



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:03 am BST

PDB ID : 2O01
Title : The Structure of a plant photosystem I supercomplex at 3.4 Angstrom resolution
Authors : Amunts, A.; Drory, O.; Nelson, N.
Deposited on : 2006-11-27
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

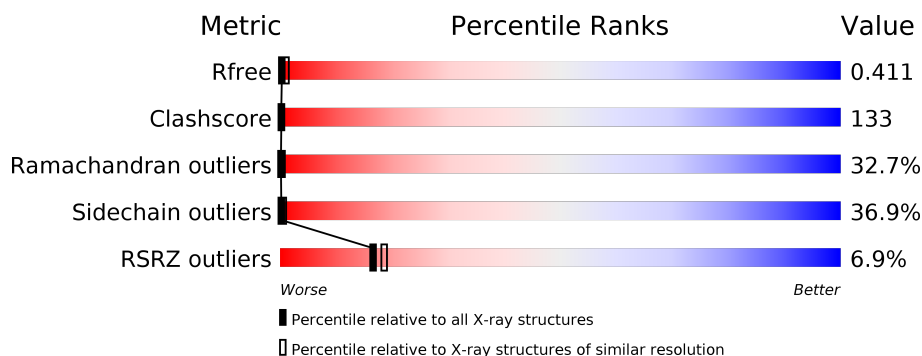
1 Overall quality at a glance

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	754	<div> <div>8%</div> <div>6%</div> <div>39%</div> <div>41%</div> <div>11%</div> <div>.</div> </div>
2	B	732	<div> <div>5%</div> <div>5%</div> <div>46%</div> <div>38%</div> <div>11%</div> </div>
3	C	80	<div> <div>14%</div> <div>.</div> <div>35%</div> <div>41%</div> <div>20%</div> </div>
4	D	138	<div> <div>4%</div> <div>5%</div> <div>35%</div> <div>43%</div> <div>17%</div> </div>
5	E	62	<div> <div>2%</div> <div>10%</div> <div>39%</div> <div>39%</div> <div>13%</div> </div>
6	F	154	<div> <div>8%</div> <div>5%</div> <div>43%</div> <div>37%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	95	
8	H	75	
9	I	30	
10	J	42	
11	K	38	
12	L	164	
13	N	85	
14	1	187	
15	2	186	
16	3	165	
17	4	165	

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
18	CLA	1	1001	X	-	-	-
18	CLA	1	1002	X	-	-	-
18	CLA	1	1003	X	-	-	-
18	CLA	1	1004	X	-	-	-
18	CLA	1	1005	X	-	-	-
18	CLA	1	1006	X	-	-	-
18	CLA	1	1007	X	-	-	-
18	CLA	1	1008	X	-	-	-
18	CLA	1	1010	X	-	-	-
18	CLA	1	1011	X	-	-	-
18	CLA	1	1012	X	-	-	-
18	CLA	1	1013	X	-	-	-
18	CLA	1	1014	X	-	-	-
18	CLA	2	2001	X	-	-	-
18	CLA	2	2002	X	-	-	-
18	CLA	2	2003	X	-	-	-
18	CLA	2	2004	X	-	-	-
18	CLA	2	2005	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	2006	X	-	-	-
18	CLA	2	2007	X	-	-	-
18	CLA	2	2008	X	-	-	-
18	CLA	2	2010	X	-	-	-
18	CLA	2	2011	X	-	-	X
18	CLA	2	2012	X	-	-	-
18	CLA	2	2013	X	-	-	-
18	CLA	2	2015	X	-	-	-
18	CLA	3	2009	X	-	-	-
18	CLA	3	3001	X	-	-	X
18	CLA	3	3002	X	-	-	-
18	CLA	3	3003	X	-	-	-
18	CLA	3	3004	X	-	-	-
18	CLA	3	3005	X	-	-	-
18	CLA	3	3006	X	-	-	-
18	CLA	3	3007	X	-	-	-
18	CLA	3	3008	X	-	-	-
18	CLA	3	3009	X	-	-	-
18	CLA	3	3010	X	-	-	-
18	CLA	3	3011	X	-	-	-
18	CLA	3	3012	X	-	-	-
18	CLA	3	3013	X	-	-	-
18	CLA	3	3015	X	-	-	-
18	CLA	4	1009	X	-	-	-
18	CLA	4	1304	X	-	-	-
18	CLA	4	4001	X	-	-	X
18	CLA	4	4002	X	-	-	-
18	CLA	4	4003	X	-	-	-
18	CLA	4	4004	X	-	-	-
18	CLA	4	4005	X	-	-	-
18	CLA	4	4006	X	-	-	-
18	CLA	4	4007	X	-	-	-
18	CLA	4	4008	X	-	-	-
18	CLA	4	4009	X	-	-	-
18	CLA	4	4010	X	-	-	-
18	CLA	4	4011	X	-	-	-
18	CLA	4	4012	X	-	-	-
18	CLA	4	4013	X	-	-	-
18	CLA	A	1101	X	-	-	-
18	CLA	A	1102	X	-	-	-
18	CLA	A	1103	X	-	-	-
18	CLA	A	1104	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	1105	X	-	-	-
18	CLA	A	1106	X	-	-	-
18	CLA	A	1107	X	-	-	-
18	CLA	A	1108	X	-	-	-
18	CLA	A	1109	X	-	-	-
18	CLA	A	1110	X	-	-	-
18	CLA	A	1111	X	-	-	-
18	CLA	A	1113	X	-	-	-
18	CLA	A	1115	X	-	-	-
18	CLA	A	1116	X	-	-	-
18	CLA	A	1117	X	-	-	-
18	CLA	A	1118	X	-	-	-
18	CLA	A	1119	X	-	-	-
18	CLA	A	1120	X	-	-	-
18	CLA	A	1122	X	-	-	-
18	CLA	A	1123	X	-	X	-
18	CLA	A	1124	X	-	-	-
18	CLA	A	1126	X	-	X	-
18	CLA	A	1127	X	-	-	-
18	CLA	A	1128	X	-	-	-
18	CLA	A	1129	X	-	-	-
18	CLA	A	1131	X	-	-	-
18	CLA	A	1132	X	-	-	-
18	CLA	A	1133	X	-	-	-
18	CLA	A	1134	X	-	-	-
18	CLA	A	1135	X	-	-	X
18	CLA	A	1136	X	-	X	-
18	CLA	A	1137	X	-	-	-
18	CLA	A	1140	X	-	X	-
18	CLA	A	1142	X	-	-	-
18	CLA	A	1143	X	-	-	-
18	CLA	A	1144	X	-	-	-
18	CLA	A	1146	X	-	-	-
18	CLA	A	1147	X	-	-	-
18	CLA	A	1148	X	-	-	-
18	CLA	A	1151	X	-	-	-
18	CLA	A	1152	X	-	-	-
18	CLA	A	1309	X	-	-	-
18	CLA	A	9011	X	-	X	-
18	CLA	A	9013	X	-	-	-
18	CLA	B	1138	X	-	X	-
18	CLA	B	1201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	1202	X	-	X	-
18	CLA	B	1203	X	-	-	-
18	CLA	B	1205	X	-	-	-
18	CLA	B	1206	X	-	-	-
18	CLA	B	1207	X	-	-	-
18	CLA	B	1208	X	-	-	-
18	CLA	B	1209	X	-	X	-
18	CLA	B	1210	X	-	-	-
18	CLA	B	1211	X	-	-	-
18	CLA	B	1212	X	-	-	X
18	CLA	B	1213	X	-	-	-
18	CLA	B	1214	X	-	X	-
18	CLA	B	1215	X	-	X	-
18	CLA	B	1216	X	-	X	-
18	CLA	B	1217	X	-	-	-
18	CLA	B	1218	X	-	X	-
18	CLA	B	1219	X	-	-	-
18	CLA	B	1220	X	-	X	-
18	CLA	B	1221	X	-	X	-
18	CLA	B	1222	X	-	-	-
18	CLA	B	1223	X	-	-	-
18	CLA	B	1224	X	-	-	-
18	CLA	B	1225	X	-	X	-
18	CLA	B	1226	X	-	-	-
18	CLA	B	1227	X	-	X	-
18	CLA	B	1228	X	-	X	-
18	CLA	B	1229	X	-	-	-
18	CLA	B	1230	X	-	-	-
18	CLA	B	1231	X	-	-	-
18	CLA	B	1232	X	-	-	-
18	CLA	B	1234	X	-	X	-
18	CLA	B	1235	X	-	-	-
18	CLA	B	1236	X	-	-	-
18	CLA	B	1237	X	-	-	-
18	CLA	B	1238	X	-	X	-
18	CLA	B	1239	X	-	X	-
18	CLA	B	1241	X	-	-	-
18	CLA	B	1242	X	-	-	-
18	CLA	B	1301	X	-	-	-
18	CLA	B	9010	X	-	X	-
18	CLA	B	9012	X	-	-	-
18	CLA	B	9022	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	9023	X	-	-	-
18	CLA	F	1139	X	-	X	-
18	CLA	F	1240	X	-	-	-
18	CLA	F	1302	X	-	-	-
18	CLA	F	1303	X	-	-	-
18	CLA	F	1305	X	-	-	-
18	CLA	F	1306	X	-	-	-
18	CLA	F	4015	X	-	-	-
18	CLA	G	1233	X	-	-	-
18	CLA	G	1248	X	-	-	-
18	CLA	H	1501	X	-	-	-
18	CLA	H	1505	X	-	-	-
18	CLA	I	1204	X	-	-	-
18	CLA	J	1307	X	-	-	-
18	CLA	J	1308	X	-	-	-
18	CLA	J	2107	X	-	-	-
18	CLA	K	1141	X	-	-	-
18	CLA	K	1150	X	-	-	-
18	CLA	K	1153	X	-	-	-
18	CLA	L	1125	X	-	-	-
18	CLA	L	1130	X	-	X	-
18	CLA	L	1502	X	-	-	-
18	CLA	L	1503	X	-	X	-
18	CLA	L	1504	X	-	-	-
19	PQN	A	5001	X	-	X	-
19	PQN	B	5002	X	-	-	X
20	BCR	B	6017	-	-	-	X
21	SF4	B	3101	-	-	X	-
21	SF4	C	3102	-	-	X	-
21	SF4	C	3103	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 29846 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5732	3758	975	981	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLY	ARG	CONFLICT	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5844	3841	996	994	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	147	ALA	PHE	CONFLICT	UNP P05311

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			611	379	107	114	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	62	Total	C	N	O	0	0	0
			503	321	90	92			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	S	0	0	0
			744	484	121	137	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	0	0	0
			577	379	96	102			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			344	236	51	56	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	37	Total	C	N	O	0	0	0
			185	111	37	37			

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	164	Total	C	N	O	S	0	0	0
			1235	815	197	218	5			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	175	Total	C	N	O	S	0	0	0
			1187	755	211	217	4			

- Molecule 15 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	166	Total	C	N	O	S	0	0	0
			1268	828	207	230	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	17	GLU	PRO	CONFLICT	UNP Q41038
2	35	SER	GLY	CONFLICT	UNP Q41038

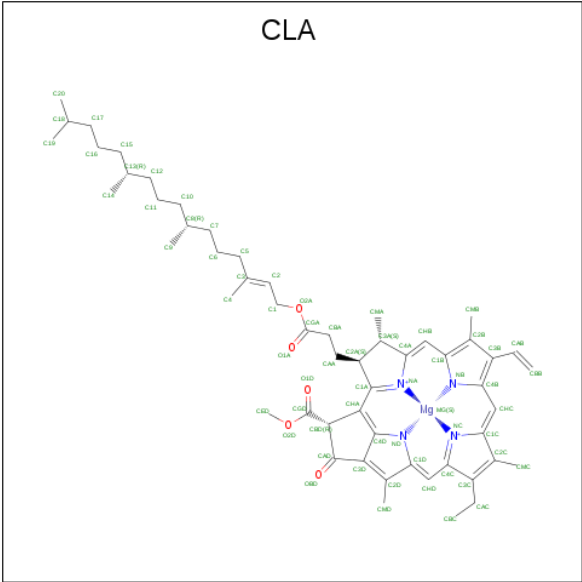
- Molecule 16 is a protein called PSI type III chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	115	Total	C	N	O	S	0	0	0
			857	559	141	153	4			

- Molecule 17 is a protein called PSI light-harvesting antenna chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	165	Total	C	N	O	S	0	0	0
			1282	839	214	226	3			

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
18	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N		0	0
			24	19	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
18	A	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			44	34	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	A	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			46	36	1	4	5	
18	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	B	1	Total	C	Mg	N	0	0
			56	46	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	B	1	Total	C	Mg	N	0	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			48	38	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	B	1	Total	C	Mg	N	0	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	0	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	B	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
18	B	1	Total 51	C 41	Mg 1	N 4 O 5	0	0
18	B	1	Total 54	C 44	Mg 1	N 4 O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	B	1	Total 47	C 37	Mg 1	N 4 O 5	0	0
18	B	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 44	C 35	Mg 1	N 4 O 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	F	1	Total 25	C 20	Mg 1	N 4	0	0
18	G	1	Total 51	C 41	Mg 1	N 4 O 5	0	0
18	G	1	Total 25	C 20	Mg 1	N 4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	H	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	I	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	J	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
18	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	L	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
18	1	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	1	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	2	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0

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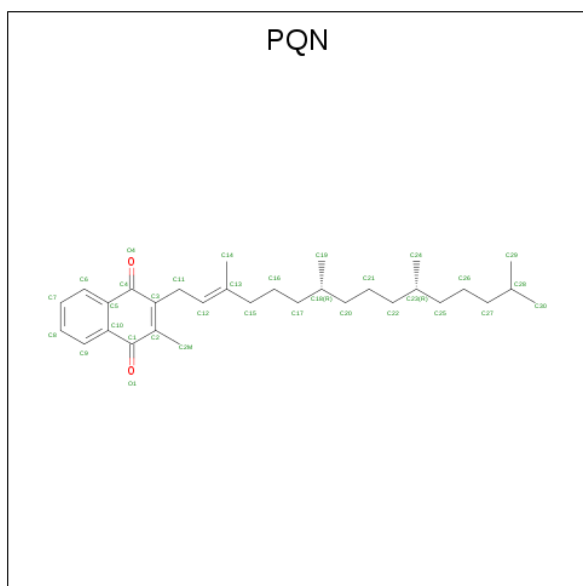
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	3	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0
18	4	1	Total 25	C 20	Mg 1	N 4	0	0

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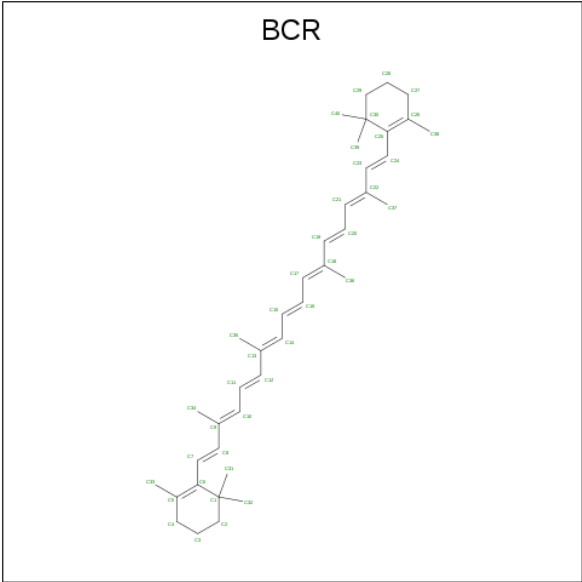
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
18	4	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



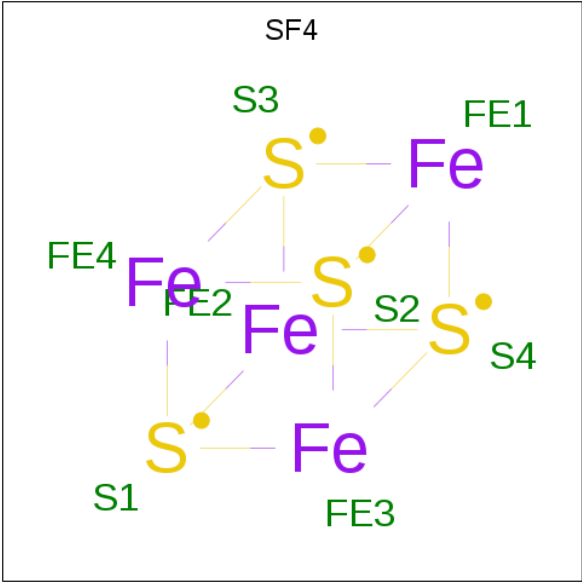
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			33	31	2		
19	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 20 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

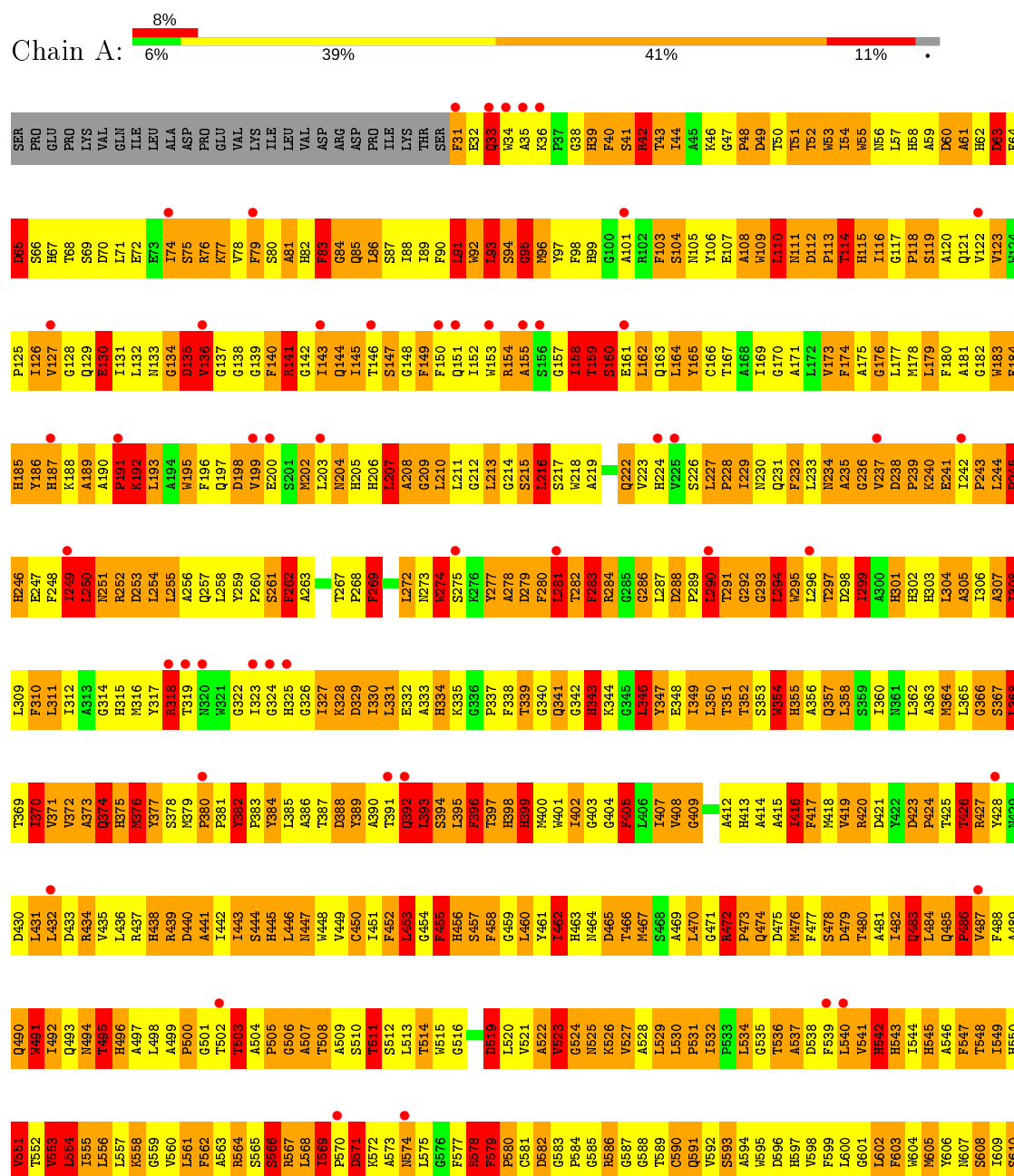


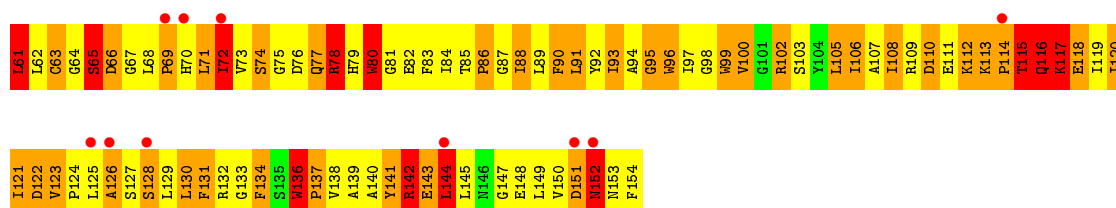
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total 8	Fe 4	S 4	0	0
21	C	1	Total 8	Fe 4	S 4	0	0
21	C	1	Total 8	Fe 4	S 4	0	0

3 Residue-property plots

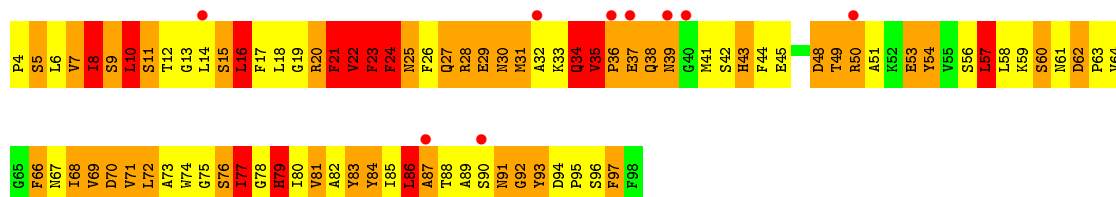
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

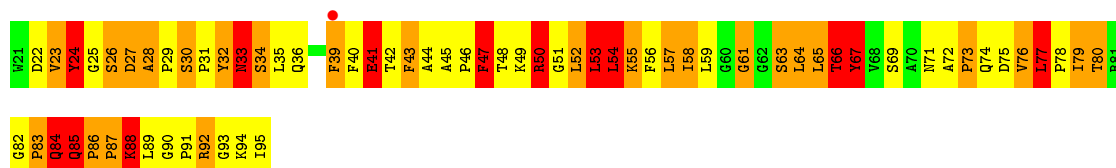




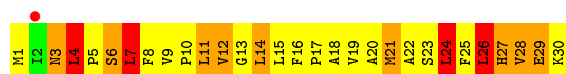
• Molecule 7: Photosystem I reaction center subunit V, chloroplast



• Molecule 8: Photosystem I reaction center subunit VI, chloroplast



• Molecule 9: Photosystem I reaction center subunit VIII



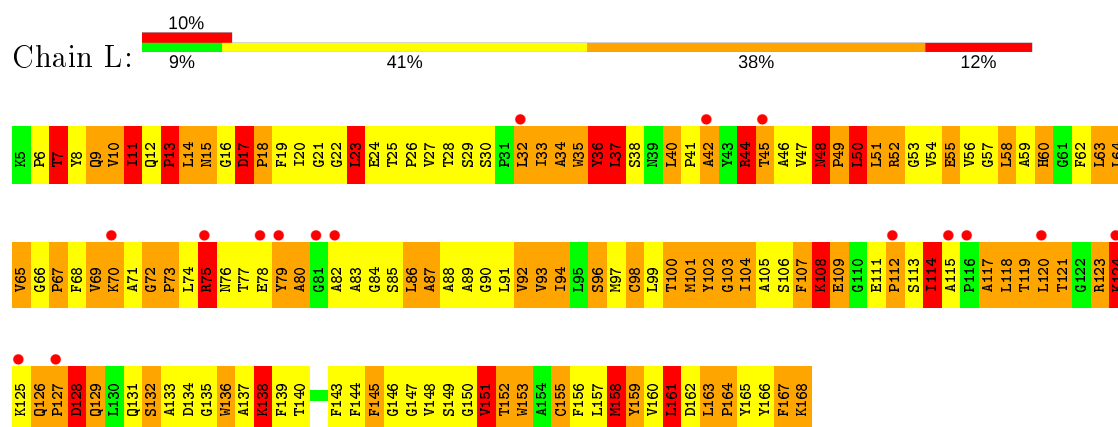
• Molecule 10: Photosystem I reaction center subunit IX



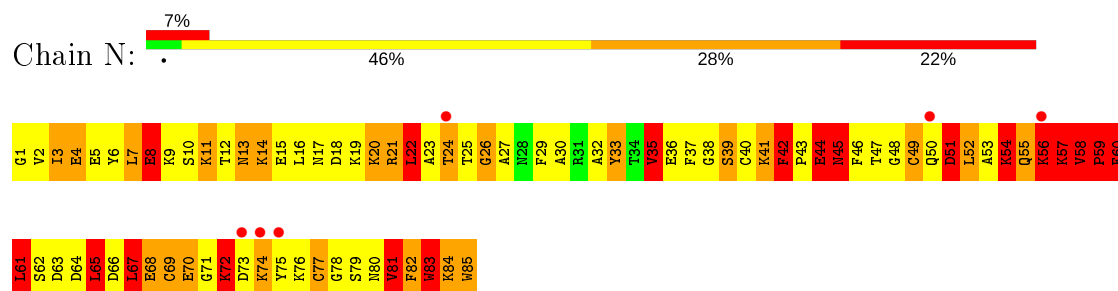
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplast



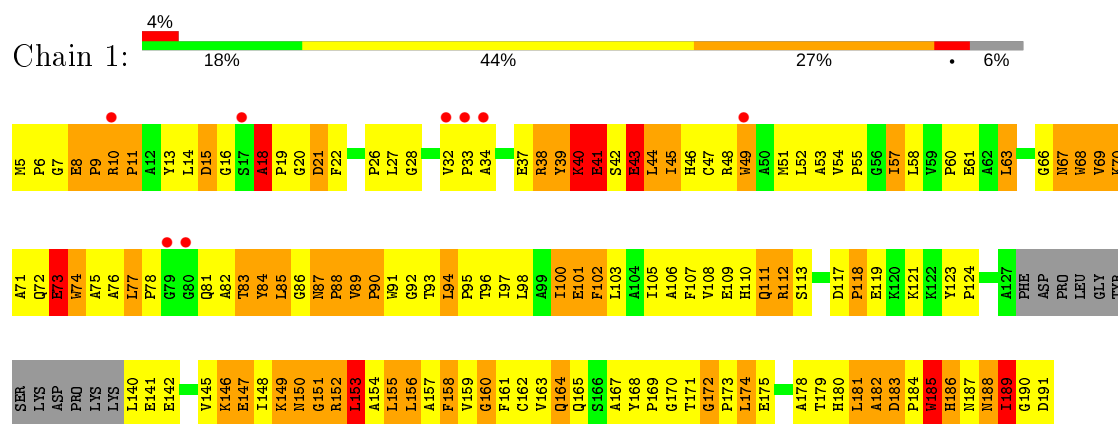
• Molecule 12: Photosystem I reaction center subunit XI, chloroplast



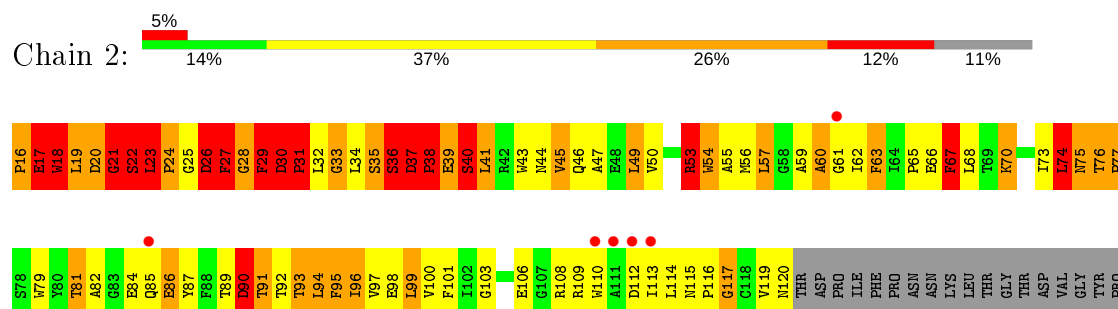
• Molecule 13: Photosystem I-N subunit



• Molecule 14: AT3g54890



• Molecule 15: Type II chlorophyll a/b binding protein from photosystem I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.05Å 188.78Å 127.52Å 90.00° 95.19° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 50.40 – 3.01	Depositor EDS
% Data completeness (in resolution range)	90.8 (40.00-3.40) 64.2 (50.40-3.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.348 , 0.409 0.353 , 0.411	Depositor DCC
R_{free} test set	3517 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	96.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 500.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	29846	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: SF4, CLA, BCR, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/5928	1.06	14/8092 (0.2%)
2	B	0.76	0/6054	1.06	16/8273 (0.2%)
3	C	0.97	1/624 (0.2%)	1.18	2/846 (0.2%)
4	D	0.82	0/1122	1.25	5/1514 (0.3%)
5	E	0.73	0/513	1.06	1/694 (0.1%)
6	F	0.78	0/1250	1.10	6/1687 (0.4%)
7	G	0.72	0/764	1.08	3/1035 (0.3%)
8	H	0.83	0/595	1.23	5/810 (0.6%)
9	I	0.75	0/235	1.20	2/320 (0.6%)
10	J	0.78	0/356	1.15	2/484 (0.4%)
12	L	0.78	0/1272	1.10	1/1736 (0.1%)
13	N	0.63	0/699	0.96	2/936 (0.2%)
14	1	0.61	0/1215	0.87	1/1666 (0.1%)
15	2	0.73	1/1309 (0.1%)	1.03	6/1787 (0.3%)
16	3	0.60	0/879	0.95	2/1194 (0.2%)
17	4	0.72	2/1319 (0.2%)	0.88	2/1797 (0.1%)
All	All	0.75	4/24134 (0.0%)	1.06	70/32871 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	32
2	B	0	32
3	C	0	4
4	D	0	14
5	E	0	3
6	F	0	9
7	G	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	4
9	I	0	2
12	L	0	4
13	N	3	11
14	1	0	5
15	2	3	21
16	3	1	14
17	4	0	13
All	All	7	174

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	21	CYS	CB-SG	5.62	1.91	1.82
17	4	190	TRP	CB-CG	-5.40	1.40	1.50
15	2	40	SER	C-N	-5.35	1.21	1.34
17	4	119	PRO	N-CD	5.04	1.54	1.47

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	SER	C-N-CD	-17.32	82.50	120.60
15	2	40	SER	C-N-CA	-12.47	90.53	121.70
4	D	119	TYR	C-N-CD	-10.41	97.69	120.60
12	L	72	GLY	C-N-CD	-9.86	98.90	120.60
16	3	196	LEU	CA-CB-CG	8.27	134.32	115.30

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	N	59	PRO	CA
13	N	61	LEU	CA
13	N	83	TRP	CA
15	2	20	ASP	CA
15	2	23	LEU	CA

5 of 174 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	SER	Peptide
1	A	117	GLY	Peptide
1	A	33	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	47	GLY	Peptide
1	A	65	ASP	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	A	5732	0	5577	1855	0
2	B	5844	0	5659	1973	0
3	C	611	0	594	257	0
4	D	1095	0	1112	364	0
5	E	503	0	510	132	0
6	F	1221	0	1250	362	0
7	G	744	0	721	208	0
8	H	577	0	587	137	0
9	I	229	0	252	97	0
10	J	344	0	347	103	0
11	K	185	0	40	12	0
12	L	1235	0	1244	370	1
13	N	685	0	672	268	0
14	1	1187	0	1019	230	1
15	2	1268	0	1177	492	1
16	3	857	0	789	220	0
17	4	1282	0	1241	271	1
18	1	325	0	39	12	0
18	2	325	0	39	15	0
18	3	375	0	45	11	0
18	4	405	0	90	16	0
18	A	1601	0	870	350	0
18	B	2078	0	1535	705	0
18	F	224	0	94	43	0
18	G	76	0	43	12	0
18	H	80	0	51	13	0
18	I	55	0	48	11	0
18	J	111	0	66	8	0
18	K	75	0	9	5	0
18	L	227	0	162	107	0
19	A	33	0	46	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	33	0	46	20	0
20	A	40	0	54	17	0
20	B	40	0	54	20	0
20	F	40	0	54	15	0
20	I	40	0	54	13	0
20	L	40	0	54	17	0
21	B	8	0	0	4	0
21	C	16	0	0	15	0
All	All	29846	0	26244	7466	2

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 133.

The worst 5 of 7466 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)
3:C:22:PRO:HG2	3:C:51:CYS:SG	1.33	1.68
15:2:192:LEU:HA	15:2:195:HIS:CE1	1.34	1.58
2:B:290:MET:CA	18:B:1218:CLA:HBC2	1.12	1.57
15:2:26:ASP:HB3	15:2:27:PHE:CB	1.34	1.56
2:B:290:MET:HA	18:B:1218:CLA:CBC	1.31	1.56

All (2) 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)
12:L:161:LEU:O	17:4:141:LEU:O[1_655]	1.55	0.65
14:1:71:ALA:CB	15:2:30:ASP:OD1[1_556]	1.96	0.24

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/754 (96%)	290 (40%)	201 (28%)	235 (32%)	0	0
2	B	730/732 (100%)	290 (40%)	209 (29%)	231 (32%)	0	0
3	C	78/80 (98%)	20 (26%)	23 (30%)	35 (45%)	0	0
4	D	136/138 (99%)	50 (37%)	28 (21%)	58 (43%)	0	0
5	E	60/62 (97%)	28 (47%)	13 (22%)	19 (32%)	0	0
6	F	152/154 (99%)	59 (39%)	40 (26%)	53 (35%)	0	0
7	G	93/95 (98%)	40 (43%)	22 (24%)	31 (33%)	0	0
8	H	73/75 (97%)	21 (29%)	18 (25%)	34 (47%)	0	0
9	I	28/30 (93%)	9 (32%)	11 (39%)	8 (29%)	0	0
10	J	40/42 (95%)	16 (40%)	14 (35%)	10 (25%)	0	0
12	L	162/164 (99%)	64 (40%)	40 (25%)	58 (36%)	0	0
13	N	83/85 (98%)	26 (31%)	26 (31%)	31 (37%)	0	0
14	1	171/187 (91%)	74 (43%)	43 (25%)	54 (32%)	0	0
15	2	162/186 (87%)	72 (44%)	46 (28%)	44 (27%)	0	0
16	3	109/165 (66%)	49 (45%)	36 (33%)	24 (22%)	0	0
17	4	163/165 (99%)	69 (42%)	48 (29%)	46 (28%)	0	0
All	All	2966/3114 (95%)	1177 (40%)	818 (28%)	971 (33%)	0	0

5 of 971 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	48	PRO
1	A	51	THR
1	A	52	THR
1	A	61	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	588/613 (96%)	350 (60%)	238 (40%)	0	0
2	B	598/598 (100%)	397 (66%)	201 (34%)	0	1
3	C	69/69 (100%)	40 (58%)	29 (42%)	0	0
4	D	118/118 (100%)	77 (65%)	41 (35%)	0	1
5	E	55/55 (100%)	36 (66%)	19 (34%)	0	1
6	F	127/127 (100%)	80 (63%)	47 (37%)	0	0
7	G	80/80 (100%)	37 (46%)	43 (54%)	0	0
8	H	62/62 (100%)	40 (64%)	22 (36%)	0	1
9	I	26/26 (100%)	18 (69%)	8 (31%)	0	1
10	J	37/37 (100%)	27 (73%)	10 (27%)	0	1
12	L	127/127 (100%)	78 (61%)	49 (39%)	0	0
13	N	74/74 (100%)	48 (65%)	26 (35%)	0	1
14	1	92/147 (63%)	63 (68%)	29 (32%)	0	1
15	2	122/151 (81%)	80 (66%)	42 (34%)	0	1
16	3	74/123 (60%)	45 (61%)	29 (39%)	0	0
17	4	130/139 (94%)	84 (65%)	46 (35%)	0	1
All	All	2379/2546 (93%)	1500 (63%)	879 (37%)	0	0

5 of 879 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	575	ASP
4	D	102	ARG
16	3	84	LEU
2	B	612	SER
3	C	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	333	GLN
2	B	595	HIS
17	4	47	ASN
2	B	363	GLN
2	B	406	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

178 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
18	CLA	H	1501	-	49,63,73	2.22	12 (24%)	55,101,113	3.61	23 (41%)
21	SF4	C	3102	3	0,12,12	0.00	-	-		
18	CLA	4	1009	-	22,32,73	1.90	5 (22%)	26,54,113	2.79	13 (50%)
18	CLA	1	1002	-	22,32,73	1.89	6 (27%)	26,54,113	2.97	15 (57%)
18	CLA	J	1308	-	22,32,73	1.87	5 (22%)	26,54,113	3.17	16 (61%)
18	CLA	3	3006	16	22,32,73	1.84	5 (22%)	26,54,113	2.92	14 (53%)
18	CLA	A	1133	-	22,32,73	1.88	5 (22%)	26,54,113	3.03	15 (57%)
18	CLA	A	1140	-	49,63,73	2.27	13 (26%)	55,101,113	3.68	21 (38%)
18	CLA	A	1122	-	49,63,73	2.28	13 (26%)	55,101,113	3.20	20 (36%)
18	CLA	A	1152	-	22,32,73	1.91	6 (27%)	26,54,113	2.97	17 (65%)
18	CLA	1	1001	-	22,32,73	1.95	6 (27%)	26,54,113	3.04	16 (61%)
18	CLA	3	3012	-	22,32,73	1.84	7 (31%)	26,54,113	2.90	15 (57%)
20	BCR	F	6016	-	41,41,41	1.56	2 (4%)	56,56,56	4.86	33 (58%)
18	CLA	H	1505	8	22,32,73	1.92	7 (31%)	26,54,113	3.04	15 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	4	4005	-	22,32,73	1.90	5 (22%)	26,54,113	3.28	14 (53%)
18	CLA	A	1101	-	22,32,73	1.91	5 (22%)	26,54,113	3.12	14 (53%)
18	CLA	3	3002	-	22,32,73	1.88	6 (27%)	26,54,113	2.98	16 (61%)
18	CLA	B	1211	2	22,32,73	1.82	7 (31%)	26,54,113	3.03	14 (53%)
18	CLA	A	1106	-	35,49,73	2.51	12 (34%)	38,84,113	3.73	19 (50%)
18	CLA	B	1216	-	50,64,73	2.27	11 (22%)	56,102,113	3.43	20 (35%)
18	CLA	3	3015	-	22,32,73	1.82	5 (22%)	26,54,113	2.98	18 (69%)
18	CLA	1	1006	-	22,32,73	1.93	7 (31%)	26,54,113	3.08	17 (65%)
18	CLA	A	1309	-	22,32,73	1.88	6 (27%)	26,54,113	2.95	15 (57%)
18	CLA	B	9010	2	41,55,73	2.44	15 (36%)	45,91,113	3.59	23 (51%)
18	CLA	G	1248	-	22,32,73	1.91	7 (31%)	26,54,113	3.14	14 (53%)
18	CLA	A	1107	1	51,65,73	2.34	13 (25%)	57,103,113	3.42	22 (38%)
18	CLA	A	1108	-	44,58,73	2.29	12 (27%)	49,95,113	3.85	18 (36%)
18	CLA	B	1238	-	48,62,73	2.32	12 (25%)	53,99,113	3.56	26 (49%)
18	CLA	B	1215	2	46,60,73	2.33	12 (26%)	51,97,113	3.06	25 (49%)
18	CLA	4	4010	-	22,32,73	1.90	5 (22%)	26,54,113	3.02	16 (61%)
18	CLA	3	3013	-	22,32,73	1.94	7 (31%)	26,54,113	3.06	17 (65%)
18	CLA	1	1005	-	22,32,73	1.90	5 (22%)	26,54,113	3.03	17 (65%)
18	CLA	A	1127	1	22,32,73	1.94	8 (36%)	26,54,113	2.87	13 (50%)
18	CLA	3	3010	-	22,32,73	1.84	5 (22%)	26,54,113	2.89	14 (53%)
18	CLA	2	2004	-	22,32,73	1.91	6 (27%)	26,54,113	3.07	15 (57%)
18	CLA	3	3001	-	22,32,73	1.91	5 (22%)	26,54,113	3.13	16 (61%)
18	CLA	B	1202	-	44,58,73	2.41	13 (29%)	49,95,113	4.00	23 (46%)
18	CLA	B	1224	-	45,59,73	2.21	13 (28%)	50,96,113	2.75	22 (44%)
18	CLA	1	1010	-	22,32,73	1.92	5 (22%)	26,54,113	3.03	17 (65%)
18	CLA	K	1141	-	22,32,73	1.84	5 (22%)	26,54,113	2.89	16 (61%)
18	CLA	B	1212	-	54,68,73	2.11	13 (24%)	61,107,113	3.28	19 (31%)
18	CLA	A	1111	-	22,32,73	1.95	5 (22%)	26,54,113	3.00	15 (57%)
18	CLA	B	1213	2	22,32,73	1.84	5 (22%)	26,54,113	2.96	16 (61%)
18	CLA	2	2006	-	22,32,73	1.82	5 (22%)	26,54,113	2.91	14 (53%)
18	CLA	4	4008	-	22,32,73	1.87	5 (22%)	26,54,113	2.94	15 (57%)
18	CLA	B	1208	-	49,63,73	2.24	12 (24%)	55,101,113	3.45	28 (50%)
18	CLA	A	1104	1	22,32,73	1.88	6 (27%)	26,54,113	3.00	15 (57%)
18	CLA	A	1142	-	22,32,73	1.91	5 (22%)	26,54,113	2.89	15 (57%)
18	CLA	F	1139	-	38,52,73	2.39	9 (23%)	40,87,113	3.37	18 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	3008	-	22,32,73	1.96	6 (27%)	26,54,113	3.08	14 (53%)
18	CLA	A	1110	-	22,32,73	1.88	6 (27%)	26,54,113	3.26	15 (57%)
18	CLA	4	4006	-	22,32,73	1.97	5 (22%)	26,54,113	3.10	16 (61%)
18	CLA	L	1502	12	45,59,73	2.31	12 (26%)	50,96,113	3.24	22 (44%)
18	CLA	B	1220	-	54,68,73	2.06	11 (20%)	61,107,113	3.76	20 (32%)
18	CLA	A	1134	-	22,32,73	1.85	6 (27%)	26,54,113	3.25	18 (69%)
18	CLA	L	1125	-	22,32,73	1.88	5 (22%)	26,54,113	2.84	14 (53%)
18	CLA	B	1206	2	22,32,73	1.91	6 (27%)	26,54,113	3.13	16 (61%)
18	CLA	B	1232	-	49,63,73	2.18	11 (22%)	55,101,113	3.61	20 (36%)
18	CLA	4	4012	-	22,32,73	2.02	7 (31%)	26,54,113	3.14	12 (46%)
21	SF4	C	3103	3	0,12,12	0.00	-	-	-	-
18	CLA	B	9023	-	41,55,73	2.37	12 (29%)	45,91,113	3.60	19 (42%)
18	CLA	1	1003	-	22,32,73	1.86	5 (22%)	26,54,113	3.04	16 (61%)
18	CLA	2	2002	-	22,32,73	1.92	7 (31%)	26,54,113	2.99	15 (57%)
18	CLA	B	9012	-	49,63,73	2.33	12 (24%)	55,101,113	3.25	24 (43%)
18	CLA	2	2003	-	22,32,73	1.89	7 (31%)	26,54,113	3.24	14 (53%)
18	CLA	B	1218	-	45,59,73	2.62	14 (31%)	50,96,113	3.57	22 (44%)
18	CLA	F	1306	-	22,32,73	1.99	6 (27%)	26,54,113	3.04	15 (57%)
18	CLA	A	1109	-	23,30,73	2.57	10 (43%)	16,49,113	2.93	8 (50%)
18	CLA	2	2015	-	22,32,73	1.86	5 (22%)	26,54,113	2.99	17 (65%)
18	CLA	F	1303	-	22,32,73	1.87	5 (22%)	26,54,113	3.02	15 (57%)
18	CLA	4	4011	-	22,32,73	1.88	6 (27%)	26,54,113	2.96	17 (65%)
18	CLA	3	2009	-	22,32,73	1.91	7 (31%)	26,54,113	3.02	15 (57%)
18	CLA	2	2010	-	22,32,73	1.89	5 (22%)	26,54,113	3.09	15 (57%)
18	CLA	L	1503	-	40,54,73	2.80	14 (35%)	48,90,113	5.25	24 (50%)
18	CLA	1	1012	-	22,32,73	1.81	5 (22%)	26,54,113	3.14	15 (57%)
18	CLA	4	4013	-	22,32,73	1.92	7 (31%)	26,54,113	3.02	14 (53%)
18	CLA	A	1117	-	22,32,73	1.78	5 (22%)	26,54,113	2.92	16 (61%)
18	CLA	B	1219	2	45,59,73	2.30	9 (20%)	50,96,113	3.09	21 (42%)
18	CLA	A	1118	-	22,32,73	1.91	7 (31%)	26,54,113	3.05	15 (57%)
18	CLA	A	1144	-	22,32,73	1.84	5 (22%)	26,54,113	3.07	15 (57%)
18	CLA	B	9022	-	48,62,73	2.27	13 (27%)	53,99,113	4.31	23 (43%)
18	CLA	F	4015	-	22,32,73	1.87	5 (22%)	26,54,113	3.15	16 (61%)
18	CLA	B	1301	-	22,32,73	1.92	5 (22%)	26,54,113	2.95	15 (57%)
18	CLA	A	1147	-	22,32,73	1.92	7 (31%)	26,54,113	2.95	15 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	F	1302	-	49,63,73	2.14	12 (24%)	55,101,113	3.43	21 (38%)
18	CLA	A	1128	-	49,63,73	2.13	14 (28%)	55,101,113	3.04	20 (36%)
18	CLA	4	1304	-	49,63,73	2.16	11 (22%)	55,101,113	3.49	19 (34%)
18	CLA	3	3009	-	22,32,73	1.90	6 (27%)	26,54,113	3.03	14 (53%)
18	CLA	B	1205	-	49,63,73	2.17	12 (24%)	55,101,113	3.86	23 (41%)
18	CLA	1	1007	-	22,32,73	1.97	7 (31%)	26,54,113	2.91	15 (57%)
18	CLA	4	4002	-	22,32,73	1.85	6 (27%)	26,54,113	3.04	14 (53%)
18	CLA	A	1123	-	49,63,73	2.30	13 (26%)	55,101,113	3.47	20 (36%)
19	PQN	A	5001	-	34,34,34	1.75	2 (5%)	42,45,45	1.35	4 (9%)
18	CLA	I	1204	-	49,63,73	2.24	12 (24%)	55,101,113	3.21	18 (32%)
18	CLA	A	1135	-	36,53,73	2.48	13 (36%)	39,89,113	3.85	15 (38%)
18	CLA	B	1229	-	43,57,73	2.54	12 (27%)	52,94,113	4.77	21 (40%)
21	SF4	B	3101	1,2	0,12,12	0.00	-	-	-	-
18	CLA	B	1225	-	36,53,73	2.53	12 (33%)	39,89,113	4.48	21 (53%)
18	CLA	B	1241	-	22,32,73	2.07	8 (36%)	26,54,113	2.94	17 (65%)
18	CLA	A	1136	-	49,63,73	2.20	12 (24%)	55,101,113	3.58	23 (41%)
18	CLA	2	2012	-	22,32,73	1.96	8 (36%)	26,54,113	3.01	16 (61%)
18	CLA	4	4007	-	22,32,73	1.96	7 (31%)	26,54,113	3.10	16 (61%)
18	CLA	1	1008	-	22,32,73	1.88	5 (22%)	26,54,113	3.01	16 (61%)
18	CLA	A	1151	-	22,32,73	1.87	6 (27%)	26,54,113	2.94	14 (53%)
20	BCR	I	6018	-	41,41,41	1.84	4 (9%)	56,56,56	4.81	33 (58%)
18	CLA	F	1305	-	22,32,73	1.84	5 (22%)	26,54,113	3.01	16 (61%)
18	CLA	A	1102	-	22,32,73	1.87	5 (22%)	26,54,113	2.91	14 (53%)
18	CLA	B	1231	-	40,54,73	2.43	13 (32%)	44,90,113	4.12	16 (36%)
18	CLA	B	1237	-	45,59,73	2.27	12 (26%)	50,96,113	3.94	20 (40%)
18	CLA	3	3005	-	22,32,73	1.88	7 (31%)	26,54,113	3.25	16 (61%)
18	CLA	A	1132	-	22,32,73	2.09	8 (36%)	26,54,113	3.08	18 (69%)
20	BCR	A	6011	-	41,41,41	1.54	3 (7%)	56,56,56	4.49	15 (26%)
18	CLA	F	1240	-	22,32,73	1.91	6 (27%)	26,54,113	3.37	15 (57%)
18	CLA	A	9011	-	49,63,73	2.15	11 (22%)	55,101,113	3.70	22 (40%)
18	CLA	2	2011	-	22,32,73	1.86	6 (27%)	26,54,113	3.06	16 (61%)
18	CLA	1	1004	-	22,32,73	1.92	7 (31%)	26,54,113	2.89	16 (61%)
18	CLA	A	1131	-	35,52,73	2.57	10 (28%)	42,88,113	4.02	21 (50%)
18	CLA	1	1013	-	22,32,73	1.90	5 (22%)	26,54,113	2.99	16 (61%)
18	CLA	A	1143	-	22,32,73	1.91	5 (22%)	26,54,113	2.98	15 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	1242	-	41,55,73	2.46	13 (31%)	45,91,113	4.04	17 (37%)
18	CLA	2	2013	-	22,32,73	1.97	6 (27%)	26,54,113	2.90	14 (53%)
18	CLA	B	1236	-	40,54,73	2.40	11 (27%)	44,90,113	4.41	17 (38%)
18	CLA	A	1120	-	22,32,73	1.95	6 (27%)	26,54,113	3.20	17 (65%)
18	CLA	B	1221	-	42,56,73	2.31	11 (26%)	46,92,113	3.17	20 (43%)
18	CLA	G	1233	-	45,59,73	2.37	13 (28%)	50,96,113	3.70	17 (34%)
18	CLA	K	1153	-	22,32,73	1.90	7 (31%)	26,54,113	2.82	15 (57%)
18	CLA	2	2001	-	22,32,73	1.87	5 (22%)	26,54,113	2.96	15 (57%)
18	CLA	A	1124	-	22,32,73	1.91	5 (22%)	26,54,113	3.17	15 (57%)
18	CLA	J	1307	-	22,32,73	1.87	5 (22%)	26,54,113	3.03	18 (69%)
18	CLA	B	1223	-	22,32,73	1.97	8 (36%)	26,54,113	2.91	14 (53%)
18	CLA	A	1115	-	41,55,73	2.38	13 (31%)	45,91,113	3.69	21 (46%)
18	CLA	B	1207	-	49,63,73	2.09	12 (24%)	55,101,113	4.16	25 (45%)
18	CLA	4	4009	-	22,32,73	1.84	5 (22%)	26,54,113	3.08	16 (61%)
18	CLA	L	1504	-	49,63,73	2.11	11 (22%)	55,101,113	3.41	16 (29%)
18	CLA	A	9013	-	40,54,73	2.34	10 (25%)	44,90,113	3.27	18 (40%)
20	BCR	L	6020	-	41,41,41	1.88	3 (7%)	56,56,56	4.82	25 (44%)
18	CLA	4	4001	-	22,32,73	1.88	5 (22%)	26,54,113	3.07	16 (61%)
18	CLA	B	1201	-	22,32,73	1.98	6 (27%)	26,54,113	3.17	14 (53%)
18	CLA	2	2005	-	22,32,73	1.94	5 (22%)	26,54,113	3.02	17 (65%)
18	CLA	4	4003	-	22,32,73	1.87	5 (22%)	26,54,113	2.87	16 (61%)
18	CLA	2	2007	-	22,32,73	1.91	6 (27%)	26,54,113	3.16	15 (57%)
18	CLA	B	1214	-	43,57,73	2.38	12 (27%)	46,93,113	3.18	21 (45%)
18	CLA	J	2107	-	55,69,73	2.04	11 (20%)	62,108,113	3.44	21 (33%)
18	CLA	3	3004	-	22,32,73	1.91	7 (31%)	26,54,113	3.07	16 (61%)
18	CLA	B	1203	18	40,56,73	2.48	12 (30%)	46,92,113	3.55	19 (41%)
18	CLA	A	1148	-	22,32,73	1.90	6 (27%)	26,54,113	3.17	16 (61%)
18	CLA	K	1150	-	22,32,73	1.86	5 (22%)	26,54,113	3.07	14 (53%)
18	CLA	3	3011	-	22,32,73	1.85	5 (22%)	26,54,113	2.91	17 (65%)
18	CLA	B	1138	-	50,64,73	2.16	14 (28%)	56,102,113	3.22	26 (46%)
18	CLA	A	1137	-	49,63,73	2.24	11 (22%)	55,101,113	3.12	23 (41%)
18	CLA	B	1227	2	44,58,73	2.22	14 (31%)	49,95,113	4.01	19 (38%)
18	CLA	B	1226	18	22,32,73	1.97	7 (31%)	26,54,113	2.91	15 (57%)
18	CLA	B	1230	-	22,32,73	1.86	6 (27%)	26,54,113	2.86	15 (57%)
18	CLA	B	1217	-	44,58,73	2.29	13 (29%)	49,95,113	4.00	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	A	1119	-	49,63,73	2.26	12 (24%)	55,101,113	3.40	18 (32%)
18	CLA	A	1113	-	44,58,73	2.35	12 (27%)	49,95,113	4.17	22 (44%)
18	CLA	1	1011	14	22,32,73	1.92	5 (22%)	26,54,113	3.05	16 (61%)
18	CLA	A	1146	-	22,32,73	1.95	7 (31%)	26,54,113	2.93	16 (61%)
18	CLA	1	1014	-	22,32,73	1.91	5 (22%)	26,54,113	2.95	14 (53%)
18	CLA	B	1239	-	49,63,73	2.22	12 (24%)	55,101,113	3.14	19 (34%)
19	PQN	B	5002	-	34,34,34	1.78	2 (5%)	42,45,45	1.65	8 (19%)
18	CLA	A	1129	-	49,63,73	2.17	12 (24%)	55,101,113	3.69	23 (41%)
18	CLA	A	1126	1	49,63,73	2.19	13 (26%)	55,101,113	4.40	26 (47%)
18	CLA	A	1105	1	22,32,73	1.88	7 (31%)	26,54,113	3.10	16 (61%)
18	CLA	A	1116	-	22,32,73	1.92	7 (31%)	26,54,113	3.18	17 (65%)
18	CLA	B	1210	-	22,32,73	1.99	6 (27%)	26,54,113	2.97	17 (65%)
20	BCR	B	6017	-	41,41,41	1.54	3 (7%)	56,56,56	4.28	24 (42%)
18	CLA	B	1209	-	49,63,73	2.15	11 (22%)	55,101,113	3.86	23 (41%)
18	CLA	B	1228	-	49,63,73	2.18	12 (24%)	55,101,113	3.94	24 (43%)
18	CLA	3	3003	-	22,32,73	1.93	6 (27%)	26,54,113	2.90	17 (65%)
18	CLA	A	1103	1	41,55,73	2.39	12 (29%)	45,91,113	3.89	21 (46%)
18	CLA	4	4004	-	22,32,73	1.93	7 (31%)	26,54,113	2.95	15 (57%)
18	CLA	B	1234	-	44,58,73	2.29	12 (27%)	49,95,113	3.43	18 (36%)
18	CLA	3	3007	-	22,32,73	1.85	7 (31%)	26,54,113	3.14	16 (61%)
18	CLA	B	1235	-	49,63,73	2.20	13 (26%)	55,101,113	3.53	19 (34%)
18	CLA	L	1130	-	44,58,73	2.25	12 (27%)	49,95,113	3.42	20 (40%)
18	CLA	2	2008	-	22,32,73	1.91	6 (27%)	26,54,113	3.02	15 (57%)
18	CLA	B	1222	-	59,73,73	1.97	11 (18%)	67,113,113	2.74	21 (31%)

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
18	CLA	H	1501	-	4/4/18/25	9/25/123/135	-
21	SF4	C	3102	3	-	-	0/6/5/5
18	CLA	4	1009	-	3/3/7/25	-	-
18	CLA	1	1002	-	3/3/7/25	-	-
18	CLA	J	1308	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	3	3006	16	3/3/7/25	-	-
18	CLA	A	1133	-	3/3/7/25	-	-
18	CLA	A	1140	-	4/4/18/25	12/25/123/135	-
18	CLA	A	1122	-	4/4/18/25	7/25/123/135	-
18	CLA	A	1152	-	3/3/7/25	-	-
18	CLA	1	1001	-	3/3/7/25	-	-
18	CLA	3	3012	-	3/3/7/25	-	-
20	BCR	F	6016	-	-	13/29/63/63	0/2/2/2
18	CLA	H	1505	8	3/3/7/25	-	-
18	CLA	4	4005	-	3/3/7/25	-	-
18	CLA	A	1101	-	3/3/7/25	-	-
18	CLA	3	3002	-	3/3/7/25	-	-
18	CLA	B	1211	2	3/3/7/25	-	-
18	CLA	A	1106	-	3/3/15/25	2/8/106/135	-
18	CLA	B	1216	-	4/4/18/25	10/27/125/135	-
18	CLA	3	3015	-	3/3/7/25	-	-
18	CLA	1	1006	-	3/3/7/25	-	-
18	CLA	A	1309	-	3/3/7/25	-	-
18	CLA	B	9010	2	3/3/16/25	9/16/114/135	-
18	CLA	G	1248	-	3/3/7/25	-	-
18	CLA	A	1107	1	4/4/18/25	17/28/126/135	-
18	CLA	A	1108	-	3/3/17/25	5/19/117/135	-
18	CLA	B	1238	-	3/3/17/25	9/24/122/135	-
18	CLA	B	1215	2	3/3/17/25	12/22/120/135	-
18	CLA	4	4010	-	3/3/7/25	-	-
18	CLA	3	3013	-	3/3/7/25	-	-
18	CLA	1	1005	-	3/3/7/25	-	-
18	CLA	A	1127	1	3/3/7/25	-	-
18	CLA	3	3010	-	3/3/7/25	-	-
18	CLA	2	2004	-	3/3/7/25	-	-
18	CLA	3	3001	-	3/3/7/25	-	-
18	CLA	B	1202	-	3/3/17/25	8/19/117/135	-
18	CLA	B	1224	-	3/3/17/25	4/21/119/135	-
18	CLA	1	1010	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	K	1141	-	3/3/7/25	-	-
18	CLA	B	1212	-	4/4/19/25	19/31/129/135	-
18	CLA	A	1111	-	3/3/7/25	-	-
18	CLA	B	1213	2	3/3/7/25	-	-
18	CLA	2	2006	-	3/3/7/25	-	-
18	CLA	4	4008	-	3/3/7/25	-	-
18	CLA	B	1208	-	4/4/18/25	15/25/123/135	-
18	CLA	A	1104	1	3/3/7/25	-	-
18	CLA	A	1142	-	3/3/7/25	-	-
18	CLA	F	1139	-	3/3/15/25	9/11/110/135	-
18	CLA	3	3008	-	3/3/7/25	-	-
18	CLA	A	1110	-	3/3/7/25	-	-
18	CLA	4	4006	-	3/3/7/25	-	-
18	CLA	L	1502	12	3/3/17/25	10/21/119/135	-
18	CLA	B	1220	-	4/4/19/25	18/31/129/135	-
18	CLA	A	1134	-	3/3/7/25	-	-
18	CLA	L	1125	-	3/3/7/25	-	-
18	CLA	B	1206	2	3/3/7/25	-	-
18	CLA	B	1232	-	4/4/18/25	9/25/123/135	-
18	CLA	4	4012	-	3/3/7/25	-	-
21	SF4	C	3103	3	-	-	0/6/5/5
18	CLA	B	9023	-	3/3/16/25	5/16/114/135	-
18	CLA	1	1003	-	3/3/7/25	-	-
18	CLA	2	2002	-	3/3/7/25	-	-
18	CLA	B	9012	-	4/4/18/25	15/25/123/135	-
18	CLA	2	2003	-	3/3/7/25	-	-
18	CLA	B	1218	-	3/3/17/25	12/21/119/135	-
18	CLA	F	1306	-	3/3/7/25	-	-
18	CLA	A	1109	-	3/3/6/25	-	-
18	CLA	2	2015	-	3/3/7/25	-	-
18	CLA	F	1303	-	3/3/7/25	-	-
18	CLA	4	4011	-	3/3/7/25	-	-
18	CLA	3	2009	-	3/3/7/25	-	-
18	CLA	2	2010	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	L	1503	-	3/3/16/25	6/16/112/135	-
18	CLA	1	1012	-	3/3/7/25	-	-
18	CLA	4	4013	-	3/3/7/25	-	-
18	CLA	A	1117	-	3/3/7/25	-	-
18	CLA	B	1219	2	3/3/17/25	11/21/119/135	-
18	CLA	A	1118	-	3/3/7/25	-	-
18	CLA	A	1144	-	3/3/7/25	-	-
18	CLA	B	9022	-	3/3/17/25	12/24/122/135	-
18	CLA	F	4015	-	3/3/7/25	-	-
18	CLA	B	1301	-	3/3/7/25	-	-
18	CLA	A	1147	-	3/3/7/25	-	-
18	CLA	F	1302	-	4/4/18/25	6/25/123/135	-
18	CLA	A	1128	-	4/4/18/25	9/25/123/135	-
18	CLA	4	1304	-	4/4/18/25	11/25/123/135	-
18	CLA	3	3009	-	3/3/7/25	-	-
18	CLA	B	1205	-	4/4/18/25	12/25/123/135	-
18	CLA	1	1007	-	3/3/7/25	-	-
18	CLA	4	4002	-	3/3/7/25	-	-
18	CLA	A	1123	-	4/4/18/25	14/25/123/135	-
19	PQN	A	5001	-	1/1/8/9	11/23/43/43	0/2/2/2
18	CLA	I	1204	-	4/4/18/25	14/25/123/135	-
18	CLA	A	1135	-	3/3/16/25	5/11/111/135	-
18	CLA	B	1229	-	3/3/17/25	8/19/115/135	-
21	SF4	B	3101	1,2	-	-	0/6/5/5
18	CLA	B	1225	-	3/3/16/25	3/11/111/135	-
18	CLA	B	1241	-	3/3/7/25	-	-
18	CLA	A	1136	-	4/4/18/25	12/25/123/135	-
18	CLA	2	2012	-	3/3/7/25	-	-
18	CLA	4	4007	-	3/3/7/25	-	-
18	CLA	1	1008	-	3/3/7/25	-	-
18	CLA	A	1151	-	3/3/7/25	-	-
20	BCR	I	6018	-	-	12/29/63/63	0/2/2/2
18	CLA	F	1305	-	3/3/7/25	-	-
18	CLA	A	1102	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1231	-	3/3/16/25	10/15/113/135	-
18	CLA	B	1237	-	3/3/17/25	11/21/119/135	-
18	CLA	3	3005	-	3/3/7/25	-	-
18	CLA	A	1132	-	3/3/7/25	-	-
20	BCR	A	6011	-	-	15/29/63/63	0/2/2/2
18	CLA	F	1240	-	3/3/7/25	-	-
18	CLA	A	9011	-	4/4/18/25	11/25/123/135	-
18	CLA	2	2011	-	3/3/7/25	-	-
18	CLA	1	1004	-	3/3/7/25	-	-
18	CLA	A	1131	-	3/3/16/25	6/11/109/135	-
18	CLA	1	1013	-	3/3/7/25	-	-
18	CLA	A	1143	-	3/3/7/25	-	-
18	CLA	B	1242	-	3/3/16/25	13/16/114/135	-
18	CLA	2	2013	-	3/3/7/25	-	-
18	CLA	B	1236	-	3/3/16/25	6/15/113/135	-
18	CLA	A	1120	-	3/3/7/25	-	-
18	CLA	B	1221	-	3/3/16/25	14/17/115/135	-
18	CLA	G	1233	-	3/3/17/25	12/21/119/135	-
18	CLA	K	1153	-	3/3/7/25	-	-
18	CLA	2	2001	-	3/3/7/25	-	-
18	CLA	A	1124	-	3/3/7/25	-	-
18	CLA	J	1307	-	3/3/7/25	-	-
18	CLA	B	1223	-	3/3/7/25	-	-
18	CLA	A	1115	-	3/3/16/25	7/16/114/135	-
18	CLA	B	1207	-	4/4/18/25	11/25/123/135	-
18	CLA	4	4009	-	3/3/7/25	-	-
18	CLA	L	1504	-	4/4/18/25	9/25/123/135	-
18	CLA	A	9013	-	3/3/16/25	4/15/113/135	-
20	BCR	L	6020	-	-	16/29/63/63	0/2/2/2
18	CLA	4	4001	-	3/3/7/25	-	-
18	CLA	B	1201	-	3/3/7/25	-	-
18	CLA	2	2005	-	3/3/7/25	-	-
18	CLA	4	4003	-	3/3/7/25	-	-
18	CLA	2	2007	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	1214	-	3/3/16/25	7/18/116/135	-
18	CLA	J	2107	-	4/4/19/25	13/33/131/135	-
18	CLA	3	3004	-	3/3/7/25	-	-
18	CLA	B	1203	18	3/3/17/25	9/17/115/135	-
18	CLA	A	1148	-	3/3/7/25	-	-
18	CLA	K	1150	-	3/3/7/25	-	-
18	CLA	3	3011	-	3/3/7/25	-	-
18	CLA	B	1138	-	4/4/18/25	12/27/125/135	-
18	CLA	A	1137	-	4/4/18/25	13/25/123/135	-
18	CLA	B	1227	2	3/3/17/25	10/19/117/135	-
18	CLA	B	1226	18	3/3/7/25	-	-
18	CLA	B	1230	-	3/3/7/25	-	-
18	CLA	B	1217	-	3/3/17/25	6/19/117/135	-
18	CLA	A	1119	-	4/4/18/25	14/25/123/135	-
18	CLA	A	1113	-	3/3/17/25	5/19/117/135	-
18	CLA	1	1011	14	3/3/7/25	-	-
18	CLA	A	1146	-	3/3/7/25	-	-
18	CLA	1	1014	-	3/3/7/25	-	-
18	CLA	B	1239	-	4/4/18/25	6/25/123/135	-
19	PQN	B	5002	-	1/1/8/9	8/23/43/43	0/2/2/2
18	CLA	A	1129	-	4/4/18/25	9/25/123/135	-
18	CLA	A	1126	1	4/4/18/25	12/25/123/135	-
18	CLA	A	1105	1	3/3/7/25	-	-
18	CLA	A	1116	-	3/3/7/25	-	-
18	CLA	B	1210	-	3/3/7/25	-	-
20	BCR	B	6017	-	-	19/29/63/63	0/2/2/2
18	CLA	B	1209	-	4/4/18/25	13/25/123/135	-
18	CLA	B	1228	-	4/4/18/25	9/25/123/135	-
18	CLA	3	3003	-	3/3/7/25	-	-
18	CLA	A	1103	1	3/3/16/25	8/16/114/135	-
18	CLA	4	4004	-	3/3/7/25	-	-
18	CLA	B	1234	-	3/3/17/25	9/19/117/135	-
18	CLA	3	3007	-	3/3/7/25	-	-
18	CLA	B	1235	-	4/4/18/25	11/25/123/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	L	1130	-	3/3/17/25	3/19/117/135	-
18	CLA	2	2008	-	3/3/7/25	-	-
18	CLA	B	1222	-	4/4/20/25	20/37/135/135	-

The worst 5 of 1418 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	5002	PQN	C3-C2	8.48	1.50	1.35
19	A	5001	PQN	C3-C2	8.17	1.50	1.35
18	B	1229	CLA	CAB-C3B	-8.17	1.34	1.51
18	A	1131	CLA	CAB-C3B	-8.10	1.34	1.51
20	L	6020	BCR	C11-C10	-7.70	1.19	1.43

The worst 5 of 3079 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	6011	BCR	C11-C10-C9	28.99	168.68	127.31
20	L	6020	BCR	C11-C10-C9	26.87	165.66	127.31
20	F	6016	BCR	C11-C10-C9	26.81	165.58	127.31
20	B	6017	BCR	C11-C10-C9	24.33	162.03	127.31
18	A	1126	CLA	OBD-CAD-CBD	-21.09	95.77	125.89

5 of 537 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	H	1501	CLA	C8
18	H	1501	CLA	NC
18	H	1501	CLA	ND
18	H	1501	CLA	NA
18	4	1009	CLA	NC

5 of 736 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	H	1501	CLA	C3A-C2A-CAA-CBA
18	A	1140	CLA	C1A-C2A-CAA-CBA
18	A	1140	CLA	C3A-C2A-CAA-CBA
18	A	1122	CLA	C1A-C2A-CAA-CBA
18	A	1122	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

131 monomers are involved in 1354 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	H	1501	CLA	13	0
21	C	3102	SF4	8	0
18	3	3006	CLA	1	0
18	A	1133	CLA	2	0
18	A	1140	CLA	25	0
18	A	1122	CLA	4	0
20	F	6016	BCR	15	0
18	H	1505	CLA	2	0
18	4	4005	CLA	1	0
18	A	1101	CLA	4	0
18	3	3002	CLA	2	0
18	B	1211	CLA	7	0
18	A	1106	CLA	13	0
18	B	1216	CLA	23	0
18	1	1006	CLA	2	0
18	B	9010	CLA	29	0
18	G	1248	CLA	4	0
18	A	1107	CLA	16	0
18	A	1108	CLA	13	0
18	B	1238	CLA	23	0
18	B	1215	CLA	23	0
18	4	4010	CLA	1	0
18	A	1127	CLA	6	0
18	3	3010	CLA	1	0
18	2	2004	CLA	3	0
18	B	1202	CLA	42	0
18	B	1224	CLA	14	0
18	K	1141	CLA	5	0
18	B	1212	CLA	13	0
18	A	1111	CLA	2	0
18	B	1213	CLA	1	0
18	2	2006	CLA	2	0
18	B	1208	CLA	13	0
18	F	1139	CLA	21	0
18	A	1110	CLA	4	0
18	L	1502	CLA	18	0
18	B	1220	CLA	26	0
18	A	1134	CLA	7	0
18	B	1206	CLA	5	0
18	B	1232	CLA	6	0
18	4	4012	CLA	1	0
21	C	3103	SF4	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	9023	CLA	17	0
18	1	1003	CLA	3	0
18	2	2002	CLA	2	0
18	B	9012	CLA	20	0
18	2	2003	CLA	1	0
18	B	1218	CLA	44	0
18	A	1109	CLA	11	0
18	F	1303	CLA	2	0
18	4	4011	CLA	1	0
18	L	1503	CLA	59	0
18	1	1012	CLA	3	0
18	4	4013	CLA	1	0
18	B	1219	CLA	13	0
18	A	1118	CLA	7	0
18	B	9022	CLA	17	0
18	F	4015	CLA	2	0
18	B	1301	CLA	3	0
18	A	1147	CLA	6	0
18	F	1302	CLA	16	0
18	A	1128	CLA	16	0
18	4	1304	CLA	11	0
18	B	1205	CLA	14	0
18	A	1123	CLA	24	0
19	A	5001	PQN	30	0
18	I	1204	CLA	11	0
18	A	1135	CLA	7	0
18	B	1229	CLA	13	0
21	B	3101	SF4	4	0
18	B	1225	CLA	43	0
18	B	1241	CLA	6	0
18	A	1136	CLA	26	0
18	2	2012	CLA	5	0
18	1	1008	CLA	1	0
20	I	6018	BCR	13	0
18	B	1231	CLA	3	0
18	B	1237	CLA	13	0
18	3	3005	CLA	5	0
18	A	1132	CLA	9	0
20	A	6011	BCR	17	0
18	F	1240	CLA	2	0
18	A	9011	CLA	24	0
18	2	2011	CLA	1	0

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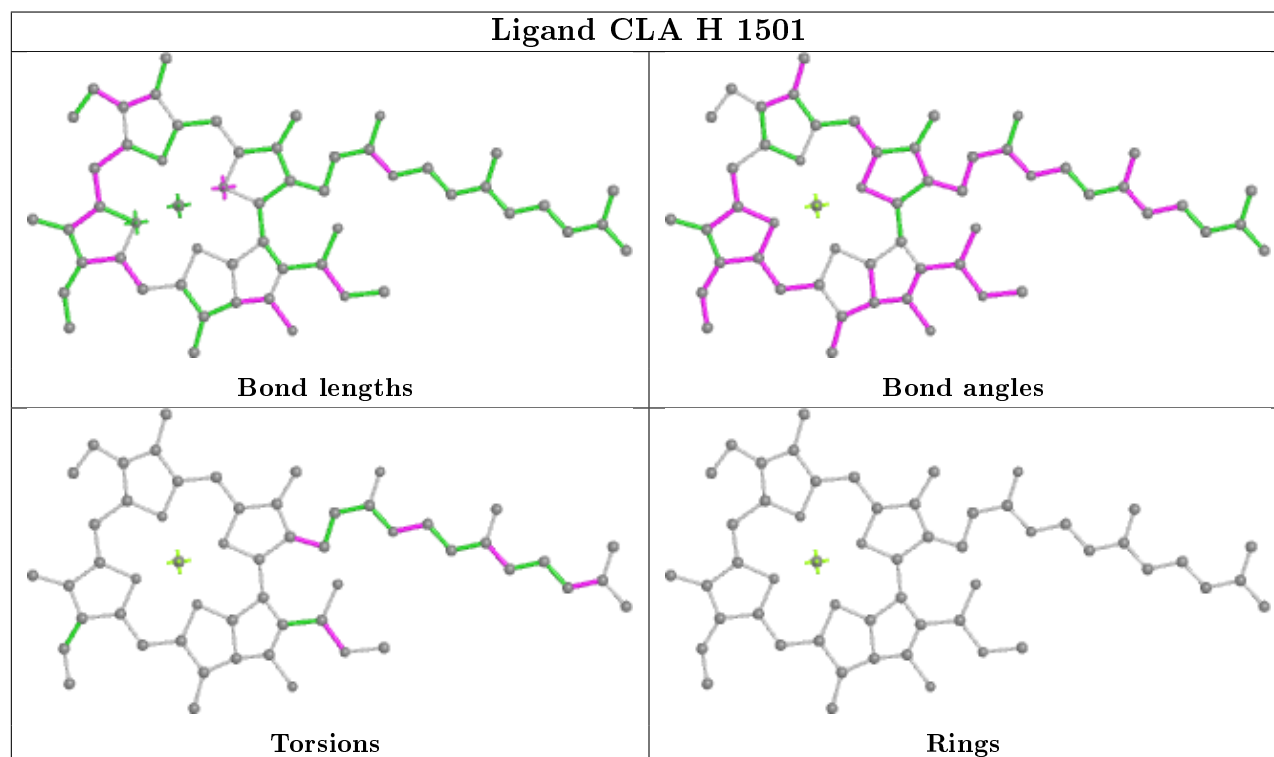
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1131	CLA	10	0
18	1	1013	CLA	3	0
18	B	1242	CLA	19	0
18	B	1236	CLA	11	0
18	A	1120	CLA	1	0
18	B	1221	CLA	23	0
18	G	1233	CLA	8	0
18	A	1124	CLA	14	0
18	B	1223	CLA	5	0
18	A	1115	CLA	8	0
18	B	1207	CLA	16	0
18	L	1504	CLA	13	0
18	A	9013	CLA	19	0
20	L	6020	BCR	17	0
18	4	4001	CLA	2	0
18	2	2005	CLA	1	0
18	2	2007	CLA	2	0
18	B	1214	CLA	32	0
18	J	2107	CLA	8	0
18	3	3004	CLA	2	0
18	B	1203	CLA	14	0
18	A	1148	CLA	4	0
18	B	1138	CLA	28	0
18	A	1137	CLA	20	0
18	B	1227	CLA	23	0
18	B	1226	CLA	4	0
18	B	1230	CLA	6	0
18	B	1217	CLA	14	0
18	A	1119	CLA	7	0
18	A	1113	CLA	6	0
18	A	1146	CLA	1	0
18	B	1239	CLA	33	0
19	B	5002	PQN	20	0
18	A	1129	CLA	17	0
18	A	1126	CLA	23	0
18	A	1105	CLA	3	0
18	A	1116	CLA	5	0
18	B	1210	CLA	15	0
20	B	6017	BCR	20	0
18	B	1209	CLA	36	0
18	B	1228	CLA	27	0
18	A	1103	CLA	19	0

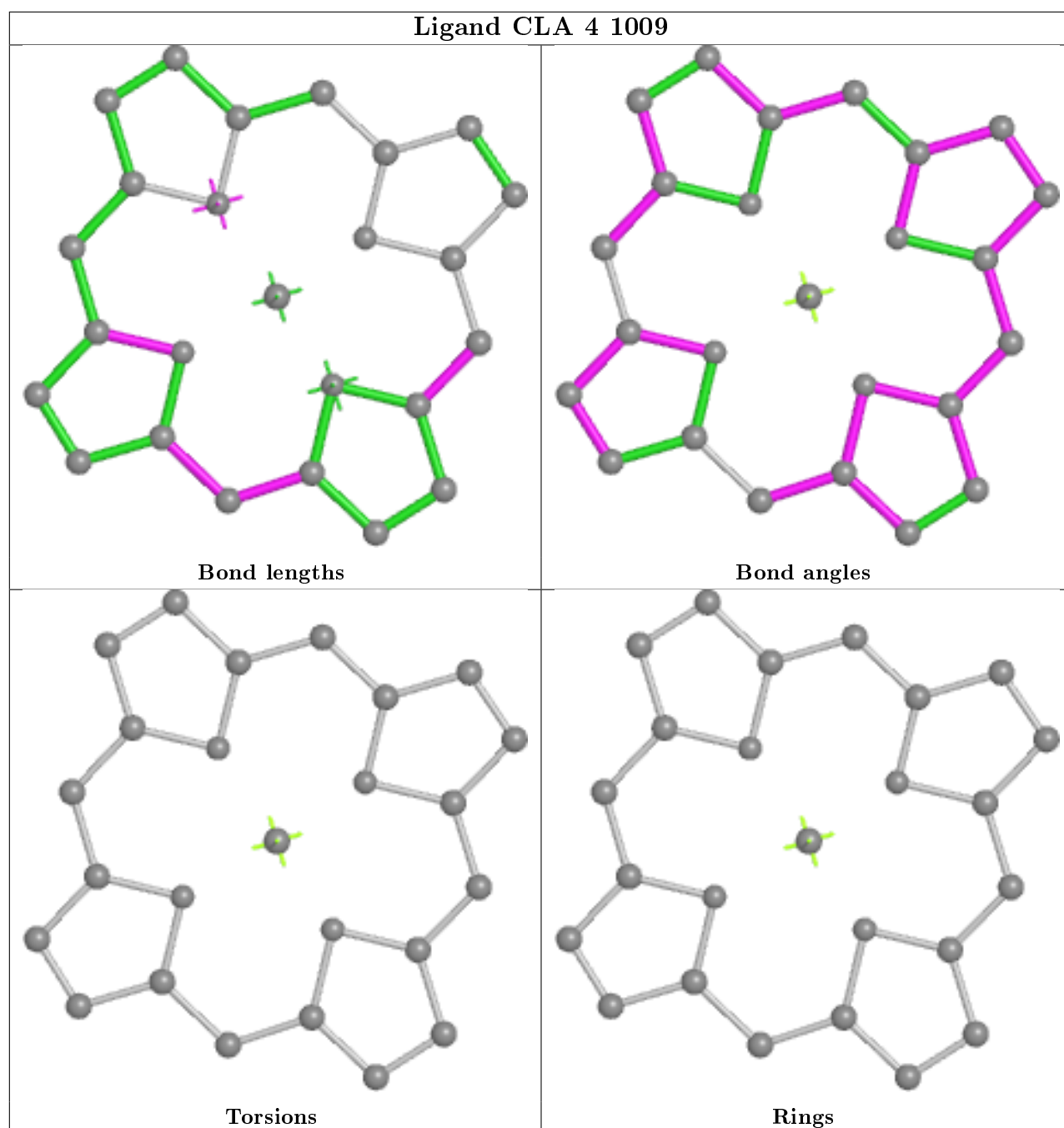
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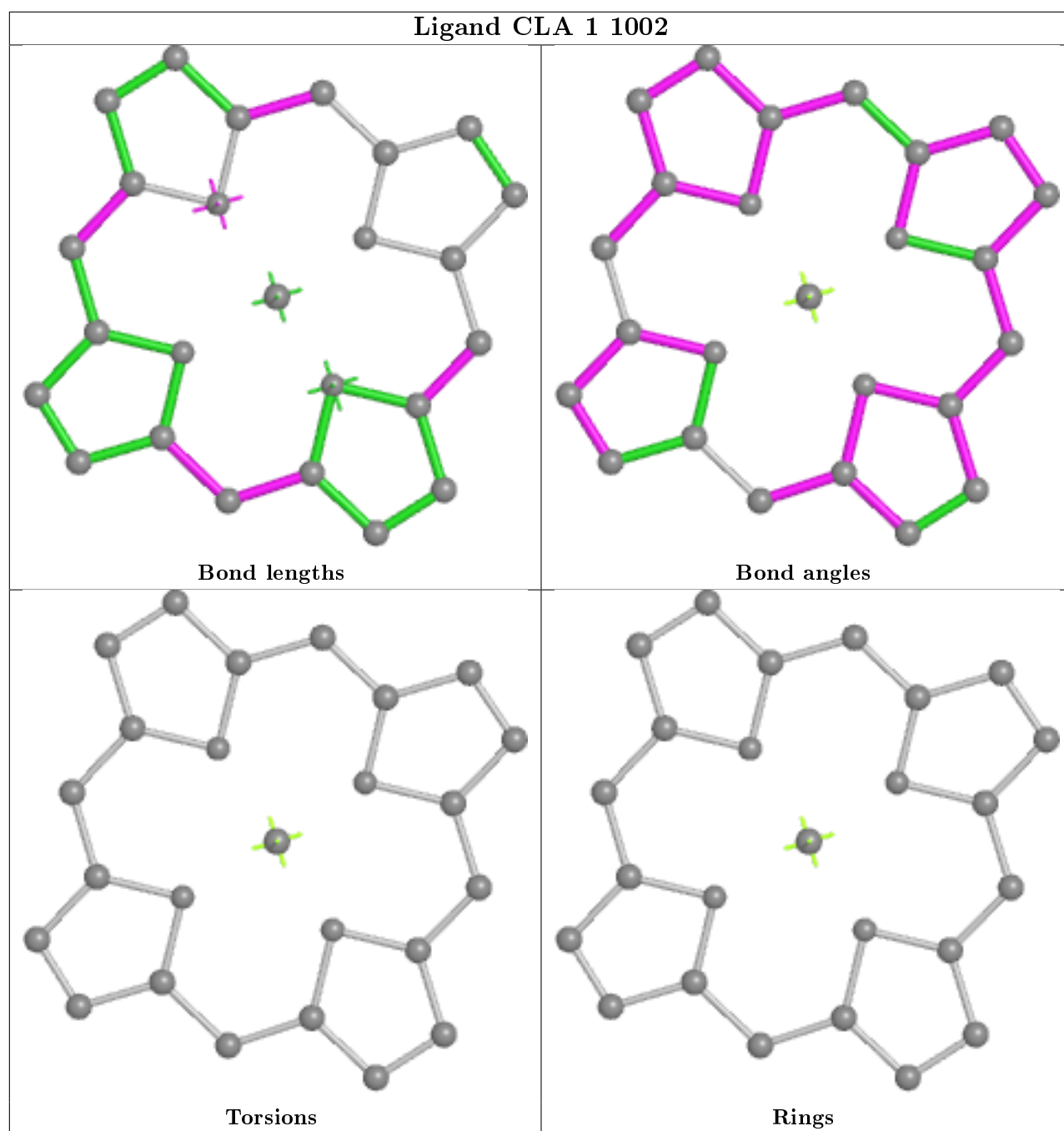
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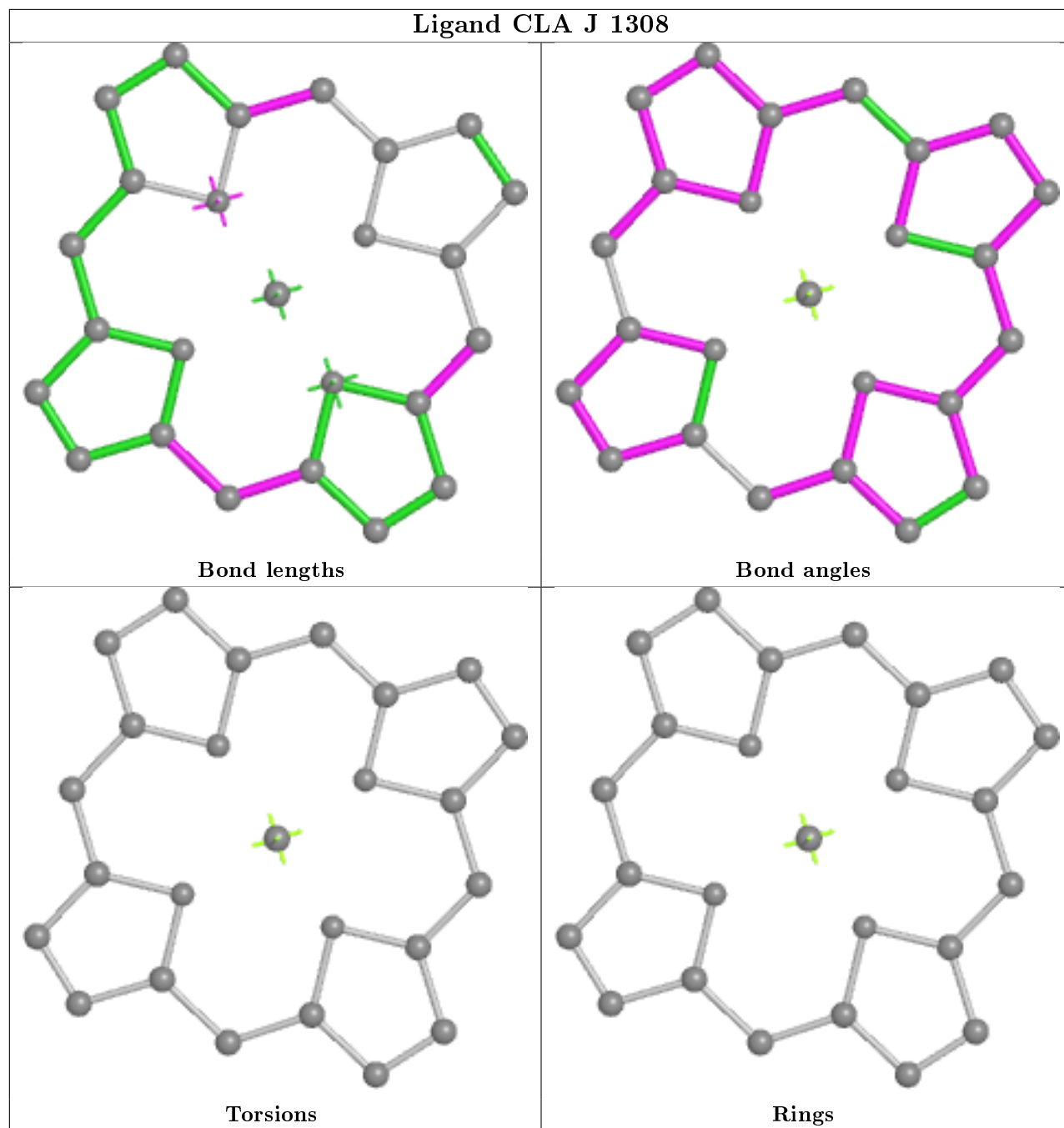
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	1234	CLA	25	0
18	3	3007	CLA	1	0
18	B	1235	CLA	20	0
18	L	1130	CLA	23	0
18	B	1222	CLA	13	0

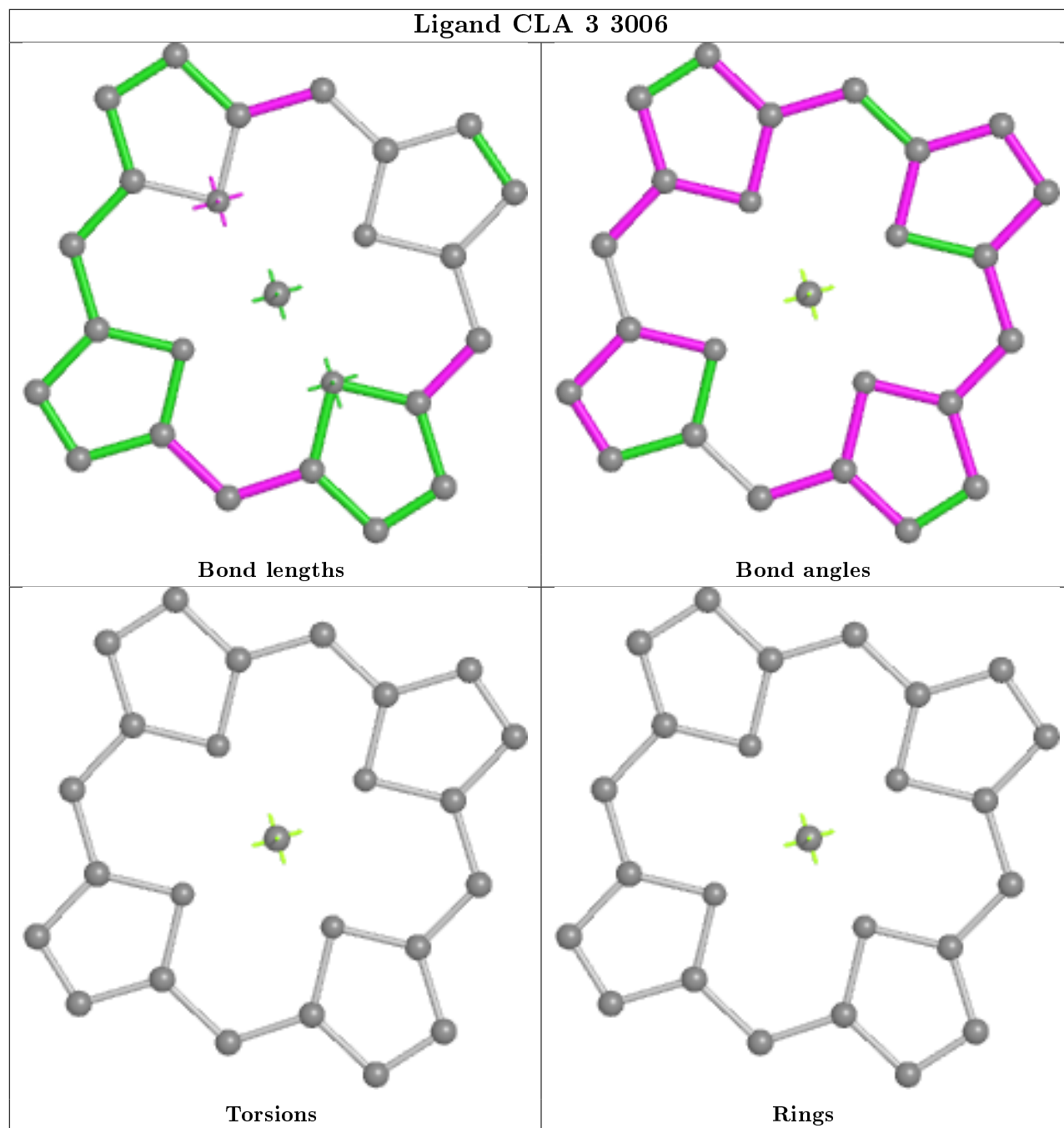
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



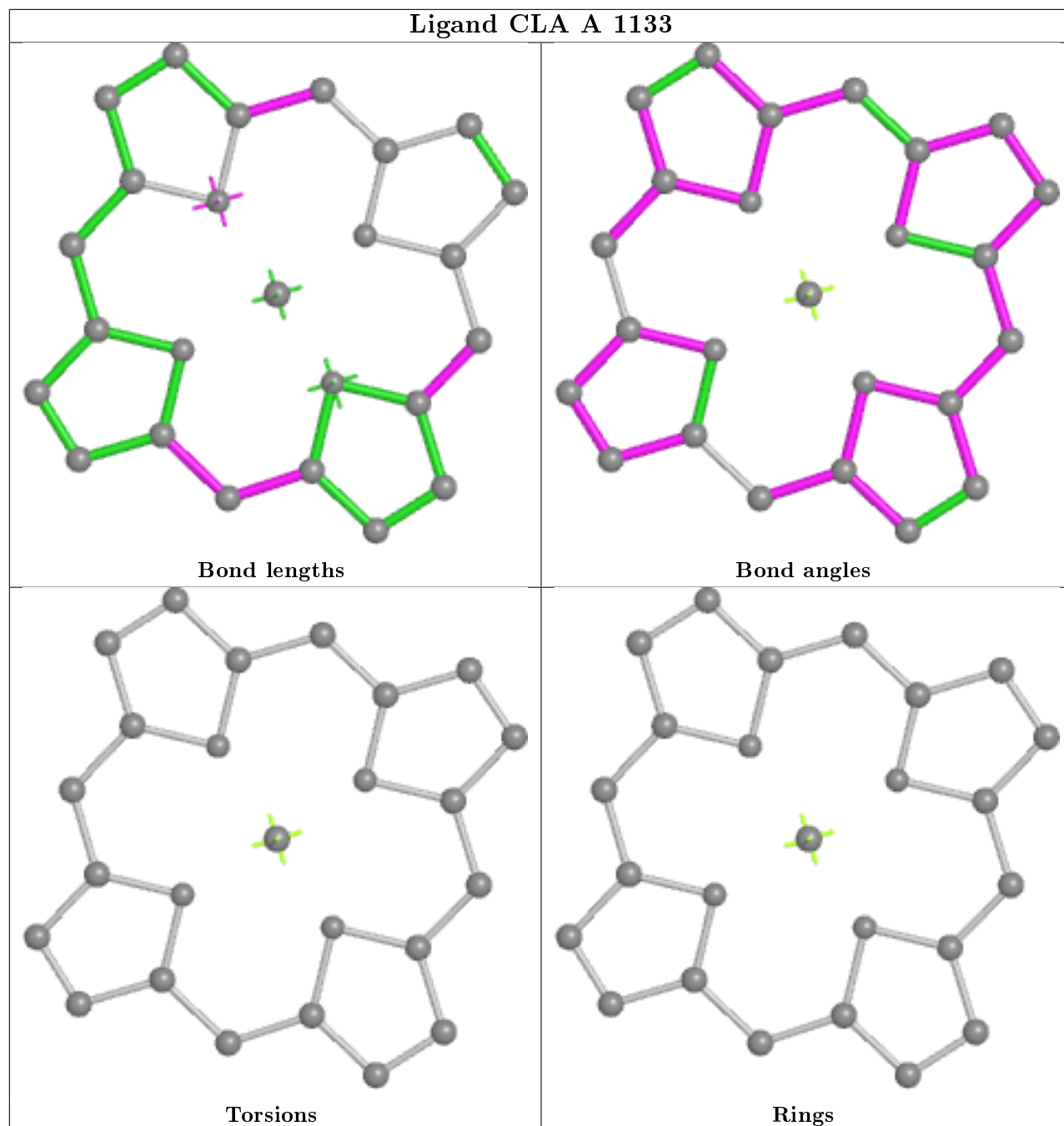




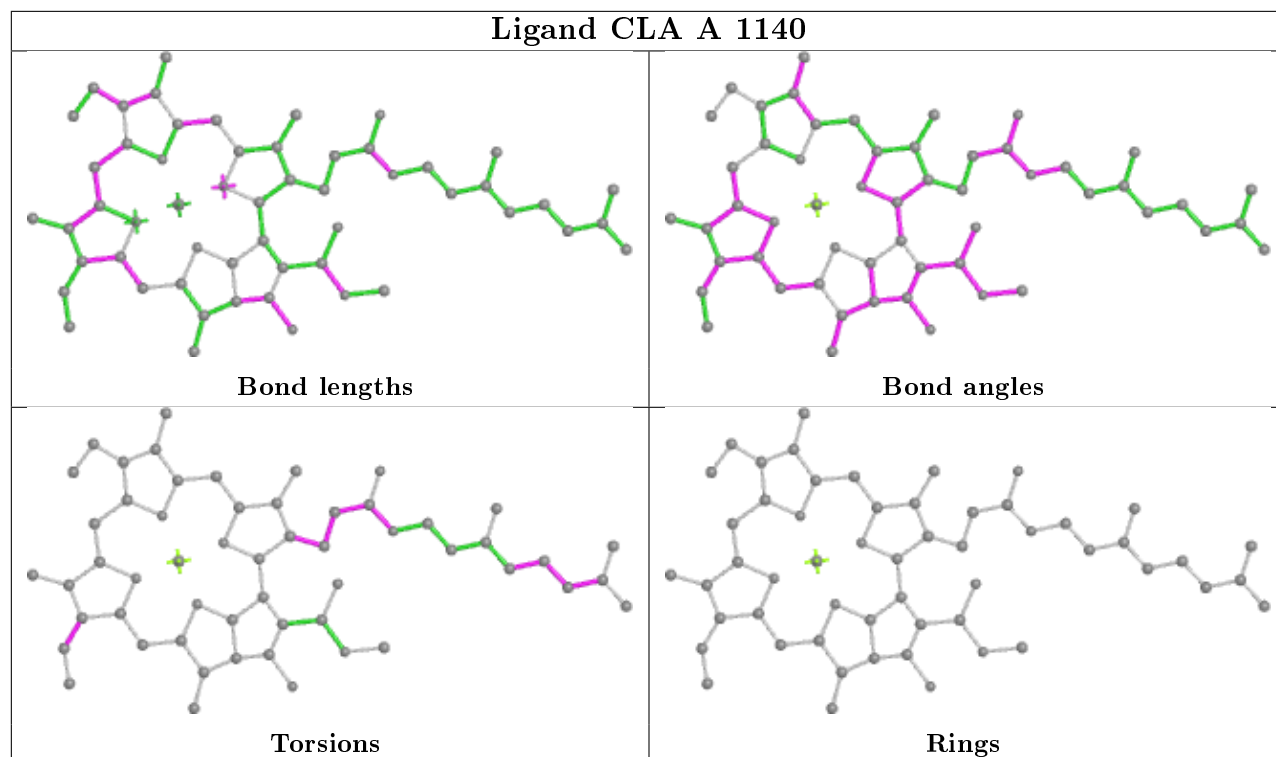




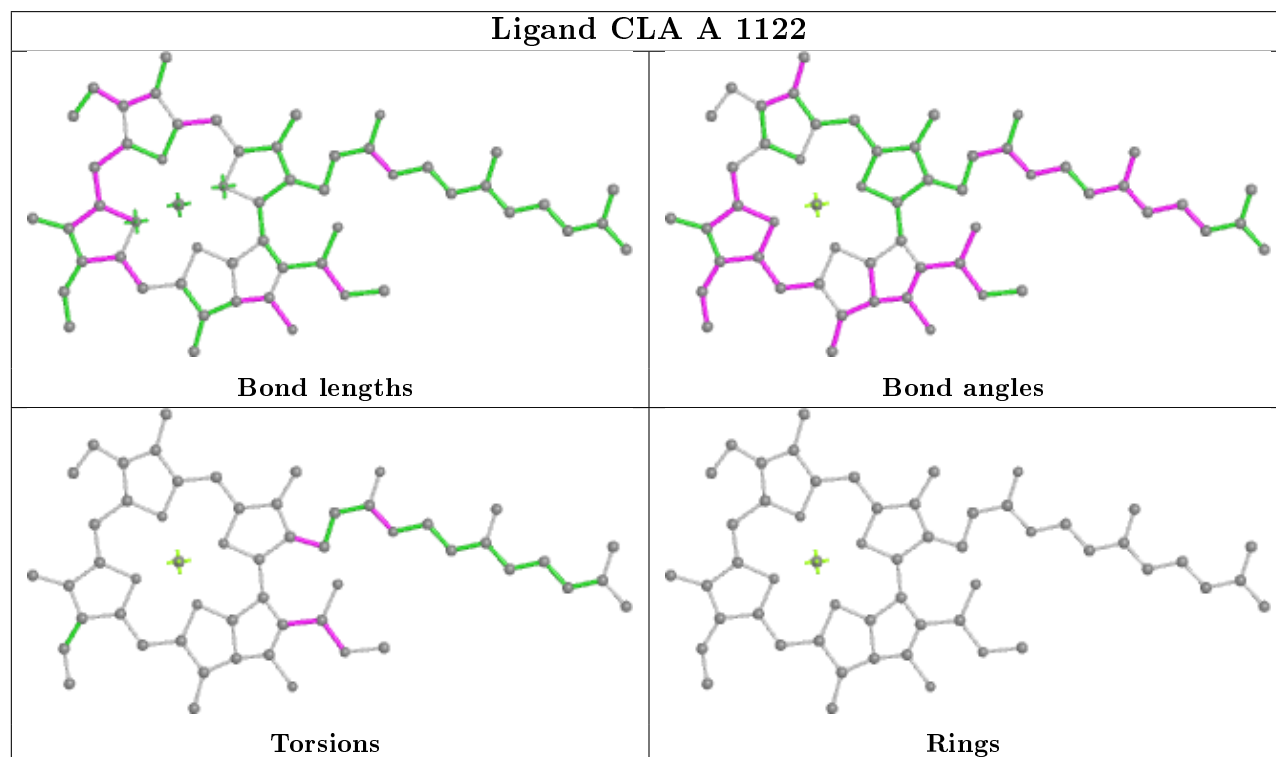
Ligand CLA A 1133



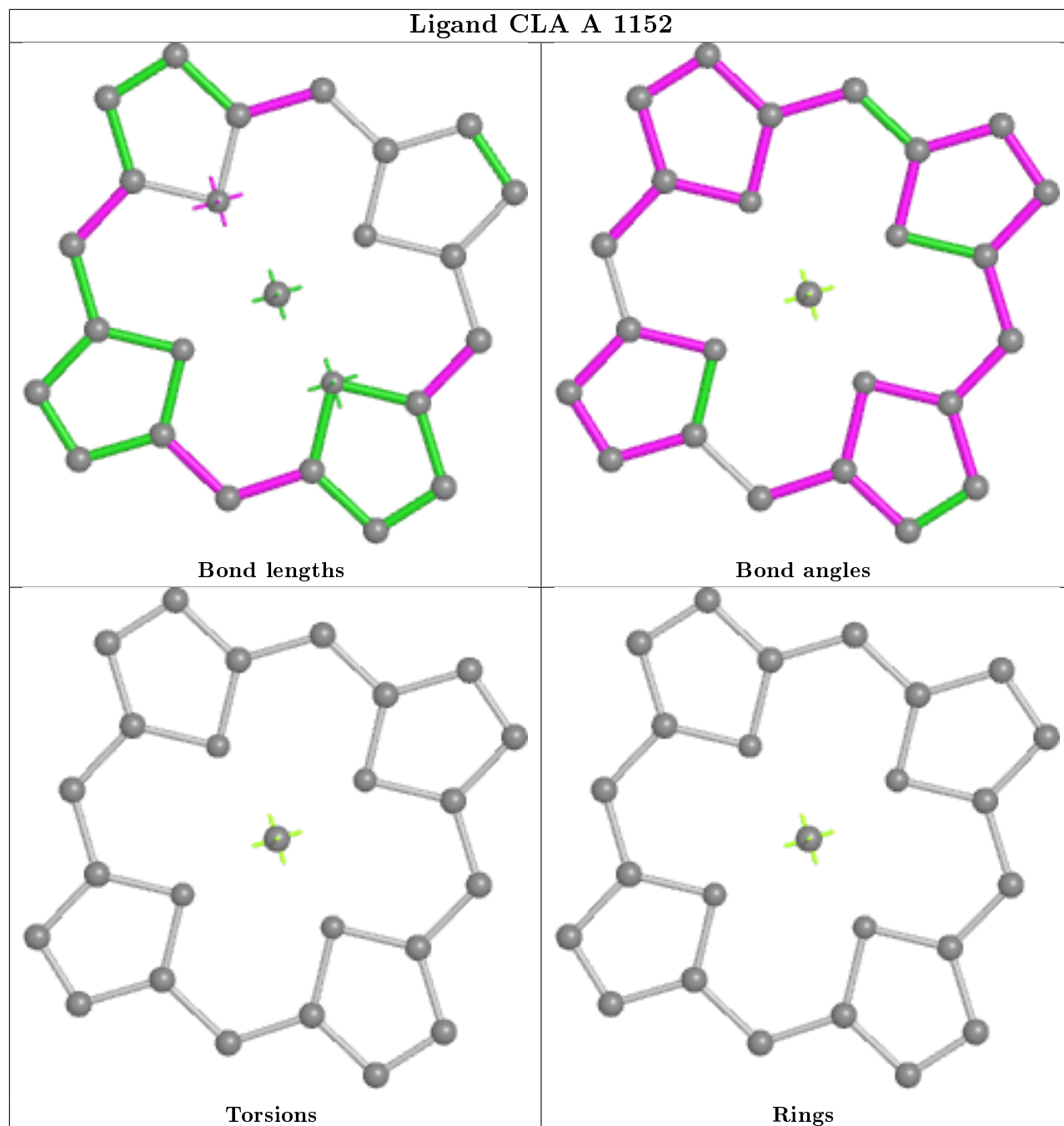
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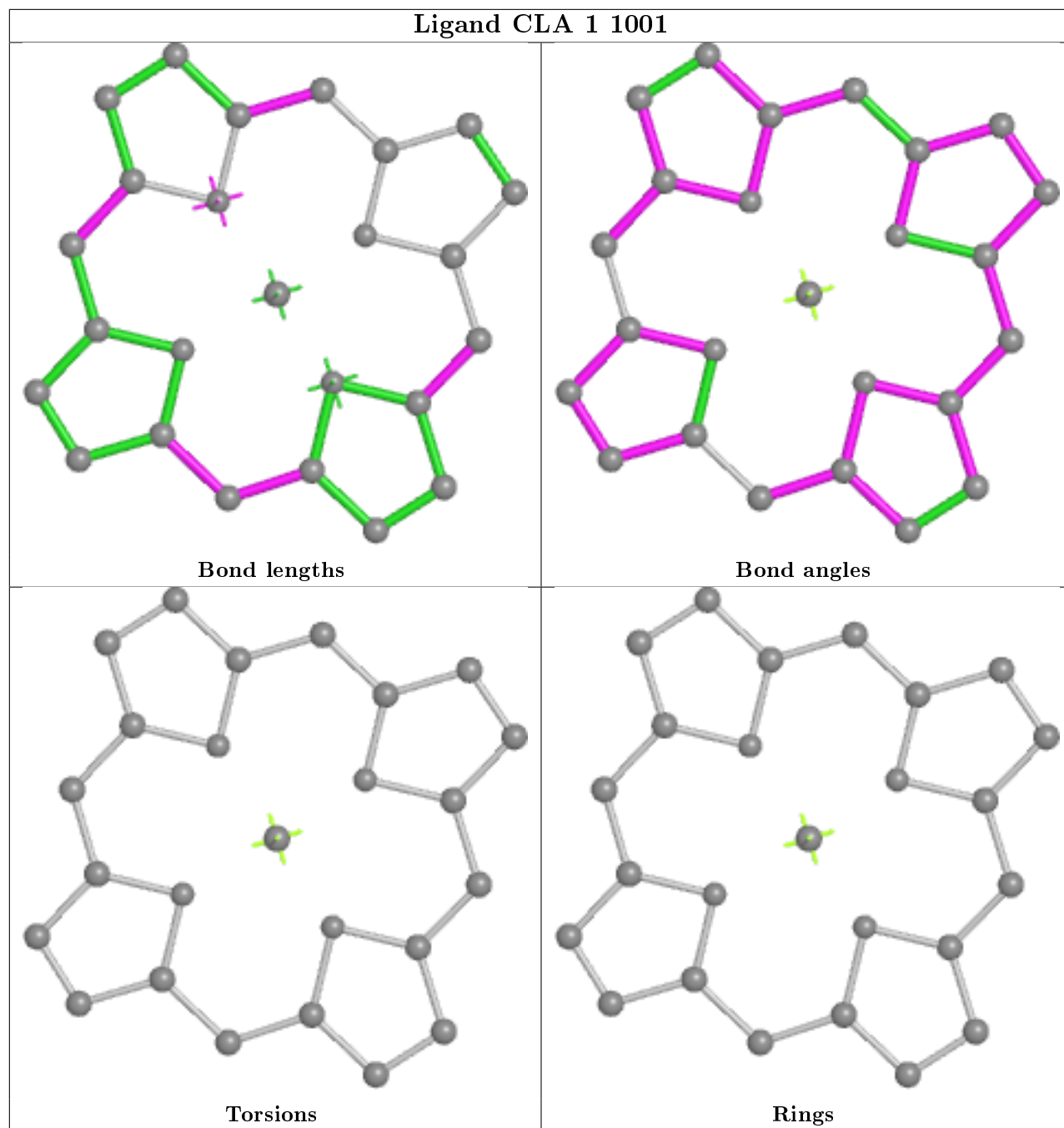


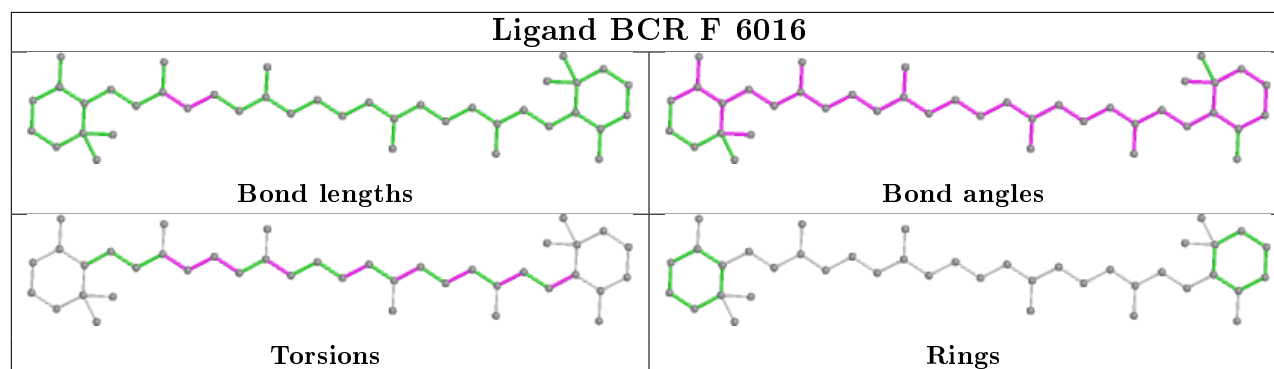
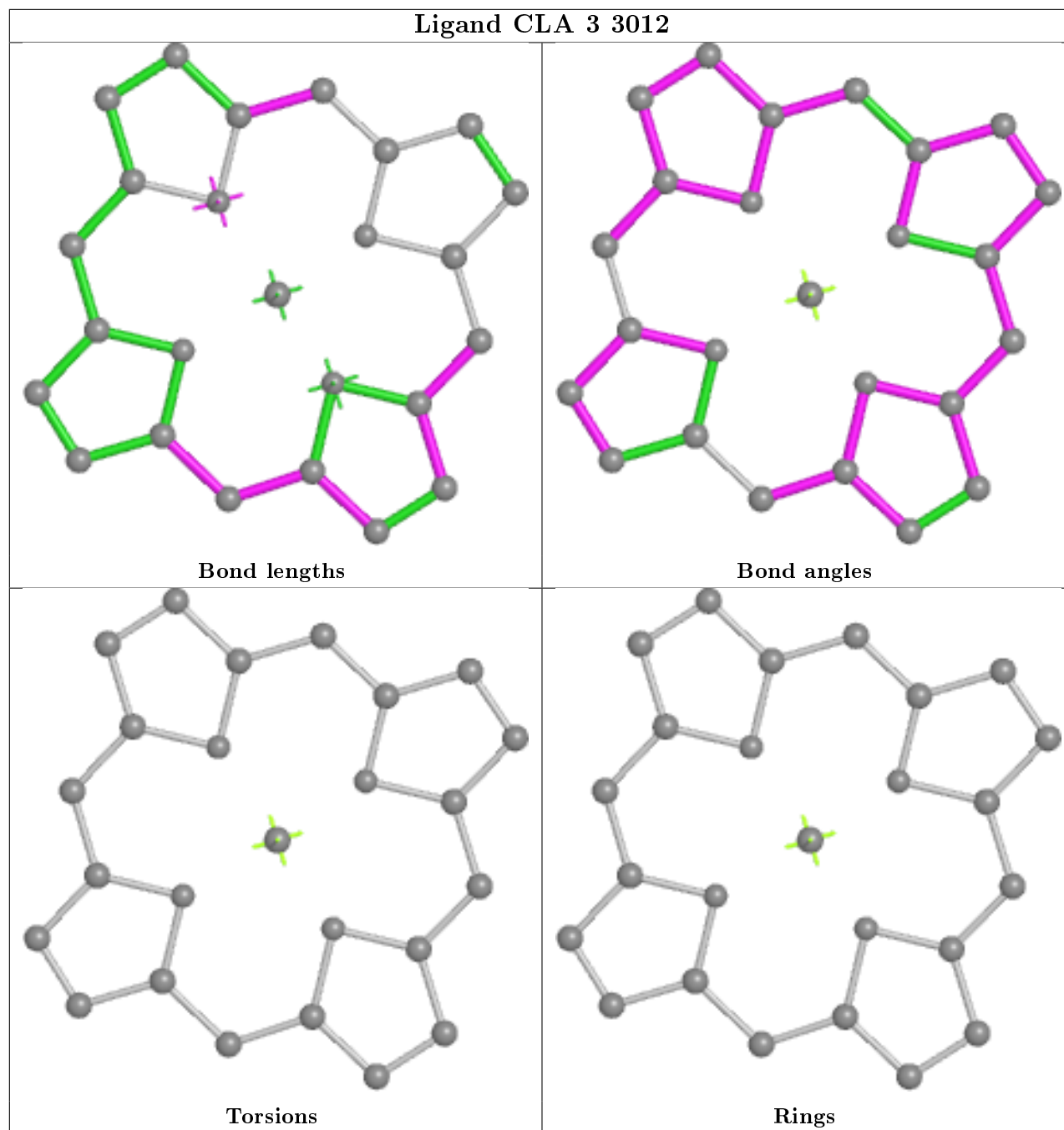
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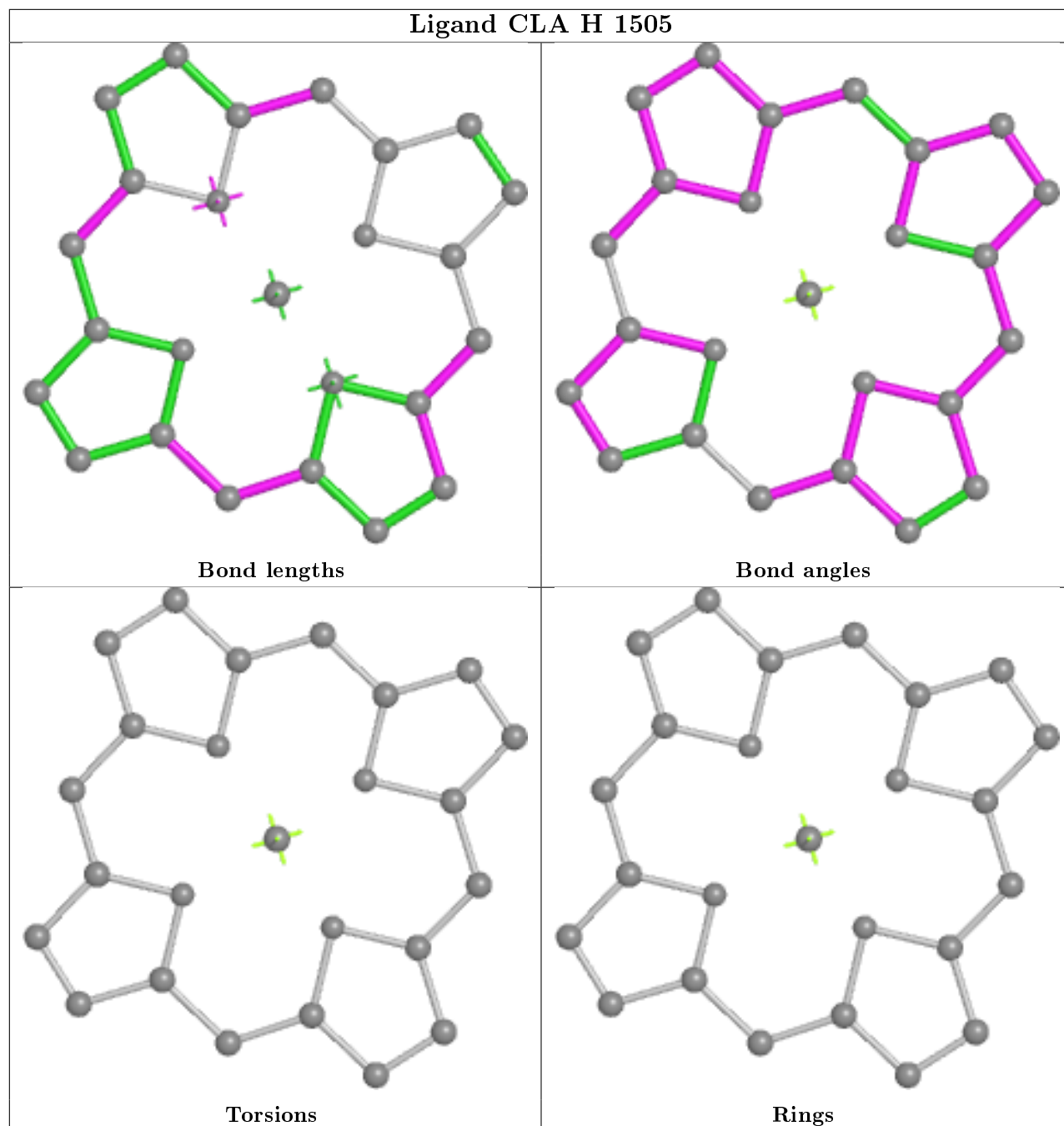
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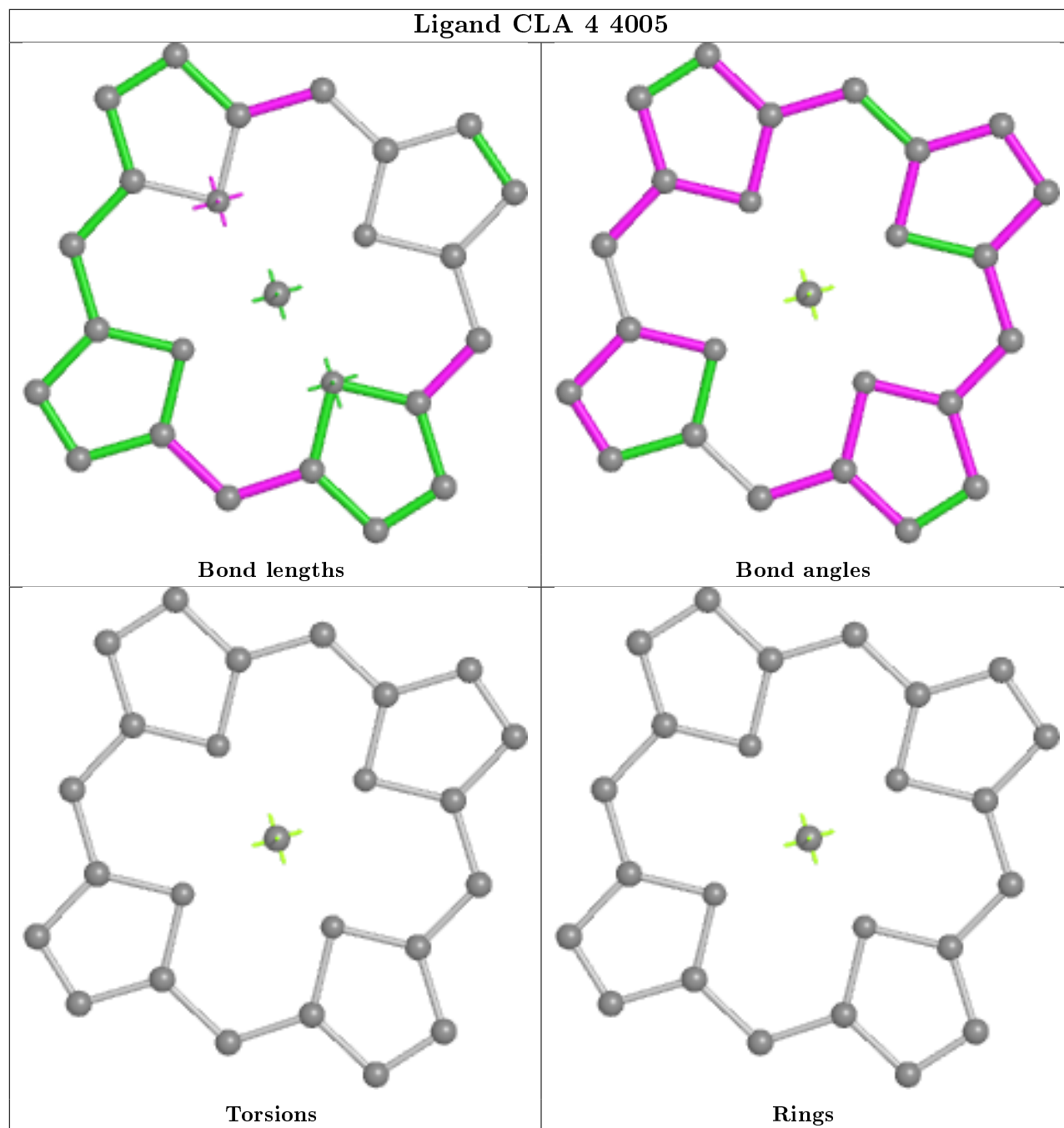




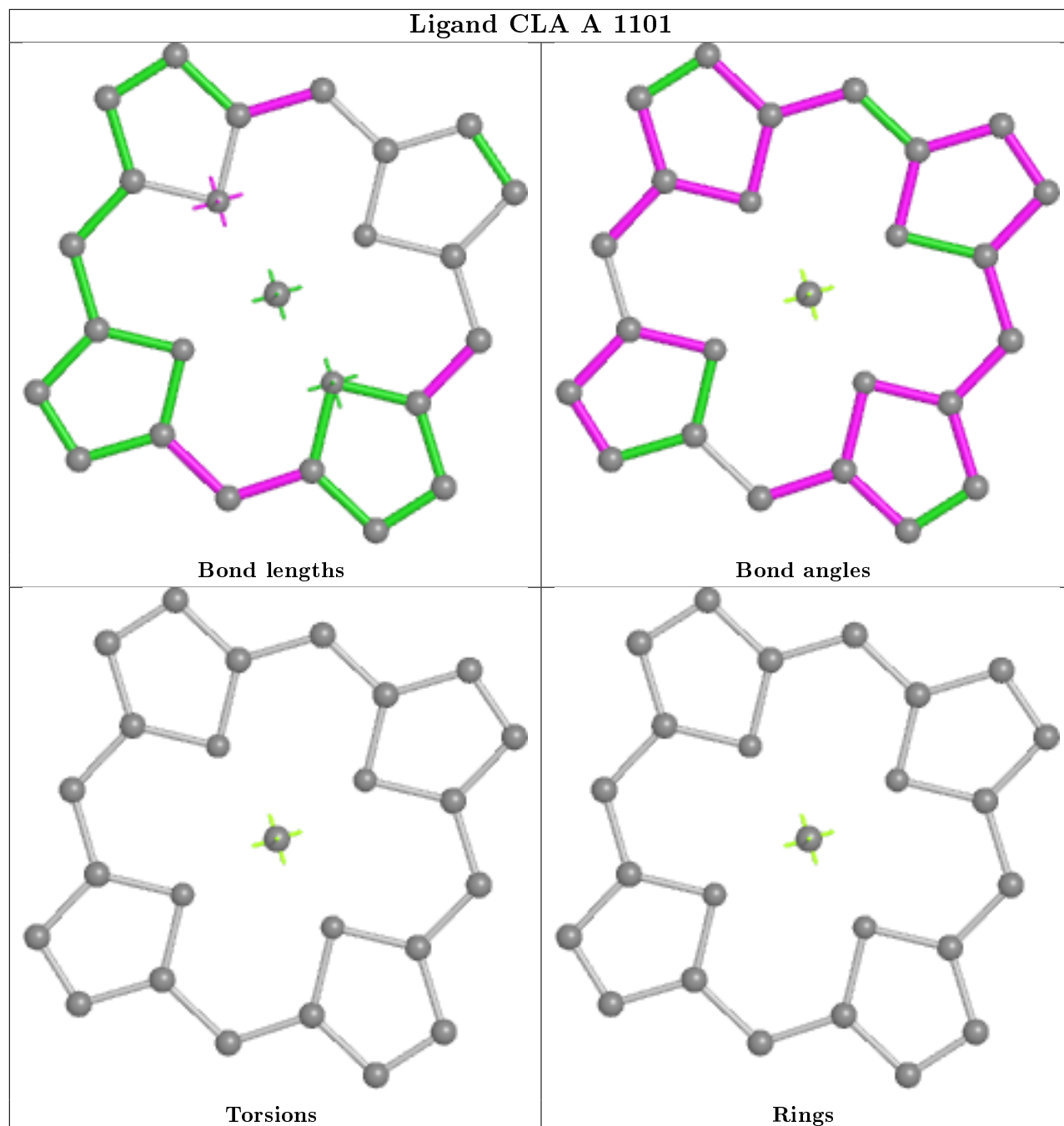


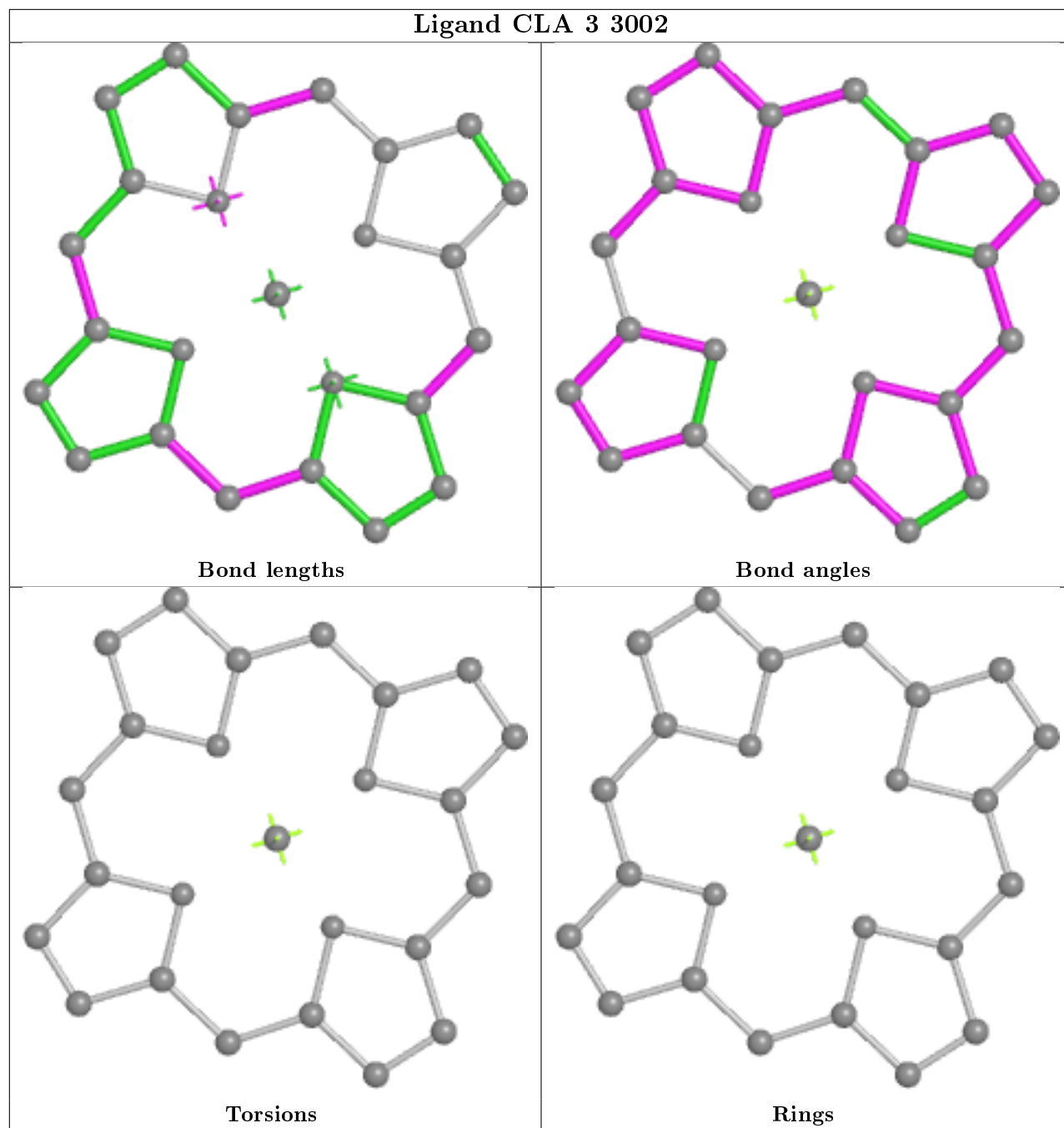
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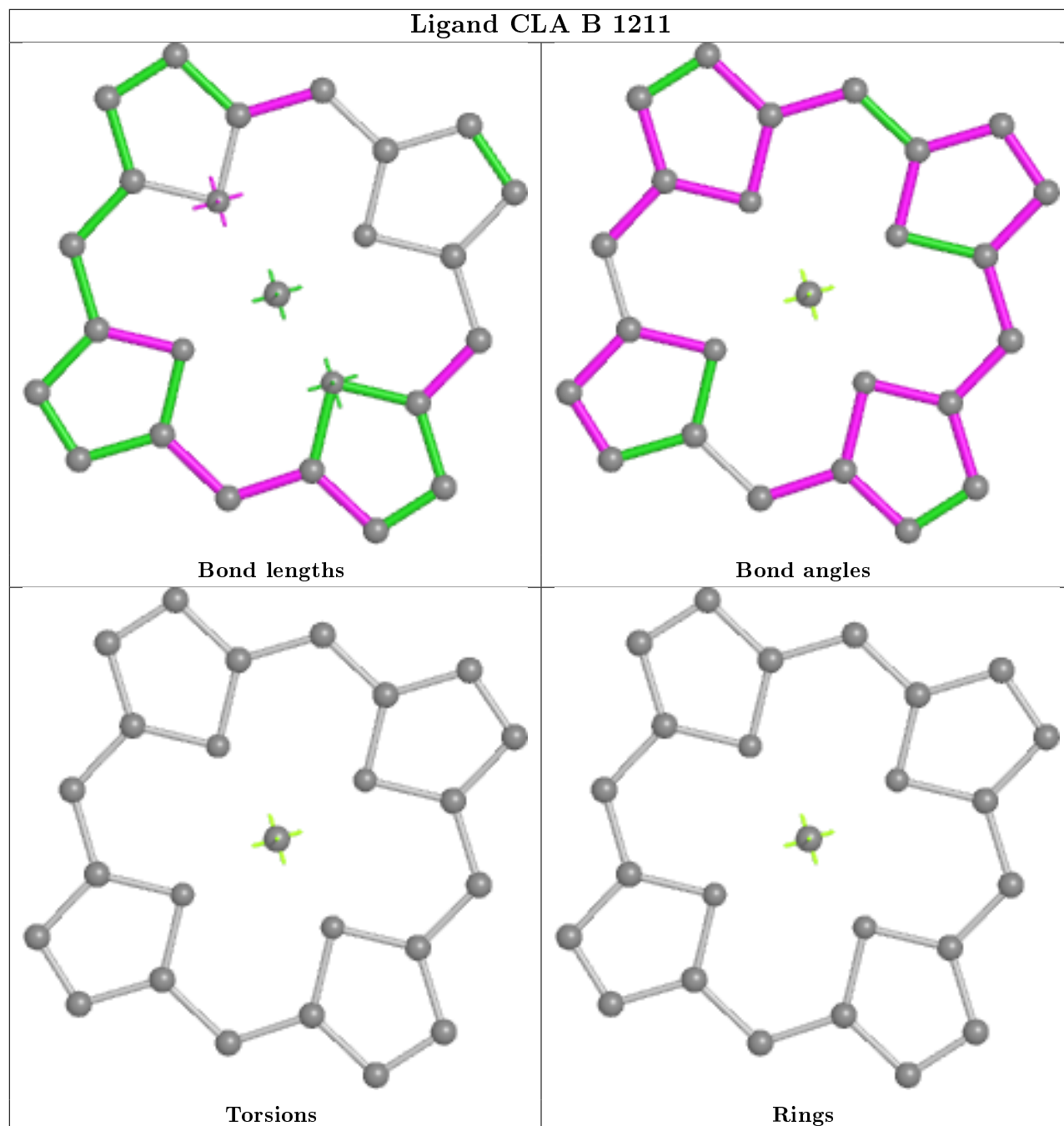


