



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 08:53 AM BST

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

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.13.1  
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) : 2.13.1

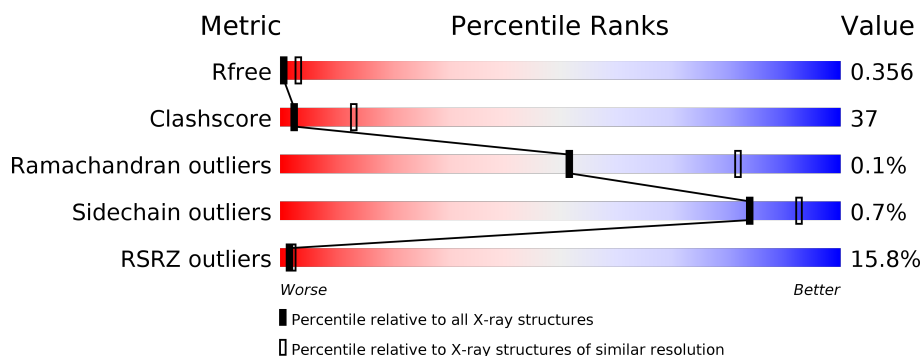
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1	195	
2	2	211	
3	3	210	
4	4	211	
5	A	739	
6	B	734	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	LUT	1	501	-	-	-	X
12	LUT	2	501	-	-	-	X
12	LUT	3	501	-	-	-	X
12	LUT	4	501	-	-	-	X
13	XAT	2	502	X	-	-	-
13	XAT	3	502	X	-	X	X
13	XAT	4	502	X	-	-	-
14	BCR	1	503	-	-	-	X
14	BCR	1	505	-	-	-	X
14	BCR	2	503	-	-	-	X
14	BCR	3	503	-	-	X	X
14	BCR	3	504	-	-	-	X
14	BCR	4	503	-	-	-	X
14	BCR	4	505	-	-	-	X
14	BCR	A	4002	-	-	-	X
14	BCR	A	4003	-	-	-	X
14	BCR	A	4004	-	-	-	X
14	BCR	A	4005	-	-	-	X
14	BCR	A	4007	-	-	-	X
14	BCR	B	4001	-	-	-	X
14	BCR	B	4002	-	-	-	X
14	BCR	B	4003	-	-	-	X
14	BCR	B	4005	-	-	-	X
14	BCR	B	4006	-	-	-	X
14	BCR	J	4001	-	-	-	X
15	CLA	1	601	X	-	-	-
15	CLA	1	602	X	-	-	-
15	CLA	1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	1	604	X	-	-	-
15	CLA	1	605	X	-	-	-
15	CLA	1	606	X	-	-	-
15	CLA	1	607	X	-	-	-
15	CLA	1	608	X	-	-	-
15	CLA	1	611	X	-	-	-
15	CLA	1	612	X	-	-	-
15	CLA	1	613	X	-	X	-
15	CLA	1	615	X	-	-	-
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	X
15	CLA	2	607	X	-	-	-
15	CLA	2	608	X	-	-	-
15	CLA	2	612	X	-	-	-
15	CLA	2	615	X	-	-	-
15	CLA	3	601	X	-	-	-
15	CLA	3	603	X	-	X	-
15	CLA	3	605	X	-	-	-
15	CLA	3	606	X	-	-	-
15	CLA	3	607	X	-	-	-
15	CLA	3	608	X	-	-	-
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	613	X	-	-	-
15	CLA	3	615	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	-
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	607	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	612	X	-	-	-
15	CLA	4	615	X	-	-	-
15	CLA	A	1012	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1013	X	-	X	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	-	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	X	-
15	CLA	A	1112	X	-	-	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	X
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	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	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1021	X	-	X	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1023	X	-	-	X
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	-	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1207	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1210	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	-	X
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-
15	CLA	B	1219	X	-	-	-
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	-	-
15	CLA	B	1224	X	-	-	X
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	-	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
16	CHL	1	609	X	-	-	-
16	CHL	1	610	X	-	-	-
16	CHL	2	609	X	-	-	-
16	CHL	2	610	X	-	-	-
16	CHL	2	611	X	-	-	-
16	CHL	2	613	X	-	-	-
16	CHL	3	604	X	-	-	X
16	CHL	4	610	X	-	-	-
16	CHL	4	611	X	-	-	-
16	CHL	4	613	X	-	-	-
21	DGD	4	811	-	-	-	X
21	DGD	J	5001	-	-	-	X
24	CL0	A	1011	X	-	X	-
25	PQN	A	2001	-	-	-	X
25	PQN	B	2002	-	-	-	X
26	SF4	C	3003	-	-	X	-

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 30870 atoms, of which 32 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Lhc2.

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

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

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

- Molecule 4 is a protein called Lhc4.

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

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

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

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

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

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

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

- Molecule 8 is a protein called PsaD.

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

- Molecule 9 is a protein called PsaE.

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

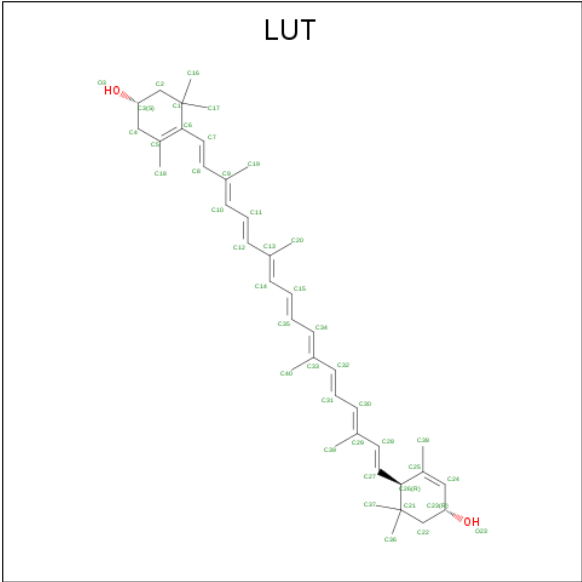
- Molecule 10 is a protein called PsaF.

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

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

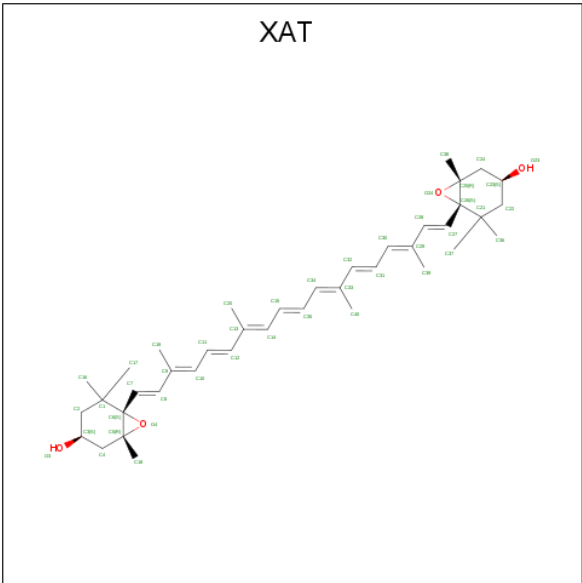
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	41	Total	C	N	O	S	0	0	0
			327	223	47	56	1			

- Molecule 12 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



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

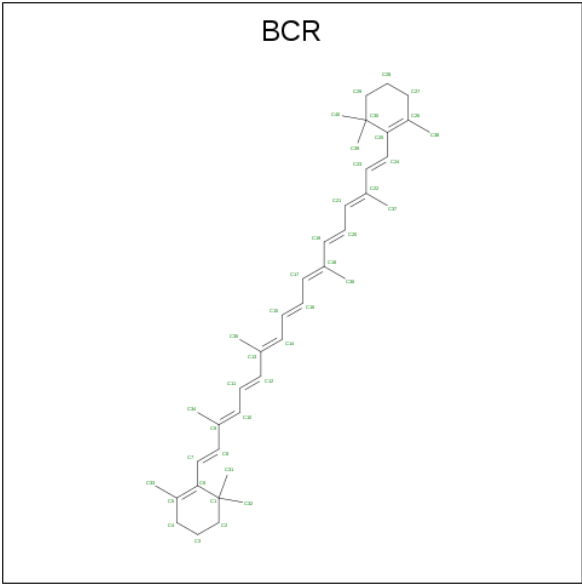
- Molecule 13 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	1	1	Total	C	O	0	0
			44	40	4		
13	2	1	Total	C	O	0	0
			44	40	4		
13	3	1	Total	C	O	0	0
			44	40	4		
13	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

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

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



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

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

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

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

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

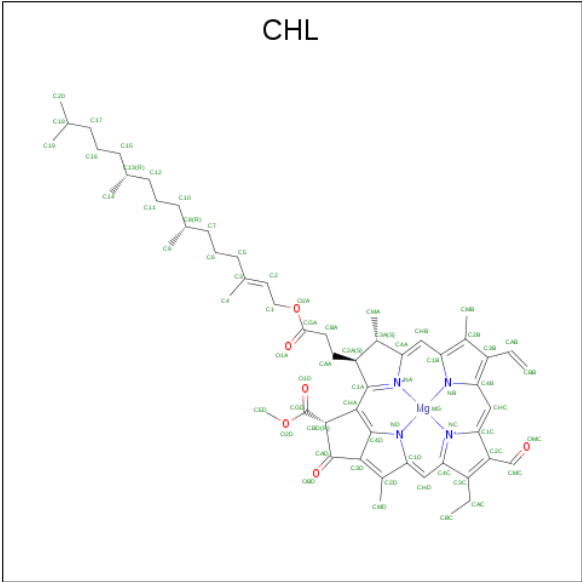
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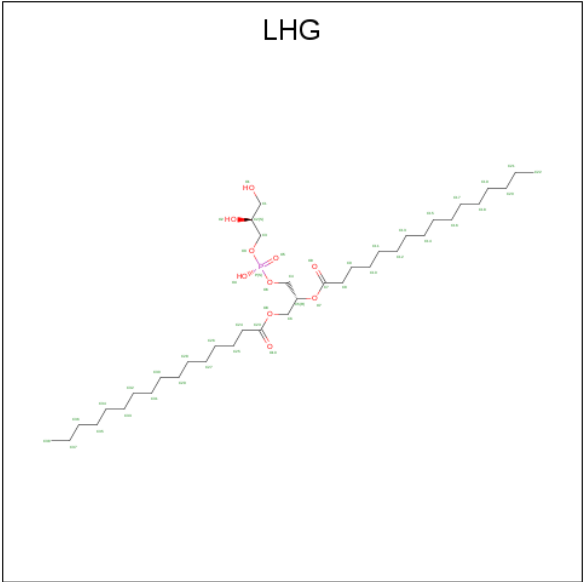
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
15	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5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

- Molecule 16 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



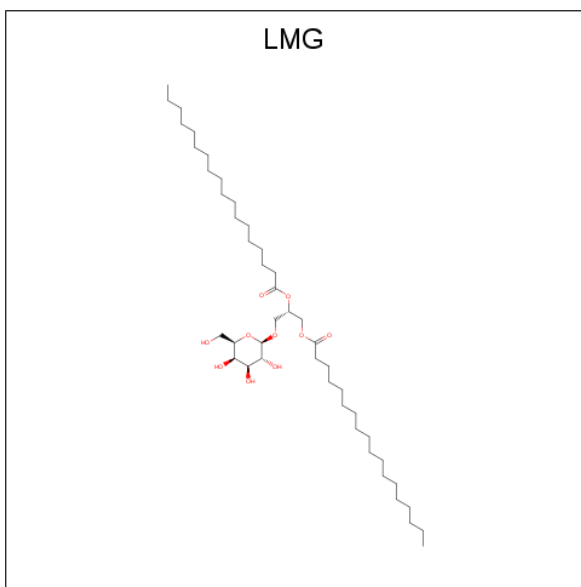
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	1	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
16	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6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

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



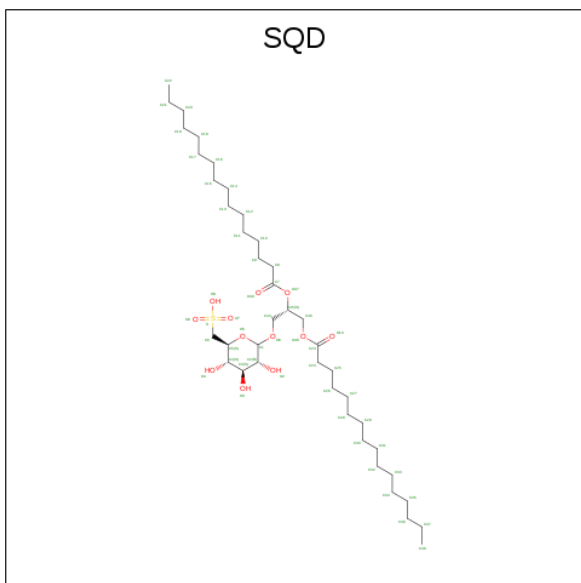
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	1	1	Total	C	O	P	0	0
			23	12	10	1		
17	2	1	Total	C	O	P	0	0
			21	10	10	1		
17	A	1	Total	C	O	P	0	0
			16	7	8	1		
17	A	1	Total	C	O	P	0	0
			24	13	10	1		
17	B	1	Total	C	O	P	0	0
			21	10	10	1		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



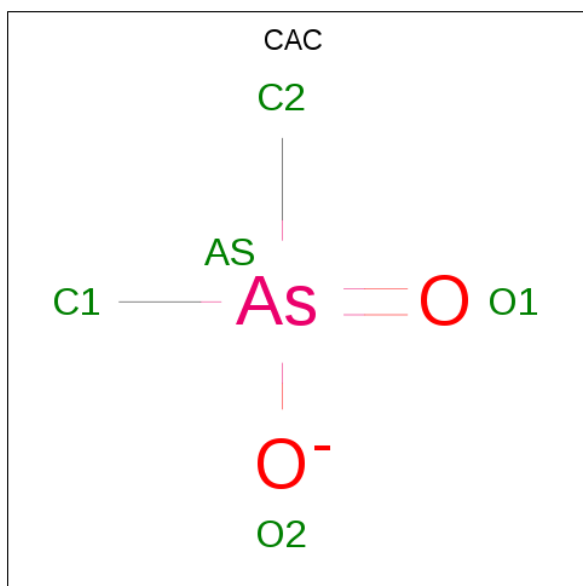
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	1	1	Total	C	O	0	0
			36	26	10		
18	1	1	Total	C	O	0	0
			23	13	10		
18	2	1	Total	C	O	0	0
			25	15	10		
18	2	1	Total	C	O	0	0
			16	9	7		

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



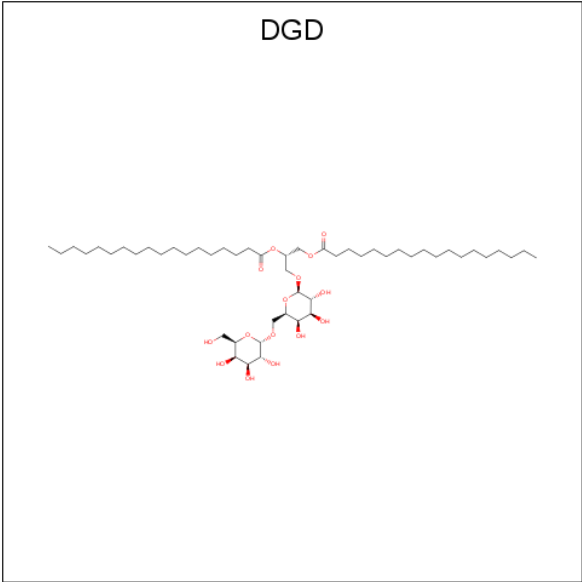
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	1	1	Total	C	O	S	0	0
			40	27	12	1		

- Molecule 20 is CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



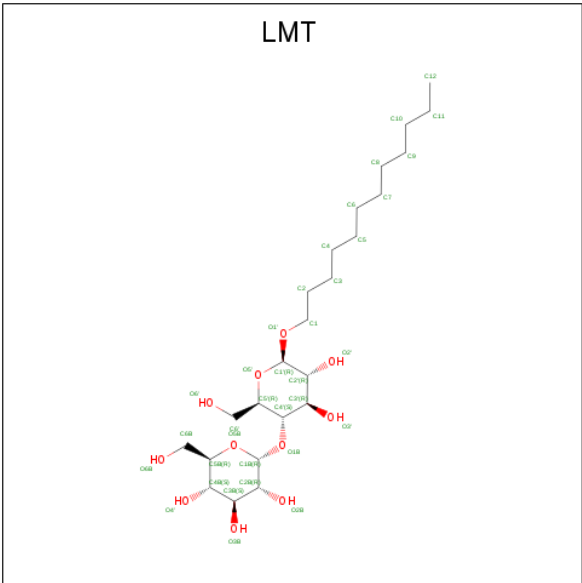
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	1	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	3	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		
20	4	1	Total	As	C	O	0	0
			5	1	2	2		

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



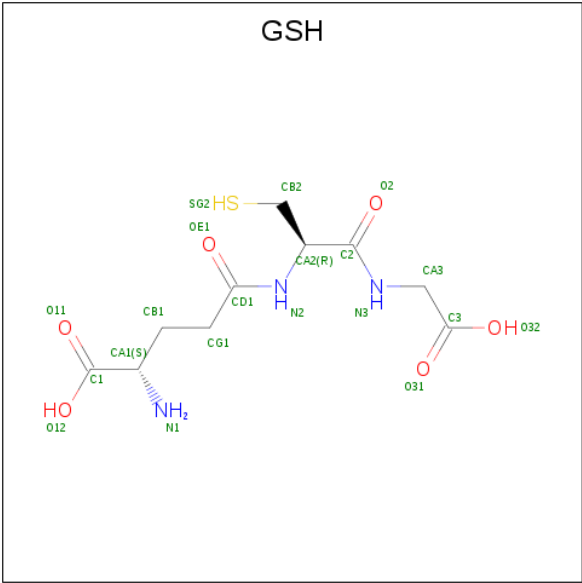
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	2	1	Total	C	O	0	0
			47	32	15		
21	4	1	Total	C	O	0	0
			45	30	15		
21	B	1	Total	C	O	0	0
			38	23	15		
21	J	1	Total	C	O	0	0
			28	15	13		

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



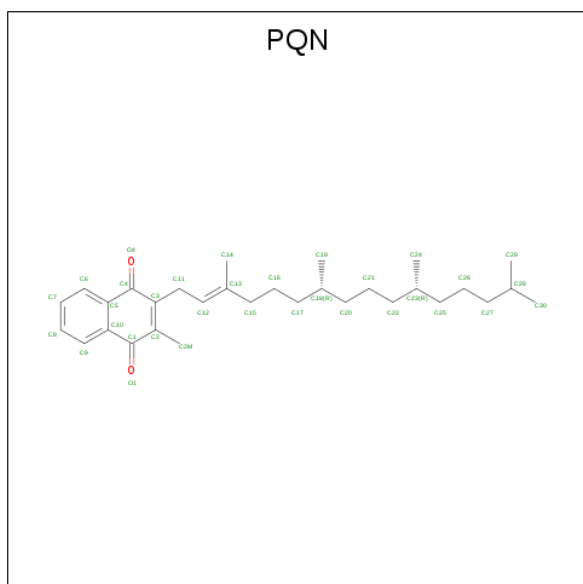
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	2	1	Total	C	O	0	0
			23	12	11		

- Molecule 23 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



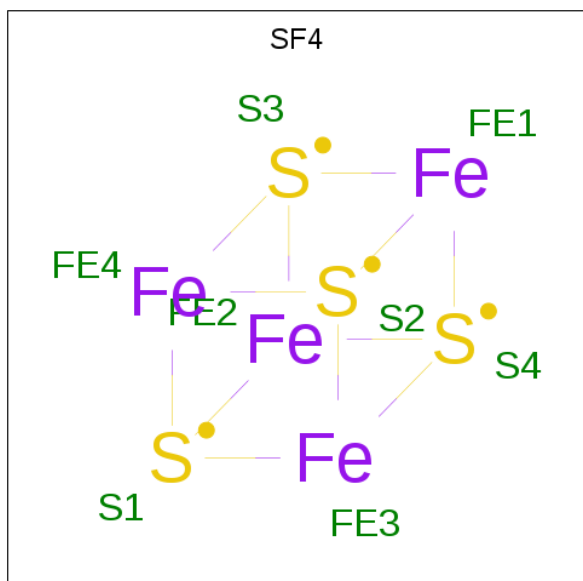
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	
			50	40	1	4	5	
							0	0

- Molecule 25 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



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

- Molecule 26 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).





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

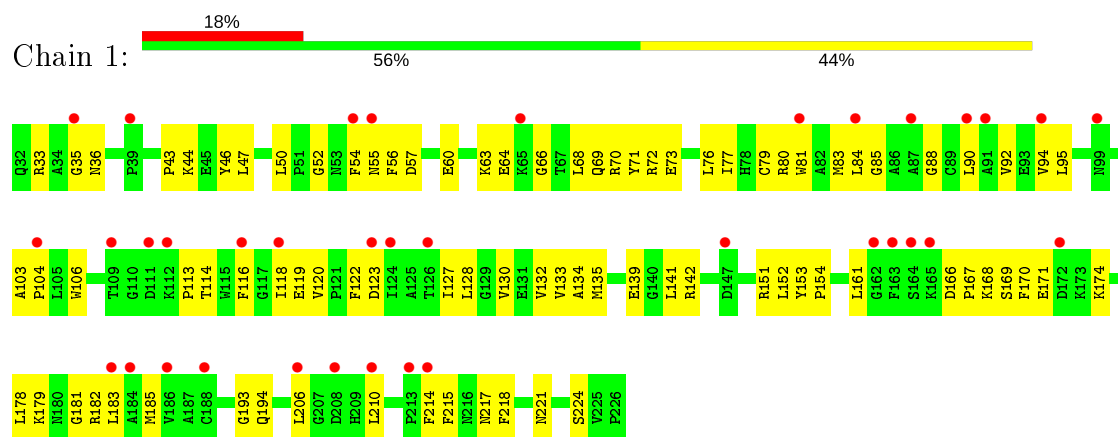
- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

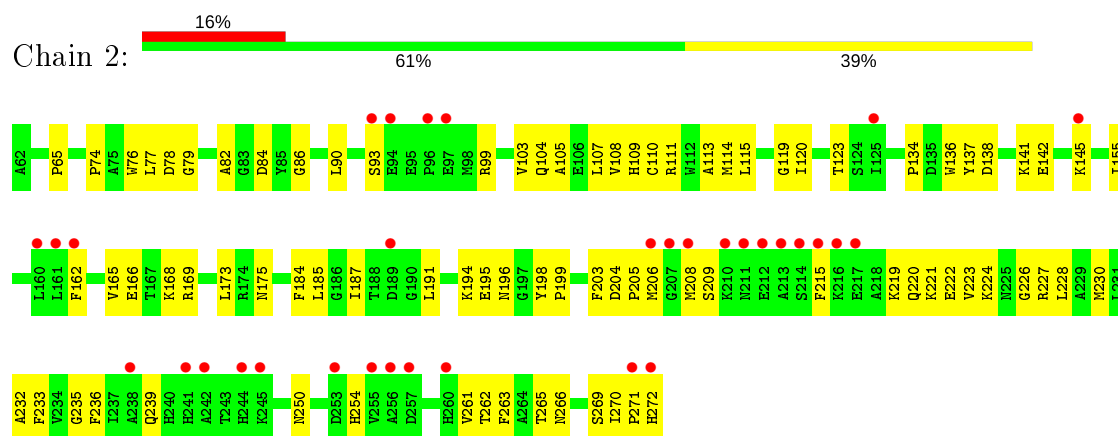
### 3 Residue-property plots [i](#)

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

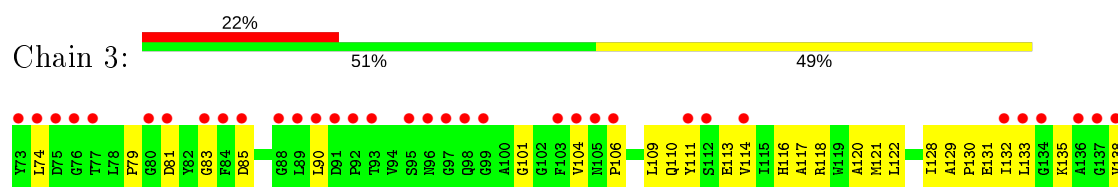
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

