



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 03:15 am BST

PDB ID : 6FOS  
Title : Cyanidioschyzon merolae photosystem I  
Authors : Nelson, N.; Hippler, M.; Antoshvili, M.; Caspy, I.  
Deposited on : 2018-02-08  
Resolution : 4.00 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](mailto: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.

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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

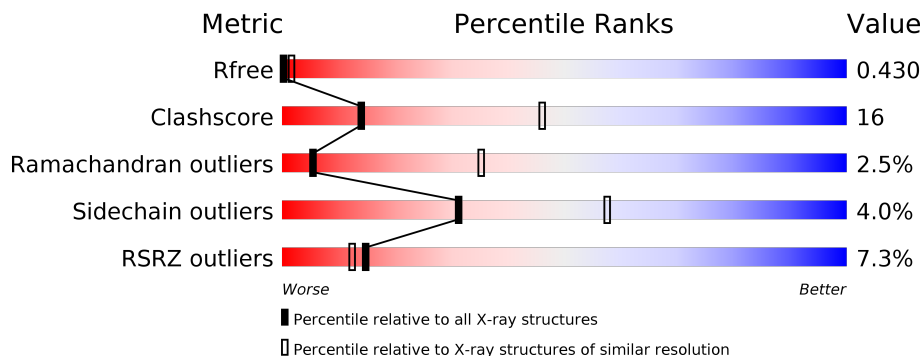
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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.



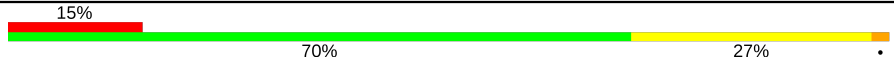





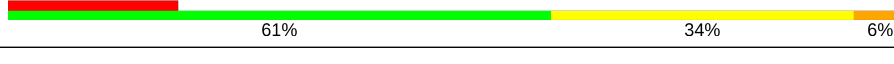
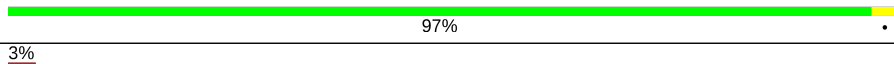
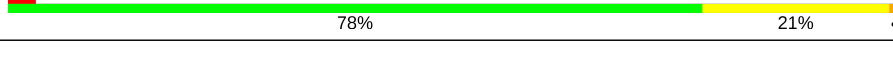
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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  $\geq 3$ , 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	2	222	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 45% 18% 35%</p>
1	3	222	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 32% 28% 6% 32%</p>
2	4	214	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 36% 15% 46%</p>
3	A	740	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">3% 64% 35%</p>
4	B	725	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">10% 66% 33%</p>
5	C	80	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">10% 59% 39%</p>

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Mol	Chain	Length	Quality of chain
6	D	124	
7	E	69	
8	F	155	
9	I	32	
10	J	38	
11	K	47	
12	L	140	
13	M	29	
14	O	98	

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
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	-
15	CLA	2	607	X	-	-	-
15	CLA	2	608	X	-	-	-
15	CLA	2	610	X	-	-	-
15	CLA	2	611	X	-	-	-
15	CLA	2	612	X	-	-	-
15	CLA	2	613	X	-	-	-
15	CLA	2	614	X	-	-	-
15	CLA	2	615	X	-	-	-
15	CLA	2	616	X	-	-	X
15	CLA	3	601	X	-	-	-
15	CLA	3	602	X	-	-	-
15	CLA	3	603	X	-	-	X
15	CLA	3	604	X	-	-	-
15	CLA	3	606	X	-	-	-
15	CLA	3	607	X	-	-	-
15	CLA	3	608	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	614	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	X
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	610	X	-	-	-
15	CLA	4	611	X	-	-	X
15	CLA	4	612	X	-	-	-
15	CLA	4	615	X	-	-	-
15	CLA	4	616	X	-	-	-
15	CLA	A	1011	X	-	-	-
15	CLA	A	1012	X	-	-	-
15	CLA	A	1013	X	-	-	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	-	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-
15	CLA	A	1121	X	-	-	-
15	CLA	A	1122	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	-	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	X	-	-	-
15	CLA	A	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1141	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1023	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1207	X	-	-	X
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1210	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1214	X	-	-	X
15	CLA	B	1215	X	-	-	-
15	CLA	B	1216	X	-	-	X
15	CLA	B	1217	X	-	-	X
15	CLA	B	1218	X	-	-	X
15	CLA	B	1219	X	-	-	-
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	X
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	X
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
15	CLA	K	1401	X	-	-	-
15	CLA	K	1402	X	-	-	-
15	CLA	L	1501	X	-	-	-
15	CLA	L	1502	X	-	-	-
15	CLA	L	1503	X	-	-	-
15	CLA	O	1601	X	-	-	-
15	CLA	O	1602	X	-	-	X
15	CLA	O	1603	X	-	-	X
16	PQN	B	2002	-	-	-	X
17	SF4	C	3002	-	-	X	-
18	BCR	A	4007	-	-	-	X
18	BCR	A	4008	-	-	-	X
18	BCR	A	4011	-	-	-	X
18	BCR	B	4008	-	-	-	X
18	BCR	I	4018	-	-	-	X

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 25611 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 Similar to chlorophyll a/b-binding protein, CP24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	2	144	1116	726	193	192	5	0	0	0
1	3	150	1181	769	200	206	6	0	0	0

- Molecule 2 is a protein called Similar to light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	4	116	935	618	157	153	7	0	0	0

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	740	5790	3787	994	982	27	0	0	0

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	725	5766	3791	974	982	19	0	0	1

- Molecule 5 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	80	597	367	104	114	12	0	0	0

- Molecule 6 is a protein called Photosystem I p700 chlorophyll A apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	124	976	618	171	182	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	69	555	360	88	106	1	0	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	153	1256	806	213	233	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	32	238	163	33	40	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	38	312	214	46	51	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	47	331	211	58	58	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	14	MET	-	initiating methionine	UNP Q85G51

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	140	1071	703	174	191	3	0	0	0

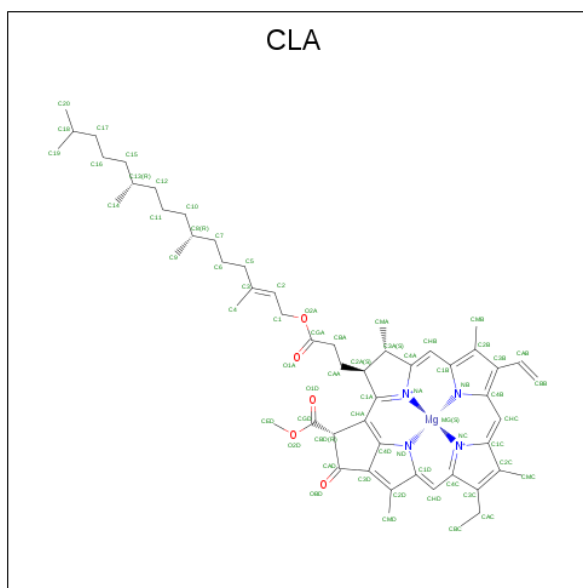
- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	29	214	142	34	36	2	0	0	0

- Molecule 14 is a protein called PsaM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	O	98	755	509	116	129	1	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	Mg	N		
15	2	1	25	20	1	4	0	0
15	2	1	25	20	1	4	0	0
15	2	1	25	20	1	4	0	0
15	2	1	25	20	1	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	3	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
15	3	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	4	1	Total	C	Mg	N	0	0	
			25	20	1	4			
15	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			

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

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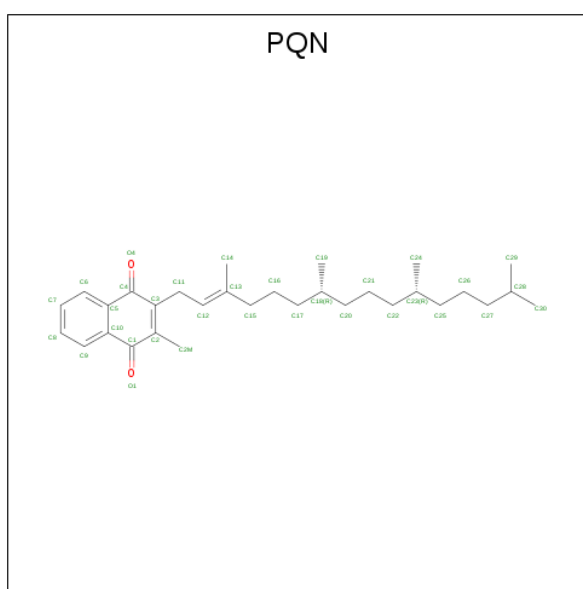
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	B	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
15	F	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
15	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	K	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	L	1	Total	C	Mg	N		0	0
			25	20	1	4			
15	L	1	Total	C	Mg	N		0	0
			25	20	1	4			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	O	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	O	1	Total	C	Mg	N	0	0
			25	20	1	4		
15	O	1	Total	C	Mg	N	0	0
			25	20	1	4		

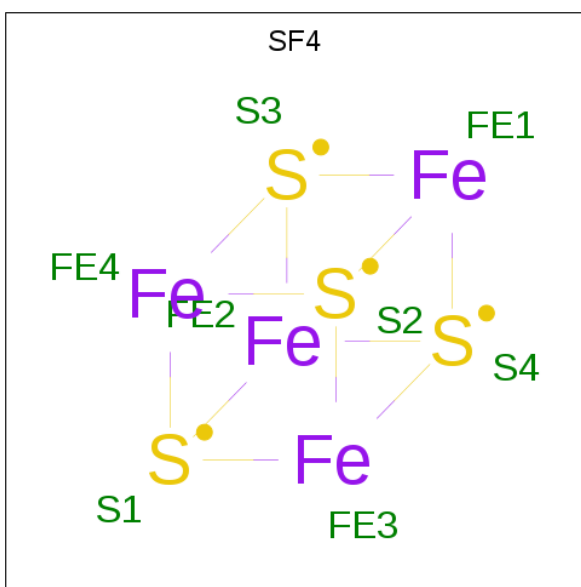
- Molecule 16 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



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

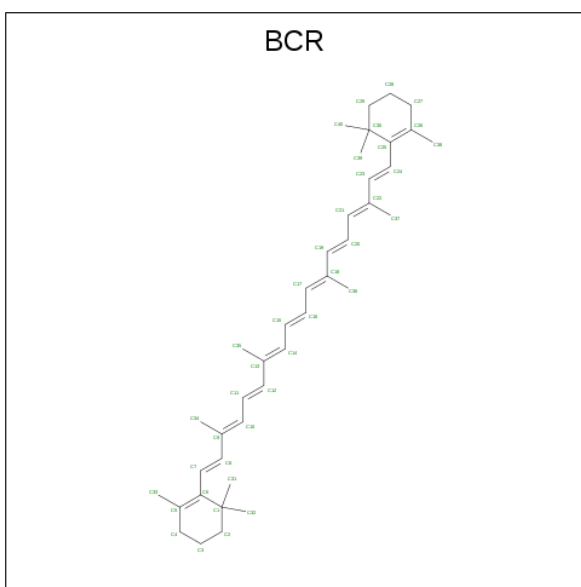
- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).





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

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

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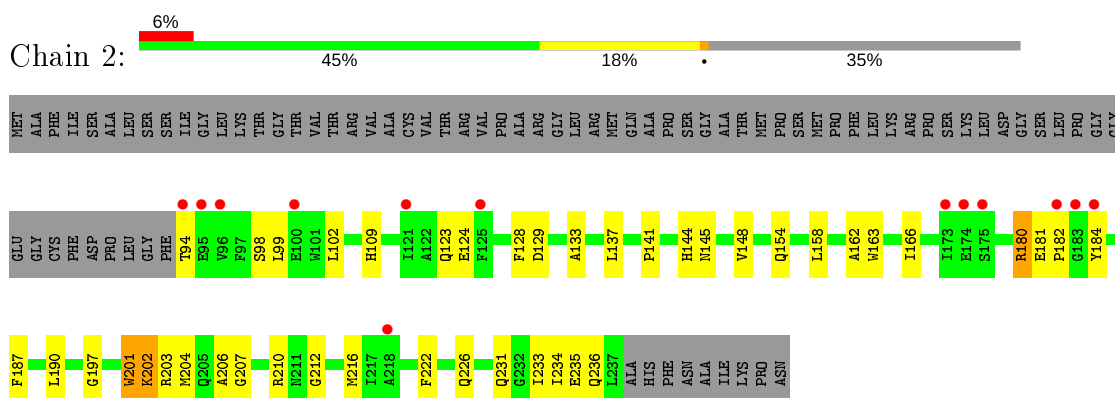
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	A	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	B	1	Total C 40 40	0	0
18	I	1	Total C 40 40	0	0

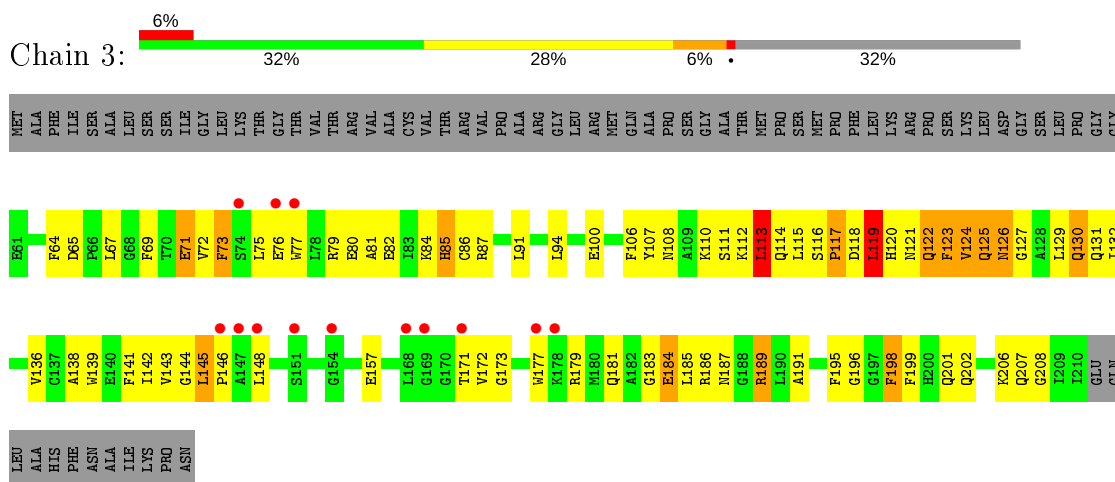
### 3 Residue-property plots [i](#)

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.

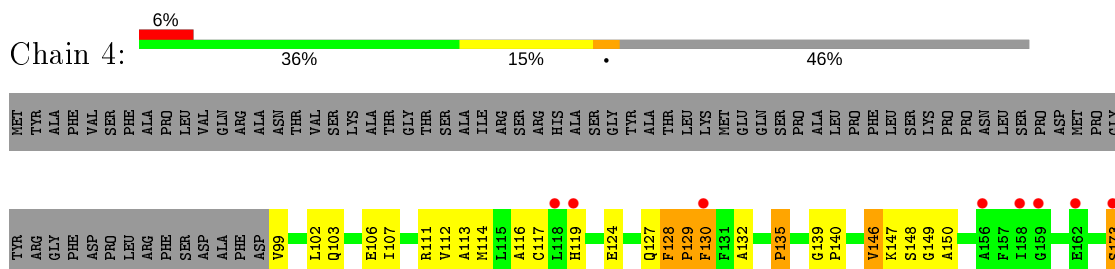
- Molecule 1: Similar to chlorophyll a/b-binding protein, CP24



- Molecule 1: Similar to chlorophyll a/b-binding protein, CP24



- Molecule 2: Similar to light harvesting protein





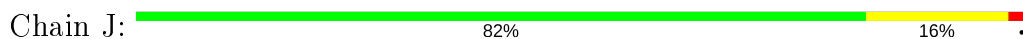




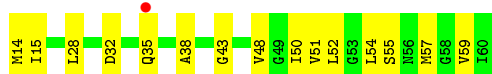
- Molecule 9: Photosystem I reaction center subunit VIII



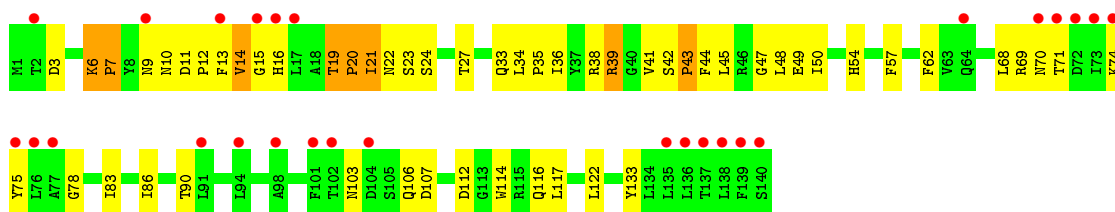
- Molecule 10: Photosystem I reaction center subunit IX



- Molecule 11: Photosystem I reaction center subunit X



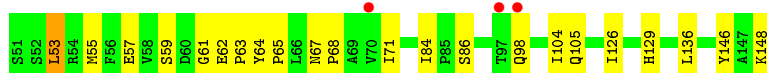
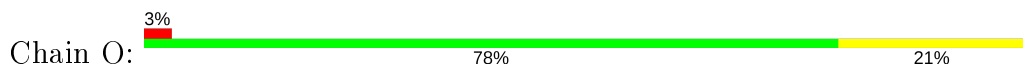
- Molecule 12: Photosystem I reaction center subunit XI



- Molecule 13: Photosystem I reaction center subunit XII



- Molecule 14: PsaM



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.13Å 213.52Å 349.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 4.00 48.53 – 3.38	Depositor EDS
% Data completeness (in resolution range)	80.9 (48.53-4.00) 53.6 (48.53-3.38)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (dev_3042: ???)	Depositor
R, $R_{free}$	0.378 , 0.430 0.378 , 0.430	Depositor DCC
$R_{free}$ test set	912 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	137.1	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.16 , 110.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	25611	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2	0.25	0/1142	0.43	0/1544
1	3	0.28	0/1210	0.59	0/1633
2	4	0.25	0/961	0.40	0/1289
3	A	0.24	0/5977	0.40	0/8146
4	B	0.24	0/5973	0.40	0/8163
5	C	0.24	0/607	0.45	0/822
6	D	0.25	0/998	0.44	0/1349
7	E	0.24	0/564	0.47	0/763
8	F	0.27	0/1289	0.43	0/1750
9	I	0.28	0/243	0.49	0/331
10	J	0.25	0/321	0.53	1/437 (0.2%)
11	K	0.22	0/333	0.42	0/448
12	L	0.26	0/1097	0.48	0/1492
13	M	0.24	0/215	0.39	0/291
14	O	0.26	0/780	0.46	0/1068
All	All	0.25	0/21710	0.43	1/29526 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
10	J	36	LEU	CA-CB-CG	6.62	130.52	115.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1116	0	1088	39	0
1	3	1181	0	1169	74	0
2	4	935	0	926	25	0
3	A	5790	0	5719	234	0
4	B	5766	0	5589	183	0
5	C	597	0	584	35	0
6	D	976	0	967	30	0
7	E	555	0	576	25	0
8	F	1256	0	1227	55	0
9	I	238	0	265	8	0
10	J	312	0	327	11	0
11	K	331	0	349	9	0
12	L	1071	0	1090	39	0
13	M	214	0	236	0	0
14	O	755	0	760	12	0
15	2	375	0	45	2	0
15	3	275	0	33	5	0
15	4	325	0	39	3	0
15	A	1546	0	801	67	0
15	B	1267	0	522	53	0
15	F	70	0	35	1	0
15	J	50	0	38	1	0
15	K	50	0	6	0	0
15	L	75	0	9	2	0
15	O	75	0	9	0	0
16	A	33	0	46	3	0
16	B	33	0	46	1	0
17	A	8	0	0	0	0
17	C	16	0	0	4	0
18	A	200	0	260	24	0
18	B	80	0	105	7	0
18	I	40	0	53	4	0
All	All	25611	0	22919	764	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 764 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)
15:A:1012:CLA:H51	4:B:436:VAL:HG13	1.54	0.87
5:C:10:ASN:HB3	5:C:60:THR:HG21	1.63	0.79
15:B:1230:CLA:HBA1	18:B:4005:BCR:H281	1.65	0.79
3:A:157:VAL:HG21	15:A:1114:CLA:HAA2	1.66	0.78
15:B:1229:CLA:HMB2	18:B:4005:BCR:H21C	1.67	0.77

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	142/222 (64%)	122 (86%)	17 (12%)	3 (2%)	7	39
1	3	148/222 (67%)	124 (84%)	18 (12%)	6 (4%)	3	25
2	4	112/214 (52%)	96 (86%)	7 (6%)	9 (8%)	1	14
3	A	738/740 (100%)	645 (87%)	82 (11%)	11 (2%)	10	45
4	B	723/725 (100%)	630 (87%)	86 (12%)	7 (1%)	15	53
5	C	78/80 (98%)	69 (88%)	8 (10%)	1 (1%)	12	48
6	D	122/124 (98%)	107 (88%)	12 (10%)	3 (2%)	5	35
7	E	67/69 (97%)	52 (78%)	9 (13%)	6 (9%)	1	12
8	F	151/155 (97%)	132 (87%)	14 (9%)	5 (3%)	4	30
9	I	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
10	J	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	33
11	K	45/47 (96%)	36 (80%)	8 (18%)	1 (2%)	6	37
12	L	138/140 (99%)	110 (80%)	20 (14%)	8 (6%)	1	19
13	M	27/29 (93%)	25 (93%)	1 (4%)	1 (4%)	3	28
14	O	96/98 (98%)	84 (88%)	10 (10%)	2 (2%)	7	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2653/2935 (90%)	2293 (86%)	295 (11%)	65 (2%)	5 35

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	113	LEU
1	3	145	LEU
1	3	172	VAL
3	A	477	PRO
7	E	56	ASP

### 5.3.2 Protein sidechains [i](#)

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	2	109/178 (61%)	105 (96%)	4 (4%)	34 60
1	3	121/178 (68%)	95 (78%)	26 (22%)	1 6
2	4	93/175 (53%)	91 (98%)	2 (2%)	52 71
3	A	597/597 (100%)	587 (98%)	10 (2%)	60 78
4	B	592/593 (100%)	576 (97%)	16 (3%)	44 66
5	C	66/66 (100%)	64 (97%)	2 (3%)	41 64
6	D	104/104 (100%)	100 (96%)	4 (4%)	33 59
7	E	66/66 (100%)	64 (97%)	2 (3%)	41 64
8	F	135/137 (98%)	120 (89%)	15 (11%)	6 26
9	I	27/27 (100%)	26 (96%)	1 (4%)	34 60
10	J	34/34 (100%)	34 (100%)	0	100 100
11	K	35/36 (97%)	35 (100%)	0	100 100
12	L	113/113 (100%)	110 (97%)	3 (3%)	44 66
13	M	22/23 (96%)	22 (100%)	0	100 100
14	O	77/77 (100%)	74 (96%)	3 (4%)	32 58
All	All	2191/2404 (91%)	2103 (96%)	88 (4%)	31 57

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	631	ASN
4	B	315	LYS
9	I	10	LEU
3	A	694	ILE
4	B	177	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	213	GLN
3	A	420	ASN
4	B	450	GLN
1	3	130	GLN
4	B	203	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

147 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
15	CLA	A	1102	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	3	601	-	22,32,73	3.05	9 (40%)	26,54,113	2.61	10 (38%)
15	CLA	4	602	-	22,32,73	3.10	9 (40%)	26,54,113	2.59	10 (38%)
15	CLA	K	1401	-	22,32,73	3.09	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1203	-	22,32,73	3.09	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	B	1222	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1201	-	22,32,73	3.10	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	A	1111	-	22,32,73	3.11	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	2	614	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1140	-	22,32,73	3.09	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	3	606	-	22,32,73	3.07	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	B	1235	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1206	-	22,32,73	3.08	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	3	603	-	22,32,73	3.08	10 (45%)	26,54,113	2.62	10 (38%)
15	CLA	A	1121	-	22,32,73	3.07	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	A	1120	-	22,32,73	3.08	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	B	1232	-	59,73,73	1.31	8 (13%)	67,113,113	1.88	10 (14%)
15	CLA	L	1501	-	22,32,73	3.06	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1137	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	4	611	-	22,32,73	3.07	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	F	1301	-	36,53,73	1.64	7 (19%)	39,89,113	2.15	8 (20%)
15	CLA	B	1231	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	4	601	-	22,32,73	3.09	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	B	1023	-	44,58,73	1.50	7 (15%)	49,95,113	2.07	10 (20%)
15	CLA	3	614	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	2	610	-	22,32,73	3.08	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	J	1302	-	44,58,73	1.53	9 (20%)	49,95,113	2.25	13 (26%)
18	BCR	A	4011	-	41,41,41	1.85	4 (9%)	56,56,56	4.34	18 (32%)
15	CLA	A	1130	-	49,63,73	1.43	8 (16%)	55,101,113	2.03	11 (20%)
15	CLA	O	1603	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1209	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1112	-	22,32,73	3.10	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	2	616	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1219	-	22,32,73	3.09	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1236	-	36,53,73	1.66	8 (22%)	39,89,113	2.16	8 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	B	1237	-	49,63,73	1.42	7 (14%)	55,101,113	2.01	11 (20%)
15	CLA	A	1124	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
17	SF4	C	3003	-	0,12,12	0.00	-	-		
15	CLA	2	606	-	22,32,73	3.08	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	A	1116	-	49,63,73	1.45	8 (16%)	55,101,113	1.92	10 (18%)
15	CLA	B	1229	-	44,58,73	1.51	7 (15%)	49,95,113	2.17	13 (26%)
15	CLA	B	1202	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	F	1302	-	22,32,73	3.07	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	3	610	-	22,32,73	3.09	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	4	605	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	3	604	-	22,32,73	3.08	9 (40%)	26,54,113	2.61	10 (38%)
15	CLA	L	1502	-	22,32,73	3.10	9 (40%)	26,54,113	2.59	10 (38%)
15	CLA	B	1227	-	22,32,73	3.08	9 (40%)	26,54,113	2.58	9 (34%)
15	CLA	B	1216	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1239	-	22,32,73	3.08	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	A	1105	-	49,63,73	1.43	8 (16%)	55,101,113	2.04	9 (16%)
15	CLA	A	1131	-	36,53,73	1.66	8 (22%)	39,89,113	2.07	6 (15%)
15	CLA	3	602	-	22,32,73	3.09	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	2	613	-	22,32,73	3.07	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	A	1136	-	22,32,73	3.07	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	A	1107	3	49,63,73	1.45	8 (16%)	55,101,113	1.99	11 (20%)
15	CLA	A	1114	-	40,54,73	1.57	8 (20%)	44,90,113	1.96	7 (15%)
15	CLA	B	1021	-	36,53,73	1.63	7 (19%)	39,89,113	2.02	8 (20%)
18	BCR	B	4005	-	41,41,41	1.86	4 (9%)	56,56,56	4.36	18 (32%)
15	CLA	2	612	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1101	-	36,53,73	1.66	8 (22%)	39,89,113	2.09	7 (17%)
15	CLA	4	608	-	22,32,73	3.07	9 (40%)	26,54,113	2.57	10 (38%)
17	SF4	A	3001	-	0,12,12	0.00	-	-		
15	CLA	A	1135	-	22,32,73	3.10	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	A	1117	-	49,63,73	1.42	7 (14%)	55,101,113	2.03	10 (18%)
15	CLA	B	1238	-	22,32,73	3.10	9 (40%)	26,54,113	2.56	10 (38%)
18	BCR	A	4017	-	41,41,41	1.85	4 (9%)	56,56,56	4.51	16 (28%)
15	CLA	B	1223	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	A	1011	-	44,58,73	1.49	7 (15%)	49,95,113	2.16	12 (24%)
15	CLA	A	1122	-	22,32,73	3.06	9 (40%)	26,54,113	2.58	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	4	612	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	2	605	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1132	-	22,32,73	3.09	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	A	1133	-	22,32,73	3.07	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1221	-	22,32,73	3.07	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	O	1601	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1141	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
18	BCR	A	4007	-	41,41,41	1.82	5 (12%)	56,56,56	4.60	18 (32%)
15	CLA	2	611	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1103	-	49,63,73	1.40	7 (14%)	55,101,113	1.99	12 (21%)
15	CLA	4	615	-	22,32,73	3.08	9 (40%)	26,54,113	2.54	10 (38%)
15	CLA	2	603	-	22,32,73	3.10	9 (40%)	26,54,113	2.54	10 (38%)
15	CLA	A	1129	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1126	-	49,63,73	1.43	8 (16%)	55,101,113	1.96	10 (18%)
15	CLA	B	1228	4	22,32,73	3.04	10 (45%)	26,54,113	2.74	10 (38%)
15	CLA	A	1104	-	49,63,73	1.43	9 (18%)	55,101,113	2.00	10 (18%)
15	CLA	4	604	-	22,32,73	3.09	9 (40%)	26,54,113	2.58	10 (38%)
18	BCR	A	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.46	17 (30%)
15	CLA	2	615	-	22,32,73	3.09	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1204	-	22,32,73	3.10	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1230	-	41,55,73	1.53	6 (14%)	45,91,113	2.32	13 (28%)
18	BCR	B	4008	-	41,41,41	1.86	4 (9%)	56,56,56	4.55	15 (26%)
15	CLA	B	1225	-	44,58,73	1.50	7 (15%)	49,95,113	2.03	9 (18%)
15	CLA	B	1224	-	49,63,73	1.42	8 (16%)	55,101,113	1.99	11 (20%)
15	CLA	A	1138	-	22,32,73	3.09	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1215	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1012	-	49,63,73	1.43	9 (18%)	55,101,113	1.95	10 (18%)
15	CLA	4	603	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	3	612	-	22,32,73	3.06	9 (40%)	26,54,113	2.54	10 (38%)
15	CLA	3	607	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1013	-	49,63,73	1.43	7 (14%)	55,101,113	1.98	11 (20%)
15	CLA	K	1402	-	22,32,73	3.06	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	A	1106	-	49,63,73	1.42	7 (14%)	55,101,113	2.00	10 (18%)
15	CLA	O	1602	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1212	-	22,32,73	3.07	9 (40%)	26,54,113	2.55	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	SF4	C	3002	-	0,12,12	0.00	-	-		
15	CLA	A	1118	-	22,32,73	3.10	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	A	1139	-	22,32,73	3.07	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	4	616	-	22,32,73	3.07	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	2	601	-	22,32,73	3.09	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	2	608	-	22,32,73	3.09	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1220	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1110	-	22,32,73	3.10	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	4	610	-	22,32,73	3.09	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	A	1108	-	22,32,73	3.10	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	2	607	1	22,32,73	3.10	9 (40%)	26,54,113	2.47	9 (34%)
16	PQN	A	2001	-	34,34,34	0.43	0	42,45,45	1.07	3 (7%)
15	CLA	3	608	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	2	602	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1207	-	22,32,73	3.06	9 (40%)	26,54,113	2.58	10 (38%)
15	CLA	B	1208	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	3	611	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1109	-	22,32,73	3.11	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	A	1123	-	22,32,73	3.10	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	L	1503	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1134	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	4	609	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	A	1128	-	22,32,73	3.10	9 (40%)	26,54,113	2.55	10 (38%)
15	CLA	4	606	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1214	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	2	604	-	22,32,73	3.11	9 (40%)	26,54,113	2.59	10 (38%)
15	CLA	A	1115	-	49,63,73	1.44	8 (16%)	55,101,113	2.00	11 (20%)
18	BCR	A	4008	-	41,41,41	1.84	4 (9%)	56,56,56	4.37	13 (23%)
15	CLA	B	1218	-	22,32,73	3.08	9 (40%)	26,54,113	2.56	10 (38%)
16	PQN	B	2002	-	34,34,34	0.39	0	42,45,45	1.16	3 (7%)
15	CLA	B	1217	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1113	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
18	BCR	I	4018	-	41,41,41	1.86	4 (9%)	56,56,56	4.33	17 (30%)
15	CLA	B	1022	-	22,32,73	3.07	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1234	-	22,32,73	3.09	9 (40%)	26,54,113	2.57	10 (38%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A	1127	-	22,32,73	3.09	8 (36%)	26,54,113	2.56	10 (38%)
15	CLA	A	1119	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1226	-	49,63,73	1.43	6 (12%)	55,101,113	2.06	10 (18%)
15	CLA	B	1210	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1211	-	22,32,73	3.10	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	A	1125	-	22,32,73	3.06	9 (40%)	26,54,113	2.56	10 (38%)
15	CLA	B	1205	-	22,32,73	3.04	9 (40%)	26,54,113	2.62	10 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1102	-	3/3/7/25	-	-
15	CLA	3	601	-	3/3/7/25	-	-
15	CLA	4	602	-	3/3/7/25	-	-
15	CLA	K	1401	-	3/3/7/25	-	-
15	CLA	B	1203	-	3/3/7/25	-	-
15	CLA	B	1222	-	3/3/7/25	-	-
15	CLA	B	1201	-	3/3/7/25	-	-
15	CLA	A	1111	-	3/3/7/25	-	-
15	CLA	2	614	-	3/3/7/25	-	-
15	CLA	A	1140	-	3/3/7/25	-	-
15	CLA	3	606	-	3/3/7/25	-	-
15	CLA	B	1235	-	3/3/7/25	-	-
15	CLA	B	1206	-	3/3/7/25	-	-
15	CLA	3	603	-	3/3/7/25	-	-
15	CLA	A	1121	-	3/3/7/25	-	-
15	CLA	A	1120	-	3/3/7/25	-	-
15	CLA	B	1232	-	3/3/20/25	17/37/135/135	-
15	CLA	L	1501	-	3/3/7/25	-	-
15	CLA	A	1137	-	3/3/7/25	-	-
15	CLA	4	611	-	3/3/7/25	-	-
15	CLA	F	1301	-	3/3/16/25	4/11/111/135	-
15	CLA	B	1231	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	4	601	-	3/3/7/25	-	-
15	CLA	B	1023	-	3/3/17/25	9/19/117/135	-
15	CLA	3	614	-	3/3/7/25	-	-
15	CLA	2	610	-	3/3/7/25	-	-
15	CLA	J	1302	-	3/3/17/25	13/19/117/135	-
18	BCR	A	4011	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1130	-	3/3/18/25	14/25/123/135	-
15	CLA	O	1603	-	3/3/7/25	-	-
15	CLA	B	1209	-	3/3/7/25	-	-
15	CLA	A	1112	-	3/3/7/25	-	-
15	CLA	2	616	-	3/3/7/25	-	-
15	CLA	B	1219	-	3/3/7/25	-	-
15	CLA	B	1236	-	3/3/16/25	6/11/111/135	-
15	CLA	B	1237	-	3/3/18/25	11/25/123/135	-
15	CLA	A	1124	-	3/3/7/25	-	-
17	SF4	C	3003	-	-	-	0/6/5/5
15	CLA	2	606	-	3/3/7/25	-	-
15	CLA	A	1116	-	3/3/18/25	16/25/123/135	-
15	CLA	B	1229	-	3/3/17/25	6/19/117/135	-
15	CLA	B	1202	-	3/3/7/25	-	-
15	CLA	F	1302	-	3/3/7/25	-	-
15	CLA	3	610	-	3/3/7/25	-	-
15	CLA	4	605	-	3/3/7/25	-	-
15	CLA	3	604	-	3/3/7/25	-	-
15	CLA	L	1502	-	3/3/7/25	-	-
15	CLA	B	1227	-	3/3/7/25	-	-
15	CLA	B	1216	-	3/3/7/25	-	-
15	CLA	B	1239	-	3/3/7/25	-	-
15	CLA	A	1105	-	3/3/18/25	9/25/123/135	-
15	CLA	A	1131	-	3/3/16/25	2/11/111/135	-
15	CLA	3	602	-	3/3/7/25	-	-
15	CLA	2	613	-	3/3/7/25	-	-
15	CLA	A	1136	-	3/3/7/25	-	-
15	CLA	A	1107	3	3/3/18/25	10/25/123/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1114	-	3/3/16/25	6/15/113/135	-
15	CLA	B	1021	-	3/3/16/25	6/11/111/135	-
18	BCR	B	4005	-	-	15/29/63/63	0/2/2/2
15	CLA	2	612	-	3/3/7/25	-	-
15	CLA	A	1101	-	3/3/16/25	5/11/111/135	-
15	CLA	4	608	-	3/3/7/25	-	-
17	SF4	A	3001	-	-	-	0/6/5/5
15	CLA	A	1135	-	3/3/7/25	-	-
15	CLA	A	1117	-	3/3/18/25	12/25/123/135	-
15	CLA	B	1238	-	3/3/7/25	-	-
18	BCR	A	4017	-	-	12/29/63/63	0/2/2/2
15	CLA	B	1223	-	3/3/7/25	-	-
15	CLA	A	1011	-	3/3/17/25	6/19/117/135	-
15	CLA	A	1122	-	3/3/7/25	-	-
15	CLA	4	612	-	3/3/7/25	-	-
15	CLA	2	605	-	3/3/7/25	-	-
15	CLA	A	1132	-	3/3/7/25	-	-
15	CLA	A	1133	-	3/3/7/25	-	-
15	CLA	B	1221	-	3/3/7/25	-	-
15	CLA	O	1601	-	3/3/7/25	-	-
15	CLA	A	1141	-	3/3/7/25	-	-
18	BCR	A	4007	-	-	18/29/63/63	0/2/2/2
15	CLA	2	611	-	3/3/7/25	-	-
15	CLA	A	1103	-	3/3/18/25	10/25/123/135	-
15	CLA	4	615	-	3/3/7/25	-	-
15	CLA	2	603	-	3/3/7/25	-	-
15	CLA	A	1129	-	3/3/7/25	-	-
15	CLA	A	1126	-	3/3/18/25	13/25/123/135	-
15	CLA	B	1228	4	3/3/7/25	-	-
15	CLA	A	1104	-	3/3/18/25	12/25/123/135	-
15	CLA	4	604	-	3/3/7/25	-	-
18	BCR	A	4002	-	-	9/29/63/63	0/2/2/2
15	CLA	2	615	-	3/3/7/25	-	-
15	CLA	B	1204	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1230	-	3/3/16/25	9/16/114/135	-
18	BCR	B	4008	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1225	-	3/3/17/25	10/19/117/135	-
15	CLA	B	1224	-	3/3/18/25	15/25/123/135	-
15	CLA	A	1138	-	3/3/7/25	-	-
15	CLA	B	1215	-	3/3/7/25	-	-
15	CLA	A	1012	-	3/3/18/25	16/25/123/135	-
15	CLA	4	603	-	3/3/7/25	-	-
15	CLA	3	612	-	3/3/7/25	-	-
15	CLA	3	607	-	3/3/7/25	-	-
15	CLA	A	1013	-	3/3/18/25	15/25/123/135	-
15	CLA	K	1402	-	3/3/7/25	-	-
15	CLA	A	1106	-	3/3/18/25	12/25/123/135	-
15	CLA	O	1602	-	3/3/7/25	-	-
15	CLA	B	1212	-	3/3/7/25	-	-
17	SF4	C	3002	-	-	-	0/6/5/5
15	CLA	A	1118	-	3/3/7/25	-	-
15	CLA	A	1139	-	3/3/7/25	-	-
15	CLA	4	616	-	3/3/7/25	-	-
15	CLA	2	601	-	3/3/7/25	-	-
15	CLA	2	608	-	3/3/7/25	-	-
15	CLA	B	1220	-	3/3/7/25	-	-
15	CLA	A	1110	-	3/3/7/25	-	-
15	CLA	4	610	-	3/3/7/25	-	-
15	CLA	A	1108	-	3/3/7/25	-	-
15	CLA	2	607	1	3/3/7/25	-	-
16	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
15	CLA	3	608	-	3/3/7/25	-	-
15	CLA	2	602	-	3/3/7/25	-	-
15	CLA	B	1207	-	3/3/7/25	-	-
15	CLA	B	1208	-	3/3/7/25	-	-
15	CLA	3	611	-	3/3/7/25	-	-
15	CLA	A	1109	-	3/3/7/25	-	-
15	CLA	A	1123	-	3/3/7/25	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	L	1503	-	3/3/7/25	-	-
15	CLA	A	1134	-	3/3/7/25	-	-
15	CLA	4	609	-	3/3/7/25	-	-
15	CLA	A	1128	-	3/3/7/25	-	-
15	CLA	4	606	-	3/3/7/25	-	-
15	CLA	B	1214	-	3/3/7/25	-	-
15	CLA	2	604	-	3/3/7/25	-	-
15	CLA	A	1115	-	3/3/18/25	15/25/123/135	-
18	BCR	A	4008	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1218	-	3/3/7/25	-	-
16	PQN	B	2002	-	-	7/23/43/43	0/2/2/2
15	CLA	B	1217	-	3/3/7/25	-	-
15	CLA	A	1113	-	3/3/7/25	-	-
18	BCR	I	4018	-	-	17/29/63/63	0/2/2/2
15	CLA	B	1022	-	3/3/7/25	-	-
15	CLA	B	1234	-	3/3/7/25	-	-
15	CLA	A	1127	-	3/3/7/25	-	-
15	CLA	A	1119	-	3/3/7/25	-	-
15	CLA	B	1226	-	3/3/18/25	11/25/123/135	-
15	CLA	B	1210	-	3/3/7/25	-	-
15	CLA	B	1211	-	3/3/7/25	-	-
15	CLA	A	1125	-	3/3/7/25	-	-
15	CLA	B	1205	-	3/3/7/25	-	-

The worst 5 of 1200 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1111	CLA	CHB-C4A	9.52	1.42	1.34
15	A	1110	CLA	CHB-C4A	9.50	1.42	1.34
15	2	607	CLA	CHB-C4A	9.50	1.42	1.34
15	A	1134	CLA	CHB-C4A	9.48	1.42	1.34
15	A	1112	CLA	CHB-C4A	9.47	1.42	1.34

The worst 5 of 1477 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4007	BCR	C10-C11-C12	18.19	179.99	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	4008	BCR	C10-C11-C12	17.90	179.09	123.22
18	A	4017	BCR	C10-C11-C12	17.72	178.52	123.22
18	B	4008	BCR	C10-C11-C12	17.61	178.17	123.22
18	B	4005	BCR	C10-C11-C12	17.51	177.87	123.22

5 of 402 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	1102	CLA	NC
15	A	1102	CLA	ND
15	A	1102	CLA	NA
15	3	601	CLA	NC
15	3	601	CLA	ND

5 of 417 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	1232	CLA	C1A-C2A-CAA-CBA
15	B	1232	CLA	C3A-C2A-CAA-CBA
15	F	1301	CLA	CAD-CBD-CGD-O1D
15	B	1023	CLA	CBD-CGD-O2D-CED
15	J	1302	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

70 monomers are involved in 158 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	601	CLA	1	0
15	B	1203	CLA	2	0
15	B	1201	CLA	1	0
15	3	606	CLA	2	0
15	B	1206	CLA	1	0
15	B	1232	CLA	3	0
15	L	1501	CLA	1	0
15	F	1301	CLA	1	0
15	B	1023	CLA	6	0
15	J	1302	CLA	1	0
18	A	4011	BCR	11	0
15	A	1130	CLA	5	0
15	A	1112	CLA	1	0
15	B	1236	CLA	1	0
15	B	1237	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1124	CLA	1	0
17	C	3003	SF4	1	0
15	A	1116	CLA	2	0
15	B	1229	CLA	5	0
15	B	1202	CLA	1	0
15	3	610	CLA	1	0
15	3	604	CLA	1	0
15	L	1502	CLA	1	0
15	B	1227	CLA	1	0
15	B	1239	CLA	1	0
15	A	1105	CLA	4	0
15	A	1131	CLA	4	0
15	A	1107	CLA	2	0
15	A	1114	CLA	1	0
15	B	1021	CLA	5	0
18	B	4005	BCR	6	0
15	2	612	CLA	1	0
15	A	1135	CLA	1	0
15	A	1117	CLA	3	0
18	A	4017	BCR	5	0
15	A	1011	CLA	6	0
15	A	1122	CLA	1	0
15	4	612	CLA	1	0
18	A	4007	BCR	4	0
15	A	1103	CLA	3	0
15	4	615	CLA	1	0
15	A	1129	CLA	1	0
15	A	1126	CLA	12	0
15	B	1228	CLA	2	0
15	A	1104	CLA	1	0
18	A	4002	BCR	3	0
15	B	1230	CLA	6	0
18	B	4008	BCR	1	0
15	B	1225	CLA	4	0
15	B	1224	CLA	7	0
15	A	1012	CLA	7	0
15	A	1013	CLA	8	0
15	A	1106	CLA	6	0
15	B	1212	CLA	1	0
17	C	3002	SF4	3	0
15	A	1139	CLA	1	0
15	2	607	CLA	1	0

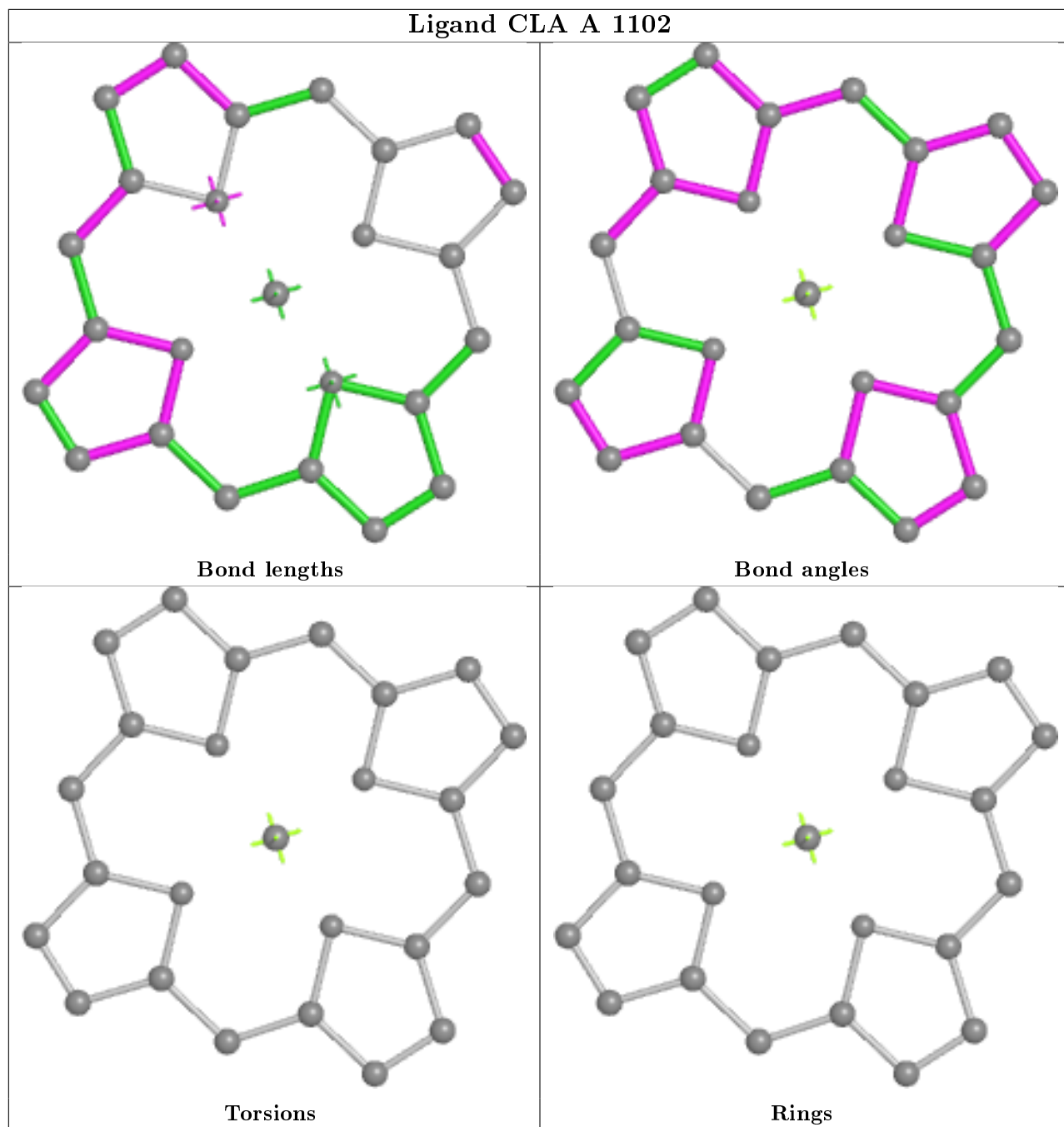
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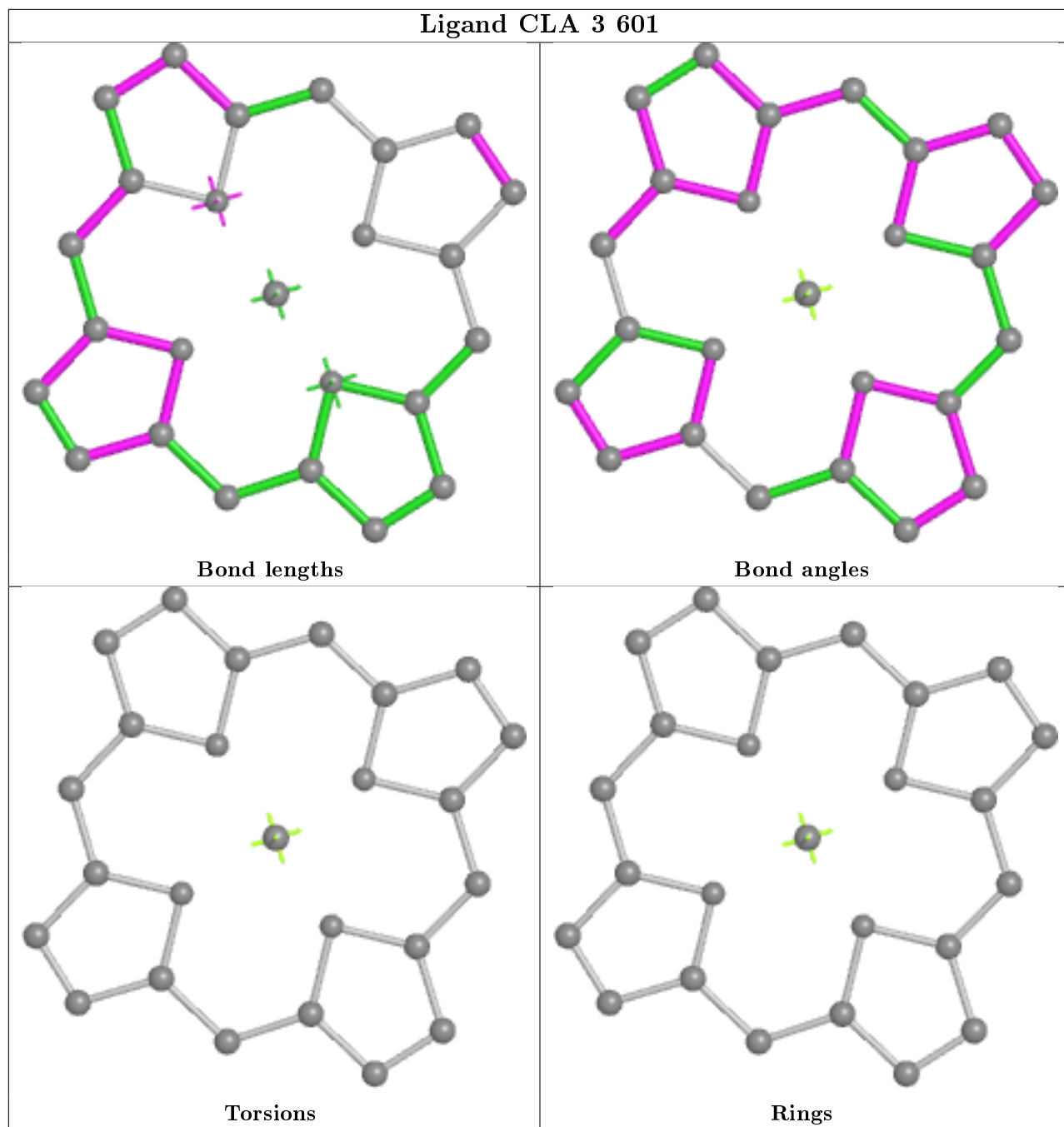
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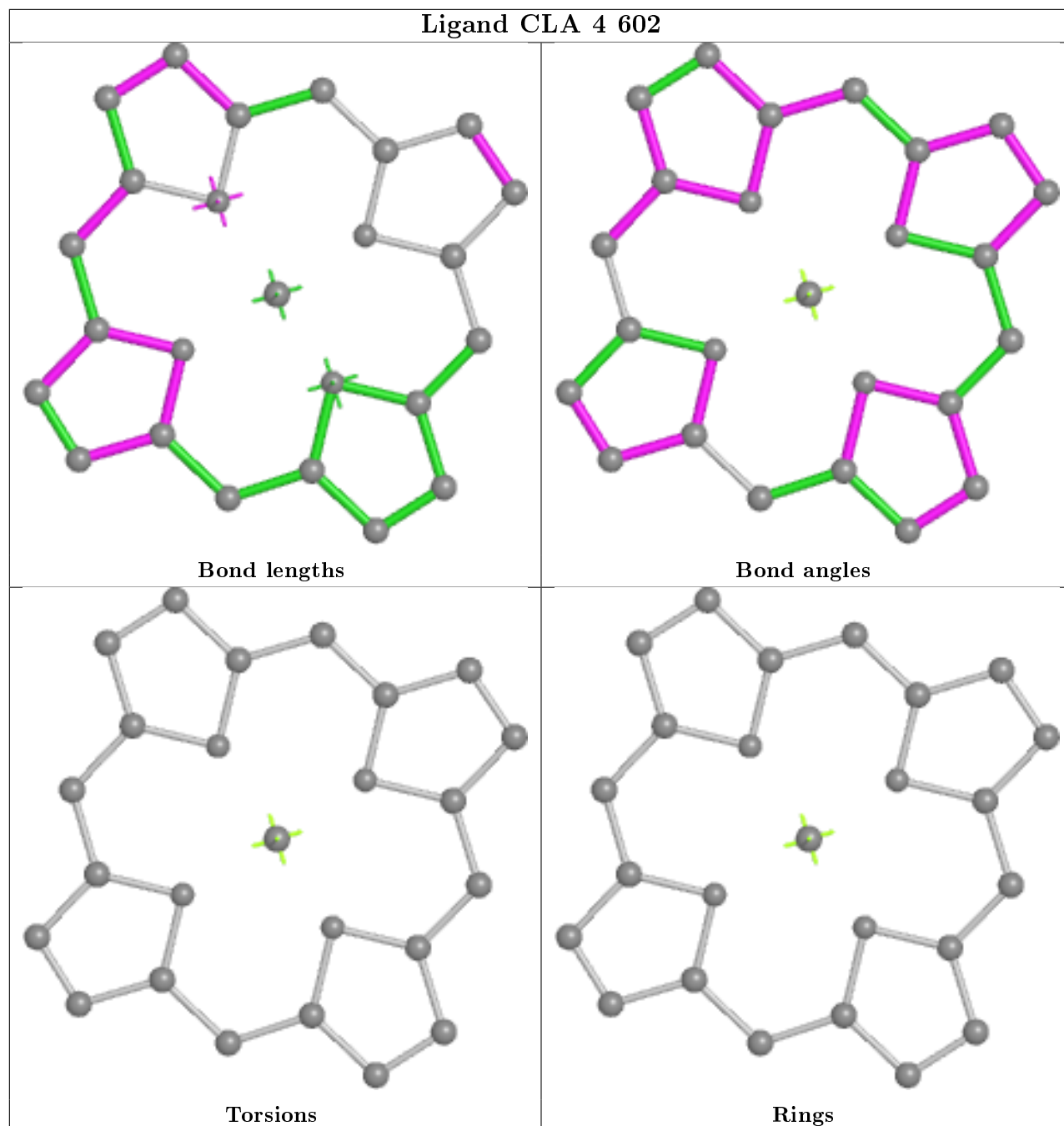
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	2001	PQN	3	0
15	B	1207	CLA	1	0
15	A	1123	CLA	1	0
15	4	606	CLA	1	0
15	A	1115	CLA	1	0
18	A	4008	BCR	1	0
16	B	2002	PQN	1	0
18	I	4018	BCR	4	0
15	B	1022	CLA	1	0
15	A	1127	CLA	1	0
15	B	1226	CLA	5	0
15	B	1210	CLA	1	0
15	B	1205	CLA	1	0

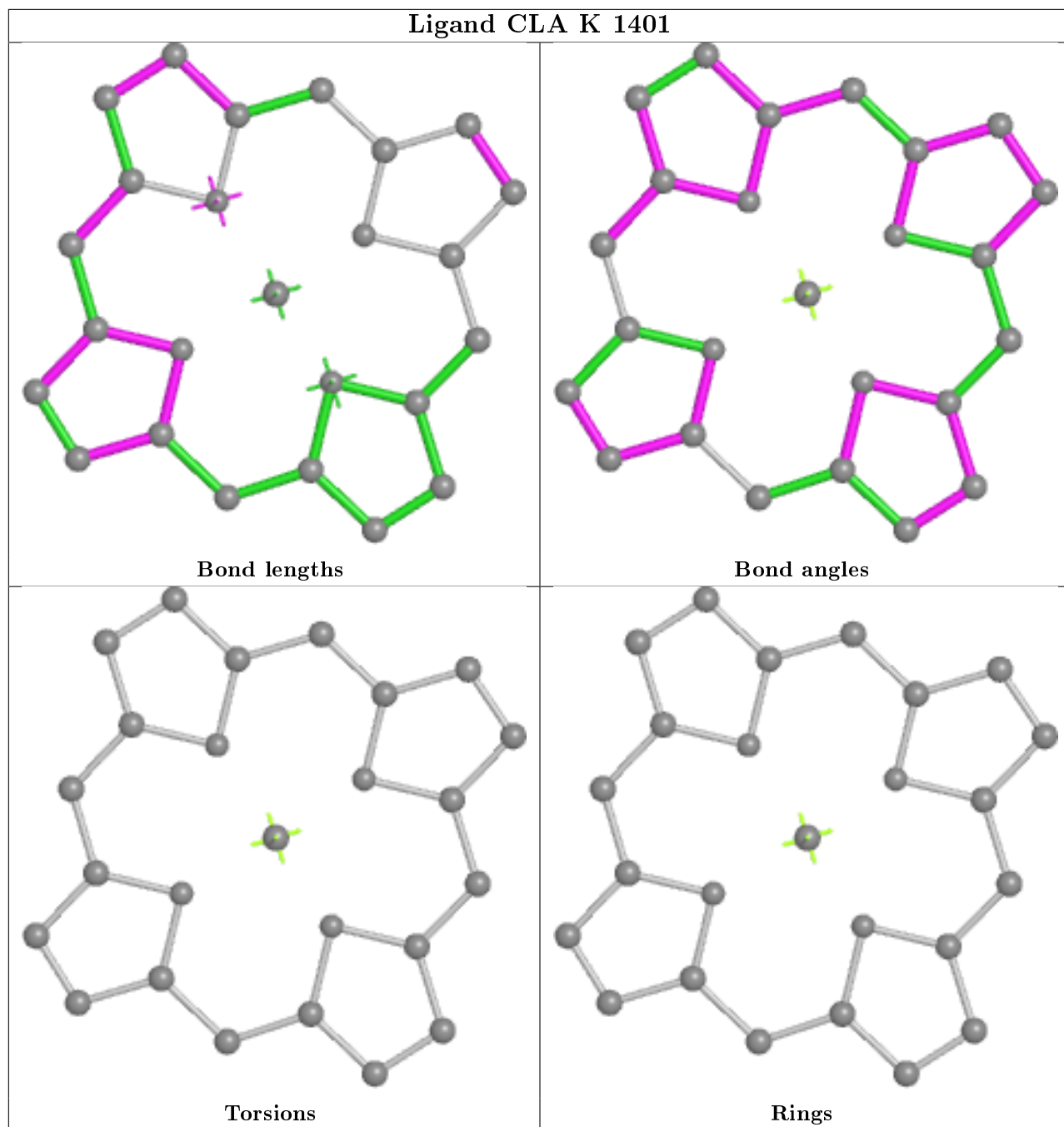
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

