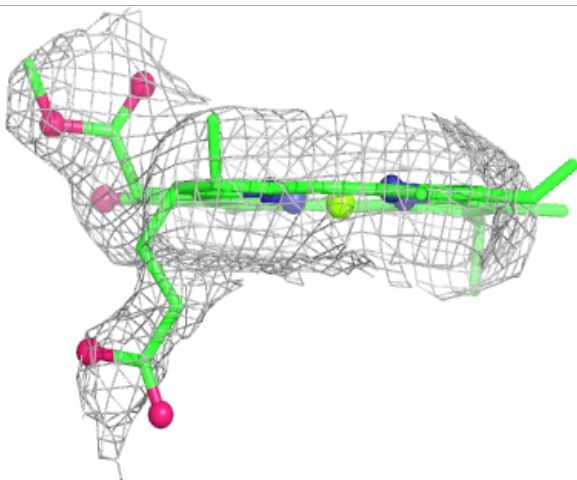
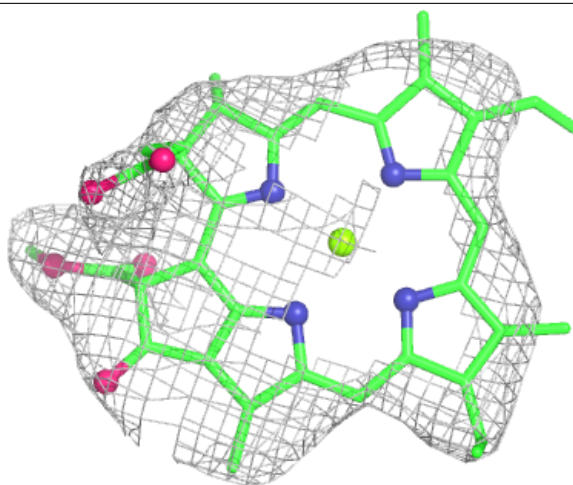
Electron density around CLA 2 611:

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



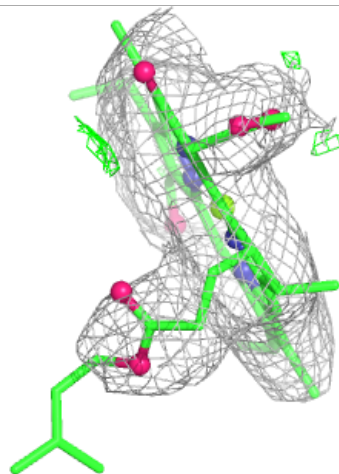
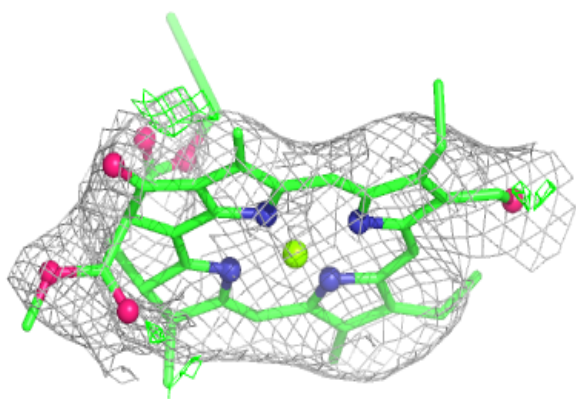
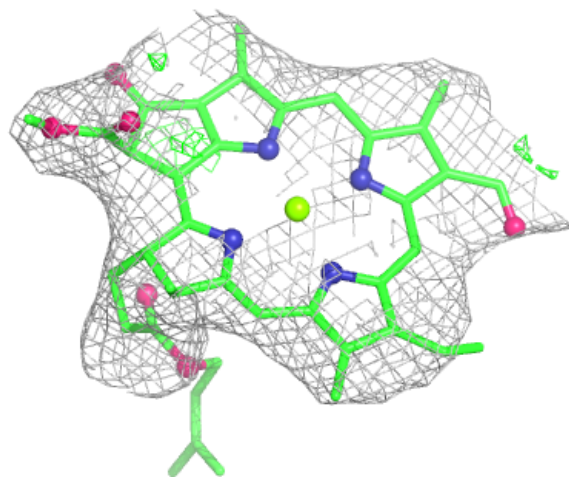
Electron density around CLA 9 613:

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



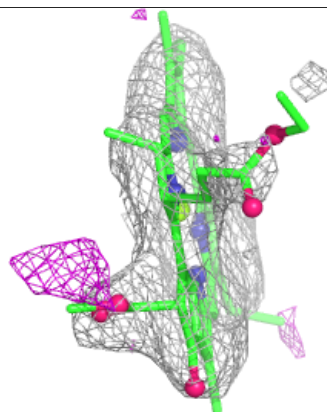
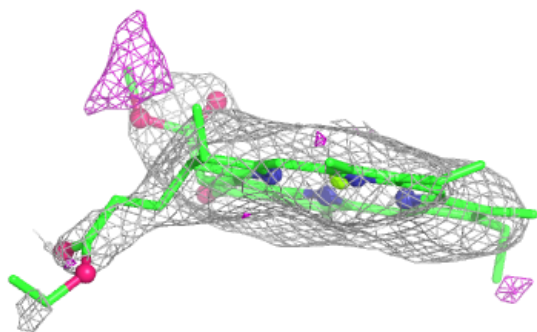
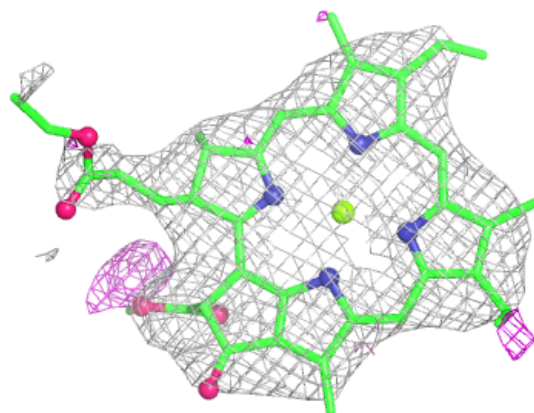
Electron density around CHL 9 606:

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

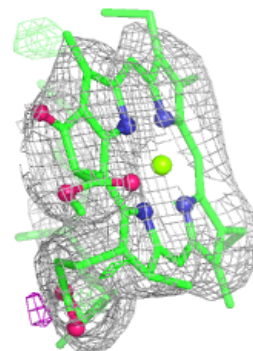
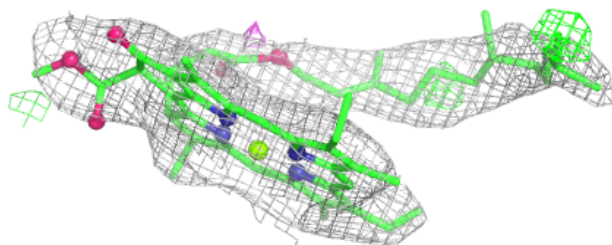
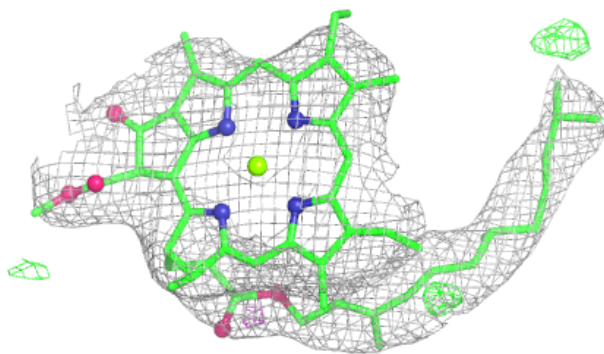


Electron density around CLA 9 614:

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

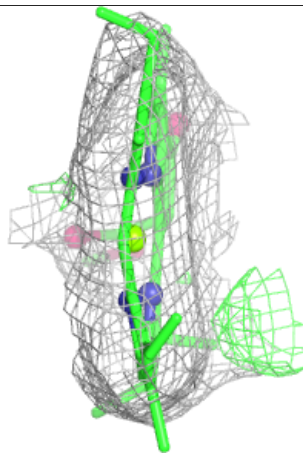
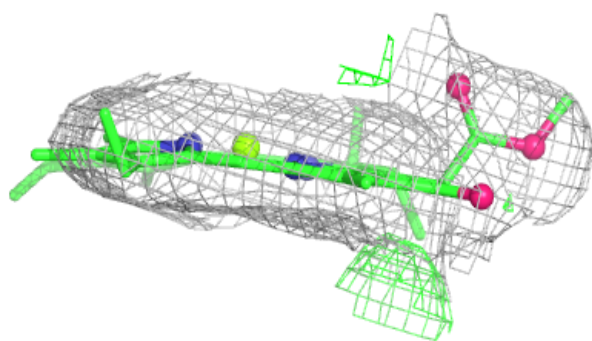
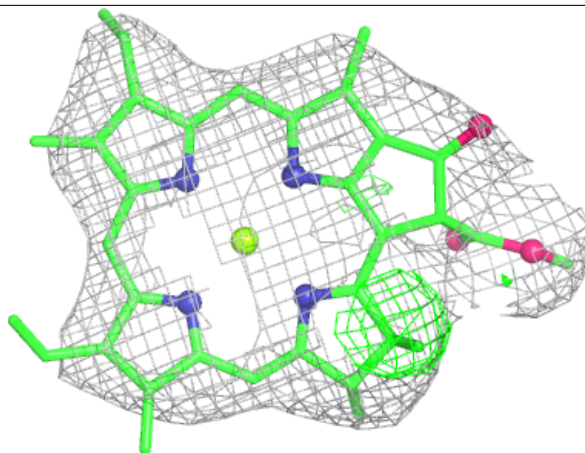
**Electron density around CLA 1 310:**

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



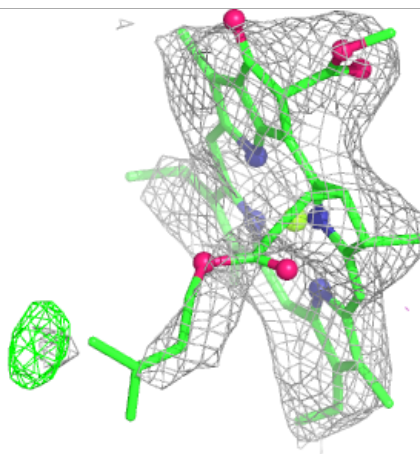
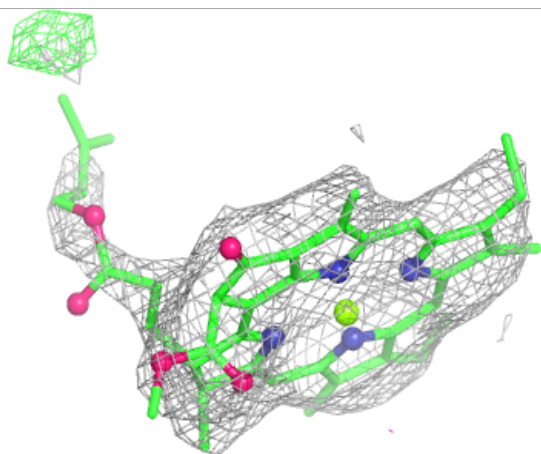
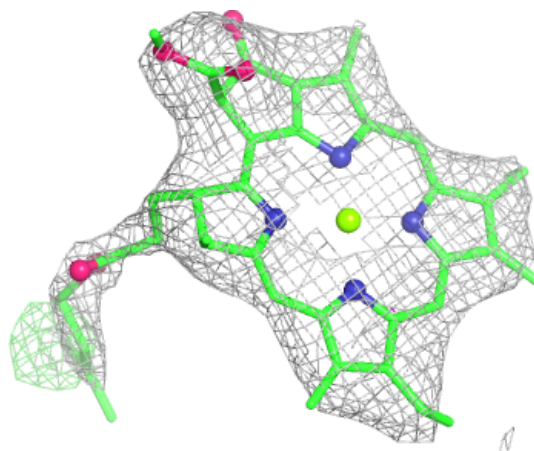
Electron density around CLA 7 610:

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



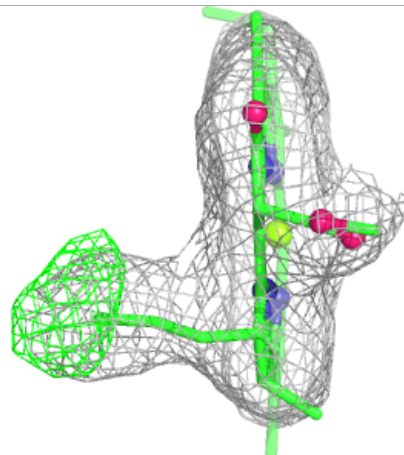
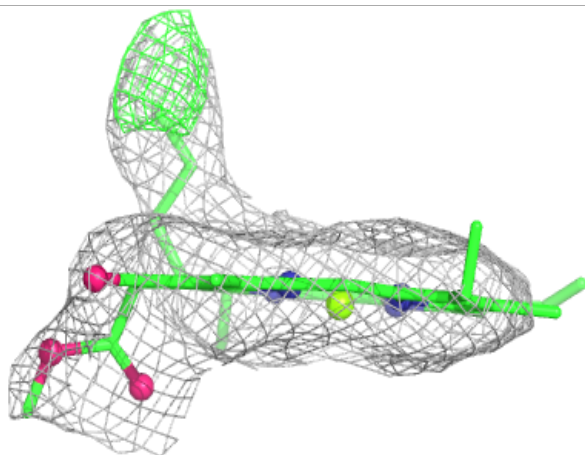
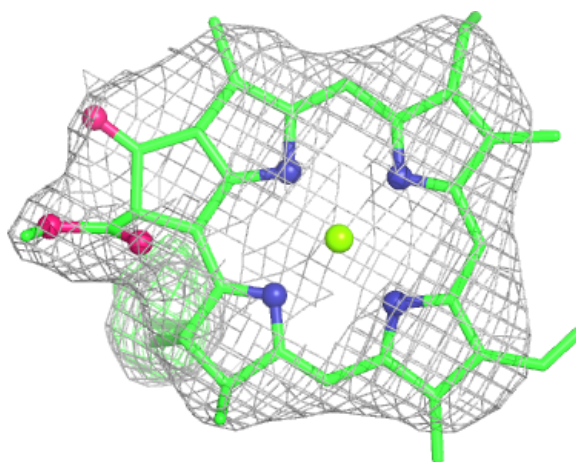
Electron density around CLA A 816:

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



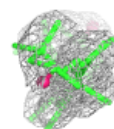
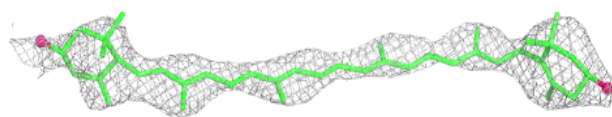
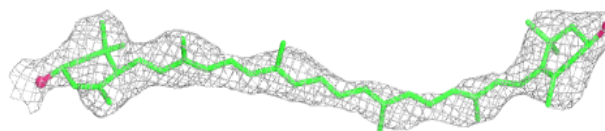
Electron density around CLA 7 613:

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

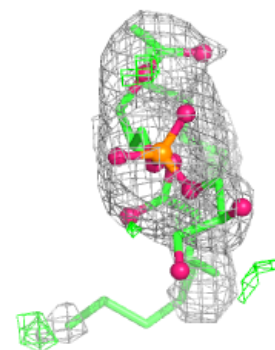
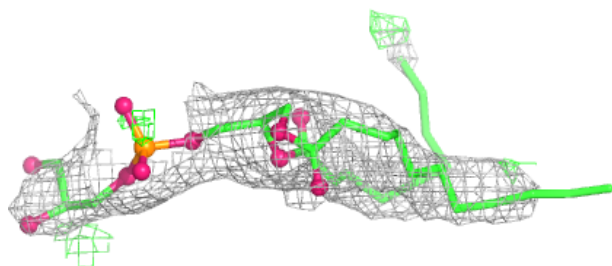
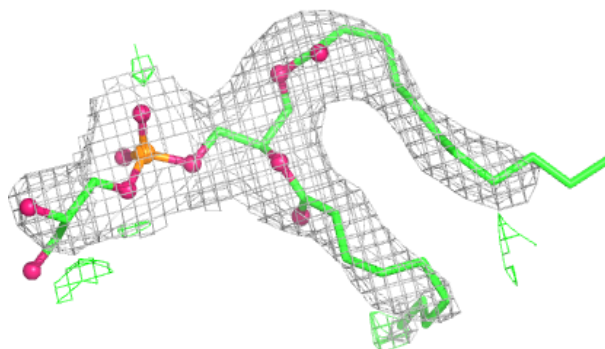


Electron density around LUT 7 615:

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

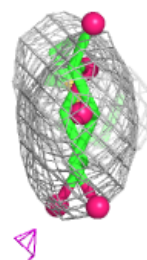
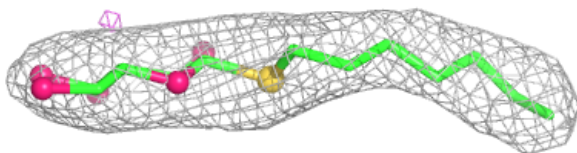
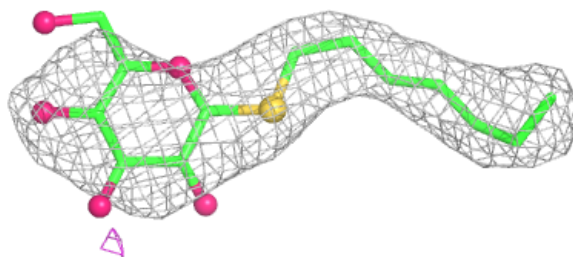
**Electron density around LHG 7 618:**

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



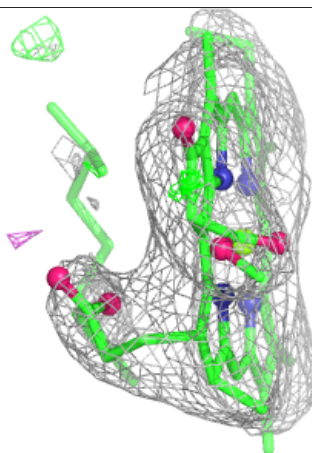
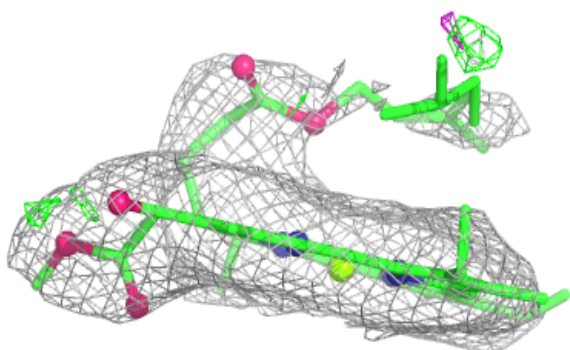
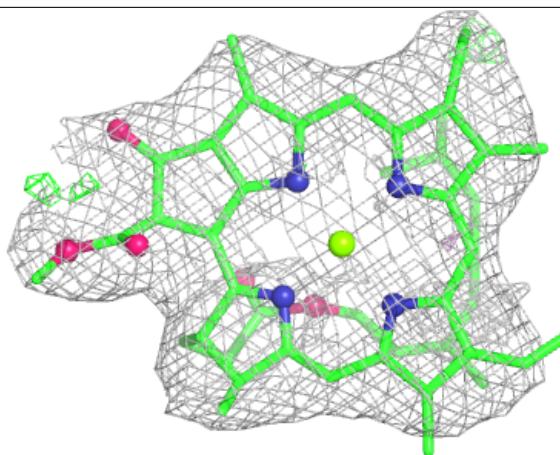
Electron density around HTG F 302:

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



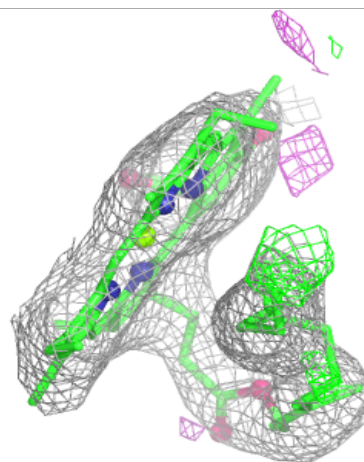
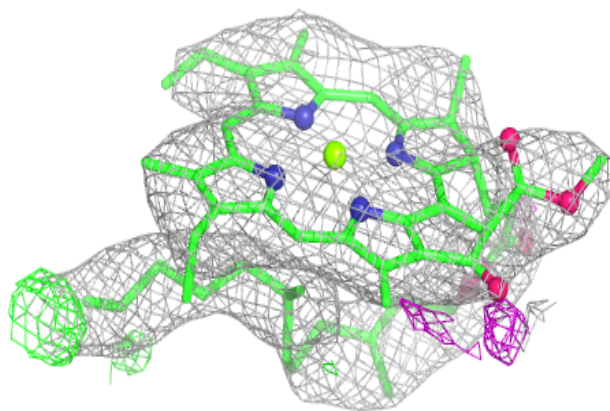
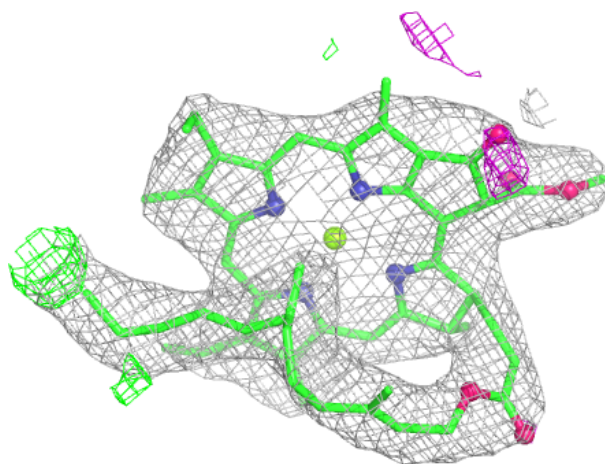
Electron density around CLA B 812:

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



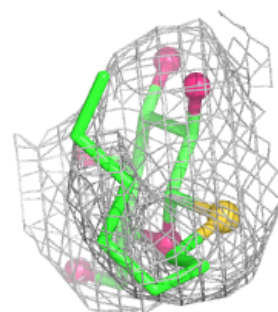
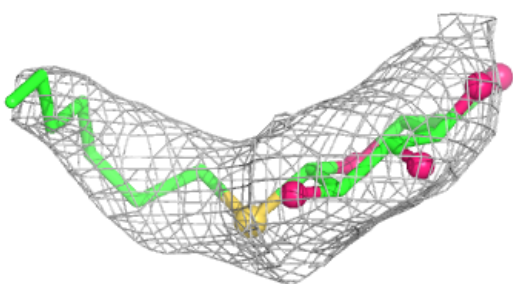
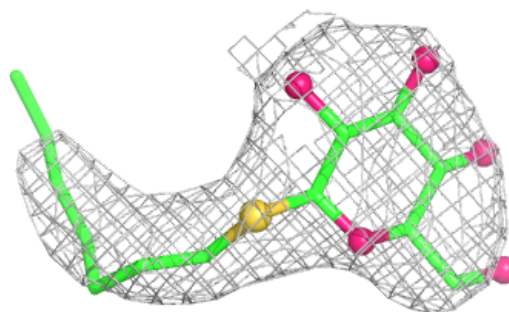
Electron density around CLA B 817:

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

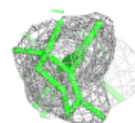
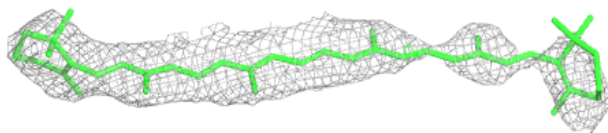
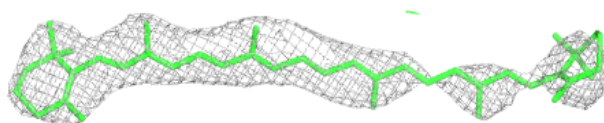


Electron density around HTG j 3001:

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

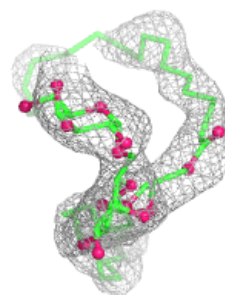
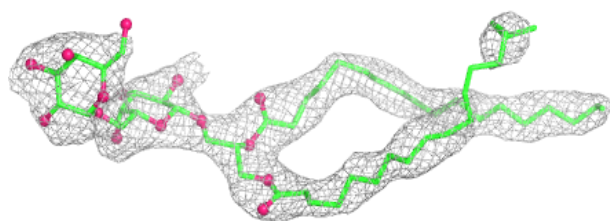
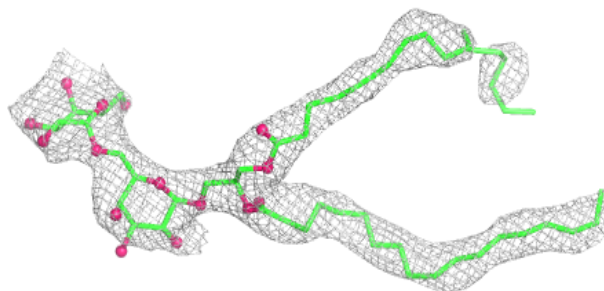
**Electron density around BCR A 850:**

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



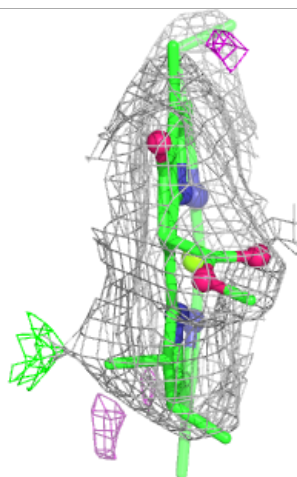
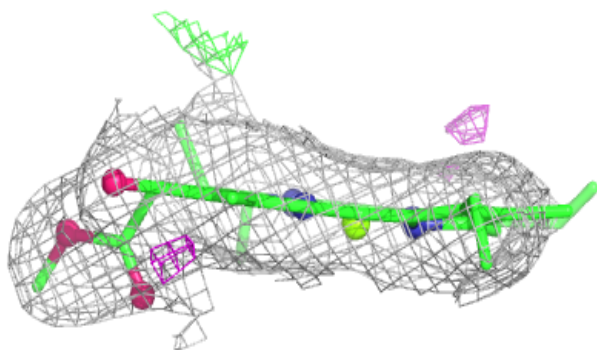
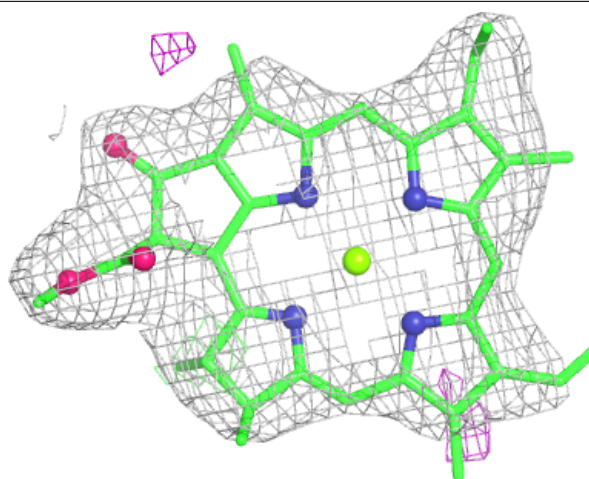
Electron density around DGD B 850:

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



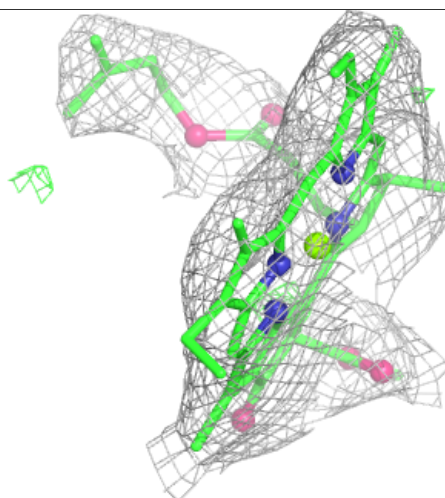
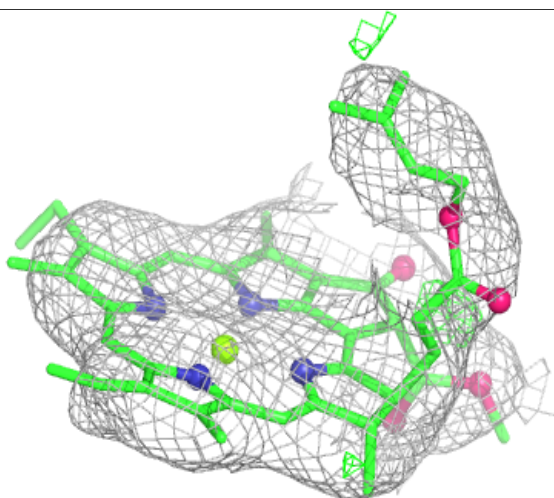
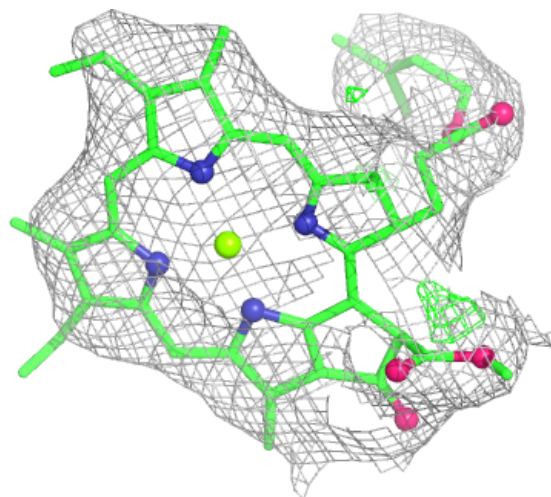
Electron density around CLA 1 311:

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



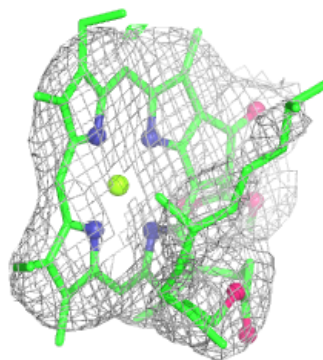
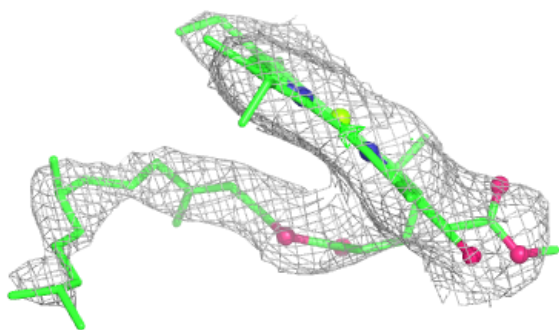
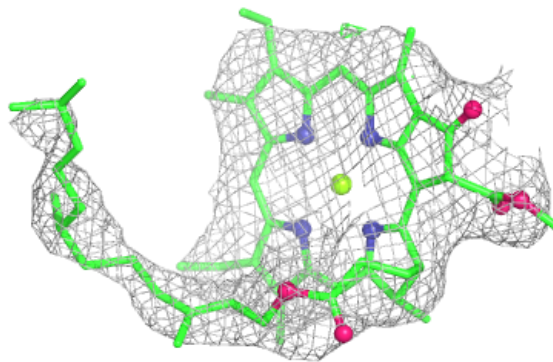
Electron density around CLA 7 608:

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



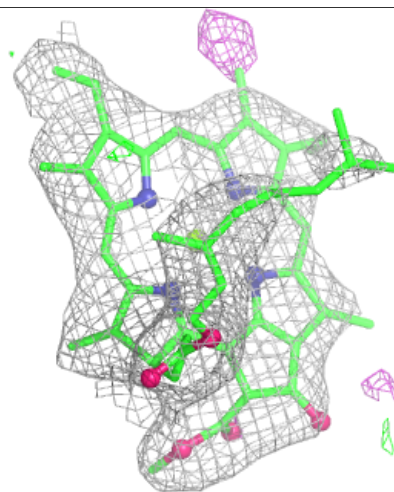
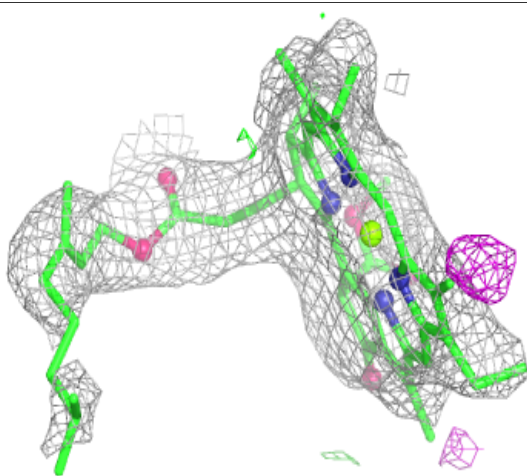
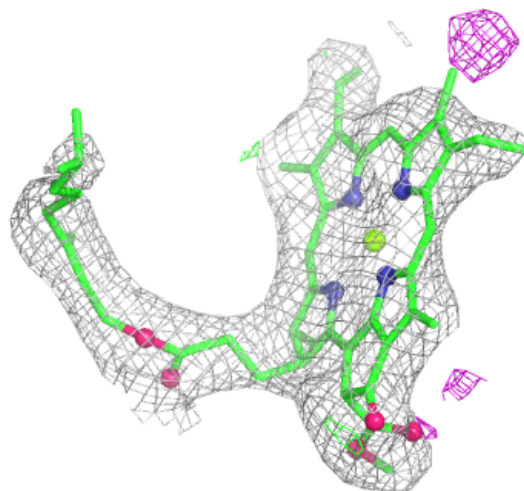
Electron density around CLA 7 609:

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



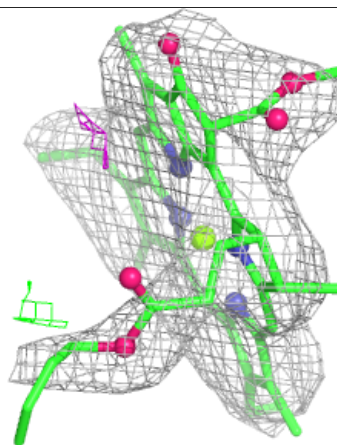
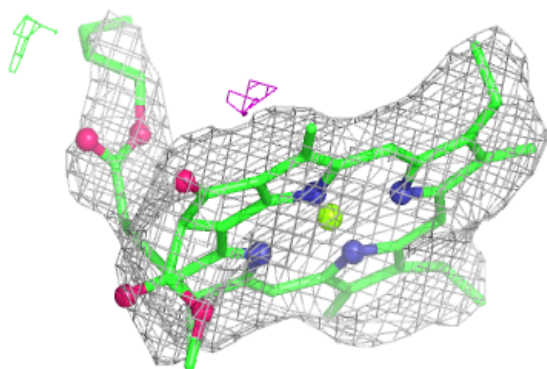
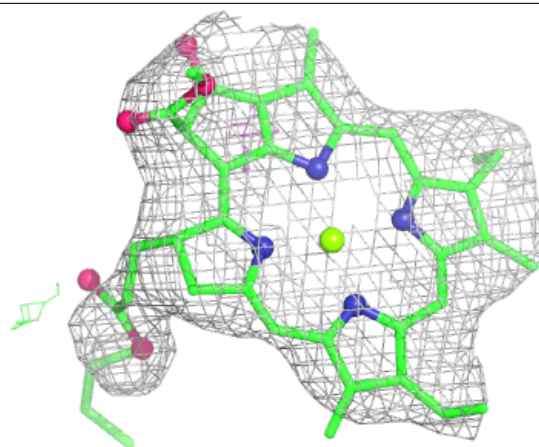
Electron density around CLA A 805:

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



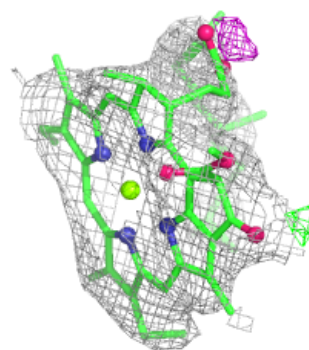
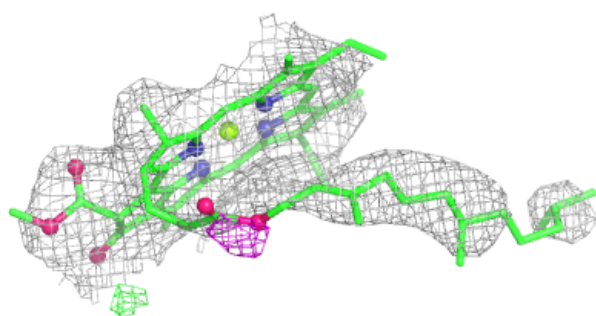
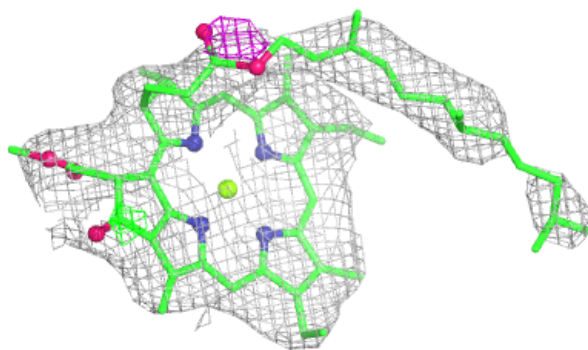
Electron density around CLA A 823:

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

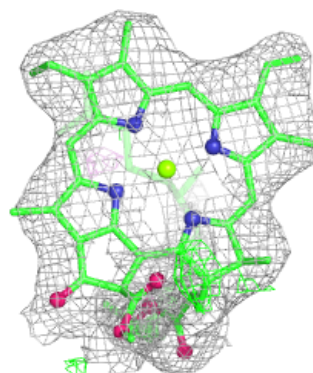
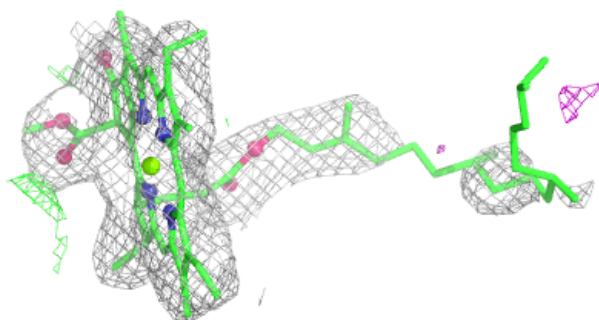
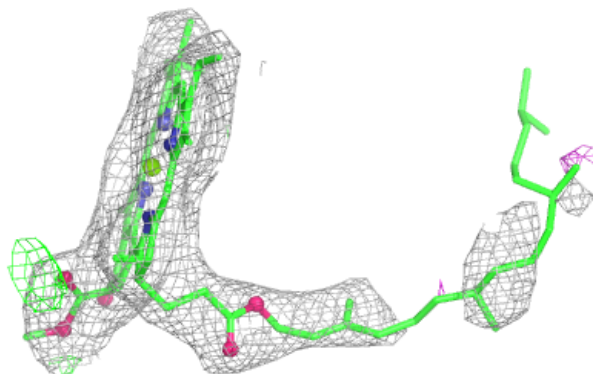


Electron density around CLA 4 609:

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

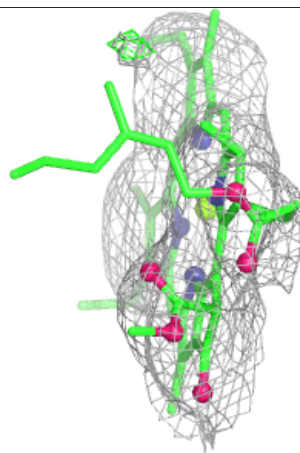
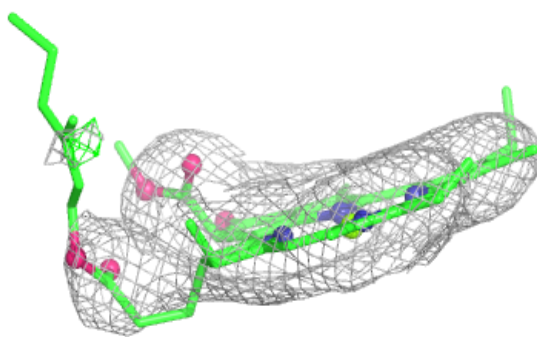
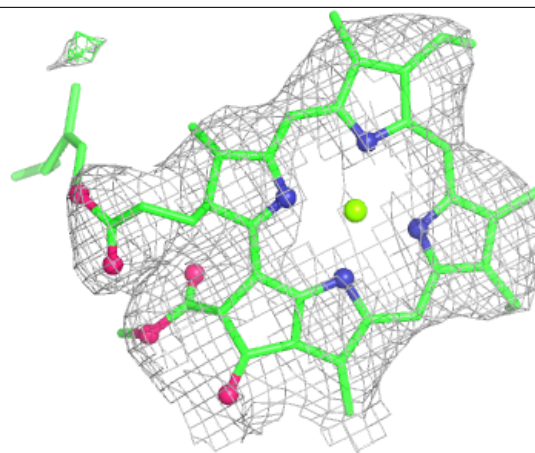
**Electron density around CLA A 808:**

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



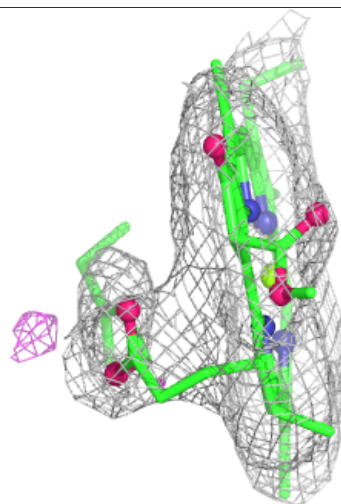
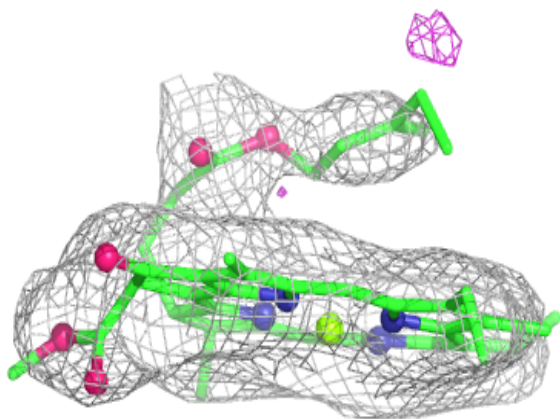
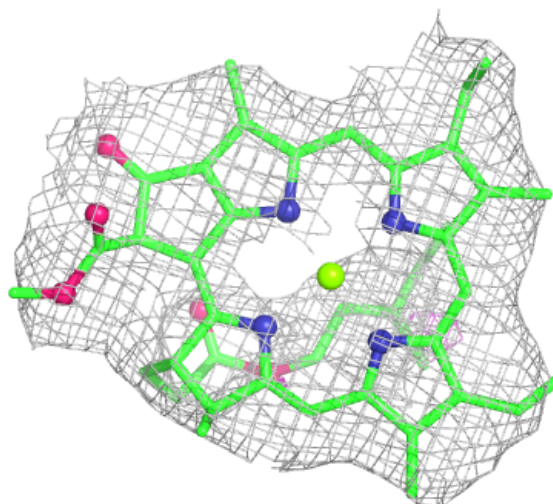
Electron density around CLA 4 611:

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



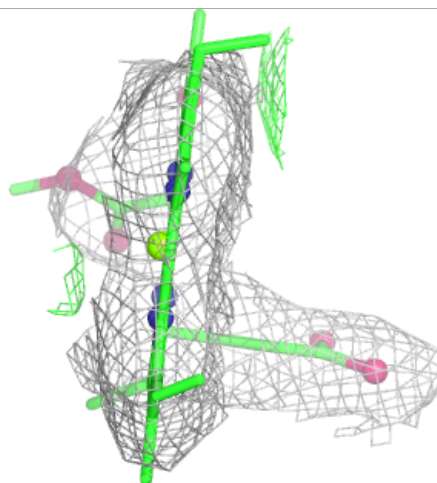
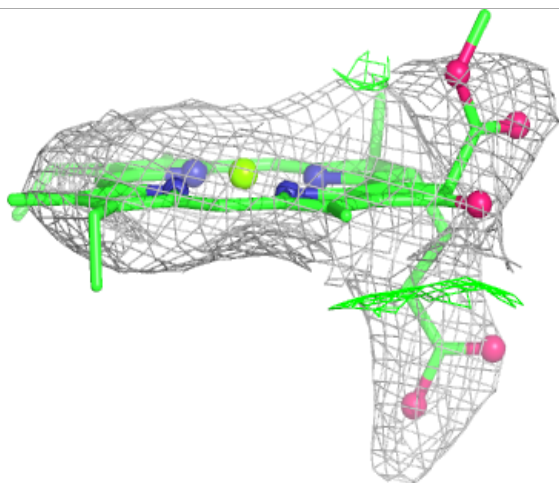
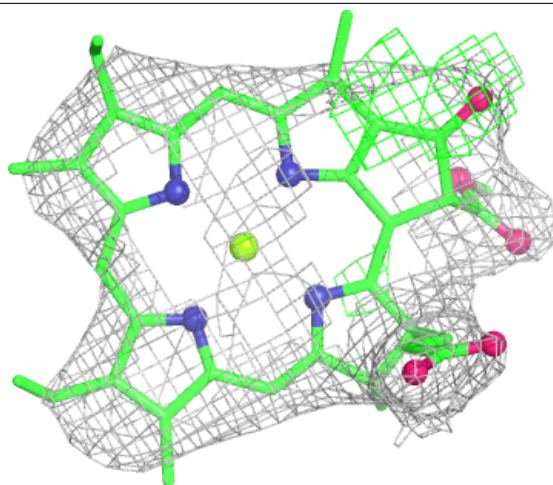
Electron density around CLA a 824:

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



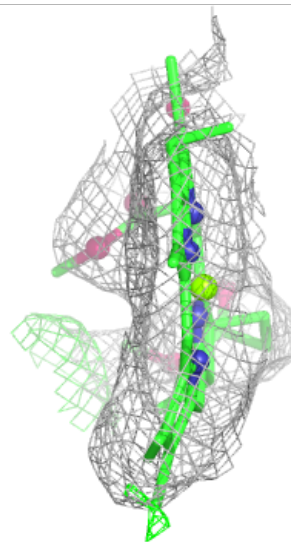
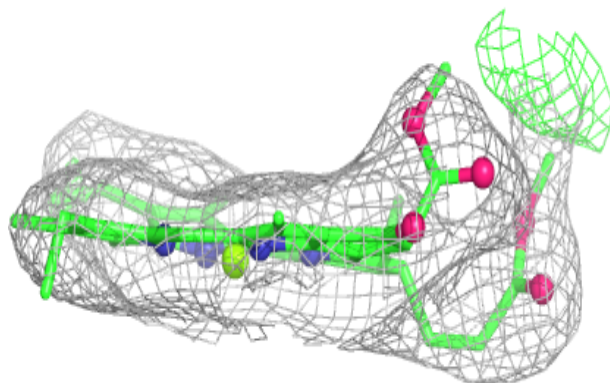
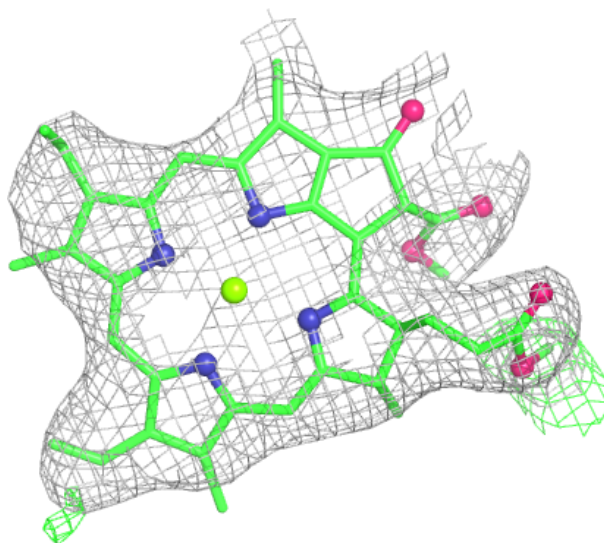
Electron density around CLA 3 304:

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



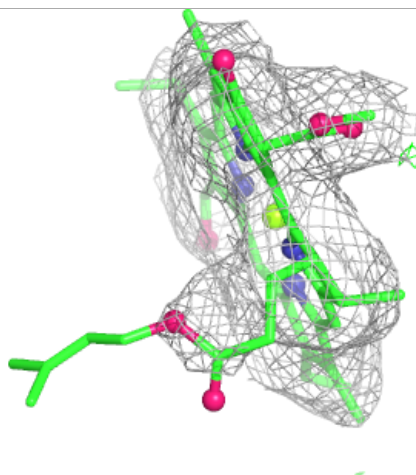
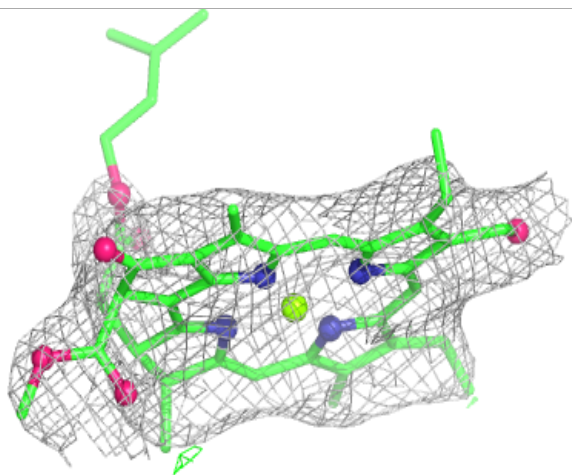
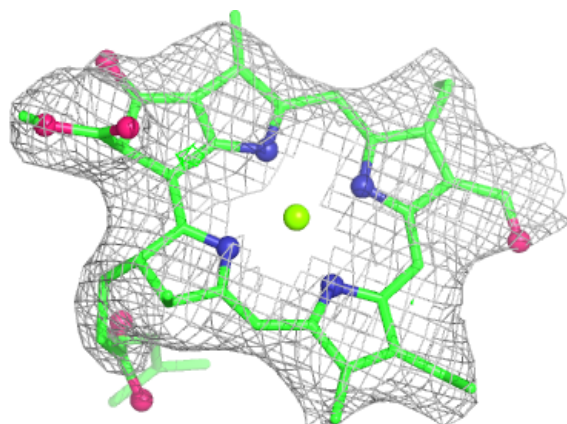
Electron density around CLA 9 603:

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



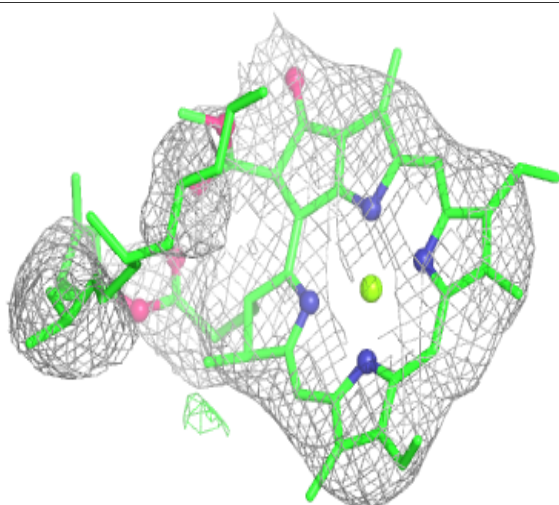
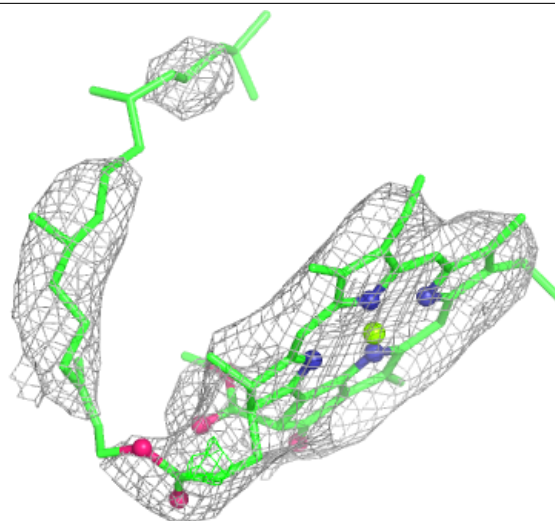
Electron density around CHL 4 606:

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



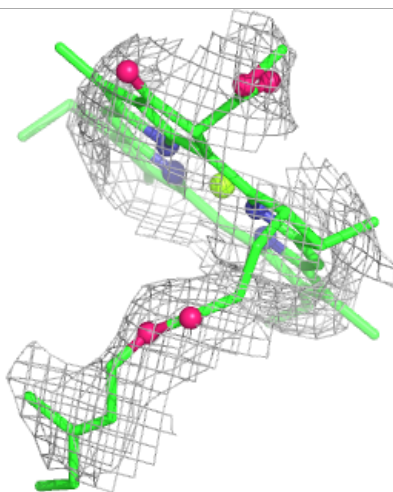
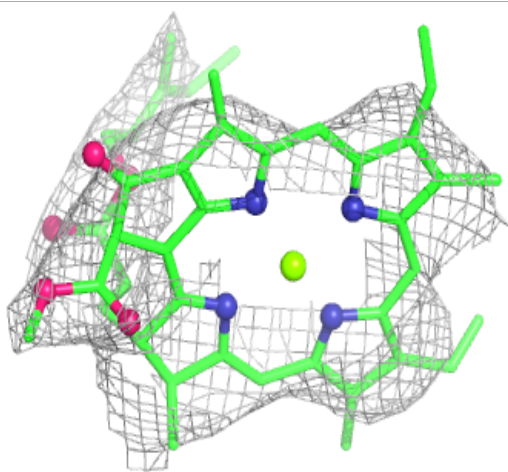
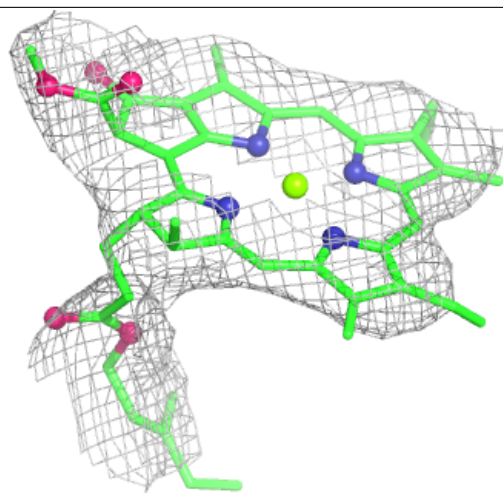
Electron density around CLA 6 305:

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



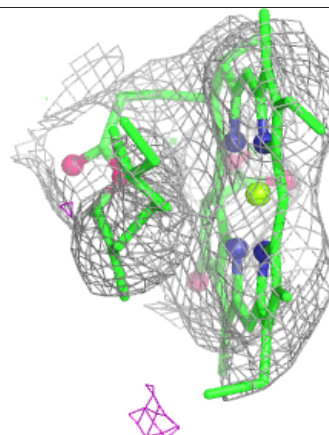
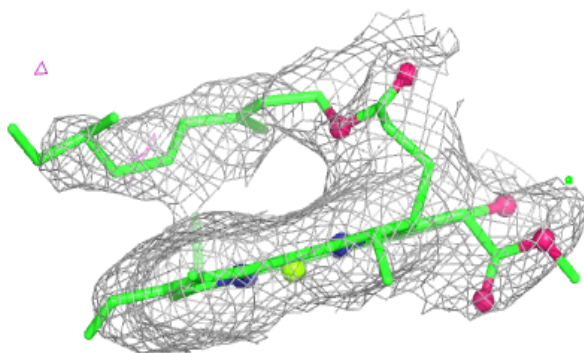
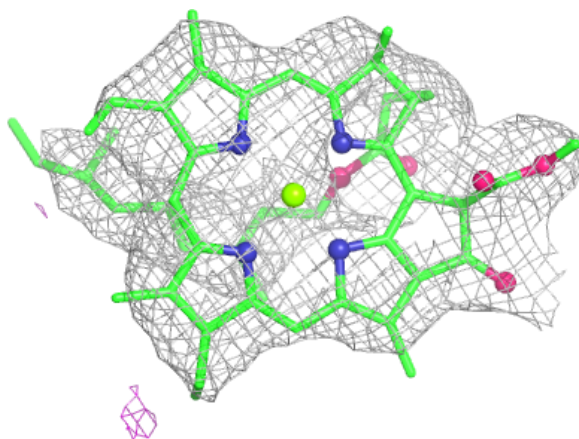
Electron density around CLA 6 306:

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

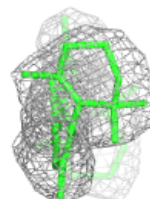
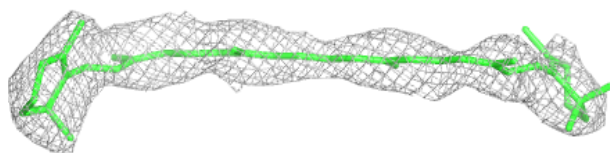
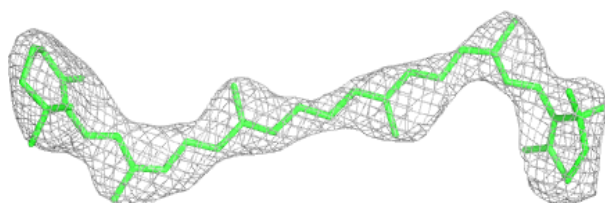


Electron density around CLA 9 612:

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

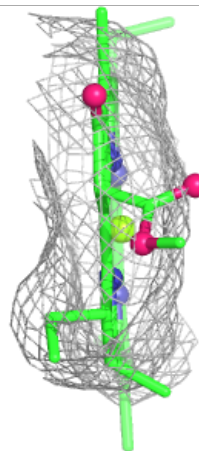
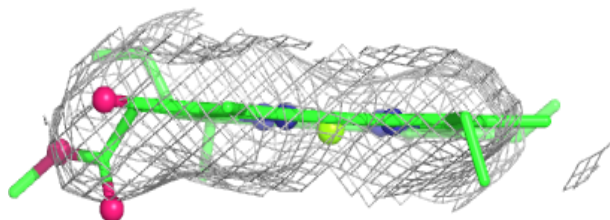
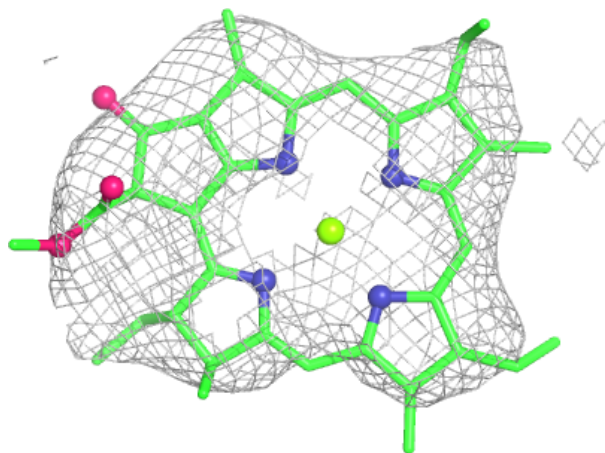
**Electron density around BCR b 845:**

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



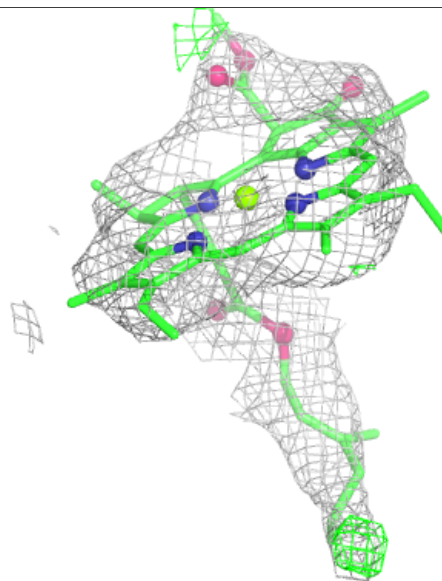
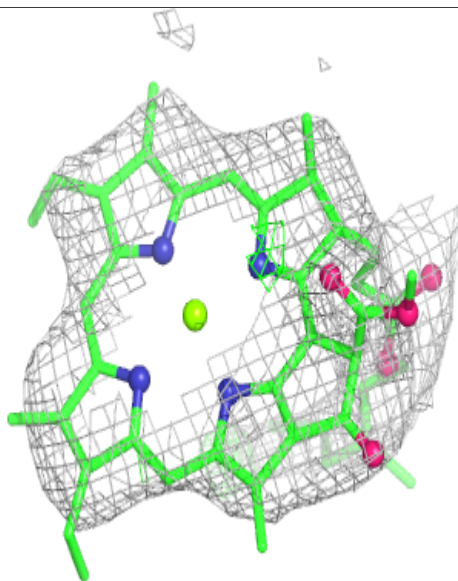
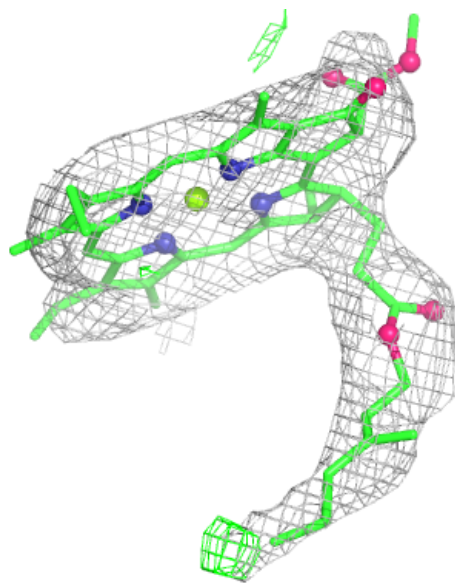
Electron density around CLA 6 307:

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



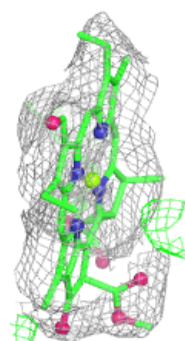
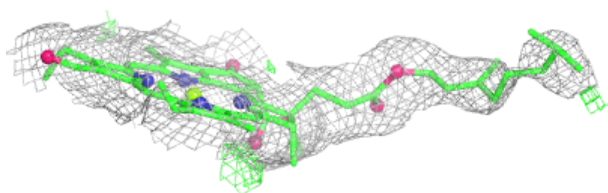
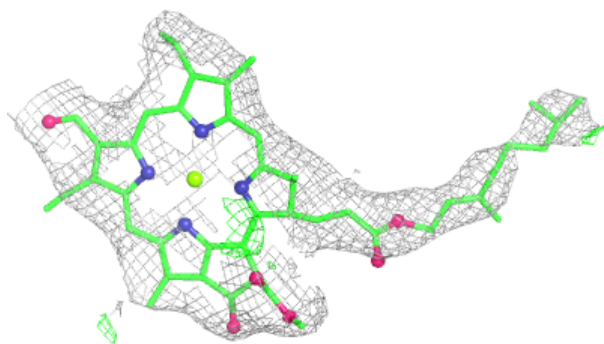
Electron density around CLA 1 305:

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

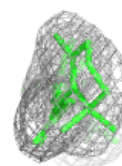
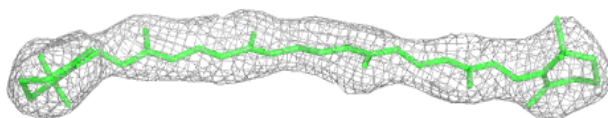
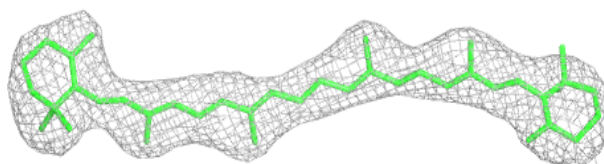


Electron density around CHL 9 605:

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

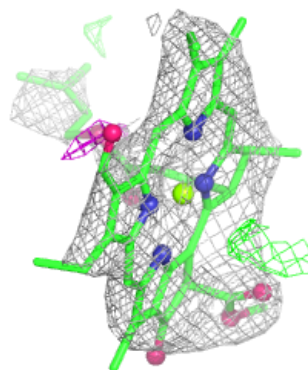
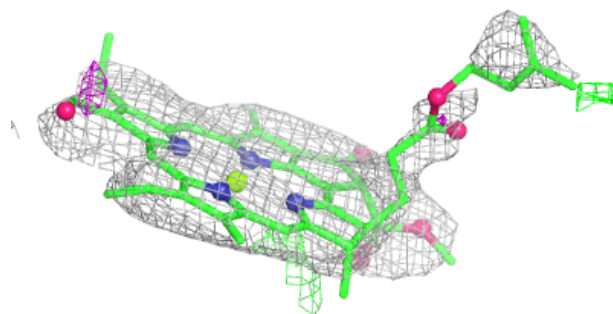
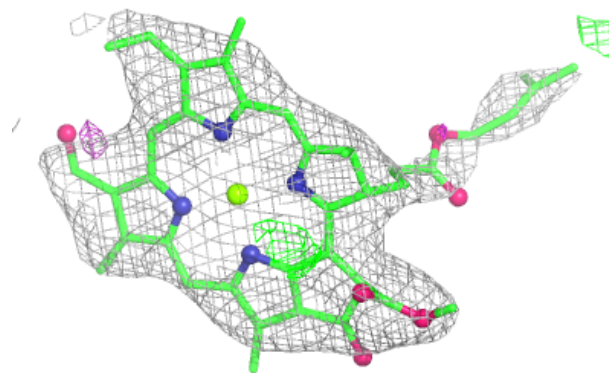
**Electron density around BCR j 3003:**

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



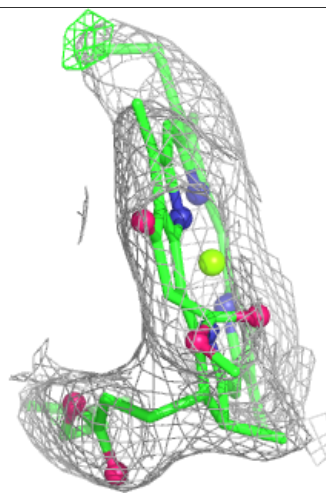
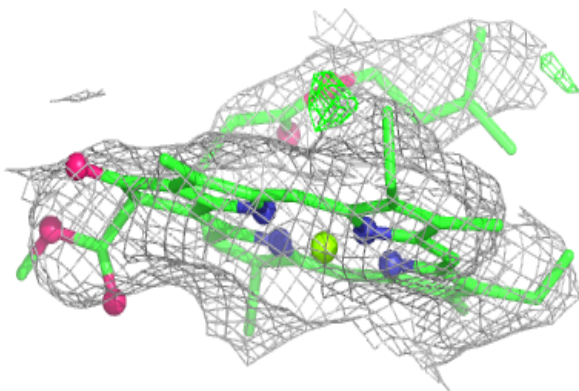
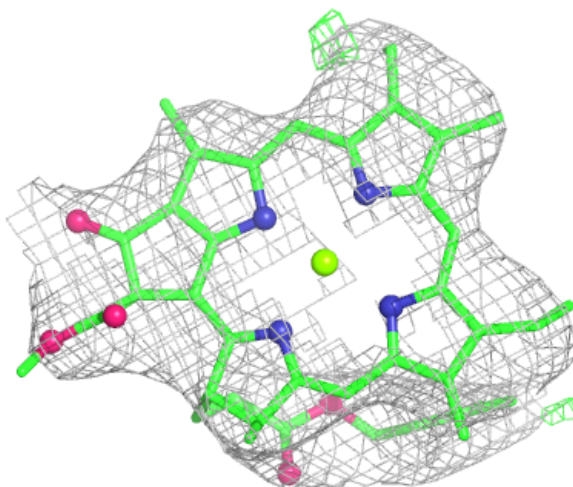
Electron density around CHL 9 607:

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



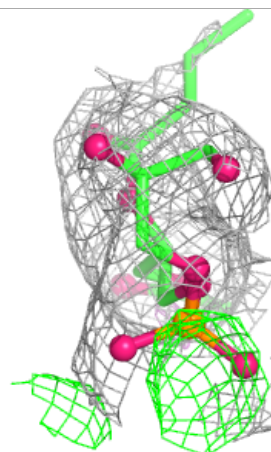
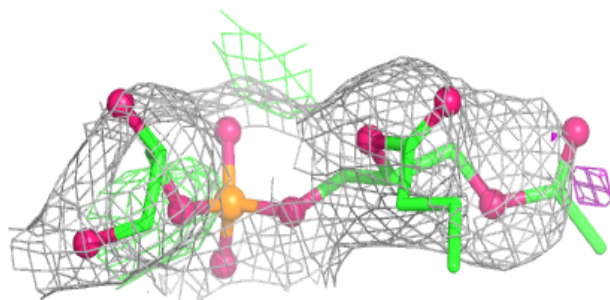
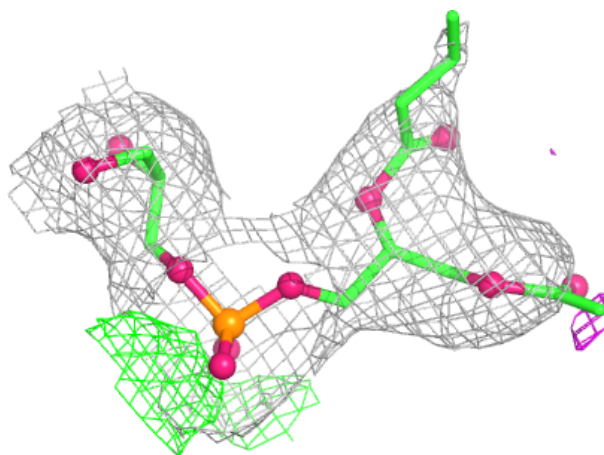
Electron density around CLA 3 309:

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



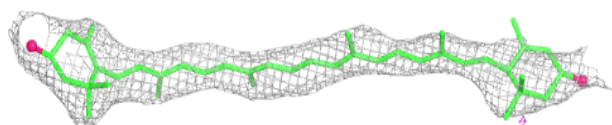
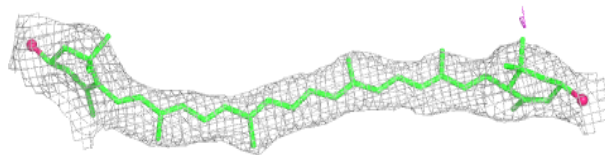
Electron density around LHG 1 301:

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

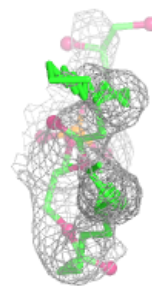
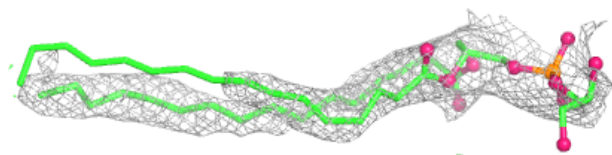
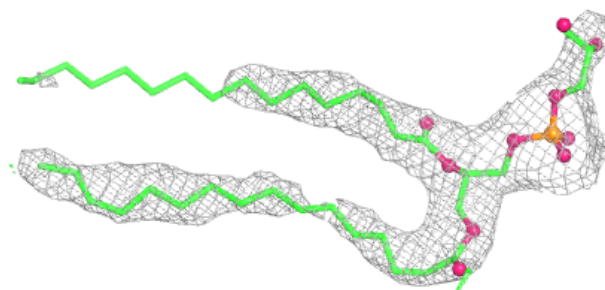


Electron density around LUT 3 316:

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

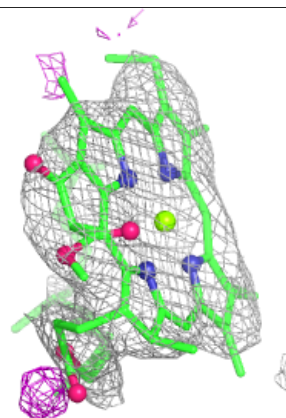
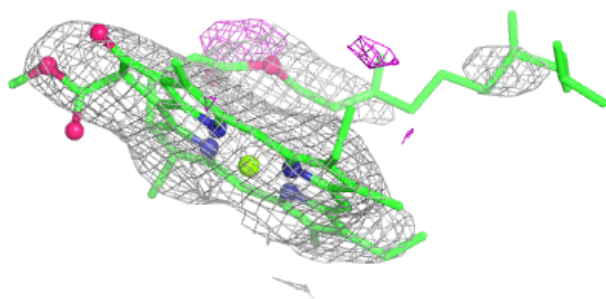
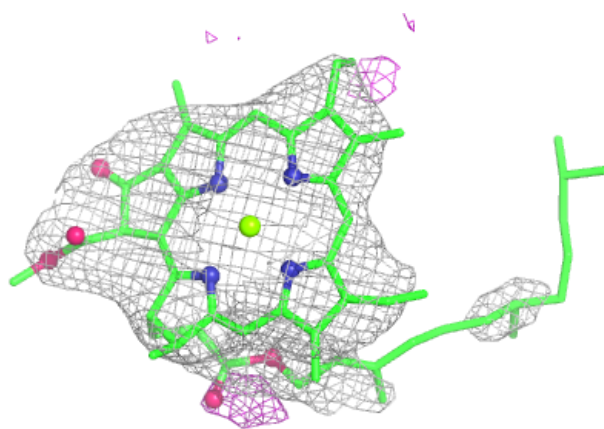
**Electron density around LHG 1 319:**

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



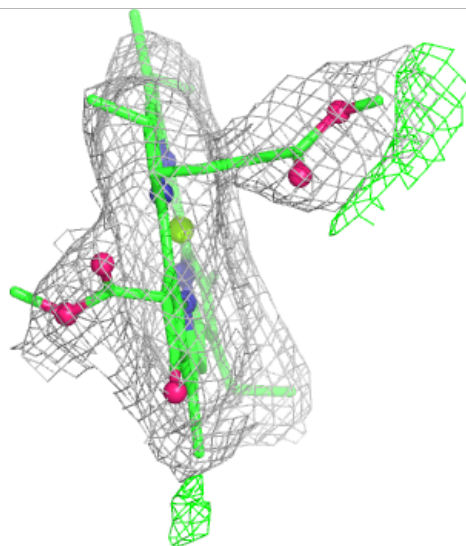
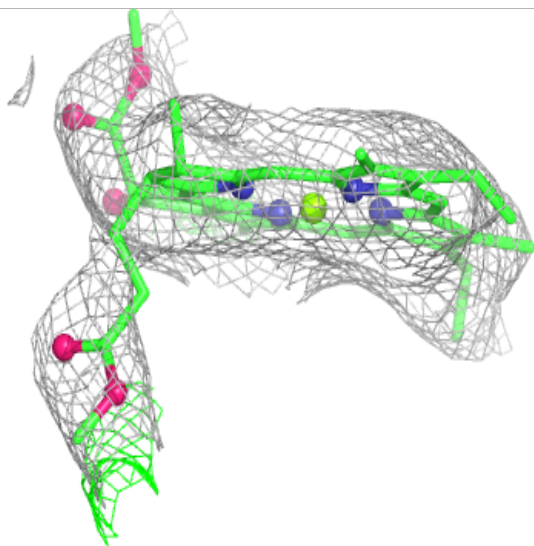
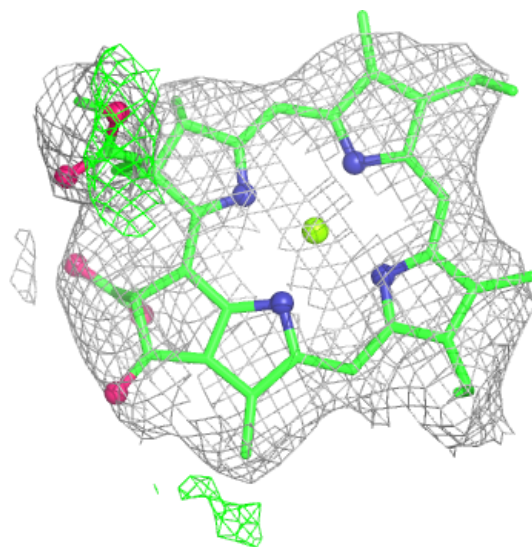
Electron density around CLA 6 311:

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



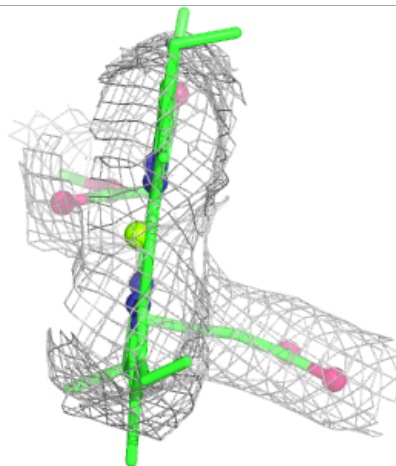
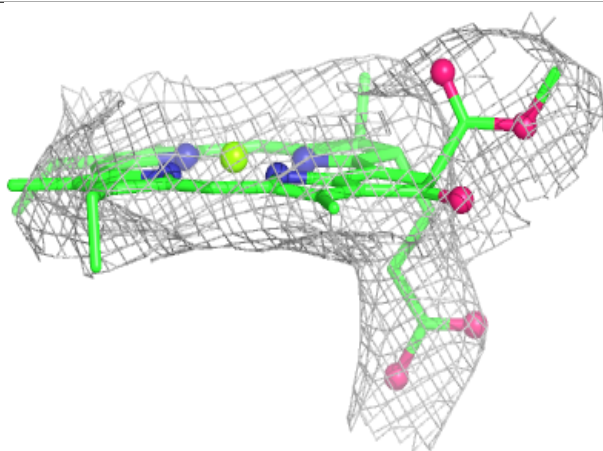
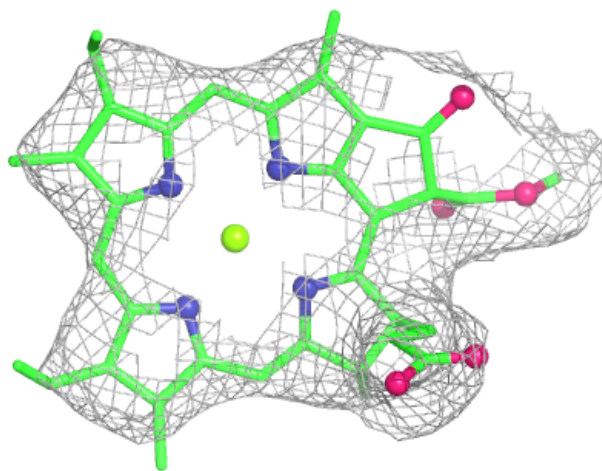
Electron density around CLA b 821:

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



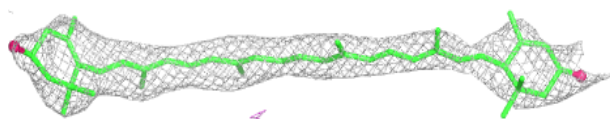
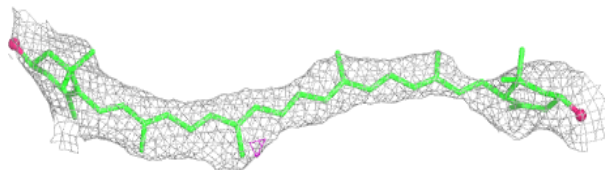
Electron density around CLA b 835:

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

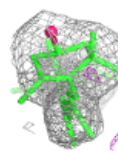
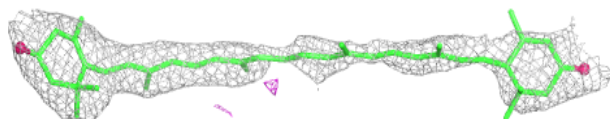
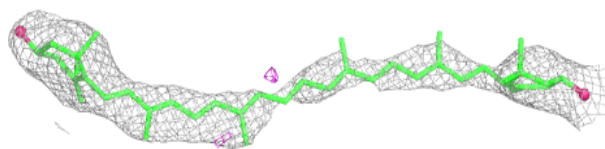


Electron density around LUT 8 314:

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

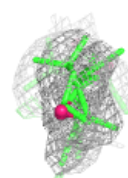
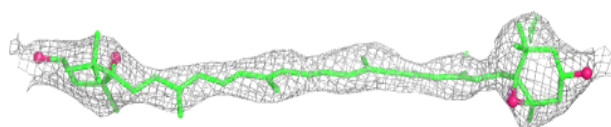
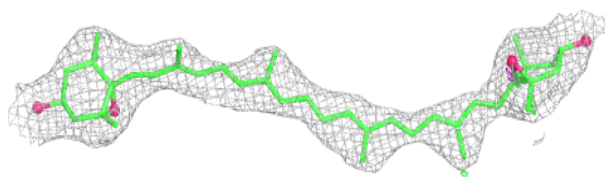
**Electron density around LUT 9 616:**

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

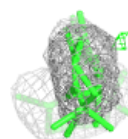
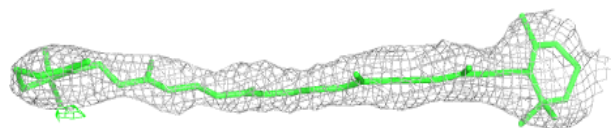
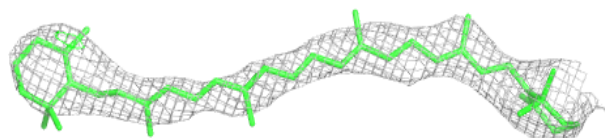


Electron density around XAT 8 315:

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

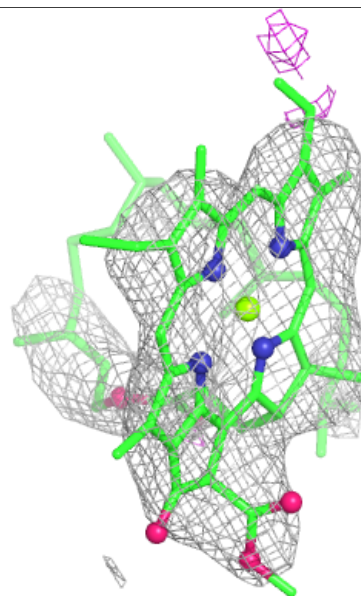
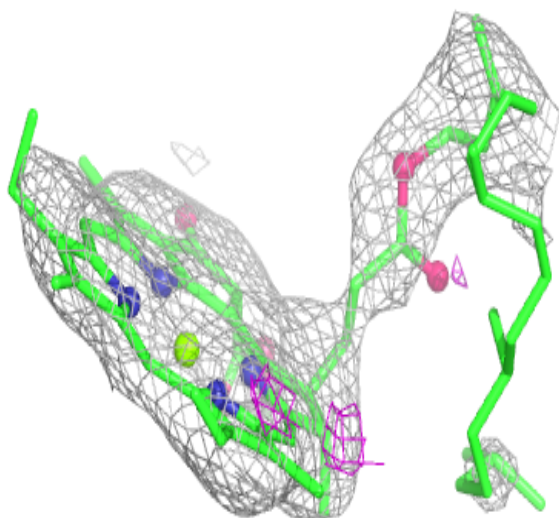
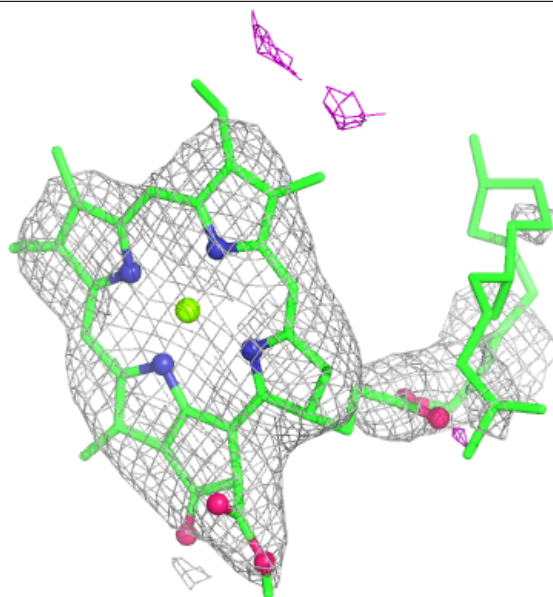
**Electron density around BCR 9 618:**

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



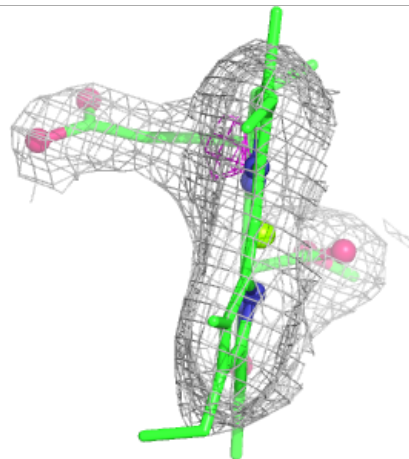
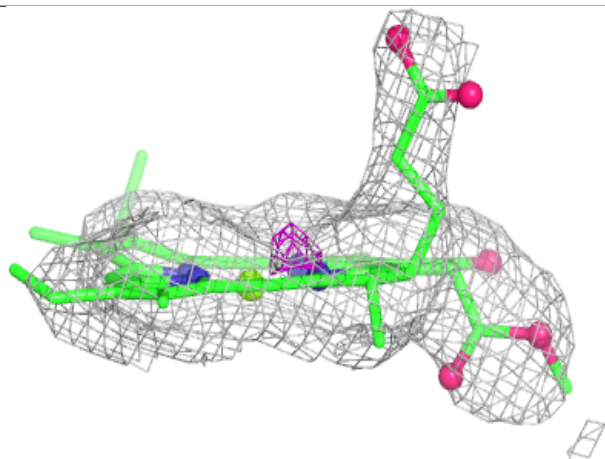
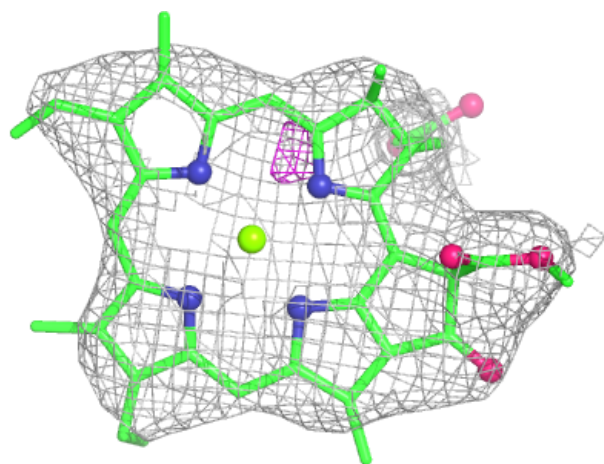
Electron density around CLA 1 308:

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



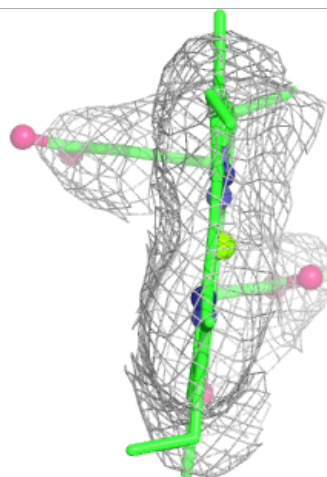
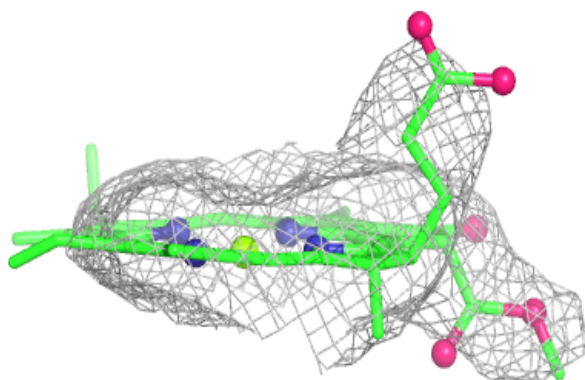
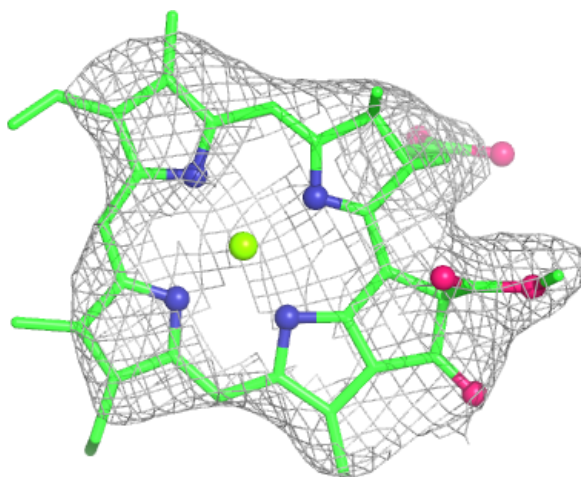
Electron density around CLA G 101:

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



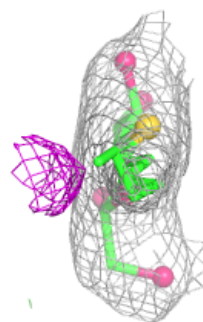
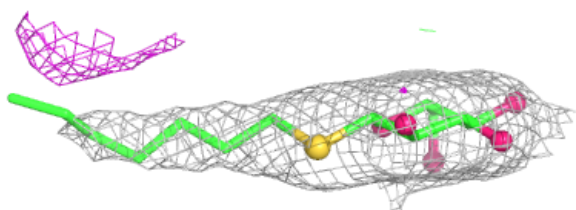
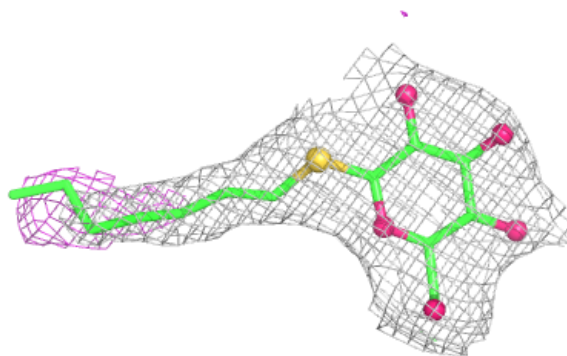
Electron density around CLA 4 613:

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



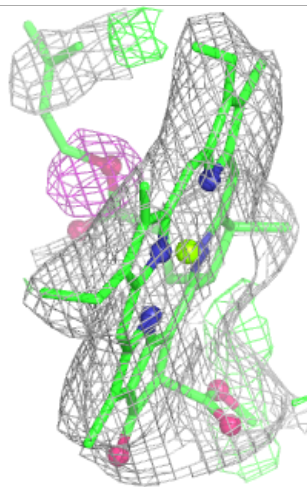
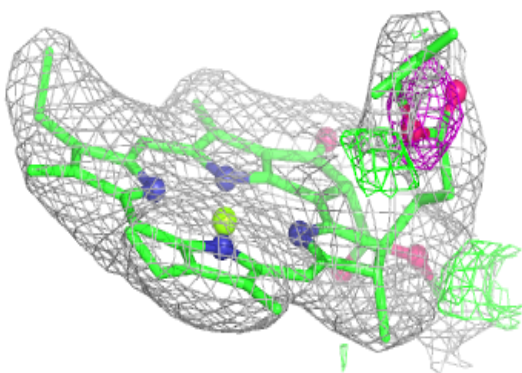
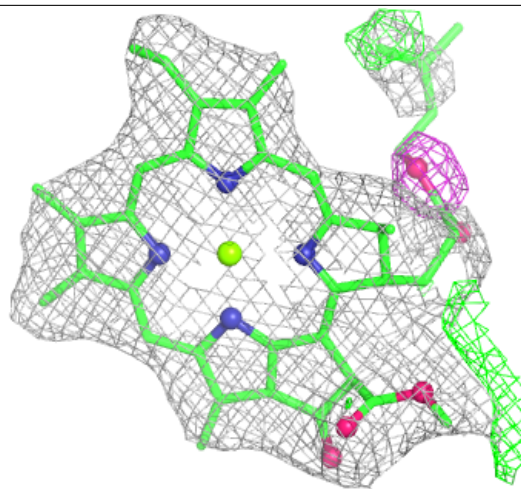
Electron density around HTG A 855:

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



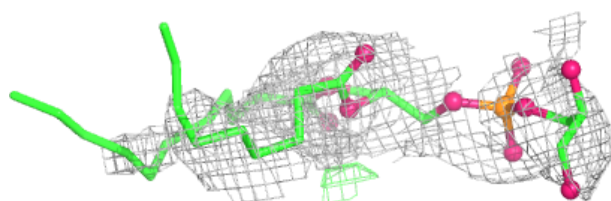
Electron density around CLA a 816:

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

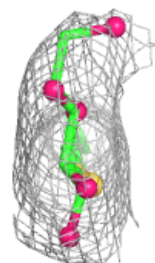
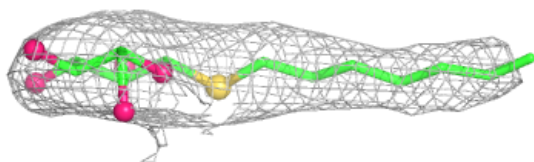
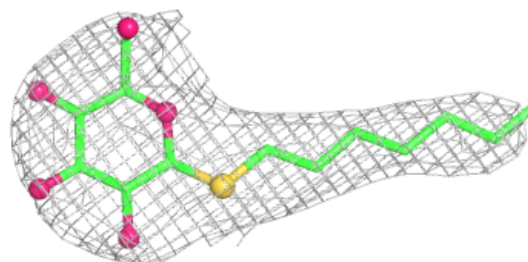


Electron density around LHG 2 618:

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

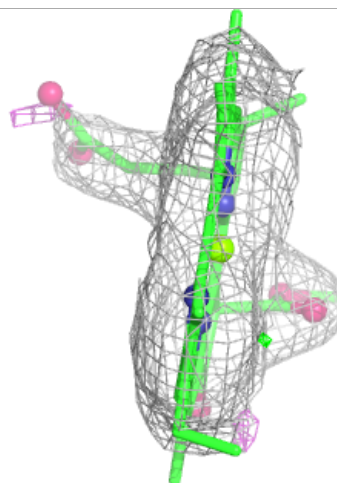
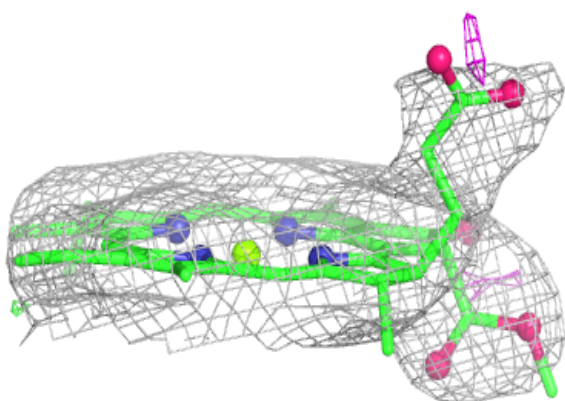
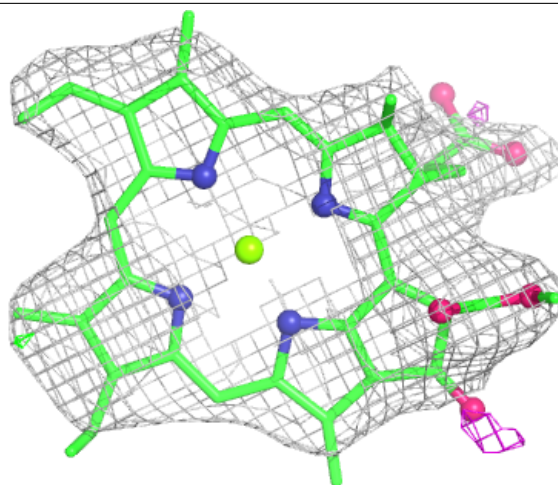
**Electron density around HTG a 857:**

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



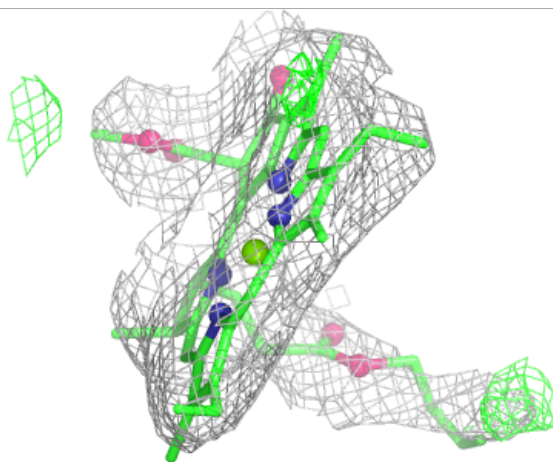
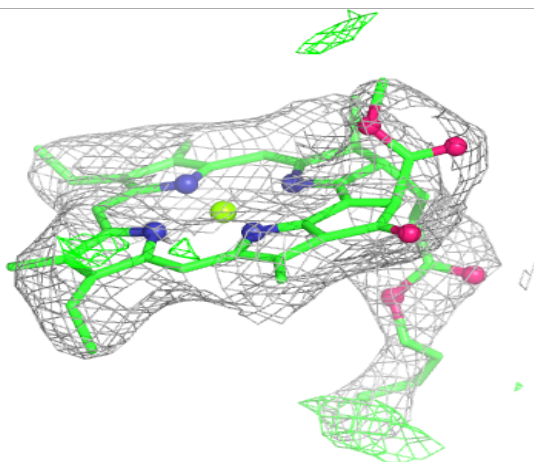
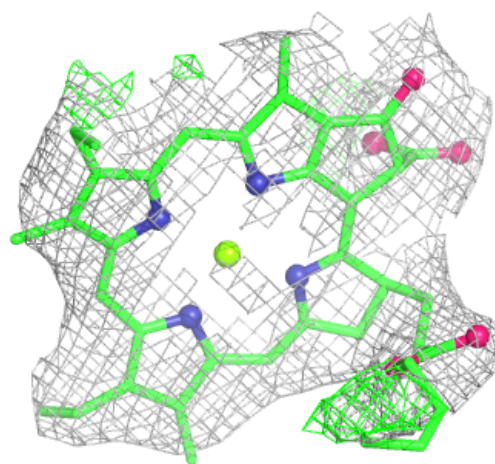
Electron density around CLA a 817:

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



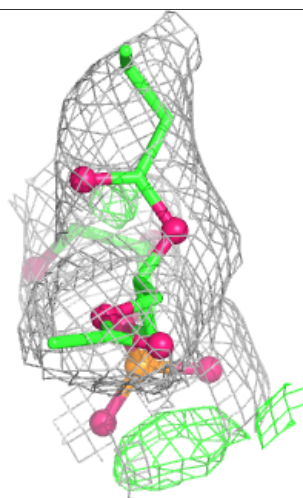
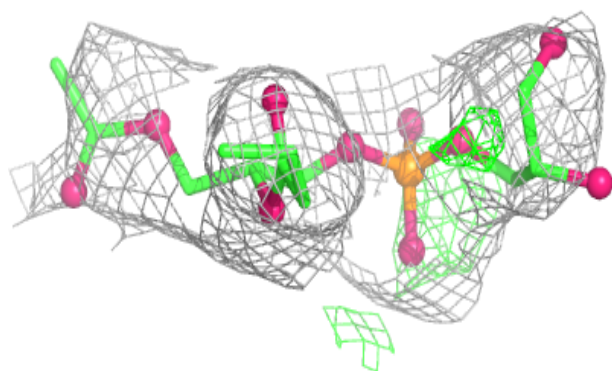
Electron density around CLA a 823:

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



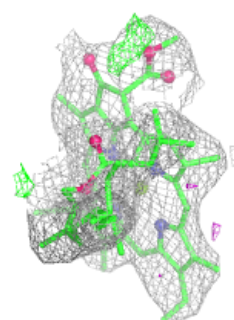
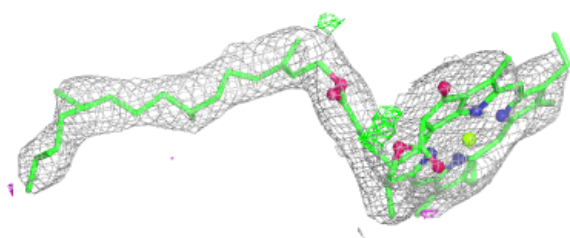
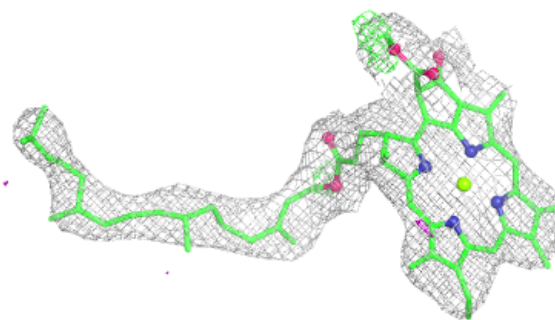
Electron density around LHG 6 301:

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



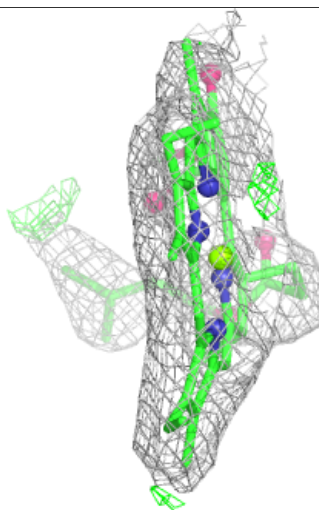
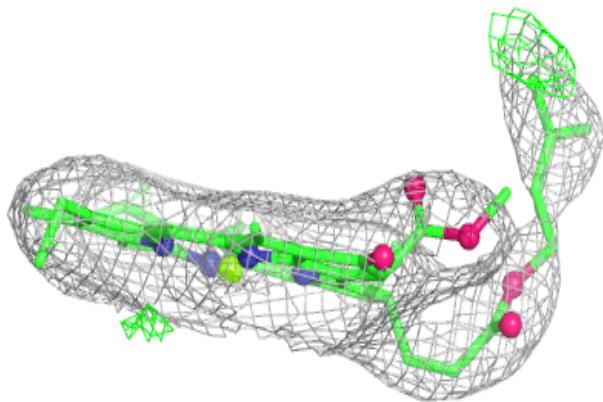
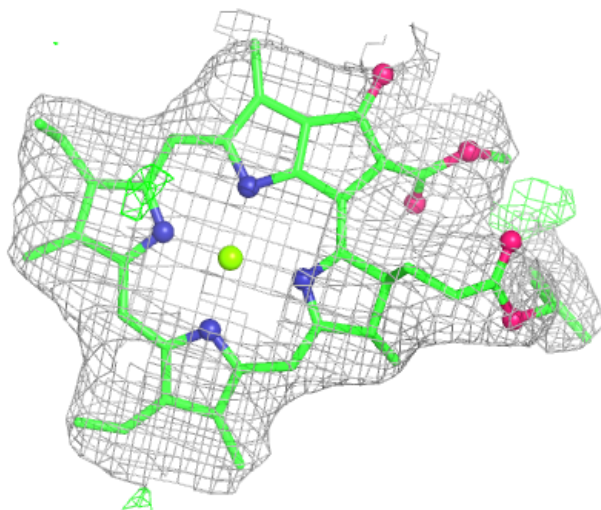
Electron density around CLA A 822:

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



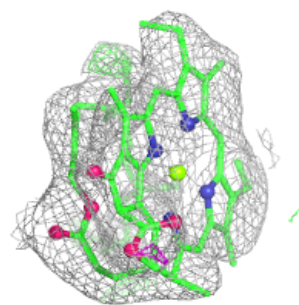
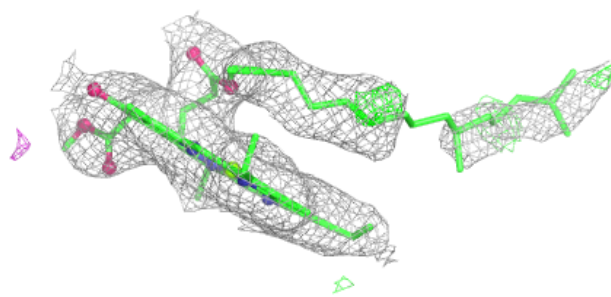
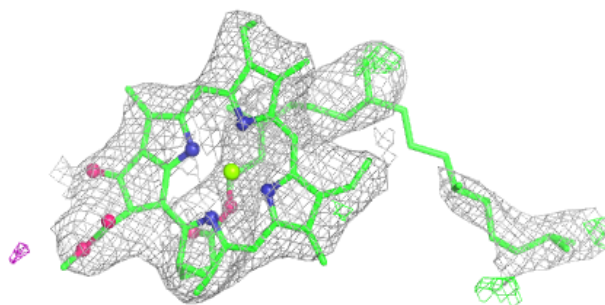
Electron density around CLA 3 303:

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

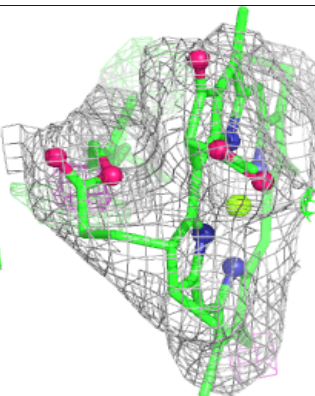
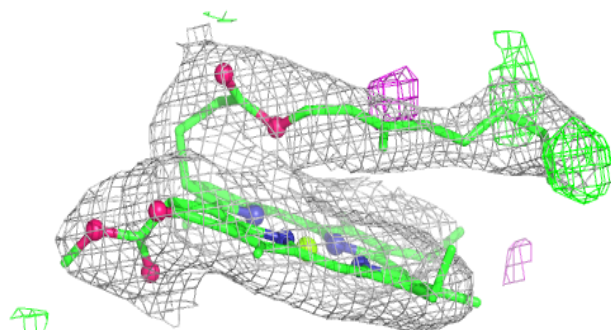
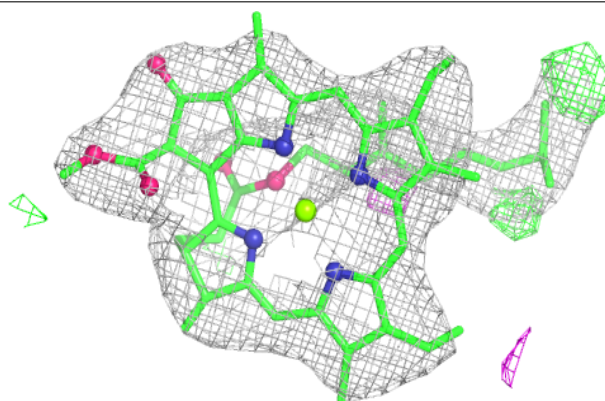


Electron density around CLA b 807:

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

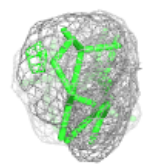
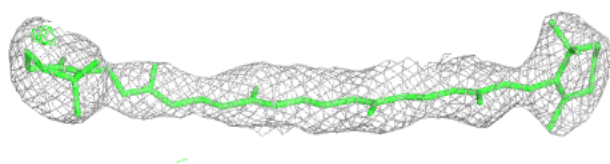
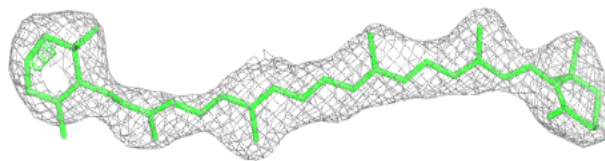
**Electron density around CLA B 816:**

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



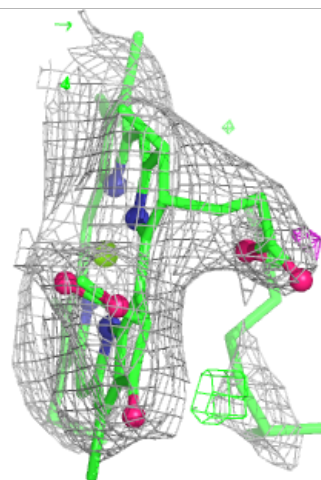
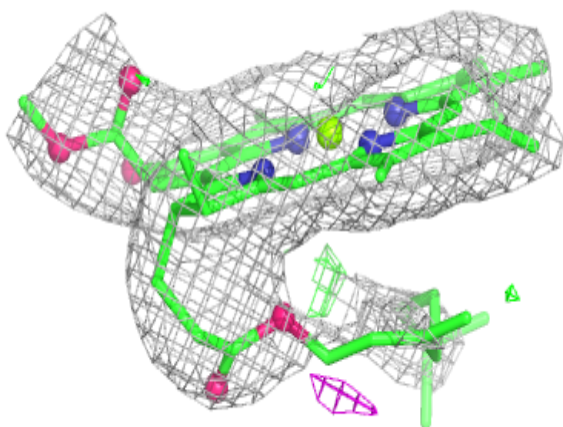
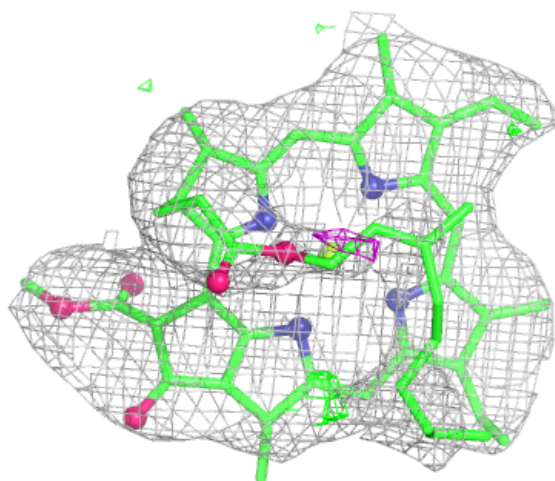
Electron density around BCR A 851:

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



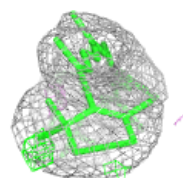
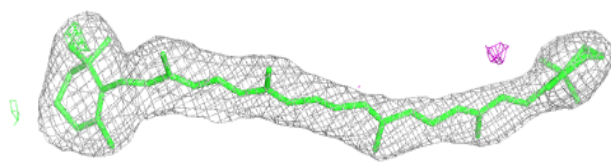
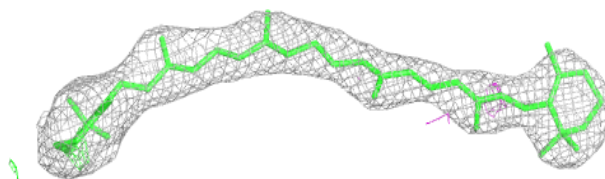
Electron density around CLA b 812:

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

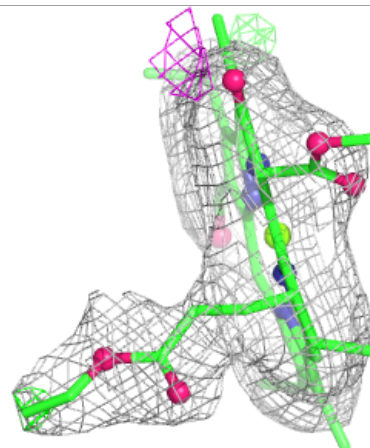
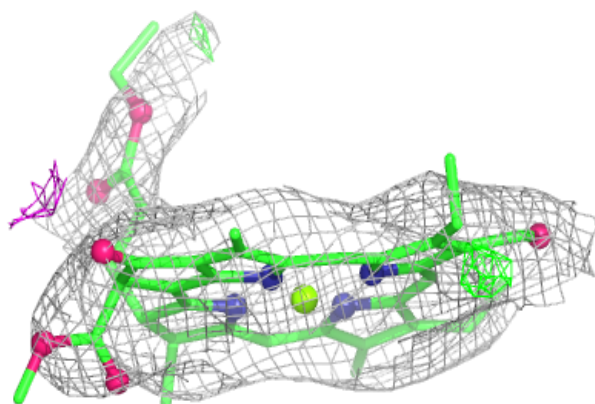
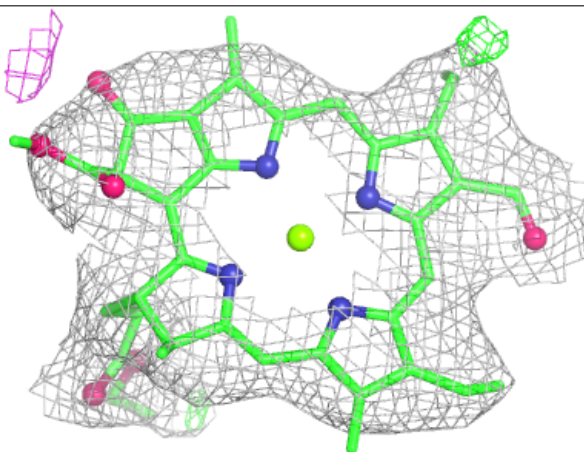


Electron density around BCR B 801:

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

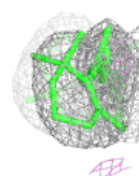
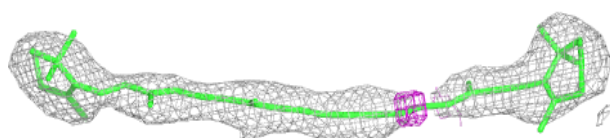
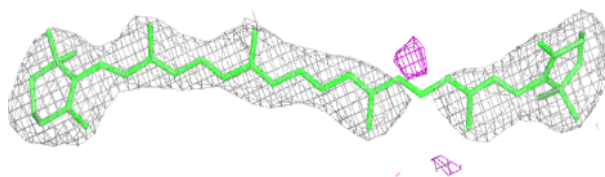
**Electron density around CHL 1 307:**

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

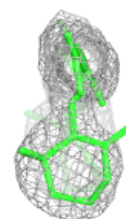
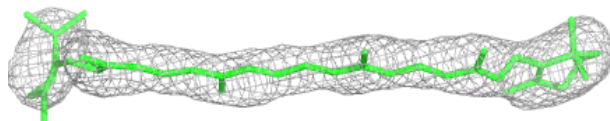
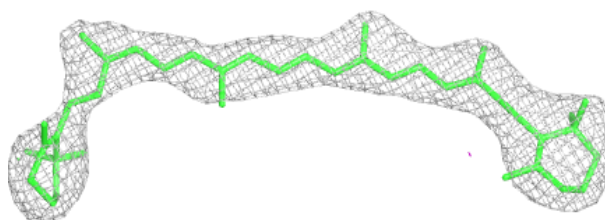


Electron density around BCR B 843:

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

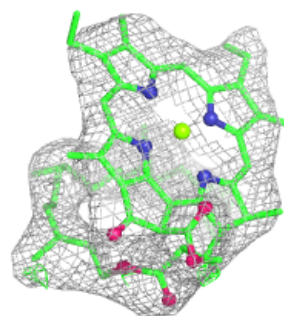
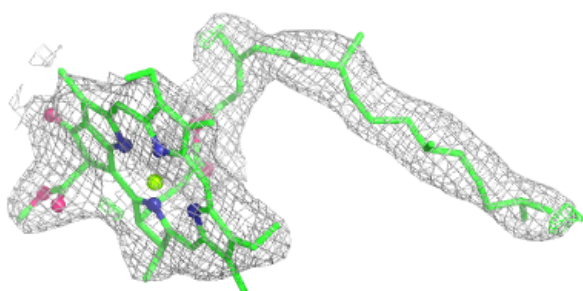
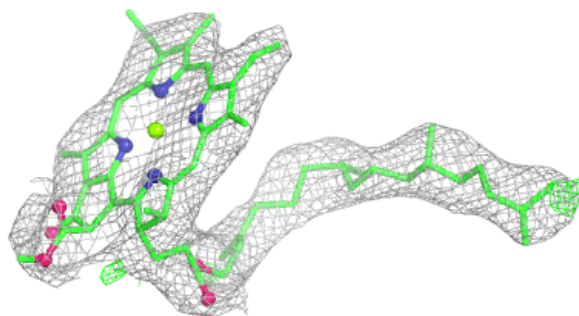
**Electron density around BCR B 844:**

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

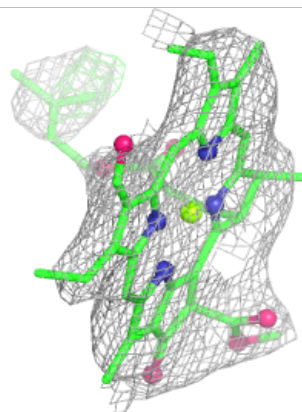
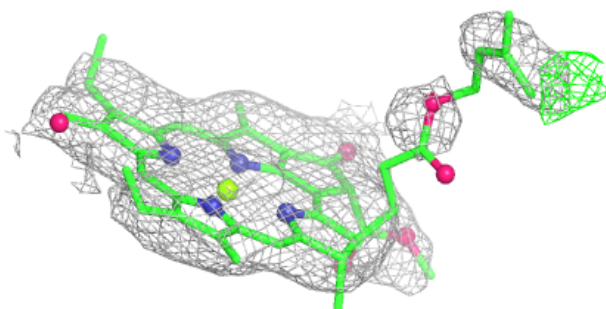
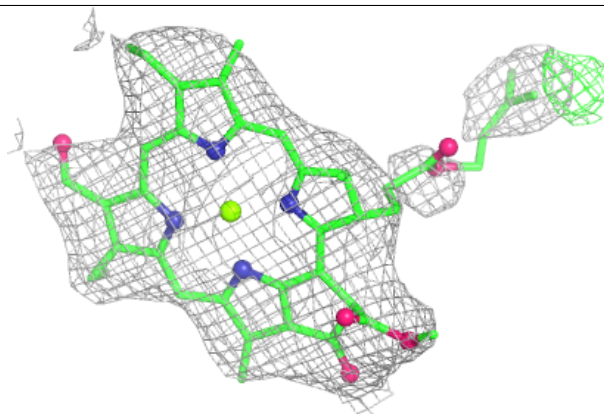


Electron density around CLA b 814:

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

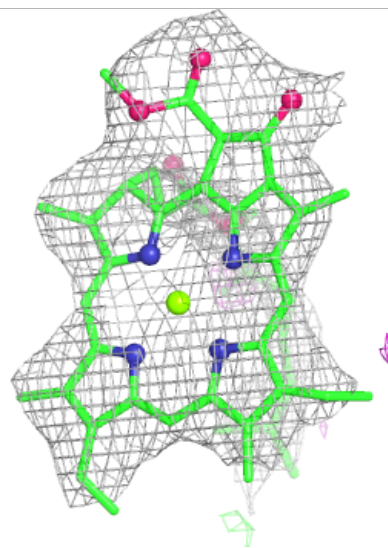
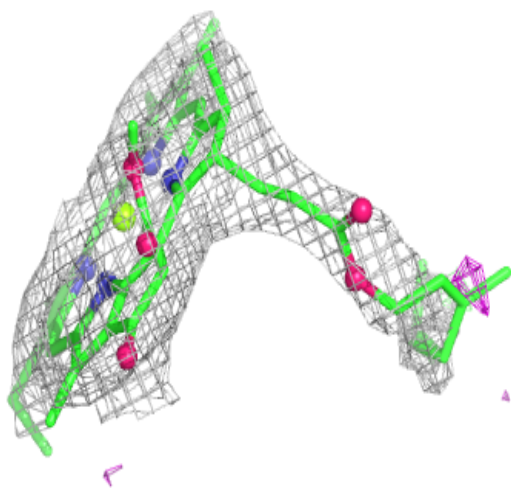
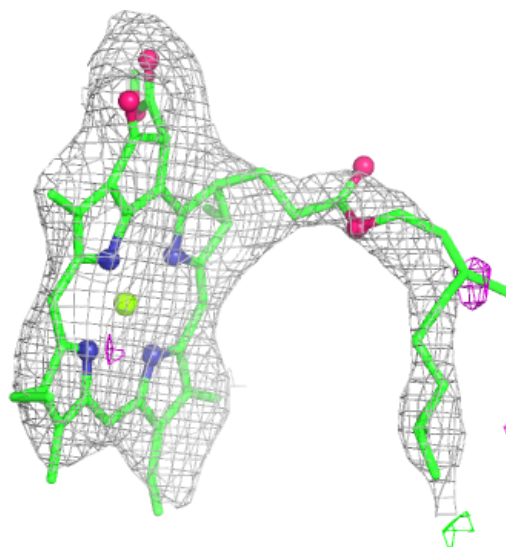
**Electron density around CHL 2 607:**

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



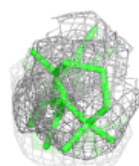
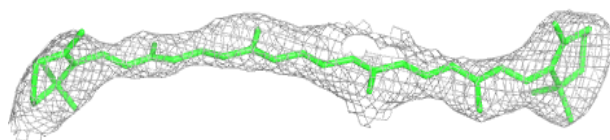
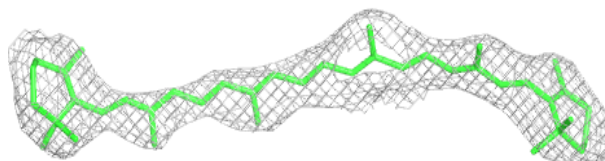
Electron density around CLA b 815:

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

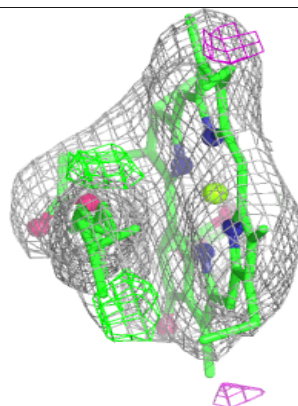
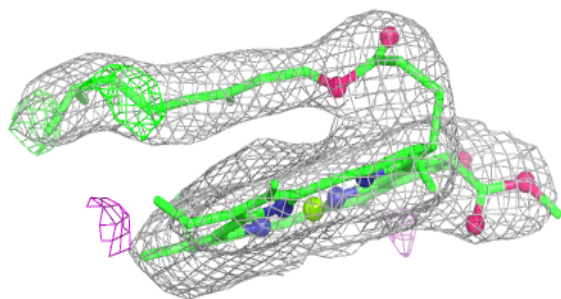
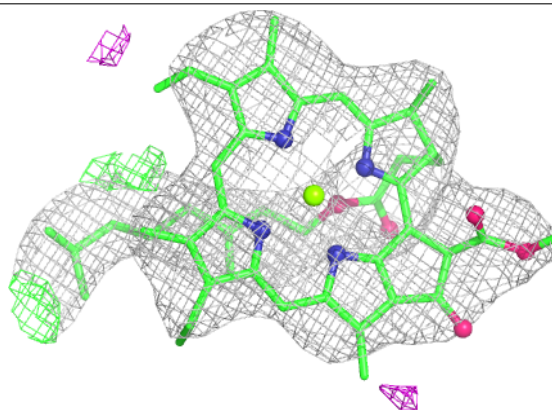