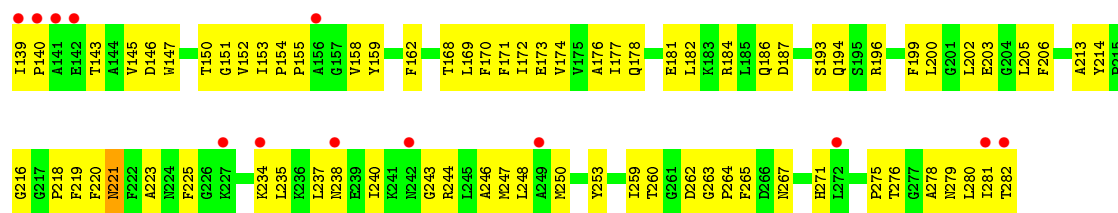


- Molecule 2: Lhc2

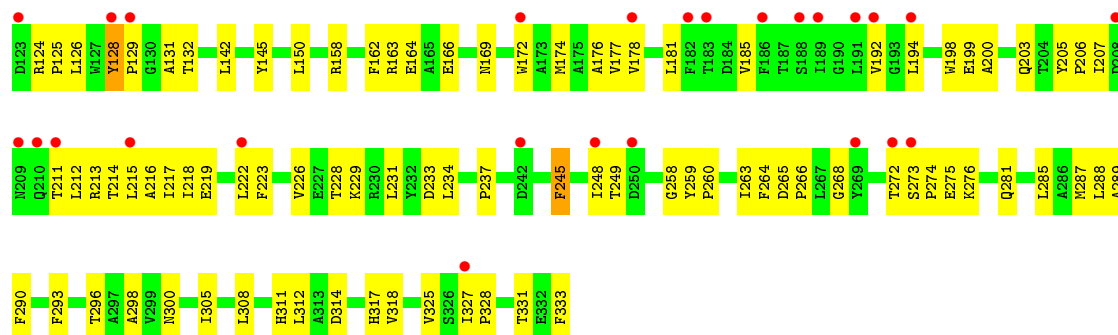


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

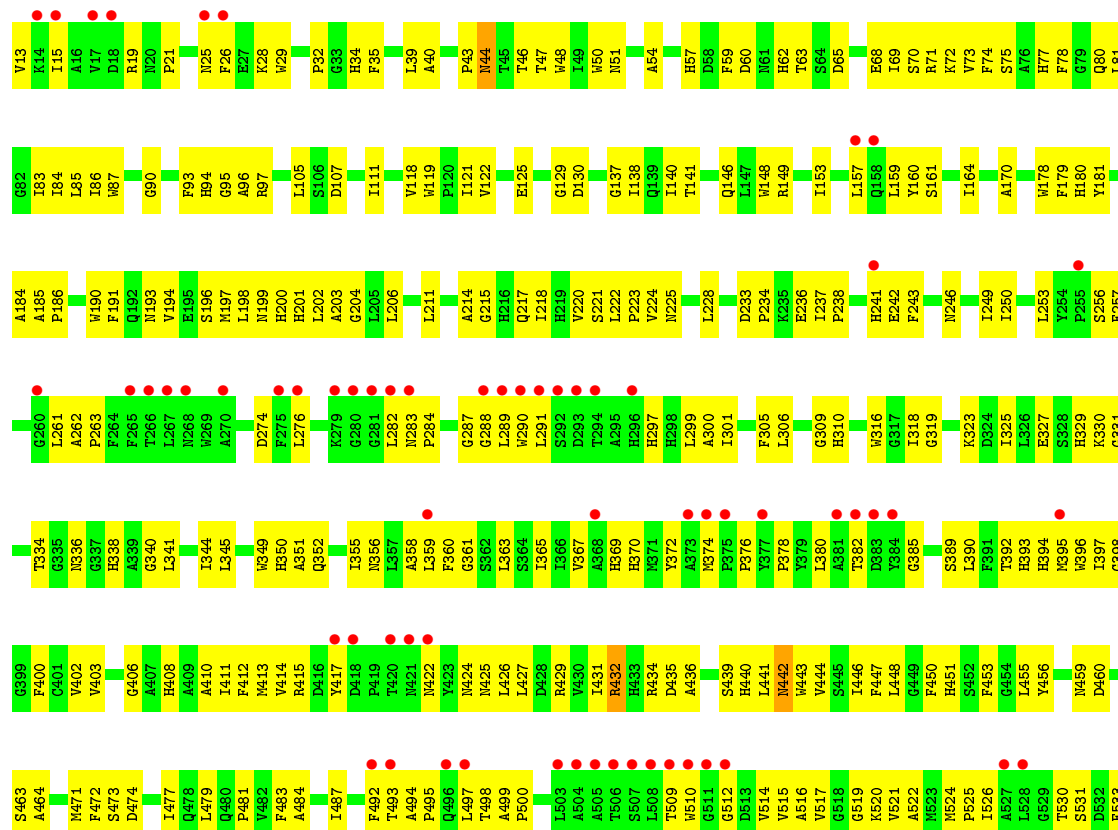


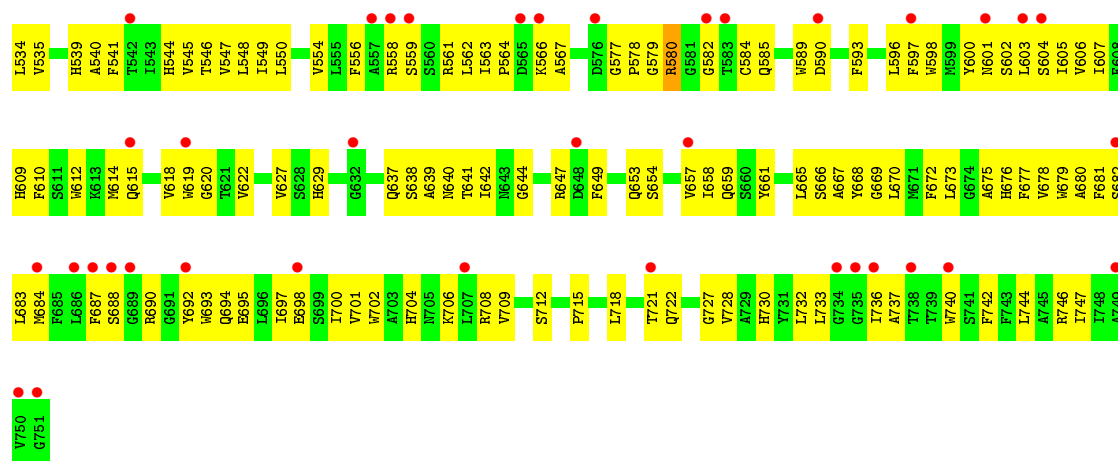


● Molecule 4: Lhc4

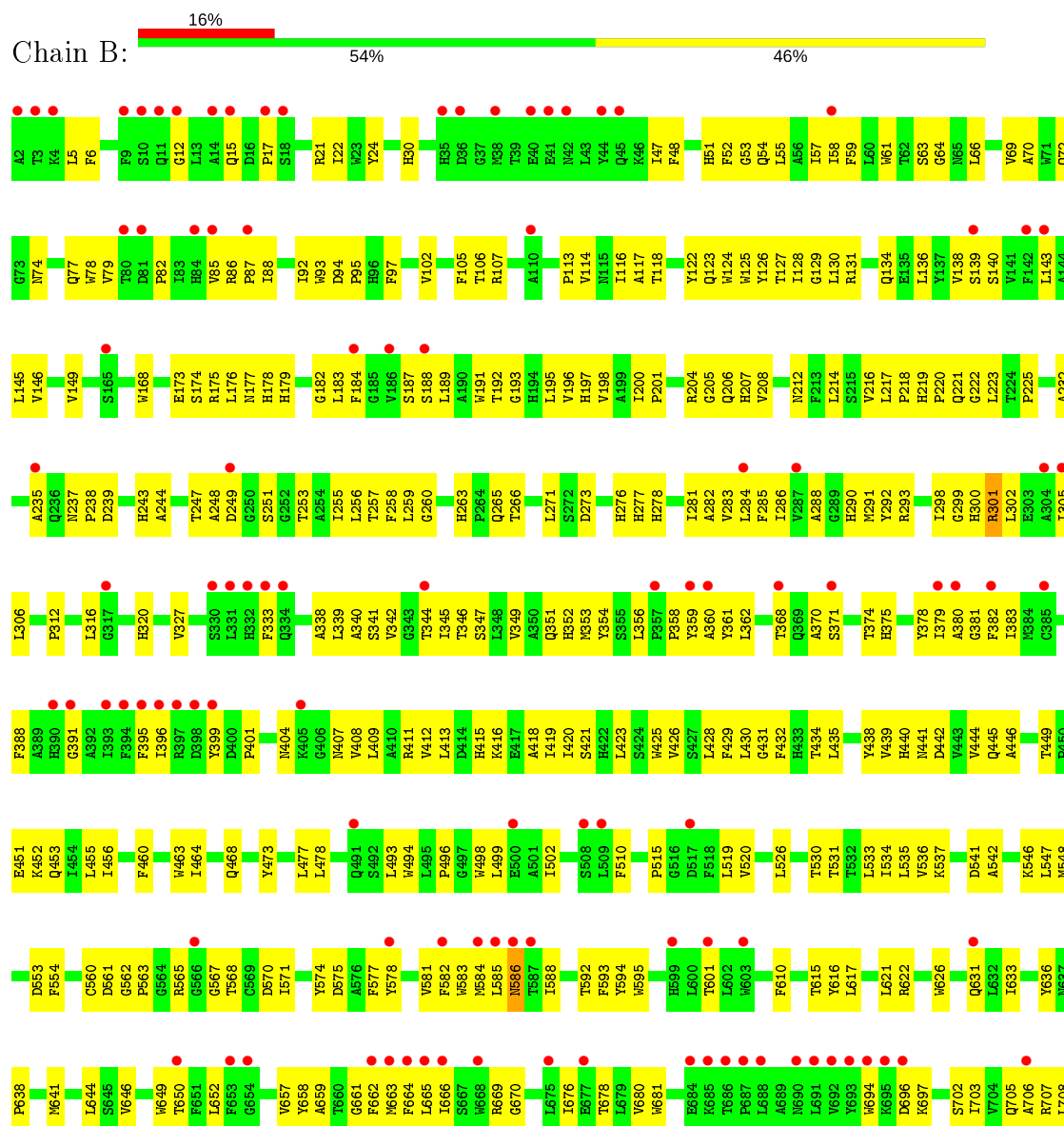


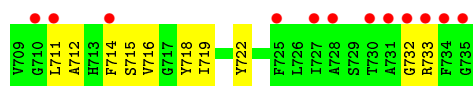
● Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



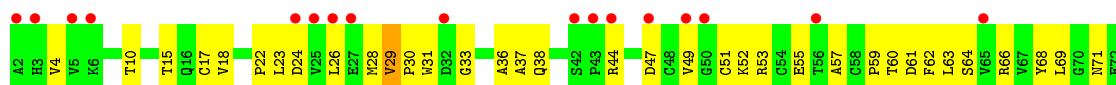


• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

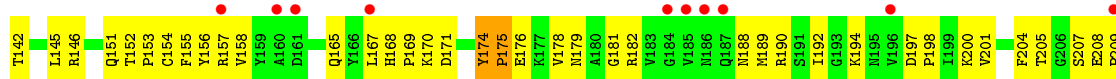
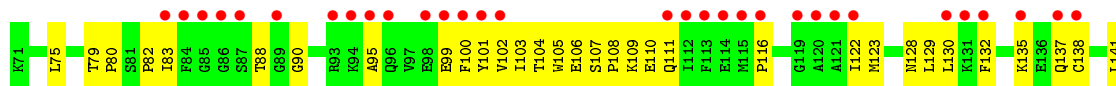




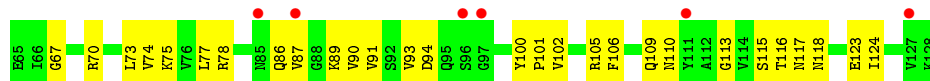
• Molecule 7: Photosystem I iron-sulfur center



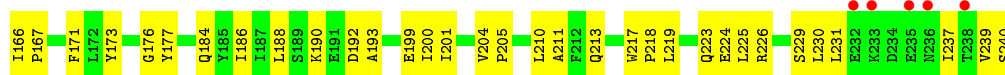
• Molecule 8: PsaD



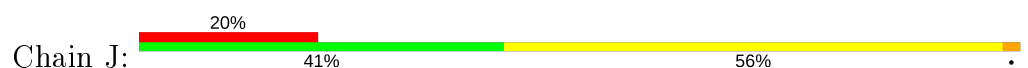
• Molecule 9: PsaE

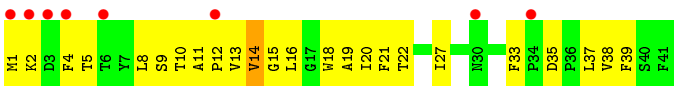


• Molecule 10: PsaF



• Molecule 11: Photosystem I reaction center subunit IX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.88Å 100.51Å 191.04Å 90.00° 91.73° 90.00°	Depositor
Resolution (Å)	48.95 – 3.40 48.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.95-3.40) 81.3 (48.95-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.22 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, $R_{free}$	0.337 , 0.356 0.337 , 0.356	Depositor DCC
$R_{free}$ test set	1593 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.3	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 4.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	30870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LUT, DGD, XAT, LMT, SF4, CHL, CLA, PQN, CAC, GSH, LMG, CL0, CA, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.33	0/1529	0.44	0/2073
2	2	0.31	0/1680	0.43	0/2277
3	3	0.28	0/1657	0.44	0/2253
4	4	0.38	0/1687	0.47	0/2300
5	A	0.29	0/5995	0.40	0/8179
6	B	0.30	0/6026	0.40	0/8237
7	C	0.29	0/610	0.45	0/828
8	D	0.29	0/1150	0.47	0/1551
9	E	0.36	0/525	0.43	0/712
10	F	0.39	0/1313	0.45	0/1776
11	J	0.38	0/338	0.49	0/461
All	All	0.31	0/22510	0.42	0/30647

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:



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

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1490	0	1457	114	1
2	2	1631	32	1575	109	0
3	3	1609	0	1567	140	0
4	4	1637	0	1579	136	0
5	A	5799	0	5629	460	0
6	B	5813	0	5565	398	0
7	C	600	0	582	48	0
8	D	1123	0	1134	77	0
9	E	515	0	508	21	0
10	F	1285	0	1304	89	0
11	J	327	0	328	43	0
12	1	42	0	55	11	0
12	2	42	0	55	12	0
12	3	42	0	55	11	0
12	4	42	0	55	18	0
13	1	44	0	56	12	0
13	2	44	0	56	15	0
13	3	44	0	56	23	0
13	4	44	0	56	5	0
14	1	80	0	105	15	0
14	2	40	0	53	8	0
14	3	80	0	105	26	0
14	4	80	0	105	12	0
14	A	240	0	318	42	0
14	B	240	0	316	34	0
14	F	40	0	52	6	0
14	J	120	0	159	26	0
15	1	593	0	468	122	0
15	2	501	0	402	66	0
15	3	525	0	391	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	4	542	0	423	95	0
15	A	2180	0	1773	325	0
15	B	2137	0	1760	280	0
15	F	96	0	72	12	0
15	J	49	0	38	8	0
16	1	97	0	66	27	0
16	2	194	0	134	31	0
16	3	47	0	30	14	0
16	4	147	0	102	21	0
17	1	23	0	16	2	0
17	2	21	0	12	2	0
17	A	40	0	30	6	0
17	B	21	0	12	2	0
18	1	59	0	58	1	0
18	2	41	0	34	1	0
19	1	40	0	46	4	0
20	1	10	0	0	0	0
20	3	10	0	0	1	0
20	4	10	0	0	1	0
21	2	47	0	52	2	0
21	4	45	0	48	7	0
21	B	38	0	34	4	0
21	J	28	0	26	0	0
22	2	23	0	21	0	0
23	4	20	0	15	0	1
23	B	20	0	15	2	0
24	A	50	0	39	23	0
25	A	33	0	46	12	0
25	B	33	0	46	6	0
26	A	8	0	0	0	0
26	C	16	0	0	2	0
27	B	1	0	0	0	0
All	All	30838	32	29094	2232	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

The worst 5 of 2232 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4005:BCR:C12	14:A:4005:BCR:C11	1.83	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4005:BCR:C10	14:A:4005:BCR:C11	1.92	1.45
7:C:29:VAL:HG12	7:C:30:PRO:HD3	1.20	1.17
5:A:197:MET:HE2	15:A:1111:CLA:HAC1	1.36	1.04
8:D:105:TRP:HB3	8:D:153:PRO:HB3	1.40	1.02

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

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

## 5.3 Torsion angles [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	1	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
2	2	209/211 (99%)	194 (93%)	15 (7%)	0	100	100
3	3	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
4	4	209/211 (99%)	184 (88%)	25 (12%)	0	100	100
5	A	737/739 (100%)	702 (95%)	35 (5%)	0	100	100
6	B	732/734 (100%)	695 (95%)	37 (5%)	0	100	100
7	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
8	D	140/142 (99%)	124 (89%)	14 (10%)	2 (1%)	11	37
9	E	62/64 (97%)	54 (87%)	8 (13%)	0	100	100
10	F	161/163 (99%)	145 (90%)	16 (10%)	0	100	100
11	J	39/41 (95%)	30 (77%)	9 (23%)	0	100	100
All	All	2768/2790 (99%)	2588 (94%)	178 (6%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	151/151 (100%)	151 (100%)	0	100	100
2	2	169/169 (100%)	169 (100%)	0	100	100
3	3	160/160 (100%)	159 (99%)	1 (1%)	86	94
4	4	169/169 (100%)	166 (98%)	3 (2%)	59	79
5	A	598/598 (100%)	594 (99%)	4 (1%)	84	92
6	B	593/593 (100%)	589 (99%)	4 (1%)	84	92
7	C	68/68 (100%)	68 (100%)	0	100	100
8	D	122/122 (100%)	121 (99%)	1 (1%)	81	91
9	E	57/57 (100%)	56 (98%)	1 (2%)	59	79
10	F	136/136 (100%)	134 (98%)	2 (2%)	65	82
11	J	36/36 (100%)	36 (100%)	0	100	100
All	All	2259/2259 (100%)	2243 (99%)	16 (1%)	84	92