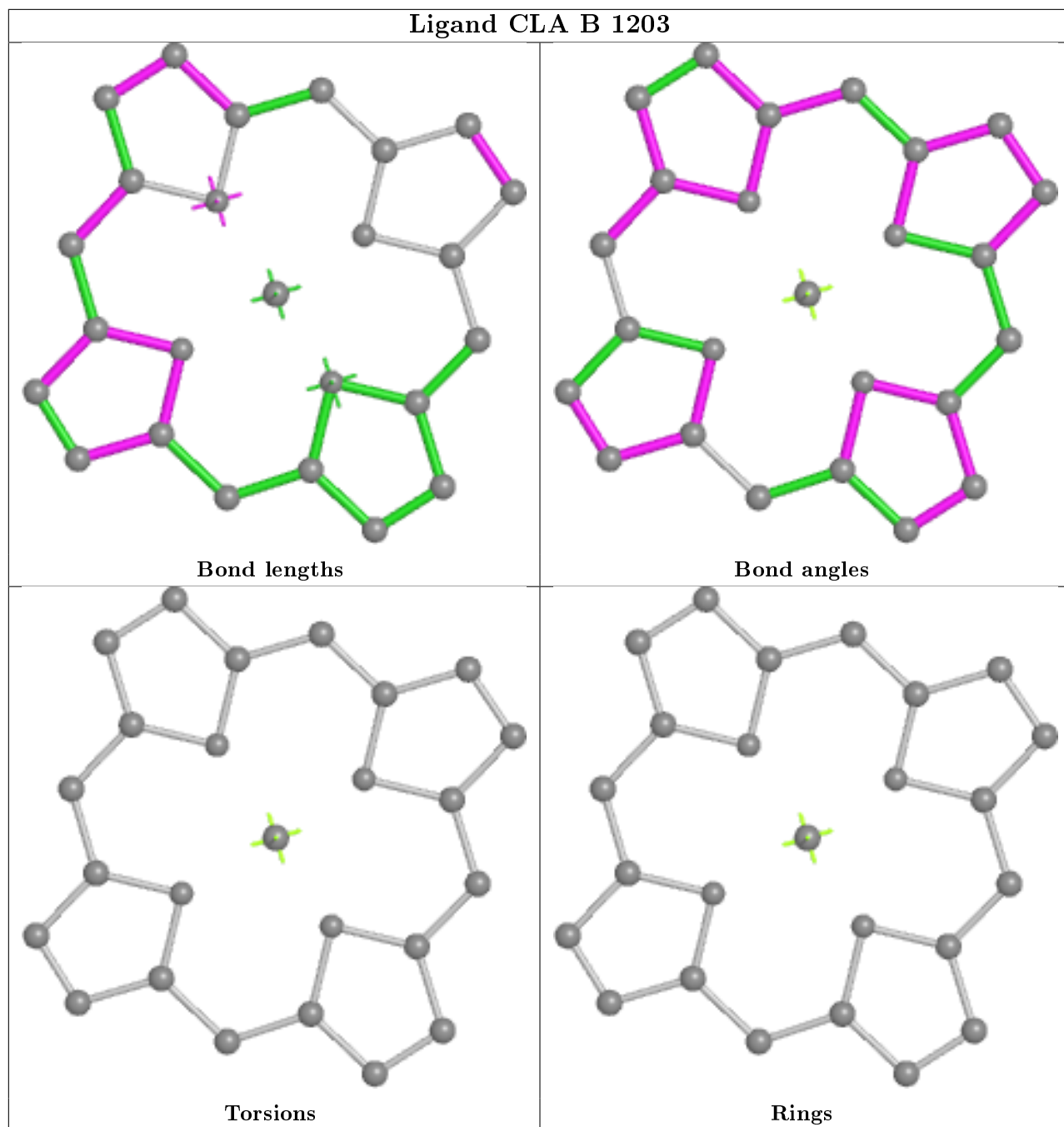


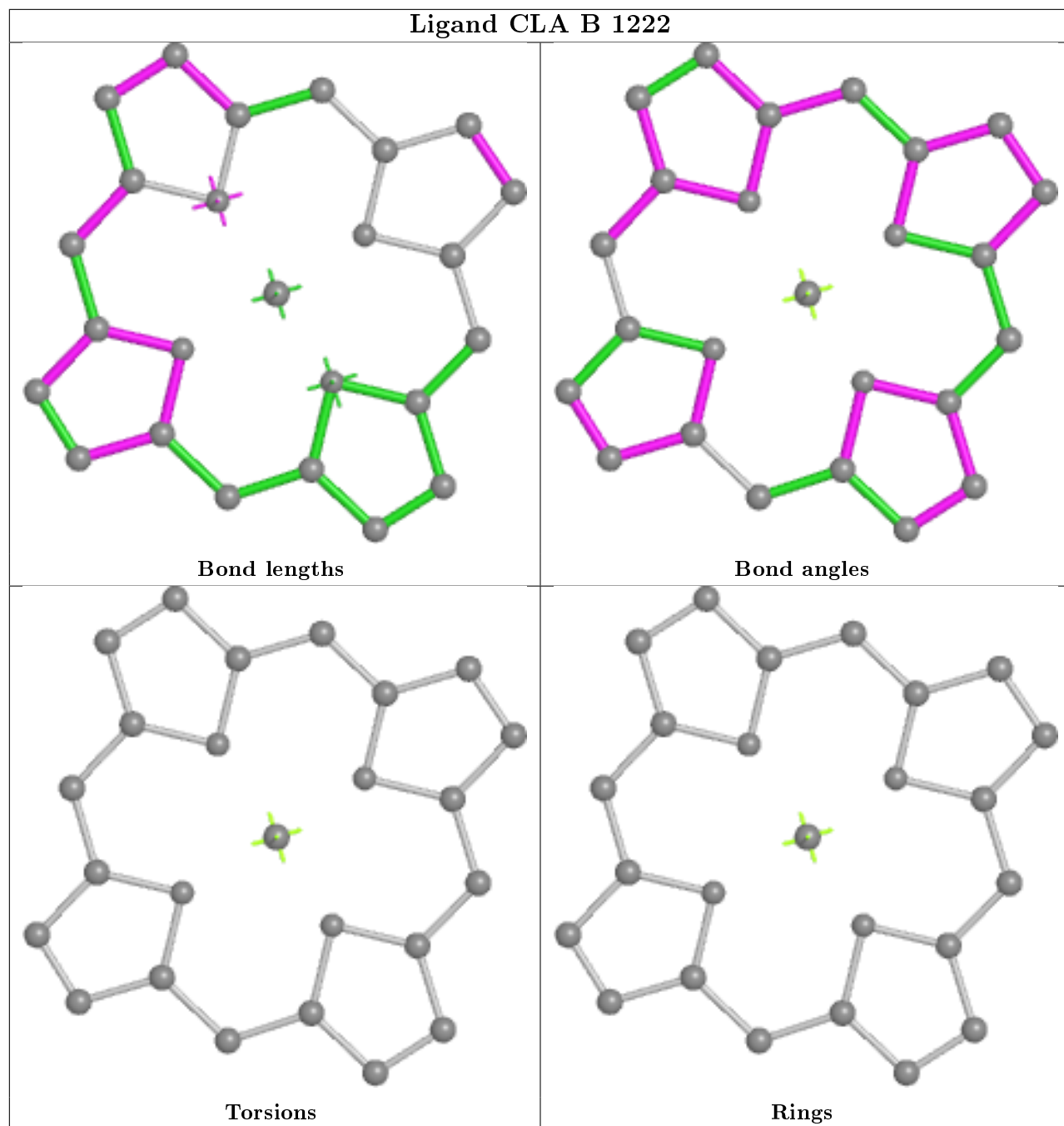


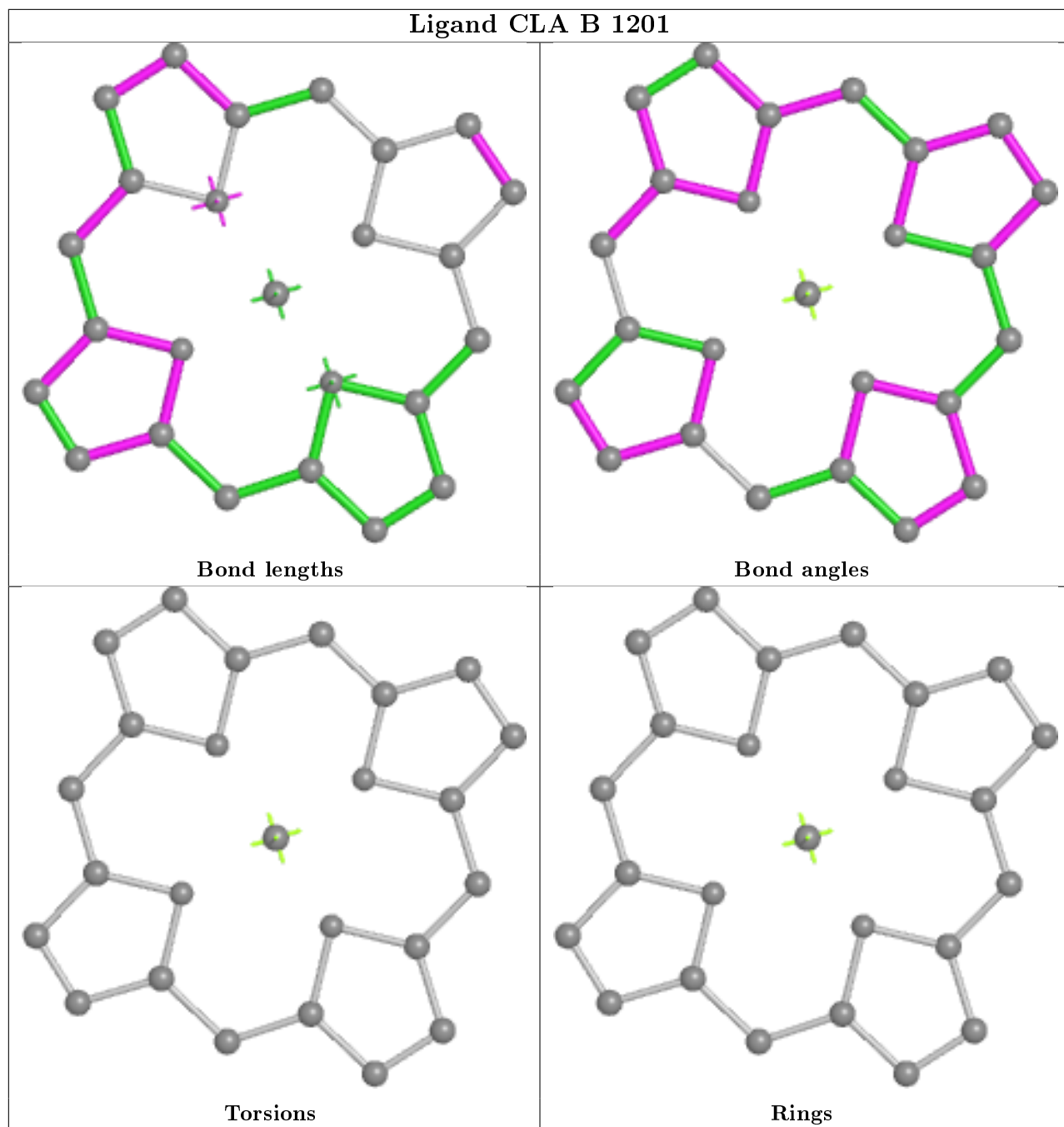


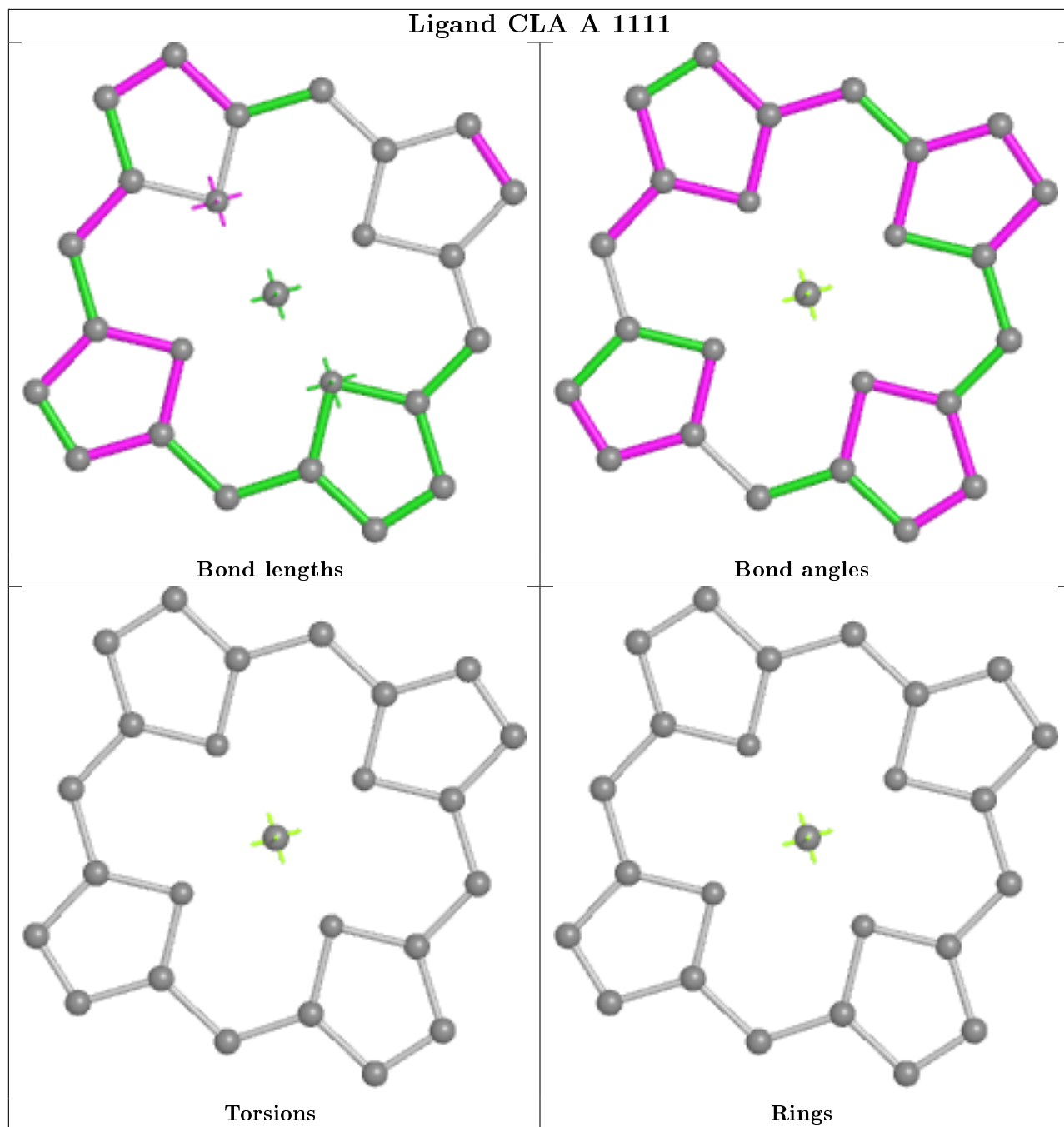




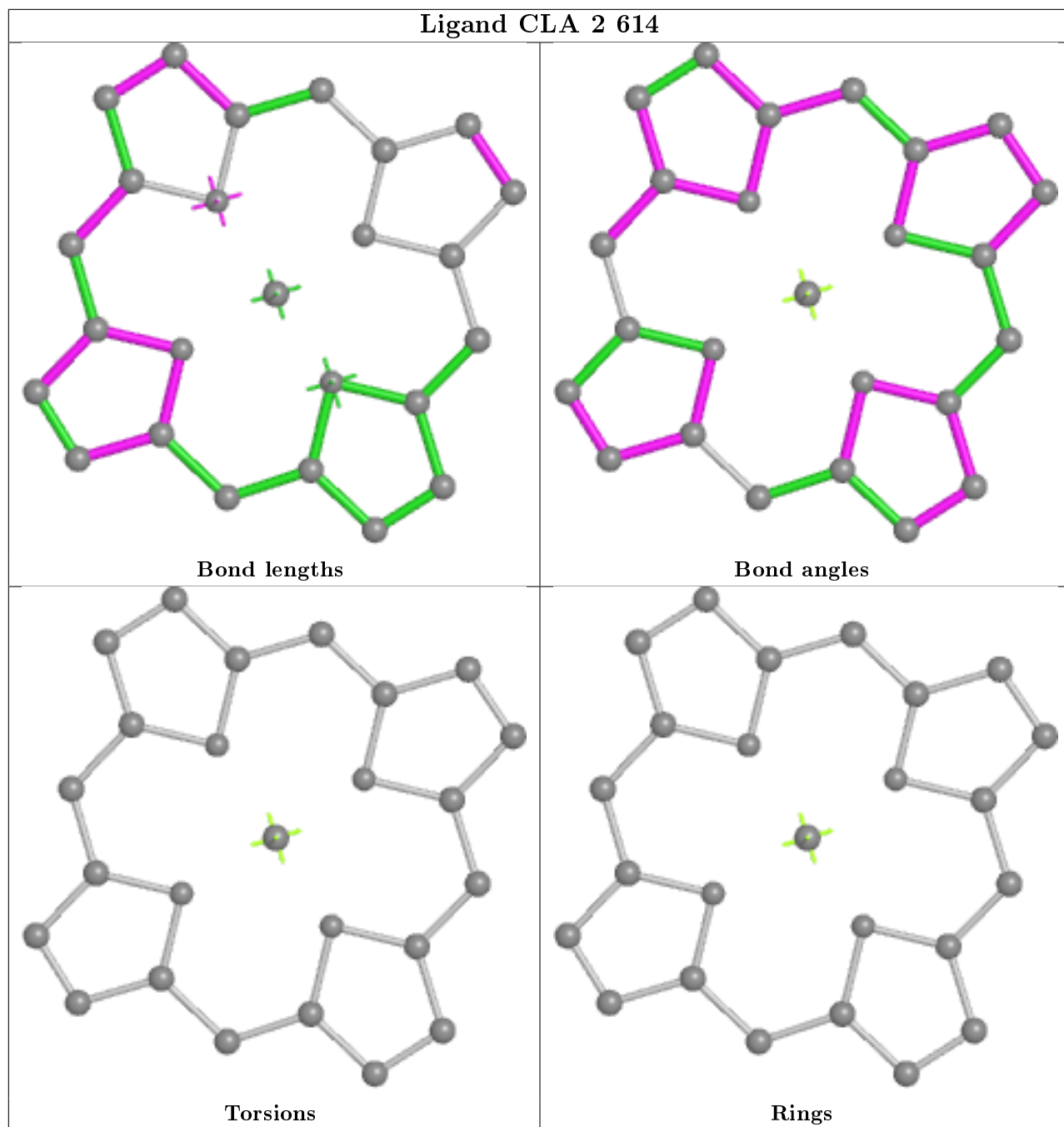


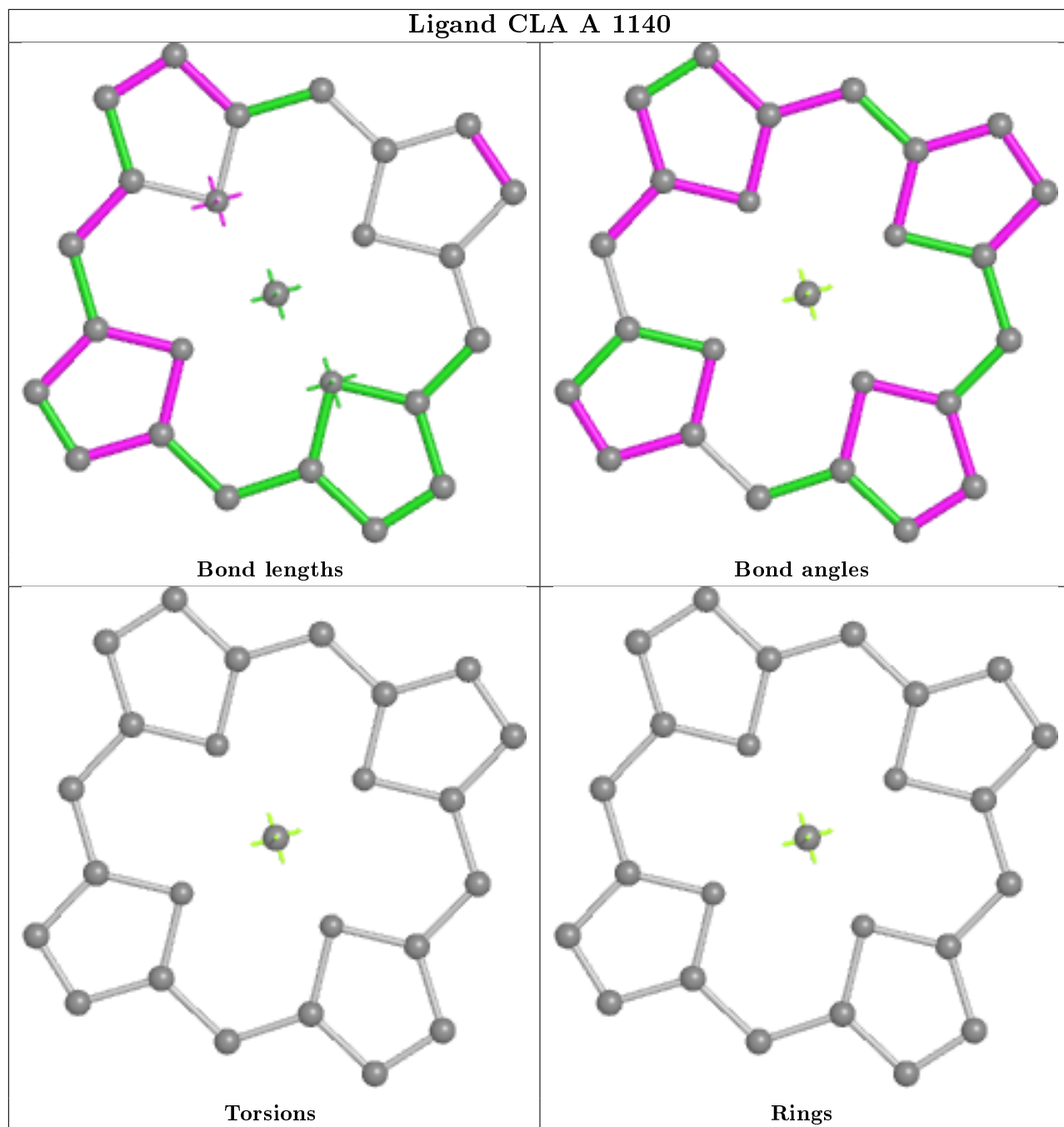


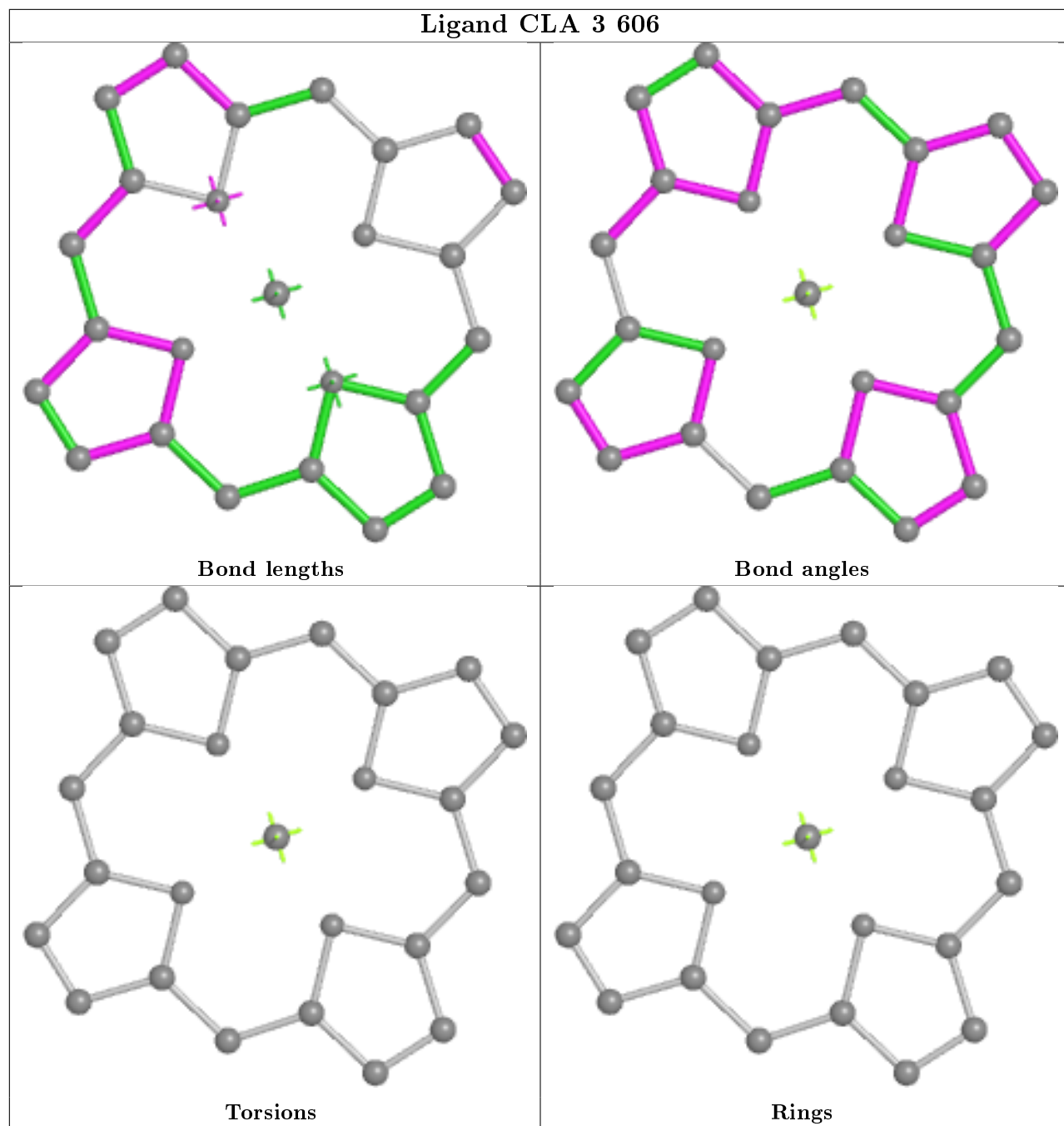


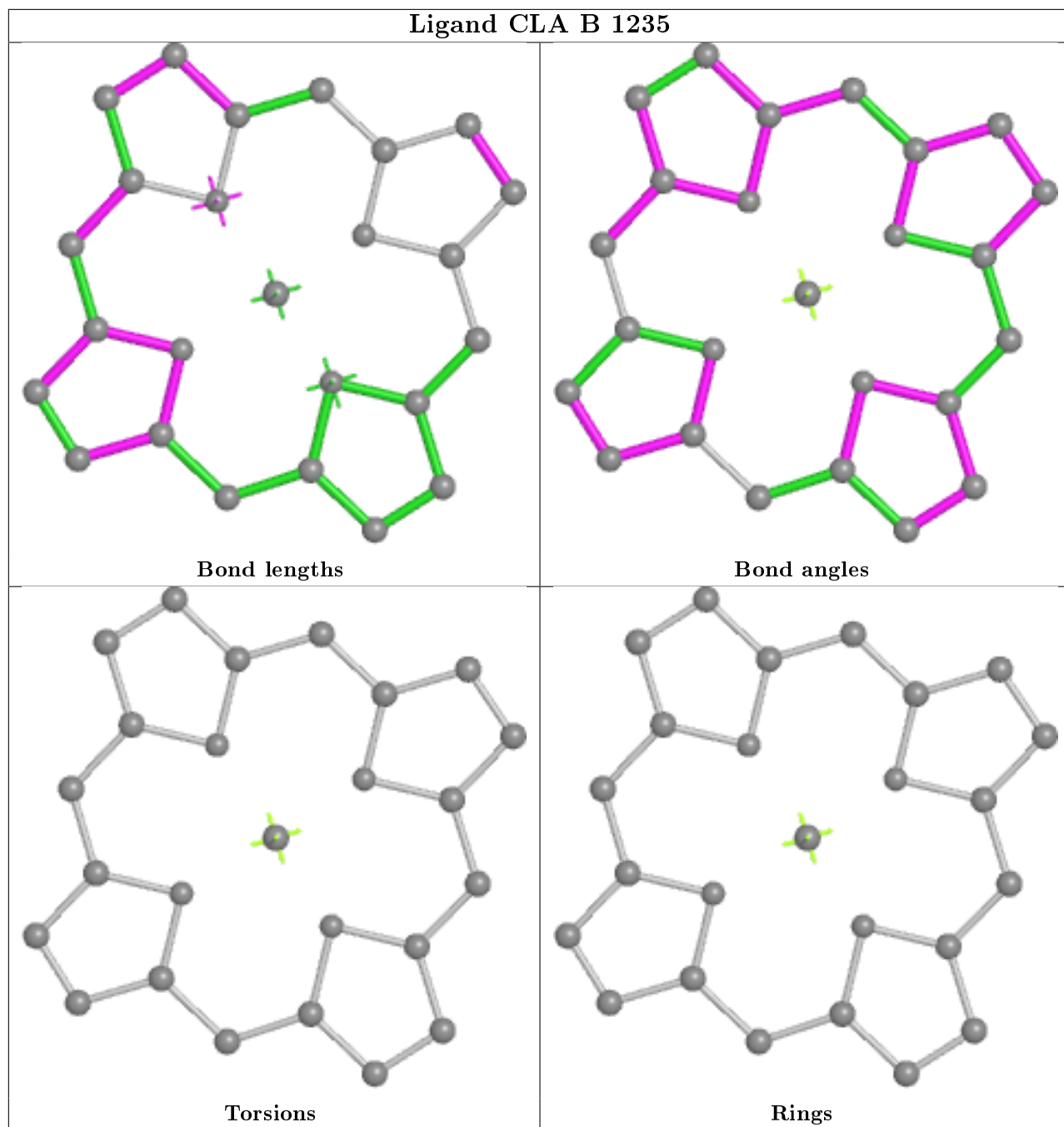


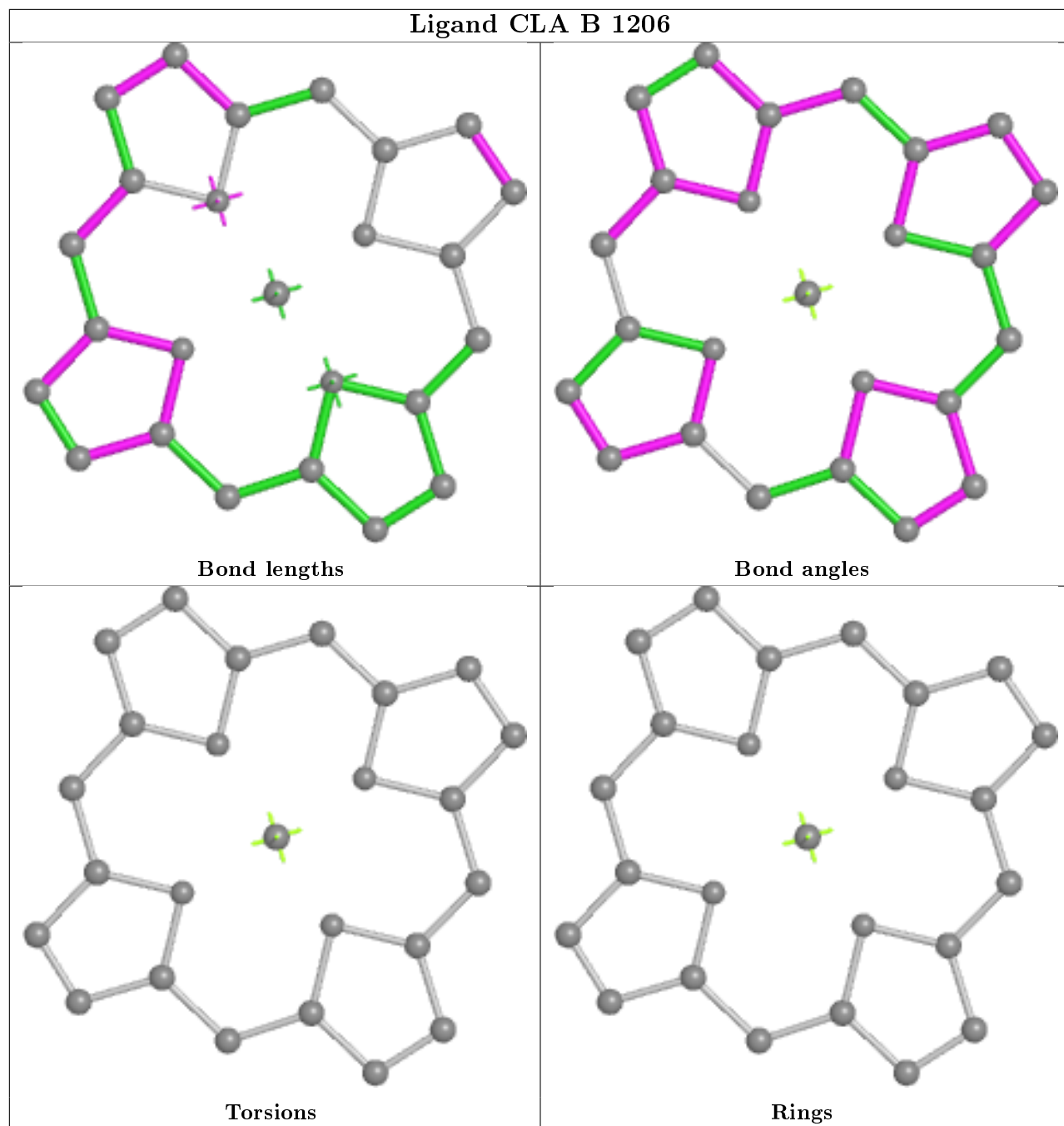


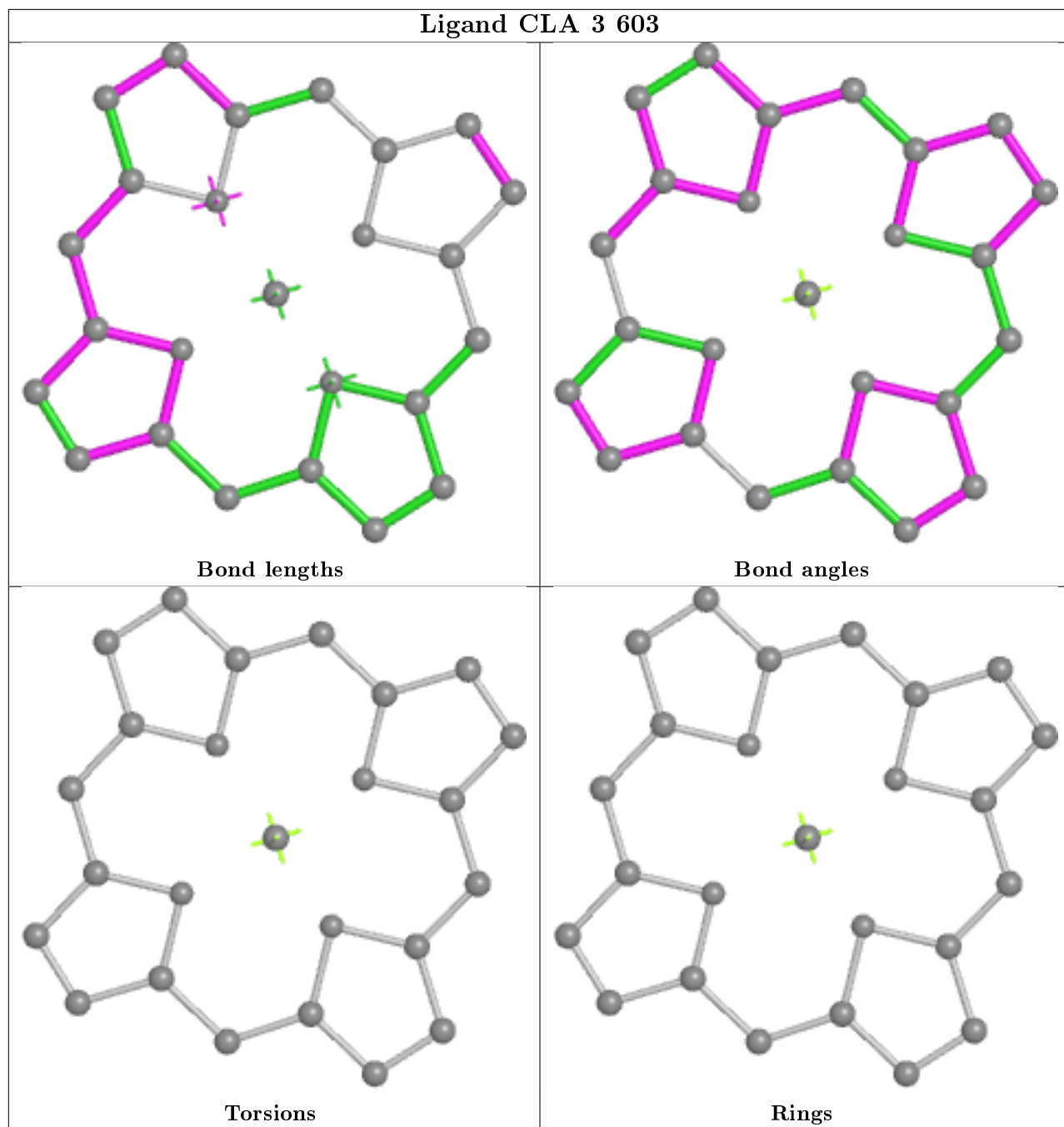


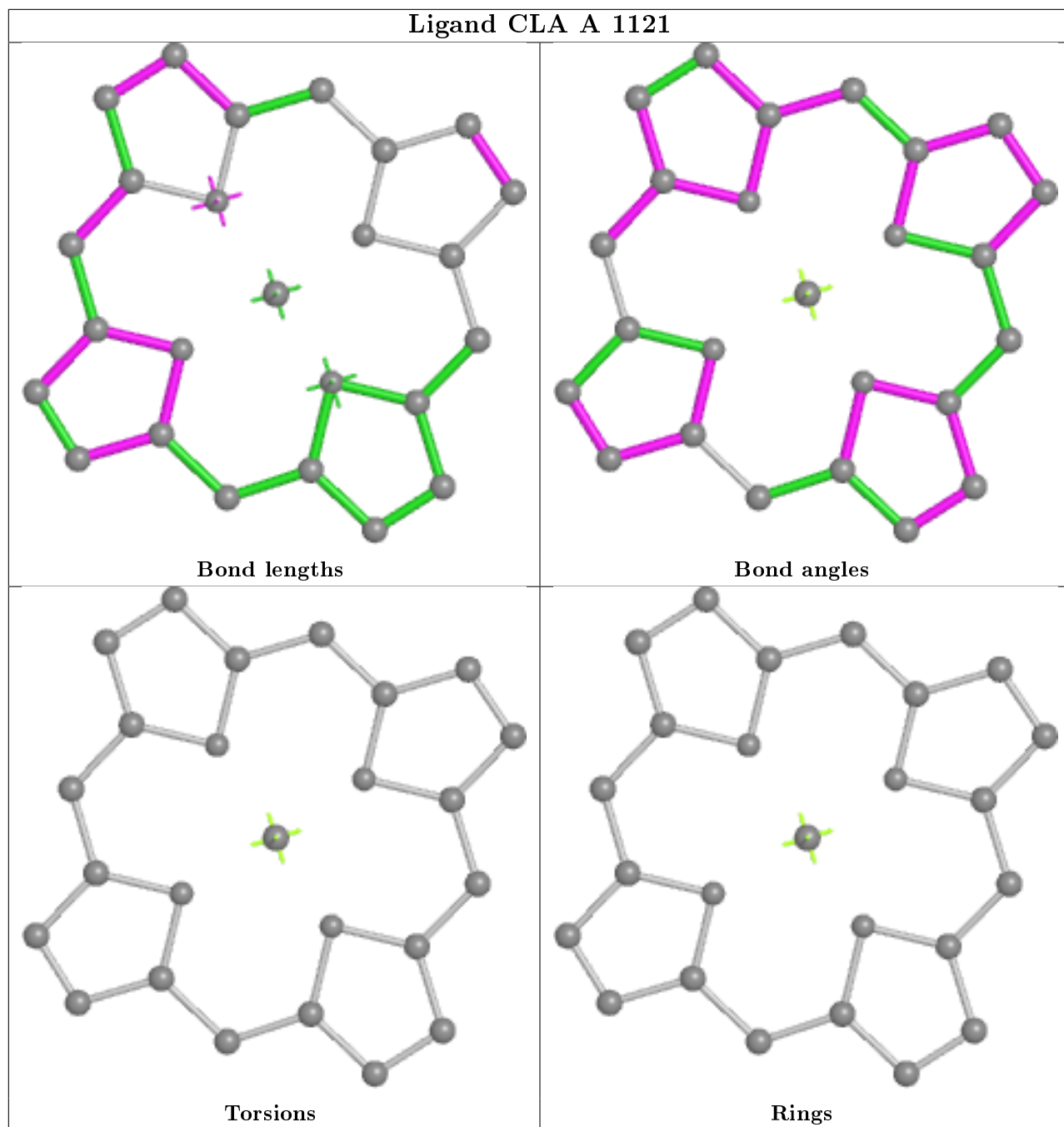


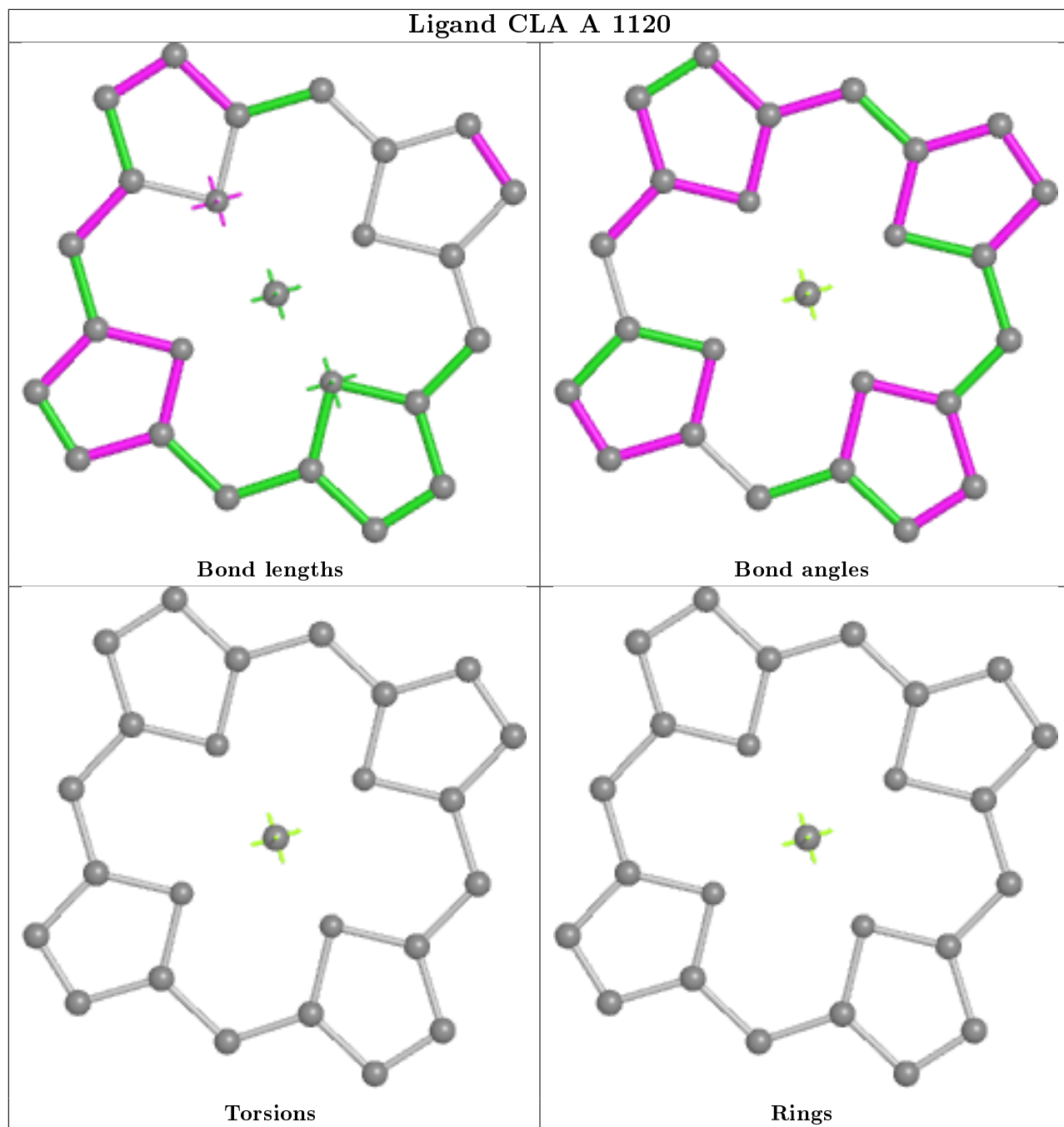




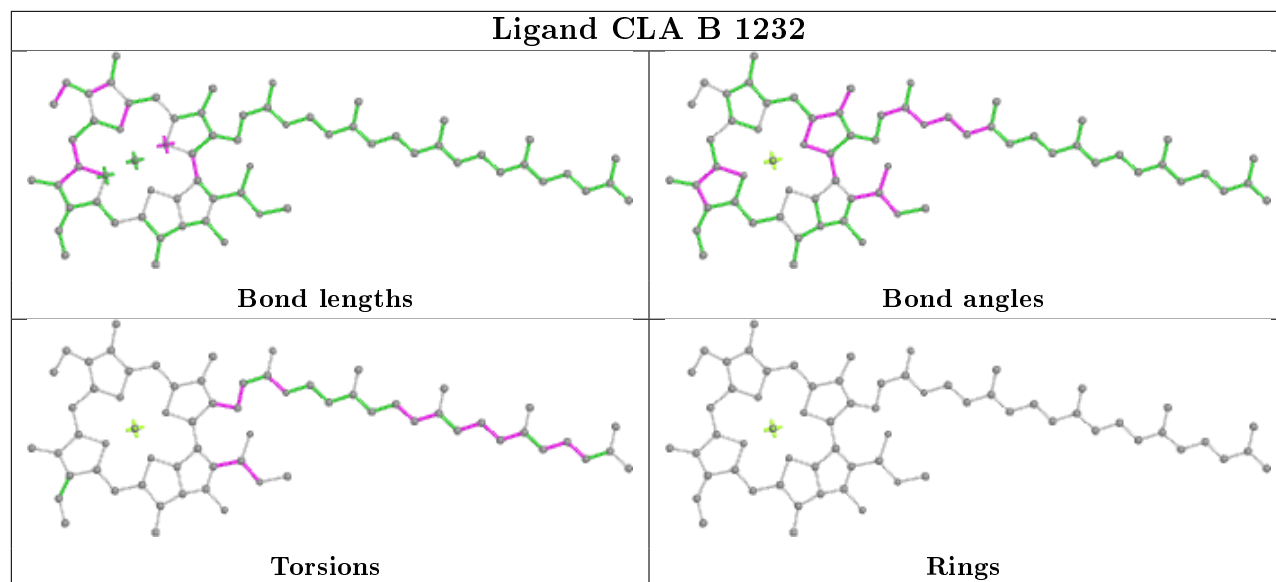


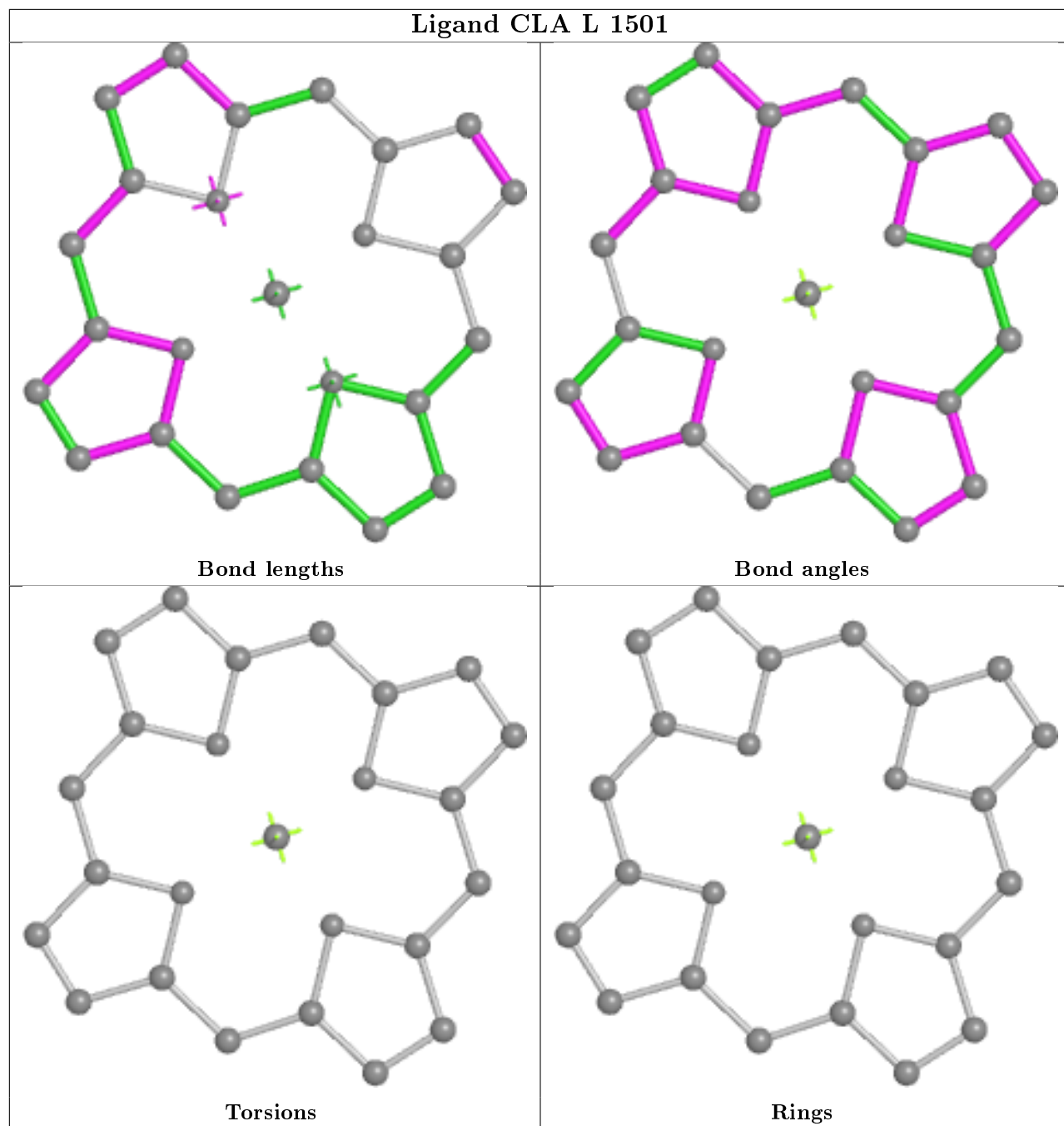


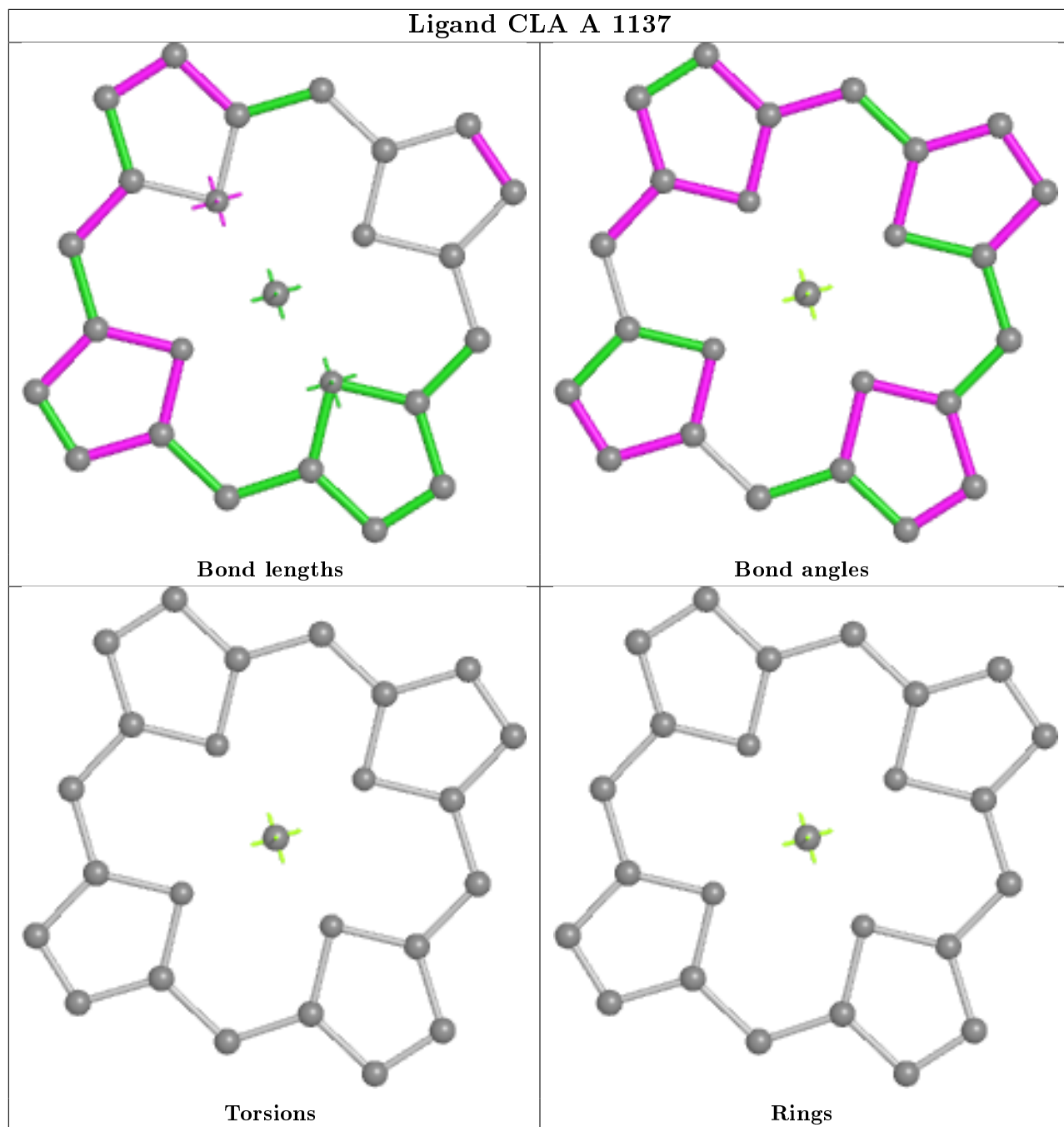


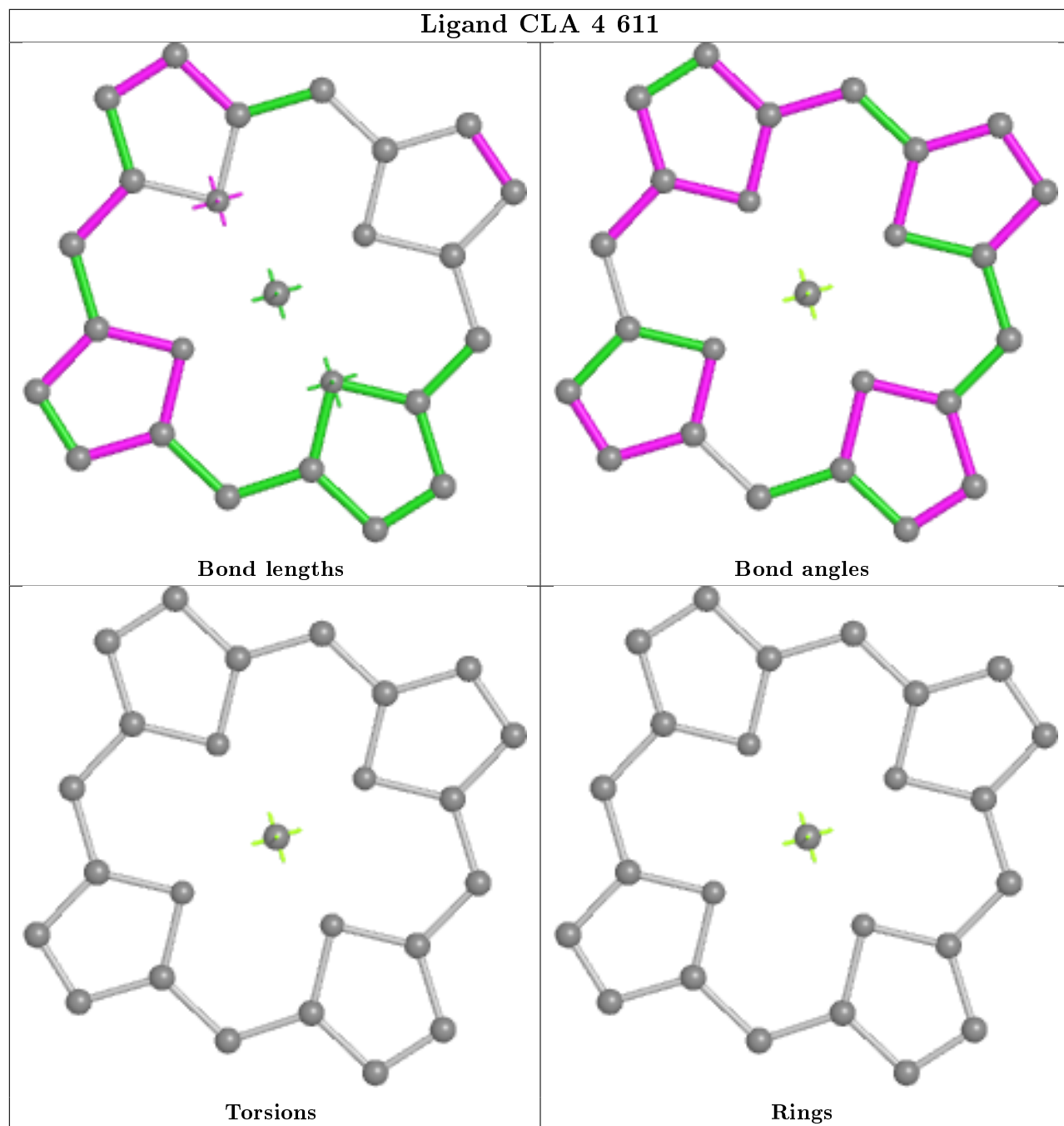


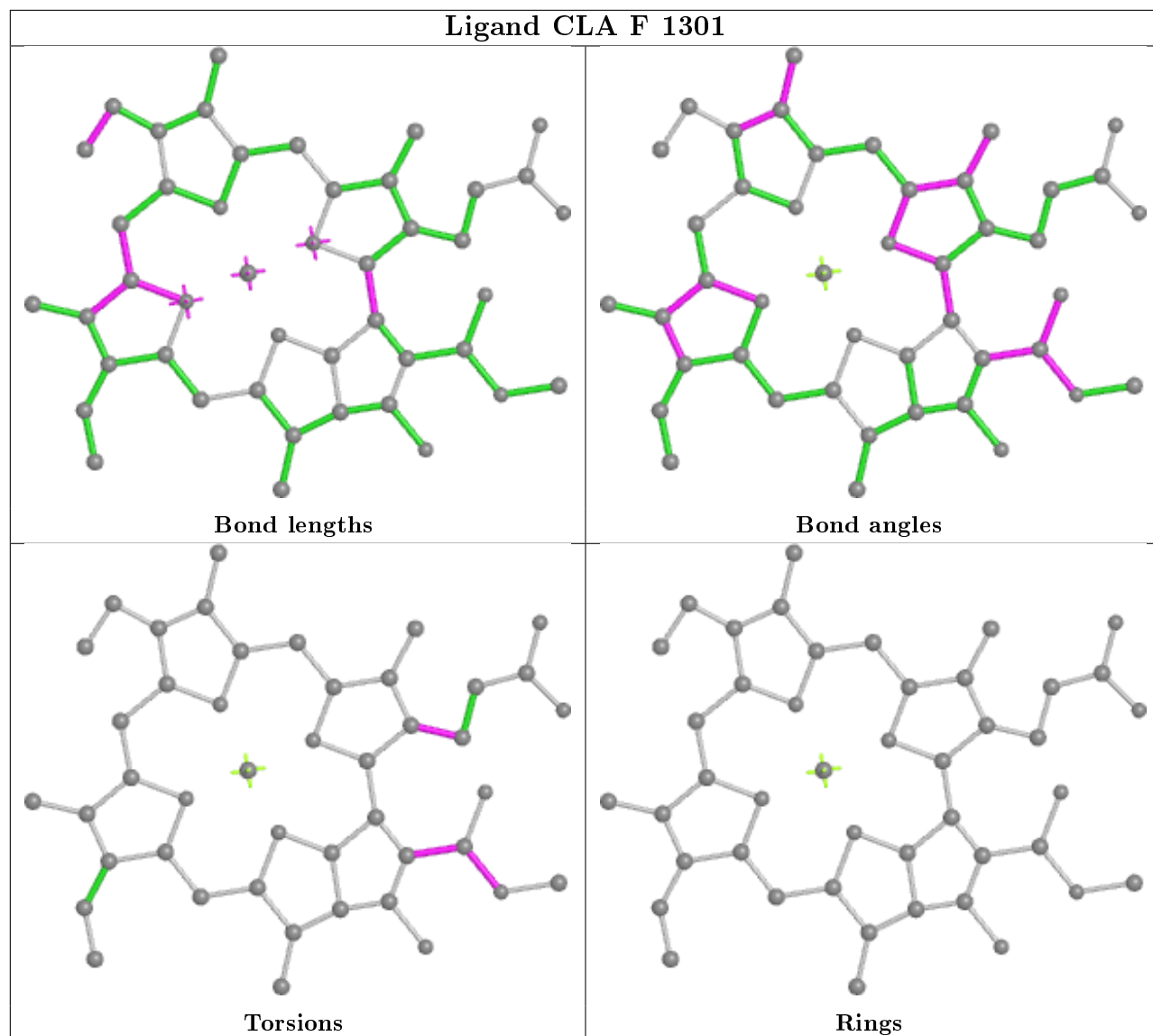


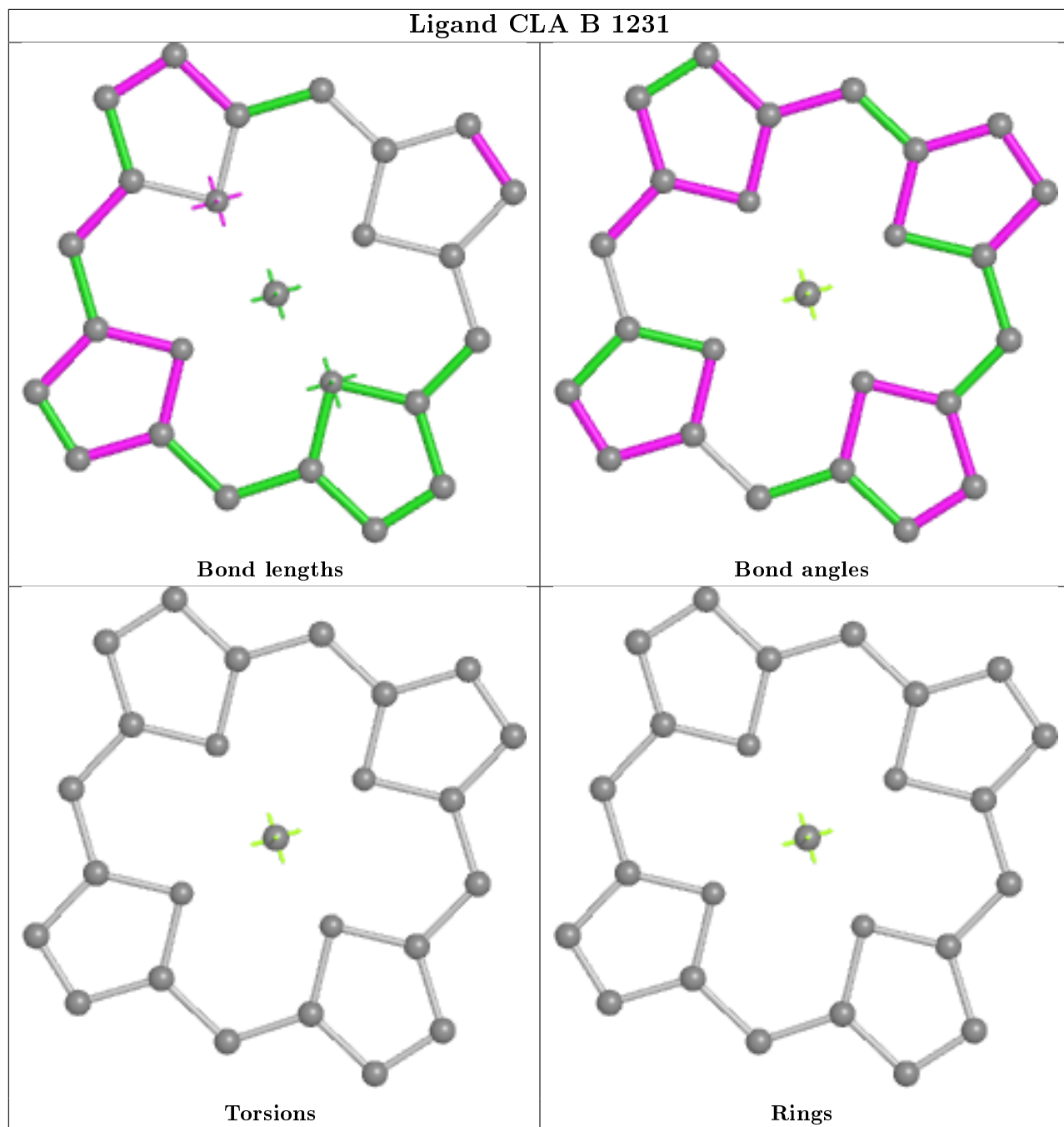


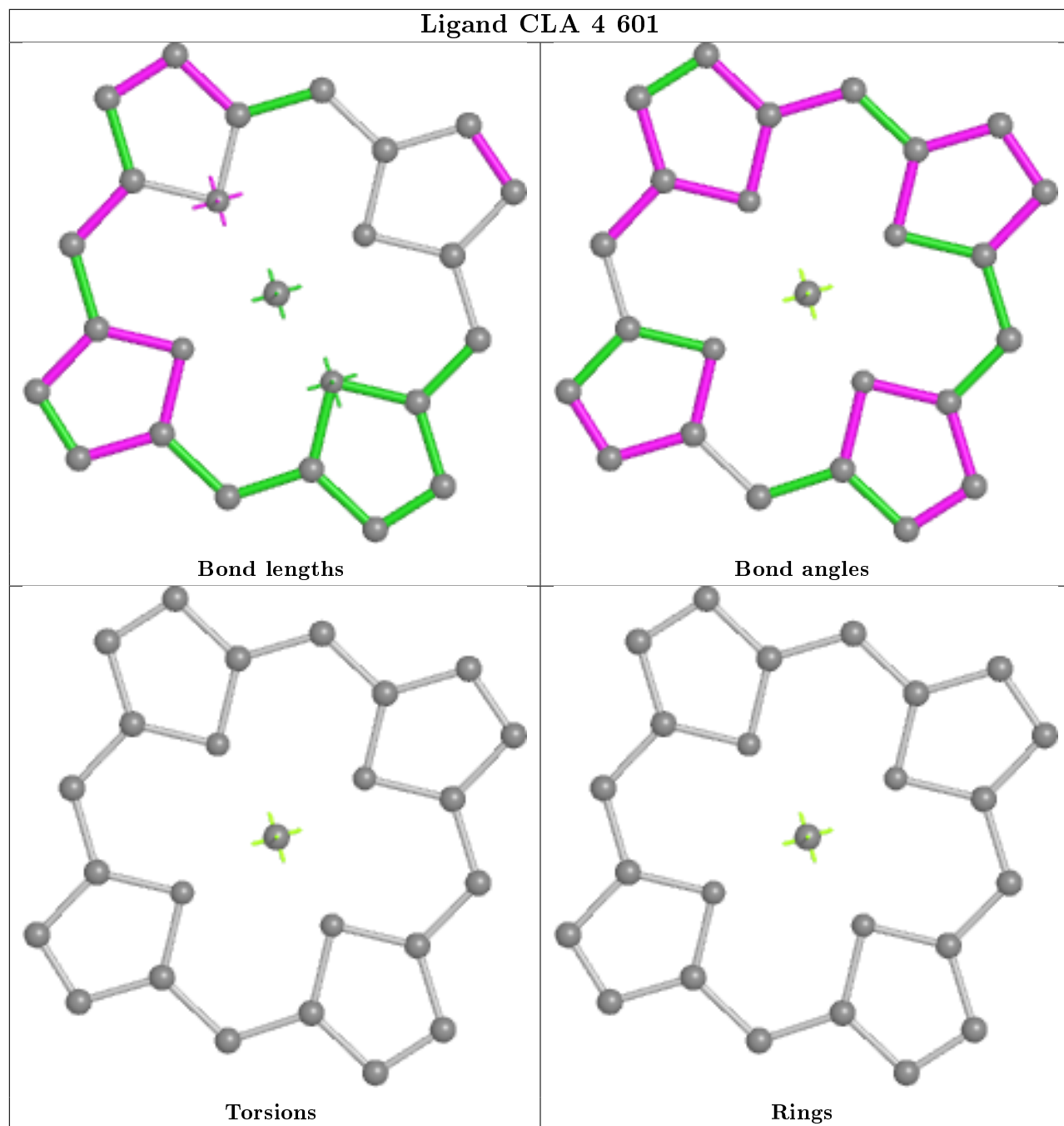


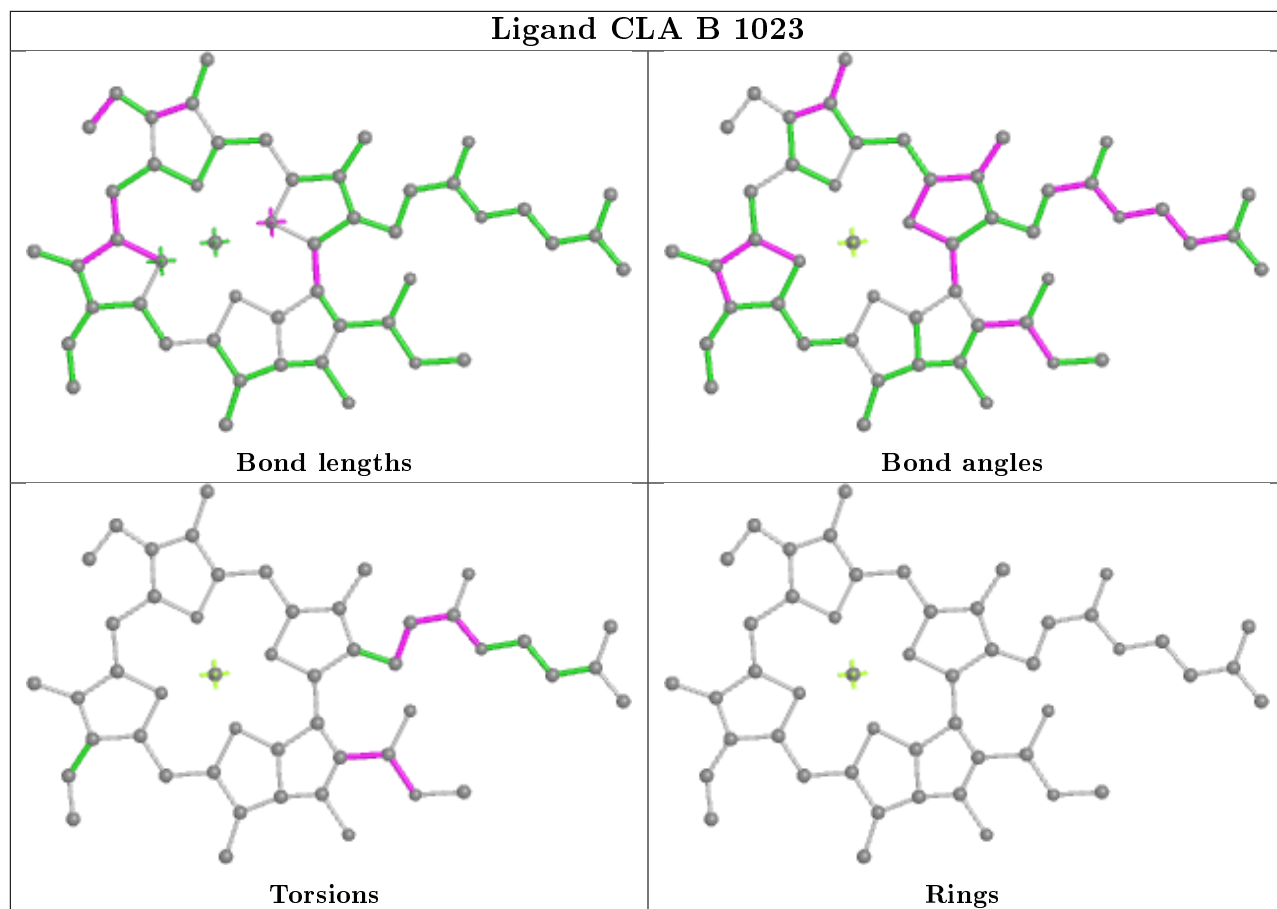




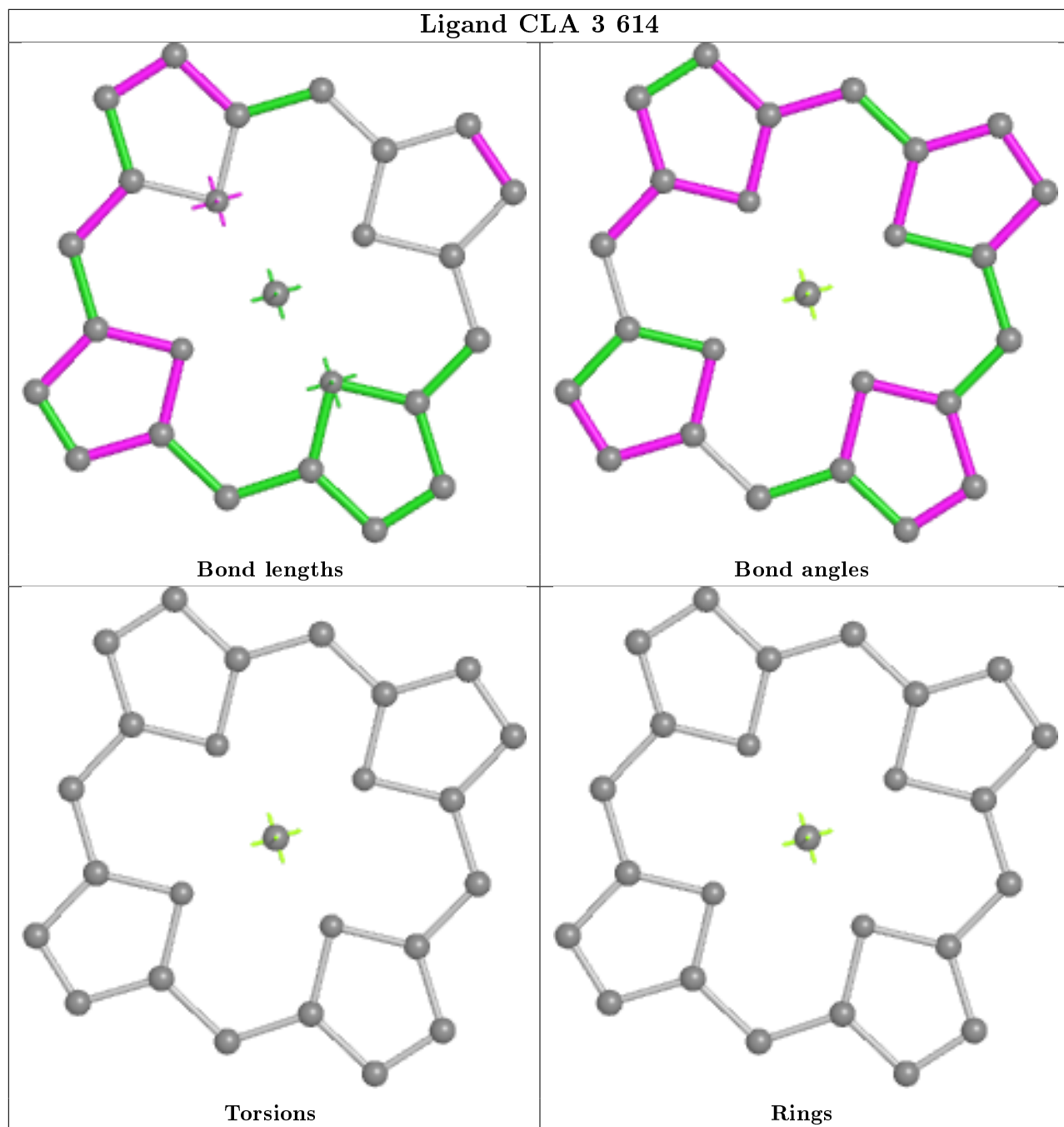


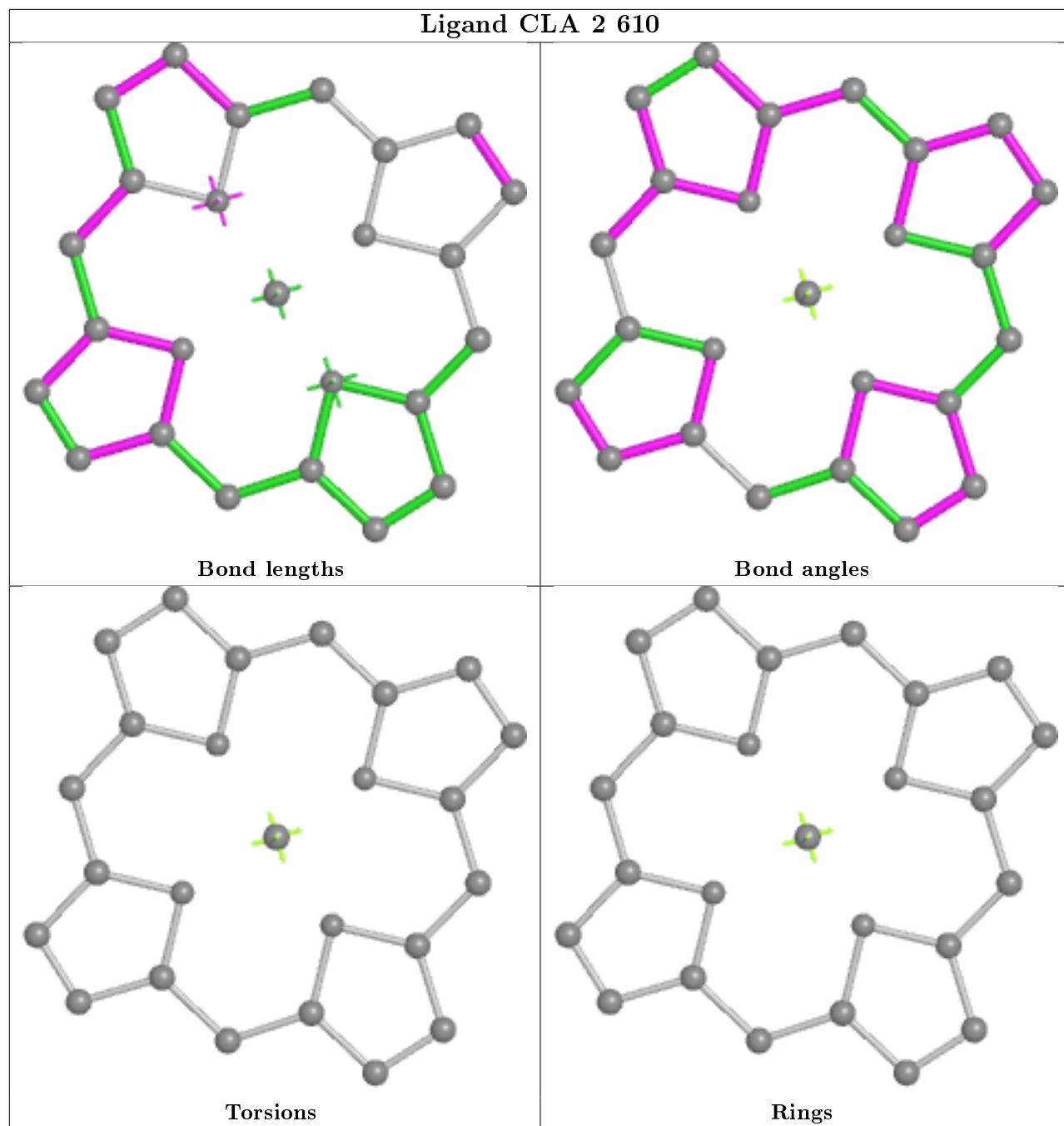


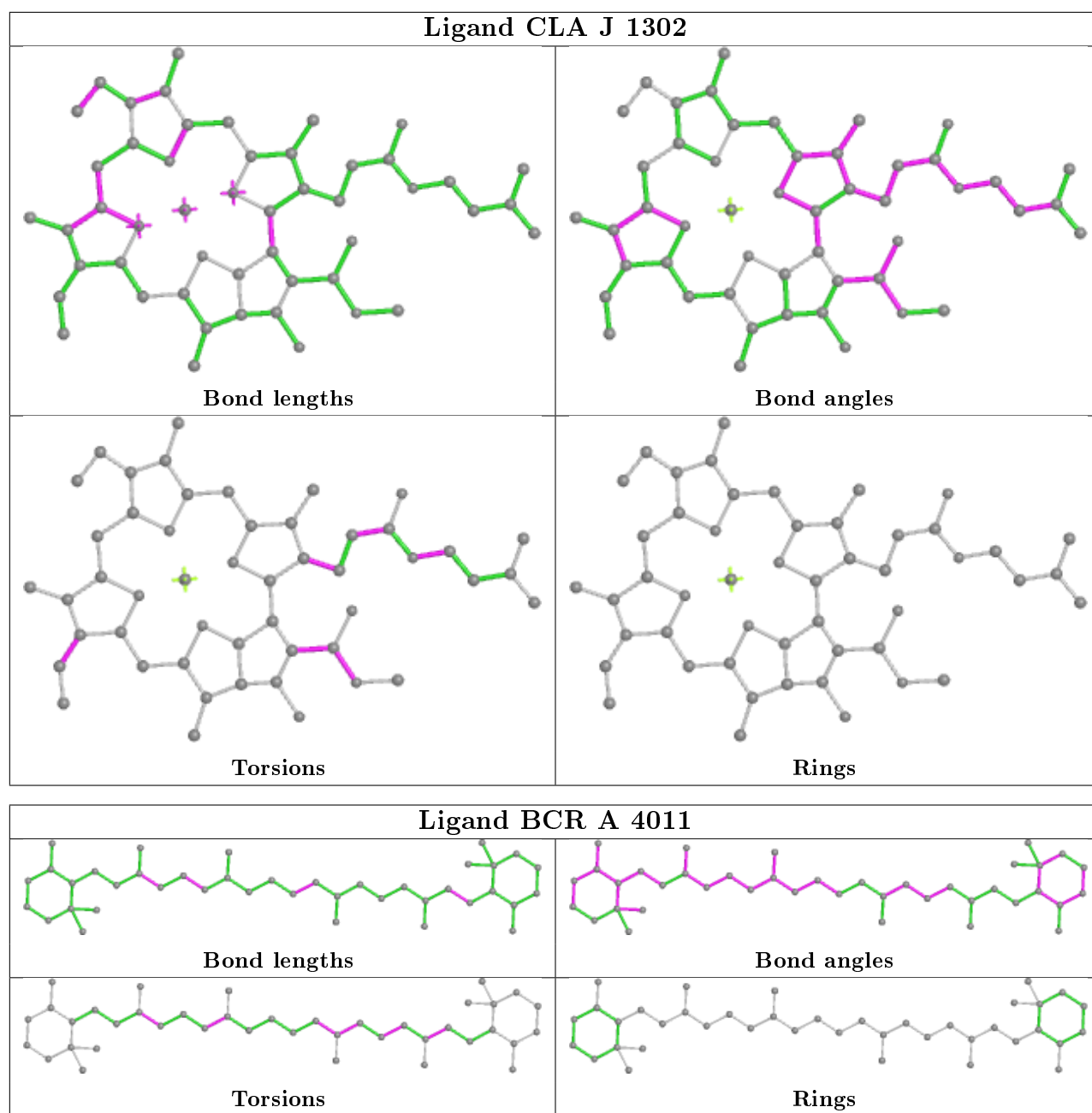


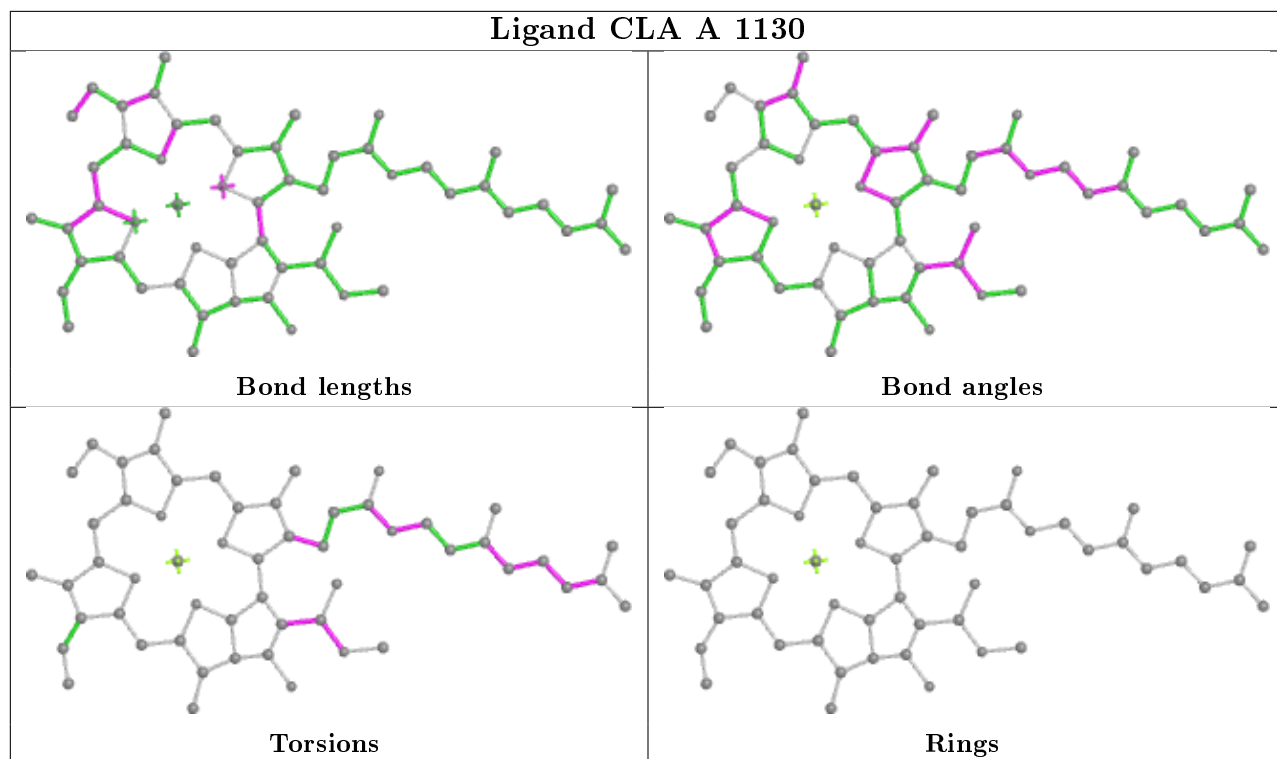


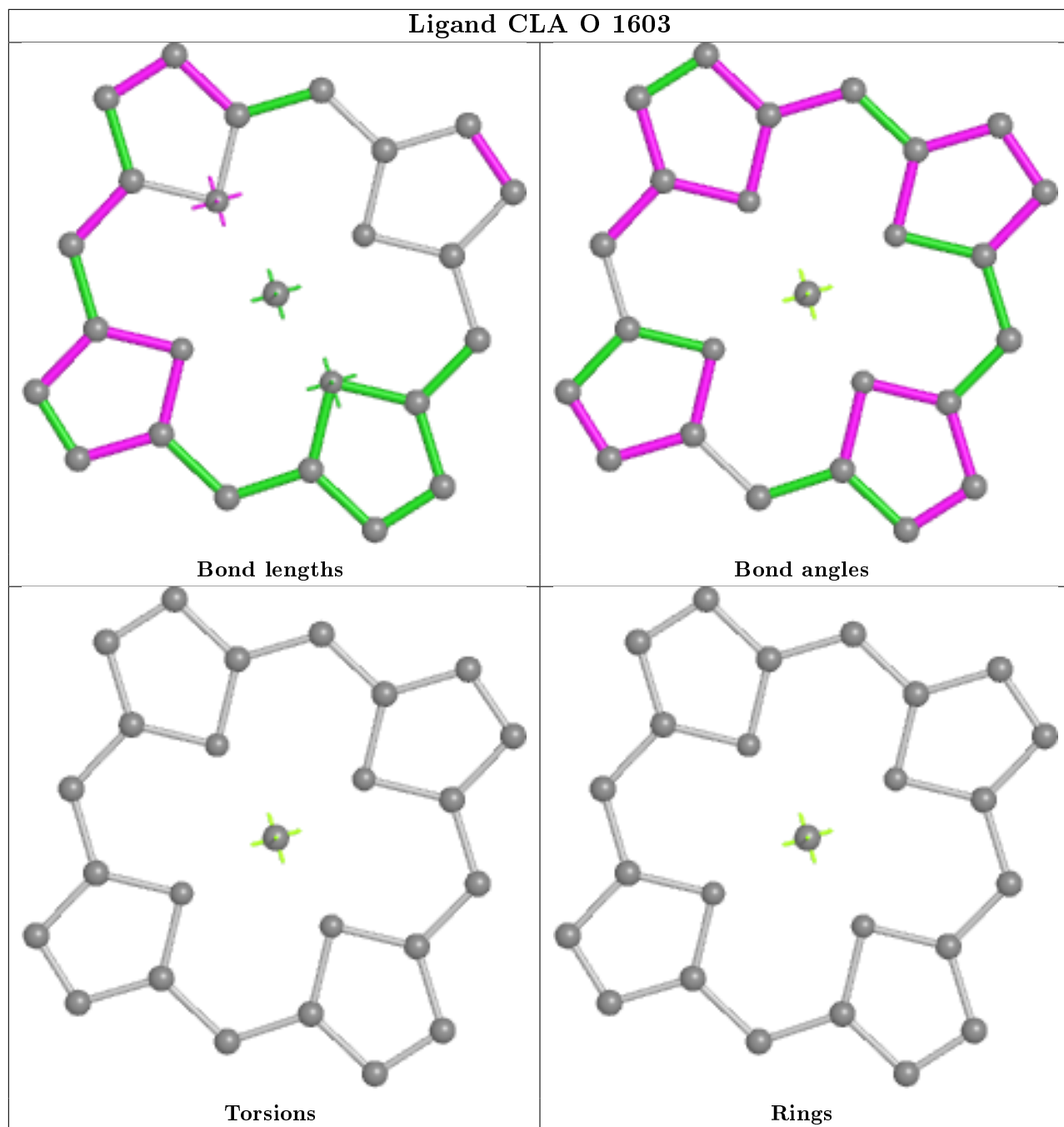


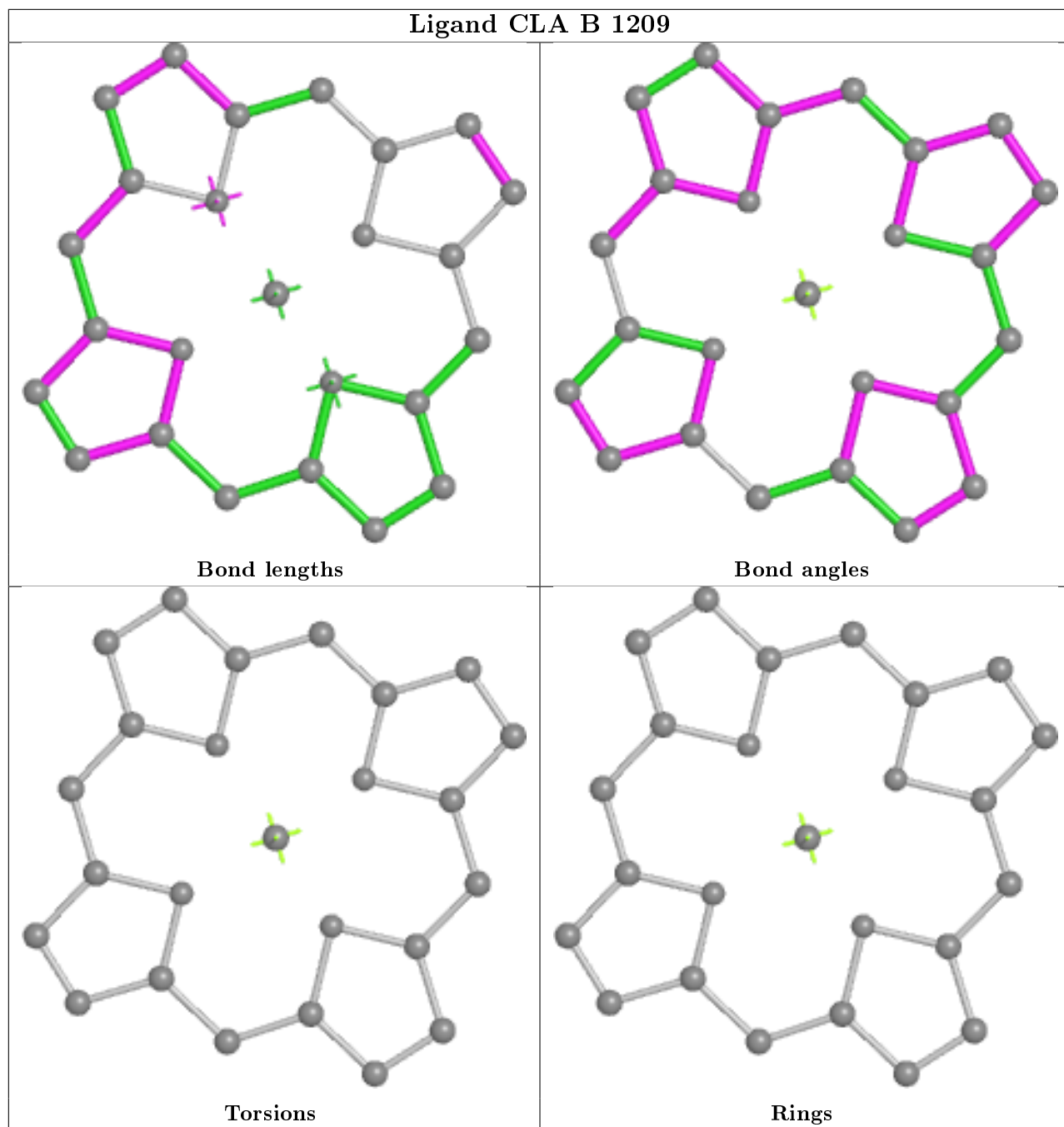


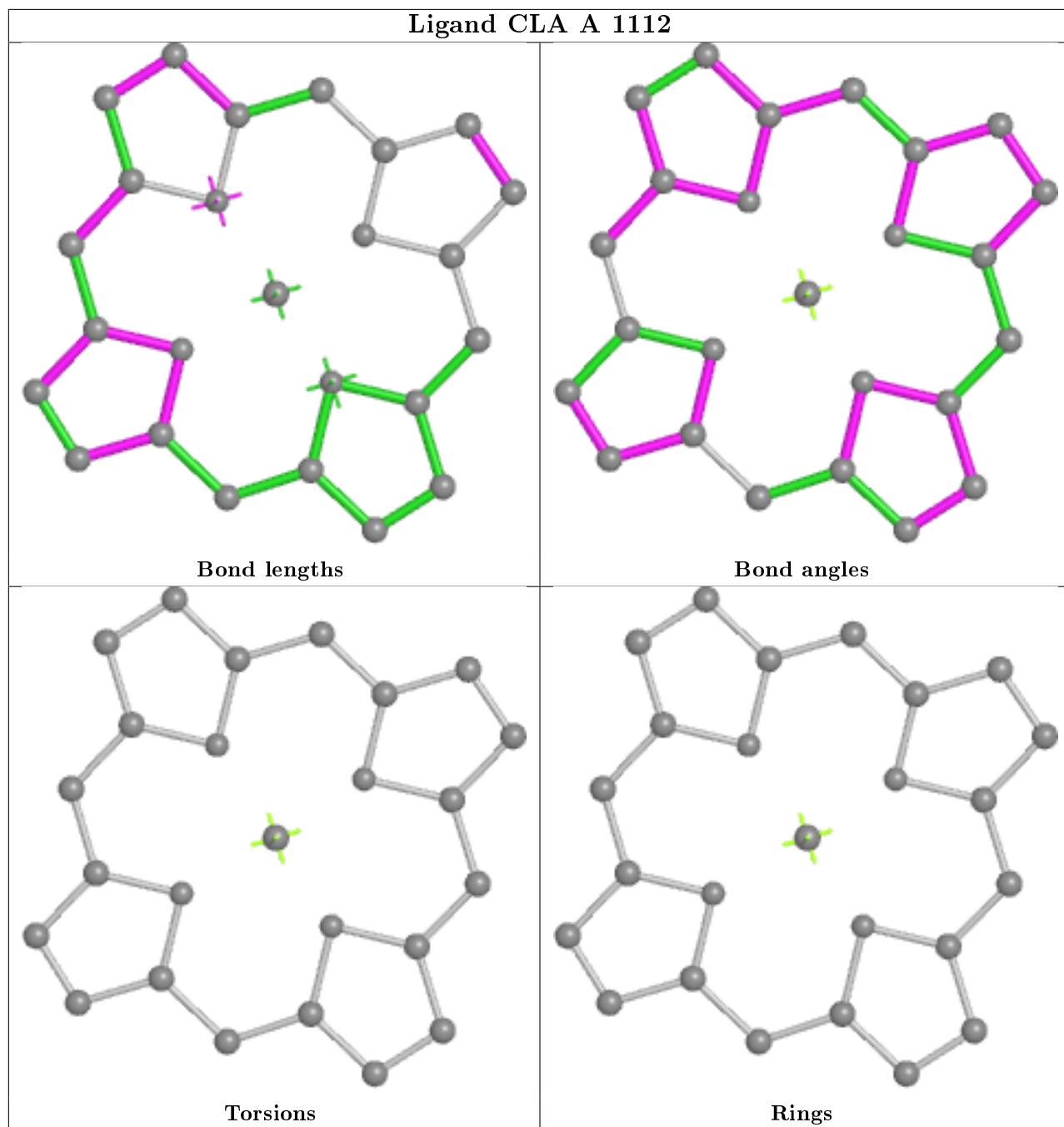


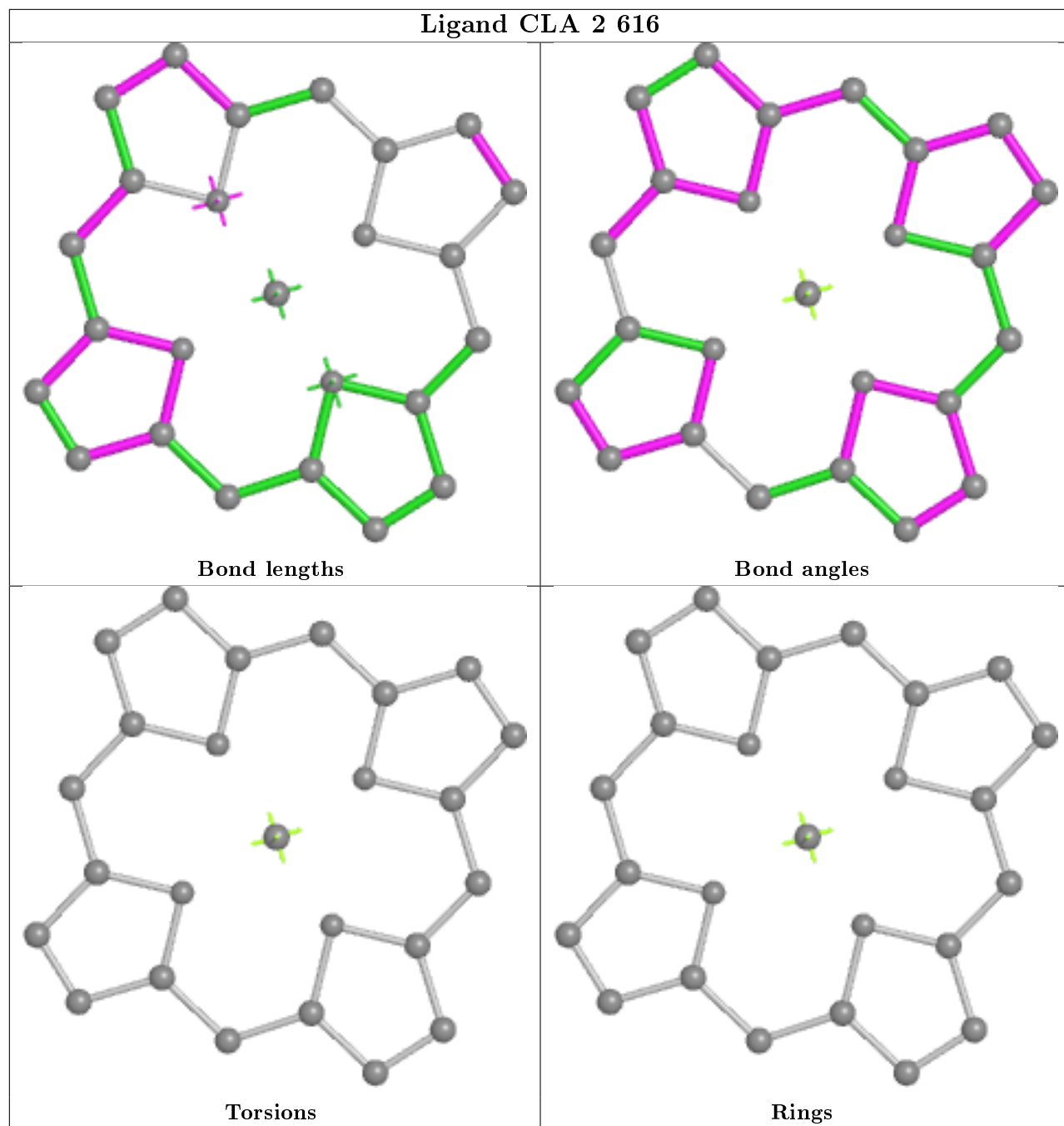




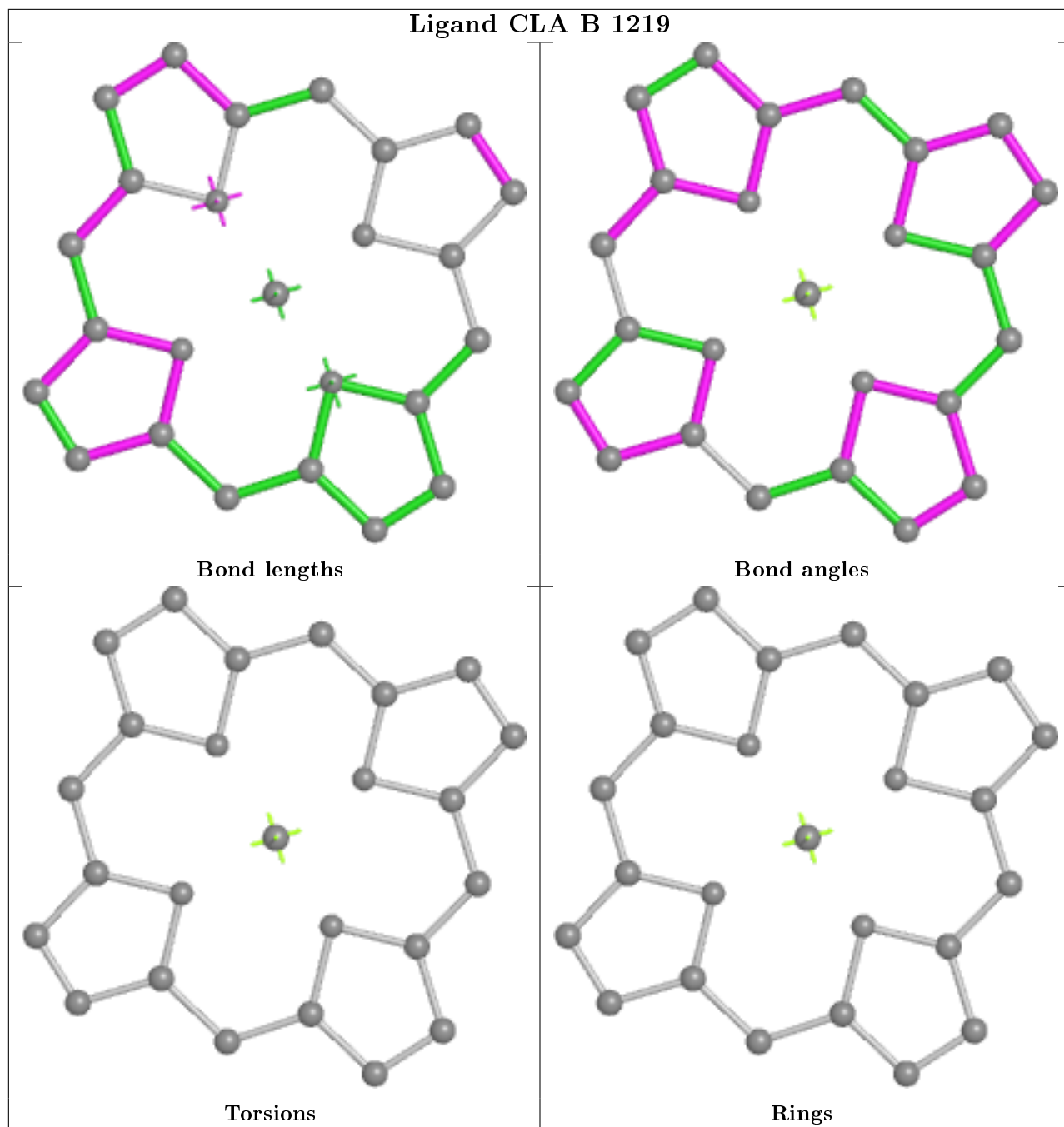


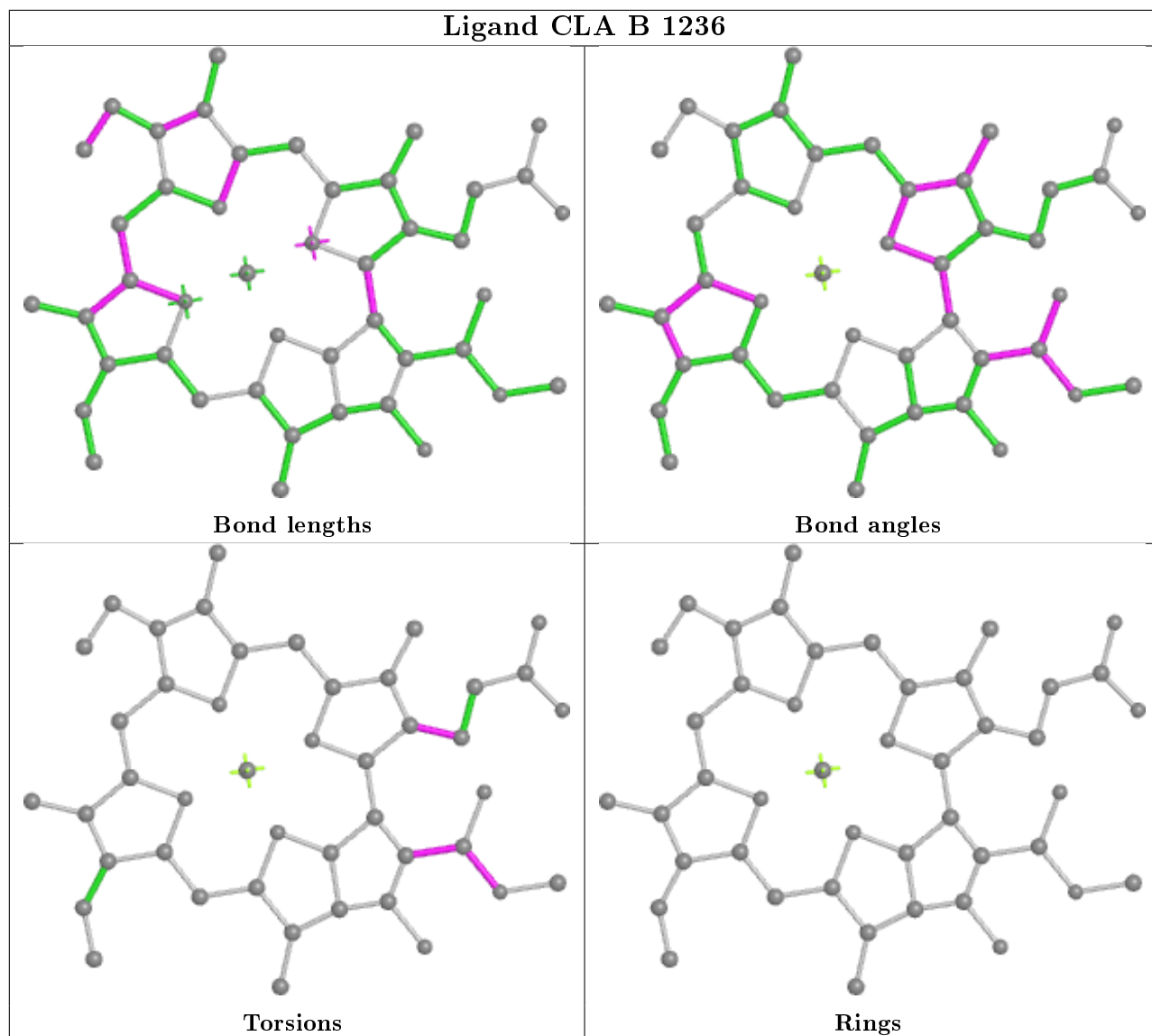


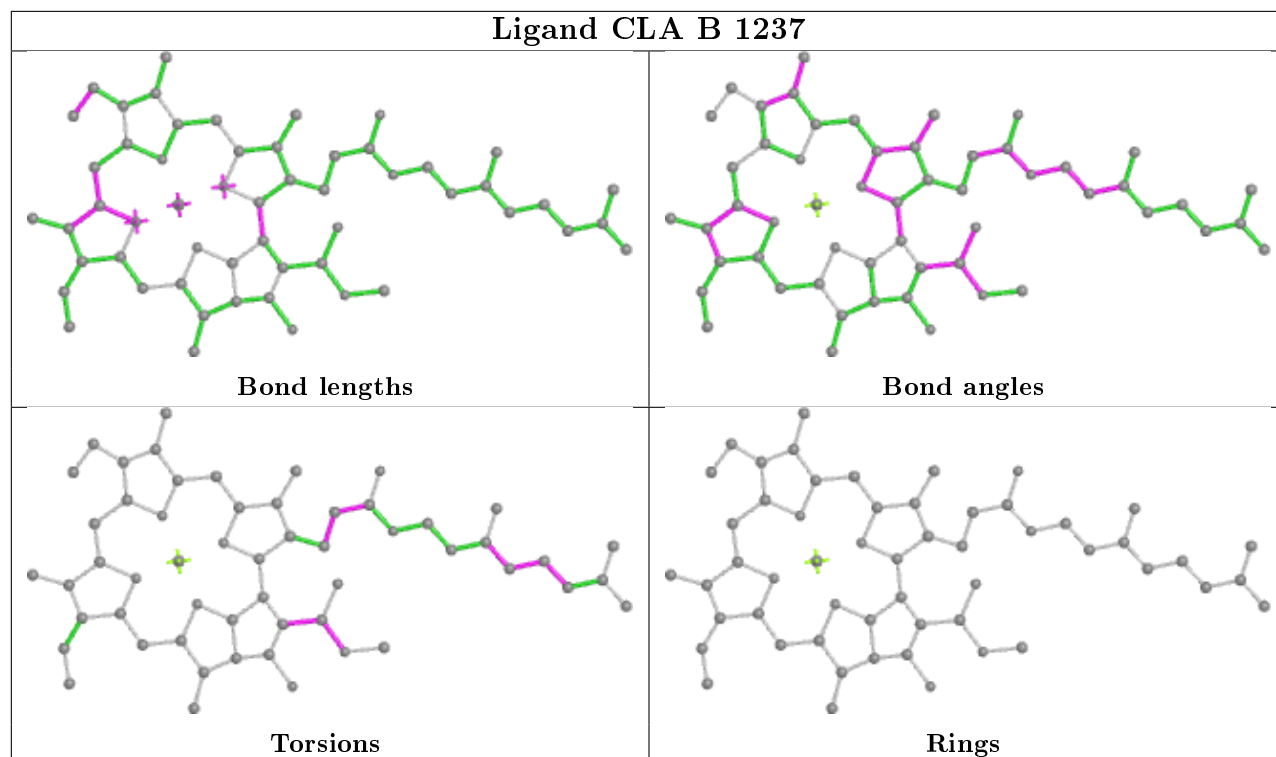


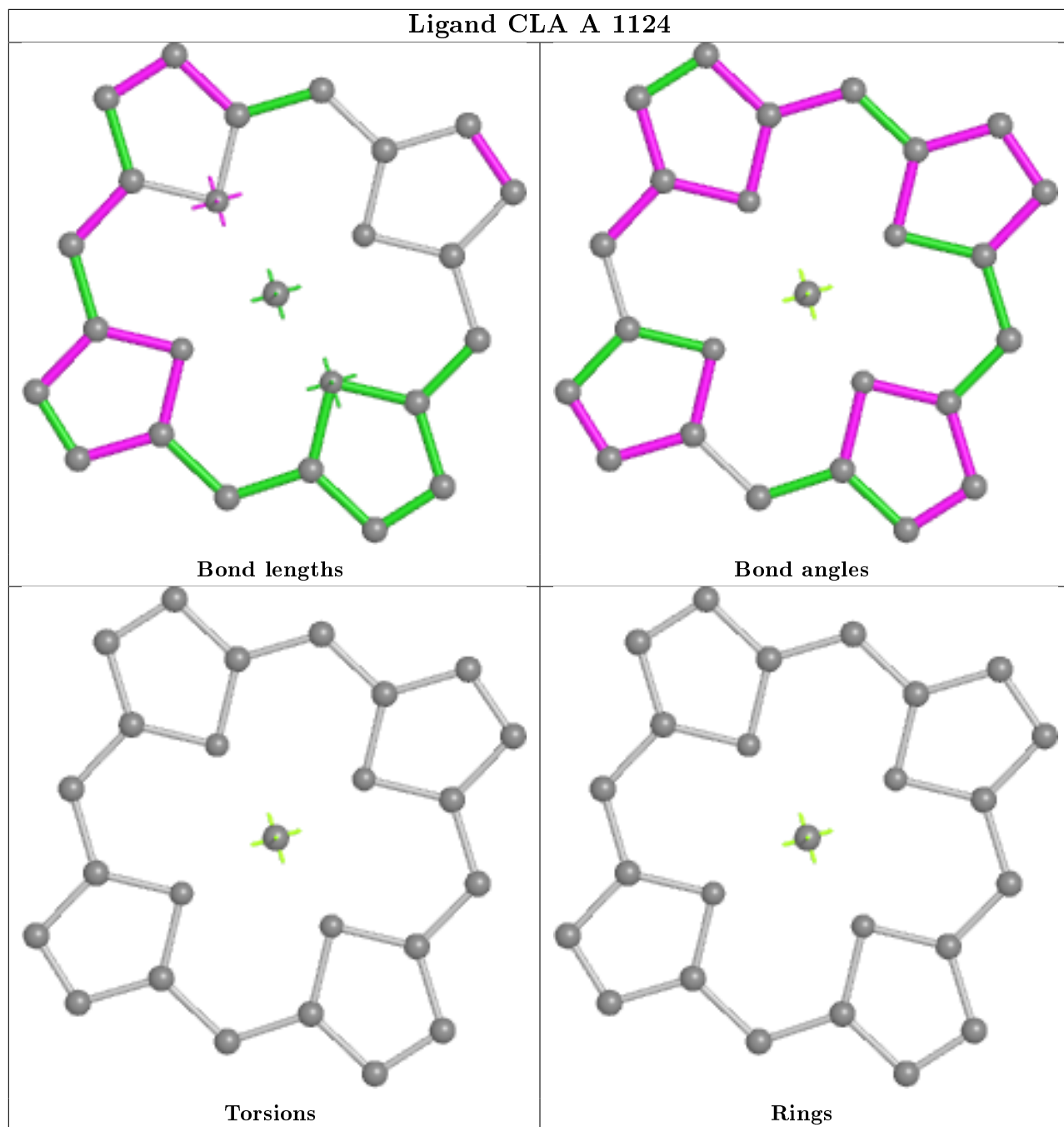


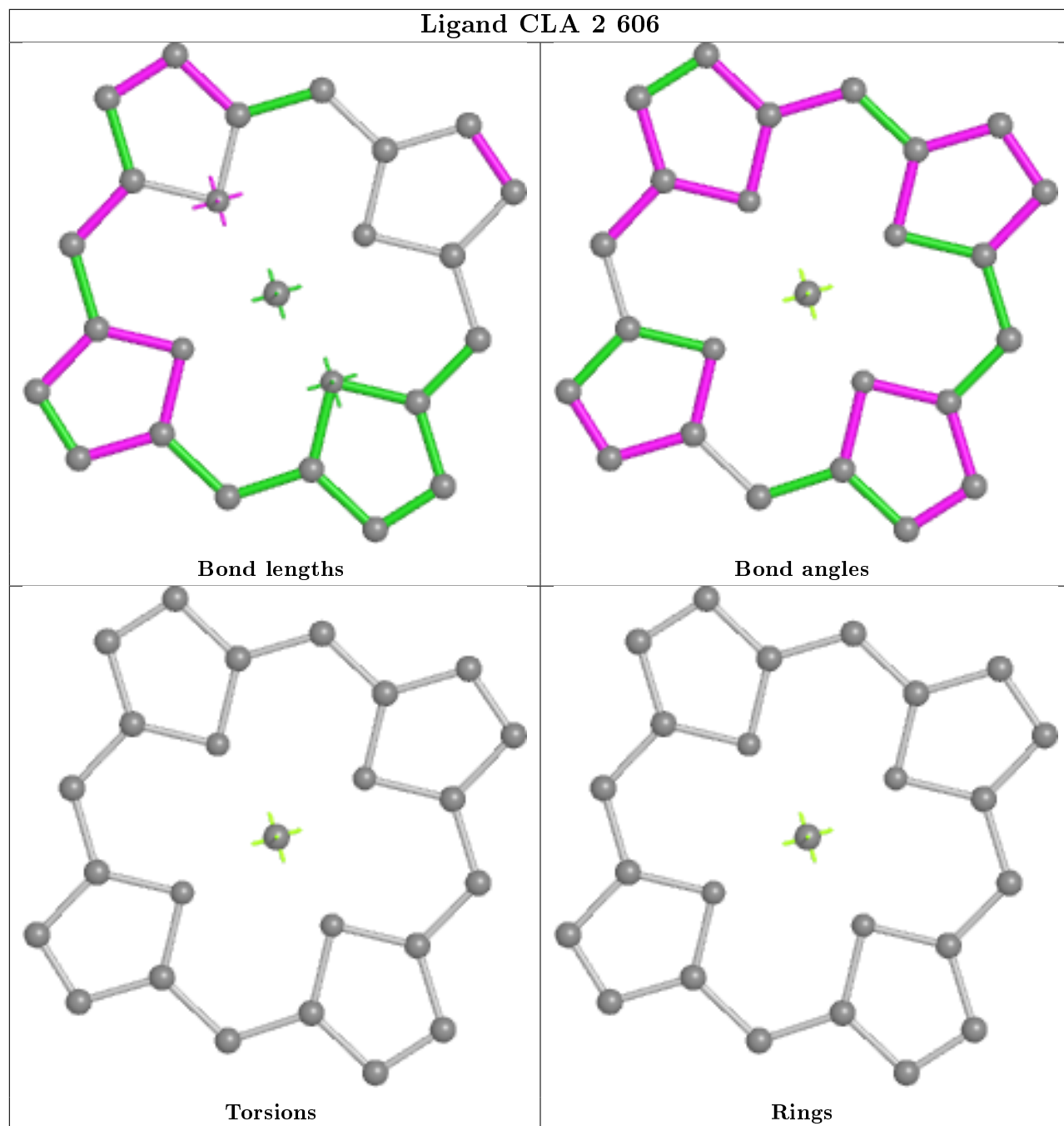


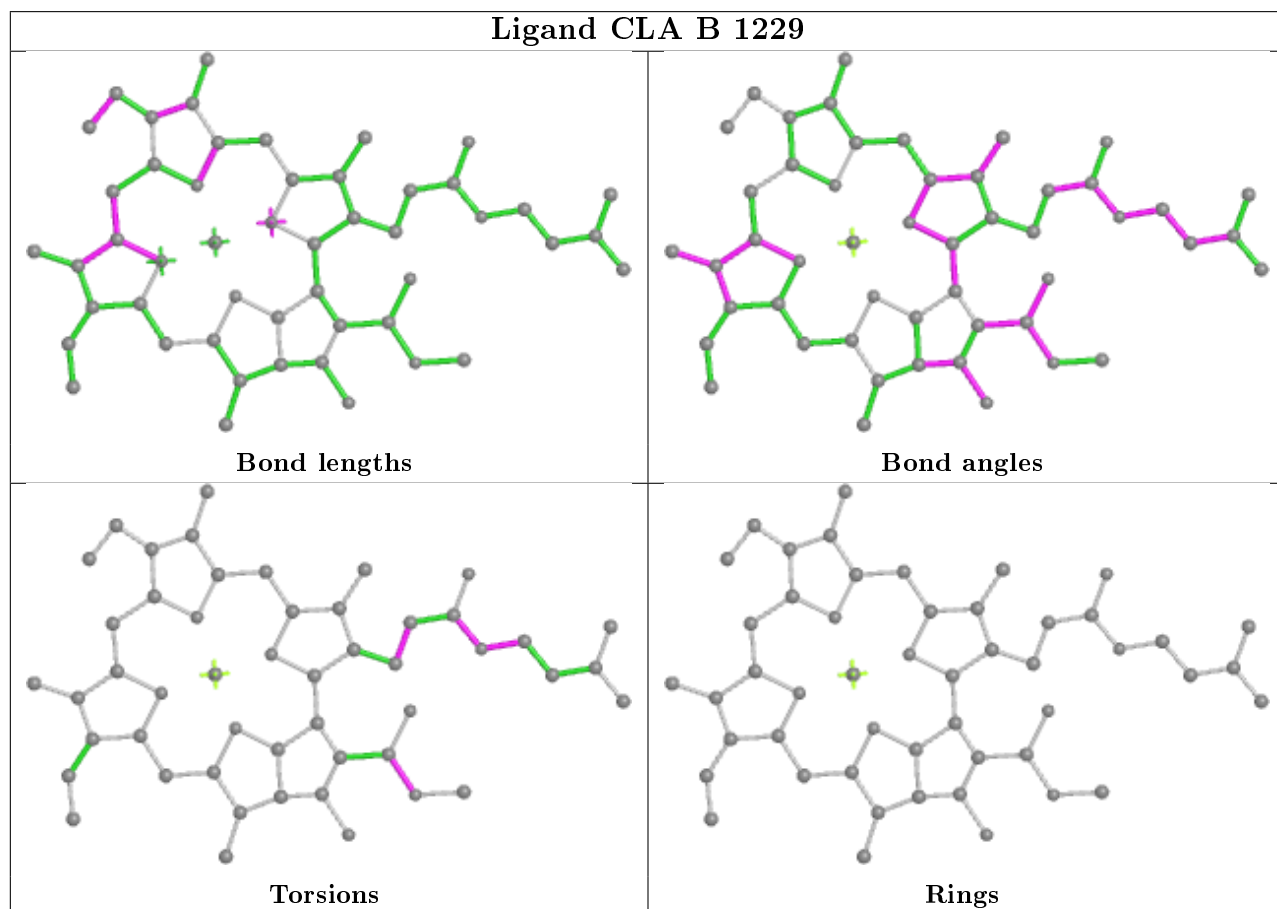
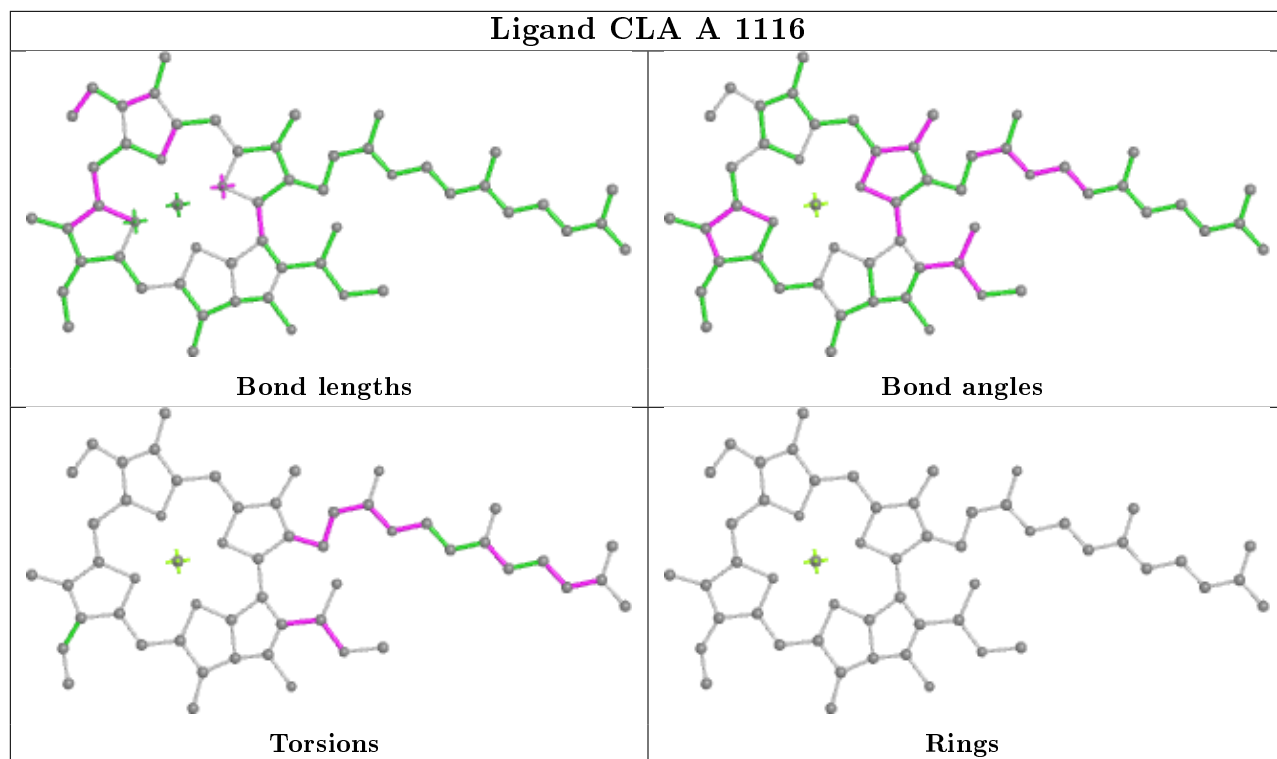