Ligand CLA A 1101

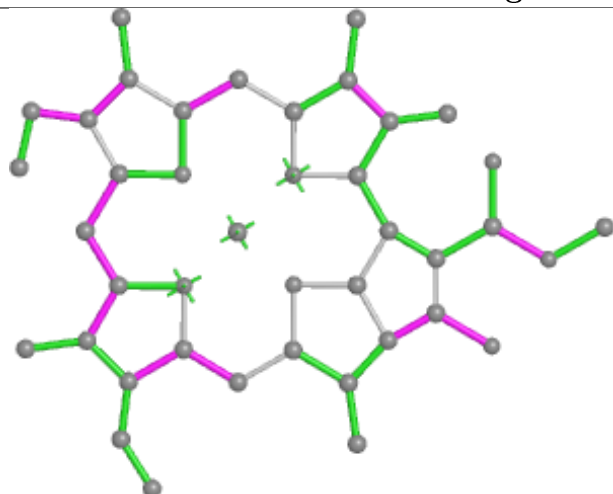




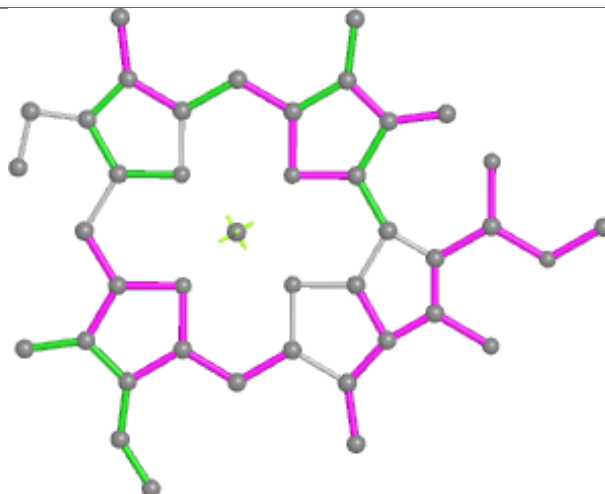
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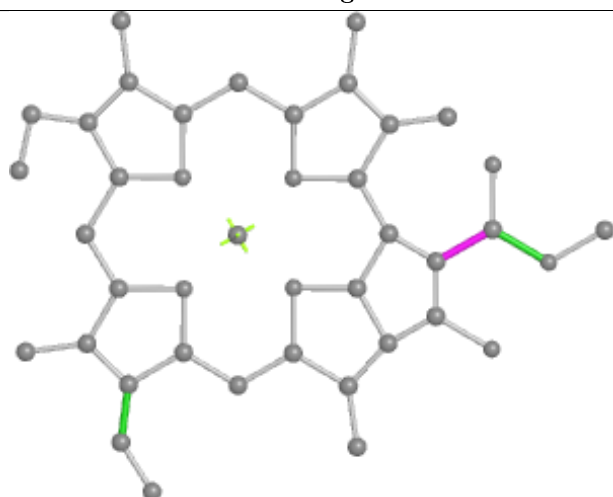
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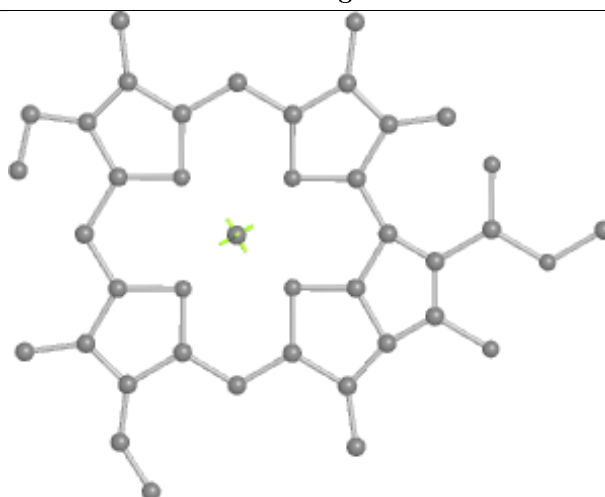
Bond lengths



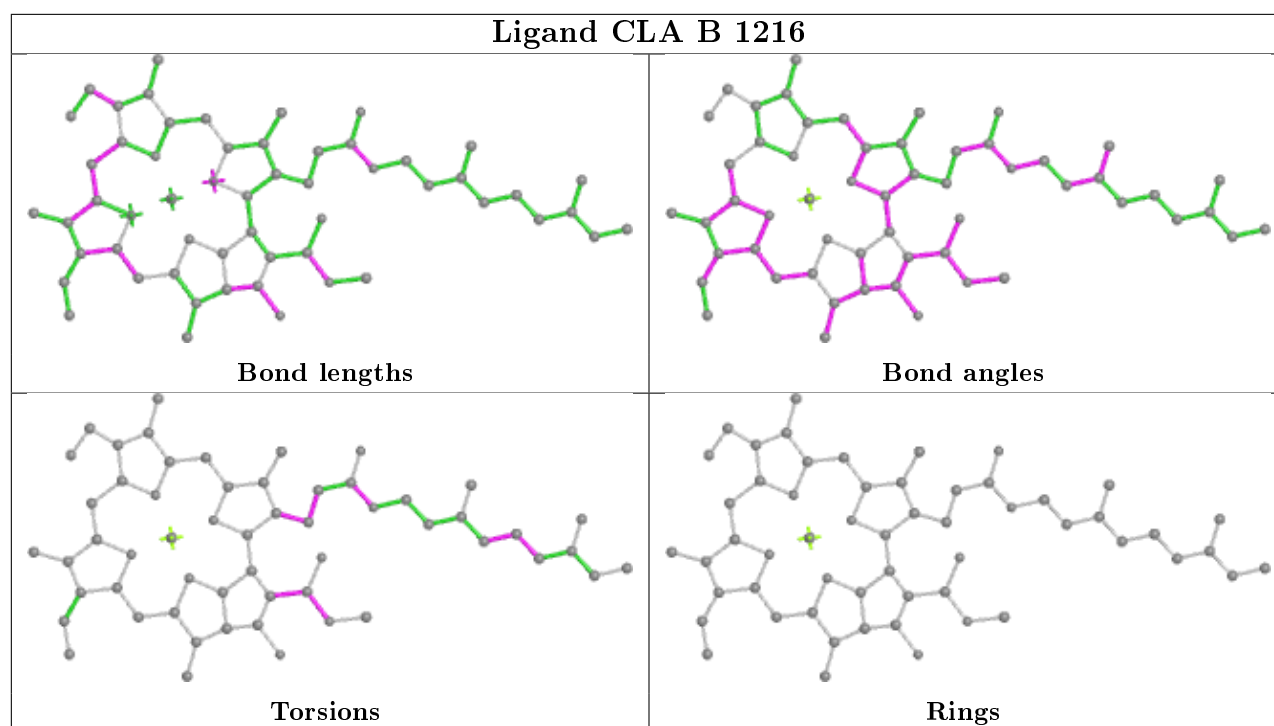
Bond angles

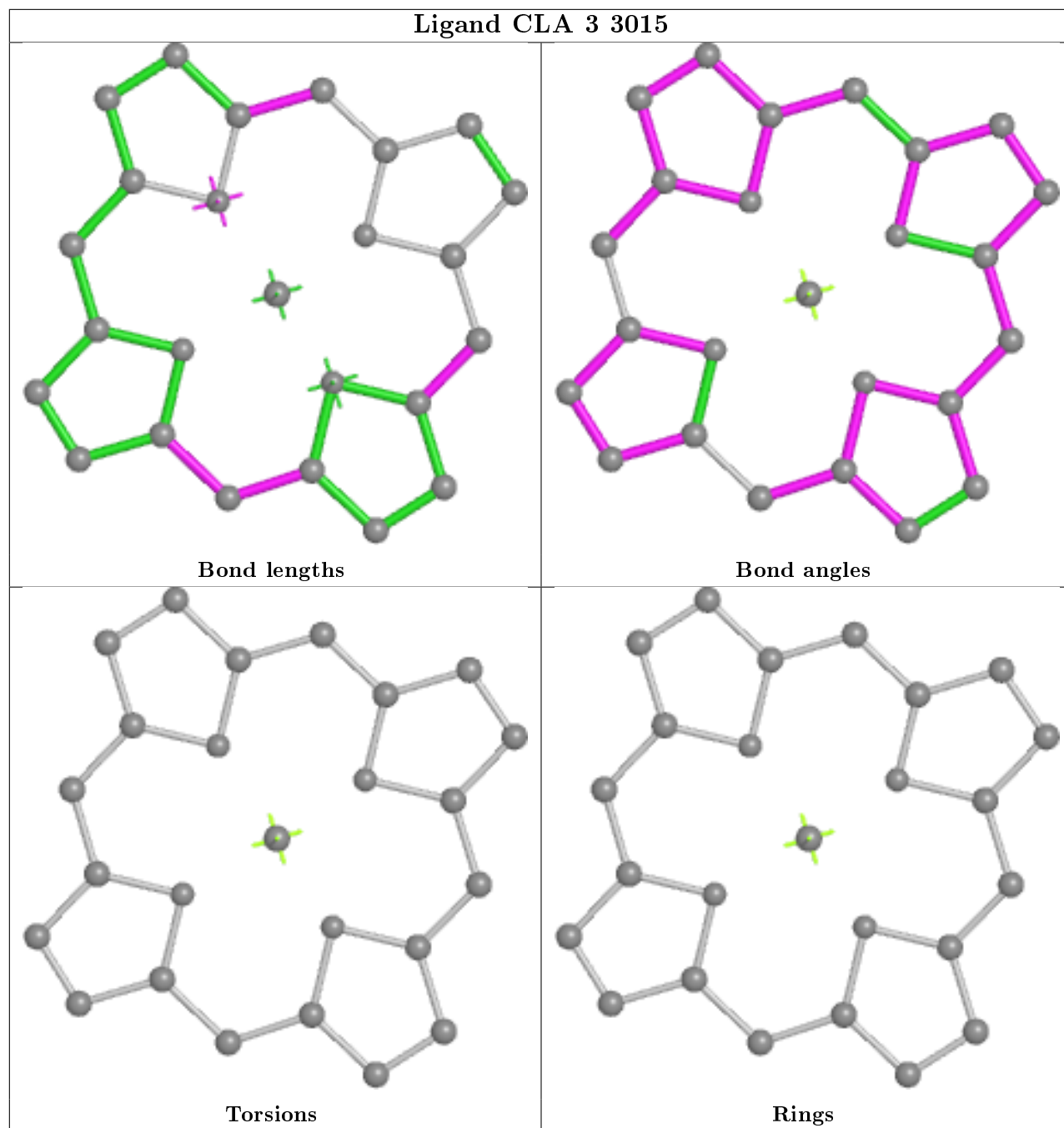


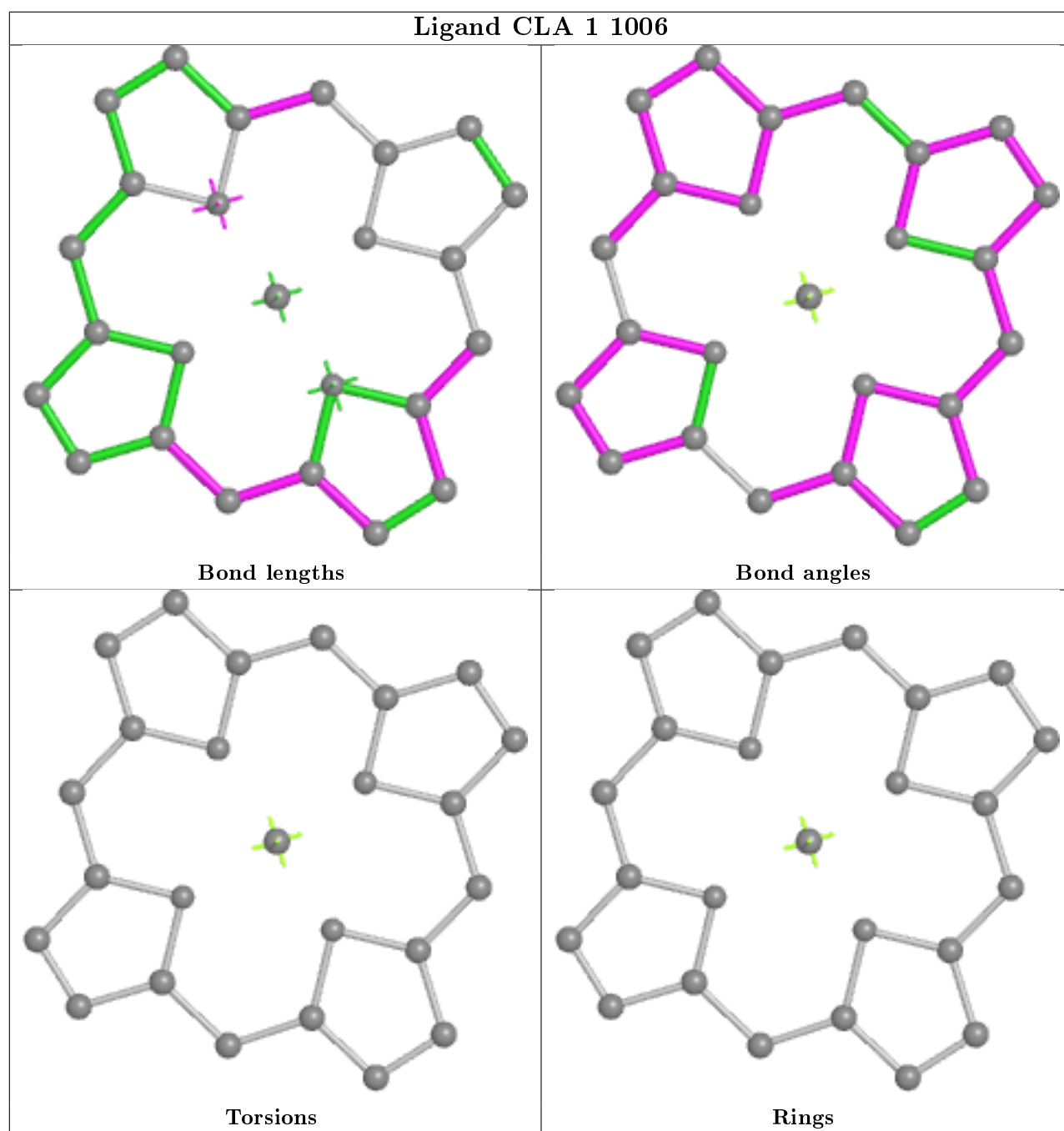
Torsions



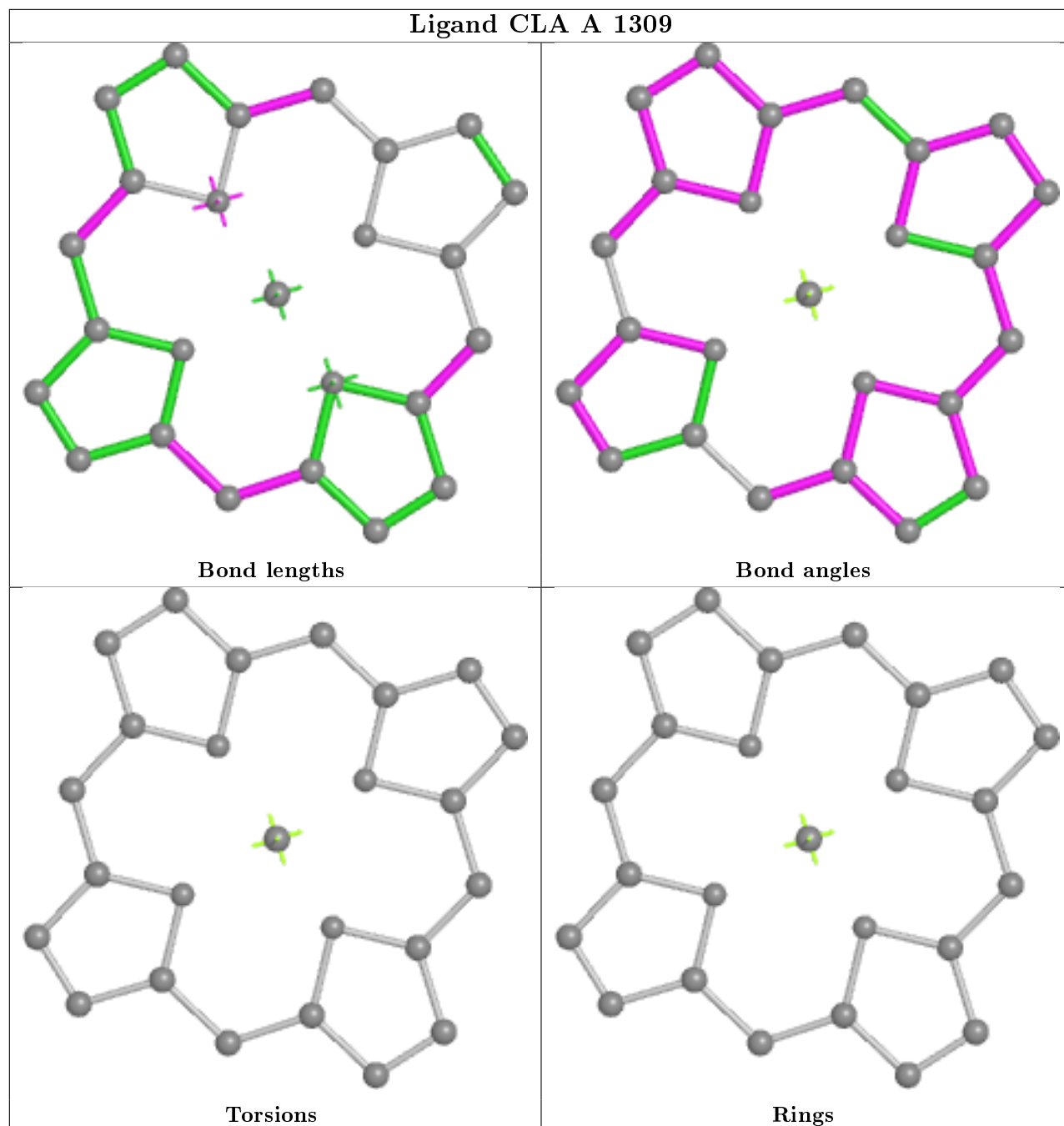
Rings

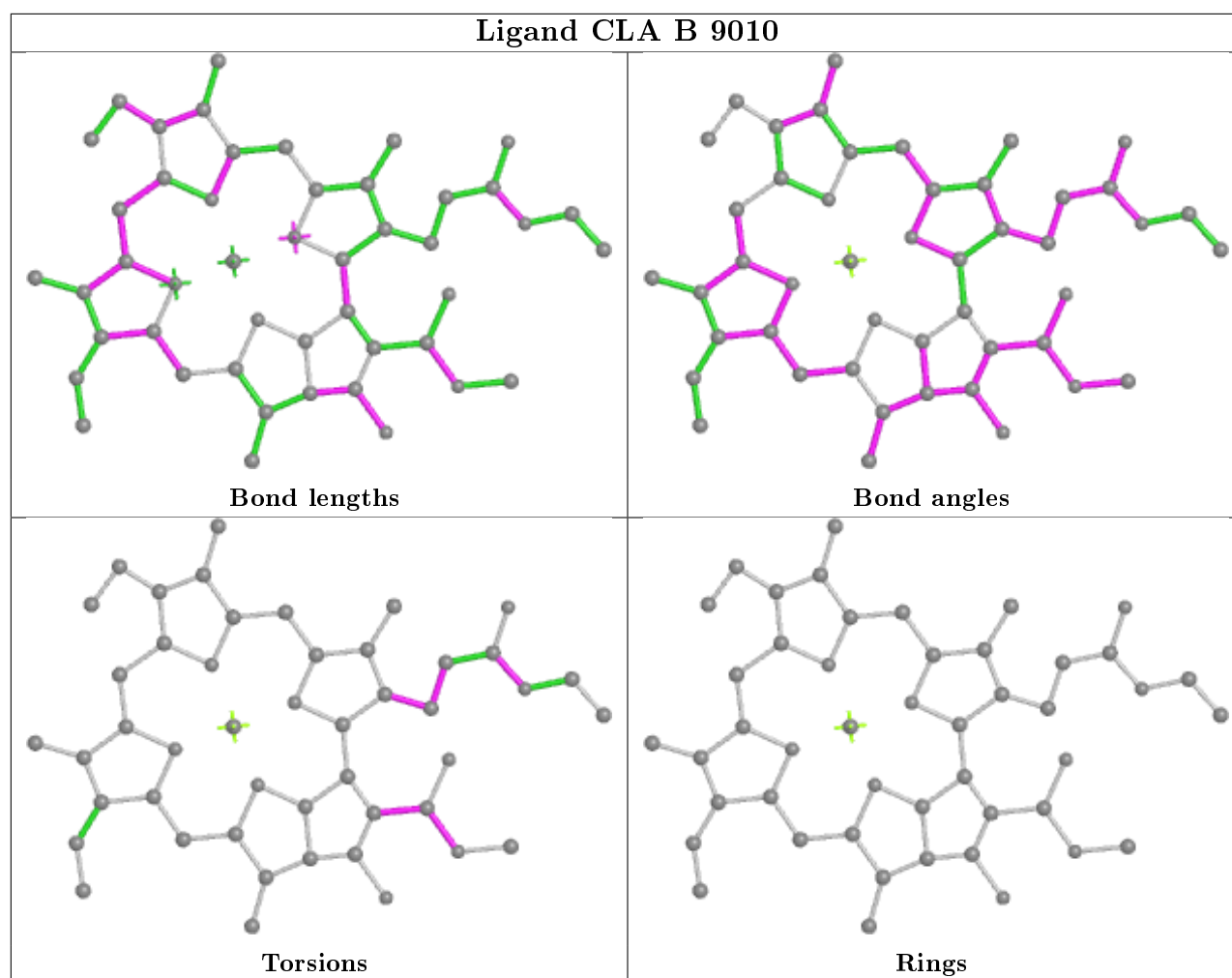




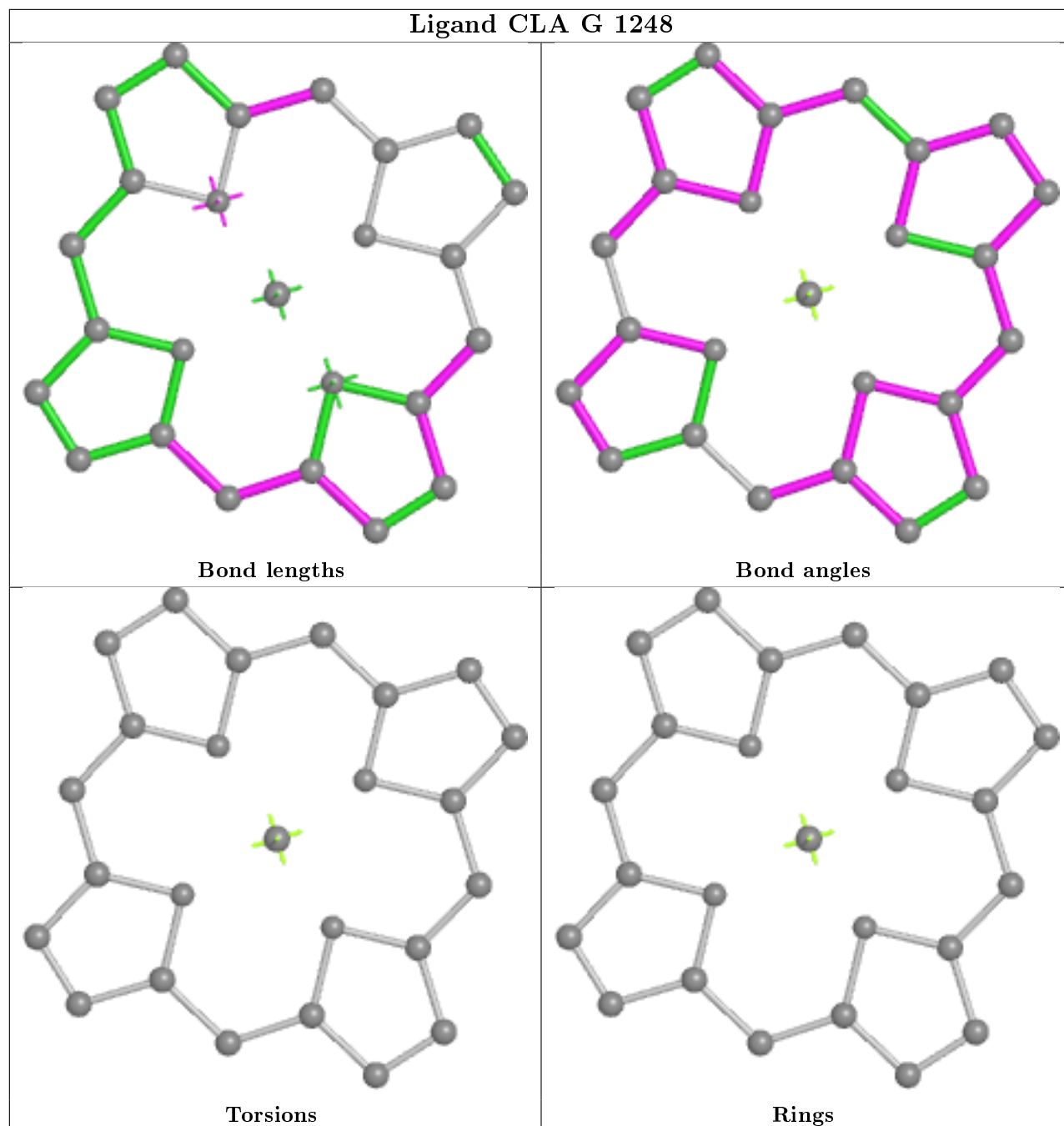


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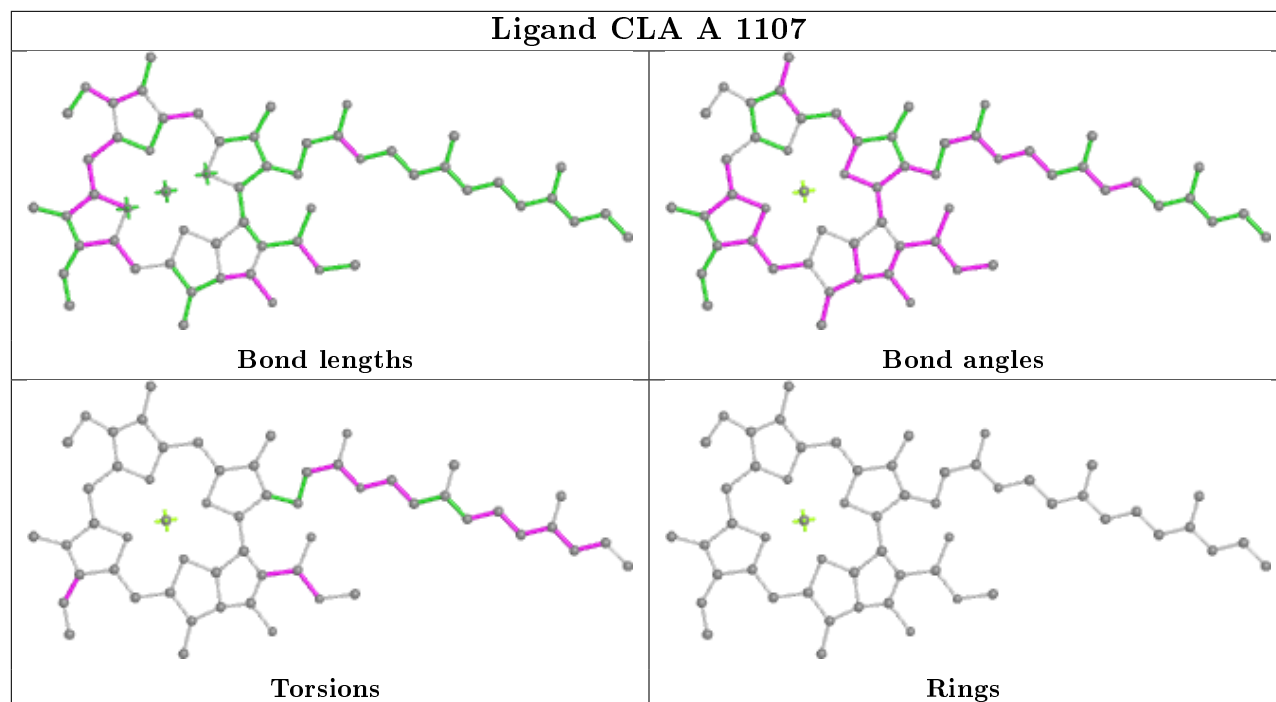




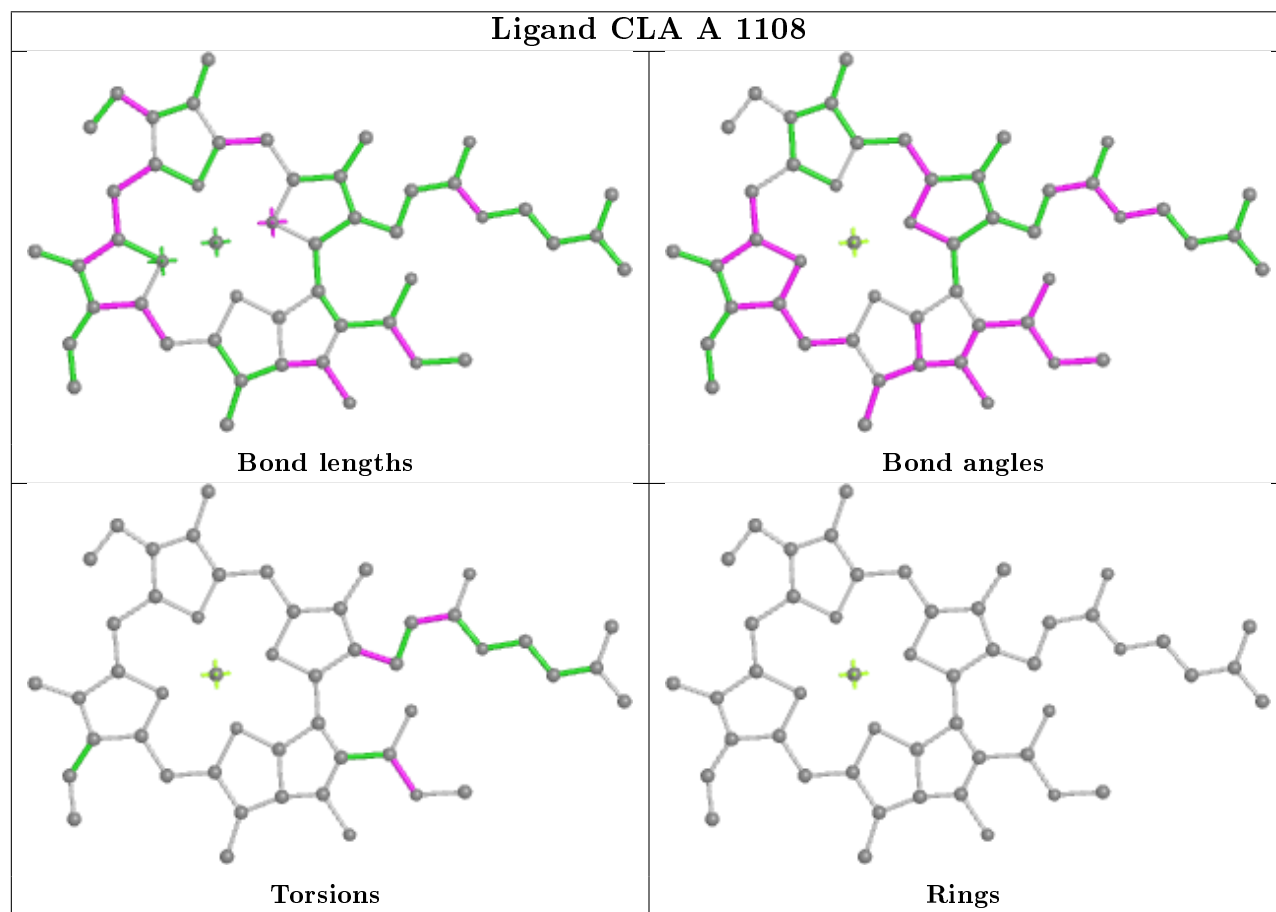
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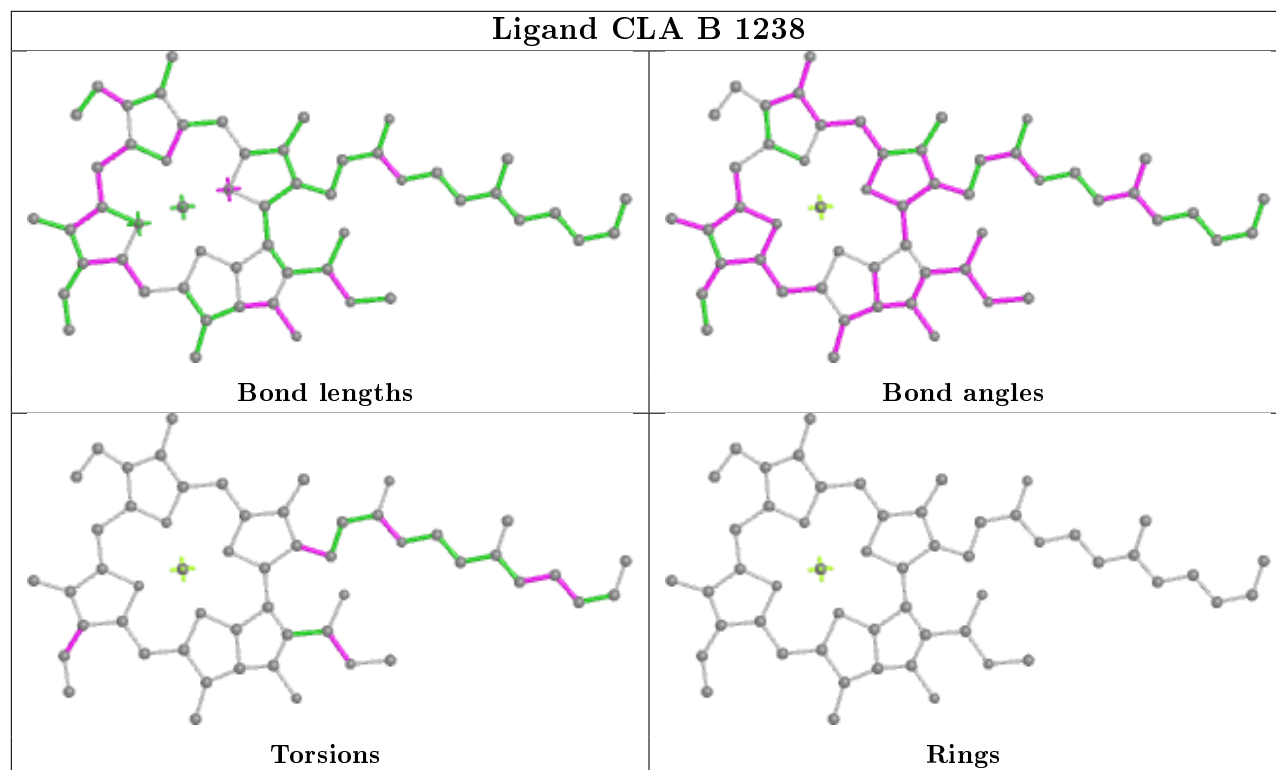
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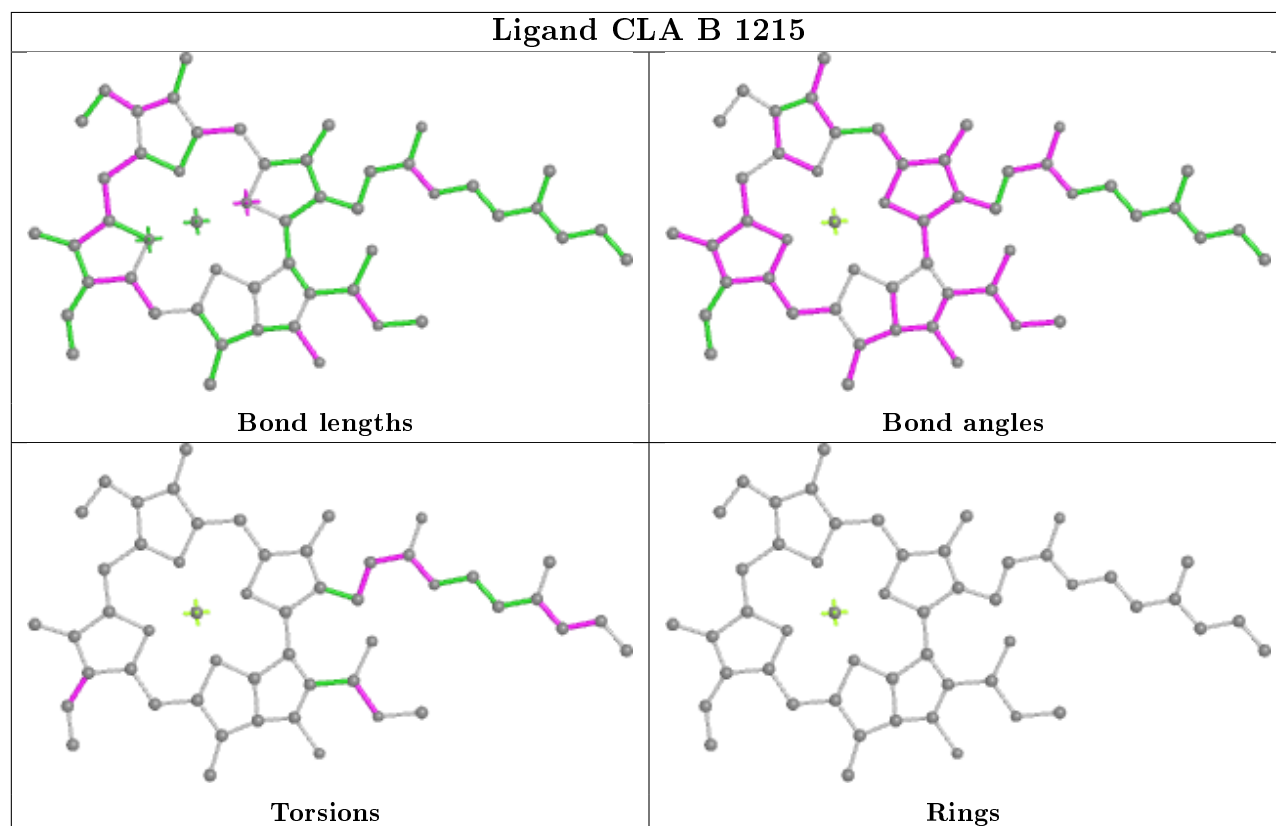
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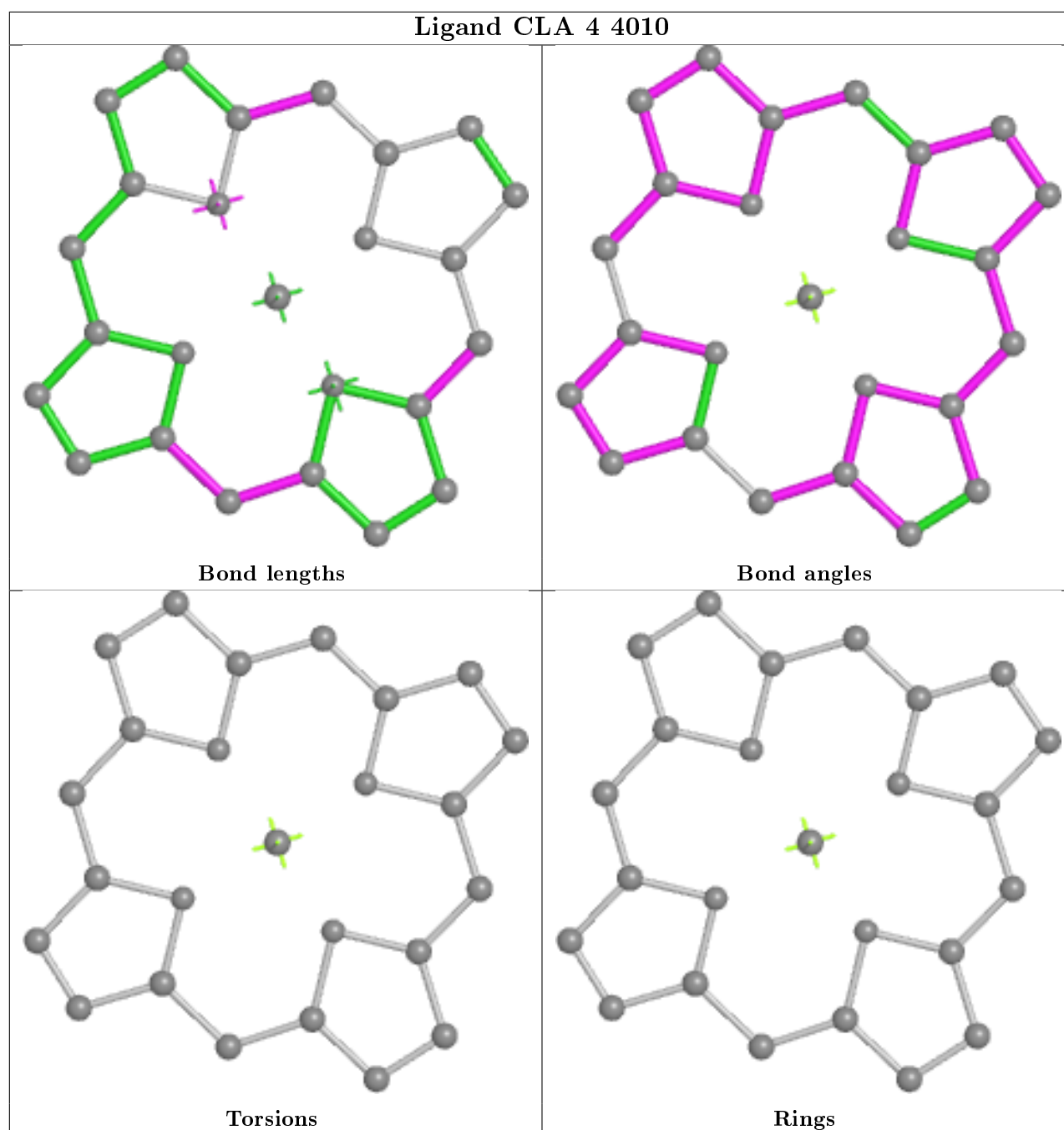


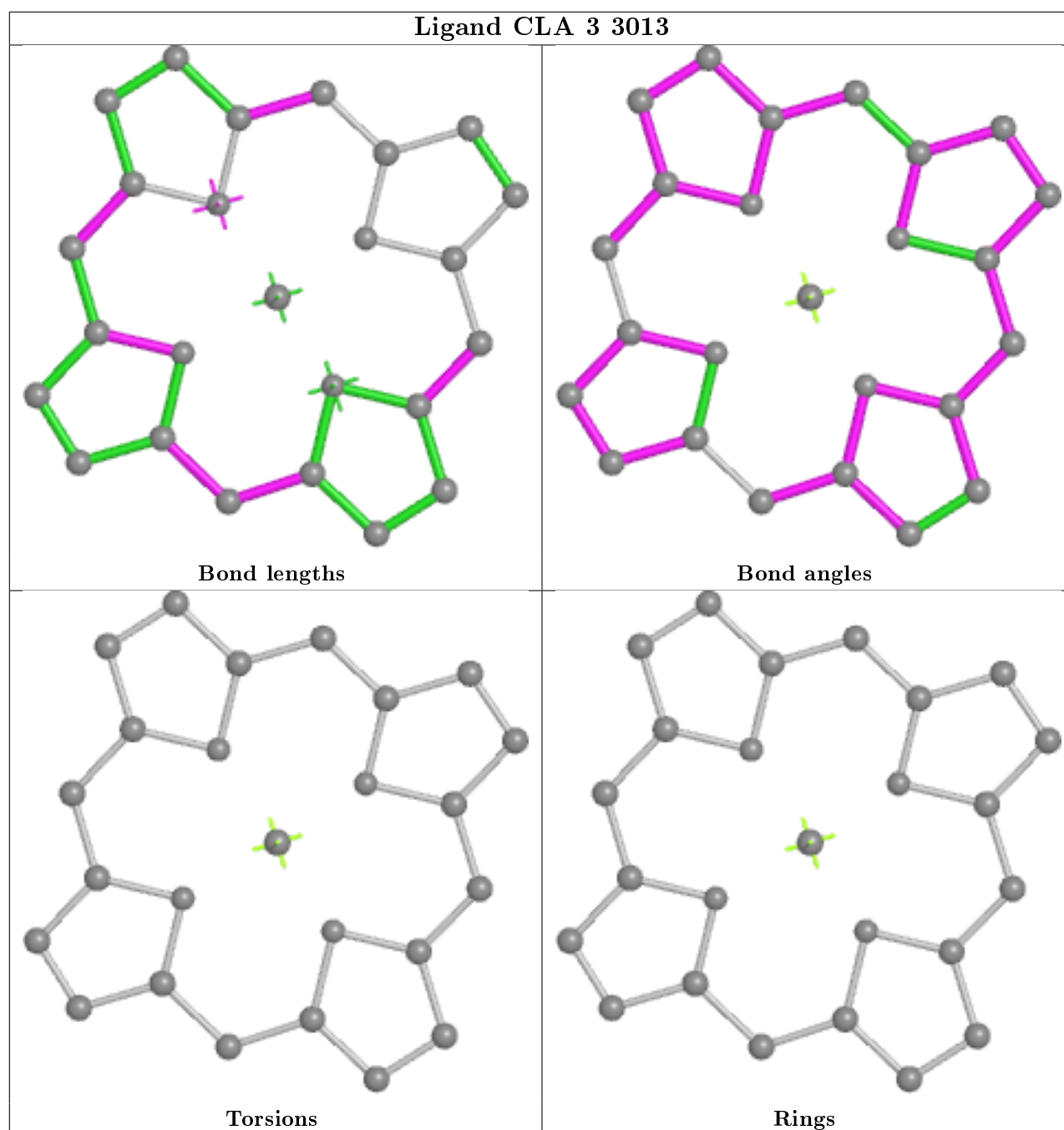
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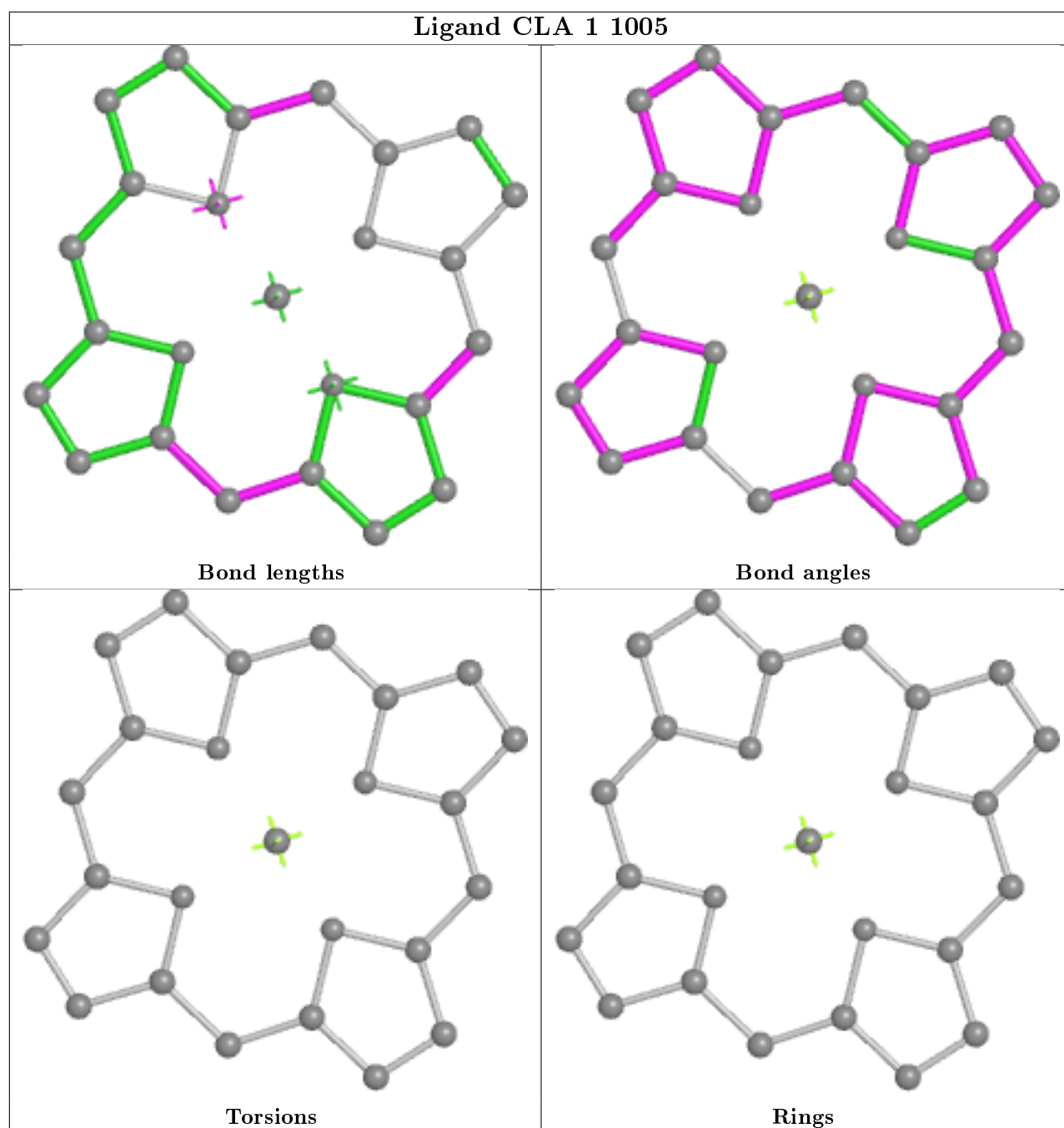


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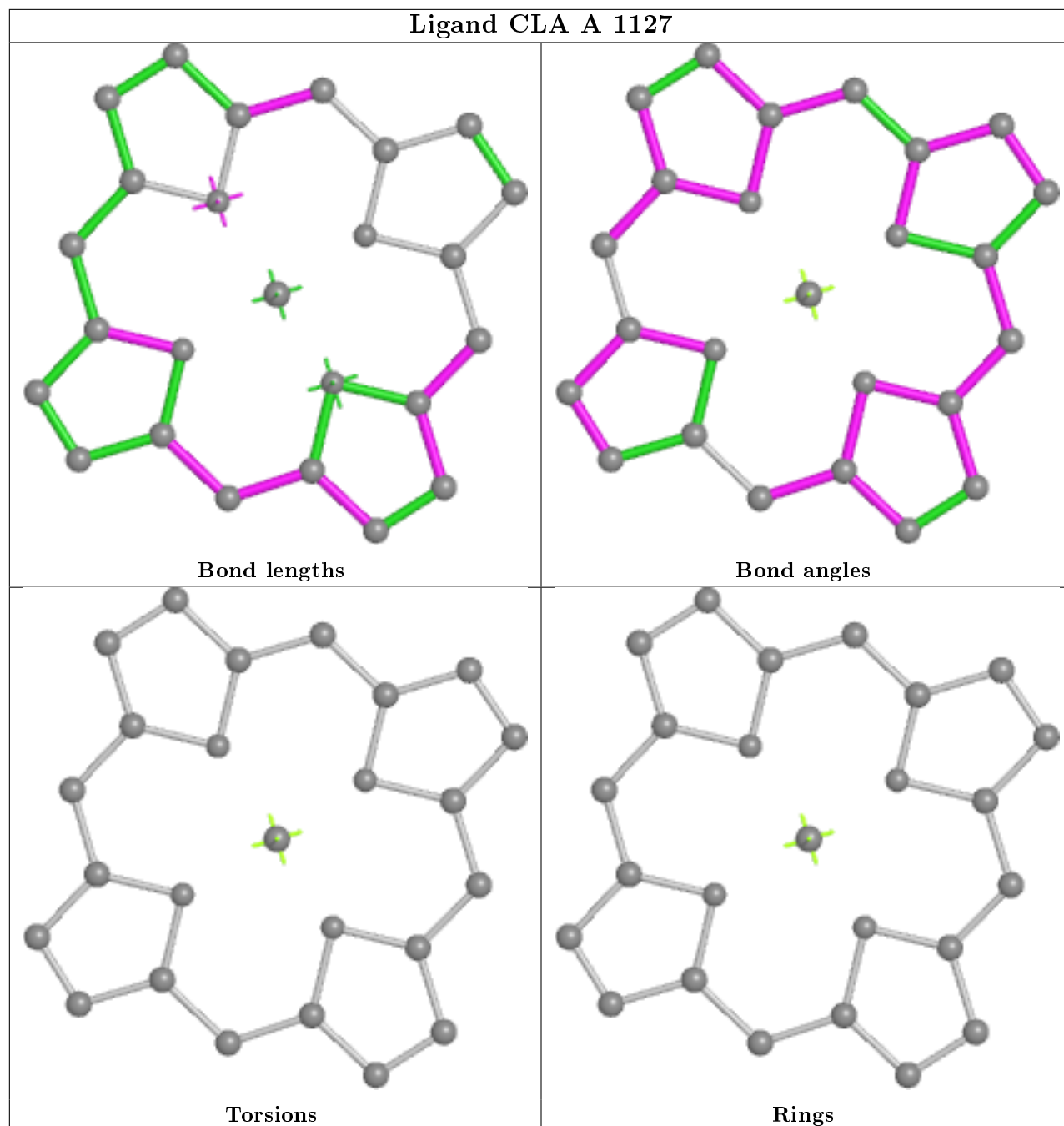


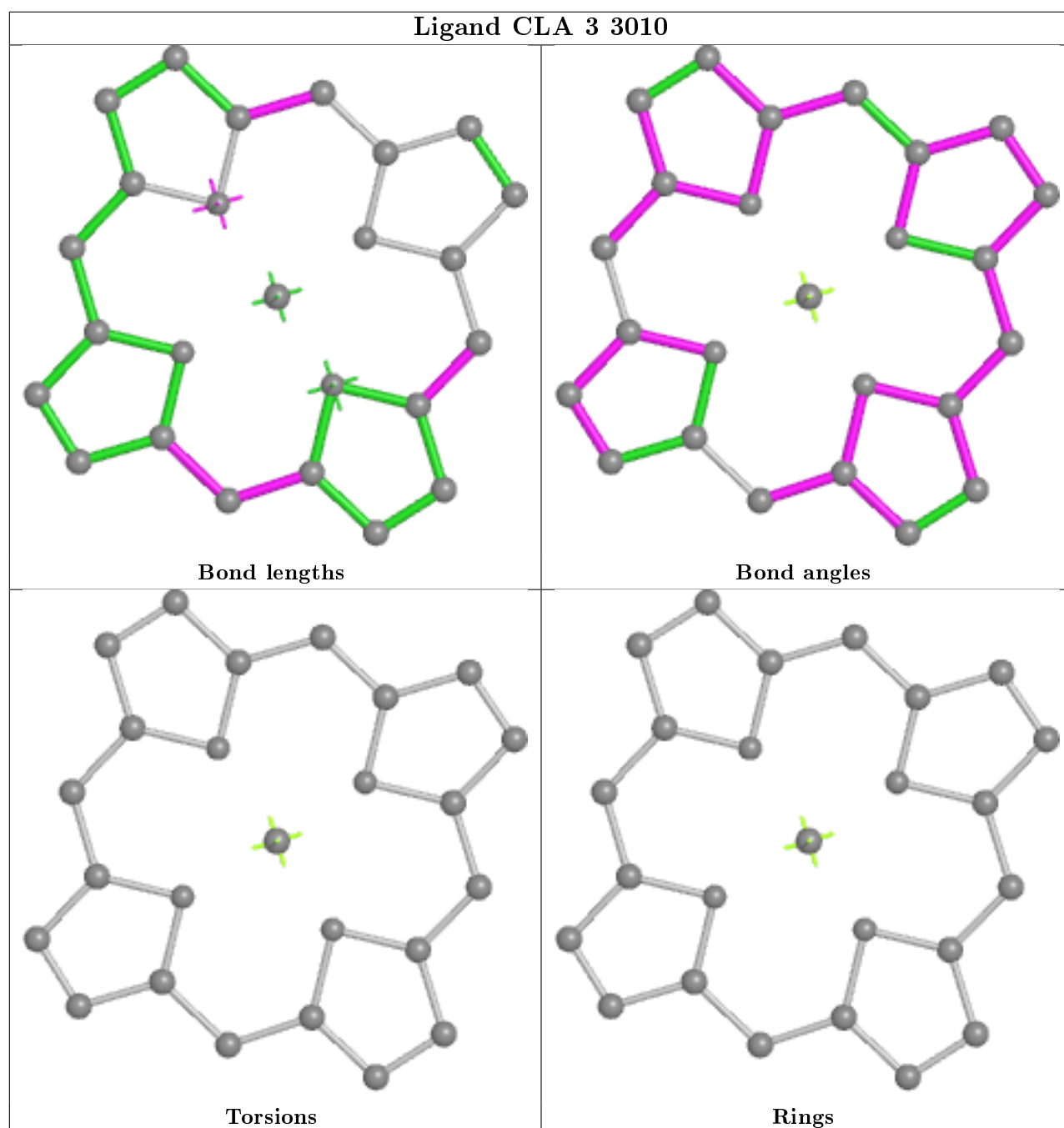


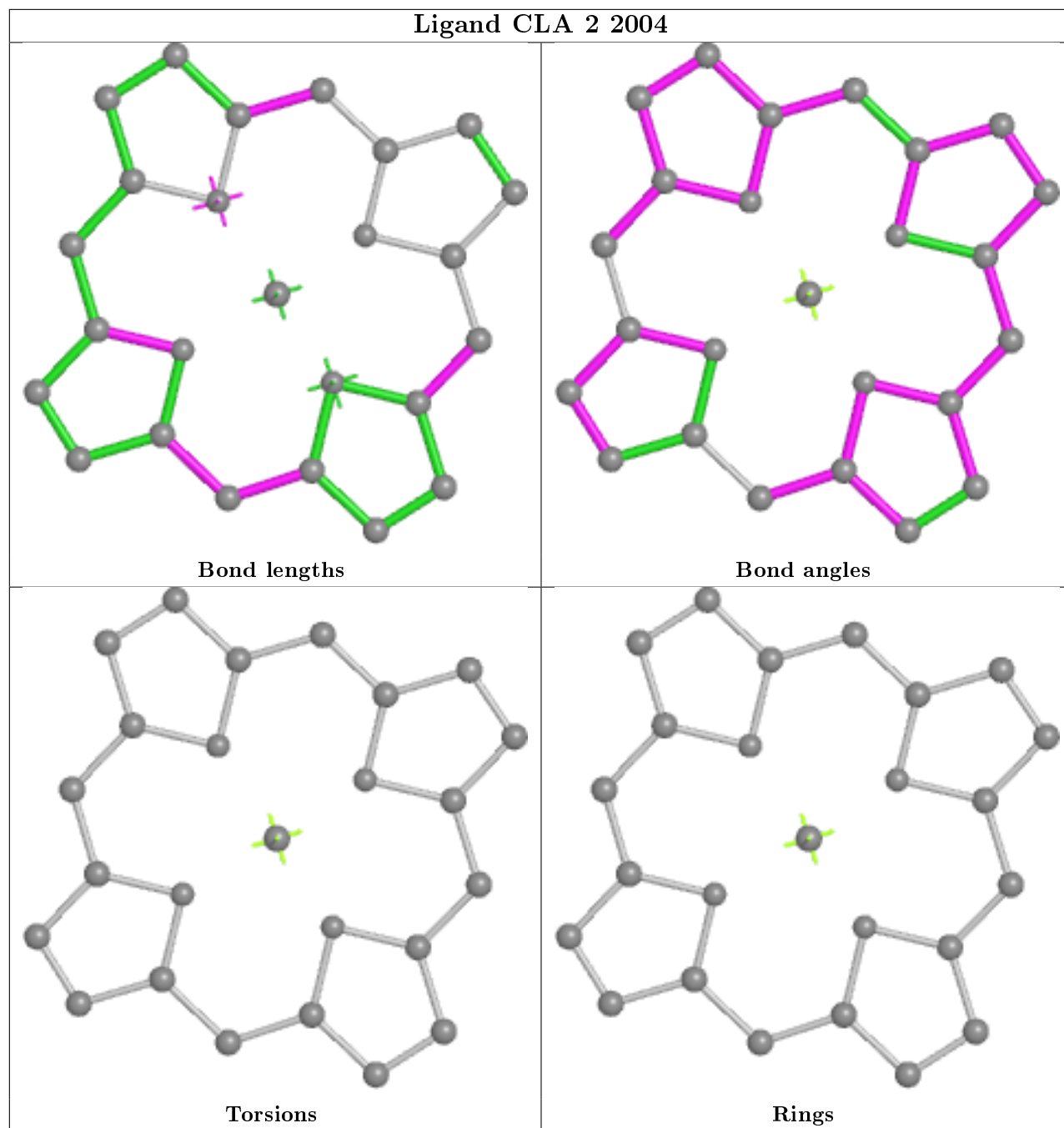


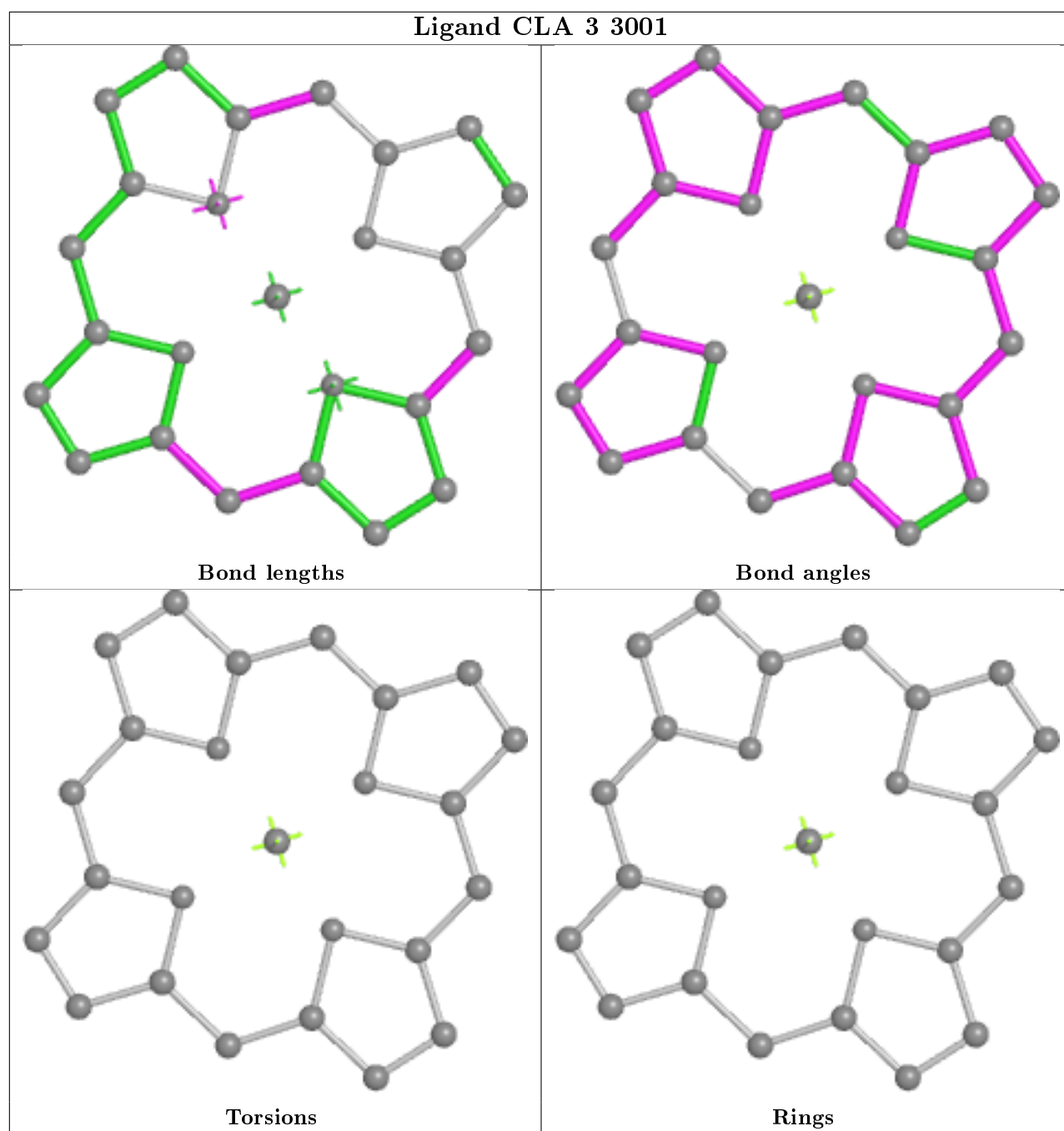


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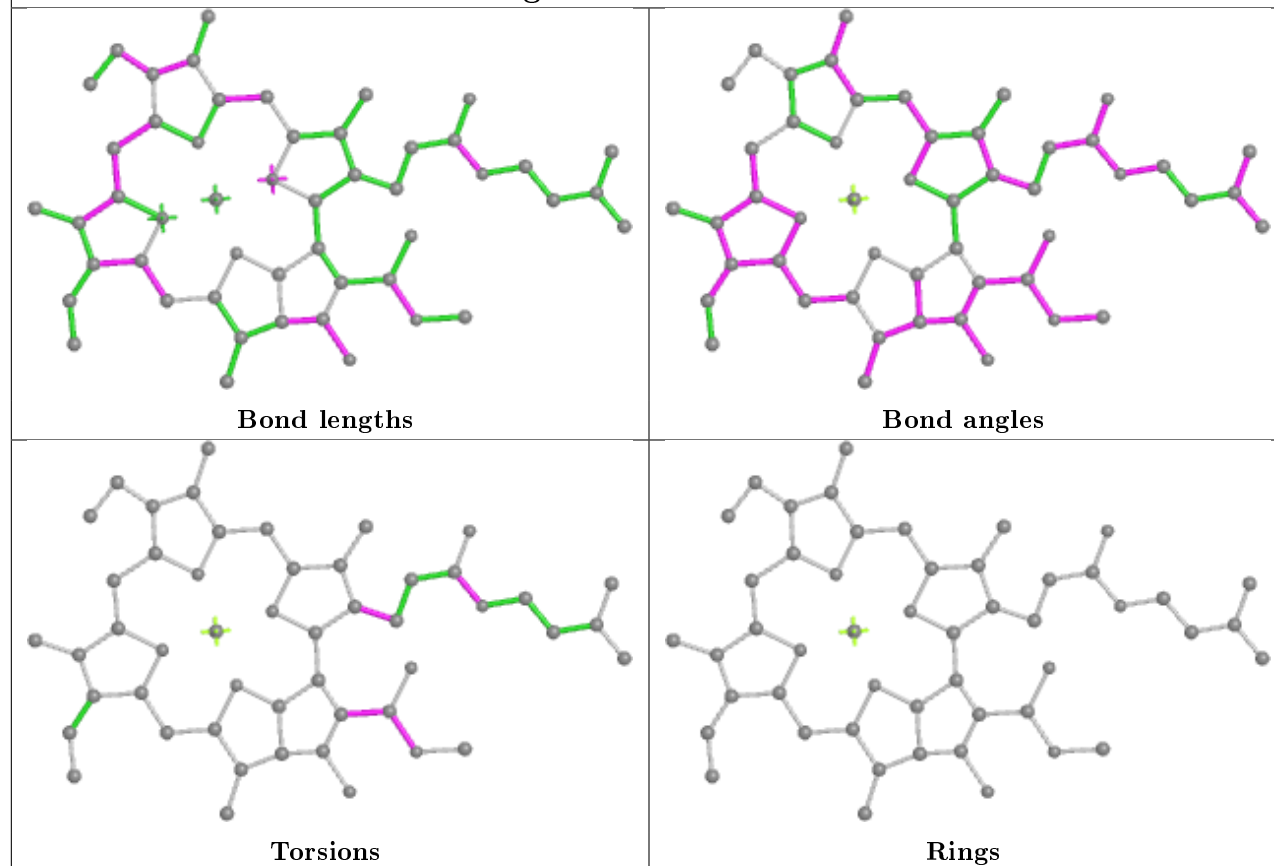




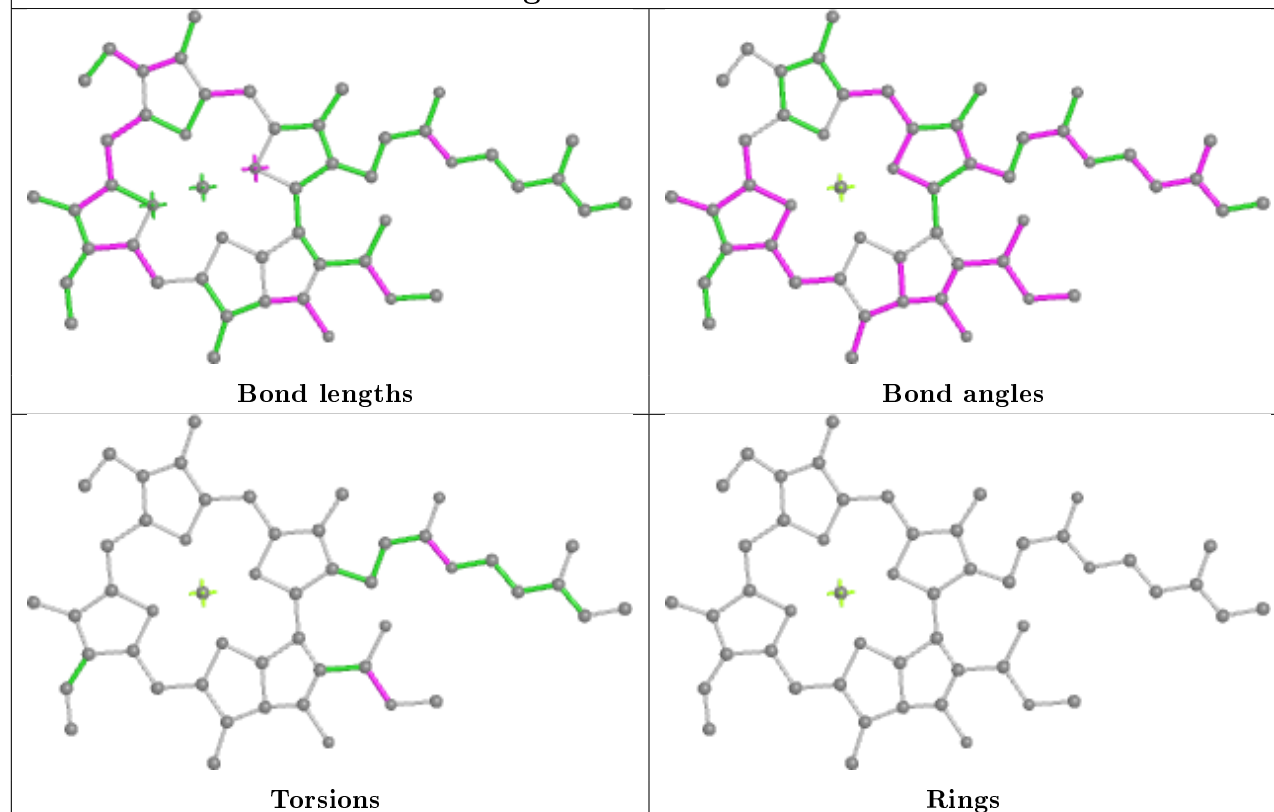


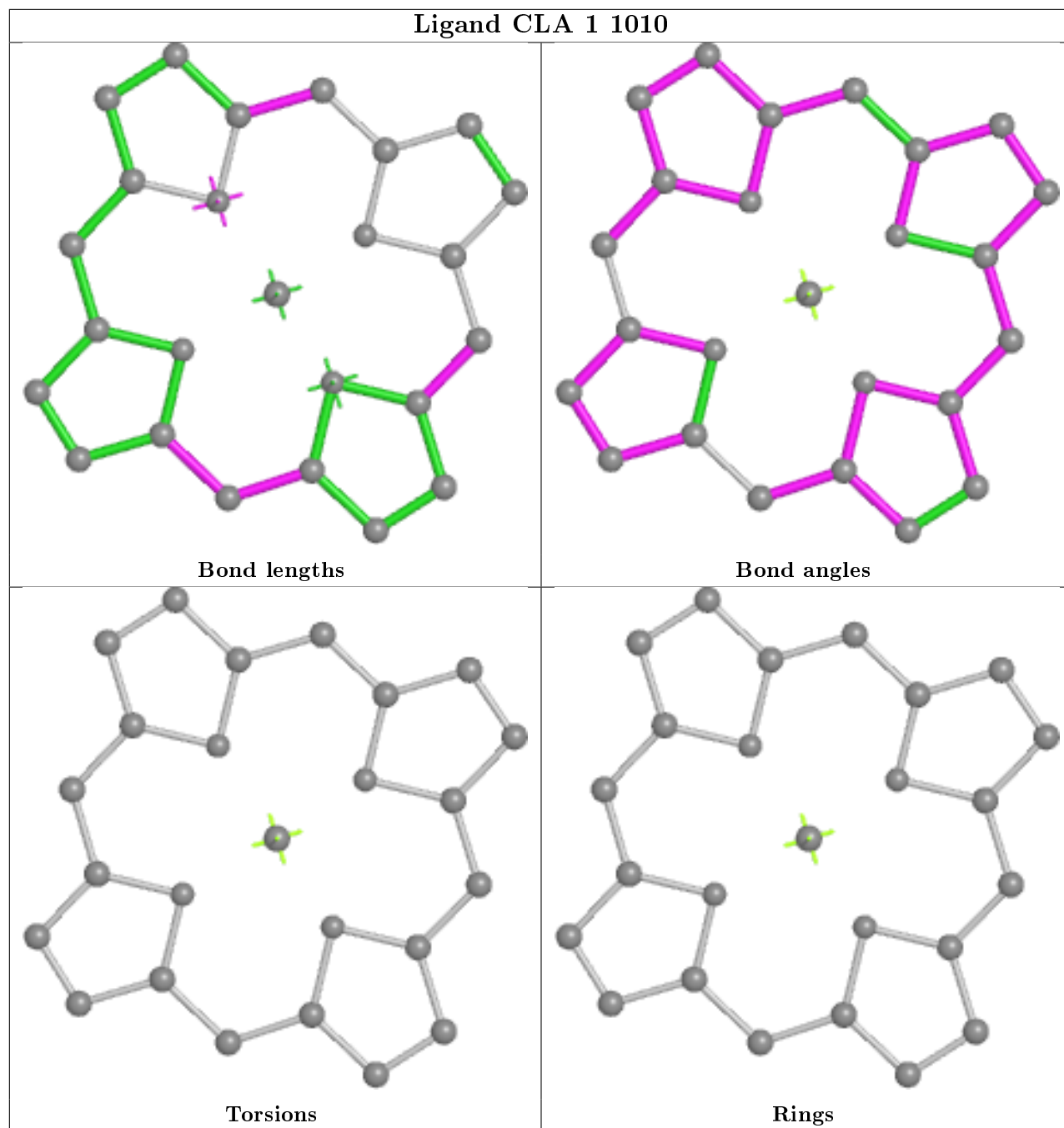


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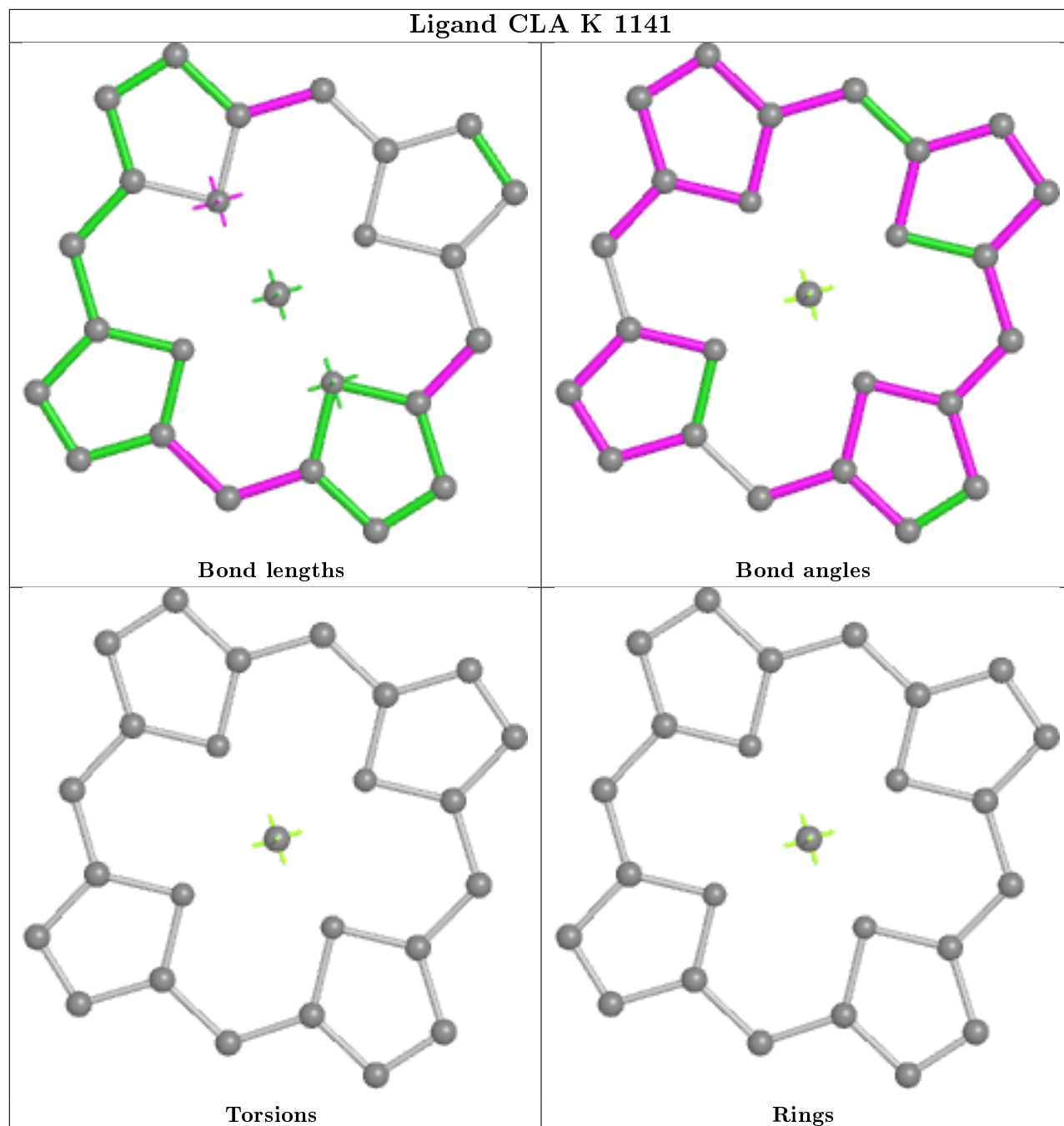


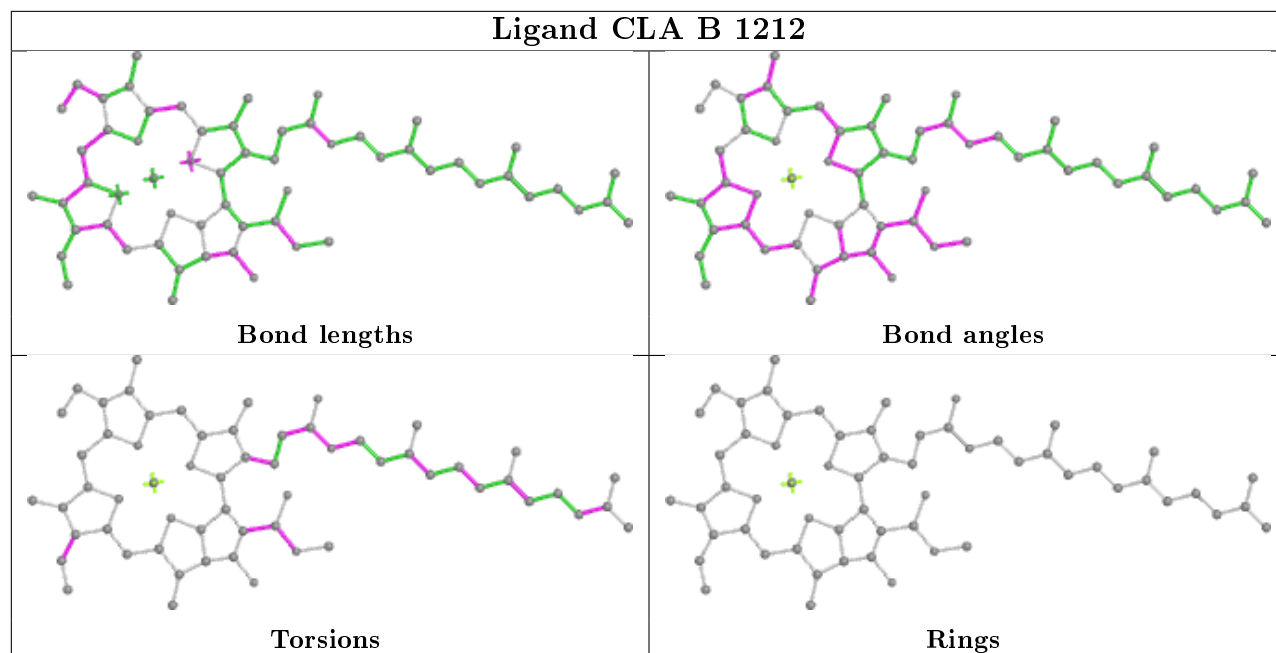
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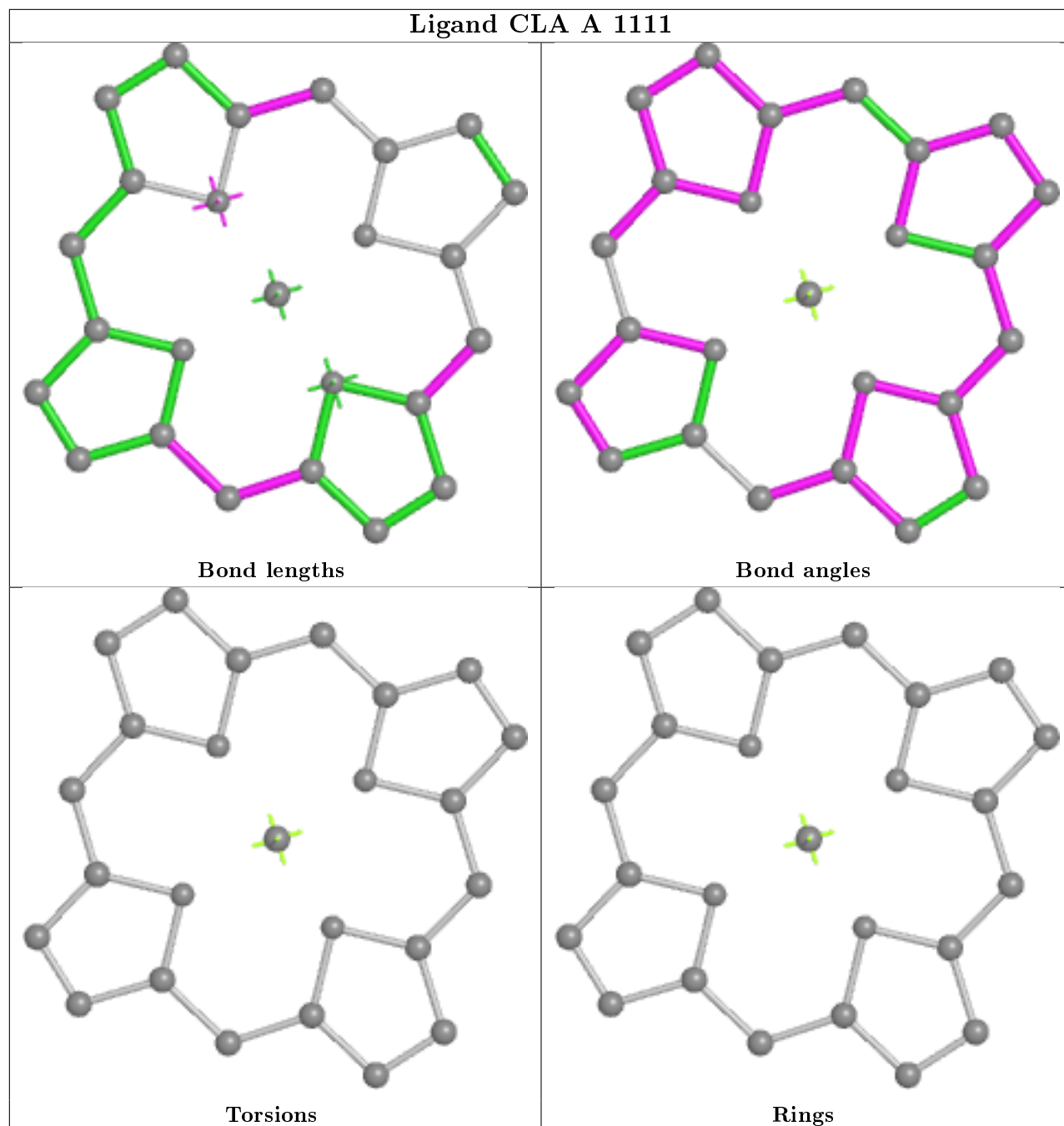


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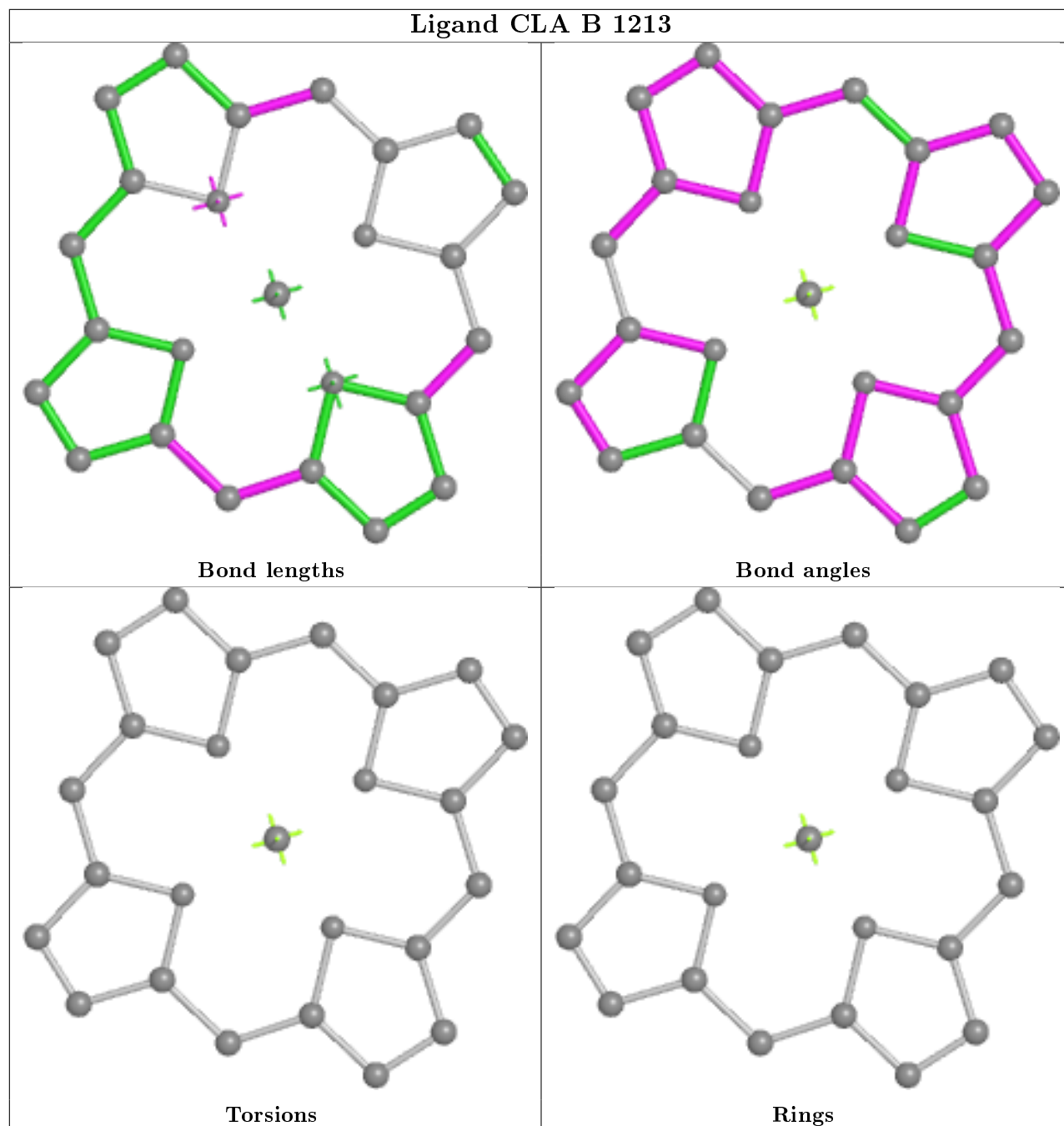


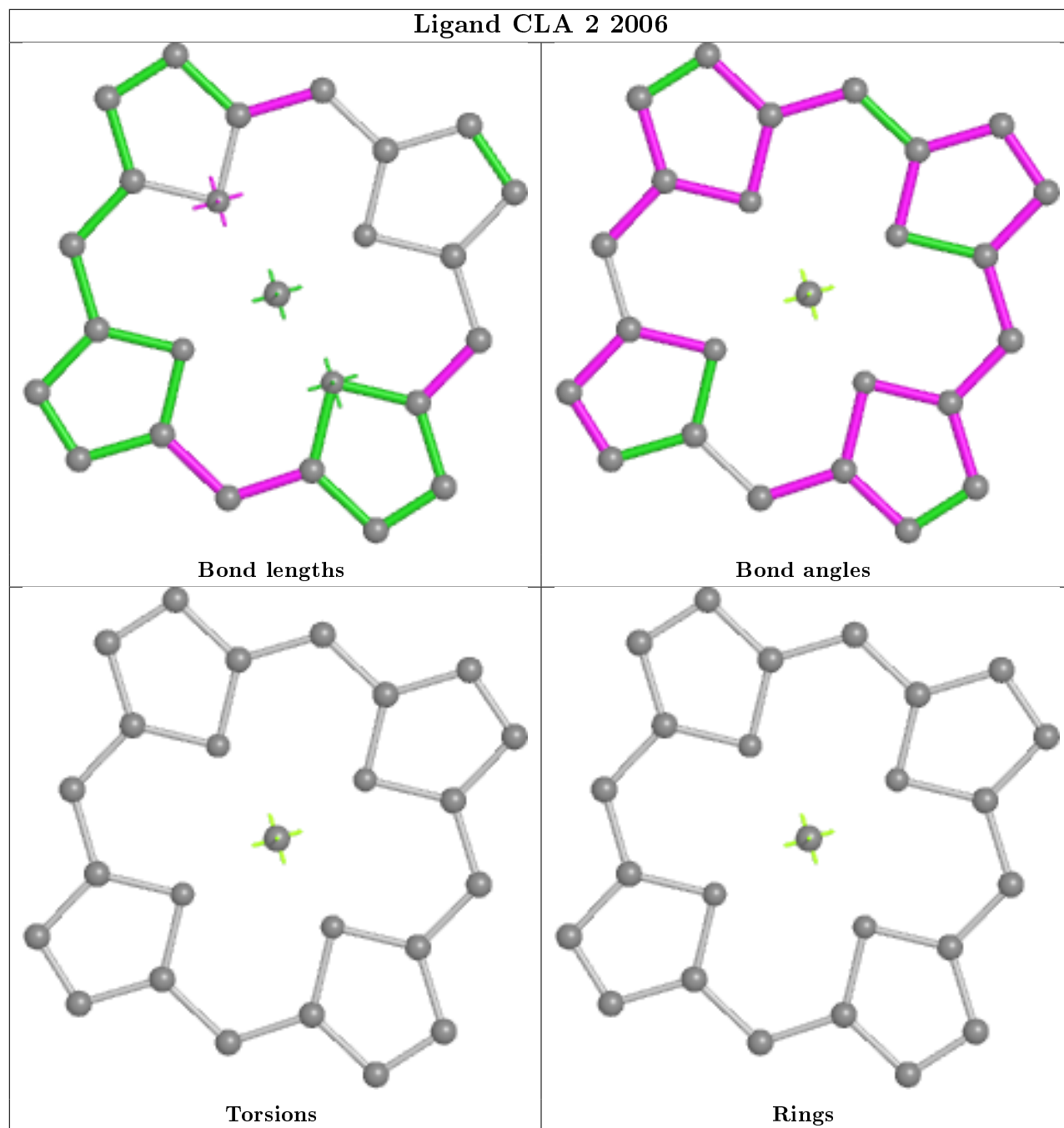


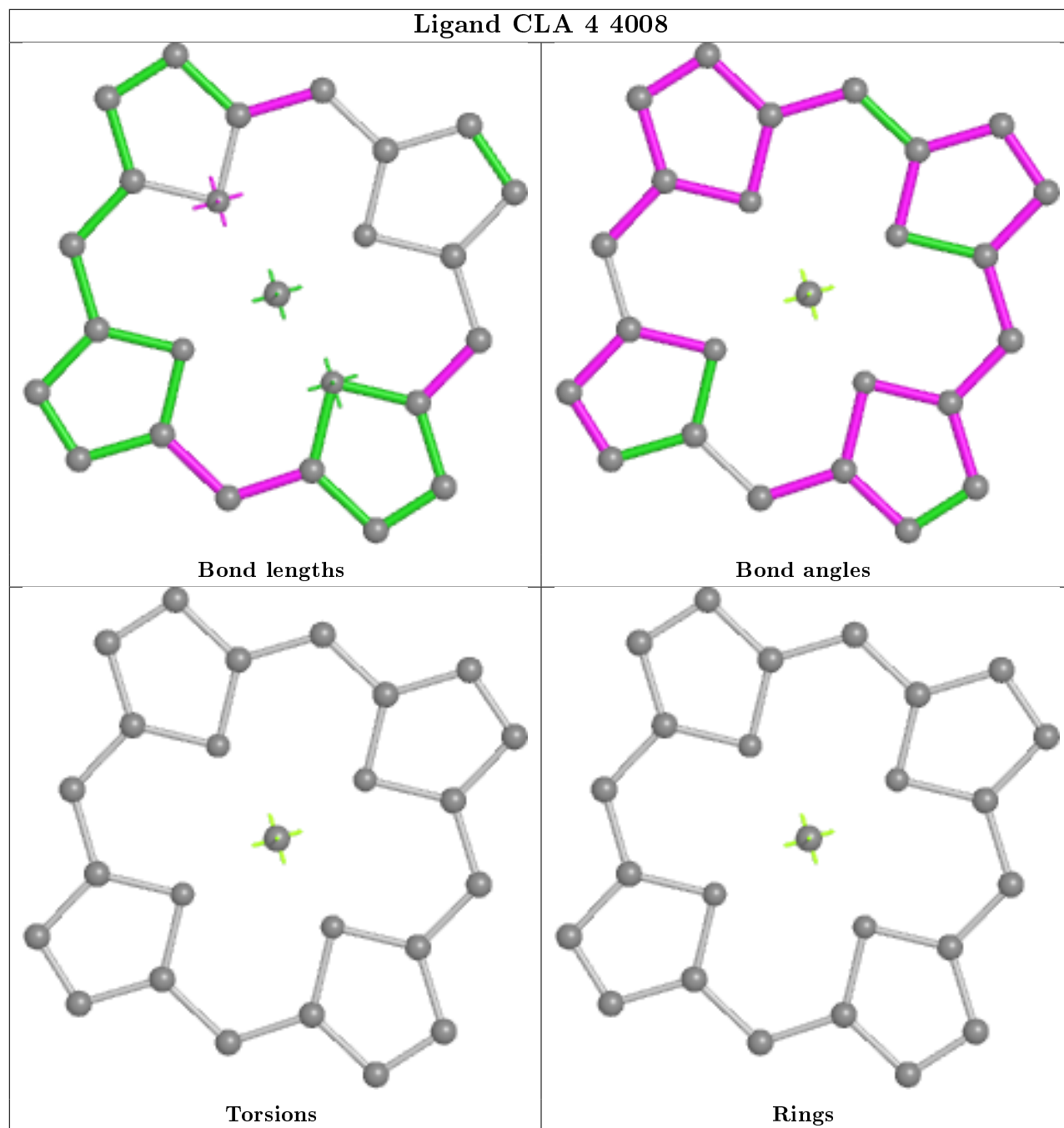
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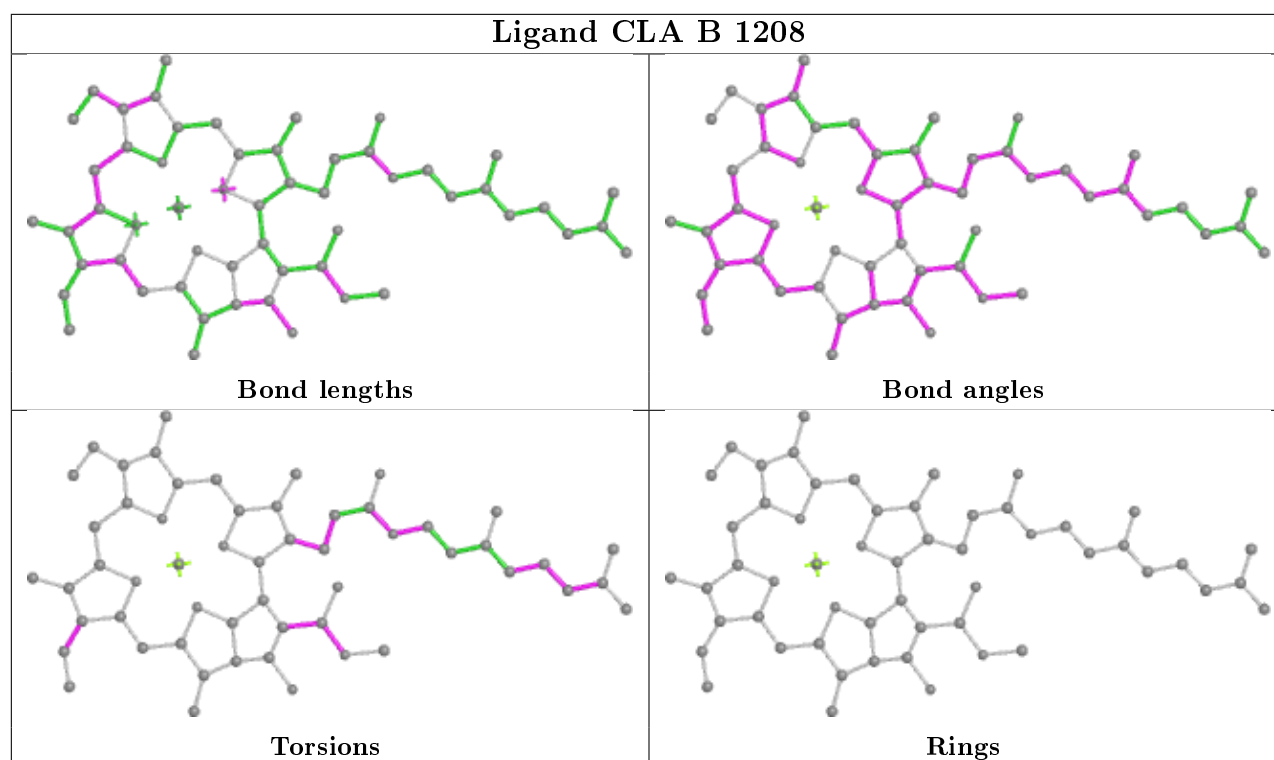


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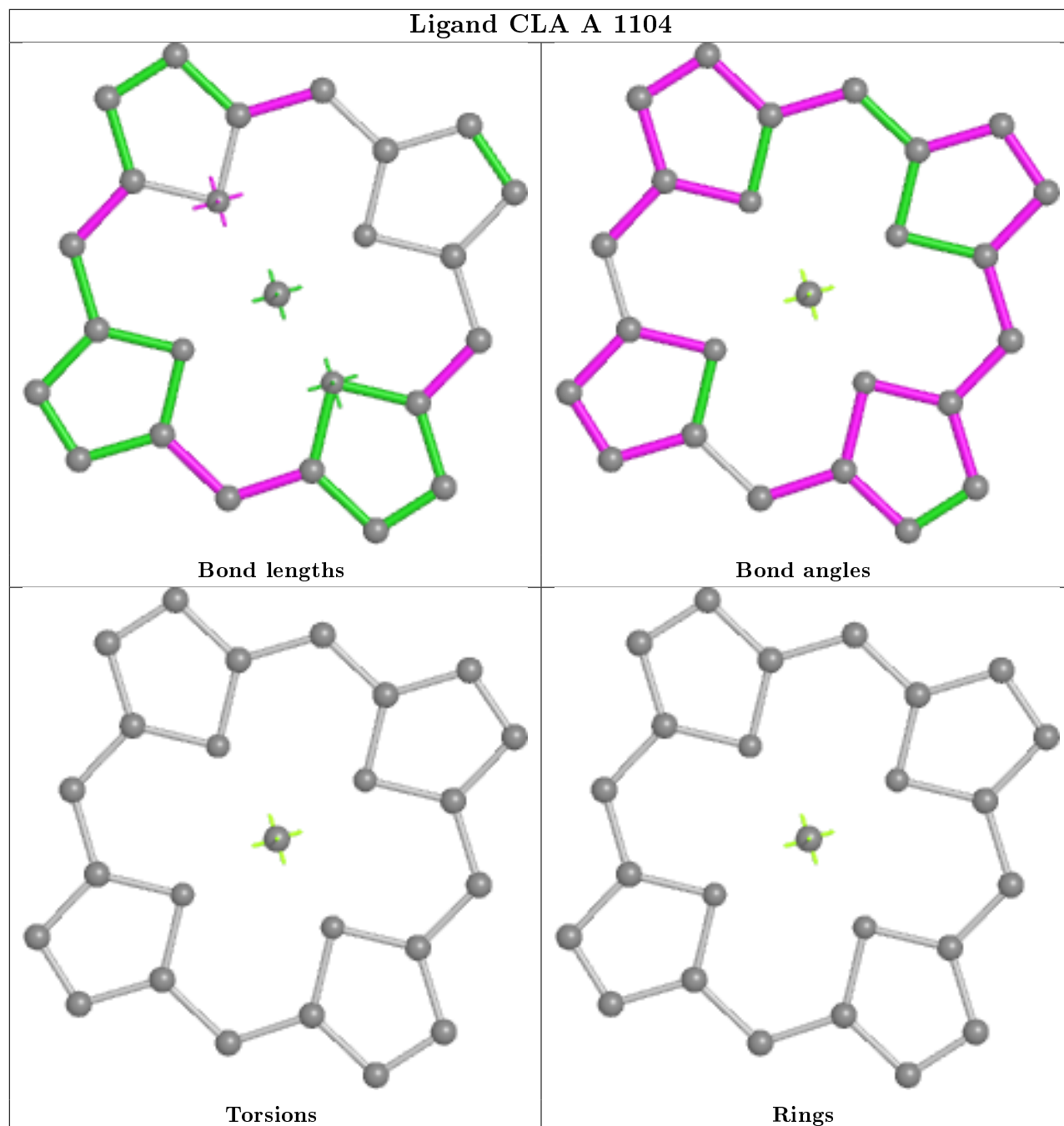




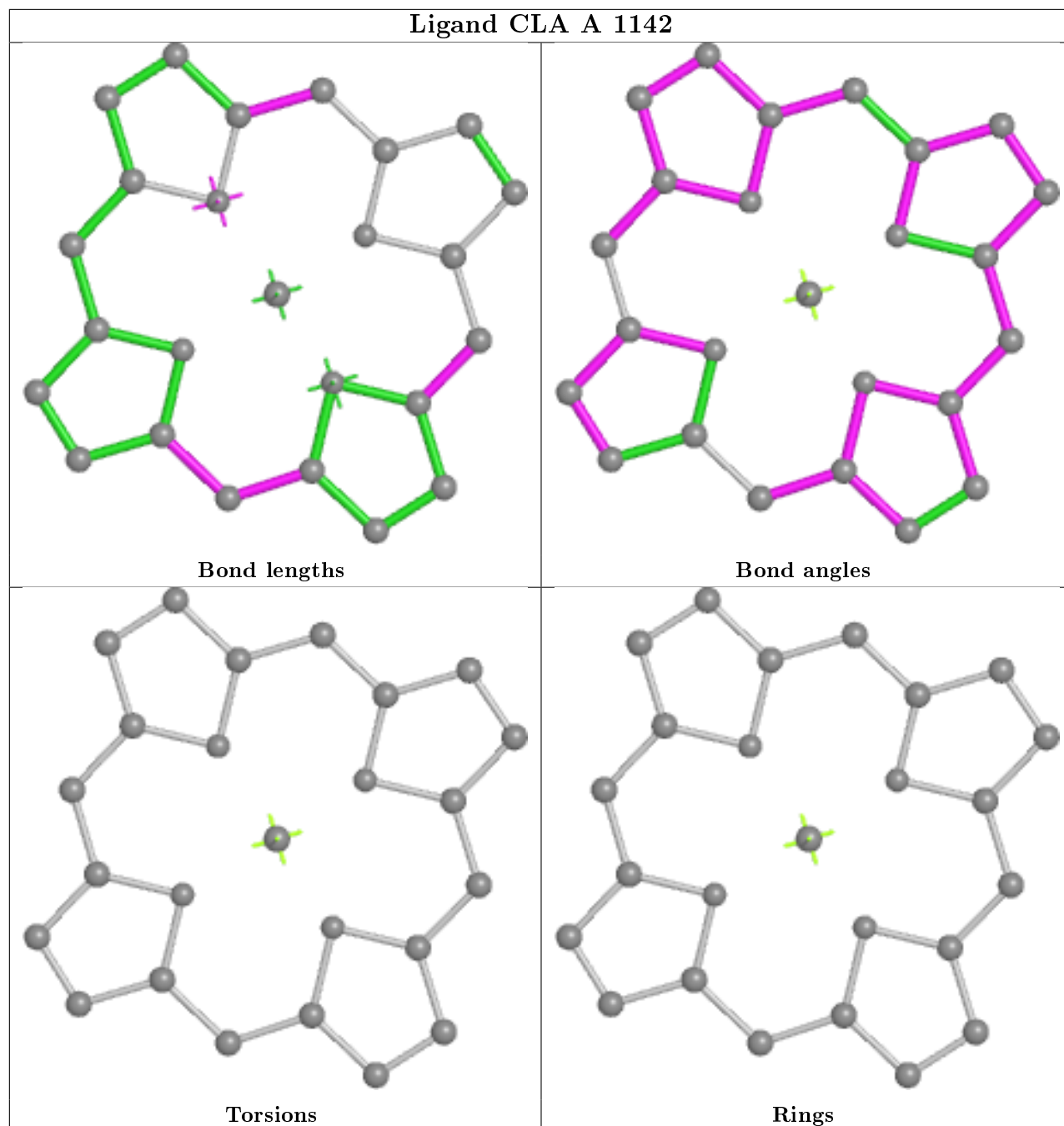


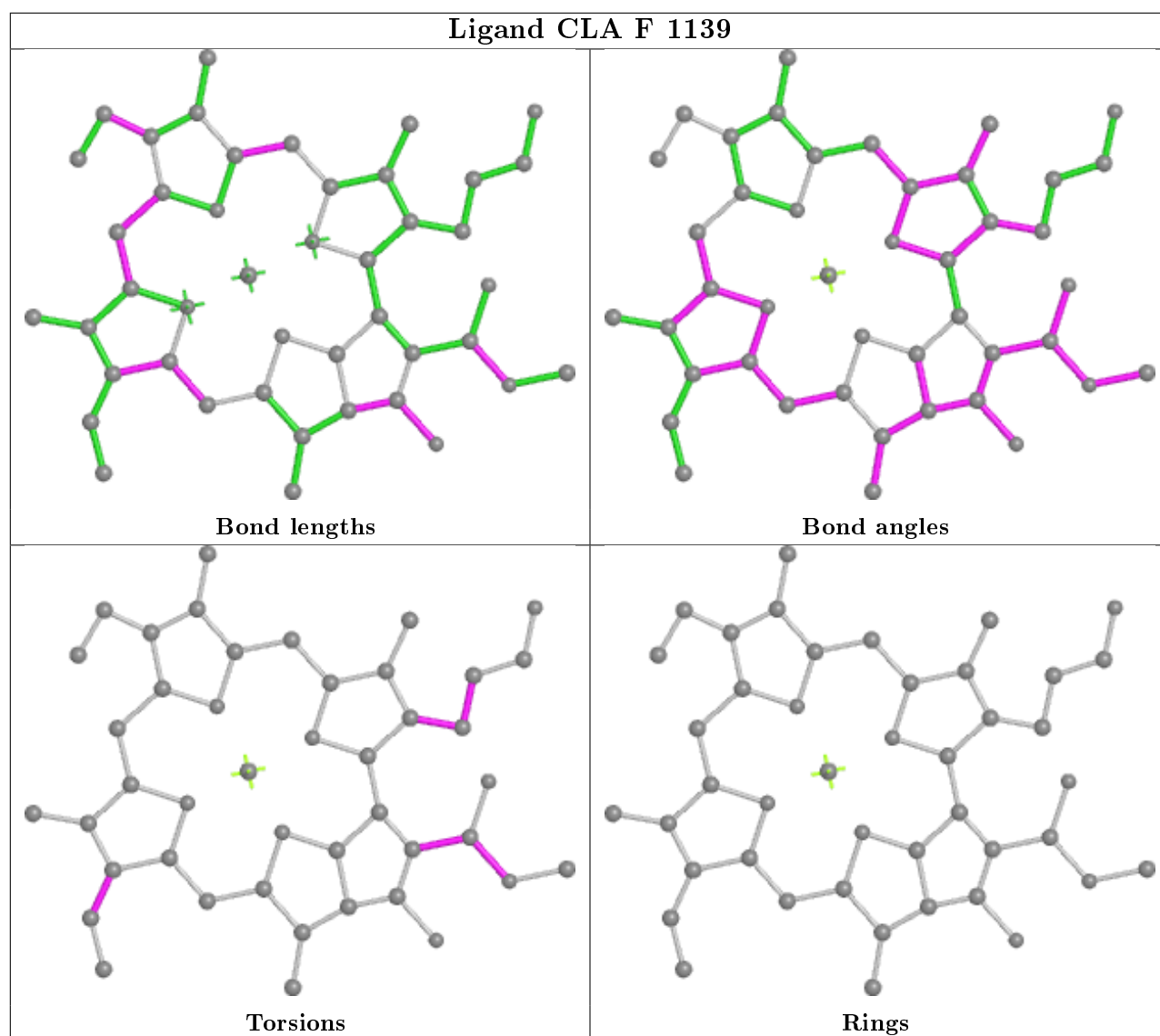


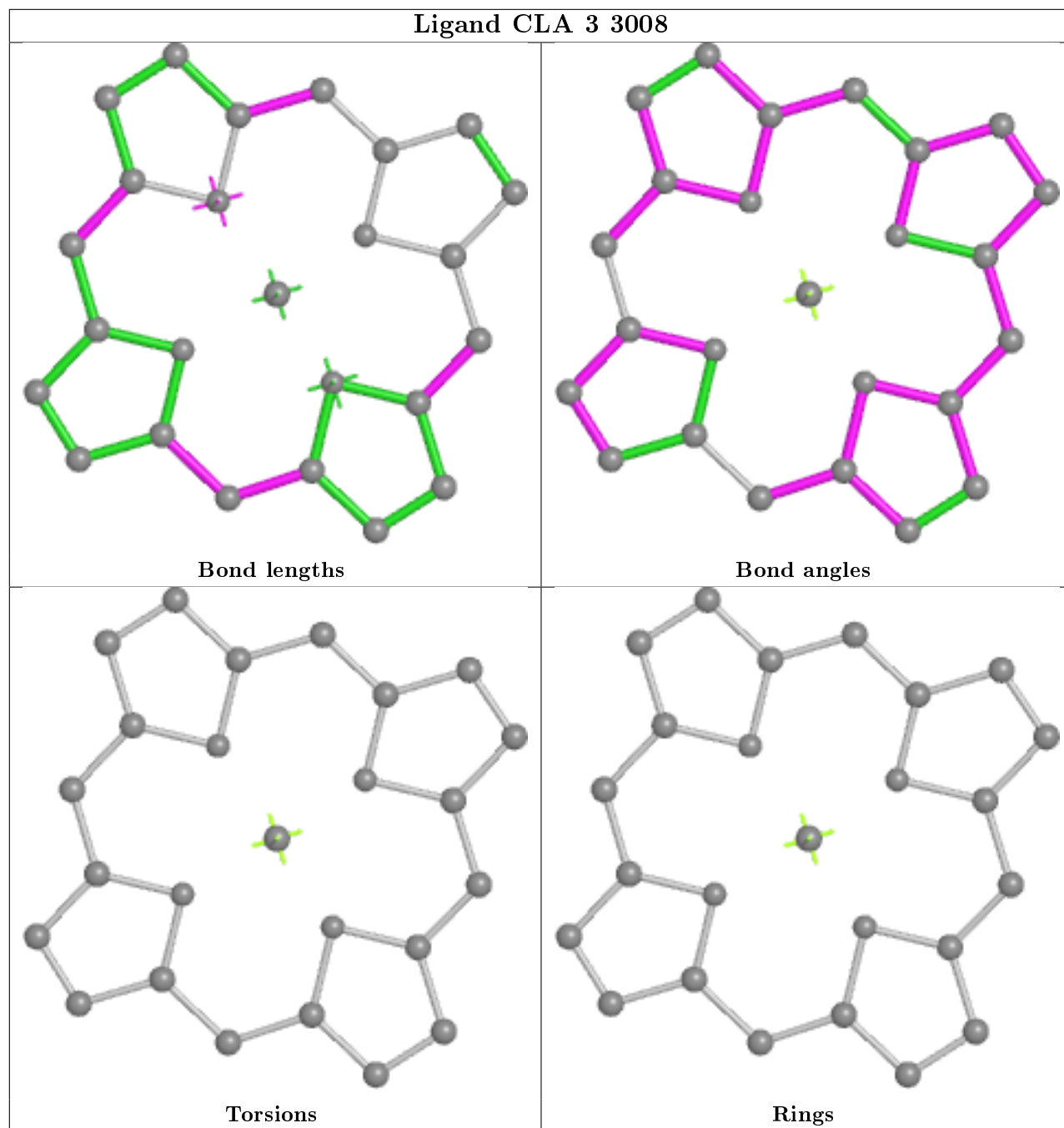
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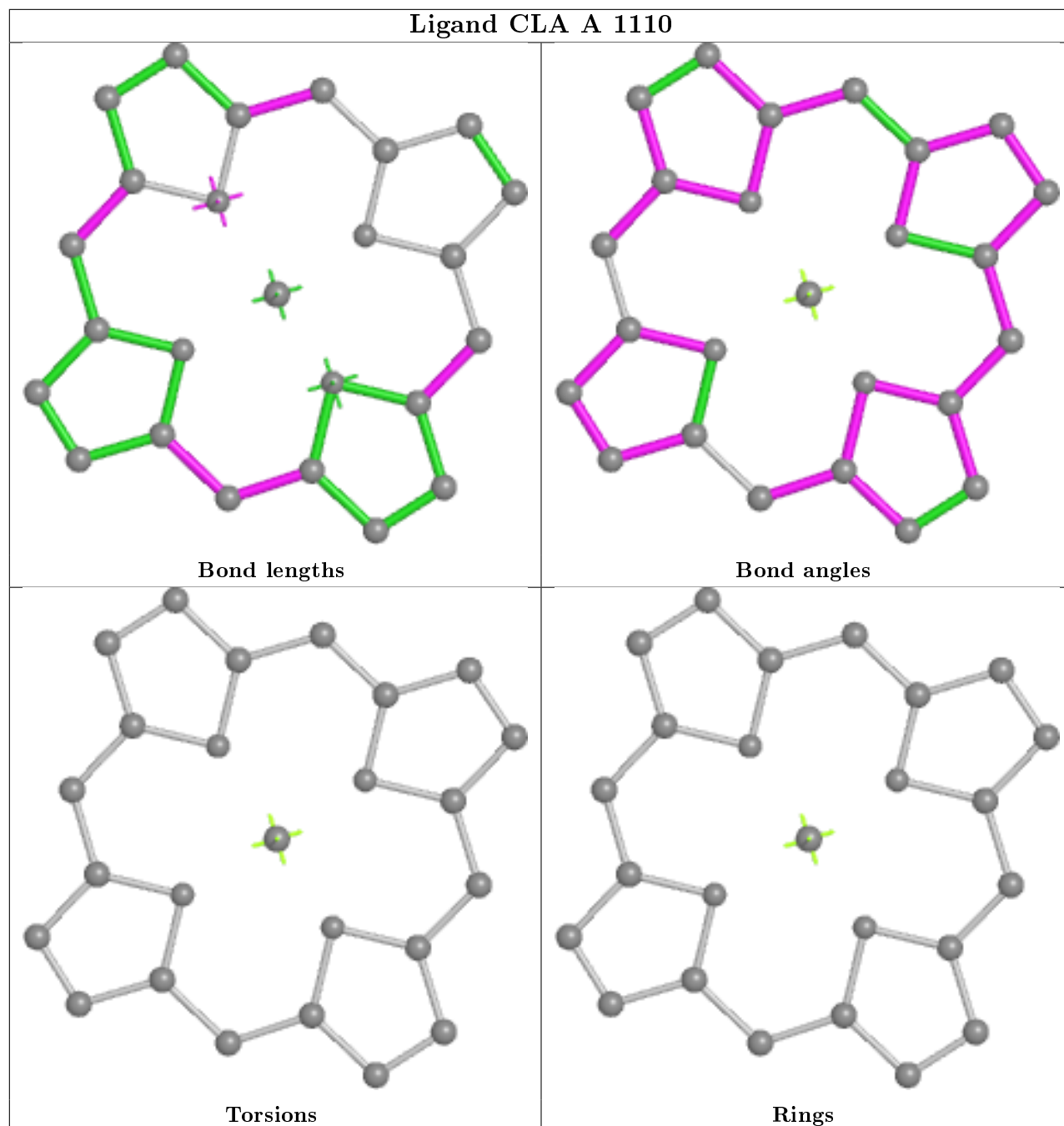
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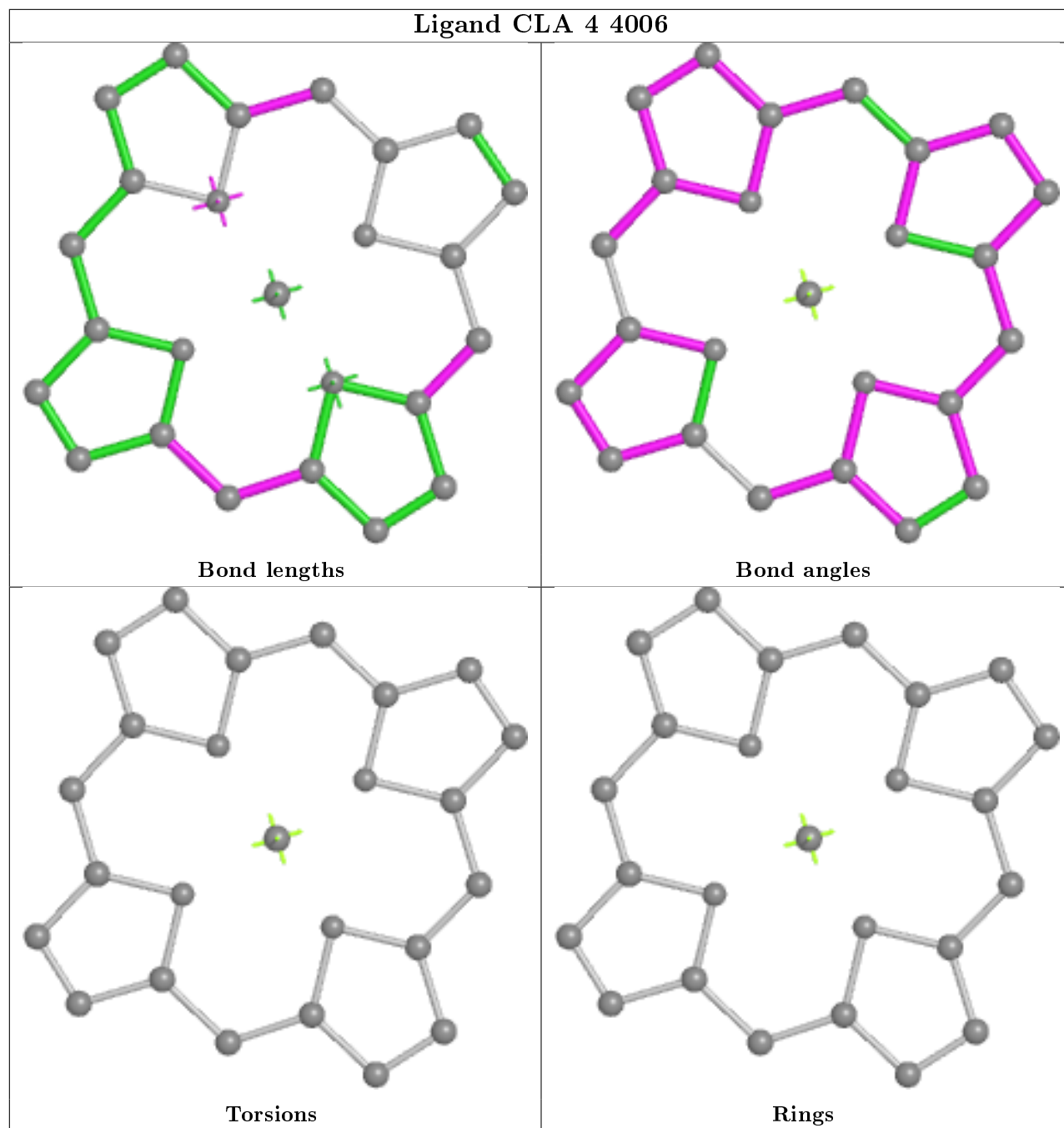


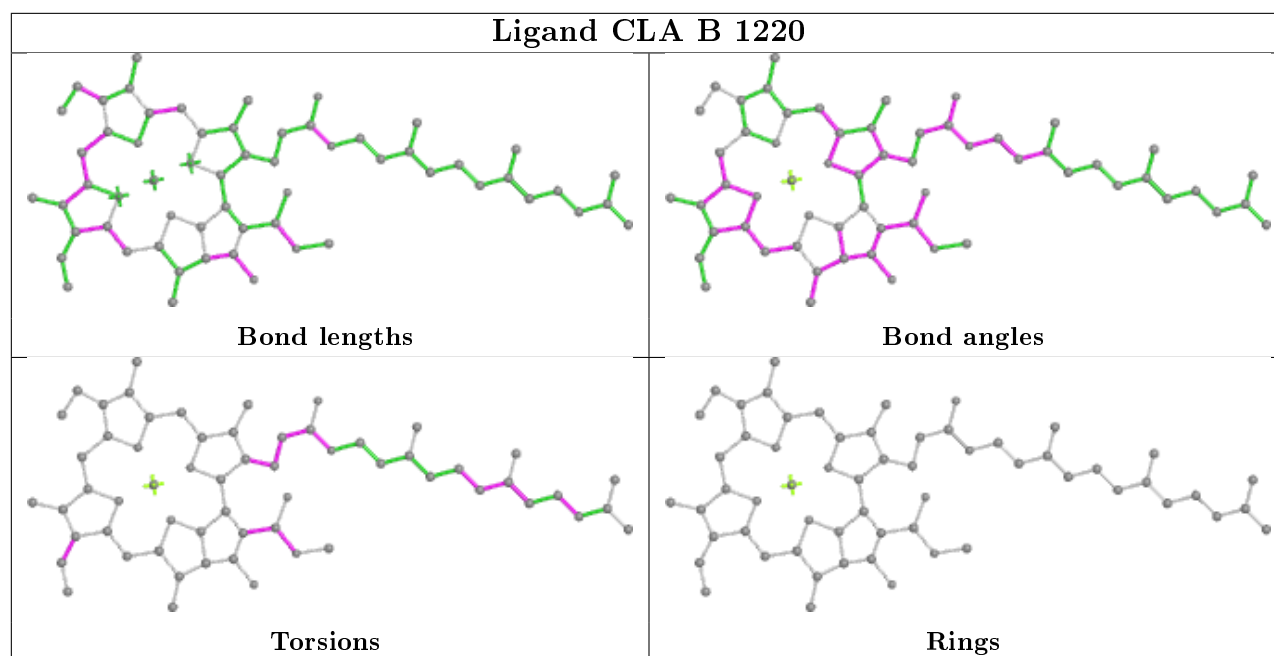
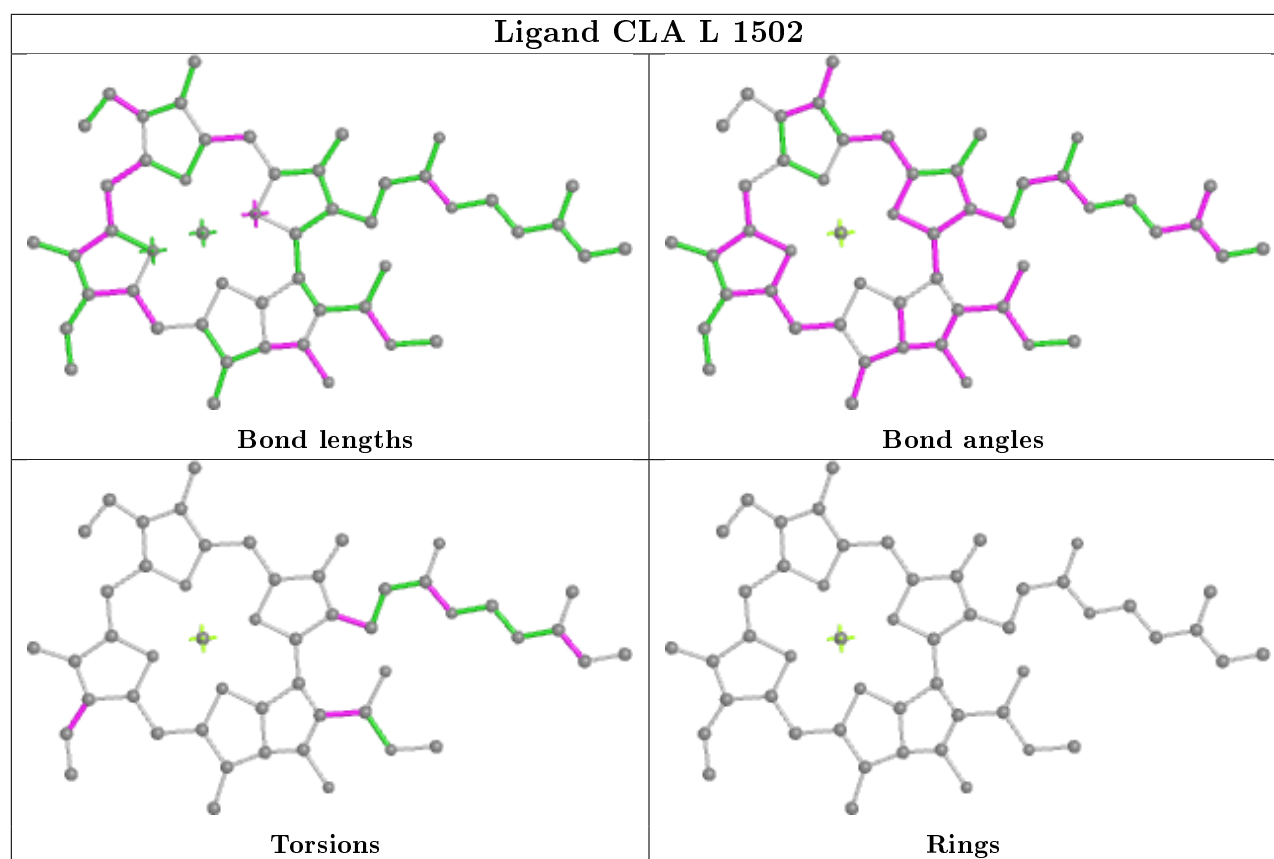




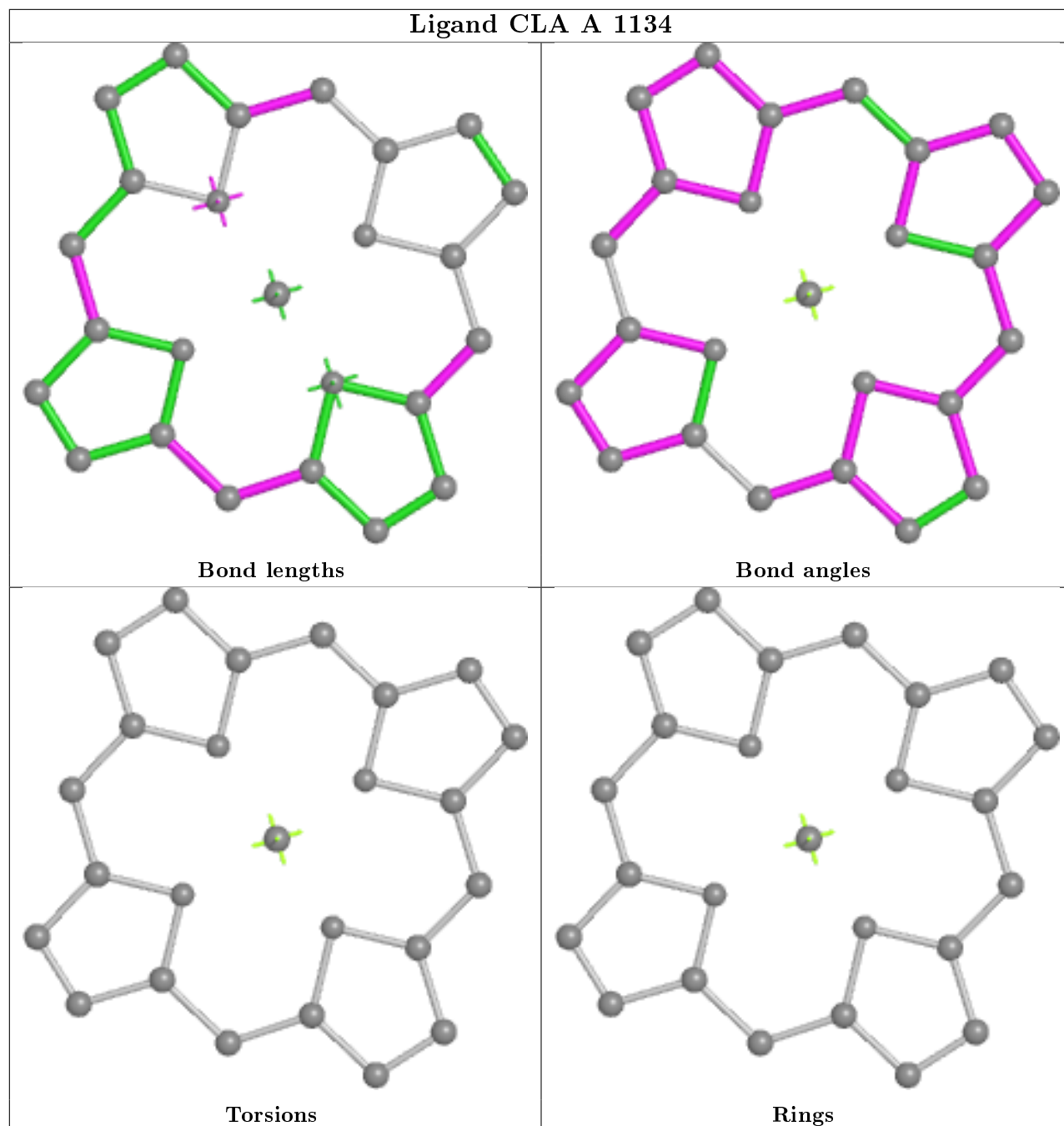
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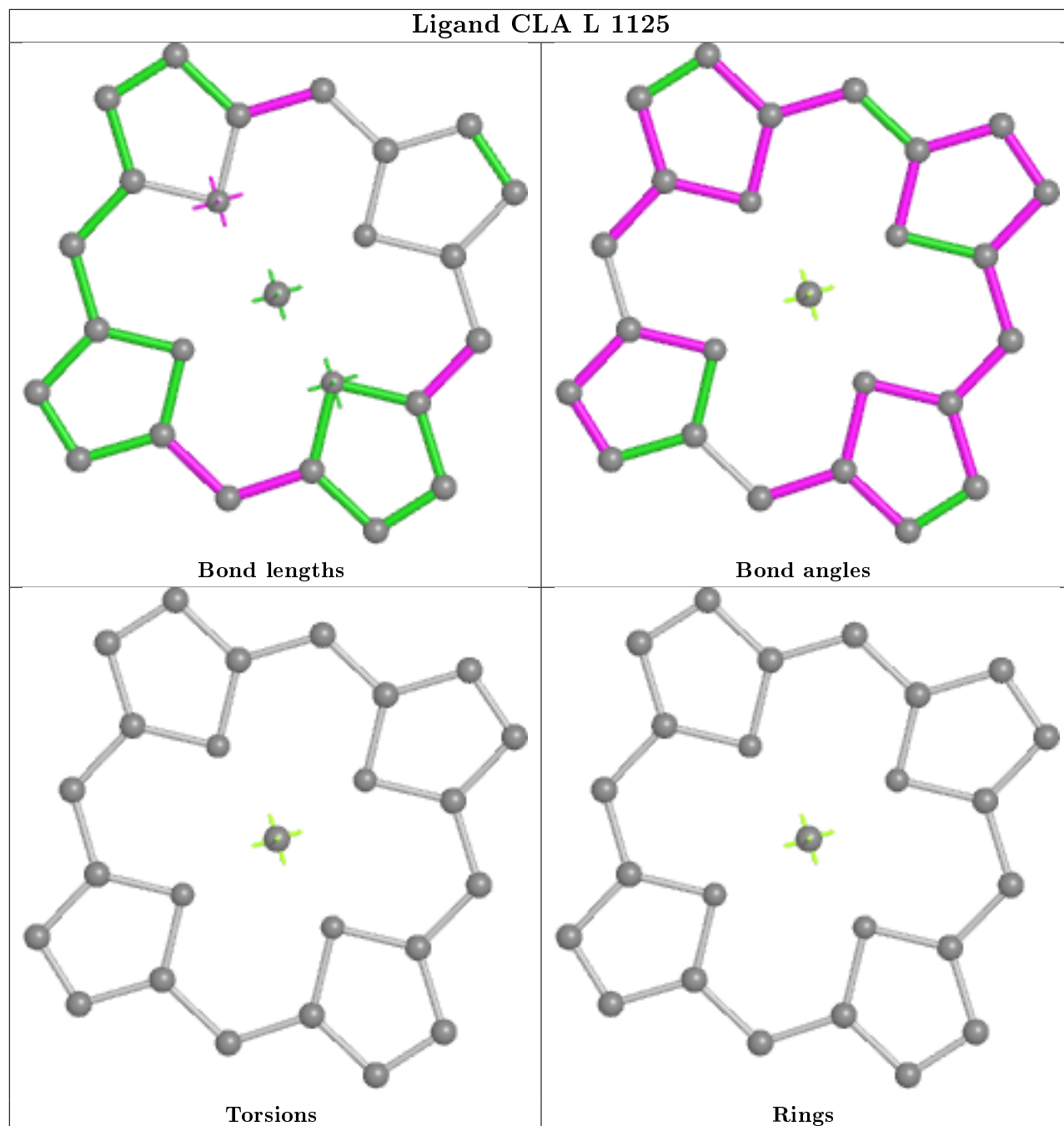