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	580	ARG
6	B	293	ARG
8	D	189	MET
5	A	442	ASN
9	E	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	3	271	HIS
3	3	279	ASN
6	B	445	GLN
3	3	267	ASN
5	A	653	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
15	CLA	4	604	4	43,57,73	1.58	9 (20%)	46,93,113	2.10	9 (19%)
15	CLA	A	1124	-	43,57,73	1.50	8 (18%)	46,93,113	2.12	10 (21%)
15	CLA	A	1133	-	43,57,73	1.56	8 (18%)	46,93,113	2.01	8 (17%)
14	BCR	B	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.60	20 (35%)
15	CLA	2	608	-	43,57,73	1.53	8 (18%)	46,93,113	2.16	10 (21%)
13	XAT	3	502	-	39,47,47	0.67	1 (2%)	54,74,74	1.92	14 (25%)
15	CLA	2	601	-	43,57,73	1.46	7 (16%)	46,93,113	1.98	10 (21%)
15	CLA	B	1218	-	43,57,73	1.54	9 (20%)	46,93,113	2.09	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A	1119	-	43,57,73	1.56	7 (16%)	46,93,113	2.08	9 (19%)
14	BCR	B	4004	-	41,41,41	1.78	4 (9%)	56,56,56	4.46	15 (26%)
15	CLA	A	1127	-	43,57,73	1.58	8 (18%)	46,93,113	2.16	10 (21%)
15	CLA	A	1134	-	43,57,73	1.53	8 (18%)	46,93,113	2.13	9 (19%)
15	CLA	A	1130	-	49,63,73	1.47	7 (14%)	55,101,113	1.99	9 (16%)
12	LUT	4	501	-	42,43,43	2.39	2 (4%)	51,60,60	1.92	14 (27%)
14	BCR	4	503	-	41,41,41	1.90	4 (9%)	56,56,56	4.47	18 (32%)
15	CLA	B	1205	-	43,57,73	1.53	9 (20%)	46,93,113	2.16	9 (19%)
15	CLA	A	1117	-	43,57,73	1.54	8 (18%)	46,93,113	2.09	8 (17%)
15	CLA	A	1013	-	59,73,73	1.35	7 (11%)	67,113,113	1.83	11 (16%)
15	CLA	B	1213	-	43,57,73	1.43	8 (18%)	46,93,113	2.00	10 (21%)
15	CLA	4	603	-	43,57,73	1.55	8 (18%)	46,93,113	2.02	9 (19%)
15	CLA	3	612	-	49,63,73	1.39	8 (16%)	55,101,113	1.96	10 (18%)
19	SQD	1	811	-	39,40,54	0.89	0	48,51,65	0.99	3 (6%)
15	CLA	1	601	-	43,57,73	1.49	8 (18%)	46,93,113	2.01	9 (19%)
15	CLA	B	1227	-	36,53,73	1.78	8 (22%)	39,89,113	2.13	8 (20%)
15	CLA	A	1108	-	40,54,73	1.65	8 (20%)	44,90,113	2.04	9 (20%)
15	CLA	B	1214	-	43,57,73	1.55	9 (20%)	46,93,113	2.08	10 (21%)
21	DGD	4	811	-	46,46,67	0.90	2 (4%)	60,60,81	0.98	3 (5%)
15	CLA	B	1229	-	59,73,73	1.40	6 (10%)	67,113,113	1.85	11 (16%)
15	CLA	3	607	-	44,58,73	1.53	8 (18%)	49,95,113	2.04	10 (20%)
25	PQN	B	2002	-	34,34,34	0.44	0	42,45,45	1.17	3 (7%)
15	CLA	B	1202	-	43,57,73	1.53	6 (13%)	46,93,113	2.08	8 (17%)
21	DGD	B	5002	-	39,39,67	0.93	2 (5%)	53,53,81	1.00	3 (5%)
15	CLA	B	1209	-	40,54,73	1.60	8 (20%)	44,90,113	1.95	7 (15%)
16	CHL	4	610	-	41,55,74	0.92	3 (7%)	41,91,114	1.45	10 (24%)
15	CLA	4	607	-	43,57,73	1.57	8 (18%)	46,93,113	2.01	10 (21%)
15	CLA	B	1204	-	43,57,73	1.56	8 (18%)	46,93,113	2.04	9 (19%)
15	CLA	A	1136	-	43,57,73	1.53	7 (16%)	46,93,113	2.10	8 (17%)
15	CLA	B	1211	-	43,57,73	1.53	9 (20%)	46,93,113	2.09	7 (15%)
15	CLA	A	1106	-	59,73,73	1.33	8 (13%)	67,113,113	1.86	9 (13%)
15	CLA	A	1113	-	36,53,73	1.68	9 (25%)	39,89,113	2.02	7 (17%)
14	BCR	J	4003	-	41,41,41	1.83	4 (9%)	56,56,56	4.39	17 (30%)
15	CLA	4	608	-	40,54,73	1.56	8 (20%)	44,90,113	1.98	6 (13%)
15	CLA	F	1301	-	41,55,73	1.59	6 (14%)	45,91,113	2.08	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	GSH	4	831	-	12,19,19	2.42	4 (33%)	15,24,24	1.73	2 (13%)
15	CLA	2	602	-	43,57,73	1.58	7 (16%)	46,93,113	2.14	9 (19%)
16	CHL	4	613	-	44,58,74	0.99	3 (6%)	43,94,114	1.52	11 (25%)
26	SF4	A	3001	5,6	0,12,12	0.00	-	-		
15	CLA	2	607	-	43,57,73	1.57	7 (16%)	46,93,113	2.12	8 (17%)
15	CLA	B	1230	-	43,57,73	1.57	8 (18%)	46,93,113	2.20	8 (17%)
14	BCR	1	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.54	21 (37%)
15	CLA	3	613	-	40,54,73	1.62	6 (15%)	44,90,113	1.92	6 (13%)
15	CLA	1	604	1	43,57,73	1.53	8 (18%)	46,93,113	2.13	11 (23%)
14	BCR	J	4002	-	41,41,41	1.82	5 (12%)	56,56,56	4.52	21 (37%)
15	CLA	2	604	-	43,57,73	1.48	7 (16%)	46,93,113	2.04	10 (21%)
18	LMG	2	803	-	15,16,55	0.51	0	20,22,63	0.54	0
14	BCR	B	4006	-	41,41,41	1.89	4 (9%)	56,56,56	4.41	15 (26%)
15	CLA	A	1138	-	59,73,73	1.33	7 (11%)	67,113,113	1.81	9 (13%)
20	CAC	4	902	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	A	1128	-	43,57,73	1.56	8 (18%)	46,93,113	2.15	8 (17%)
15	CLA	J	1302	-	43,57,73	1.55	7 (16%)	46,93,113	2.02	7 (15%)
15	CLA	B	1231	6	54,68,73	1.37	6 (11%)	61,107,113	1.88	10 (16%)
14	BCR	4	505	-	41,41,41	1.87	4 (9%)	56,56,56	4.52	18 (32%)
13	XAT	4	502	-	39,47,47	0.73	0	54,74,74	1.90	13 (24%)
15	CLA	A	1118	-	43,57,73	1.53	9 (20%)	46,93,113	2.09	8 (17%)
15	CLA	4	615	-	49,63,73	1.43	6 (12%)	55,101,113	1.91	9 (16%)
15	CLA	A	1129	-	42,56,73	1.55	7 (16%)	46,92,113	2.01	9 (19%)
18	LMG	2	802	-	25,25,55	0.58	0	33,33,63	1.19	3 (9%)
15	CLA	B	1215	-	43,57,73	1.66	7 (16%)	46,93,113	2.28	9 (19%)
15	CLA	4	605	-	43,57,73	1.64	7 (16%)	46,93,113	2.15	9 (19%)
15	CLA	B	1224	-	43,57,73	1.53	8 (18%)	46,93,113	2.04	9 (19%)
15	CLA	A	1104	-	54,68,73	1.34	8 (14%)	61,107,113	1.99	10 (16%)
20	CAC	1	902	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	2	612	-	43,57,73	1.58	8 (18%)	46,93,113	2.12	8 (17%)
15	CLA	A	1115	-	43,57,73	1.58	8 (18%)	46,93,113	2.16	9 (19%)
15	CLA	3	605	-	40,54,73	1.56	8 (20%)	44,90,113	1.87	6 (13%)
15	CLA	A	1114	-	40,54,73	1.58	9 (22%)	44,90,113	1.98	6 (13%)
15	CLA	B	1022	-	44,58,73	1.49	7 (15%)	49,95,113	2.10	12 (24%)
15	CLA	3	615	-	40,54,73	1.61	7 (17%)	44,90,113	1.96	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	4	601	4	43,57,73	1.47	6 (13%)	46,93,113	2.08	12 (26%)
15	CLA	B	1203	-	43,57,73	1.53	7 (16%)	46,93,113	2.08	7 (15%)
14	BCR	1	505	-	41,41,41	1.89	4 (9%)	56,56,56	4.53	16 (28%)
15	CLA	1	613	-	36,53,73	1.61	8 (22%)	39,89,113	2.05	7 (17%)
12	LUT	1	501	-	42,43,43	2.44	1 (2%)	51,60,60	4.93	27 (52%)
15	CLA	B	1207	-	22,32,73	3.08	9 (40%)	26,54,113	2.57	10 (38%)
15	CLA	B	1220	-	49,63,73	1.47	7 (14%)	55,101,113	1.95	11 (20%)
18	LMG	1	803	-	23,23,55	0.58	0	31,31,63	1.36	2 (6%)
15	CLA	3	610	-	43,57,73	1.53	8 (18%)	46,93,113	1.98	9 (19%)
15	CLA	B	1236	-	43,57,73	1.50	8 (18%)	46,93,113	2.14	10 (21%)
15	CLA	A	1111	-	43,57,73	1.49	7 (16%)	46,93,113	2.17	11 (23%)
17	LHG	B	5001	15	20,20,48	0.64	0	23,26,54	1.43	2 (8%)
15	CLA	4	606	-	43,57,73	1.57	8 (18%)	46,93,113	2.08	8 (17%)
15	CLA	B	1206	6	43,57,73	1.53	8 (18%)	46,93,113	2.10	9 (19%)
15	CLA	1	602	-	40,54,73	1.57	9 (22%)	44,90,113	1.93	7 (15%)
15	CLA	B	1226	-	43,57,73	1.53	8 (18%)	46,93,113	2.19	9 (19%)
15	CLA	B	1239	-	59,73,73	1.32	7 (11%)	67,113,113	1.81	9 (13%)
15	CLA	B	1216	-	43,57,73	1.47	7 (16%)	46,93,113	2.07	9 (19%)
17	LHG	1	801	15	22,22,48	0.56	0	25,28,54	1.33	3 (12%)
15	CLA	A	1012	-	54,68,73	1.44	8 (14%)	61,107,113	1.95	12 (19%)
15	CLA	A	1110	-	43,57,73	1.49	8 (18%)	46,93,113	2.10	9 (19%)
14	BCR	2	503	-	41,41,41	1.87	4 (9%)	56,56,56	4.50	17 (30%)
15	CLA	A	1109	15	43,57,73	1.52	8 (18%)	46,93,113	2.11	9 (19%)
15	CLA	A	1132	-	43,57,73	1.52	9 (20%)	46,93,113	2.13	9 (19%)
16	CHL	2	609	2	44,58,74	0.98	3 (6%)	43,94,114	1.40	10 (23%)
15	CLA	B	1240	17	59,73,73	1.34	7 (11%)	67,113,113	1.79	10 (14%)
15	CLA	B	1217	-	40,54,73	1.59	8 (20%)	44,90,113	1.90	7 (15%)
21	DGD	2	811	-	48,48,67	0.94	3 (6%)	62,62,81	1.06	3 (4%)
22	LMT	2	821	-	24,24,36	1.34	5 (20%)	35,35,47	1.04	2 (5%)
15	CLA	A	1122	-	43,57,73	1.52	8 (18%)	46,93,113	2.07	8 (17%)
15	CLA	B	1221	-	43,57,73	1.54	7 (16%)	46,93,113	2.15	10 (21%)
15	CLA	1	606	-	36,53,73	1.65	6 (16%)	39,89,113	2.12	8 (20%)
15	CLA	B	1021	-	59,73,73	1.36	8 (13%)	67,113,113	1.86	11 (16%)
14	BCR	B	4002	-	41,41,41	1.90	4 (9%)	56,56,56	4.37	17 (30%)
15	CLA	4	612	-	43,57,73	1.59	9 (20%)	46,93,113	2.13	10 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	1	611	-	43,57,73	1.56	7 (16%)	46,93,113	2.06	9 (19%)
20	CAC	3	902	-	0,4,4	0.00	-	0,6,6	0.00	-
21	DGD	J	5001	-	29,29,67	0.61	0	41,41,81	0.60	0
15	CLA	B	1235	-	54,68,73	1.35	9 (16%)	61,107,113	1.89	10 (16%)
15	CLA	3	601	-	43,57,73	1.61	7 (16%)	46,93,113	2.20	9 (19%)
13	XAT	2	502	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	14 (25%)
15	CLA	B	1223	-	44,58,73	1.63	8 (18%)	49,95,113	2.18	11 (22%)
15	CLA	A	1107	5	43,57,73	1.54	7 (16%)	46,93,113	2.08	8 (17%)
20	CAC	4	901	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	A	1120	-	43,57,73	1.54	8 (18%)	46,93,113	2.09	9 (19%)
15	CLA	A	1141	-	44,58,73	1.52	7 (15%)	49,95,113	2.07	9 (18%)
15	CLA	B	1228	-	54,68,73	1.32	7 (12%)	61,107,113	1.82	10 (16%)
18	LMG	1	802	-	36,36,55	0.73	1 (2%)	44,44,63	1.19	4 (9%)
15	CLA	4	602	-	43,57,73	1.50	7 (16%)	46,93,113	2.03	8 (17%)
16	CHL	1	610	-	41,55,74	1.07	2 (4%)	41,91,114	1.50	11 (26%)
15	CLA	2	605	-	59,73,73	1.34	8 (13%)	67,113,113	1.89	12 (17%)
15	CLA	B	1222	-	43,57,73	1.58	8 (18%)	46,93,113	2.15	8 (17%)
26	SF4	C	3002	7	0,12,12	0.00	-	-	-	-
20	CAC	1	901	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	1	612	-	53,67,73	1.41	8 (15%)	59,105,113	1.89	8 (13%)
15	CLA	2	615	2	44,58,73	1.50	9 (20%)	49,95,113	2.05	9 (18%)
14	BCR	F	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.56	19 (33%)
15	CLA	A	1140	-	49,63,73	1.47	9 (18%)	55,101,113	1.95	8 (14%)
14	BCR	A	4005	-	41,41,41	4.26	5 (12%)	56,56,56	4.55	21 (37%)
15	CLA	A	1123	-	42,56,73	1.59	8 (19%)	46,92,113	2.01	9 (19%)
17	LHG	2	801	-	20,20,48	0.62	0	23,26,54	1.48	2 (8%)
15	CLA	B	1023	-	54,68,73	1.36	8 (14%)	61,107,113	1.80	11 (18%)
15	CLA	B	1210	-	43,57,73	1.47	6 (13%)	46,93,113	2.12	8 (17%)
15	CLA	1	615	-	59,73,73	1.32	8 (13%)	67,113,113	1.84	9 (13%)
14	BCR	A	4004	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	15 (26%)
15	CLA	4	609	4	43,57,73	1.52	6 (13%)	46,93,113	2.19	10 (21%)
15	CLA	A	1116	-	43,57,73	1.51	8 (18%)	46,93,113	2.12	8 (17%)
14	BCR	B	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.54	17 (30%)
14	BCR	J	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.42	14 (25%)
14	BCR	A	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.33	17 (30%)
14	BCR	3	504	-	41,41,41	1.87	4 (9%)	56,56,56	4.57	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	B	1234	-	43,57,73	1.53	7 (16%)	46,93,113	2.10	10 (21%)
14	BCR	3	503	-	41,41,41	1.88	4 (9%)	56,56,56	4.34	17 (30%)
25	PQN	A	2001	-	34,34,34	0.49	0	42,45,45	1.17	3 (7%)
16	CHL	2	611	-	42,56,74	1.01	2 (4%)	42,92,114	1.42	12 (28%)
17	LHG	A	5001	-	15,15,48	0.75	1 (6%)	16,19,54	0.57	0
15	CLA	B	1219	-	43,57,73	1.53	9 (20%)	46,93,113	2.06	9 (19%)
14	BCR	A	4007	-	41,41,41	1.88	4 (9%)	56,56,56	4.61	18 (32%)
15	CLA	A	1126	-	43,57,73	1.59	6 (13%)	46,93,113	2.17	8 (17%)
15	CLA	2	603	-	40,54,73	1.58	7 (17%)	44,90,113	1.87	6 (13%)
15	CLA	A	1112	-	43,57,73	1.54	8 (18%)	46,93,113	2.09	9 (19%)
15	CLA	A	1139	-	46,60,73	1.51	6 (13%)	51,97,113	2.06	12 (23%)
26	SF4	C	3003	7	0,12,12	0.00	-	-	-	-
15	CLA	B	1201	-	42,56,73	1.59	9 (21%)	46,92,113	1.99	8 (17%)
15	CLA	1	603	-	36,53,73	1.78	9 (25%)	39,89,113	2.02	7 (17%)
15	CLA	B	1225	-	43,57,73	1.49	7 (16%)	46,93,113	2.07	9 (19%)
15	CLA	F	1302	-	43,57,73	1.49	8 (18%)	46,93,113	1.99	9 (19%)
15	CLA	A	1121	-	43,57,73	1.53	8 (18%)	46,93,113	2.06	8 (17%)
15	CLA	A	1135	-	43,57,73	1.52	8 (18%)	46,93,113	2.11	8 (17%)
15	CLA	A	1101	-	36,53,73	1.71	7 (19%)	39,89,113	2.15	9 (23%)
14	BCR	A	4003	-	41,41,41	1.82	4 (9%)	56,56,56	4.29	16 (28%)
15	CLA	1	608	-	40,54,73	1.60	7 (17%)	44,90,113	2.03	6 (13%)
16	CHL	2	610	-	44,58,74	0.89	2 (4%)	43,94,114	1.42	11 (25%)
15	CLA	3	608	-	42,56,73	1.56	9 (21%)	46,92,113	1.96	8 (17%)
16	CHL	3	604	-	41,55,74	0.96	2 (4%)	41,91,114	1.56	10 (24%)
15	CLA	A	1137	-	43,57,73	1.54	8 (18%)	46,93,113	2.11	10 (21%)
15	CLA	B	1238	-	44,58,73	1.53	7 (15%)	49,95,113	2.05	9 (18%)
17	LHG	A	5002	-	23,23,48	0.52	0	26,29,54	1.44	3 (11%)
15	CLA	B	1232	-	43,57,73	1.55	8 (18%)	46,93,113	2.07	8 (17%)
15	CLA	3	603	-	36,53,73	1.68	9 (25%)	39,89,113	2.43	12 (30%)
12	LUT	2	501	-	42,43,43	2.38	1 (2%)	51,60,60	2.24	15 (29%)
23	GSH	B	5031	-	12,19,19	2.46	3 (25%)	15,24,24	1.65	2 (13%)
20	CAC	3	901	-	0,4,4	0.00	-	0,6,6	0.00	-
15	CLA	B	1208	-	43,57,73	1.56	7 (16%)	46,93,113	2.06	9 (19%)
15	CLA	3	606	-	36,53,73	1.66	7 (19%)	39,89,113	2.07	9 (23%)
15	CLA	A	1131	-	44,58,73	1.53	8 (18%)	49,95,113	2.06	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A	1125	-	43,57,73	1.52	7 (16%)	46,93,113	2.05	8 (17%)
15	CLA	A	1105	-	43,57,73	1.55	8 (18%)	46,93,113	2.11	9 (19%)
16	CHL	1	609	1	44,58,74	0.96	2 (4%)	43,94,114	1.44	11 (25%)
14	BCR	B	4005	-	41,41,41	1.87	4 (9%)	56,56,56	4.47	14 (25%)
12	LUT	3	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.13	12 (23%)
15	CLA	B	1237	-	43,57,73	1.54	8 (18%)	46,93,113	2.07	9 (19%)
15	CLA	3	611	-	40,54,73	1.57	6 (15%)	44,90,113	1.99	6 (13%)
13	XAT	1	502	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
15	CLA	1	607	17	40,54,73	1.59	8 (20%)	44,90,113	1.93	6 (13%)
15	CLA	B	1212	-	36,53,73	1.65	7 (19%)	39,89,113	2.04	9 (23%)
16	CHL	2	613	-	37,54,74	1.05	3 (8%)	36,90,114	1.55	11 (30%)
15	CLA	2	606	-	40,54,73	1.63	8 (20%)	44,90,113	2.04	7 (15%)
15	CLA	A	1102	15	36,53,73	1.66	8 (22%)	39,89,113	2.11	7 (17%)
24	CL0	A	1011	-	44,58,73	2.71	16 (36%)	49,95,113	2.53	15 (30%)
15	CLA	A	1103	-	49,63,73	1.43	8 (16%)	55,101,113	1.95	10 (18%)
15	CLA	1	605	-	42,56,73	1.53	7 (16%)	46,92,113	2.04	10 (21%)
14	BCR	A	4002	-	41,41,41	1.88	4 (9%)	56,56,56	4.42	18 (32%)
16	CHL	4	611	-	44,58,74	1.02	3 (6%)	43,94,114	1.43	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	4	604	4	3/3/16/25	11/18/116/135	-
15	CLA	A	1124	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1133	-	3/3/16/25	7/18/116/135	-
14	BCR	B	4001	-	-	14/29/63/63	0/2/2/2
15	CLA	2	608	-	3/3/16/25	9/18/116/135	-
13	XAT	3	502	-	1/1/12/26	14/31/93/93	0/4/4/4
15	CLA	2	601	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1218	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1119	-	3/3/16/25	11/18/116/135	-
14	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
15	CLA	A	1127	-	3/3/16/25	11/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1134	-	3/3/16/25	8/18/116/135	-
15	CLA	A	1130	-	3/3/18/25	15/25/123/135	-
12	LUT	4	501	-	-	7/29/67/67	0/2/2/2
14	BCR	4	503	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1205	-	3/3/16/25	9/18/116/135	-
15	CLA	A	1117	-	3/3/16/25	7/18/116/135	-
15	CLA	A	1013	-	3/3/20/25	20/37/135/135	-
14	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1123	-	3/3/16/25	9/17/115/135	-
15	CLA	3	612	-	3/3/18/25	10/25/123/135	-
19	SQD	1	811	-	-	6/34/54/69	0/1/1/1
15	CLA	1	601	-	3/3/16/25	13/18/116/135	-
16	CHL	3	604	-	3/3/16/26	6/17/115/137	-
15	CLA	B	1227	-	3/3/16/25	3/11/111/135	-
15	CLA	A	1108	-	3/3/16/25	10/15/113/135	-
15	CLA	B	1214	-	3/3/16/25	10/18/116/135	-
15	CLA	4	601	4	3/3/16/25	9/18/116/135	-
21	DGD	4	811	-	-	14/34/74/95	0/2/2/2
15	CLA	B	1229	-	3/3/20/25	17/37/135/135	-
15	CLA	B	1206	6	3/3/16/25	9/18/116/135	-
25	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
21	DGD	B	5002	-	-	9/27/67/95	0/2/2/2
15	CLA	B	1209	-	3/3/16/25	8/15/113/135	-
16	CHL	4	610	-	4/4/16/26	5/17/115/137	-
15	CLA	4	607	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1204	-	3/3/16/25	8/18/116/135	-
15	CLA	A	1136	-	3/3/16/25	11/18/116/135	-
15	CLA	B	1211	-	3/3/16/25	9/18/116/135	-
15	CLA	A	1109	15	3/3/16/25	8/18/116/135	-
15	CLA	A	1113	-	3/3/16/25	6/11/111/135	-
14	BCR	J	4003	-	-	14/29/63/63	0/2/2/2
15	CLA	4	608	-	3/3/16/25	6/15/113/135	-
15	CLA	F	1301	-	3/3/16/25	10/16/114/135	-
23	GSH	4	831	-	-	3/18/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	2	602	-	3/3/16/25	7/18/116/135	-
16	CHL	4	613	-	4/4/16/26	7/20/118/137	-
26	SF4	A	3001	5,6	-	-	0/6/5/5
15	CLA	2	607	-	3/3/16/25	12/18/116/135	-
15	CLA	B	1230	-	3/3/16/25	8/18/116/135	-
15	CLA	A	1111	-	3/3/16/25	7/18/116/135	-
15	CLA	3	613	-	3/3/16/25	10/15/113/135	-
15	CLA	1	604	1	3/3/16/25	7/18/116/135	-
14	BCR	J	4002	-	-	17/29/63/63	0/2/2/2
15	CLA	2	604	-	3/3/16/25	11/18/116/135	-
18	LMG	2	803	-	-	3/7/27/70	0/1/1/1
14	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
15	CLA	A	1138	-	3/3/20/25	20/37/135/135	-
15	CLA	A	1128	-	3/3/16/25	10/18/116/135	-
15	CLA	J	1302	-	3/3/16/25	12/18/116/135	-
15	CLA	B	1231	6	3/3/19/25	11/31/129/135	-
14	BCR	4	505	-	-	19/29/63/63	0/2/2/2
13	XAT	4	502	-	1/1/12/26	6/31/93/93	0/4/4/4
15	CLA	A	1118	-	3/3/16/25	14/18/116/135	-
15	CLA	4	615	-	3/3/18/25	12/25/123/135	-
15	CLA	A	1129	-	3/3/16/25	12/17/115/135	-
18	LMG	2	802	-	-	8/20/40/70	0/1/1/1
15	CLA	B	1215	-	3/3/16/25	9/18/116/135	-
15	CLA	4	605	-	3/3/16/25	11/18/116/135	-
15	CLA	B	1224	-	3/3/16/25	11/18/116/135	-
15	CLA	A	1104	-	3/3/19/25	17/31/129/135	-
15	CLA	B	1202	-	3/3/16/25	11/18/116/135	-
15	CLA	2	612	-	3/3/16/25	14/18/116/135	-
12	LUT	2	501	-	-	6/29/67/67	0/2/2/2
15	CLA	A	1115	-	3/3/16/25	10/18/116/135	-
15	CLA	3	605	-	3/3/16/25	5/15/113/135	-
15	CLA	A	1114	-	3/3/16/25	6/15/113/135	-
15	CLA	B	1022	-	3/3/17/25	7/19/117/135	-
15	CLA	3	615	-	3/3/16/25	6/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1203	-	3/3/16/25	8/18/116/135	-
14	BCR	1	505	-	-	12/29/63/63	0/2/2/2
15	CLA	1	613	-	3/3/16/25	4/11/111/135	-
12	LUT	1	501	-	-	8/29/67/67	0/2/2/2
15	CLA	B	1207	-	3/3/7/25	-	-
15	CLA	B	1220	-	3/3/18/25	12/25/123/135	-
18	LMG	1	803	-	-	6/16/36/70	0/1/1/1
15	CLA	3	610	-	3/3/16/25	7/18/116/135	-
15	CLA	B	1236	-	3/3/16/25	10/18/116/135	-
14	BCR	1	503	-	-	16/29/63/63	0/2/2/2
17	LHG	B	5001	15	-	13/23/23/53	-
15	CLA	4	606	-	3/3/16/25	11/18/116/135	-
15	CLA	1	602	-	3/3/16/25	11/15/113/135	-
15	CLA	B	1226	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1239	-	3/3/20/25	17/37/135/135	-
15	CLA	B	1216	-	3/3/16/25	10/18/116/135	-
17	LHG	1	801	15	-	11/26/26/53	-
15	CLA	A	1012	-	3/3/19/25	11/31/129/135	-
15	CLA	A	1110	-	3/3/16/25	8/18/116/135	-
14	BCR	2	503	-	-	14/29/63/63	0/2/2/2
15	CLA	A	1132	-	3/3/16/25	12/18/116/135	-
16	CHL	2	609	2	3/3/16/26	7/20/118/137	-
15	CLA	A	1122	-	3/3/16/25	11/18/116/135	-
15	CLA	B	1240	17	3/3/20/25	19/37/135/135	-
15	CLA	B	1217	-	3/3/16/25	11/15/113/135	-
21	DGD	2	811	-	-	13/36/76/95	0/2/2/2
22	LMT	2	821	-	-	1/8/48/61	0/2/2/2
15	CLA	4	602	-	3/3/16/25	5/18/116/135	-
15	CLA	1	606	-	3/3/16/25	6/11/111/135	-
15	CLA	B	1021	-	3/3/20/25	17/37/135/135	-
14	BCR	B	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	4	612	-	3/3/16/25	11/18/116/135	-
15	CLA	1	611	-	3/3/16/25	12/18/116/135	-
21	DGD	J	5001	-	-	5/14/54/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1235	-	3/3/19/25	20/31/129/135	-
25	PQN	A	2001	-	-	12/23/43/43	0/2/2/2
15	CLA	3	601	-	3/3/16/25	12/18/116/135	-
13	XAT	2	502	-	1/1/12/26	3/31/93/93	0/4/4/4
15	CLA	B	1223	-	3/3/17/25	7/19/117/135	-
15	CLA	A	1107	5	3/3/16/25	4/18/116/135	-
15	CLA	A	1120	-	3/3/16/25	8/18/116/135	-
15	CLA	A	1141	-	3/3/17/25	9/19/117/135	-
15	CLA	B	1228	-	3/3/19/25	9/31/129/135	-
18	LMG	1	802	-	-	8/31/51/70	0/1/1/1
16	CHL	1	610	-	3/3/16/26	5/17/115/137	-
15	CLA	2	605	-	3/3/20/25	15/37/135/135	-
15	CLA	B	1222	-	3/3/16/25	9/18/116/135	-
26	SF4	C	3002	7	-	-	0/6/5/5
15	CLA	1	612	-	4/4/19/25	8/27/125/135	-
15	CLA	2	615	2	3/3/17/25	9/19/117/135	-
14	BCR	F	4002	-	-	12/29/63/63	0/2/2/2
15	CLA	A	1140	-	3/3/18/25	13/25/123/135	-
14	BCR	A	4005	-	-	8/29/63/63	0/2/2/2
15	CLA	4	603	-	3/3/16/25	4/18/116/135	-
17	LHG	2	801	-	-	10/23/23/53	-
15	CLA	B	1023	-	3/3/19/25	15/31/129/135	-
15	CLA	B	1210	-	3/3/16/25	12/18/116/135	-
15	CLA	1	615	-	3/3/20/25	20/37/135/135	-
14	BCR	A	4004	-	-	10/29/63/63	0/2/2/2
15	CLA	4	609	4	3/3/16/25	7/18/116/135	-
15	CLA	A	1116	-	3/3/16/25	8/18/116/135	-
14	BCR	B	4003	-	-	9/29/63/63	0/2/2/2
14	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
14	BCR	A	4006	-	-	15/29/63/63	0/2/2/2
14	BCR	3	504	-	-	17/29/63/63	0/2/2/2
15	CLA	B	1234	-	3/3/16/25	8/18/116/135	-
14	BCR	3	503	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1221	-	3/3/16/25	7/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CHL	2	611	-	4/4/16/26	1/18/116/137	-
17	LHG	A	5001	-	-	14/18/18/53	-
15	CLA	B	1219	-	3/3/16/25	9/18/116/135	-
14	BCR	A	4007	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1126	-	3/3/16/25	9/18/116/135	-
15	CLA	2	603	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1112	-	3/3/16/25	7/18/116/135	-
15	CLA	A	1139	-	3/3/17/25	6/22/120/135	-
26	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	B	1201	-	3/3/16/25	10/17/115/135	-
15	CLA	1	603	-	3/3/16/25	6/11/111/135	-
15	CLA	B	1225	-	3/3/16/25	8/18/116/135	-
15	CLA	F	1302	-	3/3/16/25	9/18/116/135	-
15	CLA	A	1121	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1135	-	3/3/16/25	11/18/116/135	-
15	CLA	A	1101	-	3/3/16/25	6/11/111/135	-
15	CLA	B	1213	-	3/3/16/25	9/18/116/135	-
15	CLA	1	608	-	3/3/16/25	7/15/113/135	-
16	CHL	2	610	-	4/4/16/26	8/20/118/137	-
15	CLA	3	608	-	3/3/16/25	7/17/115/135	-
15	CLA	A	1106	-	3/3/20/25	15/37/135/135	-
15	CLA	A	1137	-	3/3/16/25	10/18/116/135	-
15	CLA	B	1238	-	3/3/17/25	8/19/117/135	-
17	LHG	A	5002	-	-	18/28/28/53	-
15	CLA	B	1232	-	3/3/16/25	8/18/116/135	-
15	CLA	3	603	-	3/3/16/25	6/11/111/135	-
15	CLA	3	607	-	3/3/17/25	11/19/117/135	-
23	GSH	B	5031	-	-	7/18/24/24	-
15	CLA	B	1208	-	3/3/16/25	7/18/116/135	-
15	CLA	3	606	-	3/3/16/25	5/11/111/135	-
15	CLA	A	1131	-	3/3/17/25	10/19/117/135	-
15	CLA	A	1125	-	3/3/16/25	10/18/116/135	-
15	CLA	A	1105	-	3/3/16/25	9/18/116/135	-
16	CHL	1	609	1	4/4/16/26	6/20/118/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	B	4005	-	-	16/29/63/63	0/2/2/2
12	LUT	3	501	-	-	4/29/67/67	0/2/2/2
15	CLA	B	1237	-	3/3/16/25	11/18/116/135	-
15	CLA	3	611	-	3/3/16/25	9/15/113/135	-
13	XAT	1	502	-	-	3/31/93/93	0/4/4/4
15	CLA	1	607	17	3/3/16/25	9/15/113/135	-
14	BCR	A	4002	-	-	13/29/63/63	0/2/2/2
16	CHL	2	613	-	3/3/16/26	2/13/113/137	-
15	CLA	2	606	-	3/3/16/25	6/15/113/135	-
15	CLA	A	1102	15	3/3/16/25	5/11/111/135	-
24	CL0	A	1011	-	3/3/17/25	13/19/117/135	-
15	CLA	A	1103	-	3/3/18/25	16/25/123/135	-
15	CLA	1	605	-	3/3/16/25	10/17/115/135	-
15	CLA	B	1212	-	3/3/16/25	6/11/111/135	-
16	CHL	4	611	-	3/3/16/26	5/20/118/137	-

The worst 5 of 1175 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4005	BCR	C11-C12	19.10	1.83	1.34
14	A	4005	BCR	C11-C10	15.97	1.92	1.43
12	1	501	LUT	C24-C25	14.94	1.51	1.33
12	3	501	LUT	C24-C25	14.66	1.51	1.33
12	4	501	LUT	C24-C25	14.54	1.51	1.33

The worst 5 of 1854 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4001	BCR	C10-C11-C12	17.73	178.54	123.22
14	2	503	BCR	C10-C11-C12	17.71	178.50	123.22
14	3	504	BCR	C10-C11-C12	17.63	178.23	123.22
14	4	503	BCR	C10-C11-C12	17.61	178.18	123.22
14	A	4004	BCR	C10-C11-C12	17.60	178.13	123.22

5 of 438 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	4	604	CLA	NC

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Mol	Chain	Res	Type	Atom
15	4	604	CLA	ND
15	4	604	CLA	NA
15	A	1124	CLA	NC
15	A	1124	CLA	ND

5 of 1867 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	4	604	CLA	C1A-C2A-CAA-CBA
15	4	604	CLA	C3A-C2A-CAA-CBA
15	4	604	CLA	C2-C1-O2A-CGA
15	4	604	CLA	CHA-CBD-CGD-O1D
15	4	604	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

190 monomers are involved in 1272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	604	CLA	13	0
15	A	1124	CLA	14	0
15	A	1133	CLA	4	0
14	B	4001	BCR	2	0
15	2	608	CLA	5	0
13	3	502	XAT	23	0
15	2	601	CLA	15	0
15	B	1218	CLA	9	0
15	A	1119	CLA	5	0
14	B	4004	BCR	5	0
15	A	1127	CLA	8	0
15	A	1134	CLA	6	0
15	A	1130	CLA	4	0
12	4	501	LUT	18	0
14	4	503	BCR	8	0
15	B	1205	CLA	7	0
15	A	1117	CLA	7	0
15	A	1013	CLA	27	0
15	B	1213	CLA	4	0
15	4	603	CLA	6	0
15	3	612	CLA	9	0
19	1	811	SQD	4	0
15	1	601	CLA	12	0
15	B	1227	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1108	CLA	9	0
15	B	1214	CLA	11	0
21	4	811	DGD	7	0
15	B	1229	CLA	7	0
15	3	607	CLA	1	0
25	B	2002	PQN	6	0
15	B	1202	CLA	6	0
21	B	5002	DGD	4	0
15	B	1209	CLA	2	0
16	4	610	CHL	5	0
15	4	607	CLA	5	0
15	B	1204	CLA	7	0
15	A	1136	CLA	9	0
15	B	1211	CLA	9	0
15	A	1106	CLA	14	0
15	A	1113	CLA	6	0
14	J	4003	BCR	4	0
15	4	608	CLA	4	0
15	F	1301	CLA	6	0
23	4	831	GSH	0	1
15	2	602	CLA	7	0
16	4	613	CHL	7	0
15	2	607	CLA	8	0
15	B	1230	CLA	15	0
14	1	503	BCR	8	0
15	3	613	CLA	15	0
15	1	604	CLA	15	0
14	J	4002	BCR	15	0
15	2	604	CLA	6	0
14	B	4006	BCR	10	0
15	A	1138	CLA	13	0
20	4	902	CAC	1	0
15	A	1128	CLA	12	0
15	J	1302	CLA	8	0
15	B	1231	CLA	11	0
14	4	505	BCR	4	0
13	4	502	XAT	5	0
15	A	1118	CLA	2	0
15	4	615	CLA	7	0
15	A	1129	CLA	2	0
18	2	802	LMG	1	0
15	B	1215	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4	605	CLA	10	0
15	B	1224	CLA	5	0
15	A	1104	CLA	5	0
15	2	612	CLA	11	0
15	A	1115	CLA	6	0
15	3	605	CLA	12	0
15	A	1114	CLA	6	0
15	B	1022	CLA	10	0
15	3	615	CLA	2	0
15	4	601	CLA	13	0
15	B	1203	CLA	5	0
14	1	505	BCR	7	0
15	1	613	CLA	25	0
12	1	501	LUT	11	0
15	B	1220	CLA	5	0
15	3	610	CLA	5	0
15	B	1236	CLA	4	0
15	A	1111	CLA	23	0
17	B	5001	LHG	2	0
15	4	606	CLA	10	0
15	B	1206	CLA	5	0
15	1	602	CLA	2	0
15	B	1226	CLA	10	0
15	B	1239	CLA	11	0
15	B	1216	CLA	7	0
17	1	801	LHG	2	0
15	A	1012	CLA	30	0
15	A	1110	CLA	16	0
14	2	503	BCR	8	0
15	A	1109	CLA	13	0
15	A	1132	CLA	5	0
16	2	609	CHL	15	0
15	B	1240	CLA	5	0
15	B	1217	CLA	2	0
21	2	811	DGD	2	0
15	A	1122	CLA	5	0
15	B	1221	CLA	8	0
15	1	606	CLA	15	0
15	B	1021	CLA	25	0
14	B	4002	BCR	3	0
15	4	612	CLA	12	0
15	1	611	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	902	CAC	1	0
15	B	1235	CLA	12	0
15	3	601	CLA	15	0
13	2	502	XAT	15	0
15	B	1223	CLA	6	0
15	A	1107	CLA	11	0
15	A	1120	CLA	1	0
15	A	1141	CLA	4	0
15	B	1228	CLA	9	0
18	1	802	LMG	1	0
15	4	602	CLA	8	0
16	1	610	CHL	16	0
15	2	605	CLA	7	0
15	B	1222	CLA	9	0
15	1	612	CLA	7	0
15	2	615	CLA	1	0
14	F	4002	BCR	6	0
15	A	1140	CLA	6	0
14	A	4005	BCR	14	0
15	A	1123	CLA	11	0
17	2	801	LHG	2	0
15	B	1023	CLA	19	0
15	B	1210	CLA	9	0
15	1	615	CLA	5	0
14	A	4004	BCR	4	0
15	4	609	CLA	11	0
15	A	1116	CLA	7	0
14	B	4003	BCR	8	0
14	J	4001	BCR	7	0
14	A	4006	BCR	8	0
14	3	504	BCR	5	0
15	B	1234	CLA	7	0
14	3	503	BCR	21	0
25	A	2001	PQN	12	0
16	2	611	CHL	5	0
17	A	5001	LHG	2	0
15	B	1219	CLA	8	0
14	A	4007	BCR	8	0
15	A	1126	CLA	9	0
15	2	603	CLA	3	0
15	A	1112	CLA	1	0
15	A	1139	CLA	11	0