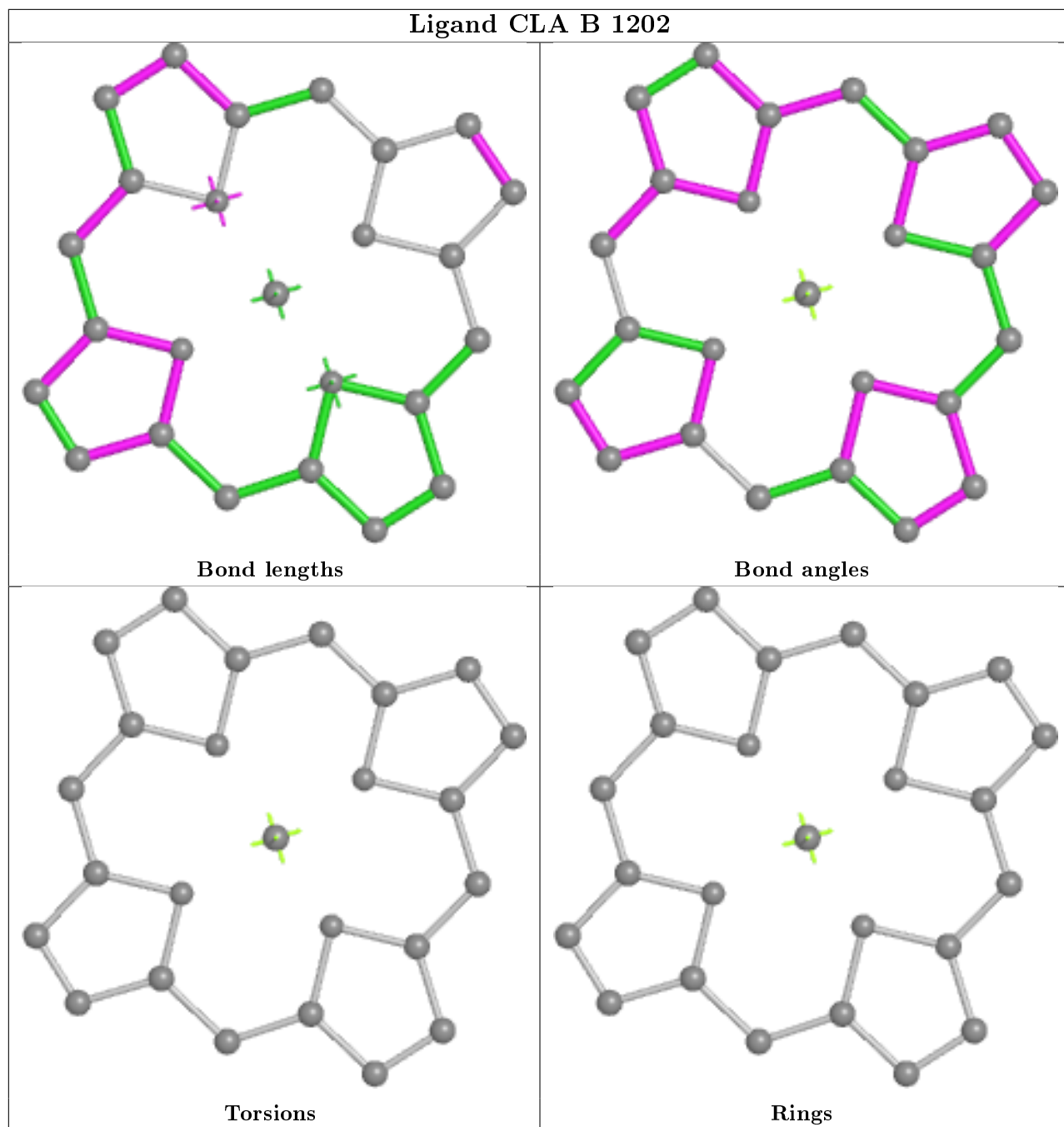


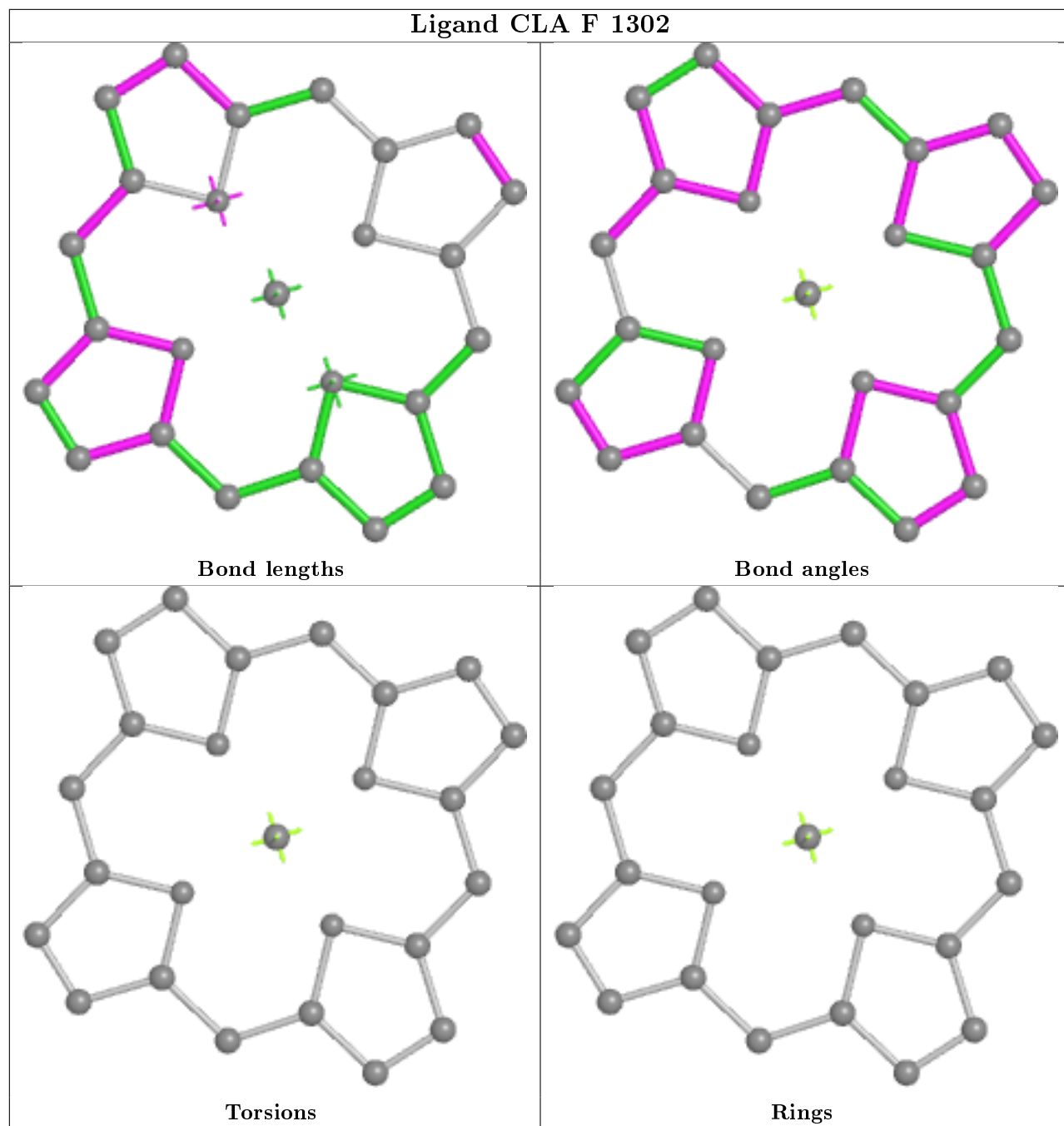




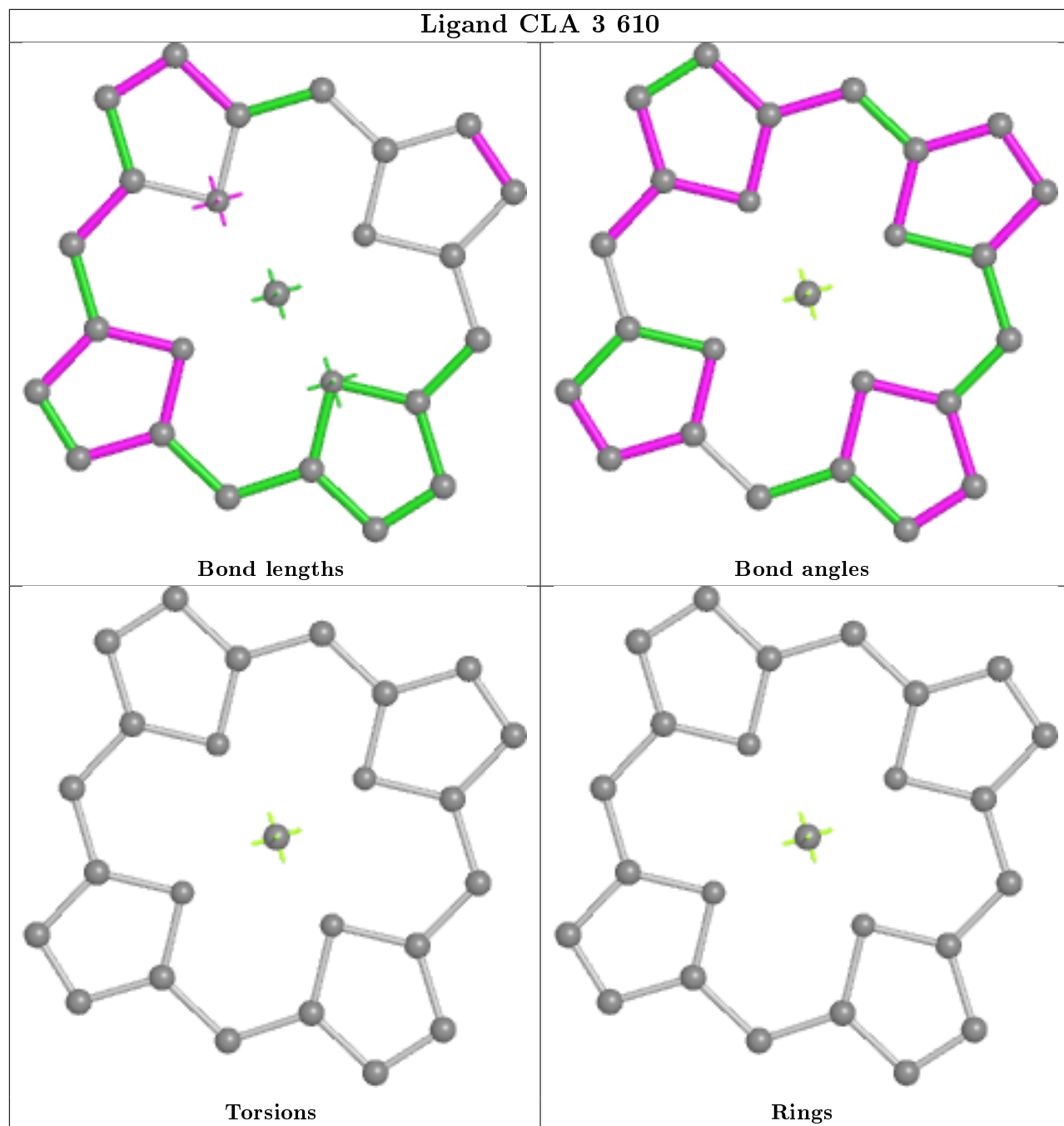


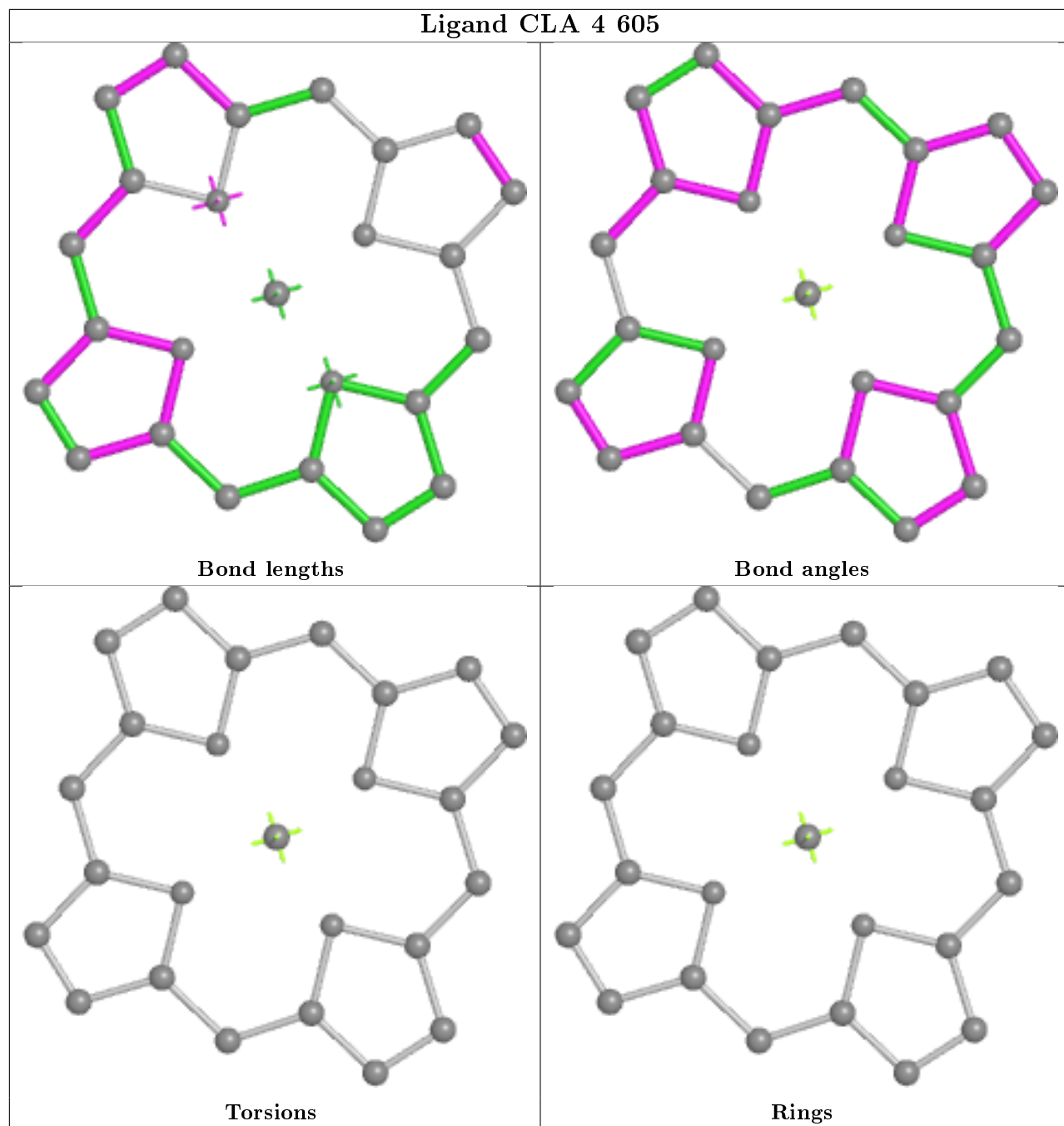


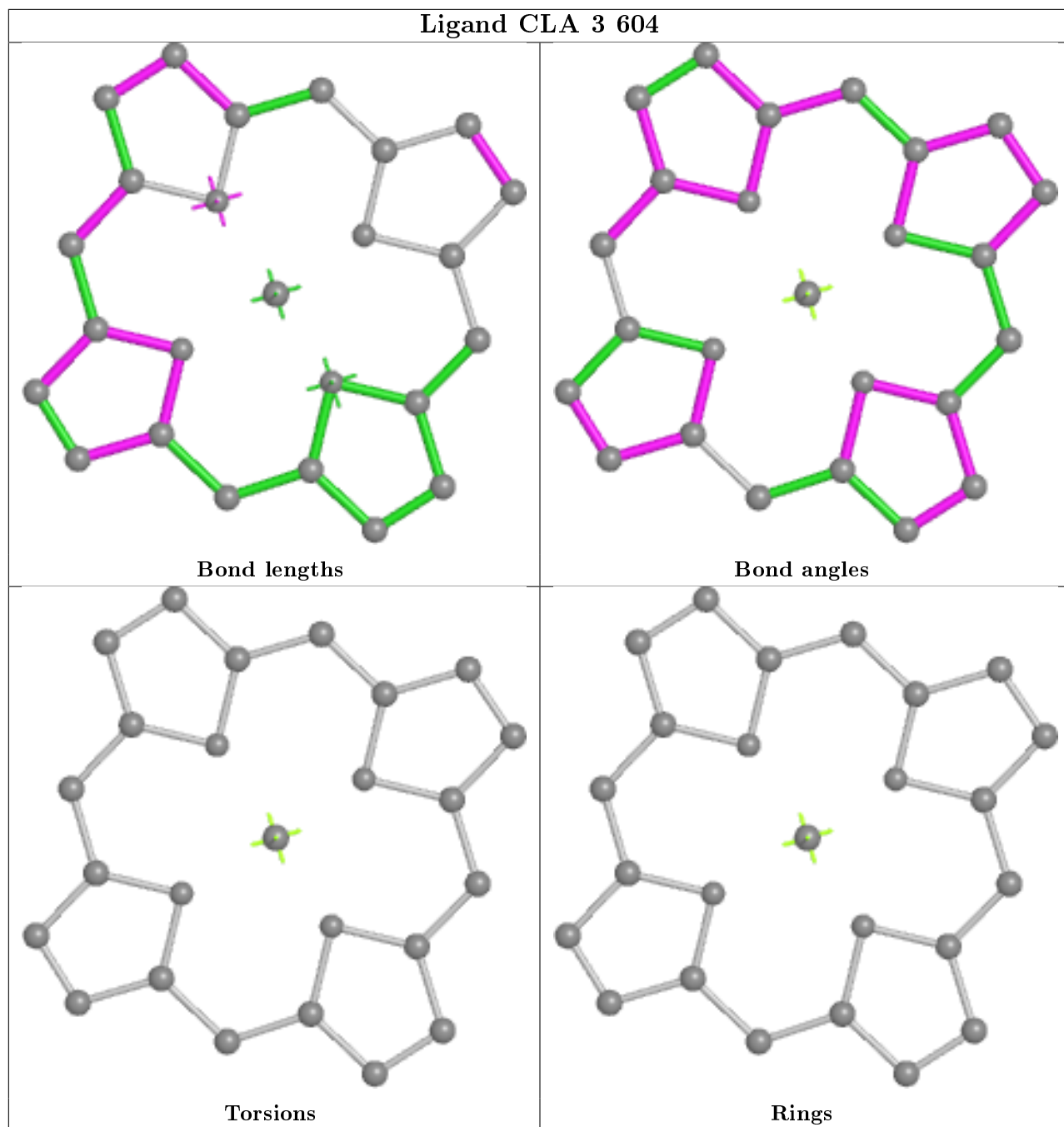


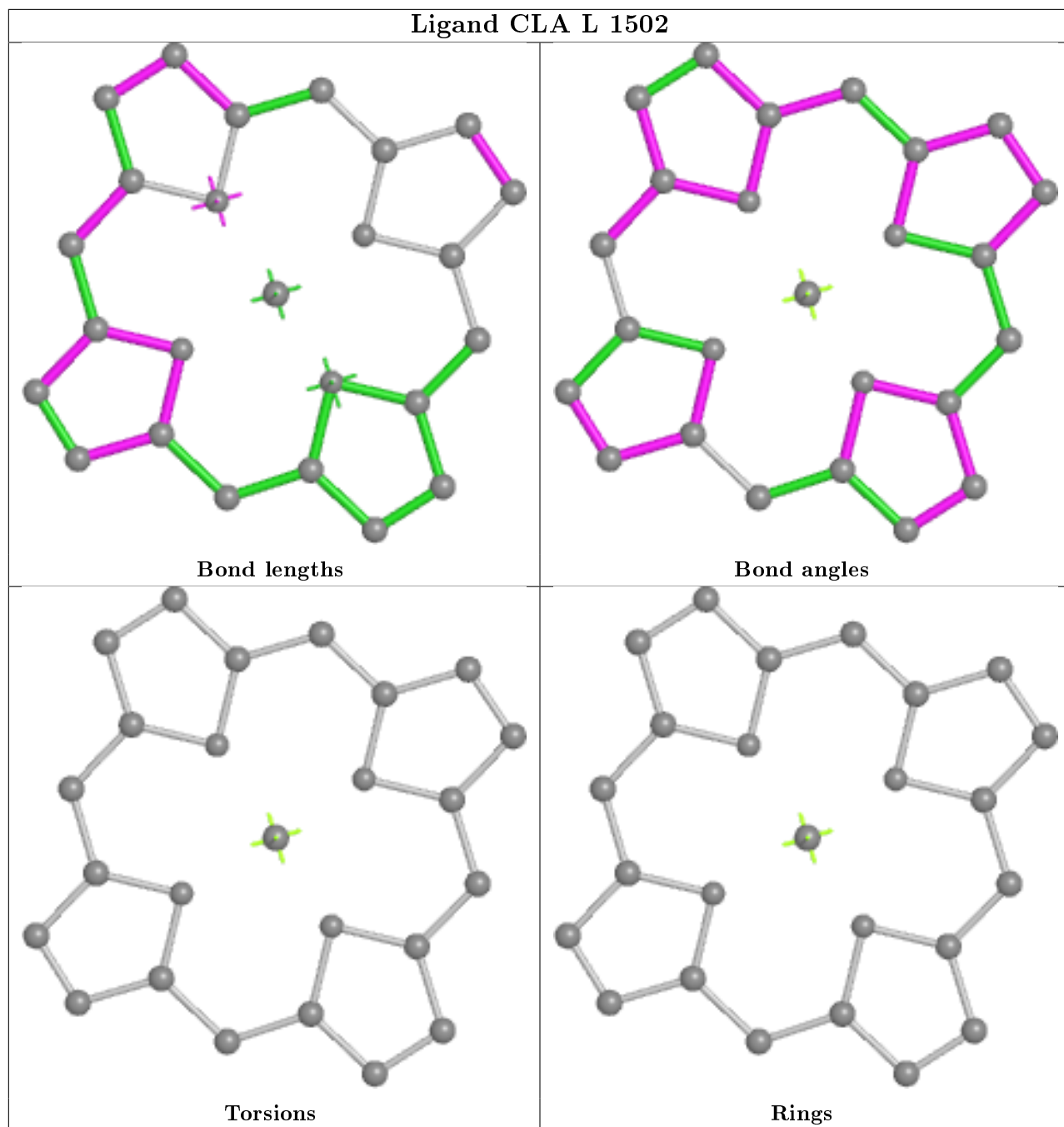


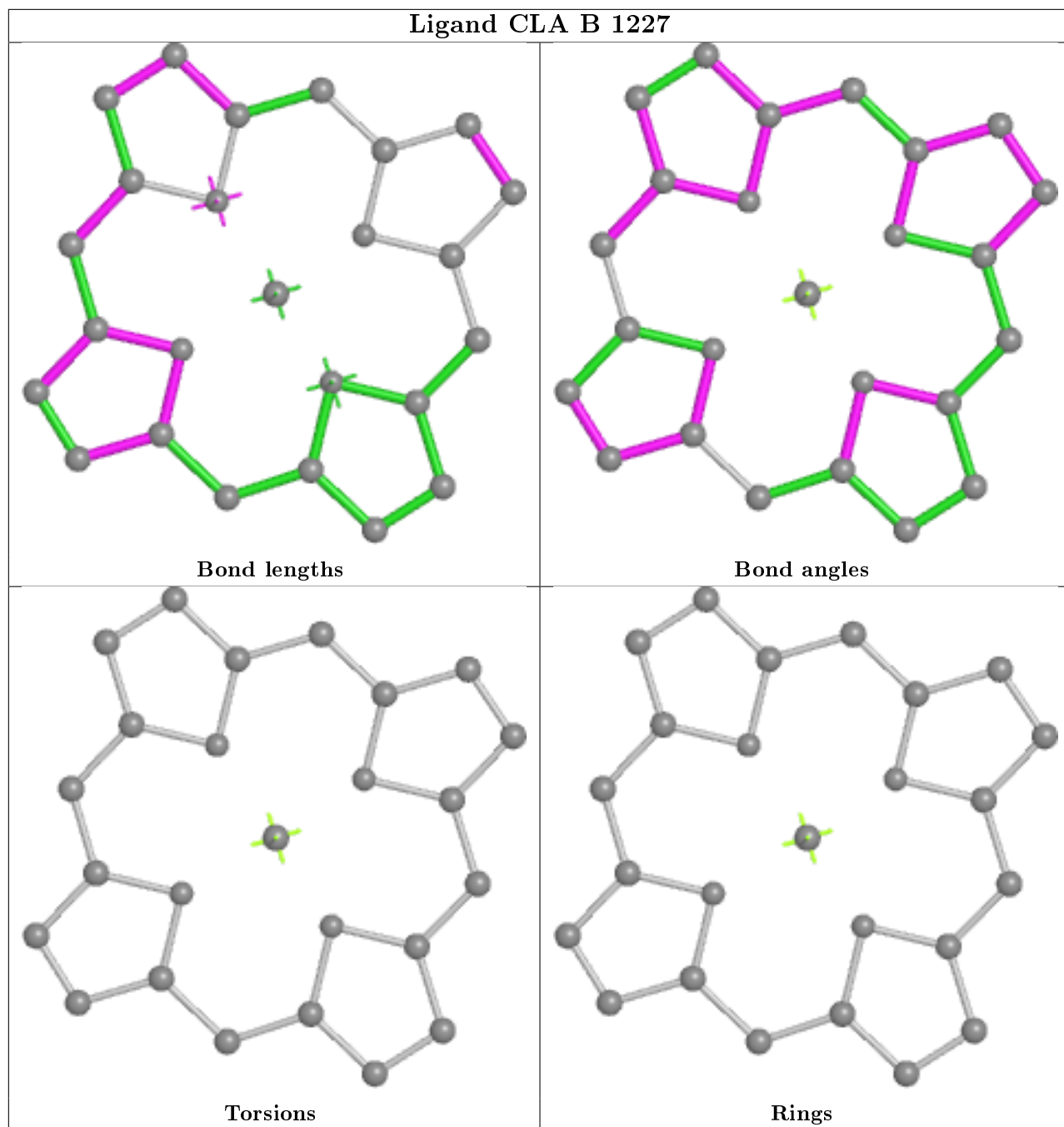


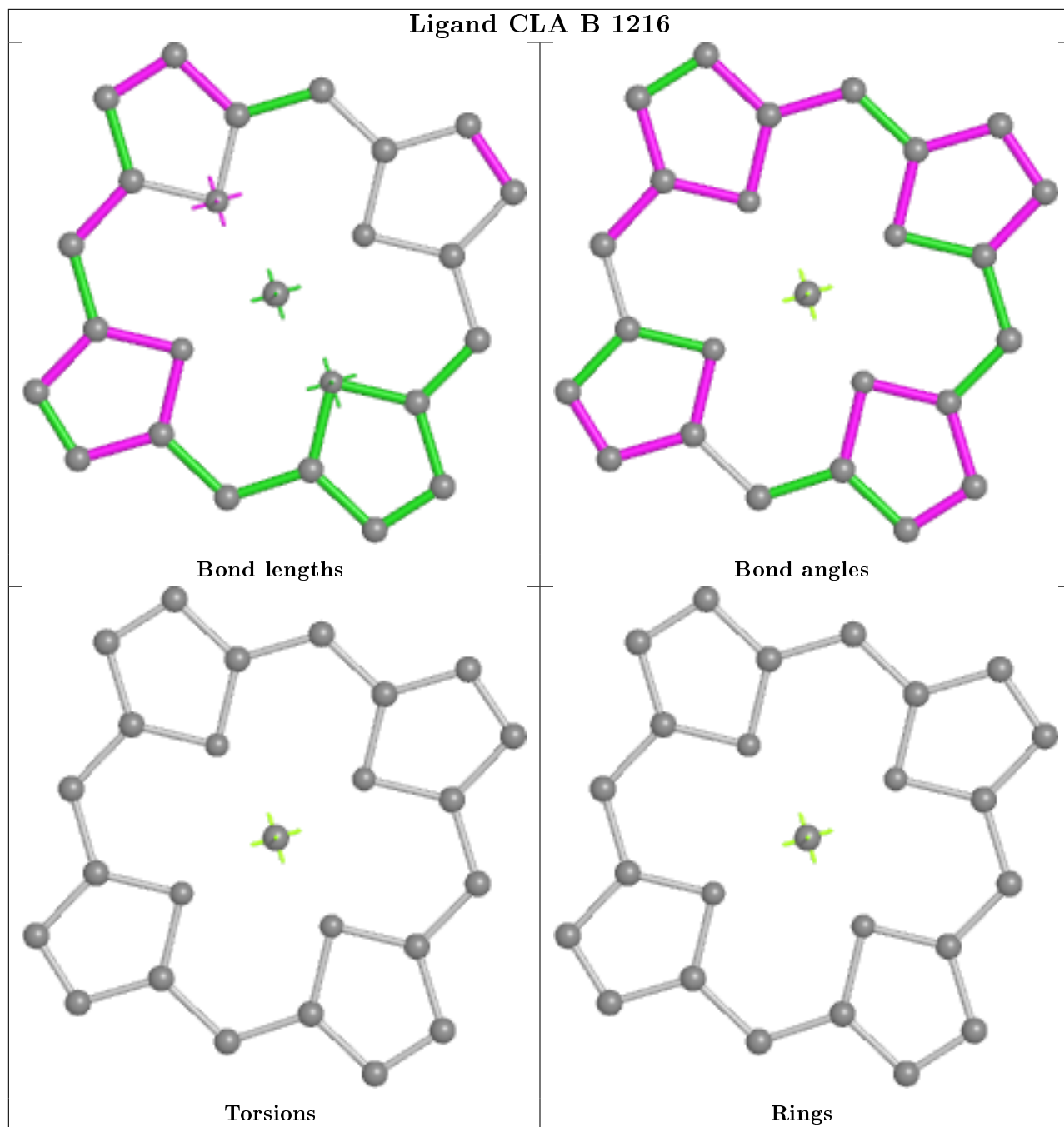


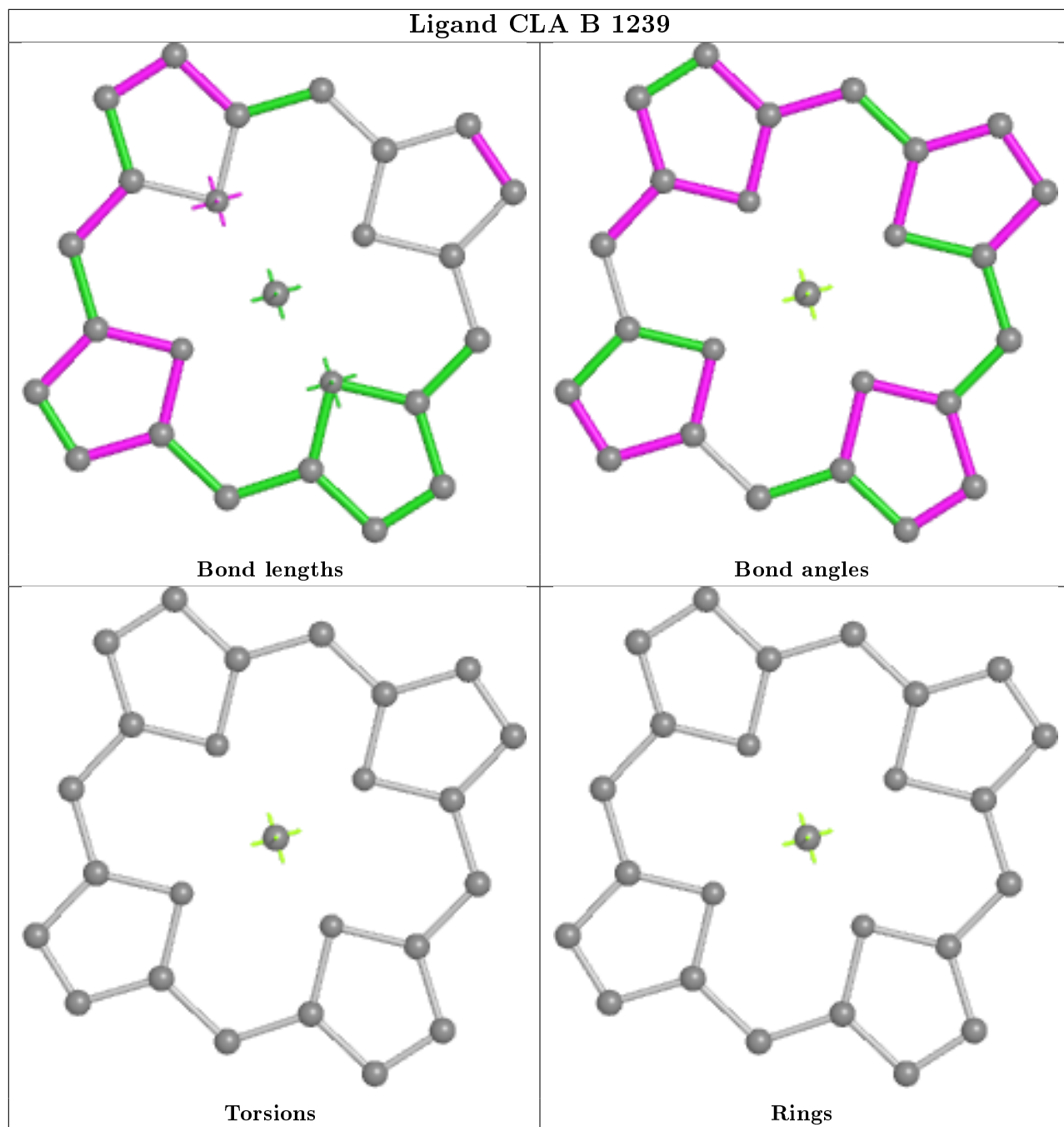


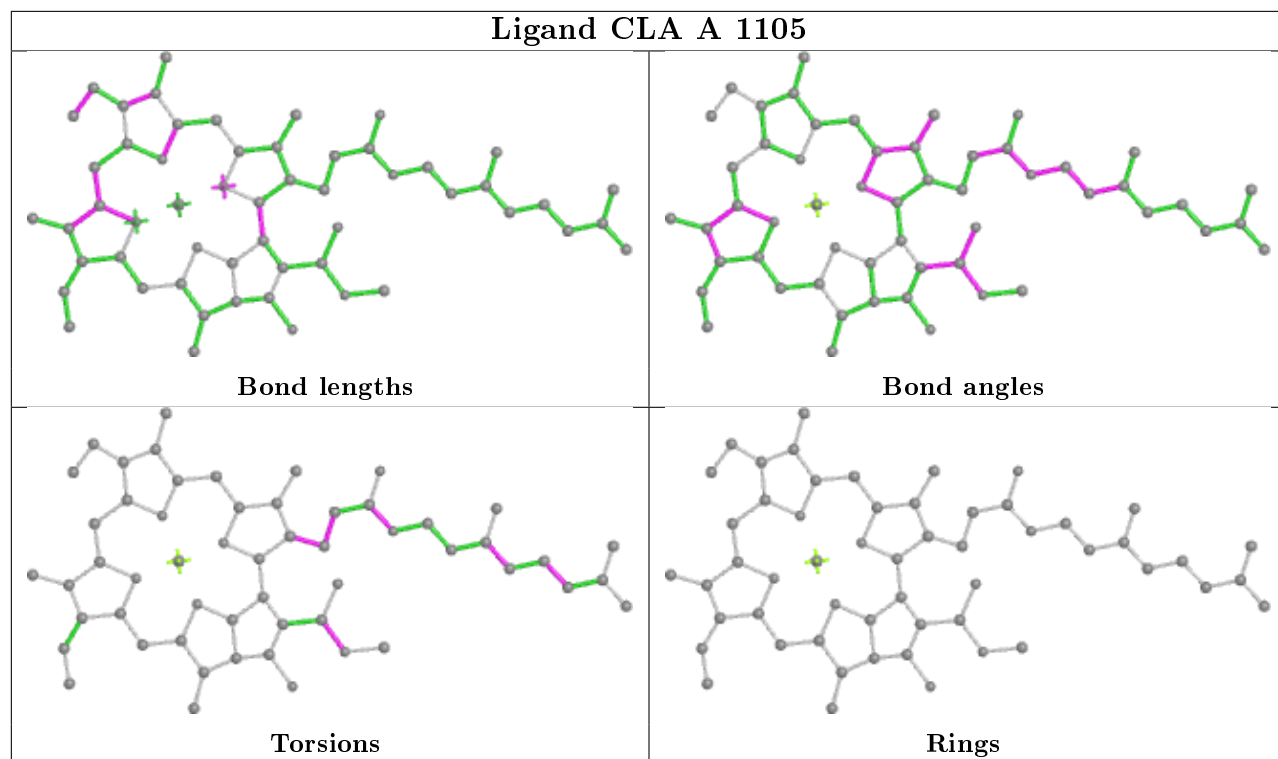




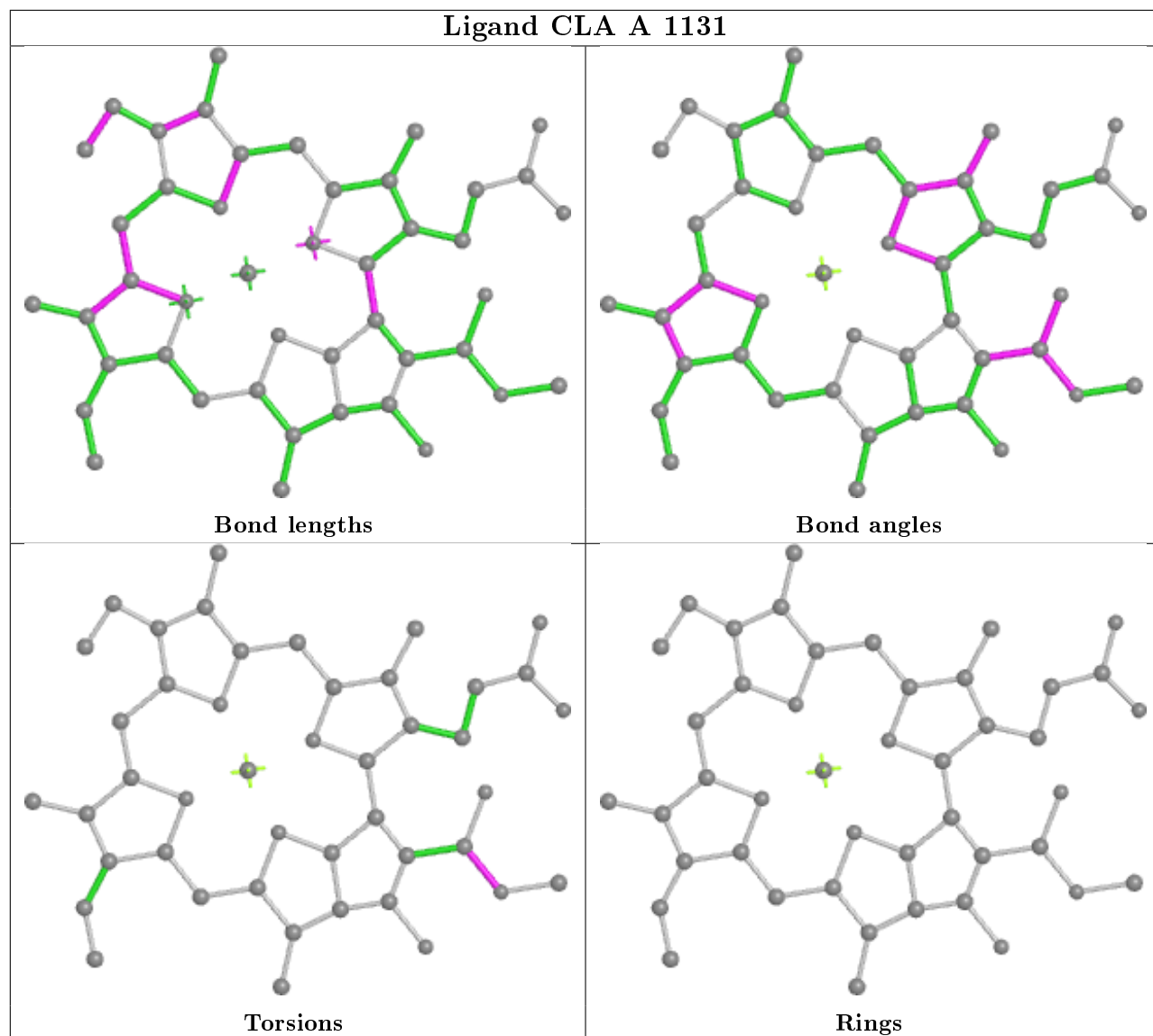


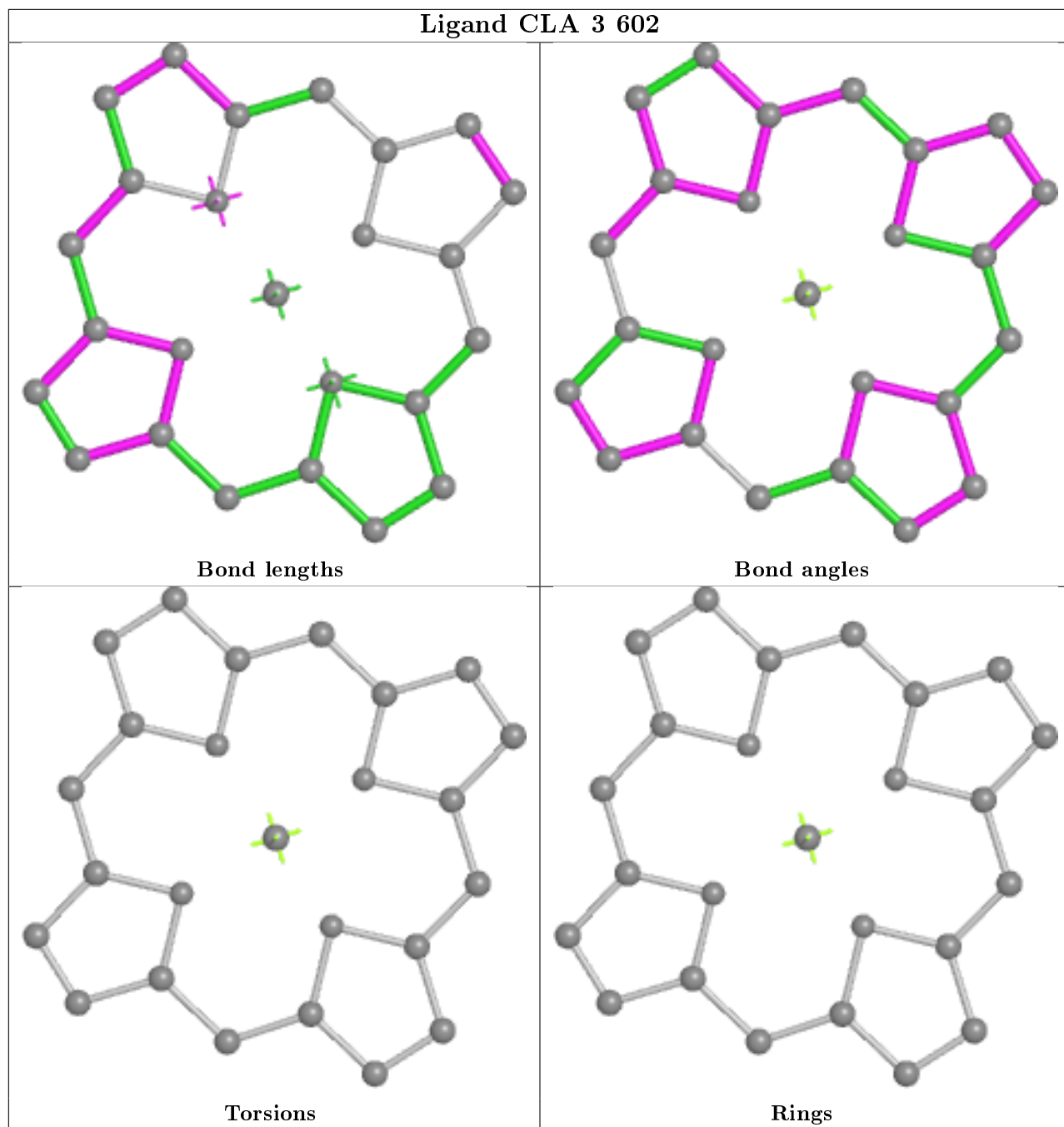


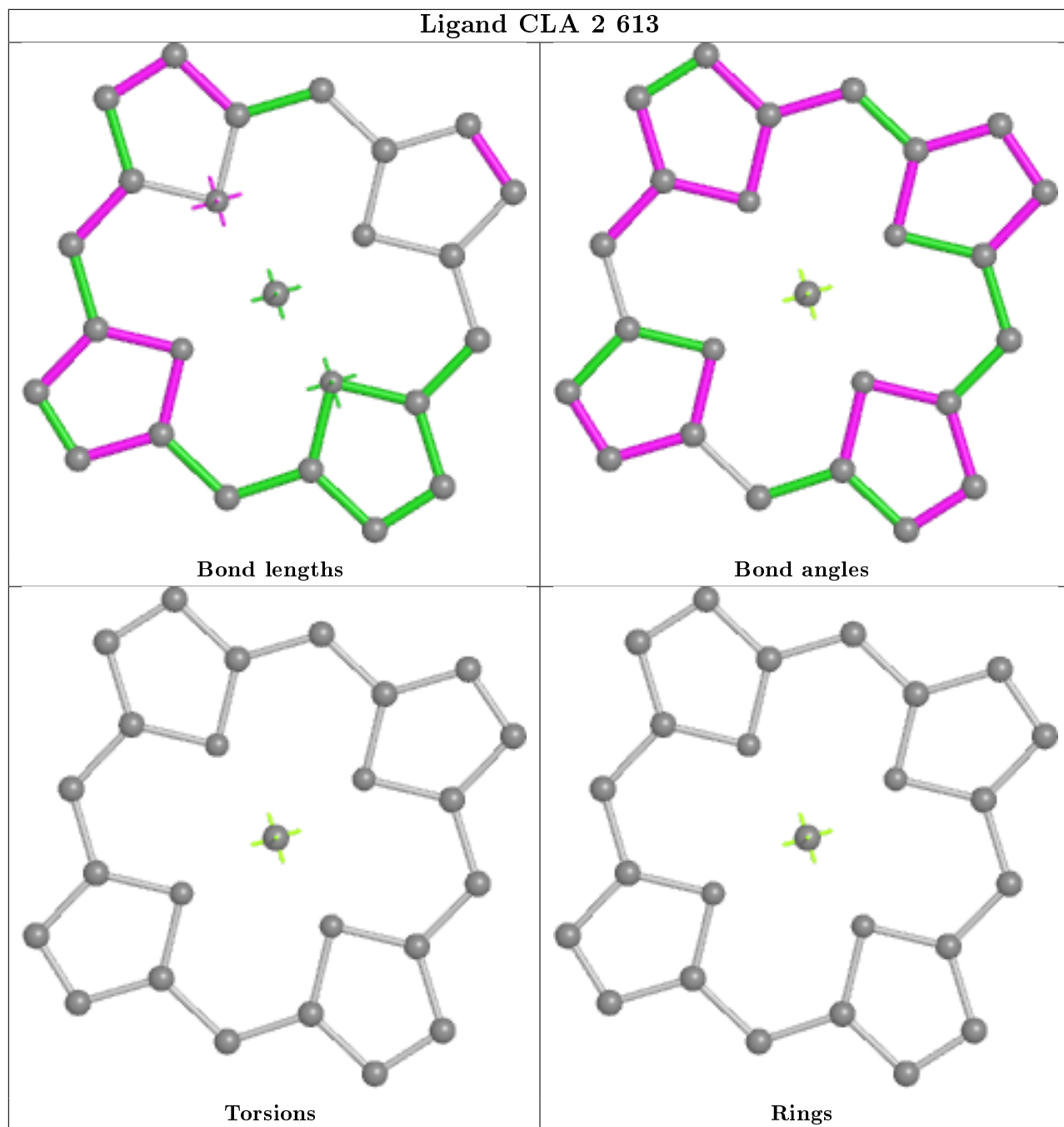


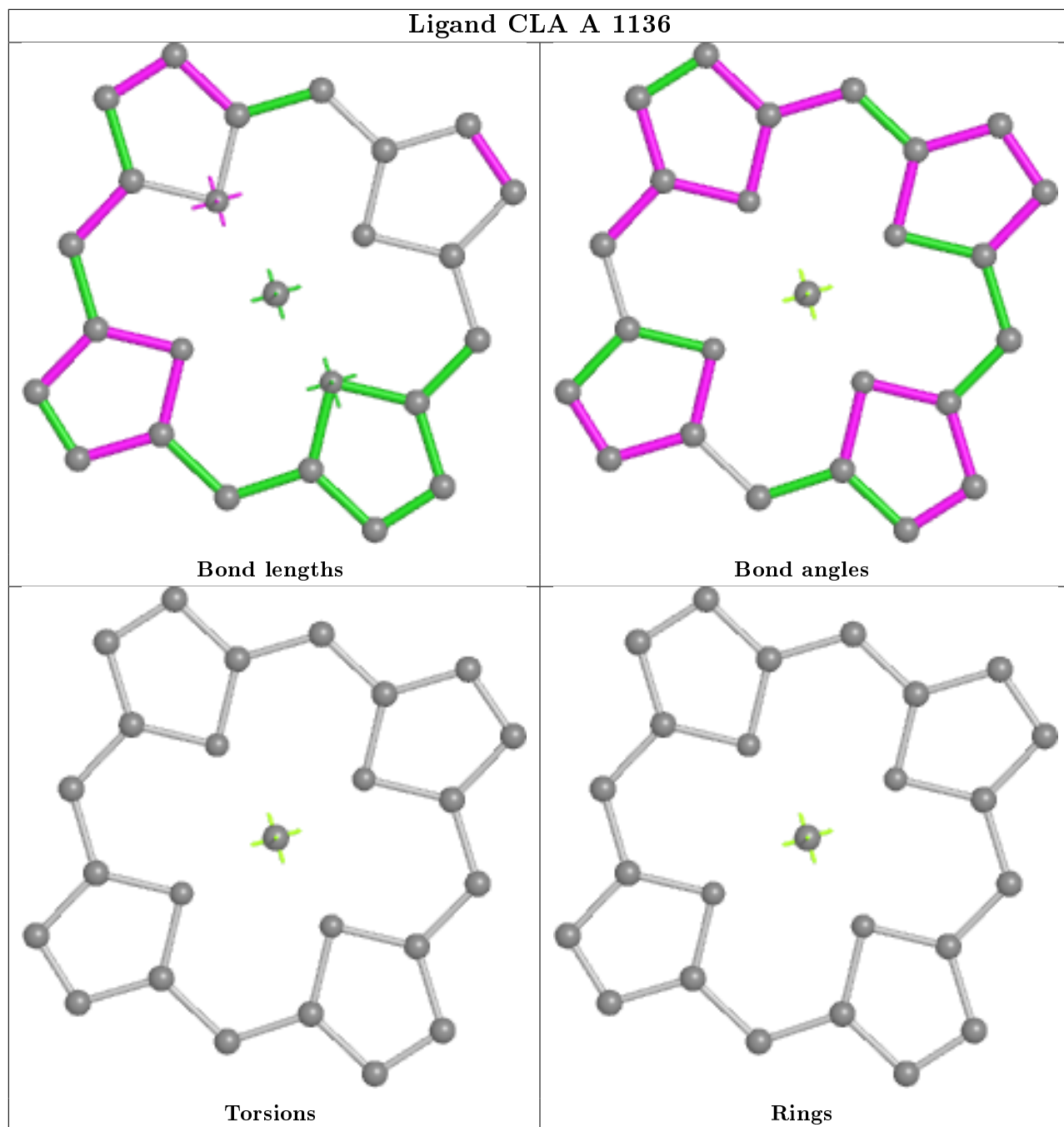


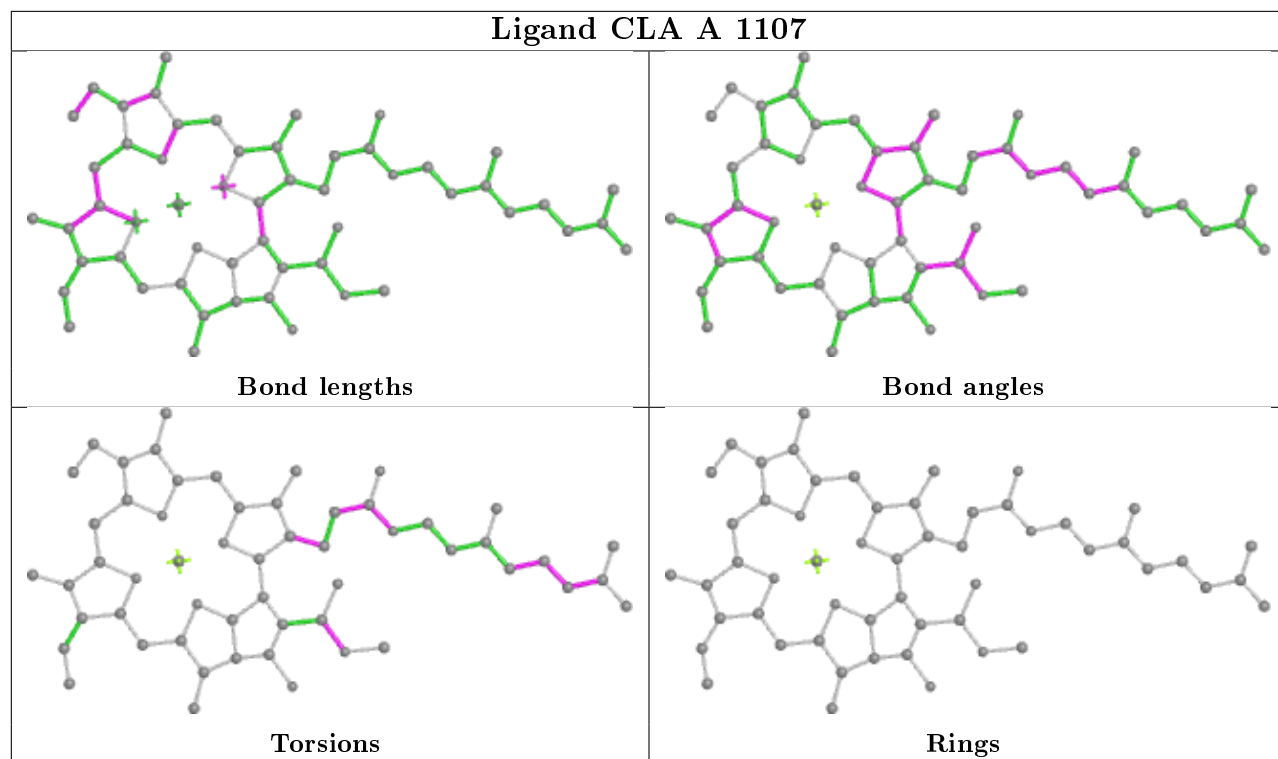


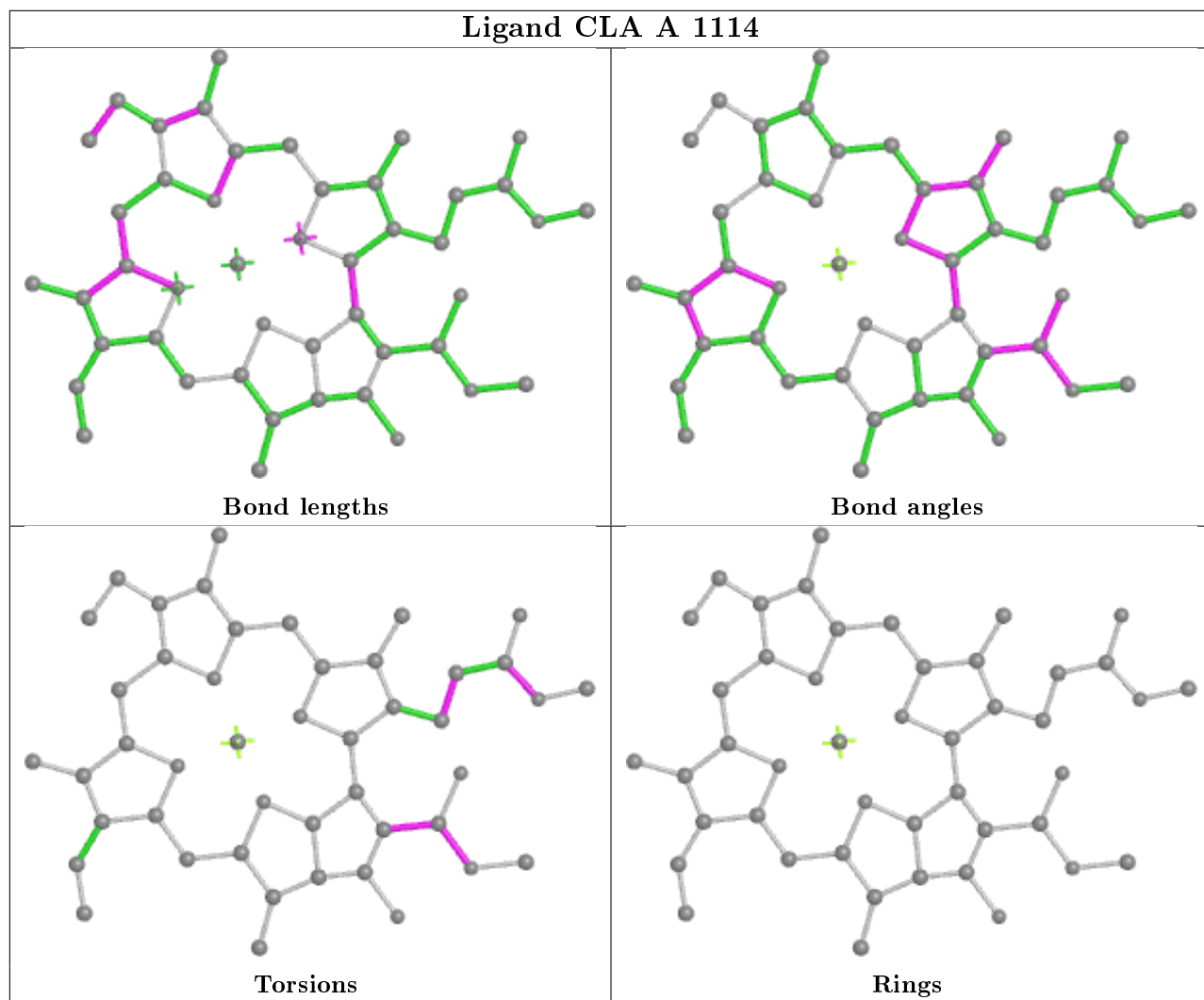


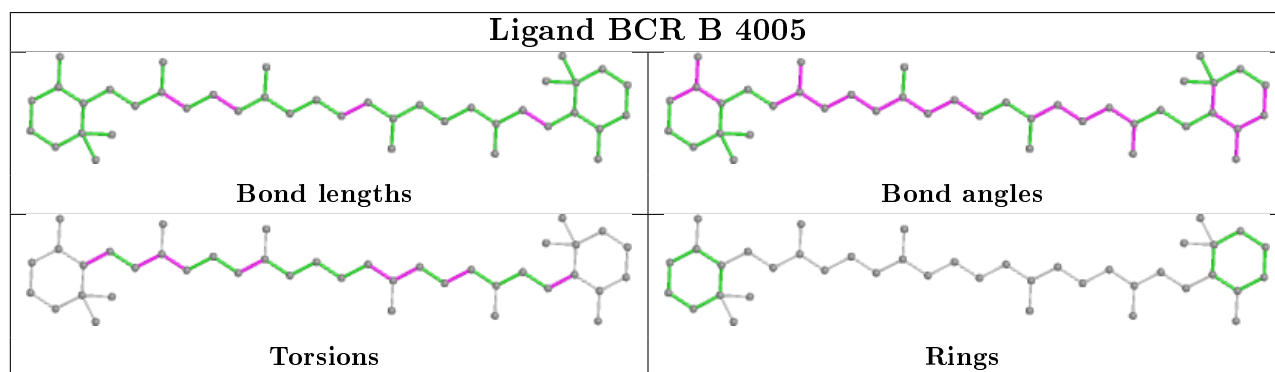
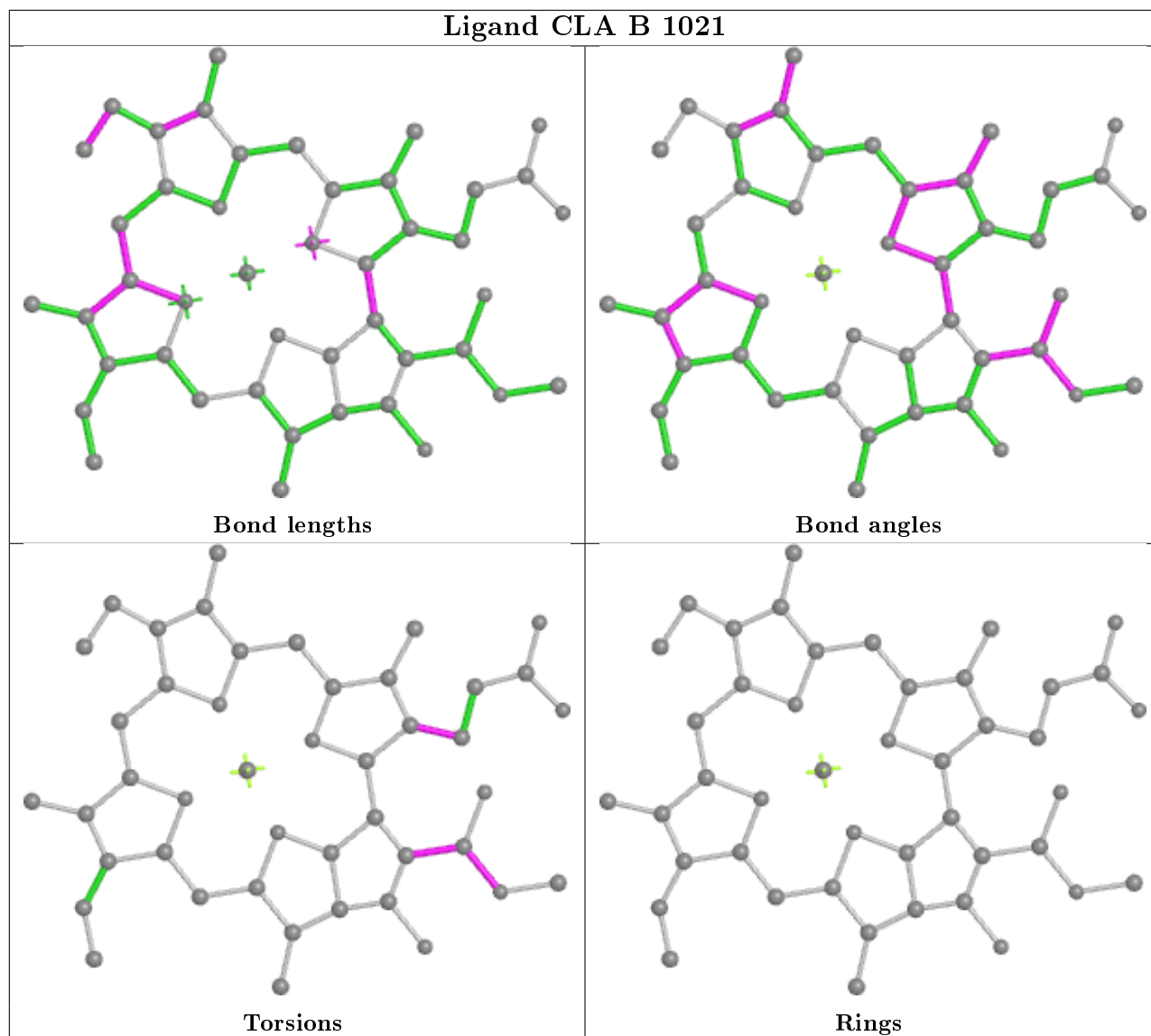


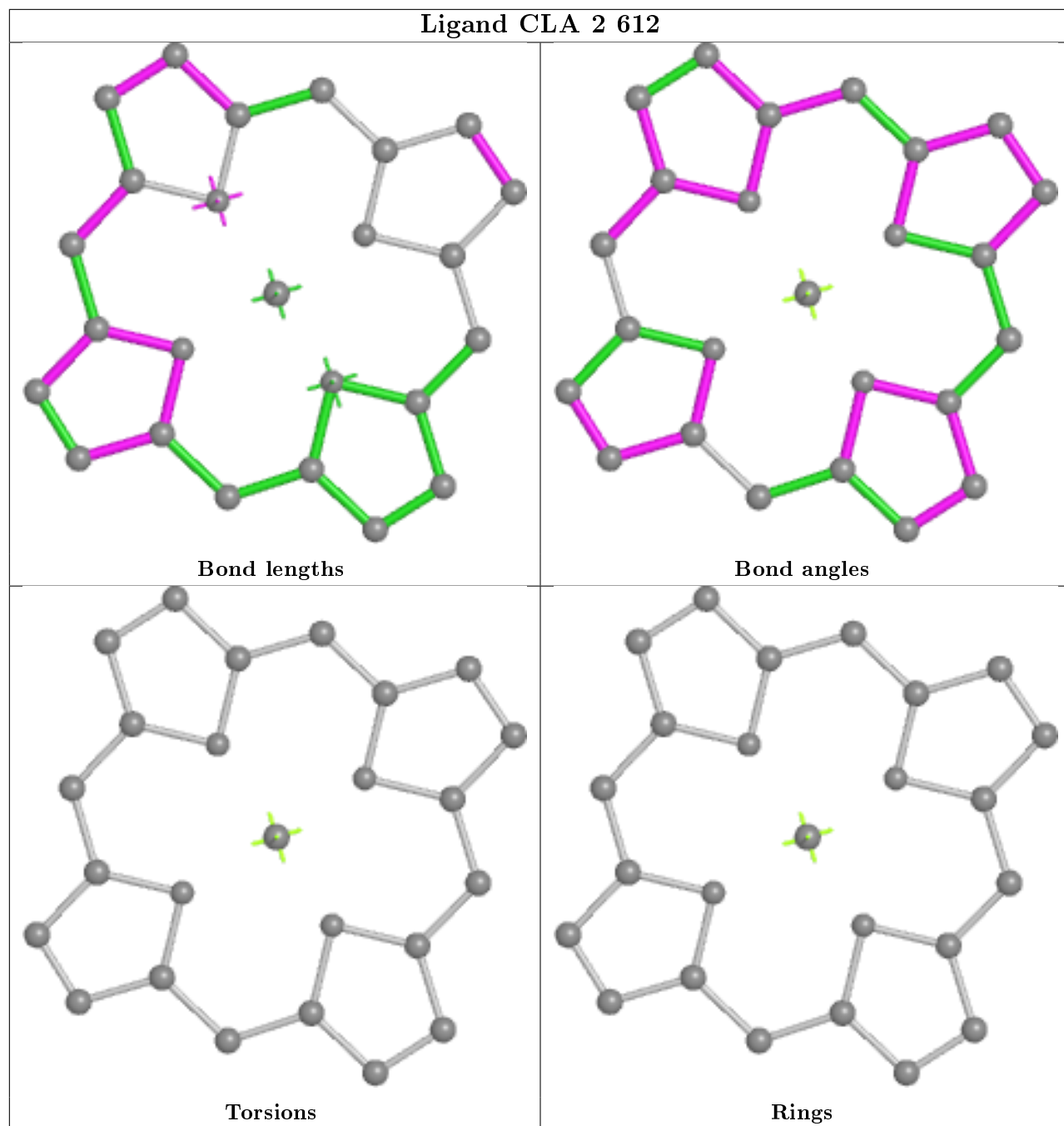




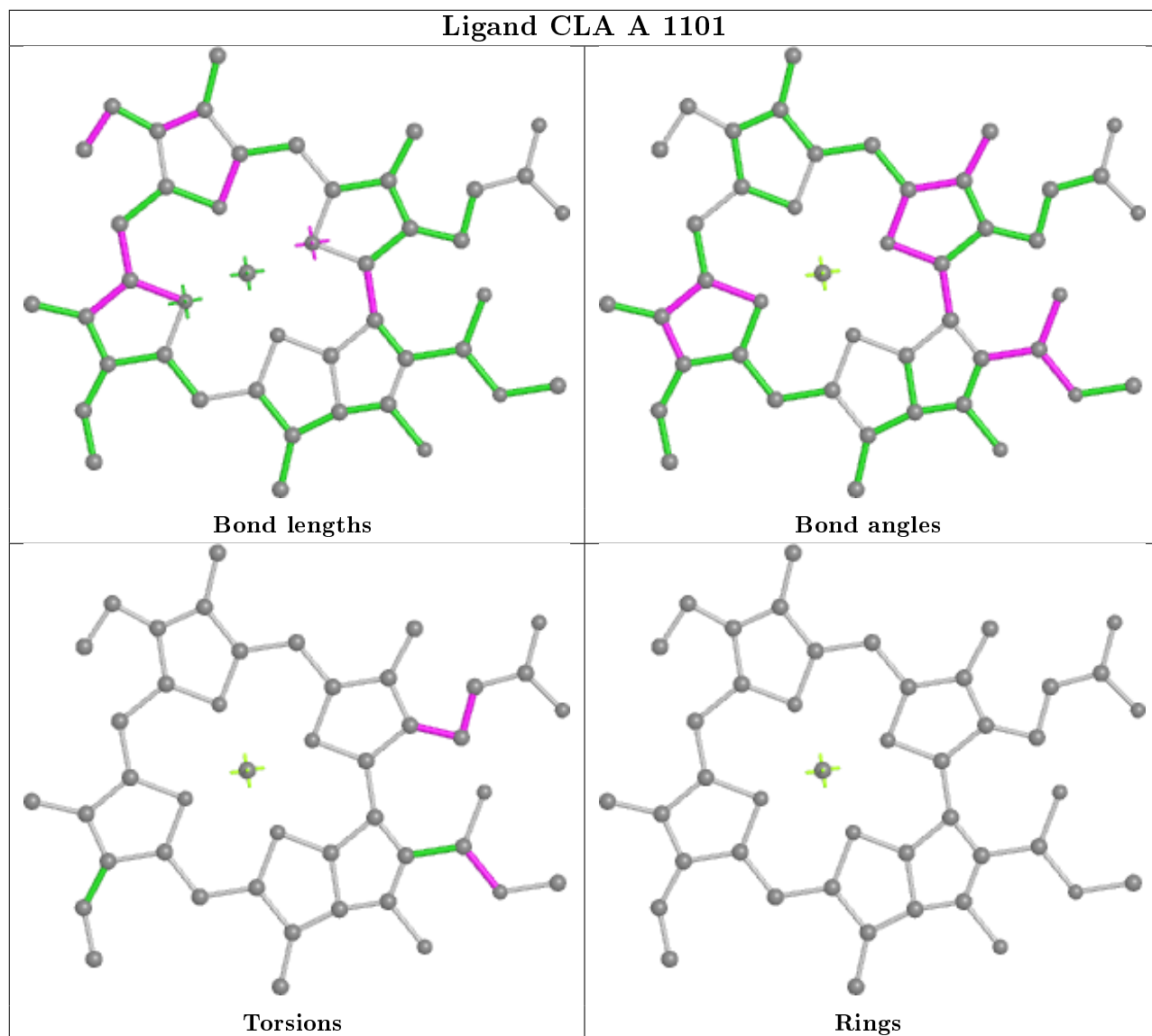


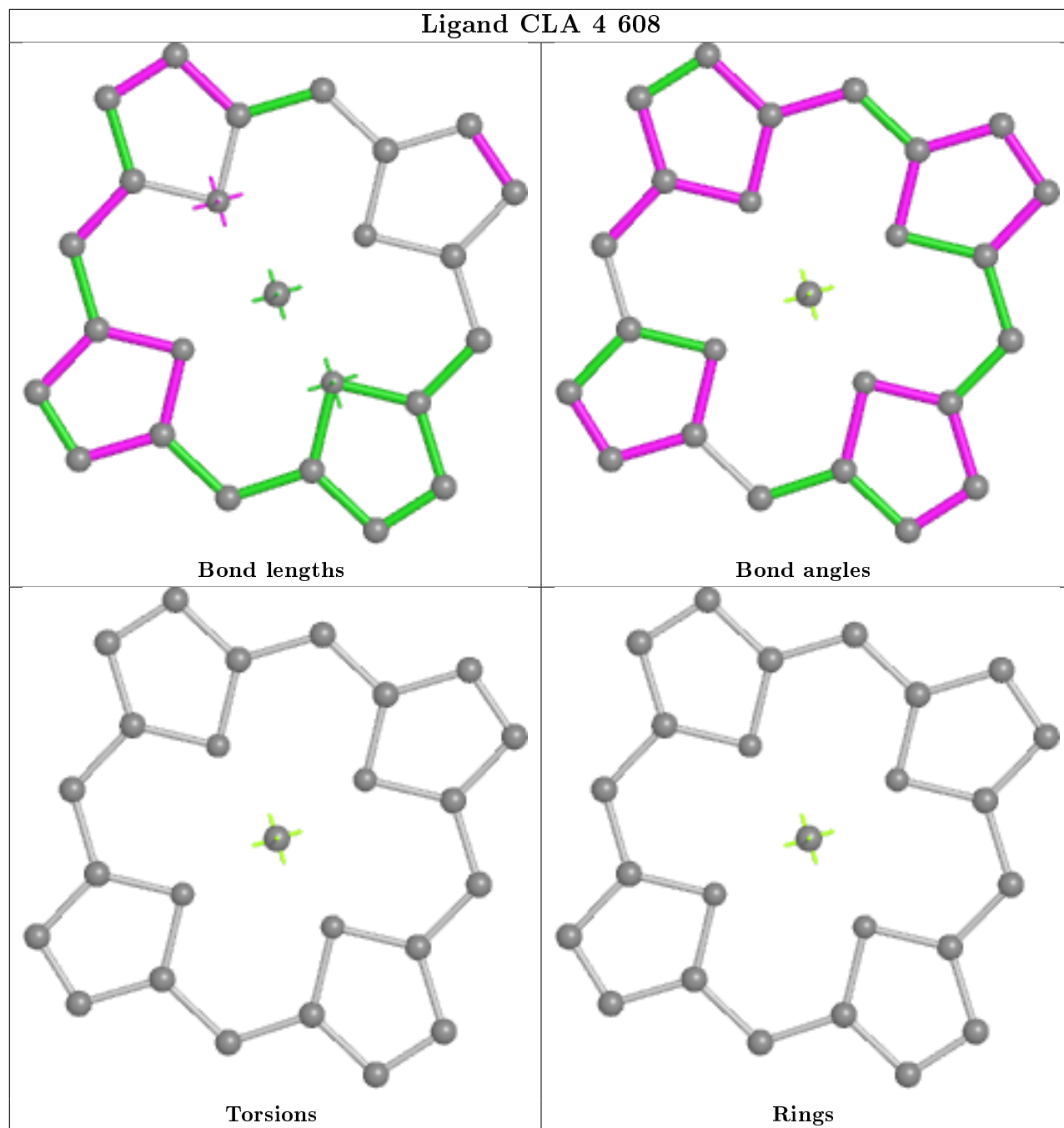


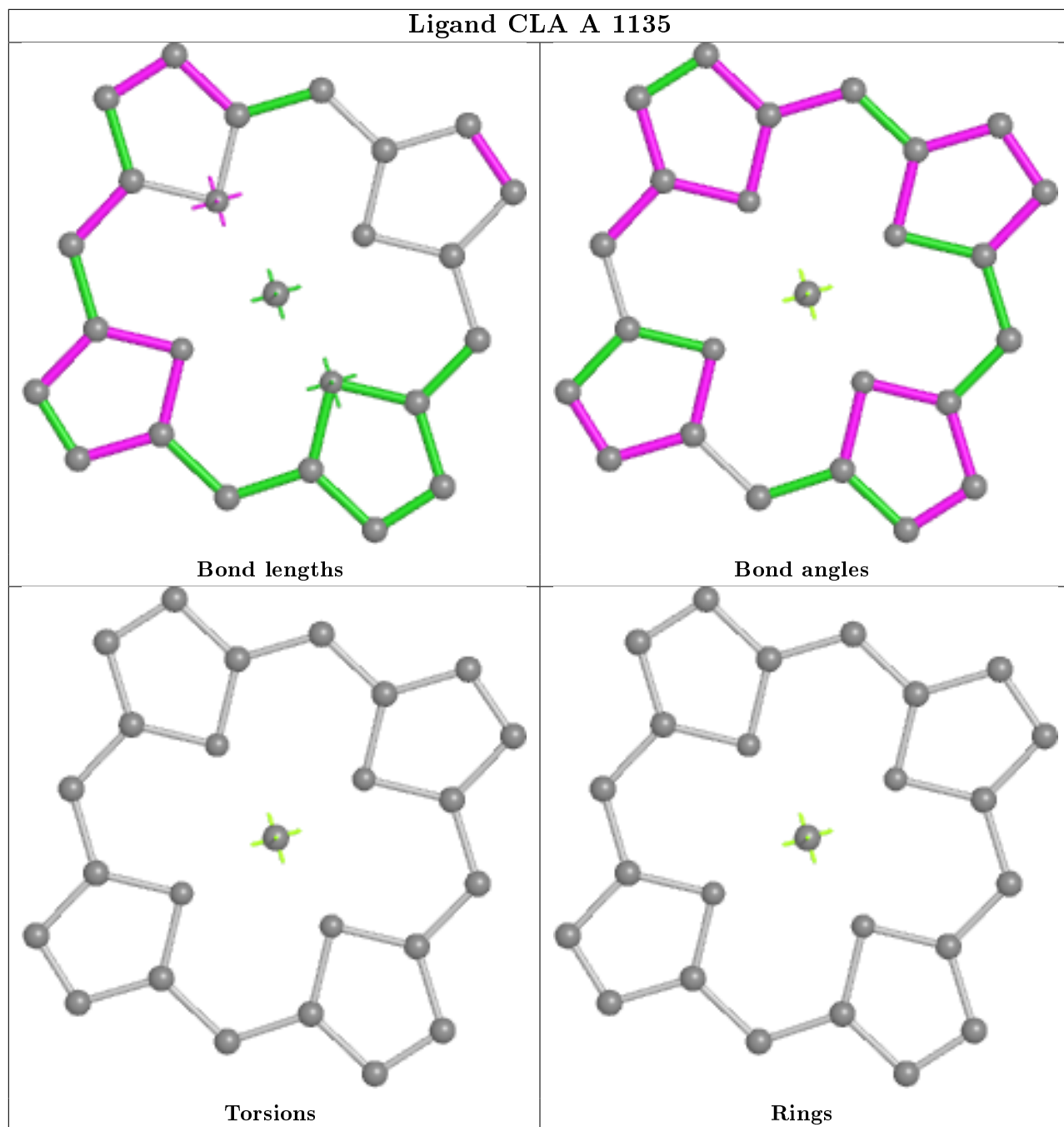


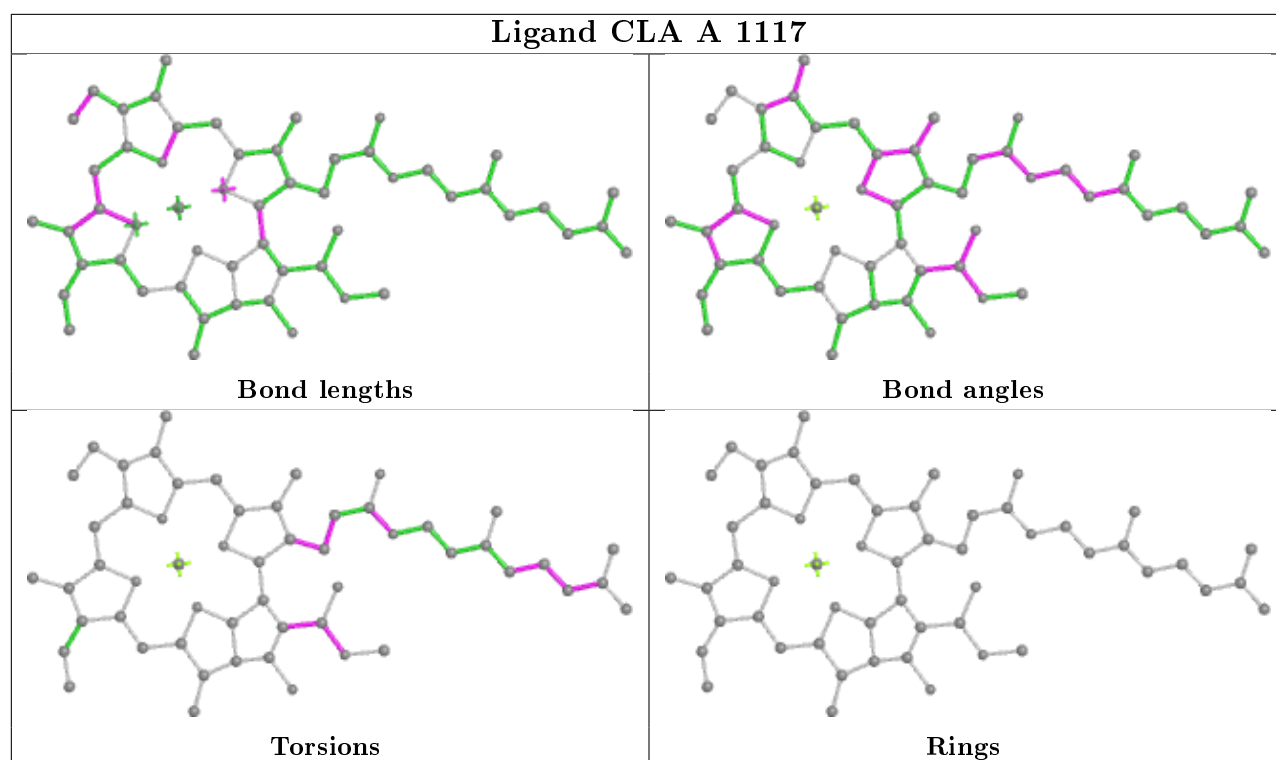


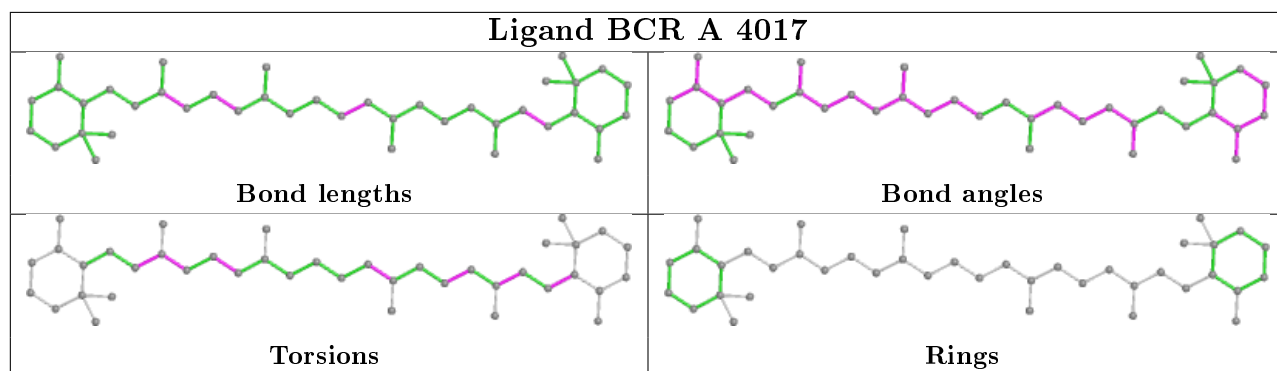
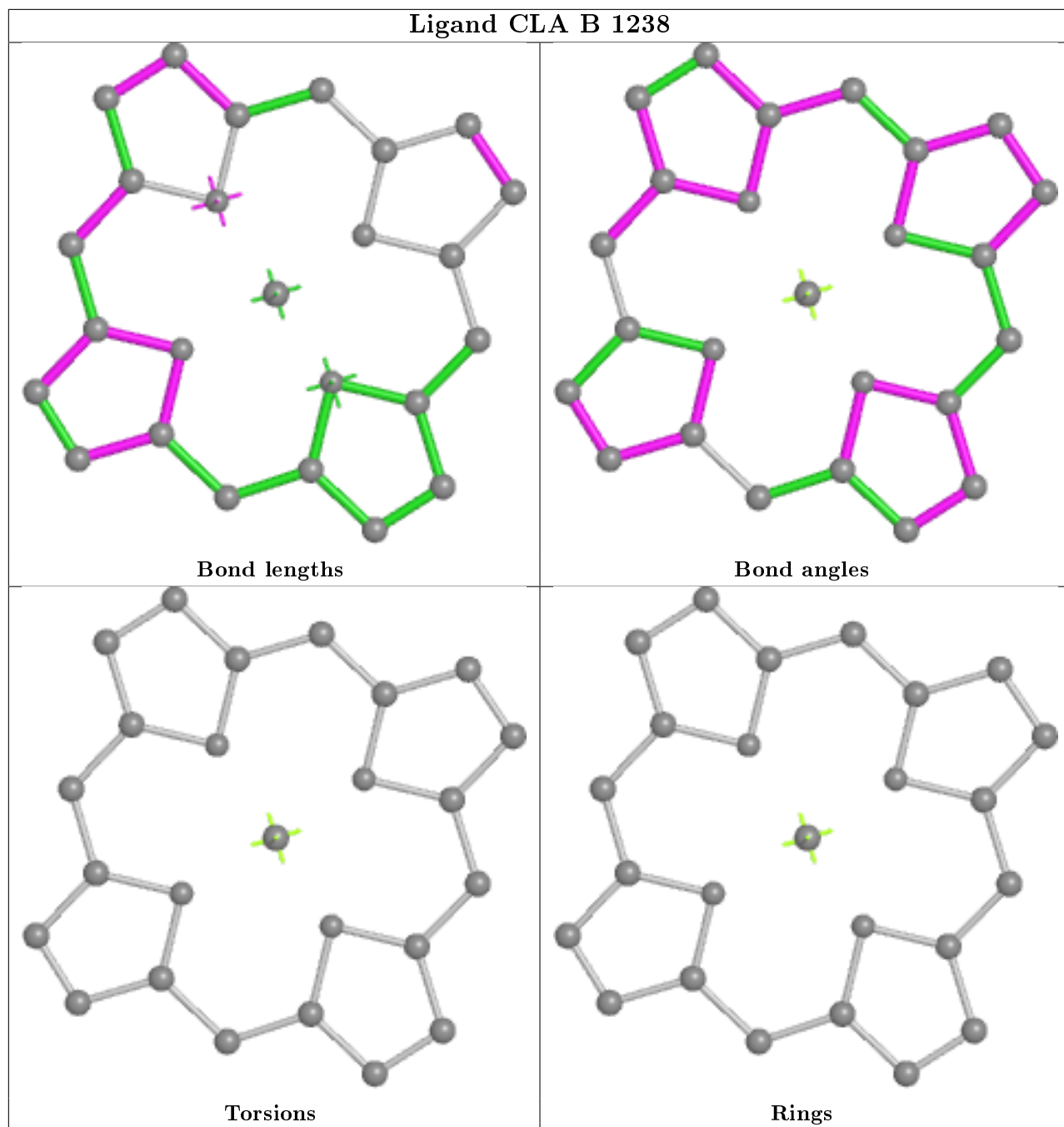


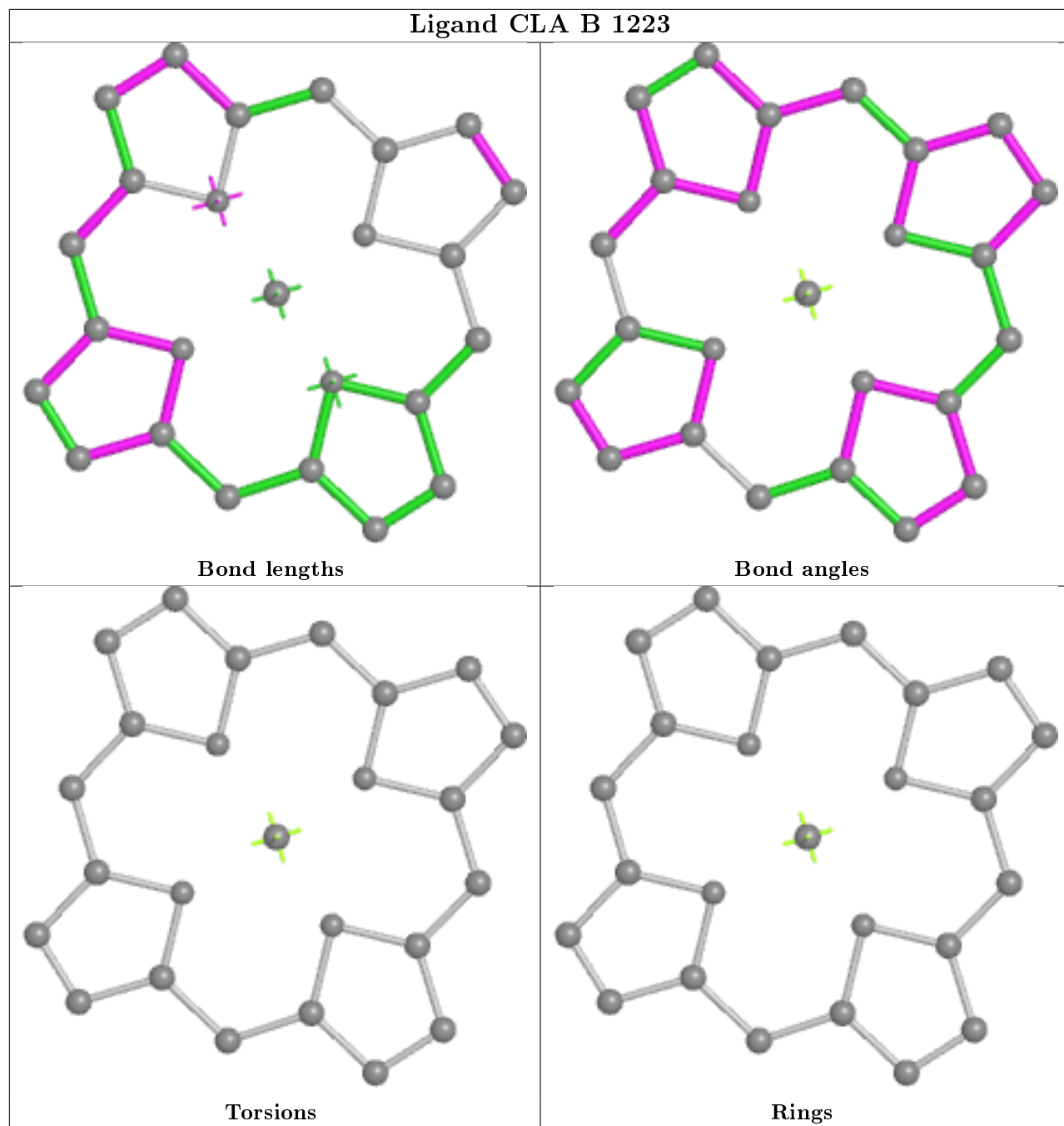


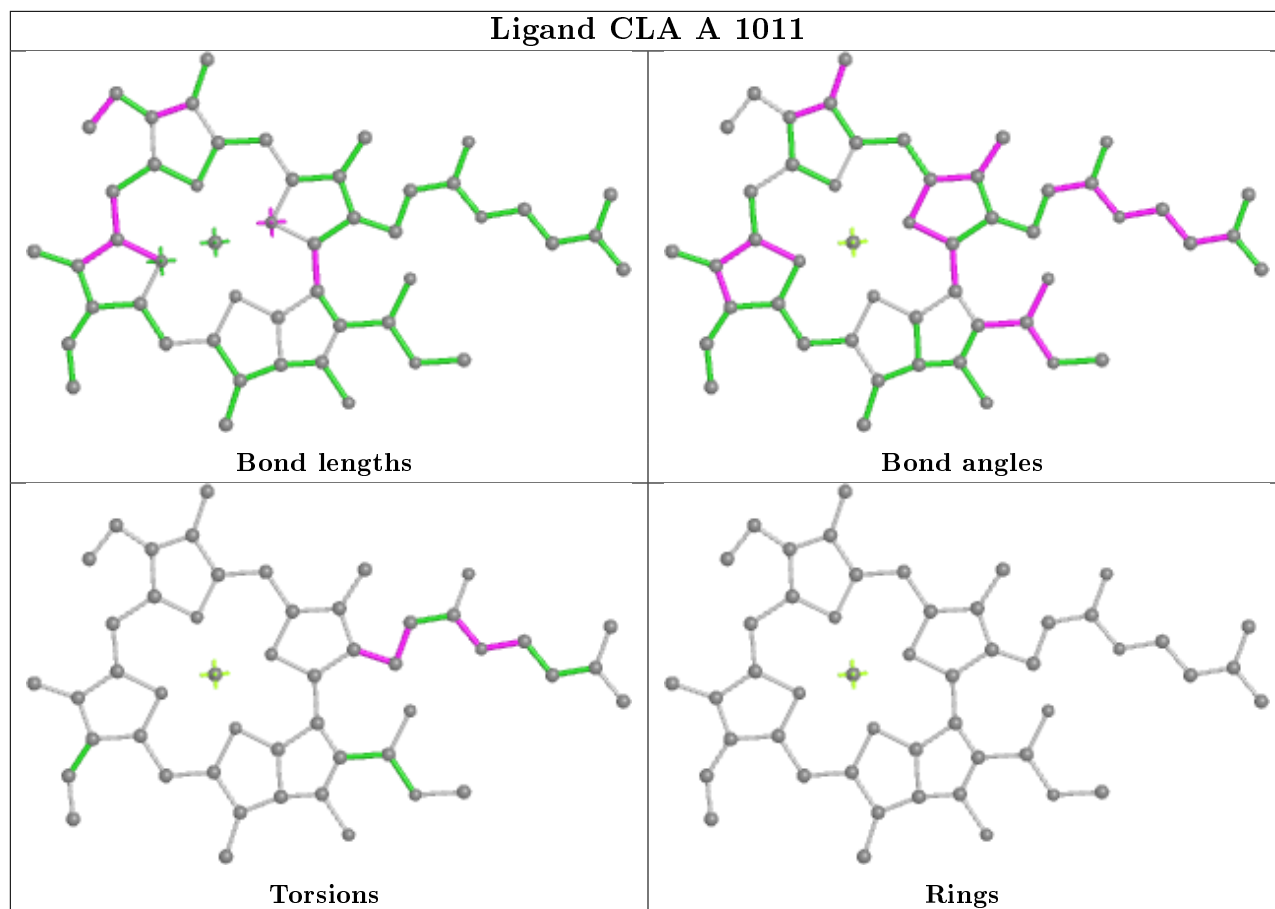


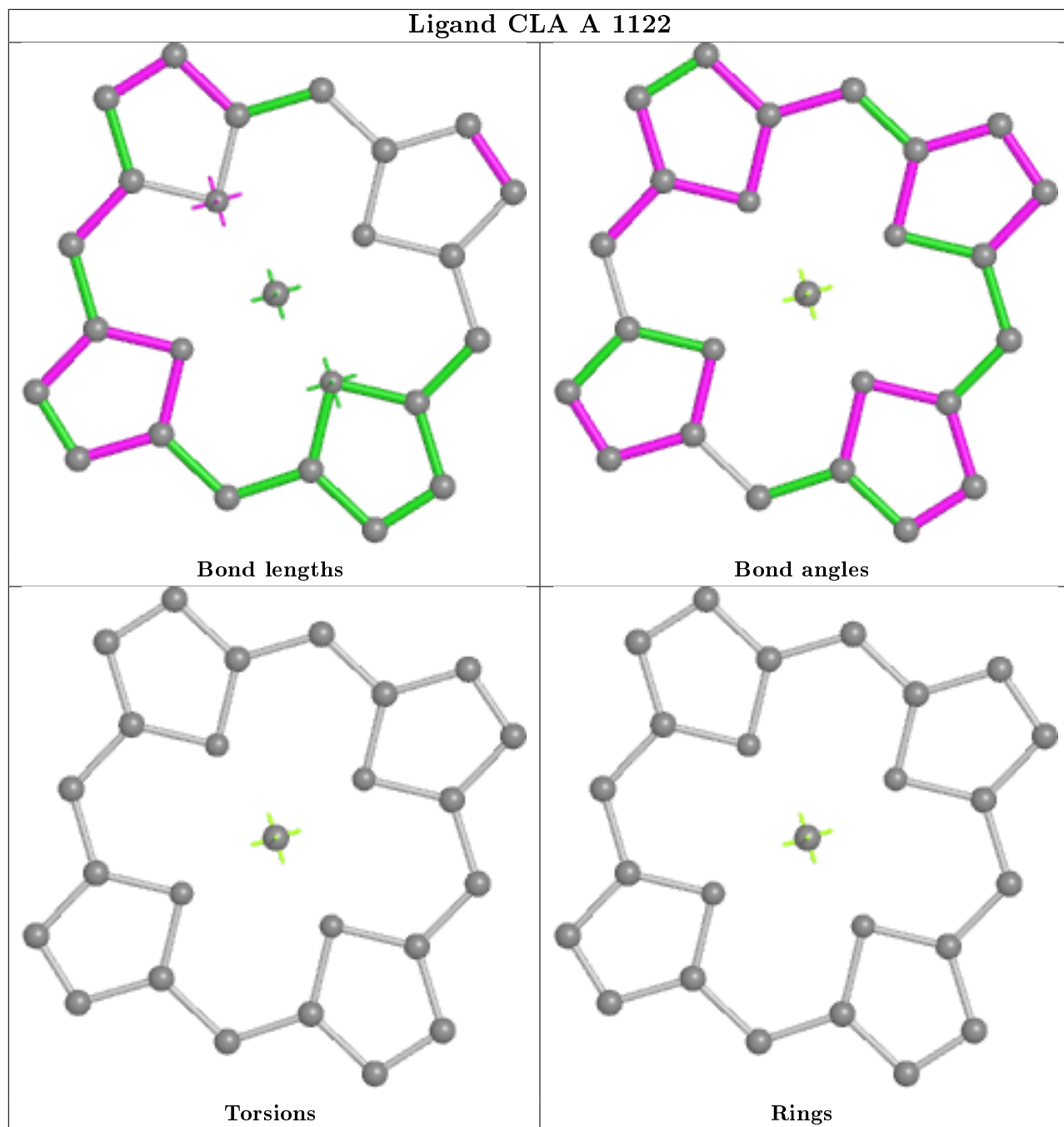




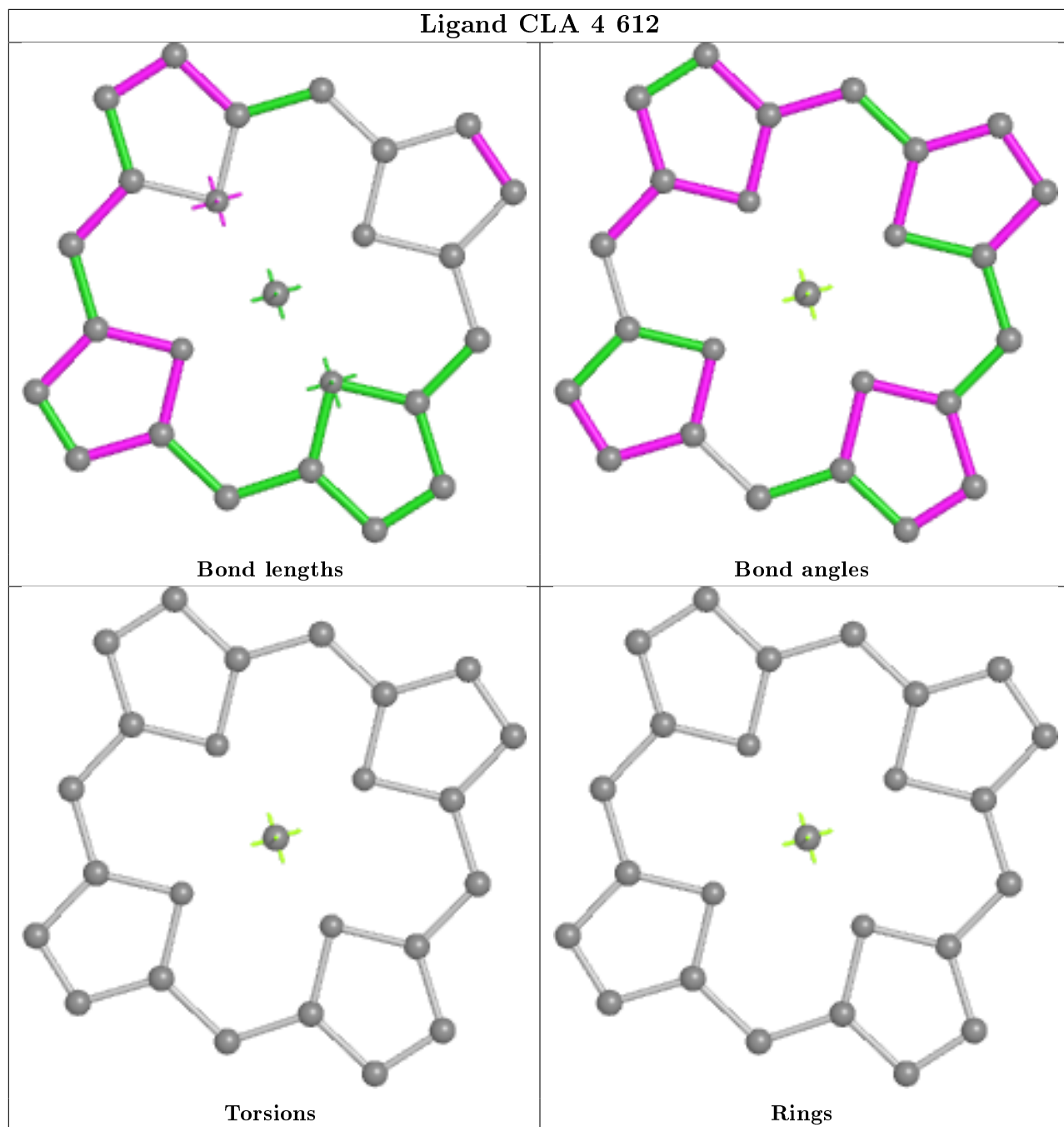


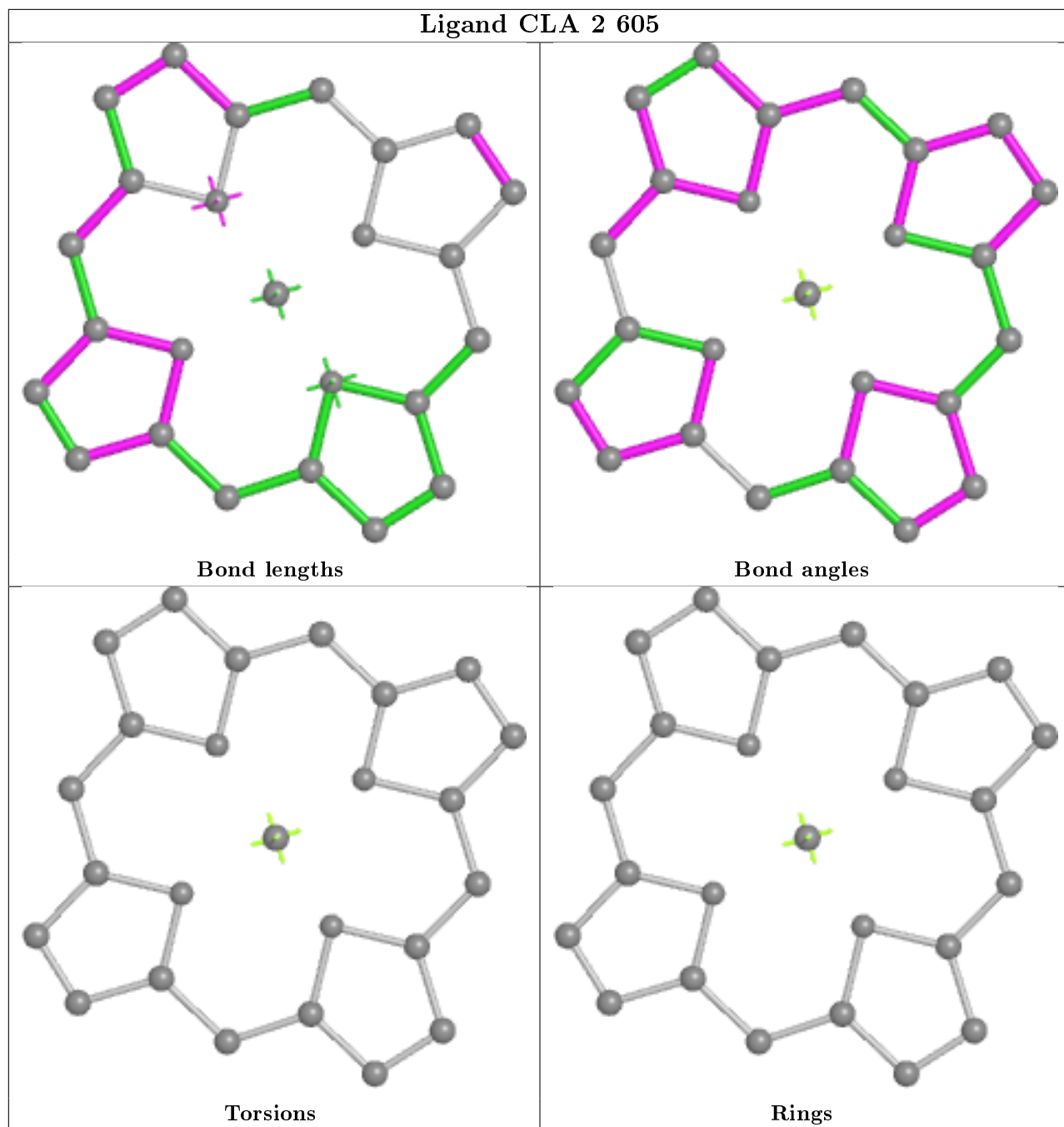


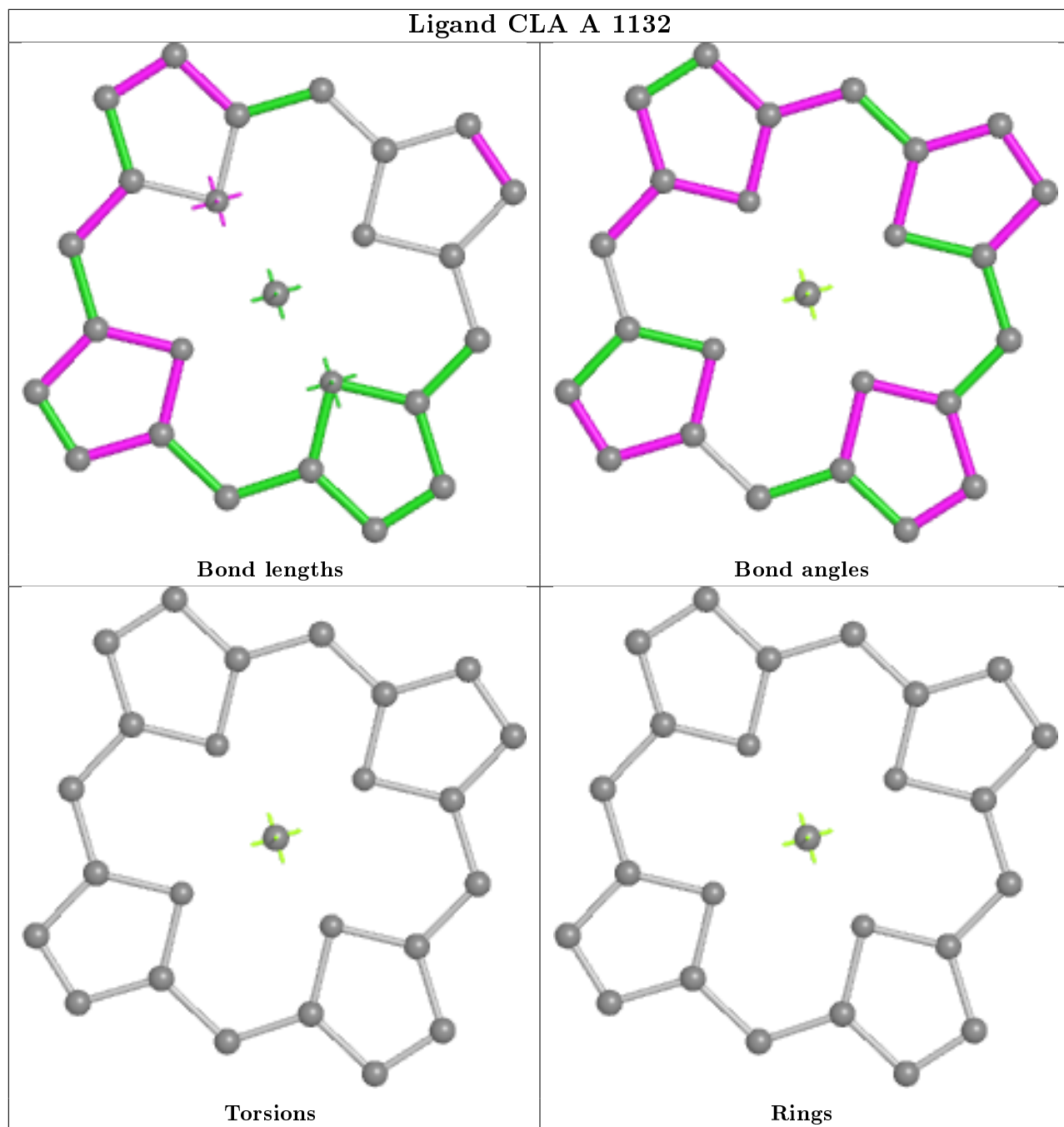


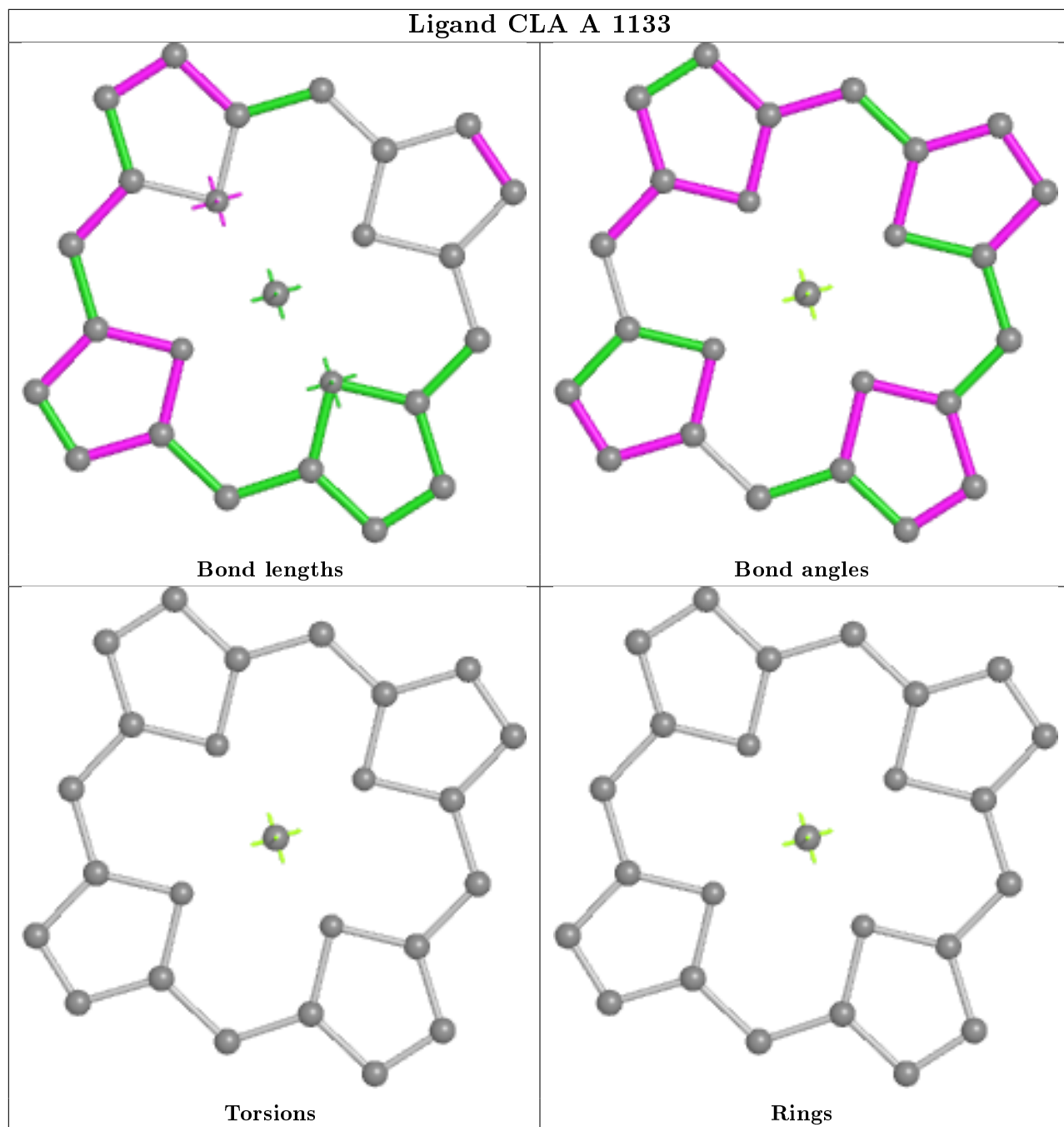


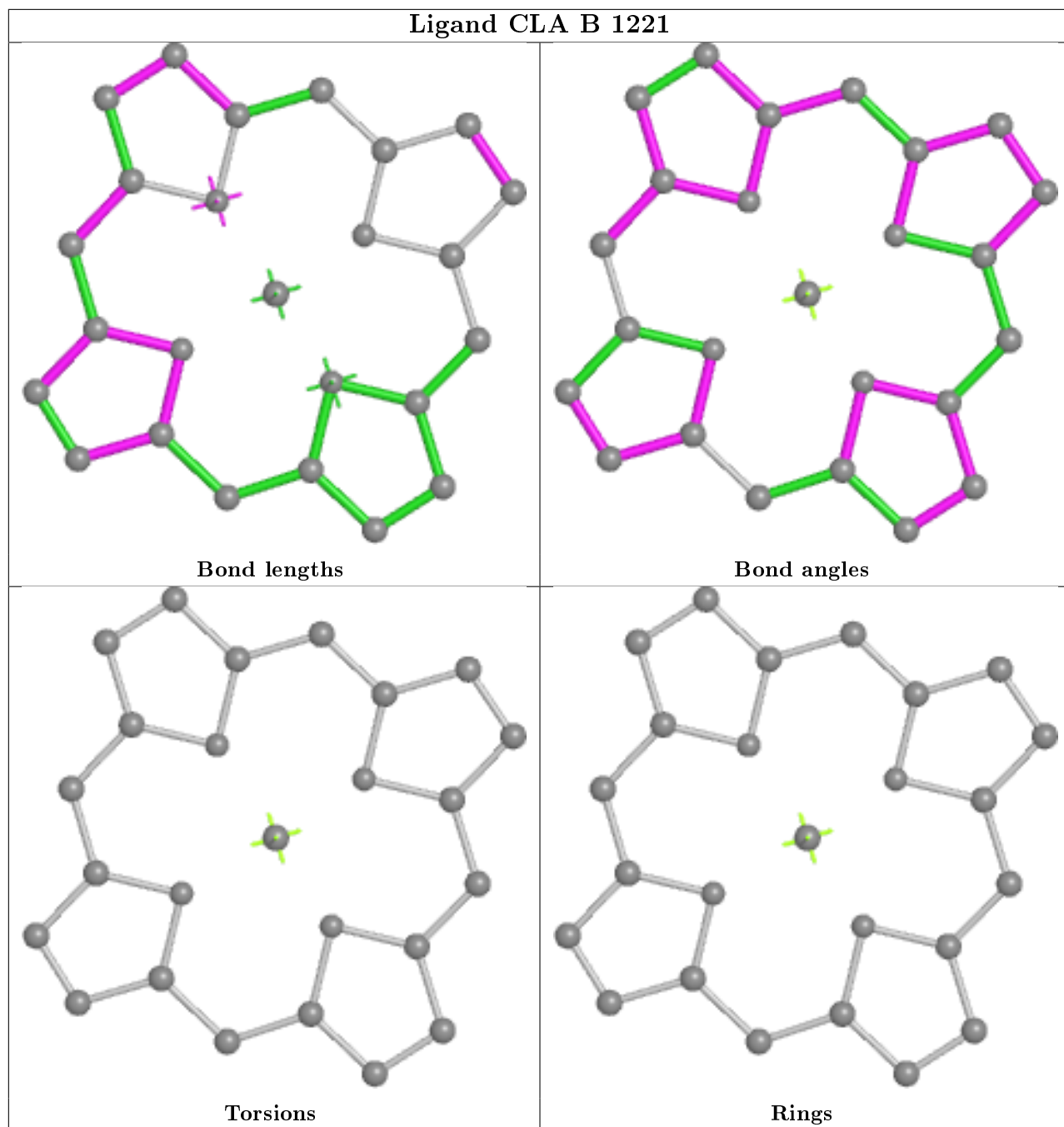


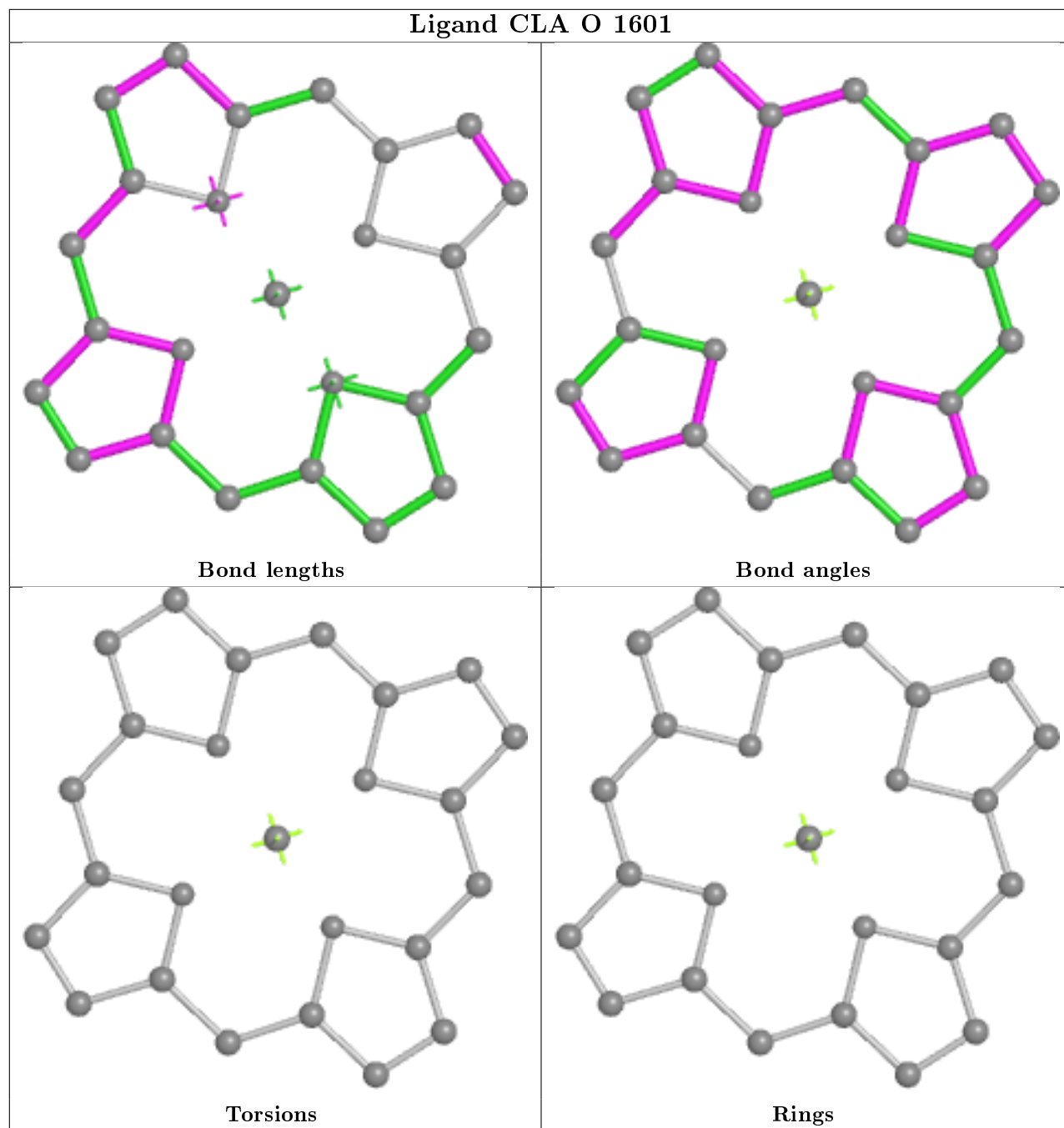


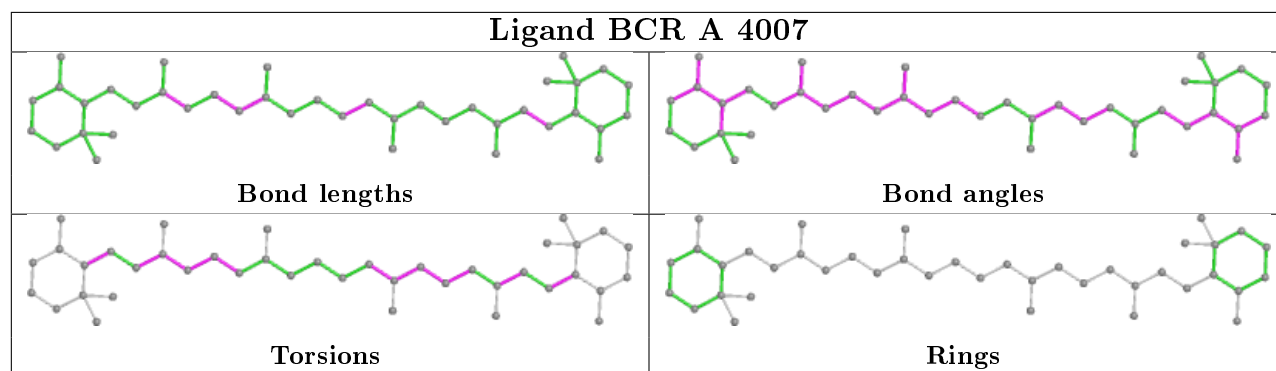
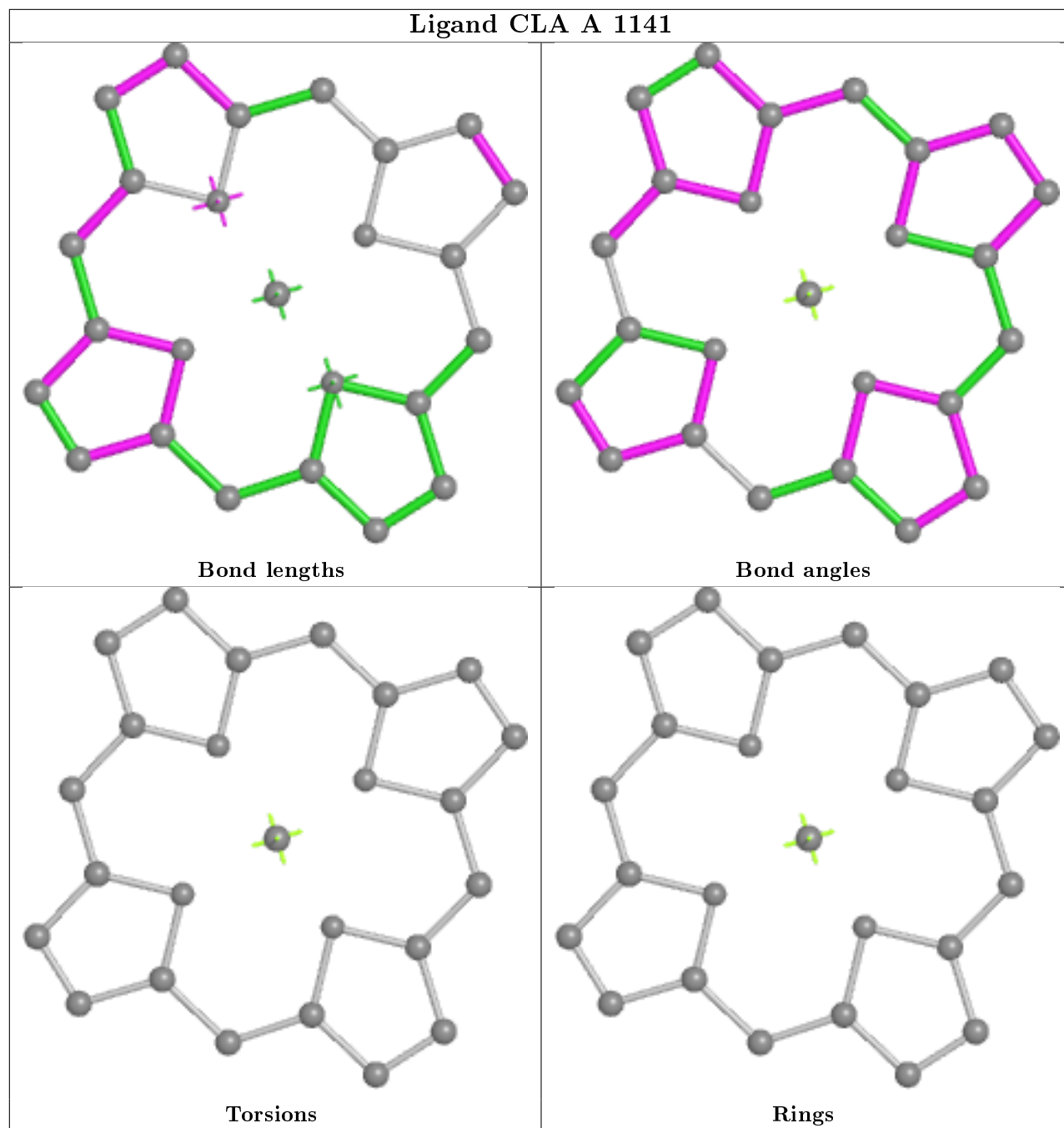


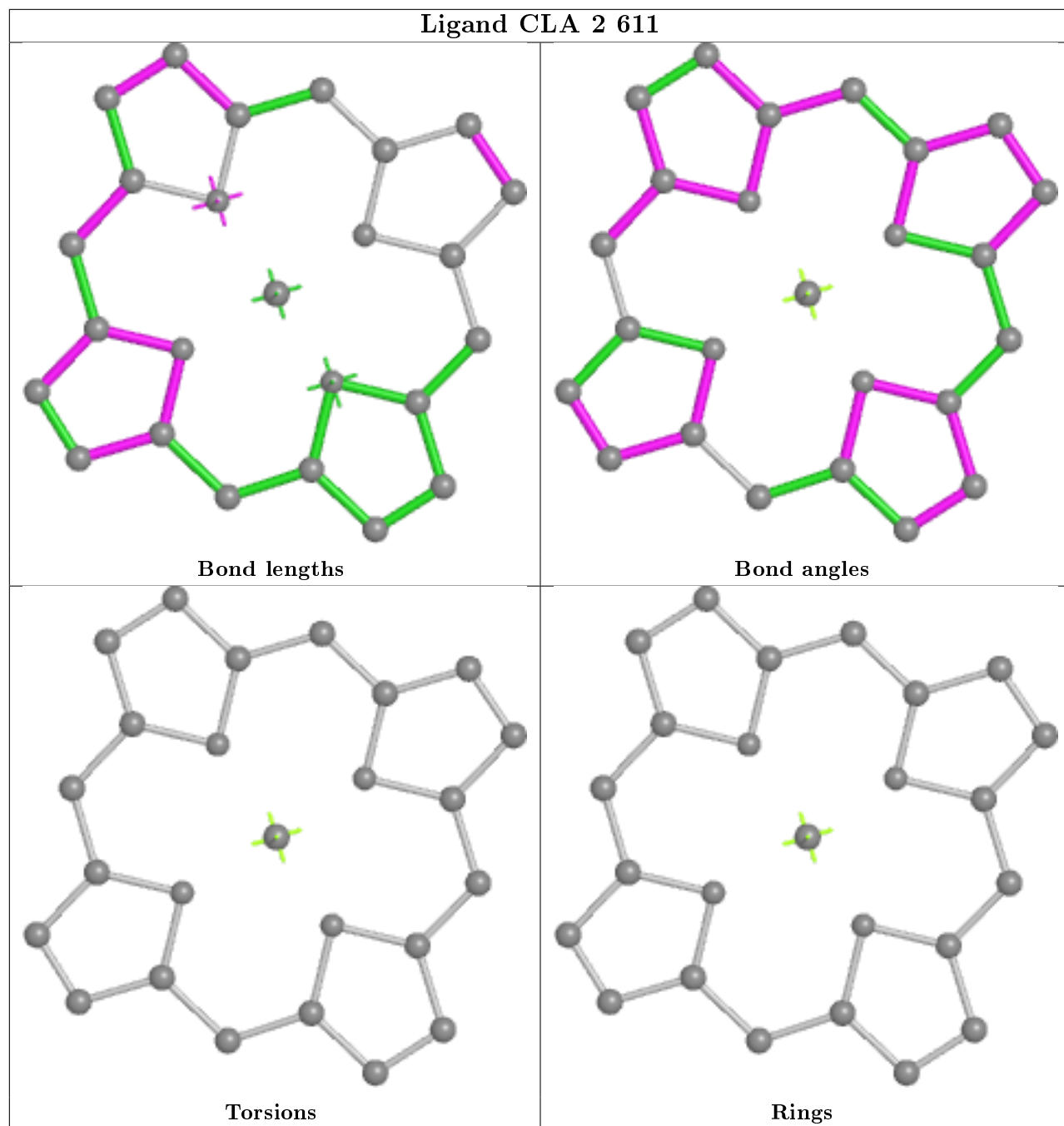




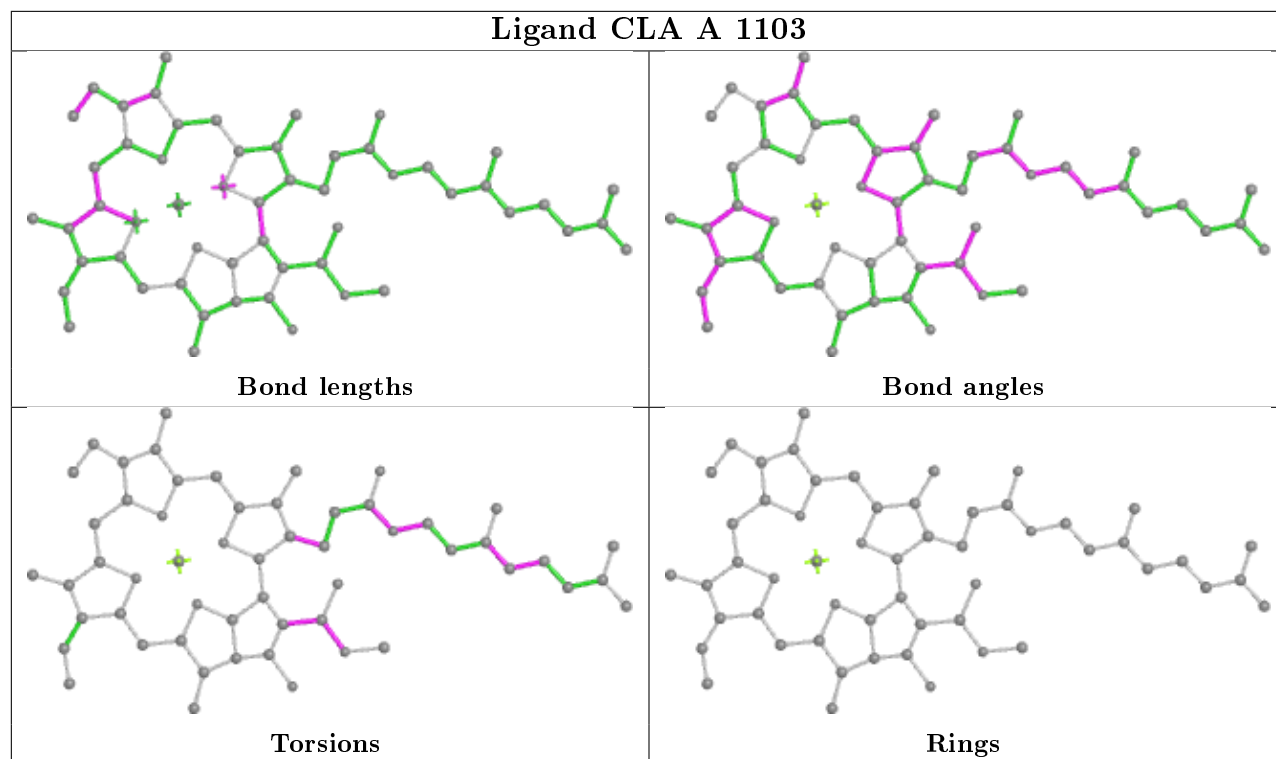


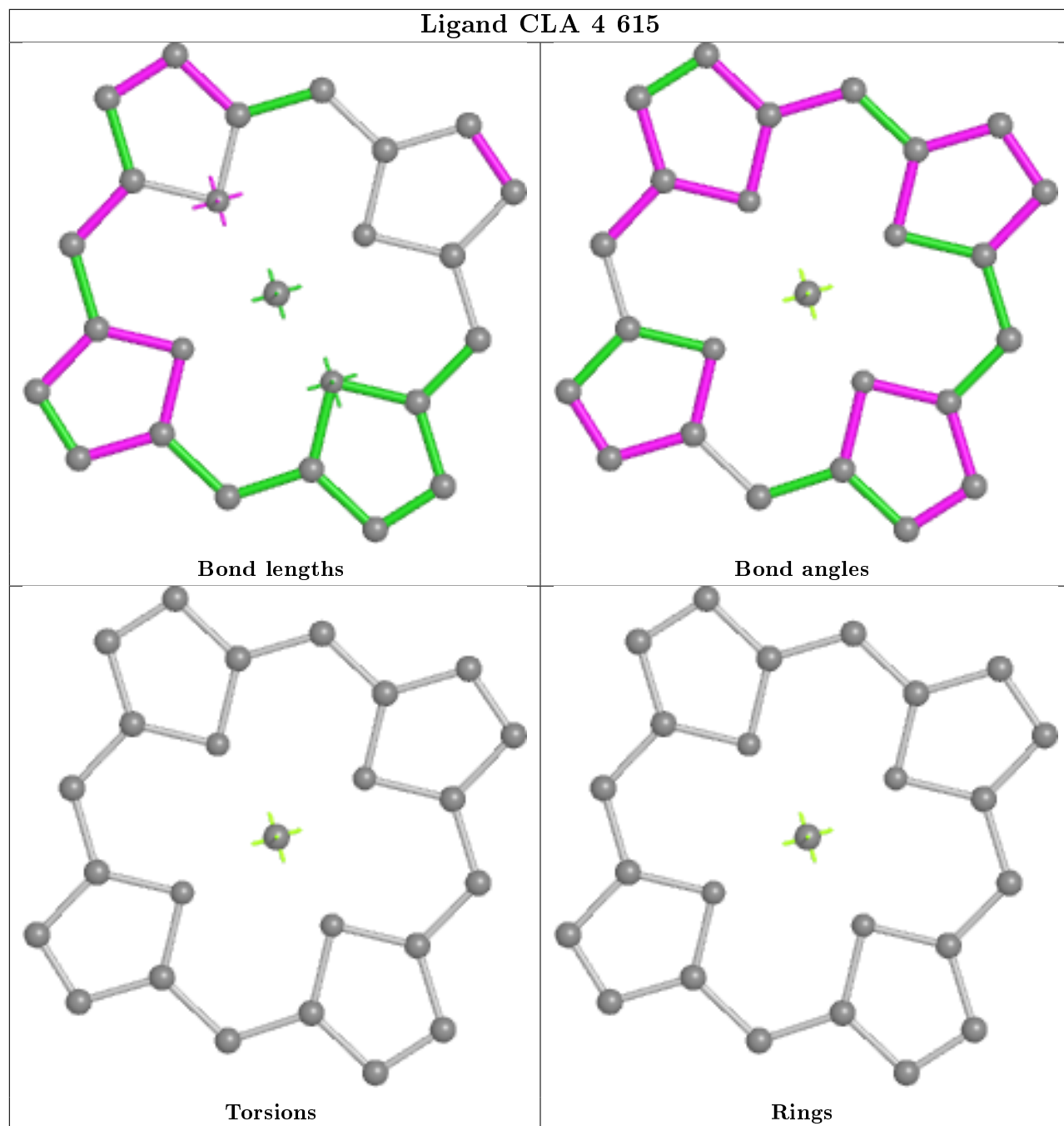


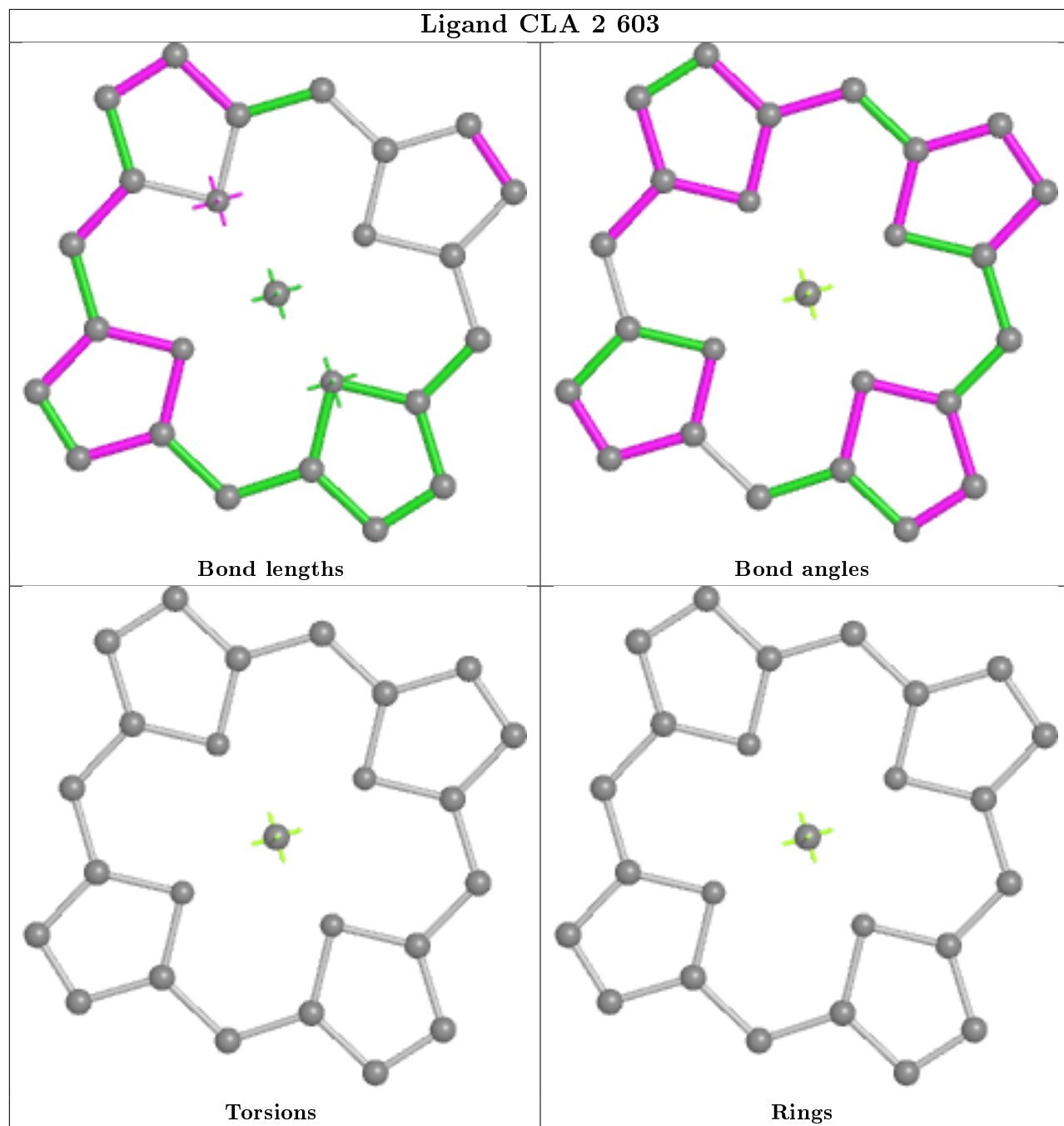


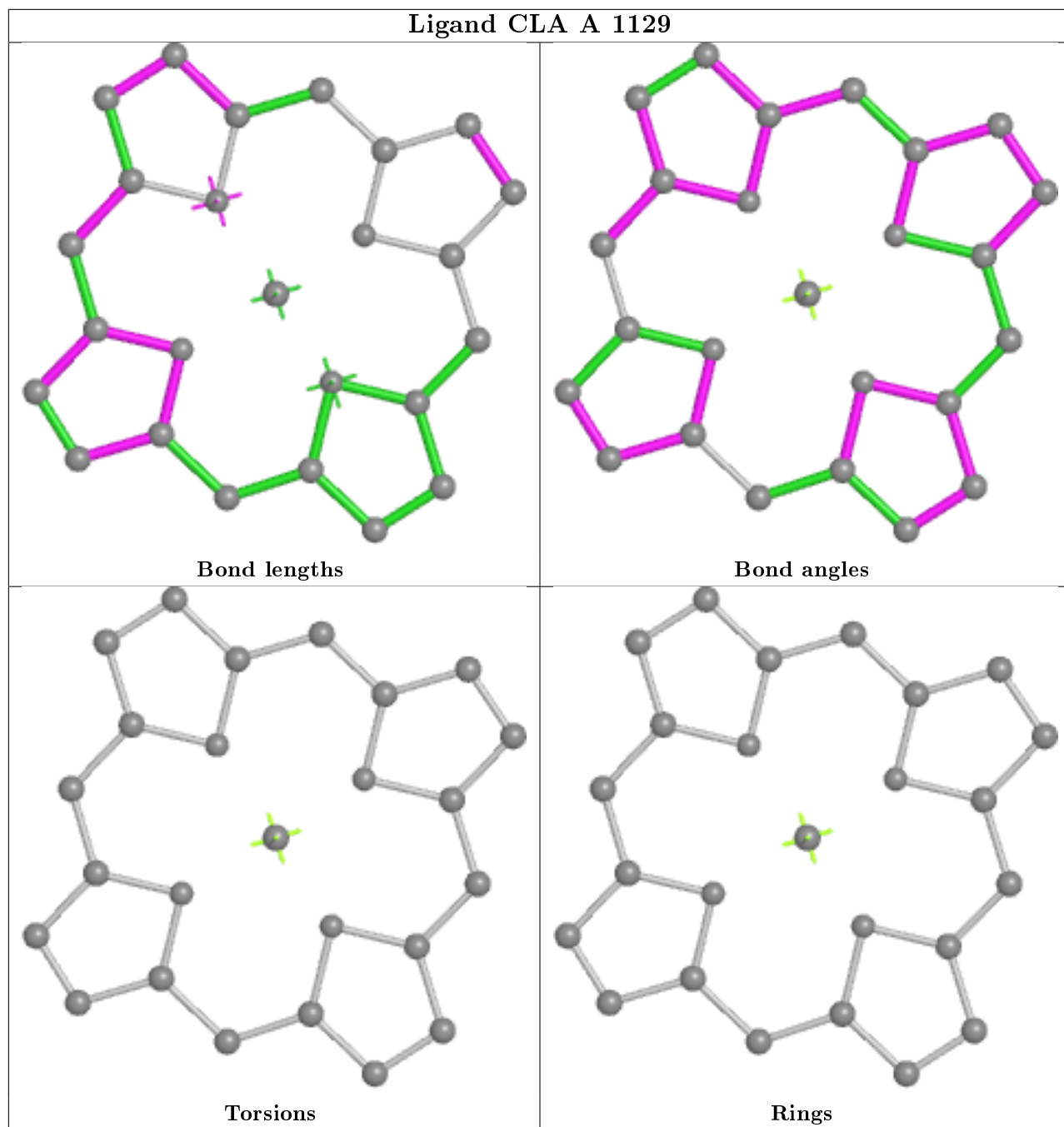


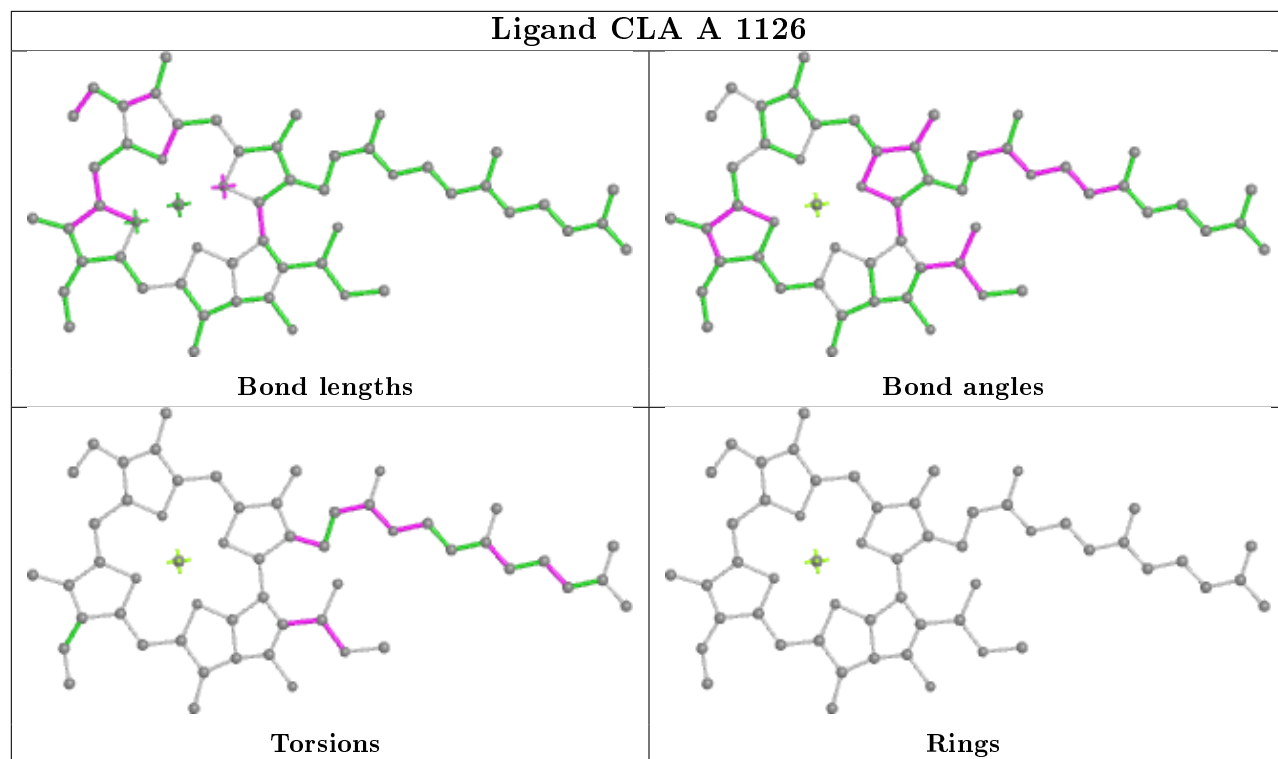


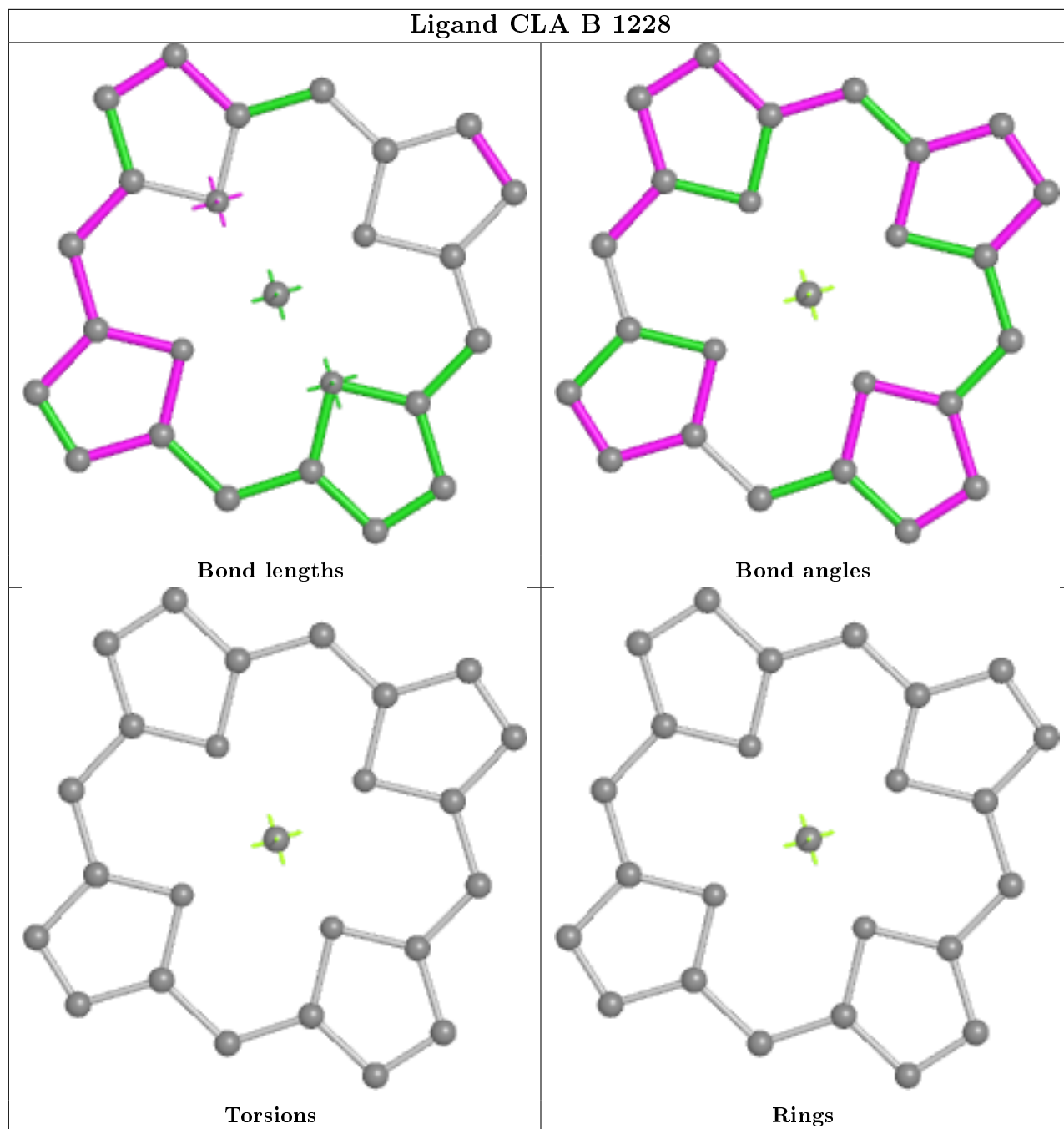


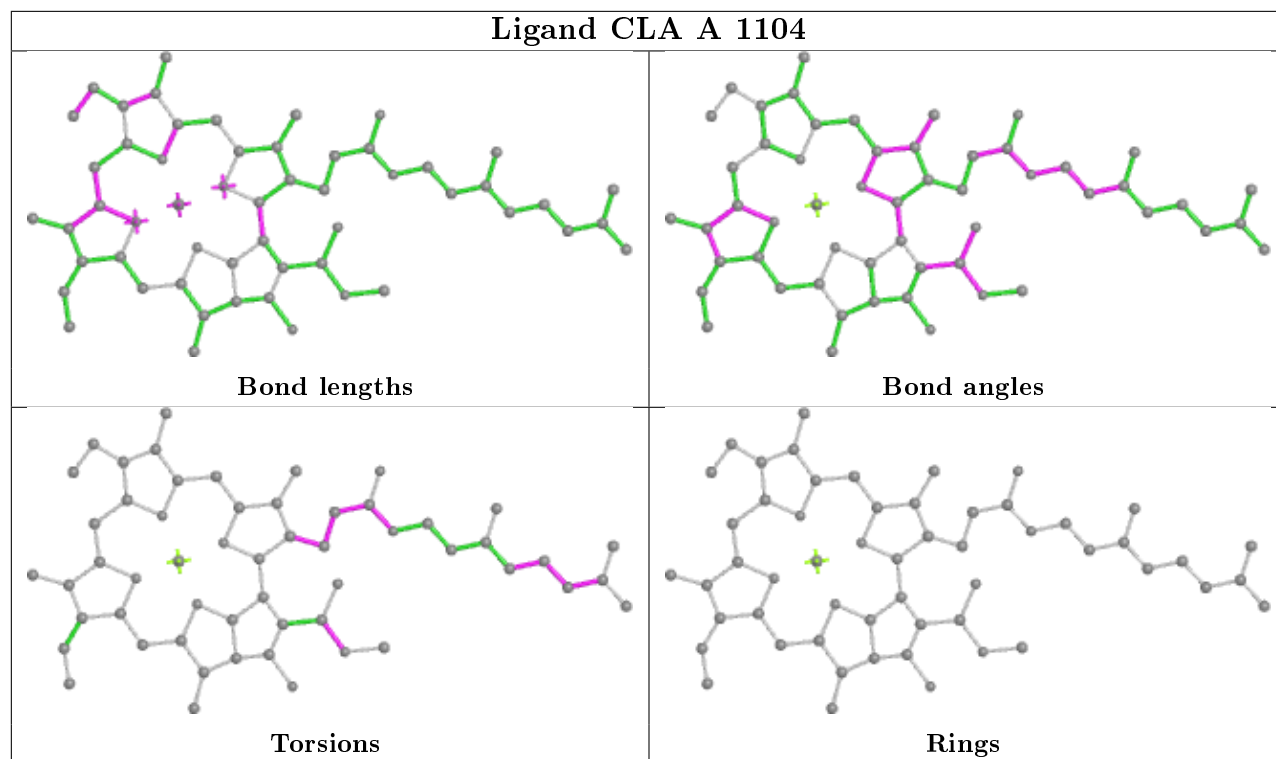


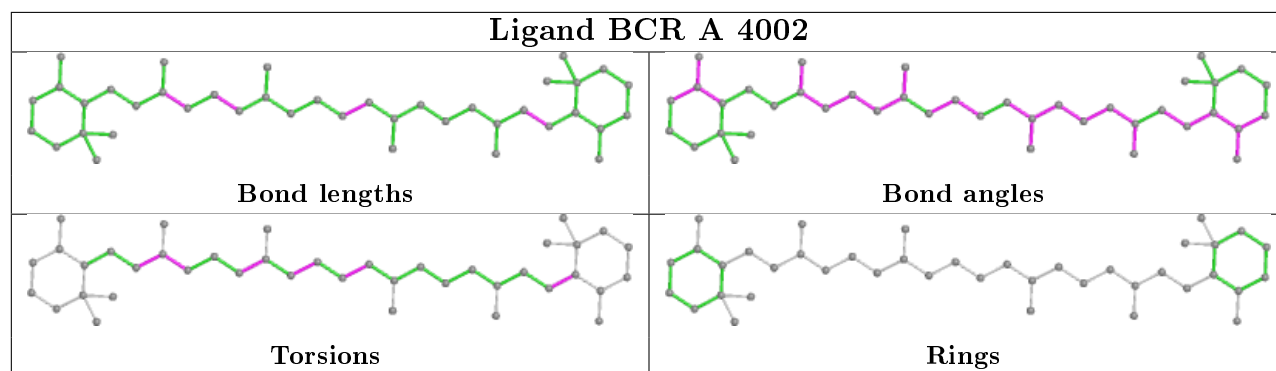
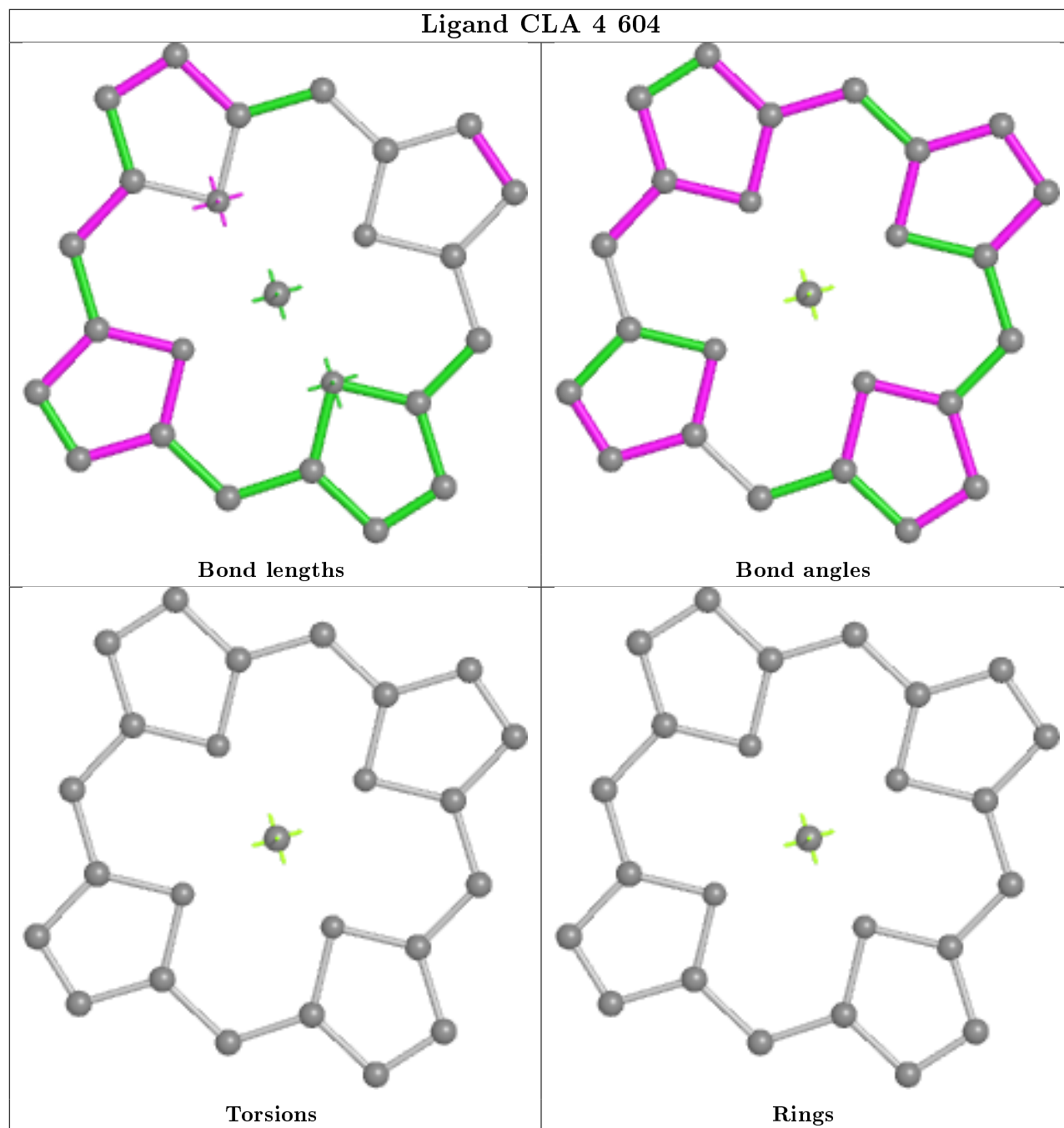






