



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:28 AM UTC

PDB ID : 6QPH / pdb_00006qph
Title : Dunaliella minimal PSI complex
Authors : Klaiman, D.; Caspy, I.; Nelson, N.
Deposited on : 2019-02-14
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

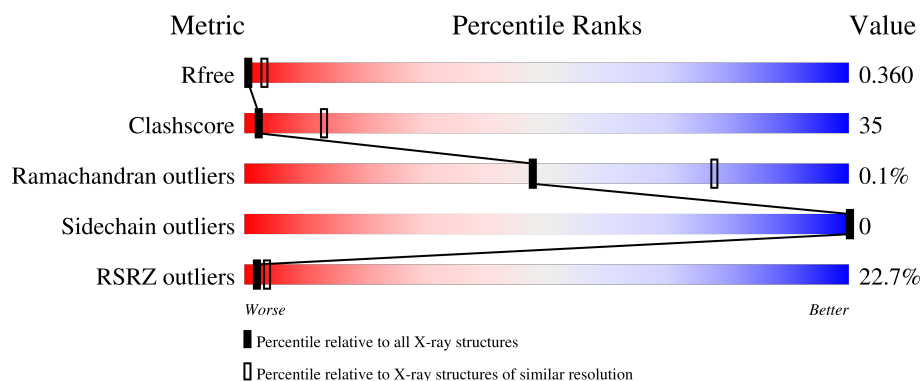
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	195	21% 57% 43%
2	2	211	23% 61% 39%
3	3	210	33% 51% 49%
4	4	211	24% 60% 40%
5	A	739	25% 48% 52%

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Mol	Chain	Length	Quality of chain
6	B	734	
7	C	80	
8	D	142	
9	E	64	
10	F	163	
11	J	41	

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
13	XAT	2	502	X	-	-	-
13	XAT	3	502	X	-	X	-
13	XAT	4	502	X	-	-	-
15	CLA	1	601	X	-	-	-
15	CLA	1	602	X	-	-	-
15	CLA	1	603	X	-	-	-
15	CLA	1	604	X	-	-	-
15	CLA	1	605	X	-	-	-
15	CLA	1	606	X	-	-	-
15	CLA	1	607	X	-	-	-
15	CLA	1	608	X	-	-	-
15	CLA	1	611	X	-	-	-
15	CLA	1	612	X	-	-	-
15	CLA	1	613	X	-	X	-
15	CLA	1	615	X	-	-	-
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	-
15	CLA	2	607	X	-	-	-
15	CLA	2	608	X	-	-	-
15	CLA	2	612	X	-	-	-
15	CLA	2	615	X	-	-	-
15	CLA	3	601	X	-	-	-
15	CLA	3	603	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	3	605	X	-	-	-
15	CLA	3	606	X	-	-	-
15	CLA	3	607	X	-	-	-
15	CLA	3	608	X	-	-	-
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	613	X	-	-	-
15	CLA	3	615	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	-
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	607	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	612	X	-	-	-
15	CLA	4	615	X	-	-	-
15	CLA	A	1012	X	-	X	-
15	CLA	A	1013	X	-	X	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	X	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	-	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	X	-	-	-
15	CLA	A	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1141	X	-	-	-
15	CLA	B	1021	X	-	X	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1023	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1207	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1210	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	-	-
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1219	X	-	-	-
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
16	CHL	1	609	X	-	-	-
16	CHL	1	610	X	-	-	-
16	CHL	2	609	X	-	-	-
16	CHL	2	610	X	-	-	-
16	CHL	2	611	X	-	-	-
16	CHL	2	613	X	-	-	-
16	CHL	3	604	X	-	-	-
16	CHL	4	610	X	-	-	-
16	CHL	4	611	X	-	-	-
16	CHL	4	613	X	-	-	-
24	CL0	A	1011	X	-	-	-
26	SF4	C	3003	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 30870 atoms, of which 32 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	195	Total	C	N	O	S	0	0	0
			1490	956	253	274	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 2 is a protein called Lhc2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	211	Total	C	H	N	O	S	0	0
			1663	1047	32	277	300	7		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	210	Total	C	N	O	S	0	0	0
			1609	1050	263	291	5			

- Molecule 4 is a protein called Lhc4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	211	Total	C	N	O	S	0	0	0
			1637	1058	272	303	4			

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	739	Total	C	N	O	S	0	0	0
			5799	3789	991	1001	18			

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	734	Total	C	N	O	S	0	0	0
			5813	3818	975	1007	13			

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	80	Total	C	N	O	S	0	0	0
			600	370	104	115	11			

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	142	Total	C	N	O	S	0	0	0
			1123	718	195	204	6			

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	64	Total	C	N	O	0	0	0
			515	327	89	99			

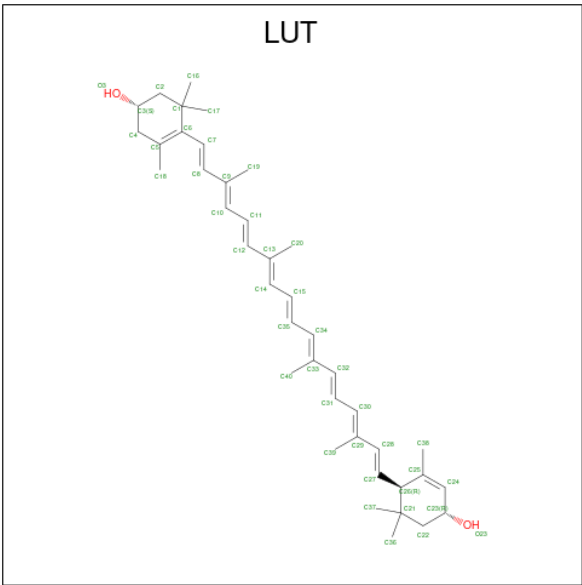
- Molecule 10 is a protein called PsaF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	163	Total	C	N	O	S	0	0	0
			1285	828	218	237	2			

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

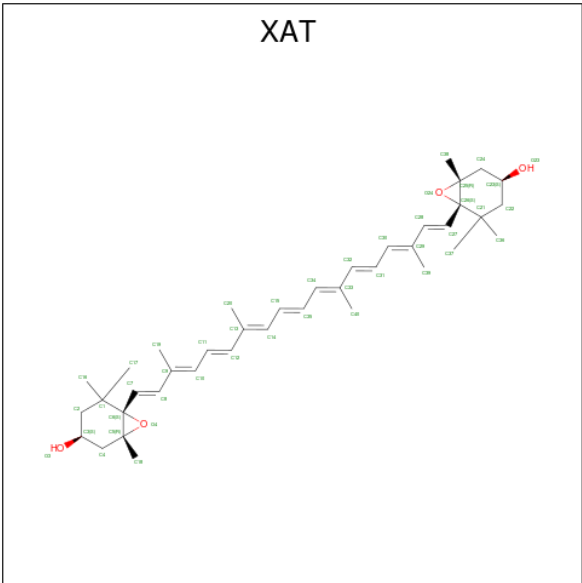
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	41	Total	C	N	O	S	0	0	0
			327	223	47	56	1			

- Molecule 12 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



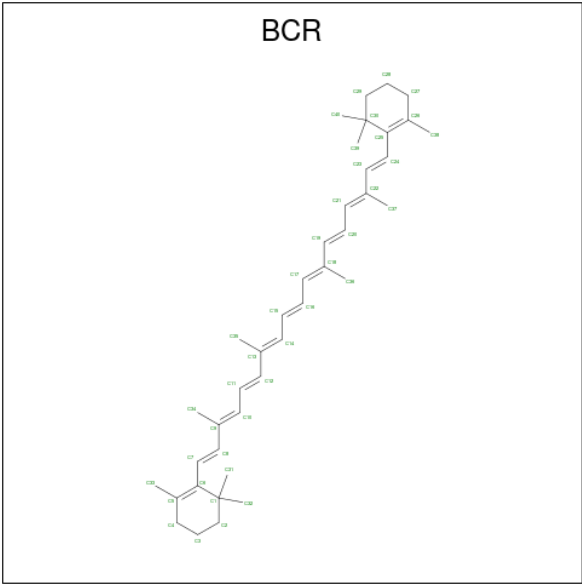
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			42	40	2		
12	2	1	Total	C	O	0	0
			42	40	2		
12	3	1	Total	C	O	0	0
			42	40	2		
12	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 13 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
13	1	1	Total	C	O	0	0
			44	40	4		
13	2	1	Total	C	O	0	0
			44	40	4		
13	3	1	Total	C	O	0	0
			44	40	4		
13	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



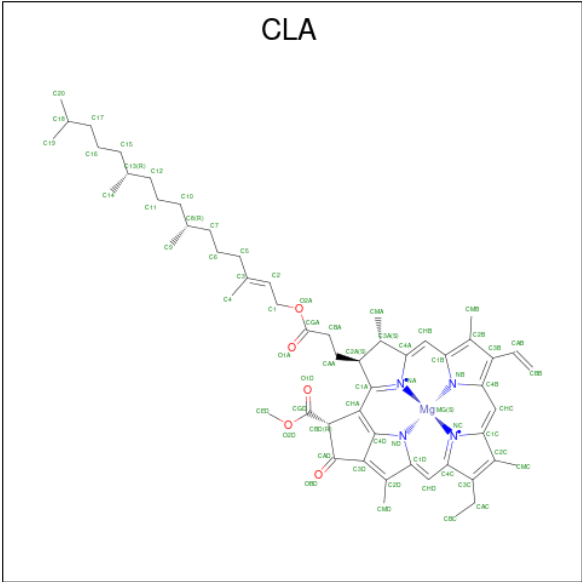
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	1	1	Total	C	0	0
			40	40		
14	1	1	Total	C	0	0
			40	40		
14	2	1	Total	C	0	0
			40	40		
14	3	1	Total	C	0	0
			40	40		
14	3	1	Total	C	0	0
			40	40		
14	4	1	Total	C	0	0
			40	40		
14	4	1	Total	C	0	0
			40	40		
14	A	1	Total	C	0	0
			40	40		

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

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	4	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	4	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
15	A	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	A	1	Total 48	C 38	Mg 1	N 4	O 5	0	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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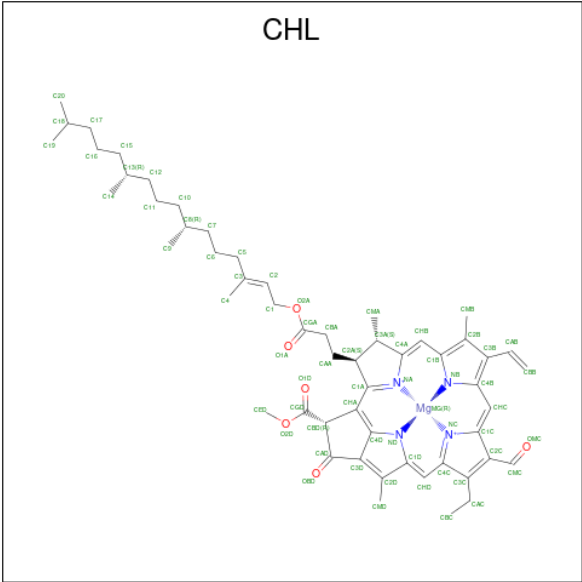
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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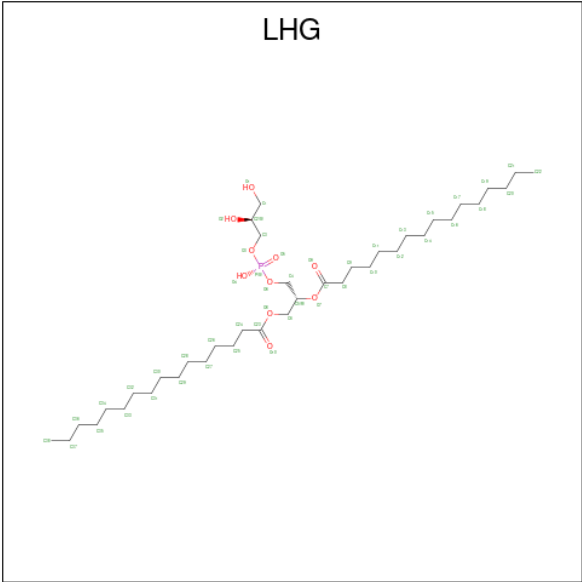
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
15	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
15	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	B	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
15	F	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
15	F	1	Total 49	C 39	Mg 1	N 4	O 5	0	0
15	J	1	Total 49	C 39	Mg 1	N 4	O 5	0	0

- Molecule 16 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



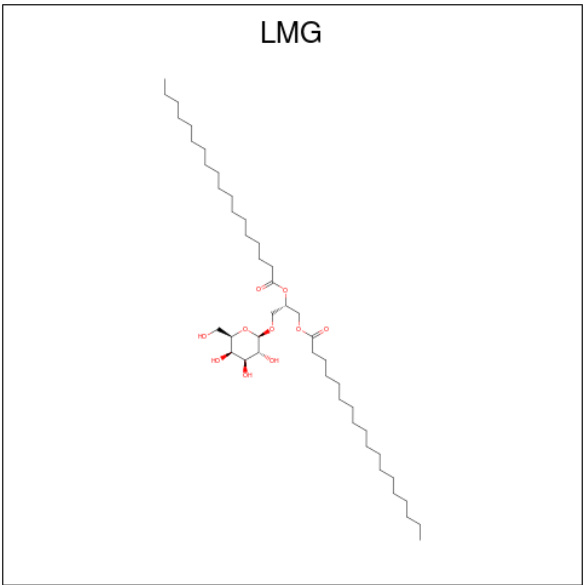
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	1	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
16	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	4	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



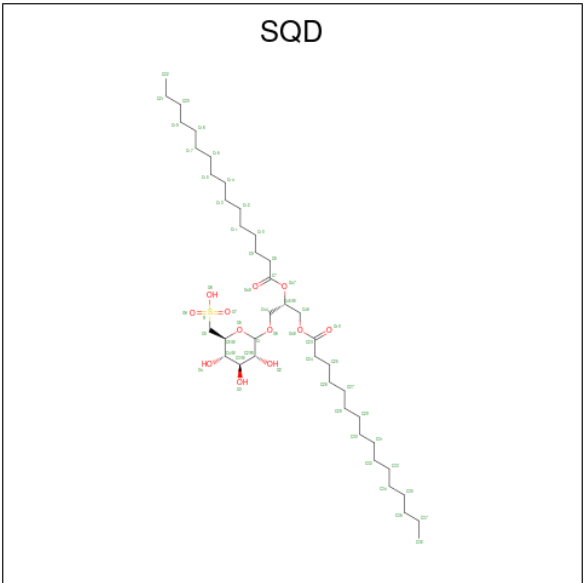
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	1	1	Total	C	O	P	0	0
			23	12	10	1		
17	2	1	Total	C	O	P	0	0
			21	10	10	1		
17	A	1	Total	C	O	P	0	0
			16	7	8	1		
17	A	1	Total	C	O	P	0	0
			24	13	10	1		
17	B	1	Total	C	O	P	0	0
			21	10	10	1		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



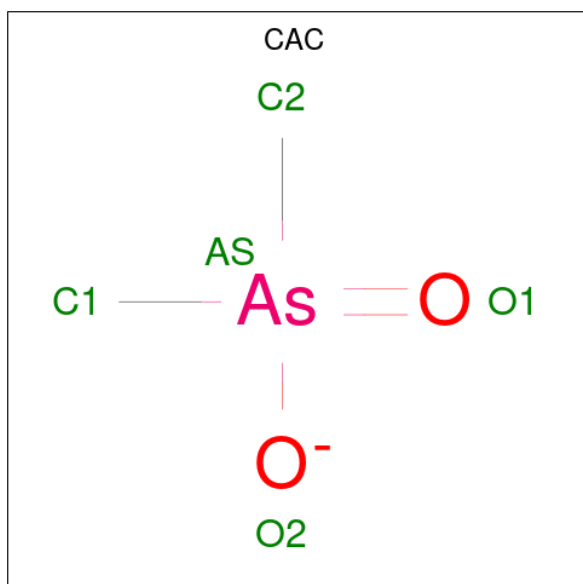
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	1	1	Total	C	O	0	0
			36	26	10		
18	1	1	Total	C	O	0	0
			23	13	10		
18	2	1	Total	C	O	0	0
			25	15	10		
18	2	1	Total	C	O	0	0
			16	9	7		

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



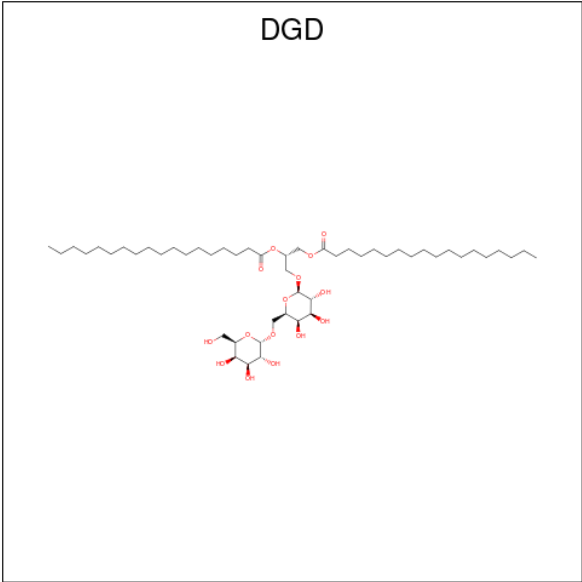
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	1	1	Total	C	O	S	0	0
			40	27	12	1		

- Molecule 20 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



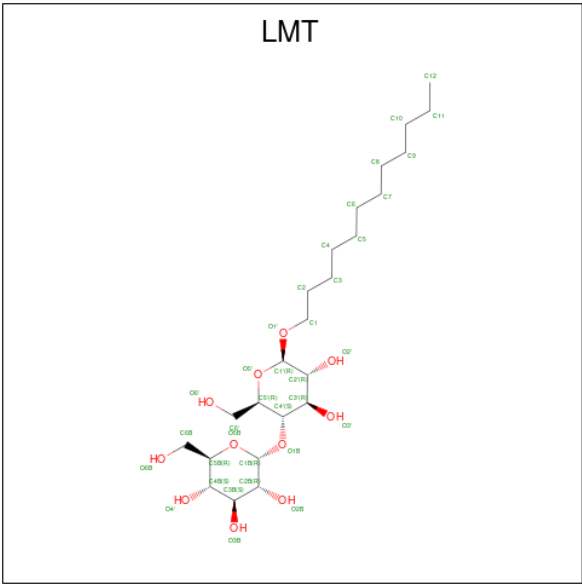
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 21 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



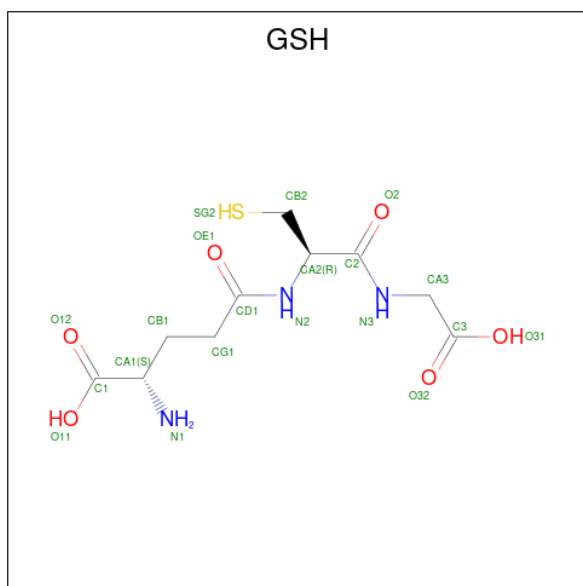
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			47	32	15		
21	4	1	Total	C	O	0	0
			45	30	15		
21	B	1	Total	C	O	0	0
			38	23	15		
21	J	1	Total	C	O	0	0
			28	15	13		

- Molecule 22 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



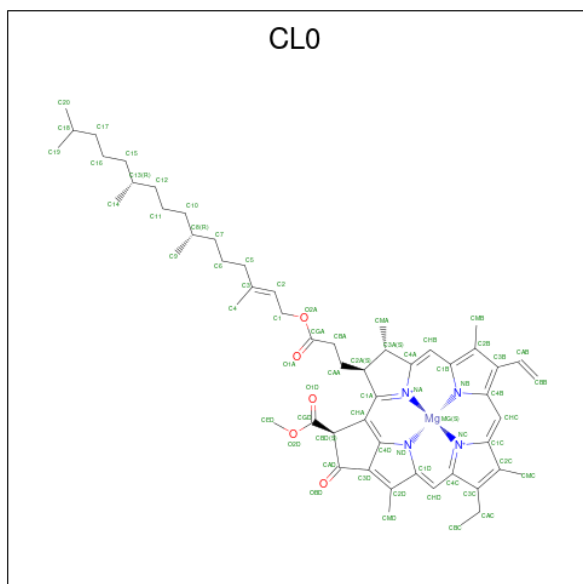
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	2	1	Total	C	O	0	0
			23	12	11		

- Molecule 23 is GLUTATHIONE (CCD ID: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



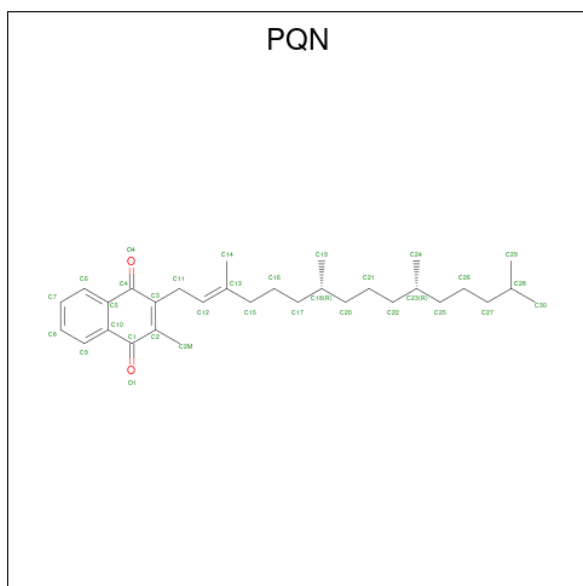
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	4	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
23	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



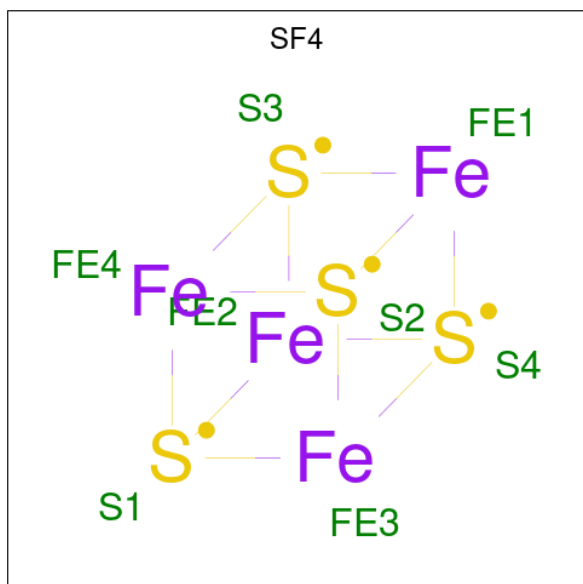
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	
			50	40	1	4	5	
							0	0

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

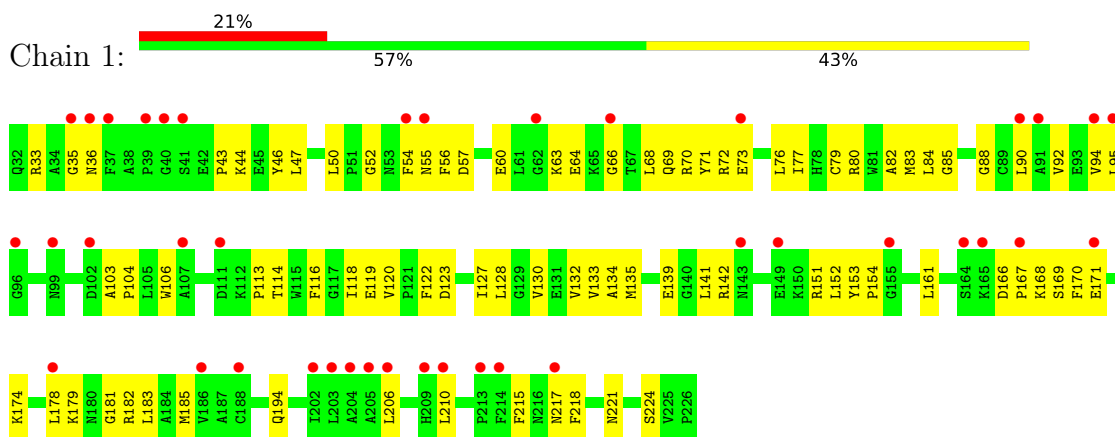
- Molecule 27 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total 1	Ca 1	0	0

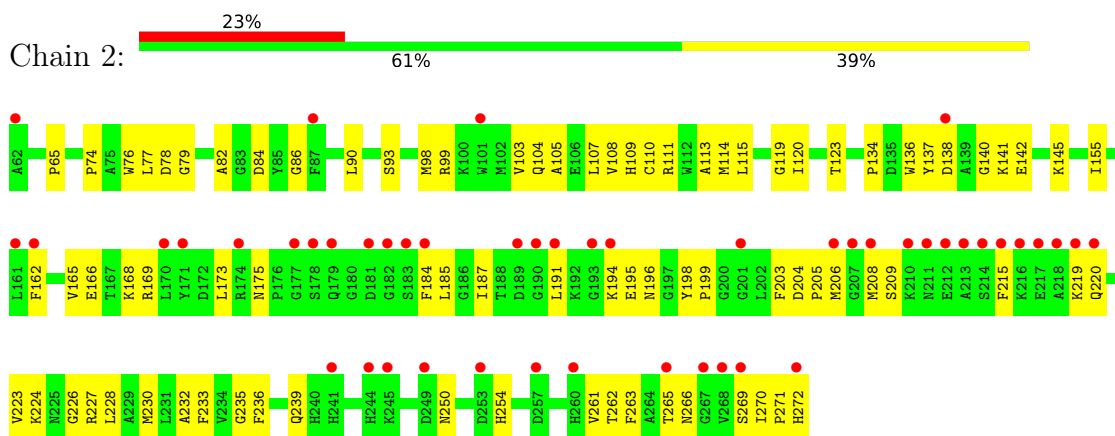
3 Residue-property plots [i](#)

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

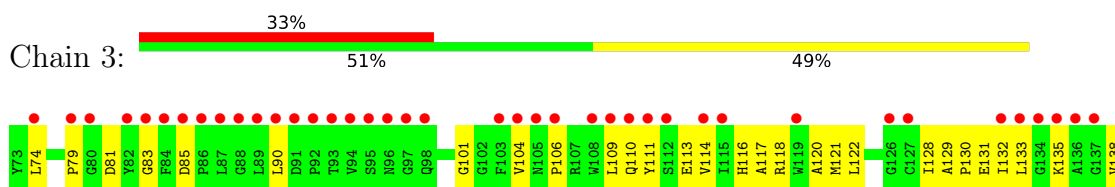
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

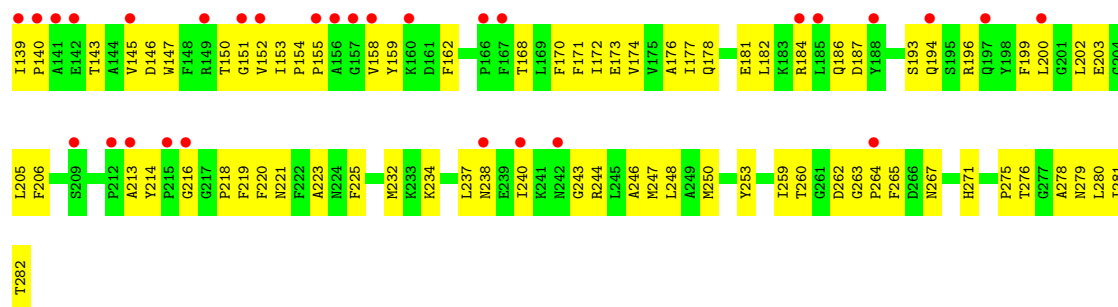


- Molecule 2: Lhc2

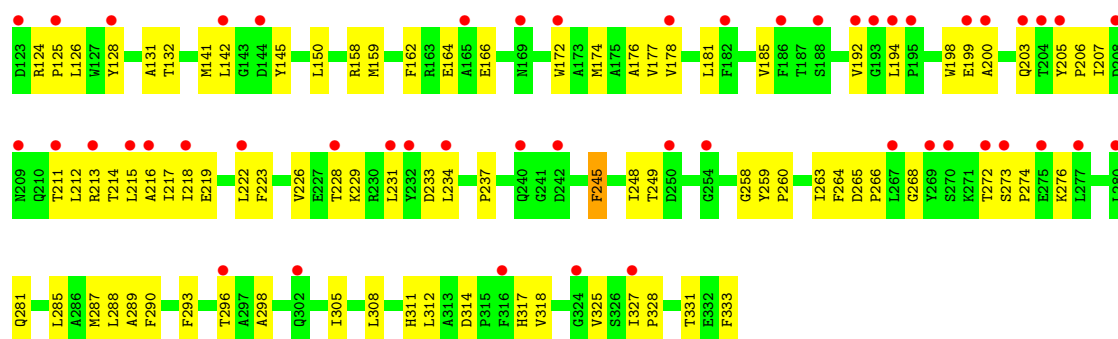


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

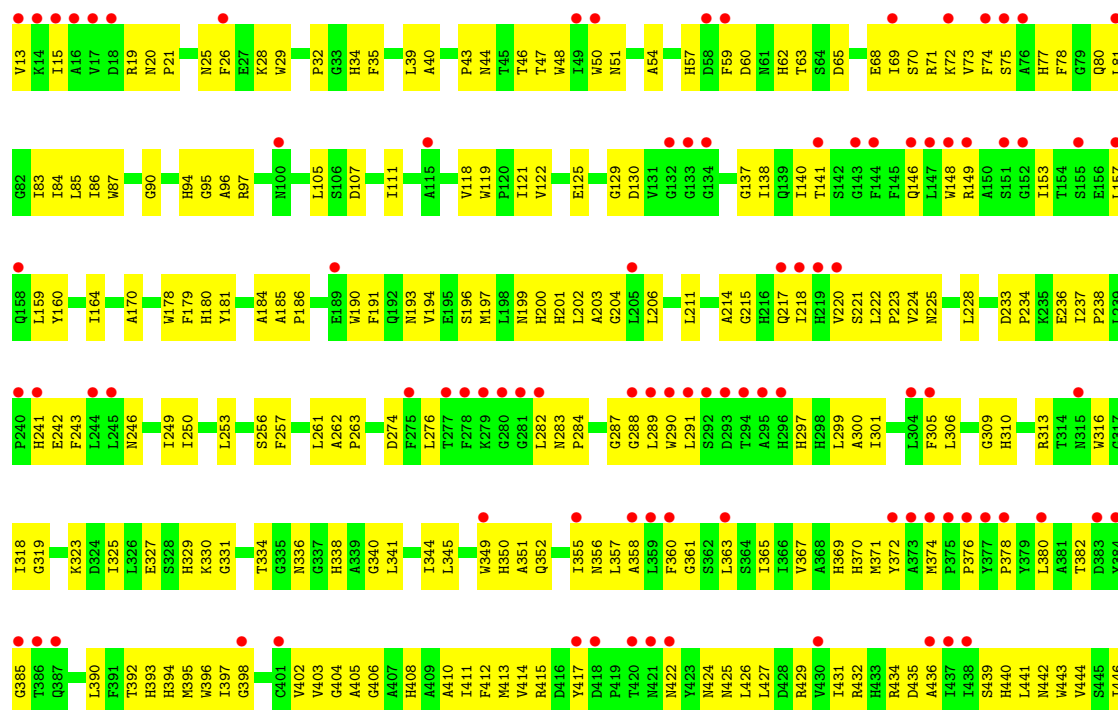


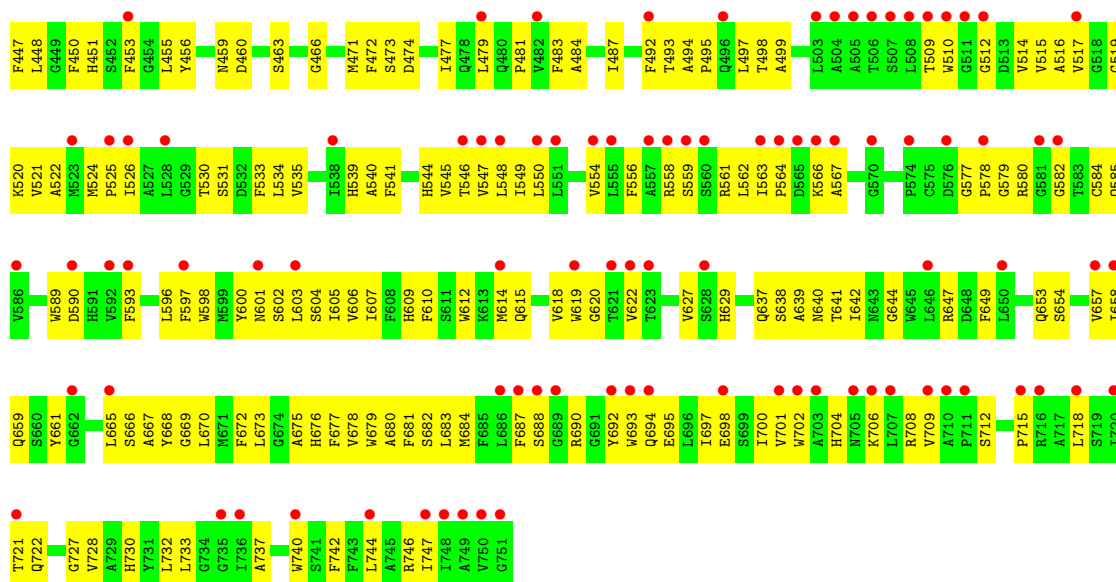


● Molecule 4: Lhc4

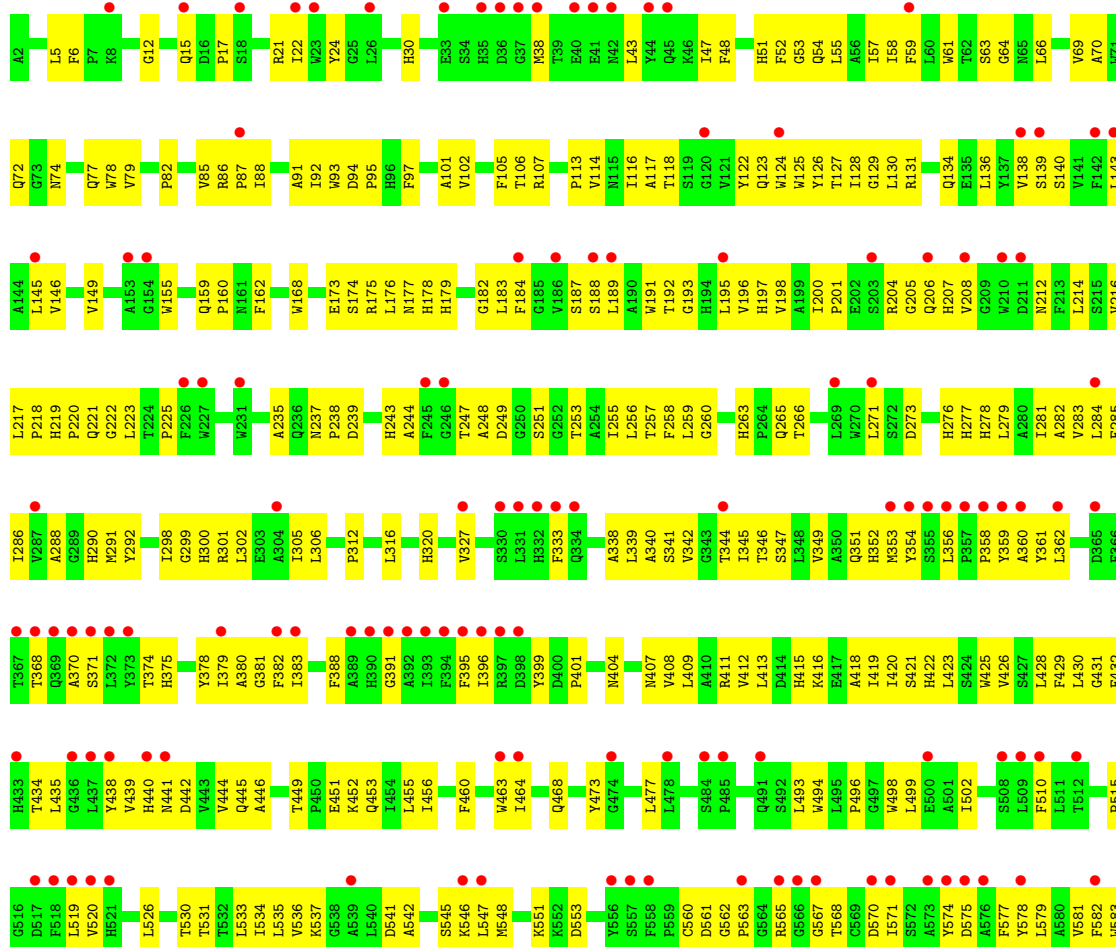


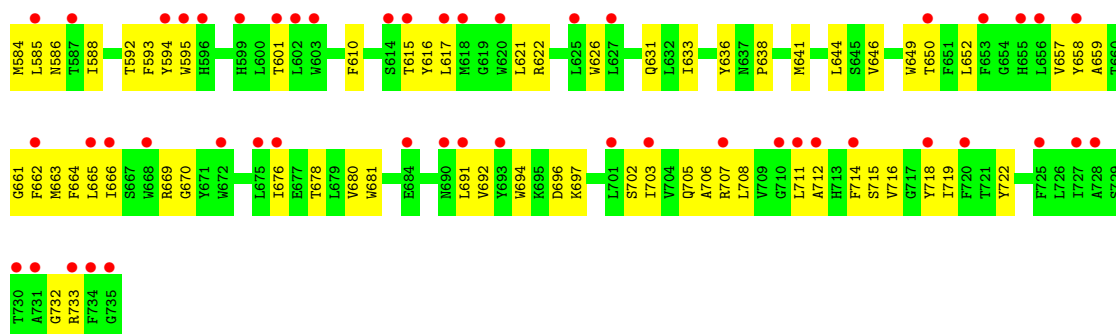
● Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



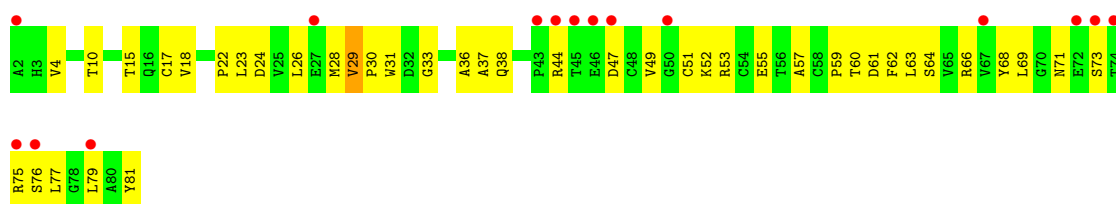


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

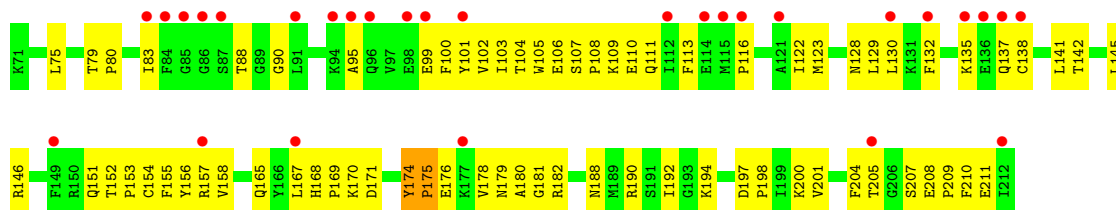




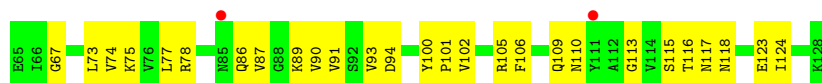
• Molecule 7: Photosystem I iron-sulfur center



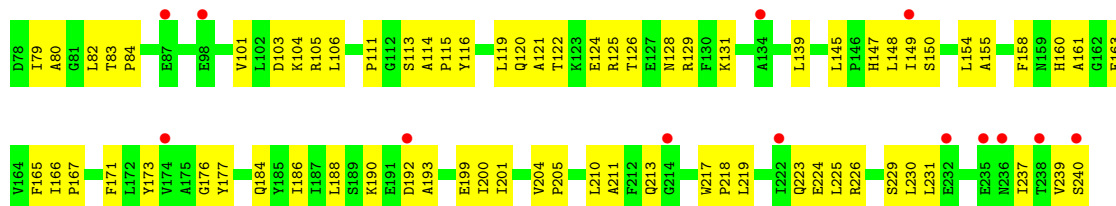
• Molecule 8: PsaD



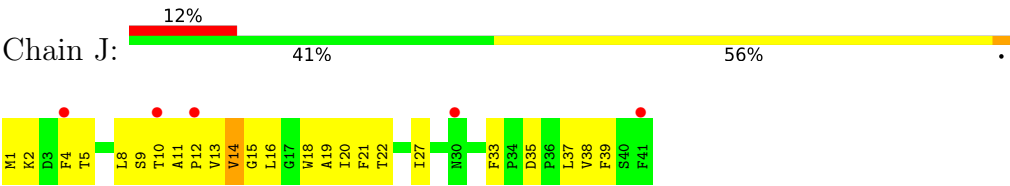
• Molecule 9: PsaE



• Molecule 10: PsaF



● Molecule 11: Photosystem I reaction center subunit IX



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	158.88Å 100.51Å 191.04Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	48.95 – 3.40 48.95 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.95-3.40) 89.4 (48.95-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.337 , 0.356 0.339 , 0.360	Depositor DCC
R_{free} test set	1593 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 17.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	30870	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: SQD, SF4, XAT, DGD, LHG, CHL, BCR, CA, CLA, LUT, LMT, LMG, CL0, GSH, PQN, CAC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.31	0/1529	0.34	0/2073
2	2	0.27	0/1680	0.34	0/2277
3	3	0.16	0/1657	0.36	0/2253
4	4	0.39	0/1687	0.41	0/2300
5	A	0.23	1/5995 (0.0%)	0.27	0/8179
6	B	0.26	0/6026	0.28	0/8237
7	C	0.24	0/610	0.30	0/828
8	D	0.21	0/1150	0.40	0/1551
9	E	0.34	0/525	0.31	0/712
10	F	0.40	0/1313	0.38	0/1776
11	J	0.38	0/338	0.45	0/461
All	All	0.28	1/22510 (0.0%)	0.32	0/30647

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	4	0	2
7	C	0	1
11	J	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	20	ASN	C-O	-5.06	1.21	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	213	ARG	Peptide
4	4	245	PHE	Peptide
7	C	29	VAL	Peptide
11	J	14	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1490	0	1457	108	1
2	2	1631	32	1575	112	0
3	3	1609	0	1567	138	0
4	4	1637	0	1579	139	0
5	A	5799	0	5629	446	0
6	B	5813	0	5565	403	0
7	C	600	0	582	52	0
8	D	1123	0	1134	83	0
9	E	515	0	508	21	0
10	F	1285	0	1304	91	0
11	J	327	0	328	46	0
12	1	42	0	55	10	0
12	2	42	0	55	13	0
12	3	42	0	55	11	0
12	4	42	0	55	18	0
13	1	44	0	56	11	0
13	2	44	0	56	13	0
13	3	44	0	56	21	0
13	4	44	0	56	5	0
14	1	80	0	105	15	0
14	2	40	0	53	8	0
14	3	80	0	105	25	0
14	4	80	0	105	12	0
14	A	240	0	318	39	0
14	B	240	0	316	34	0
14	F	40	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	J	120	0	159	27	0
15	1	593	0	468	105	0
15	2	501	0	402	58	0
15	3	525	0	391	96	0
15	4	542	0	423	82	0
15	A	2180	0	1773	276	0
15	B	2137	0	1760	230	0
15	F	96	0	72	7	0
15	J	49	0	38	9	0
16	1	97	0	66	26	0
16	2	194	0	134	25	0
16	3	47	0	30	15	0
16	4	147	0	102	22	0
17	1	23	0	16	2	0
17	2	21	0	12	2	0
17	A	40	0	30	5	0
17	B	21	0	12	2	0
18	1	59	0	58	1	0
18	2	41	0	34	1	0
19	1	40	0	46	4	0
20	1	10	0	0	0	0
20	3	10	0	0	1	0
20	4	10	0	0	1	0
21	2	47	0	52	2	0
21	4	45	0	48	7	0
21	B	38	0	34	5	0
21	J	28	0	26	0	0
22	2	23	0	21	0	0
23	4	20	0	15	0	1
23	B	20	0	15	2	0
24	A	50	0	39	19	0
25	A	33	0	46	9	0
25	B	33	0	46	8	0
26	A	8	0	0	0	0
26	C	16	0	0	2	0
27	B	1	0	0	0	0
All	All	30838	32	29094	2127	1

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 35.

The worst 5 of 2127 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)
14:A:4005:BCR:C11	14:A:4005:BCR:C12	1.83	1.49
14:A:4005:BCR:C11	14:A:4005:BCR:C10	1.92	1.45
7:C:29:VAL:HG12	7:C:30:PRO:HD3	1.20	1.17
8:D:105:TRP:HB3	8:D:153:PRO:HB3	1.40	1.02
6:B:5:LEU:HD13	6:B:6:PHE:H	1.24	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:168:LYS:NZ	23:4:831:GSH:O31[2_555]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
2	2	209/211 (99%)	194 (93%)	15 (7%)	0	100	100
3	3	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
4	4	209/211 (99%)	184 (88%)	25 (12%)	0	100	100
5	A	737/739 (100%)	702 (95%)	35 (5%)	0	100	100
6	B	732/734 (100%)	695 (95%)	37 (5%)	0	100	100
7	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
8	D	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	9	31
9	E	62/64 (97%)	54 (87%)	8 (13%)	0	100	100
10	F	161/163 (99%)	145 (90%)	16 (10%)	0	100	100
11	J	39/41 (95%)	30 (77%)	9 (23%)	0	100	100
All	All	2768/2790 (99%)	2588 (94%)	178 (6%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	175	PRO
8	D	174	TYR

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	1	151/151 (100%)	151 (100%)	0	100	100
2	2	169/169 (100%)	169 (100%)	0	100	100
3	3	160/160 (100%)	160 (100%)	0	100	100
4	4	169/169 (100%)	169 (100%)	0	100	100
5	A	598/598 (100%)	598 (100%)	0	100	100
6	B	593/593 (100%)	593 (100%)	0	100	100
7	C	68/68 (100%)	68 (100%)	0	100	100
8	D	122/122 (100%)	122 (100%)	0	100	100
9	E	57/57 (100%)	57 (100%)	0	100	100
10	F	136/136 (100%)	136 (100%)	0	100	100
11	J	36/36 (100%)	36 (100%)	0	100	100
All	All	2259/2259 (100%)	2259 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	90	HIS
6	B	320	HIS
10	F	136	GLN
6	B	159	GLN
6	B	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 203 ligands modelled in this entry, 1 is monoatomic - leaving 202 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	CLA	4	601	4	53,57,73	1.53	9 (16%)	61,93,113	2.10	20 (32%)
15	CLA	B	1240	17	69,73,73	1.38	7 (10%)	82,113,113	1.83	17 (20%)
23	GSH	4	831	-	18,19,19	2.05	4 (22%)	21,24,24	1.56	2 (9%)
26	SF4	A	3001	6,5	0,12,12	-	-	-		
15	CLA	2	606	-	50,54,73	1.65	8 (16%)	59,90,113	2.09	16 (27%)
15	CLA	A	1132	-	53,57,73	1.54	8 (15%)	61,93,113	2.14	16 (26%)
17	LHG	1	801	15	22,22,48	0.57	0	25,28,54	1.36	3 (12%)
15	CLA	A	1110	-	53,57,73	1.52	7 (13%)	61,93,113	2.14	18 (29%)
15	CLA	A	1138	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	16 (19%)
15	CLA	B	1211	-	53,57,73	1.54	8 (15%)	61,93,113	2.10	15 (24%)
15	CLA	1	611	-	53,57,73	1.57	7 (13%)	61,93,113	2.10	18 (29%)
26	SF4	C	3002	7	0,12,12	-	-	-		
15	CLA	3	607	-	54,58,73	1.53	7 (12%)	64,95,113	2.05	18 (28%)
15	CLA	B	1203	-	53,57,73	1.54	6 (11%)	61,93,113	2.12	16 (26%)
20	CAC	3	902	-	2,4,4	2.75	2 (100%)	4,6,6	1.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1136	-	53,57,73	1.56	7 (13%)	61,93,113	2.10	15 (24%)
14	BCR	4	505	-	41,41,41	1.61	4 (9%)	56,56,56	4.68	19 (33%)
14	BCR	B	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.76	19 (33%)
15	CLA	A	1012	-	64,68,73	1.48	9 (14%)	76,107,113	1.91	18 (23%)
15	CLA	A	1120	-	53,57,73	1.55	7 (13%)	61,93,113	2.13	18 (29%)
15	CLA	4	608	-	50,54,73	1.57	7 (14%)	59,90,113	2.02	14 (23%)
15	CLA	A	1141	-	54,58,73	1.53	7 (12%)	64,95,113	2.07	18 (28%)
15	CLA	B	1219	-	53,57,73	1.52	8 (15%)	61,93,113	2.09	16 (26%)
15	CLA	A	1117	-	53,57,73	1.56	8 (15%)	61,93,113	2.14	17 (27%)
13	XAT	1	502	-	41,47,47	0.73	1 (2%)	54,74,74	2.00	10 (18%)
15	CLA	2	602	-	53,57,73	1.56	8 (15%)	61,93,113	2.16	16 (26%)
15	CLA	B	1223	-	54,58,73	1.62	7 (12%)	64,95,113	2.14	19 (29%)
15	CLA	2	604	-	53,57,73	1.54	7 (13%)	61,93,113	2.10	18 (29%)
15	CLA	B	1205	-	53,57,73	1.54	8 (15%)	61,93,113	2.16	15 (24%)
16	CHL	2	610	-	44,58,74	1.35	7 (15%)	37,94,114	2.04	11 (29%)
15	CLA	B	1236	-	53,57,73	1.52	6 (11%)	61,93,113	2.18	19 (31%)
15	CLA	A	1133	-	53,57,73	1.56	7 (13%)	61,93,113	2.07	16 (26%)
15	CLA	1	608	-	50,54,73	1.59	6 (12%)	59,90,113	2.10	15 (25%)
15	CLA	A	1106	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	17 (20%)
17	LHG	2	801	-	20,20,48	0.63	0	23,26,54	1.53	3 (13%)
15	CLA	1	612	-	63,67,73	1.44	6 (9%)	74,105,113	1.93	17 (22%)
15	CLA	4	604	4	53,57,73	1.58	7 (13%)	61,93,113	2.14	17 (27%)
15	CLA	F	1301	-	51,55,73	1.64	7 (13%)	60,91,113	2.13	17 (28%)
16	CHL	4	610	-	41,55,74	1.66	9 (21%)	35,91,114	2.06	10 (28%)
14	BCR	A	4007	-	41,41,41	1.63	4 (9%)	56,56,56	4.76	18 (32%)
16	CHL	1	609	1	44,58,74	1.44	7 (15%)	37,94,114	2.03	10 (27%)
19	SQD	1	811	-	38,40,54	0.86	0	48,51,65	0.92	2 (4%)
14	BCR	A	4005	-	41,41,41	4.24	6 (14%)	56,56,56	4.64	20 (35%)
15	CLA	A	1137	-	53,57,73	1.54	7 (13%)	61,93,113	2.14	19 (31%)
15	CLA	B	1224	-	53,57,73	1.52	8 (15%)	61,93,113	2.08	16 (26%)
15	CLA	A	1134	-	53,57,73	1.54	7 (13%)	61,93,113	2.15	19 (31%)
15	CLA	B	1216	-	53,57,73	1.53	8 (15%)	61,93,113	2.11	18 (29%)
15	CLA	B	1228	-	64,68,73	1.38	7 (10%)	76,107,113	1.89	18 (23%)
15	CLA	B	1201	-	52,56,73	1.59	8 (15%)	61,92,113	2.06	16 (26%)
14	BCR	A	4004	-	41,41,41	1.61	4 (9%)	56,56,56	4.62	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1206	6	53,57,73	1.56	8 (15%)	61,93,113	2.11	16 (26%)
12	LUT	1	501	-	42,43,43	2.54	1 (2%)	51,60,60	4.95	25 (49%)
15	CLA	A	1109	15	53,57,73	1.54	8 (15%)	61,93,113	2.15	16 (26%)
15	CLA	J	1302	-	53,57,73	1.57	6 (11%)	61,93,113	2.05	16 (26%)
14	BCR	F	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.71	17 (30%)
15	CLA	2	612	-	53,57,73	1.60	7 (13%)	61,93,113	2.11	16 (26%)
14	BCR	J	4002	-	41,41,41	1.62	5 (12%)	56,56,56	4.67	19 (33%)
15	CLA	A	1118	-	53,57,73	1.52	8 (15%)	61,93,113	2.12	16 (26%)
18	LMG	1	802	-	36,36,55	0.78	1 (2%)	44,44,63	1.20	4 (9%)
18	LMG	2	802	-	25,25,55	0.59	0	33,33,63	1.10	3 (9%)
15	CLA	B	1209	-	50,54,73	1.60	8 (16%)	59,90,113	2.02	16 (27%)
14	BCR	J	4001	-	41,41,41	1.64	4 (9%)	56,56,56	4.59	13 (23%)
15	CLA	1	603	-	49,53,73	1.73	8 (16%)	58,89,113	2.02	16 (27%)
15	CLA	4	606	-	53,57,73	1.57	9 (16%)	61,93,113	2.10	15 (24%)
15	CLA	2	601	-	53,57,73	1.49	7 (13%)	61,93,113	2.02	17 (27%)
15	CLA	4	607	-	53,57,73	1.55	8 (15%)	61,93,113	2.06	17 (27%)
15	CLA	A	1103	-	59,63,73	1.47	7 (11%)	70,101,113	1.97	18 (25%)
15	CLA	4	605	-	53,57,73	1.61	8 (15%)	61,93,113	2.14	15 (24%)
15	CLA	A	1101	-	49,53,73	1.66	7 (14%)	58,89,113	2.10	17 (29%)
15	CLA	A	1108	-	50,54,73	1.63	7 (14%)	59,90,113	2.09	17 (28%)
15	CLA	B	1227	-	49,53,73	1.69	8 (16%)	58,89,113	2.09	14 (24%)
15	CLA	A	1111	-	53,57,73	1.49	6 (11%)	61,93,113	2.19	18 (29%)
16	CHL	3	604	-	41,55,74	1.59	7 (17%)	35,91,114	2.04	11 (31%)
16	CHL	4	611	-	44,58,74	1.42	8 (18%)	37,94,114	2.02	11 (29%)
14	BCR	2	503	-	41,41,41	1.63	4 (9%)	56,56,56	4.67	17 (30%)
14	BCR	1	503	-	41,41,41	1.59	4 (9%)	56,56,56	4.68	21 (37%)
15	CLA	3	606	-	49,53,73	1.61	6 (12%)	58,89,113	2.05	16 (27%)
16	CHL	2	611	-	42,56,74	1.43	8 (19%)	36,92,114	2.14	11 (30%)
15	CLA	A	1140	-	59,63,73	1.47	10 (16%)	70,101,113	1.96	15 (21%)
15	CLA	2	605	-	69,73,73	1.40	7 (10%)	82,113,113	1.92	19 (23%)
12	LUT	2	501	-	42,43,43	2.48	1 (2%)	51,60,60	2.17	14 (27%)
15	CLA	2	608	-	53,57,73	1.55	7 (13%)	61,93,113	2.17	17 (27%)
17	LHG	A	5001	-	15,15,48	0.77	1 (6%)	16,19,54	0.59	0
15	CLA	3	605	-	50,54,73	1.58	9 (18%)	59,90,113	1.94	13 (22%)
15	CLA	B	1202	-	53,57,73	1.55	6 (11%)	61,93,113	2.12	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1021	-	69,73,73	1.39	8 (11%)	82,113,113	1.88	17 (20%)
21	DGD	4	811	-	46,46,67	0.91	3 (6%)	60,60,81	0.99	3 (5%)
15	CLA	B	1217	-	50,54,73	1.60	8 (16%)	59,90,113	2.00	13 (22%)
15	CLA	F	1302	-	53,57,73	1.53	10 (18%)	61,93,113	2.03	16 (26%)
15	CLA	A	1121	-	53,57,73	1.54	7 (13%)	61,93,113	2.10	17 (27%)
15	CLA	B	1213	-	53,57,73	1.47	7 (13%)	61,93,113	2.07	19 (31%)
15	CLA	2	607	-	53,57,73	1.57	6 (11%)	61,93,113	2.14	18 (29%)
15	CLA	B	1023	-	64,68,73	1.45	8 (12%)	76,107,113	1.84	17 (22%)
15	CLA	B	1215	-	53,57,73	1.62	7 (13%)	61,93,113	2.27	18 (29%)
15	CLA	B	1220	-	59,63,73	1.48	6 (10%)	70,101,113	1.96	18 (25%)
15	CLA	A	1125	-	53,57,73	1.52	6 (11%)	61,93,113	2.10	17 (27%)
15	CLA	4	612	-	53,57,73	1.59	8 (15%)	61,93,113	2.14	18 (29%)
14	BCR	A	4003	-	41,41,41	1.57	4 (9%)	56,56,56	4.43	14 (25%)
17	LHG	B	5001	15	20,20,48	0.65	0	23,26,54	1.48	2 (8%)
15	CLA	3	612	-	59,63,73	1.44	8 (13%)	70,101,113	2.00	20 (28%)
16	CHL	4	613	-	44,58,74	1.39	8 (18%)	37,94,114	2.13	10 (27%)
14	BCR	B	4002	-	41,41,41	1.63	4 (9%)	56,56,56	4.53	15 (26%)
15	CLA	1	606	-	49,53,73	1.60	6 (12%)	58,89,113	2.10	17 (29%)
20	CAC	1	902	-	2,4,4	2.79	2 (100%)	4,6,6	1.65	0
15	CLA	A	1105	-	53,57,73	1.55	9 (16%)	61,93,113	2.13	15 (24%)
14	BCR	3	504	-	41,41,41	1.62	4 (9%)	56,56,56	4.73	15 (26%)
15	CLA	3	610	-	53,57,73	1.53	9 (16%)	61,93,113	2.04	16 (26%)
15	CLA	A	1102	15	49,53,73	1.61	8 (16%)	58,89,113	2.06	15 (25%)
14	BCR	A	4006	-	41,41,41	1.59	4 (9%)	56,56,56	4.50	17 (30%)
15	CLA	A	1126	-	53,57,73	1.60	5 (9%)	61,93,113	2.17	14 (22%)
15	CLA	B	1231	6	64,68,73	1.42	5 (7%)	76,107,113	1.92	20 (26%)
14	BCR	1	505	-	41,41,41	1.64	4 (9%)	56,56,56	4.68	18 (32%)
15	CLA	4	603	-	53,57,73	1.59	7 (13%)	61,93,113	2.06	16 (26%)
16	CHL	2	613	-	40,54,74	1.51	8 (20%)	34,90,114	2.08	9 (26%)
13	XAT	2	502	-	41,47,47	0.71	1 (2%)	54,74,74	2.00	14 (25%)
15	CLA	B	1225	-	53,57,73	1.52	7 (13%)	61,93,113	2.12	19 (31%)
12	LUT	4	501	-	42,43,43	2.48	2 (4%)	51,60,60	1.78	13 (25%)
15	CLA	A	1107	5	53,57,73	1.57	6 (11%)	61,93,113	2.10	15 (24%)
15	CLA	1	615	-	69,73,73	1.38	8 (11%)	82,113,113	1.86	17 (20%)
15	CLA	B	1207	-	24,32,73	3.32	11 (45%)	31,54,113	2.47	12 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1113	-	49,53,73	1.61	8 (16%)	58,89,113	2.01	15 (25%)
15	CLA	A	1123	-	52,56,73	1.59	7 (13%)	61,92,113	2.06	16 (26%)
15	CLA	A	1128	-	53,57,73	1.59	8 (15%)	61,93,113	2.14	18 (29%)
15	CLA	A	1131	-	54,58,73	1.55	8 (14%)	64,95,113	2.06	17 (26%)
15	CLA	A	1115	-	53,57,73	1.58	7 (13%)	61,93,113	2.16	16 (26%)
20	CAC	4	902	-	2,4,4	3.31	2 (100%)	4,6,6	1.42	0
15	CLA	3	603	-	49,53,73	1.62	7 (14%)	58,89,113	2.29	19 (32%)
15	CLA	3	611	-	50,54,73	1.58	6 (12%)	59,90,113	2.02	14 (23%)
15	CLA	B	1210	-	53,57,73	1.50	8 (15%)	61,93,113	2.11	15 (24%)
12	LUT	3	501	-	42,43,43	2.50	2 (4%)	51,60,60	2.01	10 (19%)
15	CLA	2	615	2	54,58,73	1.51	8 (14%)	64,95,113	2.04	17 (26%)
15	CLA	B	1214	-	53,57,73	1.58	10 (18%)	61,93,113	2.10	18 (29%)
15	CLA	A	1119	-	53,57,73	1.57	6 (11%)	61,93,113	2.11	16 (26%)
25	PQN	B	2002	-	34,34,34	0.46	0	43,45,45	1.18	4 (9%)
15	CLA	A	1127	-	53,57,73	1.60	8 (15%)	61,93,113	2.17	18 (29%)
15	CLA	B	1218	-	53,57,73	1.54	8 (15%)	61,93,113	2.11	17 (27%)
15	CLA	A	1112	-	53,57,73	1.55	8 (15%)	61,93,113	2.11	18 (29%)
15	CLA	B	1235	-	64,68,73	1.41	8 (12%)	76,107,113	1.93	18 (23%)
14	BCR	4	503	-	41,41,41	1.67	4 (9%)	56,56,56	4.63	17 (30%)
15	CLA	A	1129	-	52,56,73	1.57	8 (15%)	61,92,113	2.06	17 (27%)
15	CLA	A	1114	-	50,54,73	1.57	9 (18%)	59,90,113	2.04	14 (23%)
14	BCR	B	4004	-	41,41,41	1.57	4 (9%)	56,56,56	4.62	14 (25%)
15	CLA	B	1212	-	49,53,73	1.60	6 (12%)	58,89,113	2.01	16 (27%)
18	LMG	1	803	-	23,23,55	0.59	0	31,31,63	1.40	2 (6%)
13	XAT	4	502	-	41,47,47	0.66	1 (2%)	54,74,74	1.92	11 (20%)
15	CLA	A	1122	-	53,57,73	1.53	7 (13%)	61,93,113	2.11	17 (27%)
15	CLA	B	1234	-	53,57,73	1.56	9 (16%)	61,93,113	2.12	17 (27%)
14	BCR	B	4005	-	41,41,41	1.63	4 (9%)	56,56,56	4.63	13 (23%)
14	BCR	3	503	-	41,41,41	1.63	4 (9%)	56,56,56	4.50	16 (28%)
14	BCR	A	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.58	18 (32%)
15	CLA	1	605	-	52,56,73	1.53	5 (9%)	61,92,113	2.09	17 (27%)
15	CLA	2	603	-	50,54,73	1.59	7 (14%)	59,90,113	1.99	14 (23%)
26	SF4	C	3003	7	0,12,12	-	-	-	-	-
13	XAT	3	502	-	41,47,47	0.66	1 (2%)	54,74,74	1.92	12 (22%)
15	CLA	3	608	-	52,56,73	1.56	8 (15%)	61,92,113	2.03	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CL0	A	1011	-	43,58,73	3.73	17 (39%)	42,95,113	3.24	18 (42%)
25	PQN	A	2001	-	34,34,34	0.50	0	43,45,45	1.20	4 (9%)
14	BCR	J	4003	-	41,41,41	1.58	4 (9%)	56,56,56	4.56	17 (30%)
15	CLA	B	1208	-	53,57,73	1.56	6 (11%)	61,93,113	2.11	18 (29%)
15	CLA	3	601	-	53,57,73	1.59	6 (11%)	61,93,113	2.22	17 (27%)
20	CAC	3	901	-	2,4,4	2.74	2 (100%)	4,6,6	1.81	1 (25%)
20	CAC	4	901	-	2,4,4	2.79	2 (100%)	4,6,6	1.36	0
15	CLA	B	1239	-	69,73,73	1.37	8 (11%)	82,113,113	1.85	16 (19%)
15	CLA	A	1104	-	64,68,73	1.38	7 (10%)	76,107,113	2.01	19 (25%)
18	LMG	2	803	-	16,16,55	0.50	0	22,22,63	0.52	0
15	CLA	3	613	-	50,54,73	1.59	6 (12%)	59,90,113	2.02	14 (23%)
15	CLA	A	1124	-	53,57,73	1.53	7 (13%)	61,93,113	2.13	18 (29%)
16	CHL	1	610	-	41,55,74	1.42	7 (17%)	35,91,114	2.06	10 (28%)
15	CLA	4	602	-	53,57,73	1.54	6 (11%)	61,93,113	2.07	16 (26%)
21	DGD	B	5002	-	39,39,67	0.93	2 (5%)	53,53,81	0.99	3 (5%)
15	CLA	1	613	-	49,53,73	1.57	8 (16%)	58,89,113	2.03	16 (27%)
14	BCR	B	4003	-	41,41,41	1.59	4 (9%)	56,56,56	4.70	17 (30%)
15	CLA	B	1230	-	53,57,73	1.56	8 (15%)	61,93,113	2.18	14 (22%)
15	CLA	B	1022	-	54,58,73	1.50	7 (12%)	64,95,113	2.09	19 (29%)
15	CLA	B	1229	-	69,73,73	1.47	8 (11%)	82,113,113	1.87	19 (23%)
22	LMT	2	821	-	24,24,36	1.30	4 (16%)	35,35,47	1.04	2 (5%)
15	CLA	B	1222	-	53,57,73	1.60	9 (16%)	61,93,113	2.15	17 (27%)
15	CLA	B	1226	-	53,57,73	1.53	8 (15%)	61,93,113	2.17	17 (27%)
15	CLA	A	1013	-	69,73,73	1.39	8 (11%)	82,113,113	1.85	17 (20%)
15	CLA	B	1232	-	53,57,73	1.55	7 (13%)	61,93,113	2.12	16 (26%)
15	CLA	A	1130	-	59,63,73	1.49	8 (13%)	70,101,113	2.02	18 (25%)
15	CLA	A	1135	-	53,57,73	1.54	7 (13%)	61,93,113	2.13	16 (26%)
17	LHG	A	5002	-	23,23,48	0.52	0	26,29,54	1.41	3 (11%)
15	CLA	A	1139	-	56,60,73	1.55	7 (12%)	65,97,113	2.03	18 (27%)
15	CLA	B	1204	-	53,57,73	1.56	7 (13%)	61,93,113	2.08	17 (27%)
23	GSH	B	5031	-	18,19,19	2.08	4 (22%)	21,24,24	1.53	2 (9%)
16	CHL	2	609	2	44,58,74	1.47	9 (20%)	37,94,114	2.04	10 (27%)
20	CAC	1	901	-	2,4,4	2.80	2 (100%)	4,6,6	1.51	0
15	CLA	1	601	-	53,57,73	1.51	8 (15%)	61,93,113	2.06	16 (26%)
15	CLA	4	615	-	59,63,73	1.45	5 (8%)	70,101,113	1.97	18 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1116	-	53,57,73	1.53	7 (13%)	61,93,113	2.13	15 (24%)
15	CLA	B	1238	-	54,58,73	1.54	6 (11%)	64,95,113	2.05	19 (29%)
21	DGD	2	811	-	48,48,67	0.97	3 (6%)	62,62,81	1.07	4 (6%)
14	BCR	B	4006	-	41,41,41	1.63	4 (9%)	56,56,56	4.57	13 (23%)
15	CLA	B	1237	-	53,57,73	1.56	7 (13%)	61,93,113	2.10	16 (26%)
15	CLA	4	609	4	53,57,73	1.55	7 (13%)	61,93,113	2.17	17 (27%)
21	DGD	J	5001	-	29,29,67	0.62	0	41,41,81	0.59	0
15	CLA	B	1221	-	53,57,73	1.57	7 (13%)	61,93,113	2.18	19 (31%)
15	CLA	1	602	-	50,54,73	1.58	8 (16%)	59,90,113	2.03	16 (27%)
15	CLA	1	607	17	50,54,73	1.57	6 (12%)	59,90,113	2.04	15 (25%)
15	CLA	3	615	-	50,54,73	1.63	7 (14%)	59,90,113	2.02	14 (23%)
15	CLA	1	604	1	53,57,73	1.56	7 (13%)	61,93,113	2.15	20 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	4	601	4	1/1/11/20	9/20/96/115	-
15	CLA	B	1240	17	1/1/15/20	18/39/115/115	-
23	GSH	4	831	-	-	8/24/24/24	-
26	SF4	A	3001	6,5	-	-	0/6/5/5
15	CLA	2	606	-	1/1/11/20	7/17/93/115	-
15	CLA	A	1132	-	1/1/11/20	11/20/96/115	-
17	LHG	1	801	15	-	10/26/26/53	-
15	CLA	A	1110	-	1/1/11/20	8/20/96/115	-
15	CLA	A	1138	-	1/1/15/20	18/39/115/115	-
15	CLA	B	1211	-	1/1/11/20	7/20/96/115	-
15	CLA	1	611	-	1/1/11/20	10/20/96/115	-
26	SF4	C	3002	7	-	-	0/6/5/5
15	CLA	3	607	-	1/1/12/20	7/21/97/115	-
15	CLA	B	1203	-	1/1/11/20	6/20/96/115	-
15	CLA	A	1136	-	1/1/11/20	9/20/96/115	-
15	CLA	A	1012	-	1/1/14/20	11/33/109/115	-
15	CLA	B	1219	-	1/1/11/20	9/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1120	-	1/1/11/20	8/20/96/115	-
15	CLA	A	1141	-	1/1/12/20	9/21/97/115	-
15	CLA	4	608	-	1/1/11/20	4/17/93/115	-
14	BCR	4	505	-	-	19/29/63/63	0/2/2/2
14	BCR	B	4001	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1117	-	1/1/11/20	7/20/96/115	-
13	XAT	1	502	-	-	3/31/93/93	0/4/4/4
15	CLA	2	602	-	1/1/11/20	8/20/96/115	-
15	CLA	B	1223	-	1/1/12/20	6/21/97/115	-
15	CLA	2	604	-	1/1/11/20	12/20/96/115	-
15	CLA	B	1205	-	1/1/11/20	8/20/96/115	-
16	CHL	2	610	-	4/4/16/26	6/20/118/137	-
15	CLA	B	1236	-	1/1/11/20	10/20/96/115	-
15	CLA	A	1133	-	1/1/11/20	7/20/96/115	-
15	CLA	1	608	-	1/1/11/20	6/17/93/115	-
15	CLA	A	1106	-	1/1/15/20	15/39/115/115	-
17	LHG	2	801	-	-	9/23/23/53	-
15	CLA	1	612	-	2/2/14/20	10/29/105/115	-
15	CLA	4	604	4	1/1/11/20	10/20/96/115	-
15	CLA	F	1301	-	1/1/11/20	9/18/94/115	-
16	CHL	4	610	-	4/4/16/26	3/17/115/137	-
14	BCR	A	4007	-	-	11/29/63/63	0/2/2/2
16	CHL	1	609	1	4/4/16/26	8/20/118/137	-
19	SQD	1	811	-	-	7/34/54/69	0/1/1/1
14	BCR	A	4005	-	-	7/29/63/63	0/2/2/2
15	CLA	A	1137	-	1/1/11/20	8/20/96/115	-
15	CLA	B	1224	-	1/1/11/20	10/20/96/115	-
15	CLA	A	1134	-	1/1/11/20	7/20/96/115	-
15	CLA	B	1216	-	1/1/11/20	8/20/96/115	-
15	CLA	B	1228	-	1/1/14/20	6/33/109/115	-
15	CLA	B	1201	-	1/1/11/20	8/19/95/115	-
15	CLA	B	1206	6	1/1/11/20	9/20/96/115	-
15	CLA	J	1302	-	1/1/11/20	10/20/96/115	-
12	LUT	1	501	-	-	8/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1109	15	1/1/11/20	8/20/96/115	-
14	BCR	A	4004	-	-	8/29/63/63	0/2/2/2
14	BCR	F	4002	-	-	11/29/63/63	0/2/2/2
15	CLA	2	612	-	1/1/11/20	12/20/96/115	-
15	CLA	A	1118	-	1/1/11/20	12/20/96/115	-
14	BCR	J	4002	-	-	17/29/63/63	0/2/2/2
18	LMG	1	802	-	-	8/31/51/70	0/1/1/1
18	LMG	2	802	-	-	7/20/40/70	0/1/1/1
15	CLA	B	1209	-	1/1/11/20	5/17/93/115	-
14	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
15	CLA	1	603	-	1/1/11/20	6/15/91/115	-
15	CLA	4	606	-	1/1/11/20	8/20/96/115	-
15	CLA	2	601	-	1/1/11/20	8/20/96/115	-
15	CLA	4	607	-	1/1/11/20	9/20/96/115	-
15	CLA	A	1103	-	1/1/13/20	14/27/103/115	-
15	CLA	4	605	-	1/1/11/20	9/20/96/115	-
15	CLA	A	1101	-	1/1/11/20	5/15/91/115	-
15	CLA	A	1108	-	1/1/11/20	10/17/93/115	-
15	CLA	B	1227	-	1/1/11/20	6/15/91/115	-
15	CLA	A	1111	-	1/1/11/20	5/20/96/115	-
16	CHL	3	604	-	3/3/16/26	3/17/115/137	-
16	CHL	4	611	-	3/3/16/26	4/20/118/137	-
15	CLA	3	606	-	1/1/11/20	2/15/91/115	-
14	BCR	1	503	-	-	16/29/63/63	0/2/2/2
14	BCR	2	503	-	-	14/29/63/63	0/2/2/2
16	CHL	2	611	-	4/4/16/26	1/18/116/137	-
15	CLA	A	1140	-	1/1/13/20	13/27/103/115	-
15	CLA	2	605	-	1/1/15/20	16/39/115/115	-
12	LUT	2	501	-	-	6/29/67/67	0/2/2/2
15	CLA	2	608	-	1/1/11/20	7/20/96/115	-
17	LHG	A	5001	-	-	12/18/18/53	-
15	CLA	3	605	-	1/1/11/20	5/17/93/115	-
15	CLA	B	1202	-	1/1/11/20	10/20/96/115	-
15	CLA	B	1021	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	DGD	4	811	-	-	13/34/74/95	0/2/2/2
15	CLA	B	1217	-	1/1/11/20	9/17/93/115	-
15	CLA	F	1302	-	1/1/11/20	7/20/96/115	-
15	CLA	A	1121	-	1/1/11/20	9/20/96/115	-
15	CLA	B	1213	-	1/1/11/20	7/20/96/115	-
15	CLA	2	607	-	1/1/11/20	11/20/96/115	-
15	CLA	B	1023	-	1/1/14/20	12/33/109/115	-
15	CLA	B	1215	-	1/1/11/20	9/20/96/115	-
15	CLA	B	1220	-	1/1/13/20	12/27/103/115	-
15	CLA	A	1125	-	1/1/11/20	7/20/96/115	-
15	CLA	4	612	-	1/1/11/20	10/20/96/115	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
17	LHG	B	5001	15	-	12/23/23/53	-
15	CLA	3	612	-	1/1/13/20	10/27/103/115	-
16	CHL	4	613	-	4/4/16/26	5/20/118/137	-
14	BCR	B	4002	-	-	11/29/63/63	0/2/2/2
15	CLA	1	606	-	1/1/11/20	7/15/91/115	-
15	CLA	A	1105	-	1/1/11/20	10/20/96/115	-
15	CLA	3	610	-	1/1/11/20	9/20/96/115	-
15	CLA	A	1102	15	1/1/11/20	7/15/91/115	-
14	BCR	3	504	-	-	17/29/63/63	0/2/2/2
14	BCR	A	4006	-	-	15/29/63/63	0/2/2/2
15	CLA	A	1126	-	1/1/11/20	7/20/96/115	-
15	CLA	B	1231	6	1/1/14/20	9/33/109/115	-
15	CLA	4	603	-	1/1/11/20	4/20/96/115	-
16	CHL	2	613	-	3/3/16/26	1/15/113/137	-
14	BCR	1	505	-	-	12/29/63/63	0/2/2/2
13	XAT	2	502	-	1/1/12/26	4/31/93/93	0/4/4/4
15	CLA	B	1225	-	1/1/11/20	9/20/96/115	-
15	CLA	A	1107	5	1/1/11/20	4/20/96/115	-
12	LUT	4	501	-	-	7/29/67/67	0/2/2/2
15	CLA	1	615	-	1/1/15/20	21/39/115/115	-
15	CLA	B	1207	-	1/1/4/20	-	-
15	CLA	A	1113	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1123	-	1/1/11/20	7/19/95/115	-
15	CLA	A	1128	-	1/1/11/20	10/20/96/115	-
15	CLA	A	1131	-	1/1/12/20	9/21/97/115	-
15	CLA	A	1115	-	1/1/11/20	10/20/96/115	-
15	CLA	3	603	-	1/1/11/20	5/15/91/115	-
15	CLA	3	611	-	1/1/11/20	6/17/93/115	-
15	CLA	B	1210	-	1/1/11/20	11/20/96/115	-
12	LUT	3	501	-	-	3/29/67/67	0/2/2/2
15	CLA	2	615	2	1/1/12/20	7/21/97/115	-
15	CLA	B	1214	-	1/1/11/20	10/20/96/115	-
15	CLA	A	1119	-	1/1/11/20	9/20/96/115	-
25	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
15	CLA	A	1127	-	1/1/11/20	10/20/96/115	-
15	CLA	B	1218	-	1/1/11/20	8/20/96/115	-
15	CLA	A	1112	-	1/1/11/20	8/20/96/115	-
15	CLA	B	1235	-	1/1/14/20	18/33/109/115	-
14	BCR	4	503	-	-	13/29/63/63	0/2/2/2
15	CLA	A	1129	-	1/1/11/20	9/19/95/115	-
15	CLA	A	1114	-	1/1/11/20	6/17/93/115	-
15	CLA	B	1212	-	1/1/11/20	9/15/91/115	-
14	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
18	LMG	1	803	-	-	6/16/36/70	0/1/1/1
13	XAT	4	502	-	1/1/12/26	6/31/93/93	0/4/4/4
15	CLA	A	1122	-	1/1/11/20	10/20/96/115	-
15	CLA	B	1234	-	1/1/11/20	8/20/96/115	-
14	BCR	B	4005	-	-	16/29/63/63	0/2/2/2
14	BCR	3	503	-	-	13/29/63/63	0/2/2/2
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
15	CLA	1	605	-	1/1/11/20	10/19/95/115	-
15	CLA	2	603	-	1/1/11/20	3/17/93/115	-
26	SF4	C	3003	7	-	-	0/6/5/5
13	XAT	3	502	-	1/1/12/26	14/31/93/93	0/4/4/4
15	CLA	3	608	-	1/1/11/20	7/19/95/115	-
24	CL0	A	1011	-	3/3/17/25	11/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PQN	A	2001	-	-	11/23/43/43	0/2/2/2
14	BCR	J	4003	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1208	-	1/1/11/20	7/20/96/115	-
15	CLA	3	601	-	1/1/11/20	12/20/96/115	-
15	CLA	B	1239	-	1/1/15/20	15/39/115/115	-
15	CLA	A	1104	-	1/1/14/20	15/33/109/115	-
18	LMG	2	803	-	-	3/7/27/70	0/1/1/1
15	CLA	3	613	-	1/1/11/20	8/17/93/115	-
15	CLA	A	1124	-	1/1/11/20	8/20/96/115	-
16	CHL	1	610	-	3/3/16/26	6/17/115/137	-
15	CLA	4	602	-	1/1/11/20	5/20/96/115	-
21	DGD	B	5002	-	-	9/27/67/95	0/2/2/2
15	CLA	1	613	-	1/1/11/20	4/15/91/115	-
14	BCR	B	4003	-	-	9/29/63/63	0/2/2/2
15	CLA	B	1230	-	1/1/11/20	8/20/96/115	-
15	CLA	B	1022	-	1/1/12/20	8/21/97/115	-
15	CLA	B	1229	-	1/1/15/20	15/39/115/115	-
22	LMT	2	821	-	-	1/8/48/61	0/2/2/2
15	CLA	B	1222	-	1/1/11/20	10/20/96/115	-
15	CLA	B	1226	-	1/1/11/20	10/20/96/115	-
15	CLA	A	1013	-	1/1/15/20	18/39/115/115	-
15	CLA	B	1232	-	1/1/11/20	7/20/96/115	-
15	CLA	A	1130	-	1/1/13/20	13/27/103/115	-
15	CLA	A	1135	-	1/1/11/20	11/20/96/115	-
17	LHG	A	5002	-	-	16/28/28/53	-
15	CLA	A	1139	-	1/1/12/20	5/24/100/115	-
15	CLA	B	1204	-	1/1/11/20	6/20/96/115	-
23	GSH	B	5031	-	-	13/24/24/24	-
16	CHL	2	609	2	3/3/16/26	4/20/118/137	-
15	CLA	1	601	-	1/1/11/20	9/20/96/115	-
15	CLA	4	615	-	1/1/13/20	10/27/103/115	-
15	CLA	A	1116	-	1/1/11/20	8/20/96/115	-
15	CLA	B	1238	-	1/1/12/20	7/21/97/115	-
21	DGD	2	811	-	-	13/36/76/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
15	CLA	B	1237	-	1/1/11/20	11/20/96/115	-
15	CLA	4	609	4	1/1/11/20	7/20/96/115	-
21	DGD	J	5001	-	-	5/14/54/95	0/2/2/2
15	CLA	B	1221	-	1/1/11/20	7/20/96/115	-
15	CLA	1	602	-	1/1/11/20	11/17/93/115	-
15	CLA	1	607	17	1/1/11/20	12/17/93/115	-
15	CLA	3	615	-	1/1/11/20	6/17/93/115	-
15	CLA	1	604	1	1/1/11/20	7/20/96/115	-

The worst 5 of 1204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4005	BCR	C11-C12	18.82	1.83	1.34
14	A	4005	BCR	C11-C10	16.04	1.92	1.43
12	1	501	LUT	C24-C25	15.65	1.51	1.33
12	3	501	LUT	C24-C25	15.36	1.51	1.33
12	4	501	LUT	C24-C25	15.23	1.51	1.33

The worst 5 of 2866 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4001	BCR	C10-C11-C12	19.10	178.54	123.20
14	2	503	BCR	C10-C11-C12	19.08	178.50	123.20
14	3	504	BCR	C10-C11-C12	18.99	178.23	123.20
14	4	503	BCR	C10-C11-C12	18.98	178.18	123.20
14	A	4004	BCR	C10-C11-C12	18.96	178.13	123.20

5 of 174 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	2	502	XAT	C26
13	3	502	XAT	C6
13	4	502	XAT	C6
15	1	601	CLA	ND
15	1	602	CLA	ND

5 of 1743 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C13-C14-C15-C35
12	1	501	LUT	C21-C26-C27-C28
12	1	501	LUT	C25-C26-C27-C28
12	2	501	LUT	C21-C26-C27-C28
12	3	501	LUT	C21-C26-C27-C28

There are no ring outliers.

188 monomers are involved in 1127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	601	CLA	12	0
15	B	1240	CLA	4	0
23	4	831	GSH	0	1
15	2	606	CLA	4	0
15	A	1132	CLA	3	0
17	1	801	LHG	2	0
15	A	1110	CLA	16	0
15	A	1138	CLA	10	0
15	B	1211	CLA	8	0
15	1	611	CLA	7	0
15	3	607	CLA	1	0
15	B	1203	CLA	2	0
20	3	902	CAC	1	0
15	A	1136	CLA	9	0
14	4	505	BCR	4	0
14	B	4001	BCR	2	0
15	A	1012	CLA	24	0
15	4	608	CLA	4	0
15	A	1141	CLA	3	0
15	B	1219	CLA	5	0
15	A	1117	CLA	5	0
13	1	502	XAT	11	0
15	2	602	CLA	6	0
15	B	1223	CLA	5	0
15	2	604	CLA	5	0
15	B	1205	CLA	4	0
16	2	610	CHL	4	0
15	B	1236	CLA	6	0
15	A	1133	CLA	4	0
15	1	608	CLA	11	0
15	A	1106	CLA	8	0
17	2	801	LHG	2	0
15	1	612	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	604	CLA	14	0
15	F	1301	CLA	5	0
16	4	610	CHL	5	0
14	A	4007	BCR	9	0
16	1	609	CHL	11	0
19	1	811	SQD	4	0
14	A	4005	BCR	11	0
15	A	1137	CLA	6	0
15	B	1224	CLA	4	0
15	A	1134	CLA	2	0
15	B	1216	CLA	8	0
15	B	1228	CLA	8	0
15	B	1201	CLA	2	0
14	A	4004	BCR	4	0
15	B	1206	CLA	4	0
12	1	501	LUT	10	0
15	A	1109	CLA	14	0
15	J	1302	CLA	9	0
14	F	4002	BCR	5	0
15	2	612	CLA	11	0
14	J	4002	BCR	16	0
15	A	1118	CLA	3	0
18	1	802	LMG	1	0
18	2	802	LMG	1	0
15	B	1209	CLA	2	0
14	J	4001	BCR	7	0
15	1	603	CLA	9	0
15	4	606	CLA	7	0
15	2	601	CLA	15	0
15	4	607	CLA	4	0
15	A	1103	CLA	8	0
15	4	605	CLA	9	0
15	A	1101	CLA	5	0
15	A	1108	CLA	6	0
15	B	1227	CLA	7	0
15	A	1111	CLA	23	0
16	3	604	CHL	15	0
16	4	611	CHL	10	0
14	2	503	BCR	8	0
14	1	503	BCR	8	0
15	3	606	CLA	18	0
16	2	611	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1140	CLA	7	0
15	2	605	CLA	6	0
12	2	501	LUT	13	0
15	2	608	CLA	3	0
17	A	5001	LHG	1	0
15	3	605	CLA	11	0
15	B	1202	CLA	4	0
15	B	1021	CLA	21	0
21	4	811	DGD	7	0
15	B	1217	CLA	2	0
15	F	1302	CLA	2	0
15	A	1121	CLA	3	0
15	B	1213	CLA	2	0
15	2	607	CLA	8	0
15	B	1023	CLA	20	0
15	B	1215	CLA	4	0
15	B	1220	CLA	6	0
15	A	1125	CLA	10	0
15	4	612	CLA	9	0
14	A	4003	BCR	2	0
17	B	5001	LHG	2	0
15	3	612	CLA	10	0
16	4	613	CHL	7	0
14	B	4002	BCR	2	0
15	1	606	CLA	17	0
15	A	1105	CLA	2	0
14	3	504	BCR	5	0
15	3	610	CLA	4	0
15	A	1102	CLA	6	0
14	A	4006	BCR	7	0
15	A	1126	CLA	6	0
15	B	1231	CLA	10	0
14	1	505	BCR	7	0
15	4	603	CLA	3	0
16	2	613	CHL	6	0
13	2	502	XAT	13	0
15	B	1225	CLA	6	0
12	4	501	LUT	18	0
15	A	1107	CLA	6	0
15	1	615	CLA	4	0
15	A	1113	CLA	6	0
15	A	1123	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1128	CLA	10	0
15	A	1131	CLA	2	0
15	A	1115	CLA	7	0
20	4	902	CAC	1	0
15	3	603	CLA	22	0
15	3	611	CLA	8	0
15	B	1210	CLA	7	0
12	3	501	LUT	11	0
15	2	615	CLA	1	0
15	B	1214	CLA	9	0
15	A	1119	CLA	3	0
25	B	2002	PQN	8	0
15	A	1127	CLA	8	0
15	B	1218	CLA	4	0
15	A	1112	CLA	1	0
15	B	1235	CLA	11	0
14	4	503	BCR	8	0
15	A	1129	CLA	2	0
15	A	1114	CLA	6	0
14	B	4004	BCR	5	0
15	B	1212	CLA	8	0
13	4	502	XAT	5	0
15	A	1122	CLA	3	0
15	B	1234	CLA	7	0
14	B	4005	BCR	5	0
14	3	503	BCR	20	0
14	A	4002	BCR	6	0
15	1	605	CLA	9	0
15	2	603	CLA	4	0
26	C	3003	SF4	2	0
13	3	502	XAT	21	0
15	3	608	CLA	5	0
24	A	1011	CL0	19	0
25	A	2001	PQN	9	0
14	J	4003	BCR	4	0
15	3	601	CLA	15	0
15	B	1239	CLA	12	0
15	A	1104	CLA	6	0
15	3	613	CLA	14	0
15	A	1124	CLA	12	0
16	1	610	CHL	15	0
15	4	602	CLA	6	0

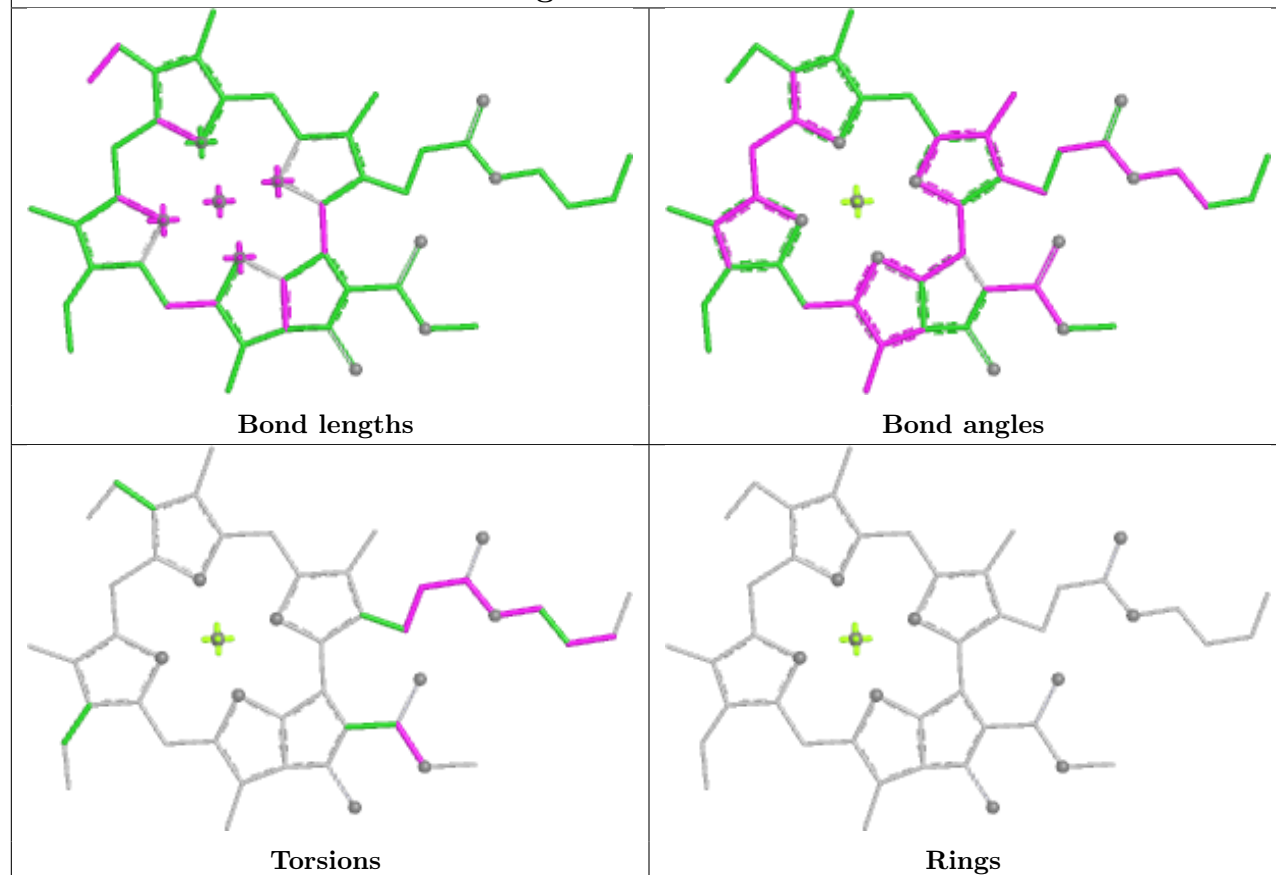
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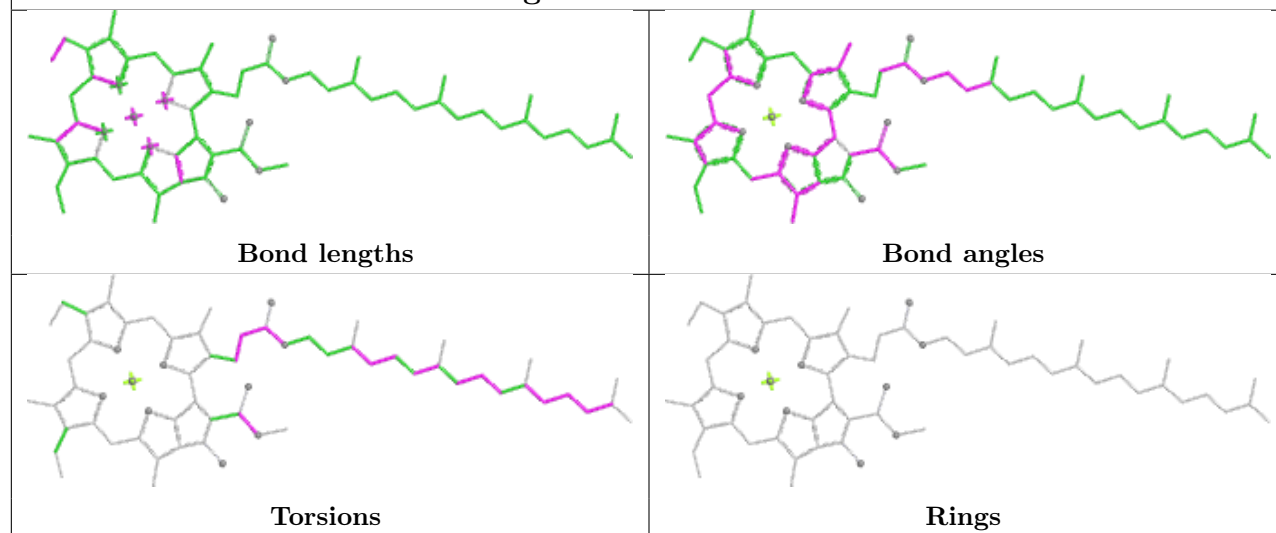
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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15	1	613	CLA	23	0
14	B	4003	BCR	9	0
15	B	1230	CLA	13	0
15	B	1022	CLA	7	0
15	B	1229	CLA	6	0
15	B	1222	CLA	6	0
15	B	1226	CLA	9	0
15	A	1013	CLA	28	0
15	B	1232	CLA	3	0
15	A	1130	CLA	4	0
15	A	1135	CLA	3	0
17	A	5002	LHG	4	0
15	A	1139	CLA	9	0
15	B	1204	CLA	5	0
23	B	5031	GSH	2	0
16	2	609	CHL	12	0
15	1	601	CLA	11	0
15	4	615	CLA	7	0
15	A	1116	CLA	6	0
15	B	1238	CLA	1	0
21	2	811	DGD	2	0
14	B	4006	BCR	11	0
15	B	1237	CLA	2	0
15	4	609	CLA	9	0
15	B	1221	CLA	5	0
15	1	602	CLA	1	0
15	1	607	CLA	4	0
15	1	604	CLA	16	0

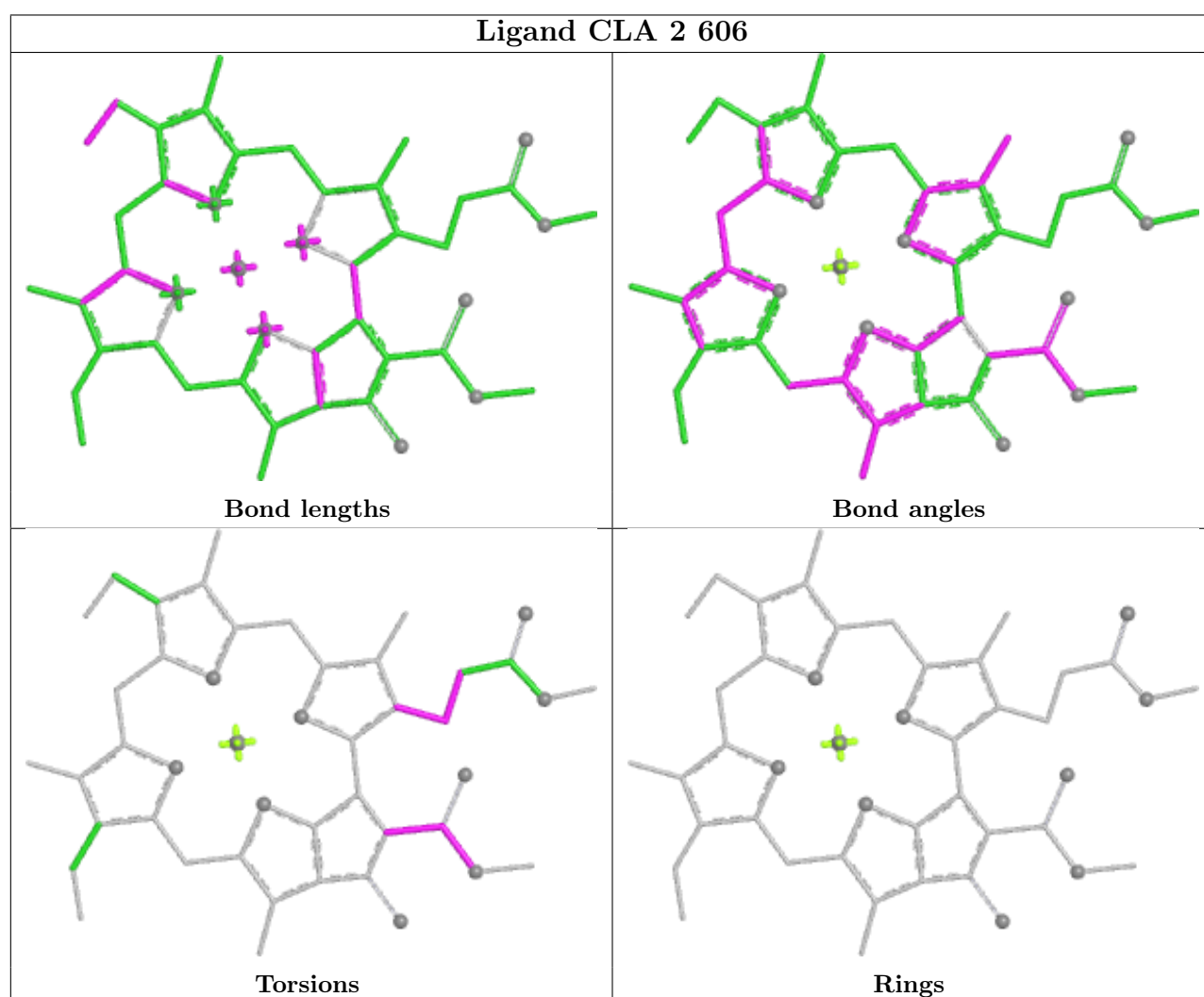
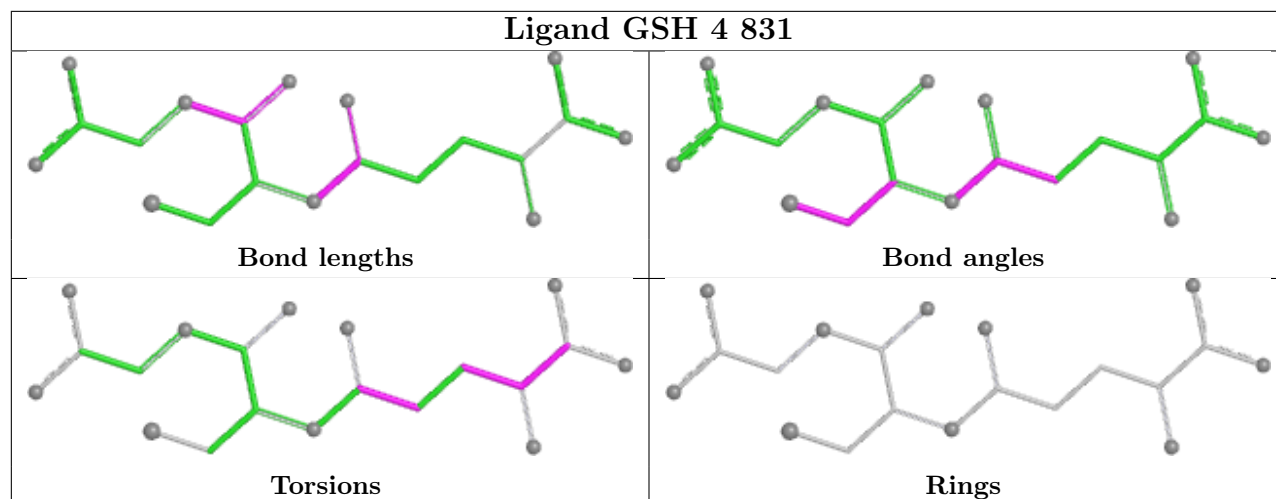
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 4 601

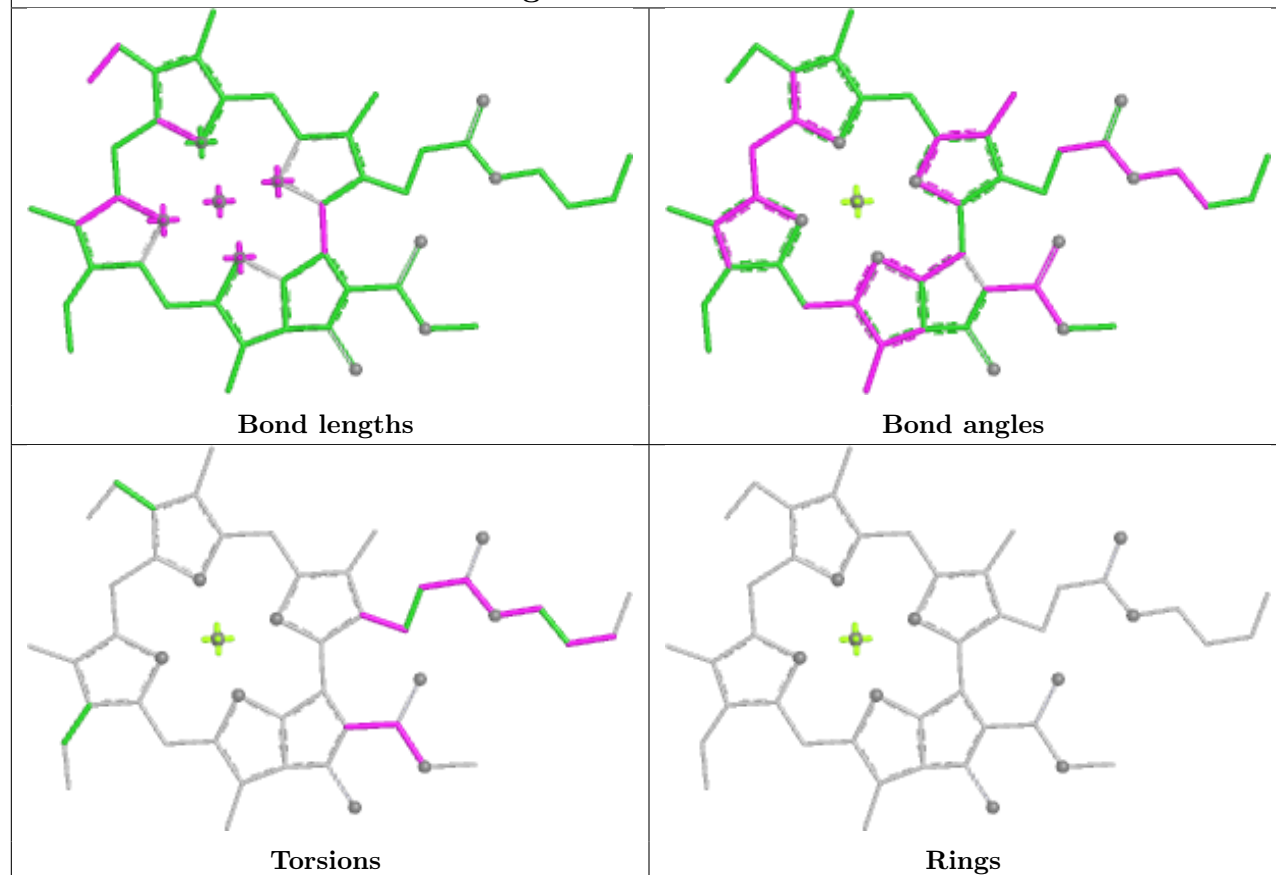


Ligand CLA B 1240

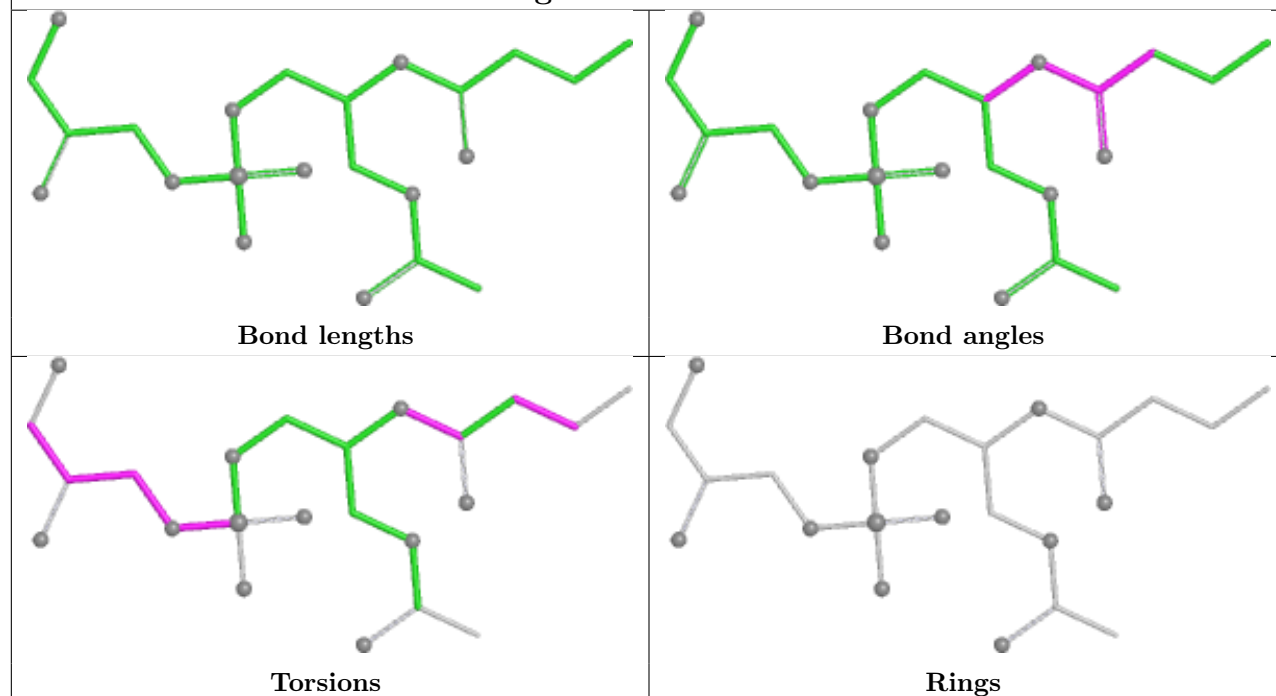


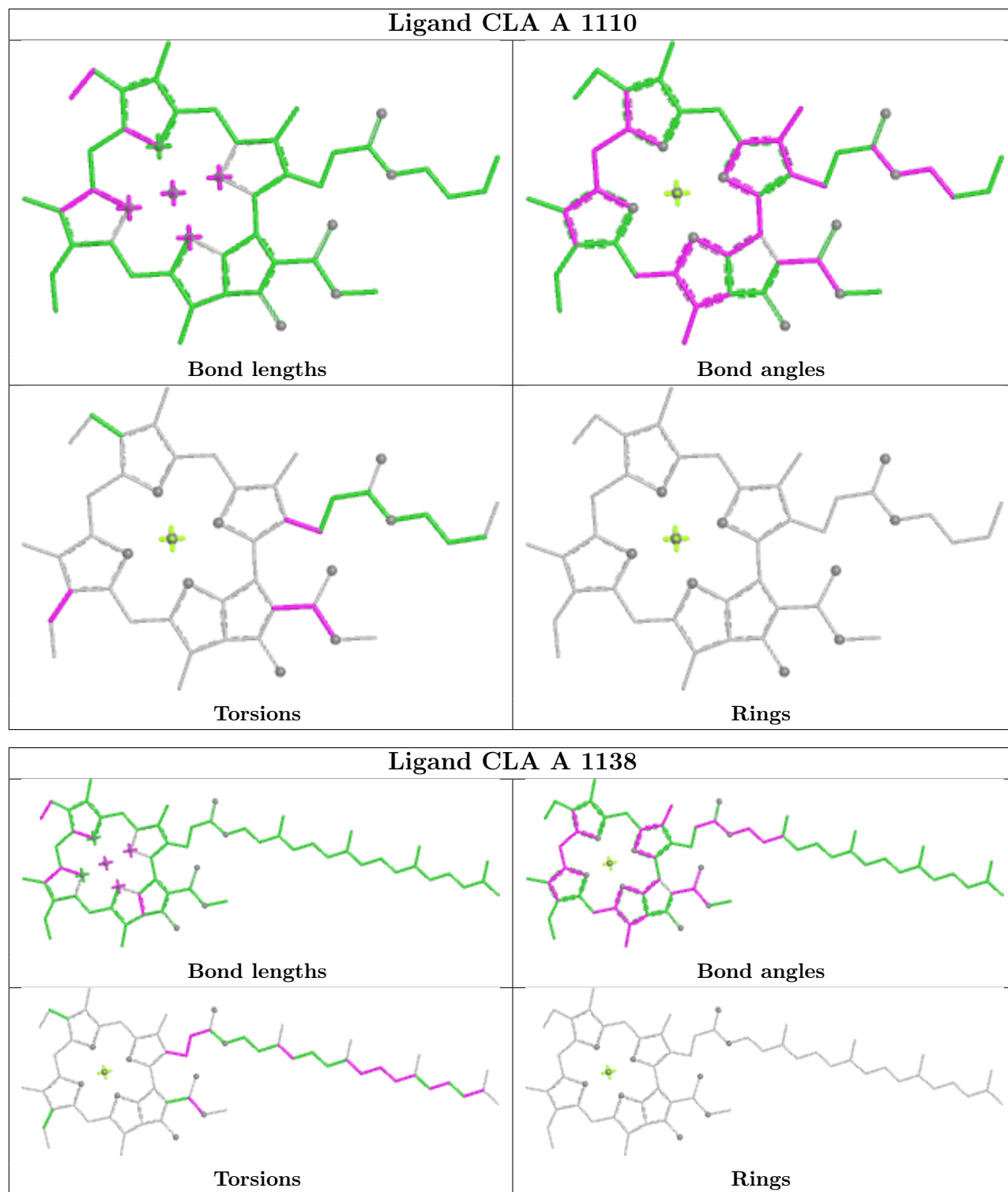


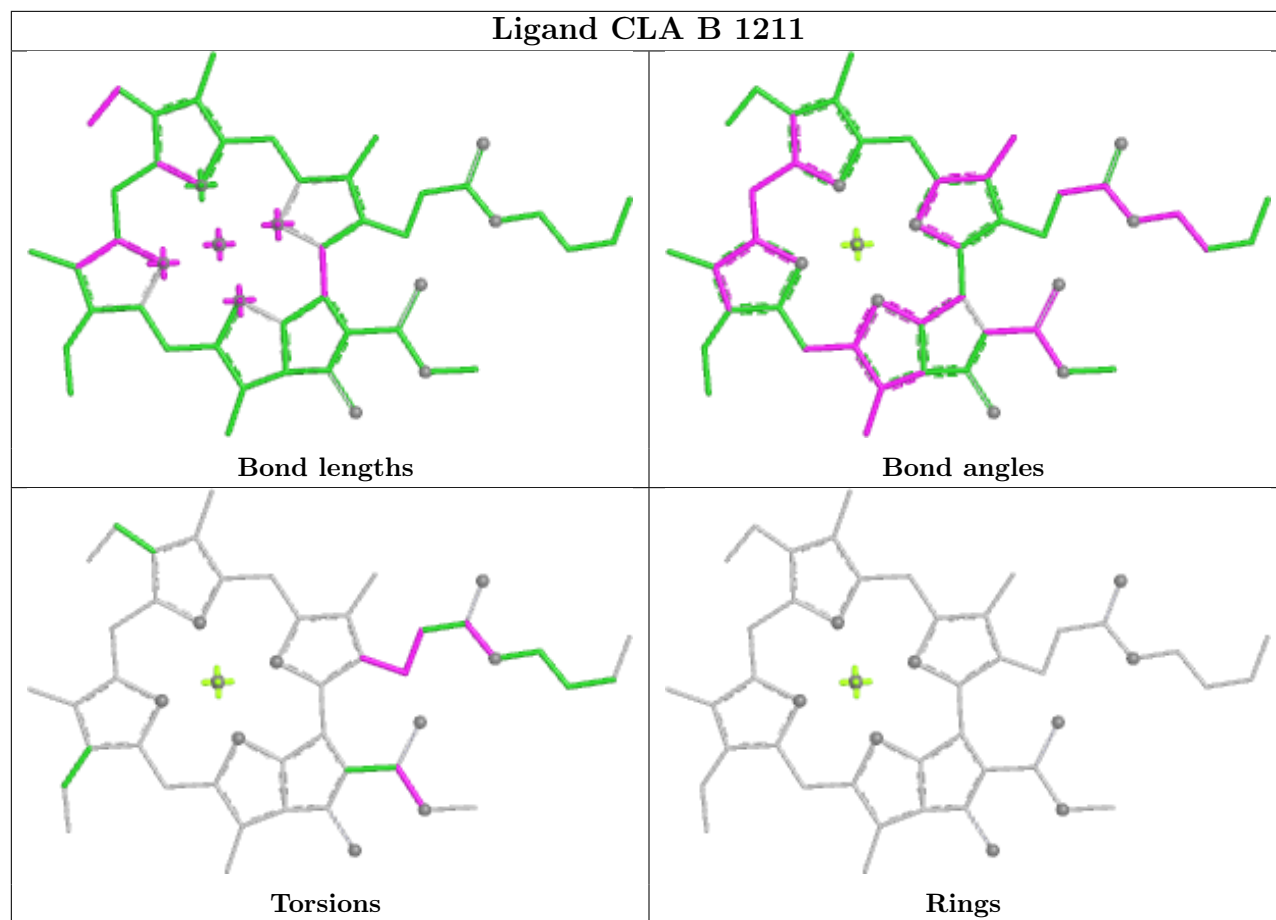
Ligand CLA A 1132



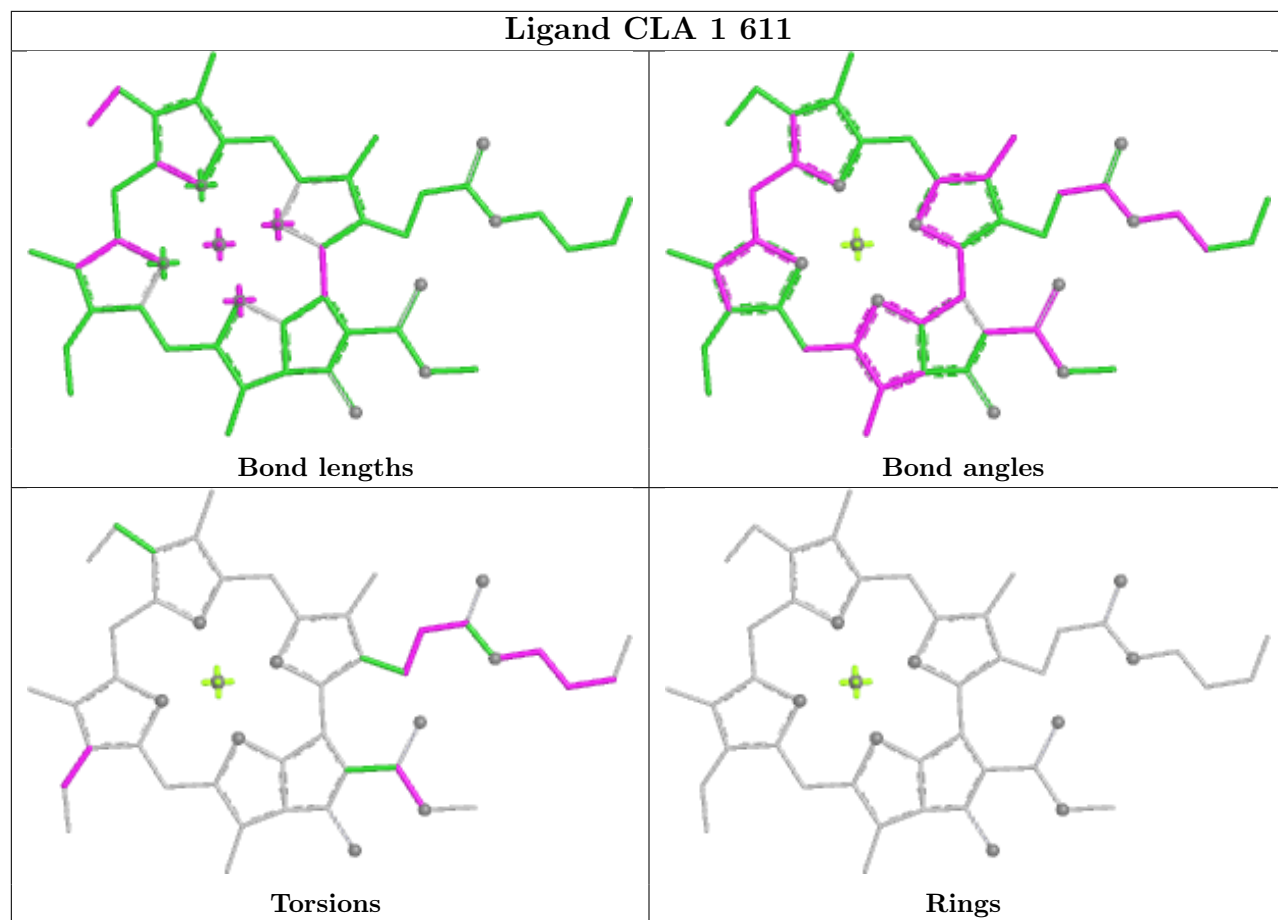
Ligand LHG 1 801



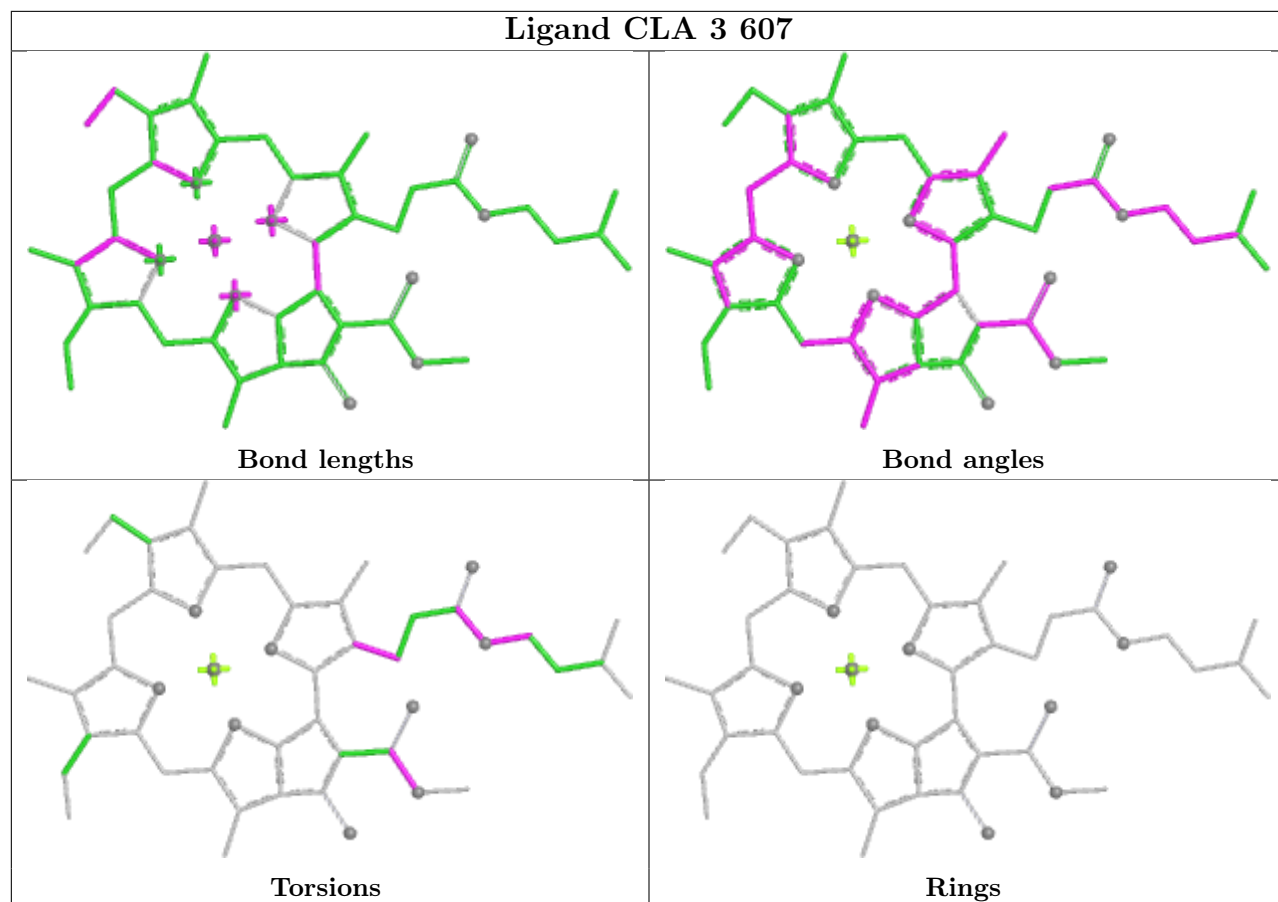


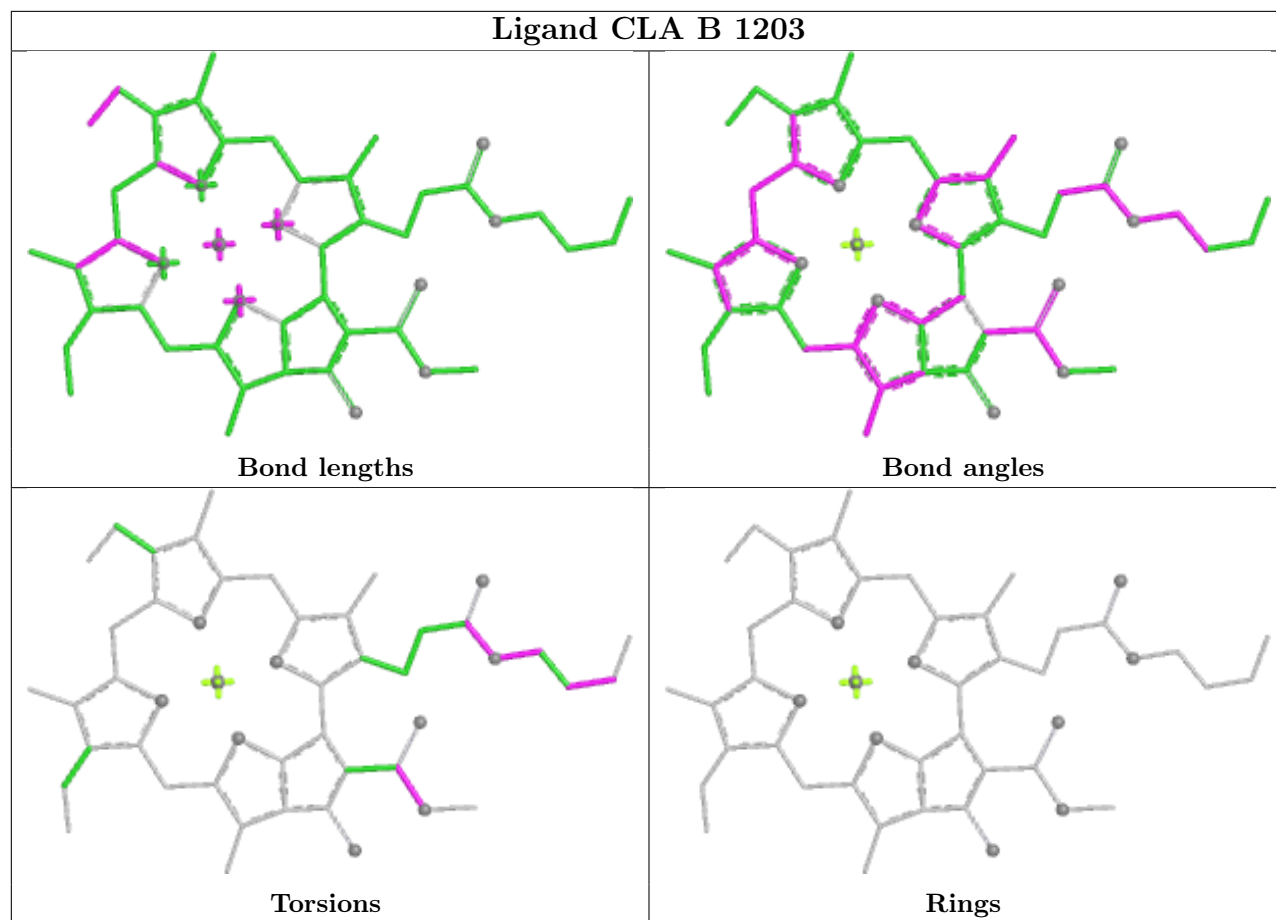


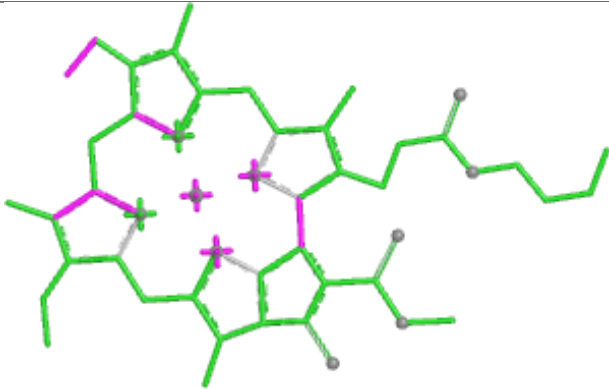
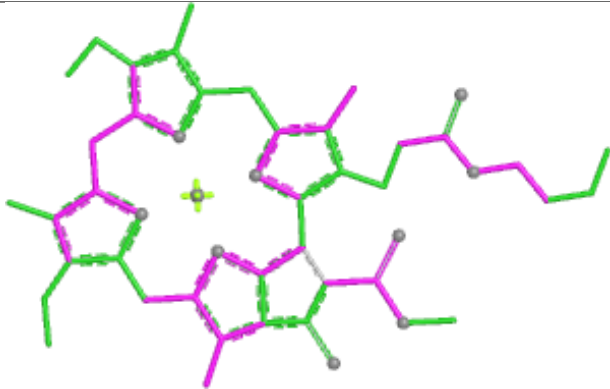
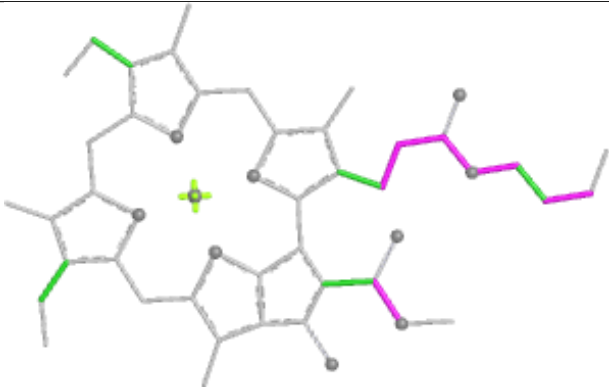
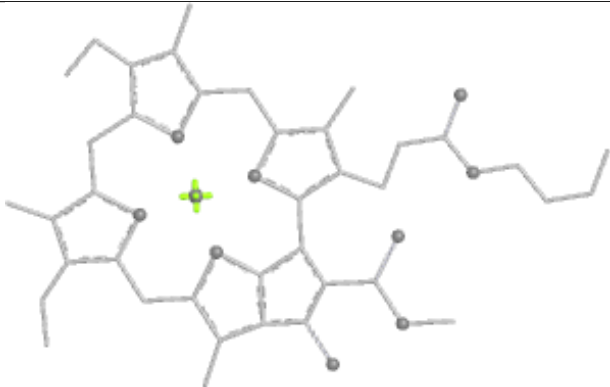
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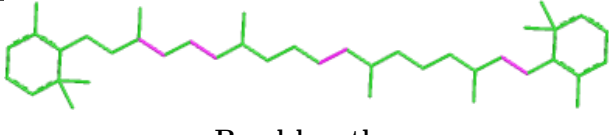
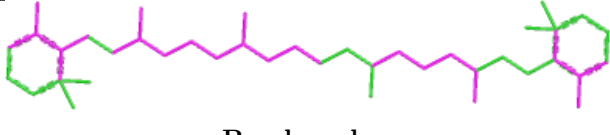
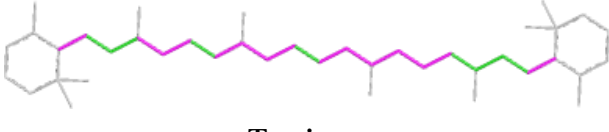
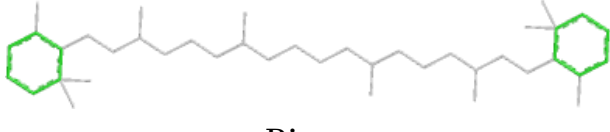