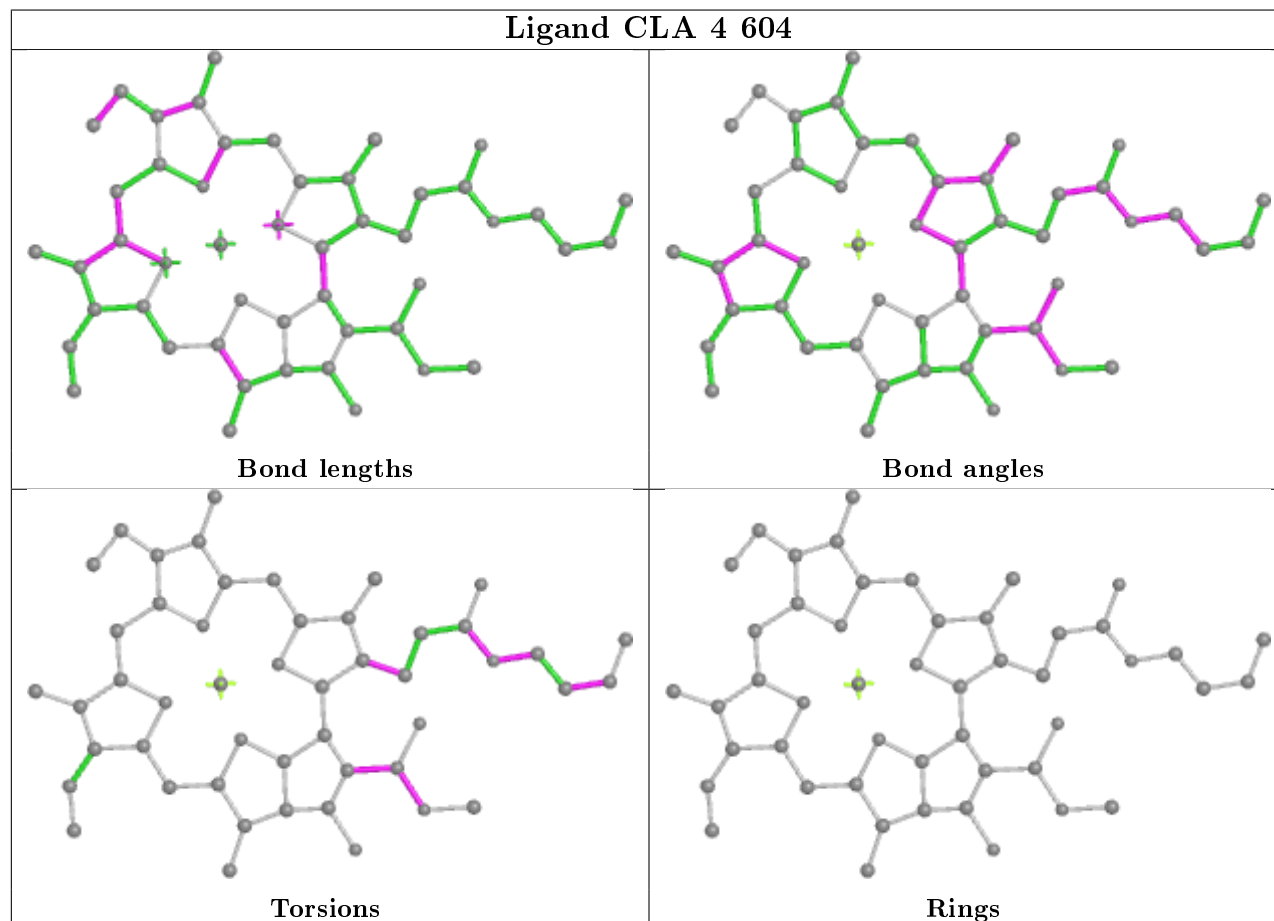
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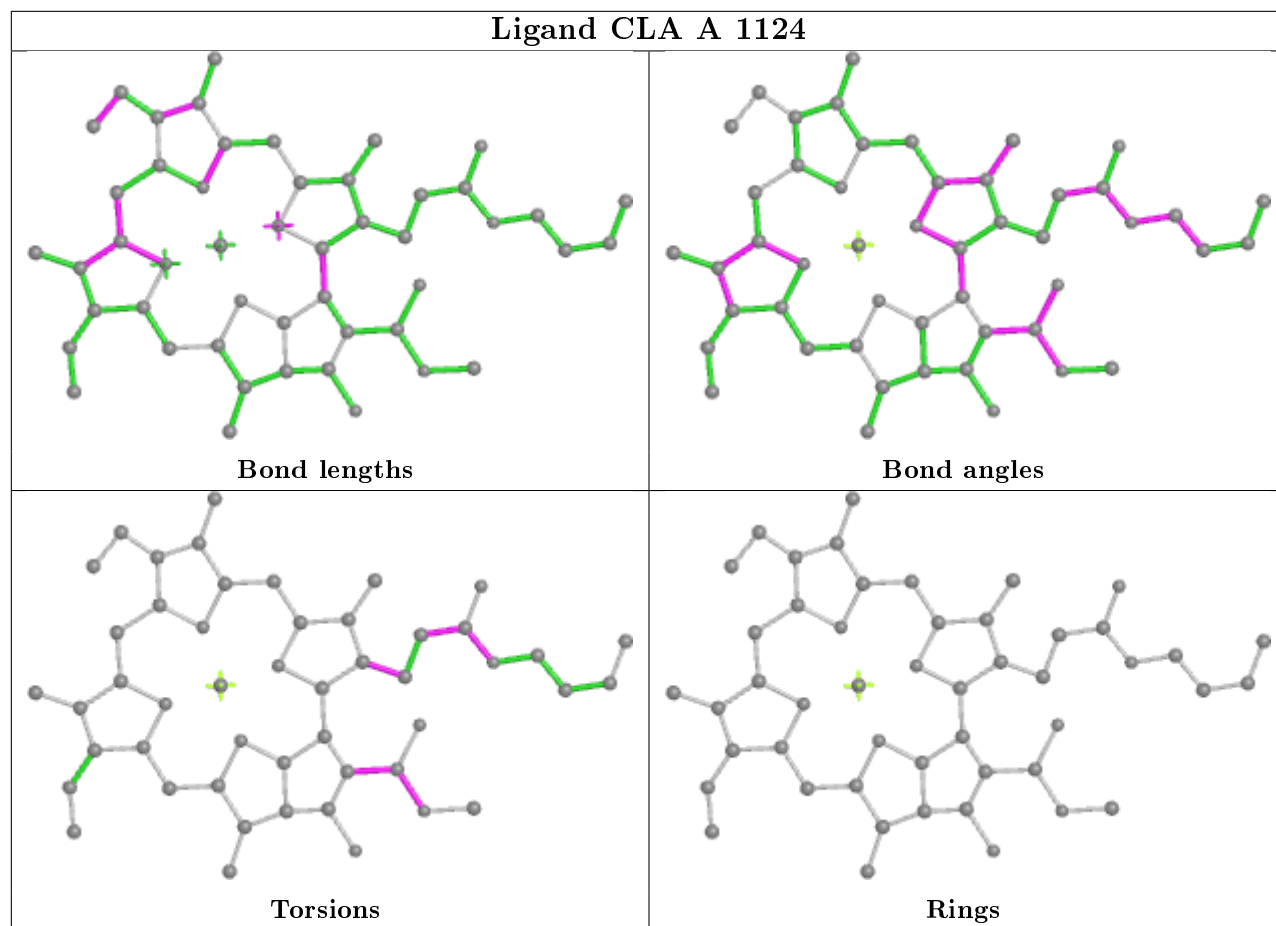
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	3003	SF4	2	0
15	B	1201	CLA	4	0
15	1	603	CLA	13	0
15	B	1225	CLA	6	0
15	F	1302	CLA	6	0
15	A	1121	CLA	4	0
15	A	1135	CLA	5	0
15	A	1101	CLA	7	0
14	A	4003	BCR	2	0
15	1	608	CLA	14	0
16	2	610	CHL	5	0
15	3	608	CLA	5	0
16	3	604	CHL	14	0
15	A	1137	CLA	7	0
15	B	1238	CLA	1	0
17	A	5002	LHG	4	0
15	B	1232	CLA	8	0
15	3	603	CLA	22	0
12	2	501	LUT	12	0
23	B	5031	GSH	2	0
15	3	606	CLA	18	0
15	A	1131	CLA	3	0
15	A	1125	CLA	11	0
15	A	1105	CLA	7	0
16	1	609	CHL	11	0
14	B	4005	BCR	6	0
12	3	501	LUT	11	0
15	B	1237	CLA	3	0
15	3	611	CLA	8	0
13	1	502	XAT	12	0
15	1	607	CLA	5	0
15	B	1212	CLA	7	0
16	2	613	CHL	6	0
15	2	606	CLA	7	0
15	A	1102	CLA	6	0
24	A	1011	CL0	23	0
15	A	1103	CLA	10	0
15	1	605	CLA	12	0
14	A	4002	BCR	6	0
16	4	611	CHL	9	0

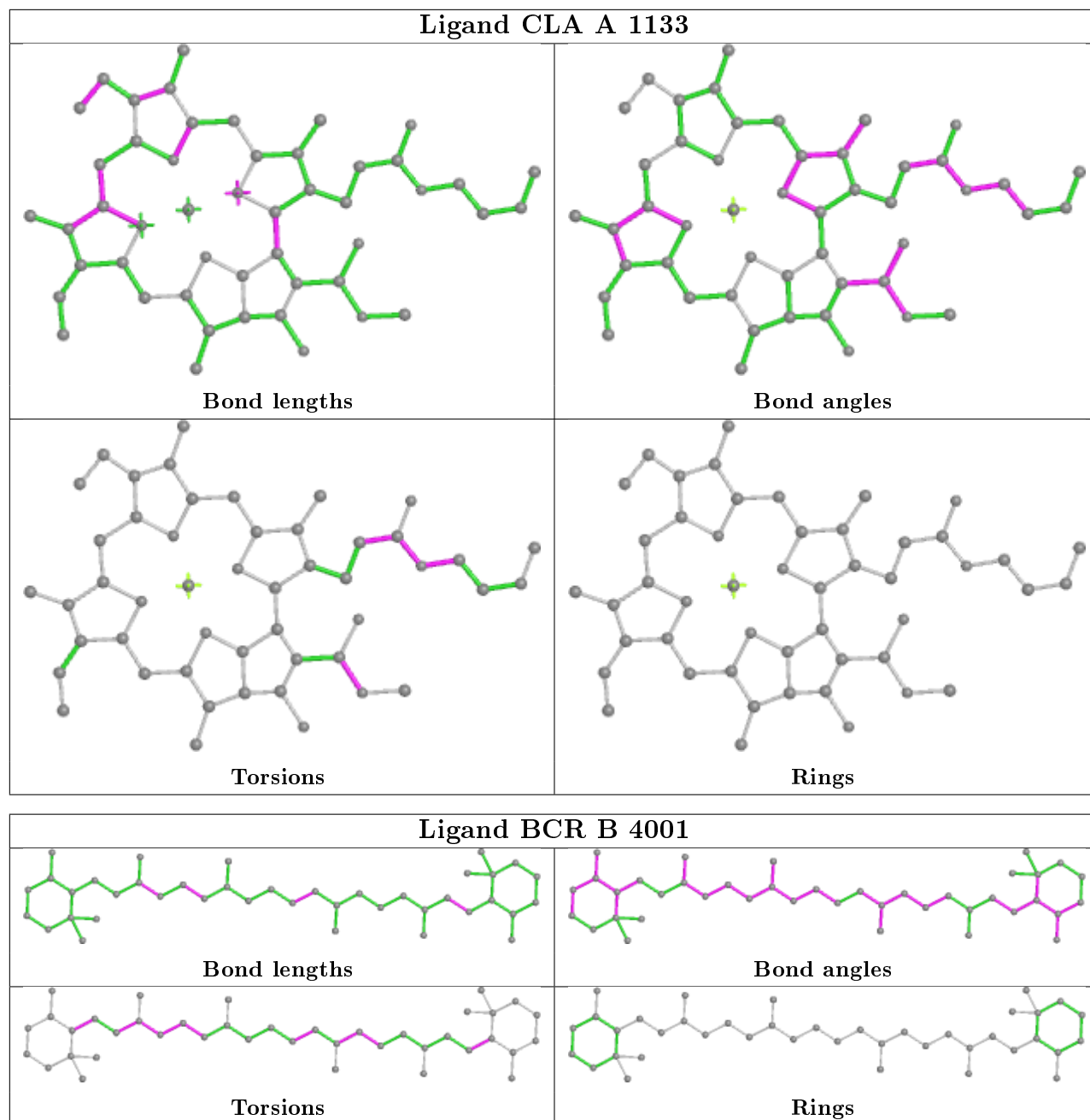
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