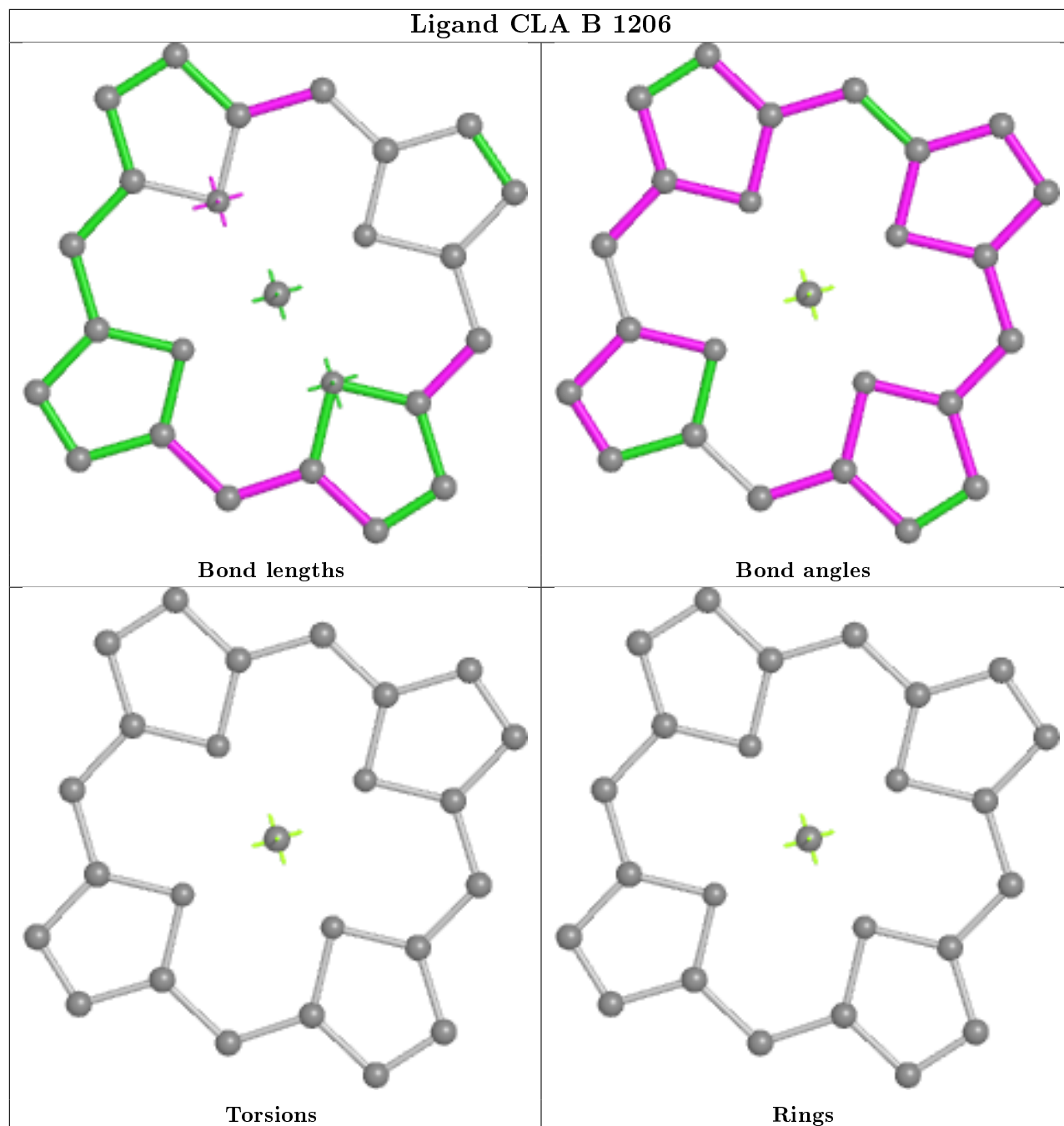
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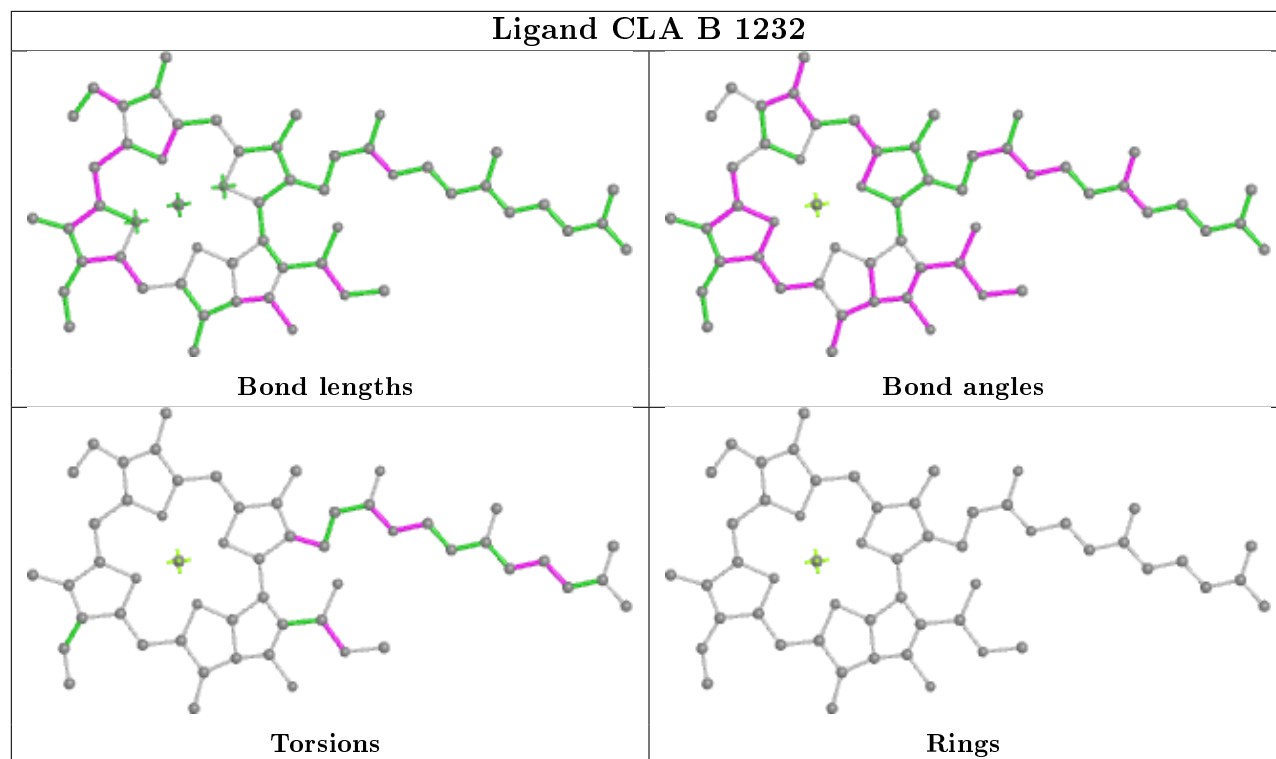


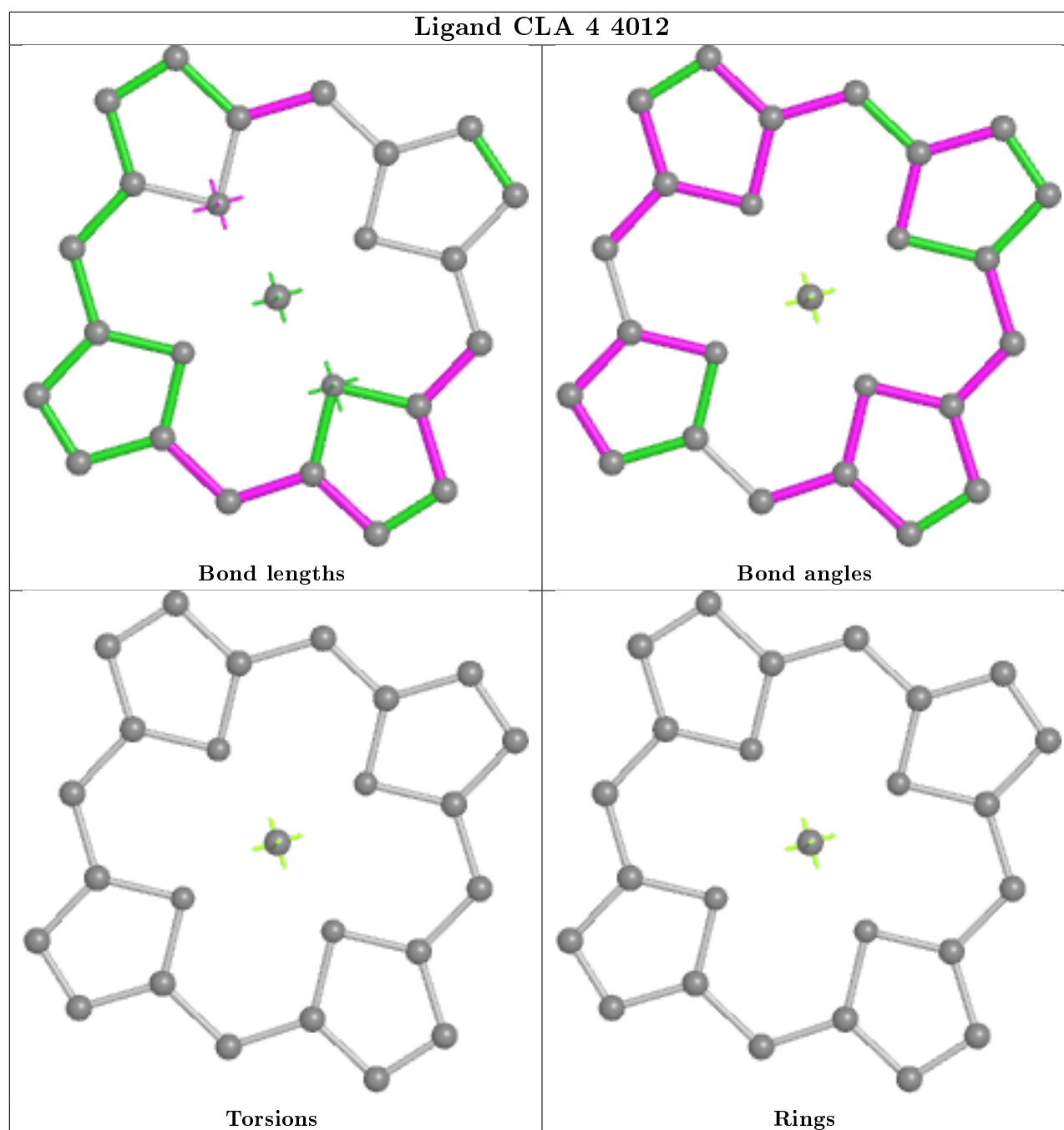
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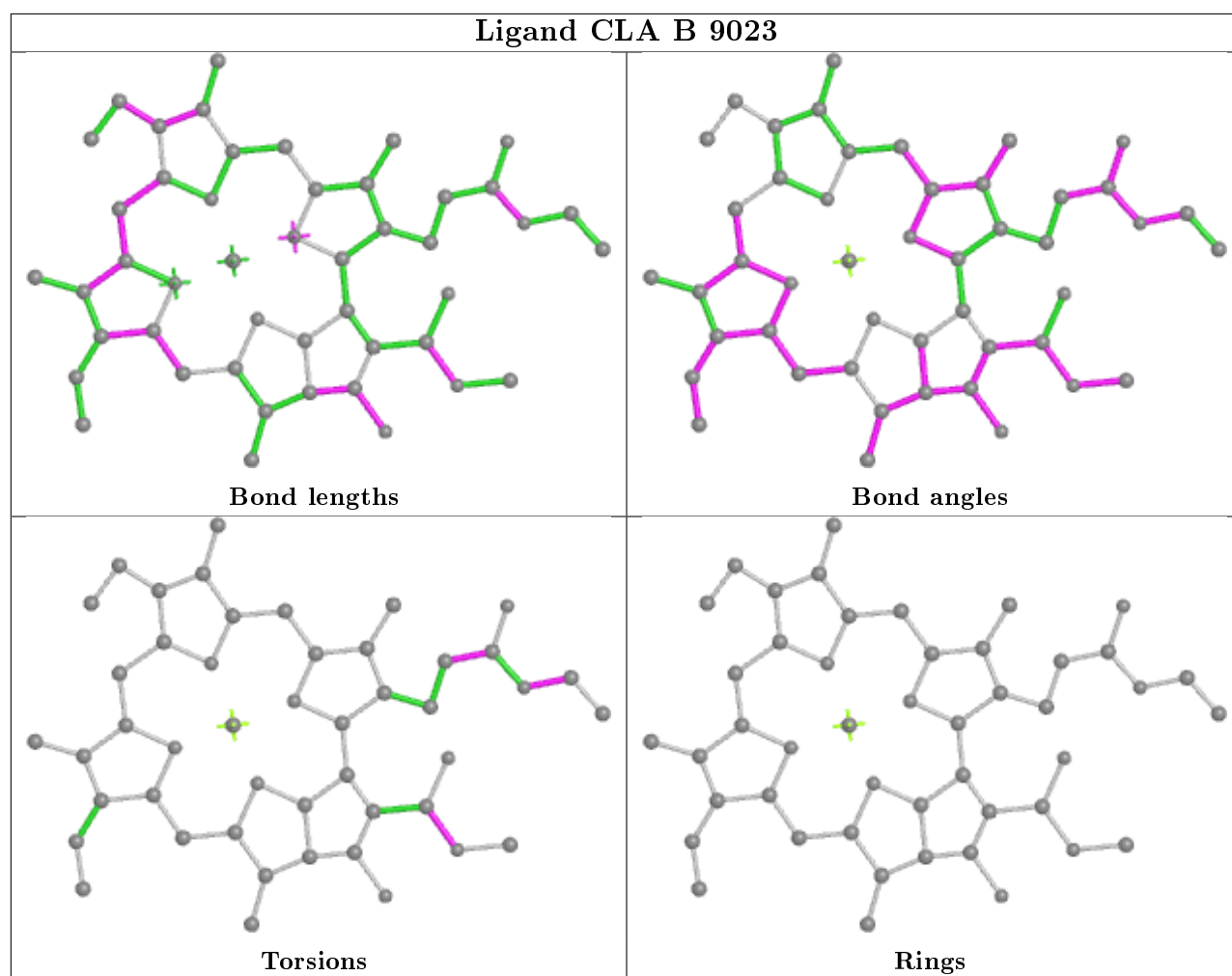


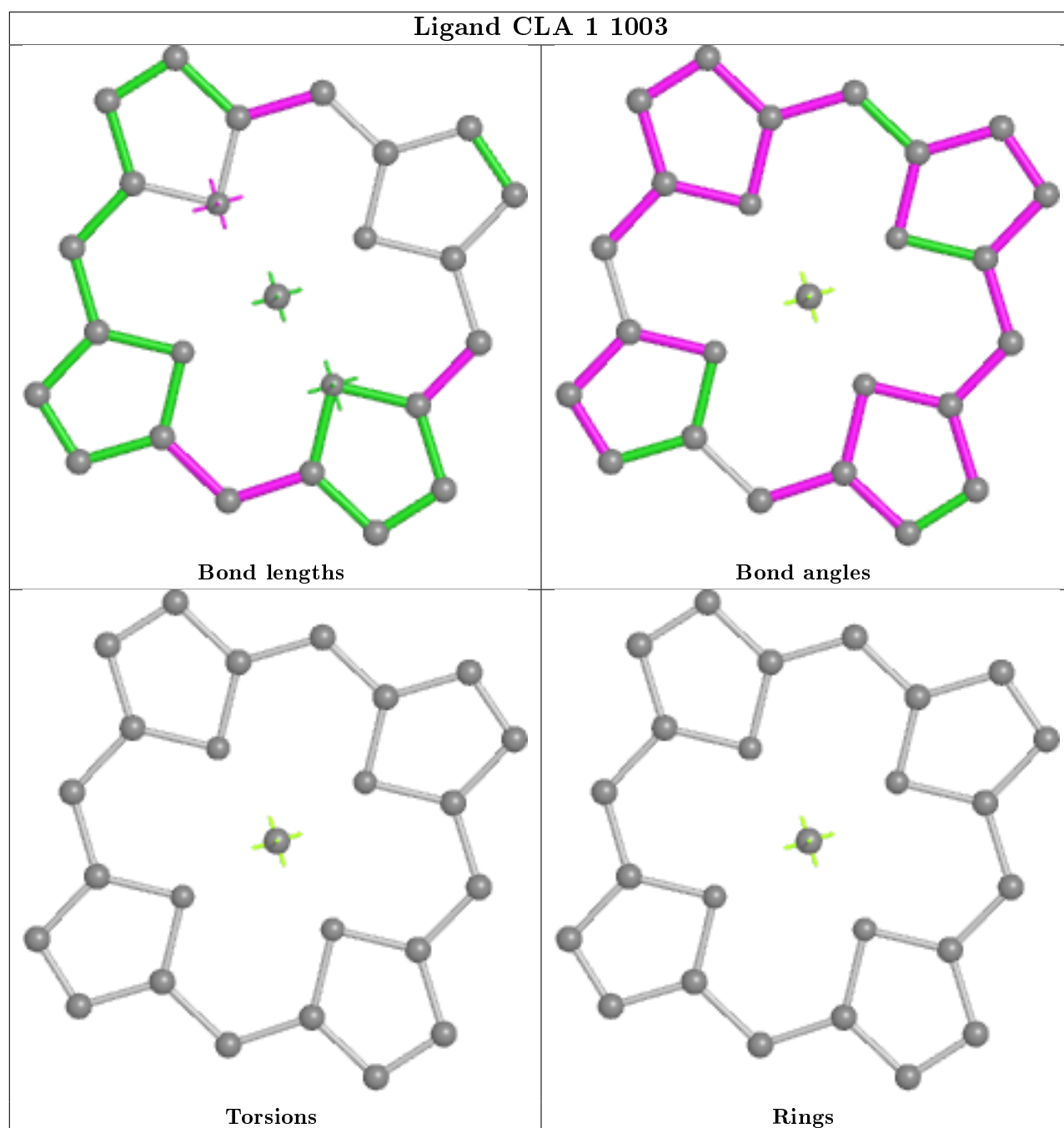
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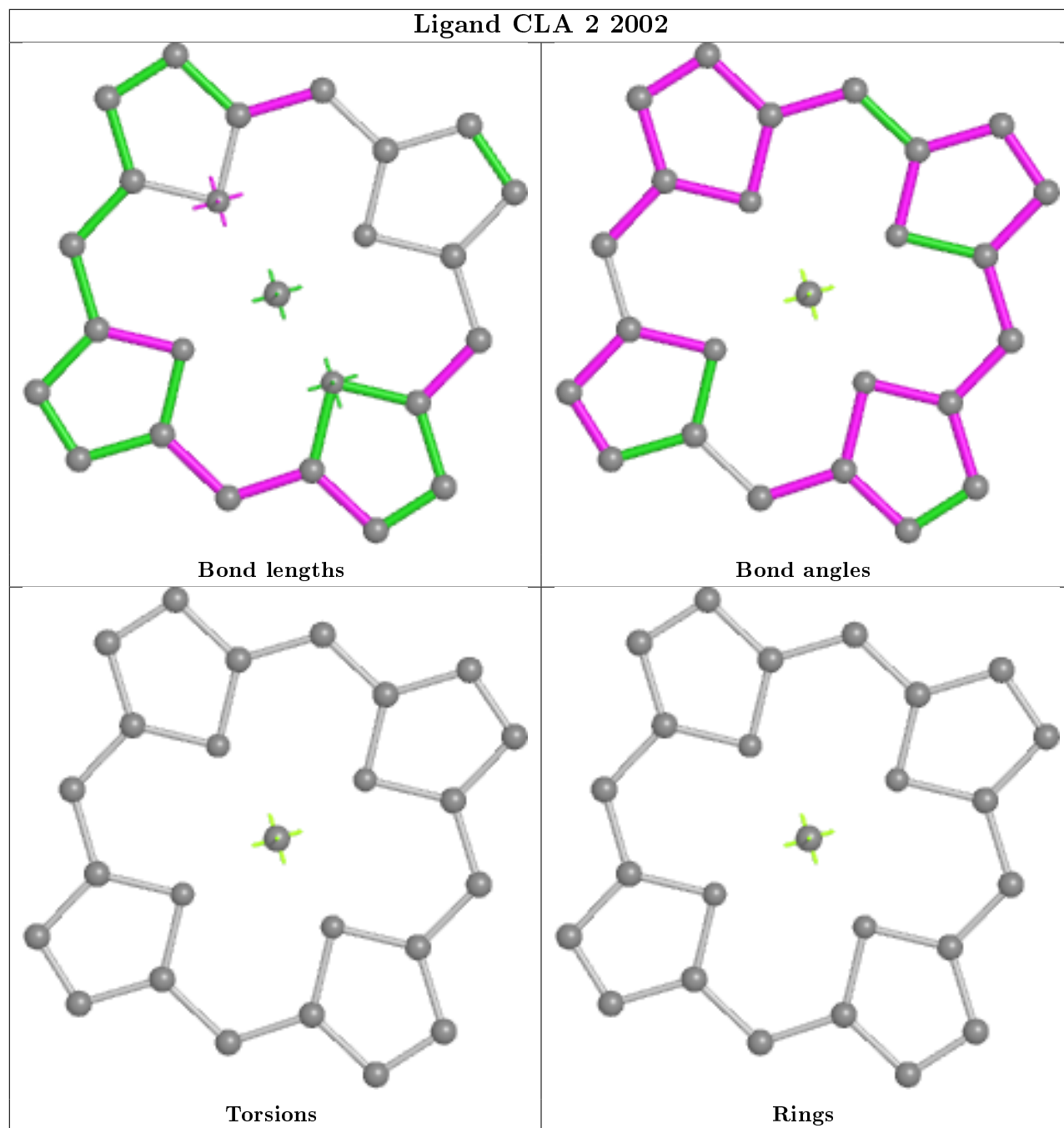


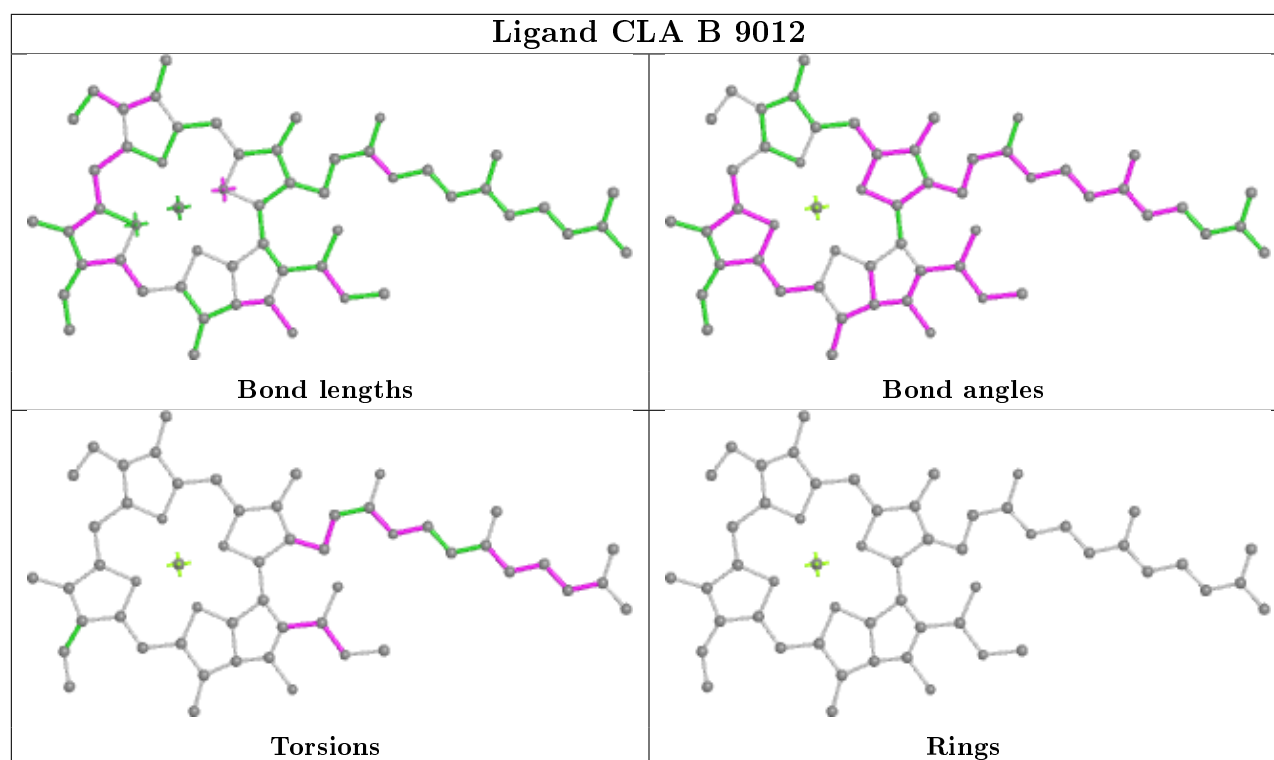


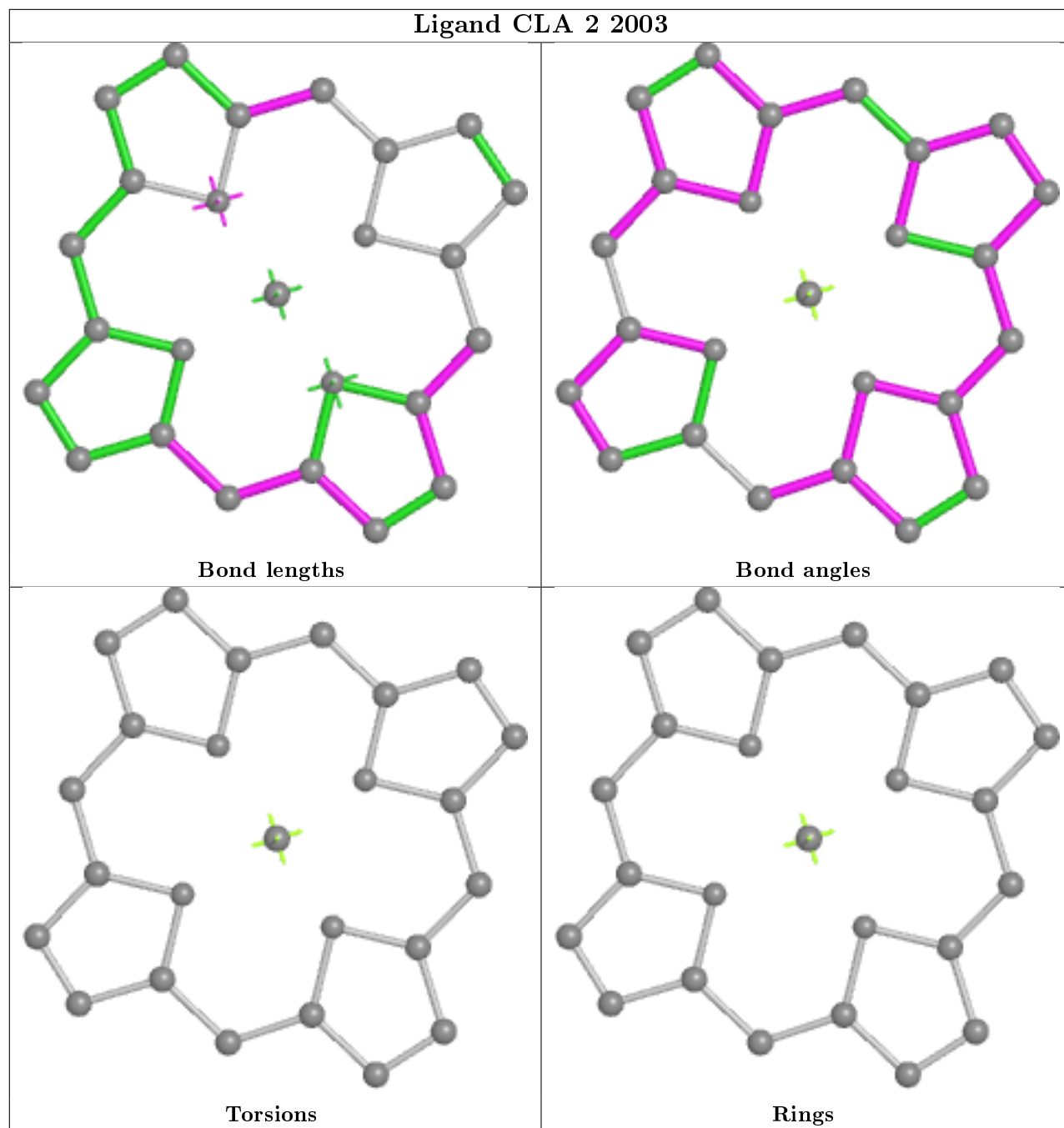


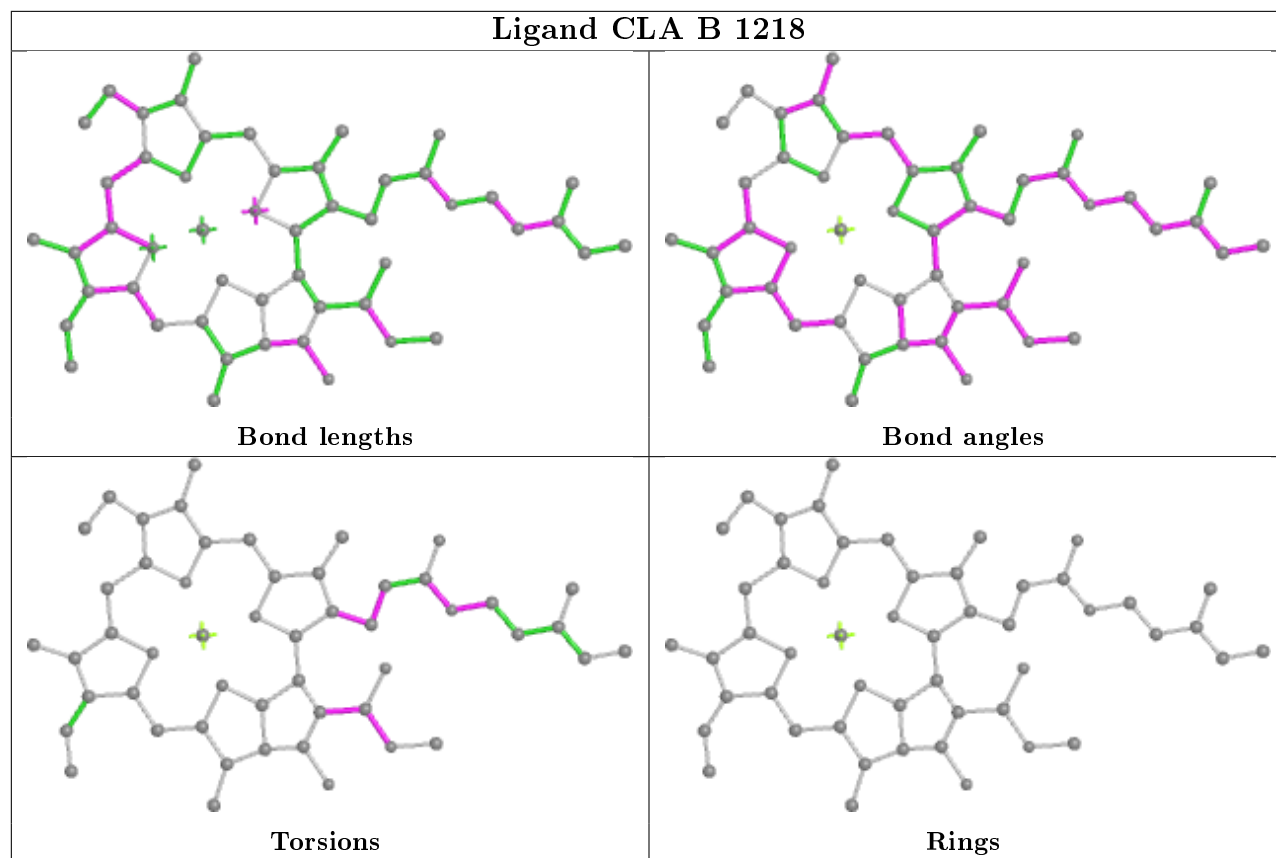


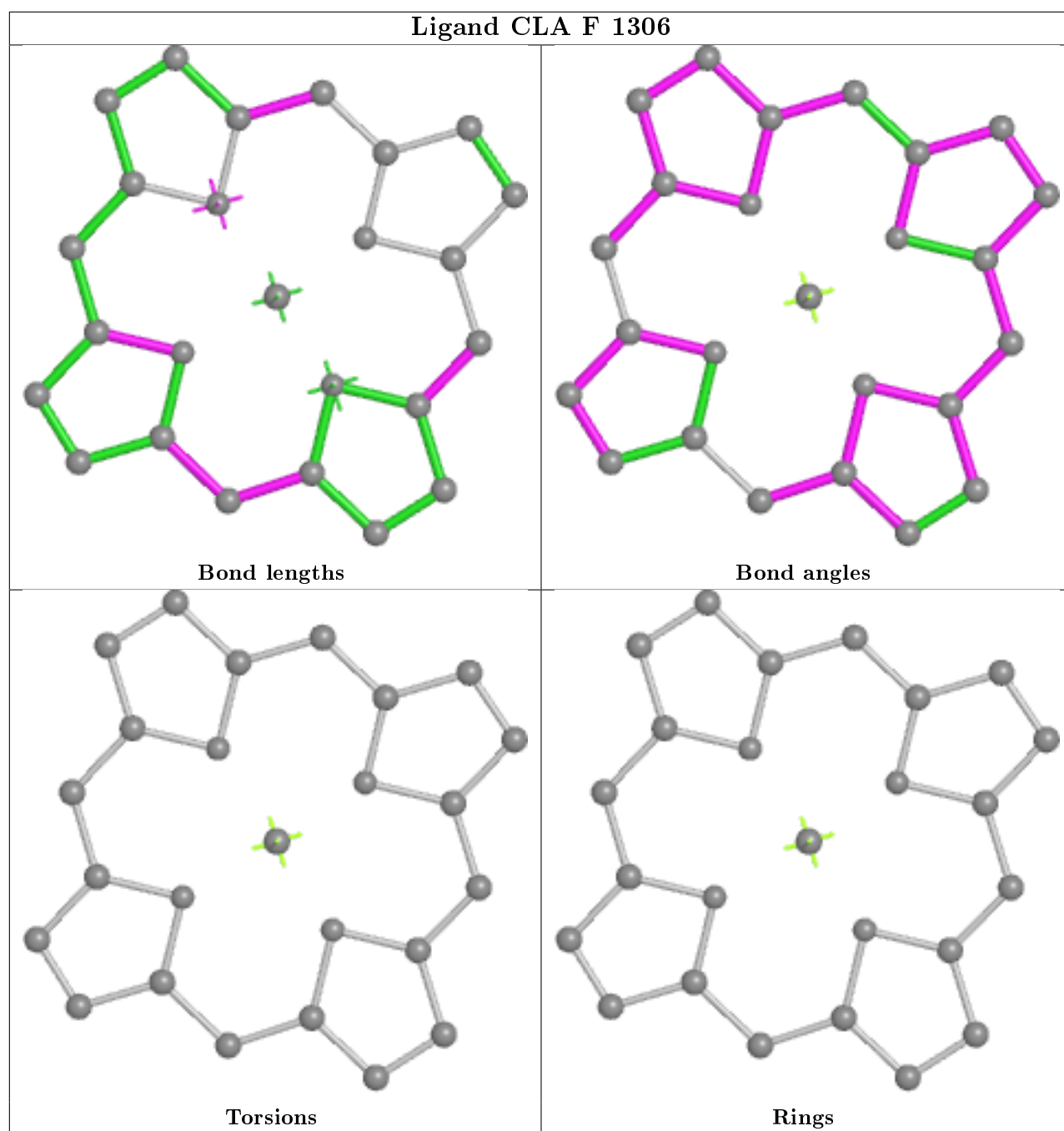


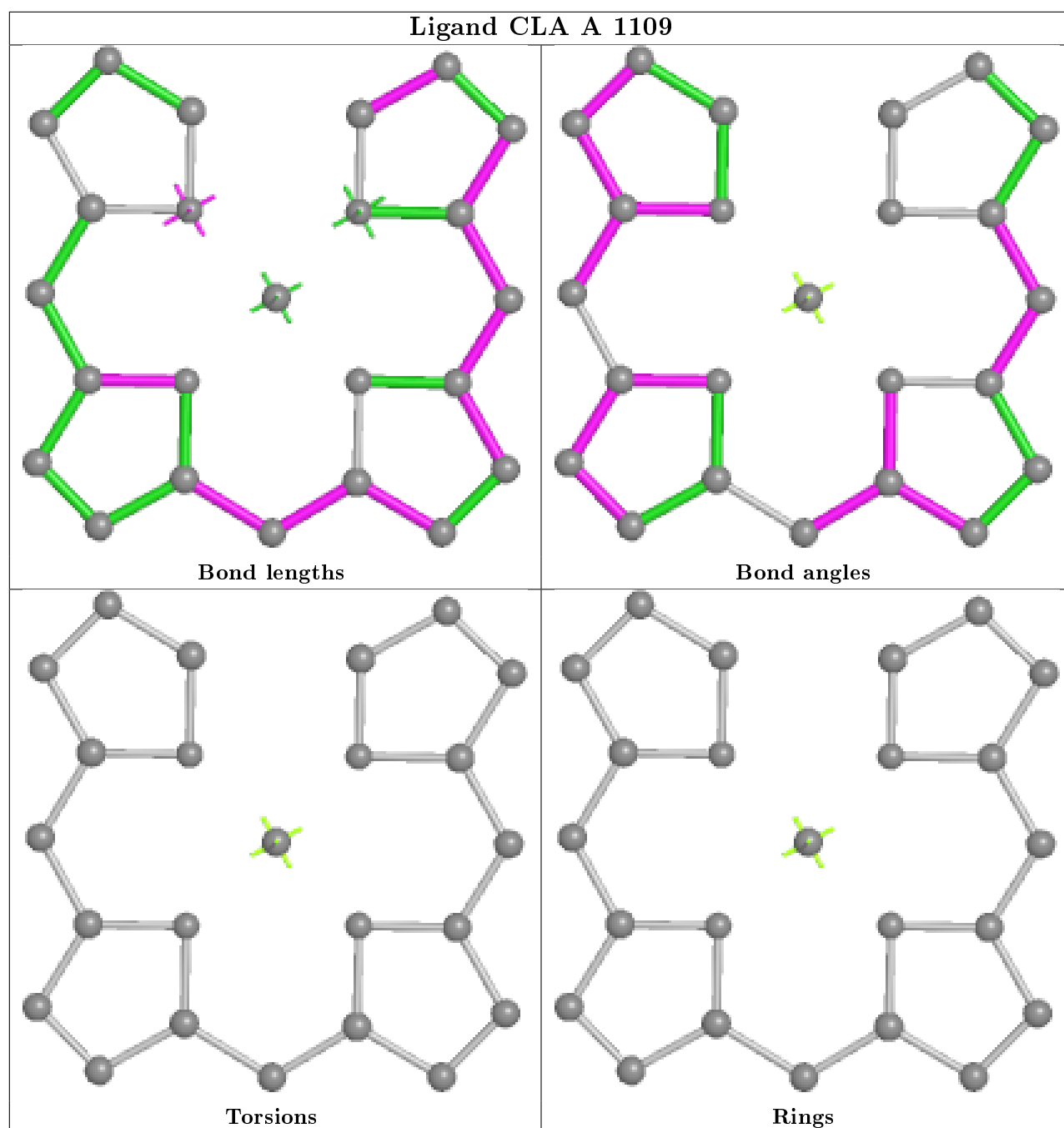


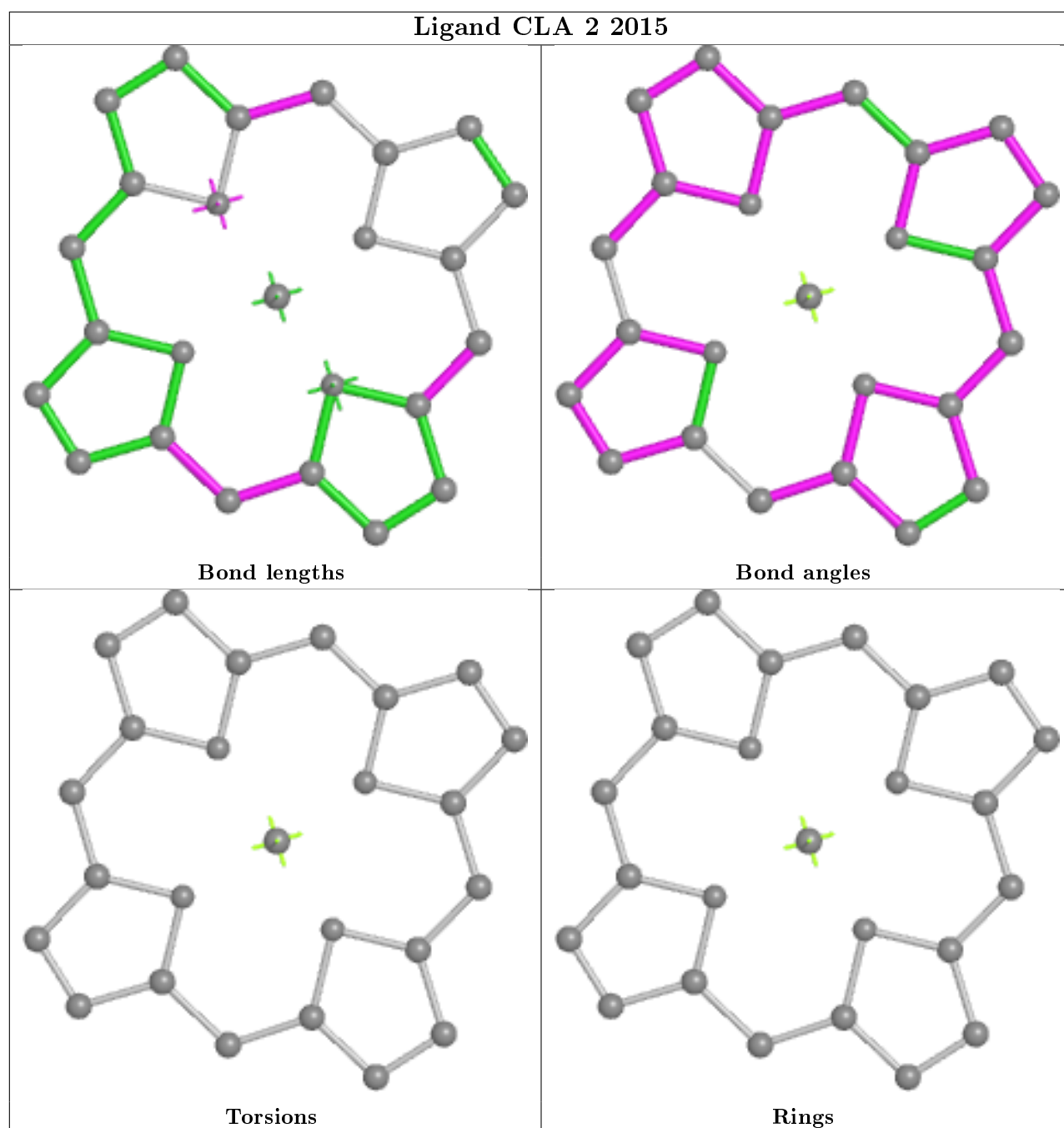




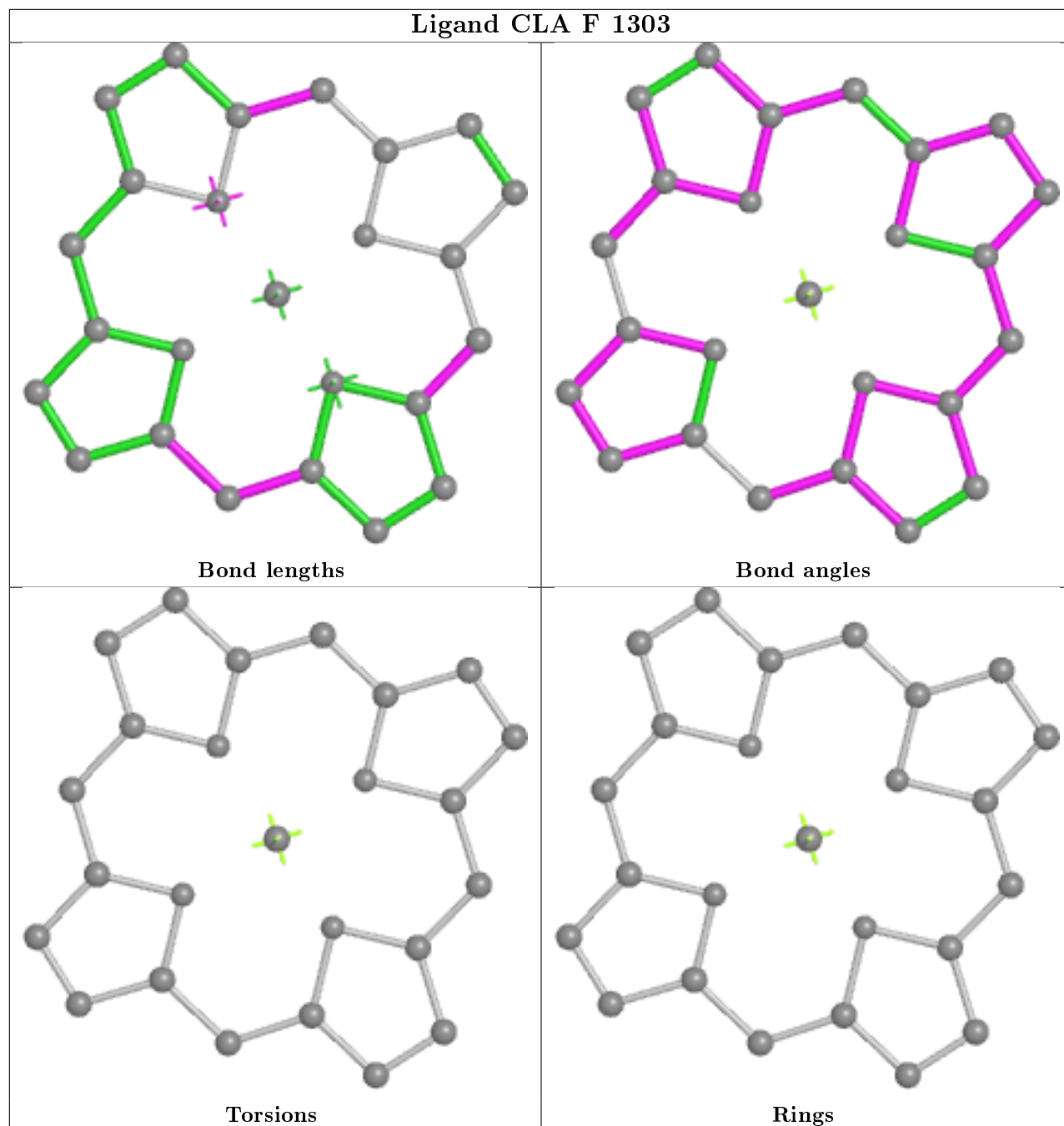








Ligand CLA F 1303

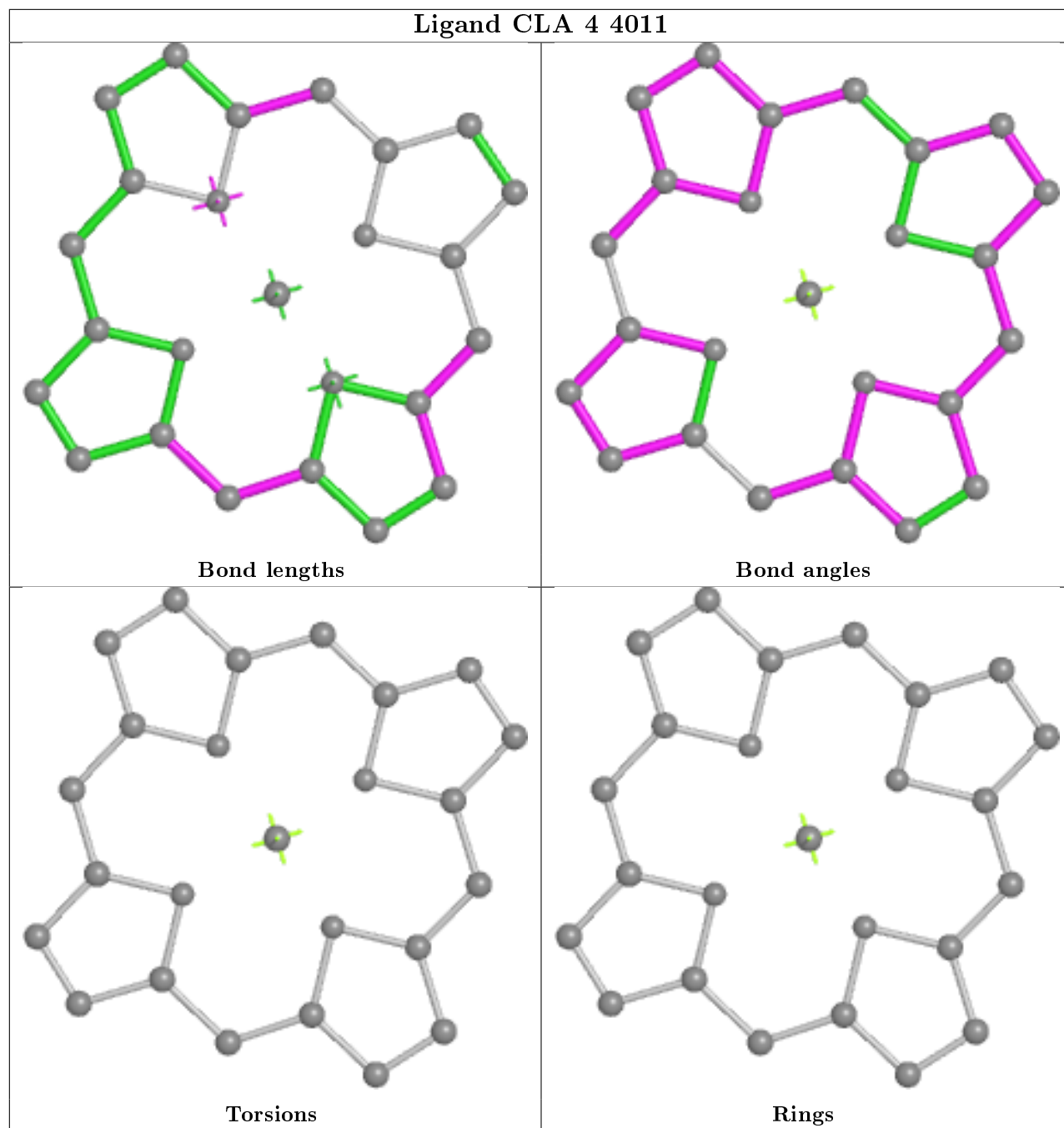


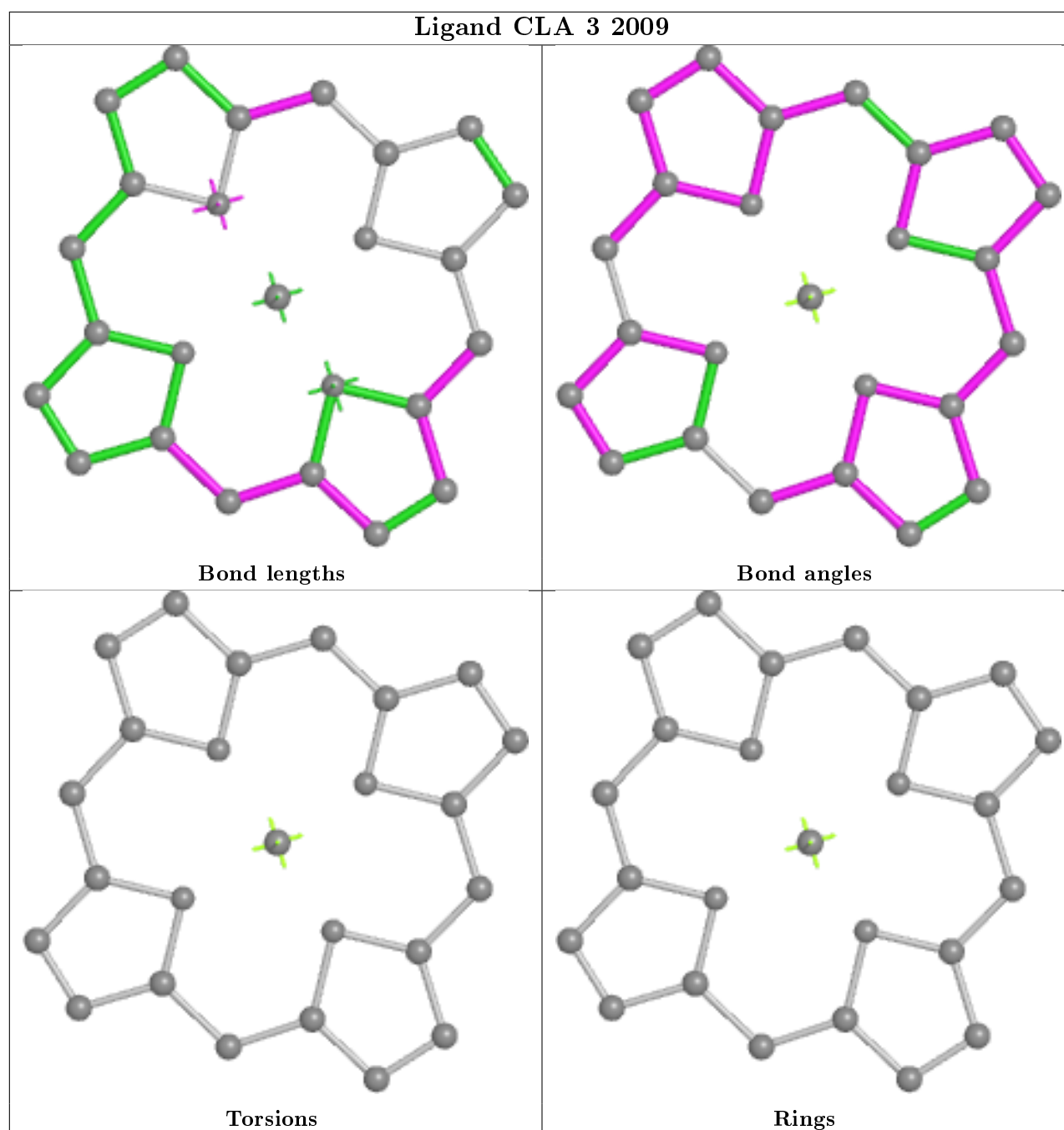
Bond lengths

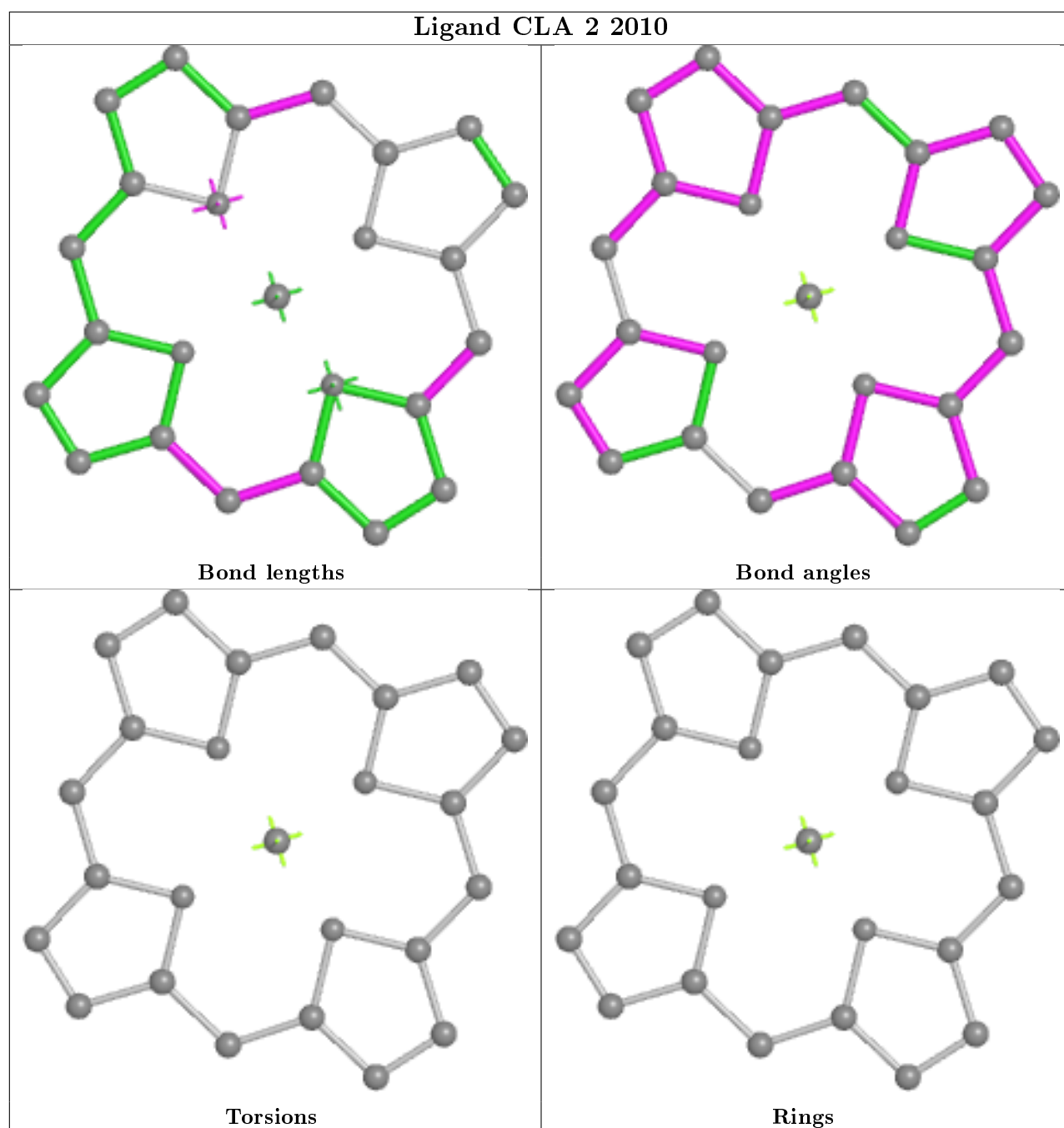
Bond angles

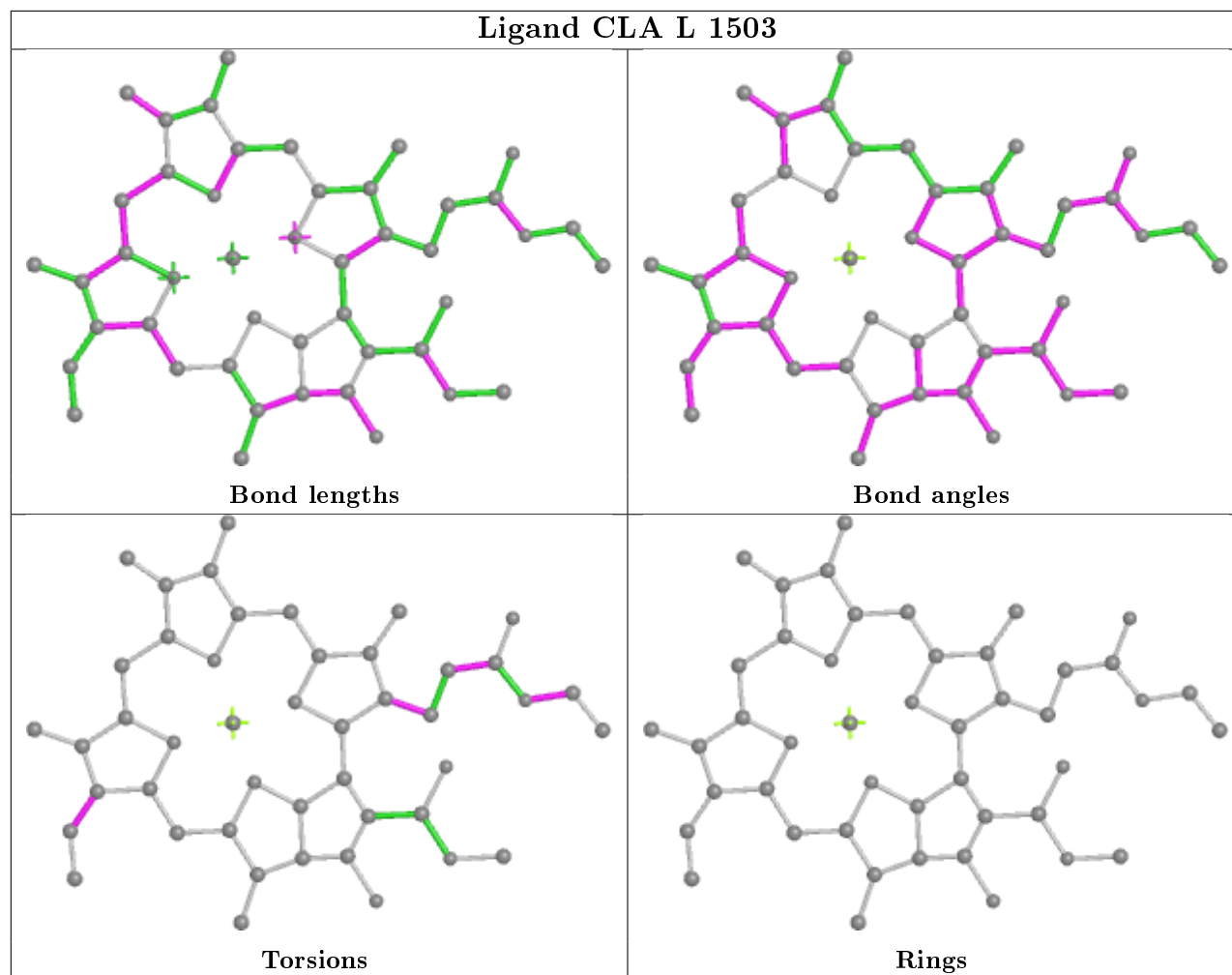
Torsions

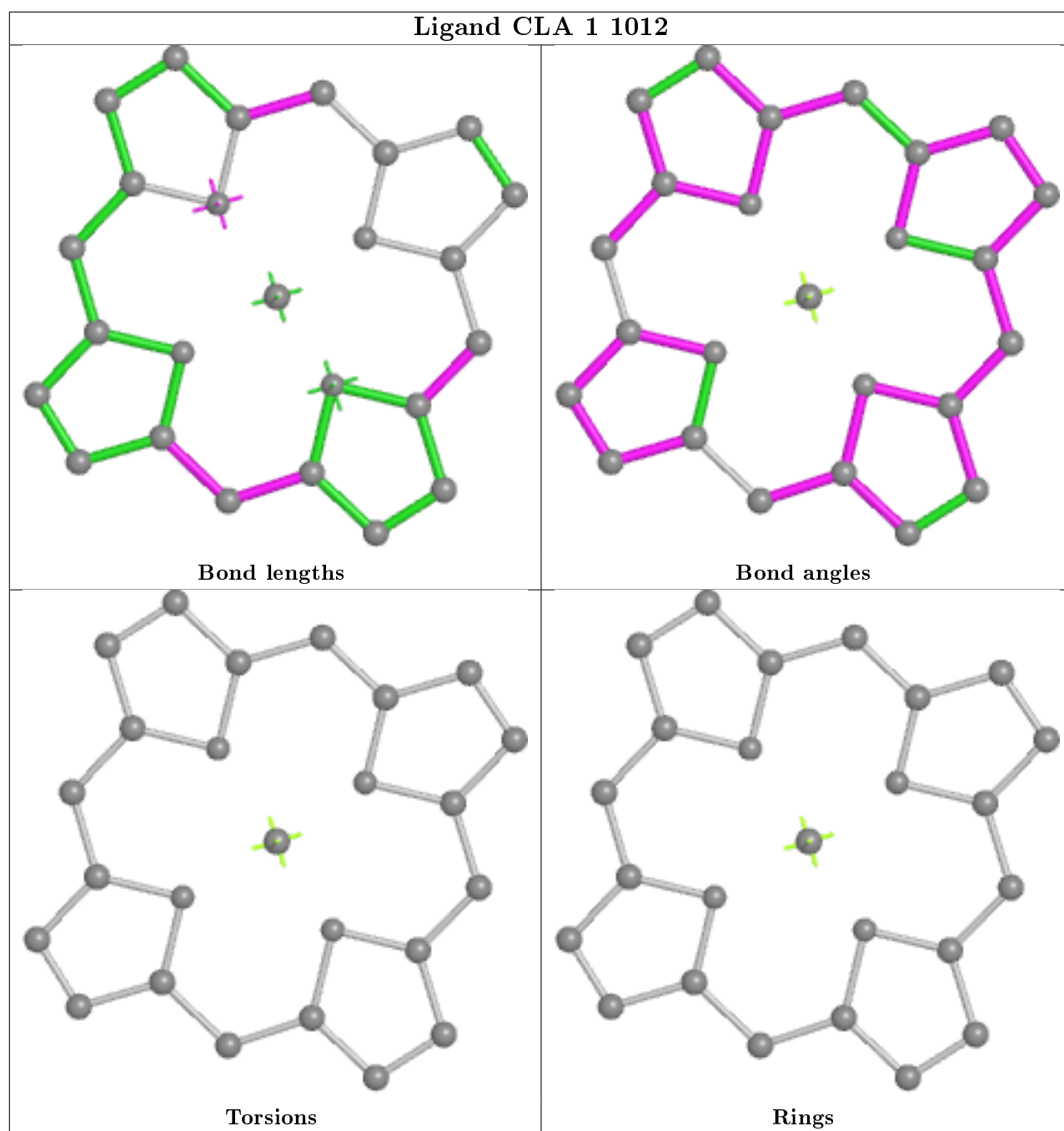
Rings

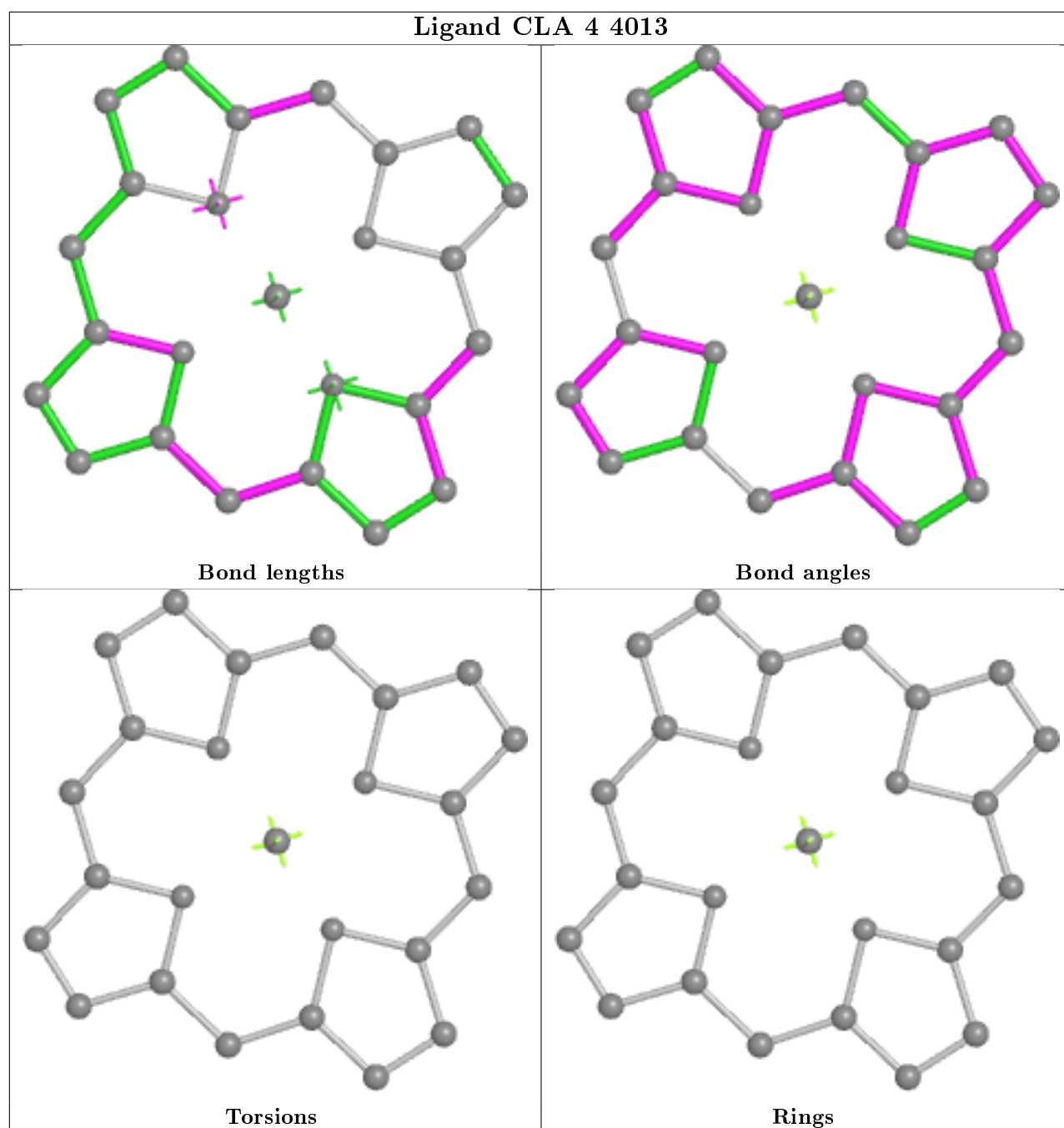




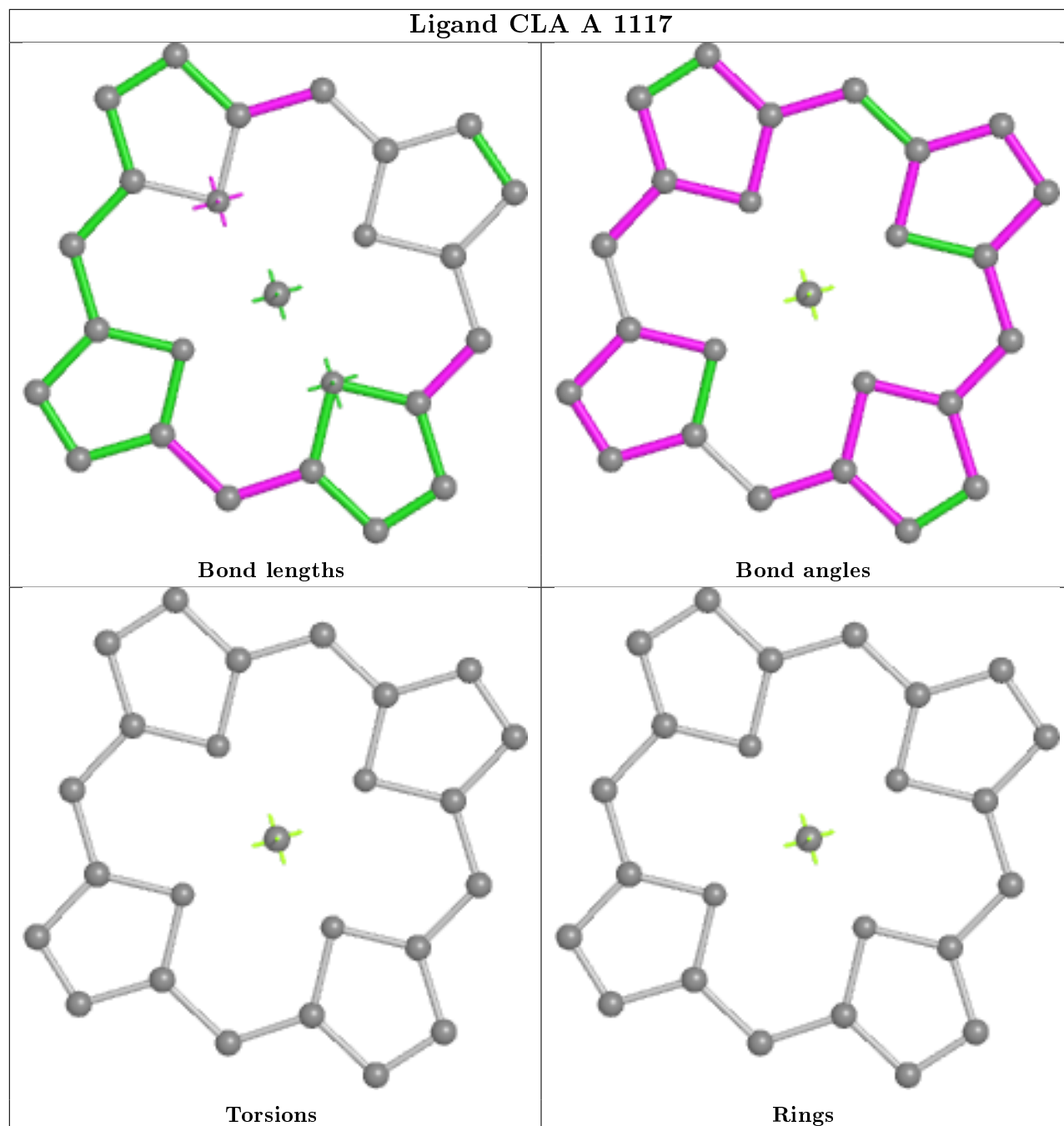


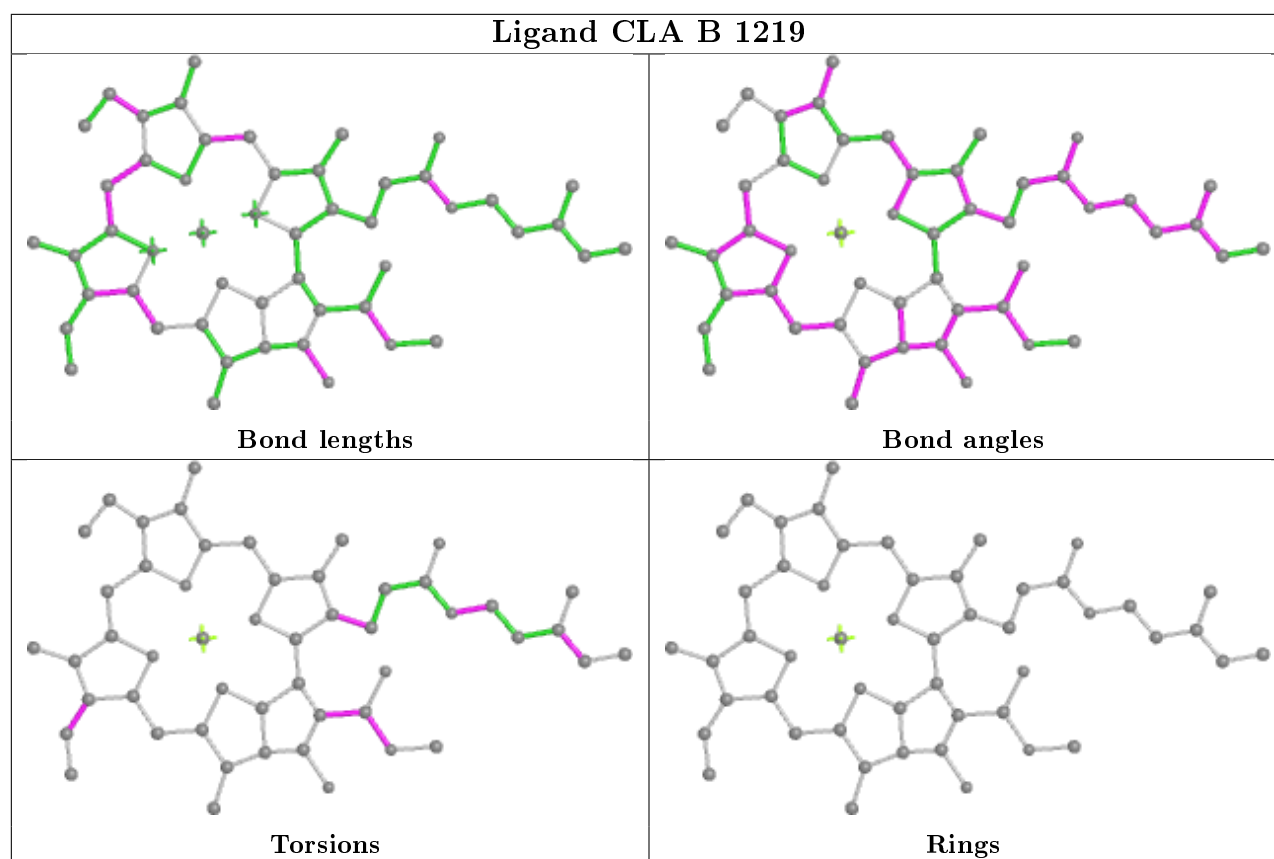




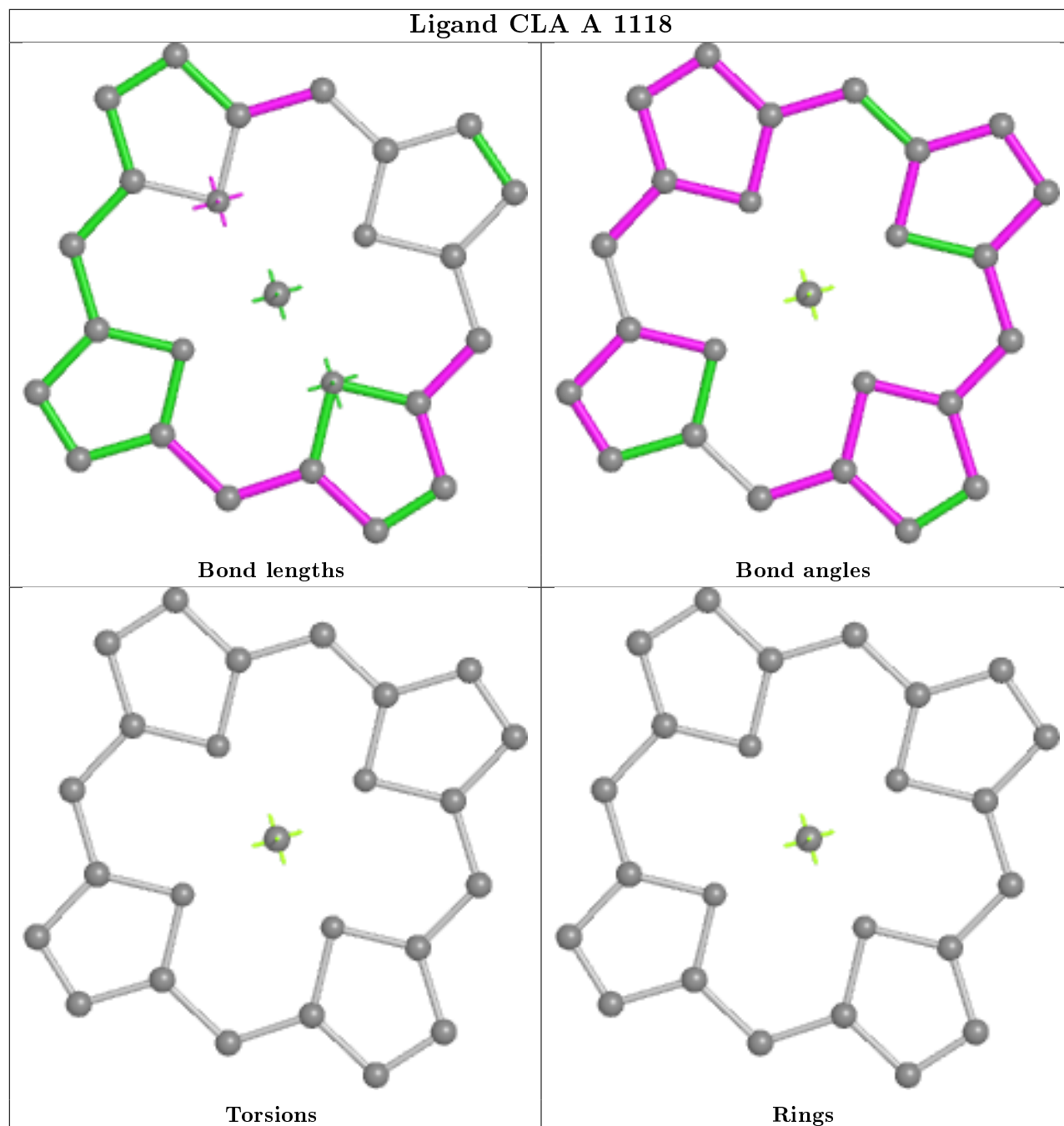


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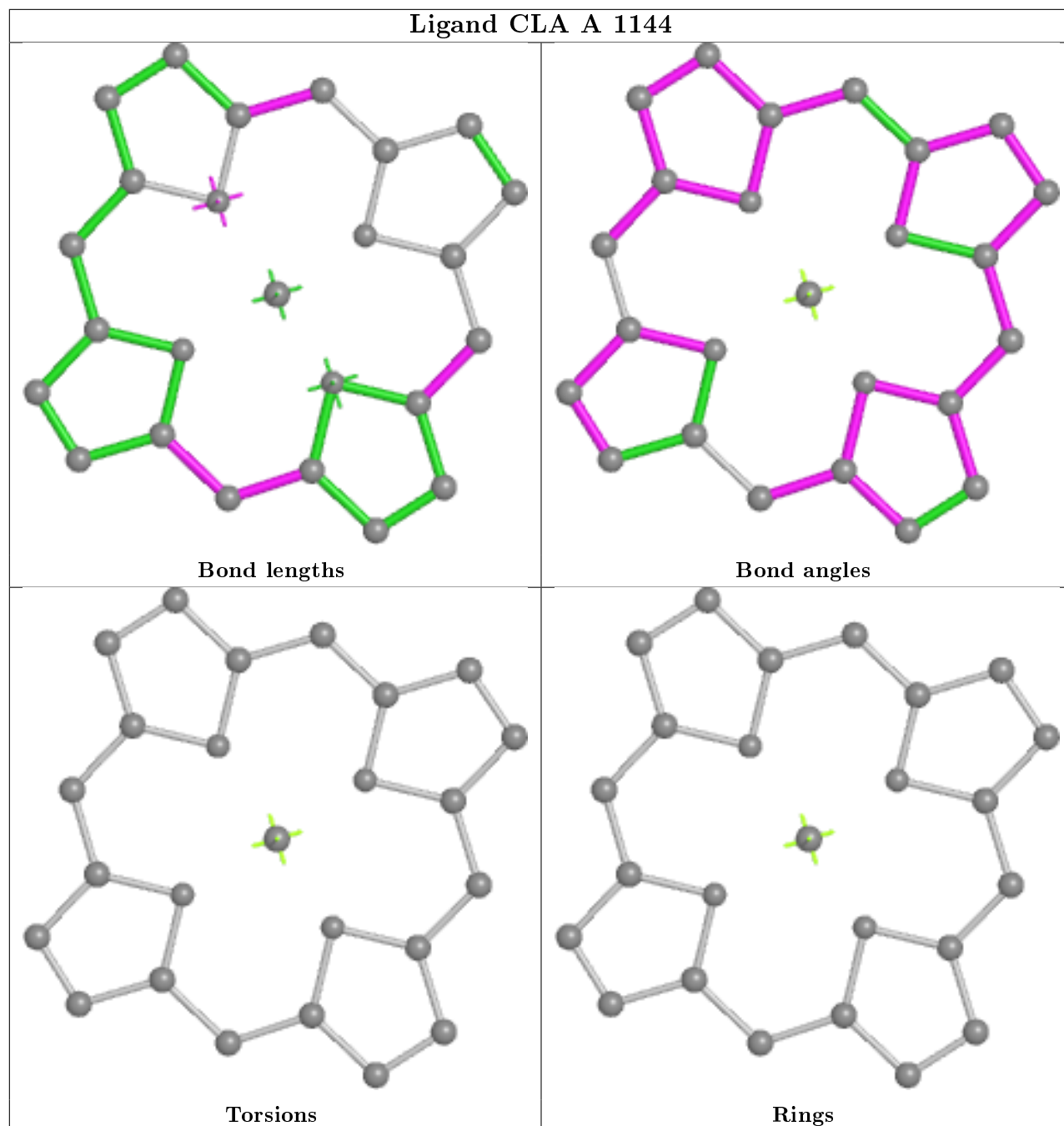


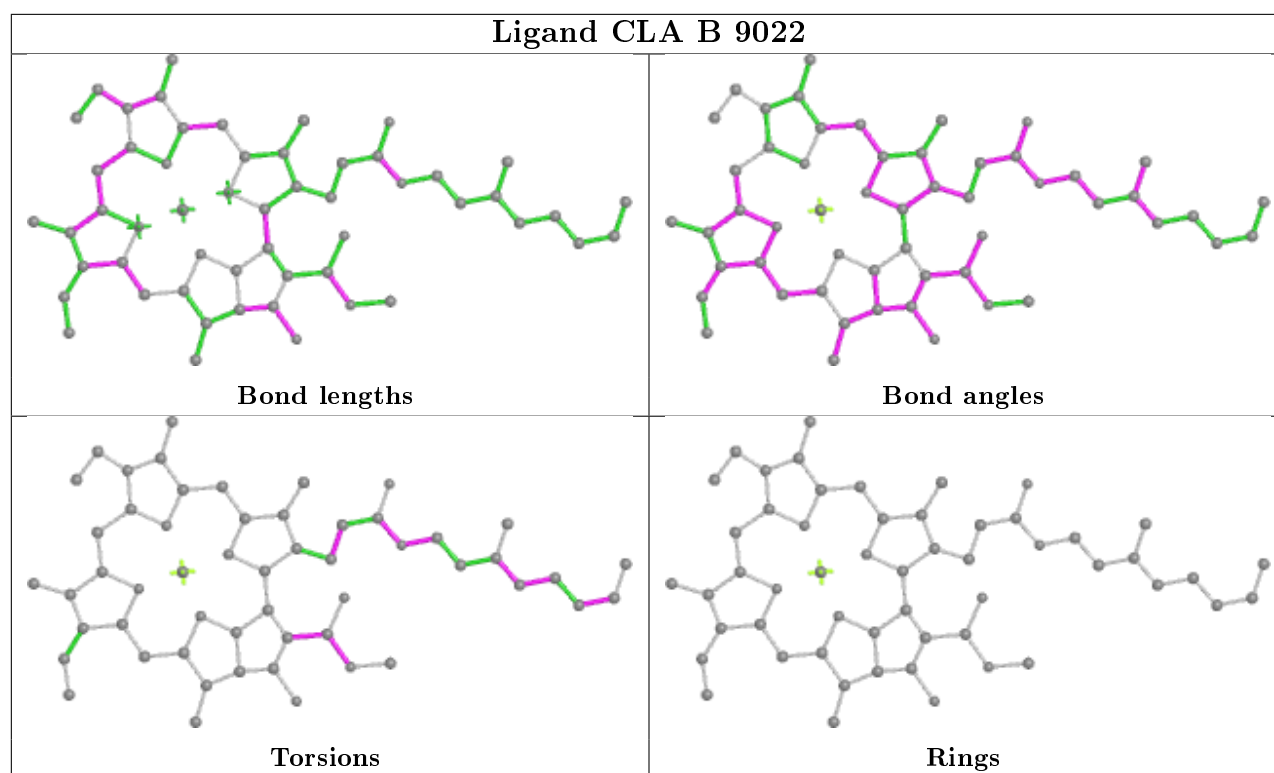


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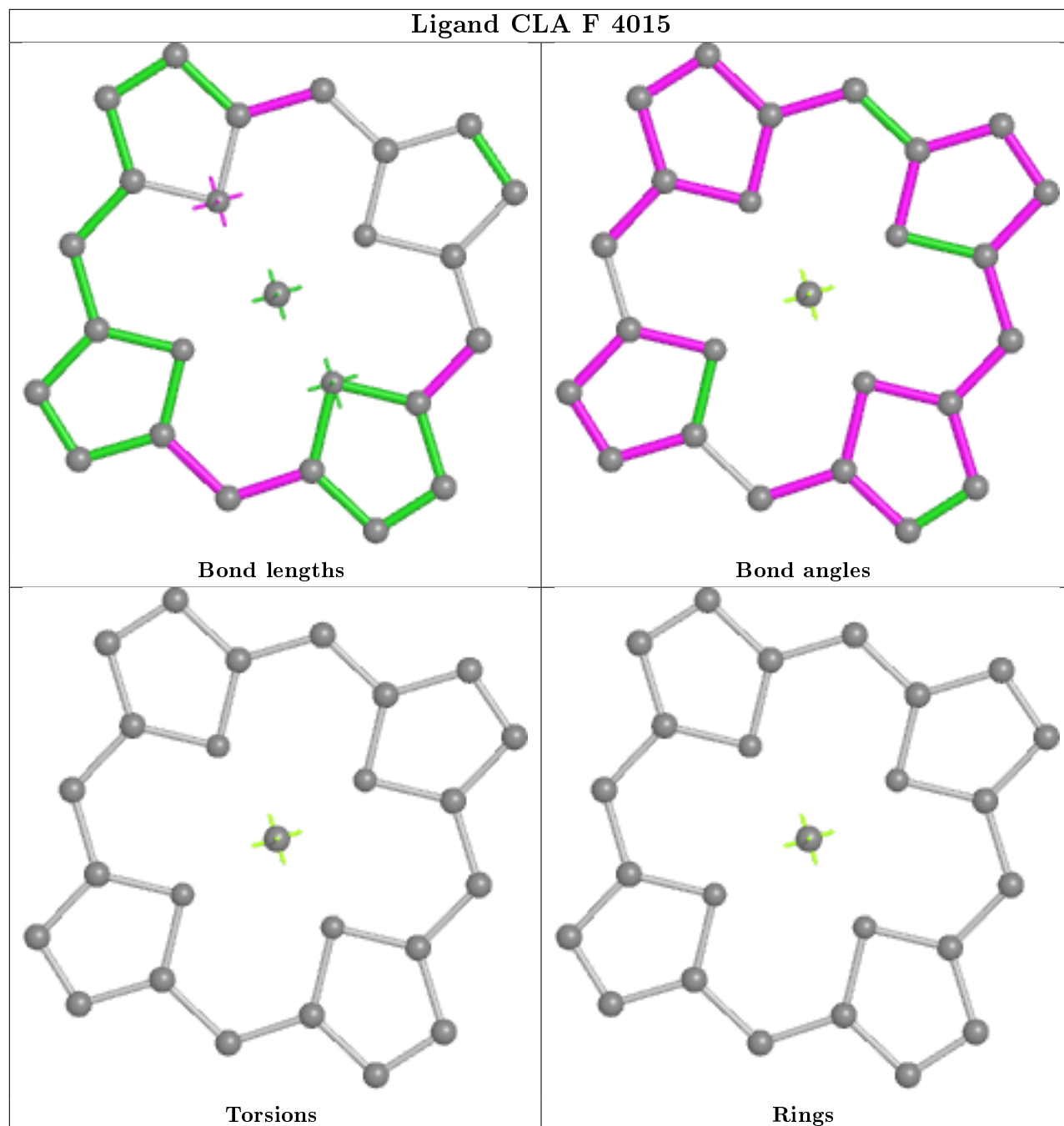


Ligand CLA A 1144

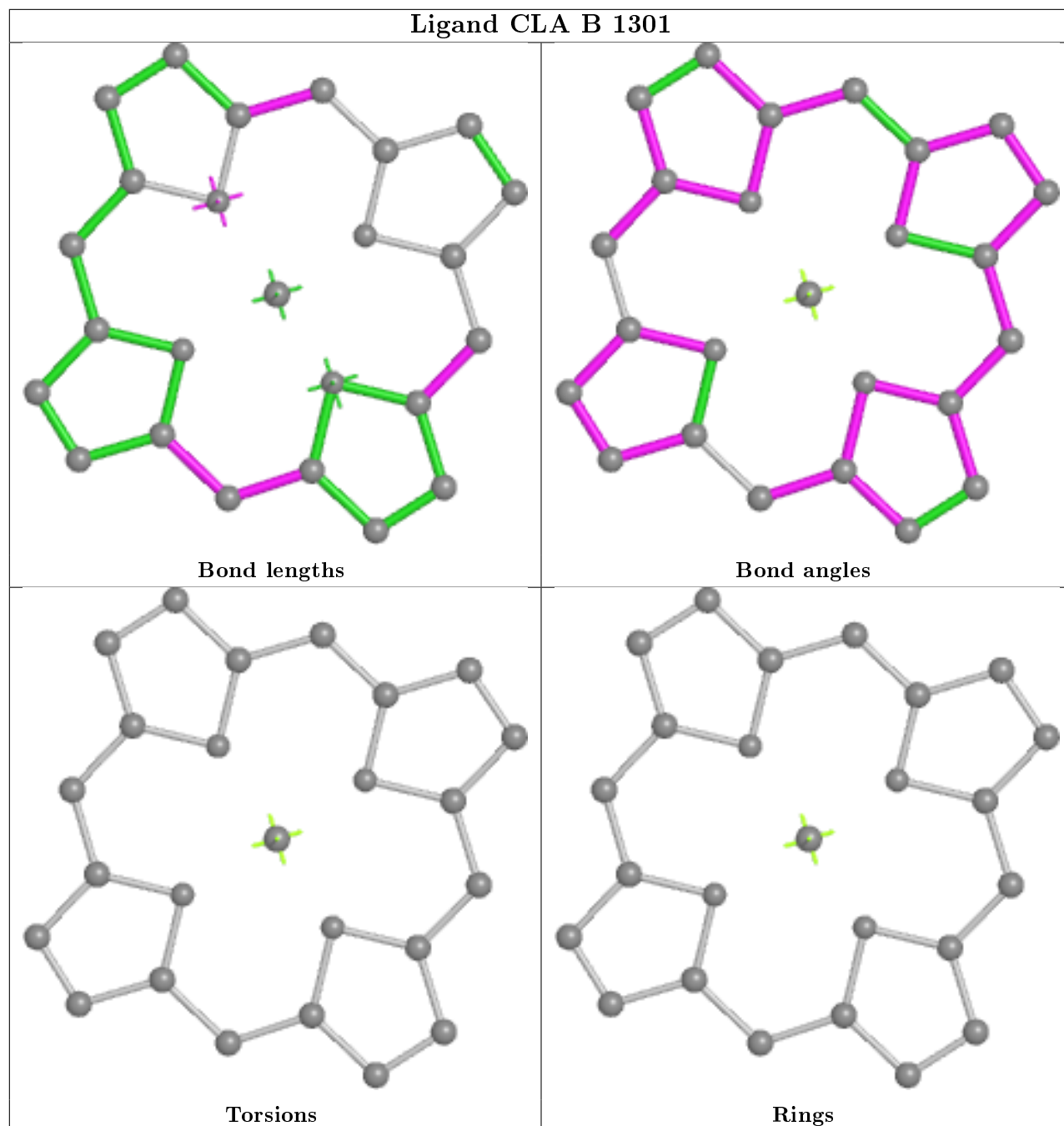




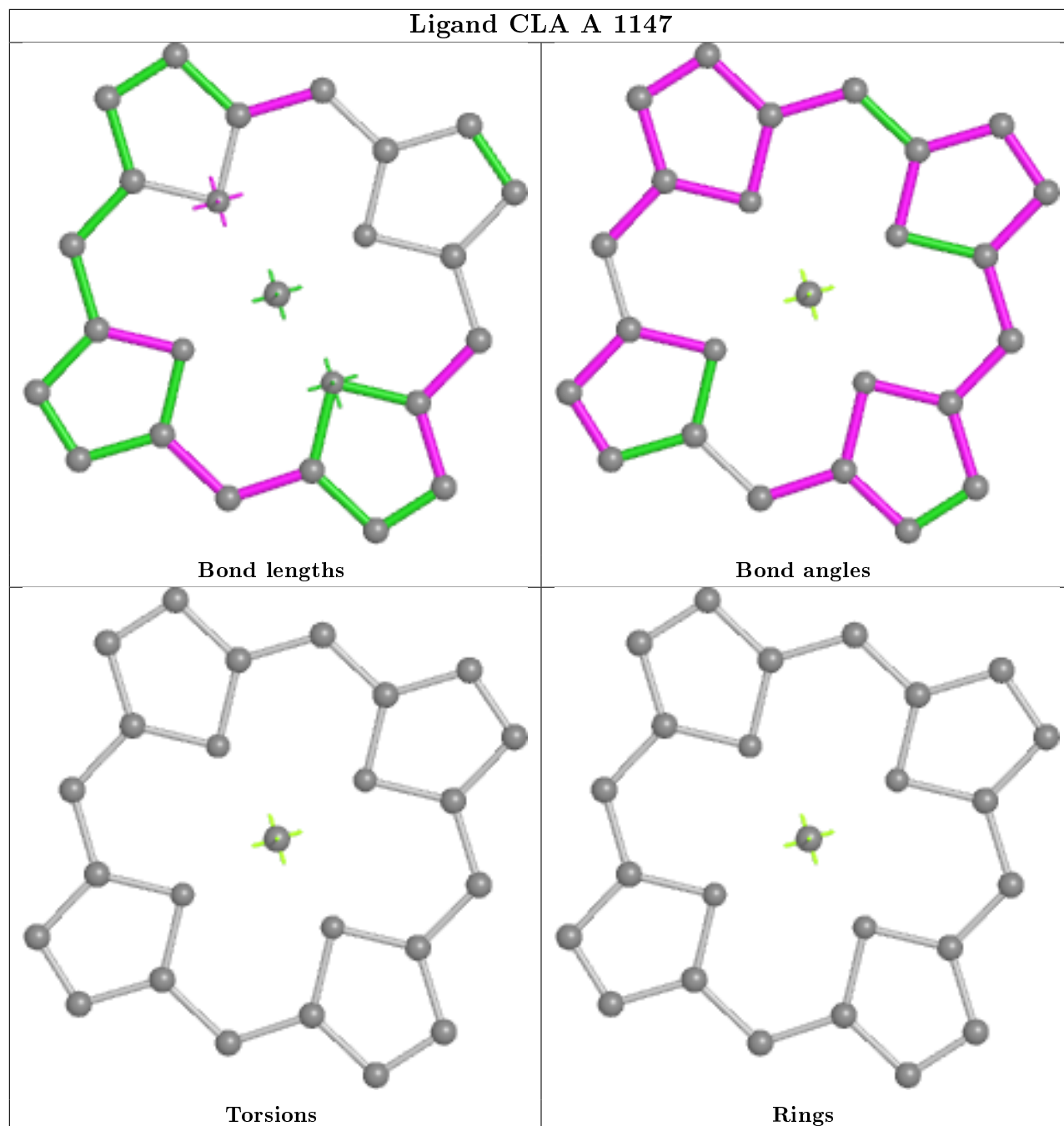
Ligand CLA F 4015



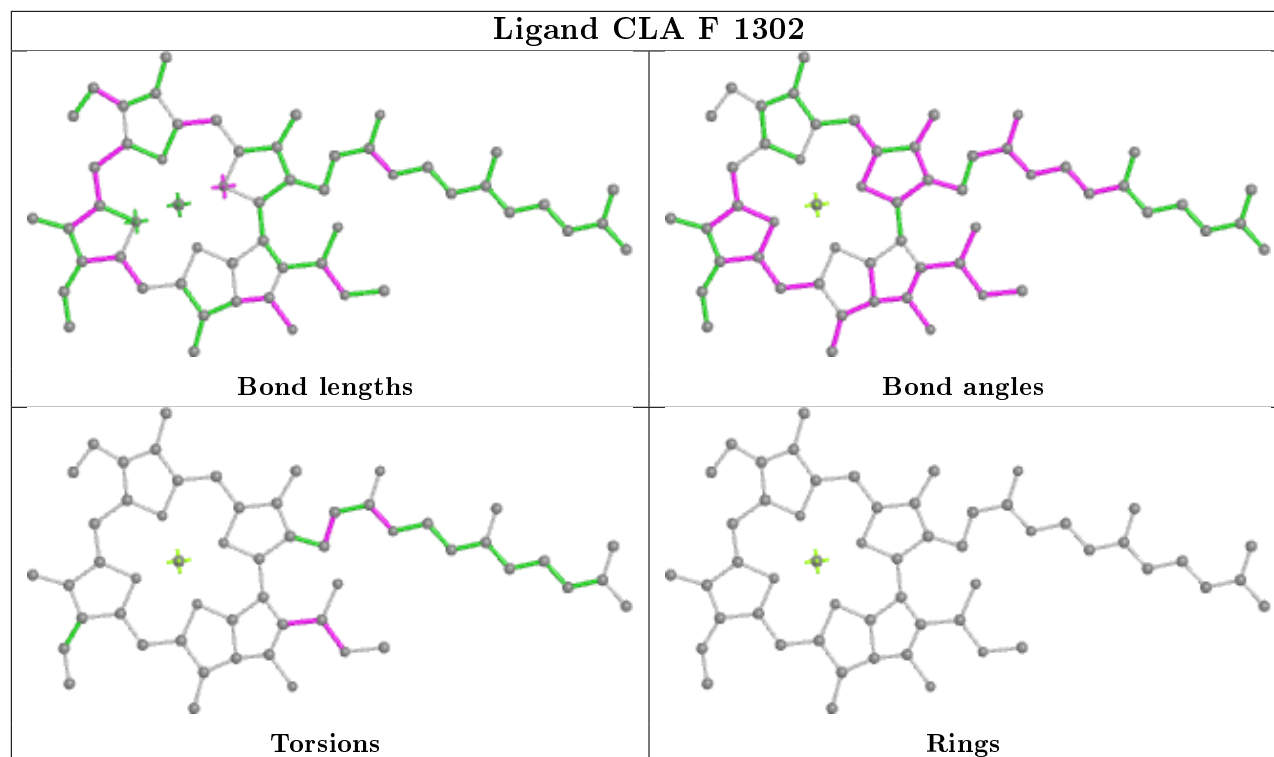
Ligand CLA B 1301



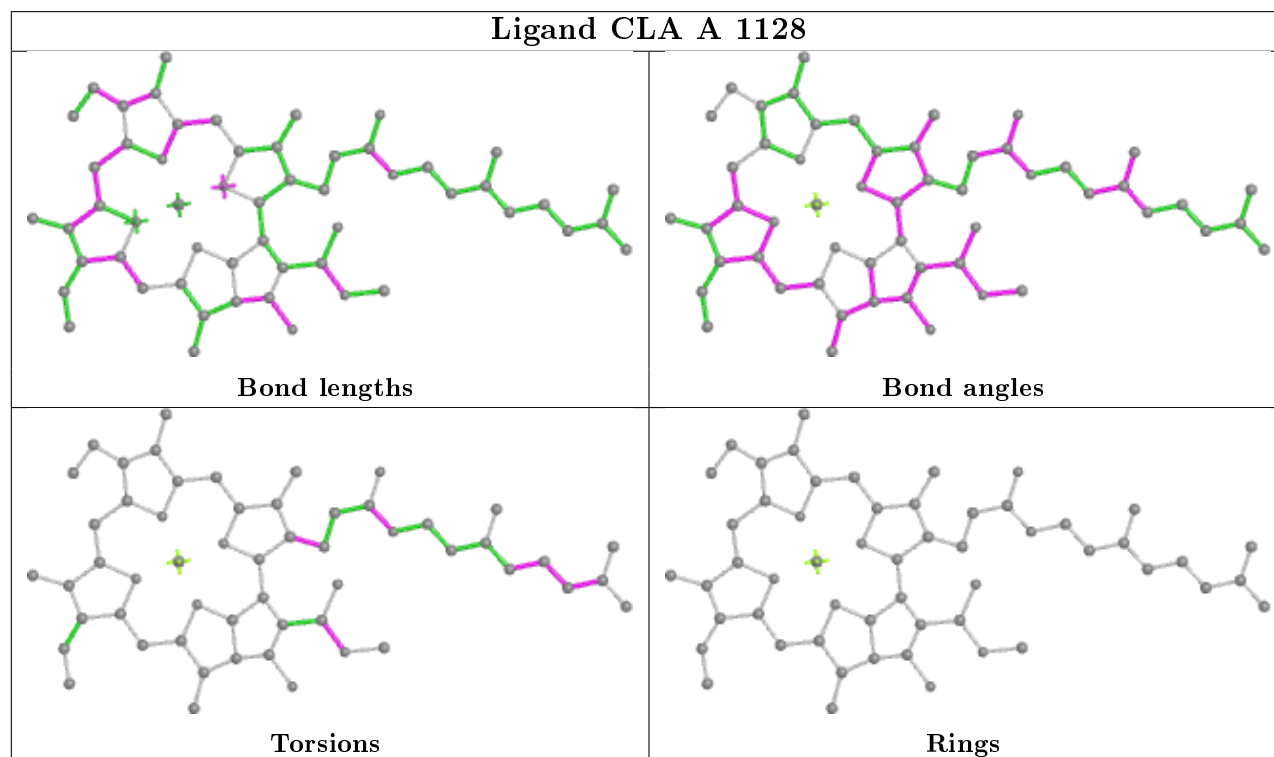
Ligand CLA A 1147

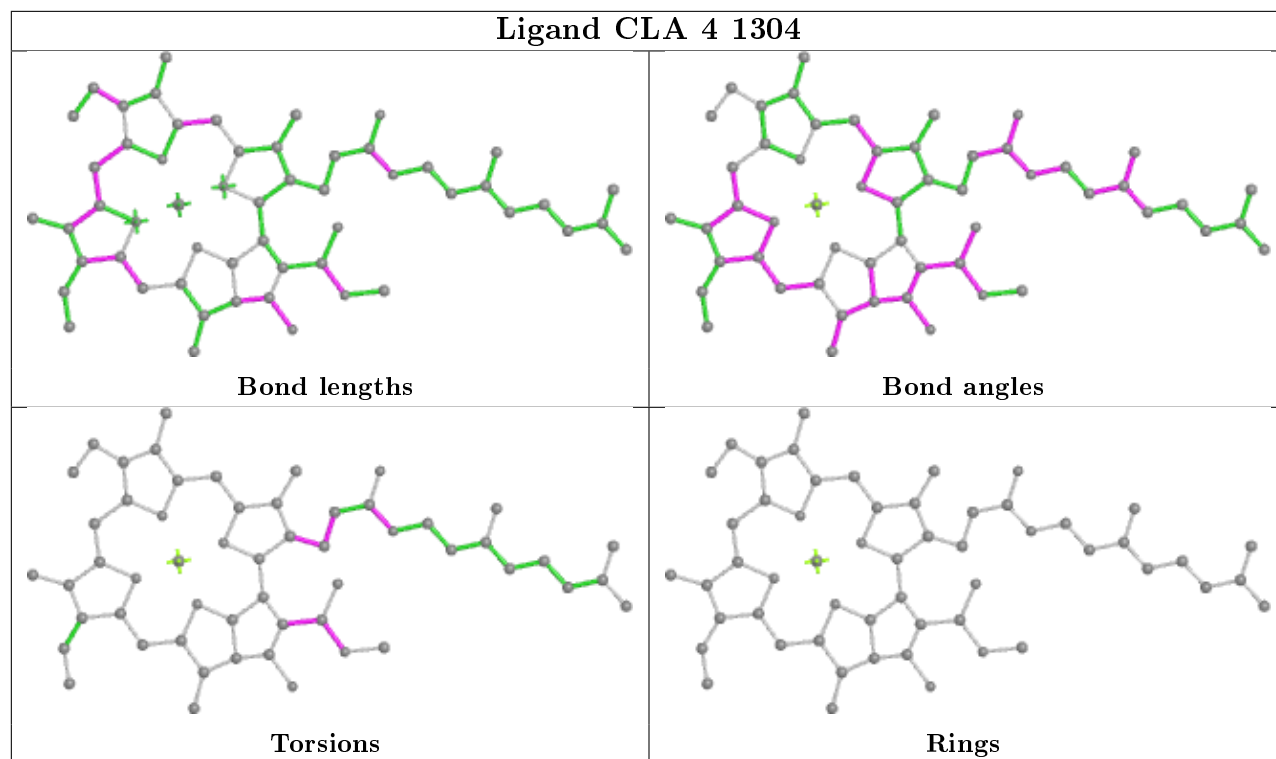


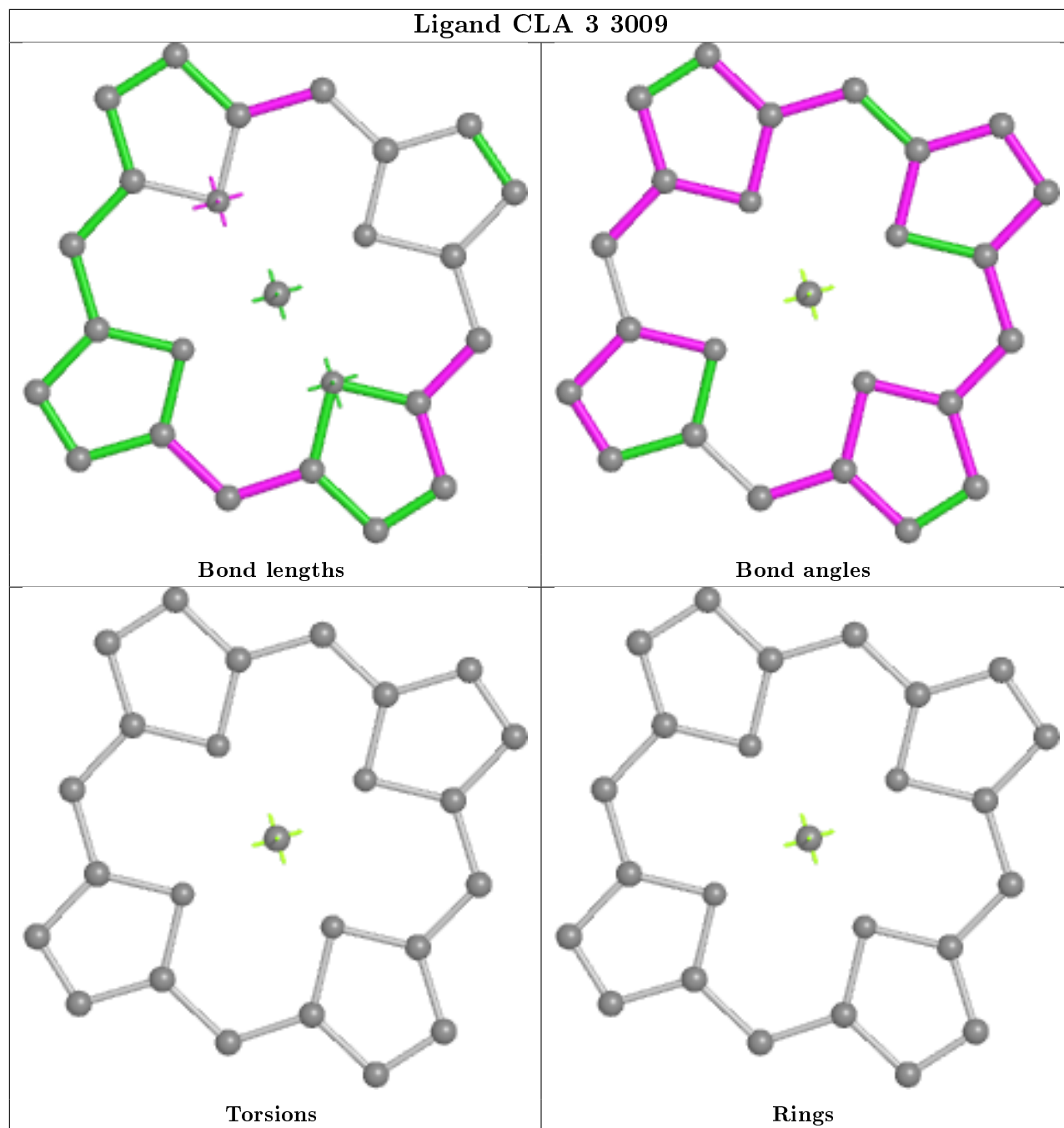
Ligand CLA F 1302

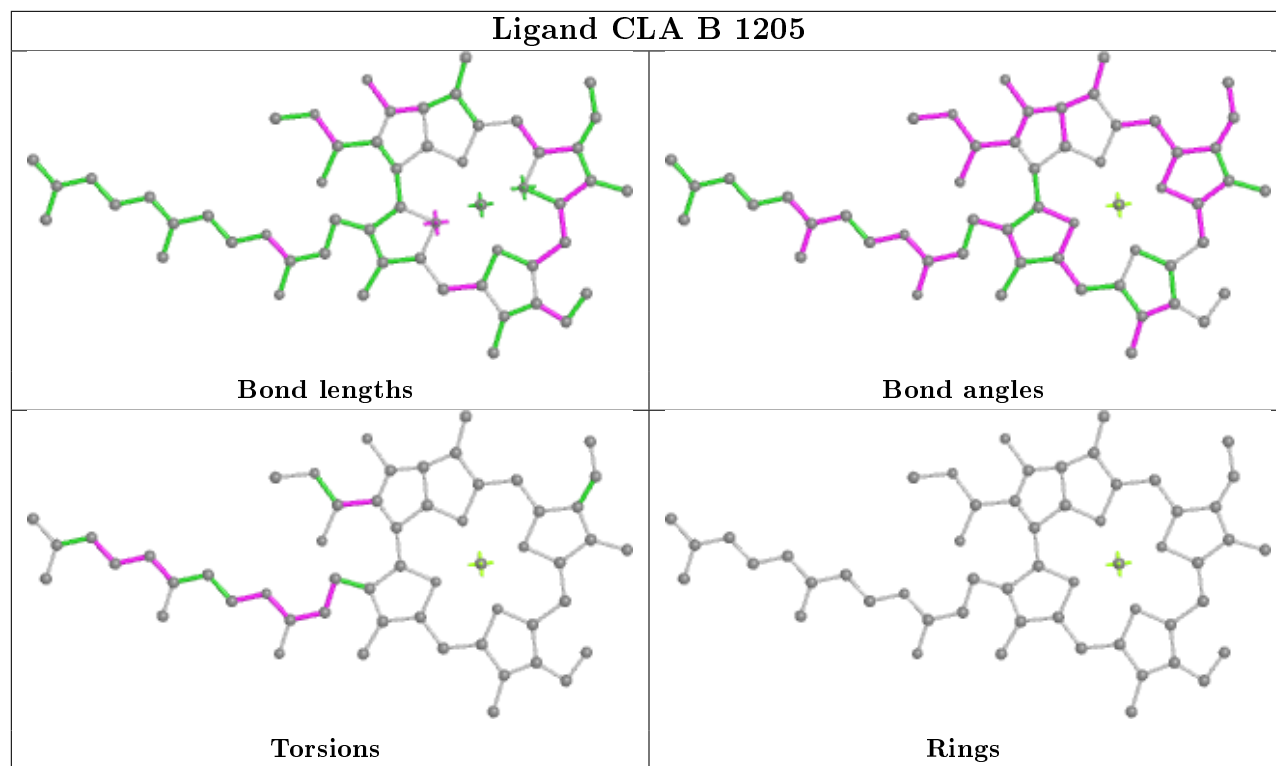


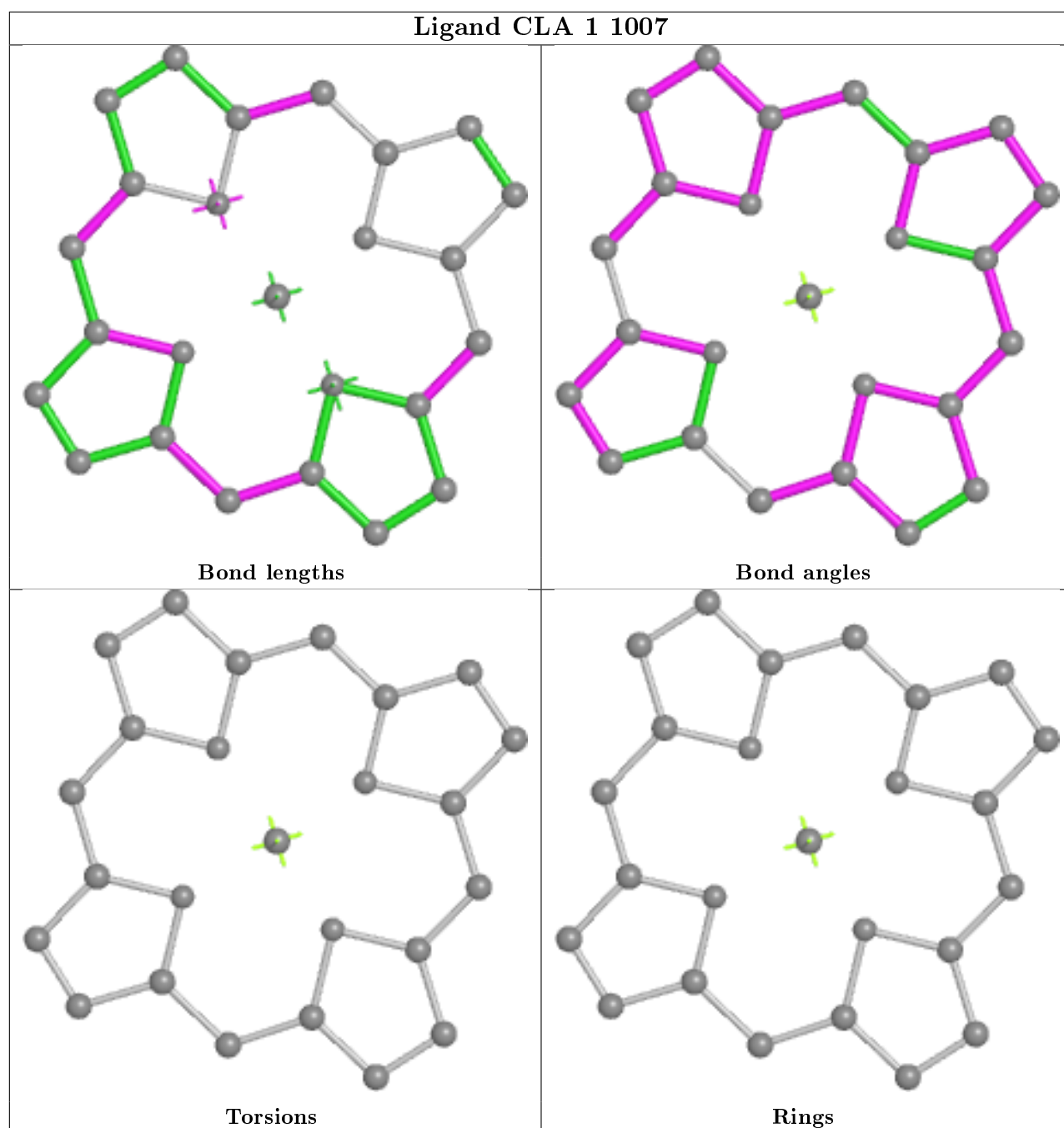
Ligand CLA A 1128

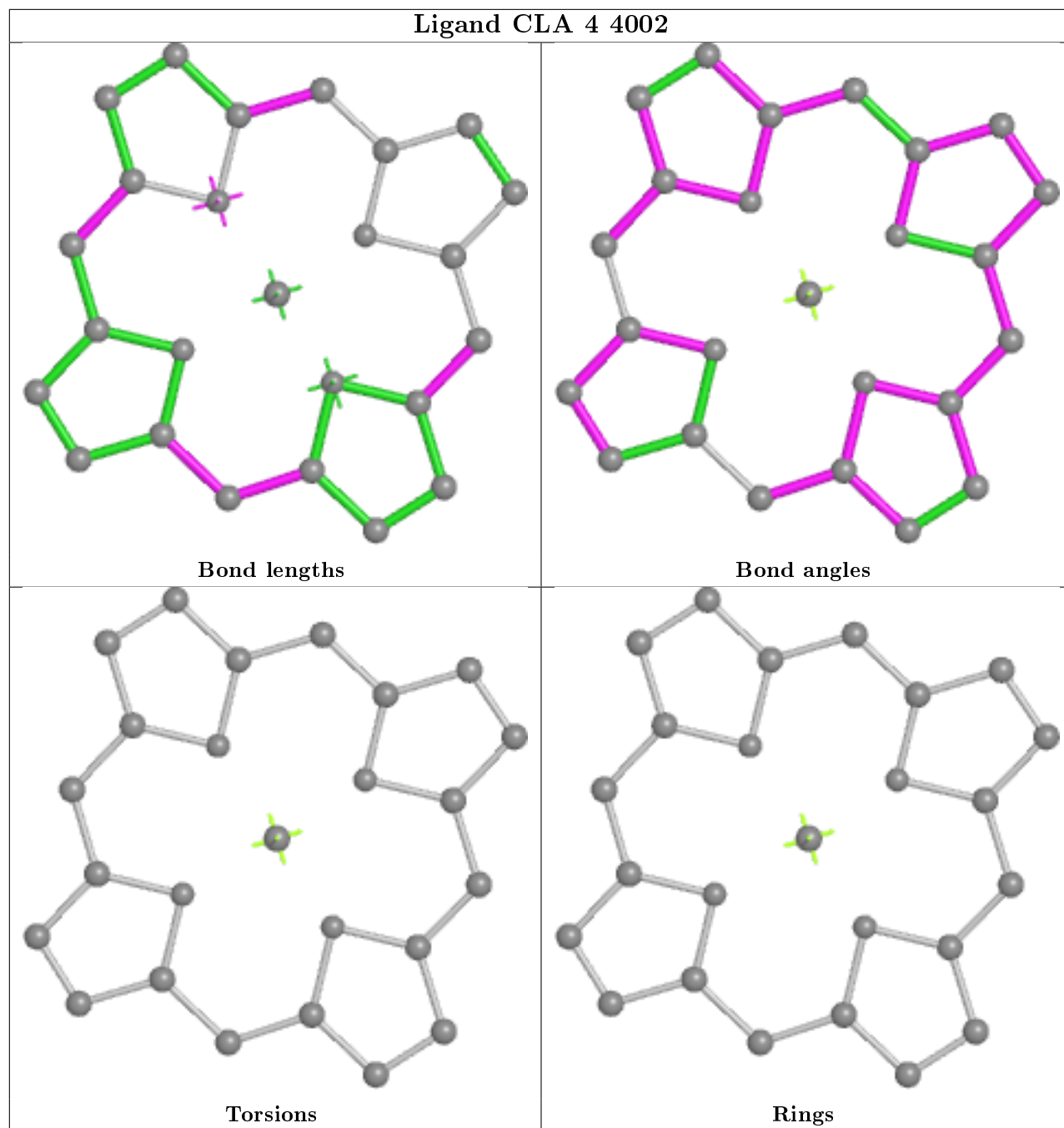


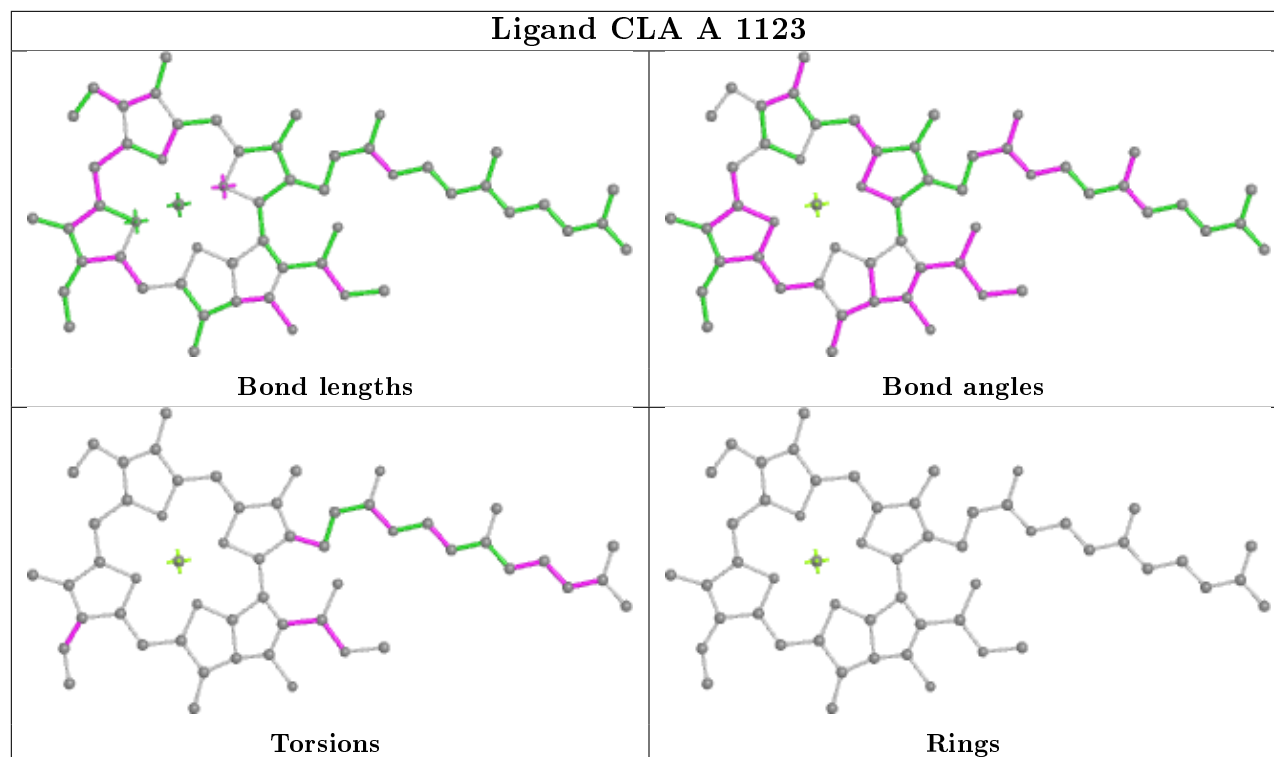
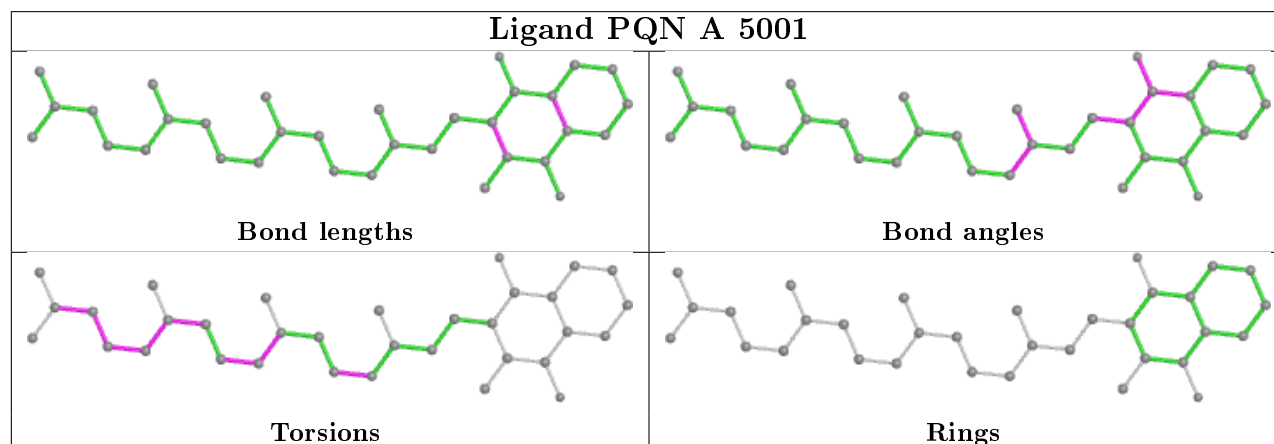