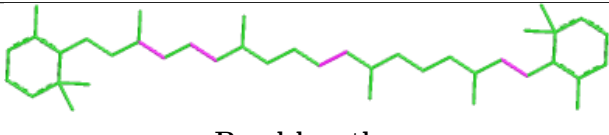
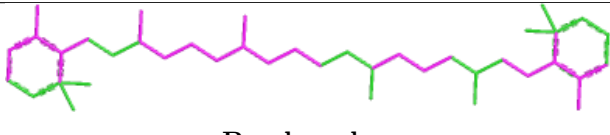
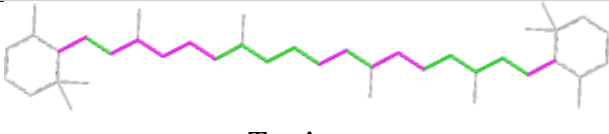
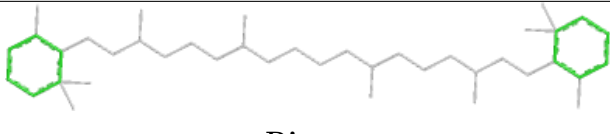
Ligand CLA 3 607



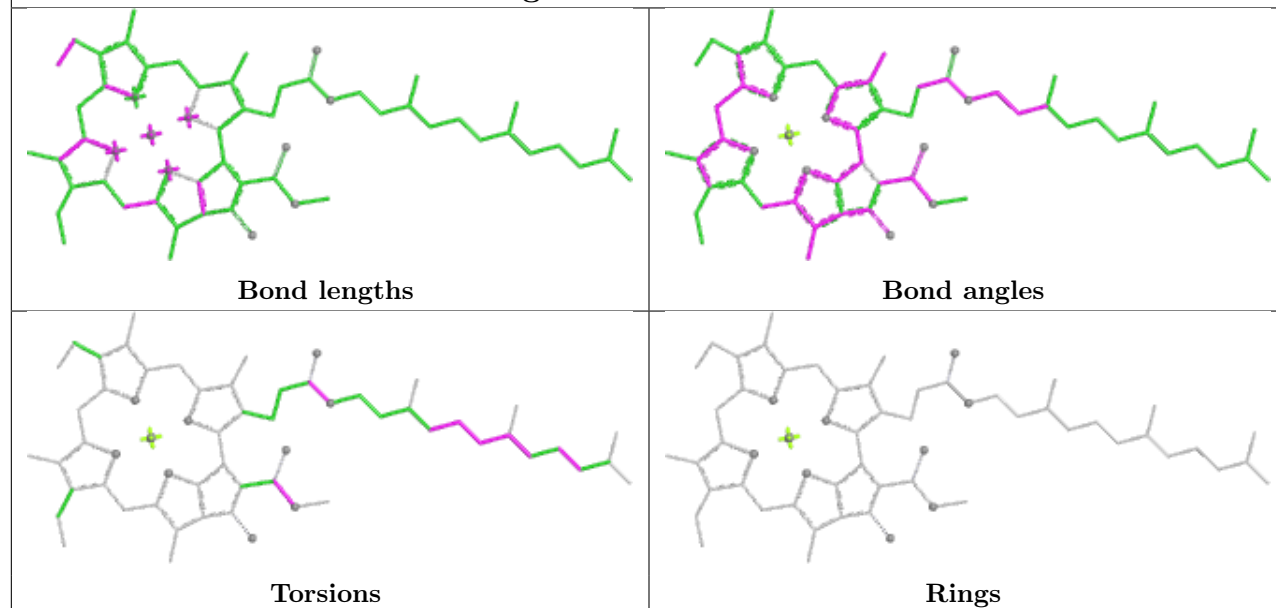


Ligand CLA A 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

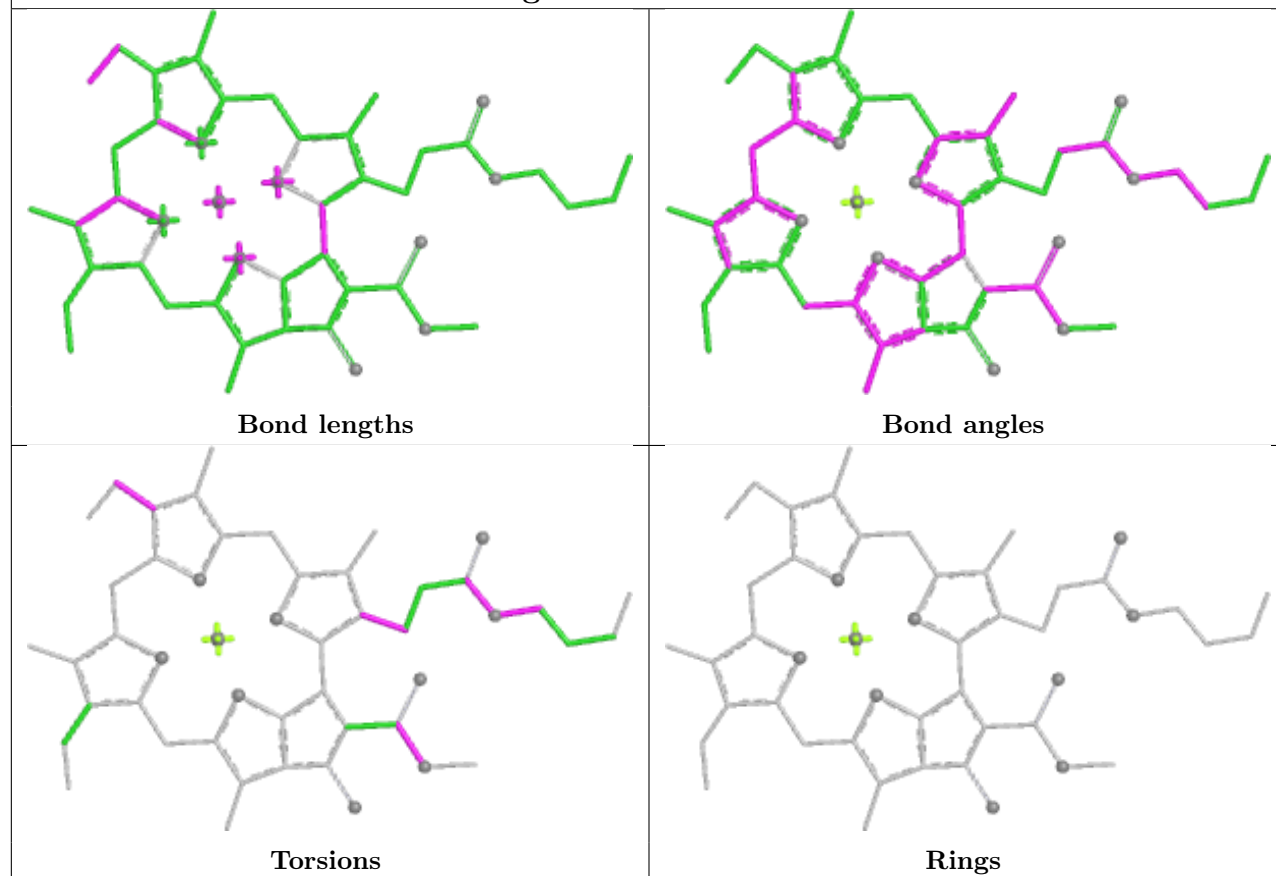
Ligand BCR 4 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

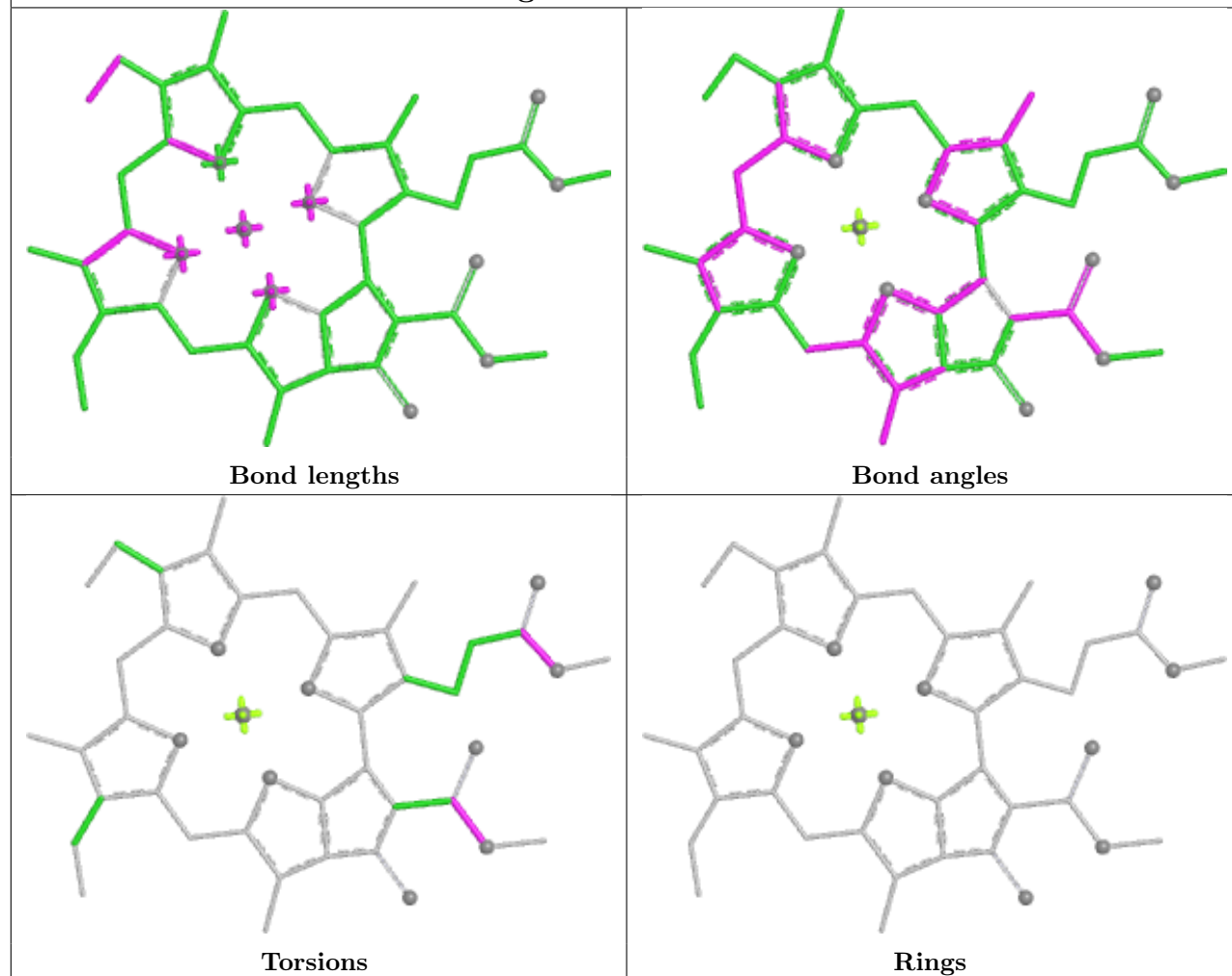
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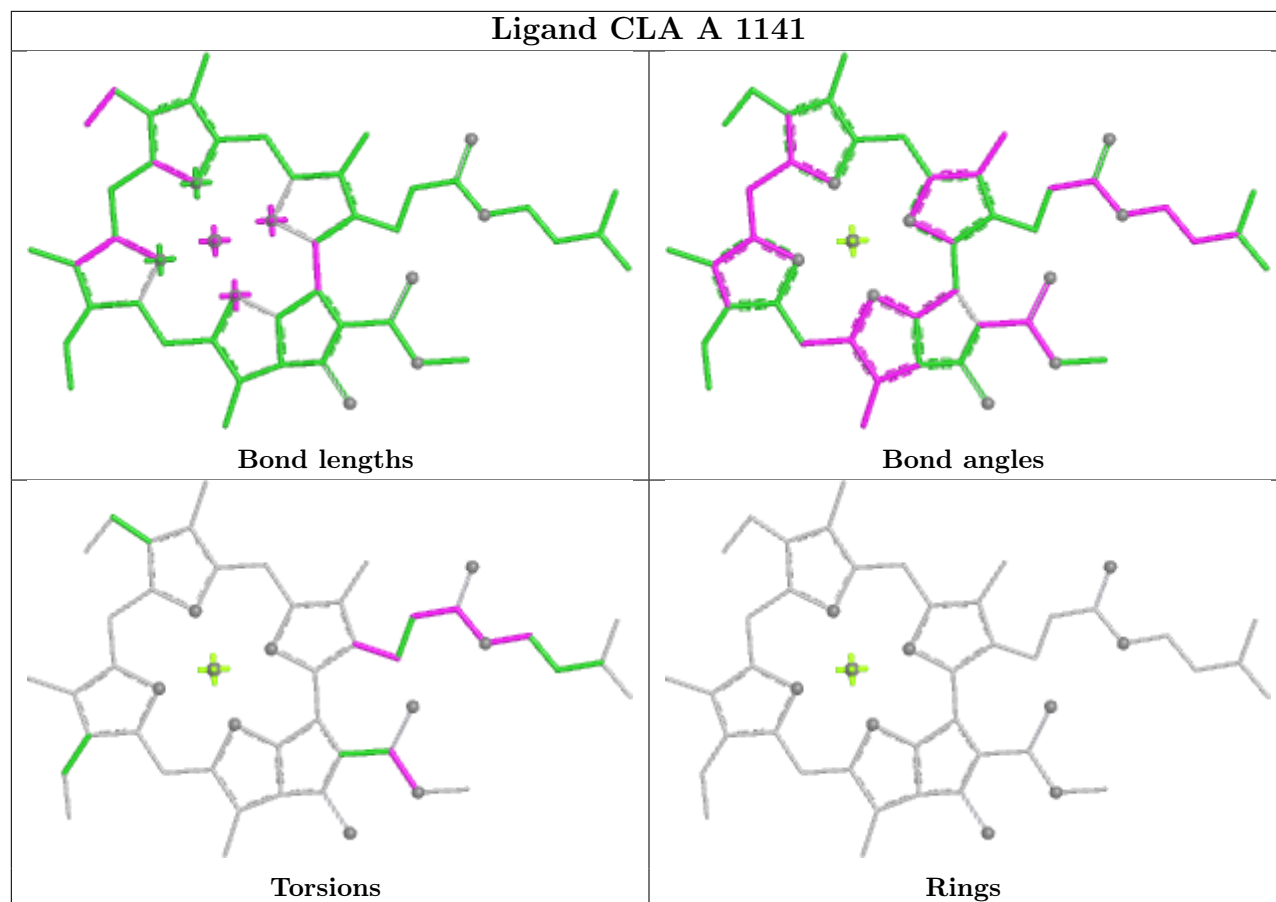
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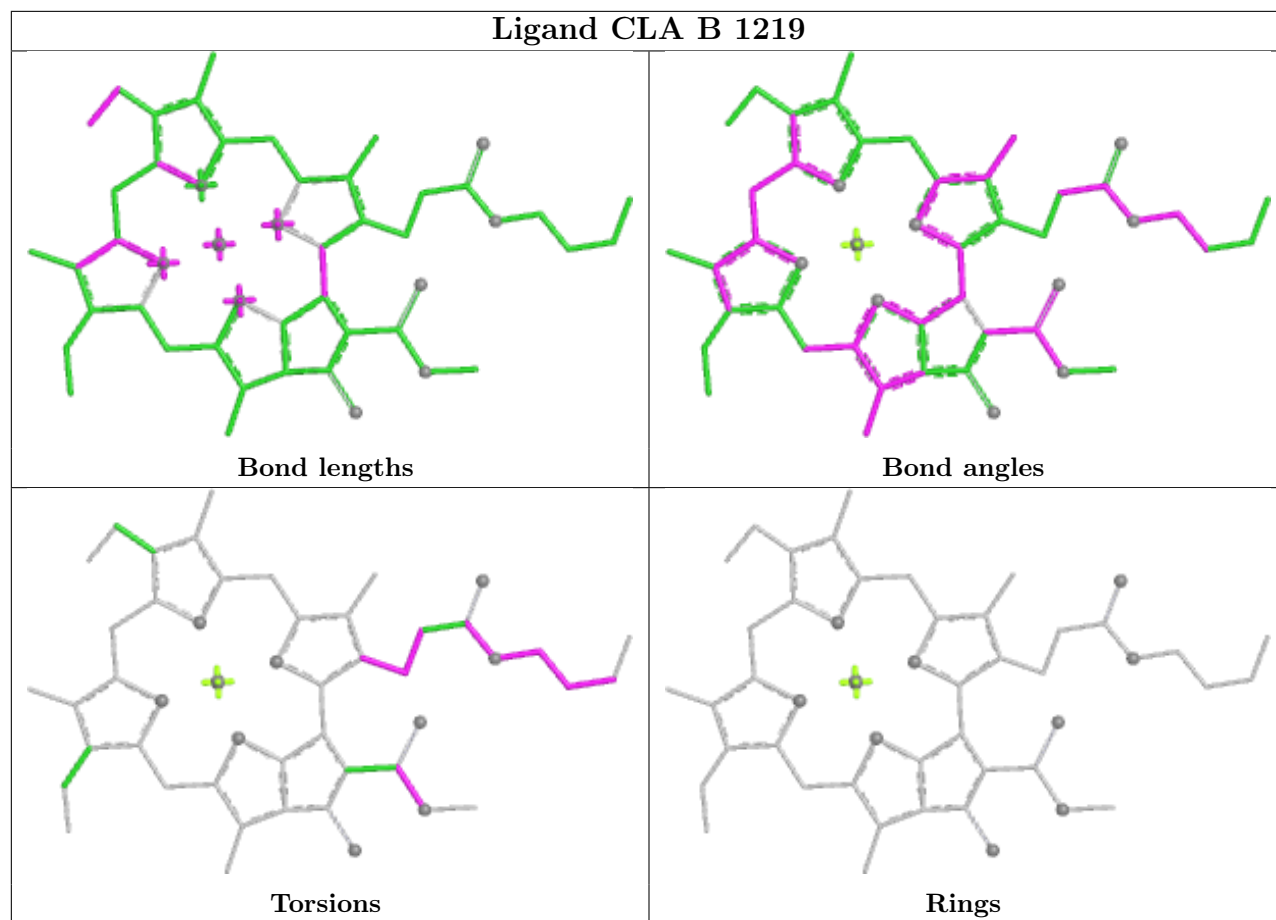


Ligand CLA 4 608

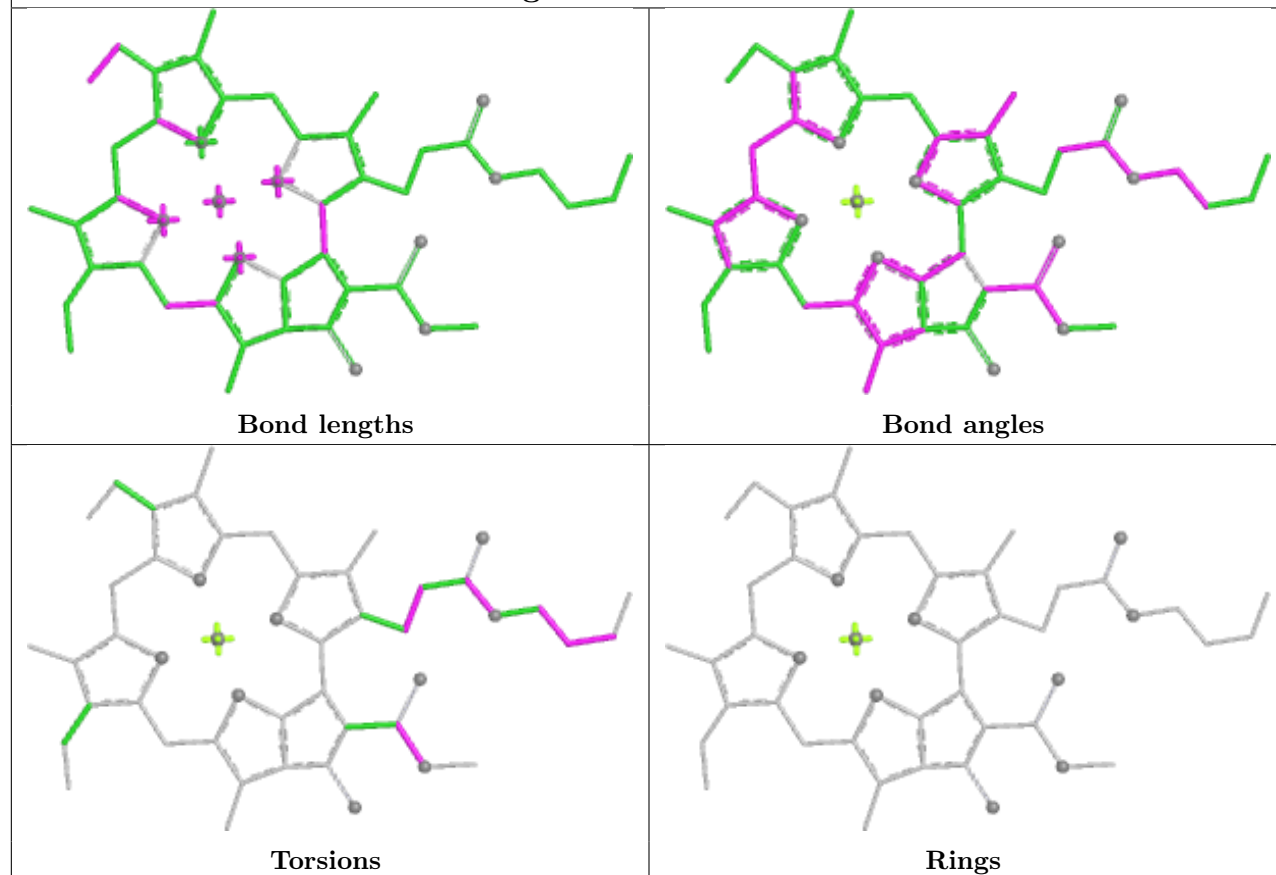


Ligand CLA A 1141

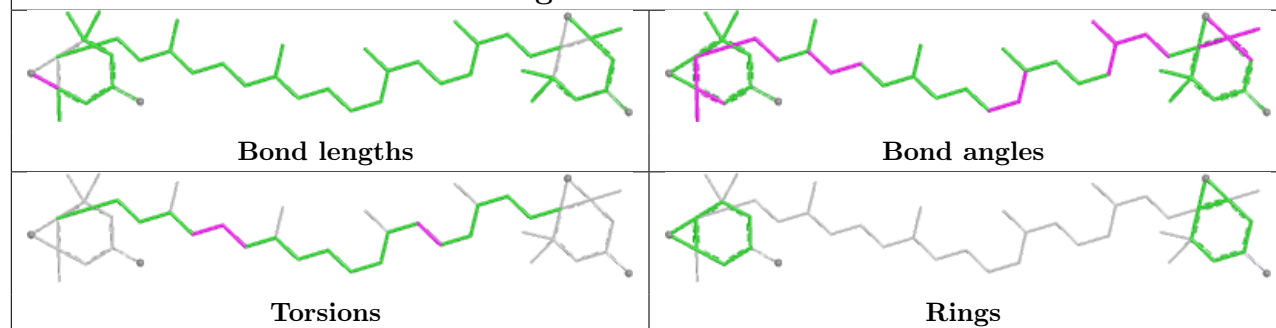




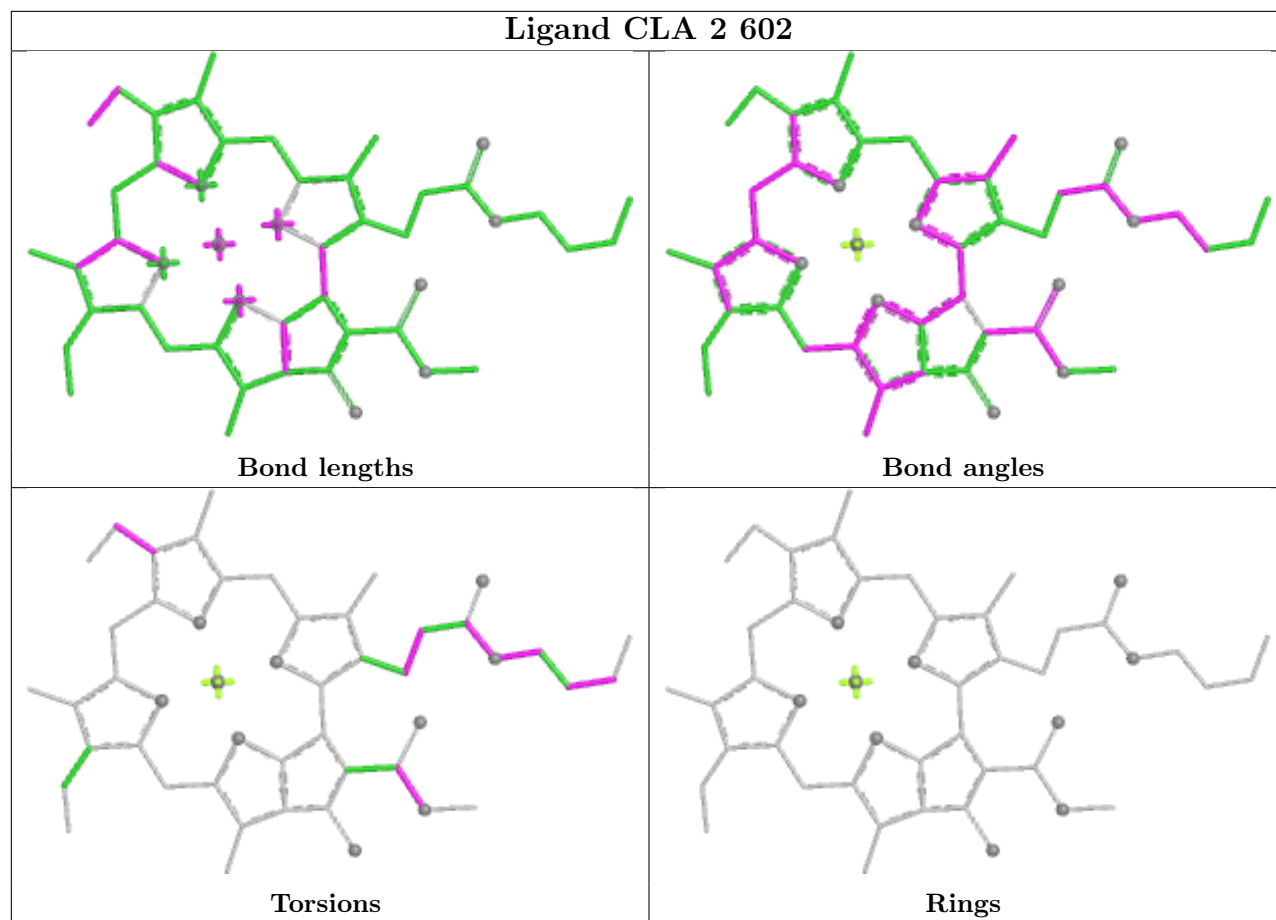
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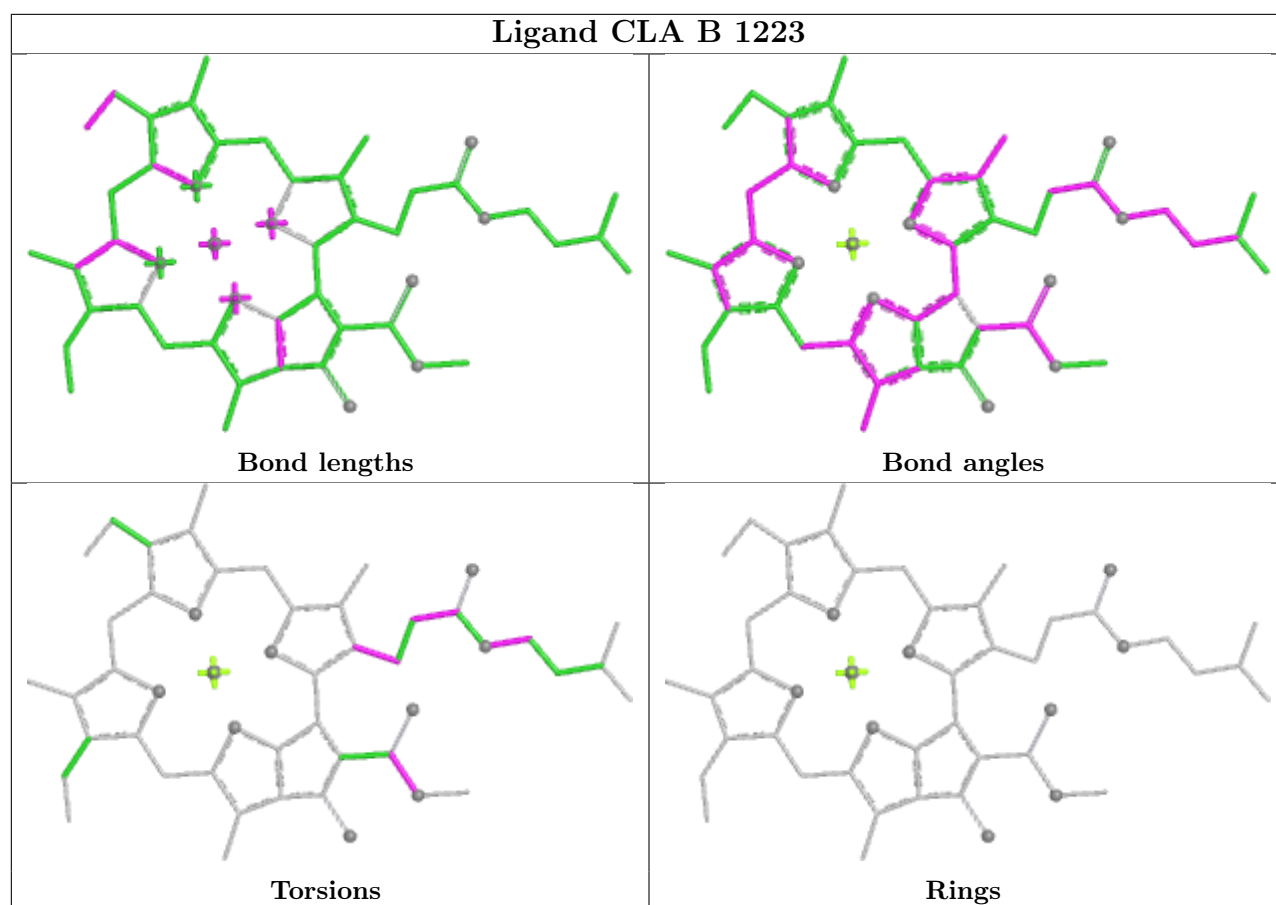


Ligand XAT 1 502

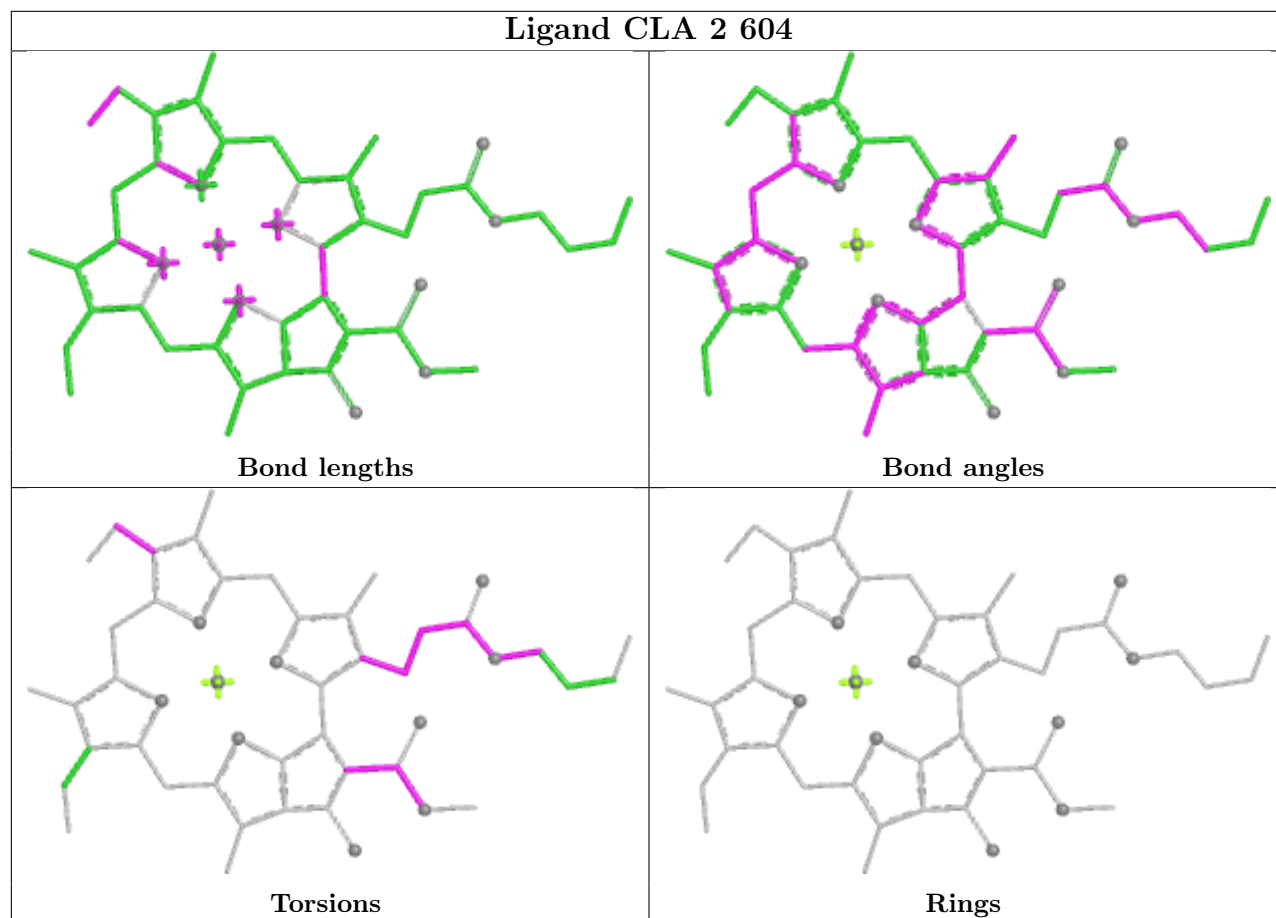


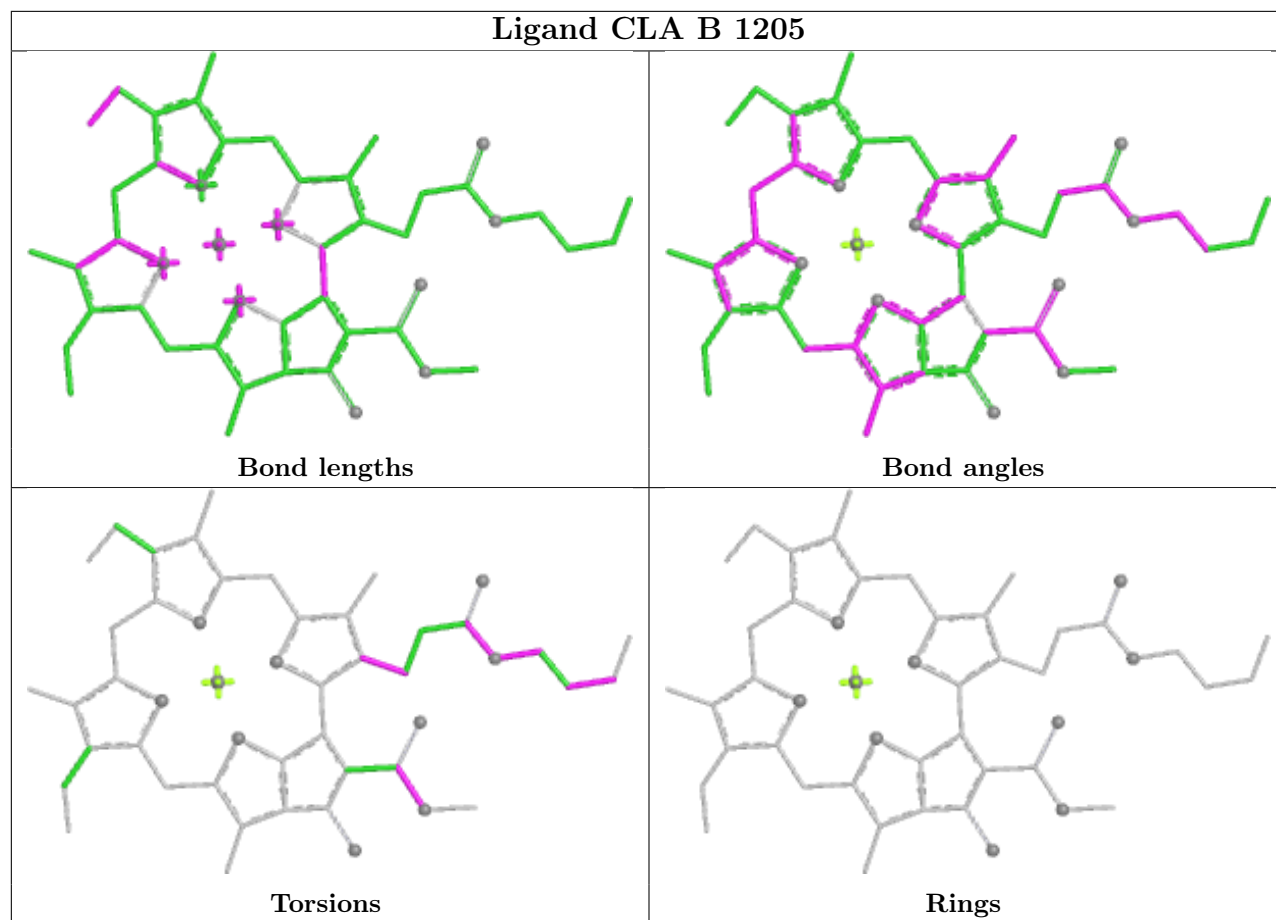
Ligand CLA 2 602

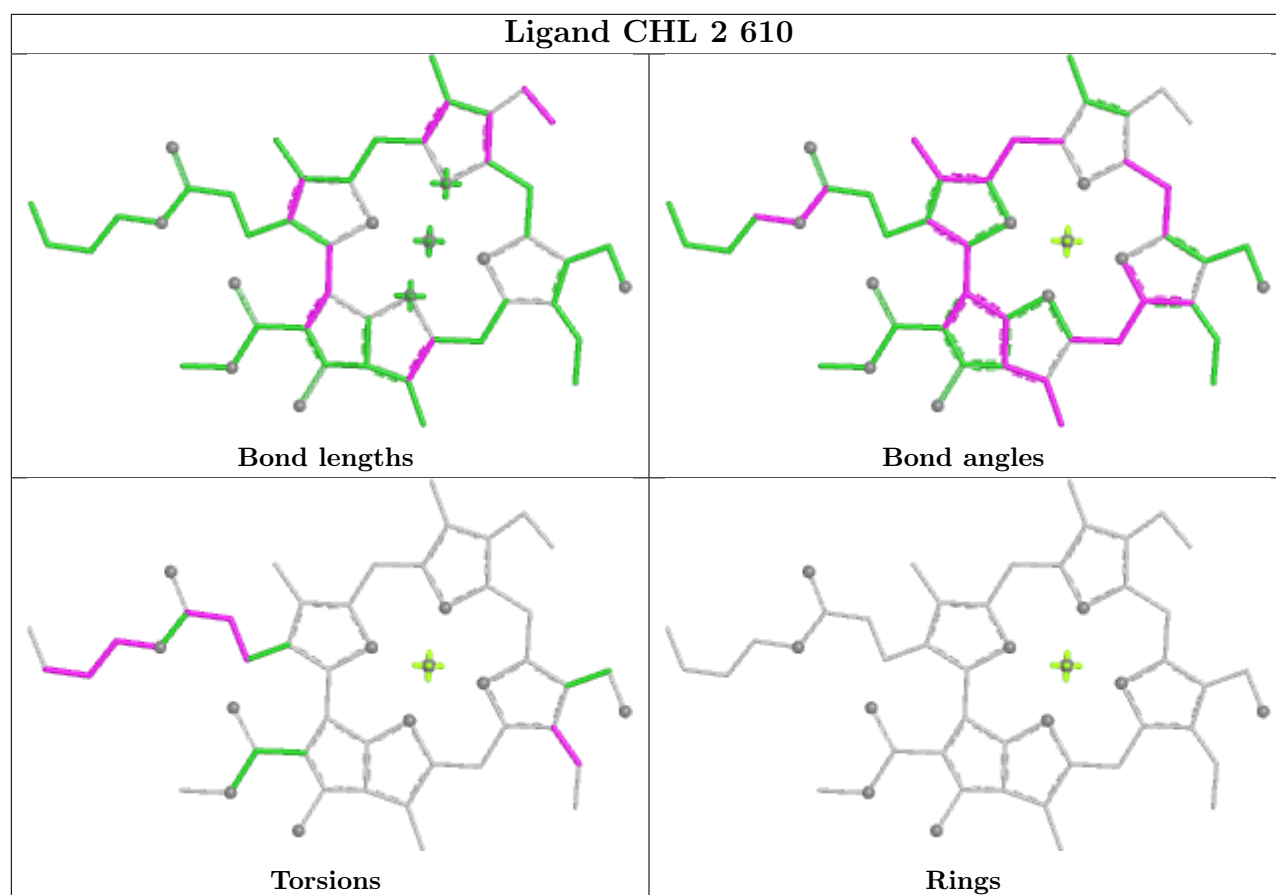


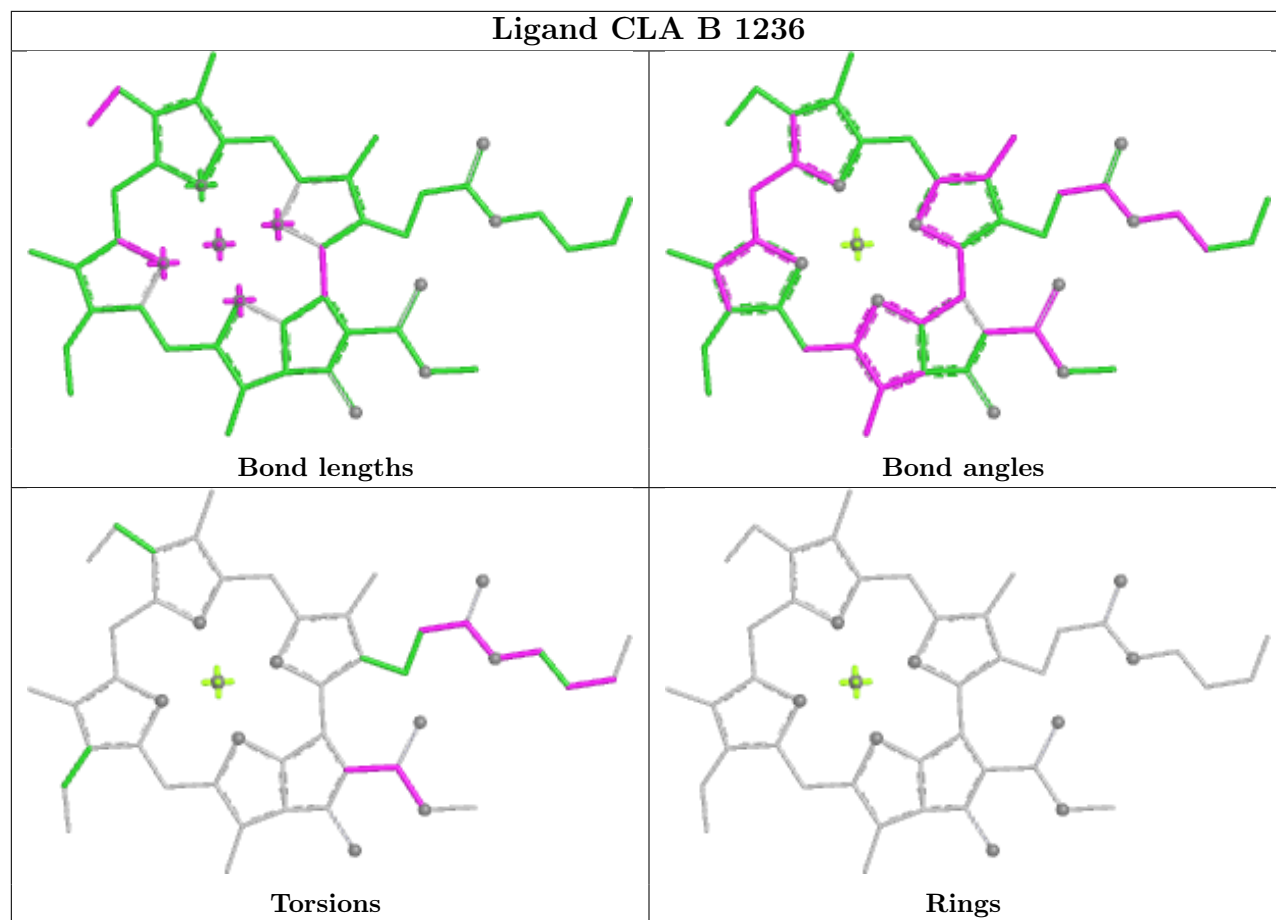


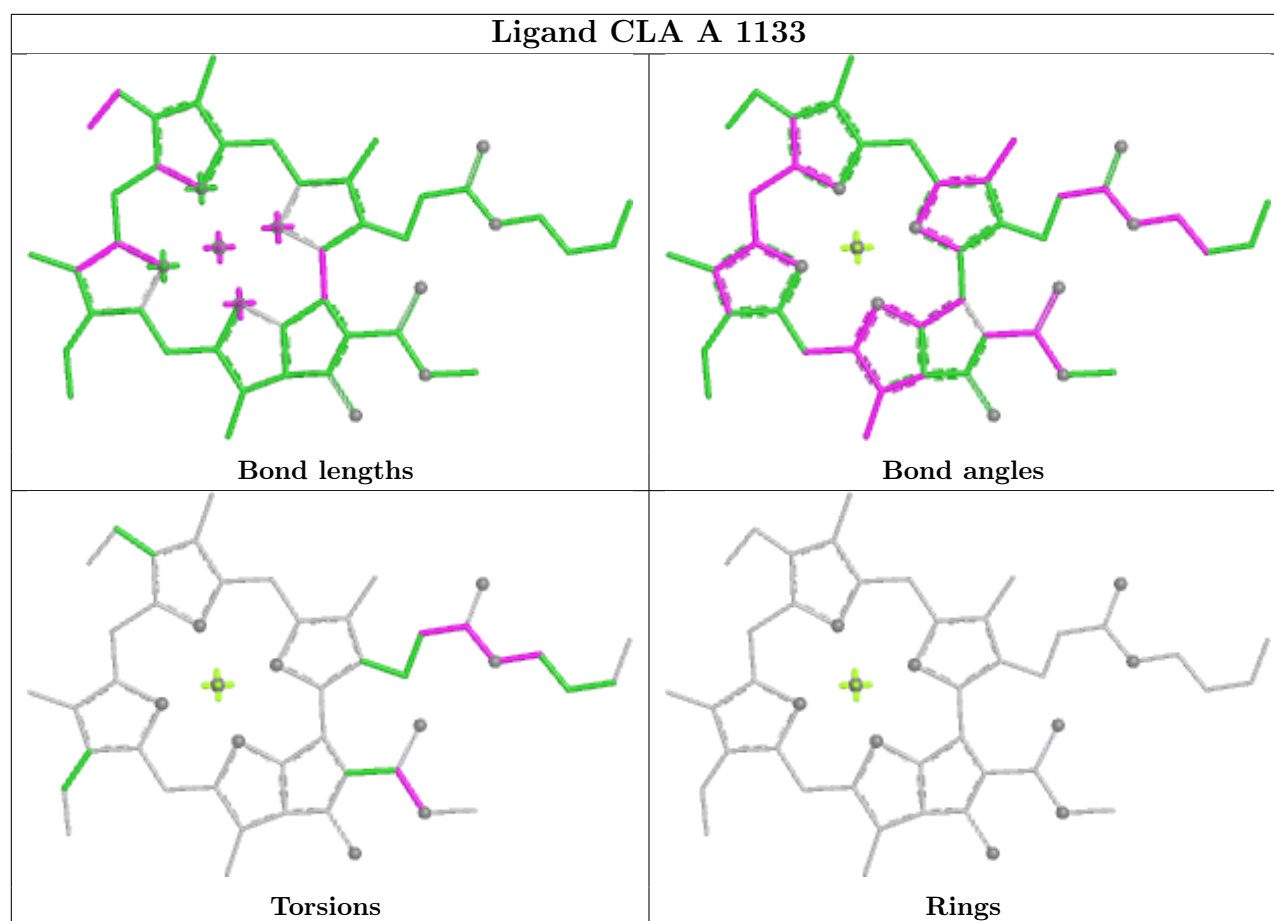
Ligand CLA 2 604



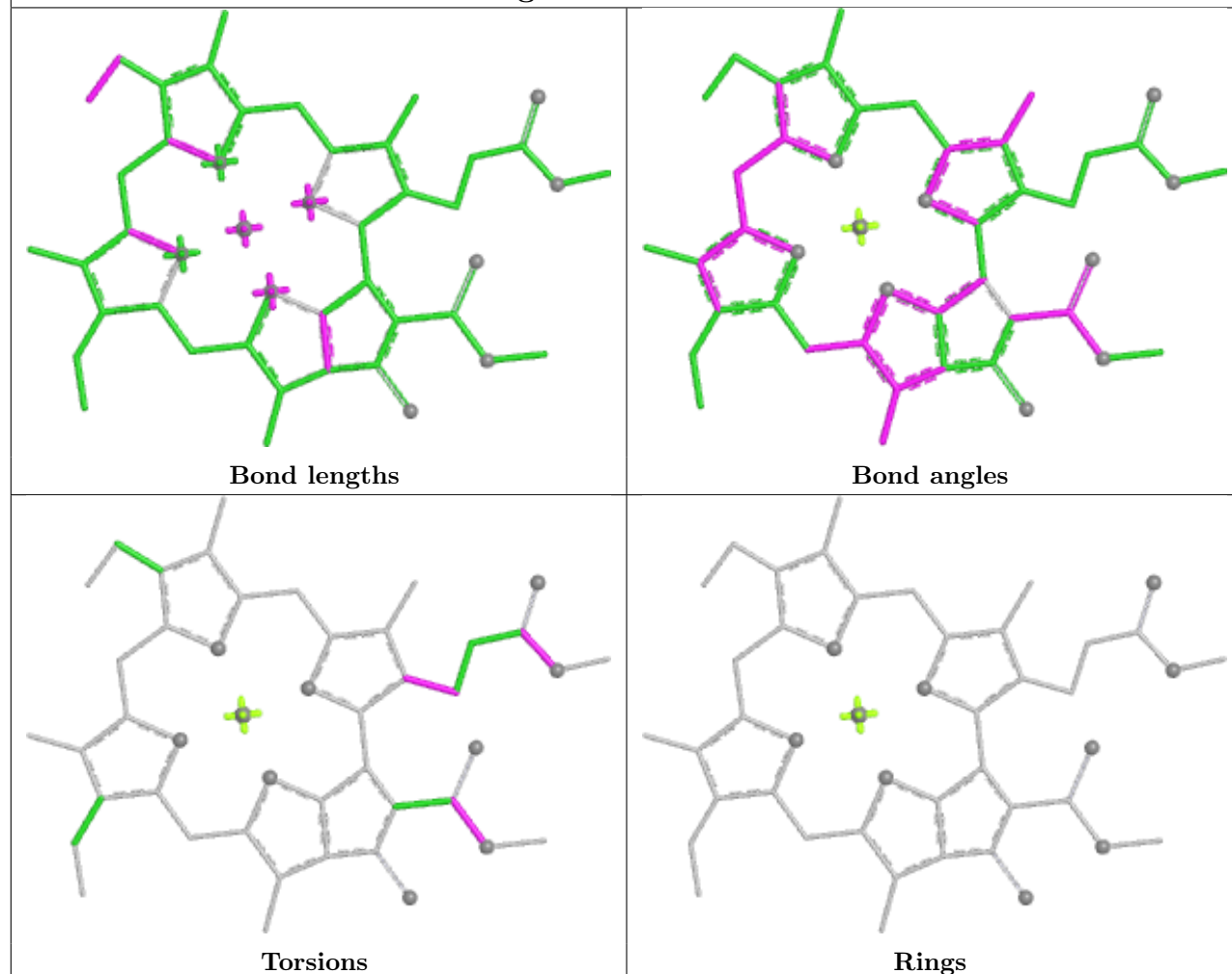




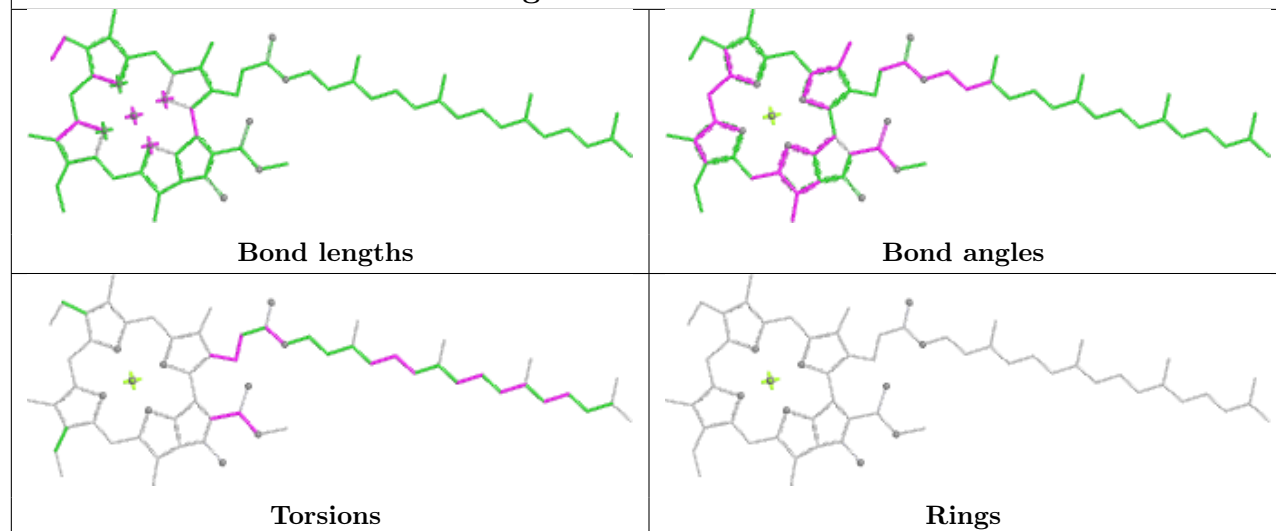


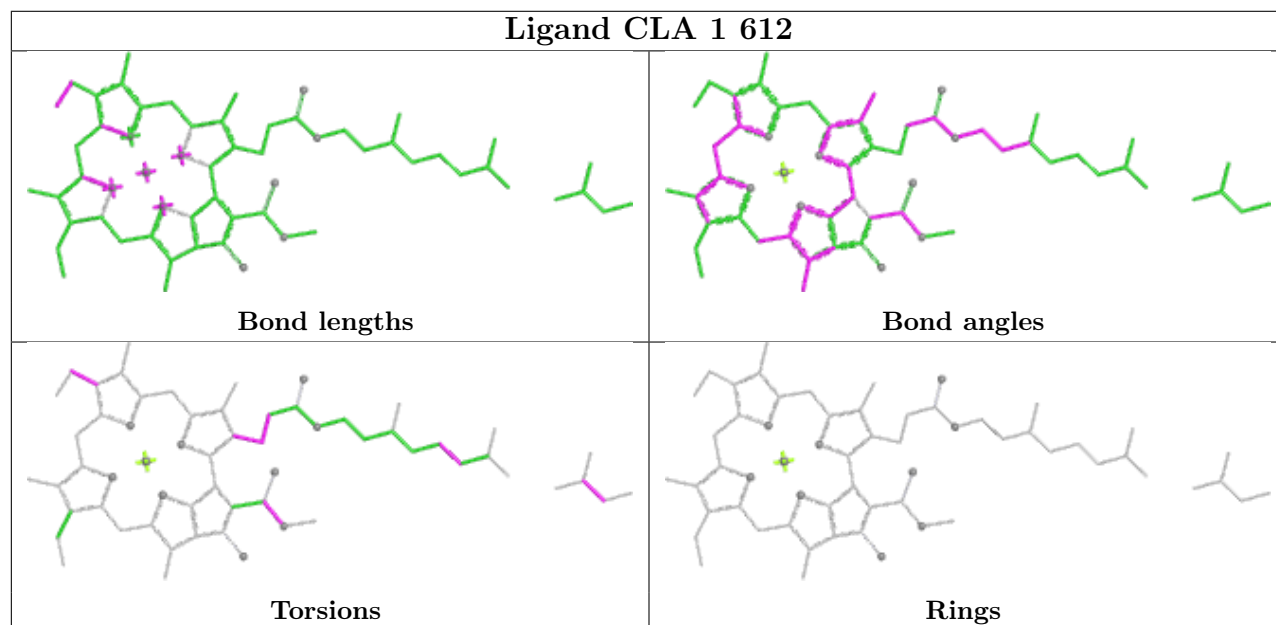
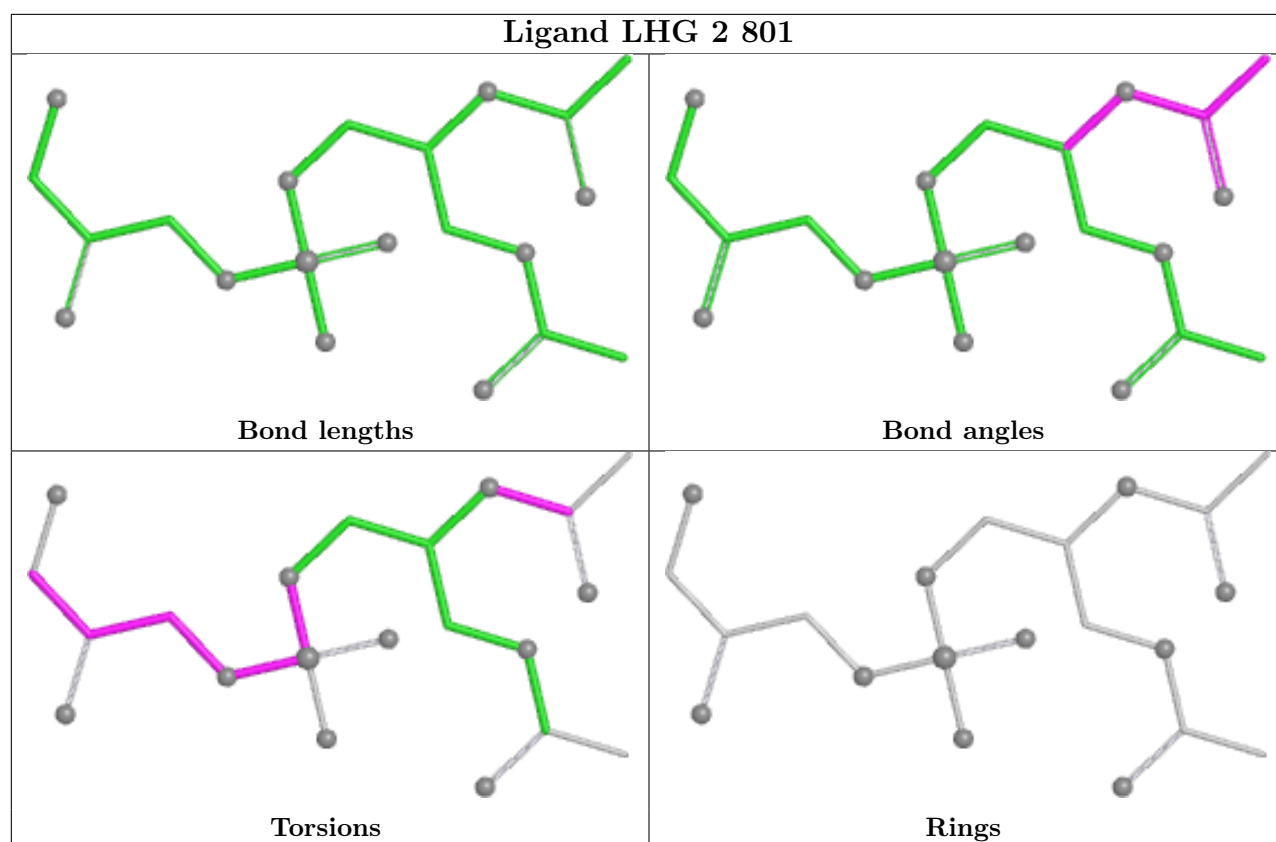


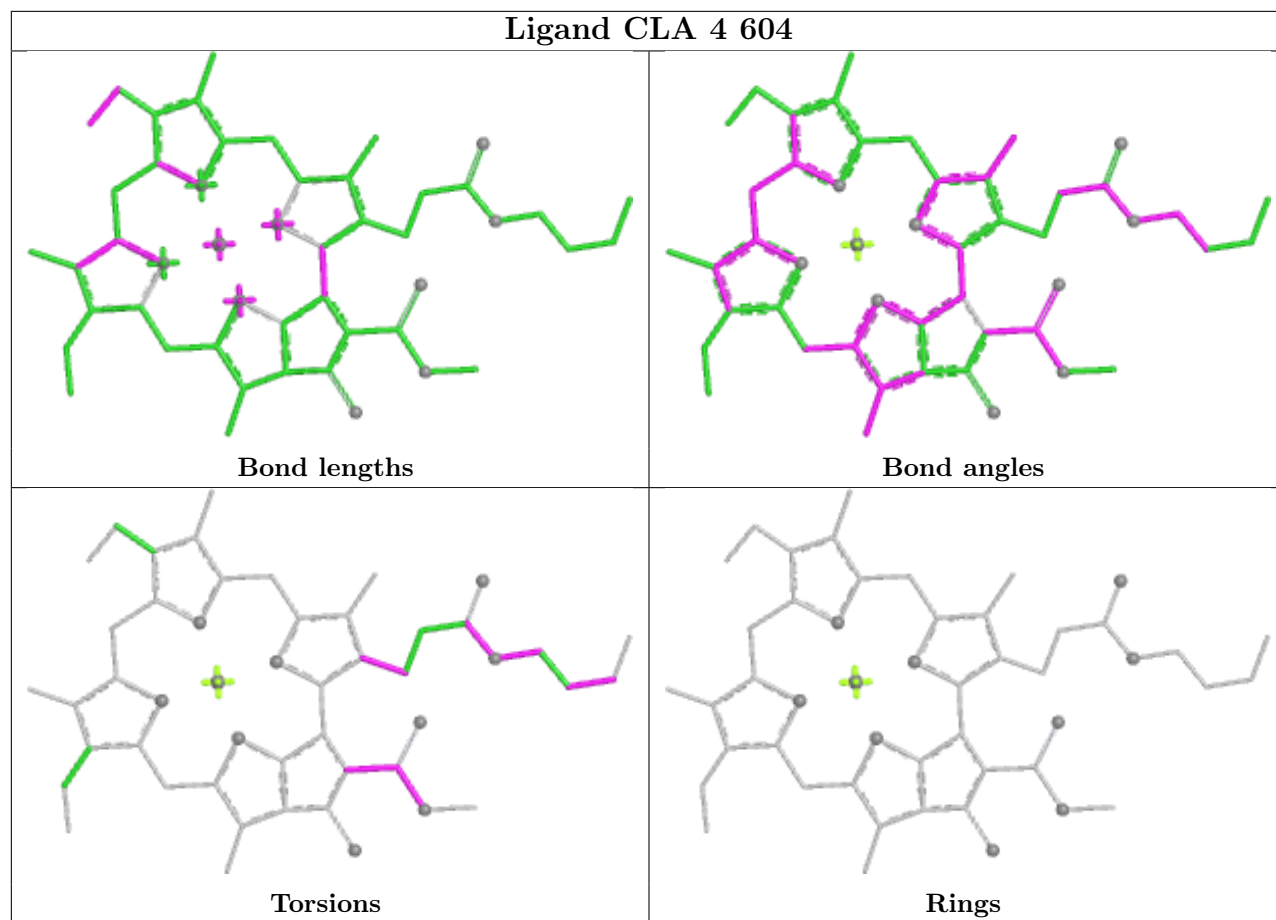
Ligand CLA 1 608

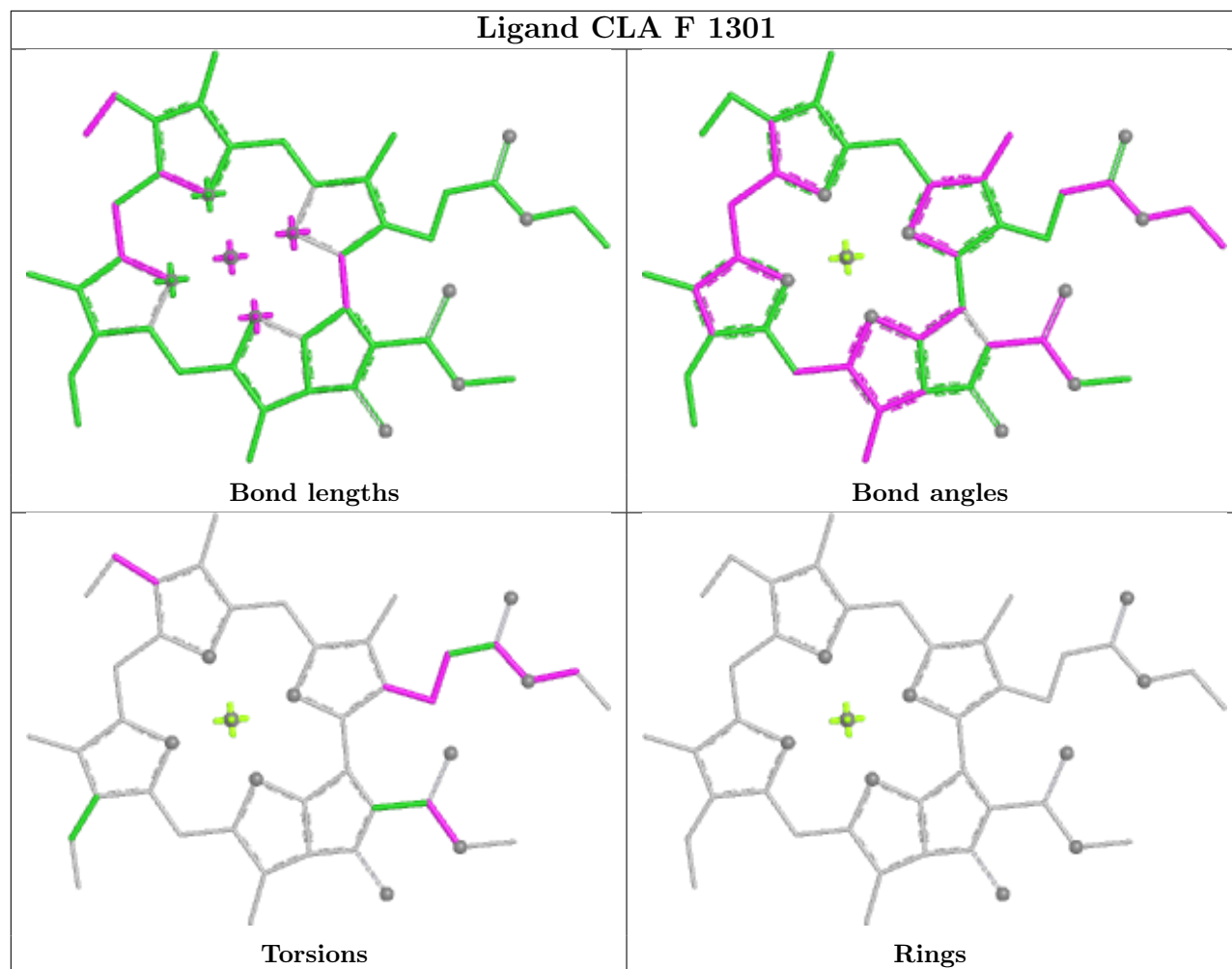


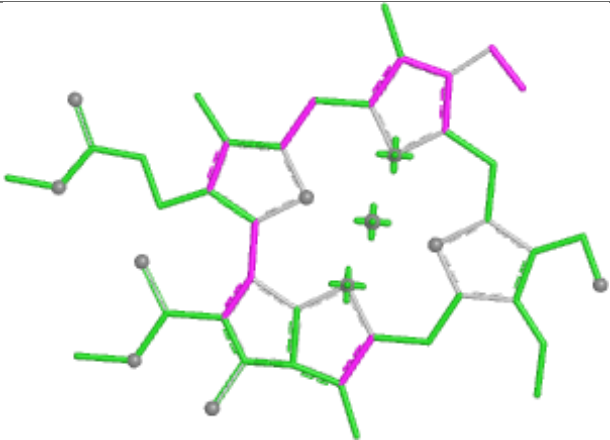
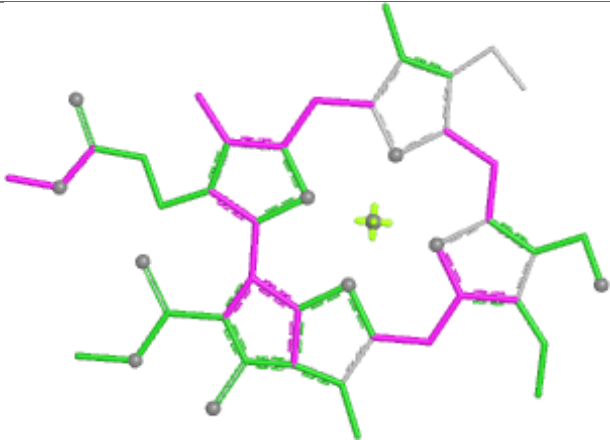
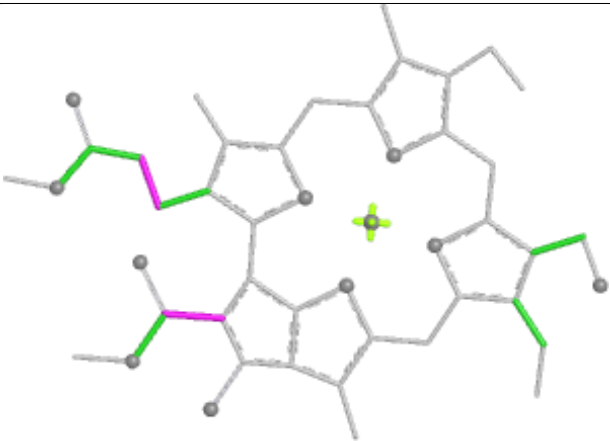
Ligand CLA A 1106

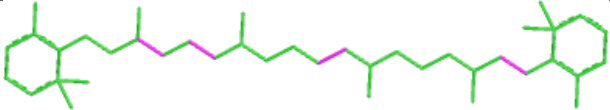
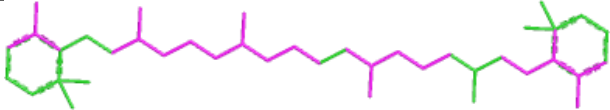
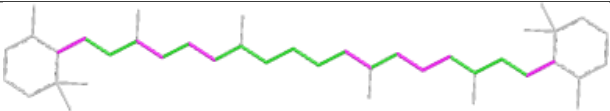
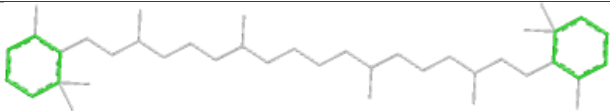


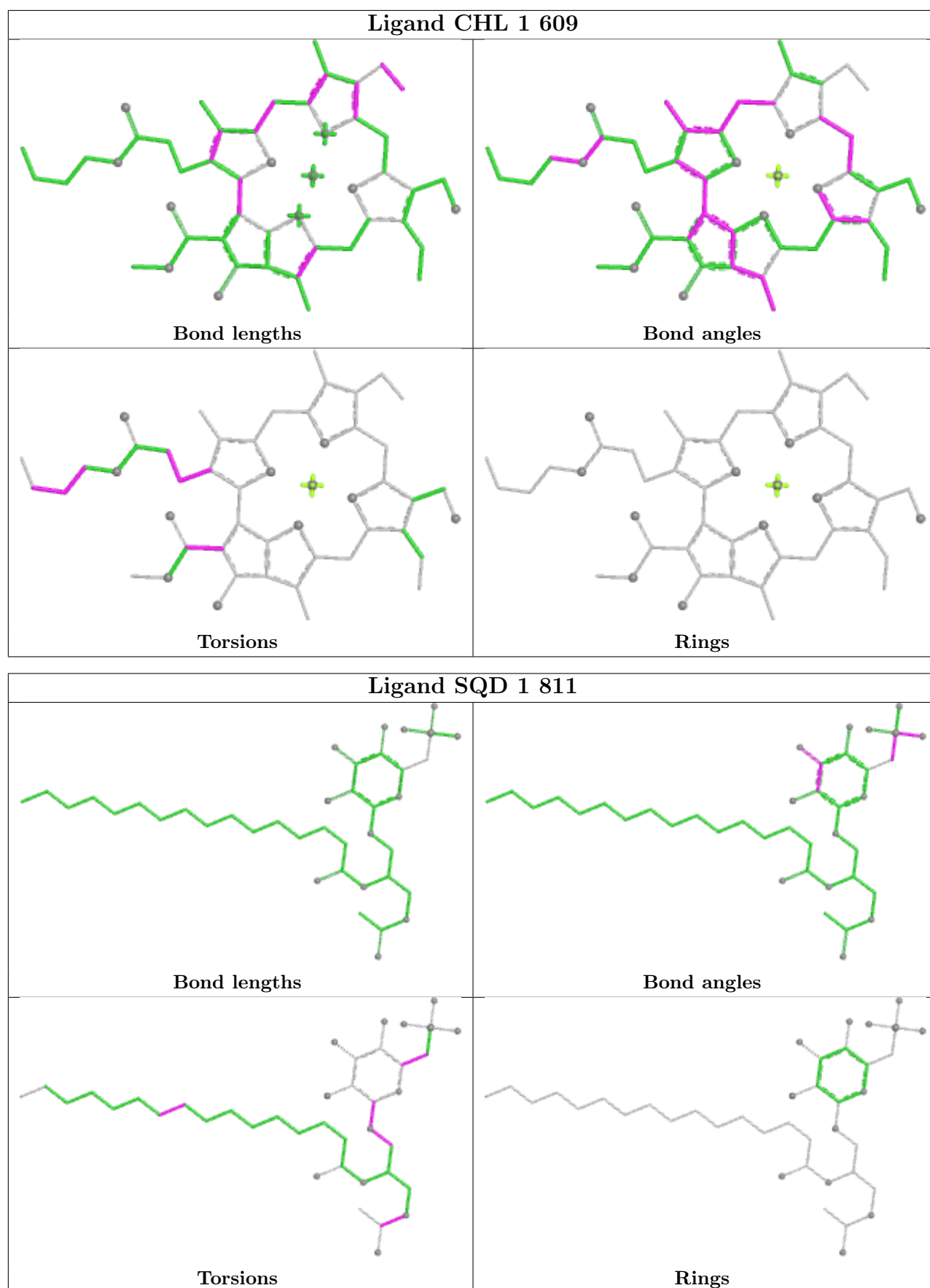


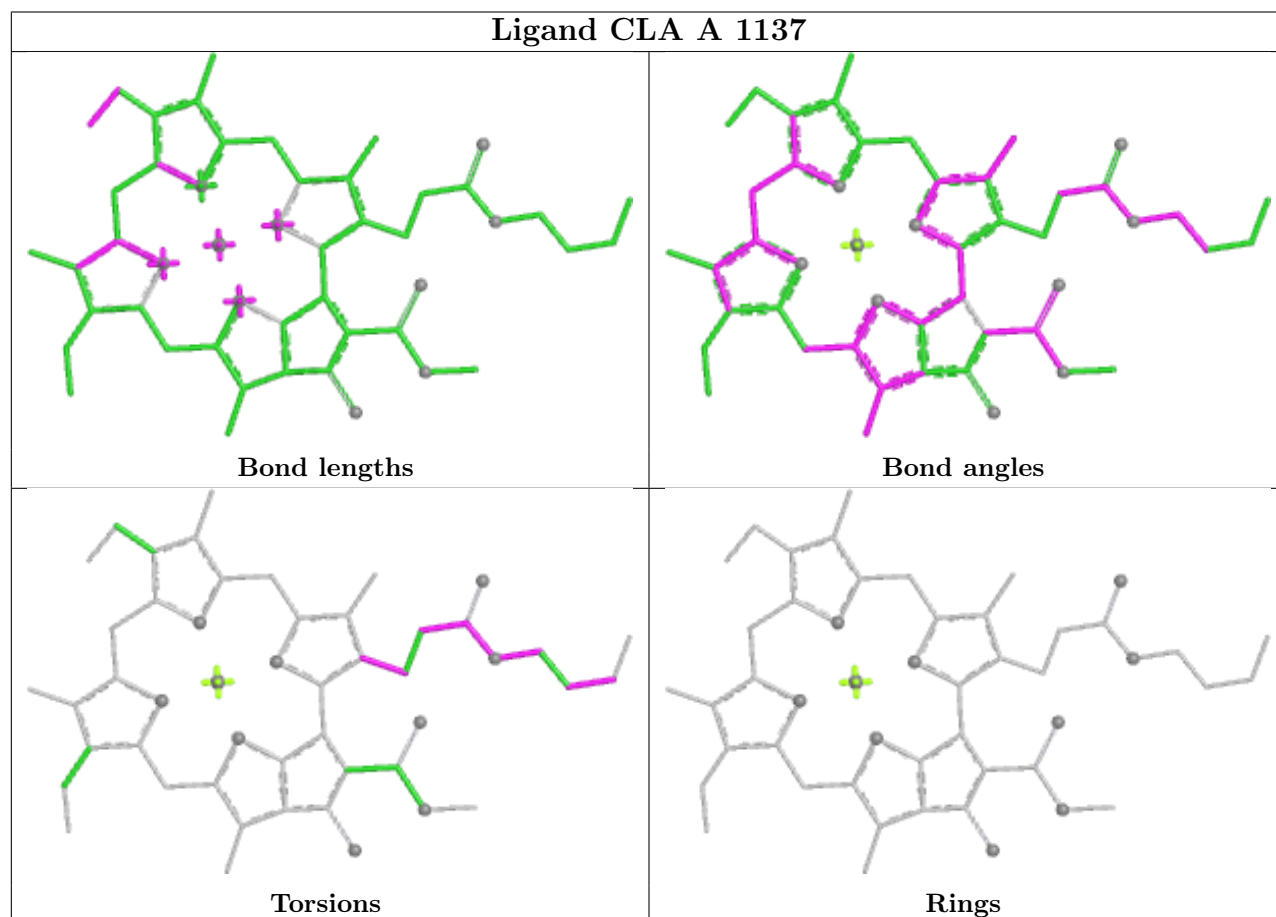
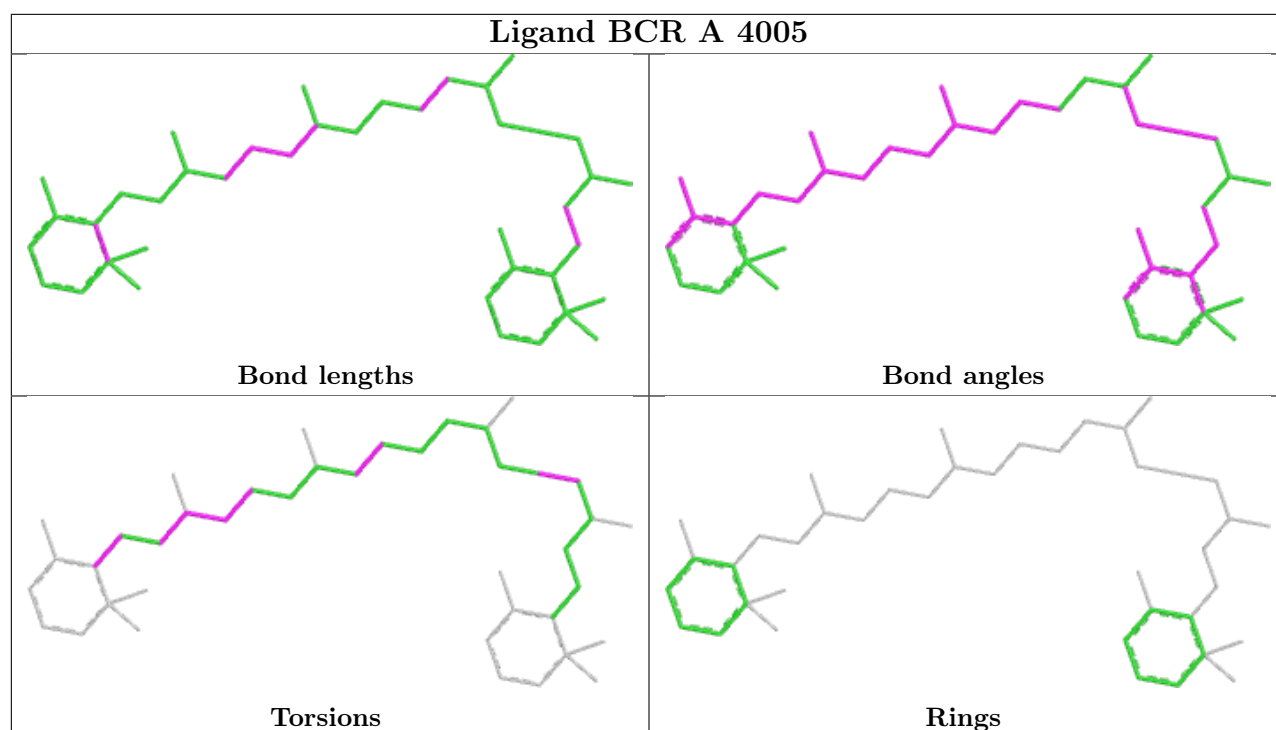


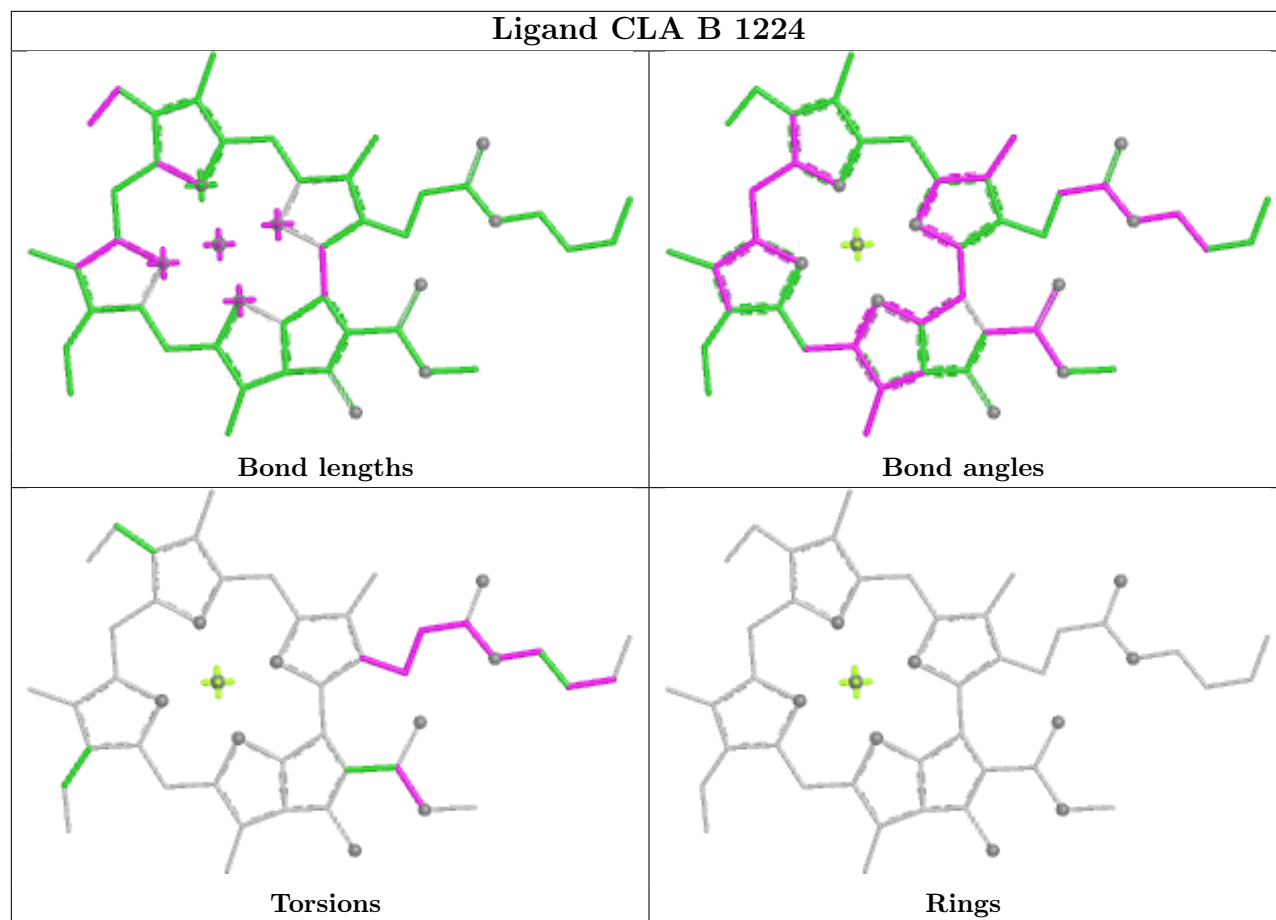


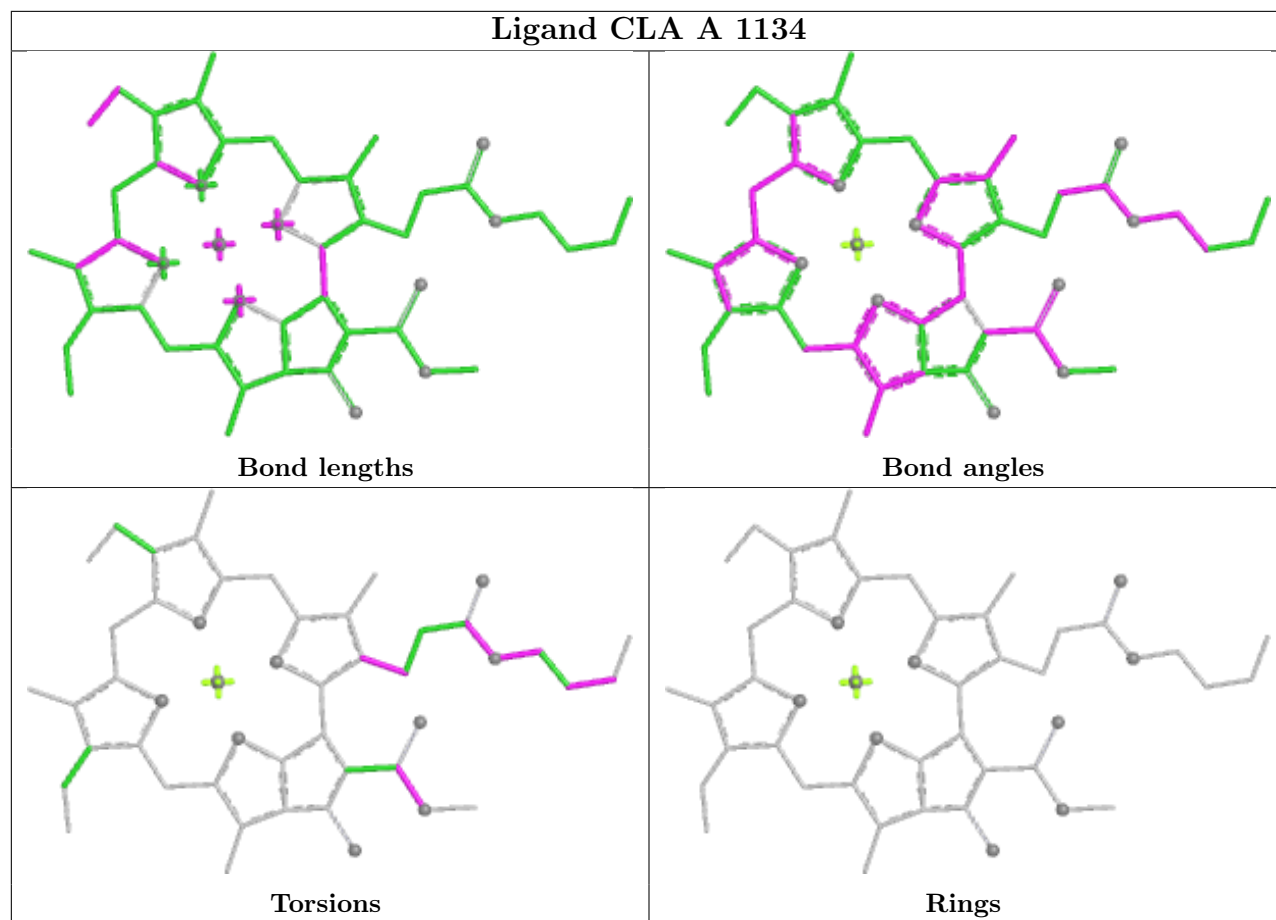
Ligand CHL 4 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 4007	
	
Bond lengths	Bond angles
	
Torsions	Rings

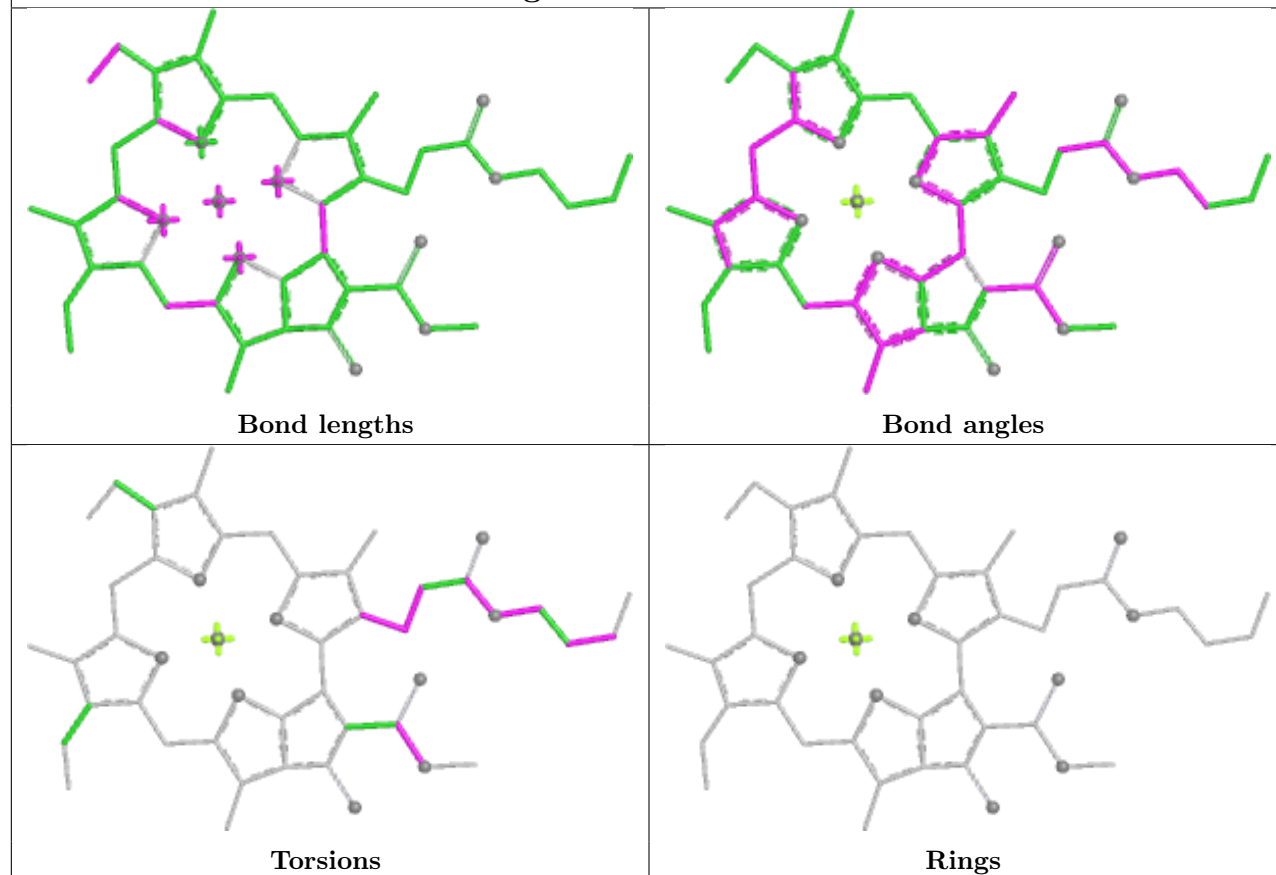




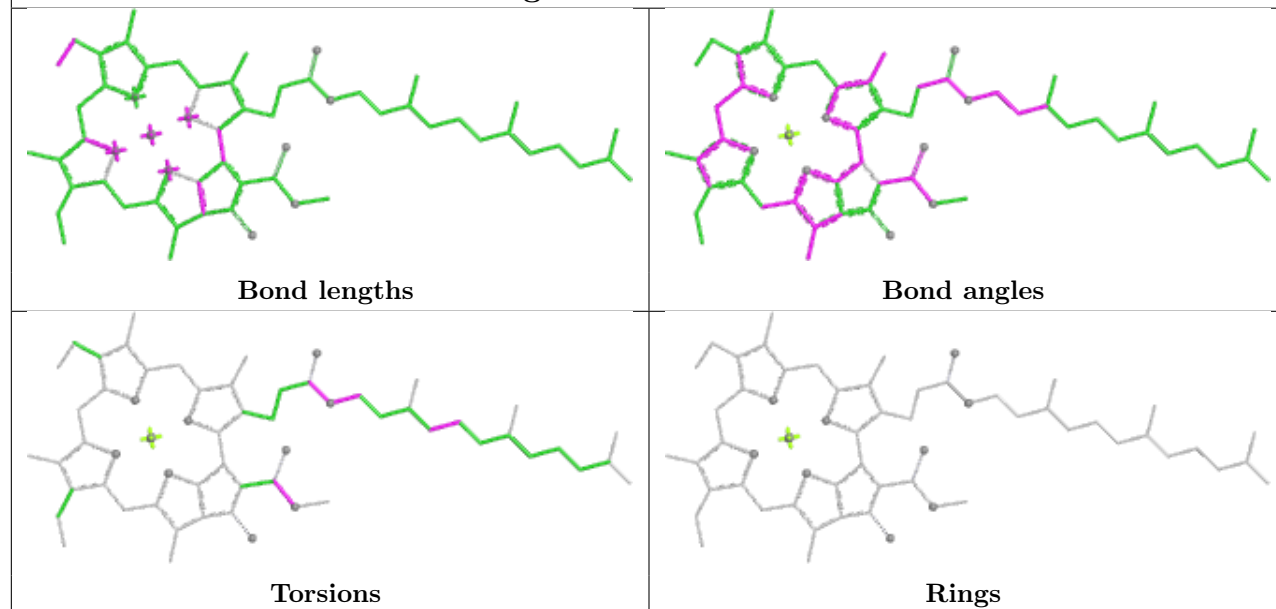


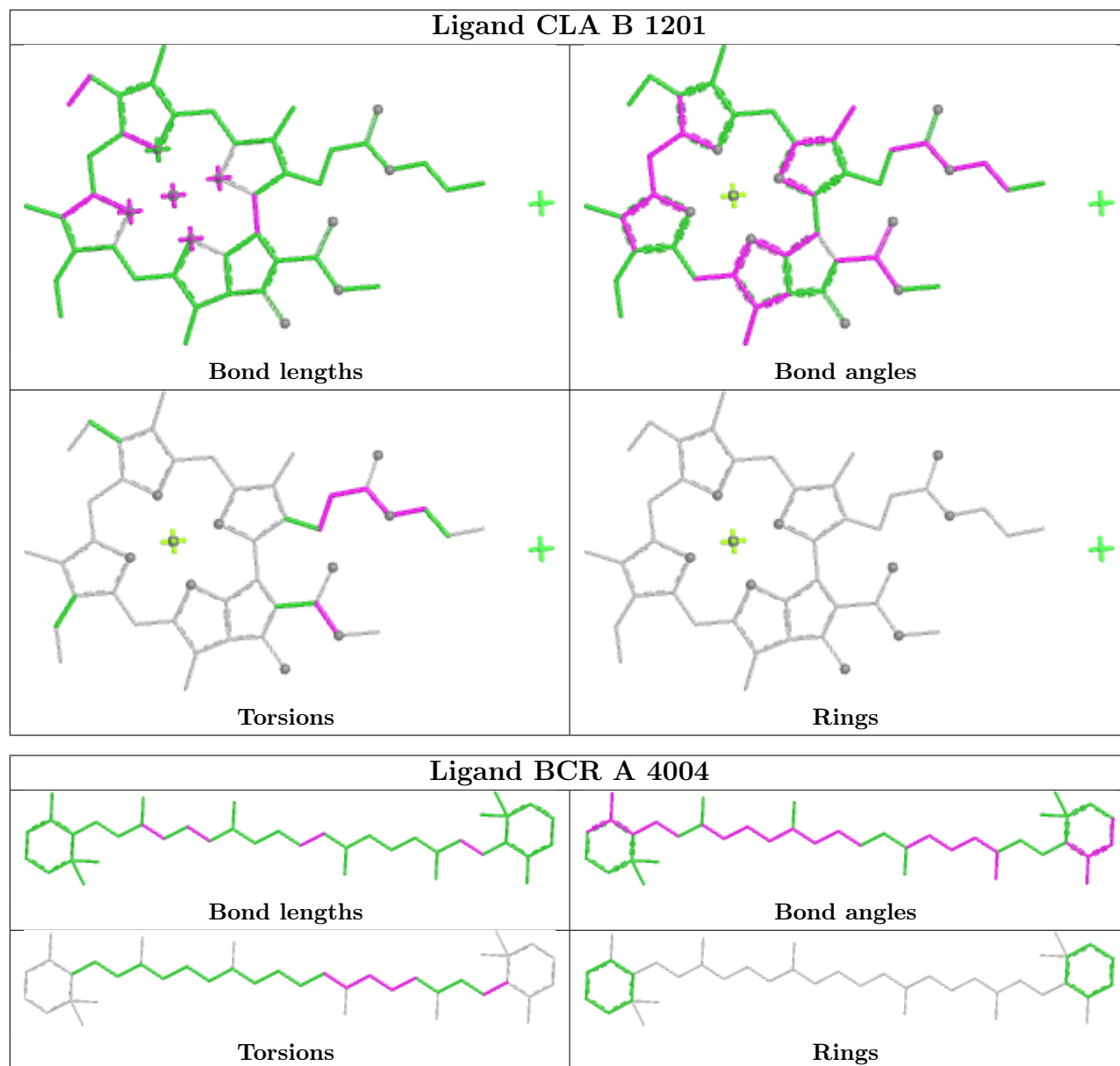


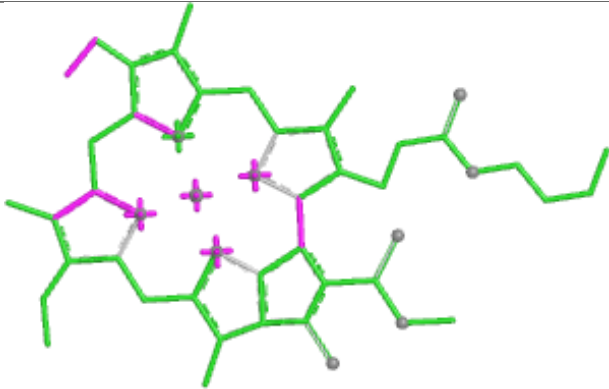
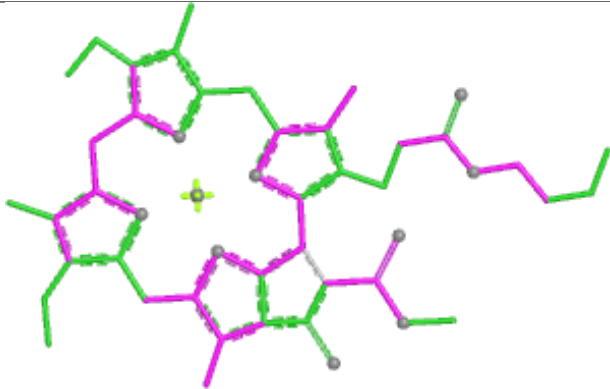
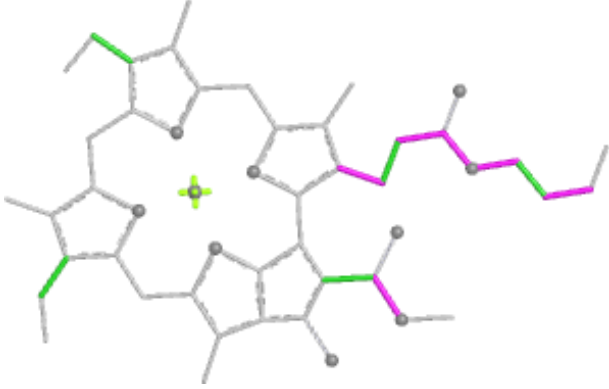
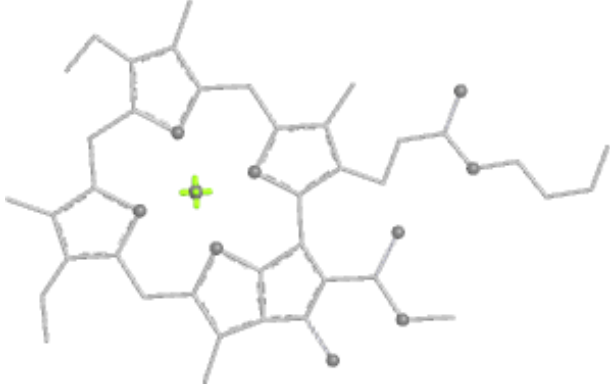
Ligand CLA B 1216

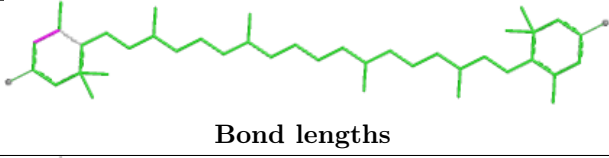
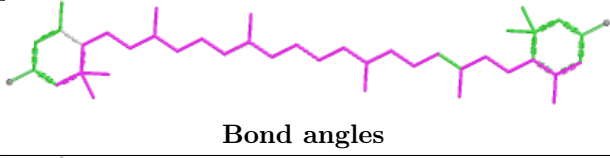
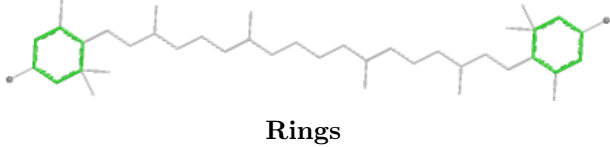


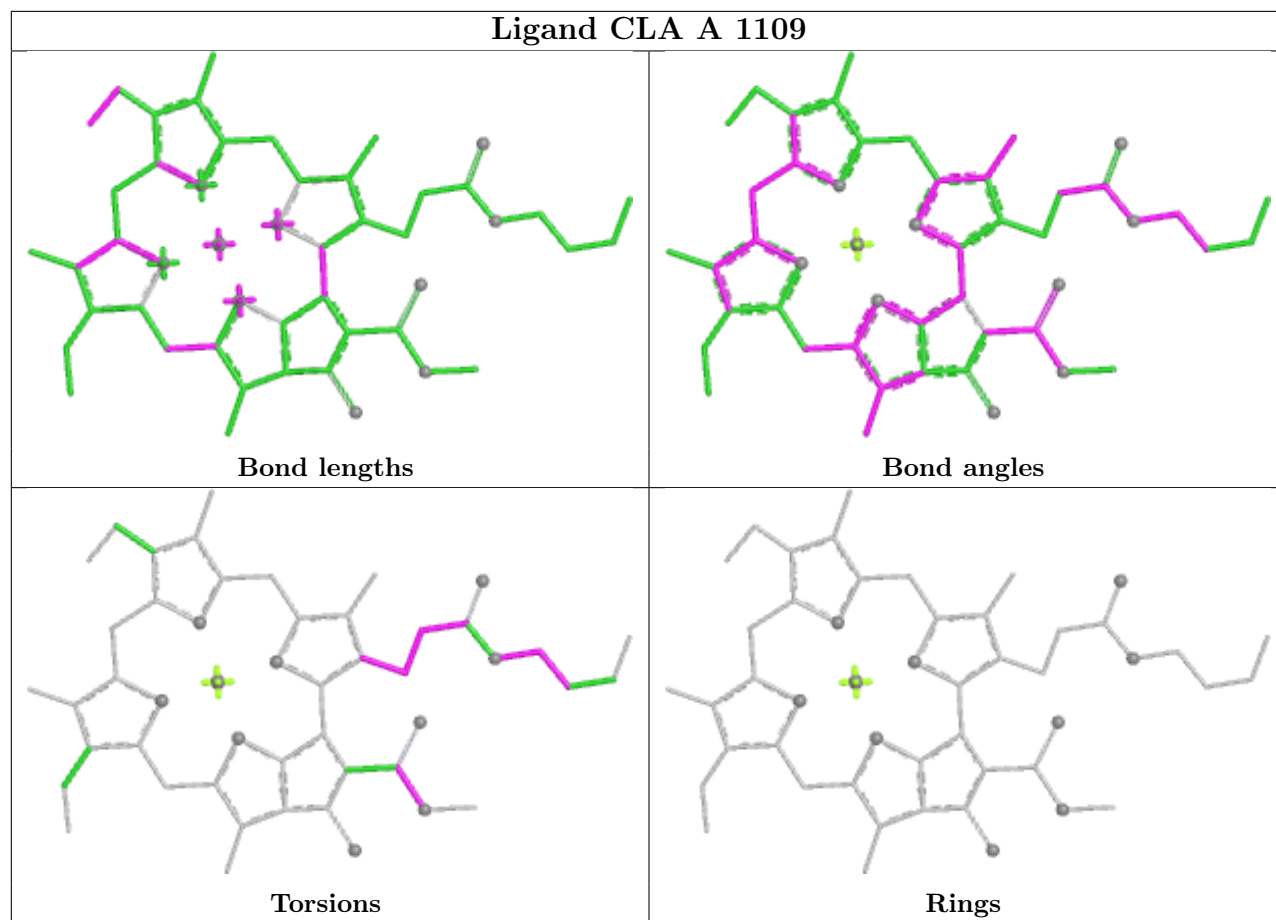
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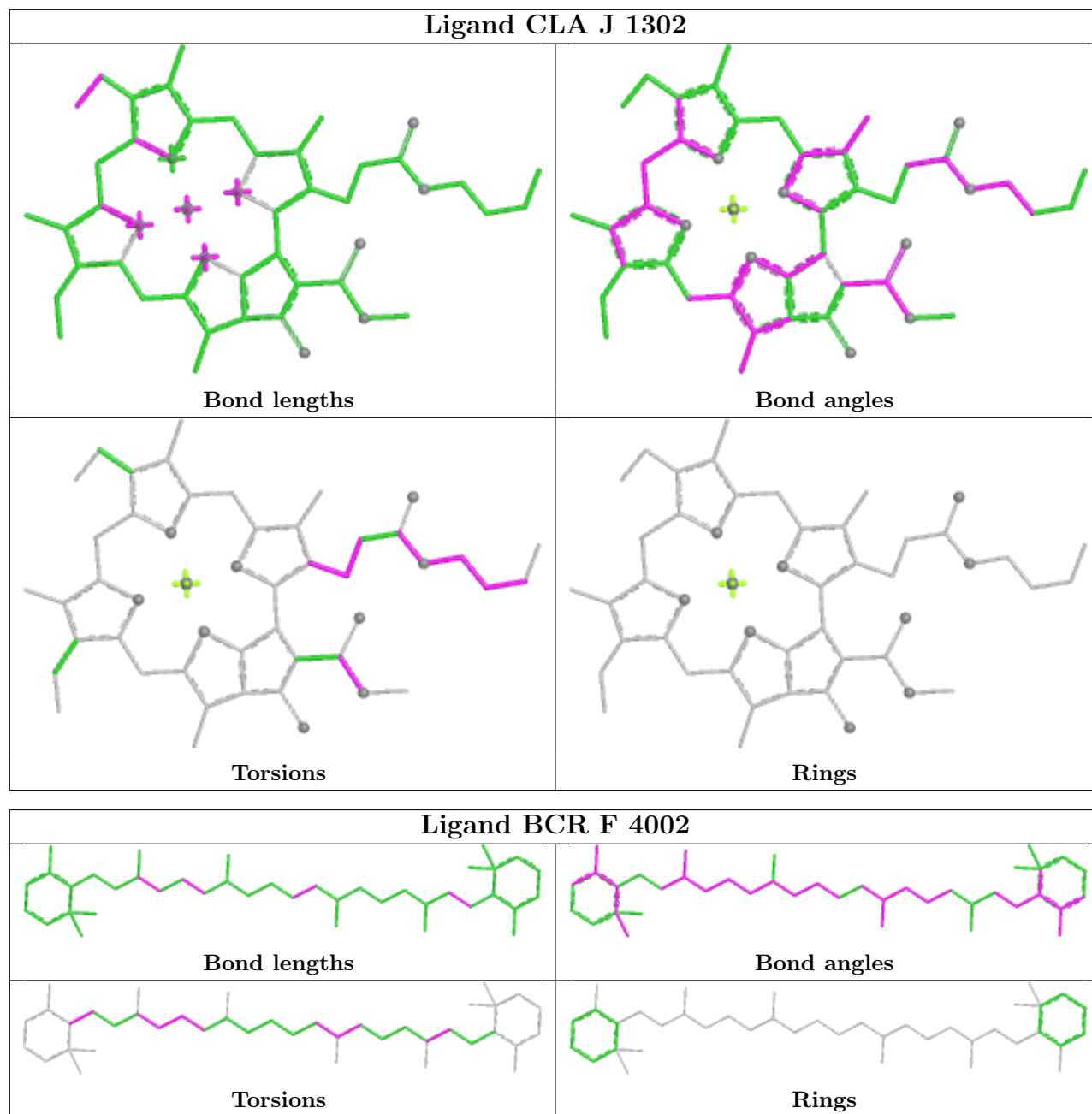




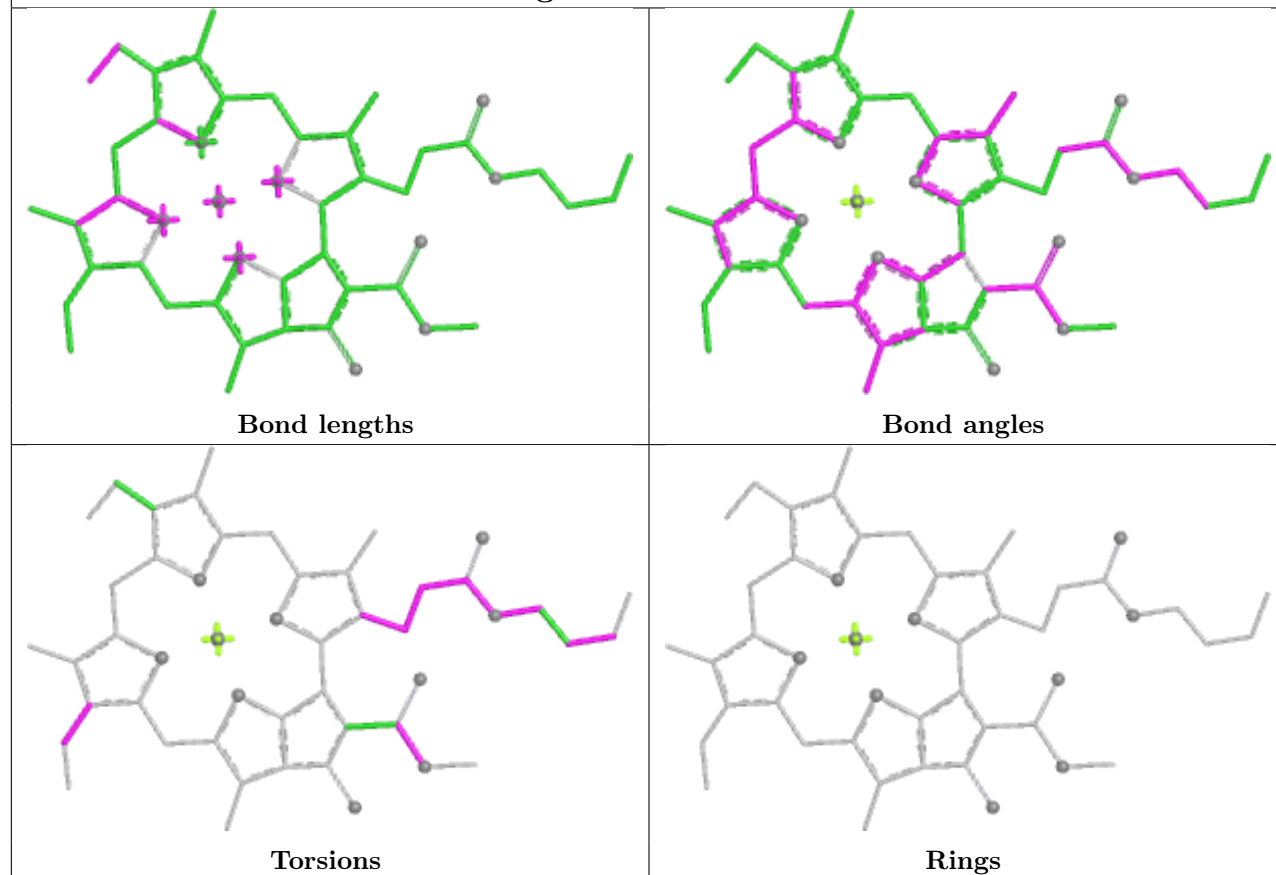
Ligand CLA B 1206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 1 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

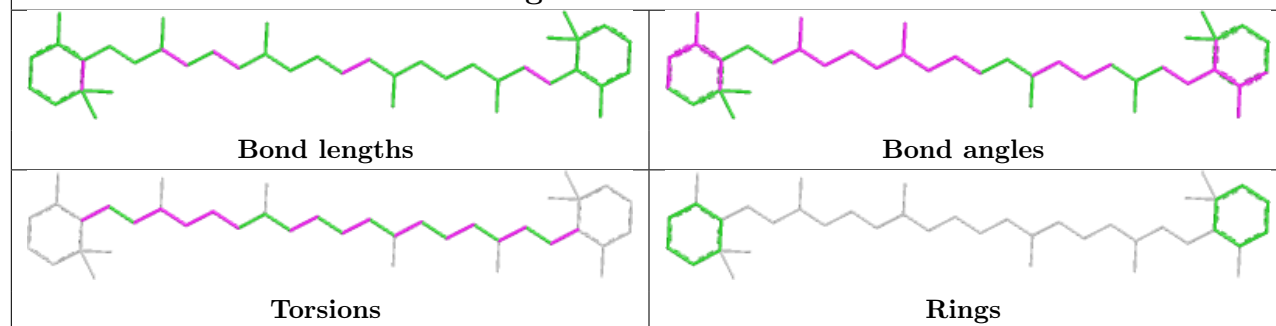




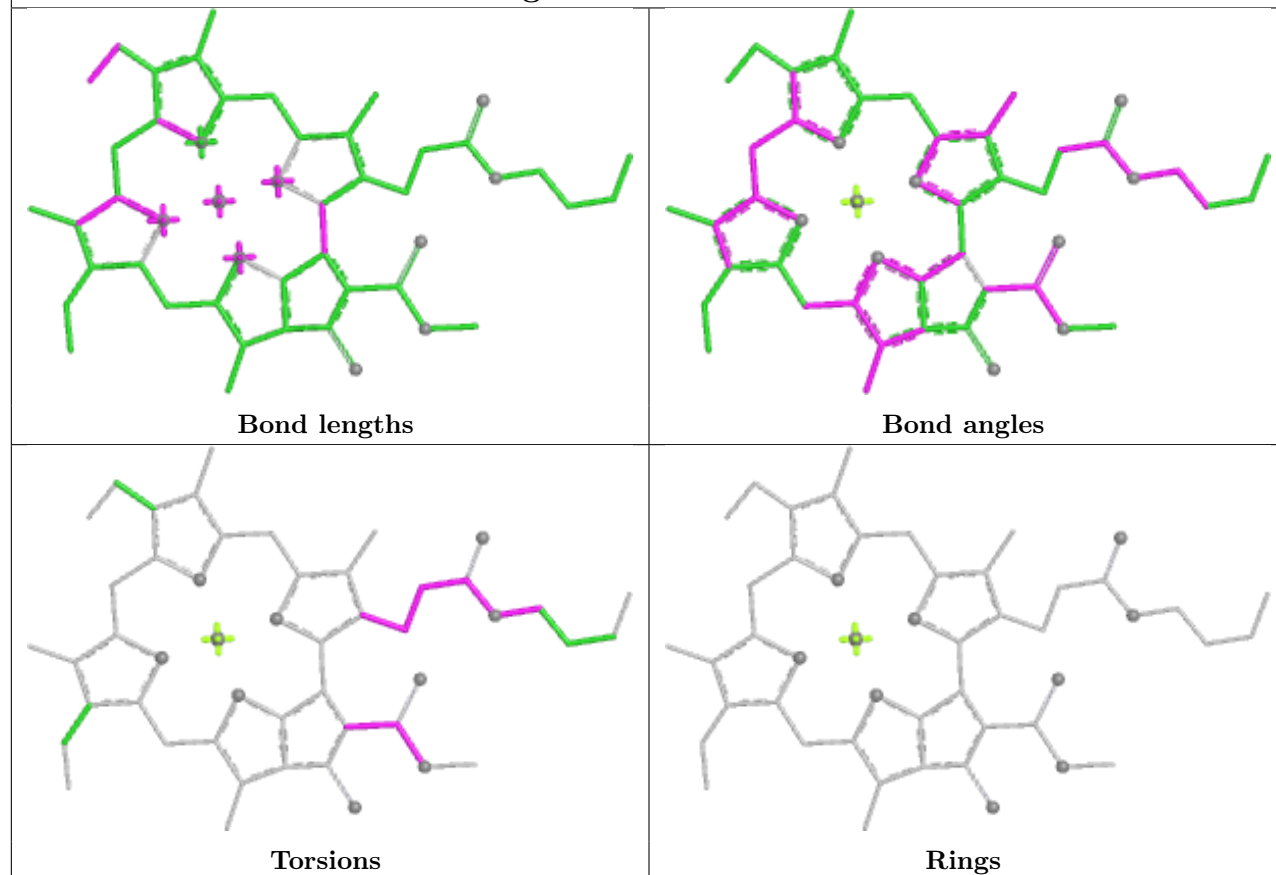
Ligand CLA 2 612



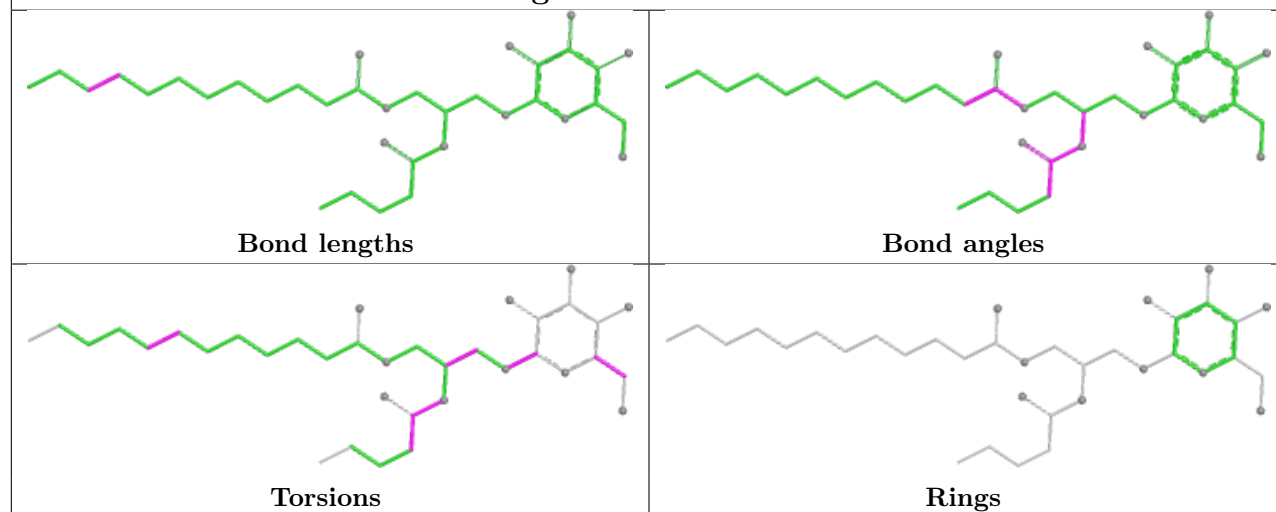
Ligand BCR J 4002

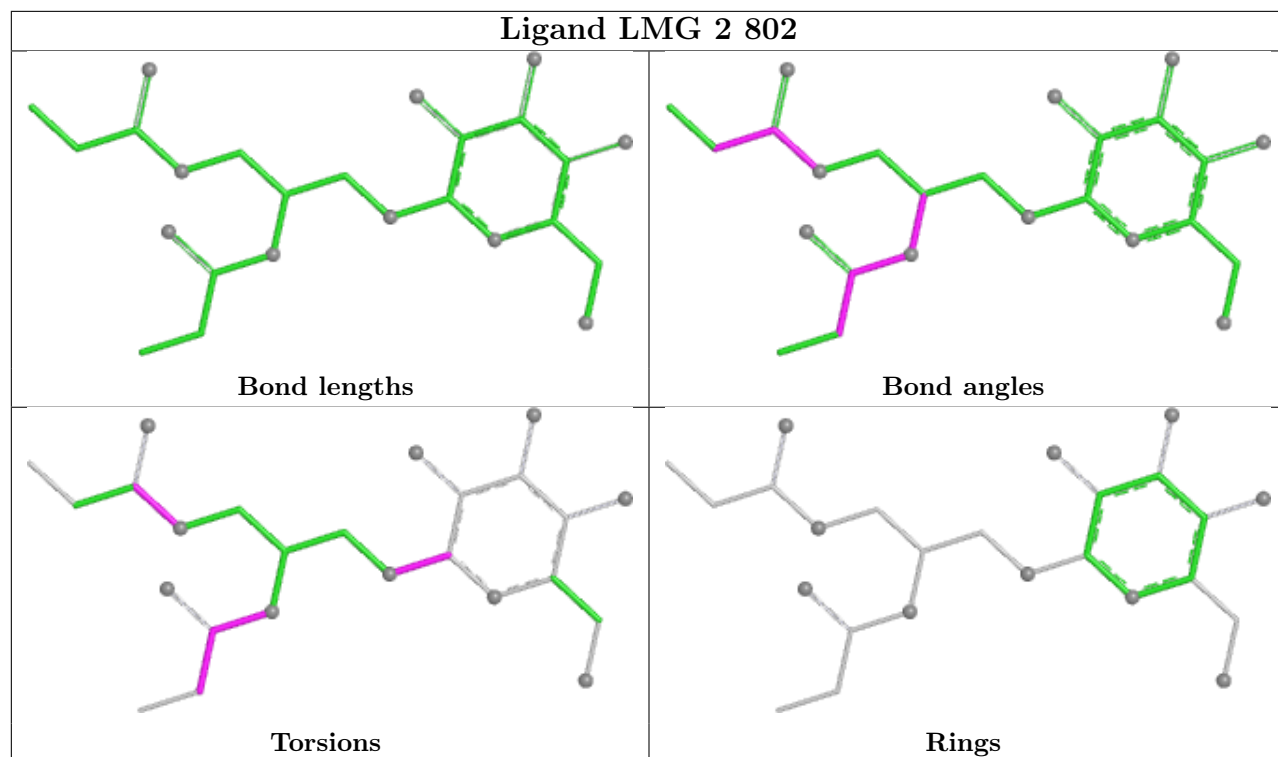


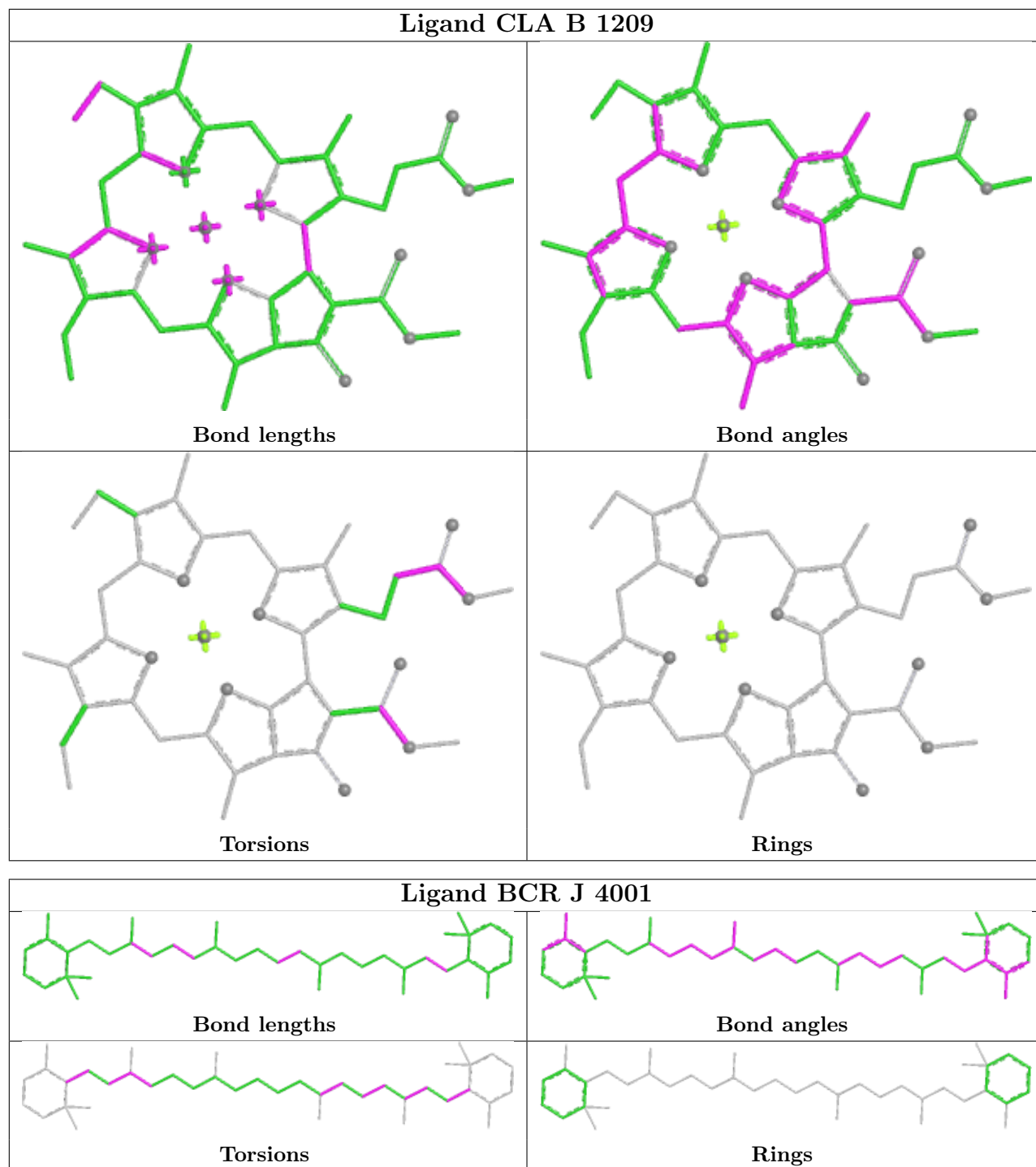
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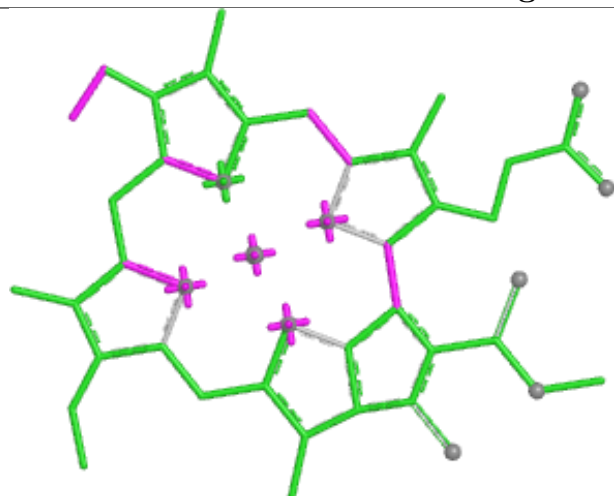
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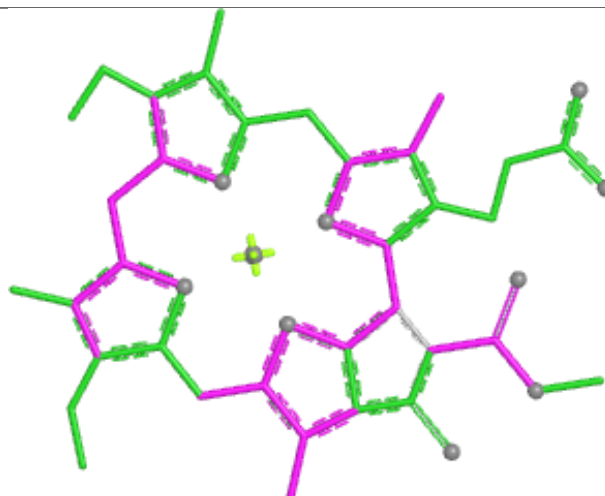