Electron density around BCR G 105:

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

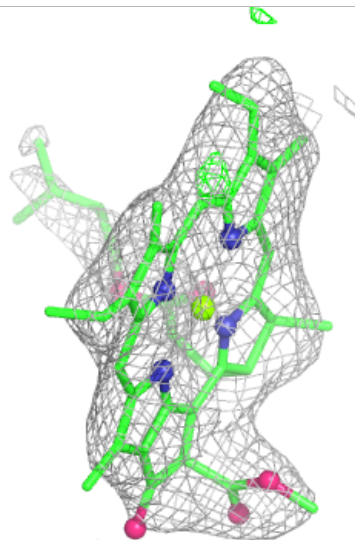
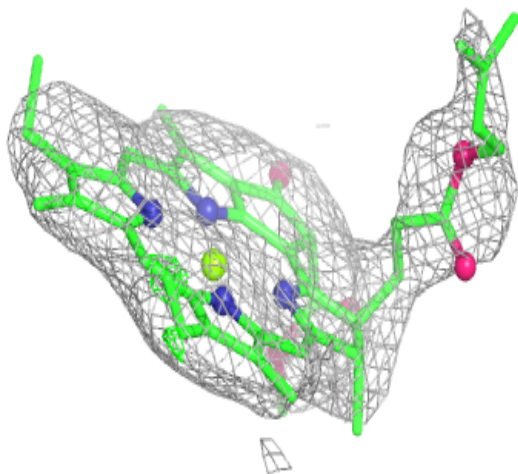
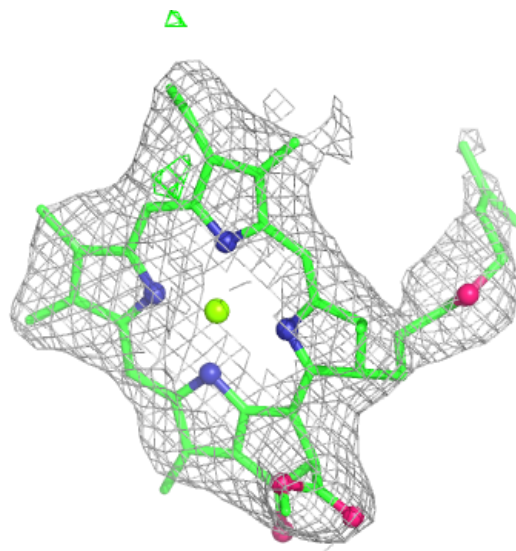
**Electron density around CLA b 816:**

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



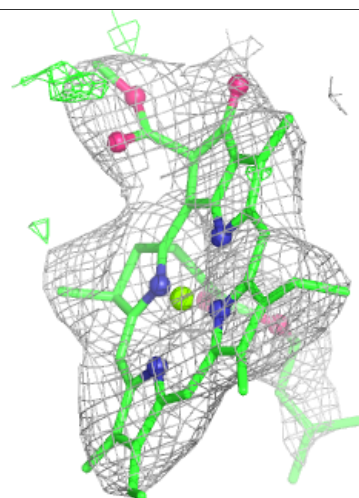
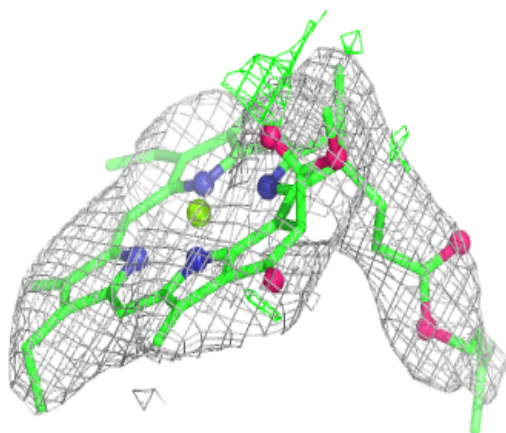
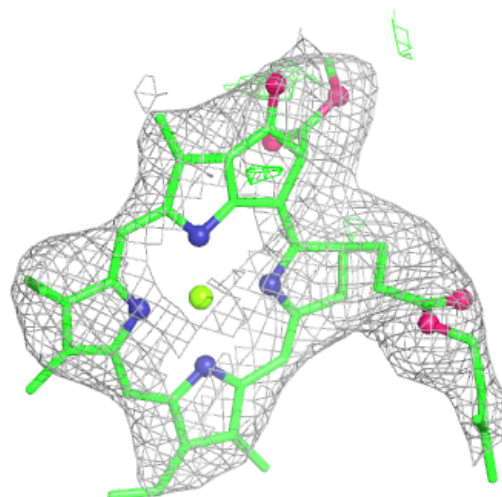
Electron density around CLA A 832:

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



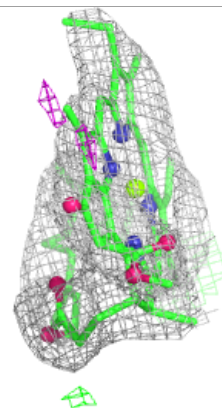
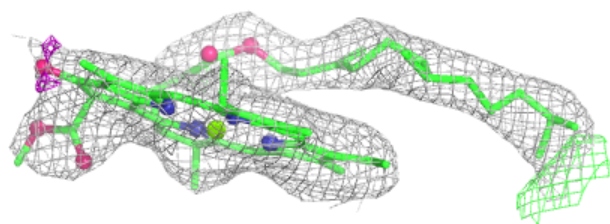
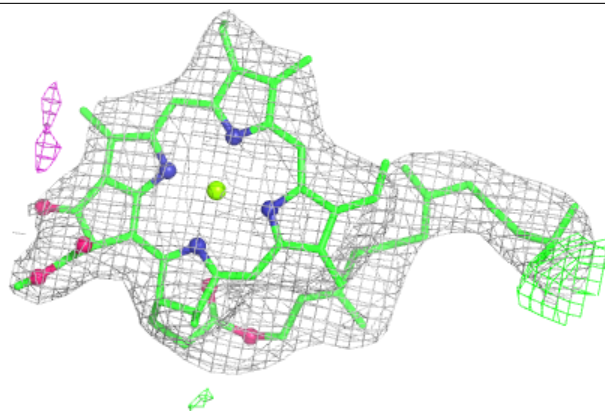
Electron density around CLA b 820:

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

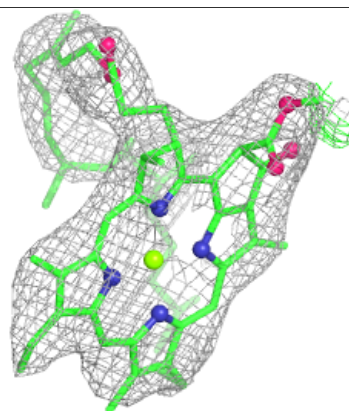
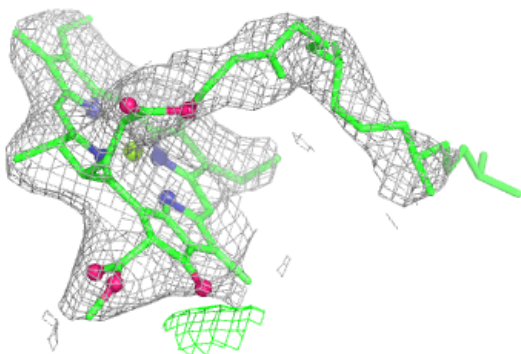
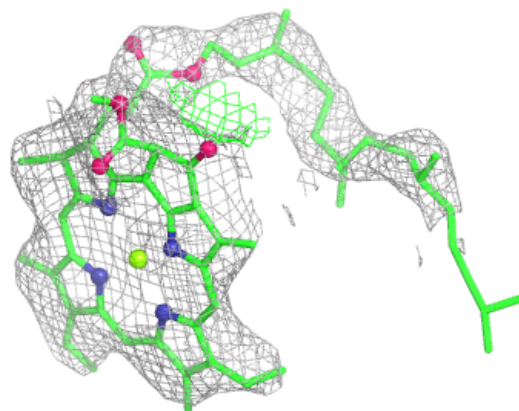


Electron density around CLA B 818:

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

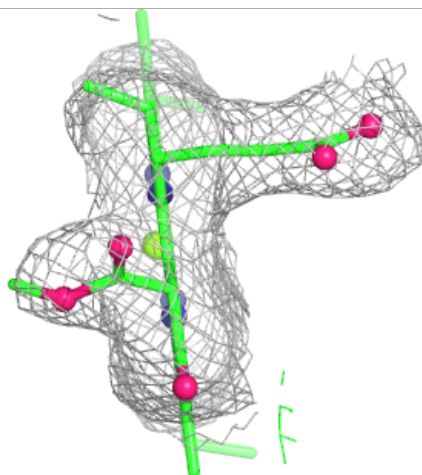
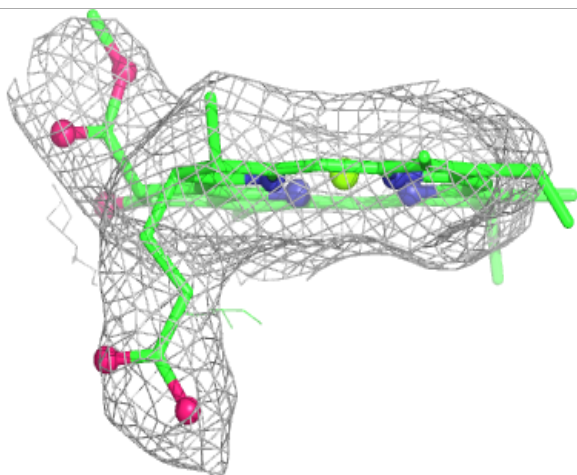
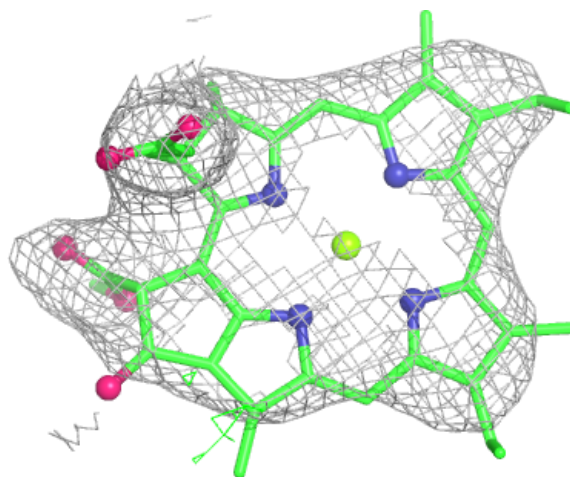
**Electron density around CLA b 834:**

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



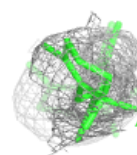
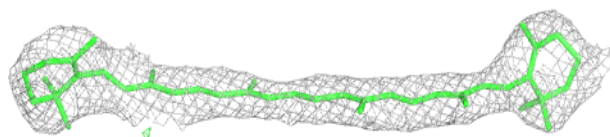
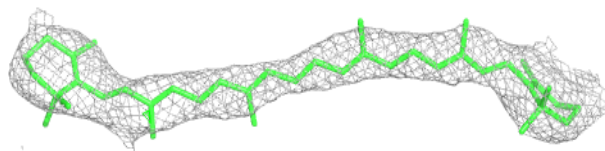
Electron density around CLA 8 303:

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



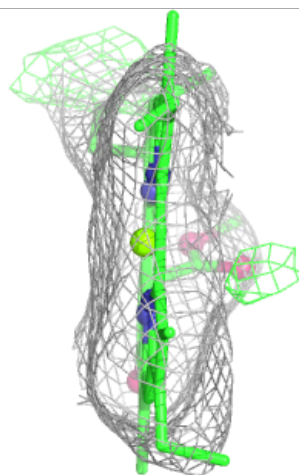
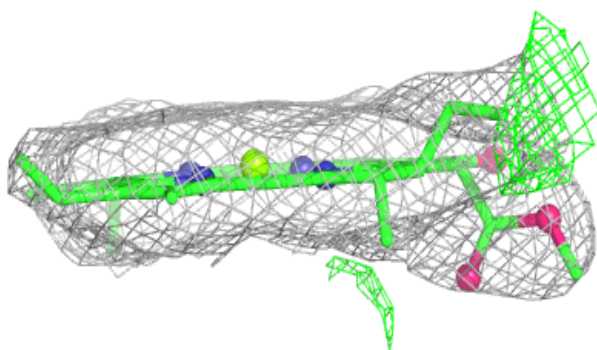
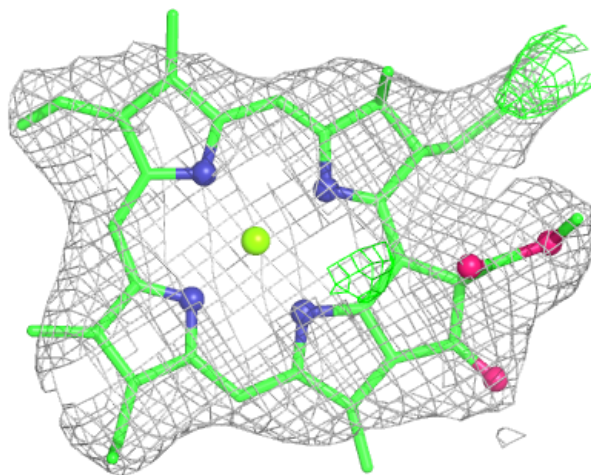
Electron density around BCR 3 318:

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



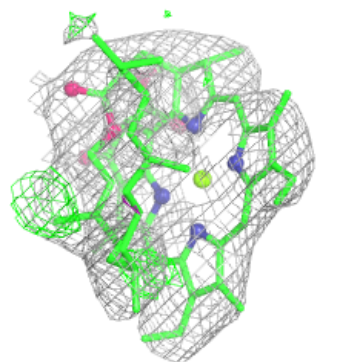
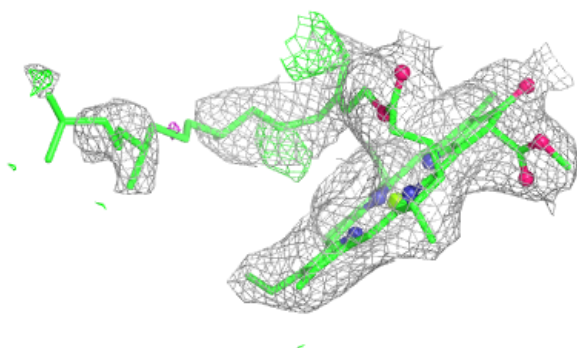
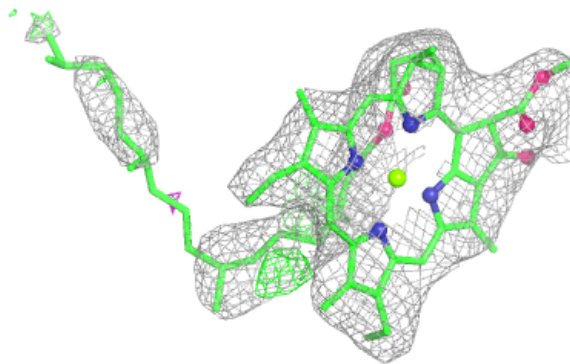
Electron density around CLA 8 304:

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



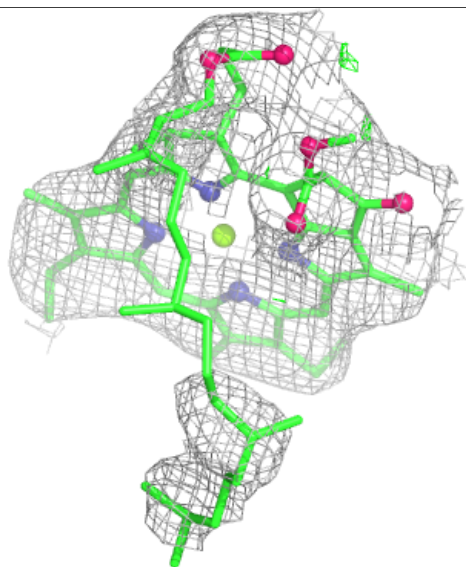
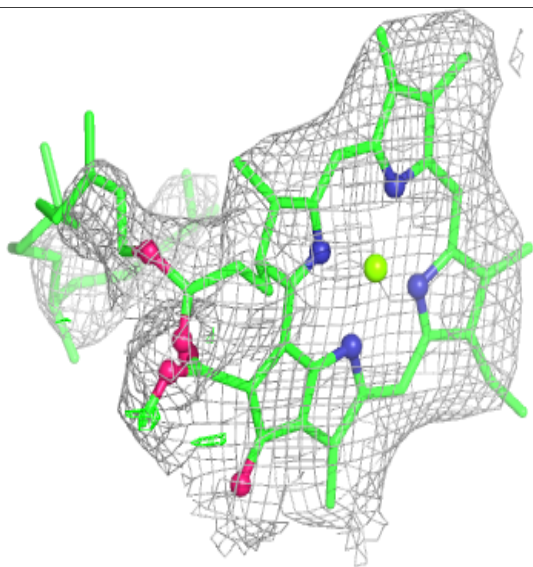
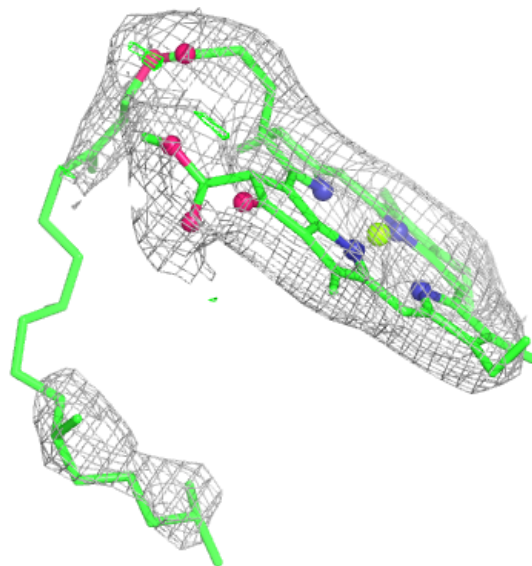
Electron density around CLA B 807:

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



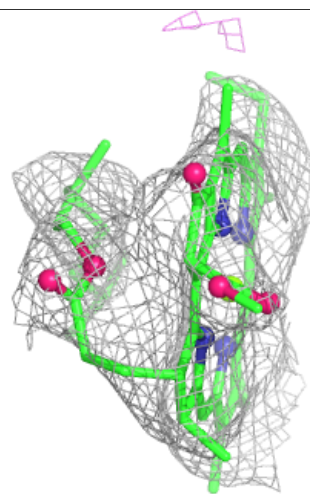
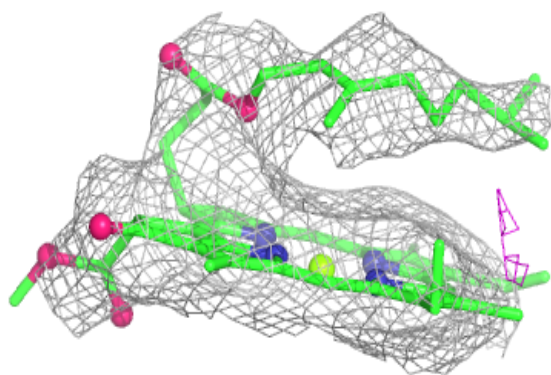
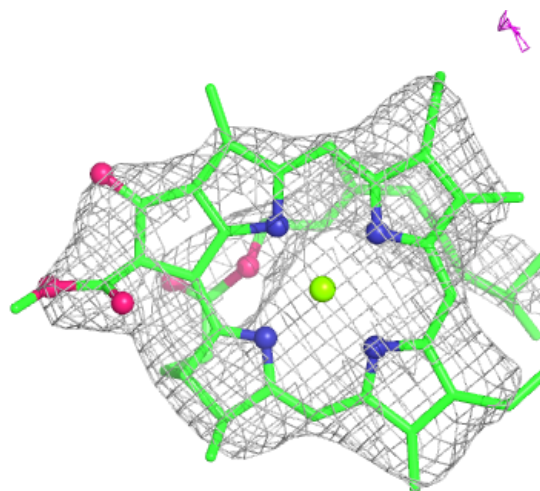
Electron density around CLA 2 603:

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



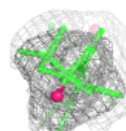
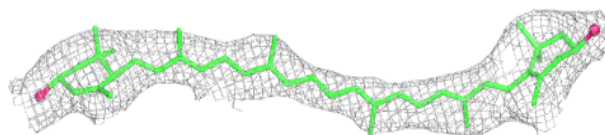
Electron density around CLA 8 310:

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

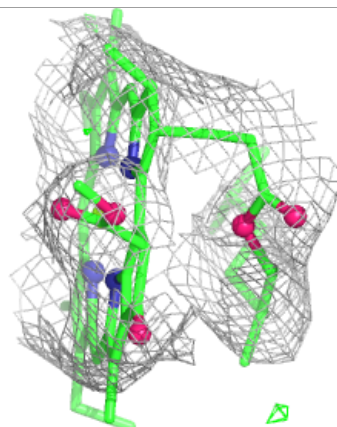
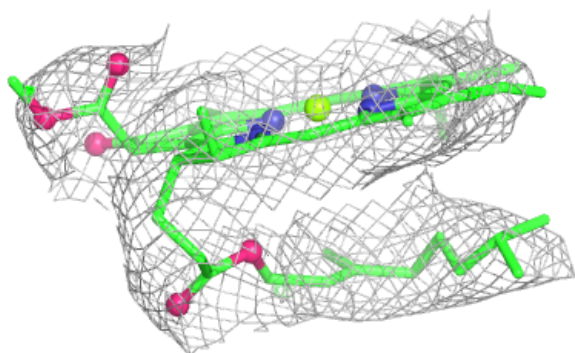
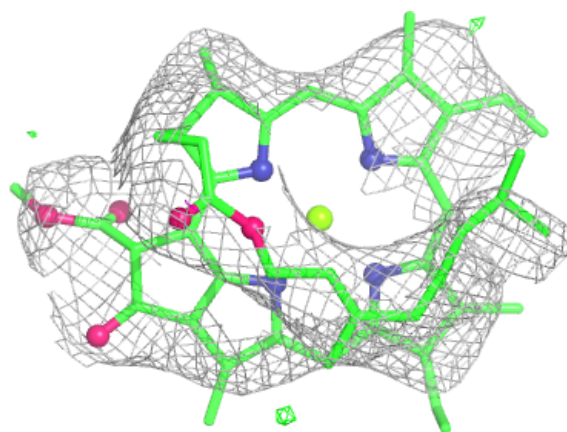


Electron density around LUT 1 316:

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

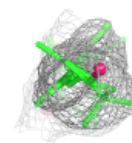
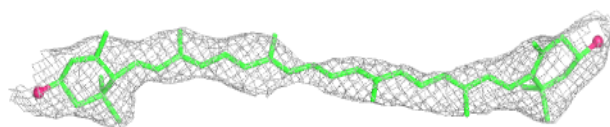
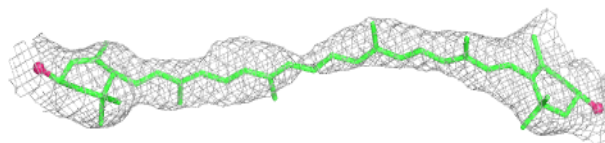
**Electron density around CLA 3 312:**

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



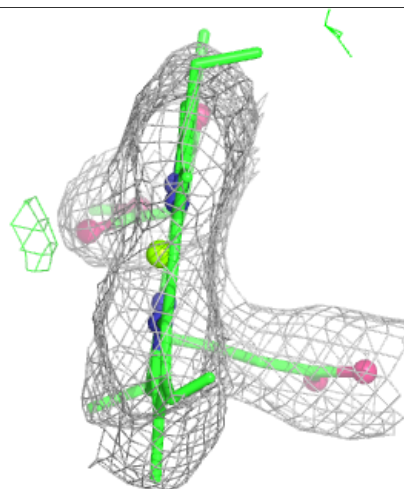
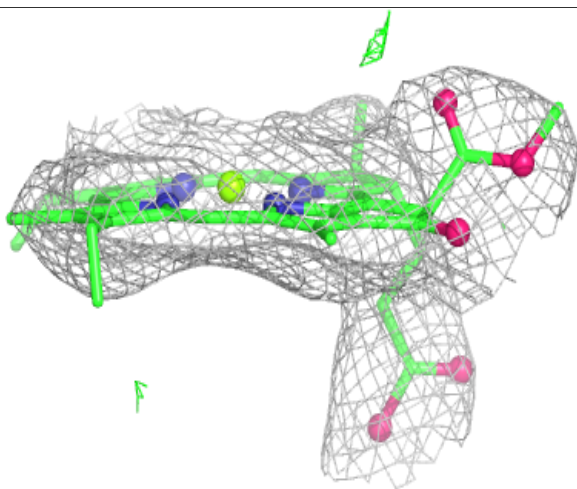
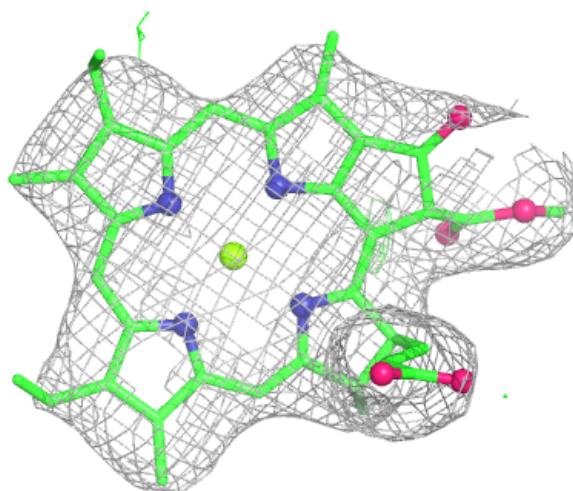
Electron density around LUT 2 615:

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



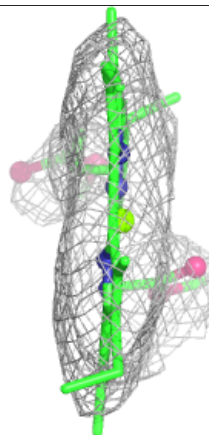
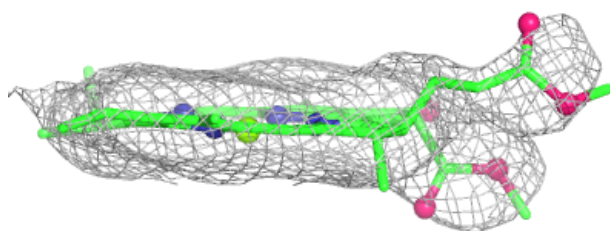
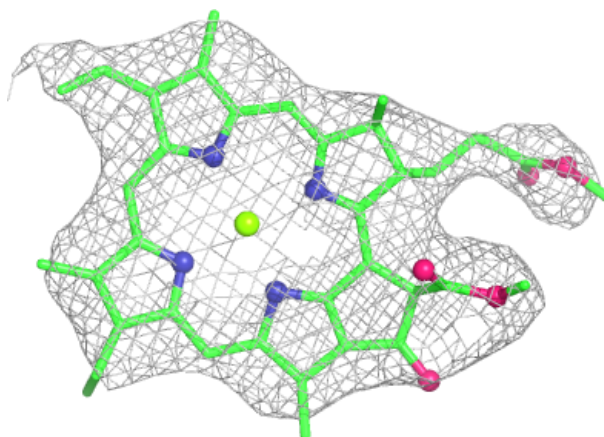
Electron density around CLA B 835:

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



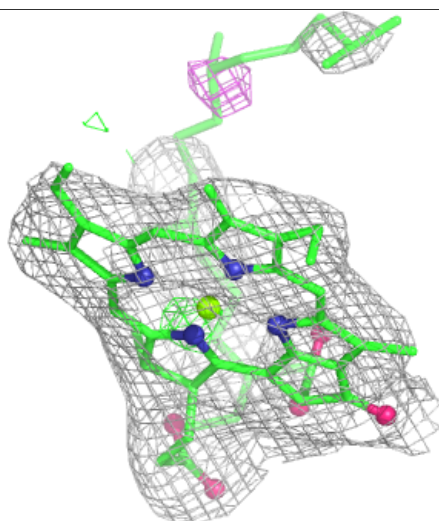
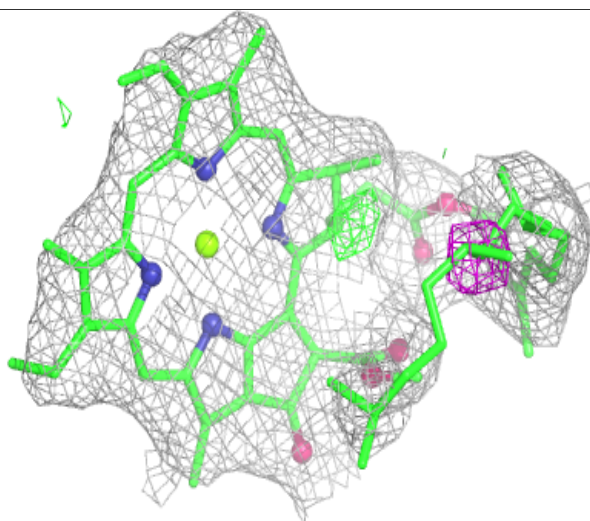
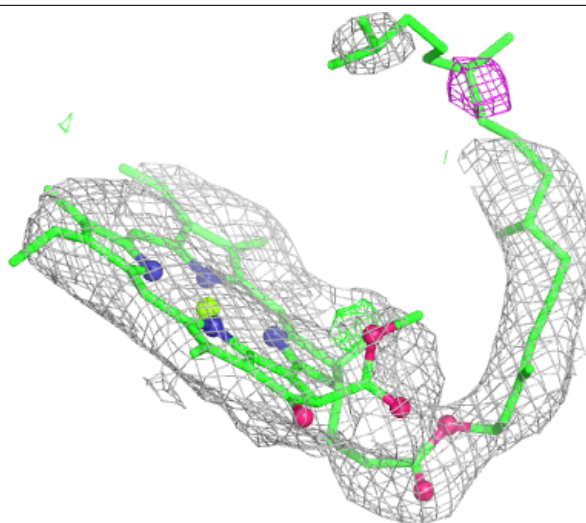
Electron density around CLA 3 314:

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



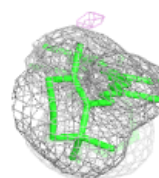
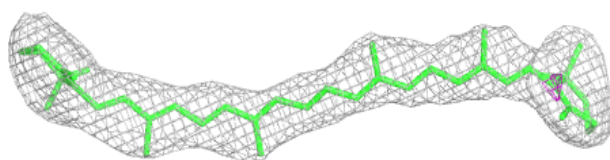
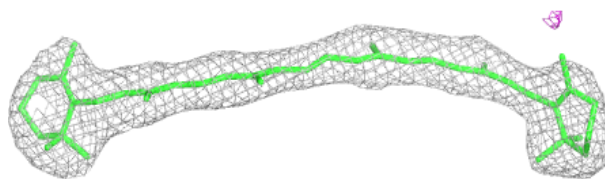
Electron density around CLA 1 304:

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

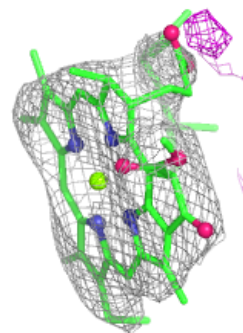
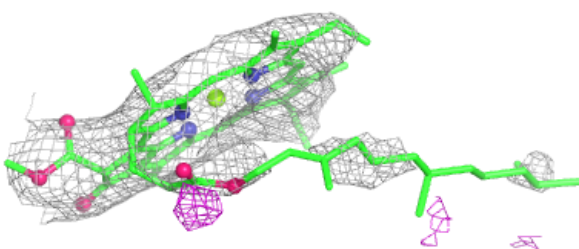
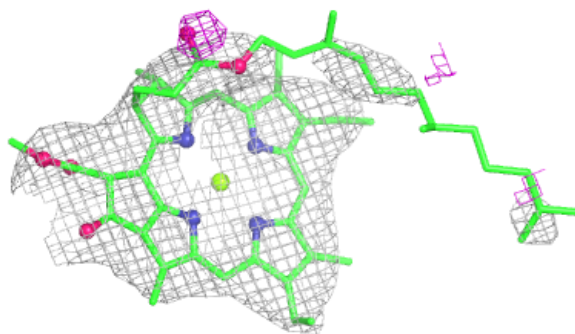


Electron density around BCR i 101:

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

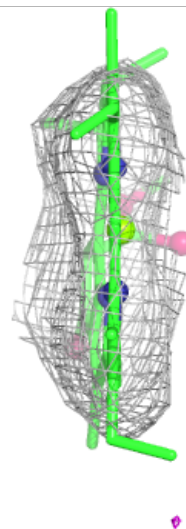
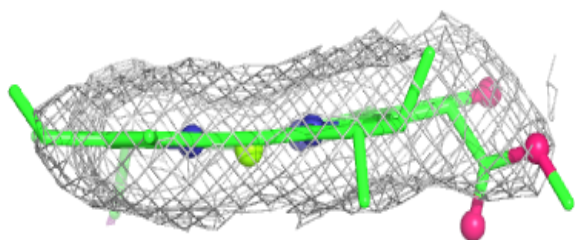
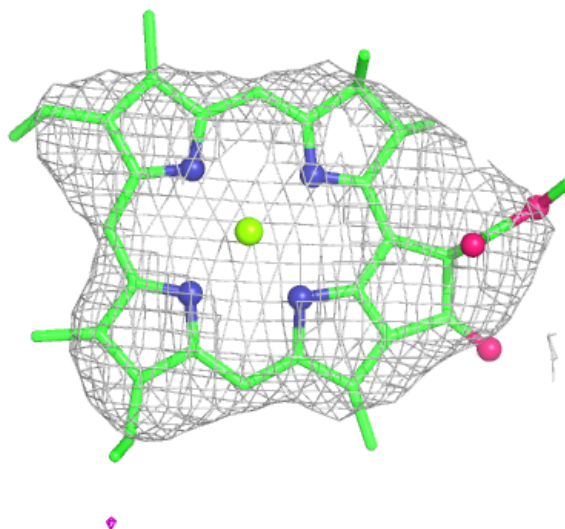
**Electron density around CLA 9 609:**

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



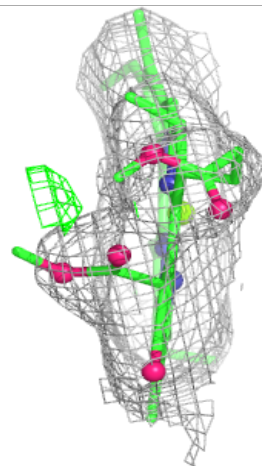
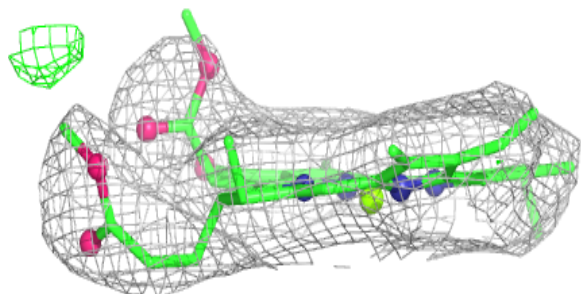
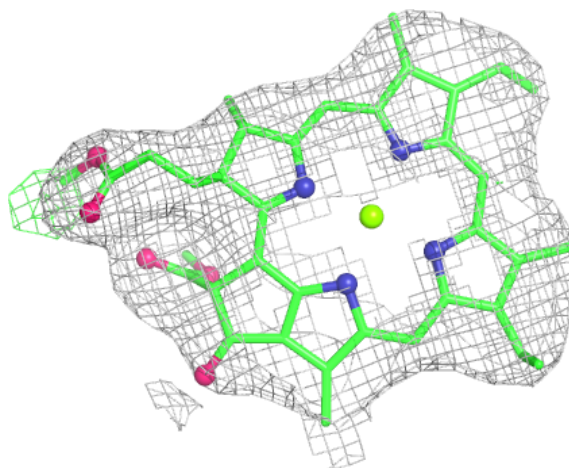
Electron density around CLA 9 610:

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



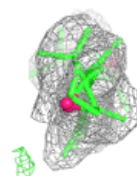
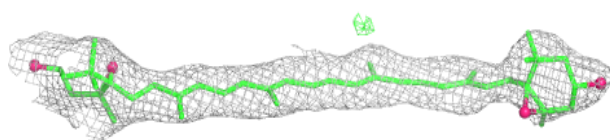
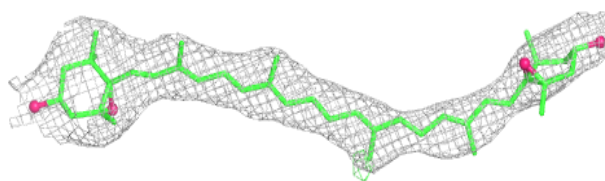
Electron density around CLA 4 603:

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

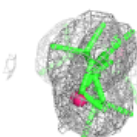
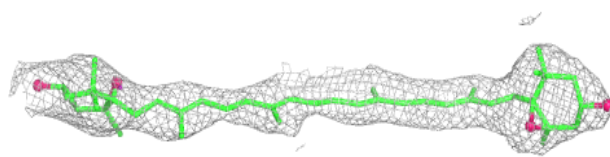
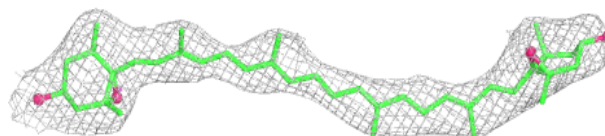


Electron density around XAT 3 317:

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

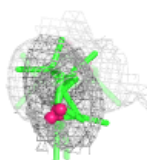
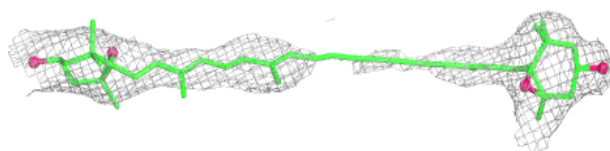
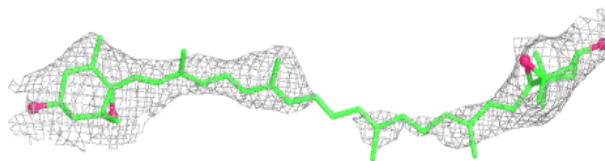
**Electron density around XAT 4 617:**

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

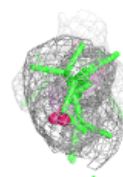
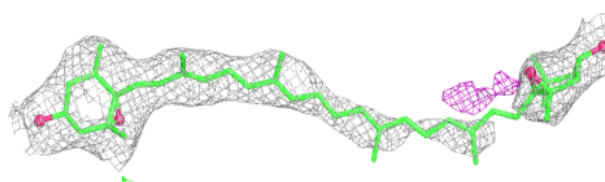


Electron density around XAT 6 318:

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

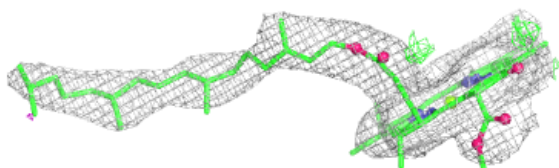
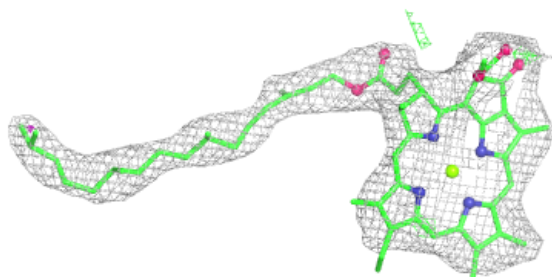
**Electron density around XAT 7 616:**

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

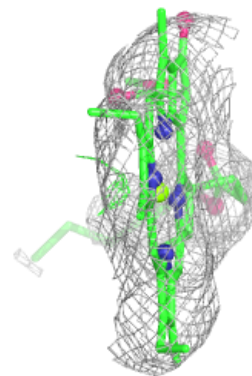
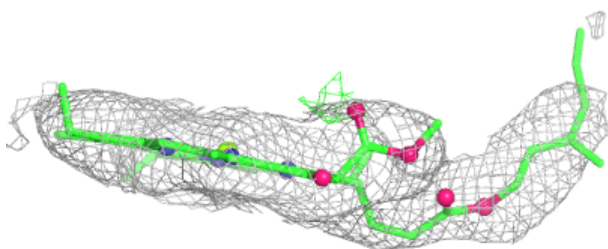
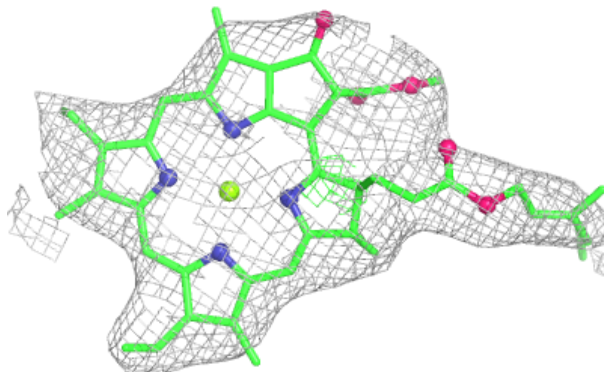


Electron density around CLA A 835:

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

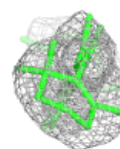
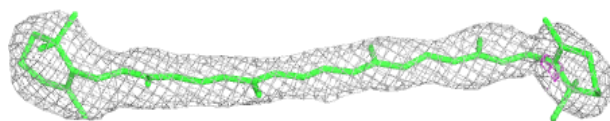
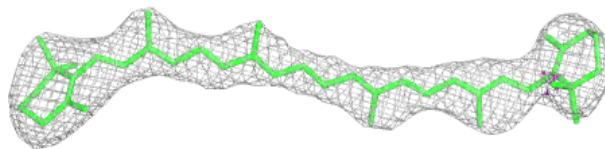
**Electron density around CLA 1 306:**

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

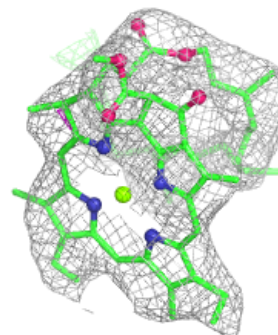
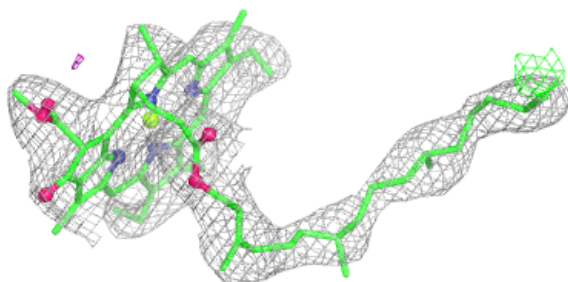
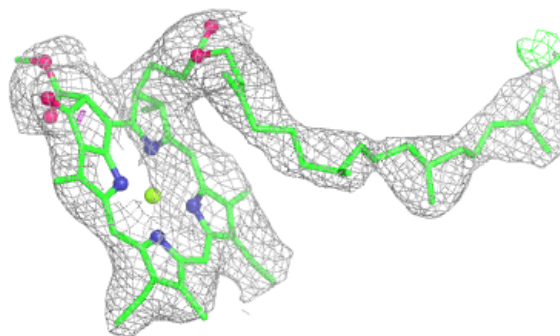


Electron density around BCR A 849:

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

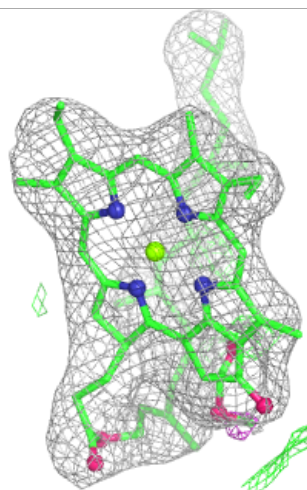
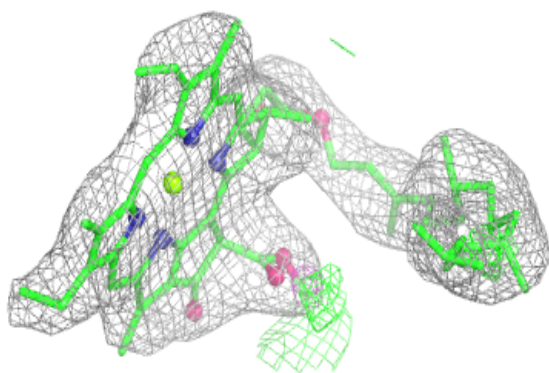
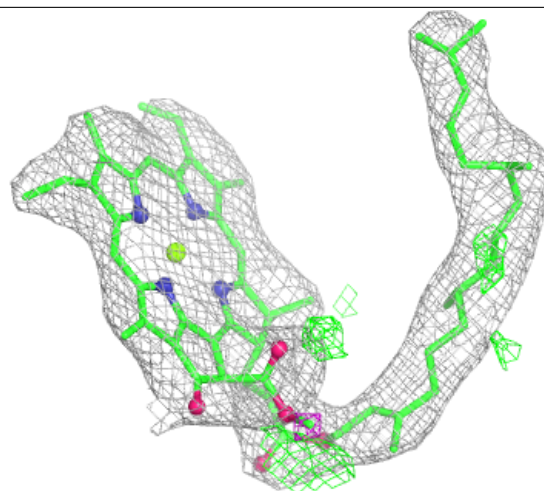
**Electron density around CLA B 814:**

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



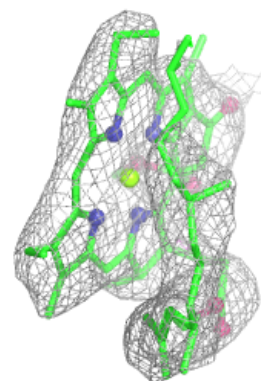
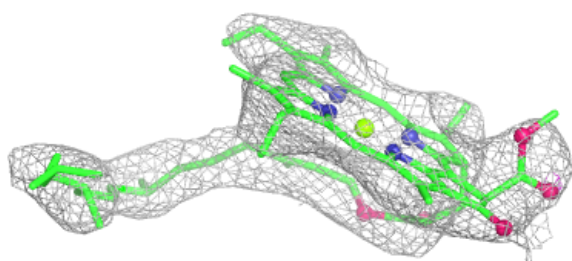
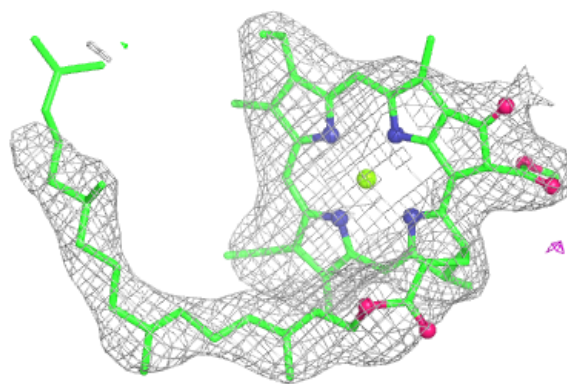
Electron density around CLA b 810:

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

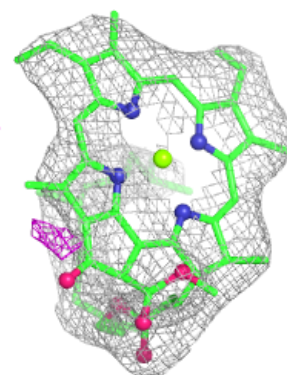
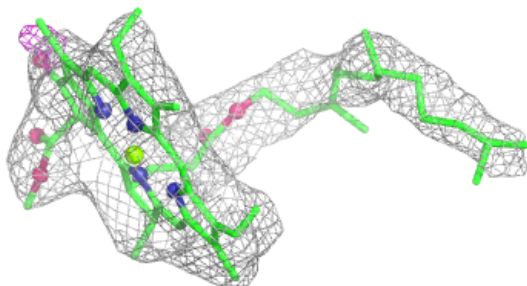
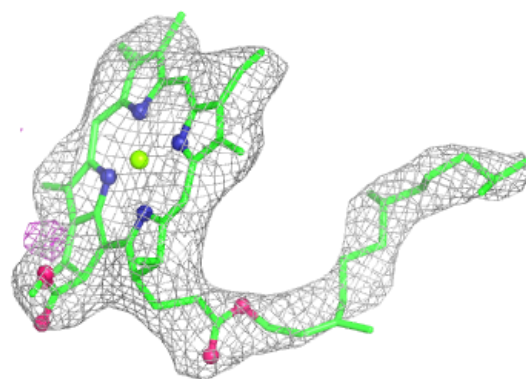


Electron density around CLA 1 303:

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

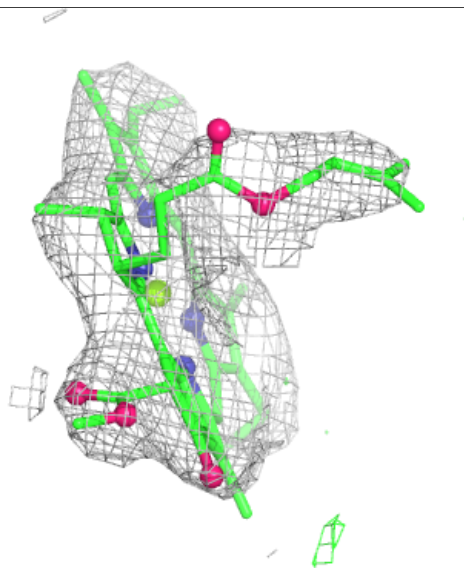
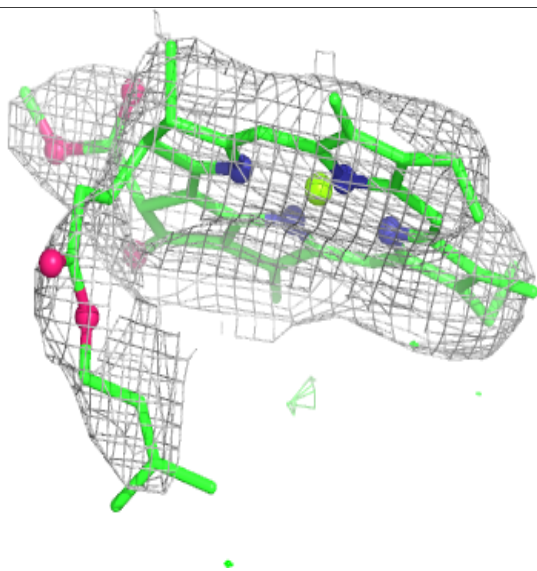
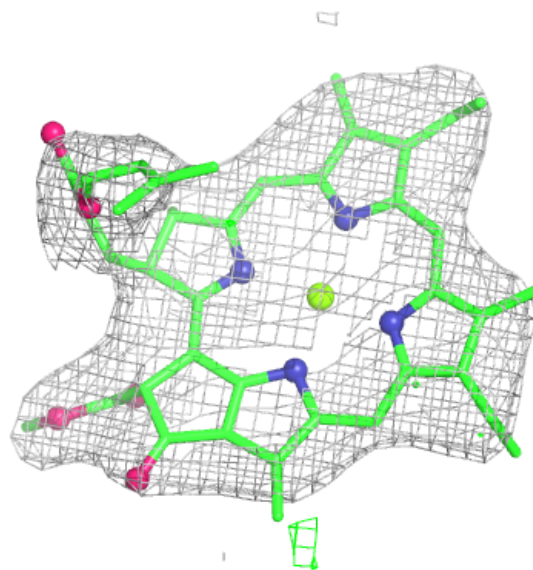
**Electron density around CLA B 815:**

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



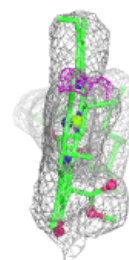
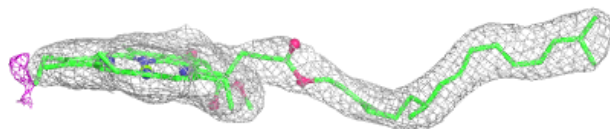
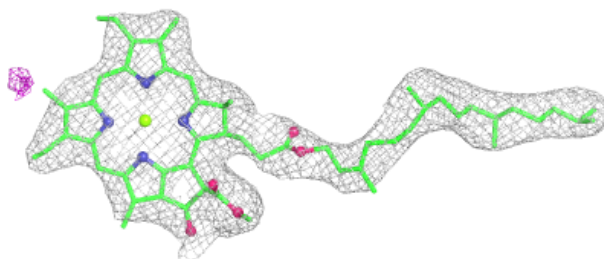
Electron density around CLA 3 308:

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

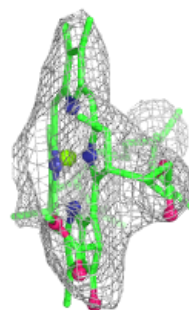
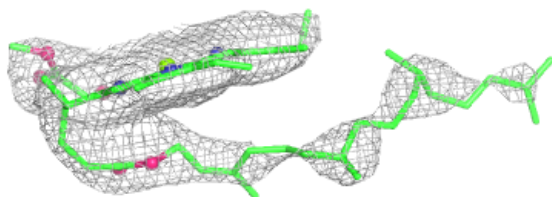
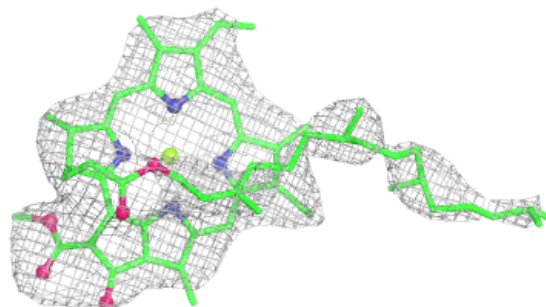


Electron density around CLA A 834:

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

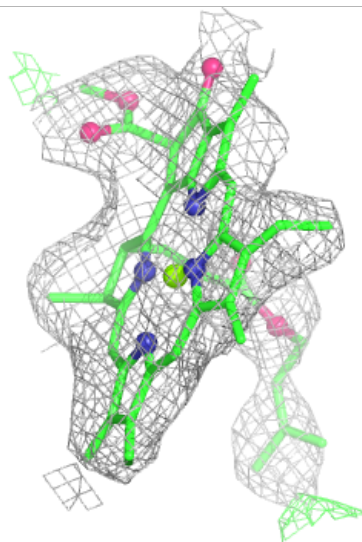
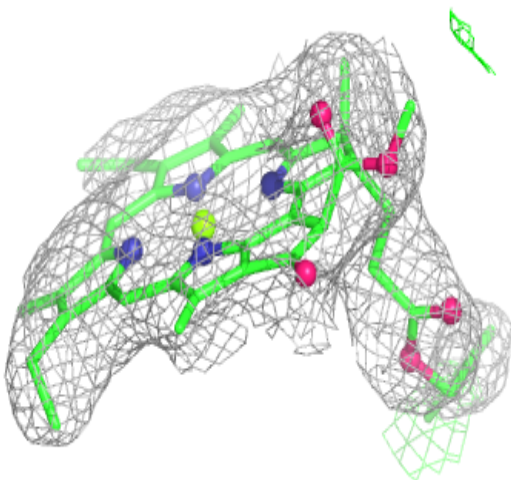
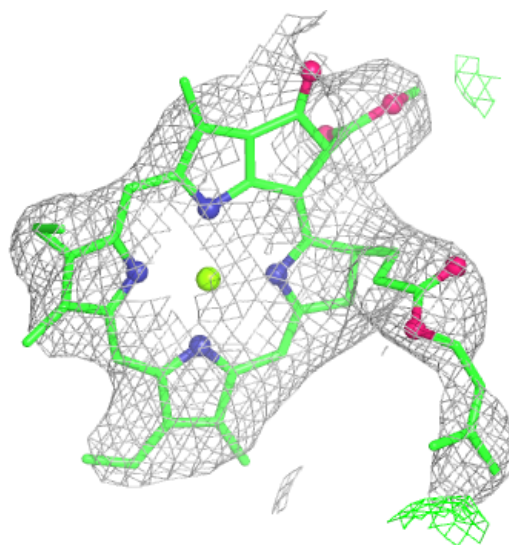
**Electron density around CLA A 818:**

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



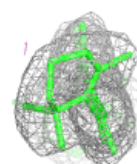
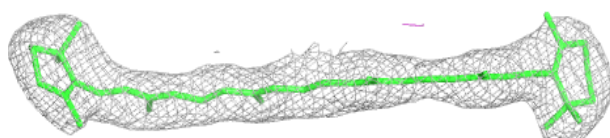
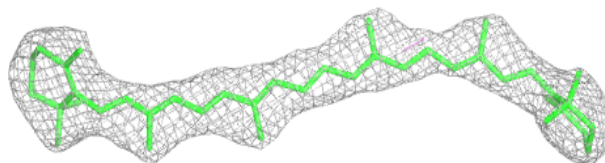
Electron density around CLA A 836:

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

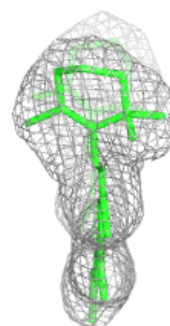
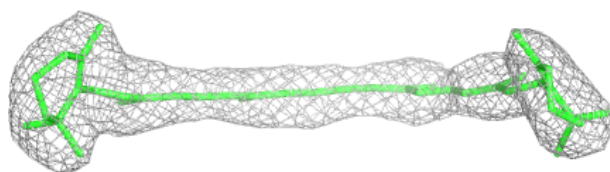
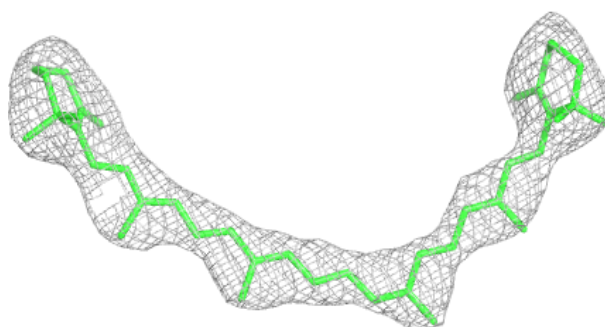


Electron density around BCR B 848:

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

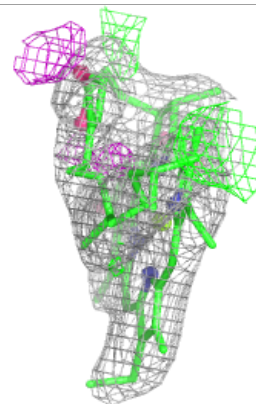
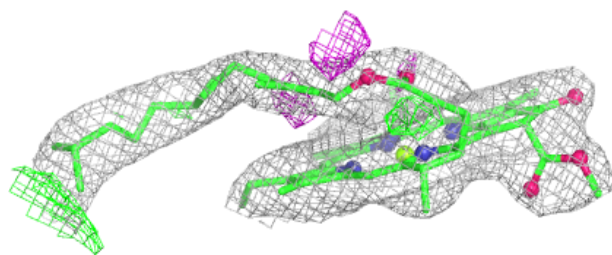
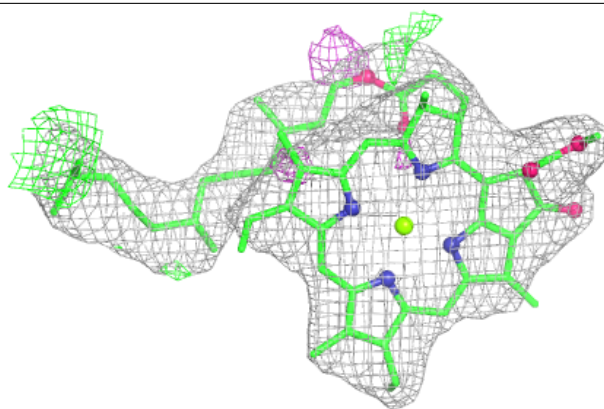
**Electron density around BCR F 305:**