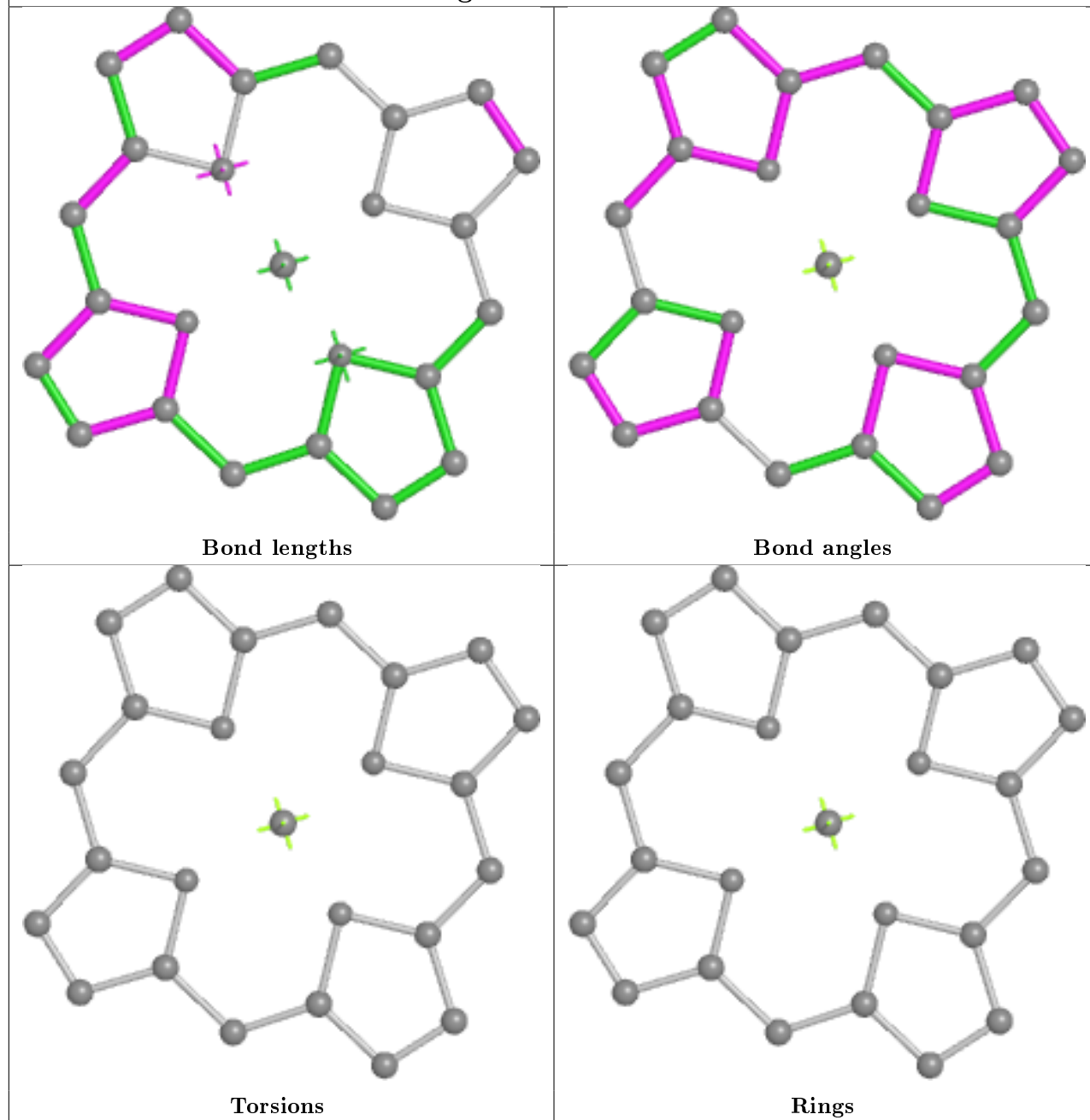


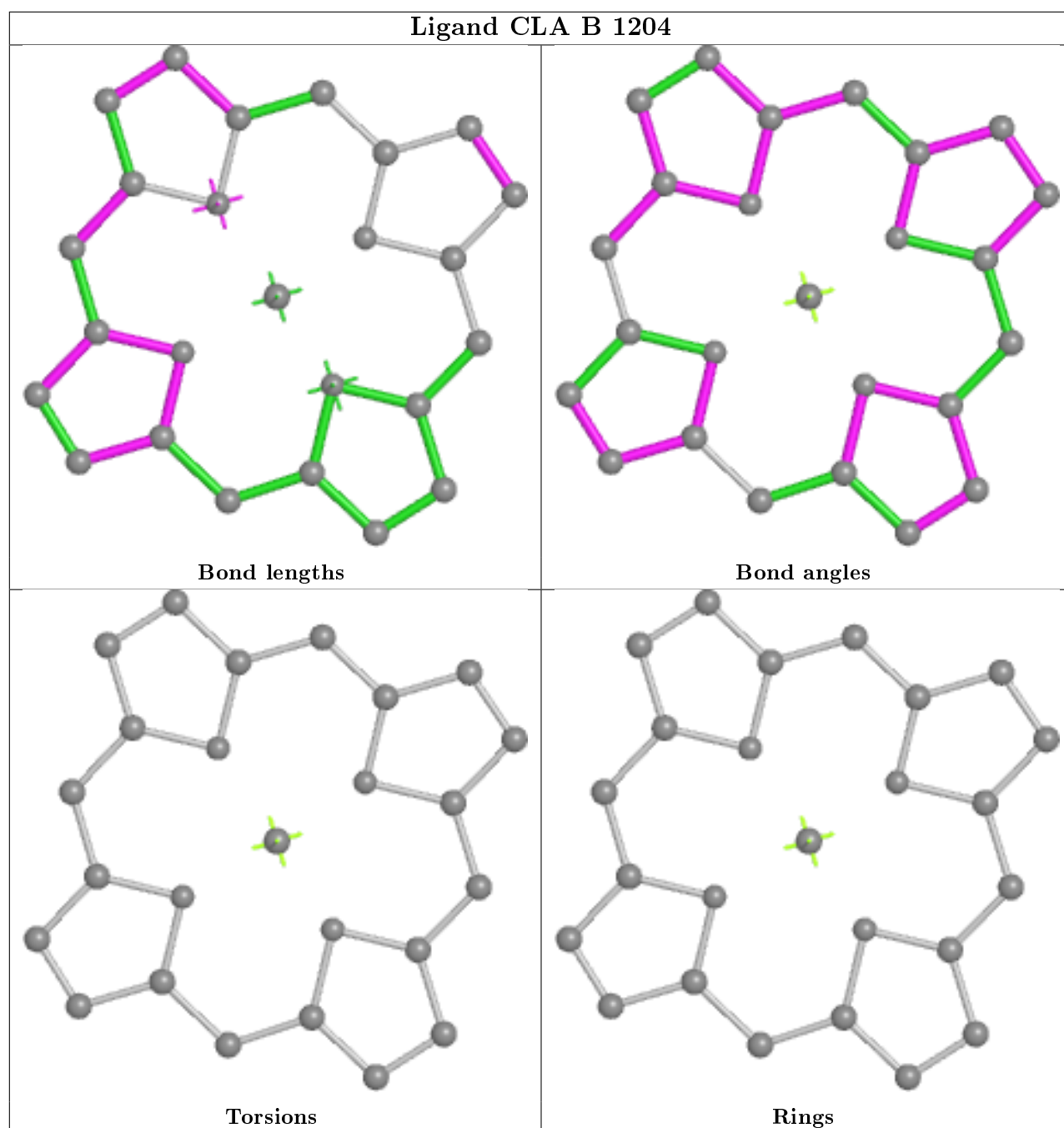


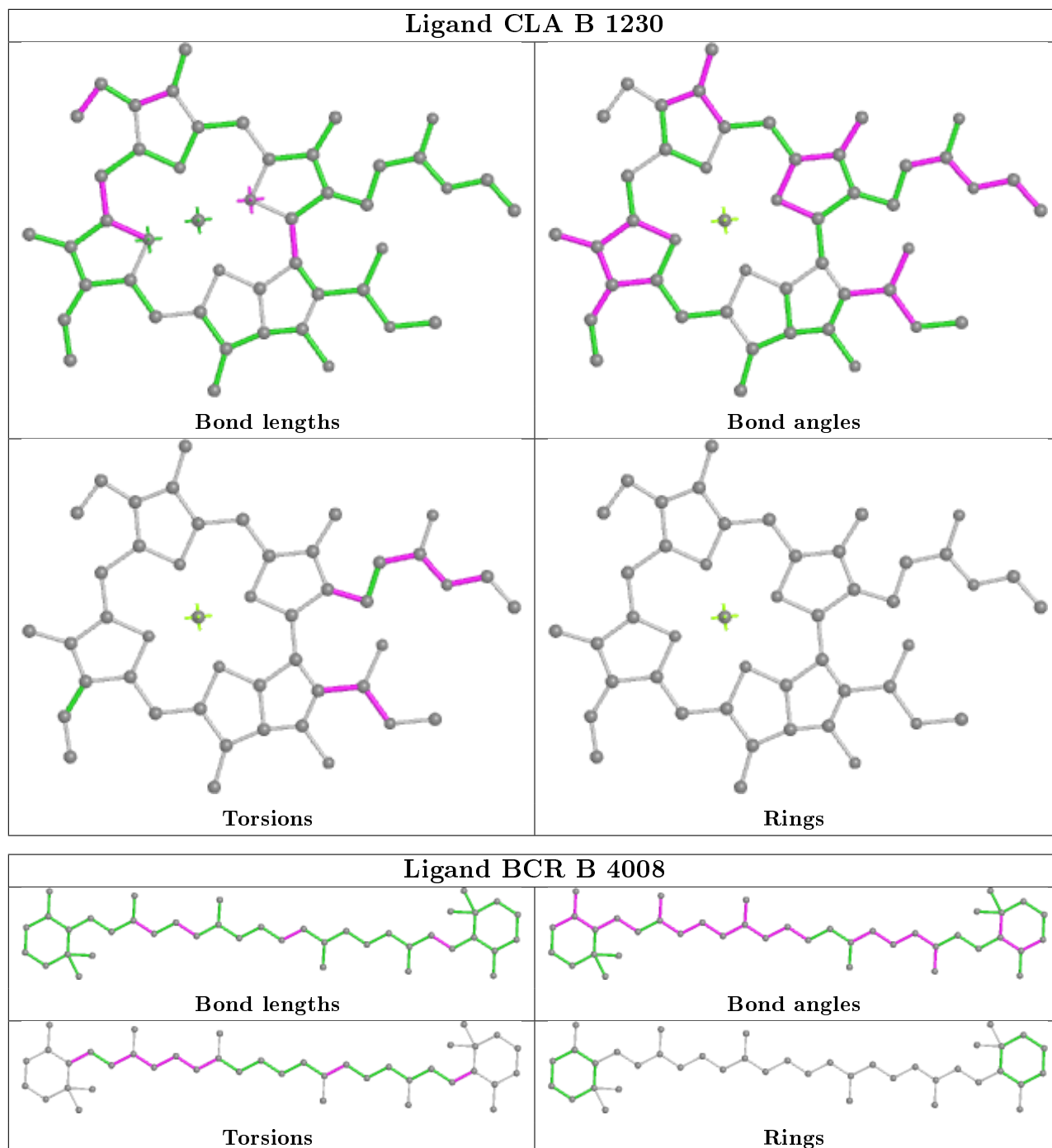


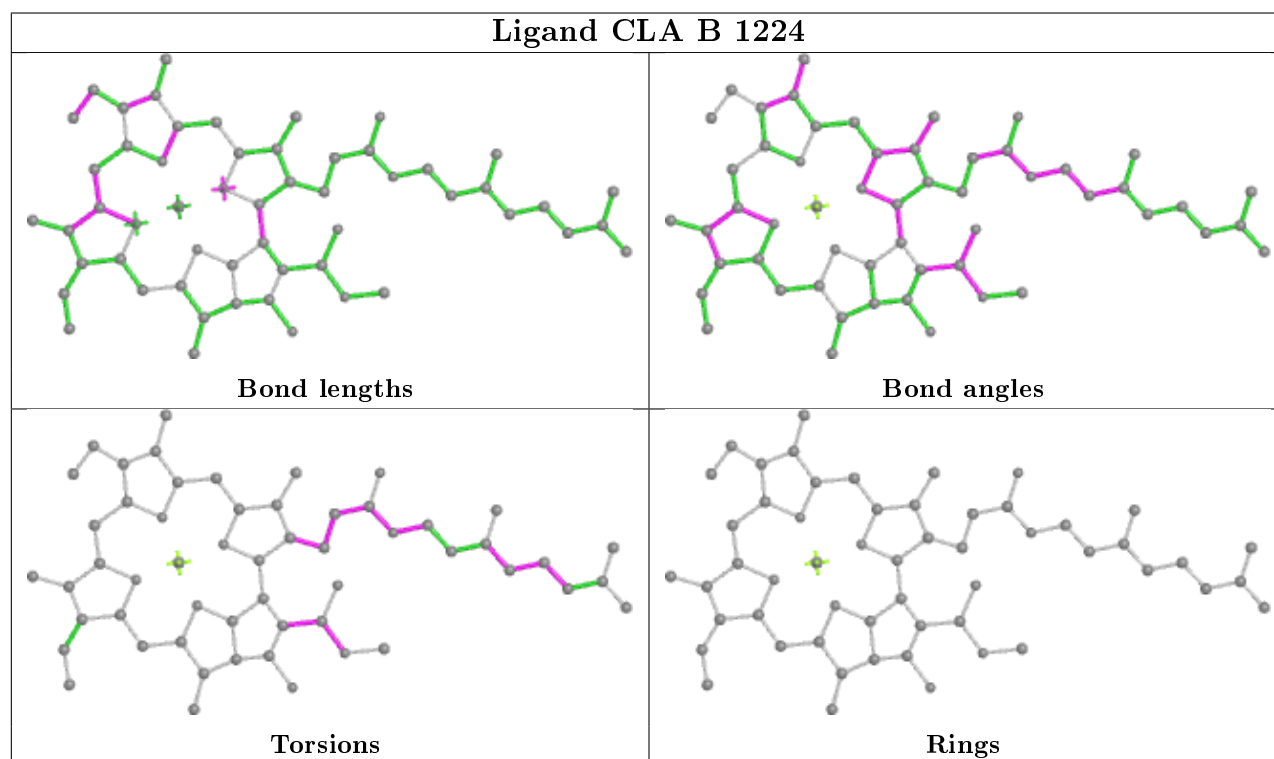
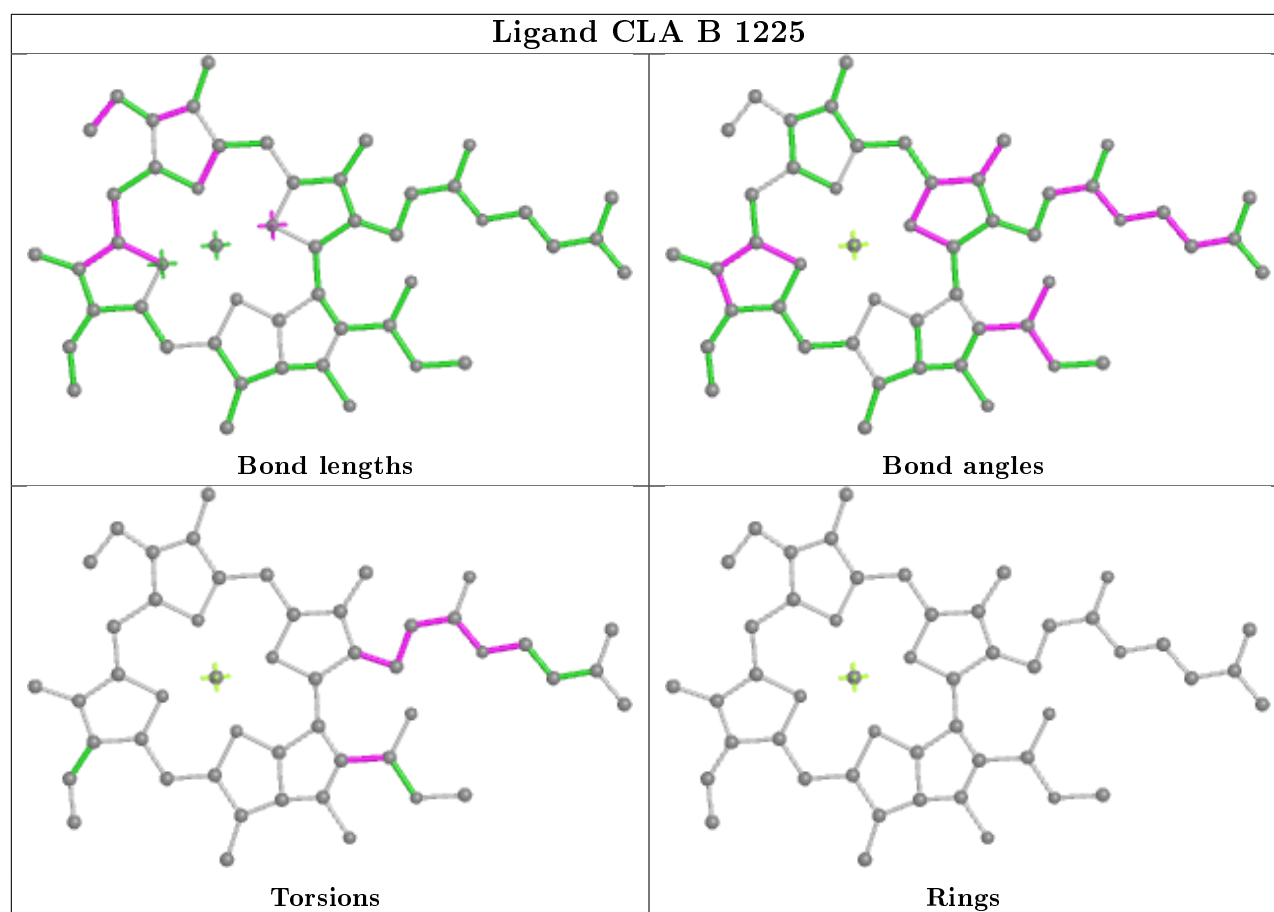


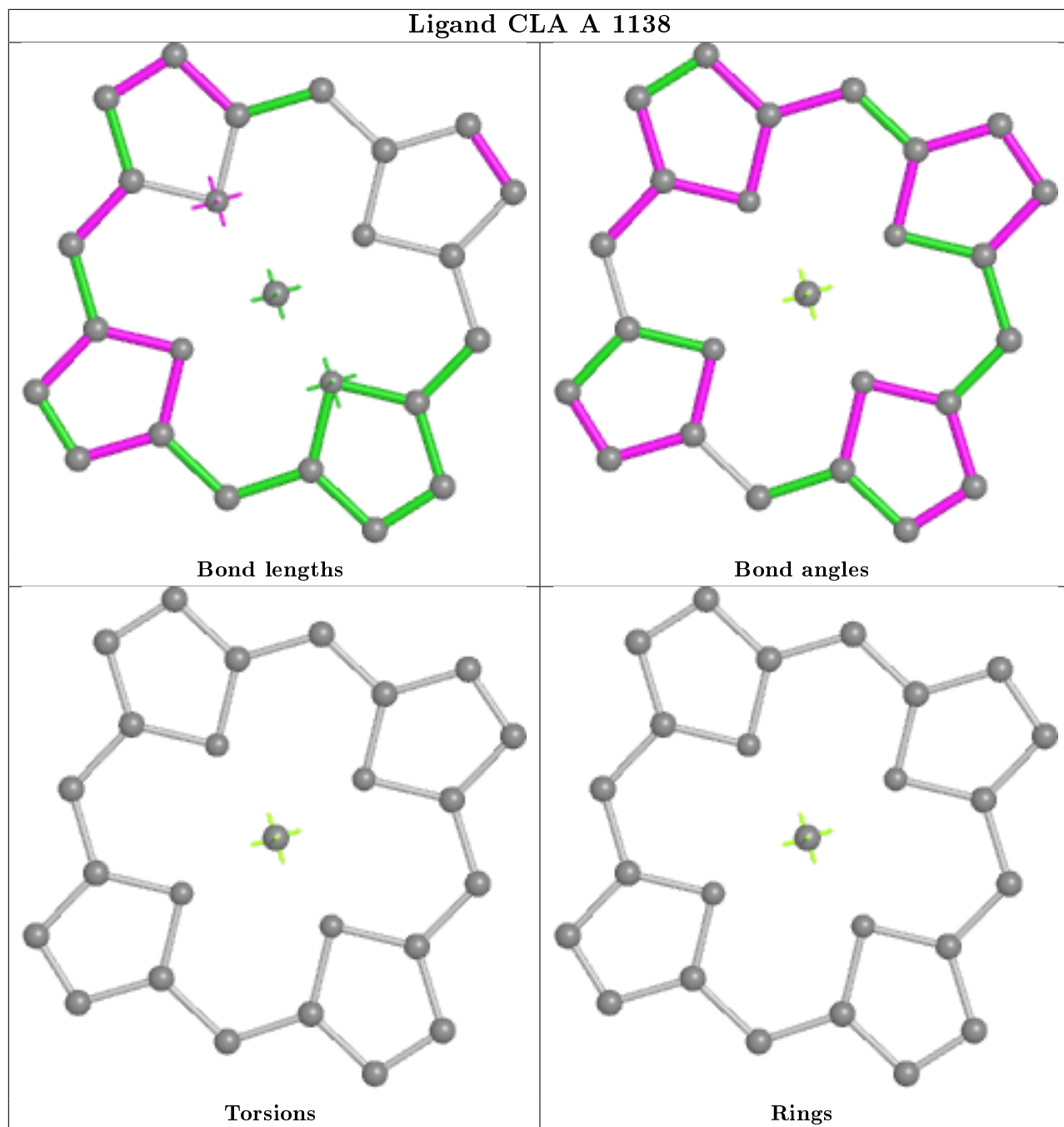
## Ligand CLA 2 615

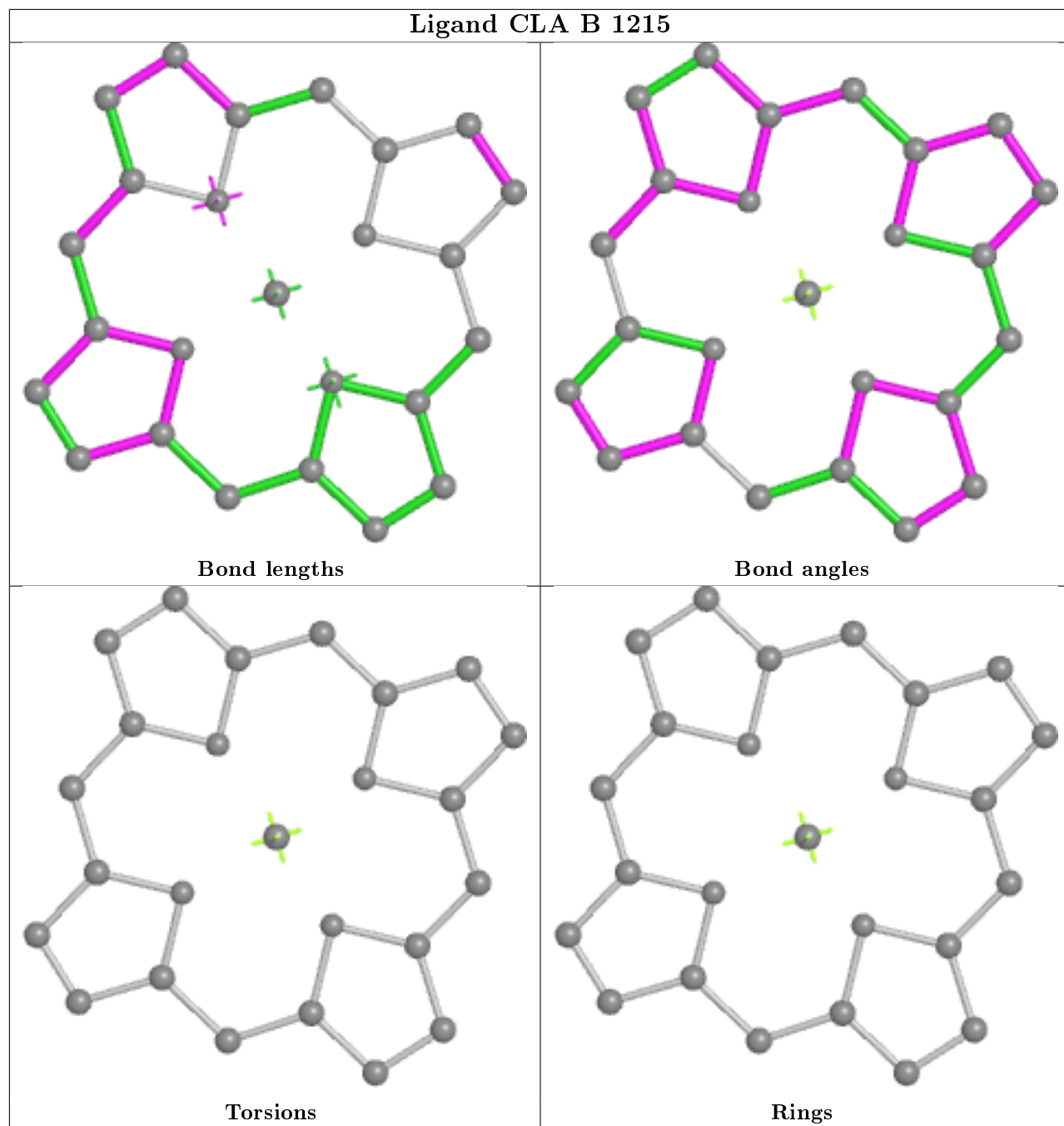


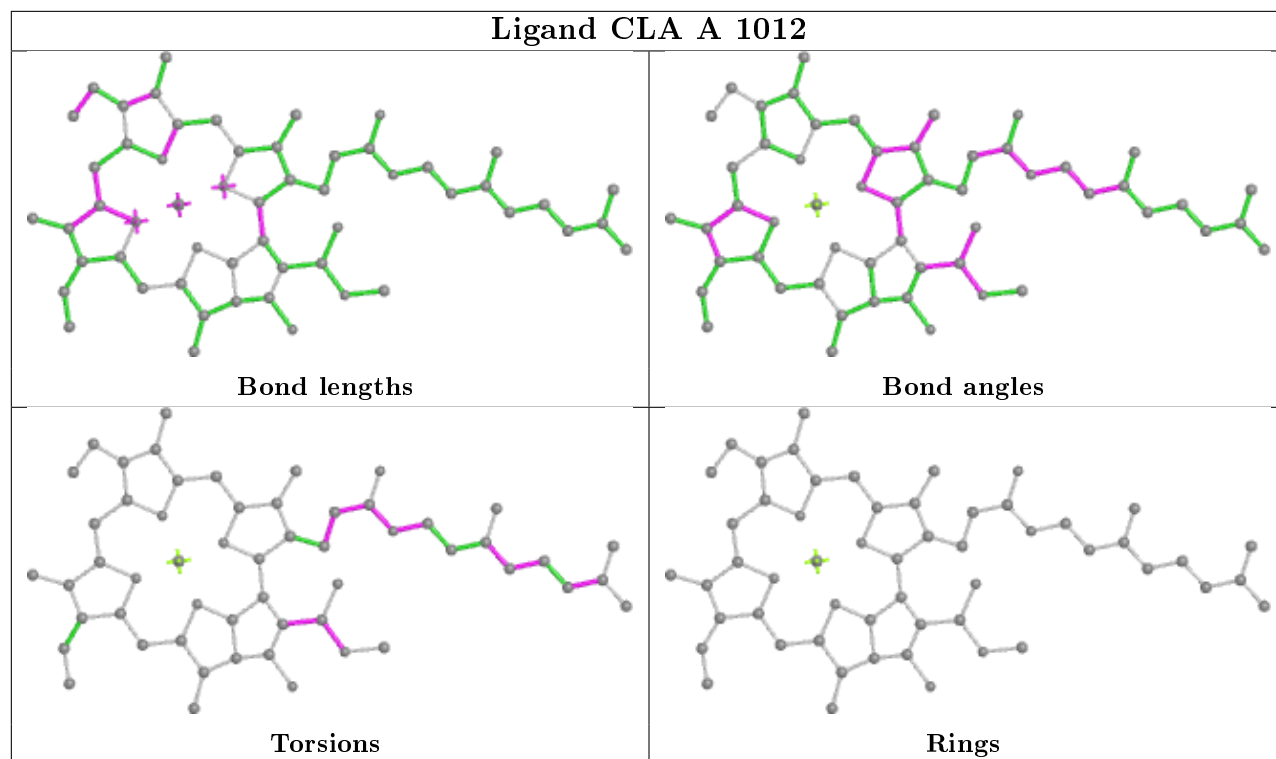


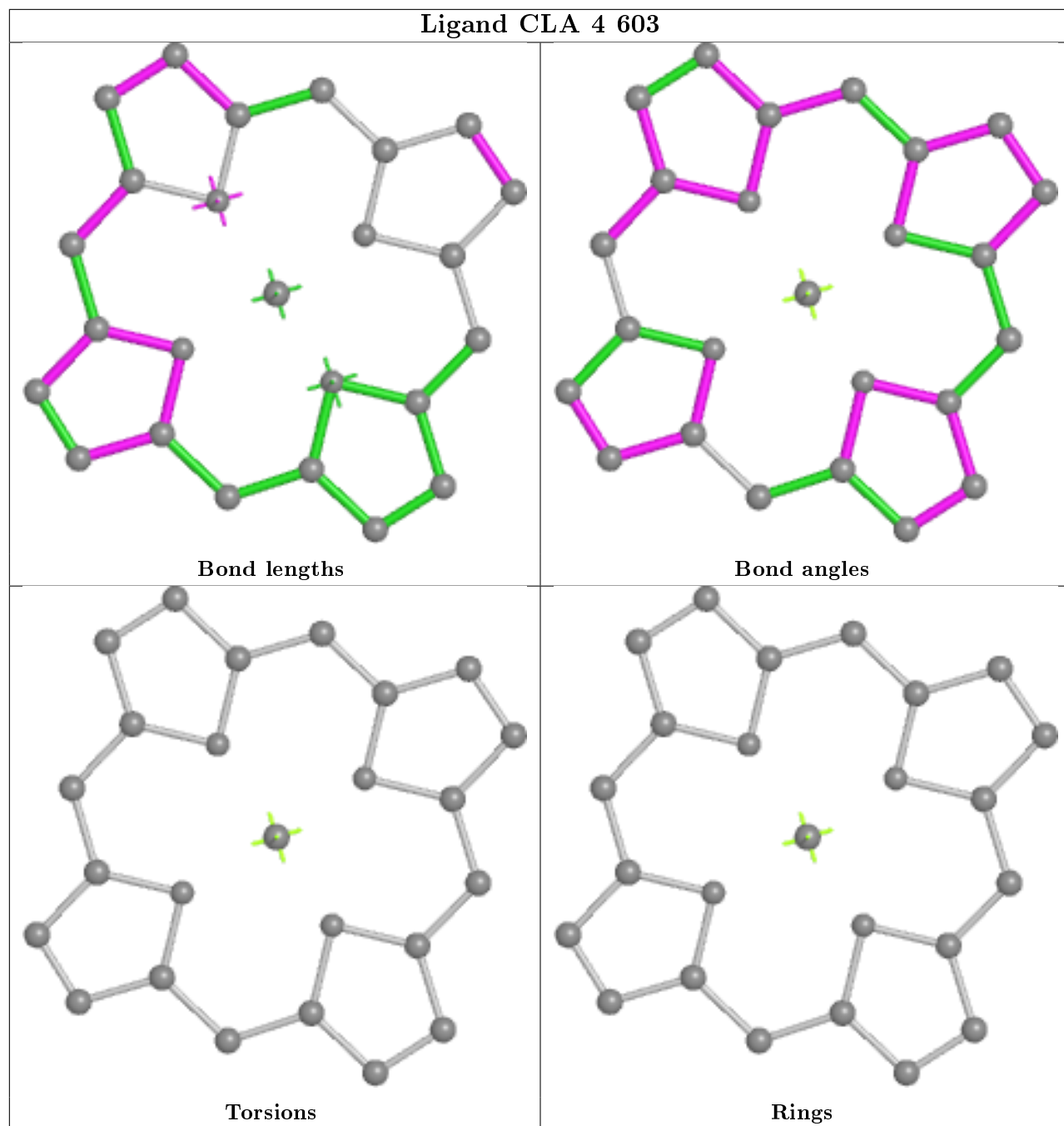




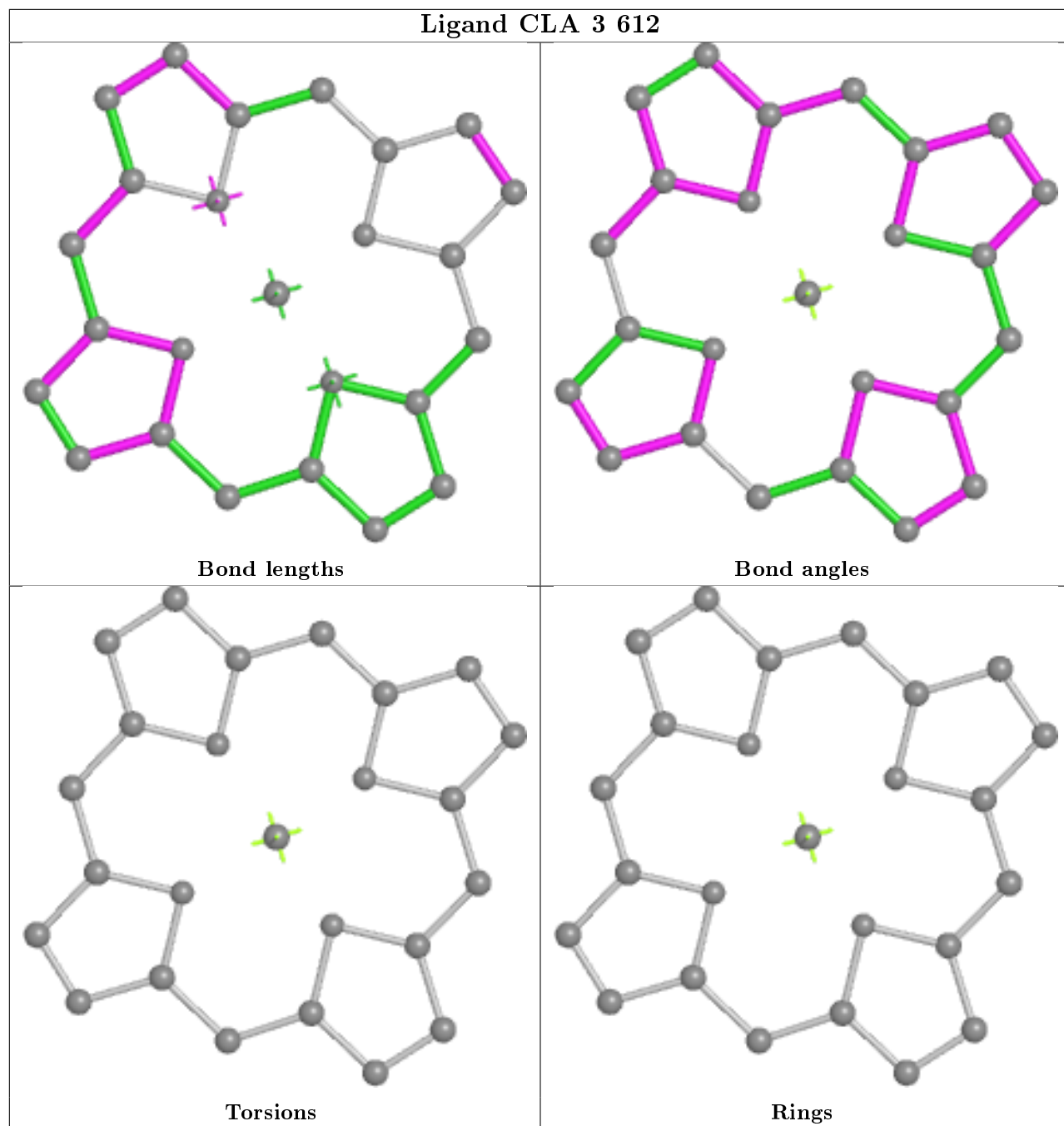




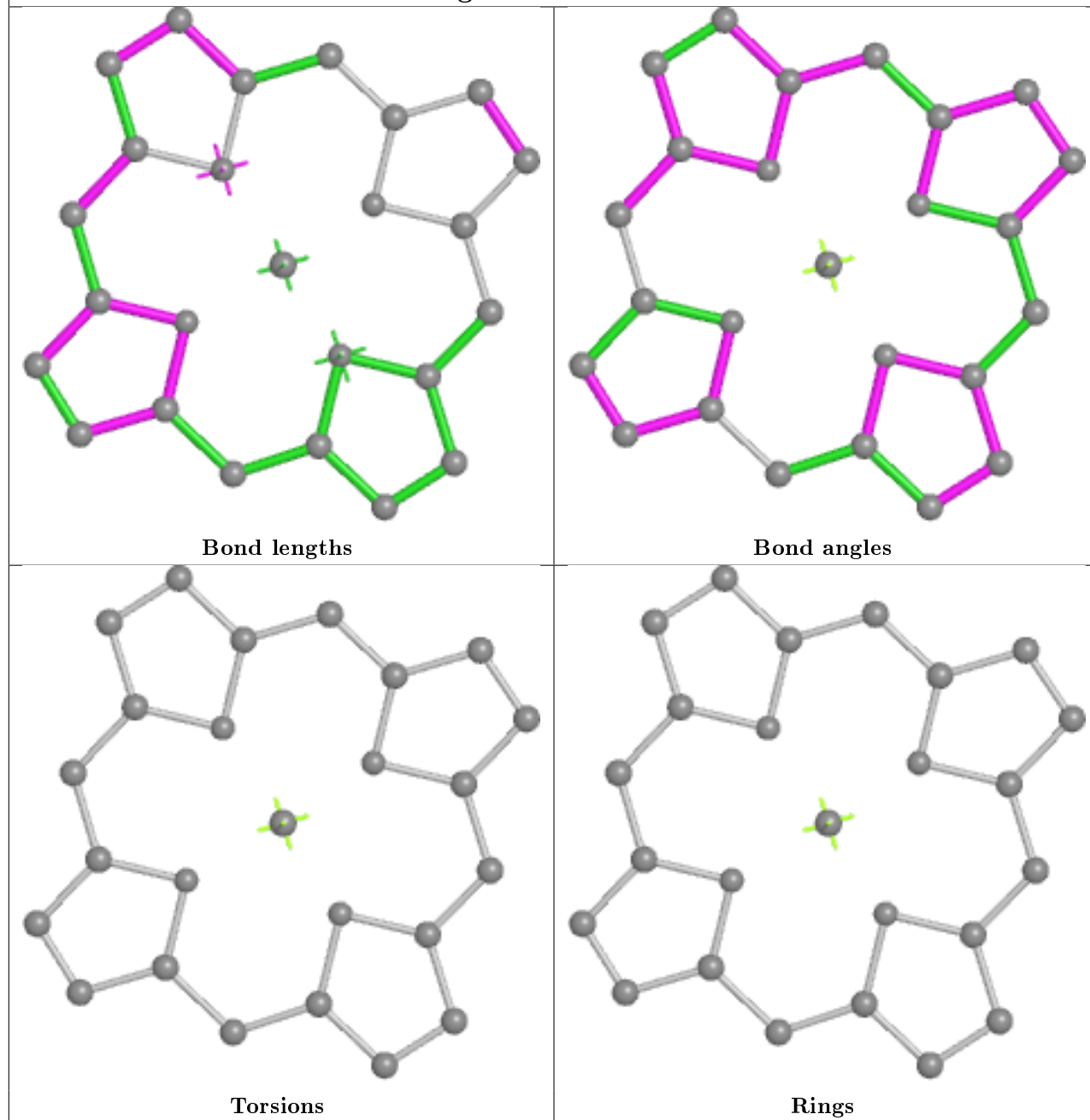


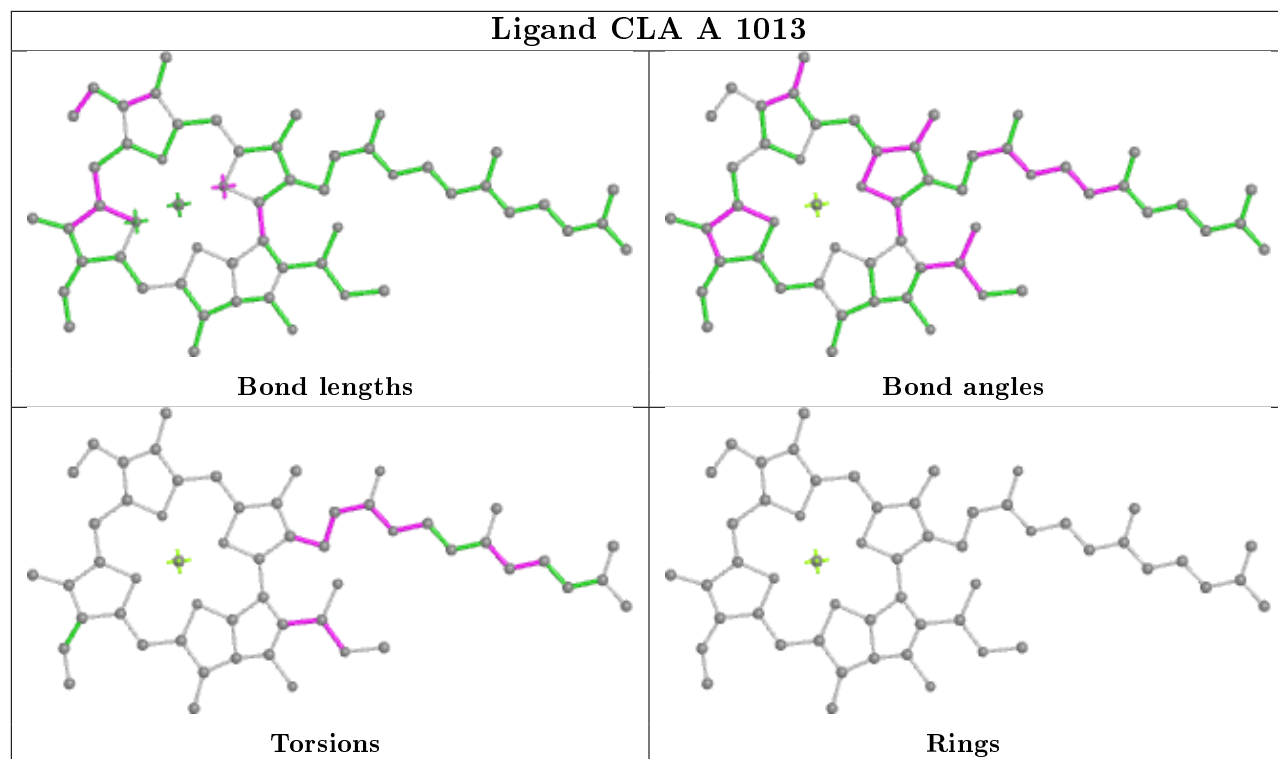


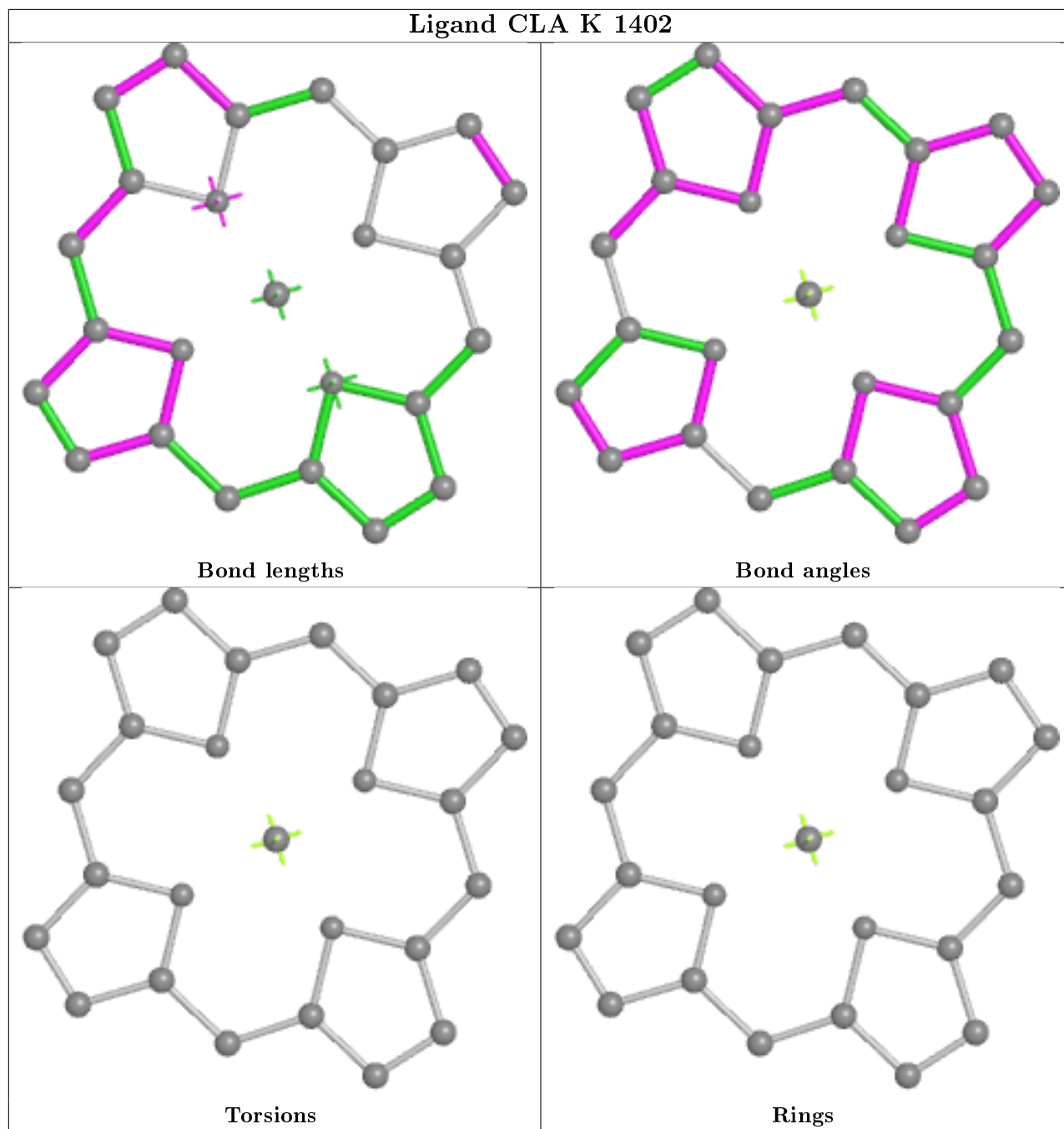


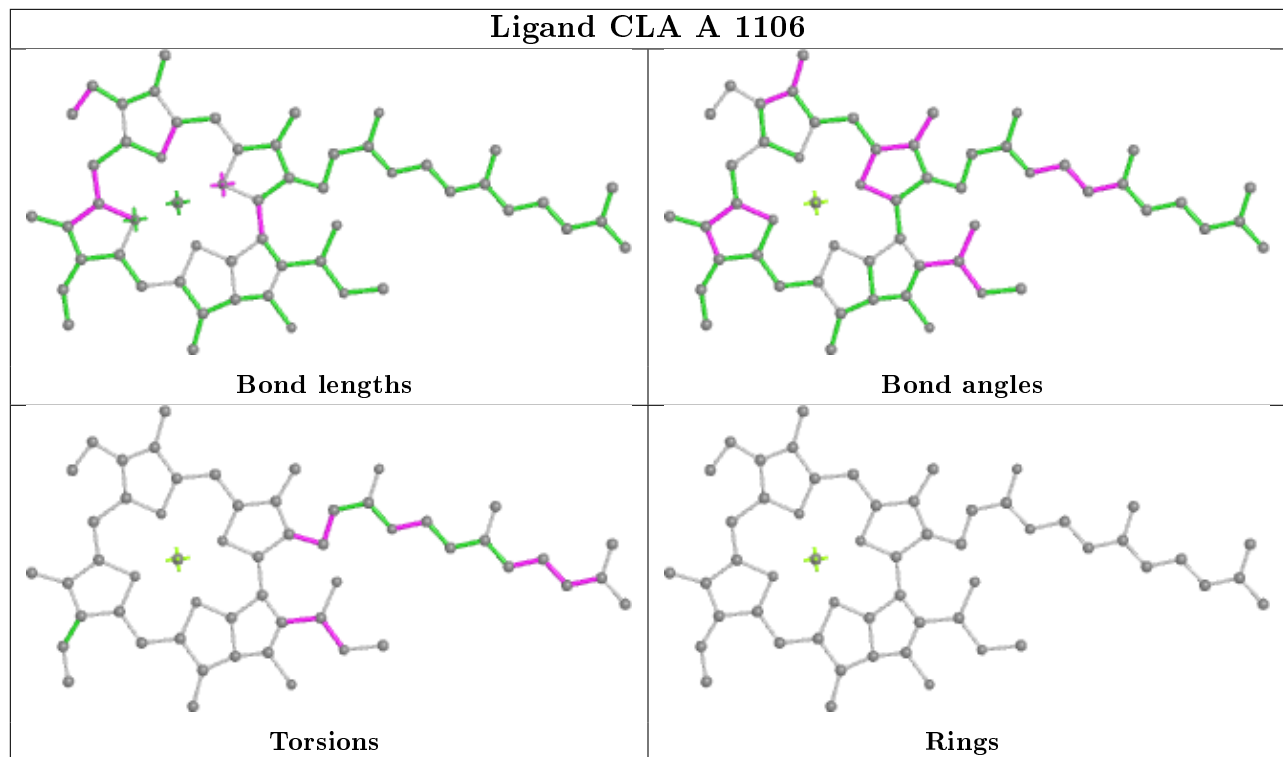


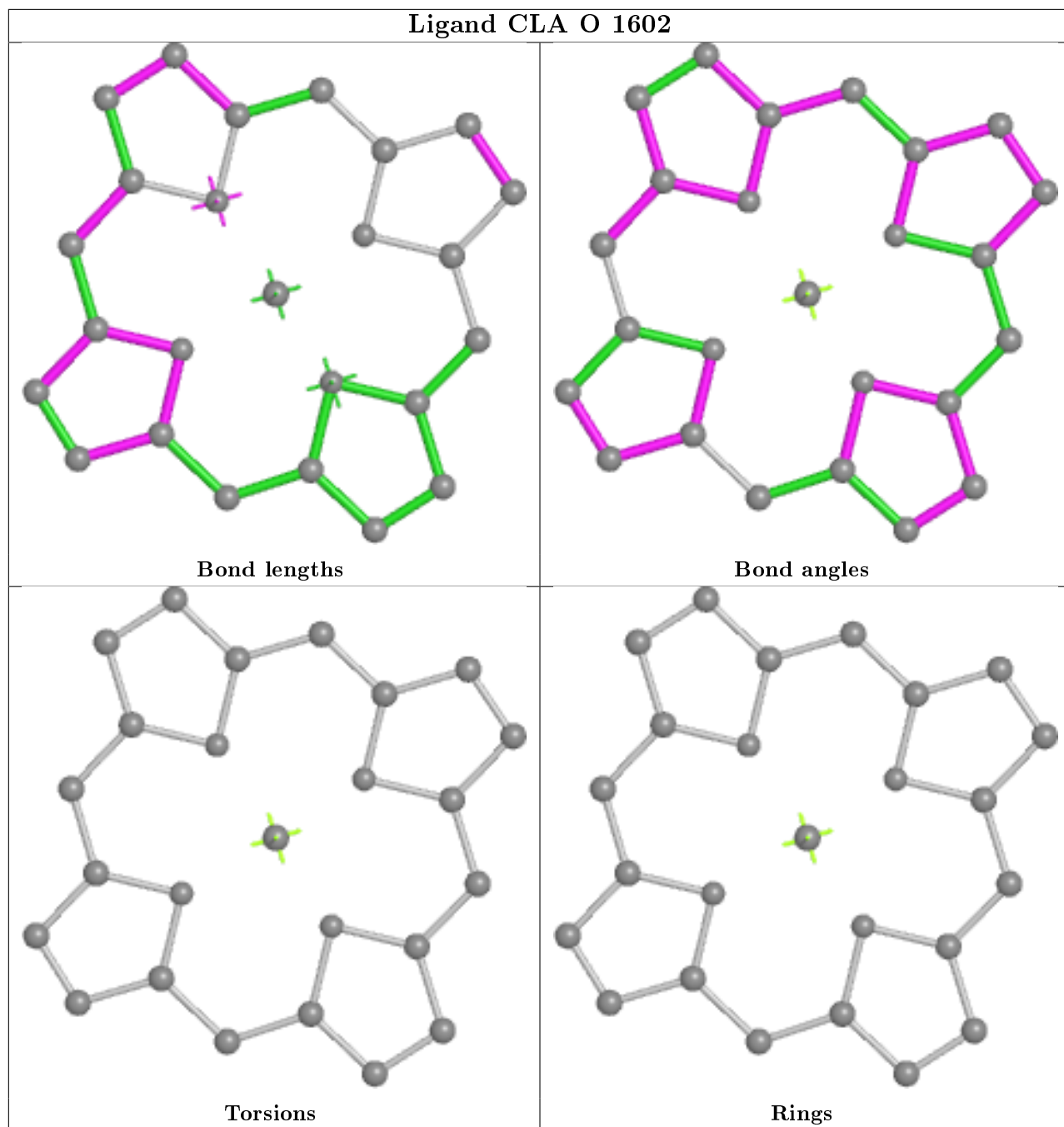
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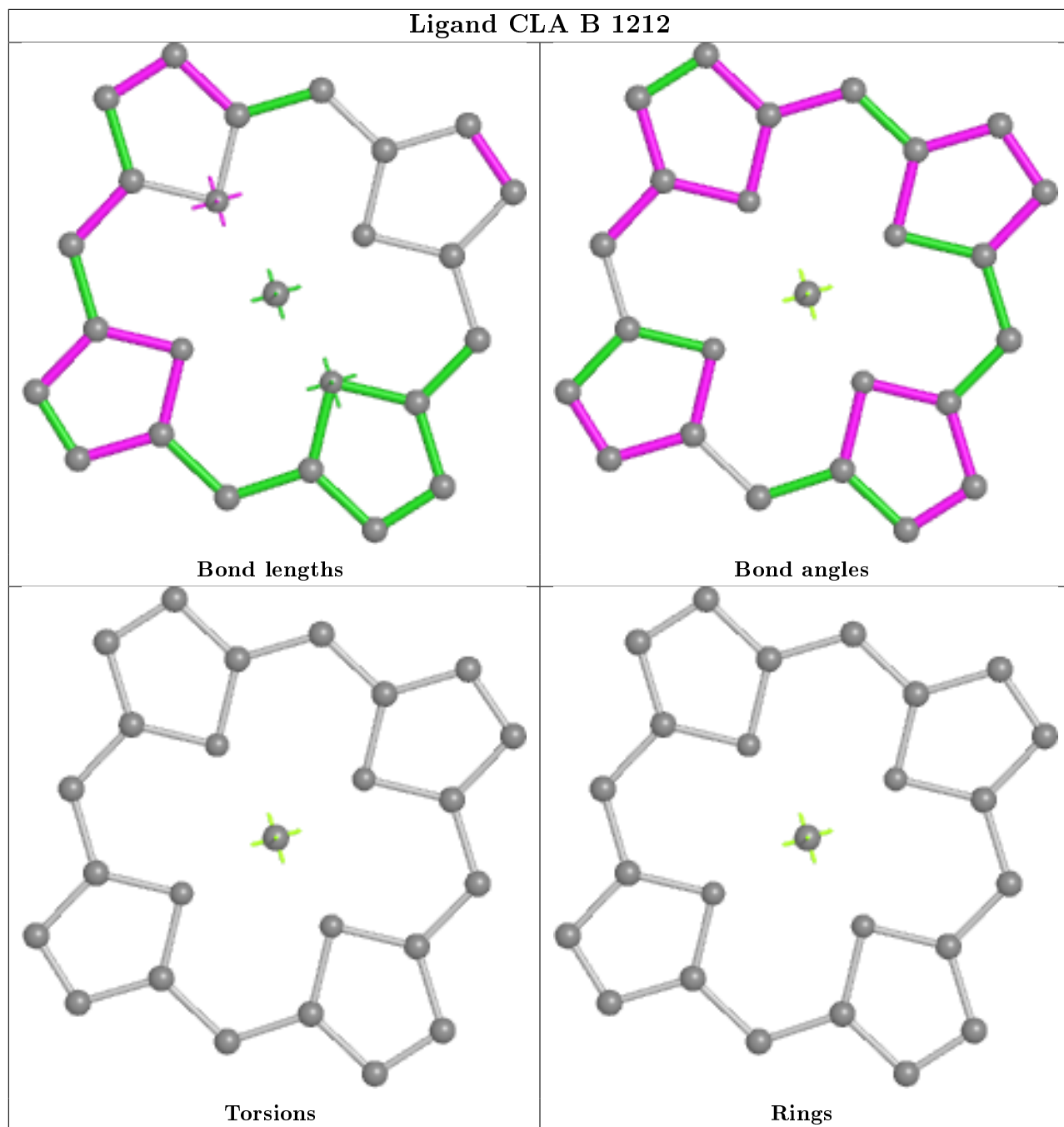


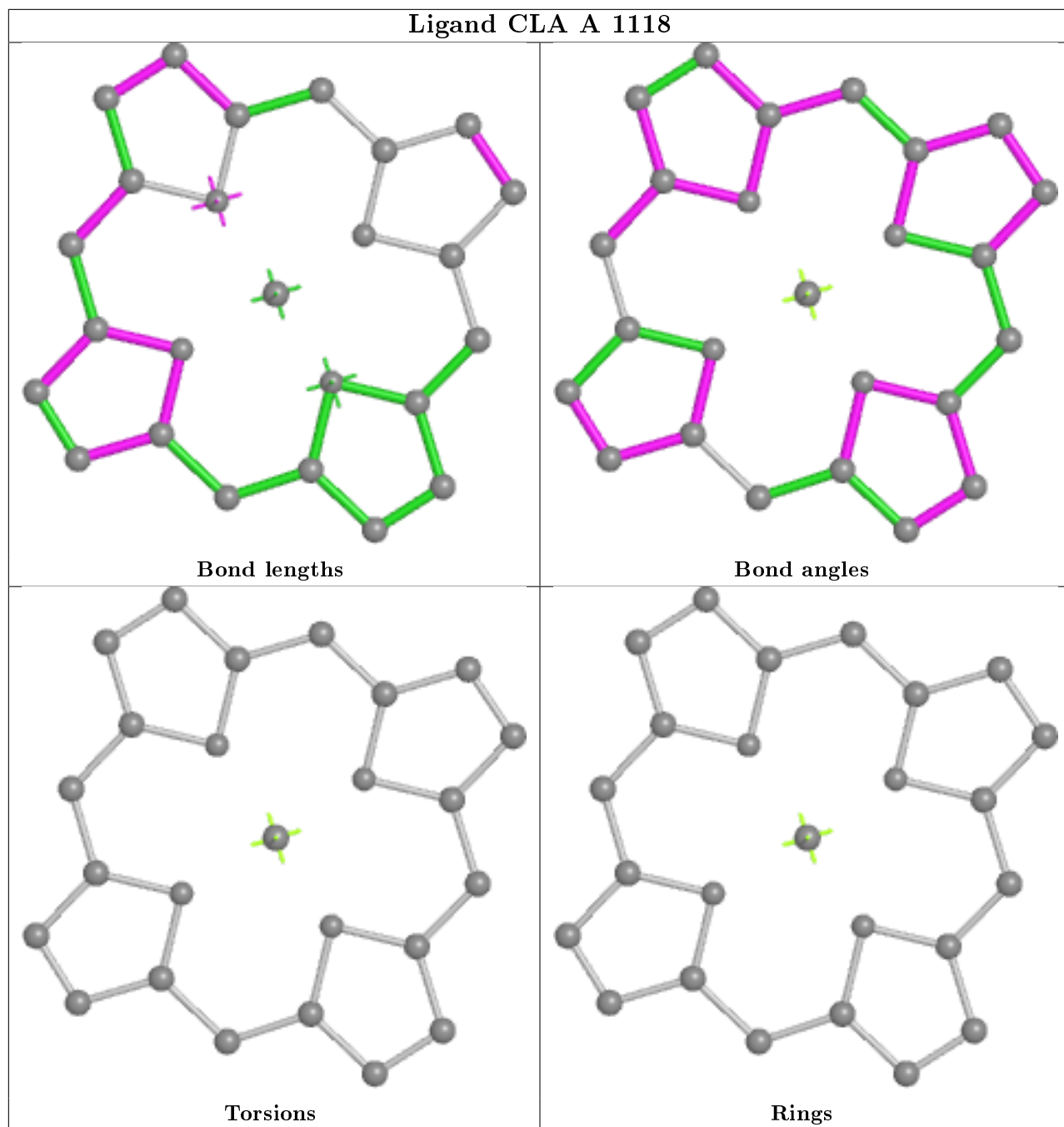




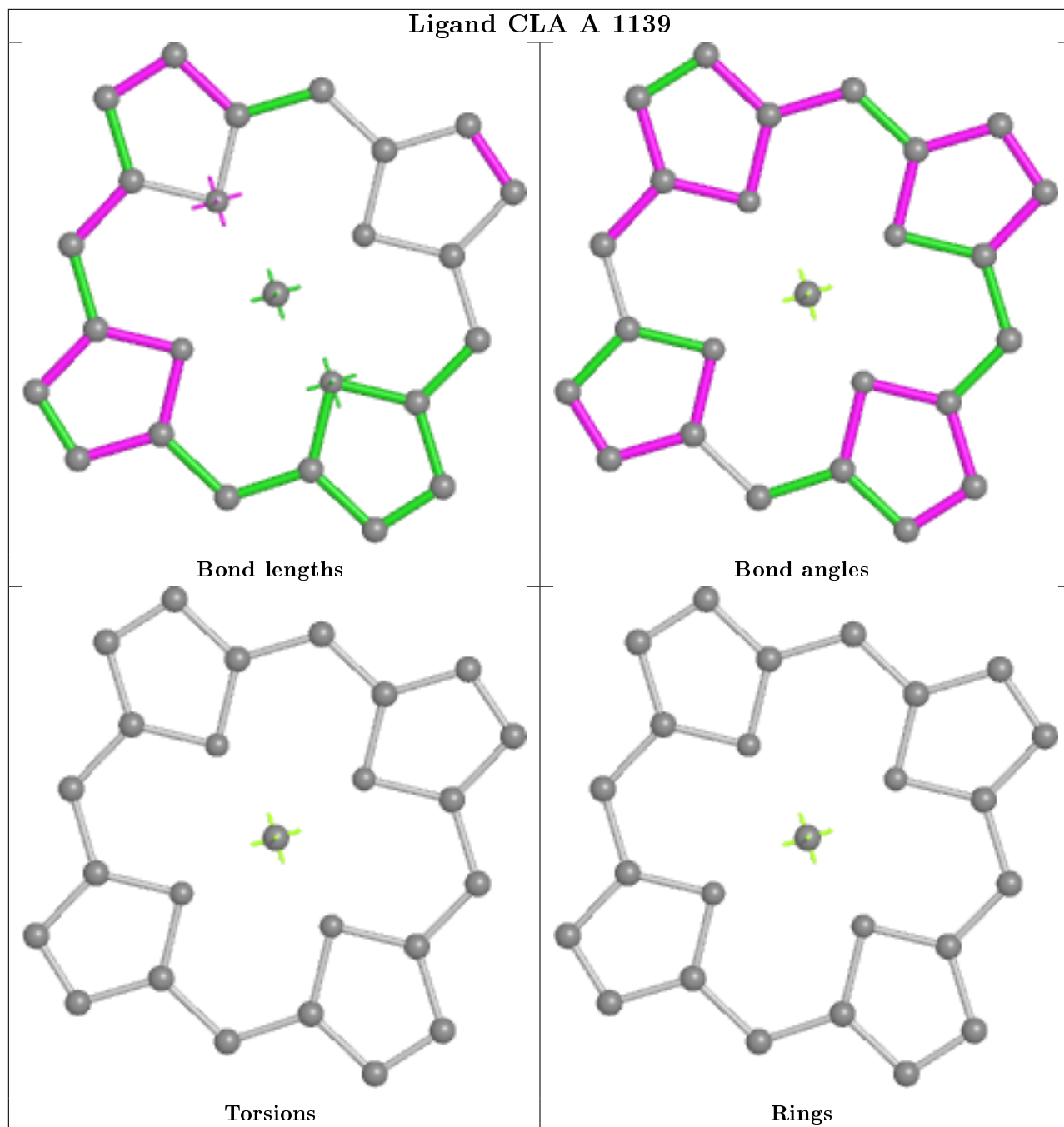


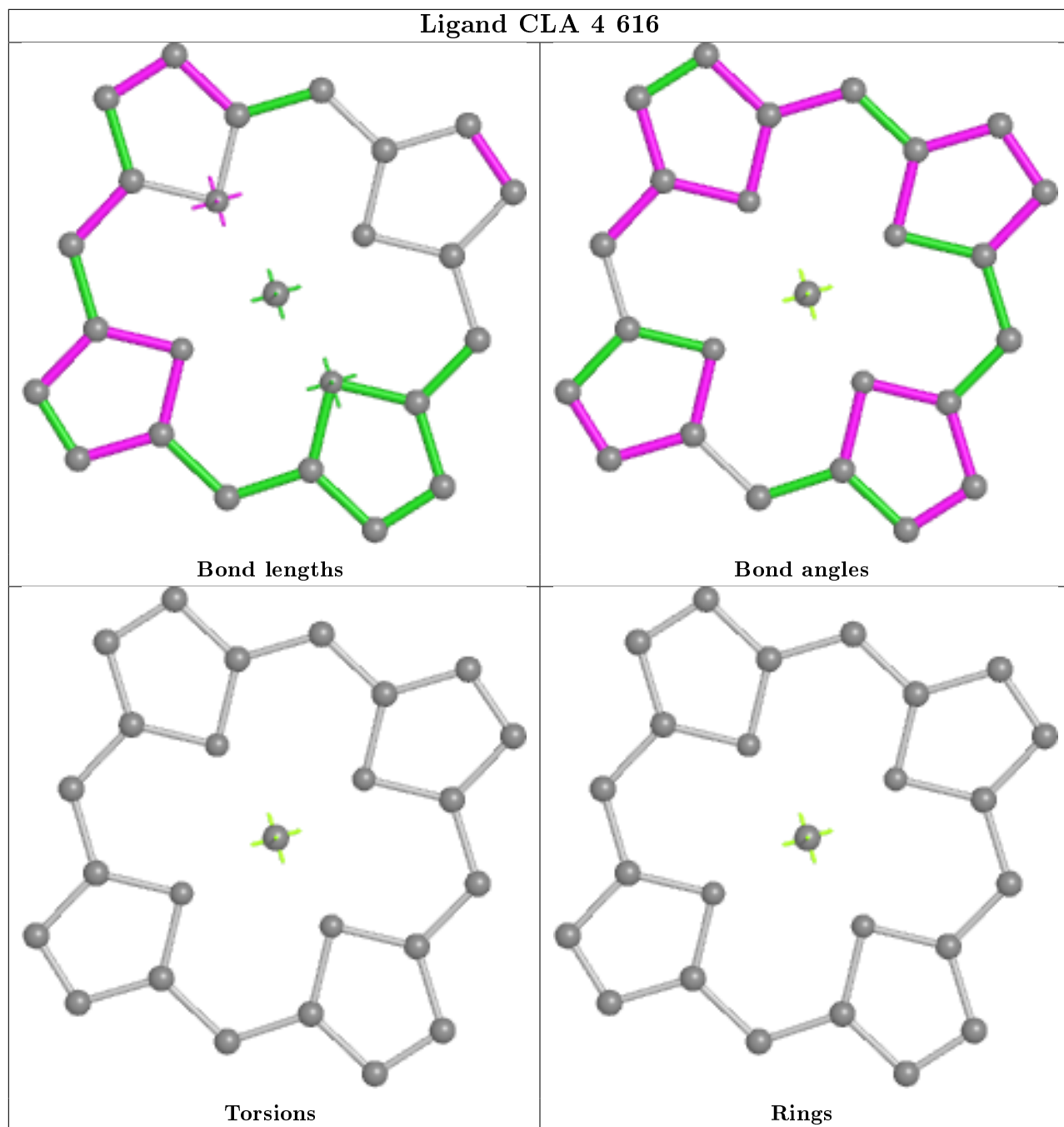


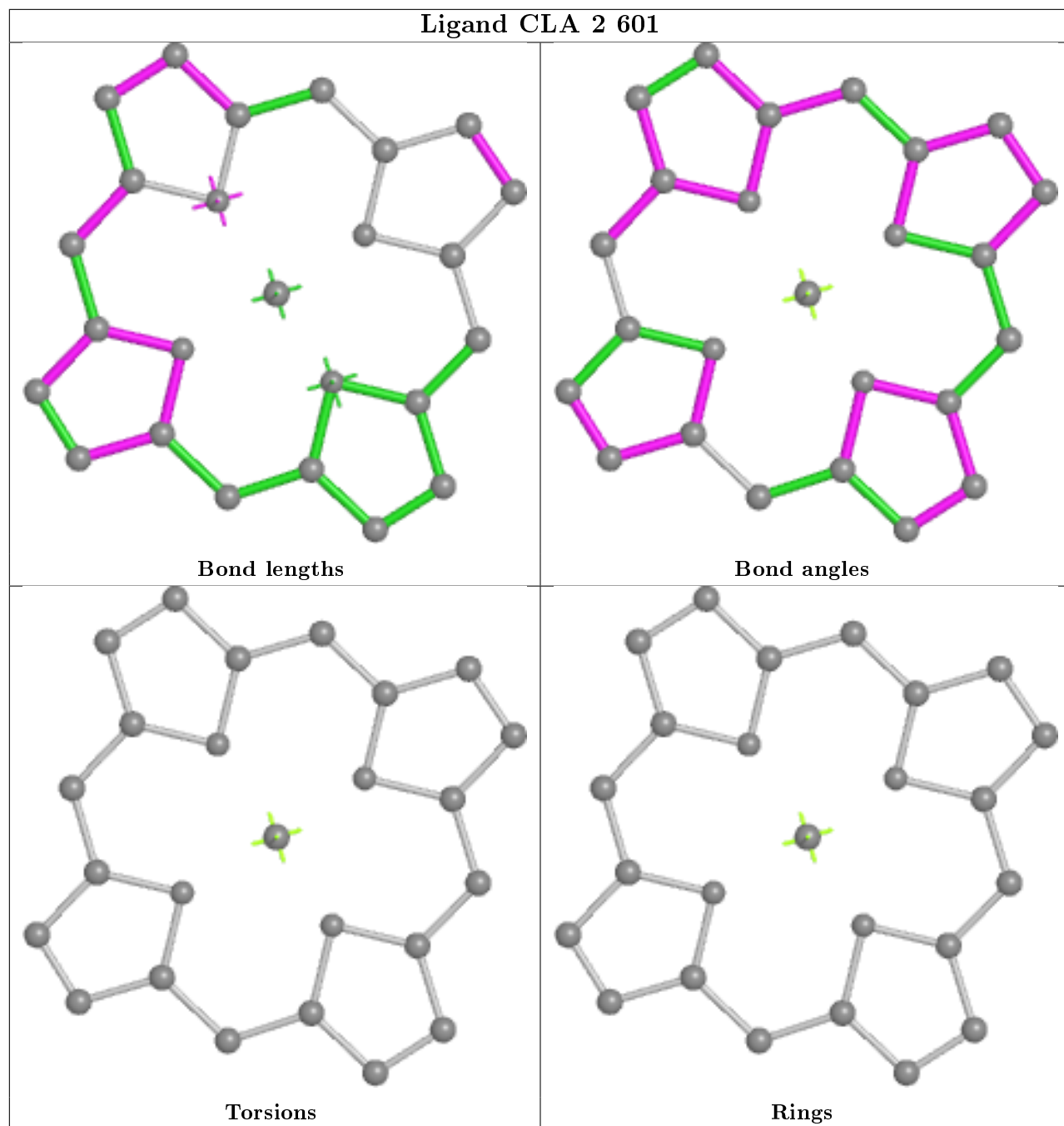




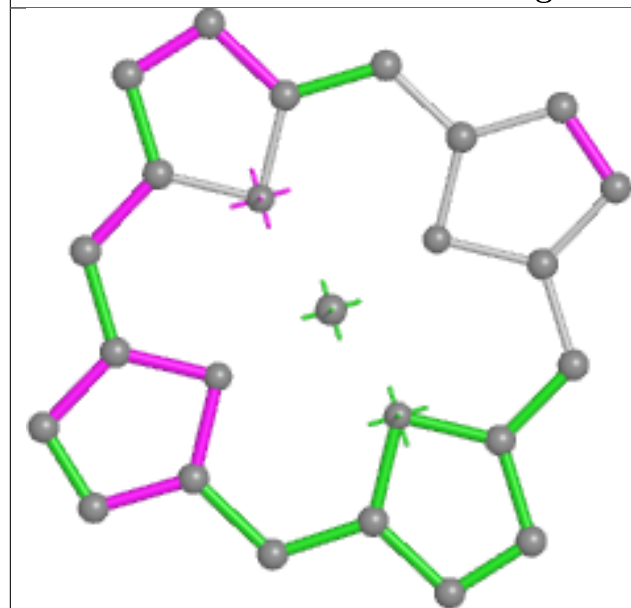




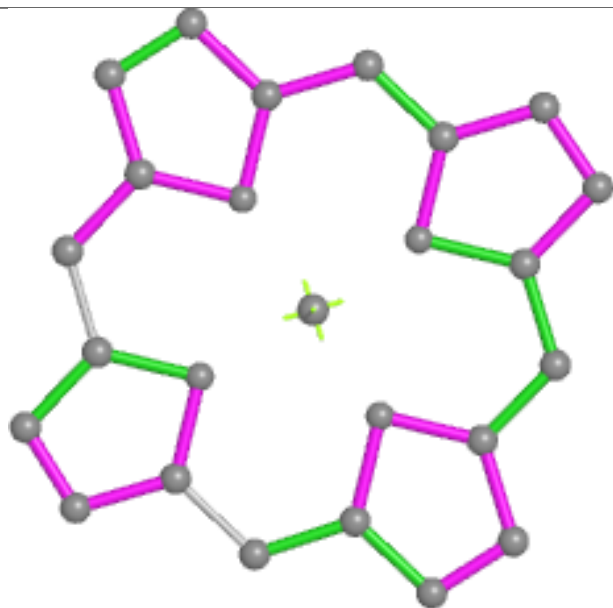




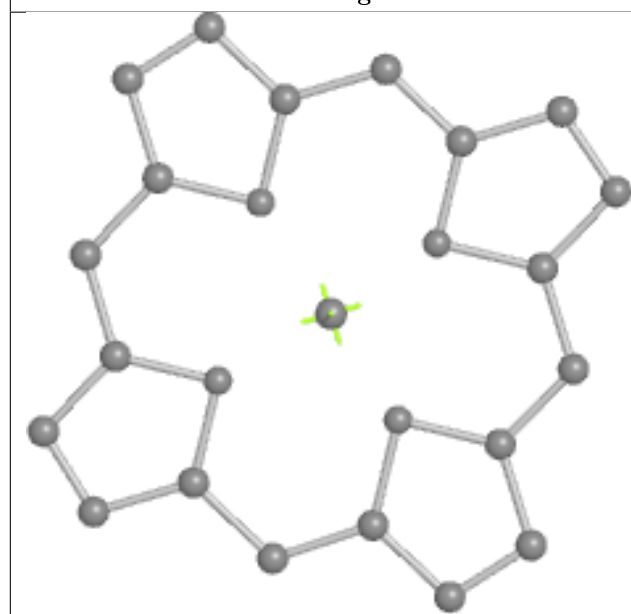
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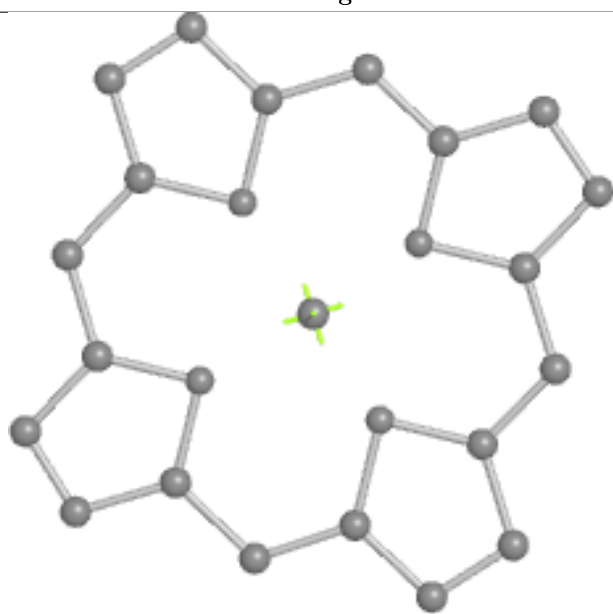
Bond lengths



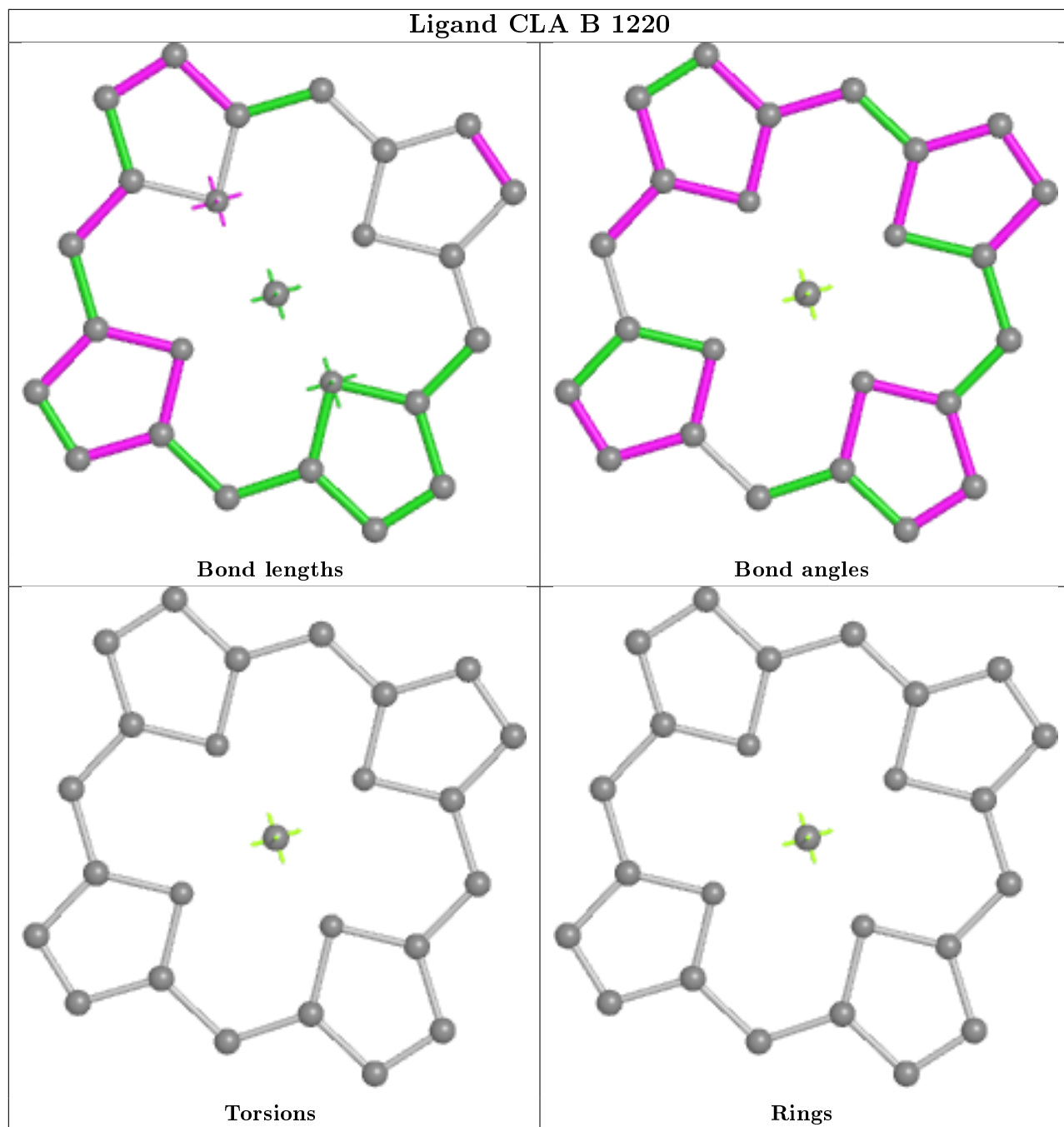
Bond angles

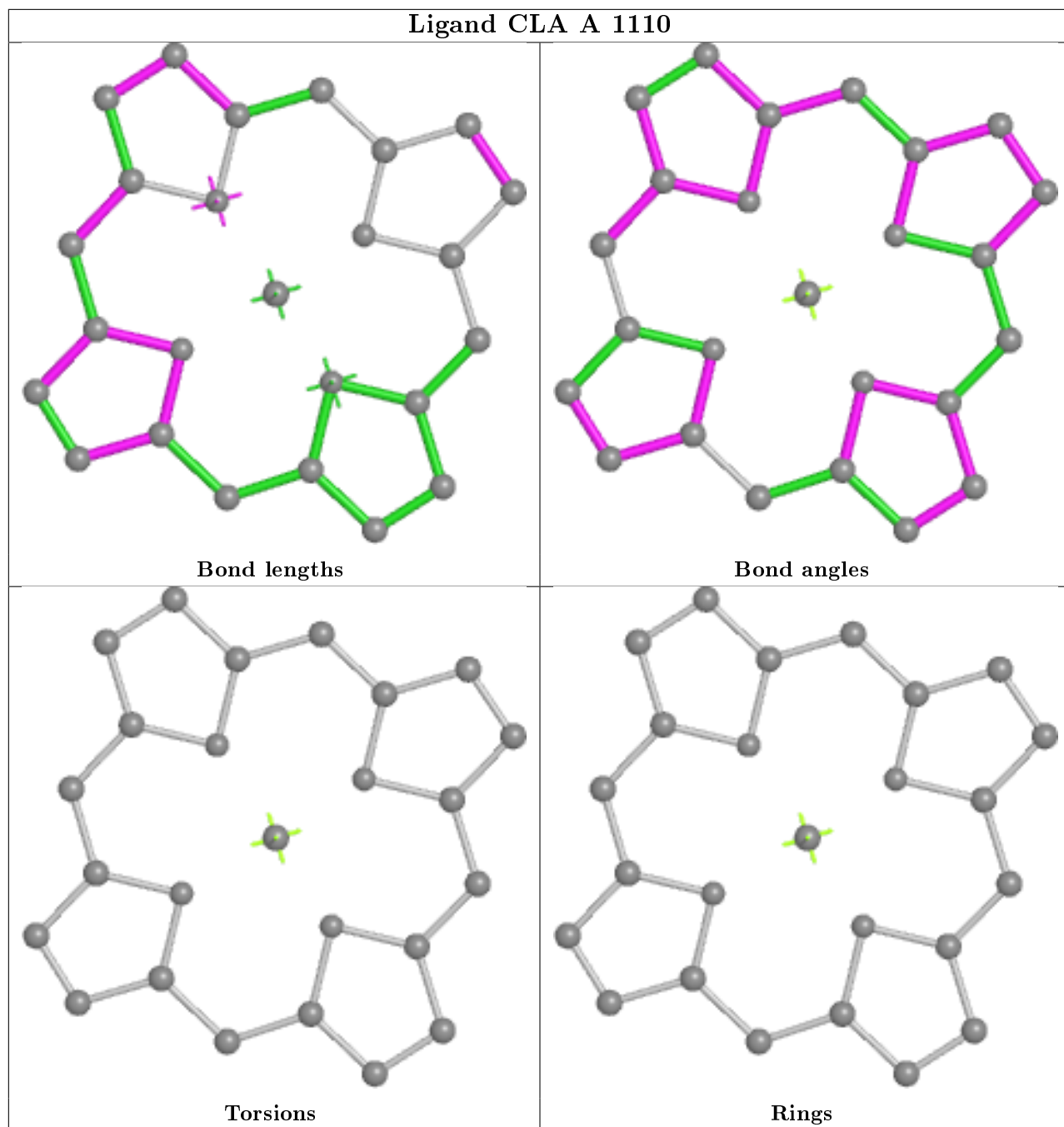


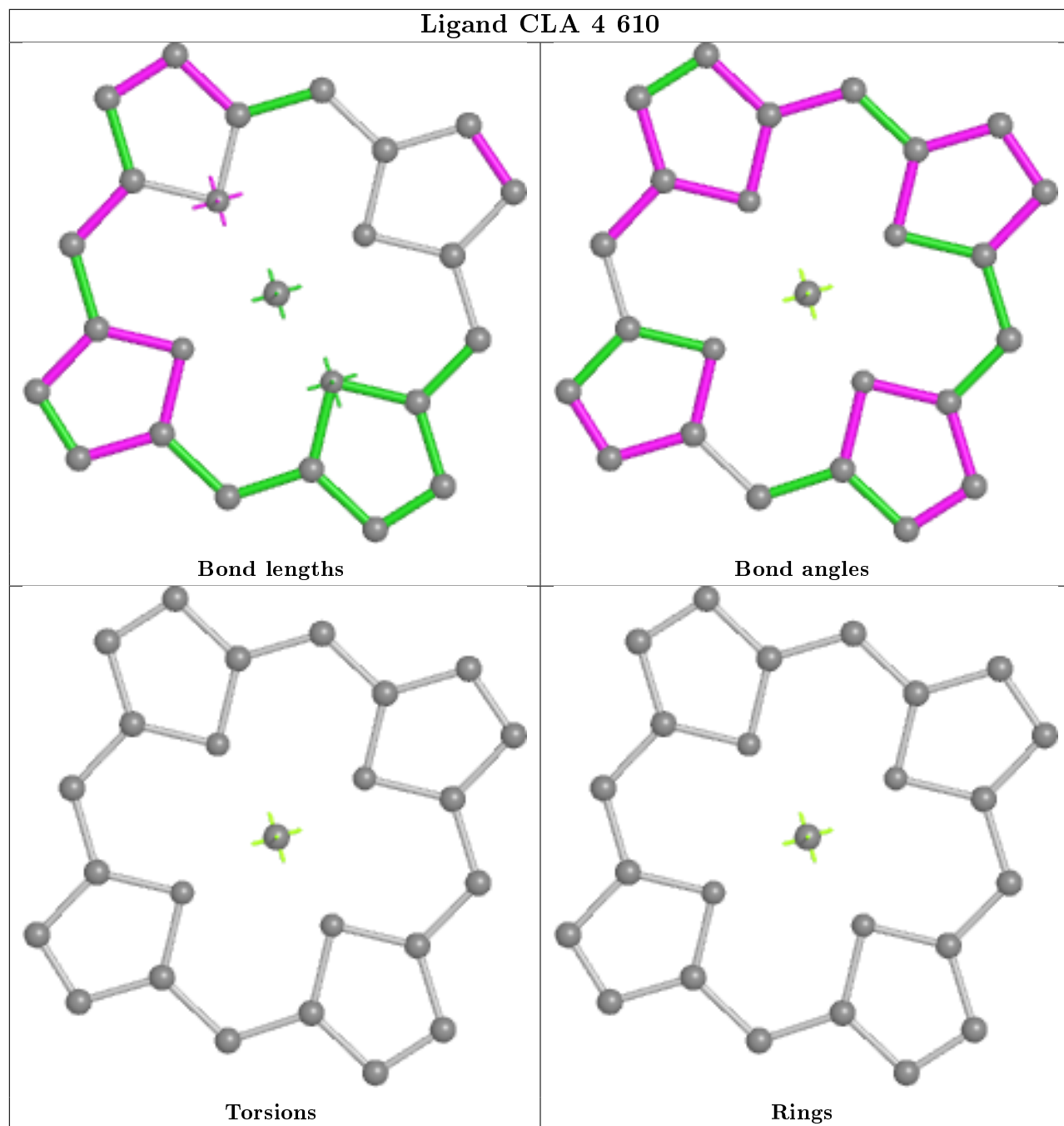
Torsions

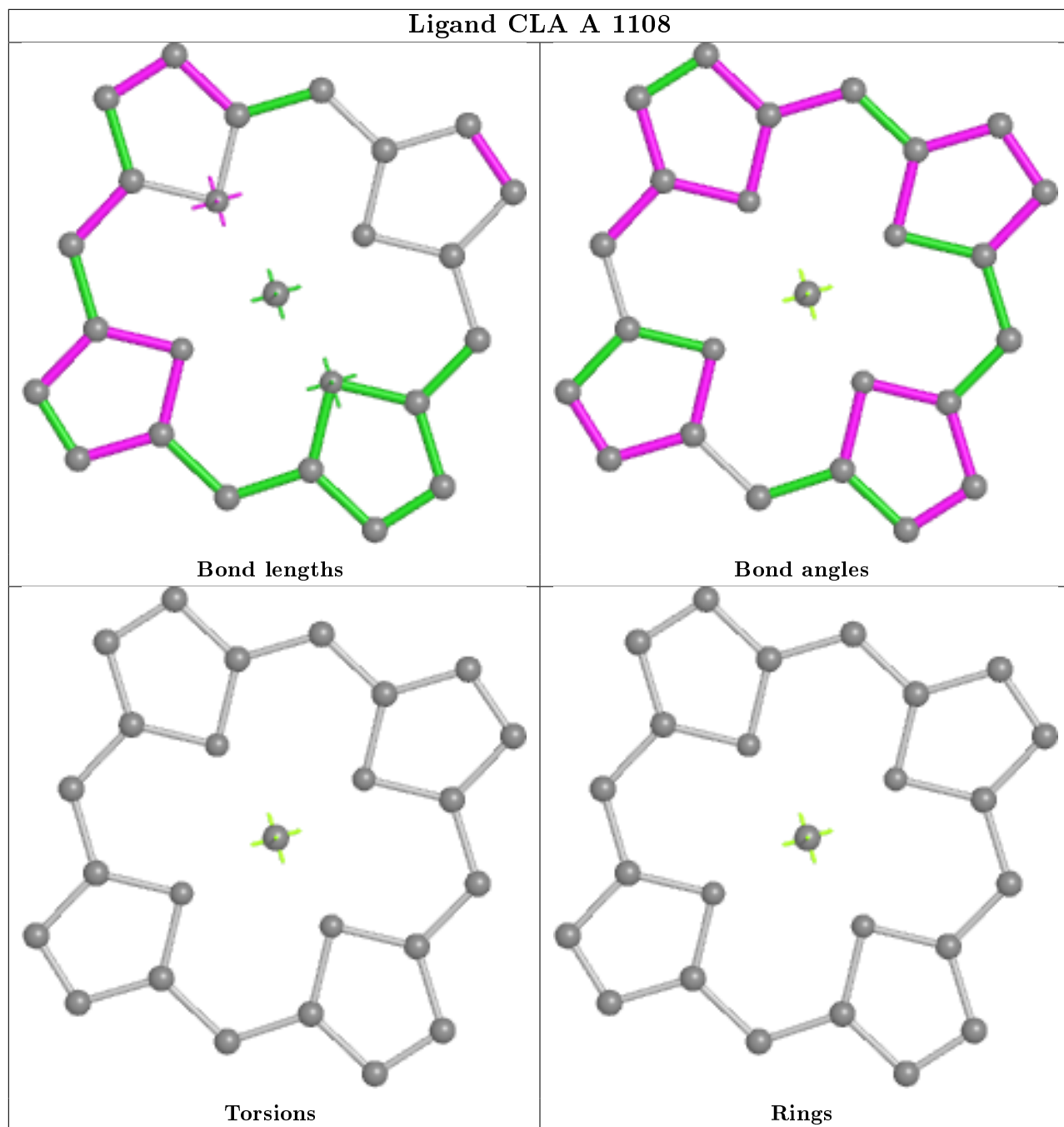


Rings

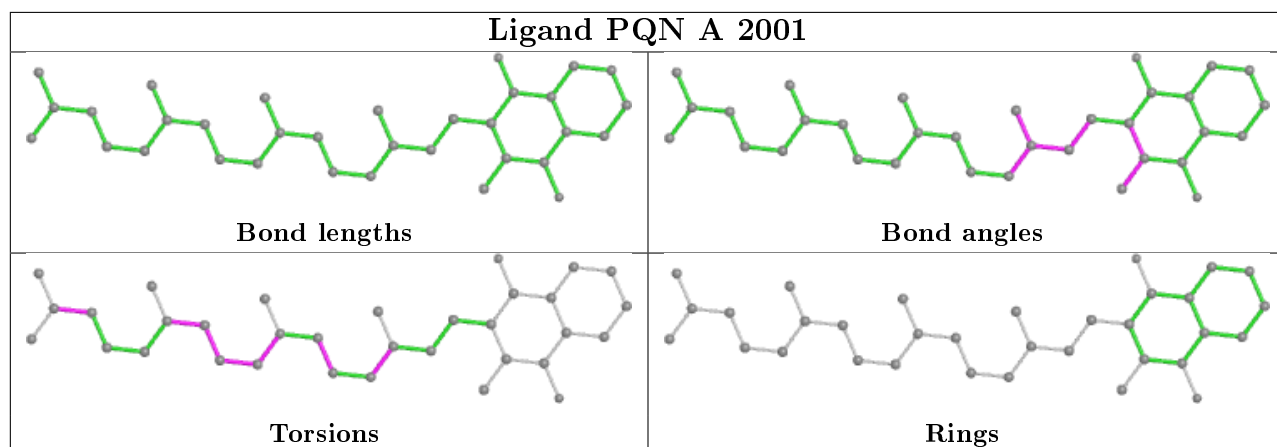
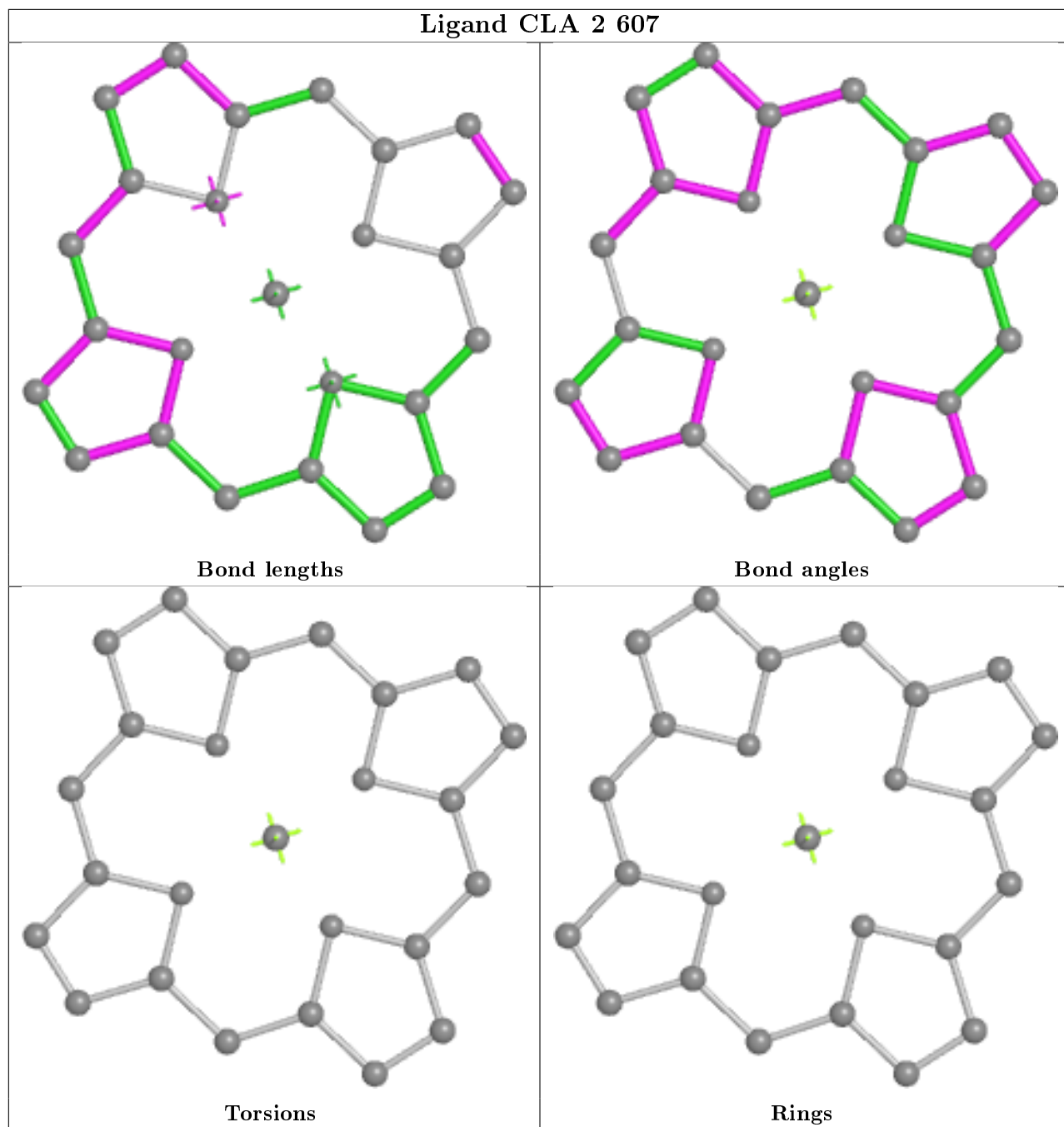


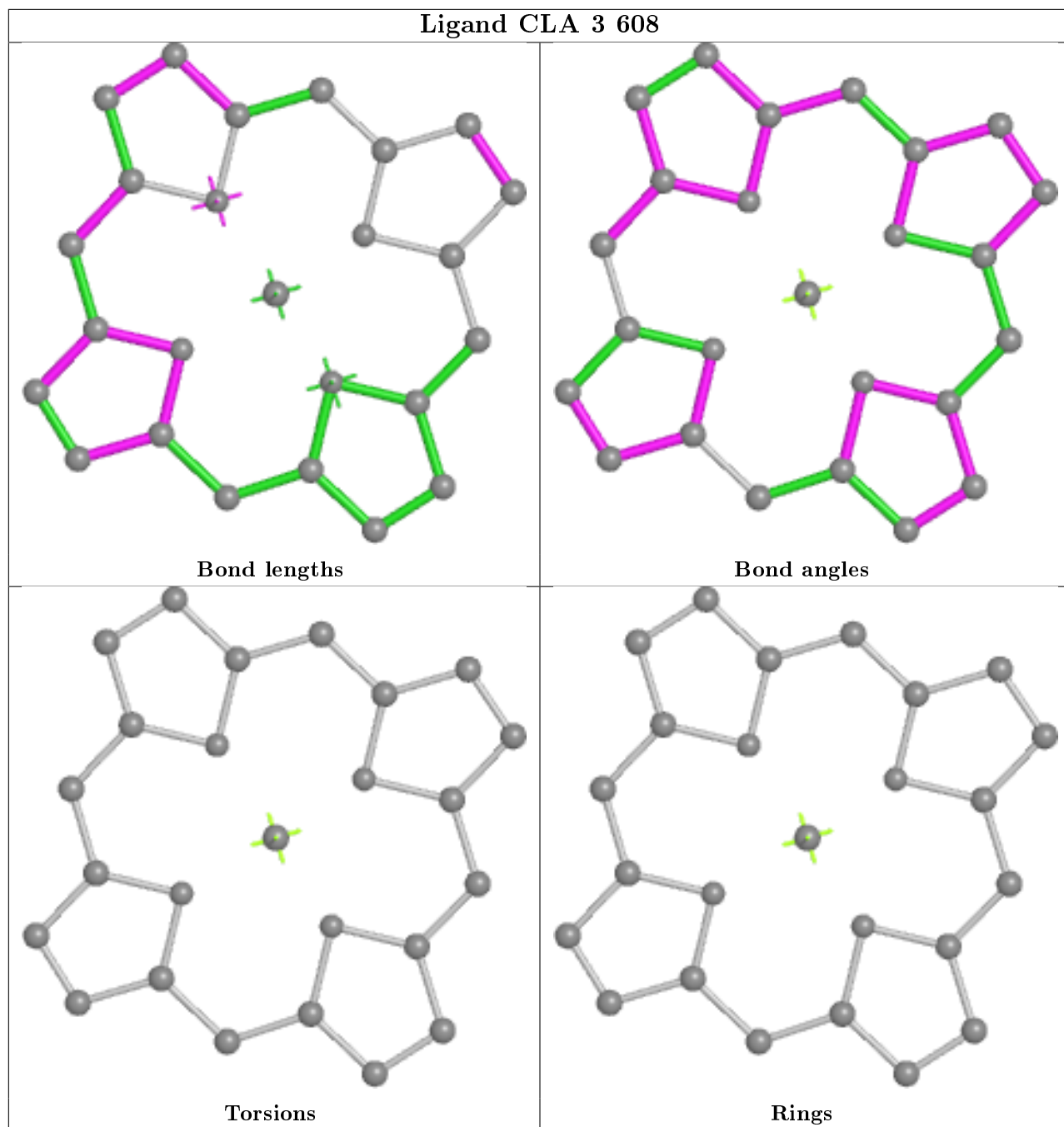


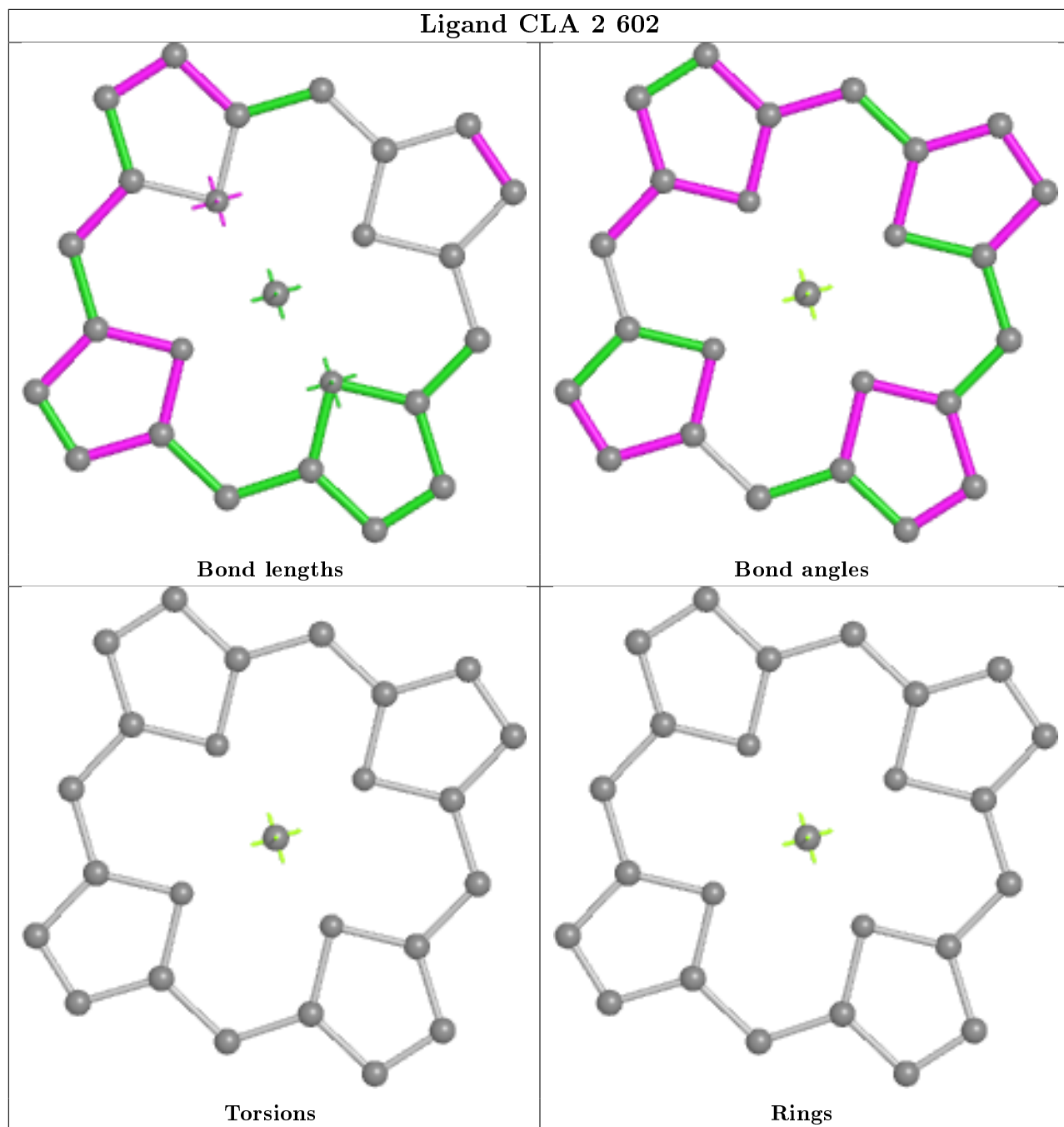


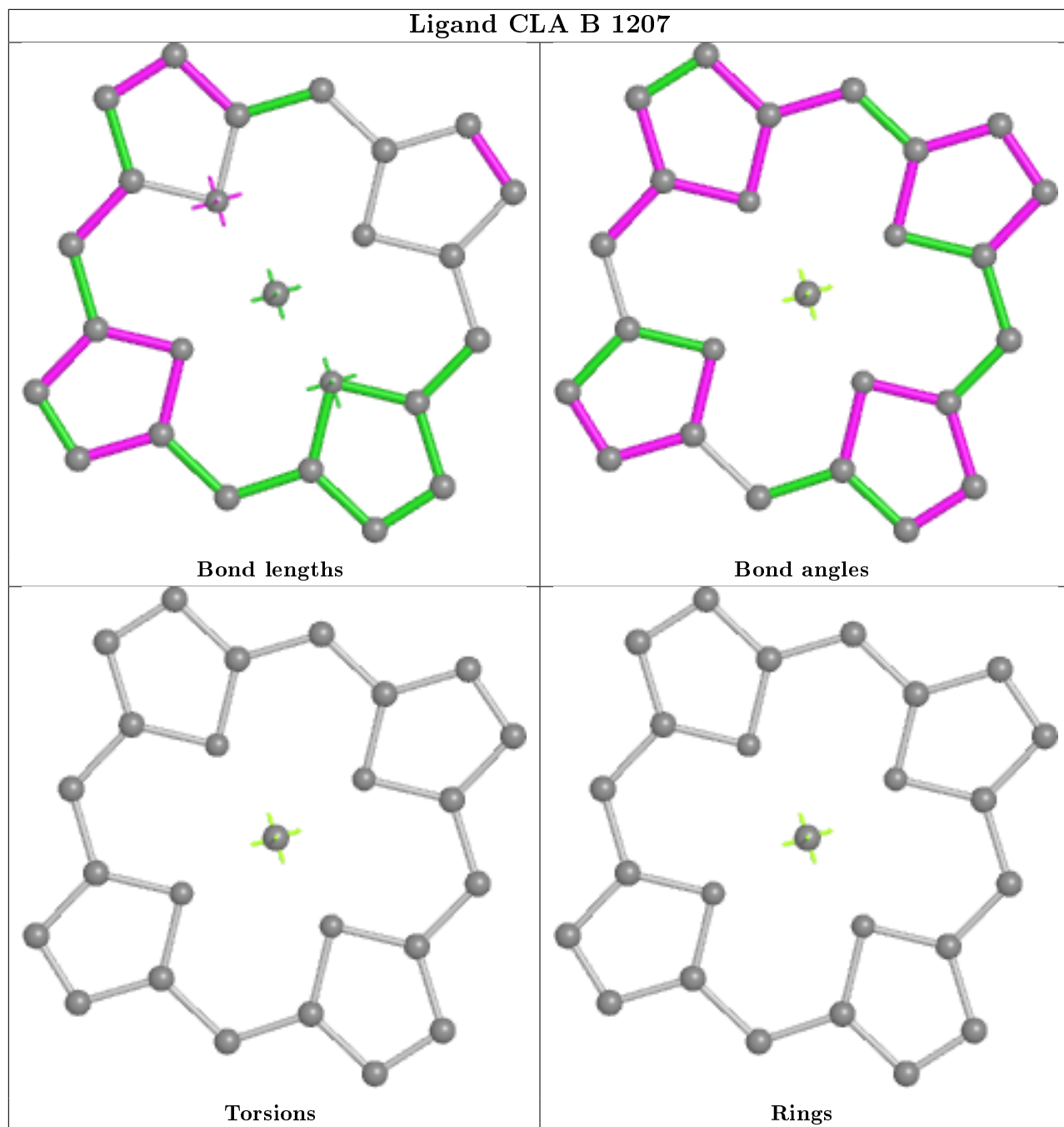


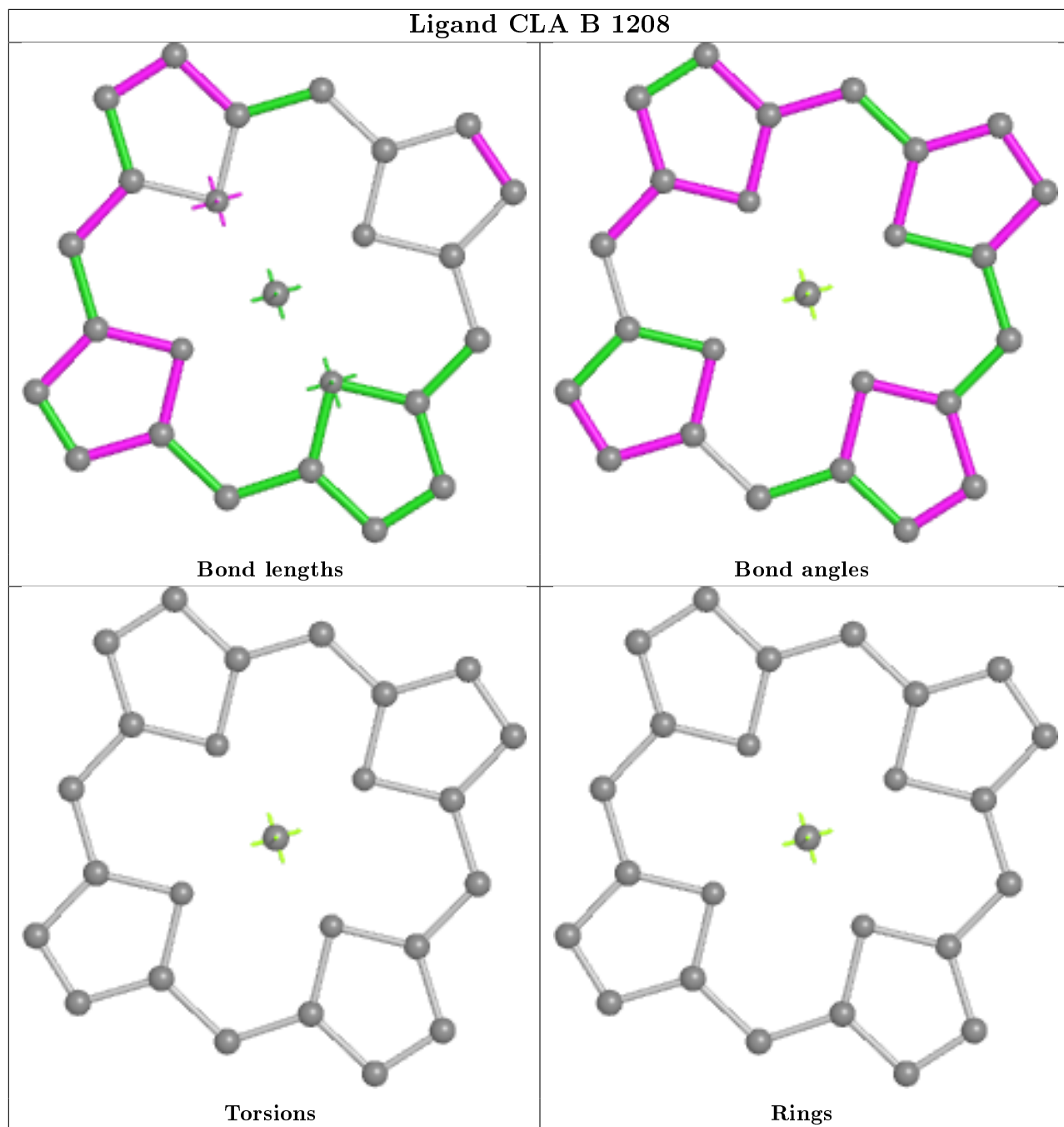




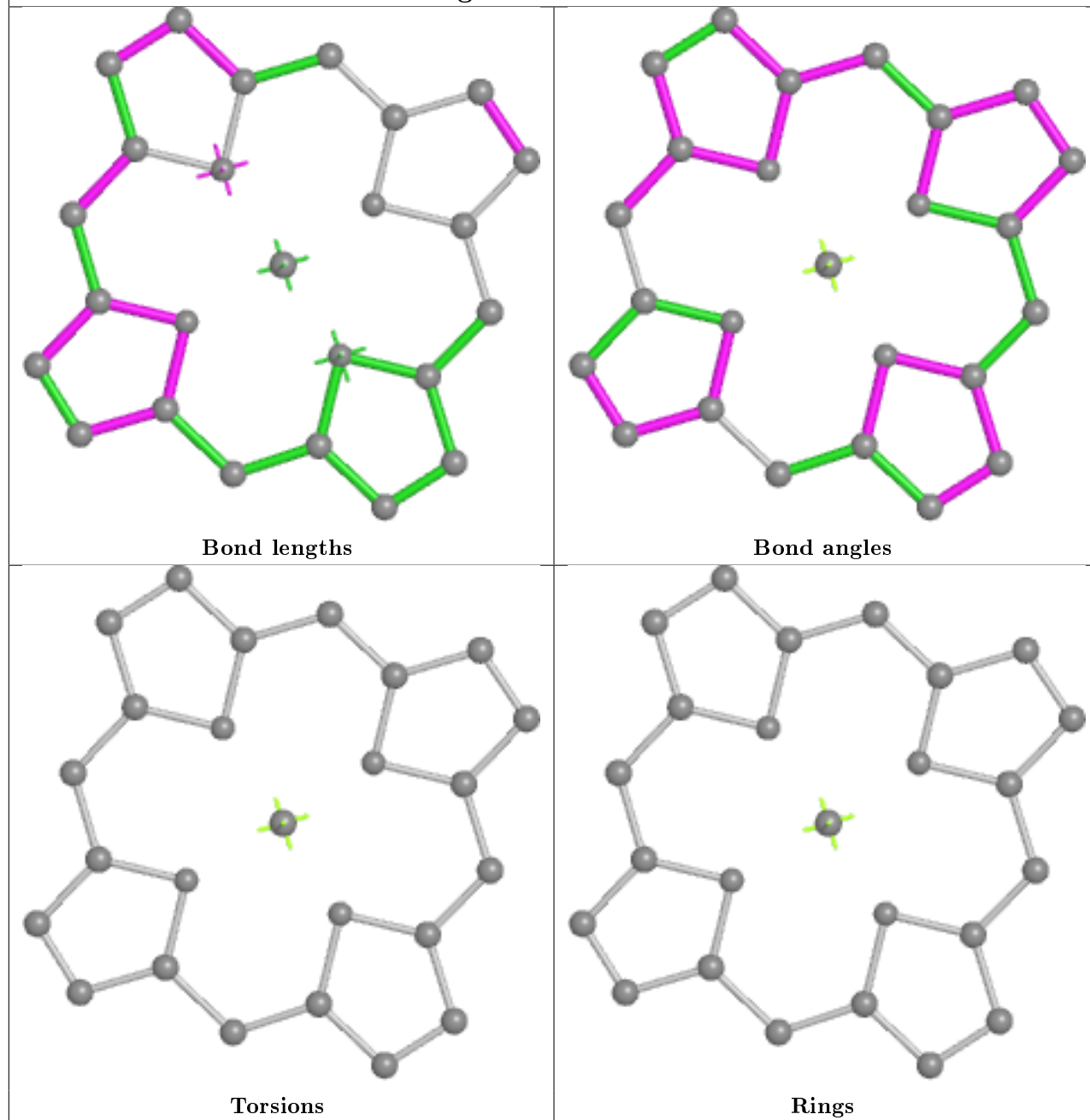


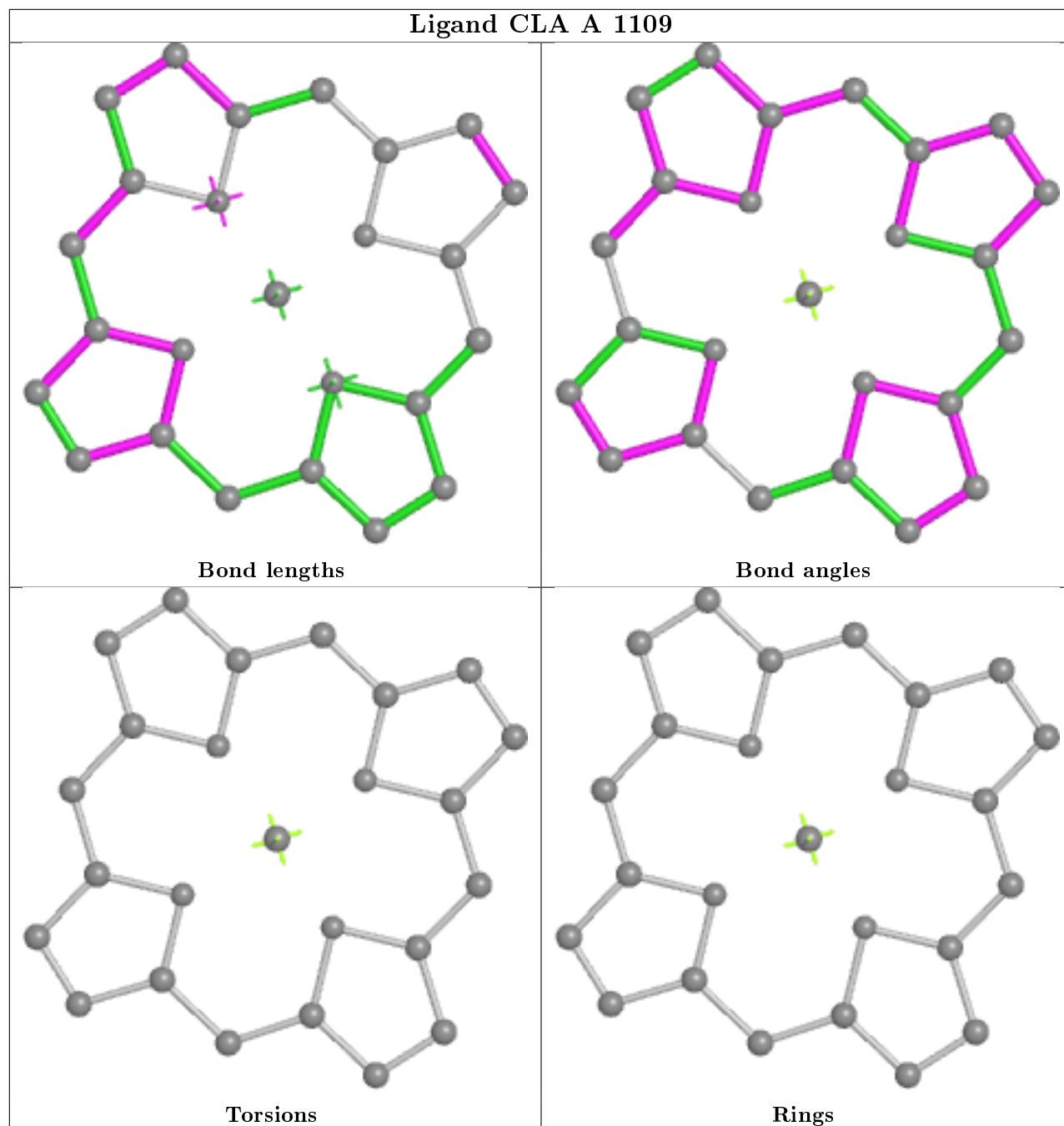


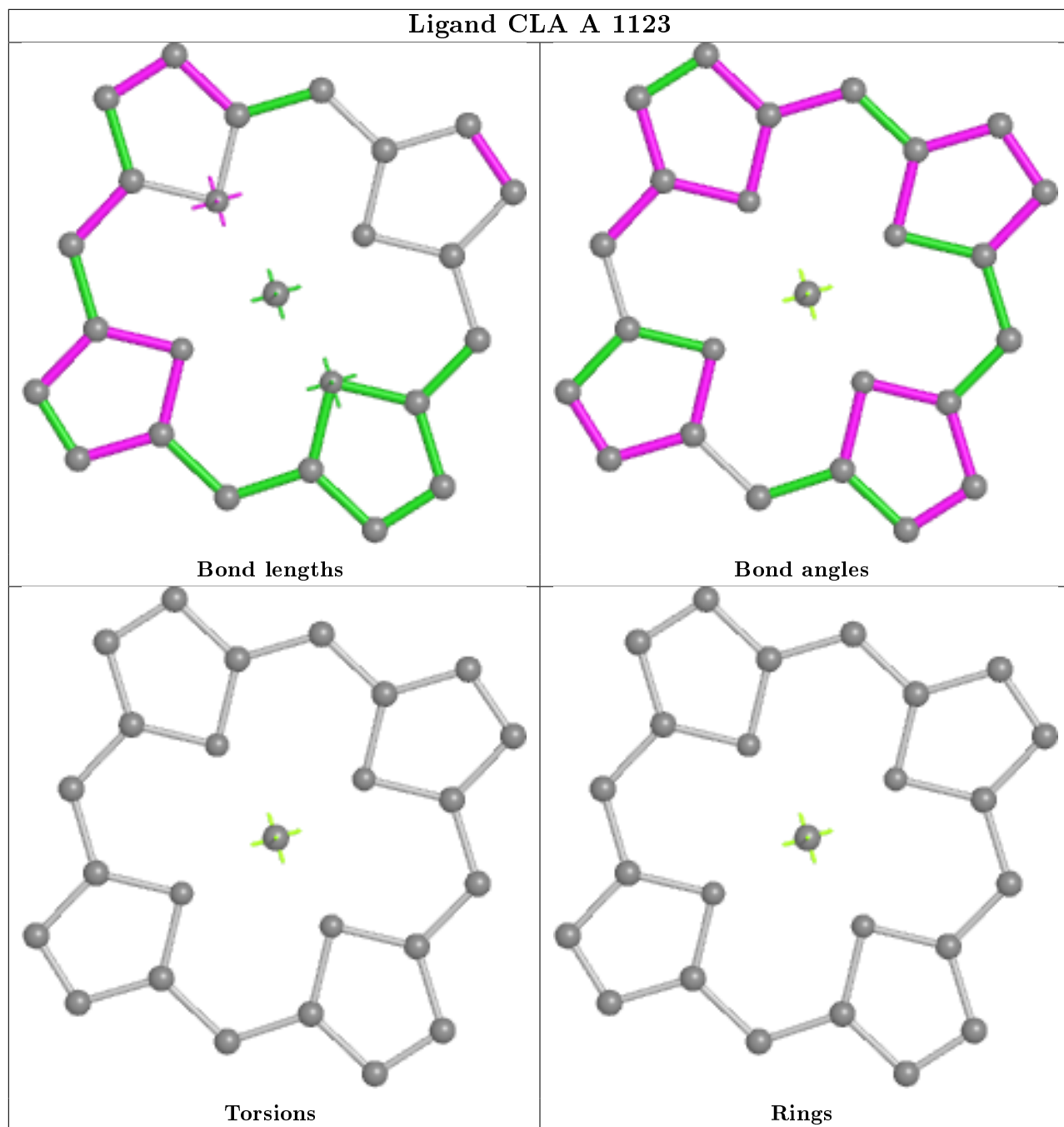




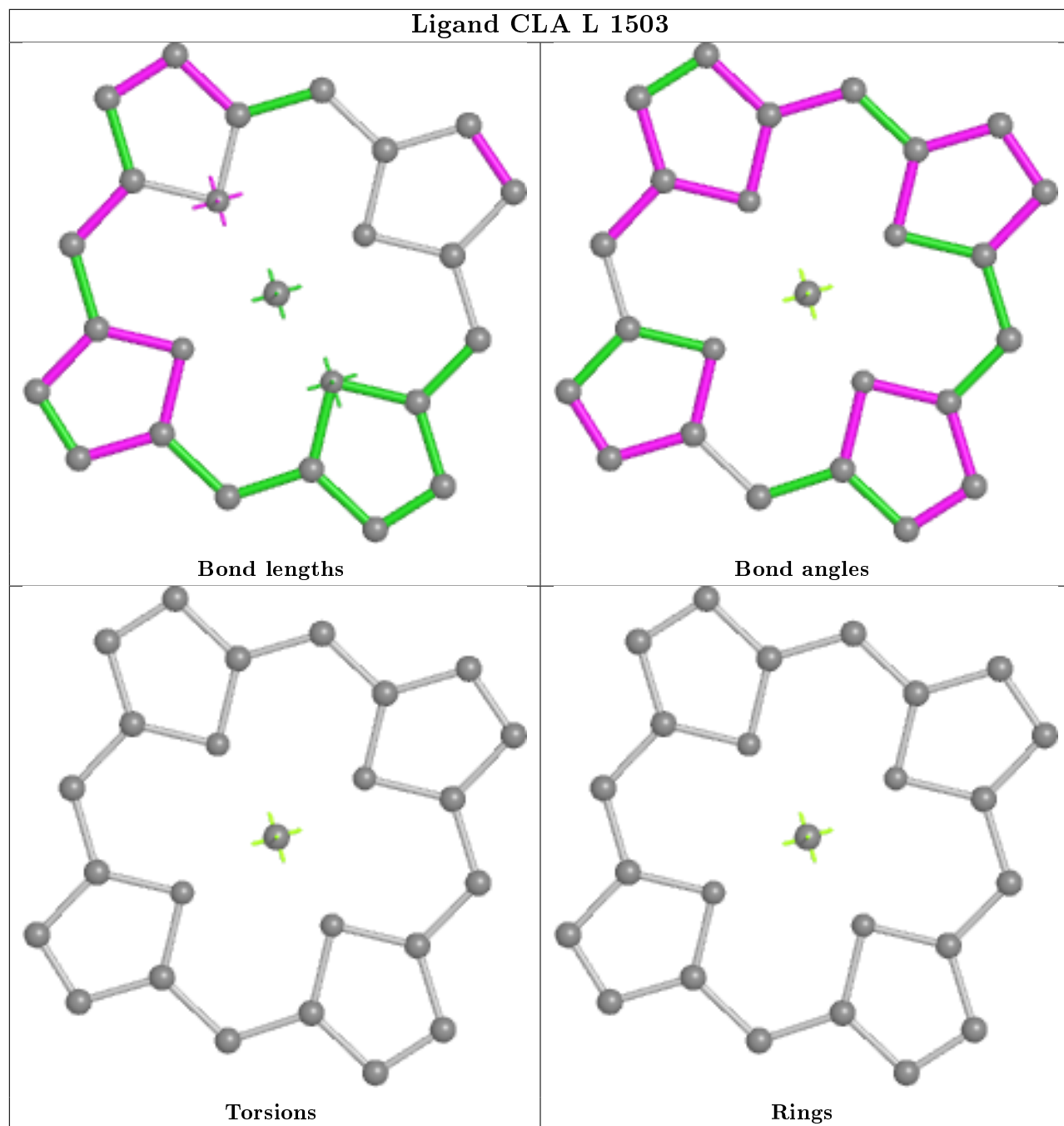
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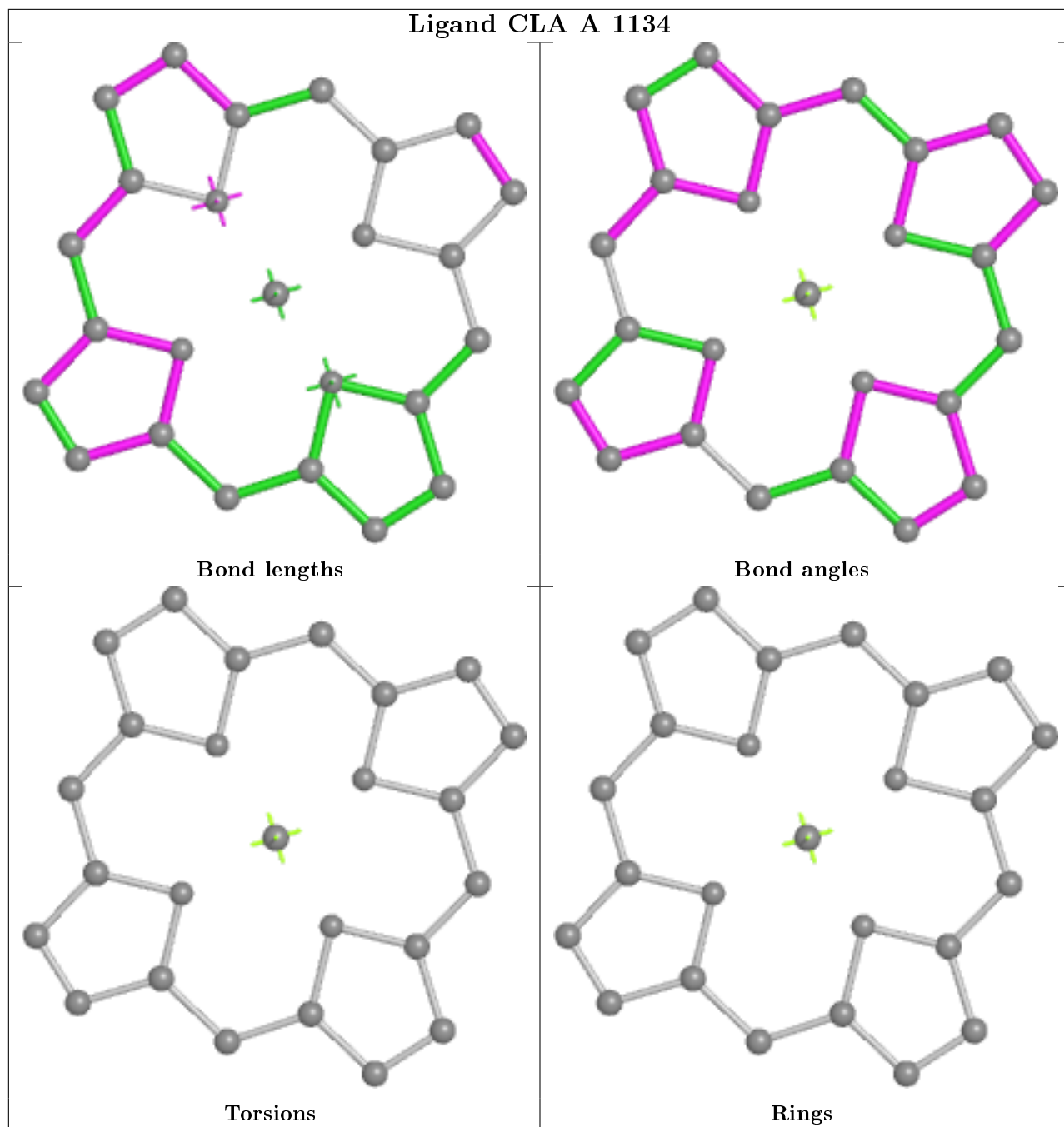