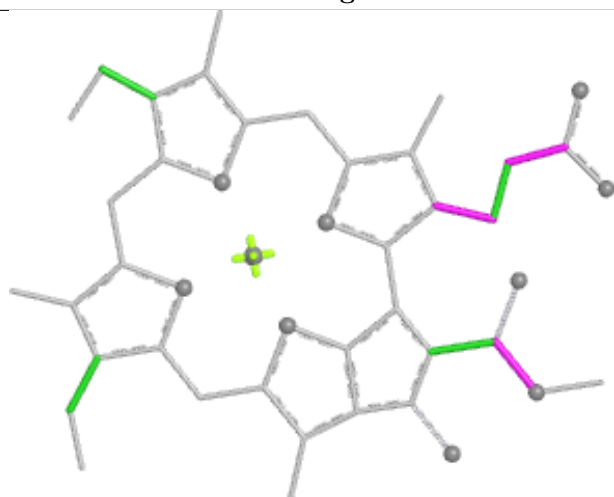
Ligand CLA 1 603



Bond lengths



Bond angles

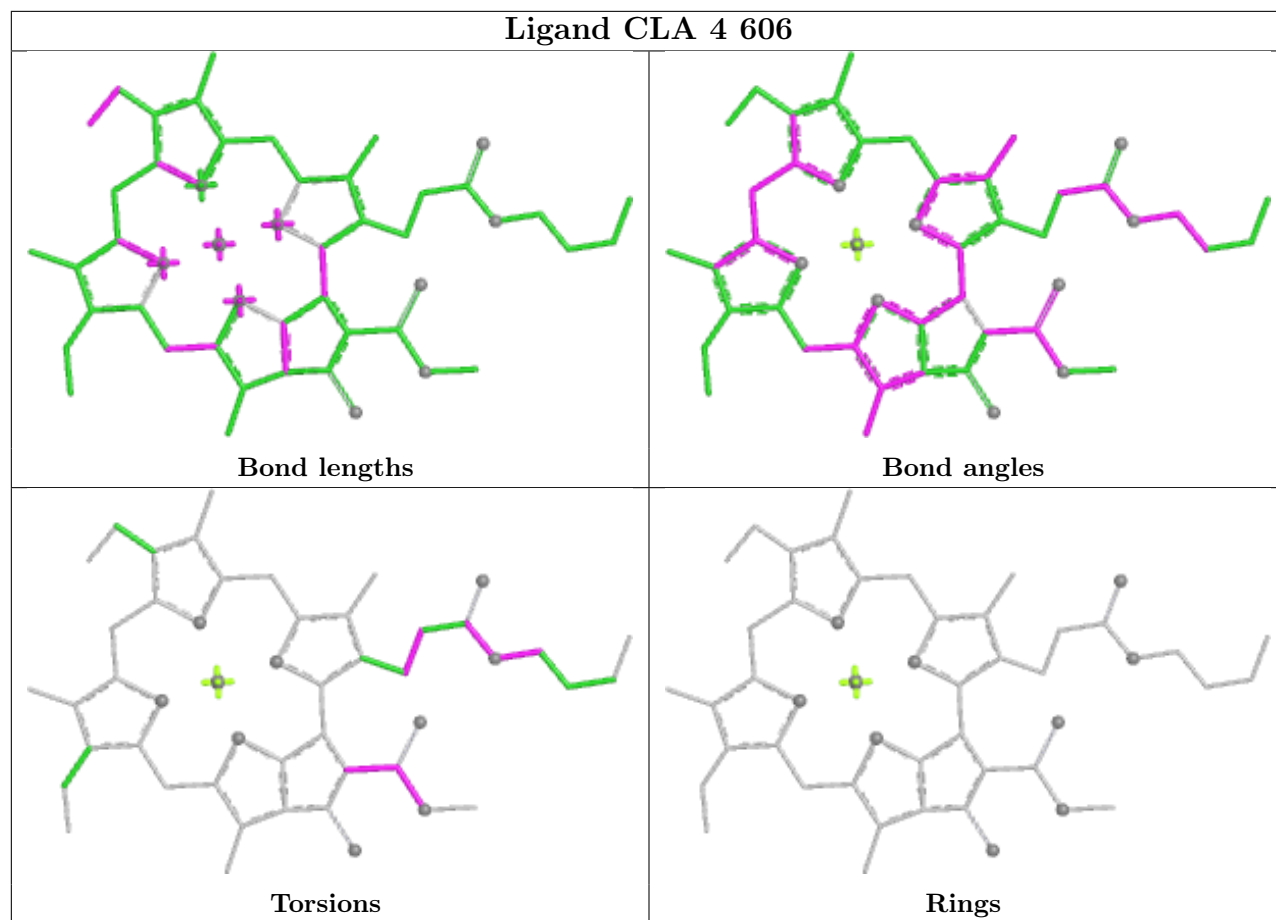


Torsions

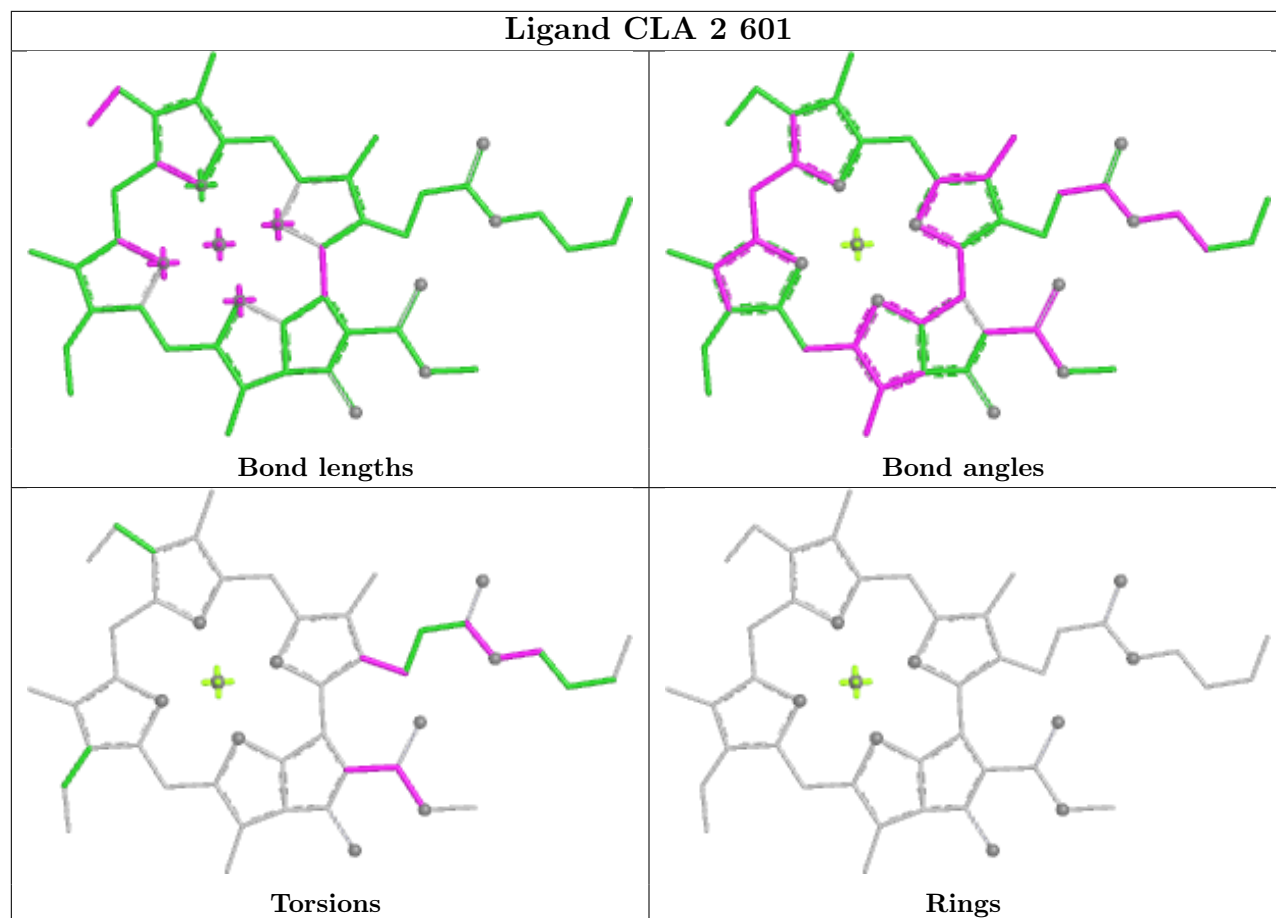


Rings

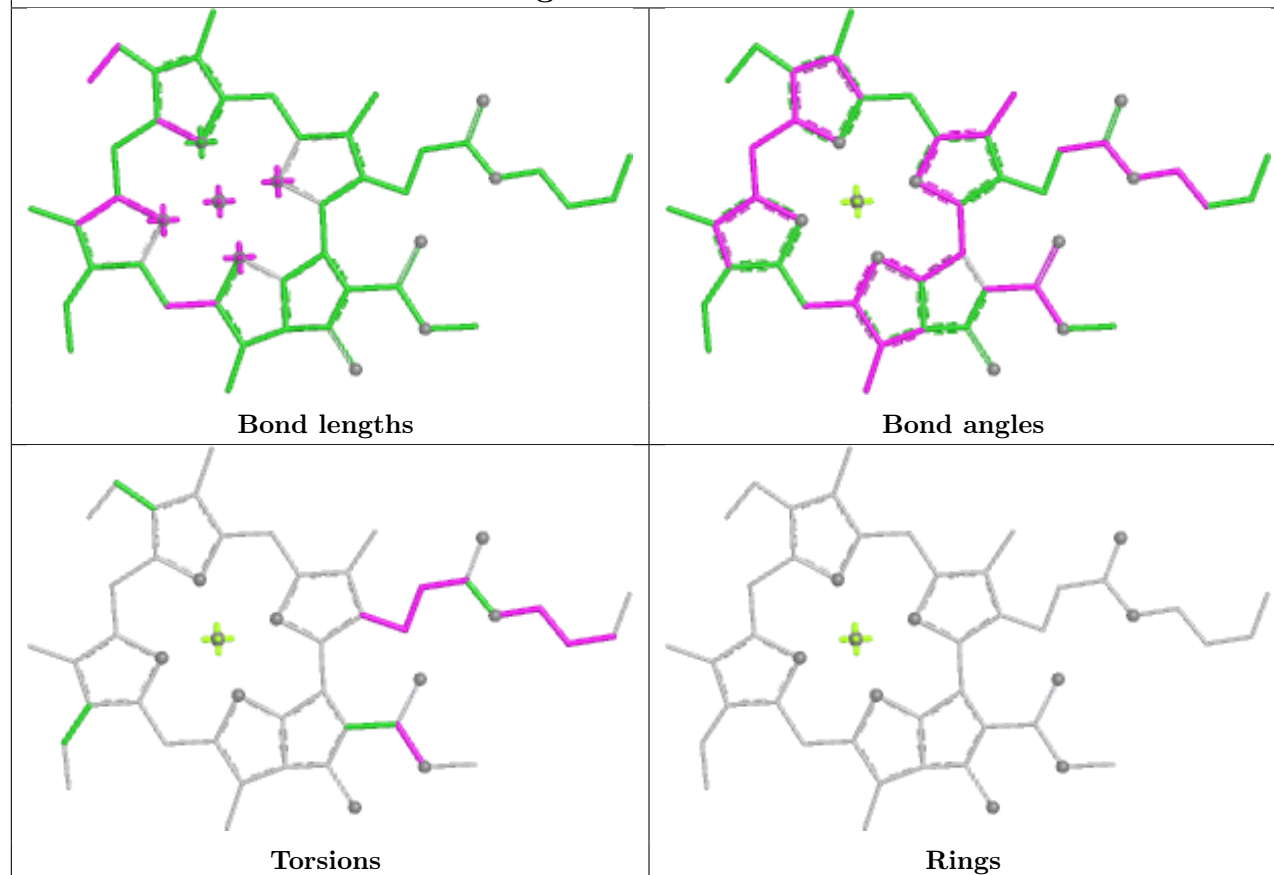
Ligand CLA 4 606



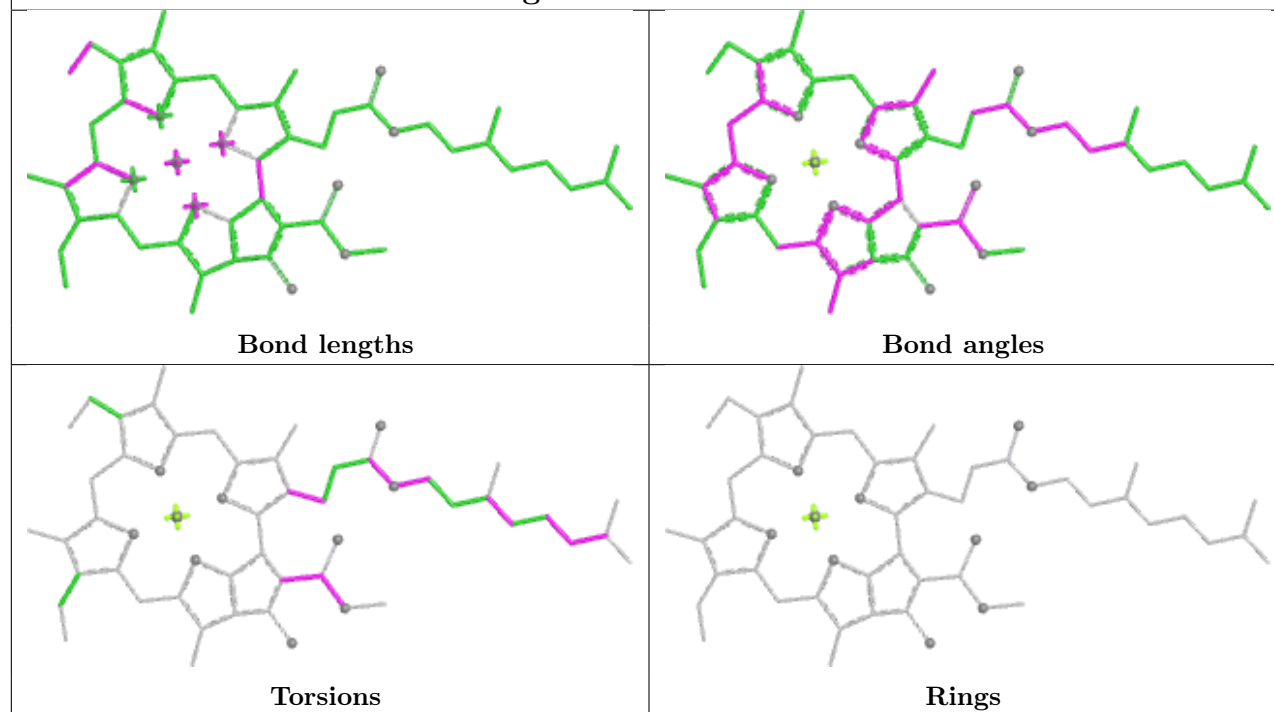
Ligand CLA 2 601



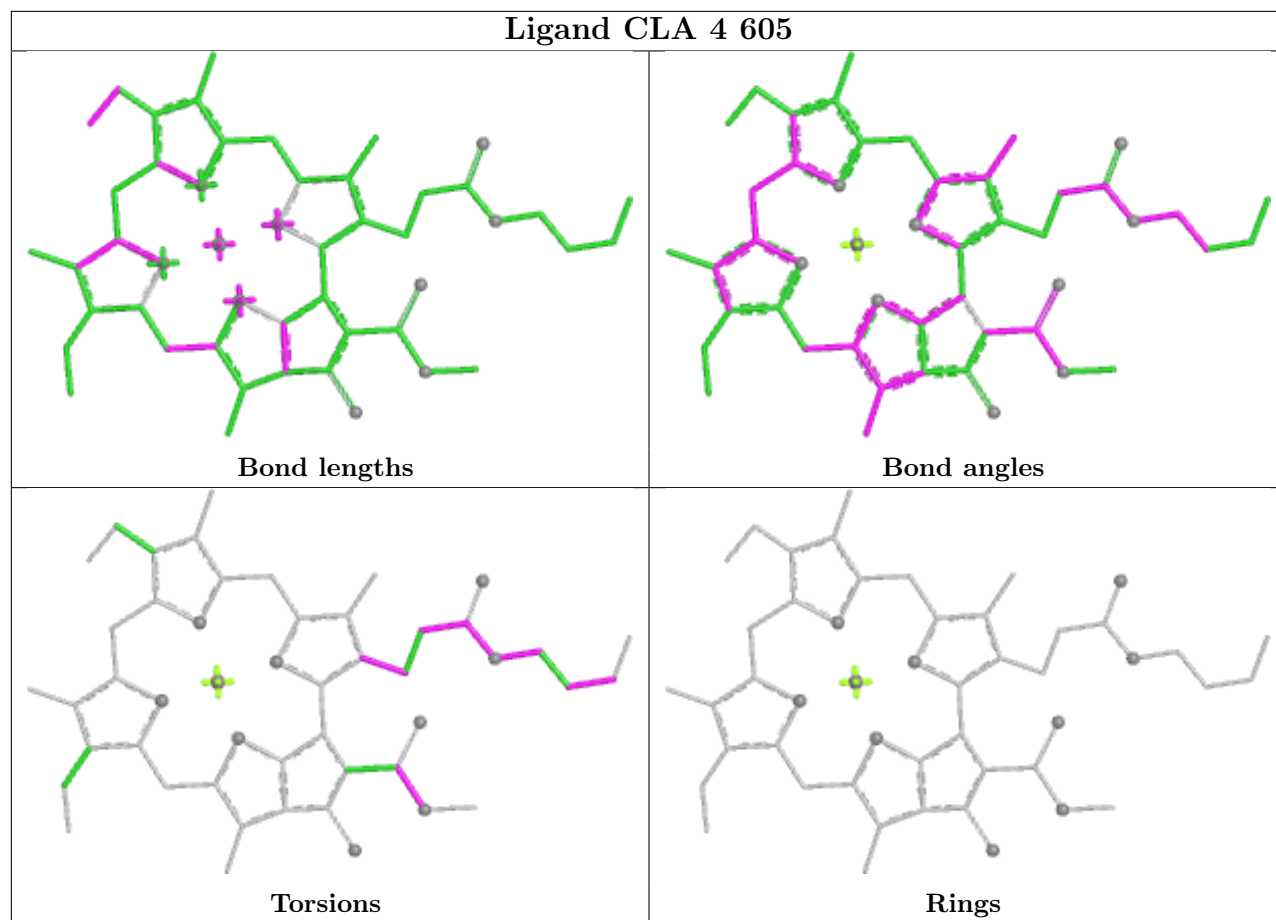
Ligand CLA 4 607



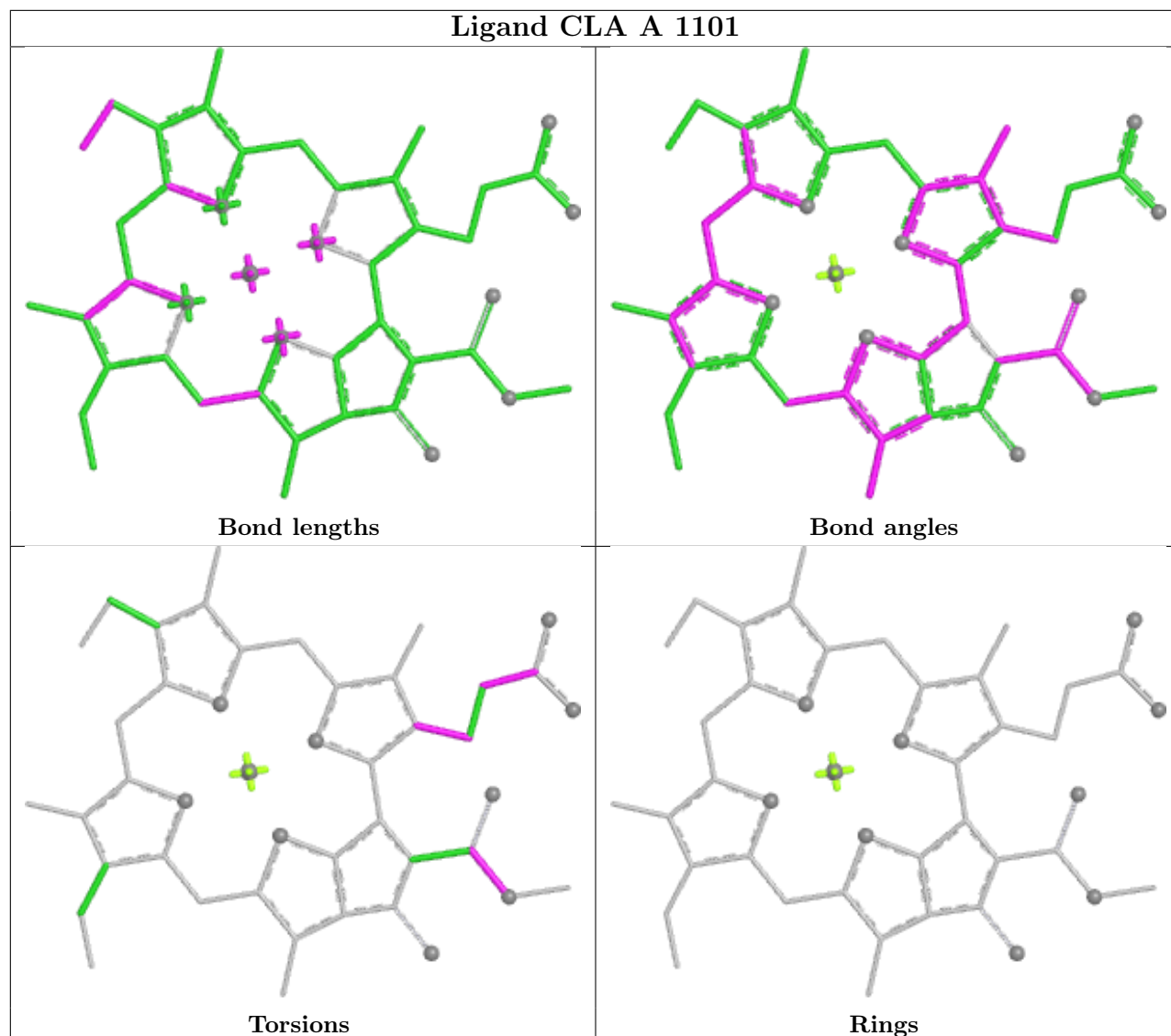
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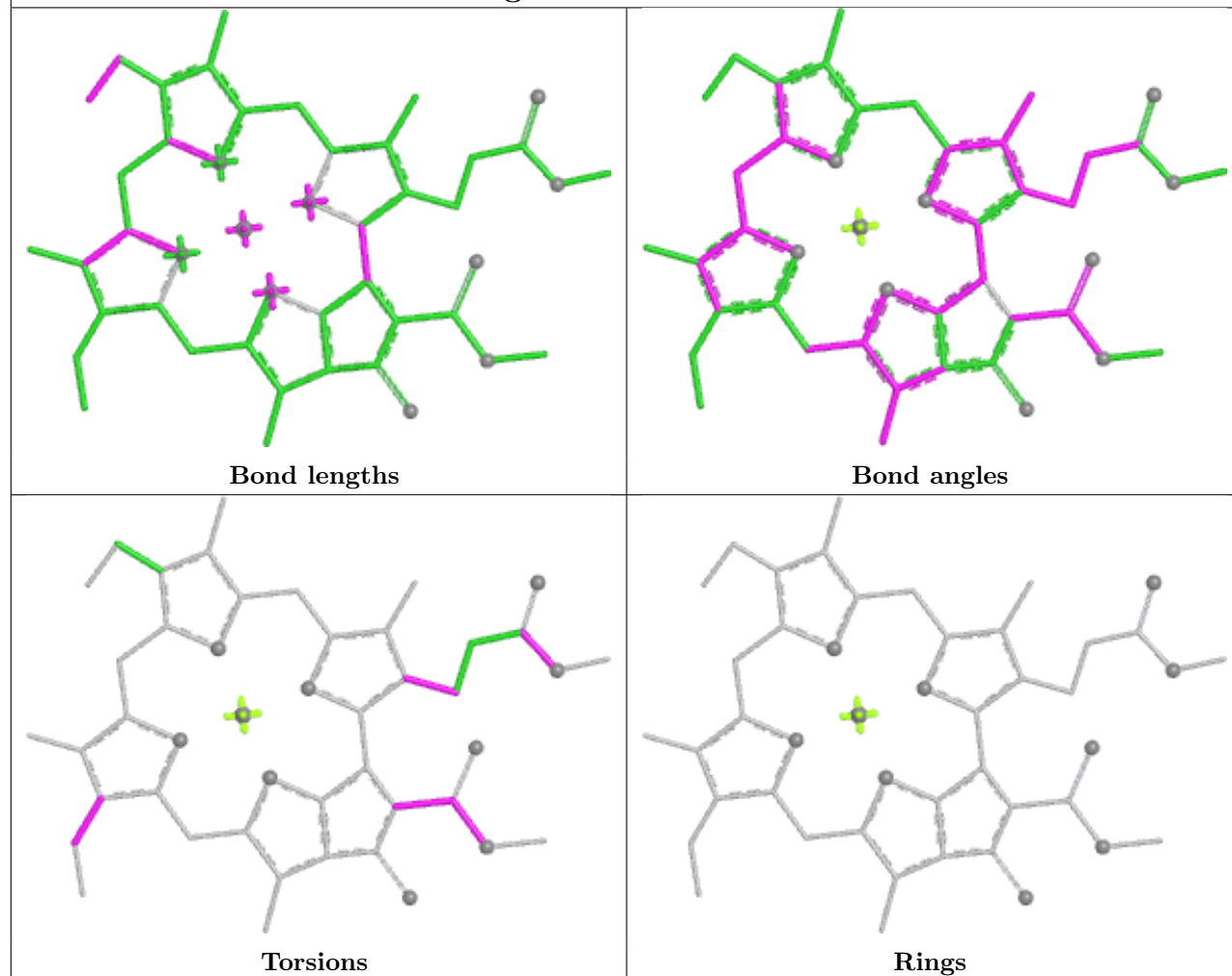
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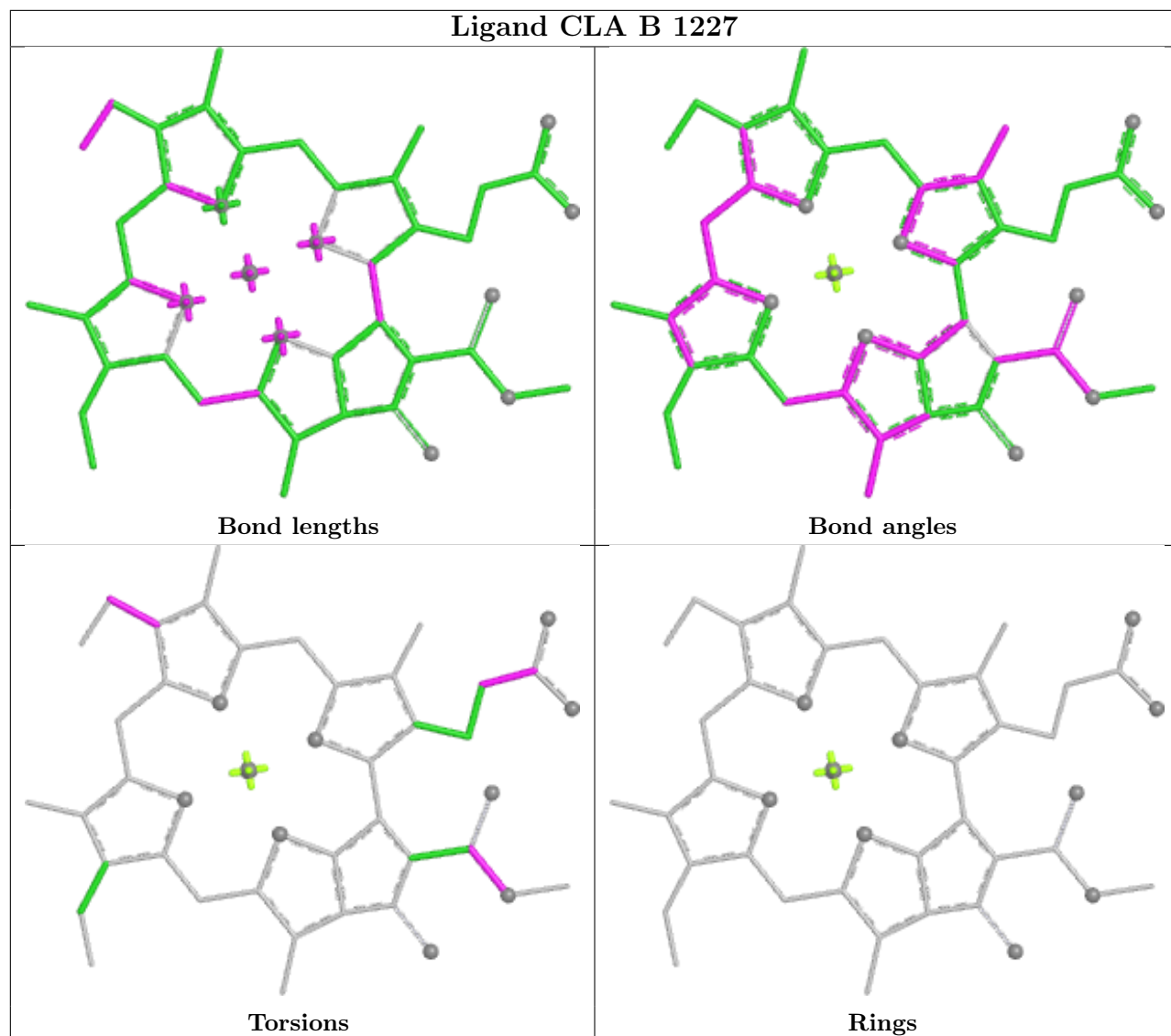
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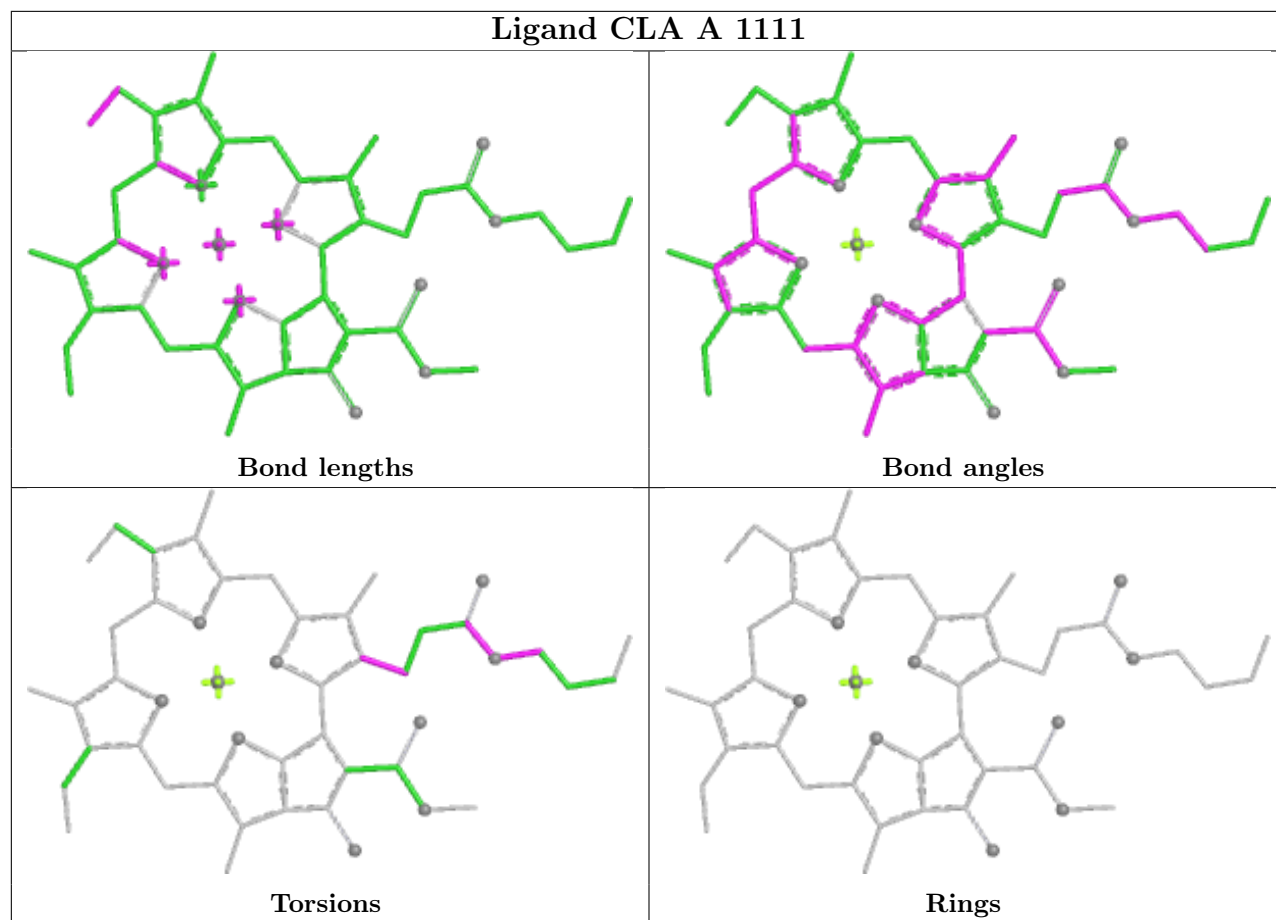


Ligand CLA A 1108

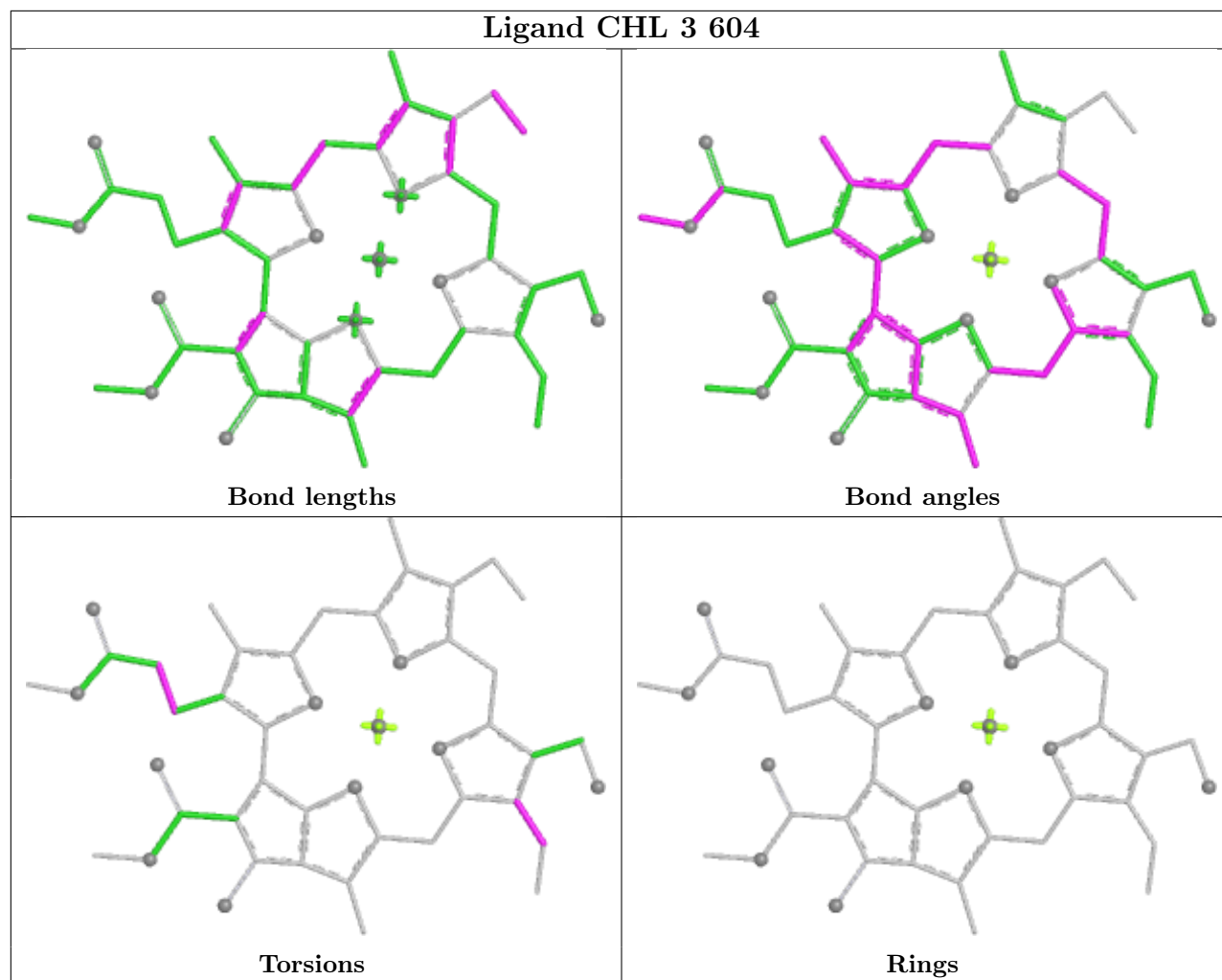


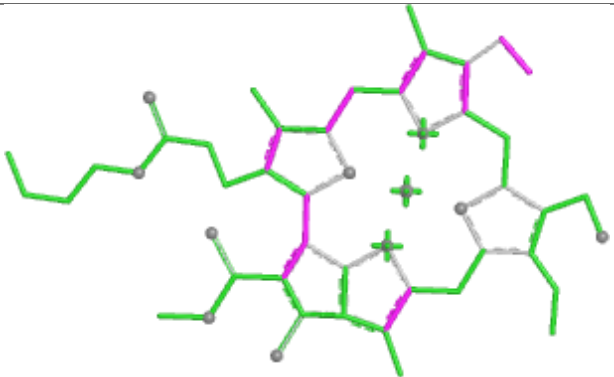
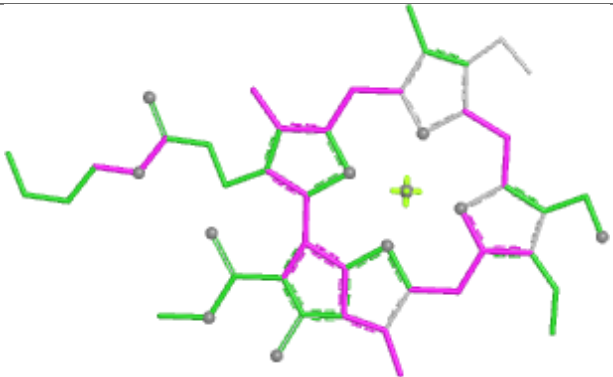
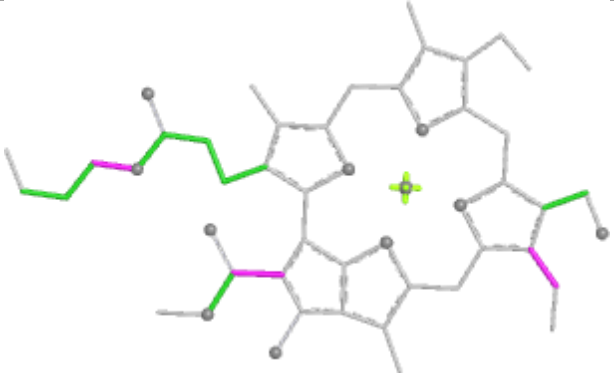
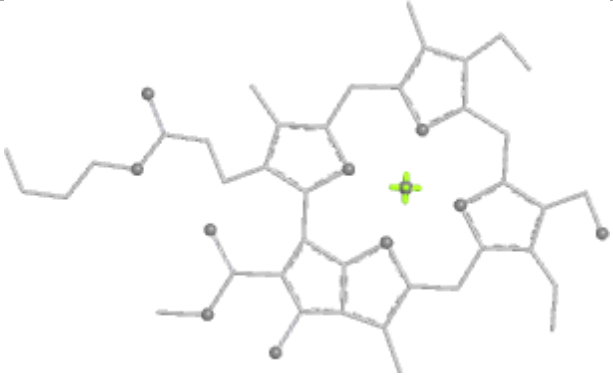
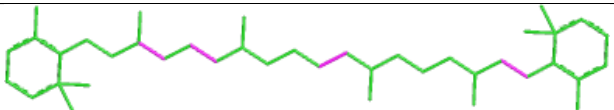
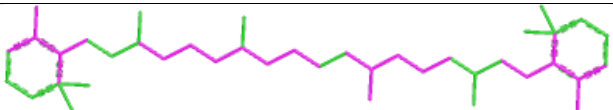
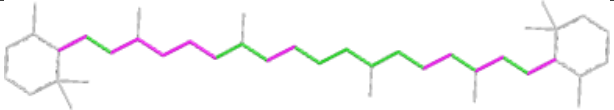
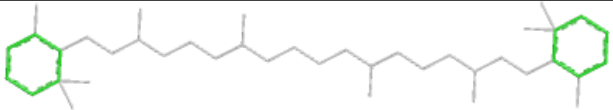
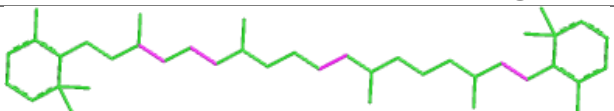
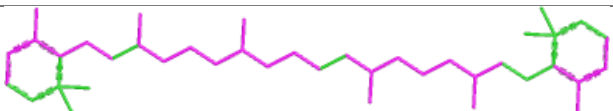
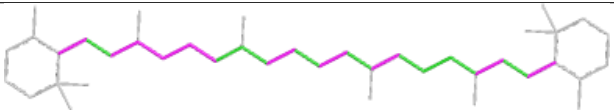
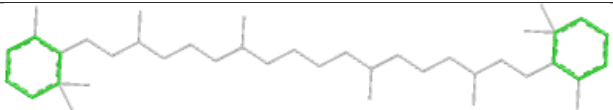
Ligand CLA B 1227



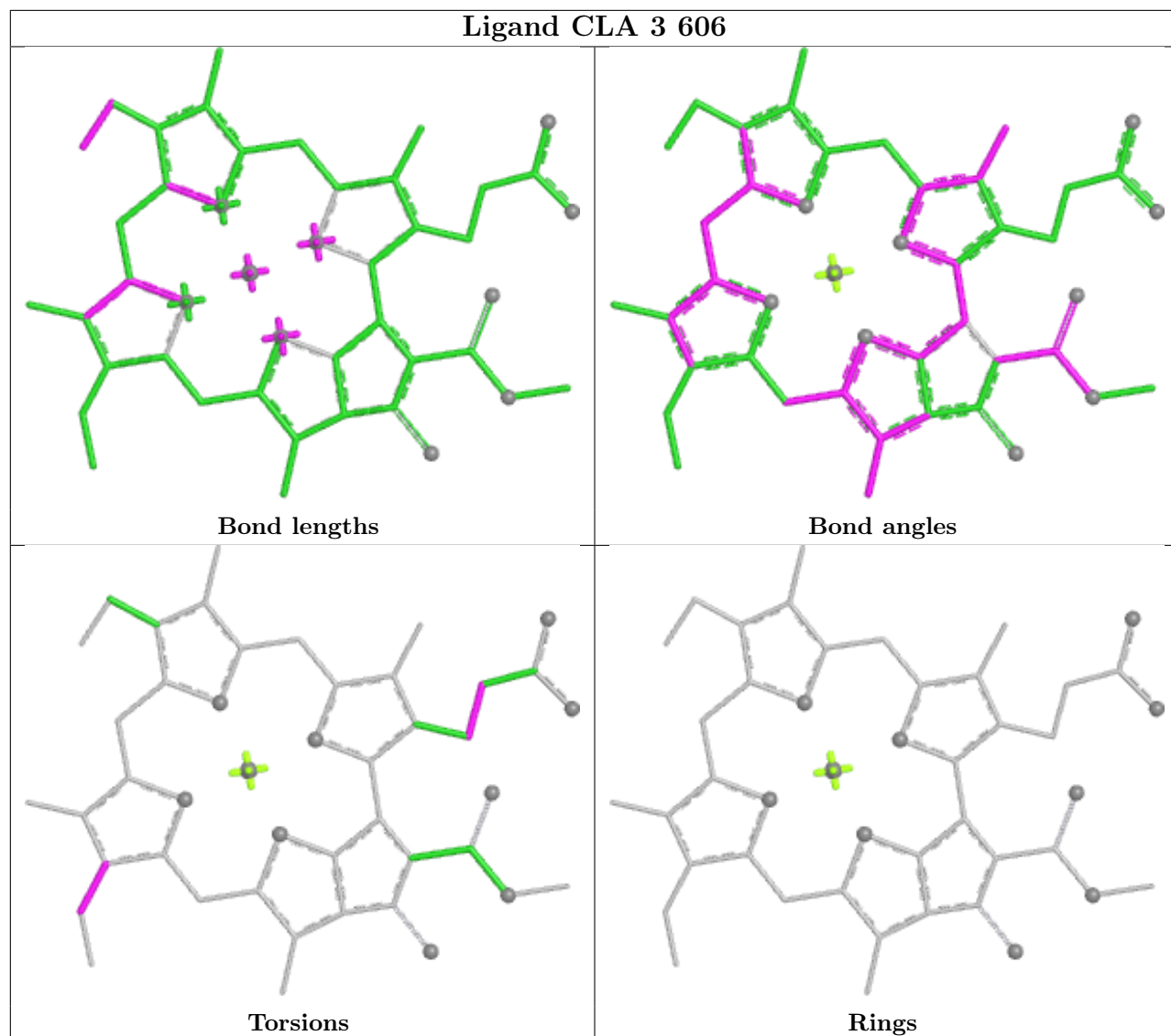


Ligand CHL 3 604

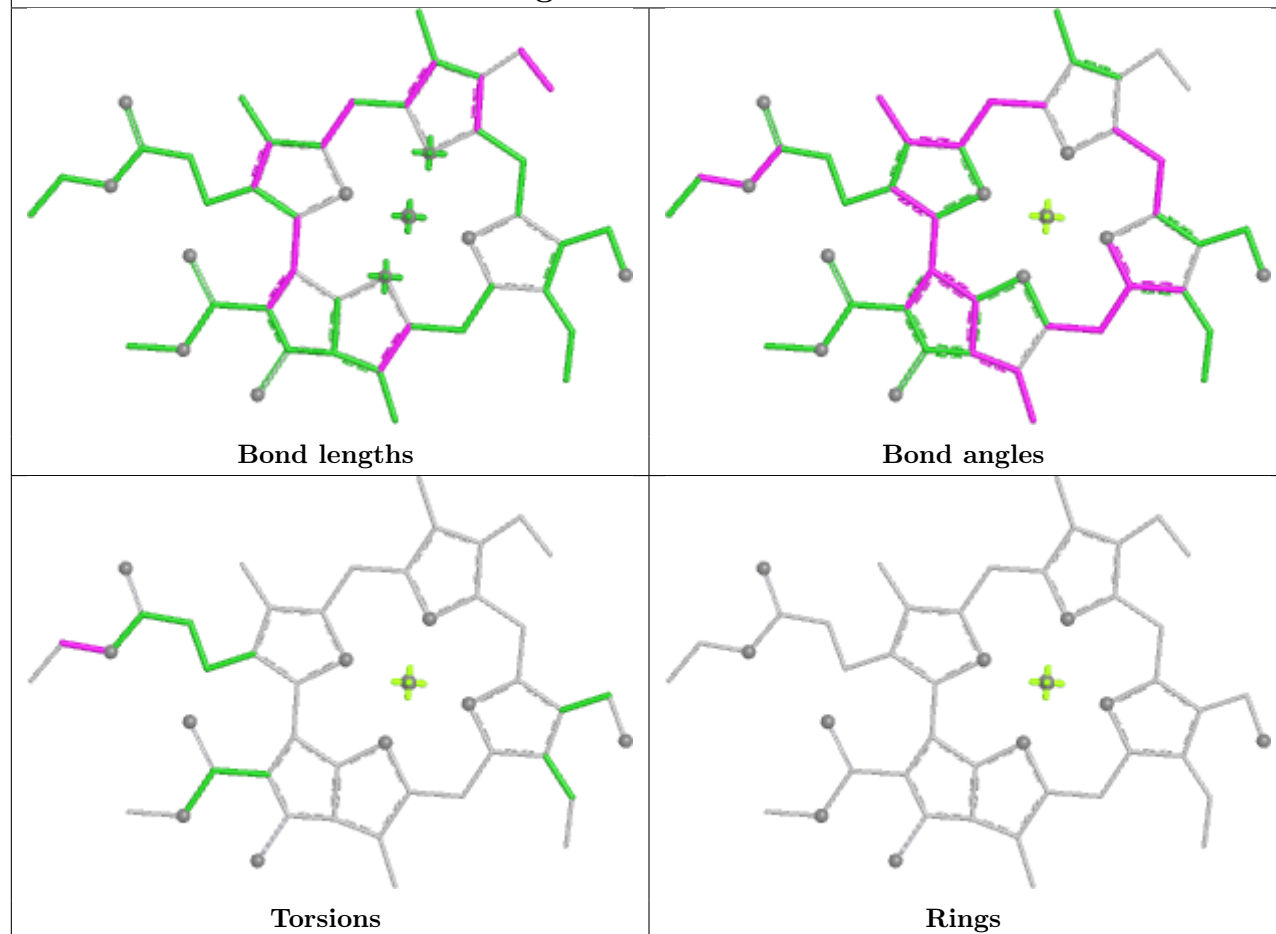


Ligand CHL 4 611	
	Bond lengths
	Bond angles
	Torsions
	Rings
Ligand BCR 2 503	
	Bond lengths
	Bond angles
	Torsions
	Rings
Ligand BCR 1 503	
	Bond lengths
	Bond angles
	Torsions
	Rings

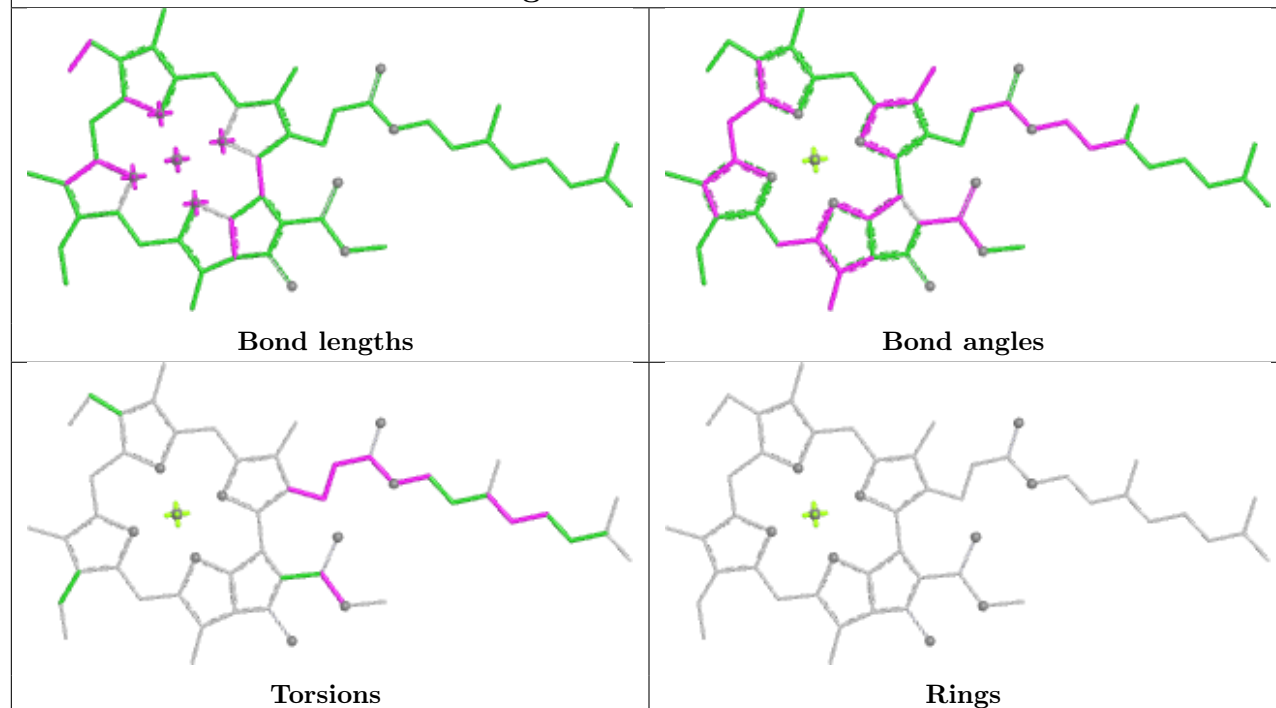
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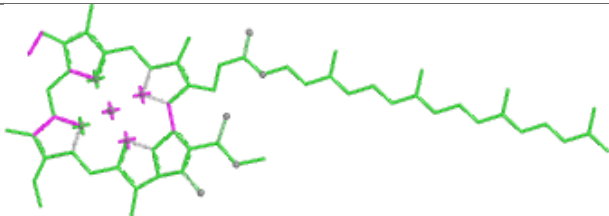
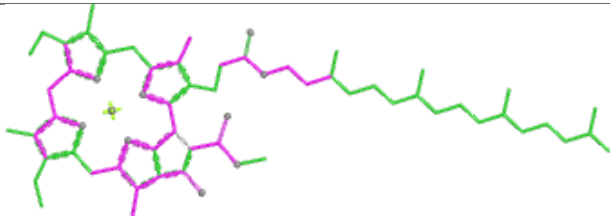
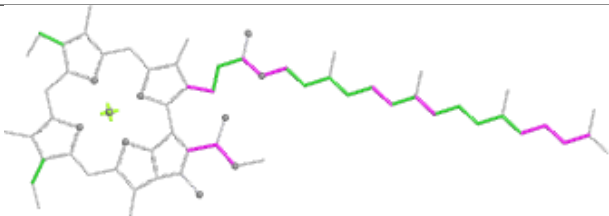
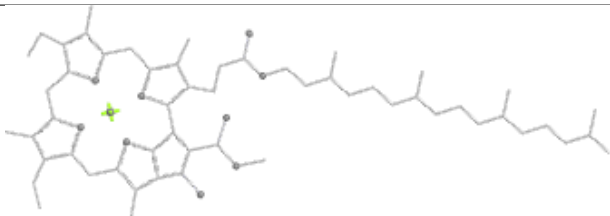


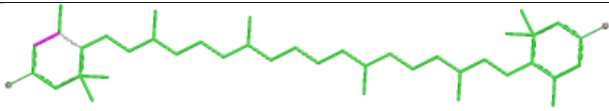
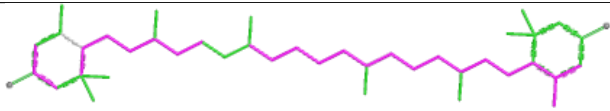
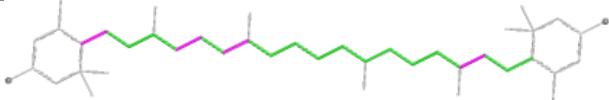
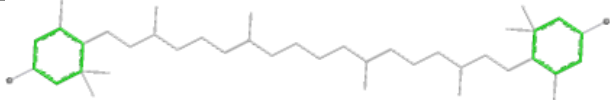
Ligand CHL 2 611



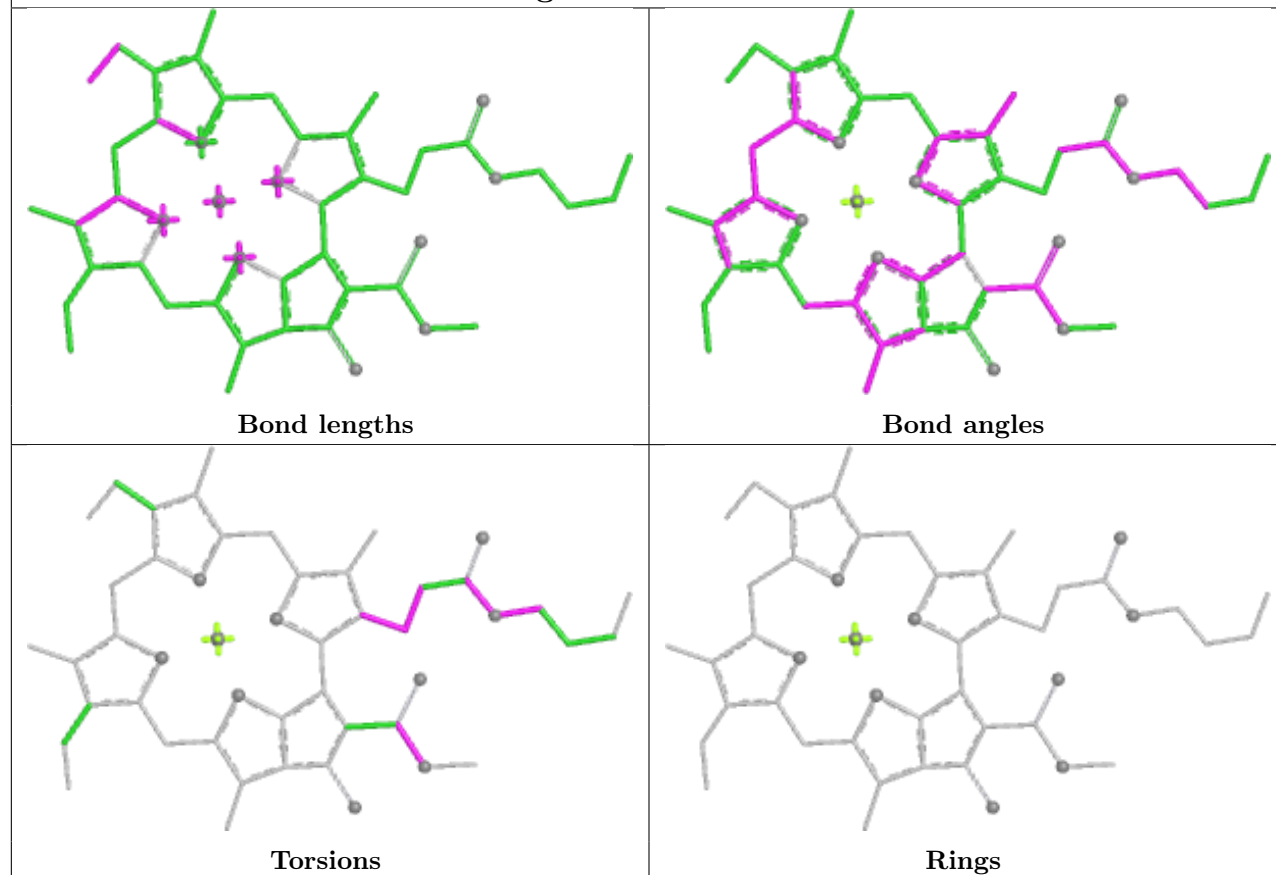
Ligand CLA A 1140



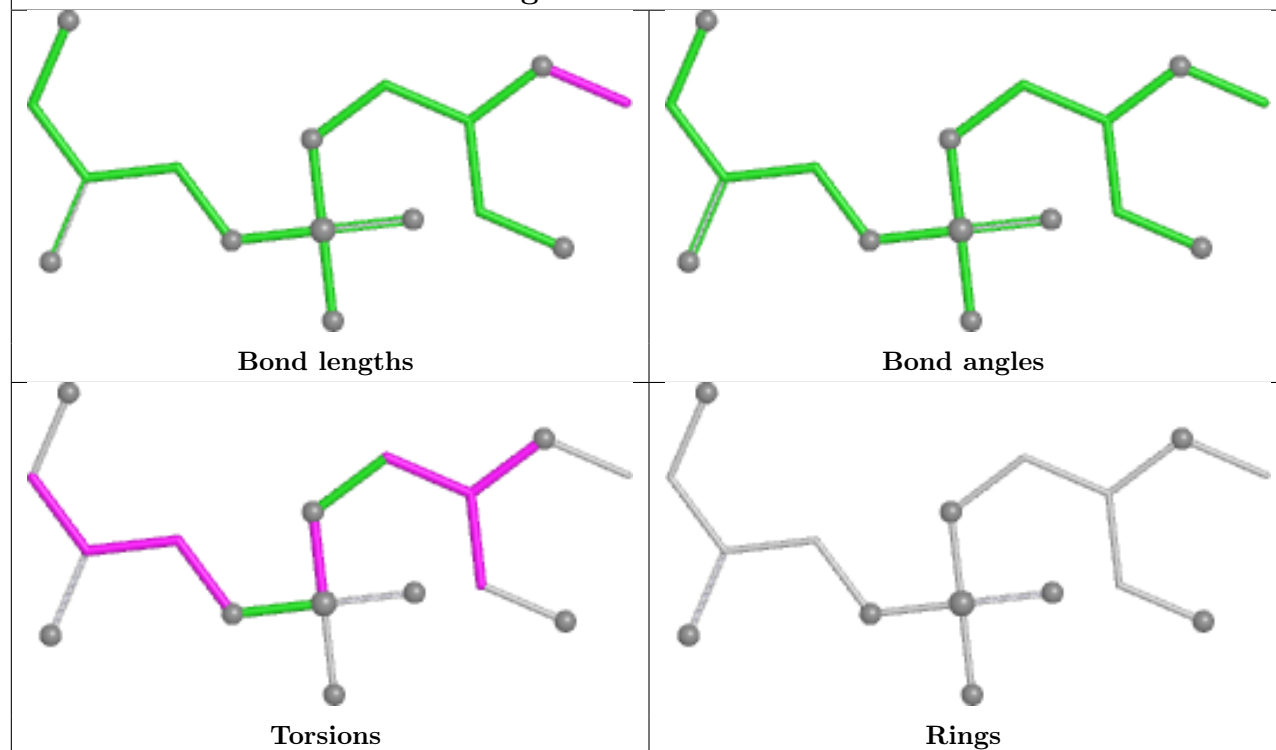
Ligand CLA 2 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 2 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

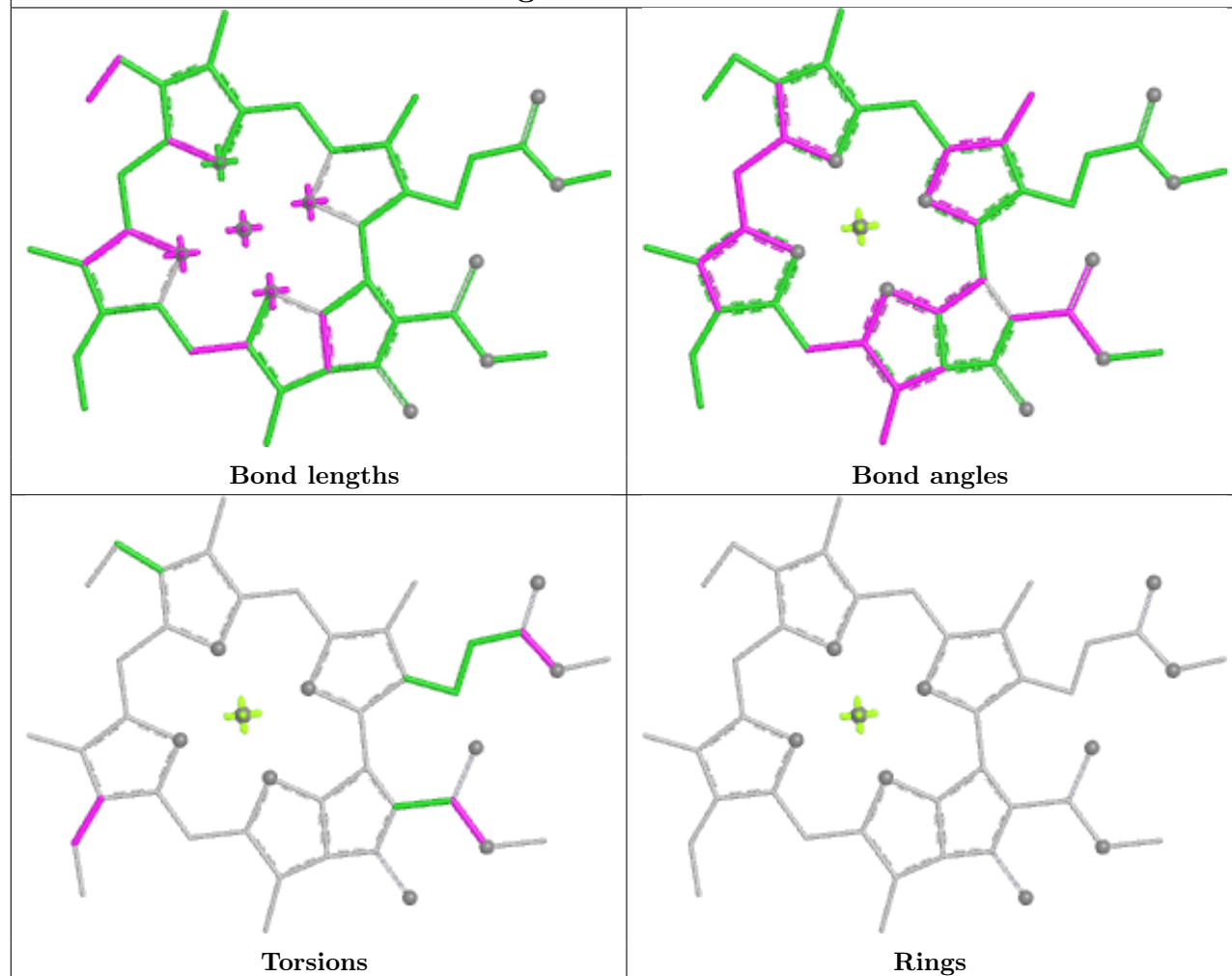
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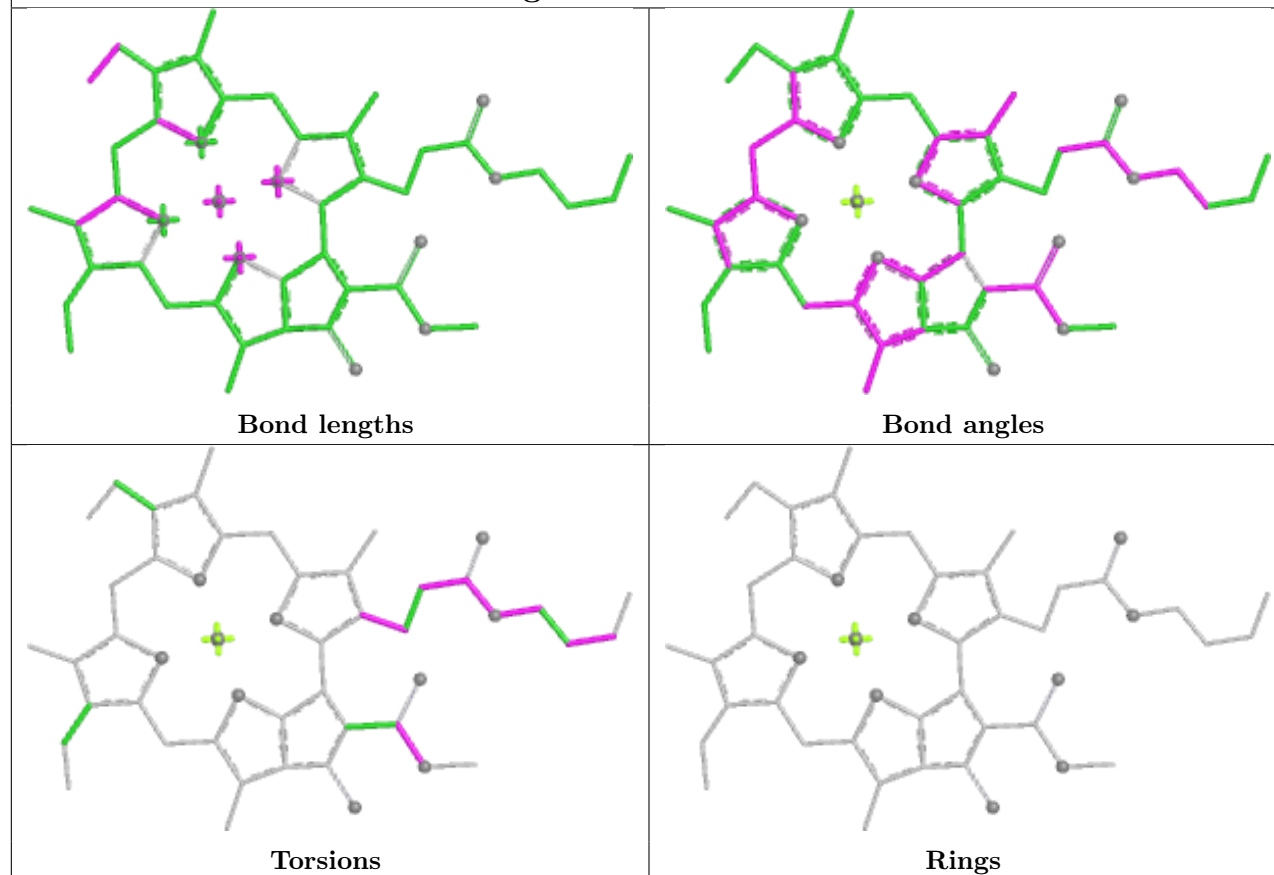
Ligand LHG A 5001



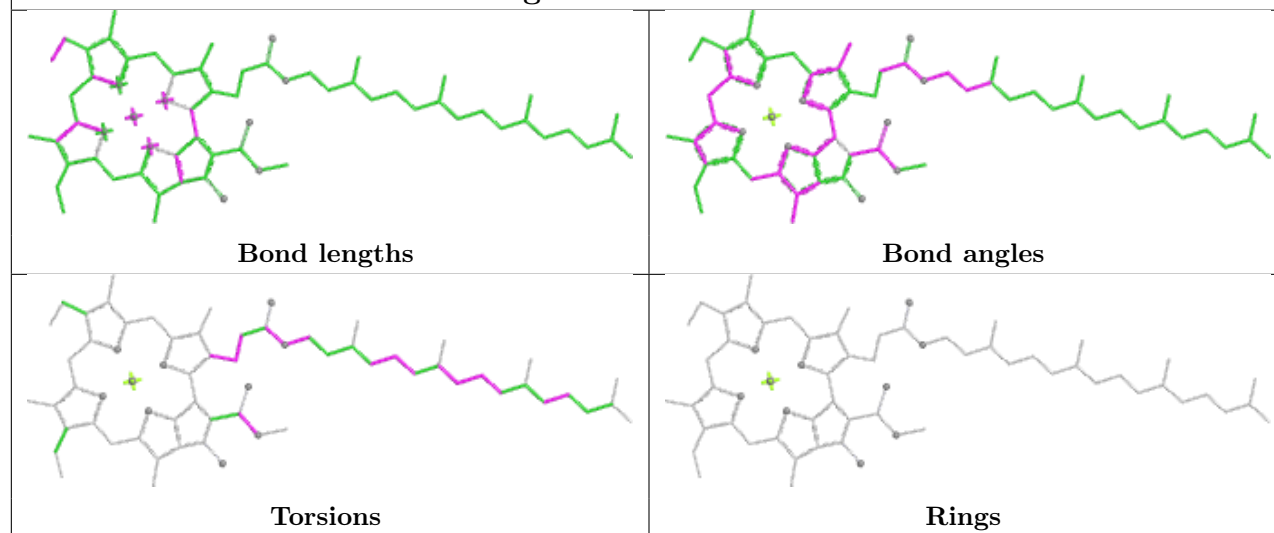
Ligand CLA 3 605



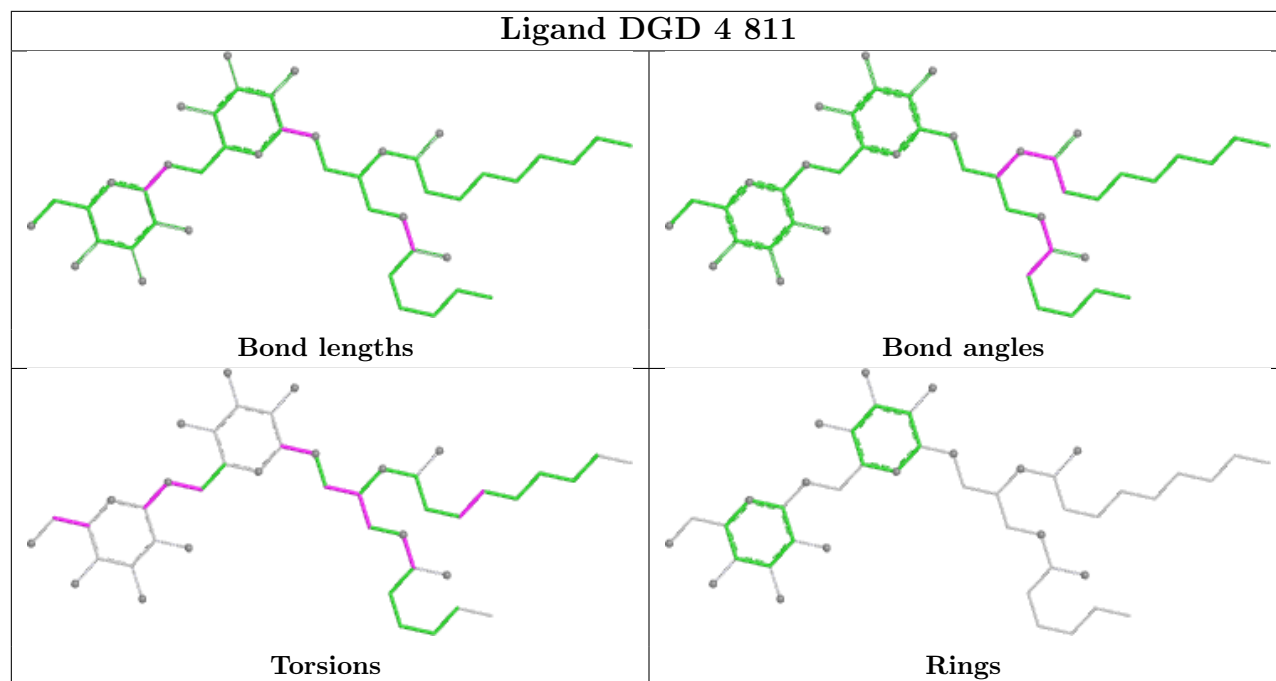
Ligand CLA B 1202



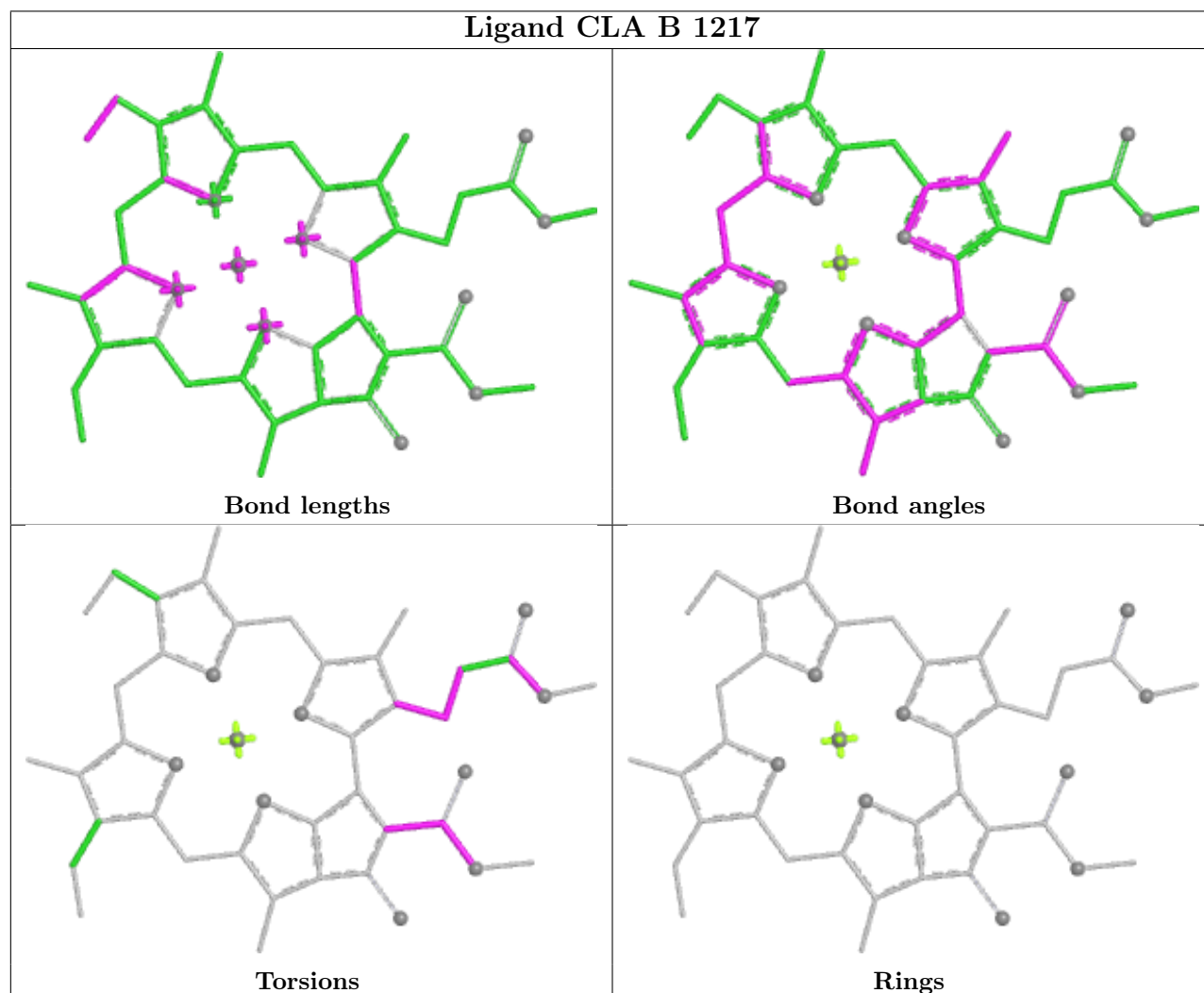
Ligand CLA B 1021

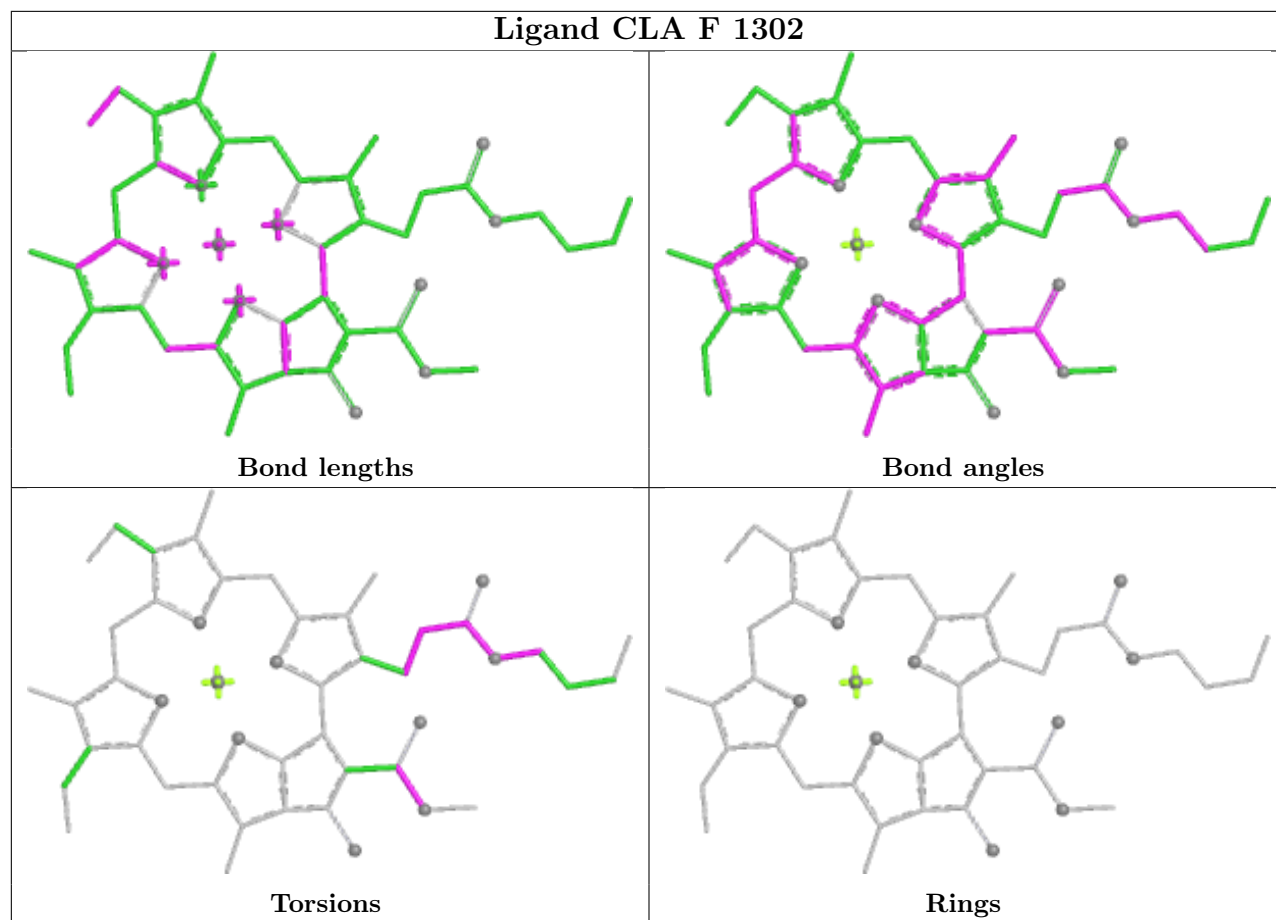


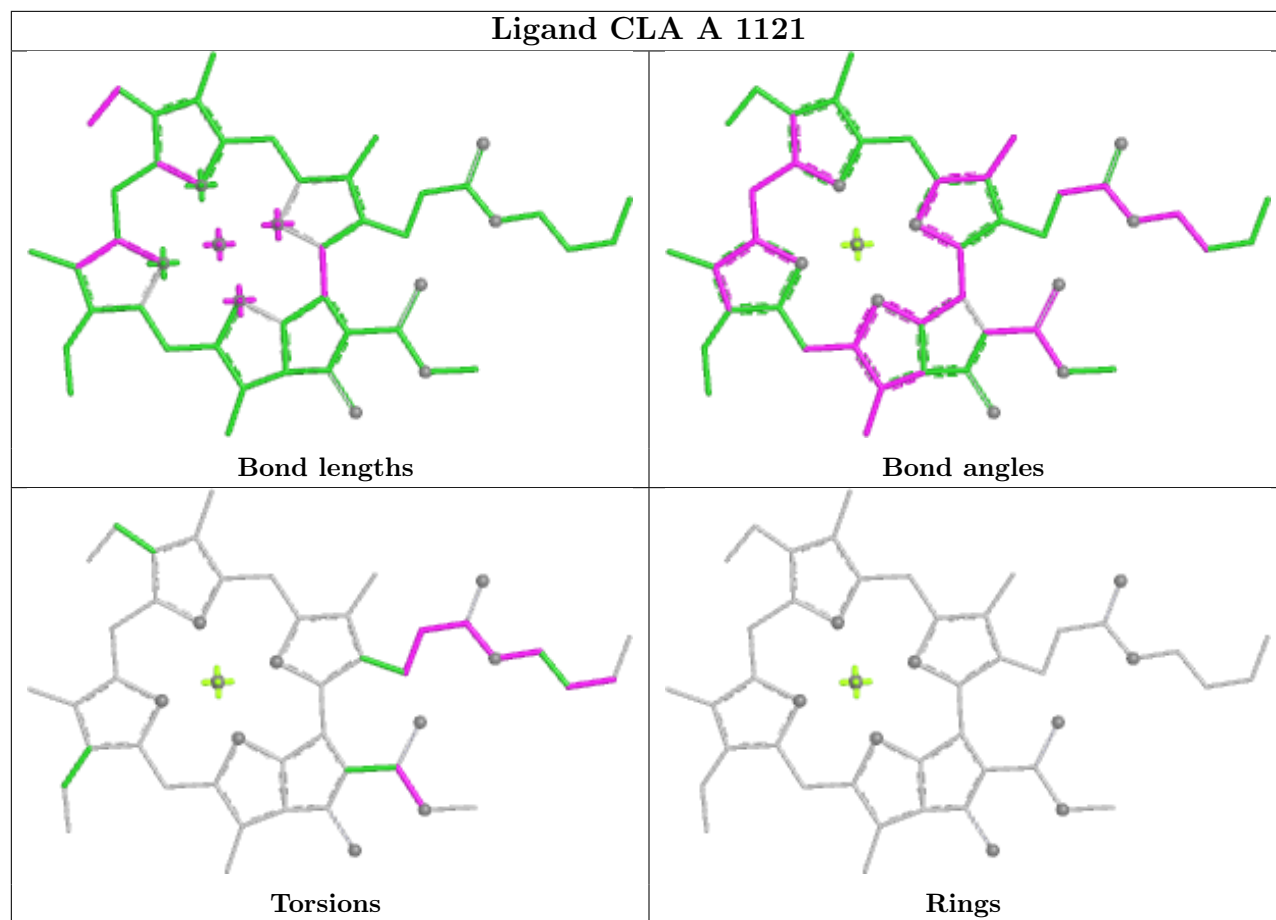
Ligand DGD 4 811

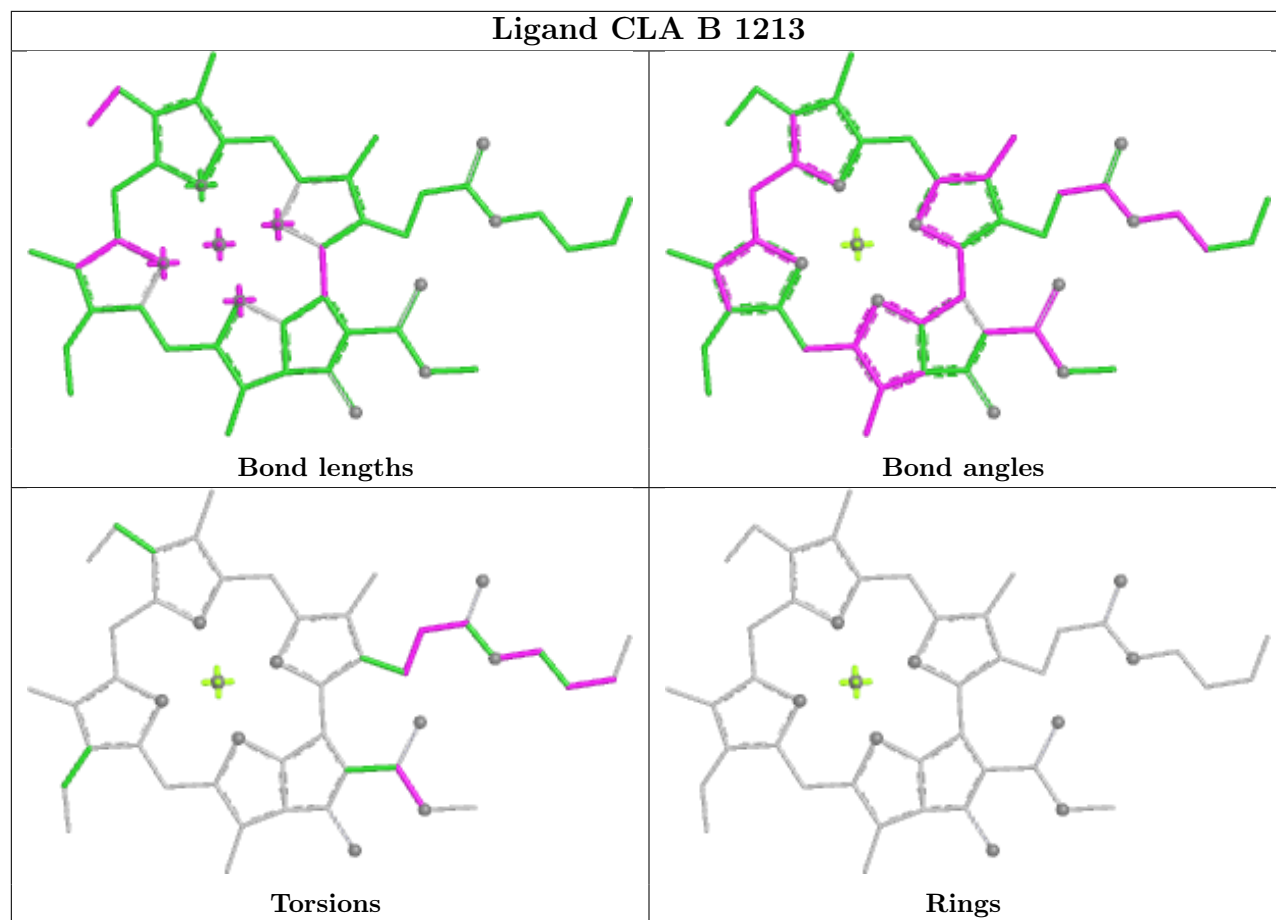


Ligand CLA B 1217

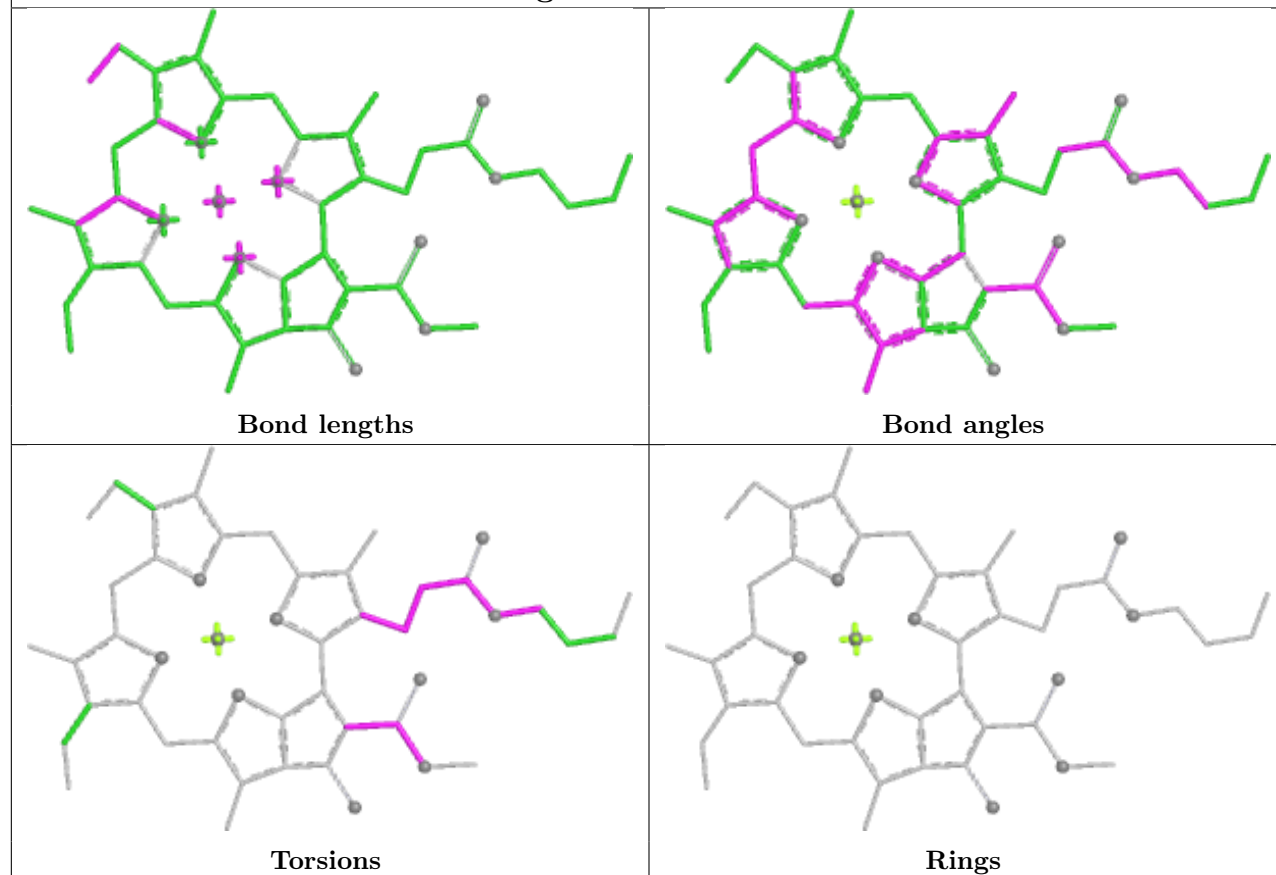




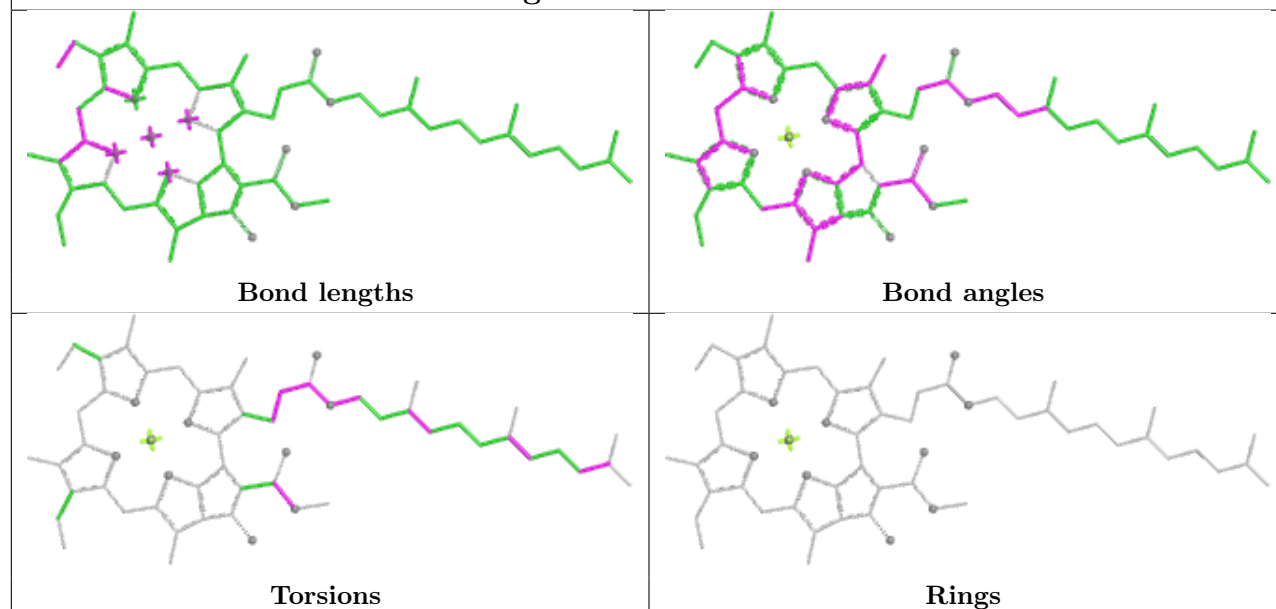




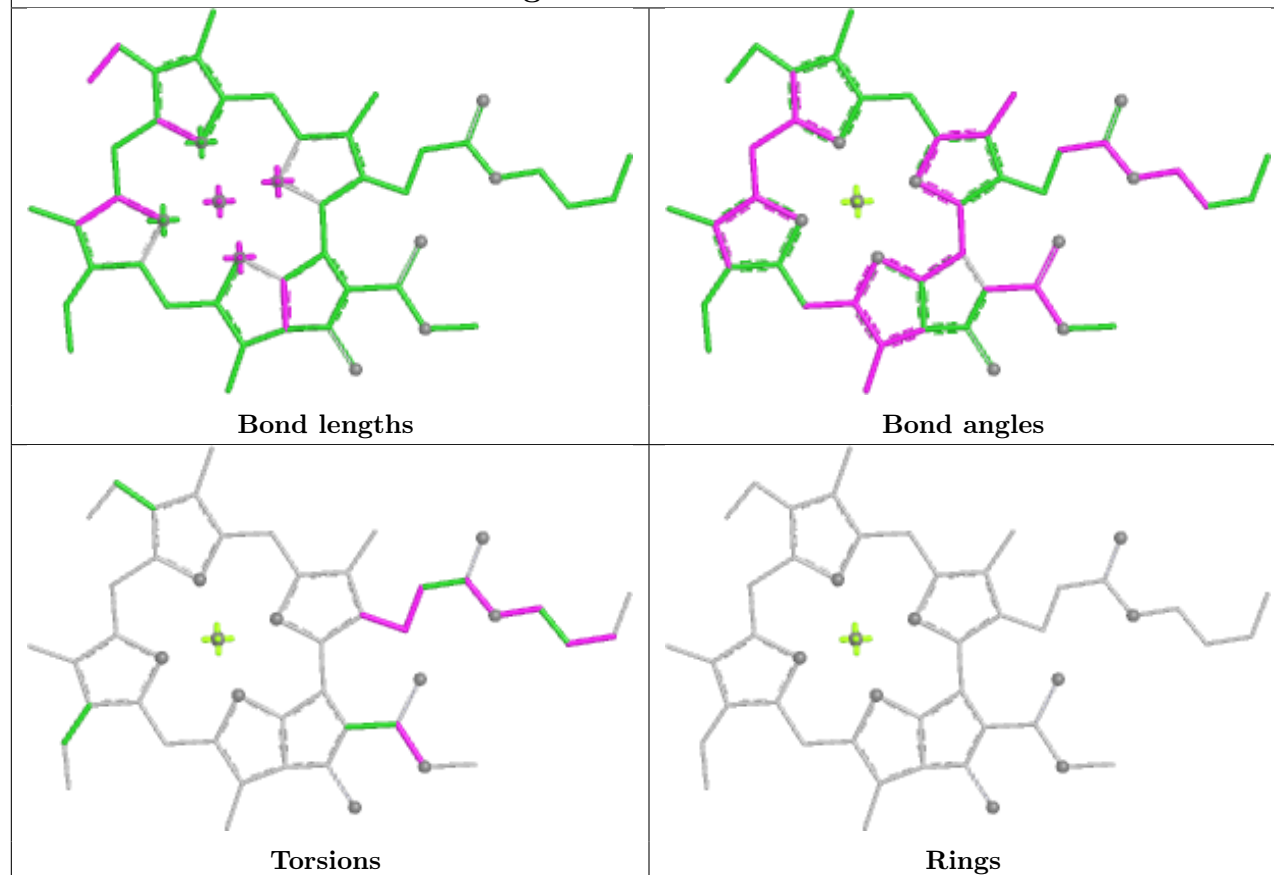
Ligand CLA 2 607



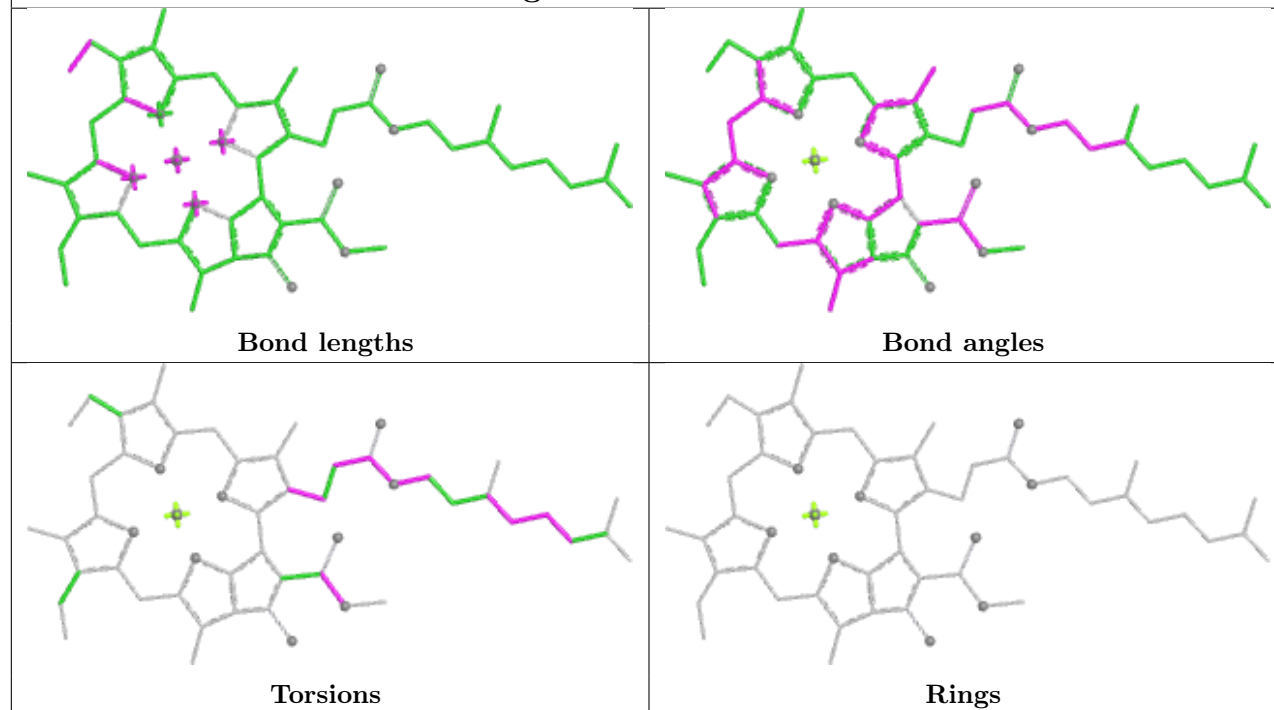
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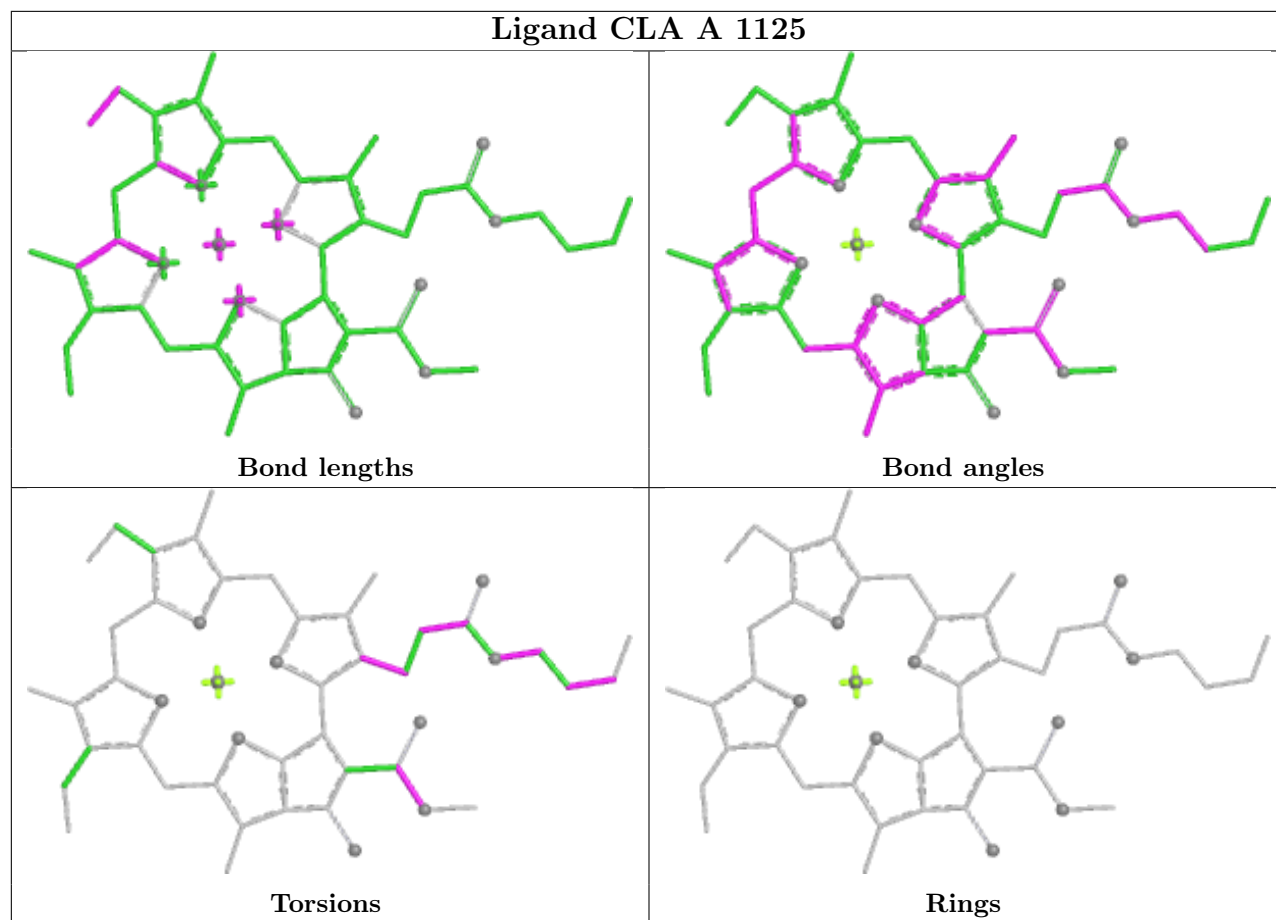


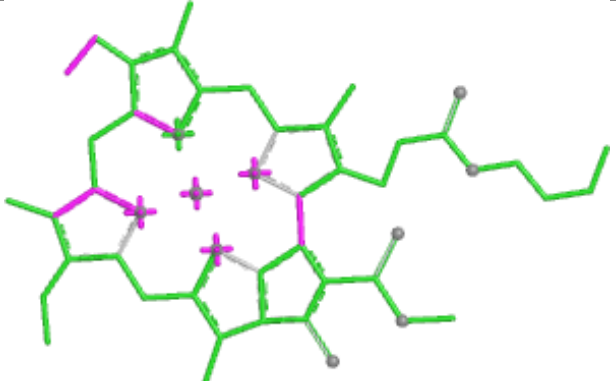
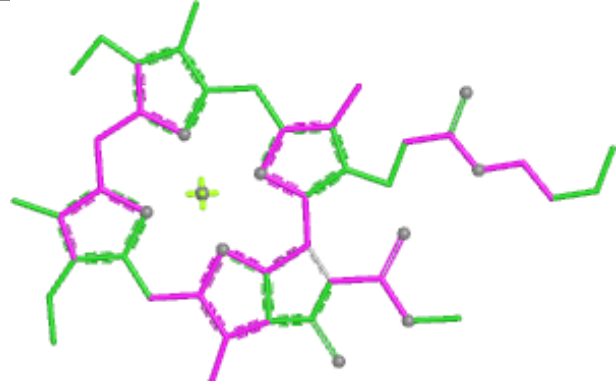
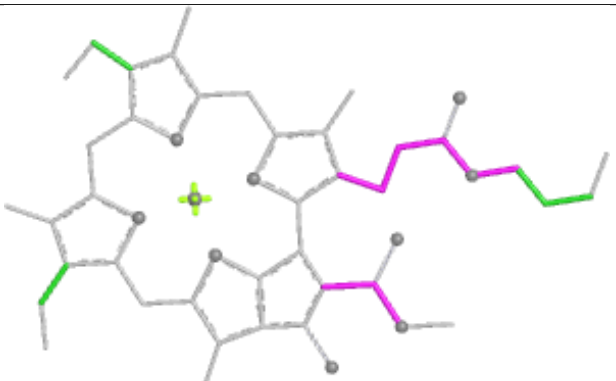
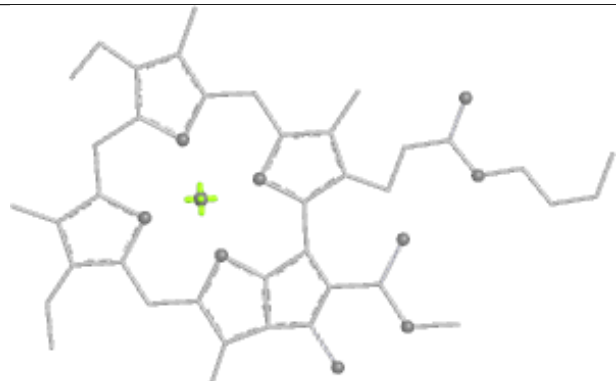
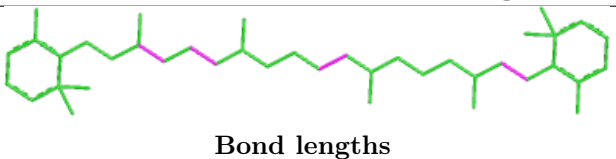
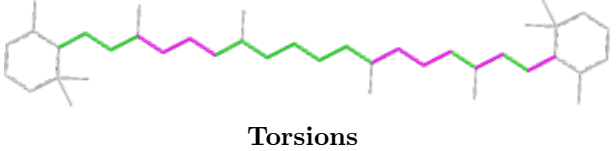
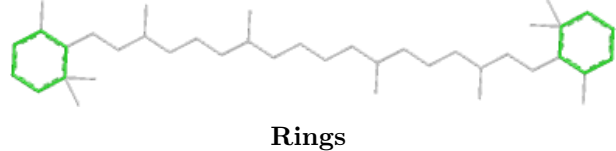
Ligand CLA B 1215

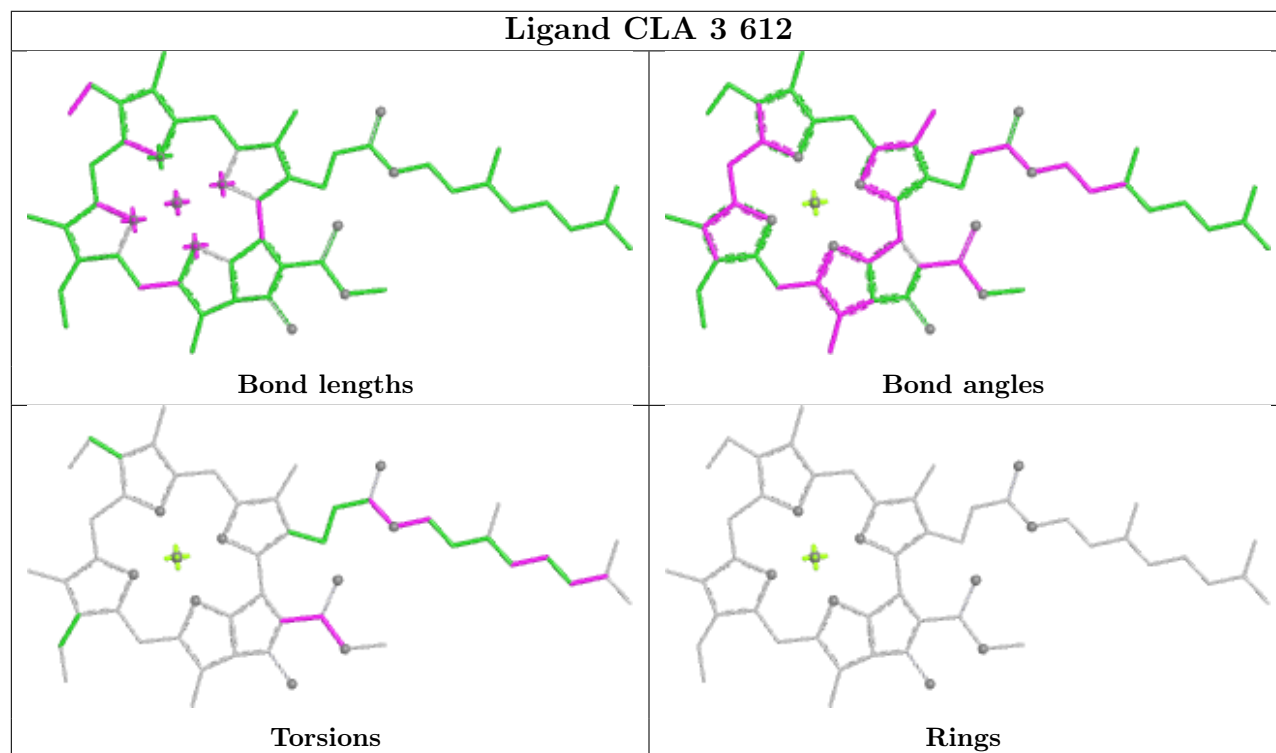
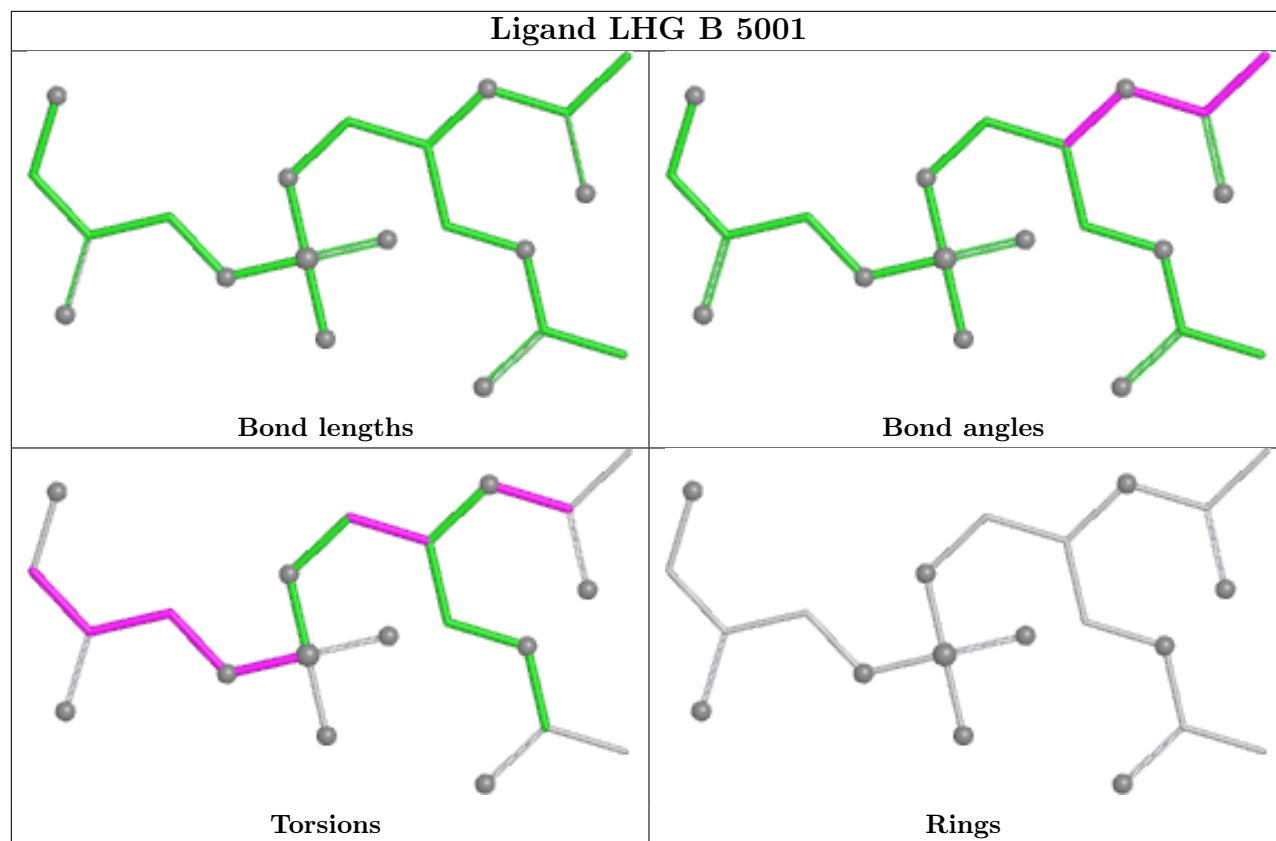


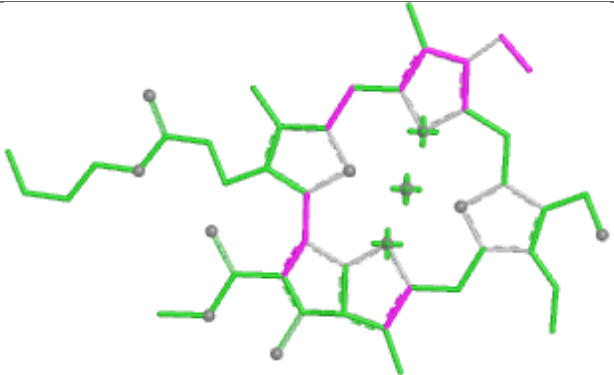
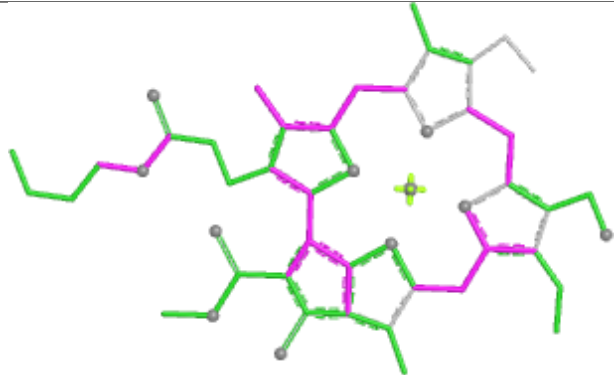
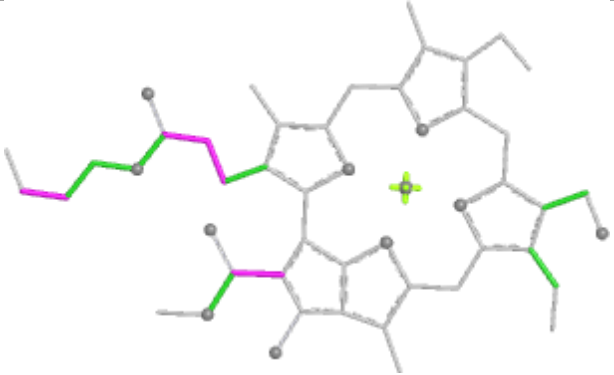
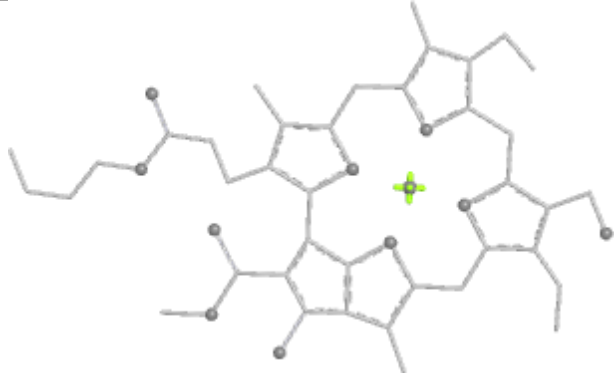
Ligand CLA B 1220

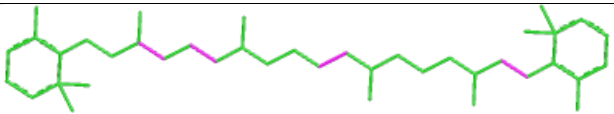
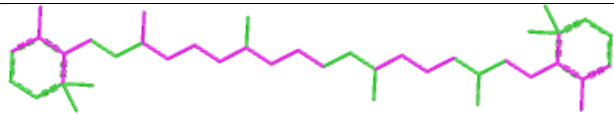
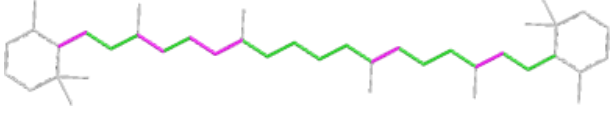
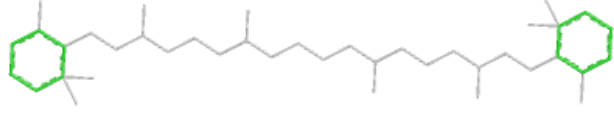




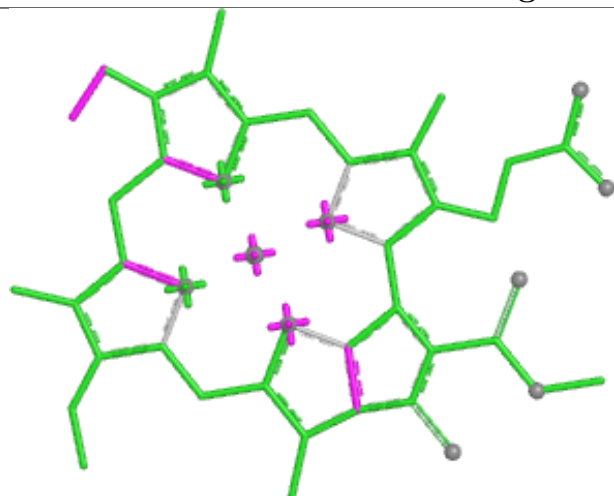
Ligand CLA 4 612	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR A 4003	
	
Bond lengths	Bond angles
	
Torsions	Rings



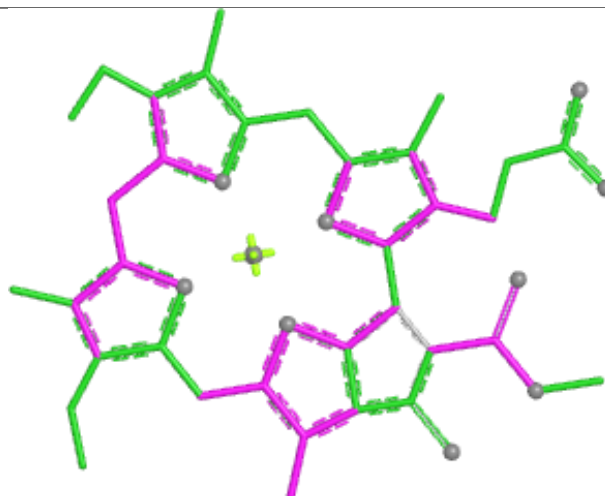
Ligand CHL 4 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