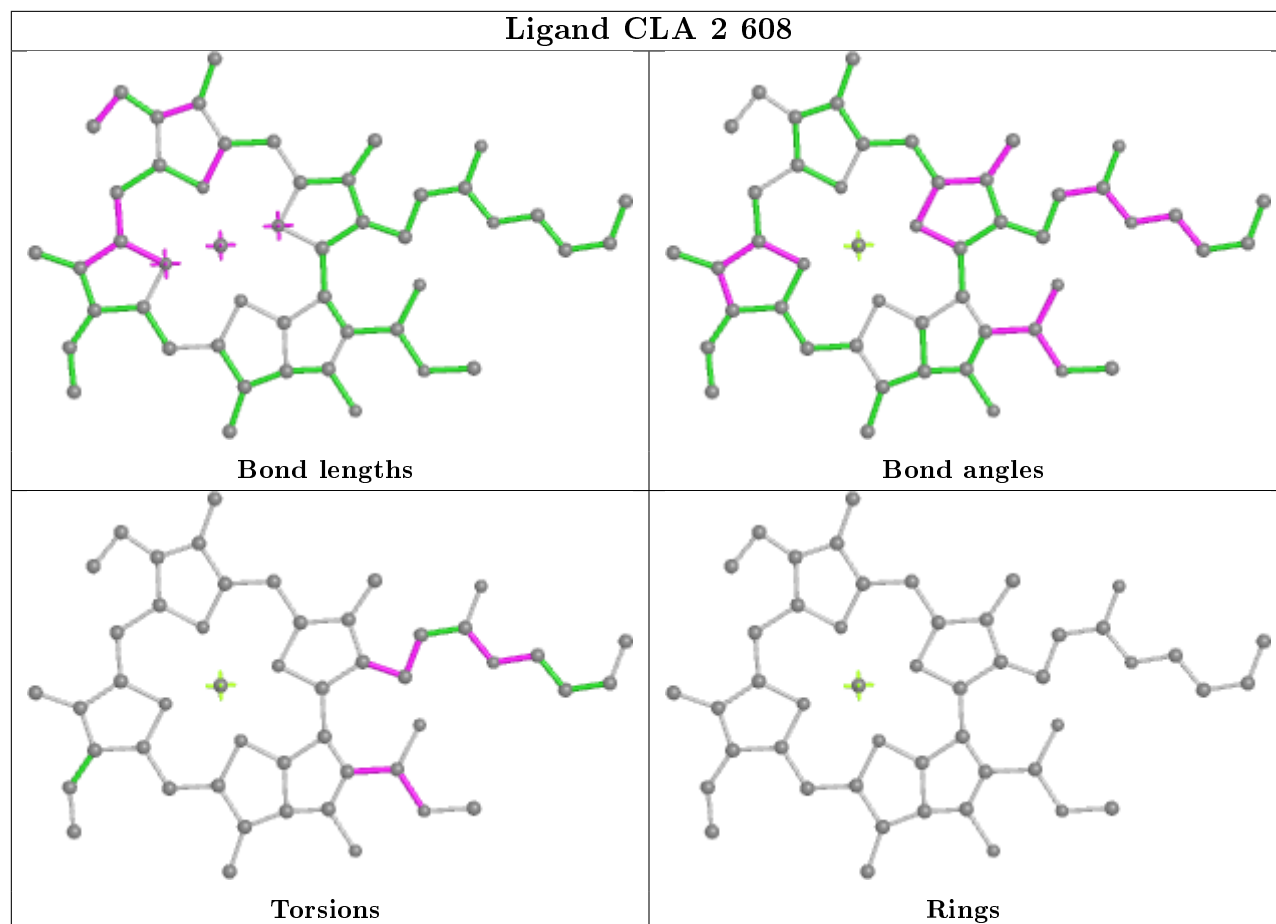




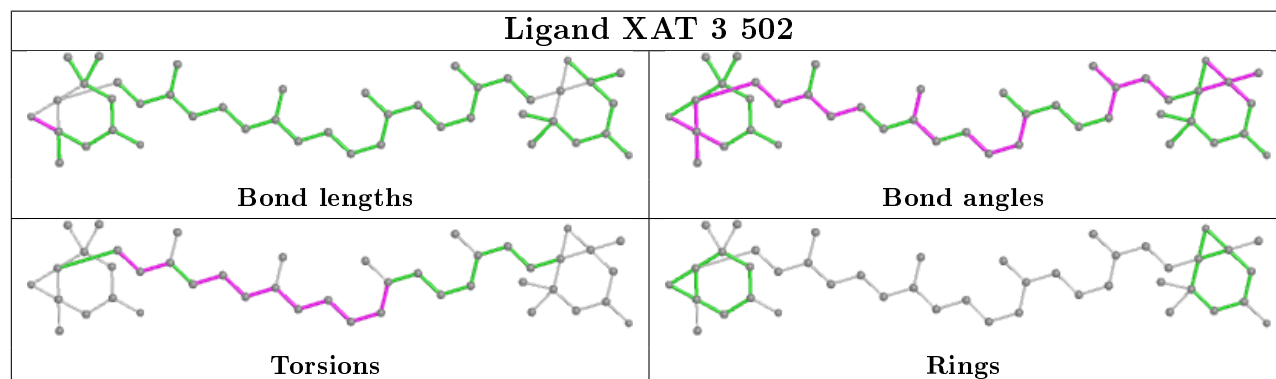


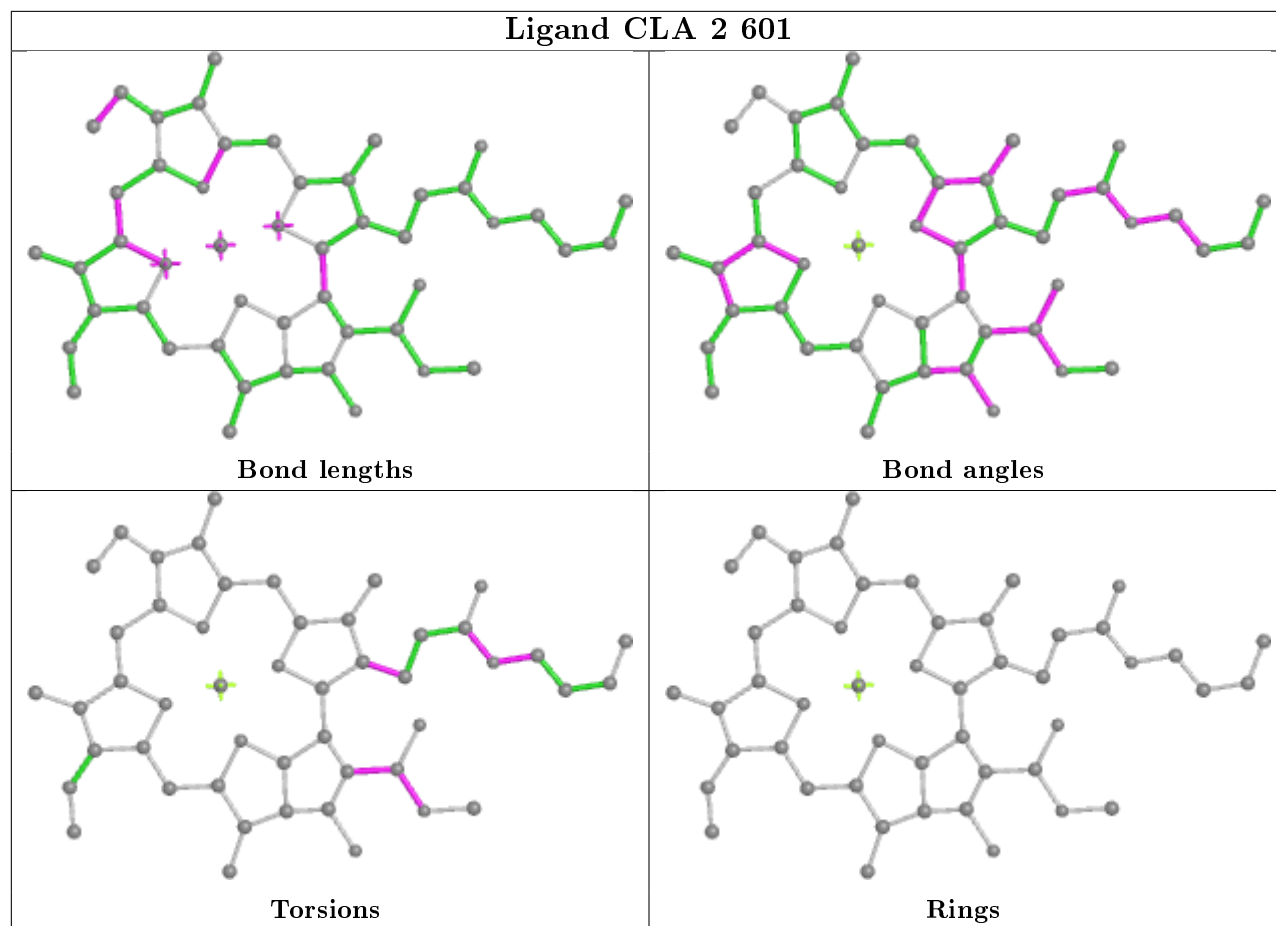


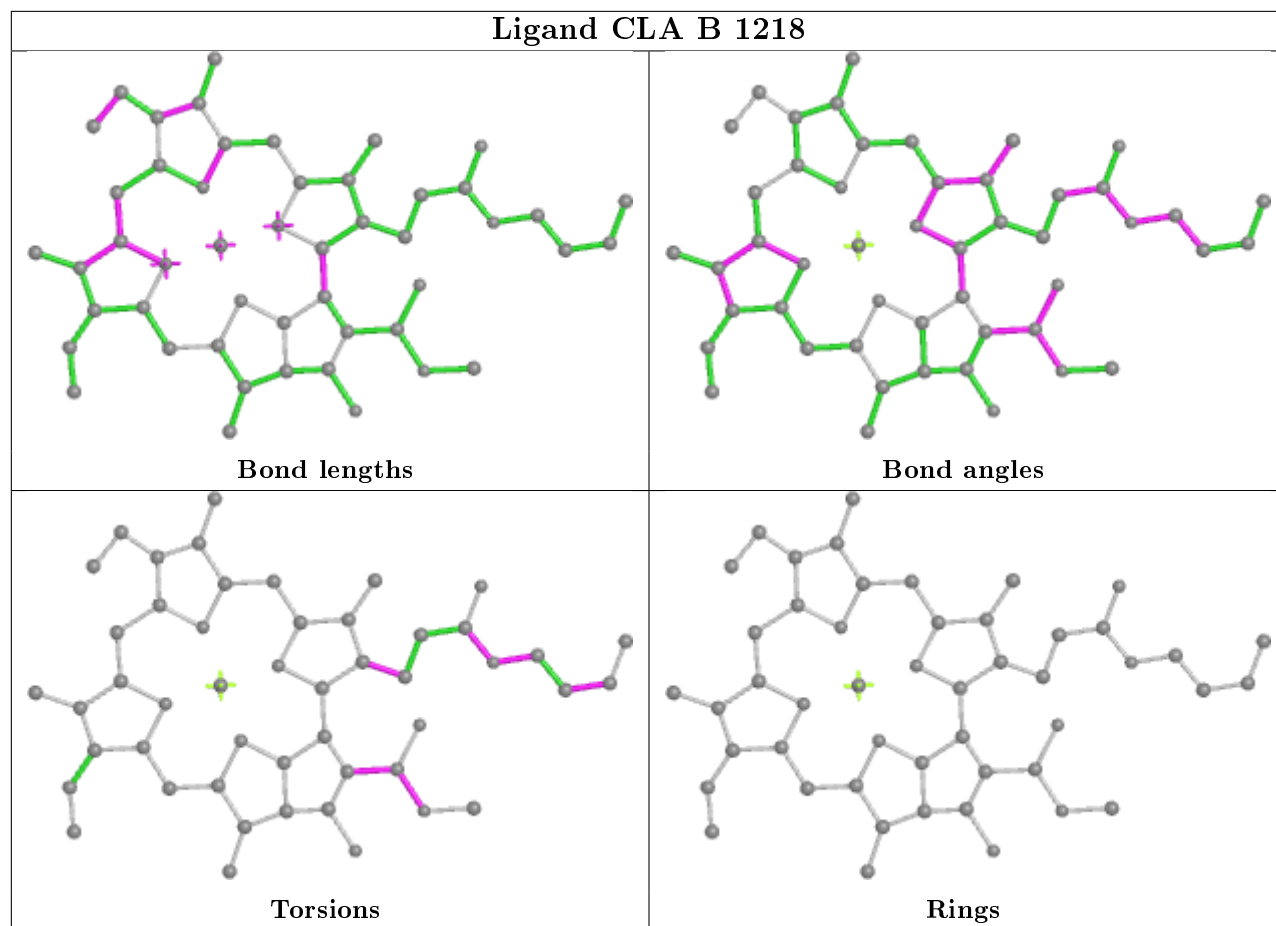
## Ligand CLA 2 608

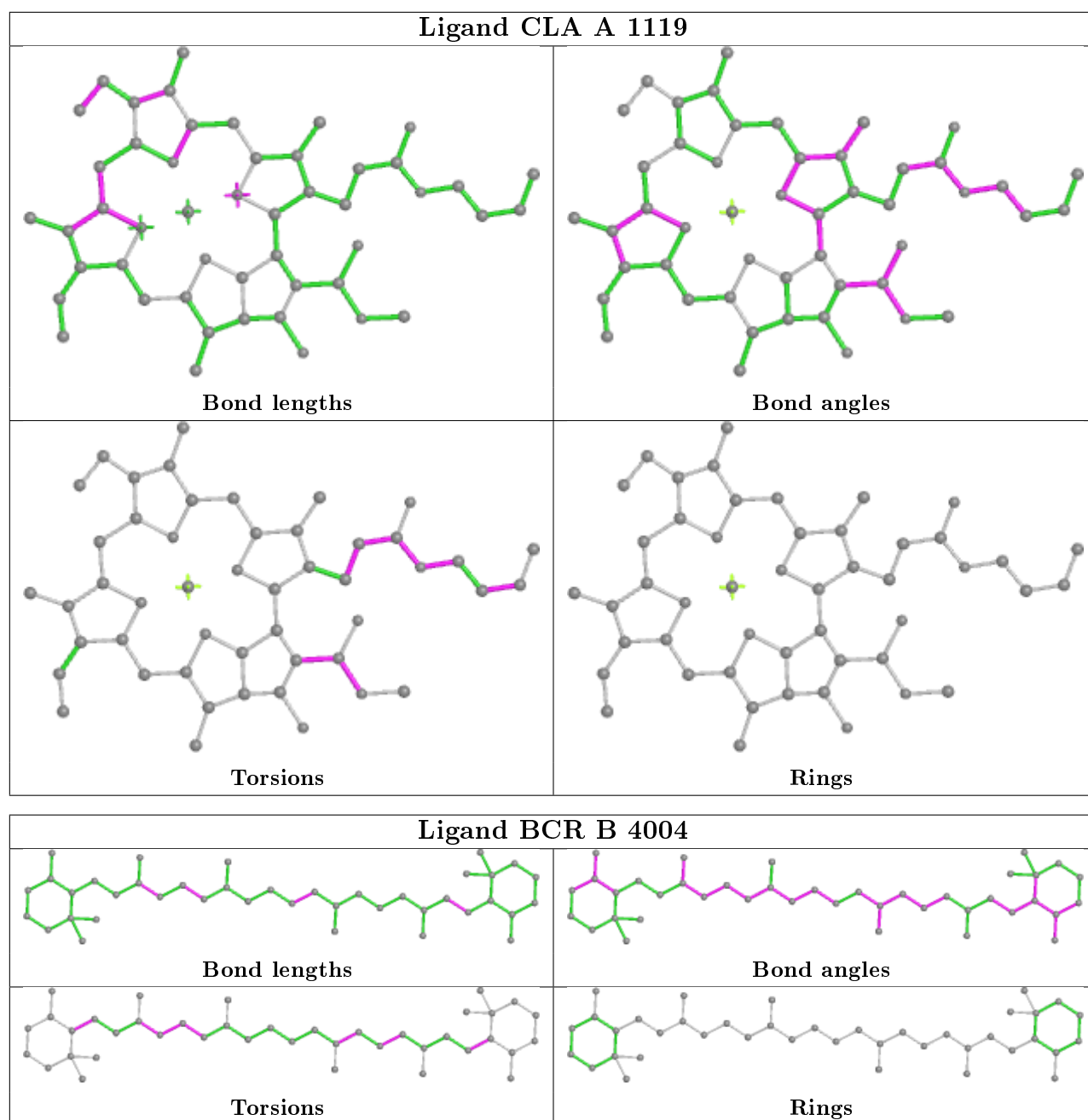


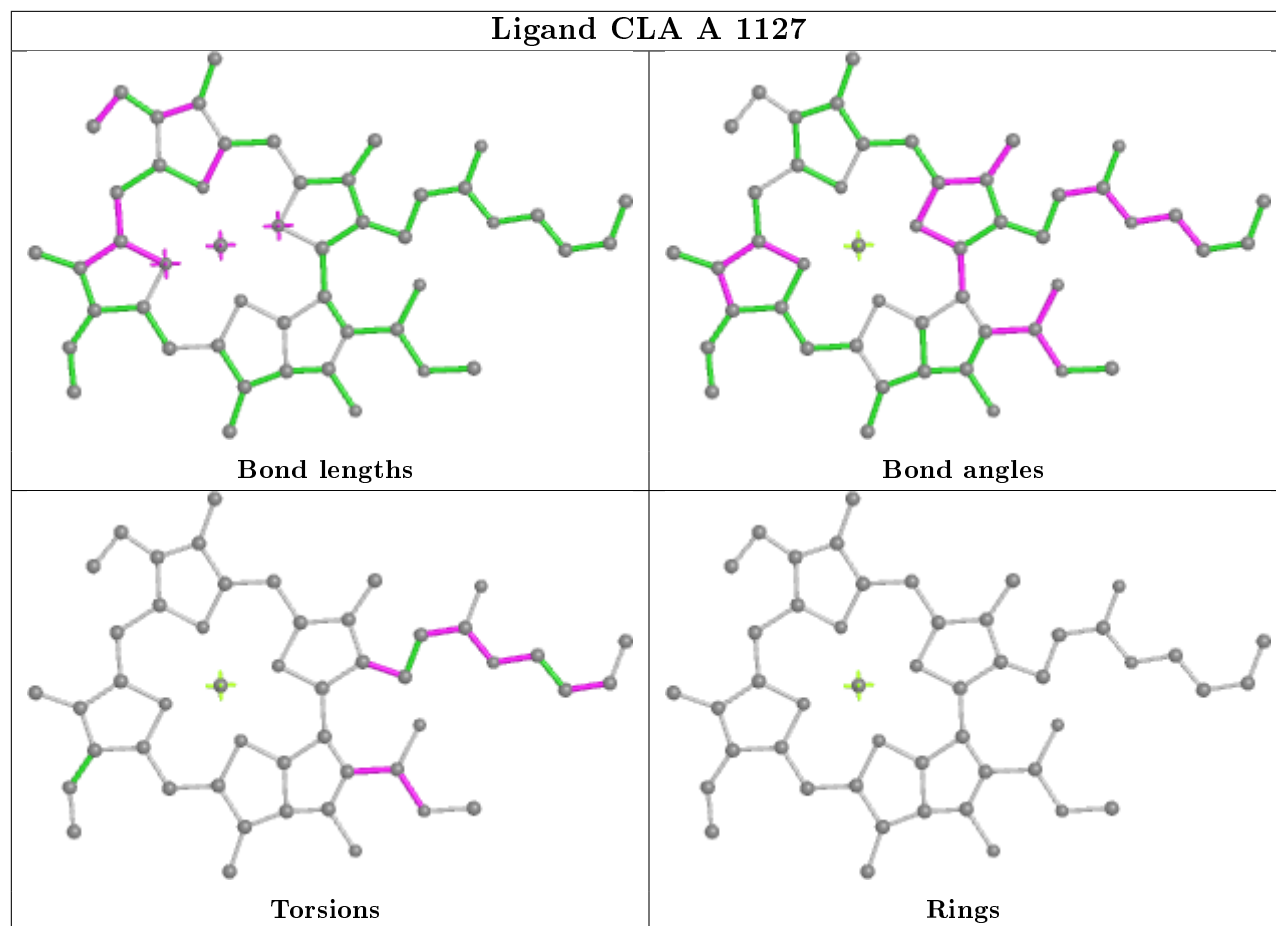
## Ligand XAT 3 502



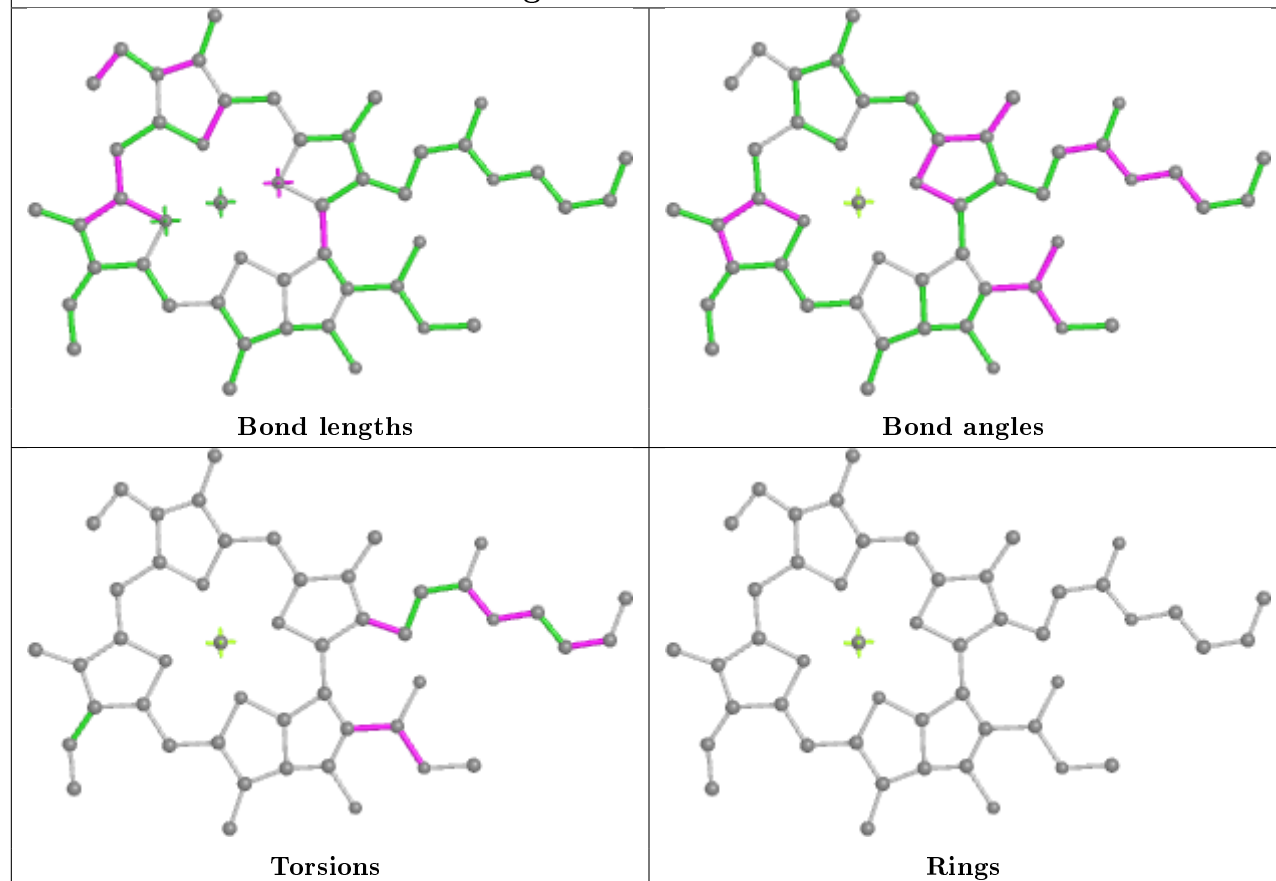




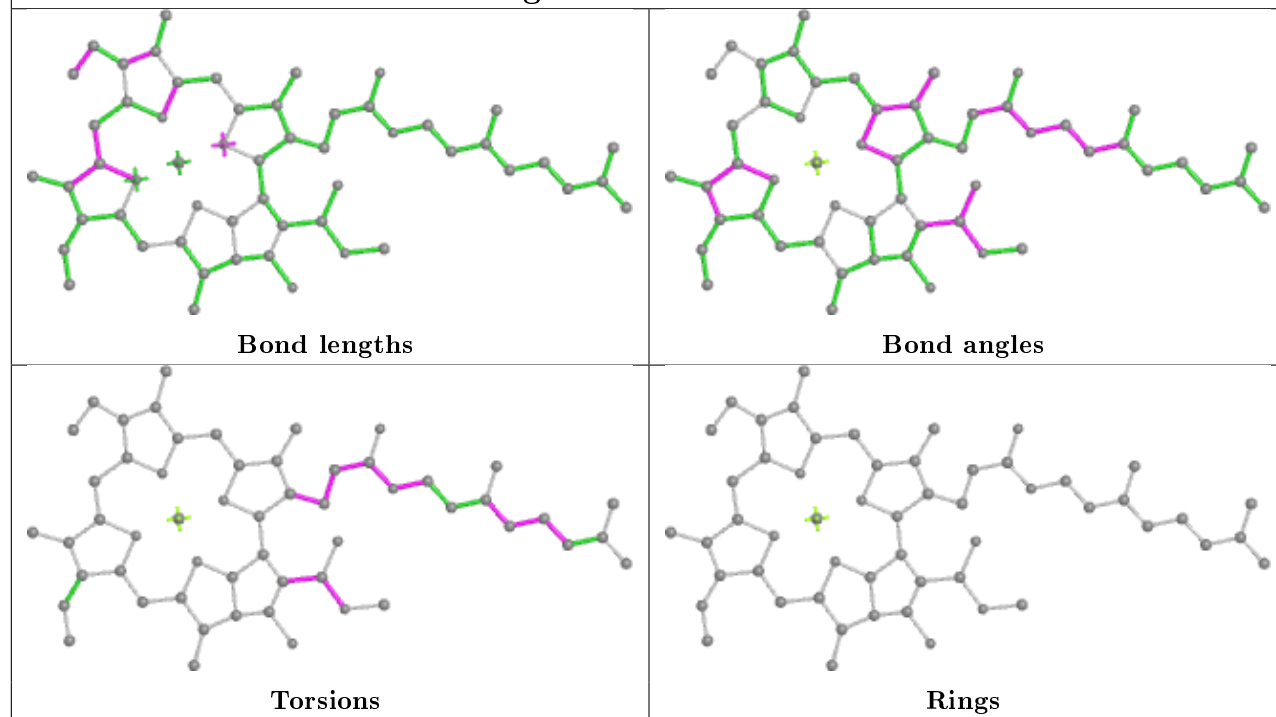


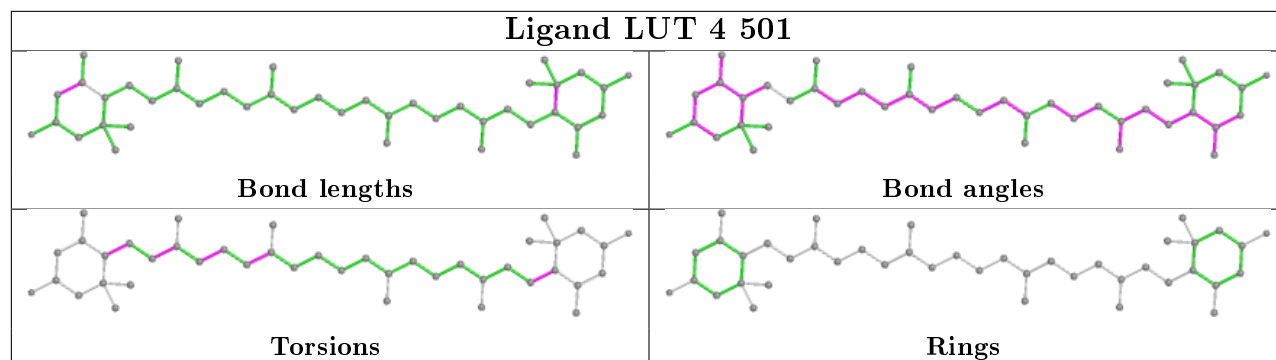
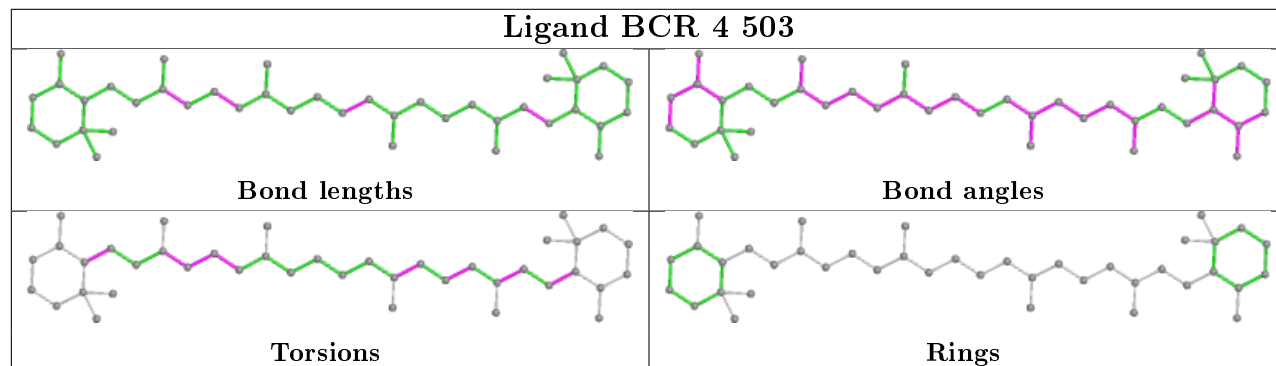
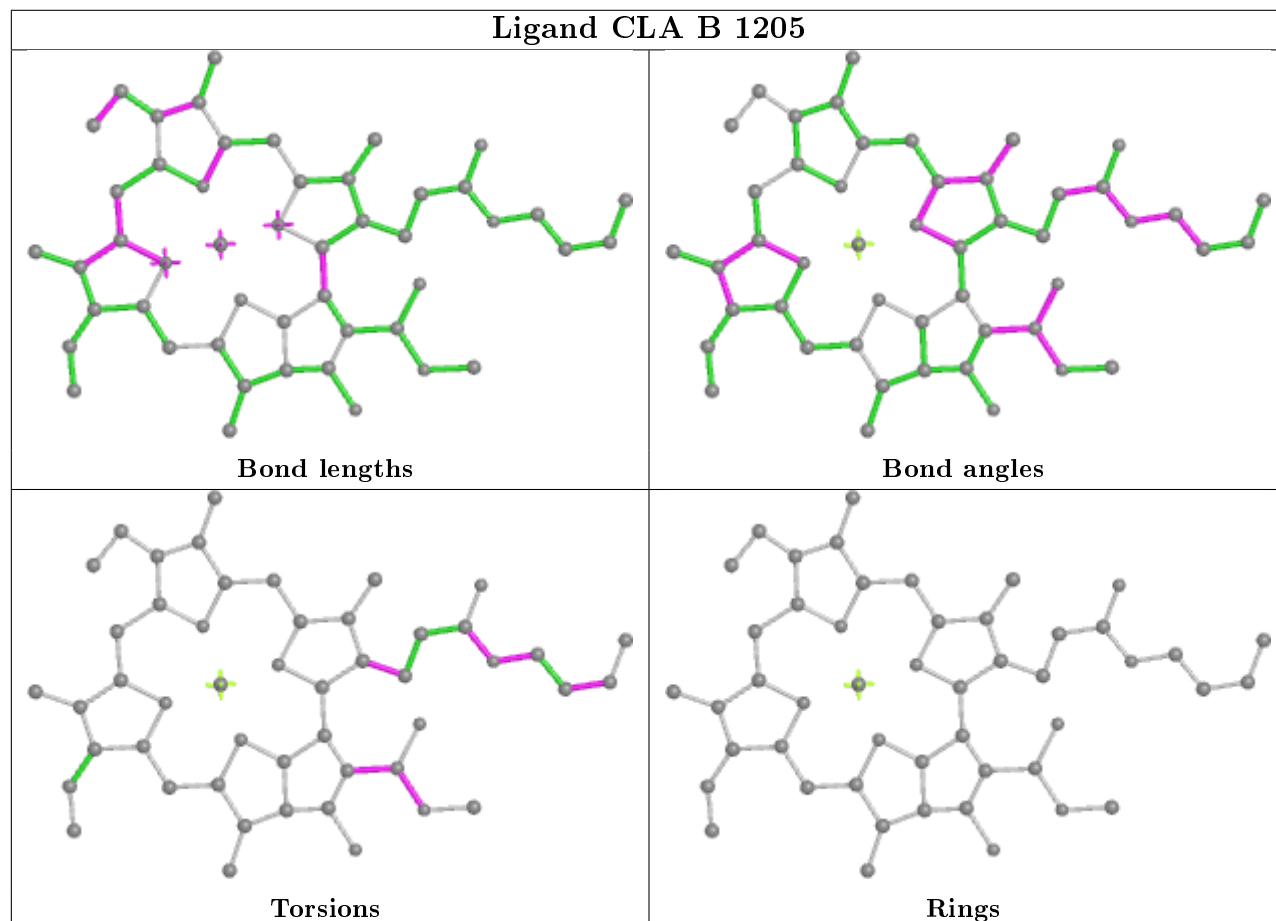


## Ligand CLA A 1134

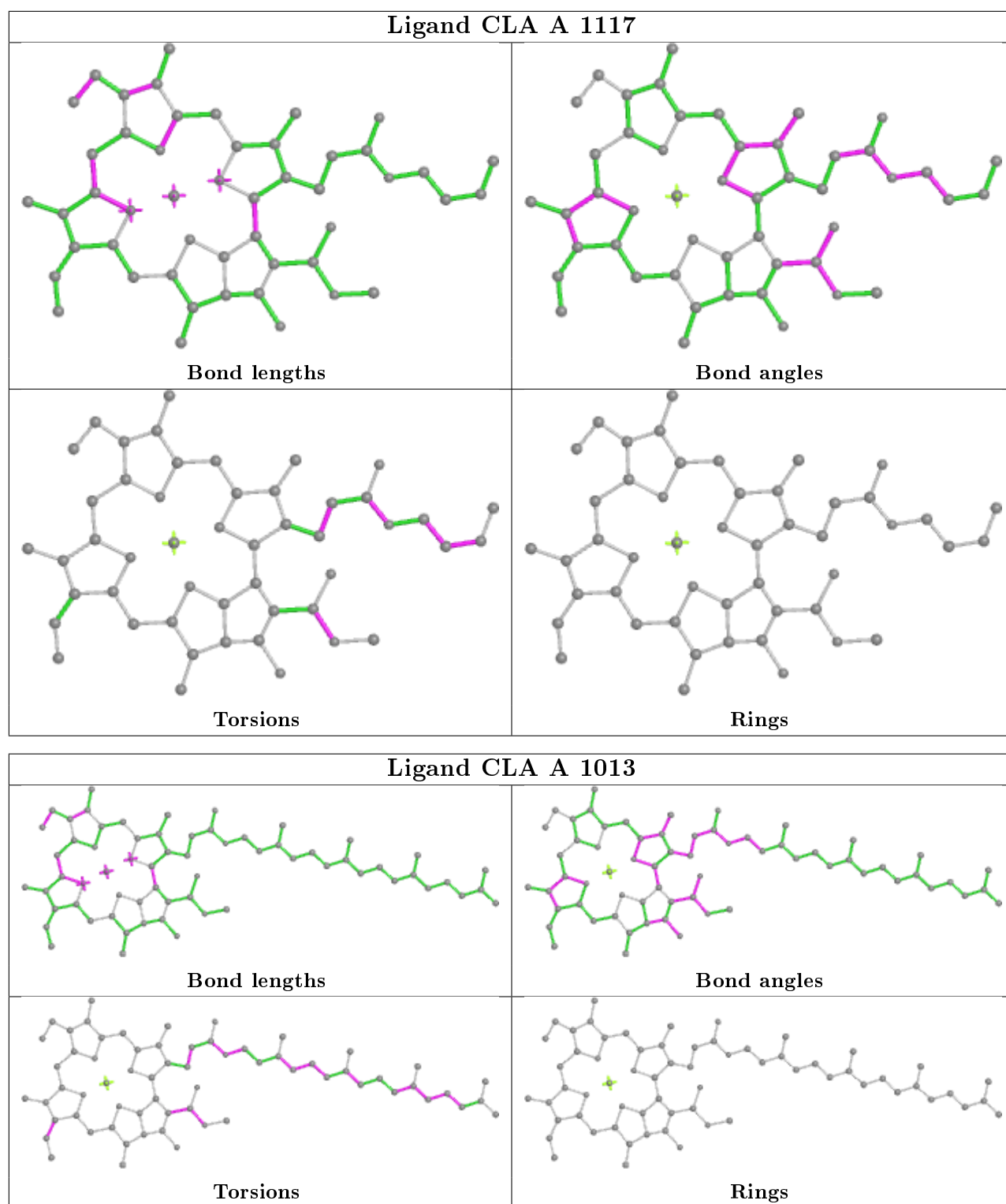


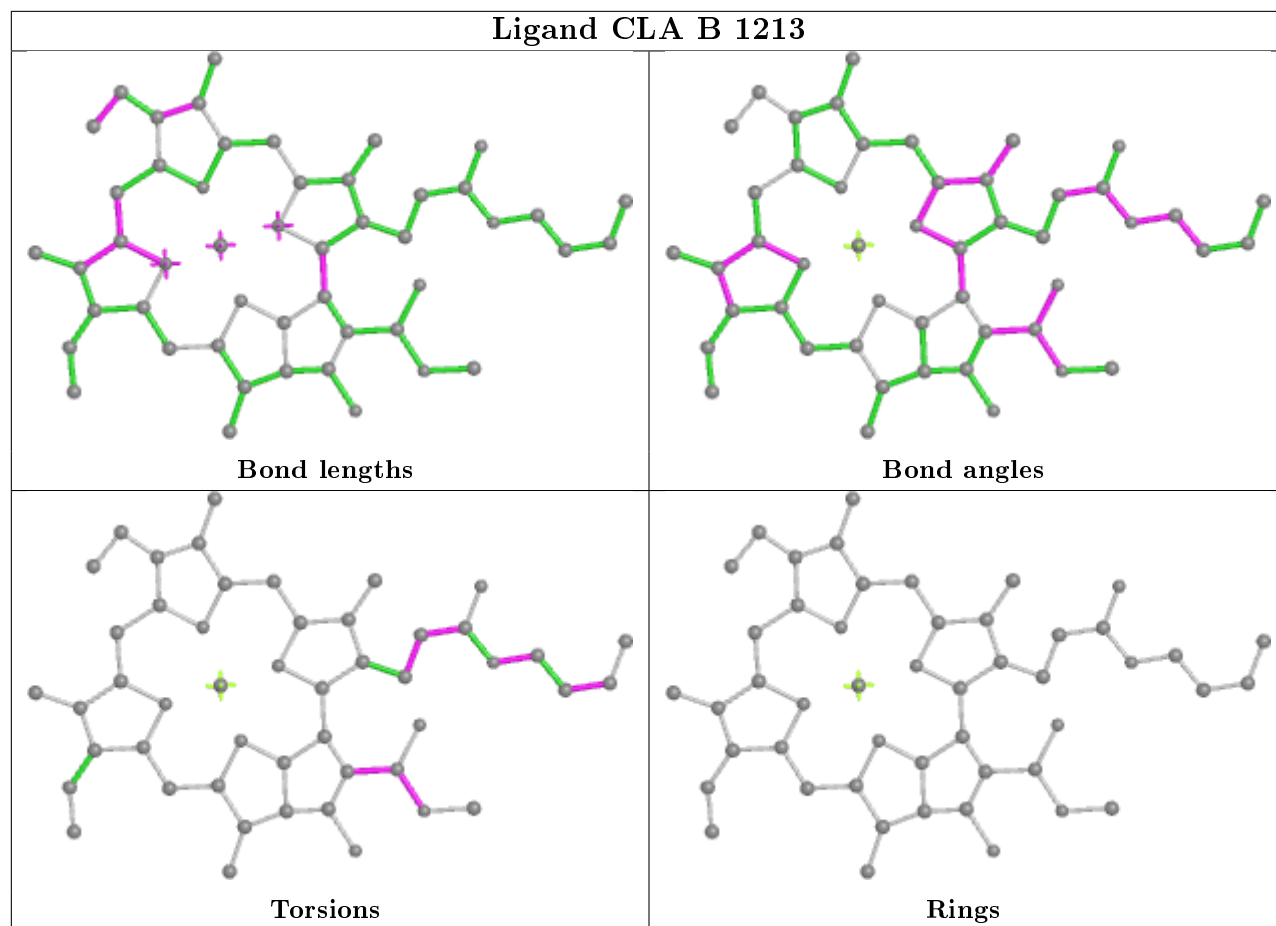
## Ligand CLA A 1130



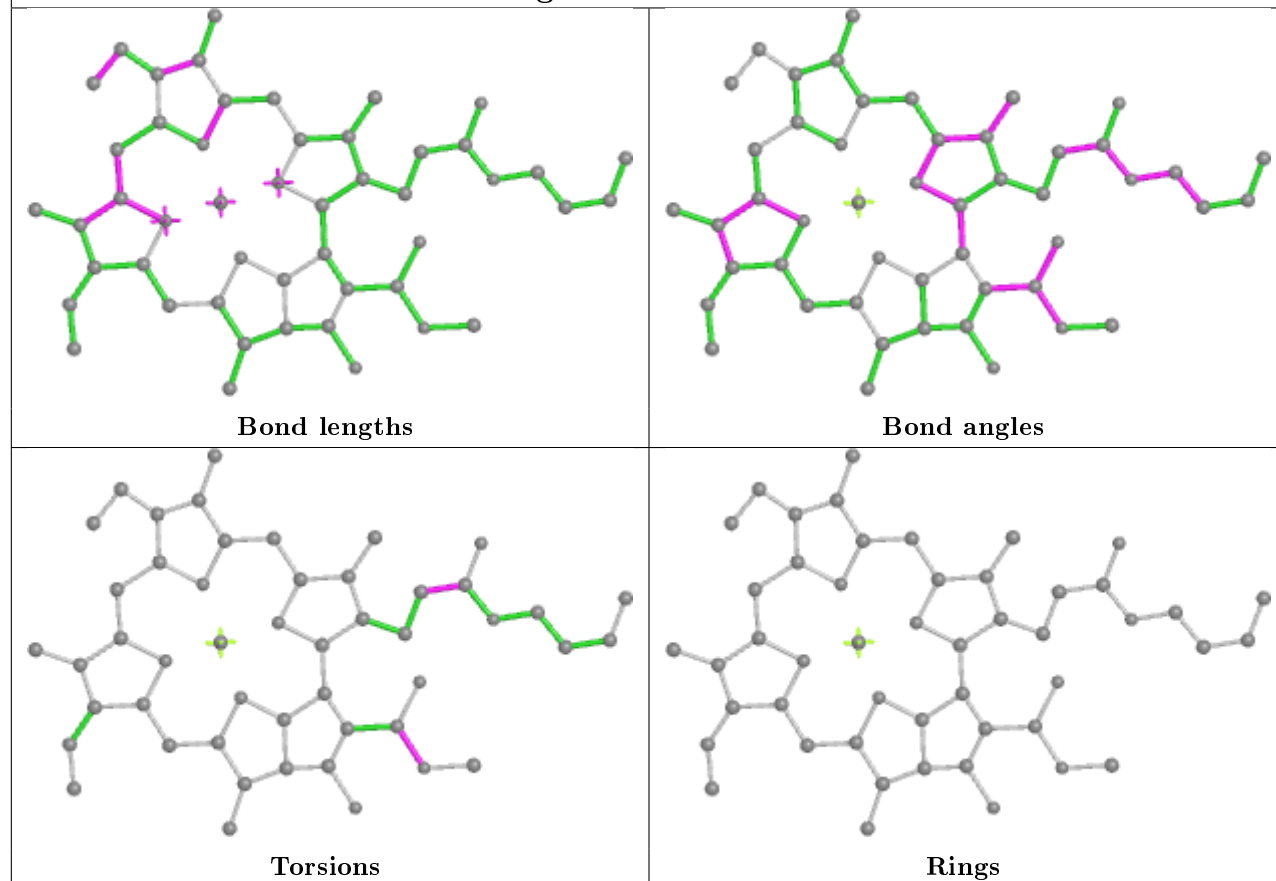
**Ligand LUT 4 501****Ligand BCR 4 503****Ligand CLA B 1205**