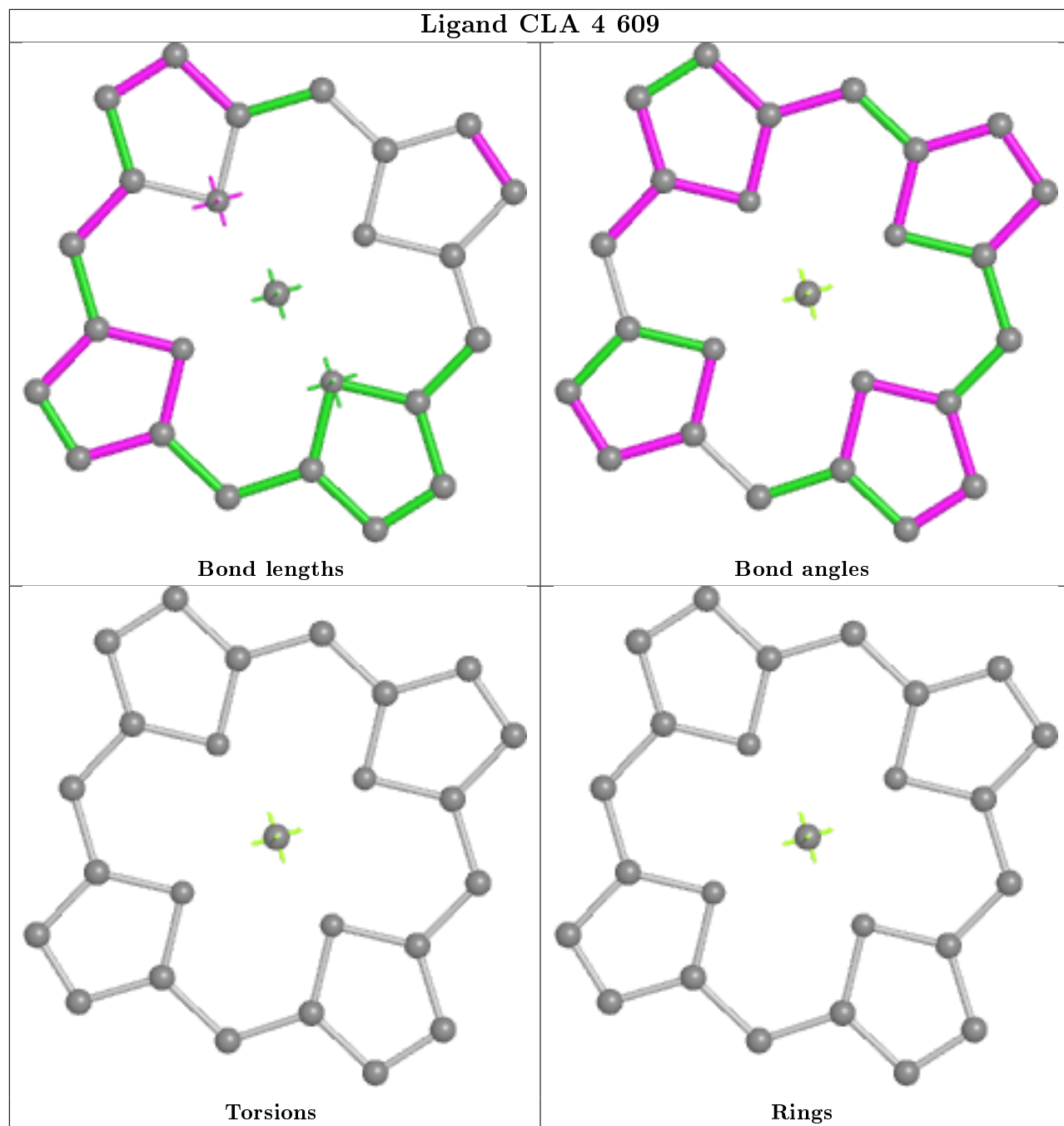


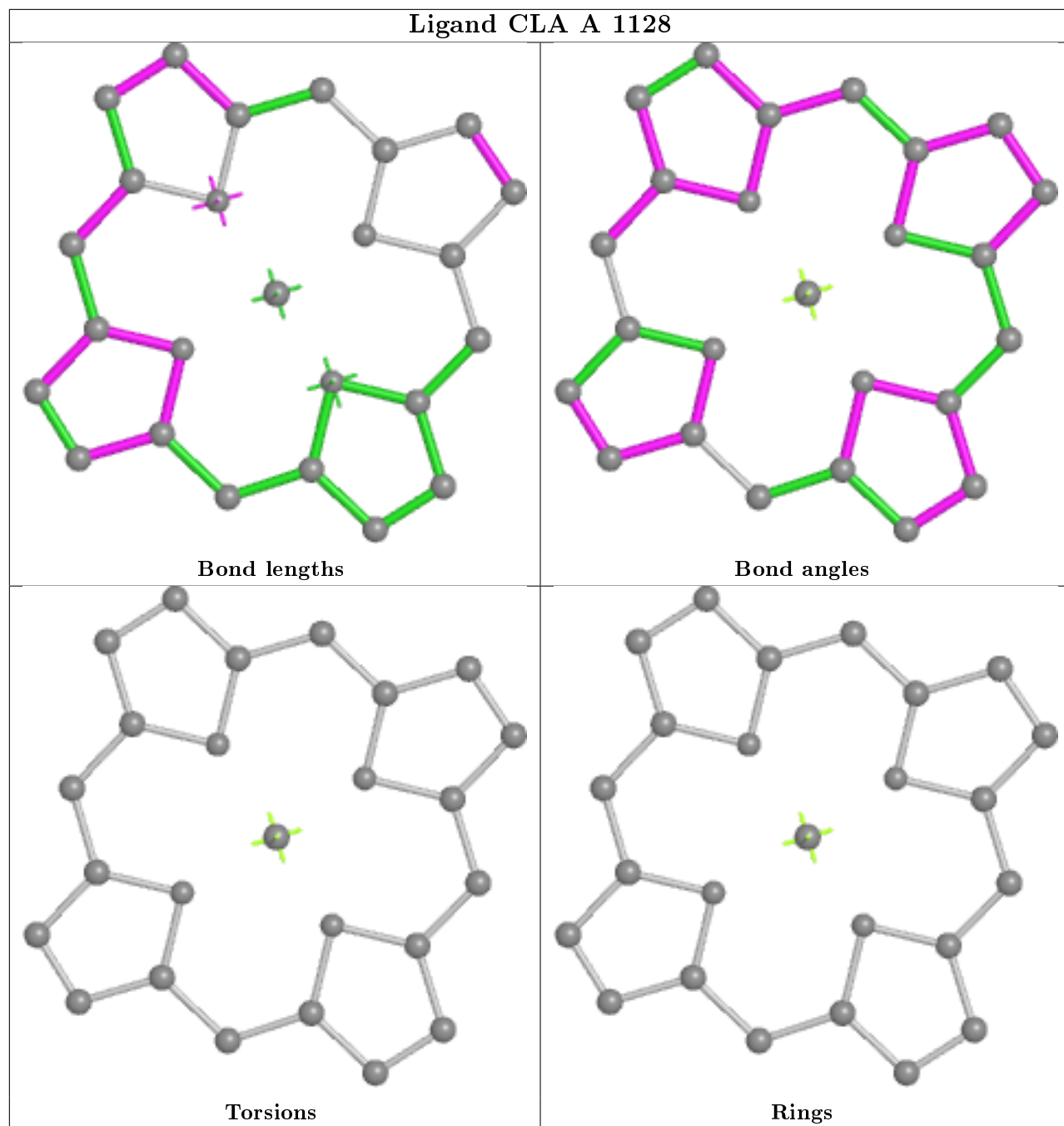




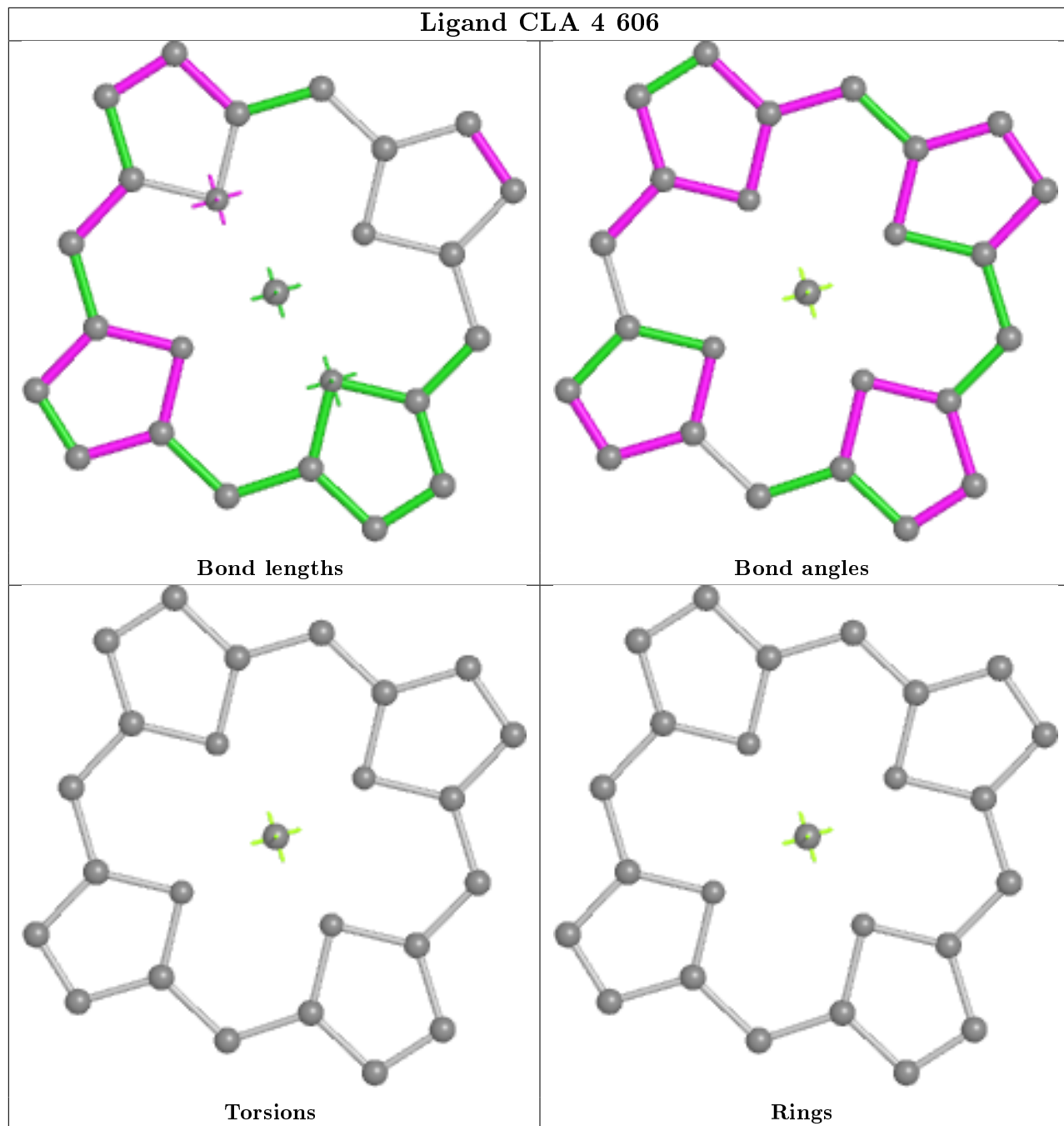


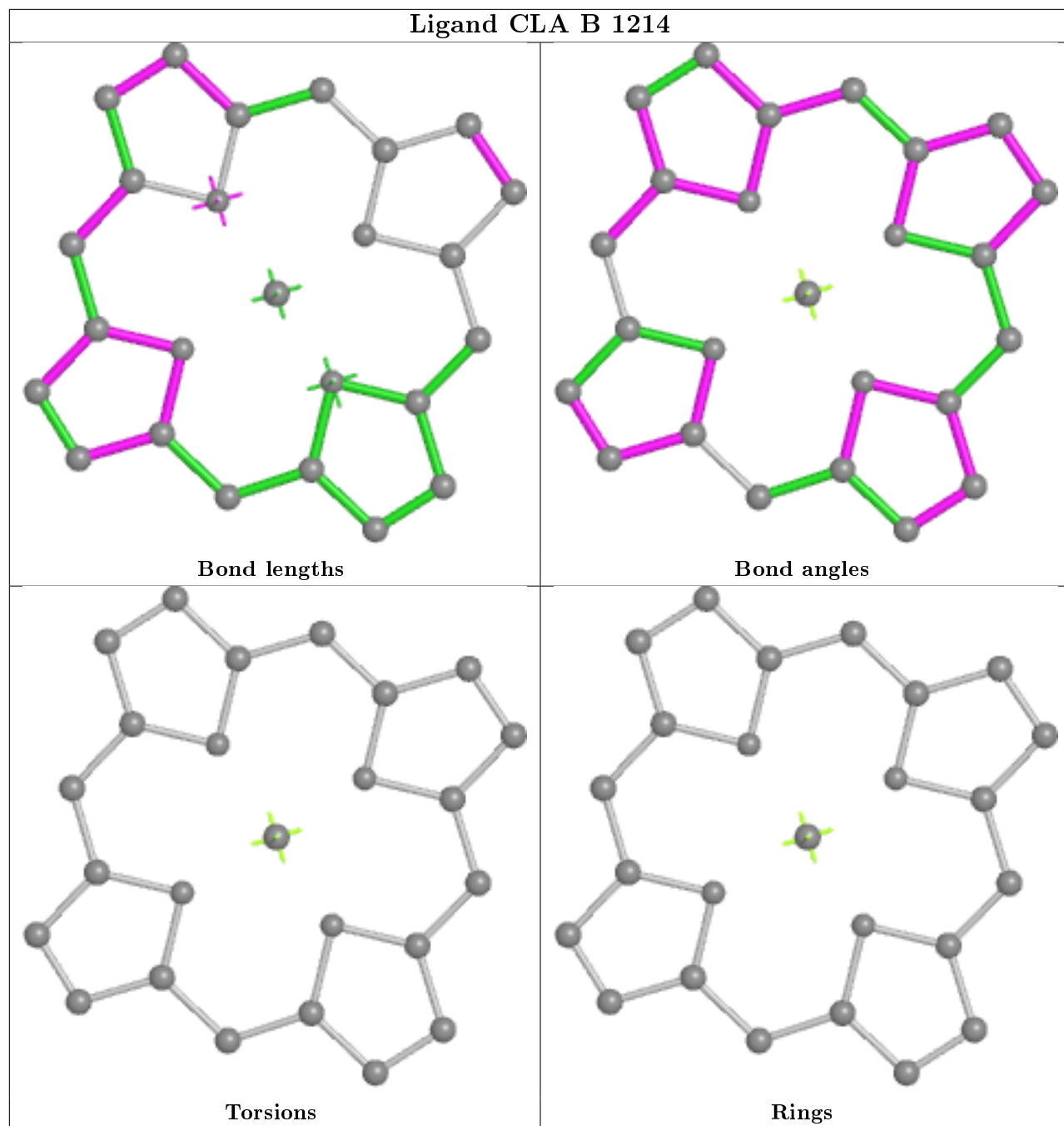




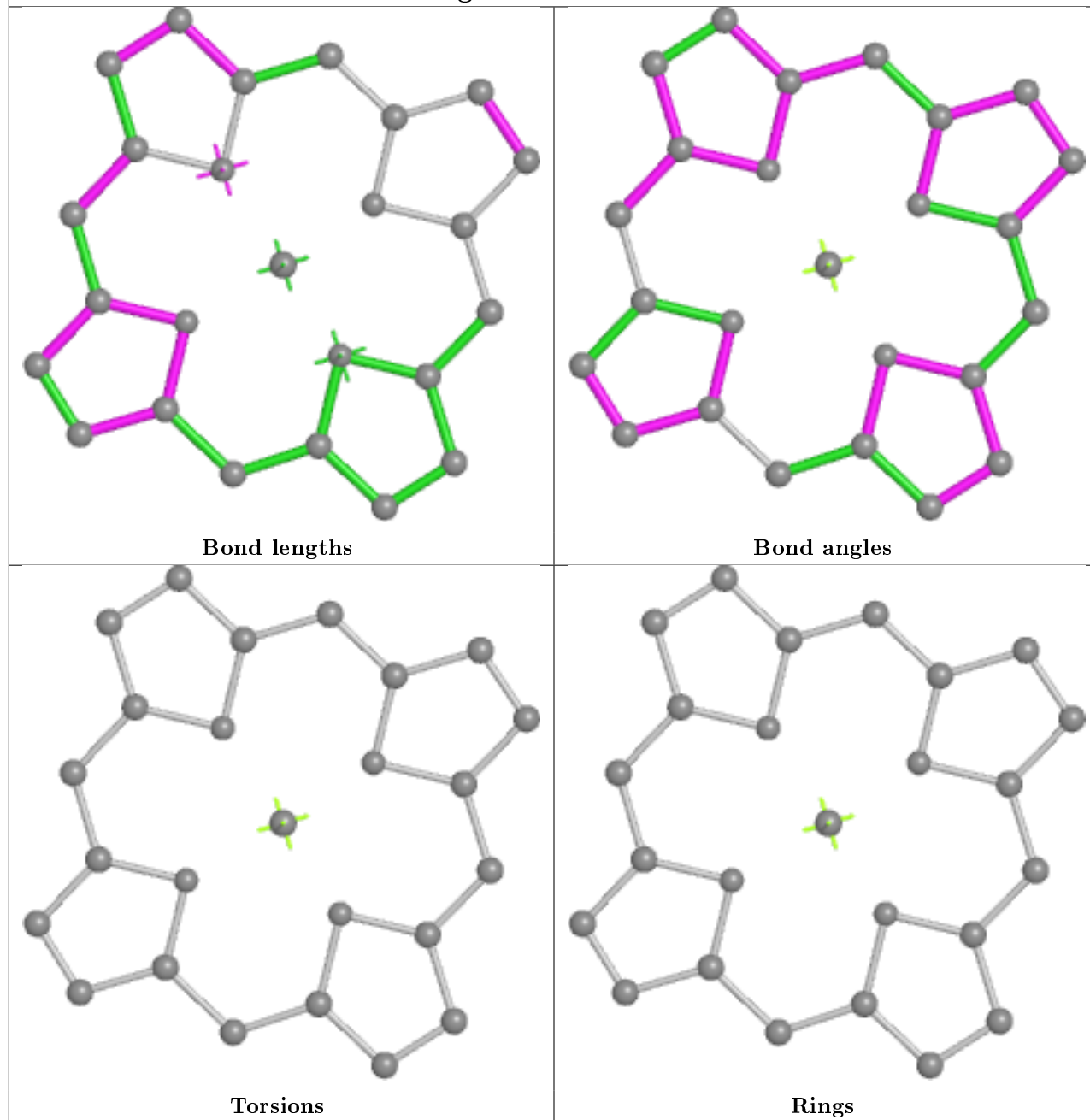


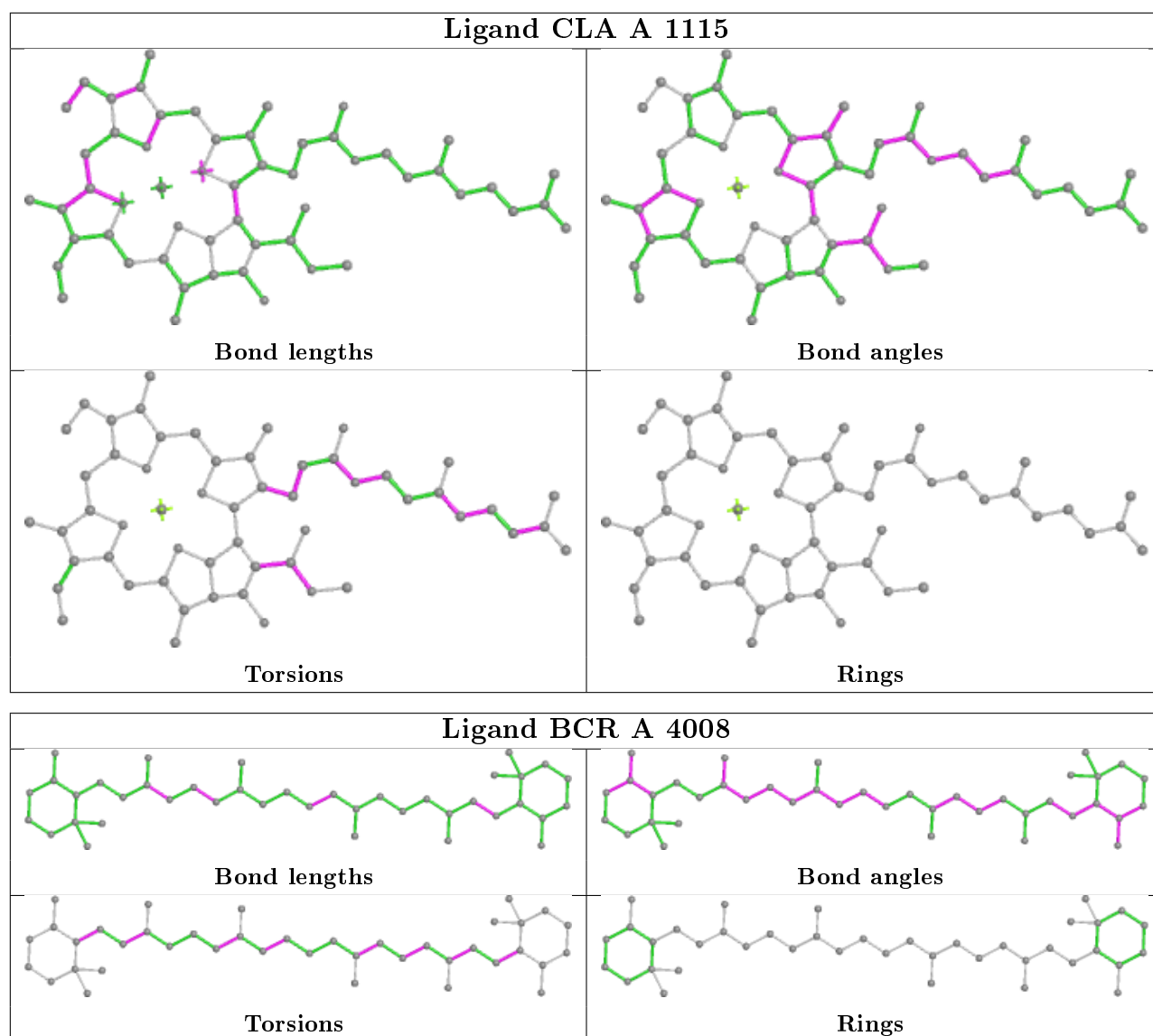
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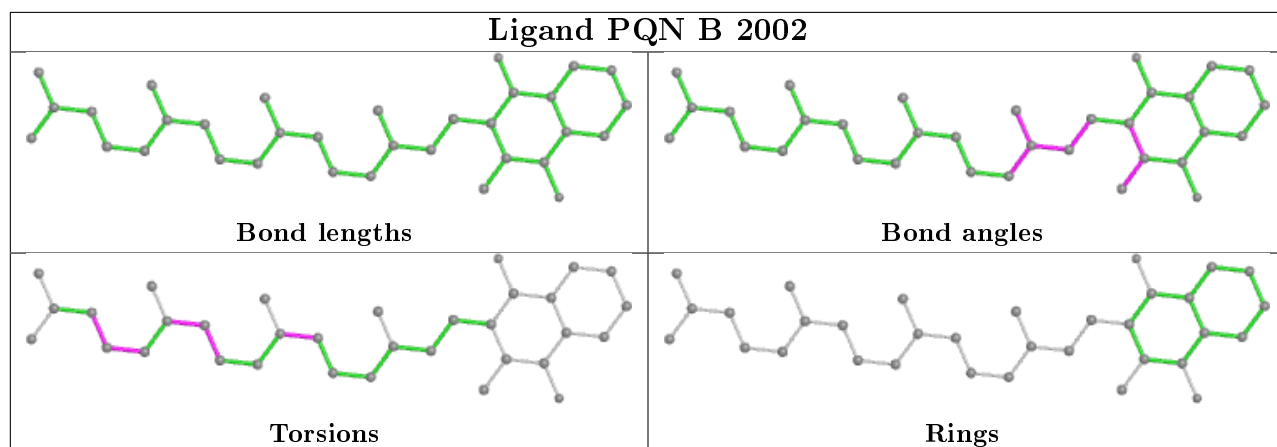
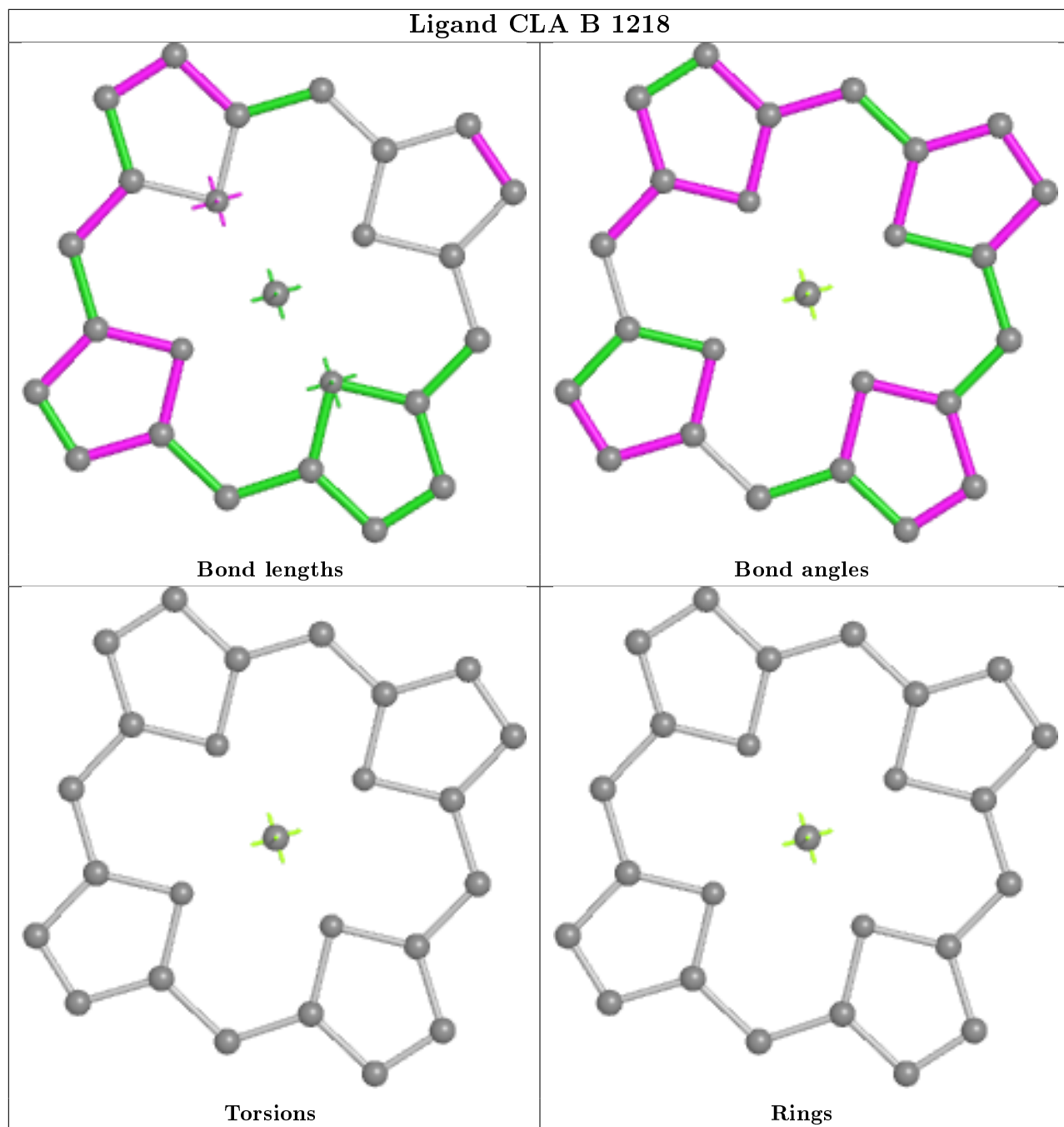


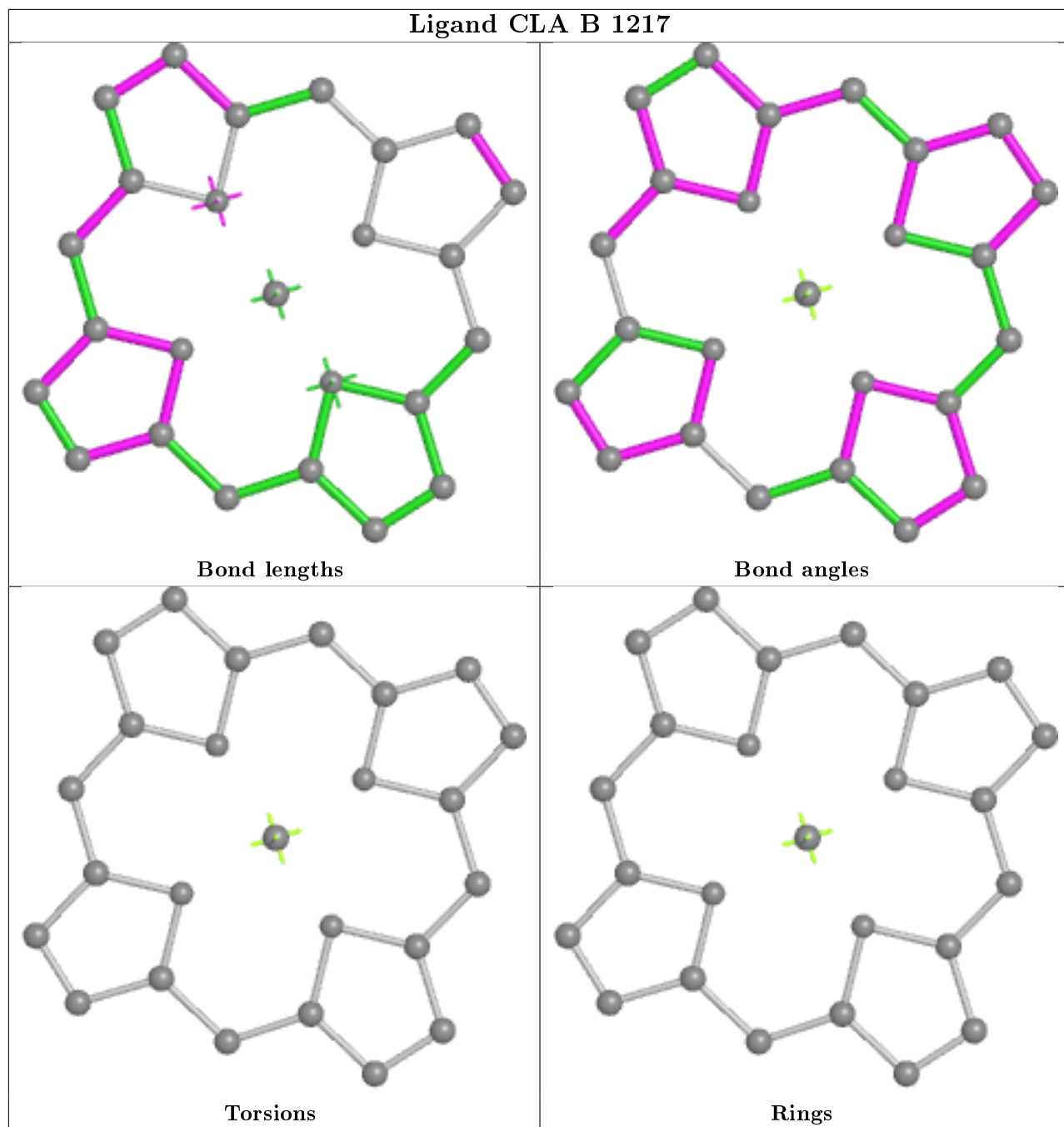
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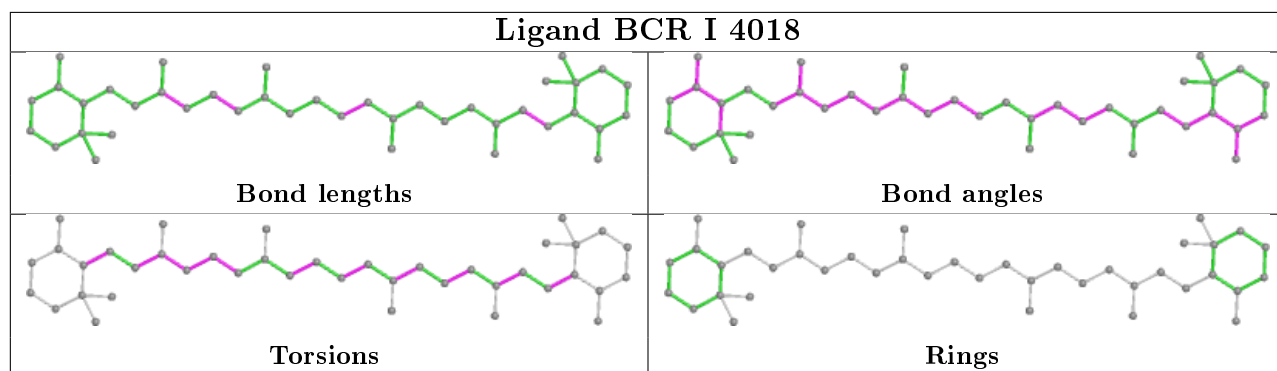
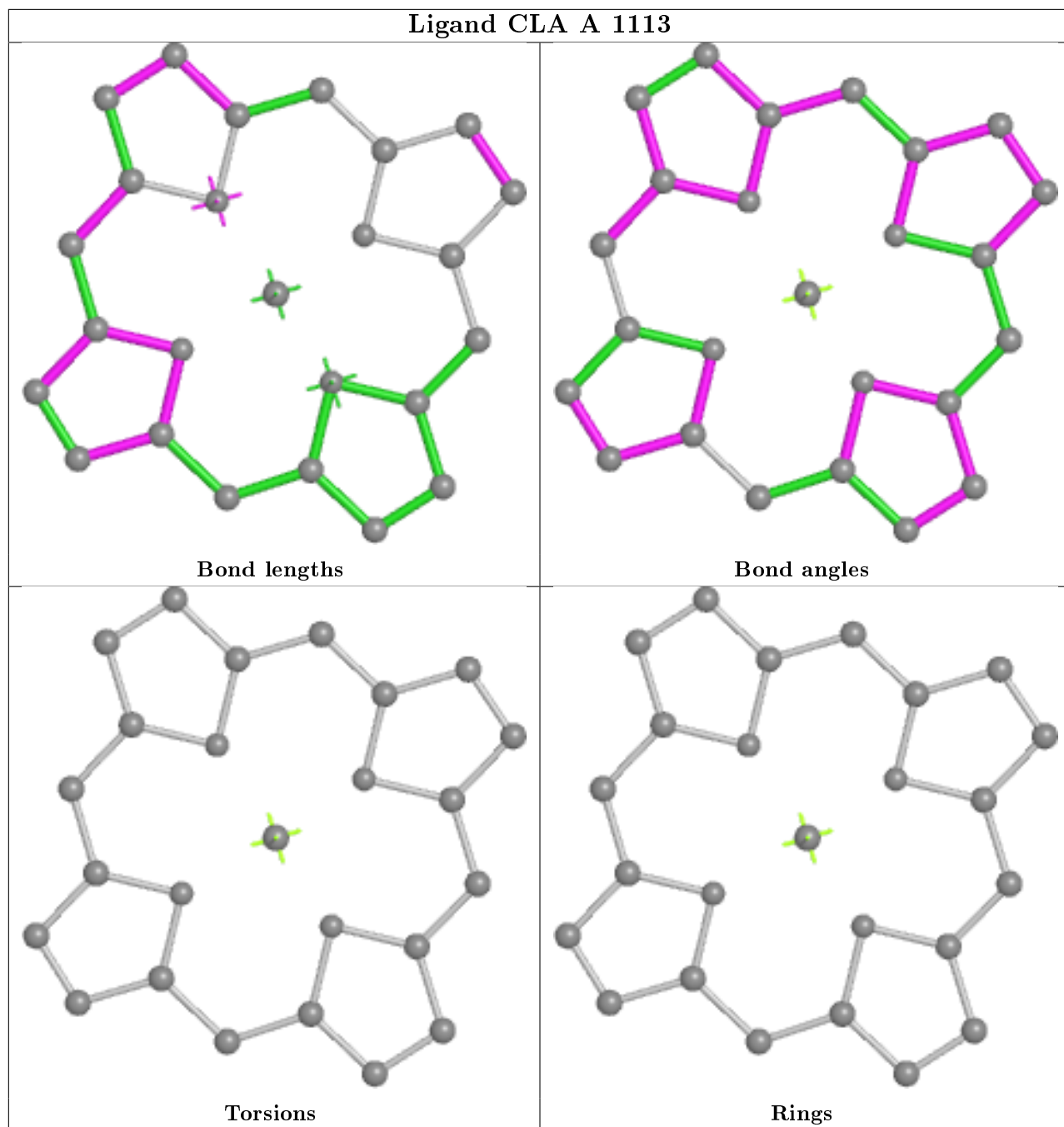


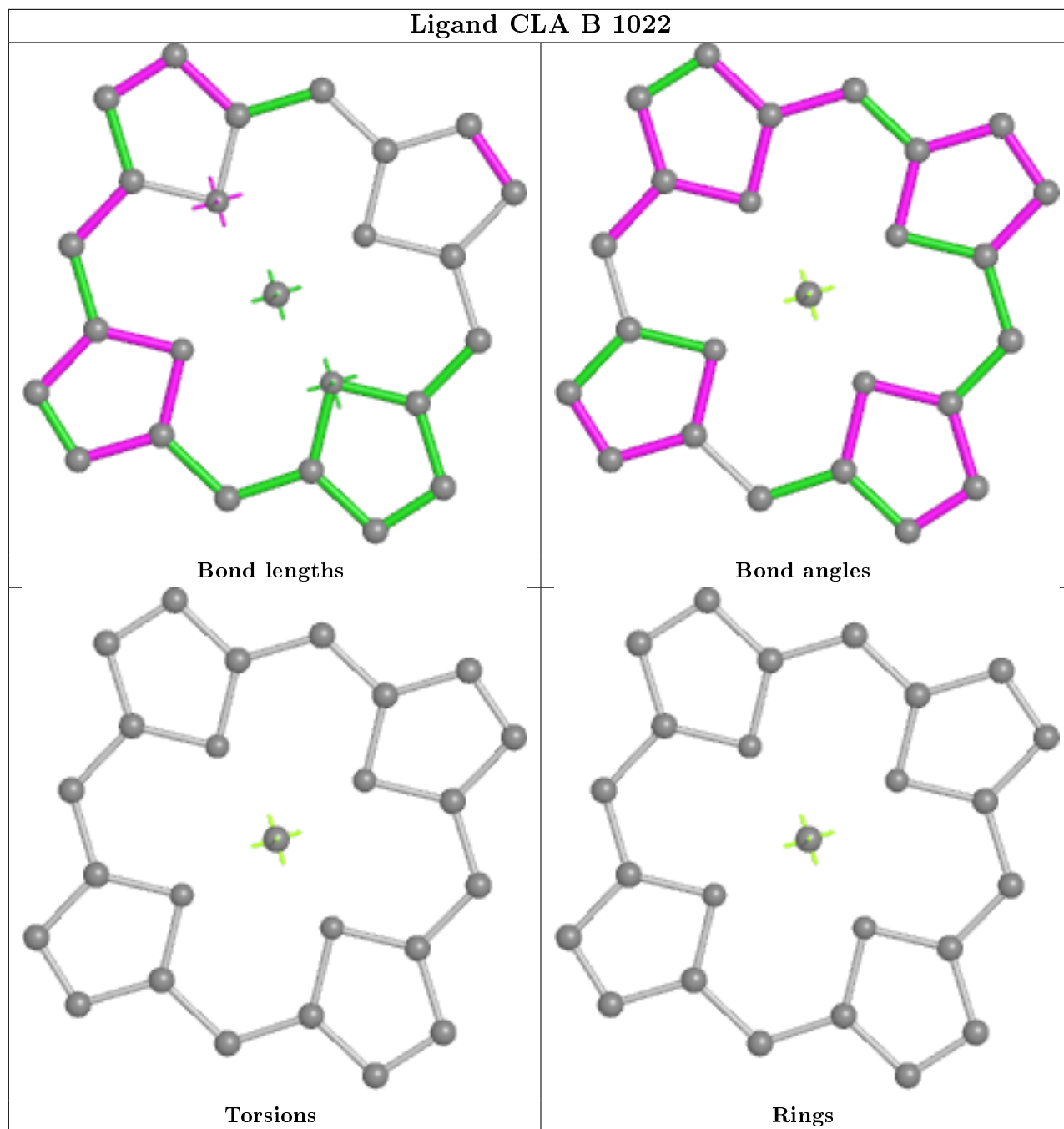


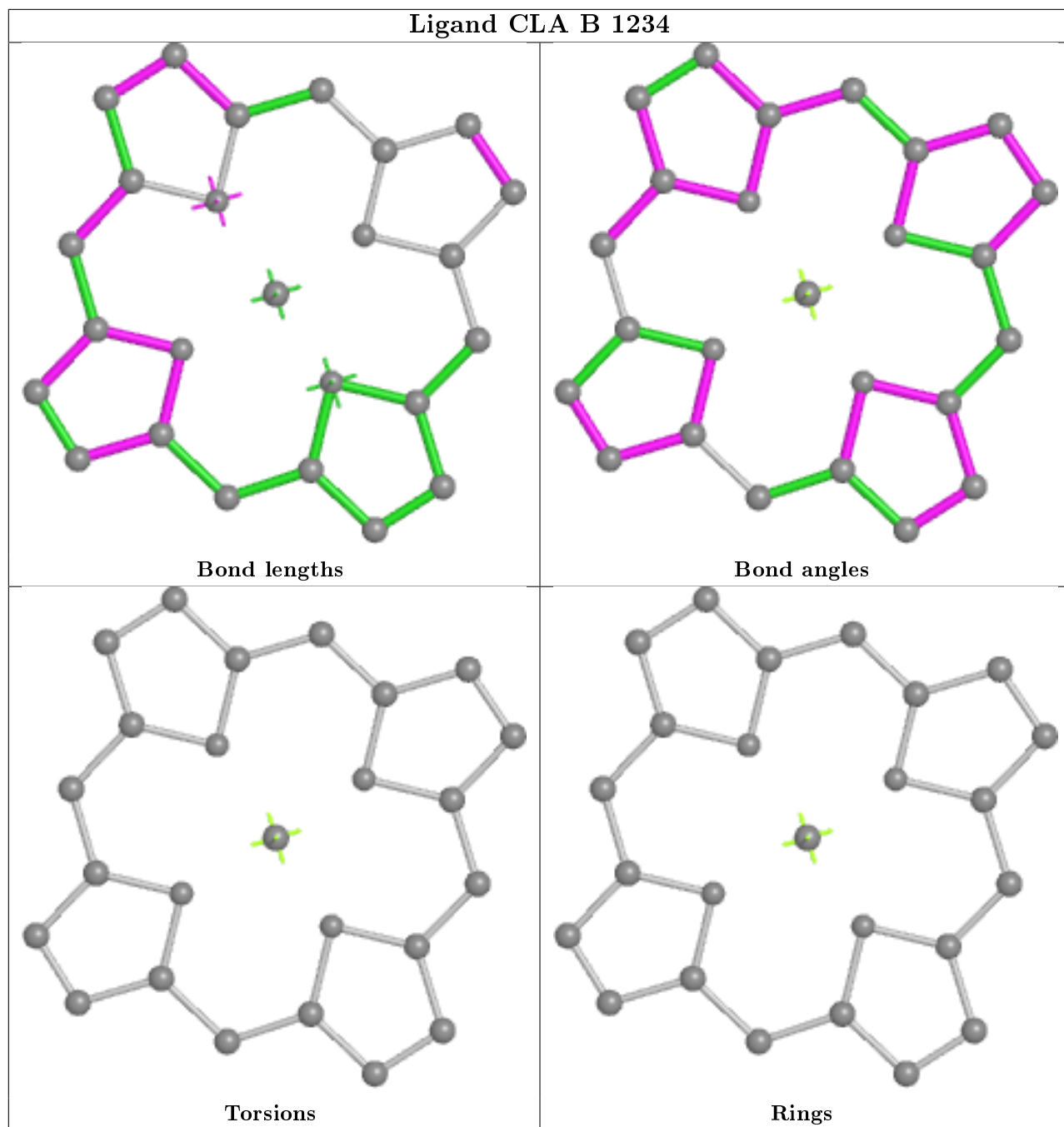


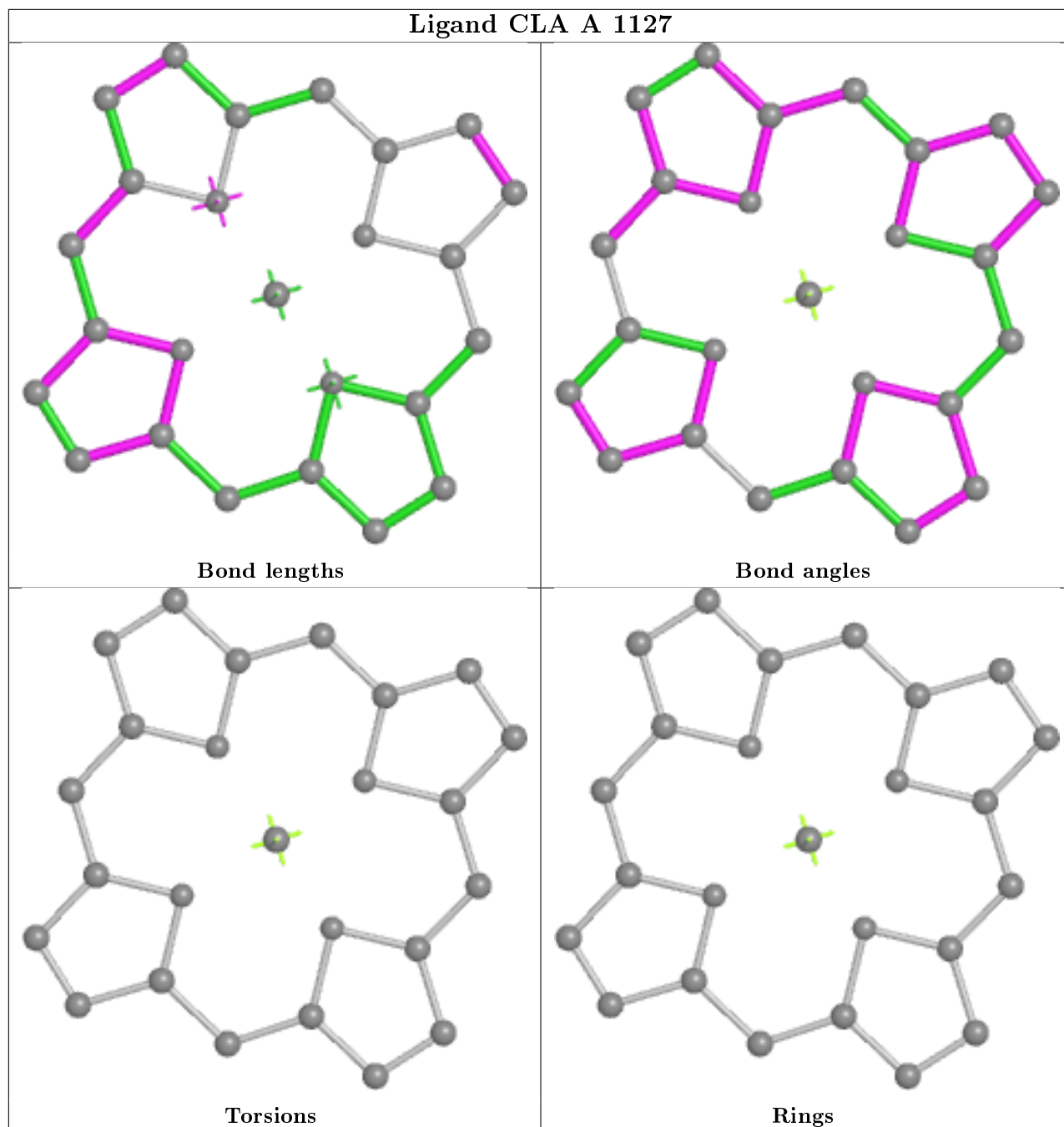


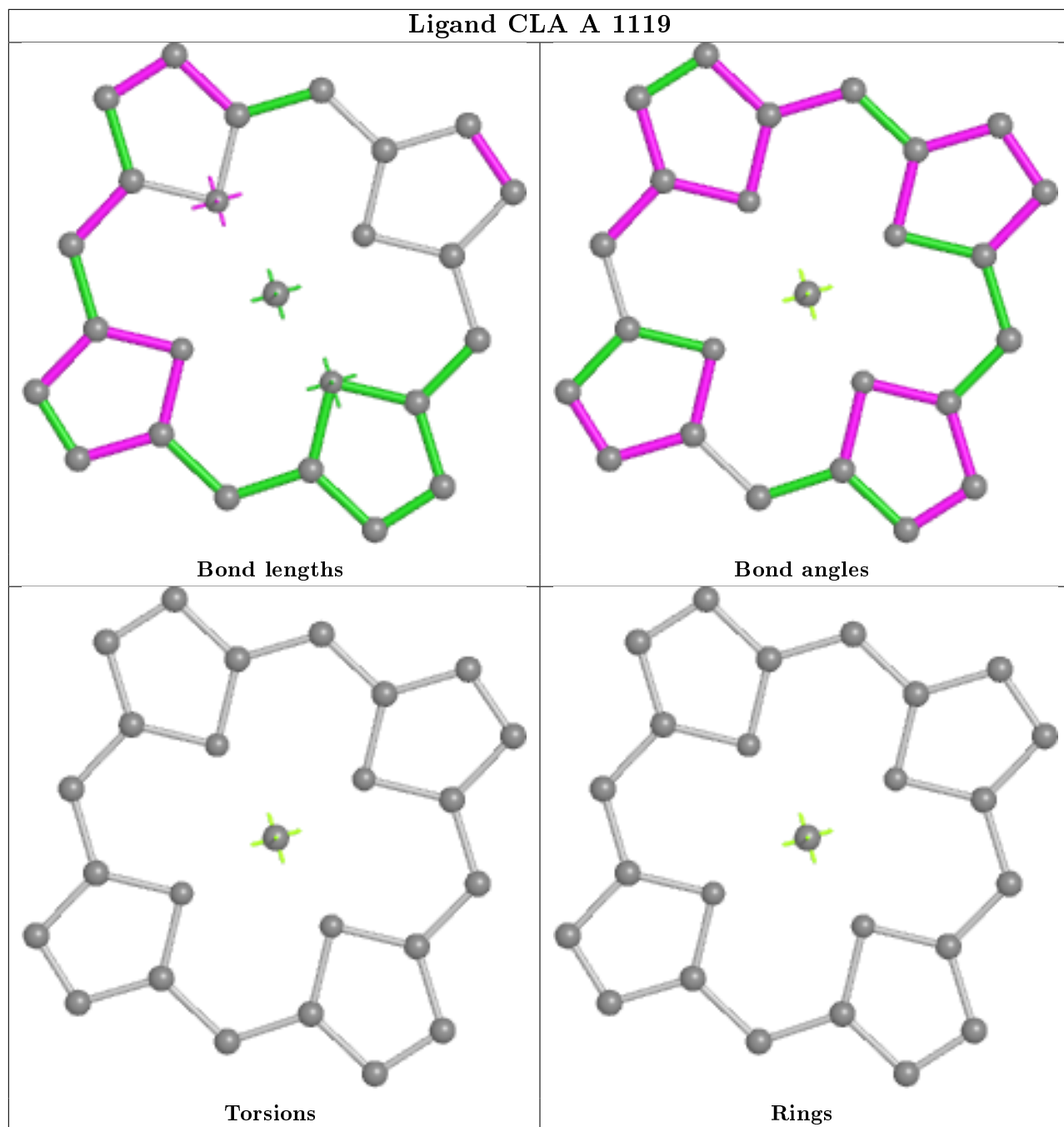


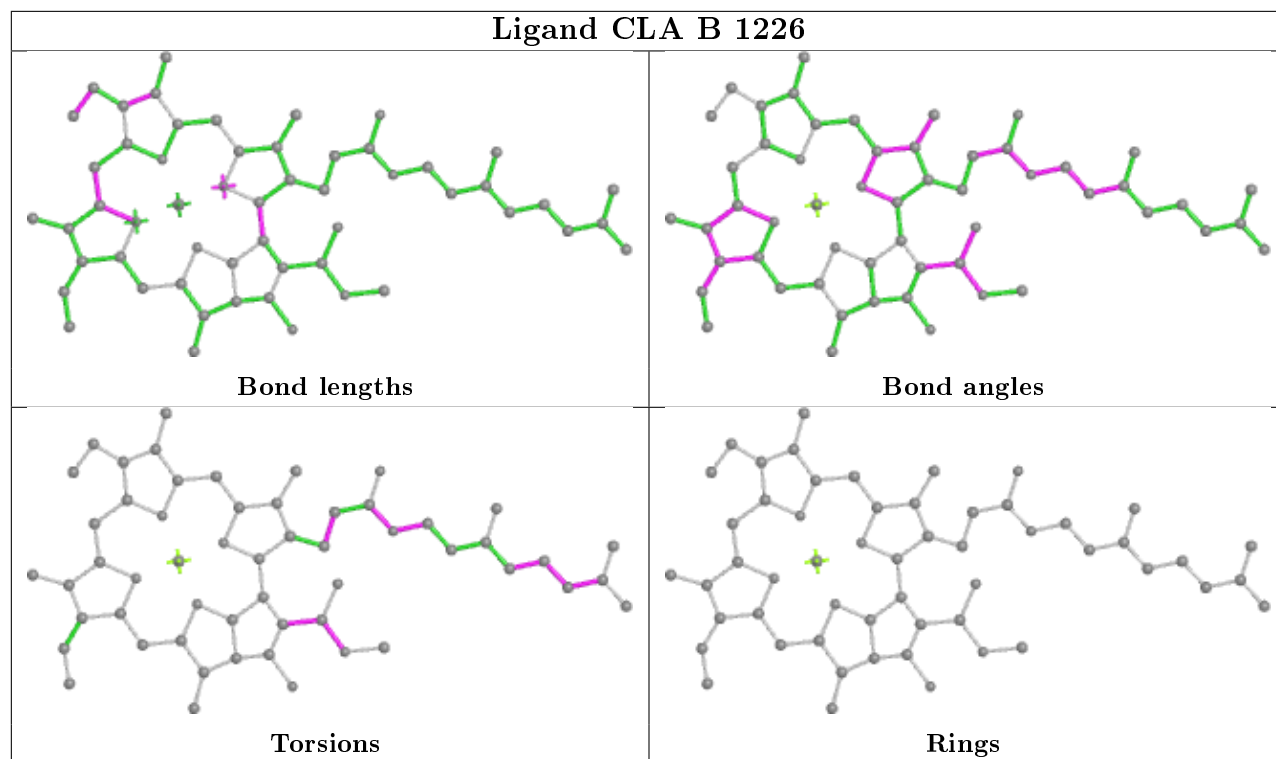




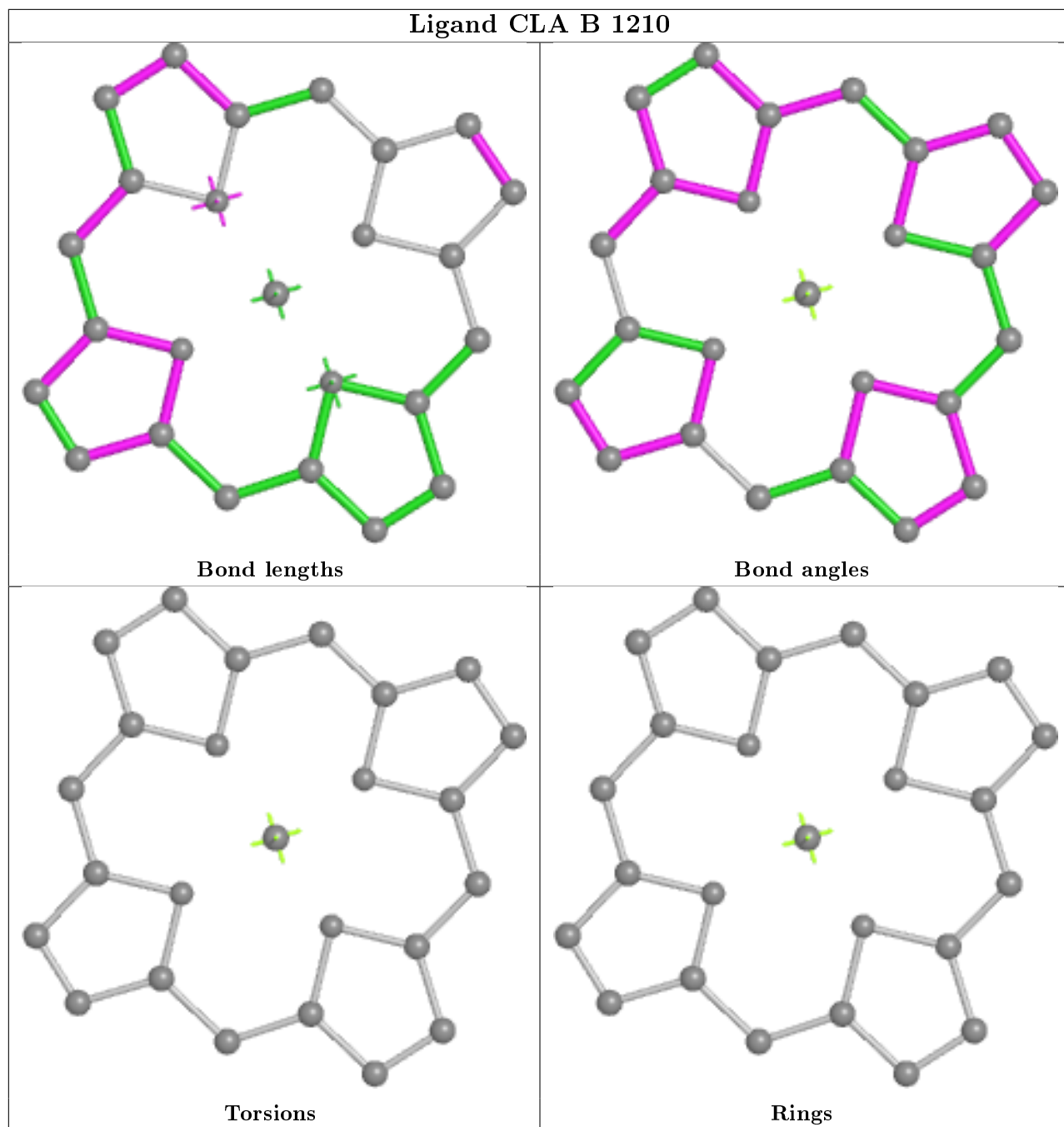


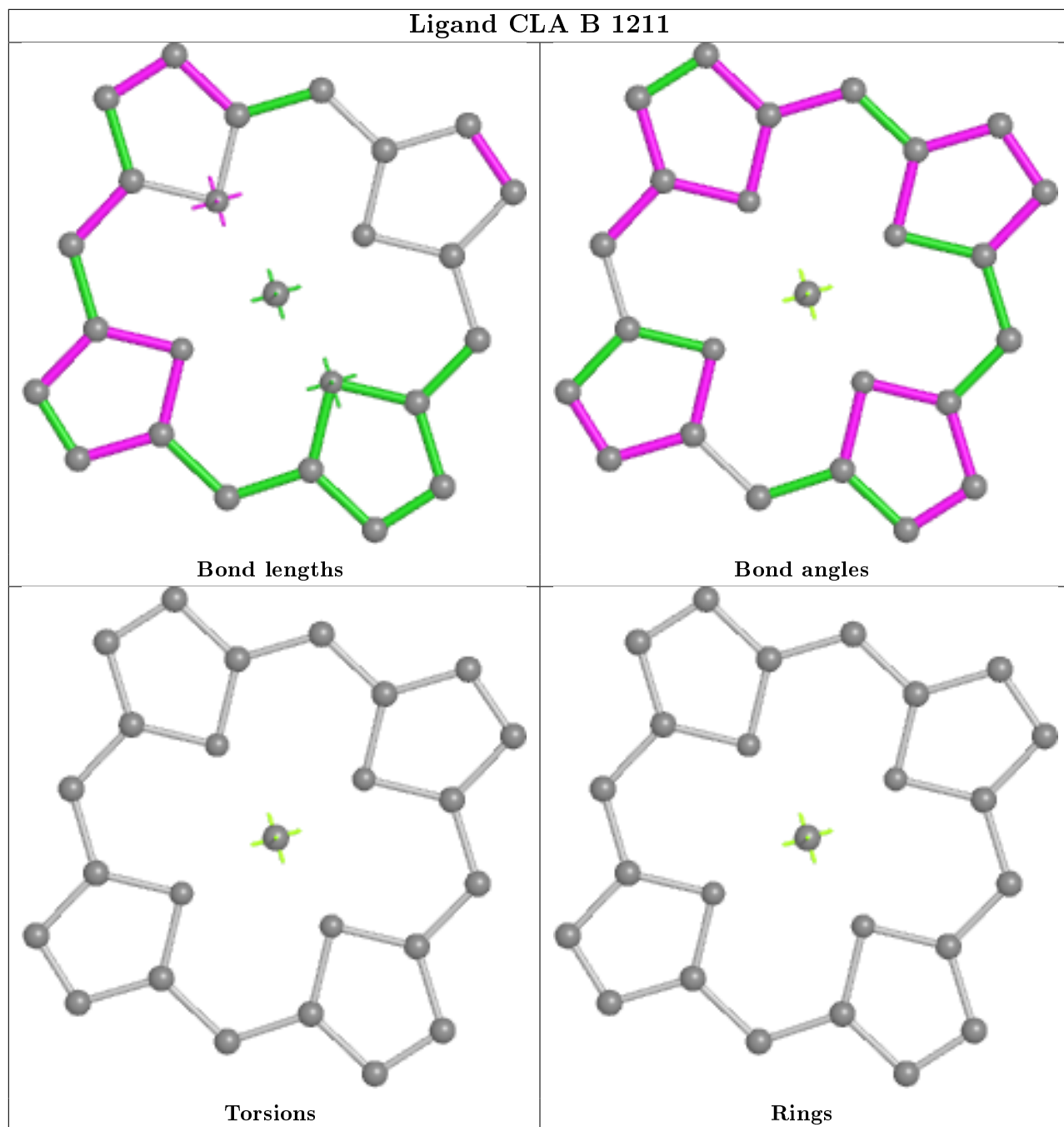


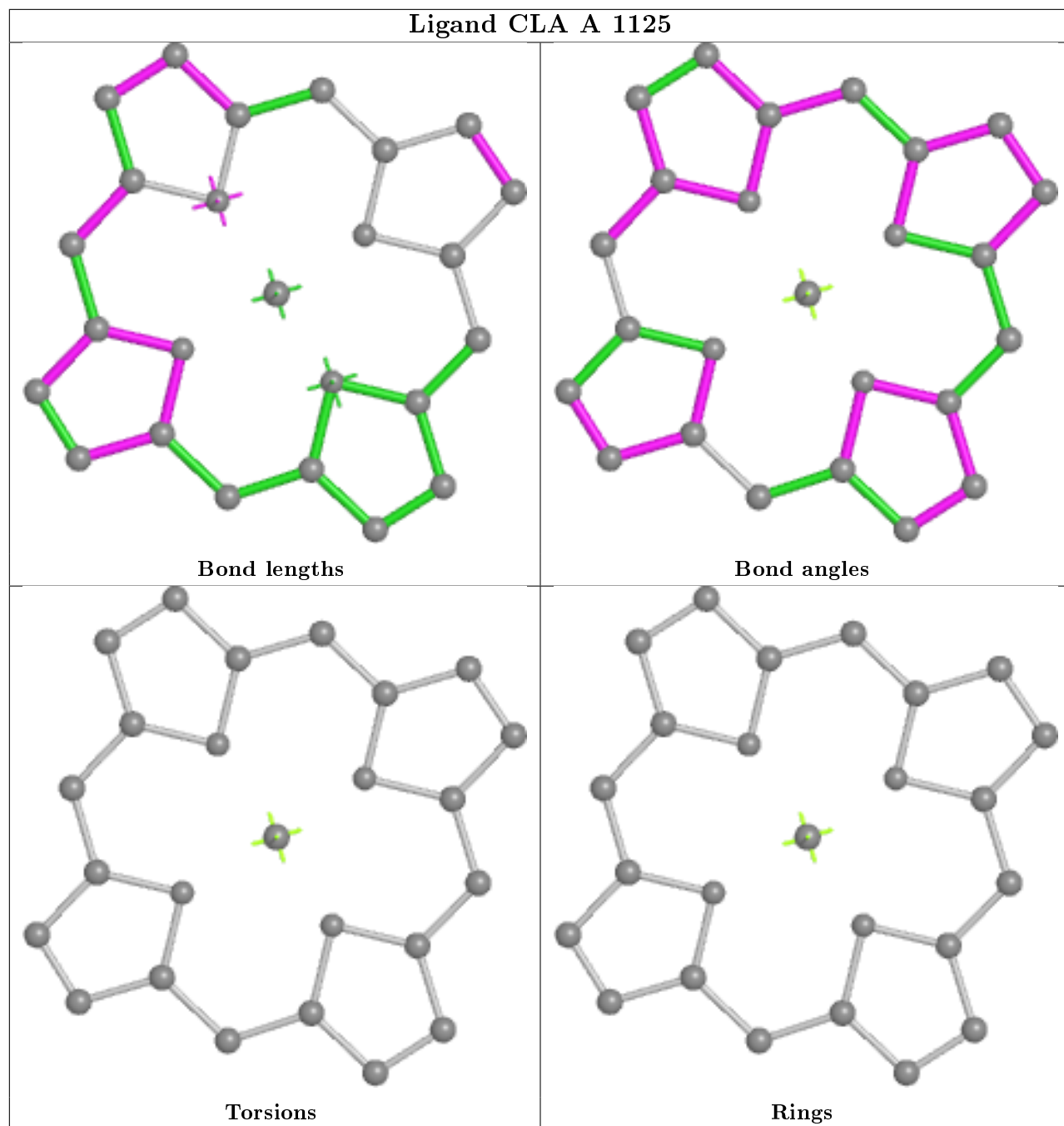


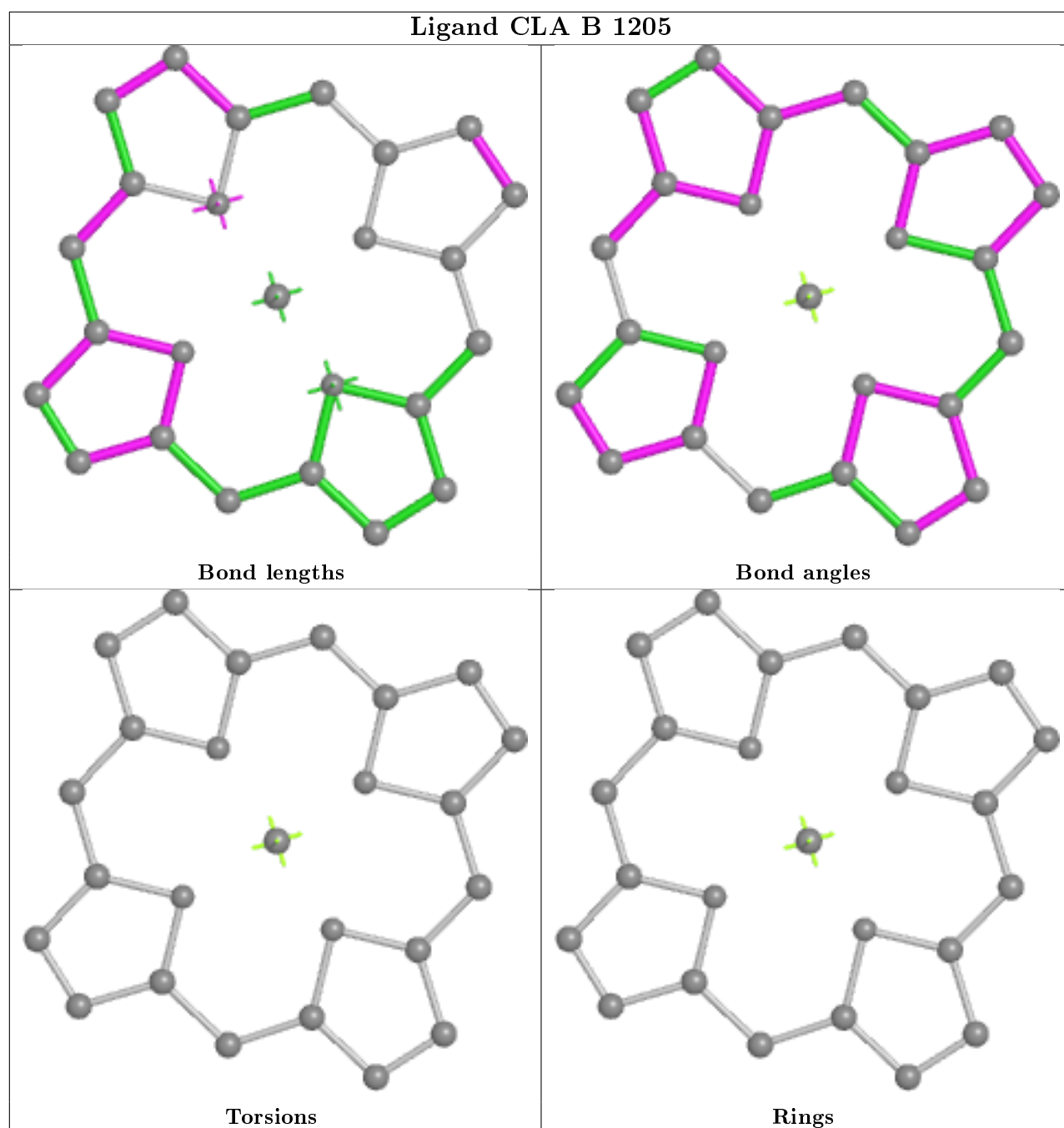












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	2	144/222 (64%)	0.11	13 (9%) 9 8	118, 215, 376, 389	0
1	3	150/222 (67%)	-0.07	13 (8%) 10 9	117, 198, 289, 310	0
2	4	116/214 (54%)	0.21	13 (11%) 5 5	169, 252, 362, 412	0
3	A	740/740 (100%)	-0.34	20 (2%) 54 44	40, 129, 195, 255	0
4	B	725/725 (100%)	0.23	72 (9%) 7 7	101, 201, 318, 438	0
5	C	80/80 (100%)	0.19	8 (10%) 7 7	113, 162, 221, 292	0
6	D	124/124 (100%)	0.22	18 (14%) 2 3	132, 186, 251, 415	0
7	E	69/69 (100%)	0.33	5 (7%) 15 12	138, 189, 265, 445	0
8	F	153/155 (98%)	-0.40	3 (1%) 65 56	117, 180, 248, 265	0
9	I	32/32 (100%)	-0.27	0 100 100	184, 254, 380, 425	0
10	J	38/38 (100%)	-0.73	0 100 100	88, 121, 212, 234	0
11	K	47/47 (100%)	-0.70	1 (2%) 63 54	132, 172, 260, 291	0
12	L	140/140 (100%)	0.62	27 (19%) 1 1	156, 233, 383, 404	0
13	M	29/29 (100%)	0.19	0 100 100	177, 247, 271, 276	0
14	O	98/98 (100%)	-0.32	3 (3%) 49 38	212, 278, 405, 427	0
All	All	2685/2935 (91%)	-0.02	196 (7%) 15 12	40, 183, 328, 445	0

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	30	SER	12.1
4	B	158	LYS	11.4
4	B	157	PRO	10.4
4	B	130	ASN	10.0
12	L	75	TYR	9.7

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CLA	3	608	25/65	0.24	0.45	298,335,354,361	0
15	CLA	3	603	25/65	0.33	0.54	246,261,286,294	0
15	CLA	B	1217	25/65	0.48	0.49	231,256,273,279	0
15	CLA	4	602	25/65	0.50	0.42	496,534,558,558	0
15	CLA	B	1227	25/65	0.50	0.76	211,262,292,303	0
15	CLA	4	601	25/65	0.55	0.24	182,213,243,269	0
15	CLA	B	1209	25/65	0.62	0.34	235,264,283,284	0
15	CLA	B	1218	25/65	0.62	0.98	300,335,347,356	0
18	BCR	B	4008	40/40	0.62	0.55	172,230,254,261	0
18	BCR	A	4007	40/40	0.66	0.55	60,129,164,195	0
15	CLA	B	1223	25/65	0.66	0.44	233,265,282,284	0
15	CLA	B	1212	25/65	0.66	0.36	184,204,223,230	0
15	CLA	4	615	25/65	0.67	0.25	236,276,298,305	0
18	BCR	A	4008	40/40	0.67	0.62	48,114,172,181	0
15	CLA	O	1602	25/65	0.68	0.44	303,330,344,350	0
15	CLA	4	608	25/65	0.69	0.27	343,352,370,376	0
15	CLA	4	611	25/65	0.69	0.73	216,237,248,253	0
15	CLA	B	1214	25/65	0.69	0.82	274,296,313,326	0
15	CLA	B	1208	25/65	0.70	0.30	203,267,283,288	0
15	CLA	4	609	25/65	0.70	0.37	252,286,299,301	0
16	PQN	B	2002	33/33	0.70	0.97	126,151,167,174	0
15	CLA	2	616	25/65	0.70	0.61	150,192,224,226	0
15	CLA	2	611	25/65	0.71	0.25	183,236,260,270	0
15	CLA	B	1221	25/65	0.72	0.70	178,214,233,234	0
15	CLA	B	1207	25/65	0.72	0.40	262,286,303,307	0
15	CLA	B	1216	25/65	0.72	1.01	337,368,376,377	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	CLA	3	611	25/65	0.72	0.17	118,182,201,208	0
15	CLA	4	604	25/65	0.72	0.33	156,208,225,230	0
18	BCR	I	4018	40/40	0.72	0.54	82,148,219,223	0
15	CLA	B	1231	25/65	0.73	0.27	247,265,279,286	0
15	CLA	2	615	25/65	0.74	0.16	232,276,300,304	0
15	CLA	O	1603	25/65	0.74	0.42	179,204,218,223	0
15	CLA	O	1601	25/65	0.74	0.26	333,342,346,354	0
15	CLA	B	1210	25/65	0.74	0.31	227,262,274,291	0
15	CLA	B	1236	45/65	0.75	0.36	123,190,211,222	0
15	CLA	2	613	25/65	0.75	0.30	182,222,233,242	0
15	CLA	2	601	25/65	0.75	0.25	164,206,231,233	0
15	CLA	L	1502	25/65	0.77	0.21	146,181,197,213	0
18	BCR	A	4011	40/40	0.78	0.50	51,112,139,162	0
15	CLA	2	603	25/65	0.78	0.21	157,184,202,206	0
15	CLA	A	1129	25/65	0.78	0.28	142,179,197,200	0
15	CLA	3	612	25/65	0.79	0.26	163,188,205,220	0
18	BCR	A	4017	40/40	0.80	0.68	86,164,194,202	0
15	CLA	4	610	25/65	0.80	0.17	157,182,206,213	0
15	CLA	3	607	25/65	0.80	0.27	213,230,253,258	0
15	CLA	K	1402	25/65	0.80	0.17	139,167,192,202	0
15	CLA	2	606	25/65	0.80	0.24	191,219,239,244	0
15	CLA	B	1232	65/65	0.80	0.34	128,185,220,230	0
15	CLA	4	616	25/65	0.80	0.29	189,214,233,237	0
18	BCR	B	4005	40/40	0.81	0.64	90,132,165,170	0
15	CLA	A	1137	25/65	0.81	0.34	71,135,157,165	0
15	CLA	3	602	25/65	0.81	0.16	135,182,210,216	0
15	CLA	B	1222	25/65	0.81	0.63	204,224,242,243	0
15	CLA	A	1011	50/65	0.81	0.43	98,141,159,202	0
15	CLA	B	1021	45/65	0.82	0.36	114,149,172,191	0
15	CLA	B	1219	25/65	0.82	0.14	159,177,201,218	0
15	CLA	2	610	25/65	0.82	0.21	164,216,237,243	0
15	CLA	B	1220	25/65	0.83	0.56	197,228,243,255	0
15	CLA	2	604	25/65	0.83	0.22	139,163,200,206	0
15	CLA	B	1023	50/65	0.83	0.45	88,147,172,183	0
15	CLA	3	614	25/65	0.83	0.33	104,155,182,201	0
15	CLA	F	1302	25/65	0.83	0.21	186,229,263,264	0
15	CLA	K	1401	25/65	0.83	0.19	151,187,207,218	0
15	CLA	B	1225	50/65	0.83	0.33	89,228,243,267	0
15	CLA	B	1234	25/65	0.83	0.36	228,248,256,260	0
15	CLA	A	1119	25/65	0.83	0.30	110,152,178,187	0
15	CLA	B	1226	55/65	0.83	0.34	72,163,196,199	0
15	CLA	3	601	25/65	0.83	0.23	144,196,210,234	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CLA	4	606	25/65	0.84	0.15	161,216,236,250	0
15	CLA	A	1101	45/65	0.84	0.27	62,120,151,173	0
15	CLA	B	1224	55/65	0.84	0.38	174,218,261,270	0
15	CLA	2	607	25/65	0.84	0.17	159,202,220,235	0
15	CLA	A	1123	25/65	0.84	0.26	90,121,141,147	0
15	CLA	4	612	25/65	0.84	0.21	87,127,149,161	0
15	CLA	2	608	25/65	0.85	0.90	188,210,232,242	0
15	CLA	A	1116	55/65	0.85	0.29	42,90,116,124	0
15	CLA	A	1110	25/65	0.85	0.30	139,192,211,225	0
15	CLA	L	1501	25/65	0.85	0.14	151,182,196,207	0
15	CLA	A	1120	25/65	0.85	0.38	109,183,229,234	0
16	PQN	A	2001	33/33	0.85	0.39	36,100,136,159	0
15	CLA	A	1121	25/65	0.85	0.26	105,146,174,178	0
15	CLA	B	1204	25/65	0.85	0.26	259,286,298,310	0
15	CLA	B	1211	25/65	0.85	0.18	166,183,201,217	0
18	BCR	A	4002	40/40	0.86	0.66	29,93,126,132	0
15	CLA	A	1138	25/65	0.86	0.53	107,137,164,202	0
15	CLA	A	1012	55/65	0.86	0.29	67,145,178,191	0
15	CLA	2	614	25/65	0.86	0.28	181,245,252,253	0
15	CLA	3	606	25/65	0.86	0.49	172,210,242,250	0
15	CLA	A	1136	25/65	0.86	0.29	87,161,186,206	0
15	CLA	A	1103	55/65	0.86	0.29	48,92,121,124	0
15	CLA	3	604	25/65	0.87	0.32	189,234,254,266	0
15	CLA	A	1013	55/65	0.87	0.33	45,141,172,184	0
15	CLA	B	1022	25/65	0.87	0.32	106,141,159,178	0
15	CLA	B	1206	25/65	0.87	0.21	148,173,194,203	0
15	CLA	A	1112	25/65	0.87	0.22	97,124,135,141	0
15	CLA	A	1133	25/65	0.87	0.29	127,167,194,209	0
15	CLA	A	1109	25/65	0.87	0.17	55,102,136,154	0
15	CLA	B	1228	25/65	0.87	0.16	132,186,206,213	0
15	CLA	L	1503	25/65	0.88	0.31	237,249,262,268	0
15	CLA	B	1238	25/65	0.88	0.23	103,134,162,167	0
15	CLA	A	1131	45/65	0.88	0.23	57,87,101,121	0
15	CLA	B	1202	25/65	0.88	0.18	128,158,167,172	0
15	CLA	2	612	25/65	0.88	0.24	142,175,184,189	0
15	CLA	A	1130	55/65	0.88	0.37	121,209,233,235	0
15	CLA	B	1237	55/65	0.88	0.40	82,150,181,203	0
15	CLA	A	1139	25/65	0.88	0.24	91,143,148,161	0
15	CLA	B	1205	25/65	0.88	0.27	260,280,296,302	0
15	CLA	A	1118	25/65	0.89	0.30	155,183,211,214	0
15	CLA	A	1134	25/65	0.89	0.16	96,146,167,169	0
15	CLA	A	1135	25/65	0.89	0.22	101,119,157,168	0

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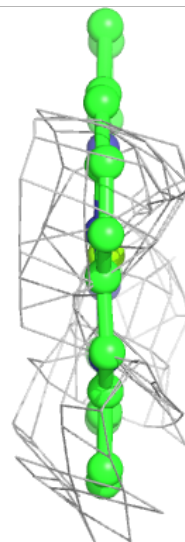
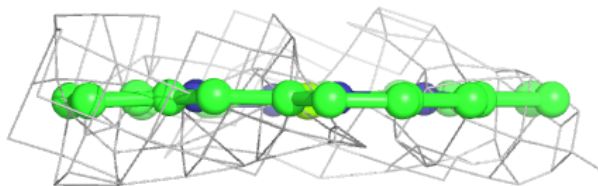
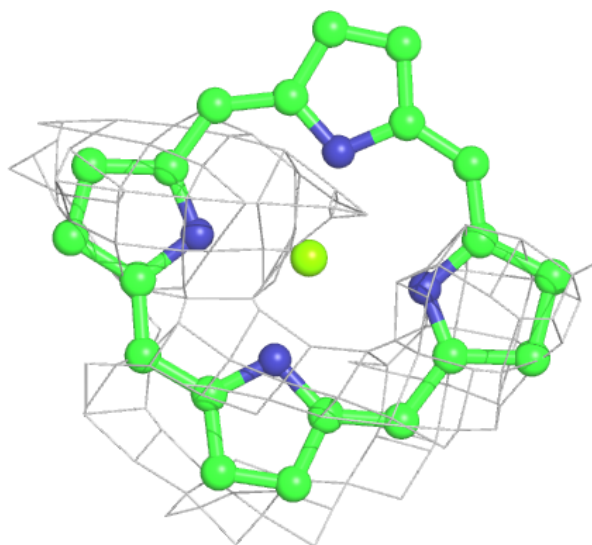
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CLA	A	1117	55/65	0.89	0.30	12,113,142,154	0
15	CLA	A	1105	55/65	0.89	0.25	39,125,150,190	0
15	CLA	A	1126	55/65	0.89	0.26	26,91,120,129	0
15	CLA	A	1132	25/65	0.89	0.28	69,121,152,153	0
15	CLA	A	1104	55/65	0.89	0.24	41,85,120,133	0
15	CLA	F	1301	45/65	0.89	0.26	96,146,168,177	0
15	CLA	B	1203	25/65	0.90	0.28	100,156,175,184	0
15	CLA	A	1106	55/65	0.90	0.29	61,117,147,168	0
15	CLA	B	1201	25/65	0.90	0.30	139,156,172,175	0
15	CLA	B	1235	25/65	0.90	0.25	105,137,154,160	0
15	CLA	B	1230	47/65	0.90	0.24	84,129,151,175	0
15	CLA	A	1108	25/65	0.90	0.17	45,123,143,151	0
15	CLA	A	1114	46/65	0.90	0.26	44,120,152,168	0
15	CLA	A	1141	25/65	0.90	0.22	145,178,193,196	0
15	CLA	2	602	25/65	0.91	0.10	132,169,184,193	0
15	CLA	J	1302	50/65	0.91	0.23	88,178,204,225	0
15	CLA	4	603	25/65	0.91	0.16	103,149,175,192	0
15	CLA	A	1127	25/65	0.91	0.18	0,57,91,97	0
15	CLA	A	1111	25/65	0.91	0.18	62,104,123,138	0
15	CLA	4	605	25/65	0.91	0.17	105,126,145,154	0
15	CLA	B	1239	25/65	0.91	0.30	131,149,167,170	0
15	CLA	B	1229	50/65	0.91	0.45	105,140,167,180	0
15	CLA	B	1215	25/65	0.91	0.21	134,189,204,215	0
15	CLA	2	605	25/65	0.92	0.15	88,123,137,147	0
15	CLA	A	1115	55/65	0.92	0.21	77,115,144,156	0
15	CLA	A	1128	25/65	0.92	0.30	46,72,86,89	0
15	CLA	A	1122	25/65	0.92	0.17	52,112,129,135	0
15	CLA	A	1125	25/65	0.92	0.19	14,51,82,84	0
15	CLA	A	1140	25/65	0.92	0.25	68,92,127,132	0
15	CLA	A	1102	25/65	0.93	0.26	58,103,120,128	0
15	CLA	A	1124	25/65	0.93	0.26	50,82,106,122	0
15	CLA	3	610	25/65	0.94	0.23	144,167,182,195	0
15	CLA	A	1107	55/65	0.94	0.28	55,115,172,216	0
15	CLA	A	1113	25/65	0.95	0.27	86,119,141,149	0
17	SF4	C	3002	8/8	0.96	0.20	137,166,186,216	0
17	SF4	A	3001	8/8	0.97	0.24	145,192,216,219	0
17	SF4	C	3003	8/8	0.98	0.24	117,158,186,198	0

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

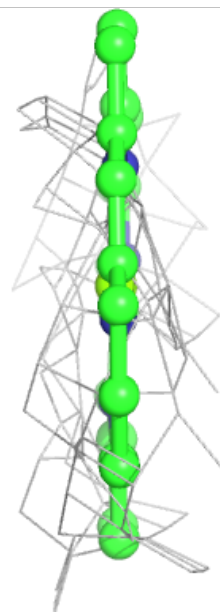
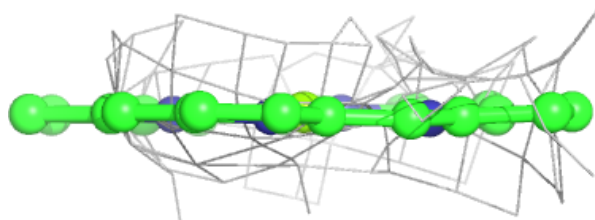
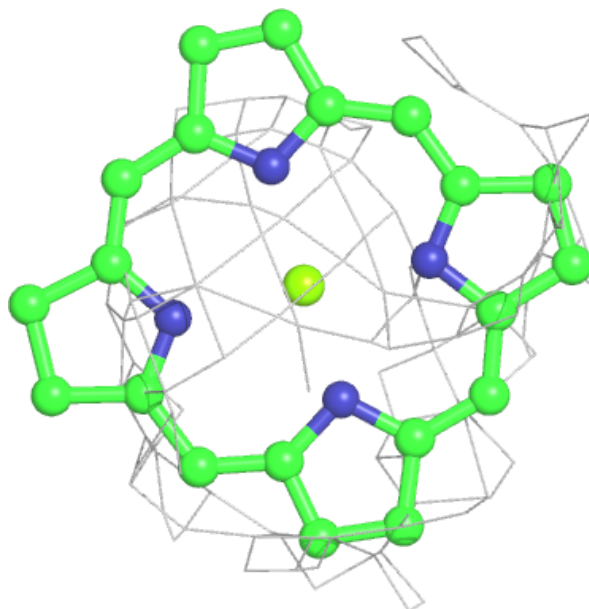
**Electron density around CLA 3 608:**

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



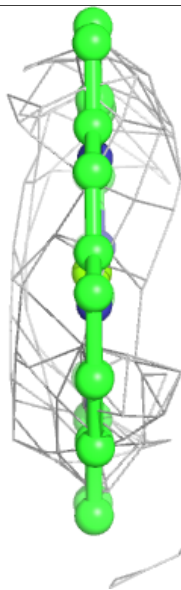
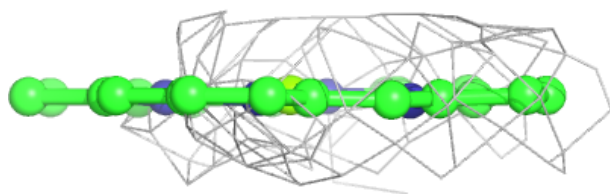
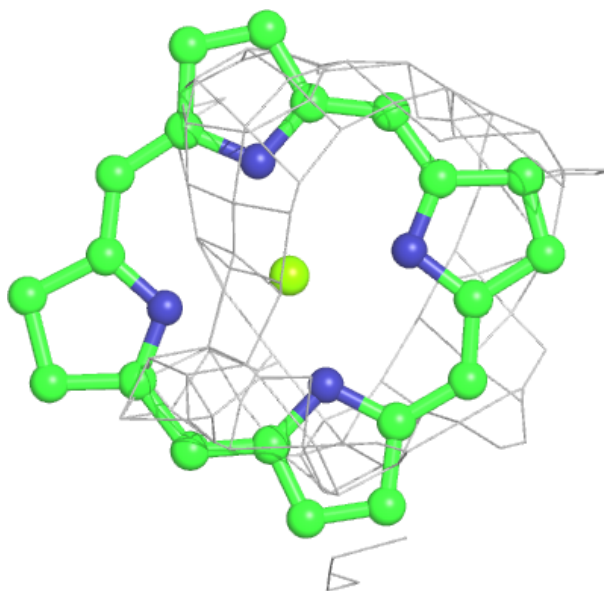
**Electron density around CLA 3 603:**

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and green (positive)



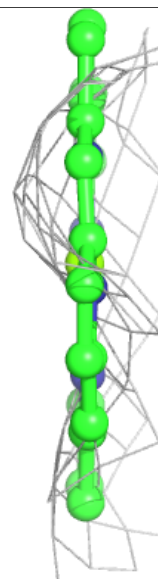
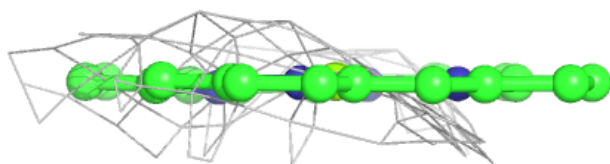
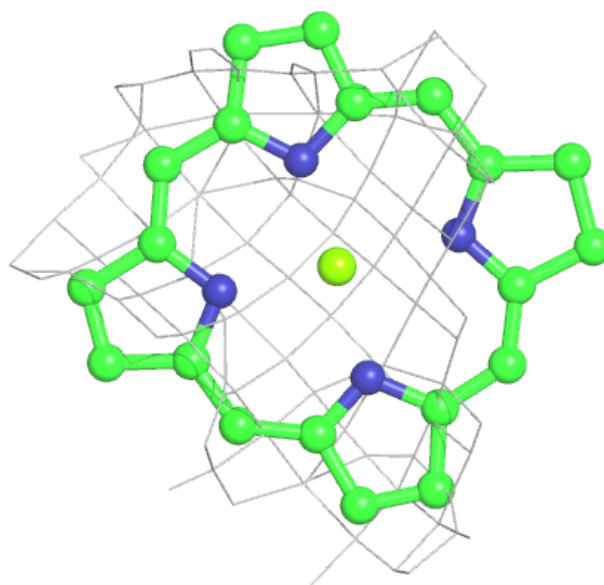
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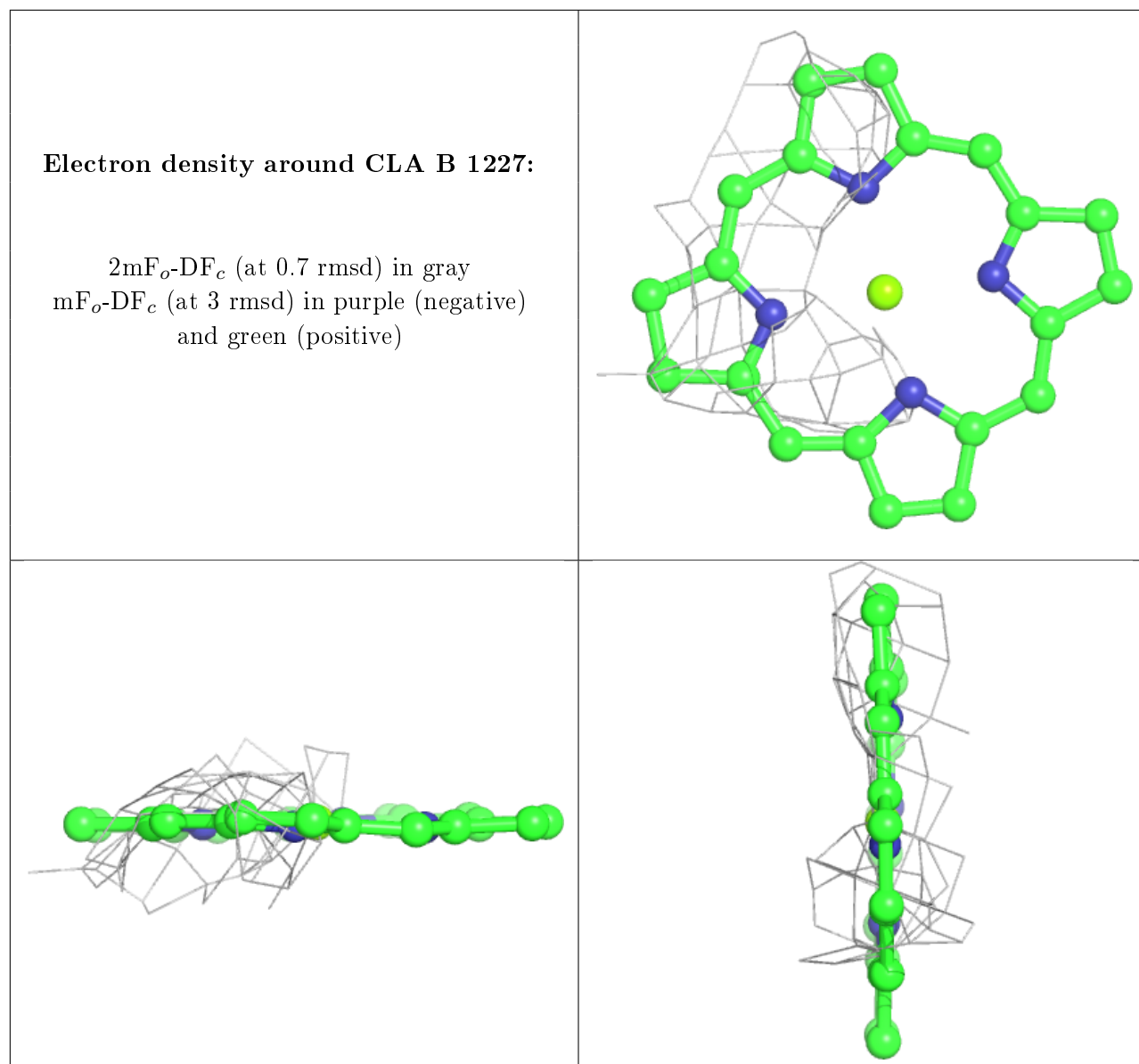
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and green (positive)



**Electron density around CLA 4 602:**

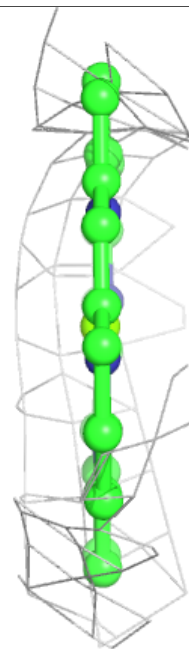
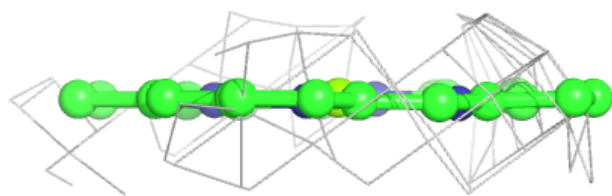
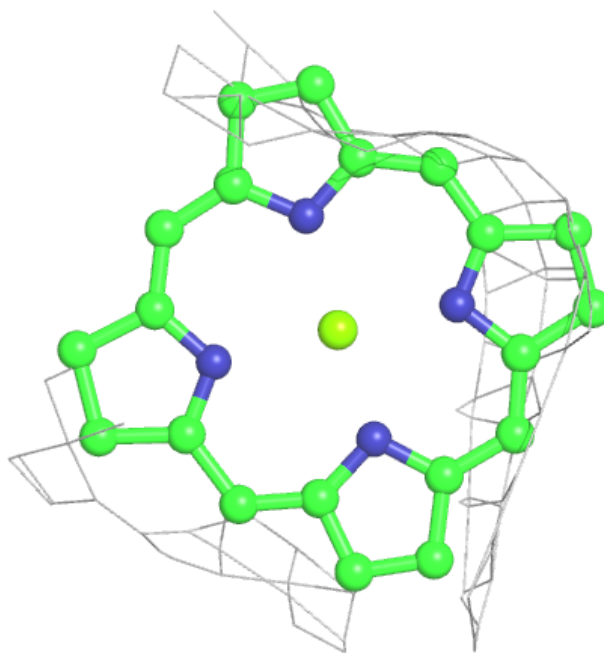
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