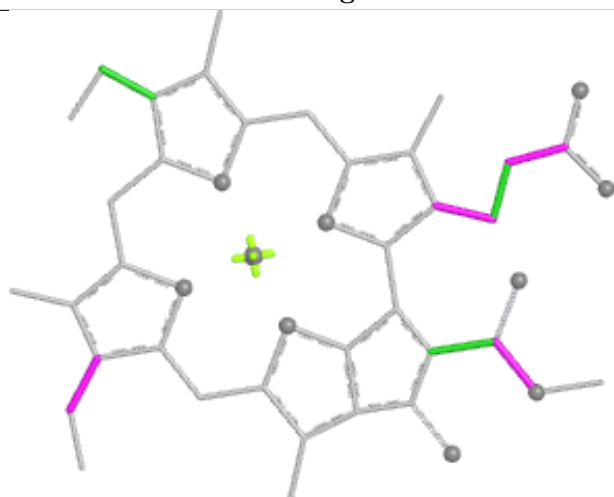
Ligand CLA 1 606



Bond lengths



Bond angles

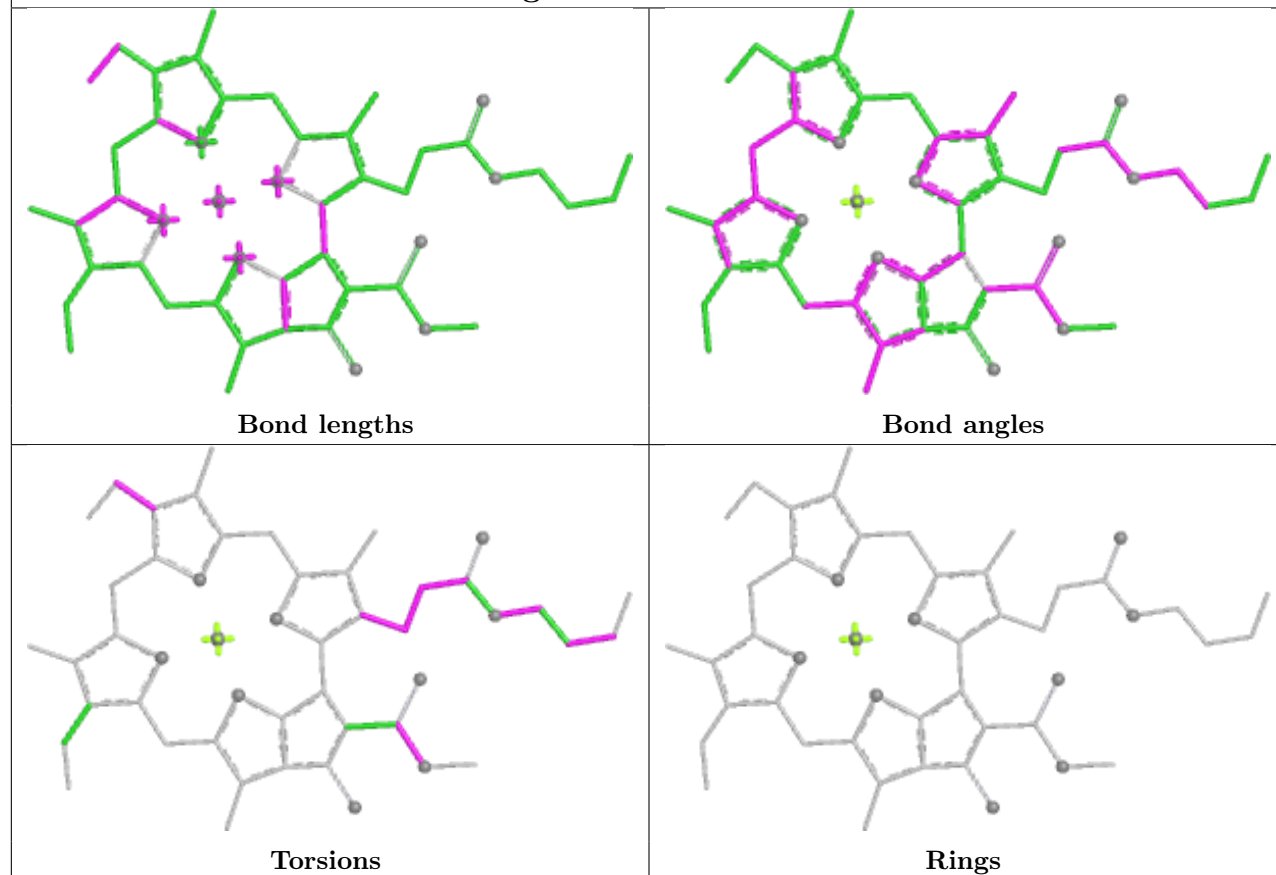


Torsions

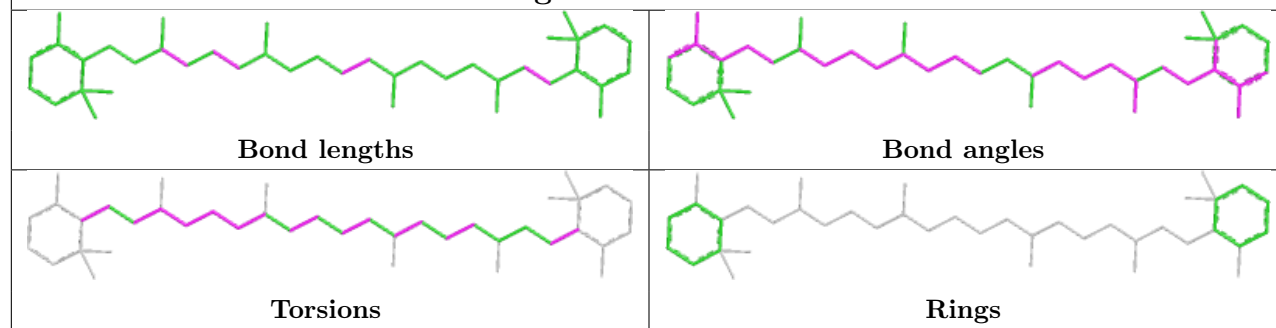


Rings

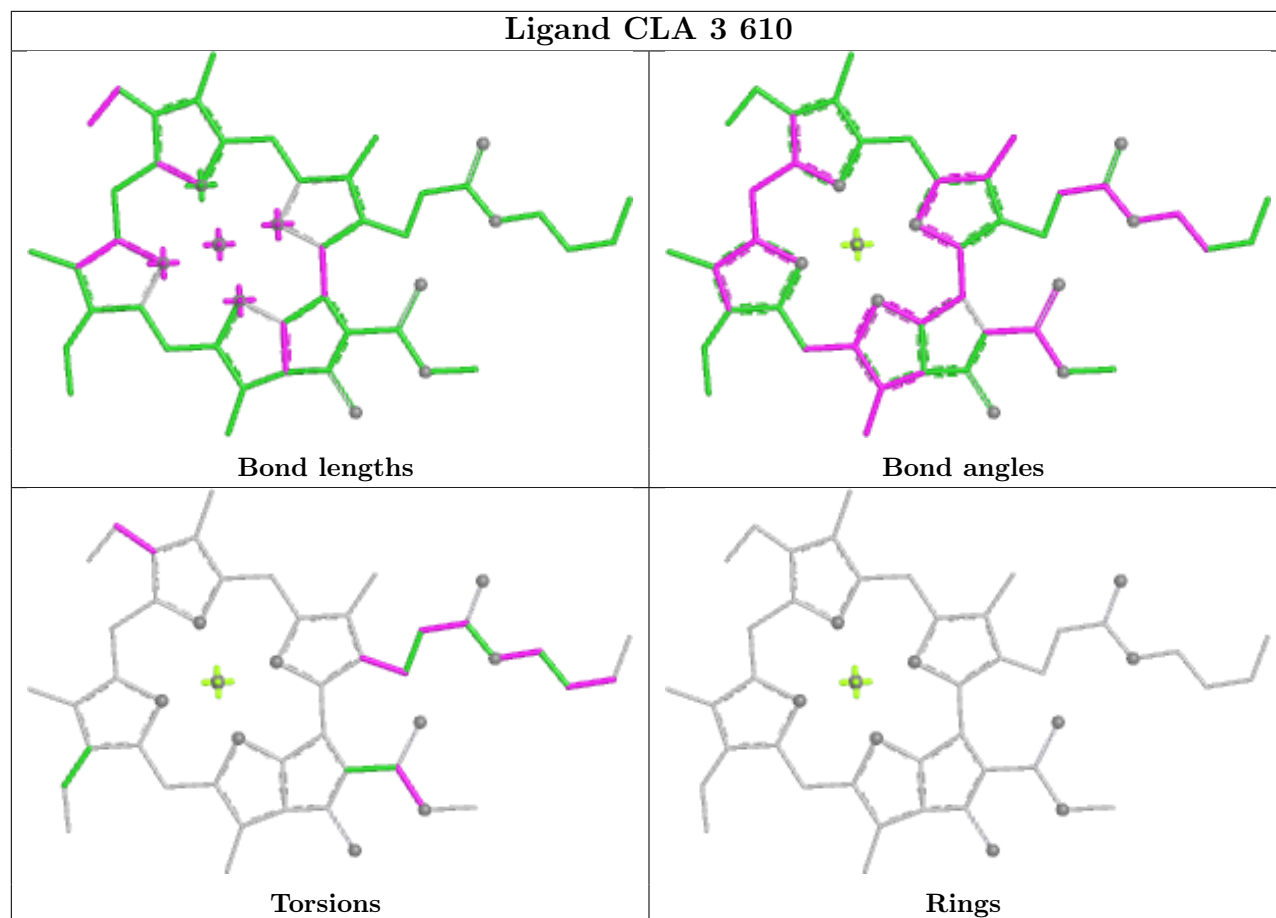
Ligand CLA A 1105



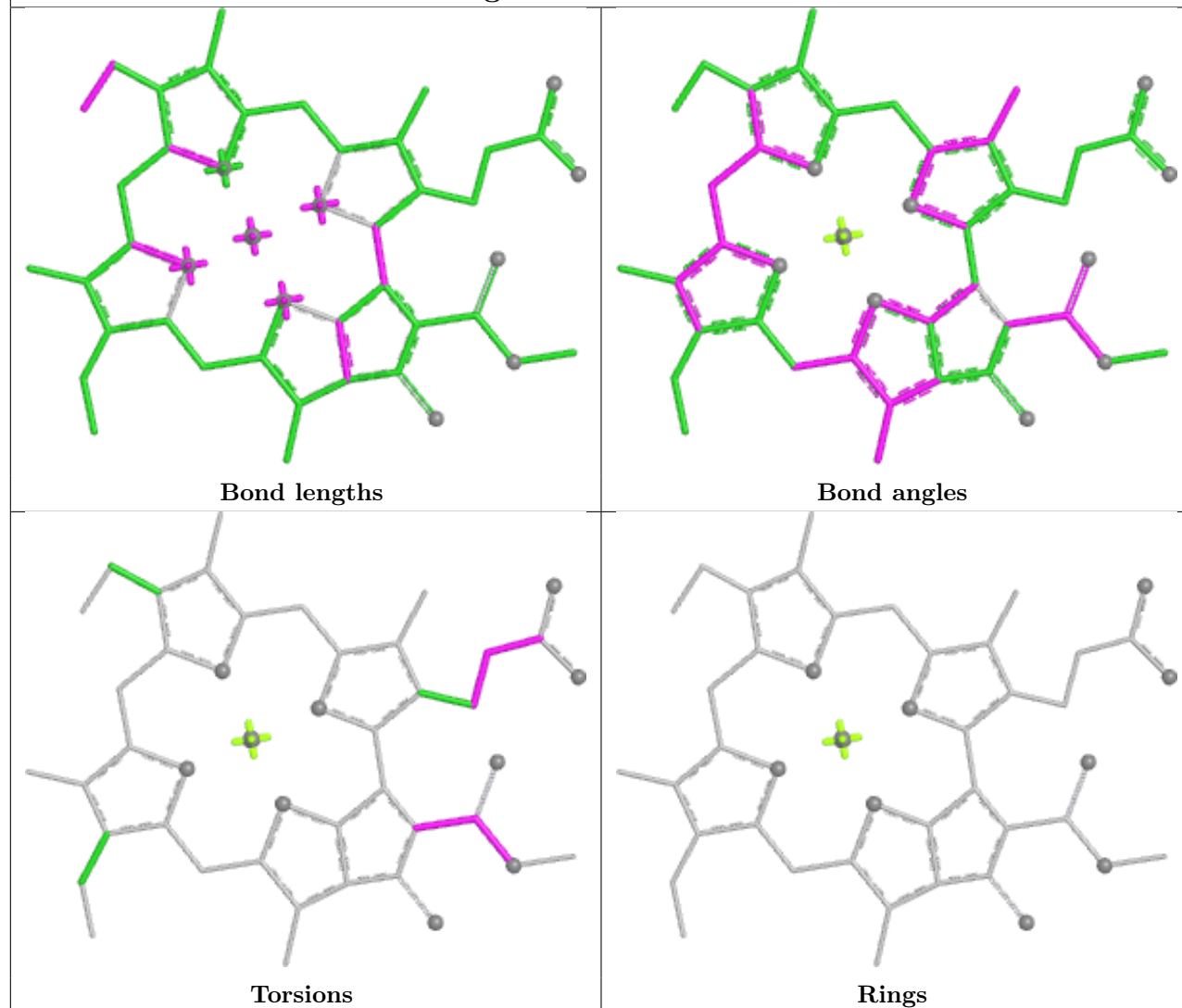
Ligand BCR 3 504



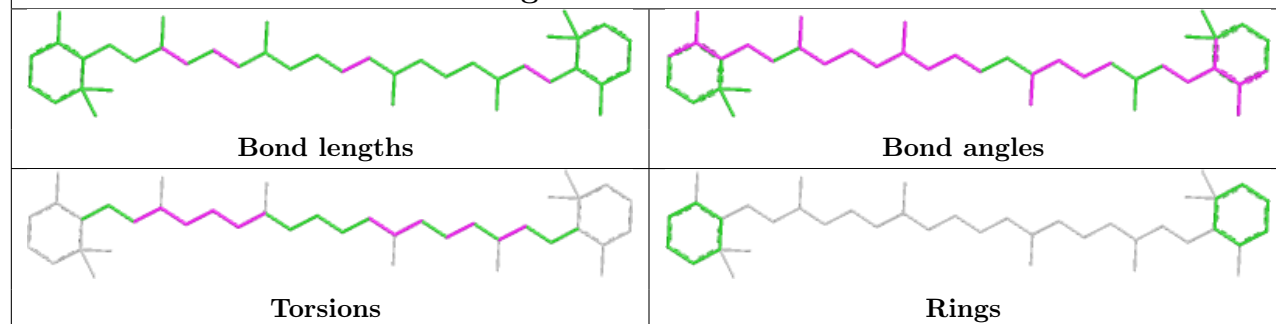
Ligand CLA 3 610



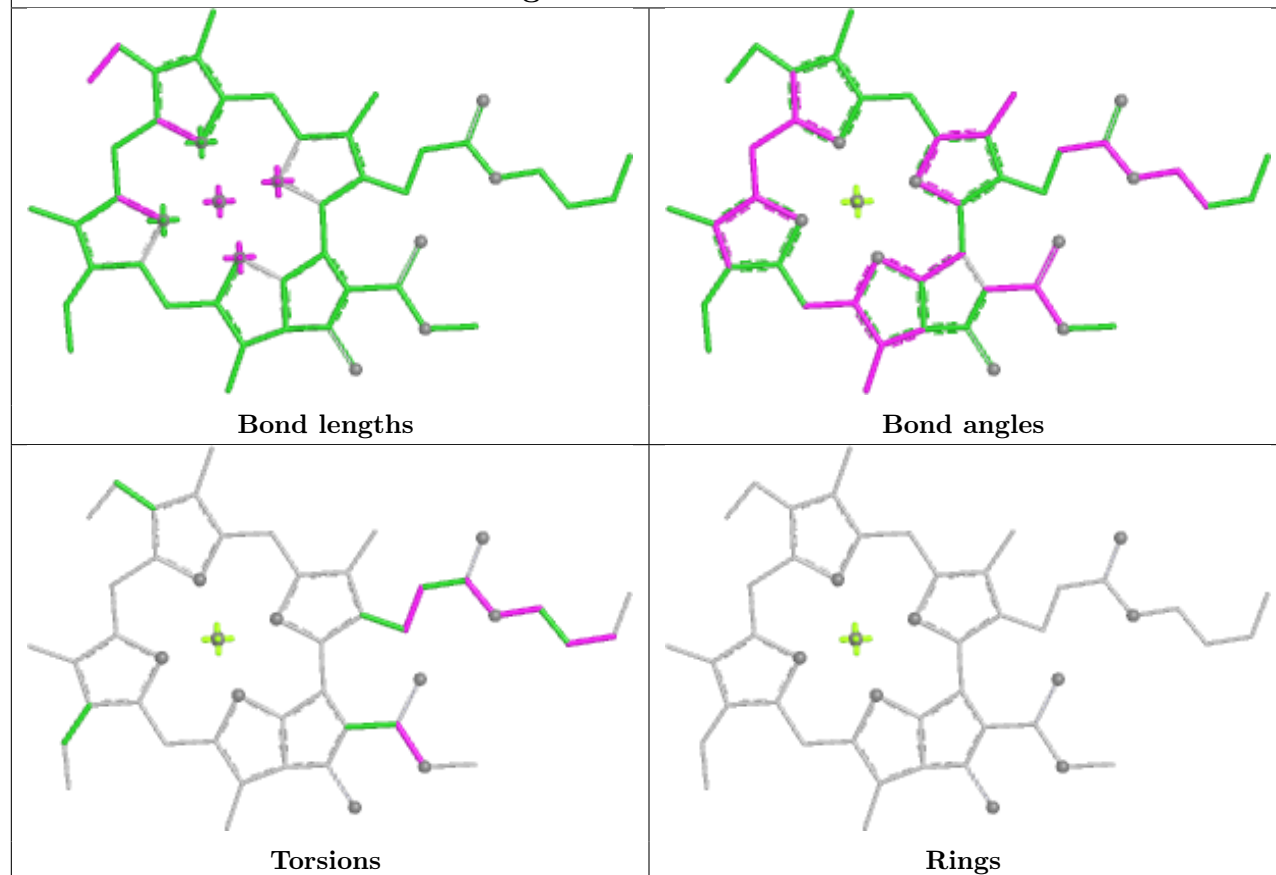
Ligand CLA A 1102



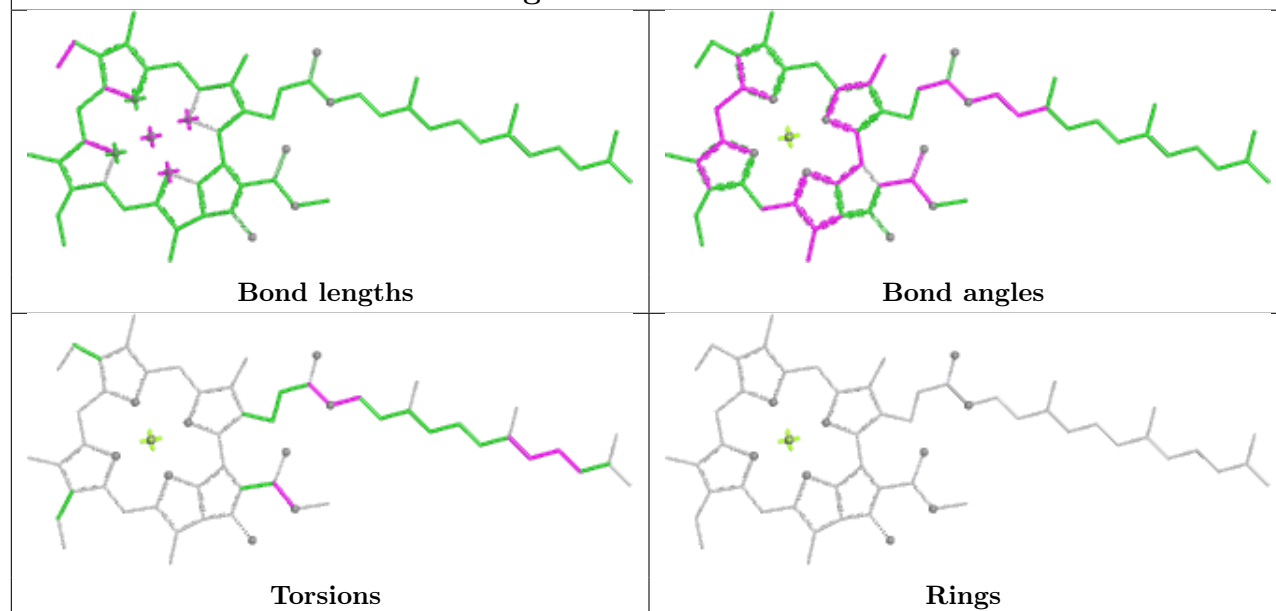
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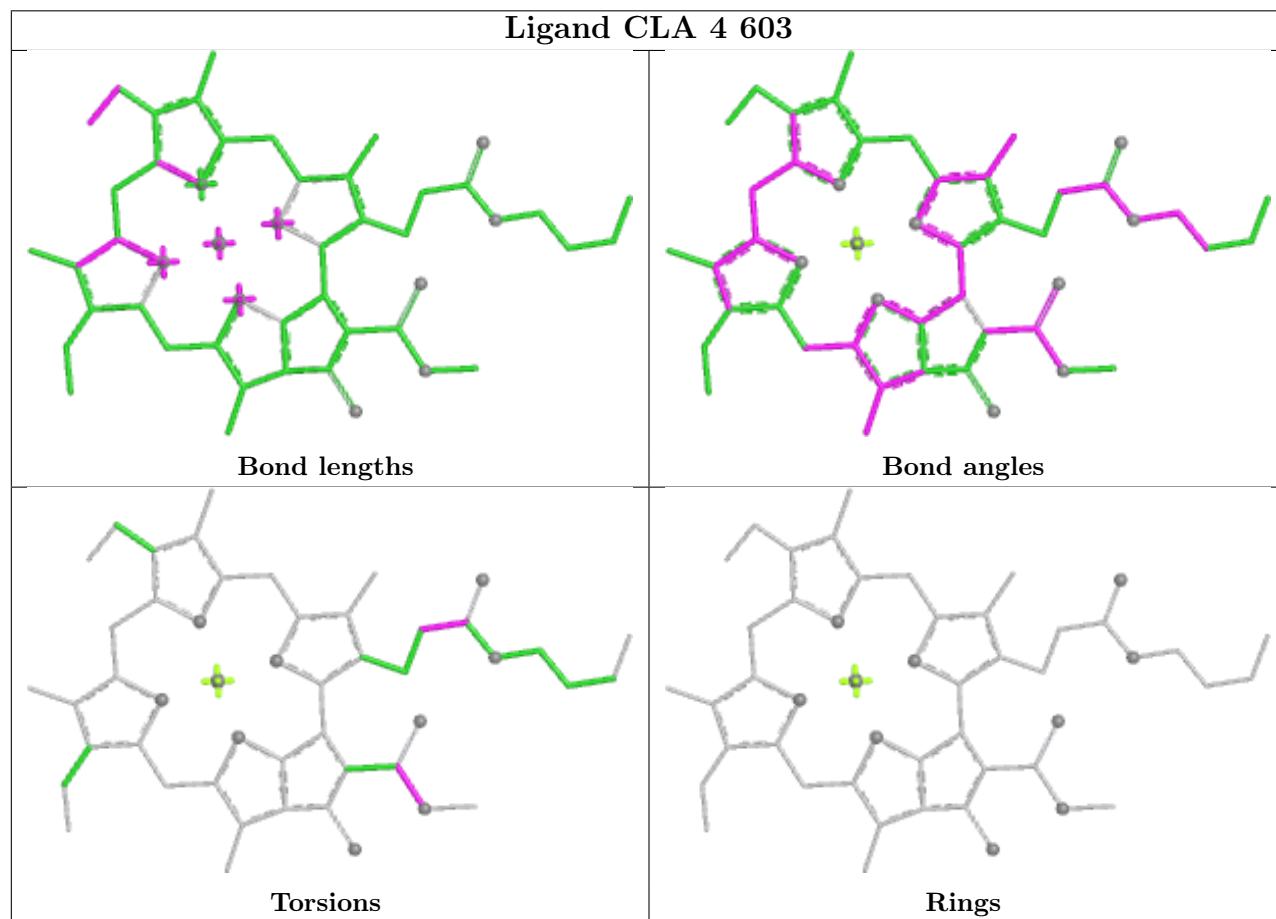
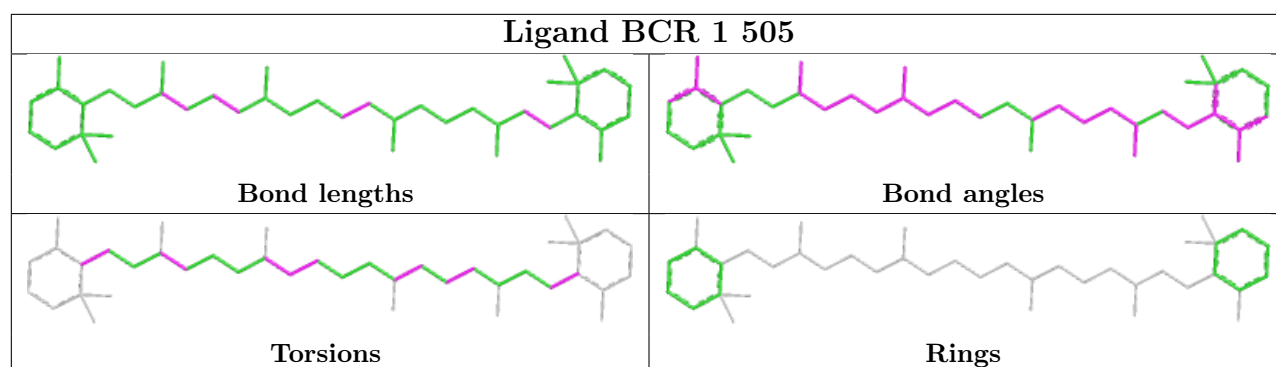


Ligand CLA A 1126

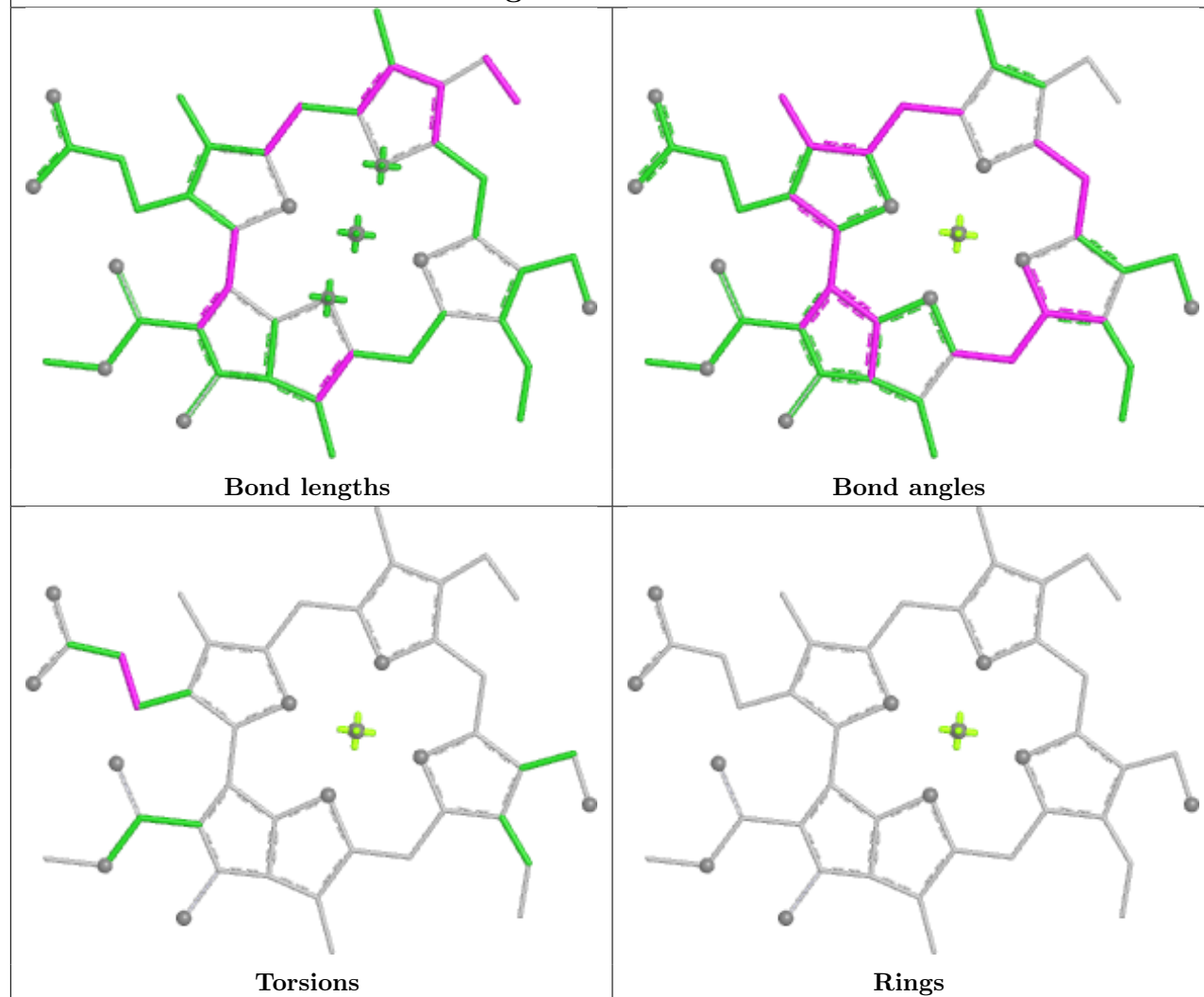


Ligand CLA B 1231

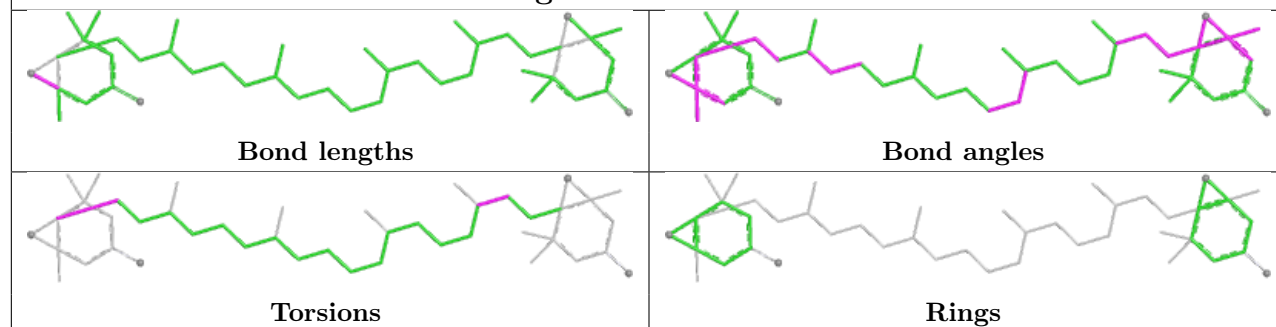


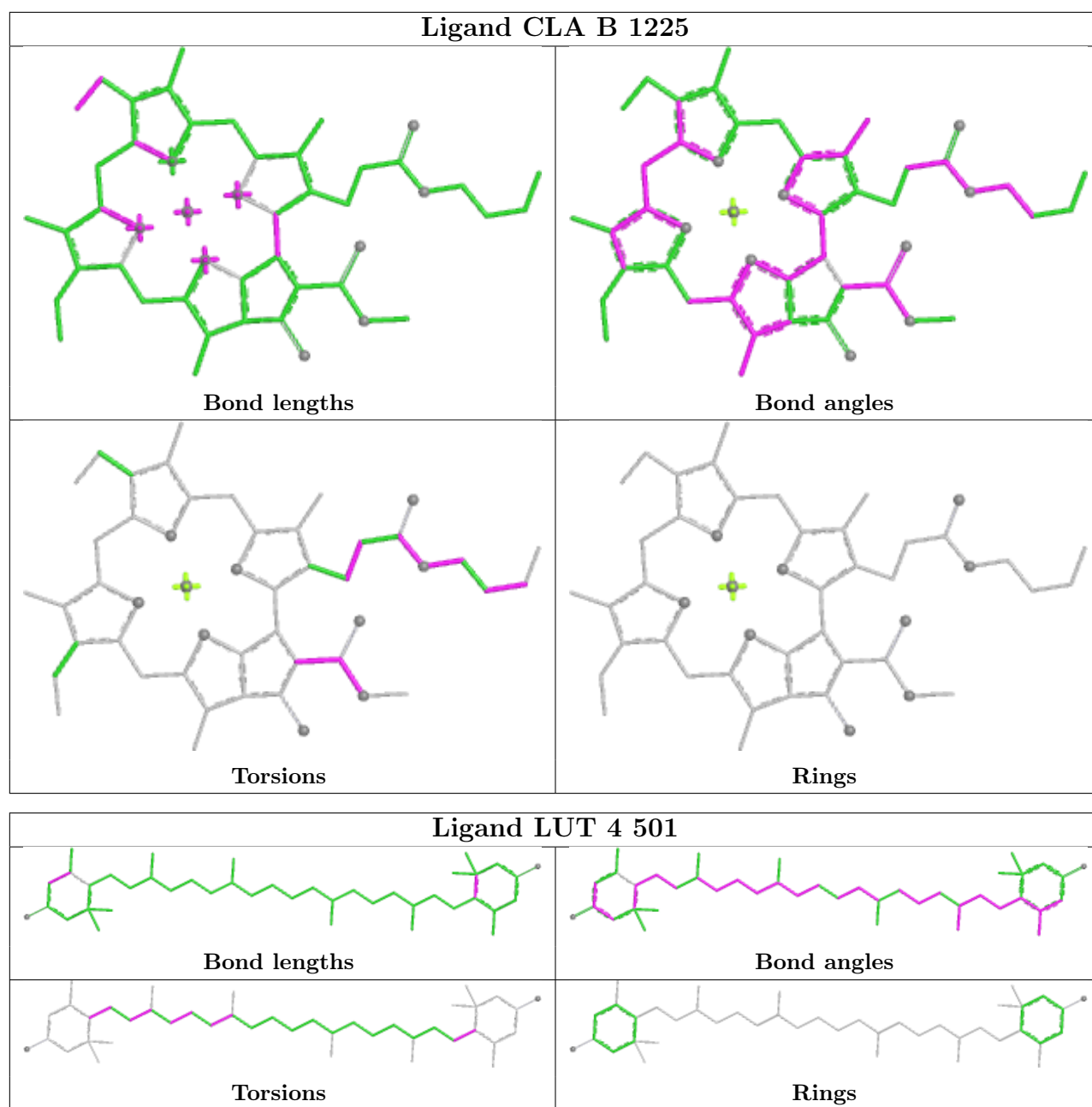


Ligand CHL 2 613

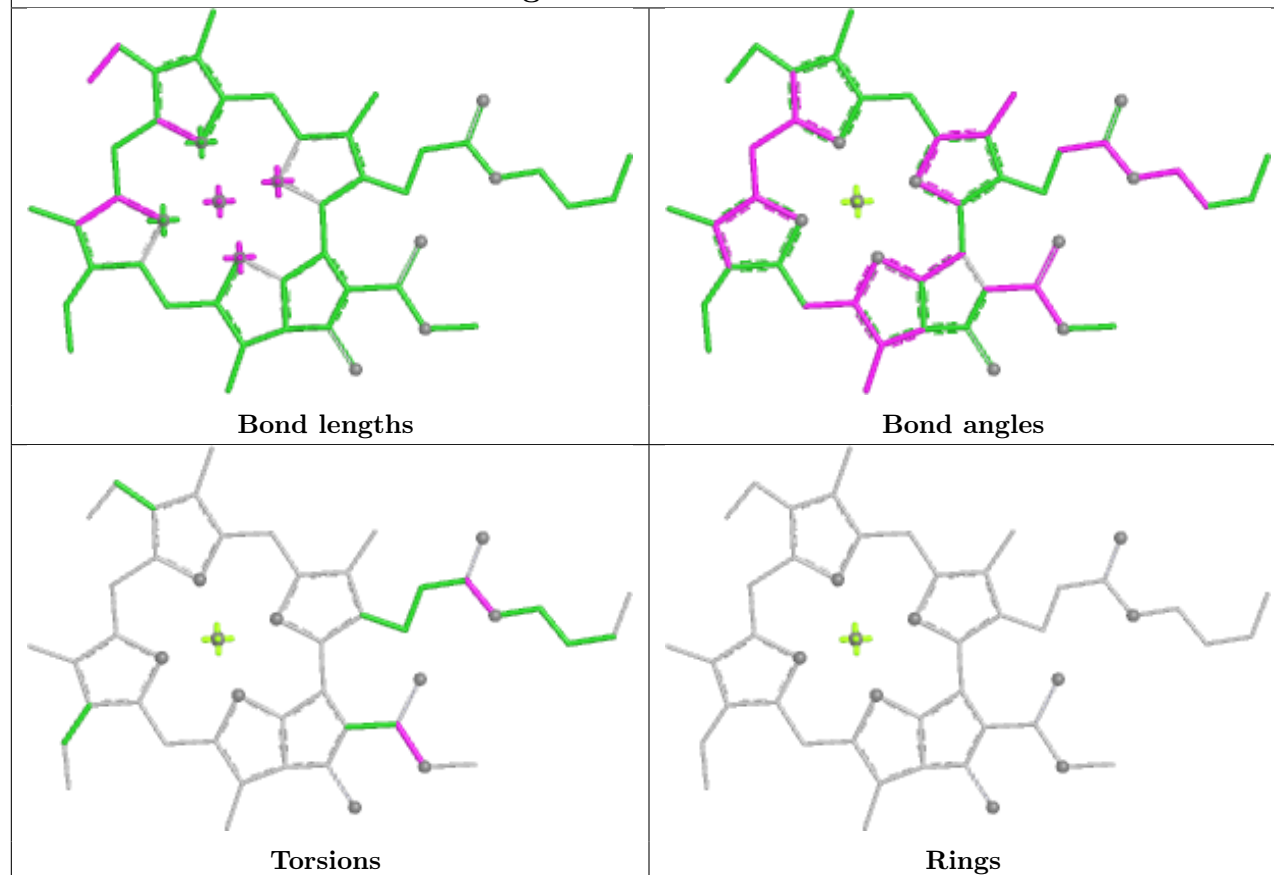


Ligand XAT 2 502

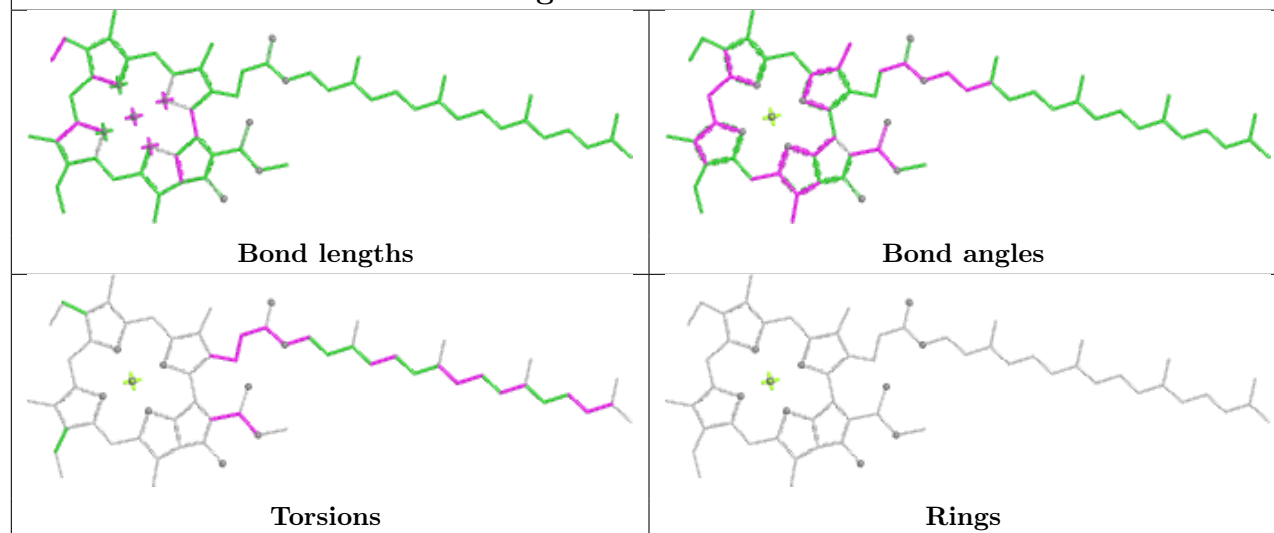




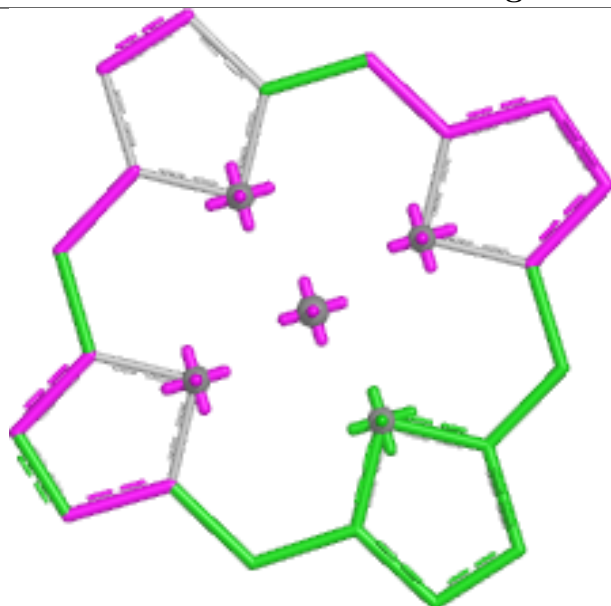
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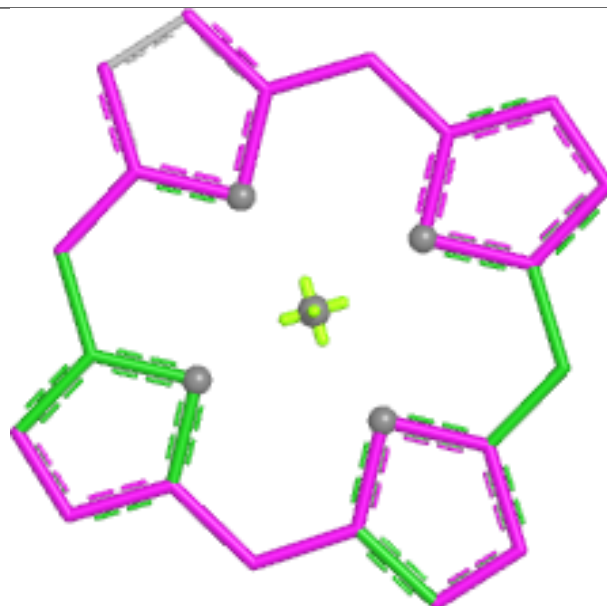
Ligand CLA 1 615



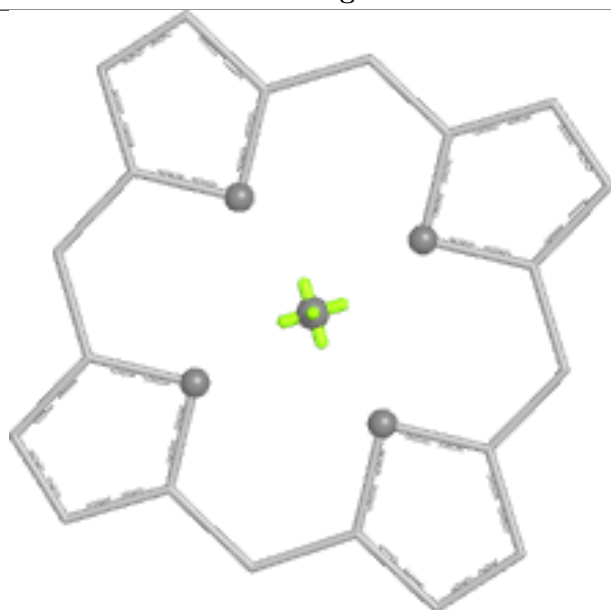
Ligand CLA B 1207



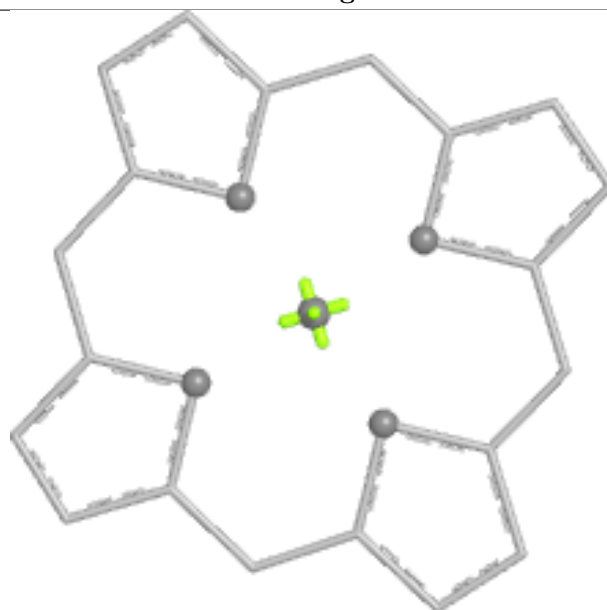
Bond lengths



Bond angles

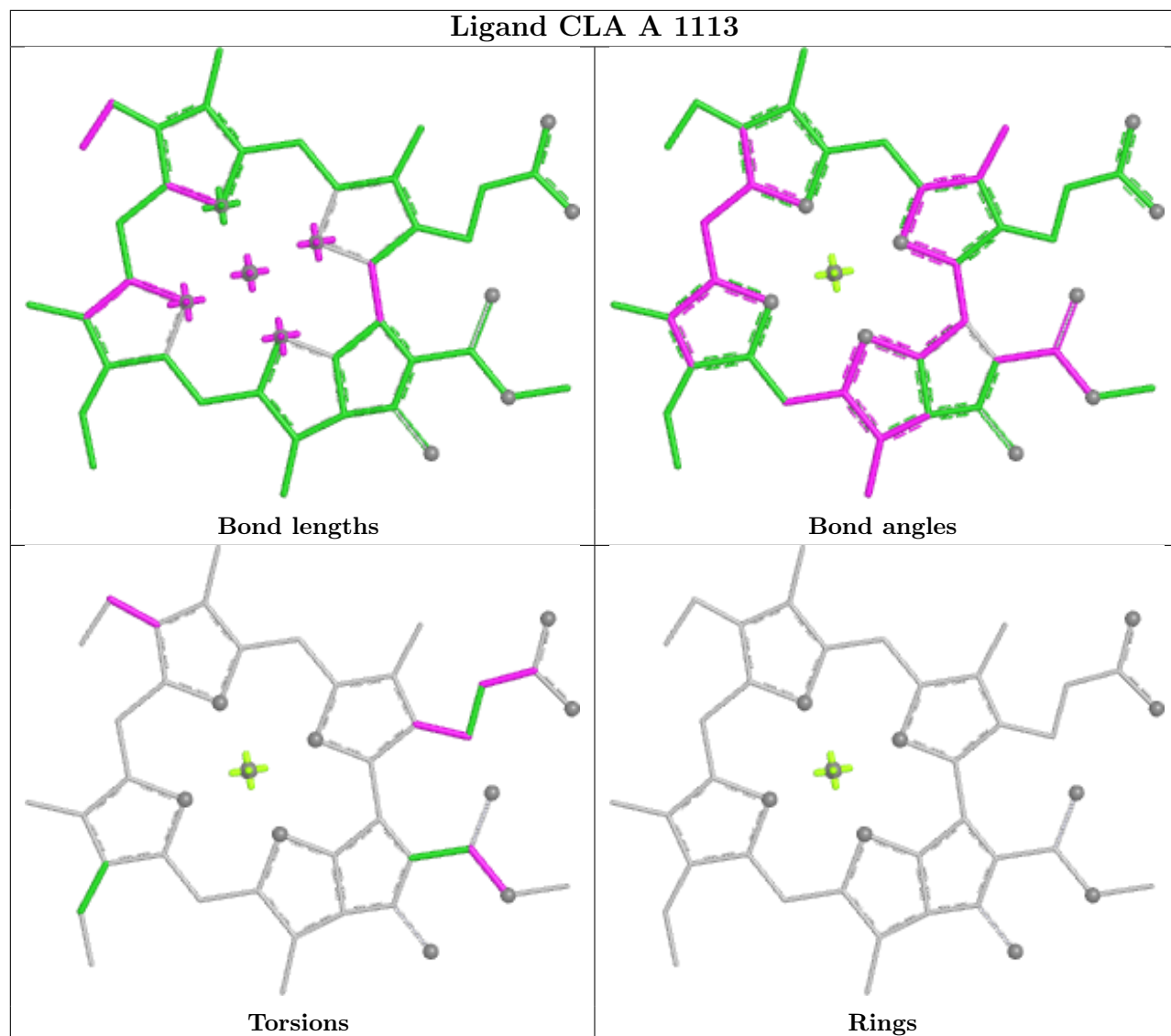


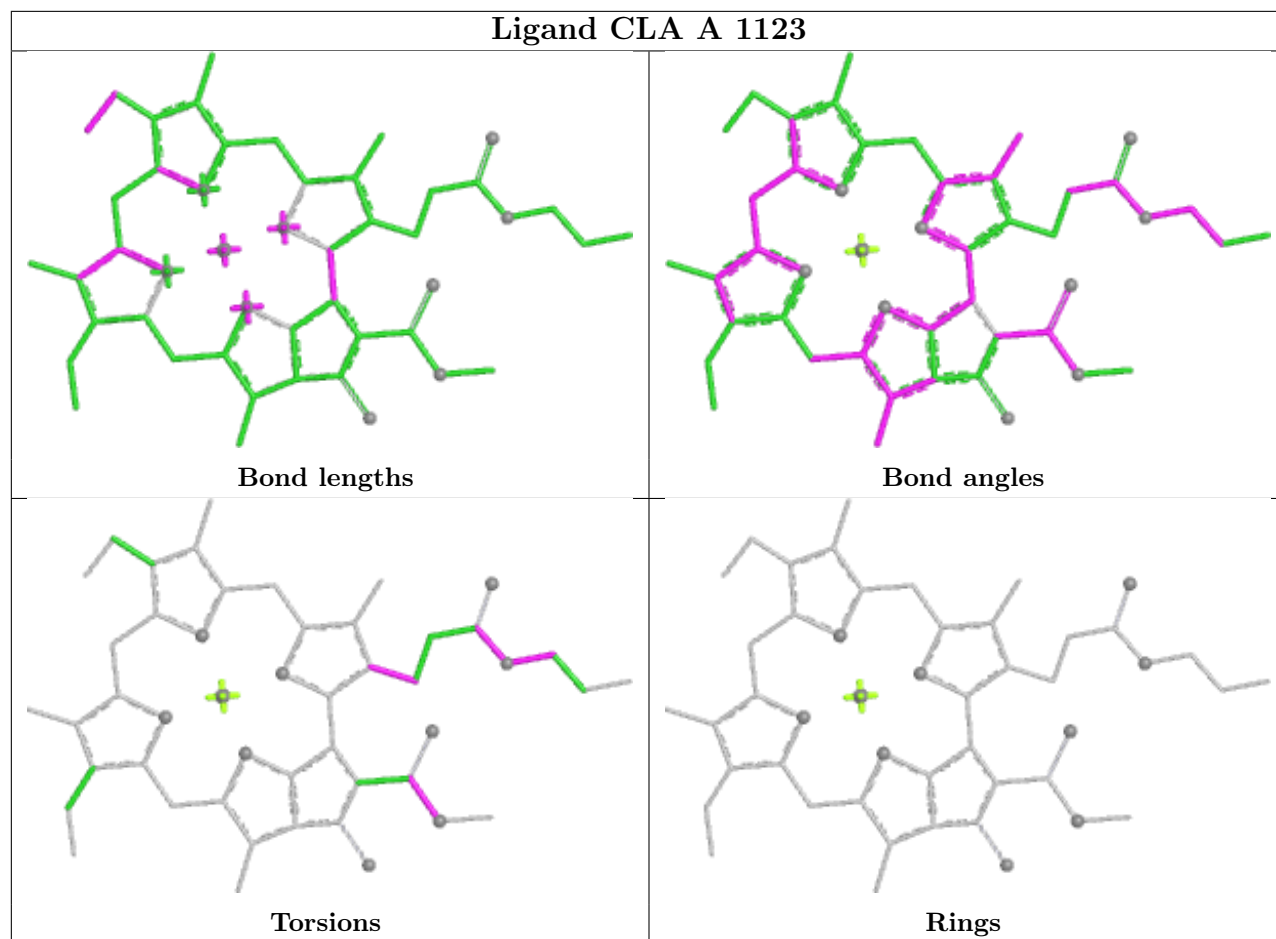
Torsions

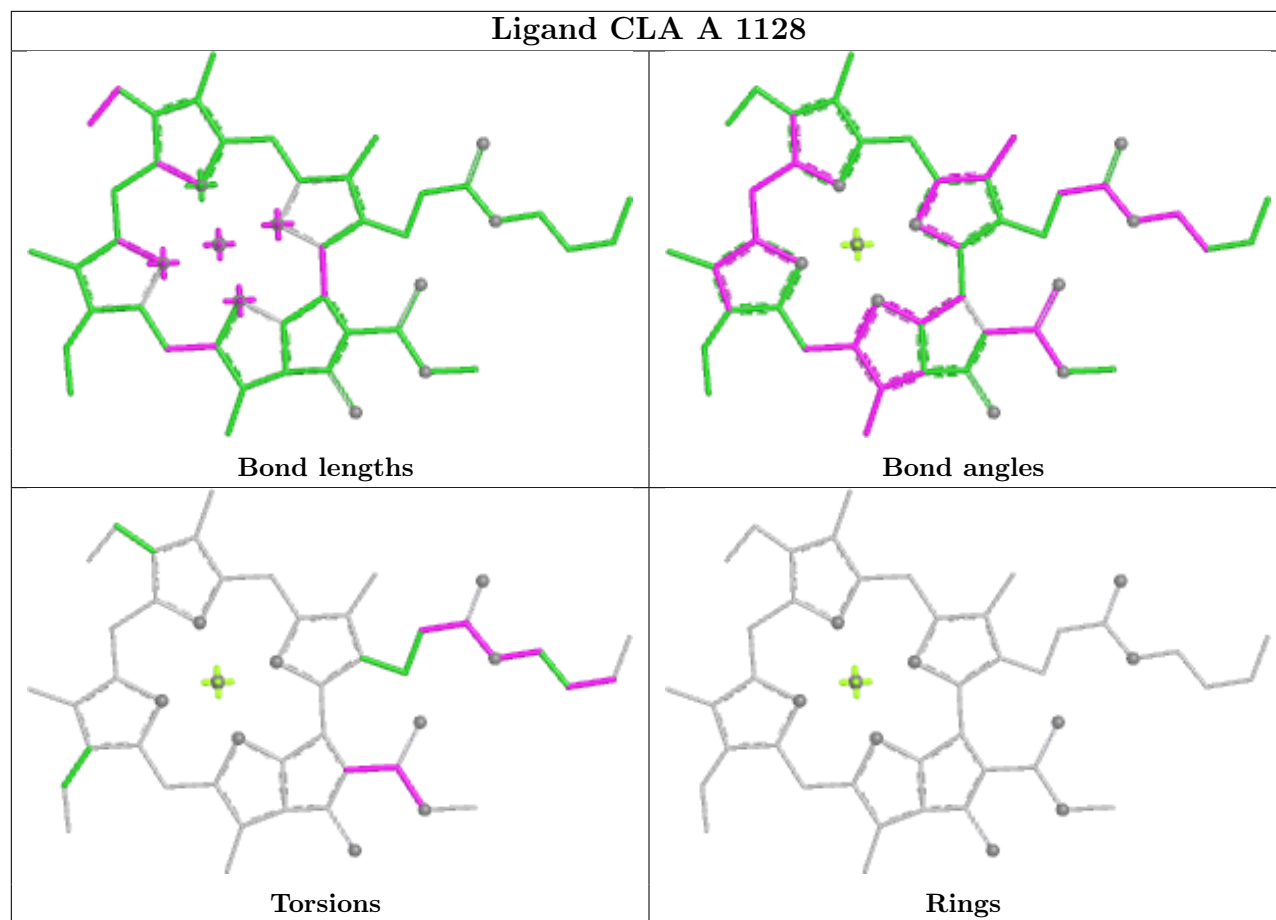


Rings

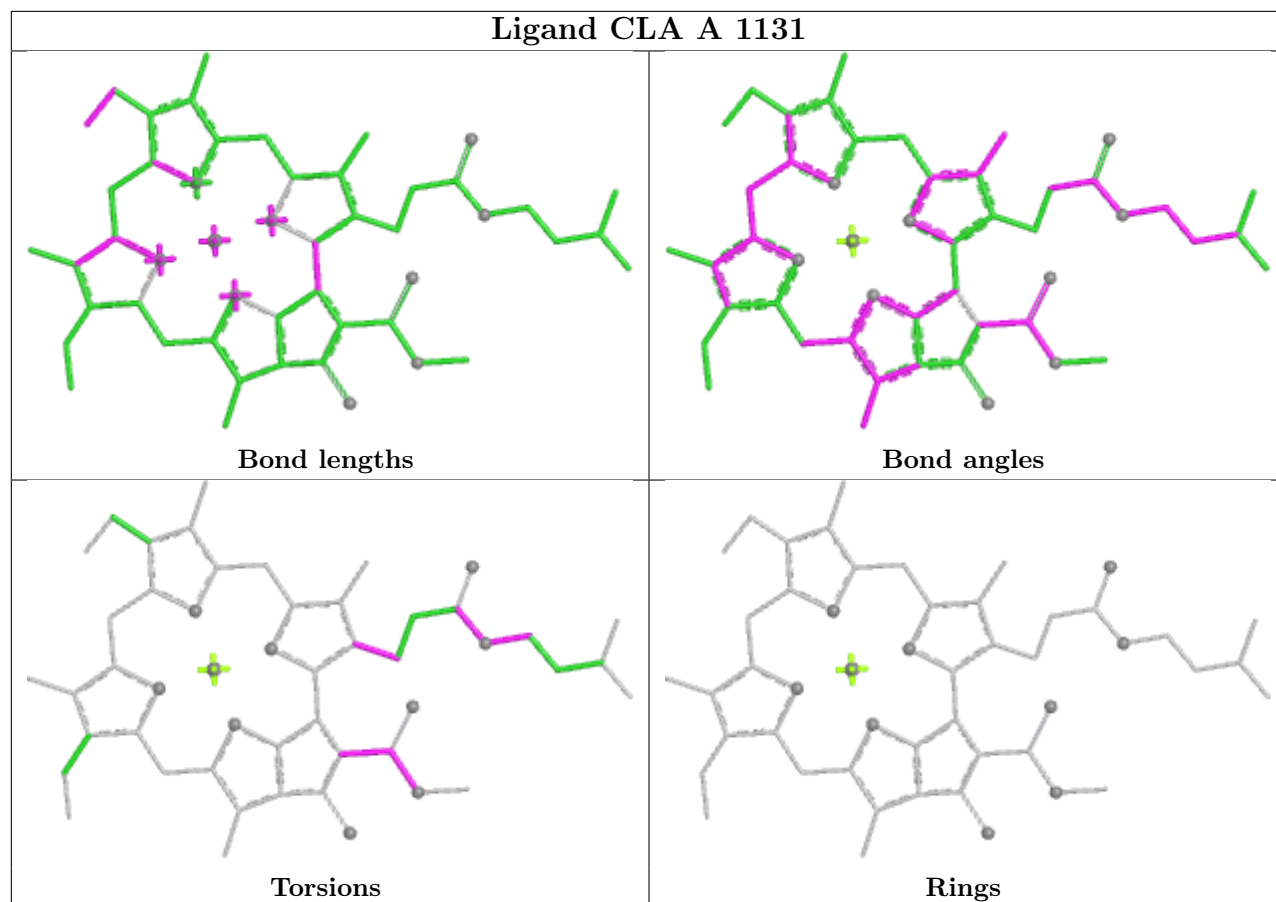
Ligand CLA A 1113

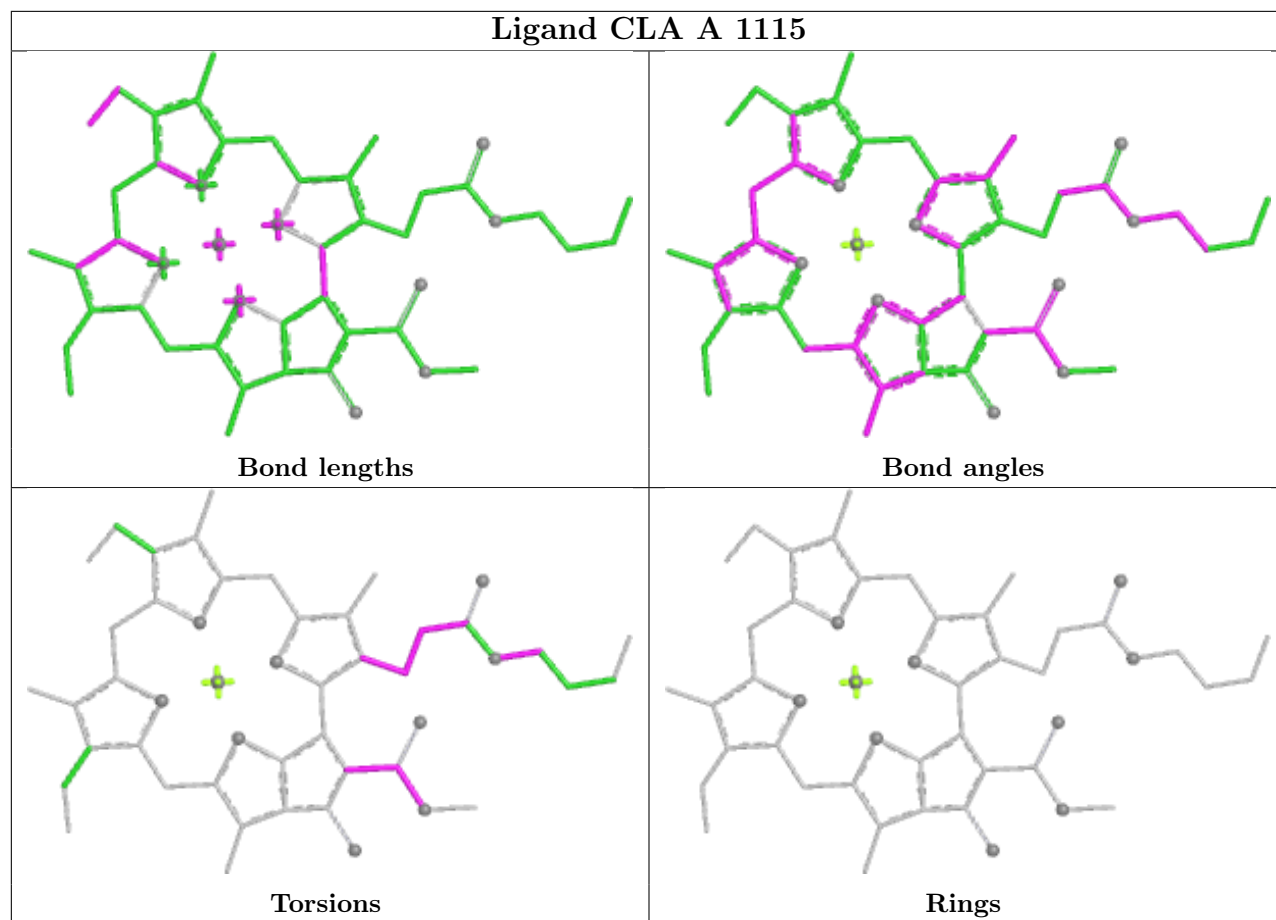




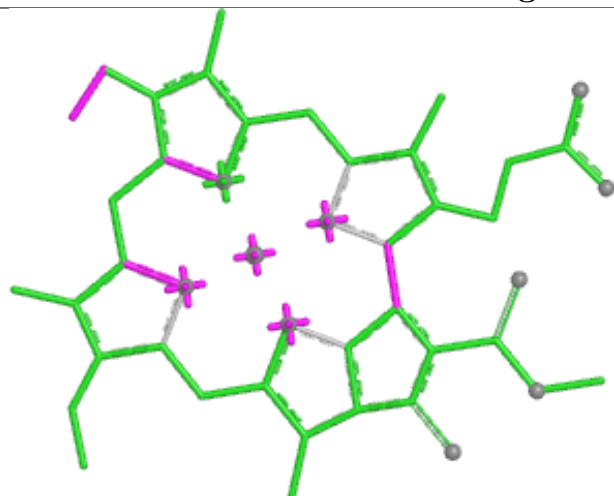


Ligand CLA A 1131

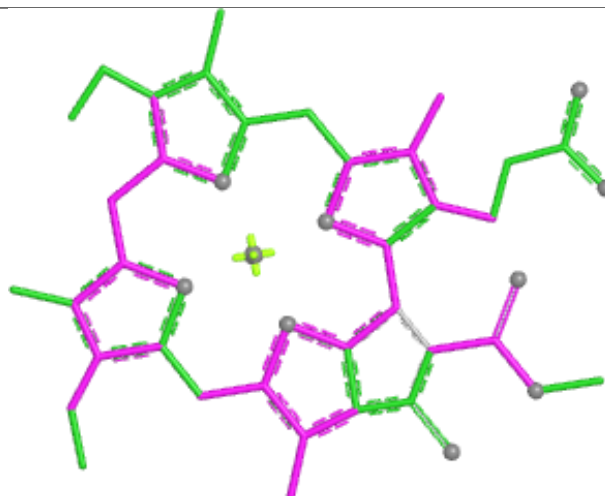




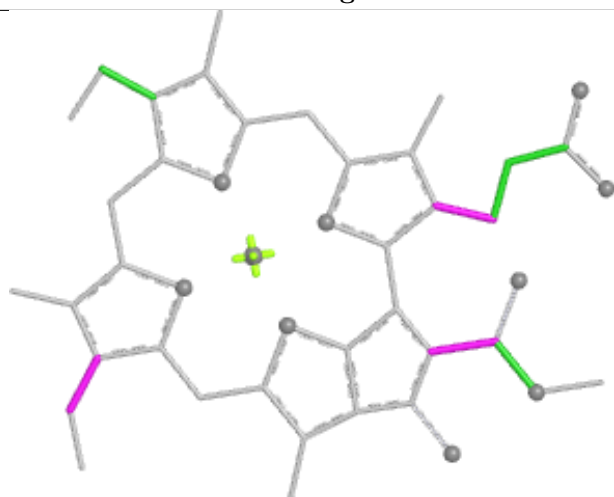
Ligand CLA 3 603



Bond lengths



Bond angles

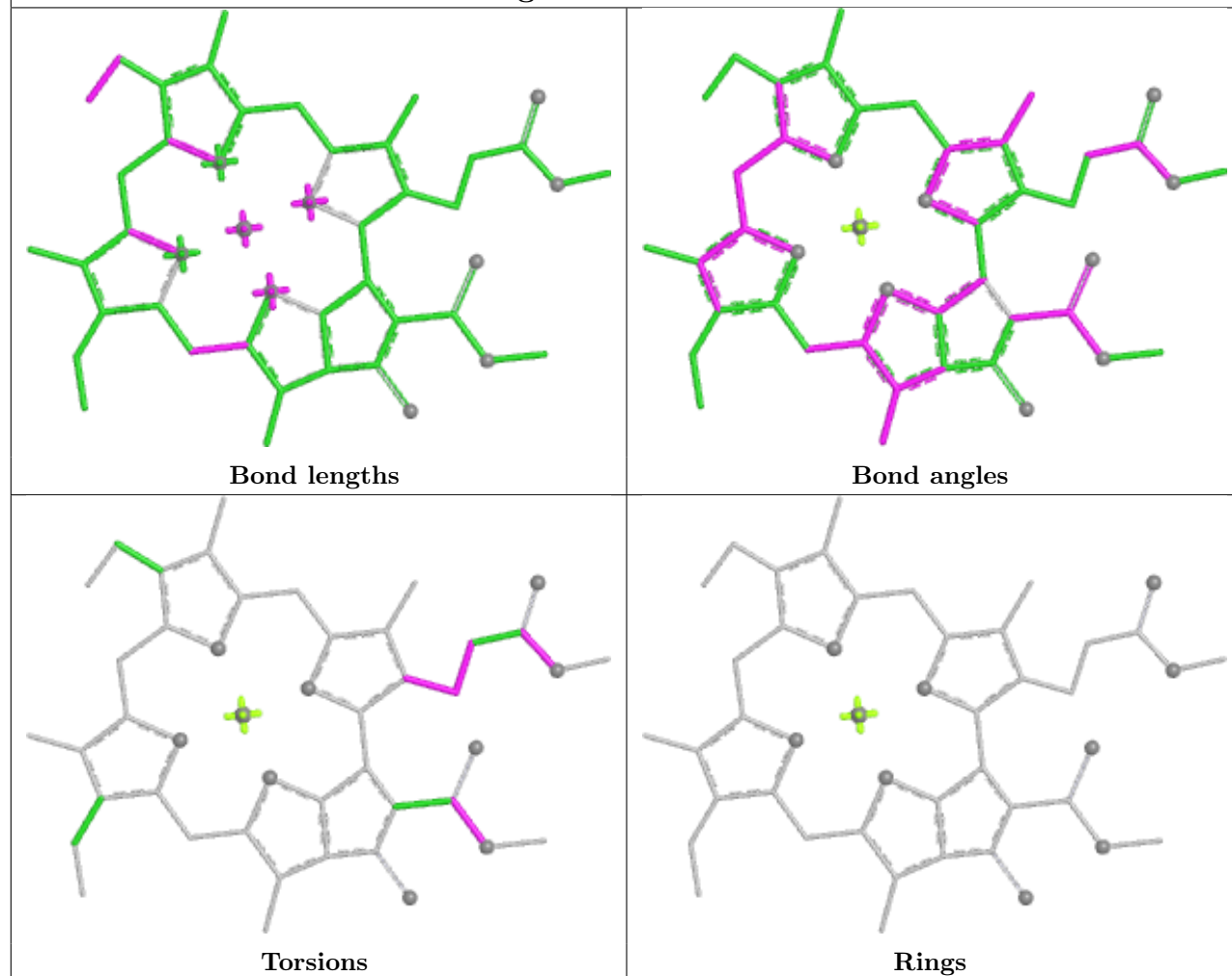


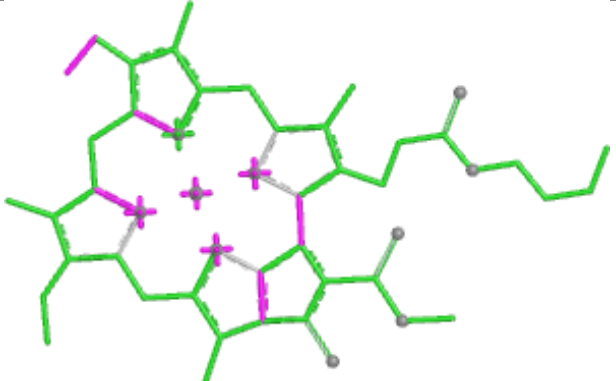
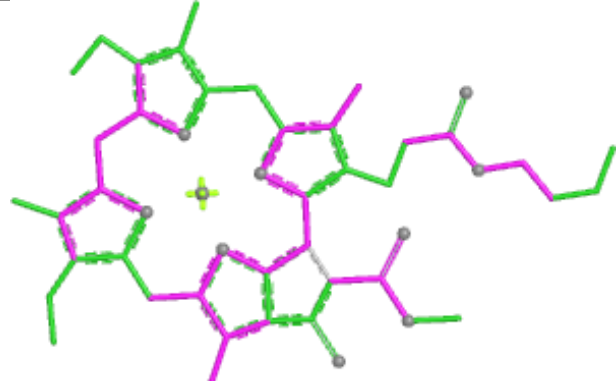
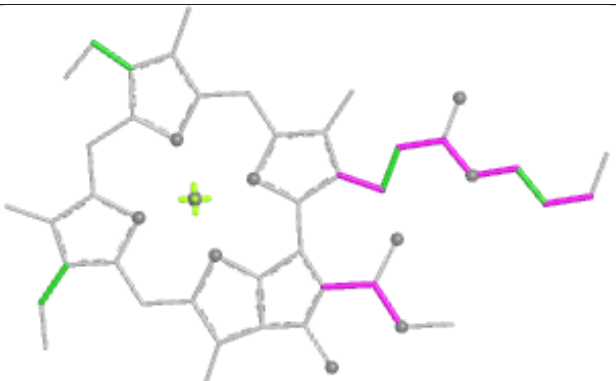
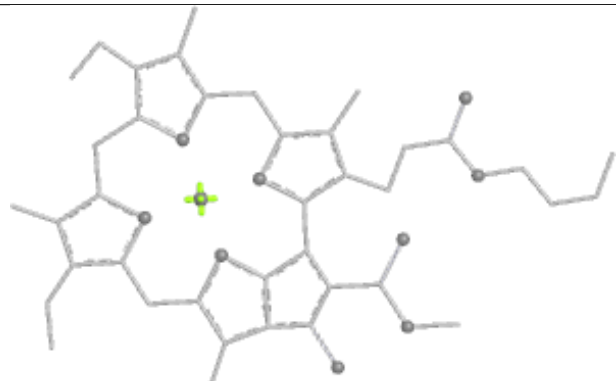
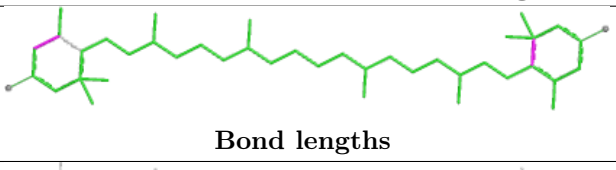
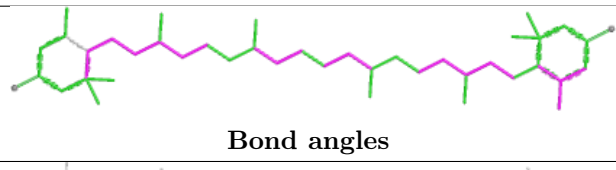
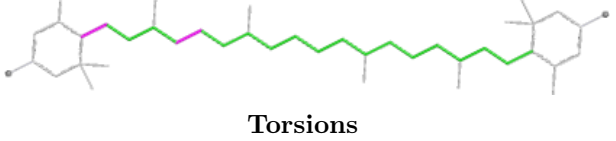
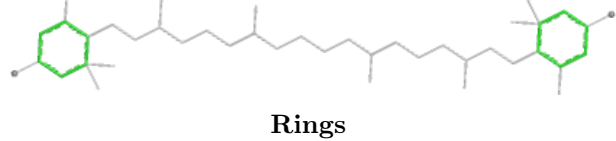
Torsions



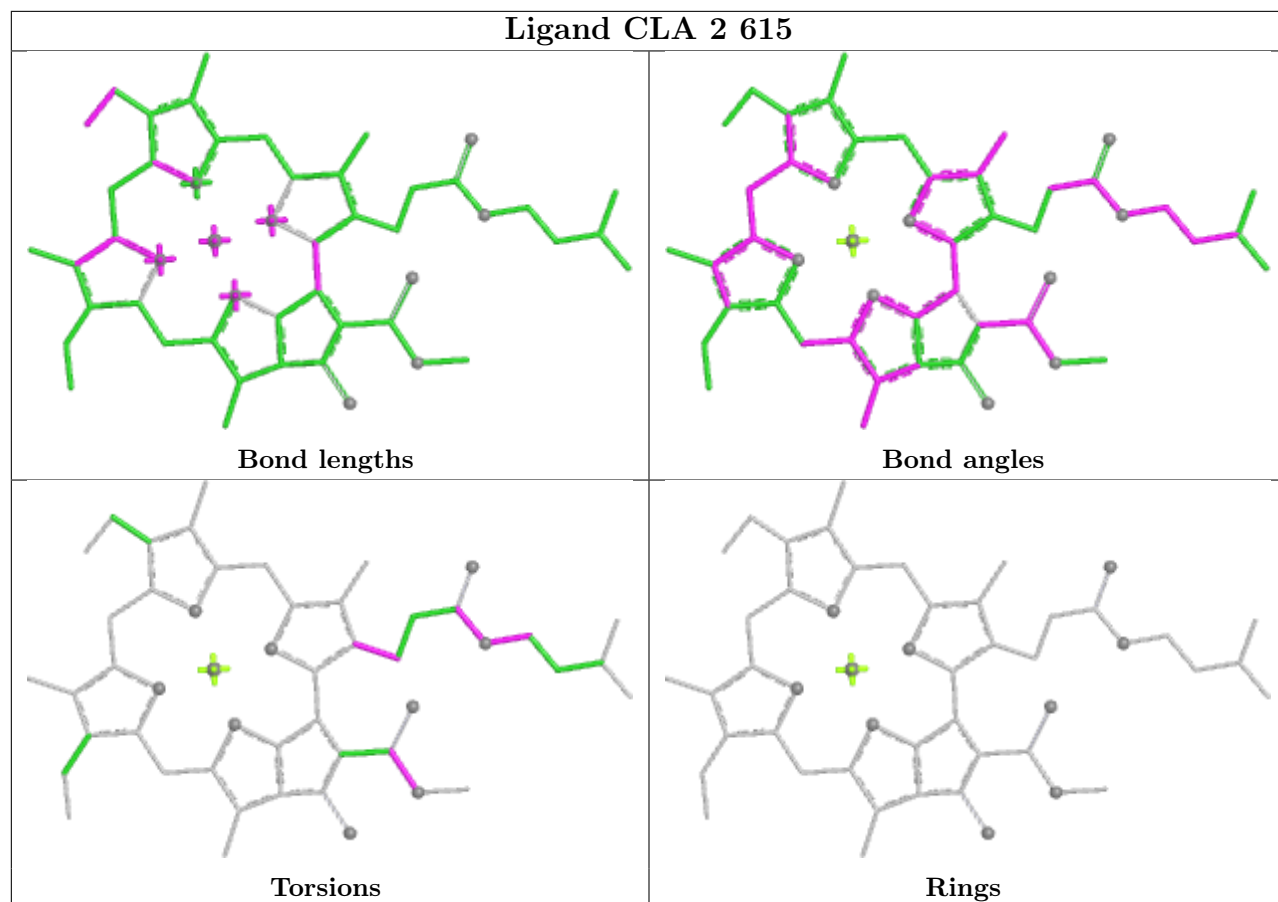
Rings

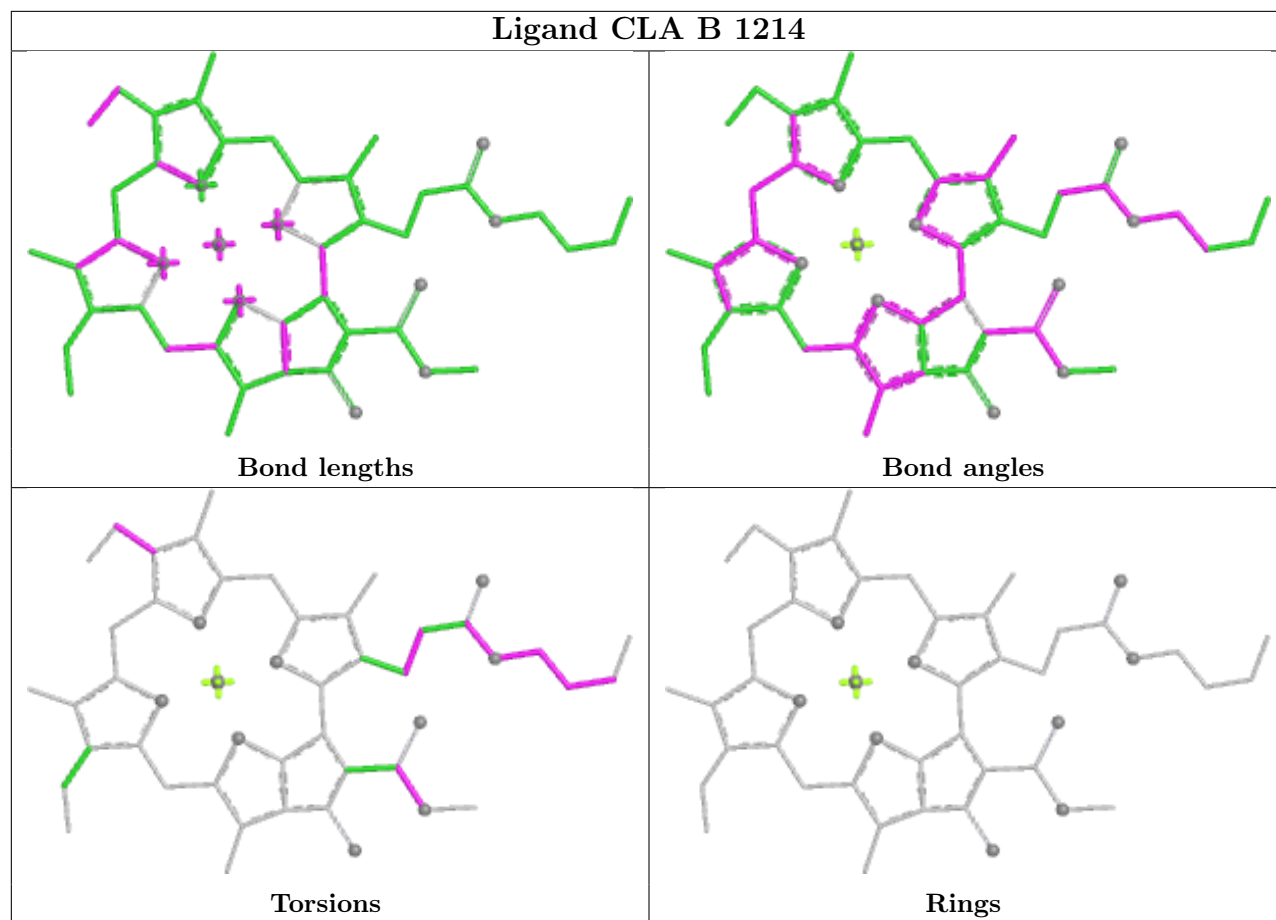
Ligand CLA 3 611

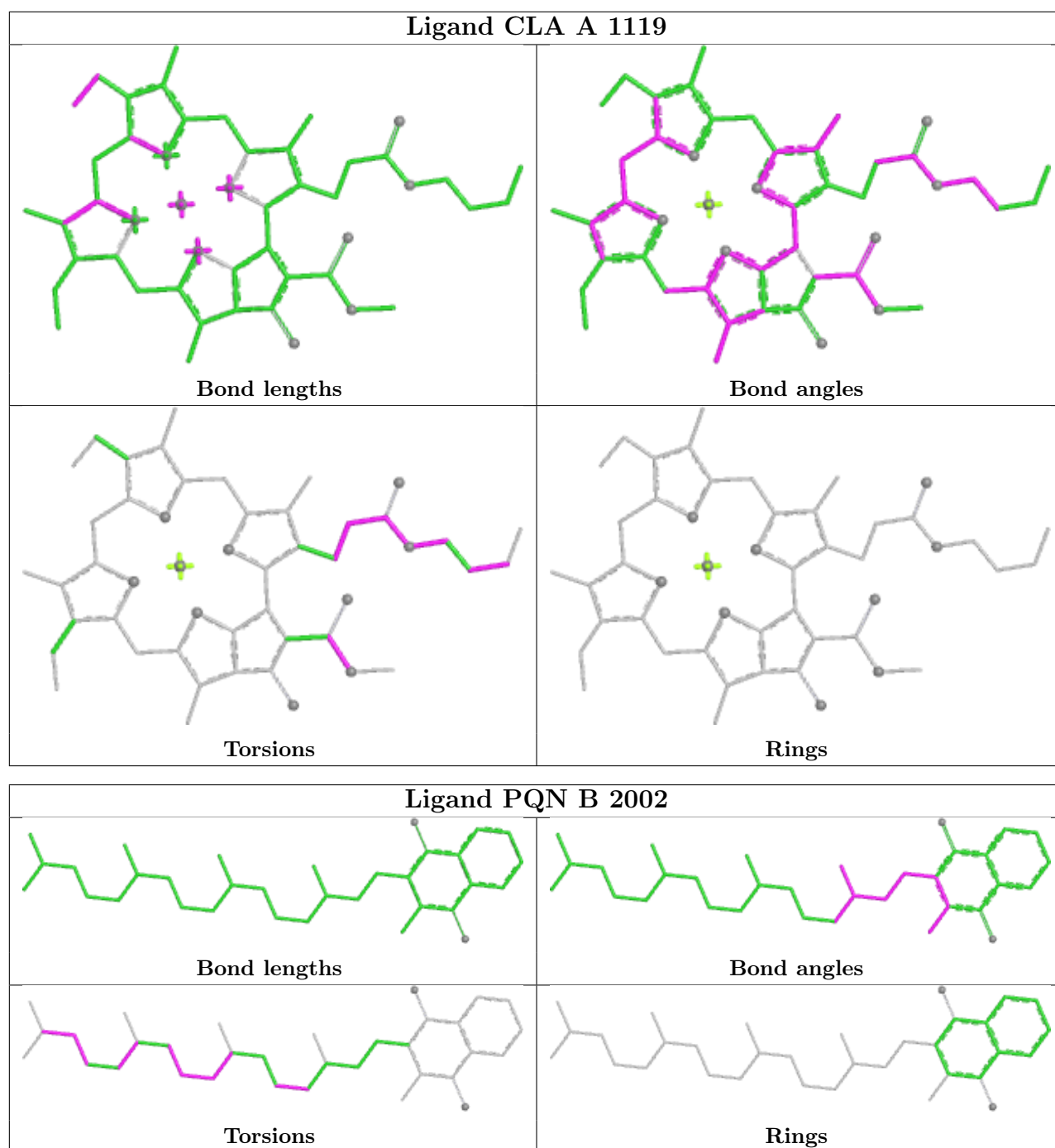


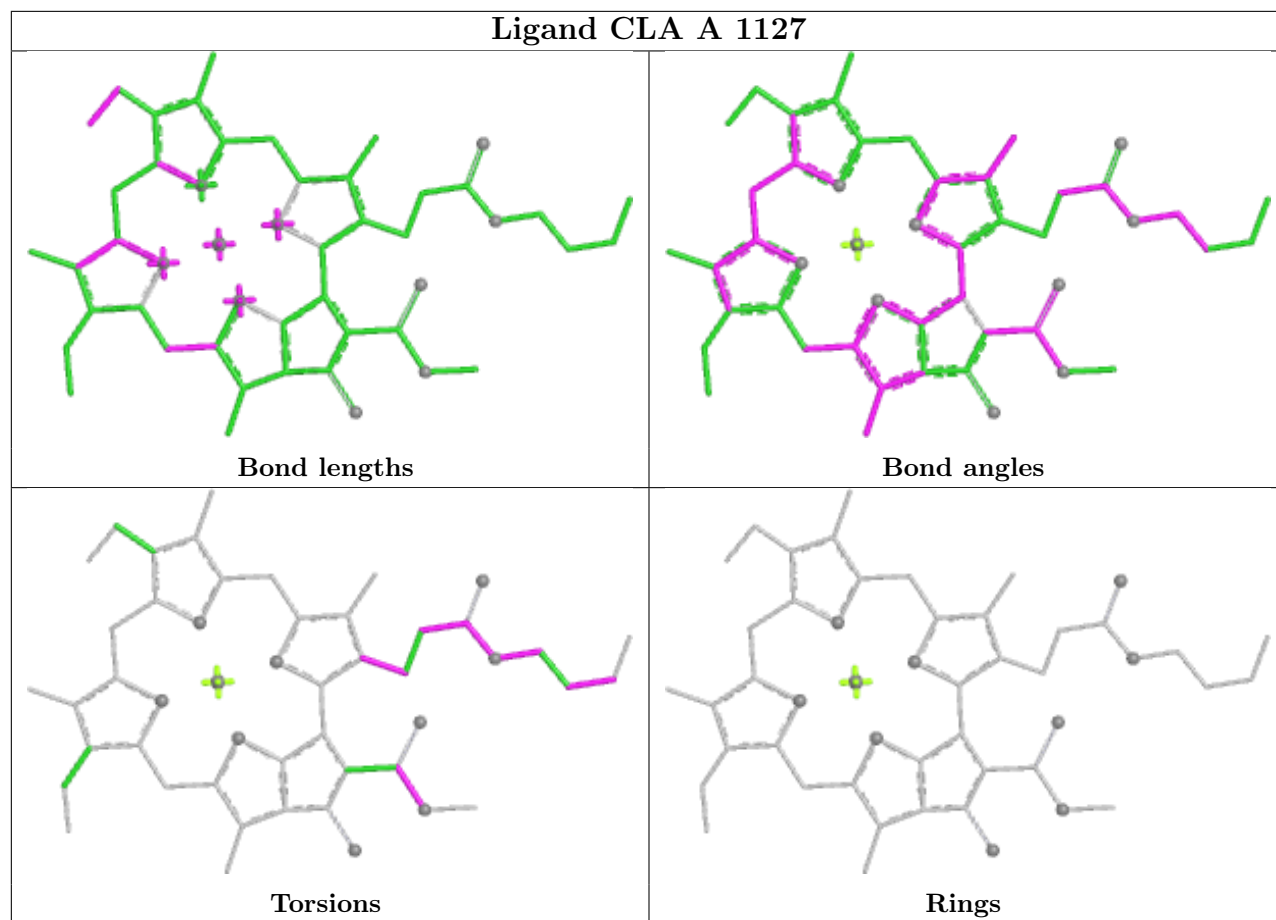
Ligand CLA B 1210	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT 3 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

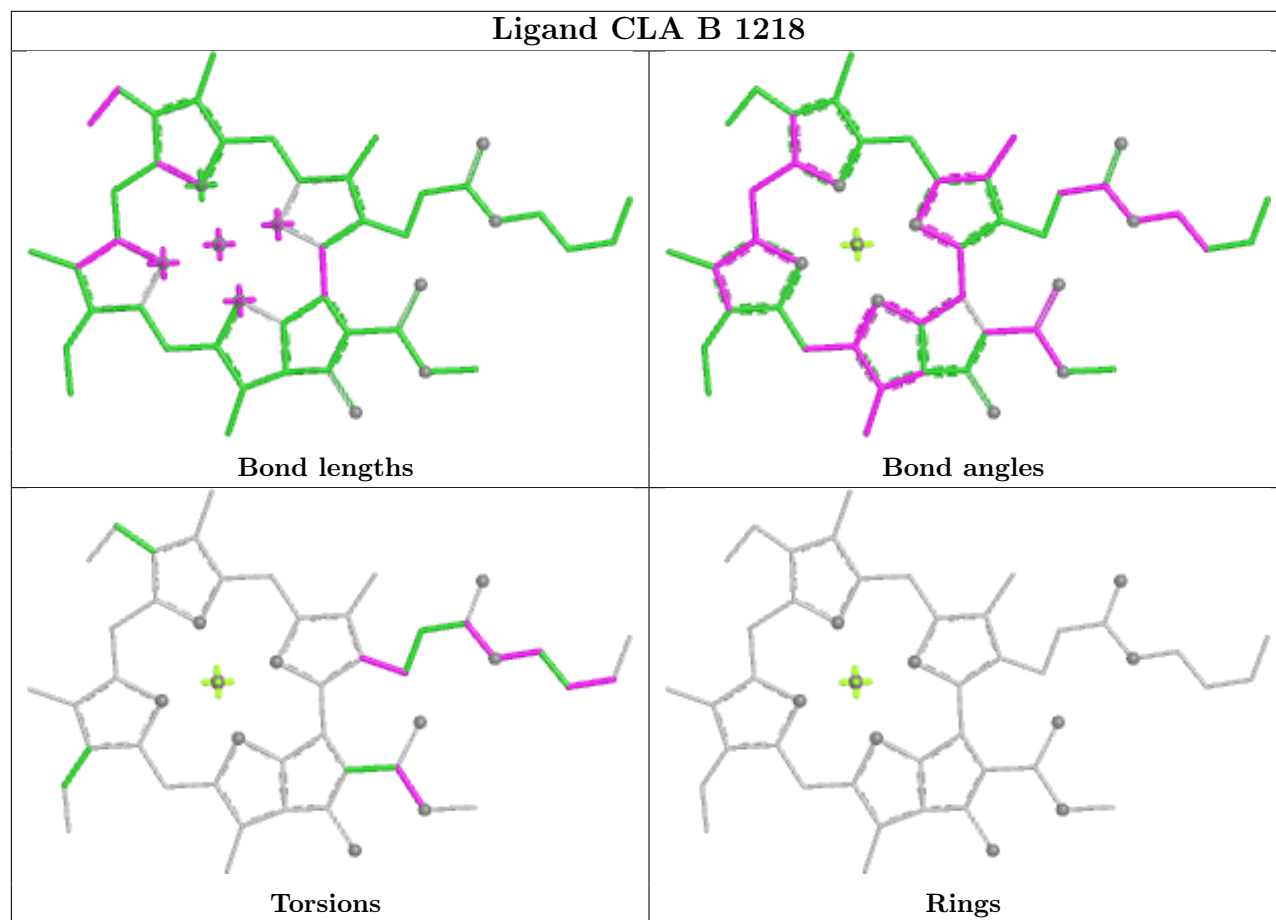
Ligand CLA 2 615



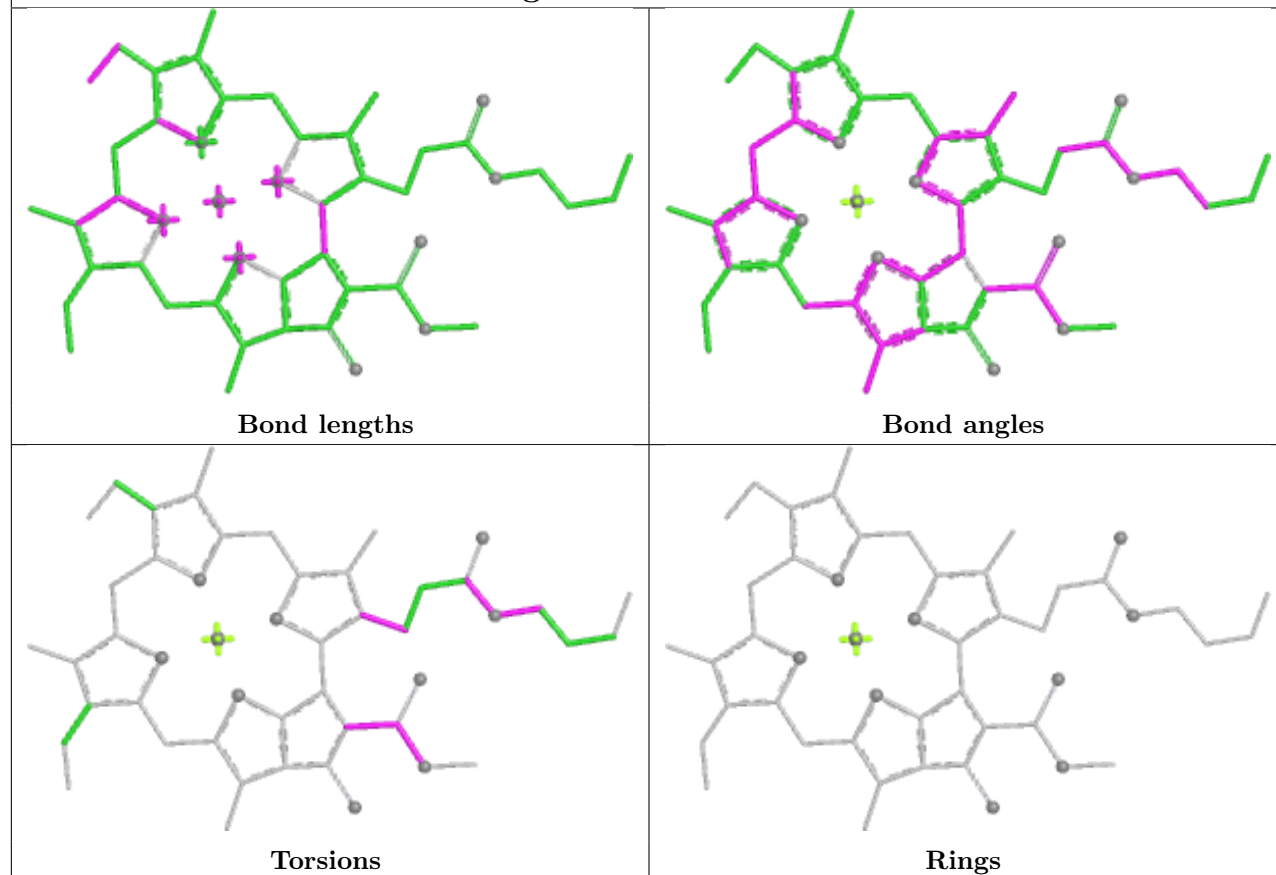




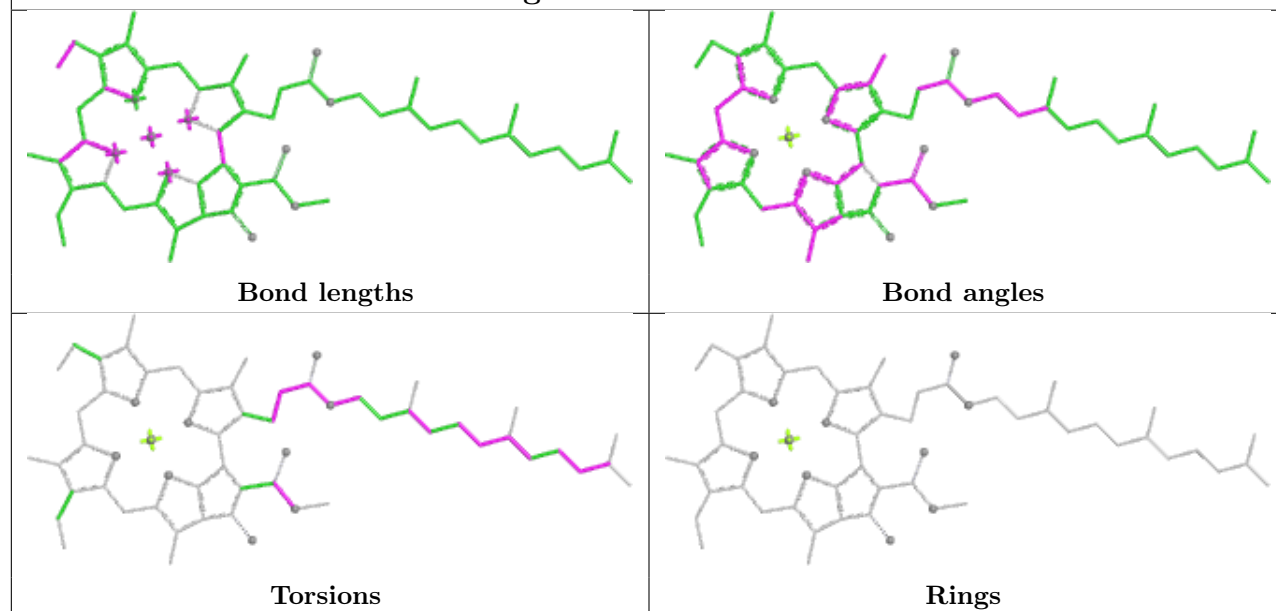


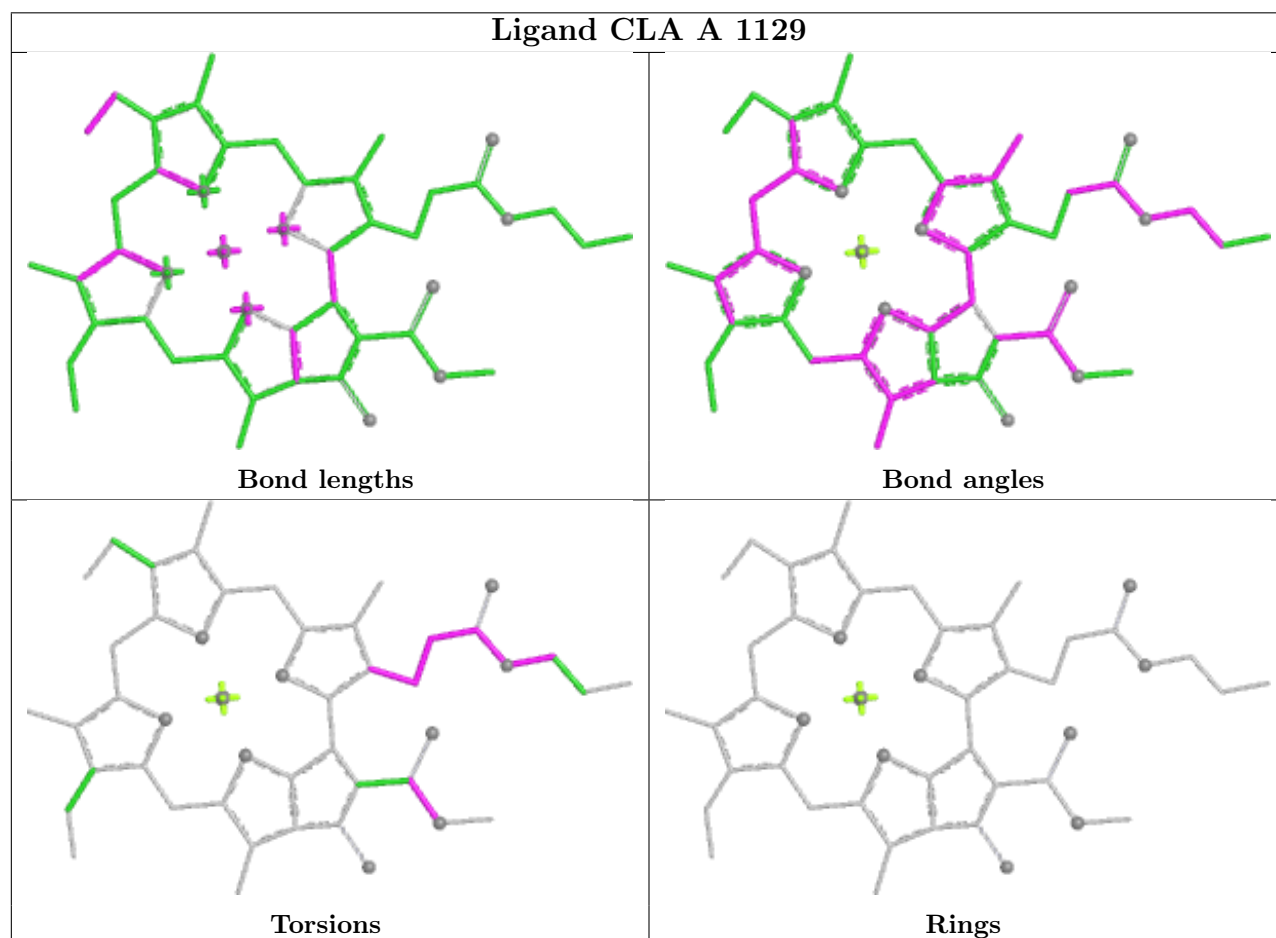
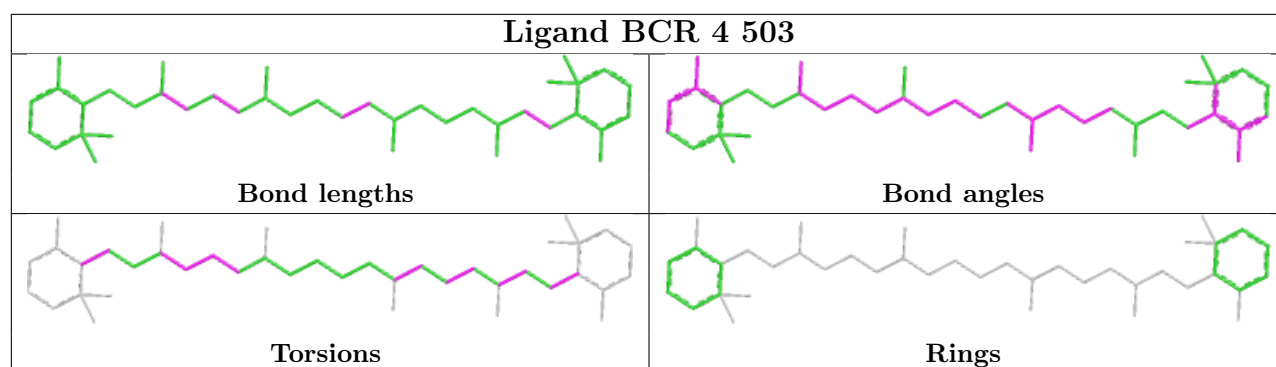


Ligand CLA A 1112

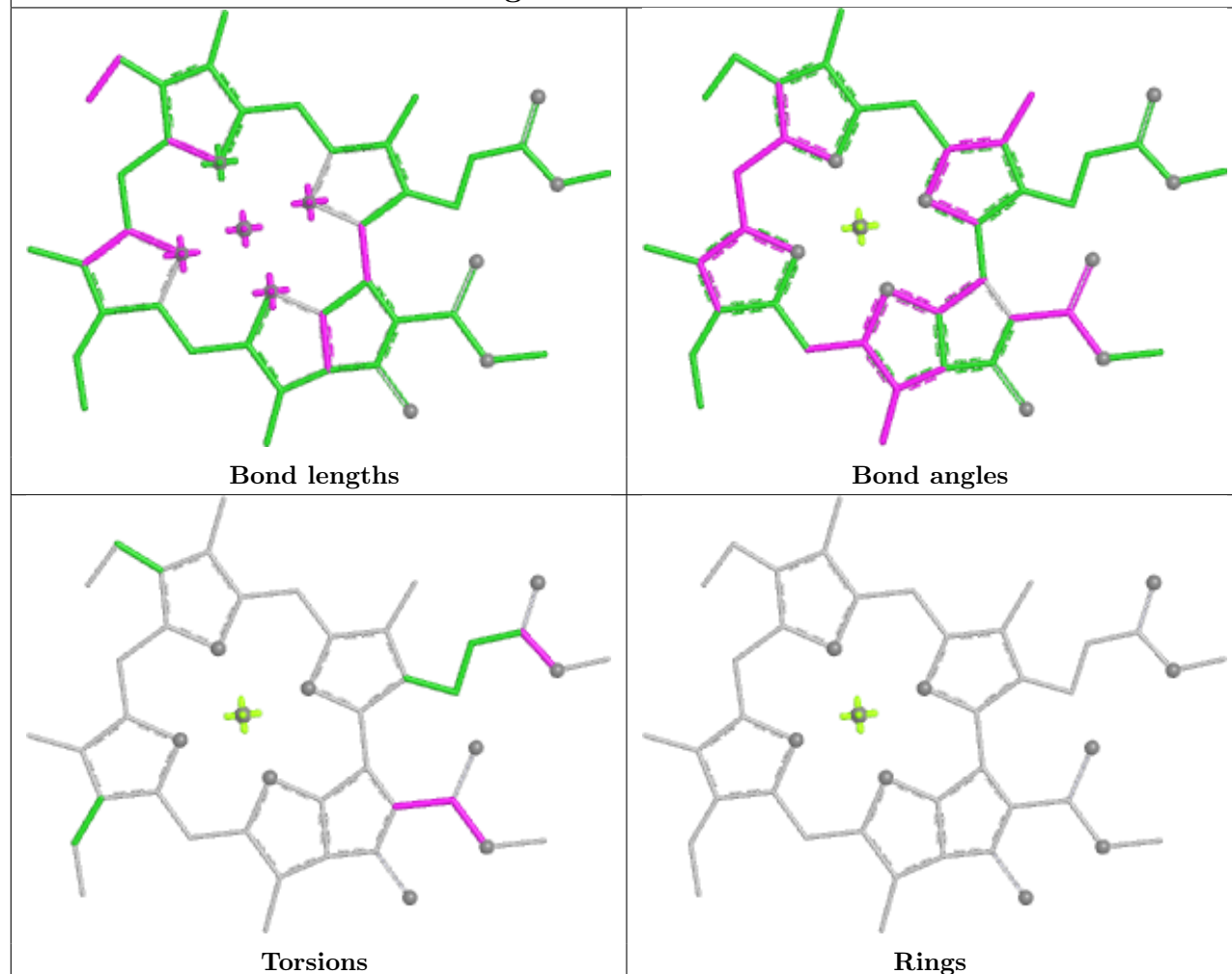


Ligand CLA B 1235

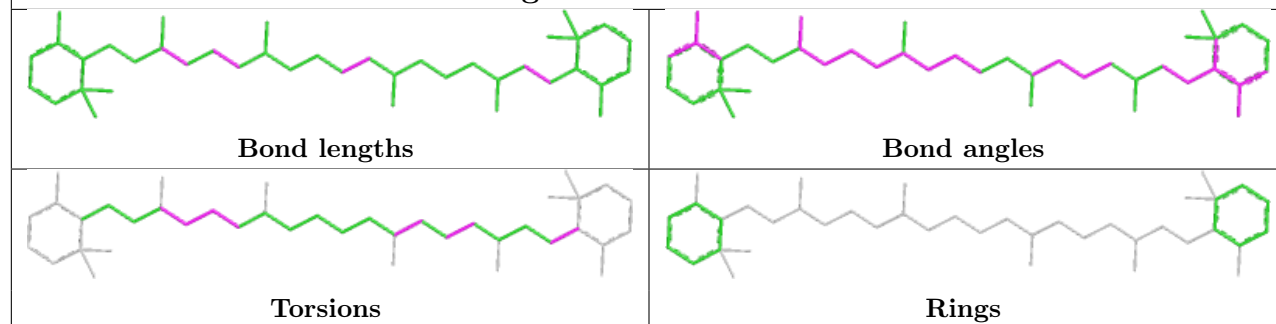




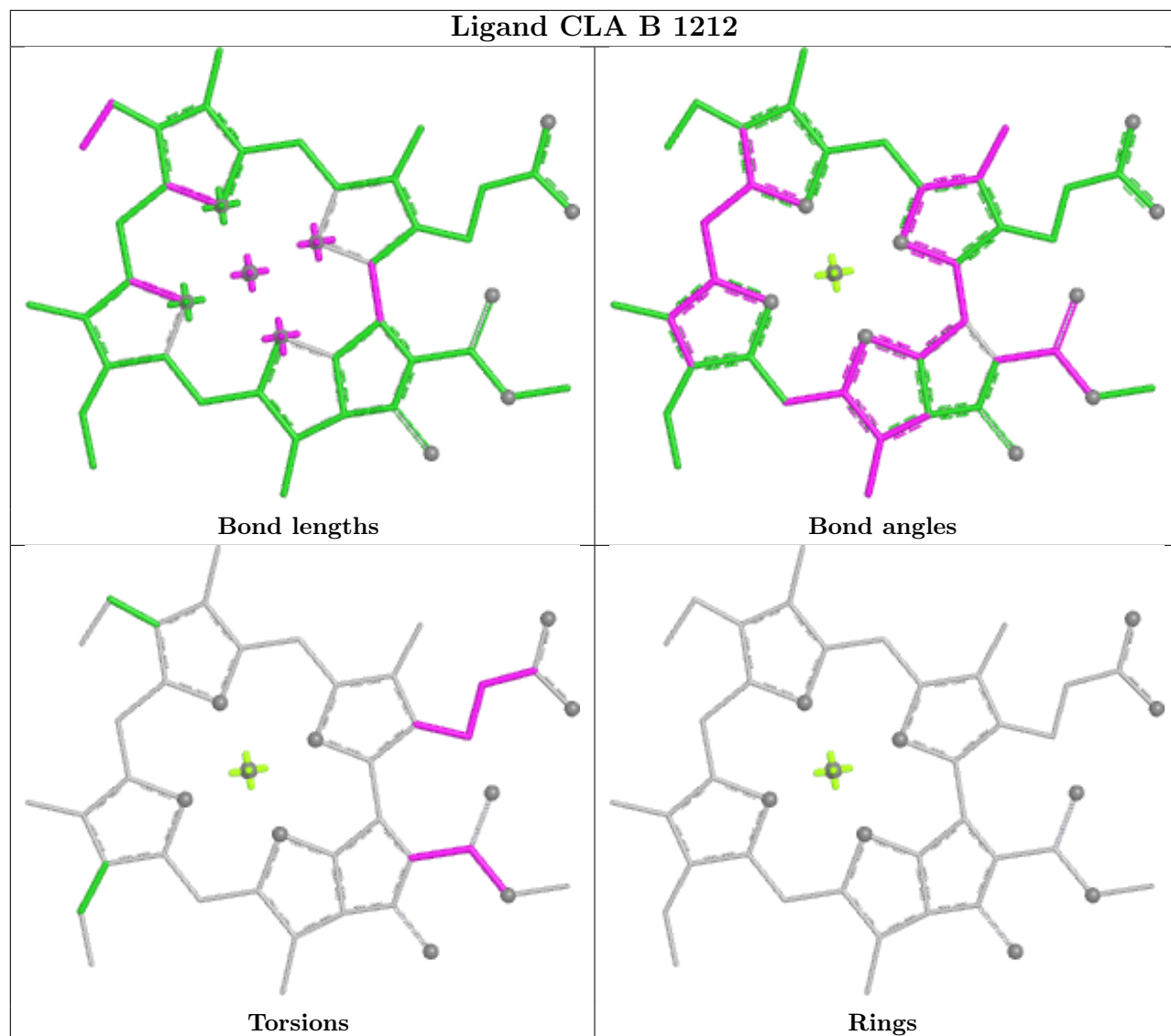
Ligand CLA A 1114

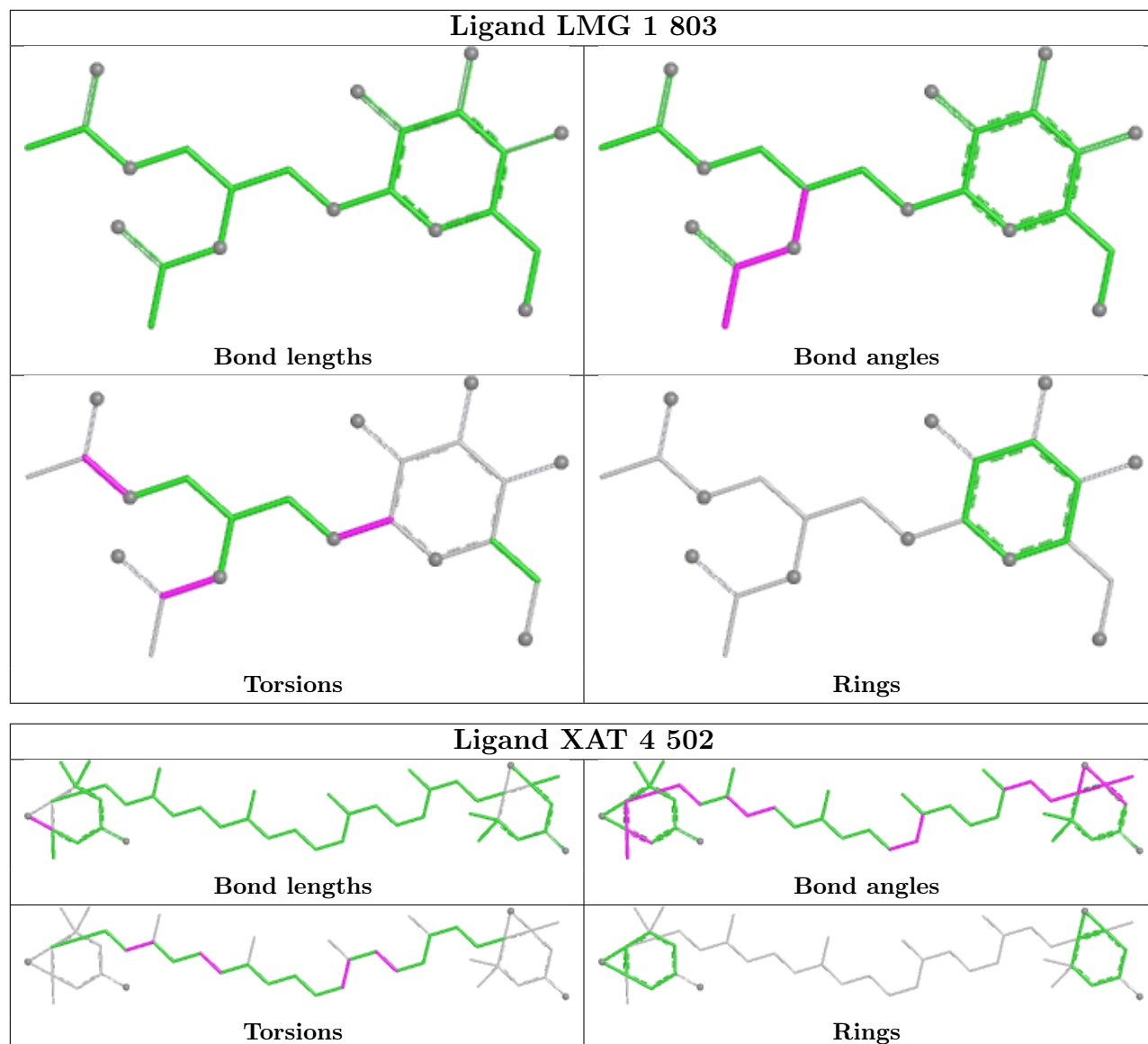


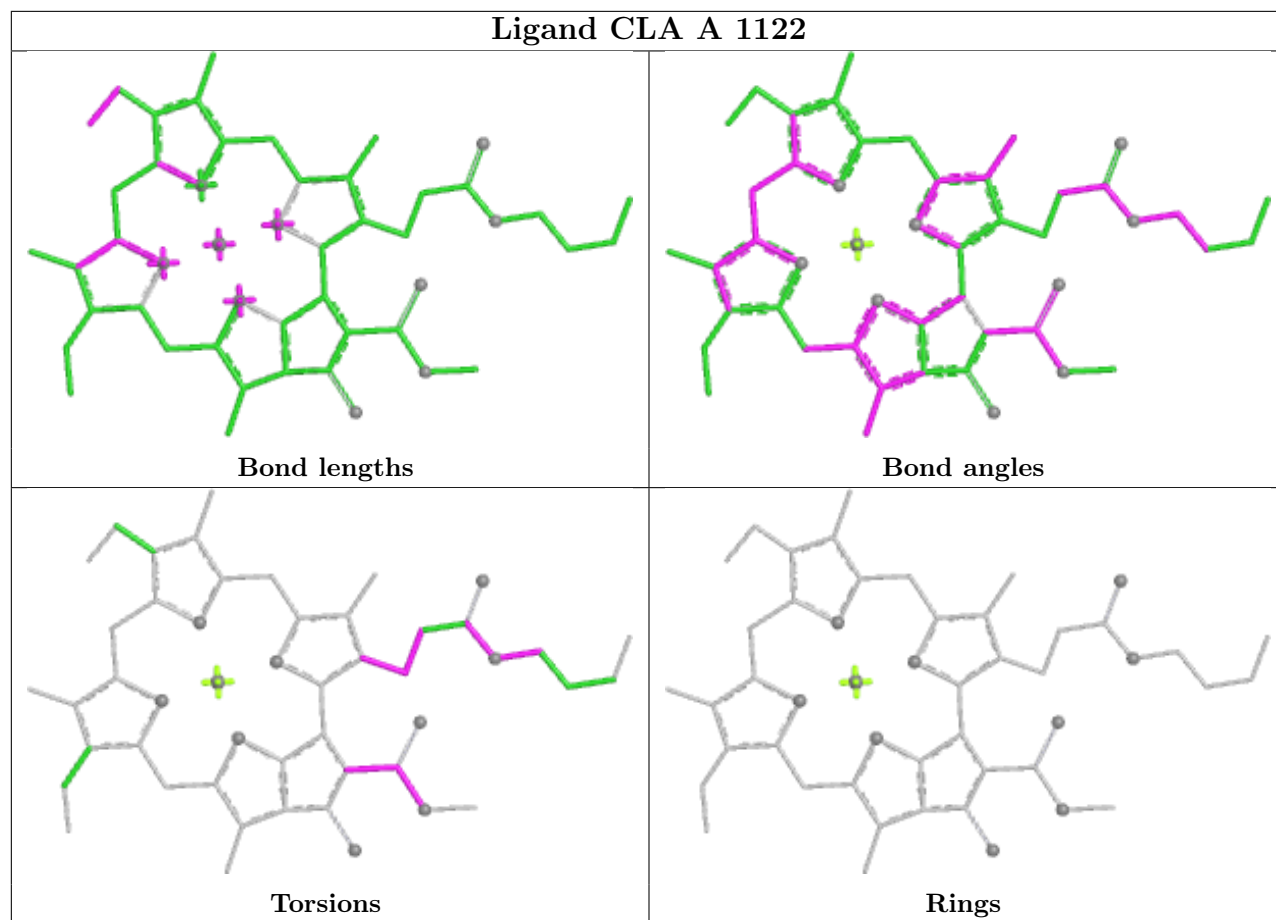
Ligand BCR B 4004

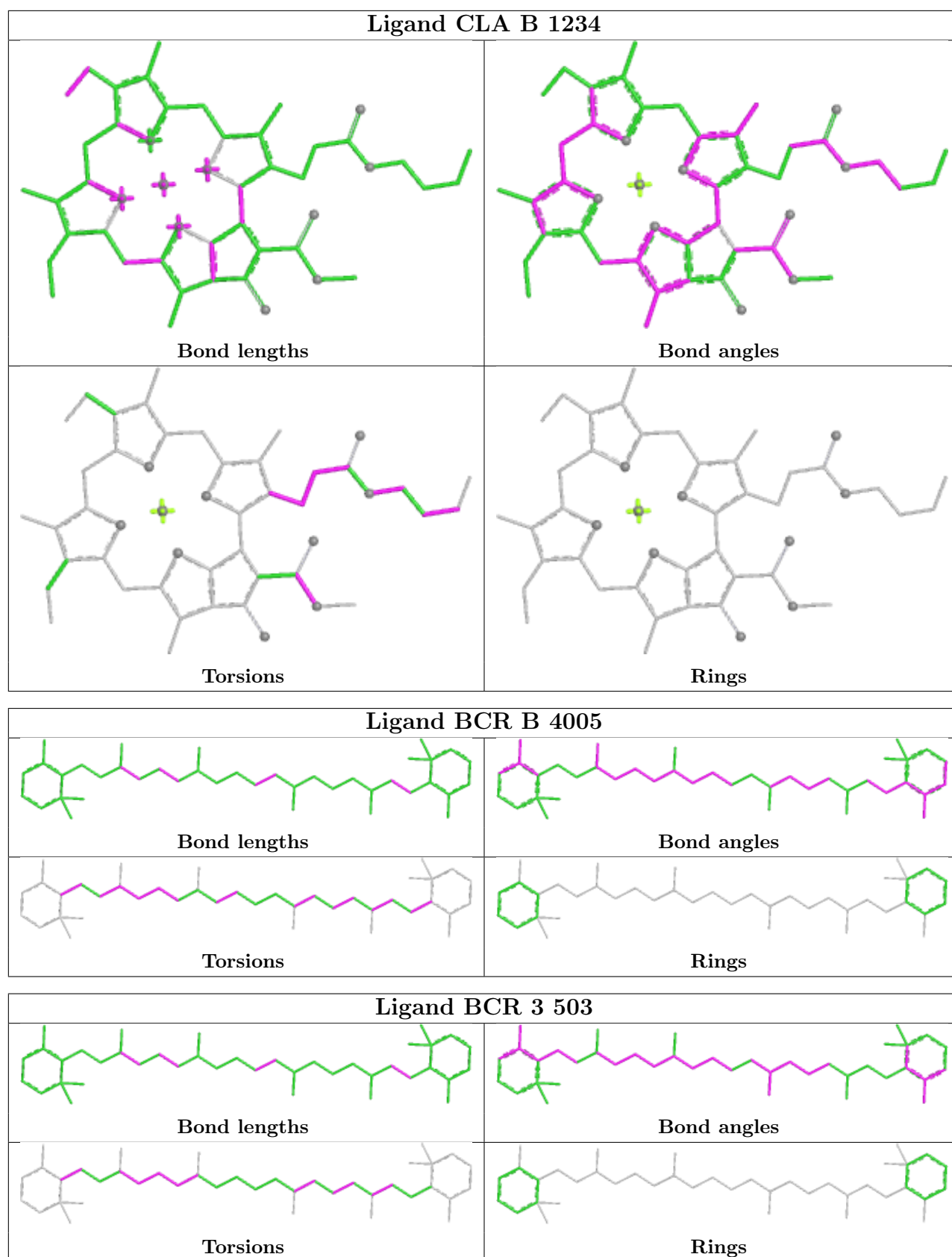


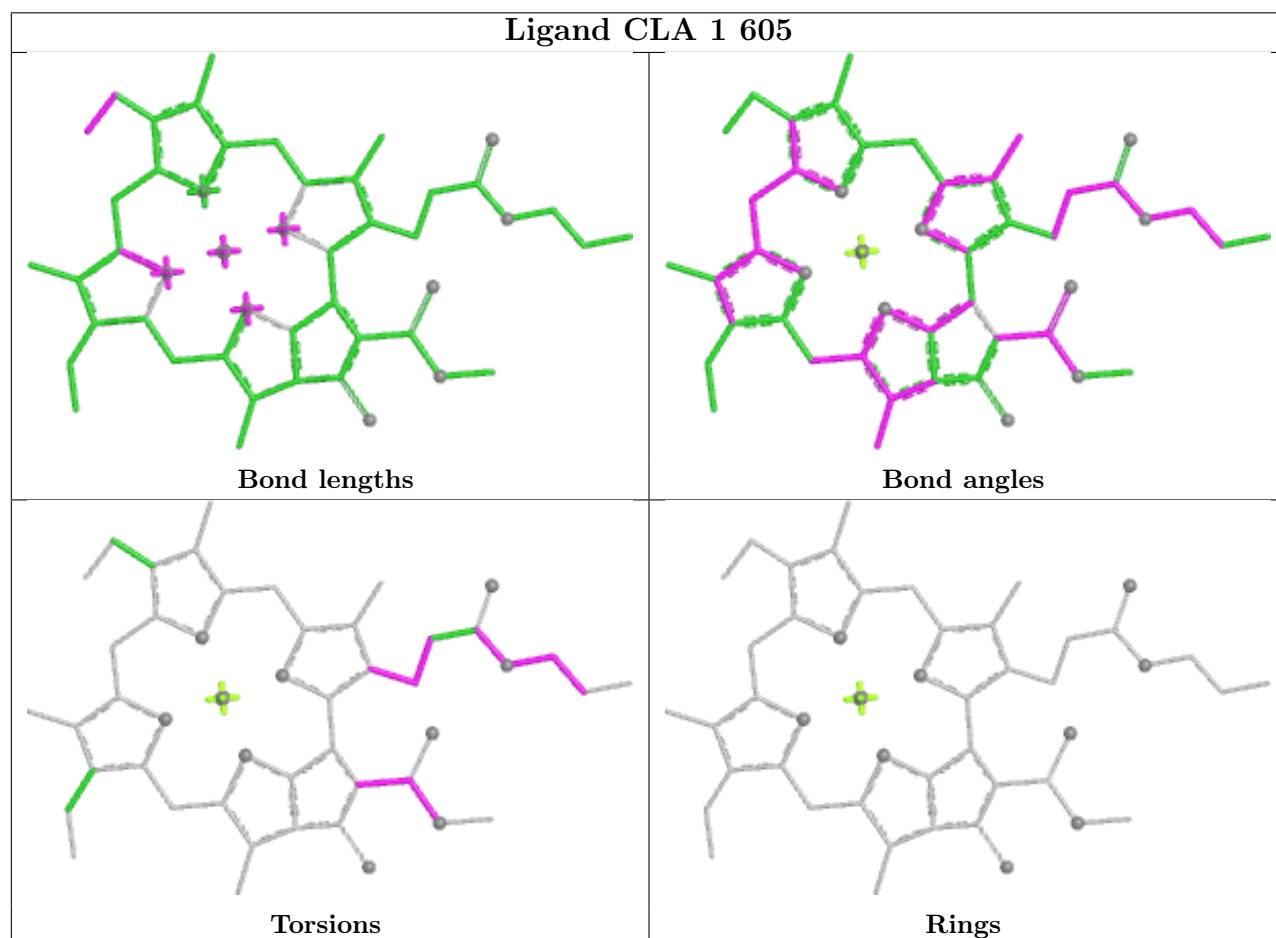
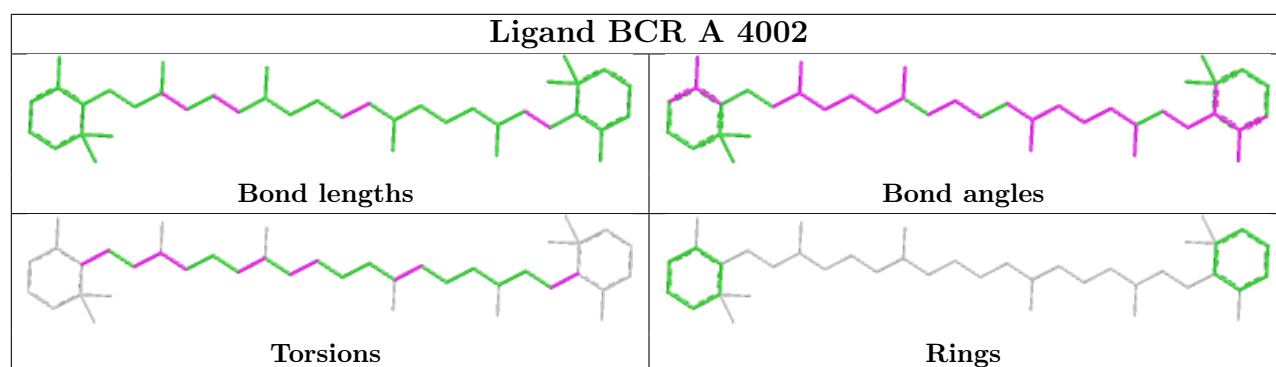
Ligand CLA B 1212