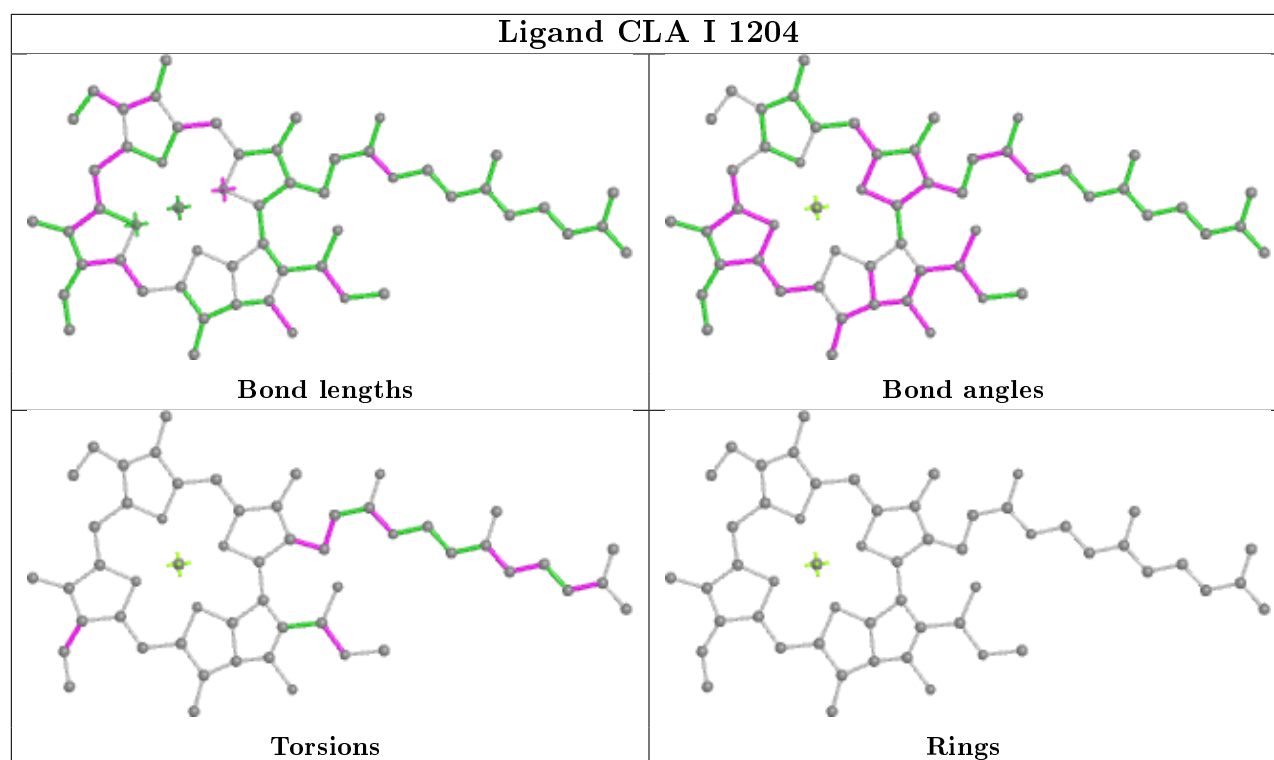




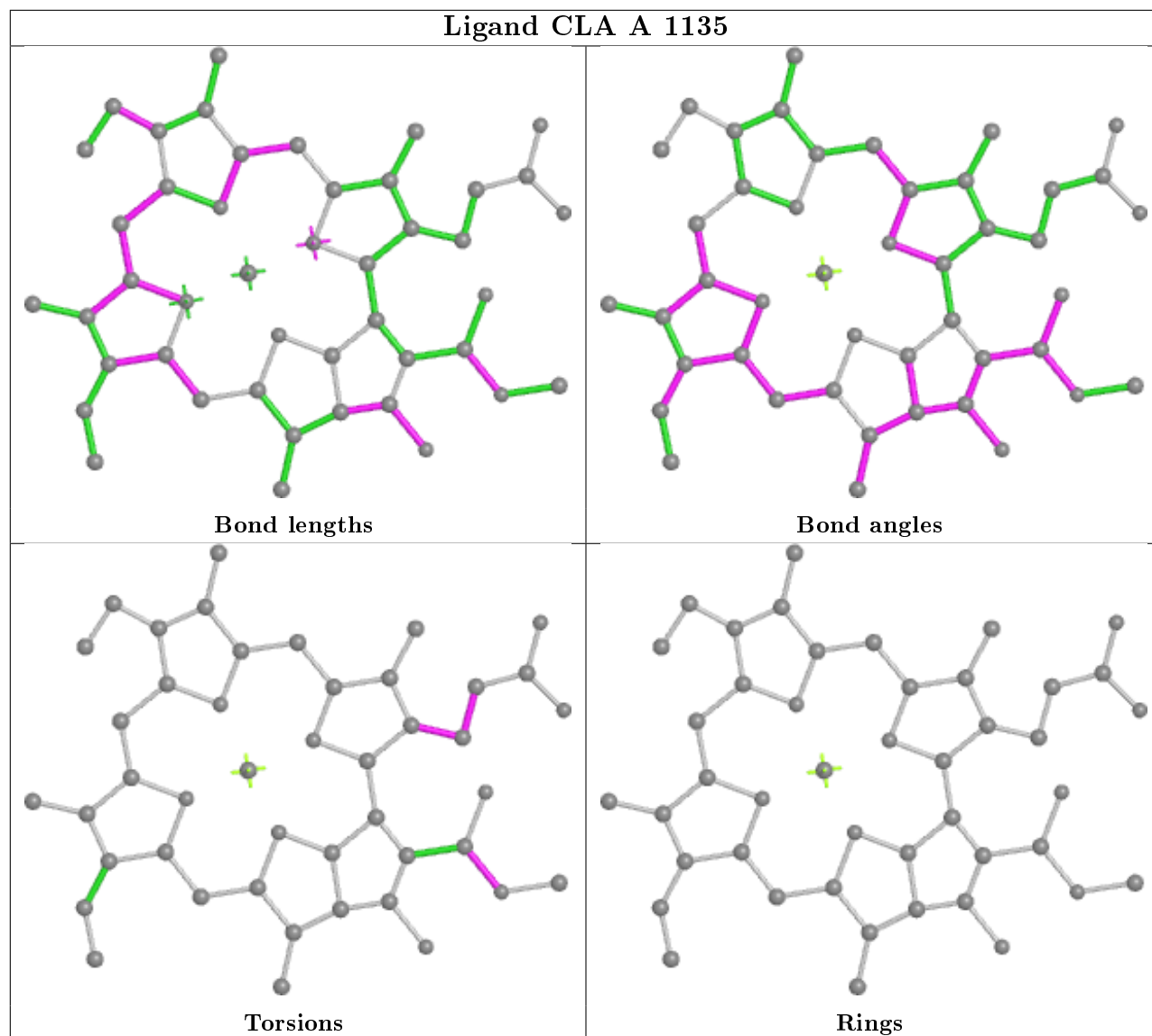


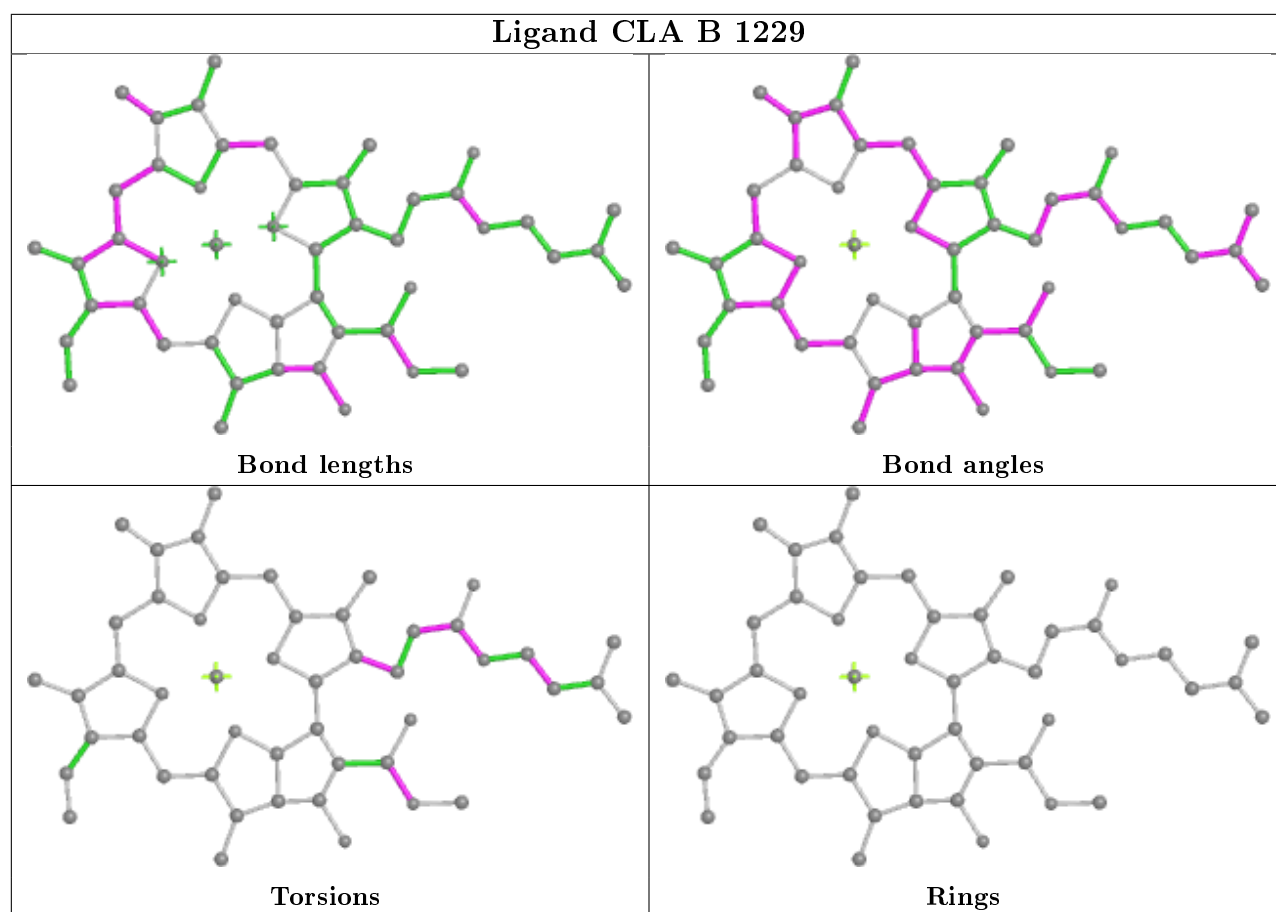


Ligand CLA A 1123**Ligand PQN A 5001**

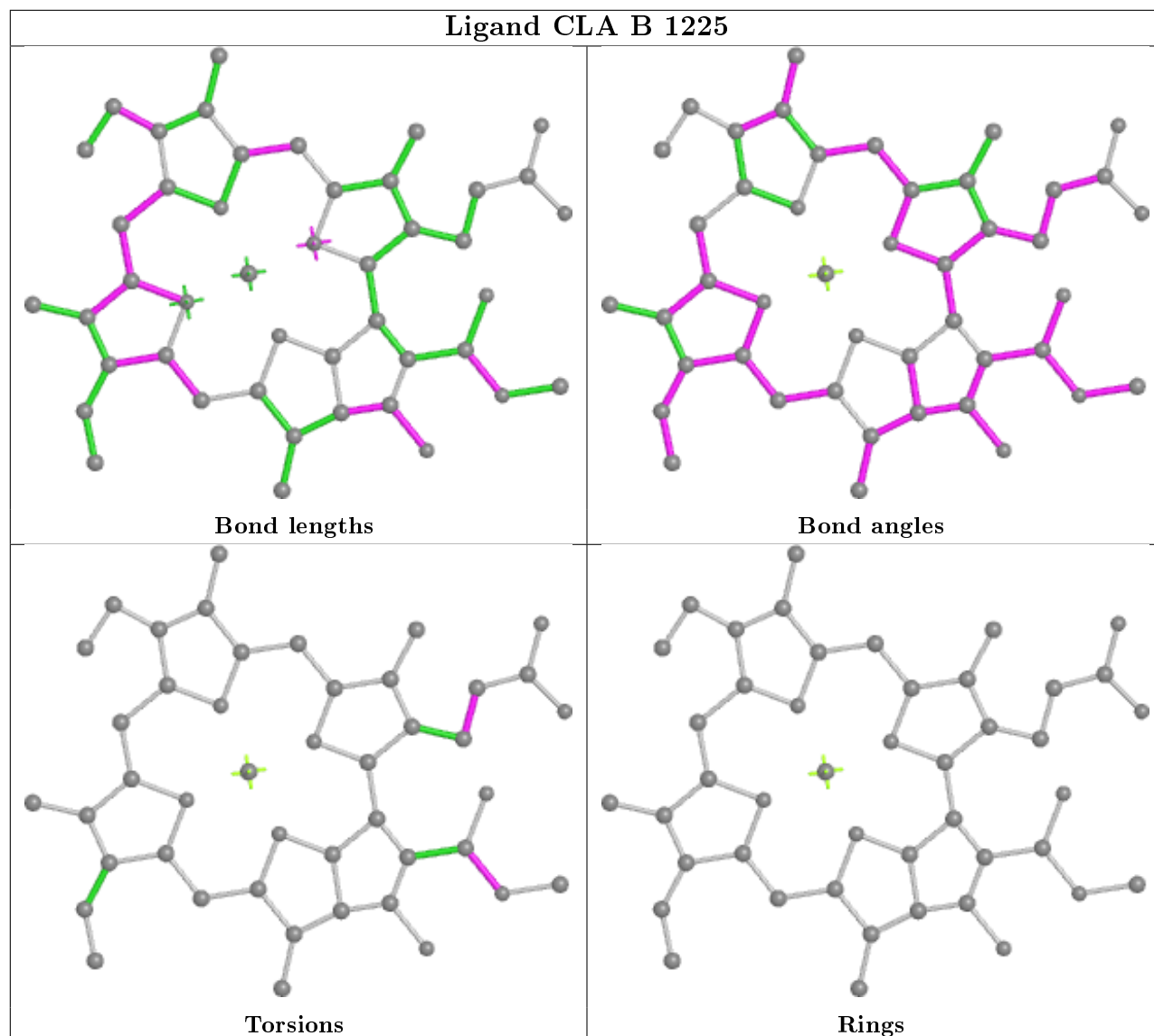


Ligand CLA A 1135

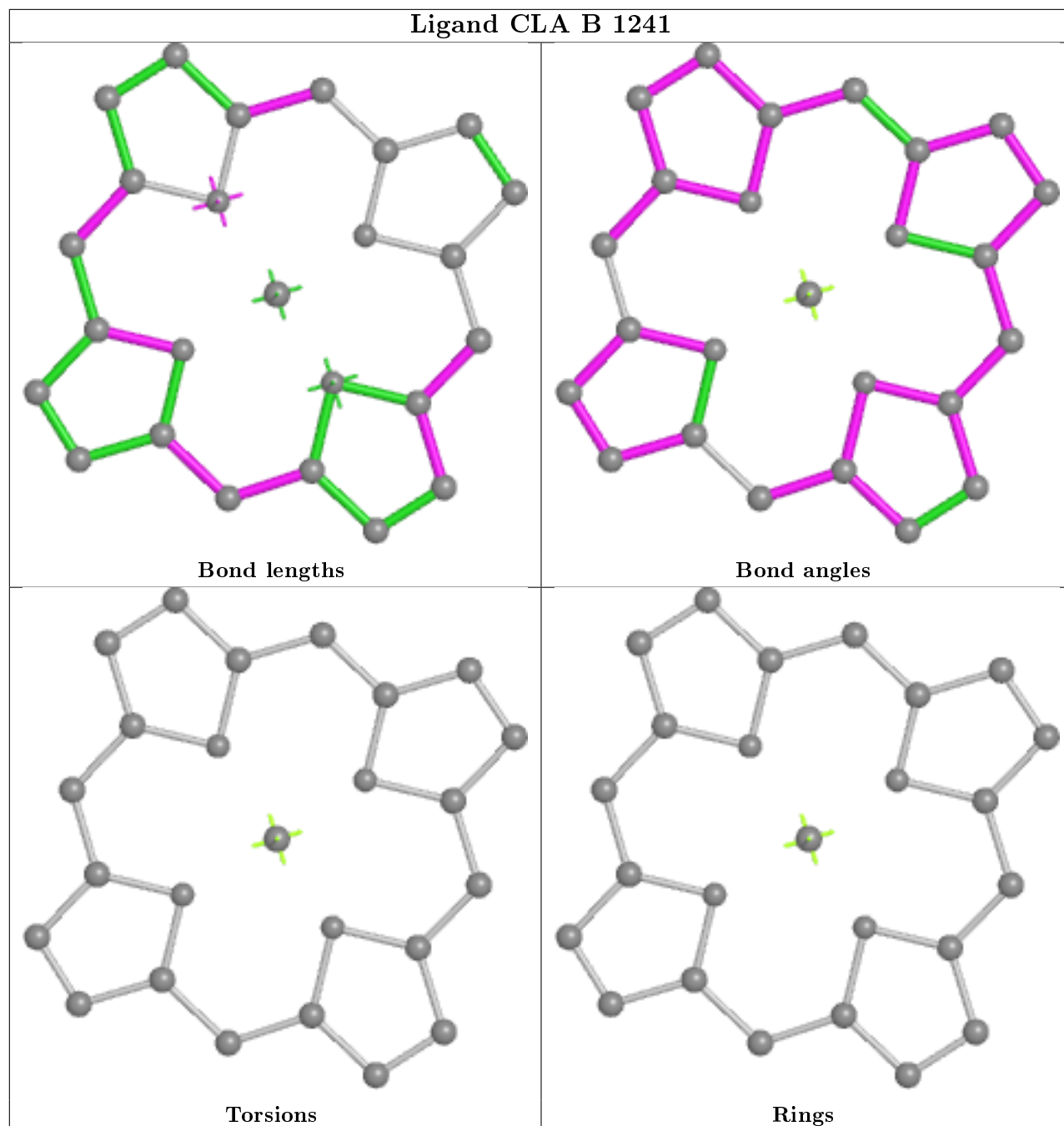


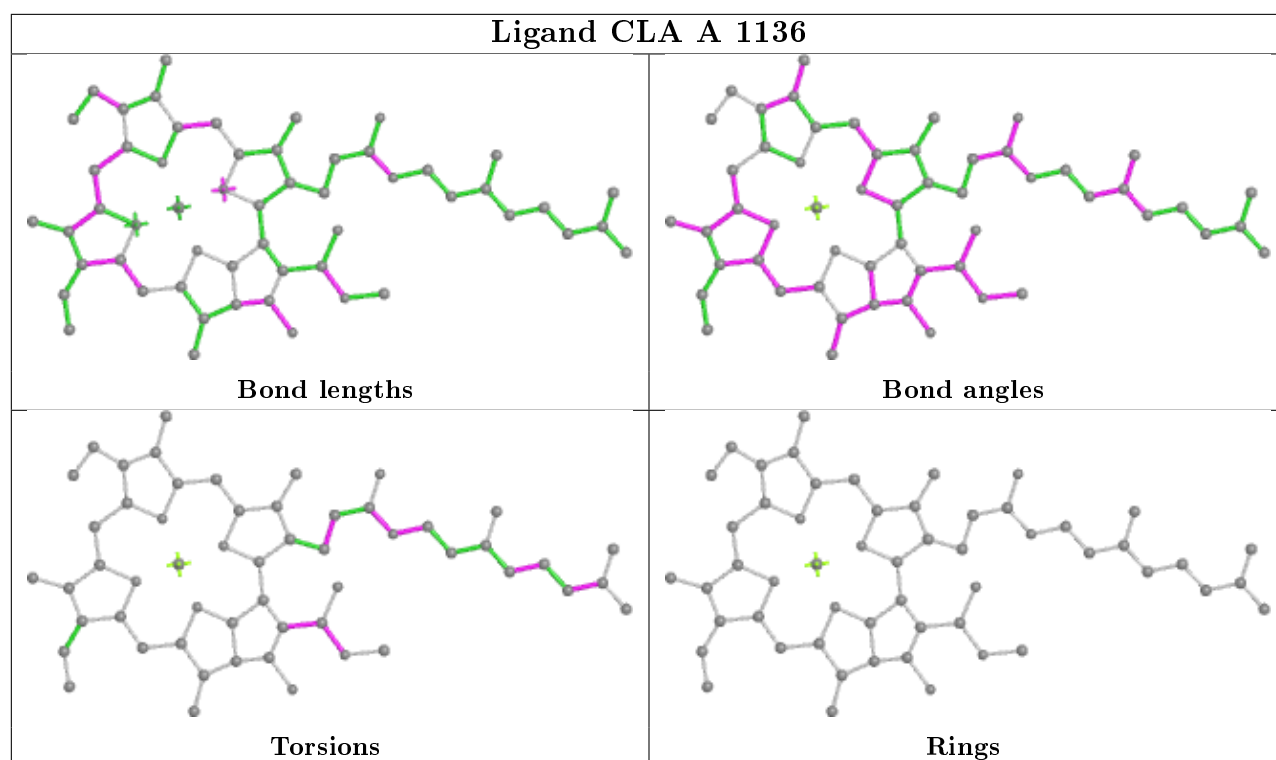


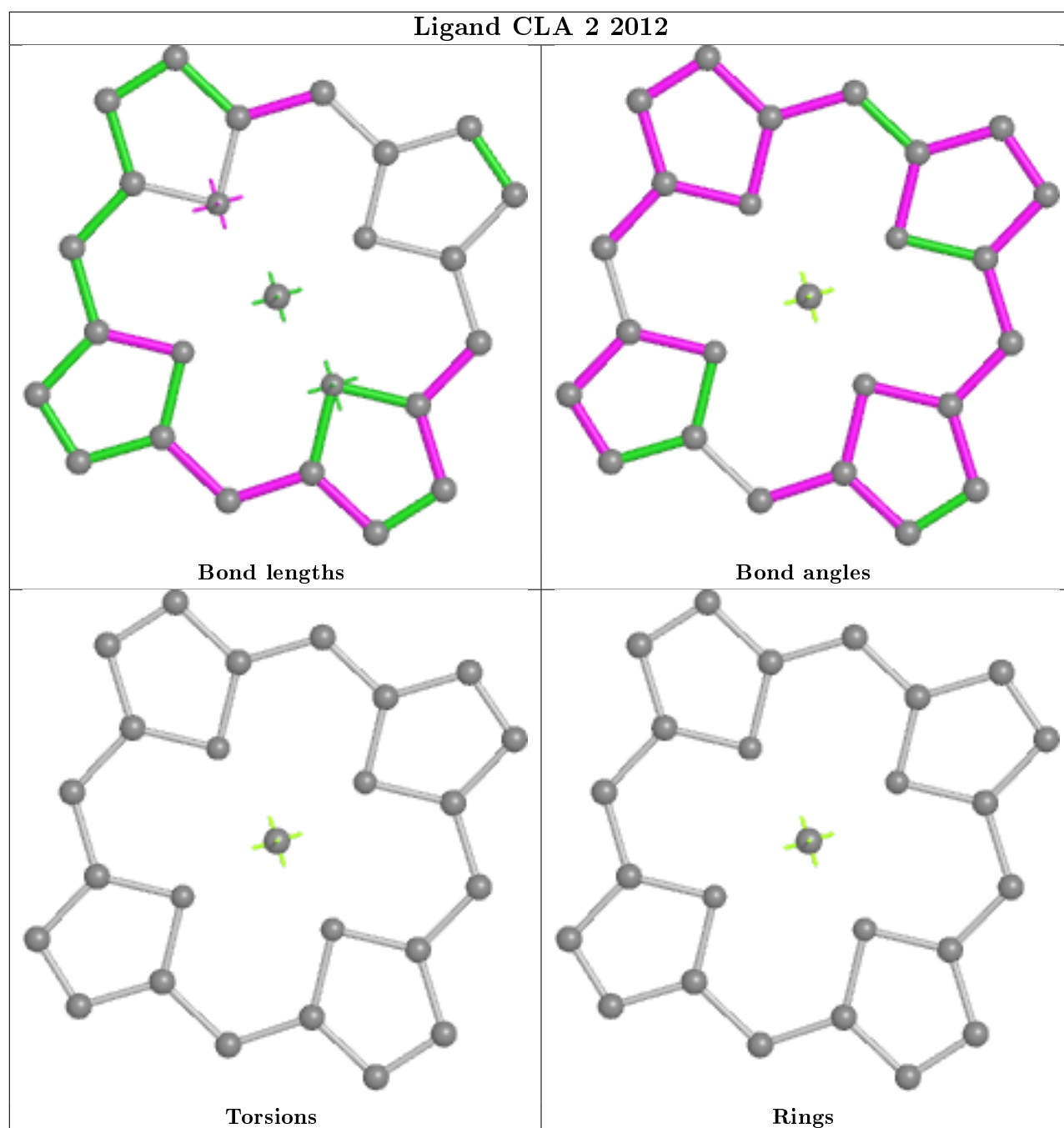
Ligand CLA B 1225

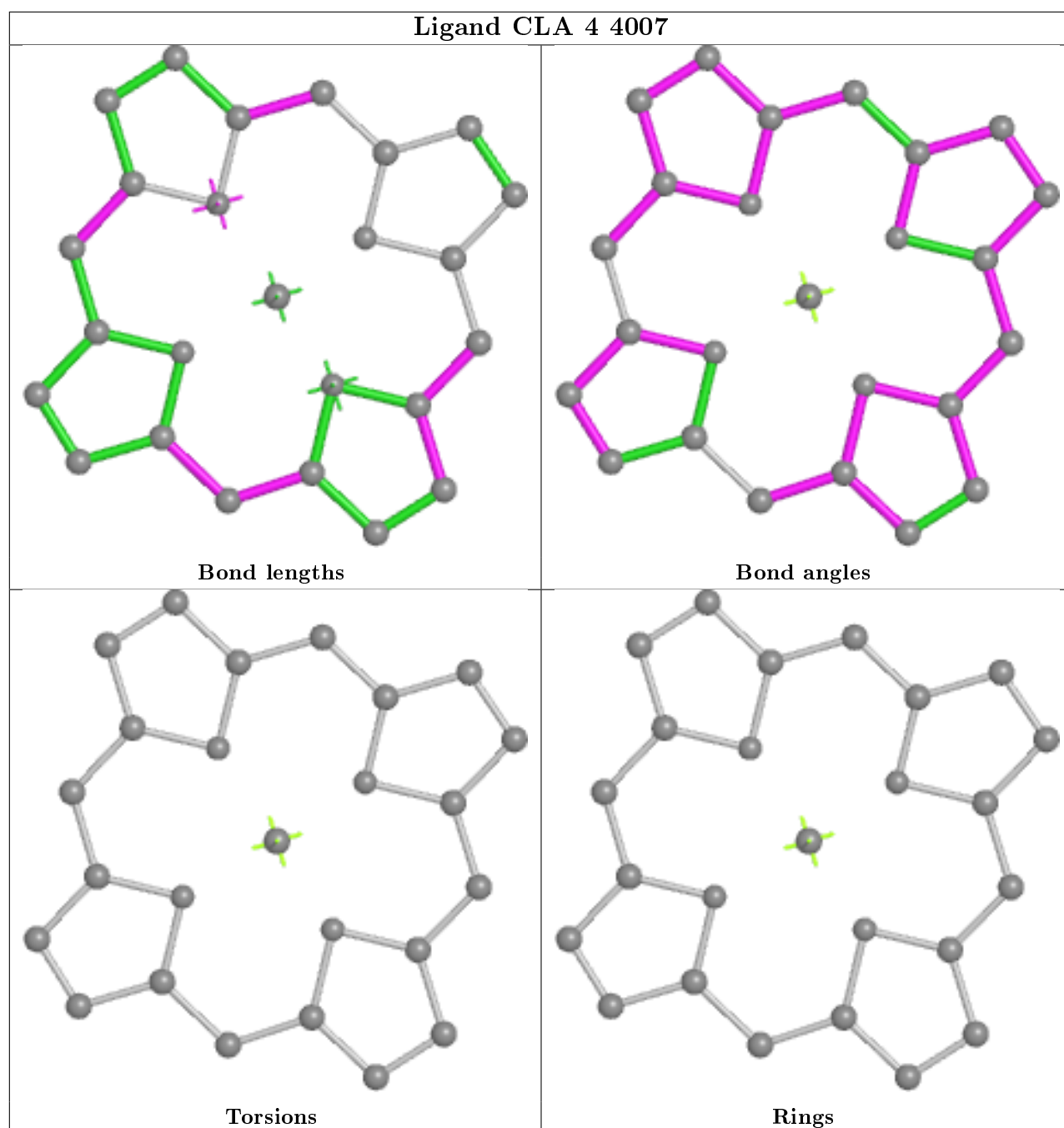


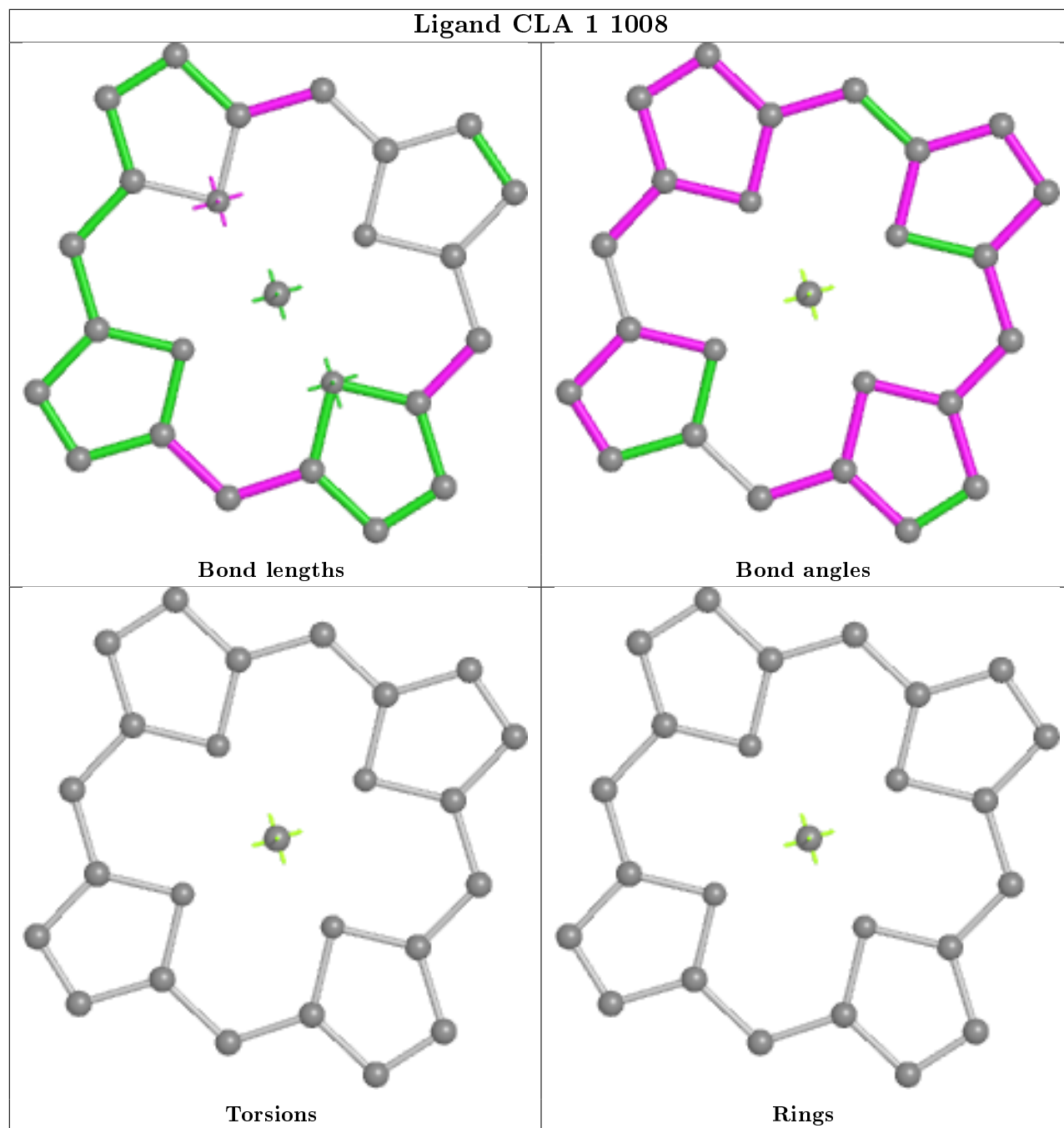
Ligand CLA B 1241



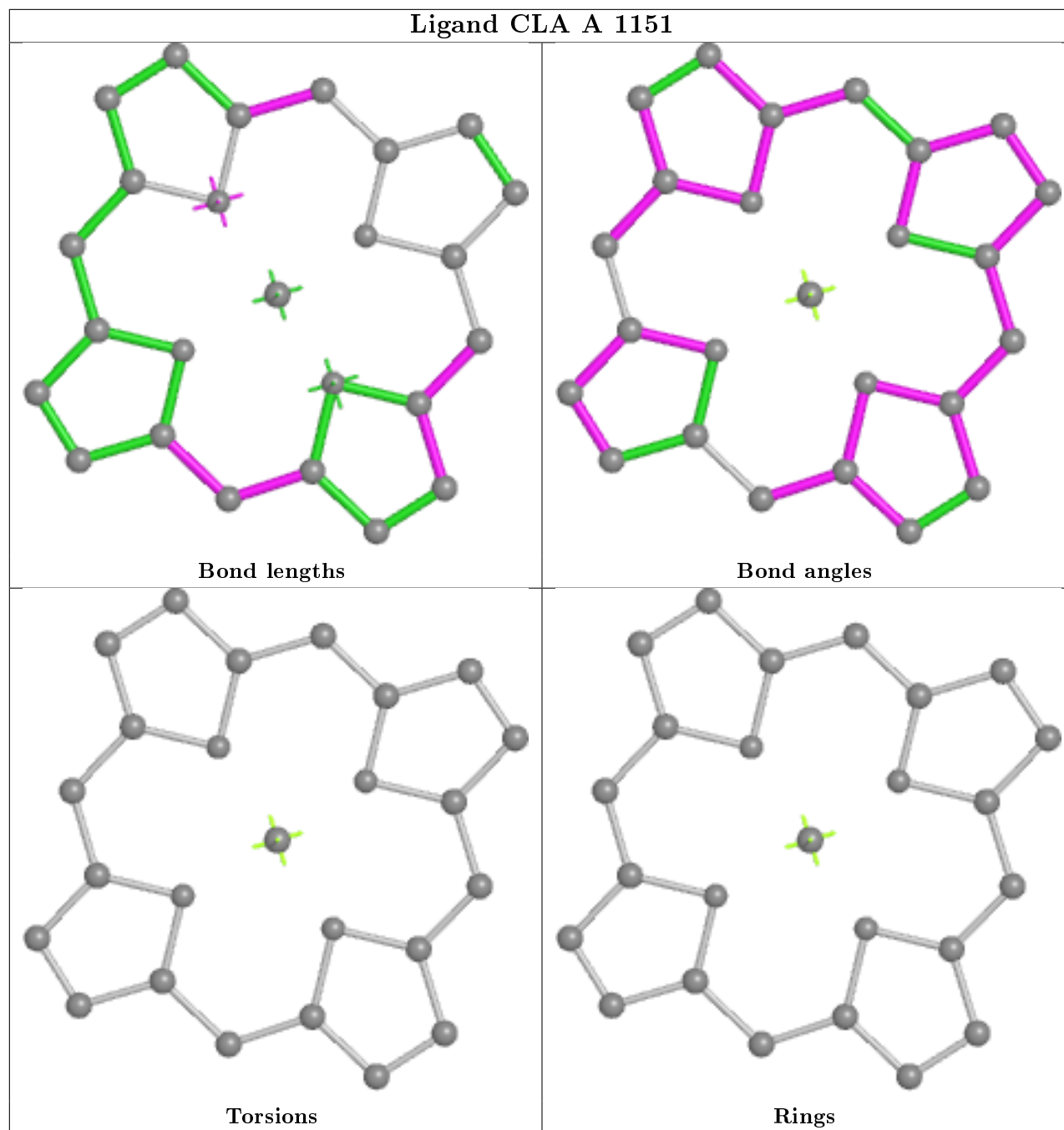




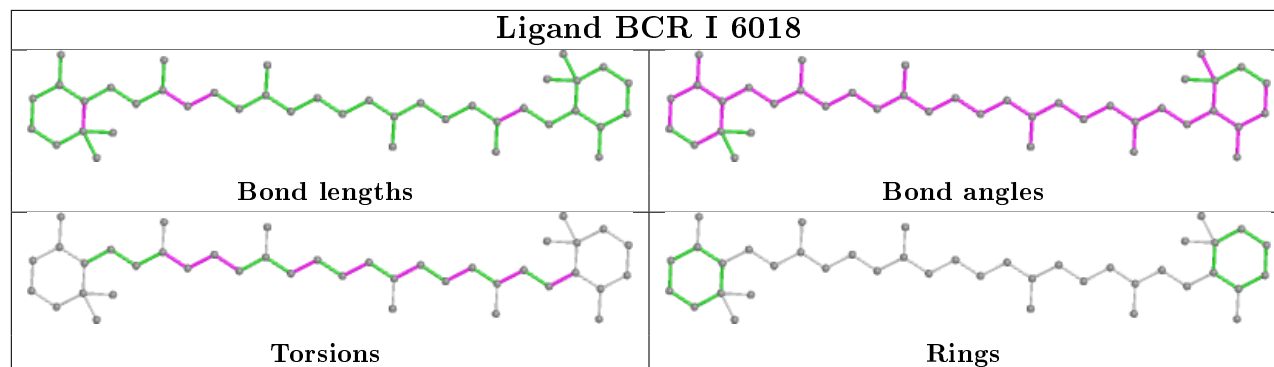




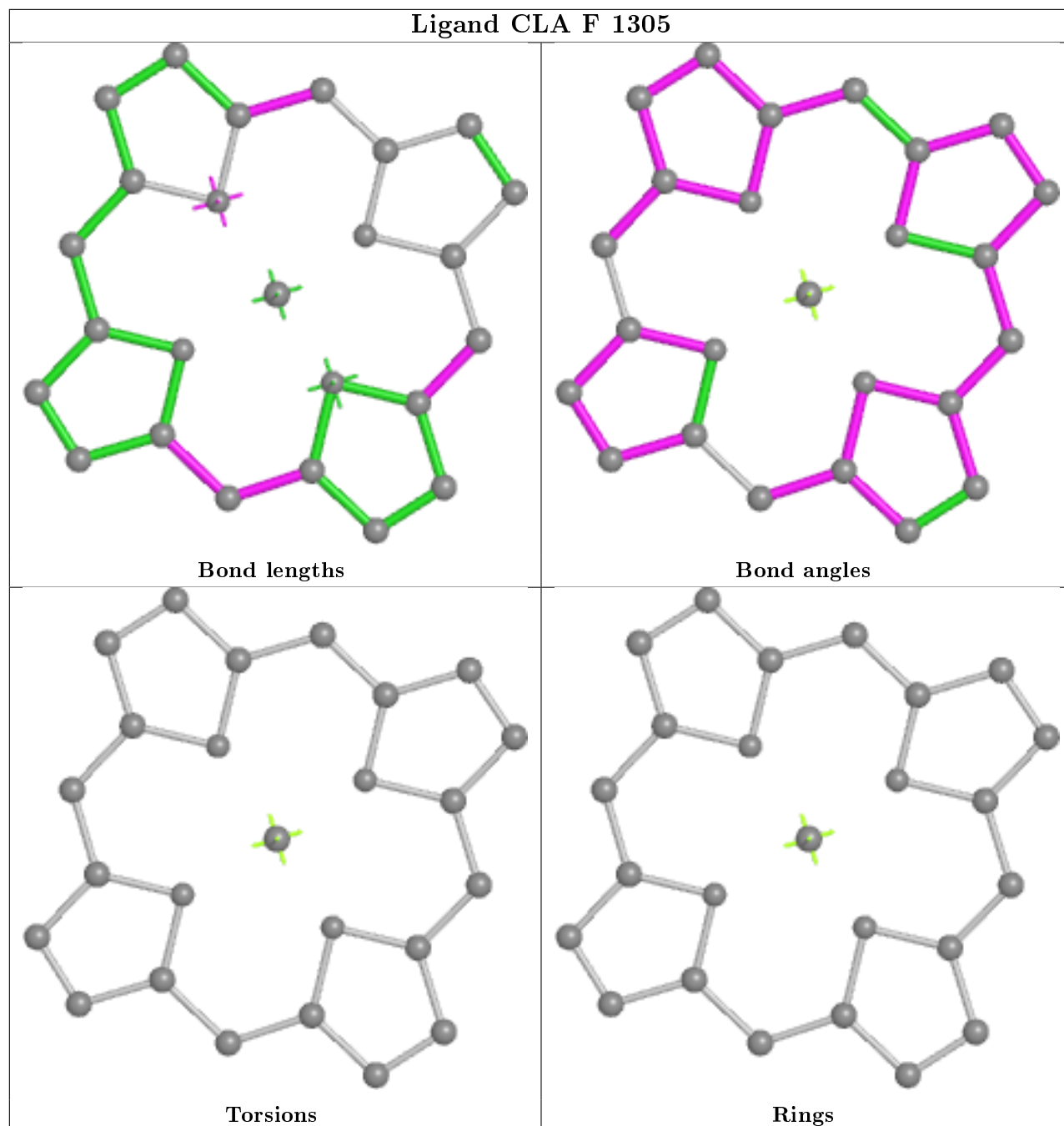
Ligand CLA A 1151



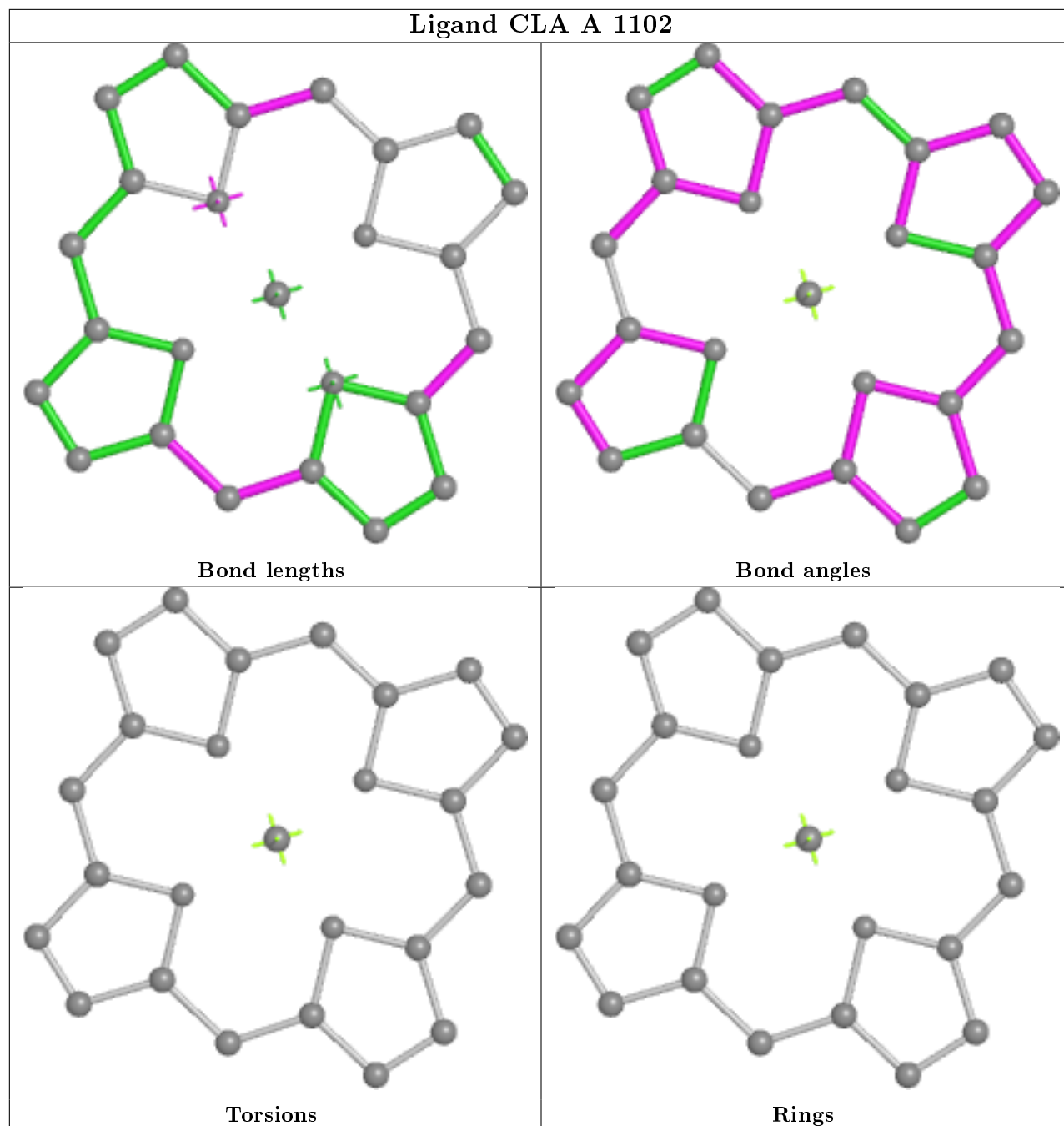
Ligand BCR I 6018



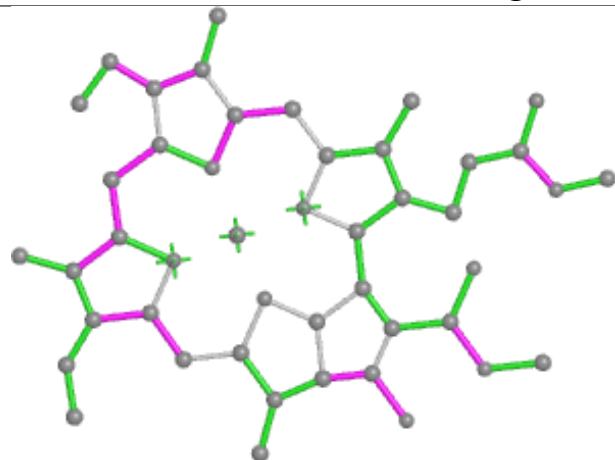
Ligand CLA F 1305



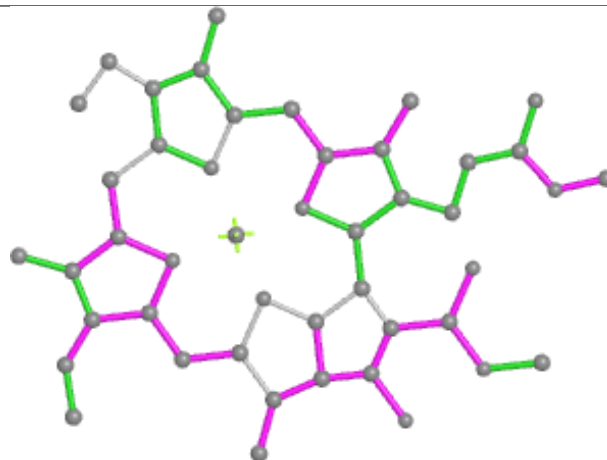
Ligand CLA A 1102



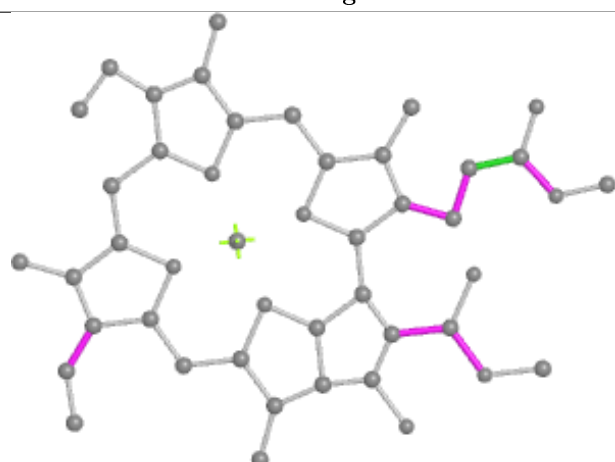
Ligand CLA B 1231



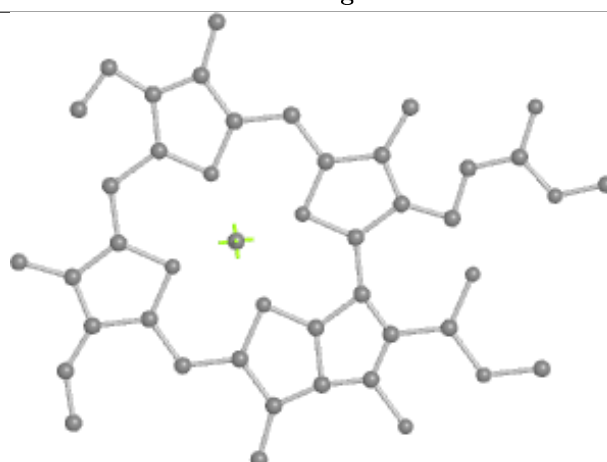
Bond lengths



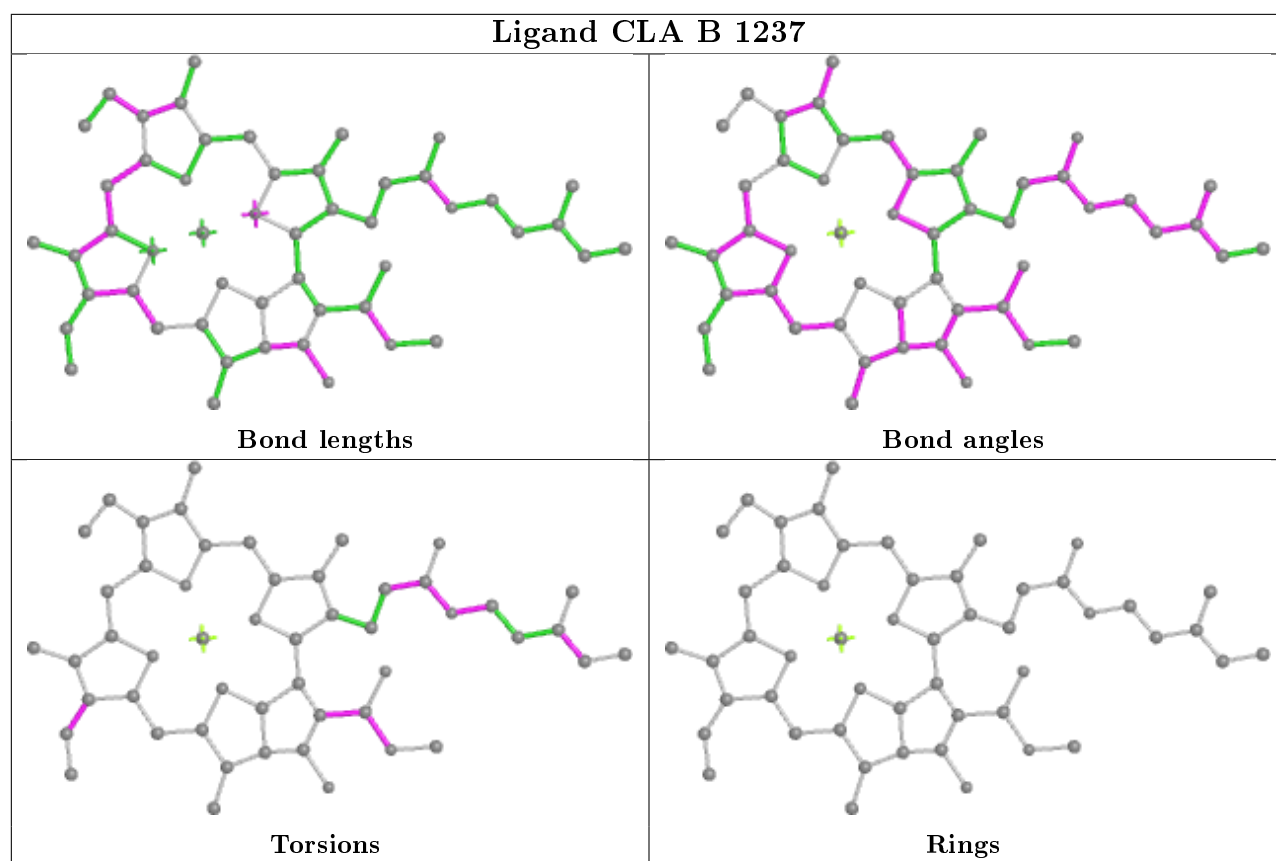
Bond angles

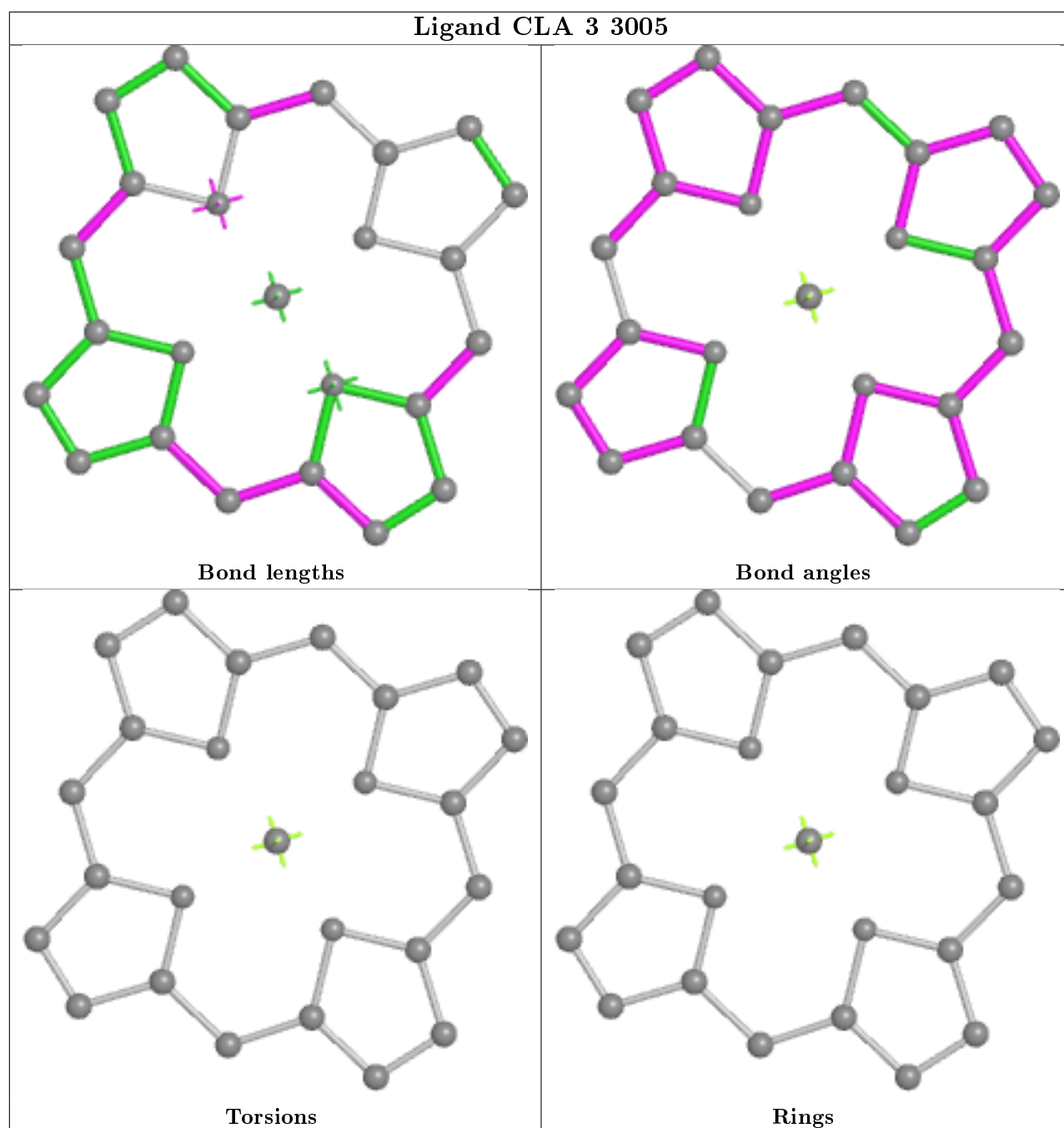


Torsions

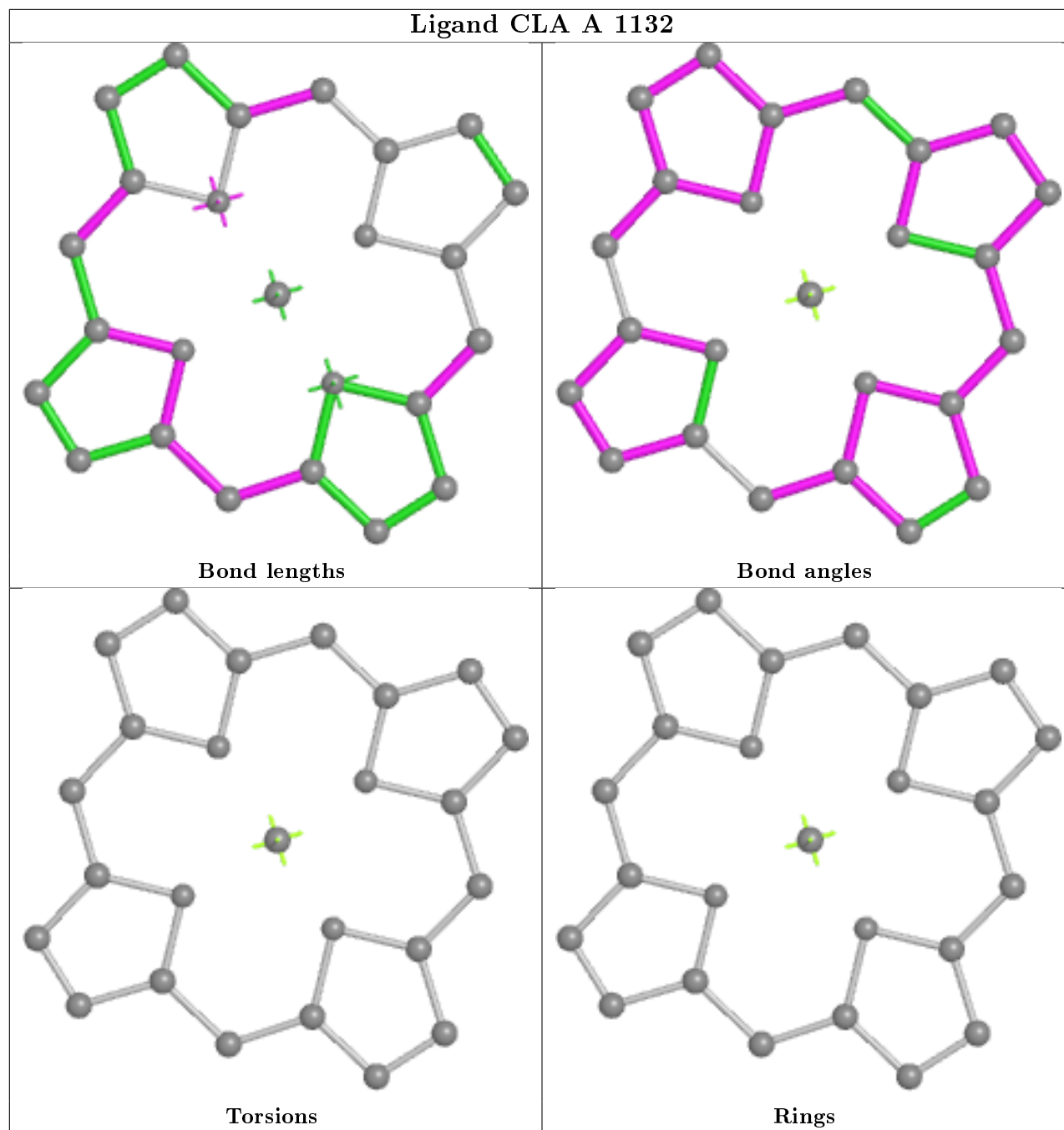


Rings

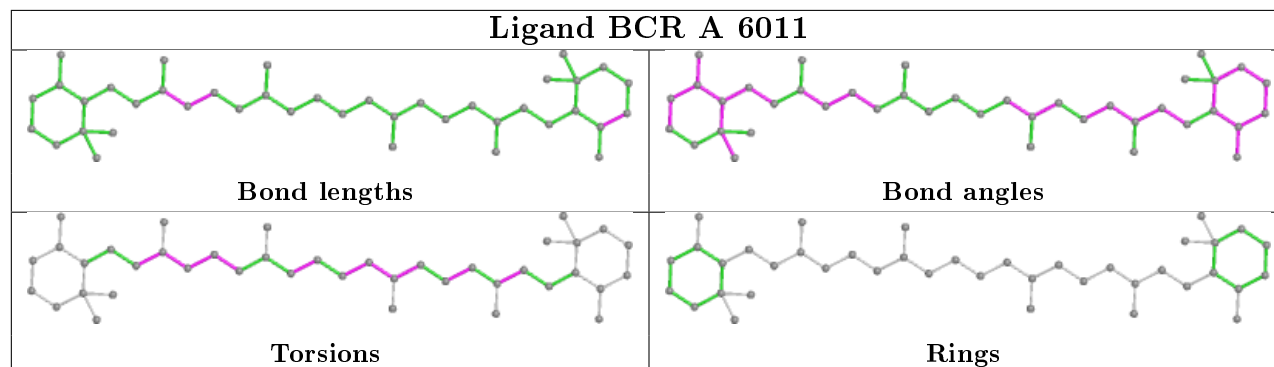




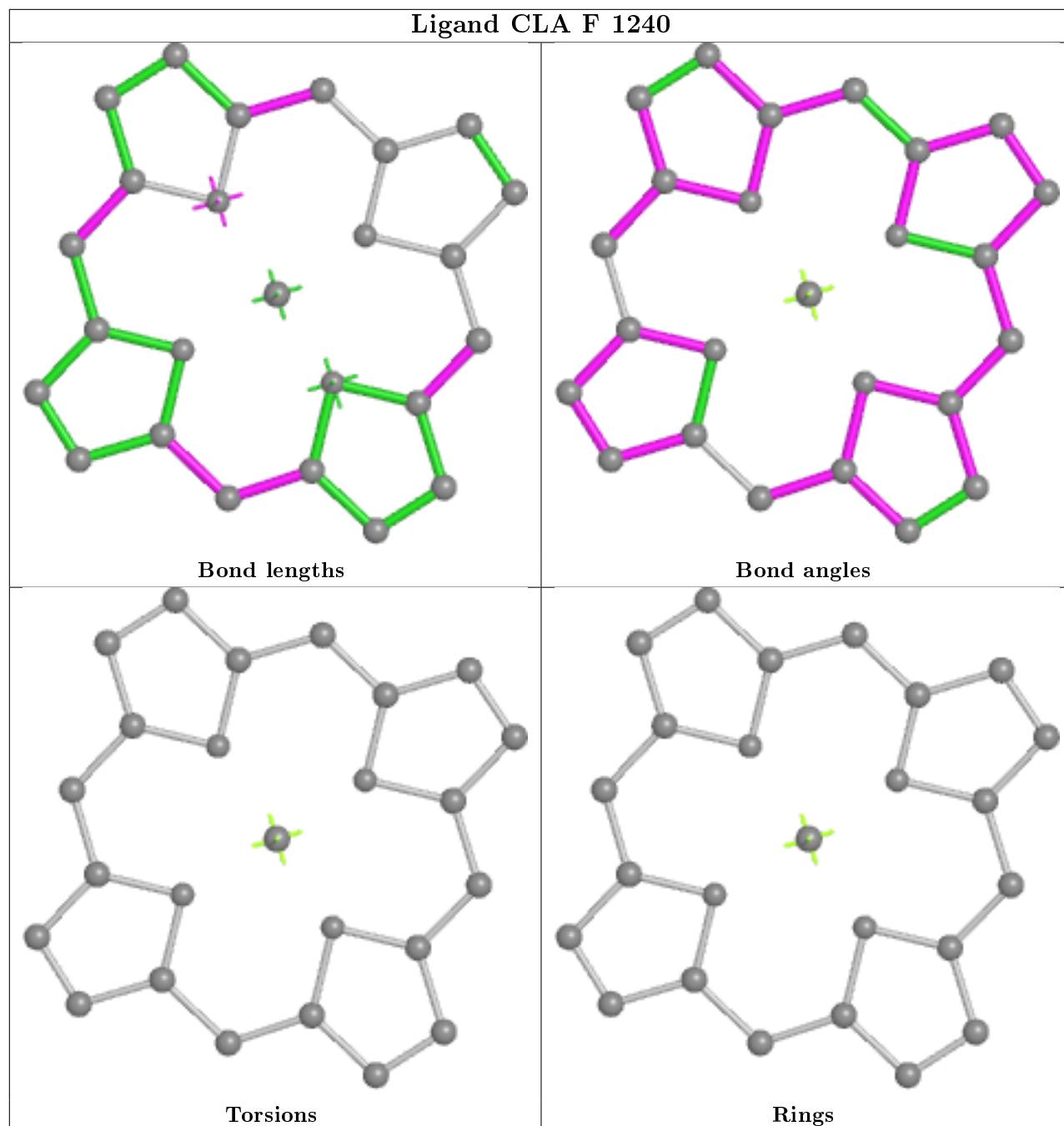
Ligand CLA A 1132

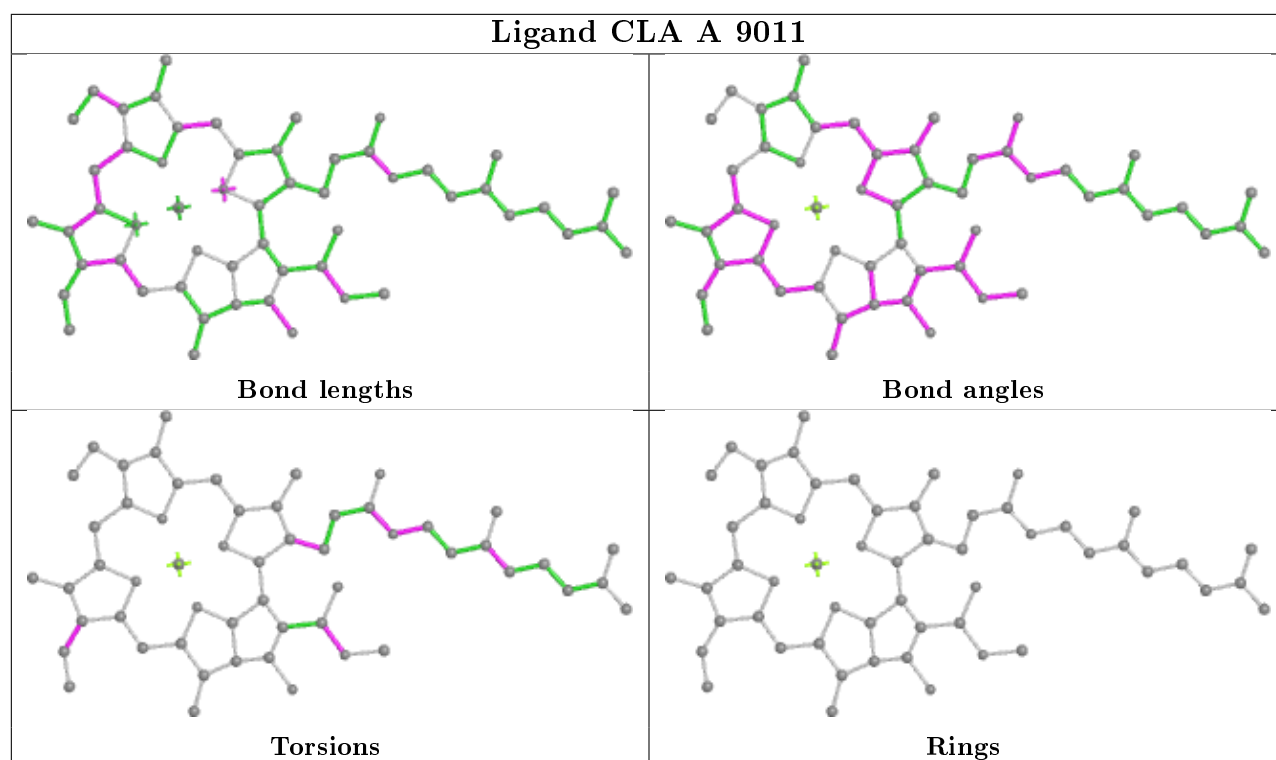


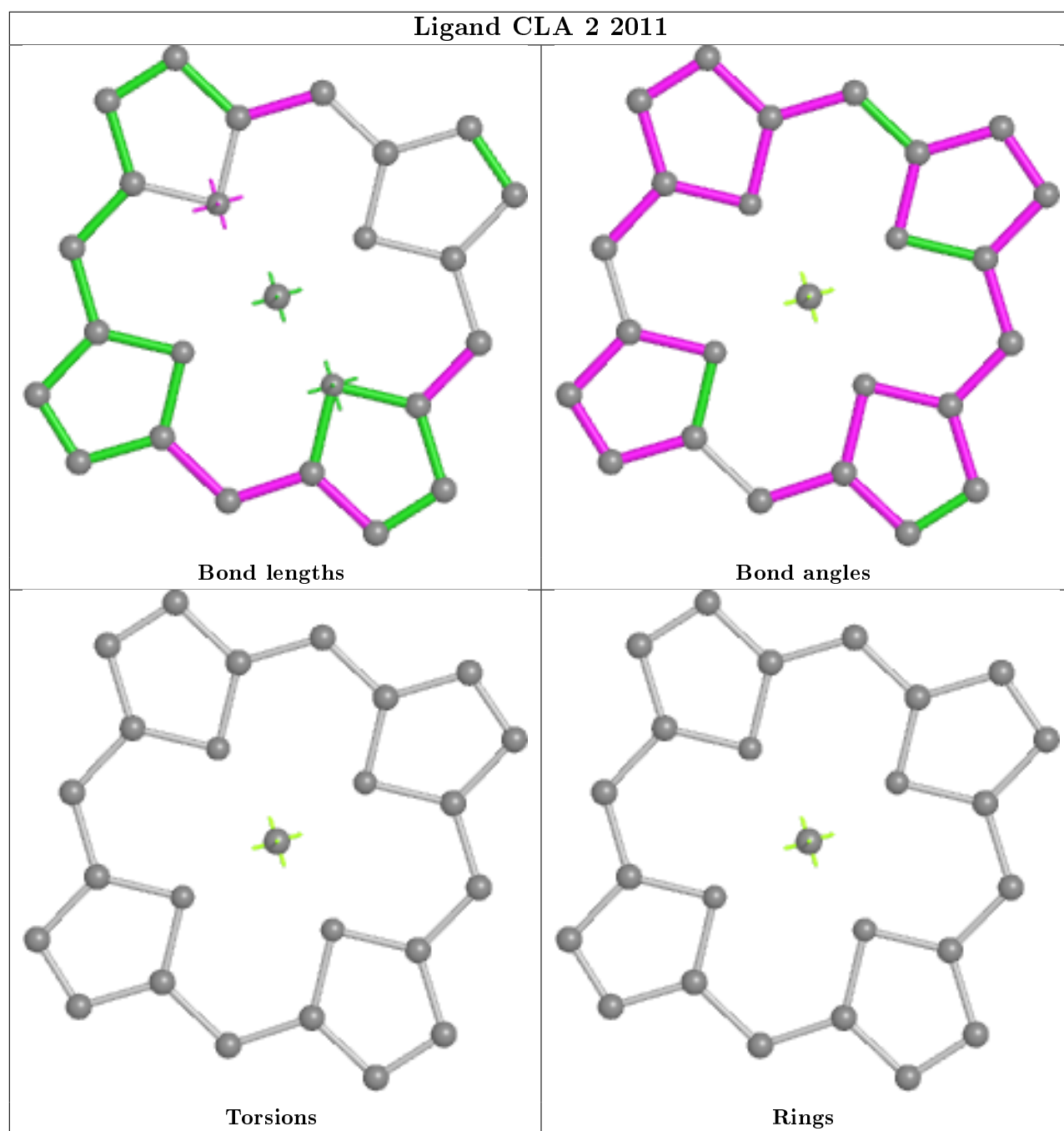
Ligand BCR A 6011

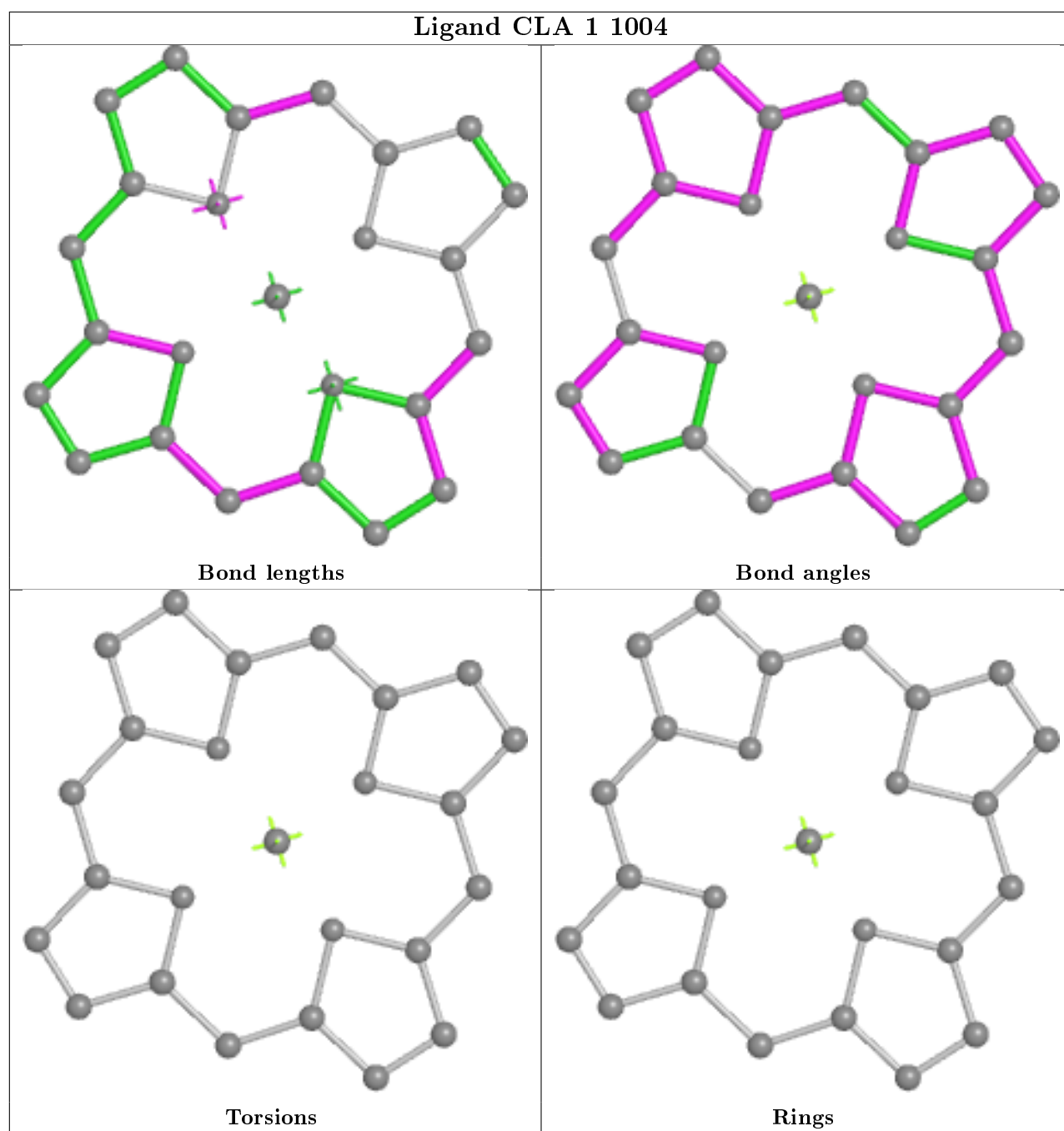


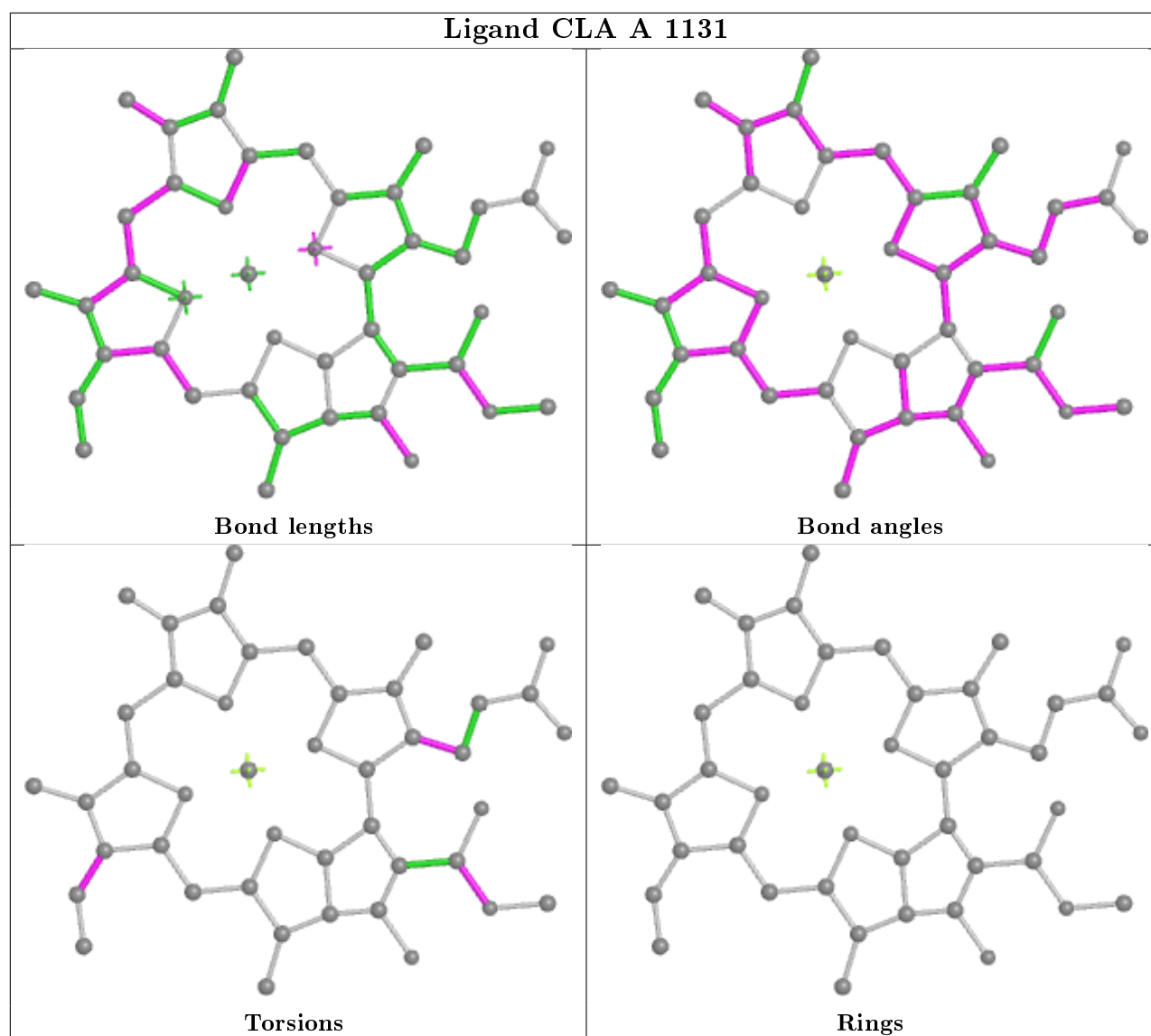
Ligand CLA F 1240

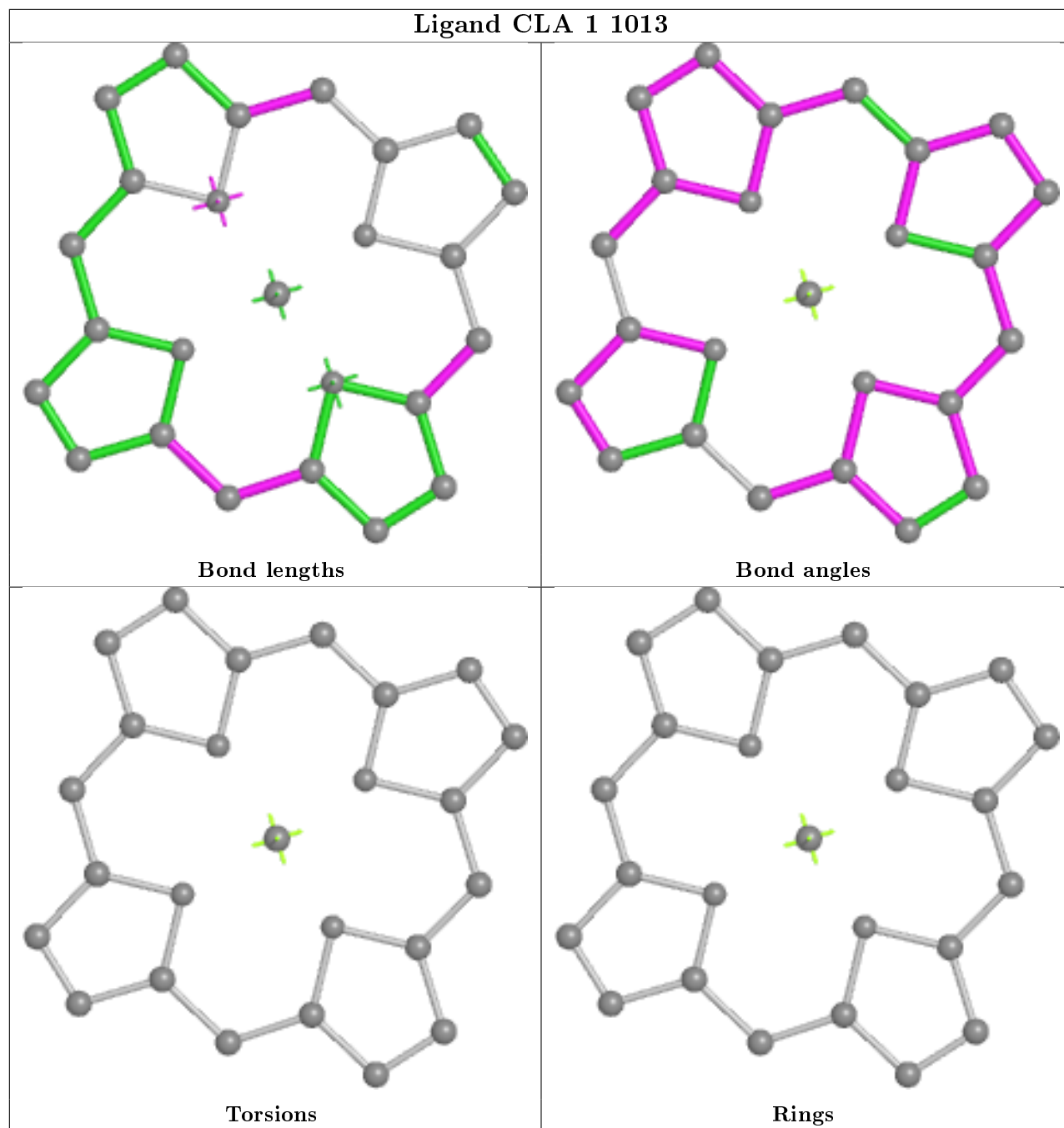




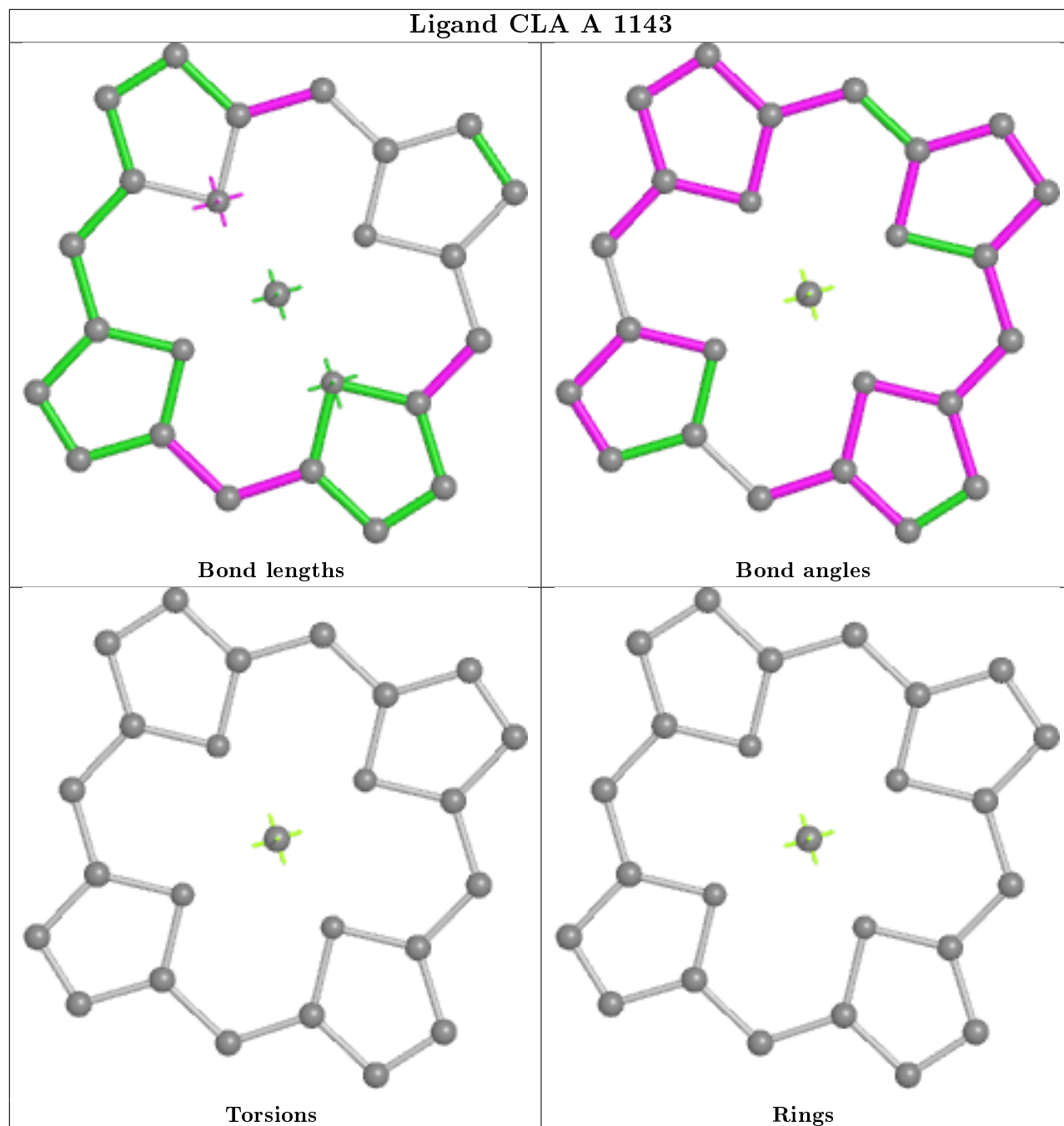




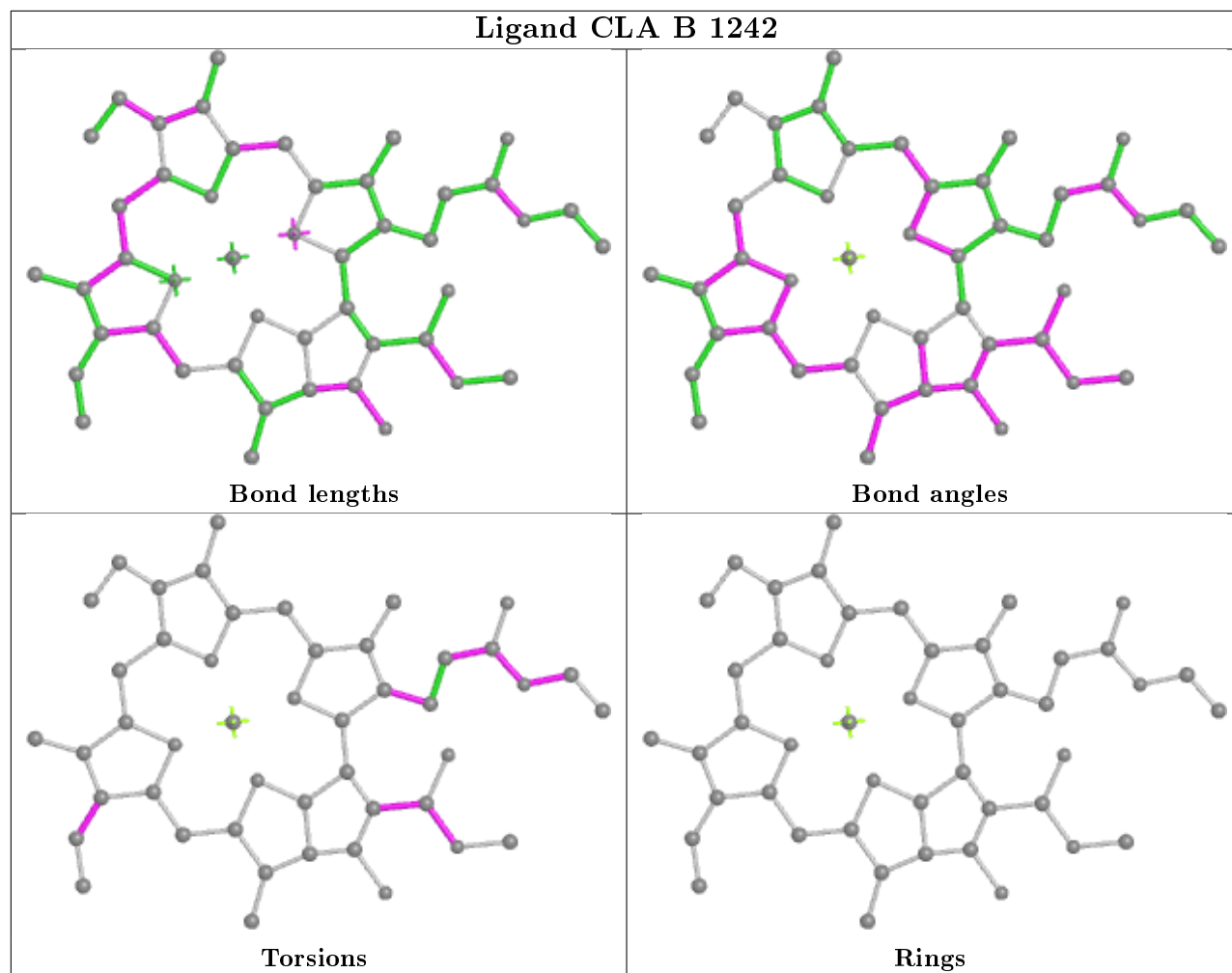


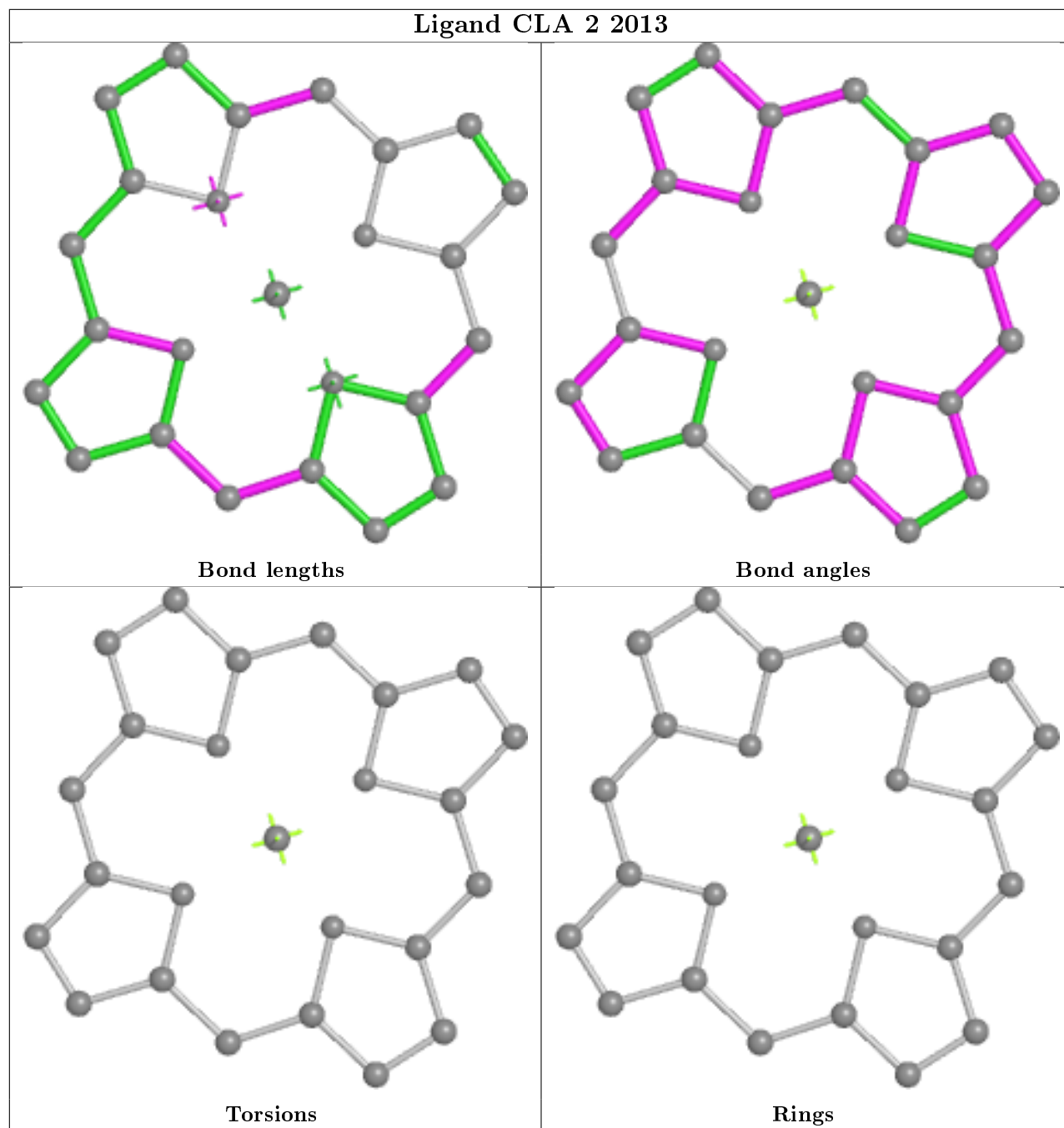


Ligand CLA A 1143

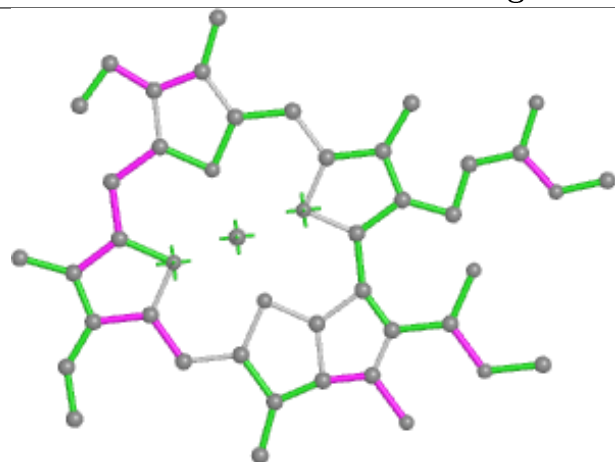


Ligand CLA B 1242

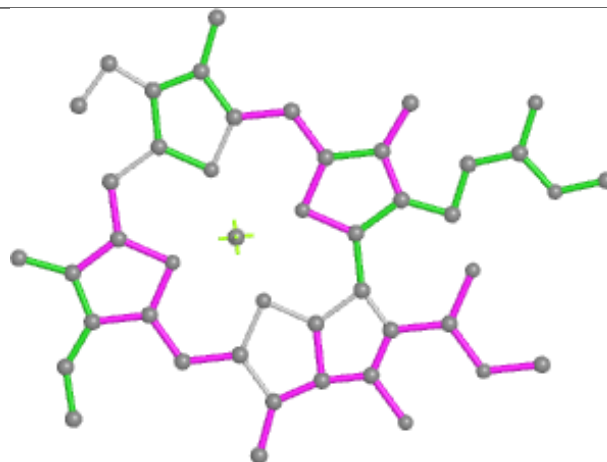




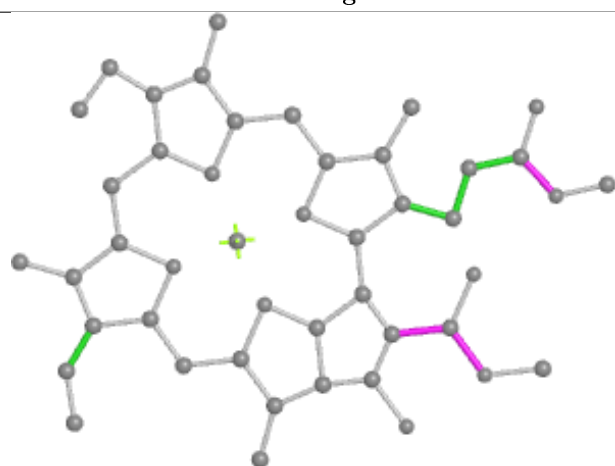
Ligand CLA B 1236



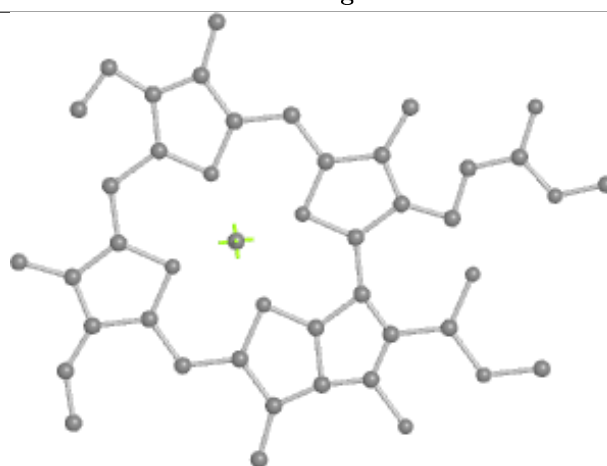
Bond lengths



Bond angles

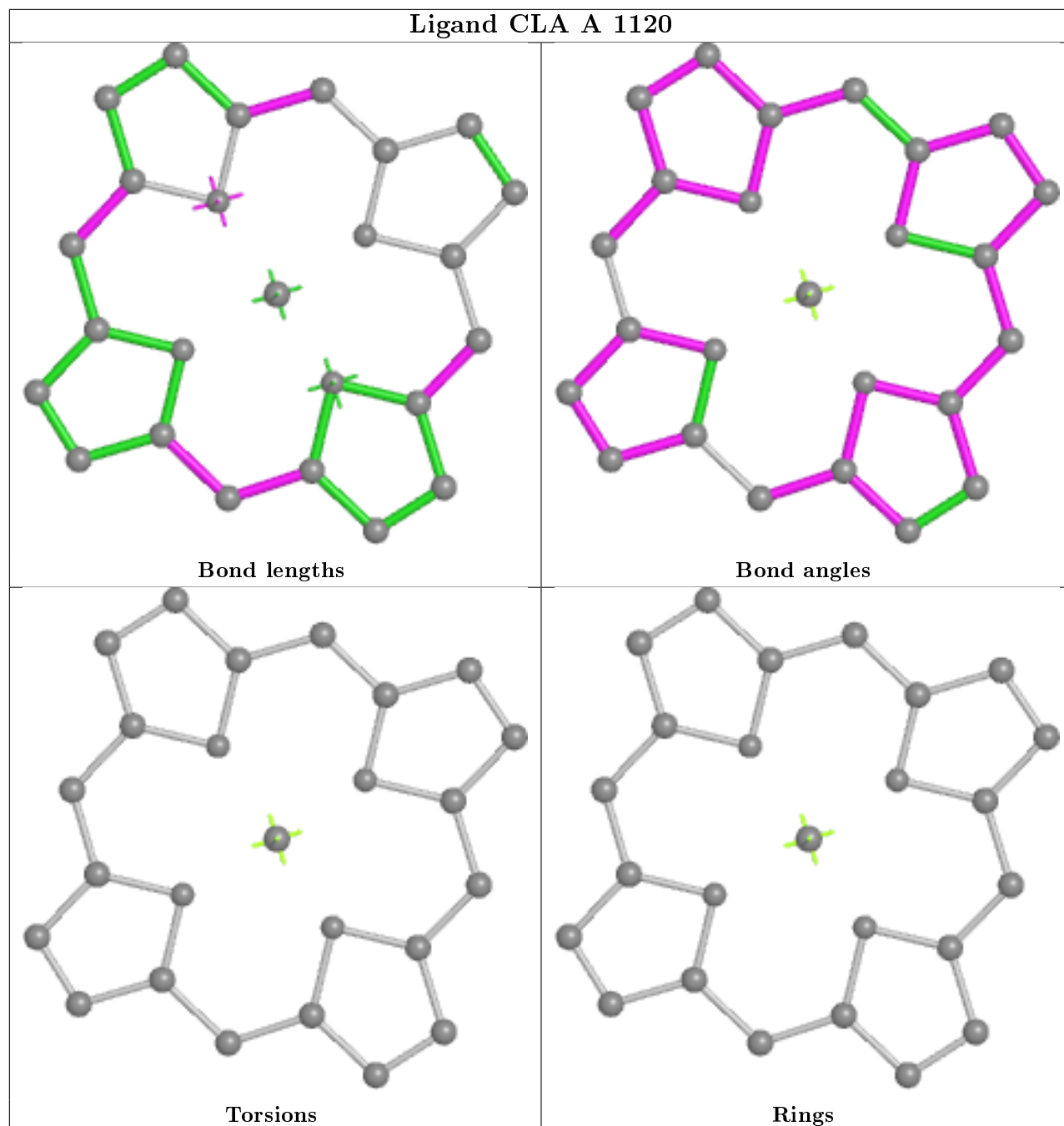


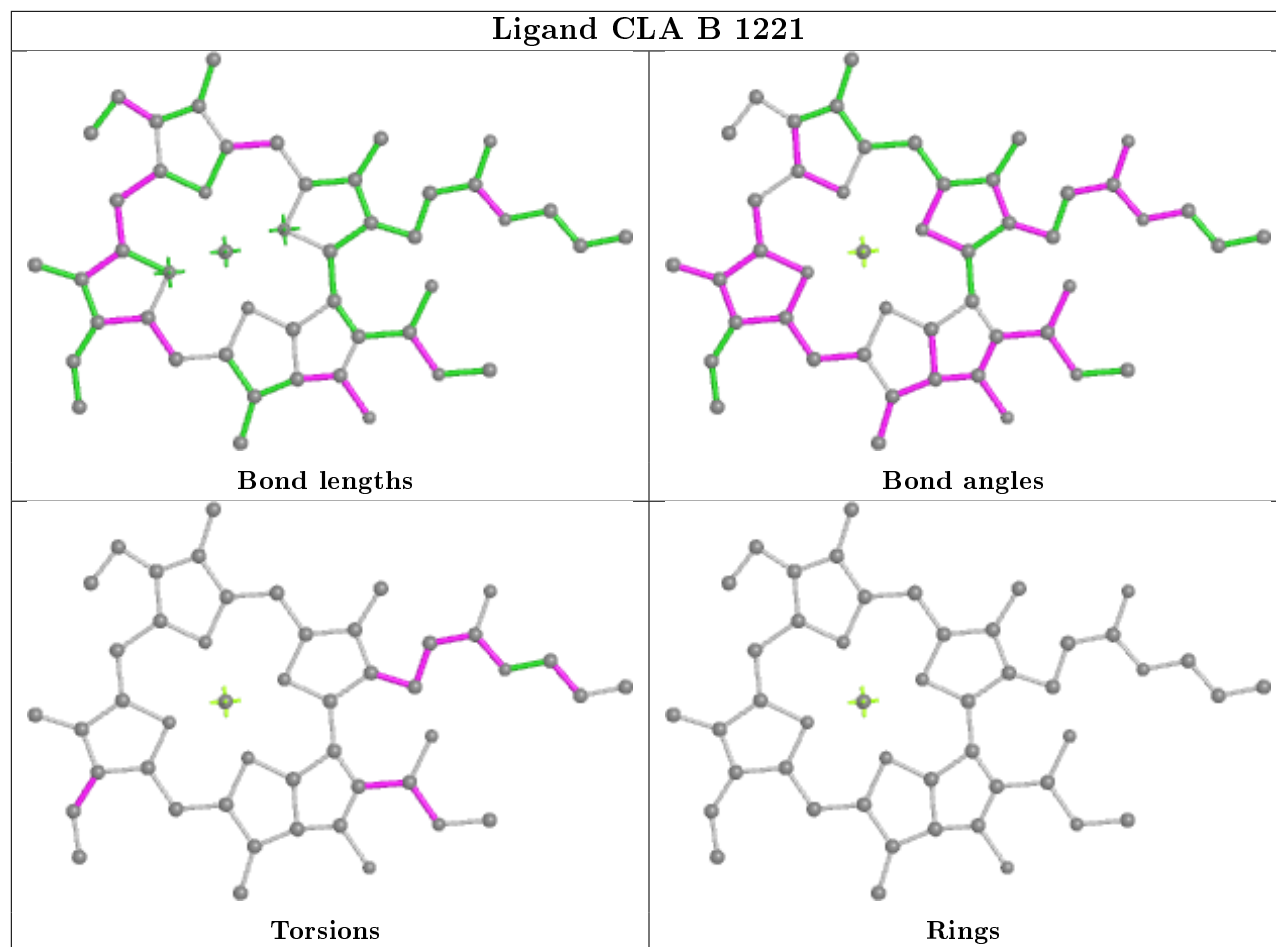
Torsions

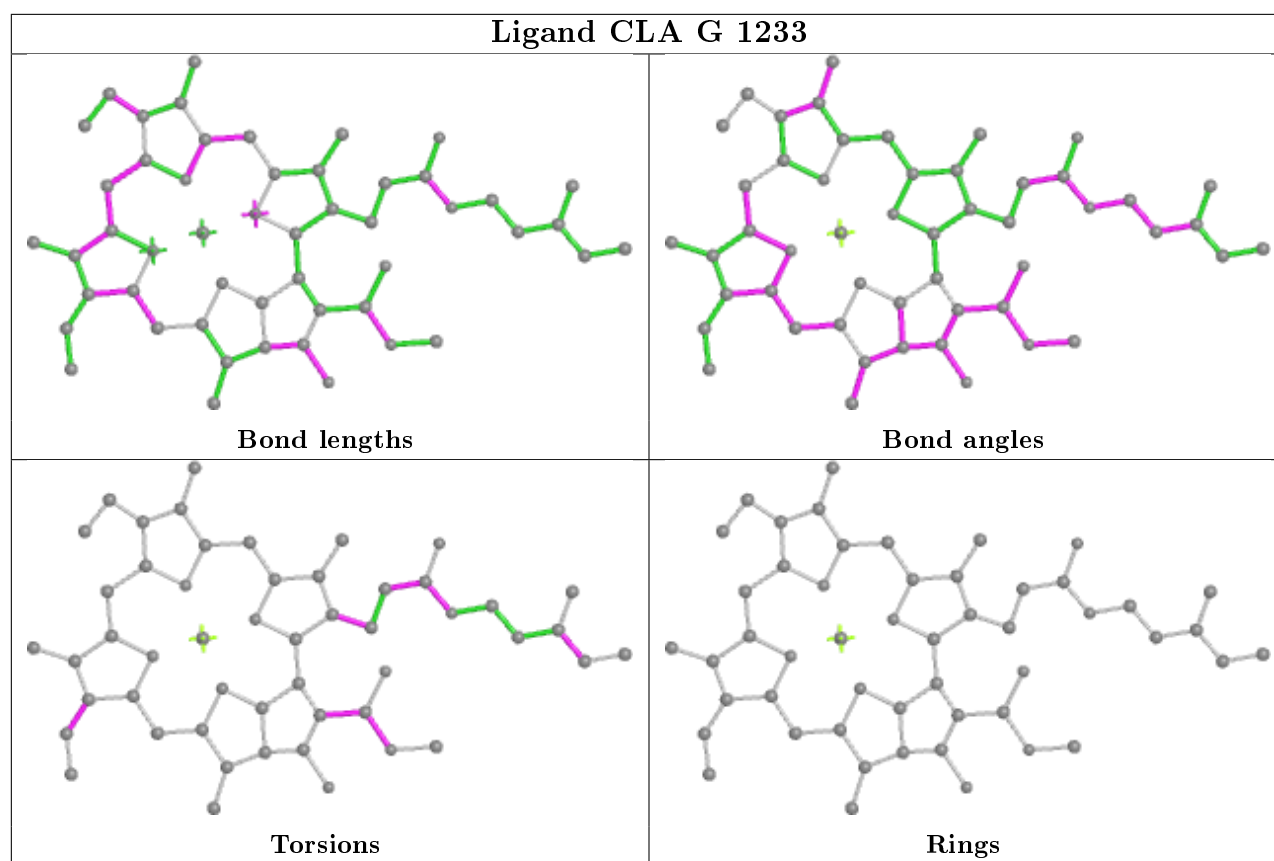


Rings

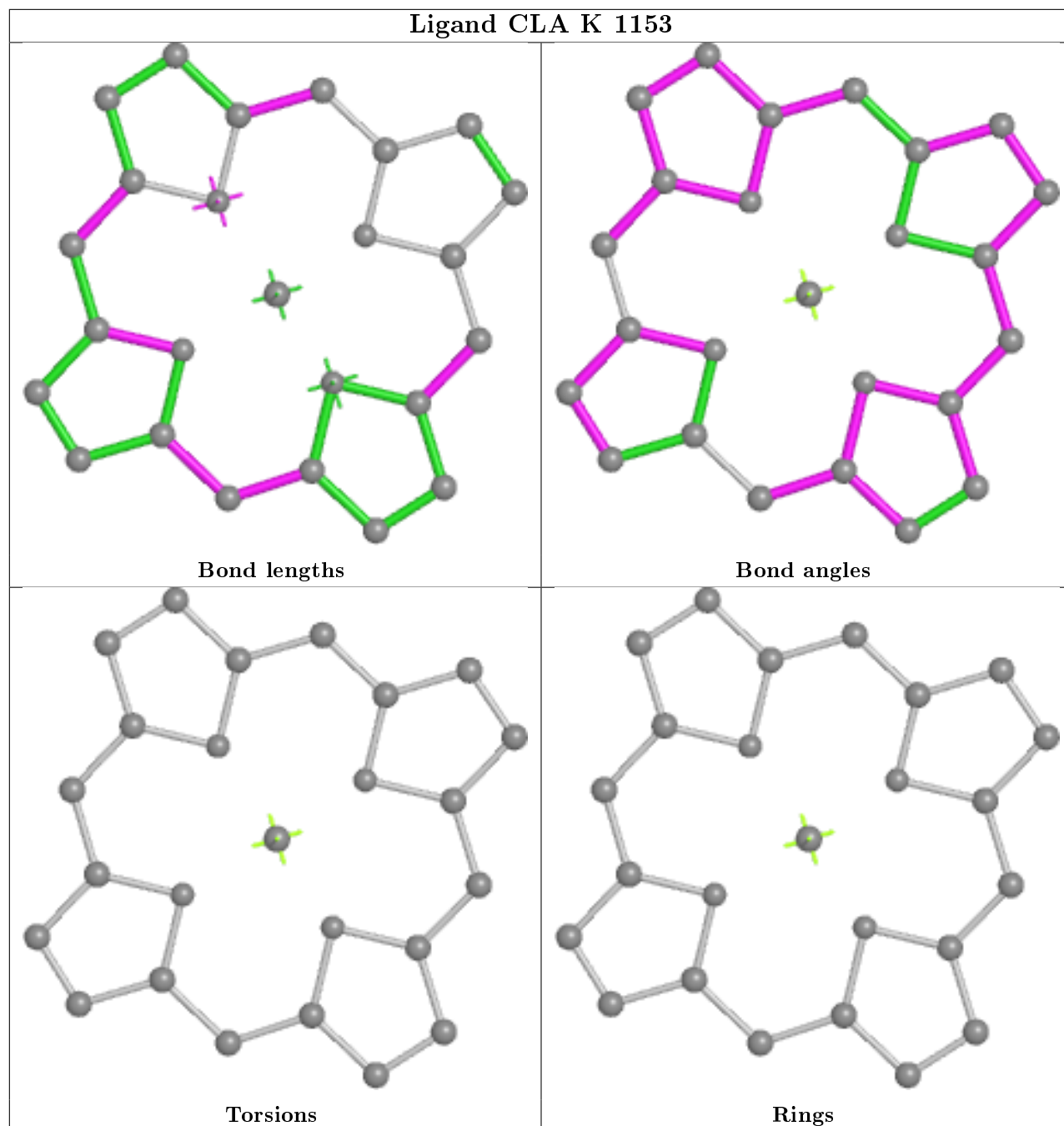
Ligand CLA A 1120







Ligand CLA K 1153

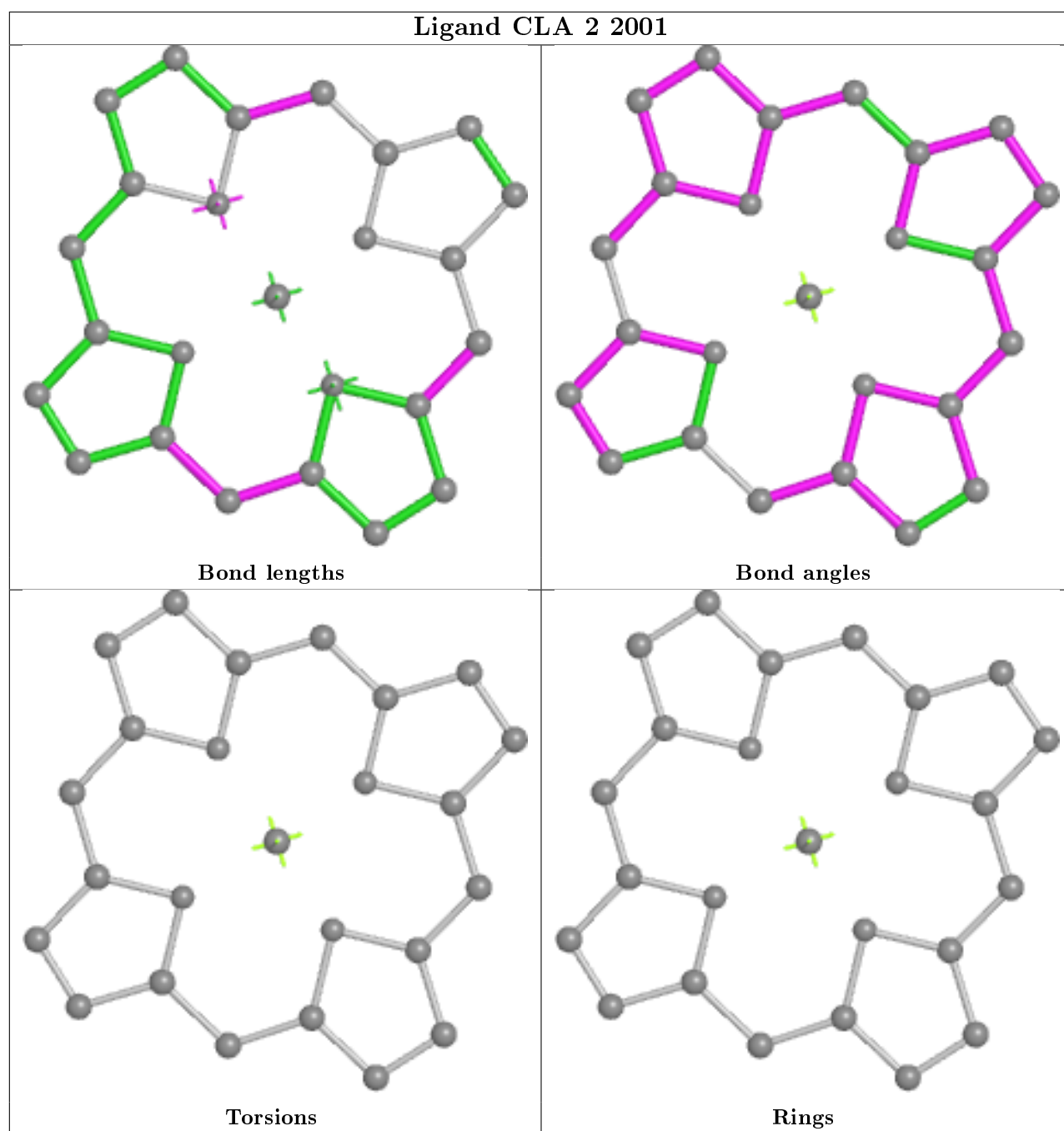


Bond lengths

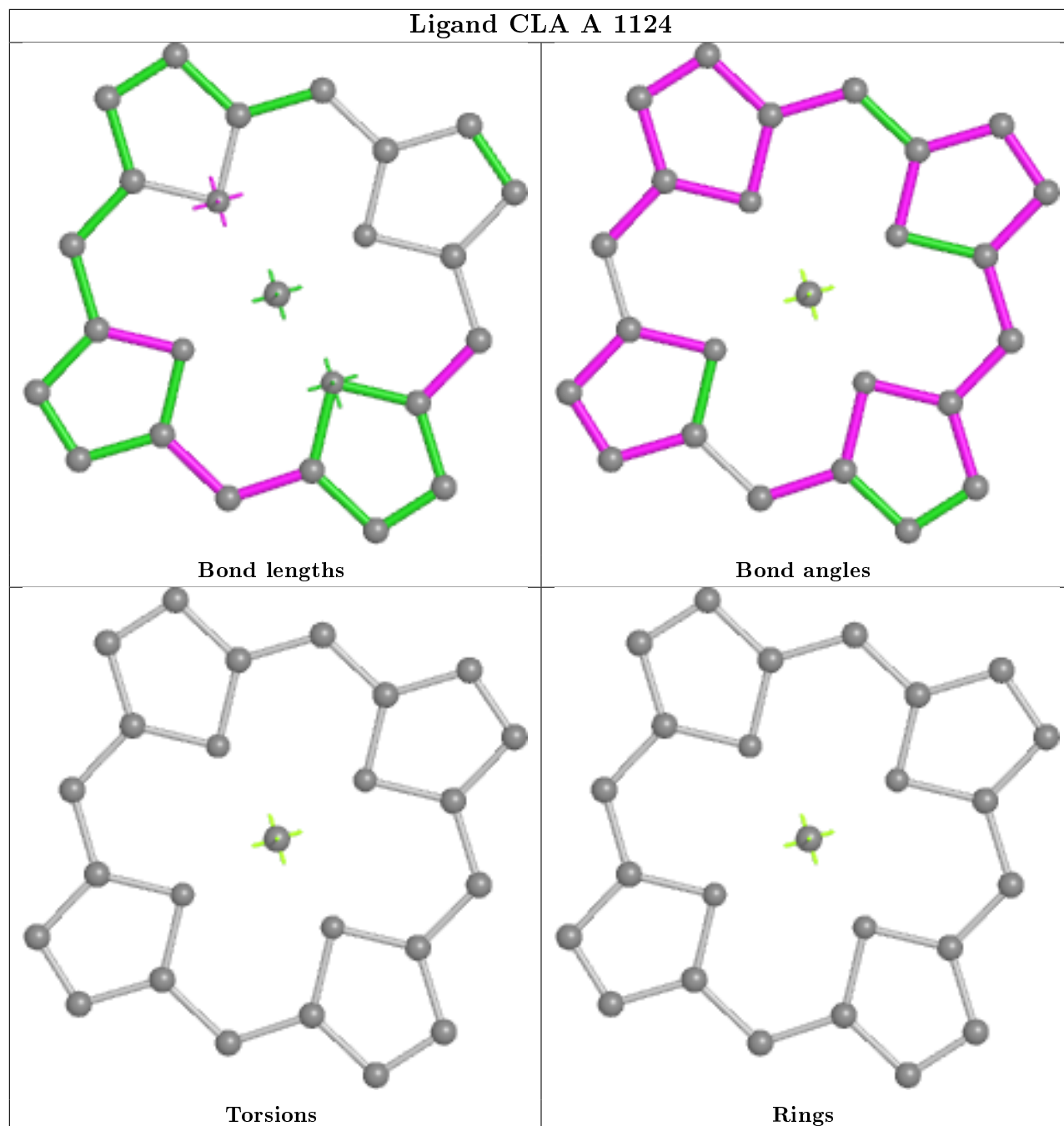
Bond angles

Torsions

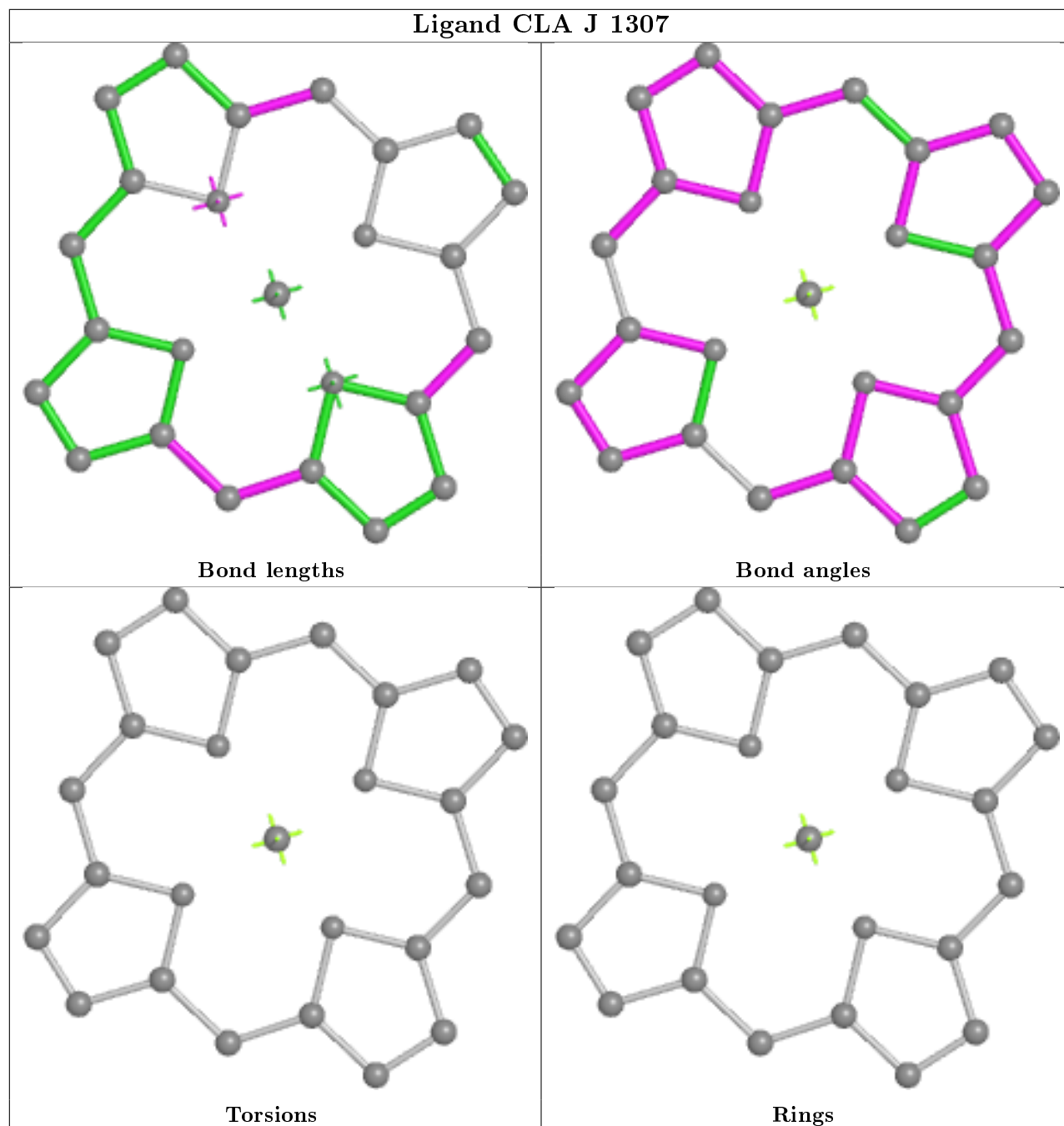
Rings



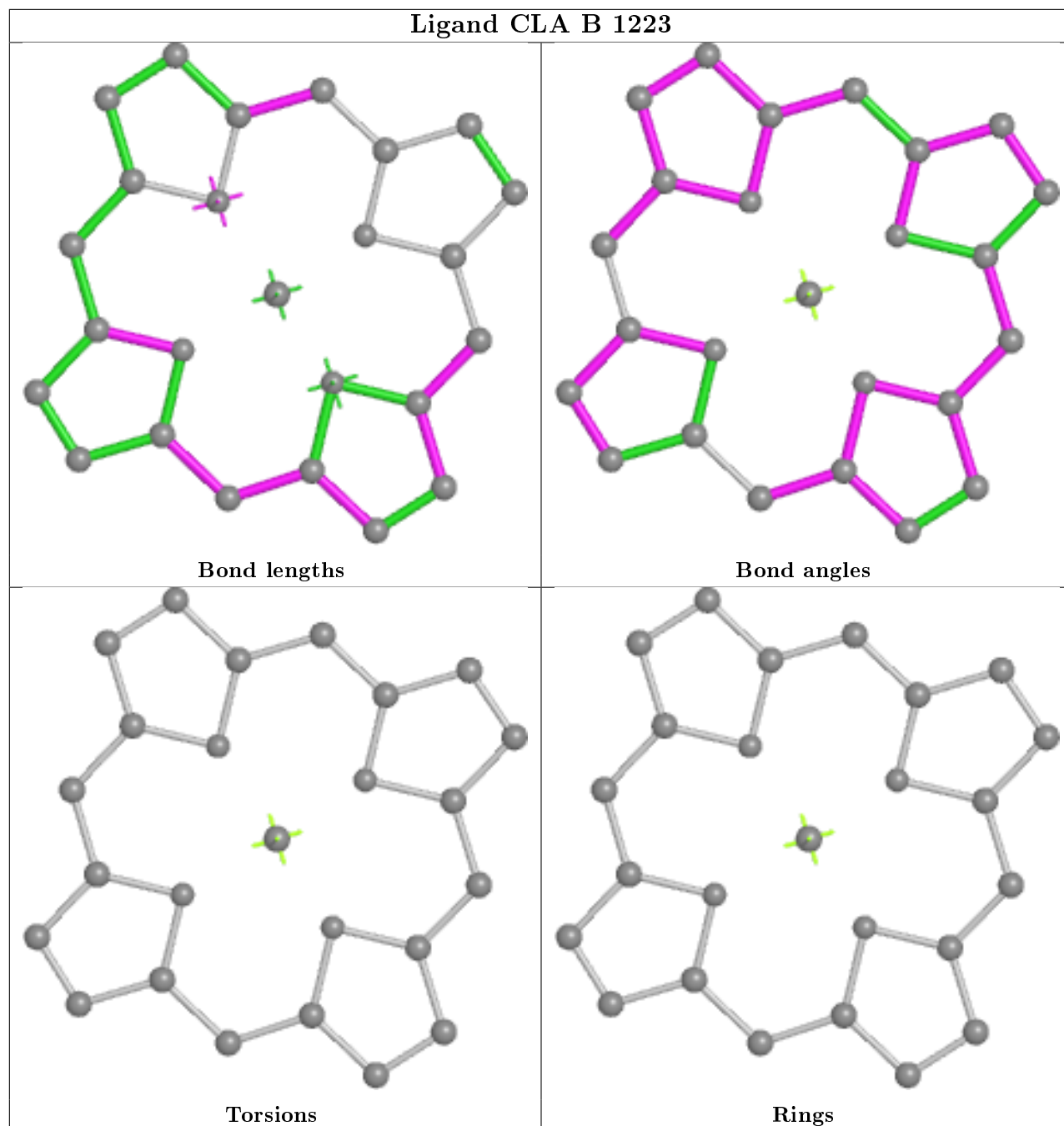
Ligand CLA A 1124



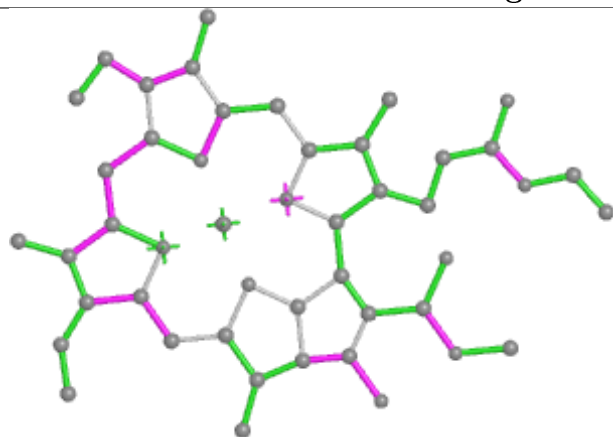
Ligand CLA J 1307



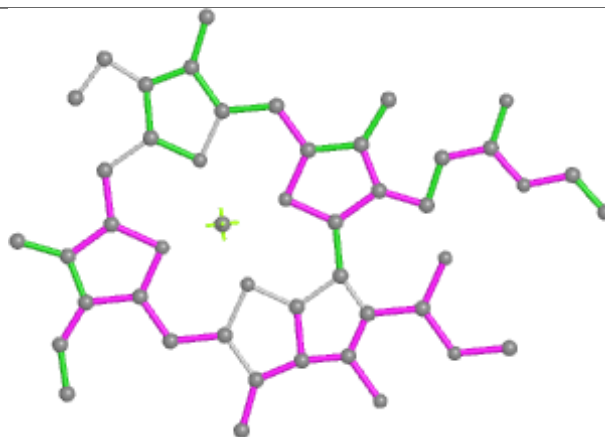
Ligand CLA B 1223



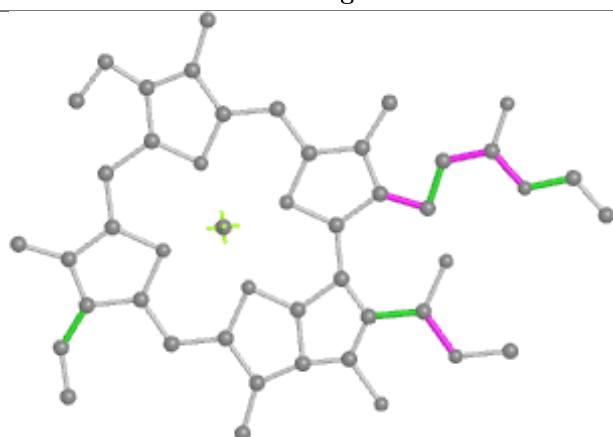
Ligand CLA A 1115



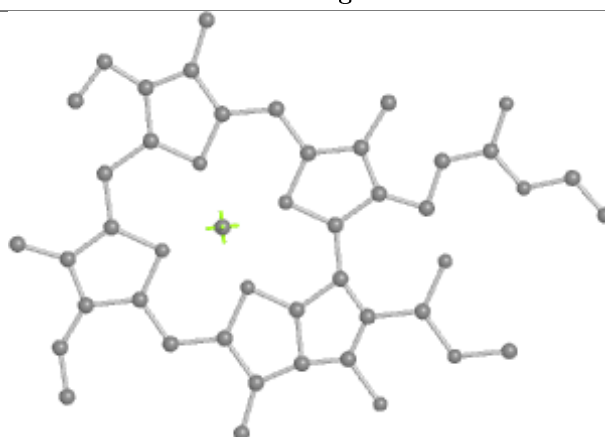
Bond lengths



Bond angles

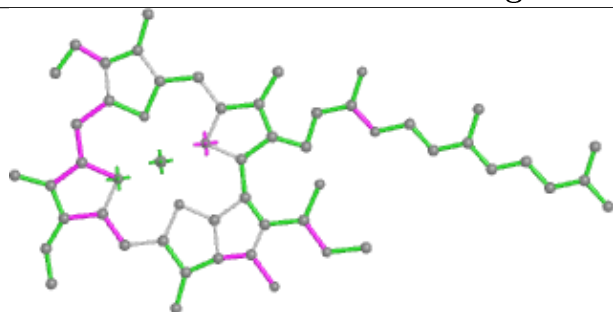


Torsions

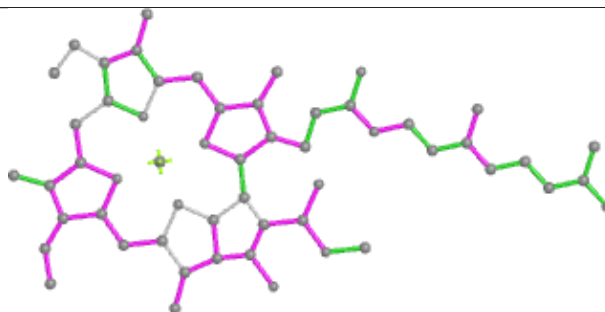


Rings

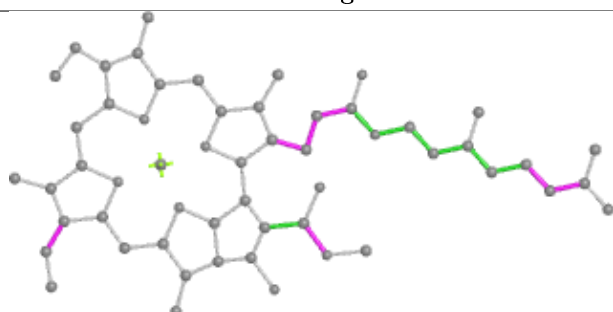