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

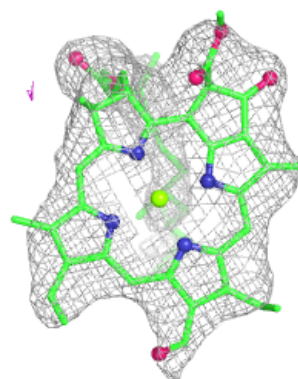
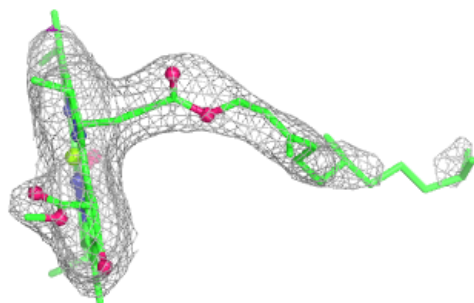
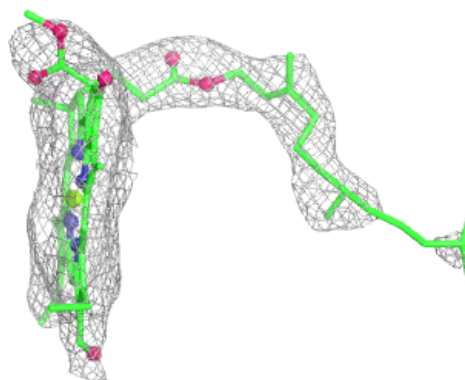


Electron density around CLA b 818:

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

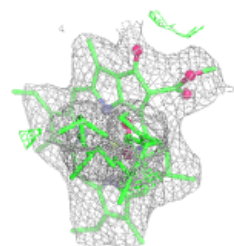
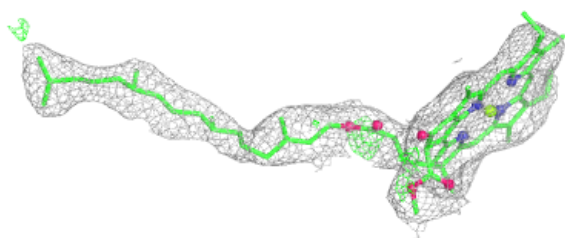
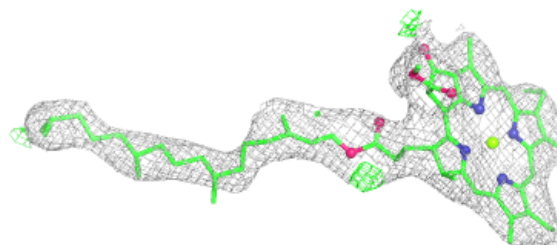
**Electron density around CHL 1 302:**

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

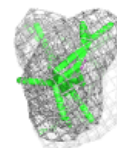
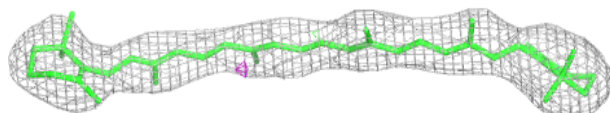
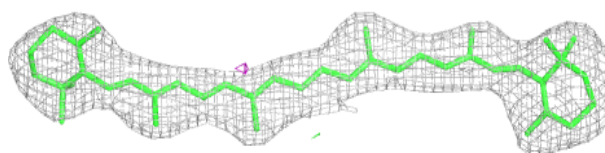


Electron density around CLA A 810:

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

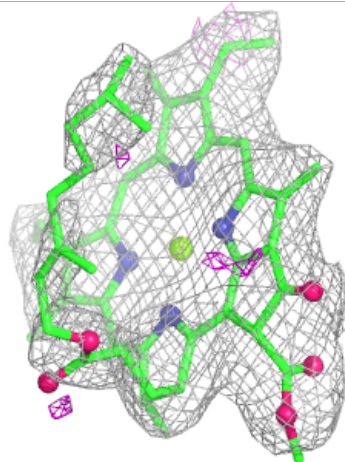
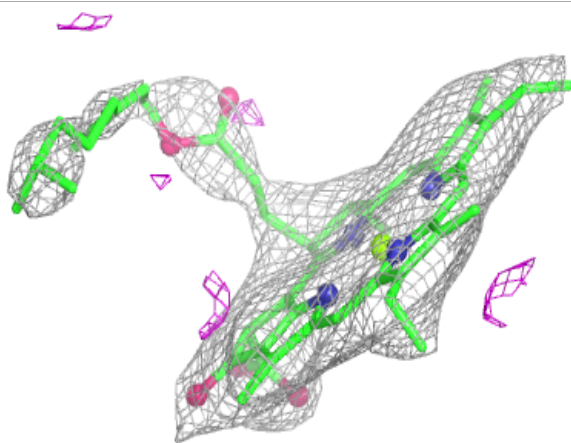
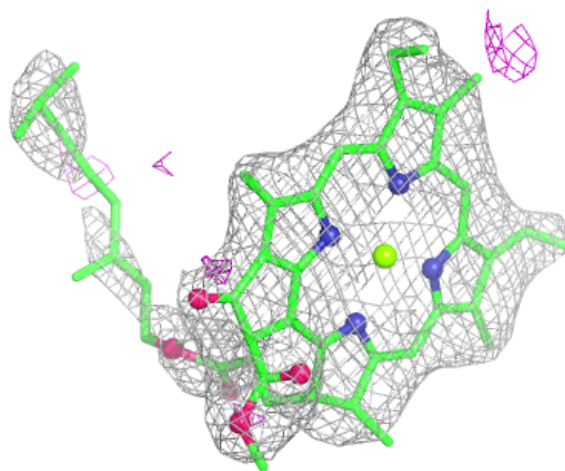
**Electron density around BCR J 3003:**

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



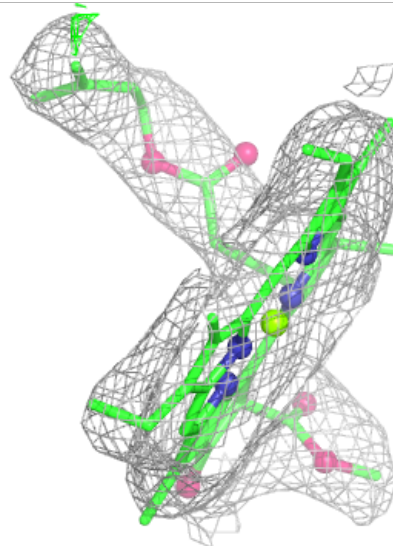
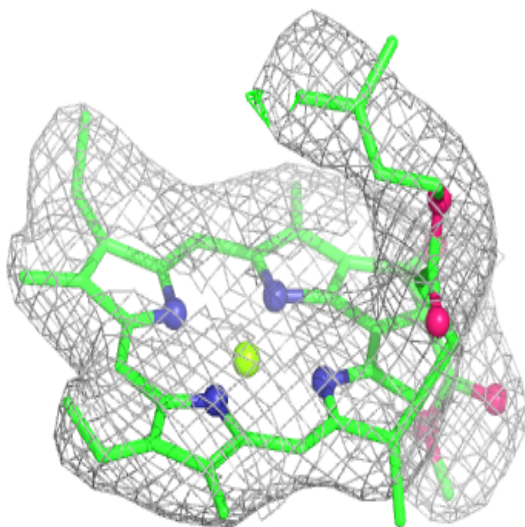
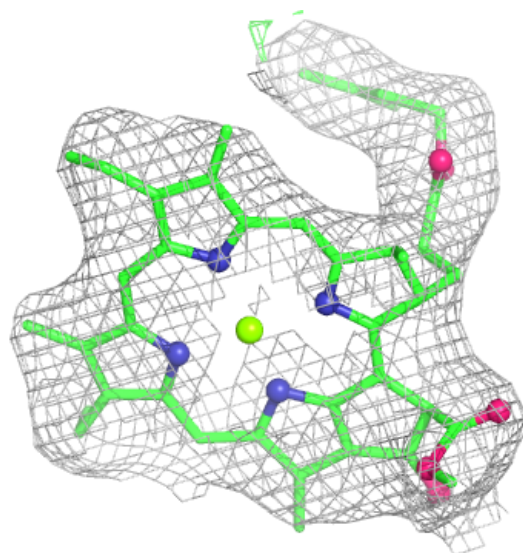
Electron density around CLA B 822:

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



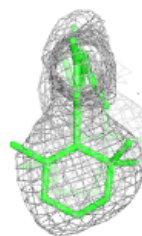
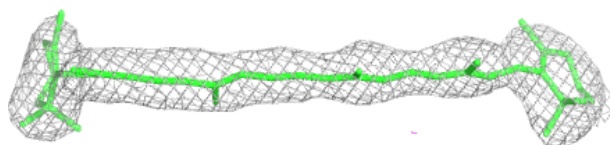
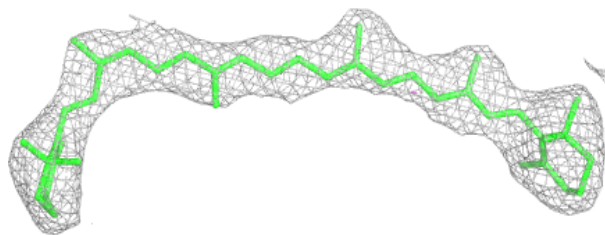
Electron density around CLA b 830:

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



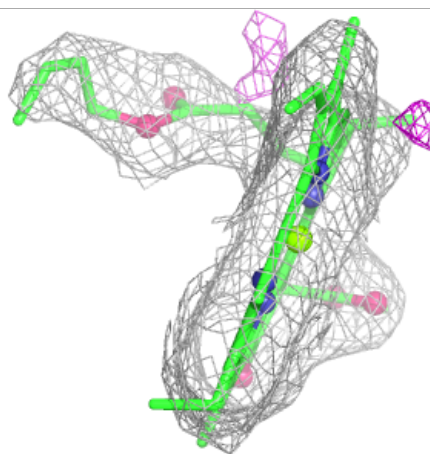
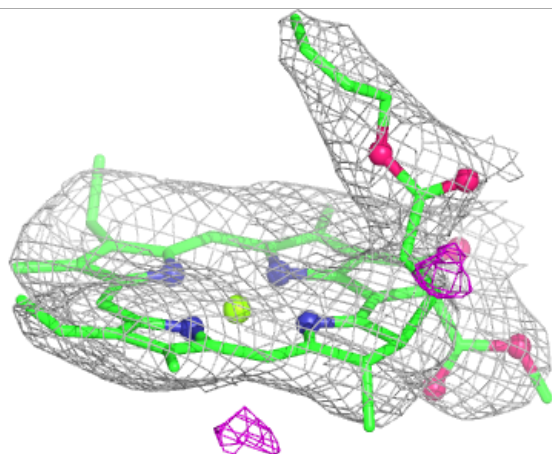
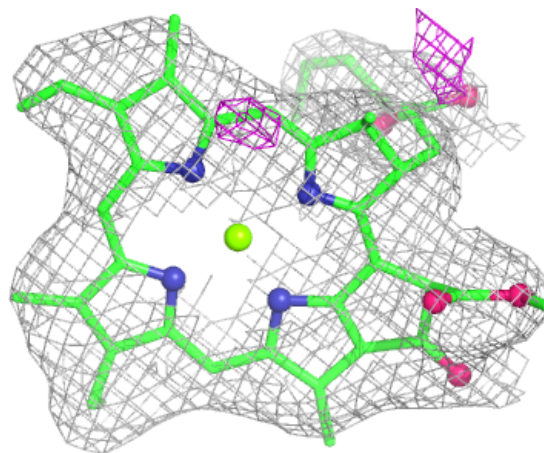
Electron density around BCR L 201:

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



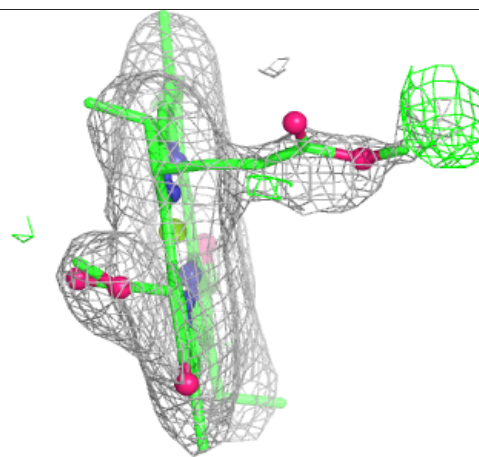
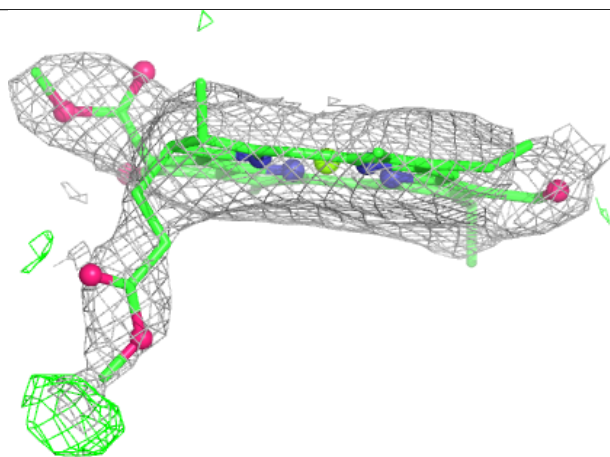
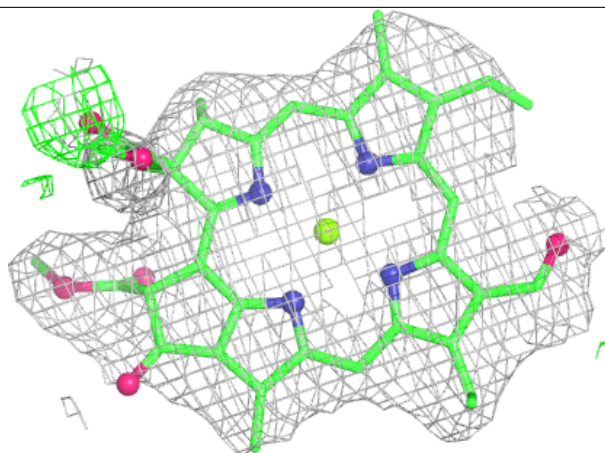
Electron density around CLA b 831:

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



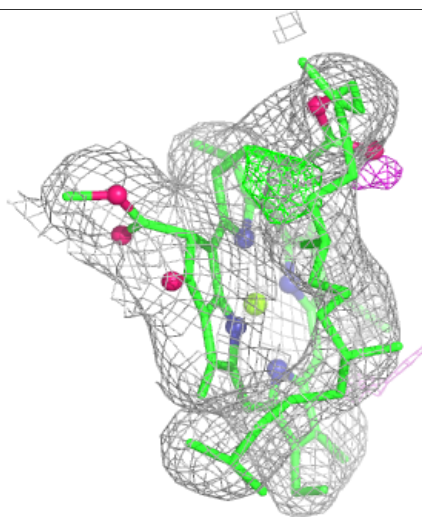
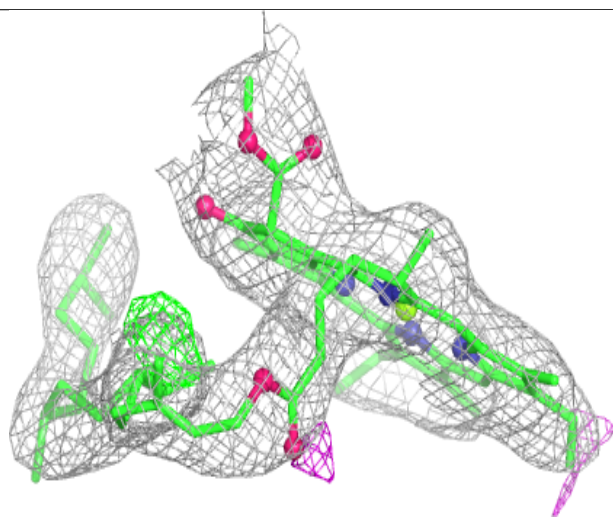
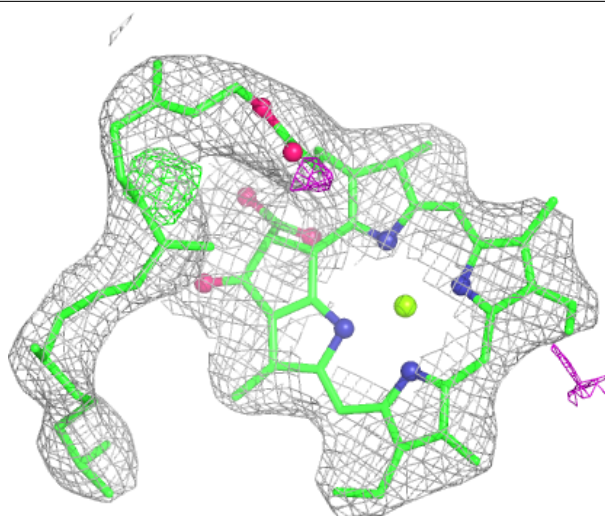
Electron density around CHL 3 307:

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



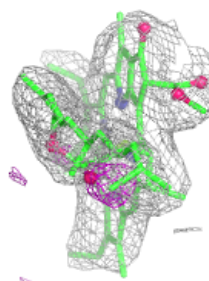
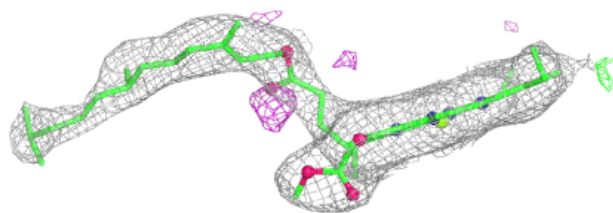
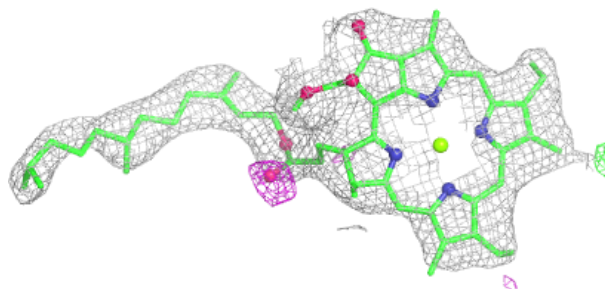
Electron density around CLA b 832:

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

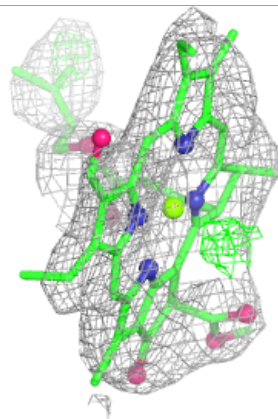
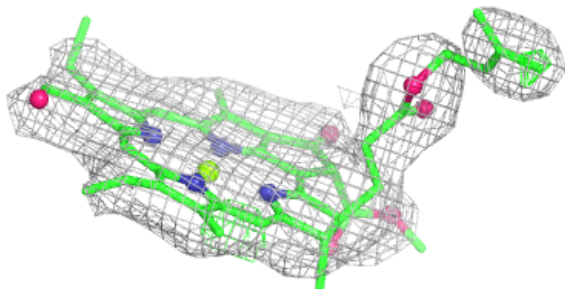
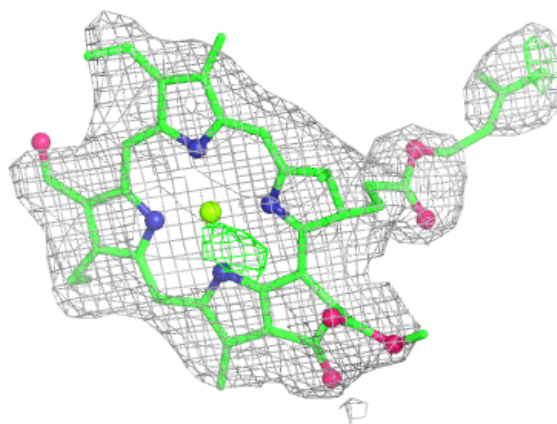


Electron density around CLA B 823:

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

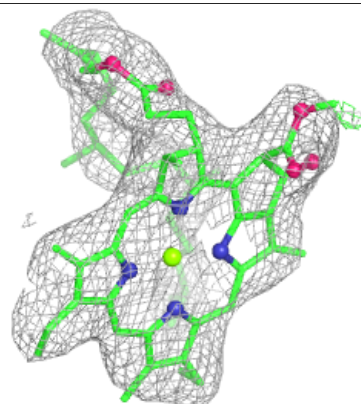
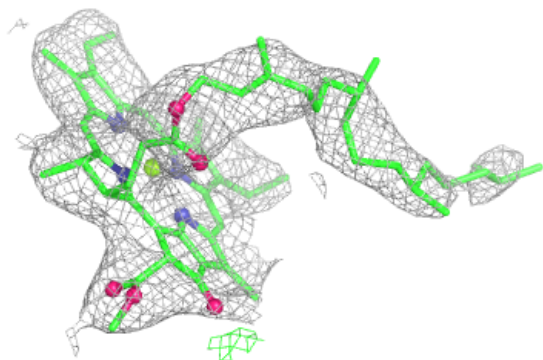
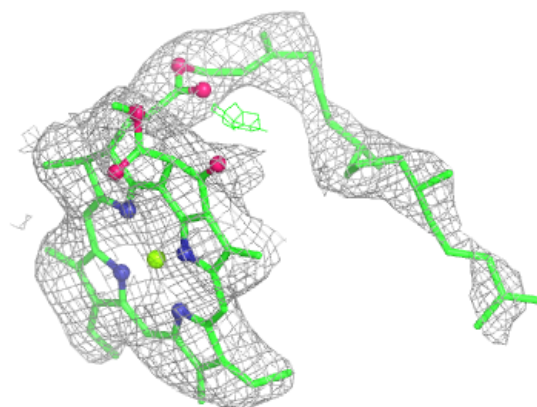
**Electron density around CHL 4 607:**

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



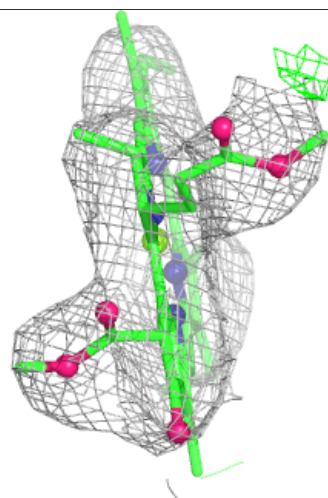
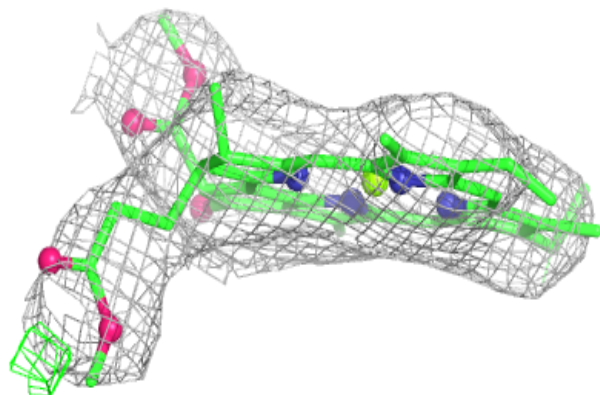
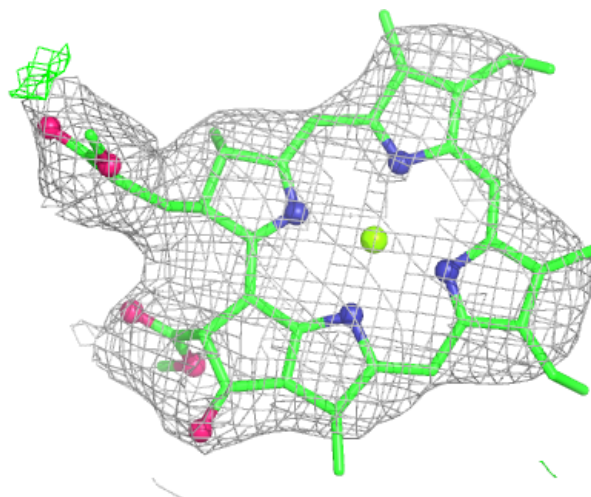
Electron density around CLA B 834:

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



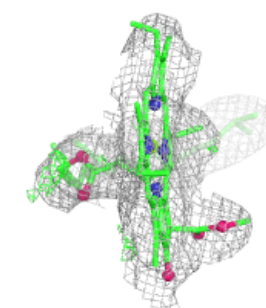
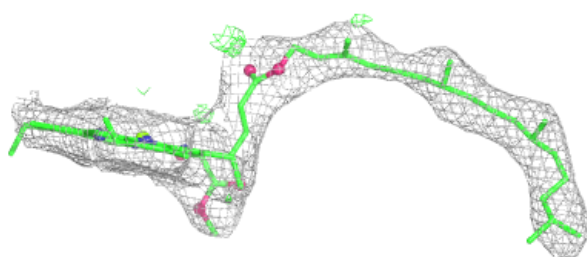
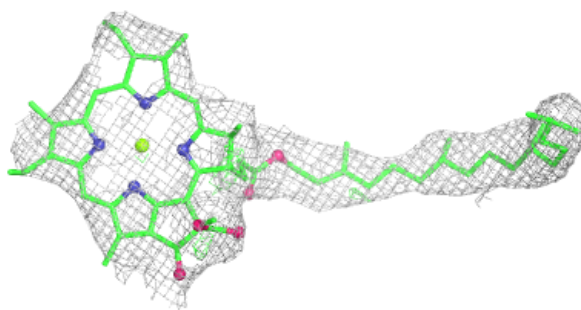
Electron density around CLA 9 601:

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

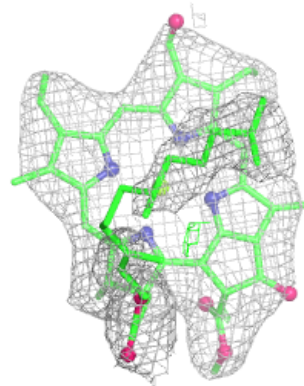
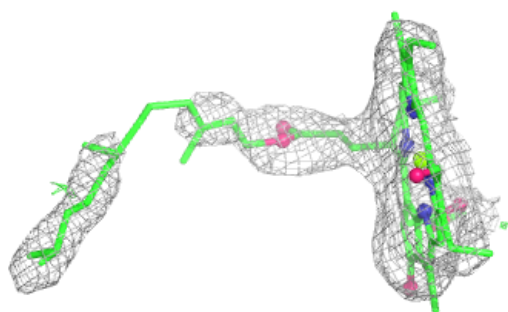
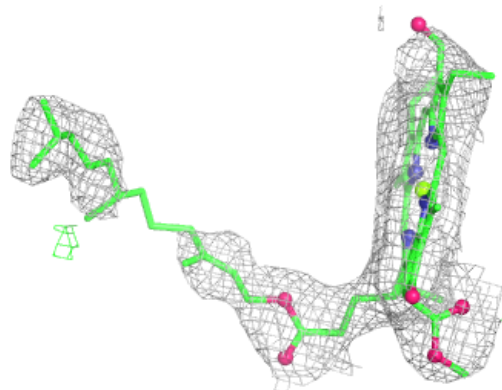


Electron density around CLA b 841:

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

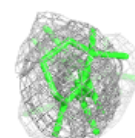
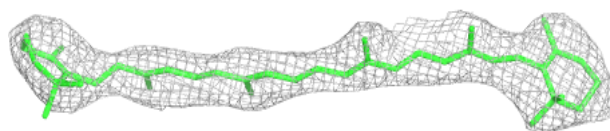
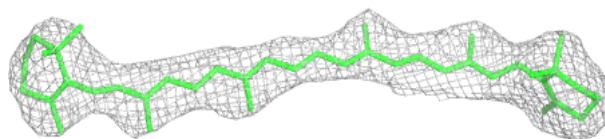
**Electron density around CHL 7 601:**

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

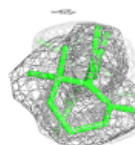
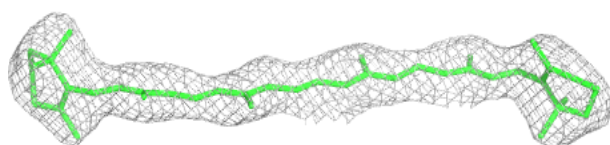
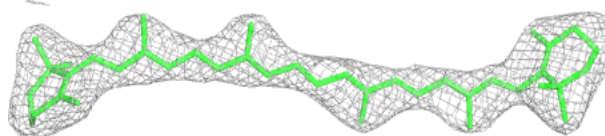


Electron density around BCR a 850:

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

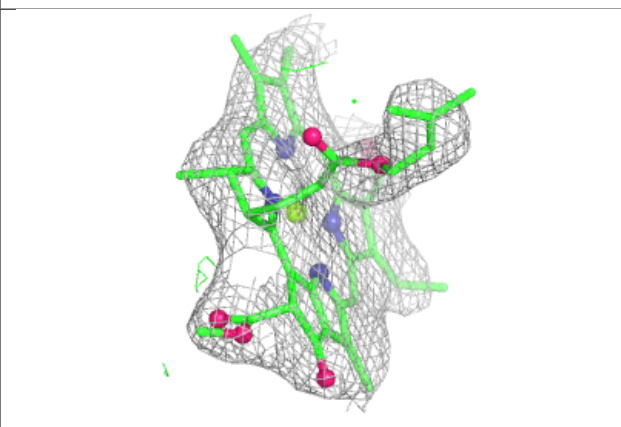
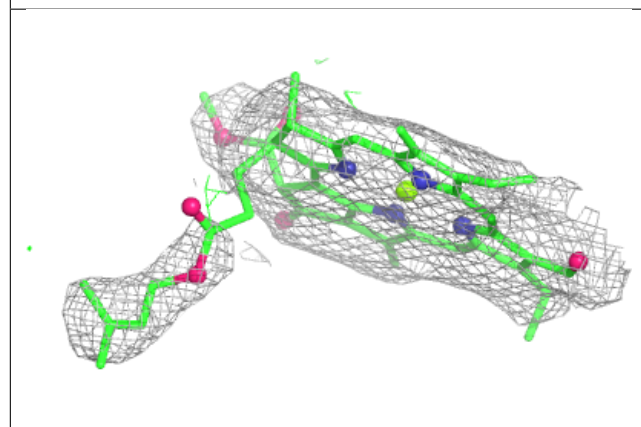
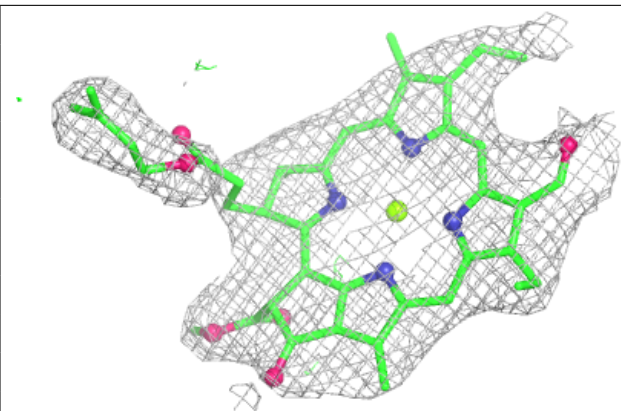
**Electron density around BCR a 851:**

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

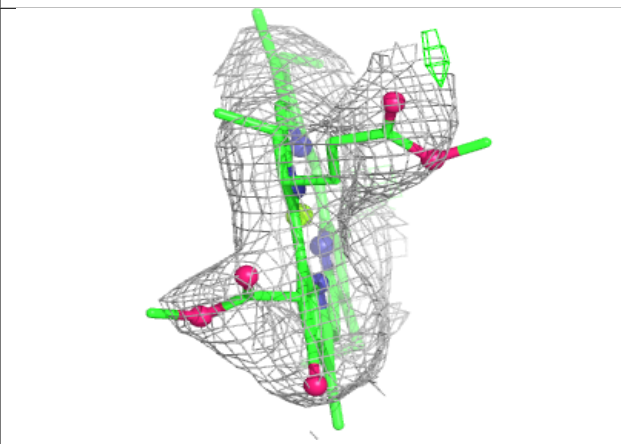
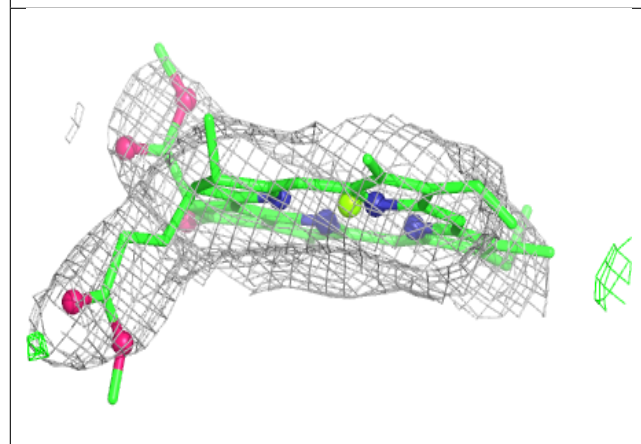
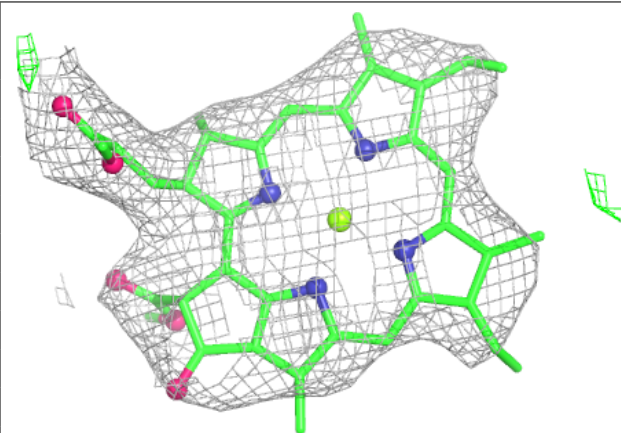


Electron density around CHL 7 607:

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

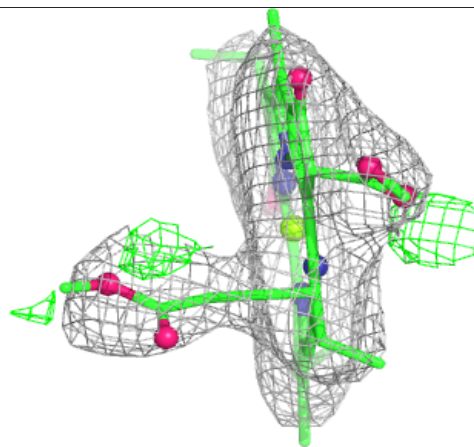
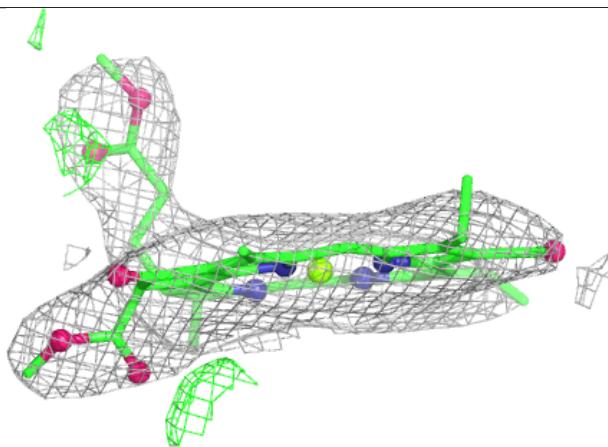
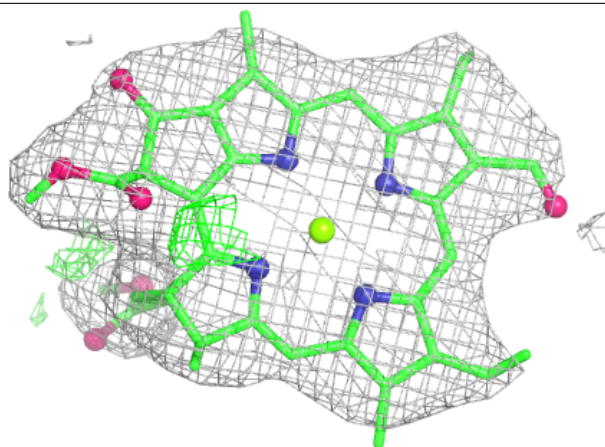
**Electron density around CLA 4 601:**

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

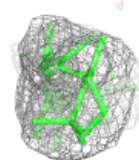
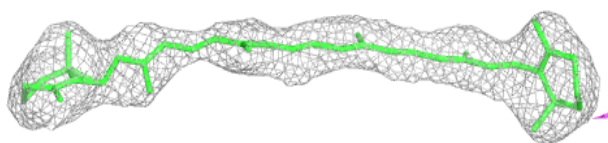
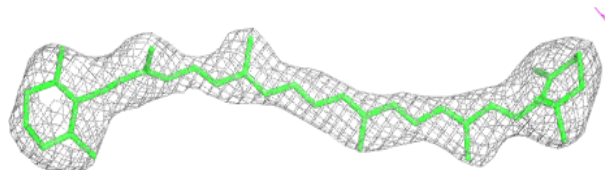


Electron density around CHL 8 306:

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

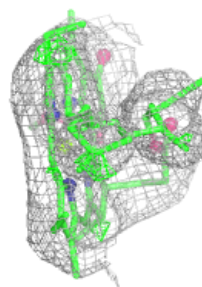
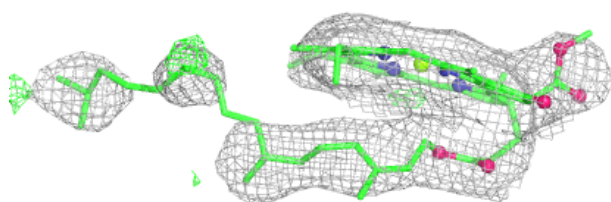
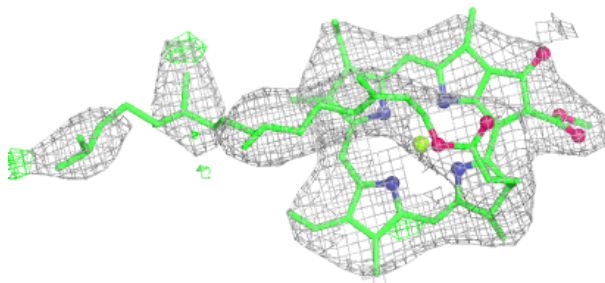
**Electron density around BCR a 853:**

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

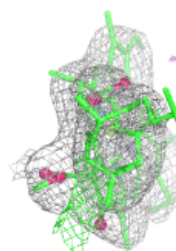
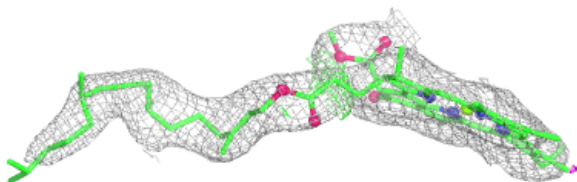
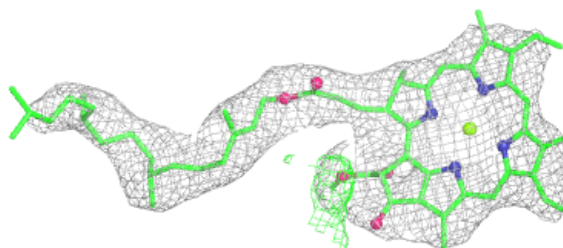


Electron density around CLA A 839:

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

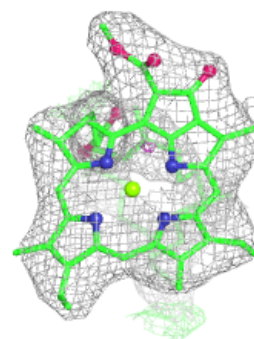
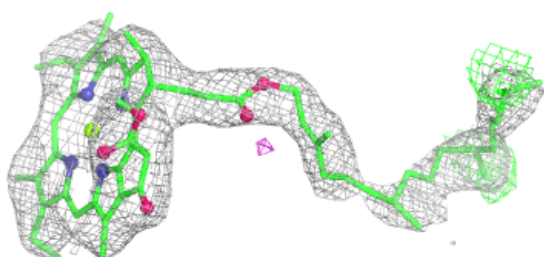
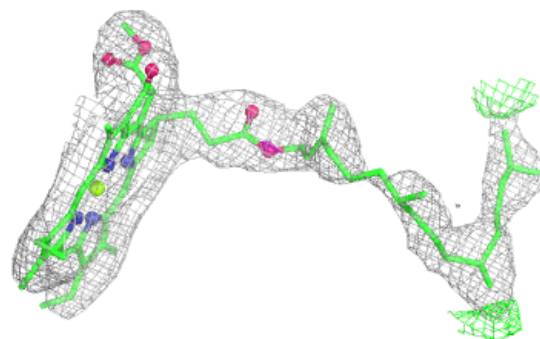
**Electron density around CLA F 301:**

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

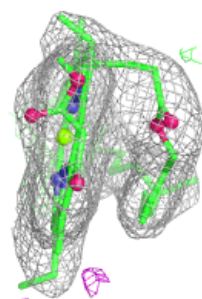
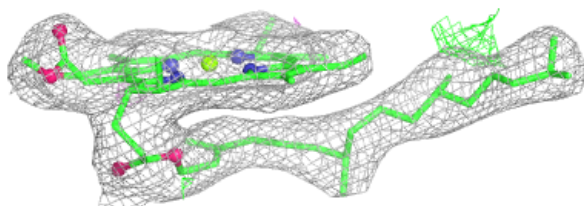
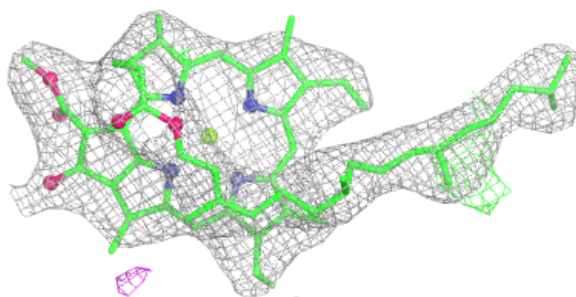


Electron density around CLA A 840:

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

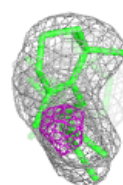
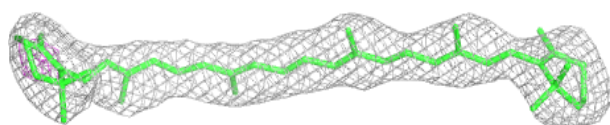
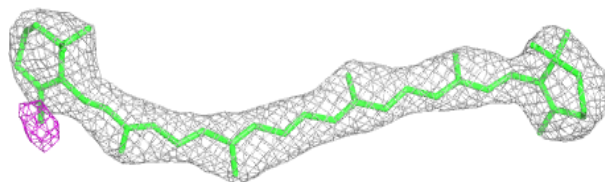
**Electron density around CLA A 841:**

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

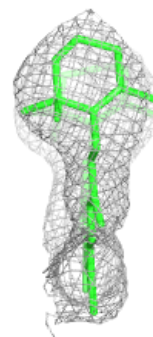
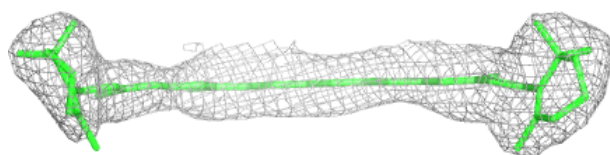
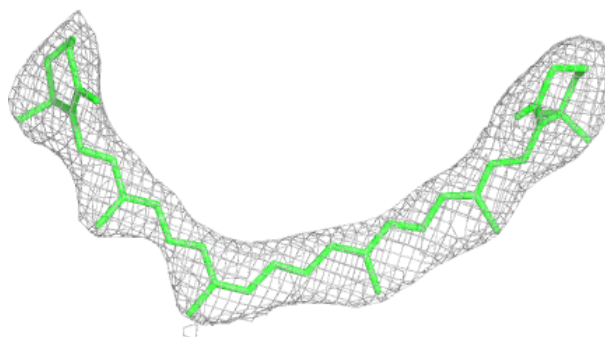


Electron density around BCR b 847:

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

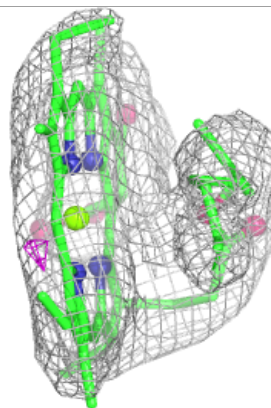
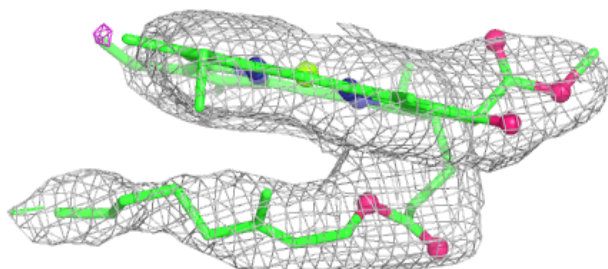
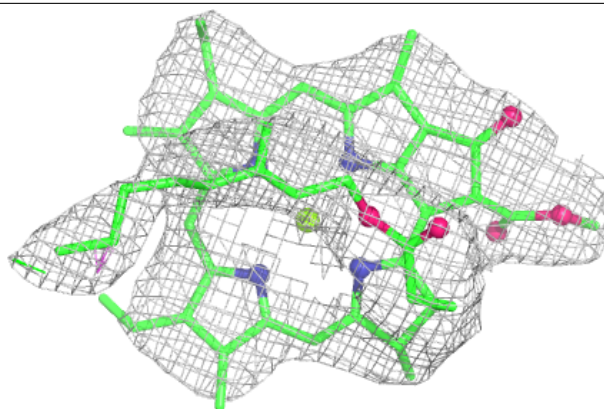
**Electron density around BCR f 7004:**

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

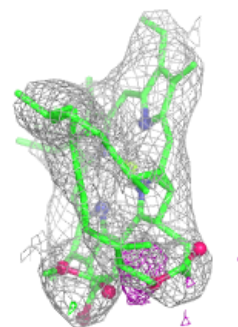
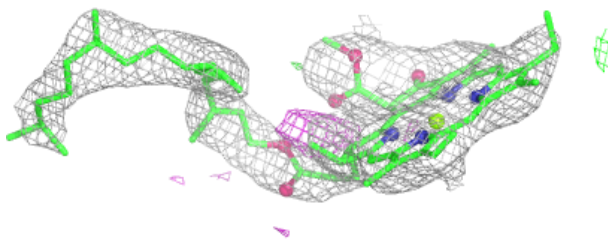
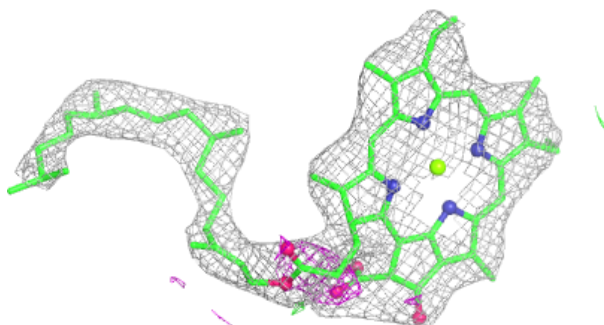


Electron density around CLA A 813:

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

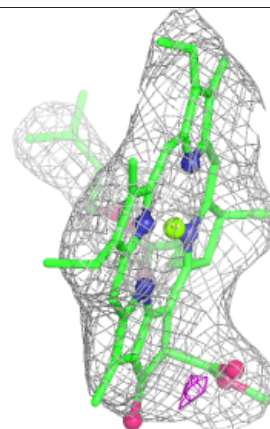
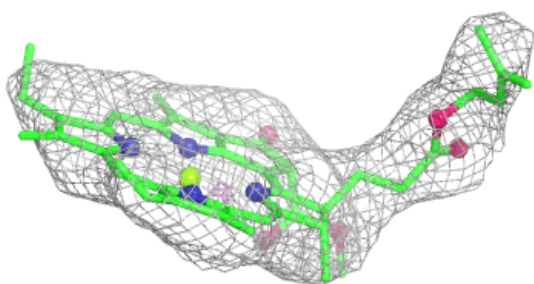
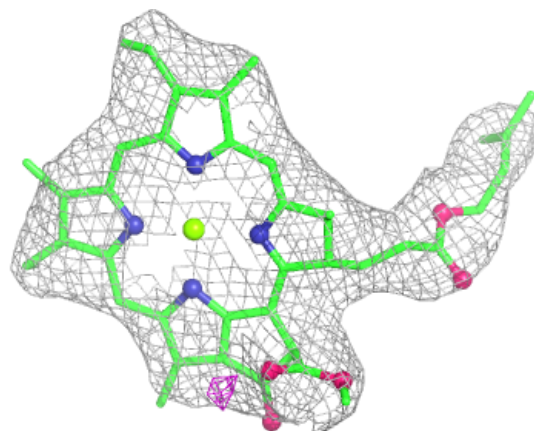
**Electron density around CLA A 804:**

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

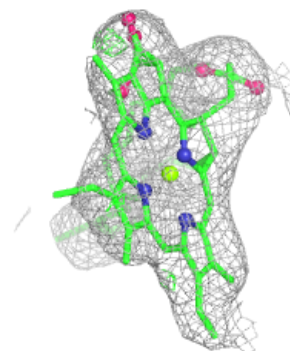
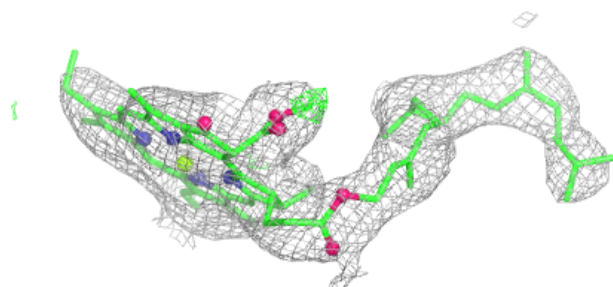
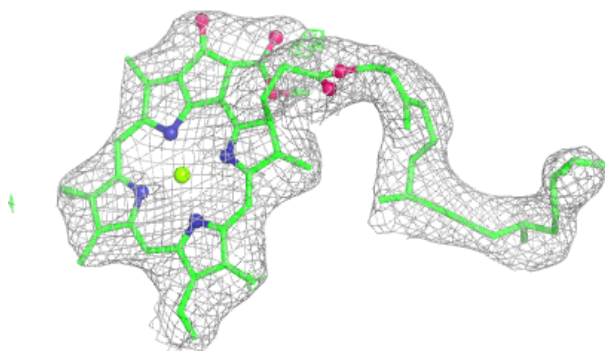


Electron density around CLA 4 614:

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

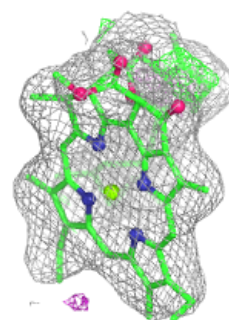
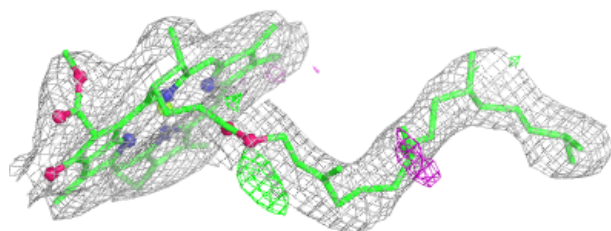
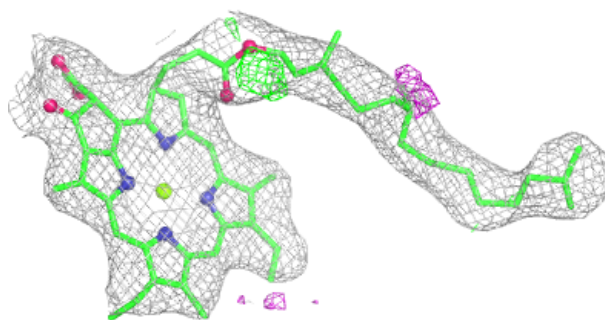
**Electron density around CLA a 804:**

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

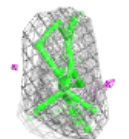
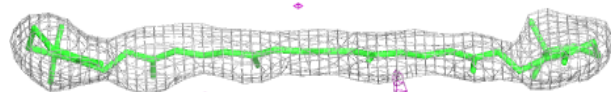
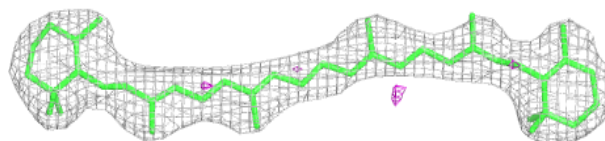


Electron density around CLA a 809:

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

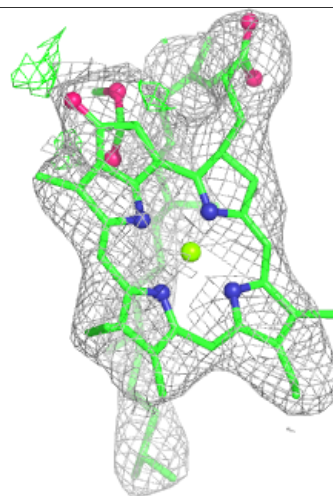
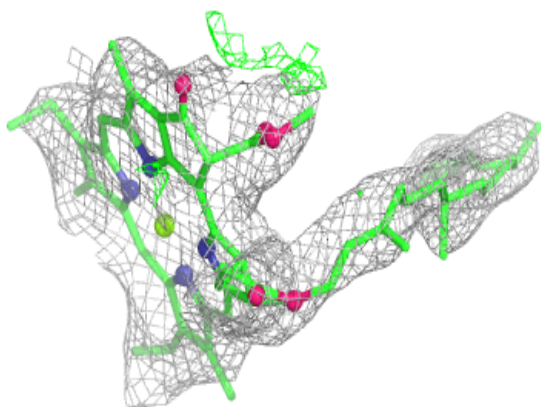
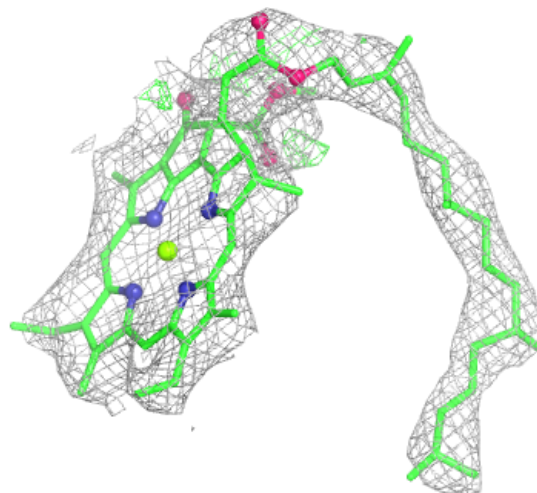
**Electron density around BCR 1 205:**

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



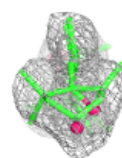
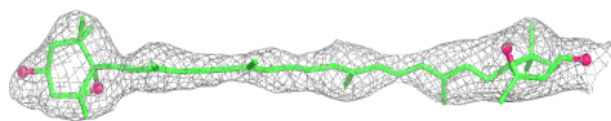
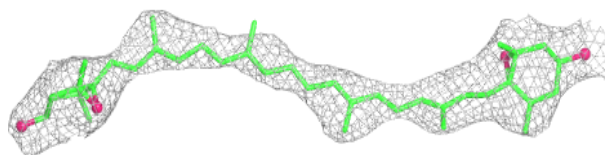
Electron density around CLA B 810:

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



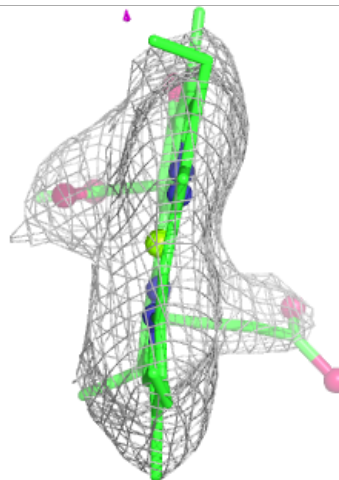
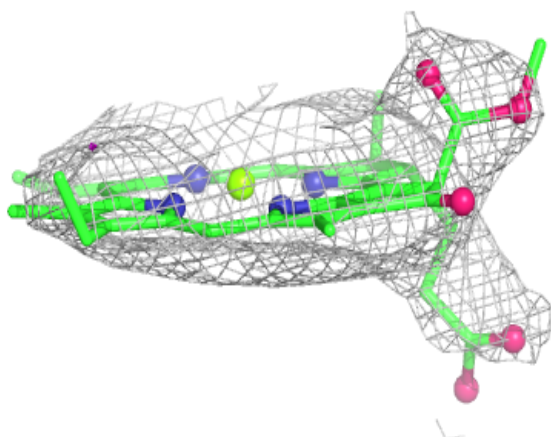
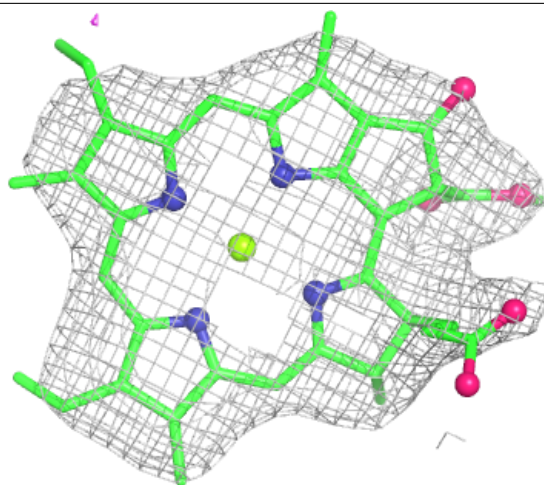
Electron density around XAT 2 616:

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



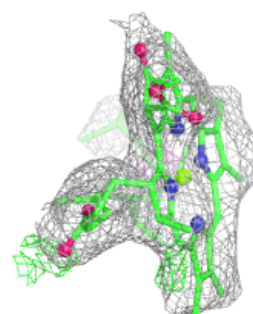
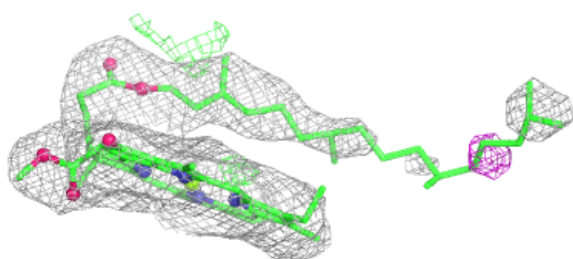
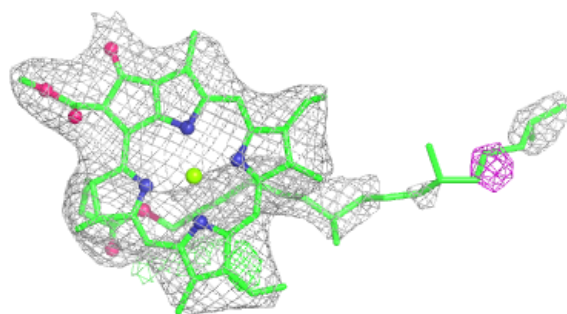
Electron density around CLA A 817:

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

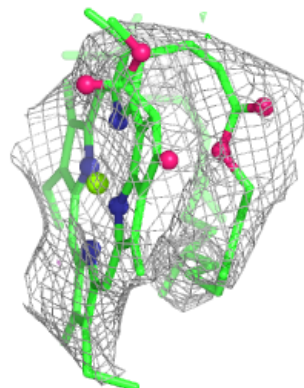
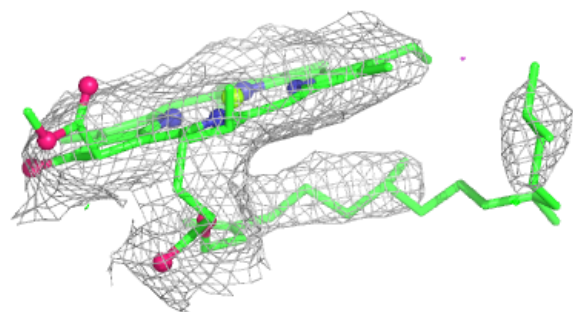
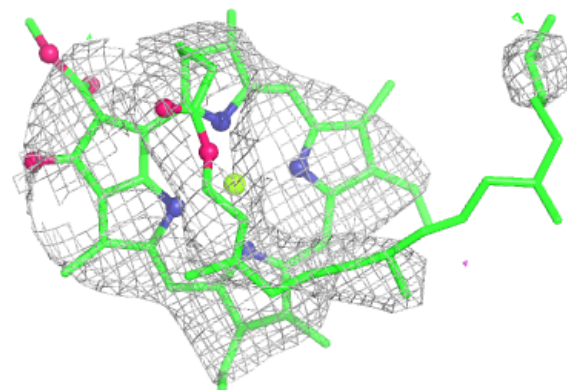


Electron density around CLA a 819:

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

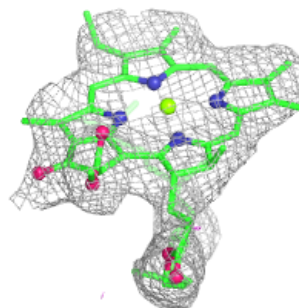
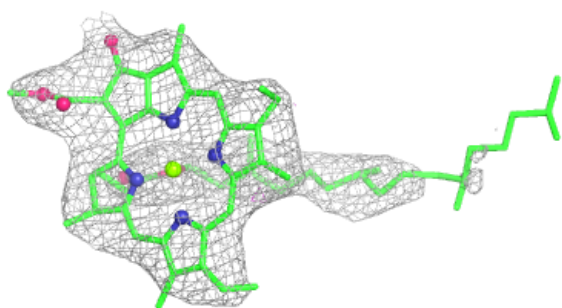
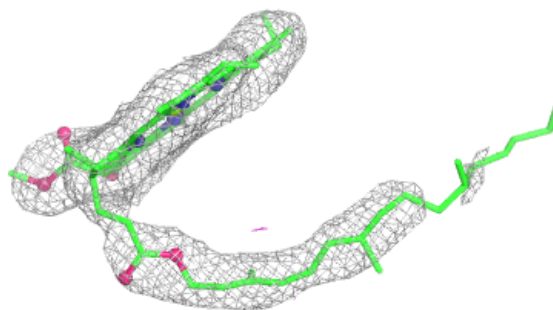
**Electron density around CLA 2 612:**