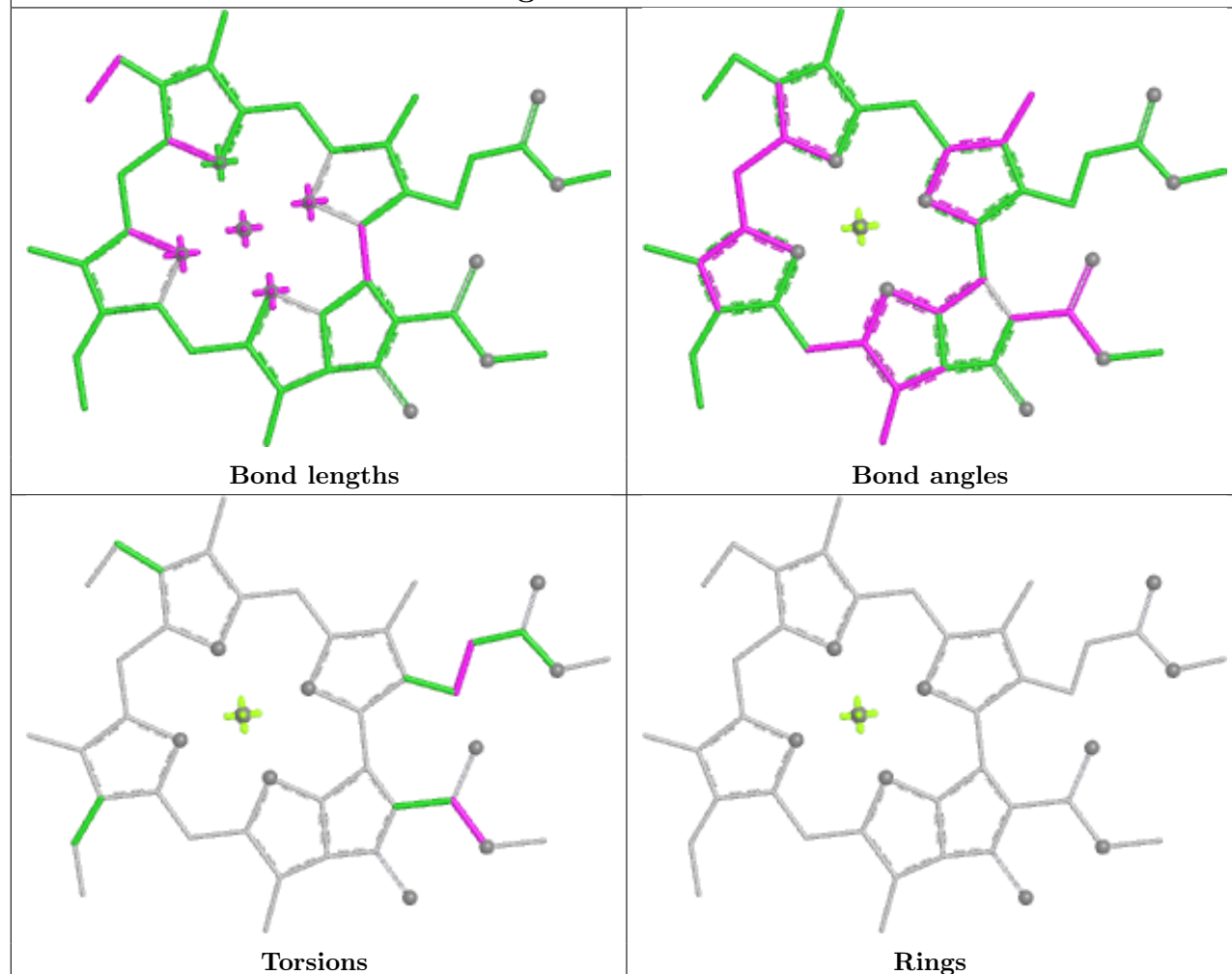




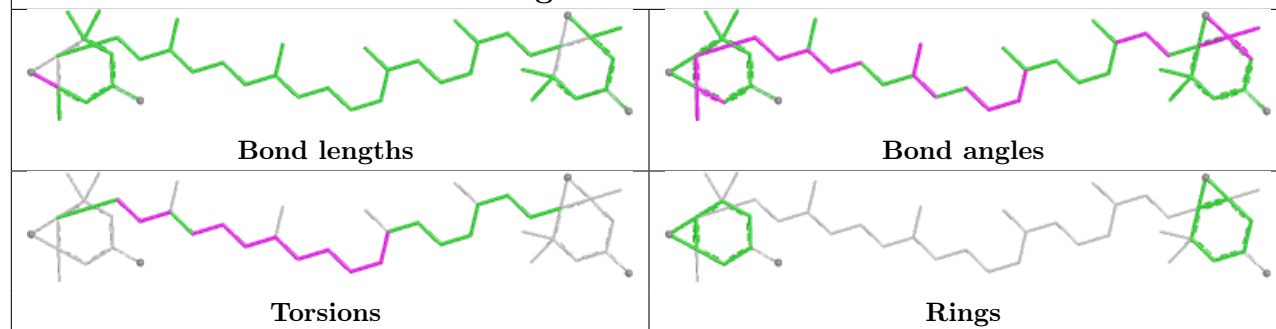




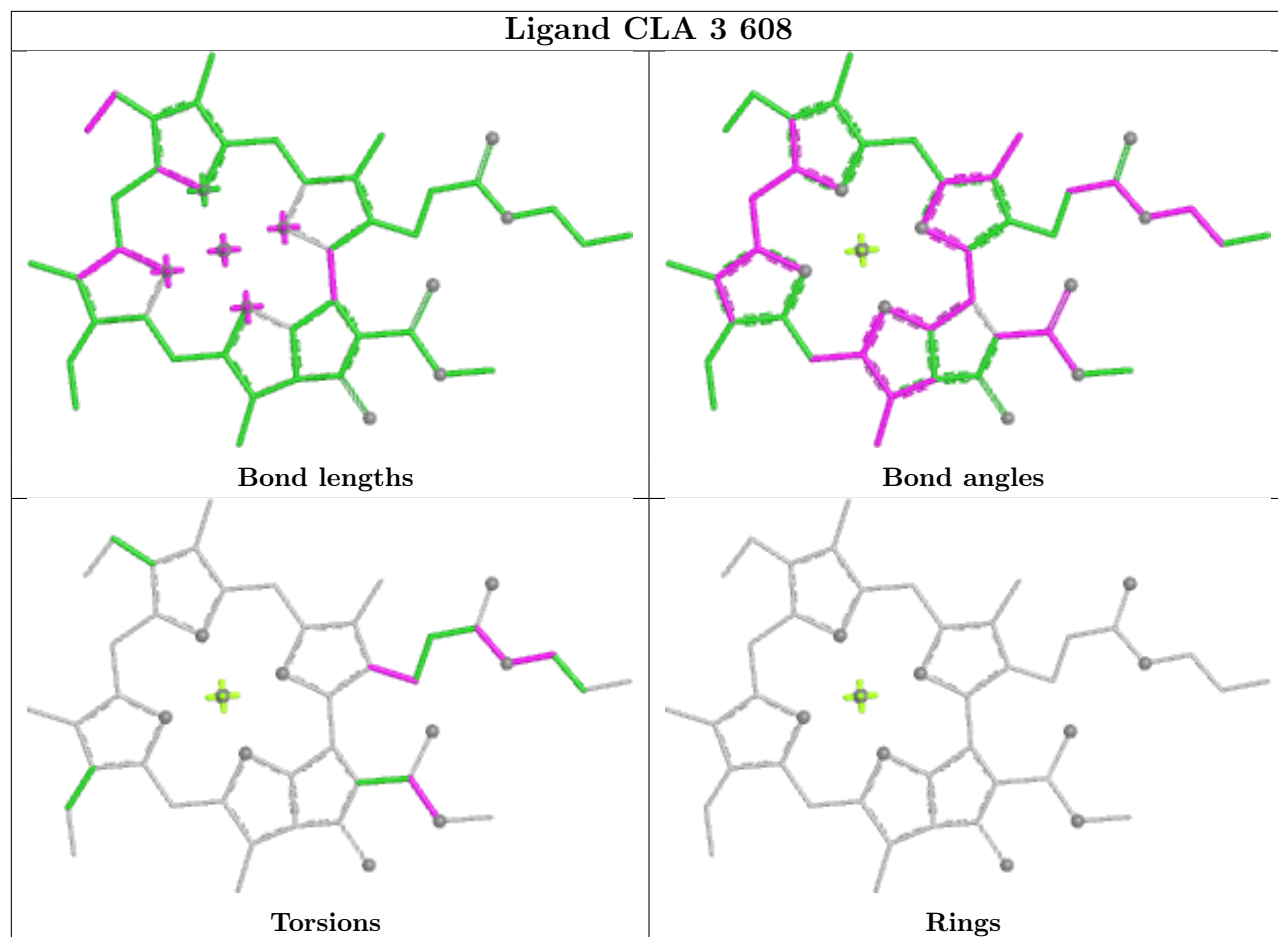
Ligand CLA 2 603

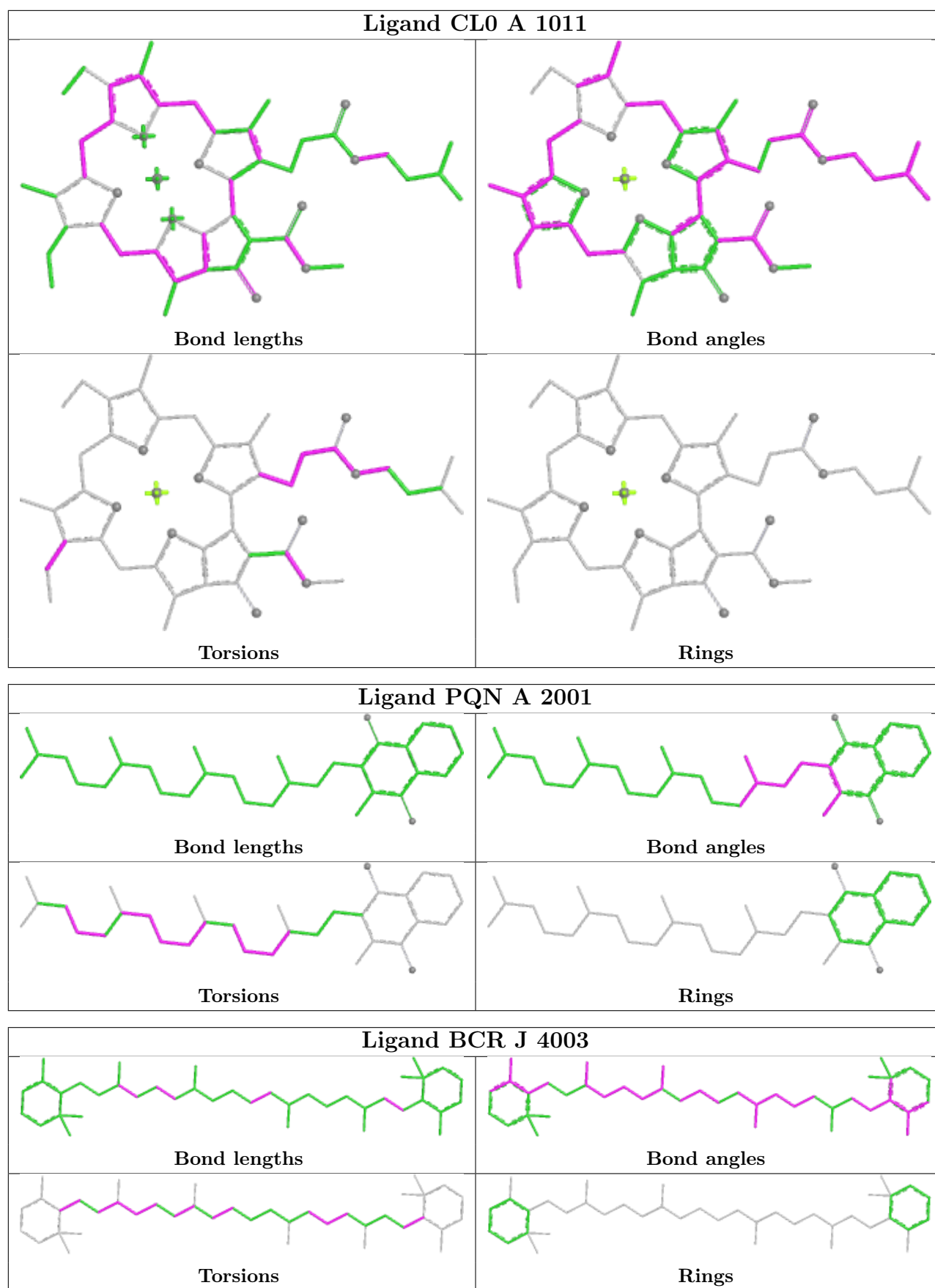


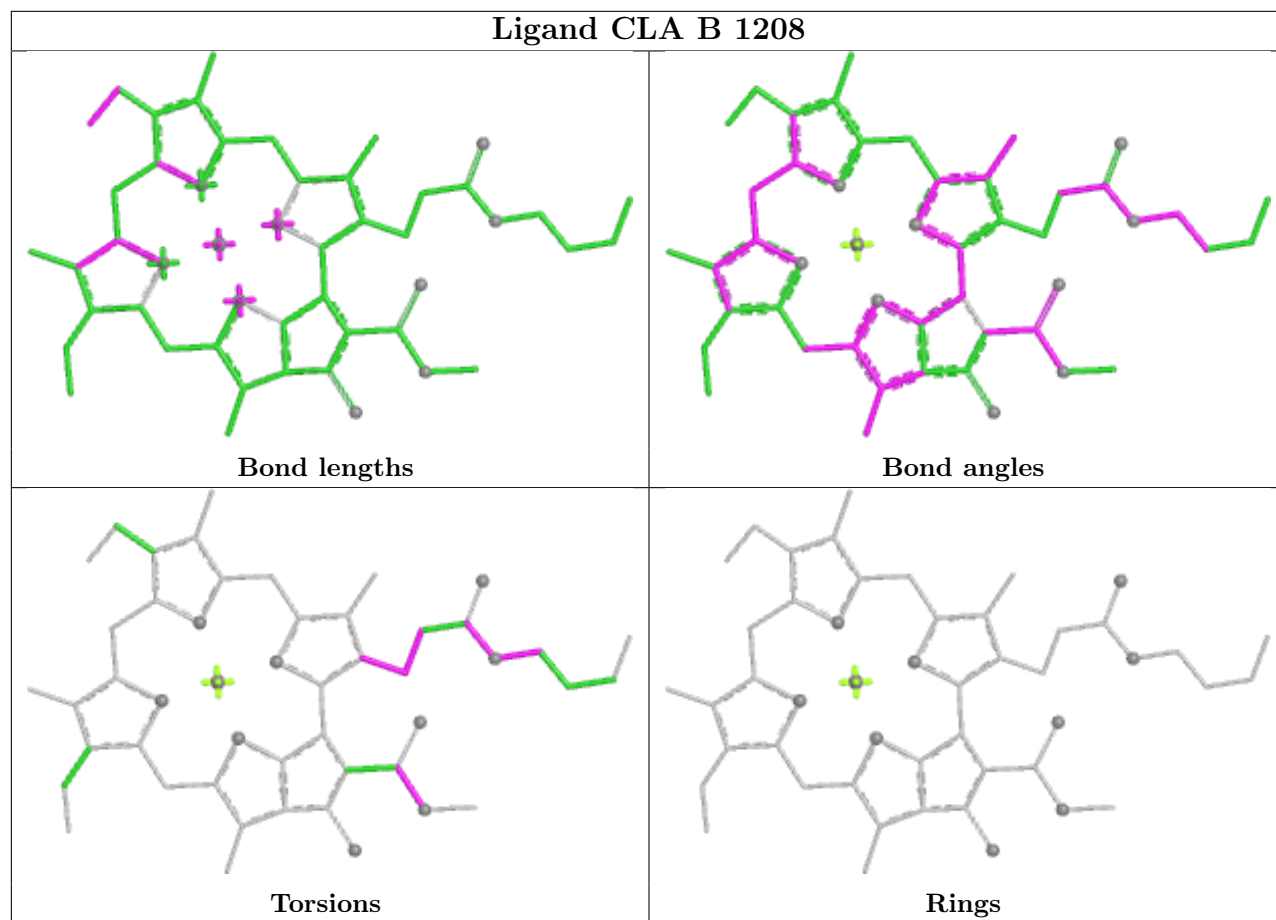
Ligand XAT 3 502



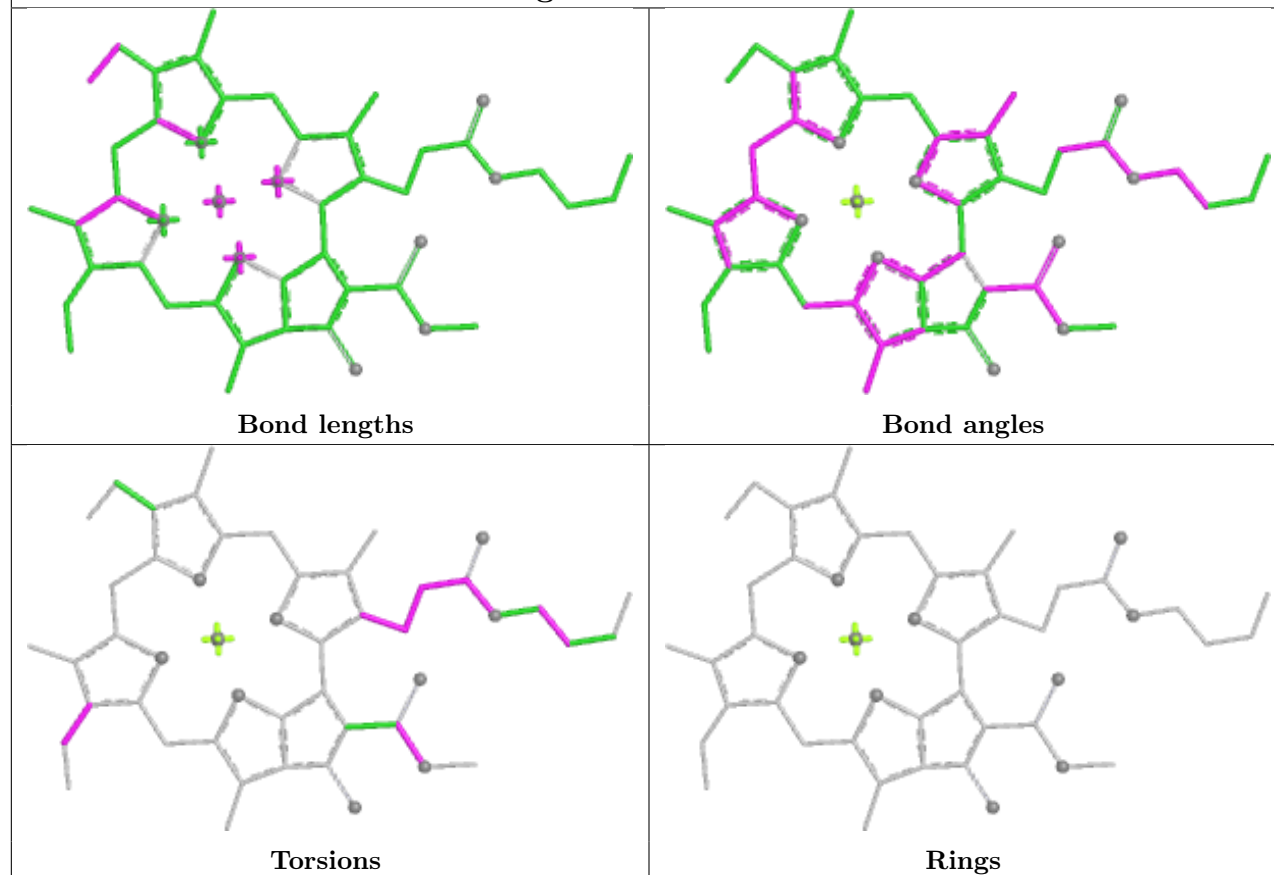
Ligand CLA 3 608



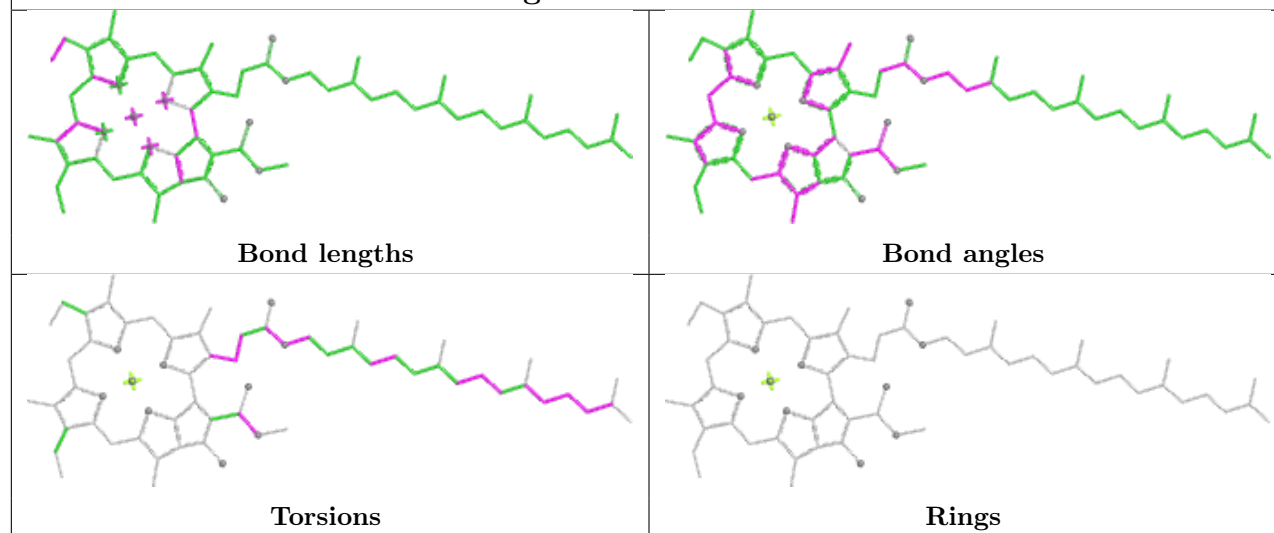




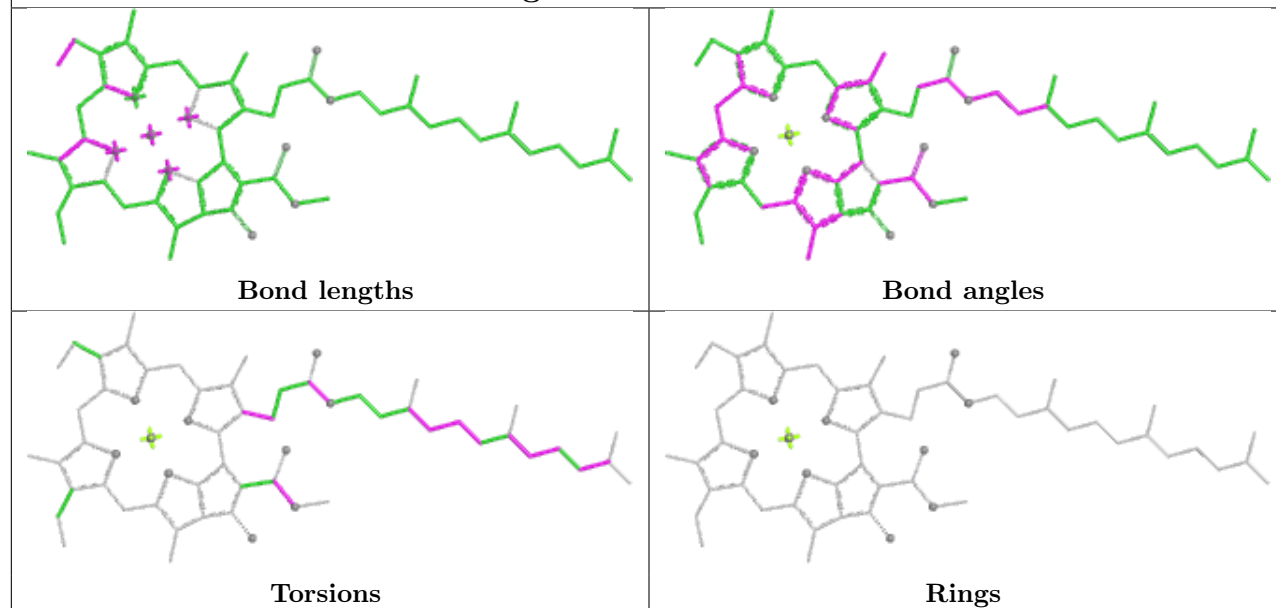
Ligand CLA 3 601



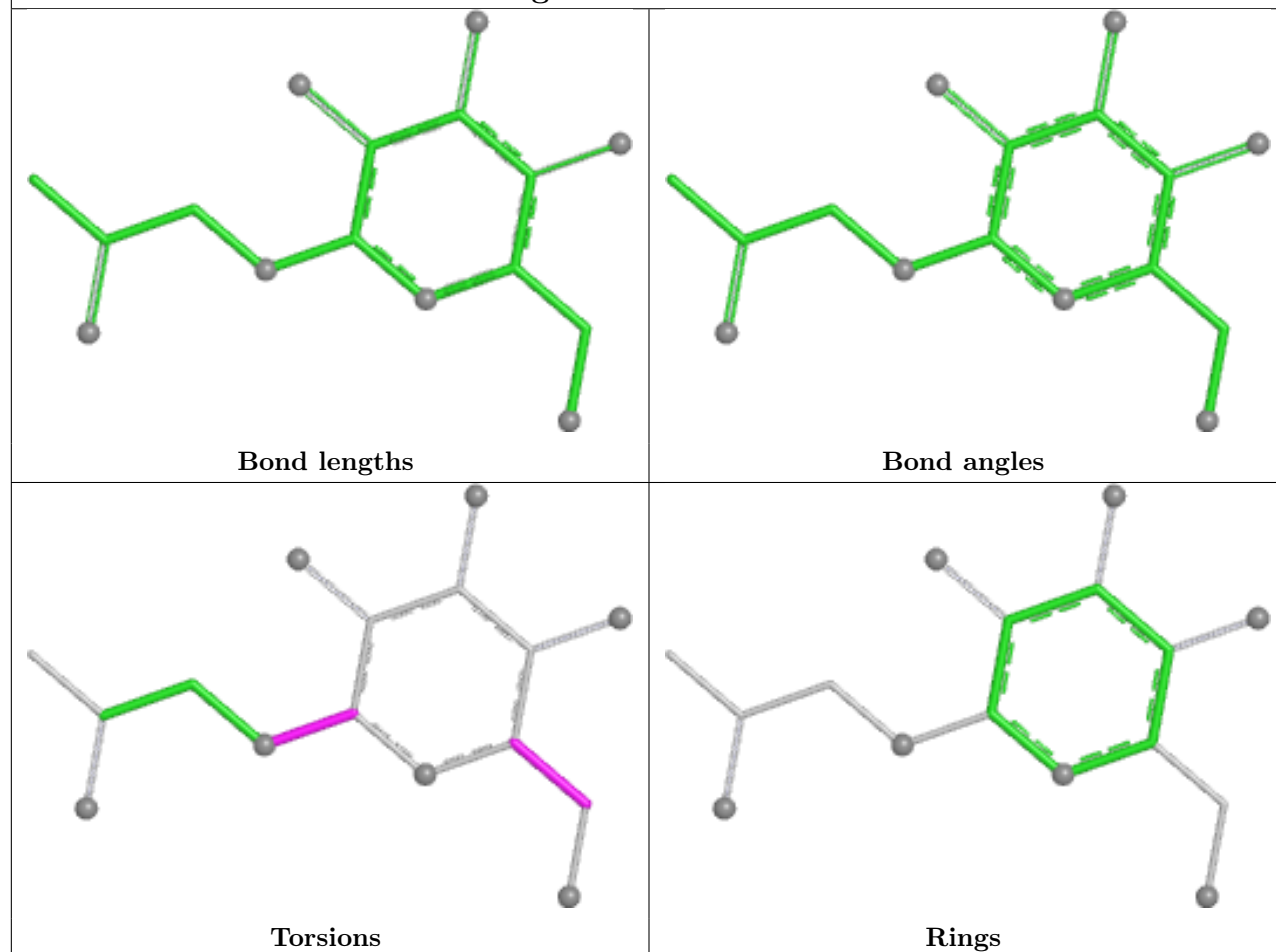
Ligand CLA B 1239



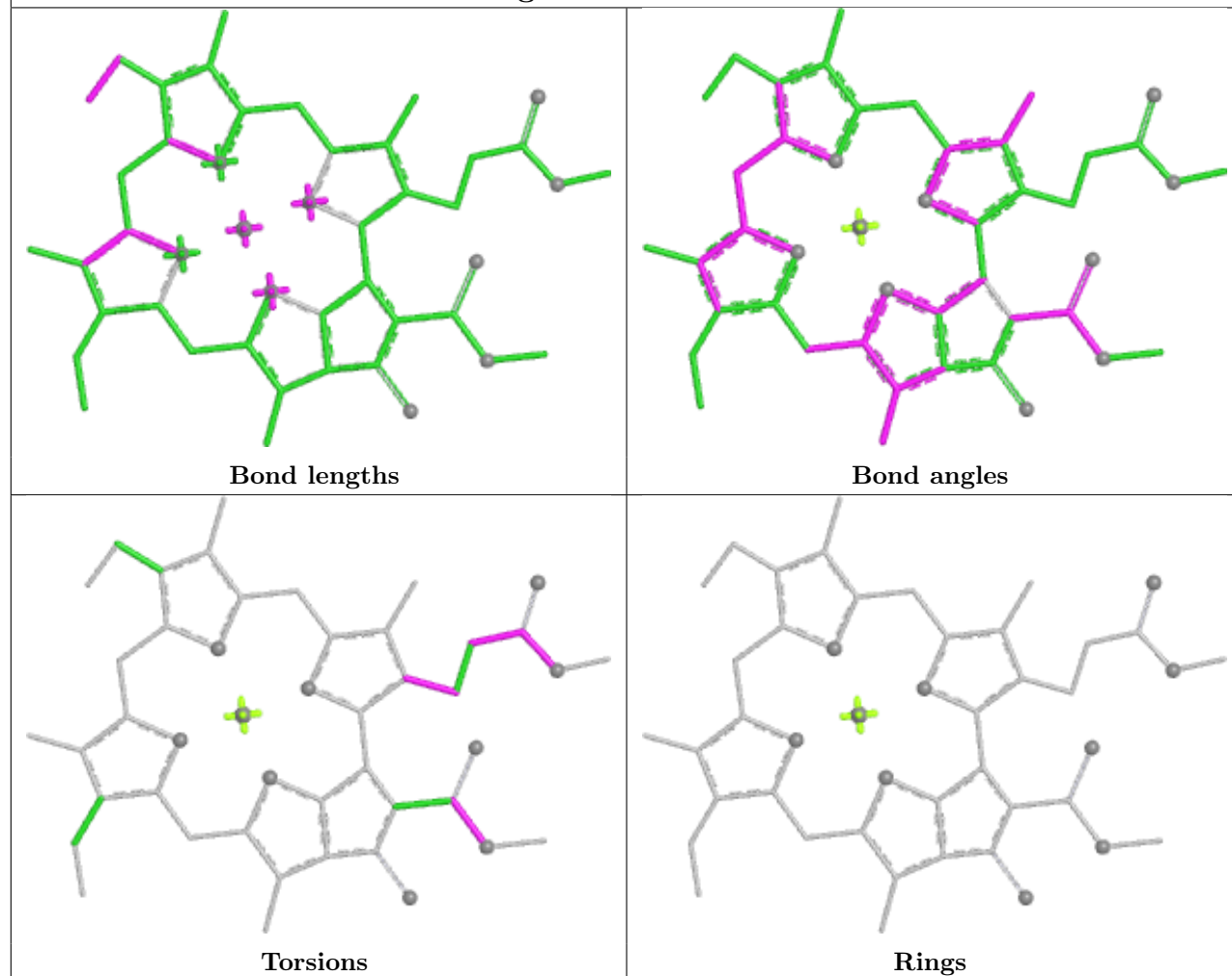
Ligand CLA A 1104

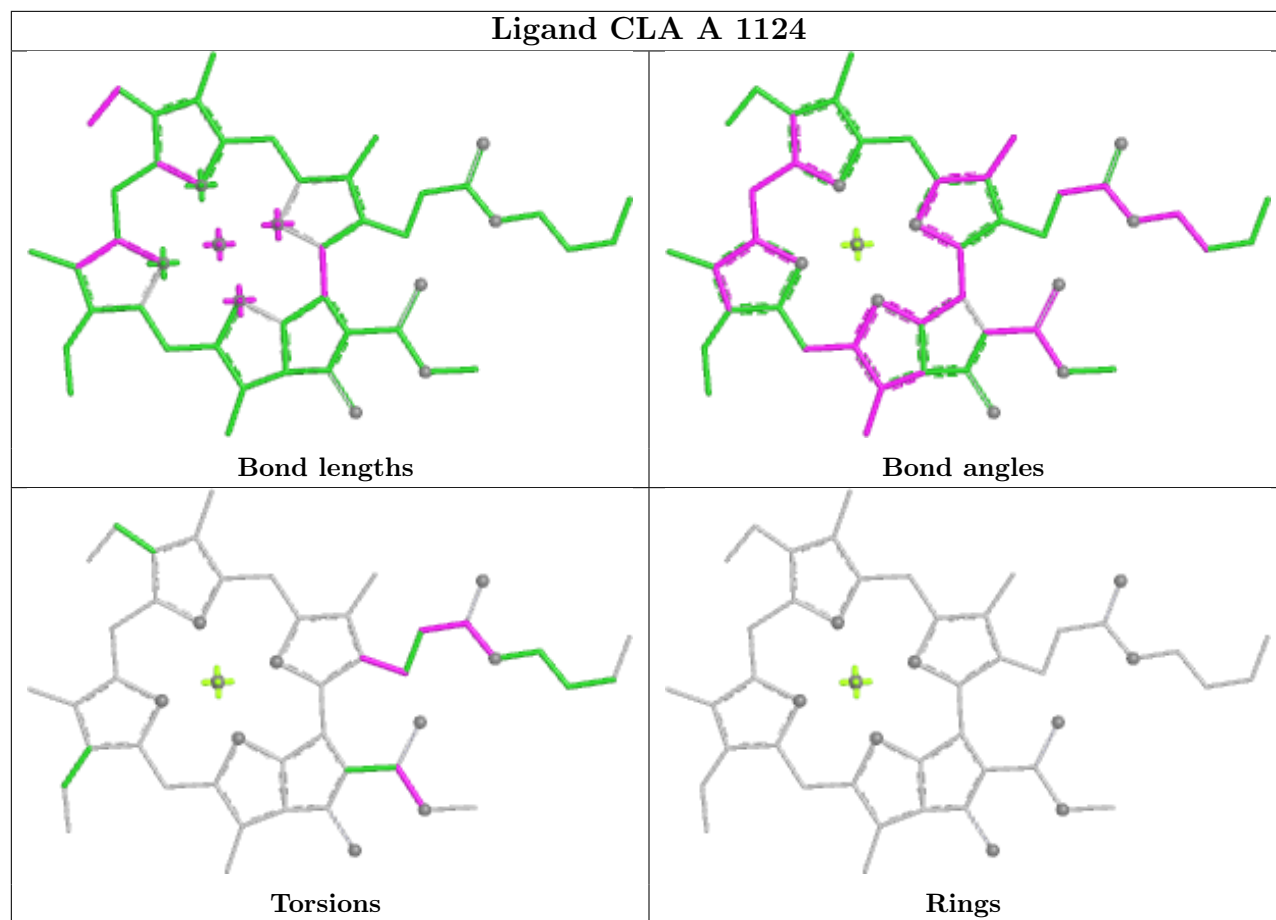


Ligand LMG 2 803

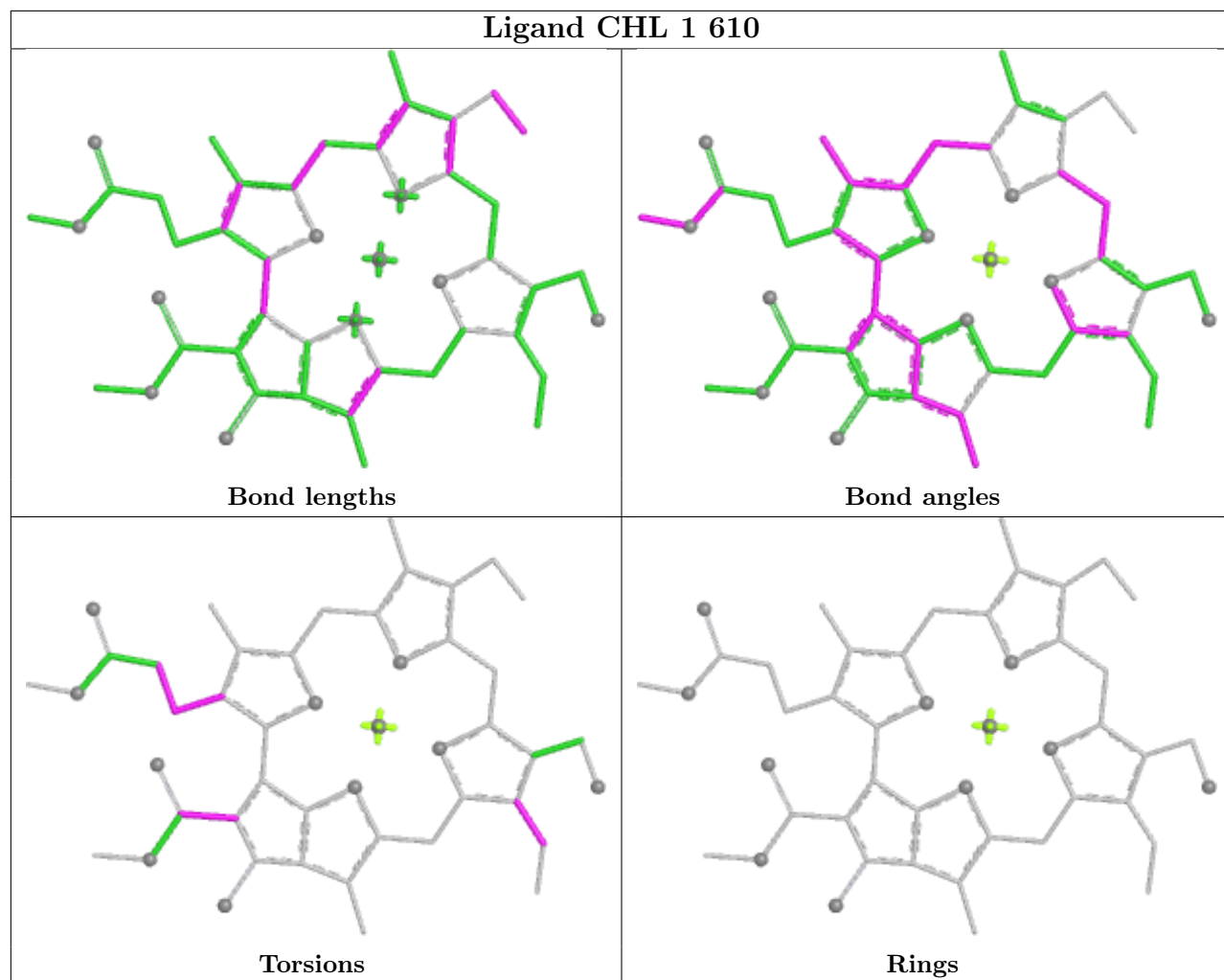


Ligand CLA 3 613

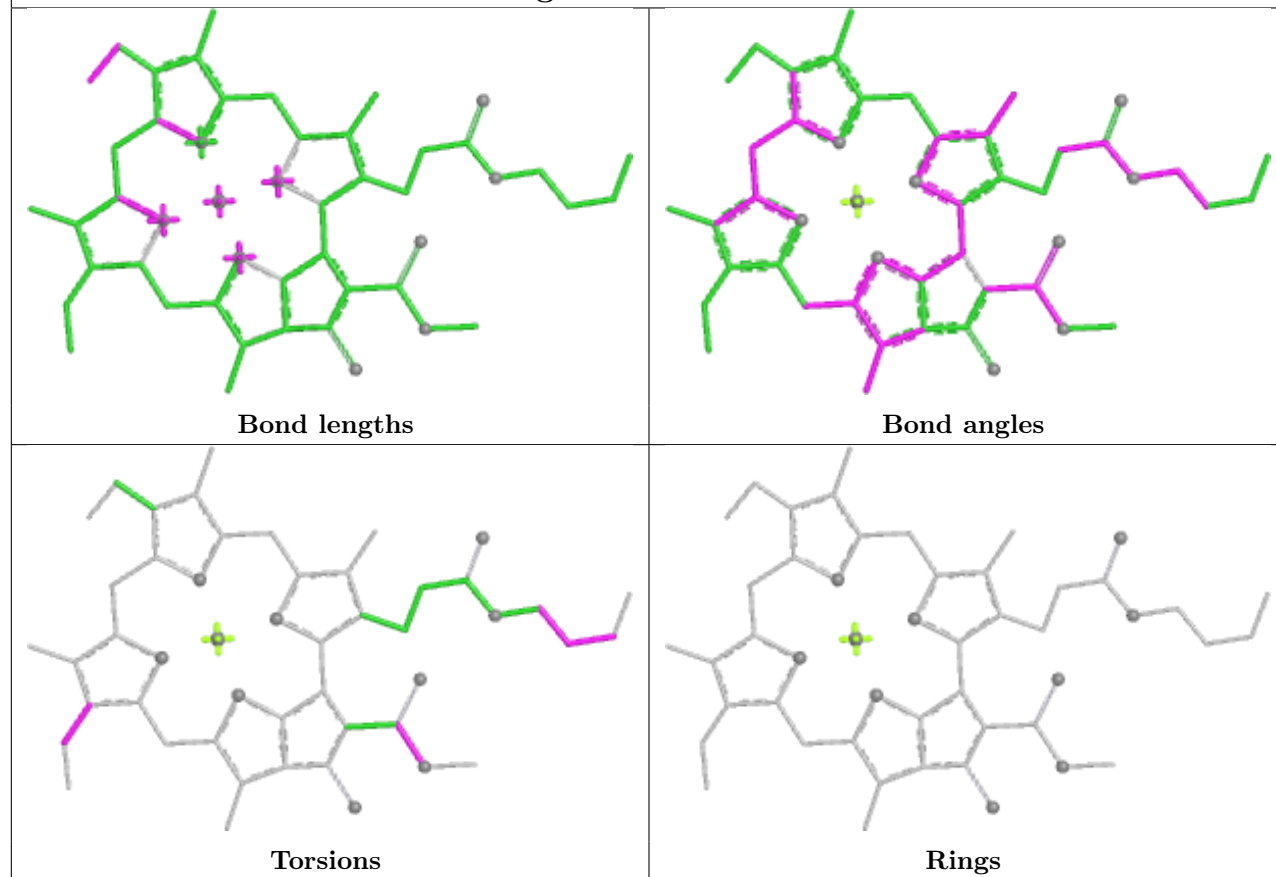




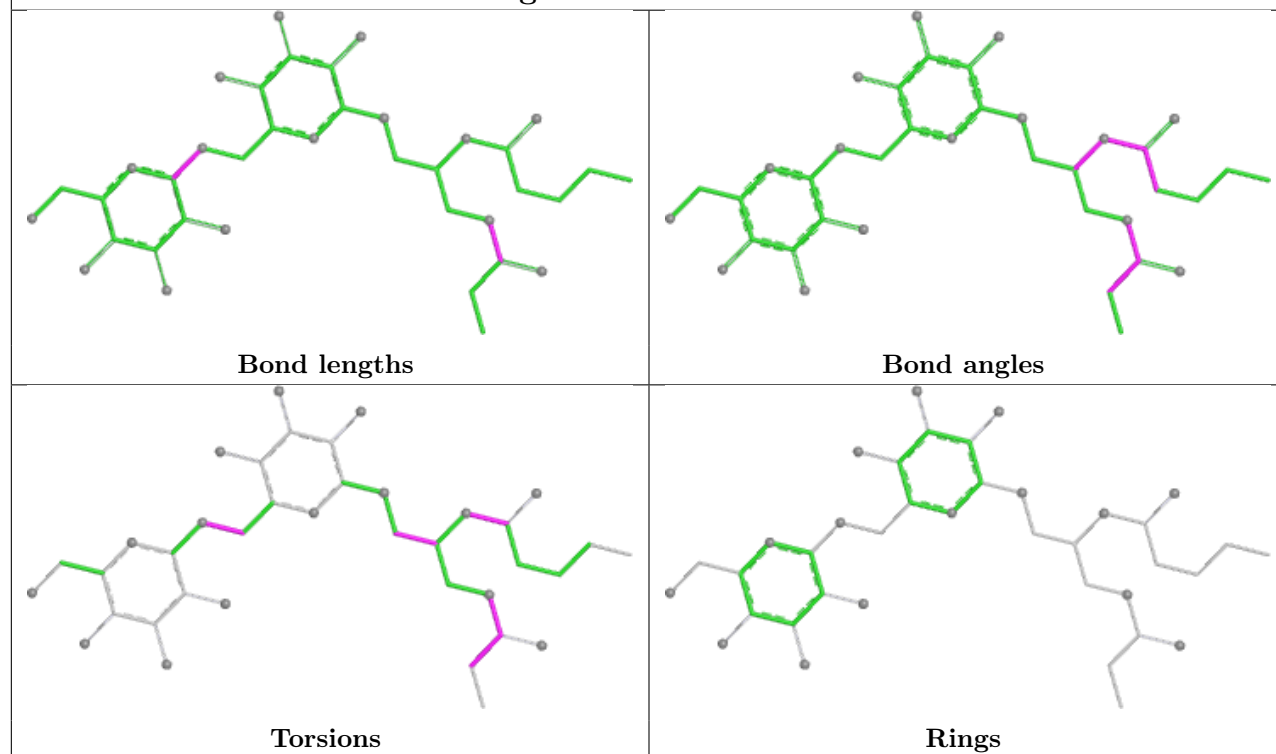
Ligand CHL 1 610



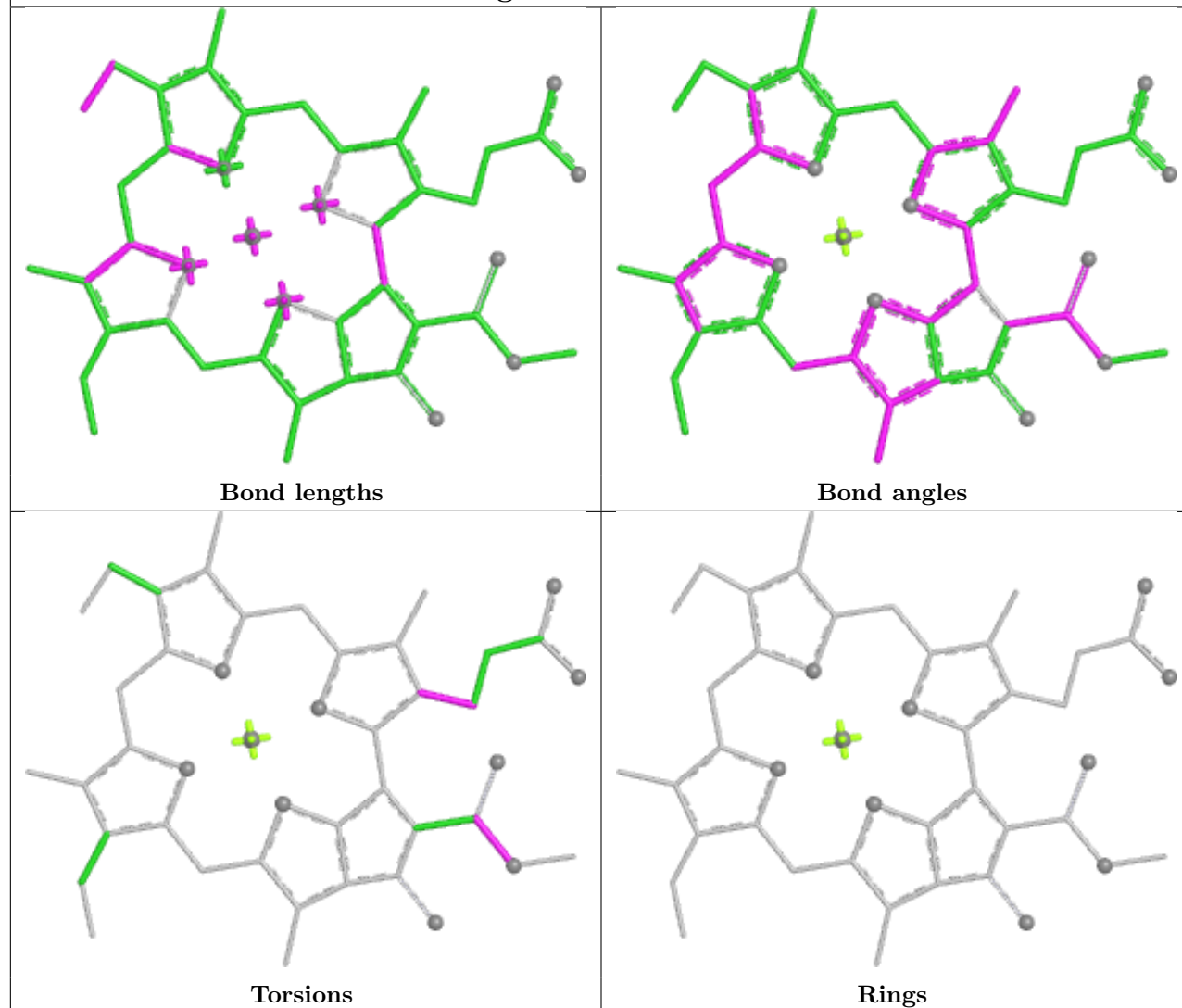
Ligand CLA 4 602



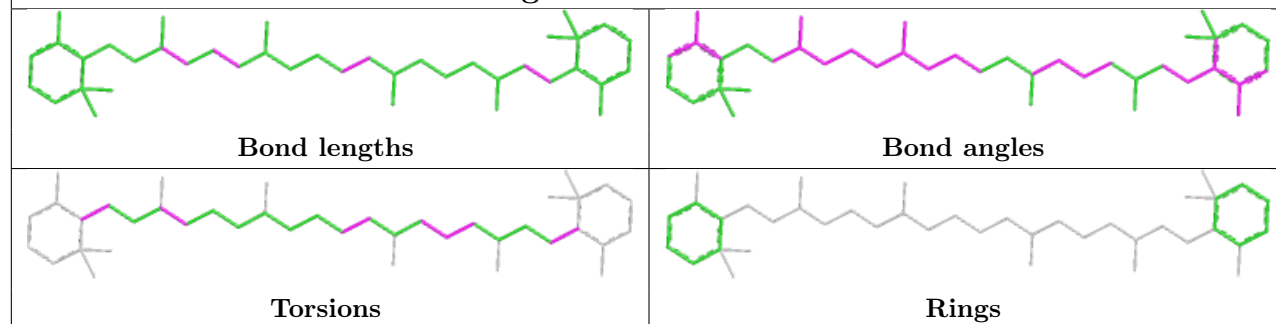
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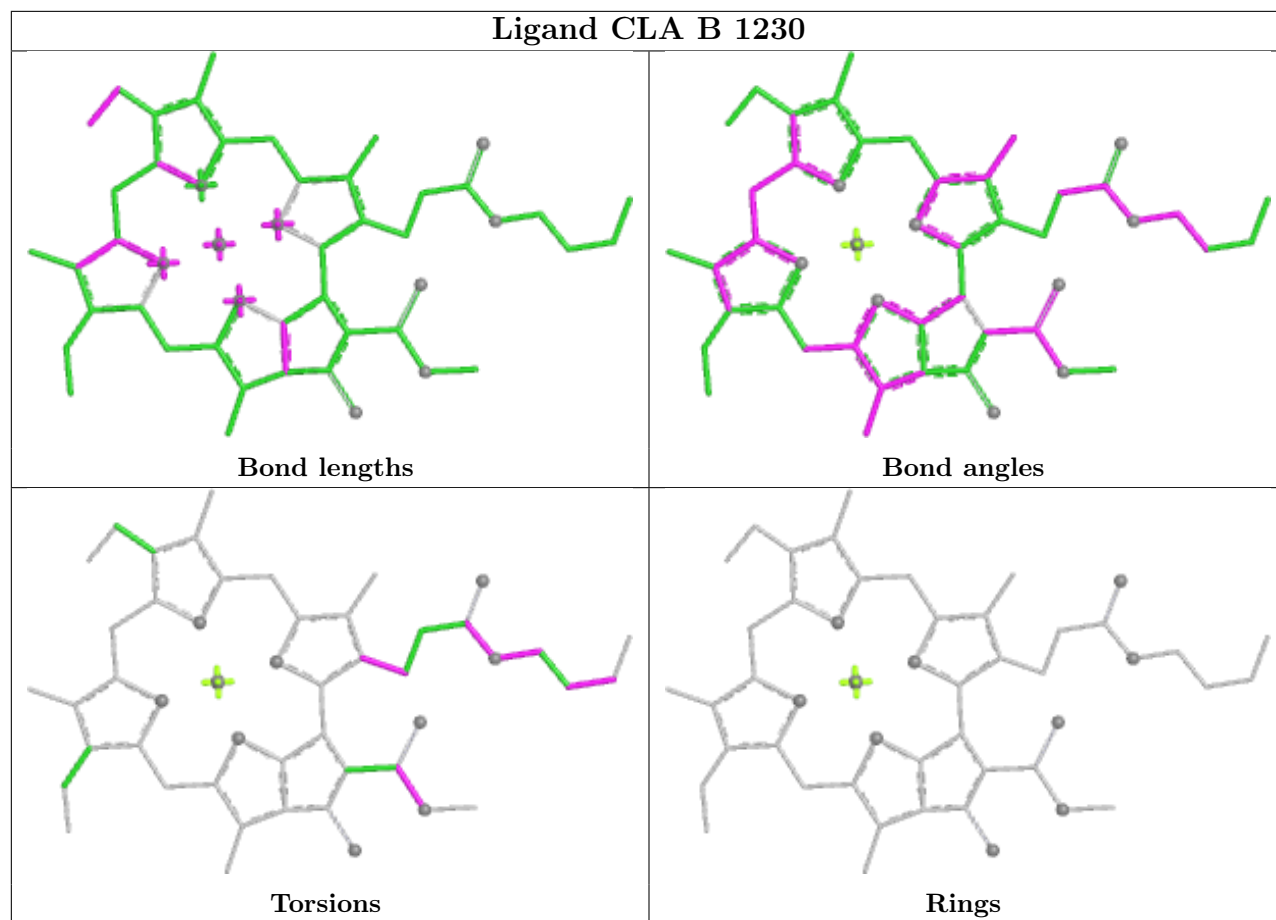


Ligand CLA 1 613

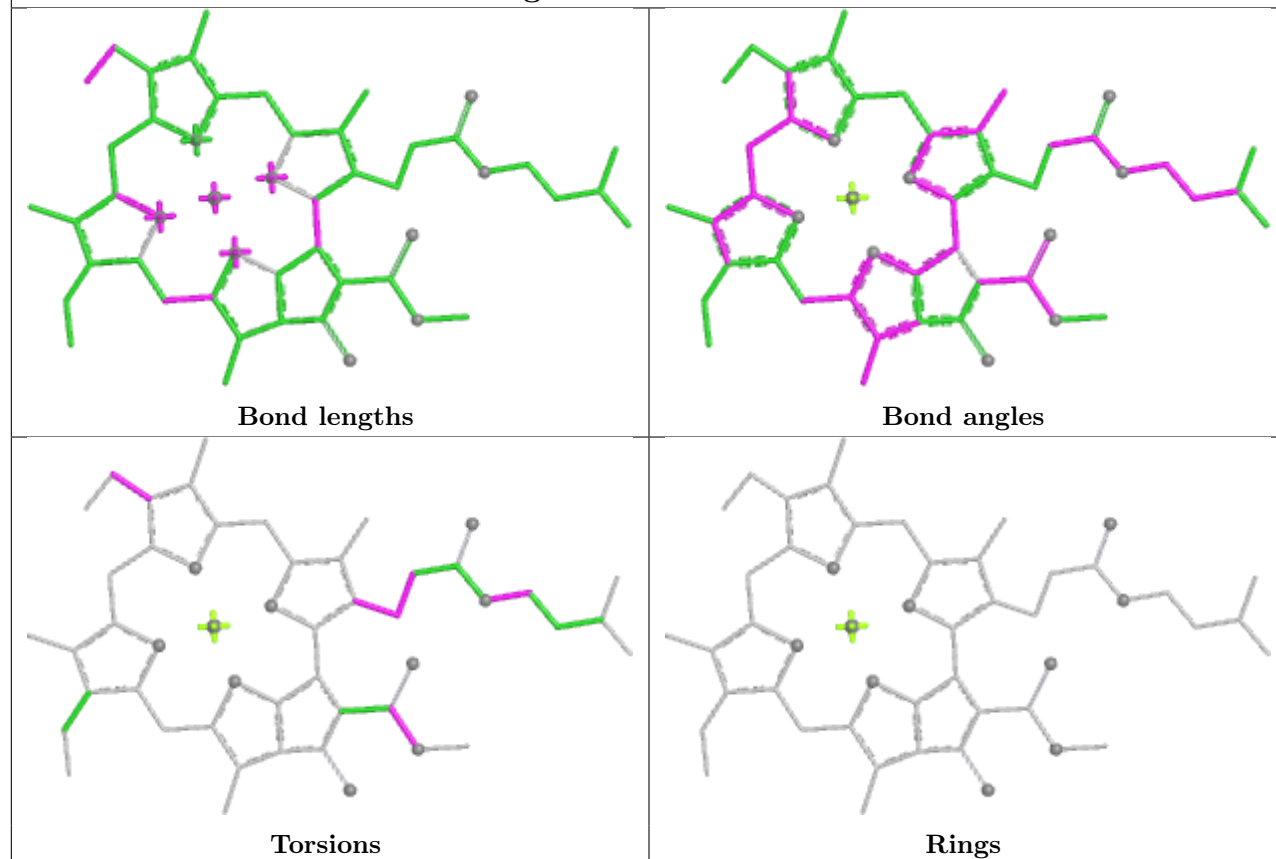


Ligand BCR B 4003

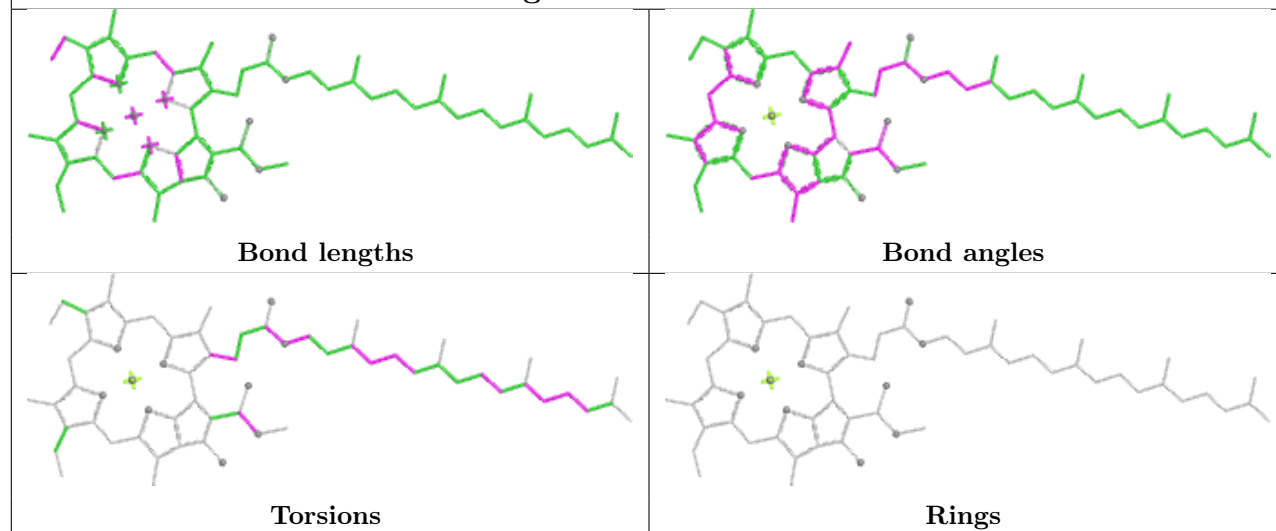




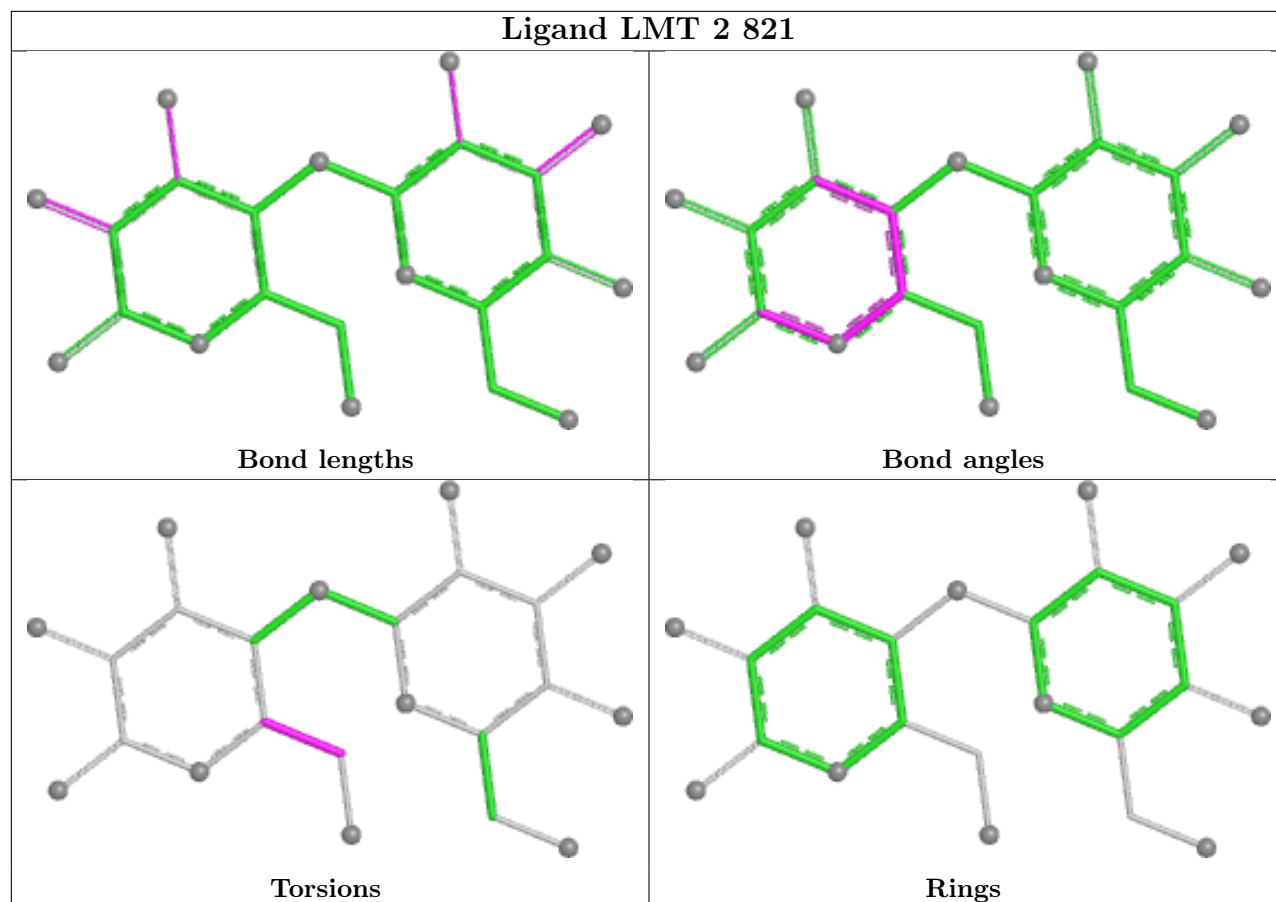
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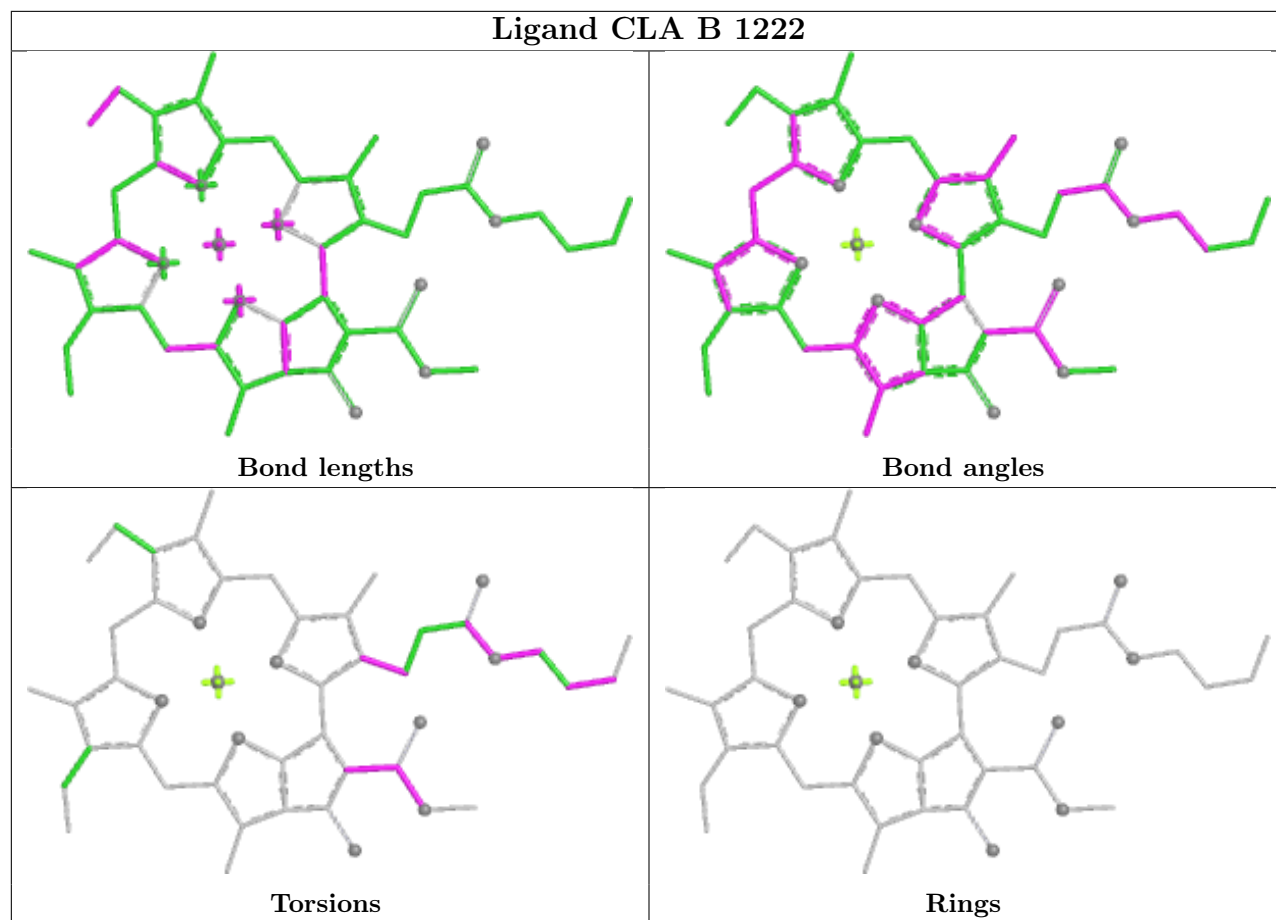


Ligand CLA B 1229

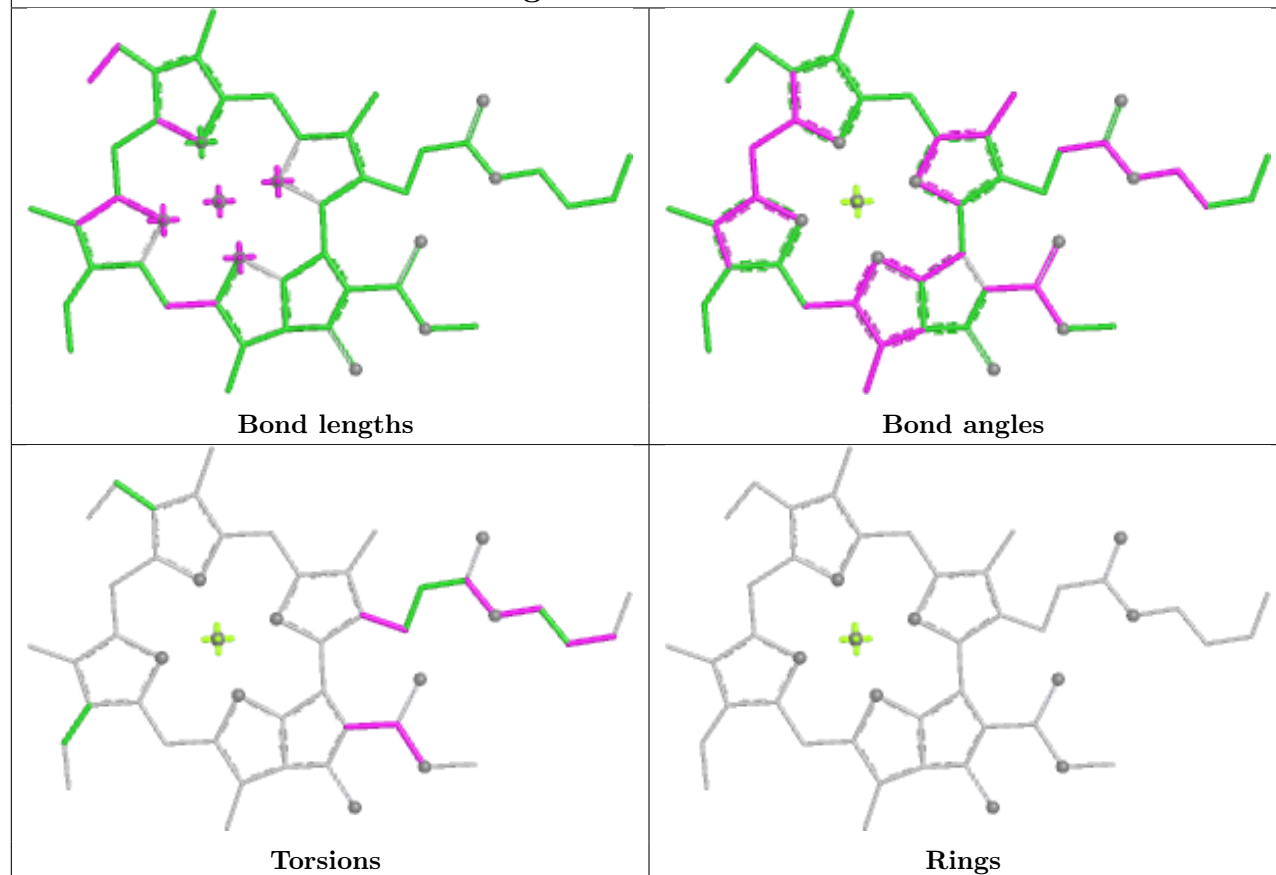


Ligand LMT 2 821

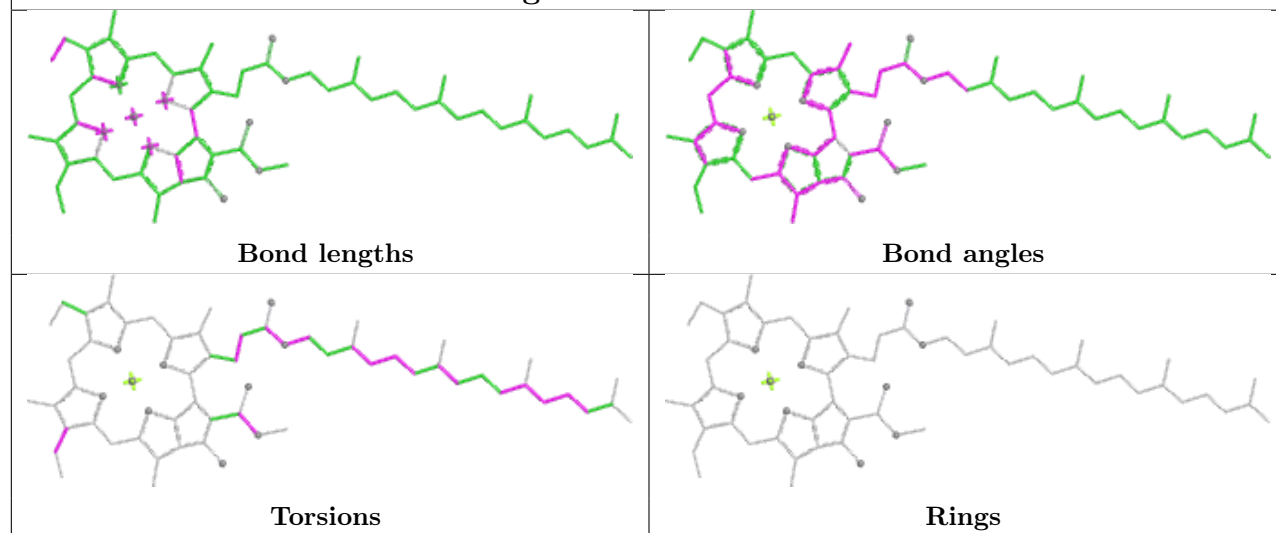




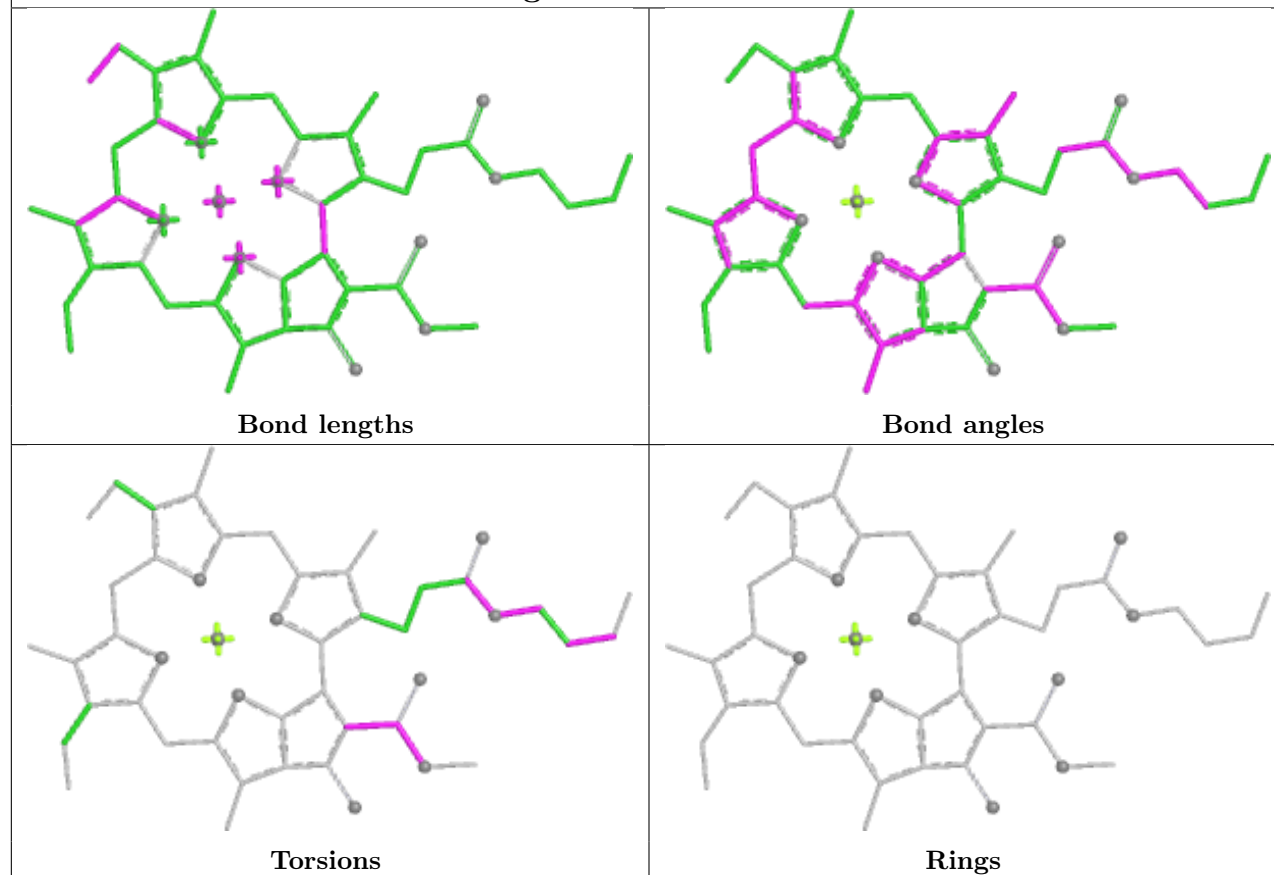
Ligand CLA B 1226



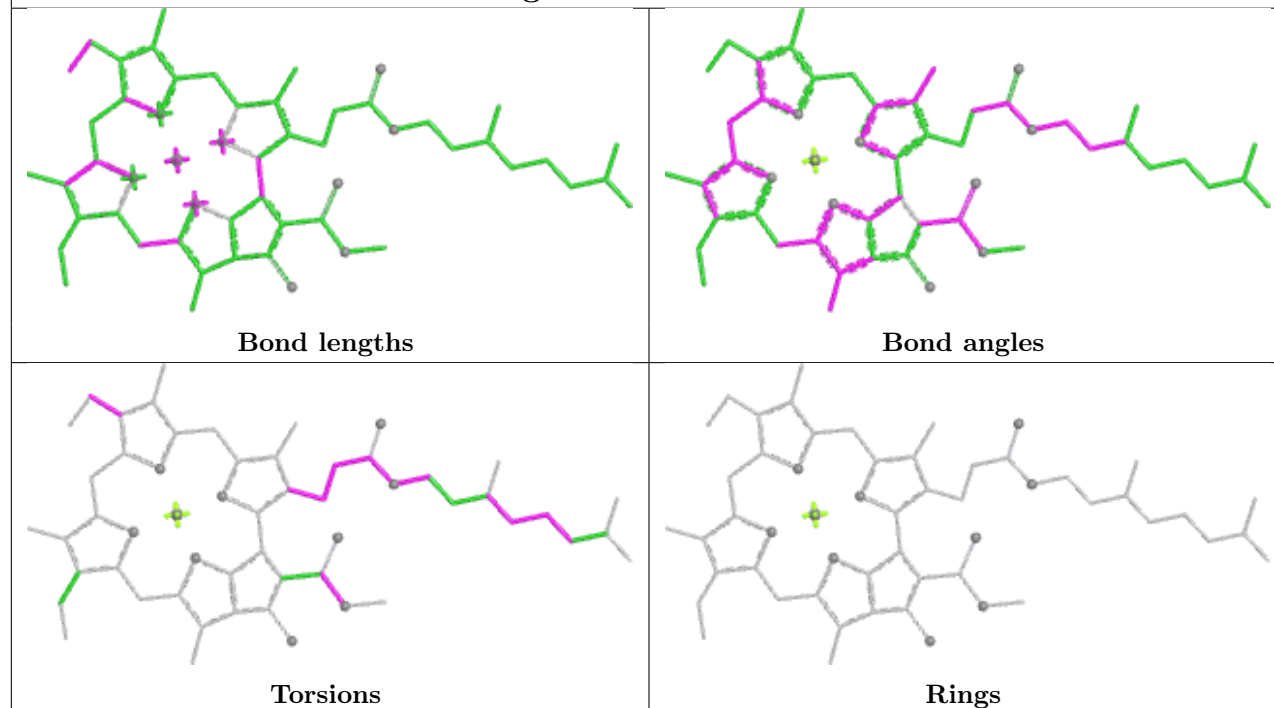
Ligand CLA A 1013



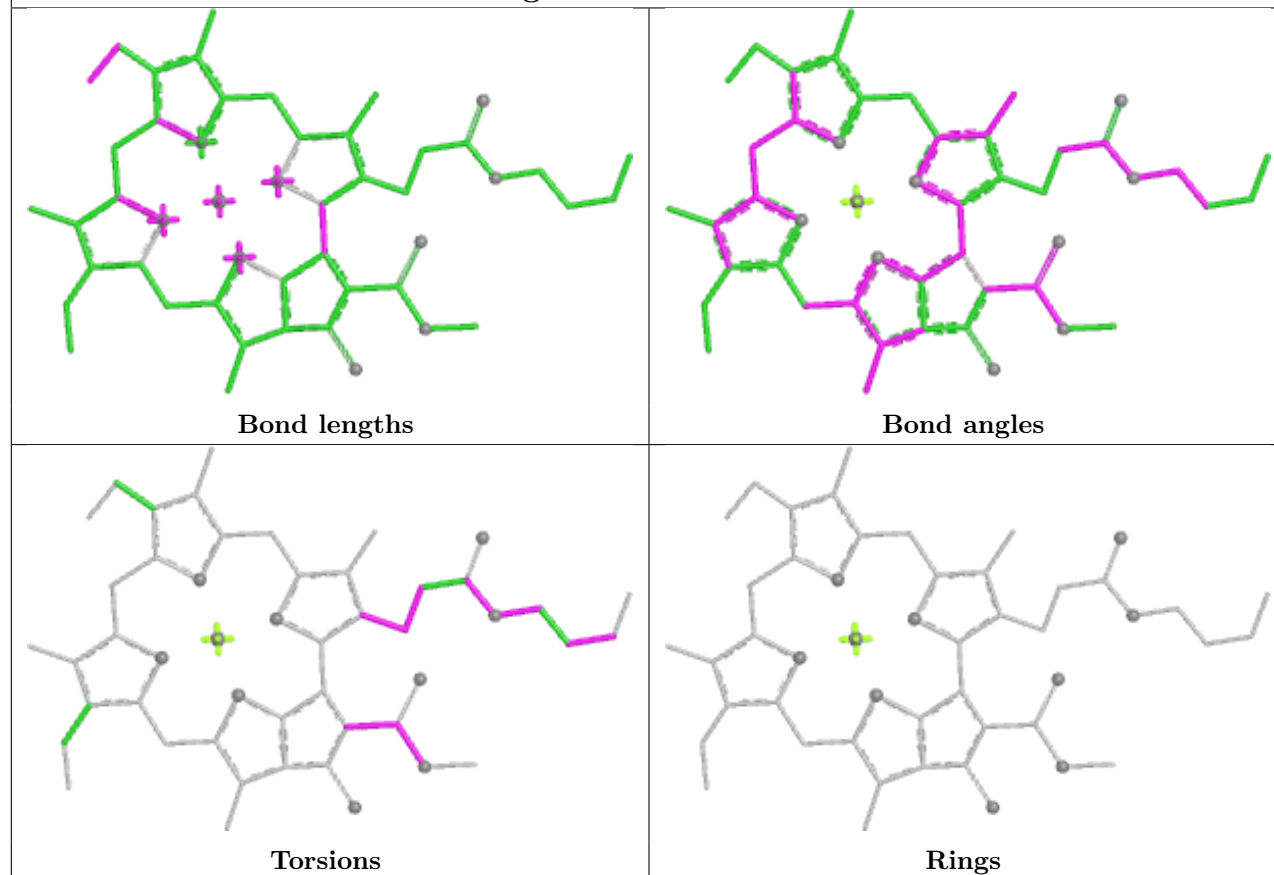
Ligand CLA B 1232



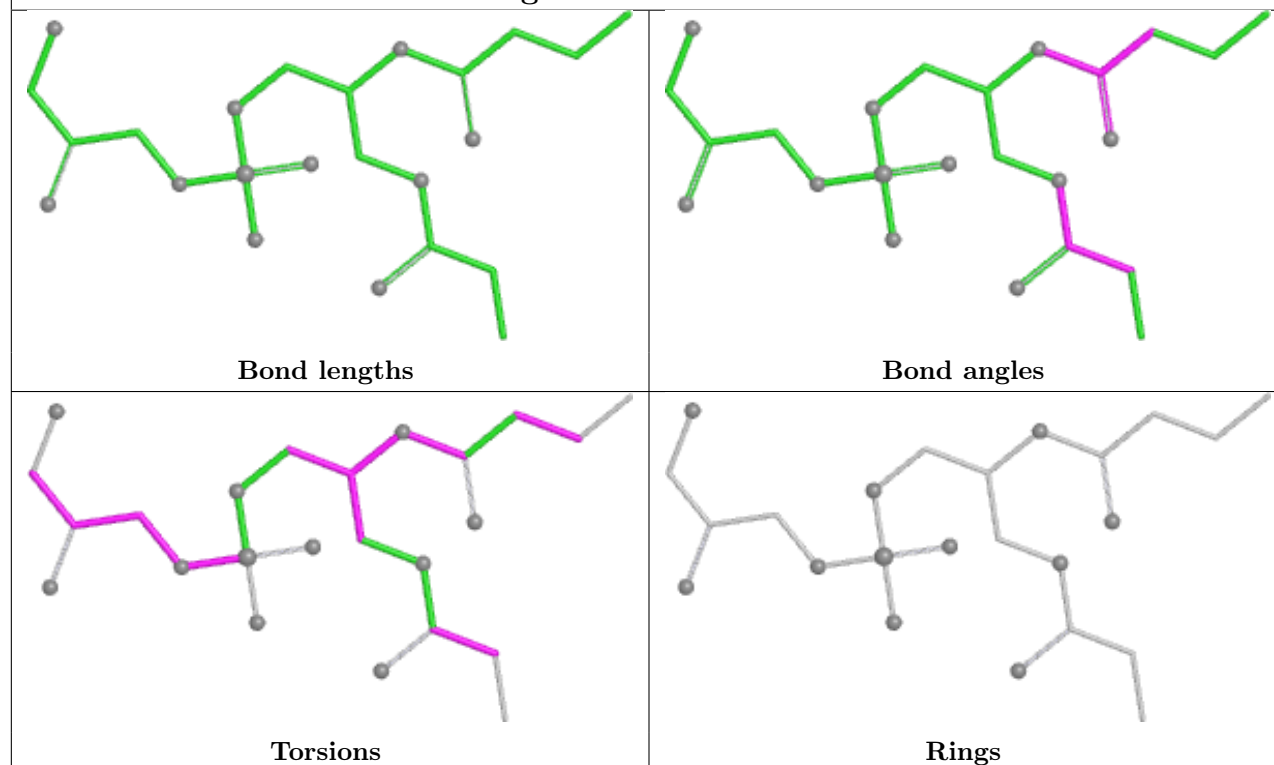
Ligand CLA A 1130



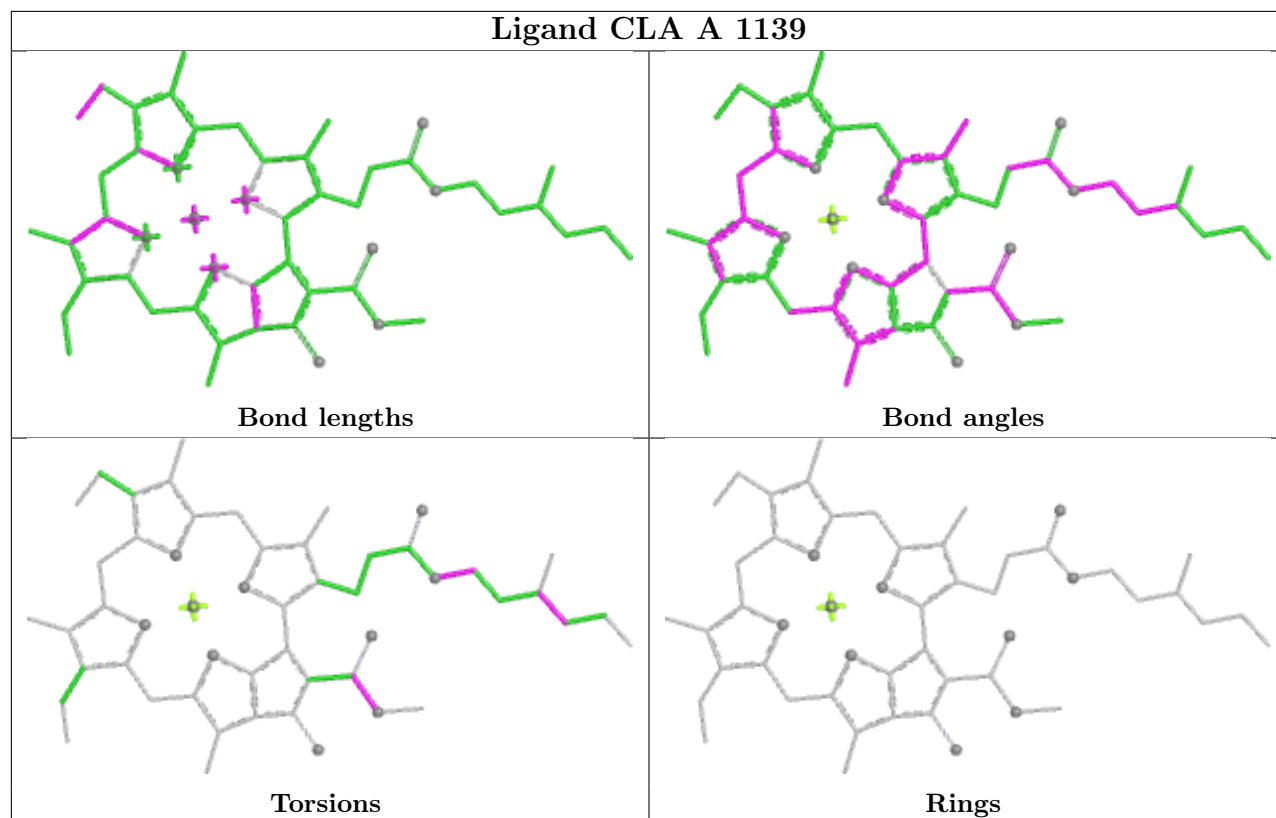
Ligand CLA A 1135



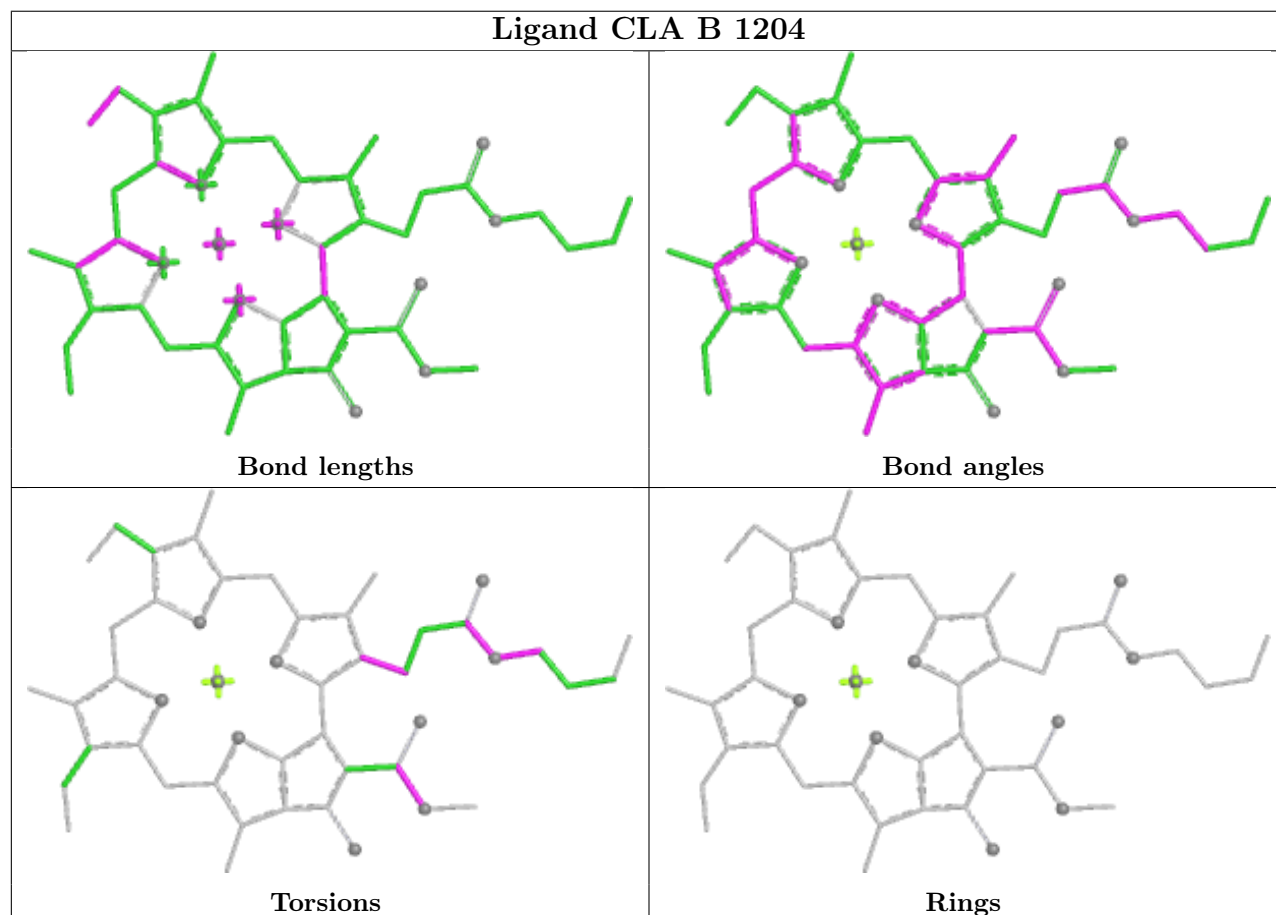
Ligand LHG A 5002

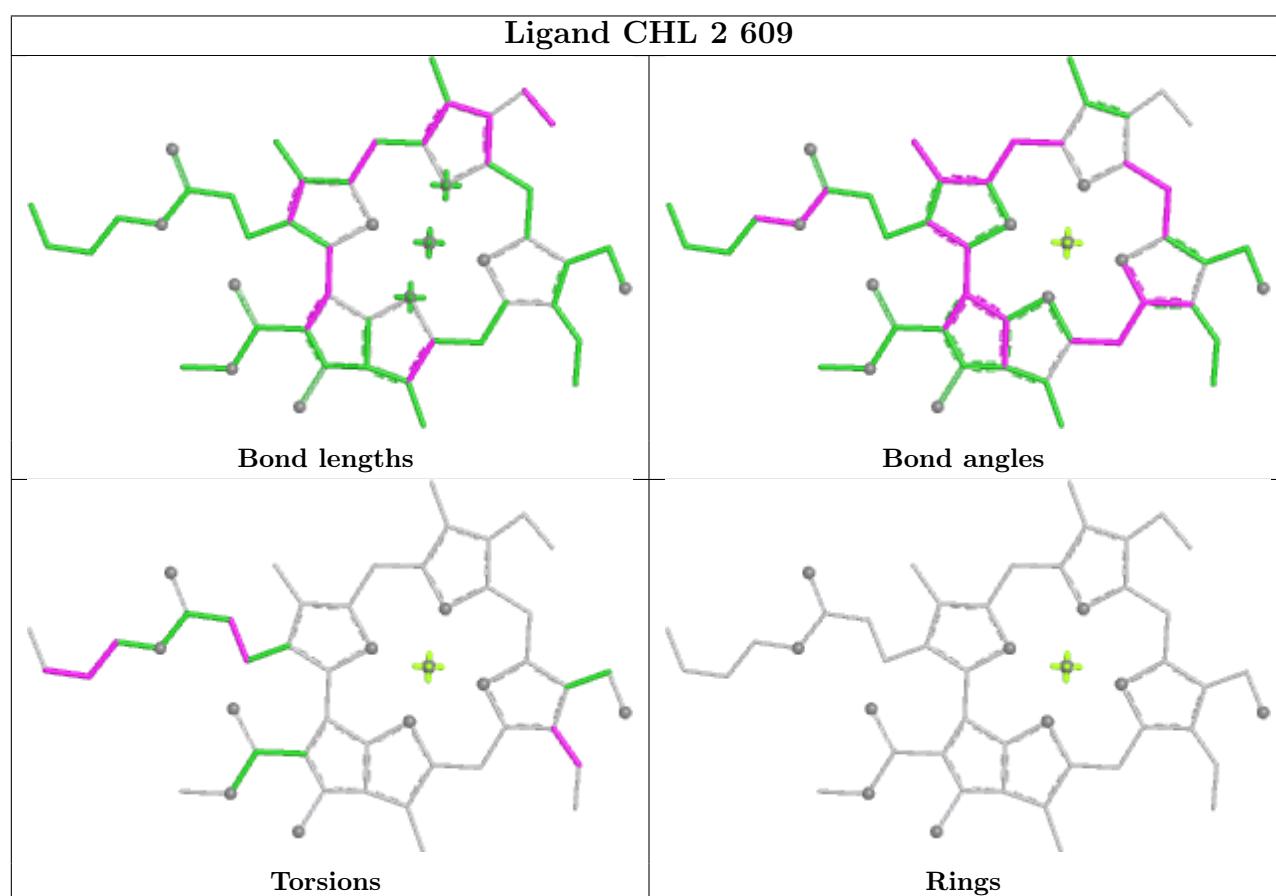
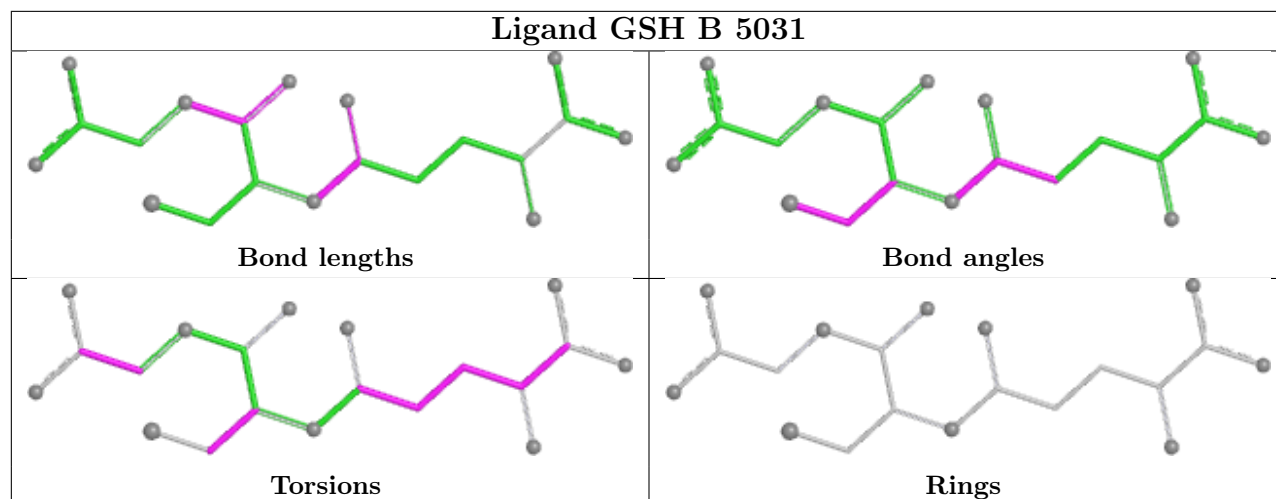


Ligand CLA A 1139

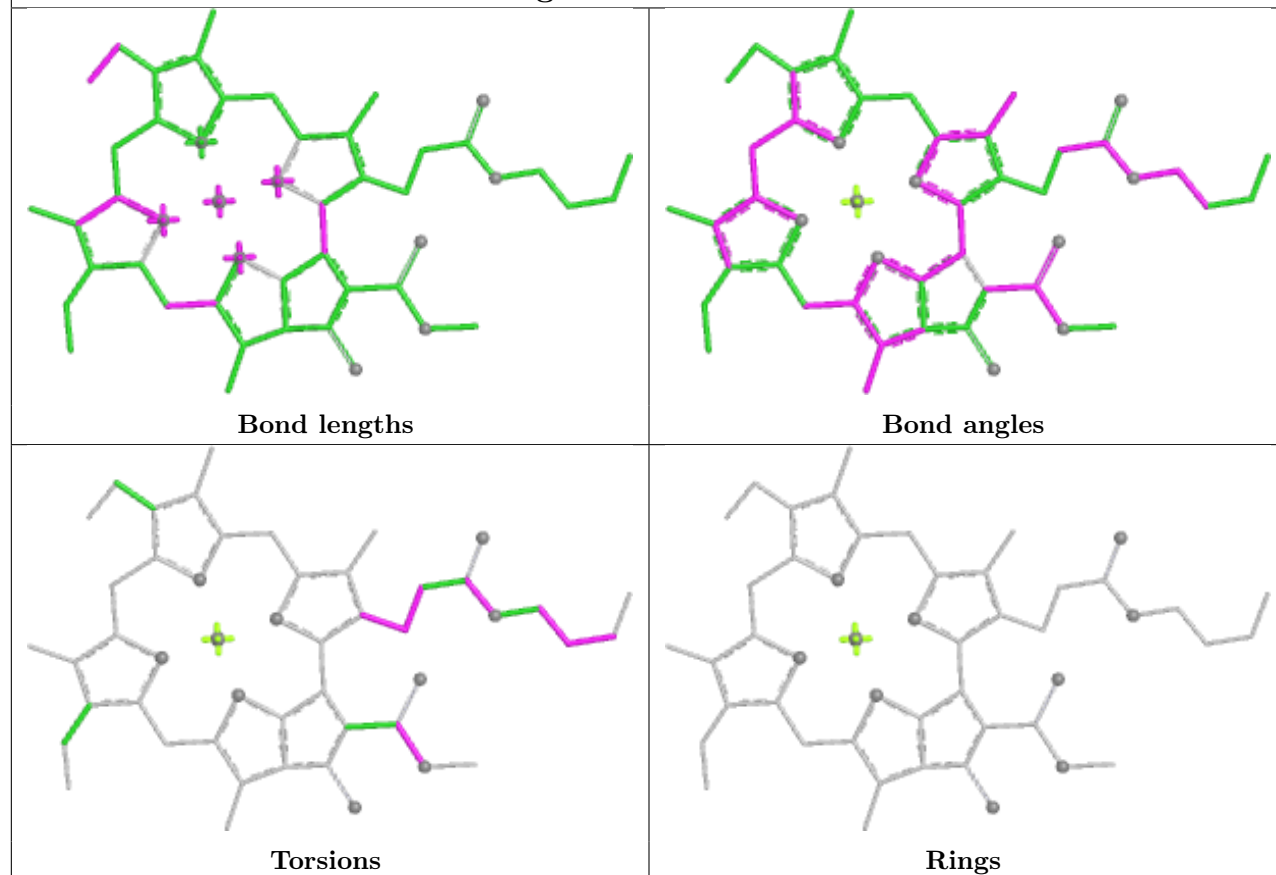


Ligand CLA B 1204

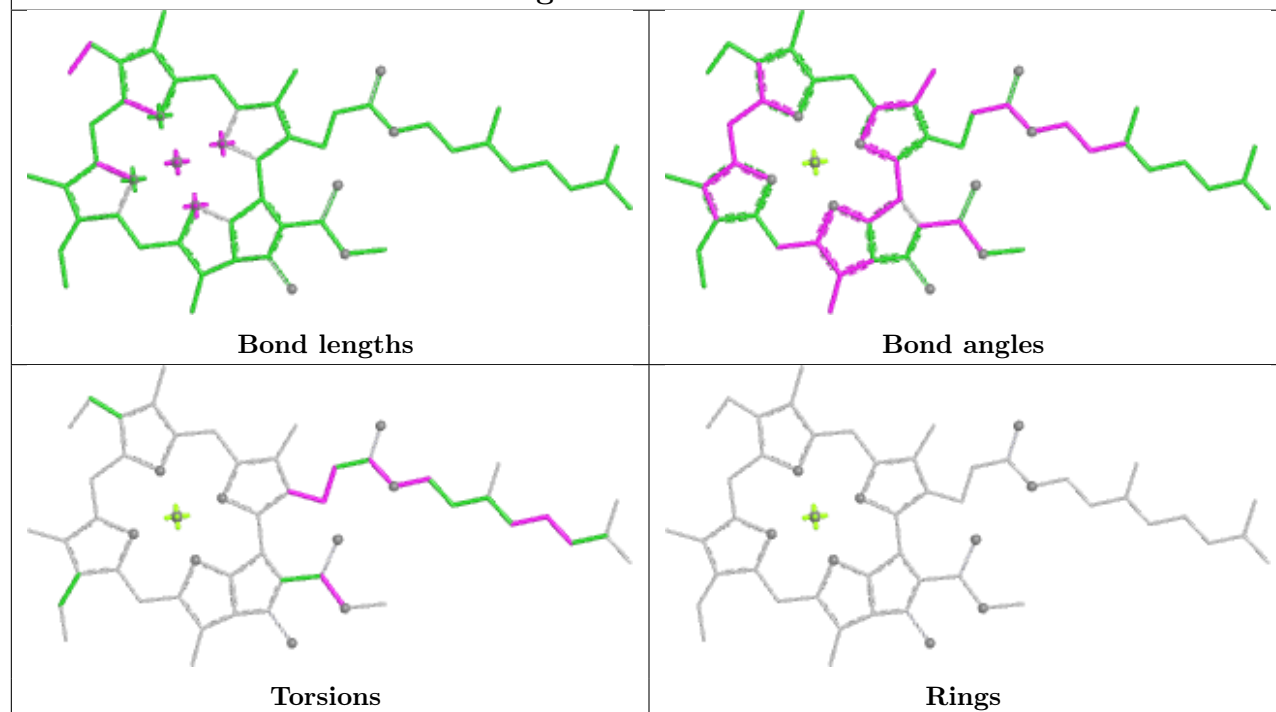


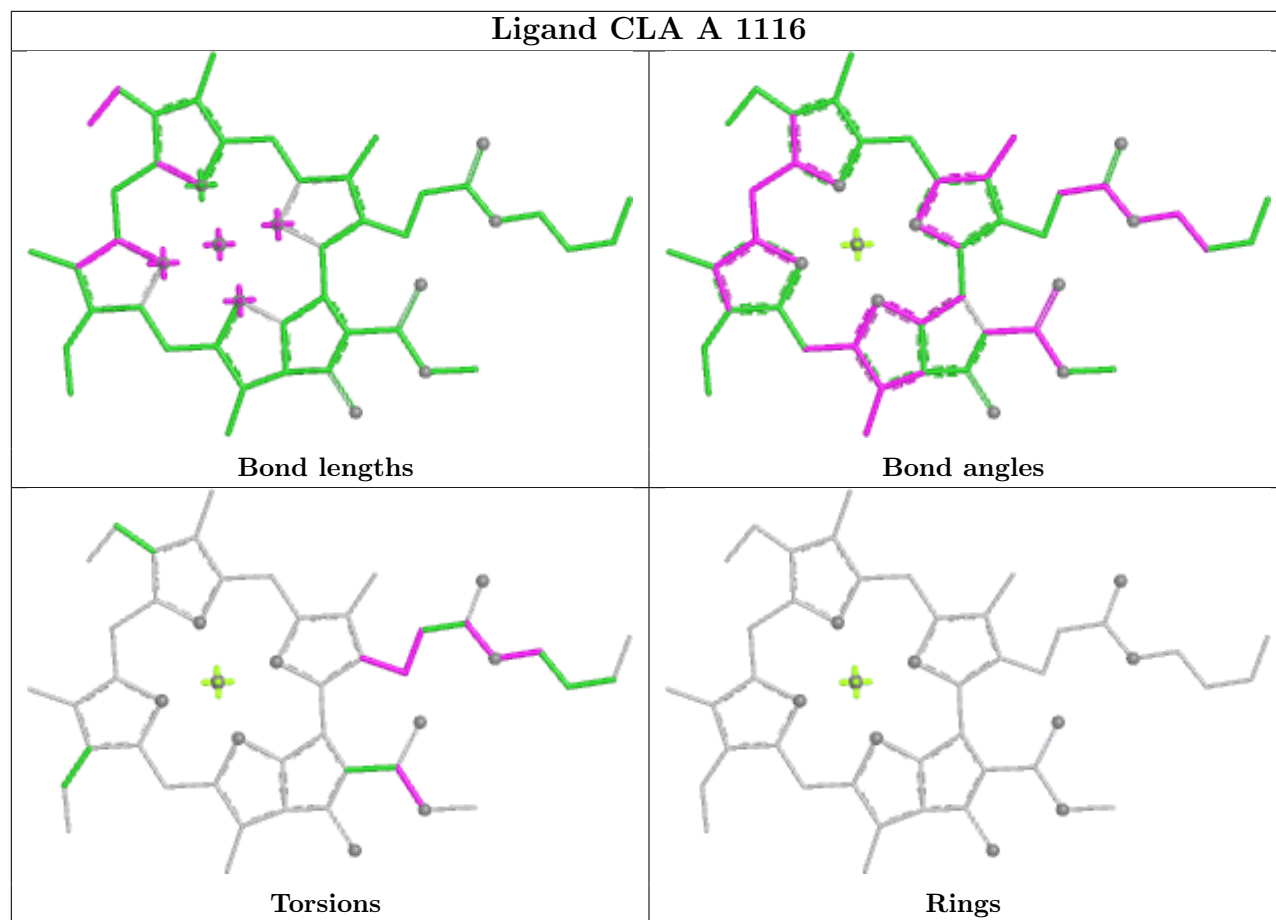


Ligand CLA 1 601

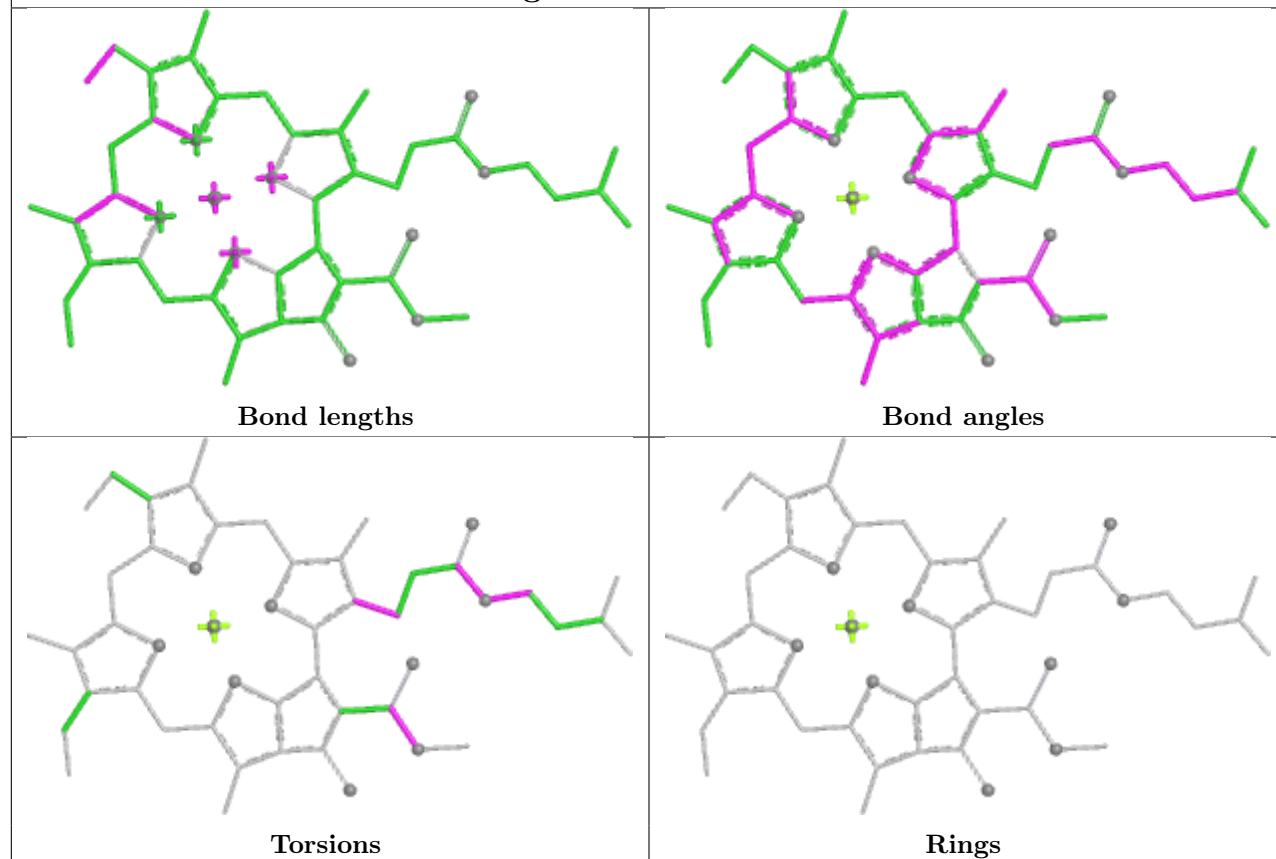


Ligand CLA 4 615

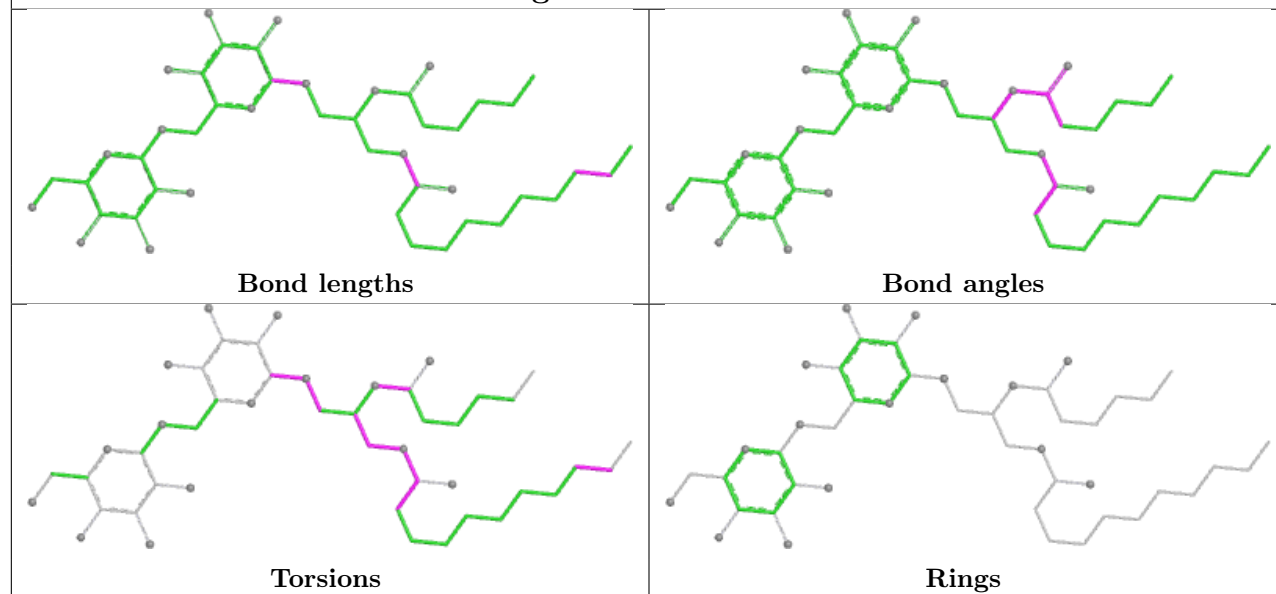


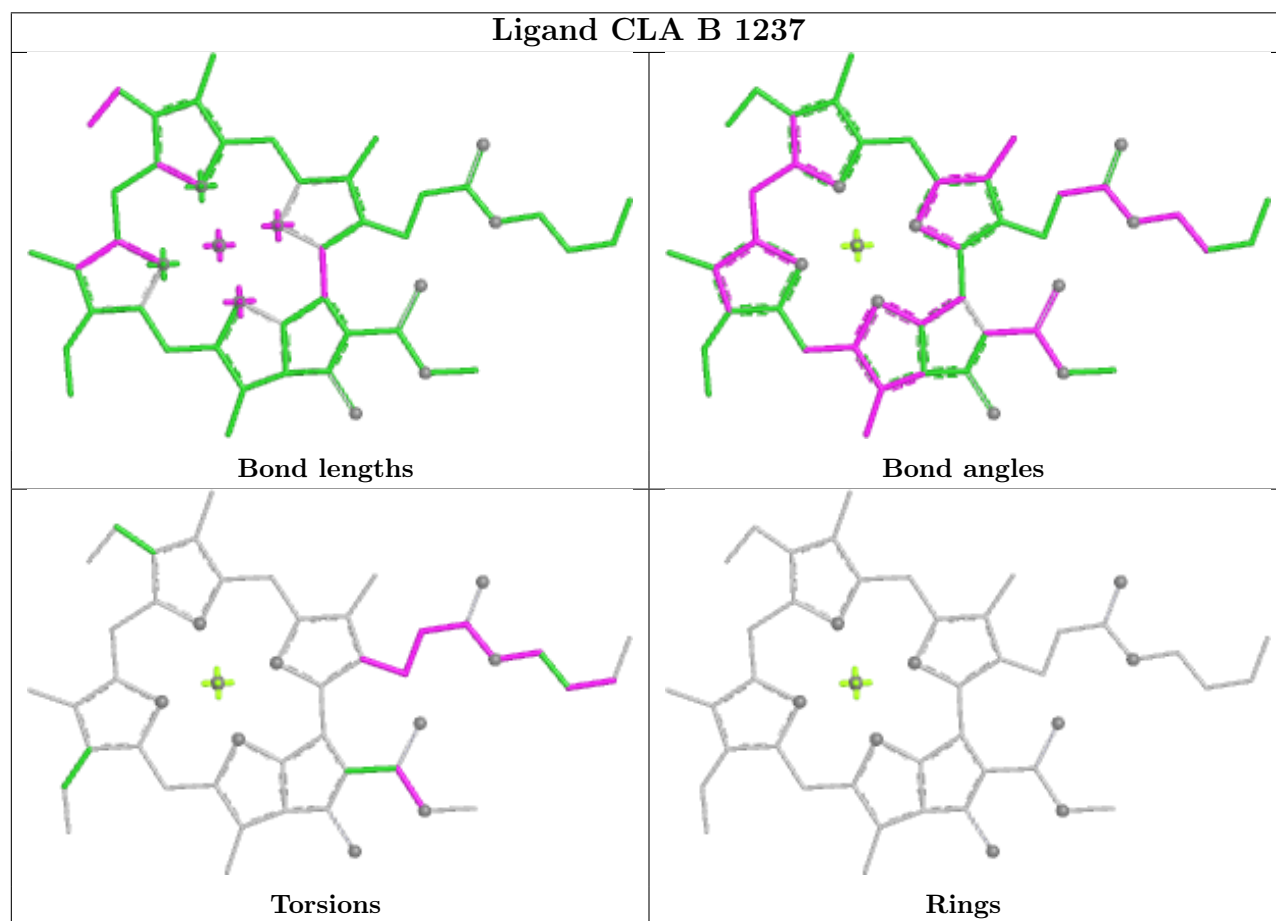
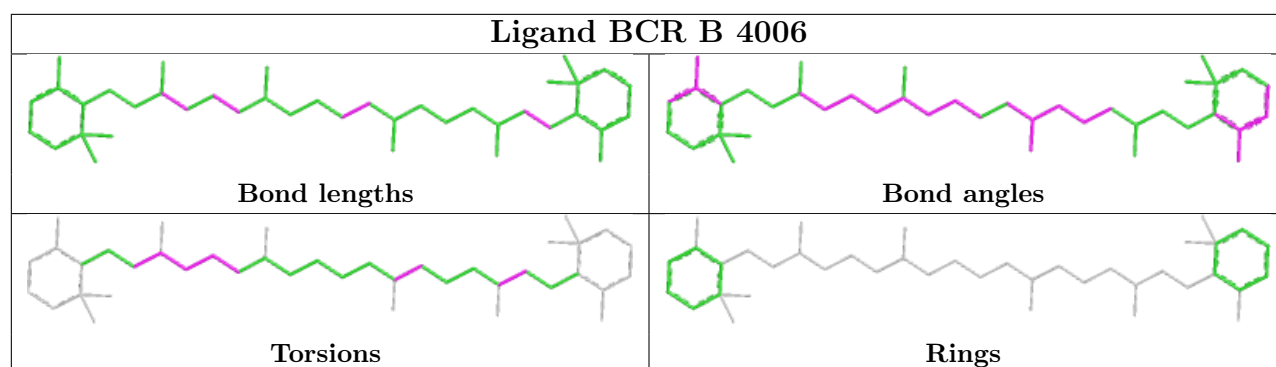