Ligand CLA B 1207



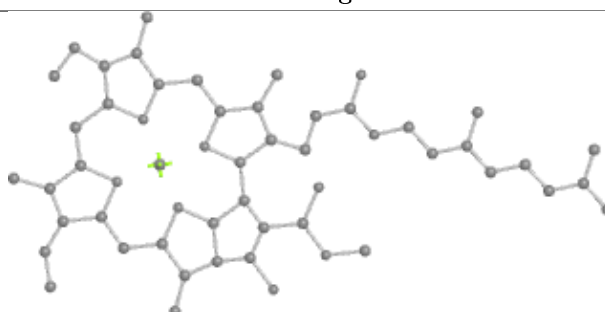
Bond lengths



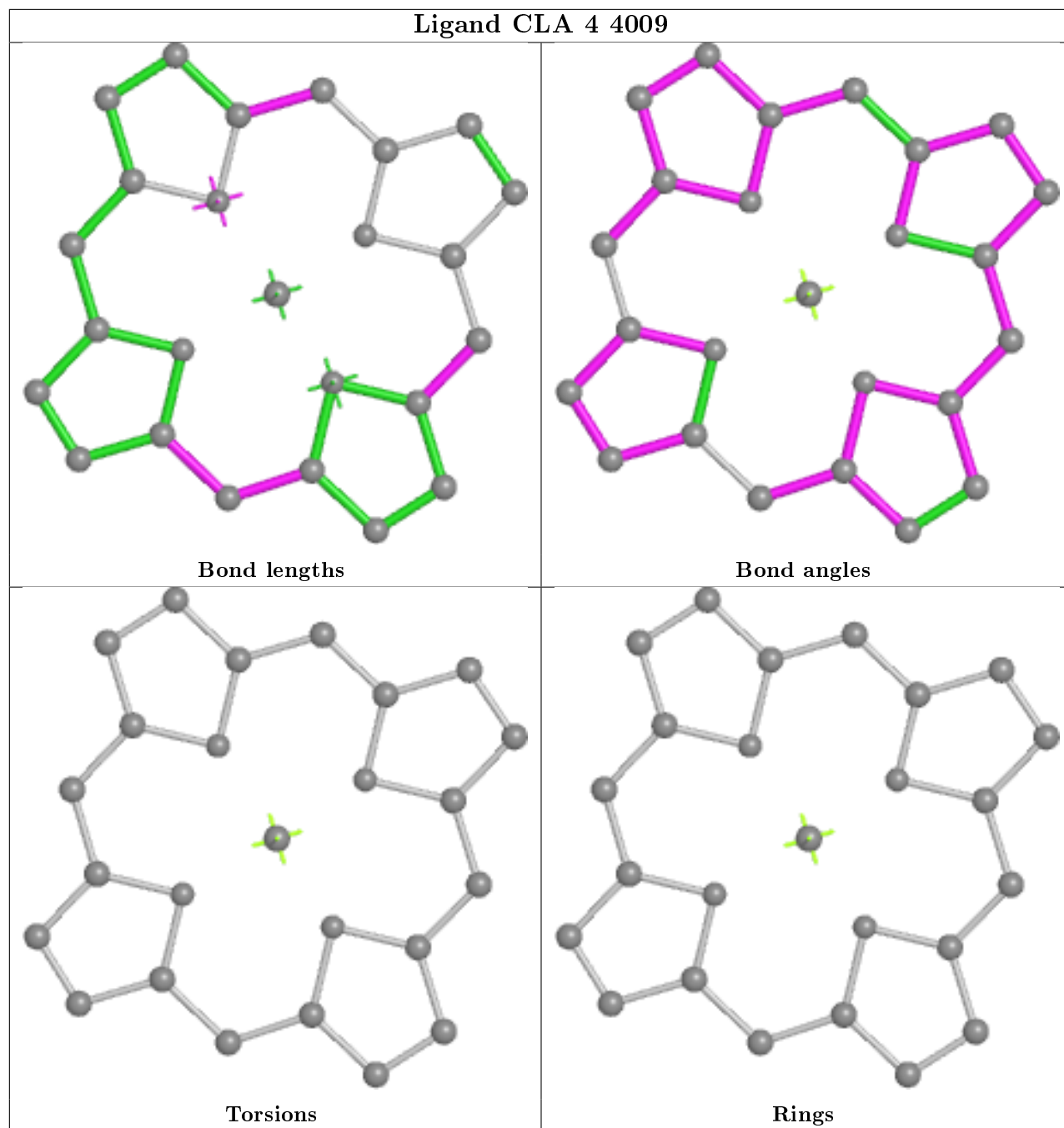
Bond angles

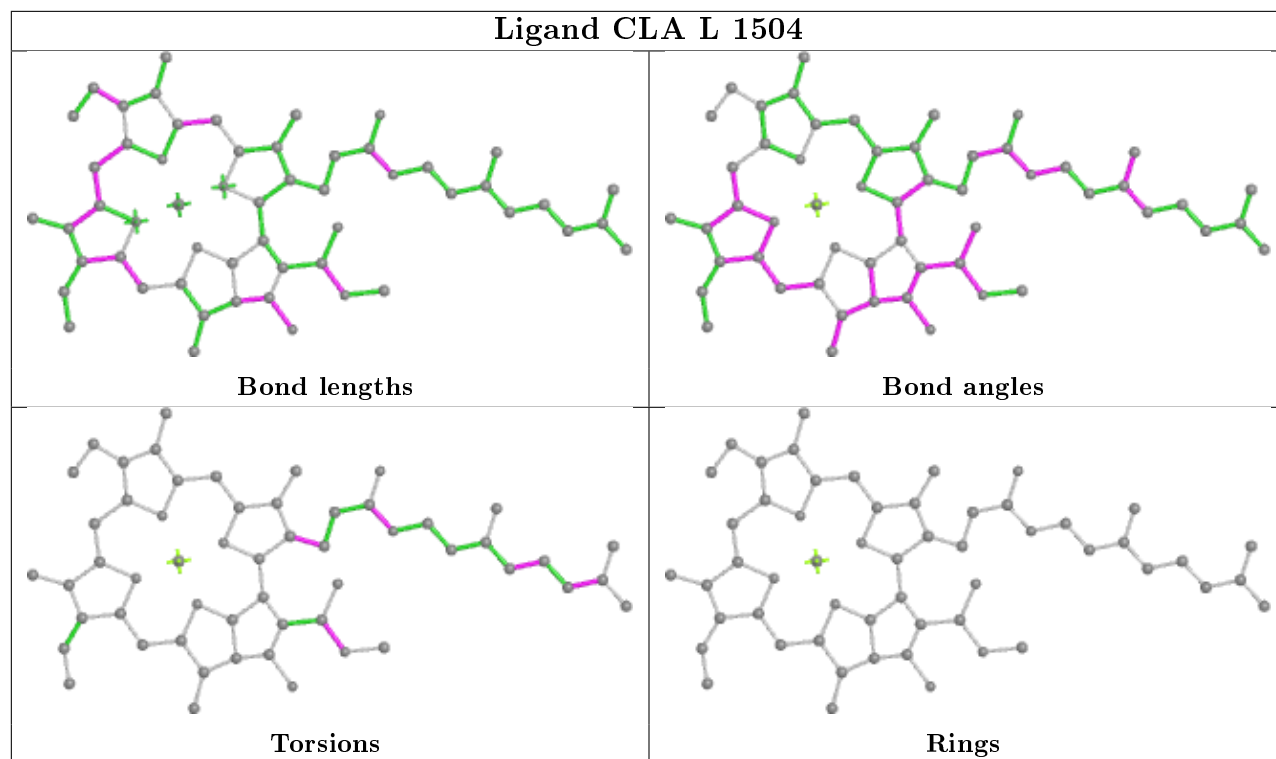


Torsions

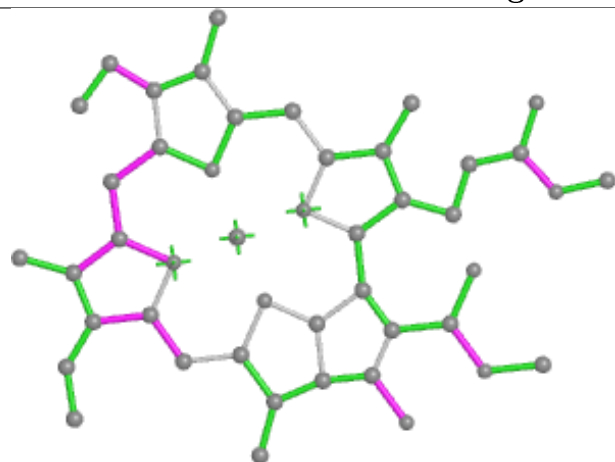


Rings

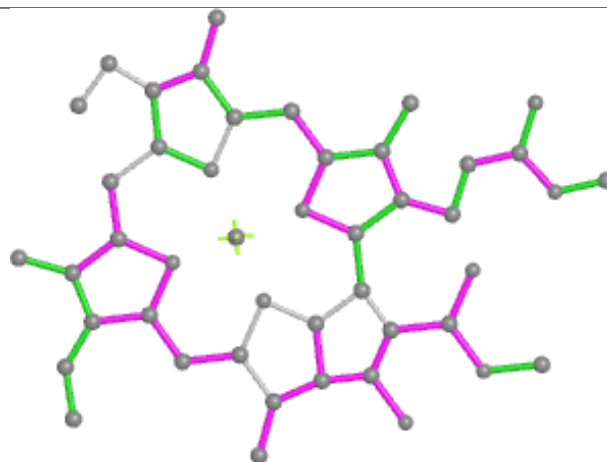




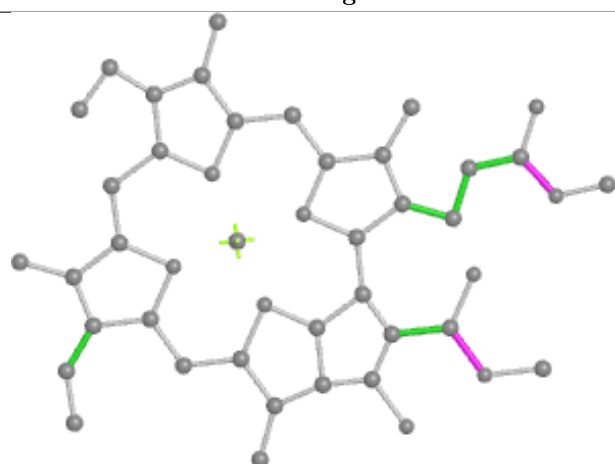
Ligand CLA A 9013



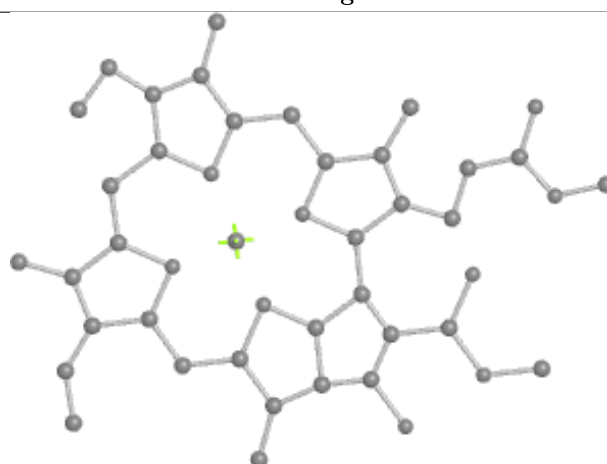
Bond lengths



Bond angles

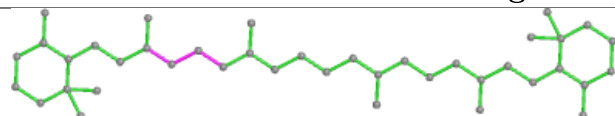


Torsions

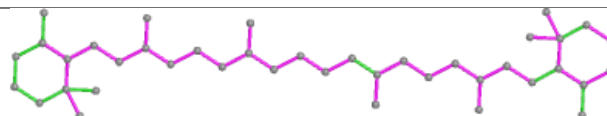


Rings

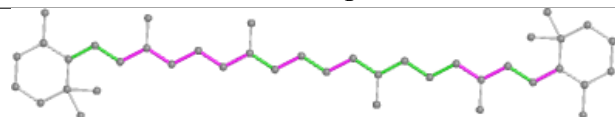
Ligand BCR L 6020



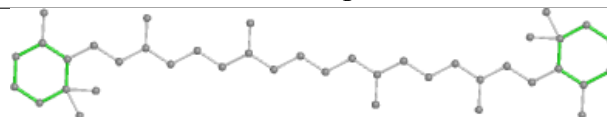
Bond lengths



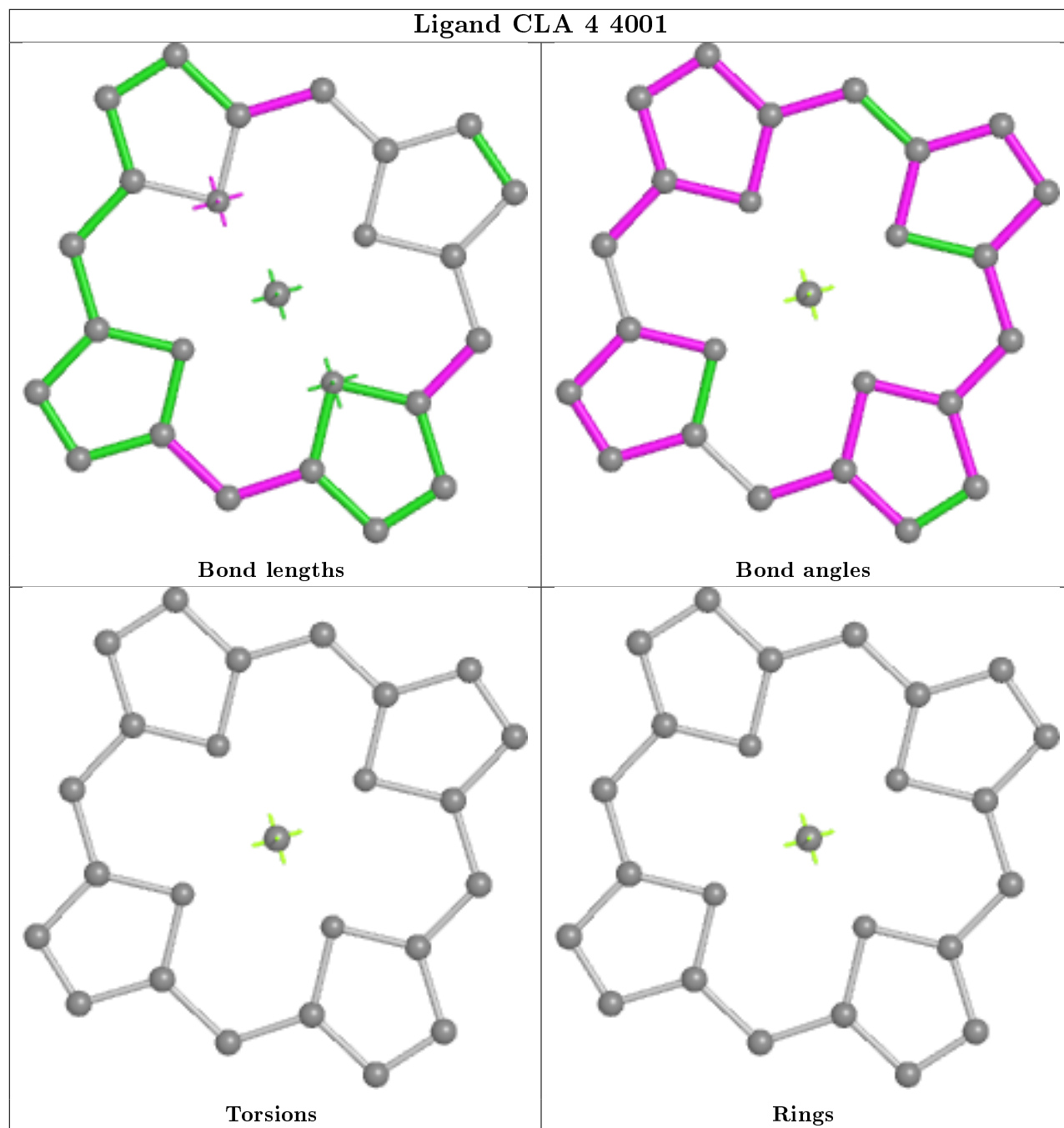
Bond angles



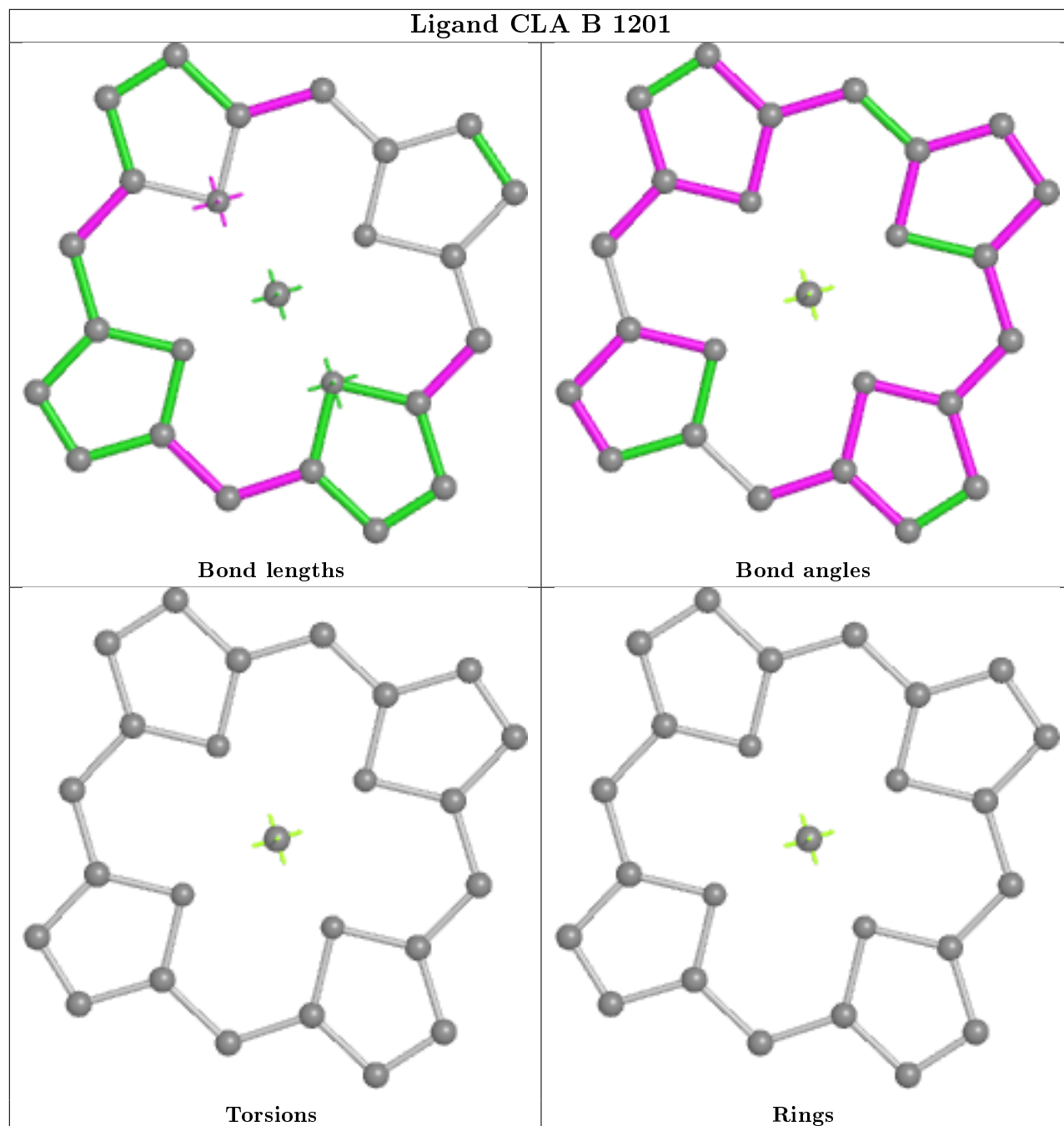
Torsions

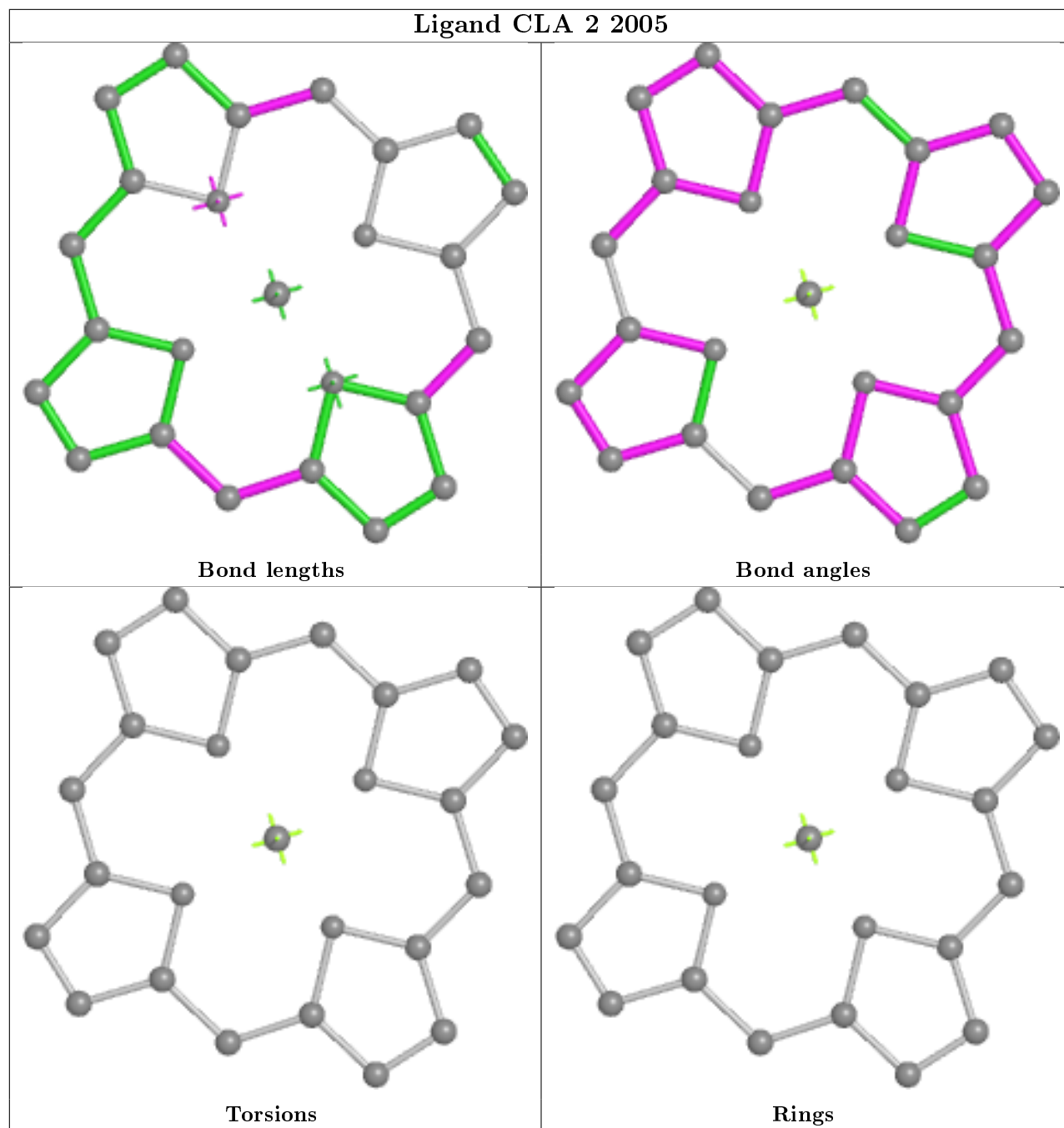


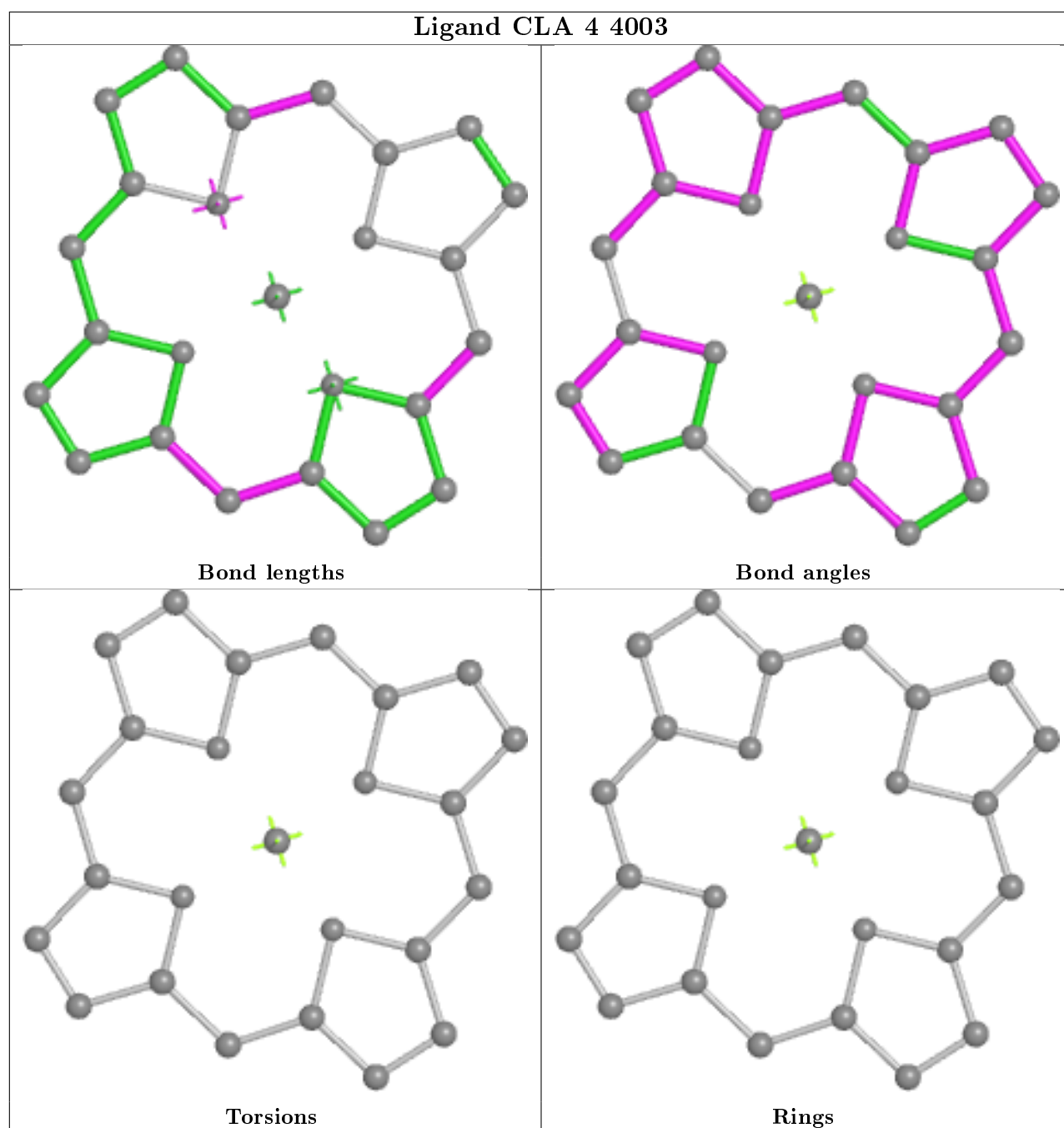
Rings

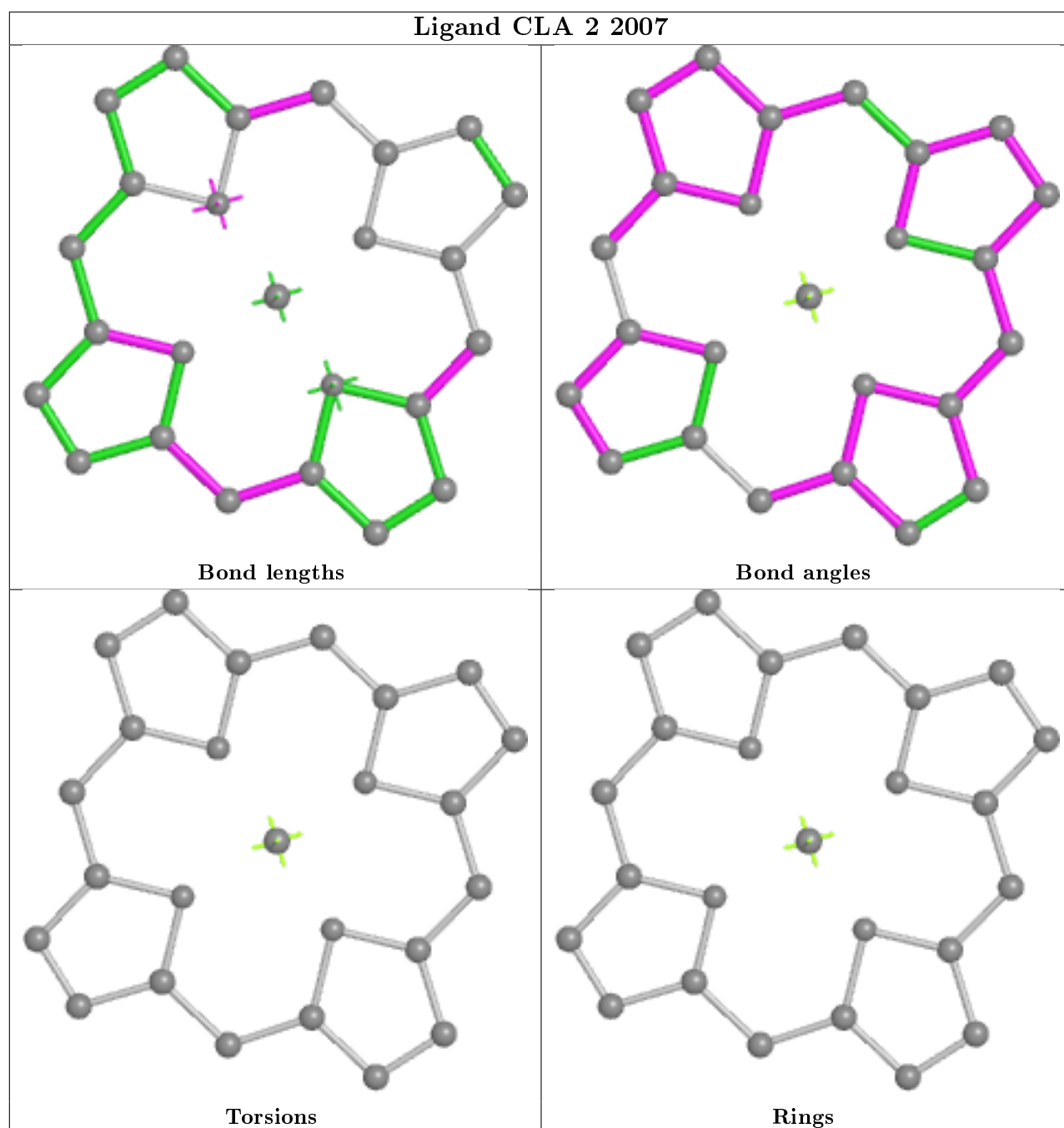


Ligand CLA B 1201

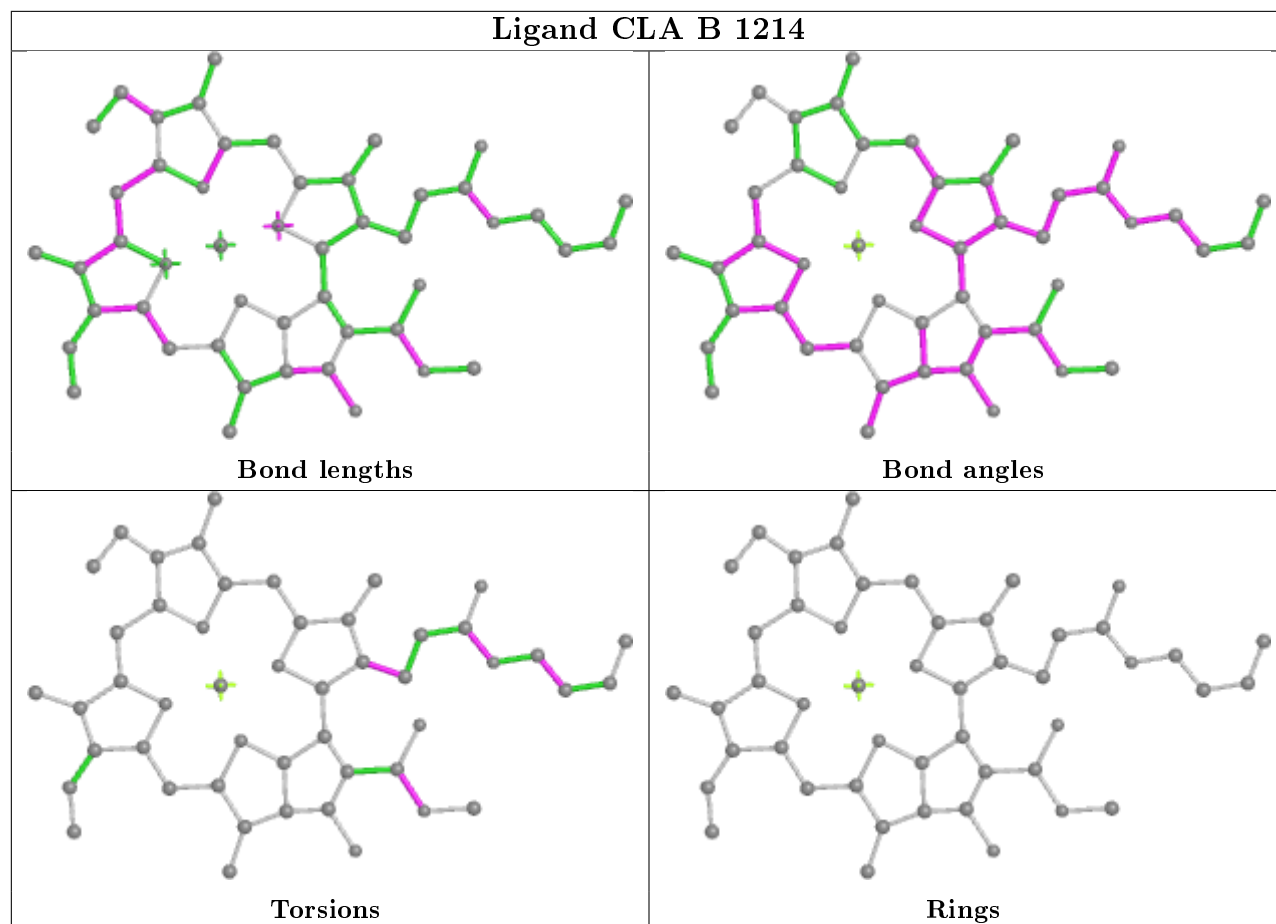




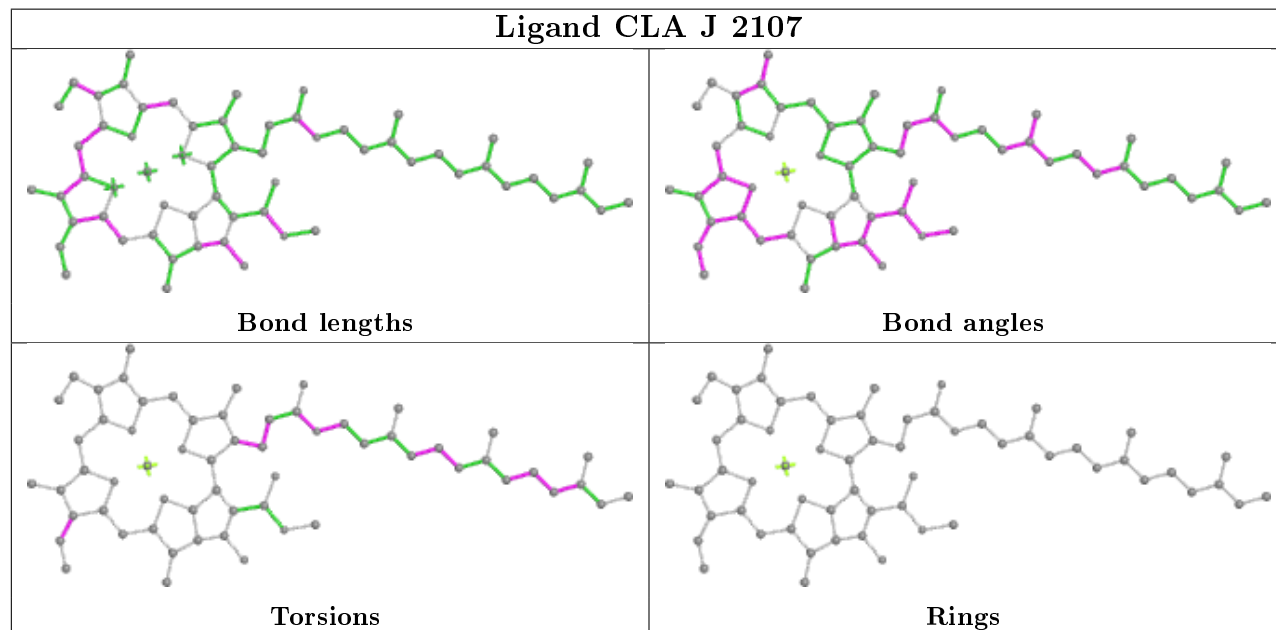


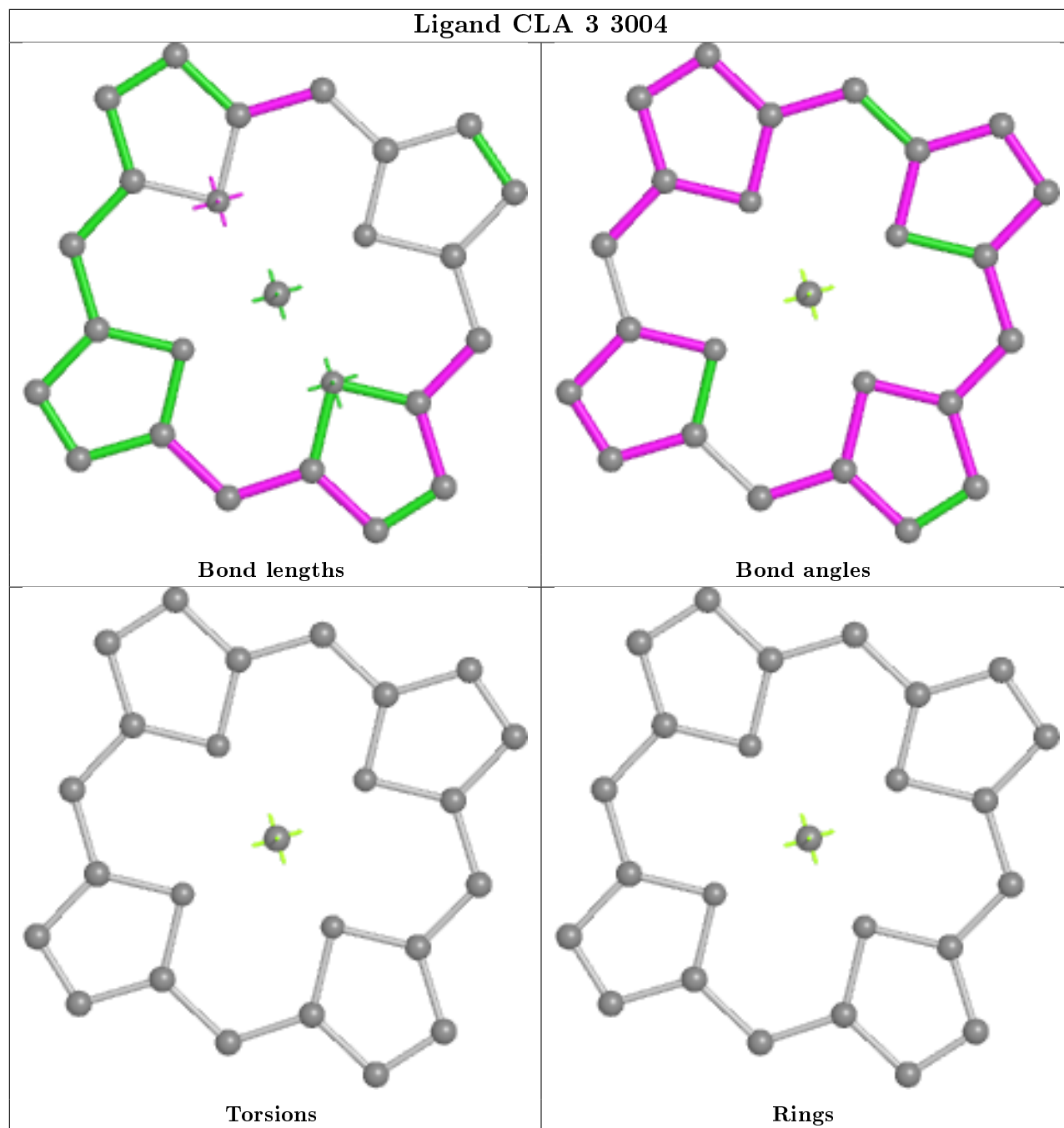


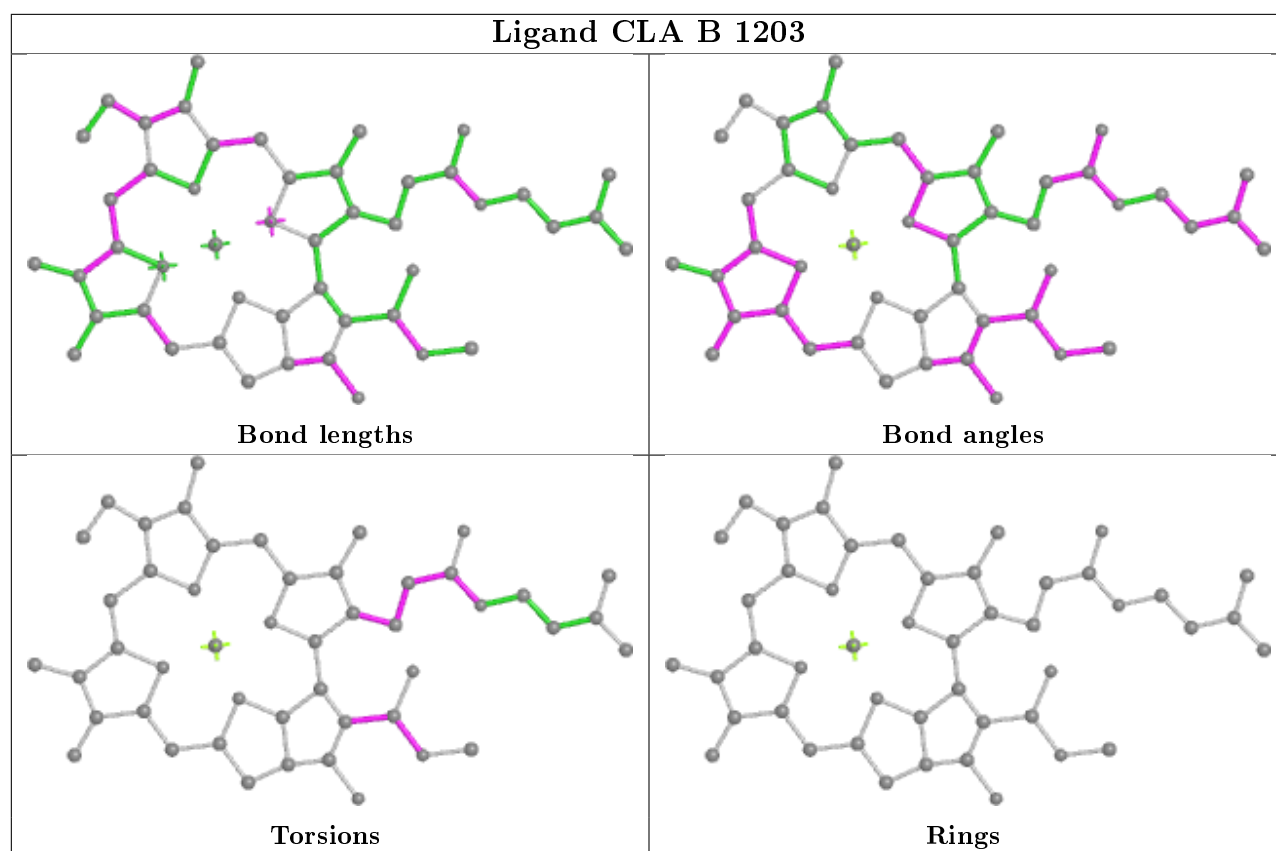
Ligand CLA B 1214



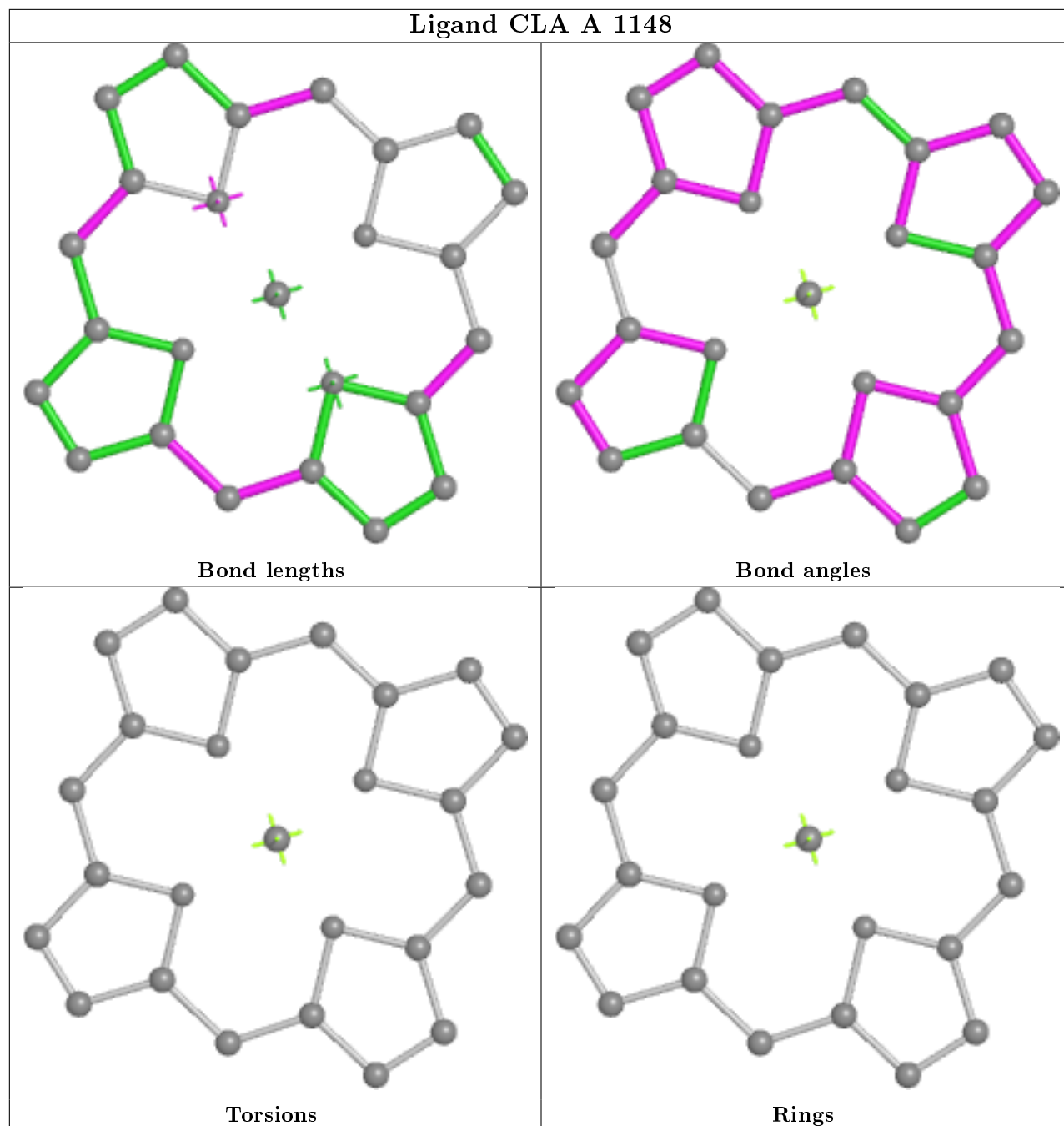
Ligand CLA J 2107



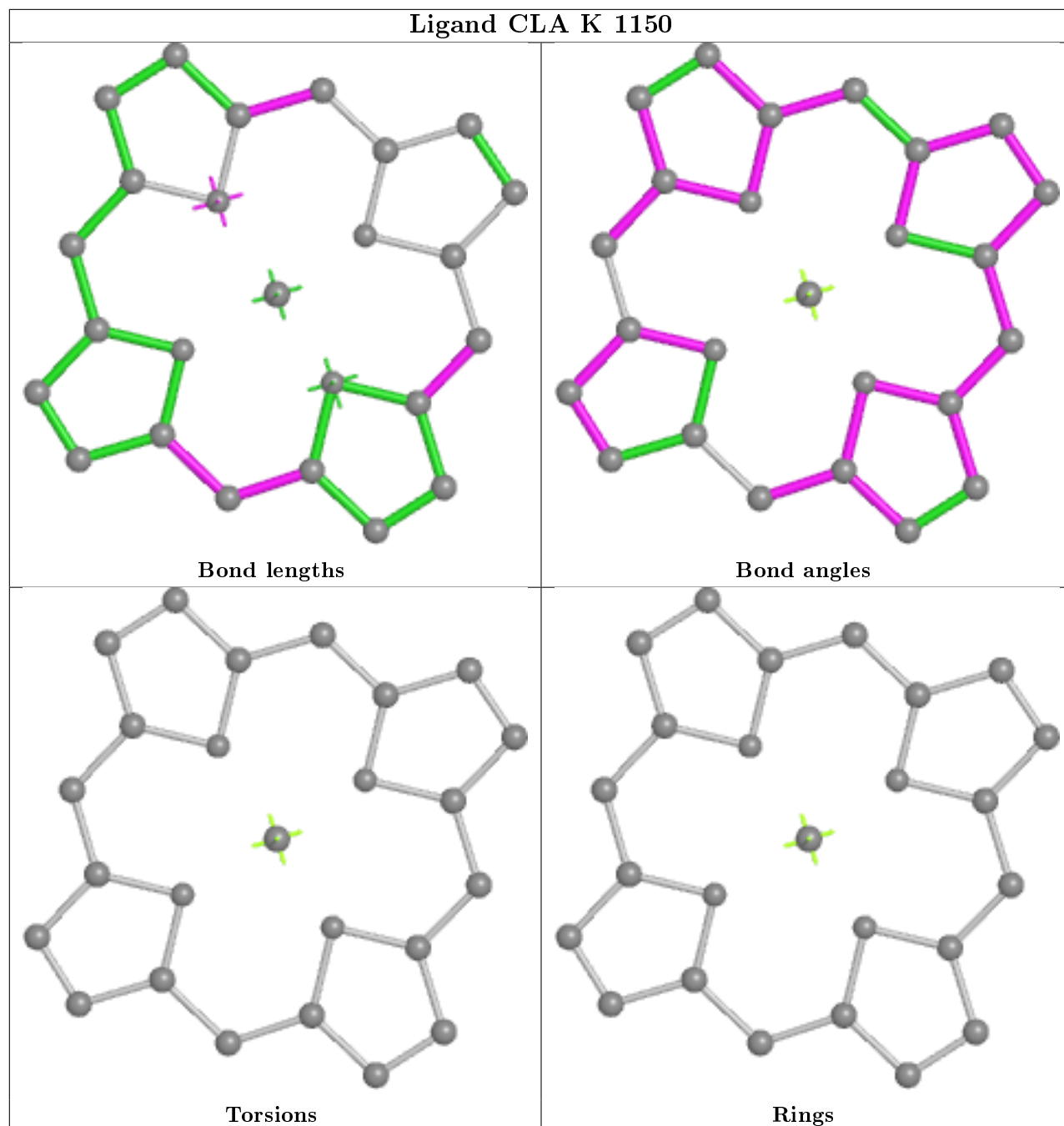


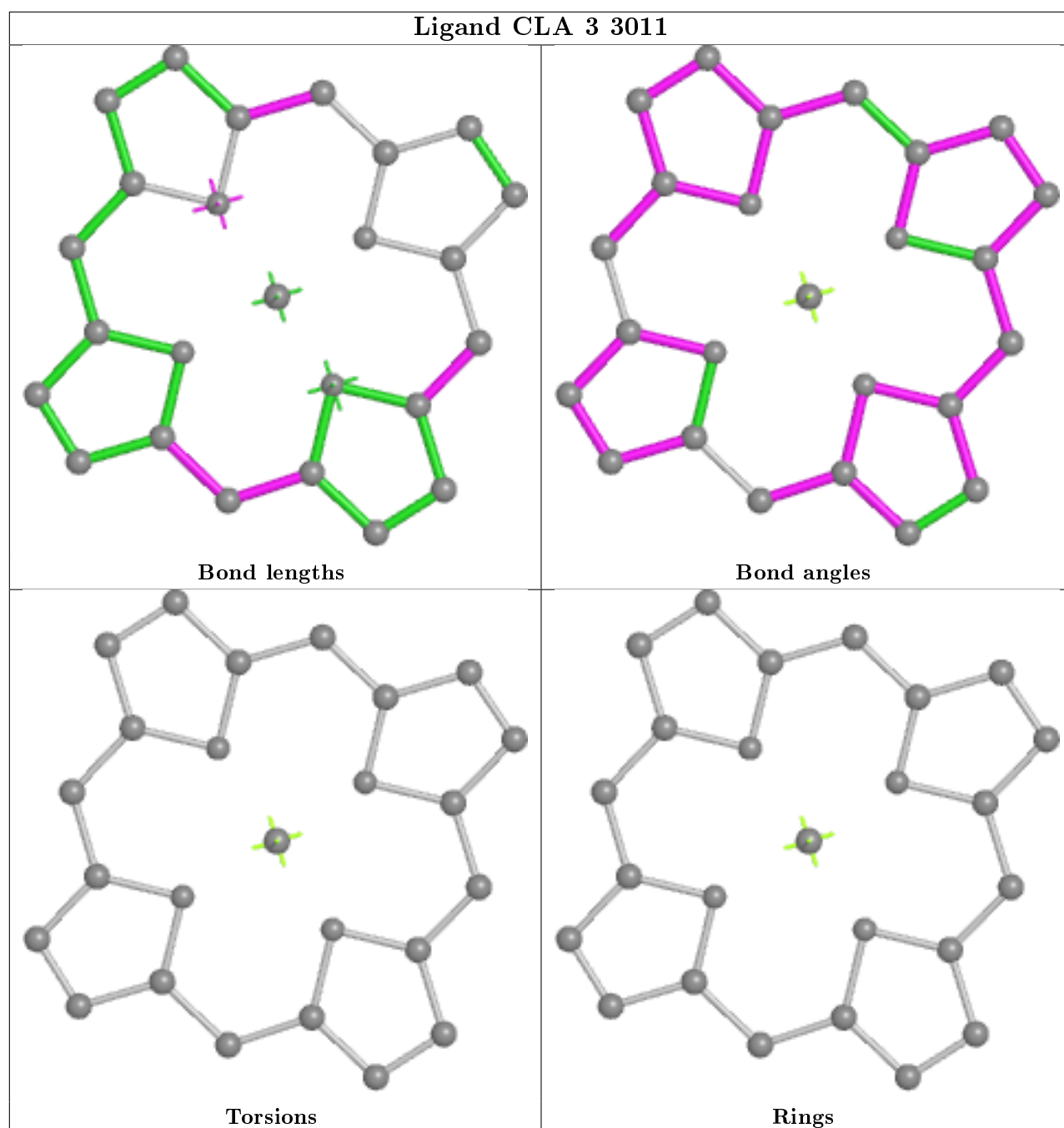


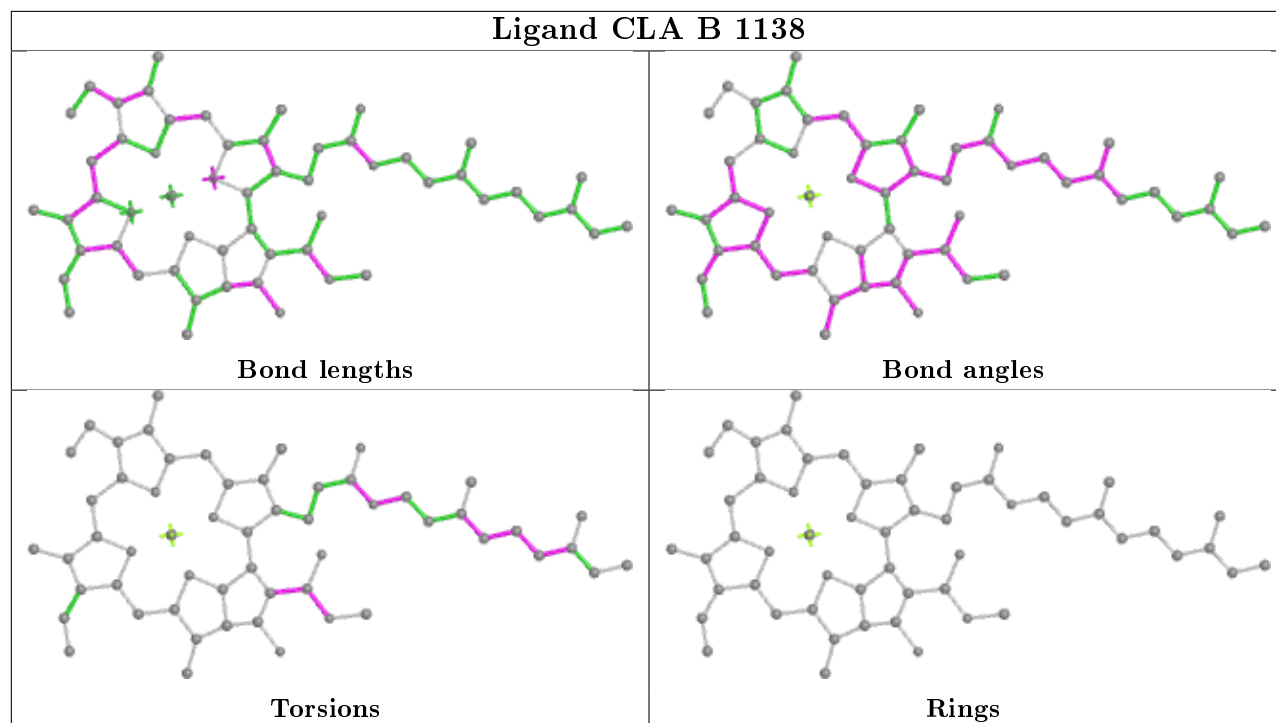
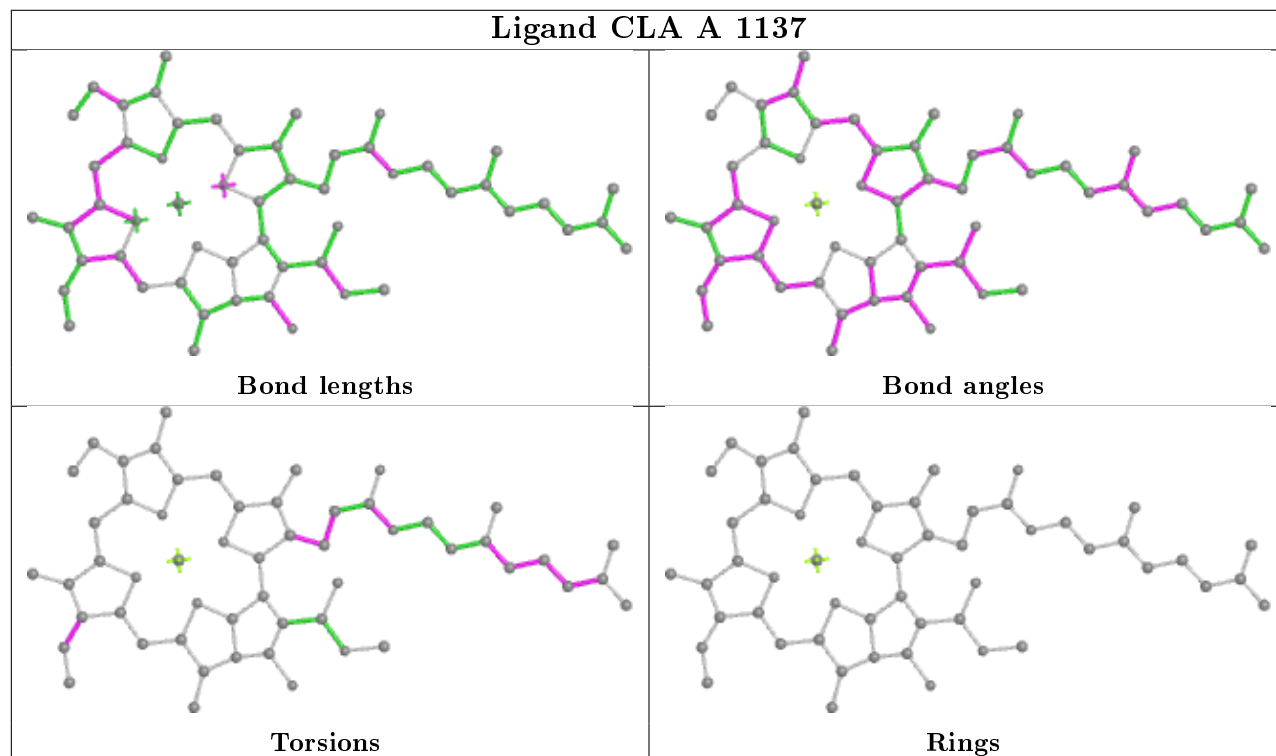
Ligand CLA A 1148

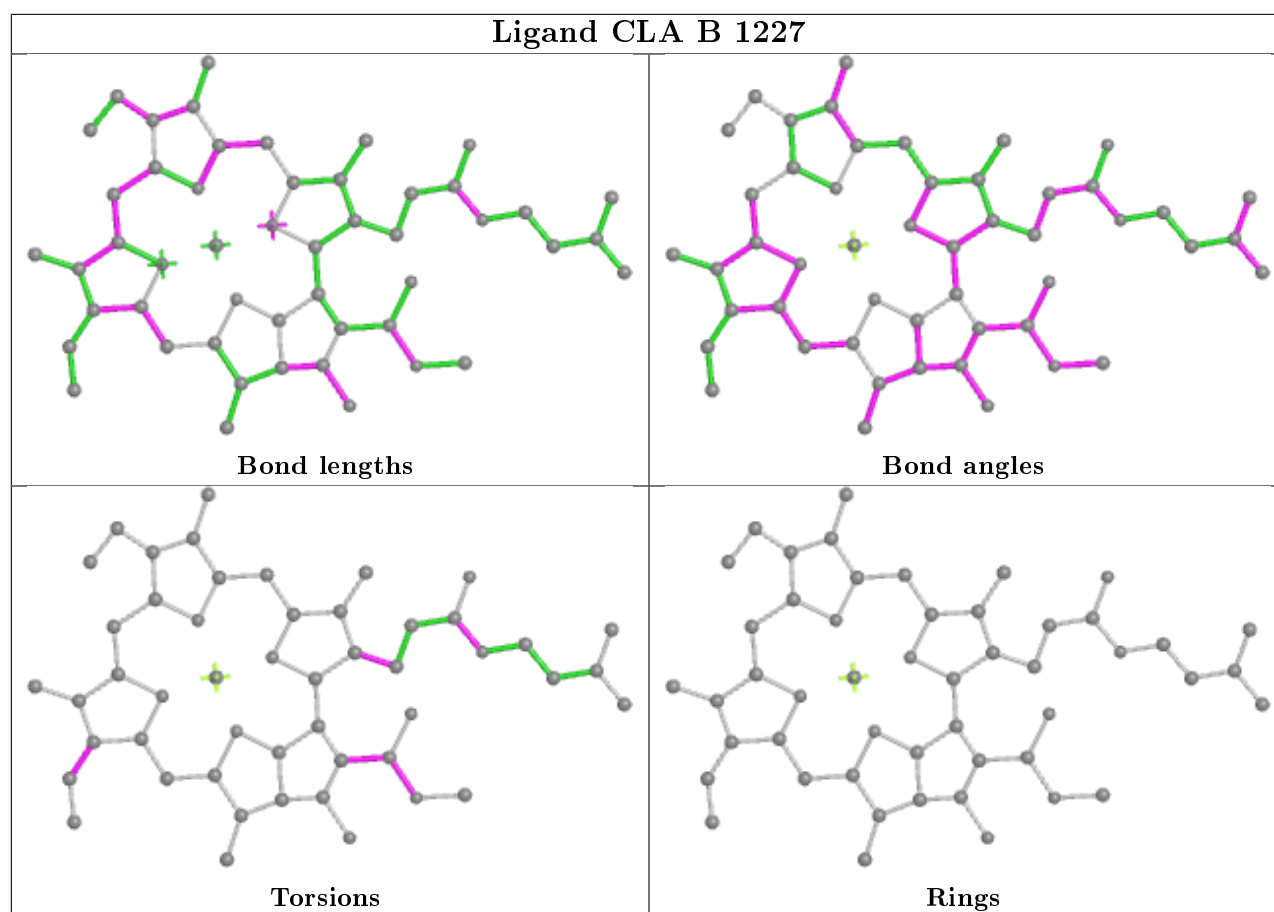


Ligand CLA K 1150

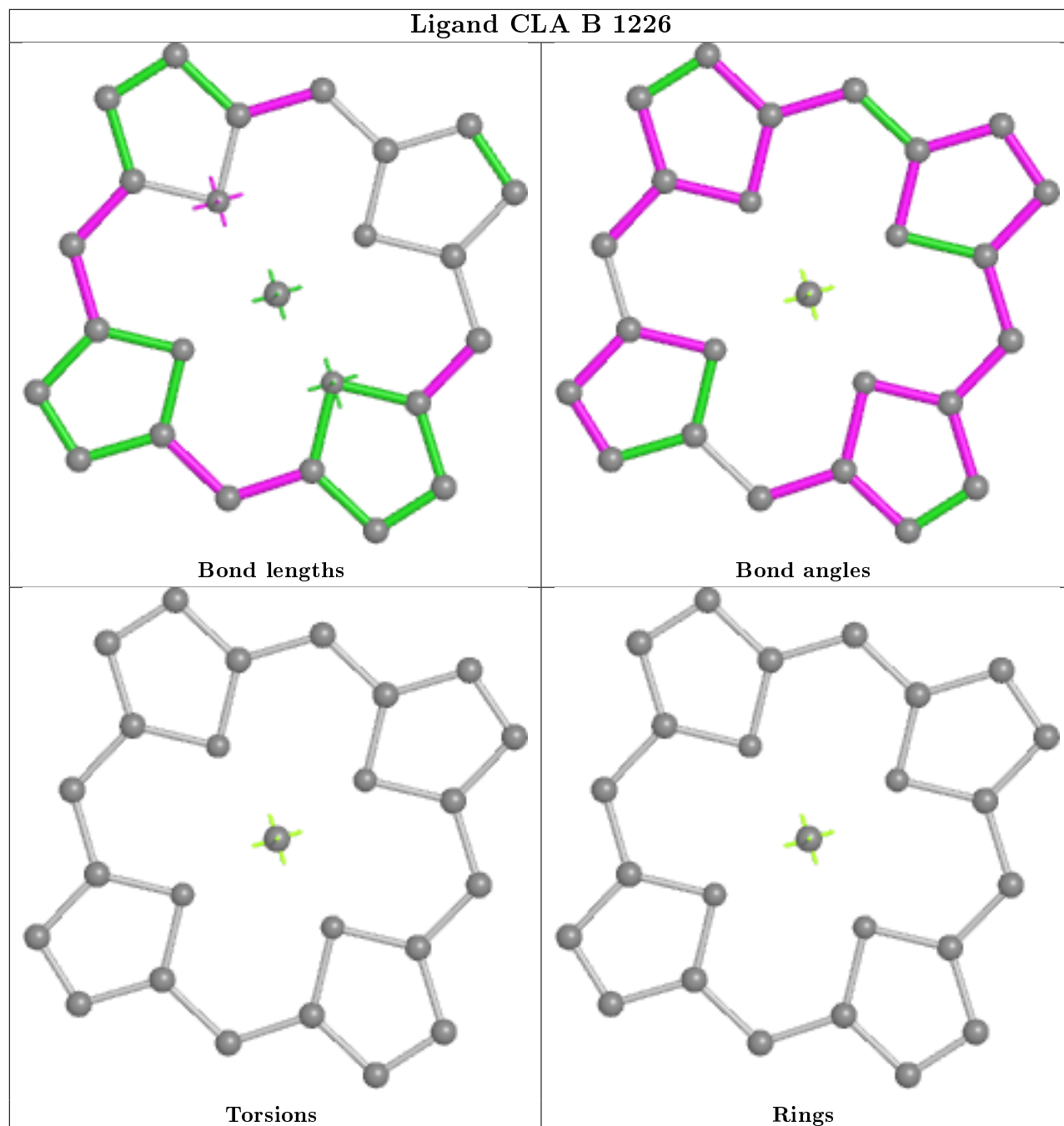




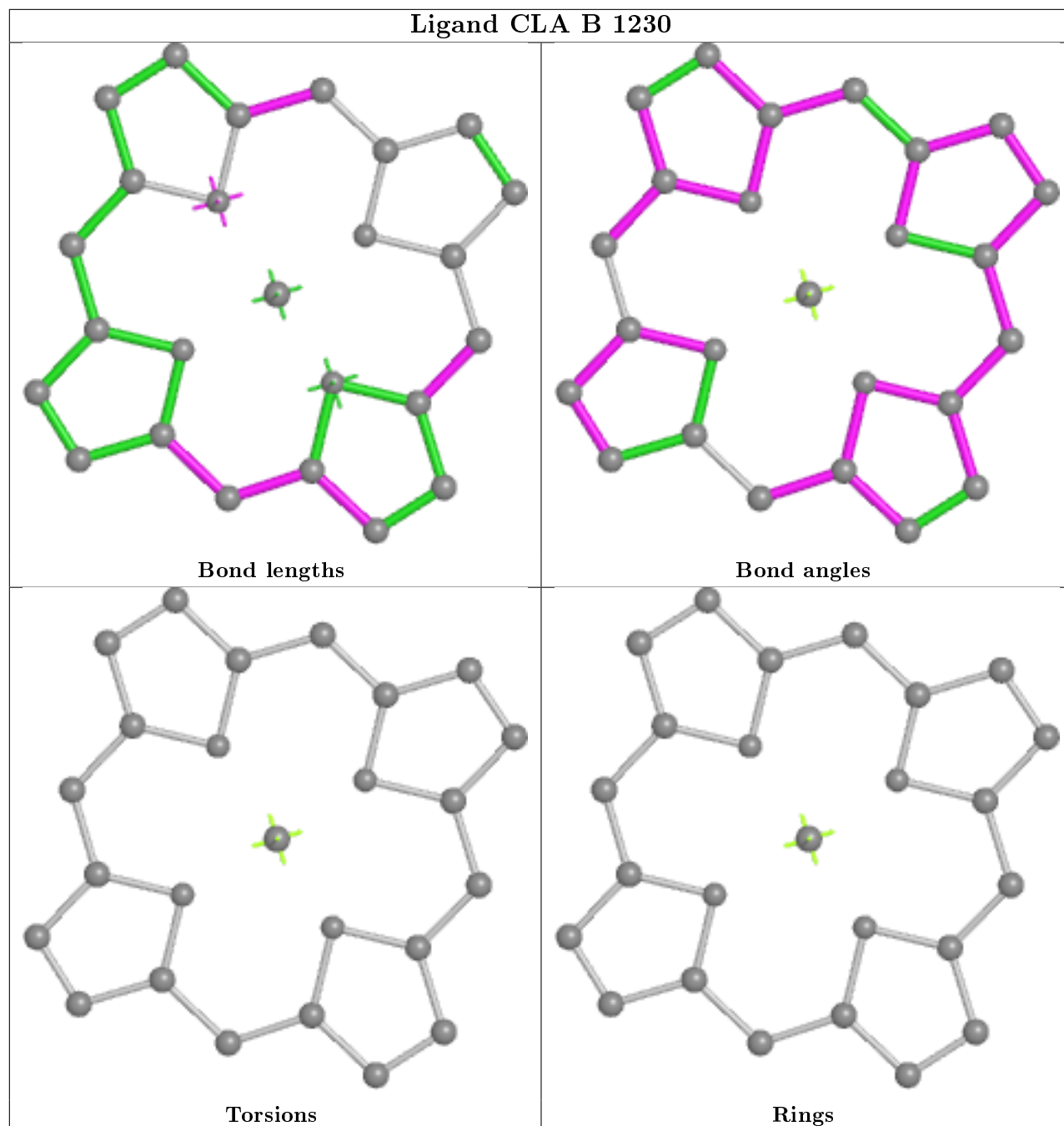
Ligand CLA B 1138**Ligand CLA A 1137**



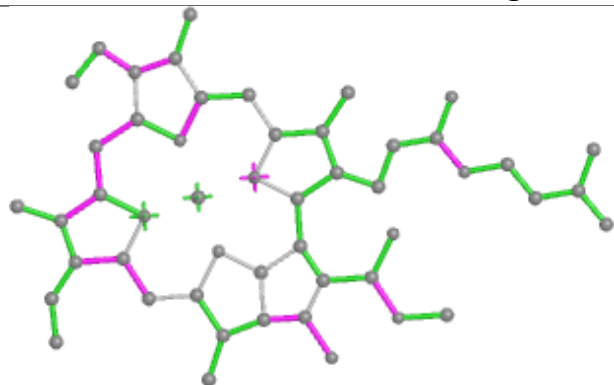
Ligand CLA B 1226



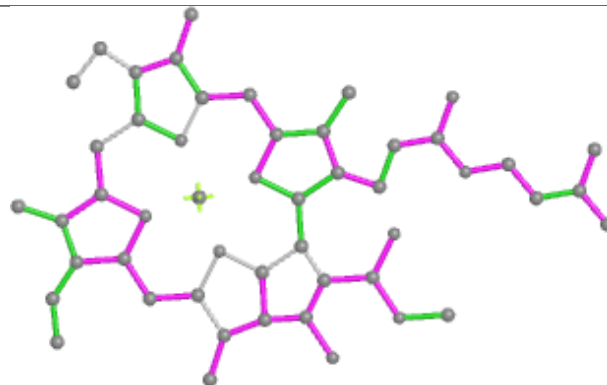
Ligand CLA B 1230



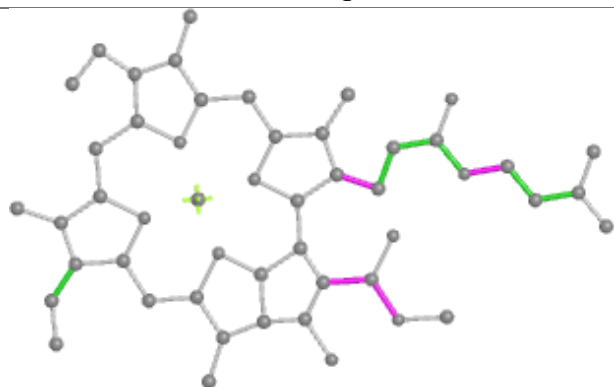
Ligand CLA B 1217



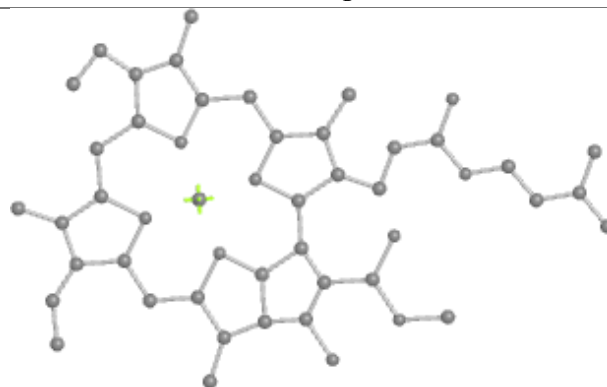
Bond lengths



Bond angles

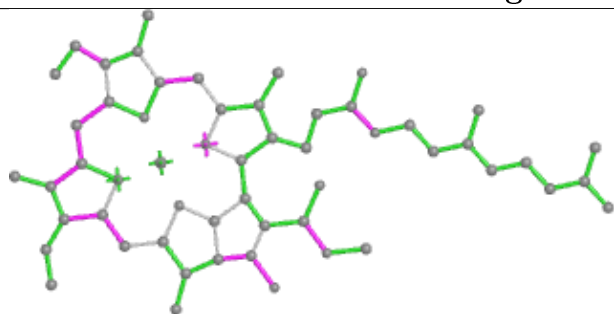


Torsions

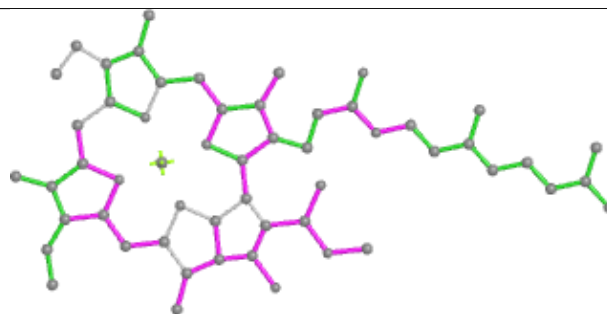


Rings

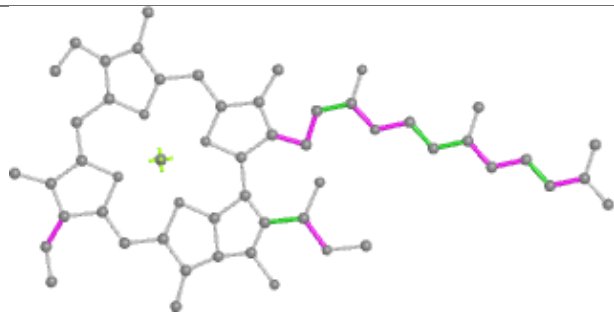
Ligand CLA A 1119



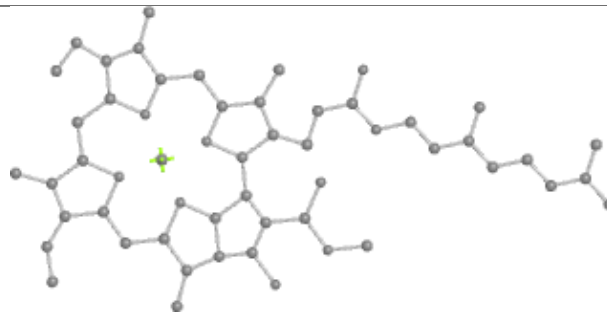
Bond lengths



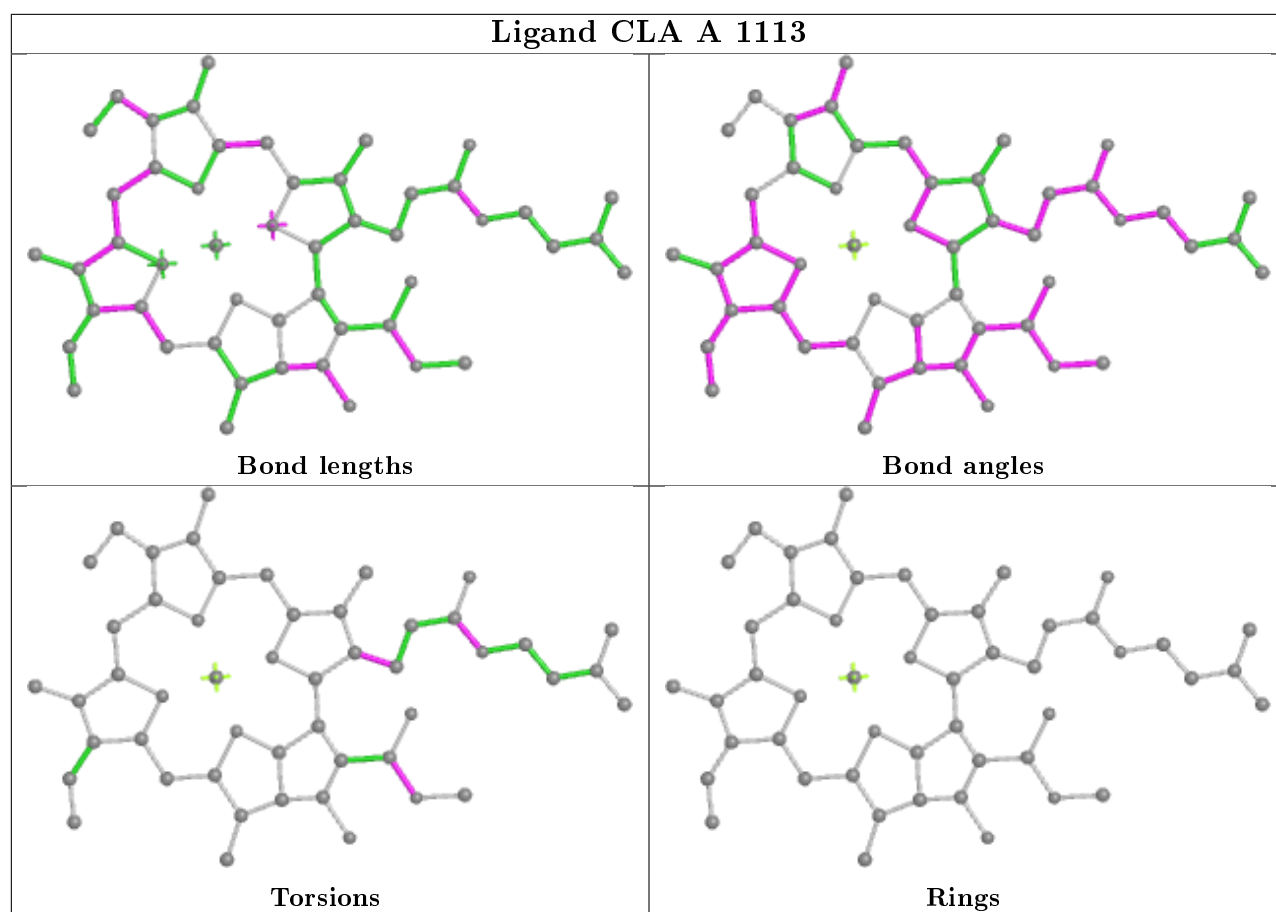
Bond angles

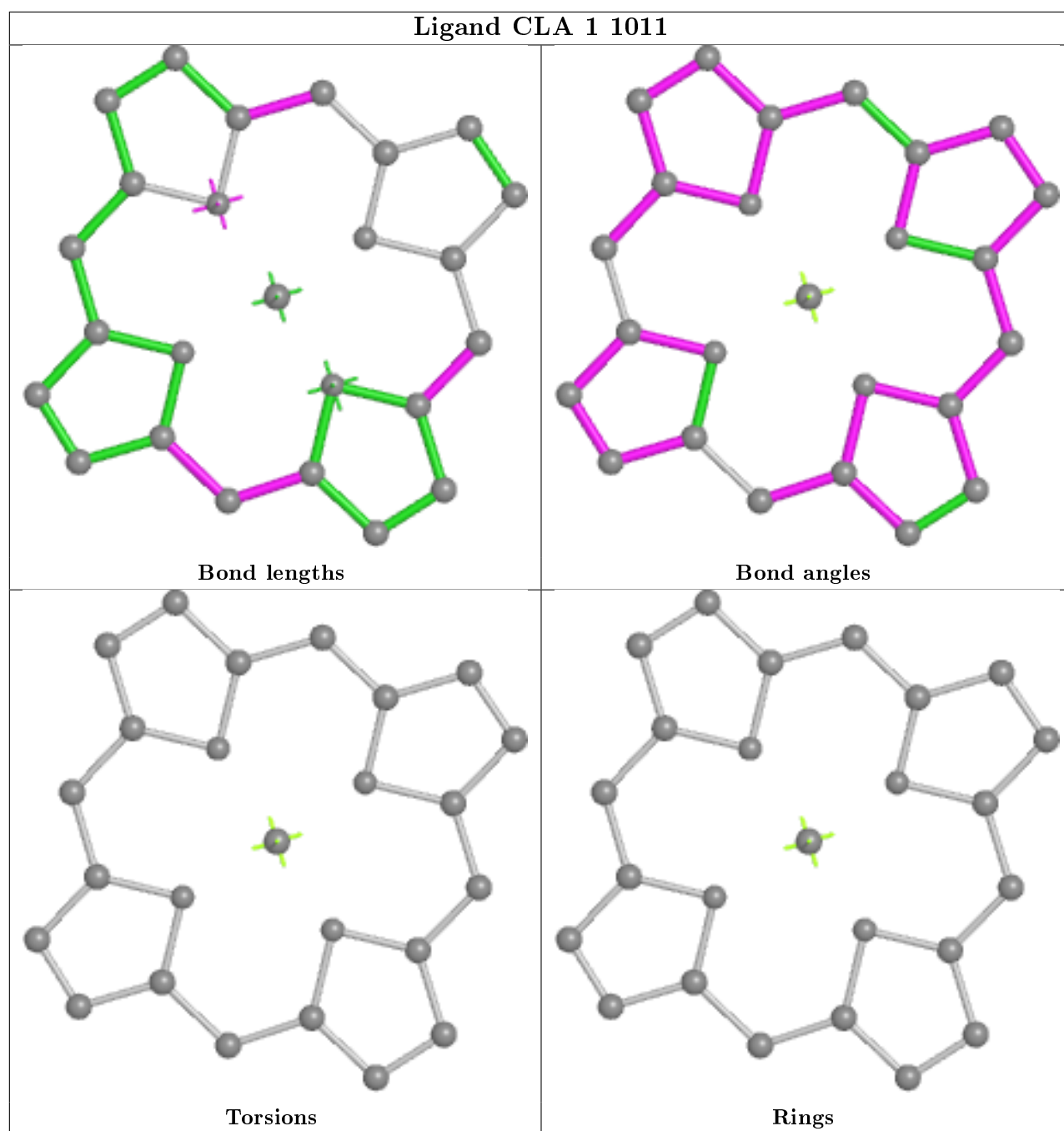


Torsions

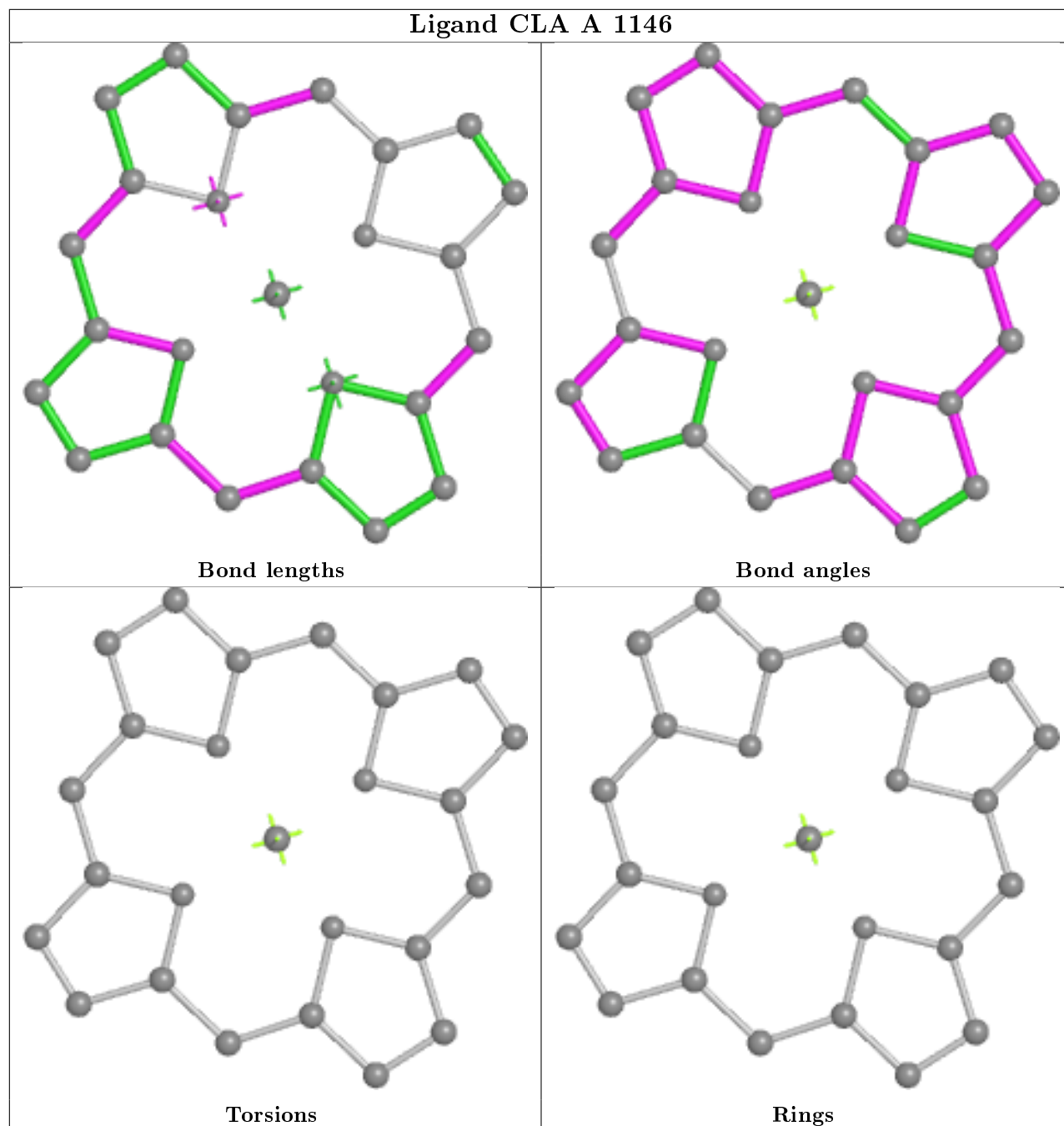


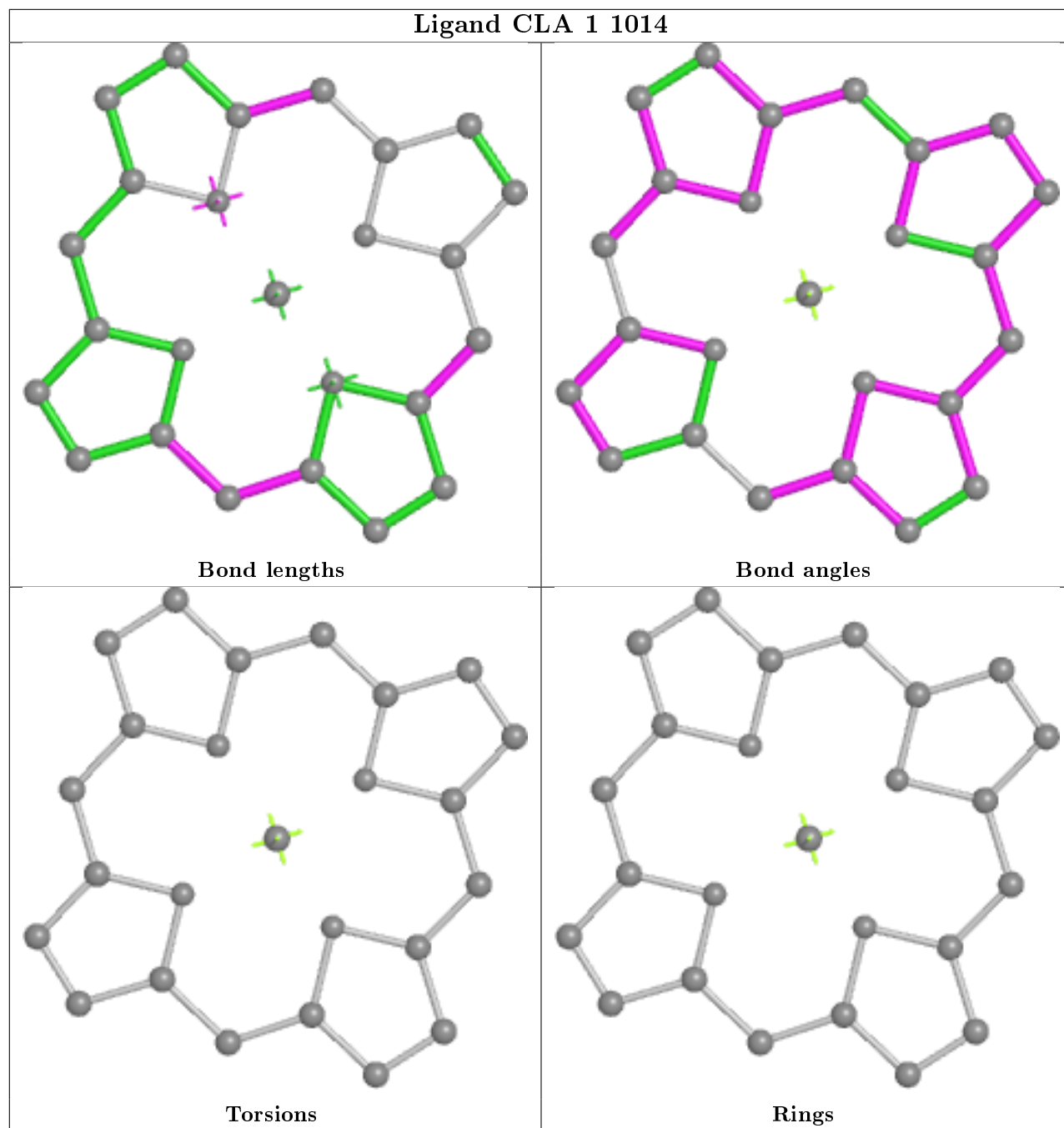
Rings

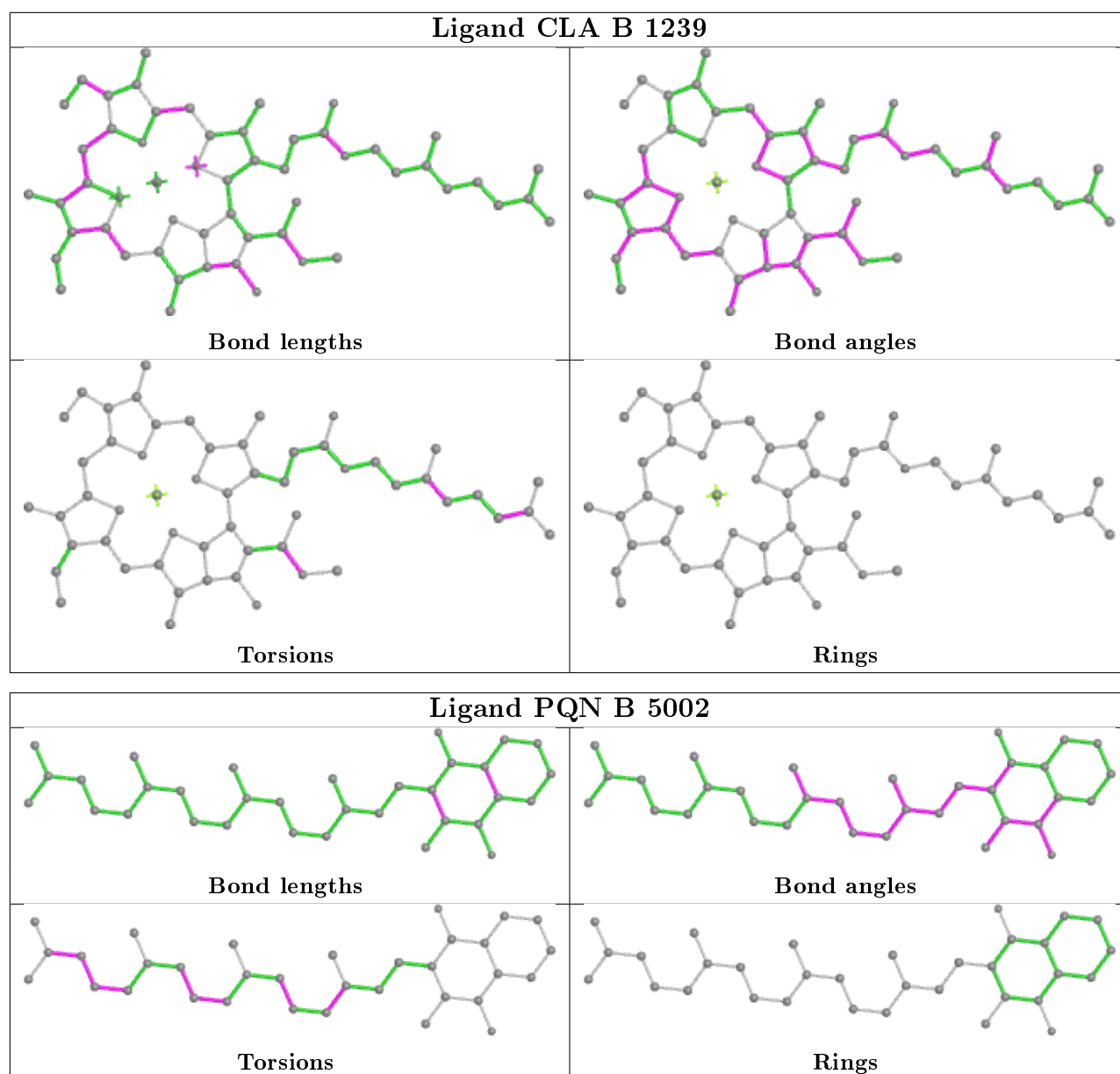




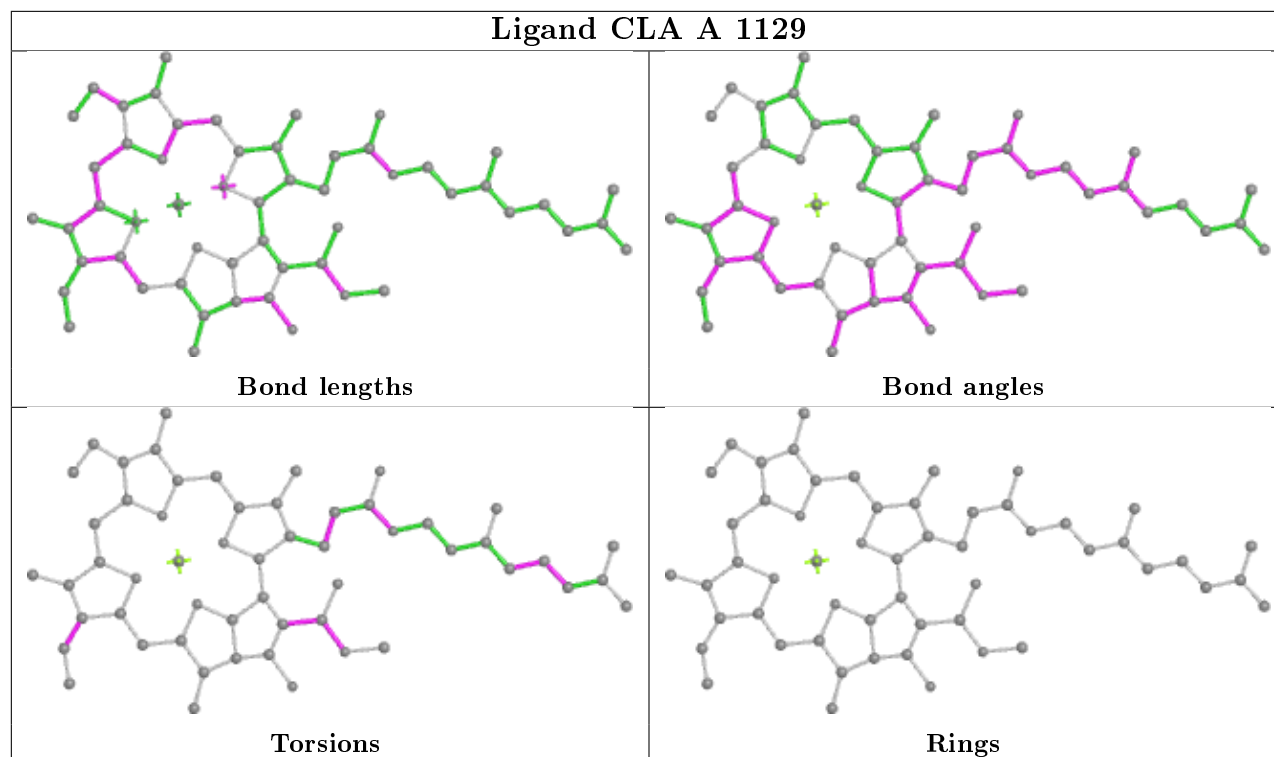
Ligand CLA A 1146



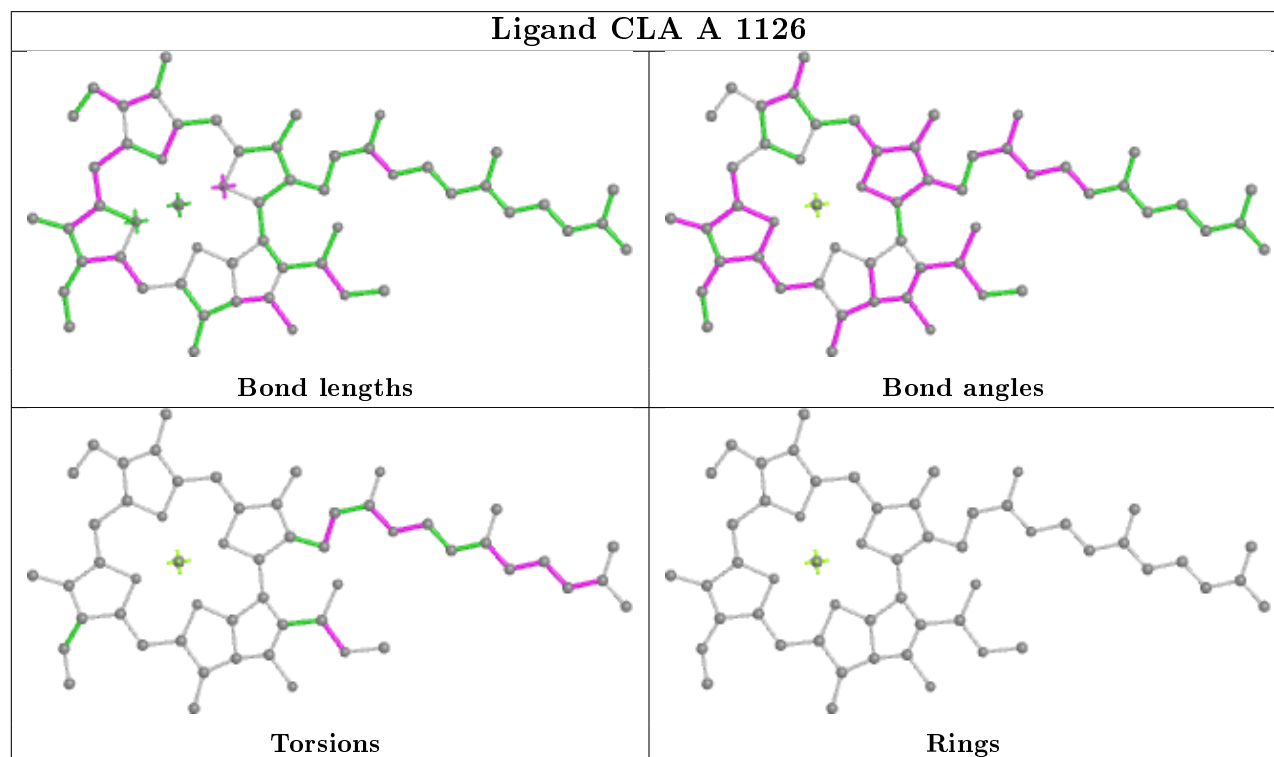




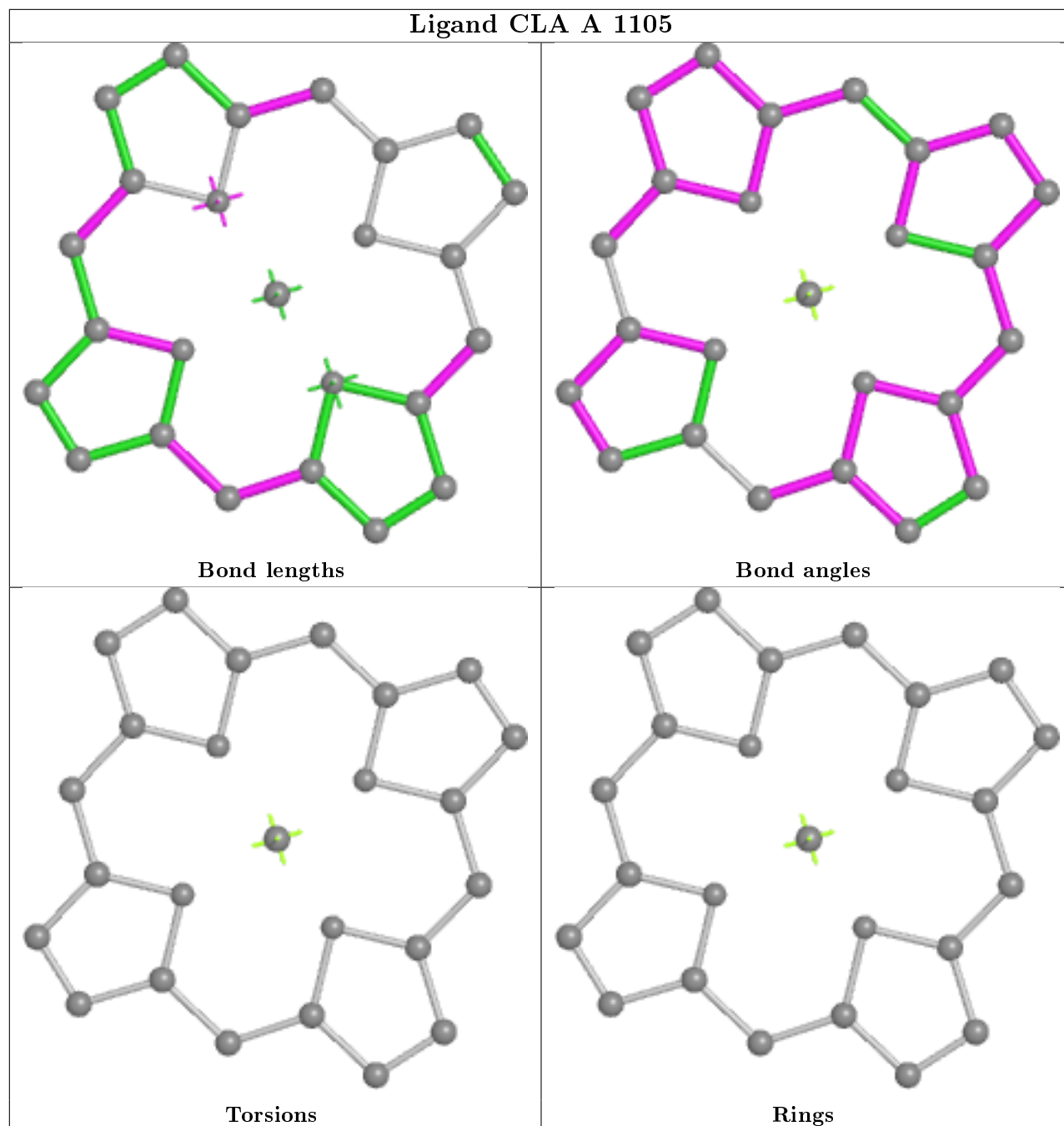
Ligand CLA A 1129



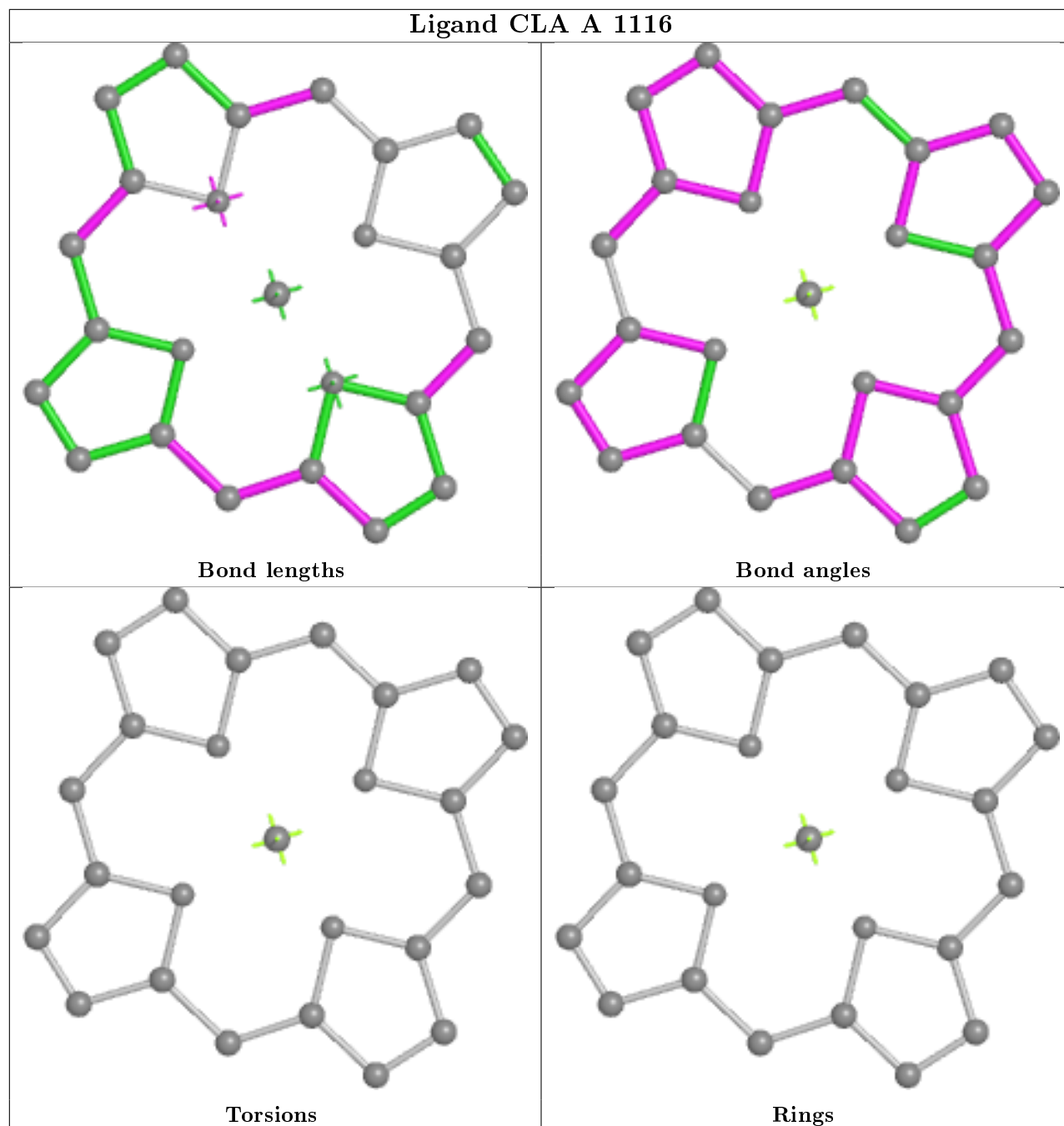
Ligand CLA A 1126



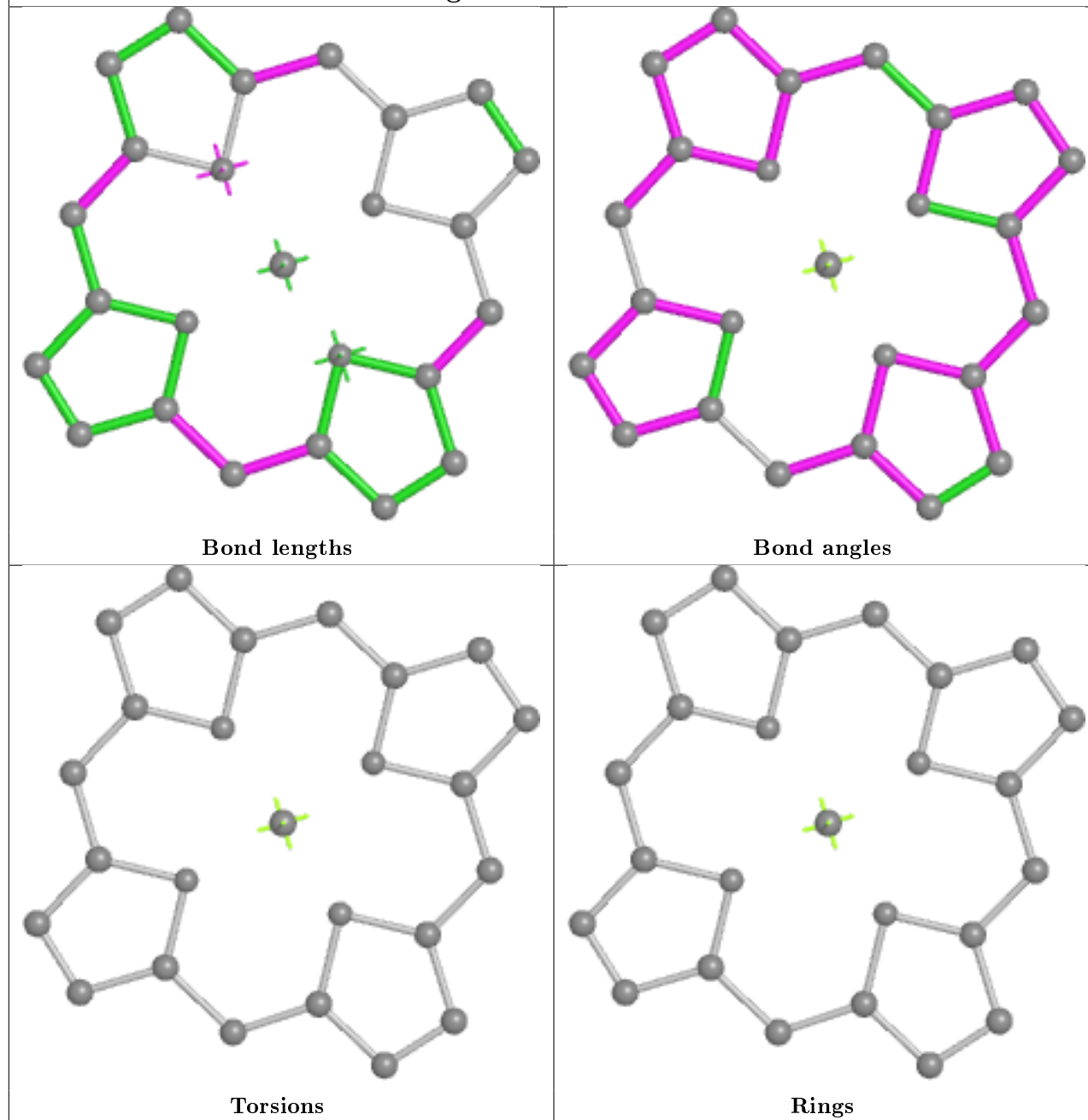
Ligand CLA A 1105



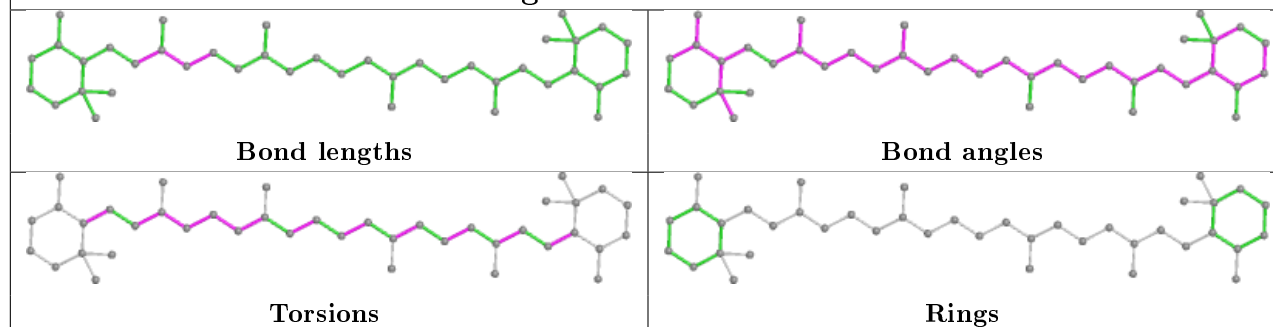
Ligand CLA A 1116

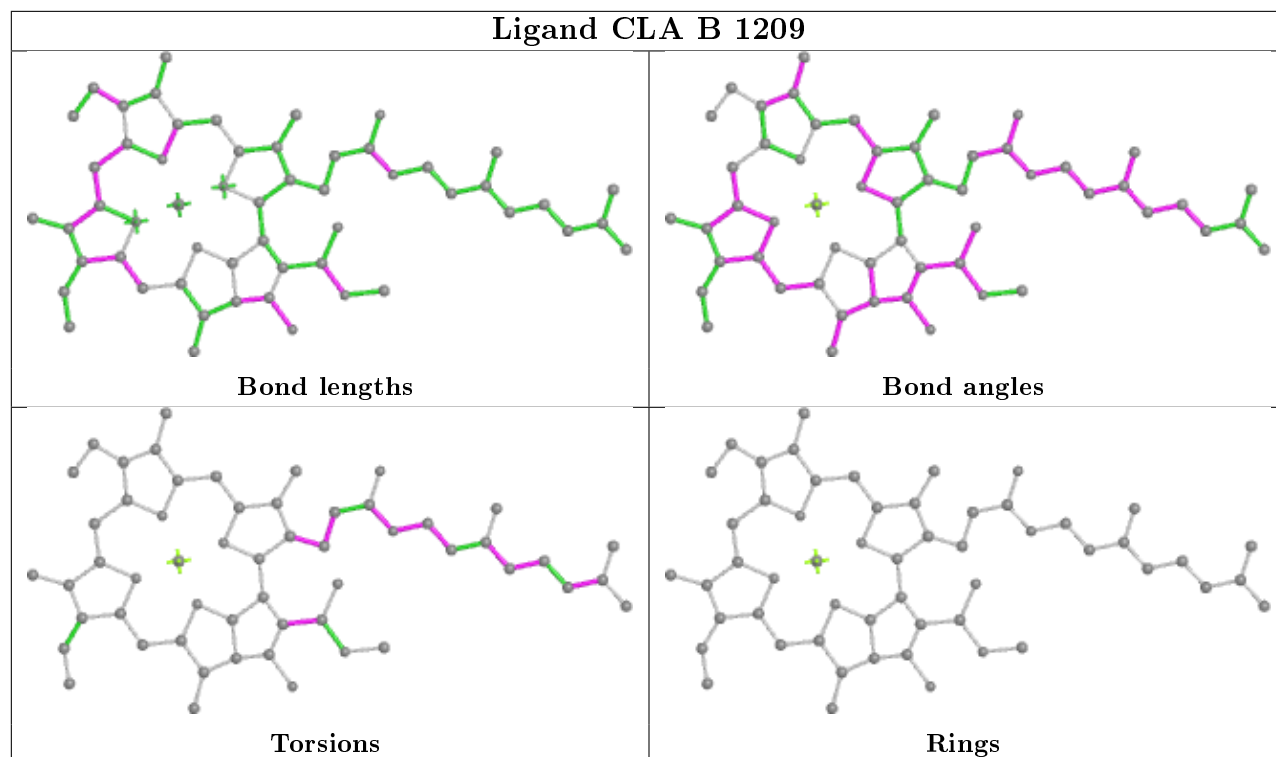
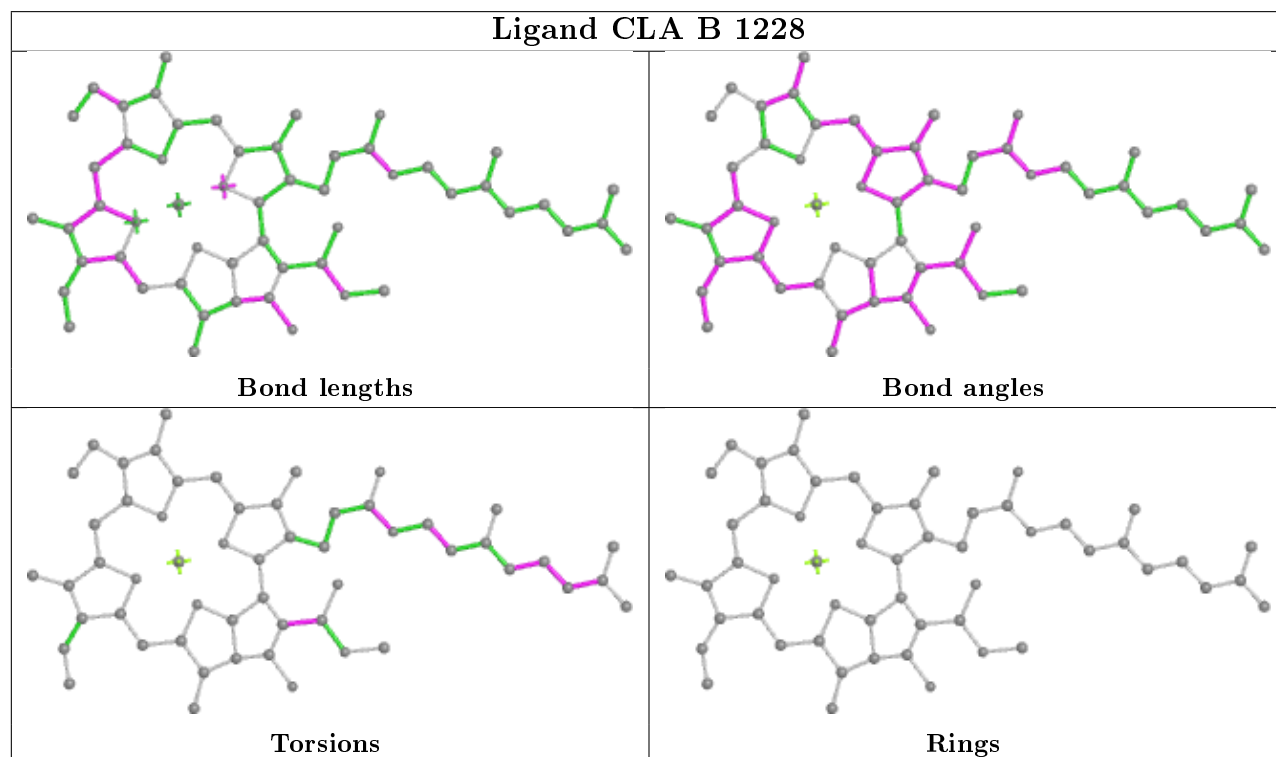