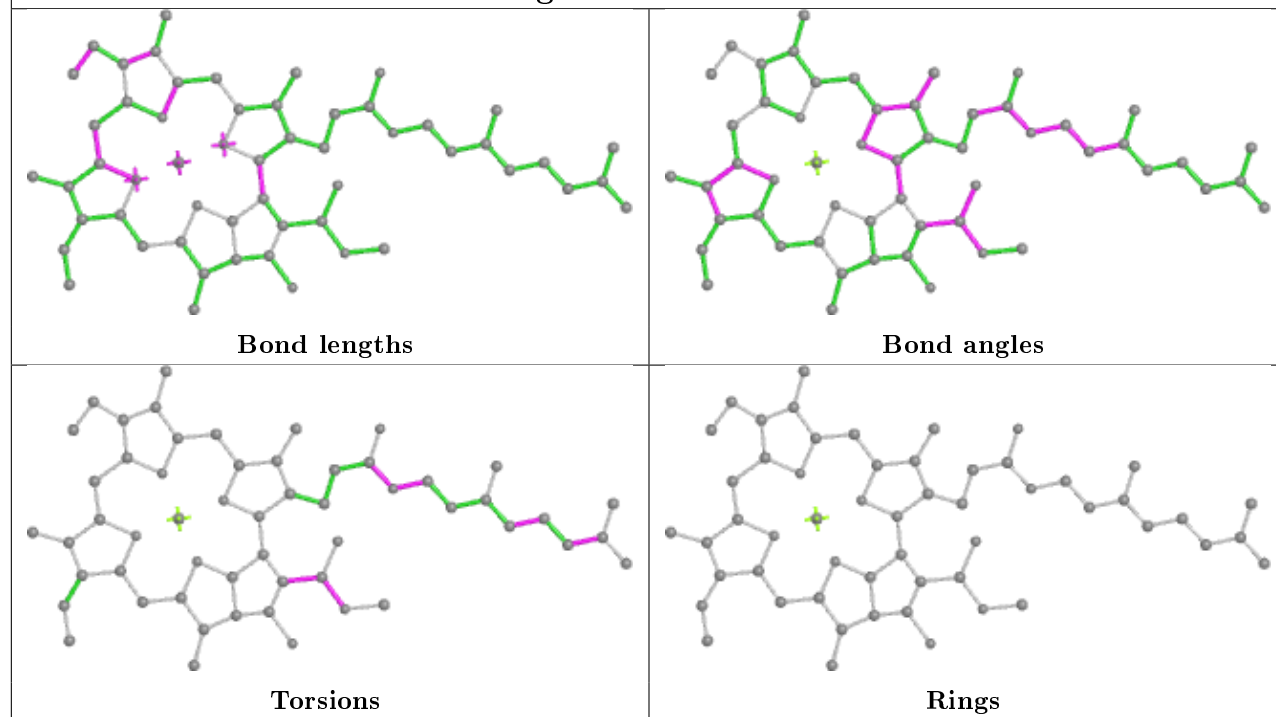




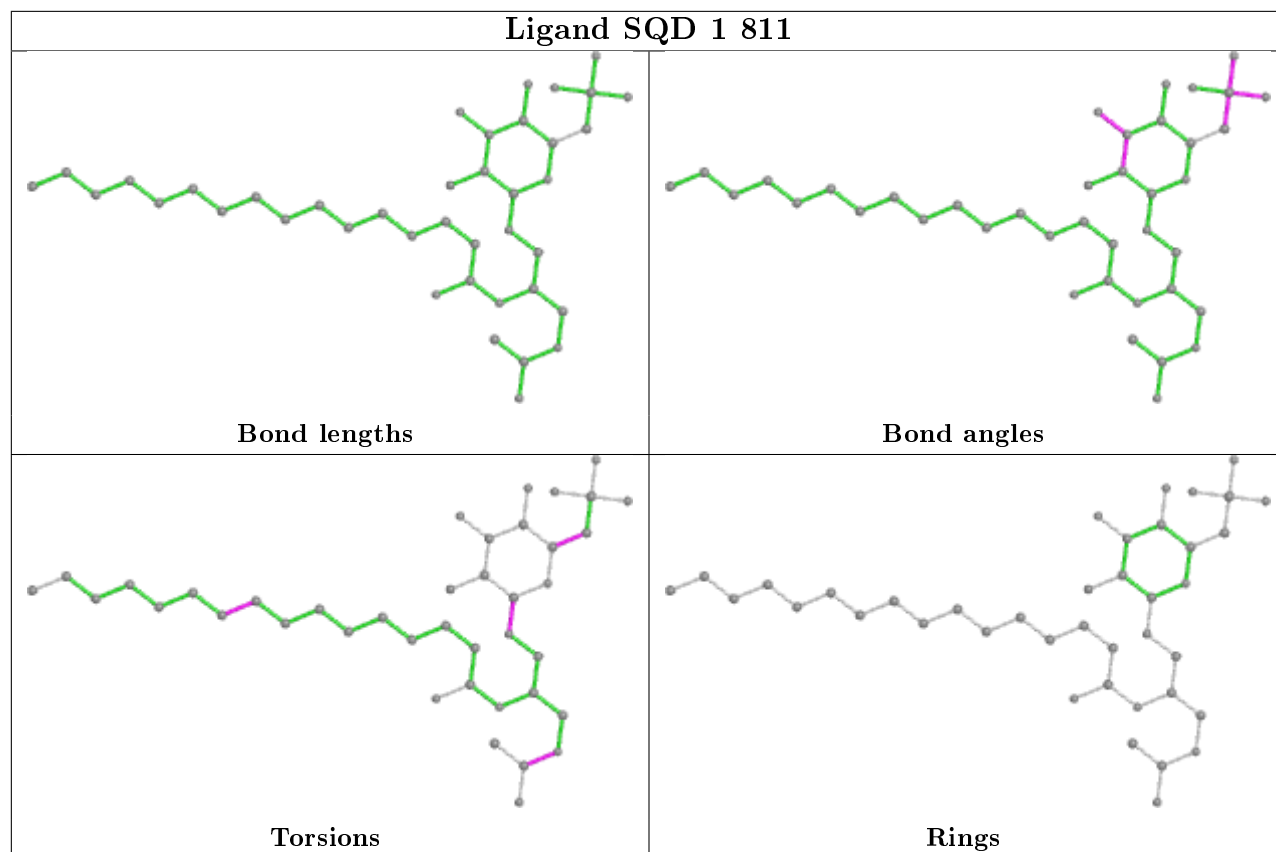
## Ligand CLA 4 603



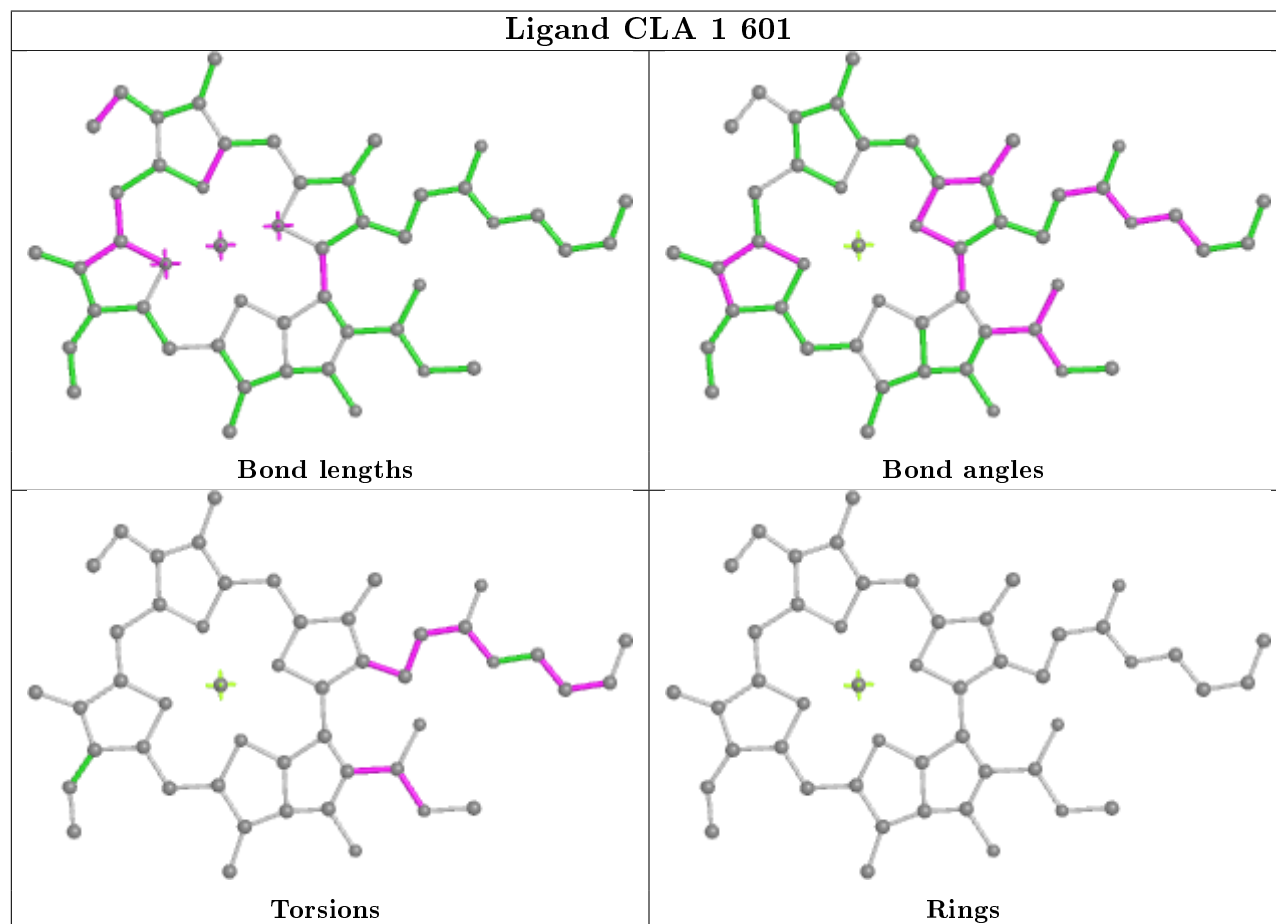
## Ligand CLA 3 612



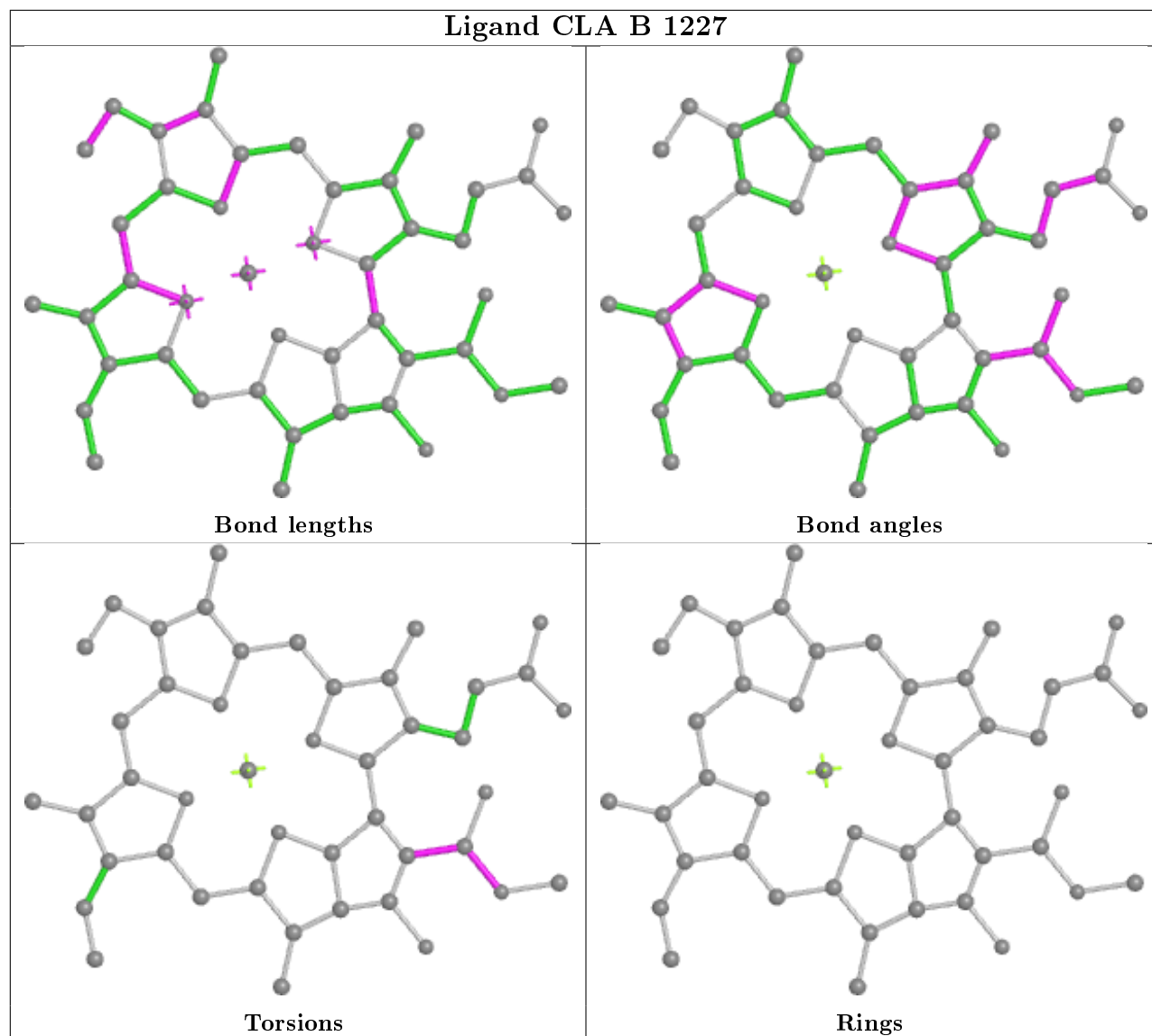
## Ligand SQD 1 811



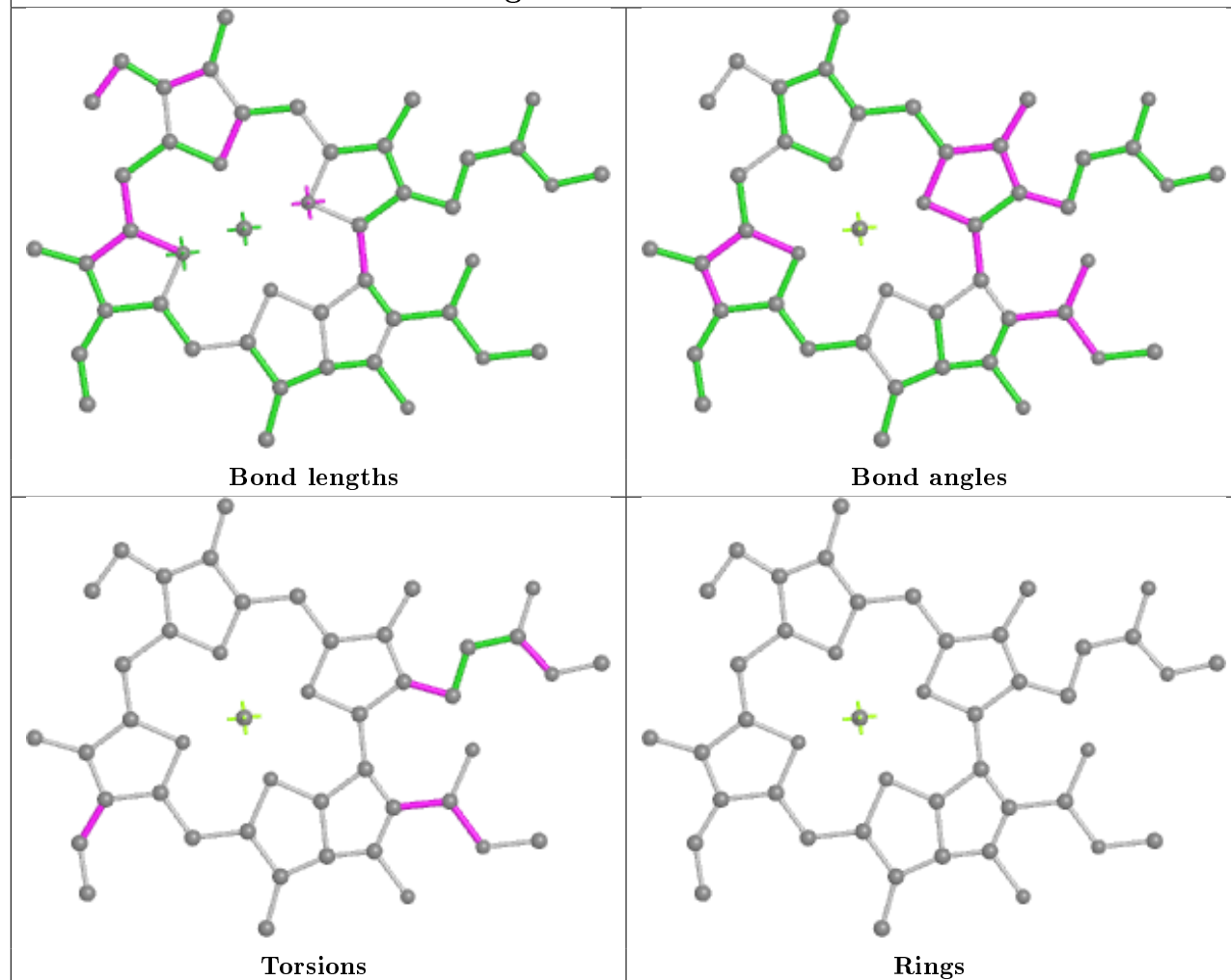
## Ligand CLA 1 601

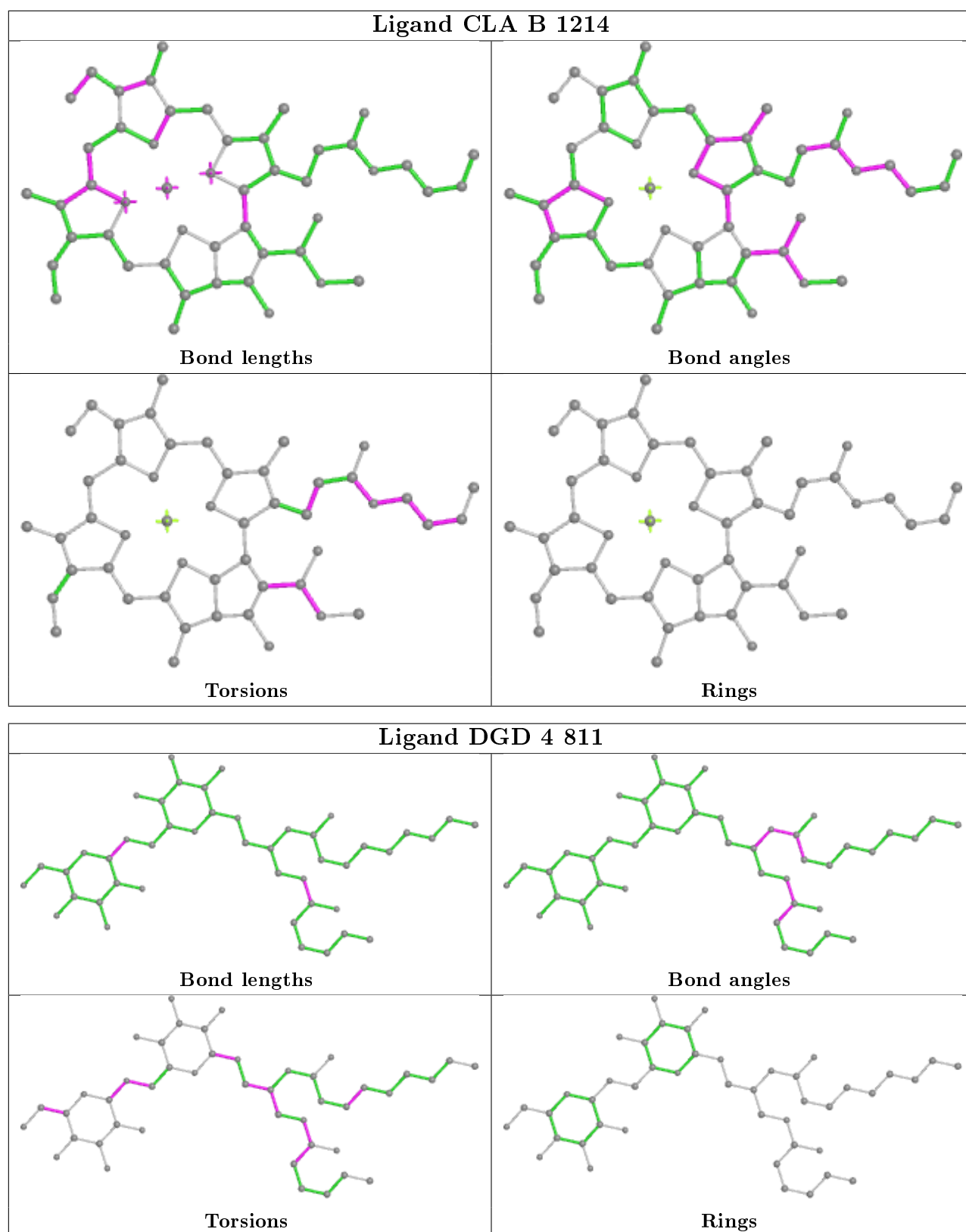


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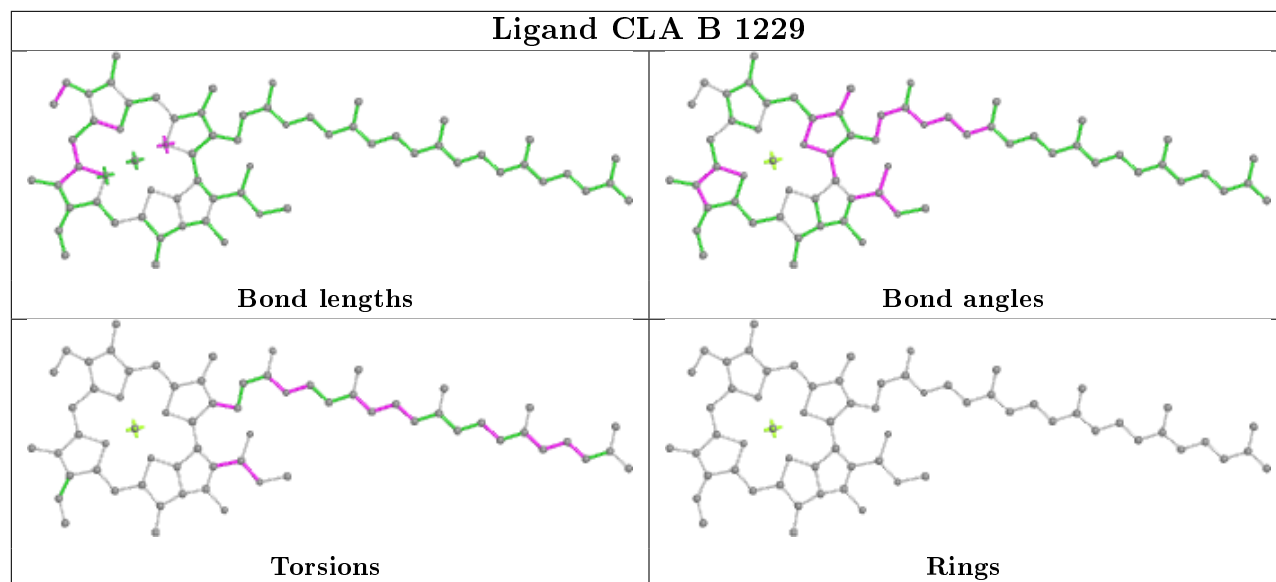


## Ligand CLA A 1108

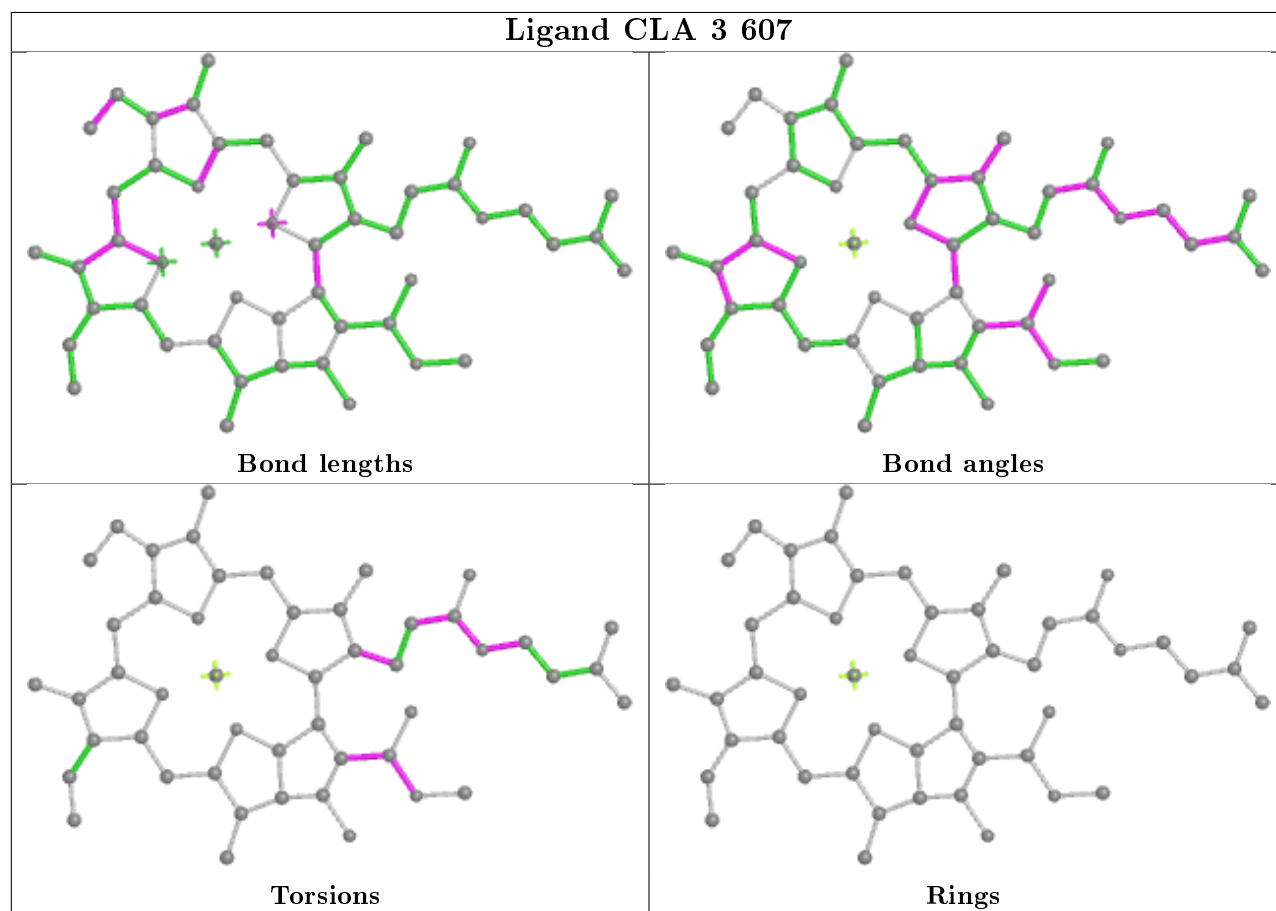




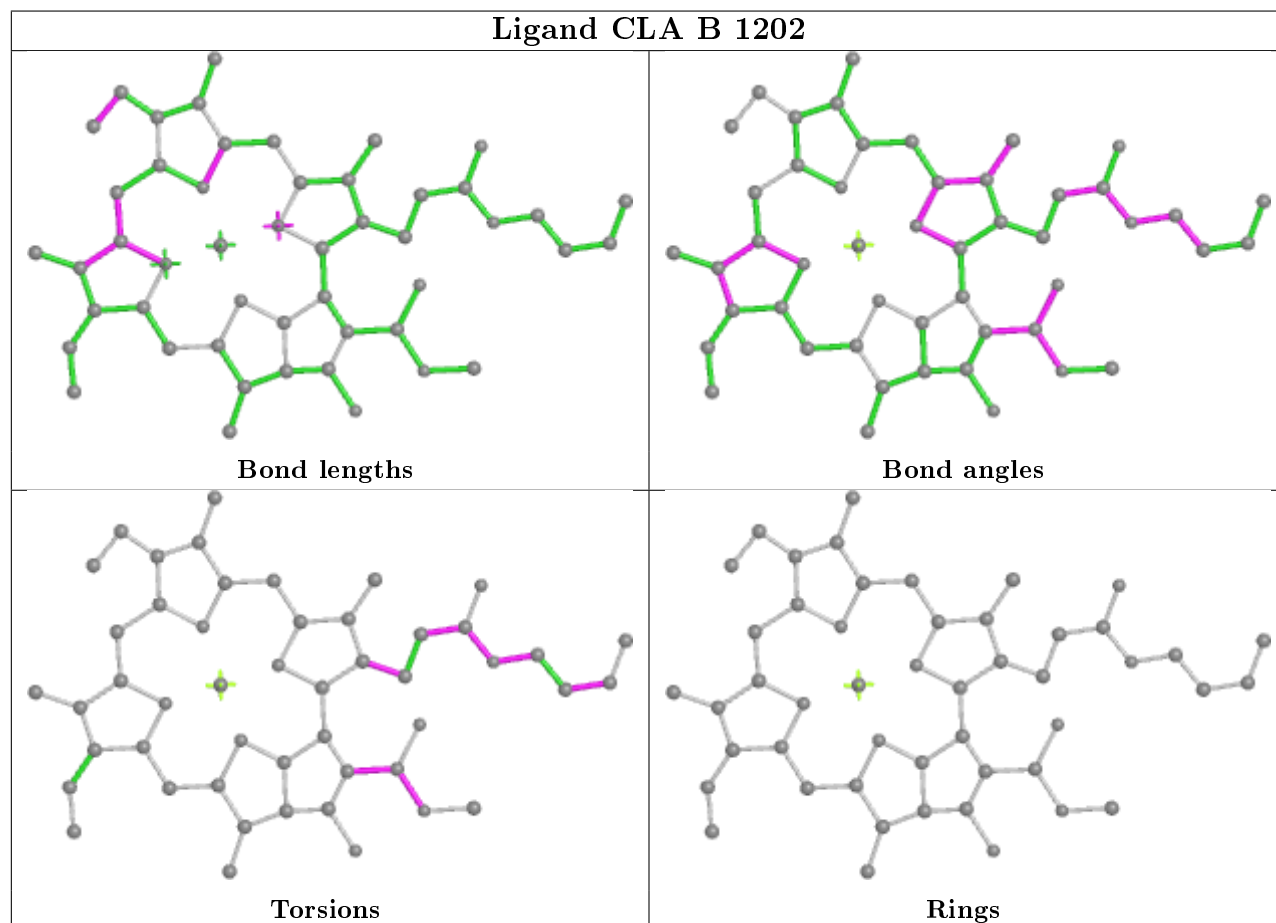
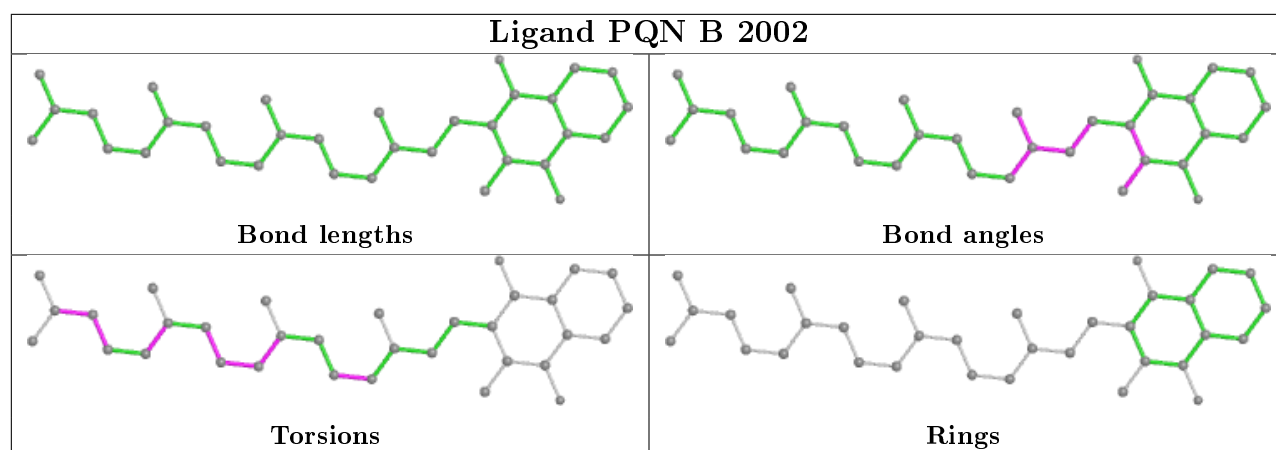
## Ligand CLA B 1229