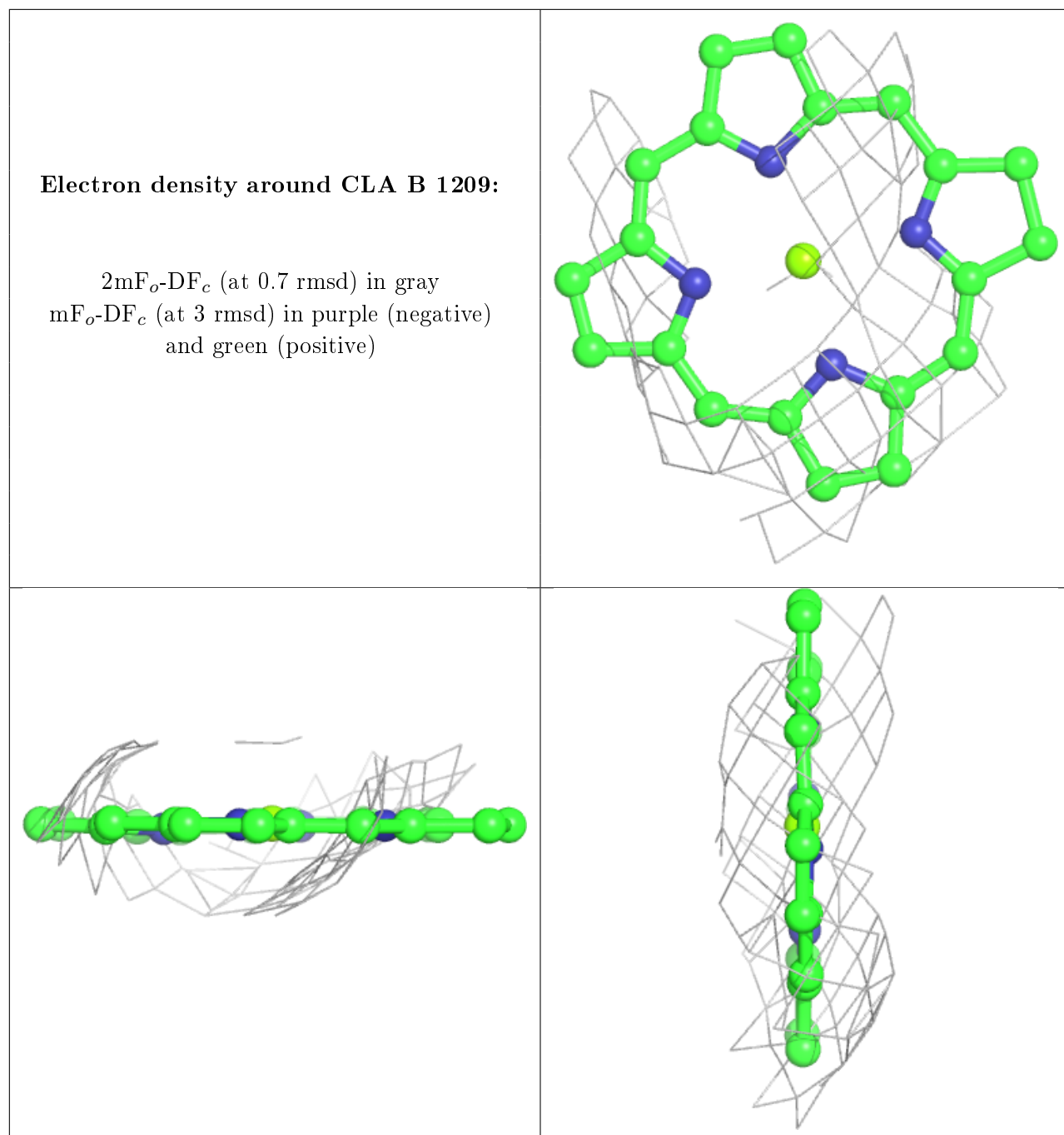




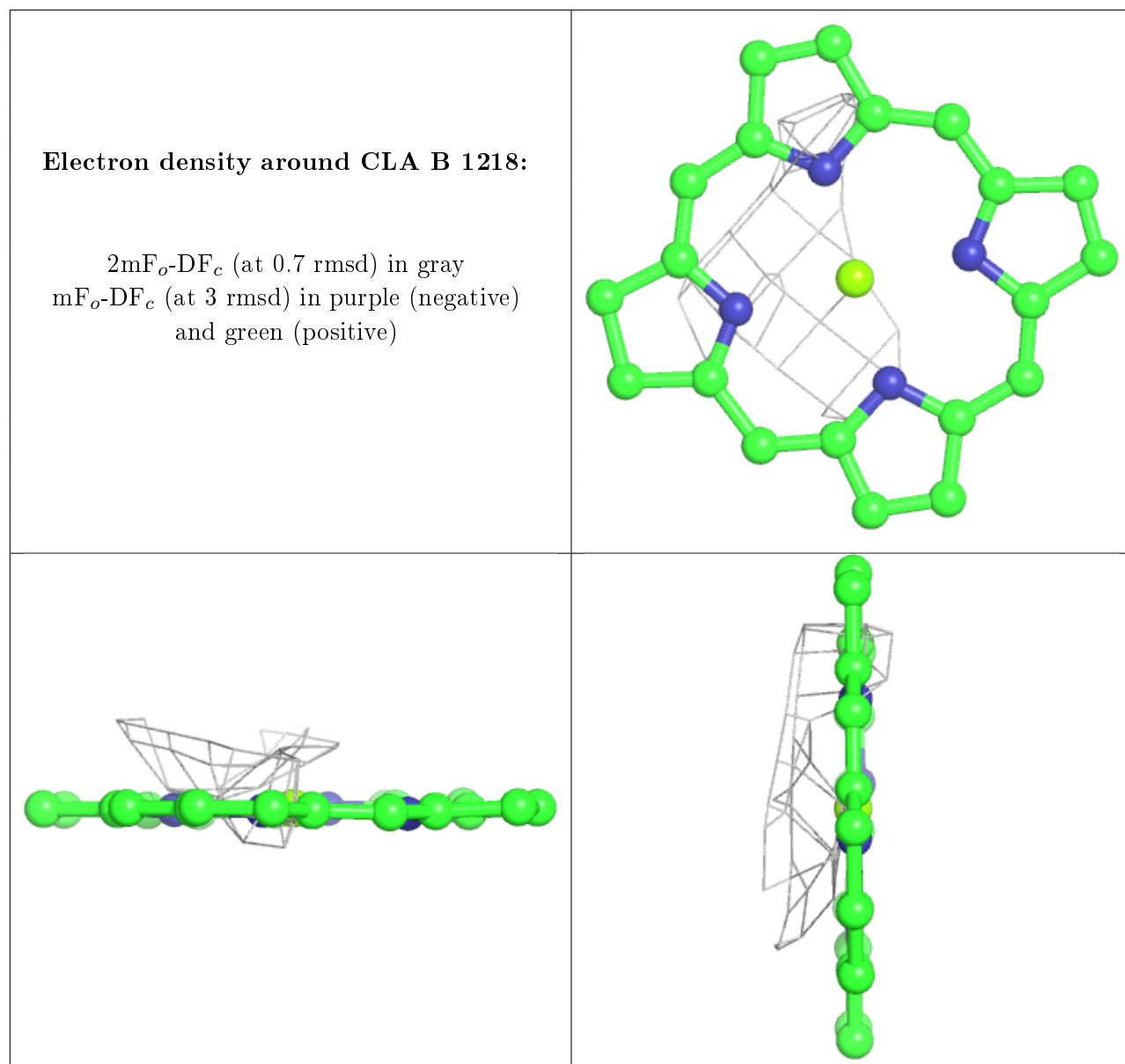
**Electron density around CLA 4 601:**

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



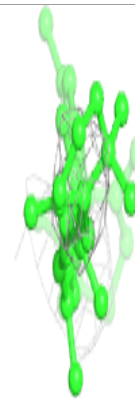
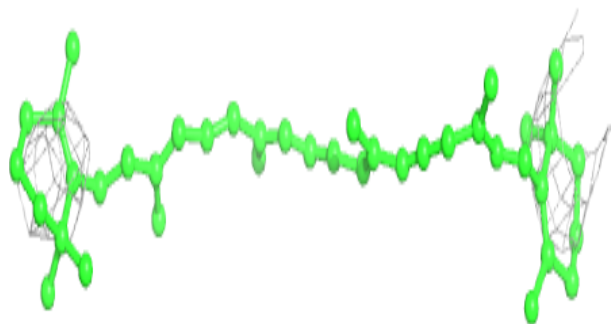
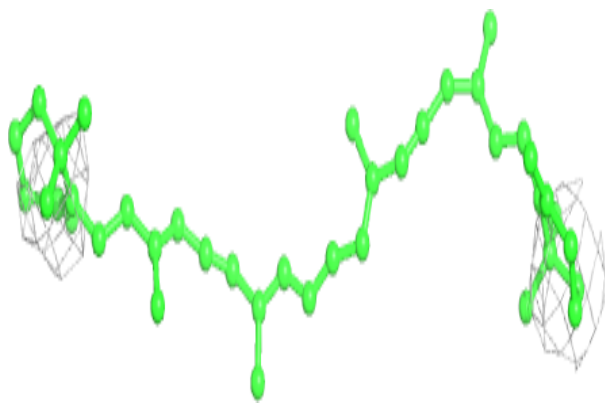




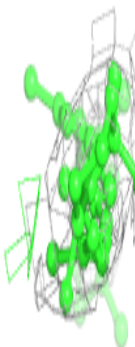
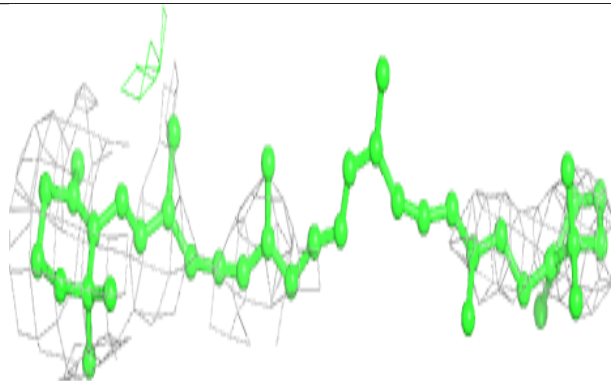
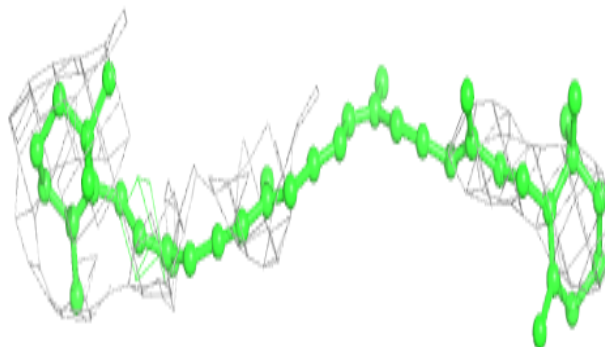


**Electron density around BCR B 4008:**

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

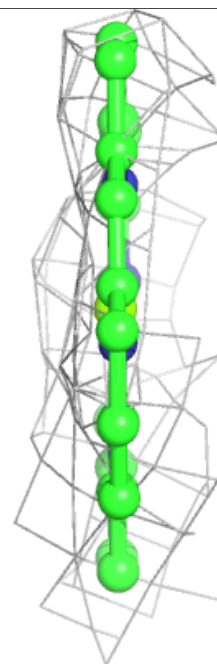
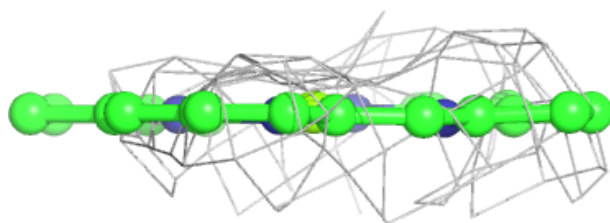
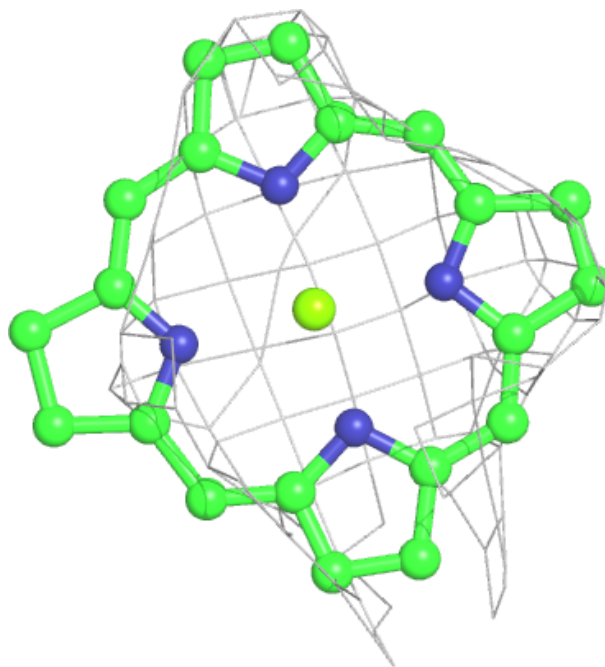
**Electron density around BCR A 4007:**

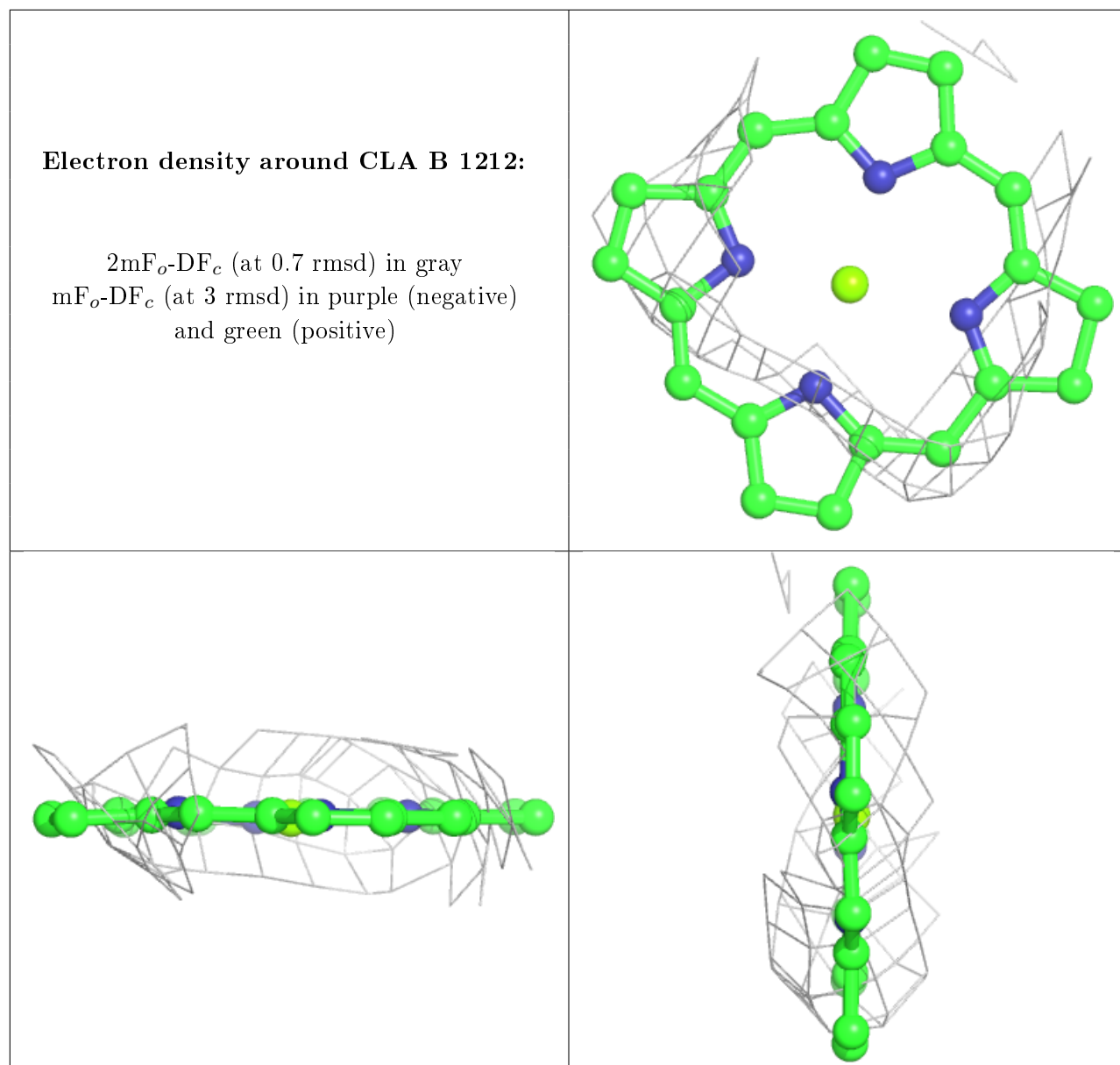
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1223:**

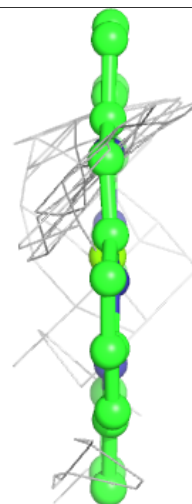
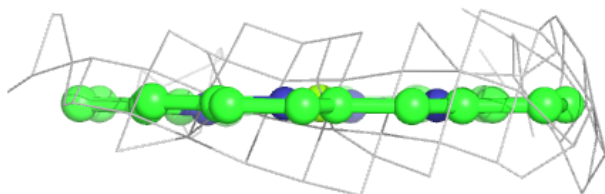
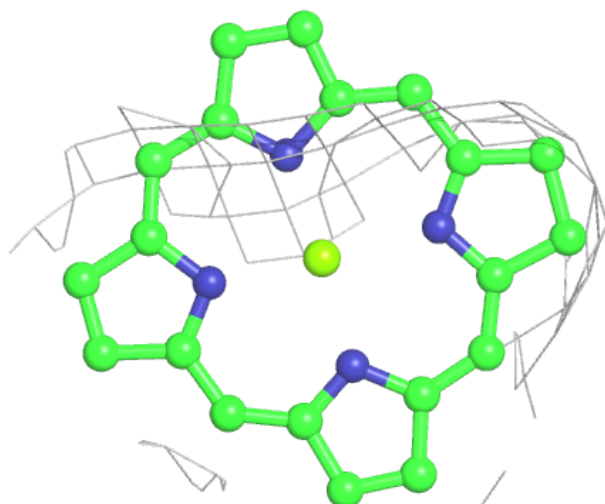
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

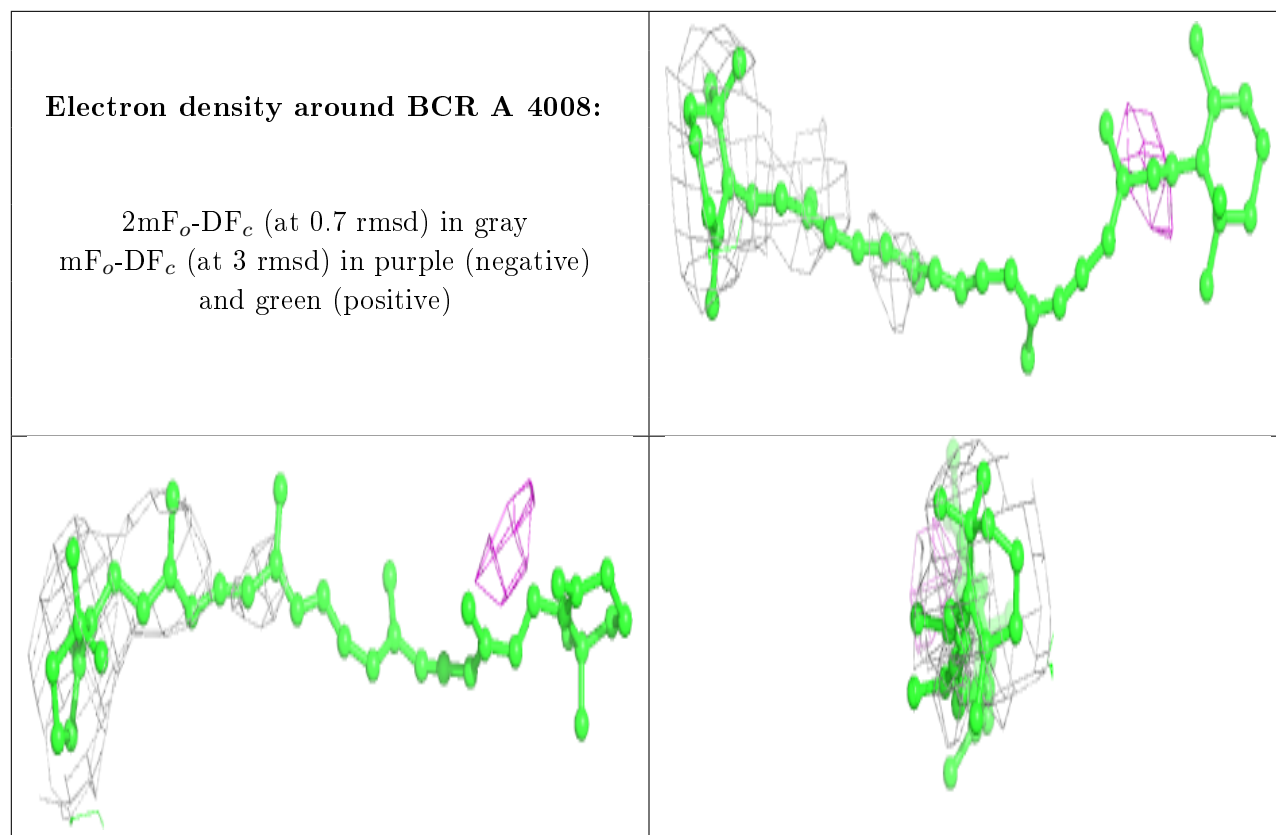




**Electron density around CLA 4 615:**

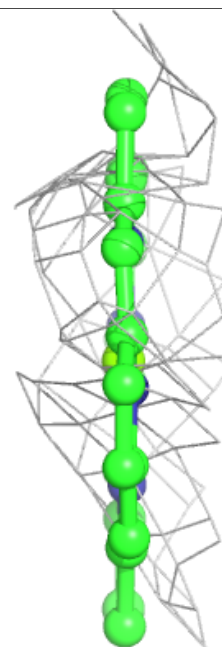
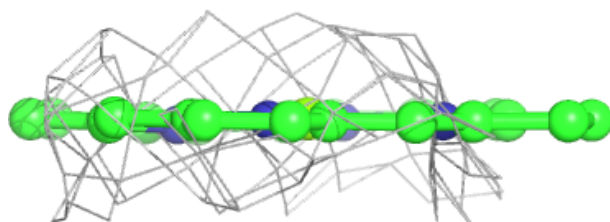
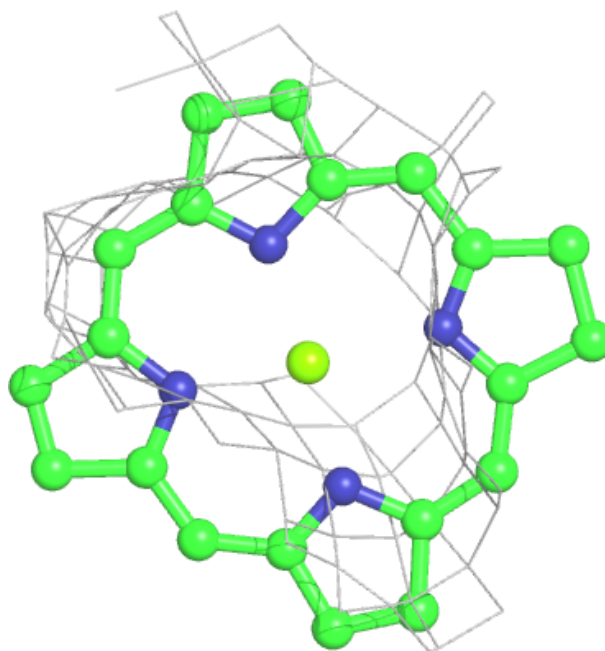
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





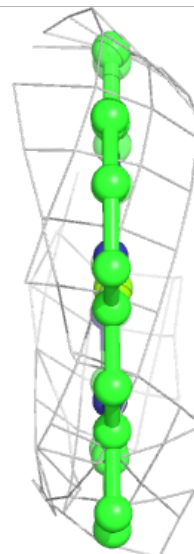
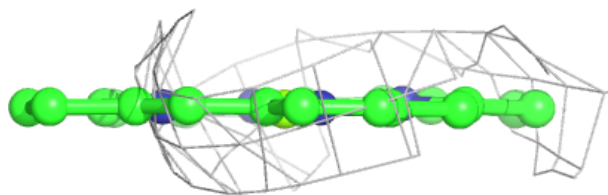
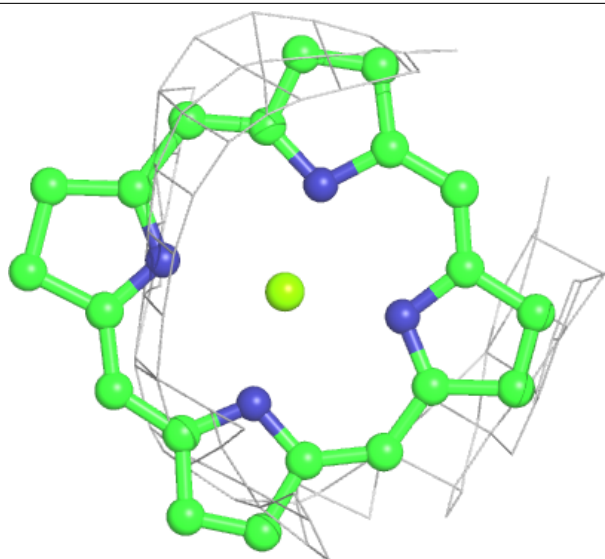
**Electron density around CLA O 1602:**

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



**Electron density around CLA 4 608:**

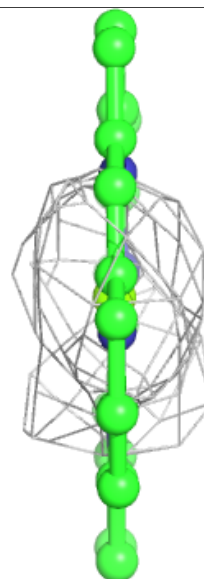
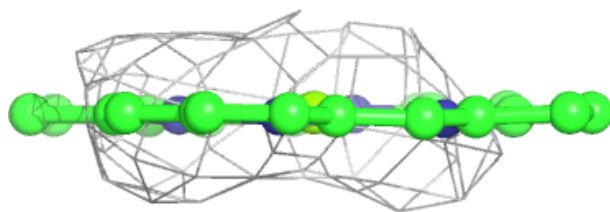
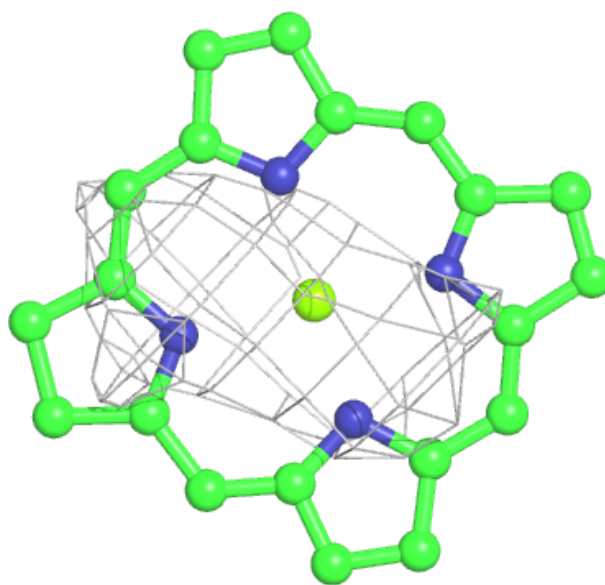
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

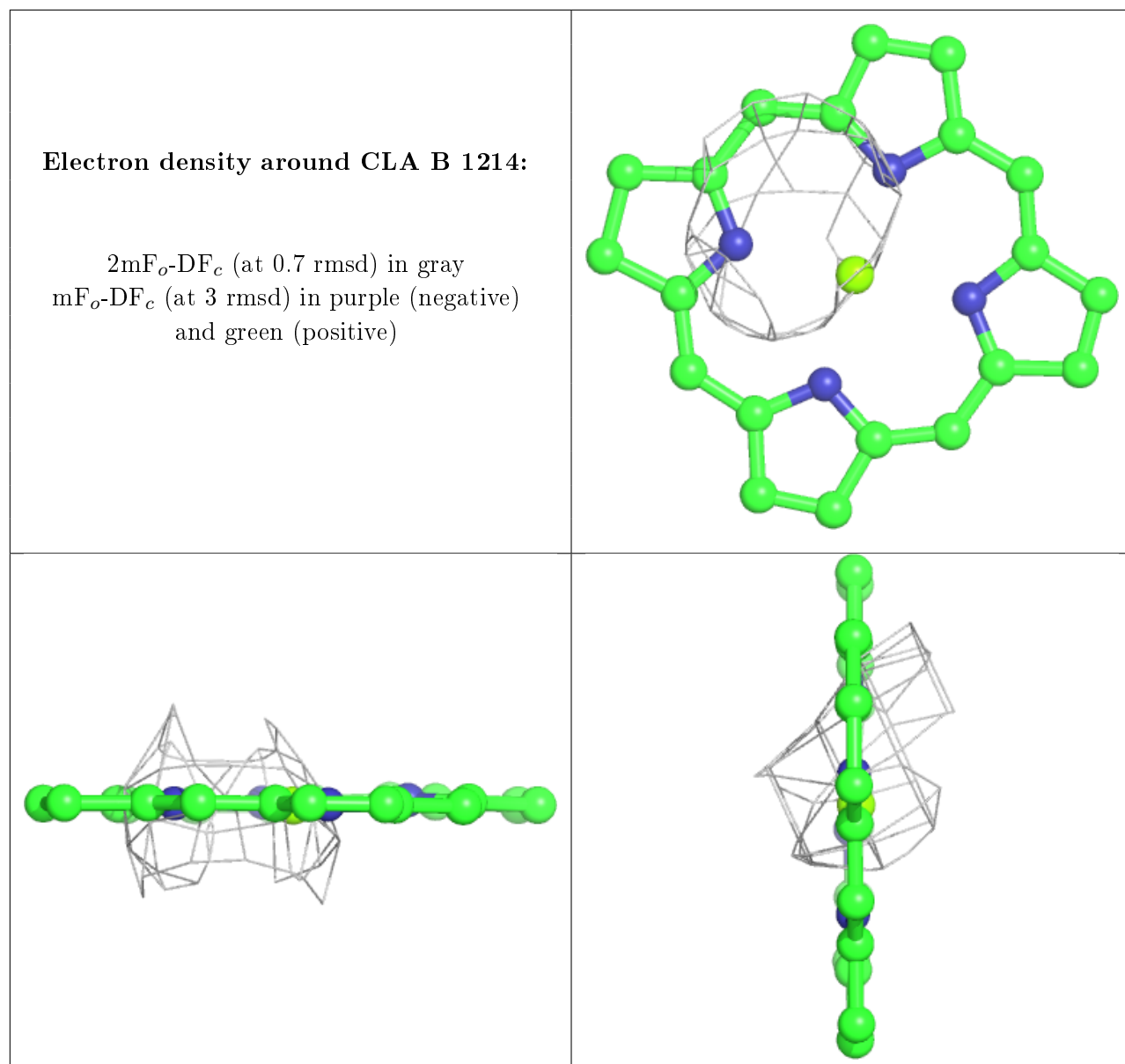




**Electron density around CLA 4 611:**

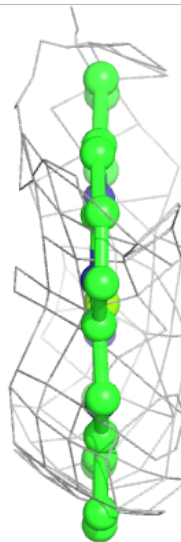
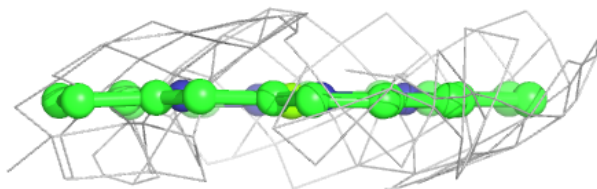
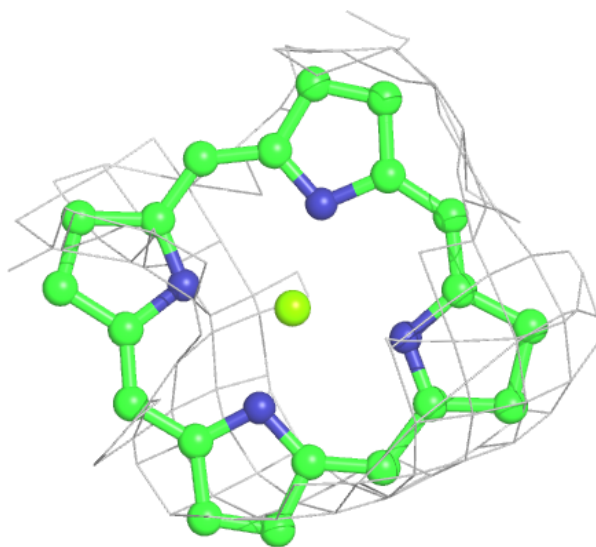
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





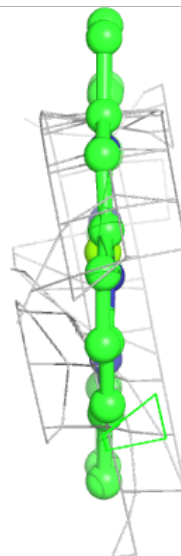
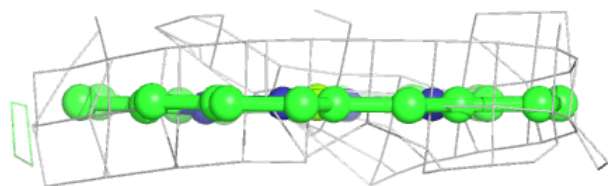
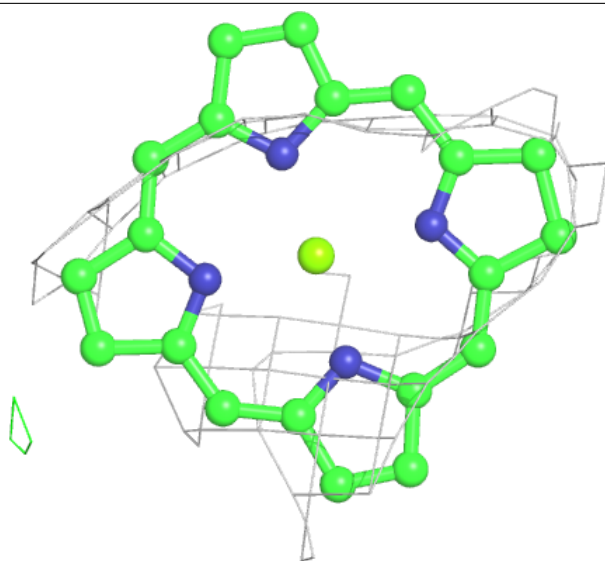
**Electron density around CLA B 1208:**

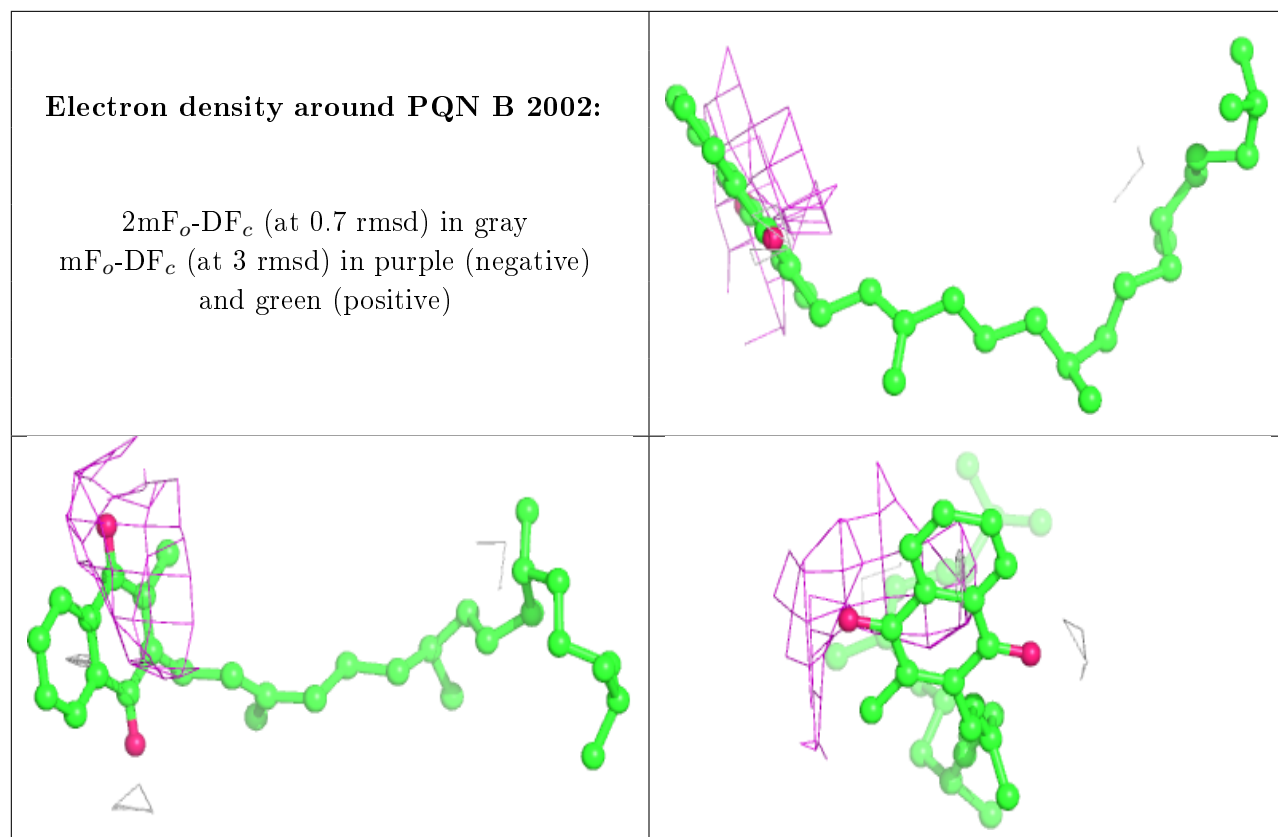
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 609:**

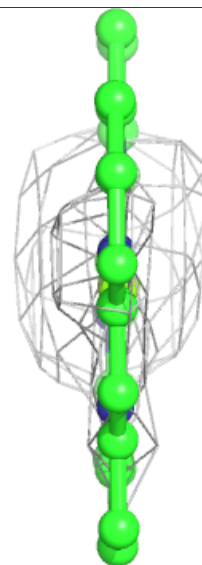
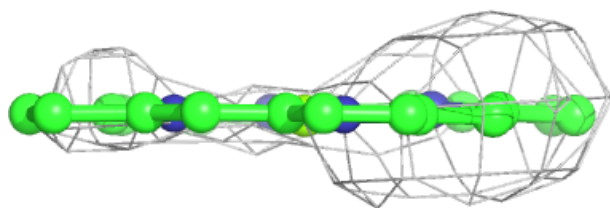
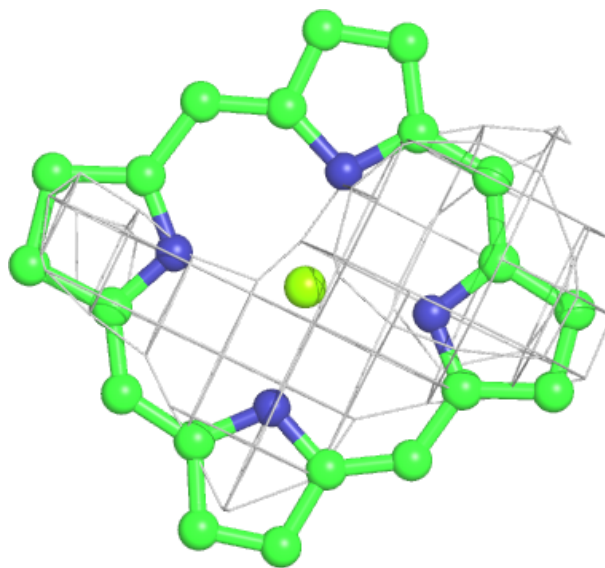
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





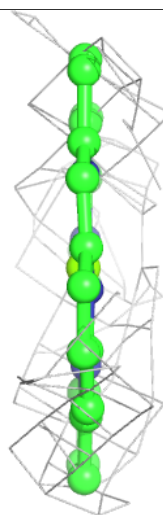
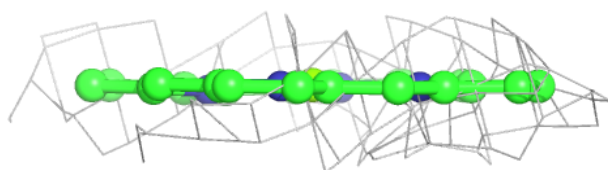
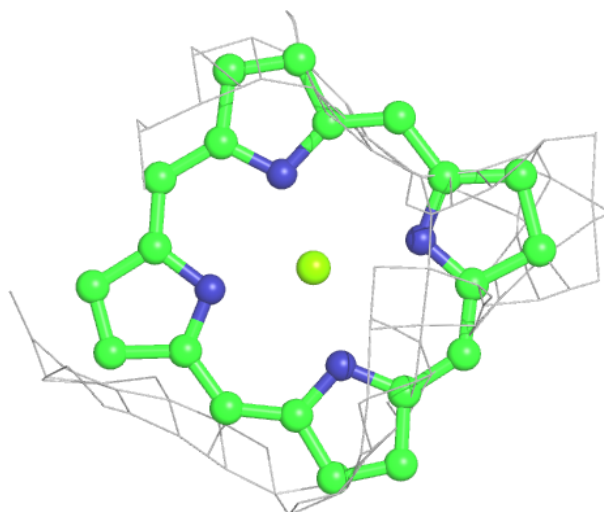
**Electron density around CLA 2 616:**

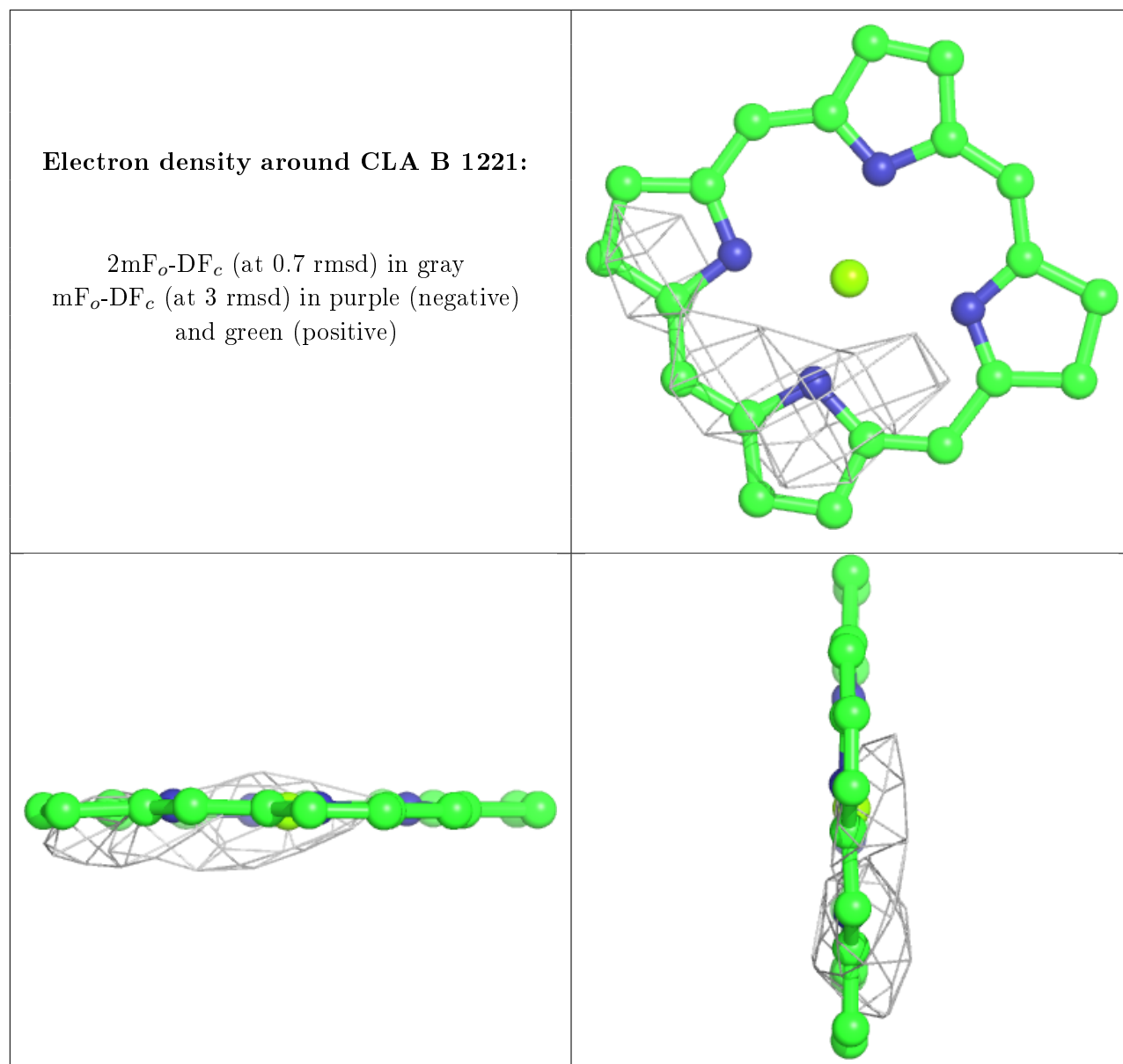
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 2 611:**

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

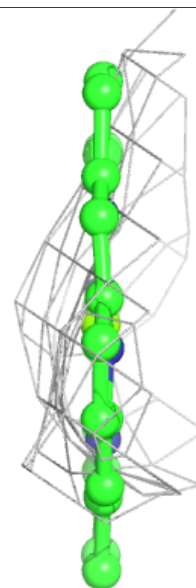
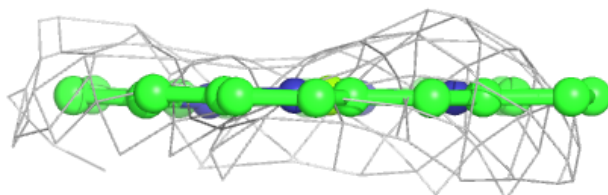
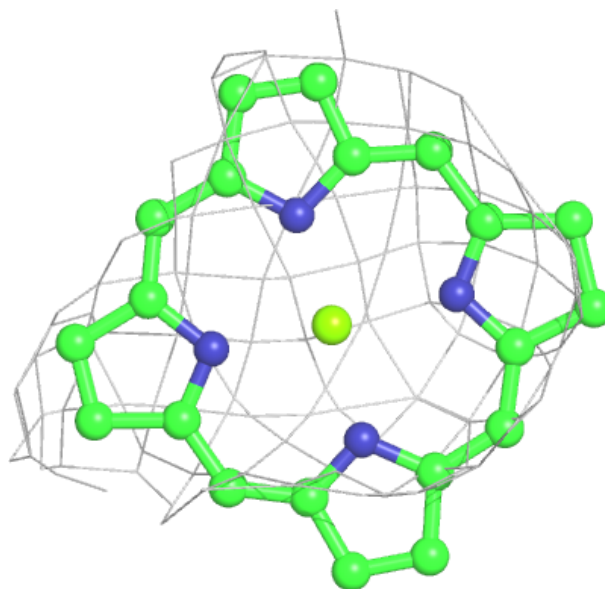


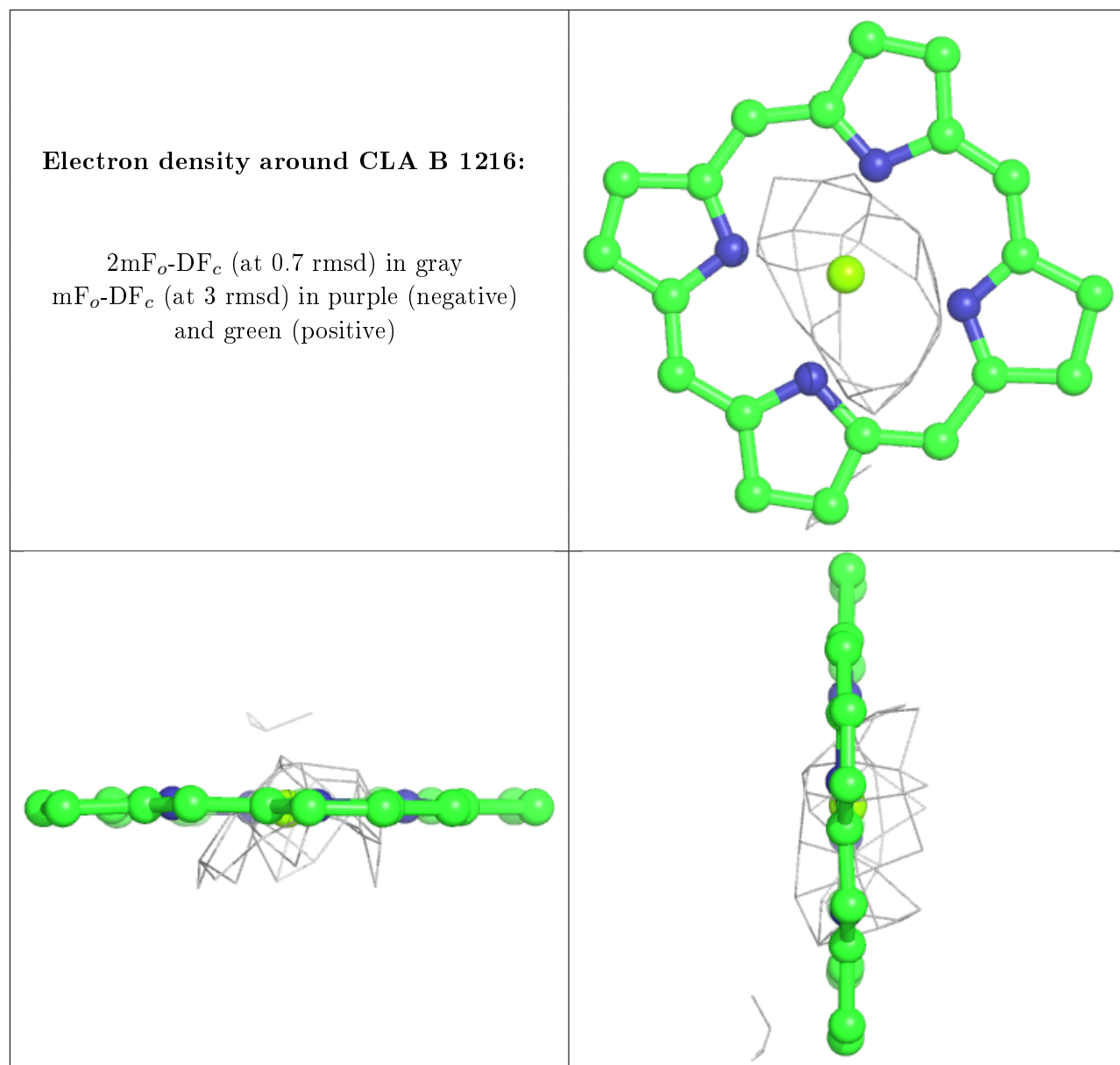




**Electron density around CLA B 1207:**

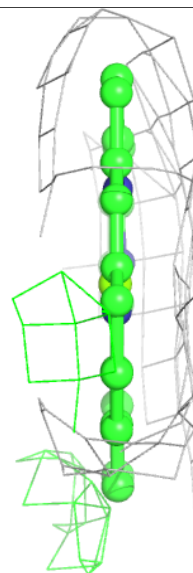
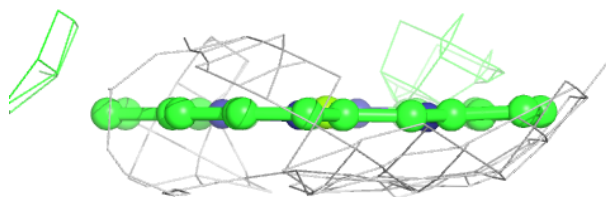
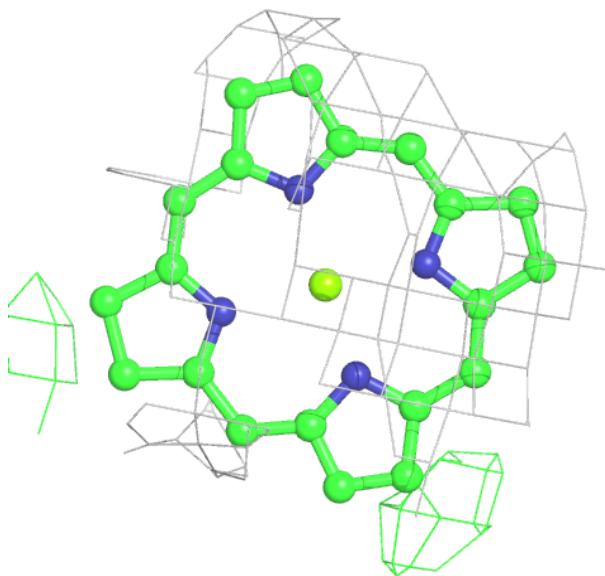
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





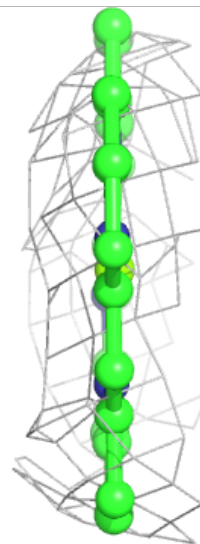
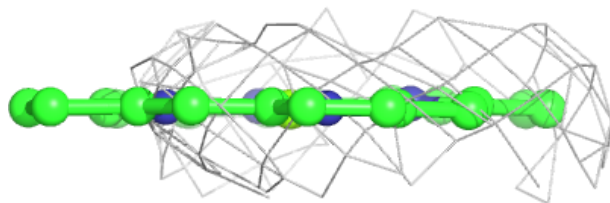
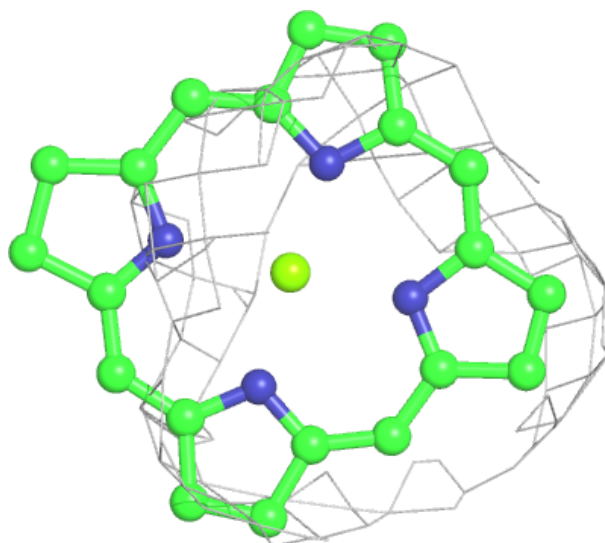
**Electron density around CLA 3 611:**

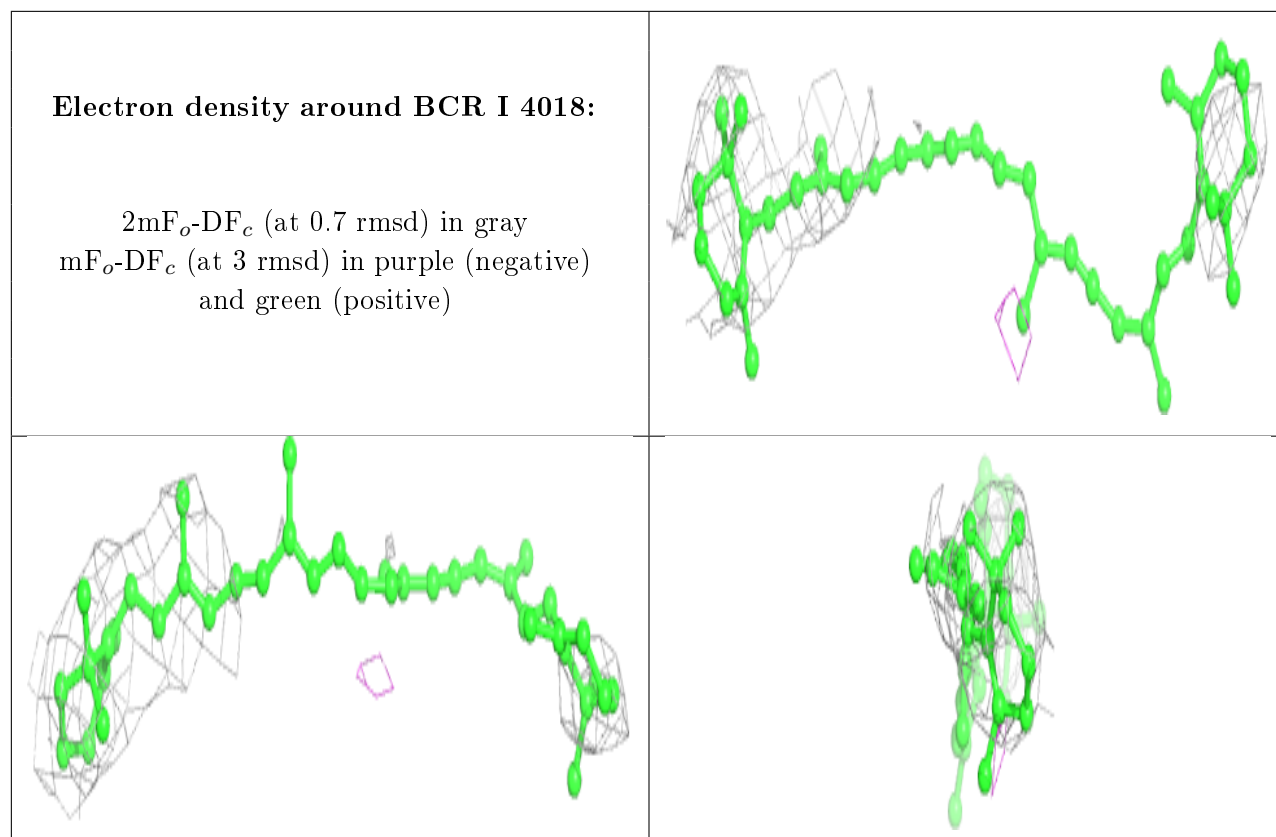
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

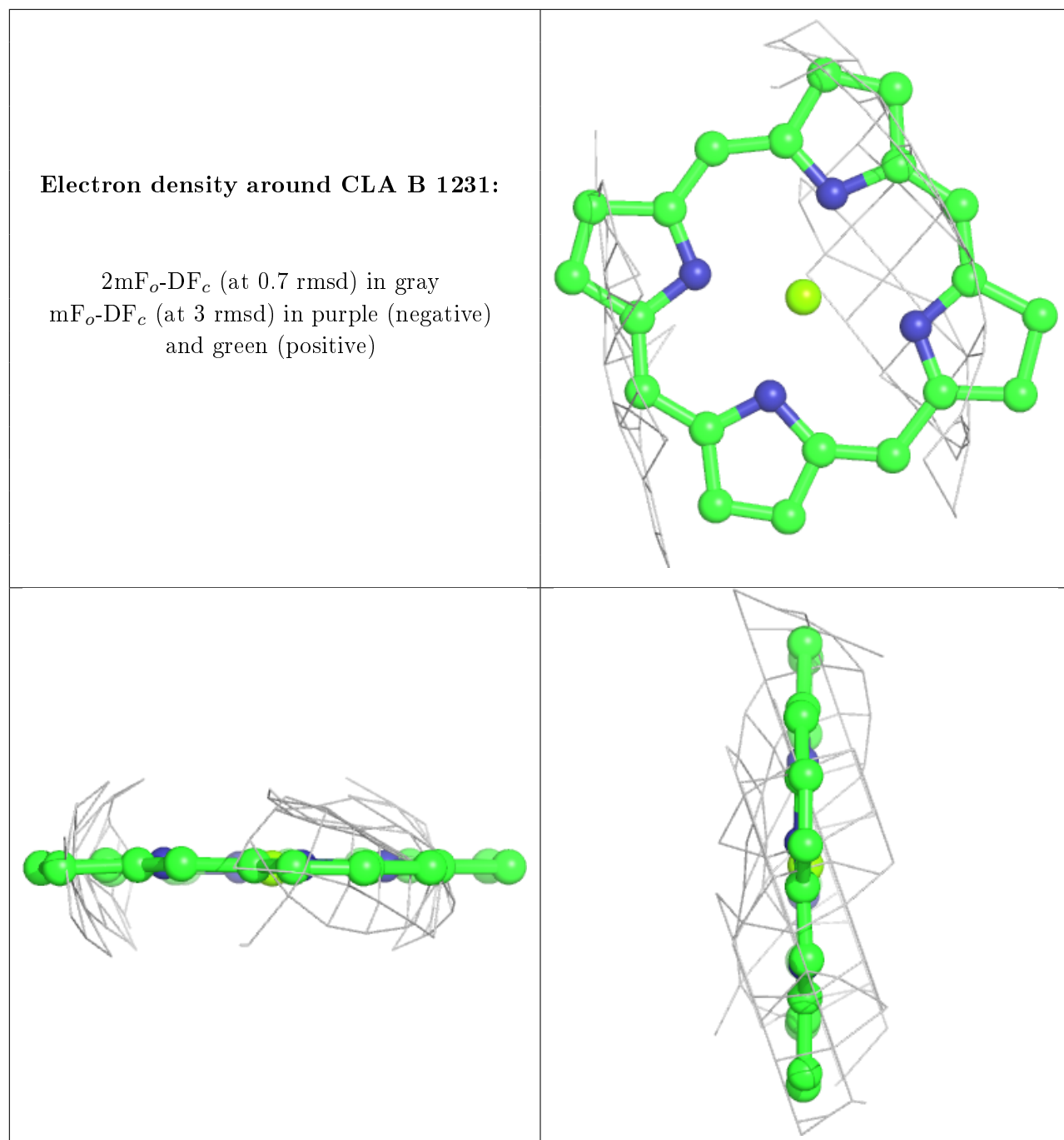


**Electron density around CLA 4 604:**

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

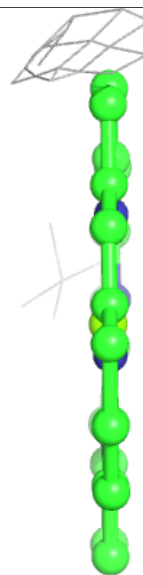
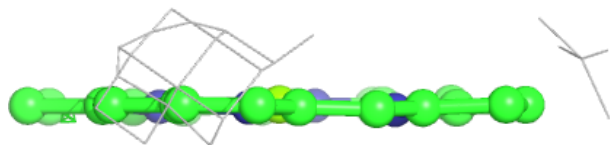
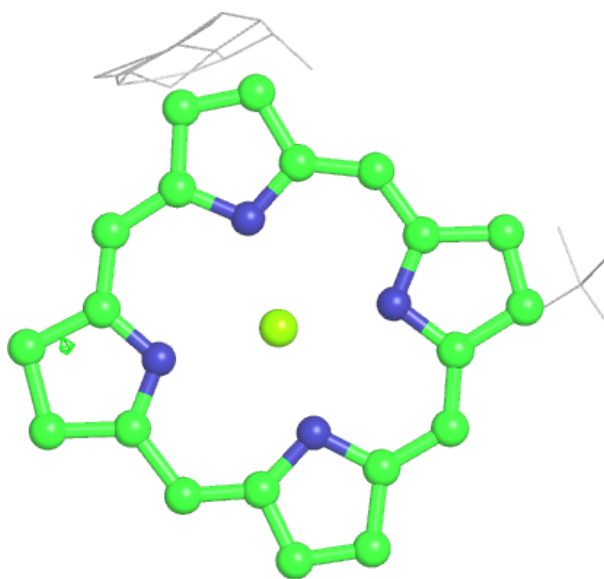






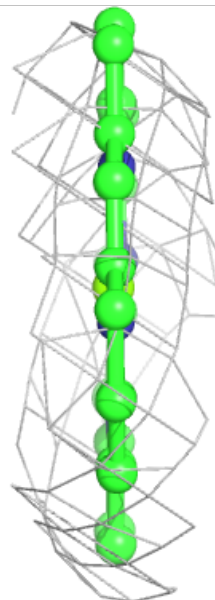
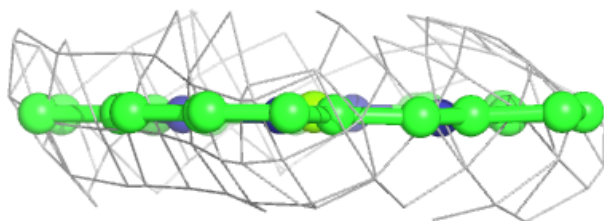
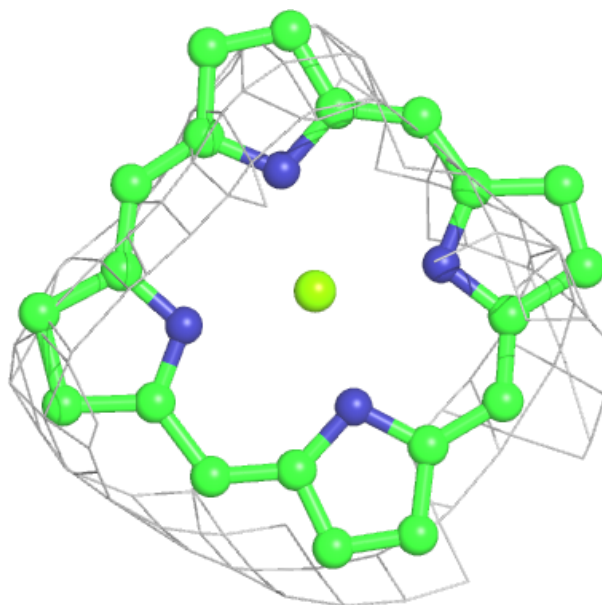
**Electron density around CLA 2 615:**

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

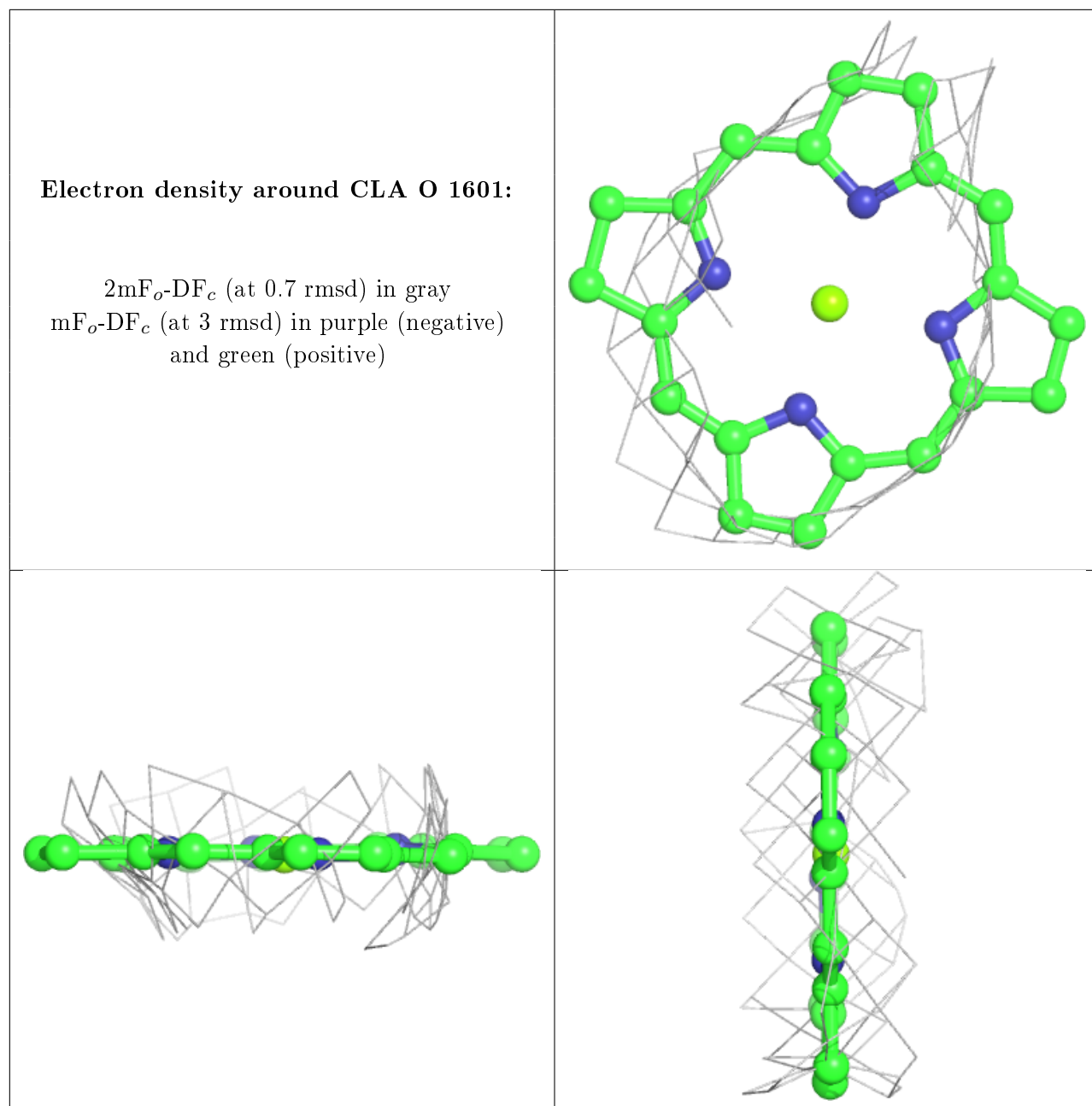


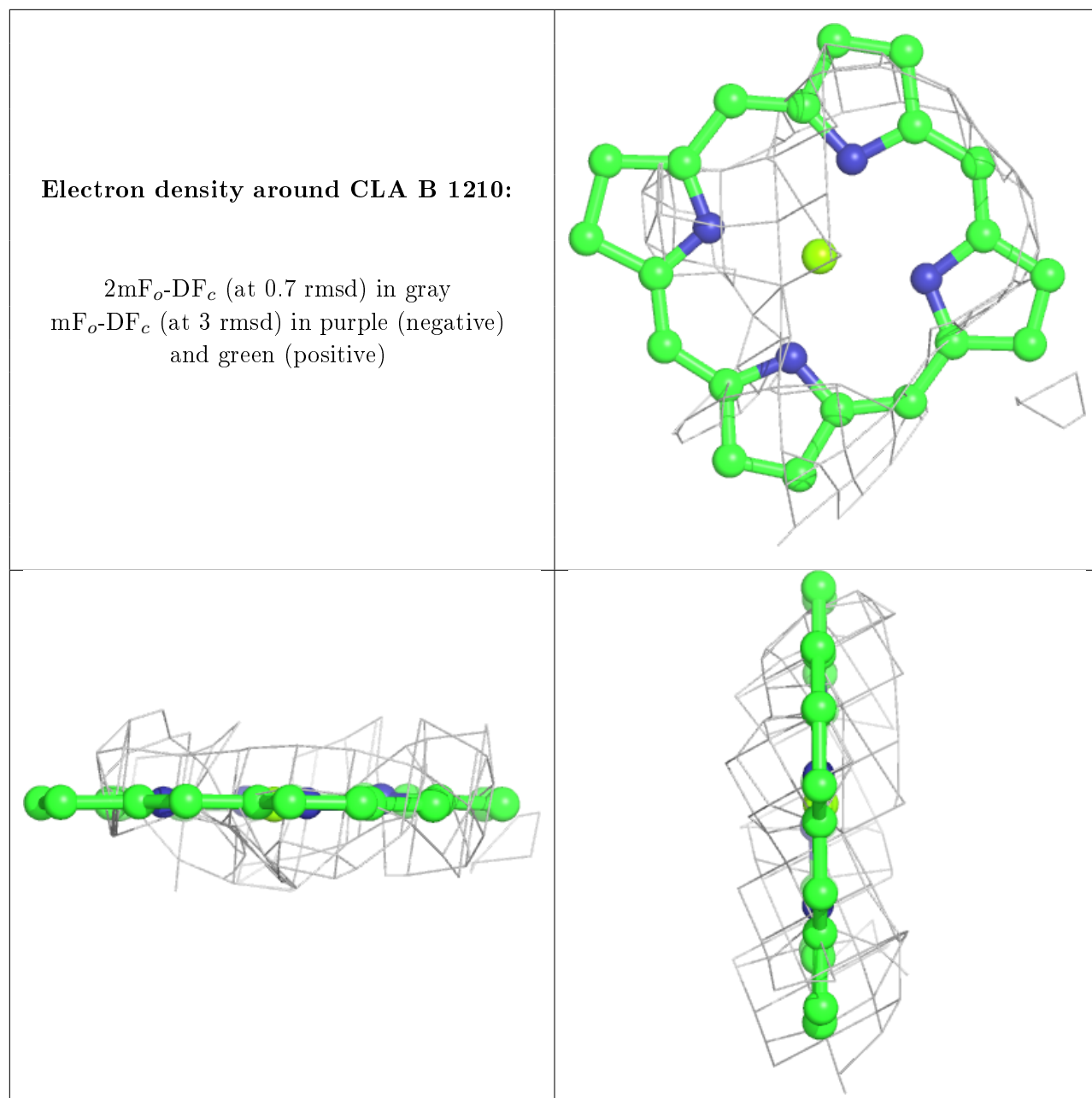
**Electron density around CLA O 1603:**

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



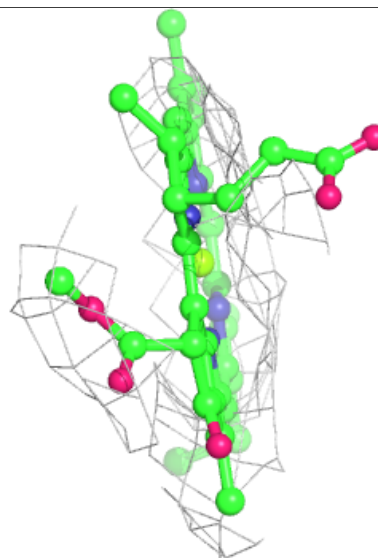
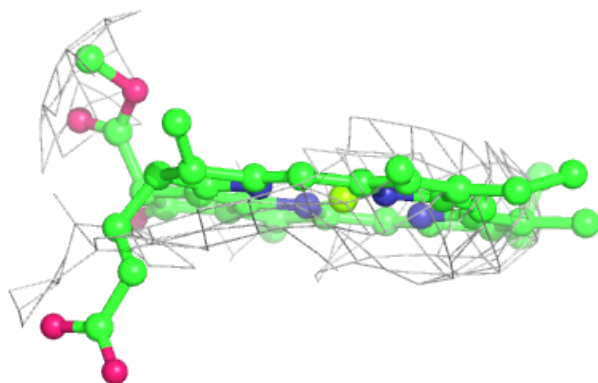
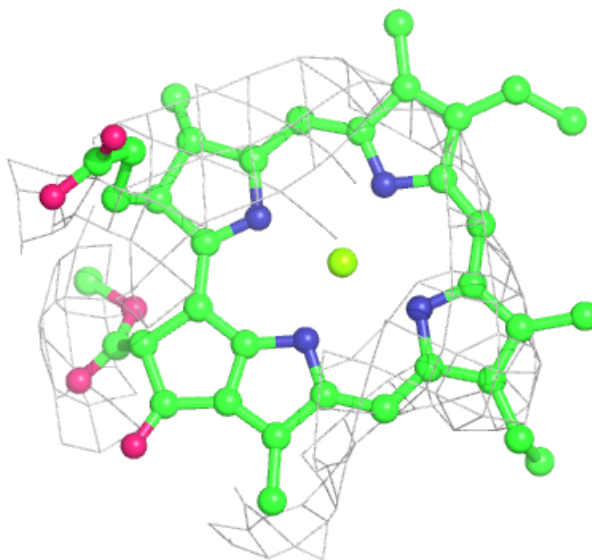






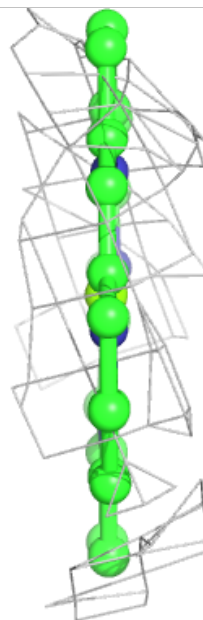
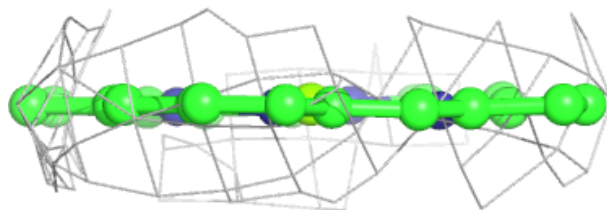
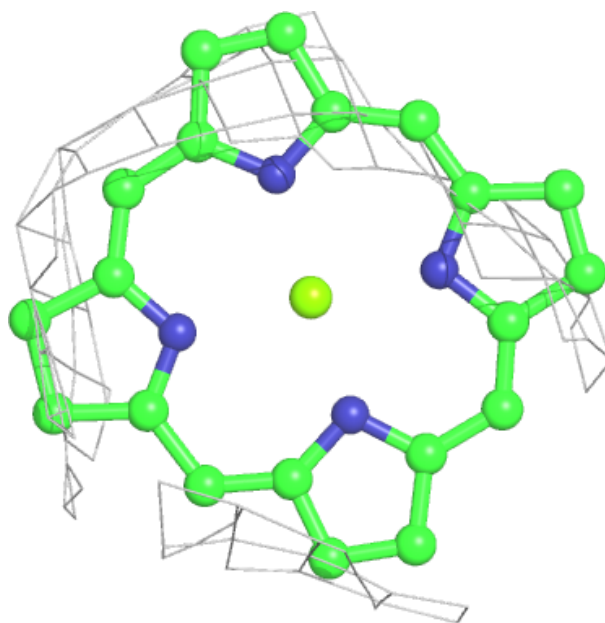
**Electron density around CLA B 1236:**

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



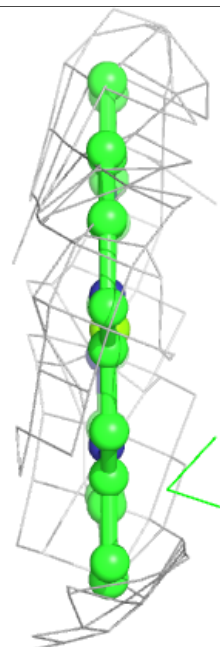
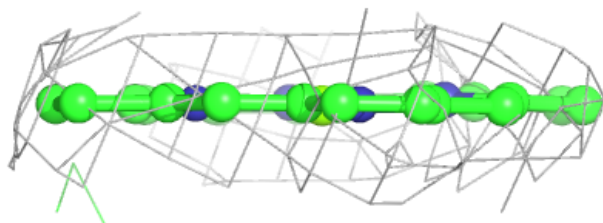
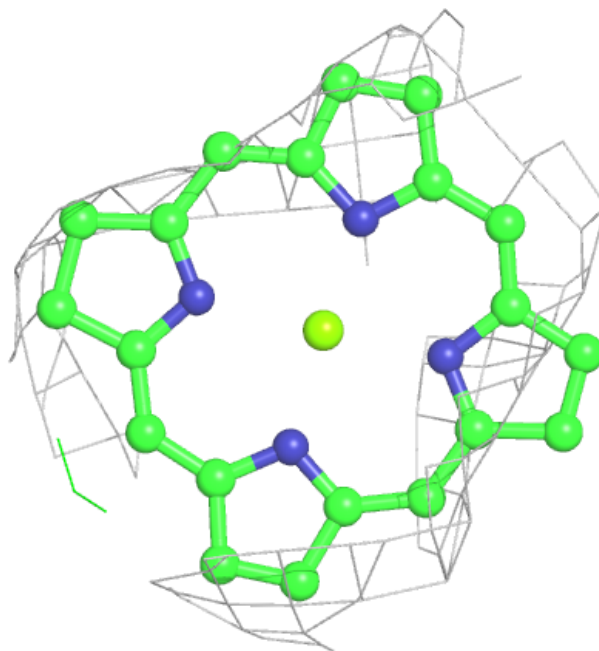
**Electron density around CLA 2 613:**

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



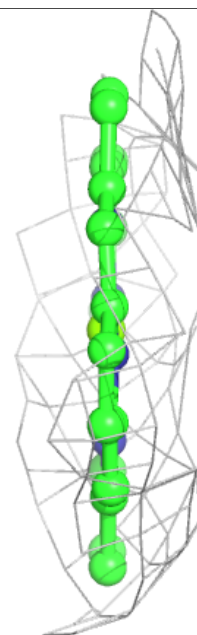
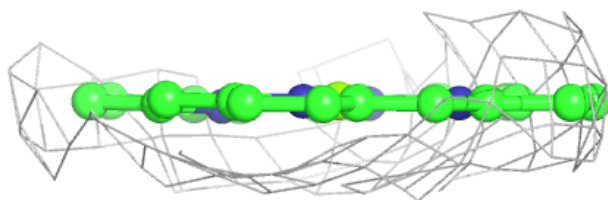
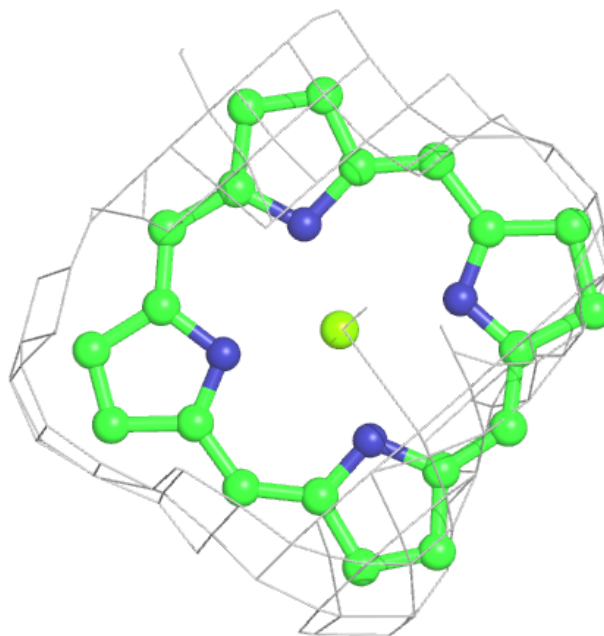
**Electron density around CLA 2 601:**

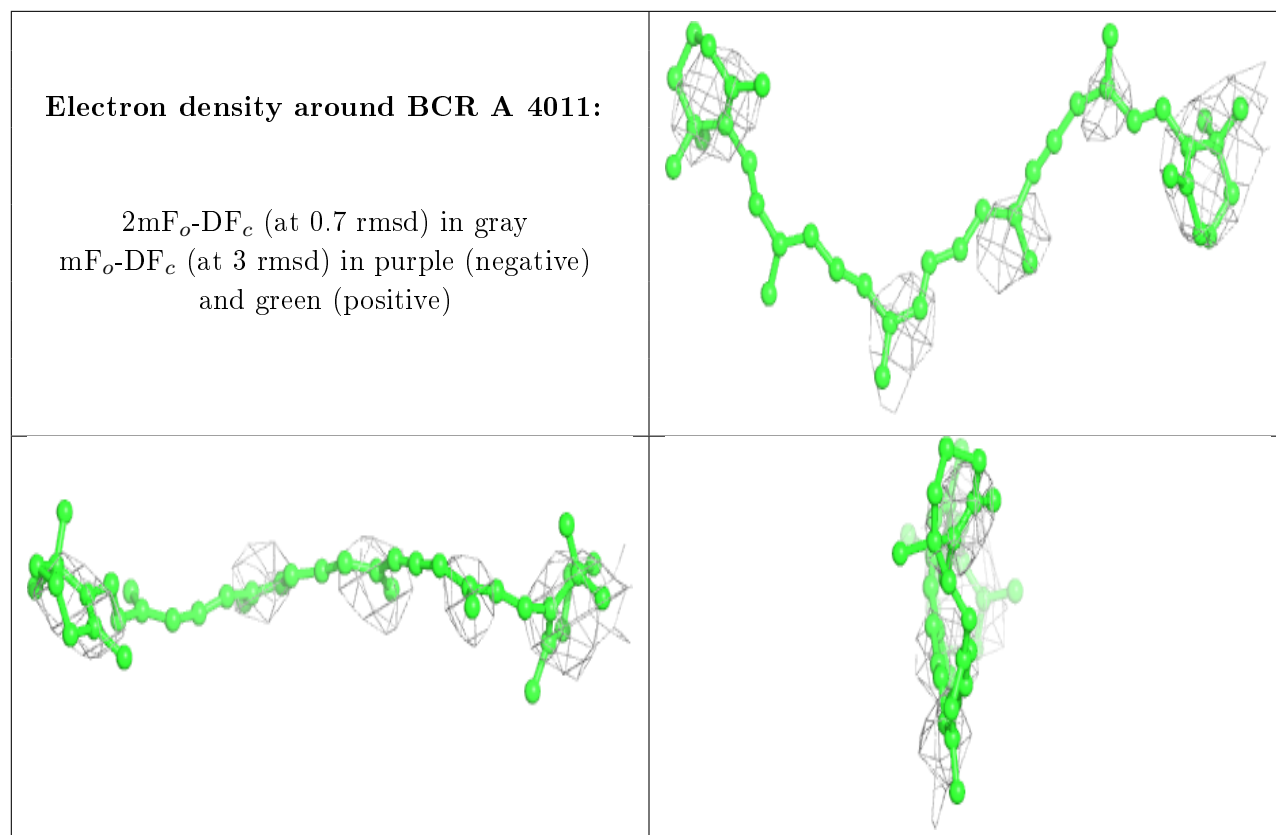
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA L 1502:**

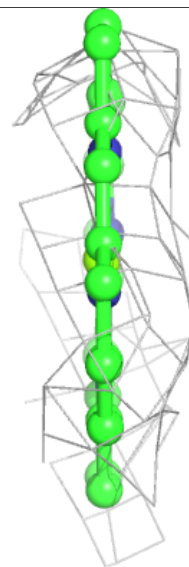
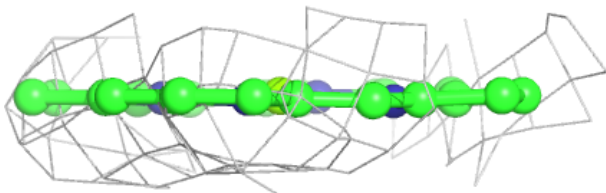
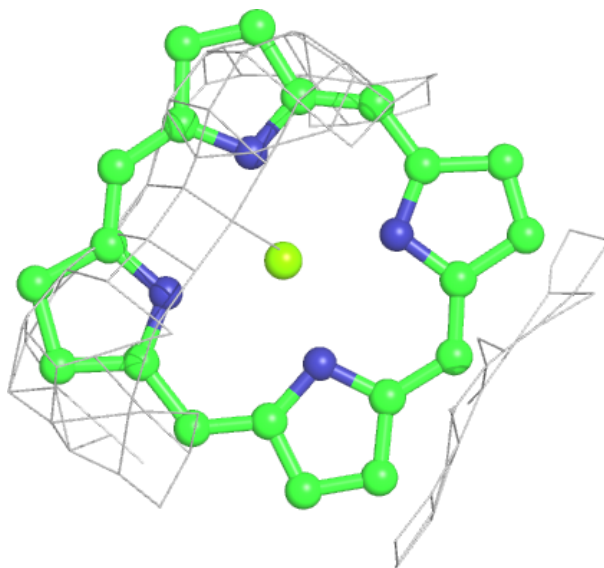
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 2 603:**

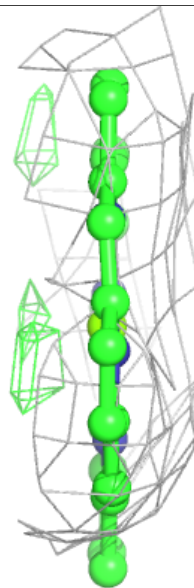
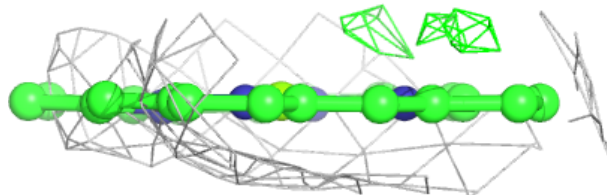
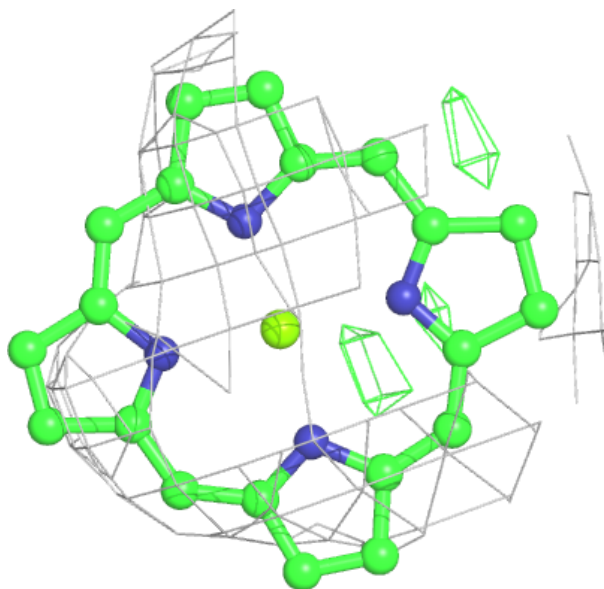
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





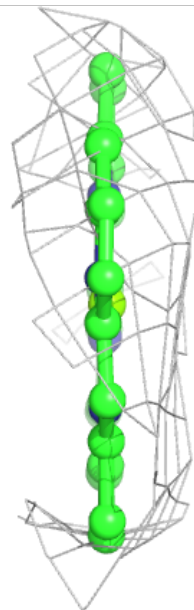
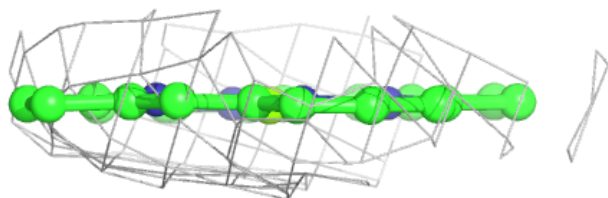
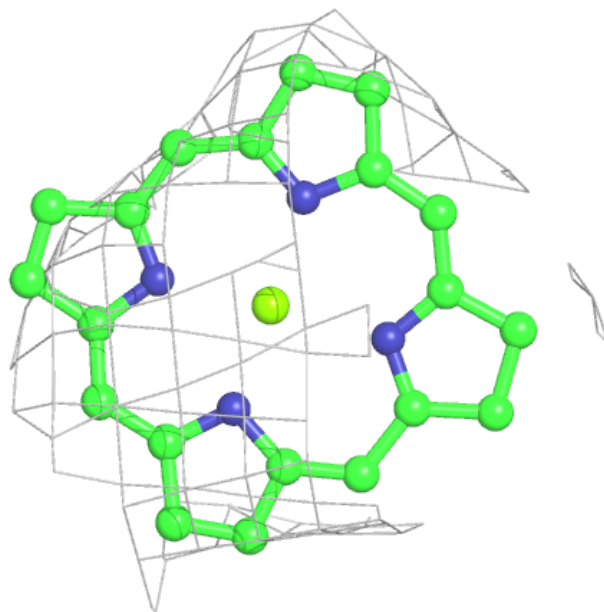
**Electron density around CLA A 1129:**

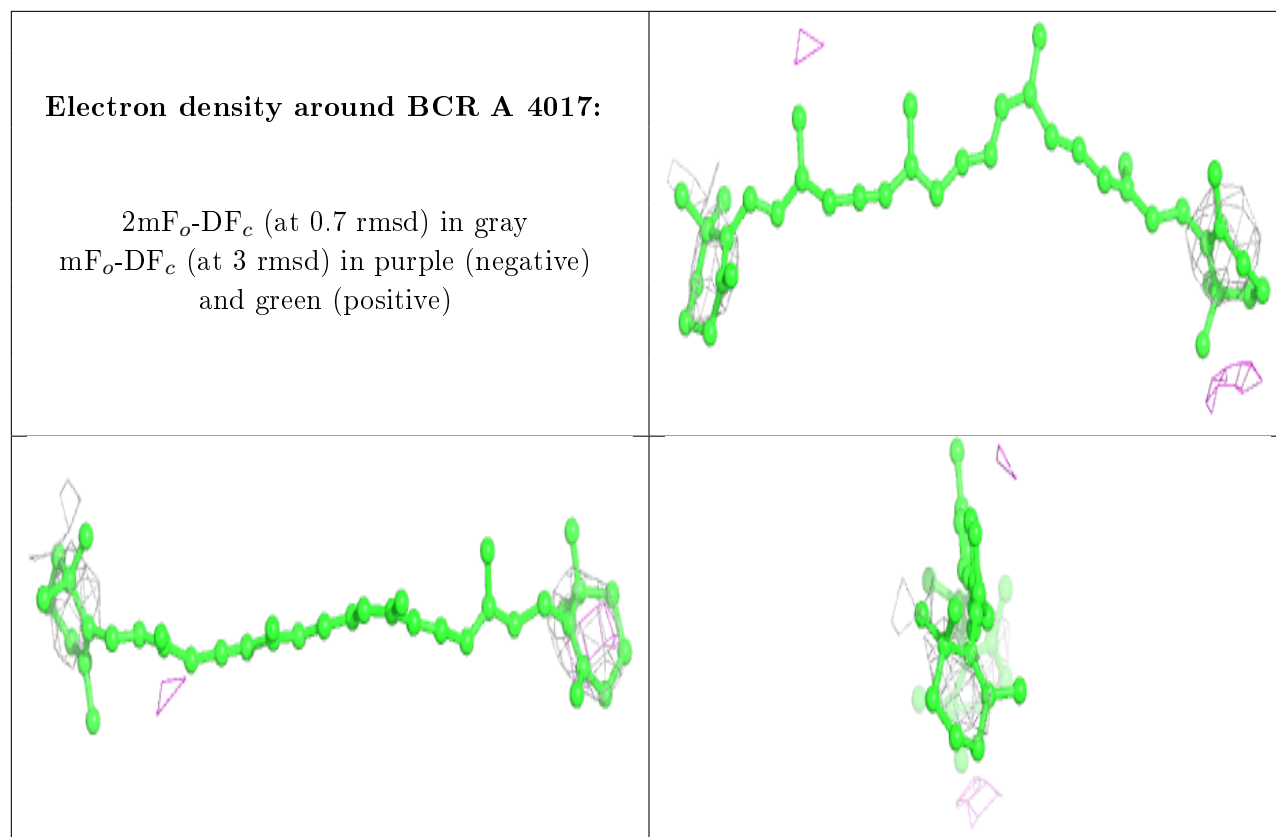
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 612:**

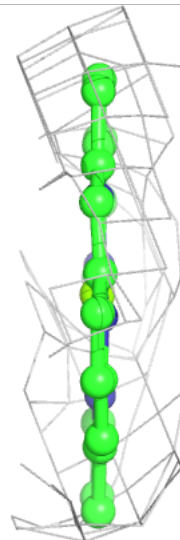
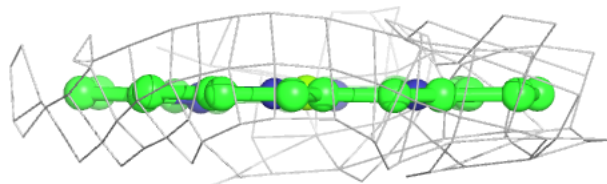
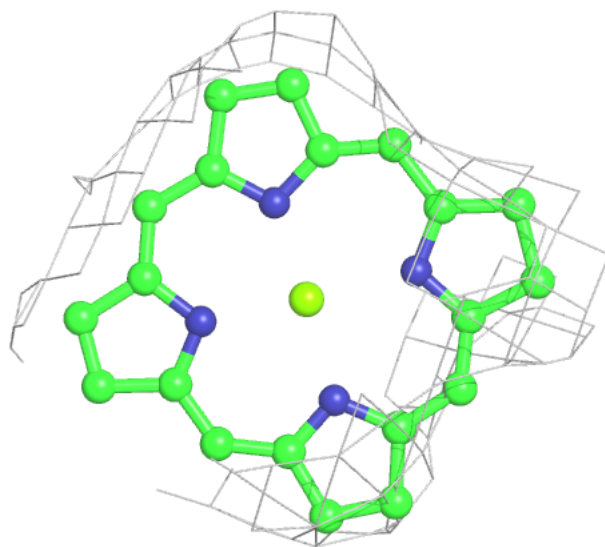
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





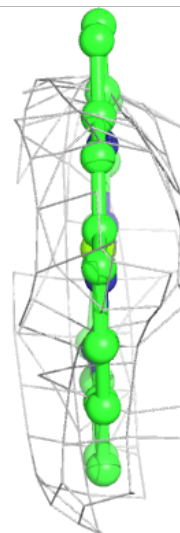
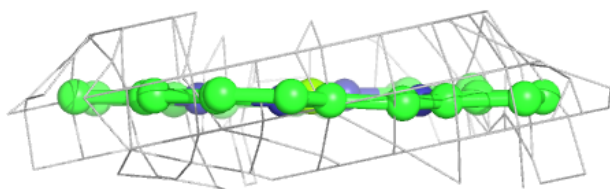
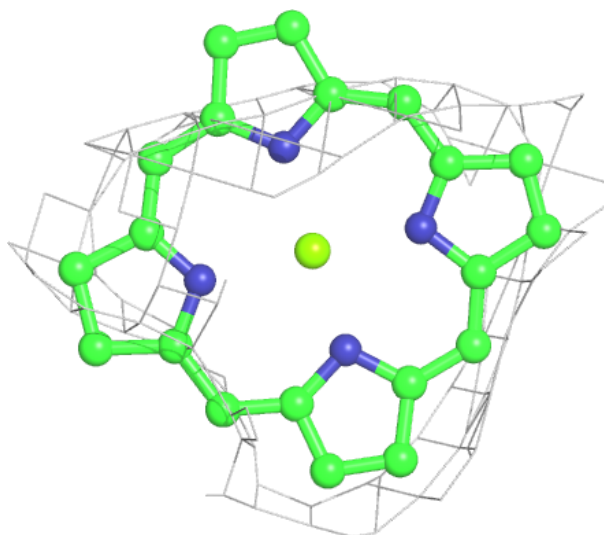
**Electron density around CLA 4 610:**

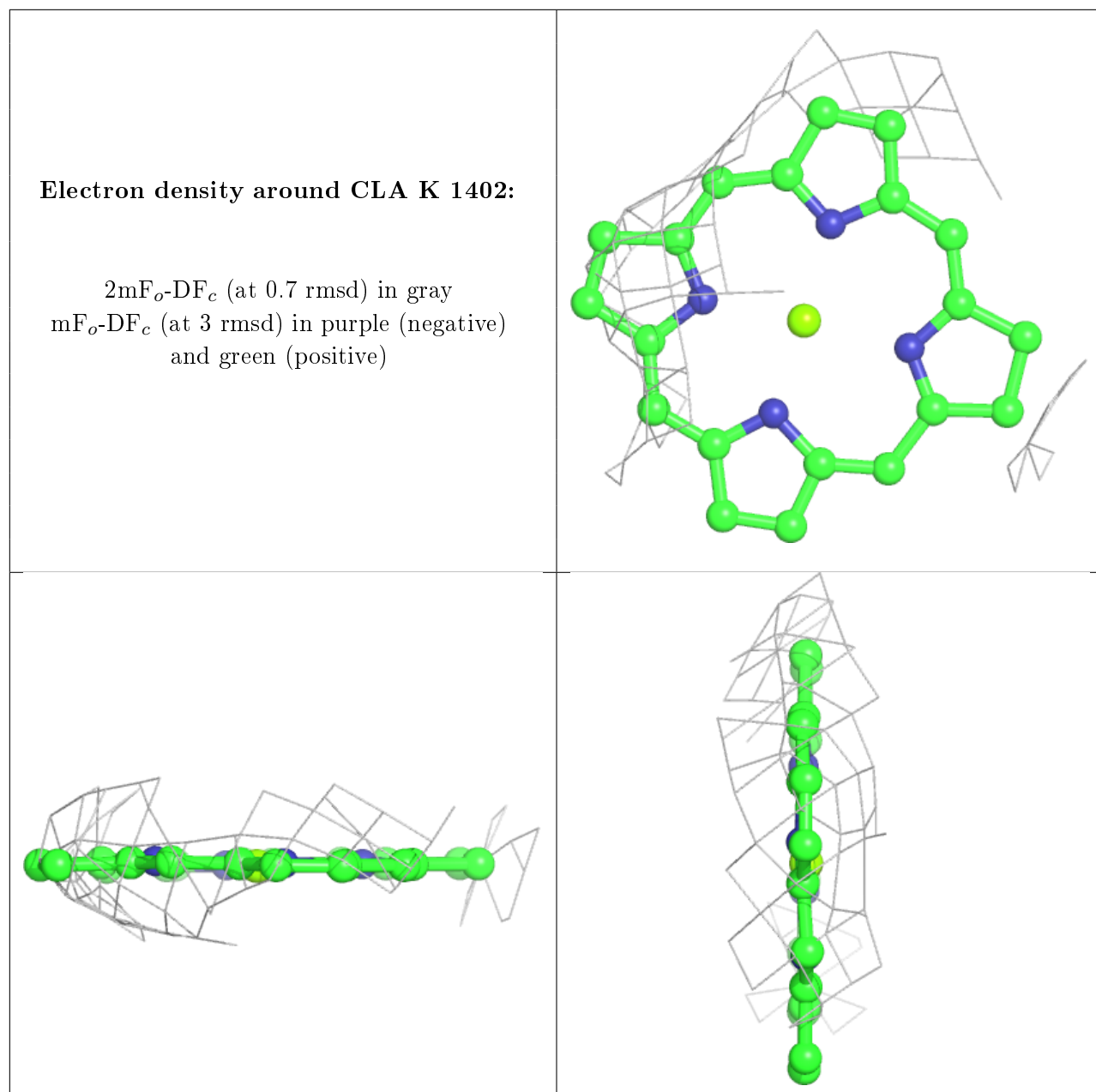
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 607:**

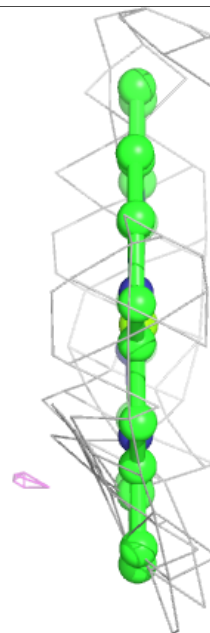
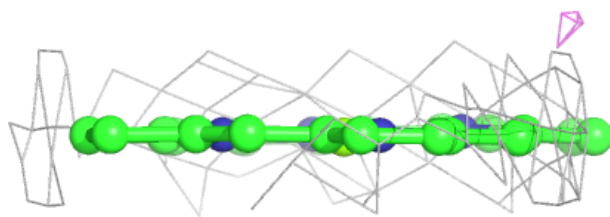
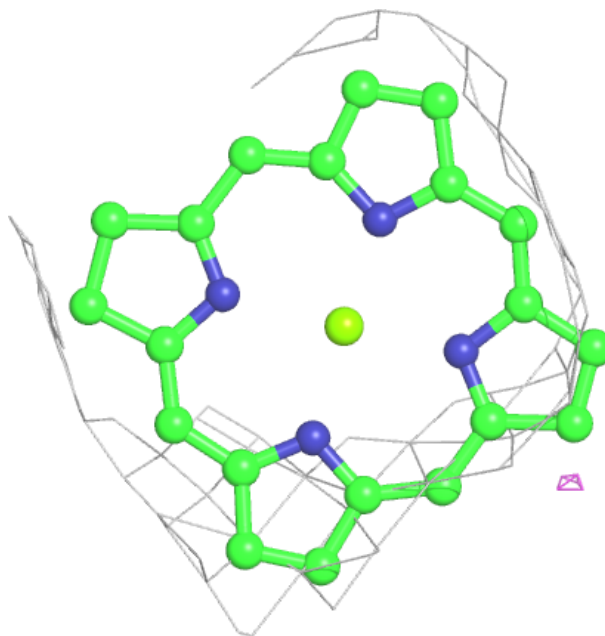
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

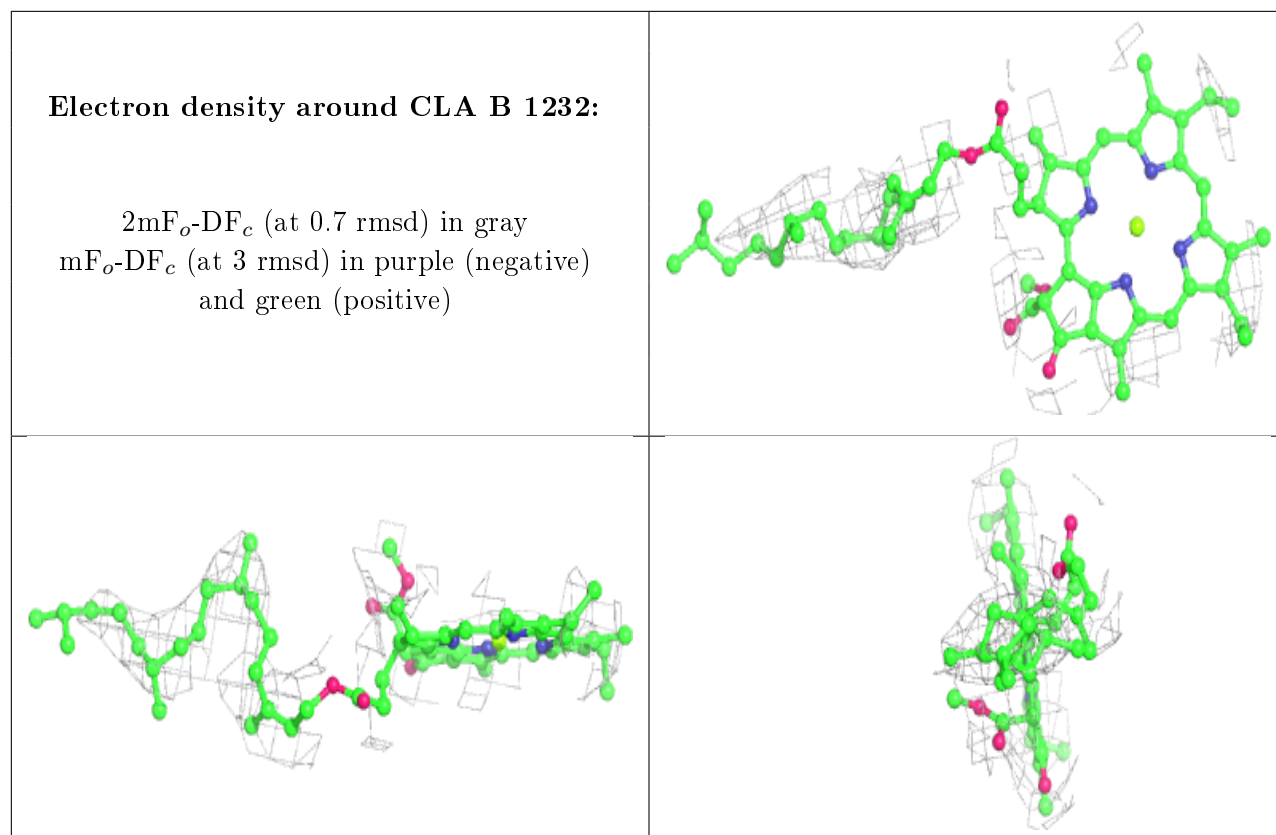




**Electron density around CLA 2 606:**

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

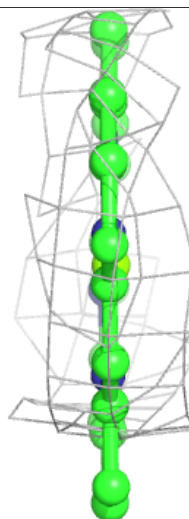
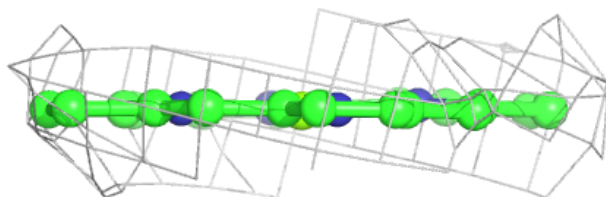
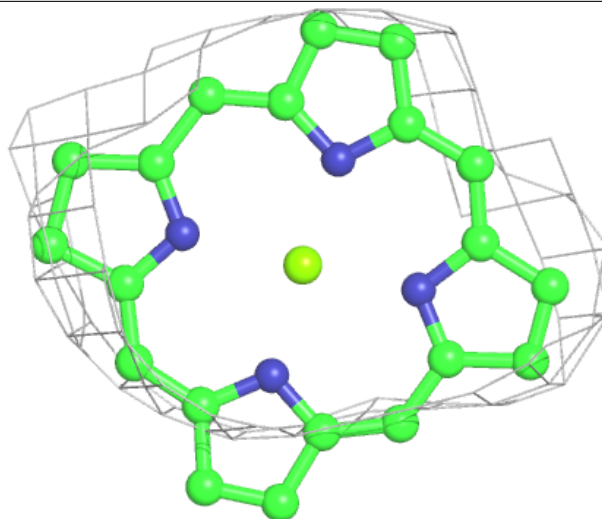


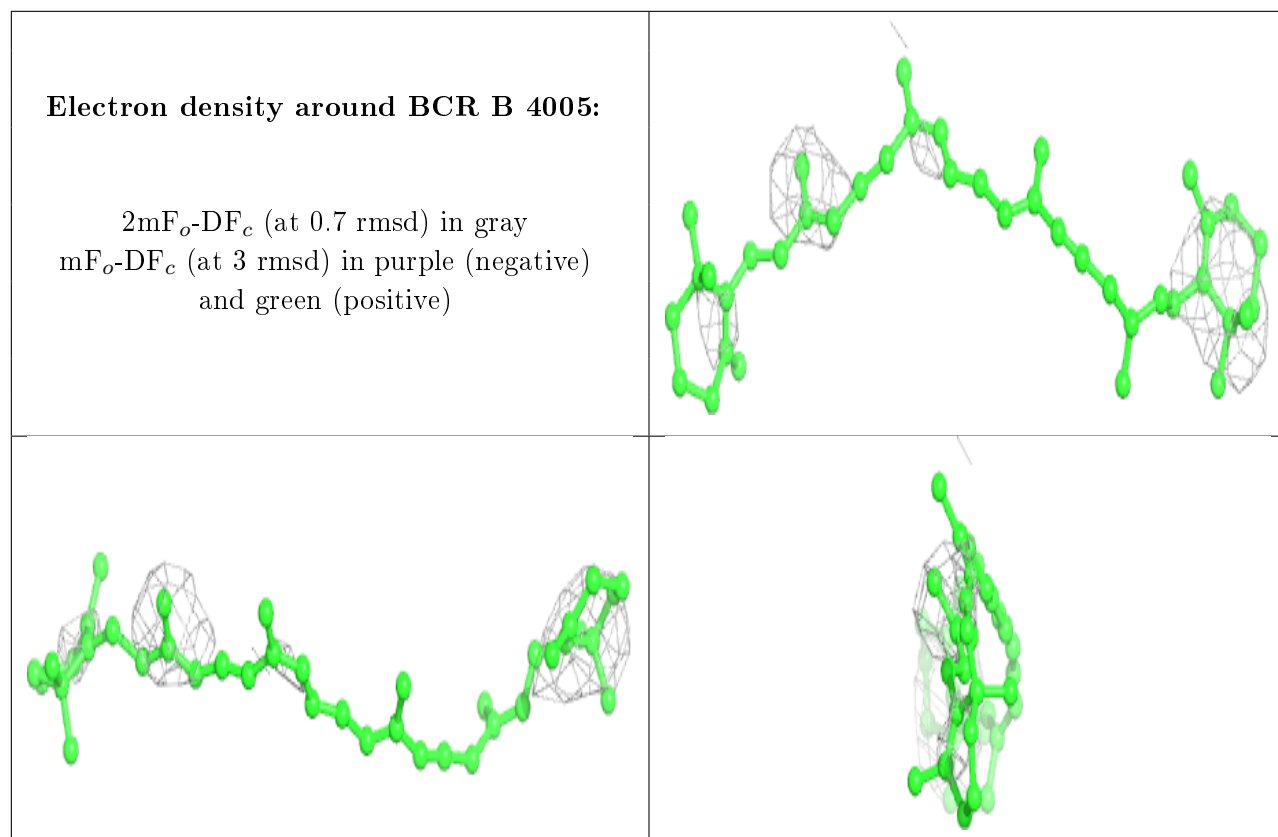




**Electron density around CLA 4 616:**

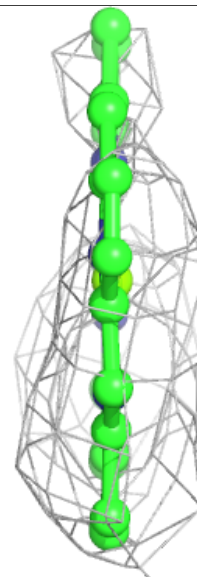
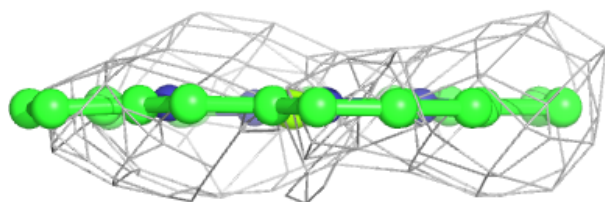
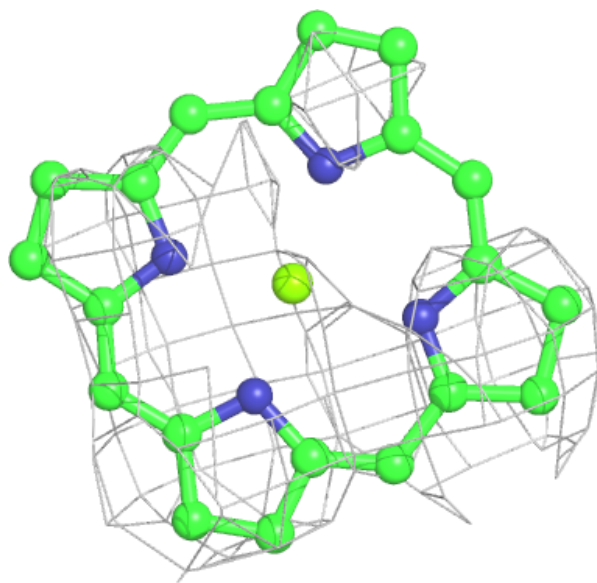
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





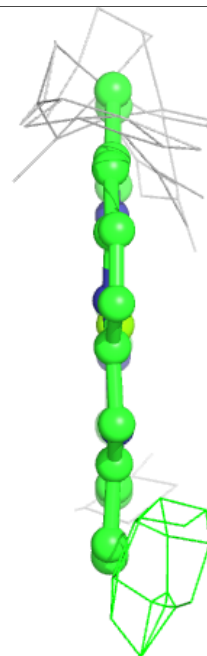
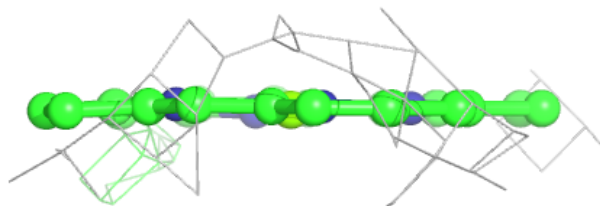
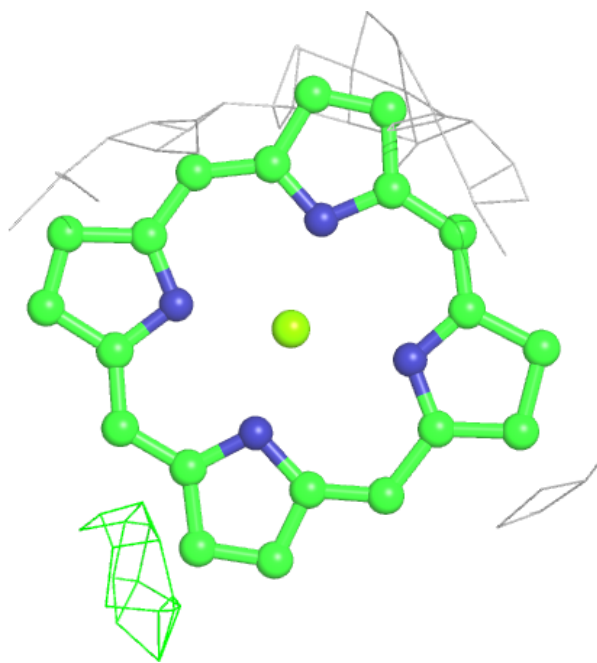
**Electron density around CLA A 1137:**