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

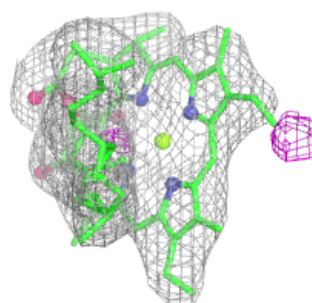
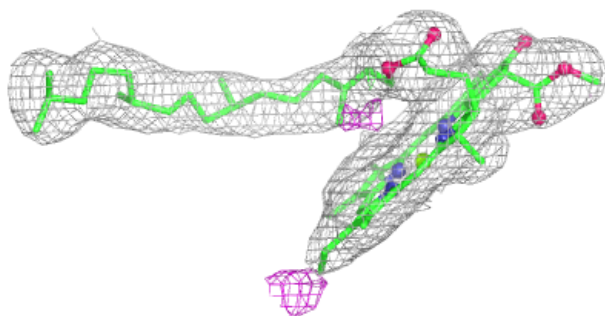
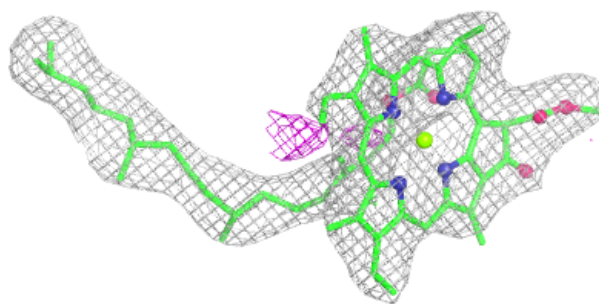


Electron density around CLA A 833:

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

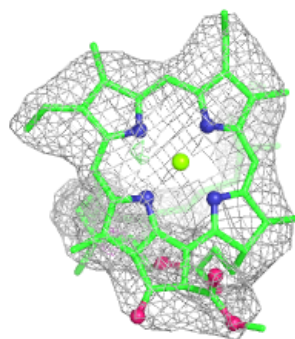
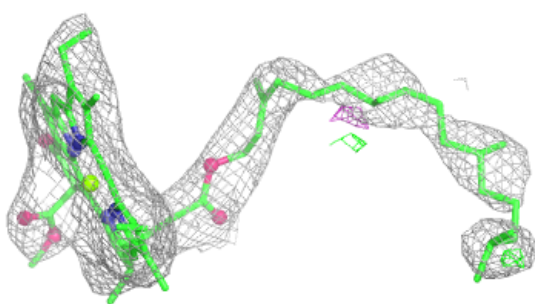
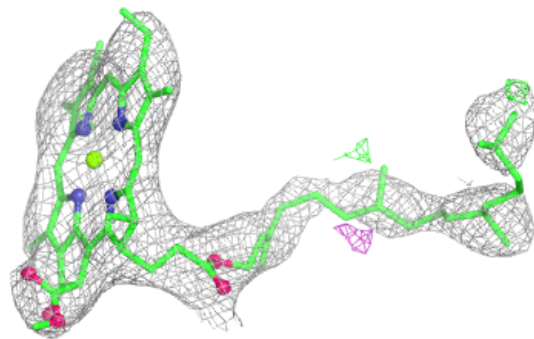
**Electron density around CLA a 843:**

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

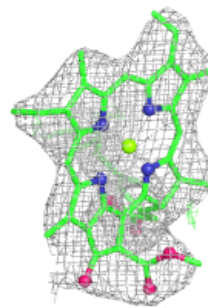
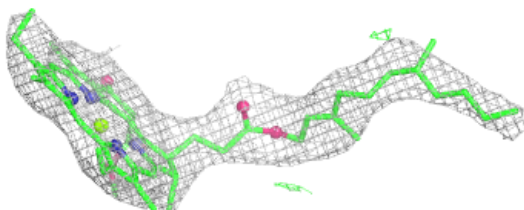
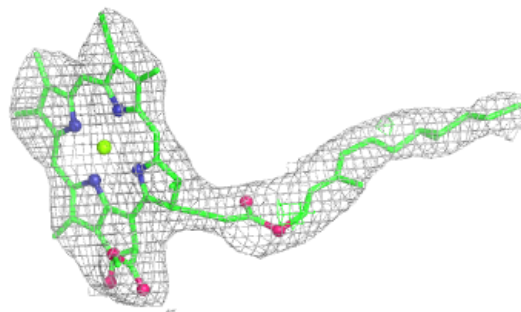


Electron density around CLA L 203:

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

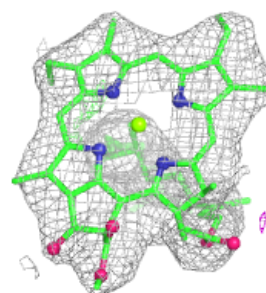
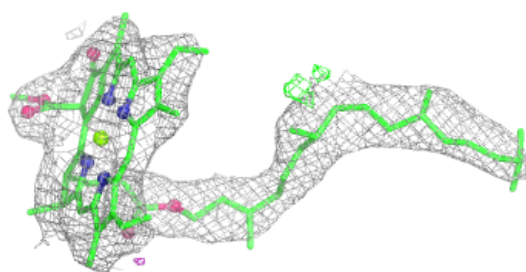
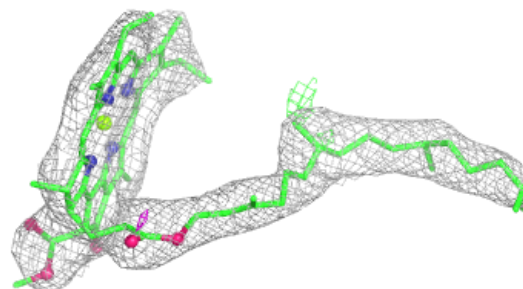
**Electron density around CLA B 833:**

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

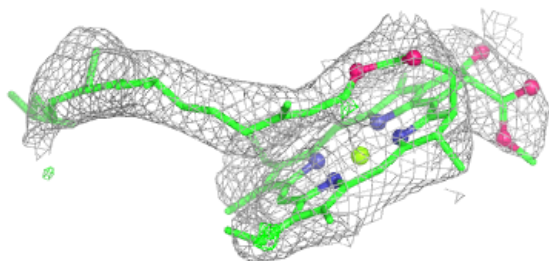
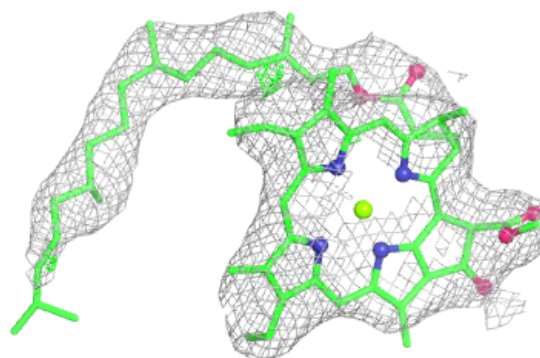


Electron density around CLA A 812:

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

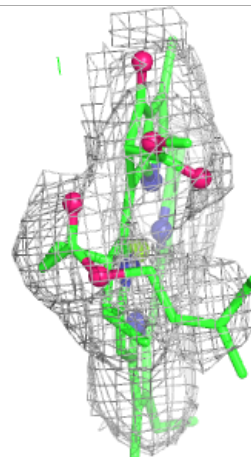
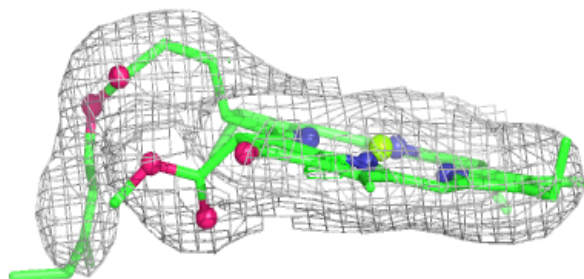
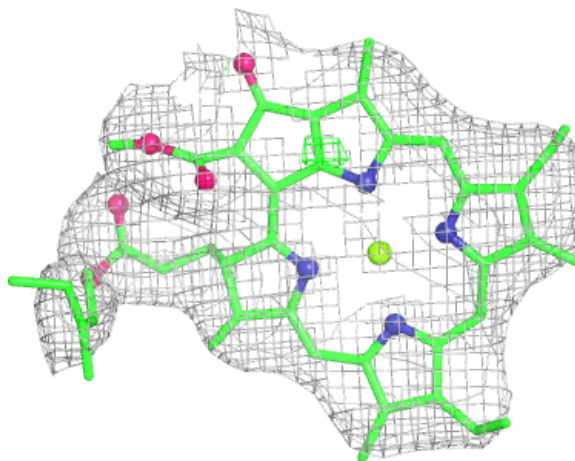
**Electron density around CLA 7 602:**

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



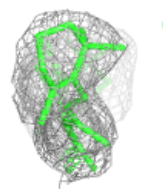
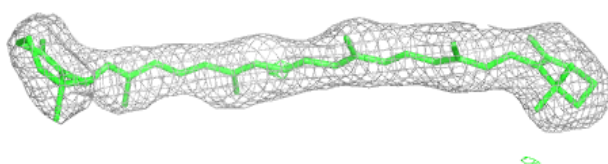
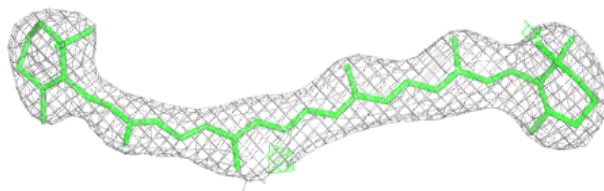
Electron density around CLA 7 603:

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



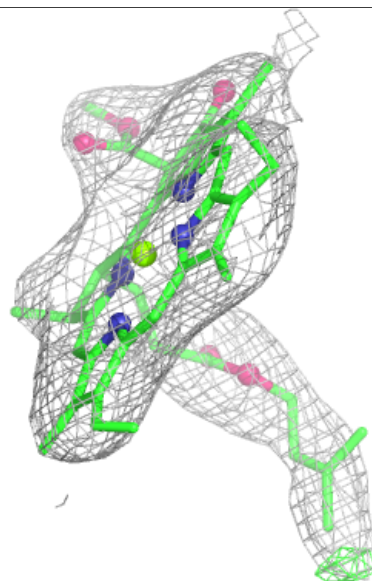
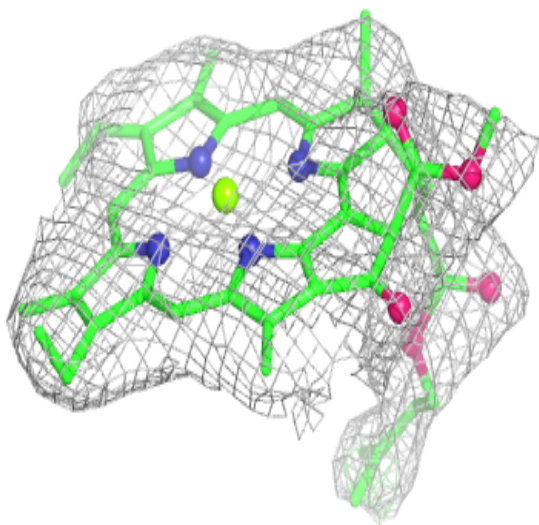
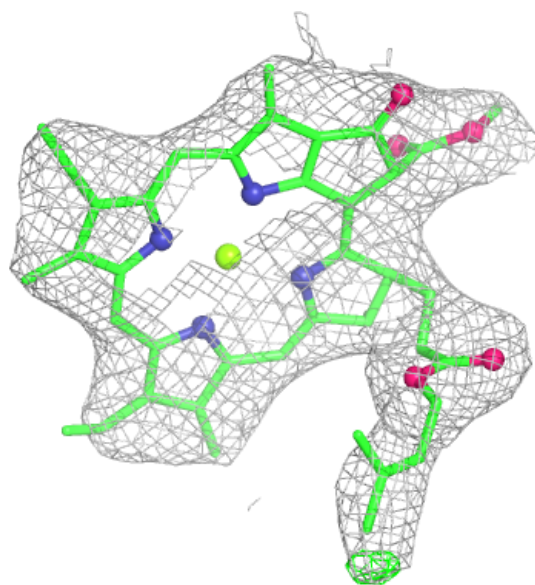
Electron density around BCR B 847:

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



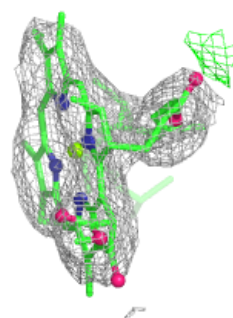
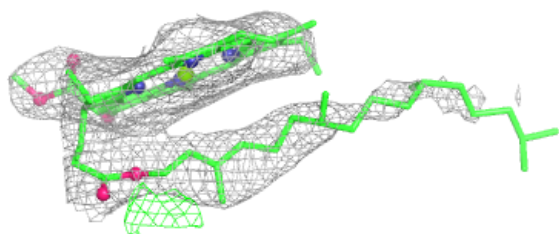
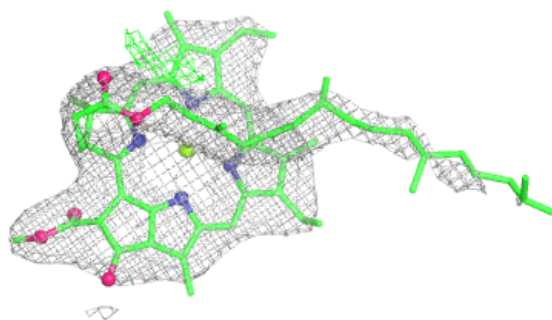
Electron density around CLA 4 608:

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

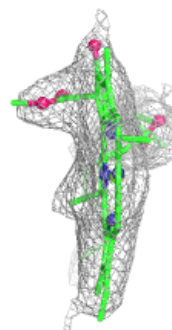
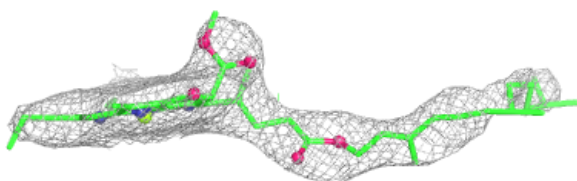
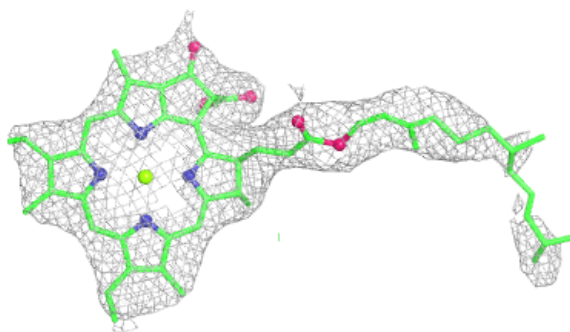


Electron density around CLA A 819:

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

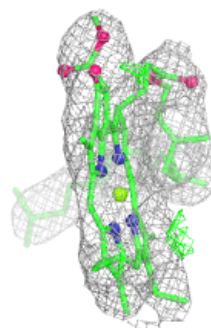
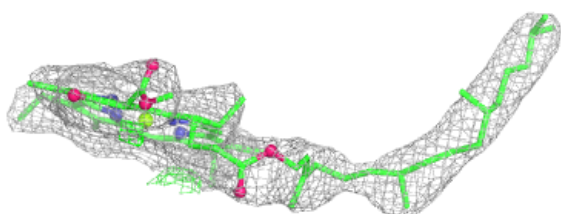
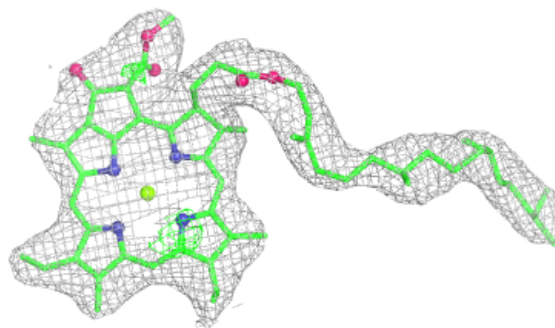
**Electron density around CLA B 836:**

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

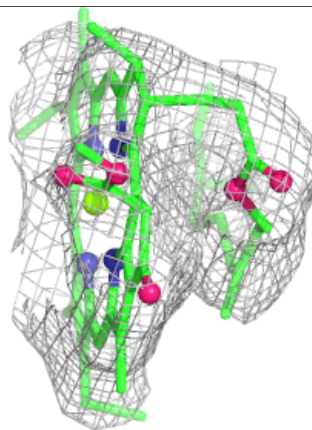
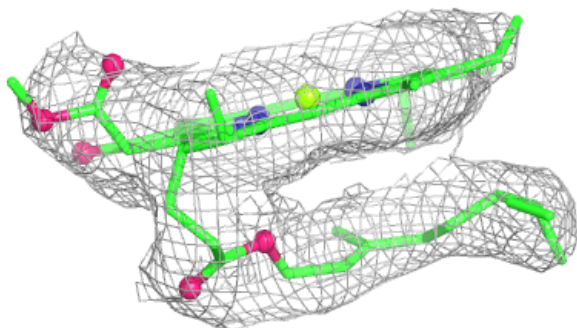
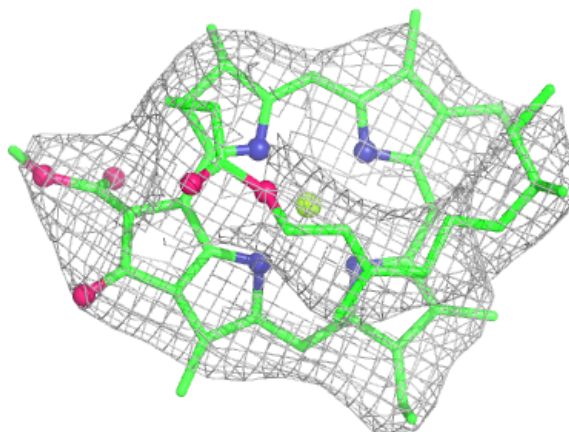


Electron density around CLA B 803:

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

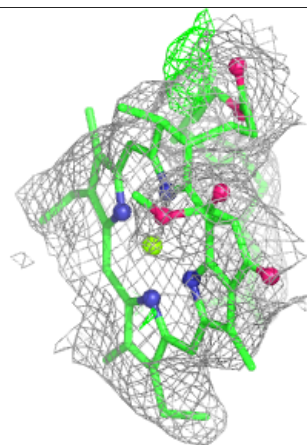
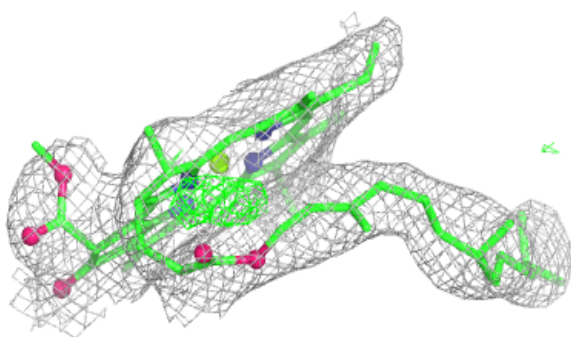
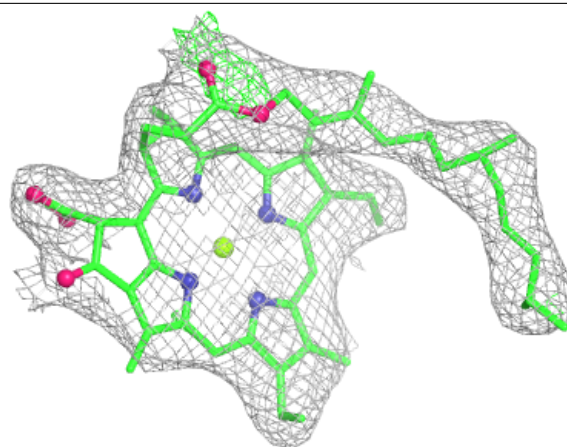
**Electron density around CLA 4 612:**

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



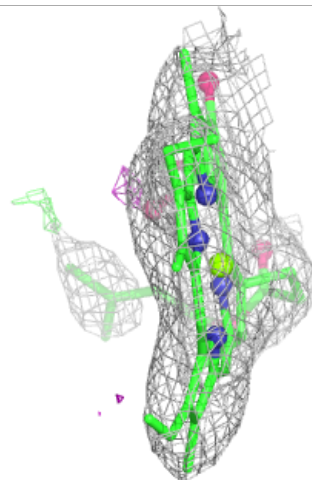
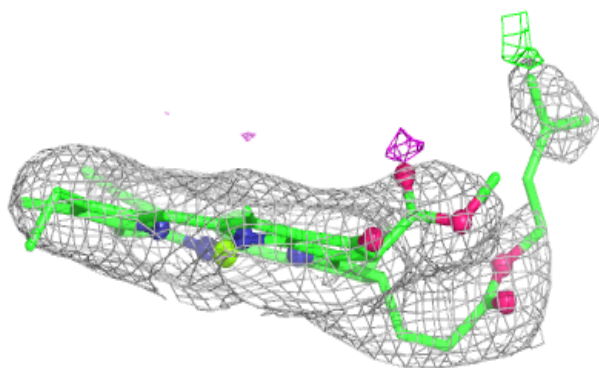
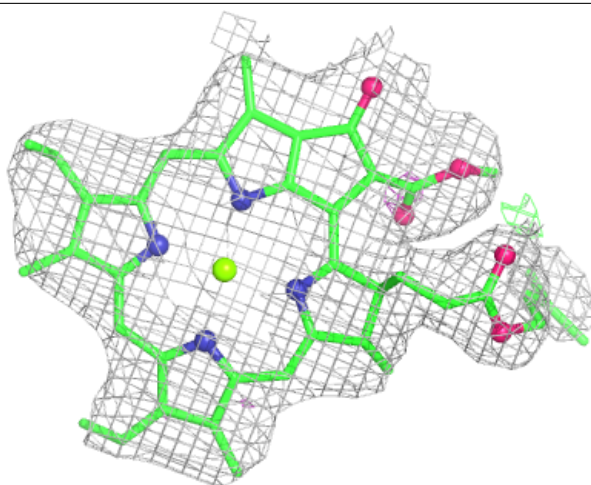
Electron density around CLA 3 302:

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



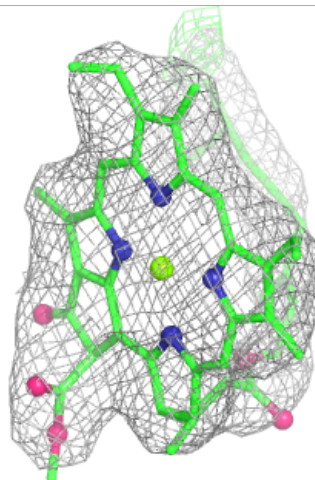
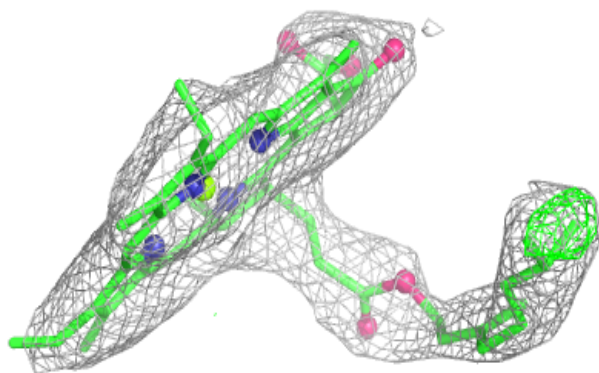
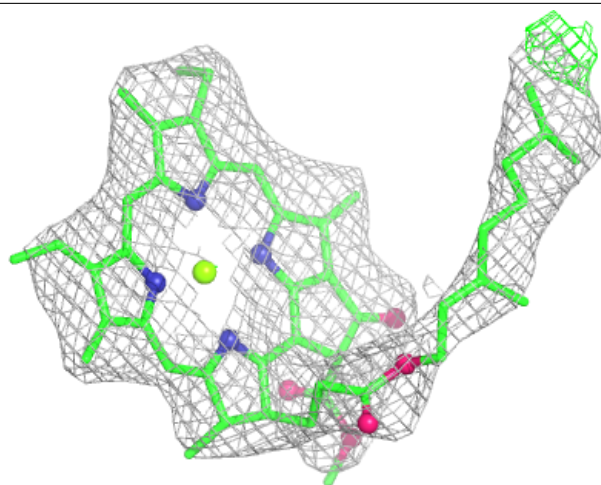
Electron density around CLA 8 302:

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



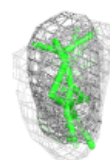
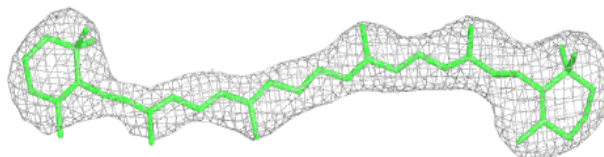
Electron density around CLA b 822:

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

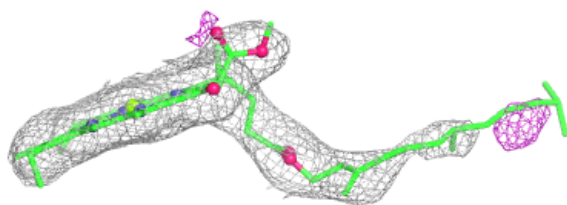
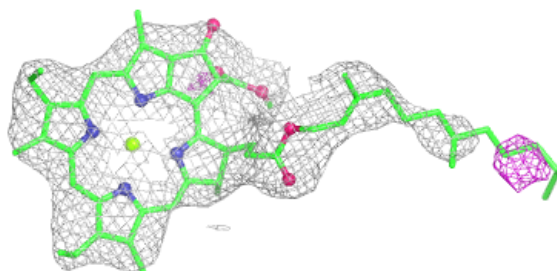


Electron density around BCR L 205:

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

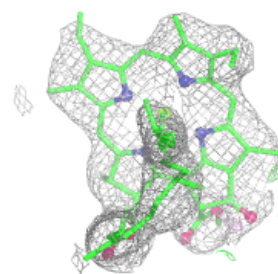
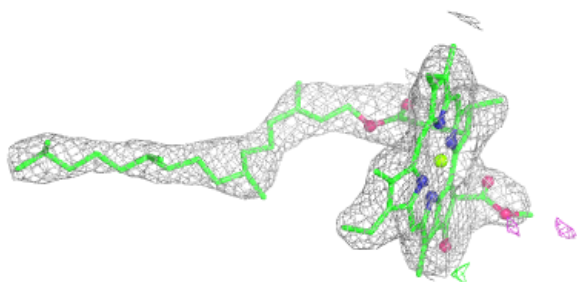
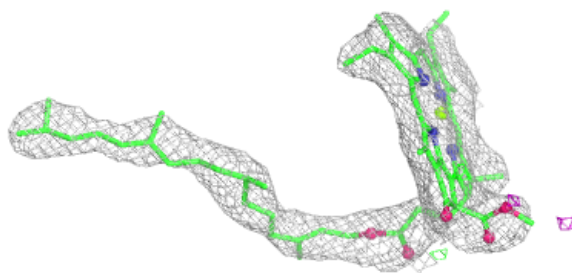
**Electron density around CLA b 823:**

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



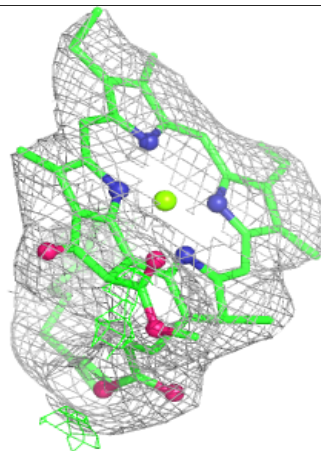
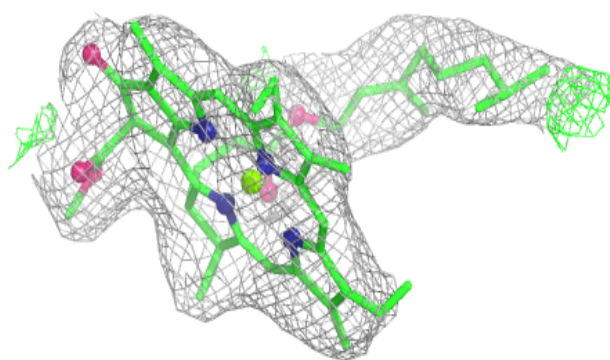
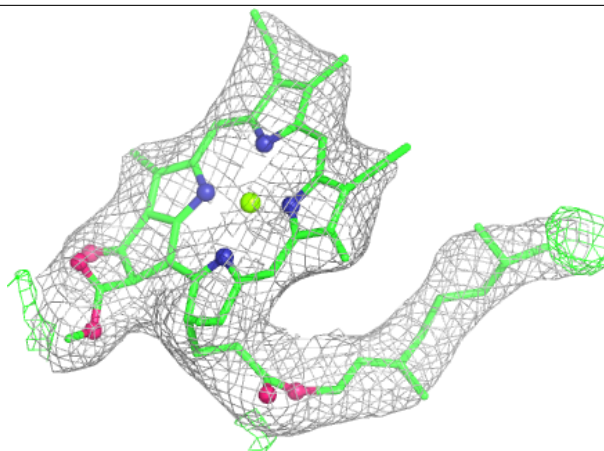
Electron density around CLA b 829:

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



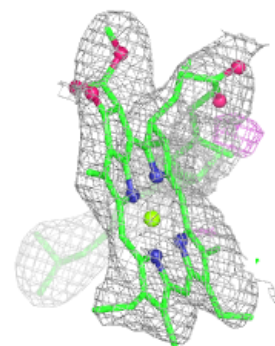
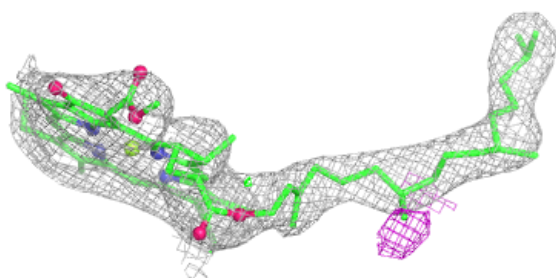
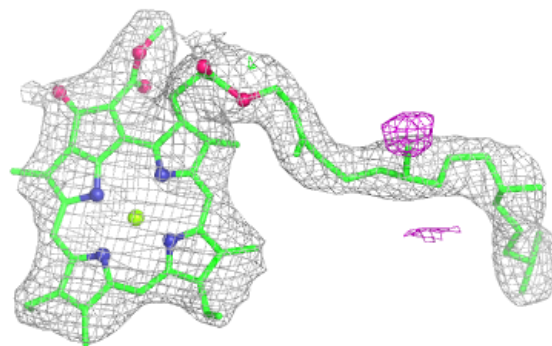
Electron density around CLA A 825:

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

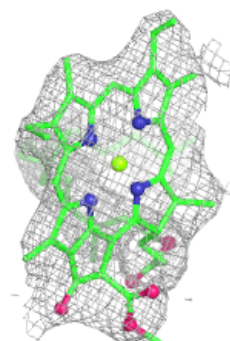
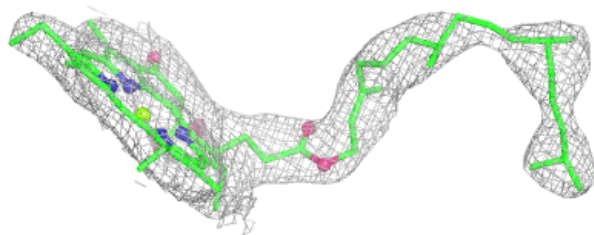
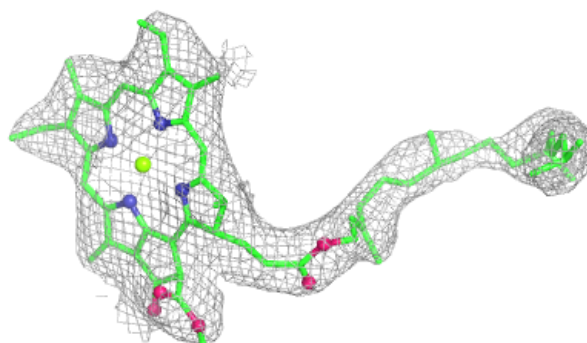


Electron density around CLA a 802:

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

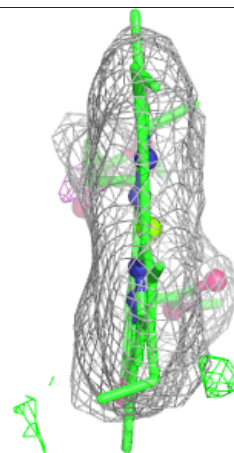
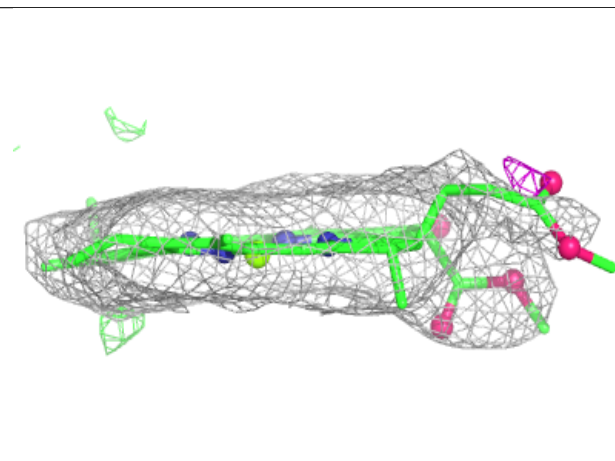
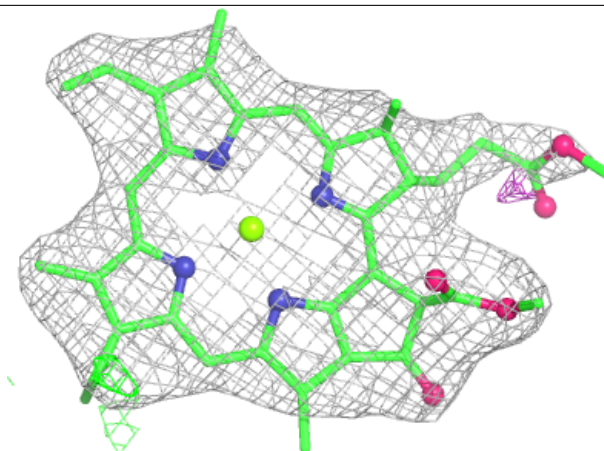
**Electron density around CLA B 809:**

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



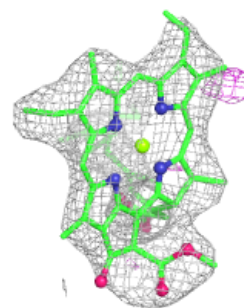
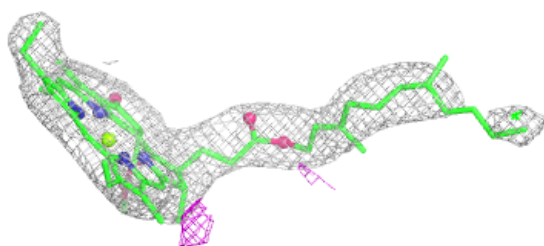
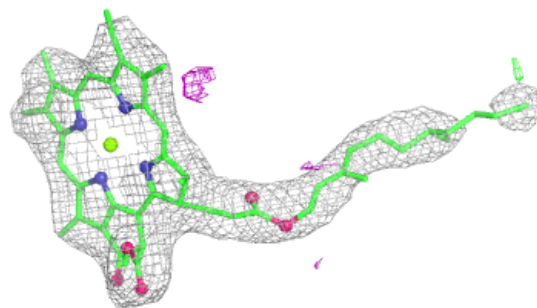
Electron density around CLA 8 312:

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

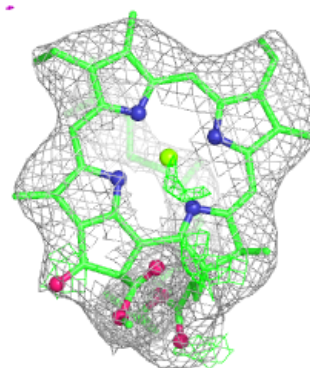
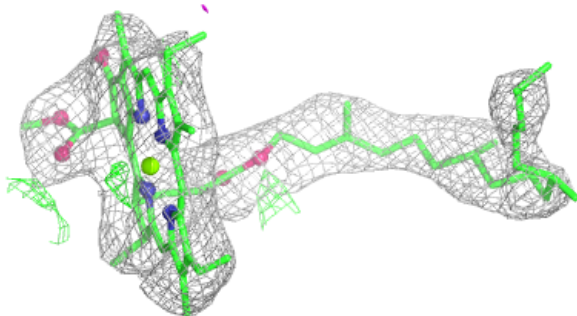
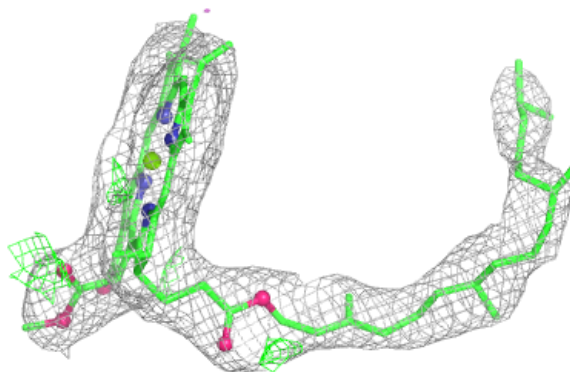


Electron density around CLA b 833:

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

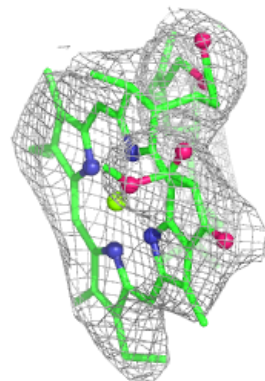
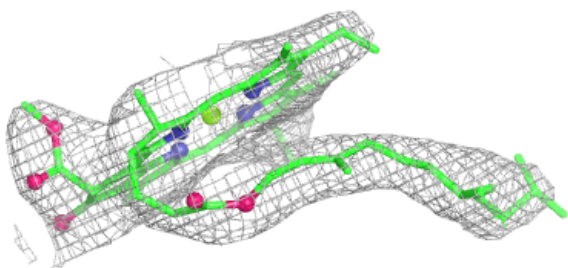
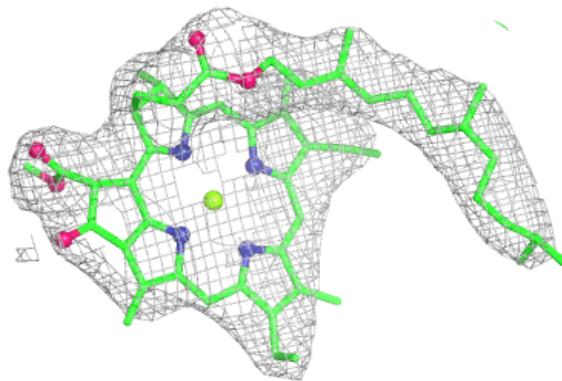
**Electron density around CLA a 808:**

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



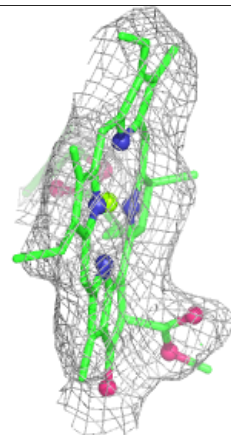
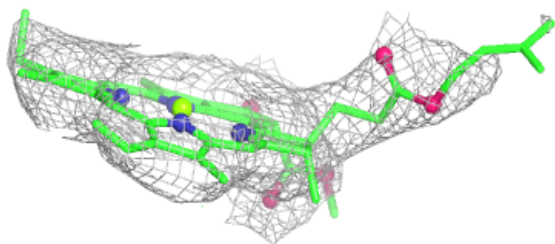
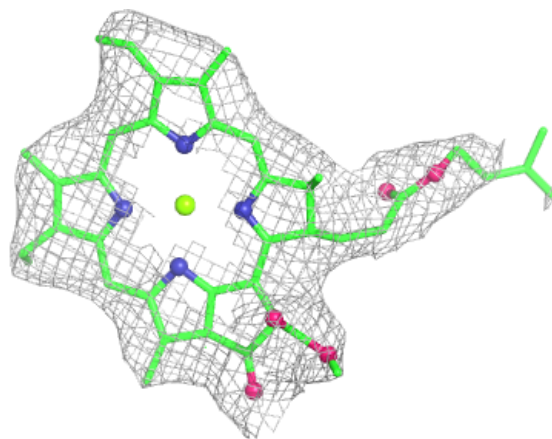
Electron density around CLA 9 602:

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



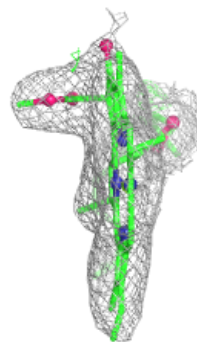
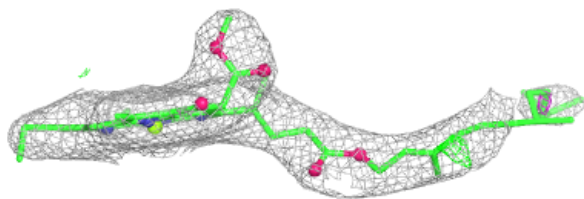
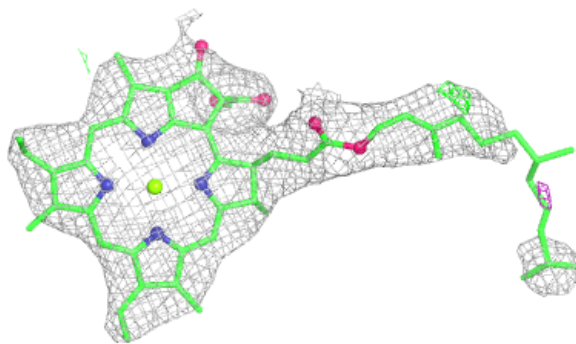
Electron density around CLA G 103:

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



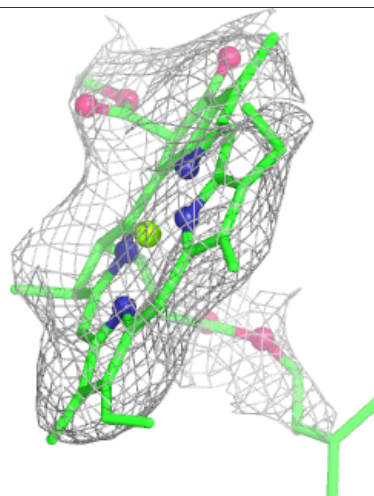
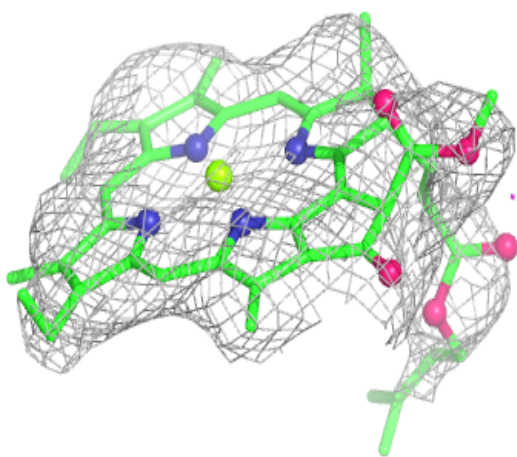
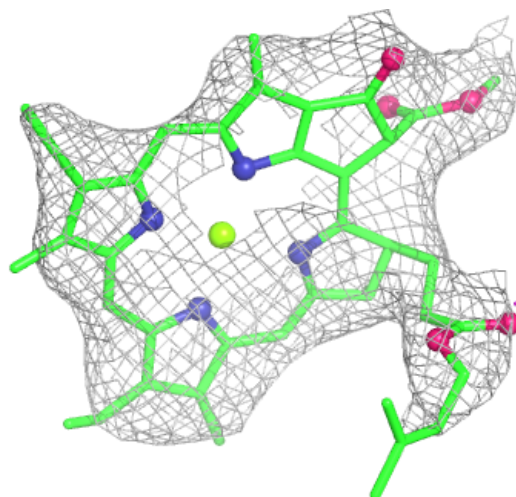
Electron density around CLA b 836:

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



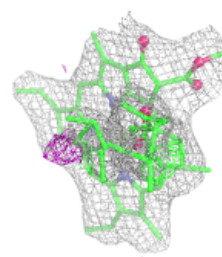
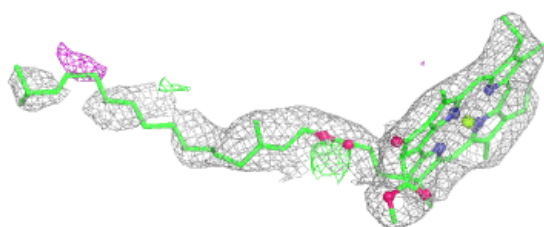
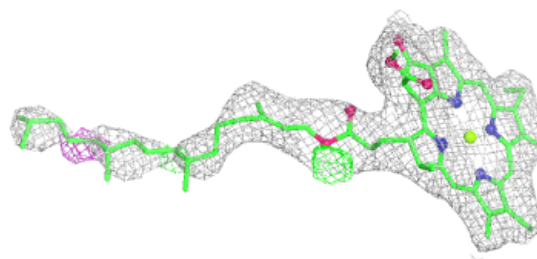
Electron density around CLA 9 608:

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

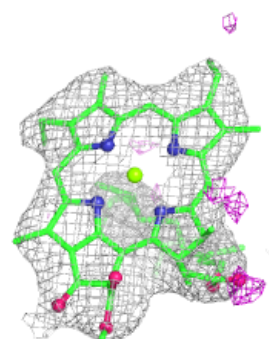
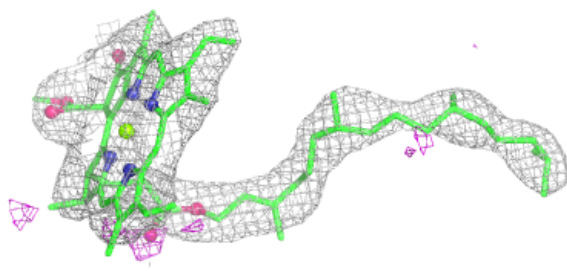
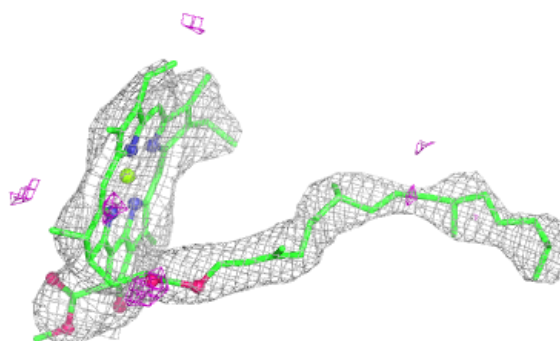


Electron density around CLA a 810:

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

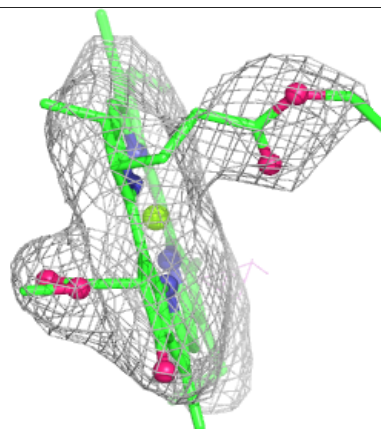
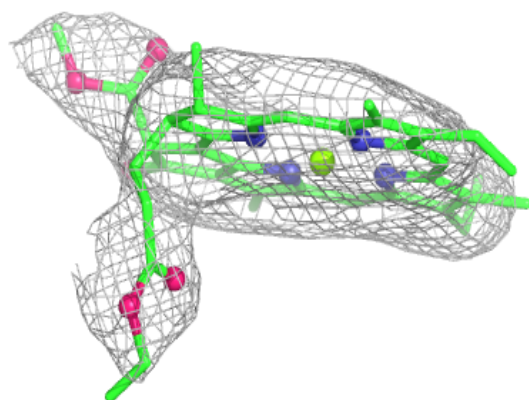
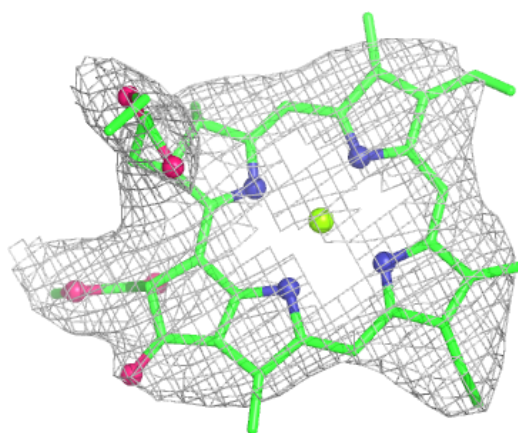
**Electron density around CLA a 812:**

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

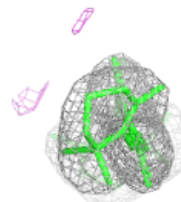
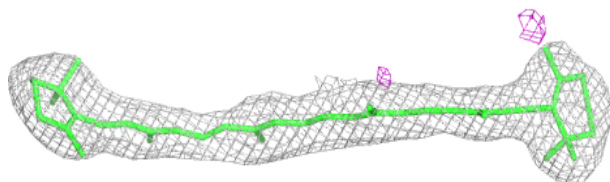
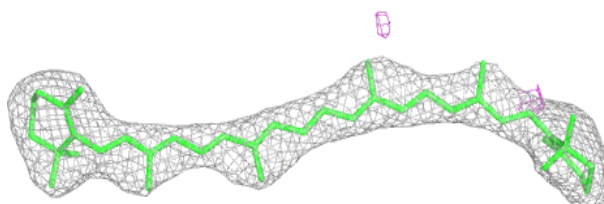


Electron density around CLA 3 306:

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

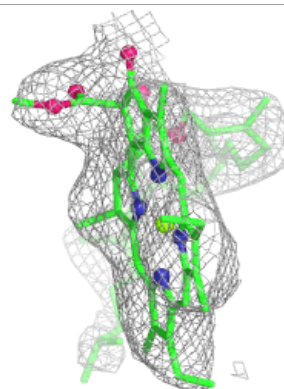
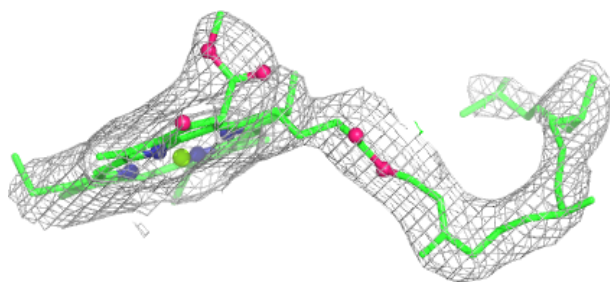
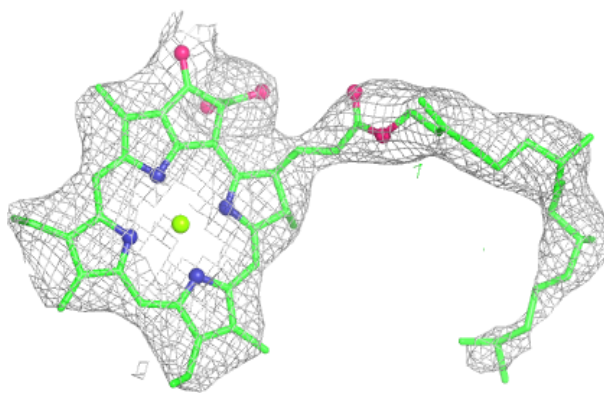
**Electron density around BCR b 848:**

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

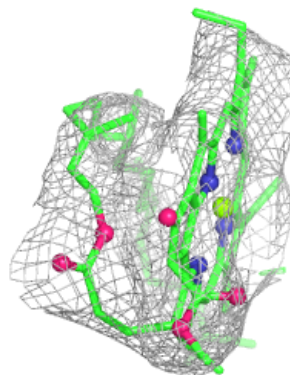
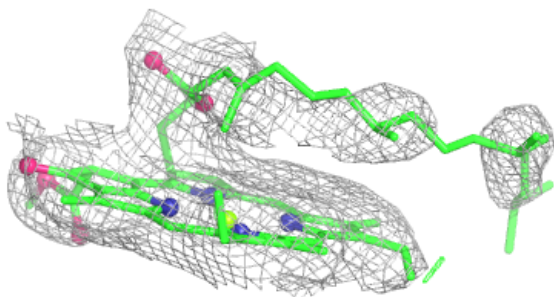
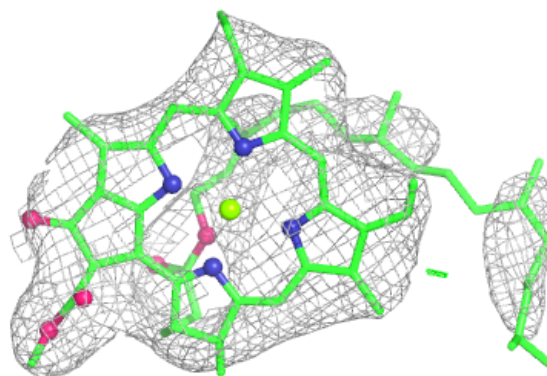


Electron density around CLA A 828:

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

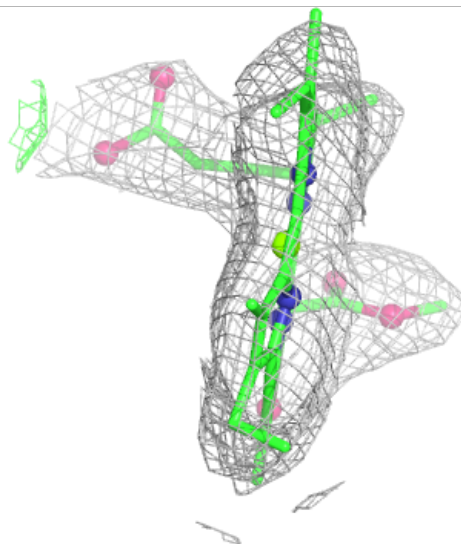
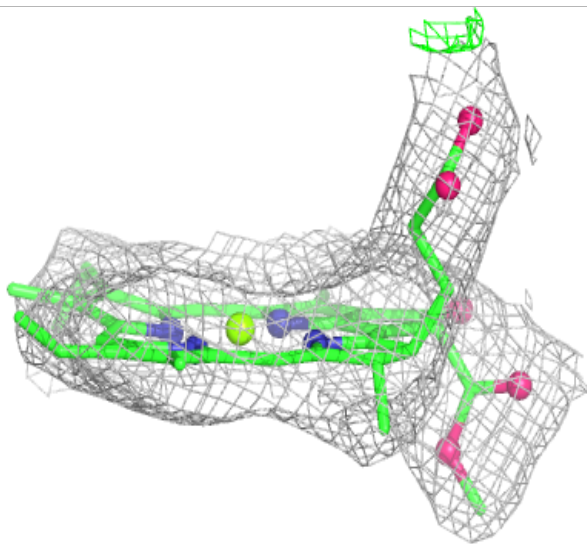
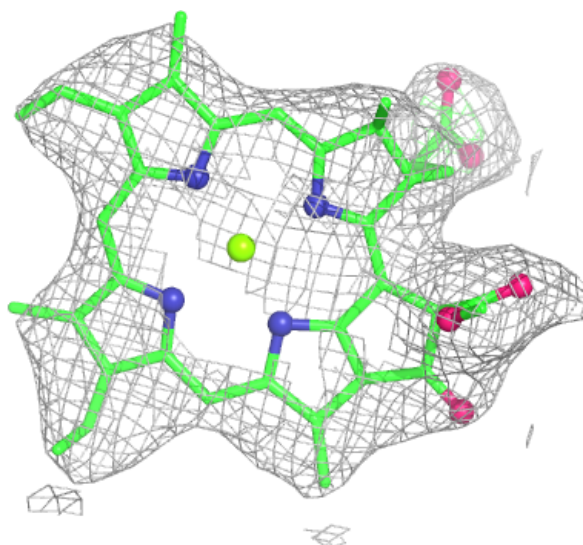
**Electron density around CLA 1 313:**

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



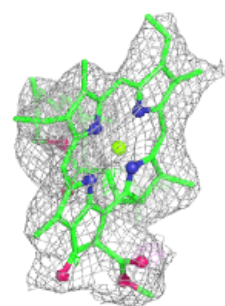
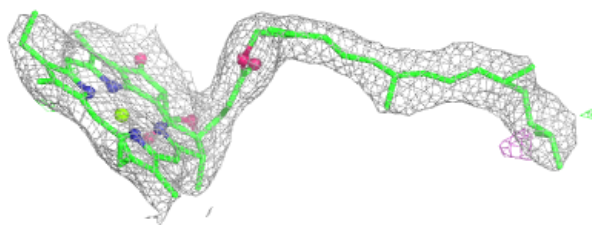
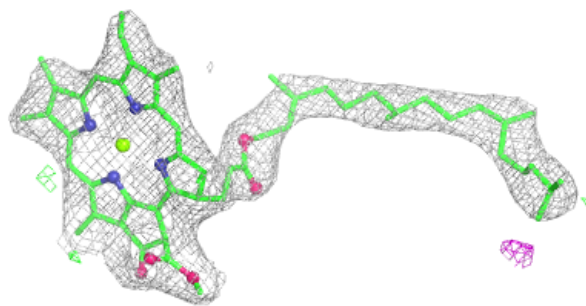
Electron density around CLA a 821:

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



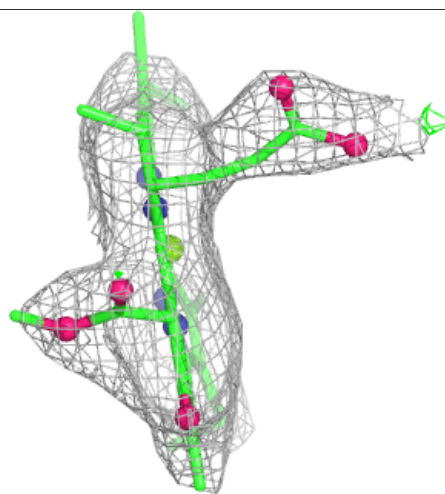
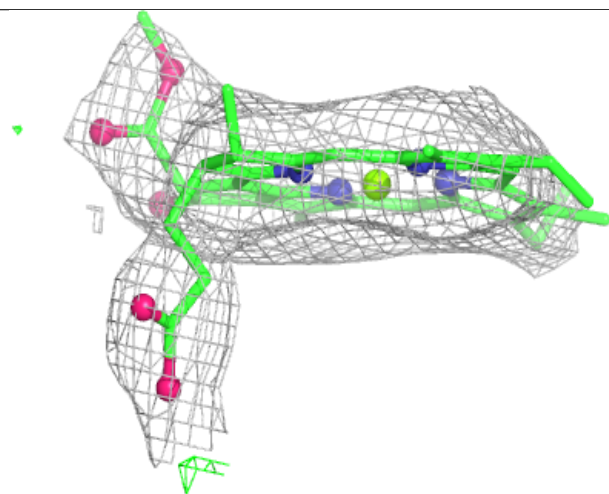
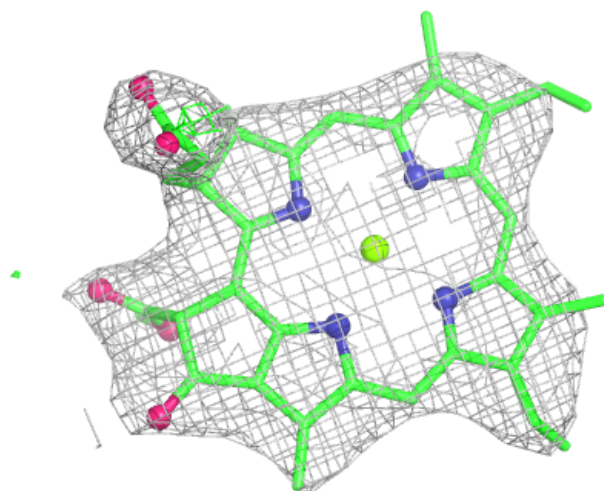
Electron density around CLA a 822:

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



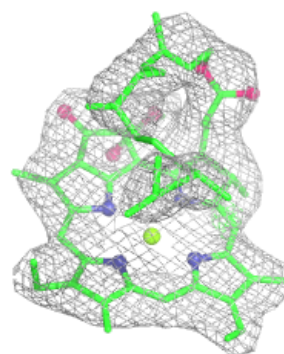
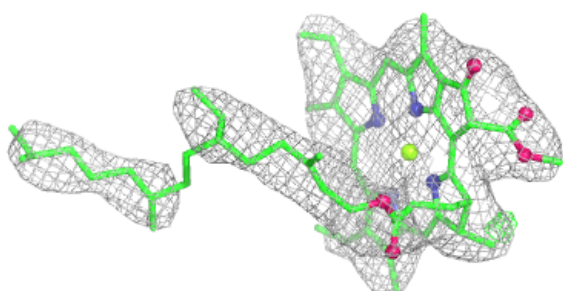
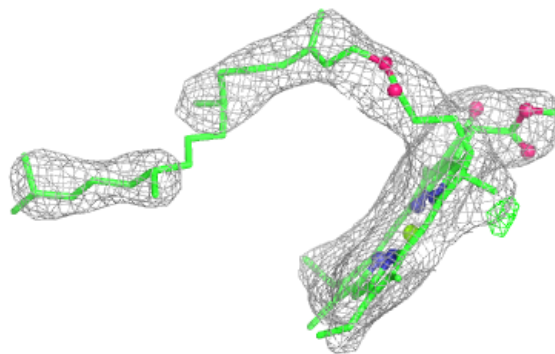
Electron density around CLA A 821:

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

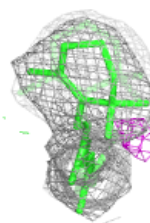
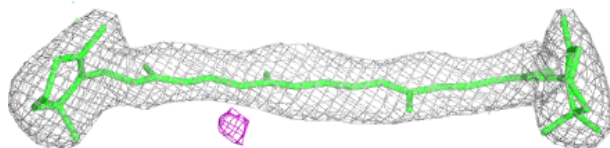
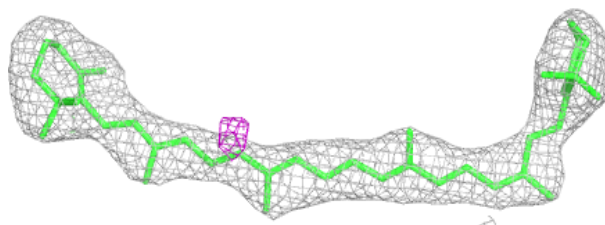


Electron density around CLA A 811:

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

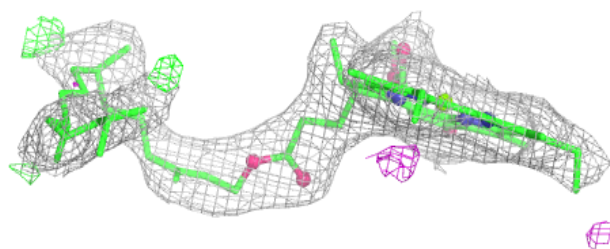
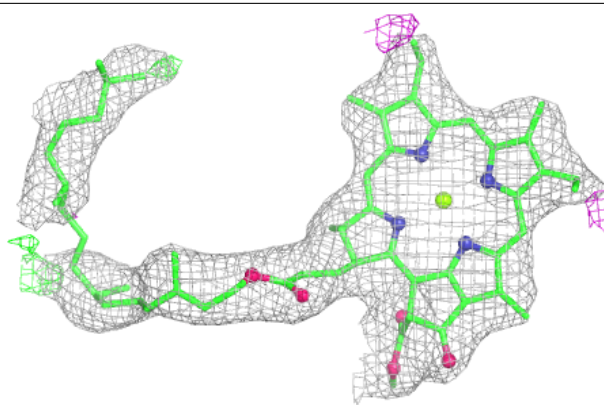
**Electron density around BCR 1 201:**

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

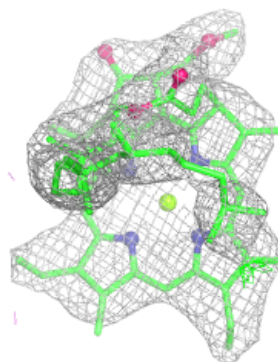
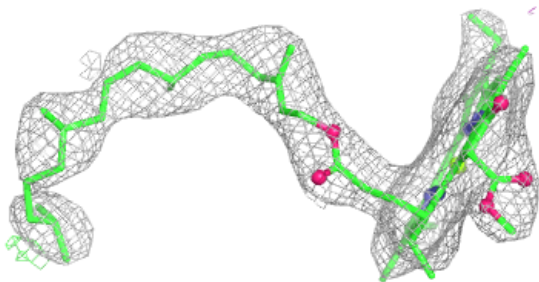
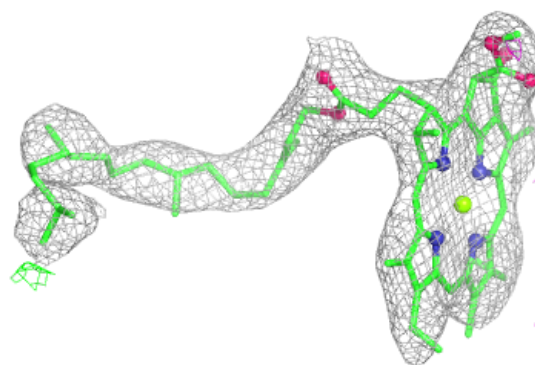


Electron density around CLA a 827:

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

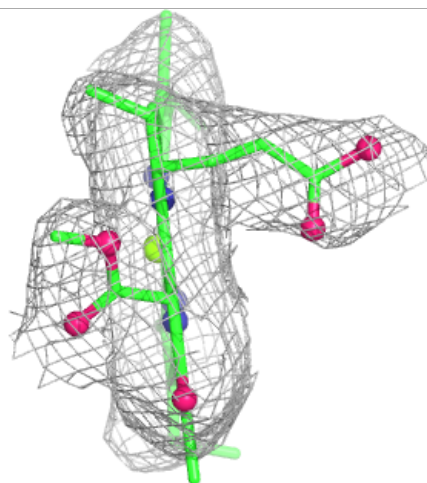
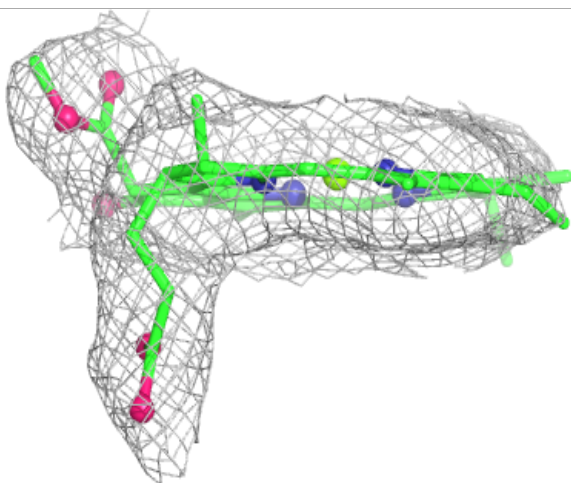
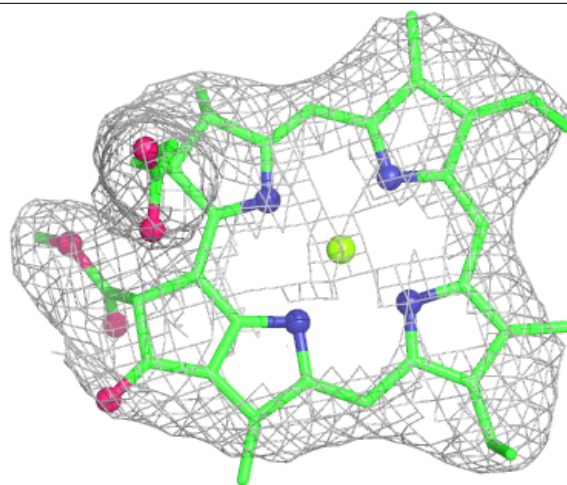
**Electron density around CLA 1 203:**

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



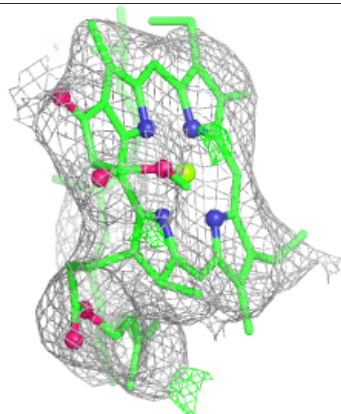
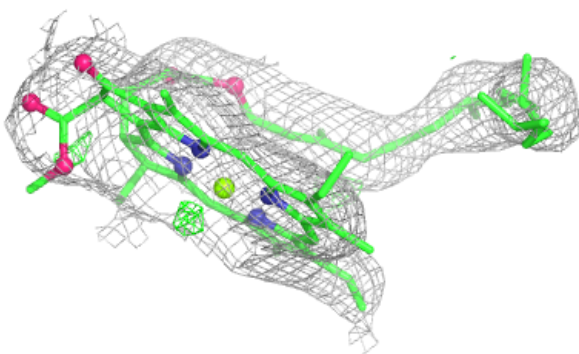
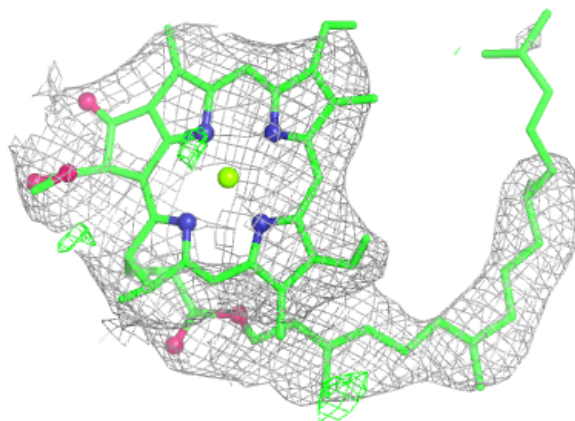
Electron density around CLA a 837:

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

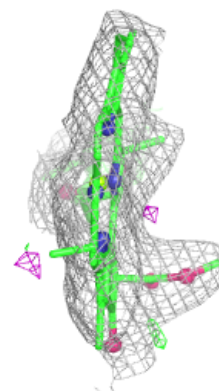
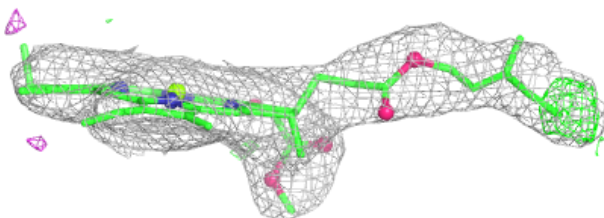
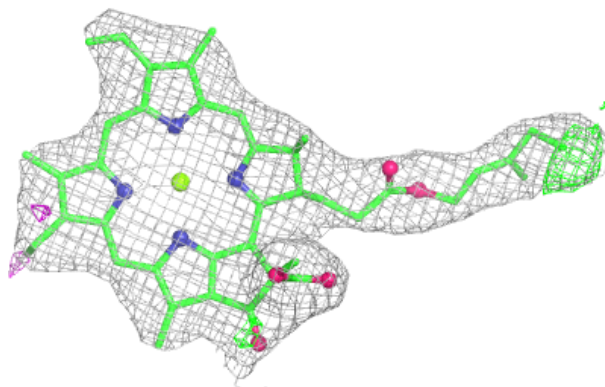


Electron density around CLA 6 304:

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

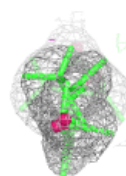
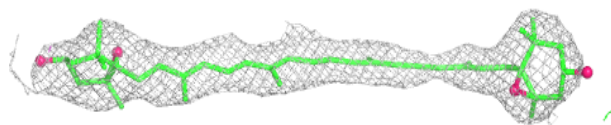
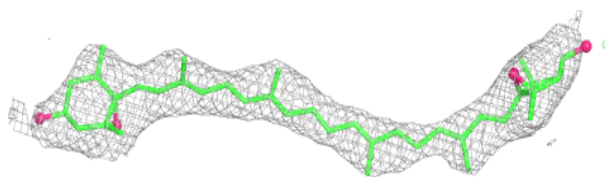
**Electron density around CLA a 838:**

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

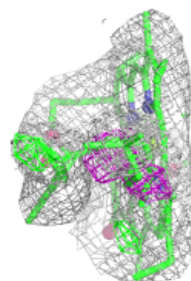
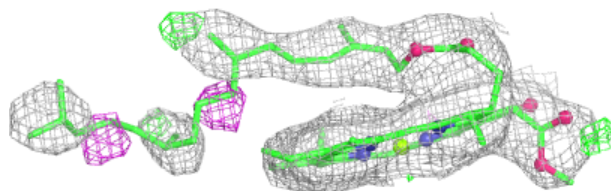
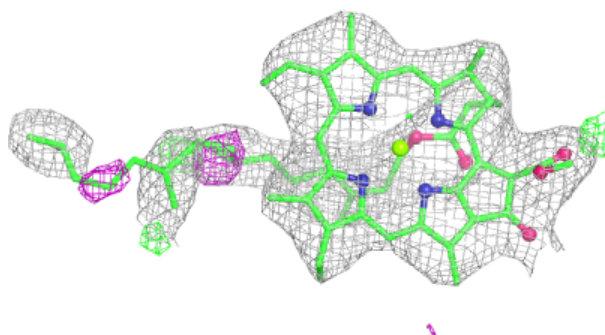


Electron density around XAT 1 317:

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

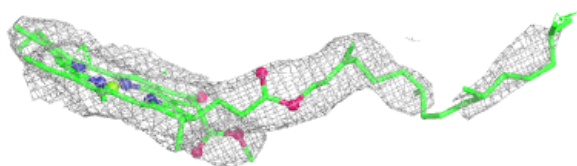
**Electron density around CLA a 839:**

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

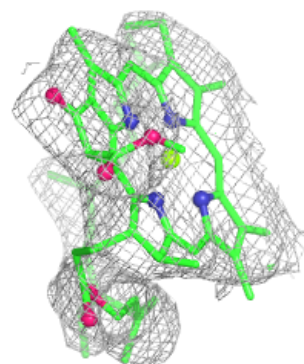
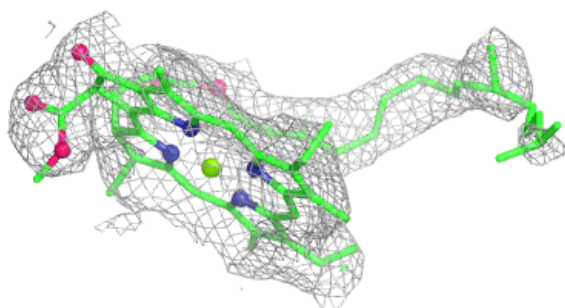
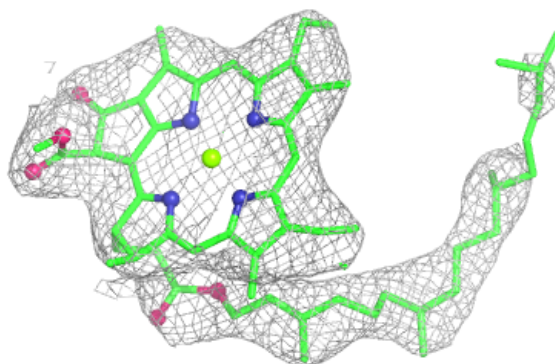


Electron density around CLA a 842:

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

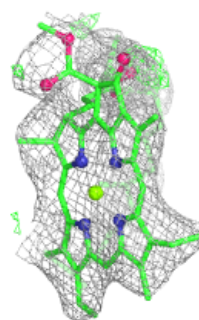
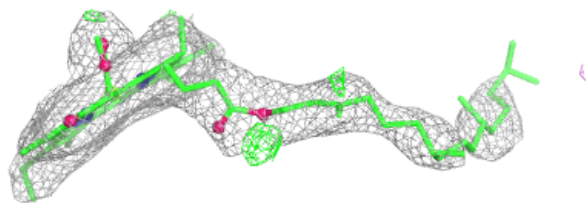
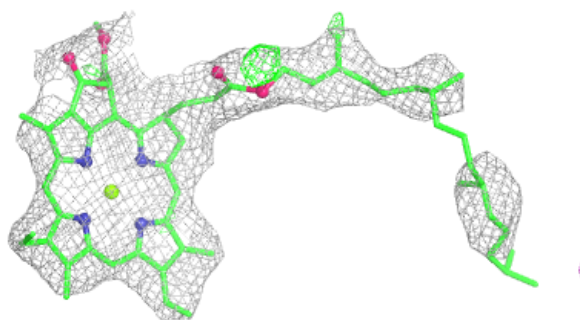
**Electron density around CLA 2 602:**

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

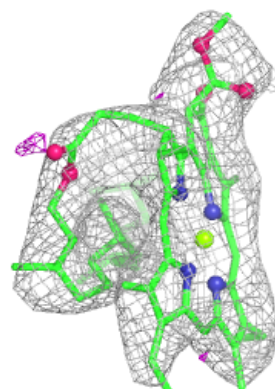
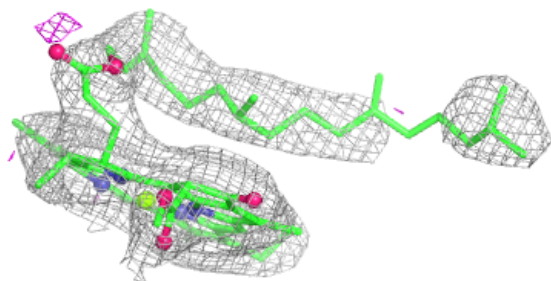
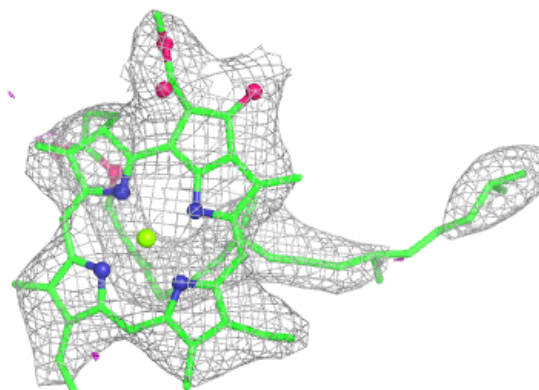


Electron density around CLA B 825:

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

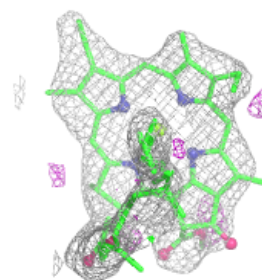
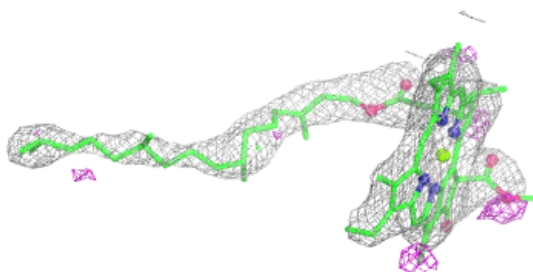
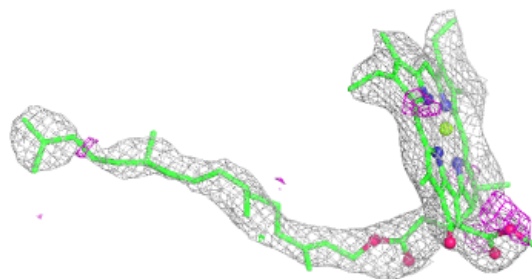
**Electron density around CLA B 827:**

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



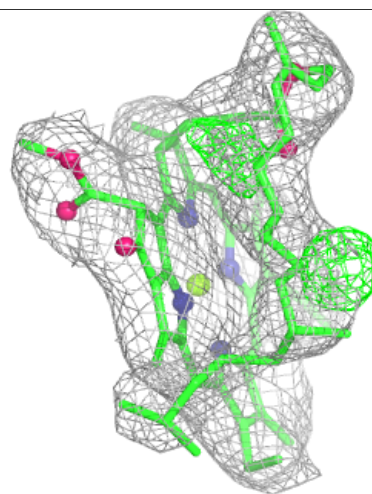
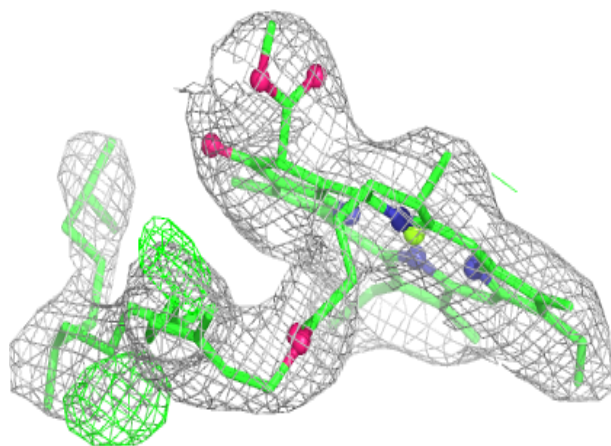
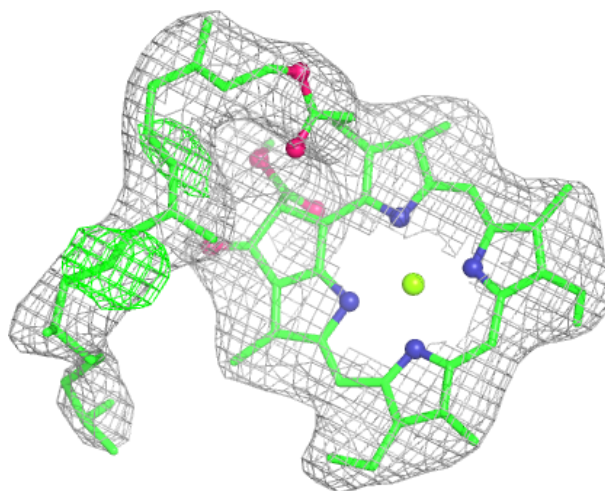
Electron density around CLA B 829:

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



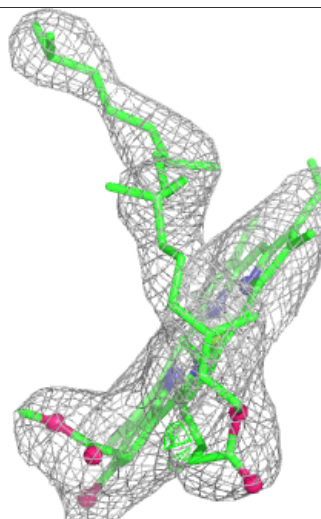
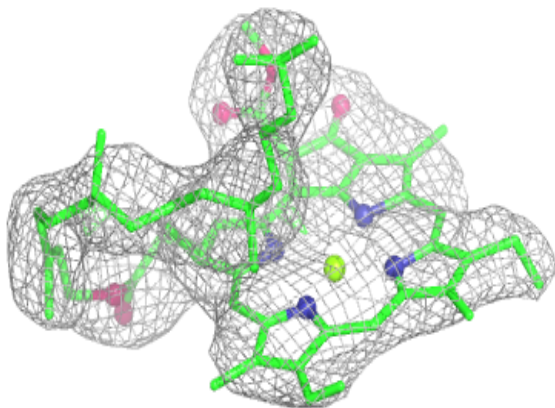
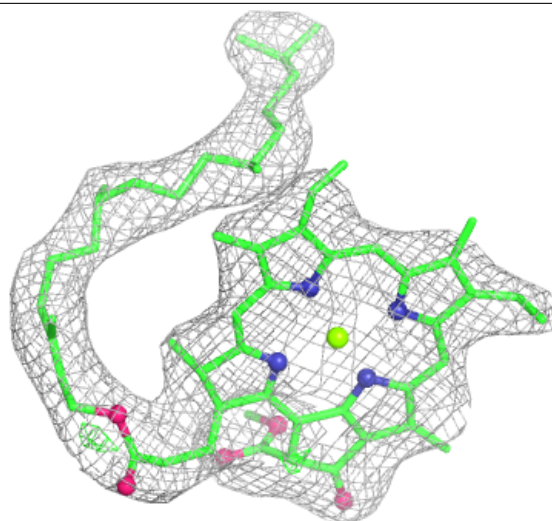
Electron density around CLA B 832:

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



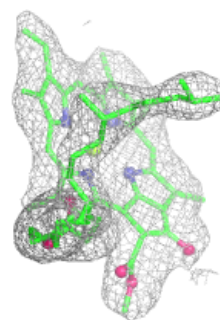
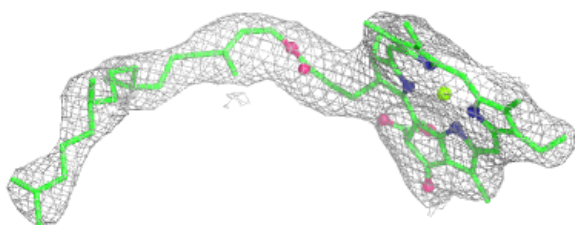
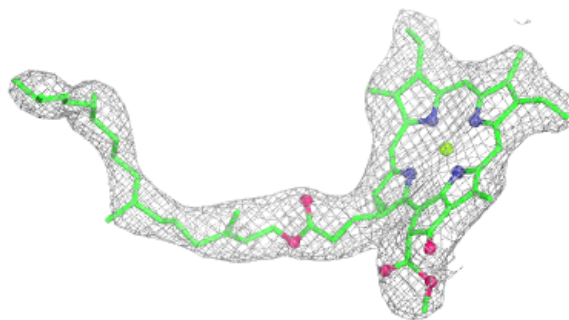
Electron density around CLA A 814:

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

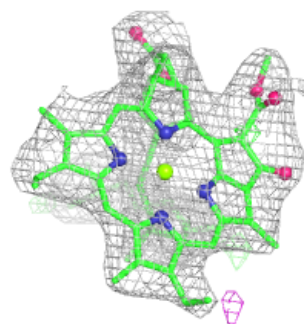
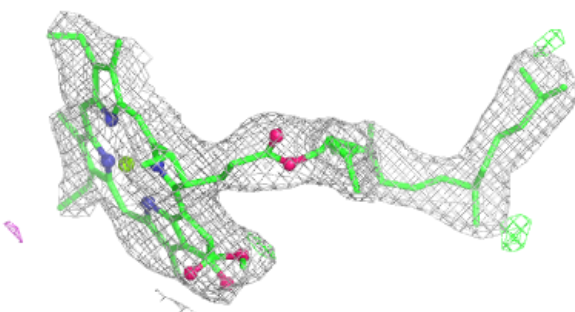
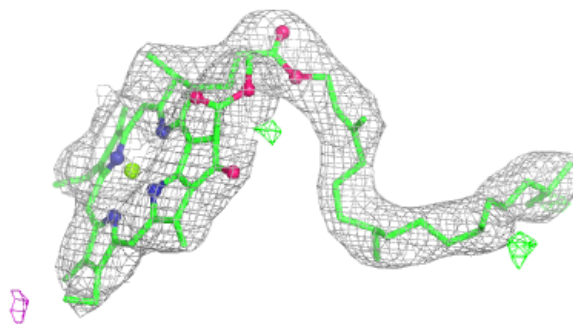


Electron density around CLA A 854:

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

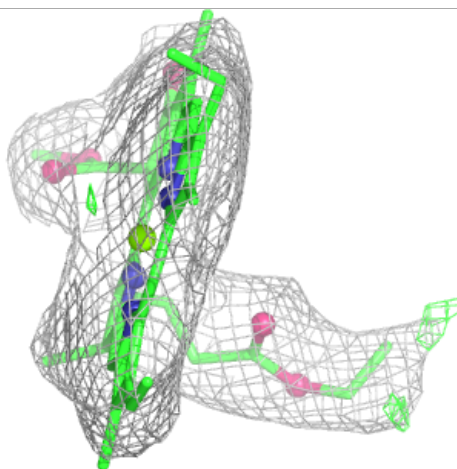
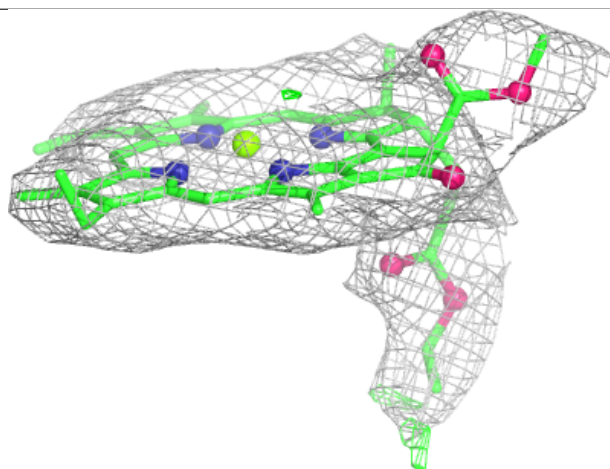
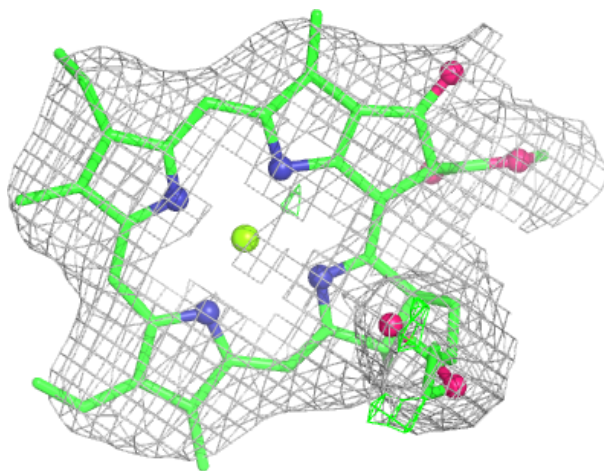
**Electron density around CLA B 802:**

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



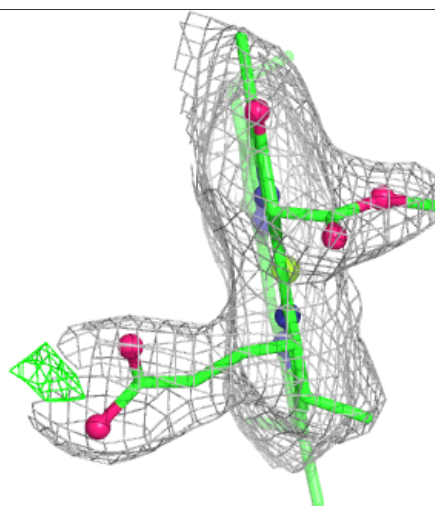
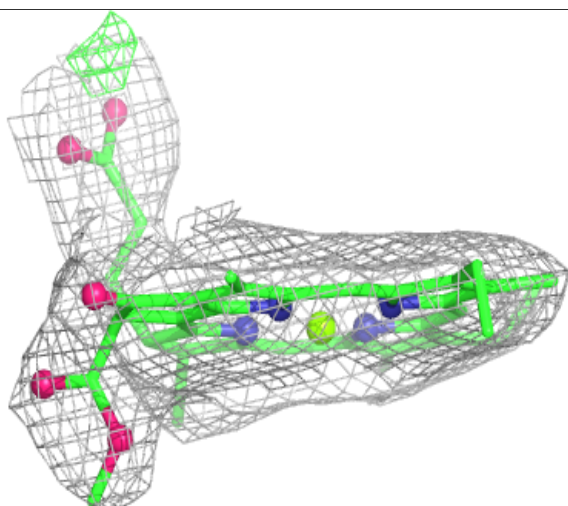
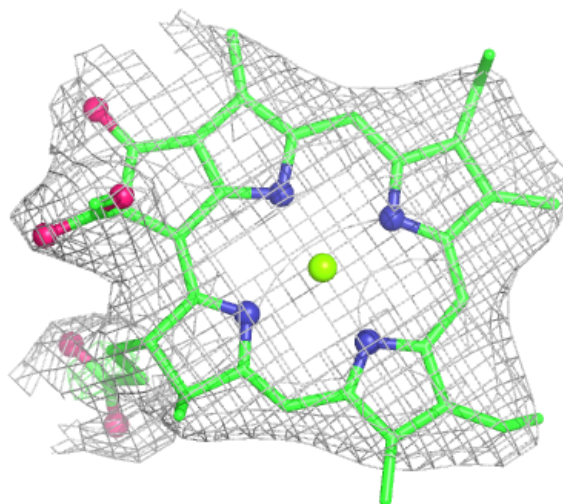
Electron density around CLA 8 305:

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



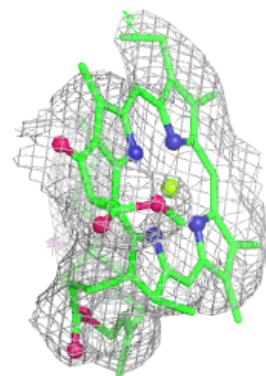
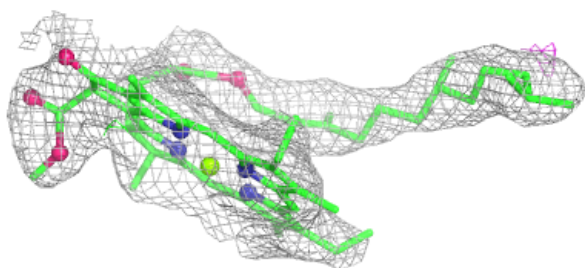
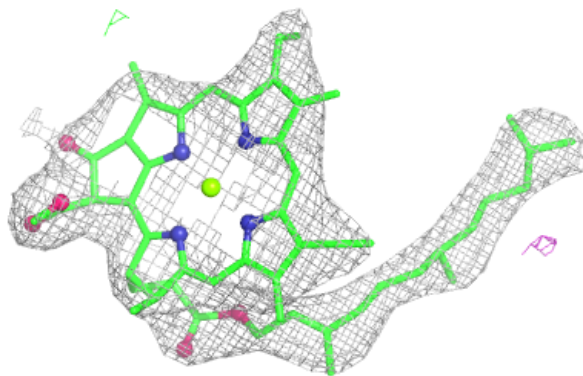
Electron density around CLA A 815:

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



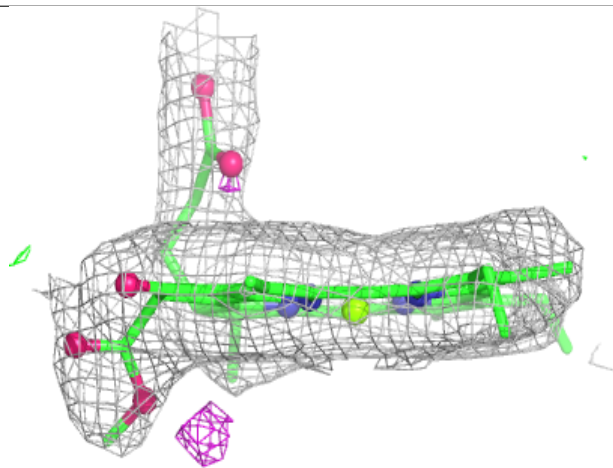
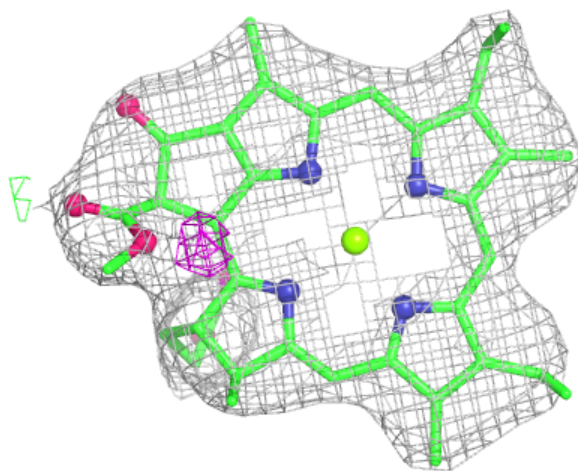
Electron density around CLA 4 602:

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



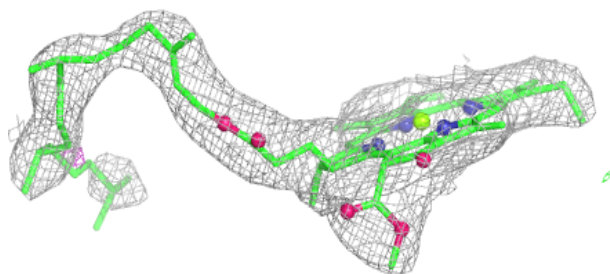
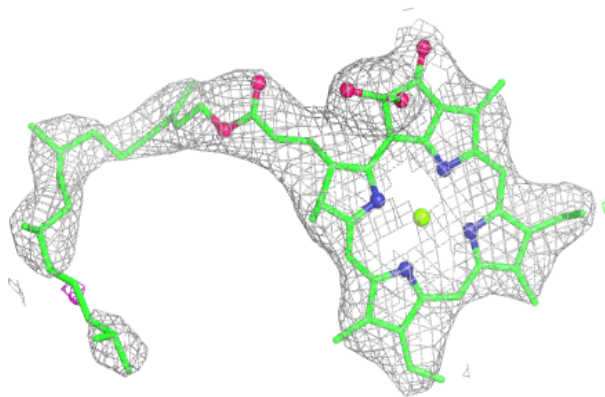
Electron density around CLA B 804:

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

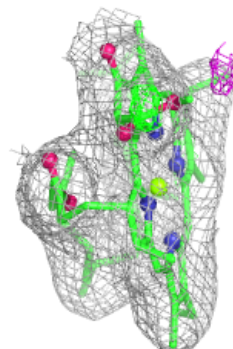
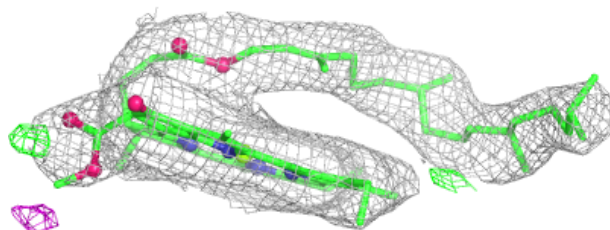
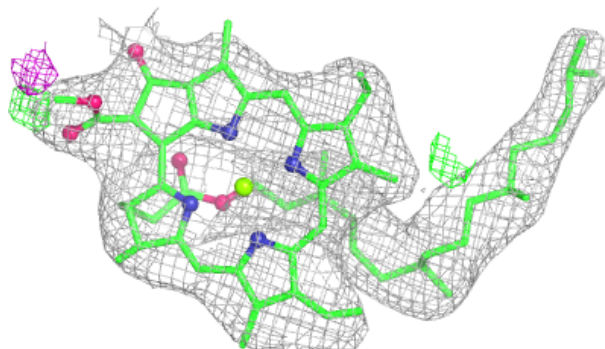


Electron density around CLA a 828:

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

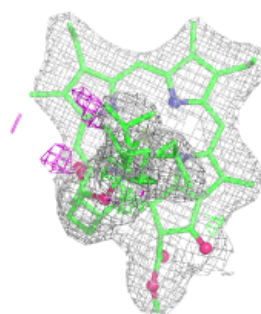
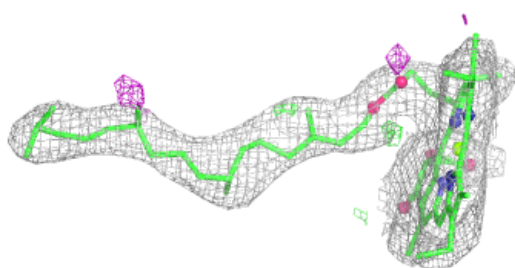
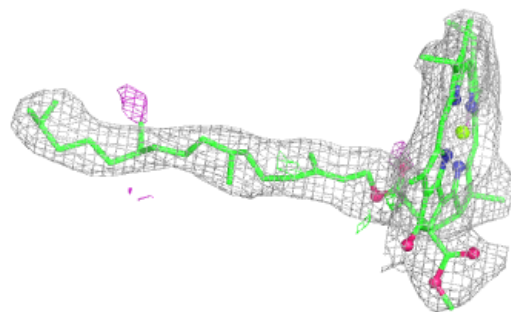
**Electron density around CLA b 837:**

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

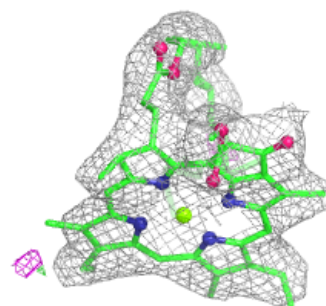
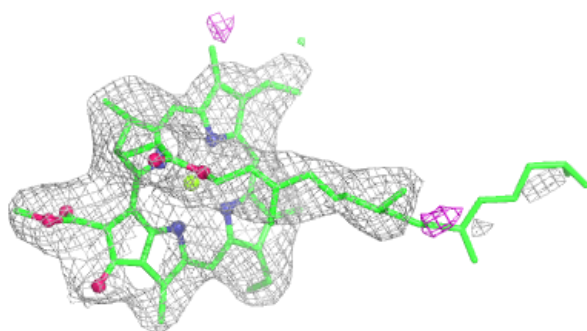
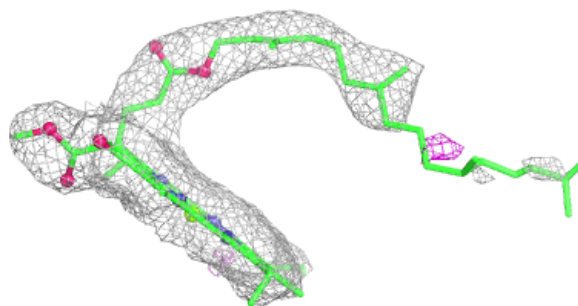


Electron density around CLA a 829:

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

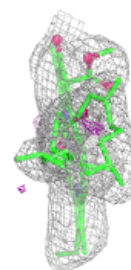
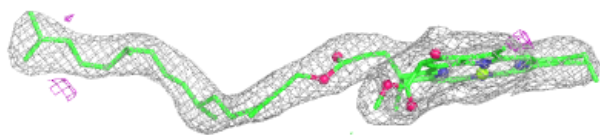
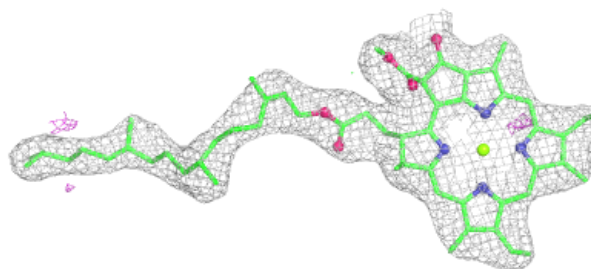
**Electron density around CLA a 833:**

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



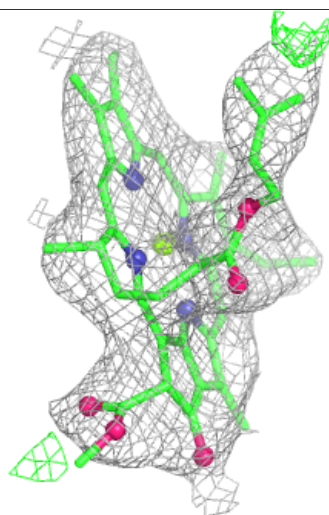
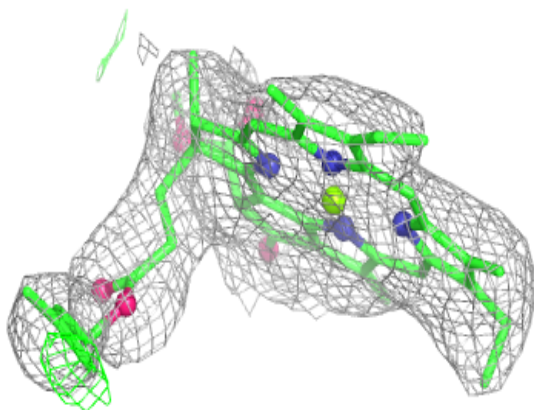
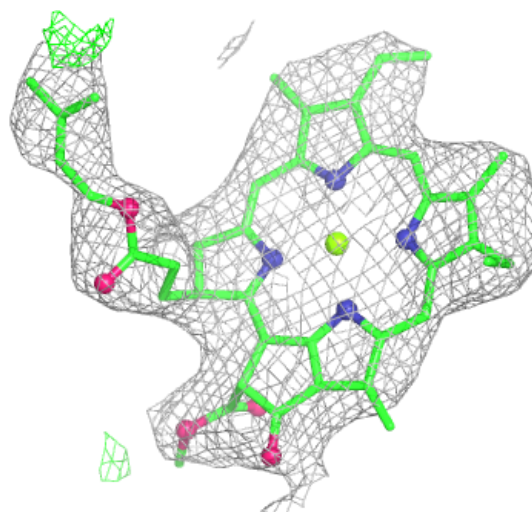
Electron density around CLA a 834:

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



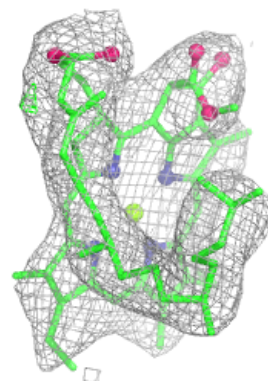
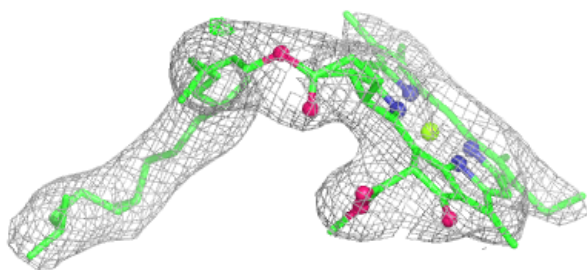
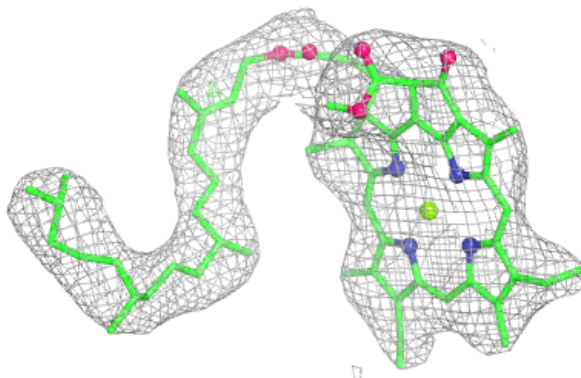
Electron density around CLA a 836:

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



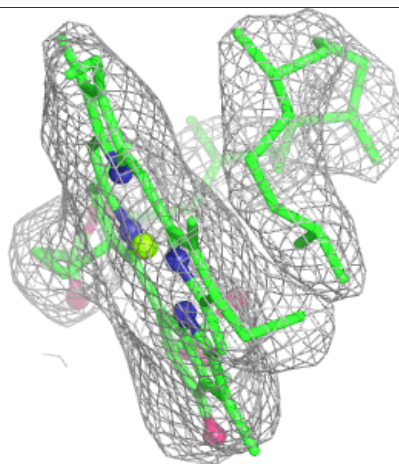
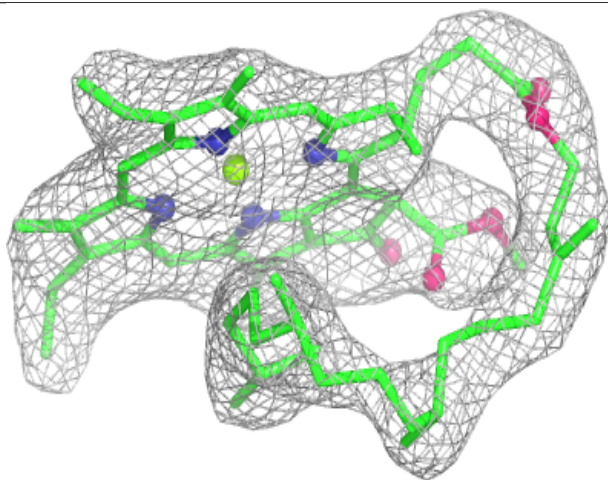
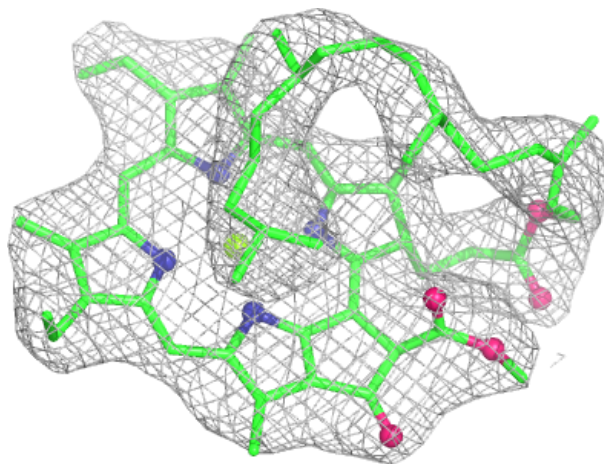
Electron density around CLA B 824:

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



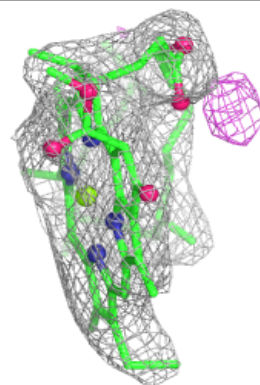
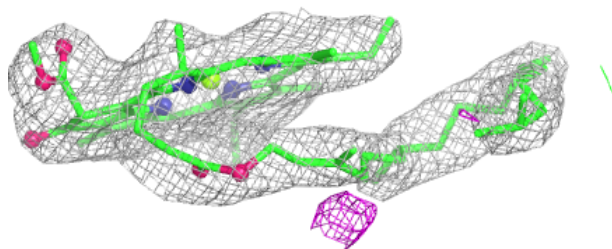
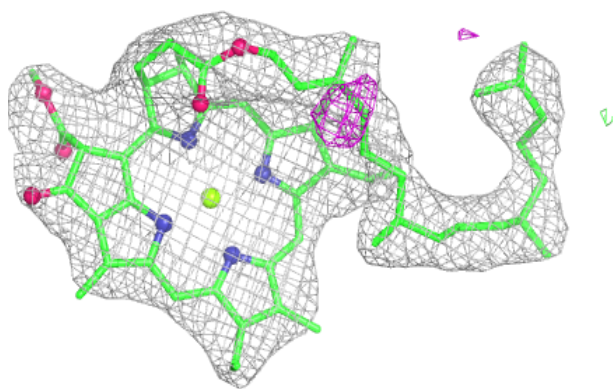
Electron density around CLA B 806:

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

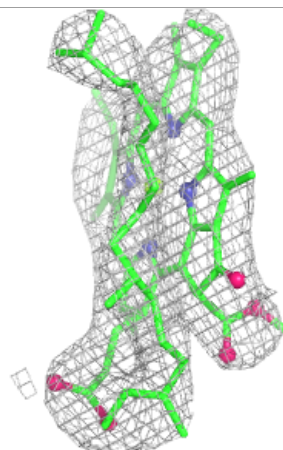
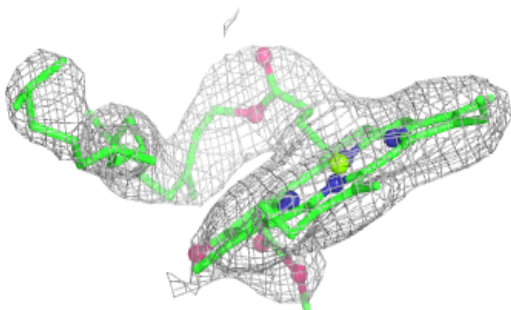
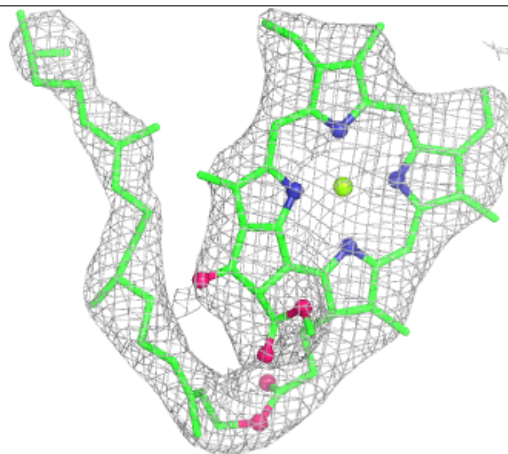


Electron density around CLA A 820:

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

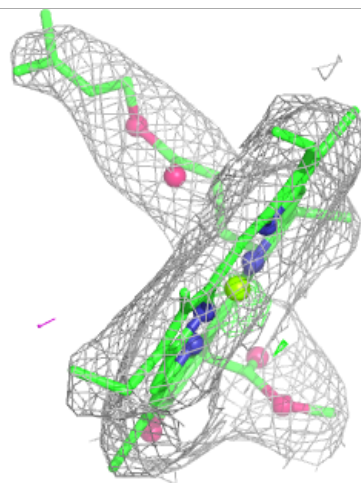
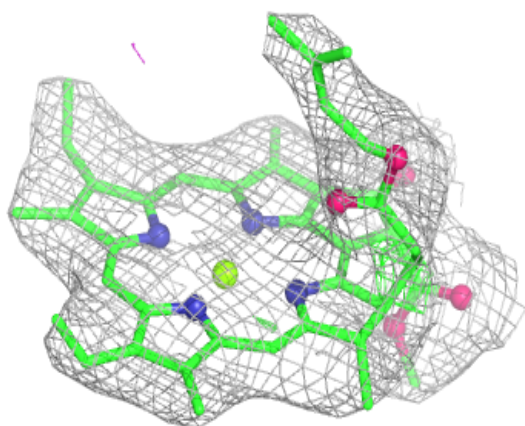
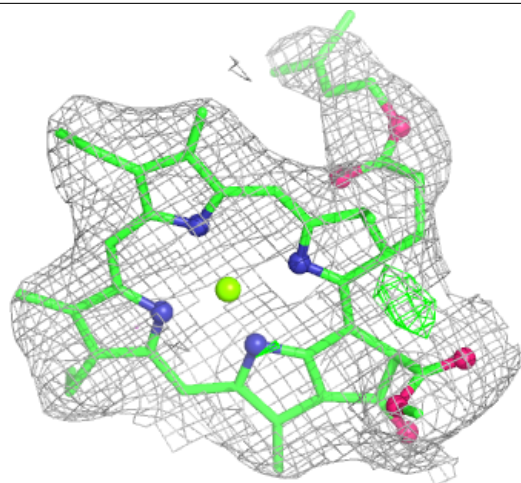
**Electron density around CLA A 826:**

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



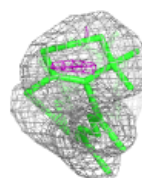
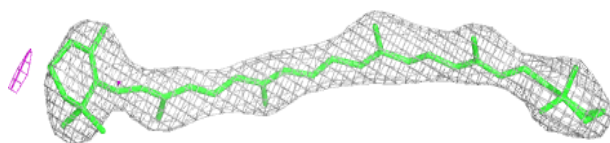
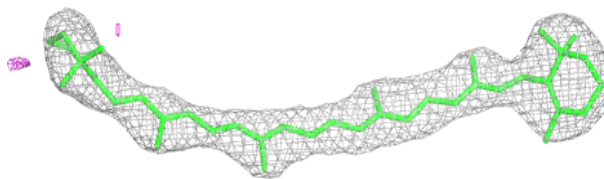
Electron density around CLA B 830:

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

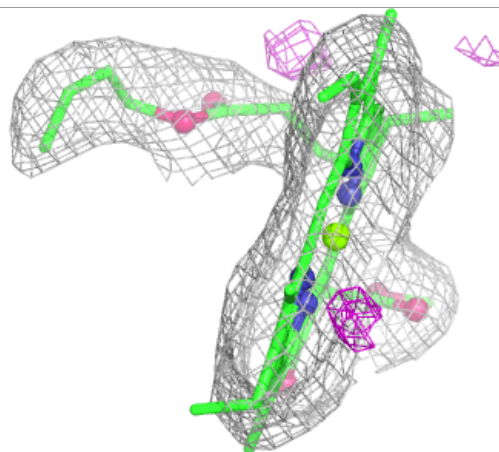
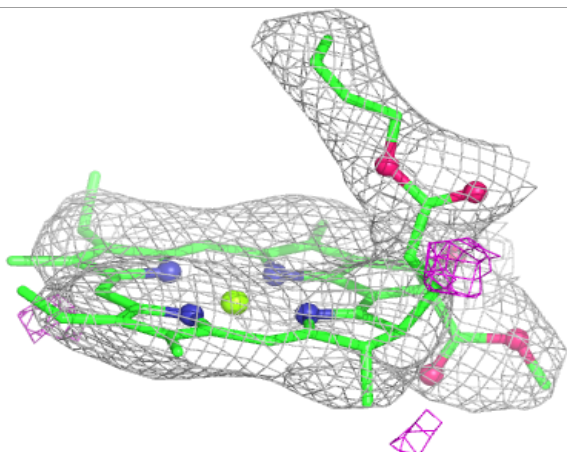
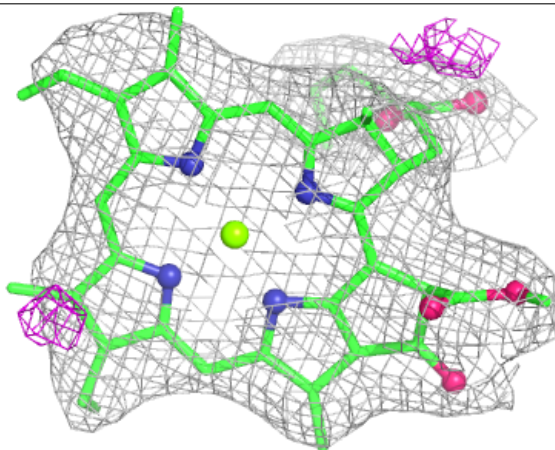


Electron density around BCR b 801:

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

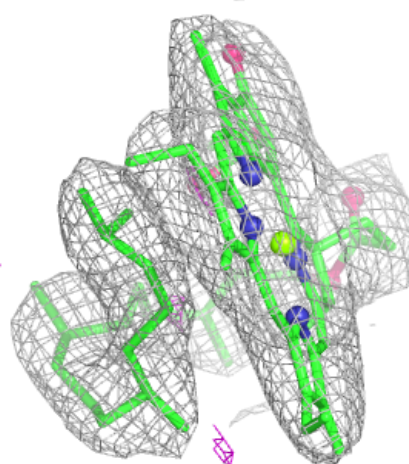
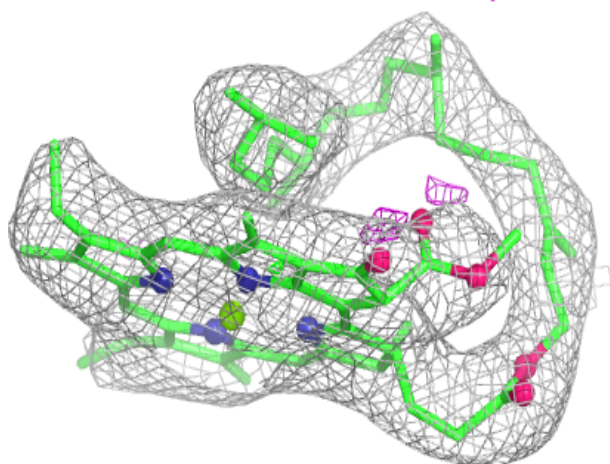
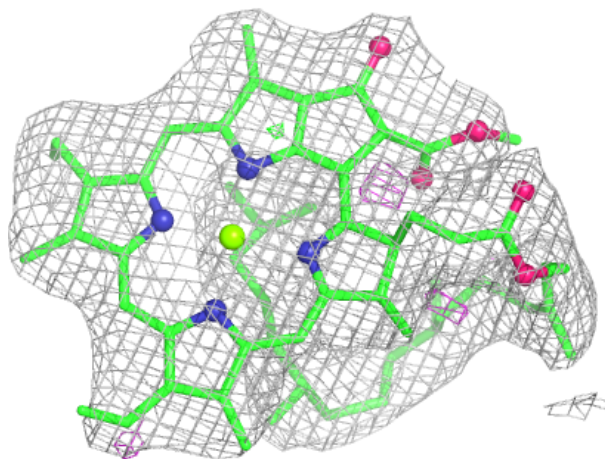
**Electron density around CLA B 831:**

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



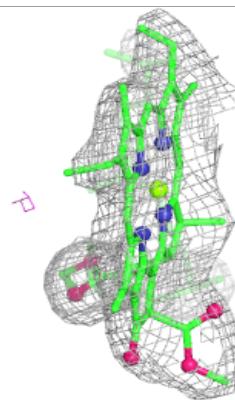
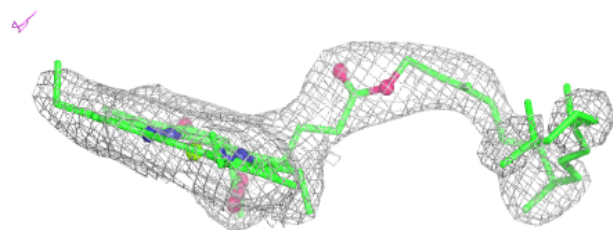
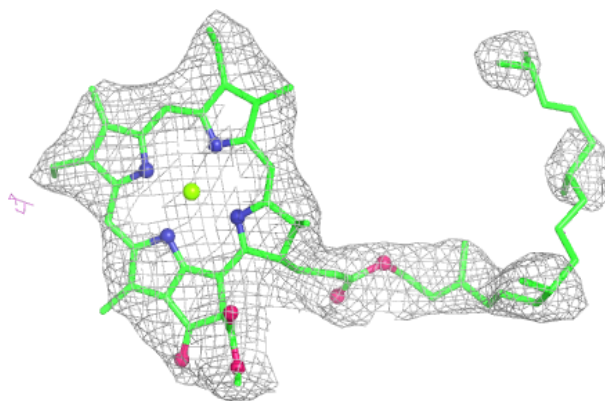
Electron density around CLA b 806:

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

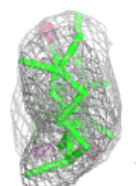
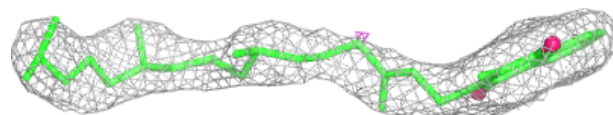
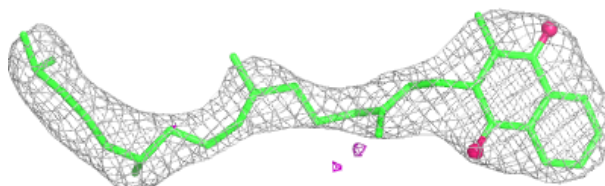


Electron density around CLA A 827:

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

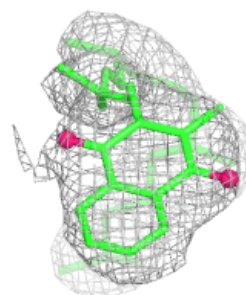
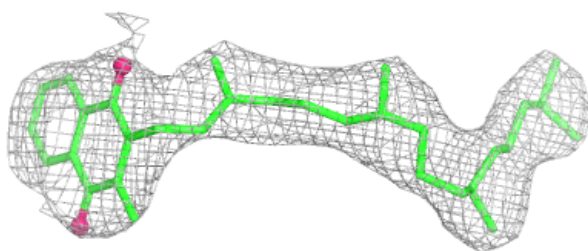
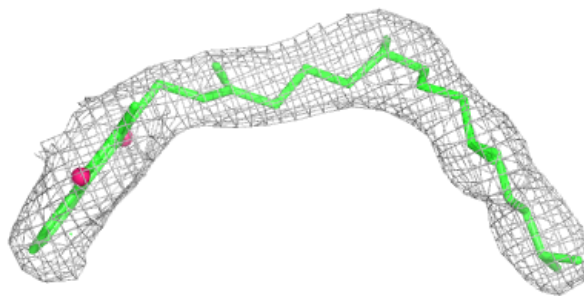
**Electron density around PQN A 844:**

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

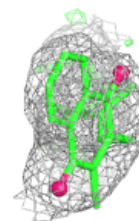
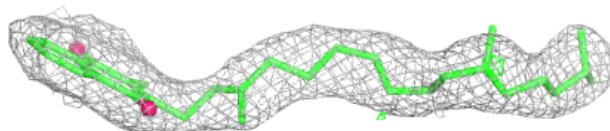
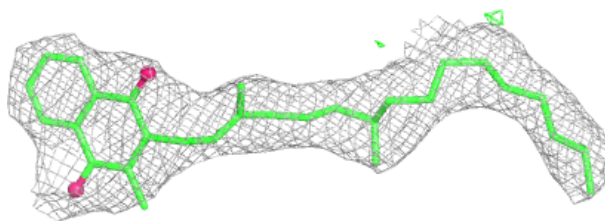


Electron density around PQN B 842:

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

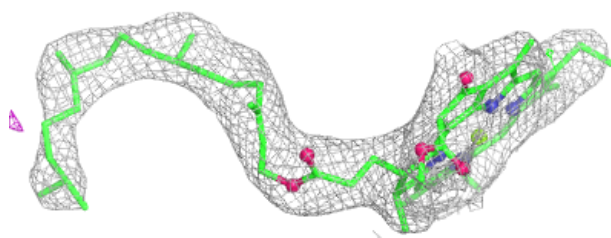
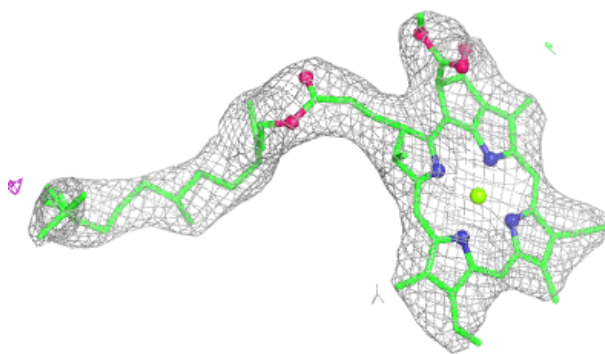
**Electron density around PQN a 845:**

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

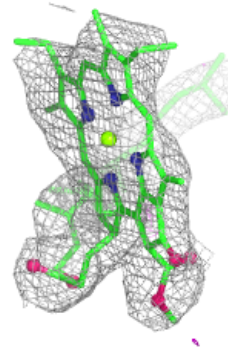
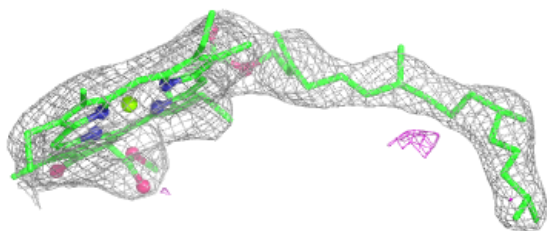
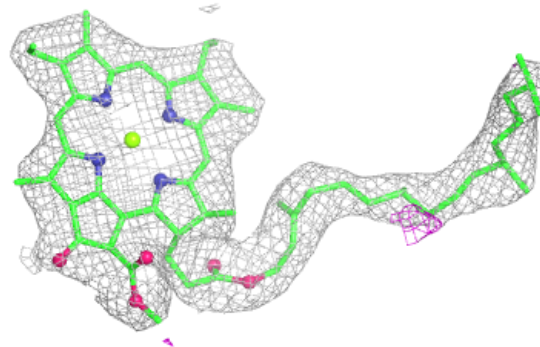


Electron density around CLA b 809:

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

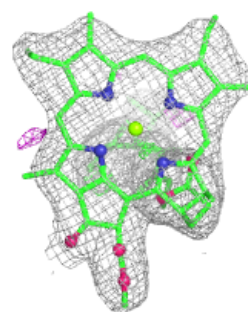
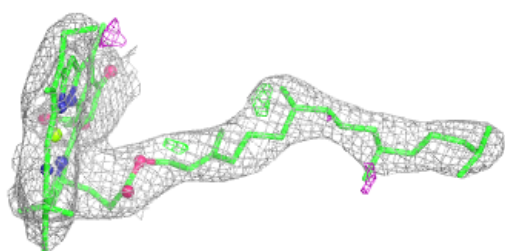
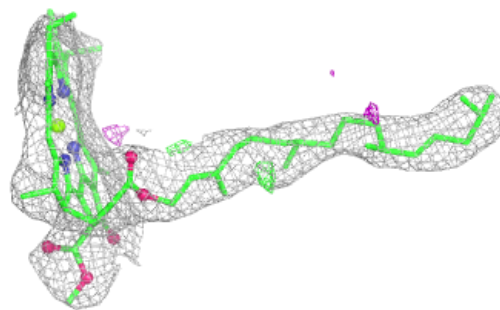
**Electron density around CLA A 802:**

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

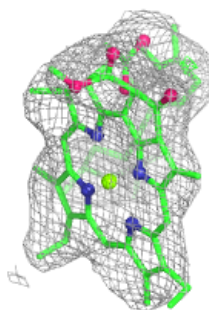
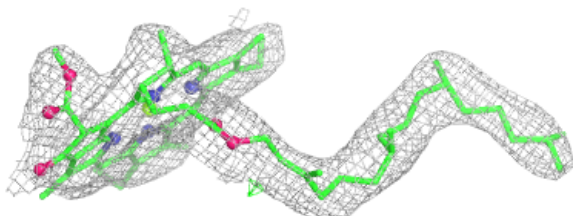
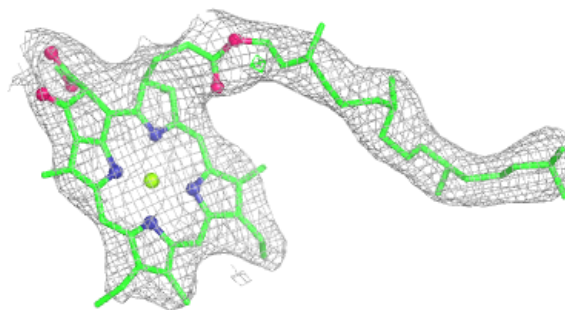


Electron density around CLA A 829:

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

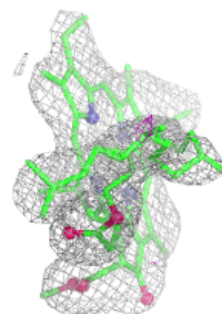
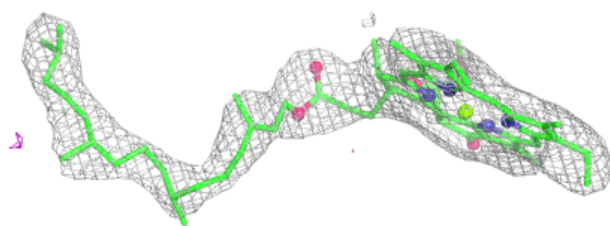
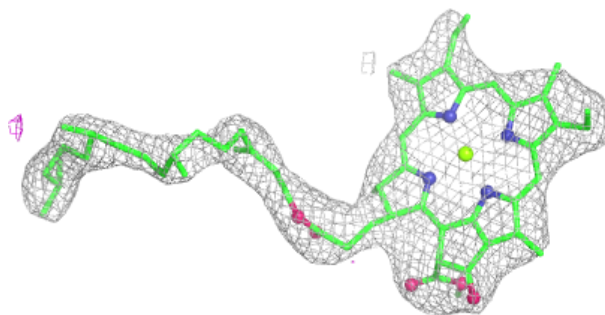
**Electron density around CLA A 809:**

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

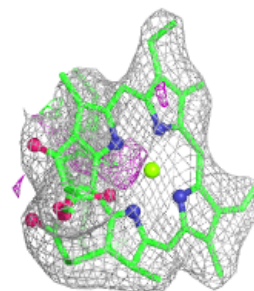
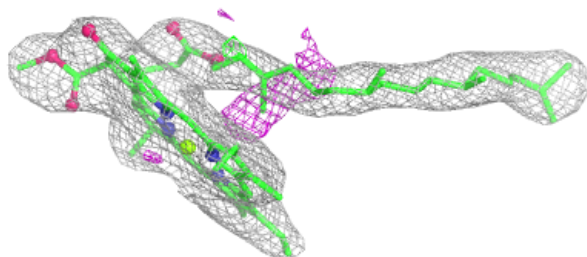
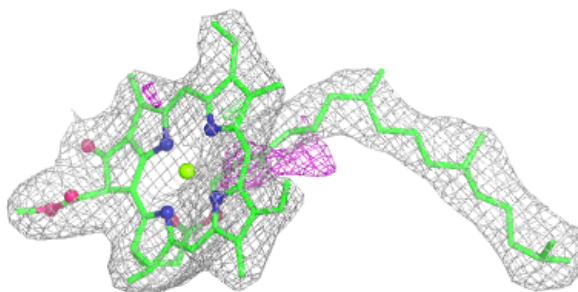


Electron density around CLA b 813:

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

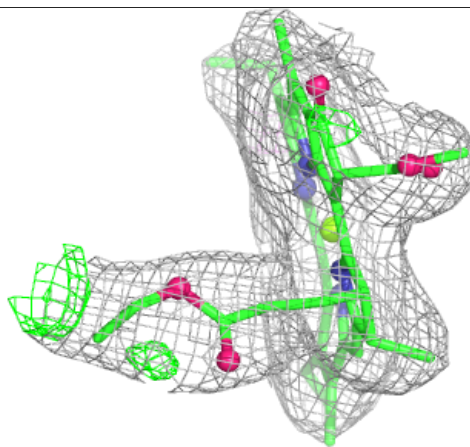
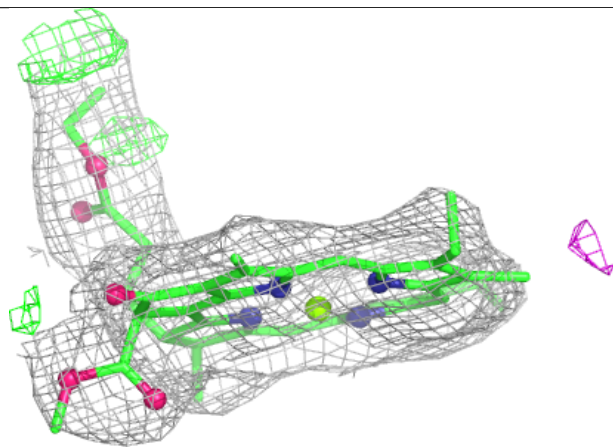
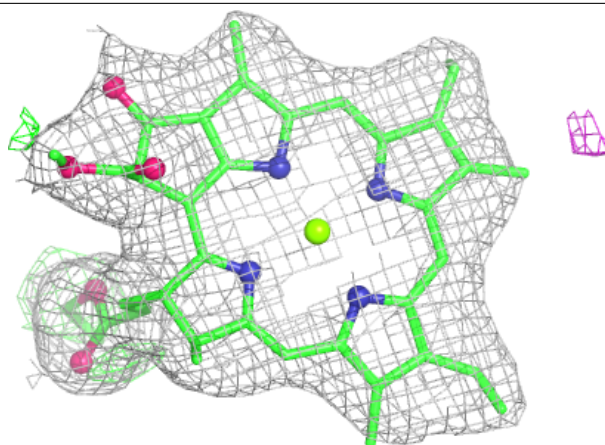
**Electron density around CLA A 842:**

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



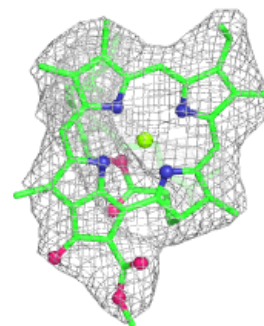
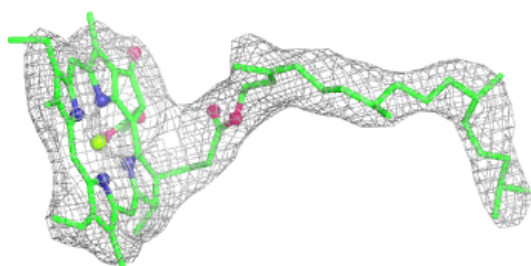
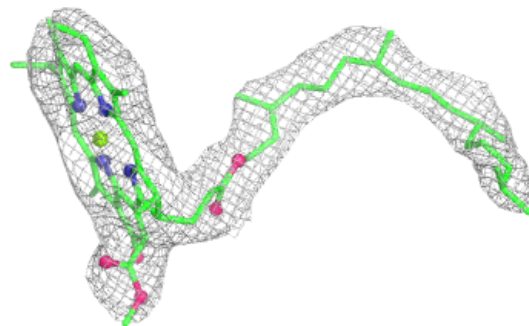
Electron density around CLA B 838:

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

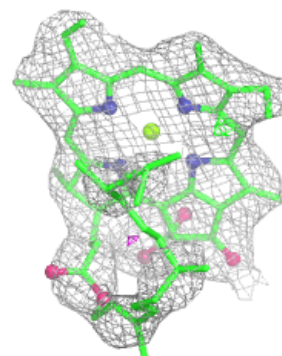
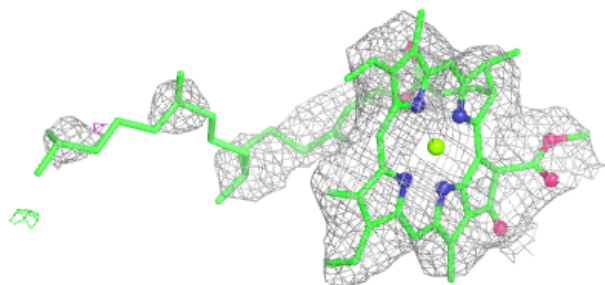
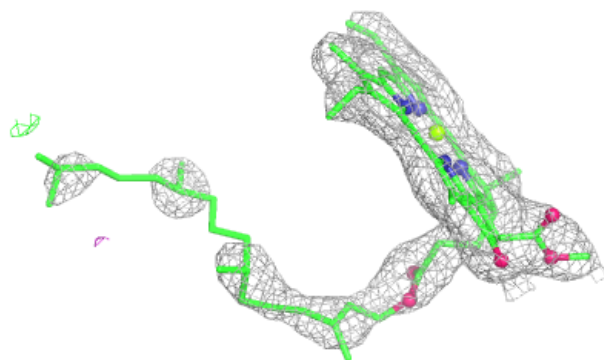


Electron density around CLA B 839:

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

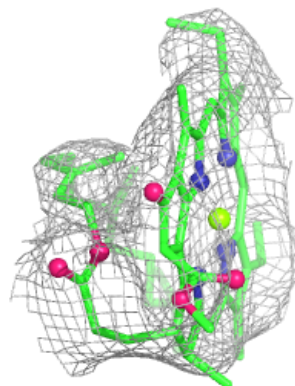
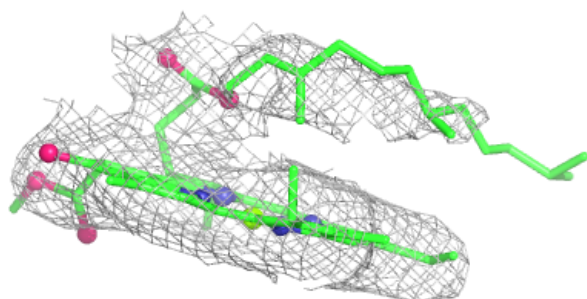
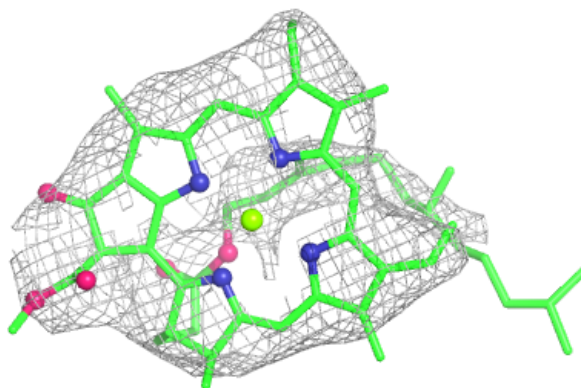
**Electron density around CLA a 811:**

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

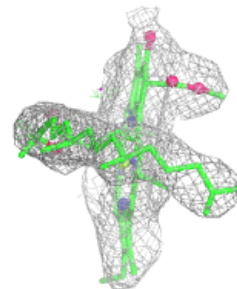
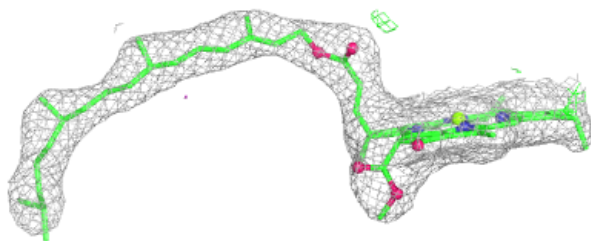
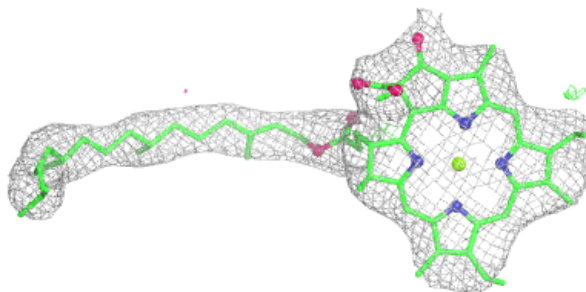


Electron density around CLA 6 314:

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

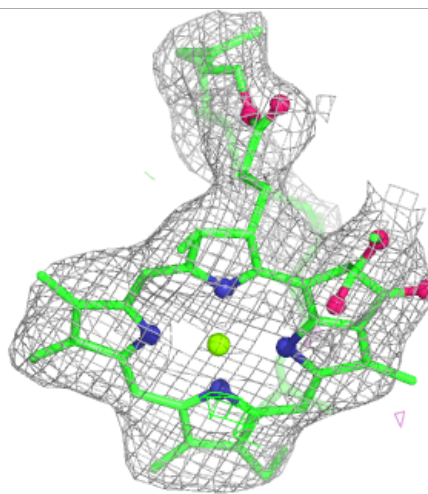
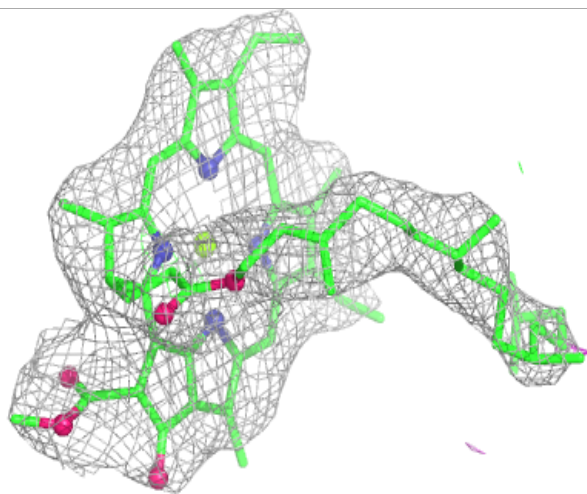
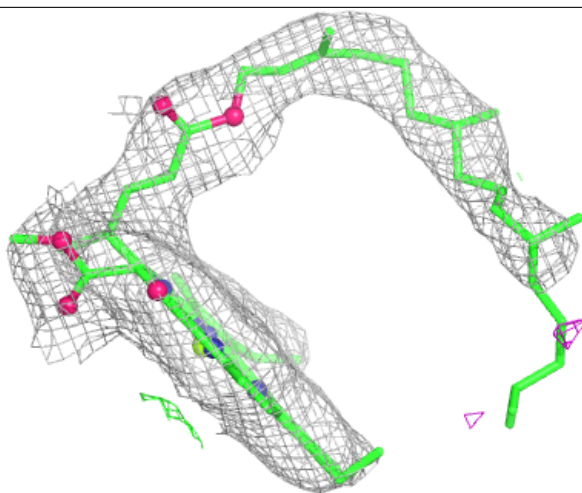
**Electron density around CLA B 841:**

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



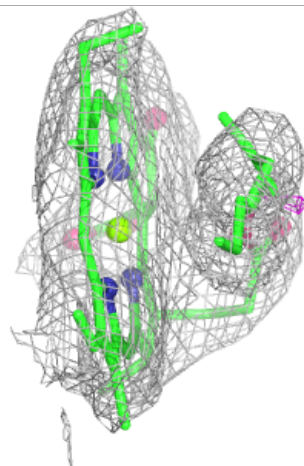
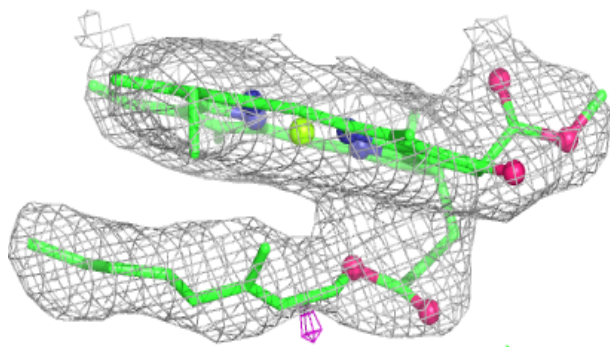
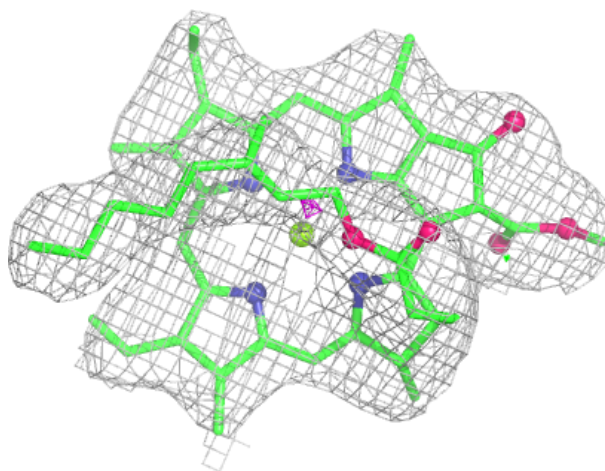
Electron density around CLA b 819:

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



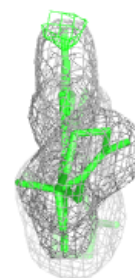
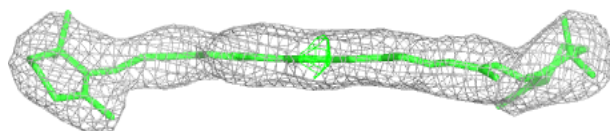
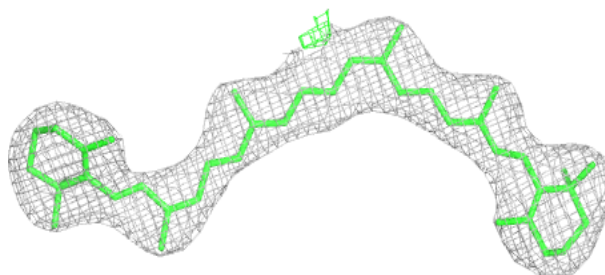
Electron density around CLA a 813:

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

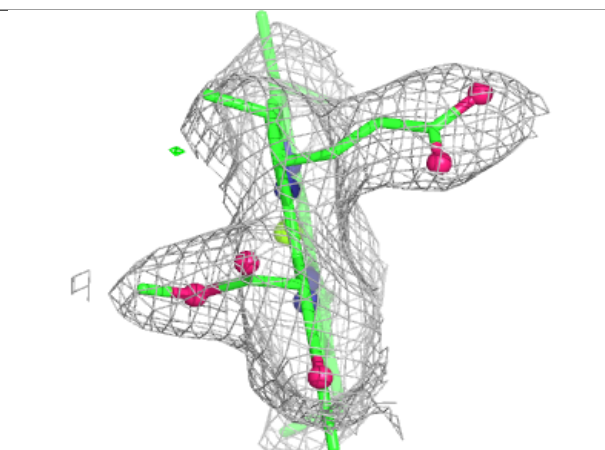
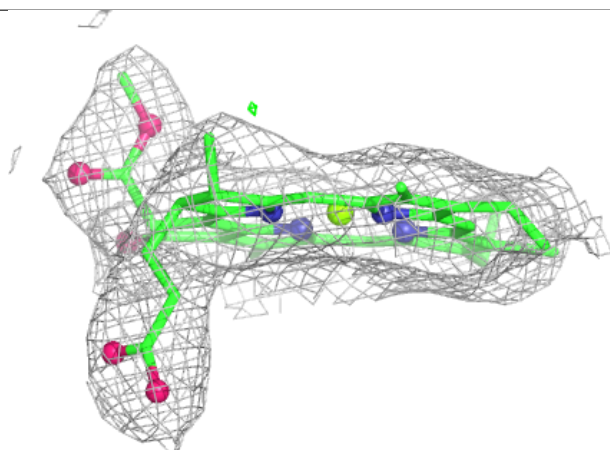
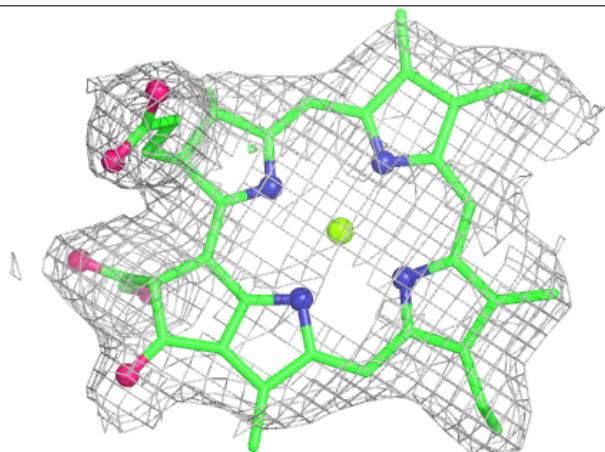


Electron density around BCR A 852:

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

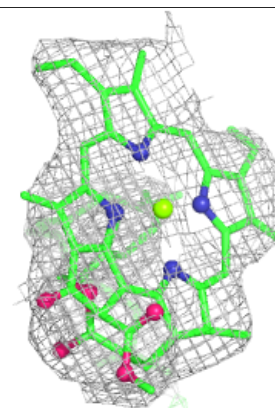
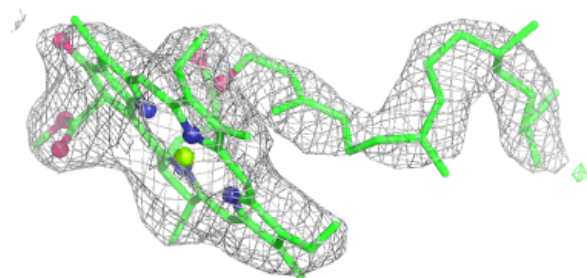
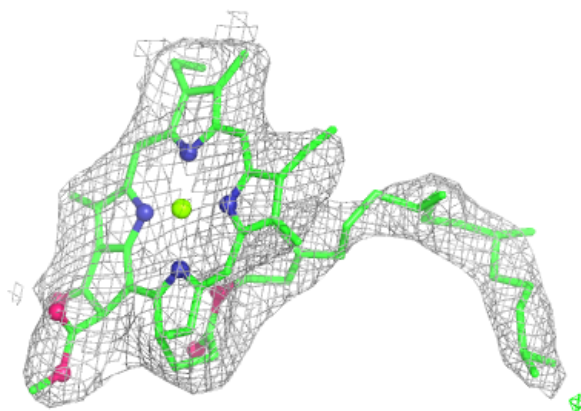
**Electron density around CLA a 815:**

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



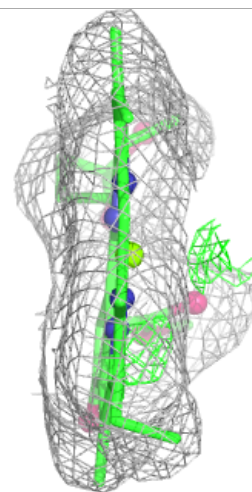
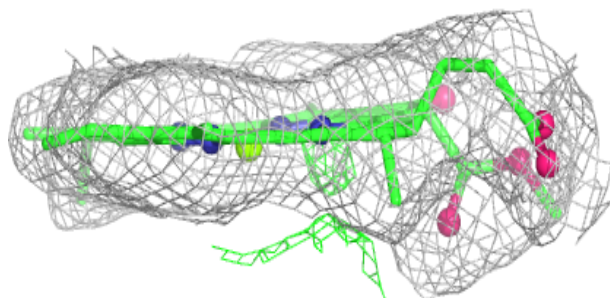
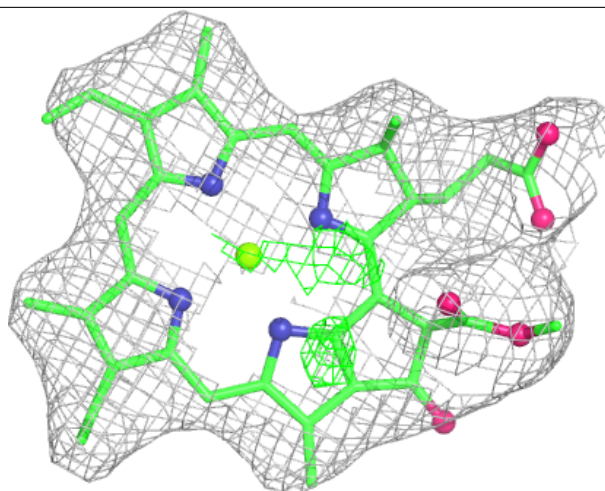
Electron density around CLA A 843:

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



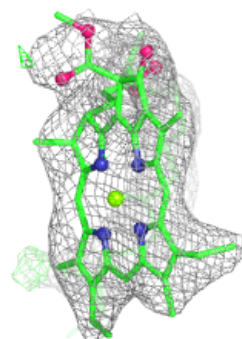
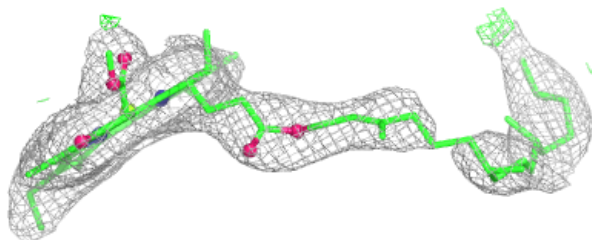
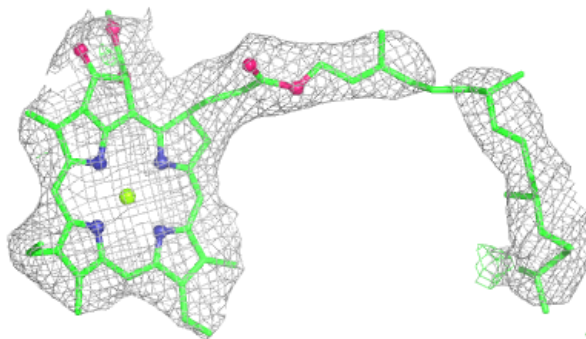
Electron density around CLA F 303:

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

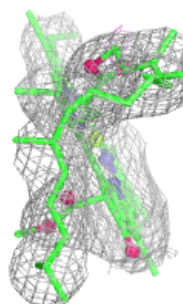
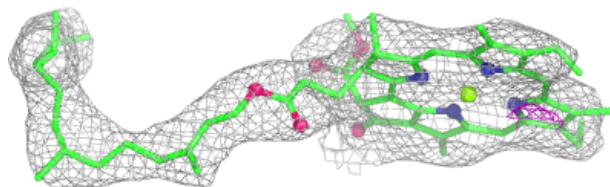
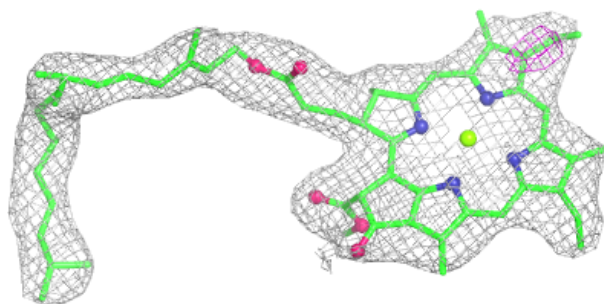


Electron density around CLA b 825:

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

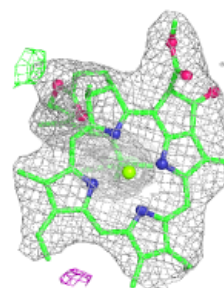
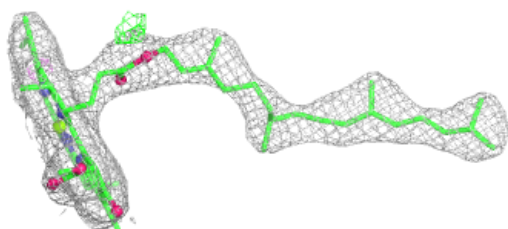
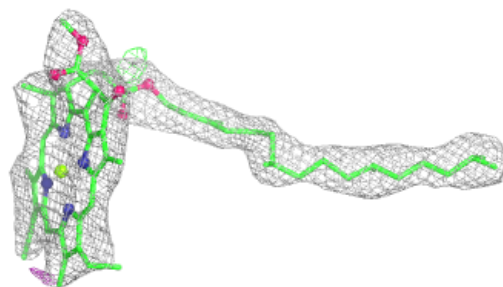
**Electron density around CLA b 826:**

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

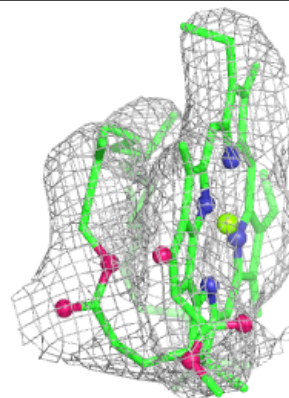
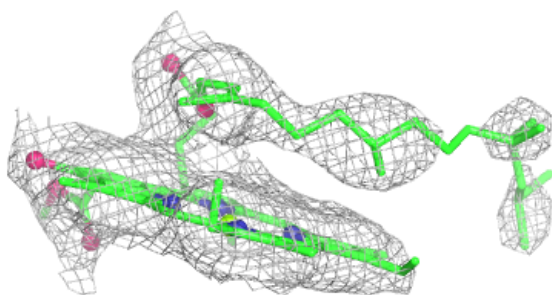
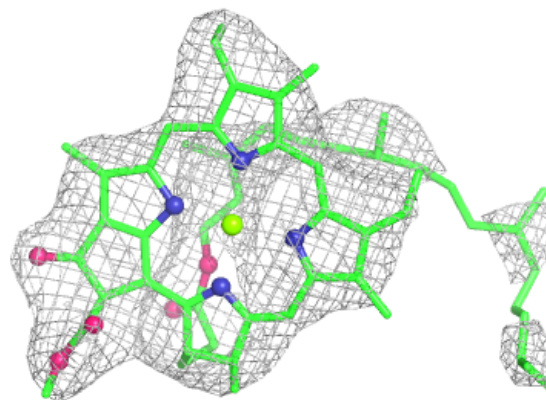


Electron density around CLA b 828:

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

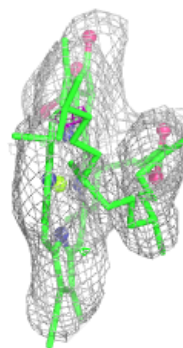
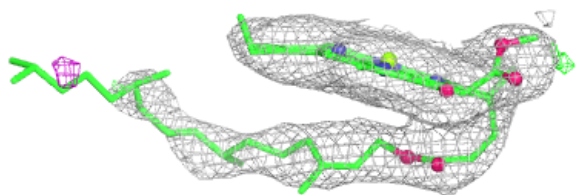
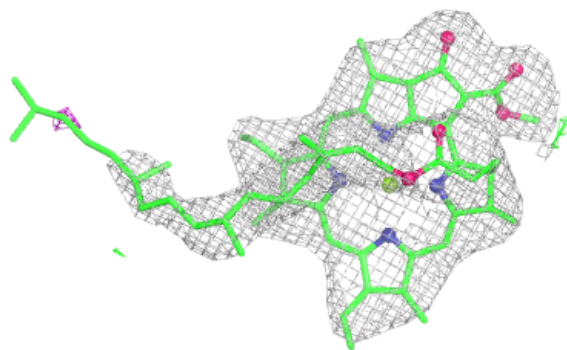
**Electron density around CLA 7 612:**

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

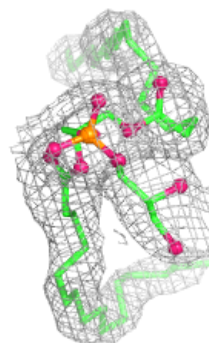
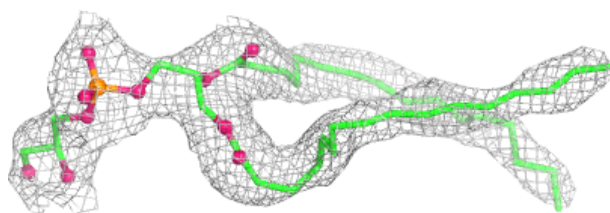
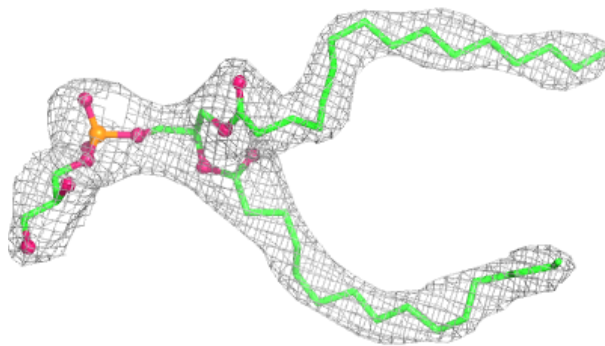


Electron density around CLA a 818:

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

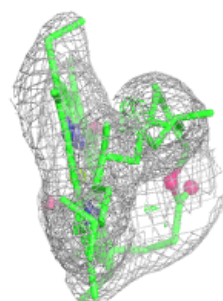
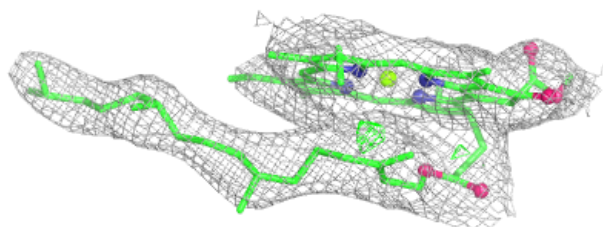
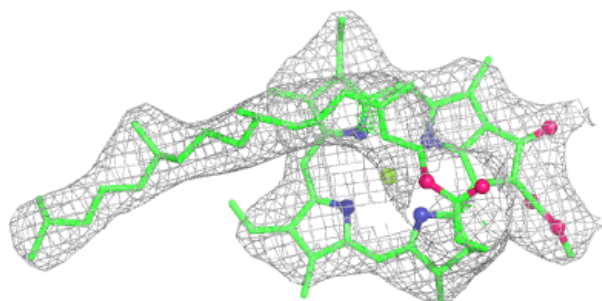
**Electron density around LHG A 846:**

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

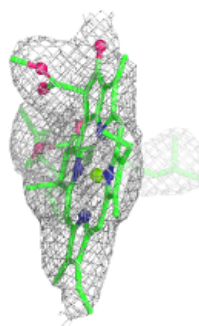
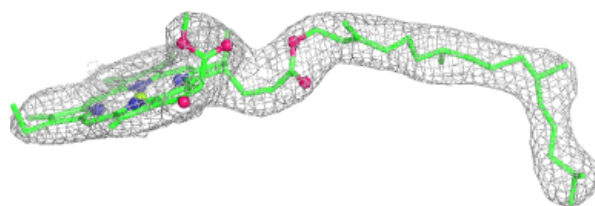
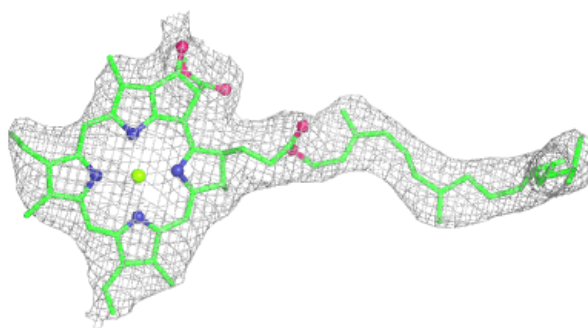


Electron density around CLA a 841:

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

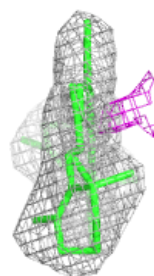
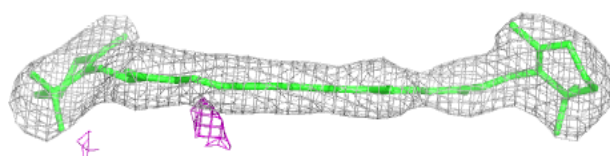
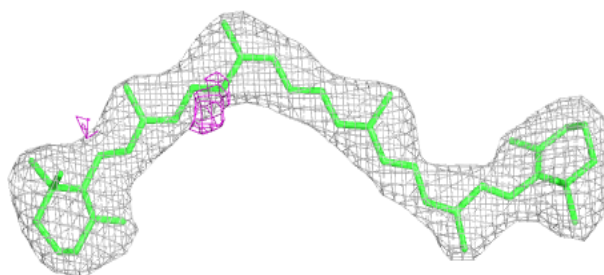
**Electron density around CLA A 806:**

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

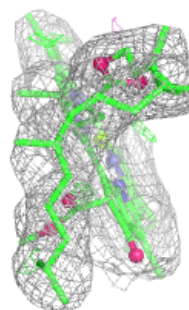
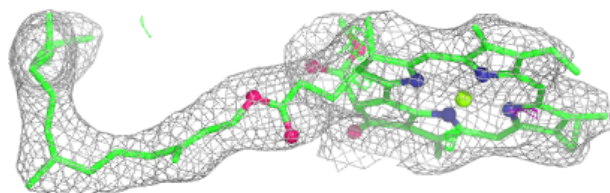
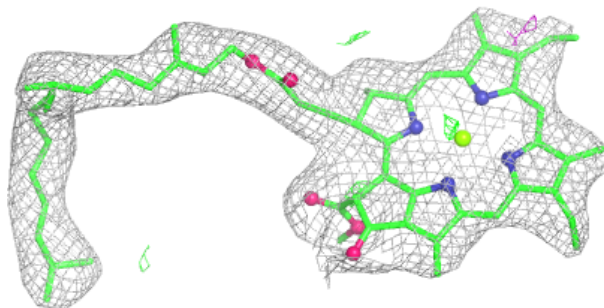


Electron density around BCR a 854:

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

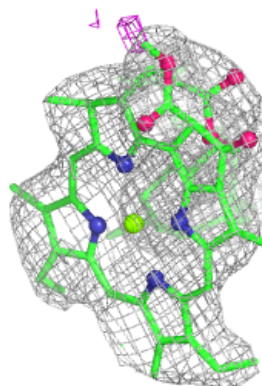
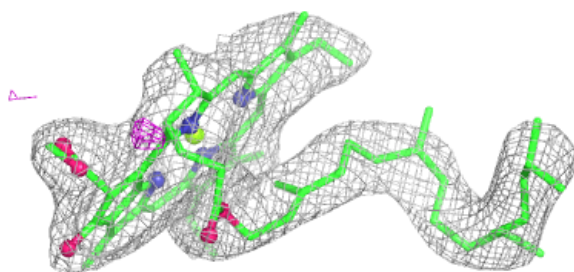
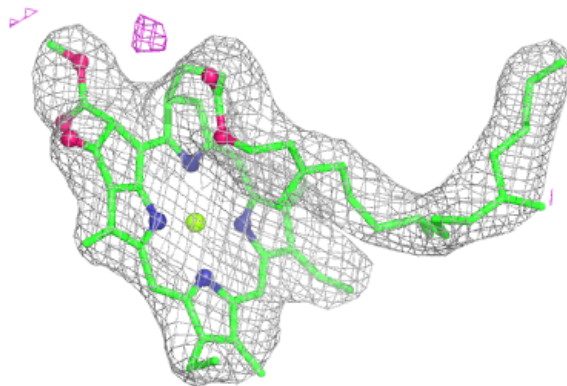
**Electron density around CLA B 826:**

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

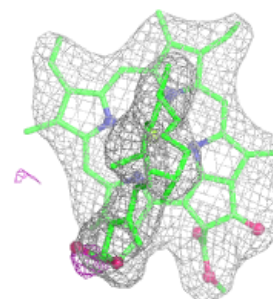
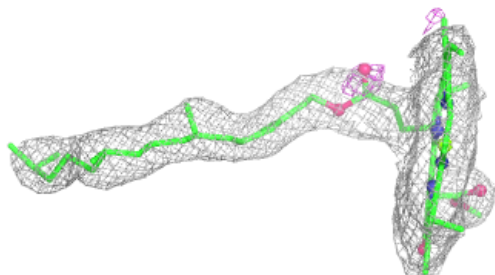
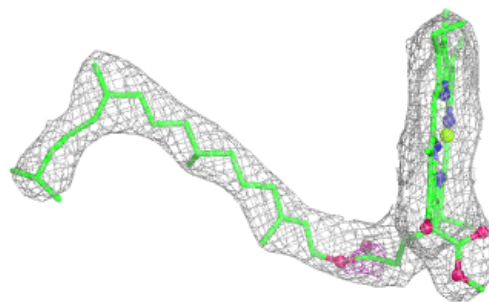


Electron density around CLA a 844:

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

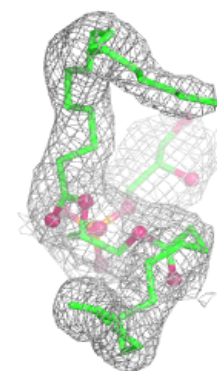
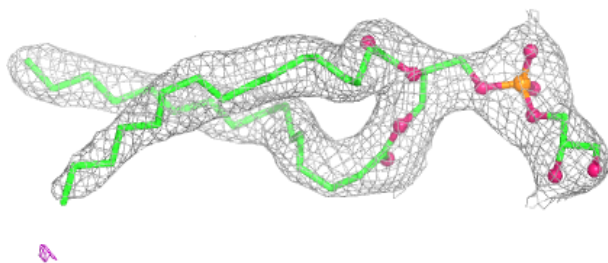
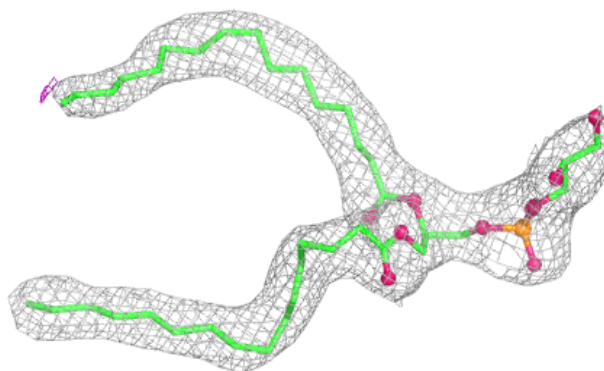
**Electron density around CLA B 840:**

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

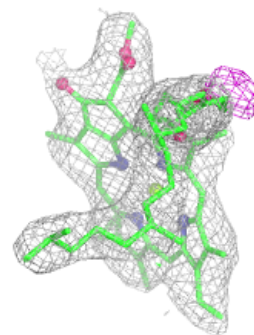
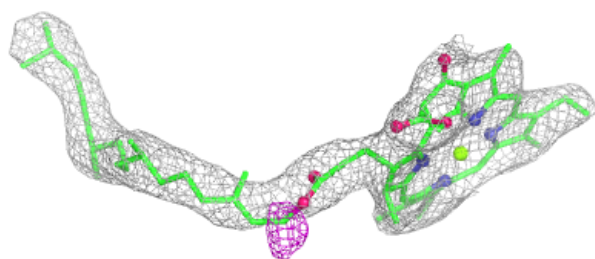
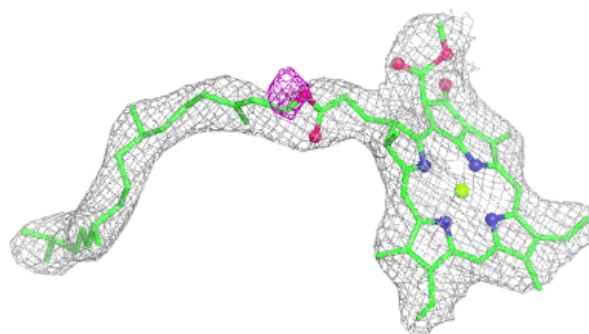


Electron density around LHG a 847:

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

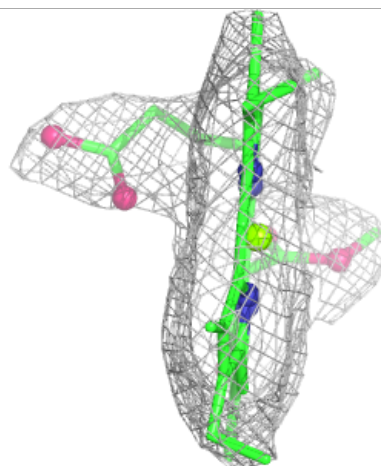
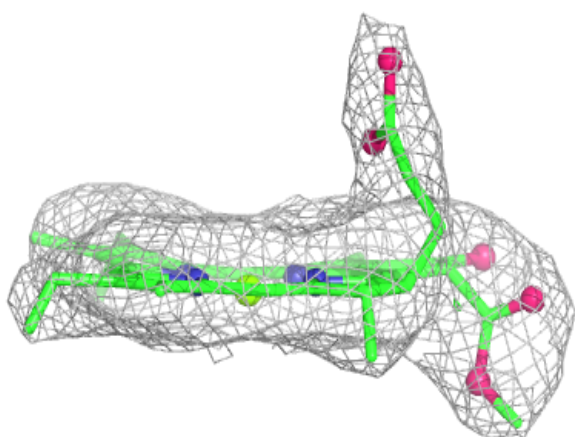
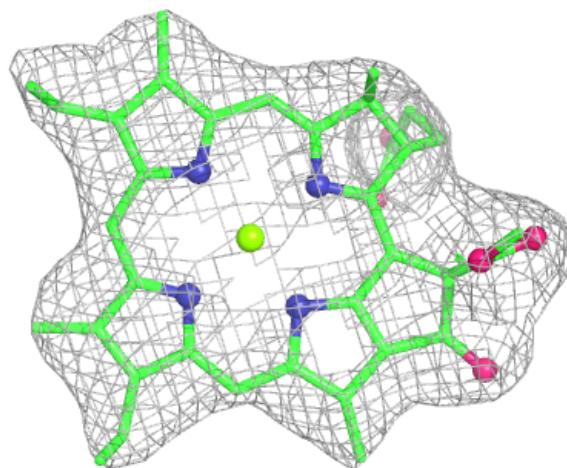
**Electron density around CLA a 856:**

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



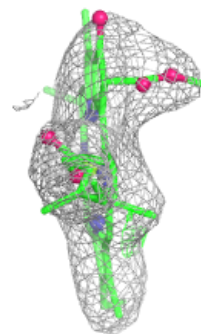
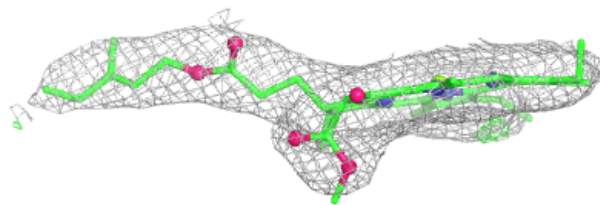
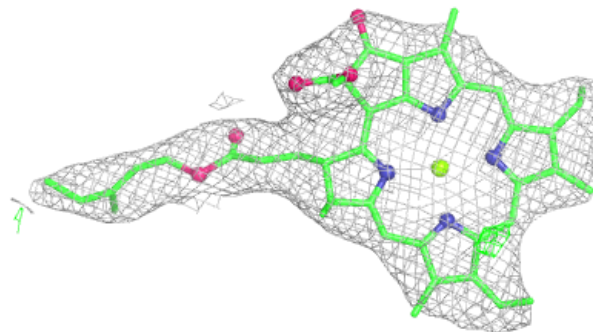
Electron density around CLA b 804:

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



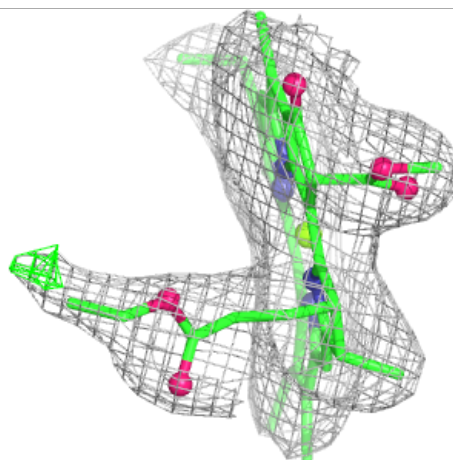
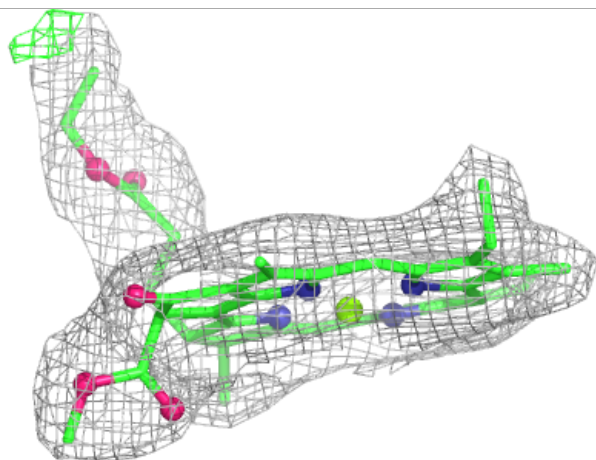
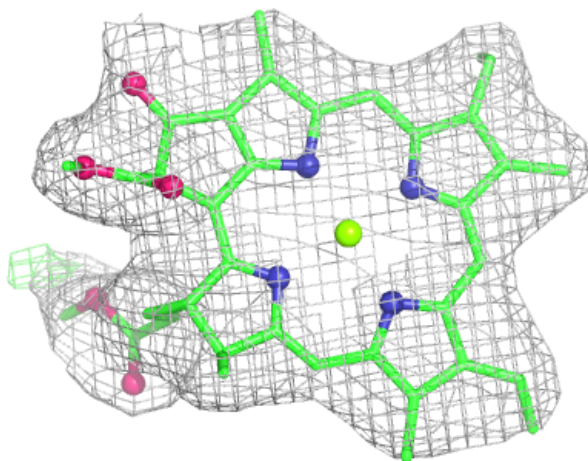
Electron density around CLA A 838:

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



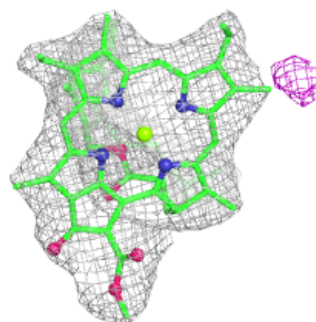
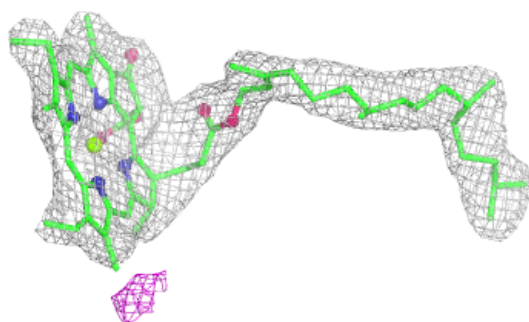
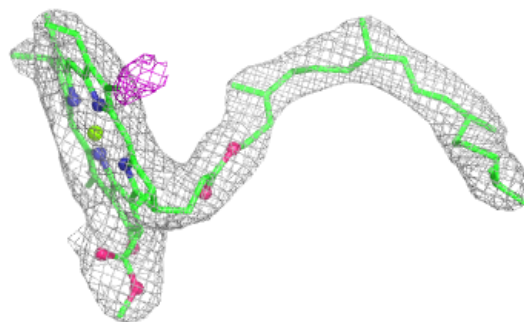
Electron density around CLA b 838:

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

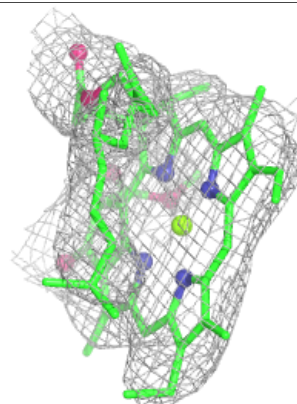
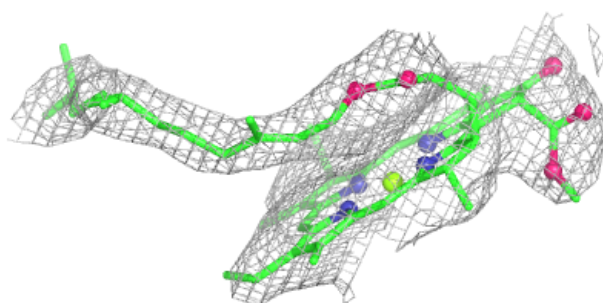
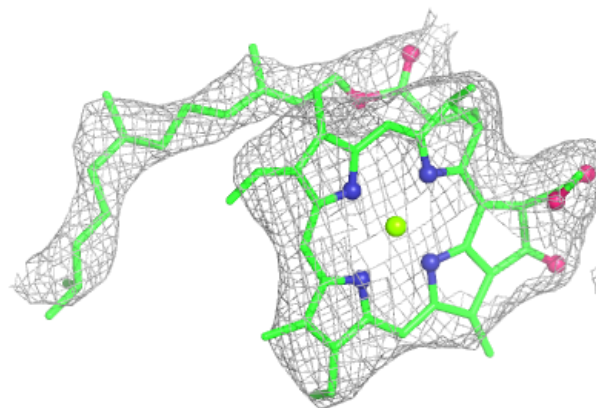


Electron density around CLA b 839:

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

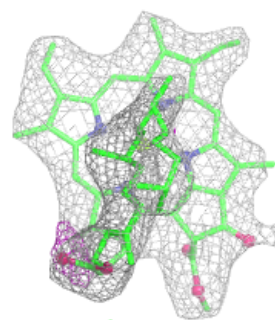
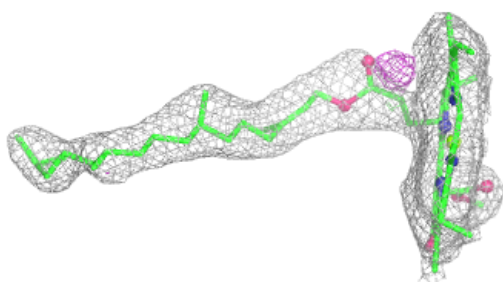
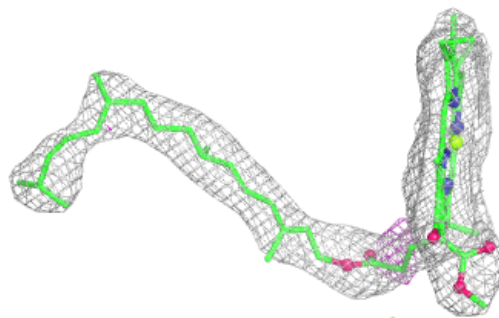
**Electron density around CLA 8 301:**

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

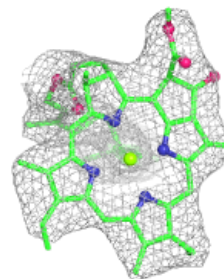
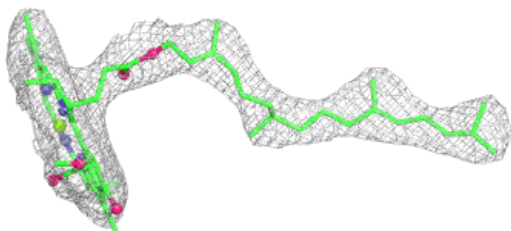
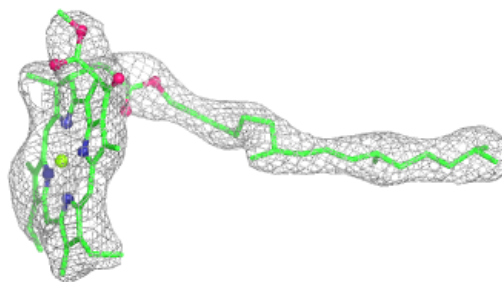


Electron density around CLA b 840:

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

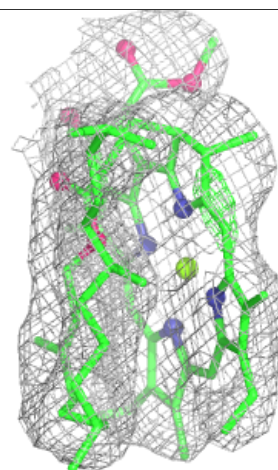
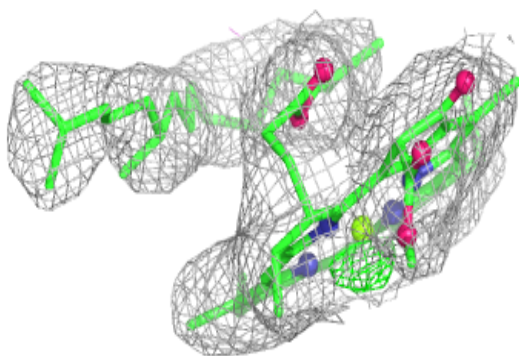
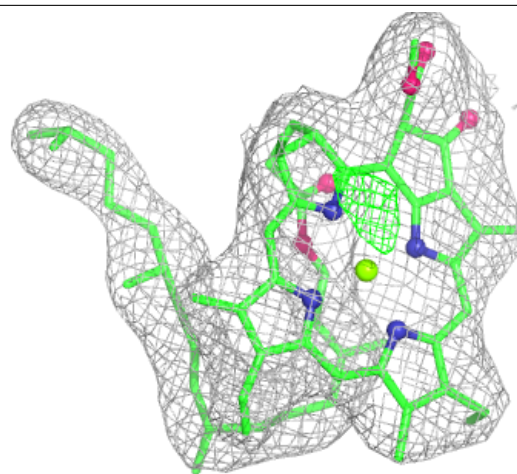
**Electron density around CLA B 828:**

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



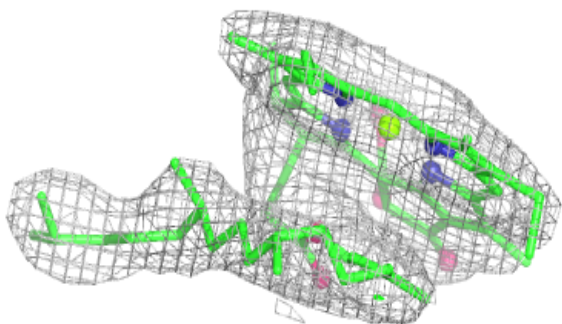
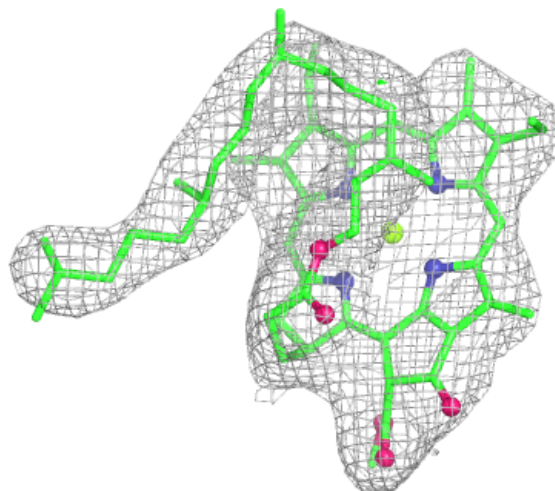
Electron density around CLA b 808:

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



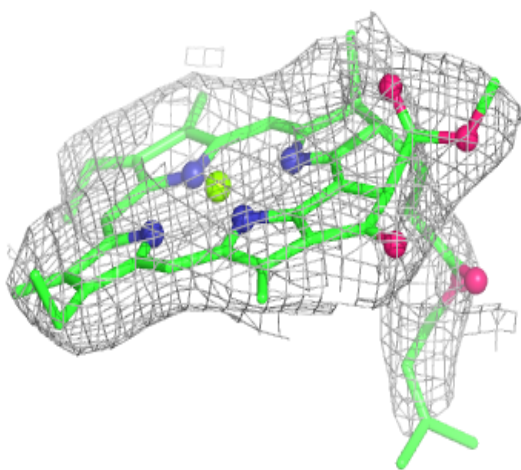
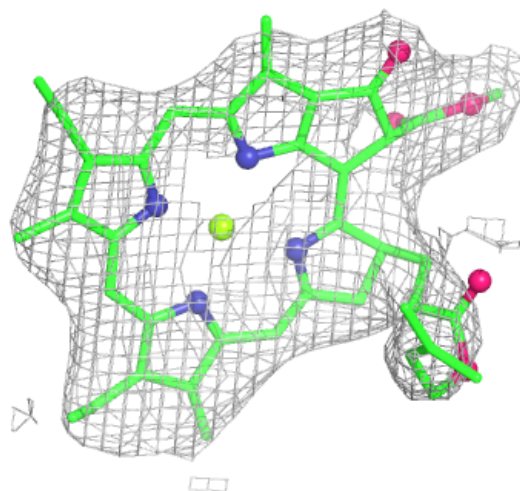
Electron density around CLA B 808:

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



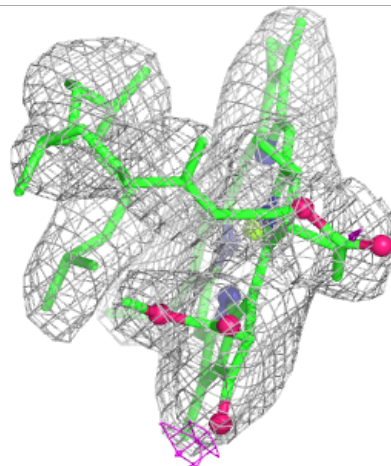
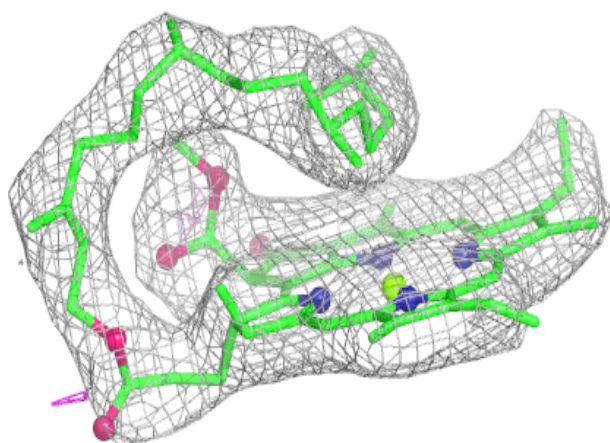
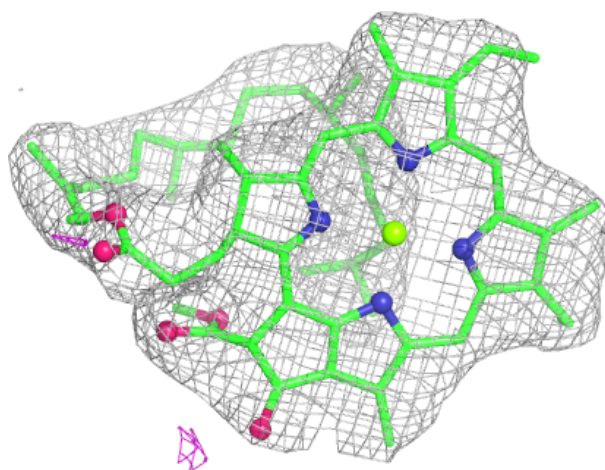
Electron density around CLA 8 307:

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



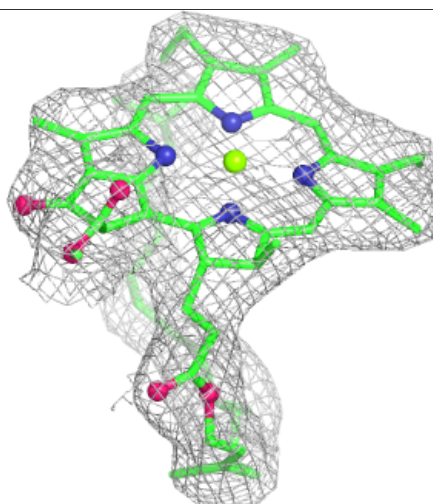
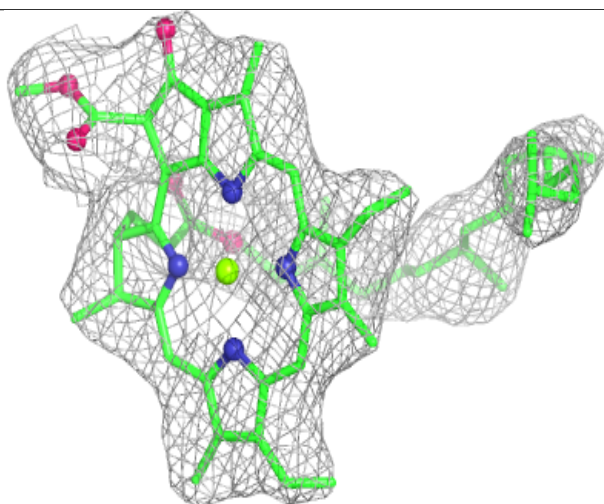
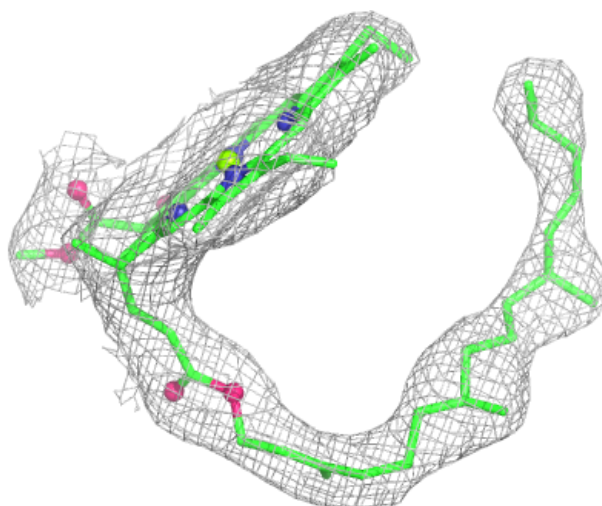
Electron density around CLA A 807:

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



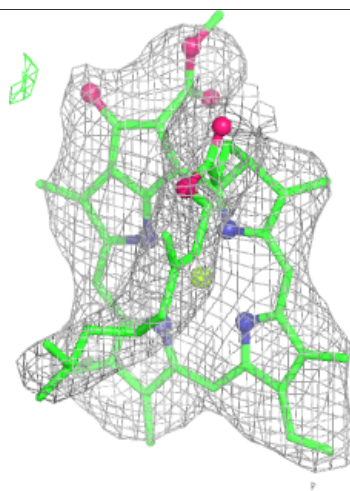
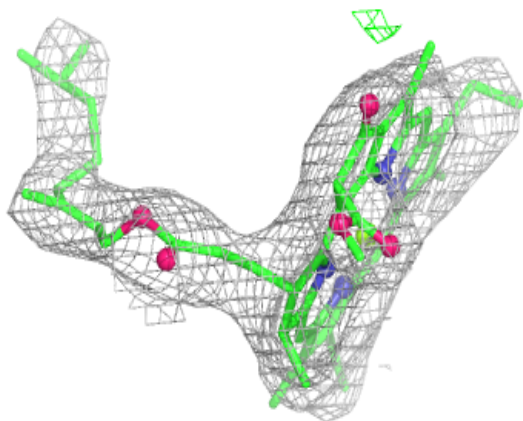
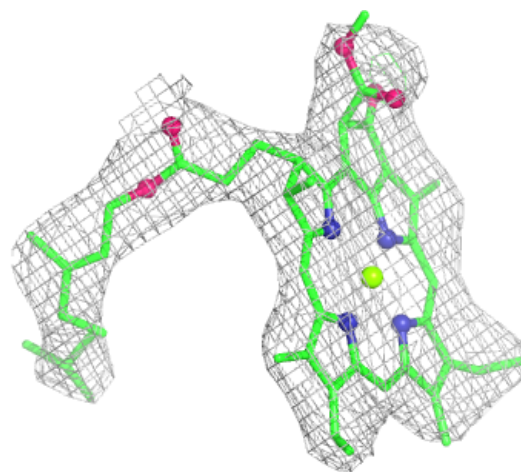
Electron density around CLA B 819:

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



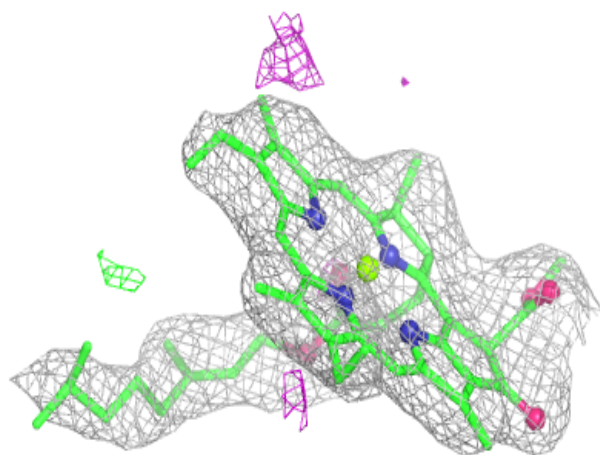
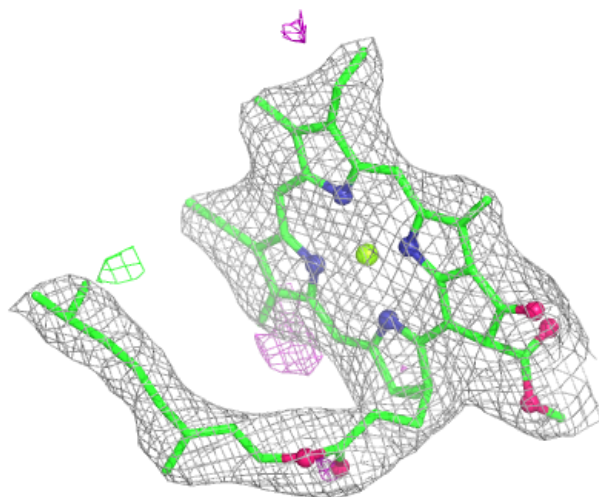
Electron density around CLA a 805:

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



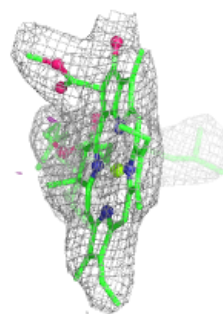
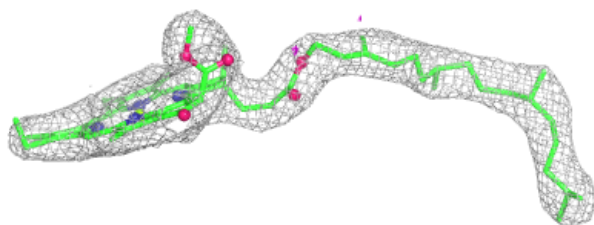
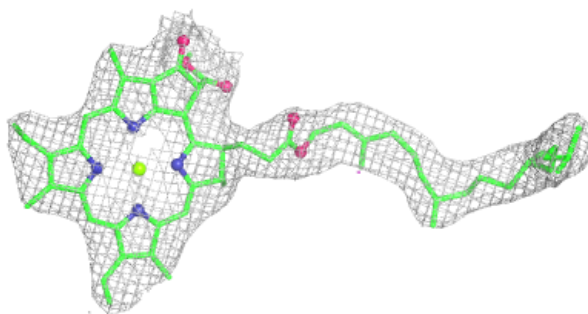
Electron density around CLA a 825:

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



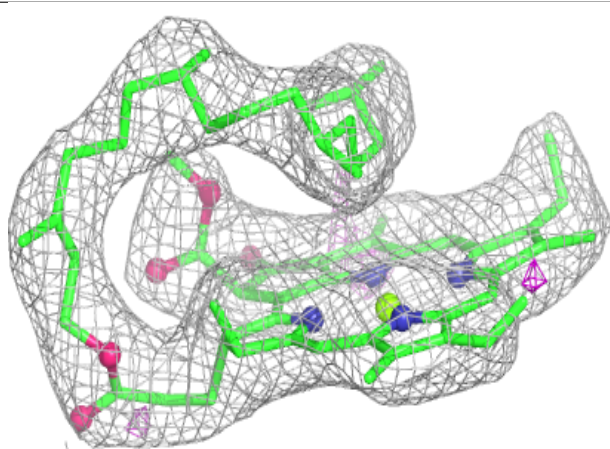
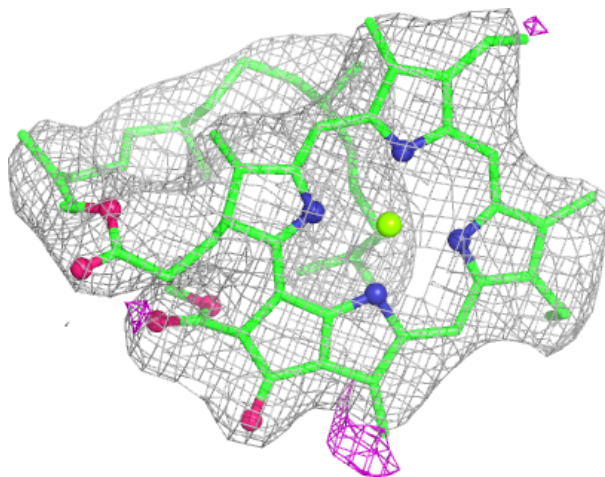
Electron density around CLA a 806:

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



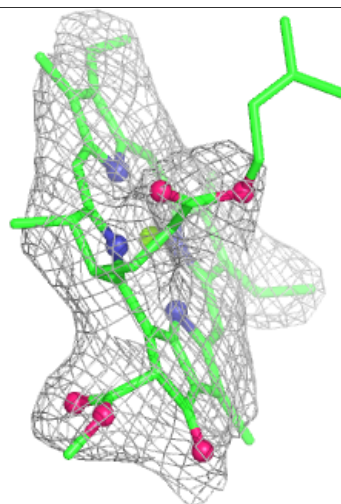
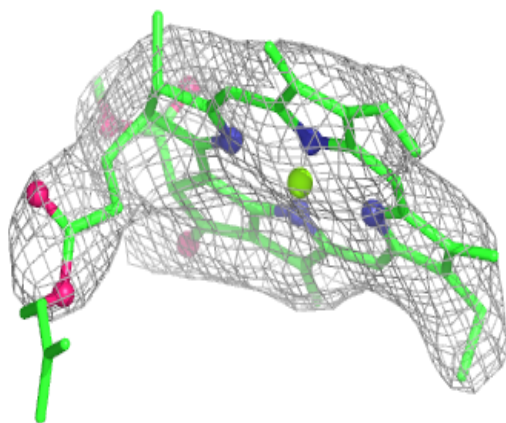
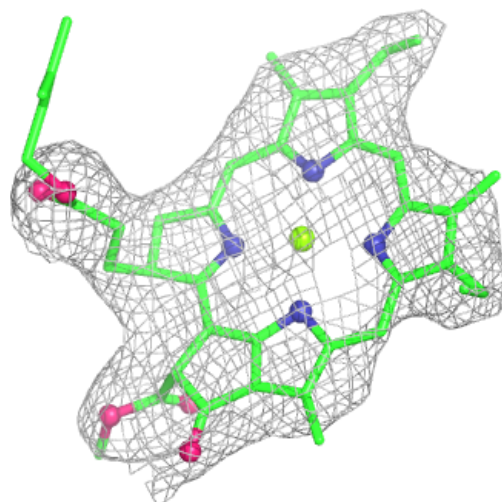
Electron density around CLA a 807:

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



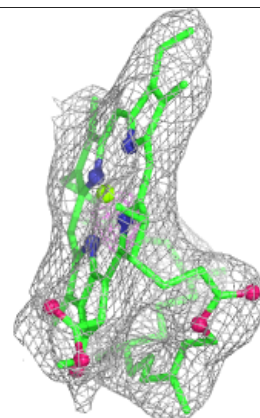
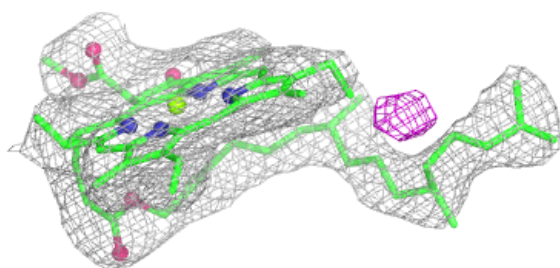
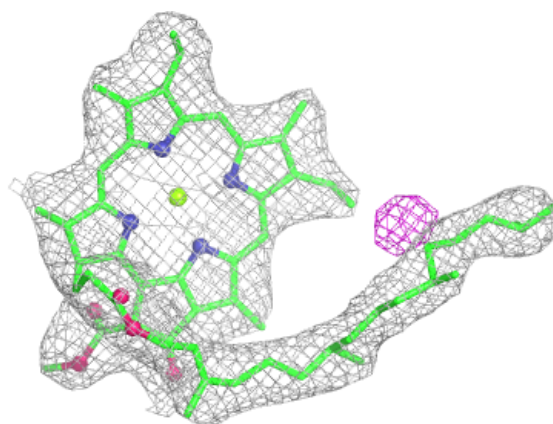
Electron density around CLA B 820:

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

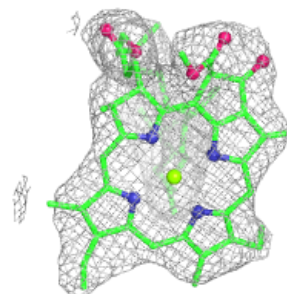
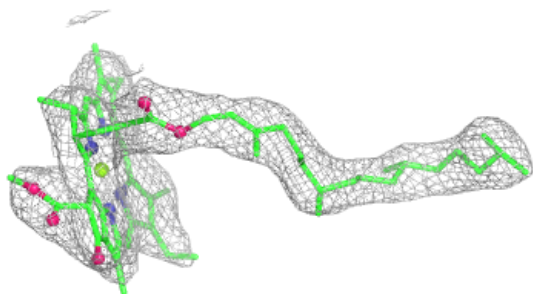
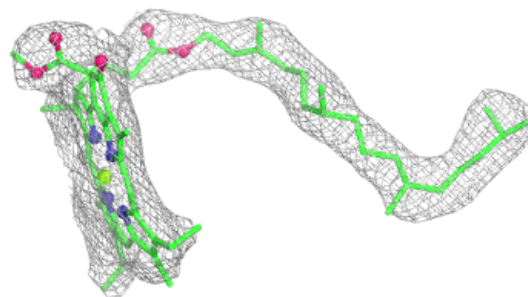


Electron density around CLA a 830:

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

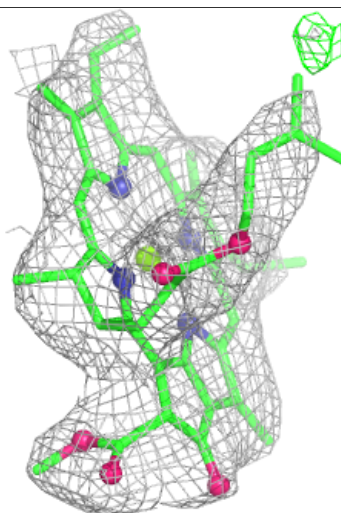
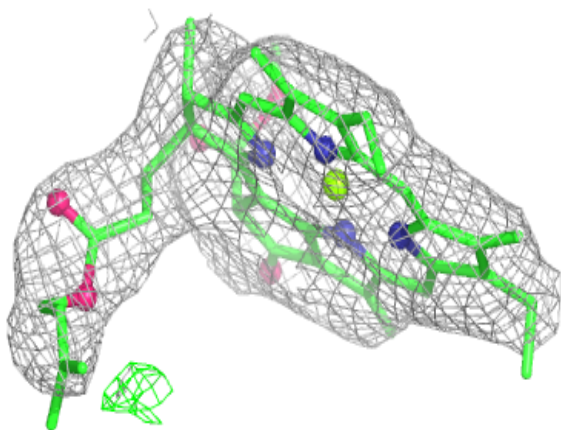
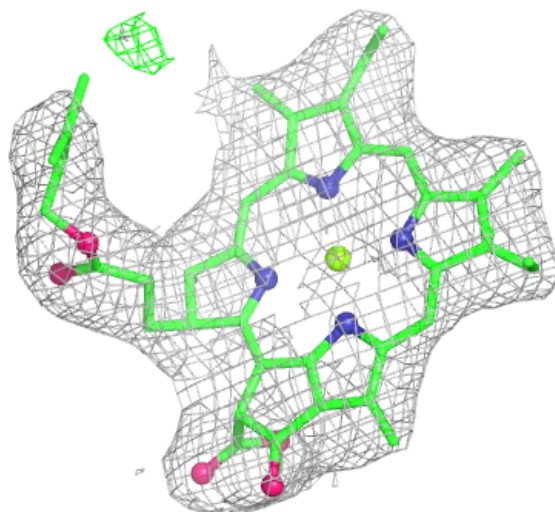
**Electron density around CLA a 831:**

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



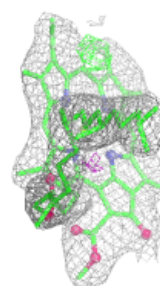
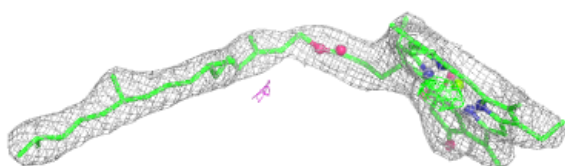
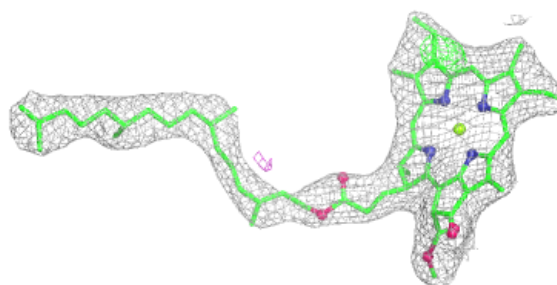
Electron density around CLA a 832:

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

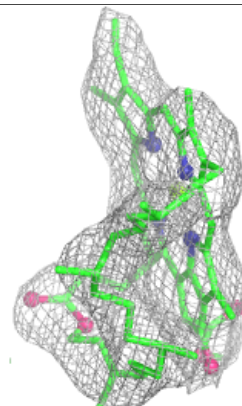
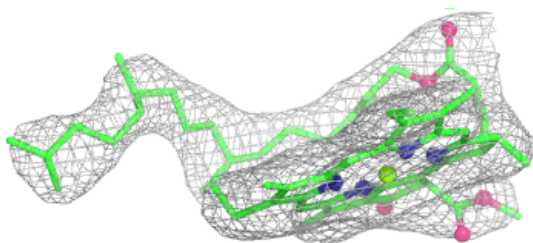
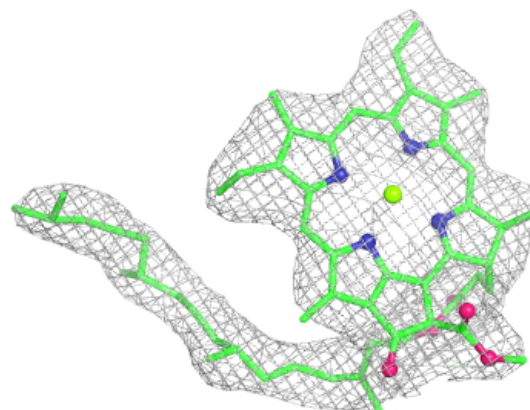


Electron density around CLA A 803:

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

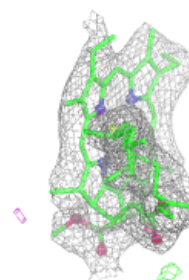
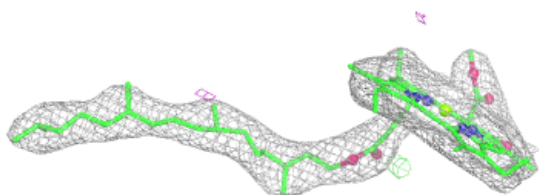
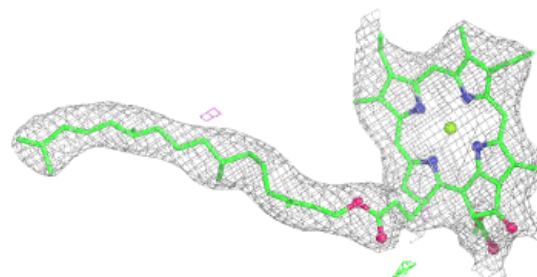
**Electron density around CLA A 830:**

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

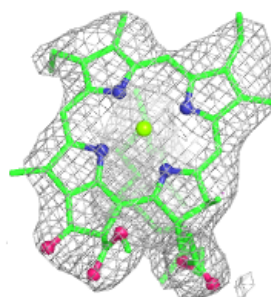
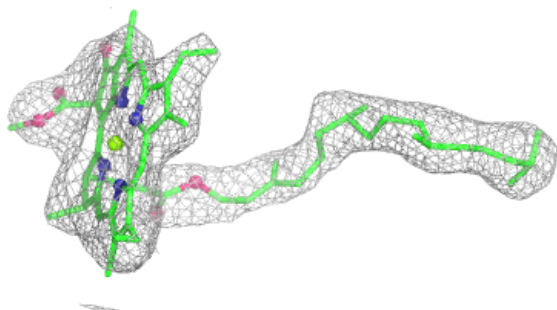
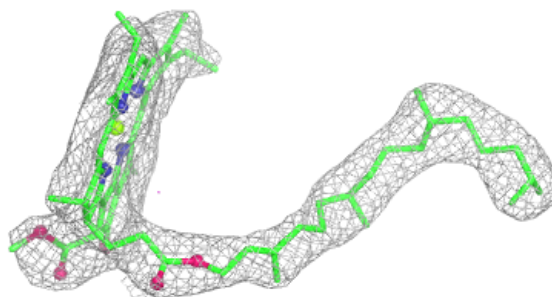


Electron density around CLA a 835:

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

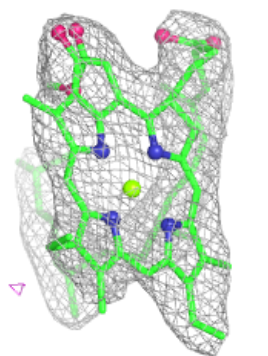
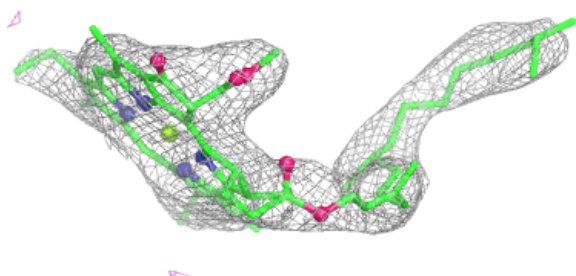
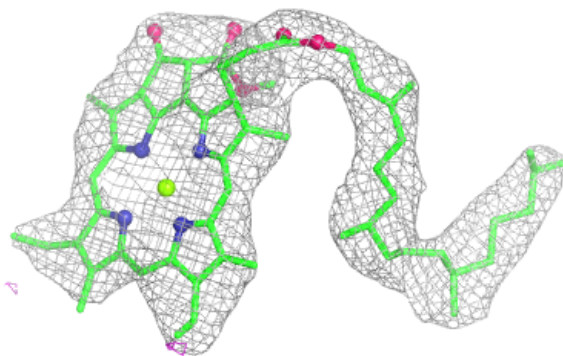
**Electron density around CLA A 831:**

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

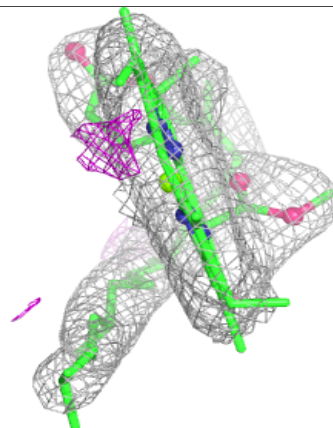
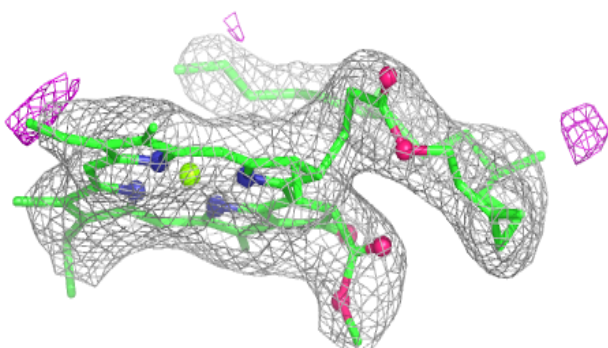
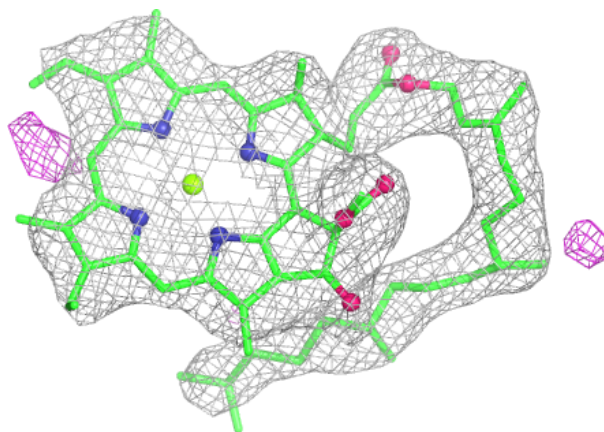


Electron density around CLA b 824:

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

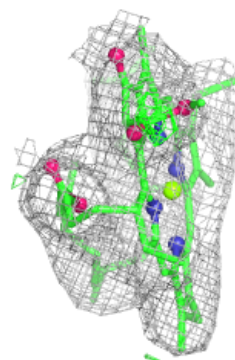
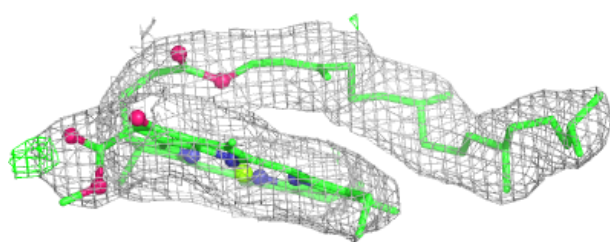
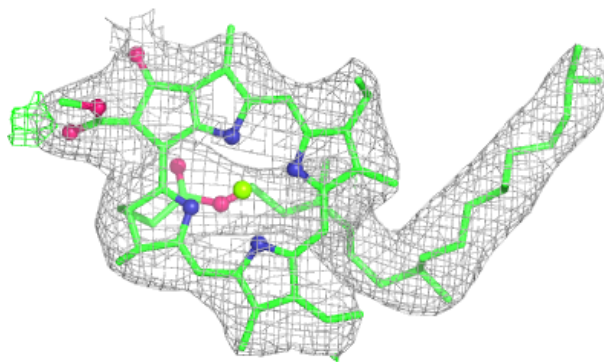
**Electron density around CLA B 805:**

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

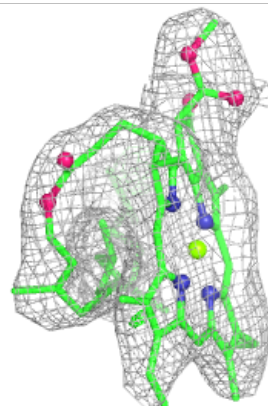
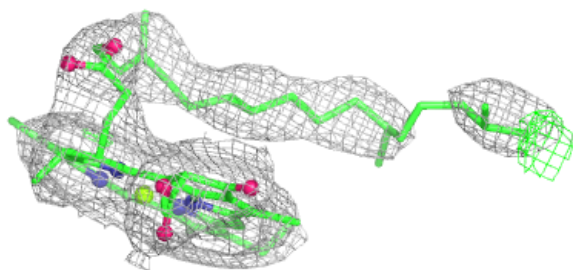
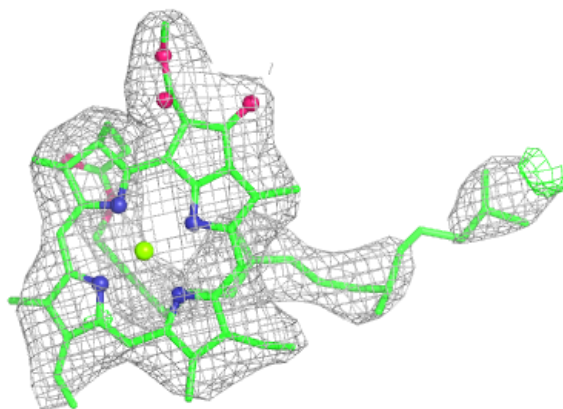


Electron density around CLA B 837:

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

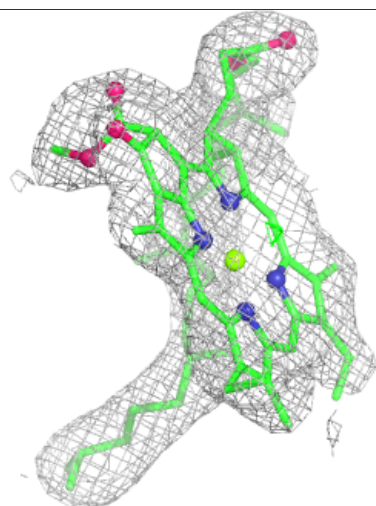
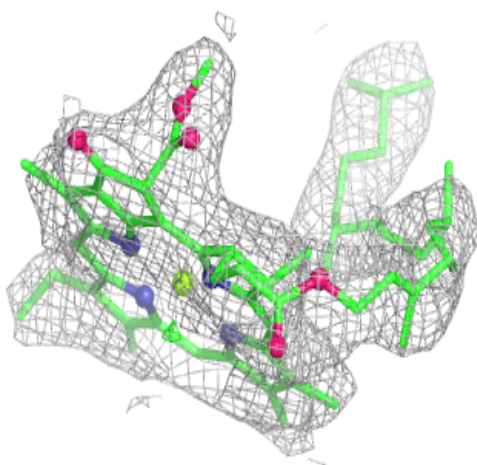
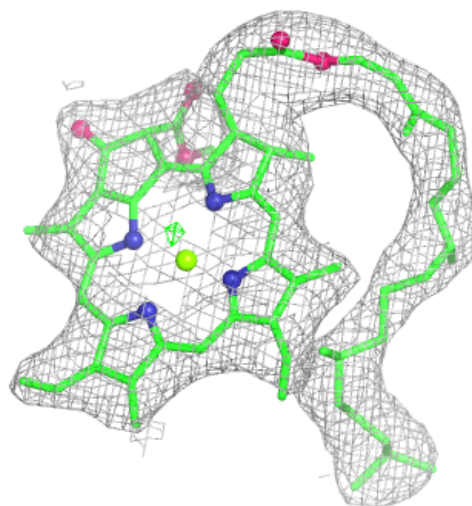
**Electron density around CLA b 827:**

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



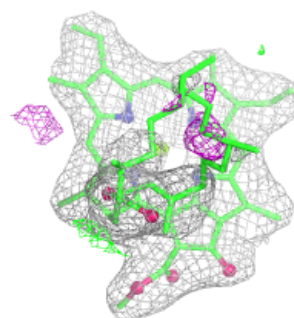
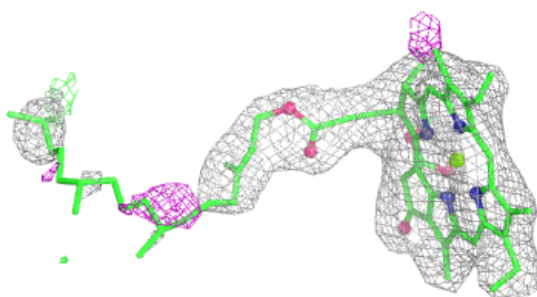
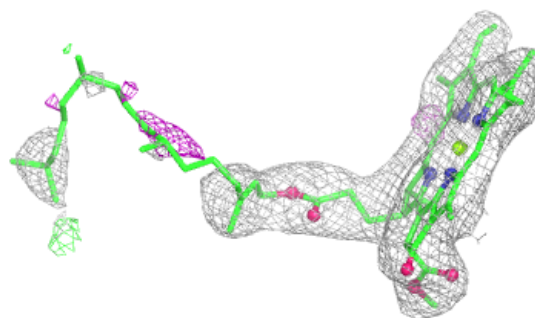
Electron density around CLA a 814:

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

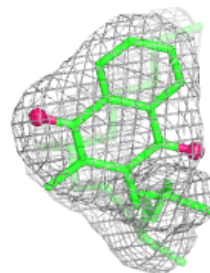
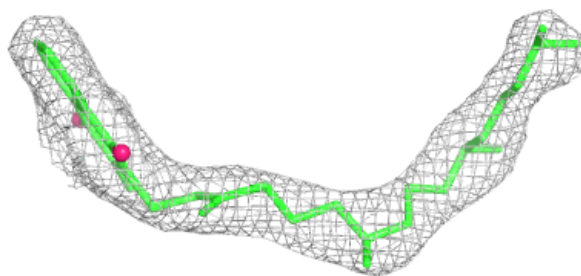


Electron density around CLA a 840:

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

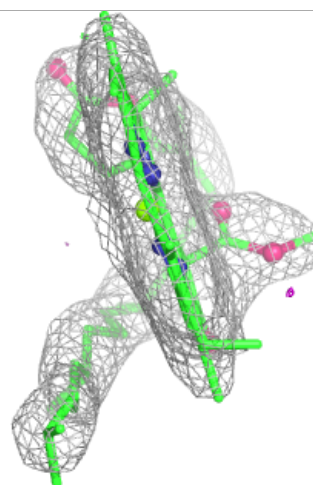
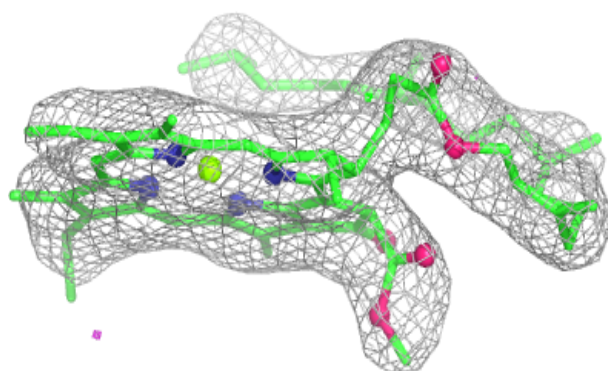
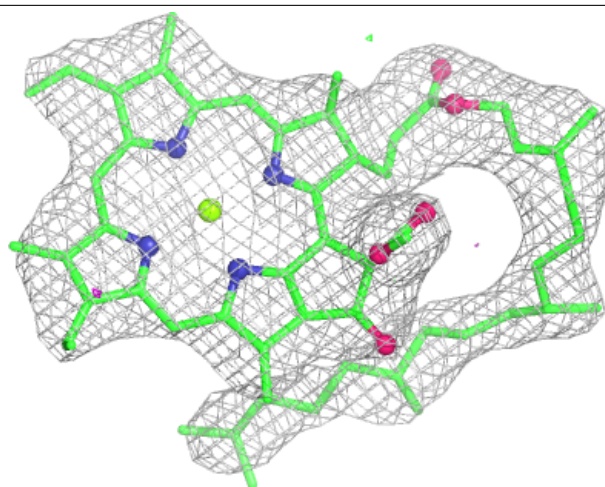
**Electron density around PQN b 842:**

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



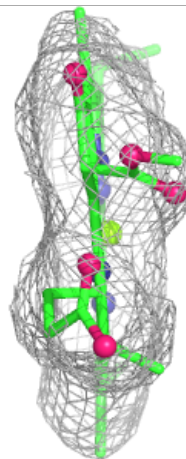
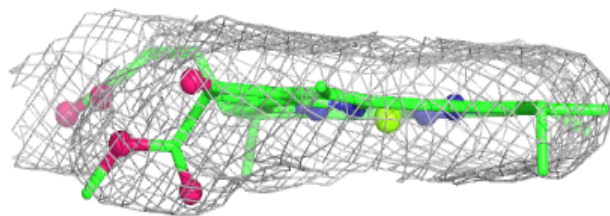
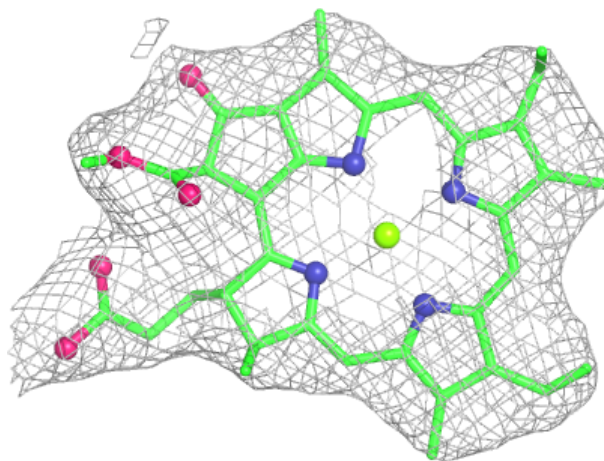
Electron density around CLA b 805:

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



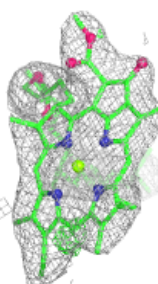
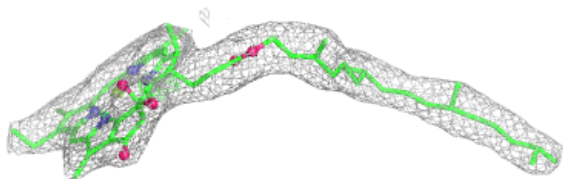
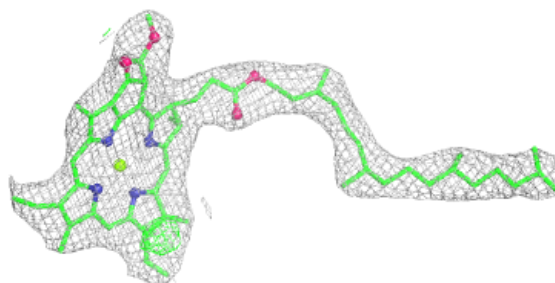
Electron density around CLA f 7002:

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

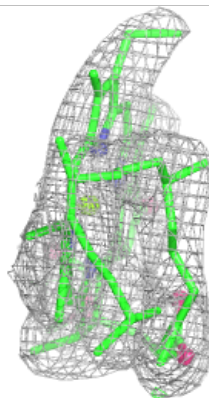
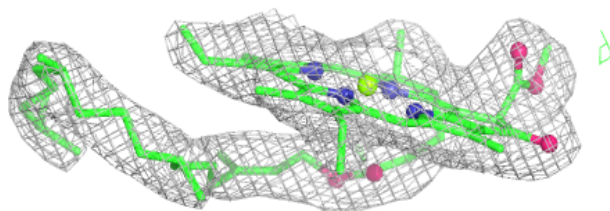
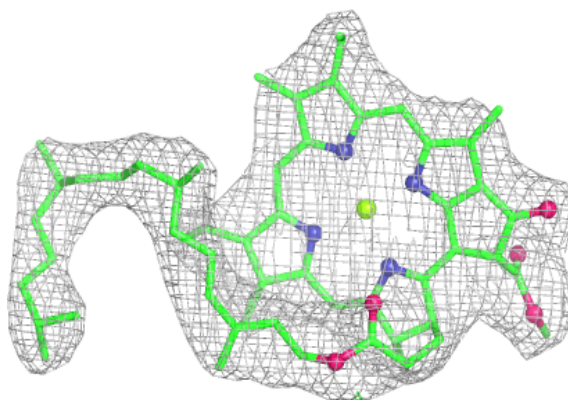


Electron density around CLA a 803:

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

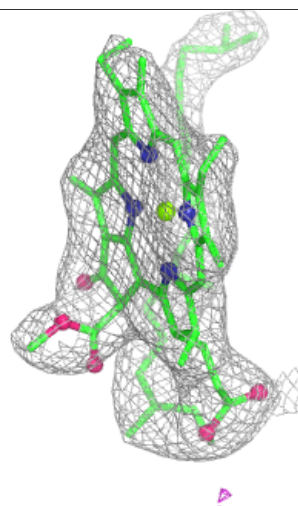
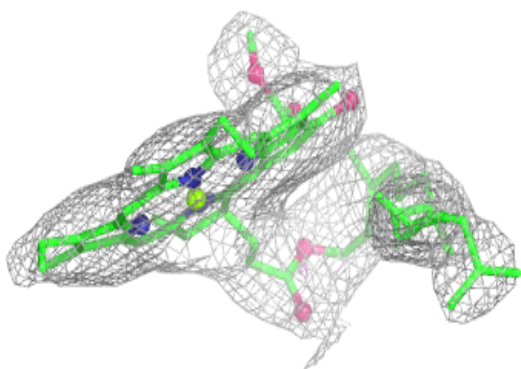
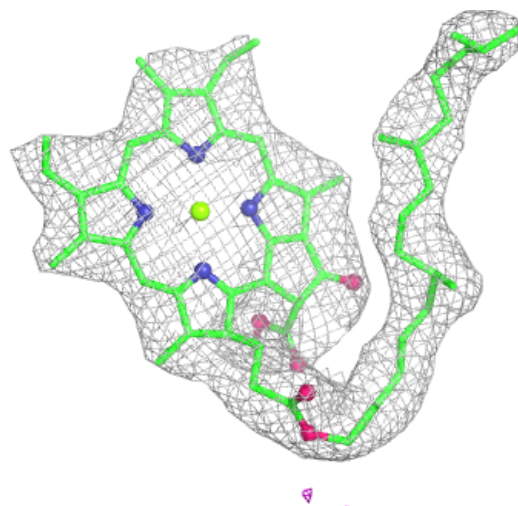
**Electron density around CLA a 820:**

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



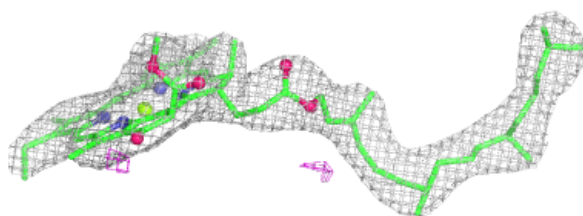
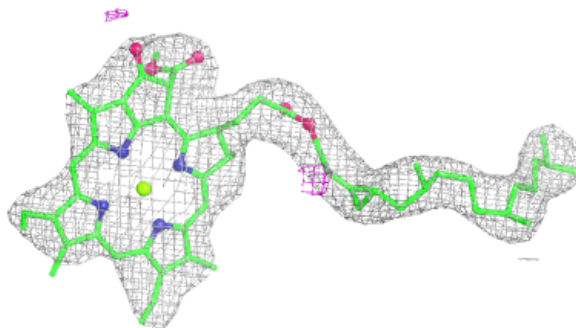
Electron density around CLA a 826:

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

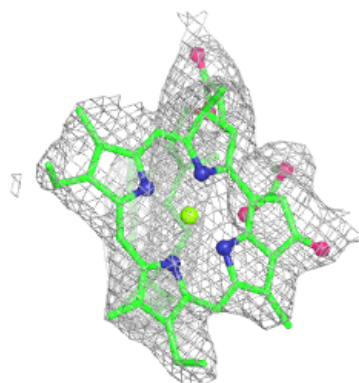
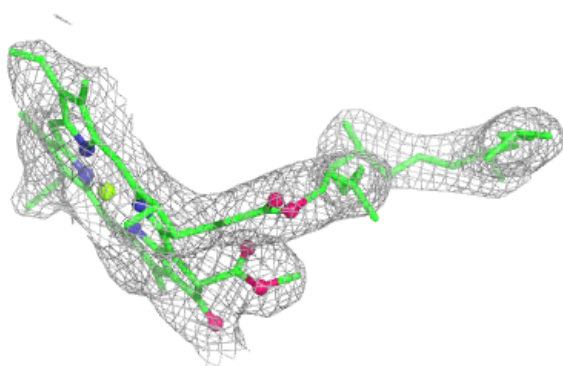
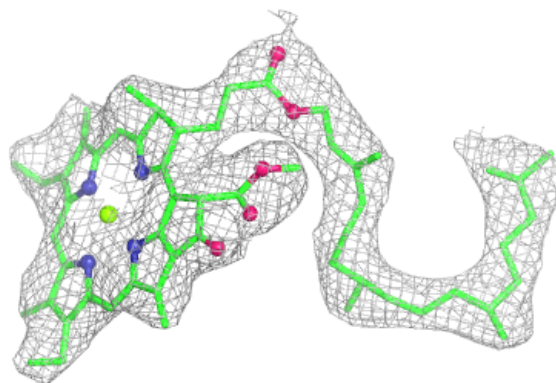


Electron density around CLA B 813:

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

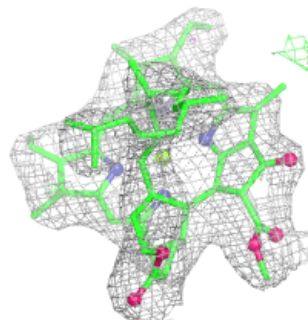
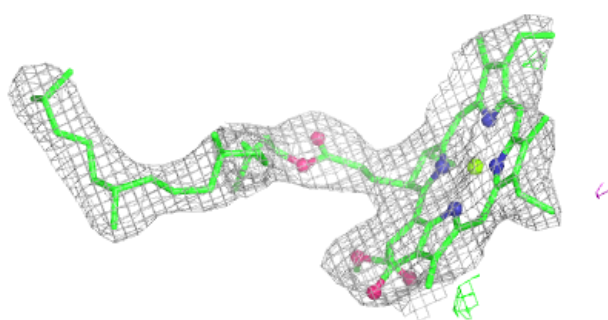
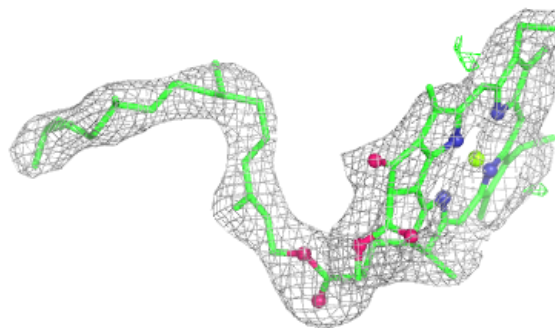
**Electron density around CLA a 801:**

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

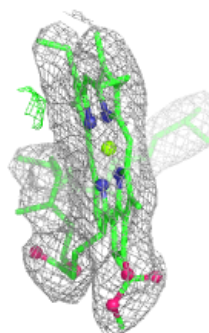
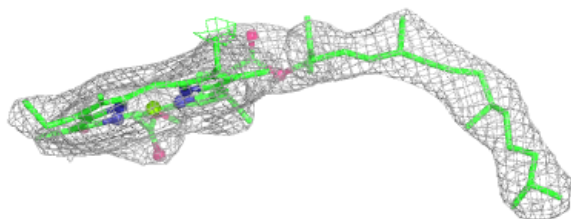
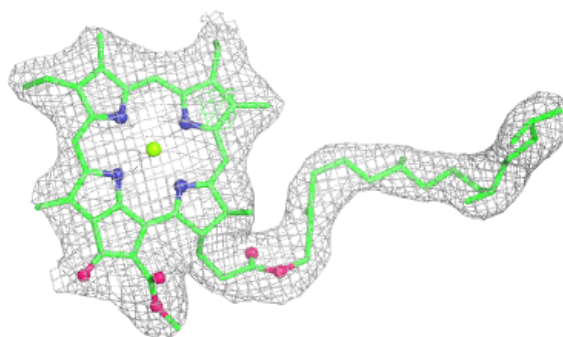


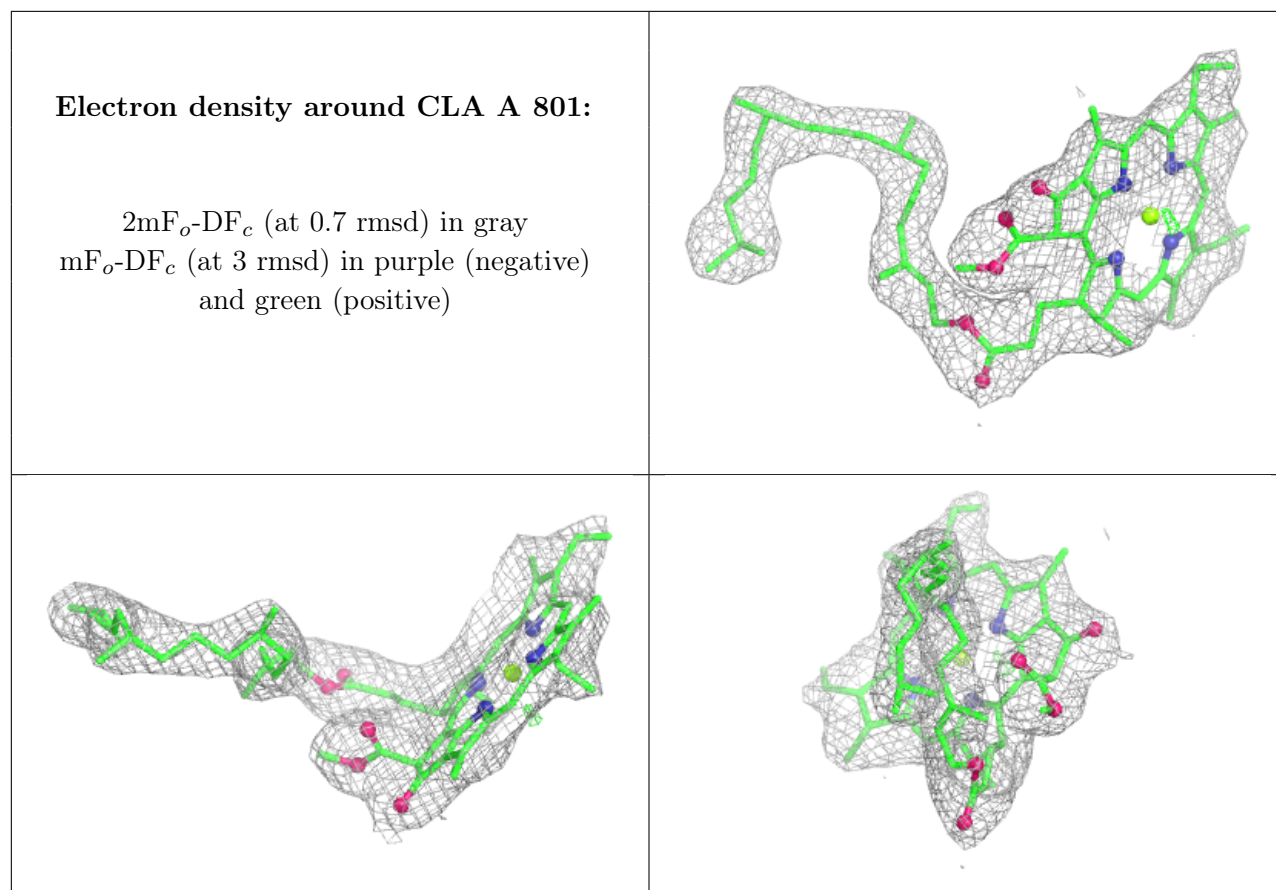
Electron density around CLA b 802:

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

**Electron density around CLA b 803:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.