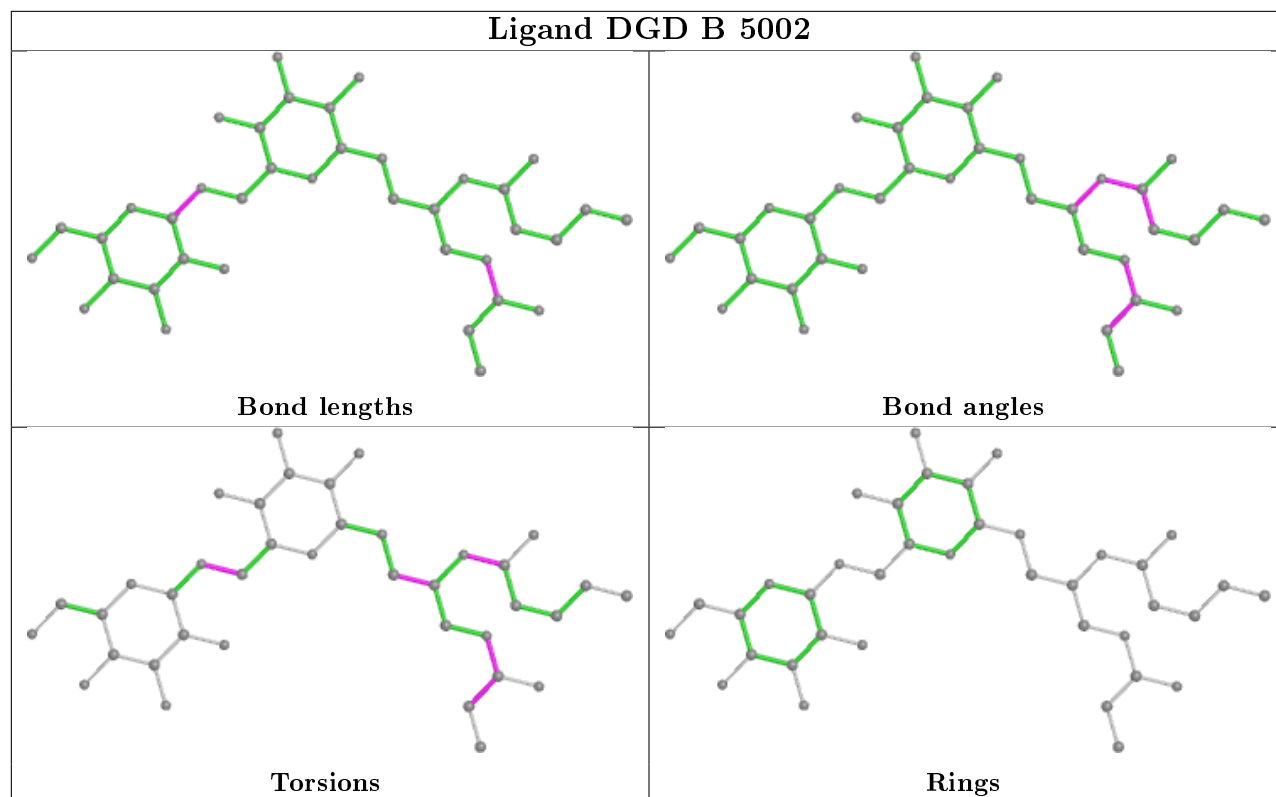


## Ligand CLA 3 607

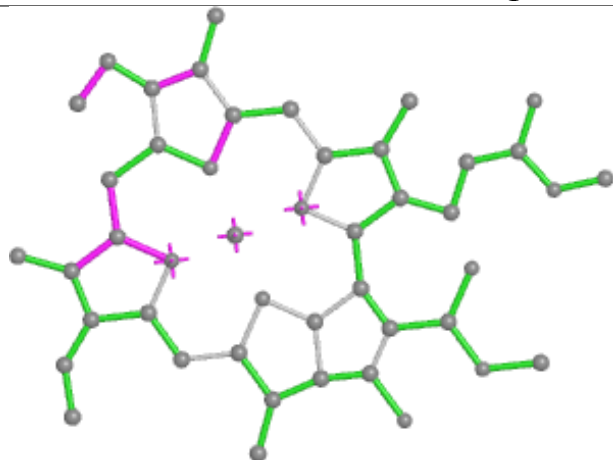




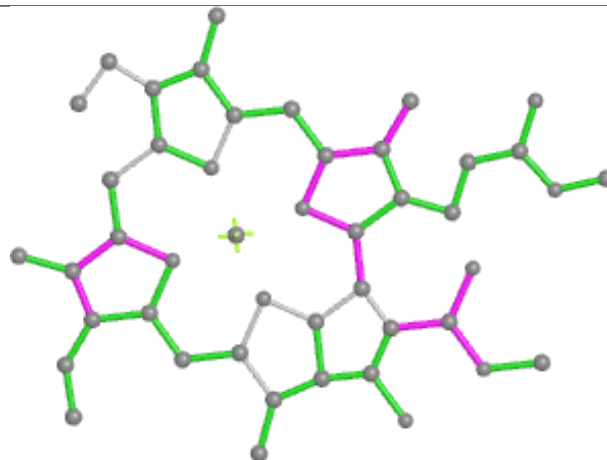




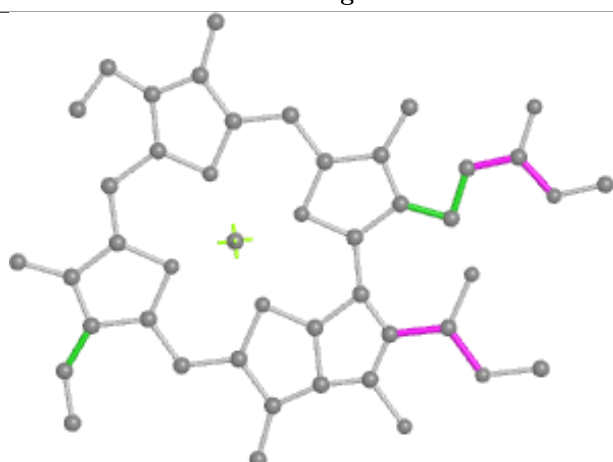
## Ligand CLA B 1209



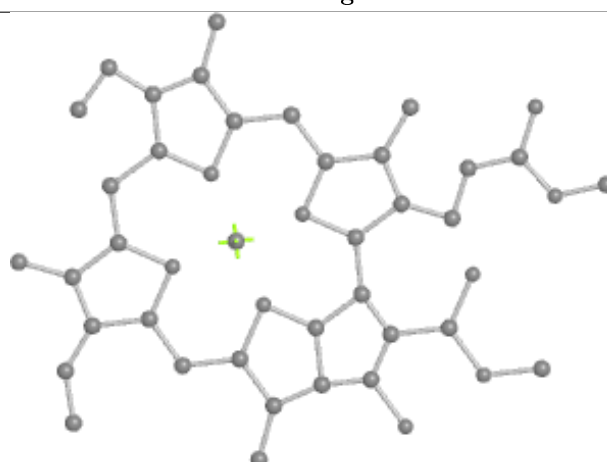
Bond lengths



Bond angles

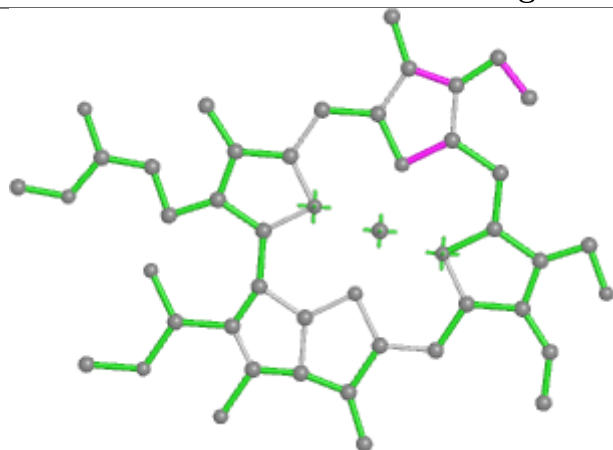


Torsions

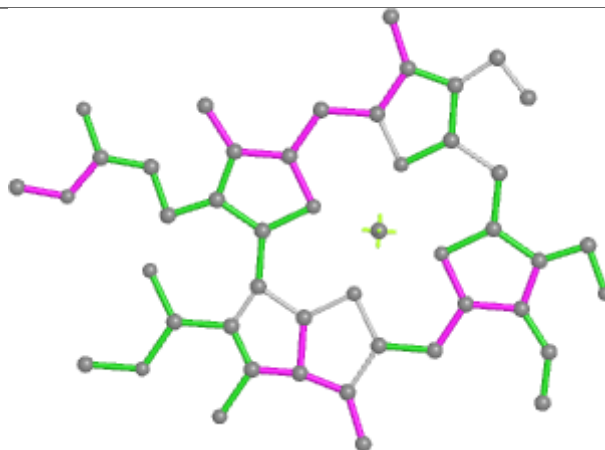


Rings

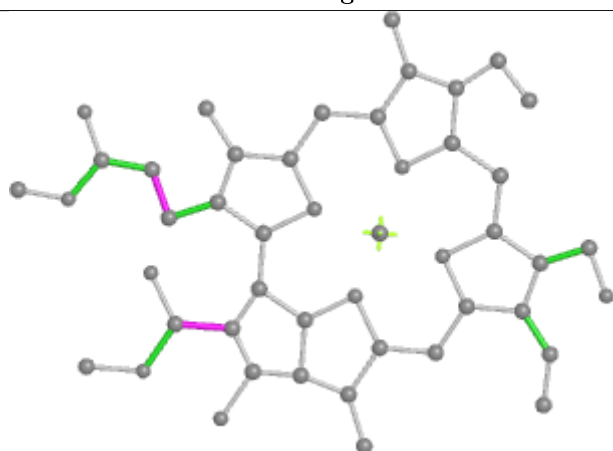
## Ligand CHL 4 610



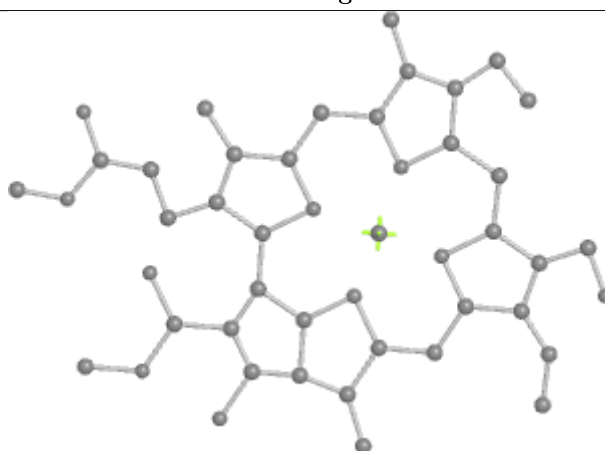
Bond lengths



Bond angles

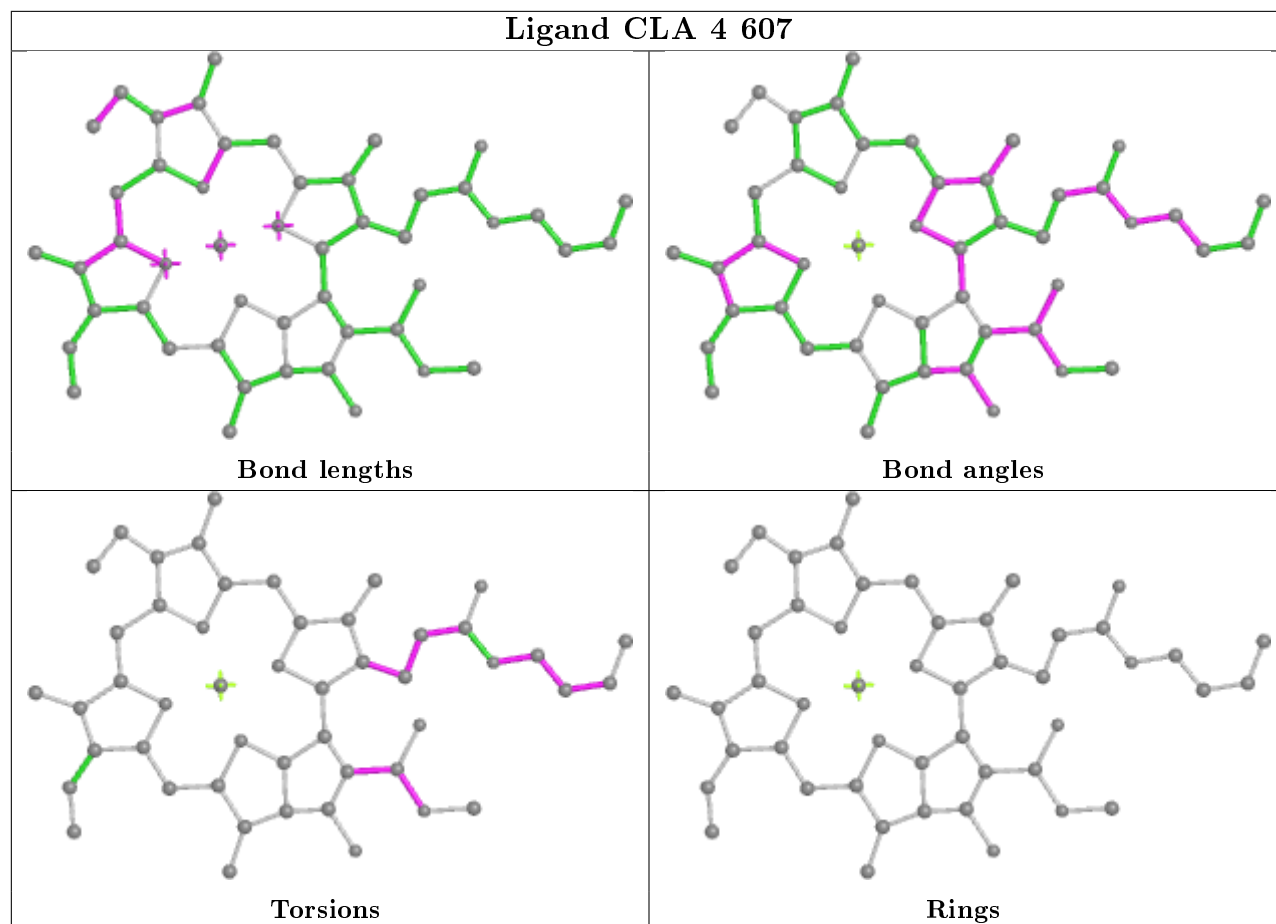


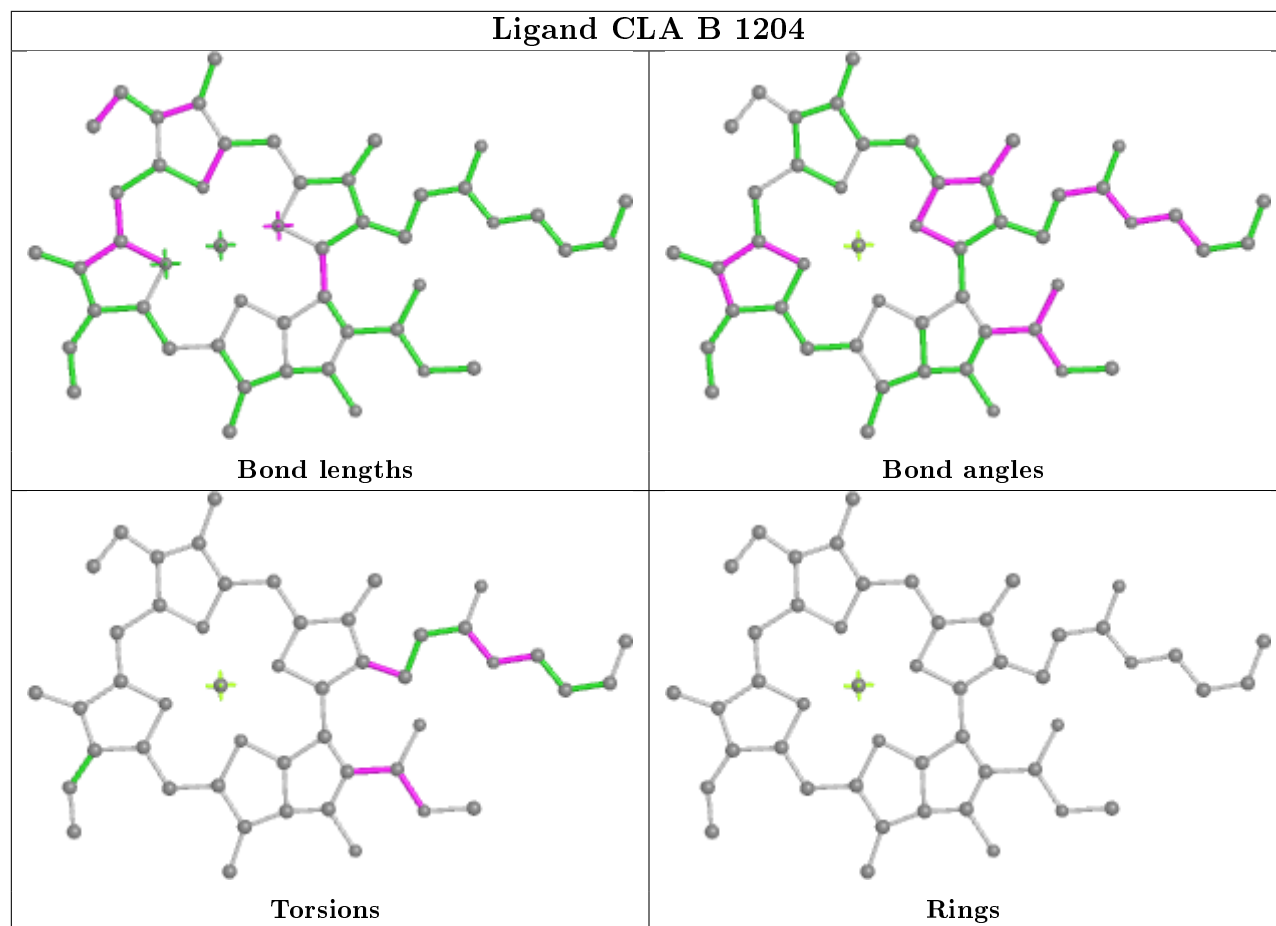
Torsions

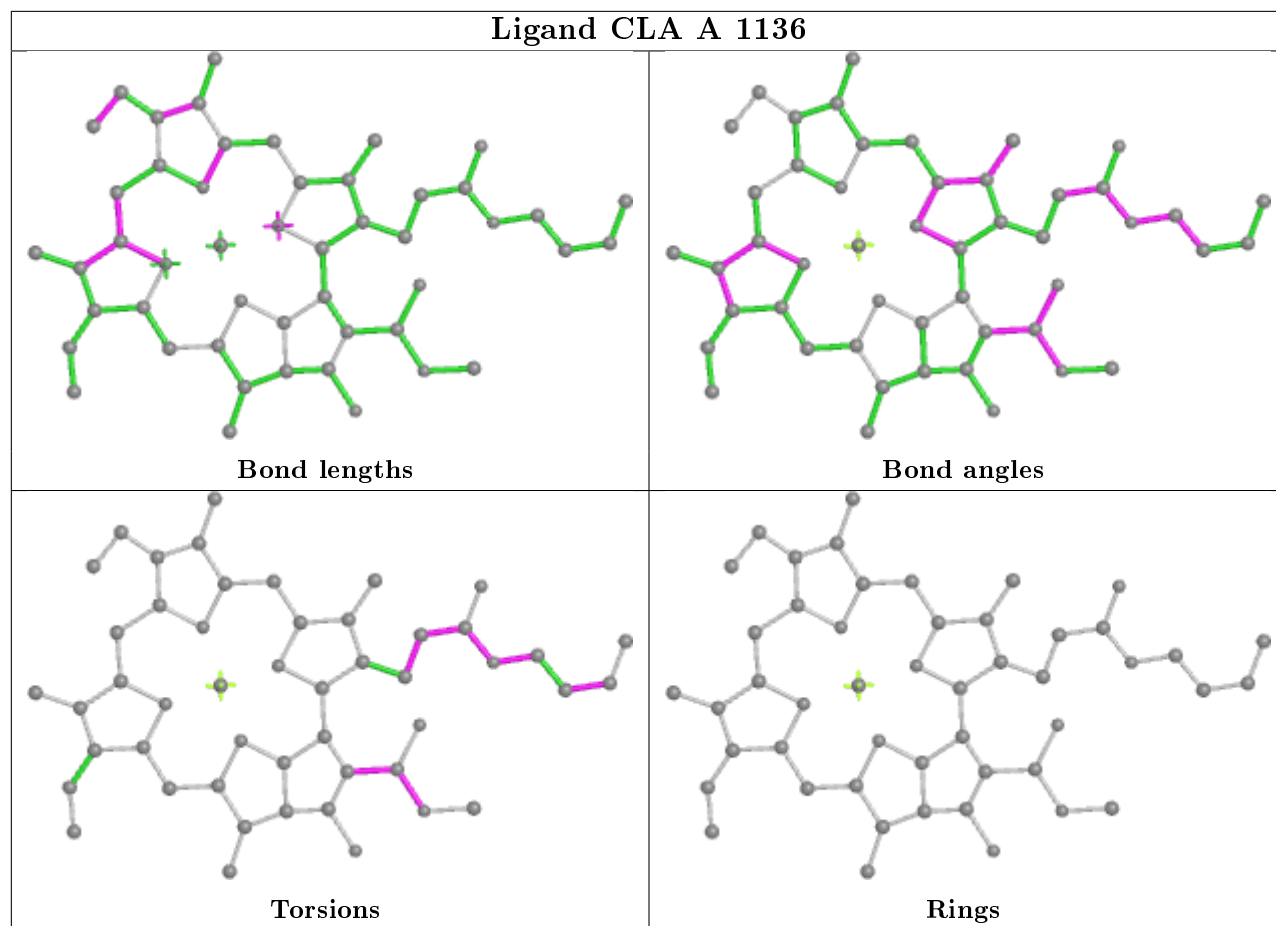


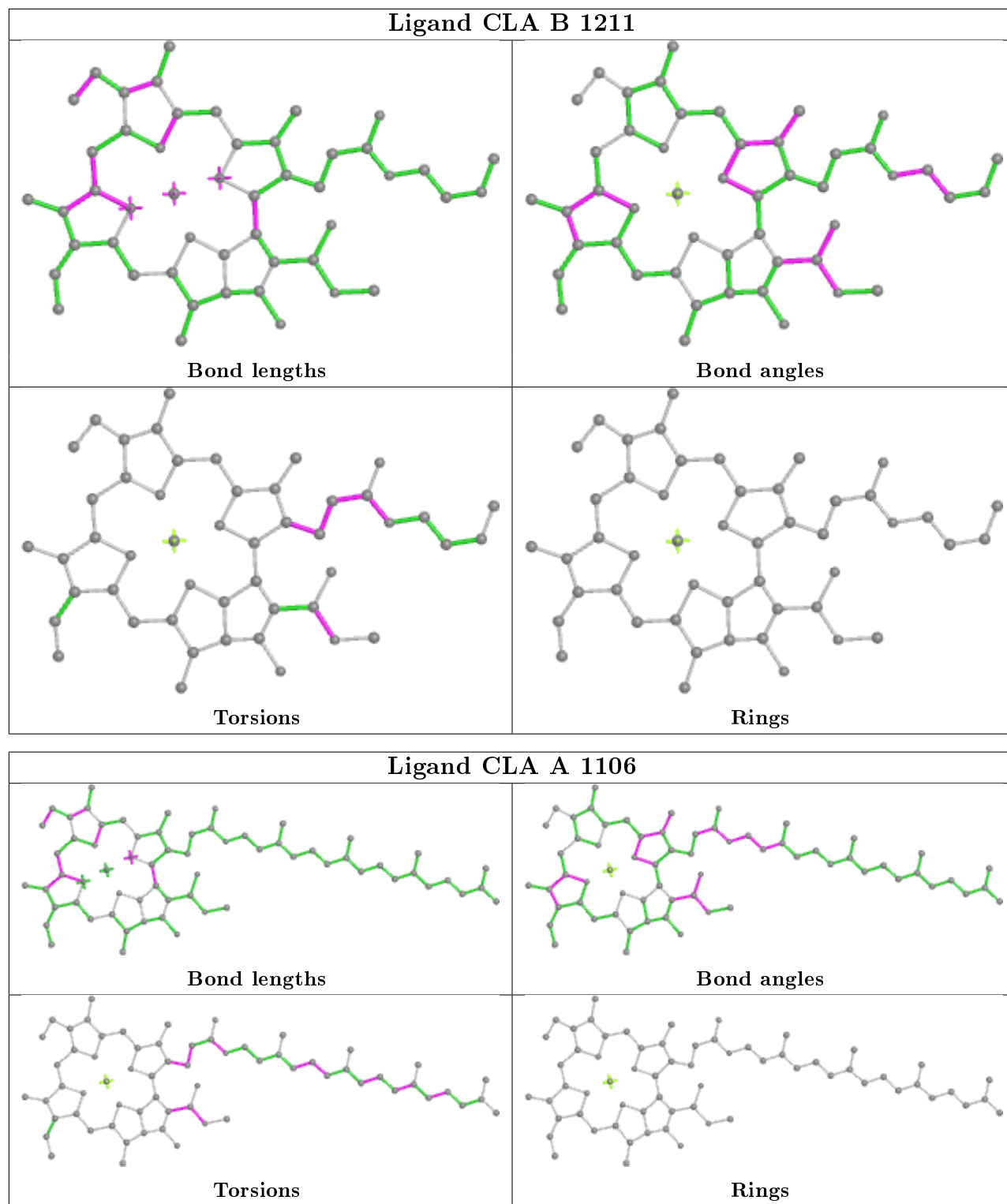
Rings