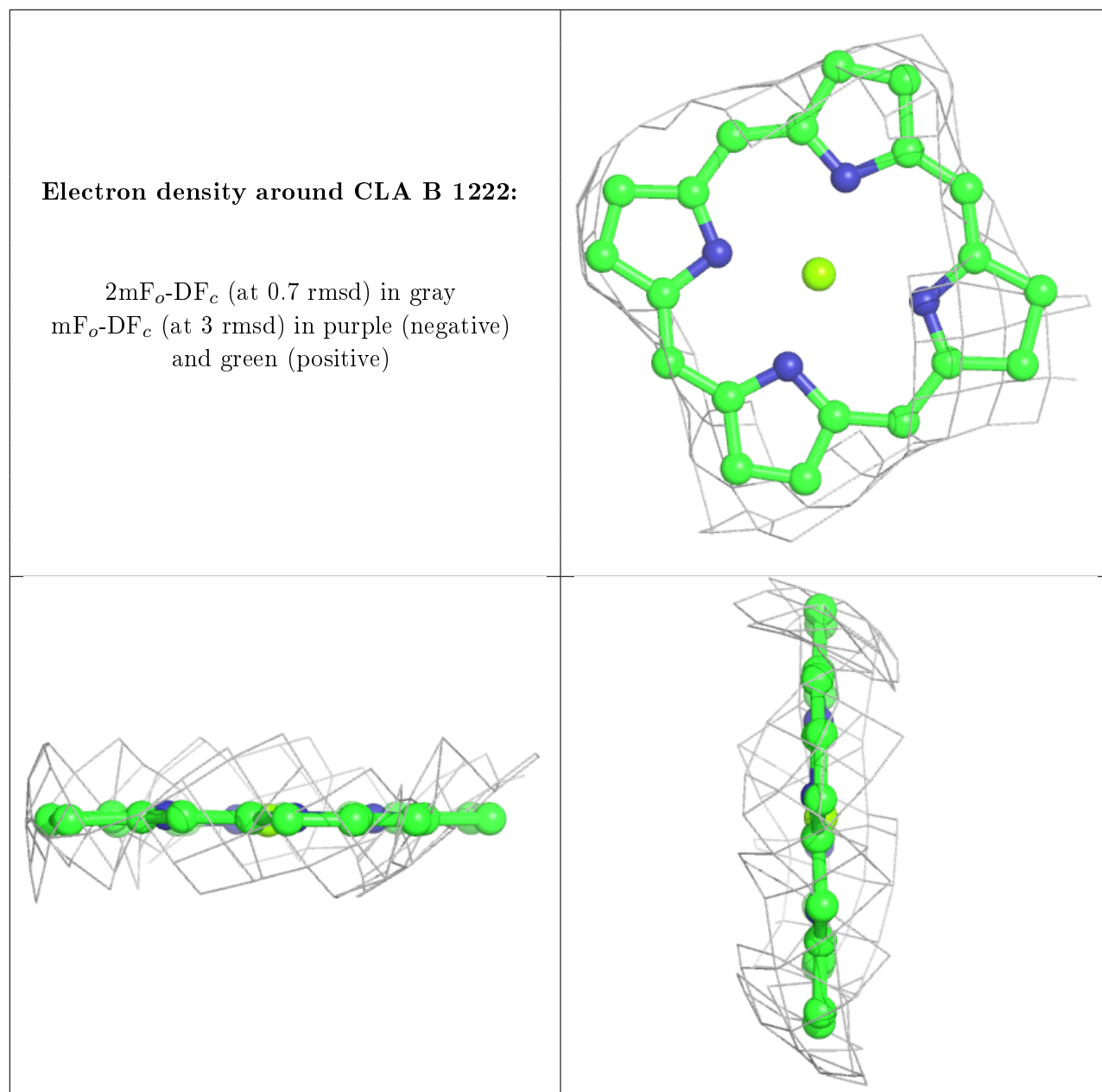
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 3 602:**

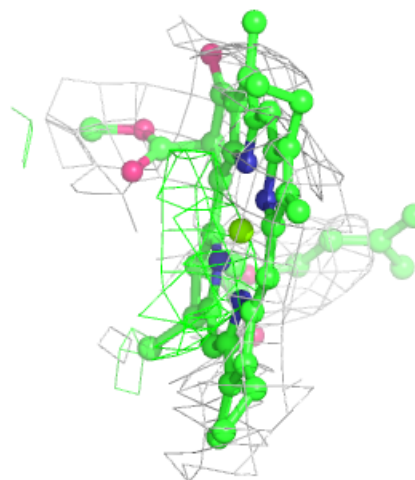
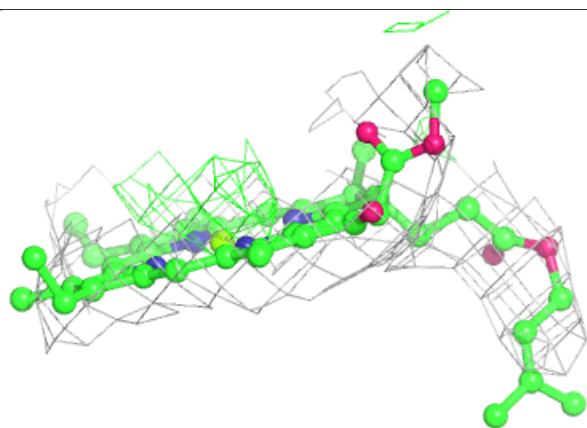
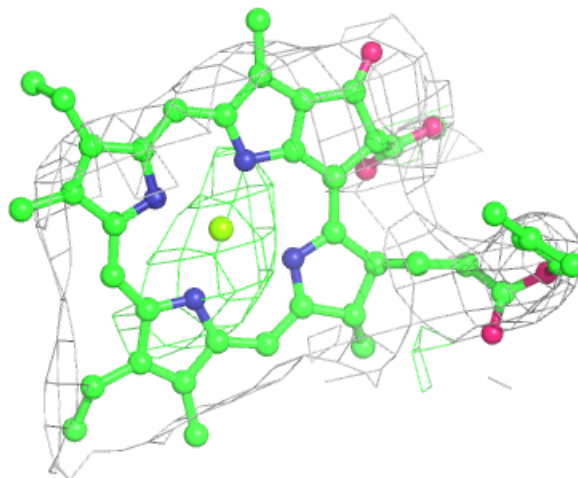
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





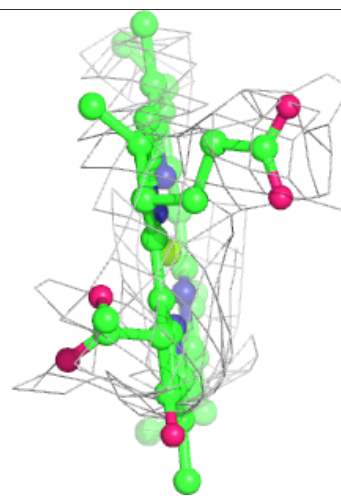
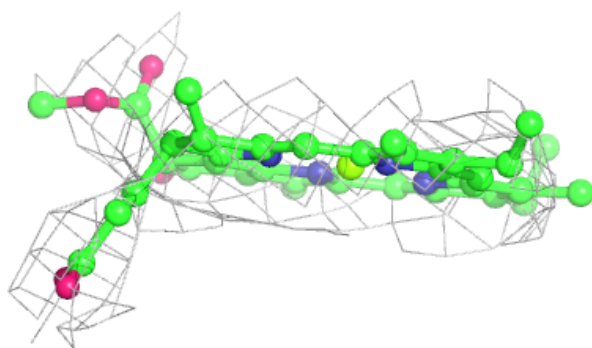
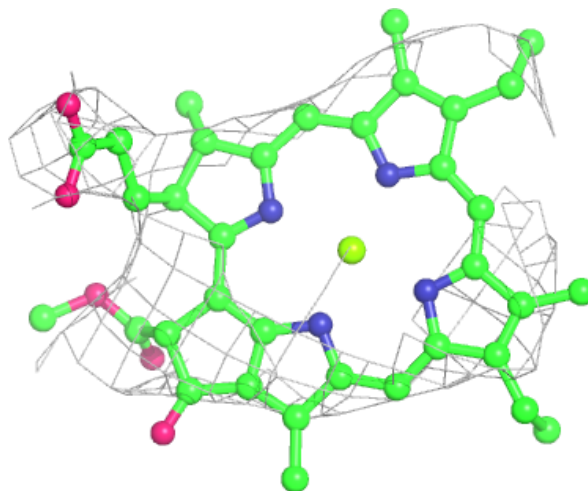
**Electron density around CLA A 1011:**

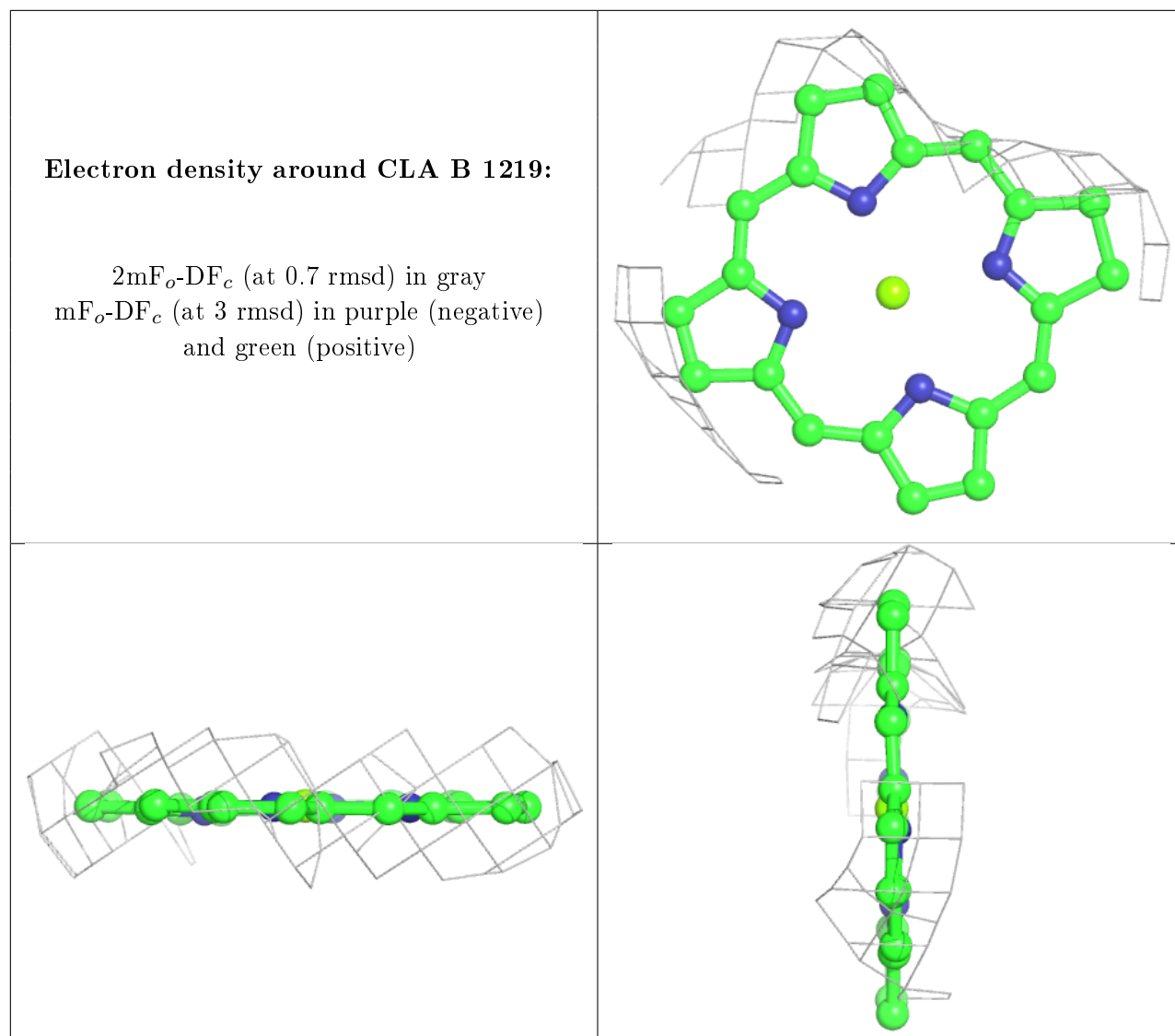
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1021:**

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

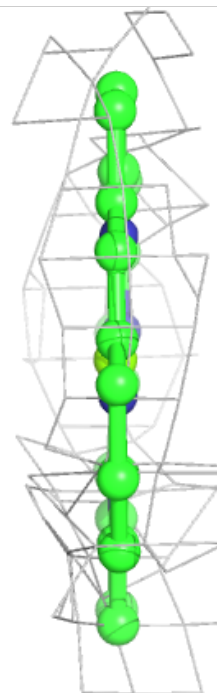
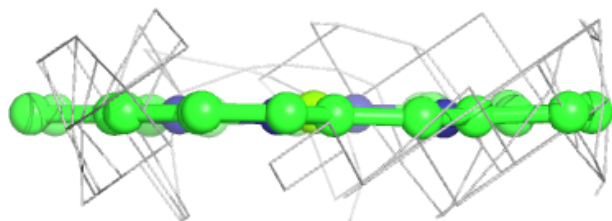
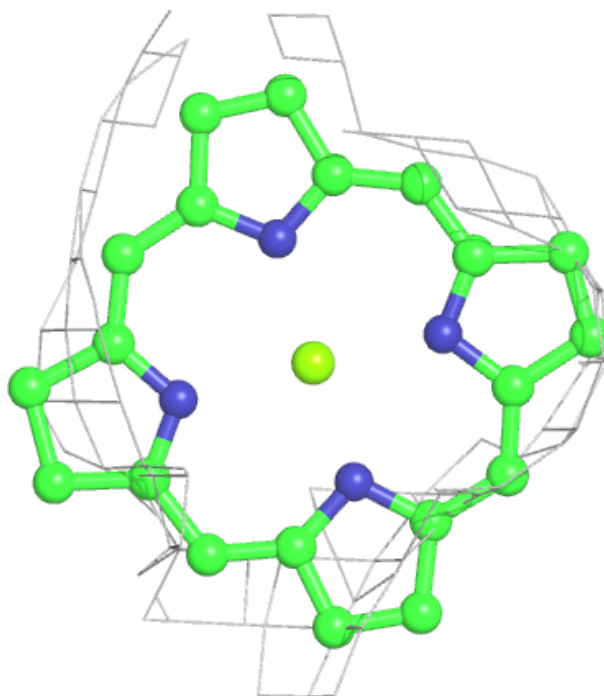


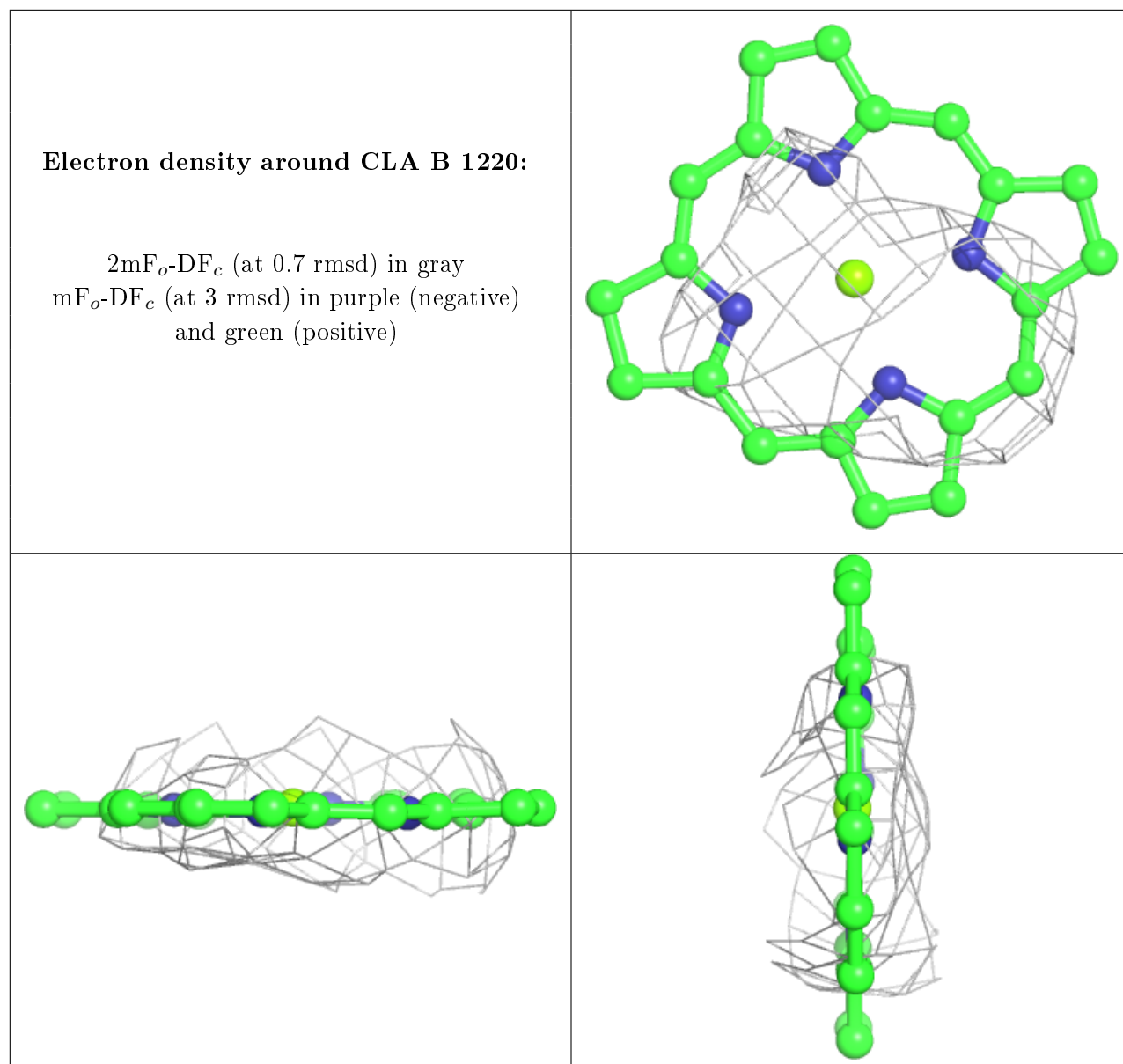




**Electron density around CLA 2 610:**

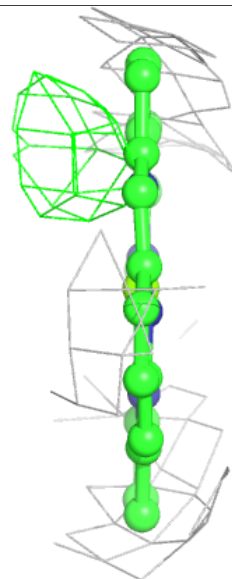
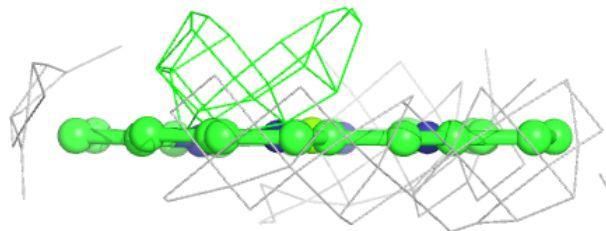
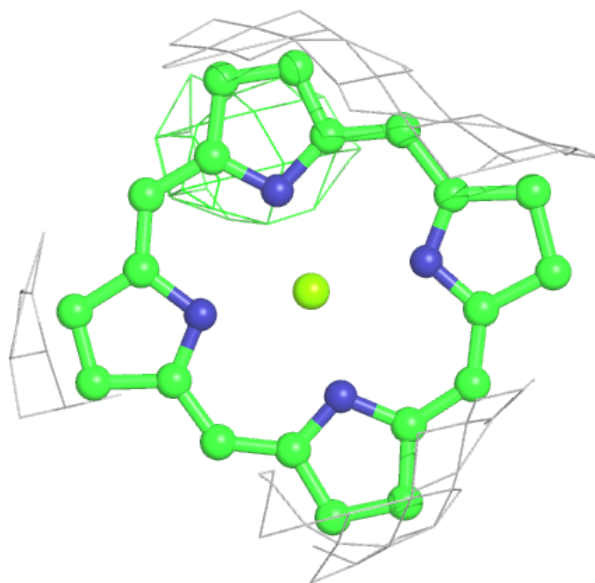
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





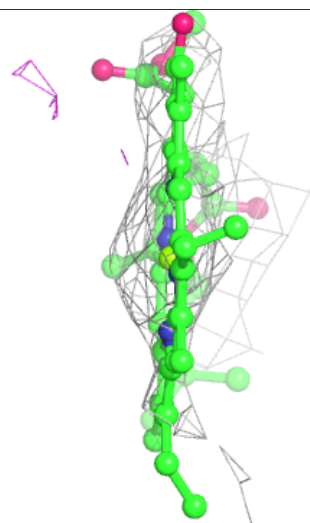
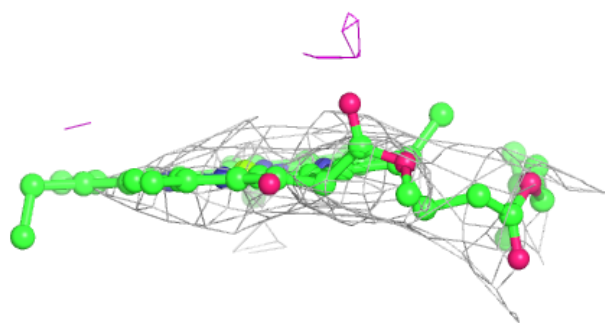
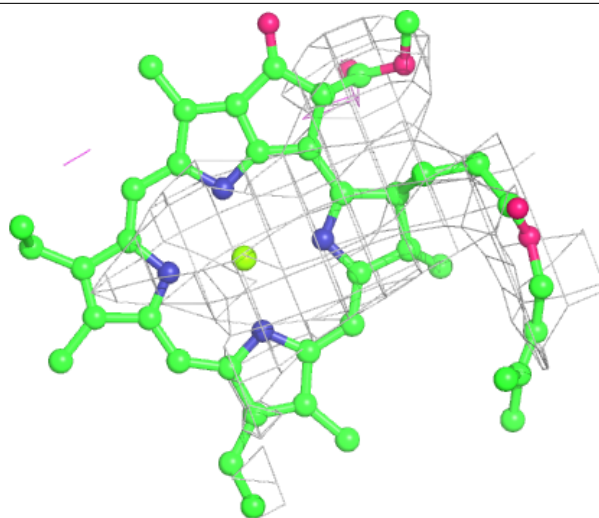
**Electron density around CLA 2 604:**

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



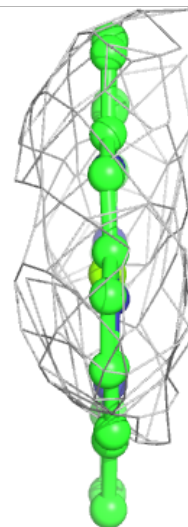
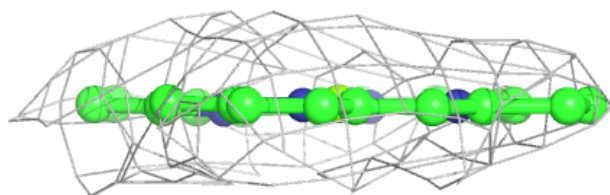
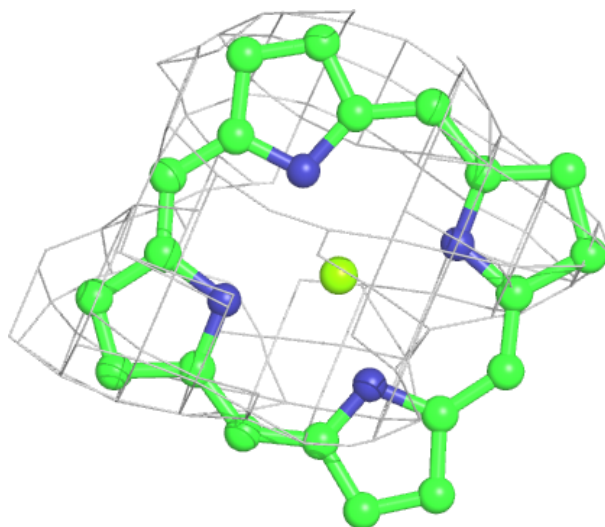
**Electron density around CLA B 1023:**

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



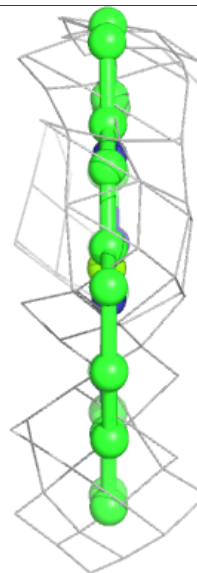
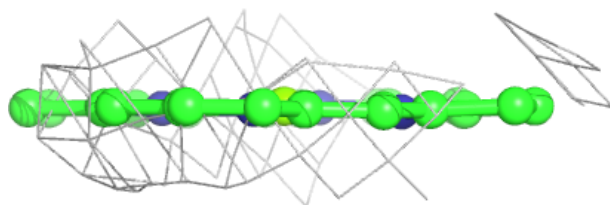
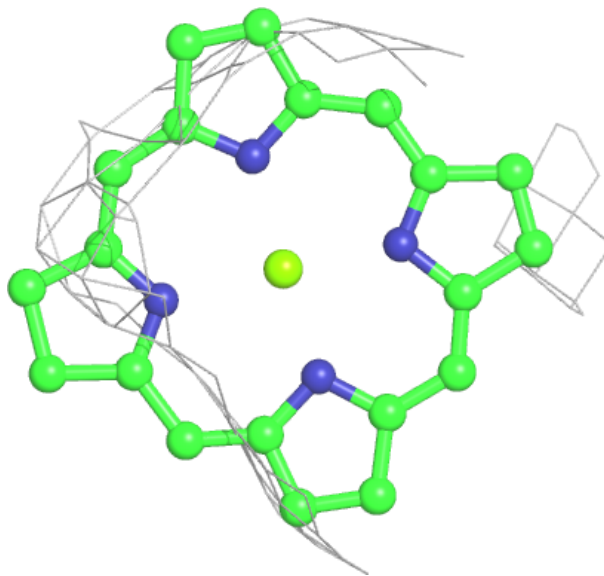
**Electron density around CLA 3 614:**

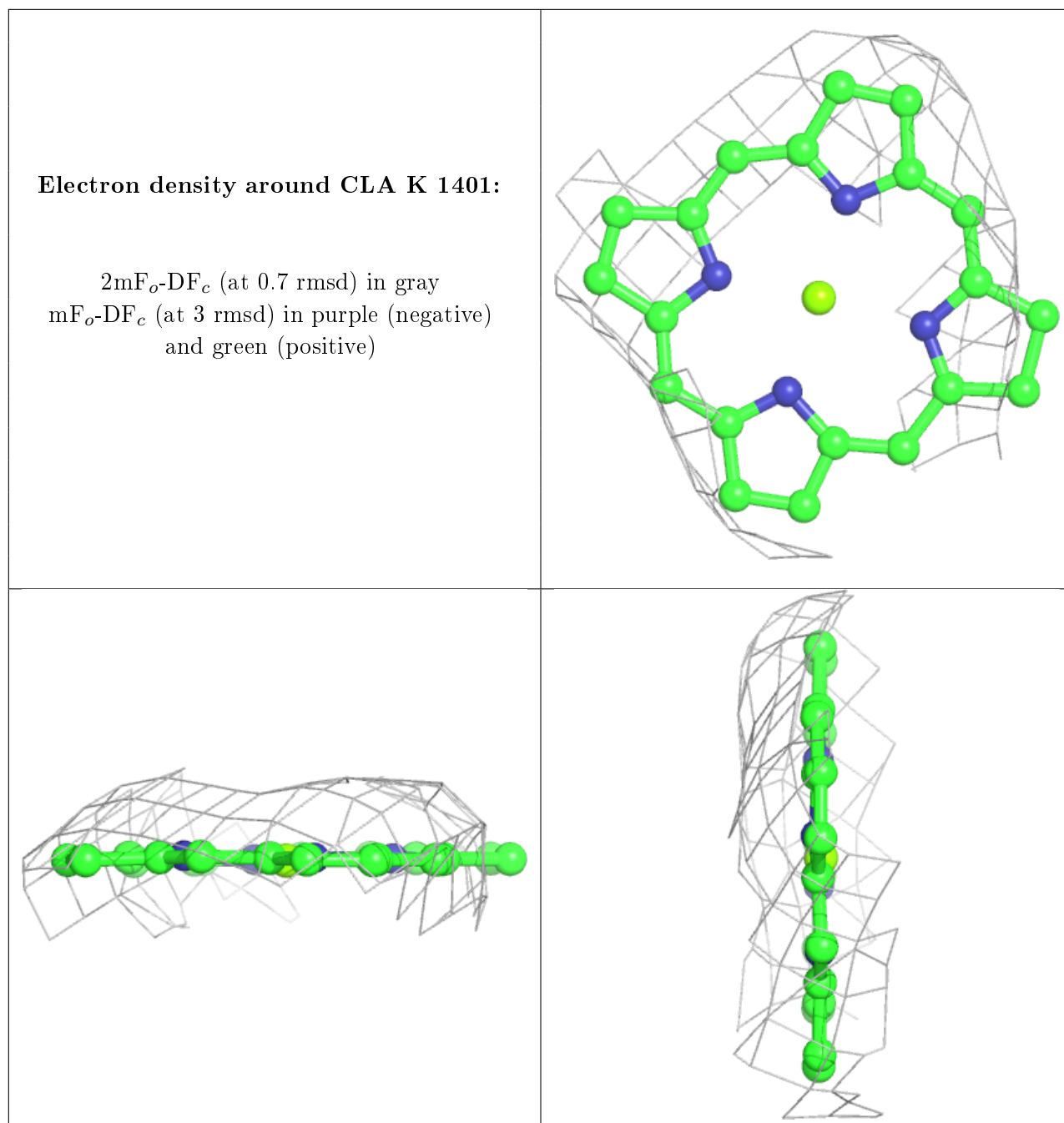
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

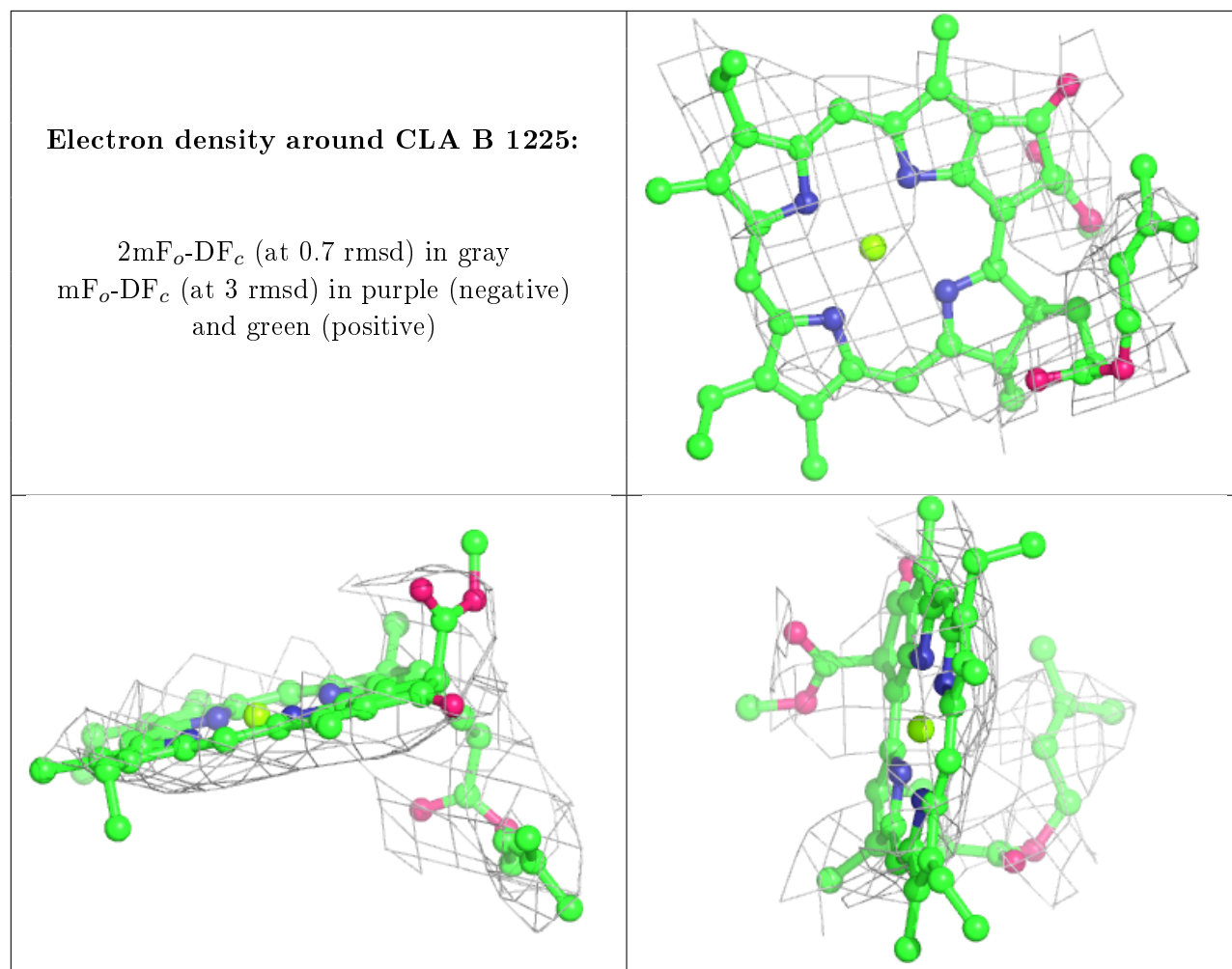


**Electron density around CLA F 1302:**

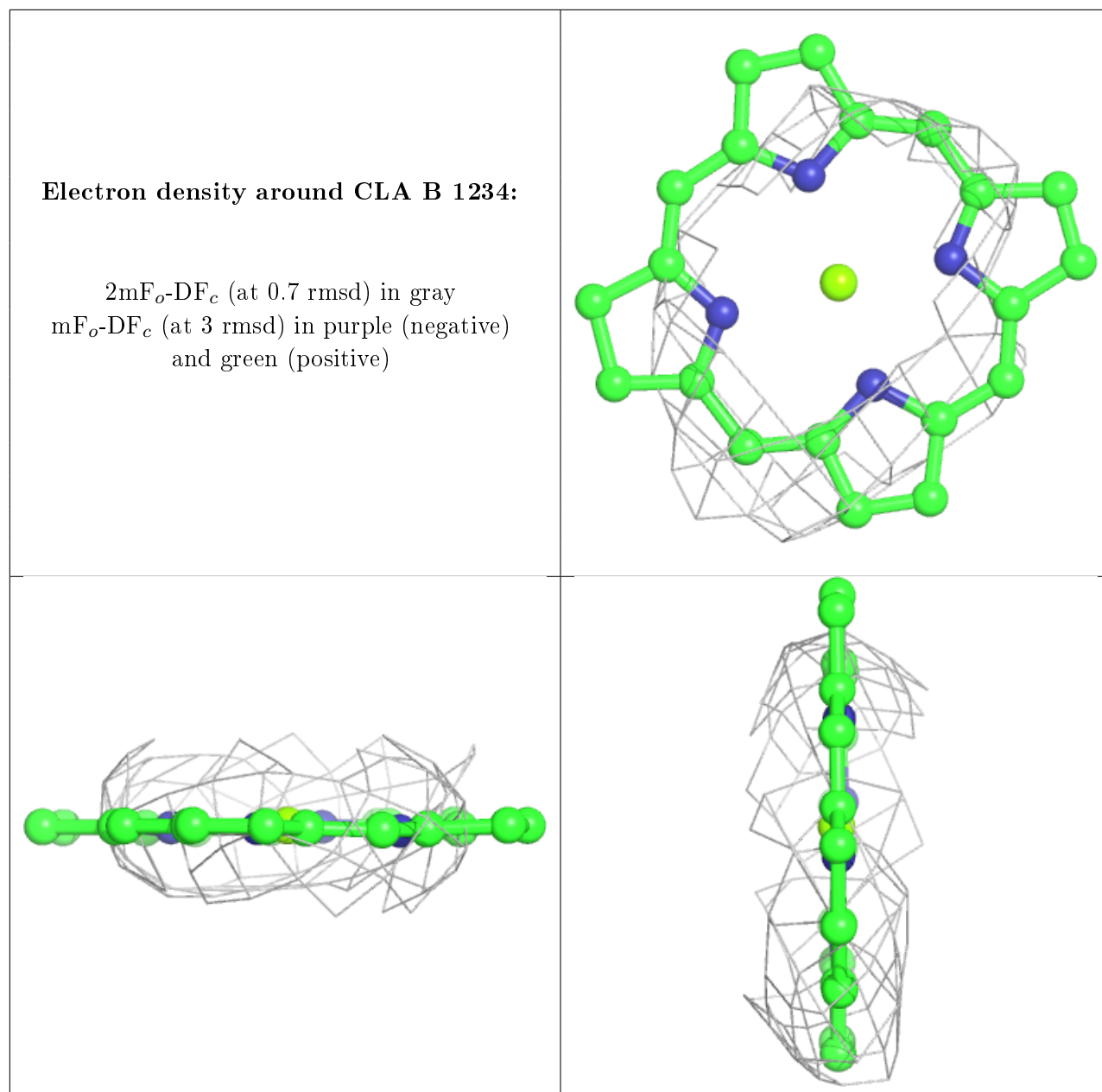
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

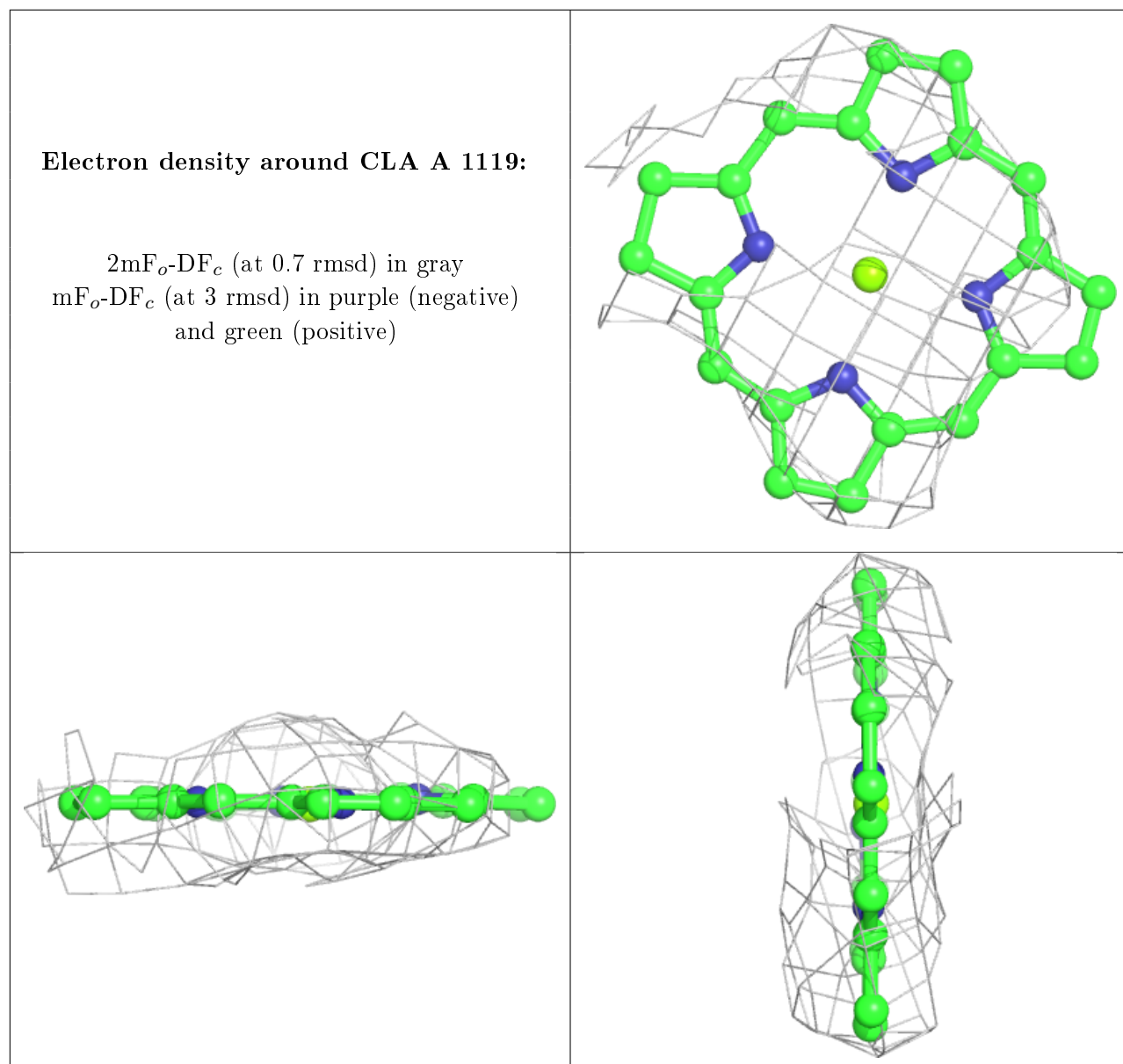






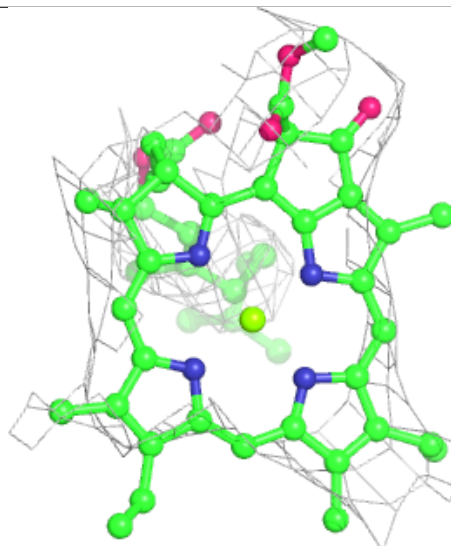
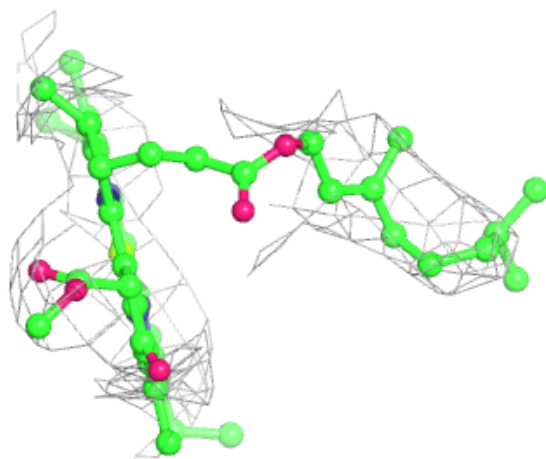
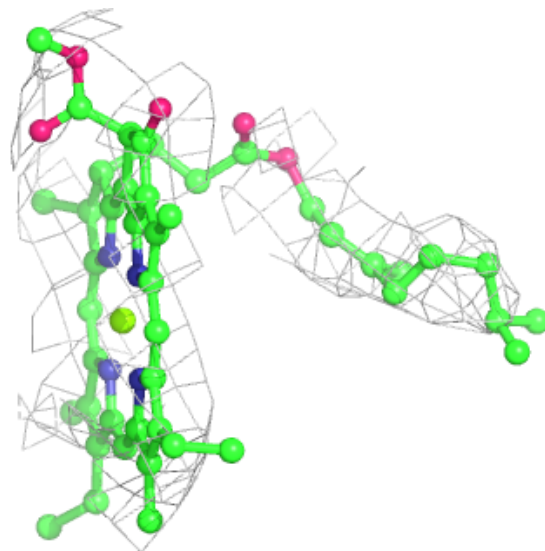






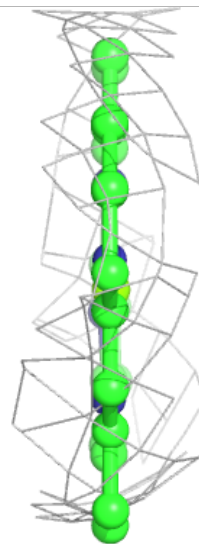
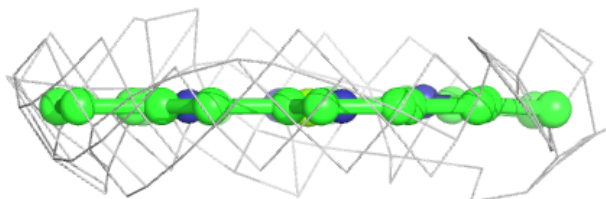
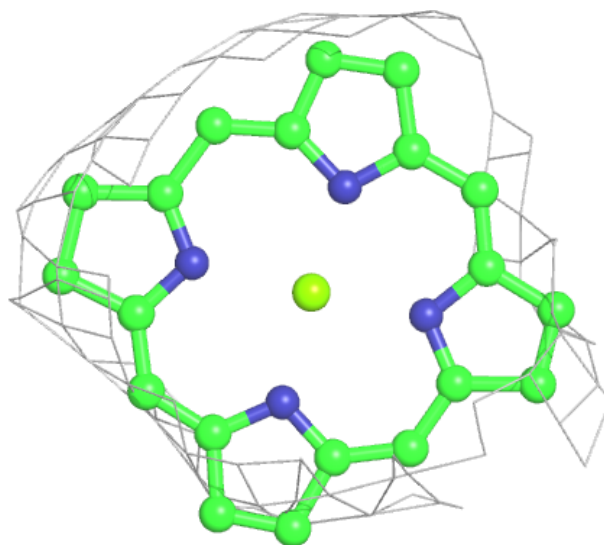
**Electron density around CLA B 1226:**

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



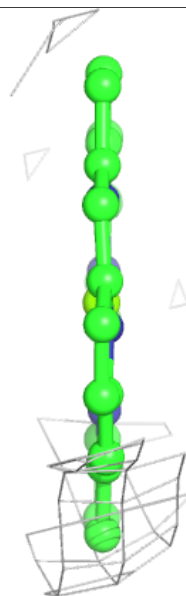
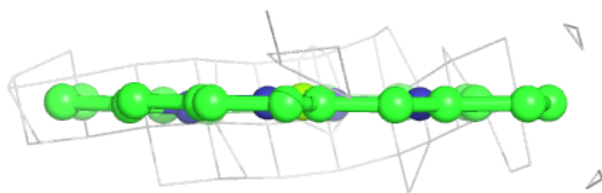
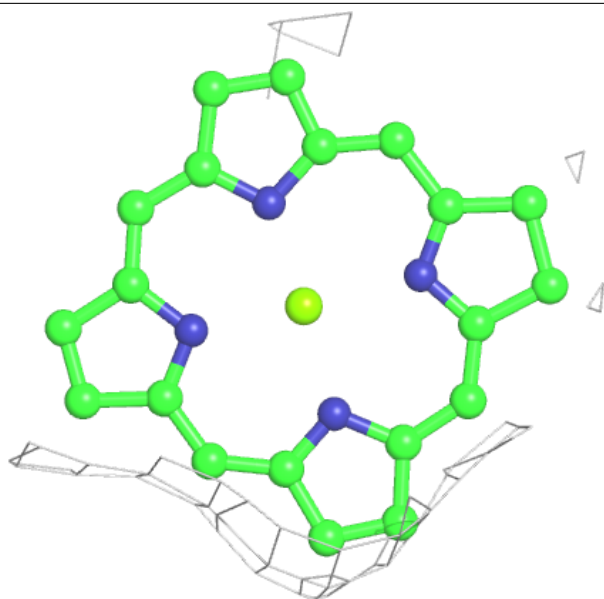
**Electron density around CLA 3 601:**

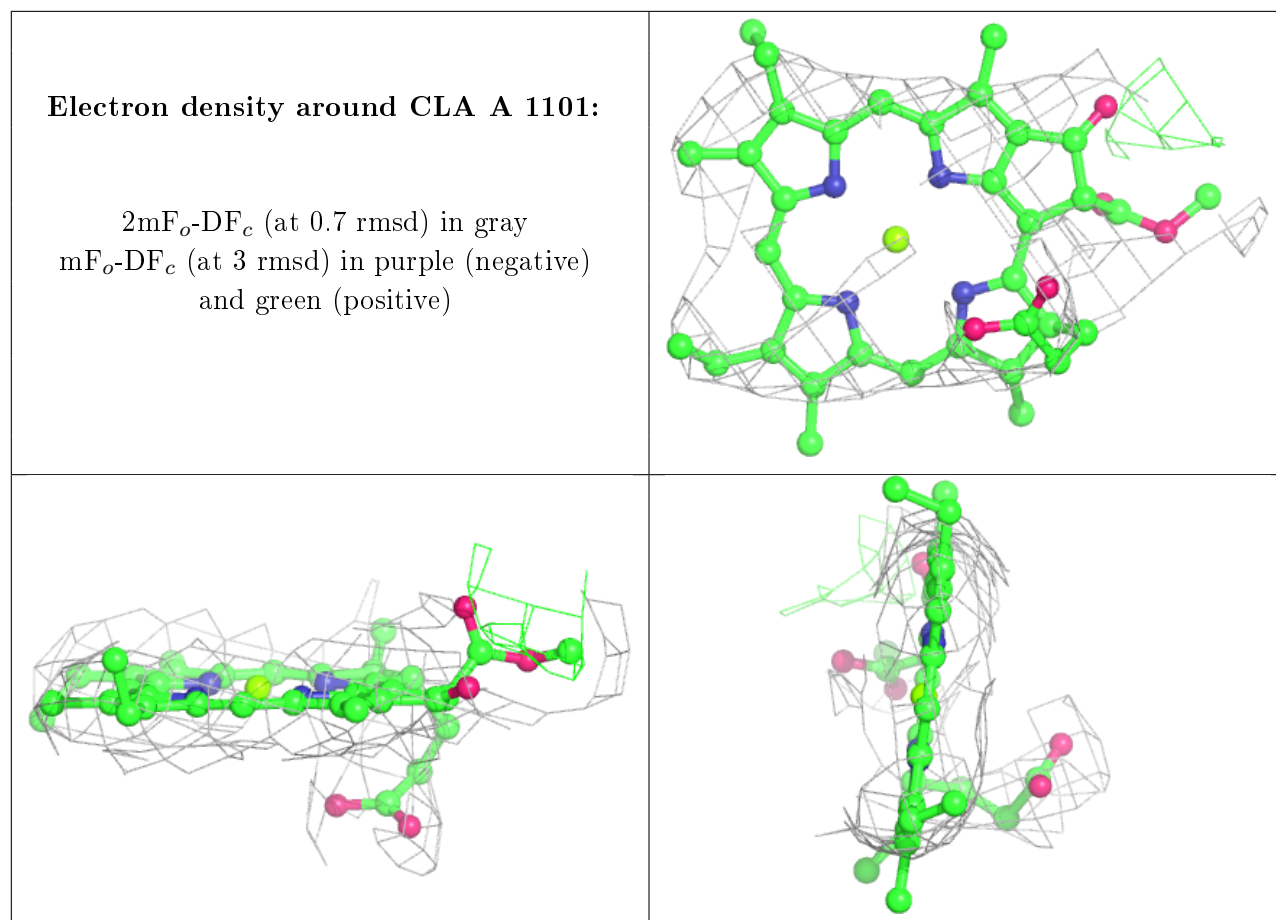
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 4 606:**

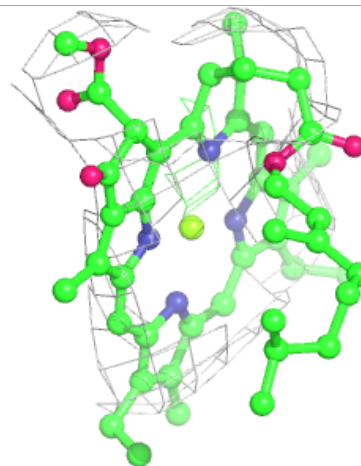
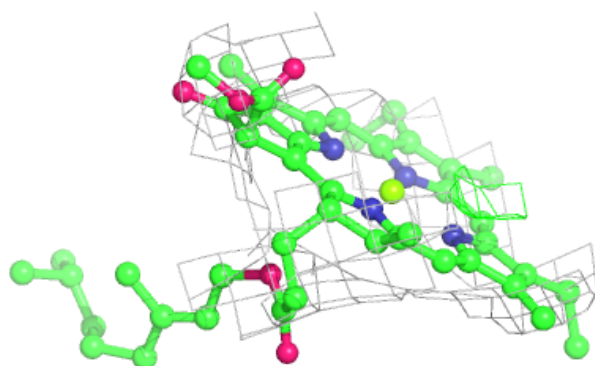
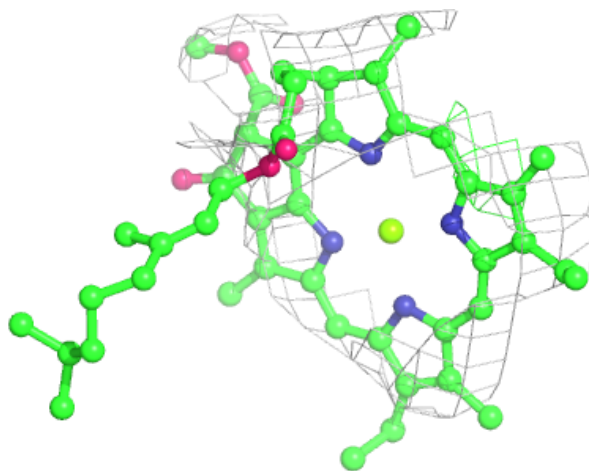
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





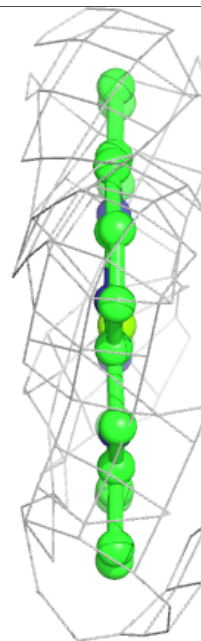
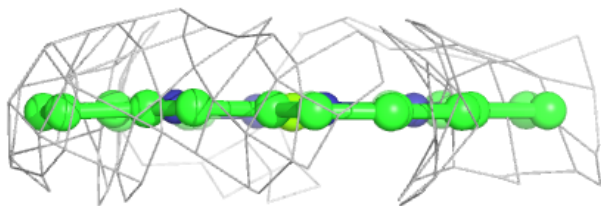
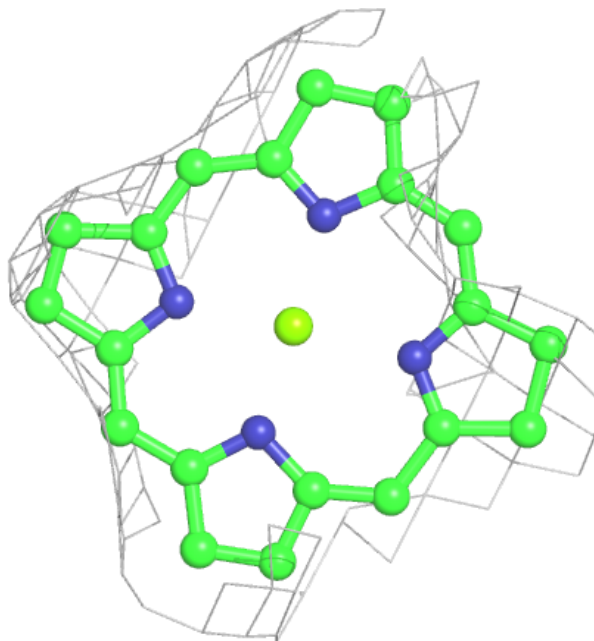
**Electron density around CLA B 1224:**

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



**Electron density around CLA 2 607:**

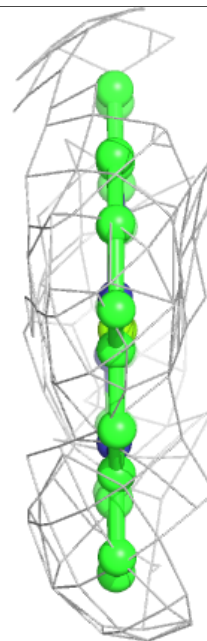
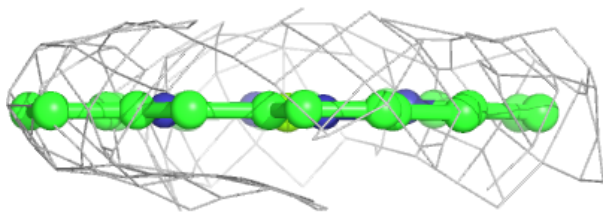
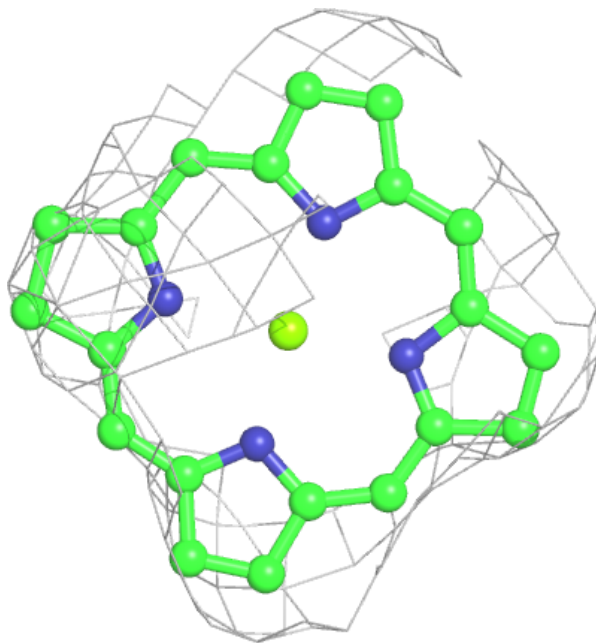
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





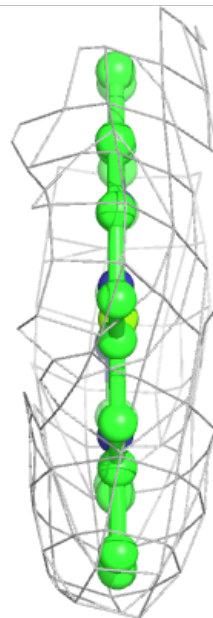
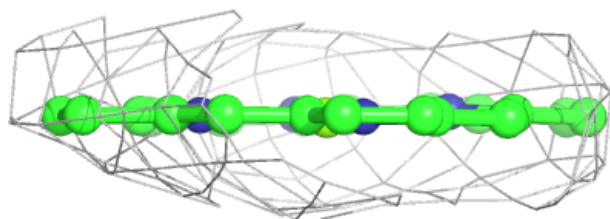
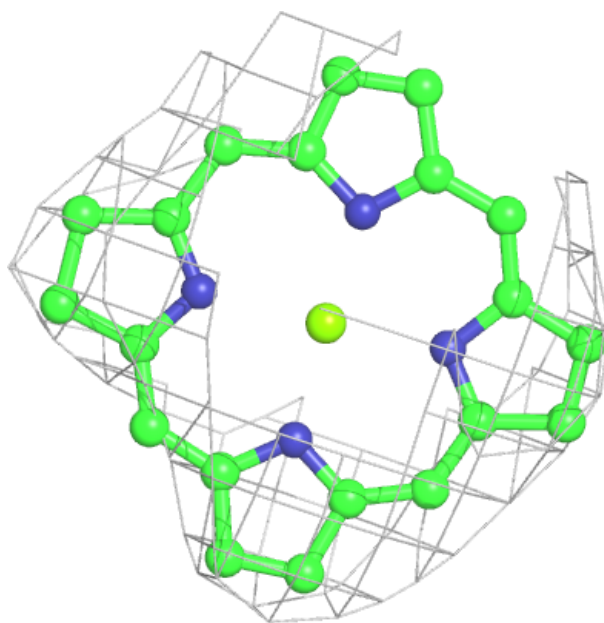
**Electron density around CLA A 1123:**

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



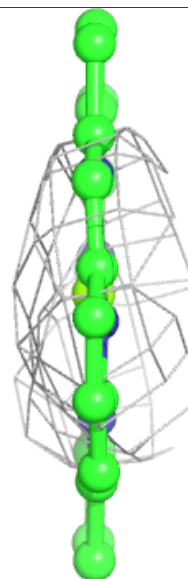
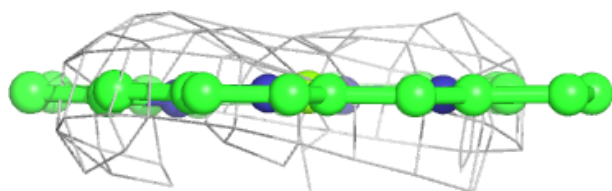
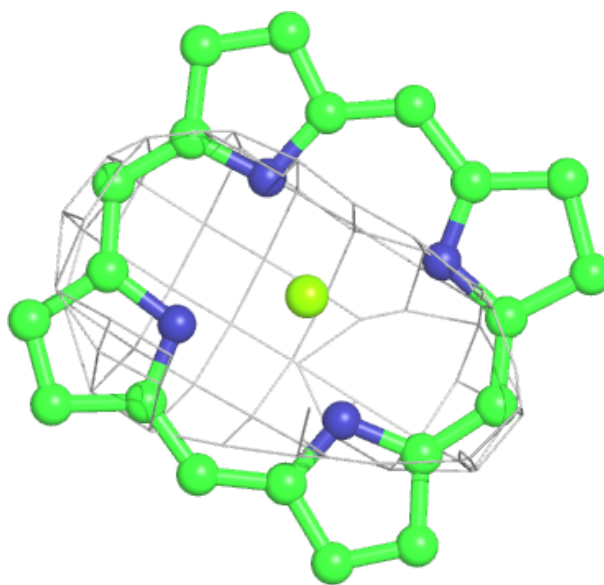
**Electron density around CLA 4 612:**

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



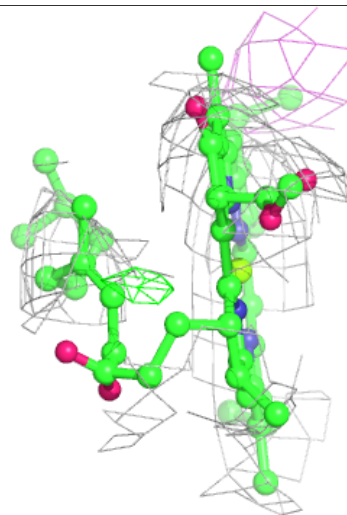
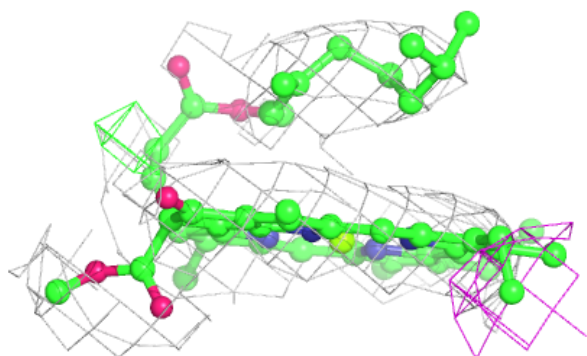
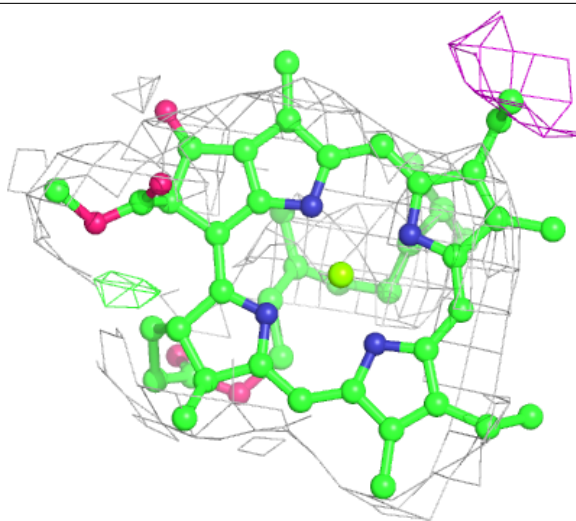
**Electron density around CLA 2 608:**

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



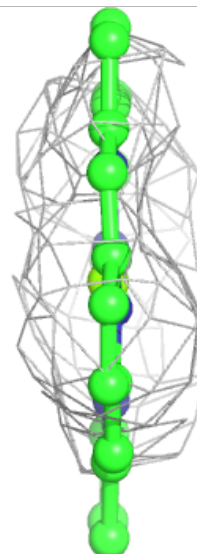
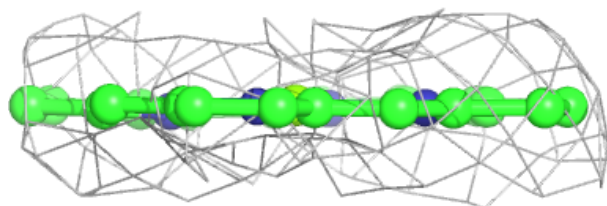
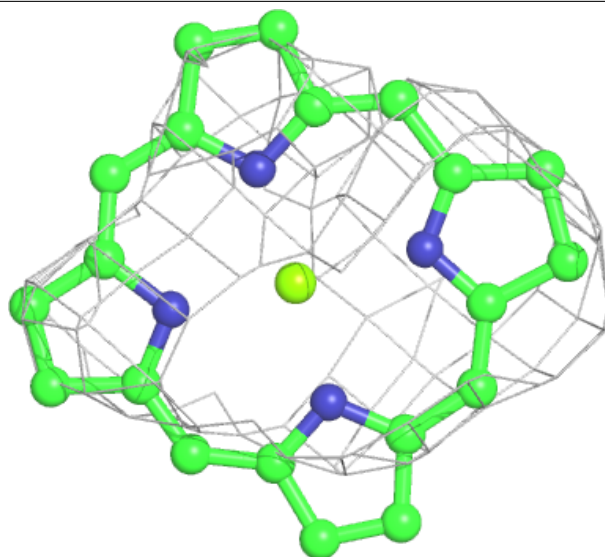
**Electron density around CLA A 1116:**

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



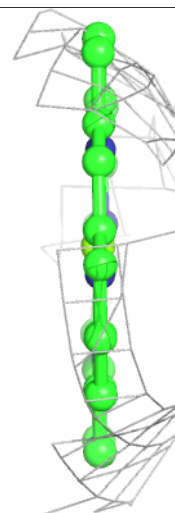
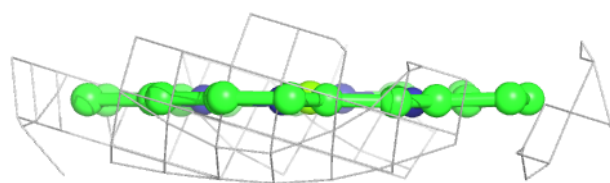
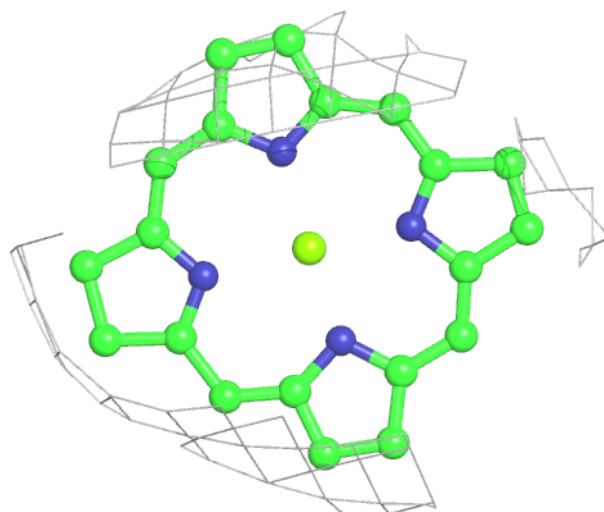
**Electron density around CLA A 1110:**

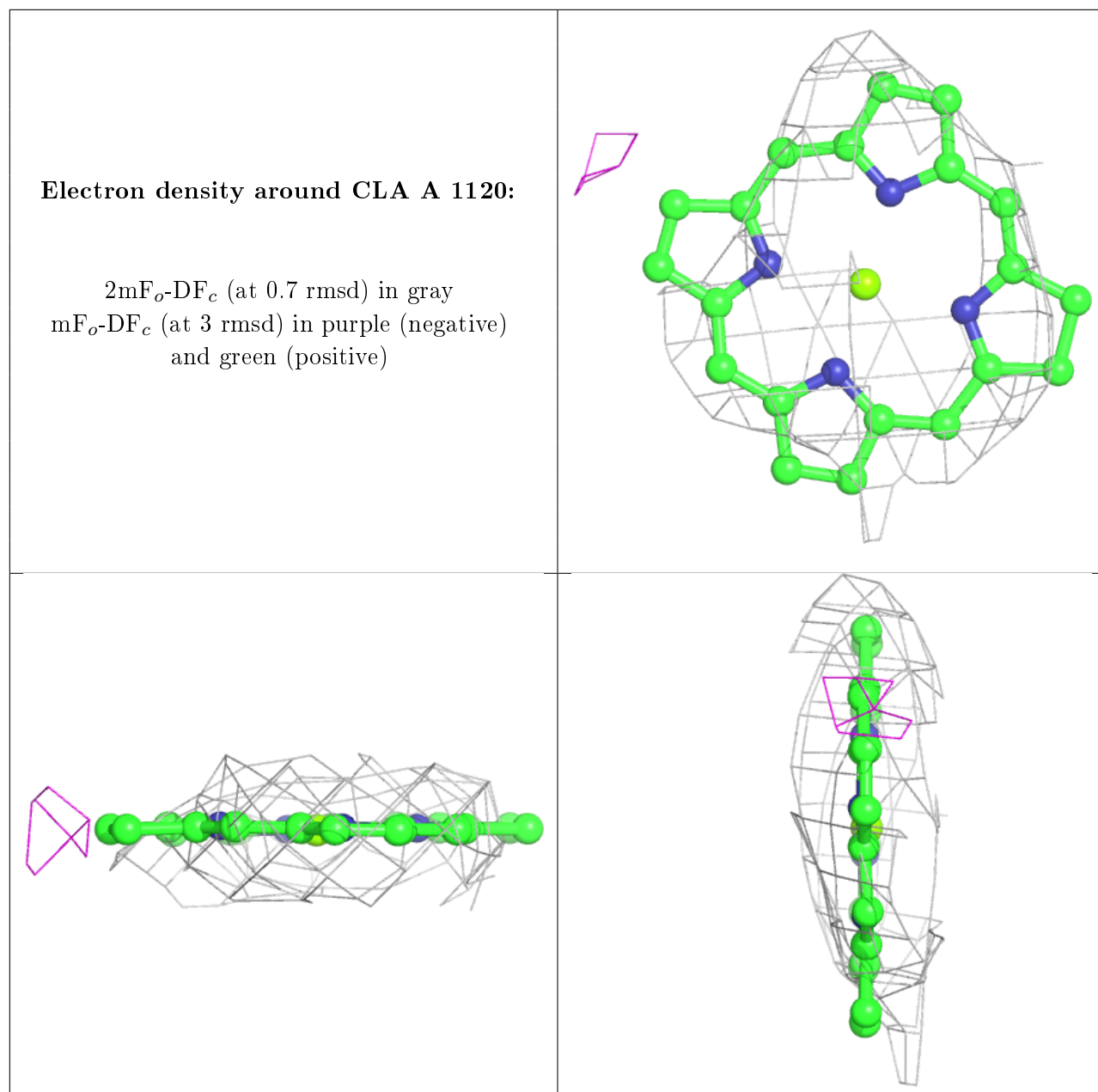
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

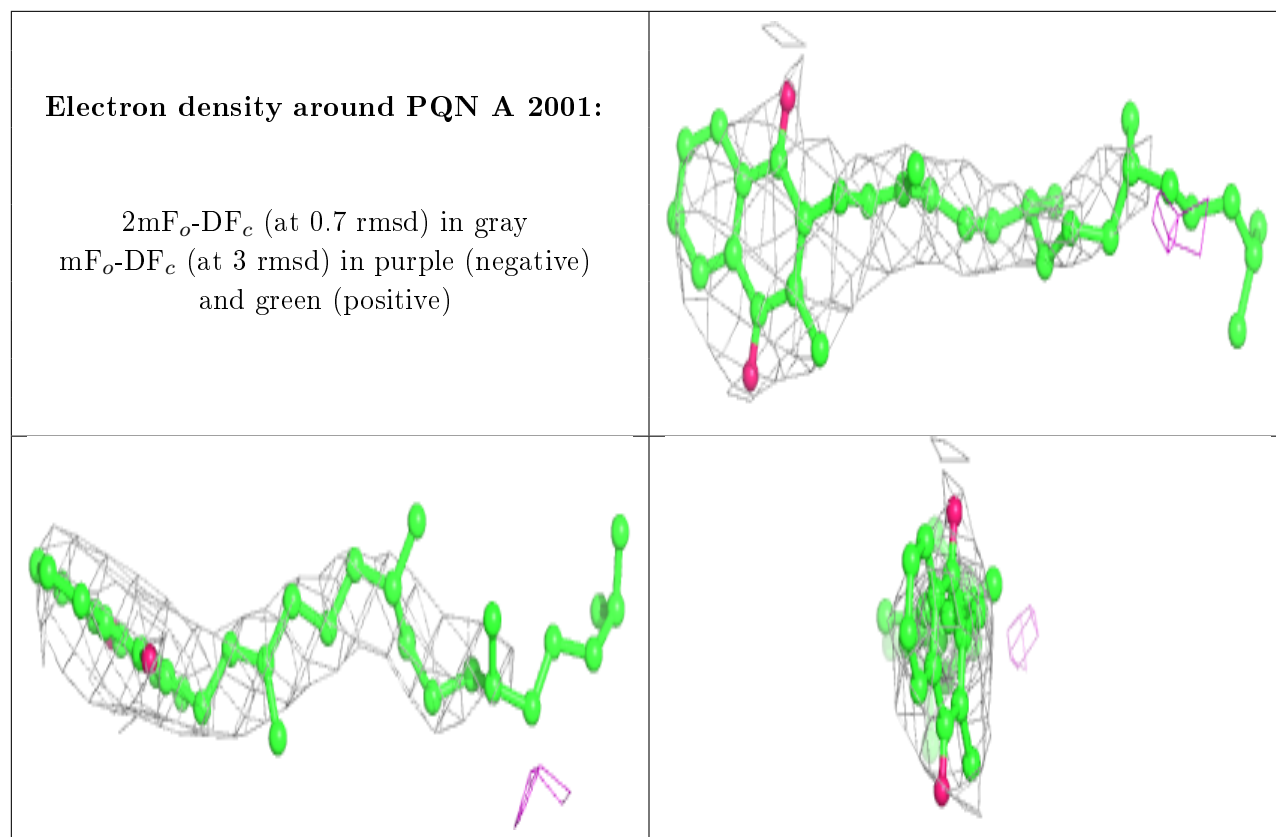


**Electron density around CLA L 1501:**

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



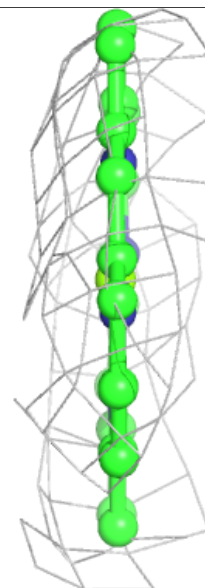
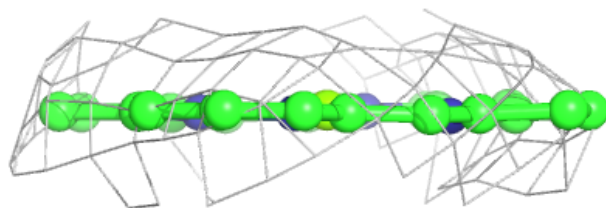
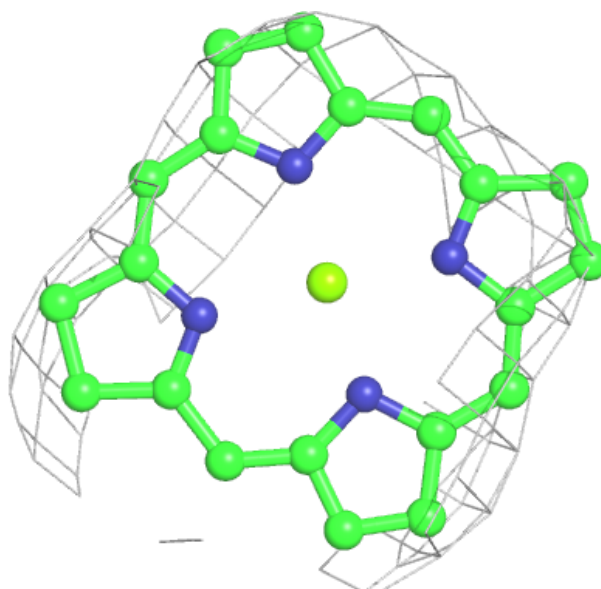






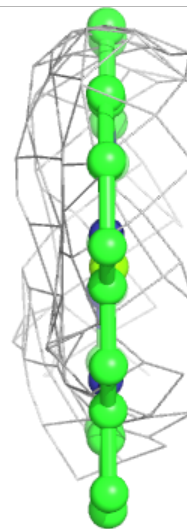
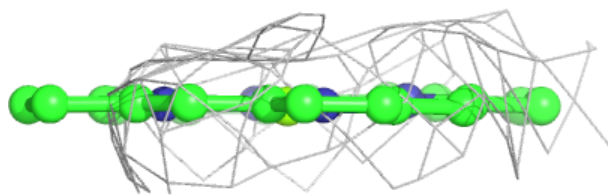
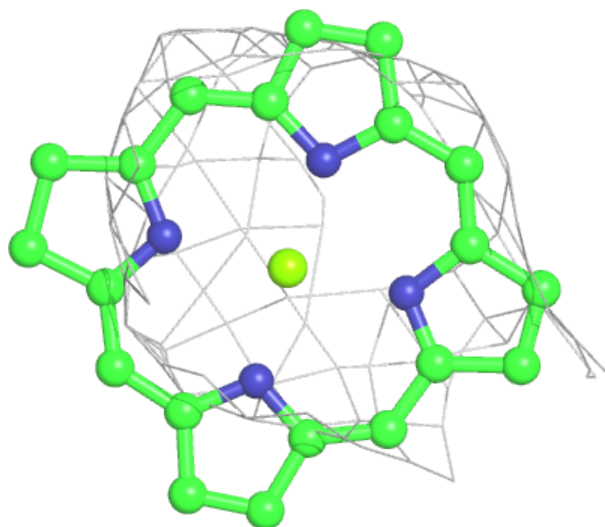
**Electron density around CLA A 1121:**

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



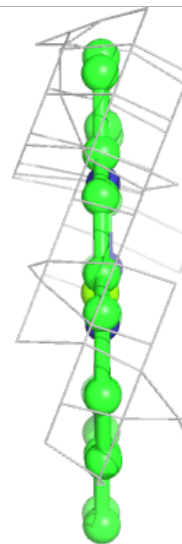
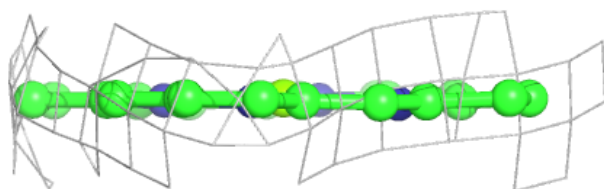
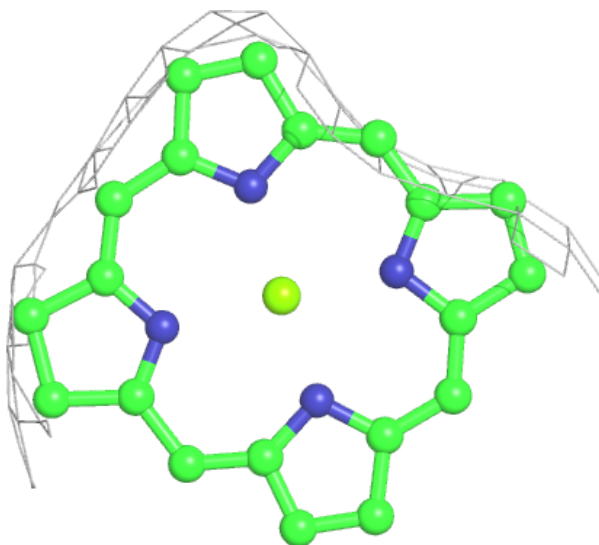
**Electron density around CLA B 1204:**

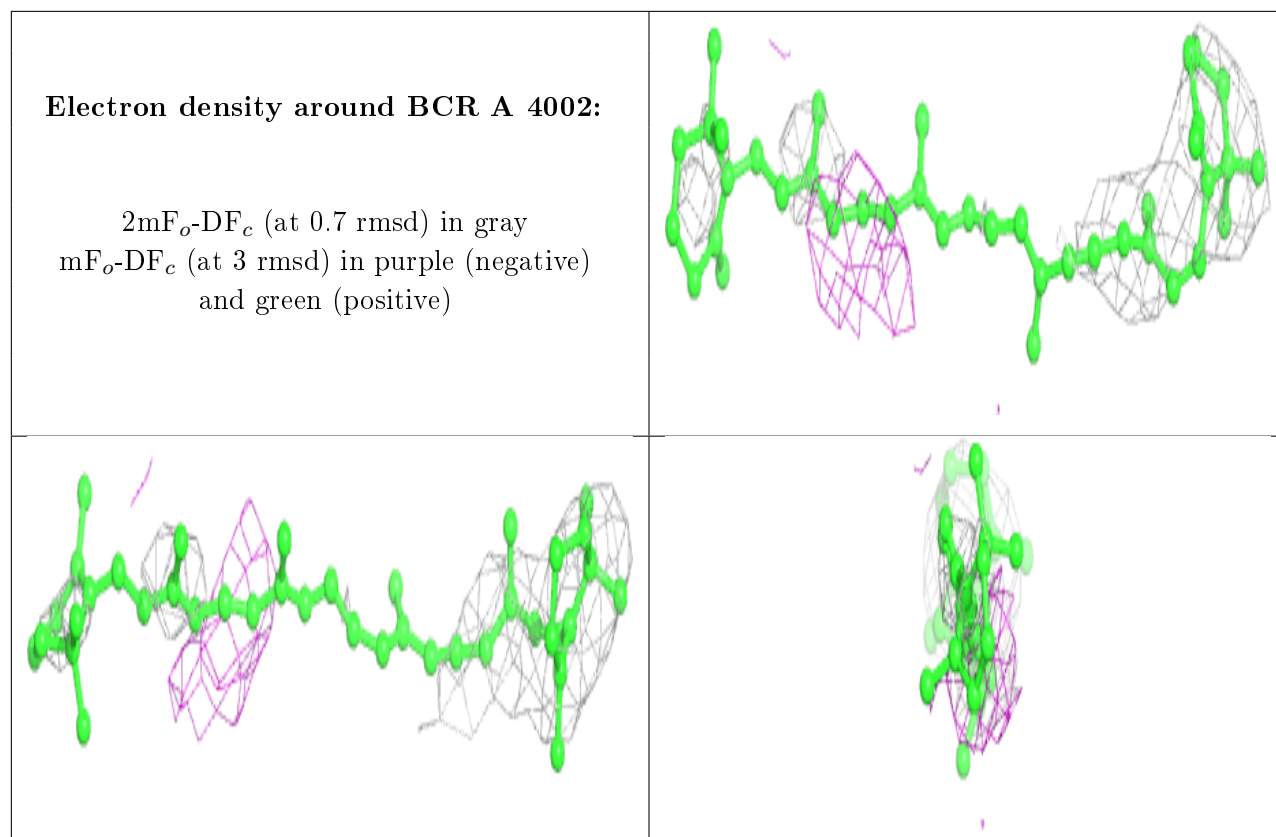
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

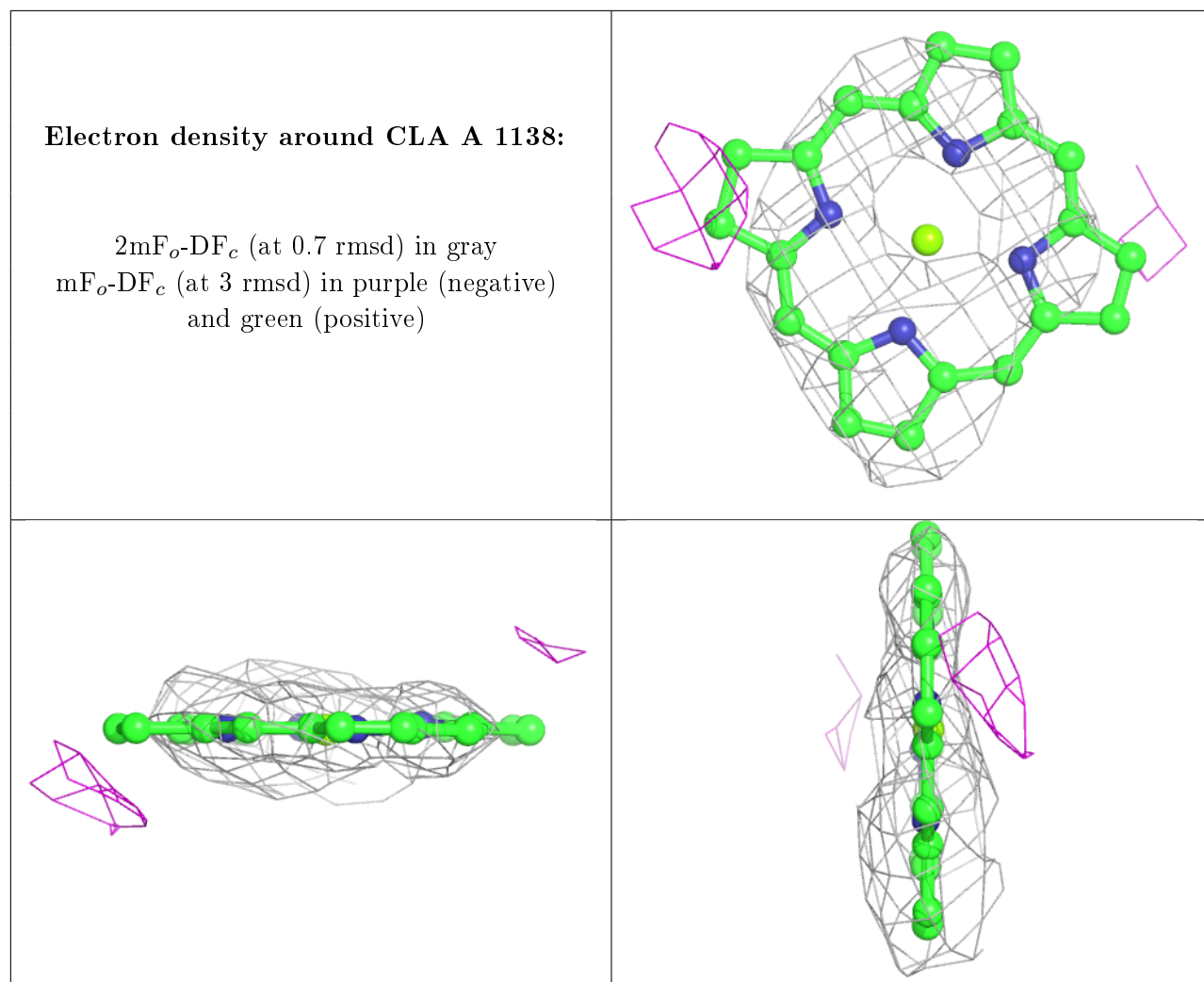


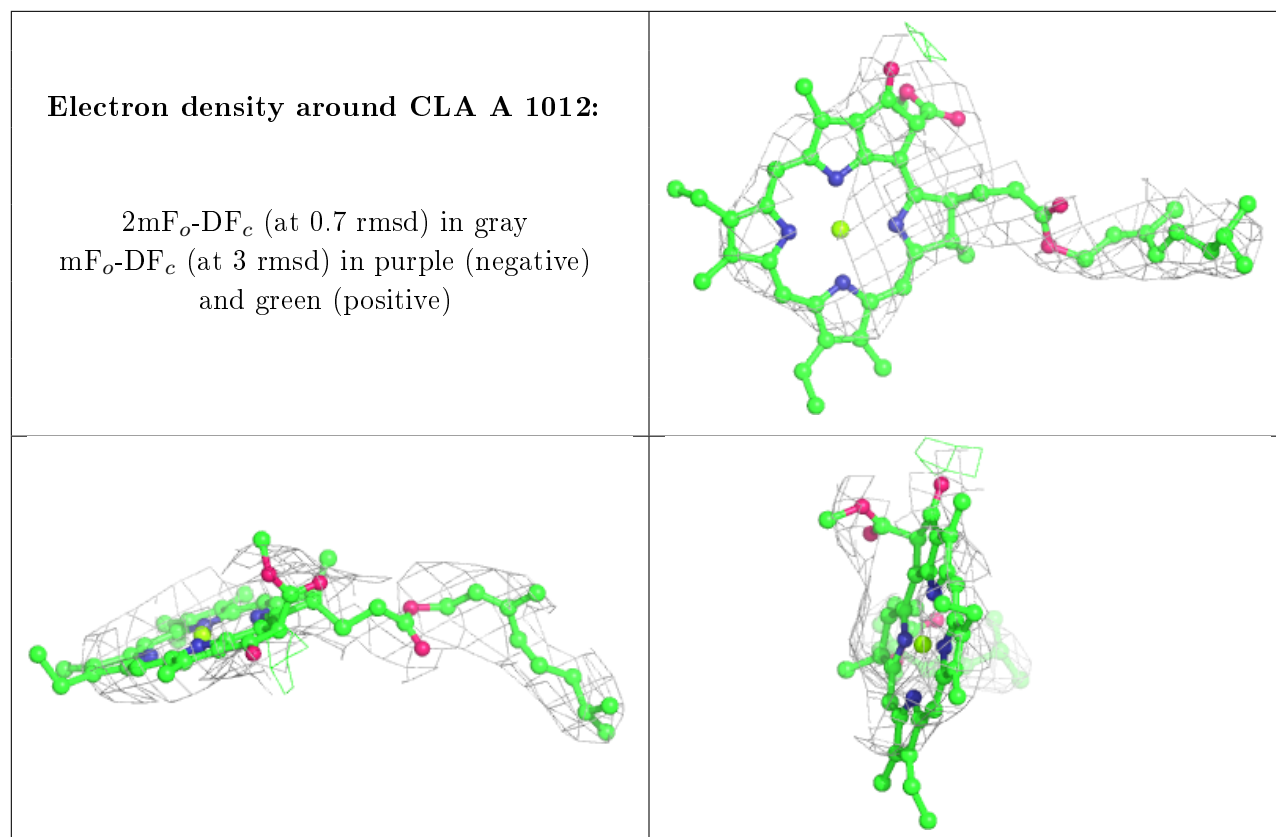
**Electron density around CLA B 1211:**

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



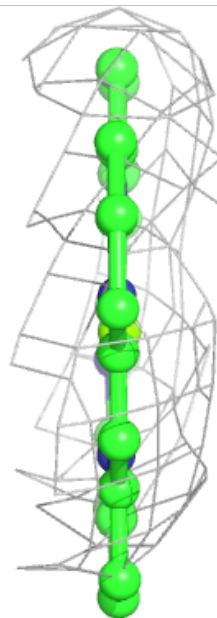
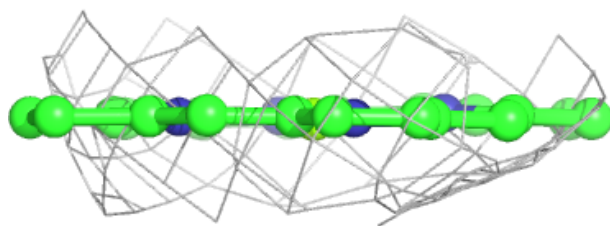
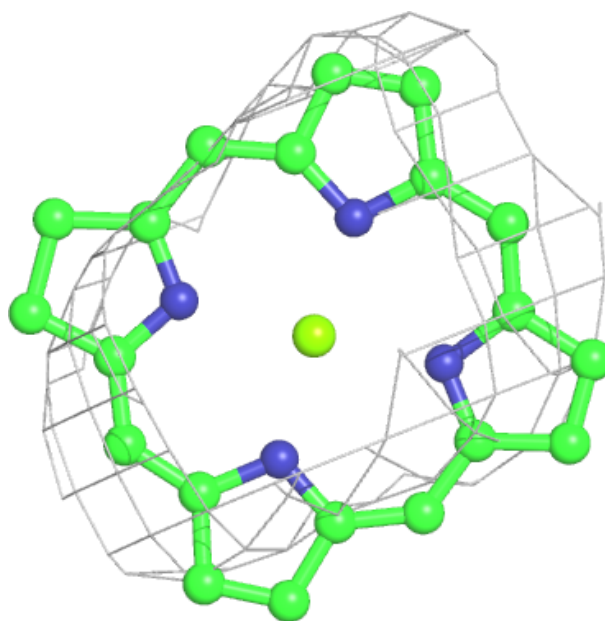






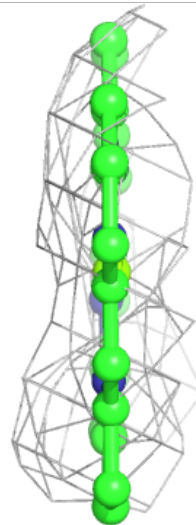
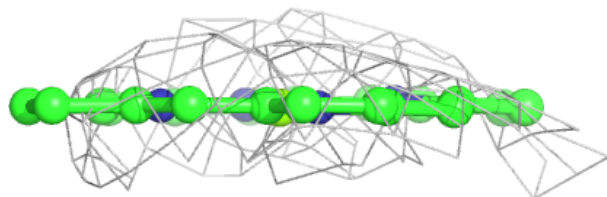
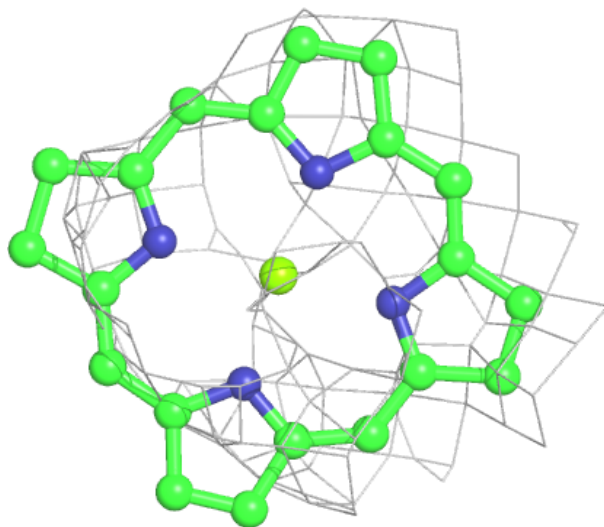
**Electron density around CLA 2 614:**

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

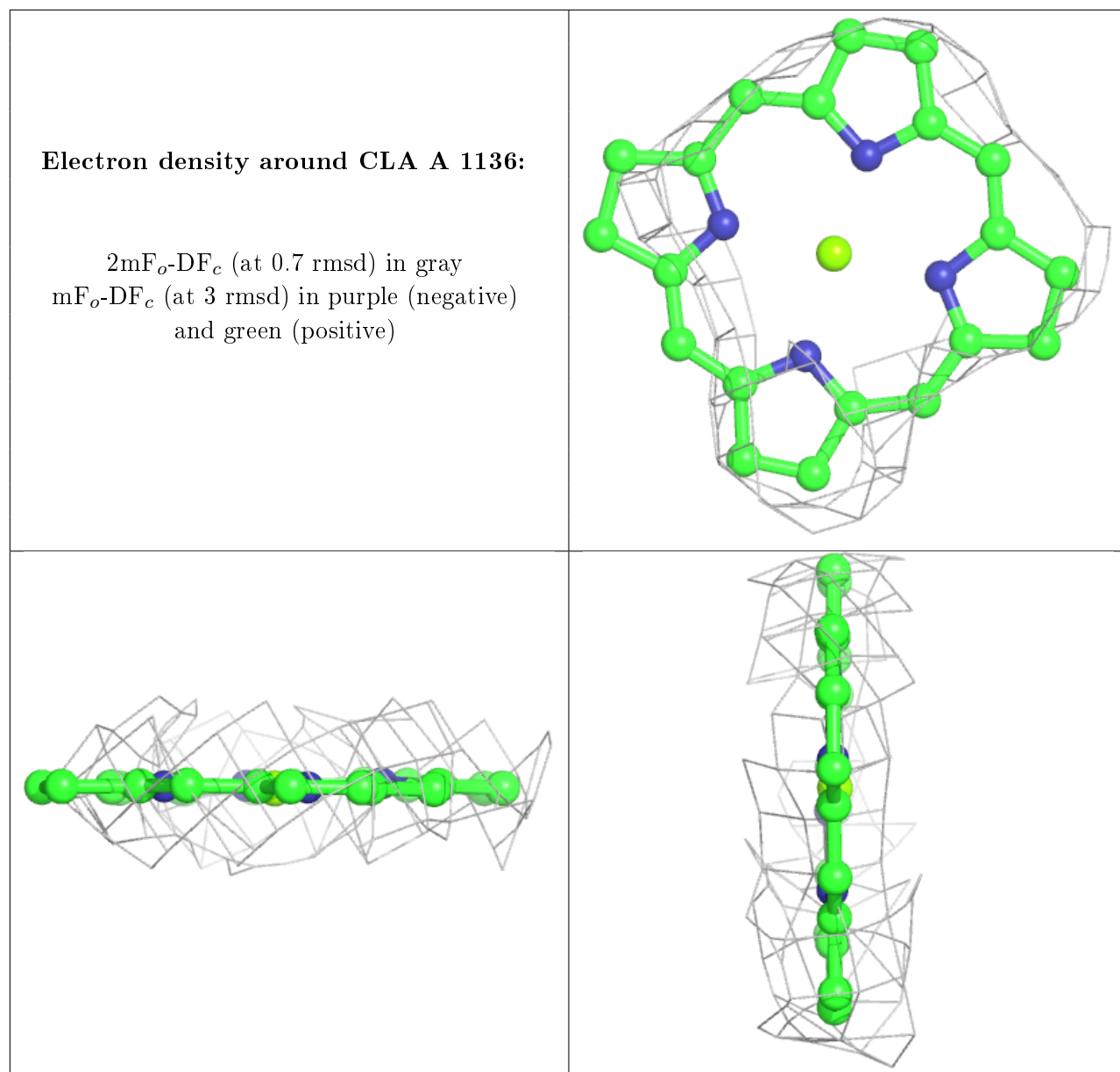


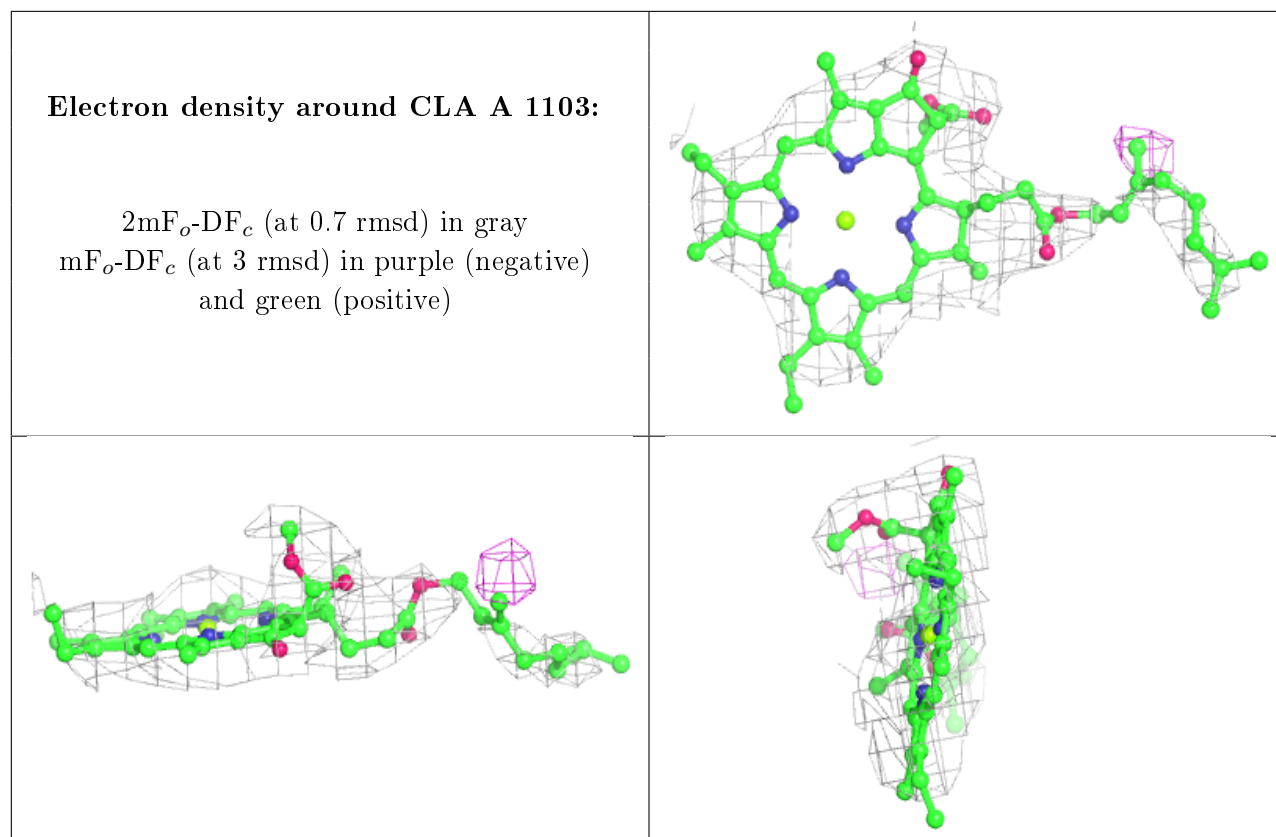
**Electron density around CLA 3 606:**

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



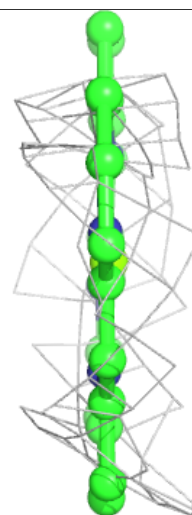
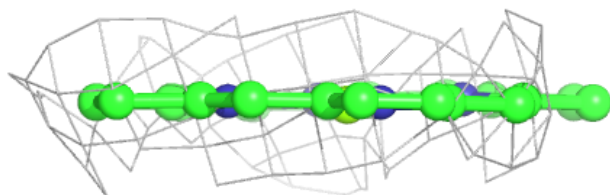
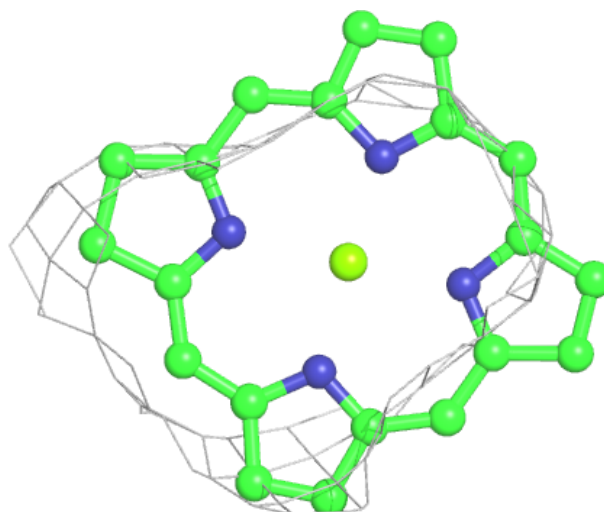






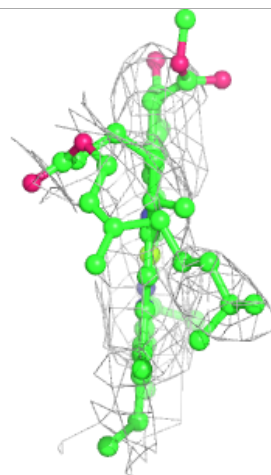
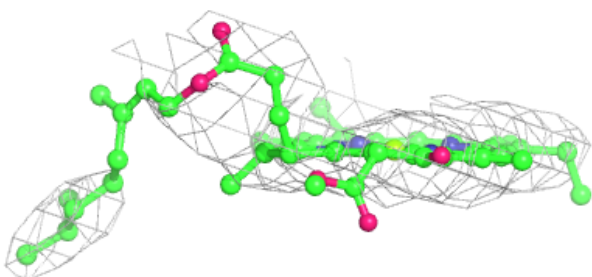
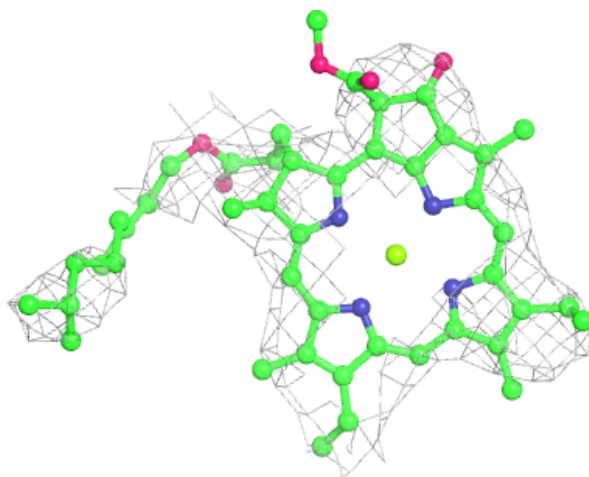
**Electron density around CLA 3 604:**

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



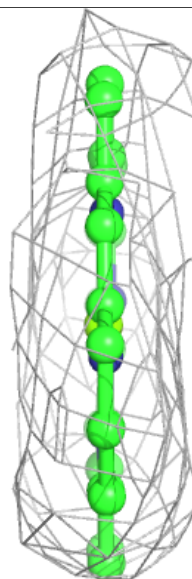
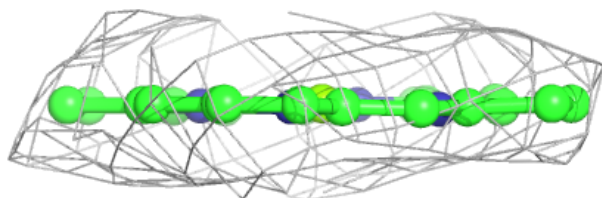
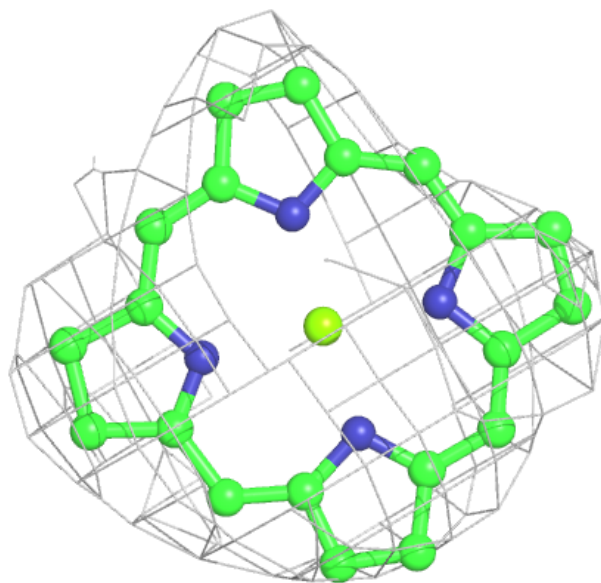
**Electron density around CLA A 1013:**

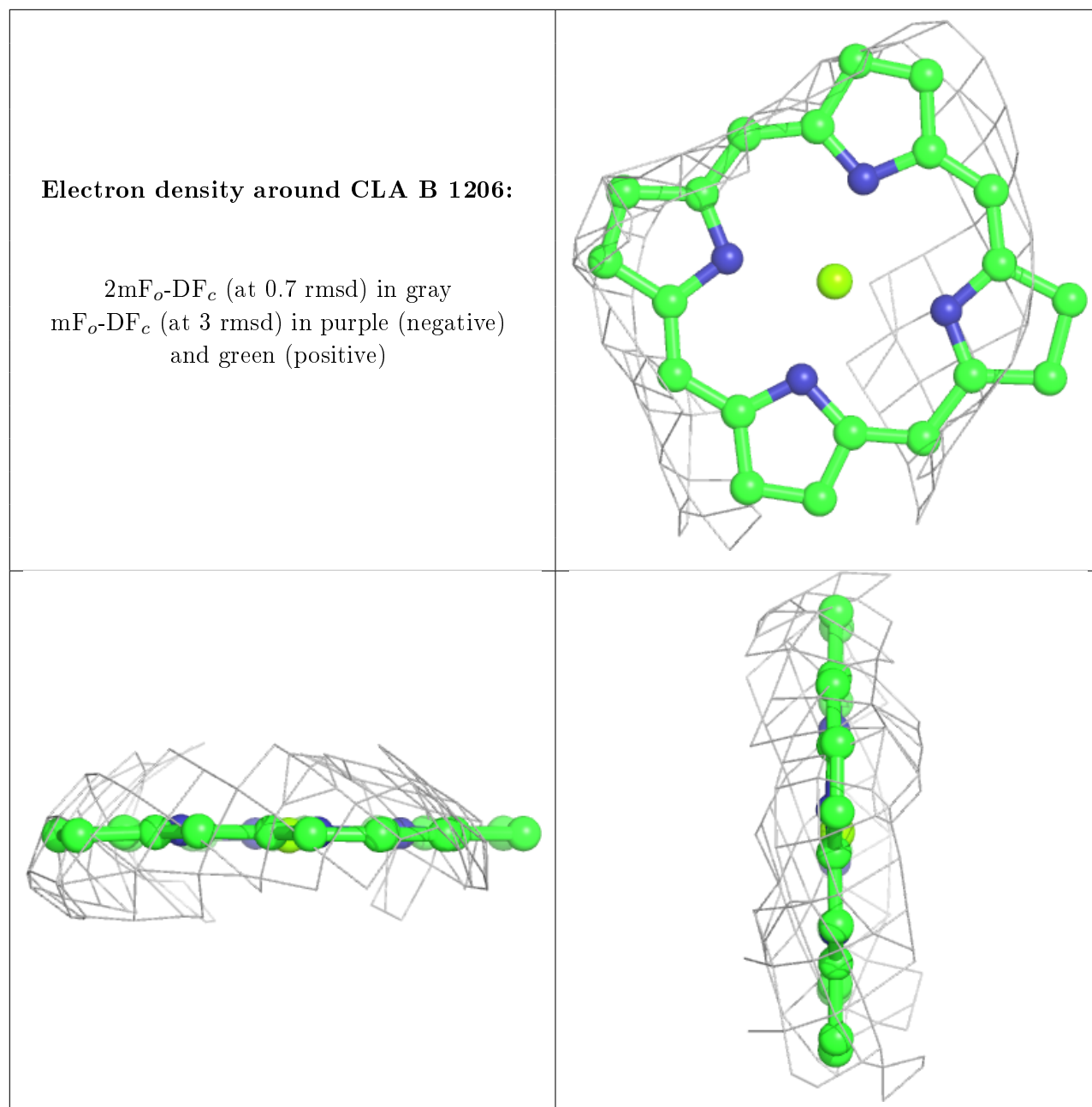
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1022:**

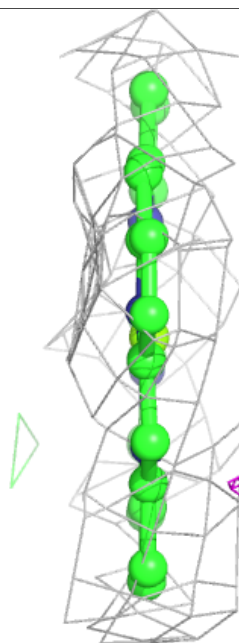
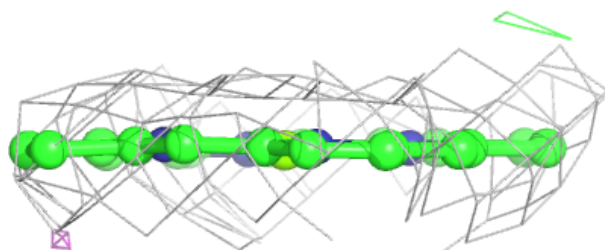
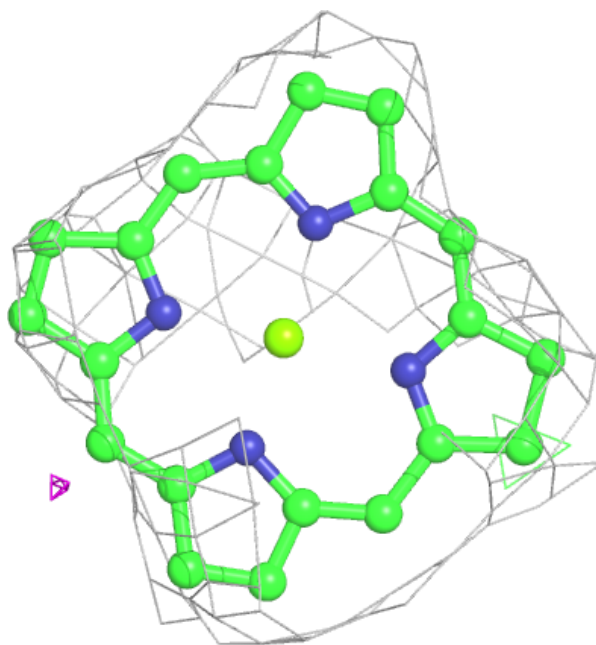
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





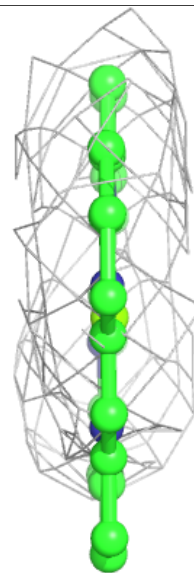
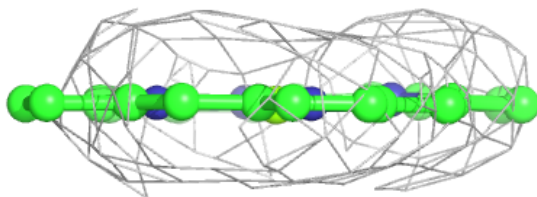
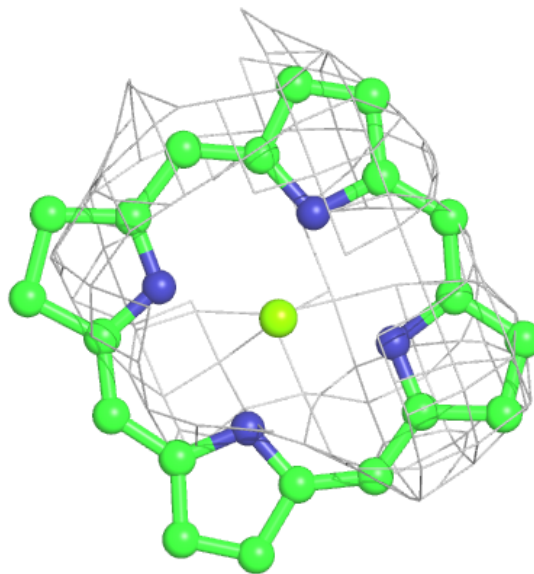
**Electron density around CLA A 1112:**