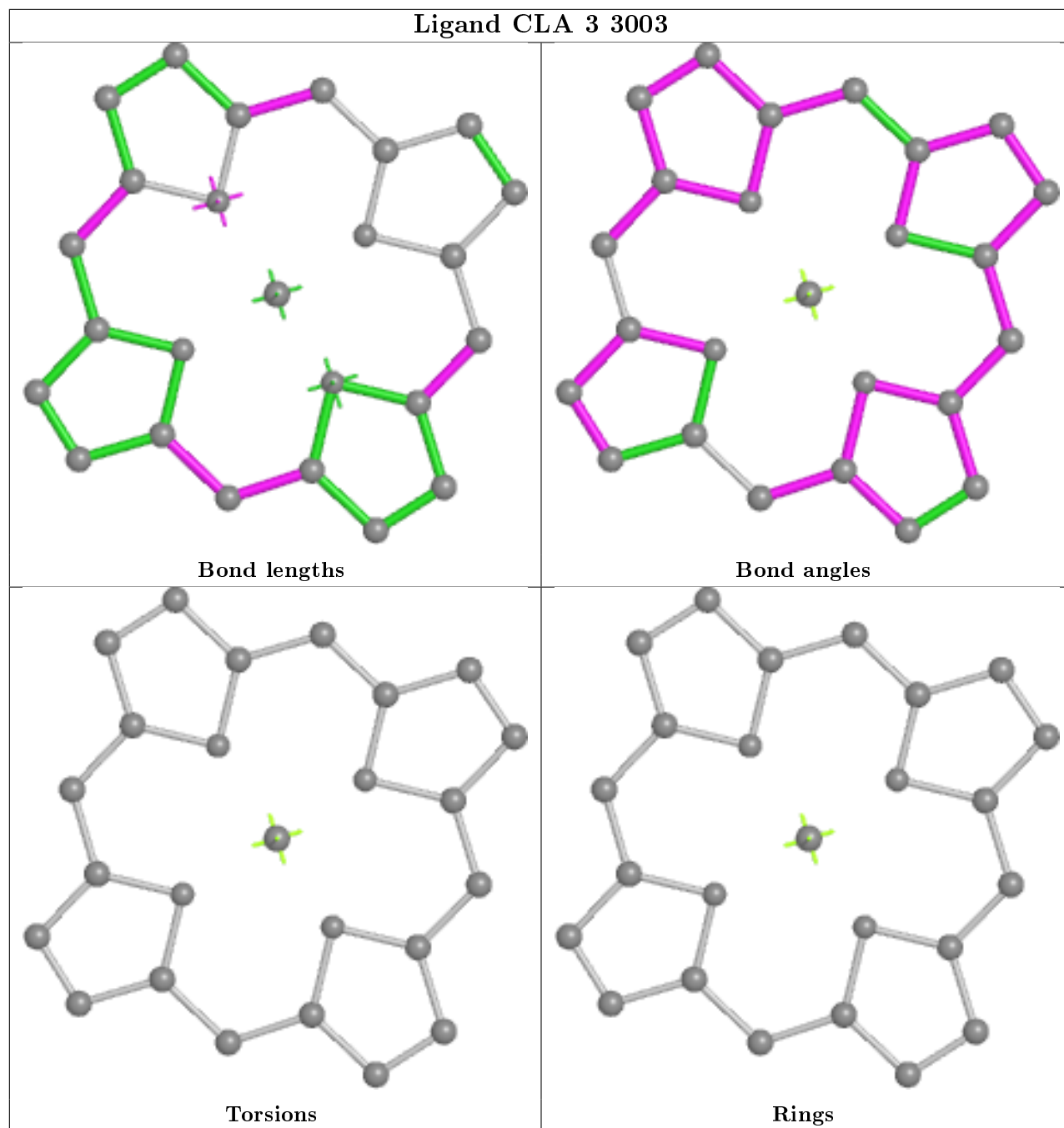
Ligand CLA B 1210



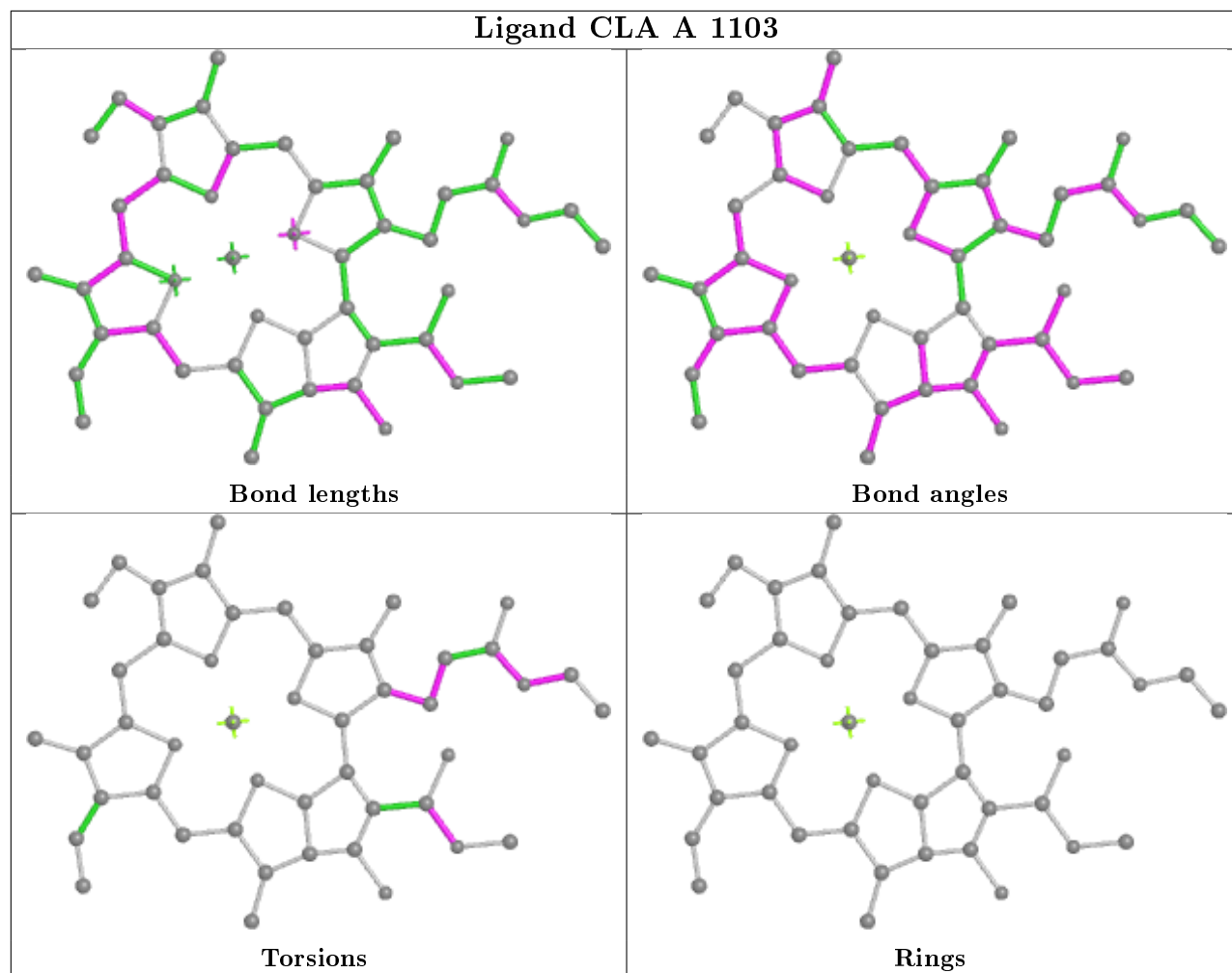
Ligand BCR B 6017

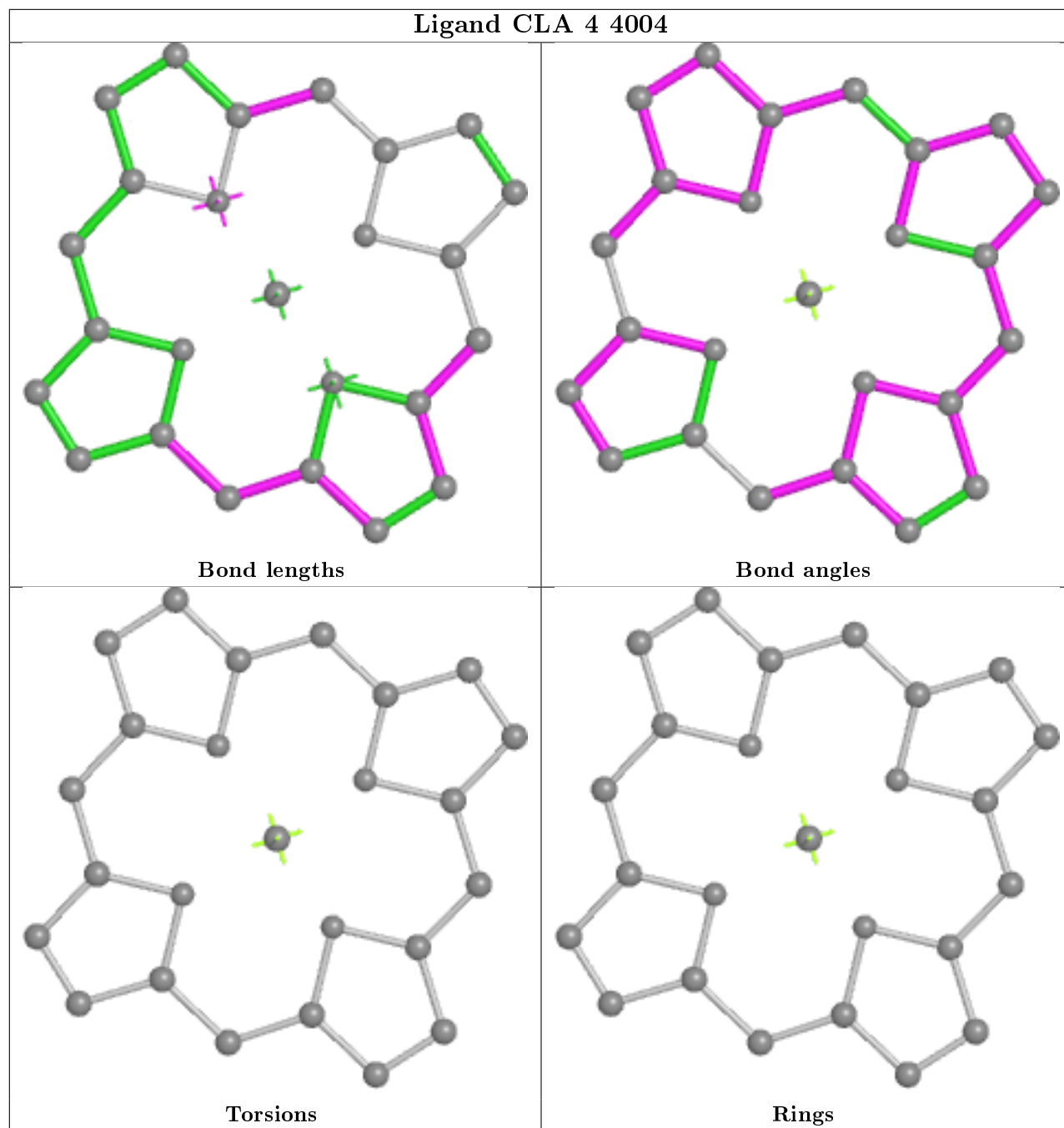


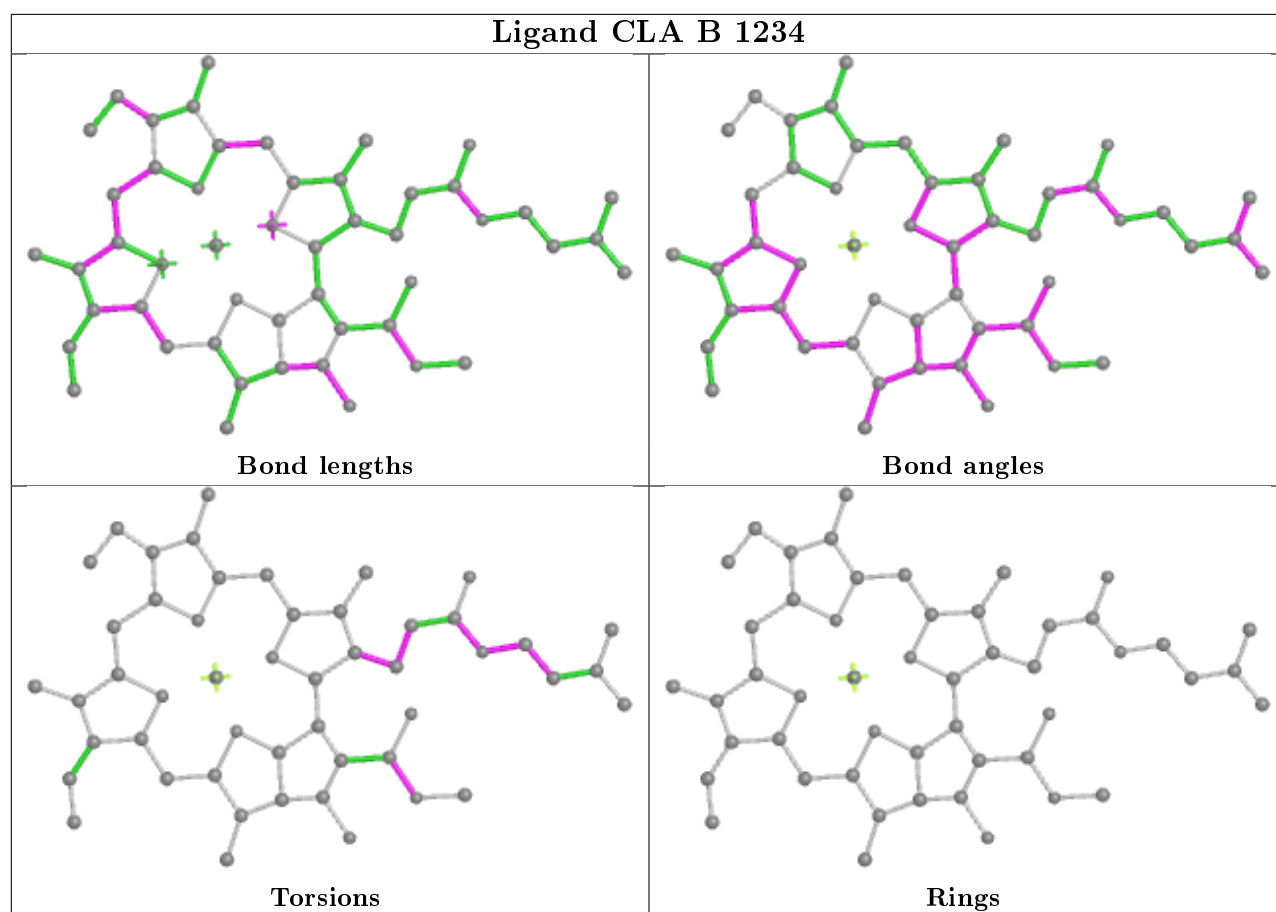
Ligand CLA B 1209**Ligand CLA B 1228**



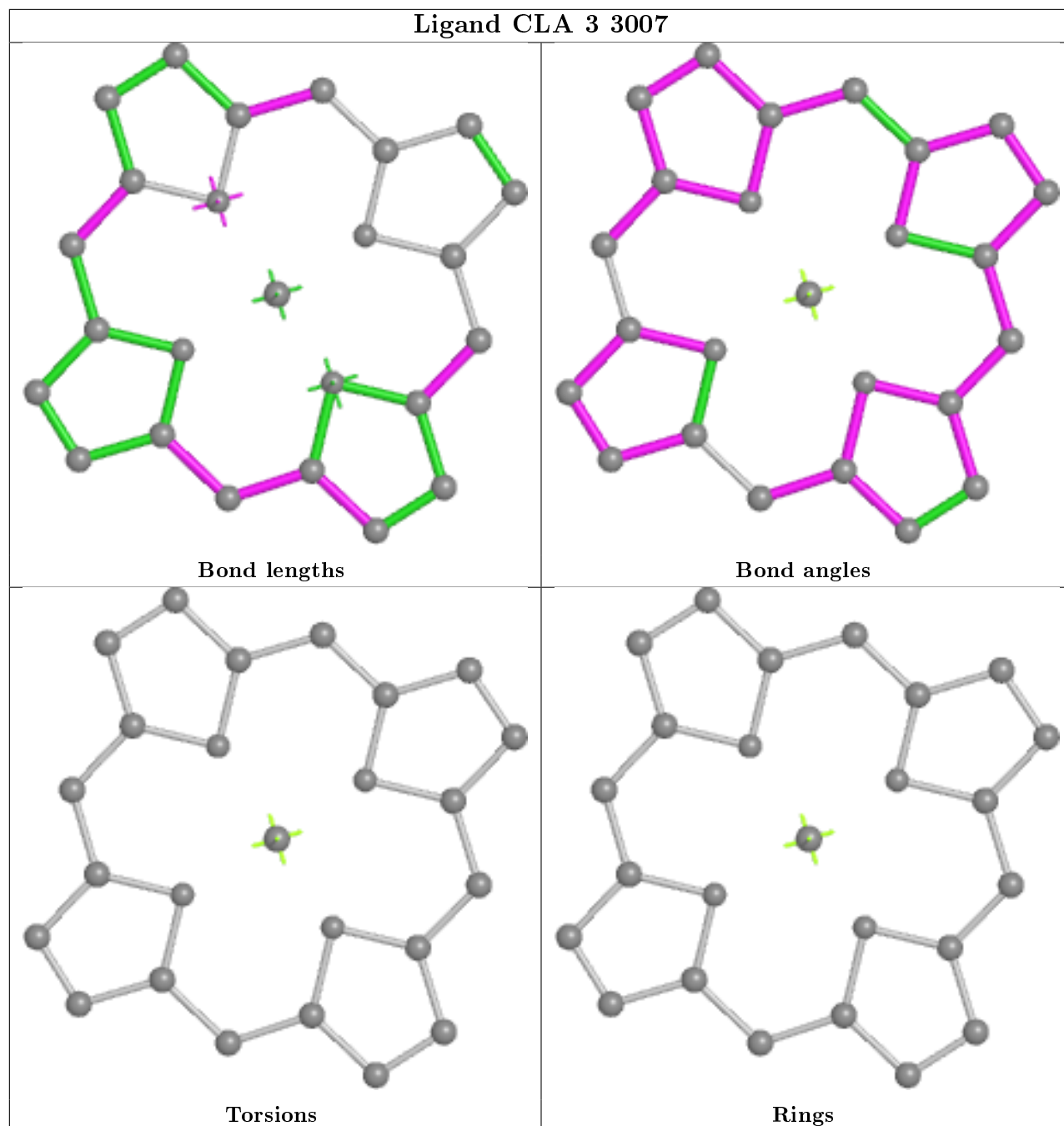
Ligand CLA A 1103



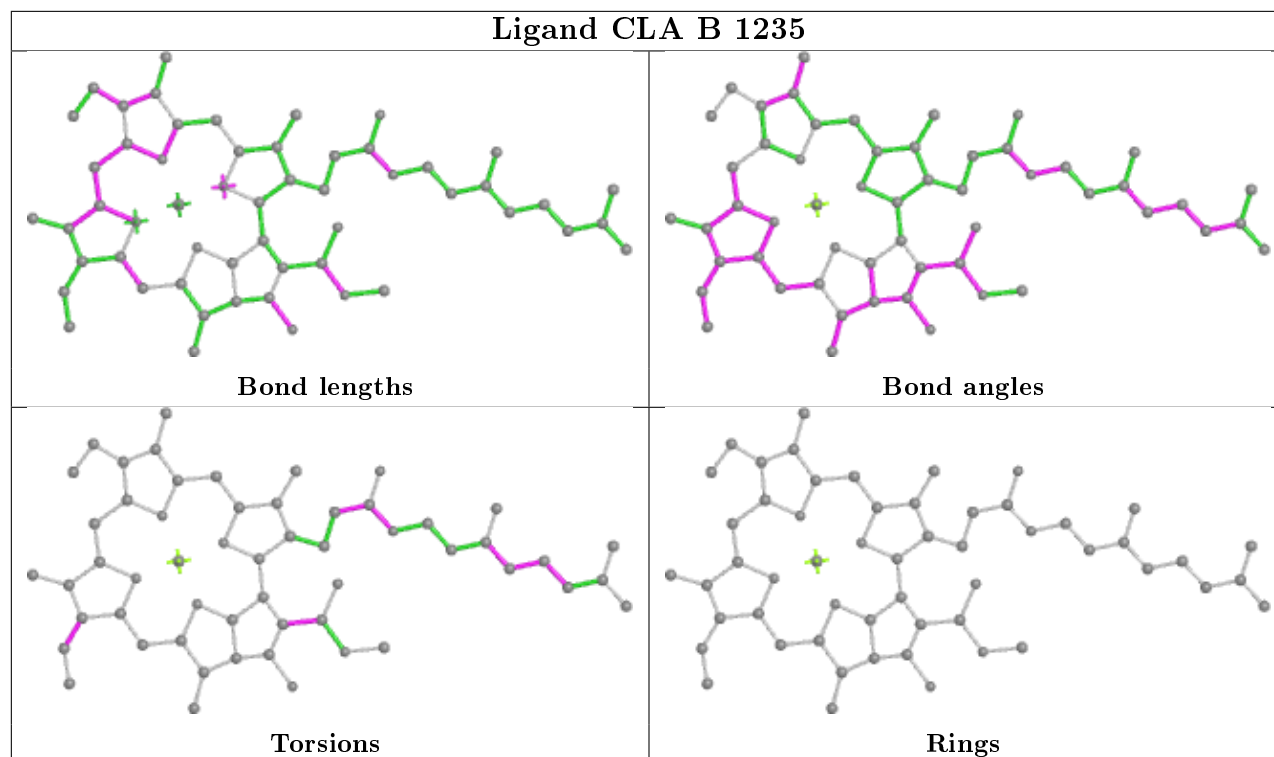




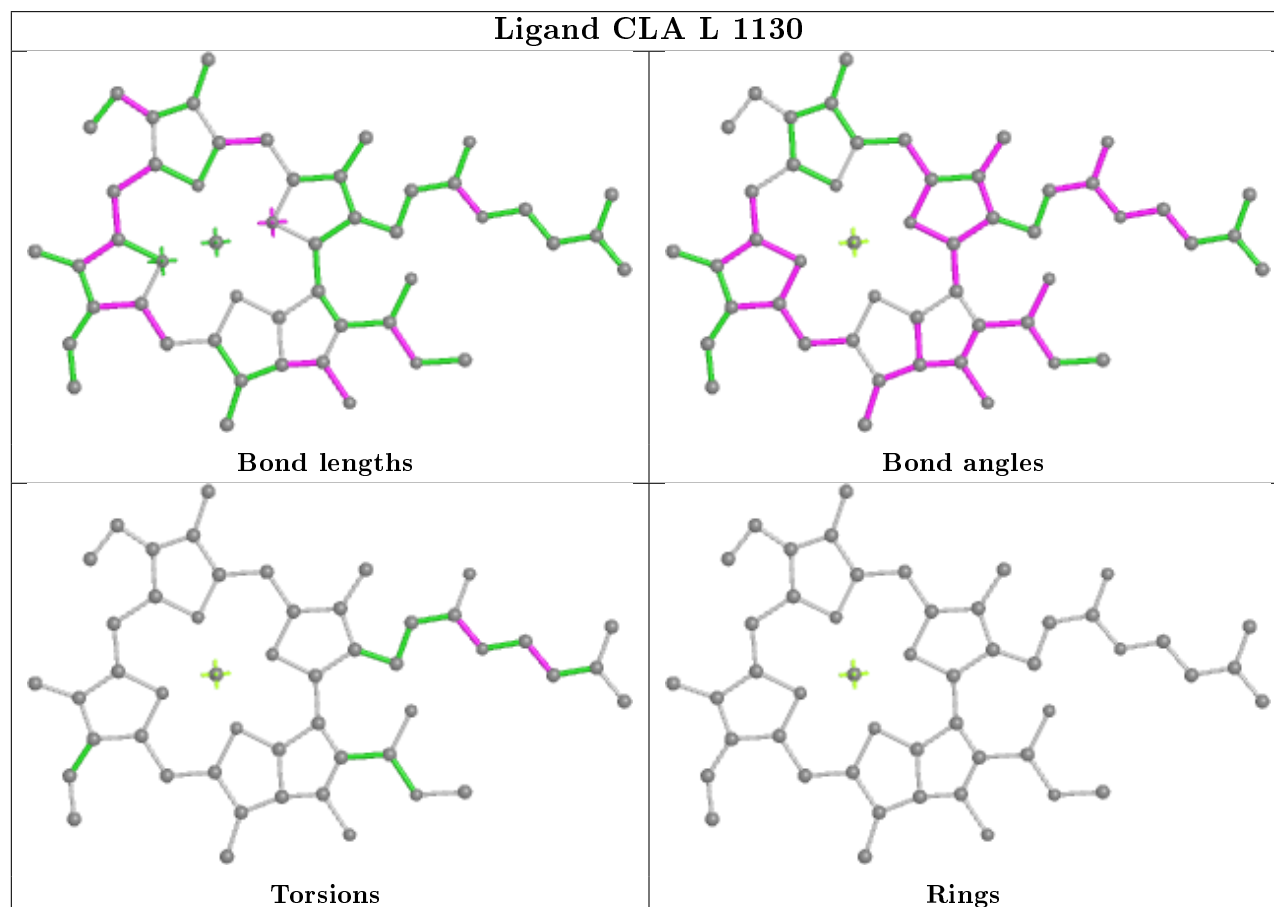
Ligand CLA 3 3007

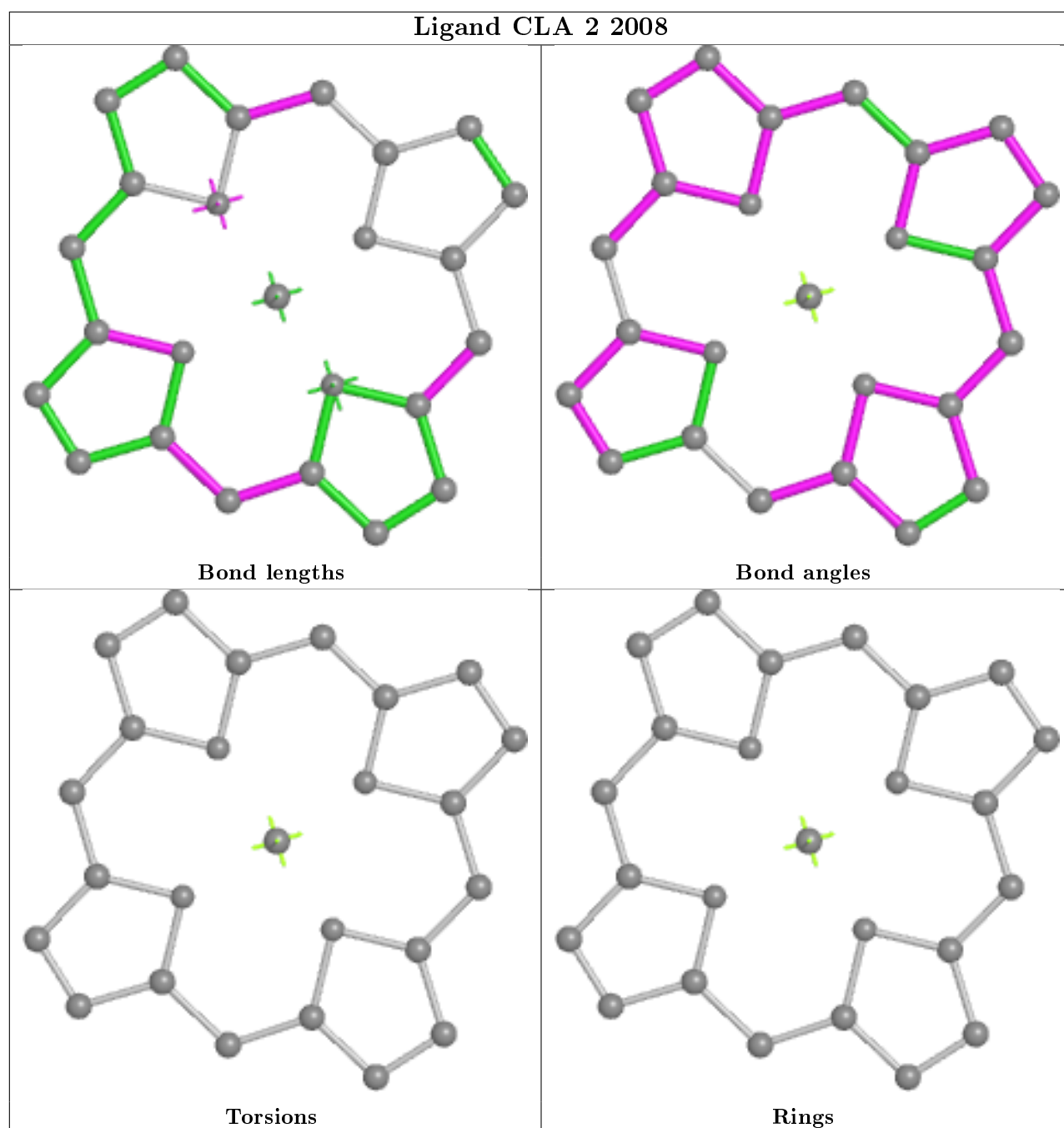


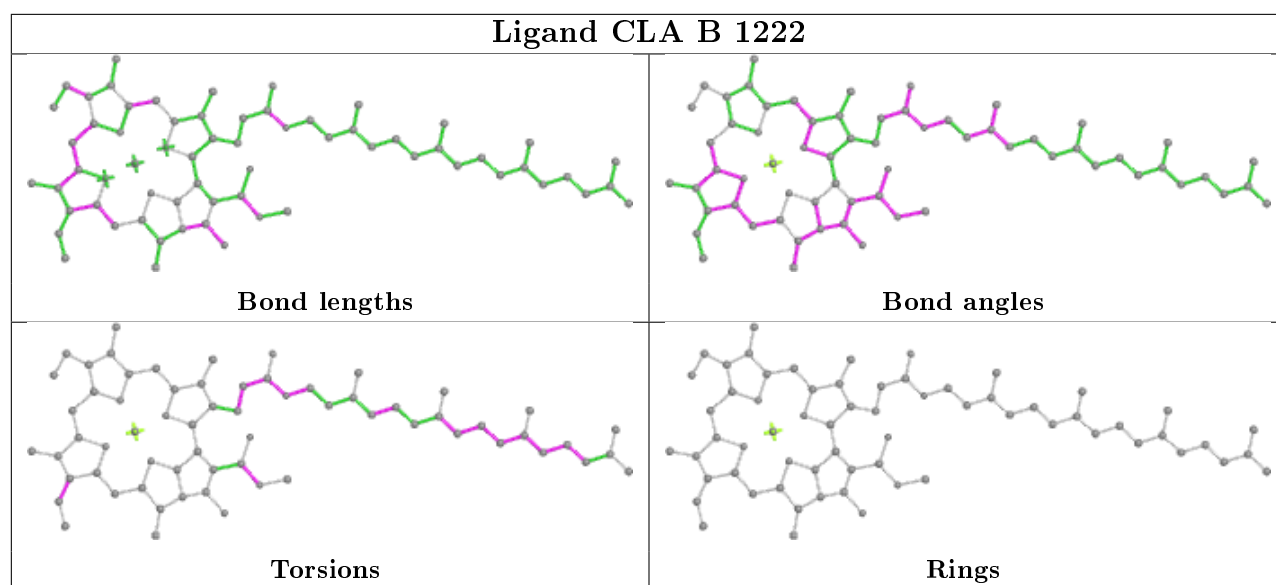
Ligand CLA B 1235



Ligand CLA L 1130







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	728/754 (96%)	0.26	60 (8%) 11 13	12, 39, 59, 72	0
2	B	732/732 (100%)	0.24	40 (5%) 25 25	13, 39, 58, 64	0
3	C	80/80 (100%)	0.42	11 (13%) 2 3	32, 38, 46, 48	0
4	D	138/138 (100%)	0.21	5 (3%) 42 42	25, 45, 53, 55	0
5	E	62/62 (100%)	0.02	1 (1%) 72 70	41, 52, 59, 59	0
6	F	154/154 (100%)	0.25	12 (7%) 13 14	25, 47, 60, 62	0
7	G	95/95 (100%)	0.49	9 (9%) 8 10	50, 61, 68, 73	0
8	H	75/75 (100%)	0.13	1 (1%) 77 76	43, 56, 75, 83	0
9	I	30/30 (100%)	-0.05	1 (3%) 46 45	39, 46, 55, 58	0
10	J	42/42 (100%)	-0.10	0 100 100	28, 55, 65, 67	0
11	K	0/38	-	-	-	-
12	L	164/164 (100%)	0.30	16 (9%) 7 9	24, 49, 62, 69	0
13	N	85/85 (100%)	0.31	6 (7%) 16 18	25, 70, 87, 90	0
14	1	175/187 (93%)	0.22	8 (4%) 32 32	28, 71, 84, 87	0
15	2	166/186 (89%)	0.23	9 (5%) 25 26	25, 71, 86, 91	0
16	3	115/165 (69%)	0.52	14 (12%) 4 5	57, 79, 88, 89	0
17	4	165/165 (100%)	0.37	14 (8%) 10 12	23, 65, 72, 75	0
All	All	3006/3152 (95%)	0.26	207 (6%) 16 18	12, 47, 78, 91	0

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	10.8
16	3	71	ALA	7.8
1	A	646	SER	7.8
1	A	319	THR	7.6
4	D	75	LEU	7.3

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	CLA	F	4015	25/65	0.43	0.34	132,133,133,133	0
18	CLA	2	2011	25/65	0.43	0.42	93,94,94,94	0
18	CLA	B	1232	55/65	0.44	0.35	74,91,93,93	0
18	CLA	J	1308	25/65	0.49	0.32	106,107,107,108	0
18	CLA	L	1504	55/65	0.52	0.34	32,67,68,71	0
18	CLA	3	3009	25/65	0.53	0.27	94,94,94,95	0
18	CLA	2	2006	25/65	0.54	0.35	81,82,82,83	0
18	CLA	2	2005	25/65	0.54	0.47	64,65,66,66	0
18	CLA	3	3001	25/65	0.55	0.51	137,137,138,138	0
18	CLA	B	1242	47/65	0.56	0.36	85,91,92,94	0
18	CLA	4	1304	55/65	0.56	0.33	40,77,78,79	0
18	CLA	K	1141	25/65	0.56	0.28	78,79,79,80	0
18	CLA	3	3010	25/65	0.57	0.25	92,93,93,93	0
18	CLA	A	1142	25/65	0.59	0.24	88,89,90,91	0
18	CLA	A	1118	25/65	0.59	0.23	89,90,91,91	0
18	CLA	A	1119	55/65	0.59	0.32	60,66,68,69	0
18	CLA	B	1301	25/65	0.61	0.26	73,74,75,75	0
18	CLA	4	4001	25/65	0.61	0.43	82,83,83,84	0
18	CLA	1	1007	25/65	0.62	0.29	68,68,69,69	0
18	CLA	B	1212	60/65	0.64	0.42	59,73,75,77	0
18	CLA	3	3011	25/65	0.64	0.27	107,107,108,108	0
18	CLA	2	2015	25/65	0.64	0.21	92,93,93,93	0
18	CLA	B	1210	25/65	0.64	0.37	75,76,76,77	0
18	CLA	A	1143	25/65	0.65	0.26	116,118,118,118	0
18	CLA	L	1125	25/65	0.65	0.20	80,80,82,82	0
18	CLA	2	2004	25/65	0.65	0.30	83,84,84,85	0
18	CLA	4	4012	25/65	0.65	0.26	63,65,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	1151	25/65	0.65	0.26	73,76,77,77	0
18	CLA	B	1216	56/65	0.65	0.33	66,72,73,73	0
18	CLA	A	1113	50/65	0.65	0.34	41,60,62,63	0
18	CLA	1	1013	25/65	0.65	0.25	86,87,88,88	0
18	CLA	F	1303	25/65	0.66	0.34	76,77,77,77	0
18	CLA	3	3006	25/65	0.66	0.24	112,113,113,114	0
18	CLA	A	1111	25/65	0.66	0.29	65,66,68,68	0
18	CLA	1	1005	25/65	0.66	0.29	77,78,78,78	0
18	CLA	3	3012	25/65	0.66	0.26	77,79,81,81	0
18	CLA	4	4006	25/65	0.66	0.26	82,83,84,85	0
18	CLA	G	1248	25/65	0.66	0.28	109,110,111,111	0
20	BCR	F	6016	40/40	0.67	0.32	28,33,39,40	0
18	CLA	4	4010	25/65	0.67	0.30	99,99,99,99	0
18	CLA	A	1134	25/65	0.67	0.30	49,51,52,52	0
18	CLA	3	3002	25/65	0.68	0.18	68,70,70,70	0
18	CLA	1	1004	25/65	0.68	0.30	88,89,89,90	0
18	CLA	1	1011	25/65	0.68	0.21	94,95,95,96	0
18	CLA	A	1116	25/65	0.68	0.22	81,82,83,83	0
18	CLA	L	1502	51/65	0.68	0.38	36,63,65,65	0
18	CLA	3	3005	25/65	0.68	0.21	95,96,97,97	0
18	CLA	A	1135	45/65	0.69	0.40	39,54,55,56	0
18	CLA	A	1129	55/65	0.69	0.27	35,58,60,61	0
18	CLA	1	1010	25/65	0.69	0.37	81,81,82,82	0
18	CLA	H	1505	25/65	0.69	0.21	84,85,86,86	0
18	CLA	B	1201	25/65	0.69	0.21	50,51,53,53	0
18	CLA	F	1302	55/65	0.70	0.25	19,75,77,79	0
18	CLA	2	2012	25/65	0.70	0.22	99,100,100,100	0
18	CLA	A	1103	47/65	0.70	0.37	67,77,78,79	0
18	CLA	B	1234	50/65	0.70	0.39	35,53,55,56	0
18	CLA	B	1222	65/65	0.70	0.30	46,69,70,73	0
18	CLA	A	1144	25/65	0.71	0.22	101,101,101,102	0
18	CLA	F	1306	25/65	0.71	0.23	87,88,89,89	0
18	CLA	2	2002	25/65	0.71	0.19	103,103,104,104	0
18	CLA	4	4007	25/65	0.72	0.24	89,91,91,91	0
18	CLA	K	1150	25/65	0.72	0.22	88,90,90,90	0
18	CLA	4	4005	25/65	0.72	0.22	60,62,63,63	0
18	CLA	2	2010	25/65	0.73	0.24	90,90,91,91	0
18	CLA	A	1309	25/65	0.73	0.24	112,112,112,112	0
18	CLA	B	1230	25/65	0.73	0.33	73,75,76,76	0
18	CLA	K	1153	25/65	0.73	0.22	54,55,56,56	0
18	CLA	J	1307	25/65	0.73	0.36	77,78,78,79	0
18	CLA	4	4004	25/65	0.73	0.23	71,72,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	1	1003	25/65	0.73	0.23	84,85,86,86	0
18	CLA	A	1110	25/65	0.73	0.22	70,71,72,72	0
18	CLA	B	1217	50/65	0.74	0.22	60,66,68,68	0
18	CLA	A	1104	25/65	0.74	0.22	40,42,43,44	0
18	CLA	B	1241	25/65	0.74	0.35	103,104,104,104	0
18	CLA	B	1237	51/65	0.74	0.28	29,59,62,62	0
20	BCR	B	6017	40/40	0.74	0.42	27,33,46,47	0
18	CLA	L	1130	50/65	0.75	0.29	57,66,69,70	0
18	CLA	2	2001	25/65	0.75	0.21	61,63,65,65	0
18	CLA	B	1219	51/65	0.75	0.23	27,47,48,49	0
18	CLA	B	1214	49/65	0.75	0.25	51,69,70,71	0
18	CLA	1	1014	25/65	0.75	0.20	67,68,70,70	0
18	CLA	A	1136	55/65	0.76	0.30	40,45,57,58	0
18	CLA	B	1211	25/65	0.76	0.27	52,54,55,55	0
20	BCR	L	6020	40/40	0.76	0.29	11,24,35,38	0
18	CLA	4	4008	25/65	0.76	0.36	72,74,74,74	0
18	CLA	A	1146	25/65	0.76	0.24	70,72,73,73	0
18	CLA	I	1204	55/65	0.76	0.30	40,44,51,52	0
18	CLA	A	1117	25/65	0.76	0.24	47,48,49,49	0
18	CLA	B	1213	25/65	0.76	0.23	79,81,82,82	0
18	CLA	H	1501	55/65	0.77	0.27	49,68,70,73	0
18	CLA	4	4009	25/65	0.77	0.21	80,81,82,82	0
18	CLA	B	1209	55/65	0.77	0.24	32,50,53,54	0
18	CLA	A	1140	55/65	0.77	0.32	12,39,41,43	0
20	BCR	A	6011	40/40	0.78	0.36	9,12,19,21	0
19	PQN	A	5001	33/33	0.78	0.26	15,23,34,36	0
18	CLA	2	2003	25/65	0.78	0.19	114,114,115,115	0
18	CLA	3	3003	25/65	0.78	0.18	67,68,70,70	0
18	CLA	A	1102	25/65	0.78	0.21	72,73,75,75	0
18	CLA	3	3004	25/65	0.78	0.25	76,77,78,78	0
18	CLA	B	1223	25/65	0.78	0.25	46,48,49,50	0
18	CLA	A	1115	47/65	0.78	0.28	40,44,48,50	0
18	CLA	A	1108	50/65	0.78	0.20	52,74,76,76	0
18	CLA	B	1224	51/65	0.79	0.32	47,55,56,57	0
18	CLA	2	2013	25/65	0.79	0.20	81,82,84,84	0
18	CLA	J	2107	61/65	0.79	0.24	40,62,63,63	0
18	CLA	B	1236	46/65	0.79	0.25	34,44,46,47	0
18	CLA	4	4002	25/65	0.79	0.20	65,66,67,67	0
18	CLA	1	1012	25/65	0.79	0.23	76,77,77,77	0
18	CLA	B	1220	60/65	0.79	0.25	31,39,50,53	0
18	CLA	3	3015	25/65	0.79	0.16	72,73,74,75	0
18	CLA	B	1229	49/65	0.79	0.23	35,48,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	PQN	B	5002	33/33	0.79	0.42	8,18,21,21	0
18	CLA	3	3013	25/65	0.79	0.26	77,78,78,78	0
18	CLA	B	1202	50/65	0.79	0.30	23,37,39,42	0
18	CLA	4	4003	25/65	0.80	0.24	80,81,81,81	0
18	CLA	B	9012	55/65	0.80	0.30	16,47,50,52	0
18	CLA	4	4011	25/65	0.80	0.25	51,52,53,54	0
18	CLA	A	9011	55/65	0.80	0.27	2,26,28,29	0
18	CLA	B	1205	55/65	0.80	0.24	17,41,43,46	0
18	CLA	1	1001	25/65	0.80	0.21	63,64,65,66	0
18	CLA	B	1228	55/65	0.80	0.24	42,46,47,49	0
18	CLA	A	1147	25/65	0.80	0.25	66,67,68,69	0
18	CLA	A	1123	55/65	0.80	0.25	37,46,49,50	0
18	CLA	B	1218	51/65	0.80	0.21	20,47,50,51	0
18	CLA	1	1006	25/65	0.80	0.18	60,62,63,63	0
18	CLA	B	1235	55/65	0.80	0.25	31,40,42,44	0
18	CLA	B	1231	46/65	0.80	0.31	36,46,49,51	0
18	CLA	B	1239	55/65	0.80	0.23	27,52,53,55	0
18	CLA	B	1221	48/65	0.81	0.32	20,31,38,42	0
18	CLA	A	1105	25/65	0.81	0.21	83,83,84,84	0
18	CLA	3	3008	25/65	0.81	0.23	90,90,91,91	0
18	CLA	L	1503	46/65	0.81	0.22	19,22,25,28	0
18	CLA	A	1122	55/65	0.81	0.25	18,39,41,43	0
18	CLA	B	1225	45/65	0.81	0.22	34,50,52,52	0
18	CLA	A	1131	44/65	0.81	0.25	35,39,42,44	0
18	CLA	1	1008	25/65	0.82	0.16	79,79,79,80	0
18	CLA	B	1226	25/65	0.82	0.20	50,53,54,54	0
18	CLA	B	1206	25/65	0.82	0.40	50,54,55,56	0
20	BCR	I	6018	40/40	0.82	0.25	6,19,26,28	0
18	CLA	A	9013	46/65	0.82	0.35	11,17,21,24	0
18	CLA	G	1233	51/65	0.82	0.16	61,66,67,67	0
18	CLA	A	1120	25/65	0.82	0.23	76,78,79,80	0
18	CLA	1	1002	25/65	0.82	0.17	86,86,87,88	0
18	CLA	A	1124	25/65	0.82	0.17	48,51,52,53	0
18	CLA	4	4013	25/65	0.82	0.17	86,86,87,87	0
18	CLA	F	1139	44/65	0.82	0.24	36,40,42,43	0
18	CLA	A	1101	25/65	0.82	0.23	61,63,64,64	0
18	CLA	A	1126	55/65	0.82	0.22	15,40,42,44	0
18	CLA	4	1009	25/65	0.83	0.19	78,79,79,79	0
18	CLA	F	1305	25/65	0.83	0.19	78,79,79,79	0
18	CLA	B	1238	54/65	0.83	0.26	13,27,32,33	0
18	CLA	B	1138	56/65	0.83	0.23	18,47,50,53	0
18	CLA	A	1137	55/65	0.83	0.23	20,28,30,32	0

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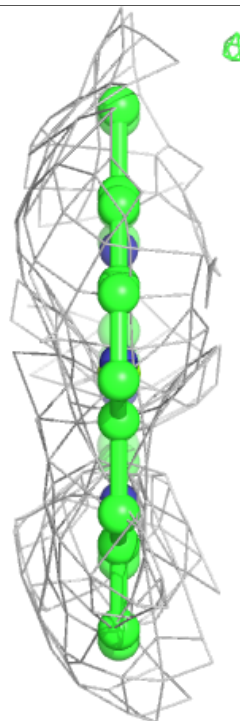
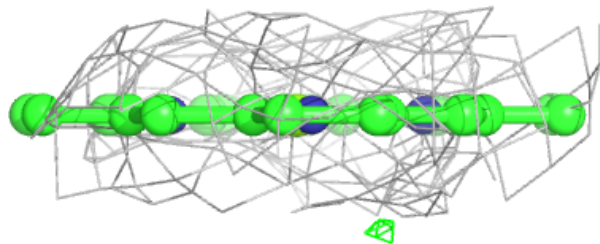
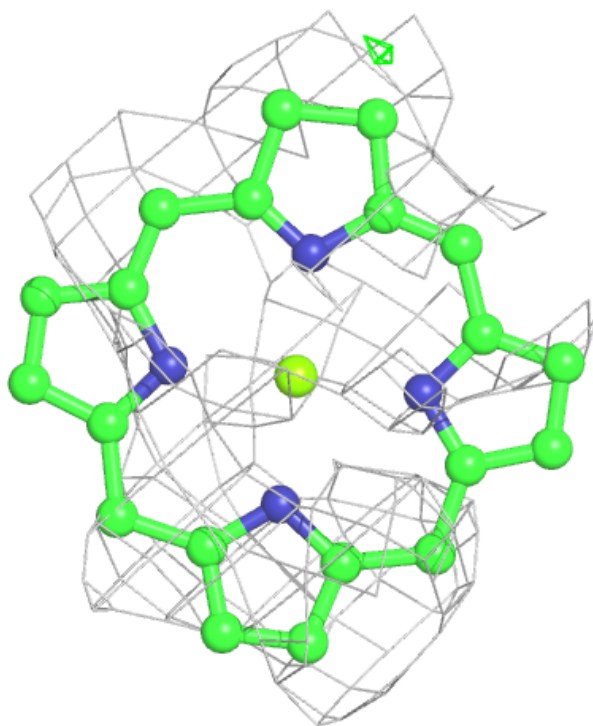
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	3	2009	25/65	0.83	0.22	94,94,95,95	0
18	CLA	A	1127	25/65	0.83	0.22	58,59,60,60	0
18	CLA	A	1132	25/65	0.83	0.20	27,29,31,32	0
18	CLA	B	1208	55/65	0.83	0.21	36,39,41,42	0
18	CLA	B	9010	47/65	0.83	0.31	23,37,40,41	0
18	CLA	A	1133	25/65	0.84	0.22	44,46,47,48	0
18	CLA	A	1109	24/65	0.84	0.20	48,49,50,51	0
18	CLA	3	3007	25/65	0.84	0.23	80,81,82,83	0
18	CLA	2	2008	25/65	0.85	0.19	60,61,62,63	0
18	CLA	B	1207	55/65	0.85	0.24	19,30,35,37	0
18	CLA	A	1148	25/65	0.86	0.26	93,94,95,95	0
18	CLA	B	1203	48/65	0.86	0.18	2,23,24,26	0
18	CLA	A	1152	25/65	0.86	0.19	68,69,70,71	0
18	CLA	B	9023	47/65	0.87	0.21	36,40,41,43	0
18	CLA	A	1107	57/65	0.87	0.19	21,26,30,33	0
18	CLA	B	1227	50/65	0.87	0.22	34,41,44,45	0
18	CLA	B	9022	54/65	0.87	0.27	28,31,41,41	0
18	CLA	A	1106	41/65	0.87	0.23	16,20,22,24	0
18	CLA	A	1128	55/65	0.87	0.19	20,37,39,40	0
18	CLA	B	1215	52/65	0.88	0.20	11,16,27,30	0
18	CLA	F	1240	25/65	0.88	0.18	43,44,45,46	0
18	CLA	2	2007	25/65	0.88	0.27	79,80,81,81	0
21	SF4	C	3102	8/8	0.92	0.15	19,21,24,26	0
21	SF4	C	3103	8/8	0.96	0.09	10,12,15,15	0
21	SF4	B	3101	8/8	0.97	0.12	14,21,22,25	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.

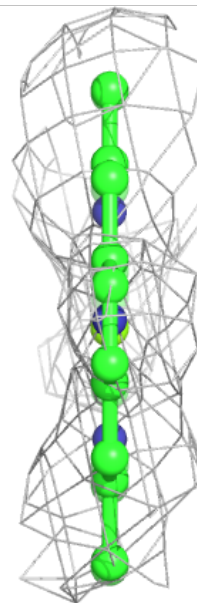
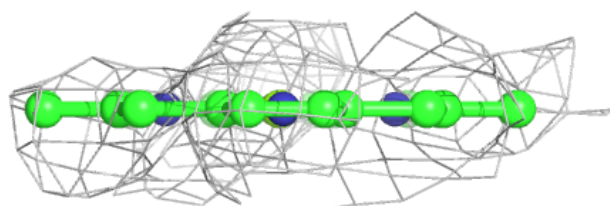
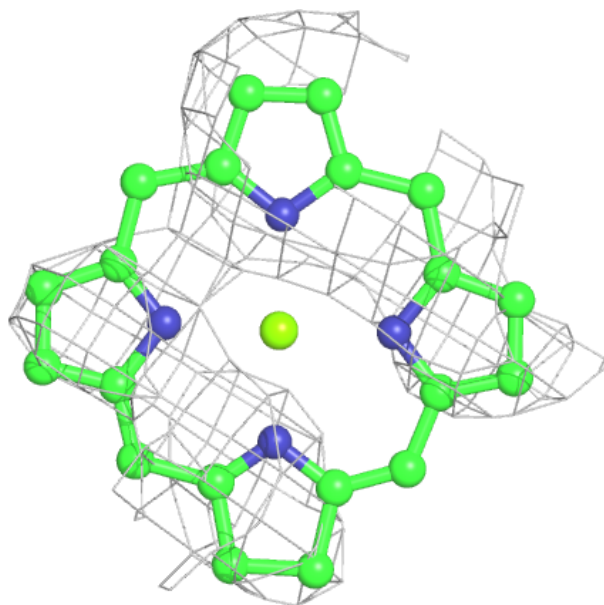
Electron density around CLA F 4015:

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



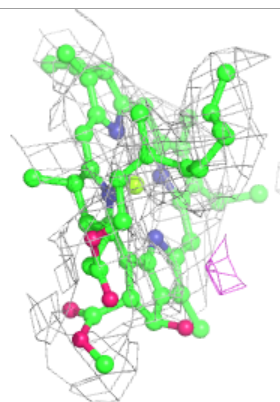
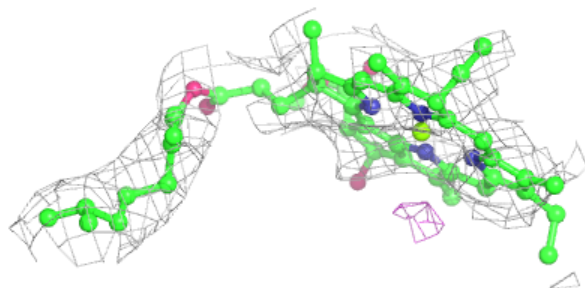
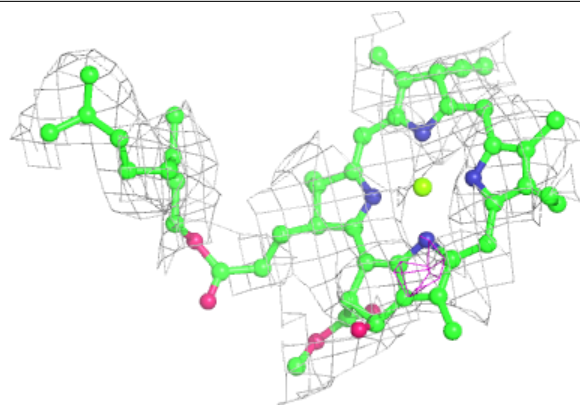
Electron density around CLA 2 2011:

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



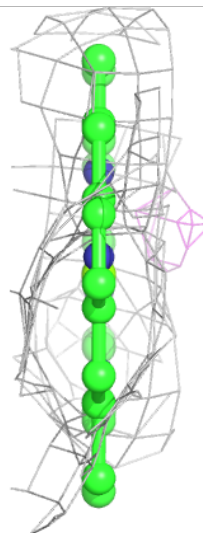
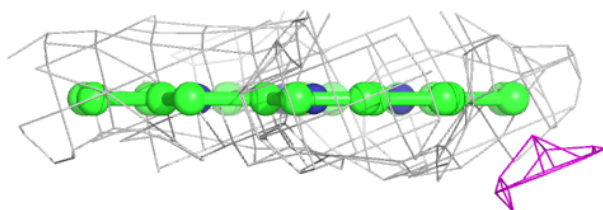
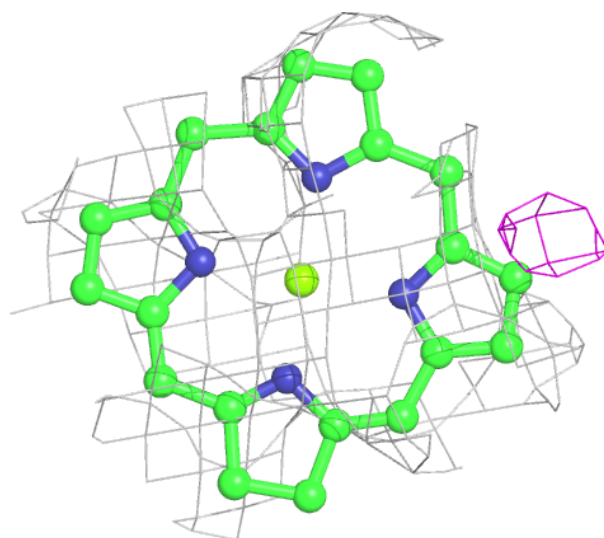
Electron density around CLA B 1232:

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



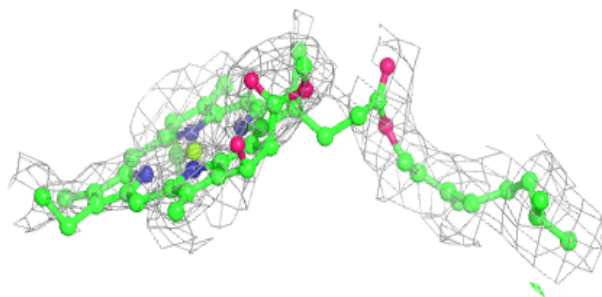
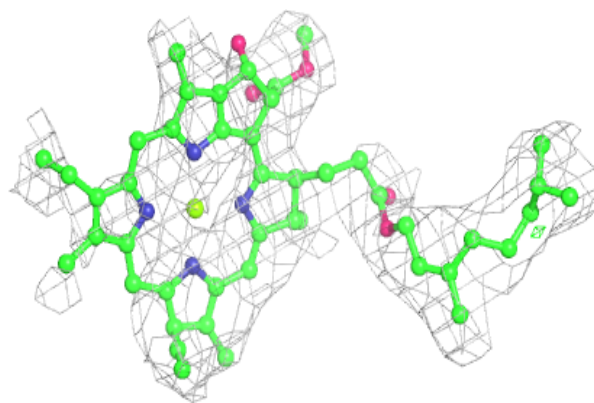
Electron density around CLA J 1308:

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



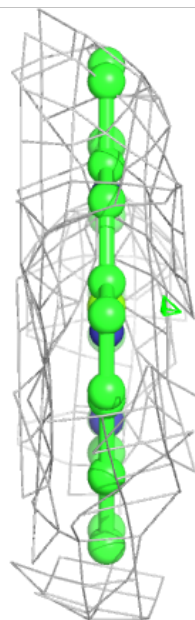
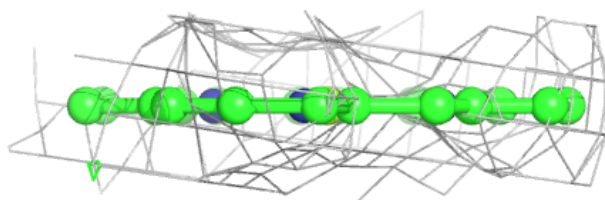
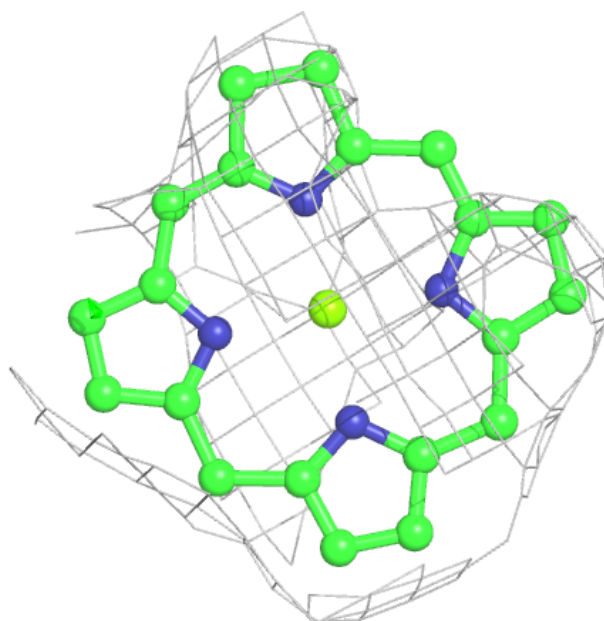
Electron density around CLA L 1504:

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



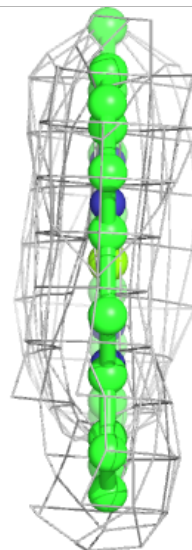
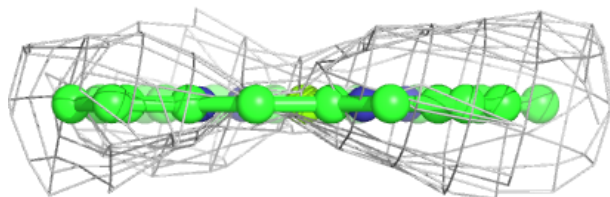
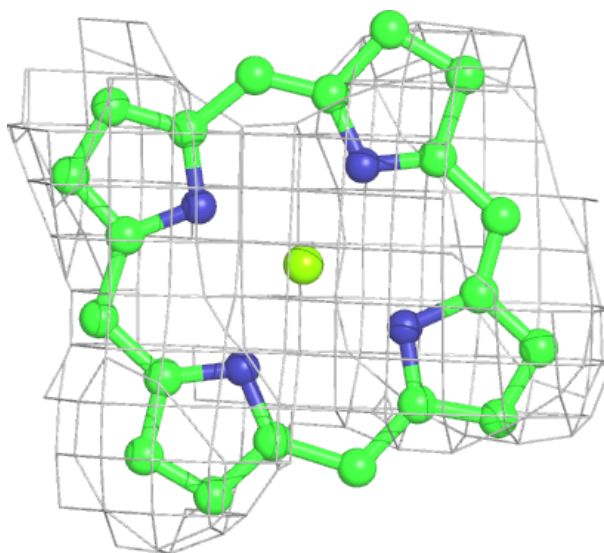
Electron density around CLA 3 3009:

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



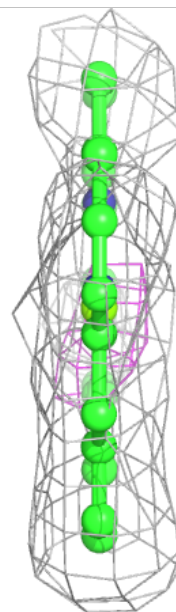
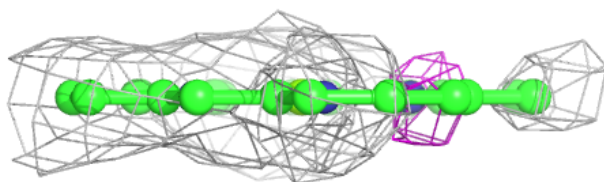
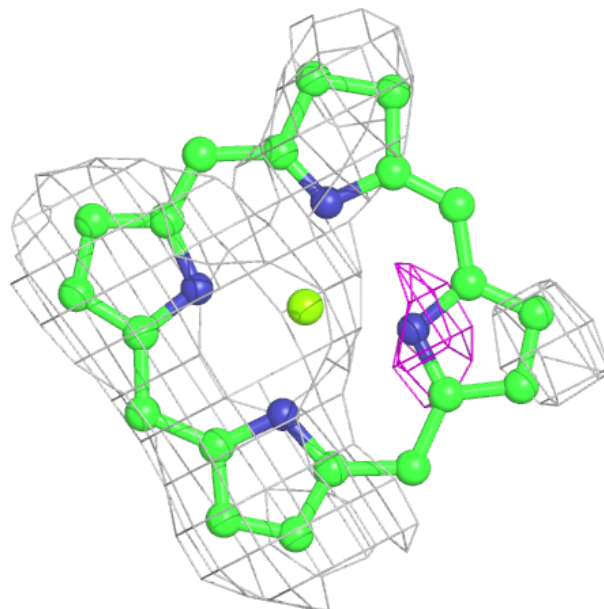
Electron density around CLA 2 2006:

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



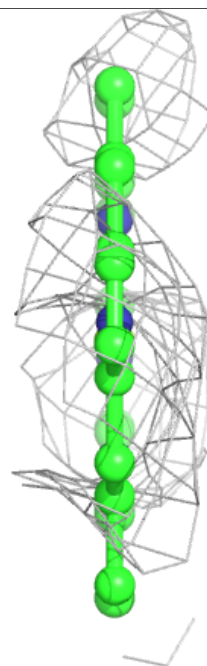
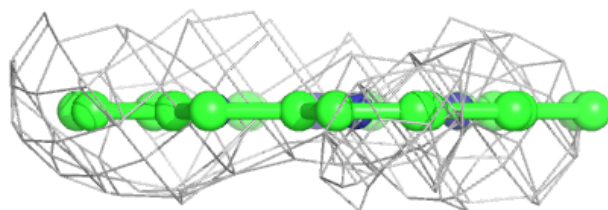
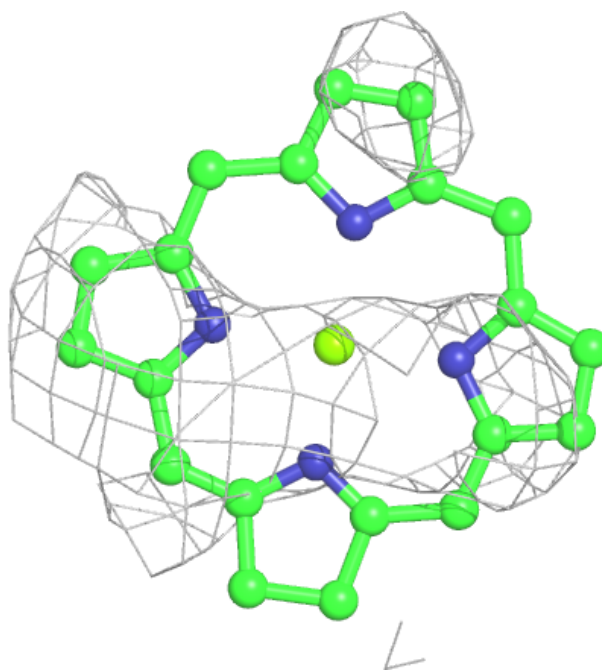
Electron density around CLA 2 2005:

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



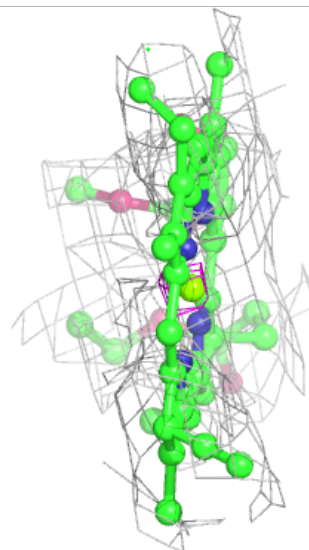
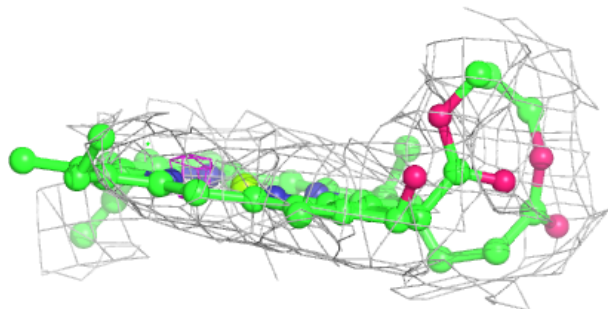
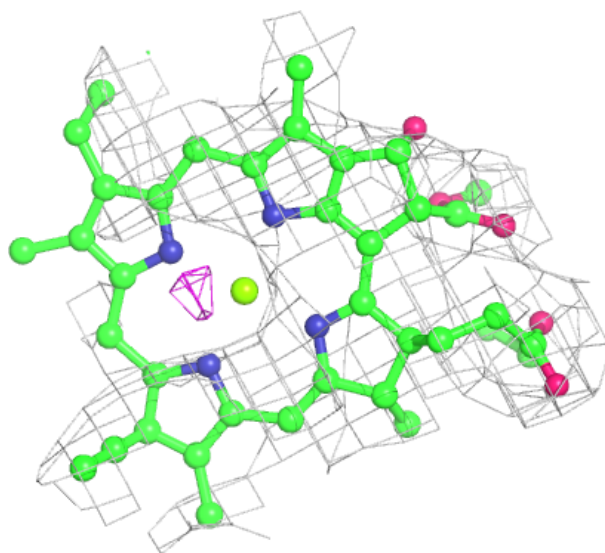
Electron density around CLA 3 3001:

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



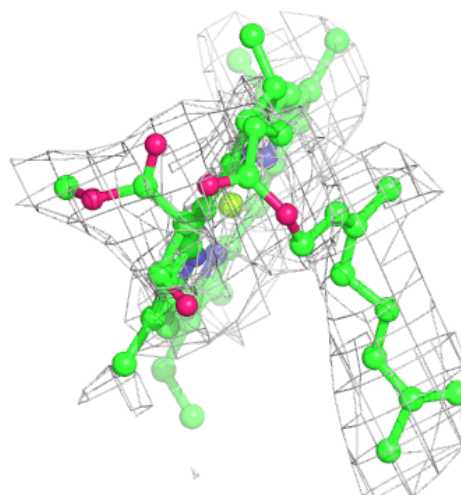
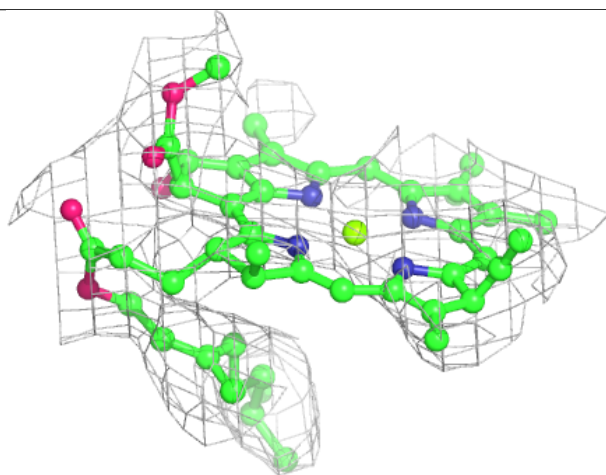
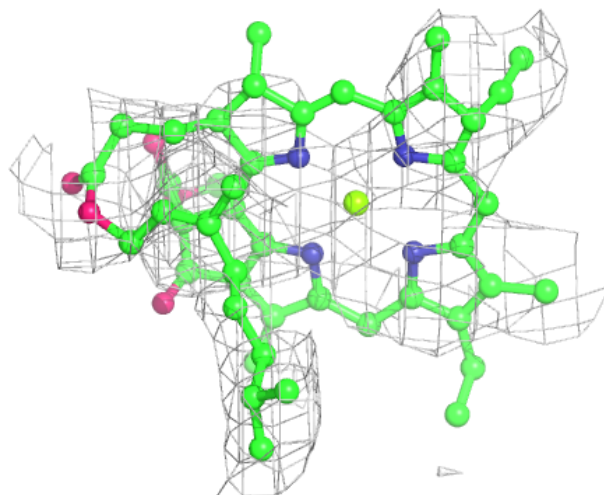
Electron density around CLA B 1242:

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



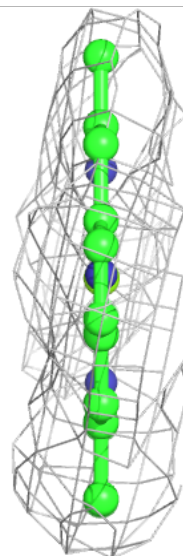
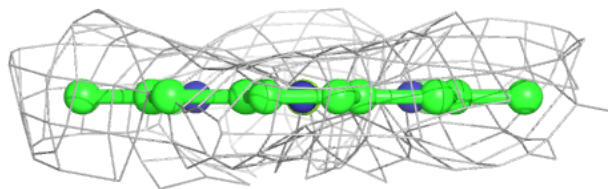
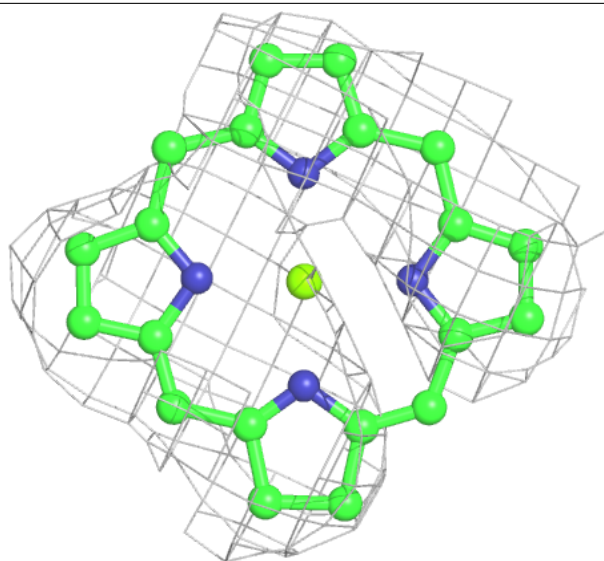
Electron density around CLA 4 1304:

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



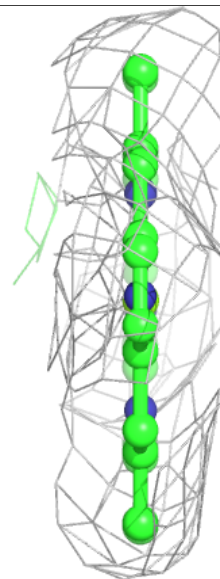
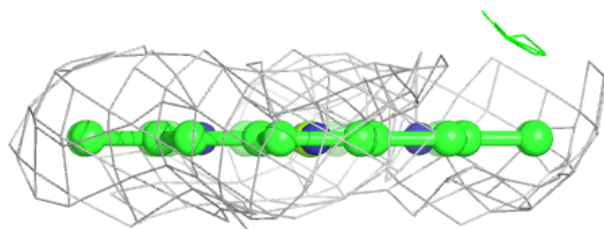
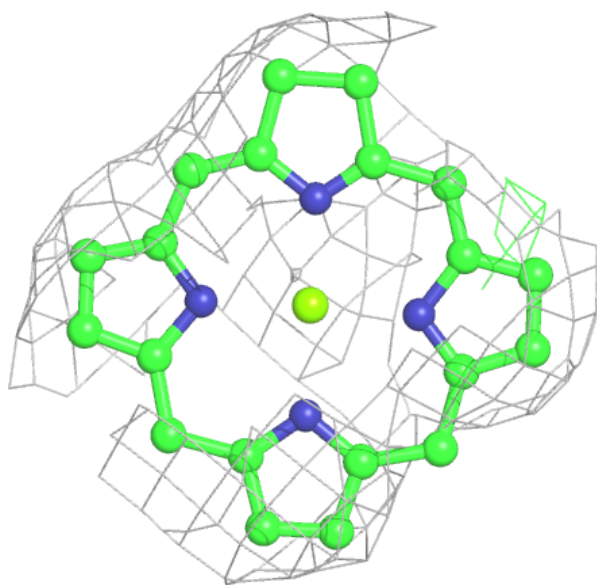
Electron density around CLA K 1141:

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



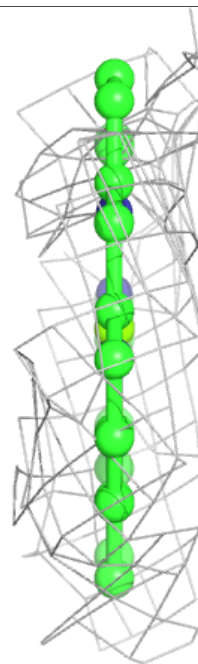
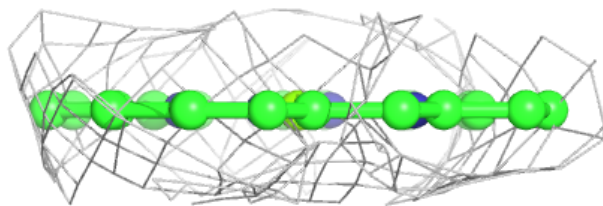
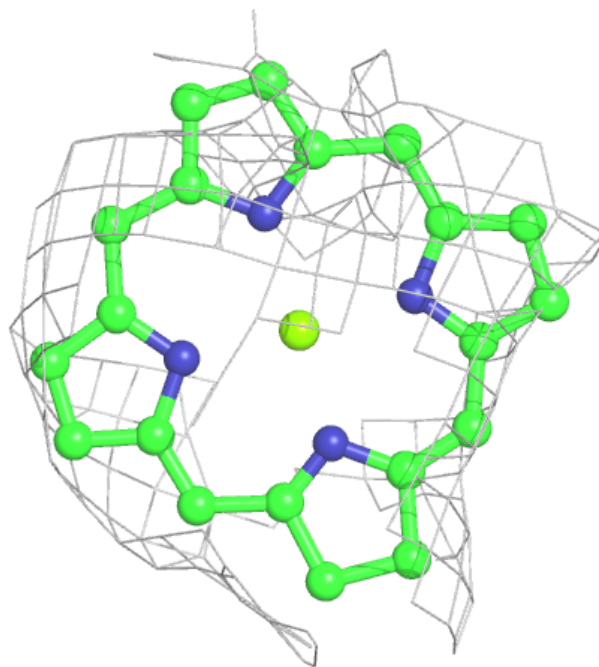
Electron density around CLA 3 3010:

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and green (positive)



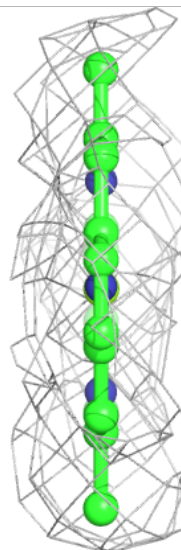
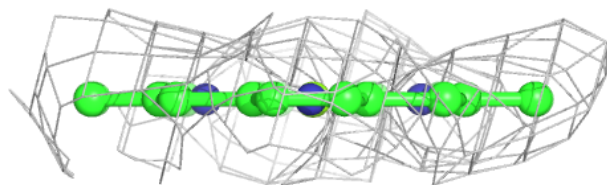
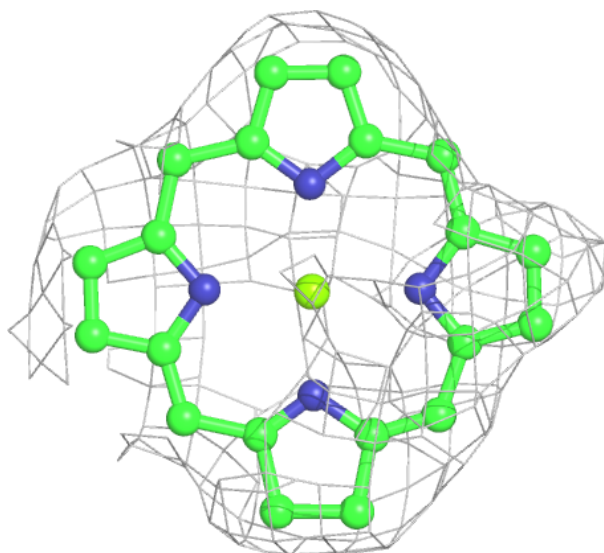
Electron density around CLA A 1142:

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and green (positive)



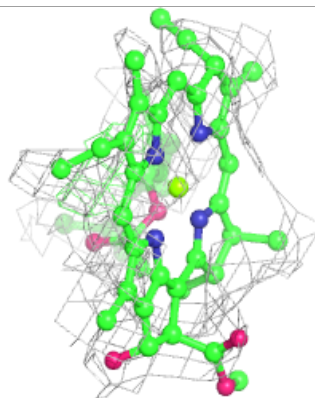
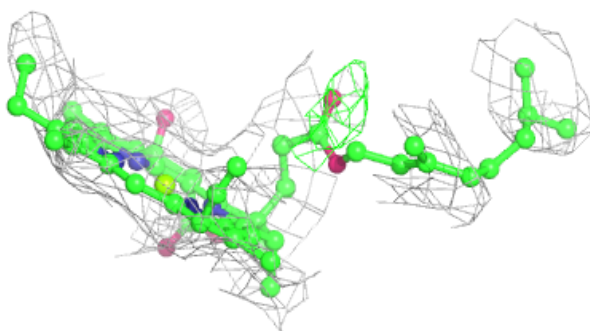
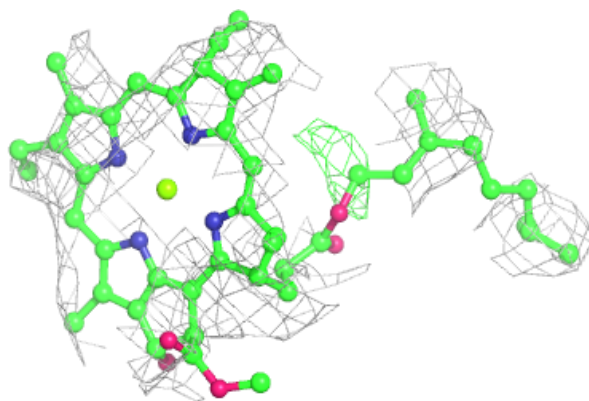
Electron density around CLA A 1118:

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and green (positive)



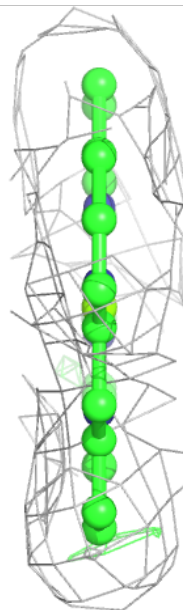
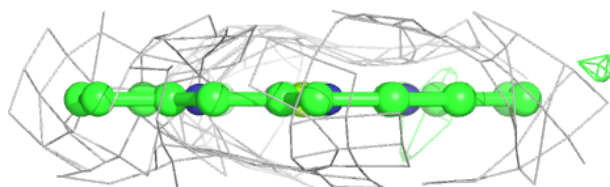
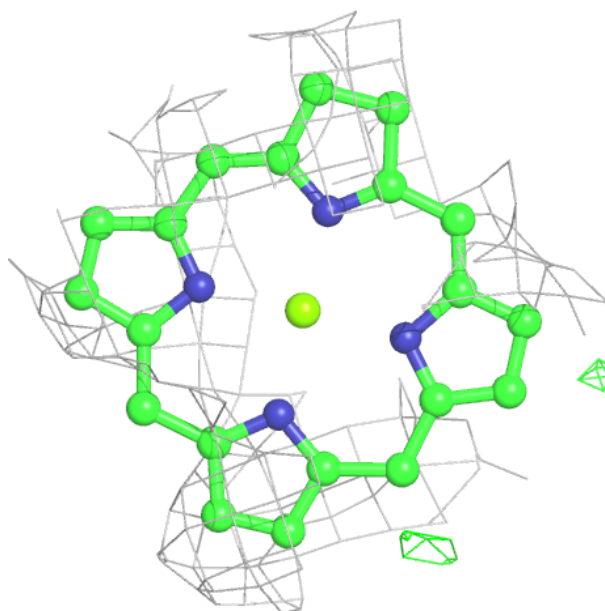
Electron density around CLA A 1119:

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and green (positive)



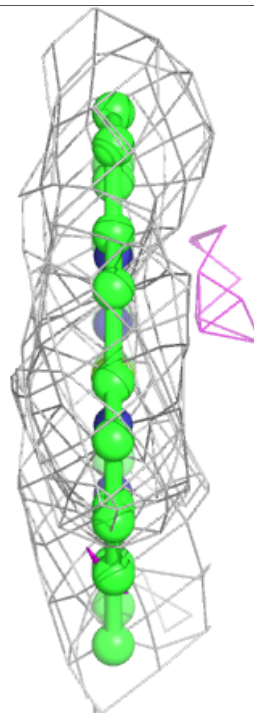
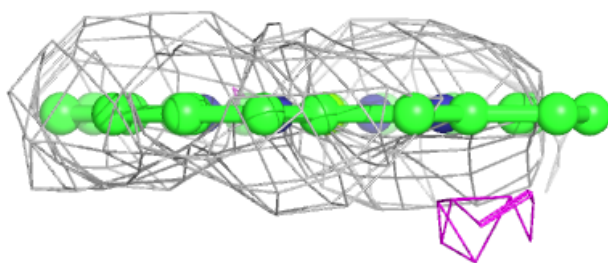
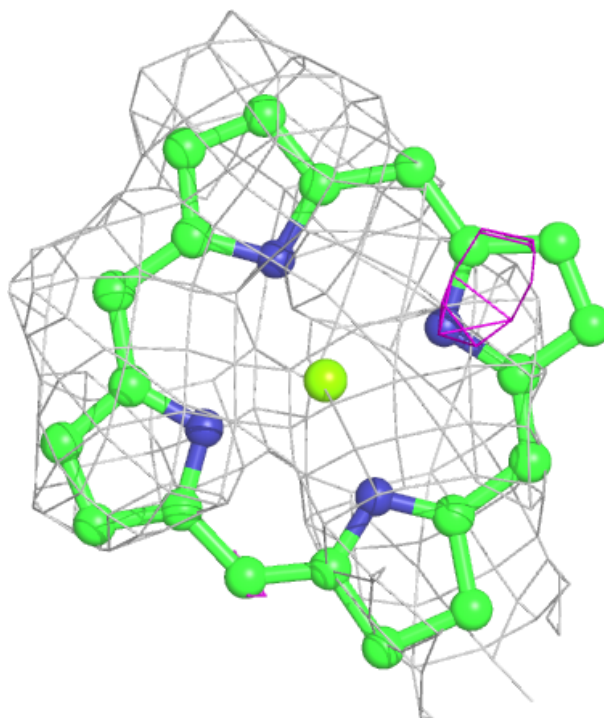
Electron density around CLA B 1301:

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and green (positive)



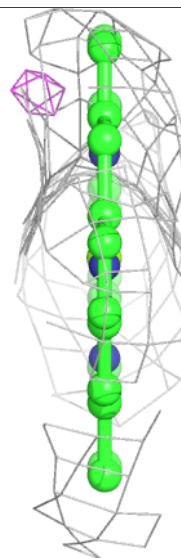
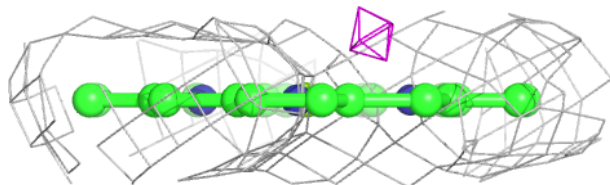
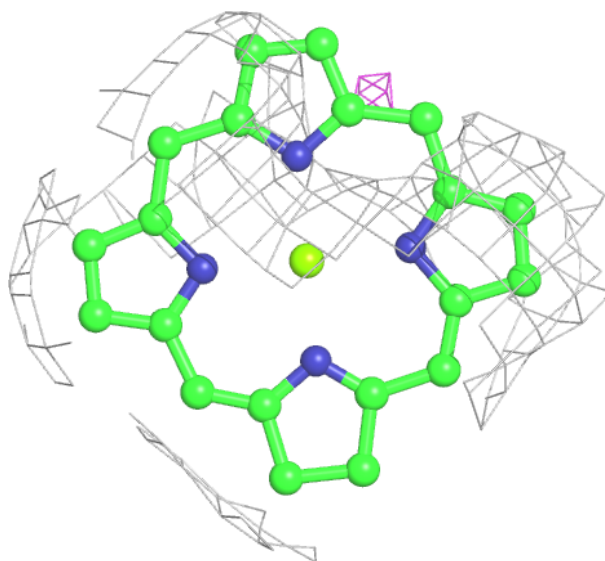
Electron density around CLA 4 4001:

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



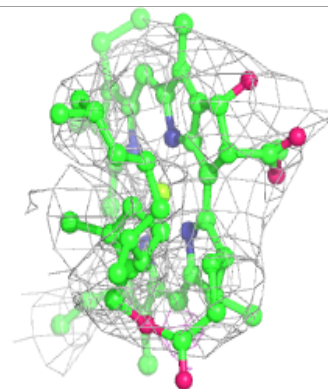
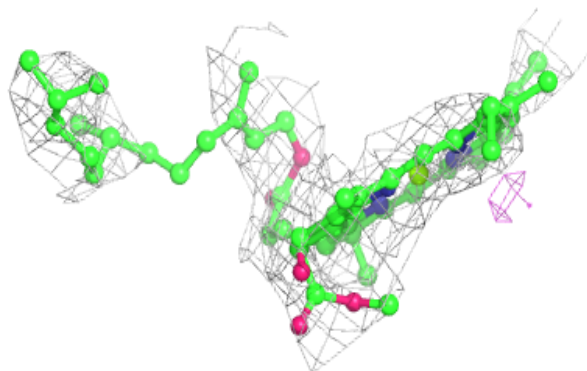
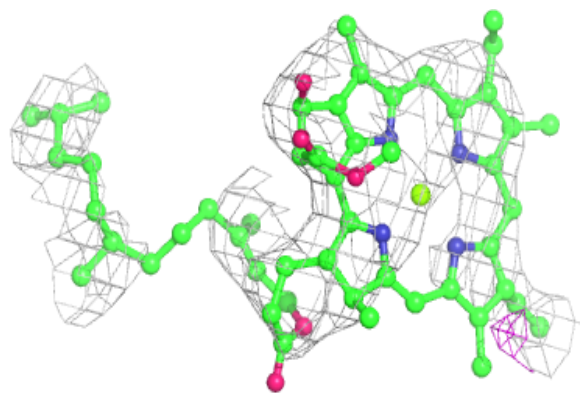
Electron density around CLA 1 1007:

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



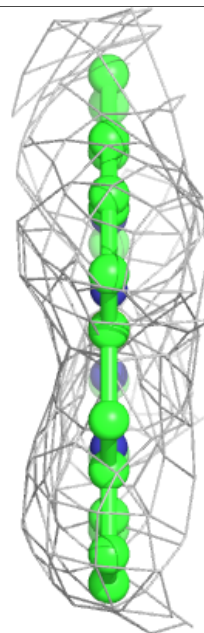
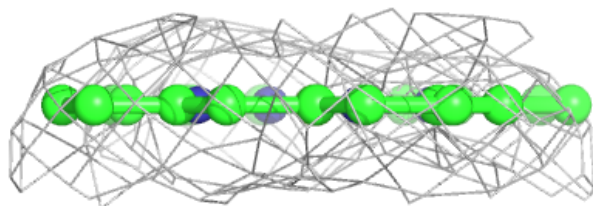
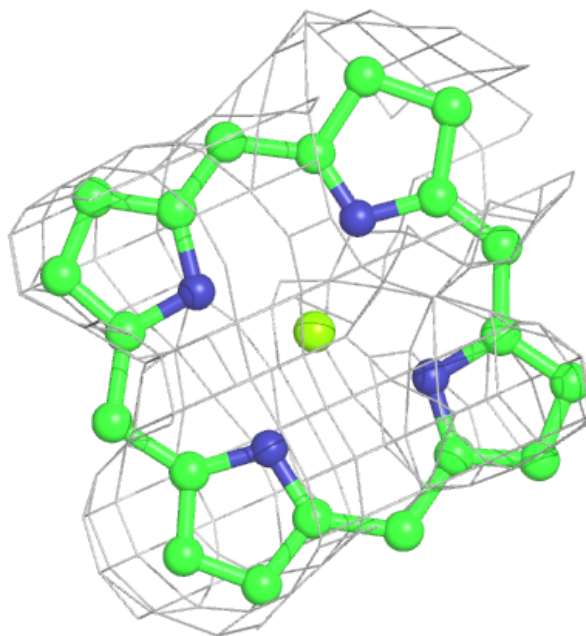
Electron density around CLA B 1212:

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and green (positive)



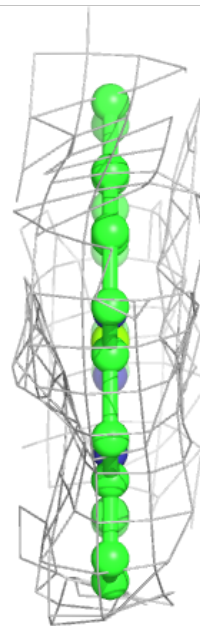
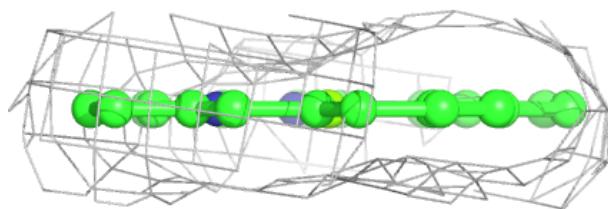
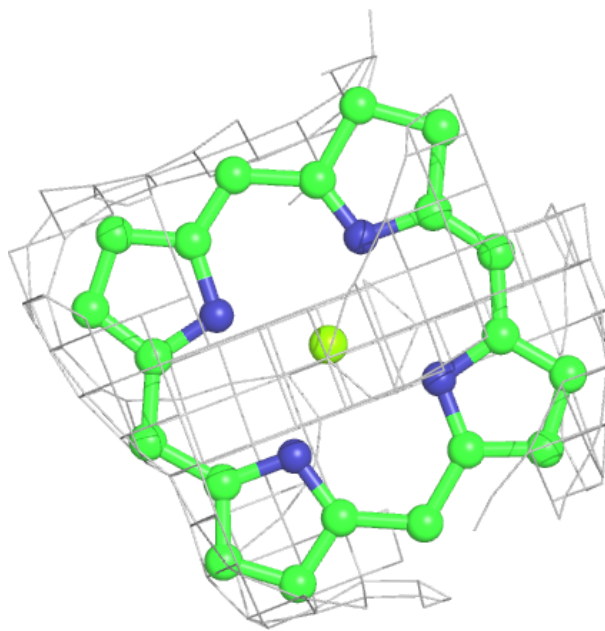
Electron density around CLA 3 3011:

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and green (positive)



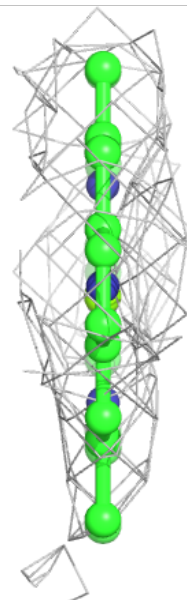
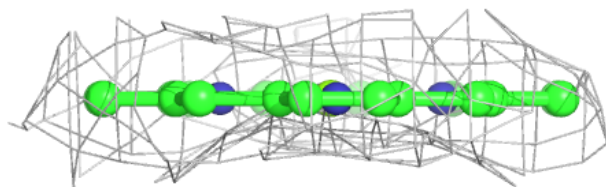
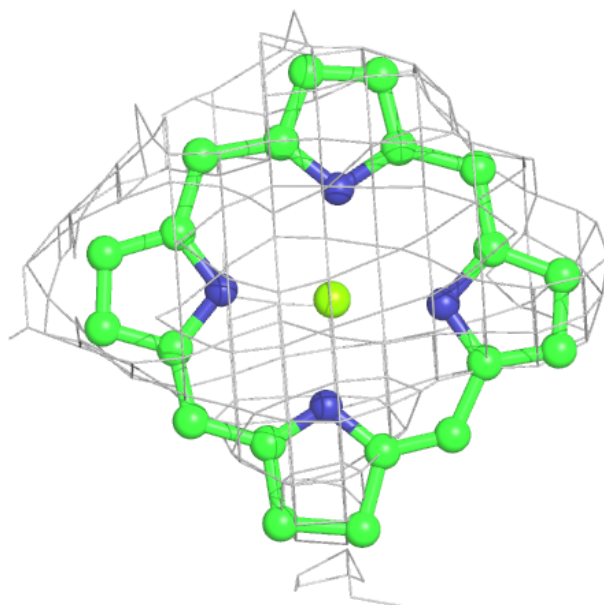
Electron density around CLA 2 2015:

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and green (positive)



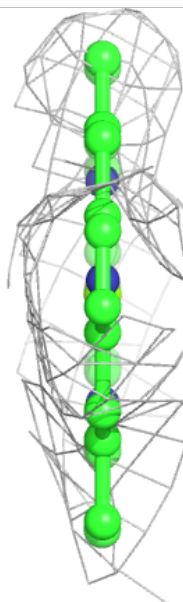
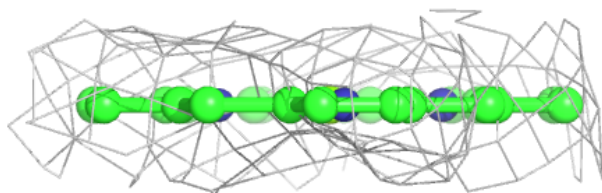
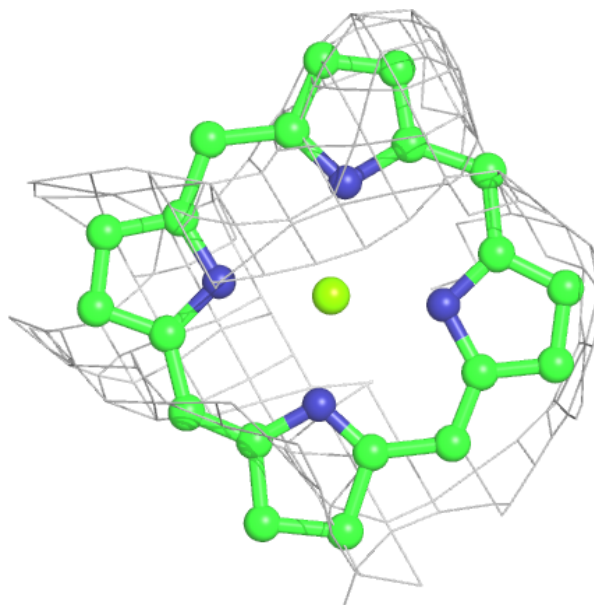
Electron density around CLA B 1210:

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



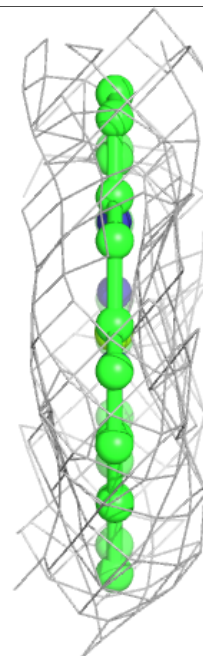
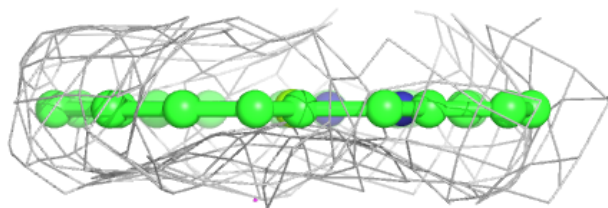
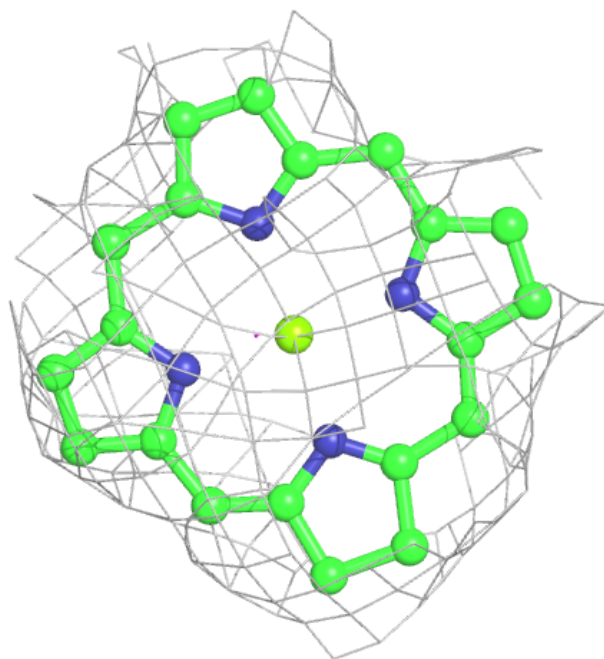
Electron density around CLA A 1143:

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



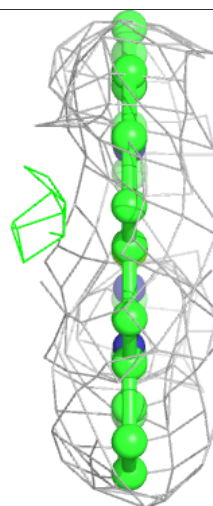
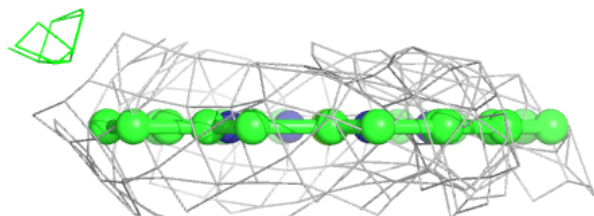
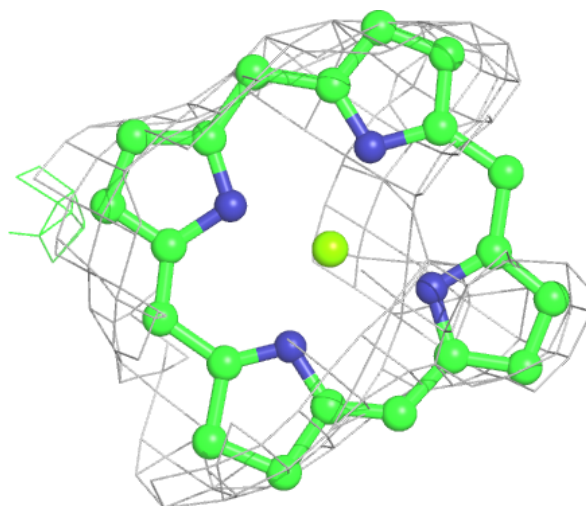
Electron density around CLA L 1125:

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



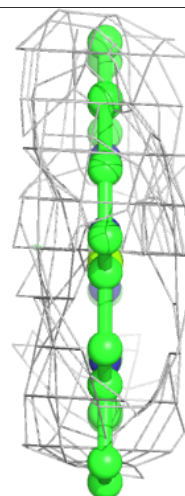
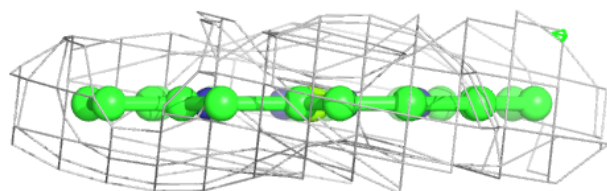
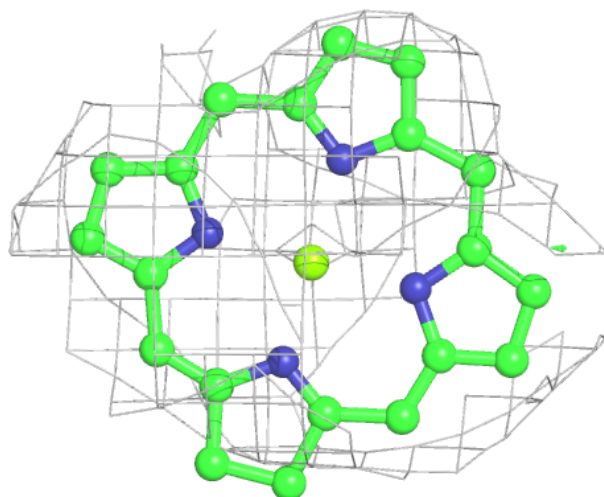
Electron density around CLA 2 2004:

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



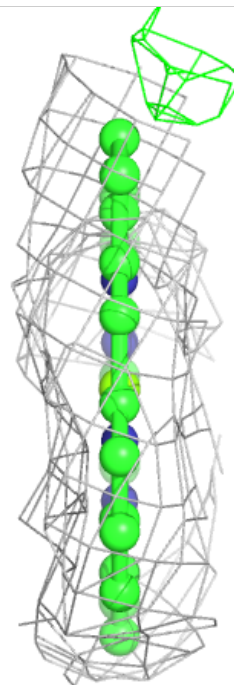
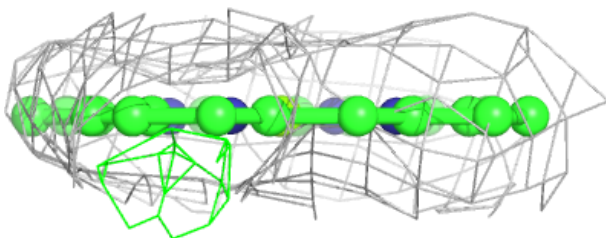
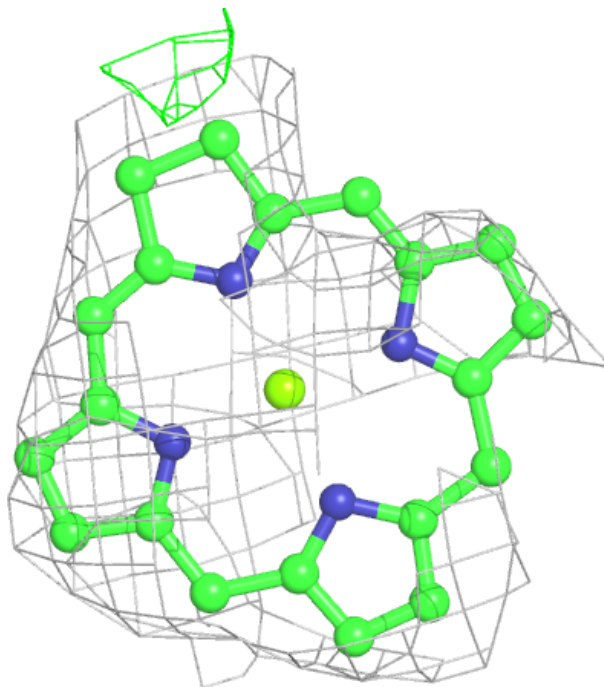
Electron density around CLA 4 4012:

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



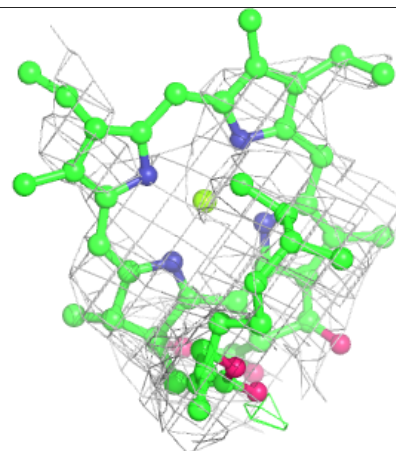
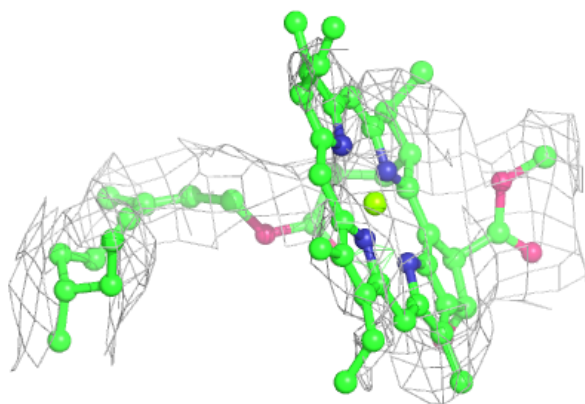
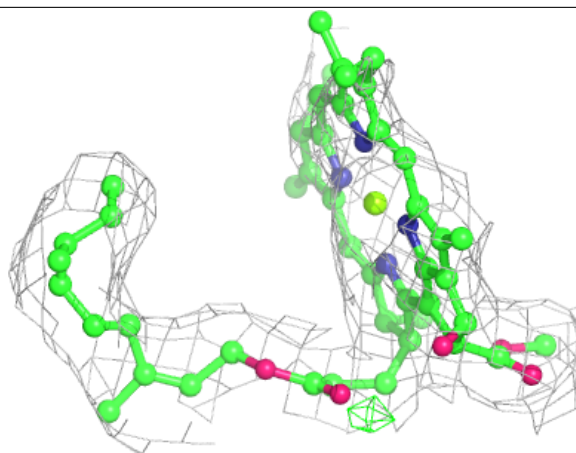
Electron density around CLA A 1151:

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



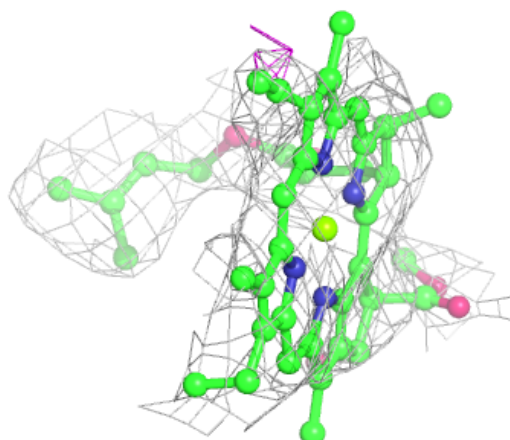
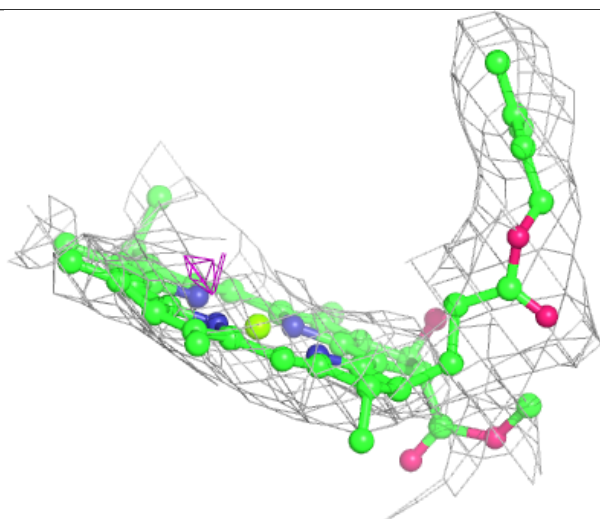
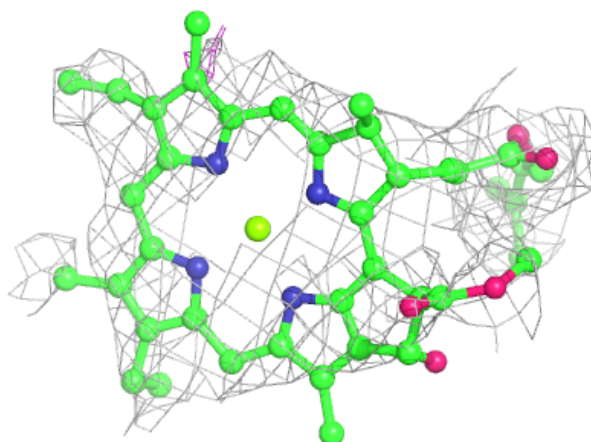
Electron density around CLA B 1216:

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



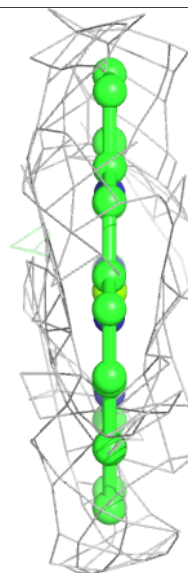
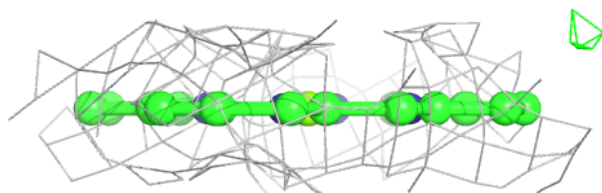
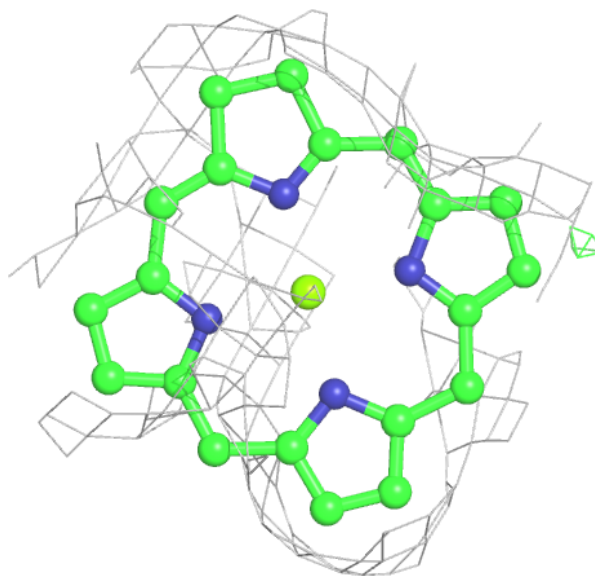
Electron density around CLA A 1113:

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



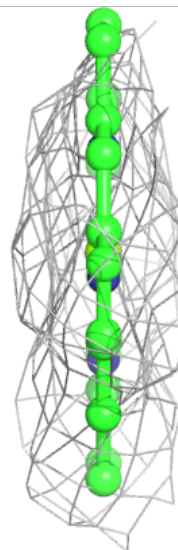
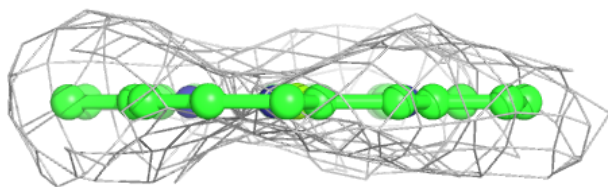
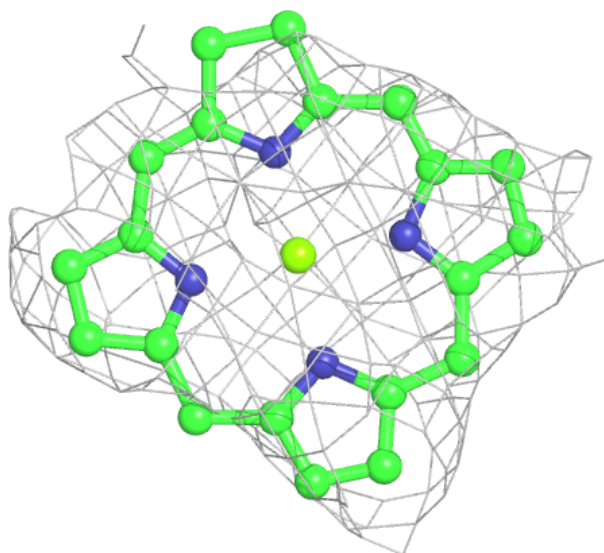
Electron density around CLA 1 1013:

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



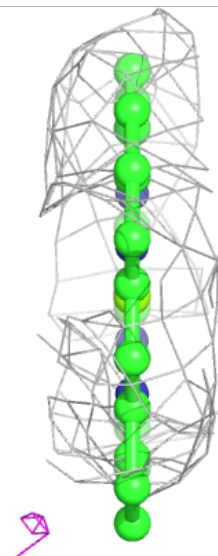
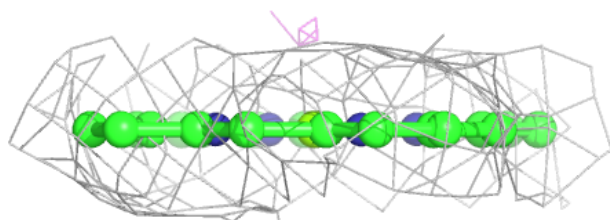
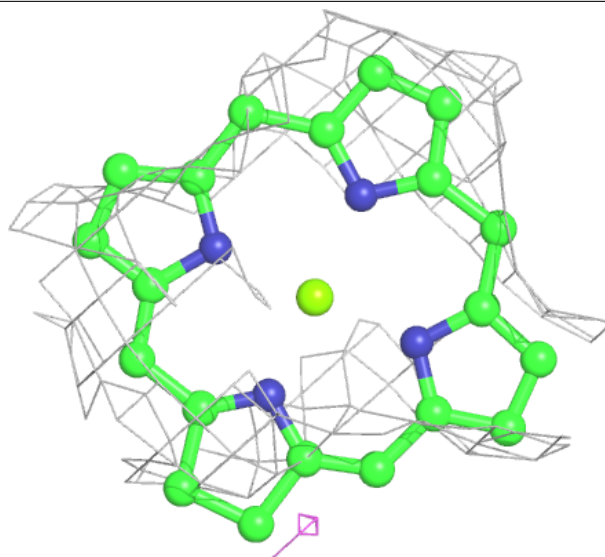
Electron density around CLA F 1303:

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



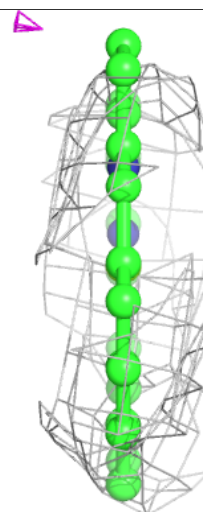
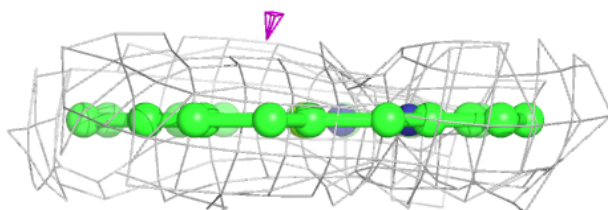
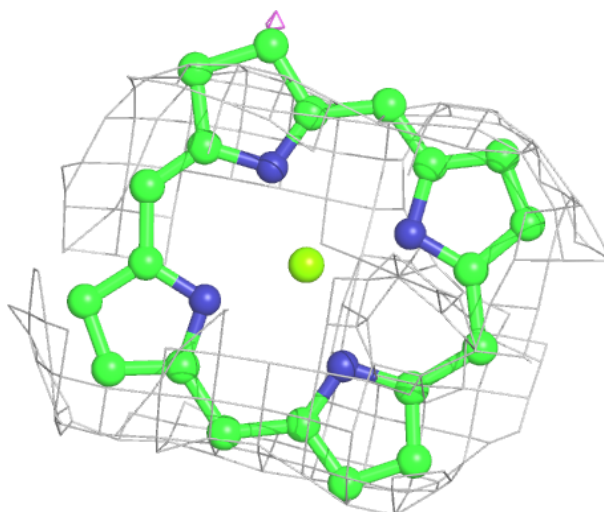
Electron density around CLA 3 3006:

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



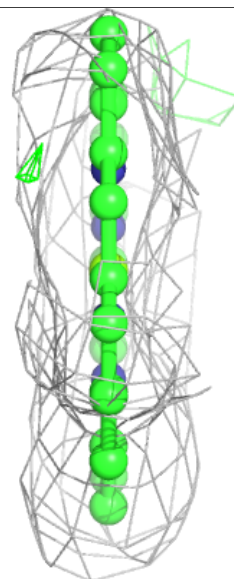
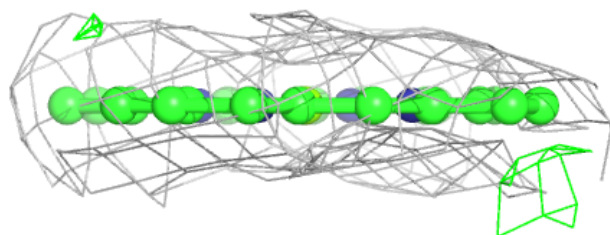
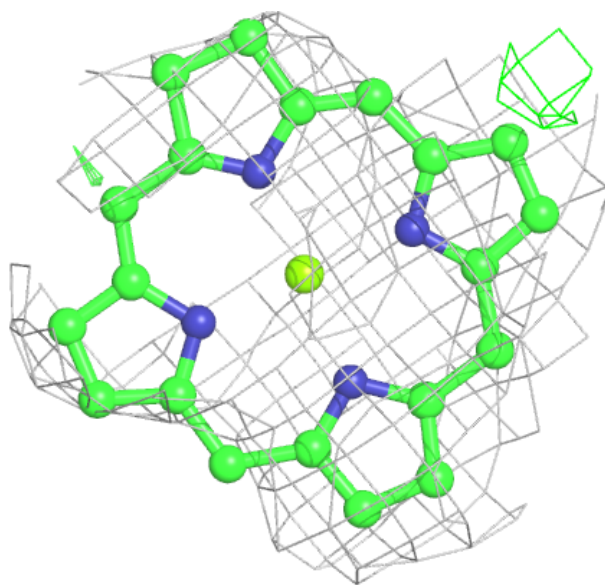
Electron density around CLA A 1111:

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



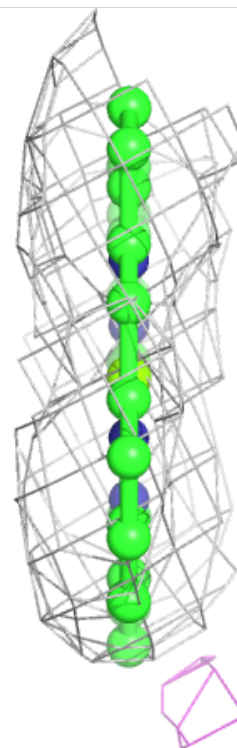
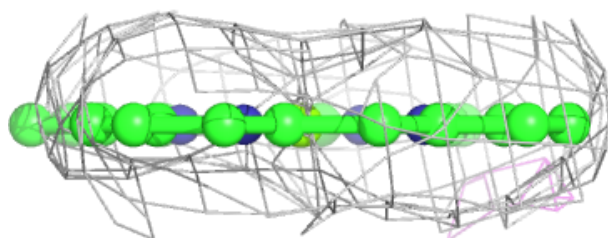
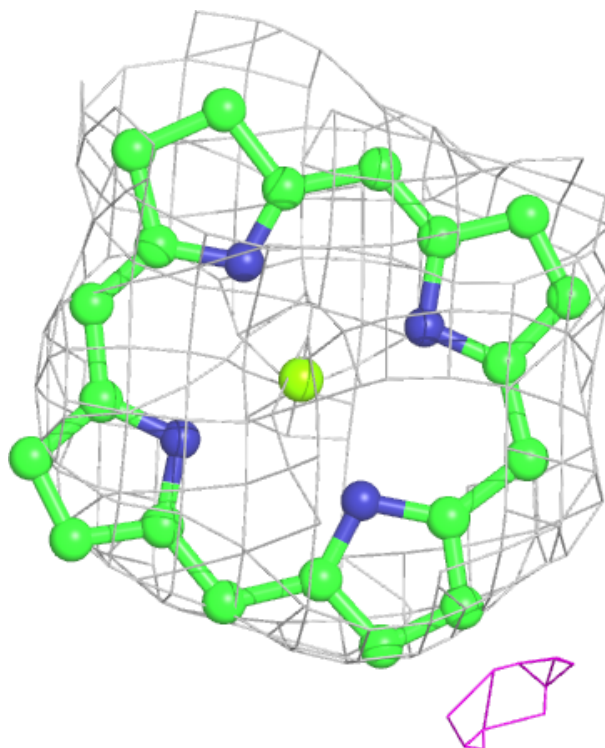
Electron density around CLA 1 1005:

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



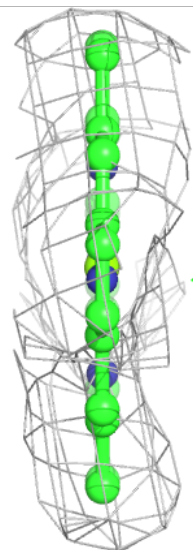
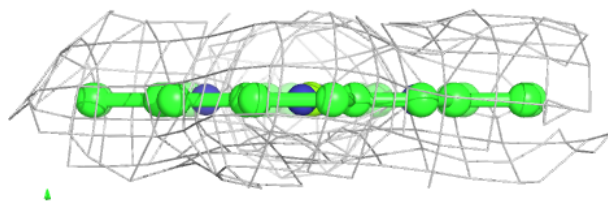
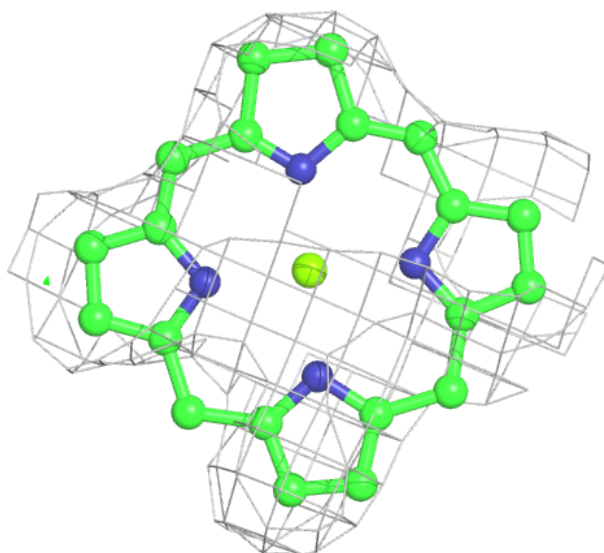
Electron density around CLA 3 3012:

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



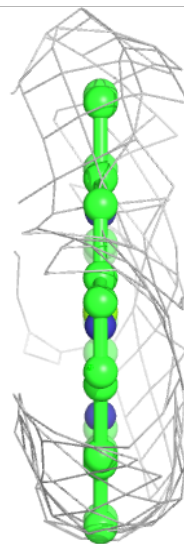
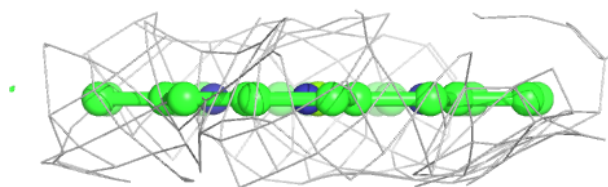
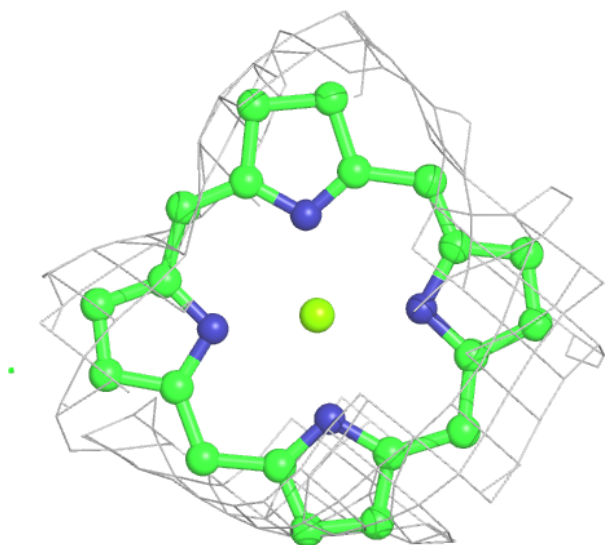
Electron density around CLA 4 4006:

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



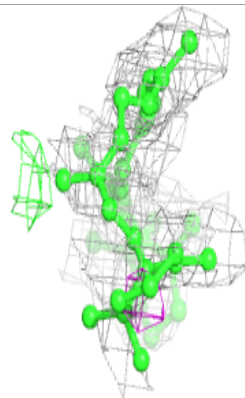
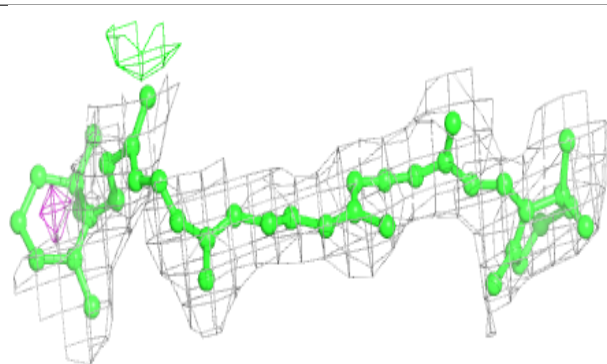
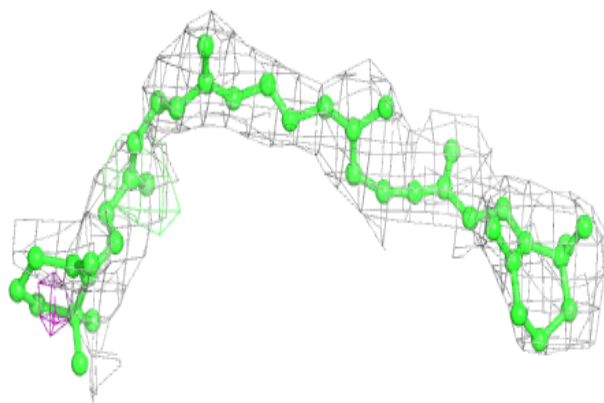
Electron density around CLA G 1248:

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



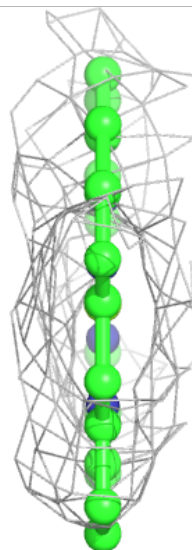
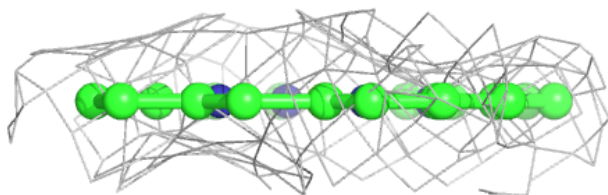
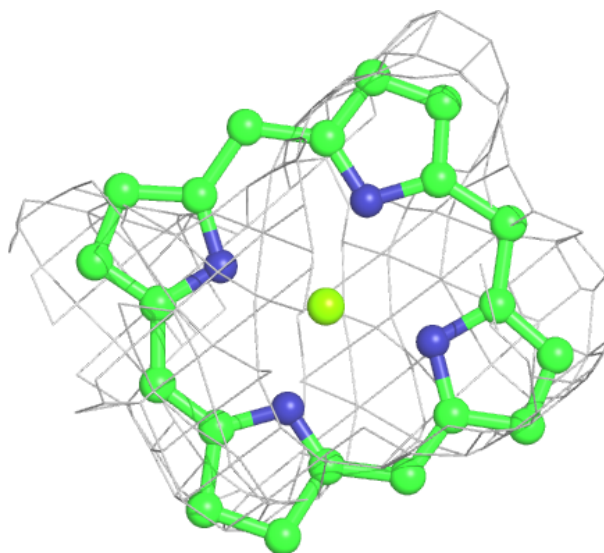
Electron density around BCR F 6016:

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



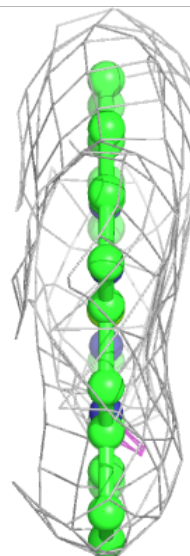
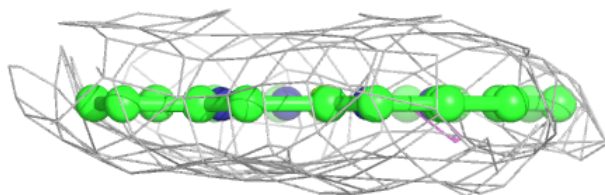
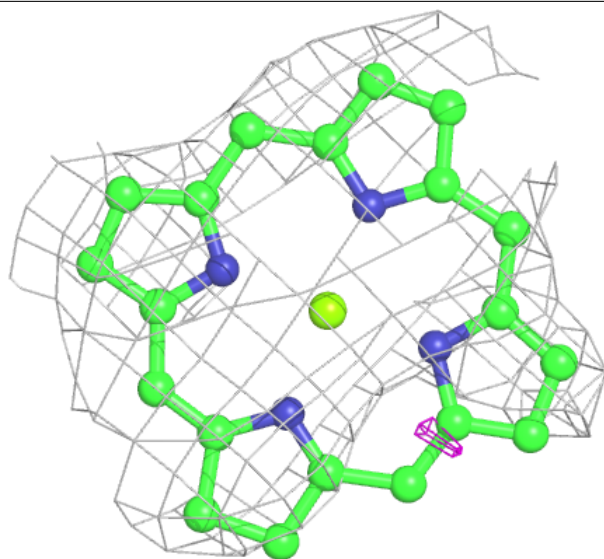
Electron density around CLA 4 4010:

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



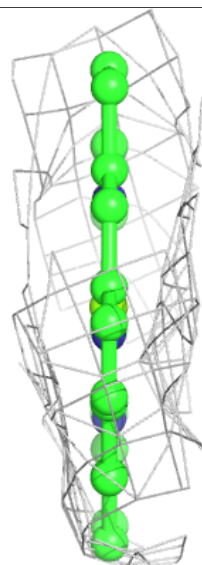
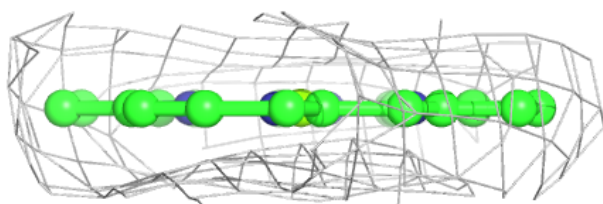
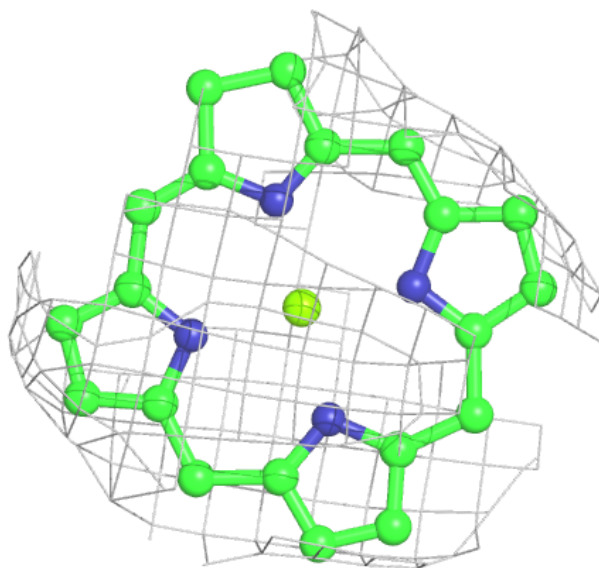
Electron density around CLA A 1134:

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



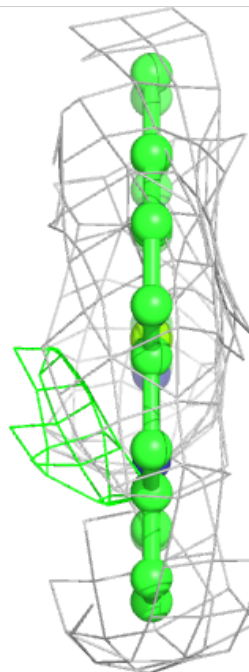
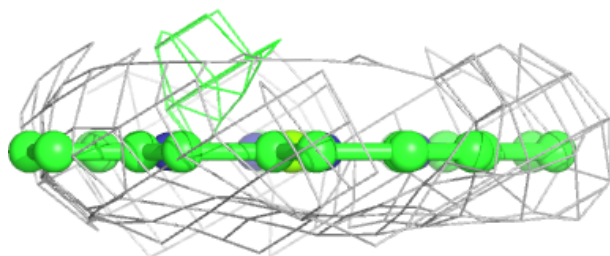
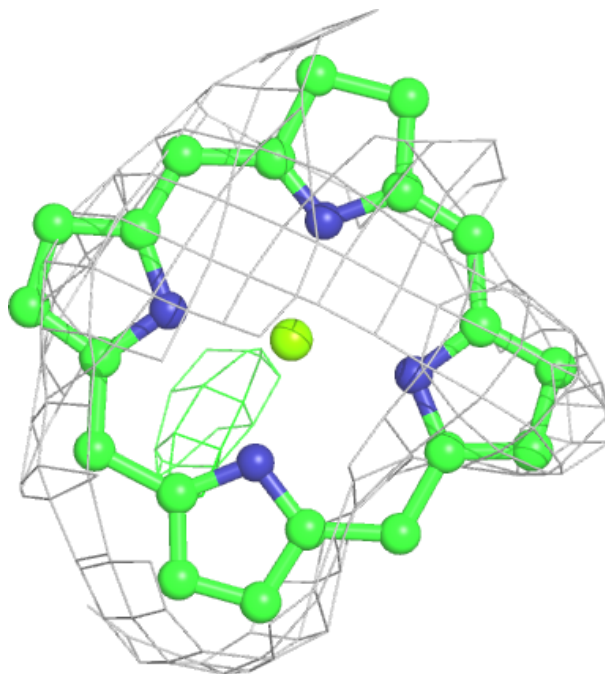
Electron density around CLA 3 3002:

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



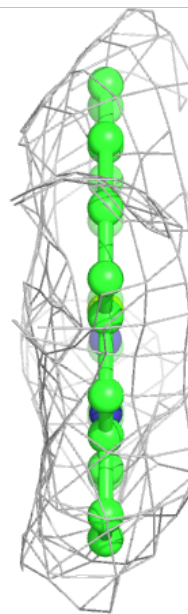
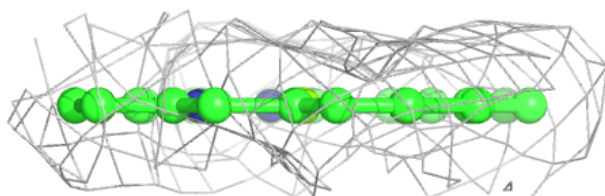
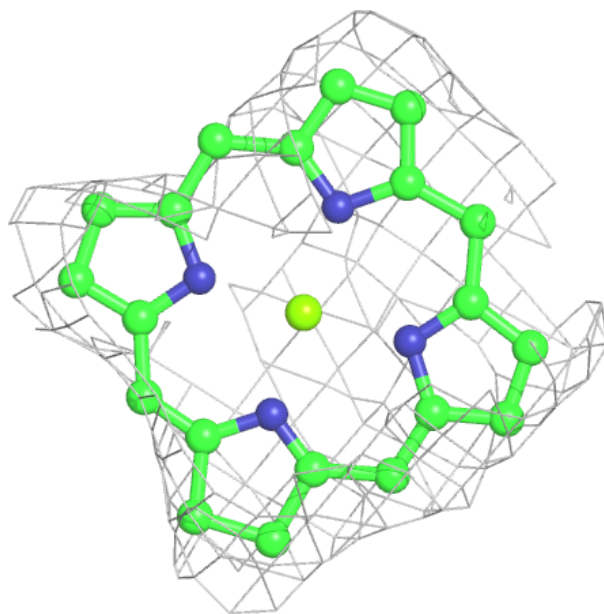
Electron density around CLA 1 1004:

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



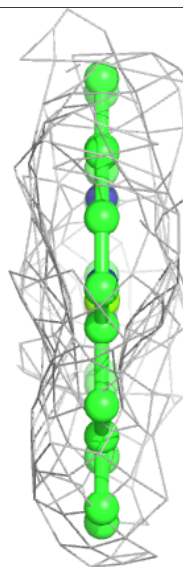
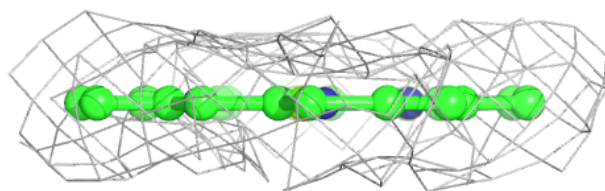
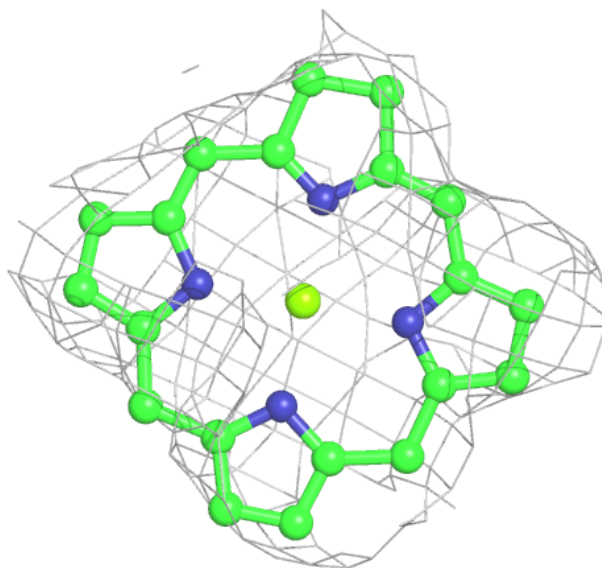
Electron density around CLA 1 1011:

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



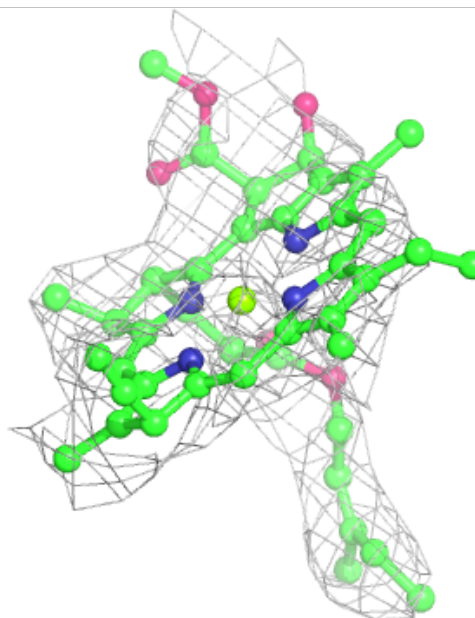
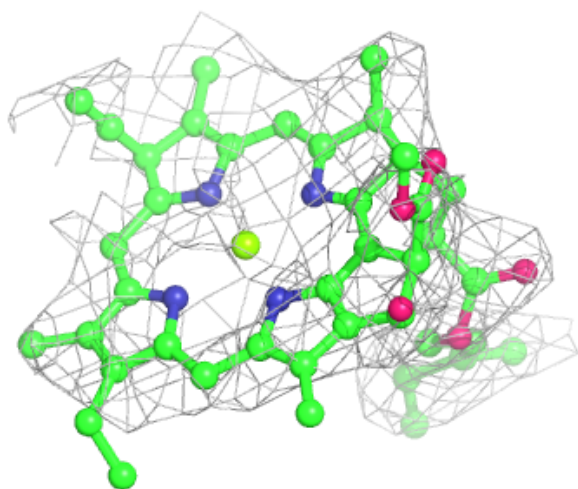
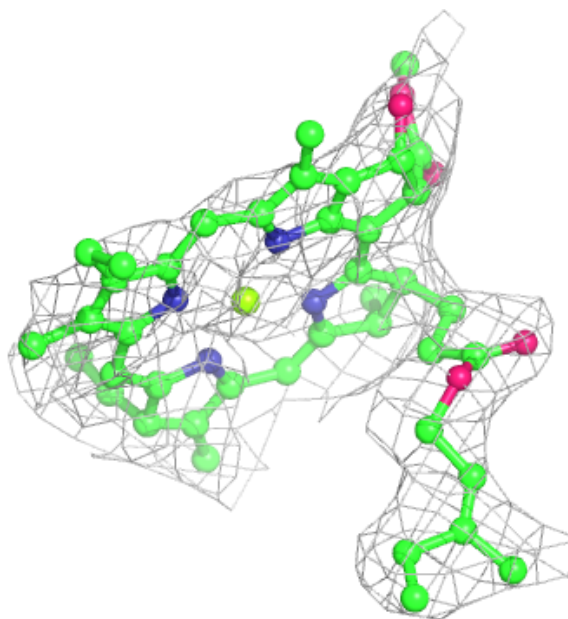
Electron density around CLA A 1116:

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



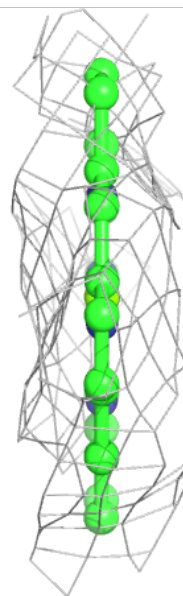
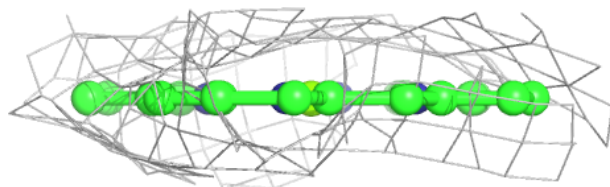
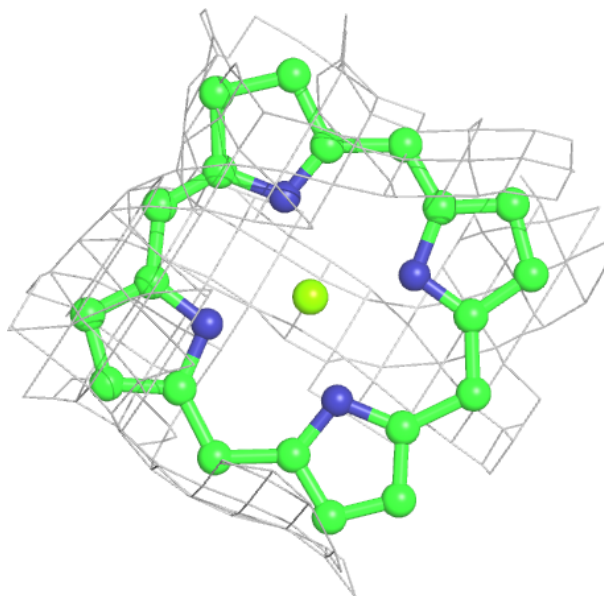
Electron density around CLA L 1502:

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



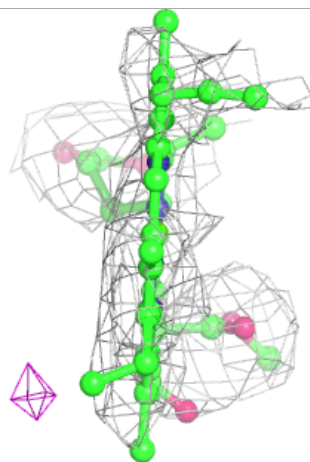
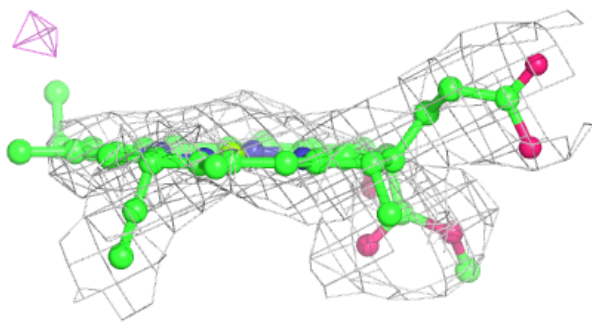
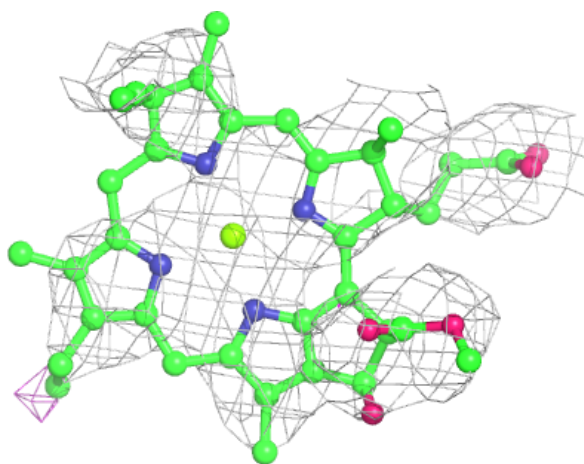
Electron density around CLA 3 3005:

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



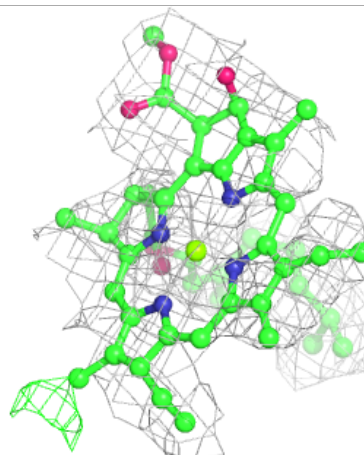
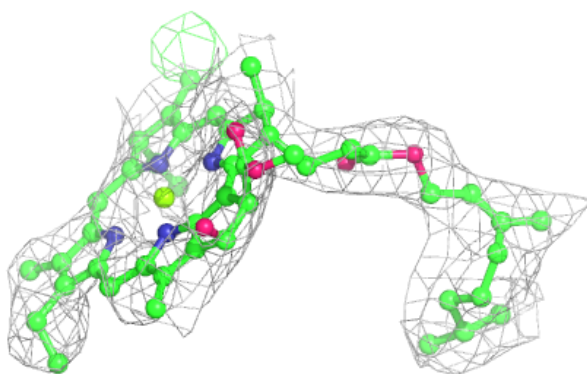
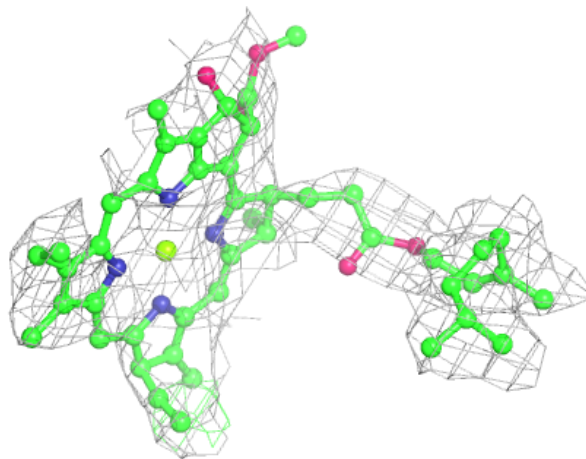
Electron density around CLA A 1135:

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



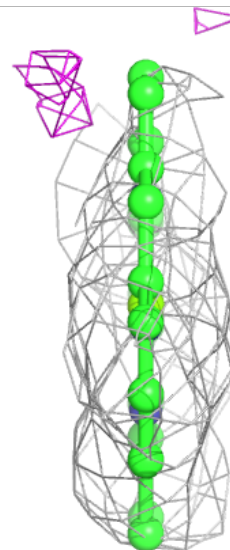
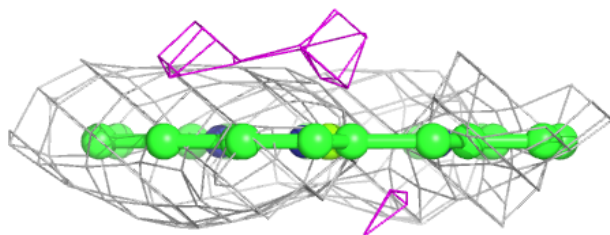
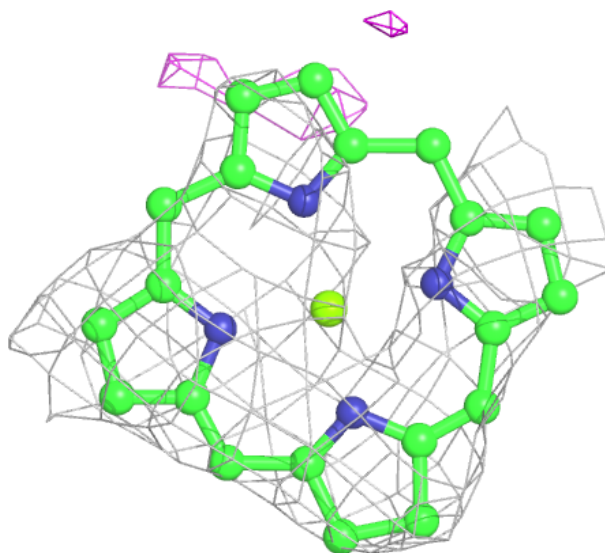
Electron density around CLA A 1129:

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



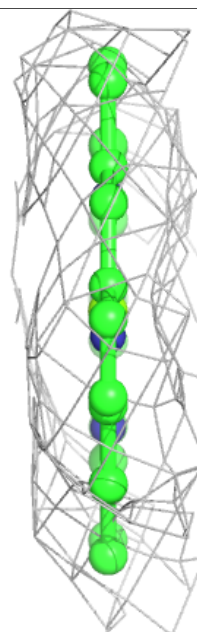
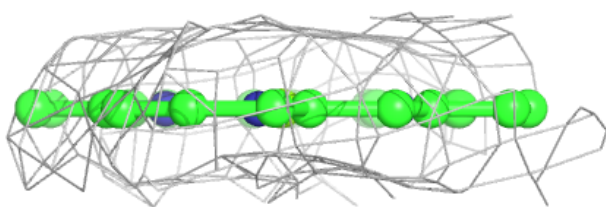
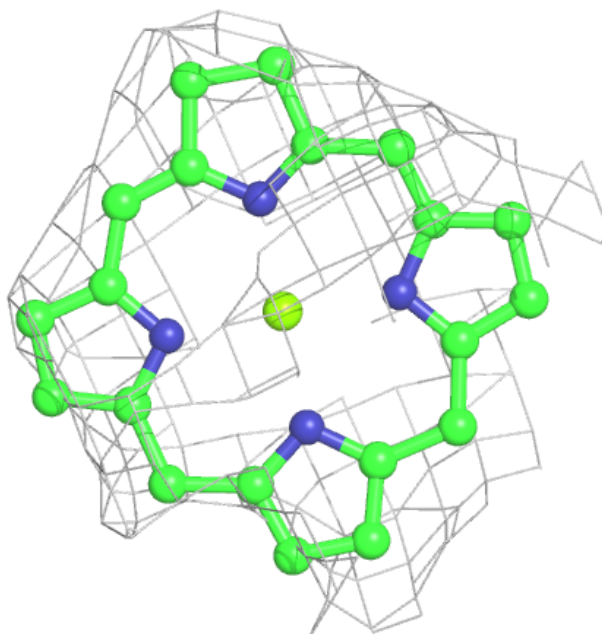
Electron density around CLA 1 1010:

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



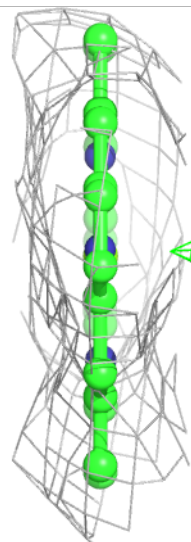
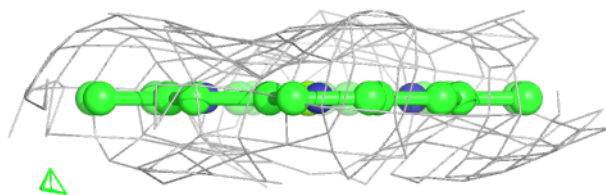
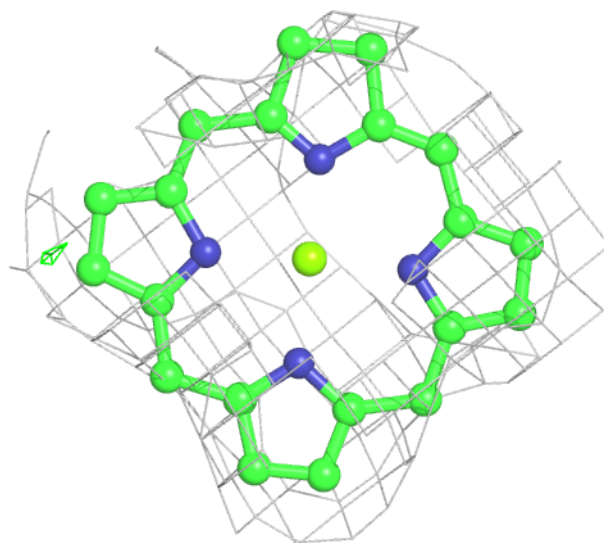
Electron density around CLA H 1505:

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



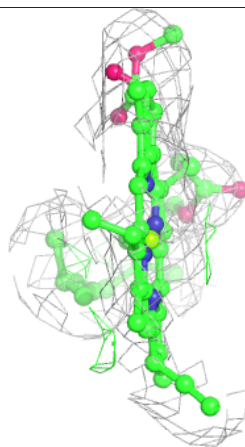
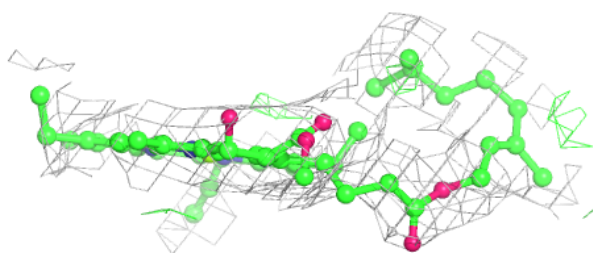
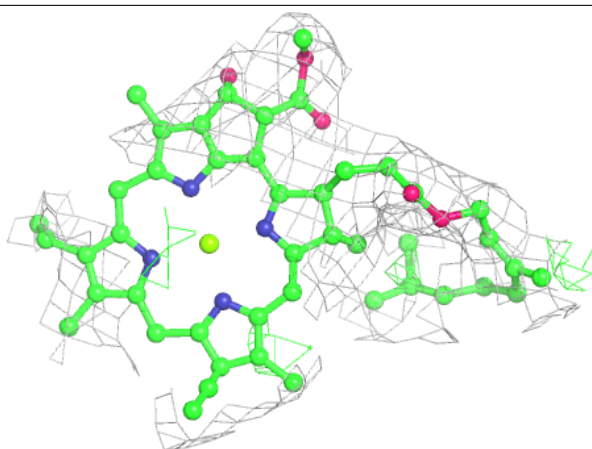
Electron density around CLA B 1201:

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



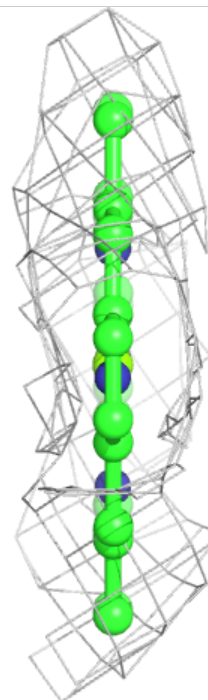
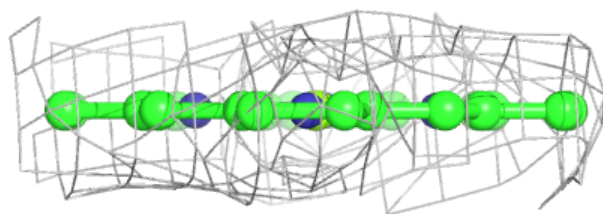
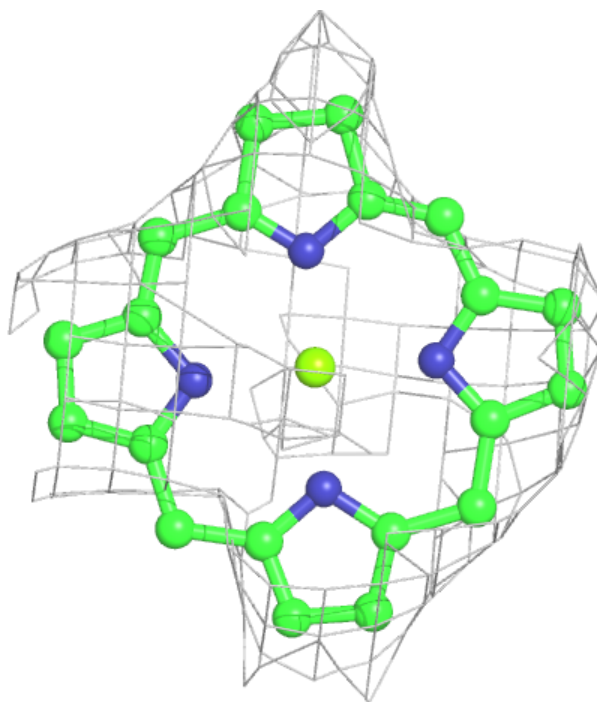
Electron density around CLA F 1302:

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



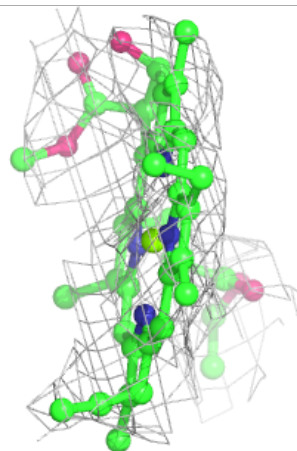
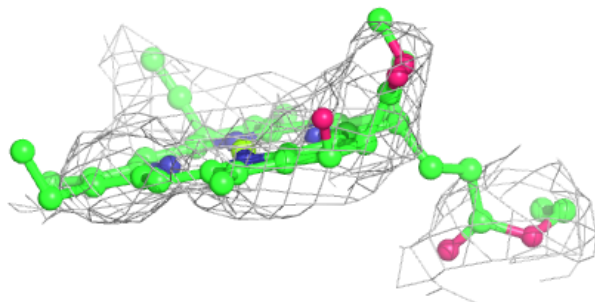
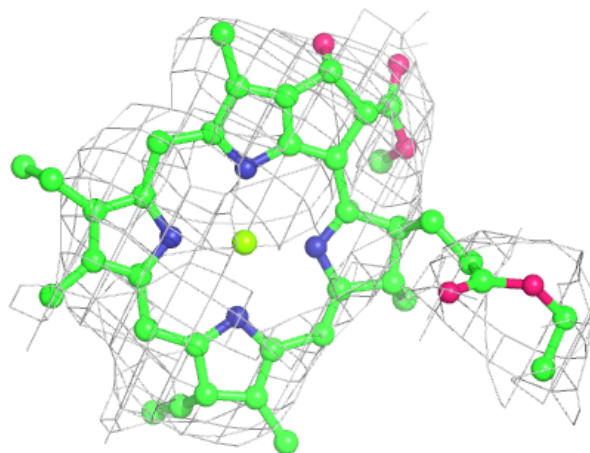
Electron density around CLA 2 2012:

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



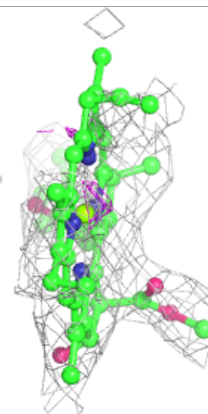
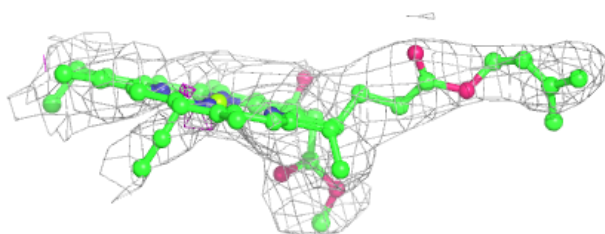
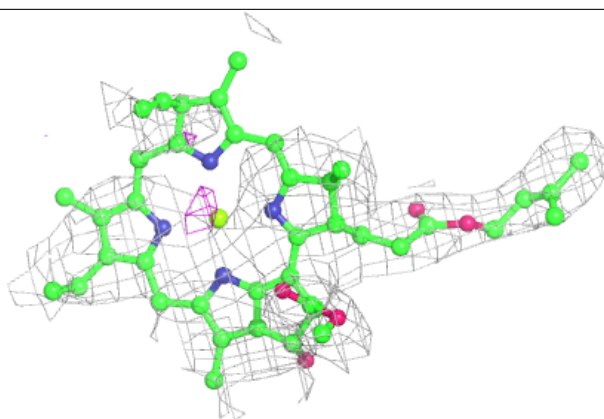
Electron density around CLA A 1103:

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

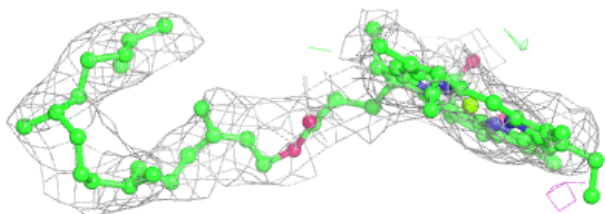
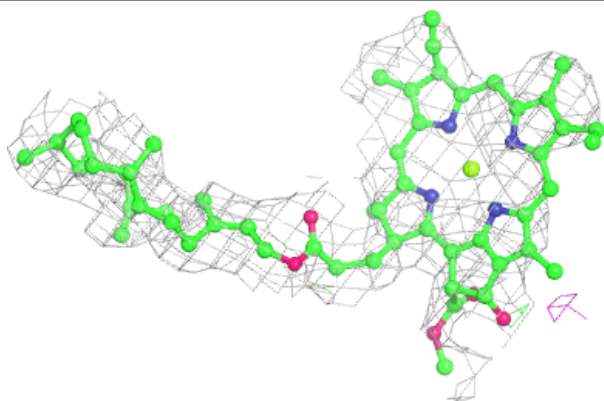


Electron density around CLA B 1234:

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

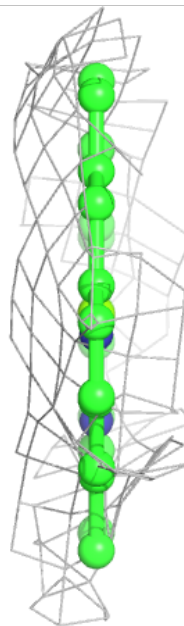
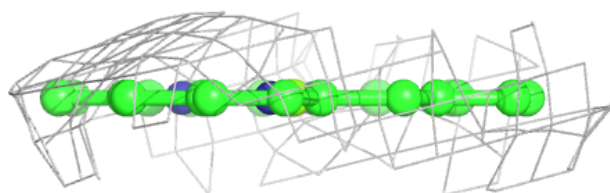
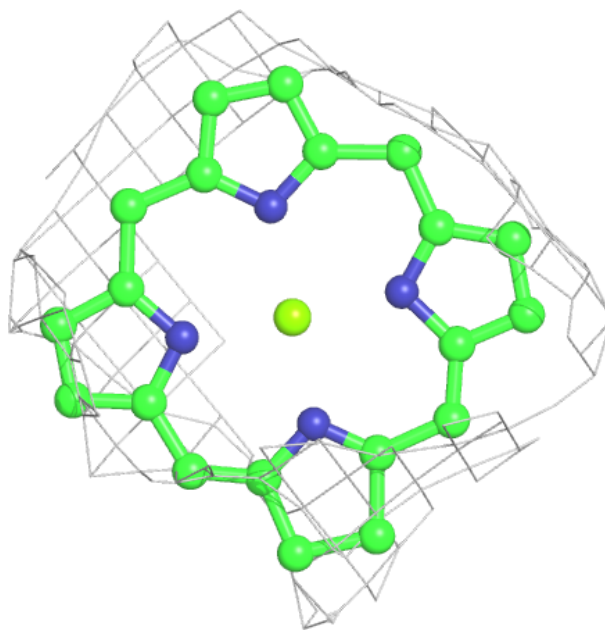
**Electron density around CLA B 1222:**

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



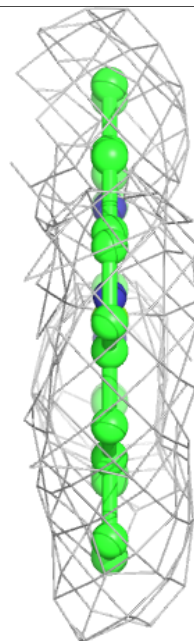
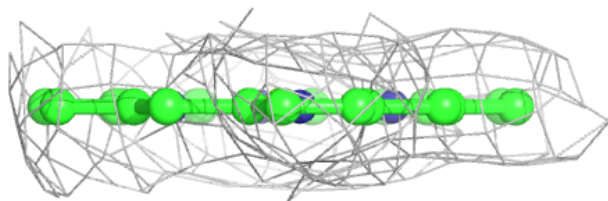
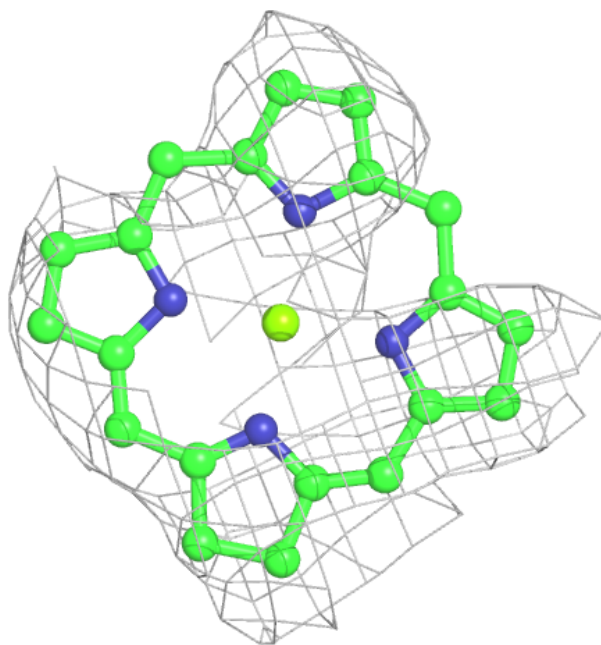
Electron density around CLA A 1144:

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



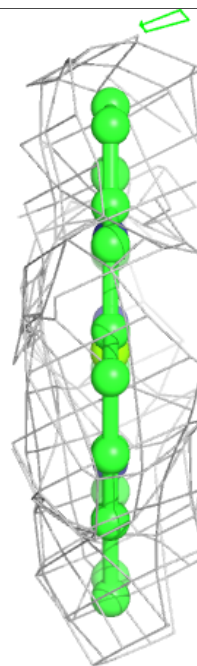
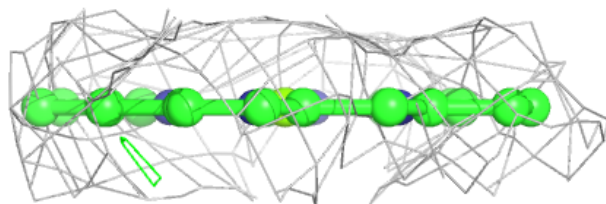
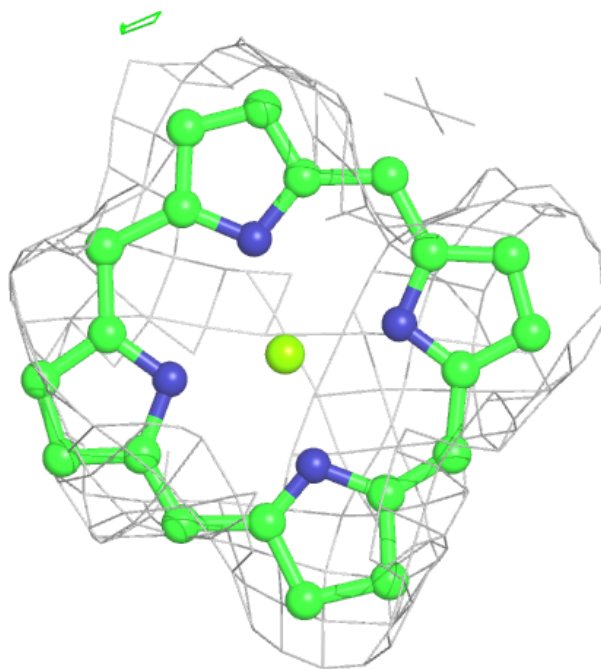
Electron density around CLA F 1306:

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



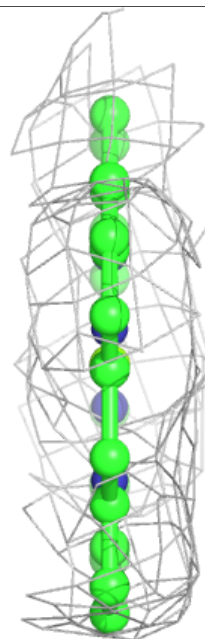
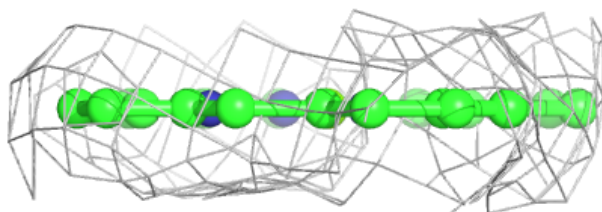
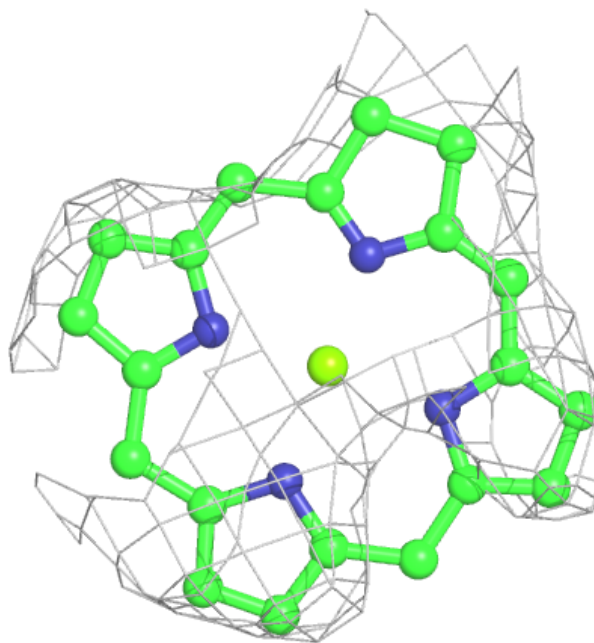
Electron density around CLA 2 2002:

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



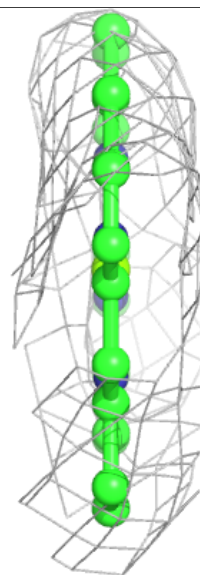
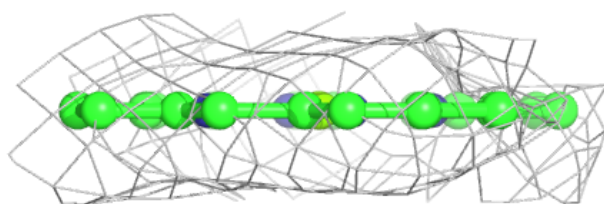
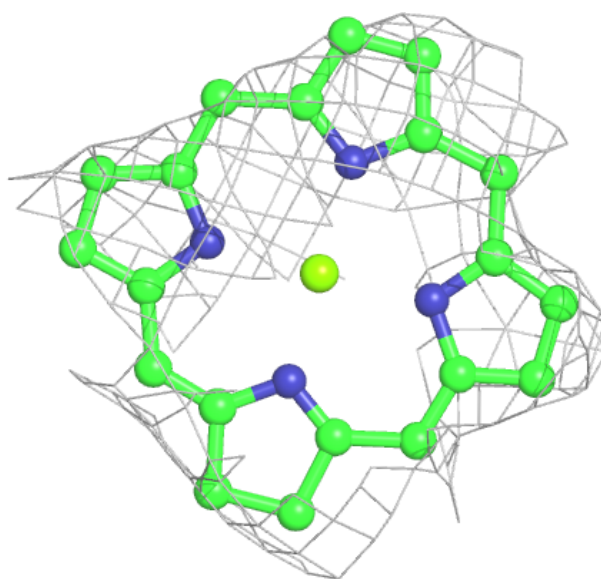
Electron density around CLA 4 4007:

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



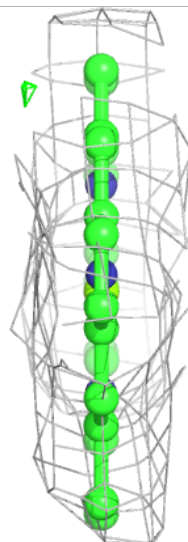
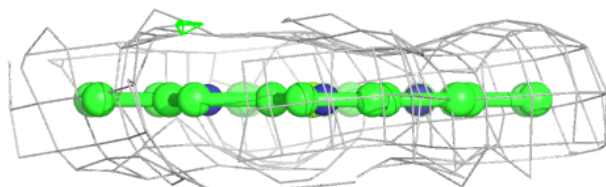
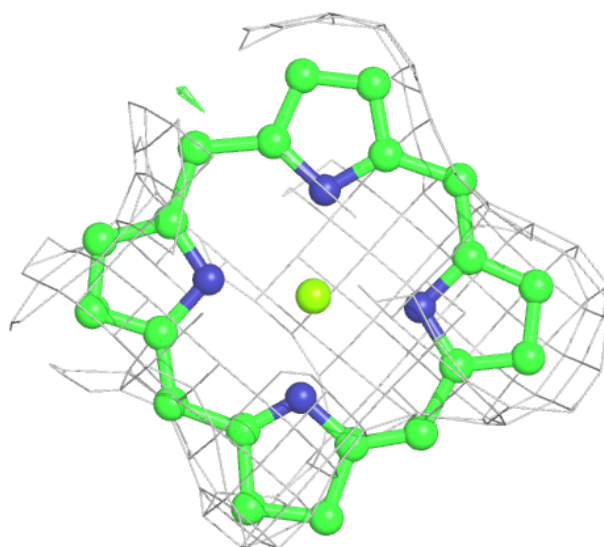
Electron density around CLA K 1150:

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



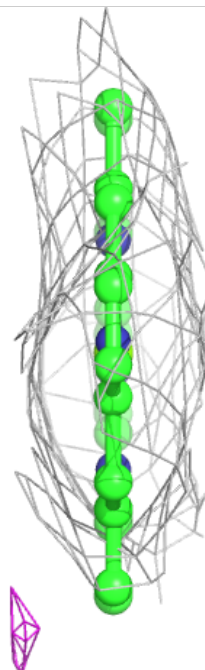
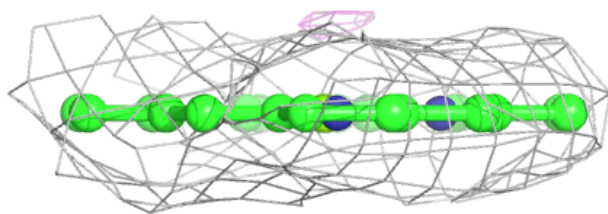
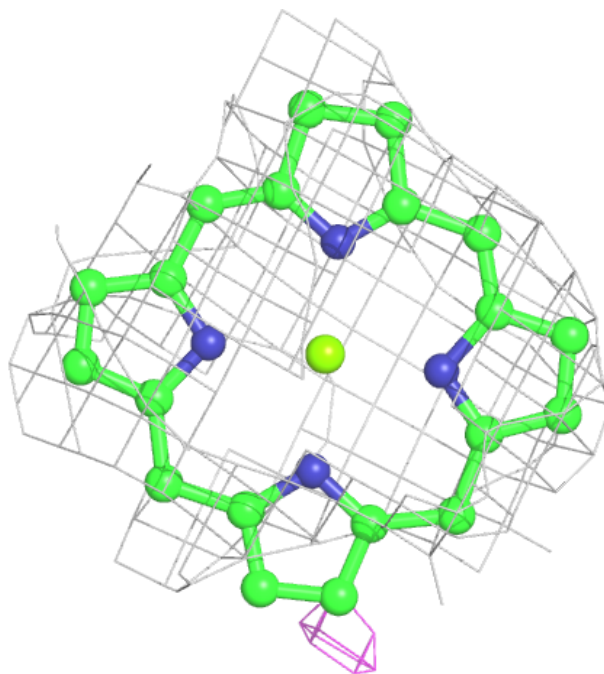
Electron density around CLA 4 4005:

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



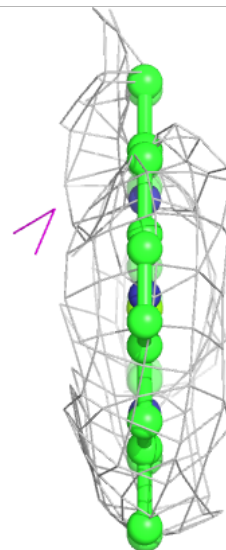
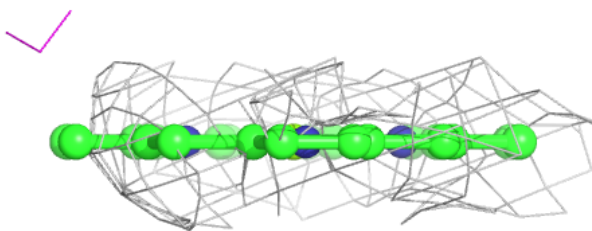
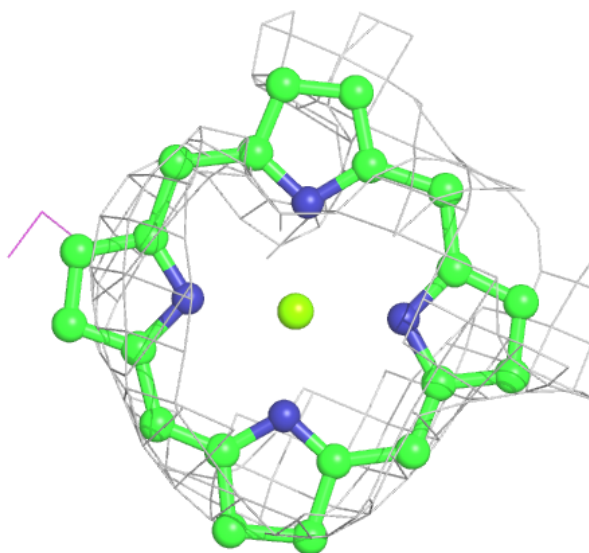
Electron density around CLA 2 2010:

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



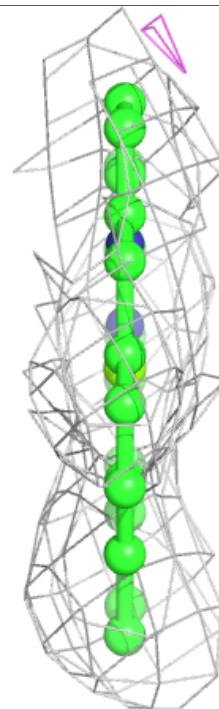
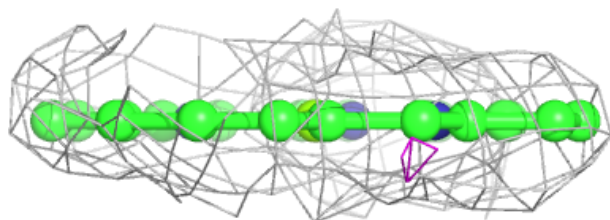
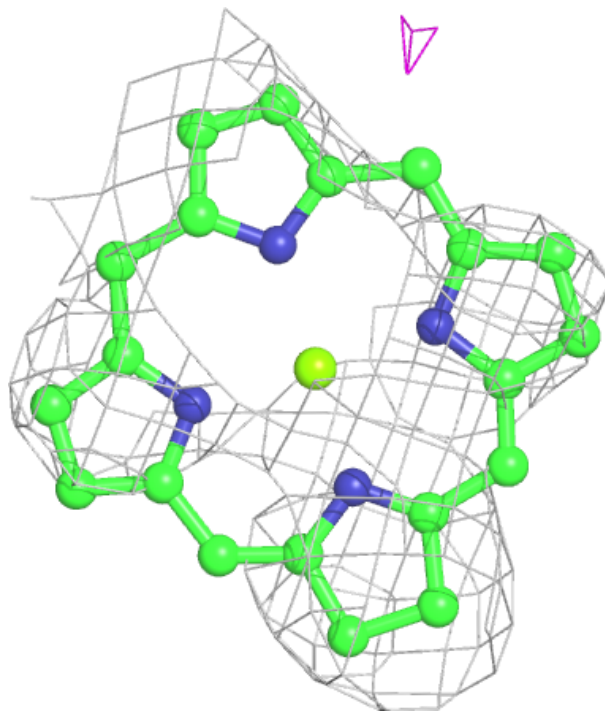
Electron density around CLA A 1309:

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



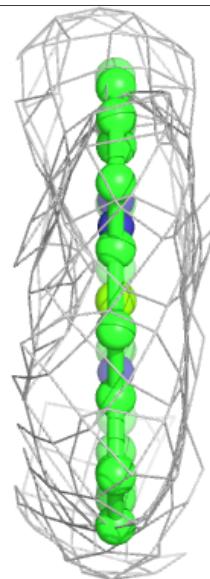
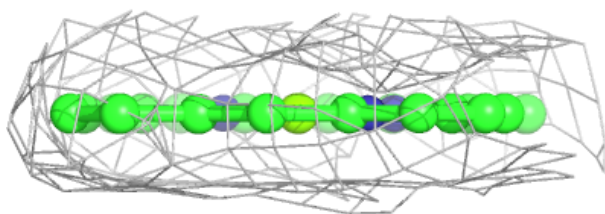
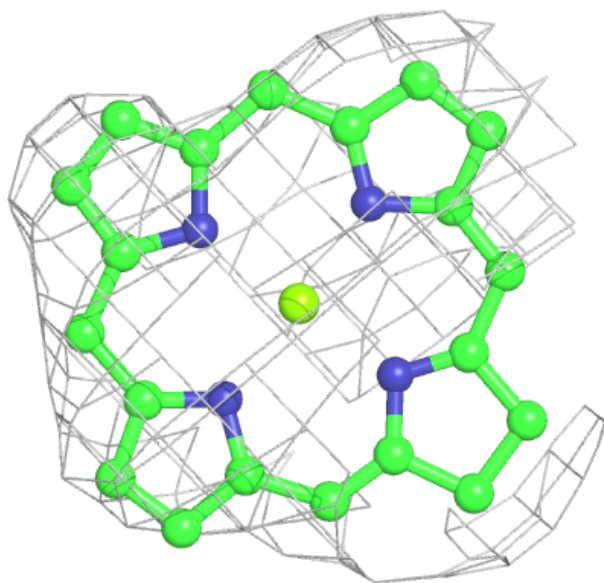
Electron density around CLA B 1230:

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



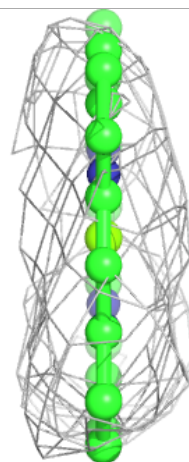
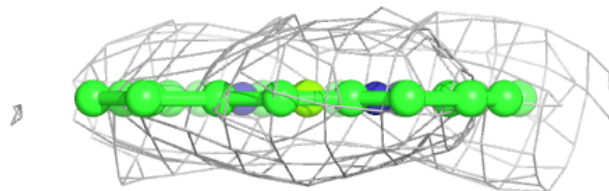
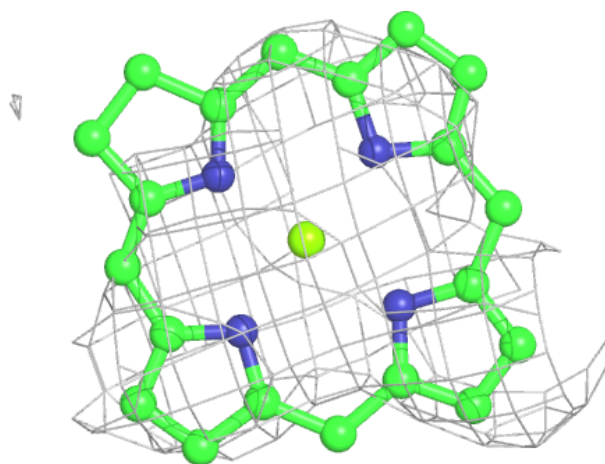
Electron density around CLA K 1153:

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



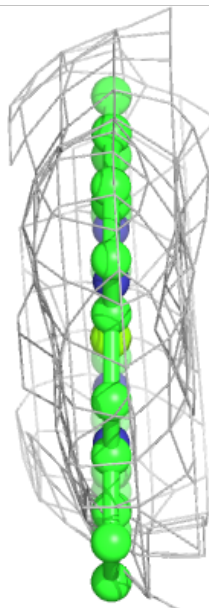
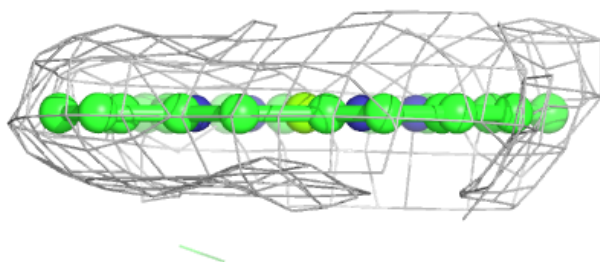
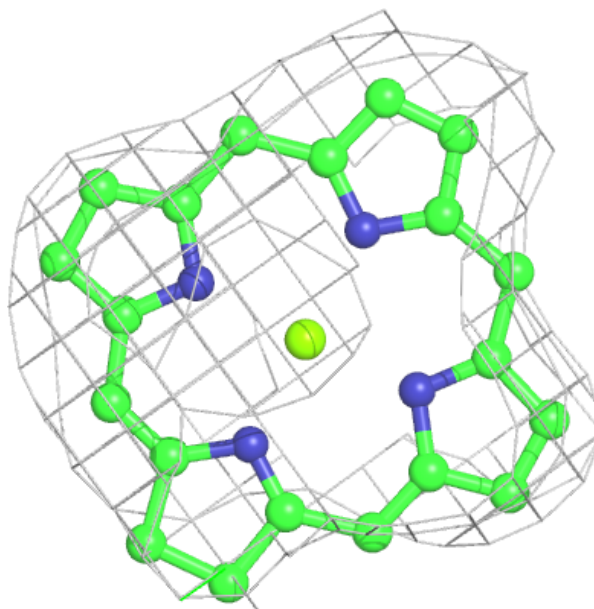
Electron density around CLA J 1307:

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



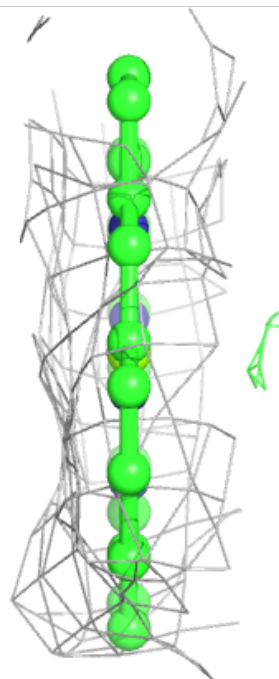
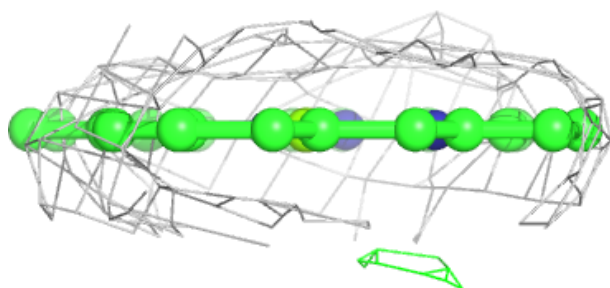
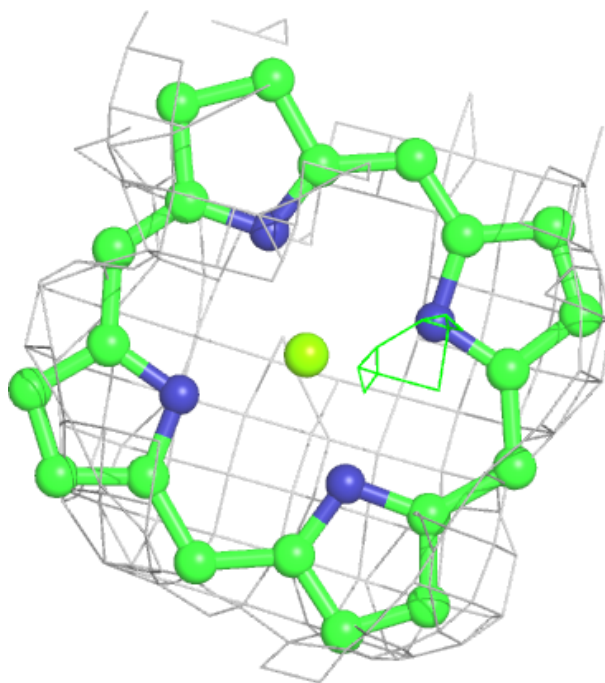
Electron density around CLA 4 4004:

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



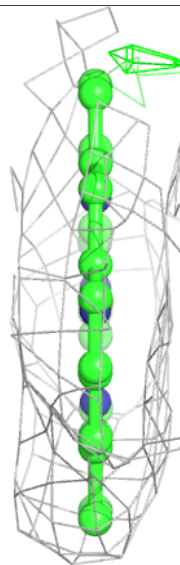
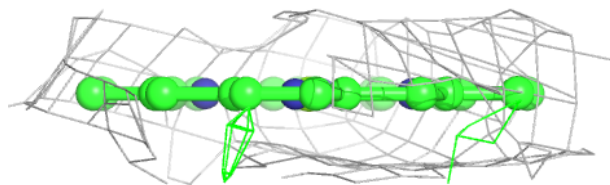
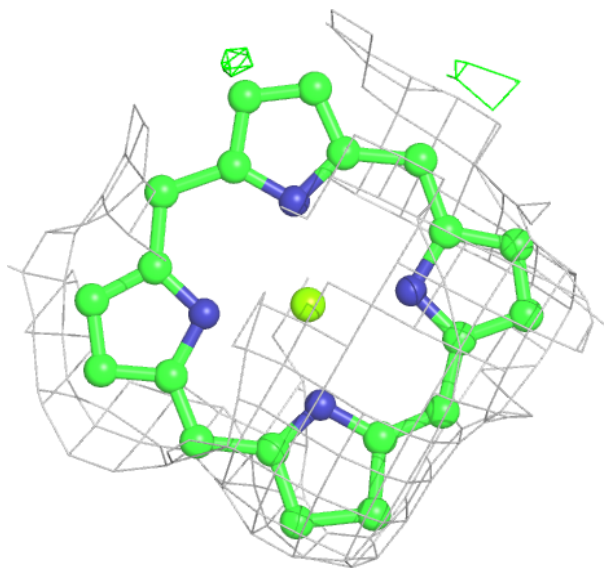
Electron density around CLA 1 1003:

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



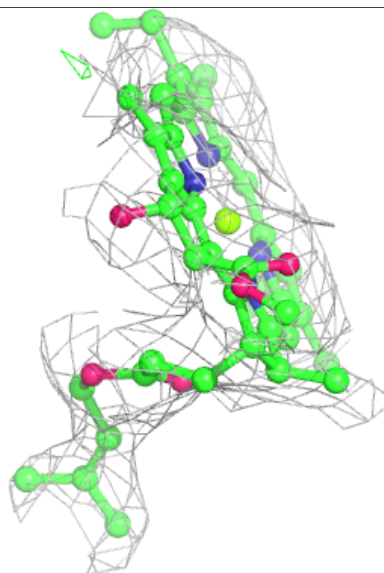
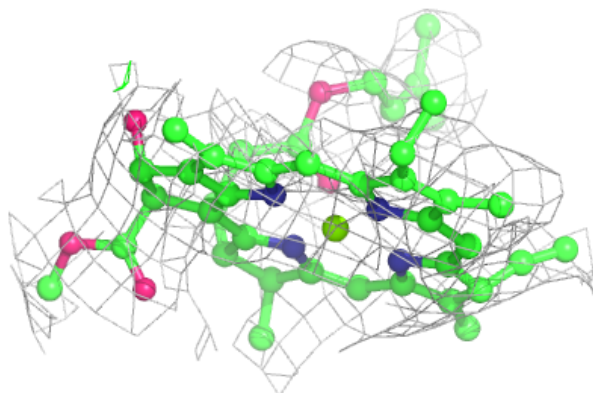
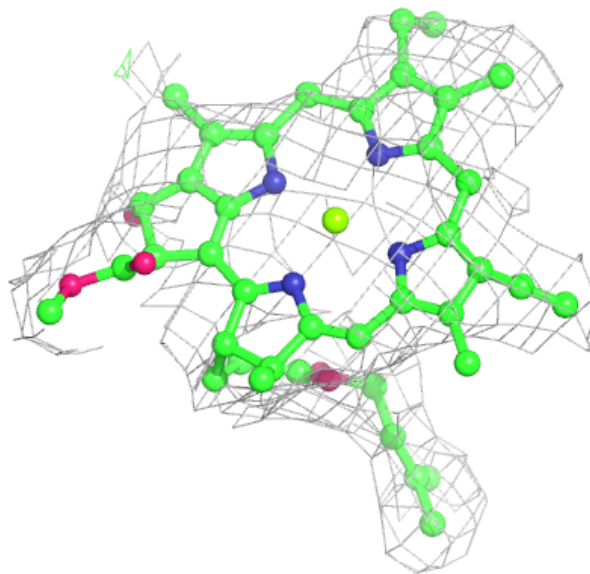
Electron density around CLA A 1110:

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



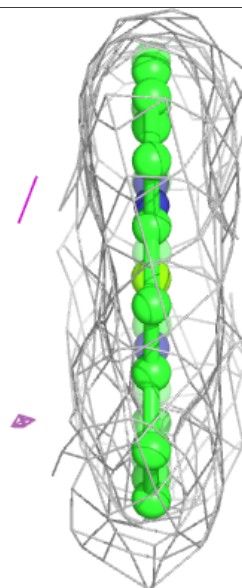
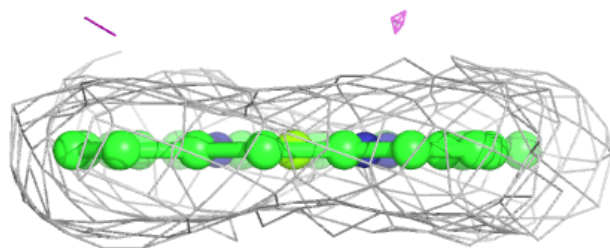
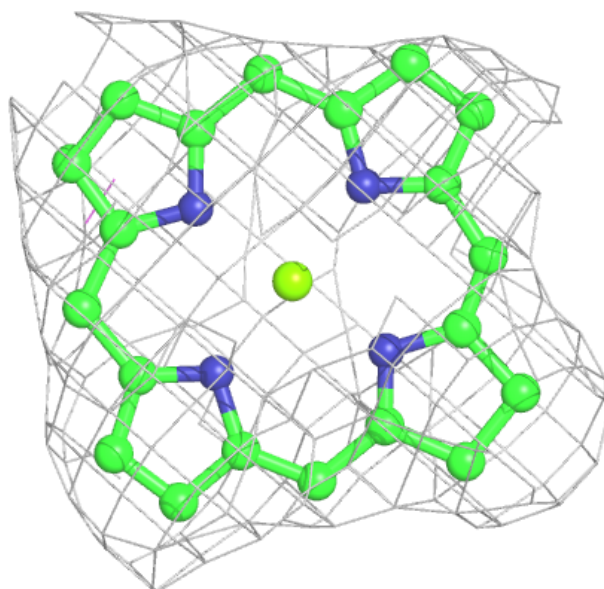
Electron density around CLA B 1217:

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



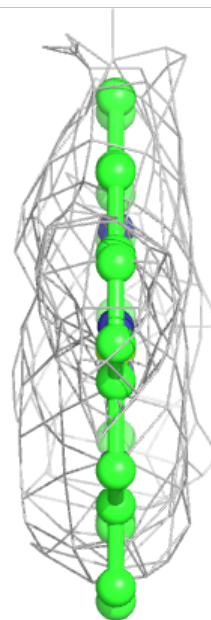
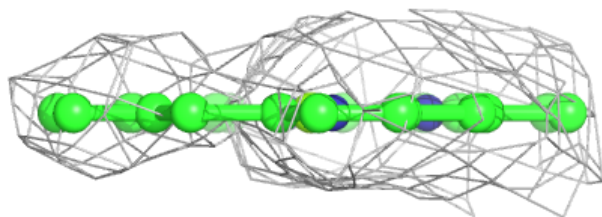
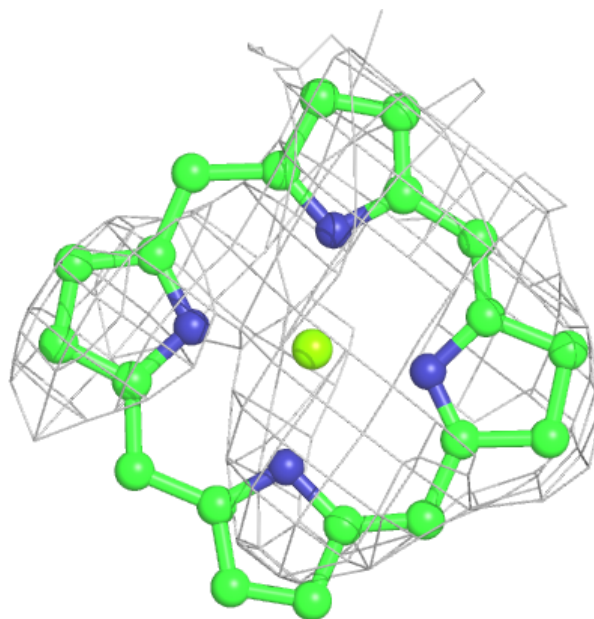
Electron density around CLA A 1104:

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



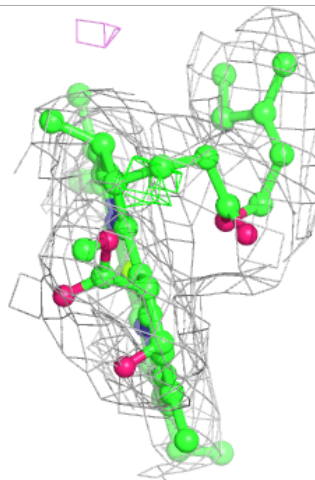
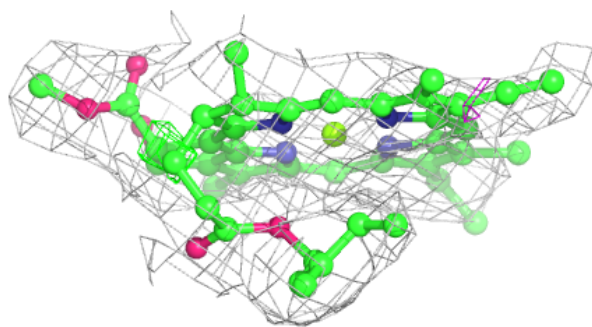
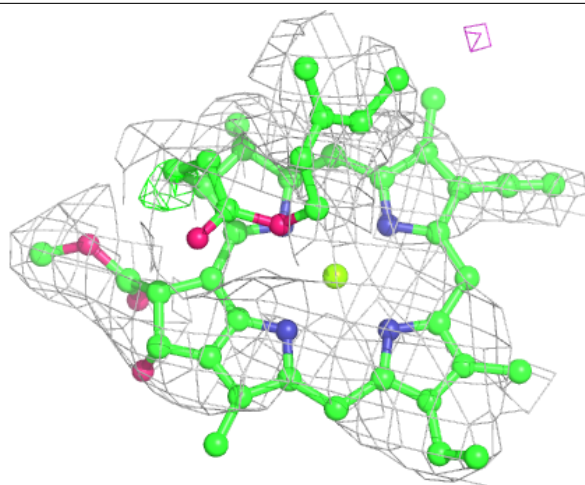
Electron density around CLA B 1241:

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



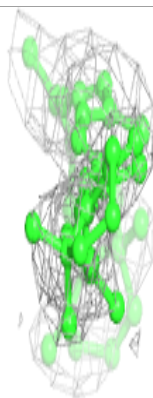
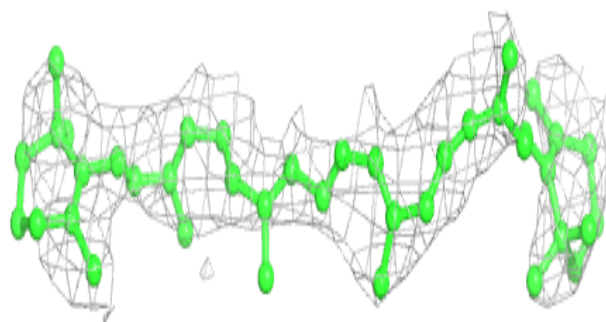
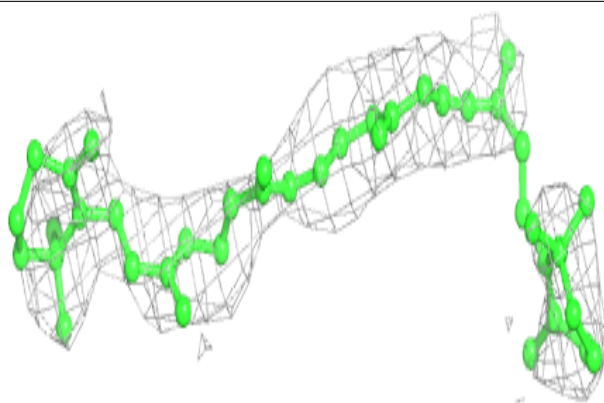
Electron density around CLA B 1237:

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



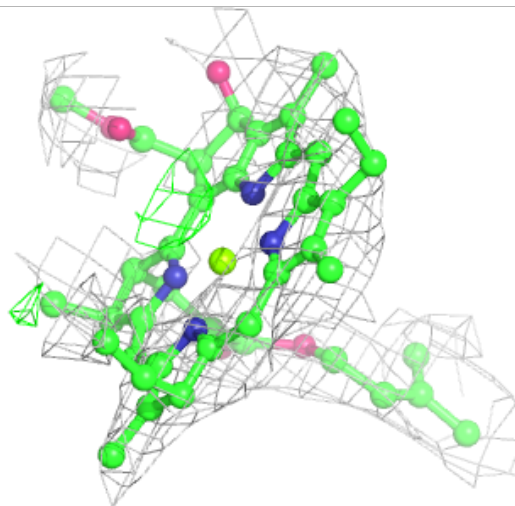
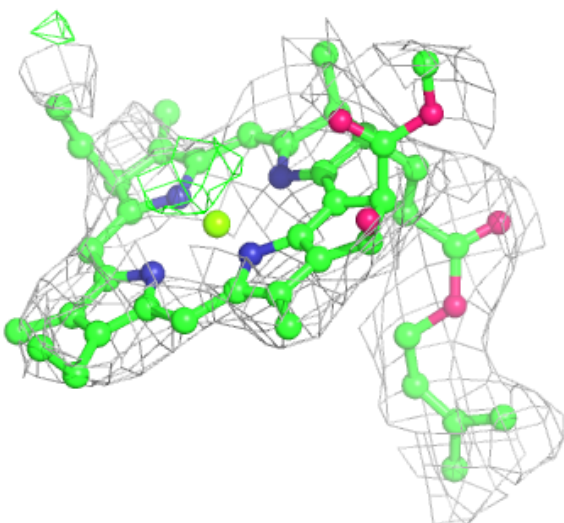
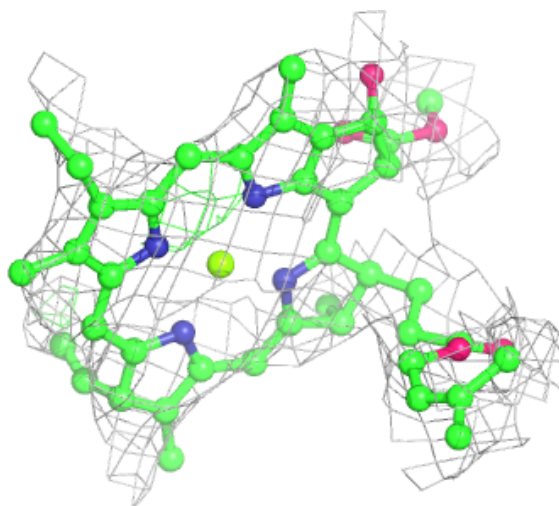
Electron density around BCR B 6017:

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



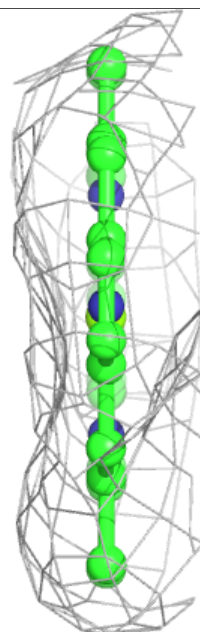
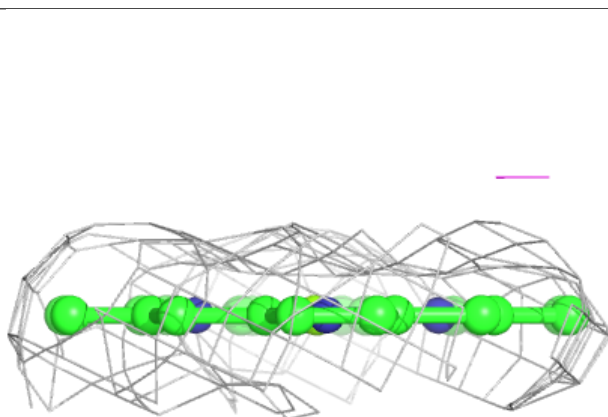
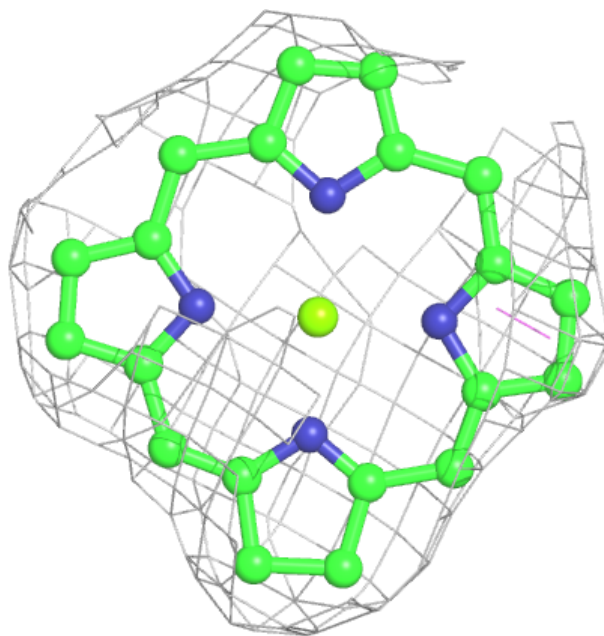
Electron density around CLA L 1130:

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



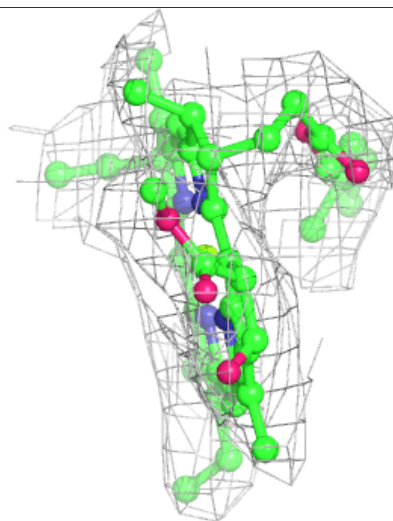
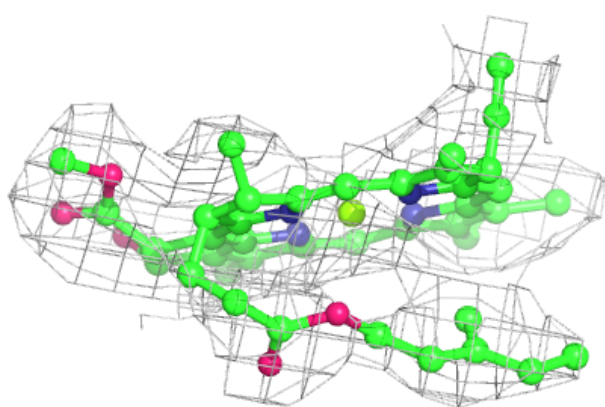
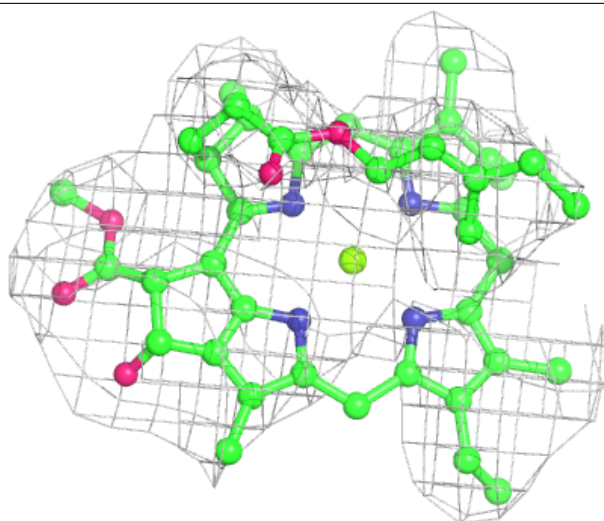
Electron density around CLA 2 2001:

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



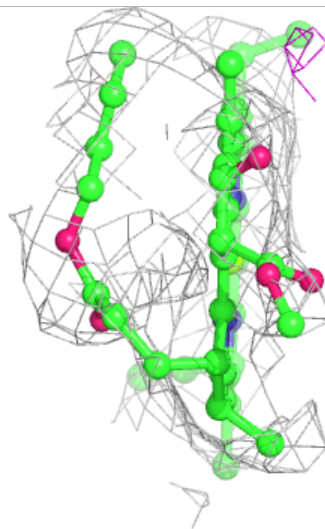
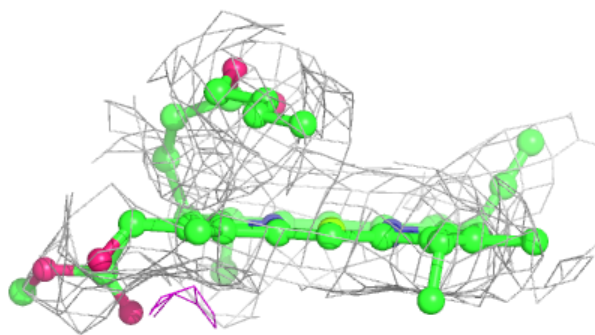
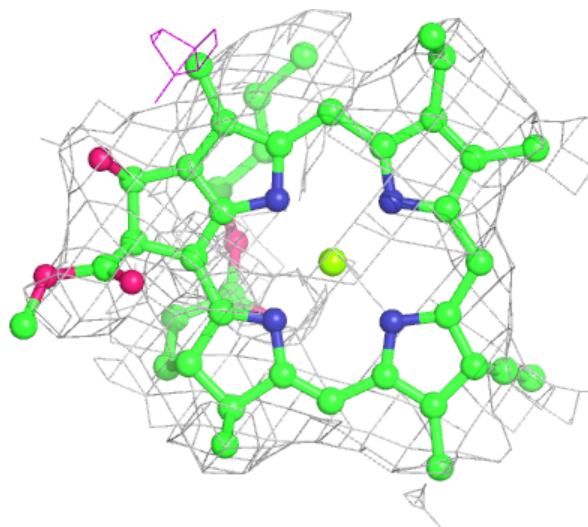
Electron density around CLA B 1219:

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



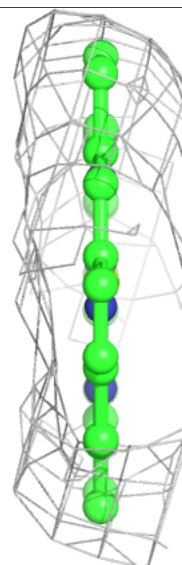
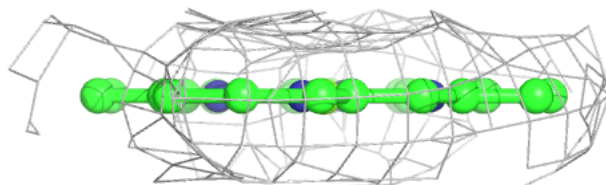
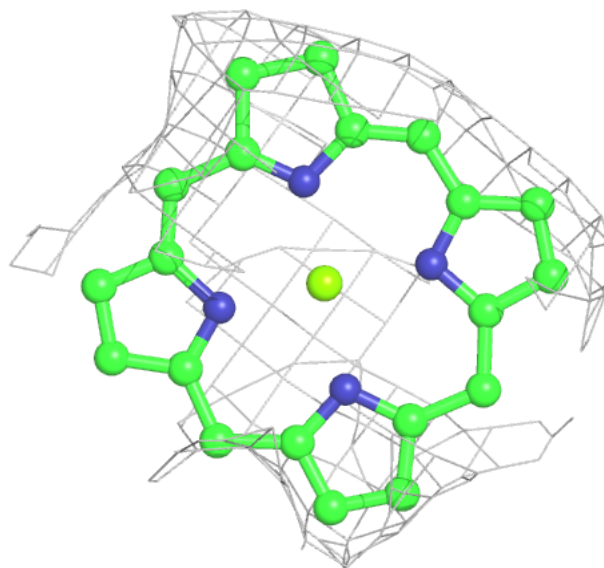
Electron density around CLA B 1214:

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



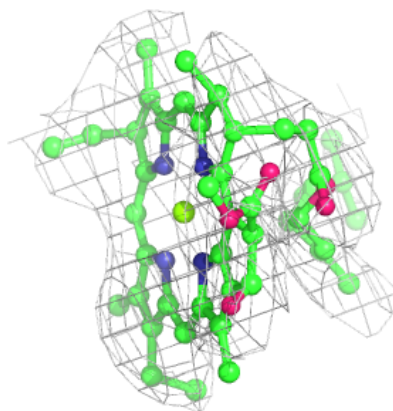
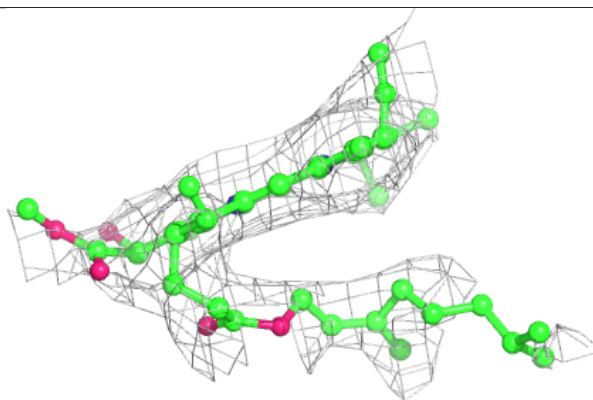
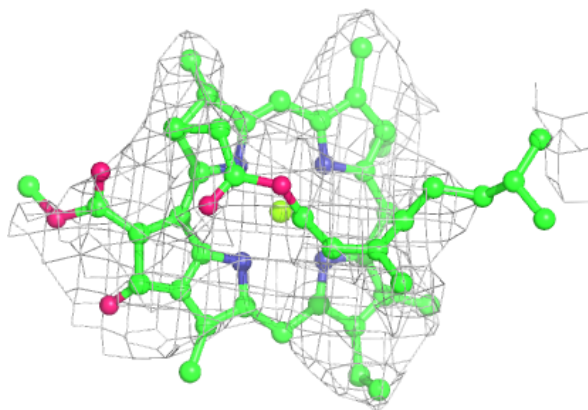
Electron density around CLA 1 1014:

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



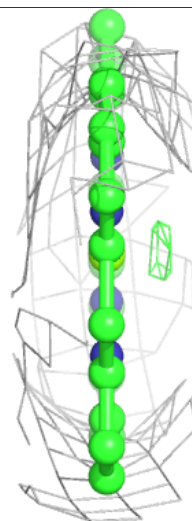
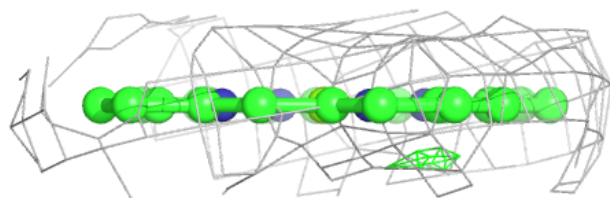
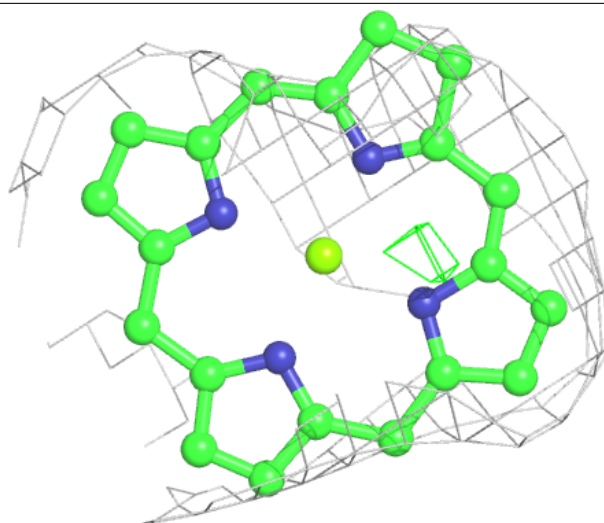
Electron density around CLA A 1136:

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



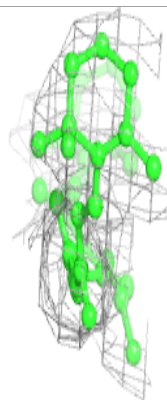
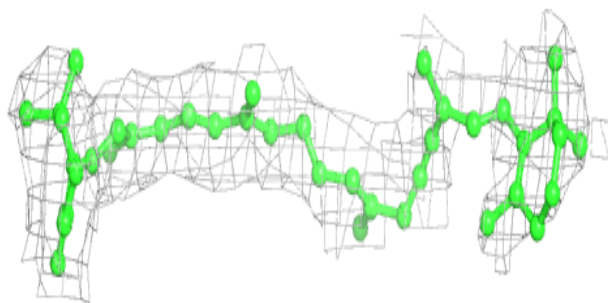
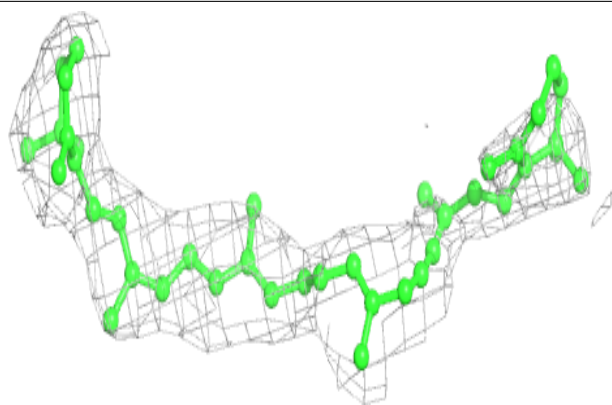
Electron density around CLA B 1211:

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



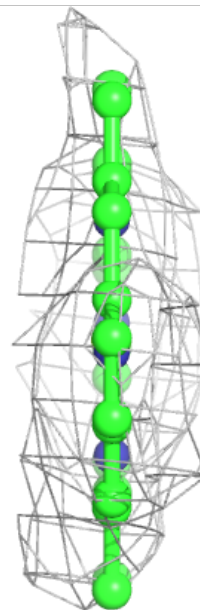
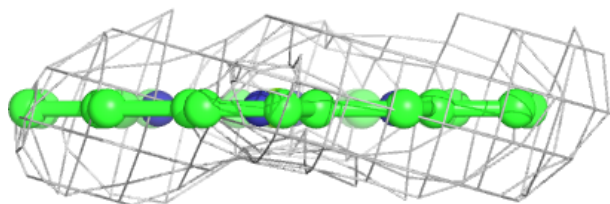
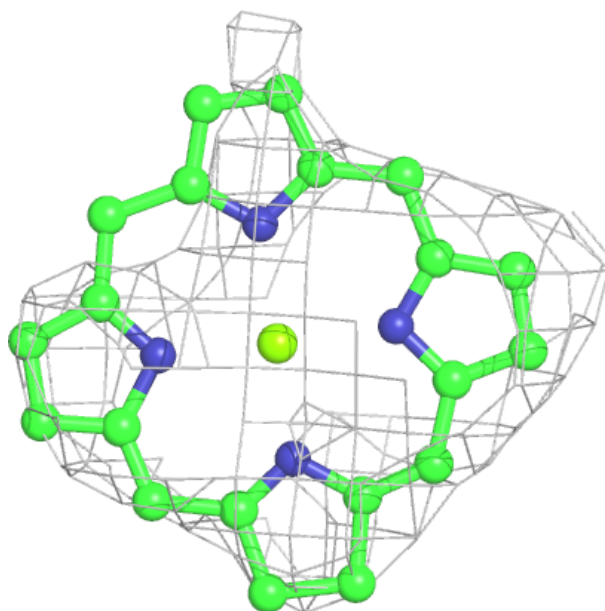
Electron density around BCR L 6020:

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



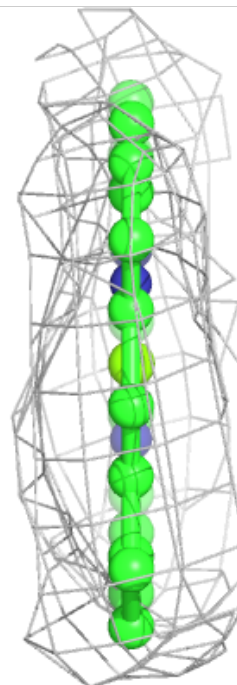
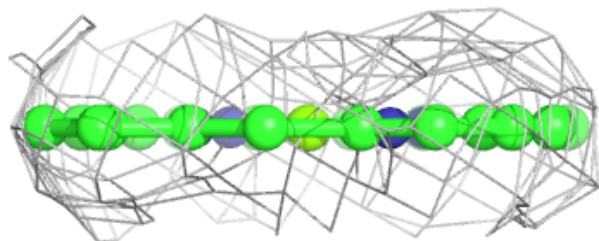
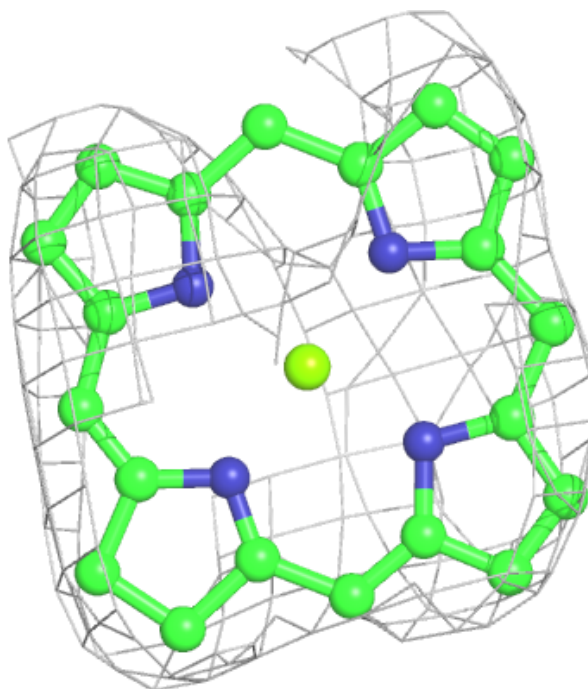
Electron density around CLA 4 4008:

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



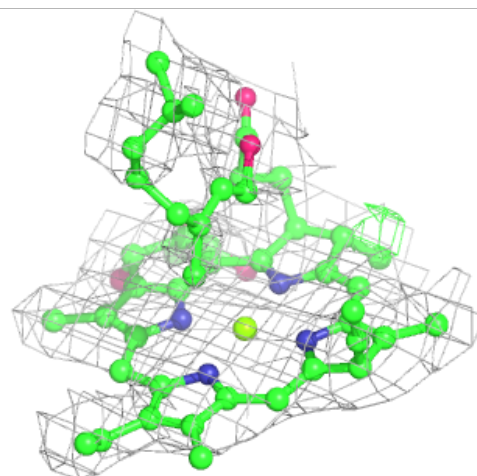
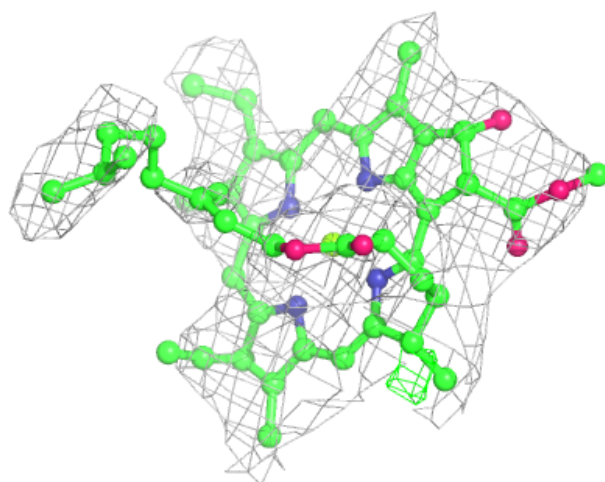
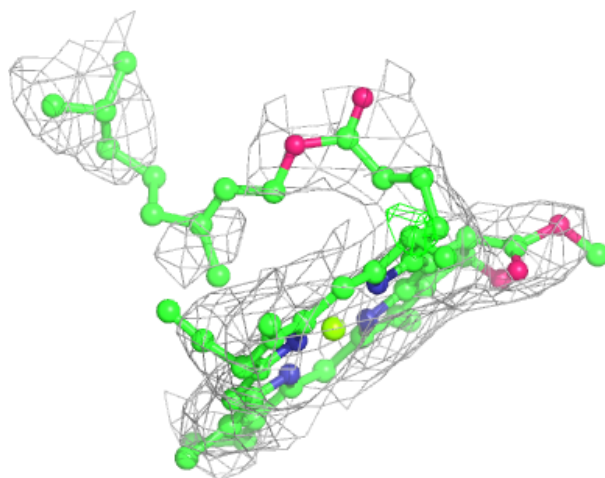
Electron density around CLA A 1146:

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



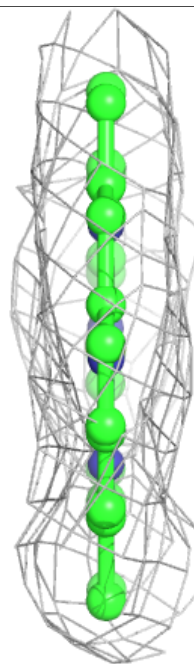
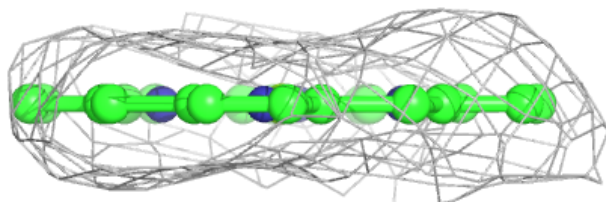
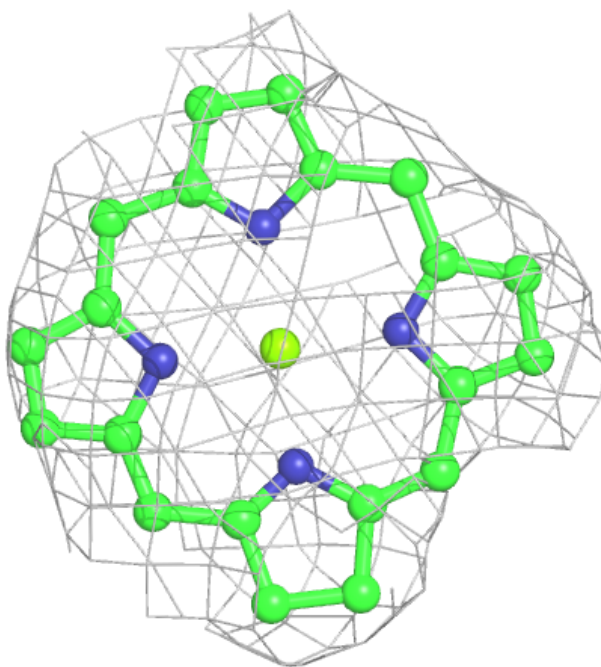
Electron density around CLA I 1204:

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



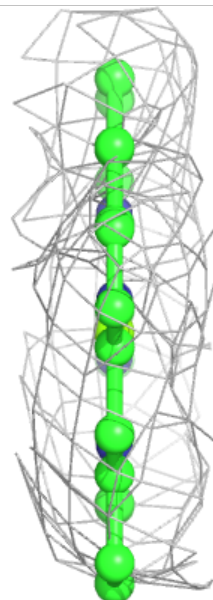
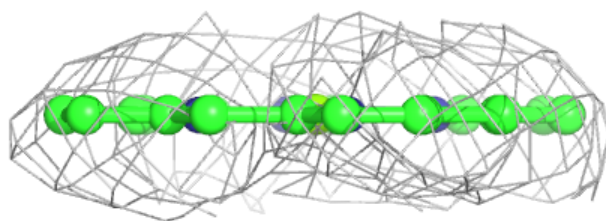
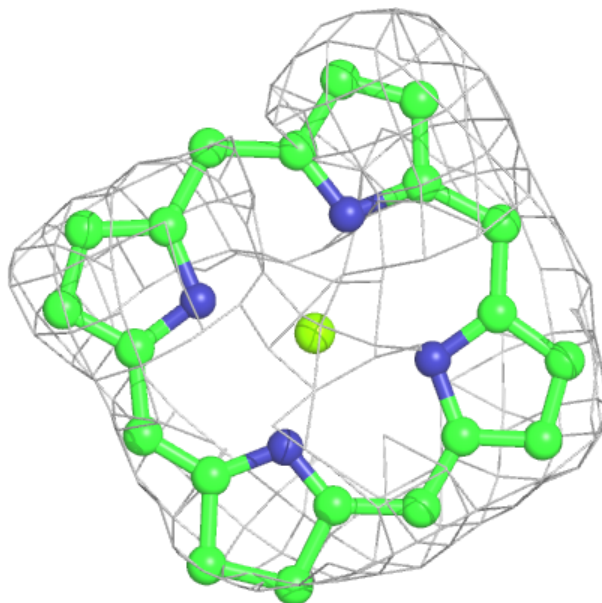
Electron density around CLA A 1117:

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



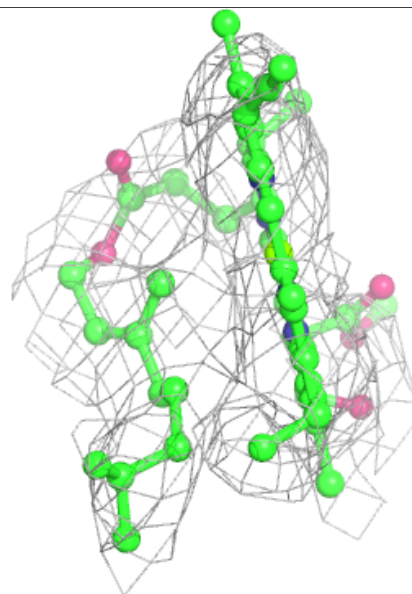
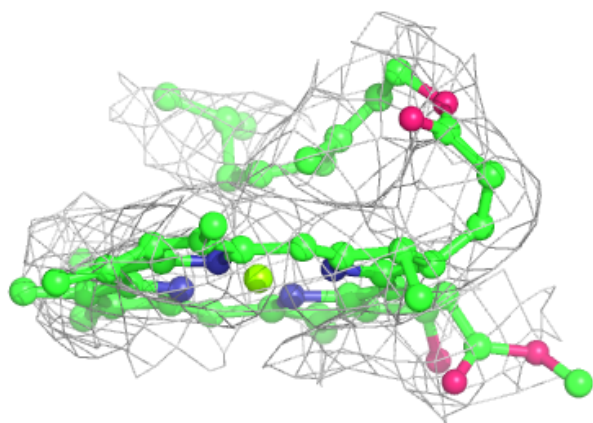
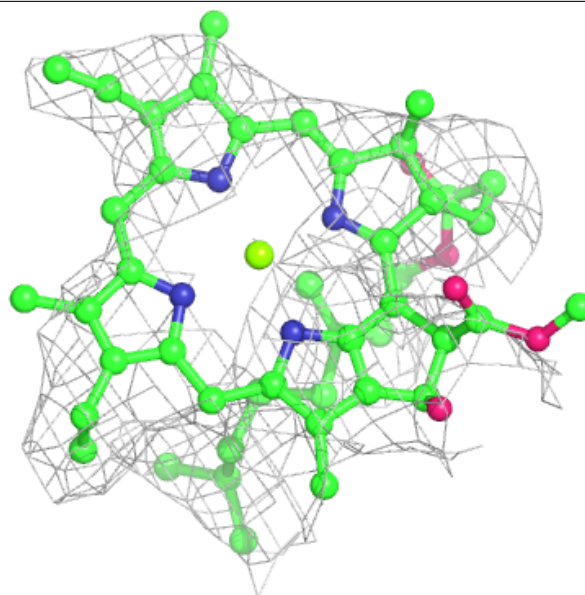
Electron density around CLA B 1213:

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



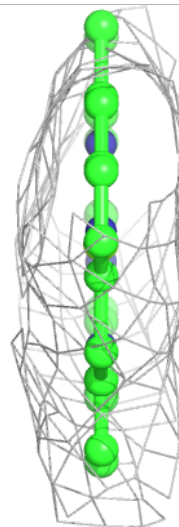
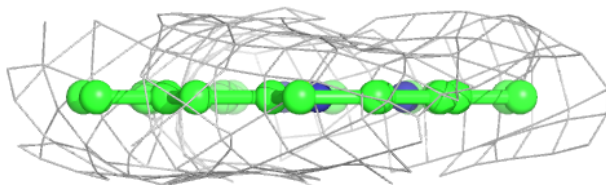
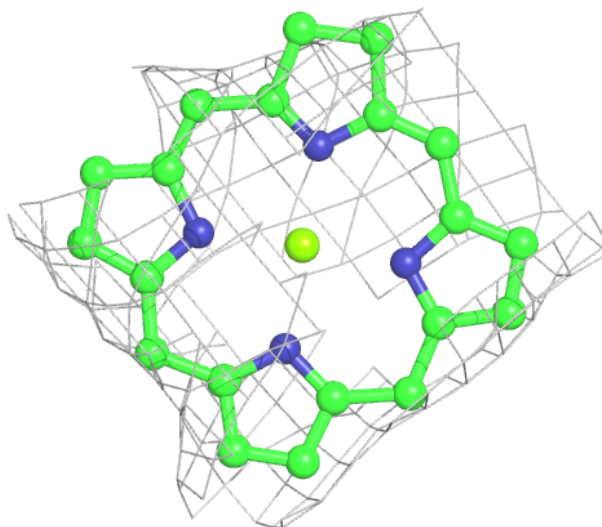
Electron density around CLA H 1501:

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



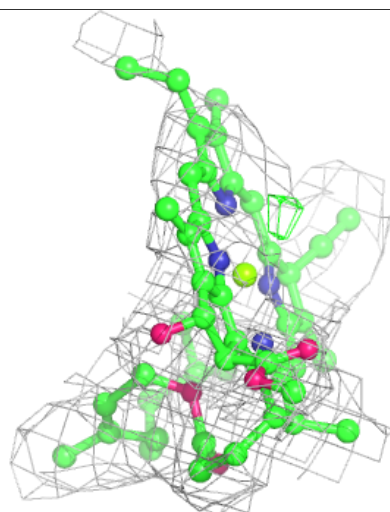
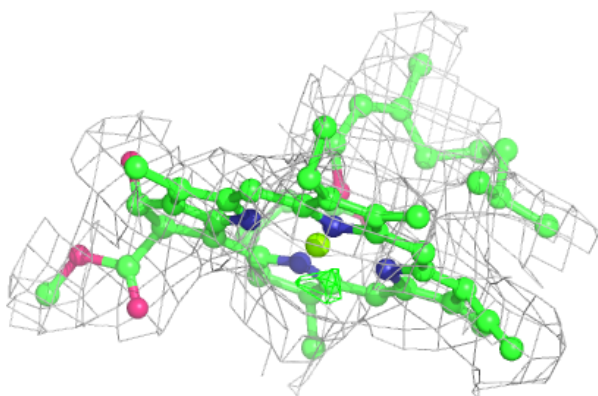
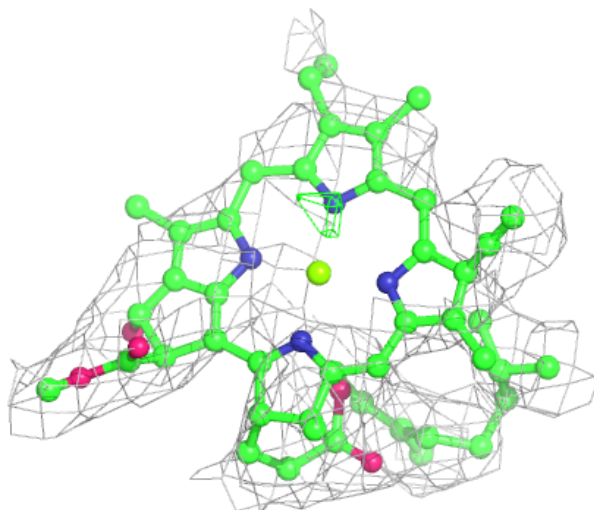
Electron density around CLA 4 4009:

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



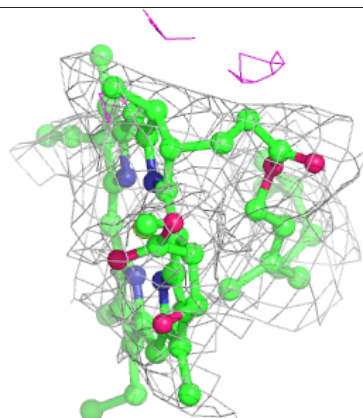
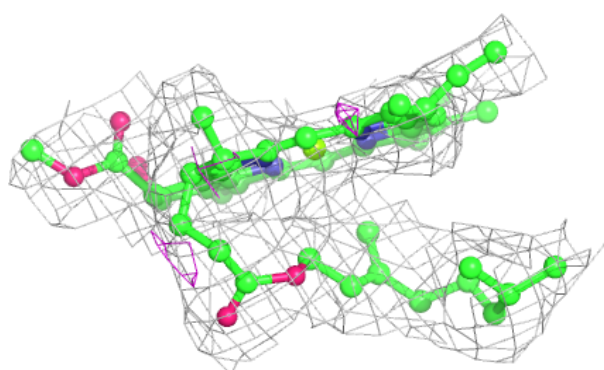
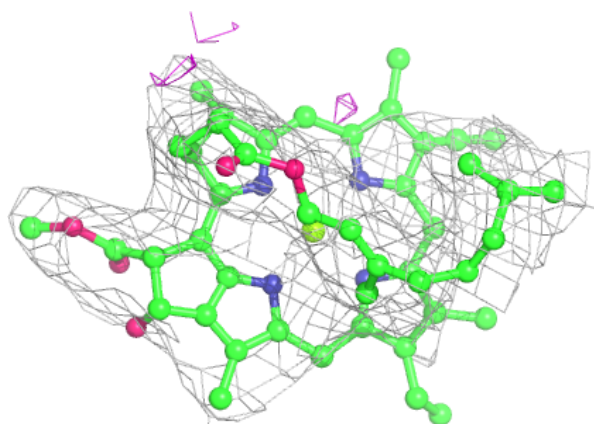
Electron density around CLA B 1209:

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

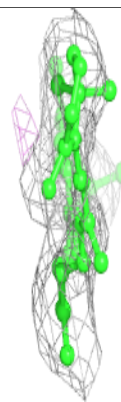
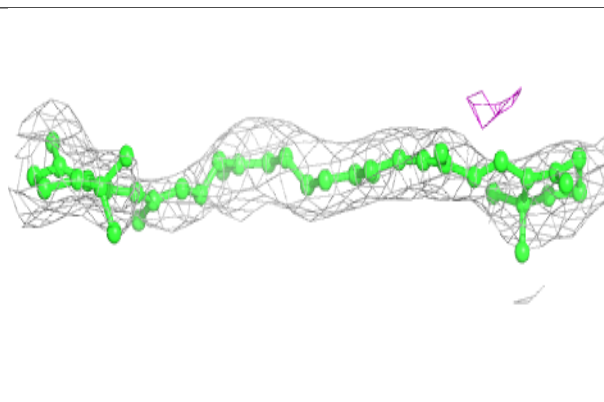
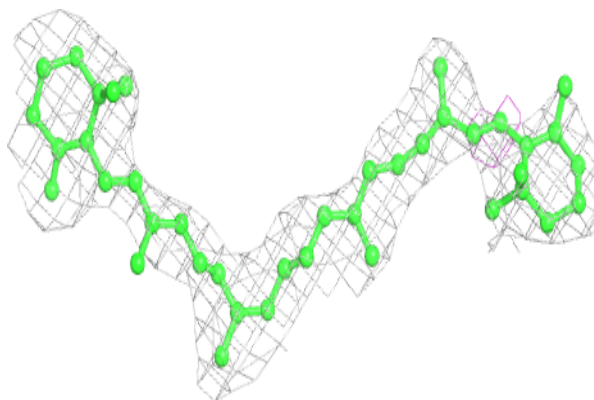


Electron density around CLA A 1140:

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

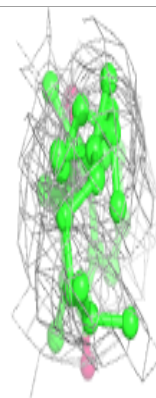
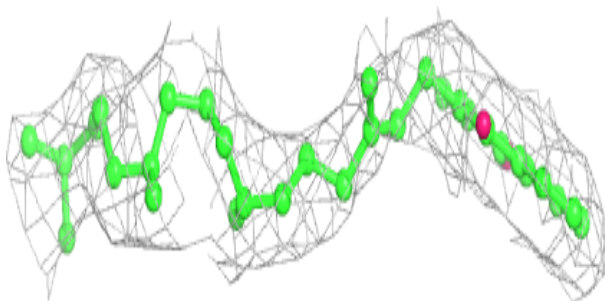
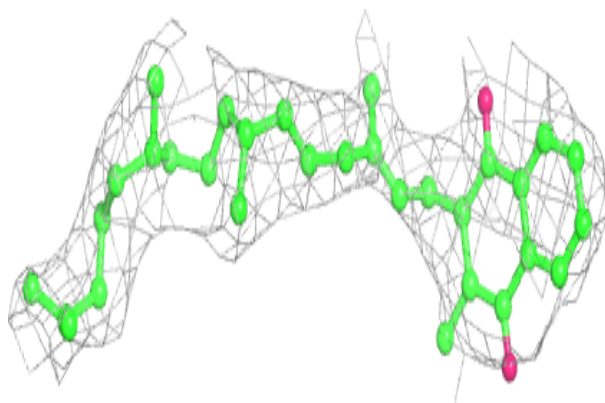
**Electron density around BCR A 6011:**

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



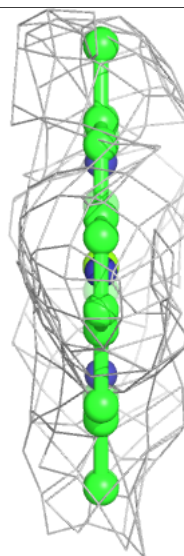
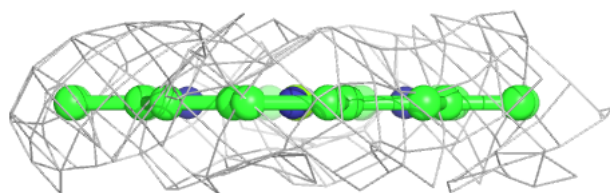
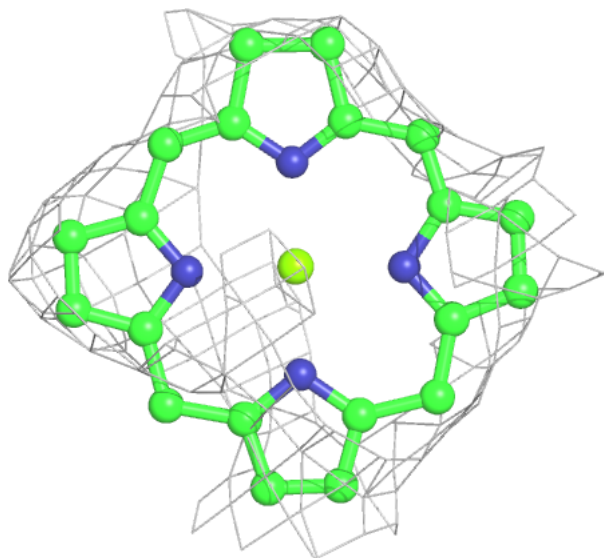
Electron density around PQN A 5001:

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



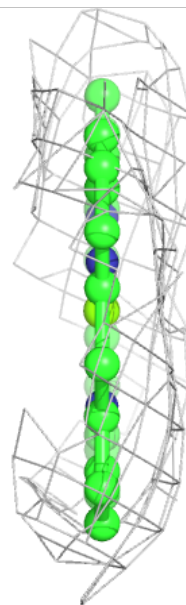
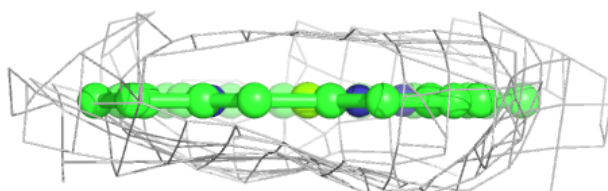
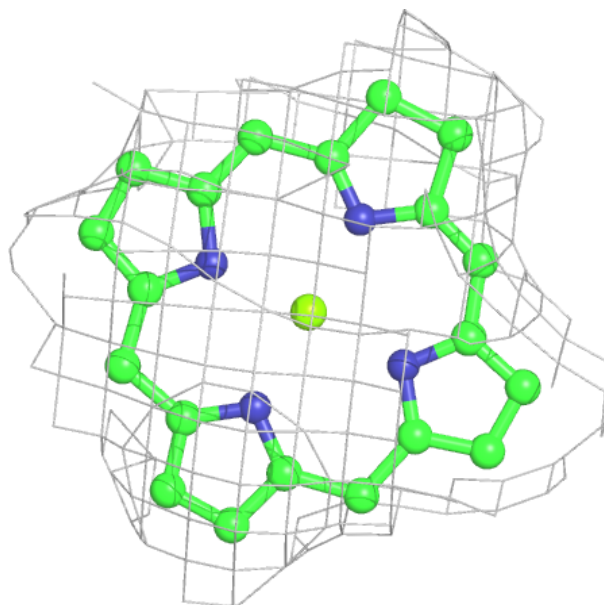
Electron density around CLA 2 2003:

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



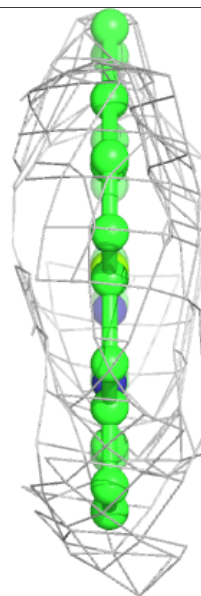
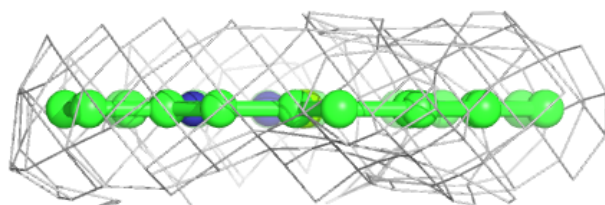
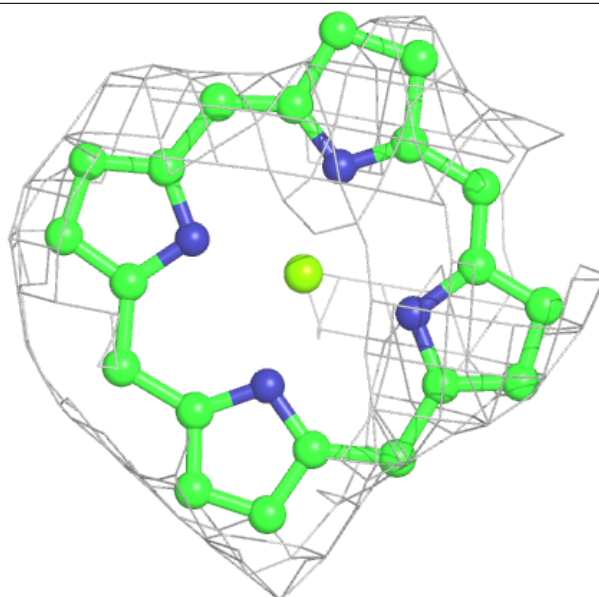
Electron density around CLA 3 3003:

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



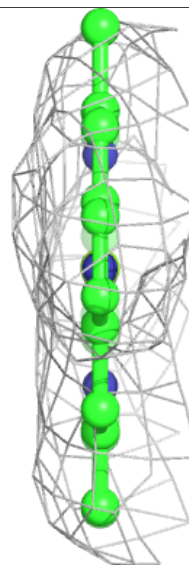
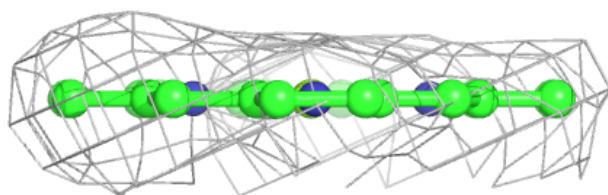
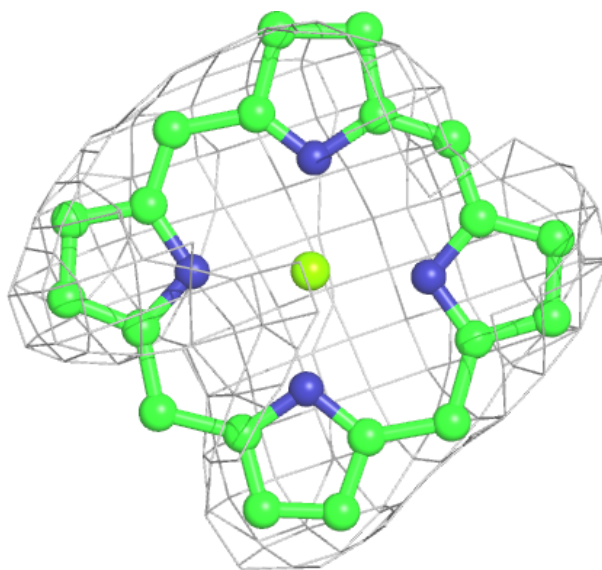
Electron density around CLA A 1102:

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



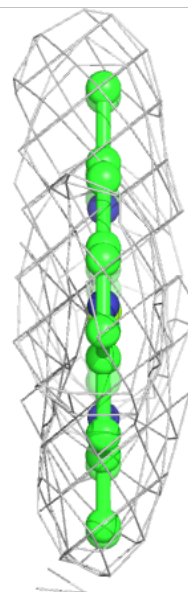
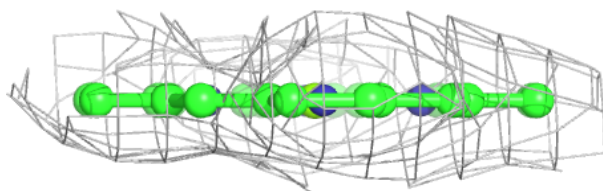
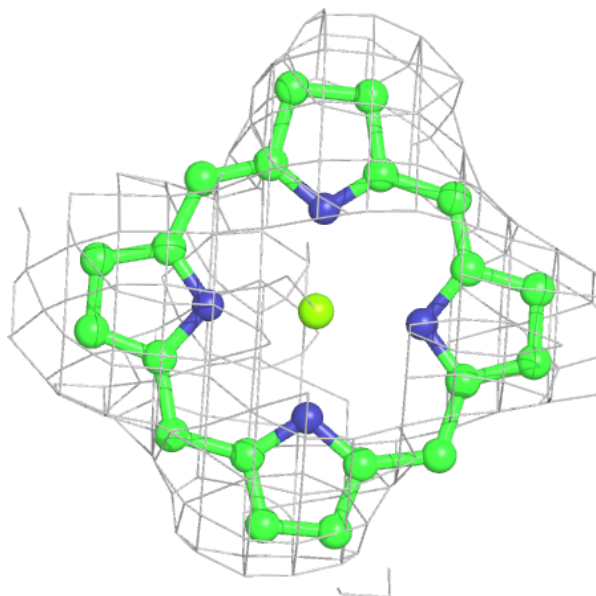
Electron density around CLA 3 3004:

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



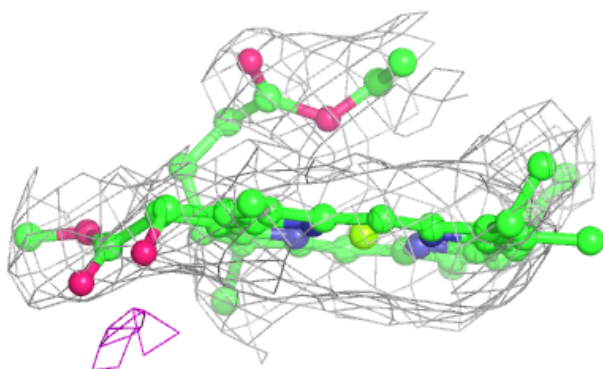
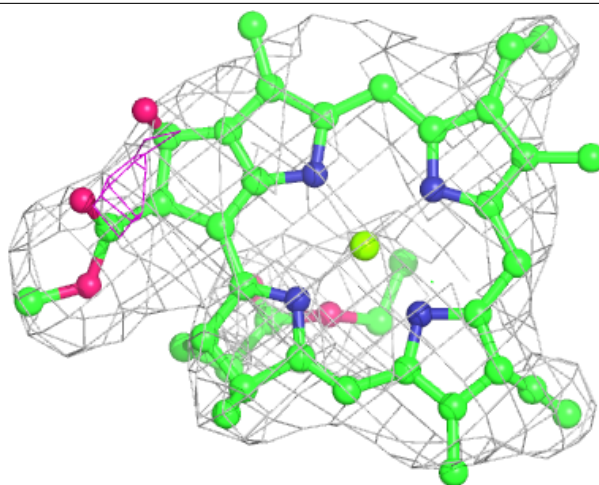
Electron density around CLA B 1223:

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



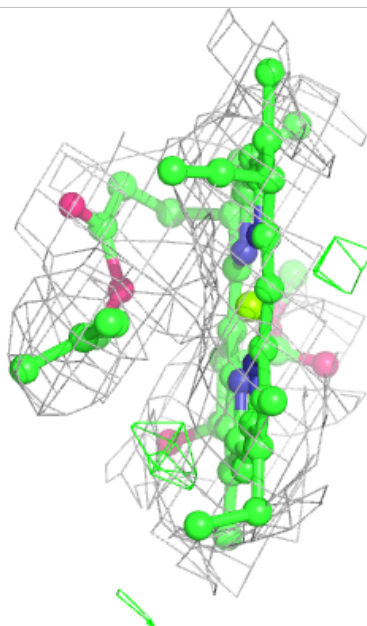
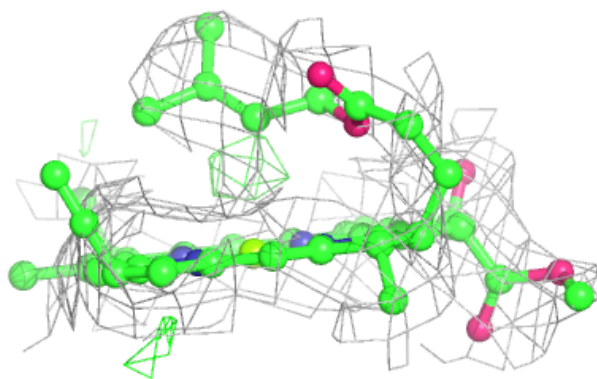
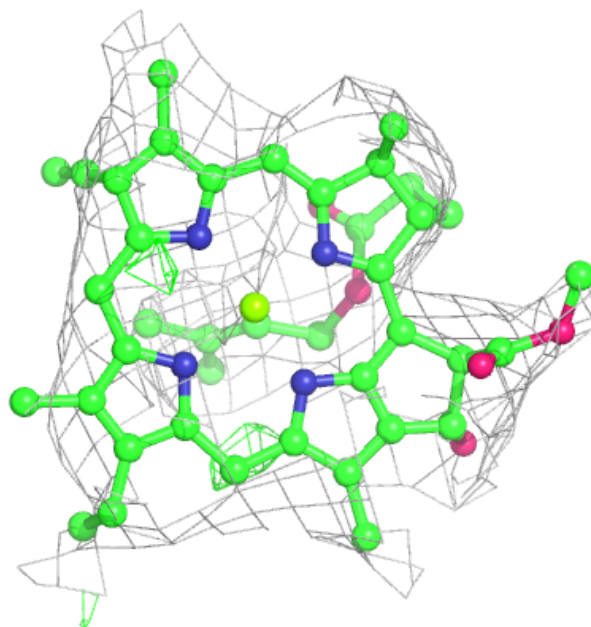
Electron density around CLA A 1115:

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



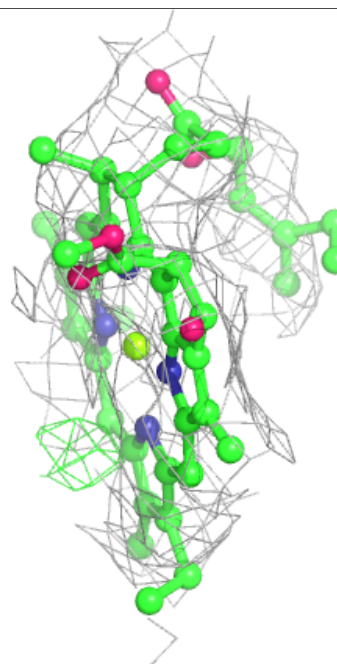
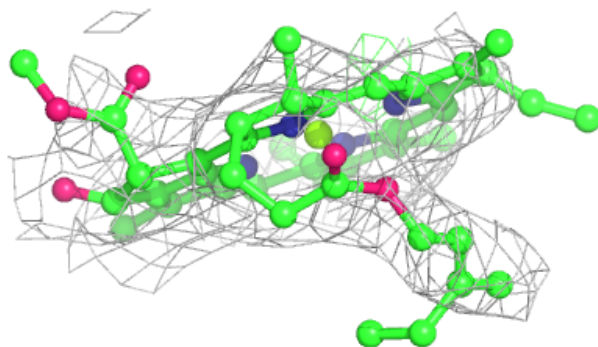
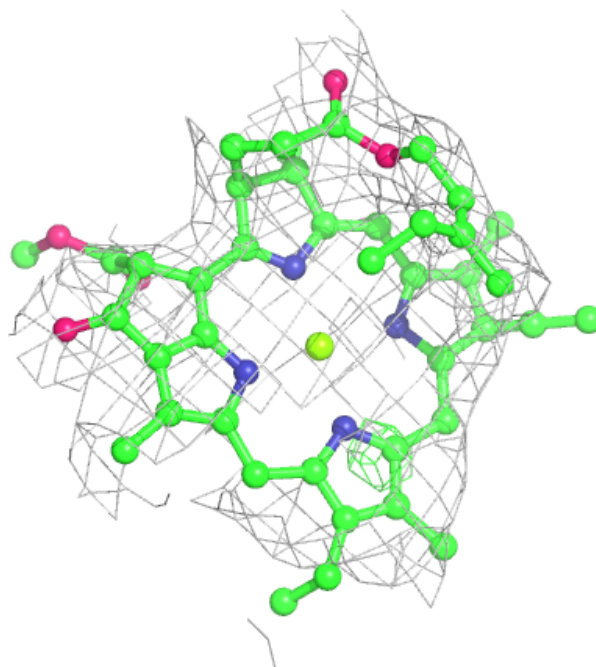
Electron density around CLA A 1108:

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



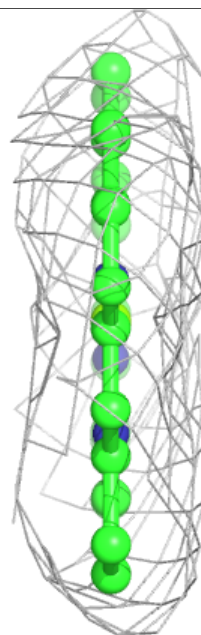
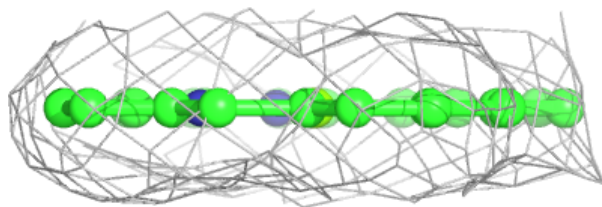
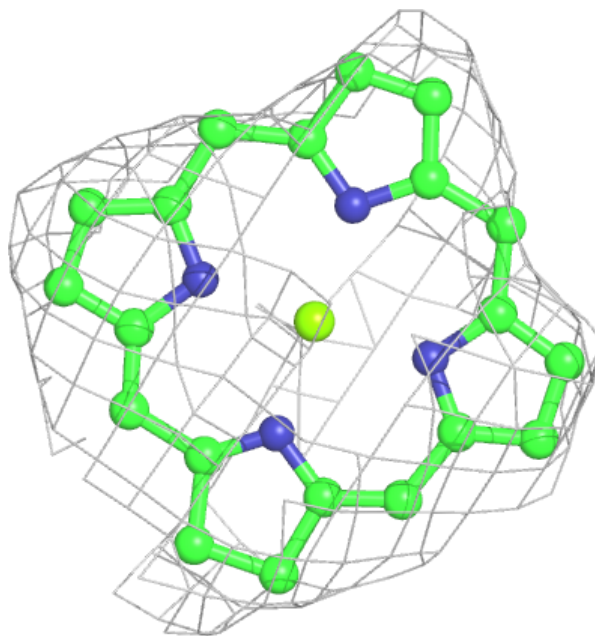
Electron density around CLA B 1224:

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



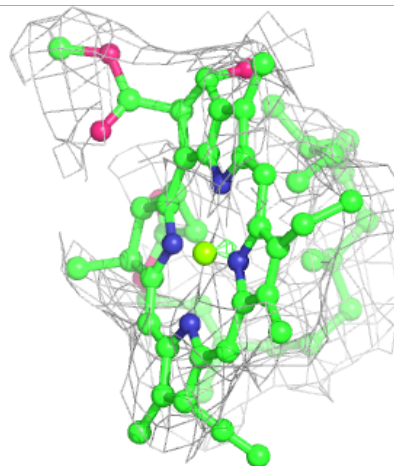
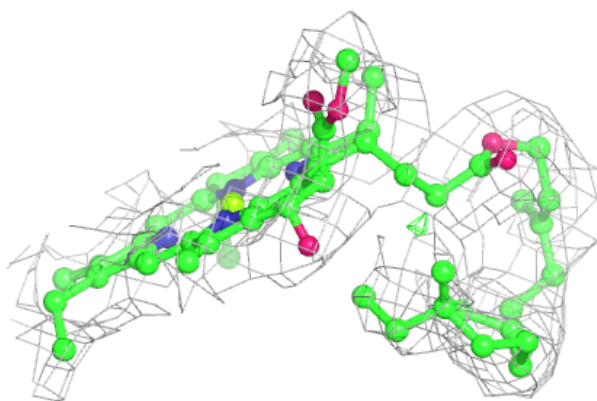
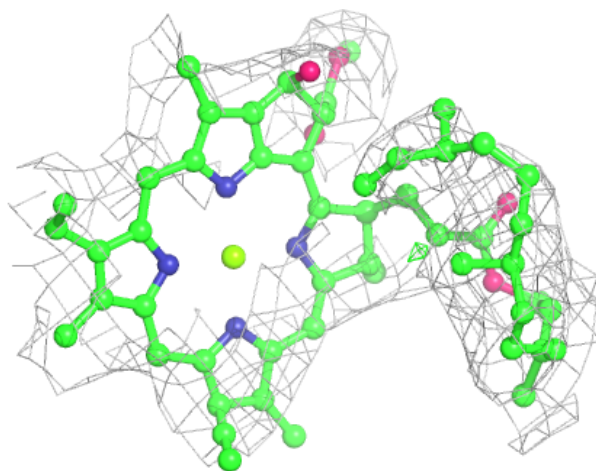
Electron density around CLA 2 2013:

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



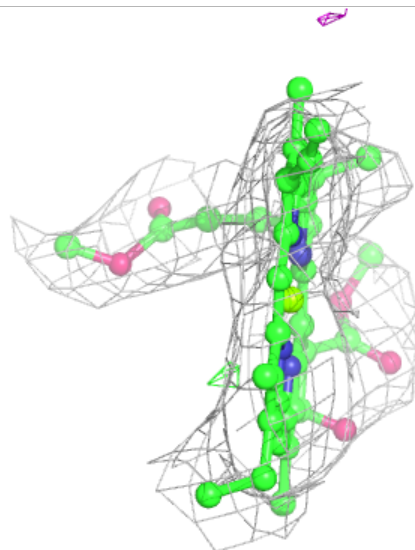
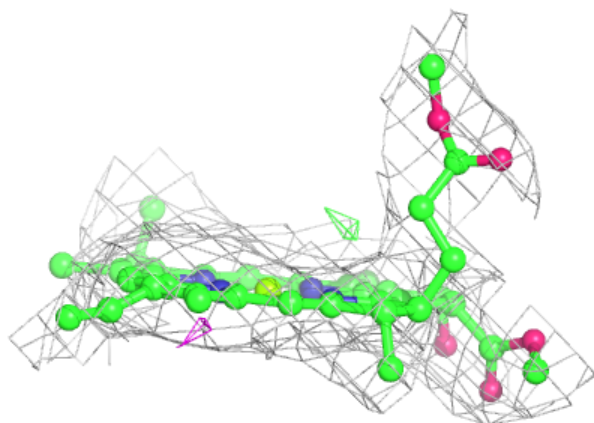
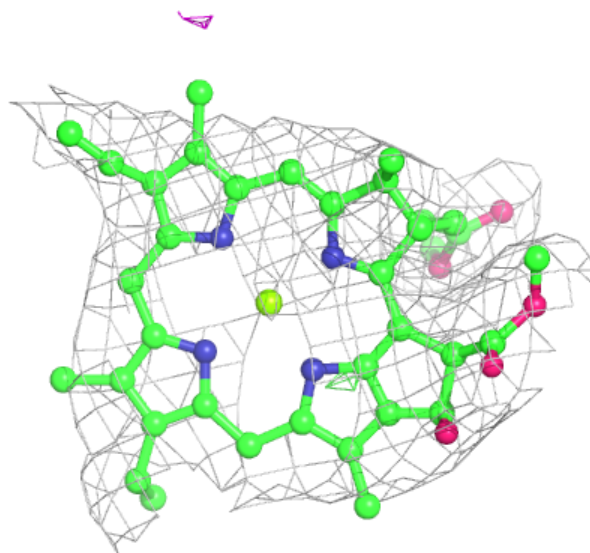
Electron density around CLA J 2107:

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



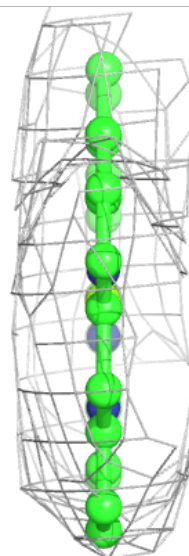
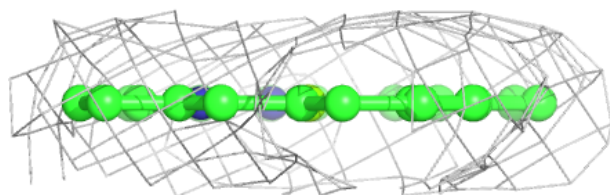
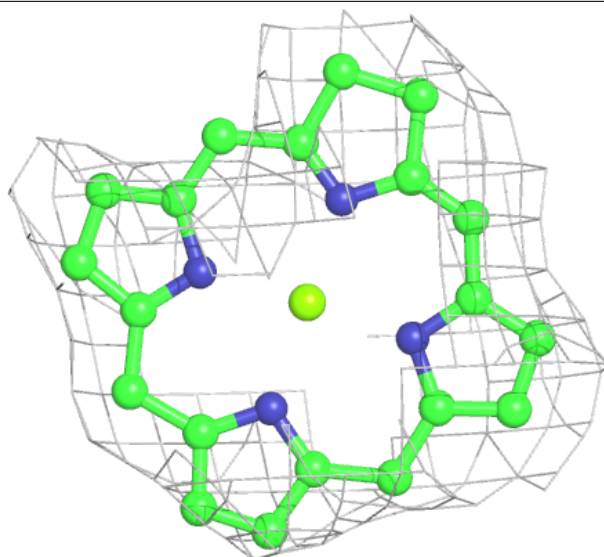
Electron density around CLA B 1236:

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



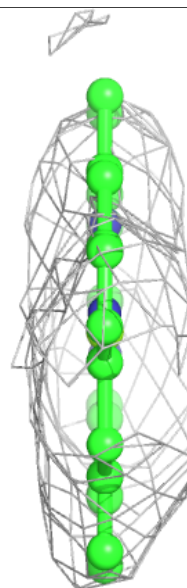
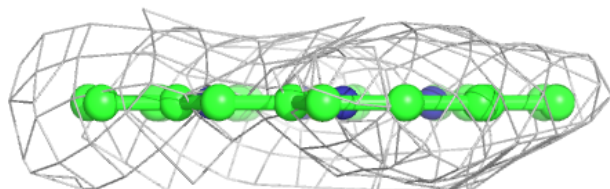
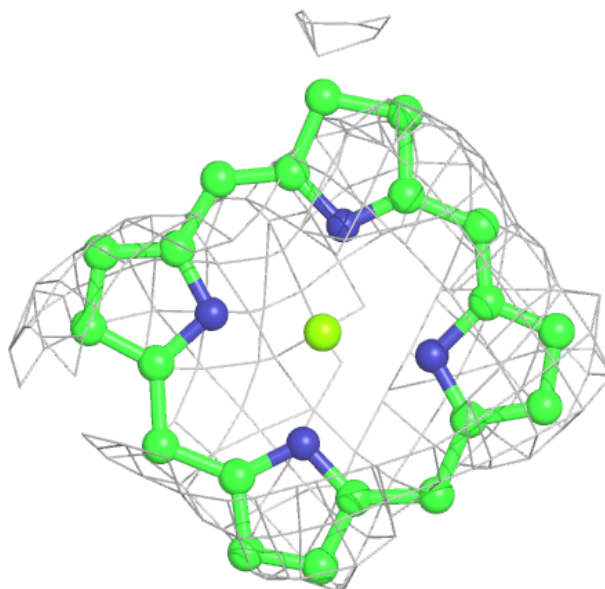
Electron density around CLA 4 4002:

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



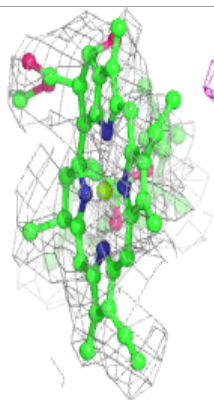
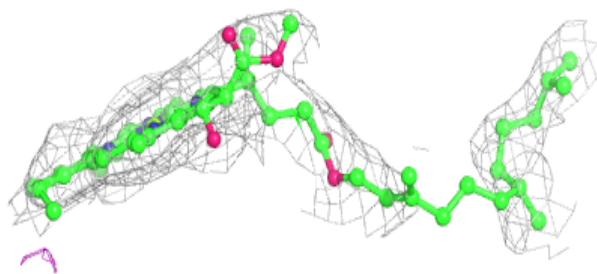
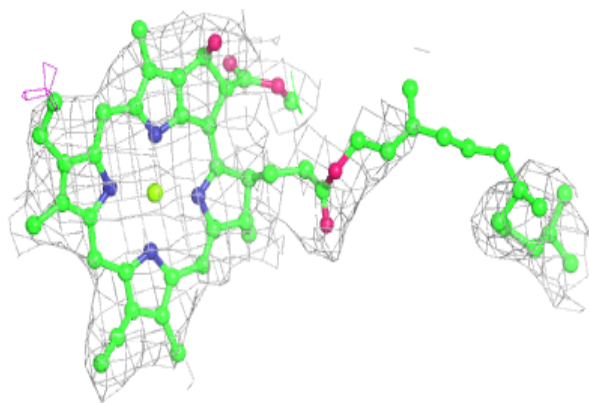
Electron density around CLA 1 1012:

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



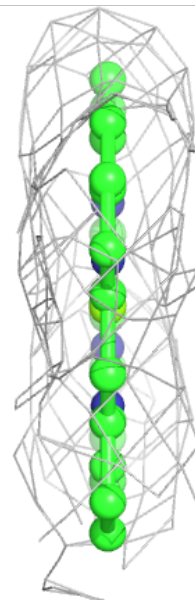
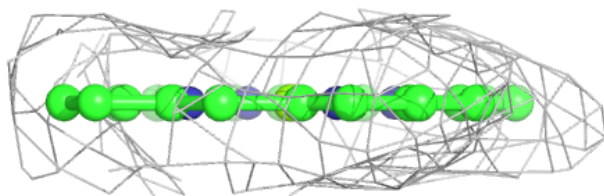
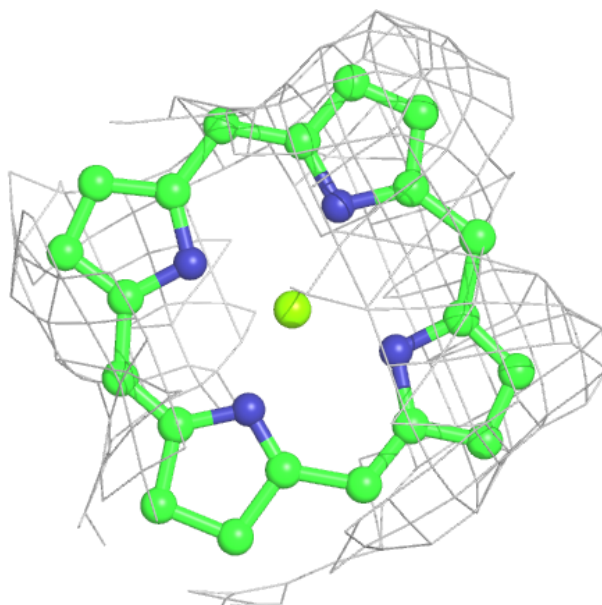
Electron density around CLA B 1220:

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



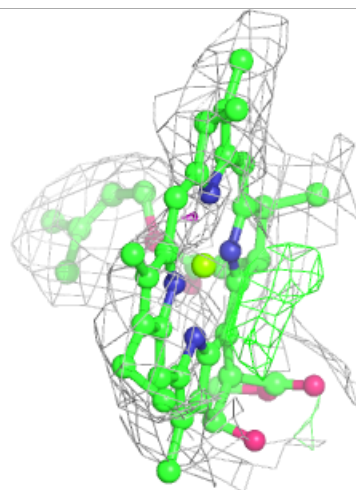
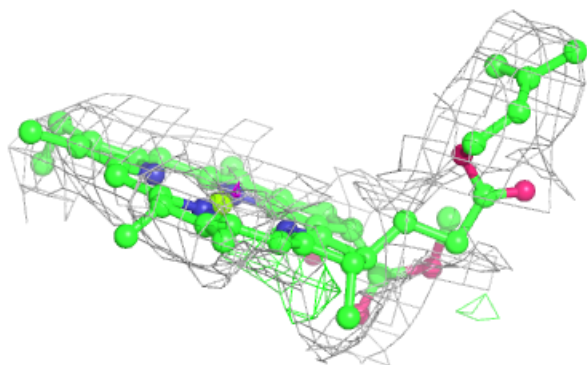
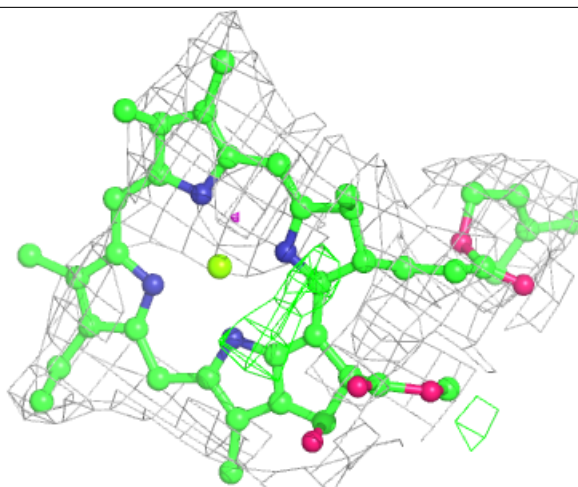
Electron density around CLA 3 3015:

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



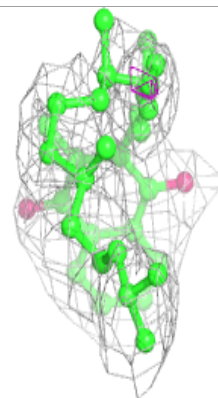
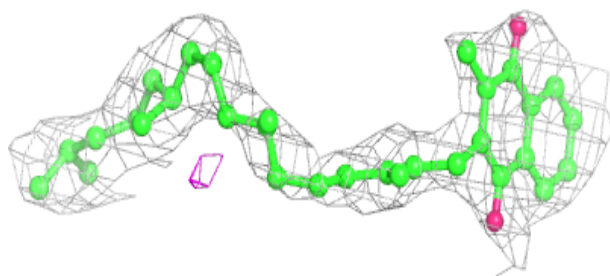
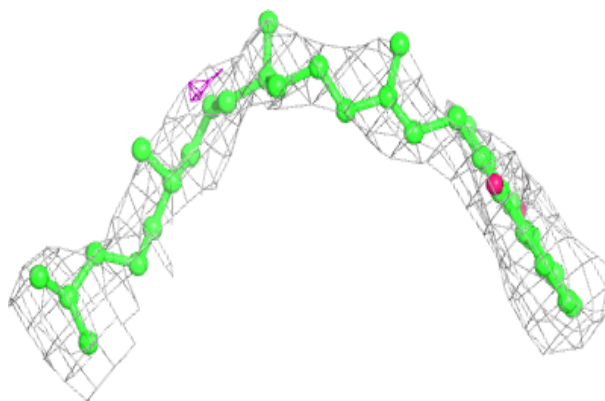
Electron density around CLA B 1229:

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



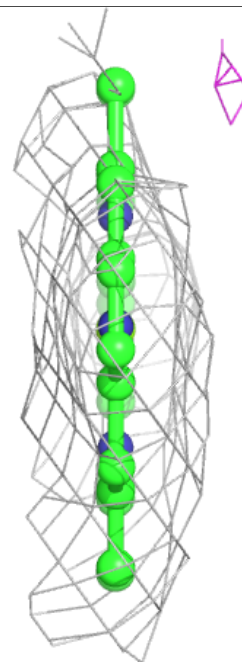
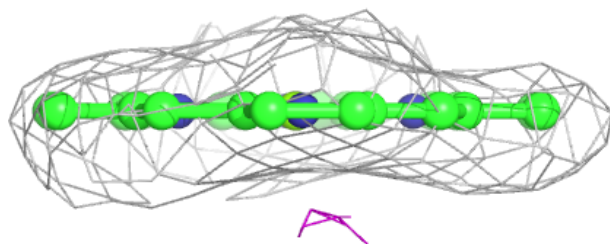
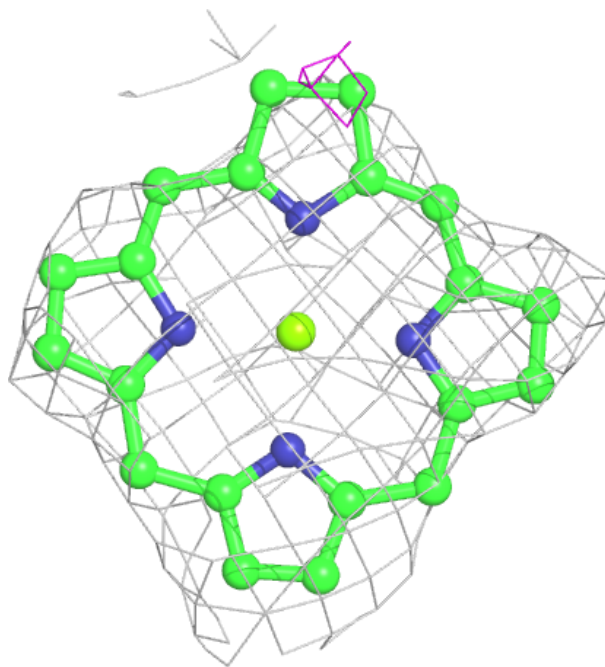
Electron density around PQN B 5002:

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



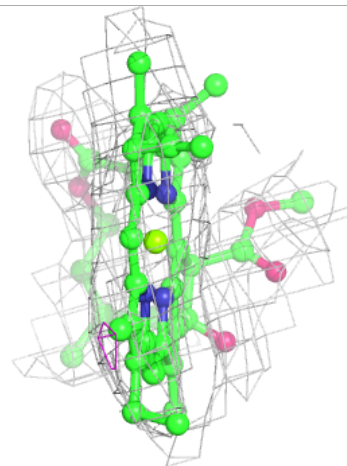
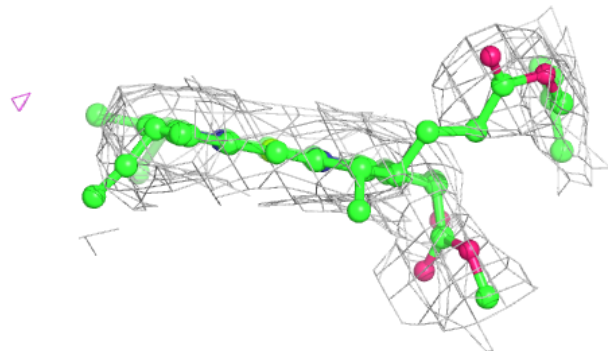
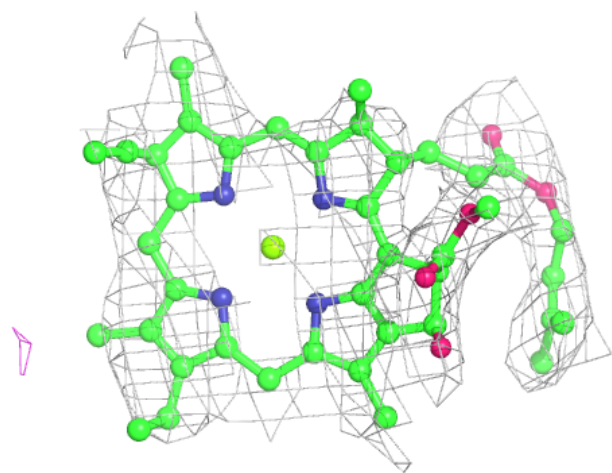
Electron density around CLA 3 3013:

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



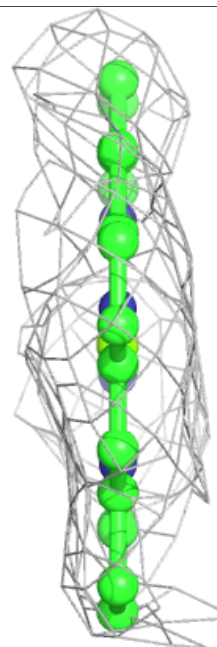
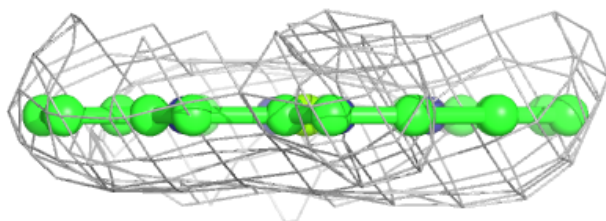
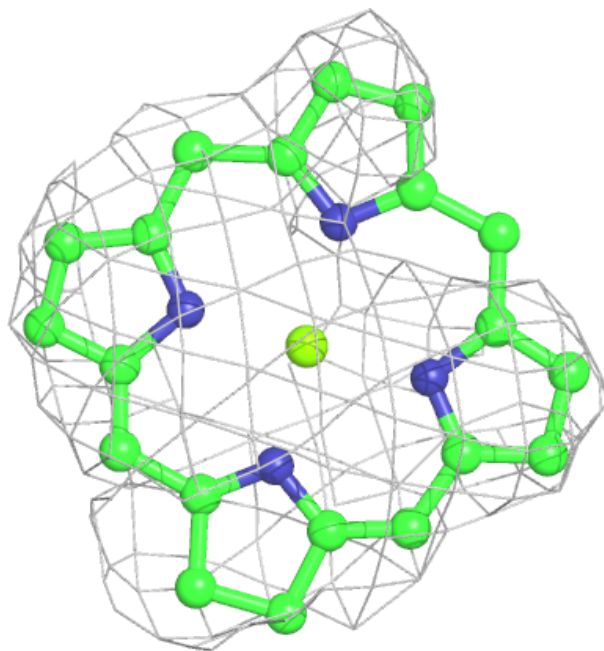
Electron density around CLA B 1202:

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



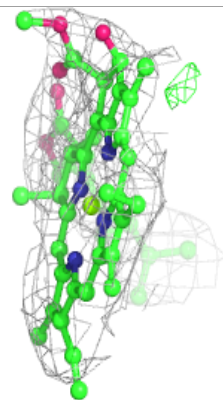
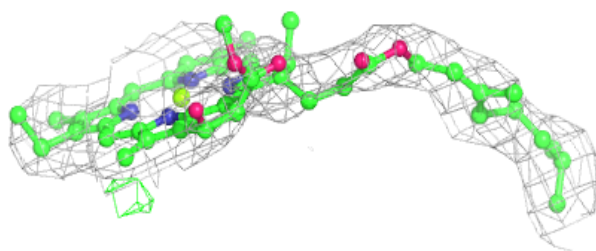
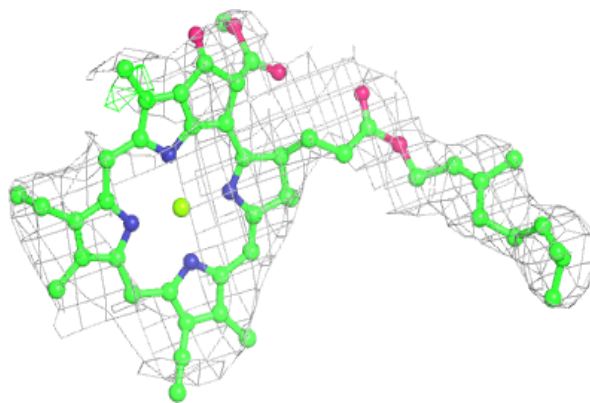
Electron density around CLA 4 4003:

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



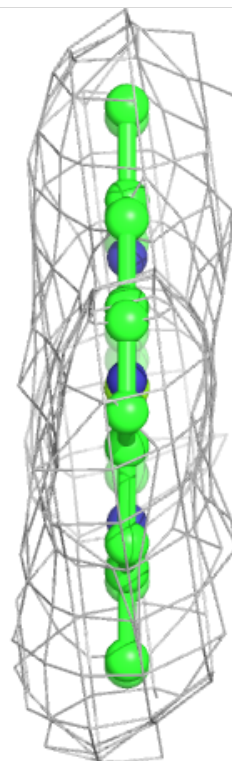
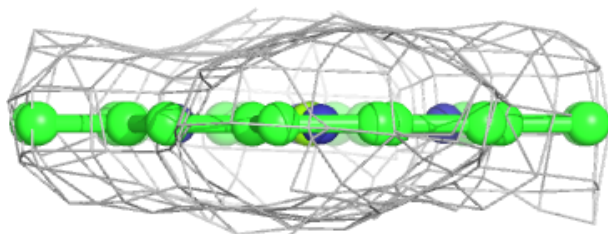
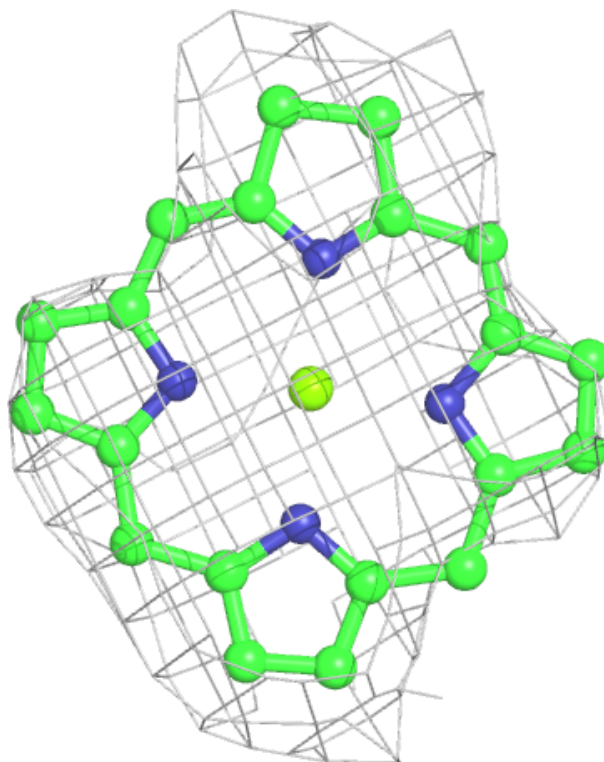
Electron density around CLA B 9012:

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



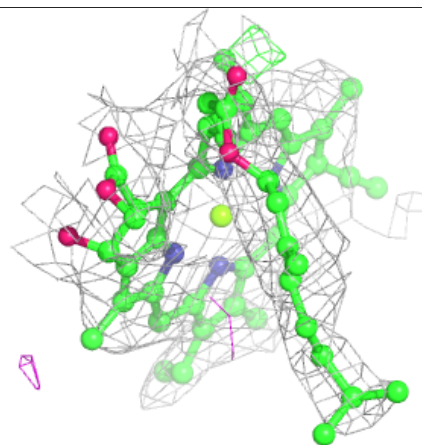
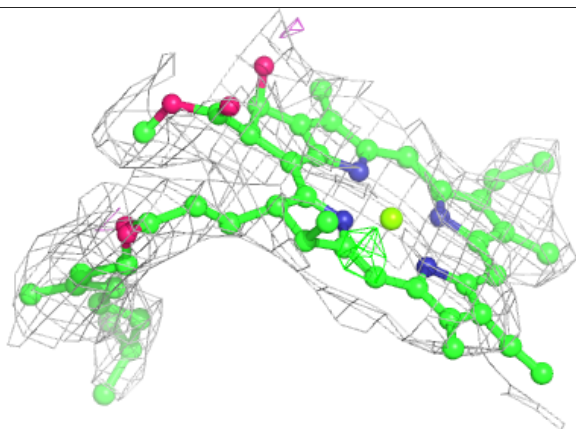
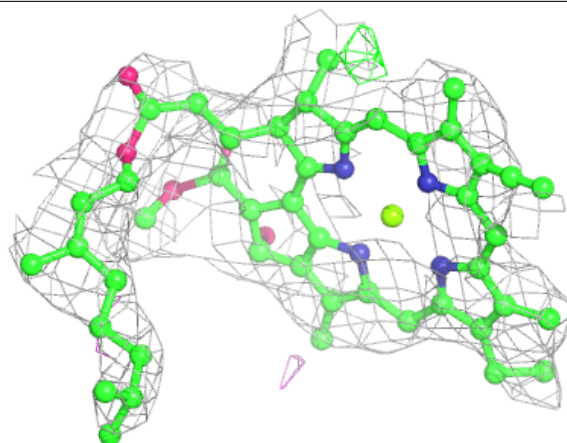
Electron density around CLA 4 4011:

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



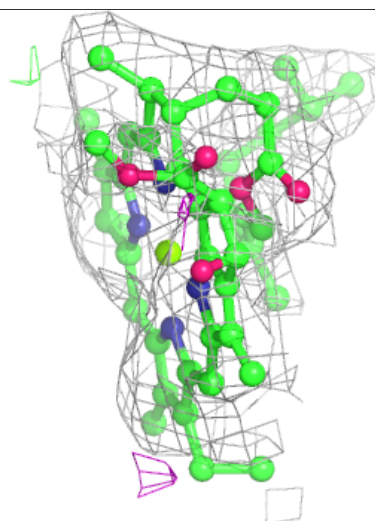
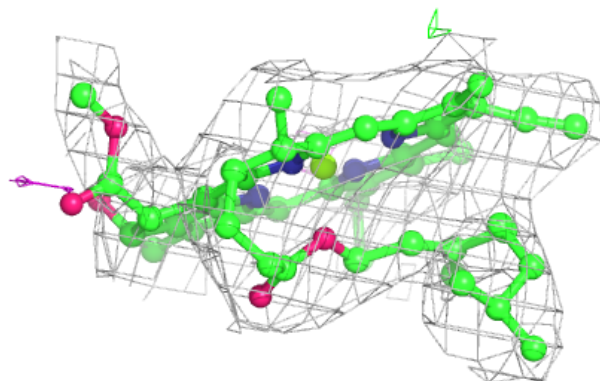
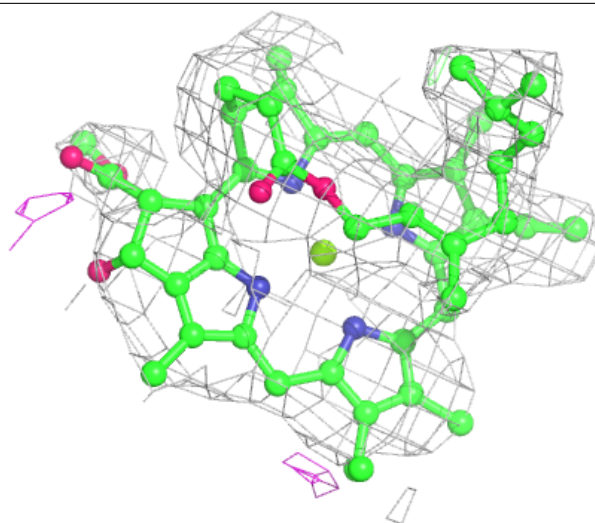
Electron density around CLA A 9011:

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



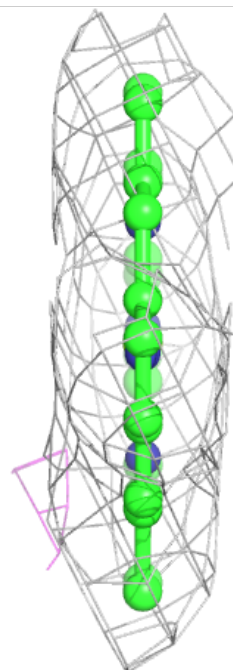
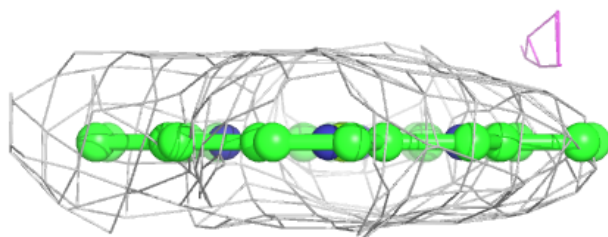
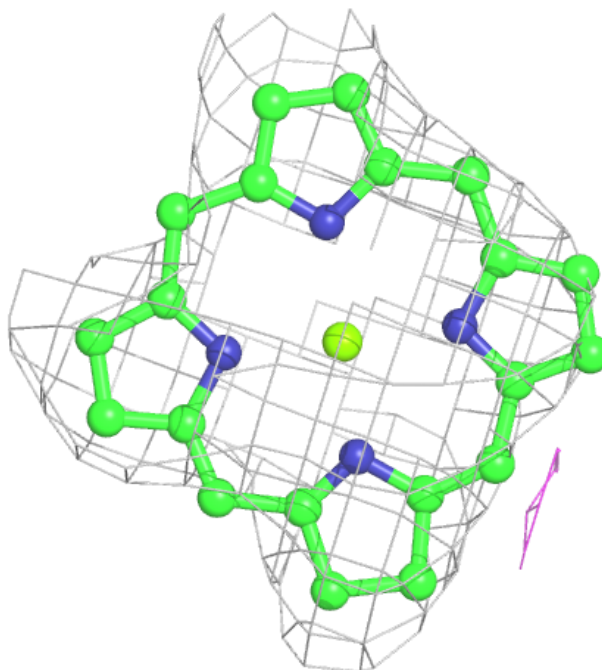
Electron density around CLA B 1205:

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



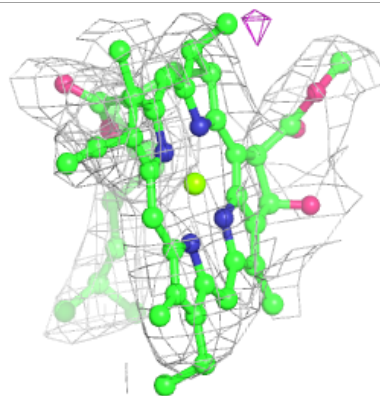
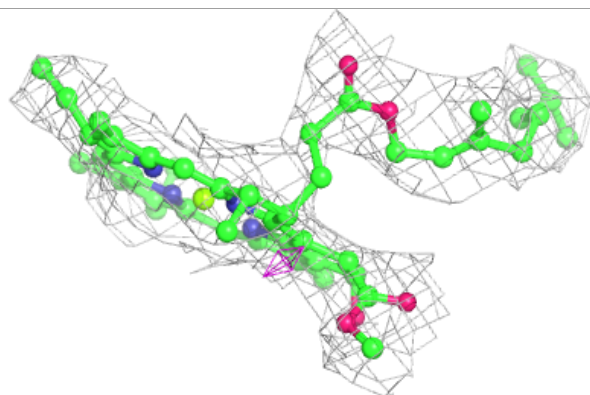
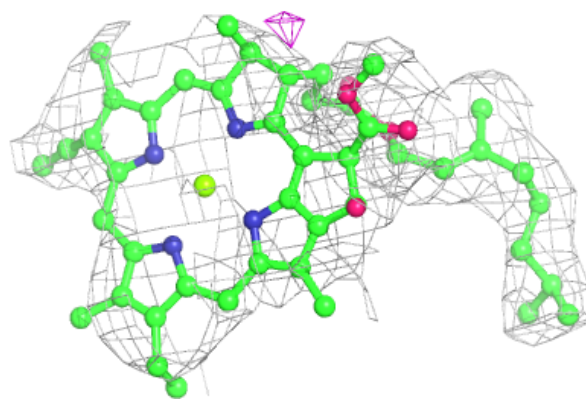
Electron density around CLA 1 1001:

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



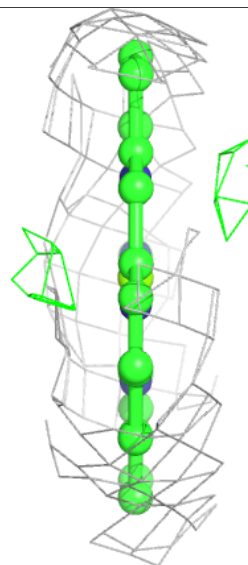
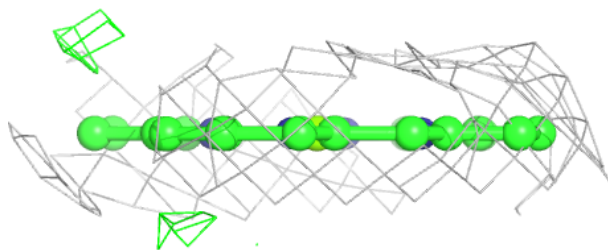
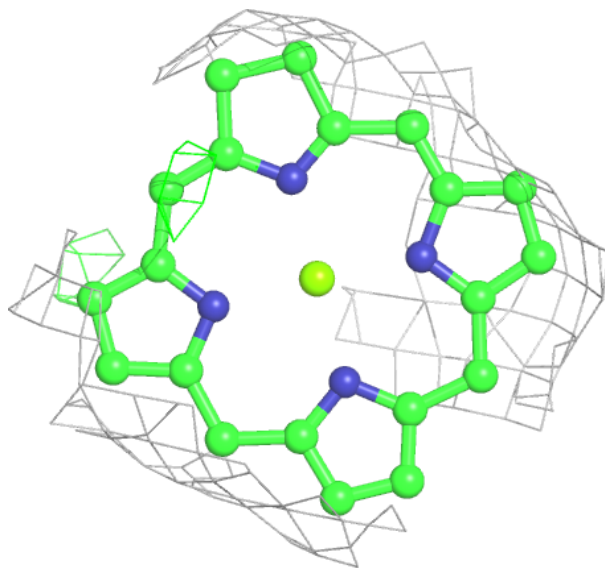
Electron density around CLA B 1228:

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



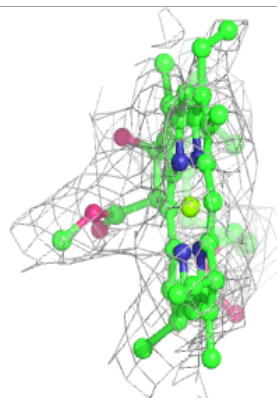
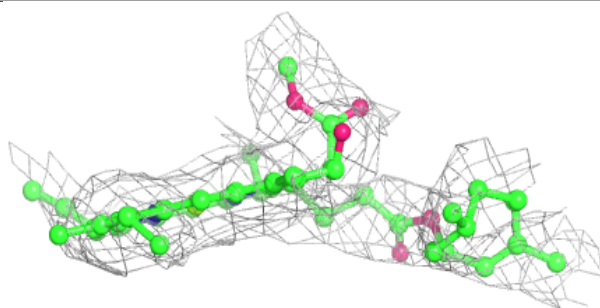
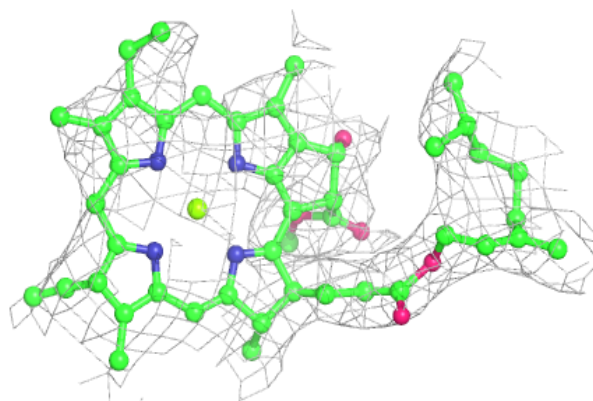
Electron density around CLA A 1147:

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

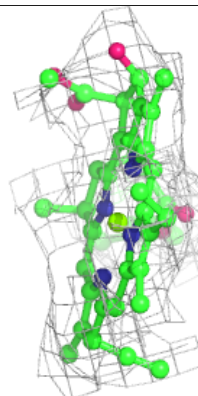
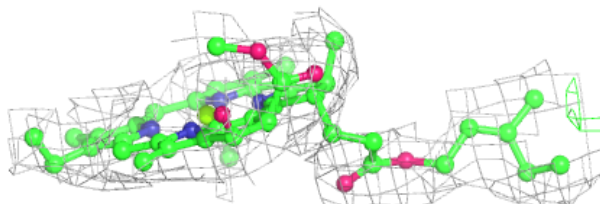
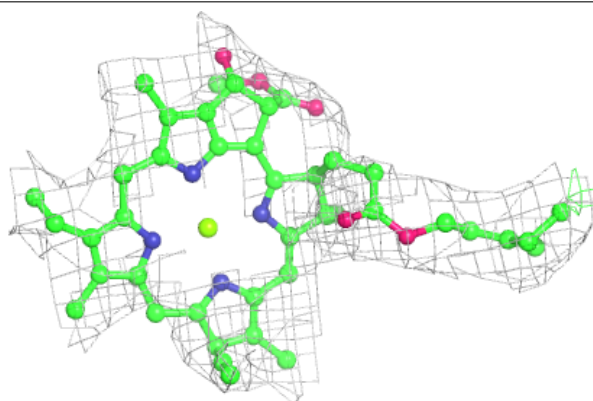


Electron density around CLA A 1123:

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

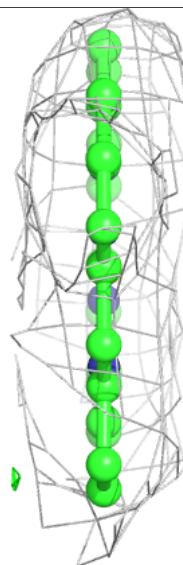
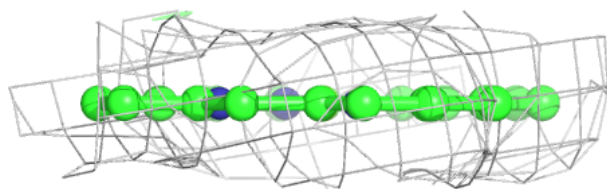
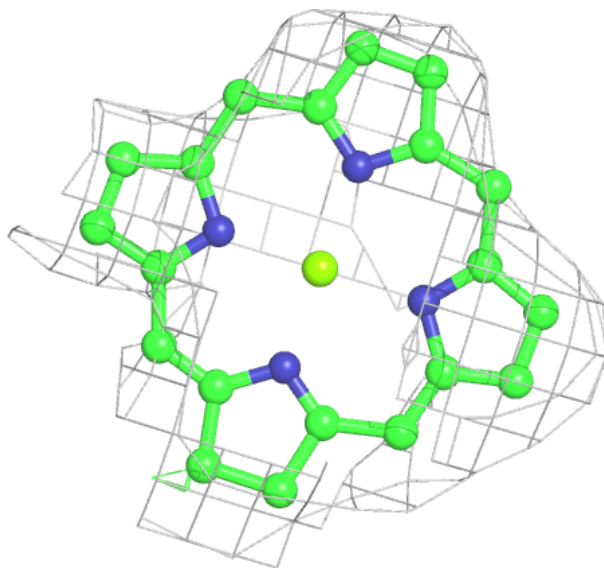
**Electron density around CLA B 1218:**

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



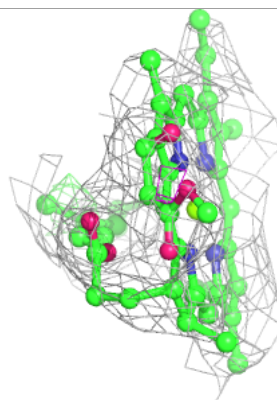
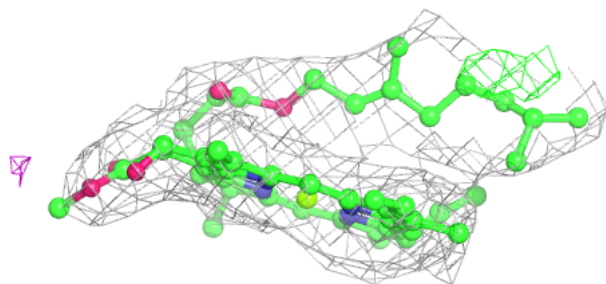
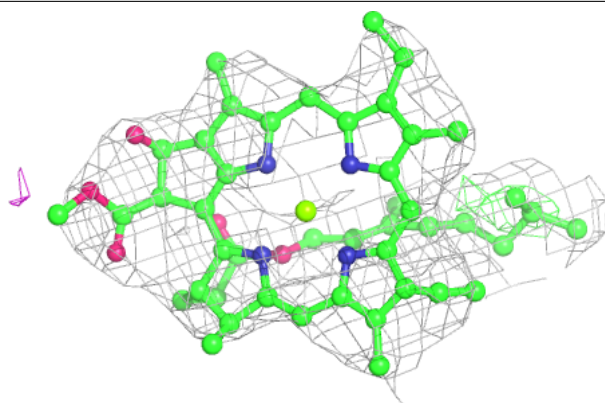
Electron density around CLA 1 1006:

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



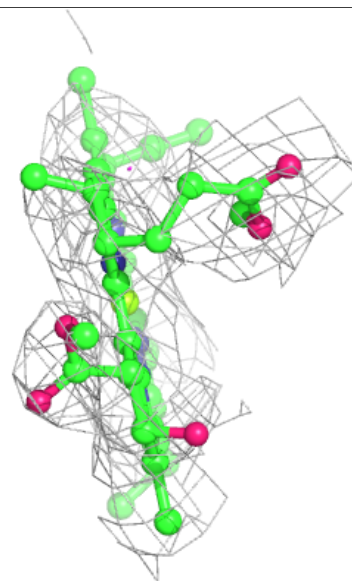
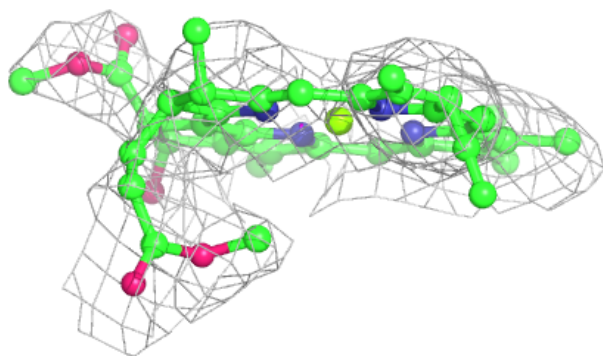
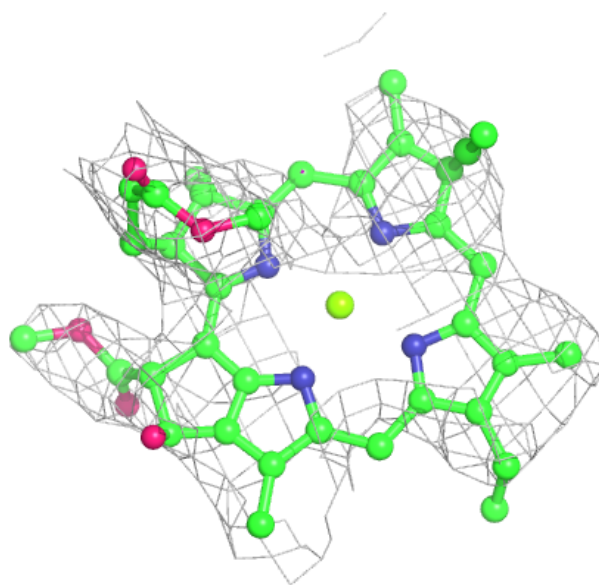
Electron density around CLA B 1235:

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



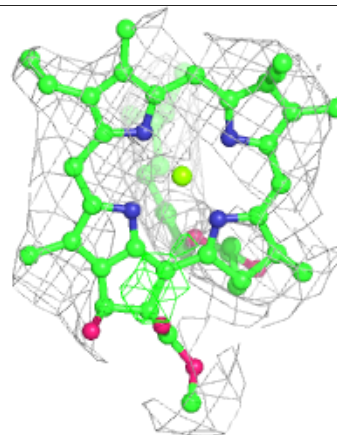
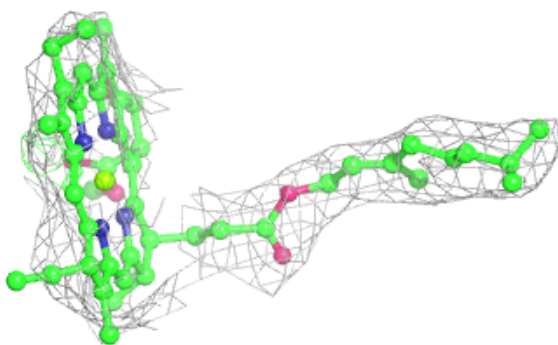
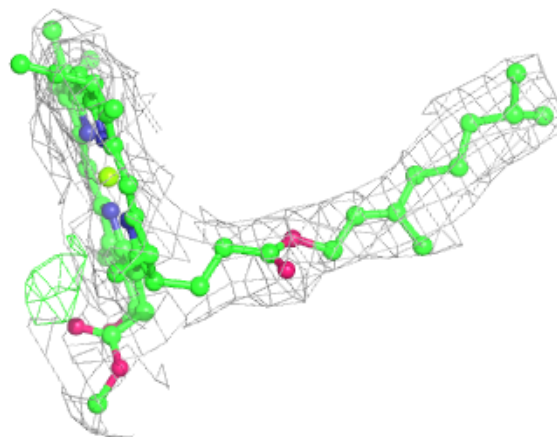
Electron density around CLA B 1231:

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



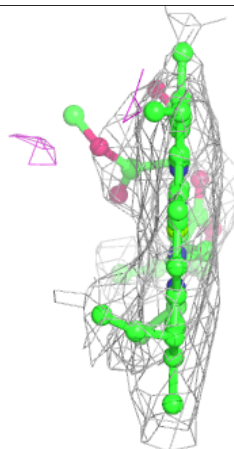
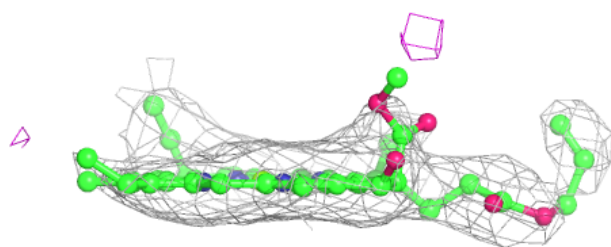
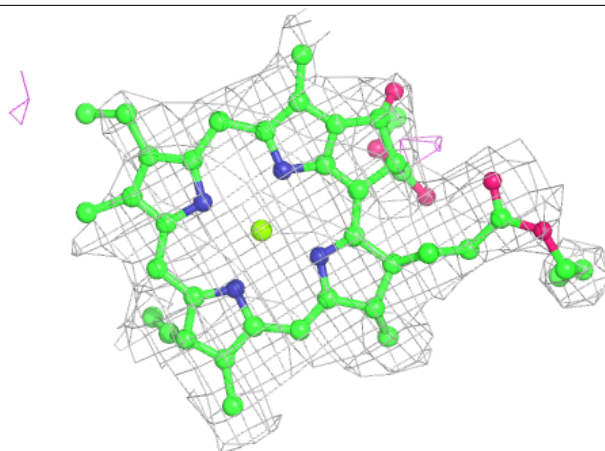
Electron density around CLA B 1239:

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



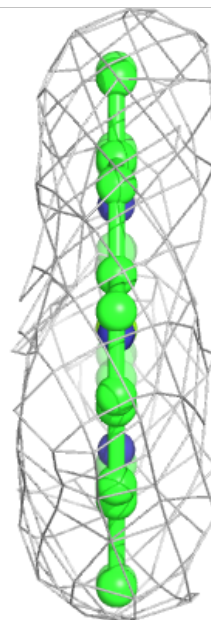
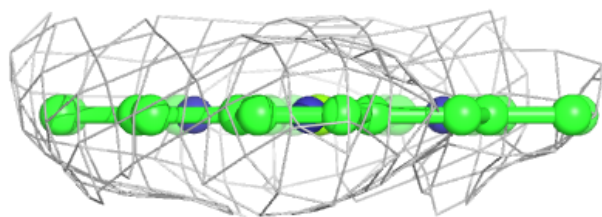
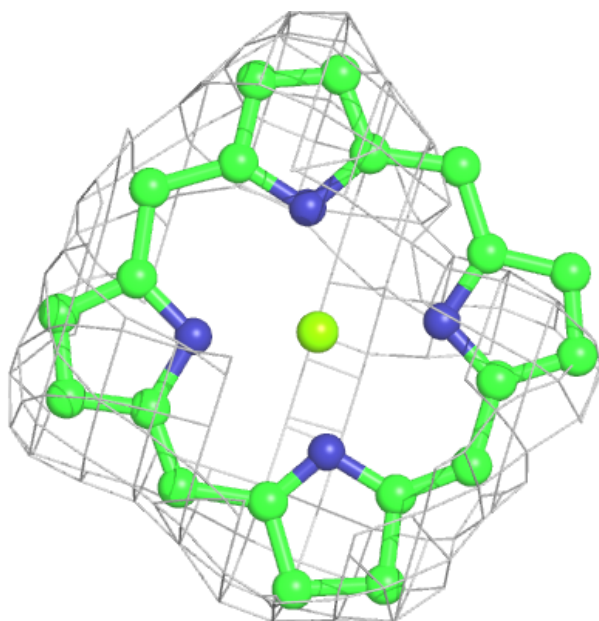
Electron density around CLA B 1221:

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



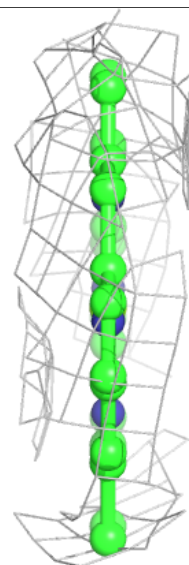
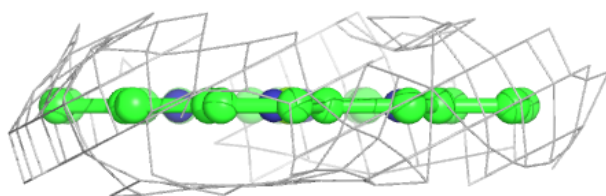
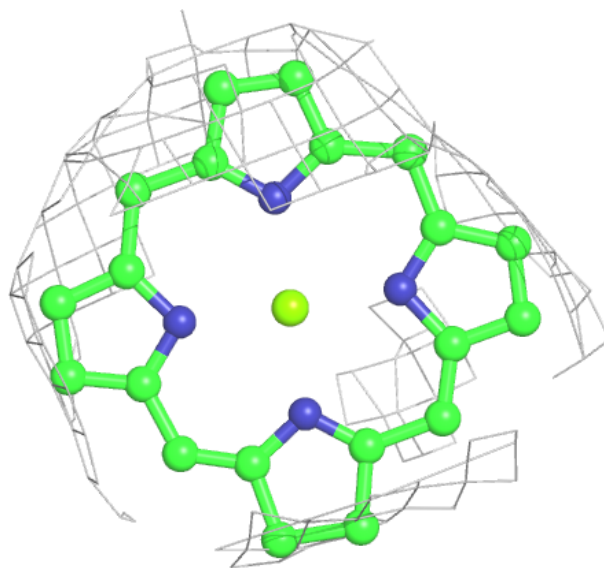
Electron density around CLA A 1105:

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



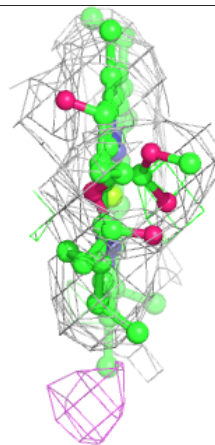
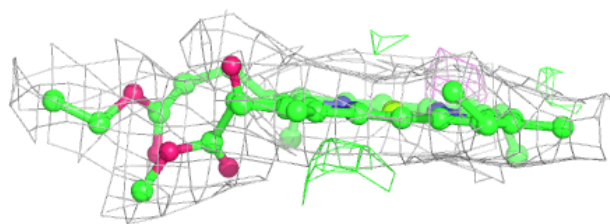
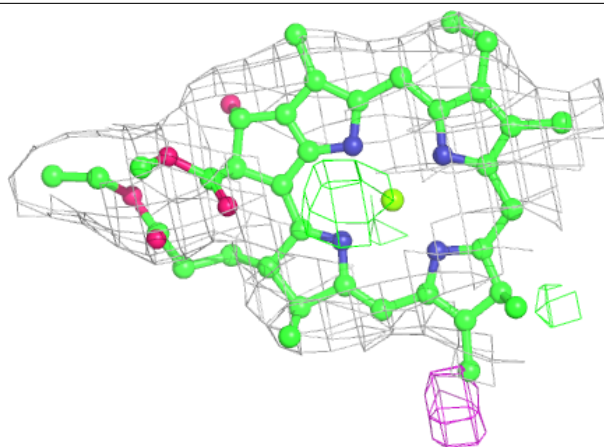
Electron density around CLA 3 3008:

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



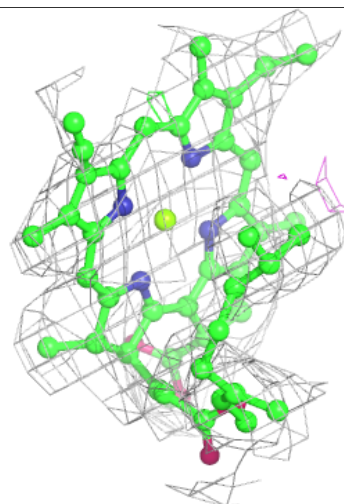
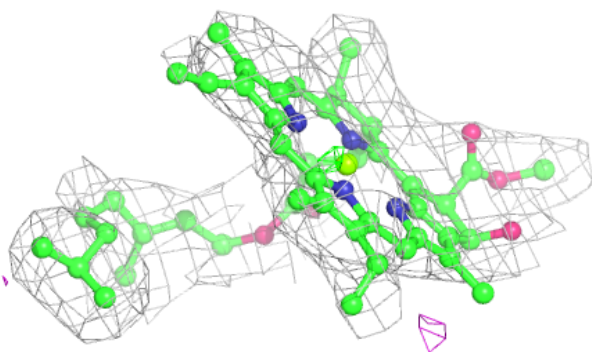
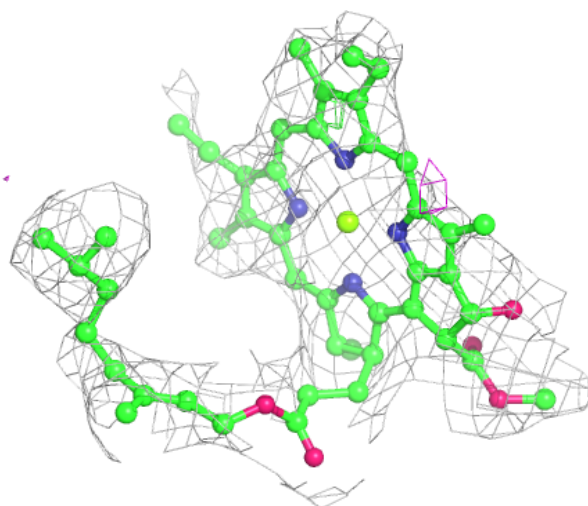
Electron density around CLA L 1503:

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



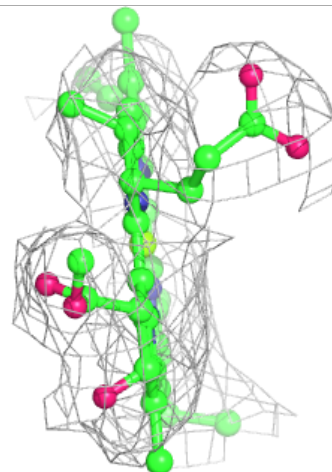
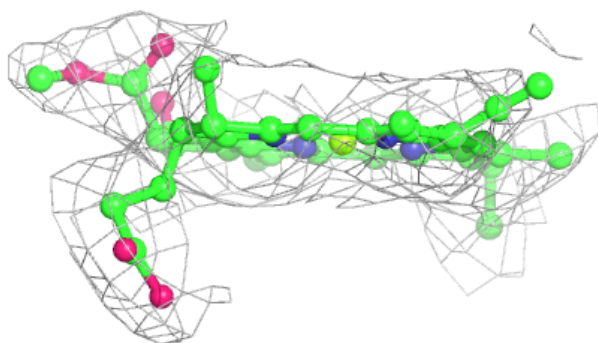
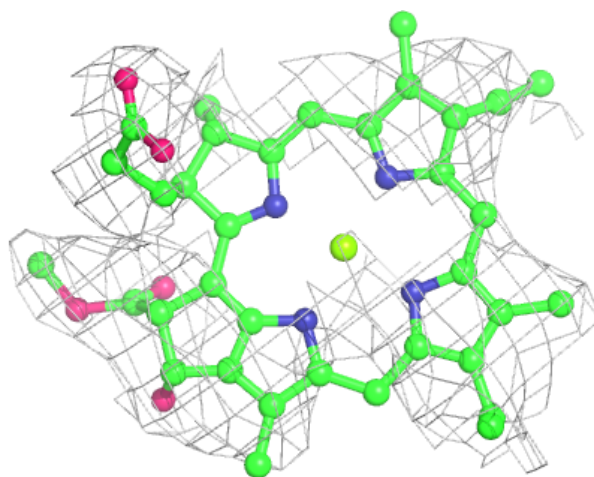
Electron density around CLA A 1122:

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



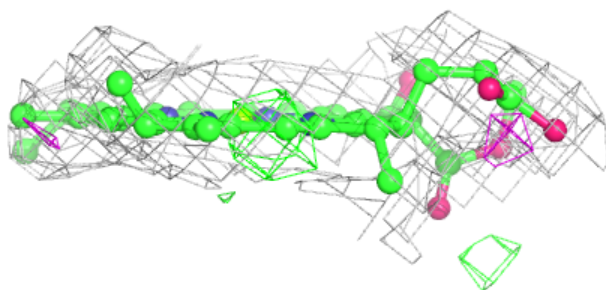
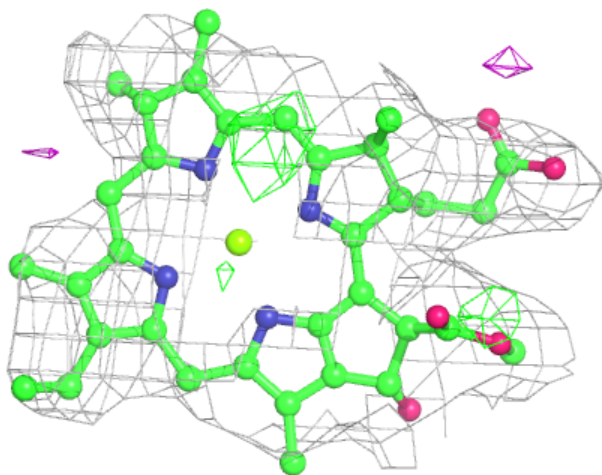
Electron density around CLA B 1225:

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



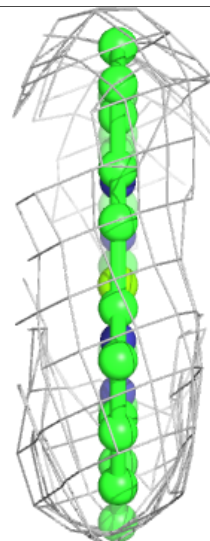
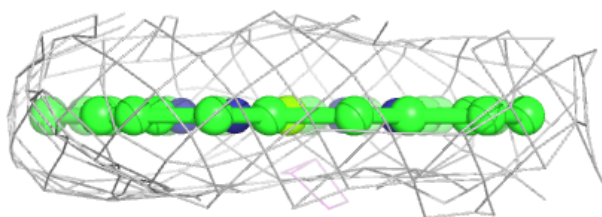
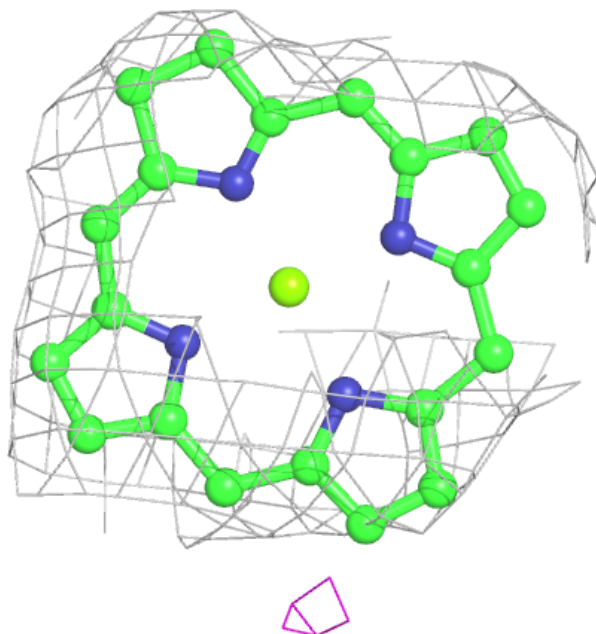
Electron density around CLA A 1131:

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



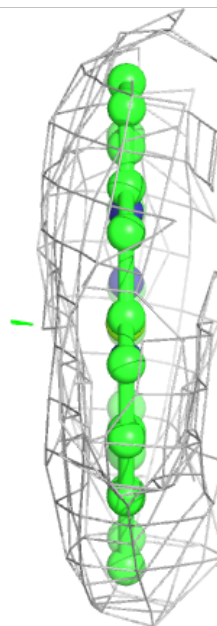
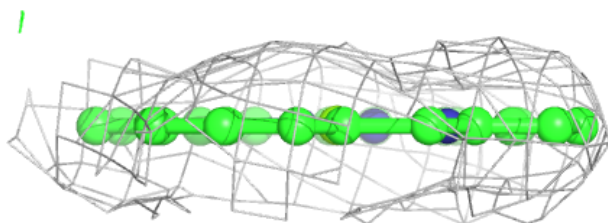
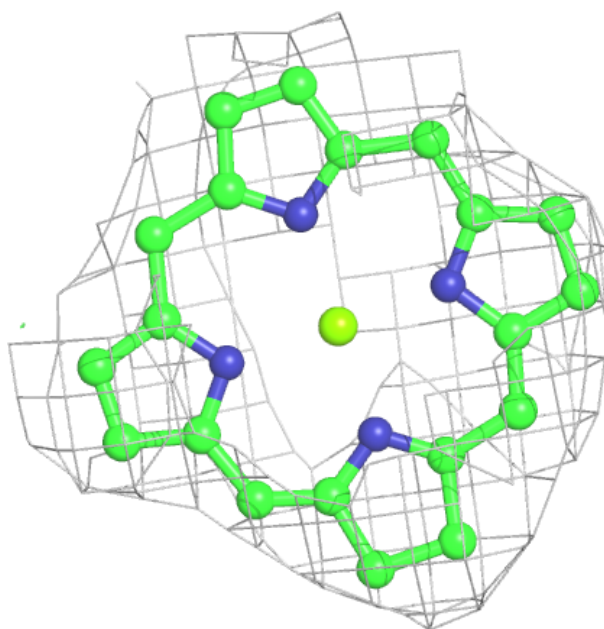
Electron density around CLA 1 1008:

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



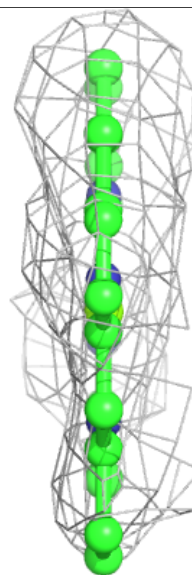
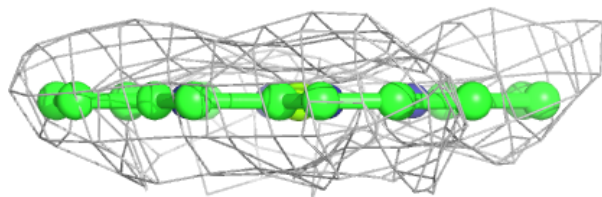
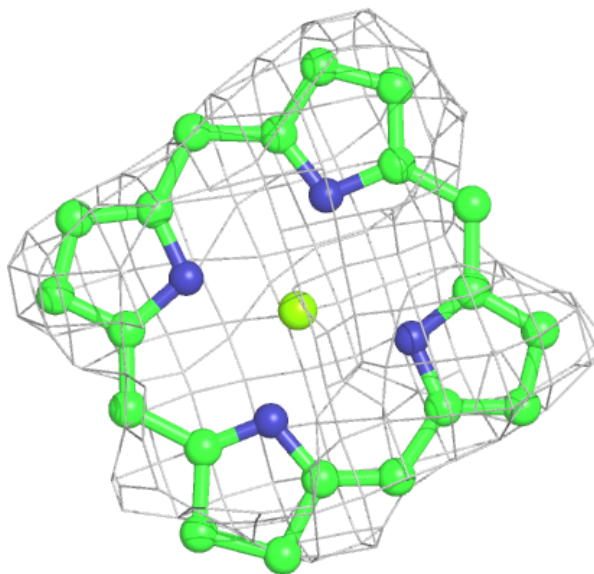
Electron density around CLA B 1226:

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



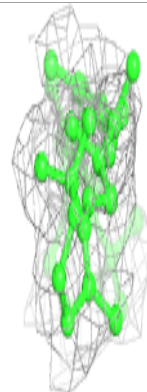
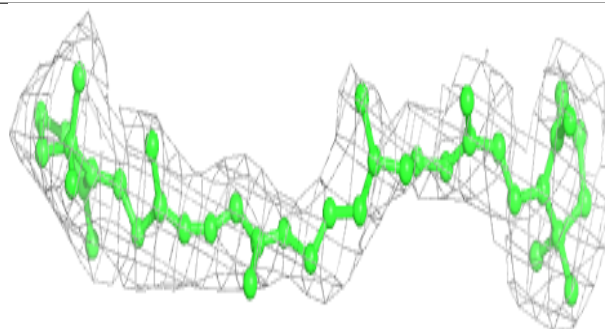
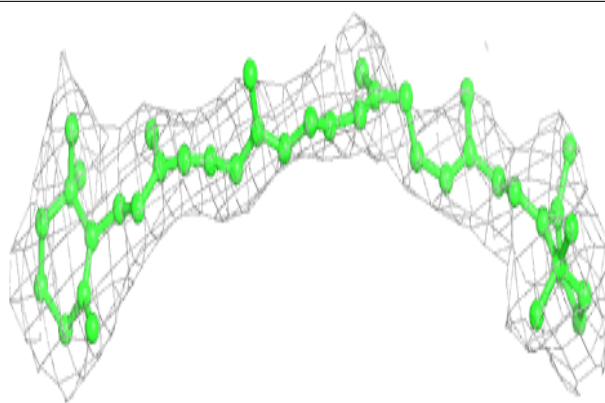
Electron density around CLA B 1206:

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



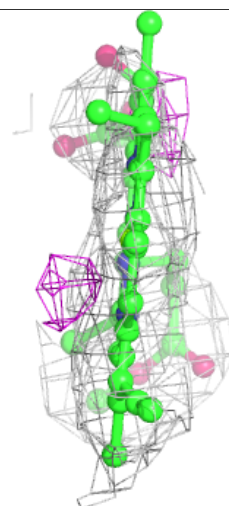
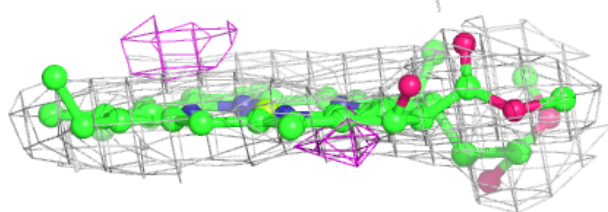
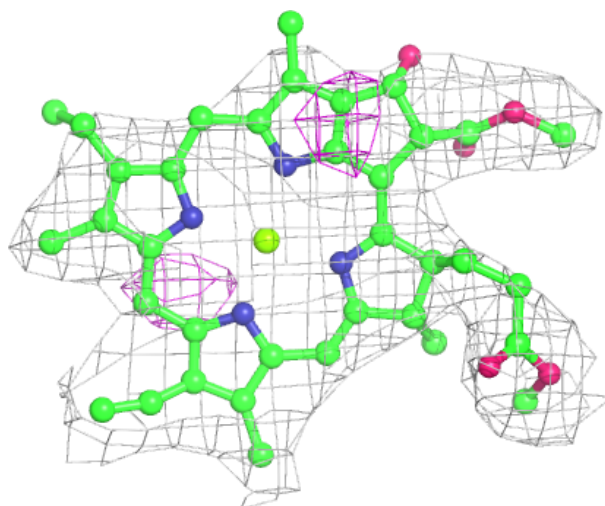
Electron density around BCR I 6018:

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



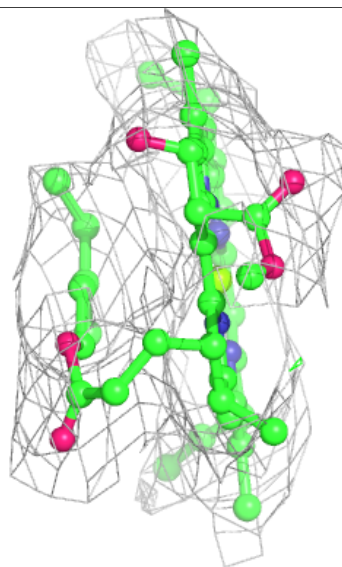
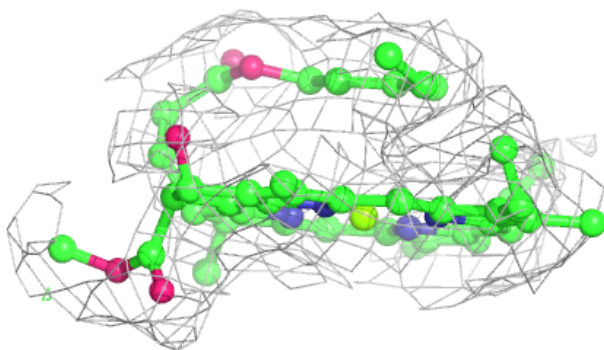
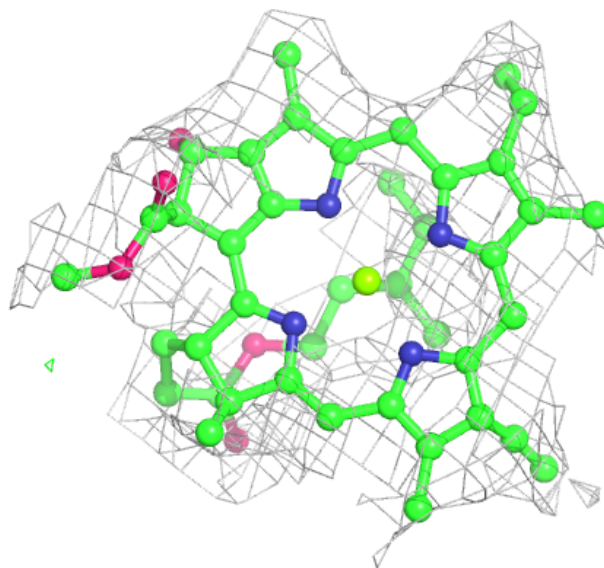
Electron density around CLA A 9013:

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



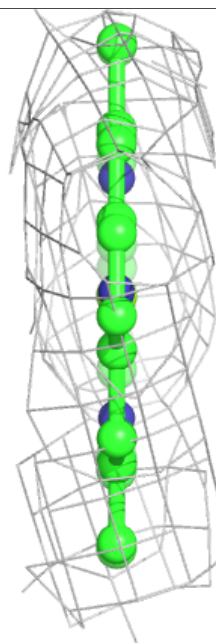
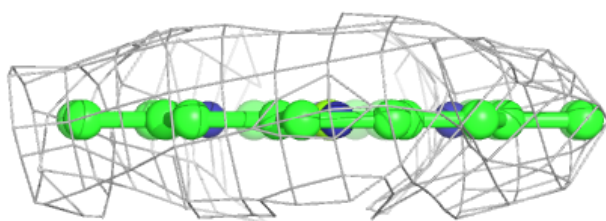
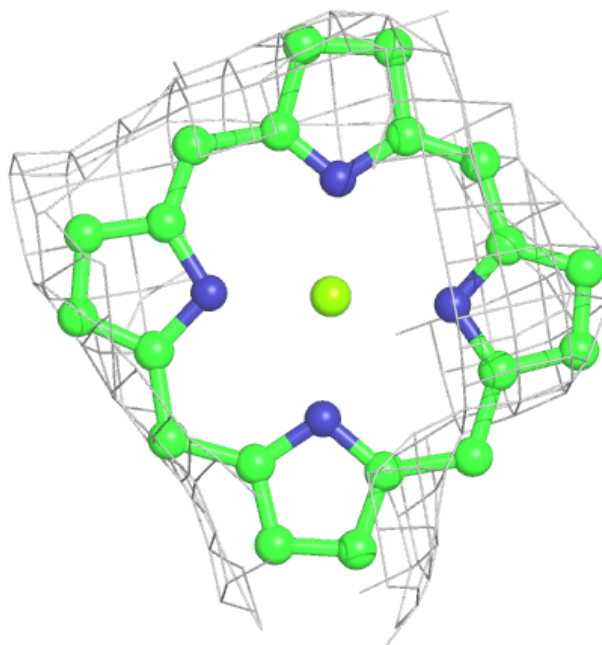
Electron density around CLA G 1233:

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



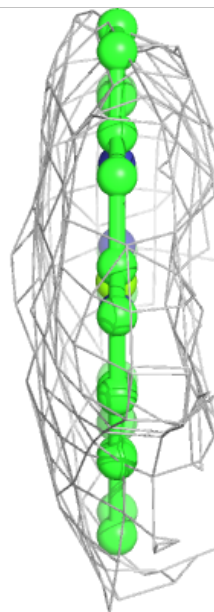
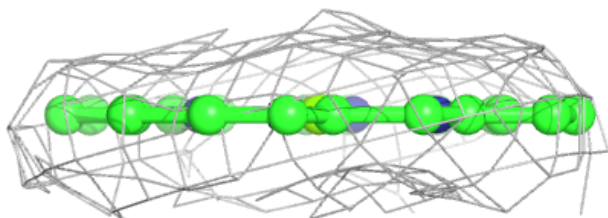
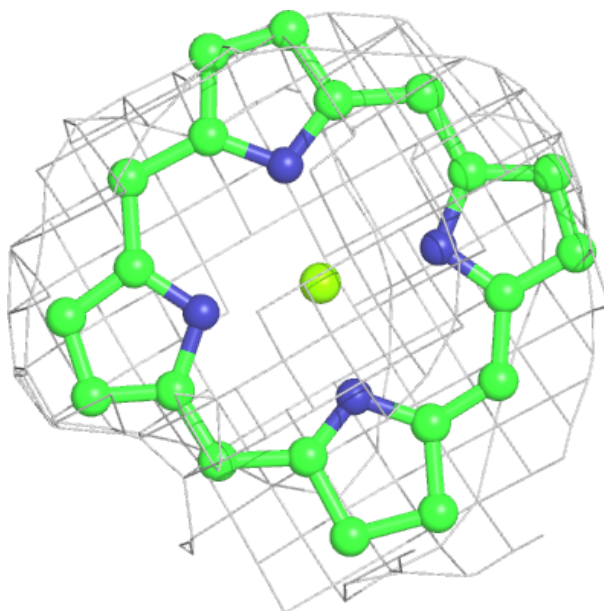
Electron density around CLA A 1120:

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



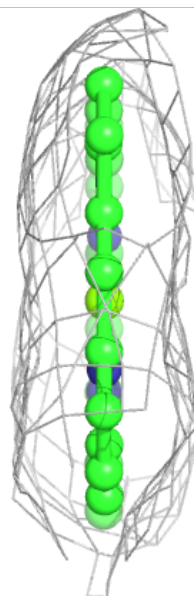
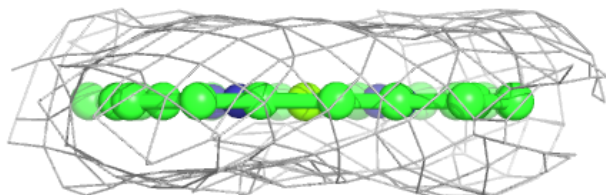
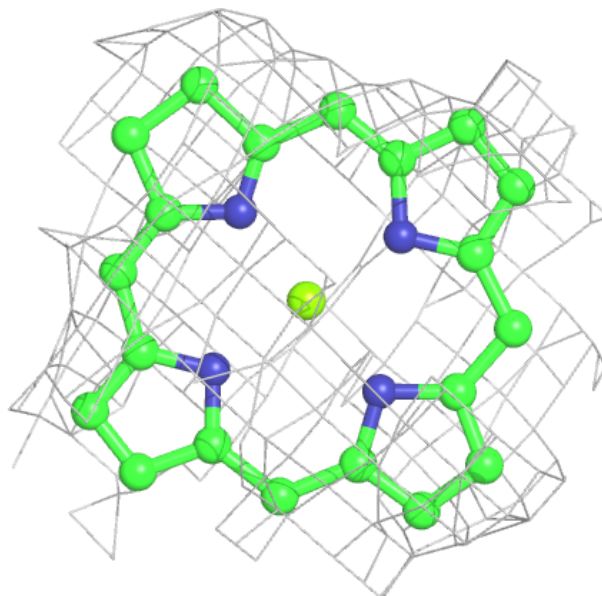
Electron density around CLA 1 1002:

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



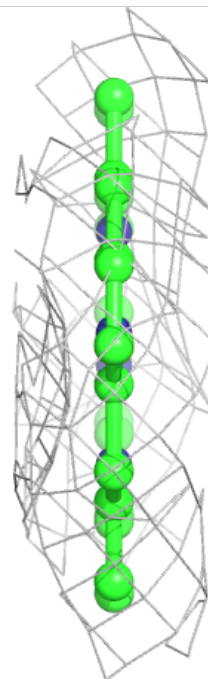
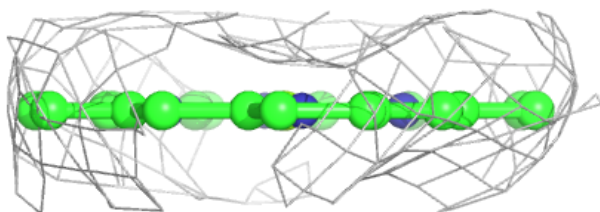
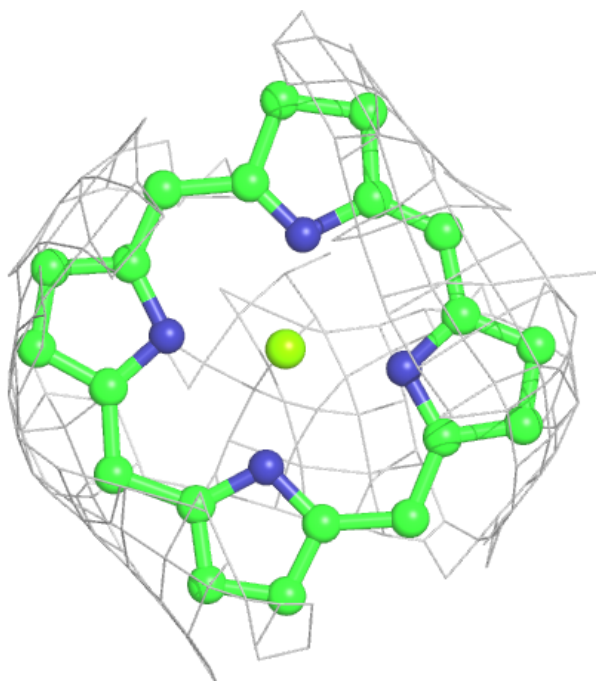
Electron density around CLA A 1124:

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



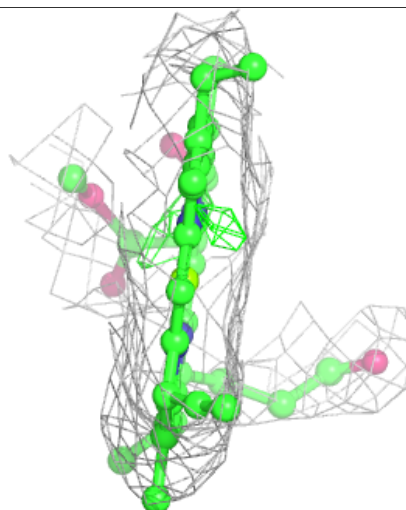
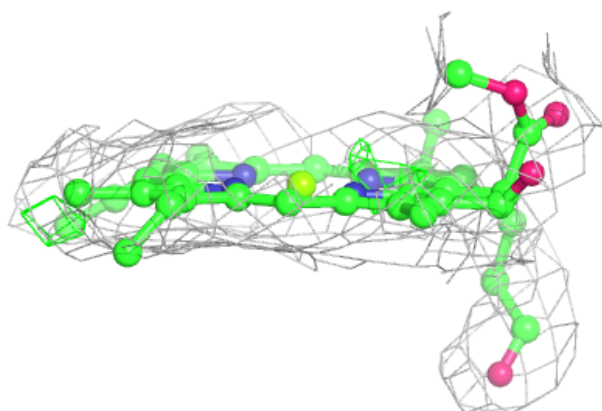
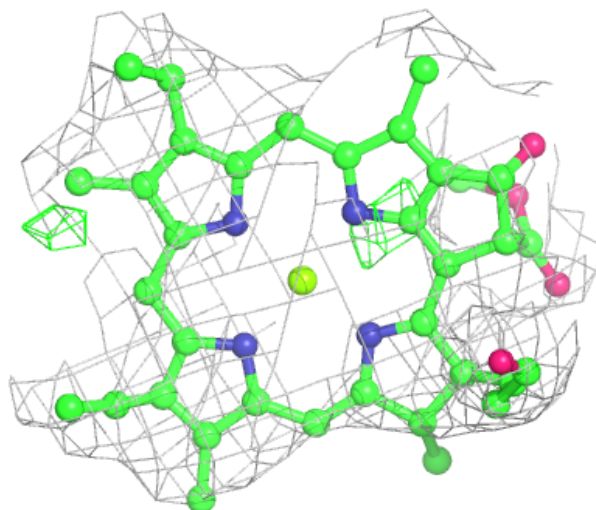
Electron density around CLA 4 4013:

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



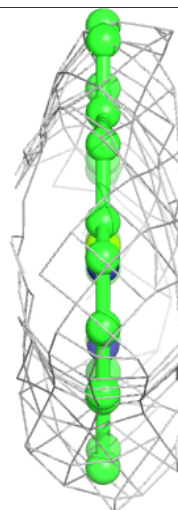
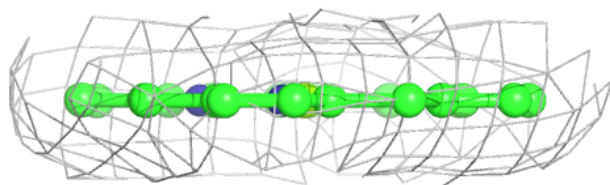
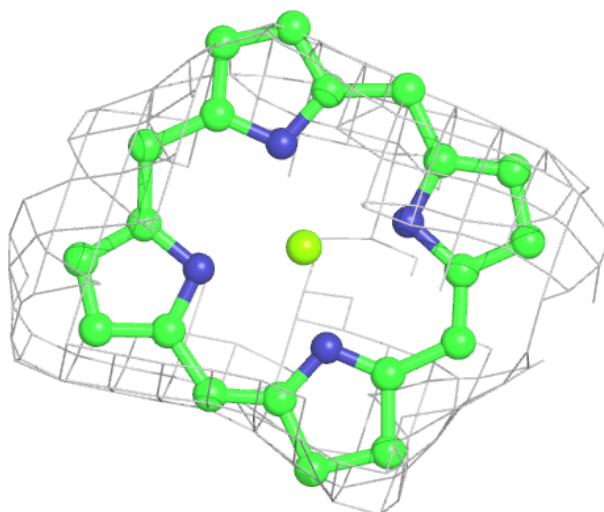
Electron density around CLA F 1139:

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



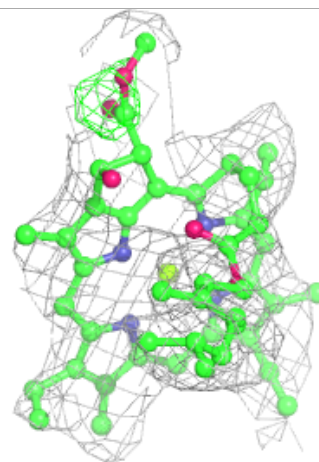
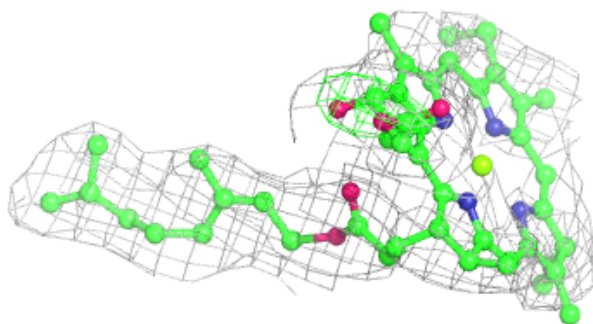
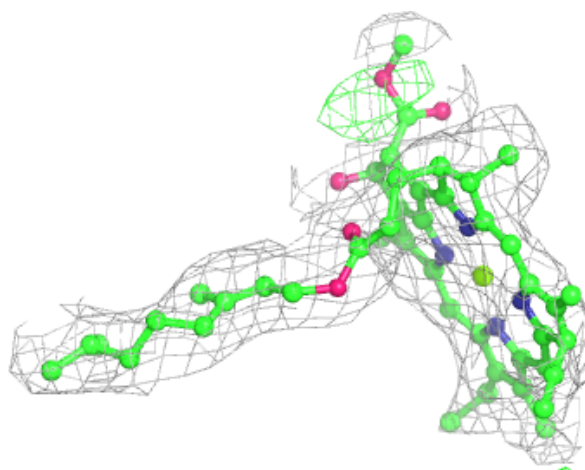
Electron density around CLA A 1101:

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



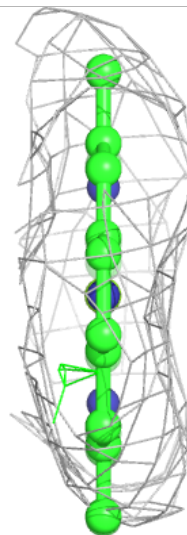
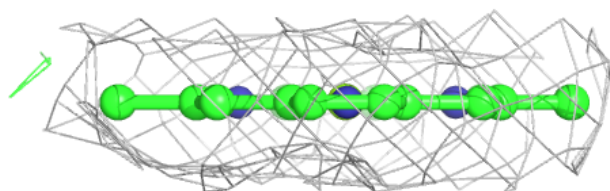
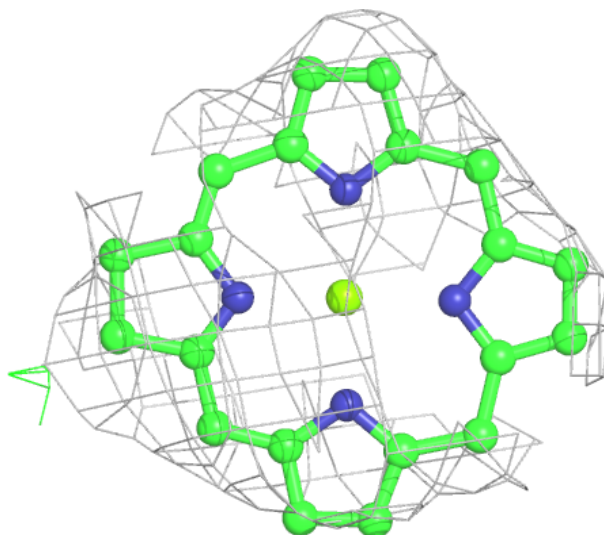
Electron density around CLA A 1126:

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



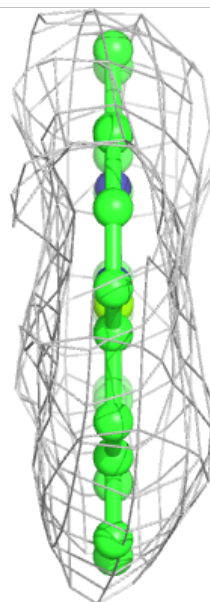
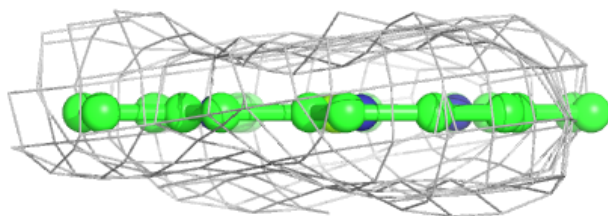
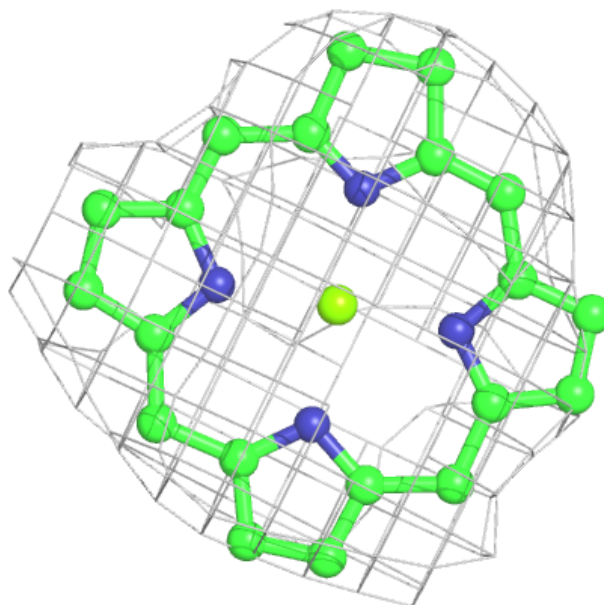
Electron density around CLA 4 1009:

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



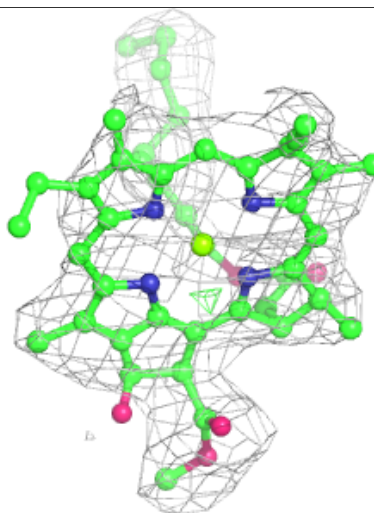
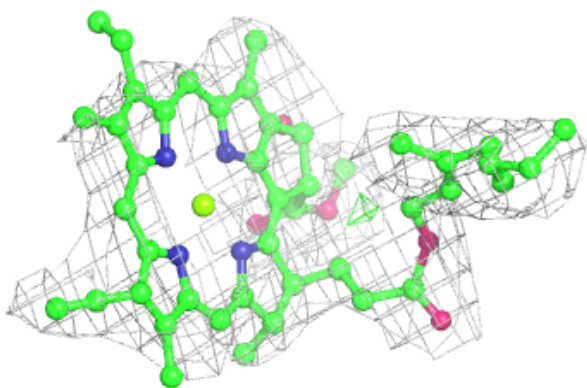
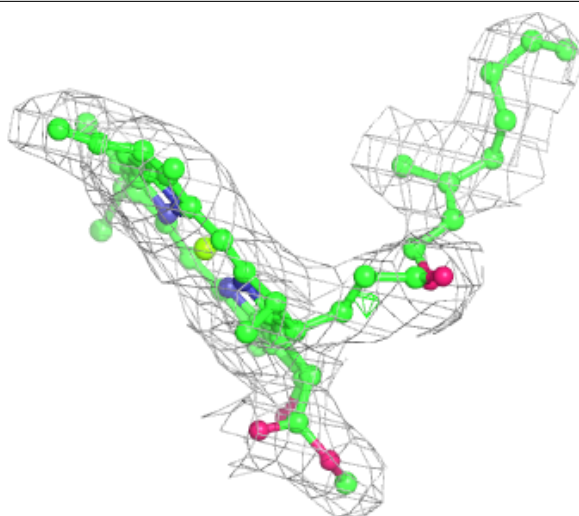
Electron density around CLA F 1305:

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



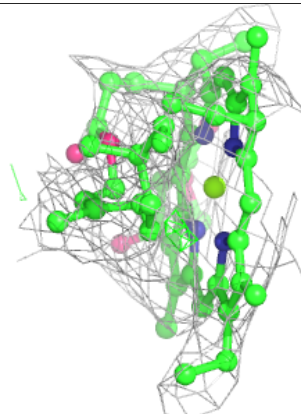
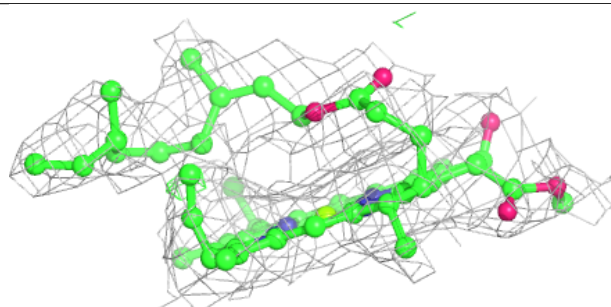
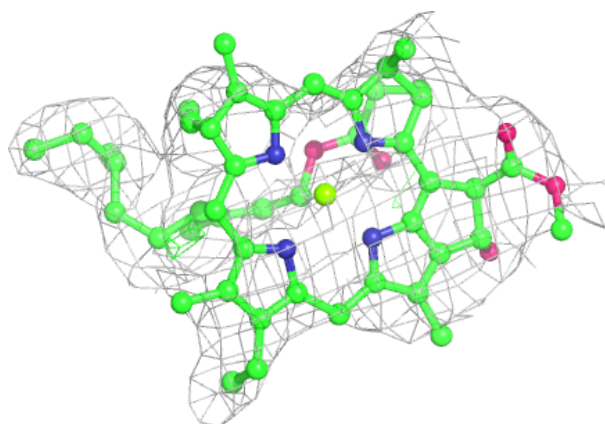
Electron density around CLA B 1238:

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

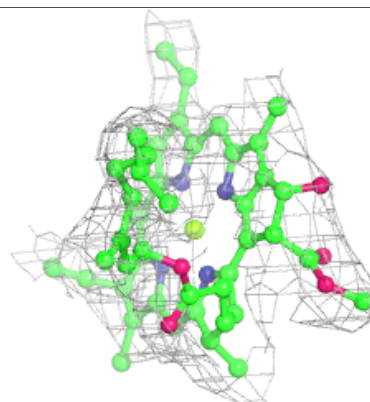
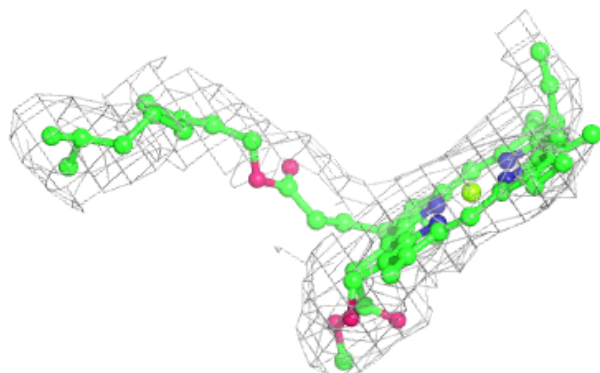
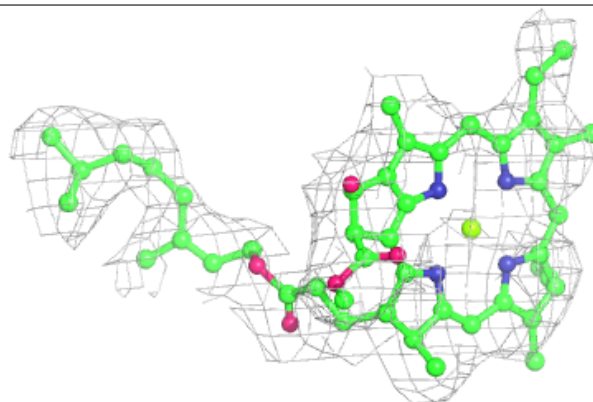


Electron density around CLA B 1138:

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

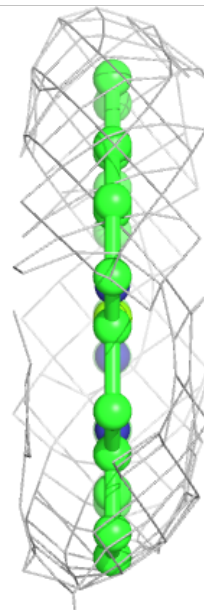
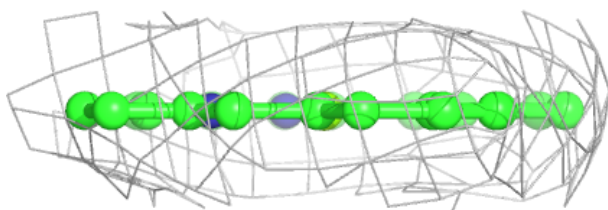
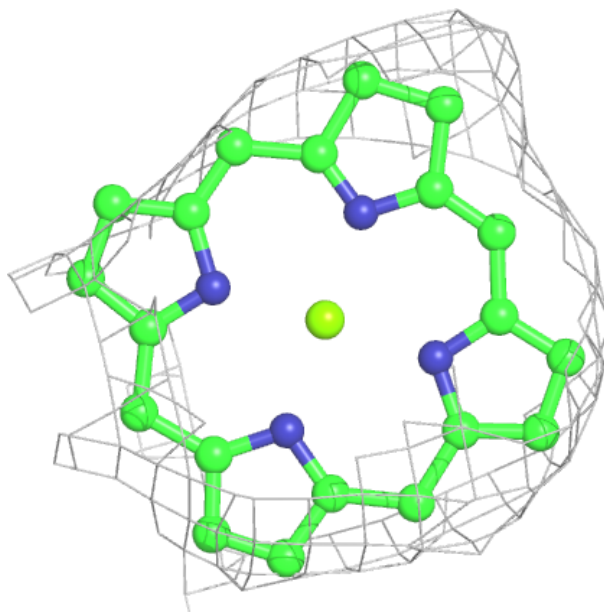
**Electron density around CLA A 1137:**

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



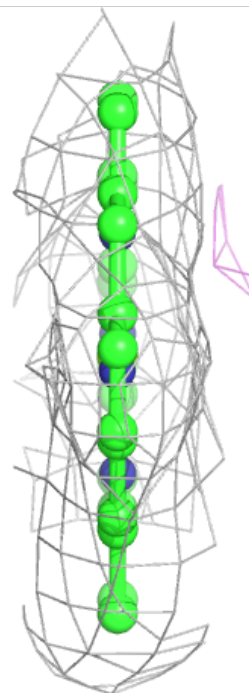
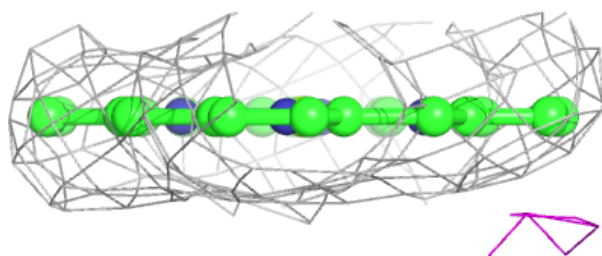
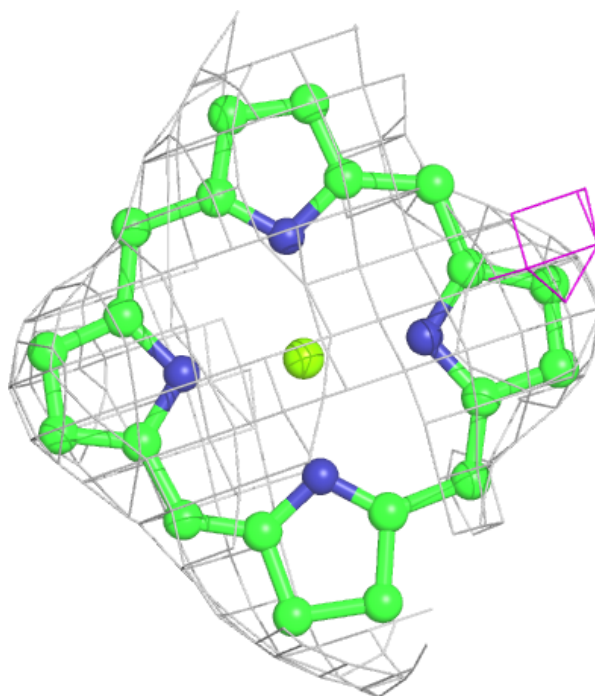
Electron density around CLA 3 2009:

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



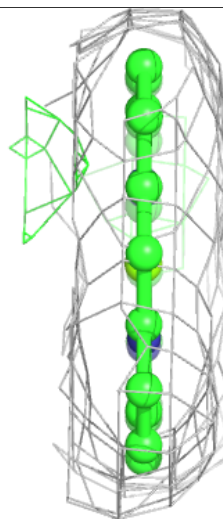
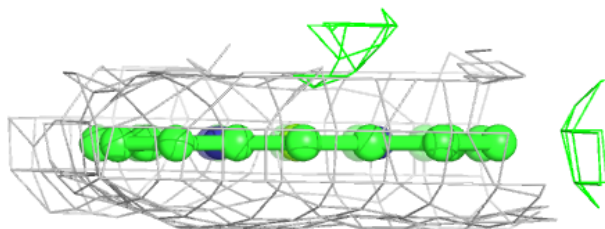
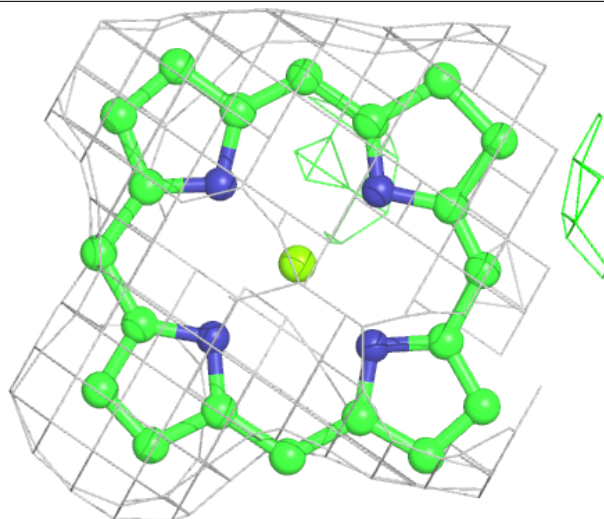
Electron density around CLA A 1127:

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



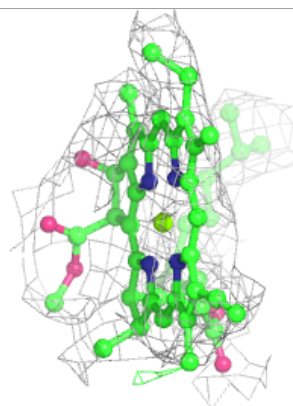
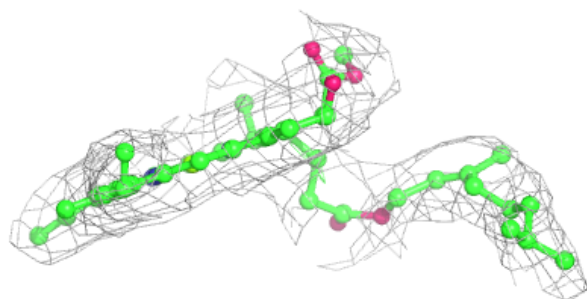
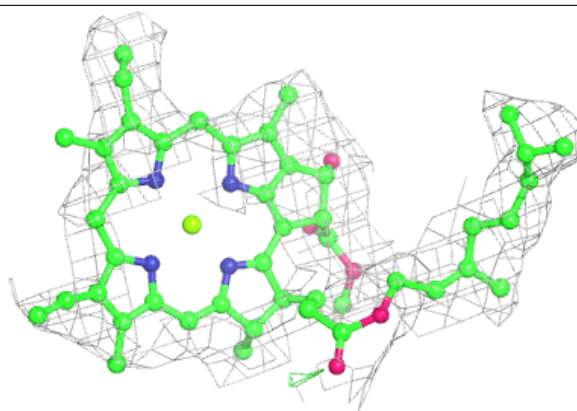
Electron density around CLA A 1132:

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



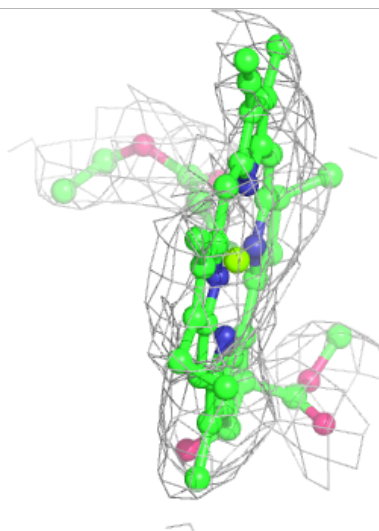
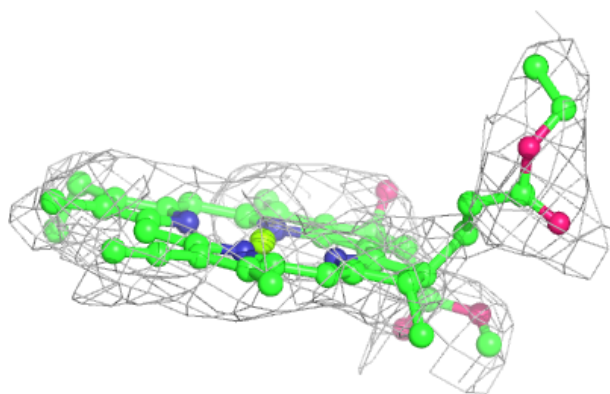
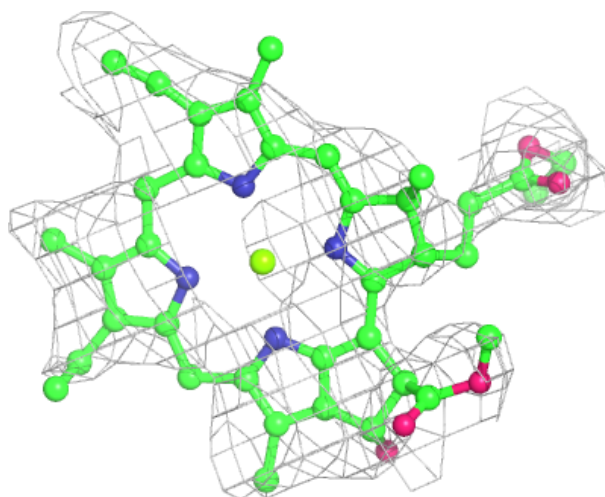
Electron density around CLA B 1208:

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



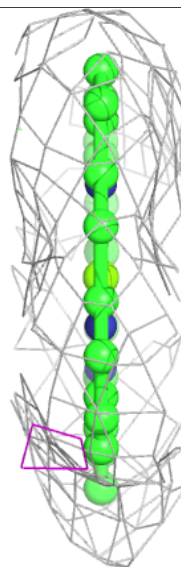
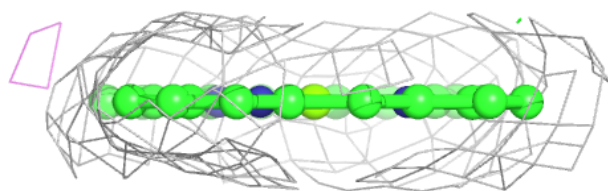
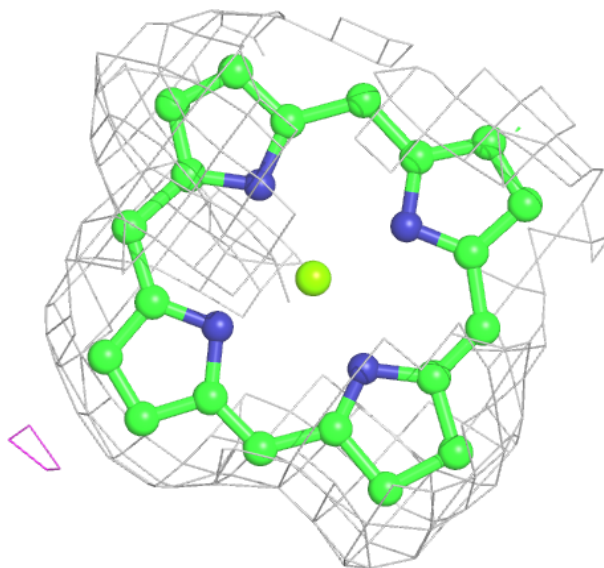
Electron density around CLA B 9010:

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



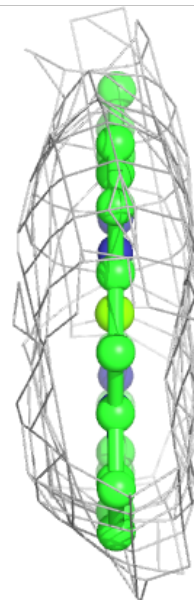
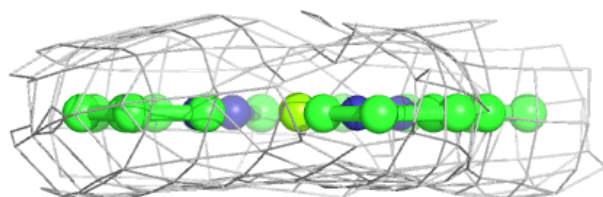
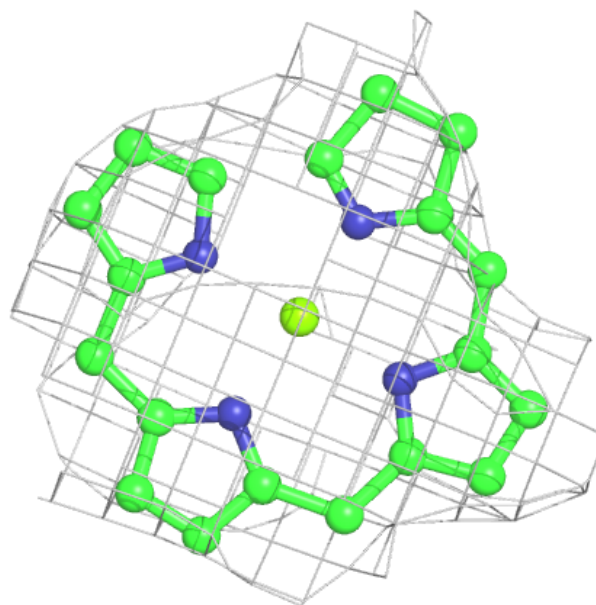
Electron density around CLA A 1133:

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



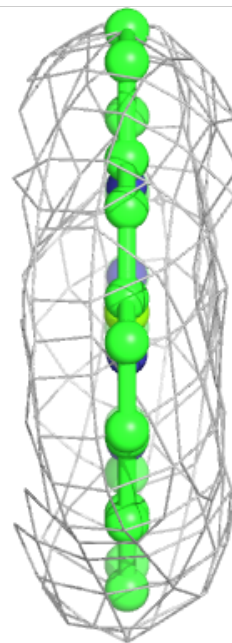
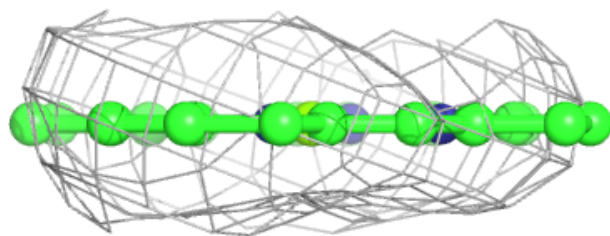
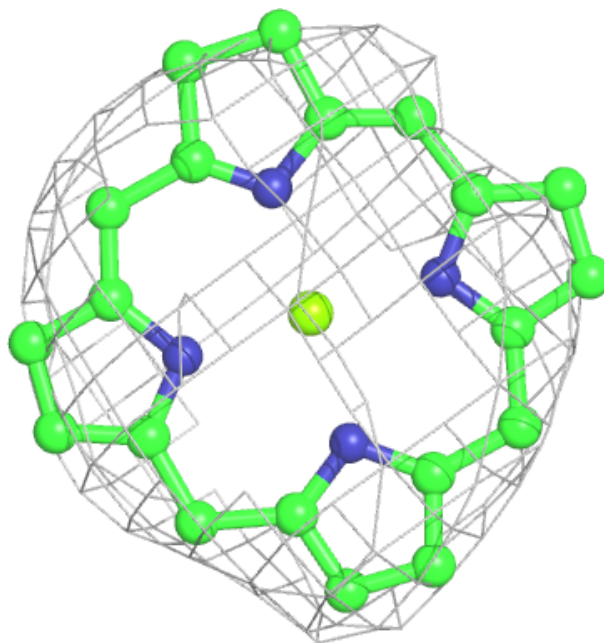
Electron density around CLA A 1109:

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



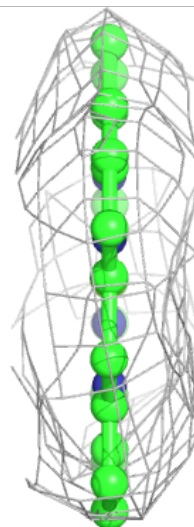
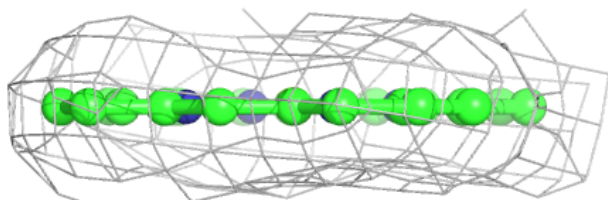
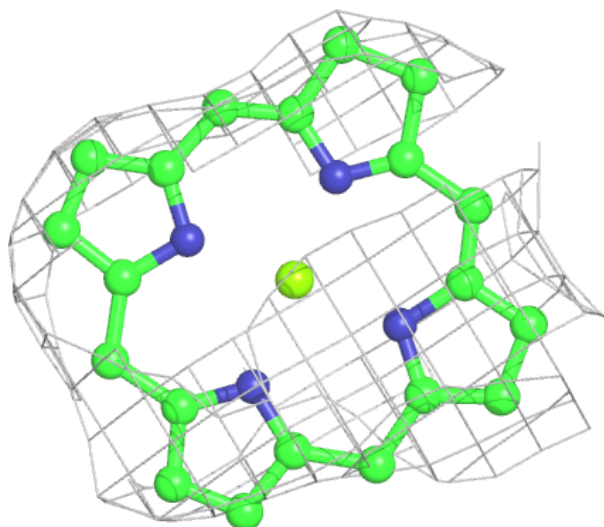
Electron density around CLA 3 3007:

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



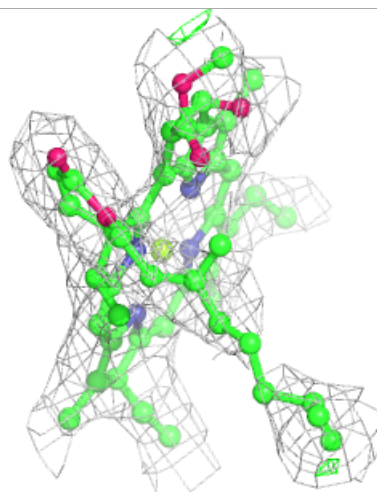
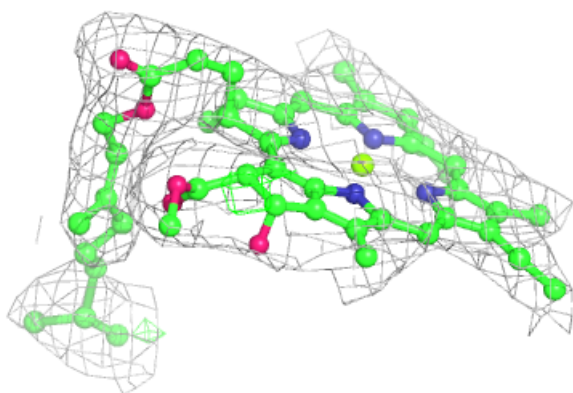
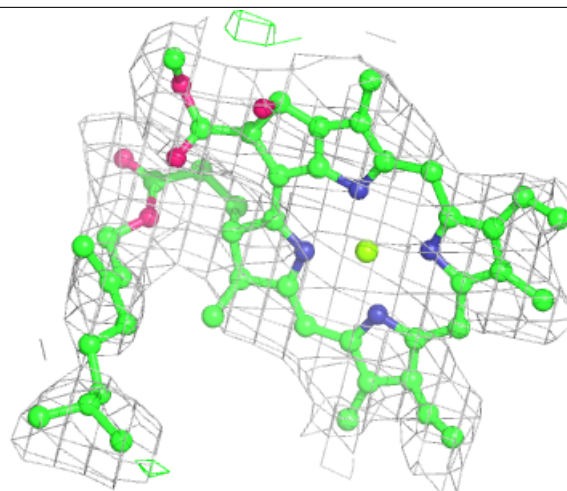
Electron density around CLA 2 2008:

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



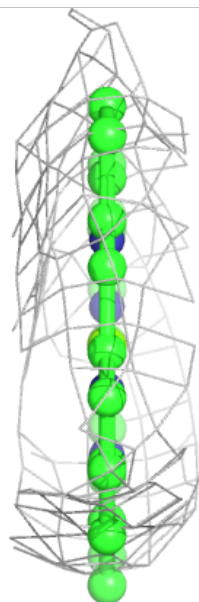
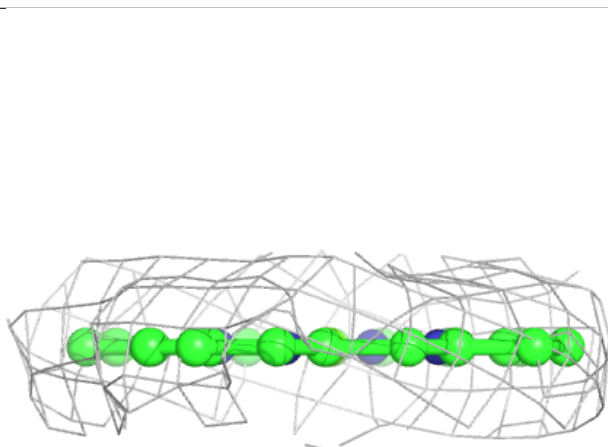
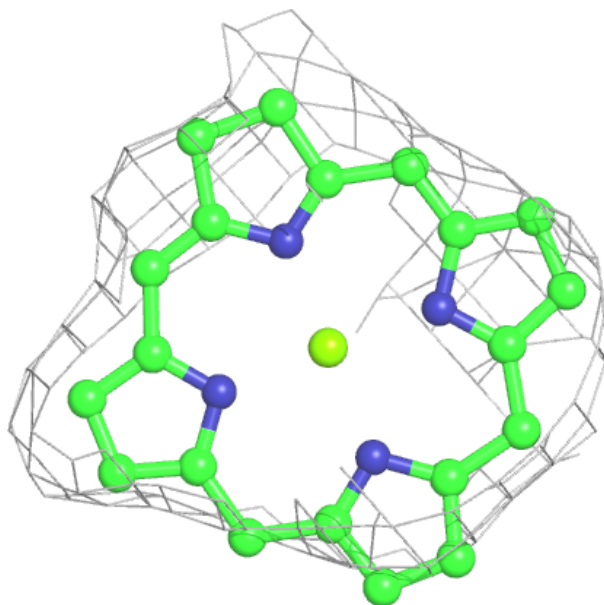
Electron density around CLA B 1207:

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



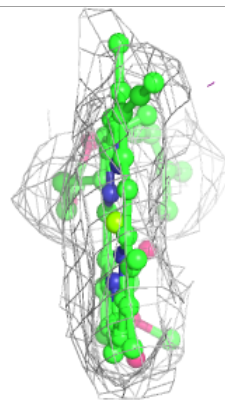
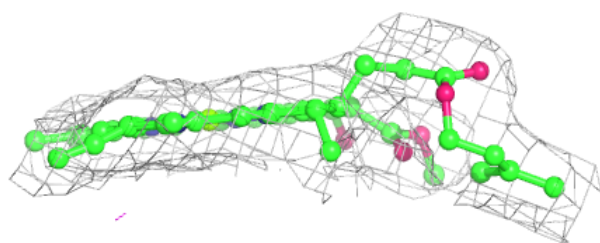
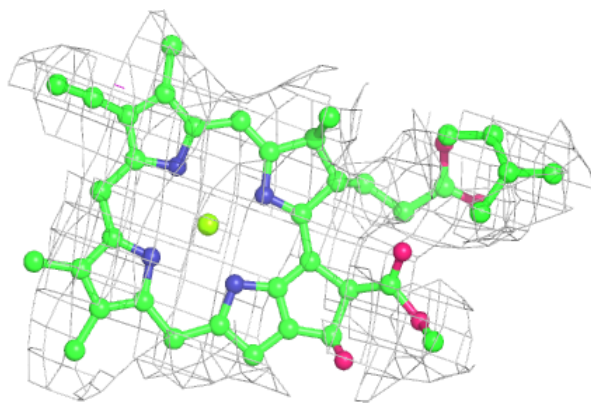
Electron density around CLA A 1148:

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



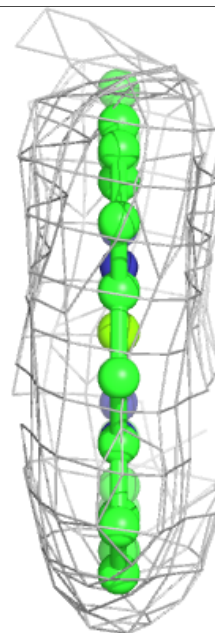
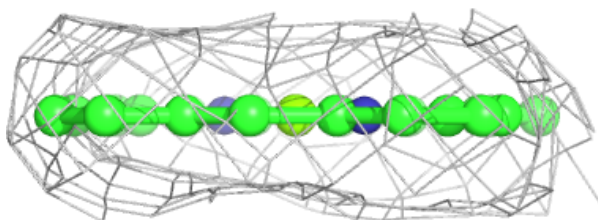
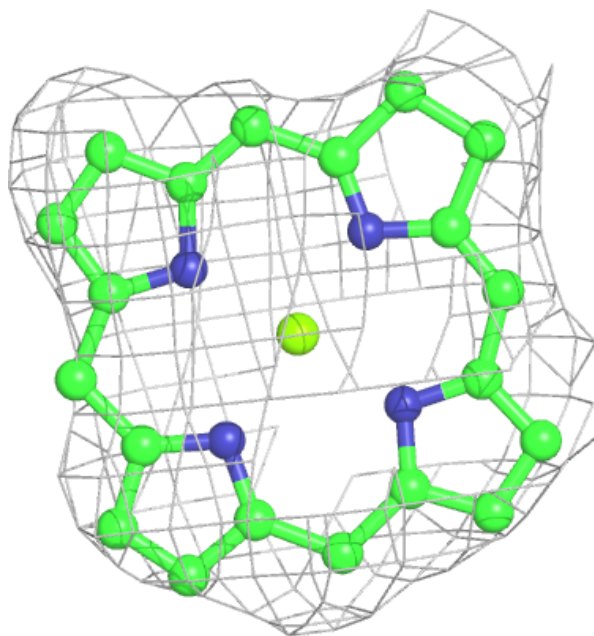
Electron density around CLA B 1203:

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



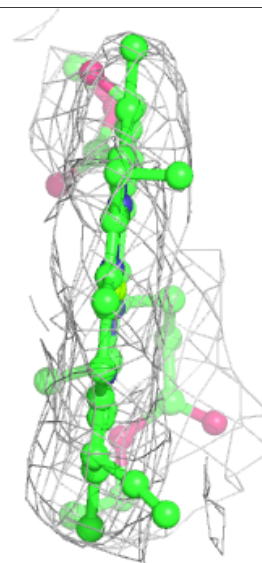
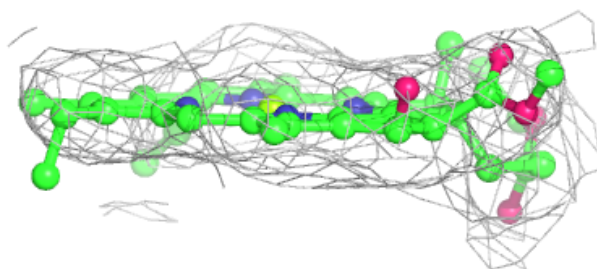
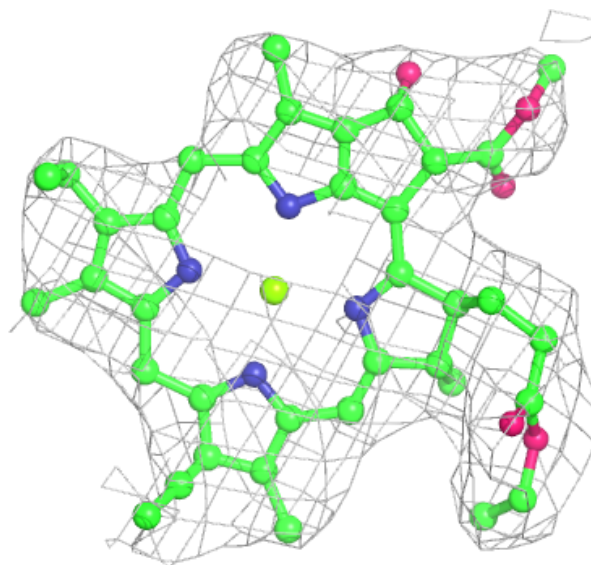
Electron density around CLA A 1152:

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



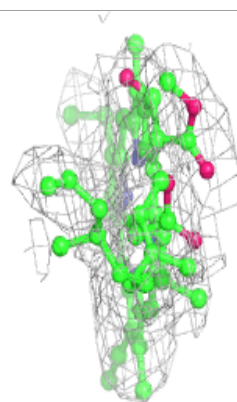
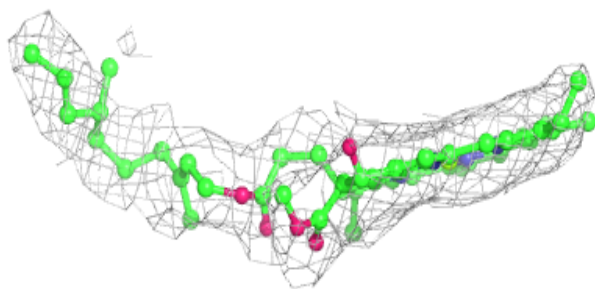
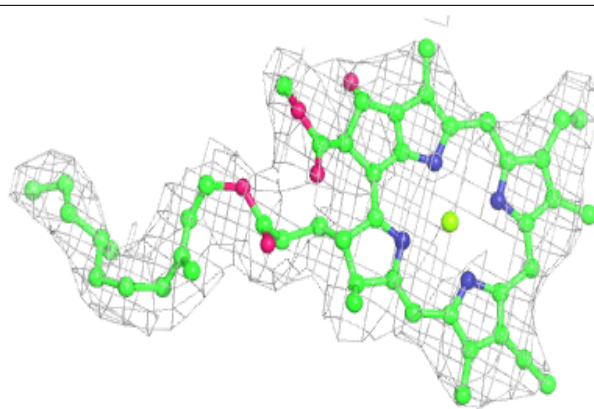
Electron density around CLA B 9023:

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



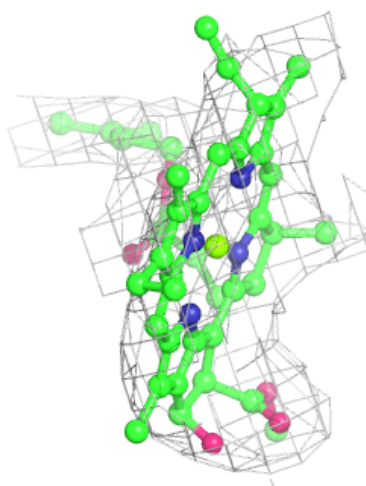
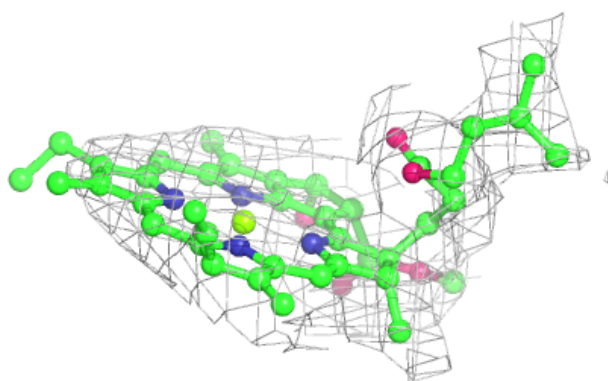
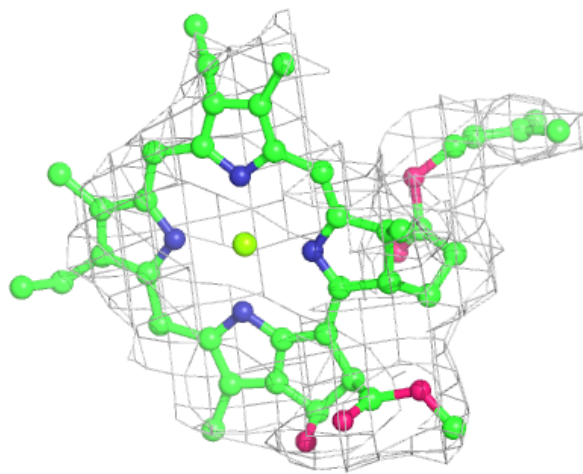
Electron density around CLA A 1107:

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



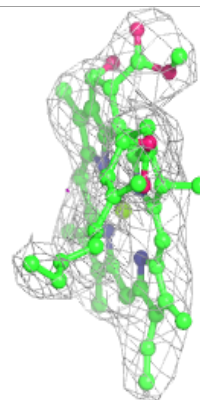
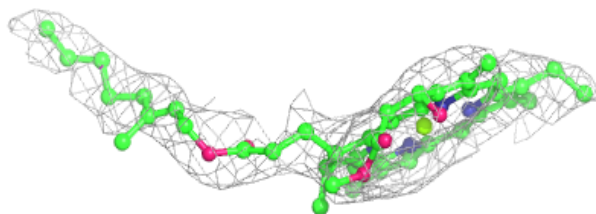
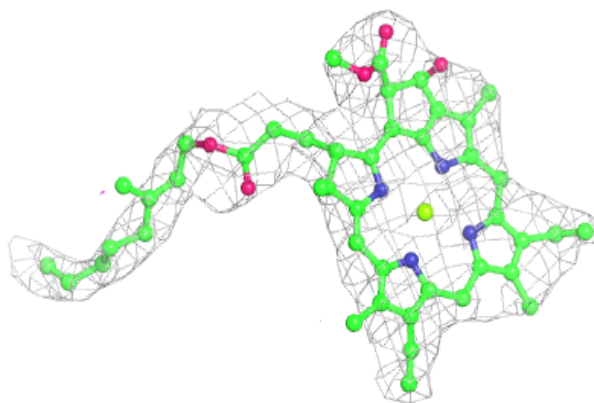
Electron density around CLA B 1227:

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



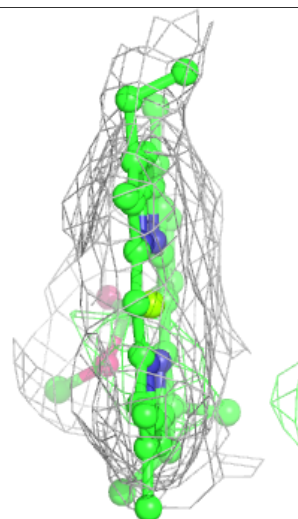
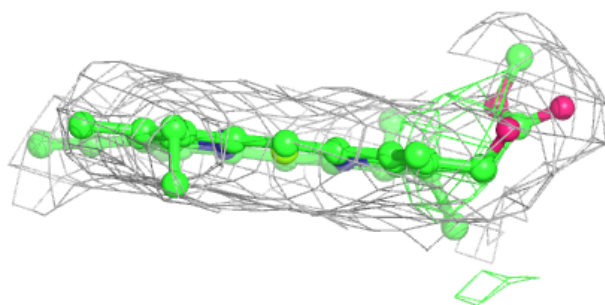
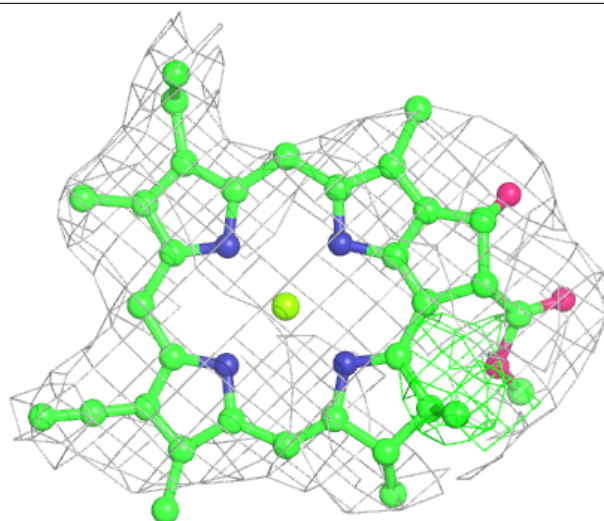
Electron density around CLA B 9022:

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



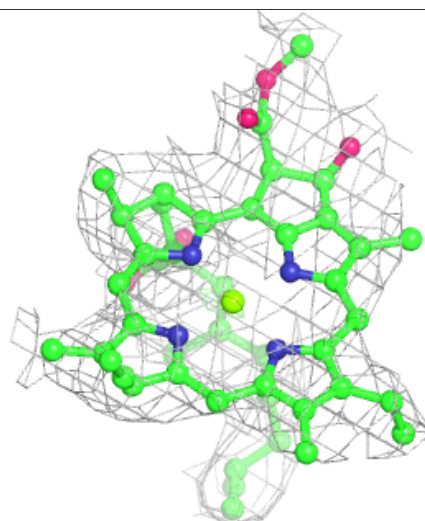
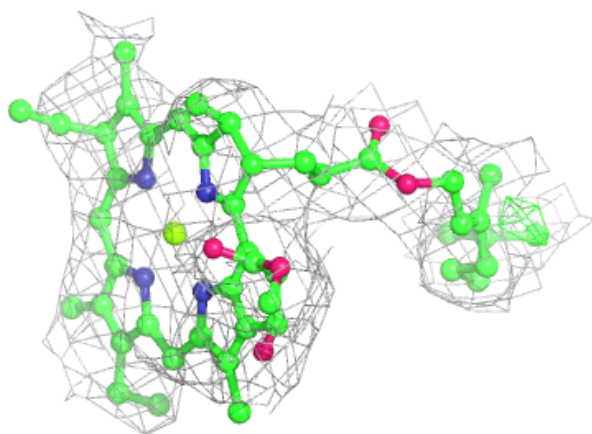
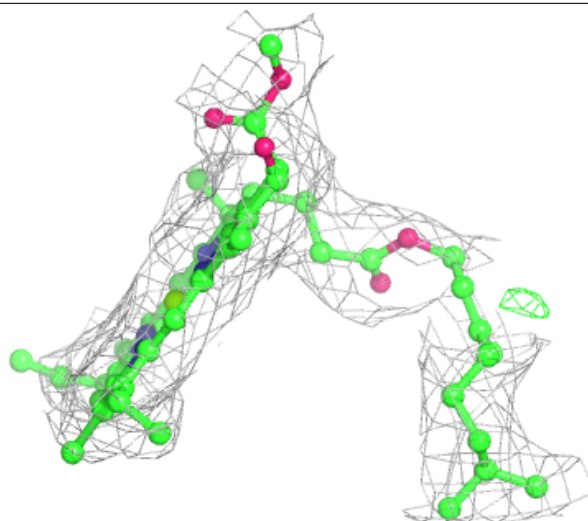
Electron density around CLA A 1106:

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



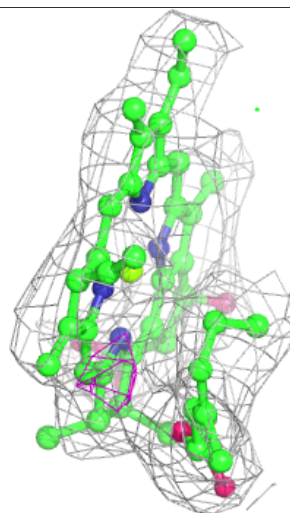
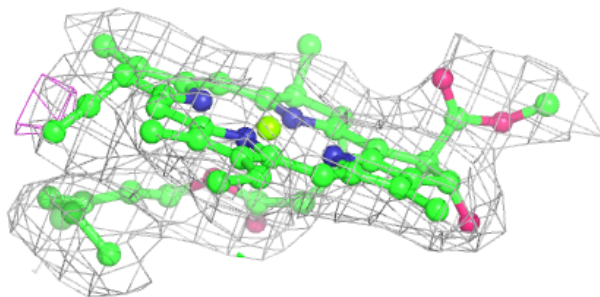
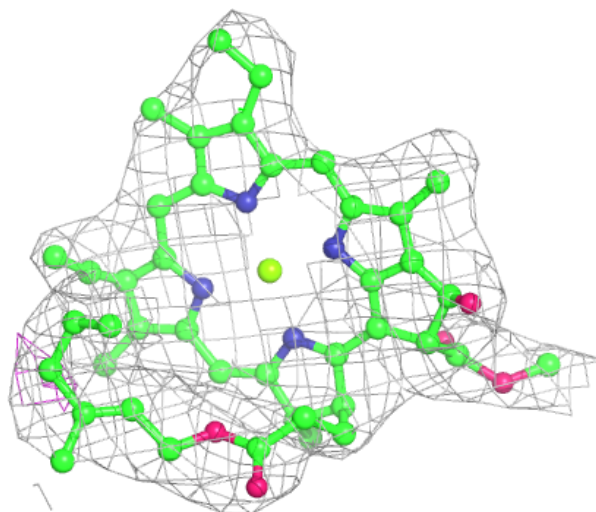
Electron density around CLA A 1128:

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



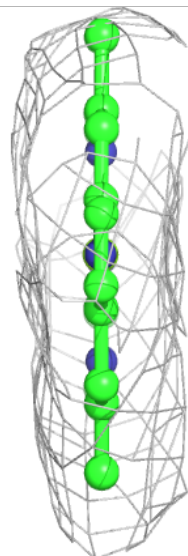
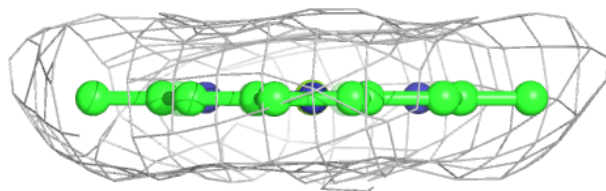
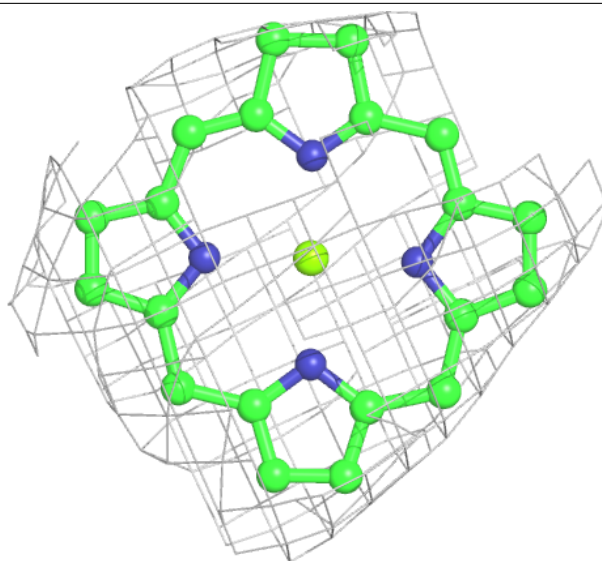
Electron density around CLA B 1215:

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



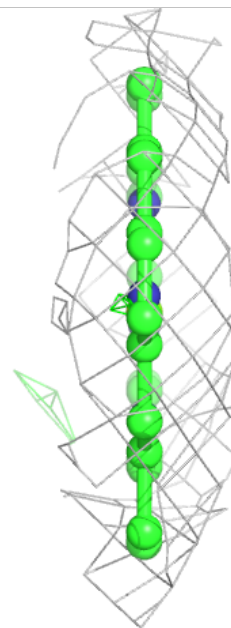
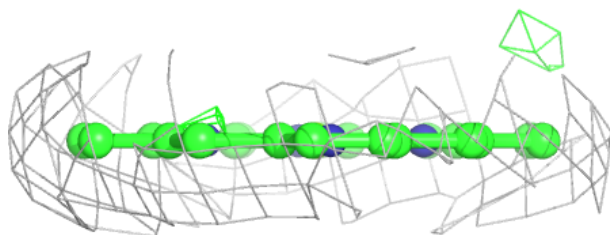
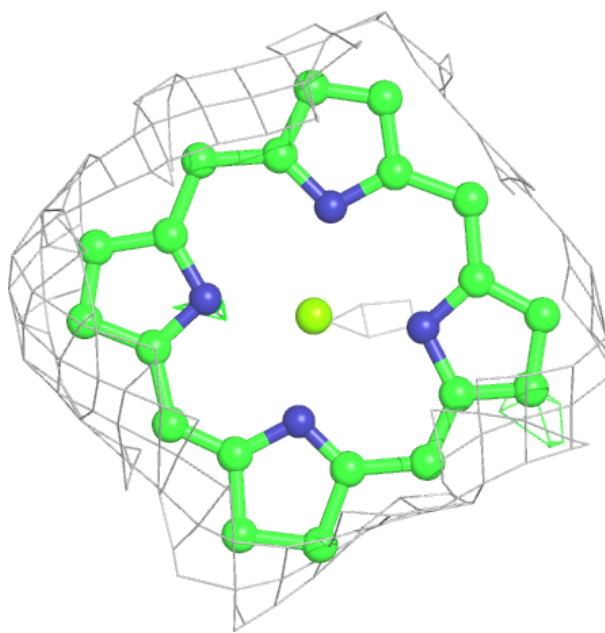
Electron density around CLA F 1240:

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



Electron density around CLA 2 2007:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.