Ligand CLA B 1238

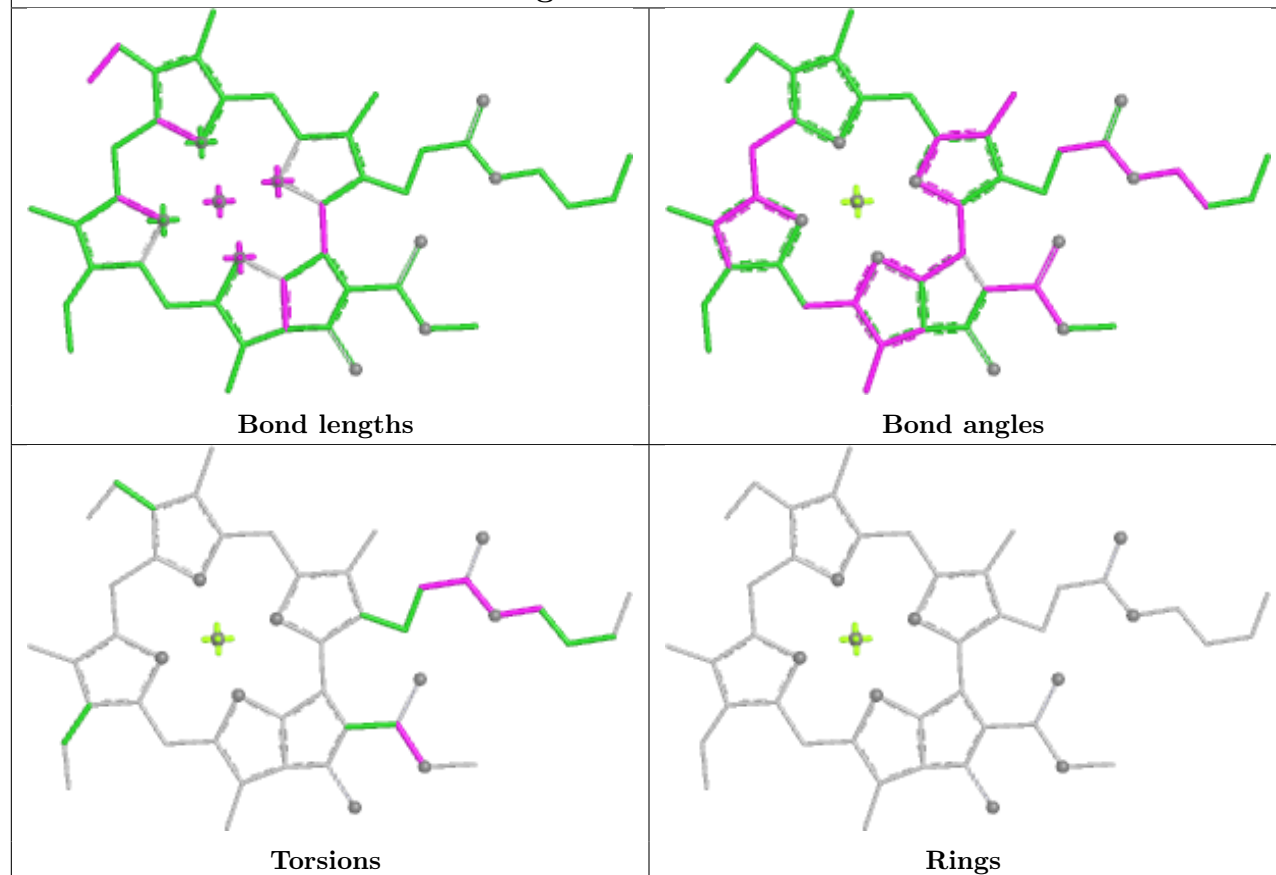


Ligand DGD 2 811

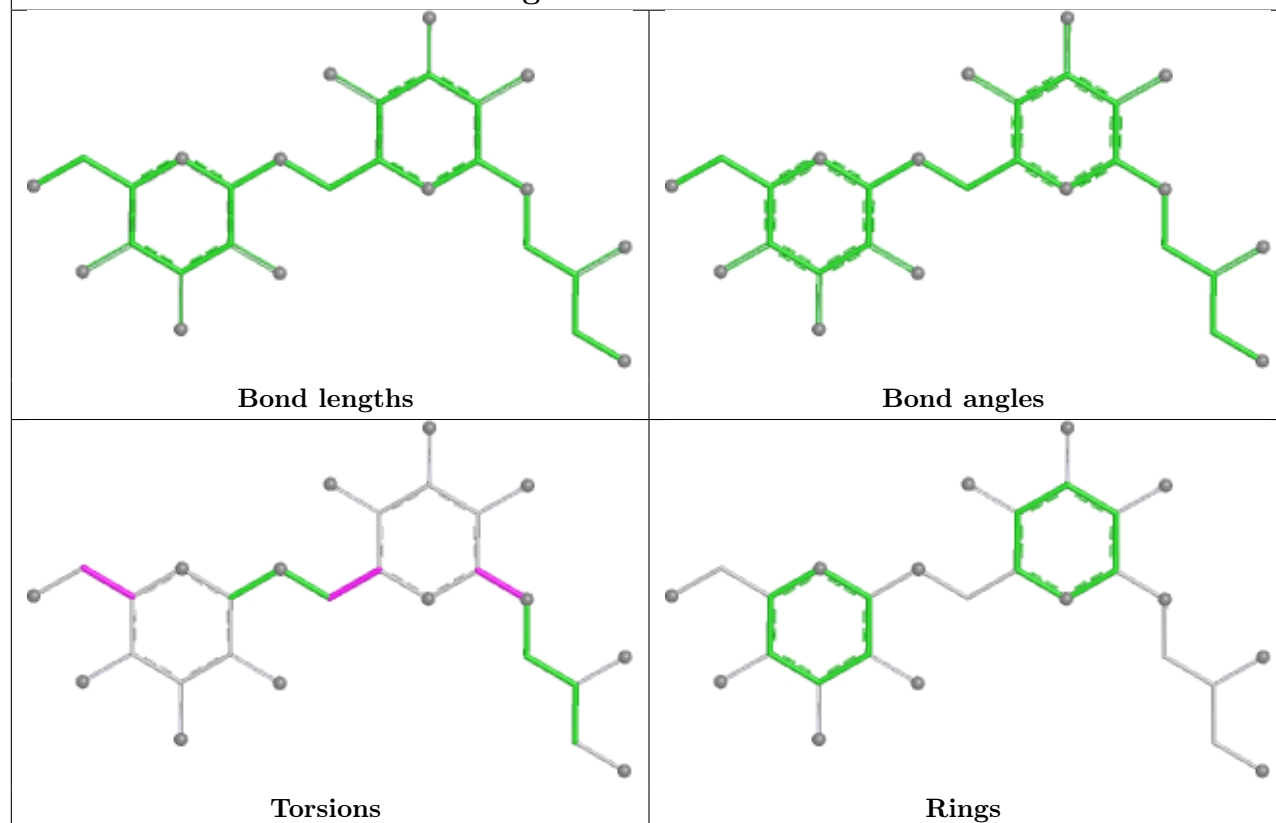


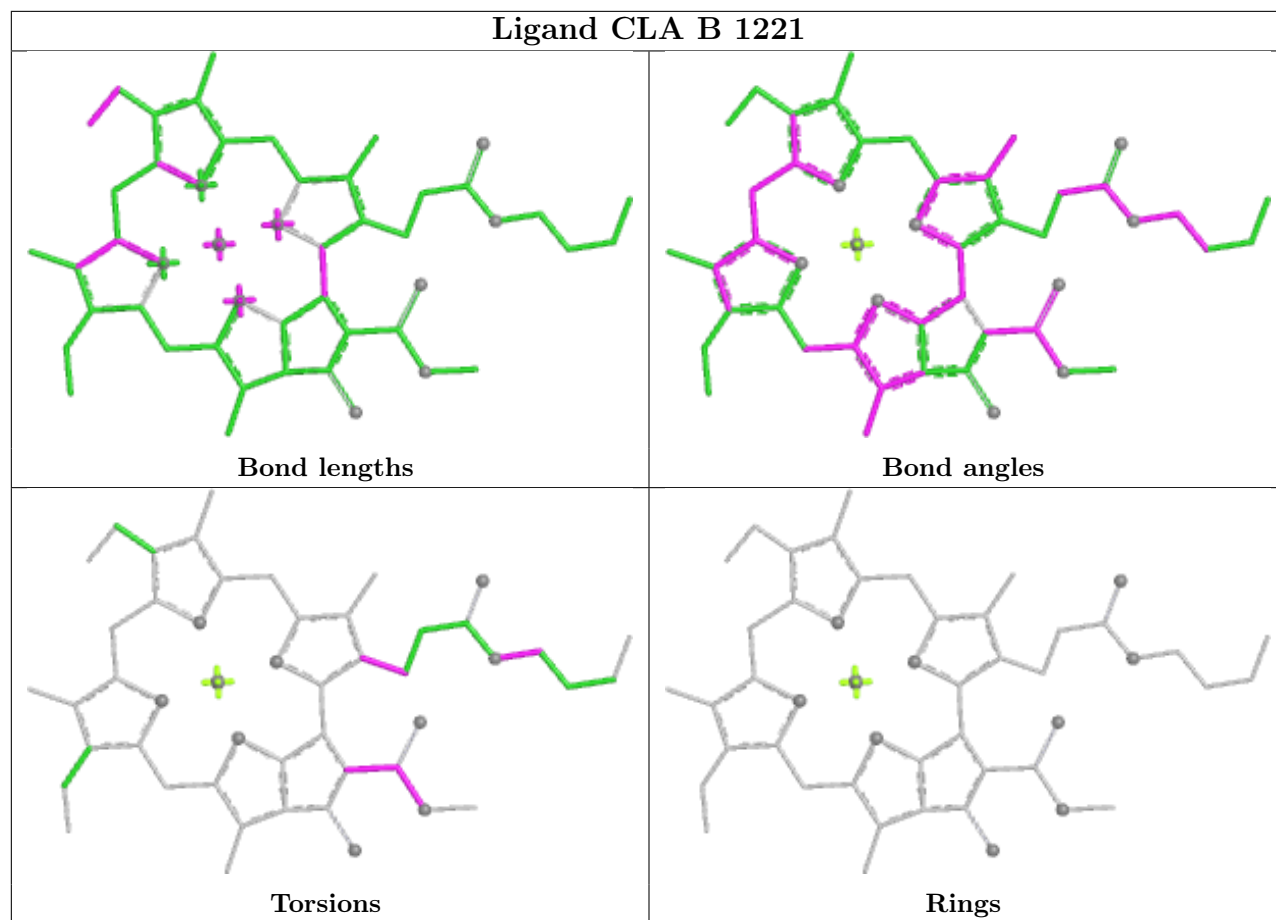


Ligand CLA 4 609

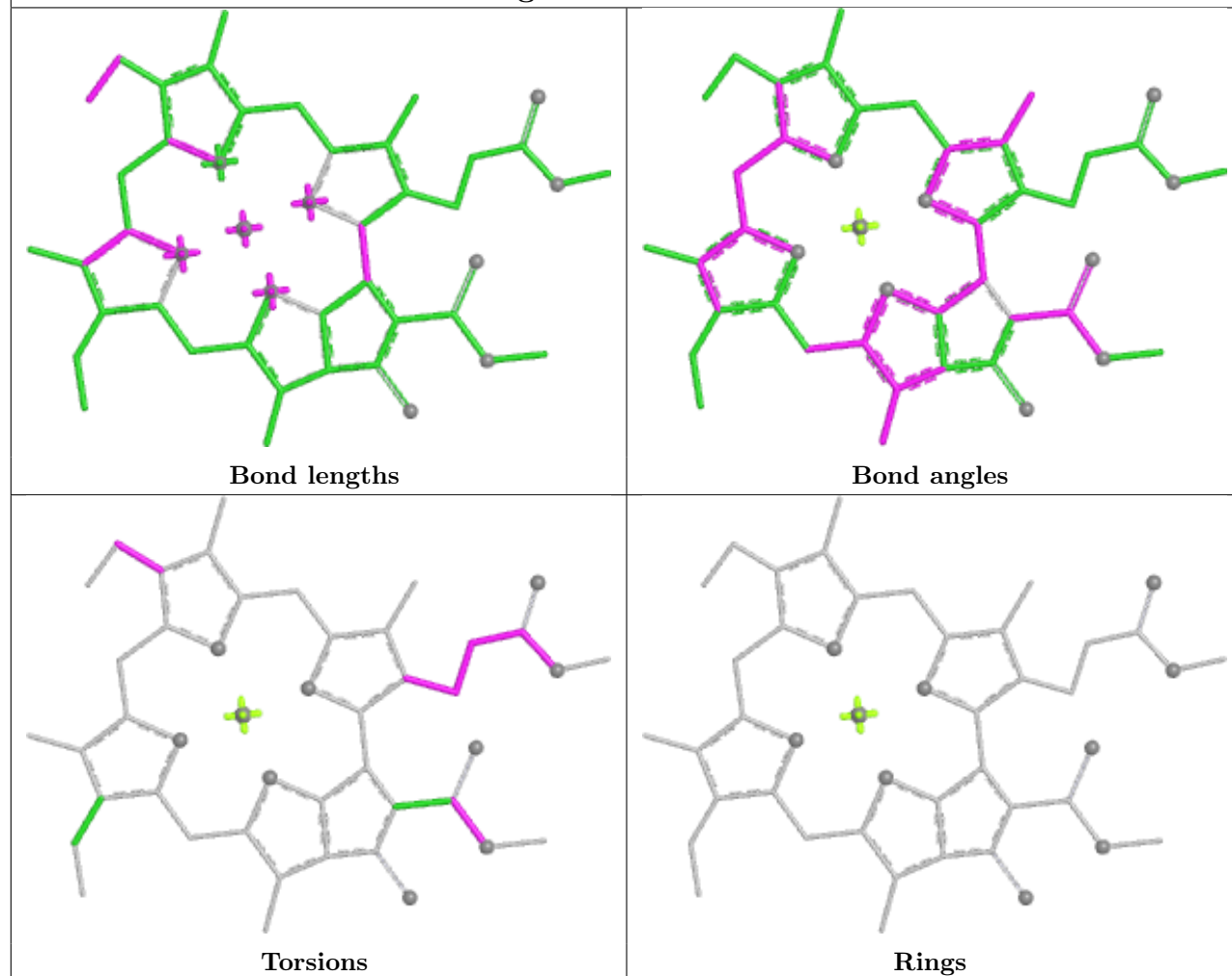


Ligand DGD J 5001

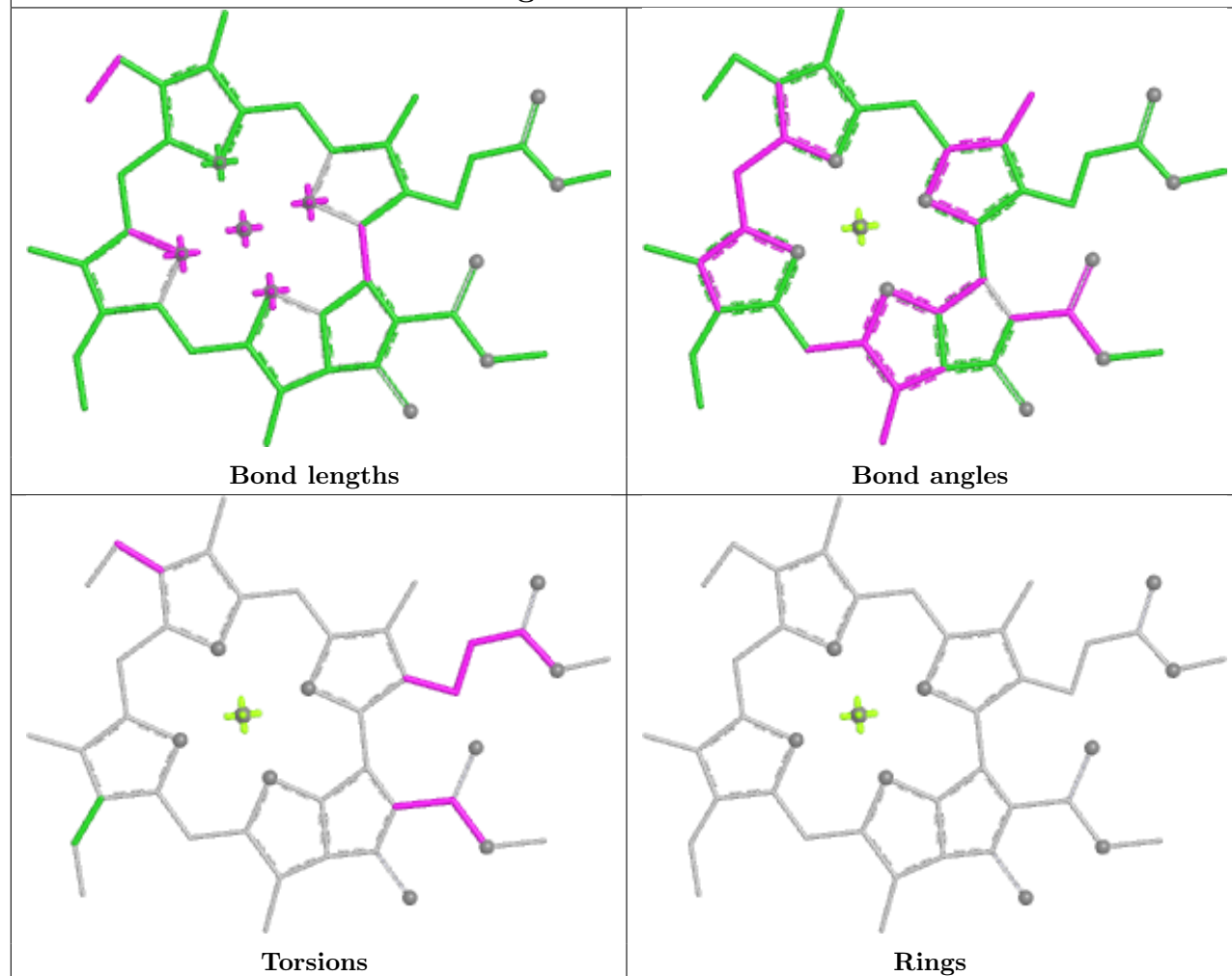




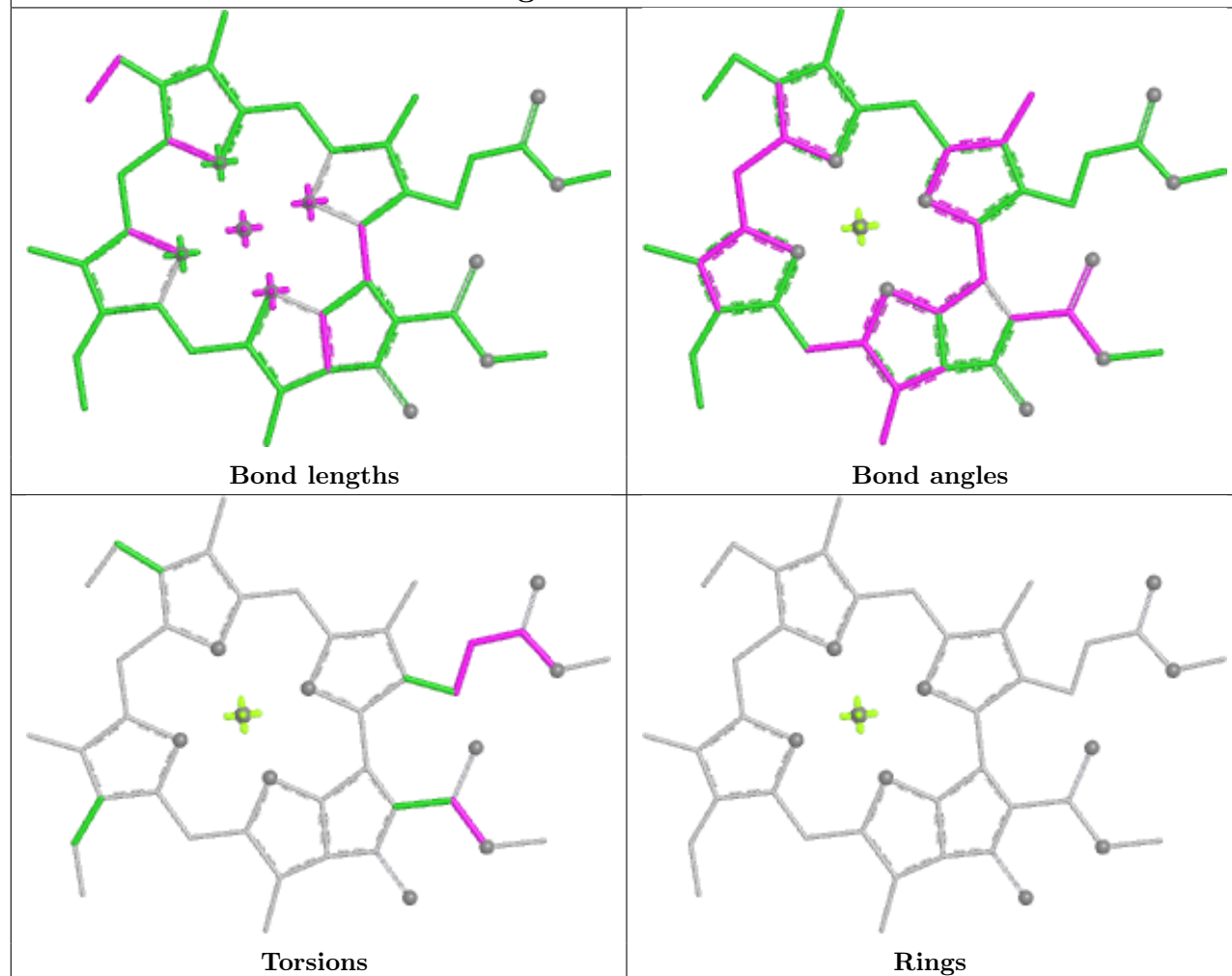
Ligand CLA 1 602

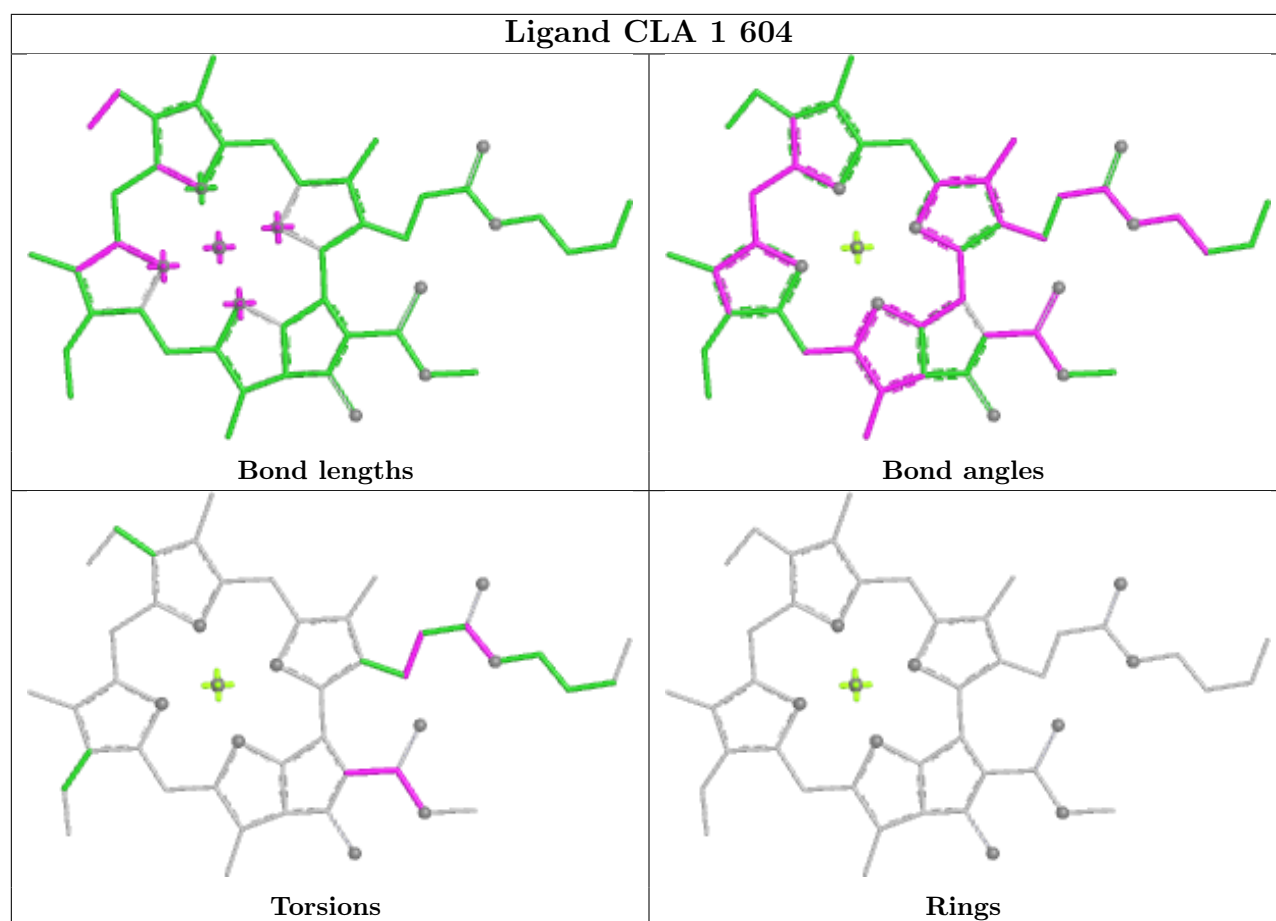


Ligand CLA 1 607



Ligand CLA 3 615





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	1	195/195 (100%)	1.26	40 (20%) 2 4	85, 106, 128, 134	0
2	2	211/211 (100%)	1.29	48 (22%) 2 4	91, 115, 139, 155	0
3	3	210/210 (100%)	1.95	70 (33%) 1 1	134, 167, 199, 210	0
4	4	211/211 (100%)	1.48	50 (23%) 2 3	84, 93, 107, 125	0
5	A	739/739 (100%)	1.57	186 (25%) 1 3	84, 127, 168, 187	0
6	B	734/734 (100%)	1.38	174 (23%) 2 3	83, 114, 149, 180	0
7	C	80/80 (100%)	1.30	15 (18%) 3 4	104, 128, 142, 146	0
8	D	142/142 (100%)	1.15	29 (20%) 3 4	108, 153, 174, 189	0
9	E	64/64 (100%)	0.33	2 (3%) 51 38	93, 103, 115, 120	0
10	F	163/163 (100%)	0.55	13 (7%) 18 16	80, 87, 99, 105	0
11	J	41/41 (100%)	0.79	5 (12%) 8 9	82, 87, 103, 105	0
All	All	2790/2790 (100%)	1.37	632 (22%) 2 4	80, 117, 171, 210	0

The worst 5 of 632 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	506	THR	19.0
5	A	280	GLY	16.4
5	A	377	TYR	16.2
5	A	375	PRO	15.1
6	B	735	GLY	13.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CAC	3	901	5/5	0.16	0.19	190,190,194,197	0
15	CLA	A	1121	49/65	0.31	0.13	177,193,206,211	0
15	CLA	3	607	50/65	0.37	0.22	195,209,223,228	0
15	CLA	3	608	48/65	0.41	0.12	196,222,240,247	0
20	CAC	1	902	5/5	0.42	0.21	136,142,150,152	0
23	GSH	4	831	20/20	0.42	0.12	136,138,145,146	0
18	LMG	2	802	25/55	0.47	0.18	92,104,127,134	0
18	LMG	1	802	36/55	0.47	0.15	88,102,125,128	0
20	CAC	1	901	5/5	0.48	0.25	130,132,142,147	0
21	DGD	4	811	45/66	0.49	0.19	83,91,111,119	0
21	DGD	J	5001	28/66	0.50	0.12	92,95,97,97	0
14	BCR	4	505	40/40	0.50	0.25	83,85,118,119	0
20	CAC	3	902	5/5	0.53	0.17	200,204,206,207	0
14	BCR	1	505	40/40	0.55	0.33	83,86,98,110	0
14	BCR	J	4003	40/40	0.57	0.21	89,99,105,106	0
18	LMG	1	803	23/55	0.57	0.16	114,119,150,154	0
15	CLA	A	1120	49/65	0.57	0.17	162,176,190,191	0
14	BCR	4	503	40/40	0.57	0.21	90,93,98,99	0
15	CLA	A	1141	50/65	0.57	0.12	170,186,196,199	0
15	CLA	A	1131	50/65	0.58	0.17	145,153,157,158	0
15	CLA	B	1218	49/65	0.59	0.16	104,112,117,137	0
23	GSH	B	5031	20/20	0.59	0.10	151,157,163,166	0
14	BCR	B	4003	40/40	0.61	0.30	125,141,149,153	0
18	LMG	2	803	16/55	0.63	0.12	121,129,134,134	0
15	CLA	3	603	45/65	0.65	0.12	179,187,200,210	0
22	LMT	2	821	23/35	0.66	0.08	109,113,132,138	0
15	CLA	B	1207	25/65	0.66	0.13	145,151,156,158	0
15	CLA	1	615	65/65	0.66	0.19	83,85,89,91	0
15	CLA	A	1114	46/65	0.67	0.20	127,141,157,160	0
14	BCR	A	4002	40/40	0.68	0.31	120,140,167,169	0
15	CLA	2	602	49/65	0.69	0.18	123,128,133,137	0
14	BCR	1	503	40/40	0.70	0.15	115,121,136,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	BCR	J	4001	40/40	0.70	0.26	83,90,102,103	0
20	CAC	4	902	5/5	0.70	0.21	85,105,119,122	0
14	BCR	B	4001	40/40	0.70	0.20	121,129,137,138	0
12	LUT	4	501	42/42	0.71	0.16	90,93,101,102	0
15	CLA	B	1238	50/65	0.71	0.15	134,148,155,158	0
14	BCR	2	503	40/40	0.72	0.22	96,102,110,110	0
15	CLA	B	1201	49/65	0.73	0.14	127,132,139,152	0
14	BCR	3	503	40/40	0.73	0.20	134,148,166,169	0
12	LUT	1	501	42/42	0.74	0.22	100,109,122,125	0
12	LUT	2	501	42/42	0.75	0.16	117,120,125,127	0
19	SQD	1	811	40/54	0.75	0.15	100,104,109,109	0
14	BCR	A	4004	40/40	0.75	0.29	136,156,183,186	0
16	CHL	1	610	47/66	0.75	0.15	101,105,111,114	0
15	CLA	A	1111	49/65	0.76	0.18	122,129,139,142	0
15	CLA	B	1203	49/65	0.76	0.20	112,118,123,126	0
17	LHG	2	801	21/49	0.76	0.14	121,128,134,137	0
14	BCR	A	4007	40/40	0.76	0.29	125,132,135,137	0
15	CLA	4	607	49/65	0.76	0.16	92,98,104,105	0
15	CLA	B	1224	49/65	0.76	0.24	106,114,119,121	0
15	CLA	A	1108	46/65	0.77	0.21	123,132,140,143	0
15	CLA	2	605	65/65	0.77	0.18	95,100,104,108	0
12	LUT	3	501	42/42	0.77	0.18	173,180,186,189	0
16	CHL	3	604	47/66	0.77	0.19	157,171,179,185	0
15	CLA	3	611	46/65	0.77	0.18	147,154,162,167	0
21	DGD	2	811	47/66	0.77	0.15	122,126,134,137	0
15	CLA	3	606	45/65	0.77	0.14	156,165,173,177	0
15	CLA	B	1208	49/65	0.77	0.14	131,141,150,152	0
15	CLA	B	1211	49/65	0.77	0.18	127,137,141,143	0
15	CLA	A	1130	55/65	0.77	0.14	157,163,172,174	0
15	CLA	B	1219	49/65	0.77	0.13	95,103,107,108	0
15	CLA	B	1230	49/65	0.78	0.17	81,83,85,86	0
15	CLA	3	601	49/65	0.78	0.15	165,175,188,190	0
20	CAC	4	901	5/5	0.78	0.17	133,136,139,139	0
15	CLA	4	615	55/65	0.78	0.20	82,84,86,87	0
14	BCR	J	4002	40/40	0.78	0.20	88,91,99,100	0
13	XAT	2	502	44/44	0.79	0.21	103,107,110,110	0
14	BCR	A	4003	40/40	0.79	0.31	116,130,150,152	0
17	LHG	A	5001	16/49	0.79	0.14	165,168,172,175	0
15	CLA	2	608	49/65	0.79	0.17	128,136,143,146	0
25	PQN	B	2002	33/33	0.79	0.19	117,129,134,136	0
15	CLA	A	1115	49/65	0.80	0.14	160,166,178,179	0
15	CLA	B	1239	65/65	0.80	0.19	120,125,155,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CLA	3	613	46/65	0.80	0.16	150,153,186,194	0
15	CLA	B	1215	49/65	0.80	0.25	105,112,119,121	0
15	CLA	2	606	46/65	0.80	0.16	105,111,116,119	0
15	CLA	A	1124	49/65	0.80	0.17	123,133,142,148	0
15	CLA	B	1205	49/65	0.80	0.22	122,126,132,134	0
15	CLA	1	601	49/65	0.80	0.14	111,114,118,119	0
15	CLA	1	607	46/65	0.81	0.17	99,104,109,111	0
15	CLA	A	1132	49/65	0.81	0.12	137,148,163,168	0
15	CLA	A	1134	49/65	0.81	0.15	162,171,183,186	0
15	CLA	B	1240	65/65	0.81	0.18	84,92,97,99	0
15	CLA	F	1302	49/65	0.81	0.15	81,83,86,86	0
15	CLA	A	1101	45/65	0.81	0.20	90,95,99,100	0
14	BCR	B	4002	40/40	0.81	0.25	114,129,145,146	0
13	XAT	3	502	44/44	0.81	0.31	154,161,165,166	0
25	PQN	A	2001	33/33	0.81	0.27	87,91,98,99	0
15	CLA	2	615	50/65	0.81	0.18	112,124,141,146	0
15	CLA	2	604	49/65	0.82	0.13	104,111,117,119	0
16	CHL	2	610	50/66	0.82	0.14	97,100,102,103	0
15	CLA	3	612	55/65	0.82	0.22	135,143,151,153	0
15	CLA	A	1113	45/65	0.82	0.16	147,155,160,161	0
15	CLA	1	605	48/65	0.82	0.15	93,97,101,103	0
15	CLA	4	606	49/65	0.82	0.13	89,94,97,98	0
15	CLA	A	1116	49/65	0.82	0.20	136,151,156,161	0
15	CLA	B	1237	49/65	0.82	0.12	140,150,158,161	0
14	BCR	A	4005	40/40	0.82	0.33	129,142,162,163	0
14	BCR	3	504	40/40	0.82	0.25	137,152,173,173	0
13	XAT	4	502	44/44	0.82	0.21	83,84,88,89	0
15	CLA	A	1129	48/65	0.82	0.18	147,160,175,178	0
15	CLA	4	601	49/65	0.83	0.12	92,95,100,101	0
14	BCR	F	4002	40/40	0.83	0.18	80,81,81,82	0
15	CLA	3	610	49/65	0.83	0.18	134,143,160,173	0
15	CLA	4	612	49/65	0.83	0.15	81,84,85,86	0
13	XAT	1	502	44/44	0.83	0.19	89,97,109,110	0
15	CLA	A	1136	49/65	0.83	0.12	140,148,154,159	0
15	CLA	1	603	45/65	0.83	0.15	91,95,97,99	0
14	BCR	B	4005	40/40	0.83	0.29	92,95,99,101	0
16	CHL	4	613	50/66	0.83	0.13	86,91,96,98	0
15	CLA	A	1109	49/65	0.83	0.13	103,111,114,115	0
15	CLA	B	1229	65/65	0.84	0.16	80,81,82,83	0
15	CLA	B	1209	46/65	0.84	0.13	130,133,140,141	0
15	CLA	B	1232	49/65	0.84	0.18	92,99,103,105	0
15	CLA	A	1126	49/65	0.84	0.23	98,106,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	LHG	B	5001	21/49	0.84	0.12	88,89,92,93	0
14	BCR	B	4006	40/40	0.84	0.26	80,83,89,90	0
21	DGD	B	5002	38/66	0.84	0.14	114,119,125,127	0
14	BCR	A	4006	40/40	0.84	0.28	83,91,102,103	0
15	CLA	A	1137	49/65	0.84	0.16	137,144,151,153	0
15	CLA	B	1220	55/65	0.84	0.16	91,98,102,103	0
15	CLA	4	604	49/65	0.84	0.17	82,86,89,89	0
15	CLA	B	1226	49/65	0.84	0.17	105,112,118,120	0
16	CHL	2	613	46/66	0.84	0.14	100,102,103,105	0
15	CLA	2	607	49/65	0.85	0.14	125,132,139,141	0
15	CLA	B	1023	60/65	0.85	0.19	113,126,138,141	0
15	CLA	A	1119	49/65	0.85	0.15	140,151,159,162	0
15	CLA	A	1112	49/65	0.85	0.16	124,131,141,144	0
15	CLA	A	1102	45/65	0.85	0.19	100,106,109,111	0
15	CLA	B	1221	49/65	0.85	0.17	99,108,113,115	0
15	CLA	J	1302	49/65	0.85	0.13	86,89,91,92	0
15	CLA	B	1206	49/65	0.85	0.15	131,139,145,148	0
15	CLA	A	1122	49/65	0.85	0.15	144,154,161,164	0
15	CLA	1	612	60/65	0.85	0.15	97,105,110,112	0
15	CLA	2	601	49/65	0.85	0.14	110,116,125,129	0
16	CHL	4	610	47/66	0.85	0.14	82,85,87,87	0
17	LHG	1	801	23/49	0.86	0.15	95,99,101,103	0
15	CLA	B	1022	50/65	0.86	0.20	108,116,124,126	0
15	CLA	4	609	49/65	0.86	0.17	87,92,96,97	0
15	CLA	A	1133	49/65	0.86	0.18	147,157,165,169	0
15	CLA	B	1228	60/65	0.86	0.16	79,82,84,85	0
15	CLA	A	1128	49/65	0.86	0.23	102,113,116,117	0
15	CLA	B	1216	49/65	0.86	0.15	97,105,108,108	0
15	CLA	4	602	49/65	0.86	0.11	95,99,104,107	0
15	CLA	B	1234	49/65	0.86	0.16	86,91,94,95	0
15	CLA	A	1123	48/65	0.86	0.20	128,139,146,148	0
16	CHL	4	611	50/66	0.86	0.14	88,92,96,99	0
15	CLA	1	602	46/65	0.86	0.13	106,110,115,118	0
15	CLA	B	1227	45/65	0.87	0.13	85,88,91,92	0
15	CLA	4	605	49/65	0.87	0.14	80,82,83,84	0
16	CHL	2	611	48/66	0.87	0.17	103,104,111,114	0
15	CLA	A	1140	55/65	0.87	0.20	89,93,98,100	0
15	CLA	1	613	45/65	0.87	0.11	109,119,126,129	0
15	CLA	F	1301	47/65	0.87	0.16	81,82,83,85	0
15	CLA	B	1217	46/65	0.87	0.10	121,128,132,134	0
15	CLA	A	1125	49/65	0.87	0.22	137,141,146,148	0
15	CLA	4	608	46/65	0.88	0.11	92,96,101,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	CHL	2	609	50/66	0.88	0.13	119,129,136,138	0
15	CLA	A	1135	49/65	0.88	0.15	126,139,154,160	0
15	CLA	A	1118	49/65	0.88	0.16	151,164,172,175	0
15	CLA	1	608	46/65	0.88	0.12	91,96,101,103	0
15	CLA	2	603	46/65	0.88	0.14	115,122,128,129	0
15	CLA	1	611	49/65	0.88	0.13	110,118,124,126	0
15	CLA	2	612	49/65	0.88	0.16	91,97,100,102	0
15	CLA	B	1213	49/65	0.88	0.17	111,117,123,125	0
15	CLA	1	606	45/65	0.88	0.12	110,116,120,122	0
15	CLA	A	1105	49/65	0.88	0.12	94,98,104,105	0
15	CLA	A	1117	49/65	0.89	0.20	132,136,143,147	0
14	BCR	B	4004	40/40	0.89	0.20	92,94,97,98	0
15	CLA	B	1212	45/65	0.89	0.16	128,138,147,148	0
15	CLA	A	1106	65/65	0.89	0.21	89,98,104,105	0
15	CLA	A	1110	49/65	0.89	0.14	140,149,157,161	0
15	CLA	B	1223	50/65	0.89	0.18	91,97,99,101	0
16	CHL	1	609	50/66	0.89	0.13	88,91,96,97	0
15	CLA	A	1139	52/65	0.89	0.18	85,88,91,92	0
15	CLA	B	1236	49/65	0.89	0.15	83,87,90,90	0
15	CLA	B	1225	49/65	0.89	0.23	108,114,122,126	0
15	CLA	B	1021	65/65	0.90	0.19	89,103,107,108	0
15	CLA	B	1204	49/65	0.90	0.14	134,146,151,153	0
15	CLA	A	1104	60/65	0.90	0.20	103,109,115,118	0
15	CLA	B	1214	49/65	0.91	0.20	102,105,111,112	0
15	CLA	3	615	46/65	0.91	0.15	118,127,131,133	0
15	CLA	B	1235	60/65	0.91	0.12	80,83,86,87	0
15	CLA	A	1012	60/65	0.91	0.19	89,92,98,100	0
15	CLA	A	1013	65/65	0.91	0.17	86,90,97,99	0
15	CLA	A	1138	65/65	0.91	0.15	82,84,86,87	0
15	CLA	A	1107	49/65	0.91	0.17	85,91,94,96	0
24	CL0	A	1011	50/65	0.91	0.17	100,104,112,115	0
15	CLA	4	603	49/65	0.91	0.14	85,89,92,93	0
15	CLA	1	604	49/65	0.91	0.15	93,95,97,98	0
15	CLA	B	1202	49/65	0.92	0.17	111,117,121,125	0
15	CLA	A	1103	55/65	0.92	0.17	111,121,125,128	0
15	CLA	B	1210	49/65	0.92	0.12	116,124,127,128	0
15	CLA	A	1127	49/65	0.92	0.18	109,118,123,125	0
27	CA	B	6000	1/1	0.92	0.14	97,97,97,97	0
17	LHG	A	5002	24/49	0.93	0.18	99,105,107,108	0
15	CLA	3	605	46/65	0.93	0.16	142,151,156,159	0
15	CLA	B	1231	60/65	0.93	0.16	88,95,99,101	0
15	CLA	B	1222	49/65	0.94	0.12	87,93,96,96	0

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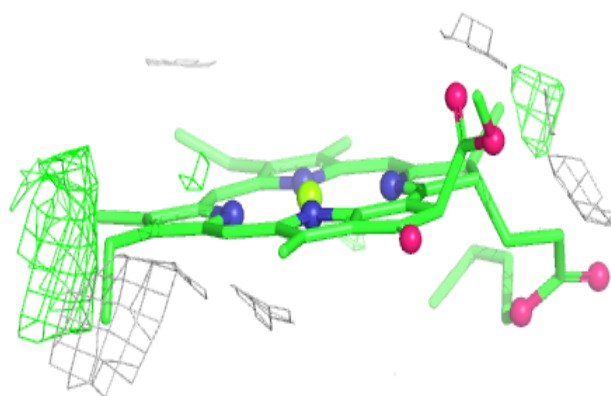
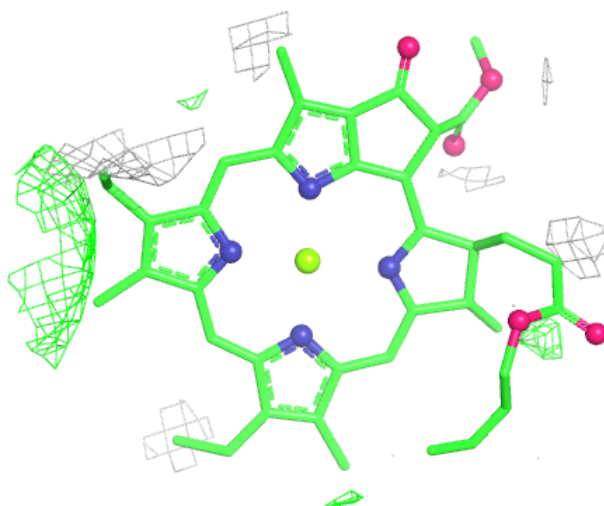
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	SF4	C	3003	8/8	0.96	0.09	115,117,119,120	0
26	SF4	A	3001	8/8	0.98	0.07	108,110,111,113	0
26	SF4	C	3002	8/8	0.98	0.06	121,123,127,198	0

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

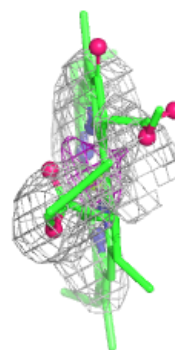
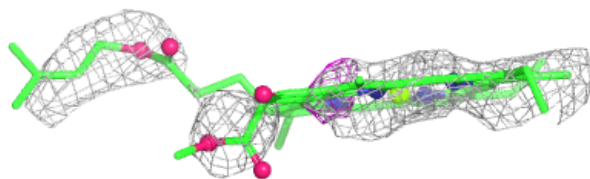
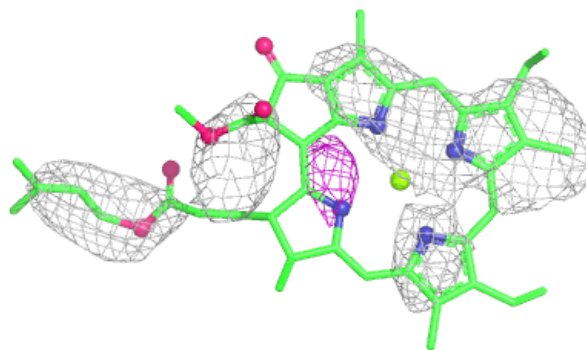
Electron density around CLA A 1121:

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

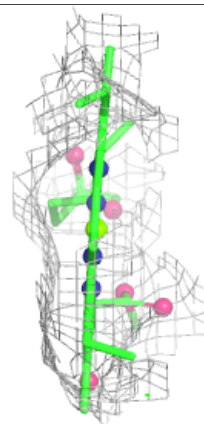
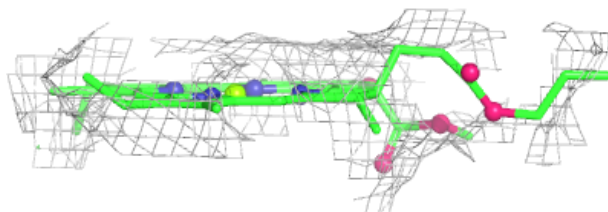
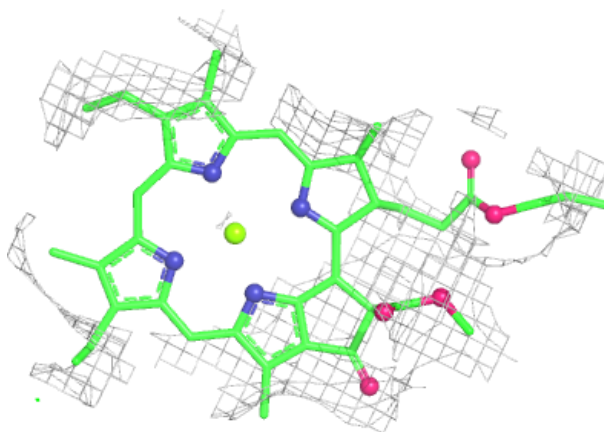


Electron density around CLA 3 607:

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and green (positive)

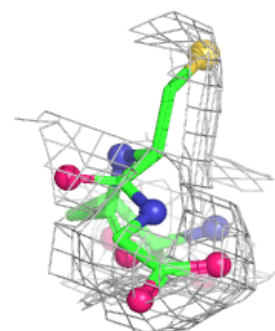
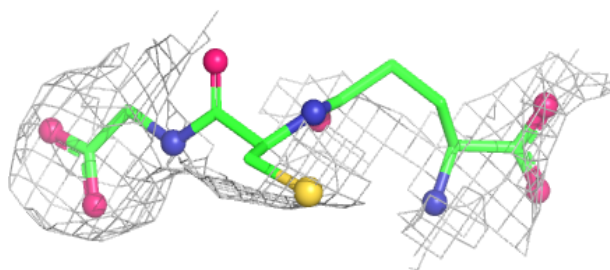
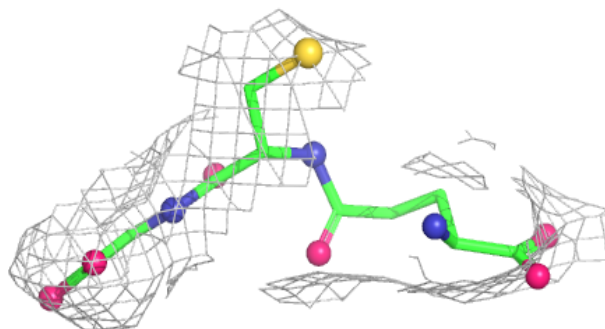
**Electron density around CLA 3 608:**

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

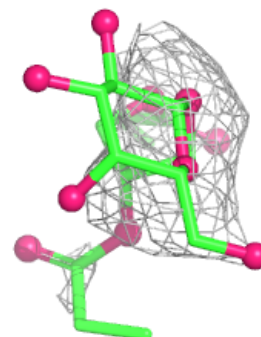
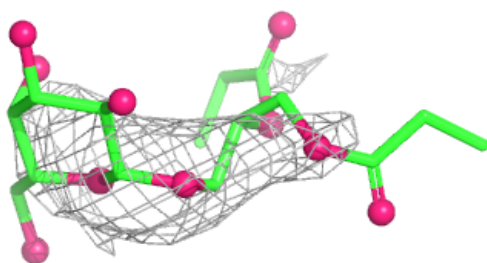
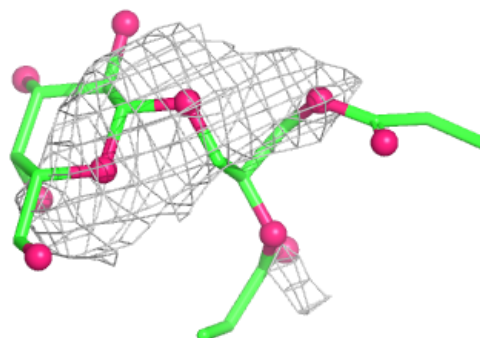


Electron density around GSH 4 831:

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

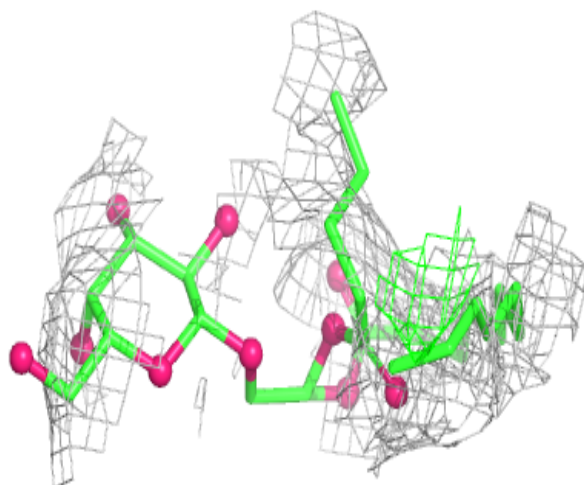
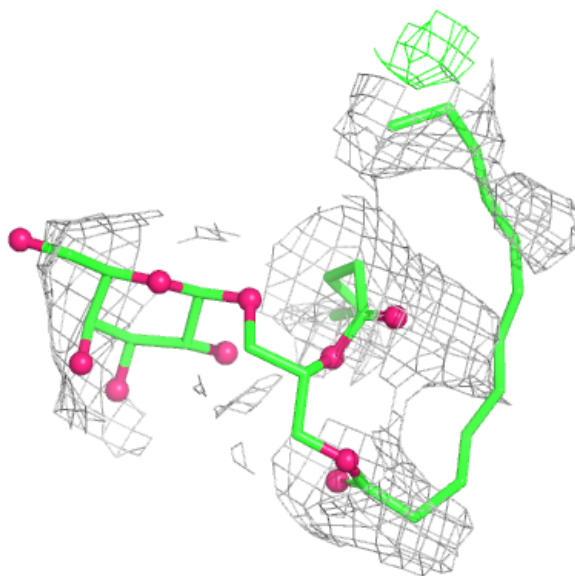
**Electron density around LMG 2 802:**

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



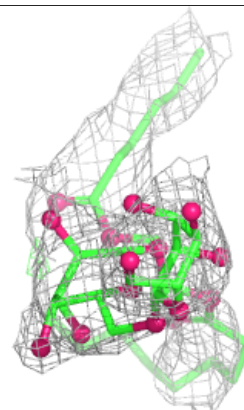
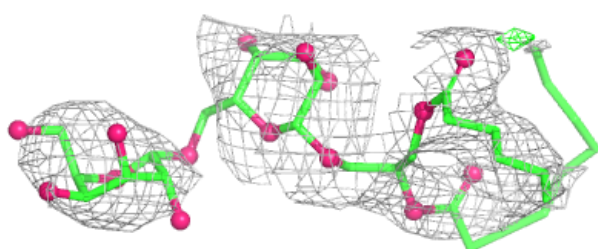
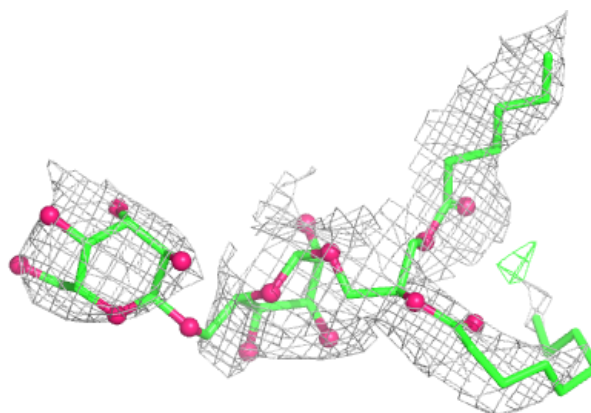
Electron density around LMG 1 802:

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

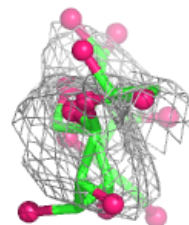
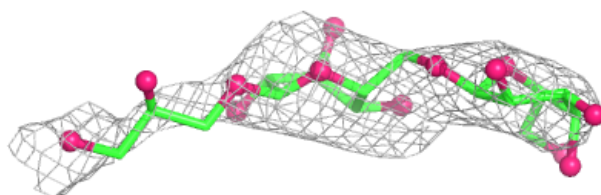
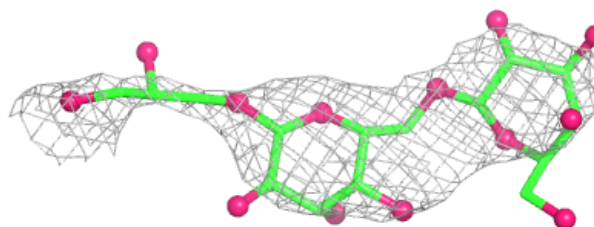


Electron density around DGD 4 811:

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

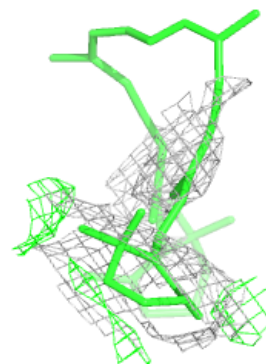
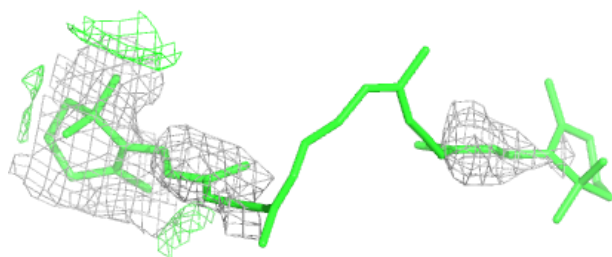
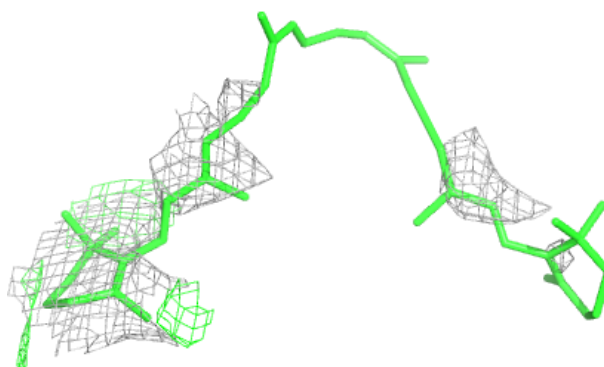
**Electron density around DGD J 5001:**

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

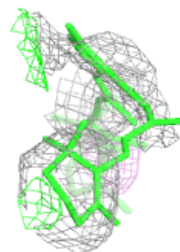
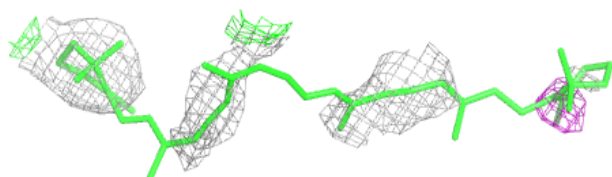
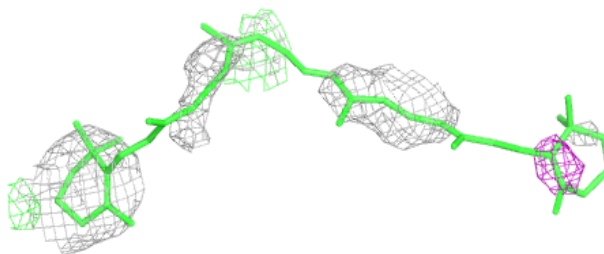


Electron density around BCR 4 505:

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and green (positive)

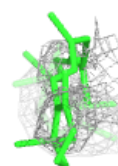
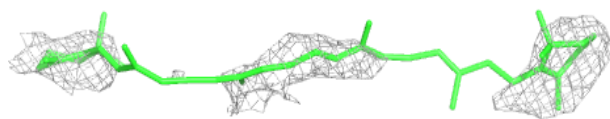
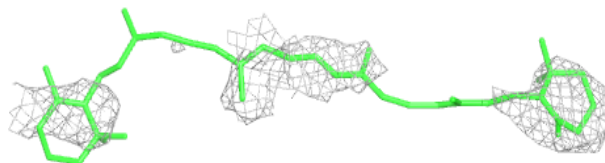
**Electron density around BCR 1 505:**

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

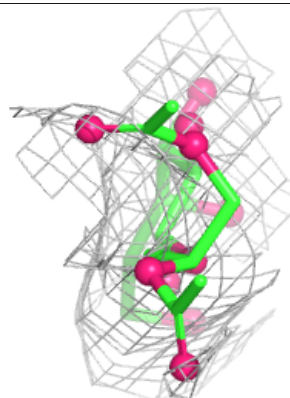
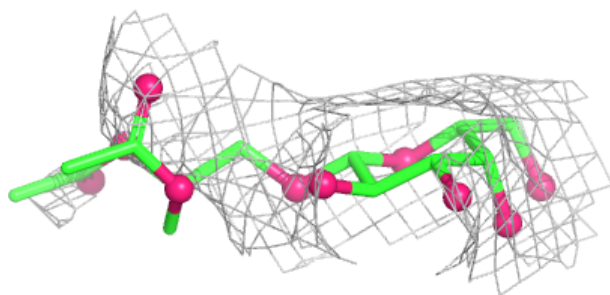
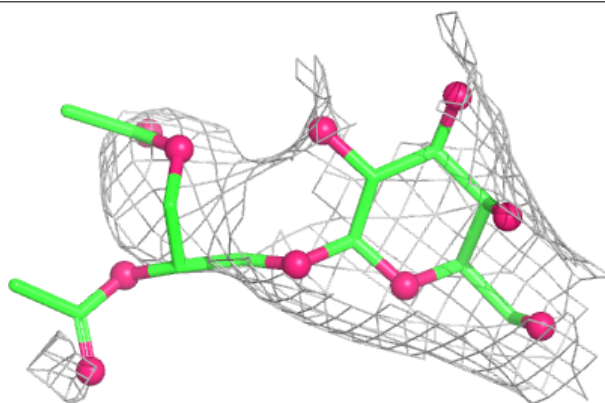


Electron density around BCR J 4003:

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and green (positive)

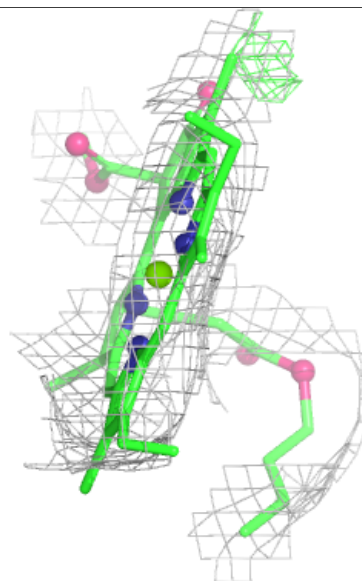
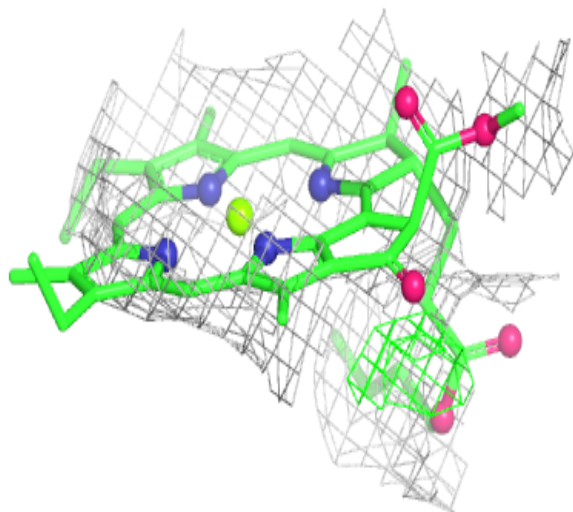
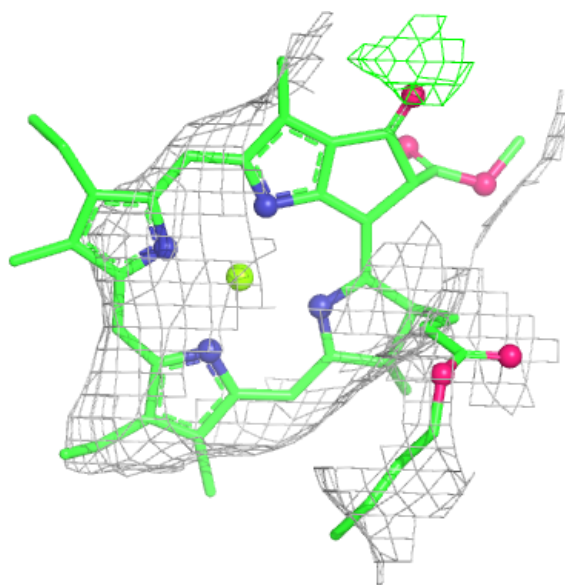
**Electron density around LMG 1 803:**

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



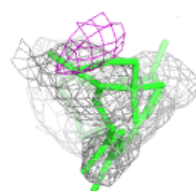
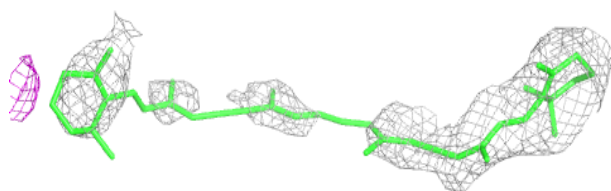
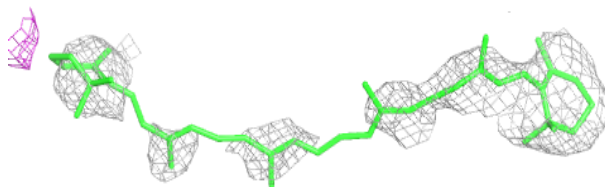
Electron density around CLA A 1120:

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and green (positive)

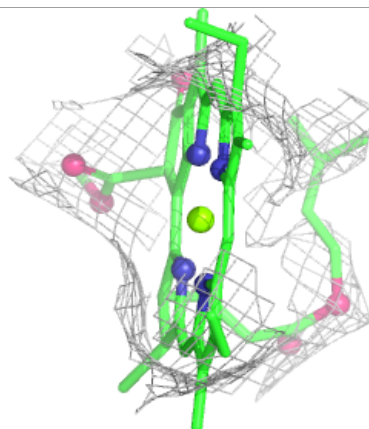
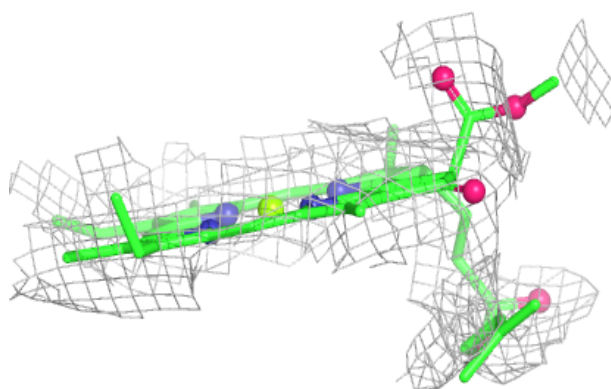
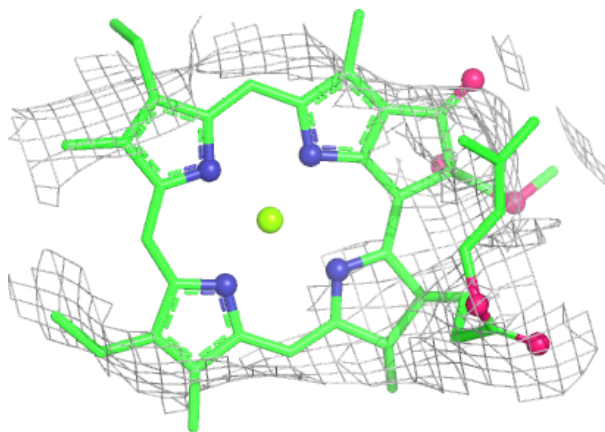


Electron density around BCR 4 503:

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and green (positive)

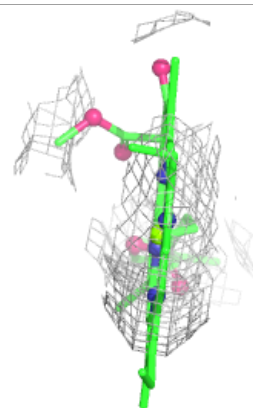
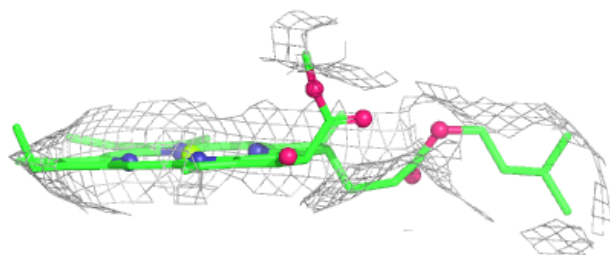
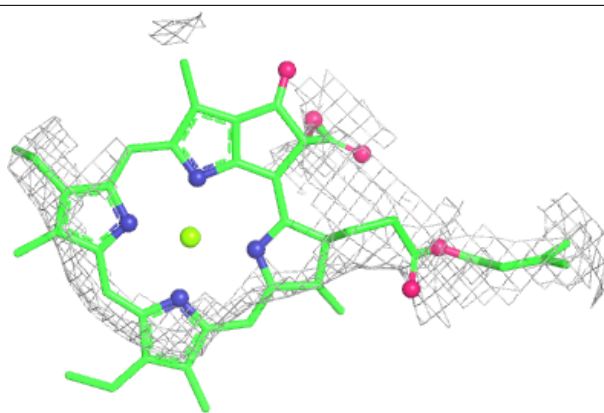
**Electron density around CLA A 1141:**

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



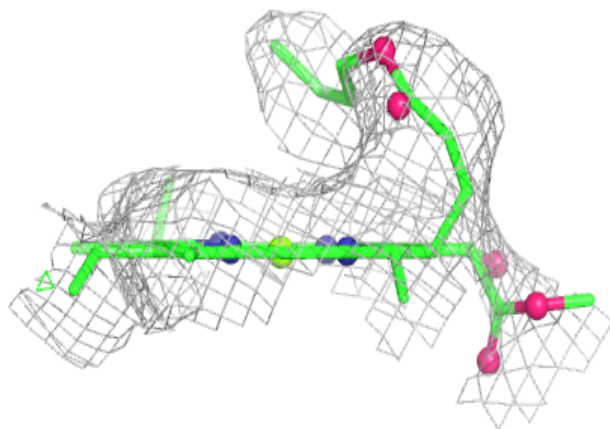
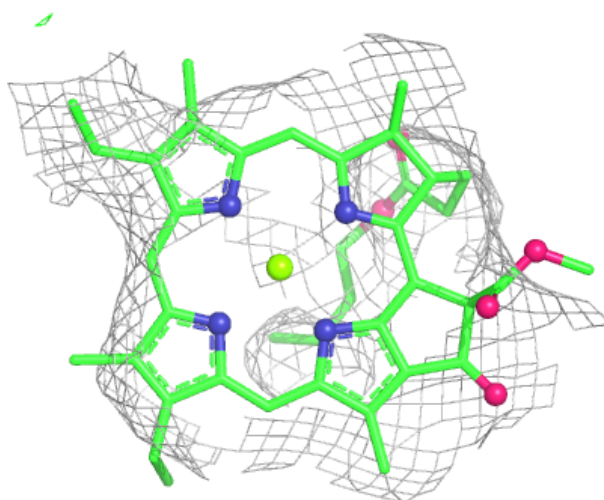
Electron density around CLA A 1131:

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



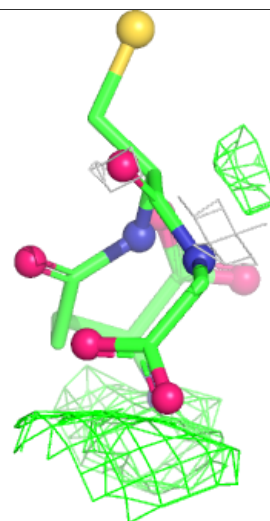
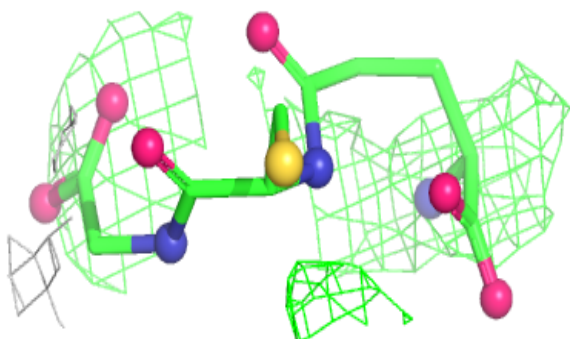
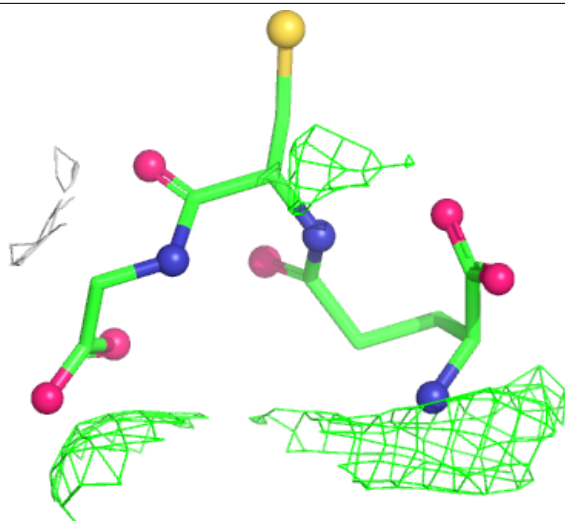
Electron density around CLA B 1218:

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and green (positive)



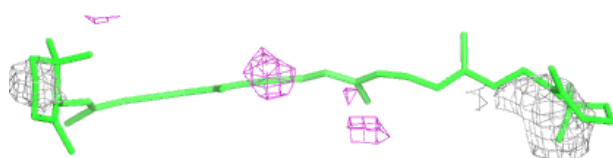
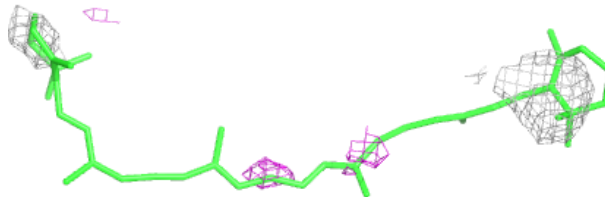
Electron density around GSH B 5031:

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and green (positive)

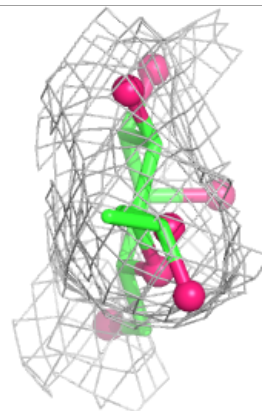
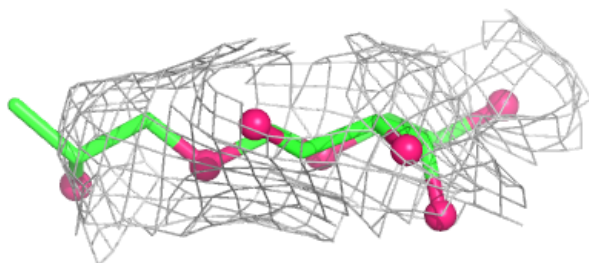
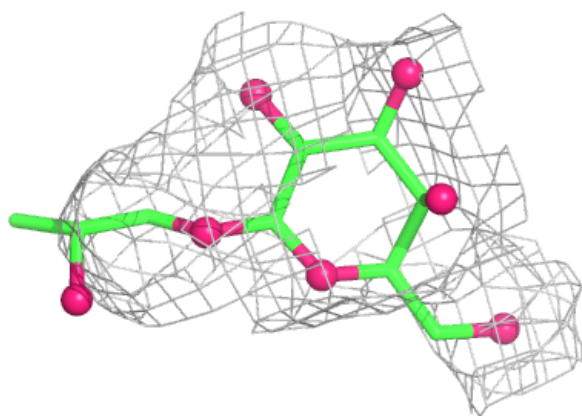


Electron density around BCR B 4003:

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and green (positive)

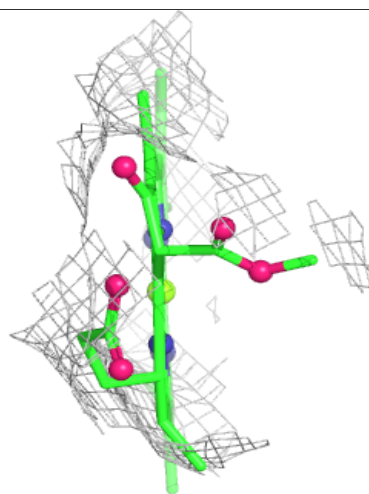
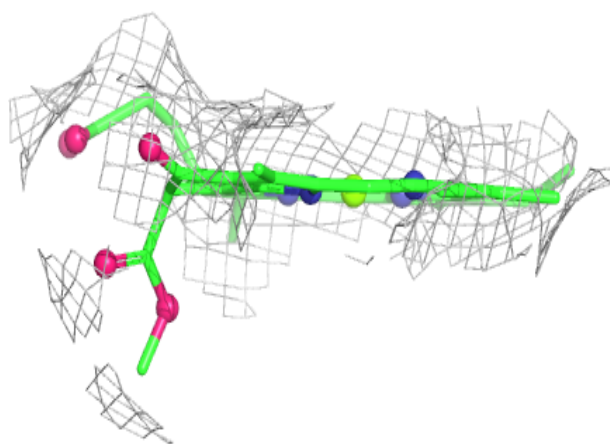
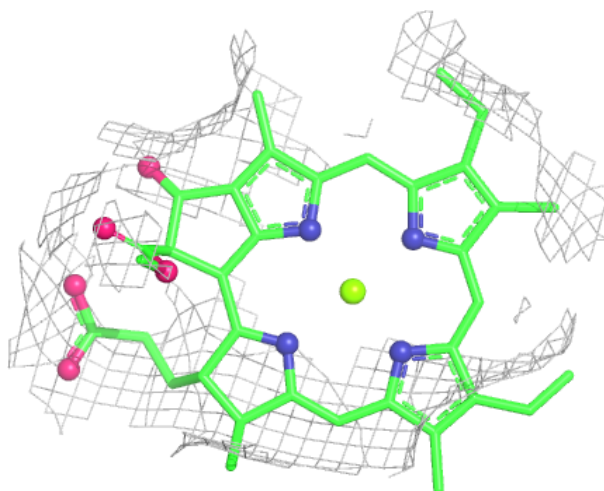
**Electron density around LMG 2 803:**

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and green (positive)



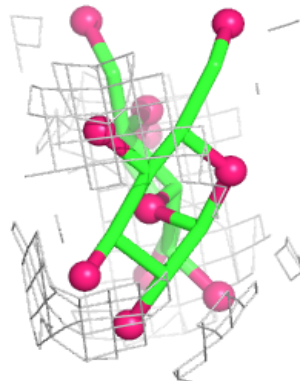
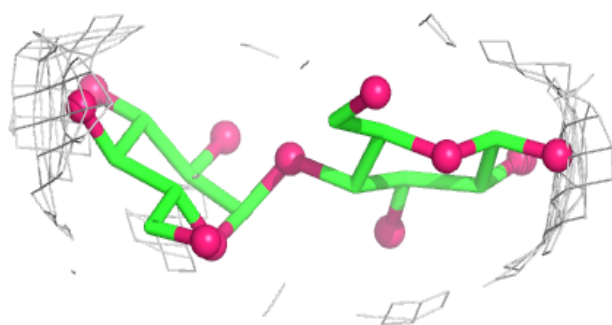
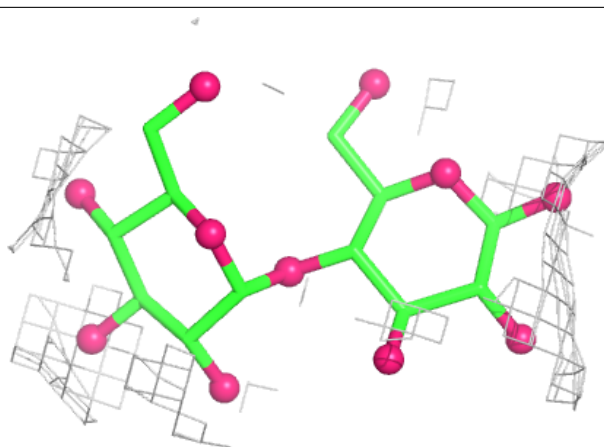
Electron density around CLA 3 603:

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and green (positive)



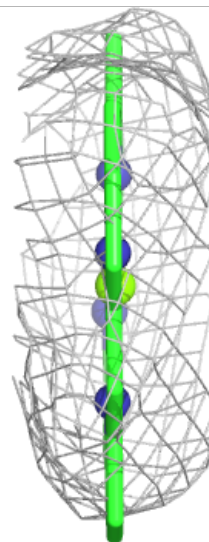
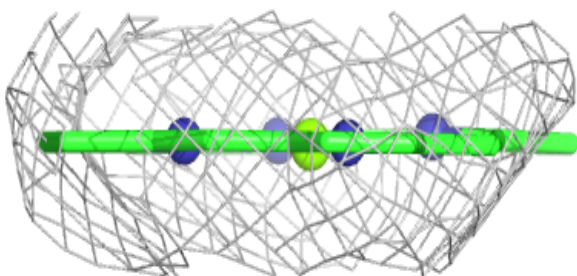
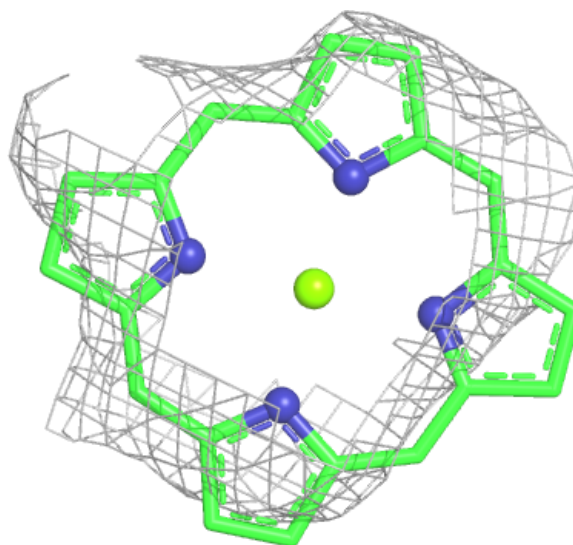
Electron density around LMT 2 821:

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



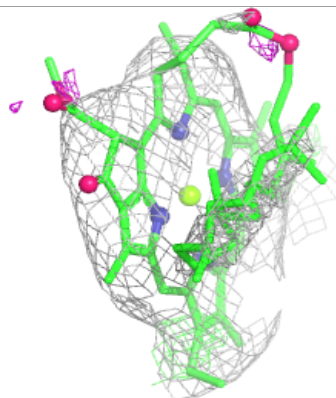
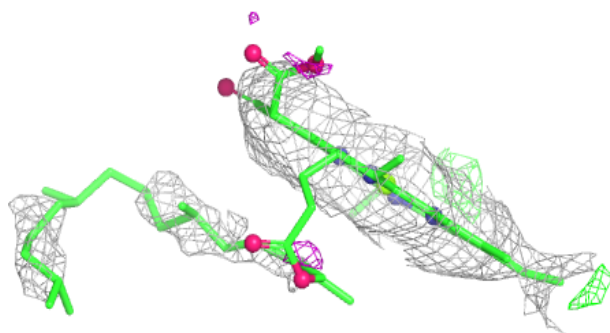
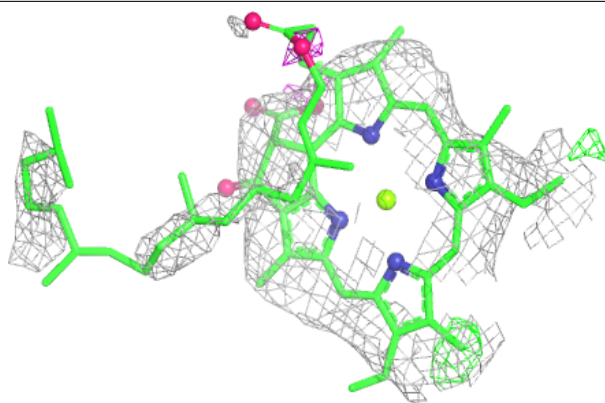
Electron density around CLA B 1207:

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



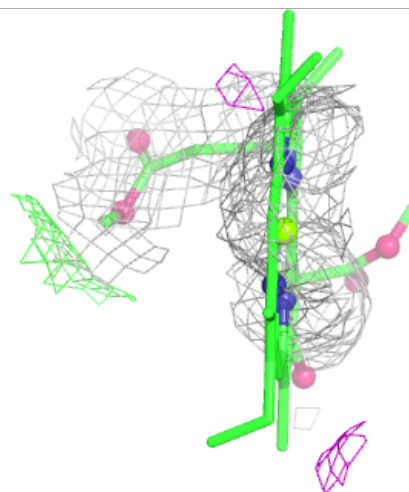
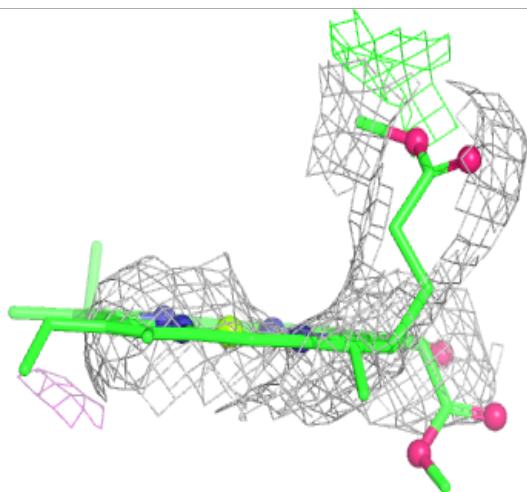
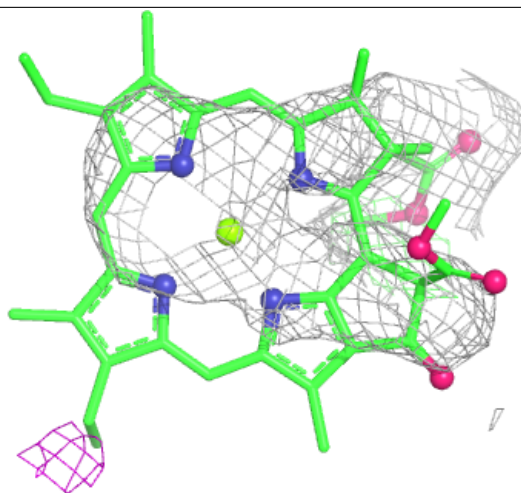
Electron density around CLA 1 615:

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



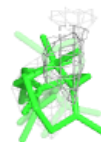
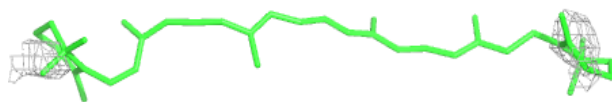
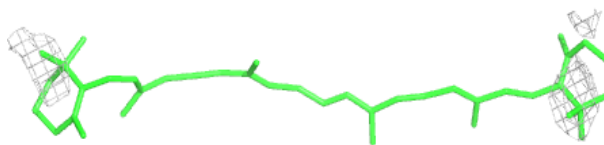
Electron density around CLA A 1114:

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



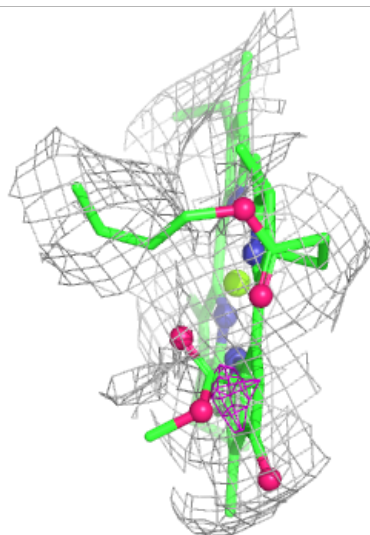
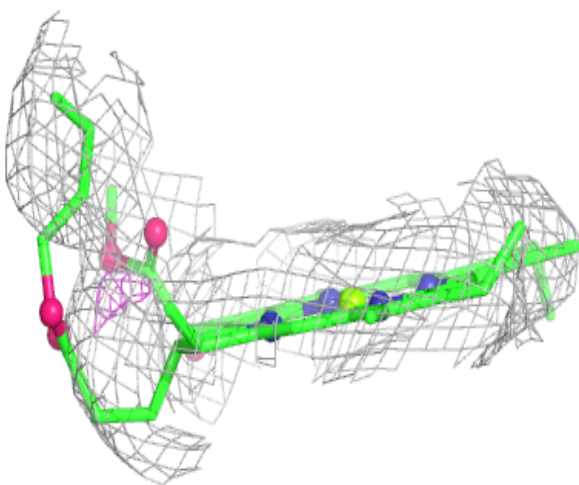
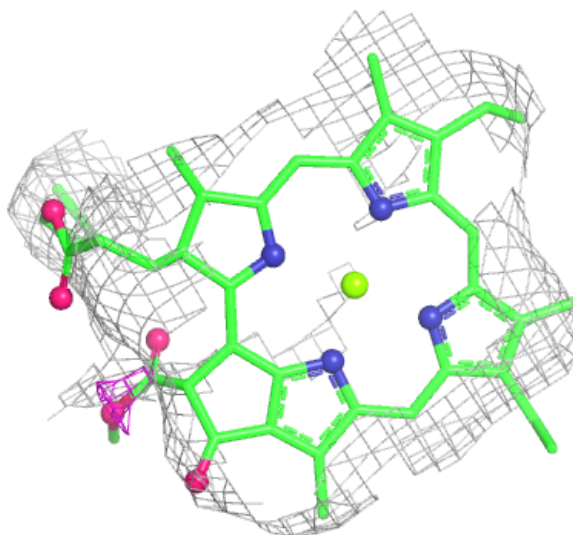
Electron density around BCR A 4002:

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



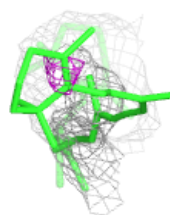
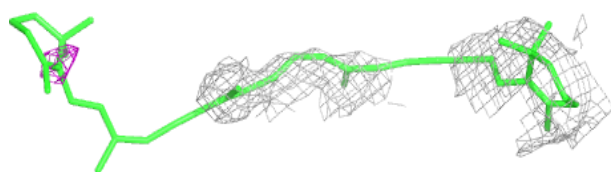
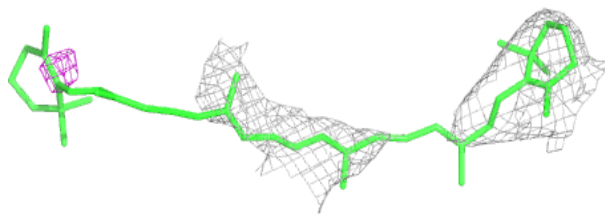
Electron density around CLA 2 602:

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

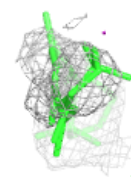
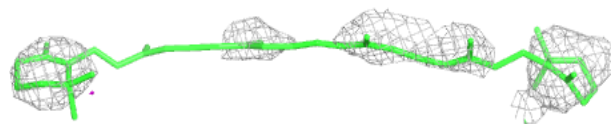
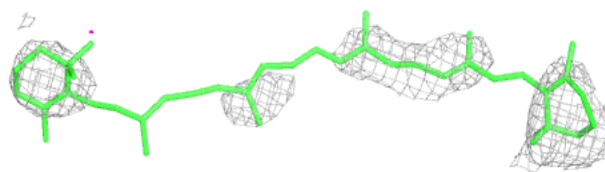


Electron density around BCR 1 503:

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

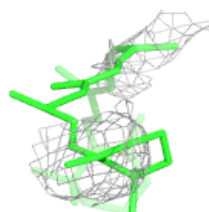
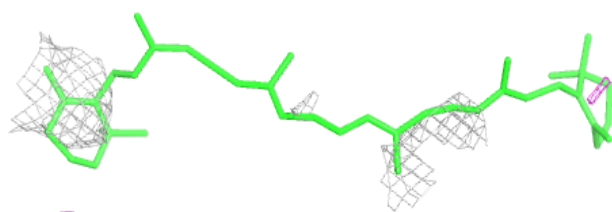
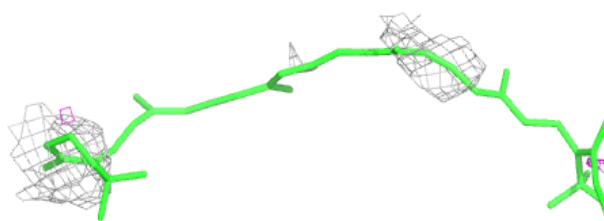
**Electron density around BCR J 4001:**

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

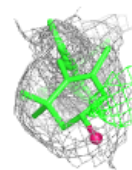
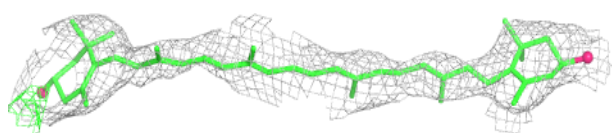
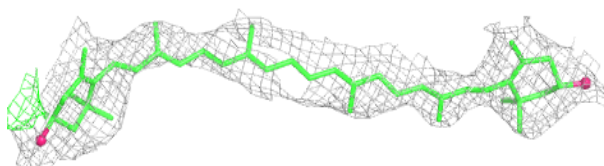


Electron density around BCR B 4001:

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

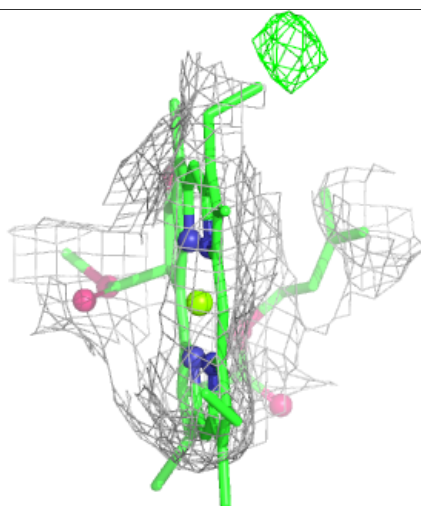
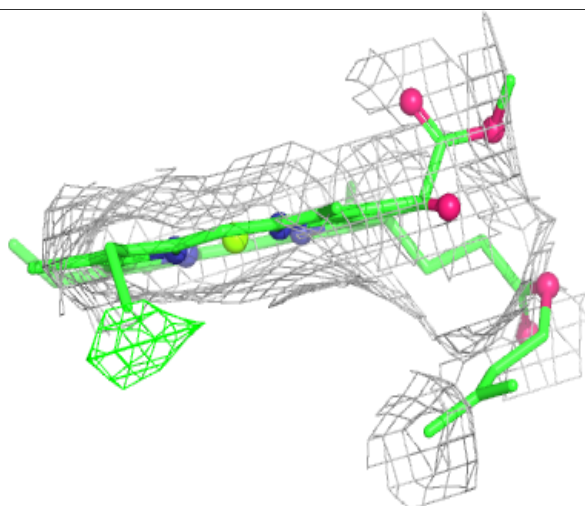
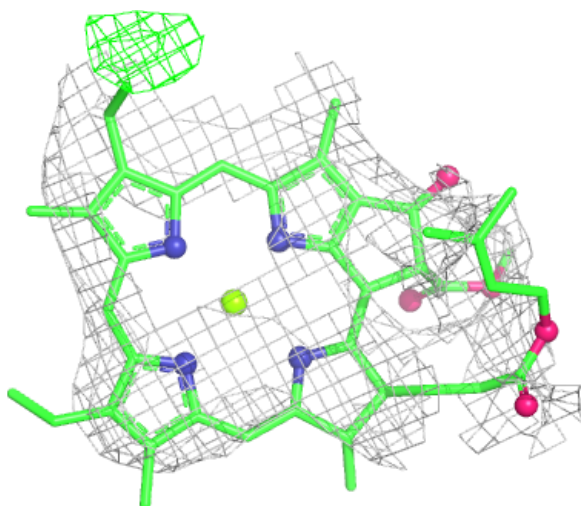
**Electron density around LUT 4 501:**

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



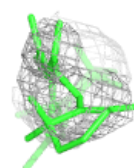
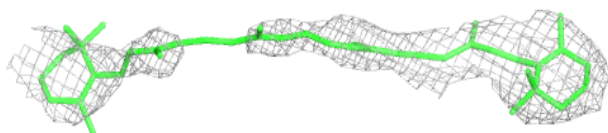
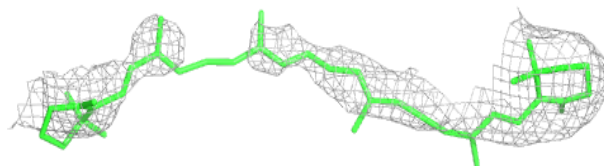
Electron density around CLA B 1238:

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

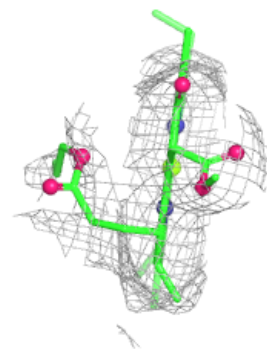
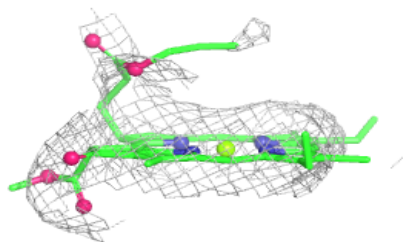
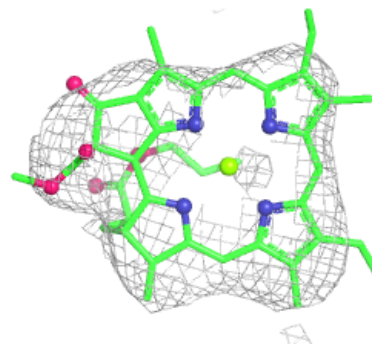


Electron density around BCR 2 503:

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

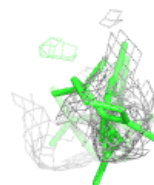
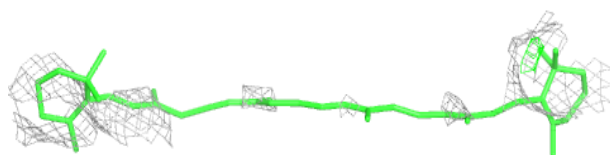
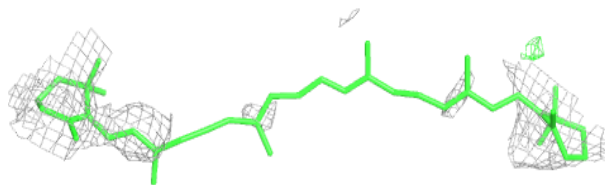
**Electron density around CLA B 1201:**

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

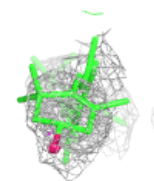
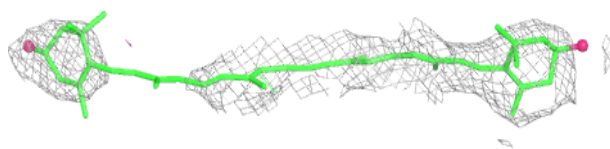
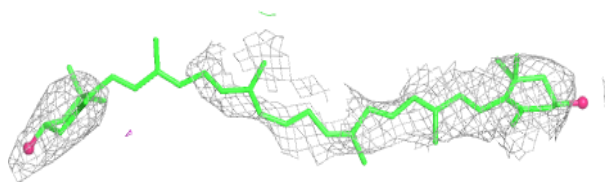


Electron density around BCR 3 503:

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

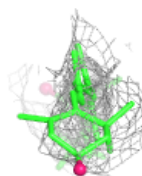
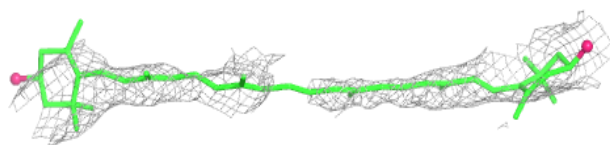
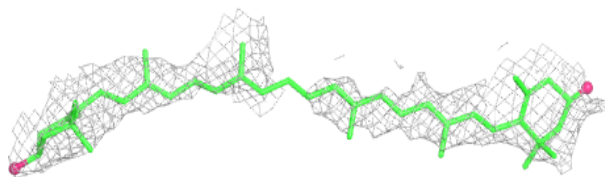
**Electron density around LUT 1 501:**

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

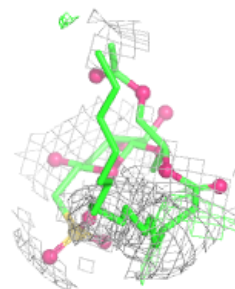
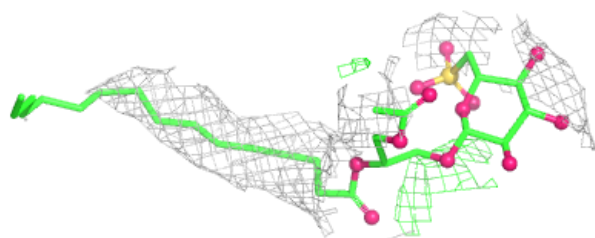
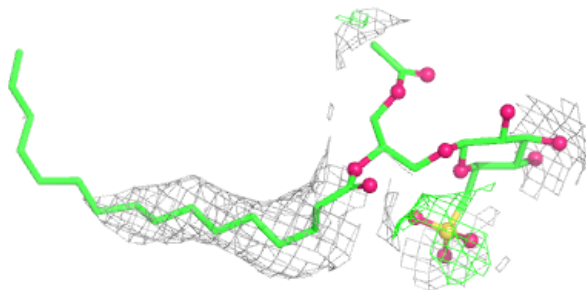


Electron density around LUT 2 501:

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

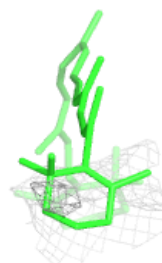
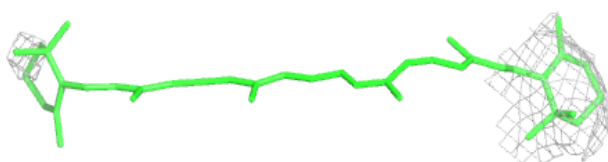
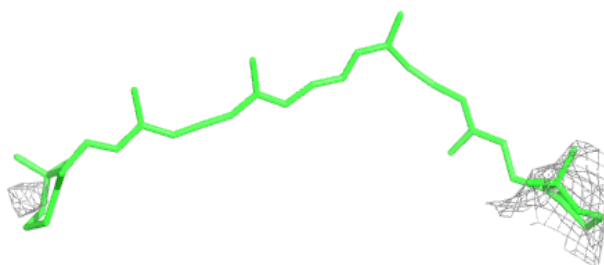
**Electron density around SQD 1 811:**

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

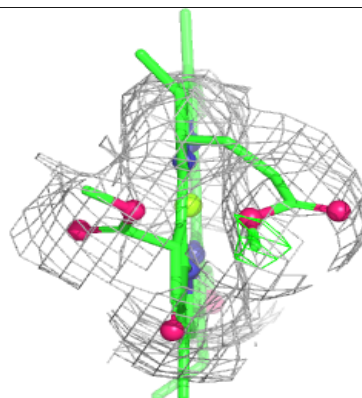
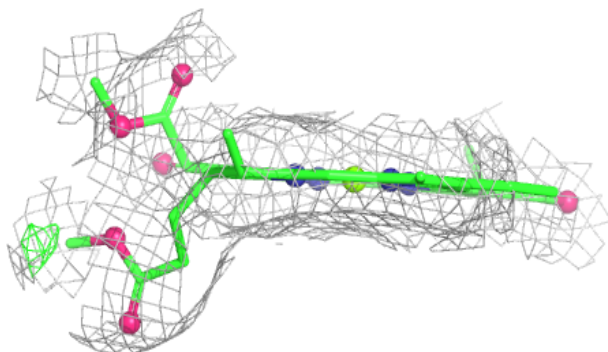
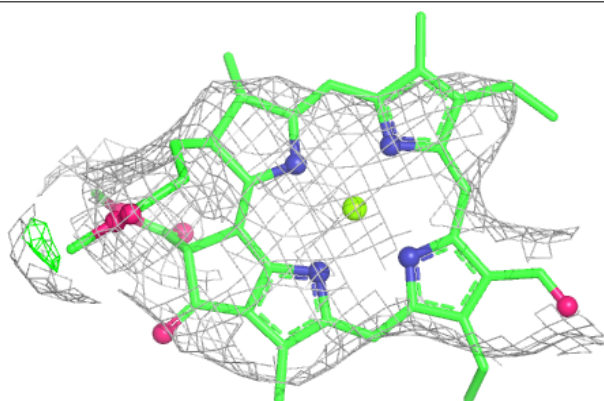


Electron density around BCR A 4004:

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

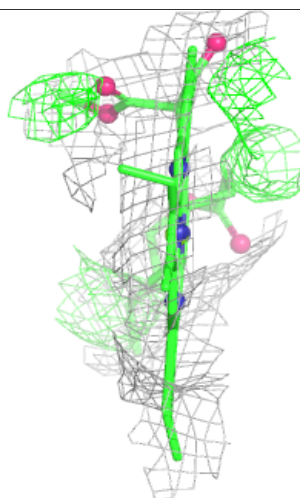
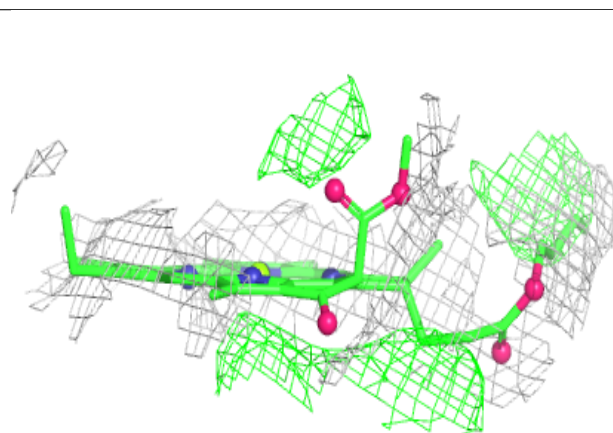
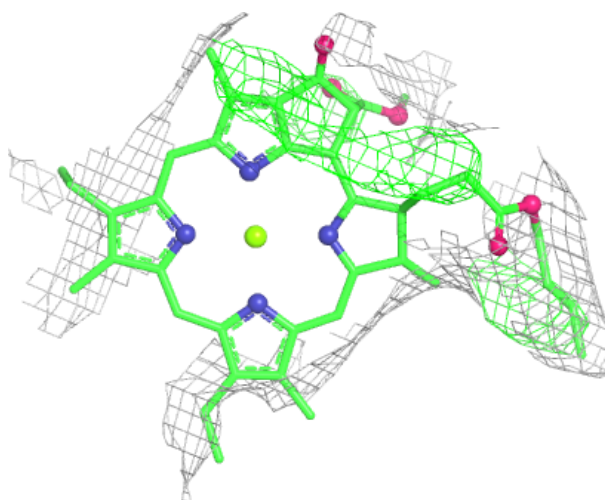
**Electron density around CHL 1 610:**

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



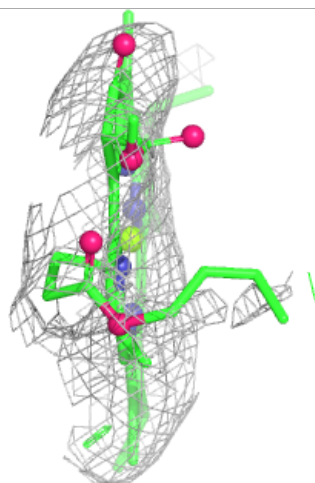
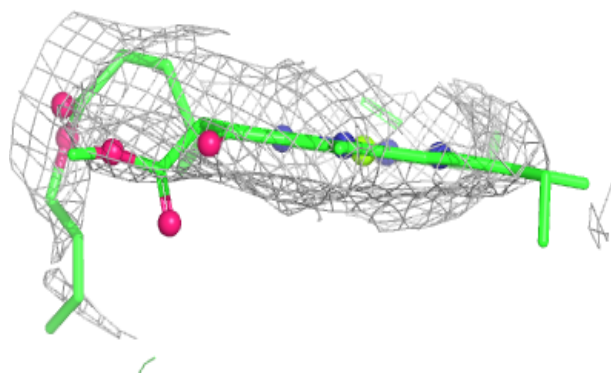
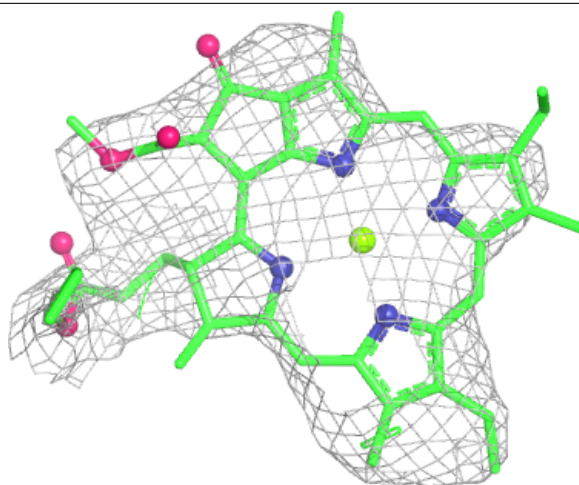
Electron density around CLA A 1111:

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



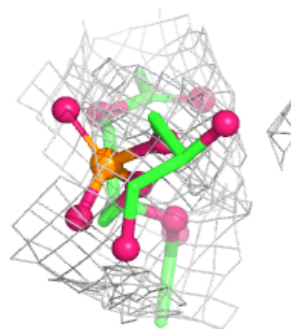
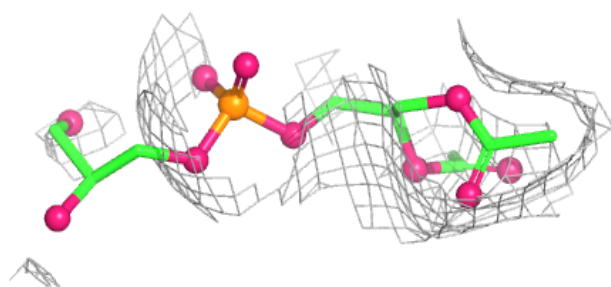
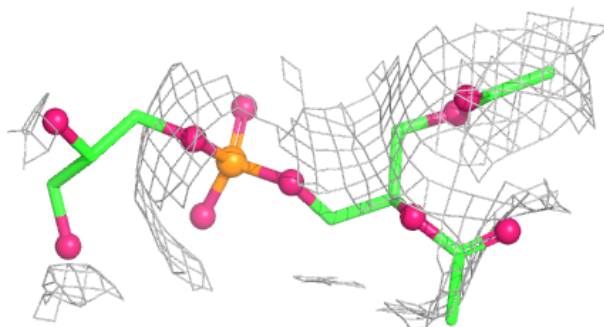
Electron density around CLA B 1203:

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

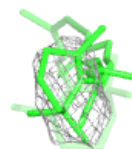
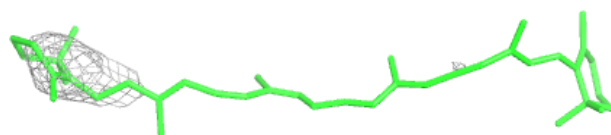
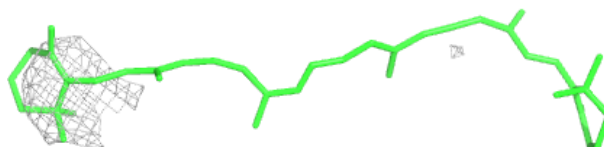


Electron density around LHG 2 801:

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

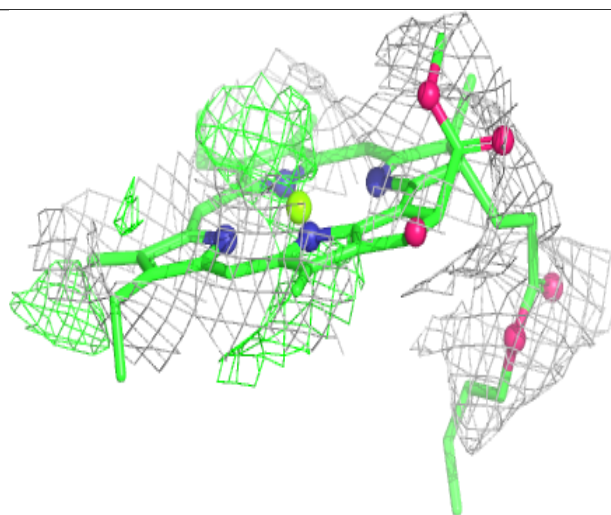
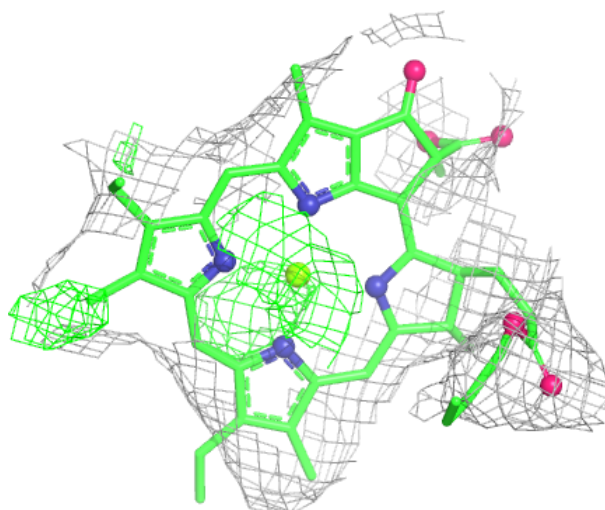
**Electron density around BCR A 4007:**

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



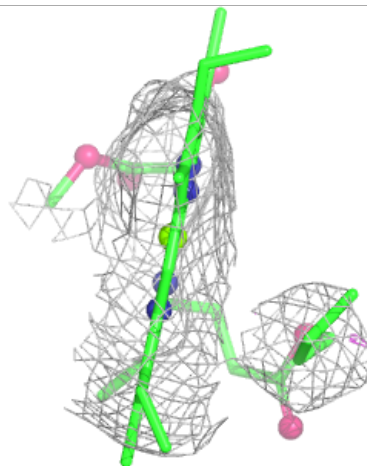
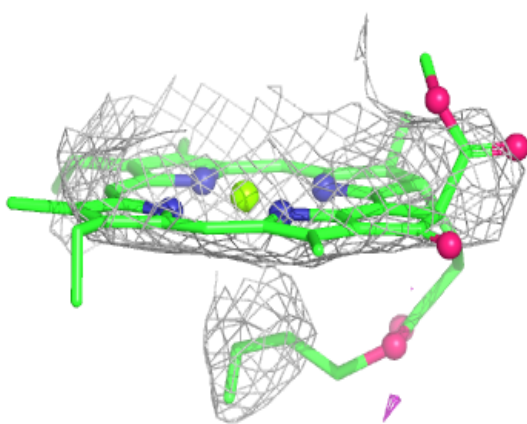
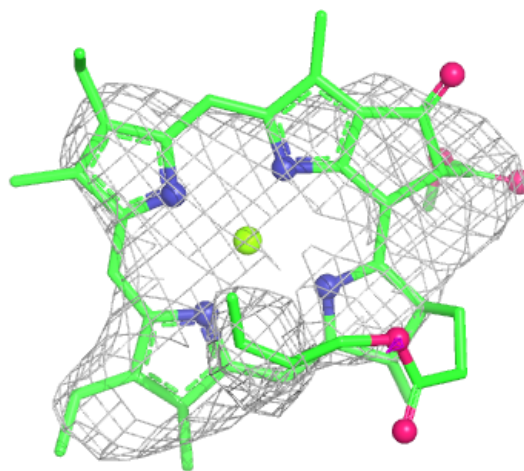
Electron density around CLA 4 607:

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



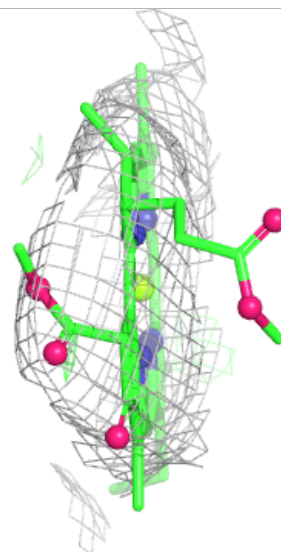
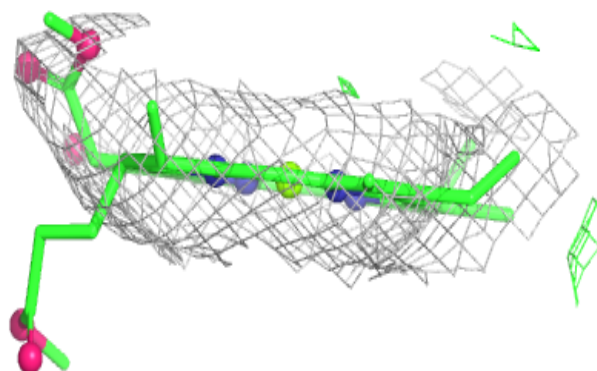
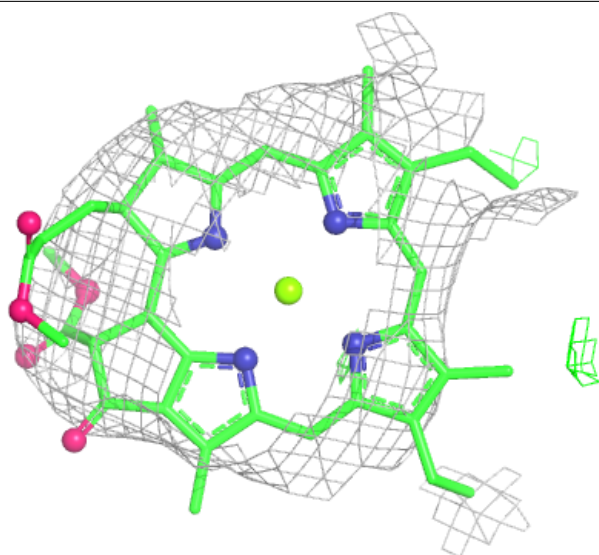
Electron density around CLA B 1224:

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



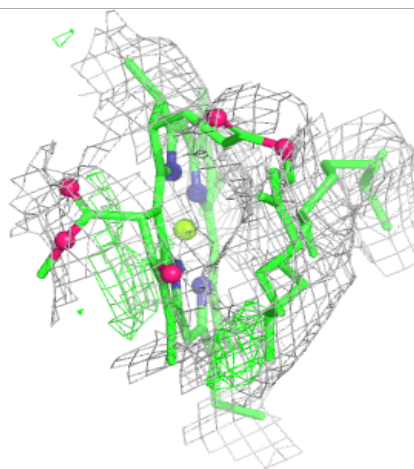
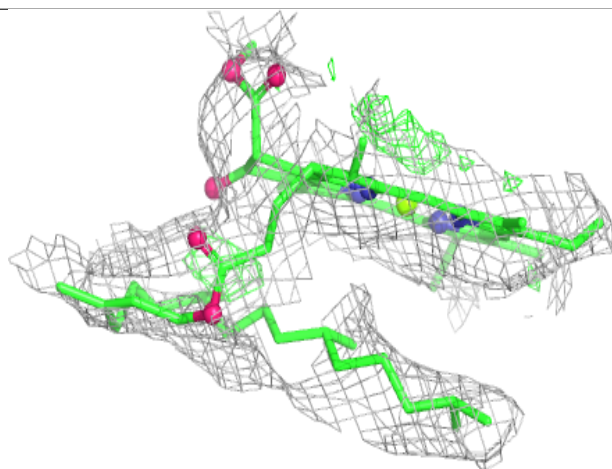
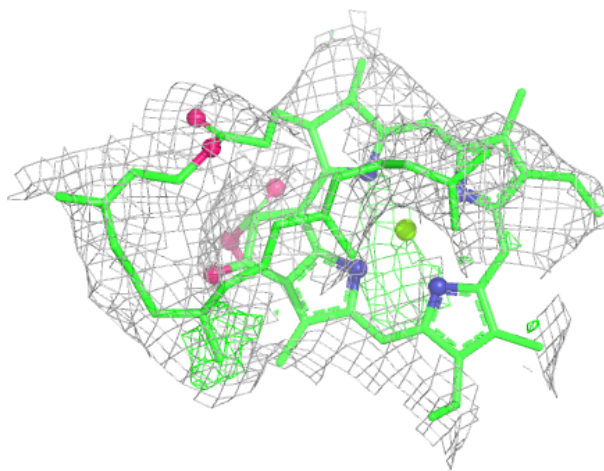
Electron density around CLA A 1108:

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



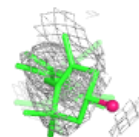
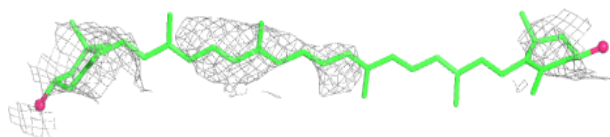
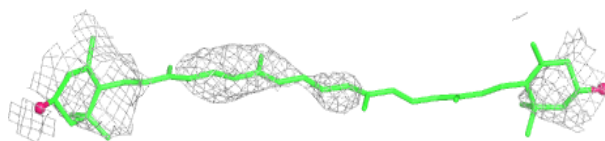
Electron density around CLA 2 605:

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



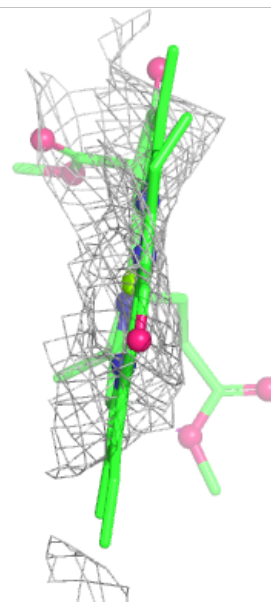
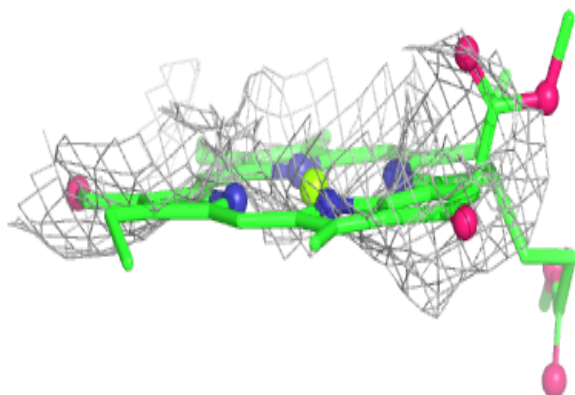
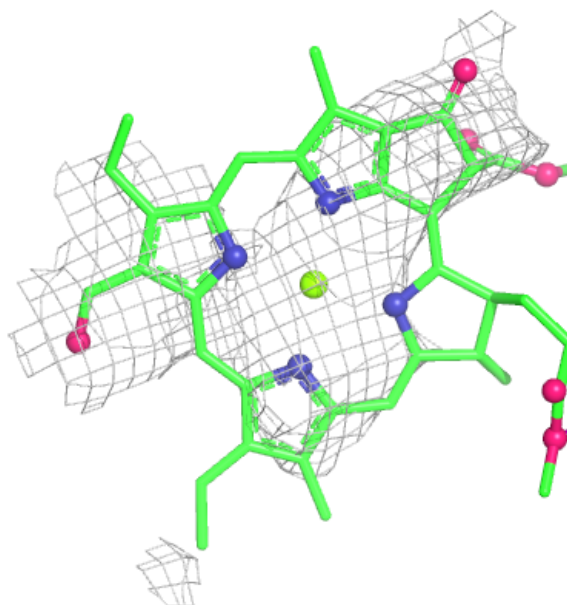
Electron density around LUT 3 501:

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



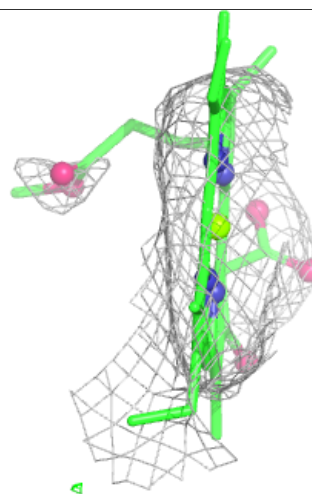
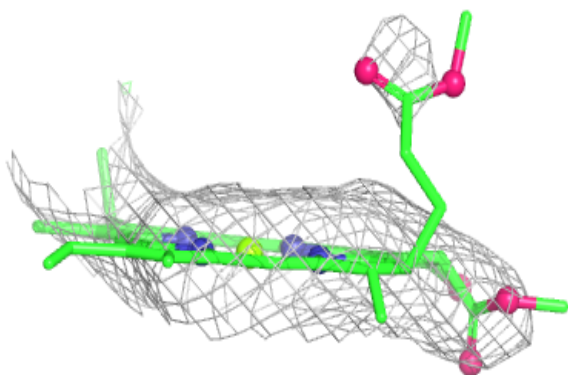
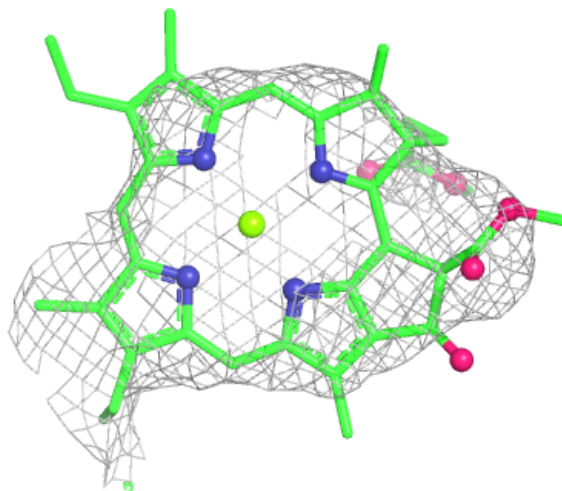
Electron density around CHL 3 604:

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



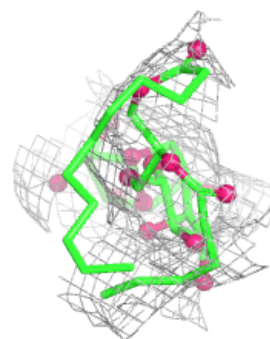
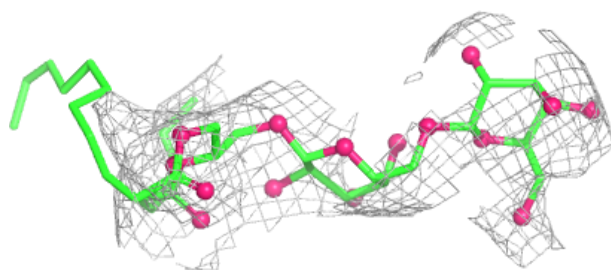
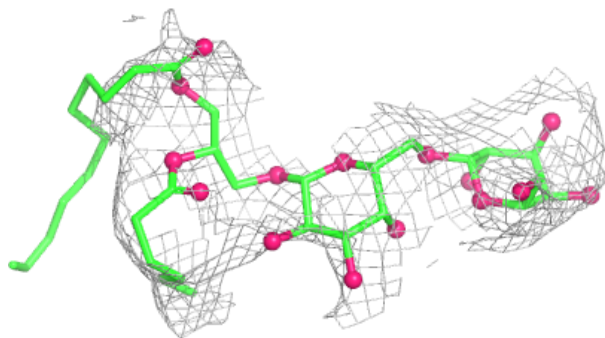
Electron density around CLA 3 611:

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



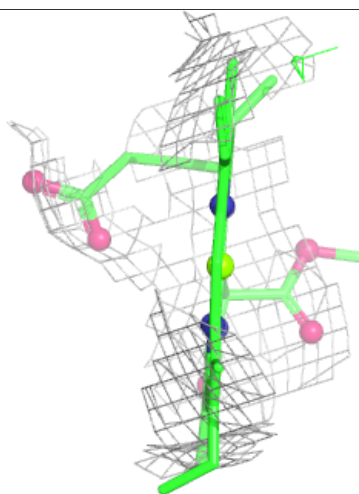
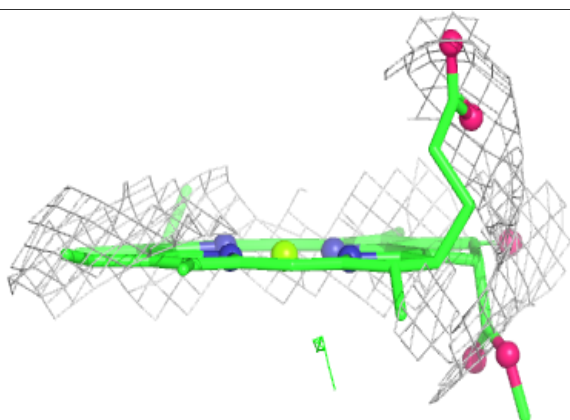
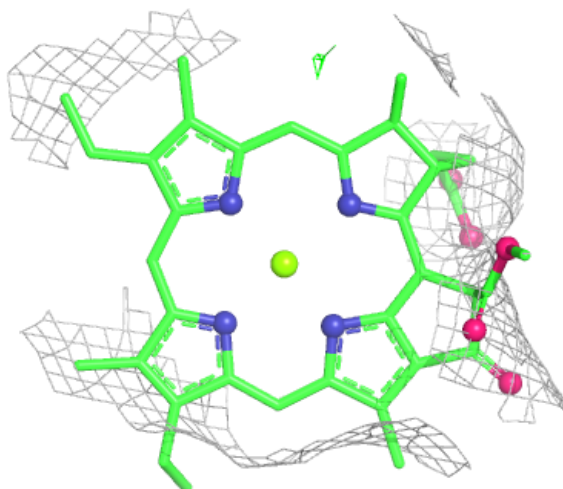
Electron density around DGD 2 811:

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



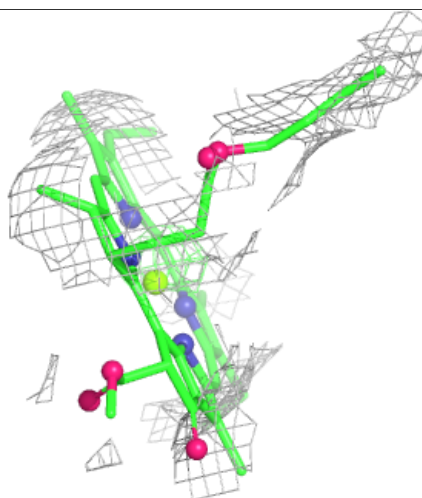
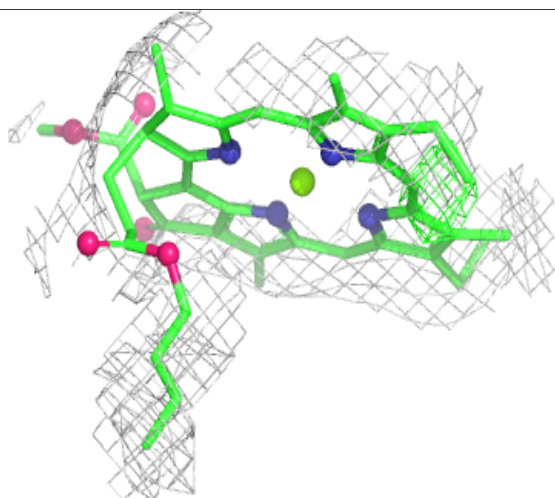
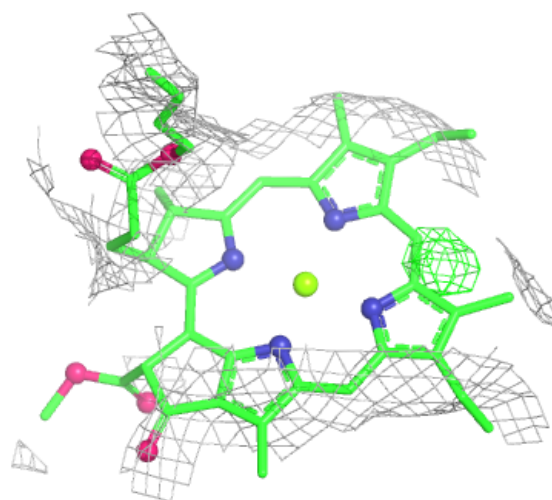
Electron density around CLA 3 606:

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



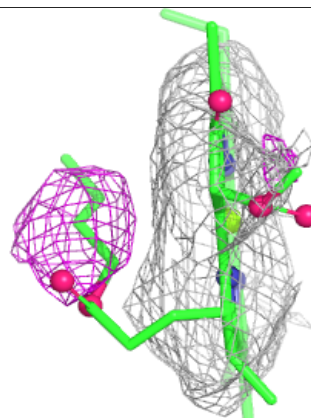
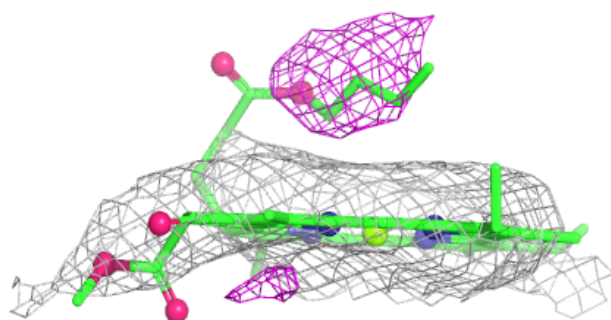
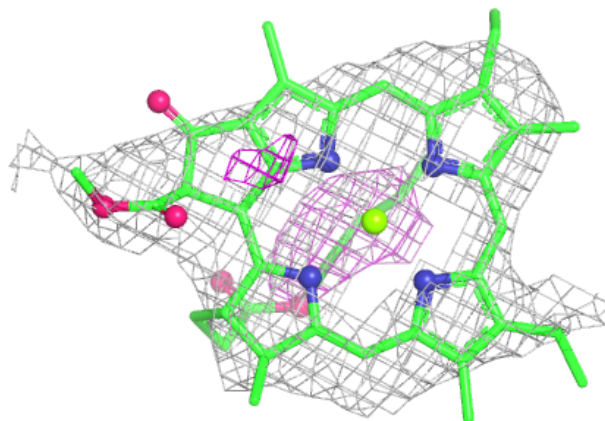
Electron density around CLA B 1208:

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



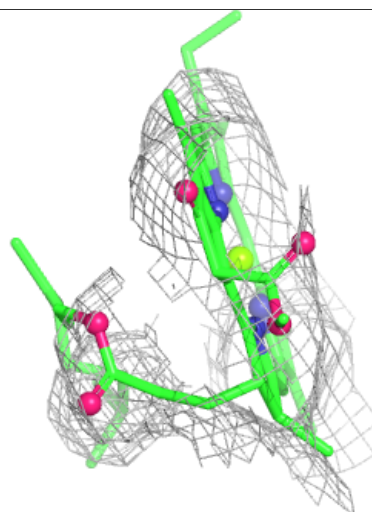
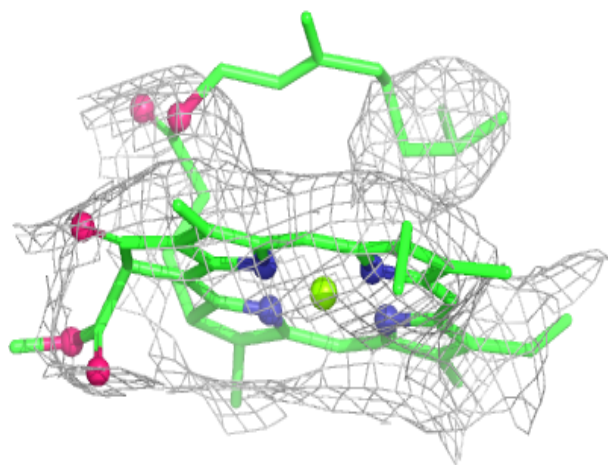
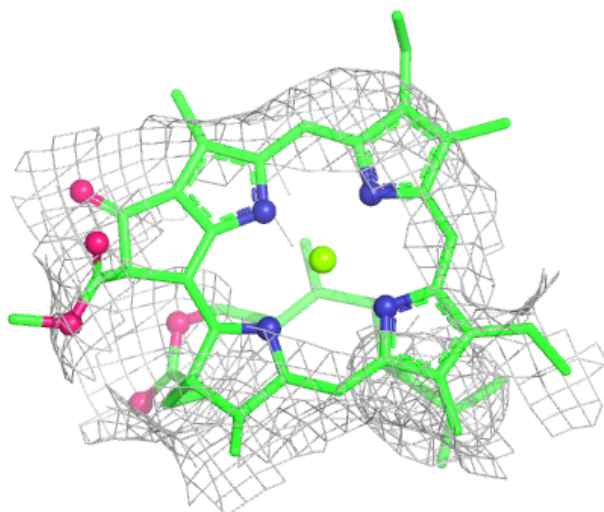
Electron density around CLA B 1211:

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



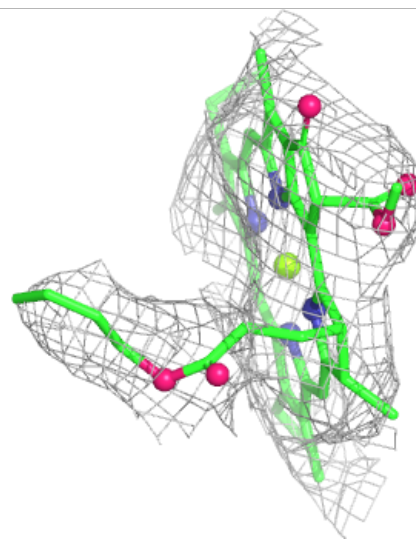
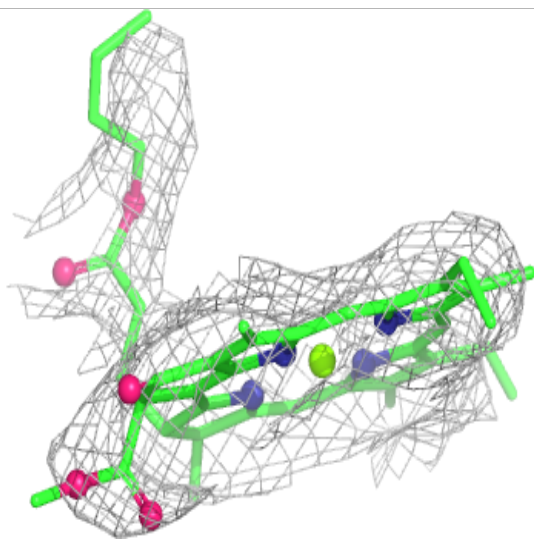
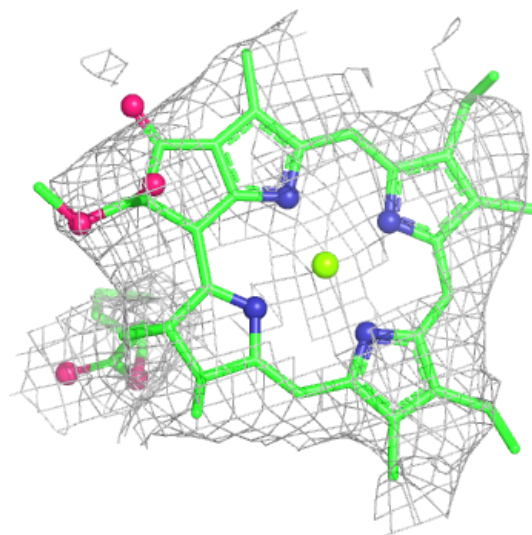
Electron density around CLA A 1130:

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



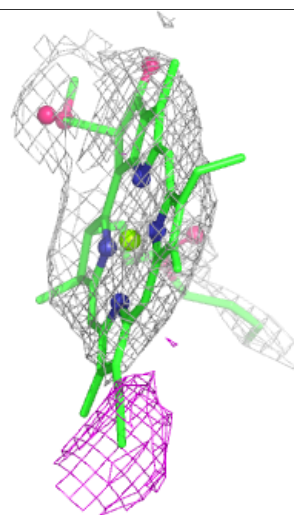
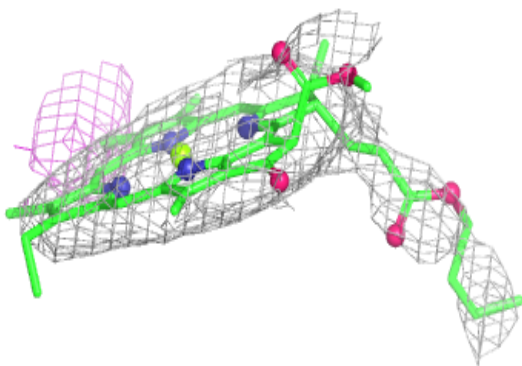
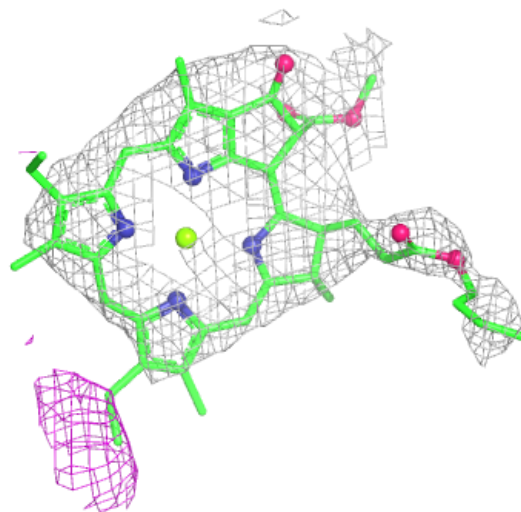
Electron density around CLA B 1219:

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



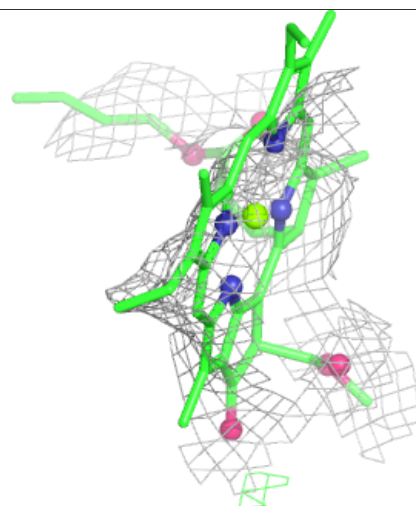
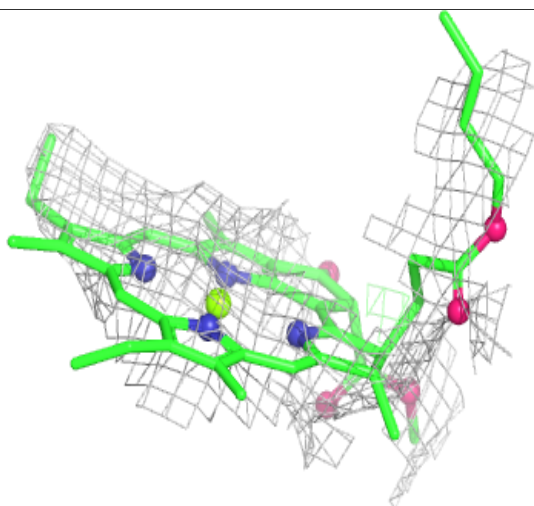
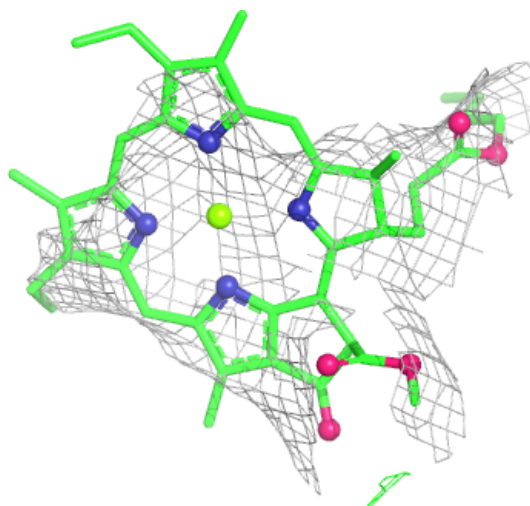
Electron density around CLA B 1230:

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



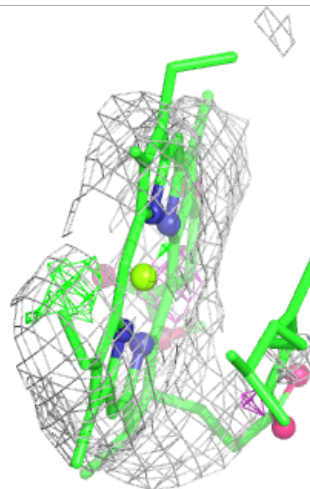
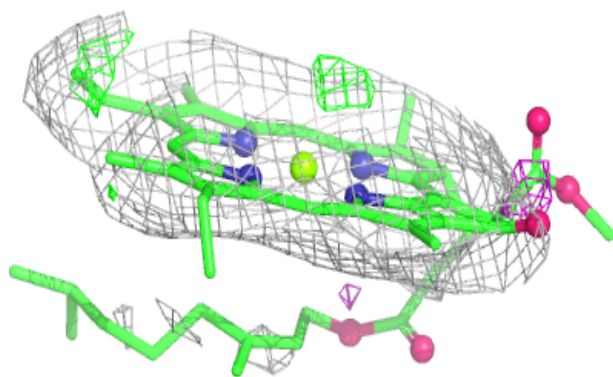
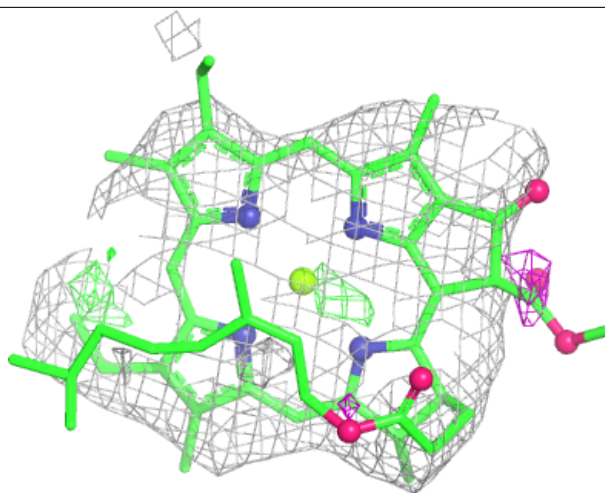
Electron density around CLA 3 601:

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



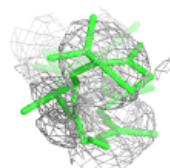
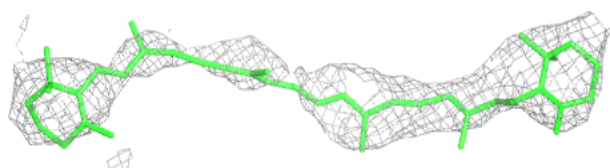
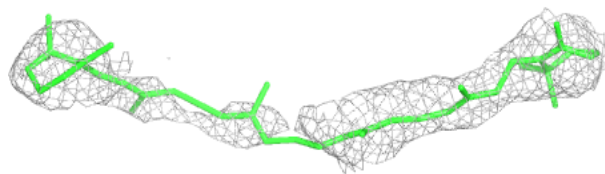
Electron density around CLA 4 615:

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

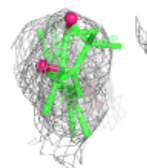
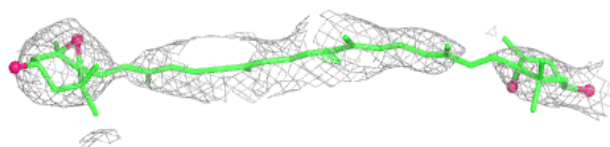
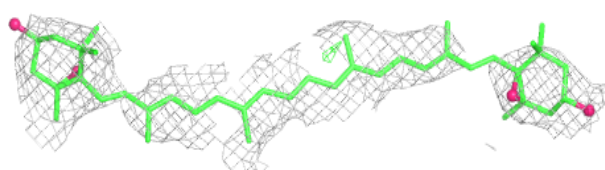


Electron density around BCR J 4002:

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

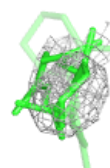
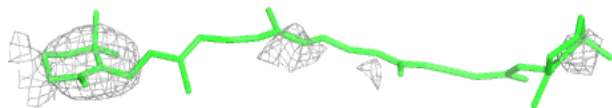
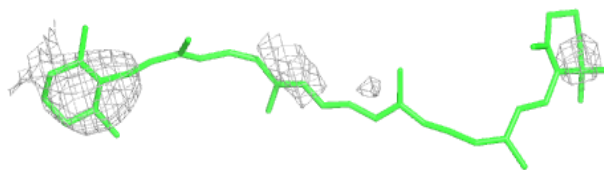
**Electron density around XAT 2 502:**

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

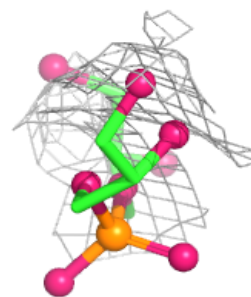
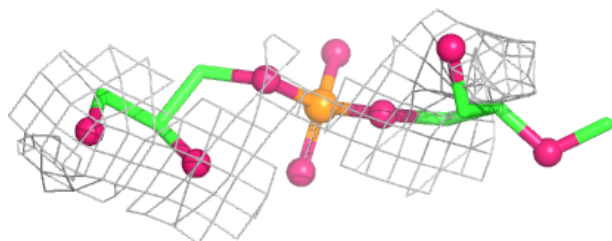
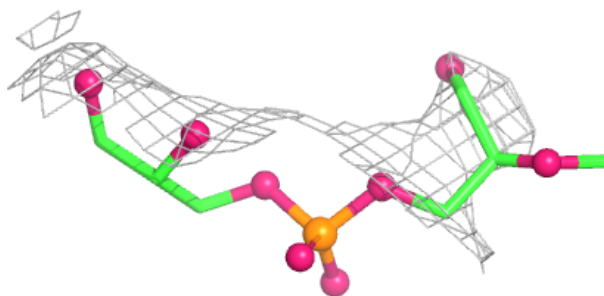


Electron density around BCR A 4003:

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

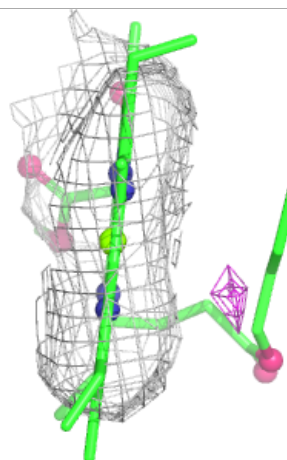
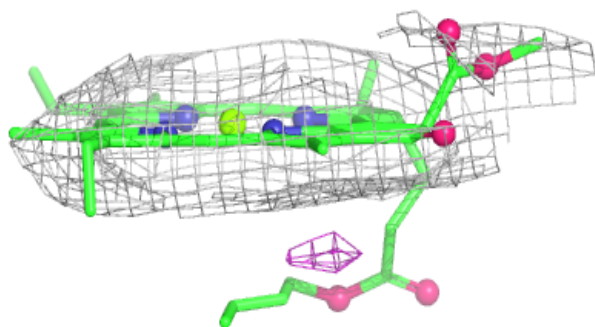
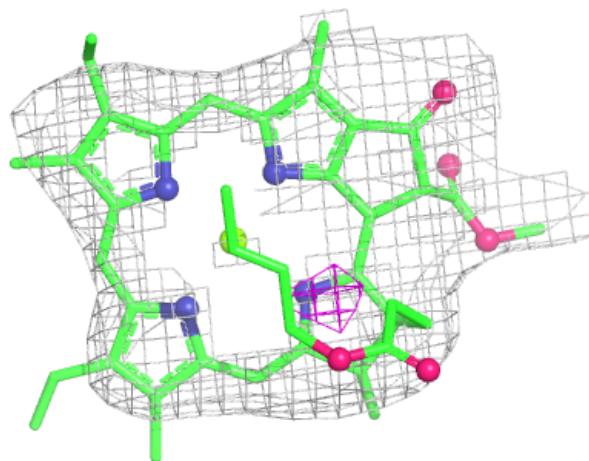
**Electron density around LHG A 5001:**

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



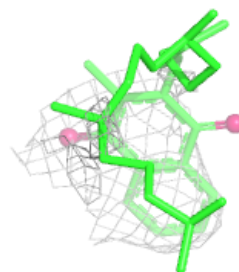
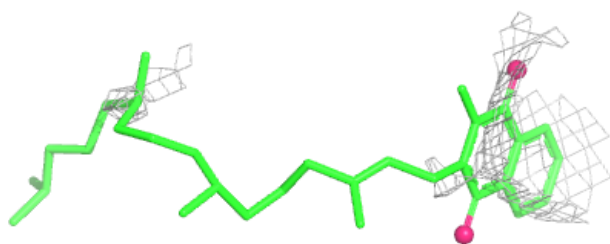
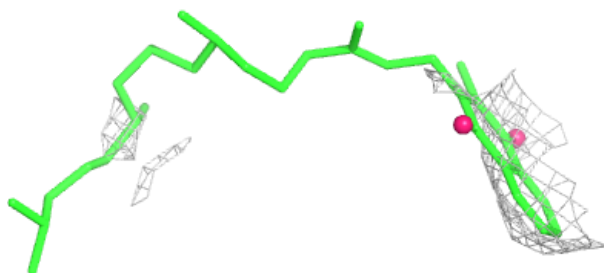
Electron density around CLA 2 608:

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



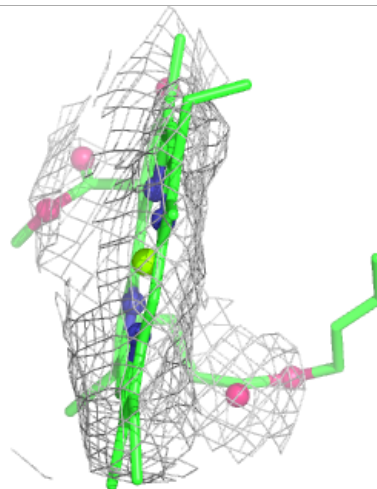
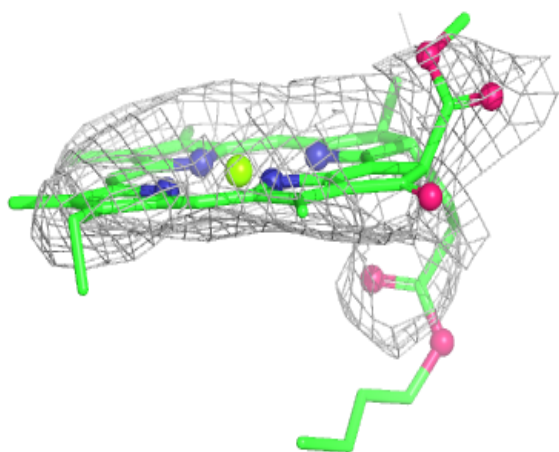
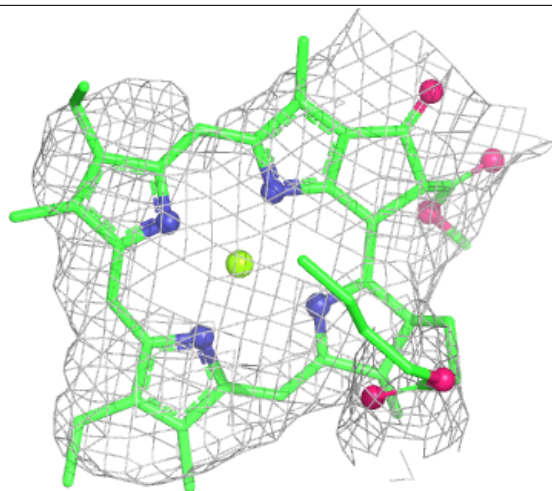
Electron density around PQN B 2002:

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



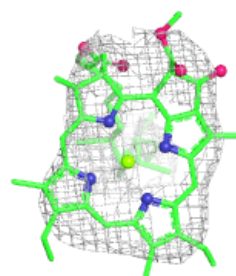
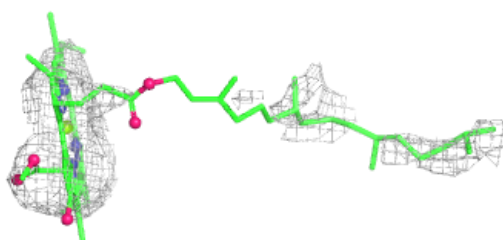
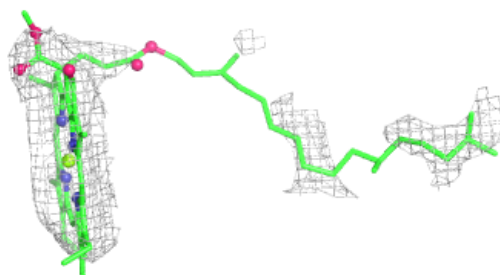
Electron density around CLA A 1115:

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



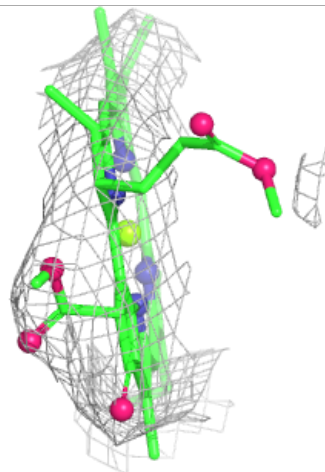
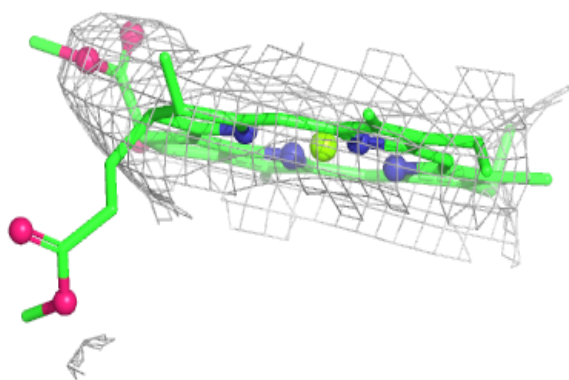
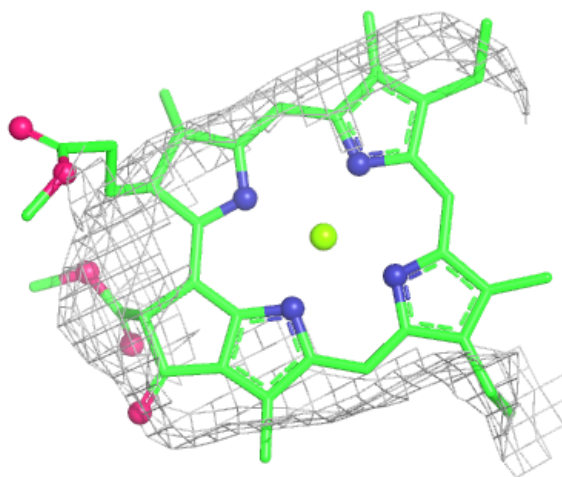
Electron density around CLA B 1239:

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



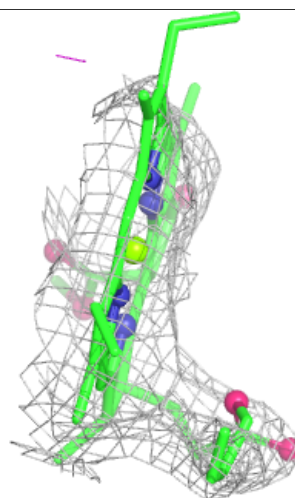
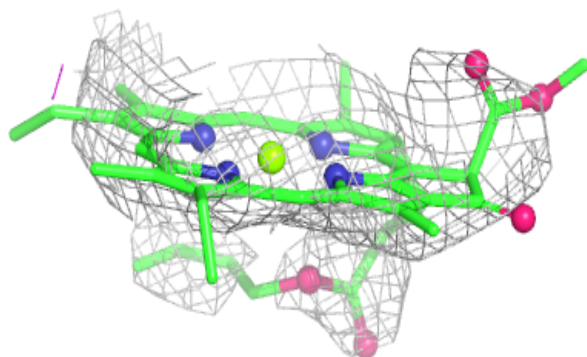
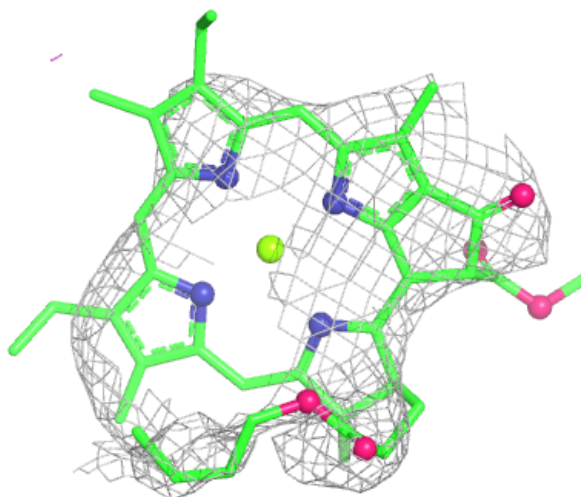
Electron density around CLA 3 613:

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



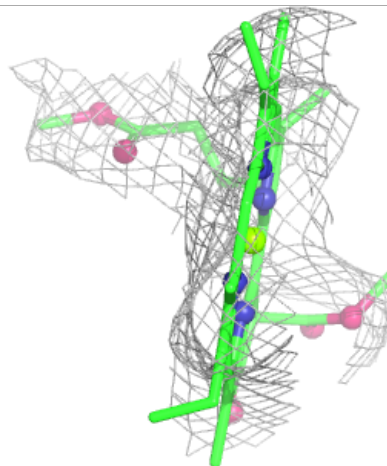
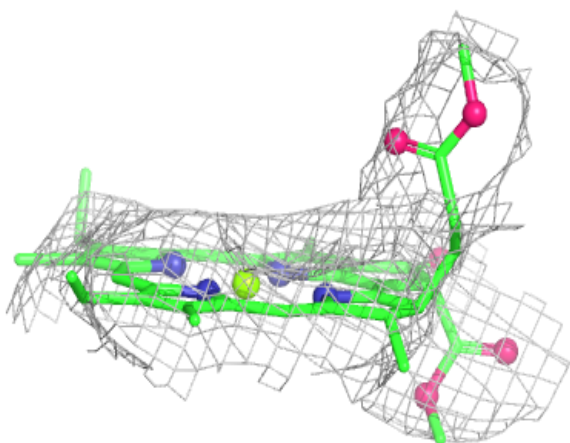
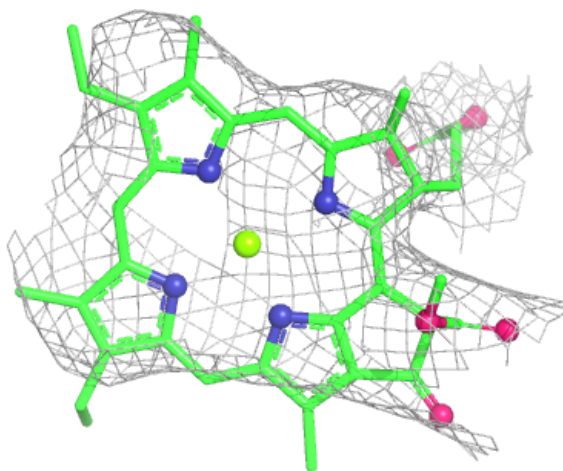
Electron density around CLA B 1215:

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



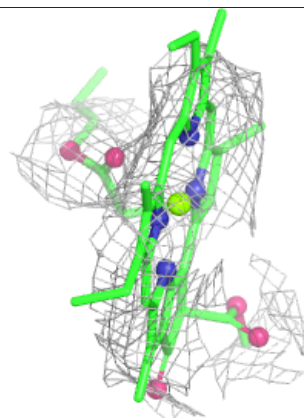
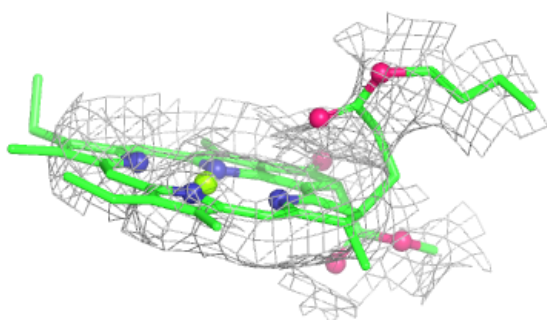
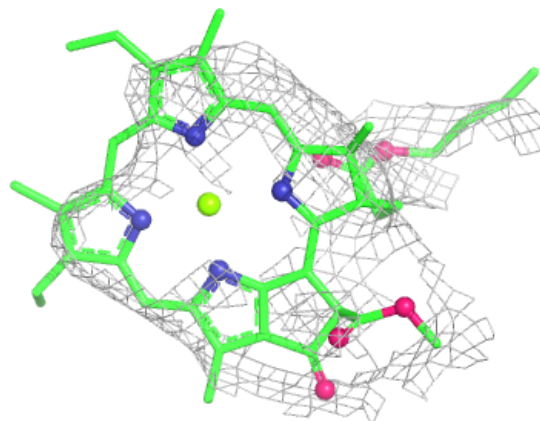
Electron density around CLA 2 606:

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



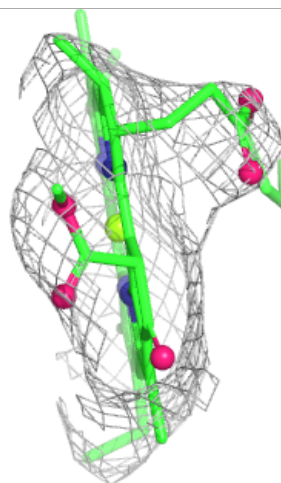
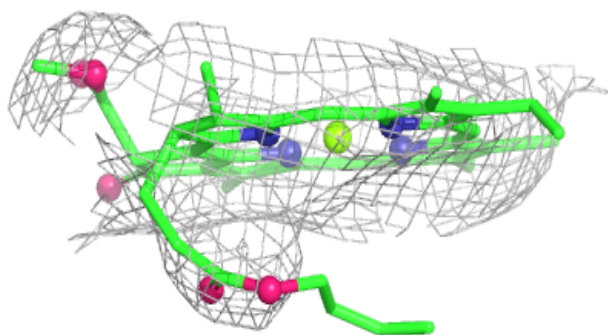
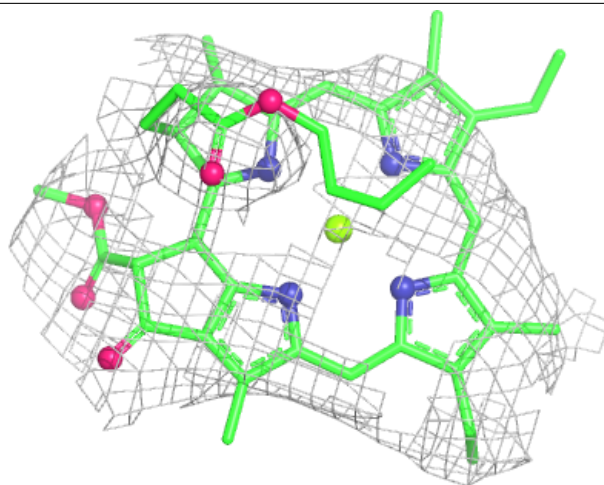
Electron density around CLA A 1124:

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



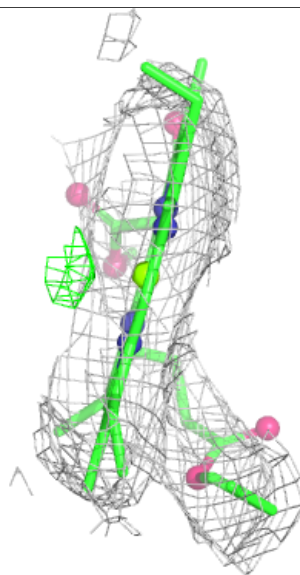
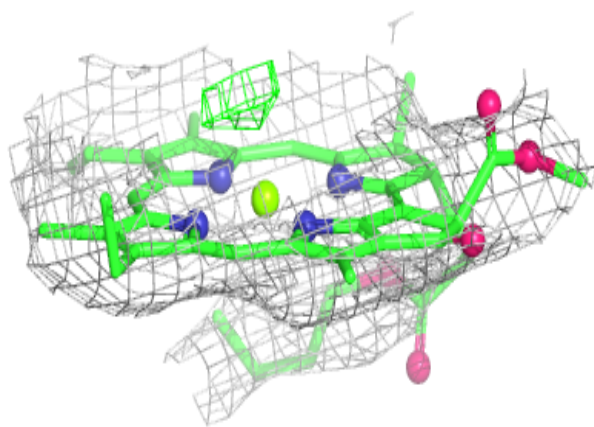
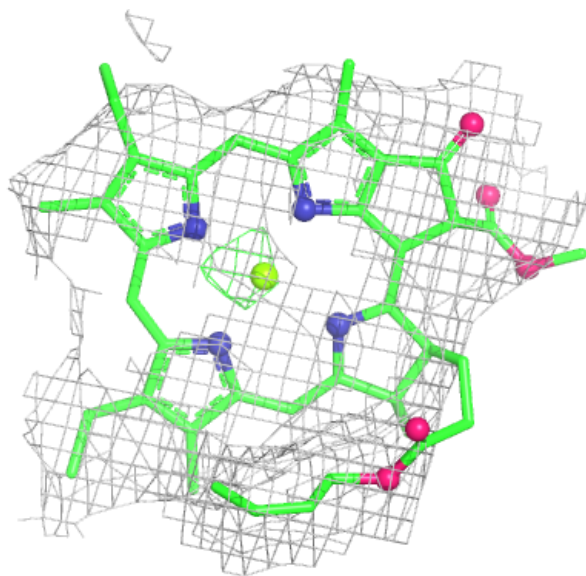
Electron density around CLA B 1205:

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



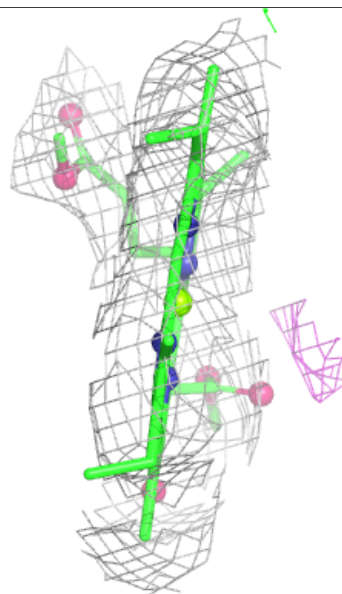
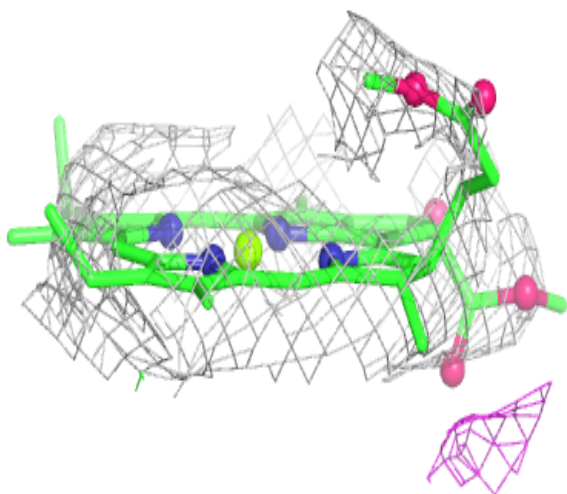
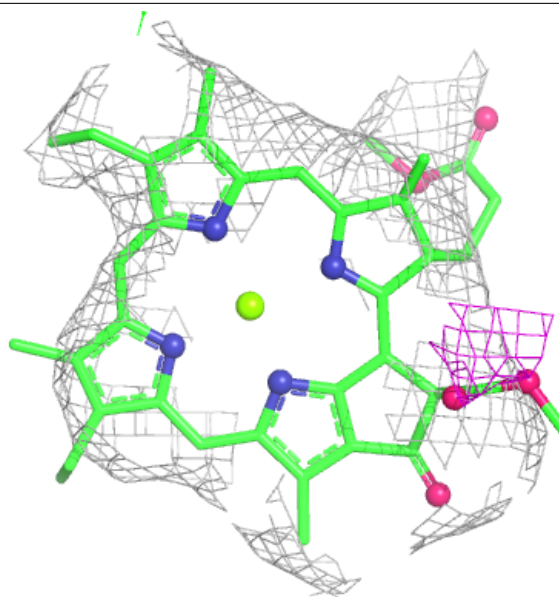
Electron density around CLA 1 601:

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



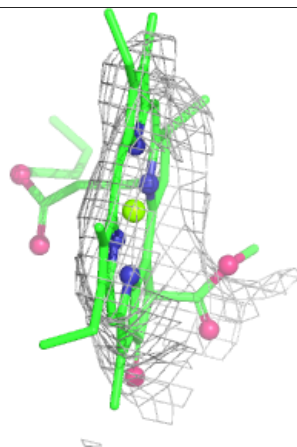
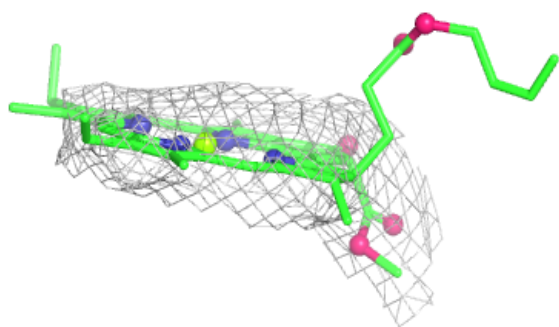
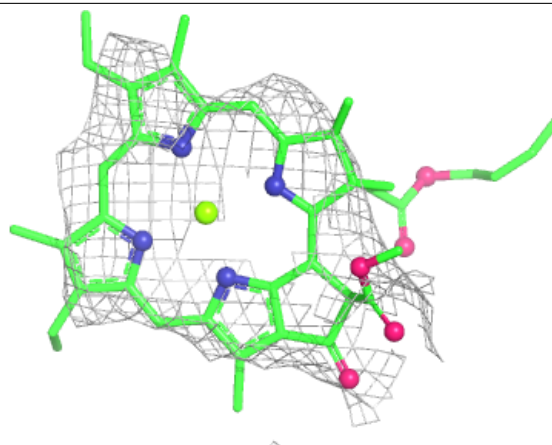
Electron density around CLA 1 607:

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



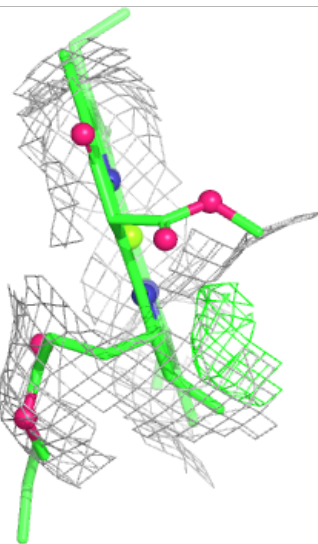
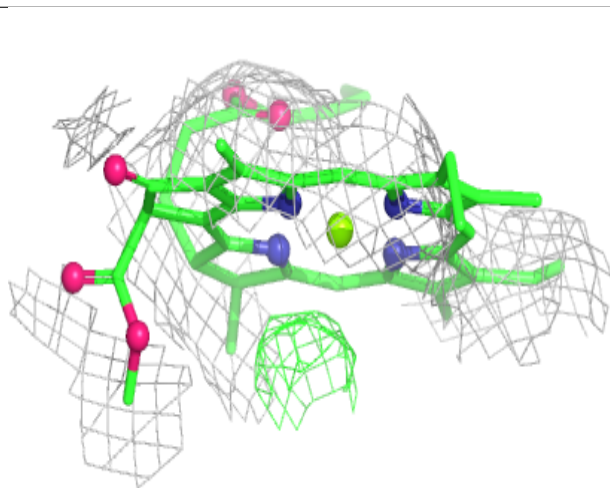
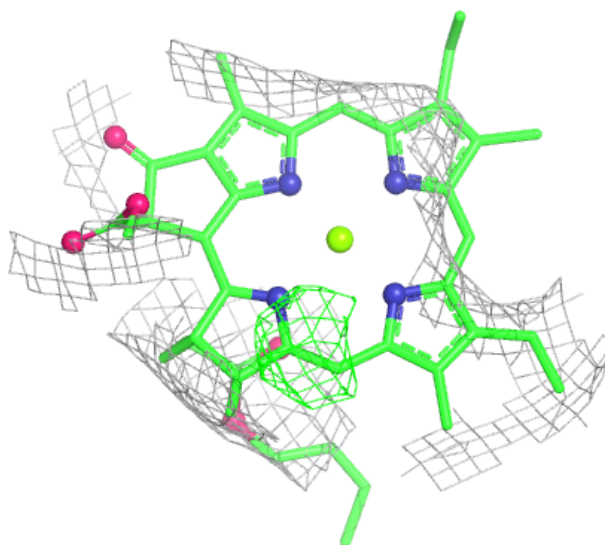
Electron density around CLA A 1132:

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



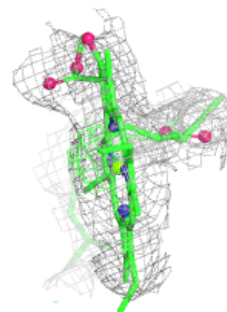
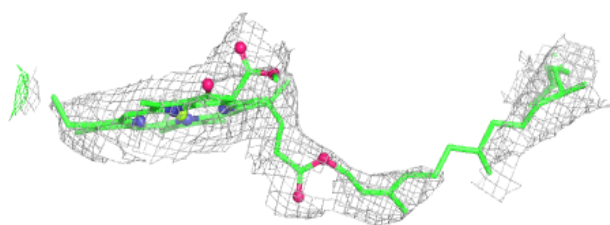
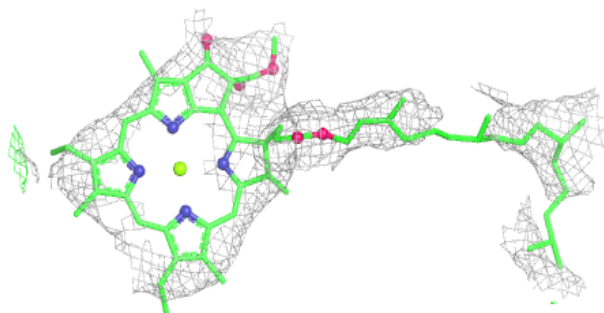
Electron density around CLA A 1134:

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



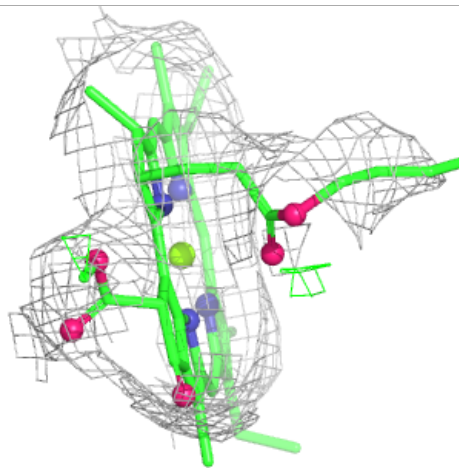
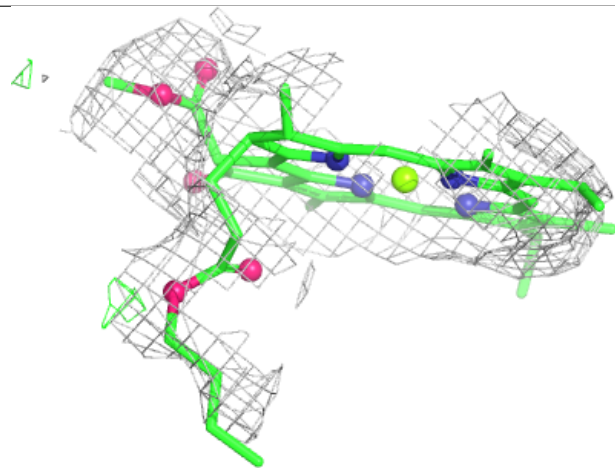
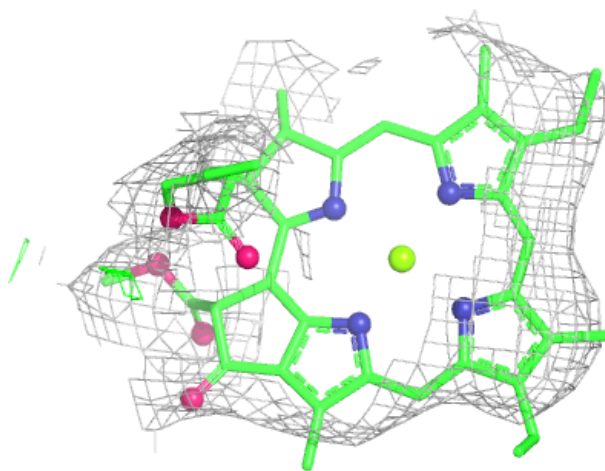
Electron density around CLA B 1240:

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



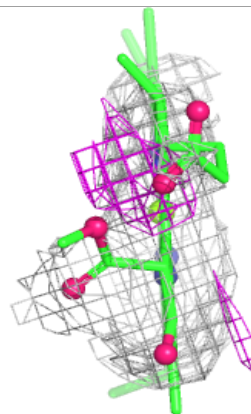
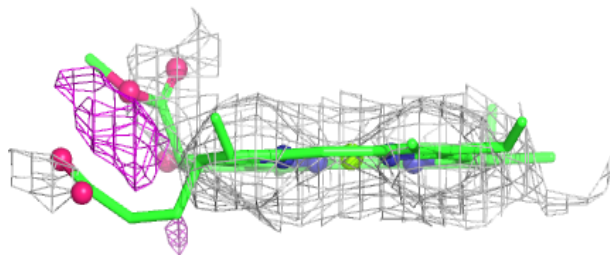
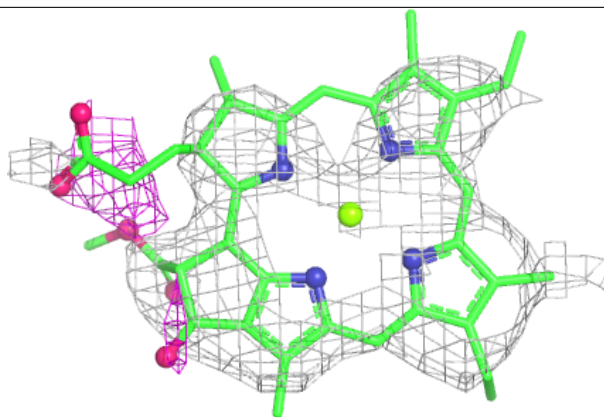
Electron density around CLA F 1302:

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

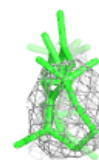
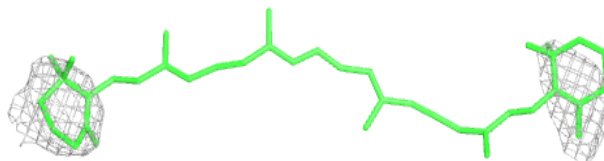


Electron density around CLA A 1101:

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

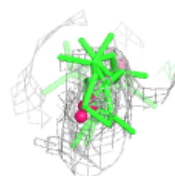
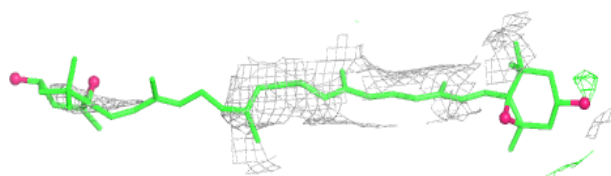
**Electron density around BCR B 4002:**

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

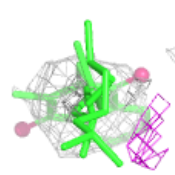
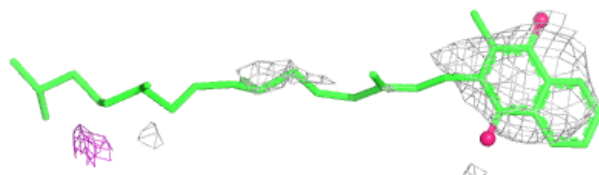
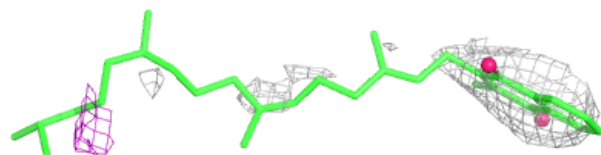


Electron density around XAT 3 502:

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

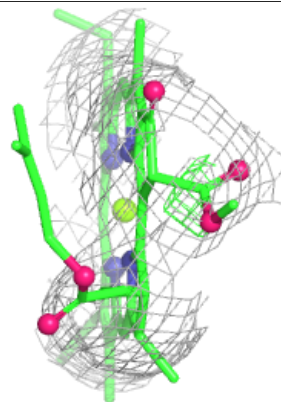
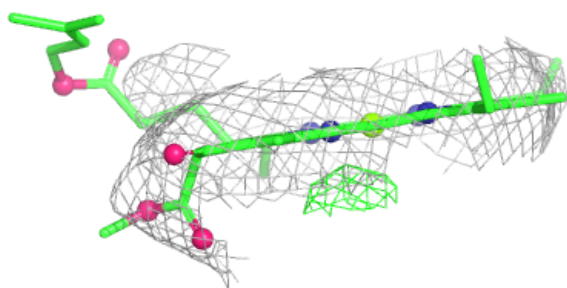
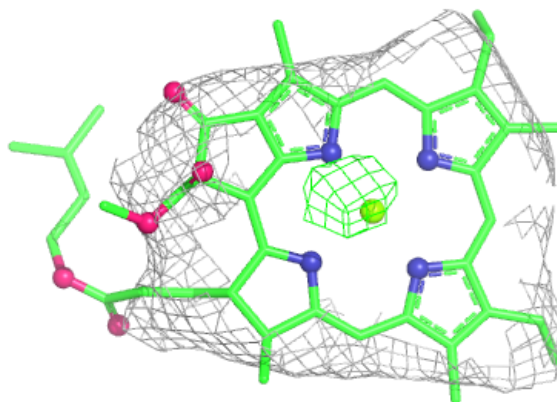
**Electron density around PQN A 2001:**

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



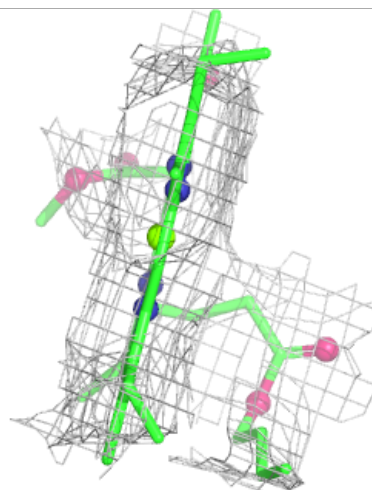
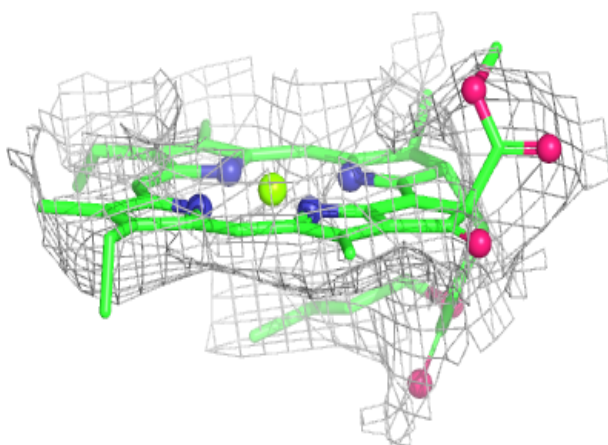
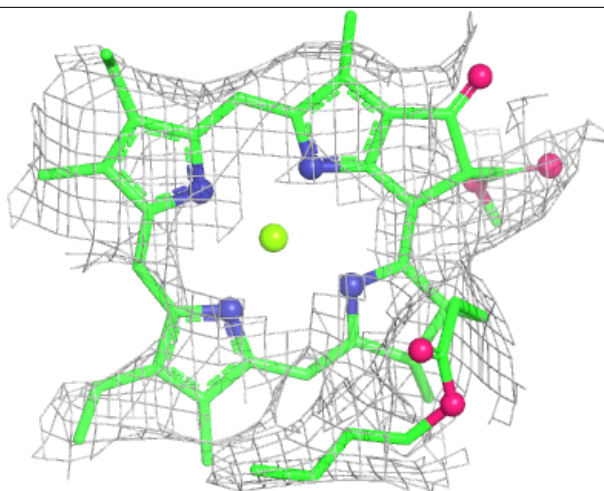
Electron density around CLA 2 615:

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



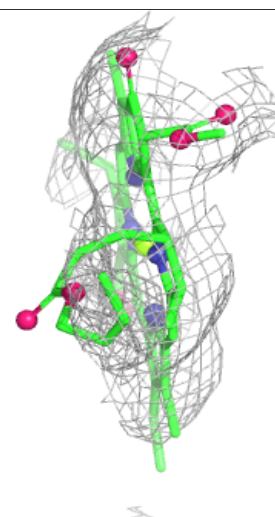
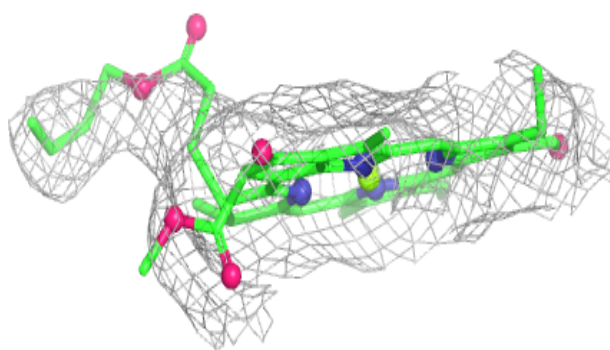
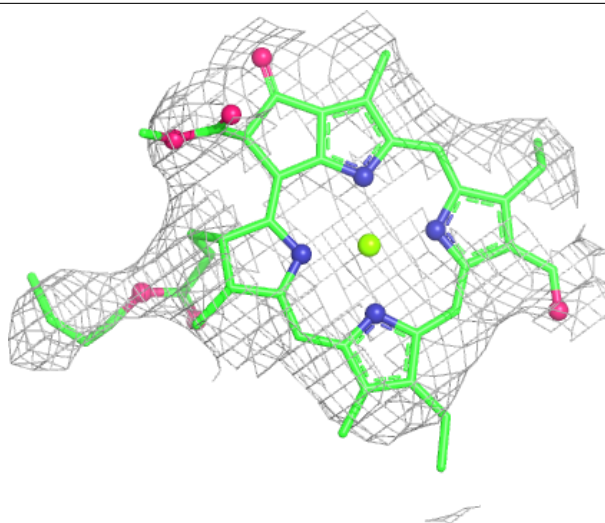
Electron density around CLA 2 604:

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



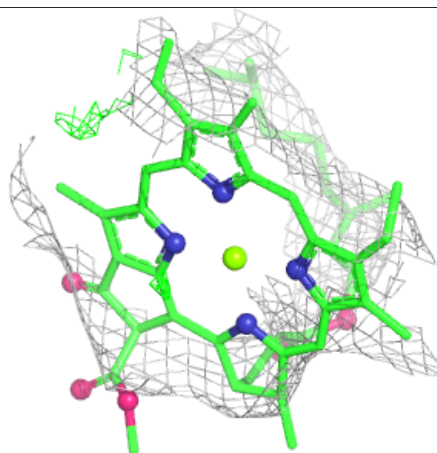
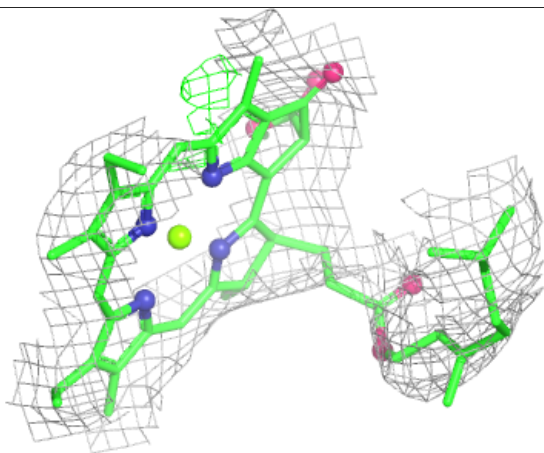
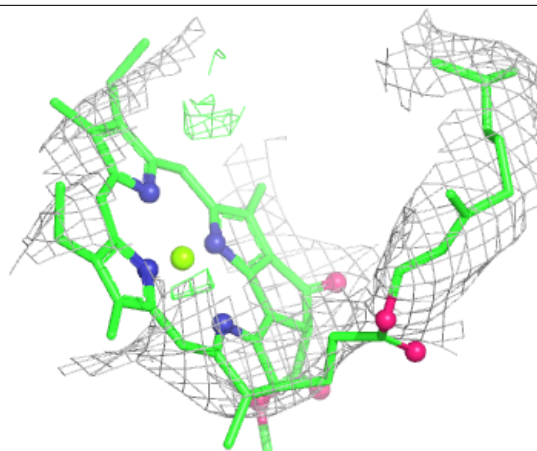
Electron density around CHL 2 610:

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



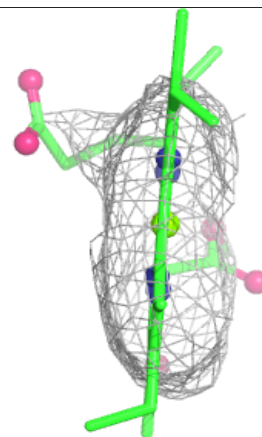
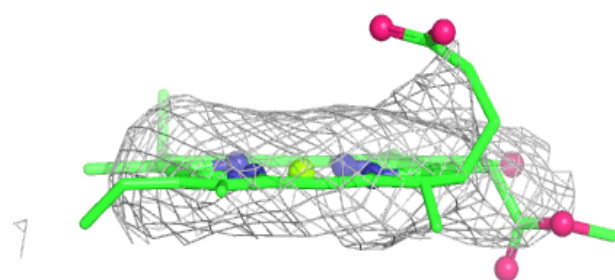
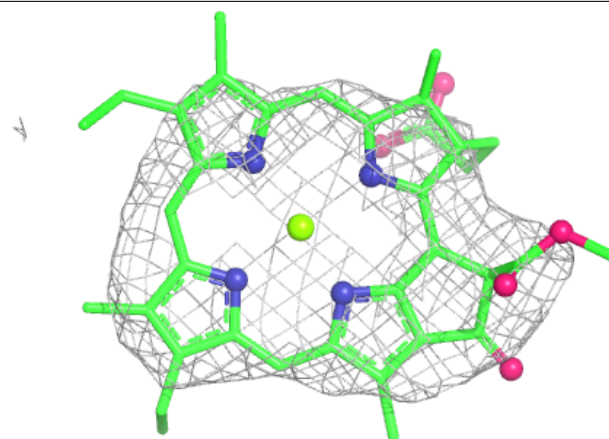
Electron density around CLA 3 612:

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



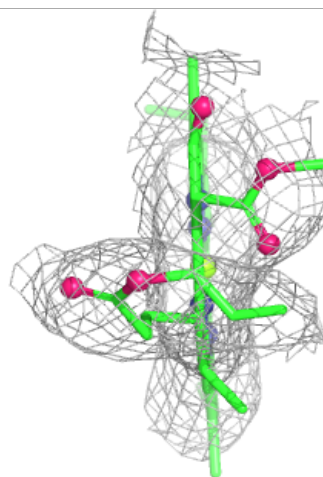
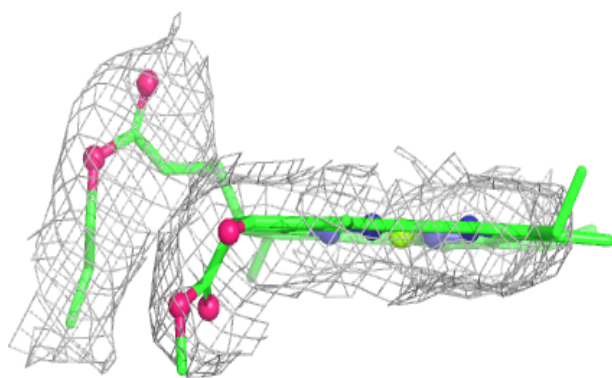
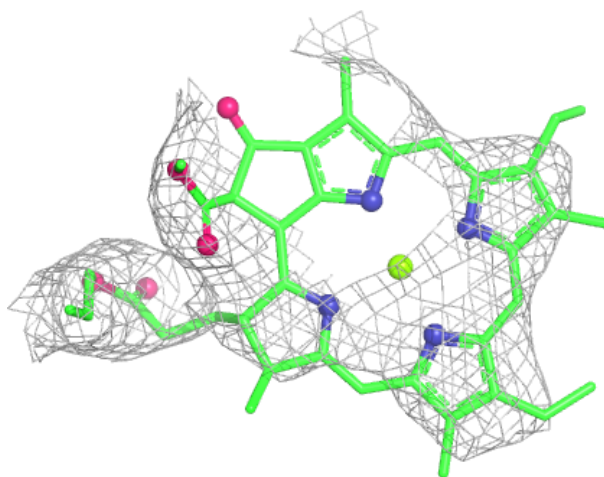
Electron density around CLA A 1113:

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



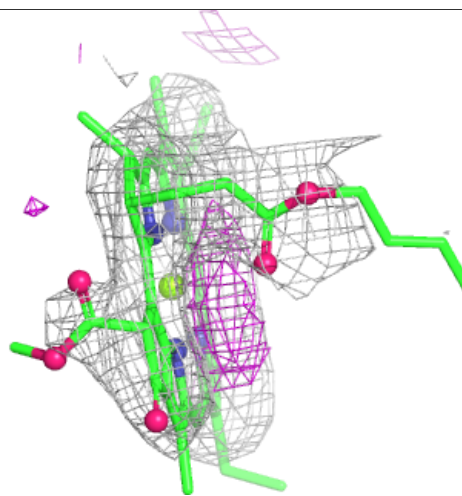
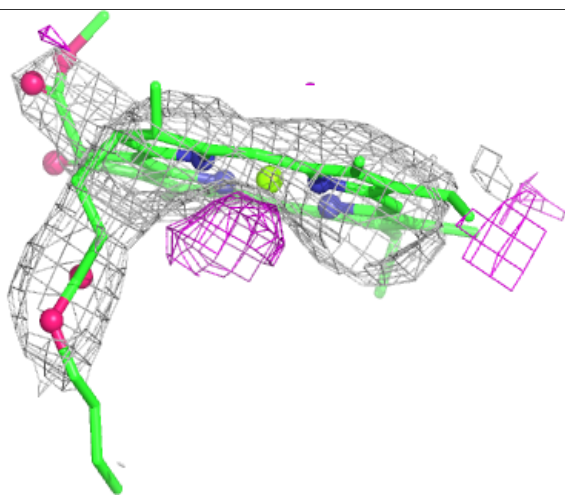
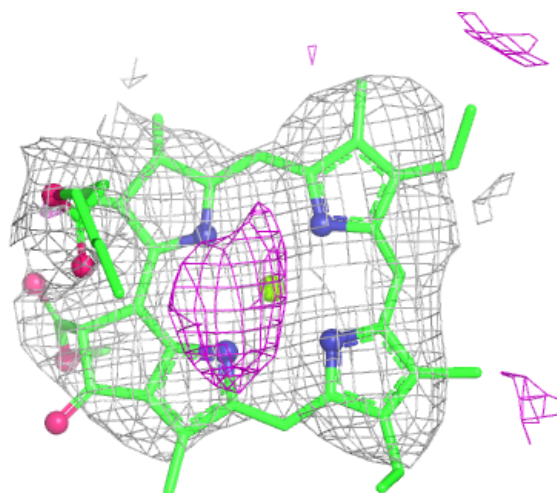
Electron density around CLA 1 605:

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



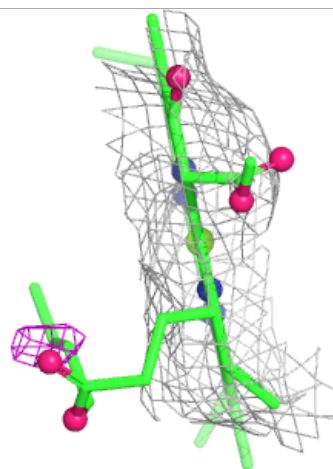
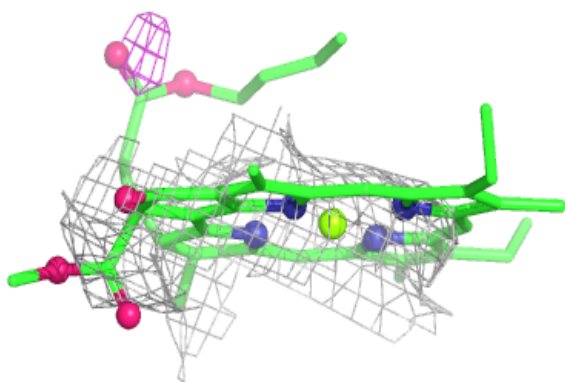
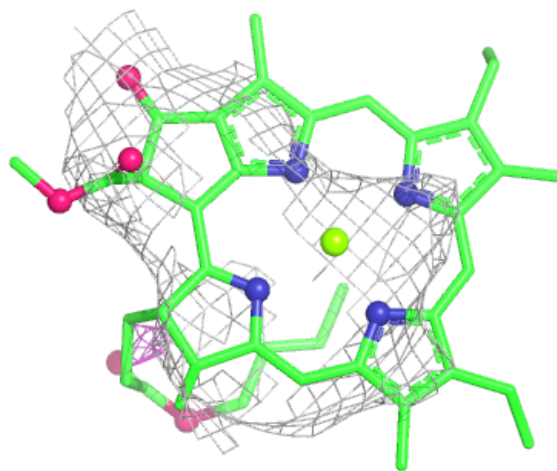
Electron density around CLA 4 606:

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



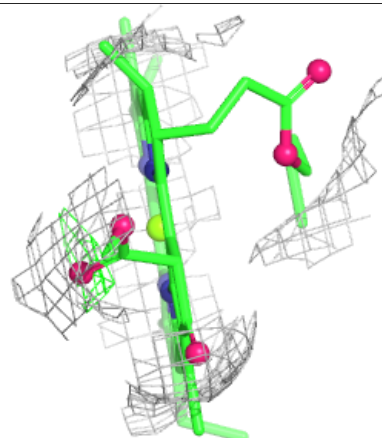
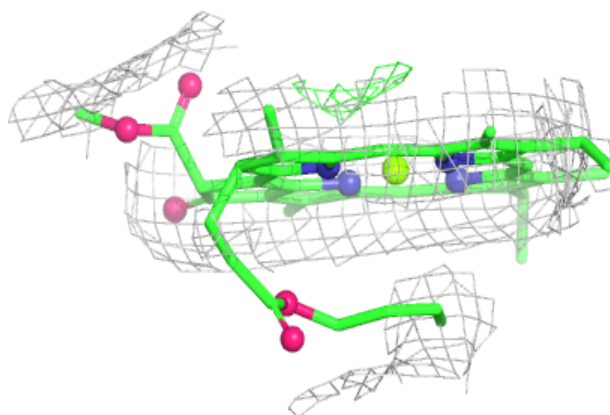
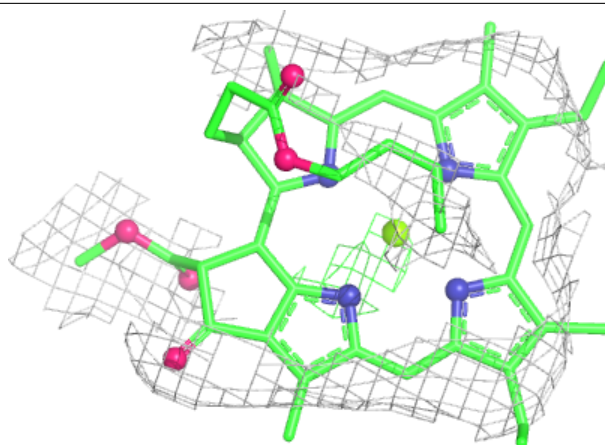
Electron density around CLA A 1116:

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

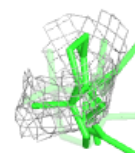
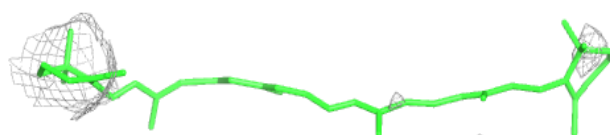
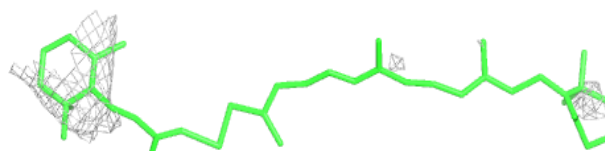


Electron density around CLA B 1237:

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

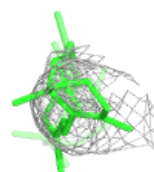
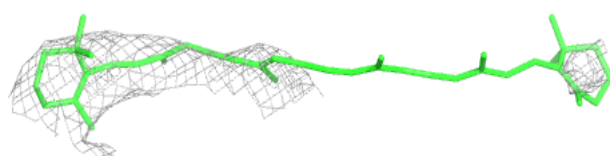
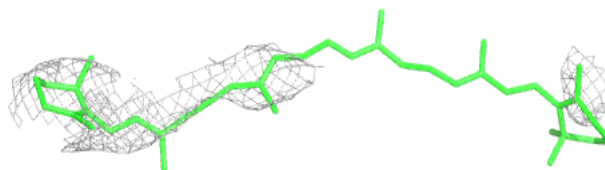
**Electron density around BCR A 4005:**

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

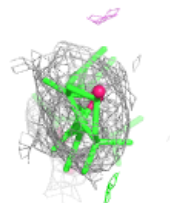
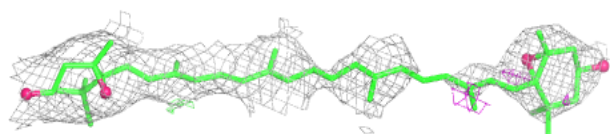
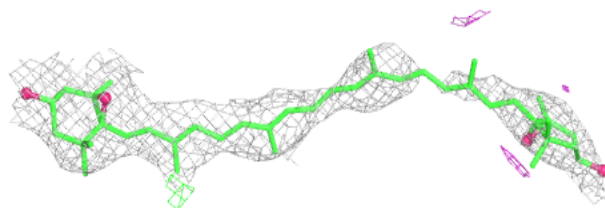


Electron density around BCR 3 504:

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

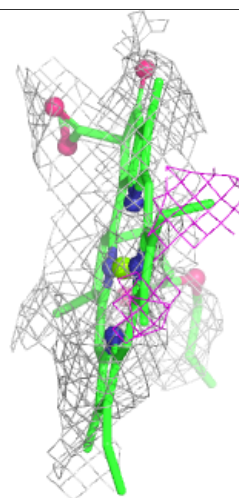
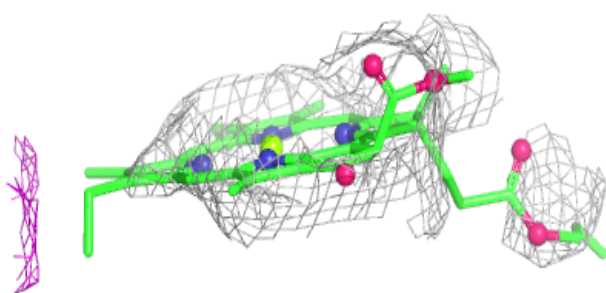
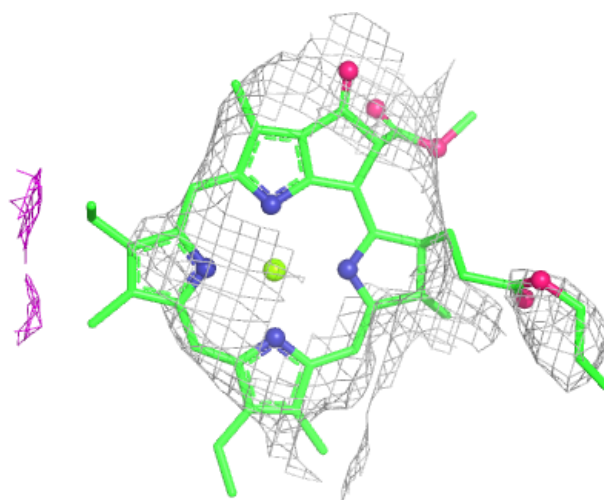
**Electron density around XAT 4 502:**

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



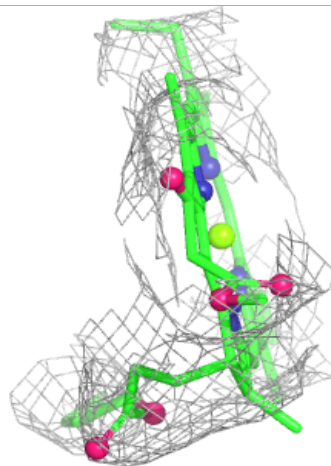
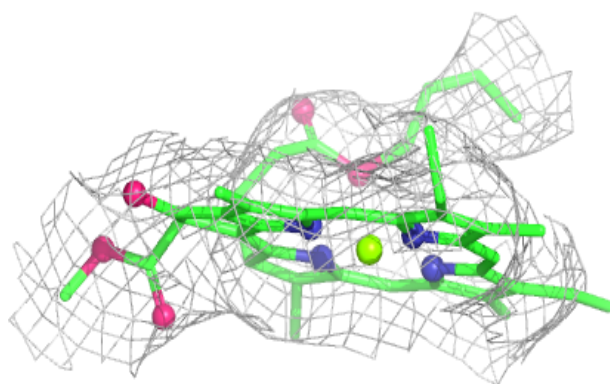
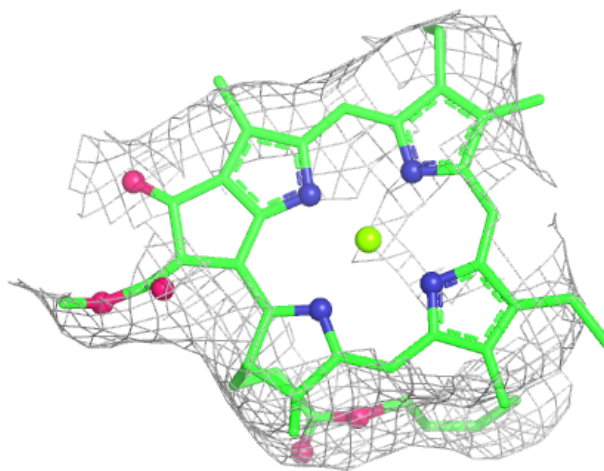
Electron density around CLA A 1129:

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



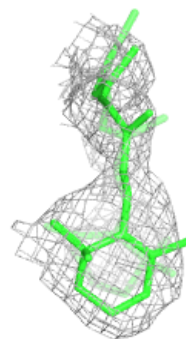
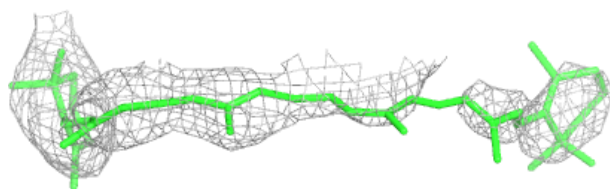
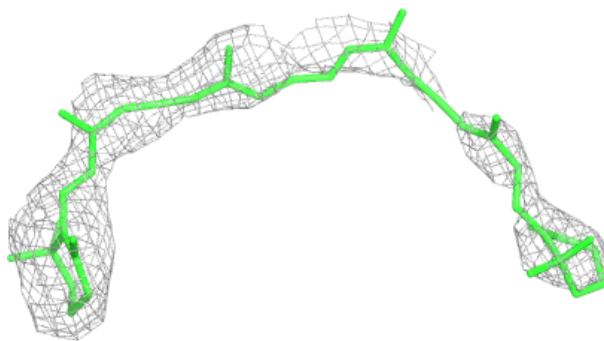
Electron density around CLA 4 601:

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



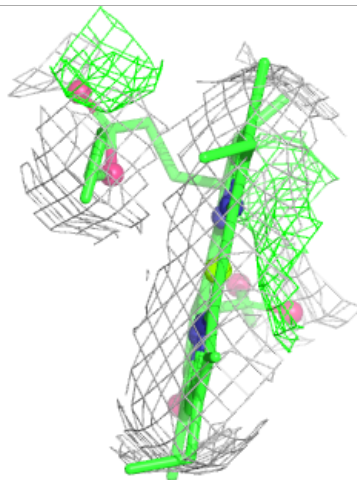
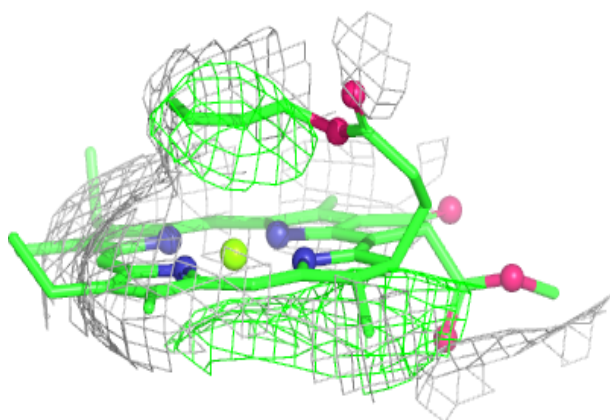
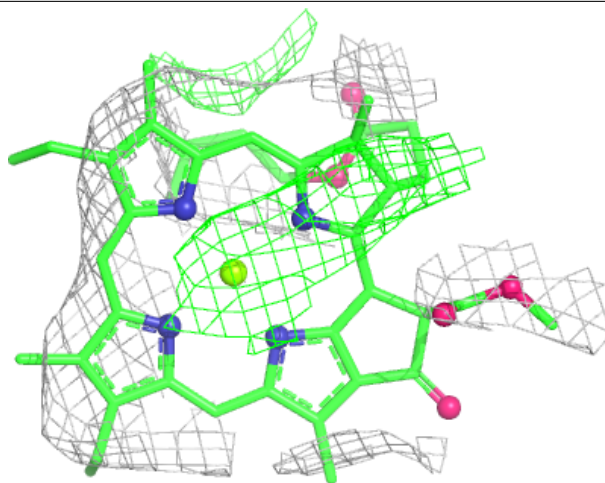
Electron density around BCR F 4002:

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



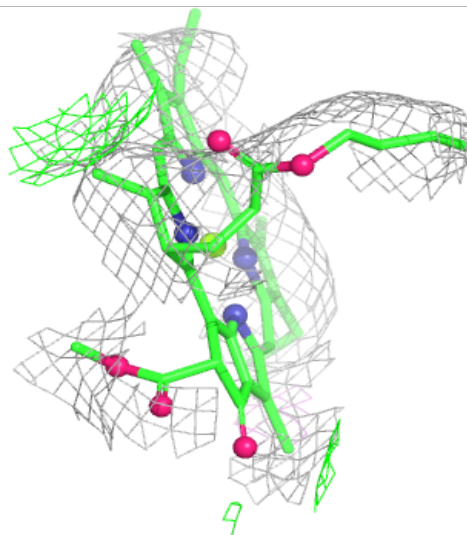
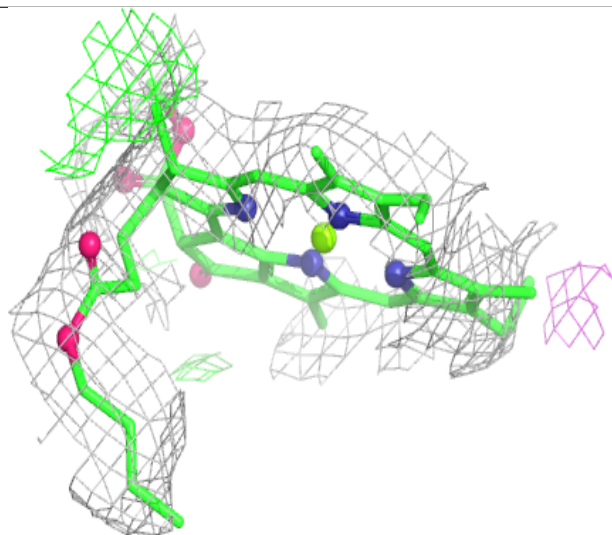
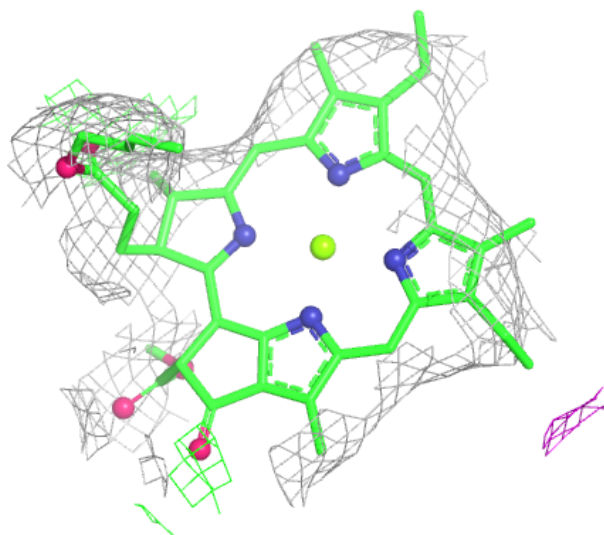
Electron density around CLA 3 610:

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



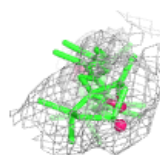
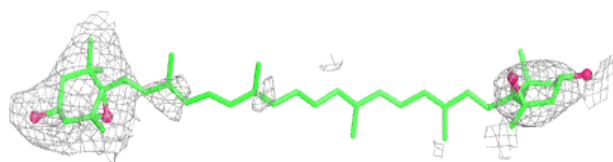
Electron density around CLA 4 612:

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



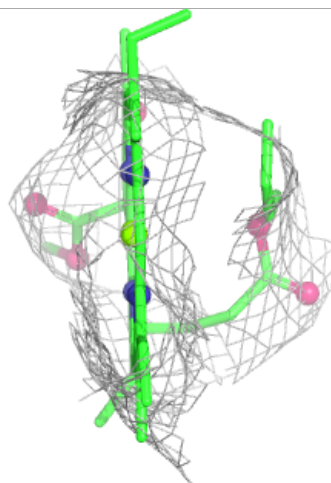
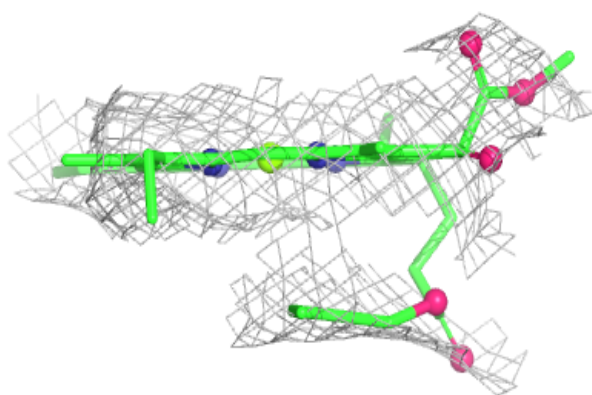
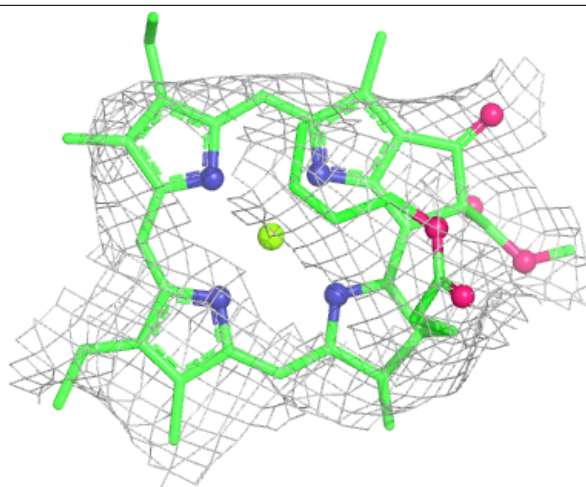
Electron density around XAT 1 502:

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



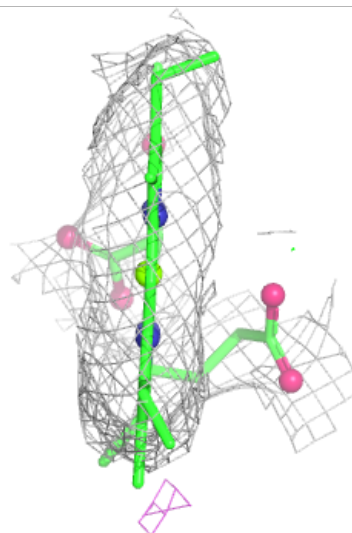
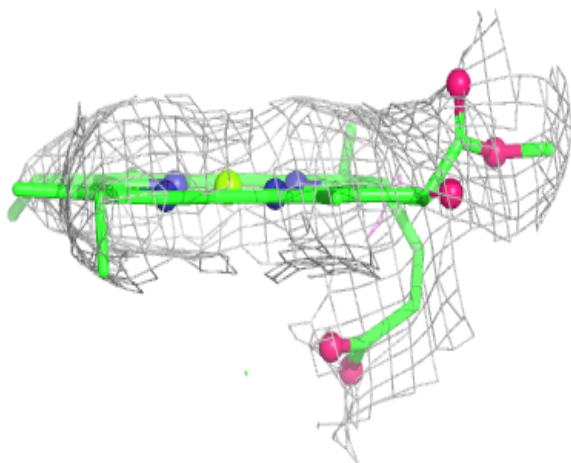
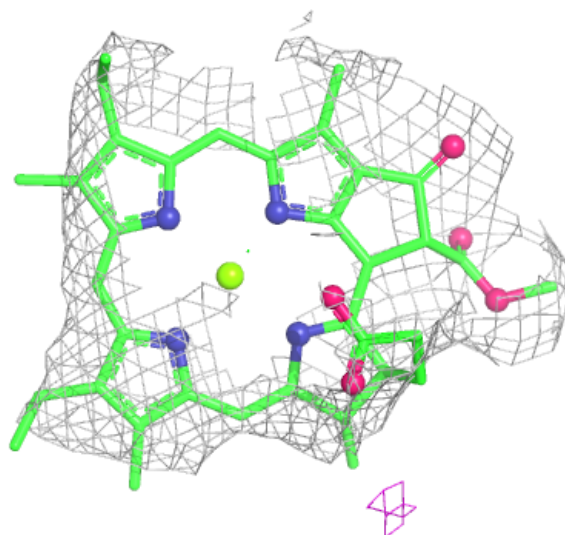
Electron density around CLA A 1136:

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



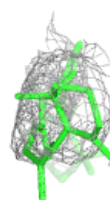
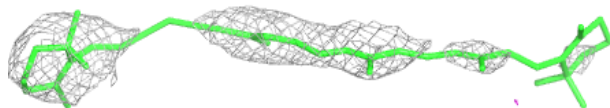
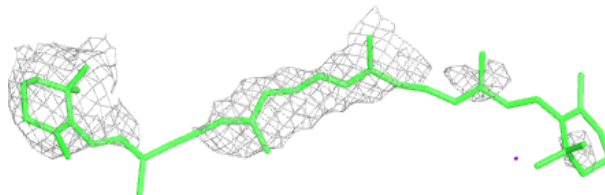
Electron density around CLA 1 603:

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

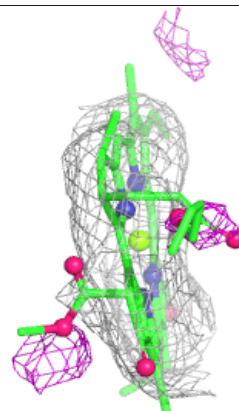
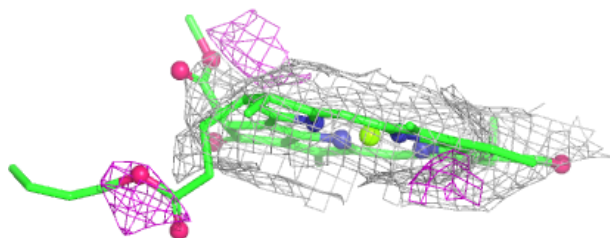
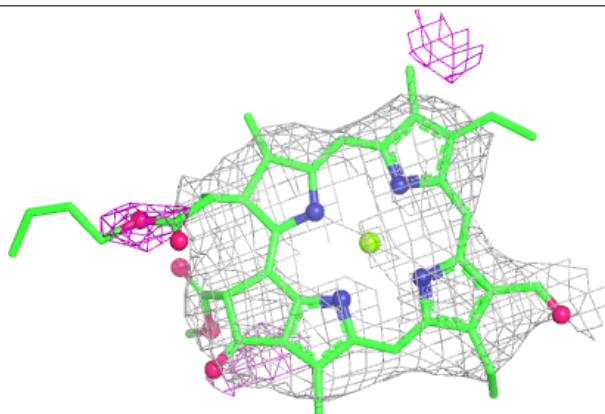


Electron density around BCR B 4005:

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

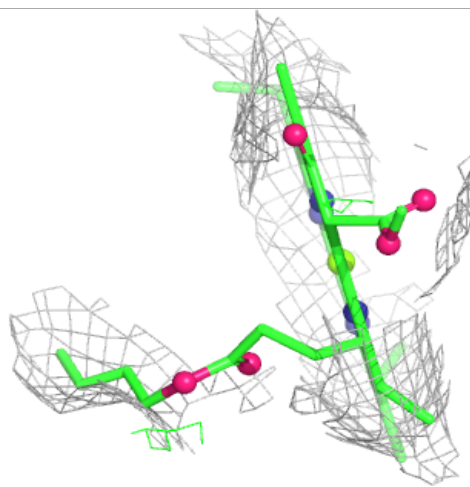
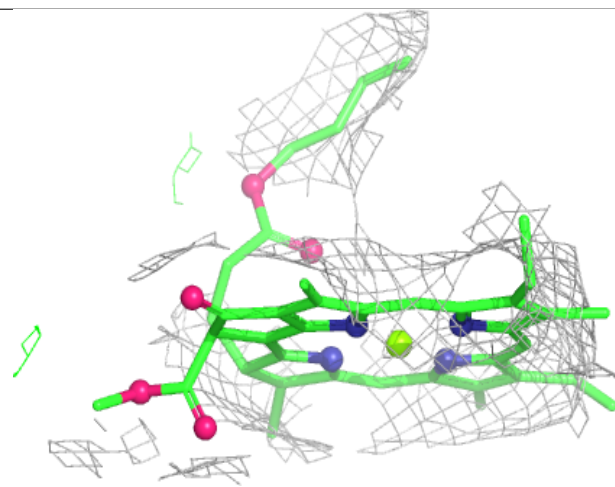
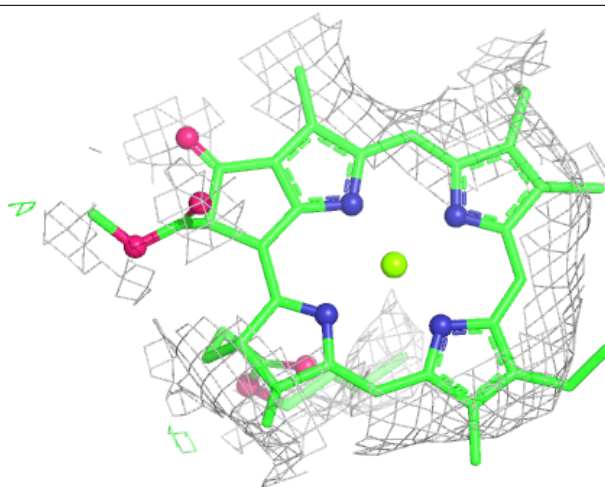
**Electron density around CHL 4 613:**

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



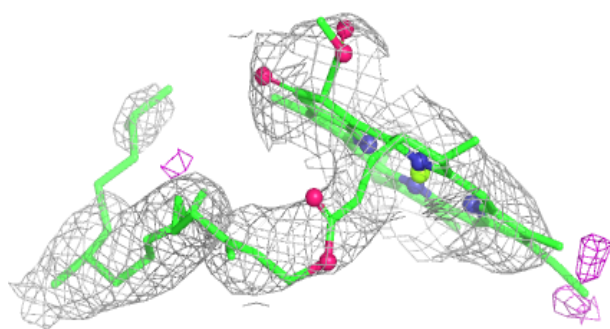
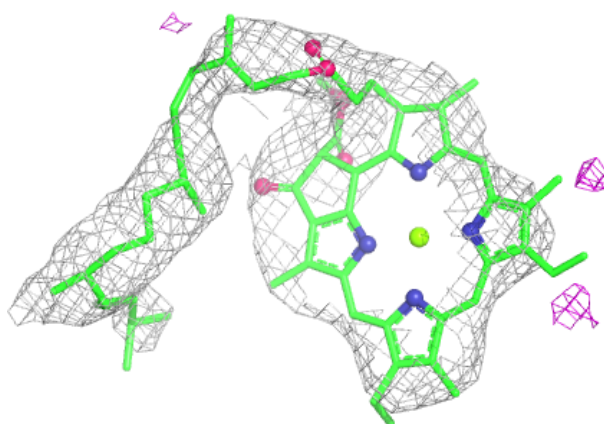
Electron density around CLA A 1109:

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



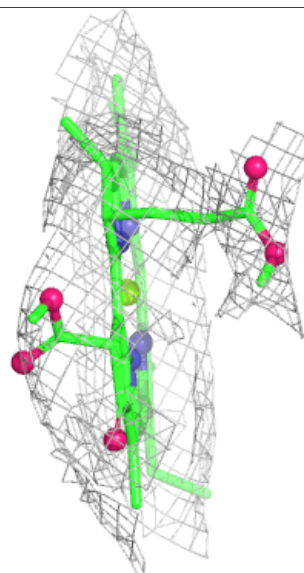
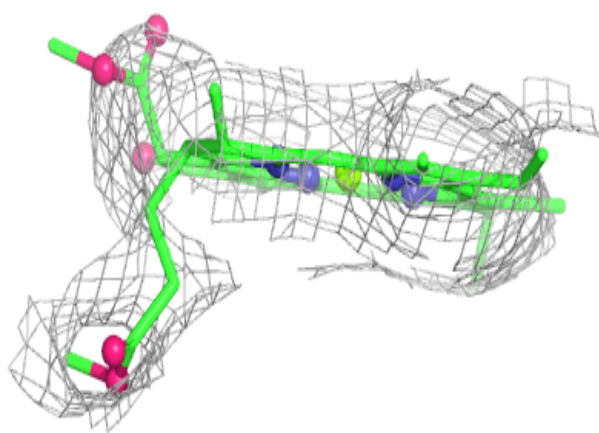
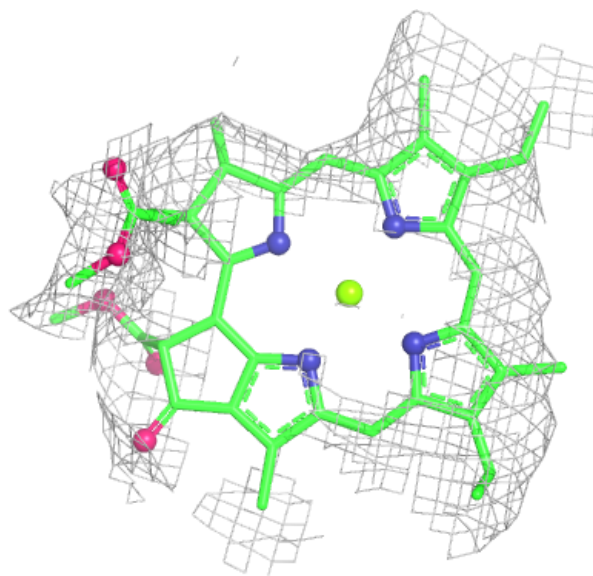
Electron density around CLA B 1229:

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



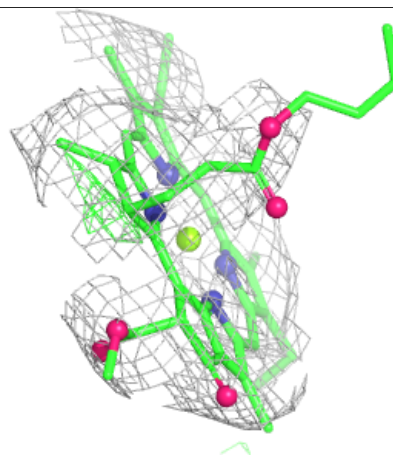
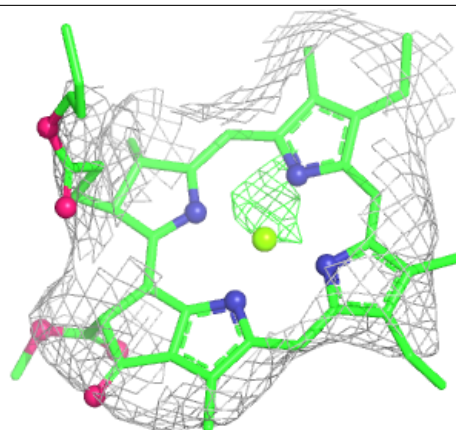
Electron density around CLA B 1209:

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



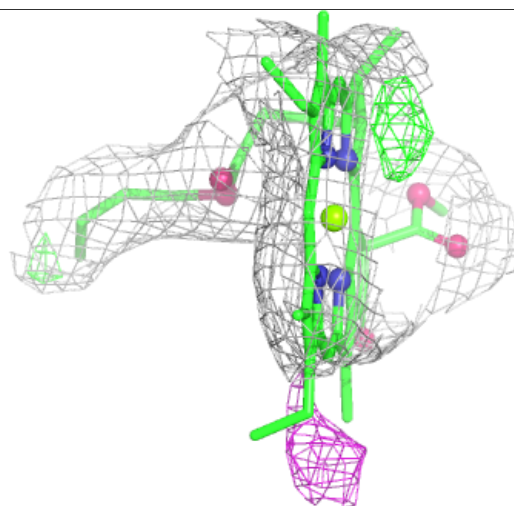
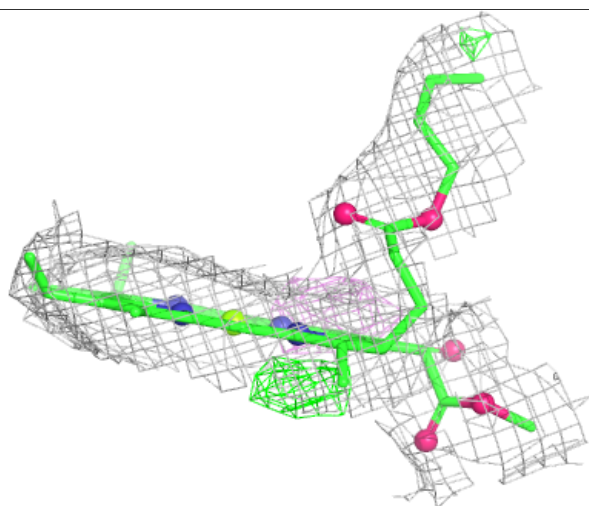
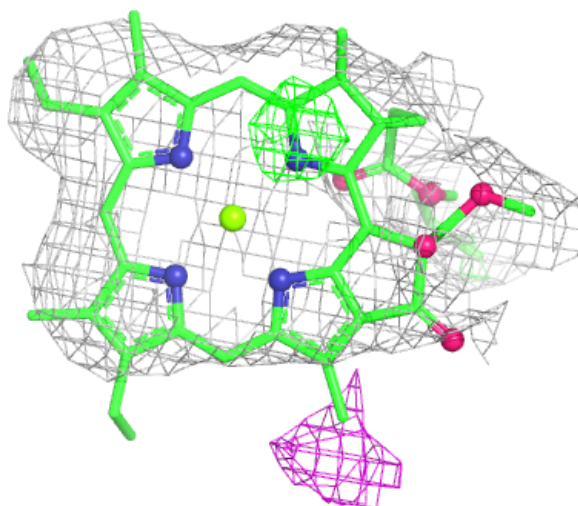
Electron density around CLA B 1232:

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



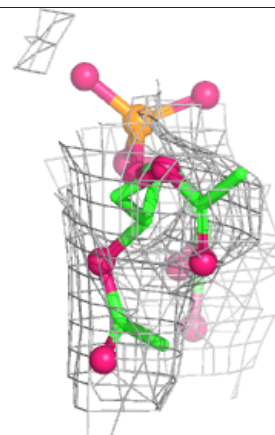
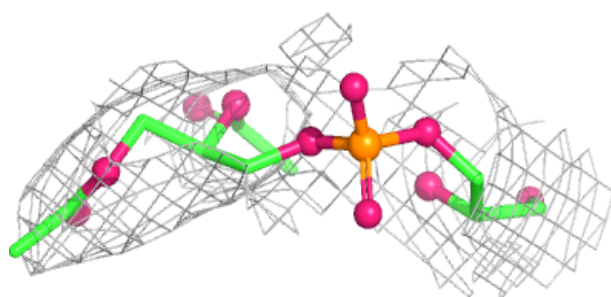
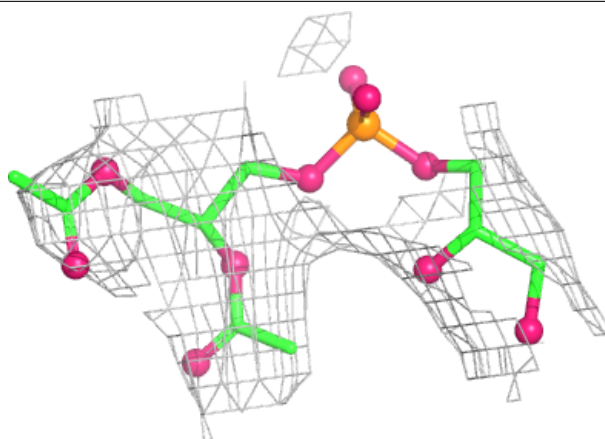
Electron density around CLA A 1126:

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

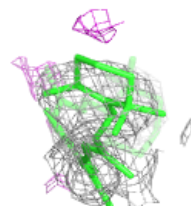
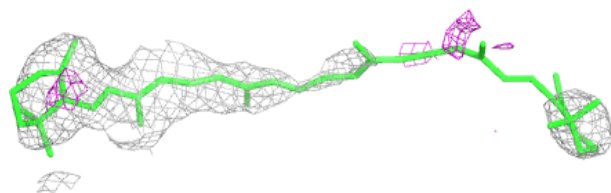
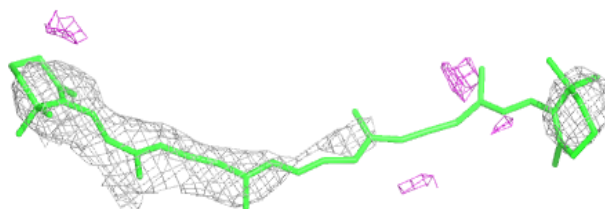


Electron density around LHG B 5001:

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

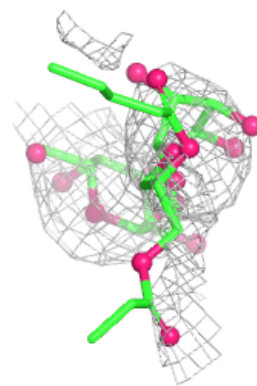
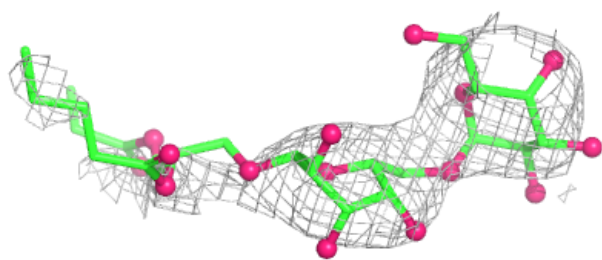
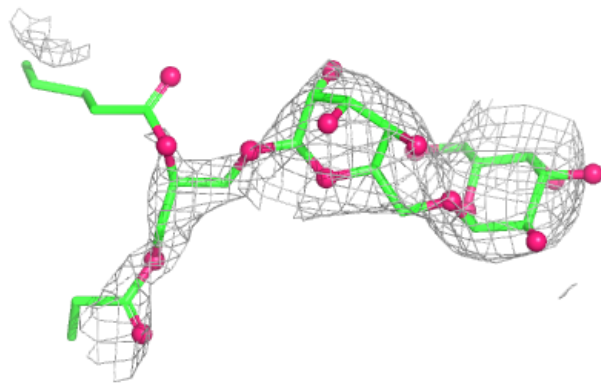
**Electron density around BCR B 4006:**

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

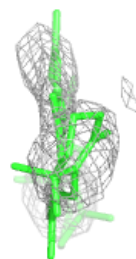
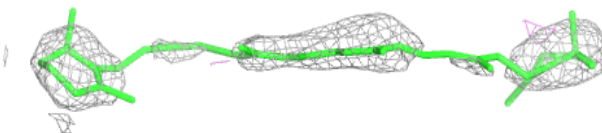
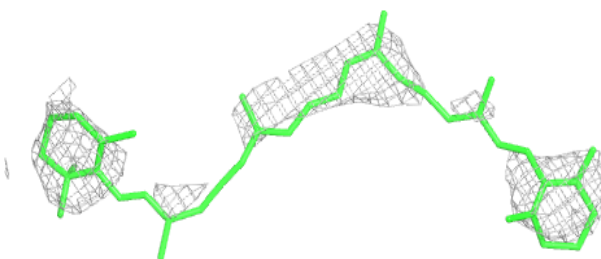


Electron density around DGD B 5002:

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

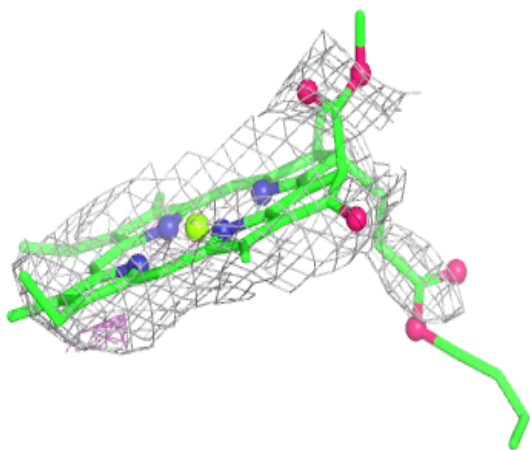
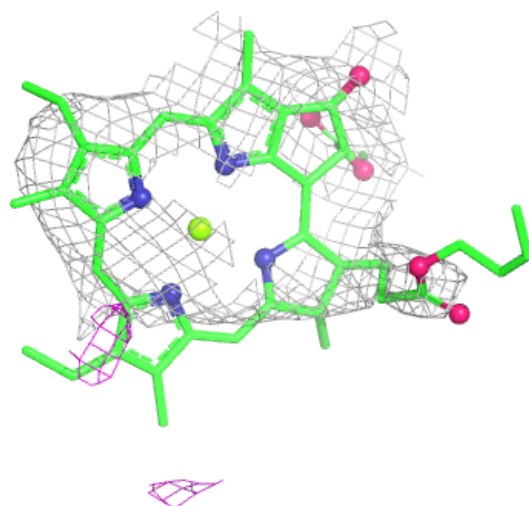
**Electron density around BCR A 4006:**

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



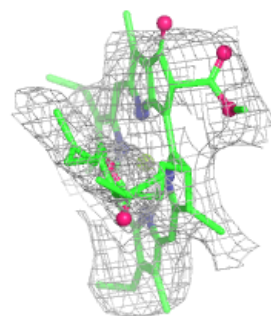
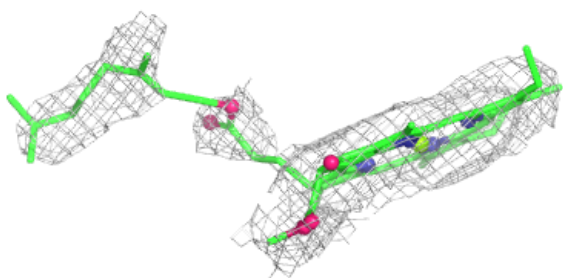
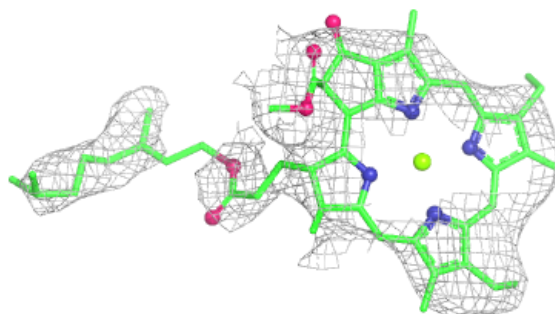
Electron density around CLA A 1137:

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



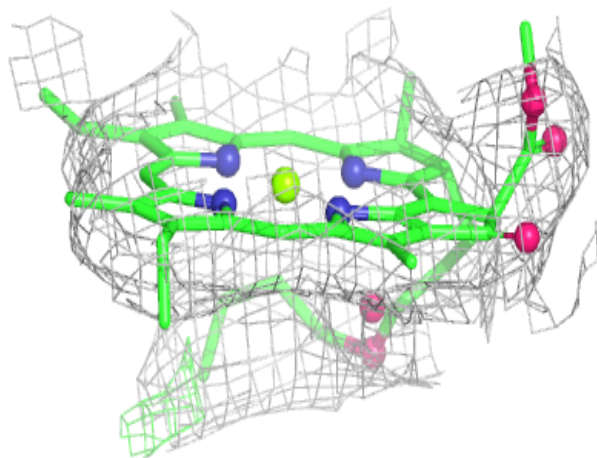
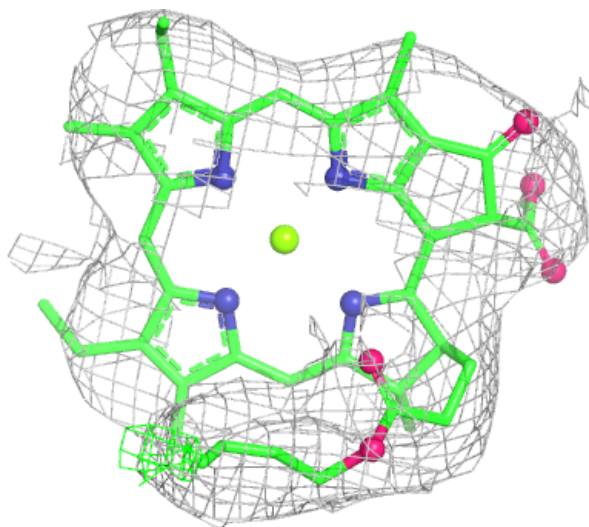
Electron density around CLA B 1220:

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



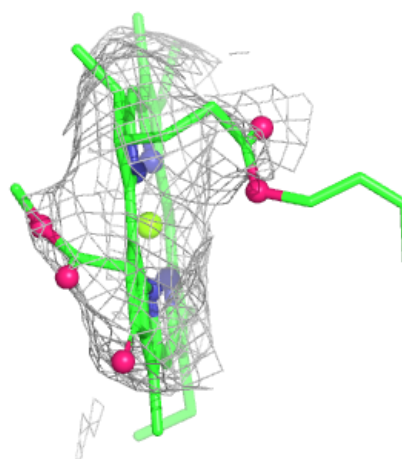
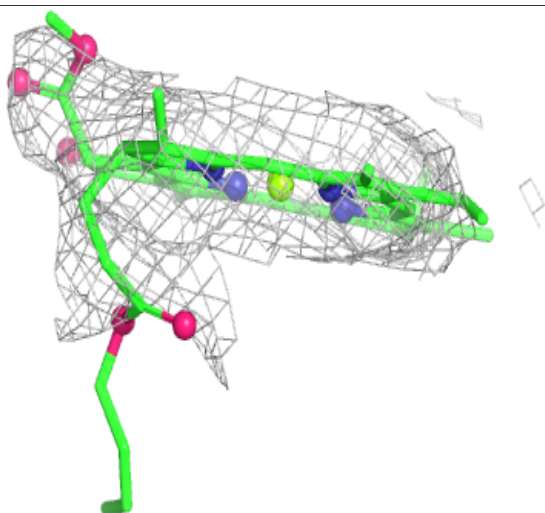
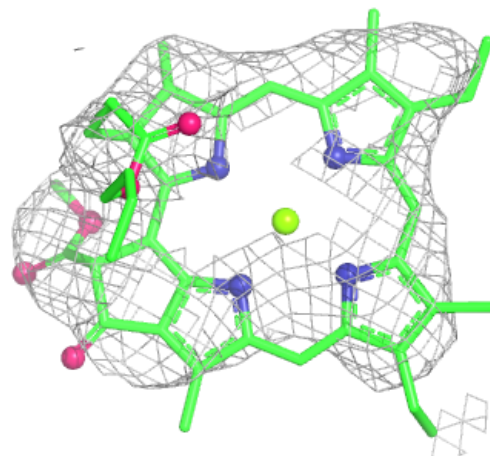
Electron density around CLA 4 604:

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



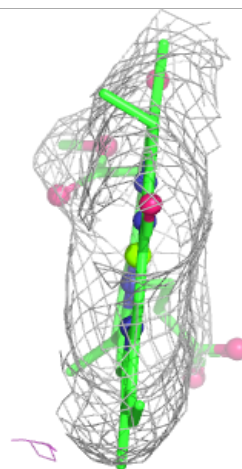
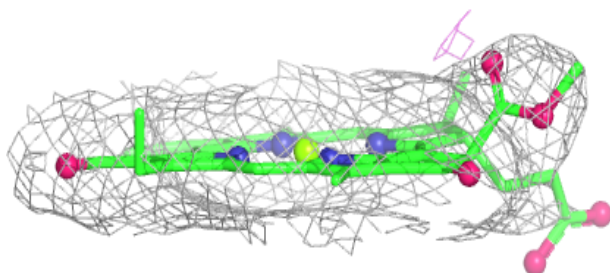
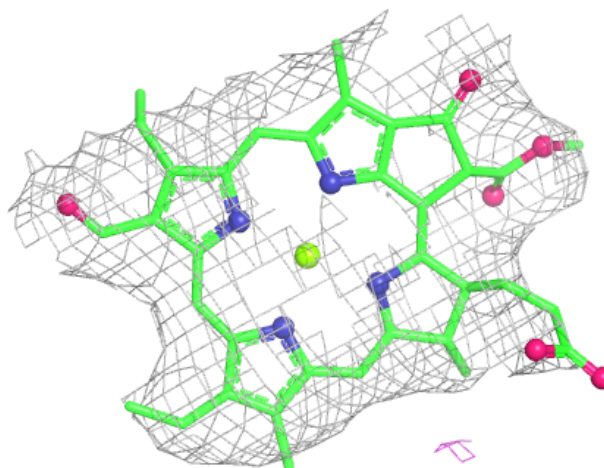
Electron density around CLA B 1226:

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



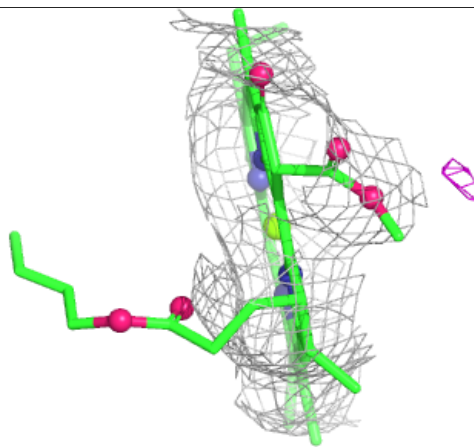
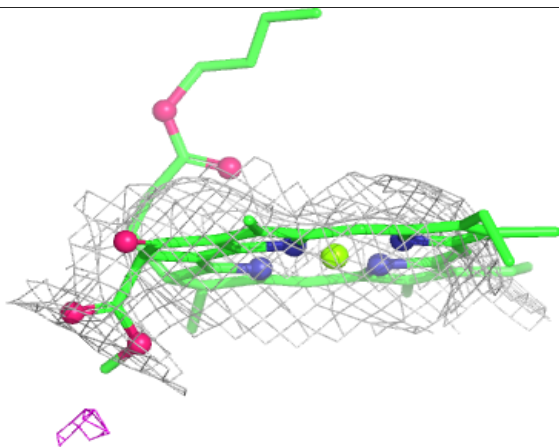
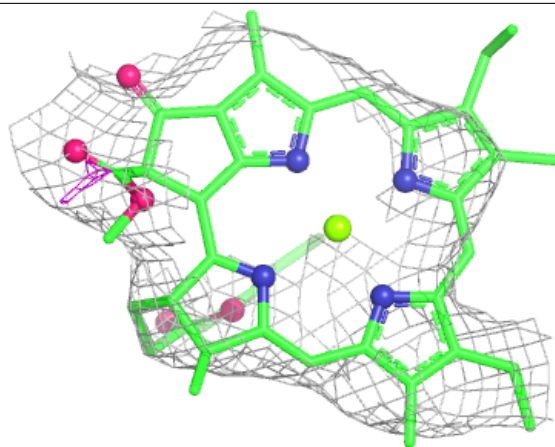
Electron density around CHL 2 613:

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



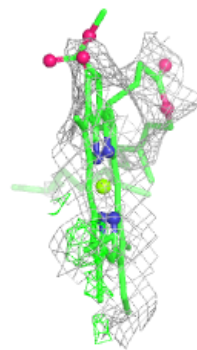
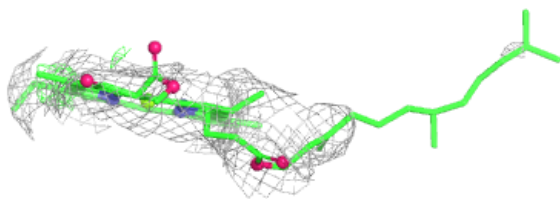
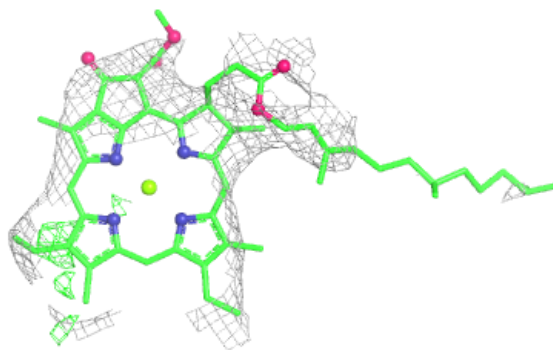
Electron density around CLA 2 607:

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



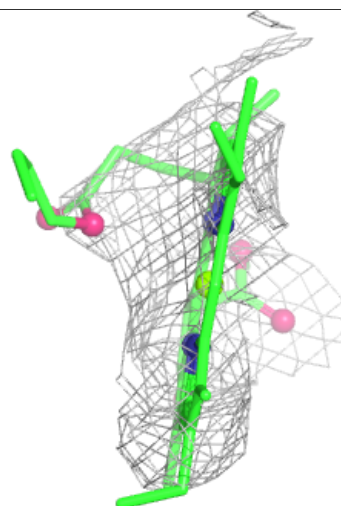
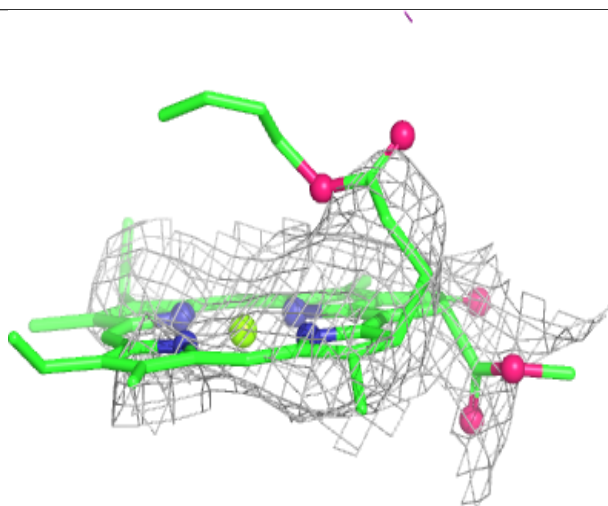
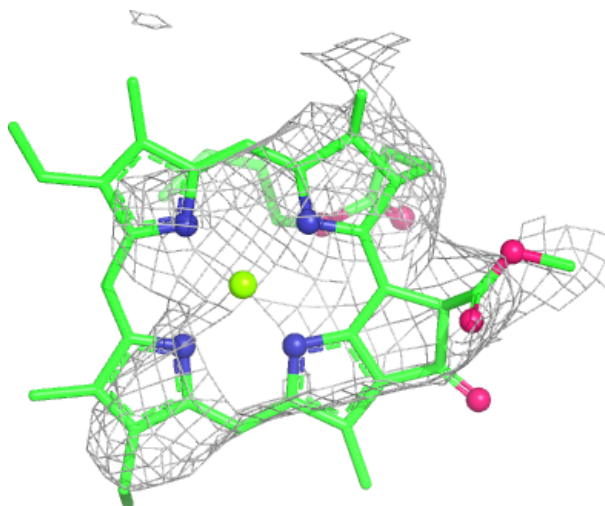
Electron density around CLA B 1023:

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



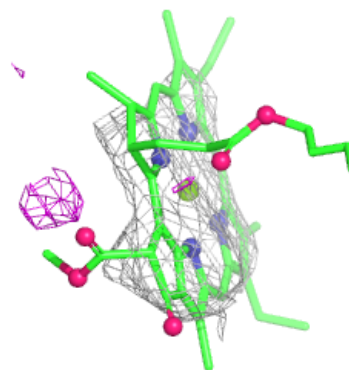
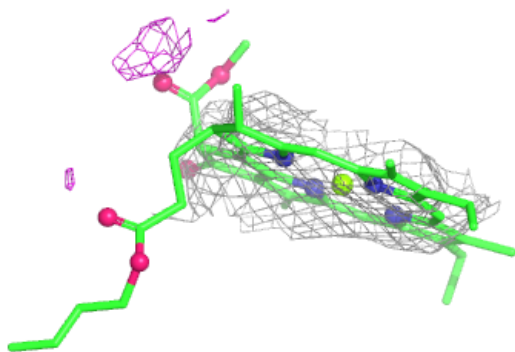
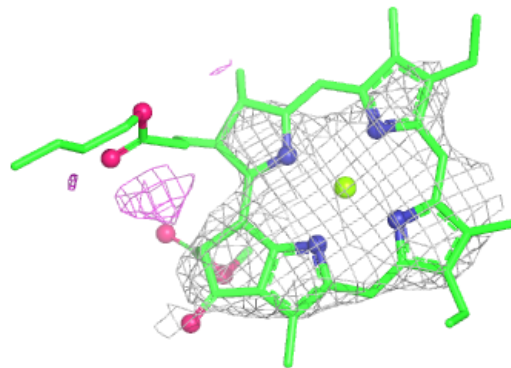
Electron density around CLA A 1119:

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



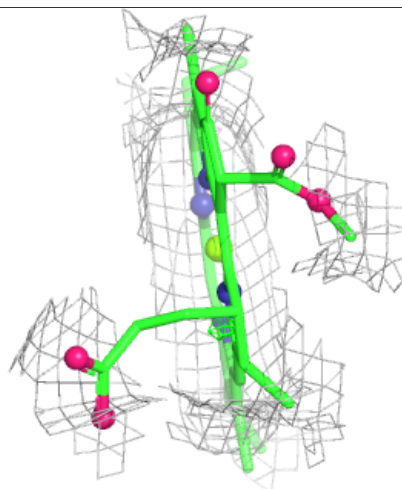
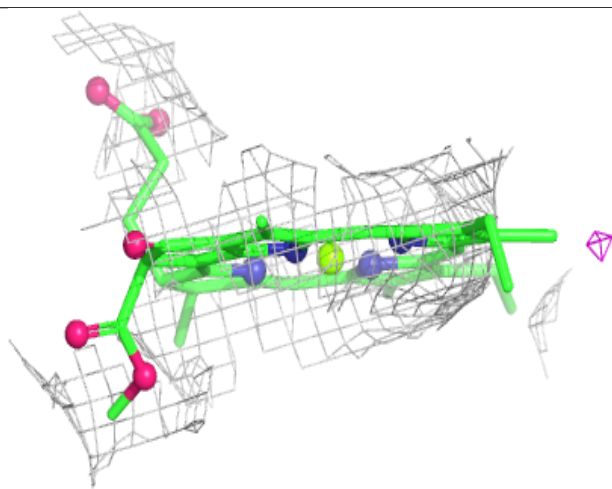
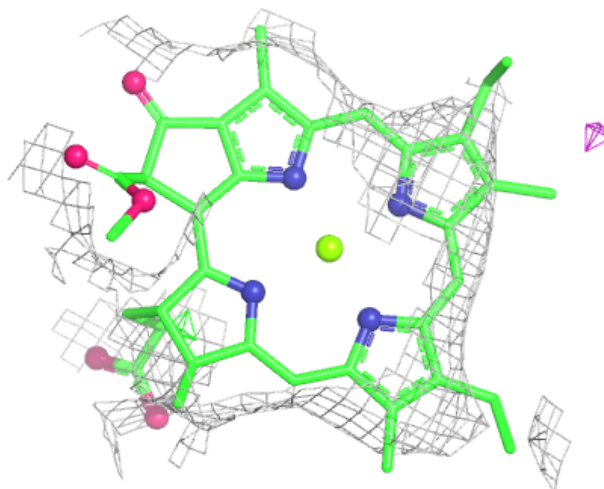
Electron density around CLA A 1112:

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



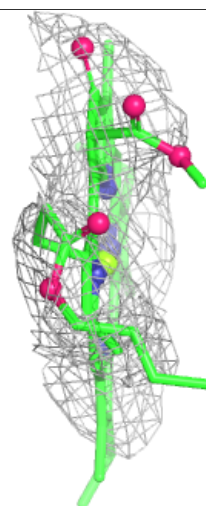
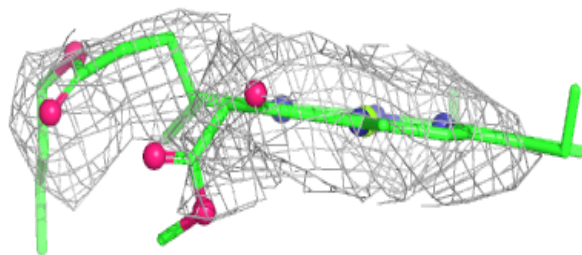
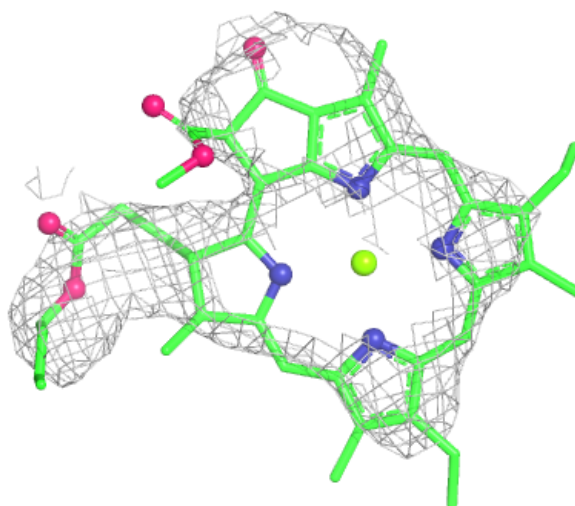
Electron density around CLA A 1102:

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



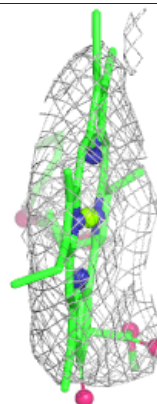
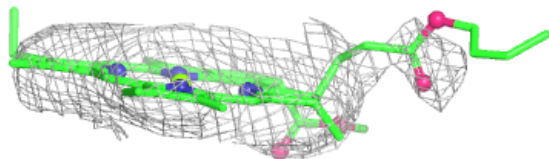
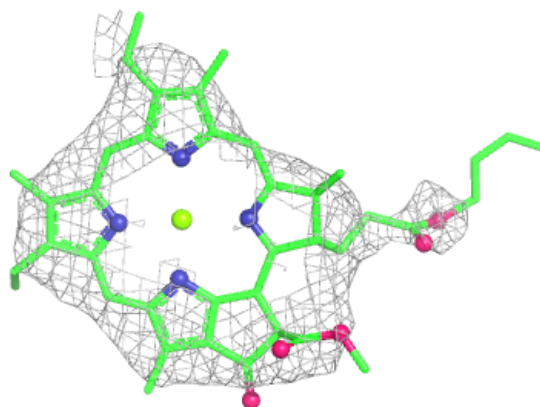
Electron density around CLA B 1221:

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



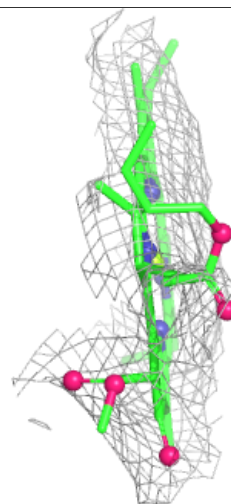
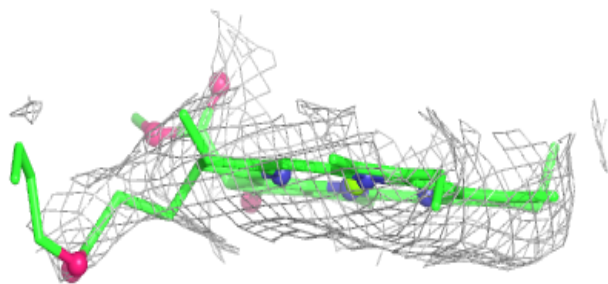
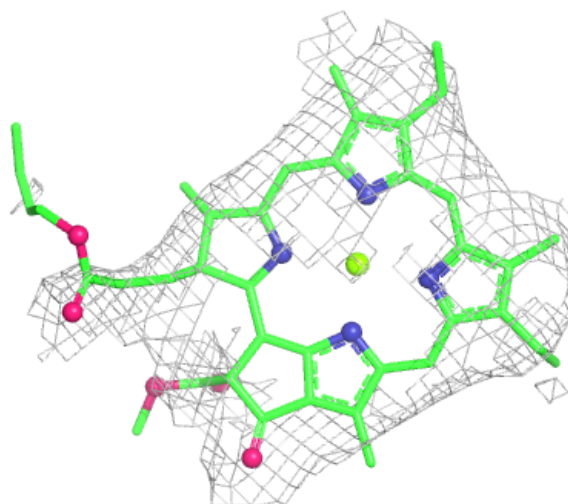
Electron density around CLA J 1302:

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



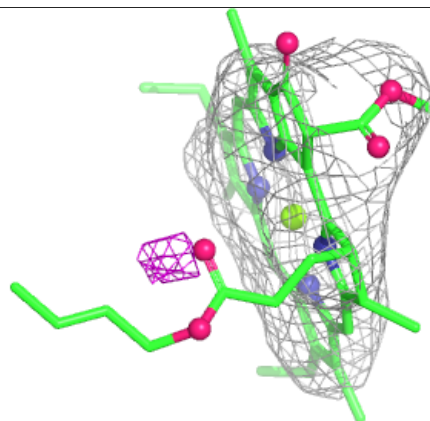
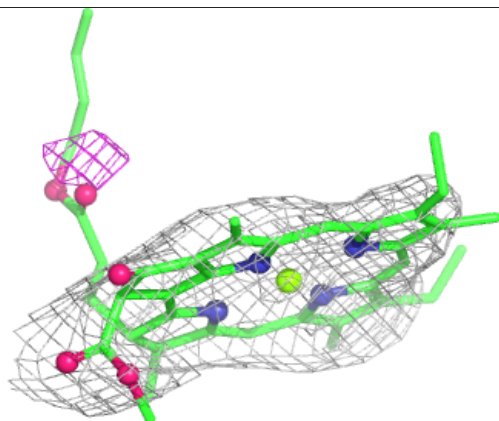
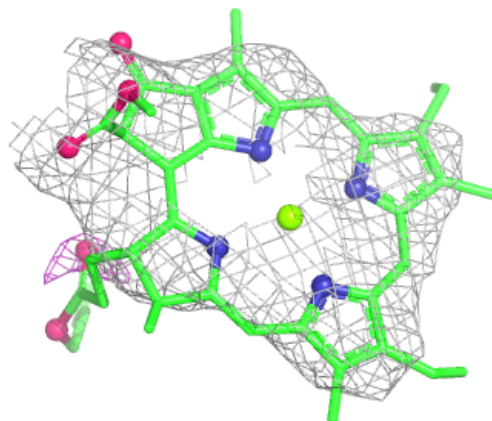
Electron density around CLA B 1206:

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



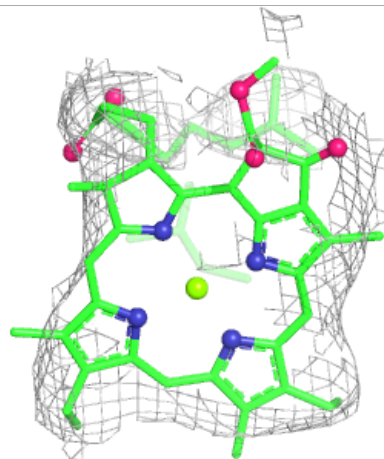
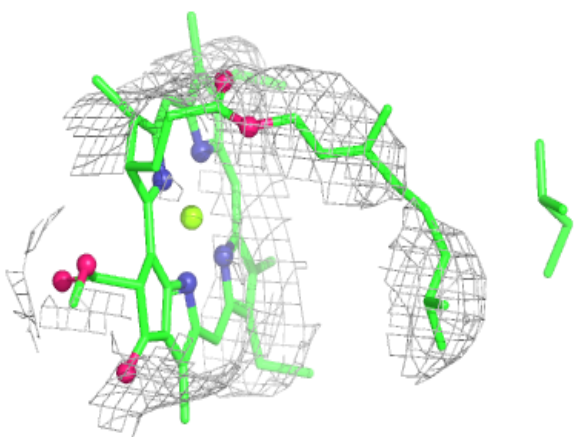
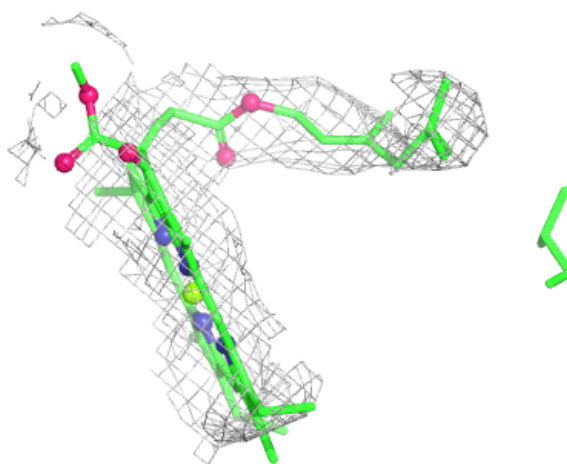
Electron density around CLA A 1122:

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



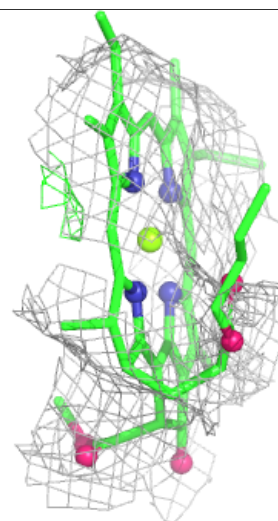
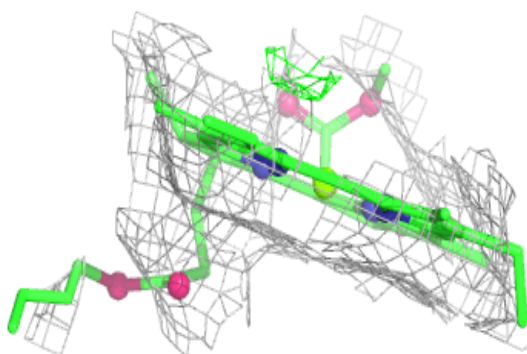
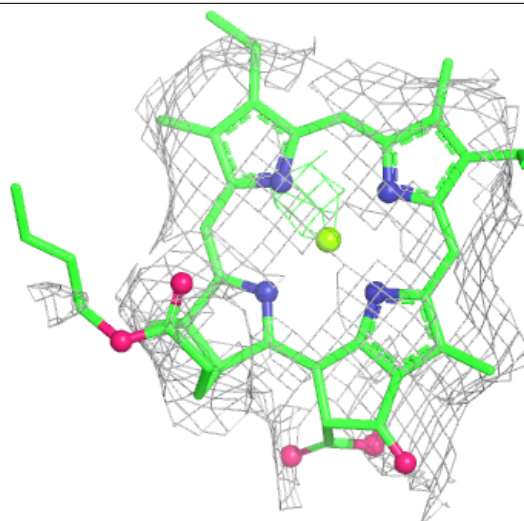
Electron density around CLA 1 612:

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



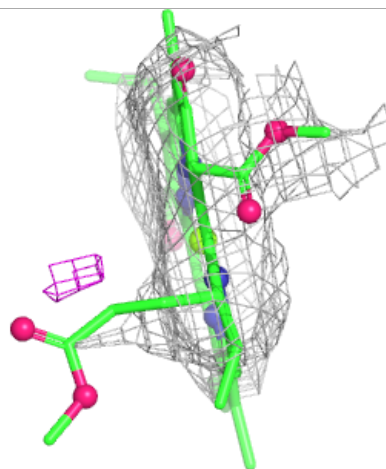
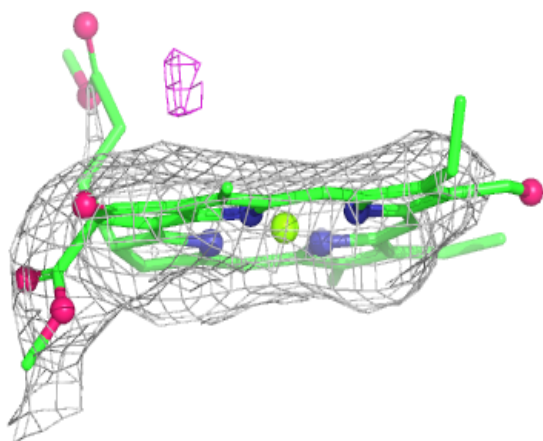
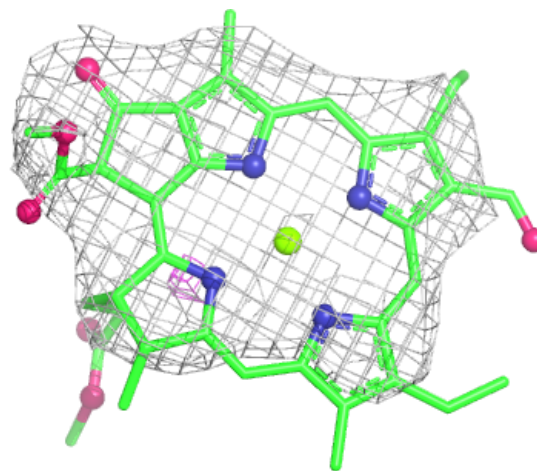
Electron density around CLA 2 601:

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



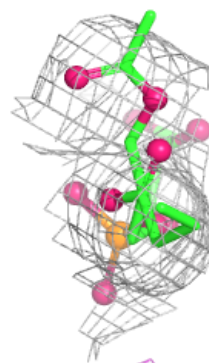
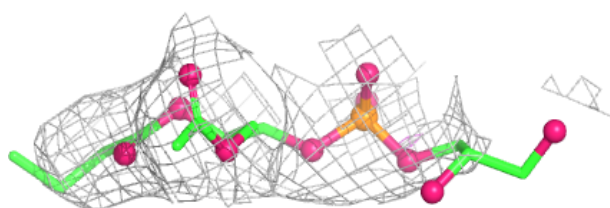
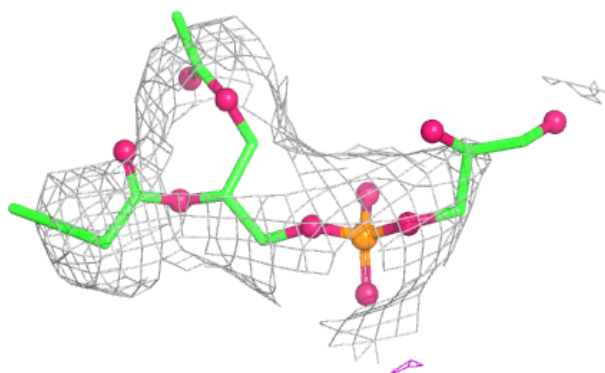
Electron density around CHL 4 610:

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

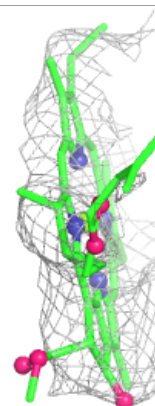
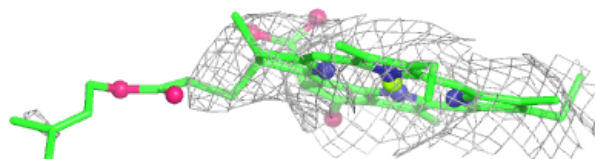
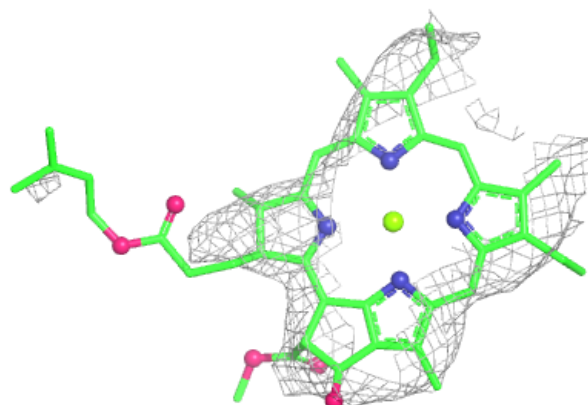


Electron density around LHG 1 801:

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

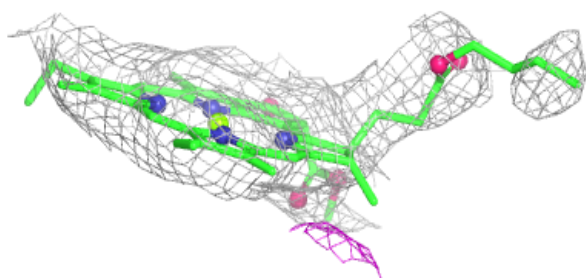
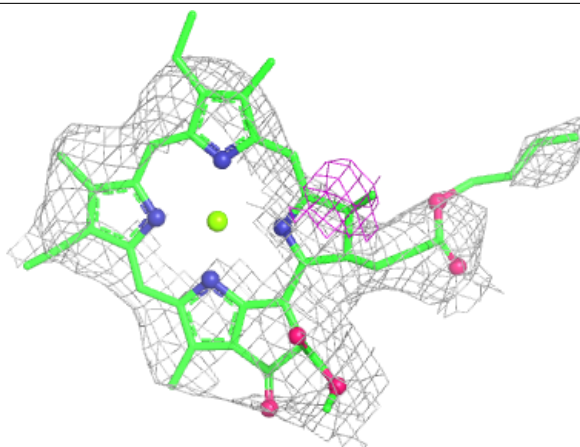
**Electron density around CLA B 1022:**

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



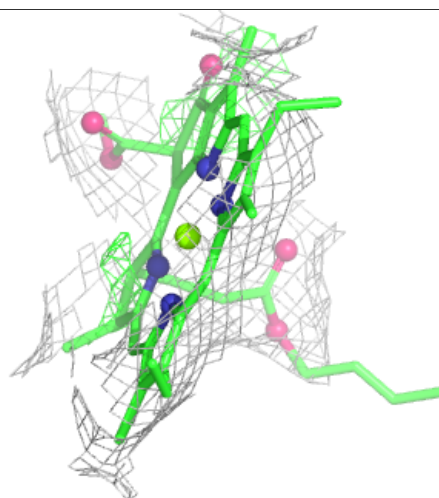
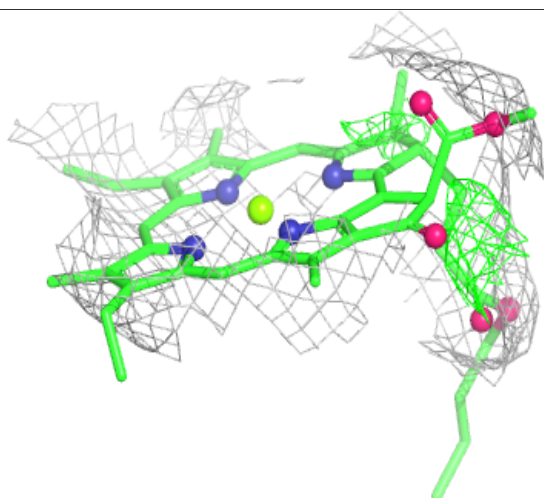
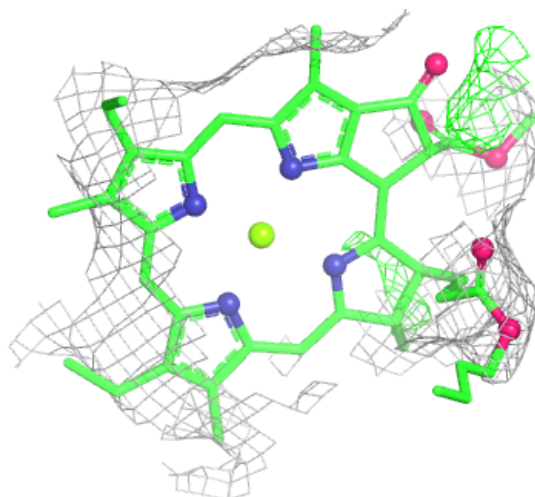
Electron density around CLA 4 609:

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



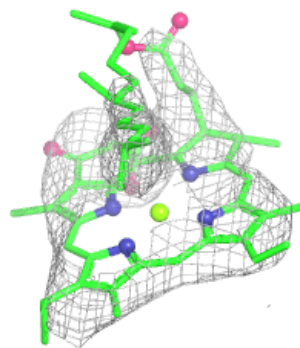
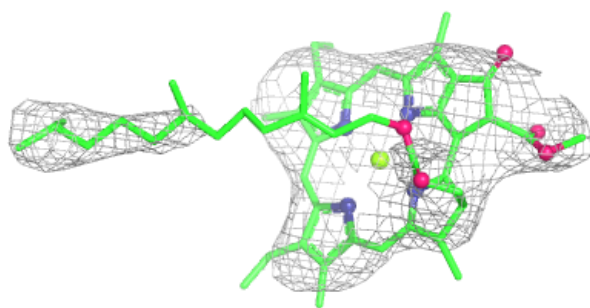
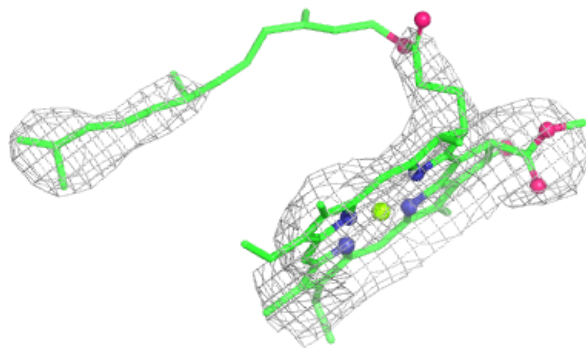
Electron density around CLA A 1133:

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



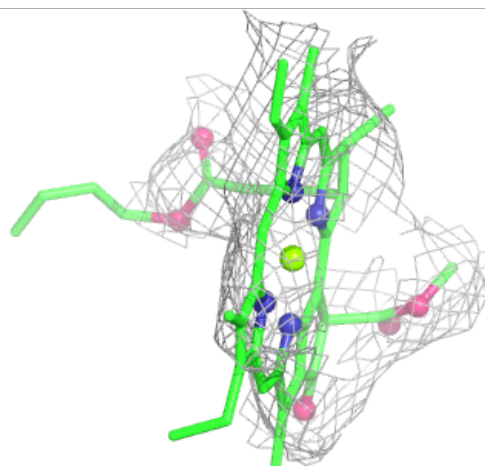
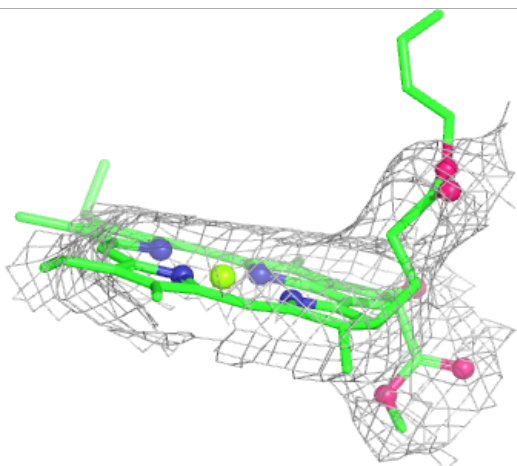
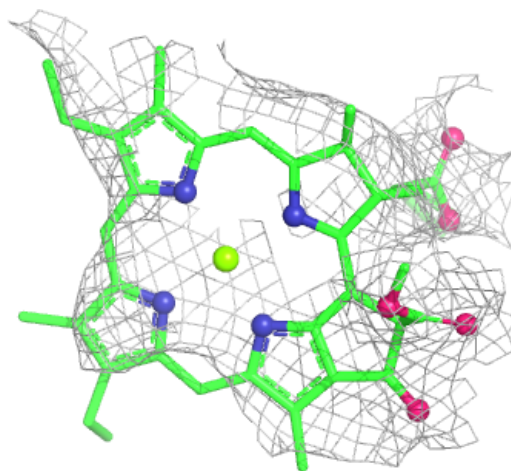
Electron density around CLA B 1228:

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



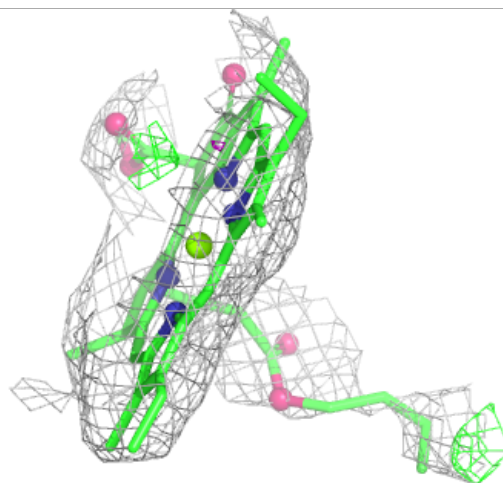
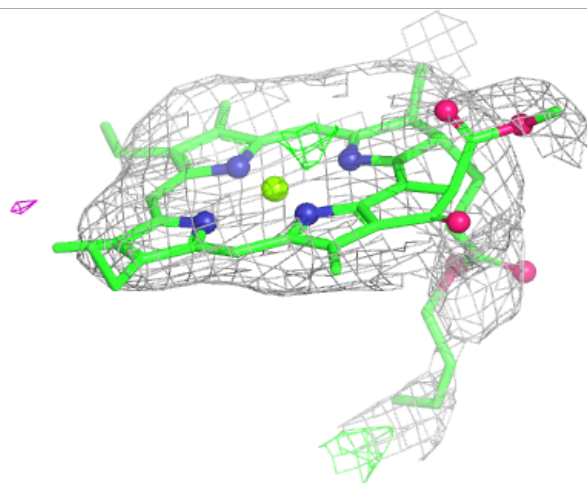
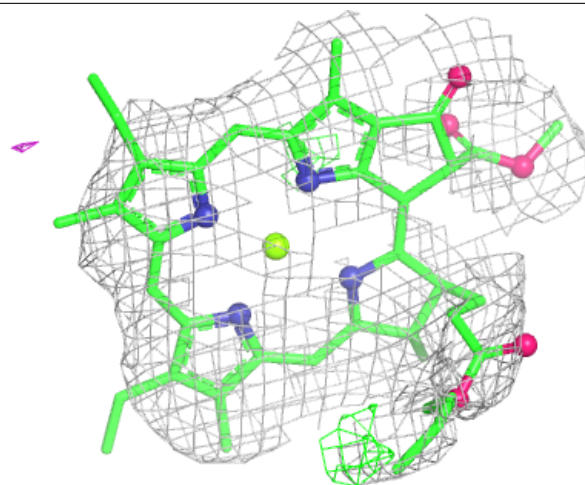
Electron density around CLA A 1128:

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



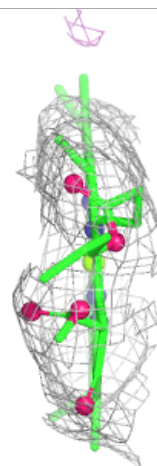
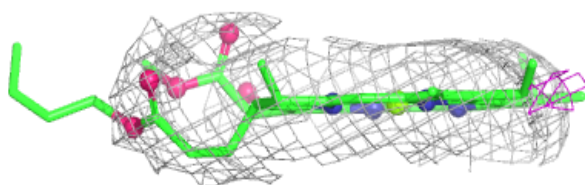
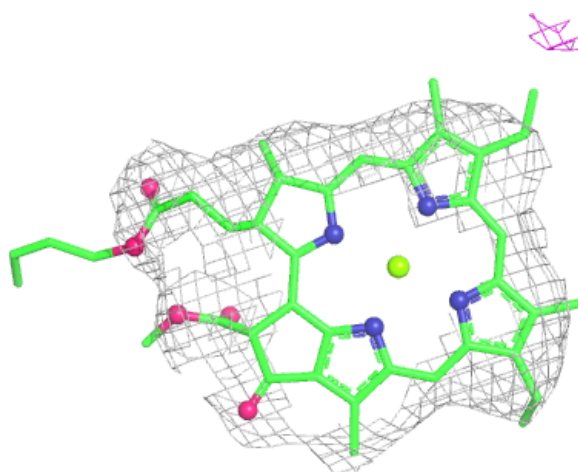
Electron density around CLA B 1216:

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



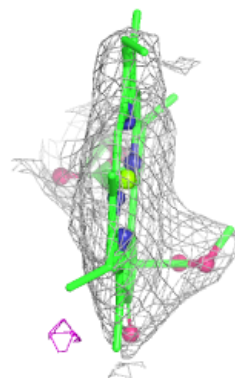
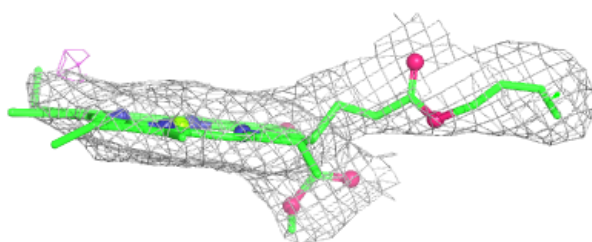
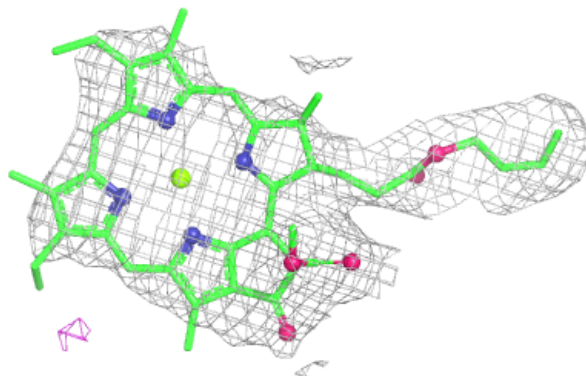
Electron density around CLA 4 602:

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

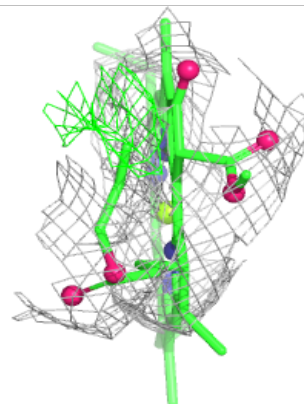
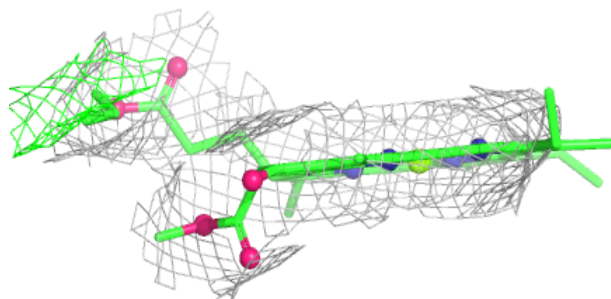
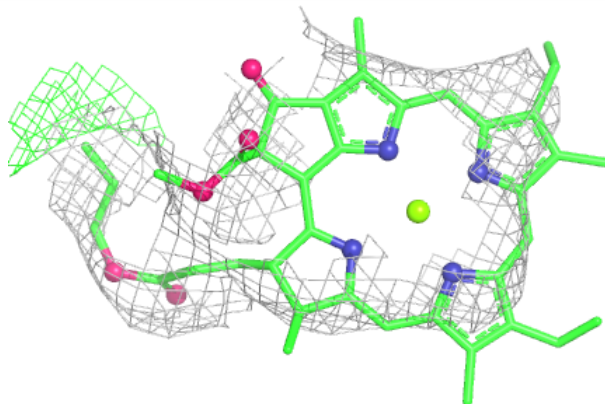


Electron density around CLA B 1234:

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

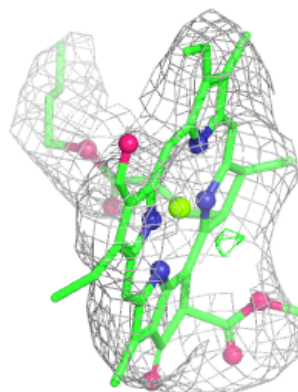
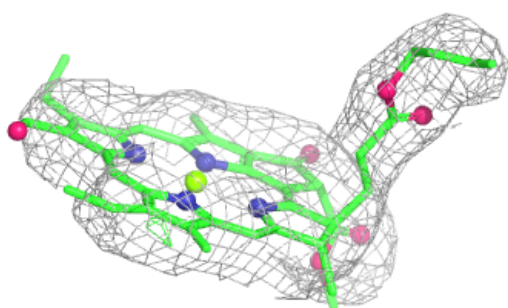
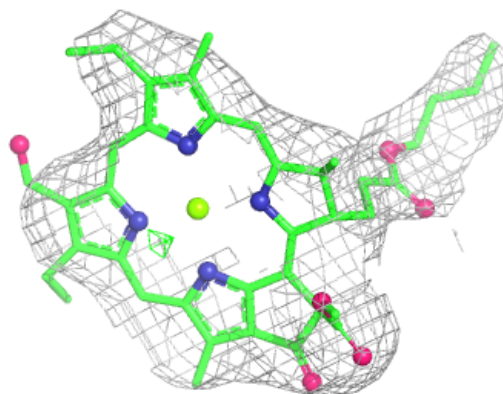
**Electron density around CLA A 1123:**

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



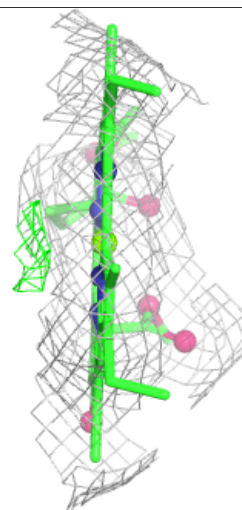
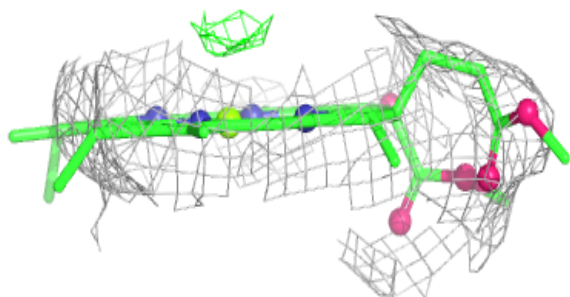
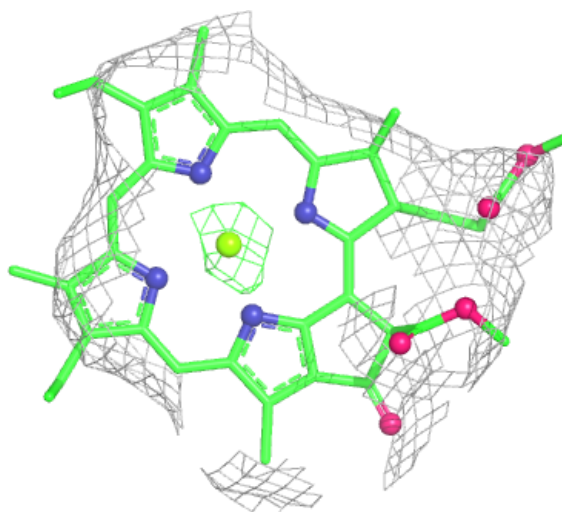
Electron density around CHL 4 611:

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



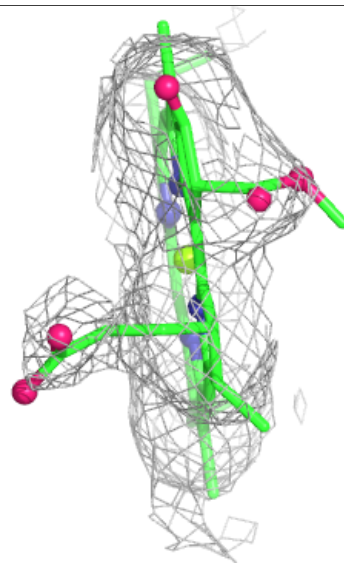
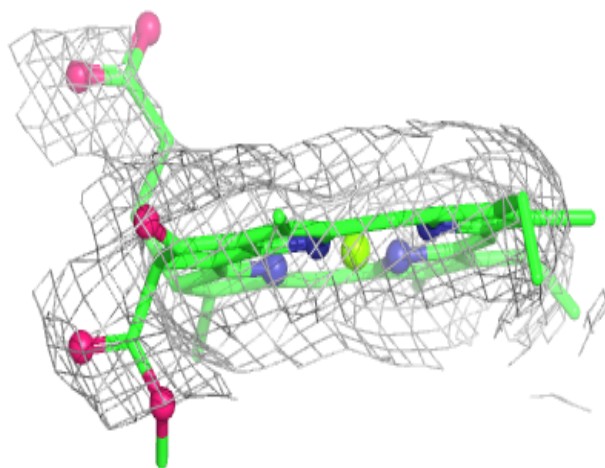
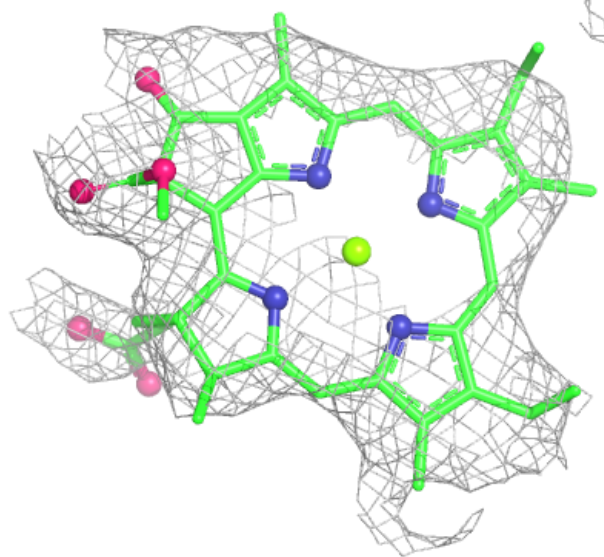
Electron density around CLA 1 602:

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



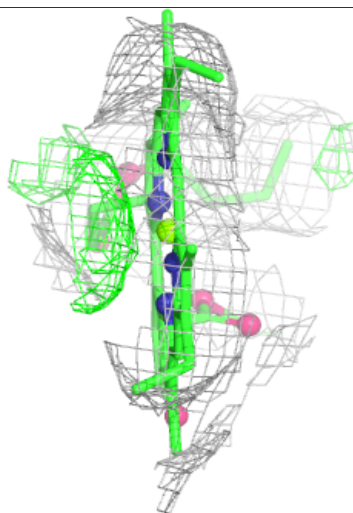
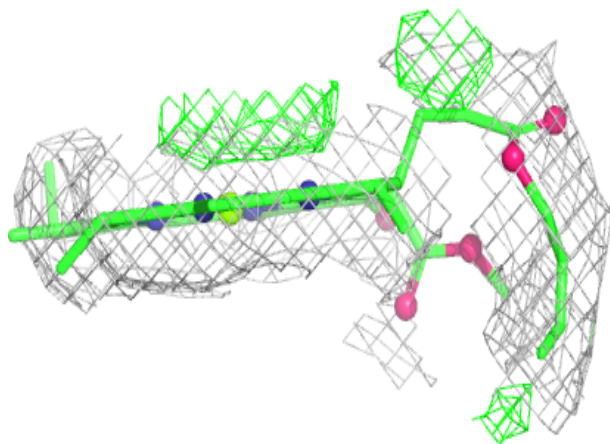
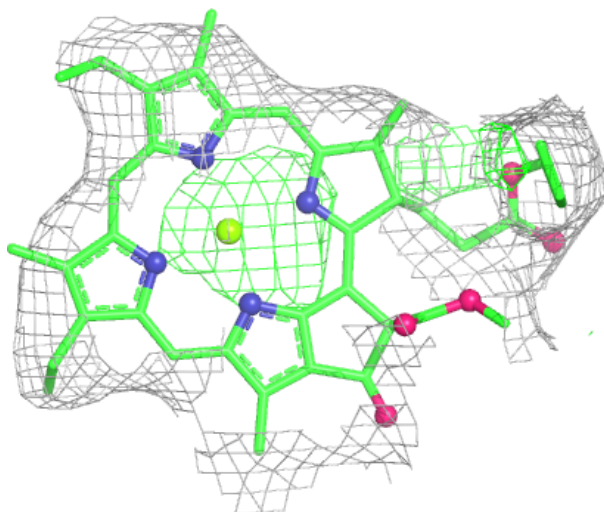
Electron density around CLA B 1227:

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



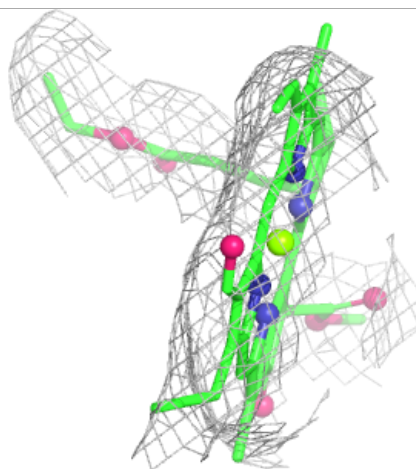
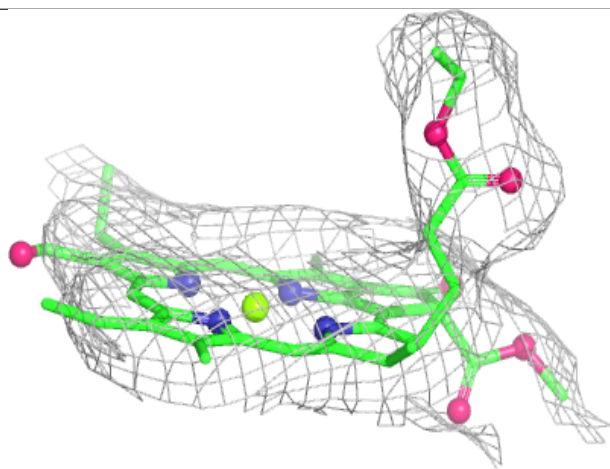
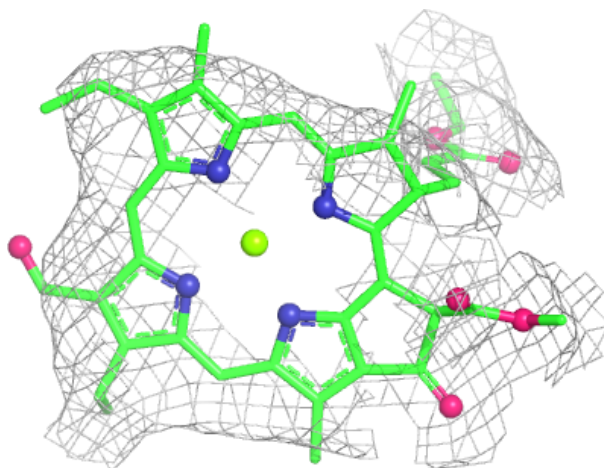
Electron density around CLA 4 605:

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



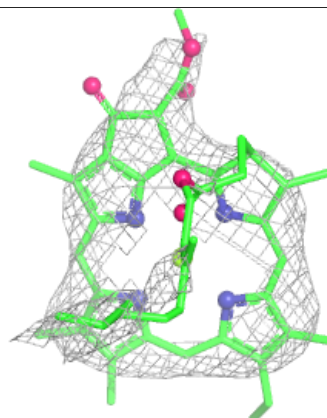
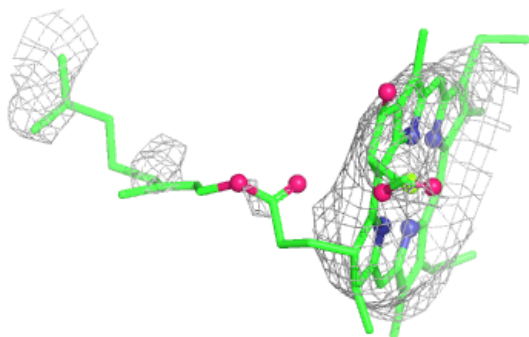
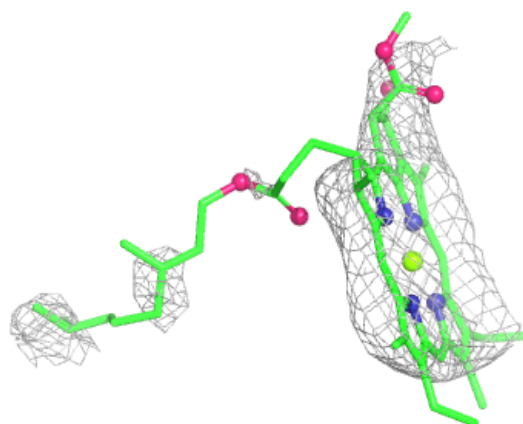
Electron density around CHL 2 611:

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



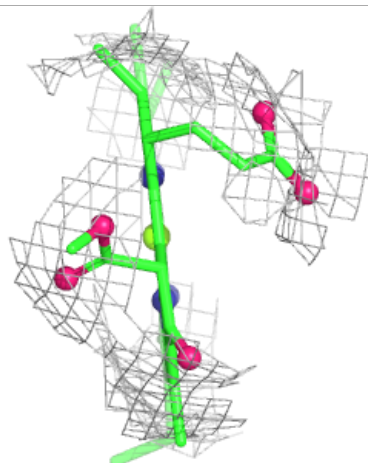
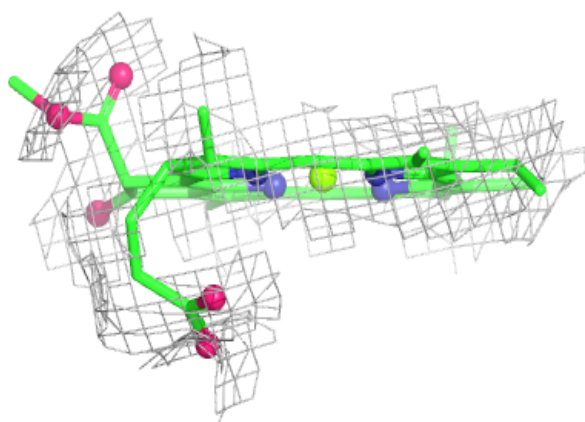
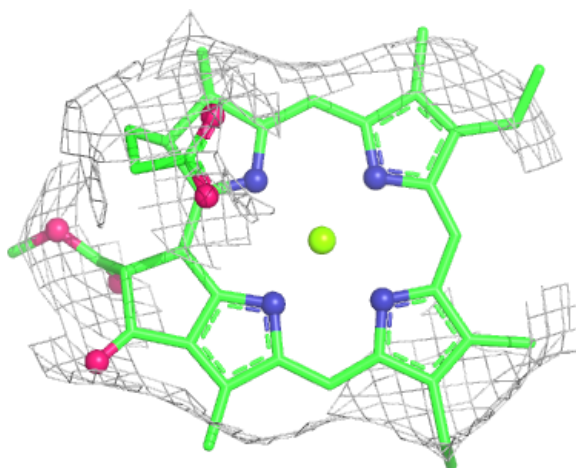
Electron density around CLA A 1140:

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



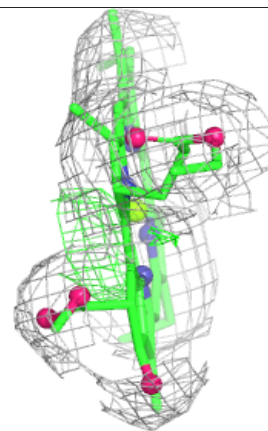
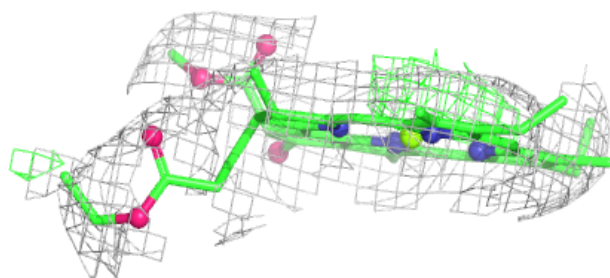
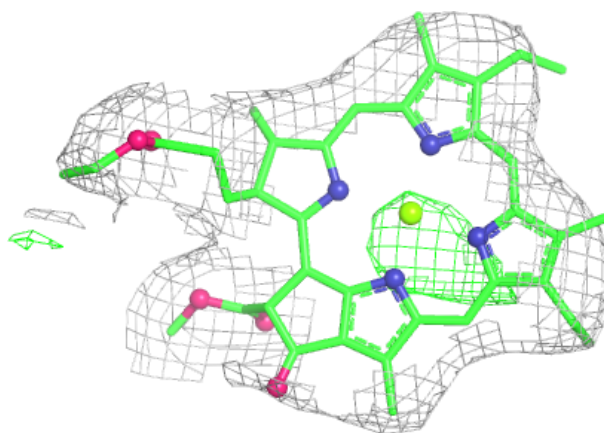
Electron density around CLA 1 613:

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



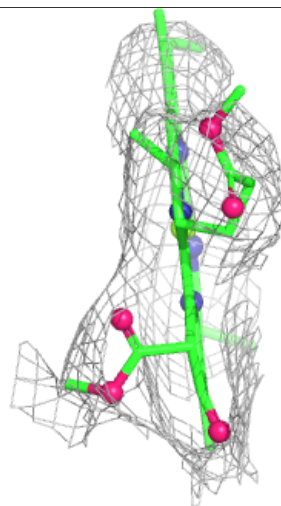
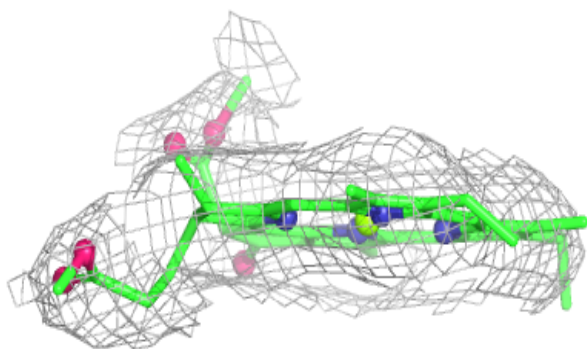
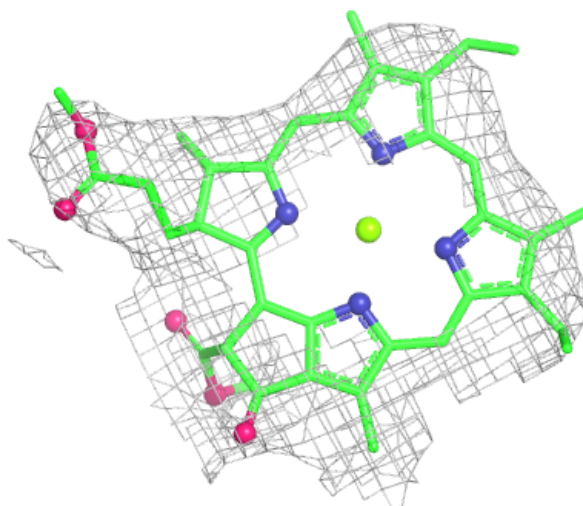
Electron density around CLA F 1301:

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



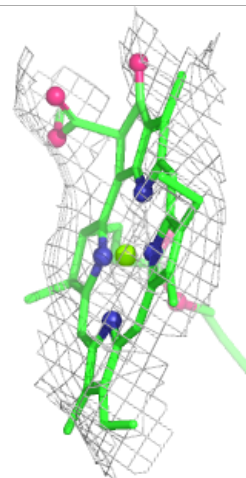
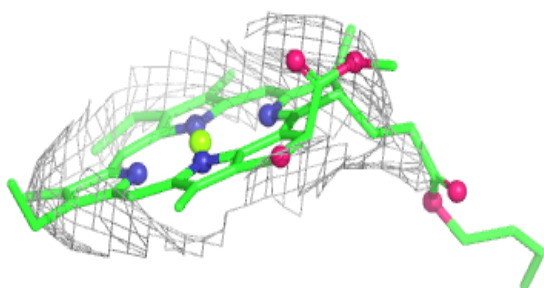
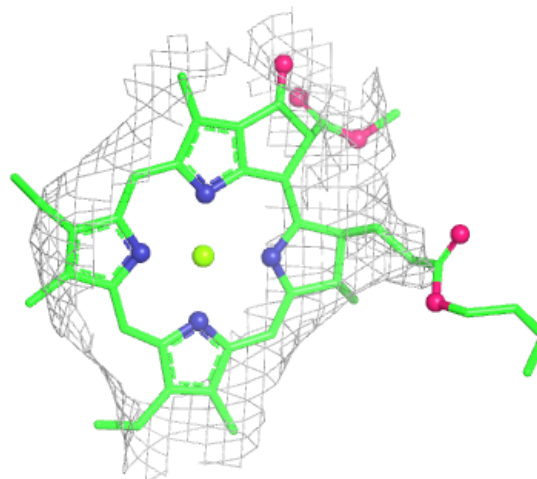
Electron density around CLA B 1217:

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



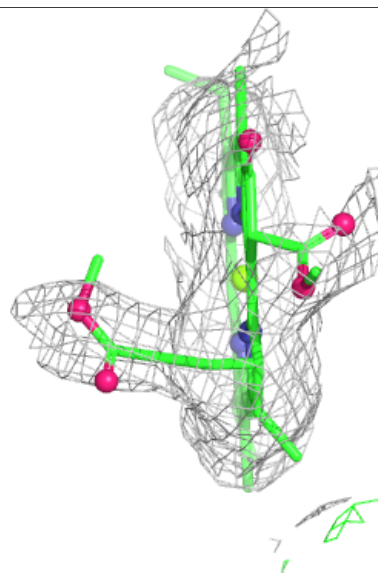
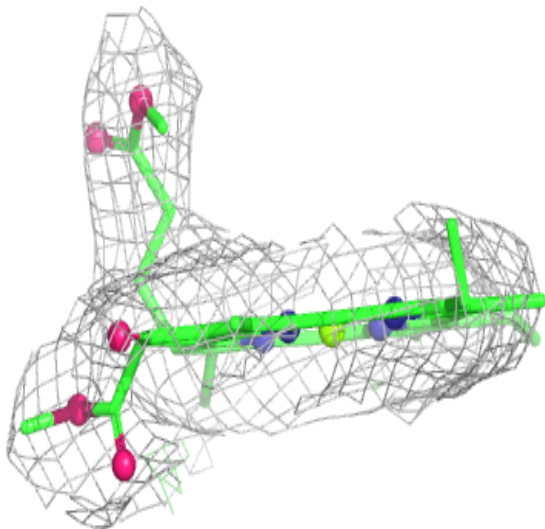
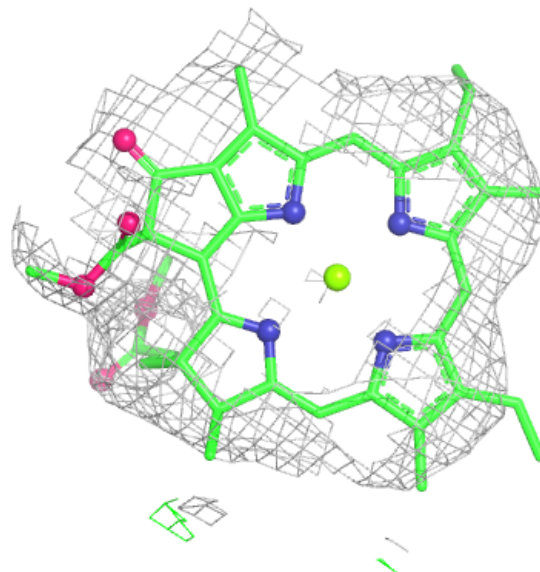
Electron density around CLA A 1125:

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



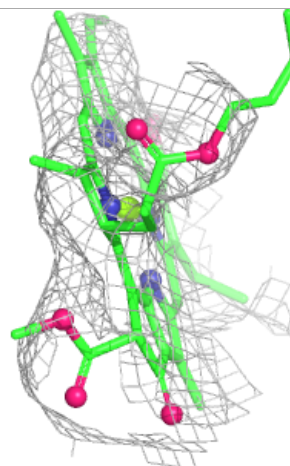
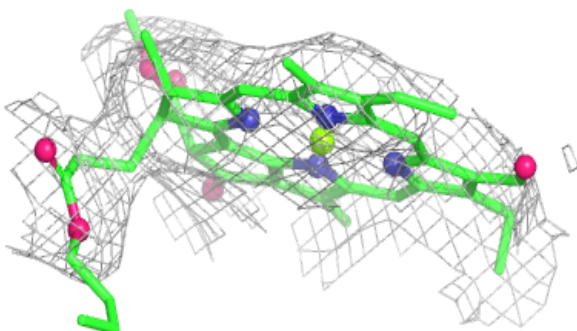
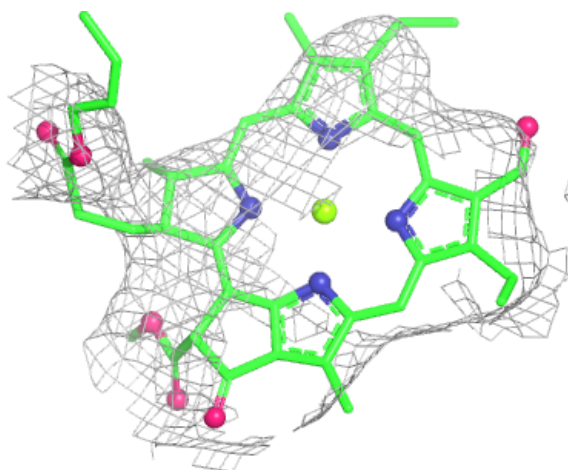
Electron density around CLA 4 608:

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



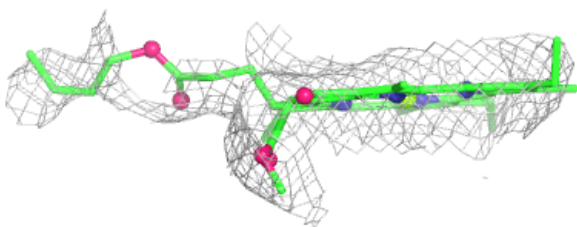
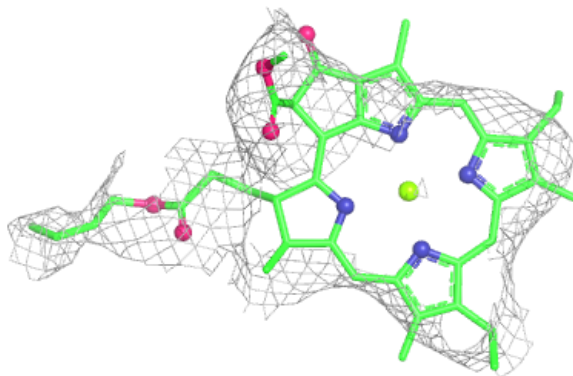
Electron density around CHL 2 609:

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



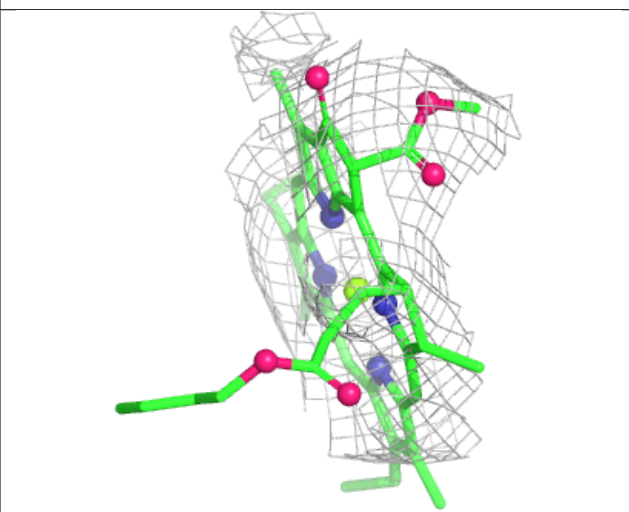
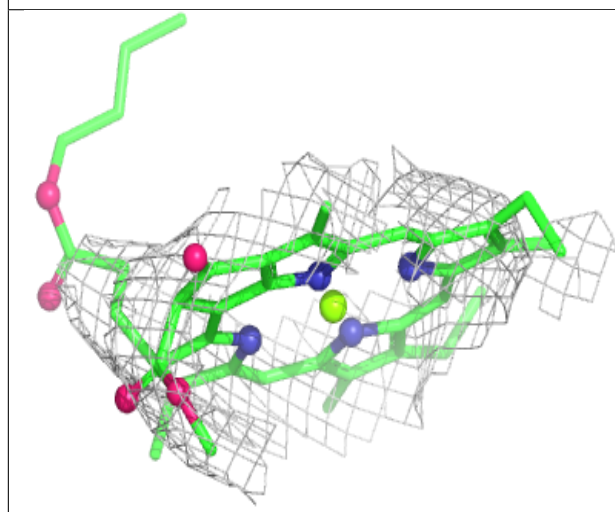
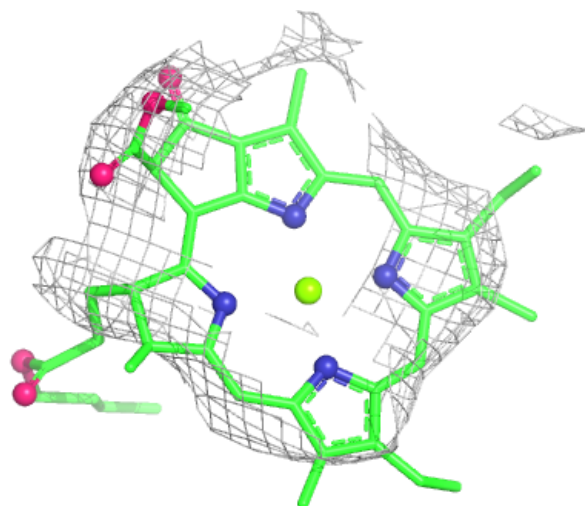
Electron density around CLA A 1135:

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



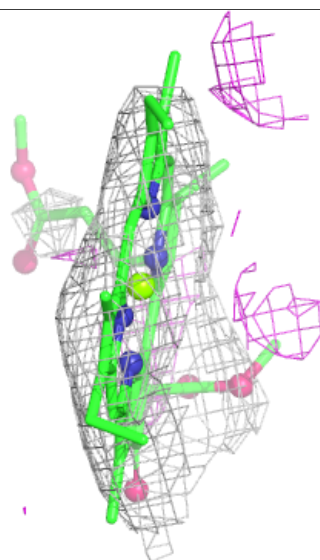
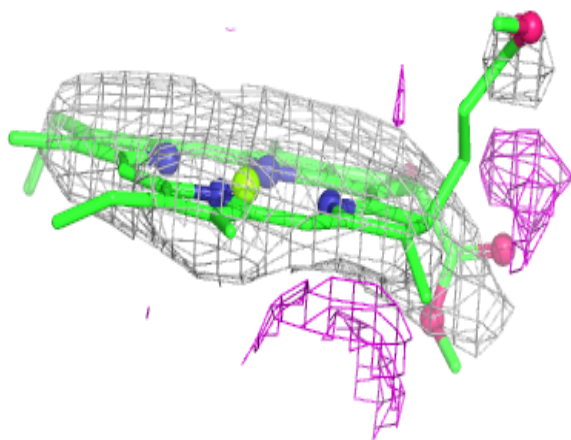
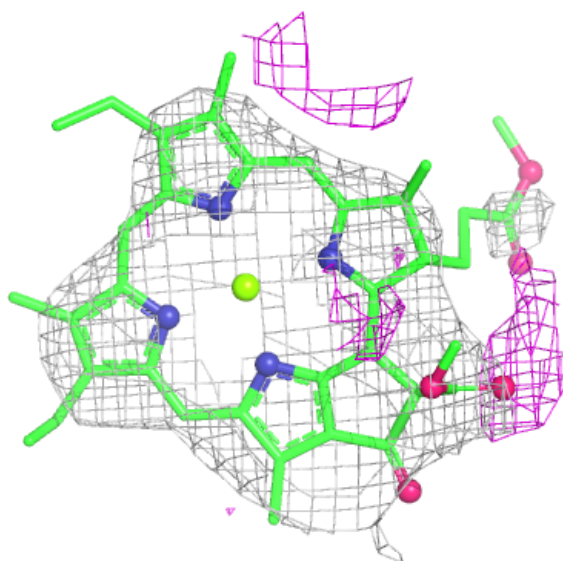
Electron density around CLA A 1118:

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



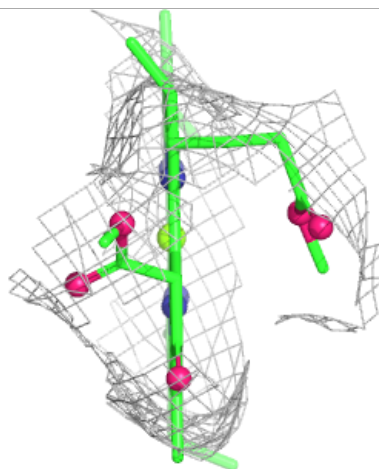
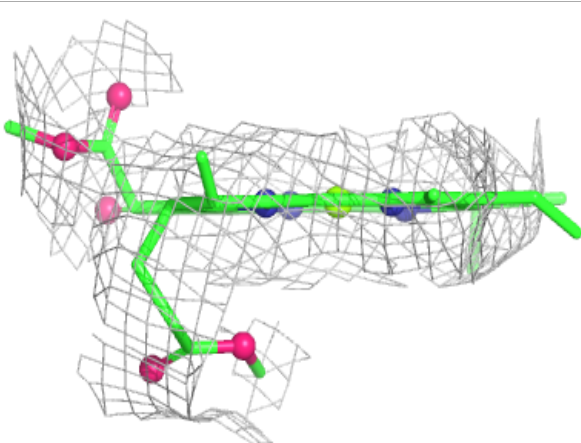
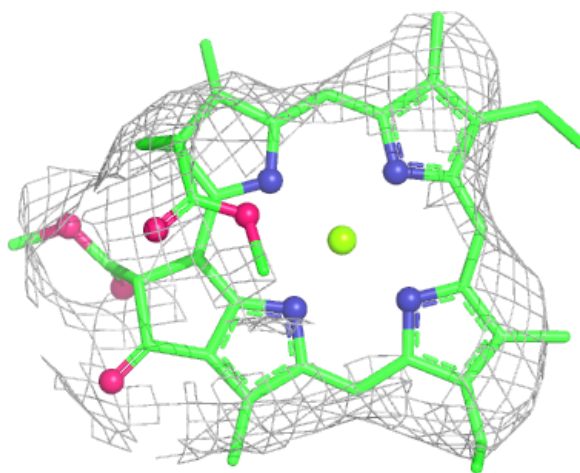
Electron density around CLA 1 608:

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



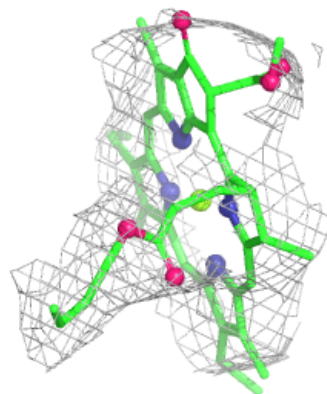
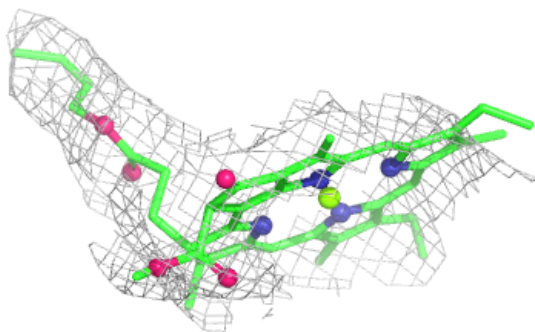
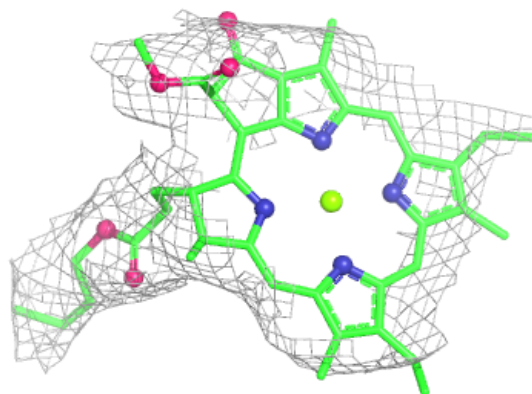
Electron density around CLA 2 603:

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



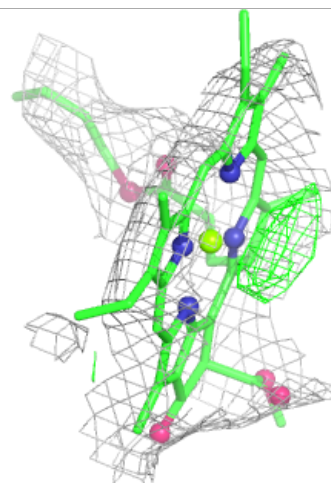
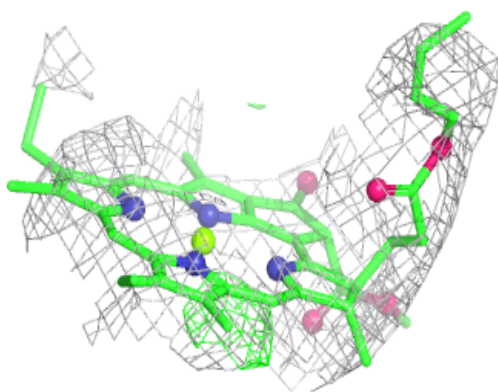
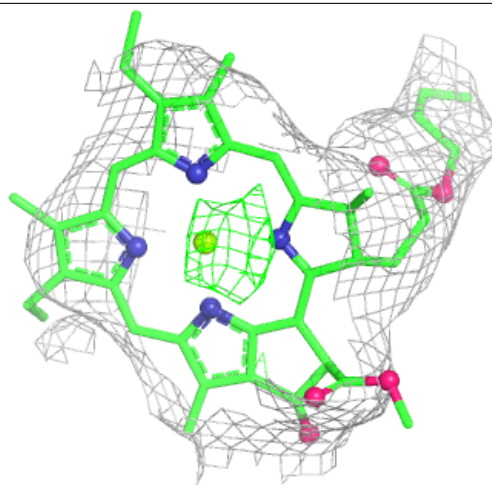
Electron density around CLA 1 611:

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



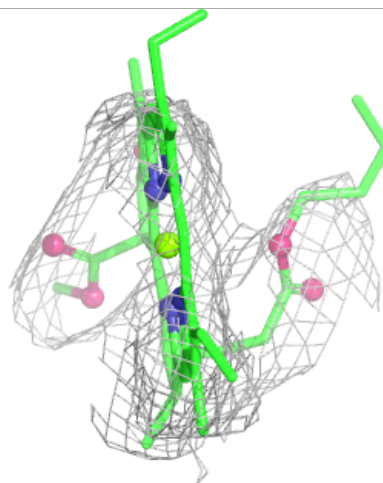
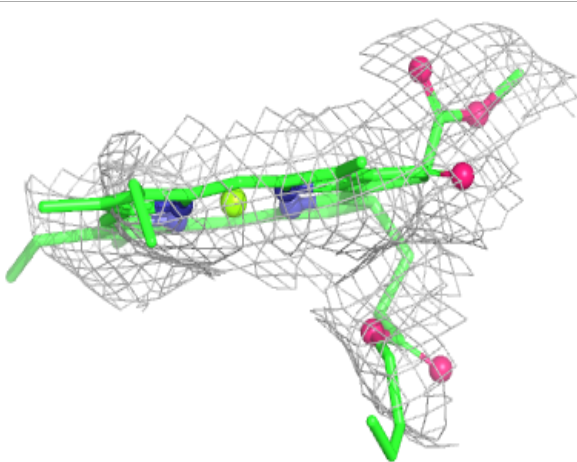
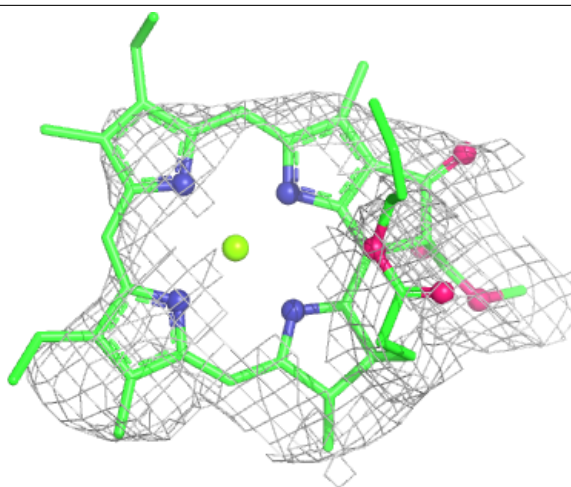
Electron density around CLA 2 612:

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



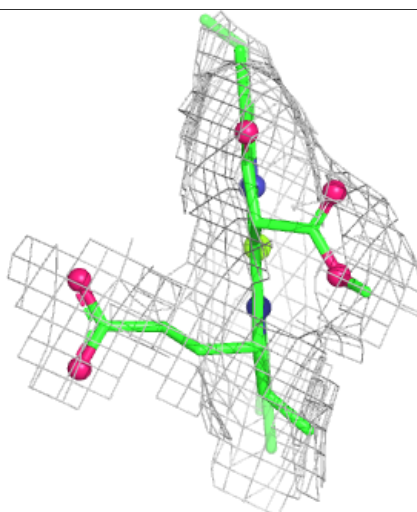
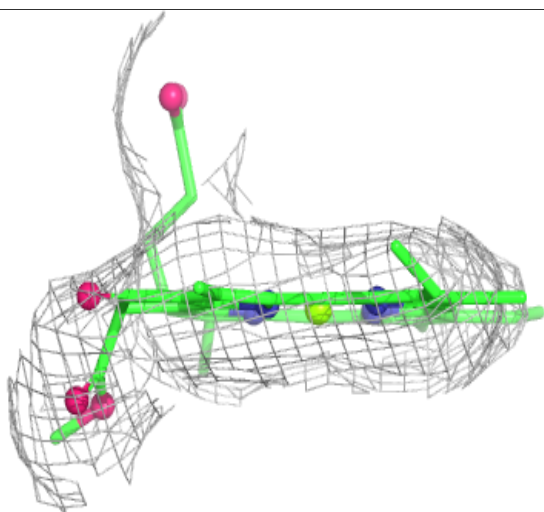
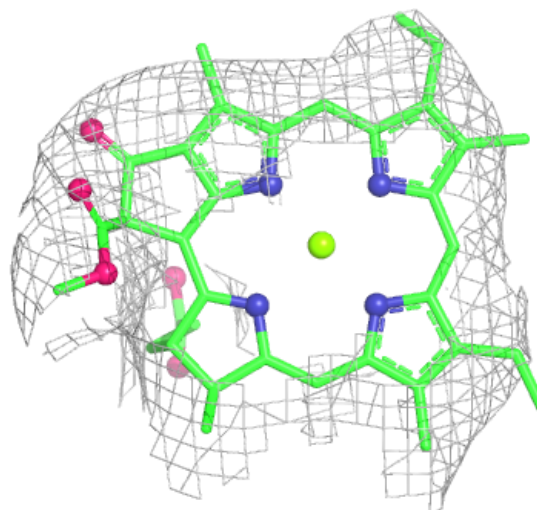
Electron density around CLA B 1213:

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



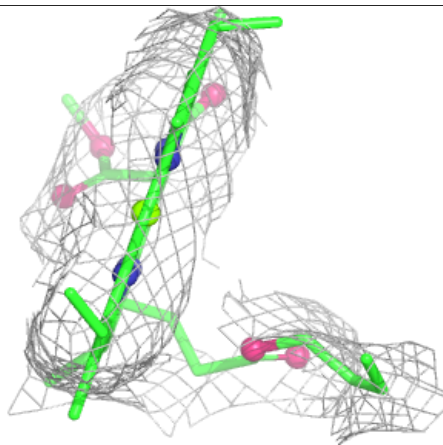
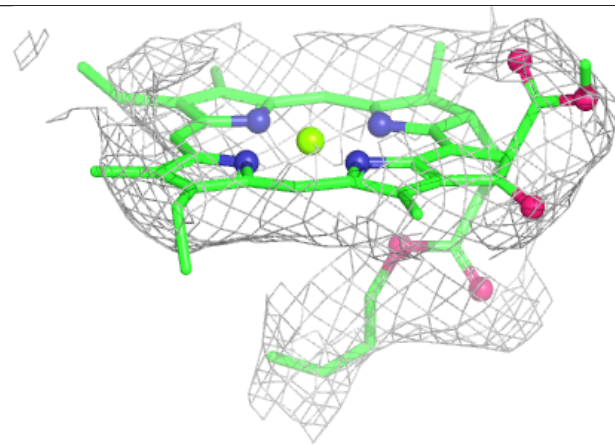
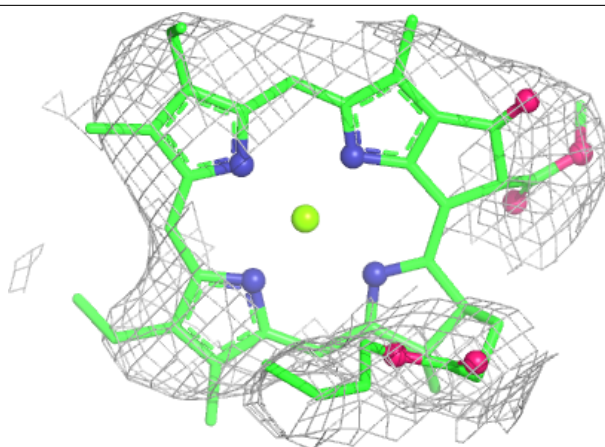
Electron density around CLA 1 606:

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



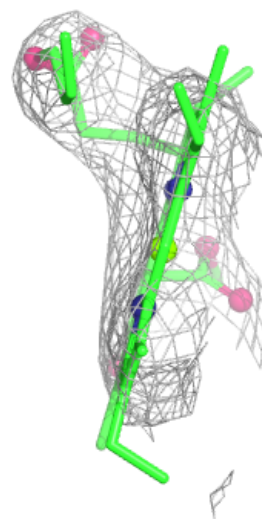
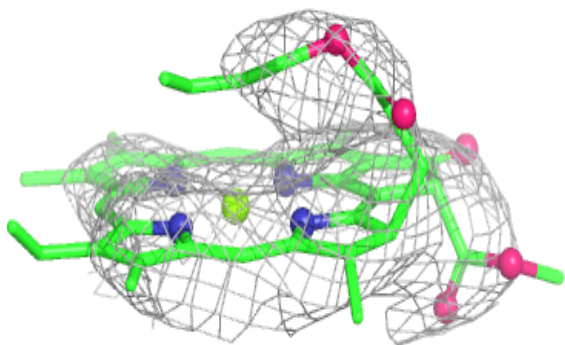
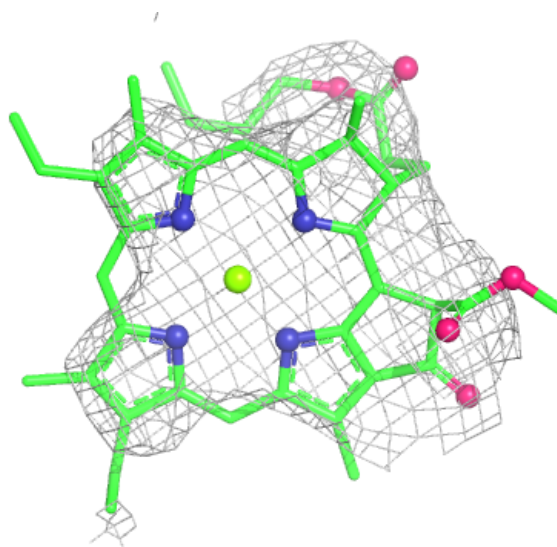
Electron density around CLA A 1105:

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



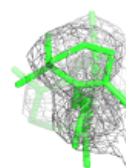
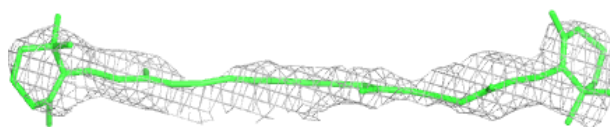
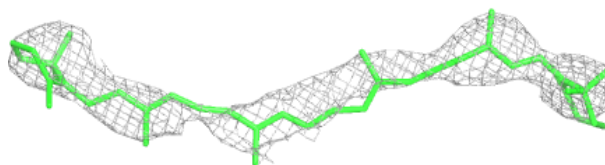
Electron density around CLA A 1117:

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



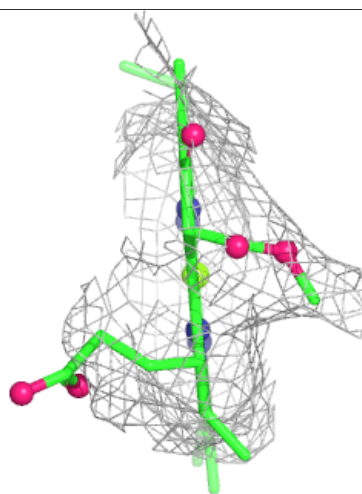
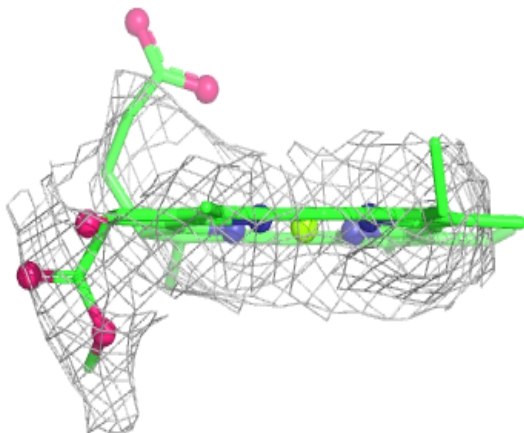
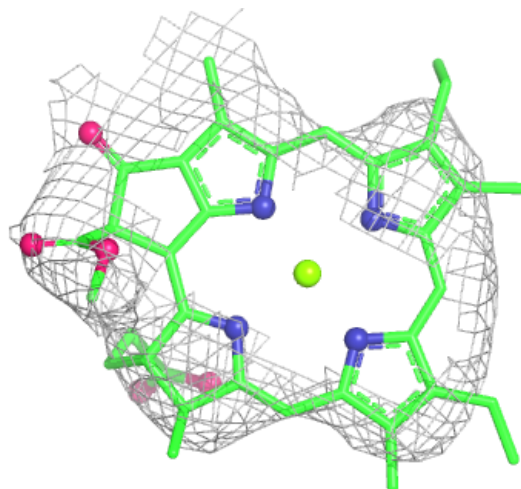
Electron density around BCR B 4004:

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



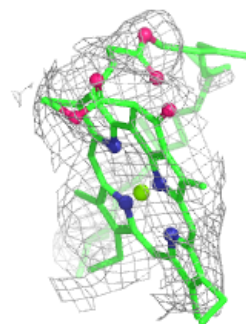
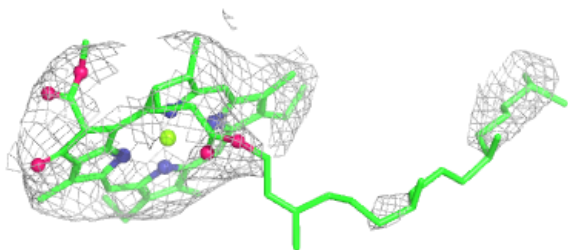
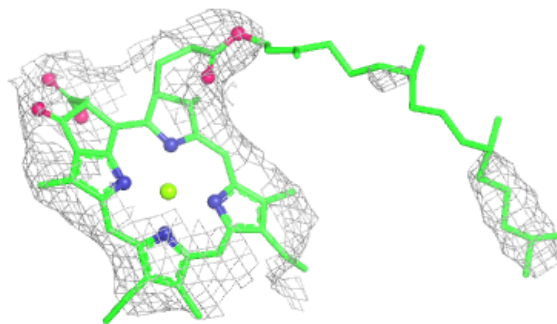
Electron density around CLA B 1212:

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



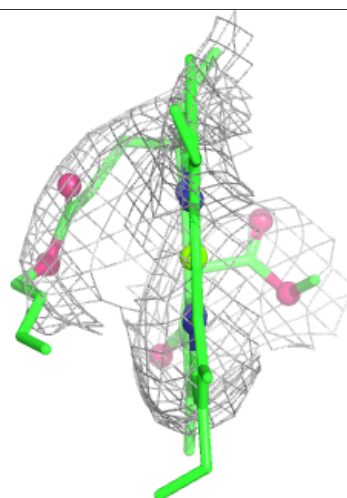
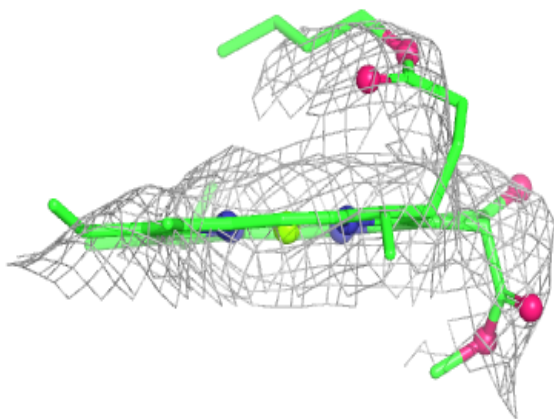
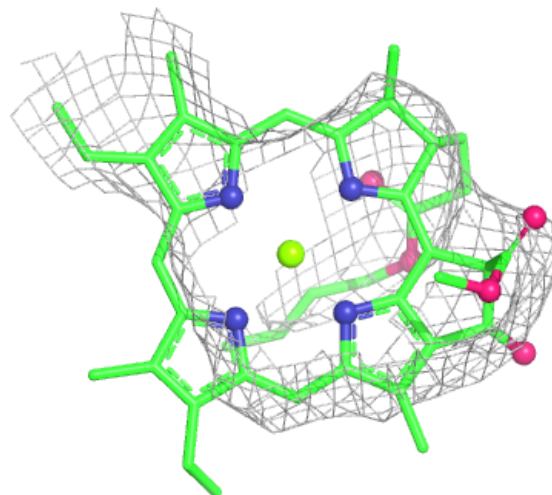
Electron density around CLA A 1106:

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



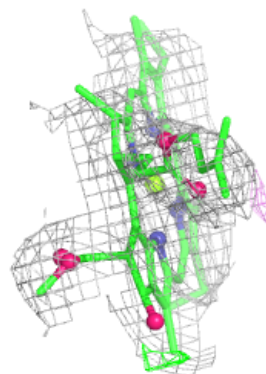
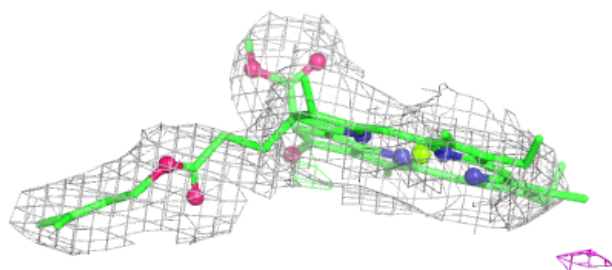
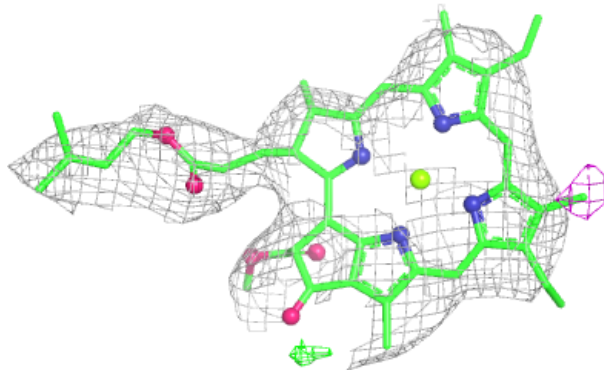
Electron density around CLA A 1110:

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



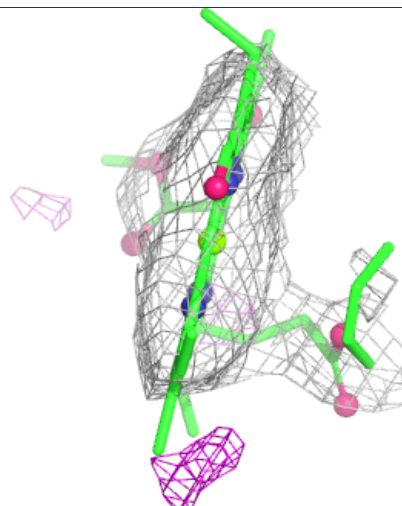
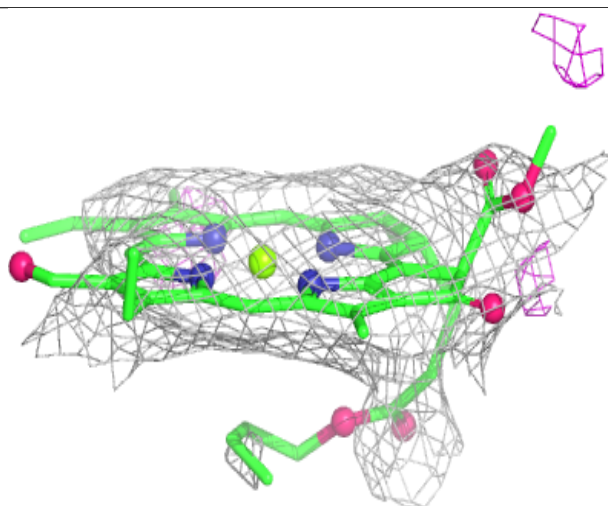
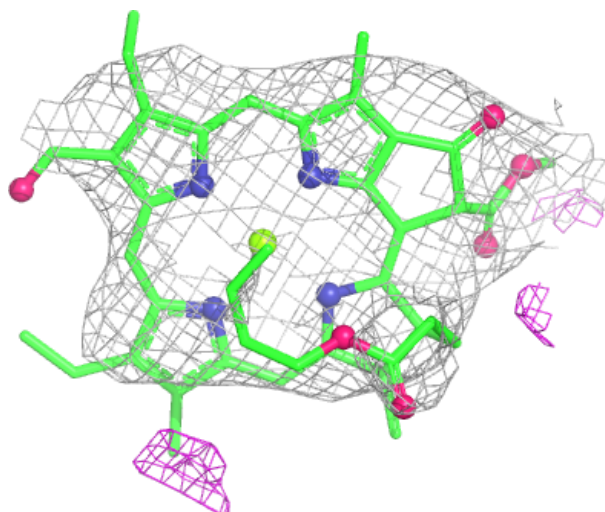
Electron density around CLA B 1223:

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



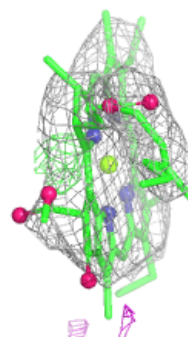
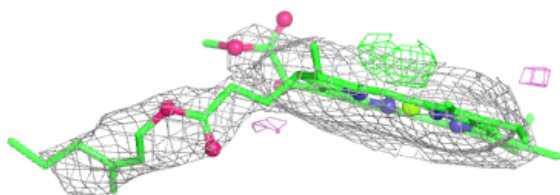
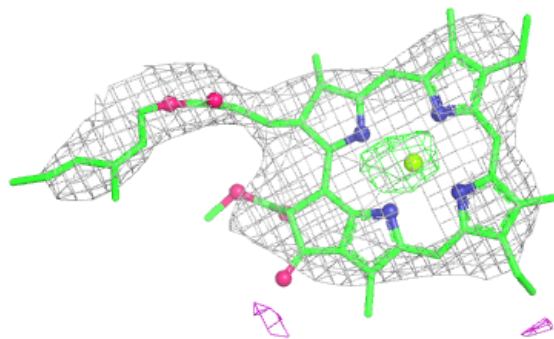
Electron density around CHL 1 609:

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

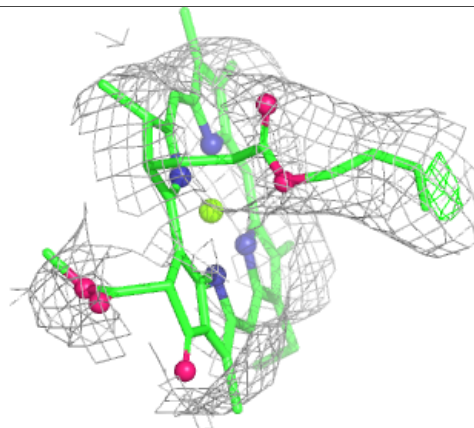
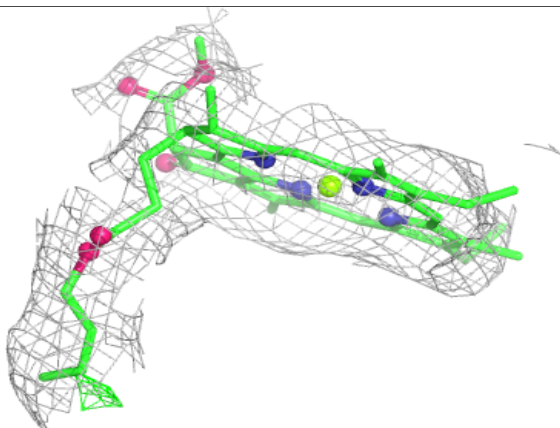
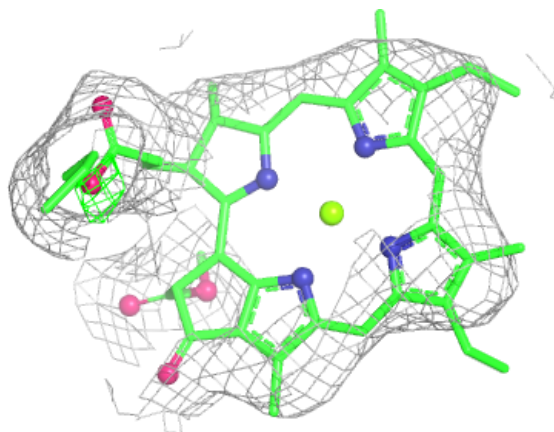


Electron density around CLA A 1139:

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

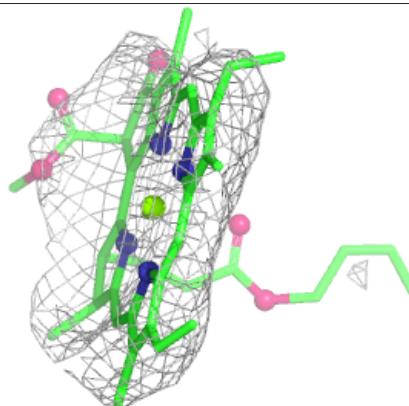
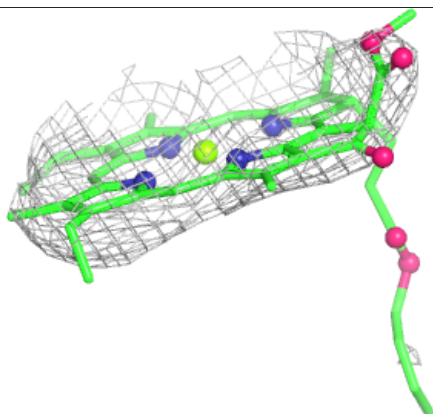
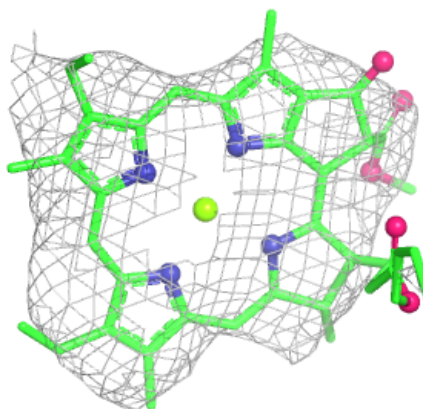
**Electron density around CLA B 1236:**

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

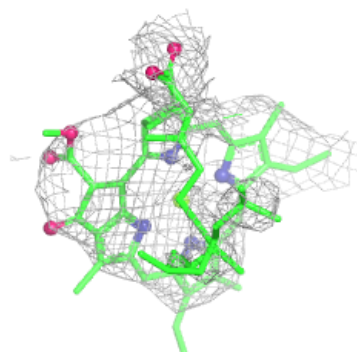
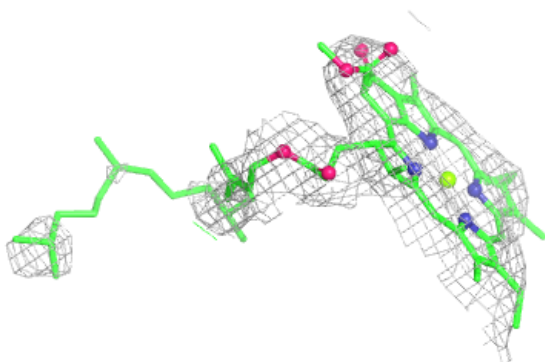
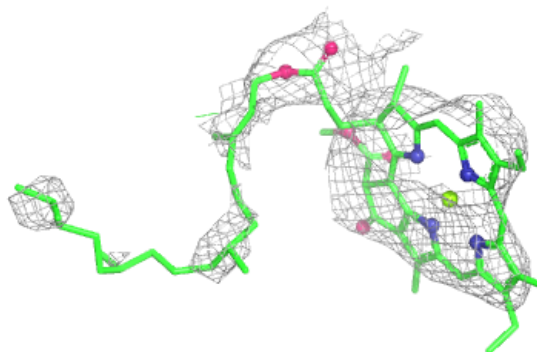


Electron density around CLA B 1225:

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

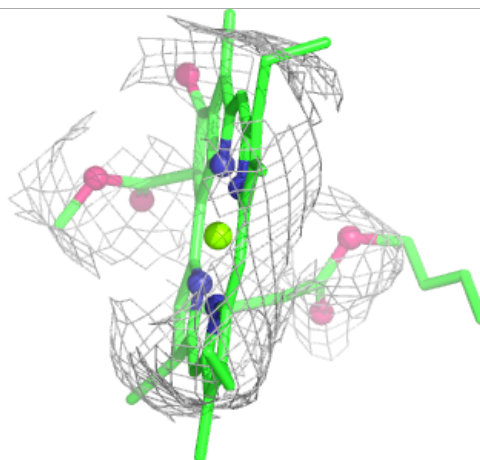
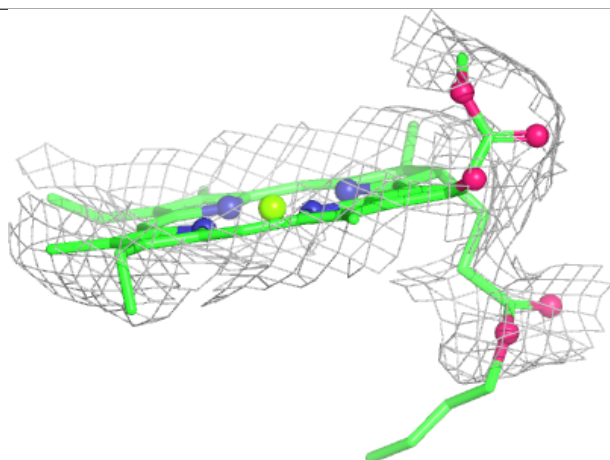
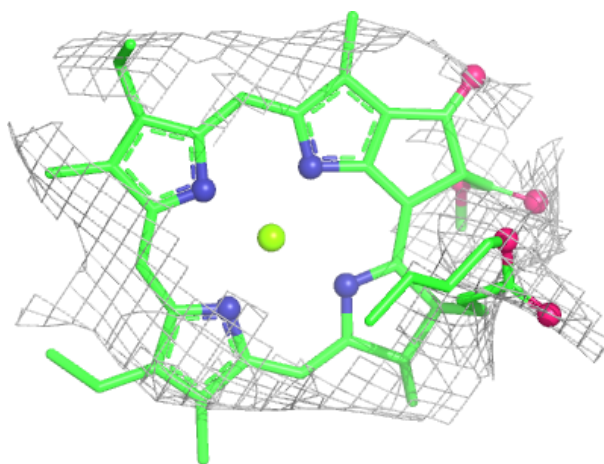
**Electron density around CLA B 1021:**

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



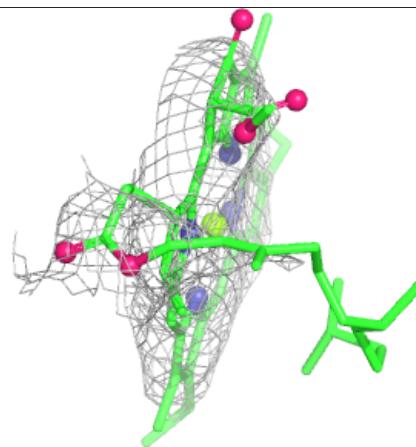
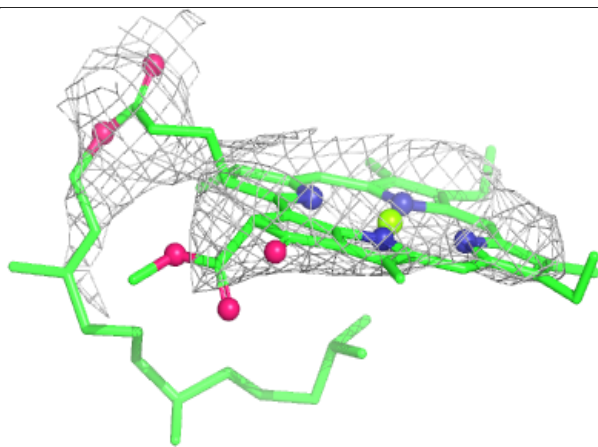
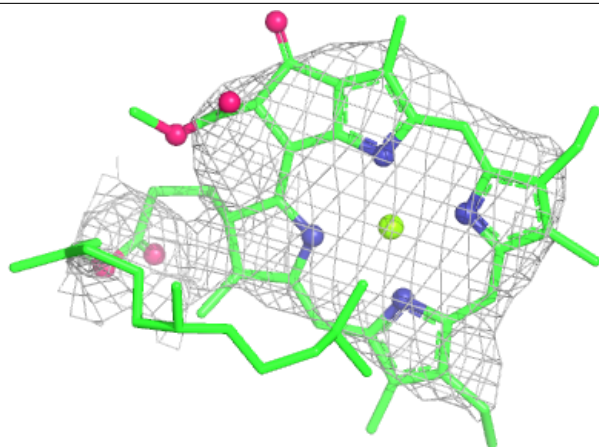
Electron density around CLA B 1204:

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



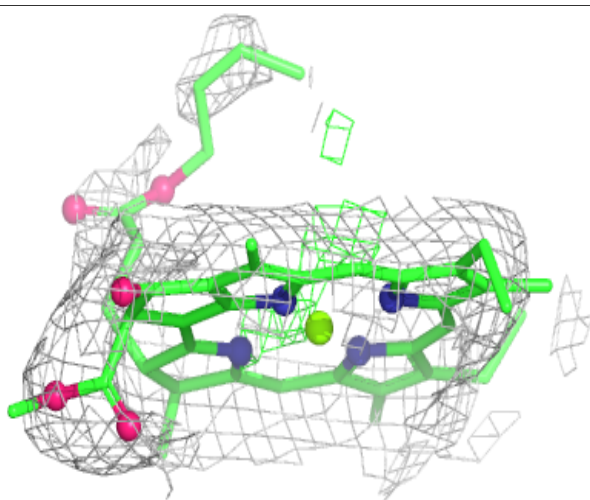
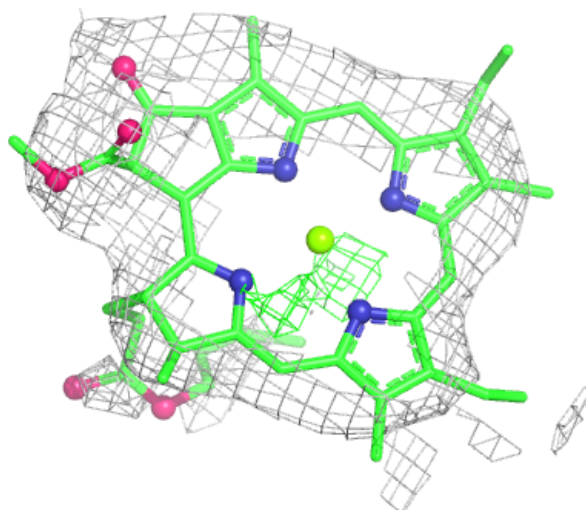
Electron density around CLA A 1104:

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



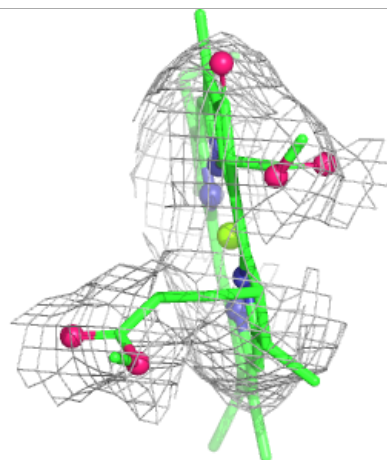
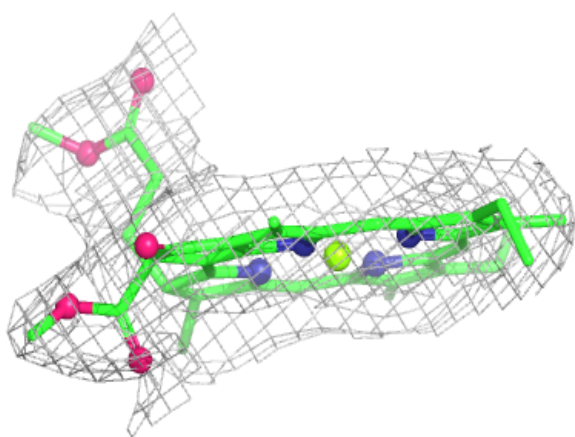
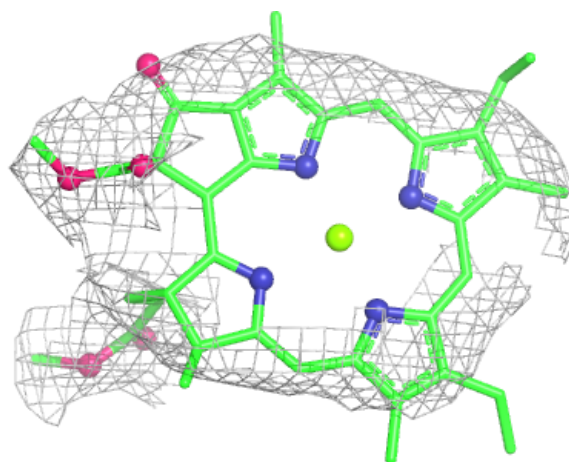
Electron density around CLA B 1214:

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



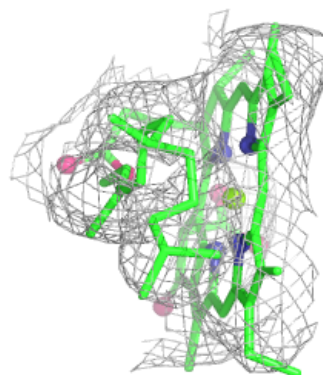
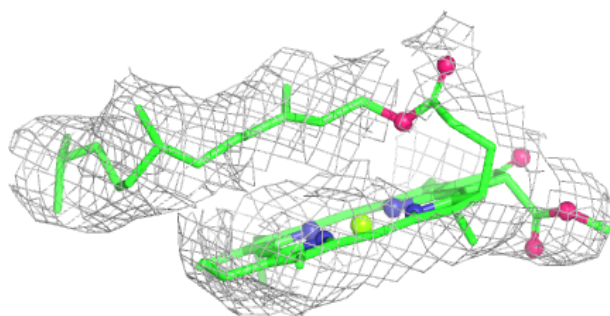
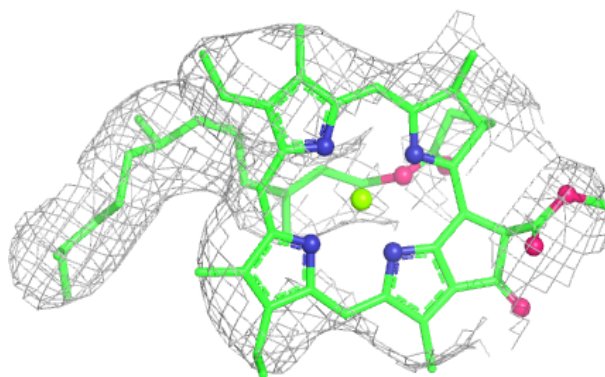
Electron density around CLA 3 615:

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

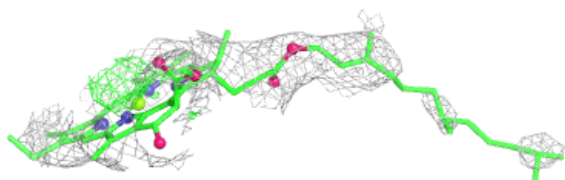
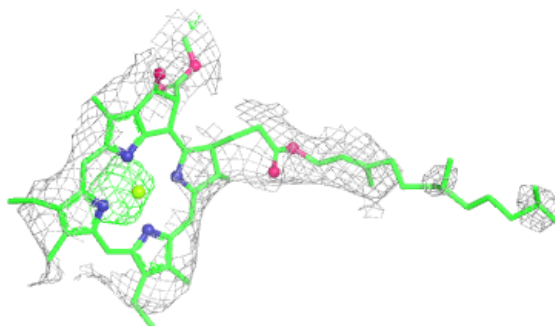


Electron density around CLA B 1235:

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

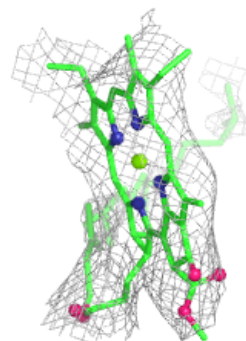
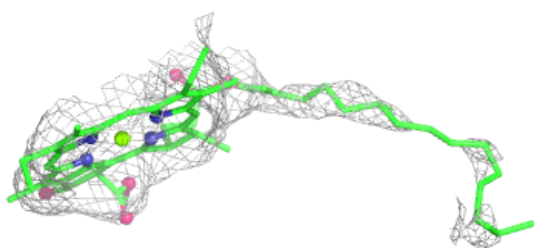
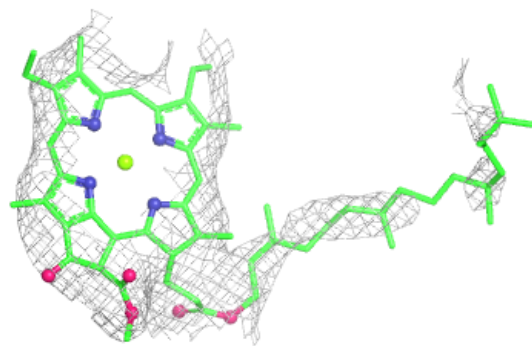
**Electron density around CLA A 1012:**

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

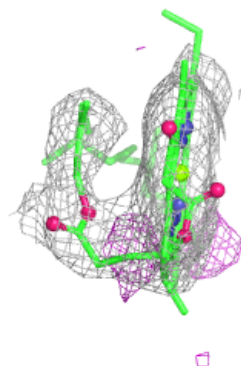
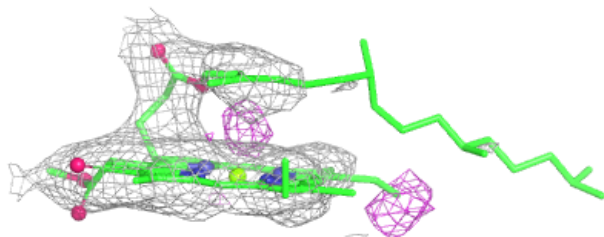
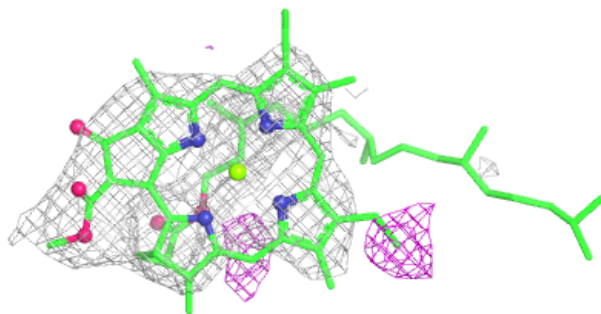


Electron density around CLA A 1013:

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

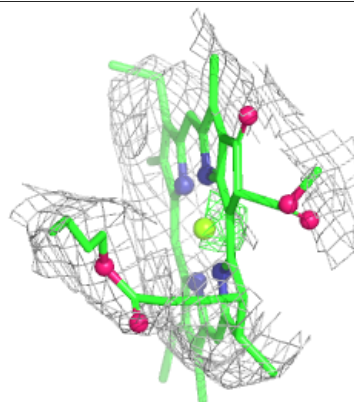
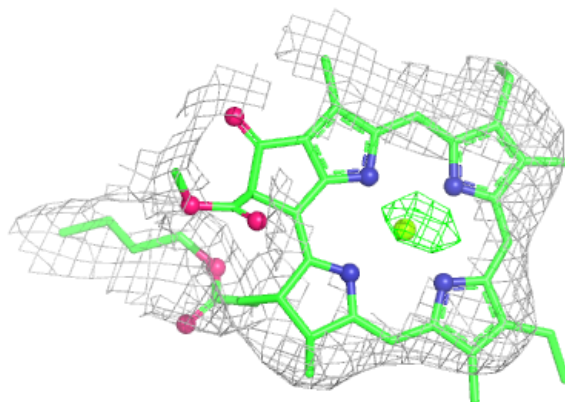
**Electron density around CLA A 1138:**

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



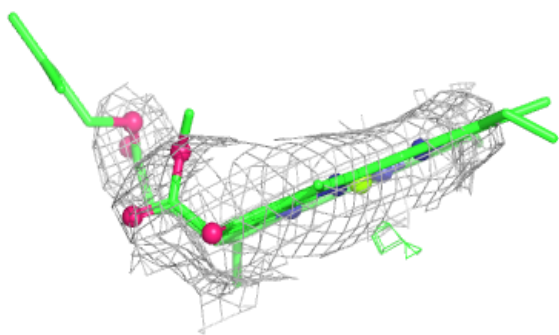
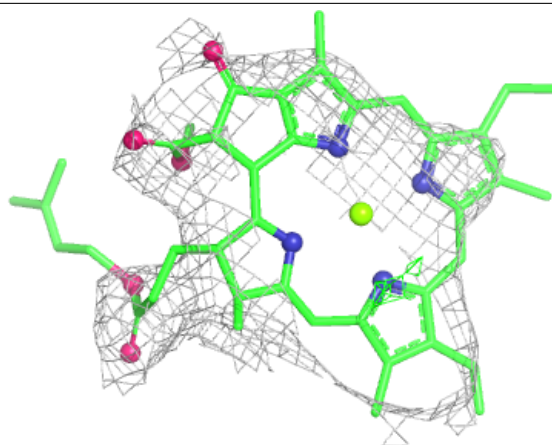
Electron density around CLA A 1107:

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



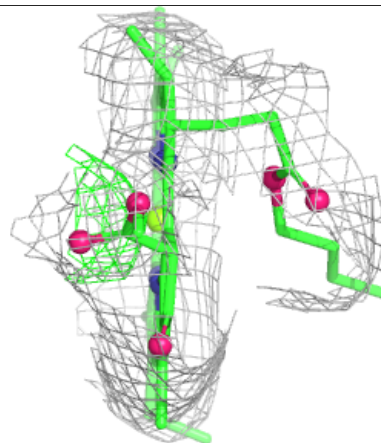
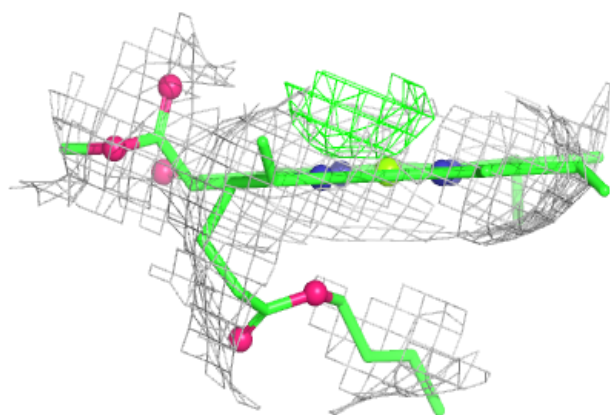
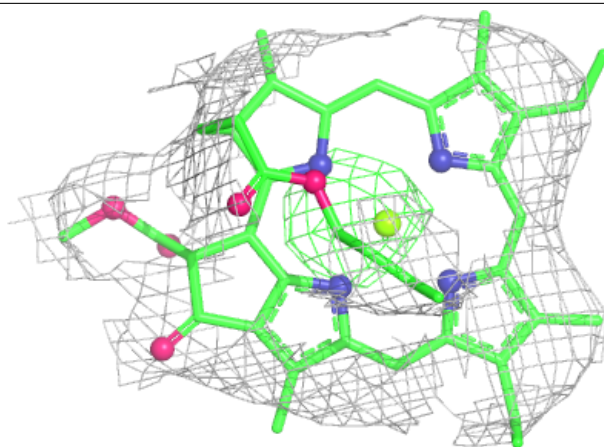
Electron density around CL0 A 1011:

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



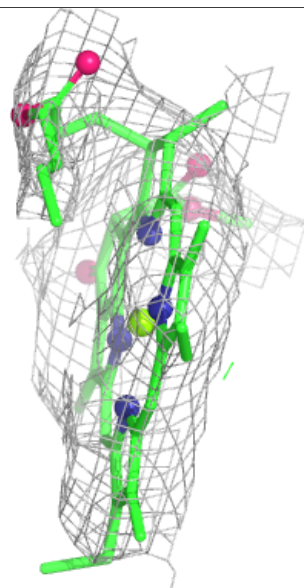
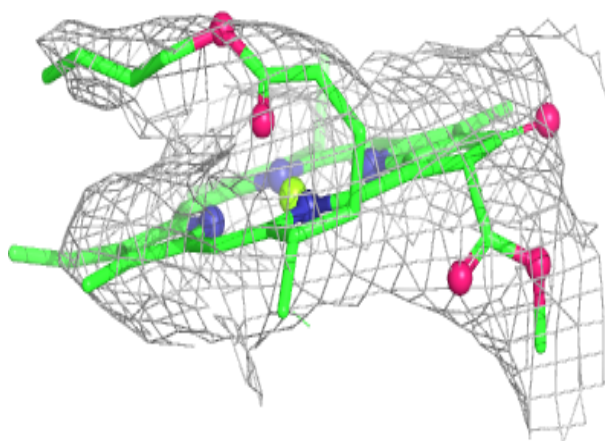
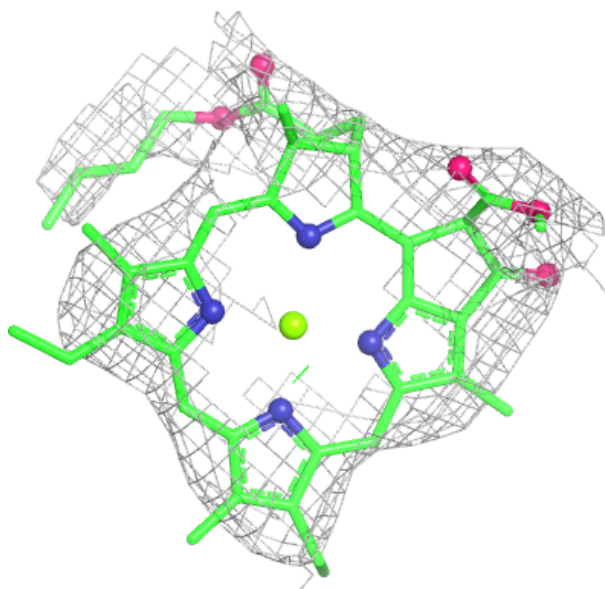
Electron density around CLA 4 603:

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



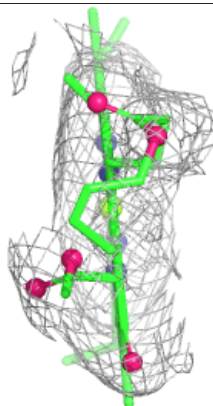
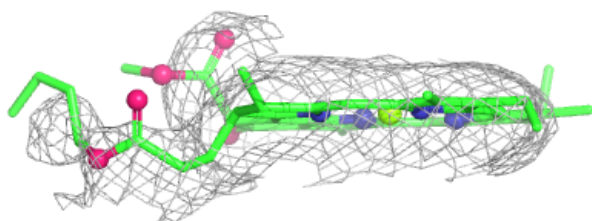
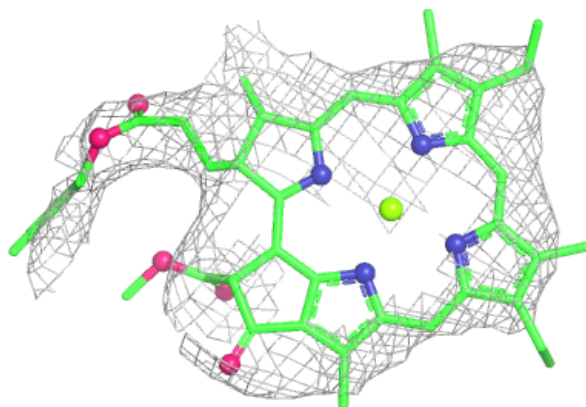
Electron density around CLA 1 604:

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

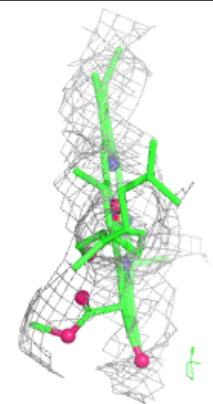
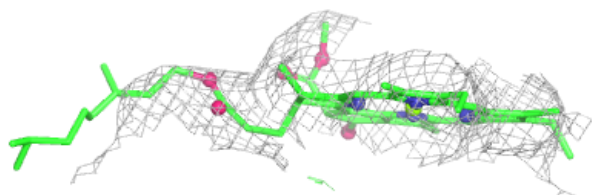
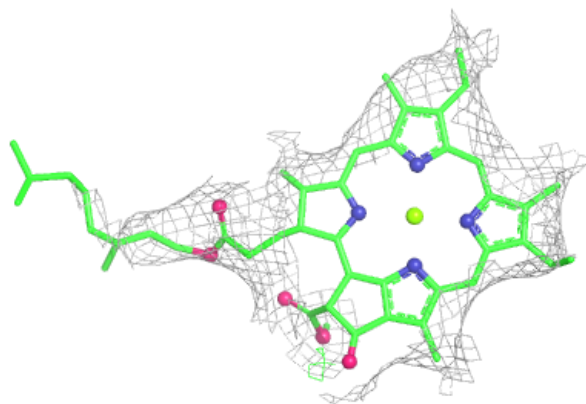


Electron density around CLA B 1202:

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

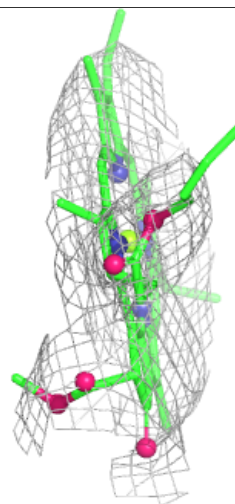
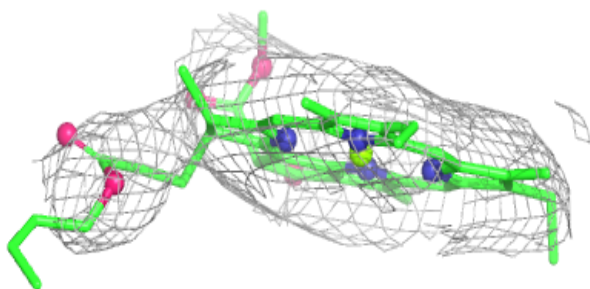
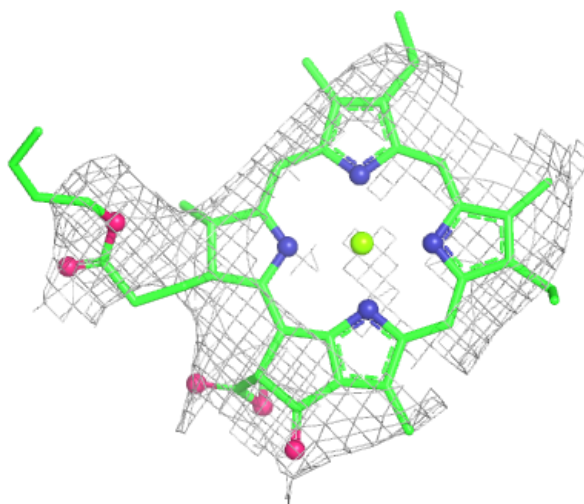
**Electron density around CLA A 1103:**

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



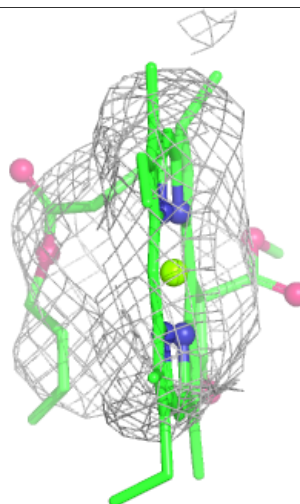
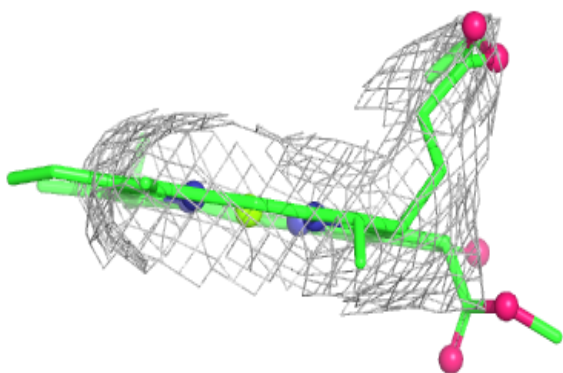
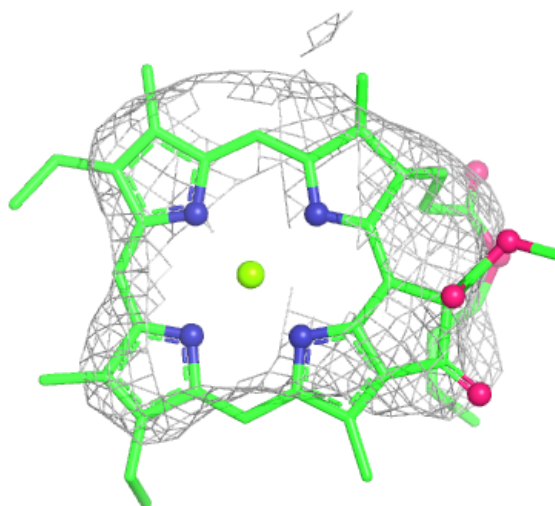
Electron density around CLA B 1210:

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



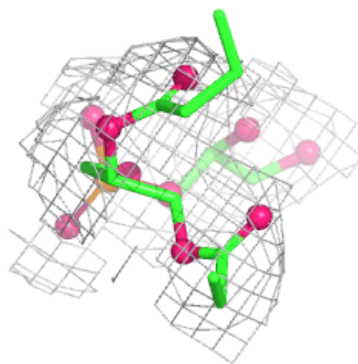
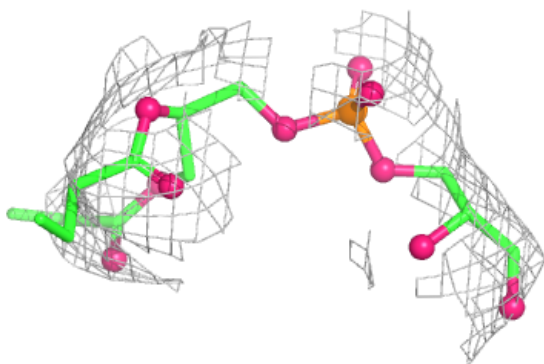
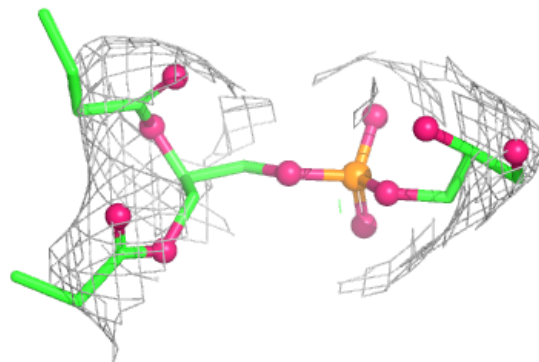
Electron density around CLA A 1127:

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



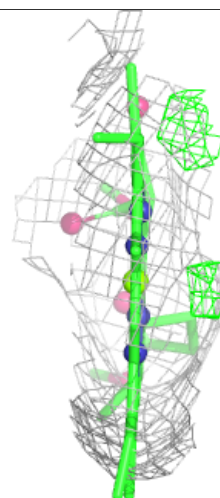
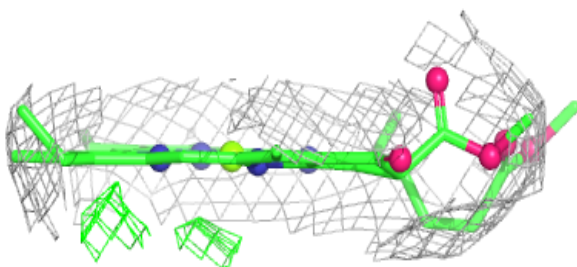
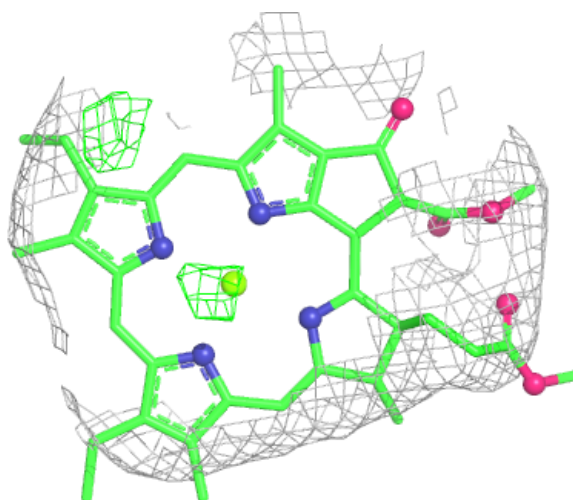
Electron density around LHG A 5002:

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



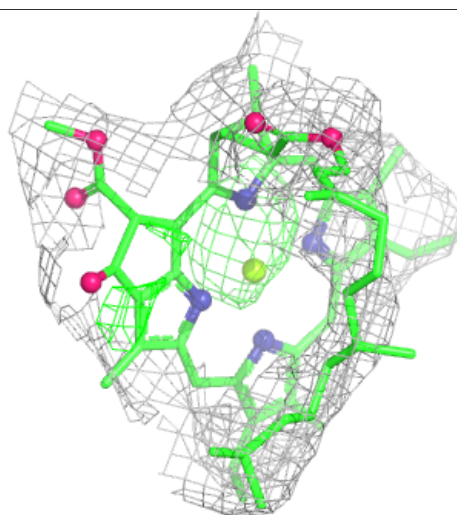
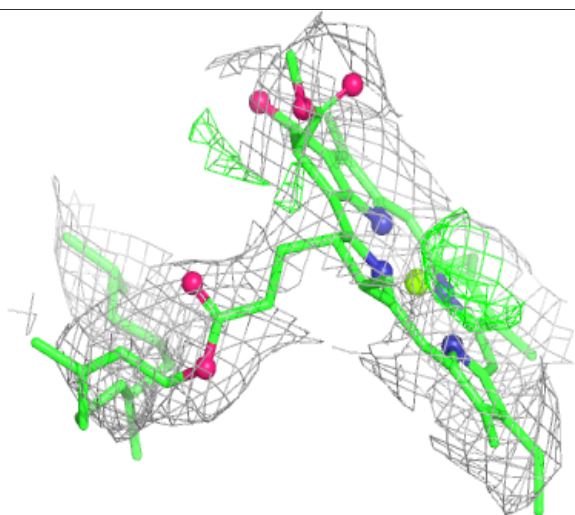
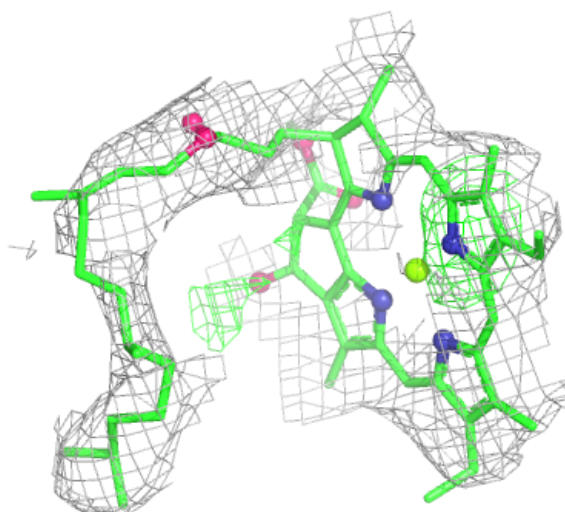
Electron density around CLA 3 605:

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



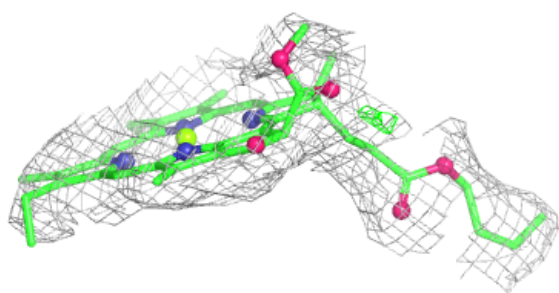
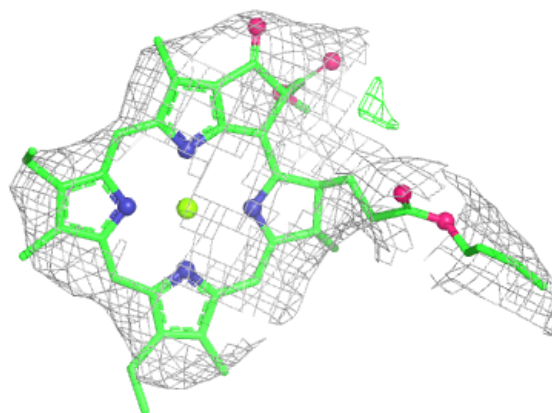
Electron density around CLA B 1231:

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



Electron density around CLA B 1222:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.