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



**Electron density around CLA A 1133:**

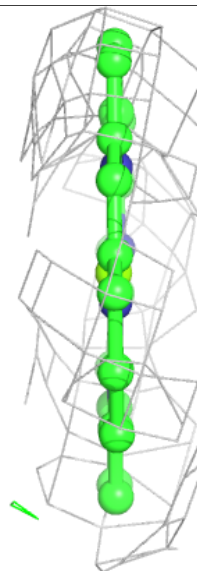
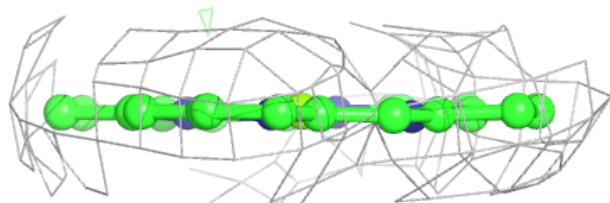
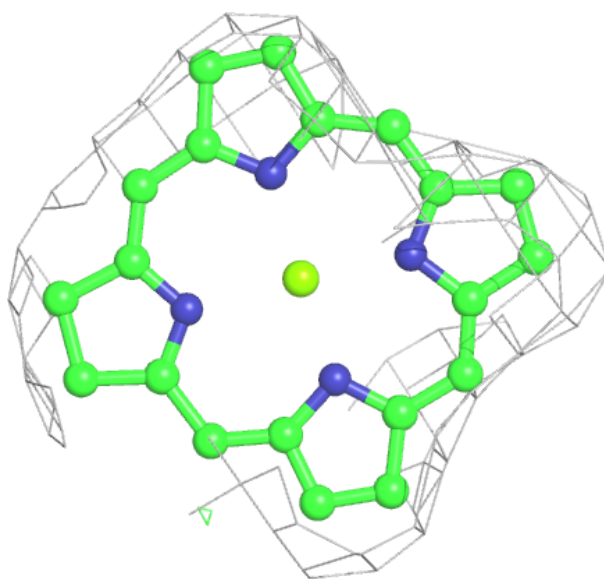
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





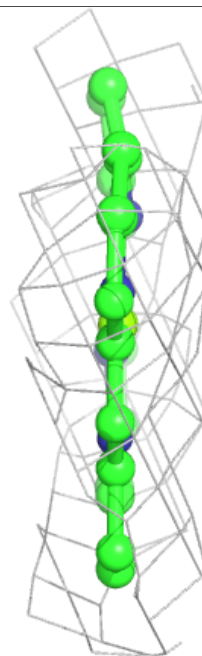
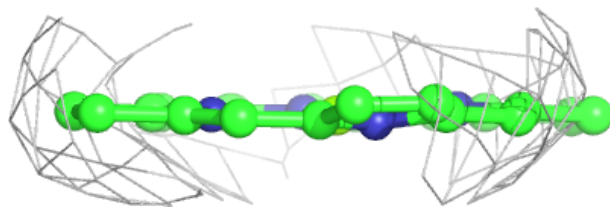
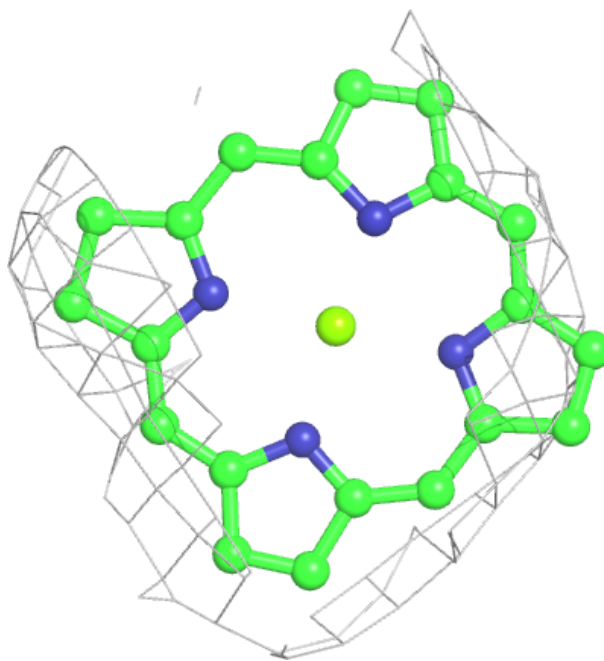
**Electron density around CLA A 1109:**

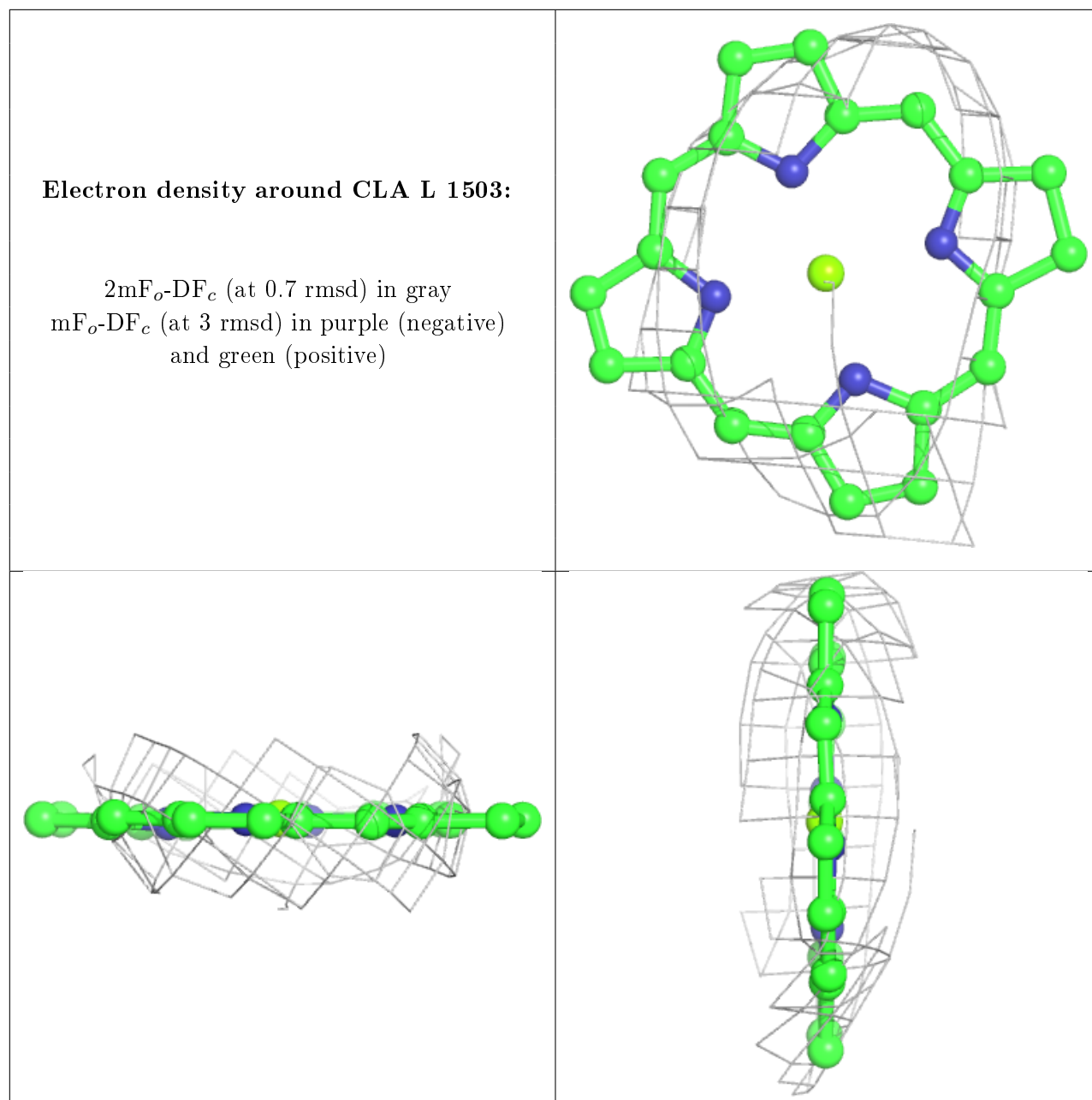
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1228:**

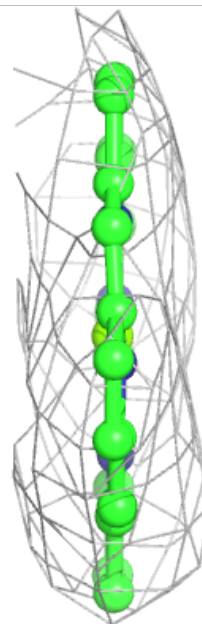
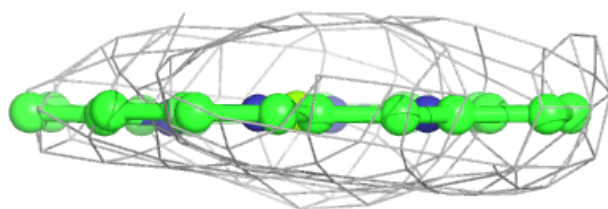
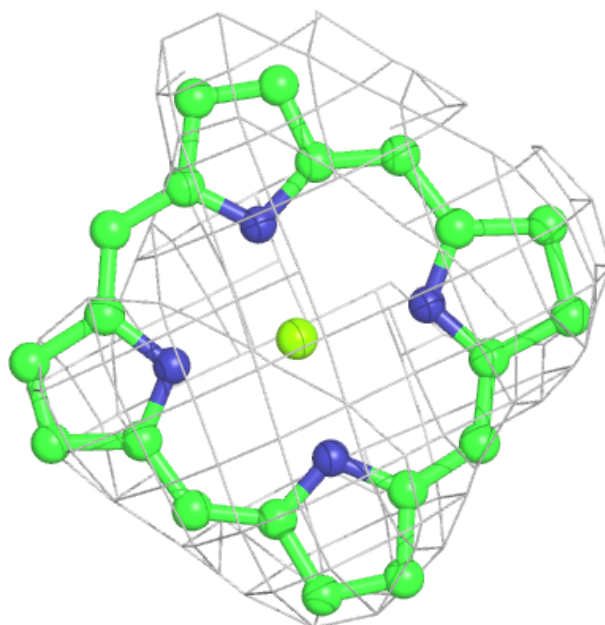
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





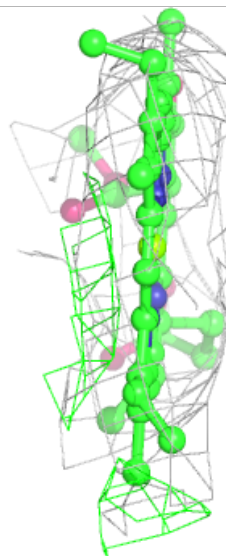
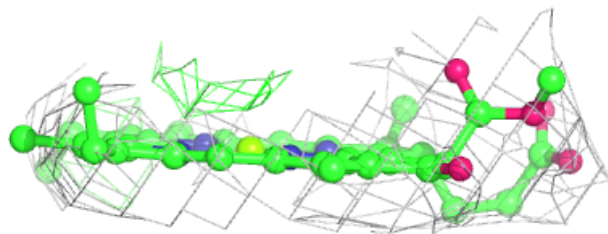
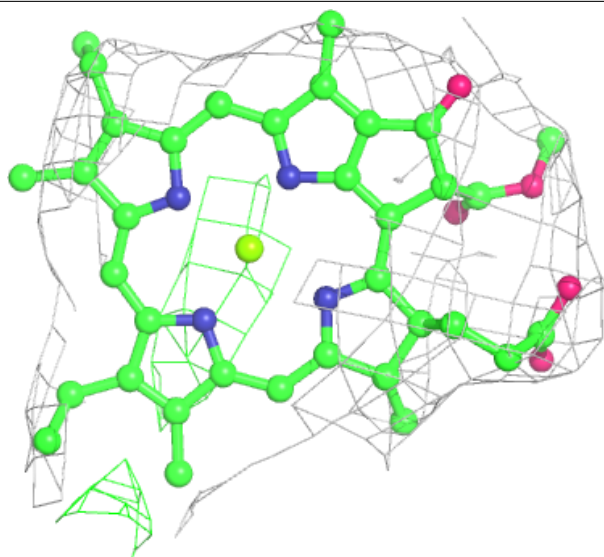
**Electron density around CLA B 1238:**

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



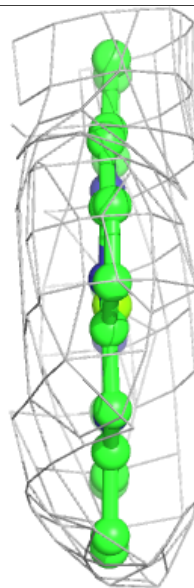
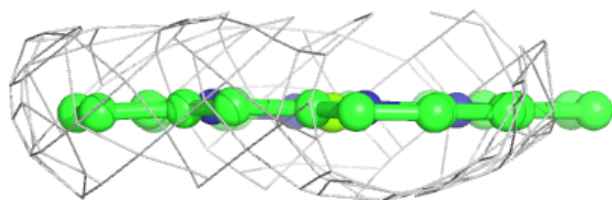
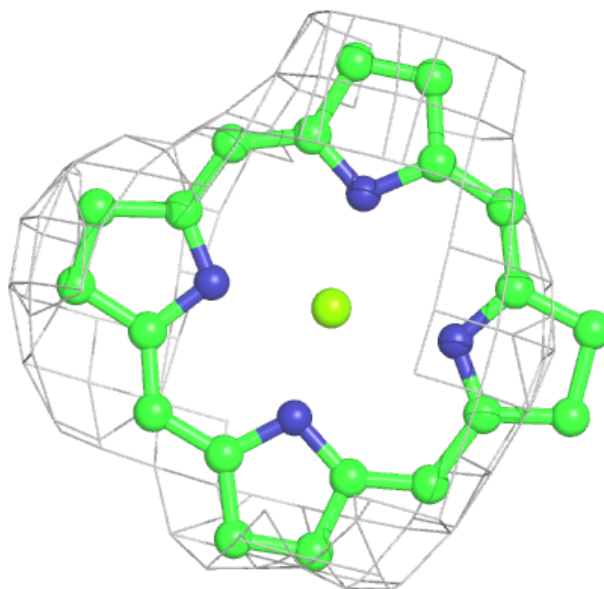
**Electron density around CLA A 1131:**

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



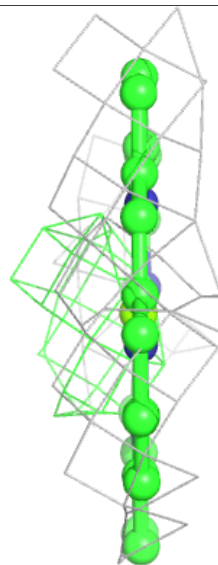
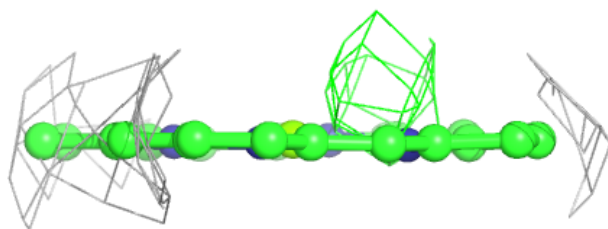
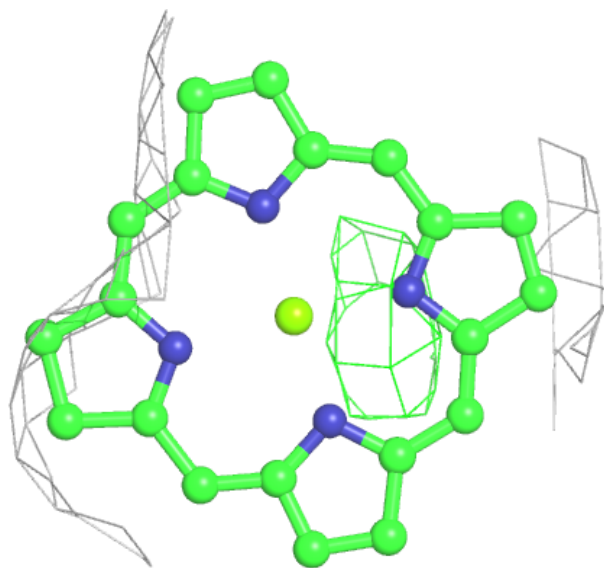
**Electron density around CLA B 1202:**

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



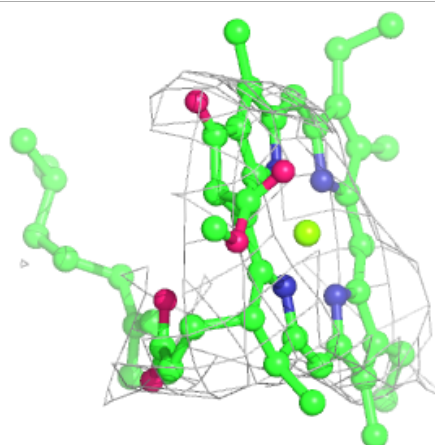
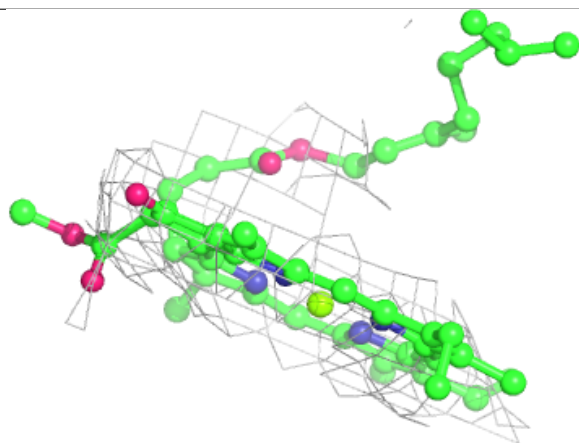
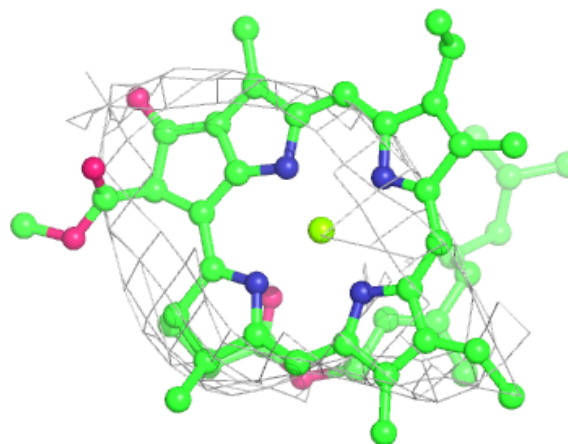
**Electron density around CLA 2 612:**

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

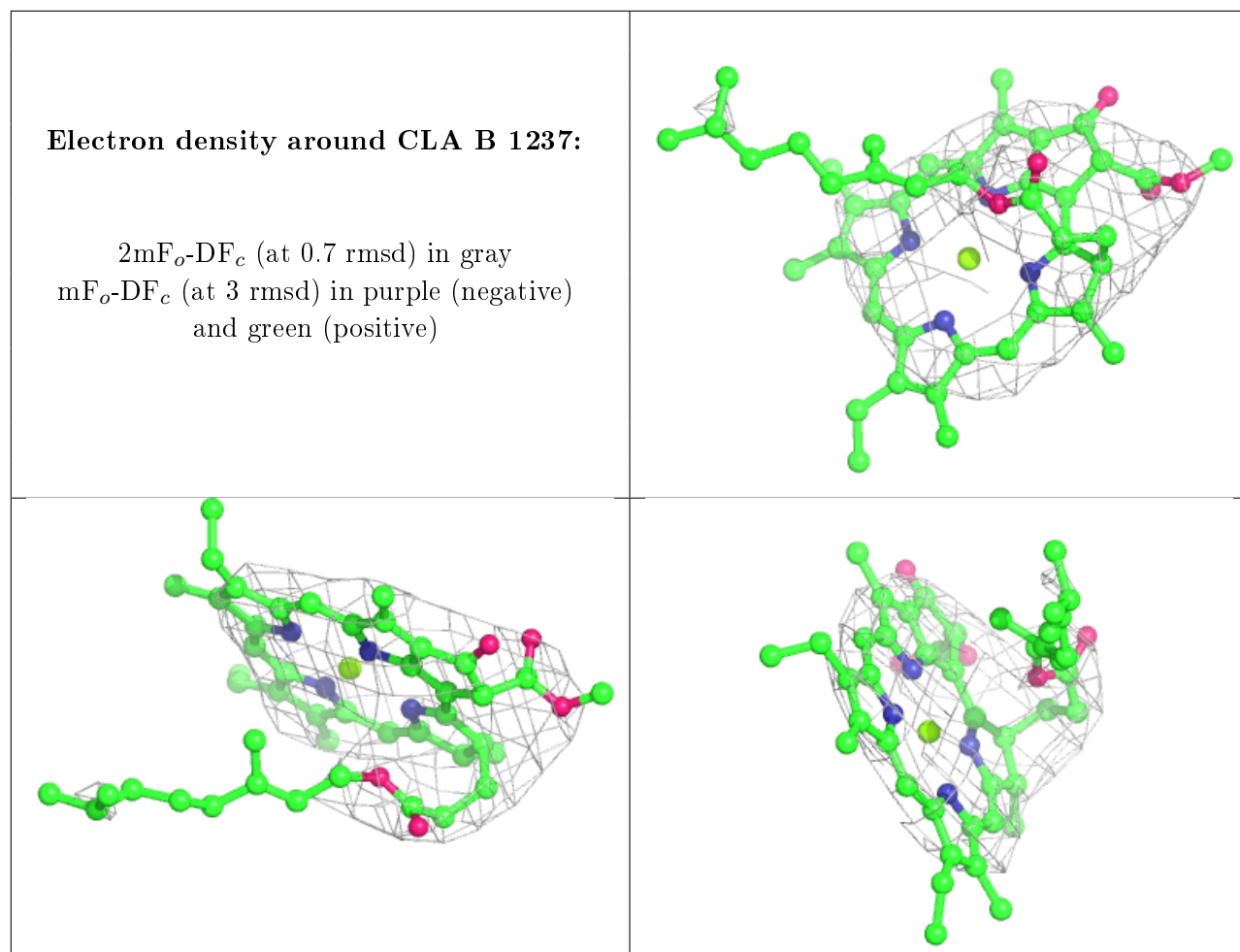


**Electron density around CLA A 1130:**

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

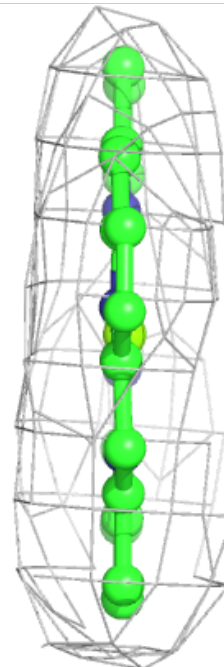
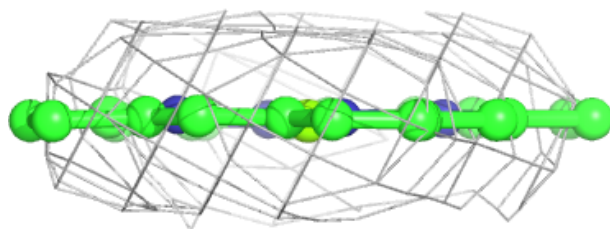
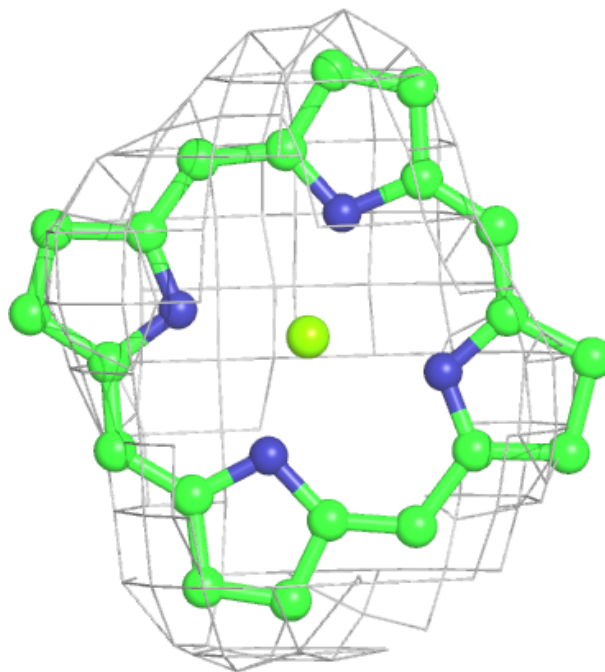


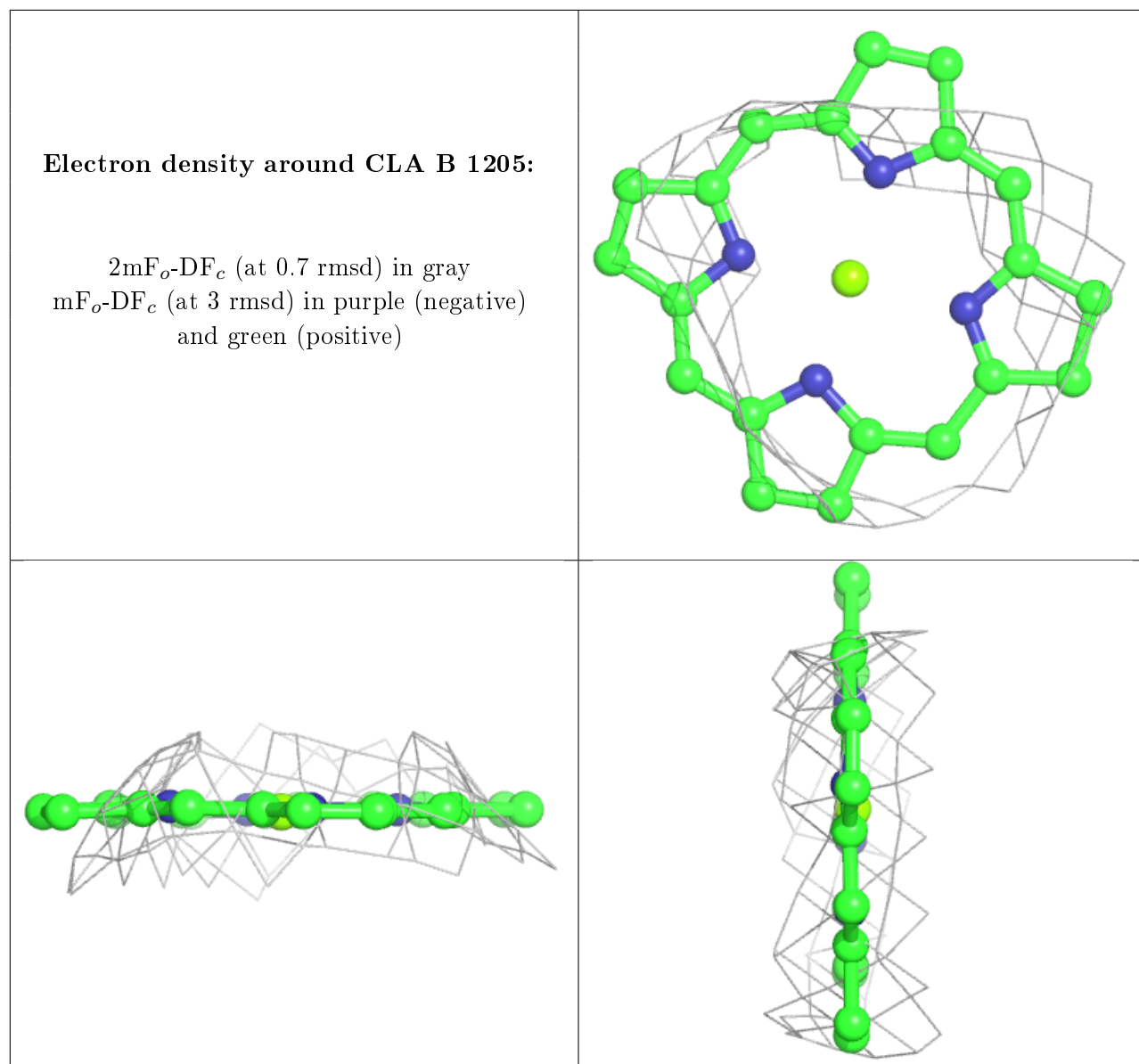


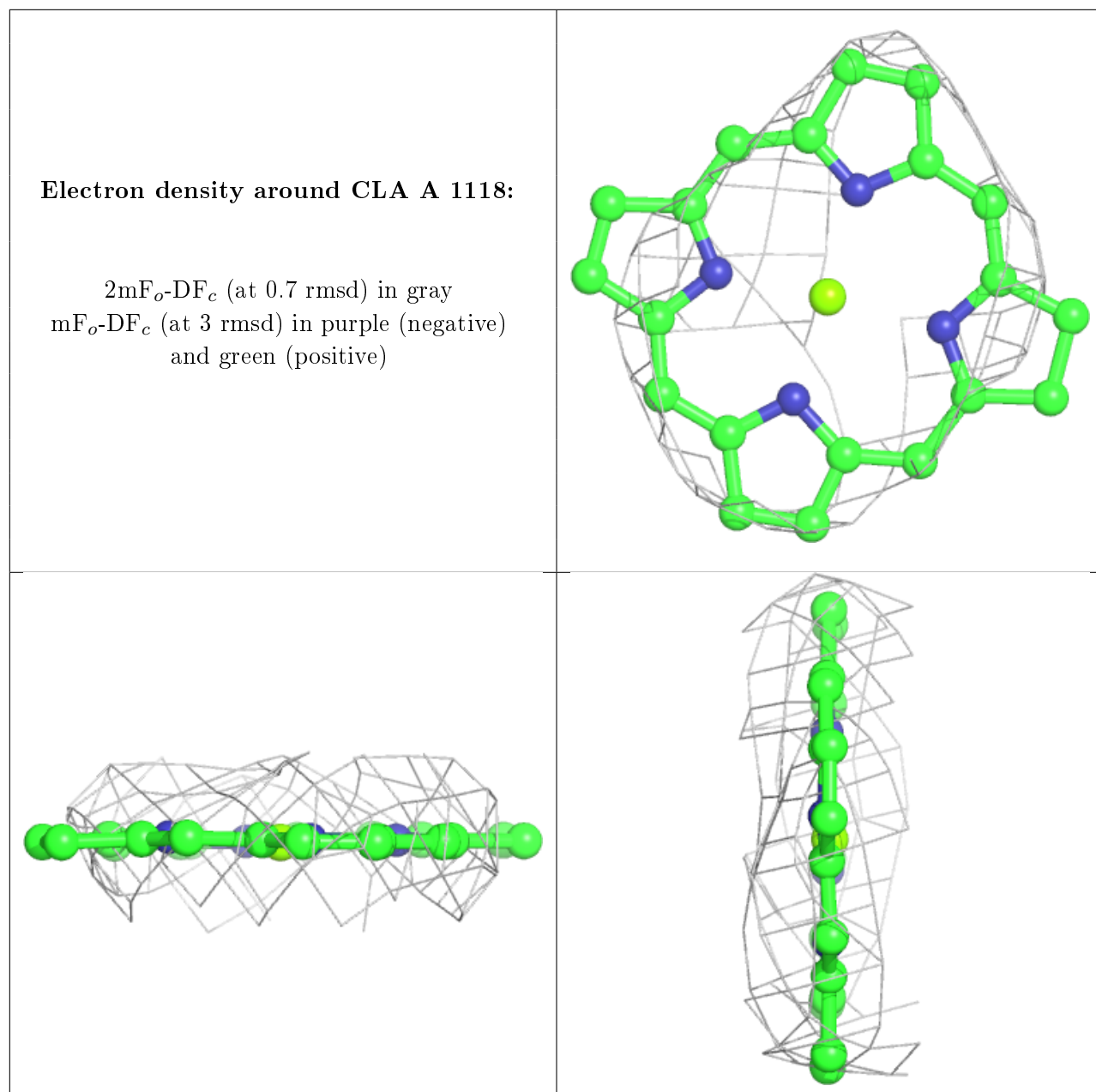


**Electron density around CLA A 1139:**

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

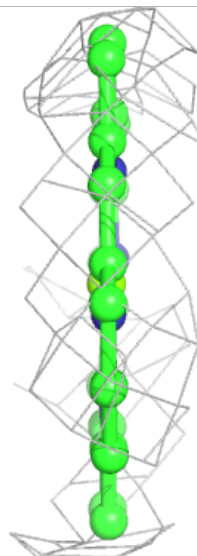
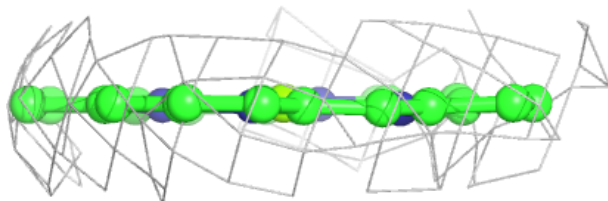
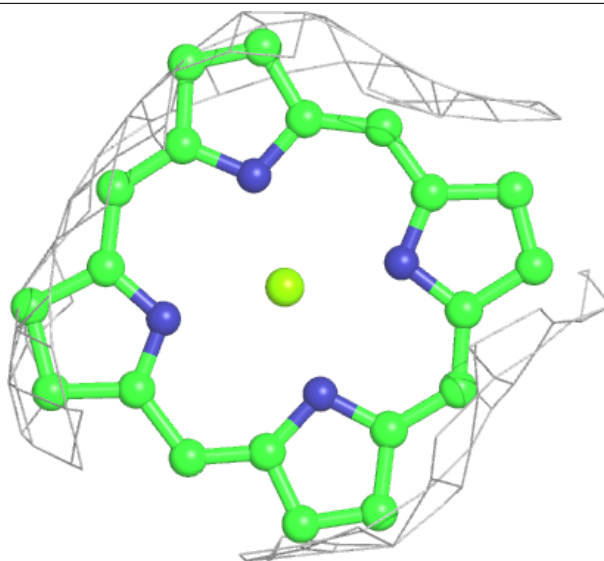






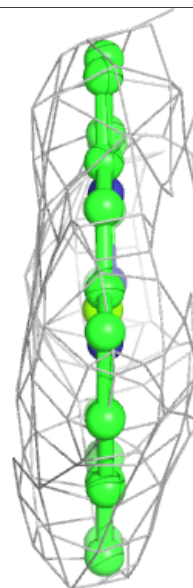
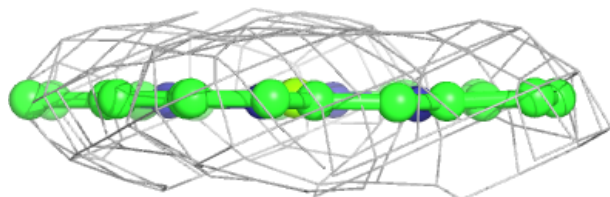
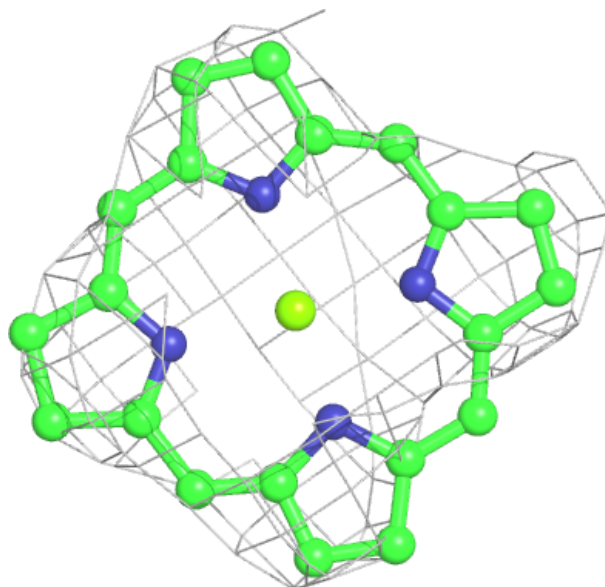
**Electron density around CLA A 1134:**

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



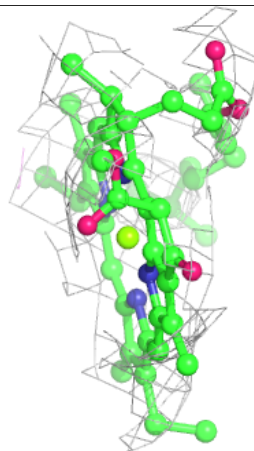
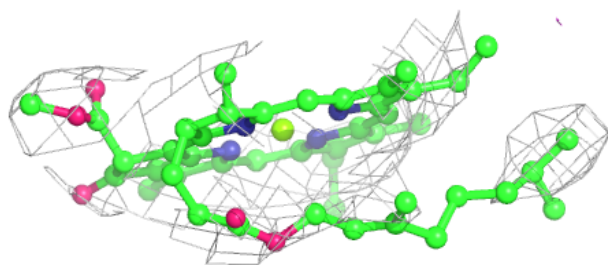
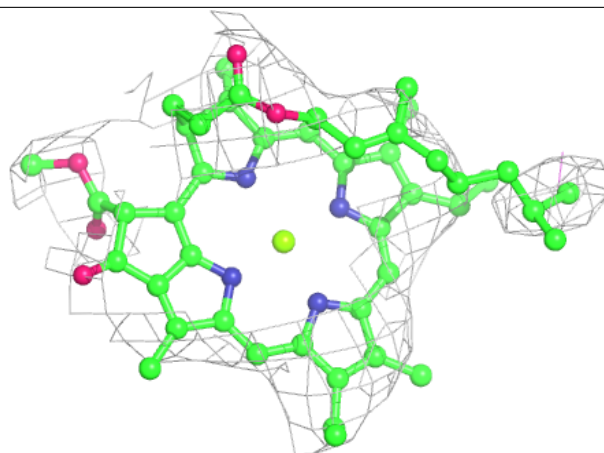
**Electron density around CLA A 1135:**

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



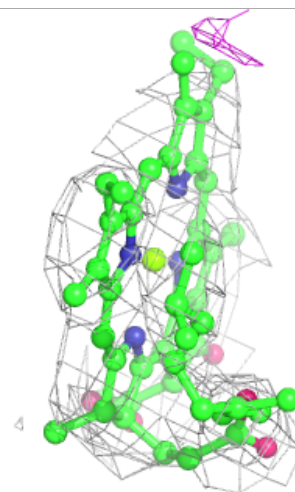
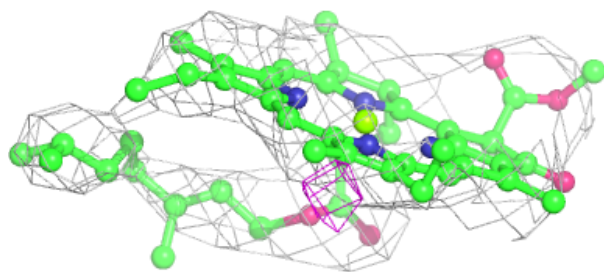
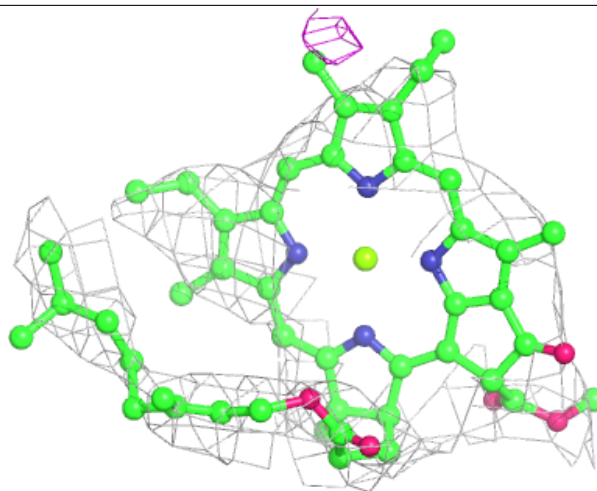
**Electron density around CLA A 1117:**

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



**Electron density around CLA A 1105:**

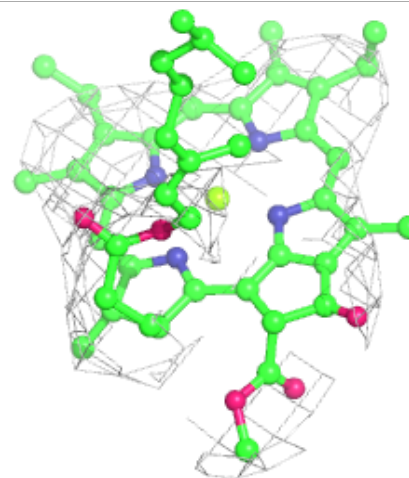
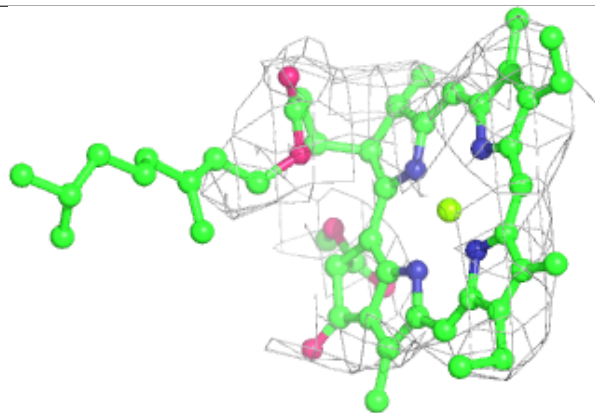
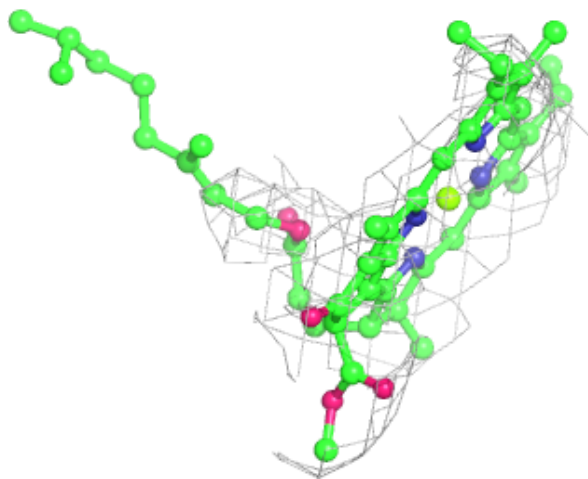
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

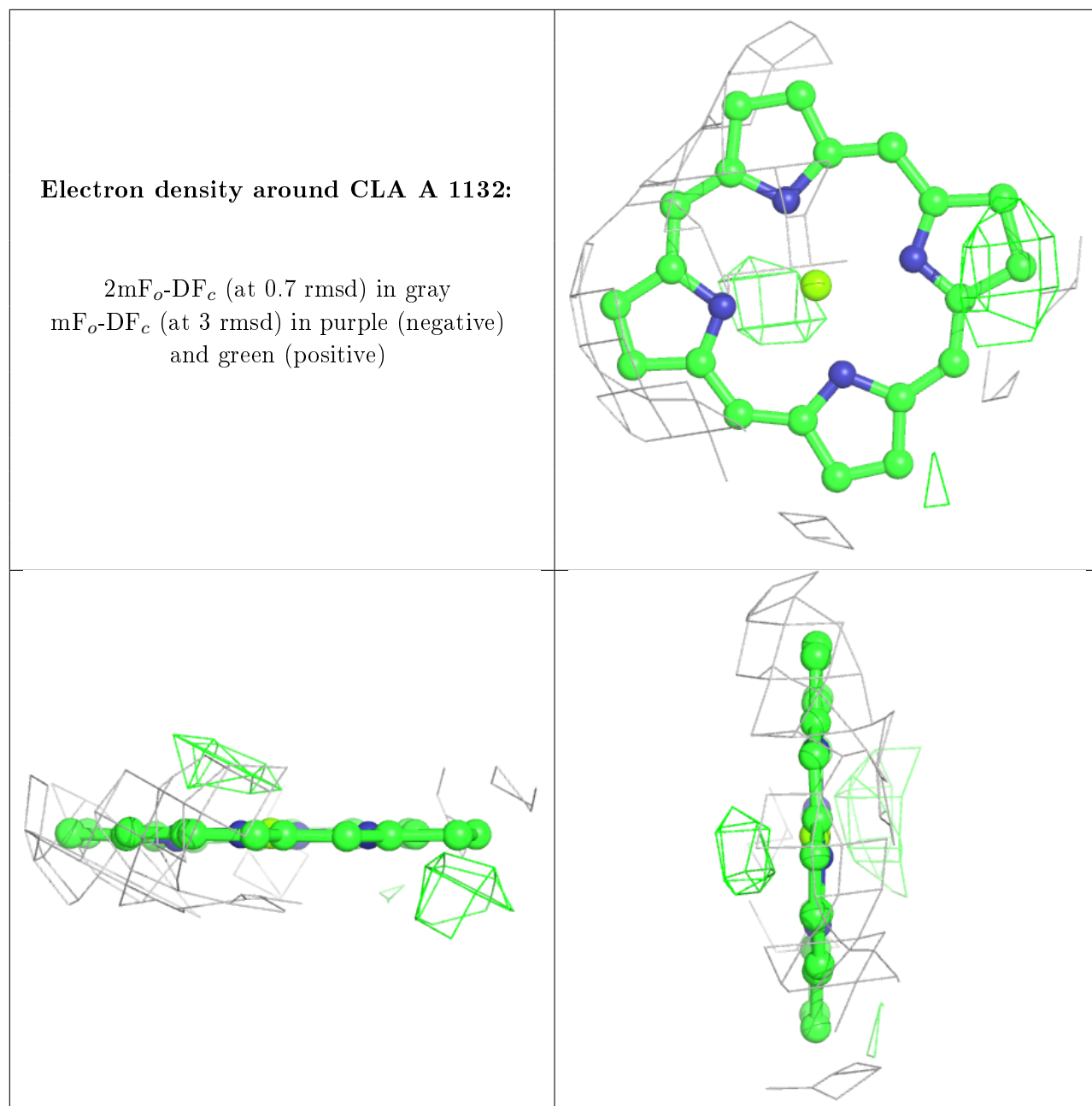




**Electron density around CLA A 1126:**

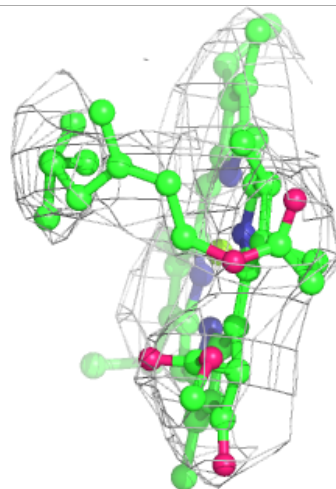
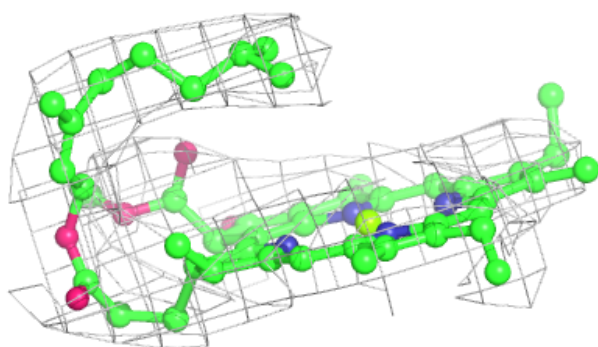
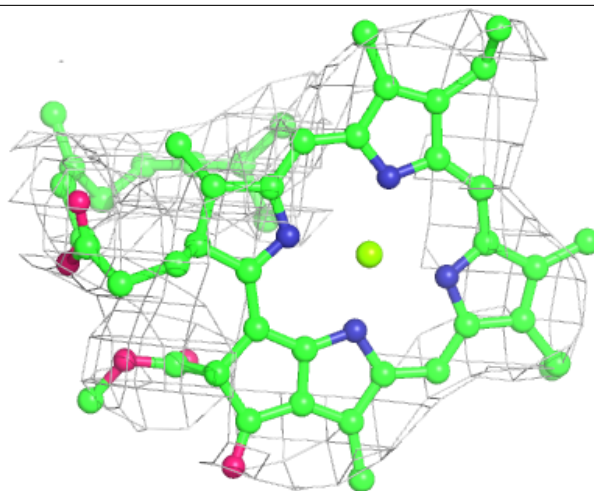
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





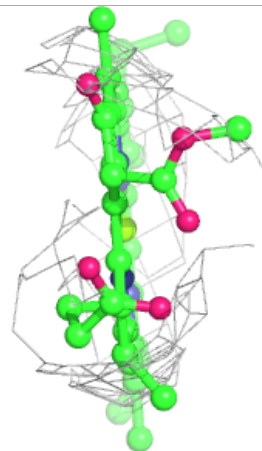
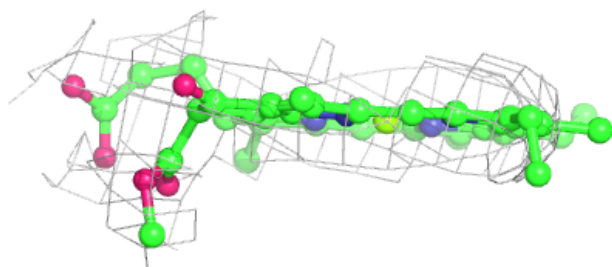
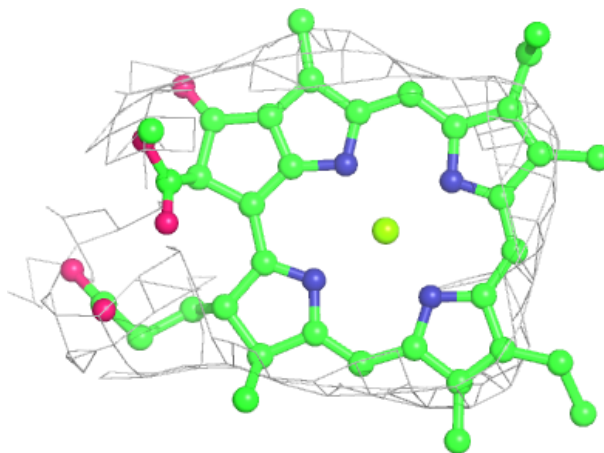
**Electron density around CLA A 1104:**

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



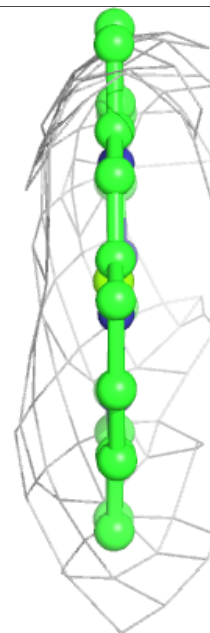
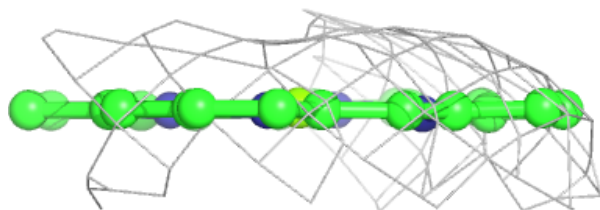
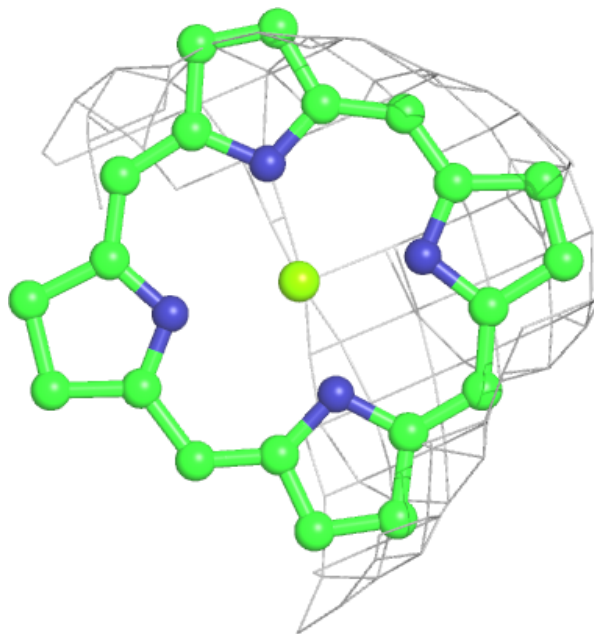
**Electron density around CLA F 1301:**

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



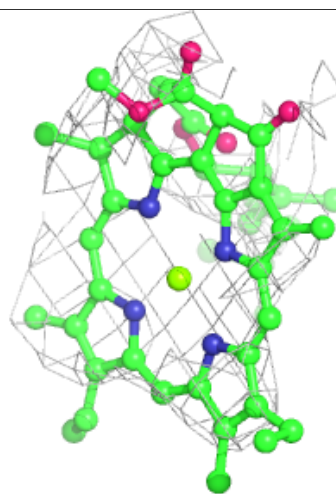
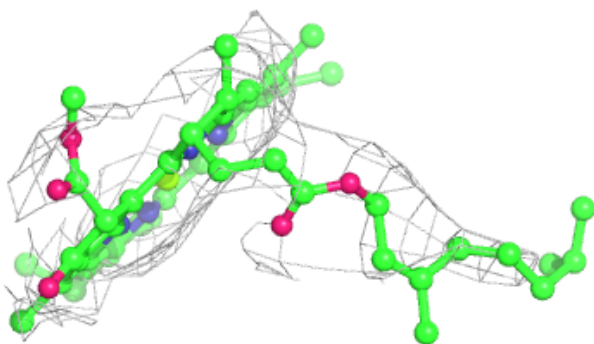
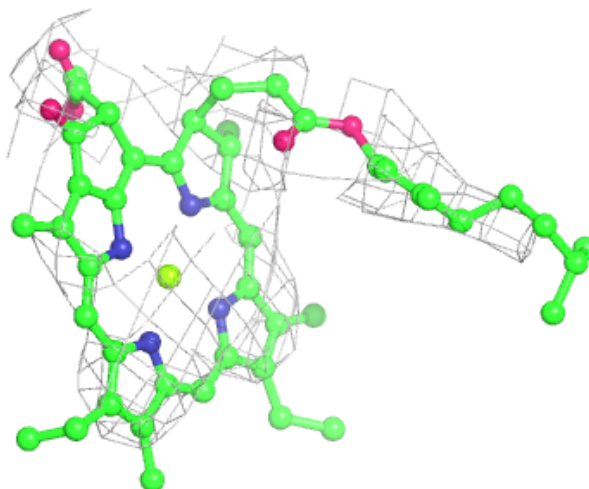
**Electron density around CLA B 1203:**

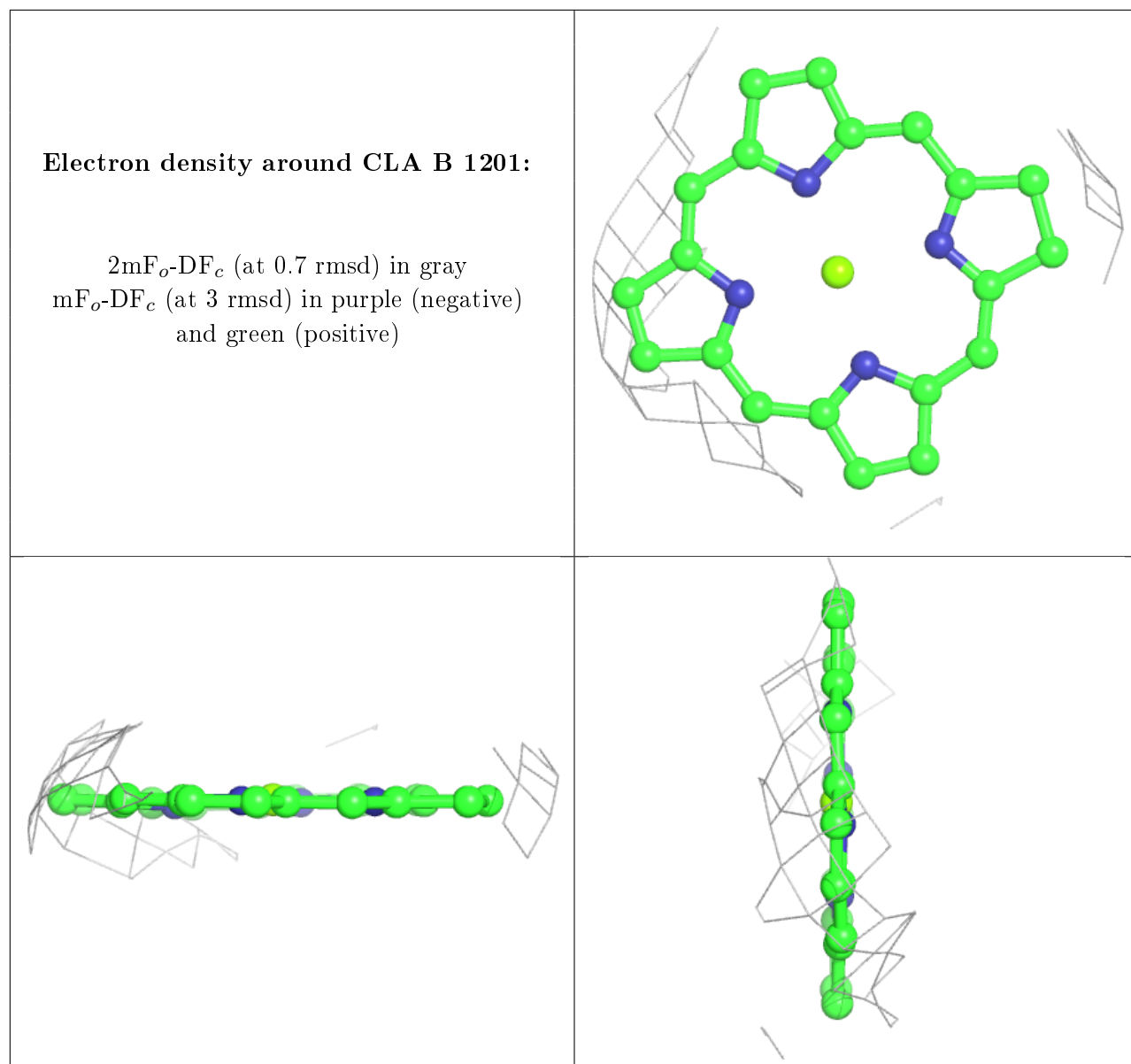
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 1106:**

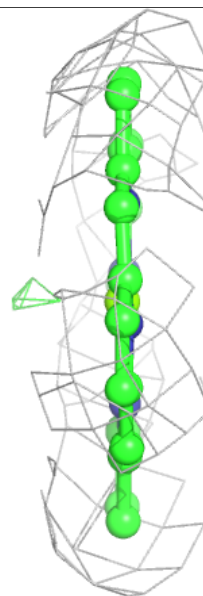
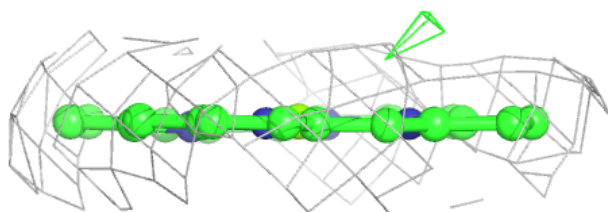
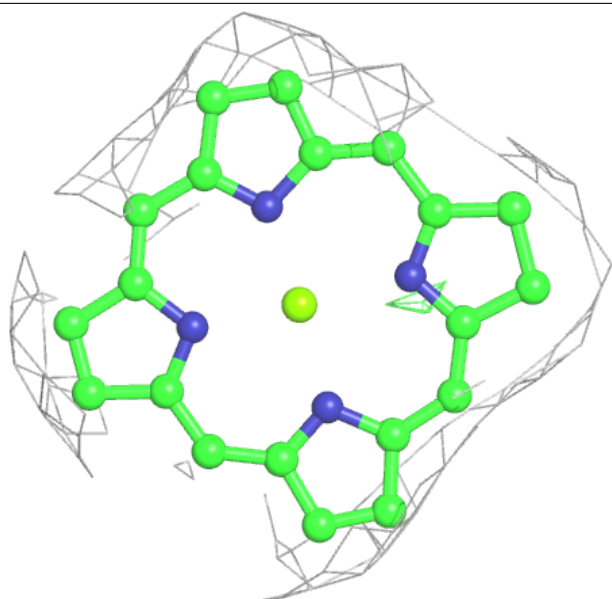
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA B 1235:**

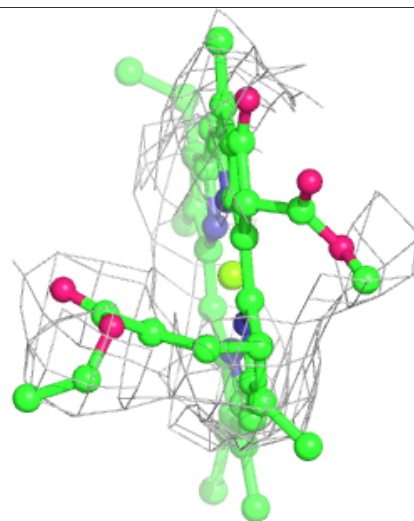
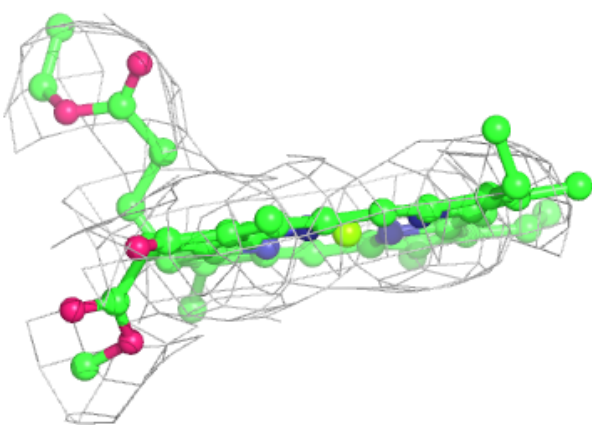
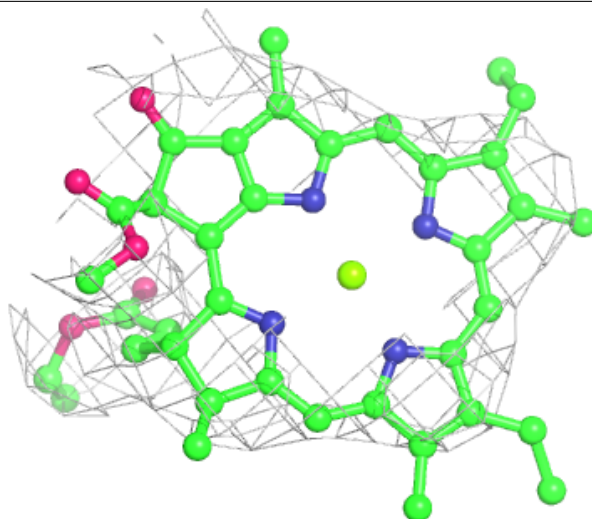
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





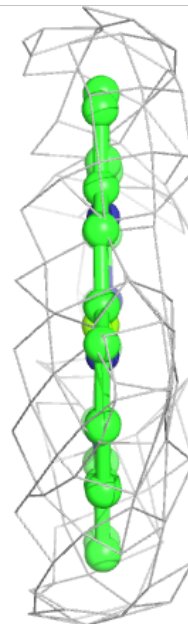
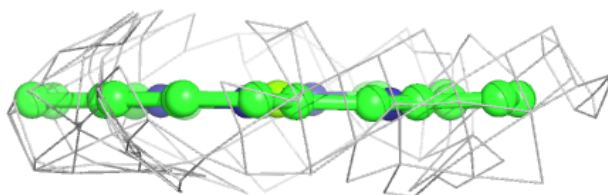
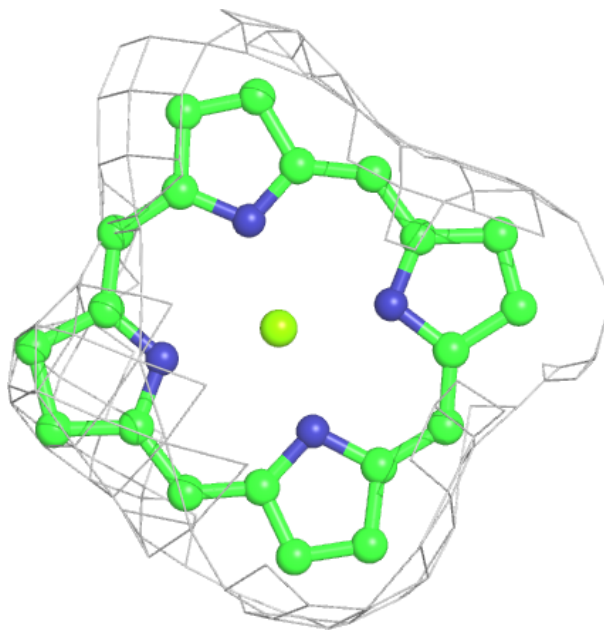
**Electron density around CLA B 1230:**

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



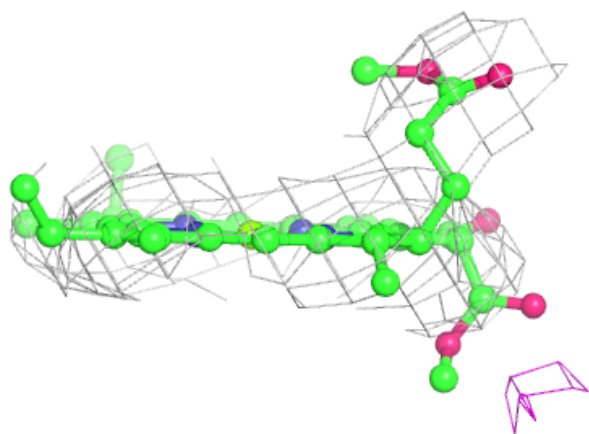
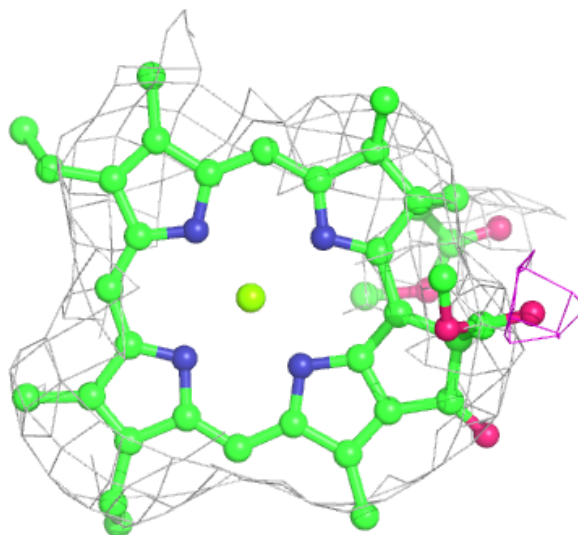
**Electron density around CLA A 1108:**

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



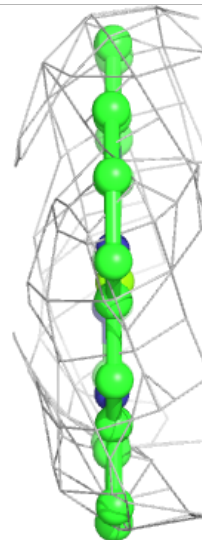
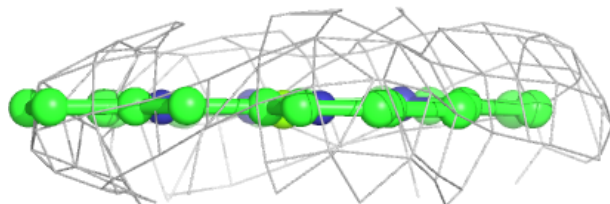
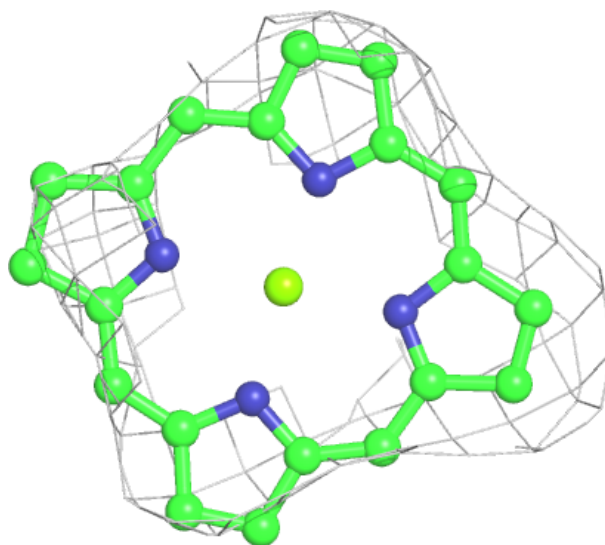
**Electron density around CLA A 1114:**

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



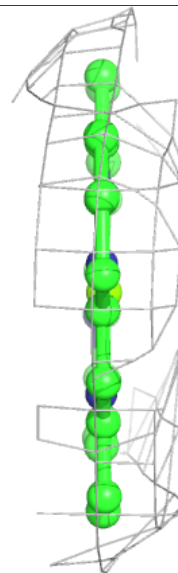
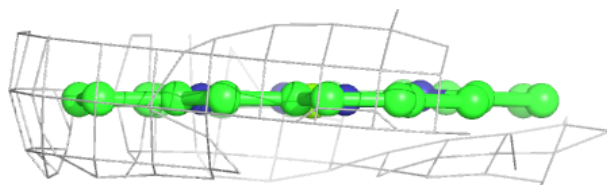
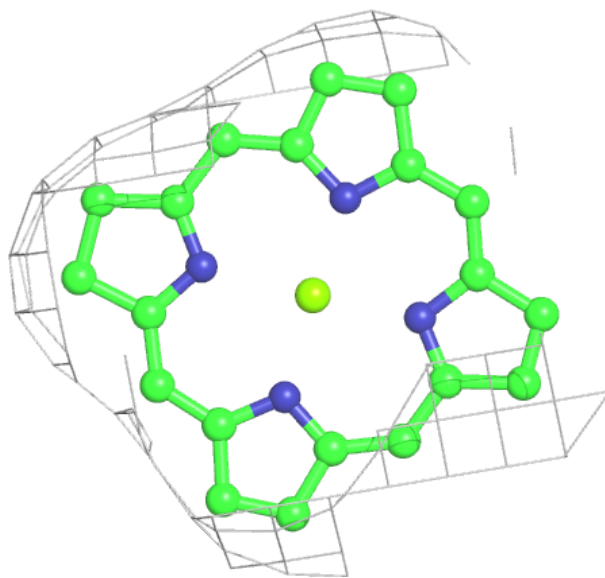
**Electron density around CLA A 1141:**

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



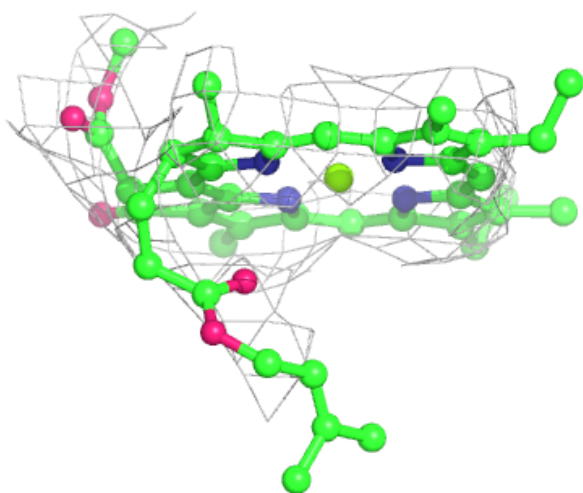
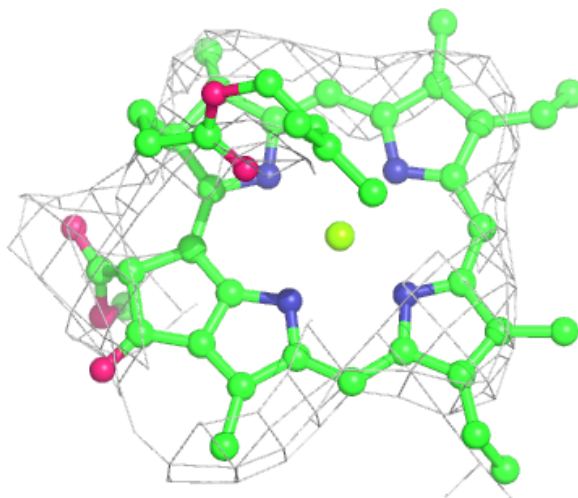
**Electron density around CLA 2 602:**

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



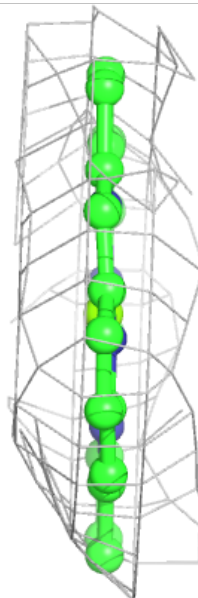
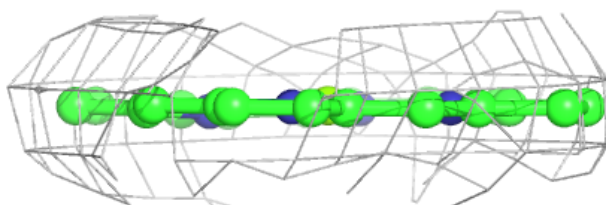
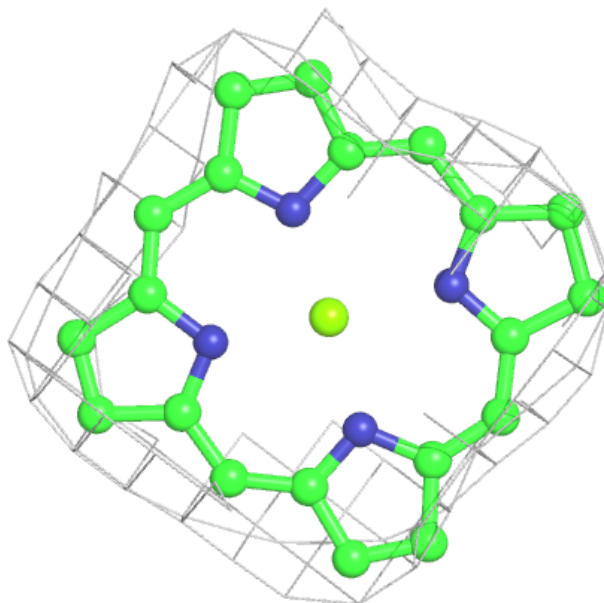
**Electron density around CLA J 1302:**

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



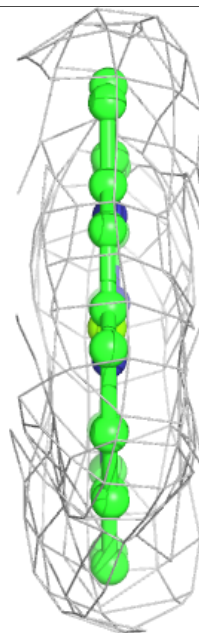
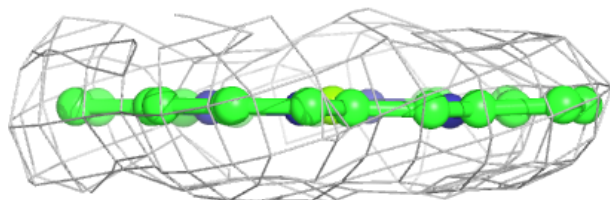
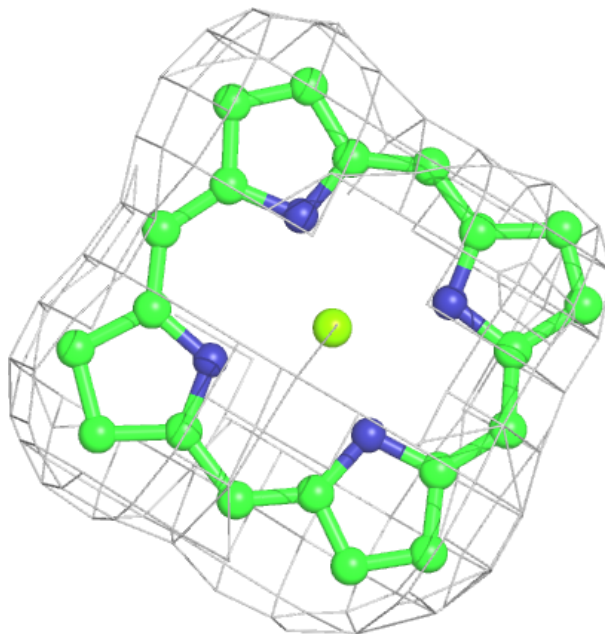
**Electron density around CLA 4 603:**

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



**Electron density around CLA A 1127:**

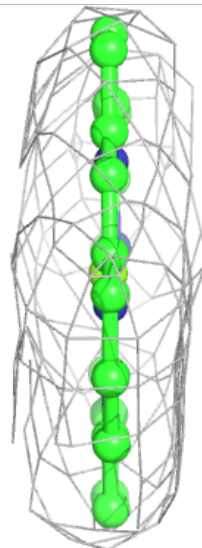
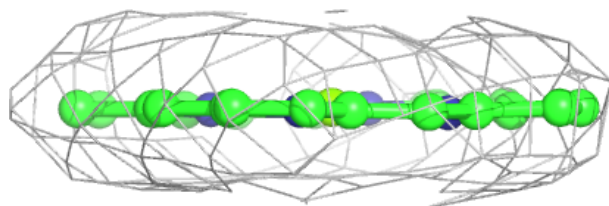
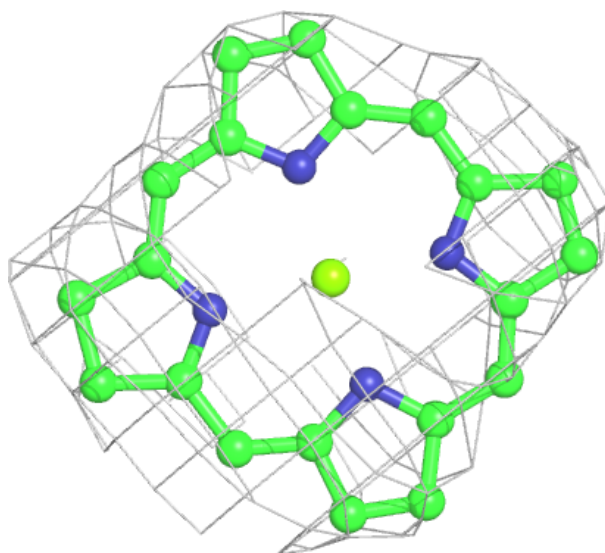
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





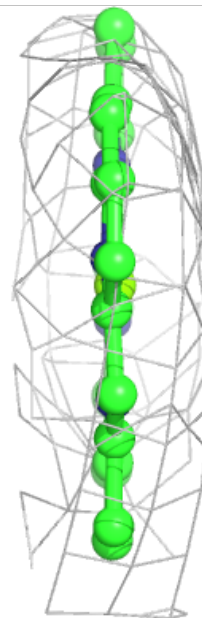
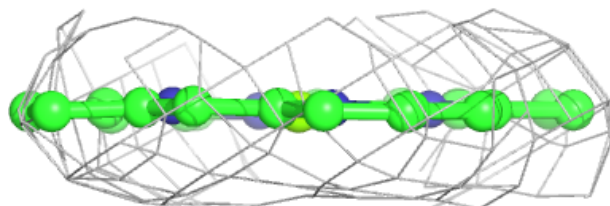
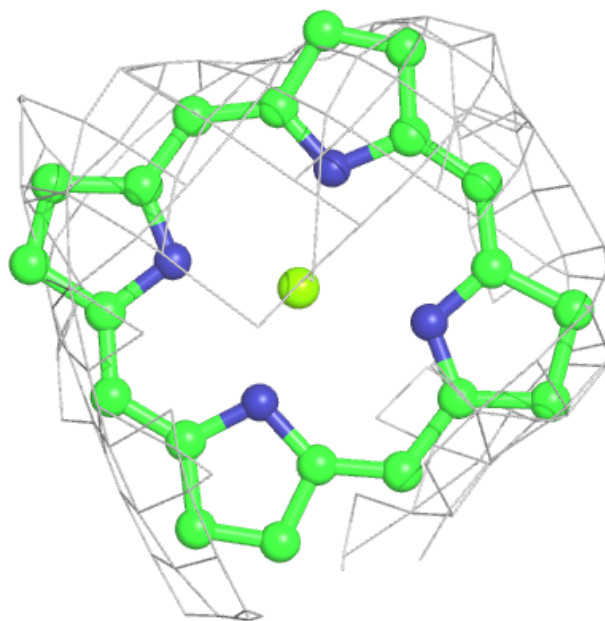
**Electron density around CLA A 1111:**

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



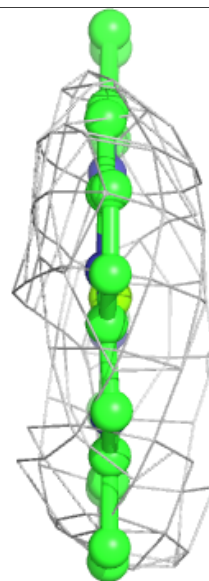
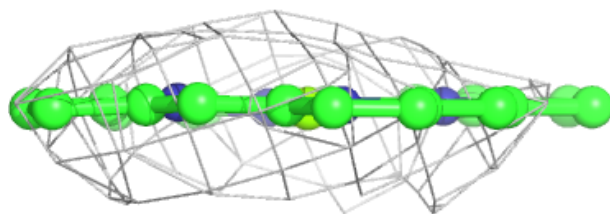
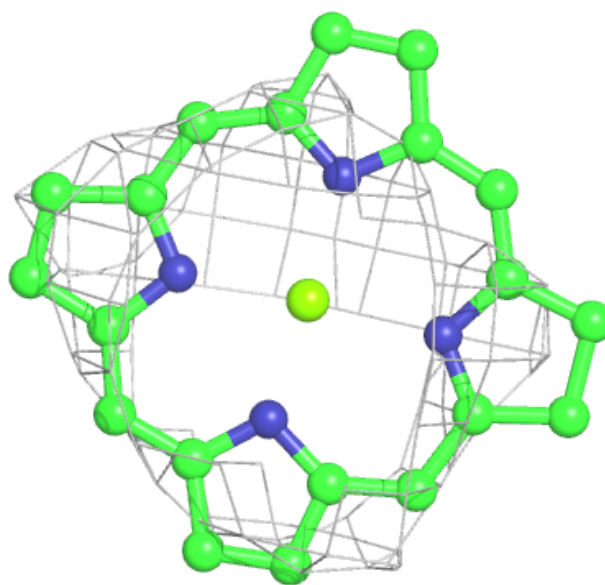
**Electron density around CLA 4 605:**

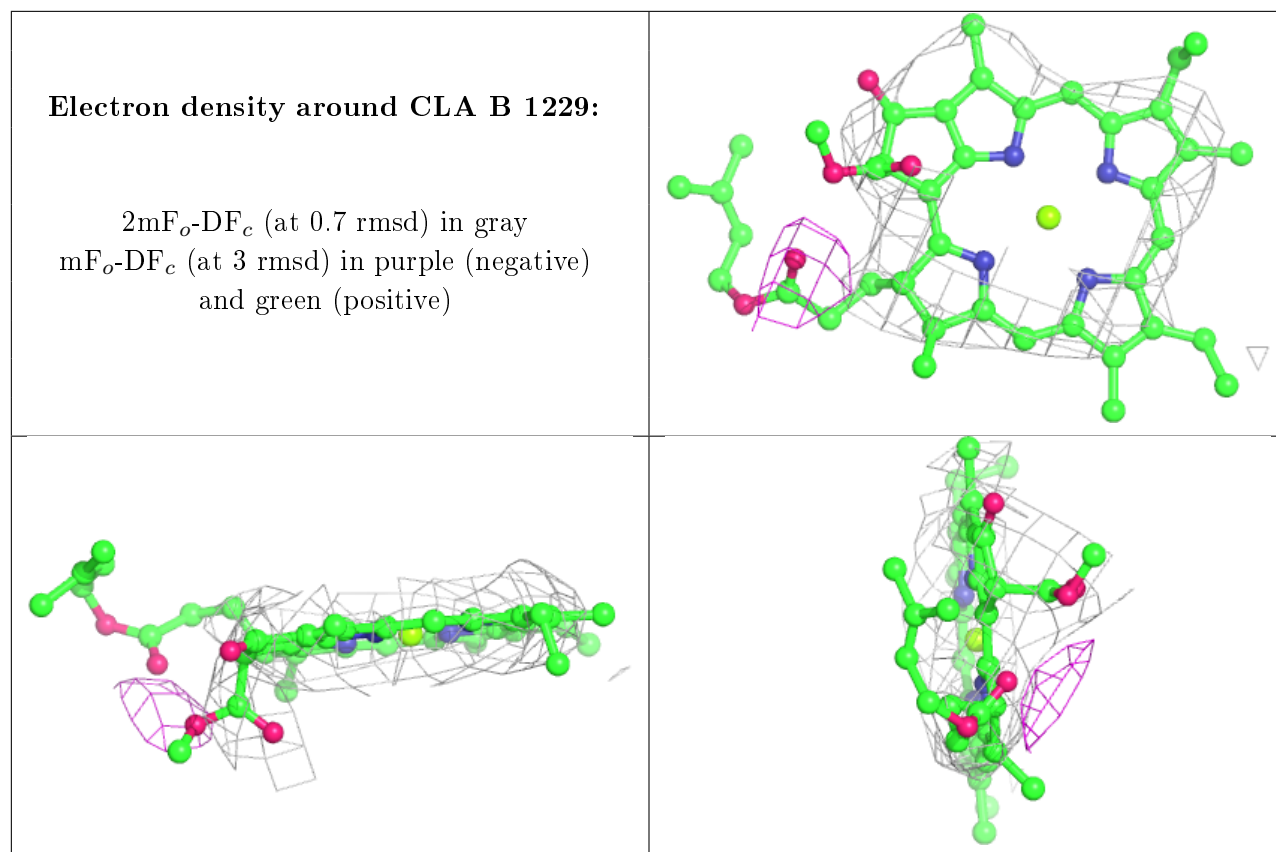
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1239:**

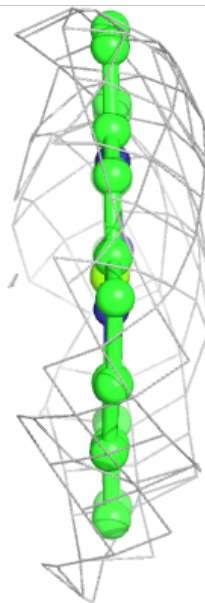
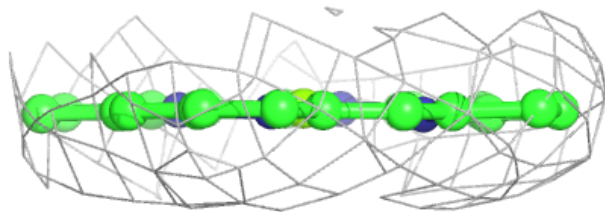
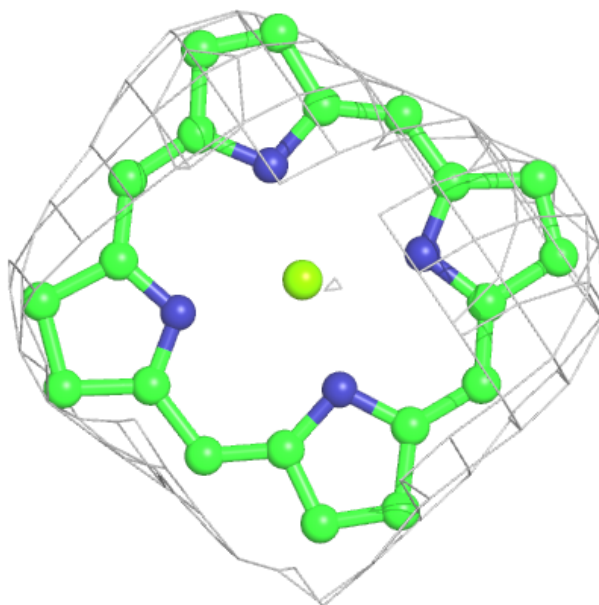
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





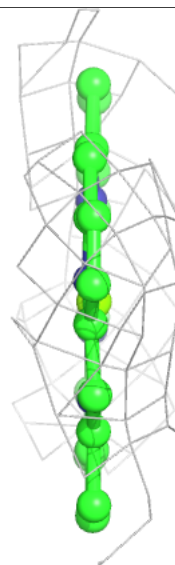
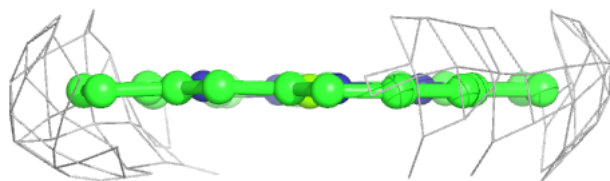
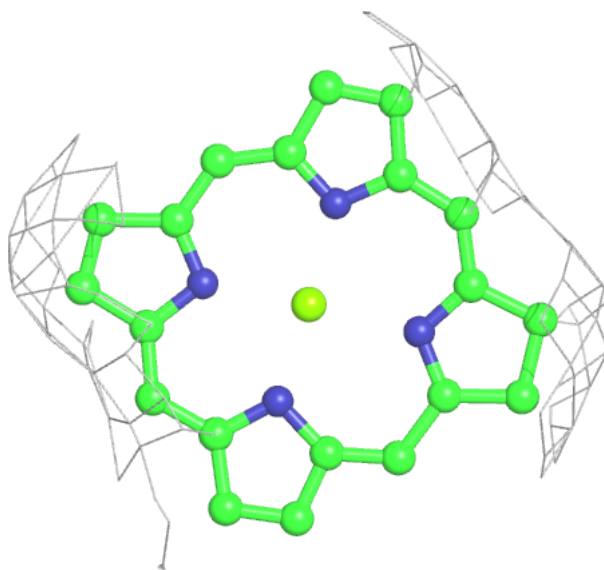
**Electron density around CLA B 1215:**

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



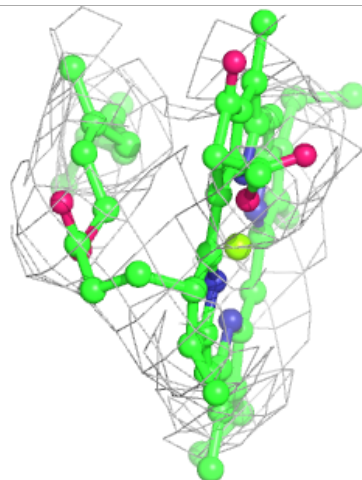
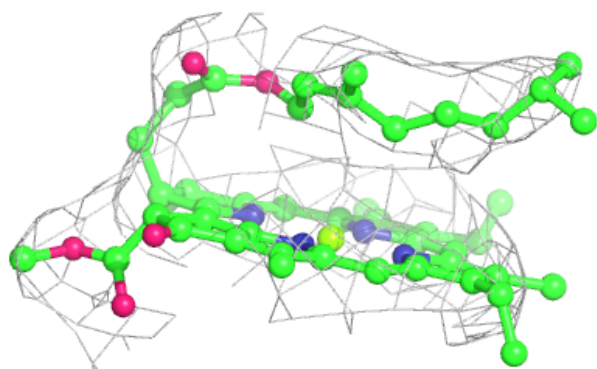
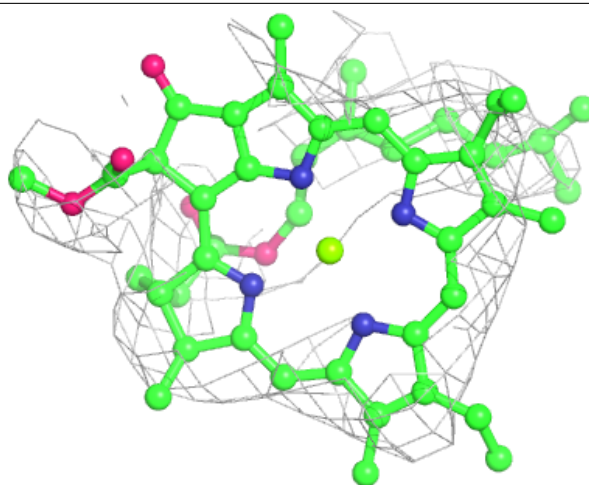
**Electron density around CLA 2 605:**

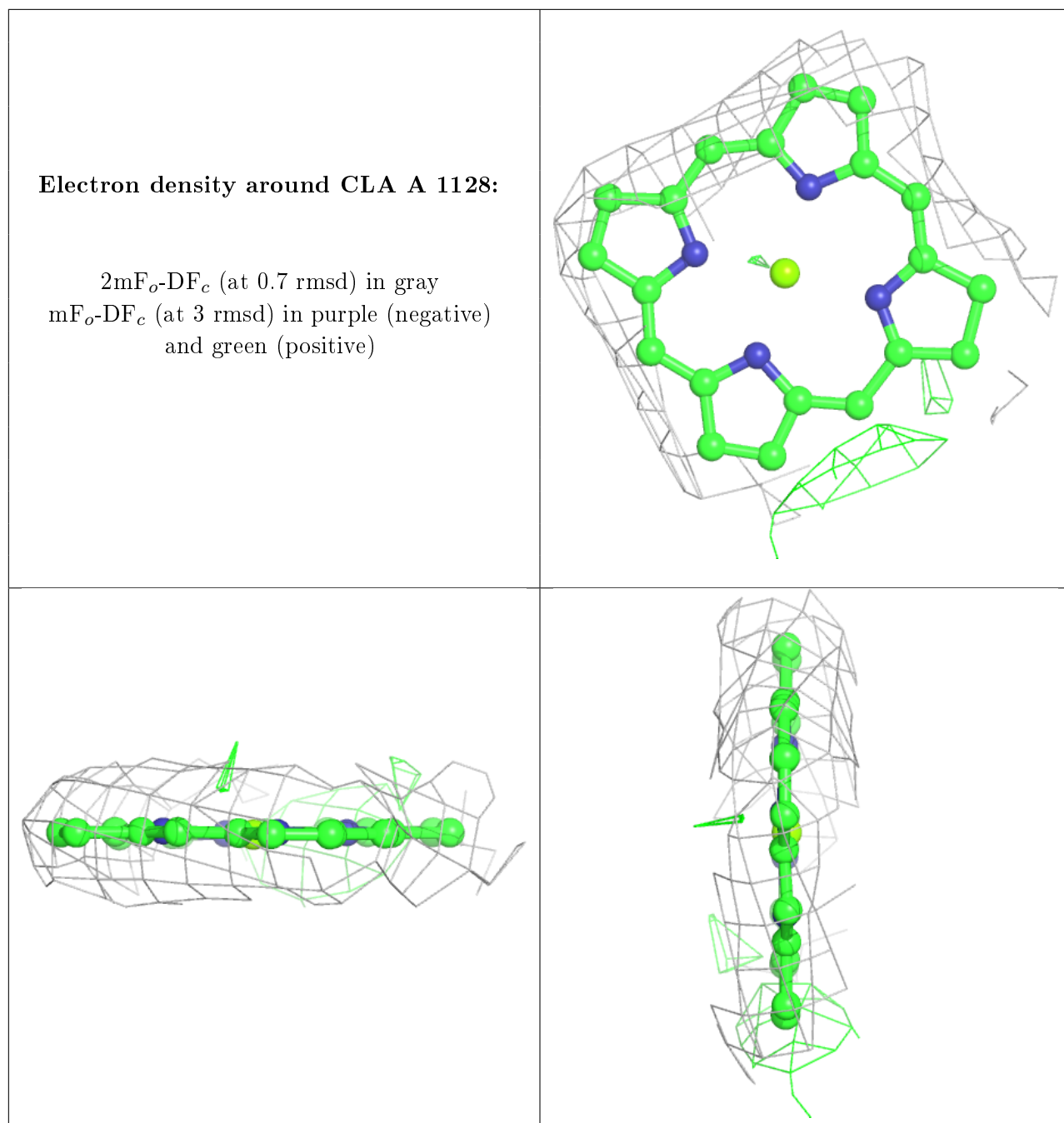
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA A 1115:**

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

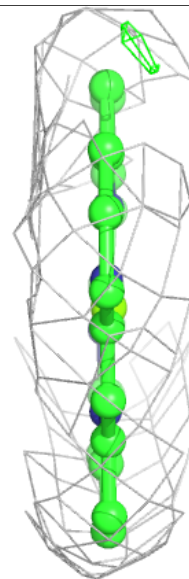
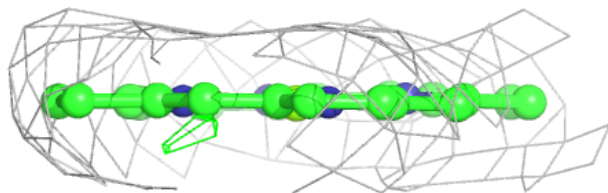
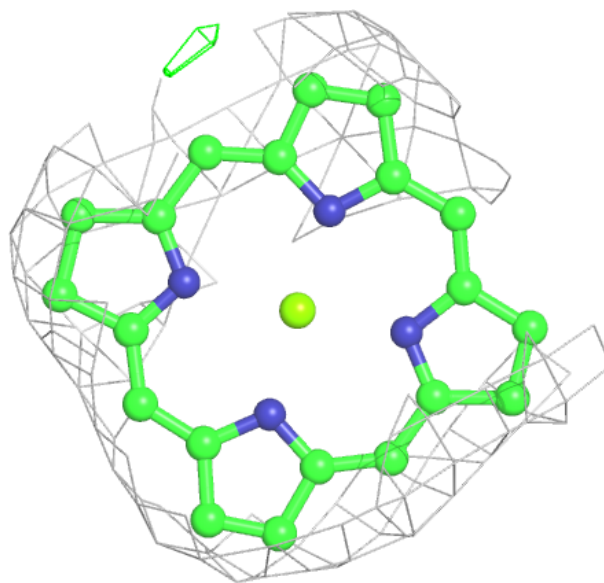






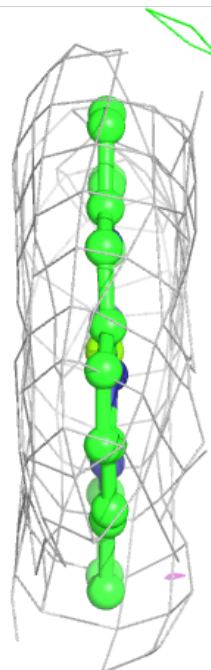
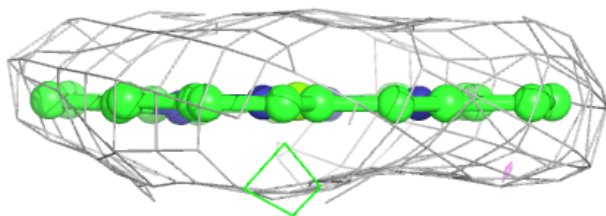
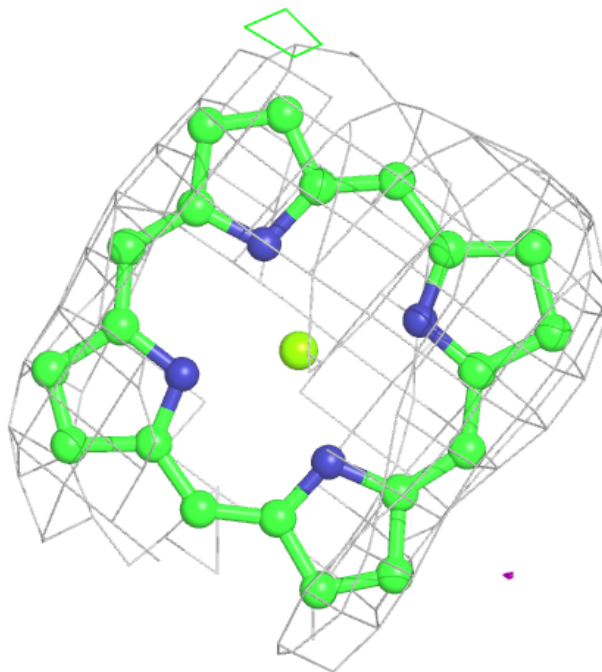
**Electron density around CLA A 1122:**

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



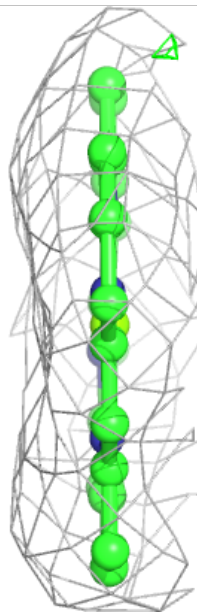
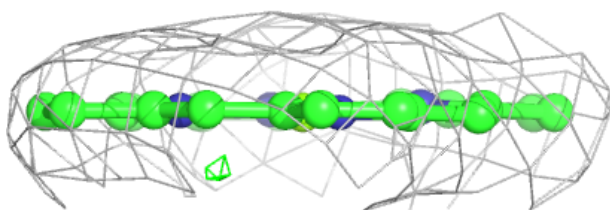
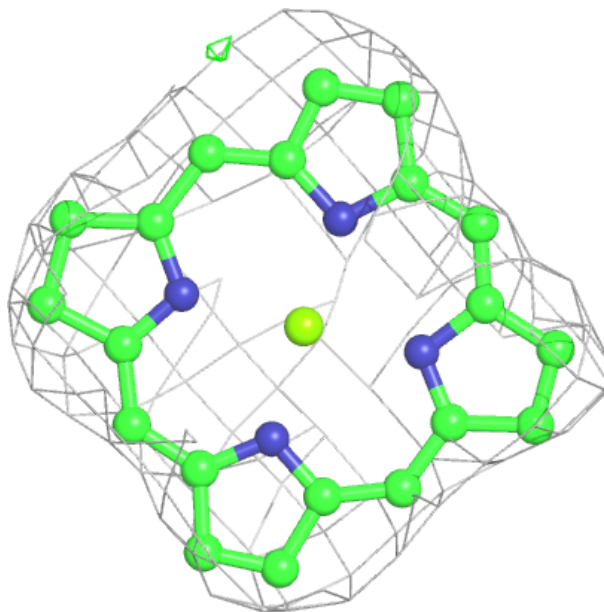
**Electron density around CLA A 1125:**

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



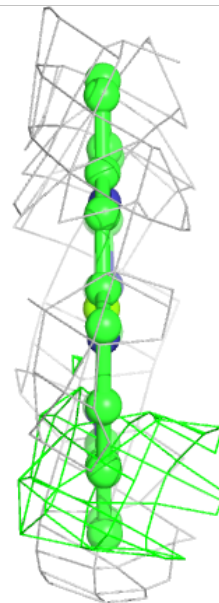
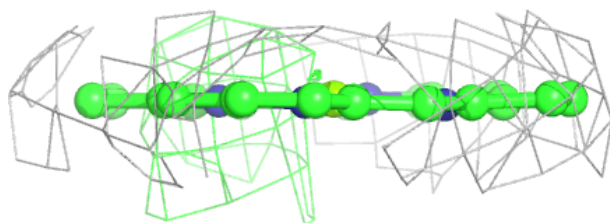
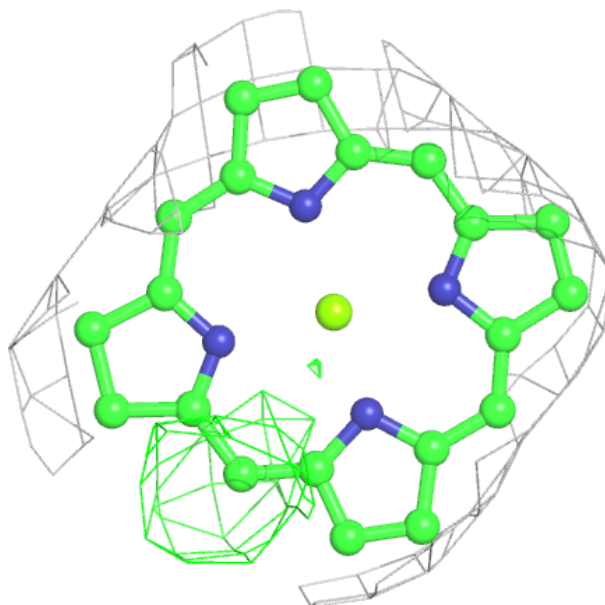
**Electron density around CLA A 1140:**

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



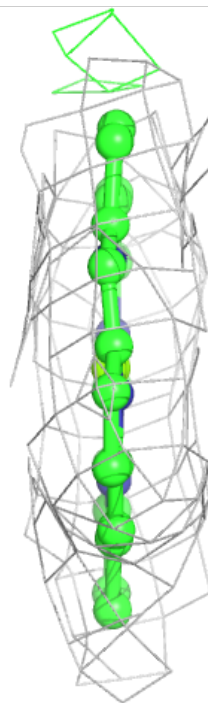
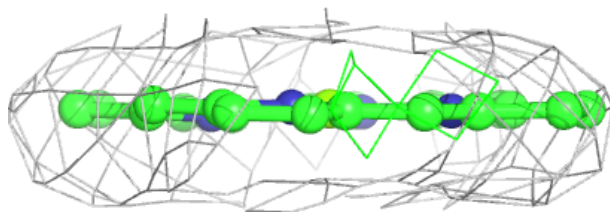
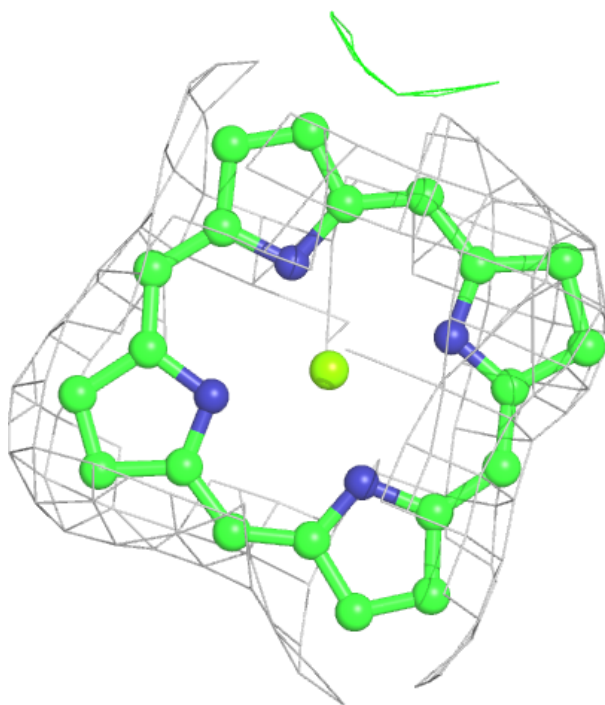
**Electron density around CLA A 1102:**

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



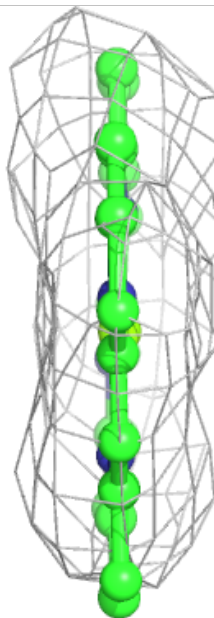
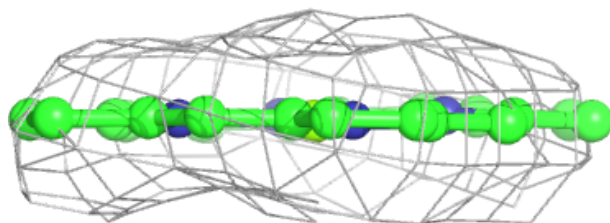
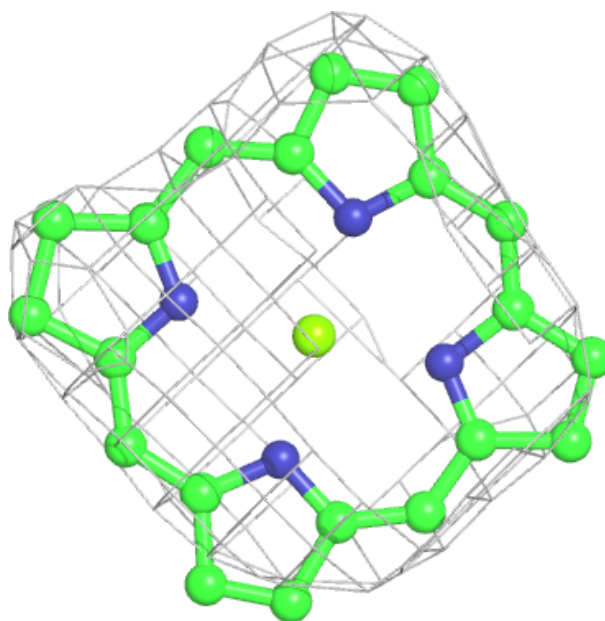
**Electron density around CLA A 1124:**

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



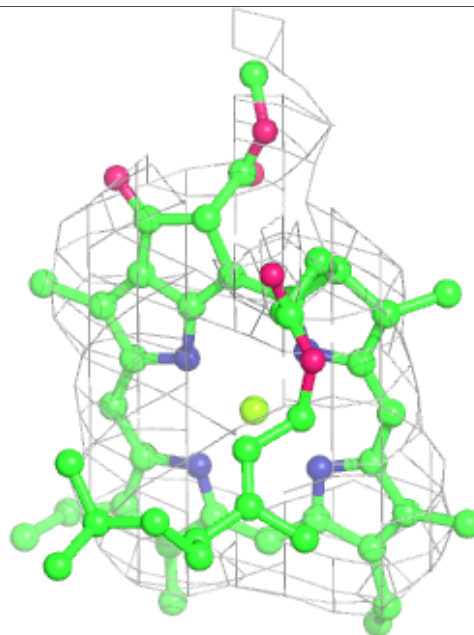
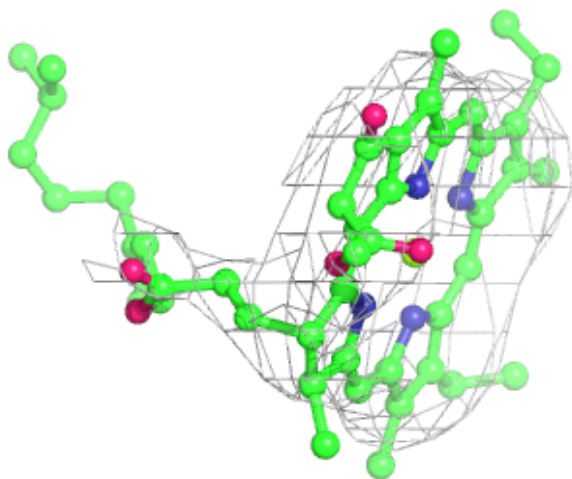
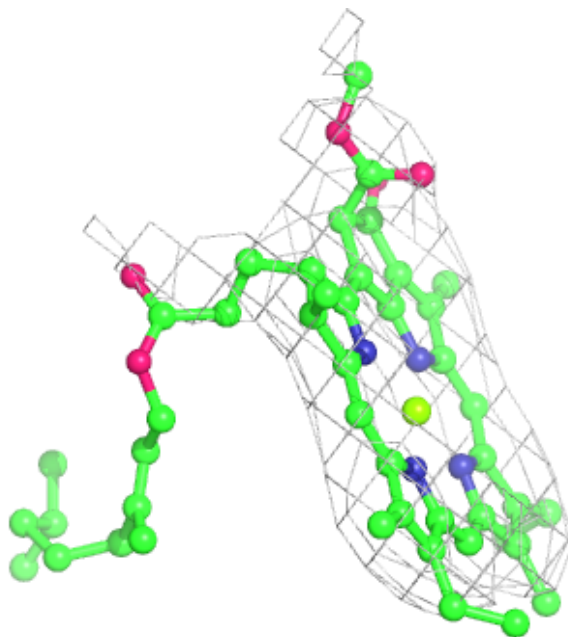
**Electron density around CLA 3 610:**

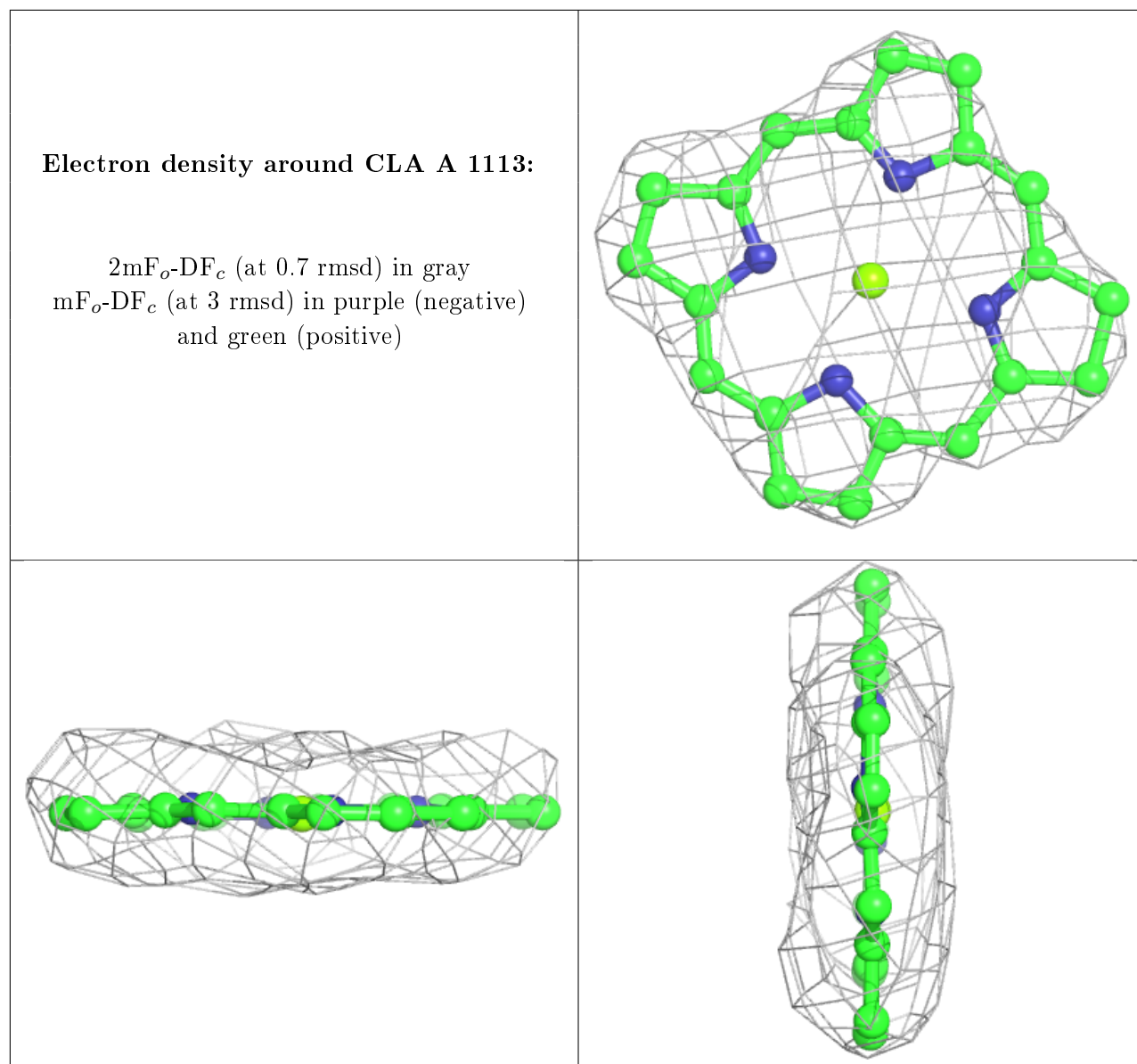
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA 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)





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

There are no such residues in this entry.