## Ligand CLA 4 607



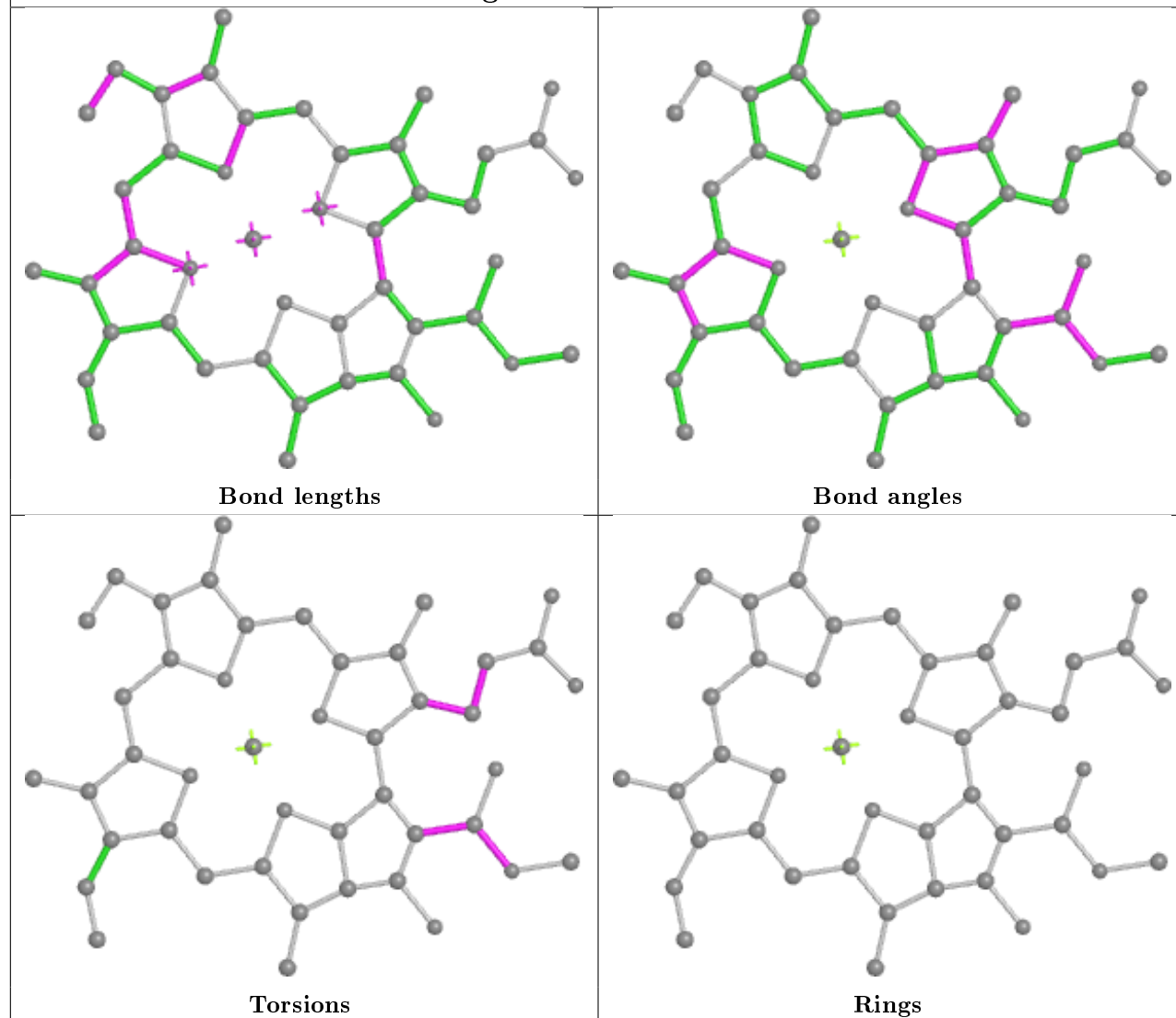




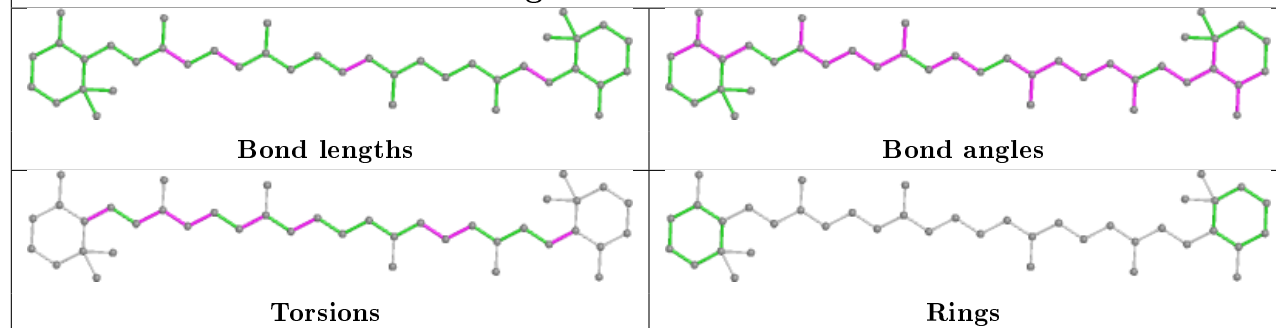




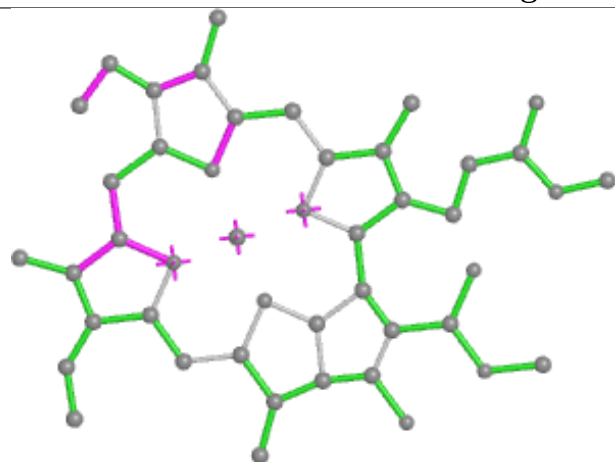
## Ligand CLA A 1113



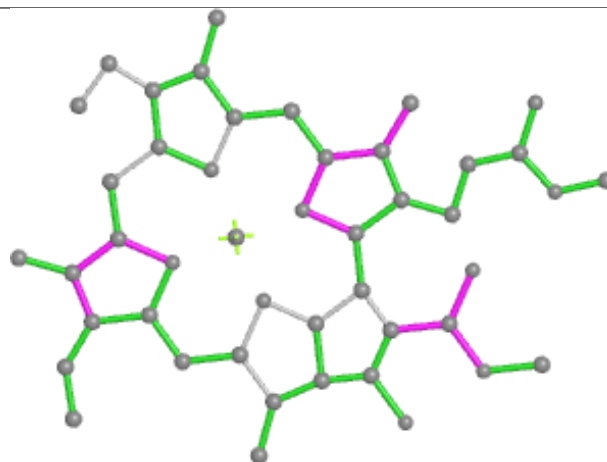
## Ligand BCR J 4003



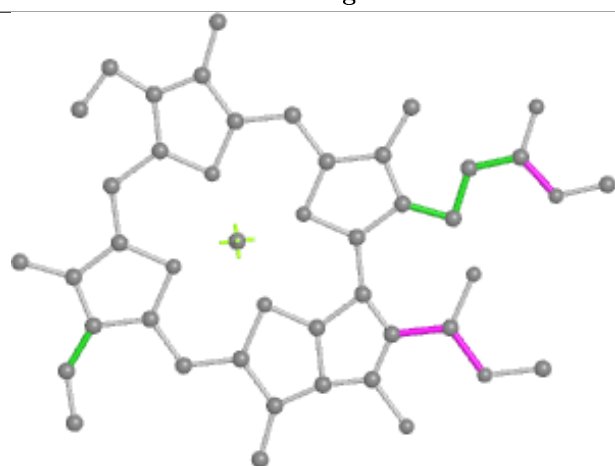
## Ligand CLA 4 608



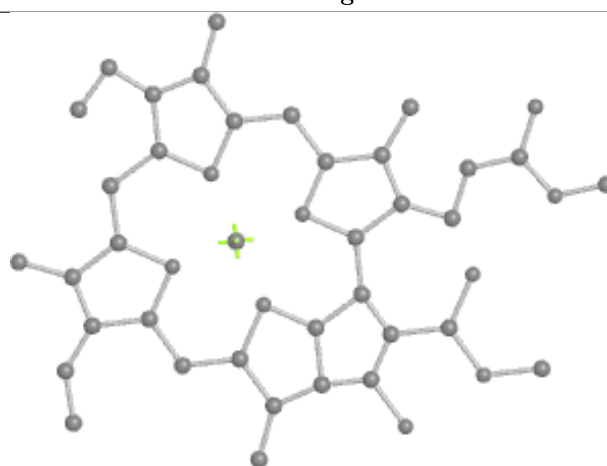
Bond lengths



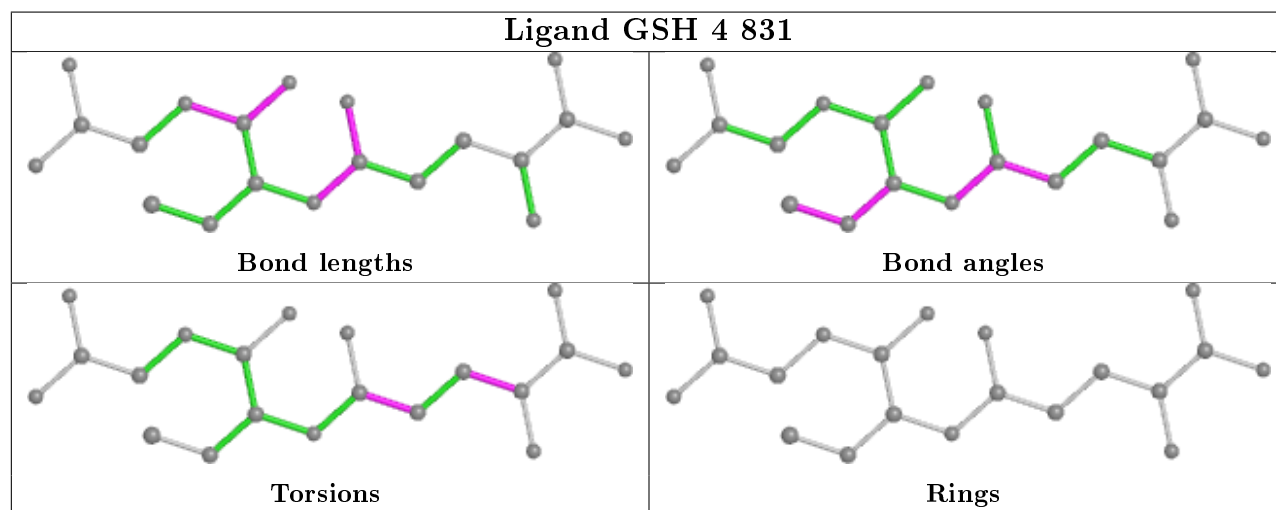
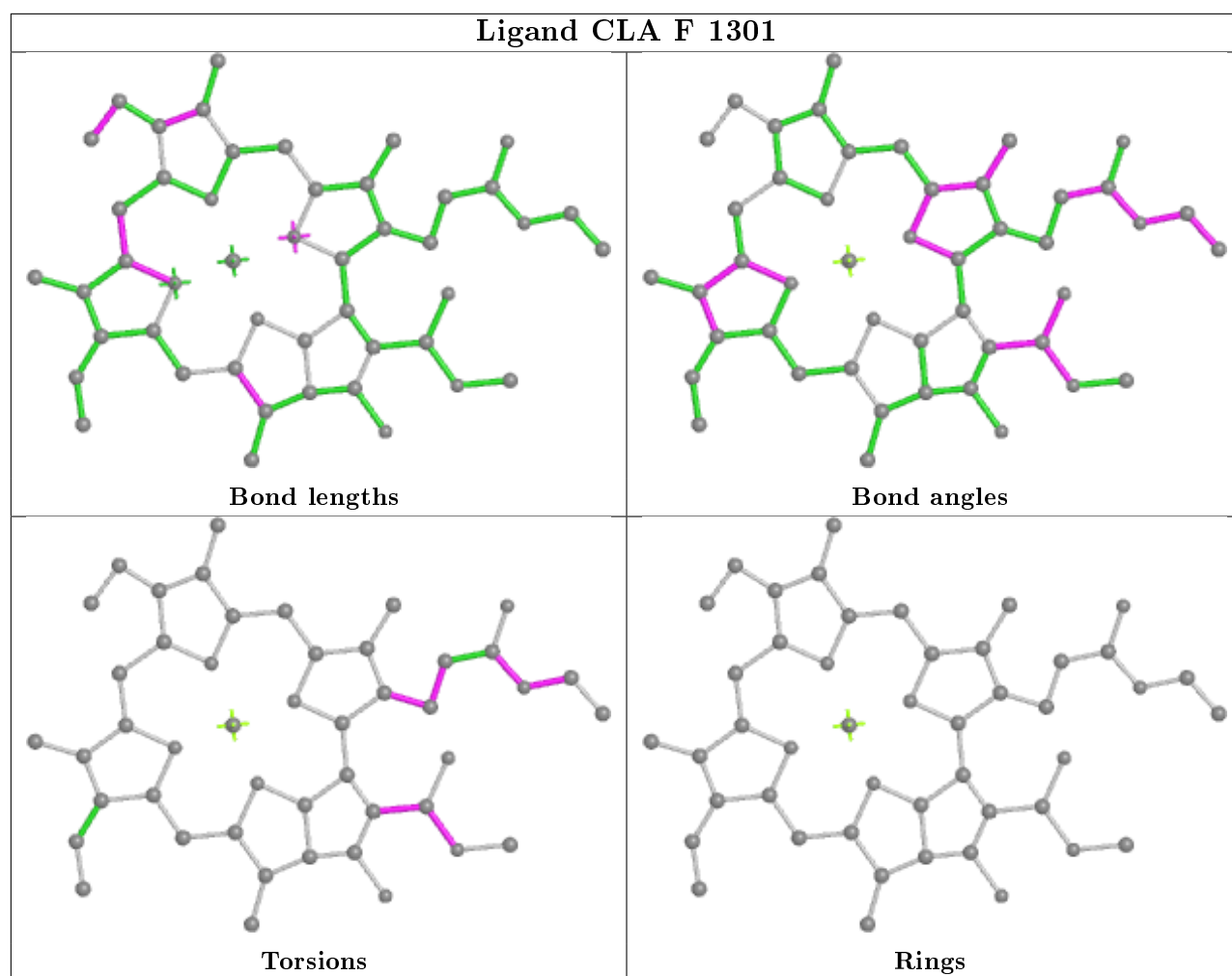
Bond angles

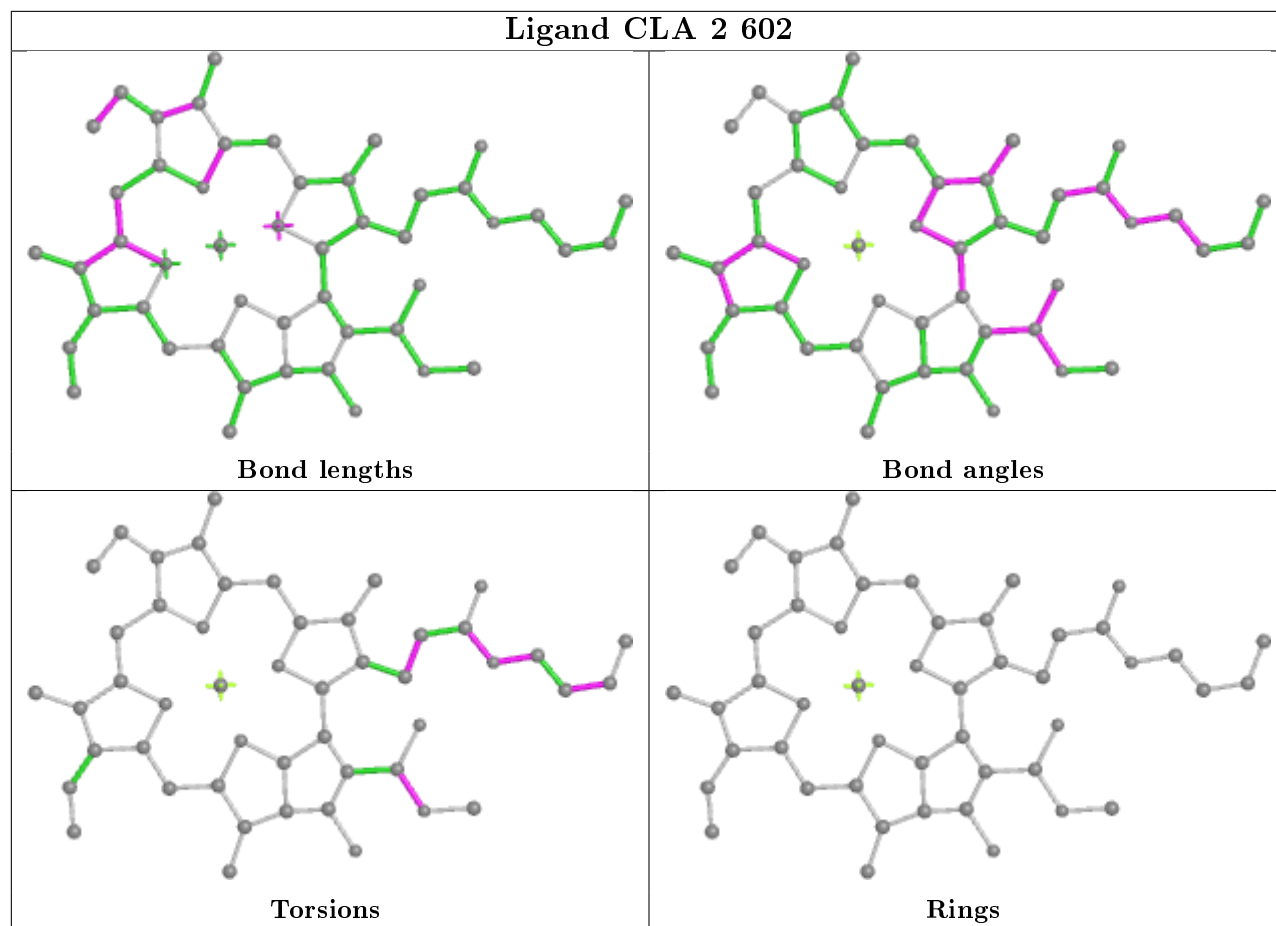


Torsions

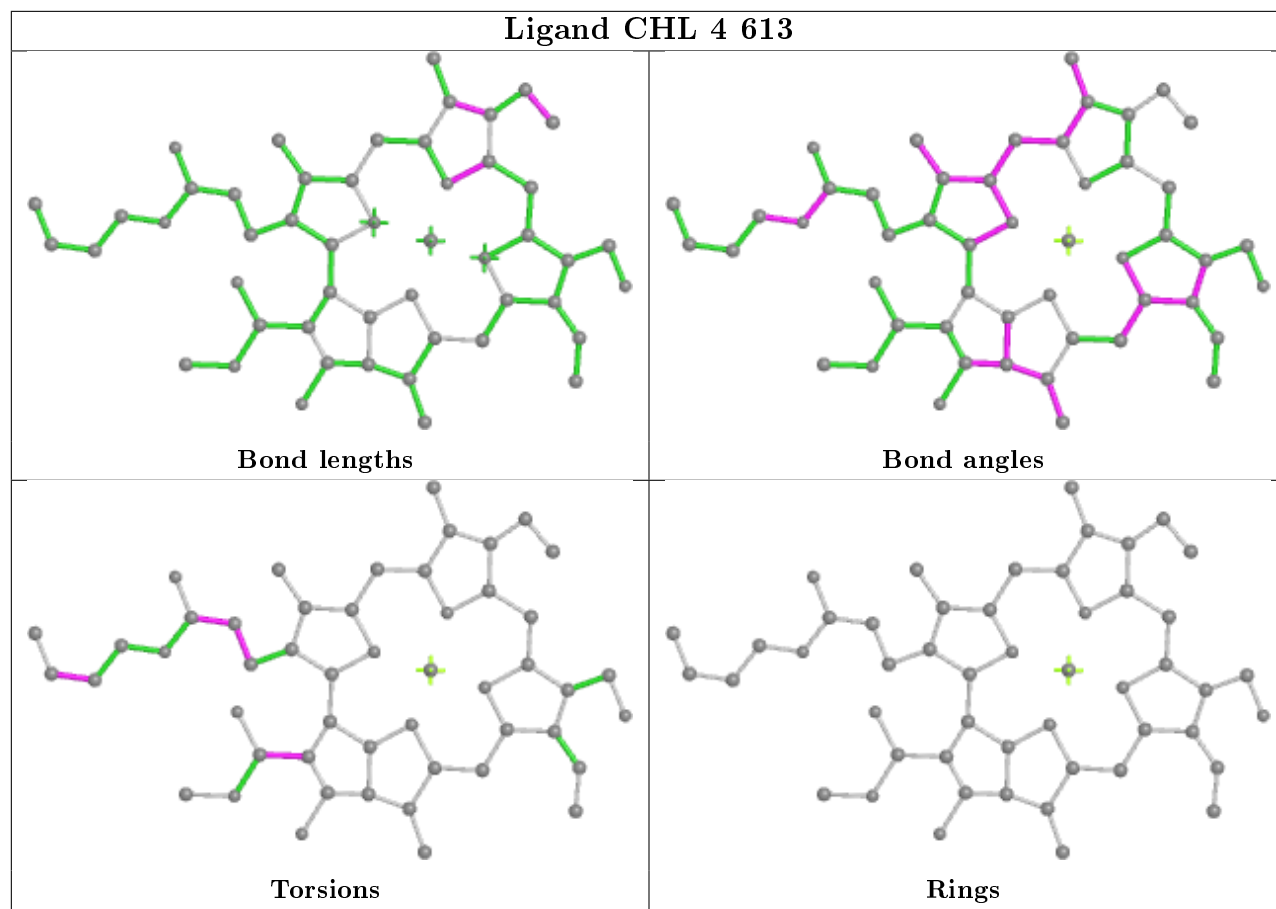


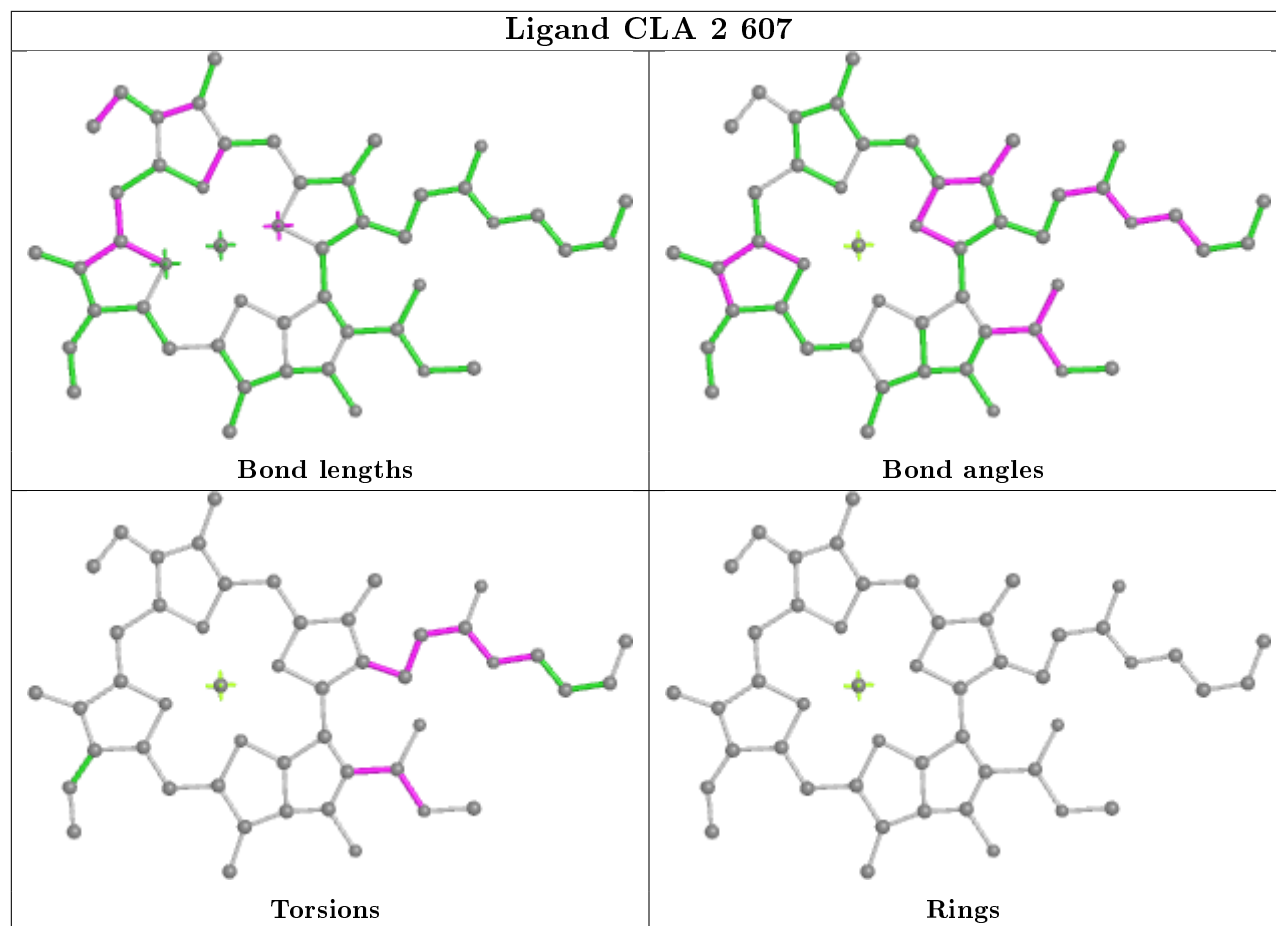
Rings

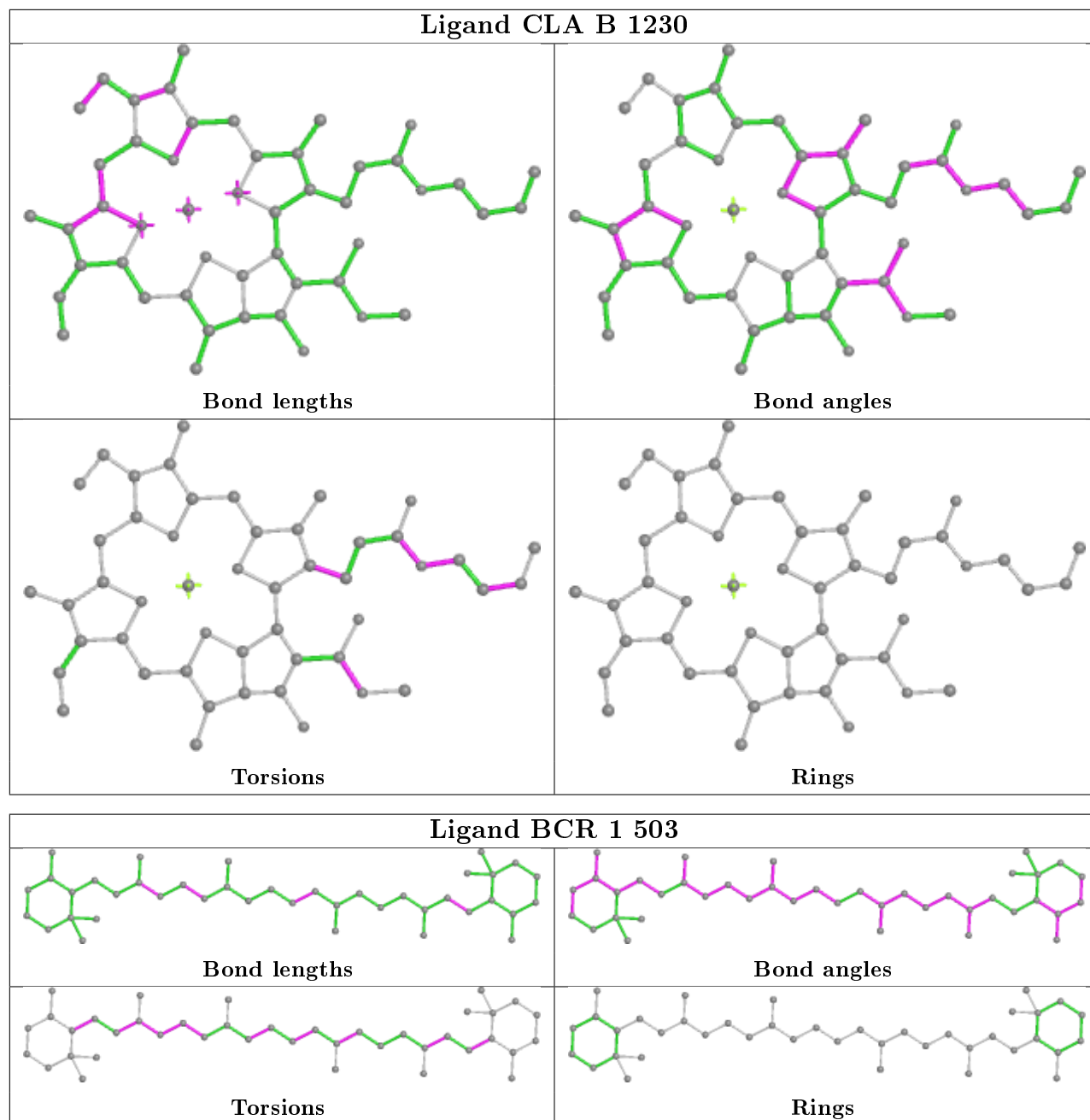




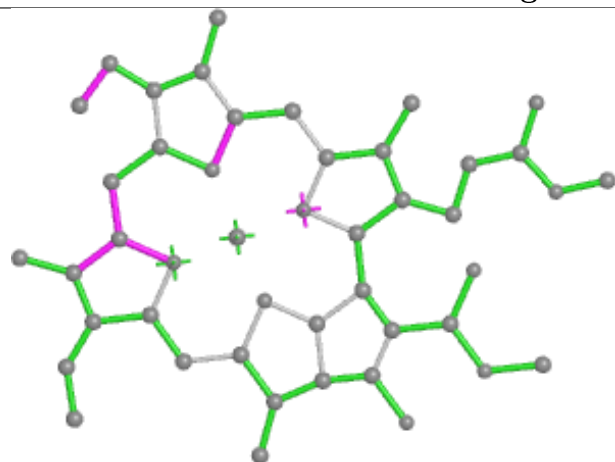
## Ligand CHL 4 613



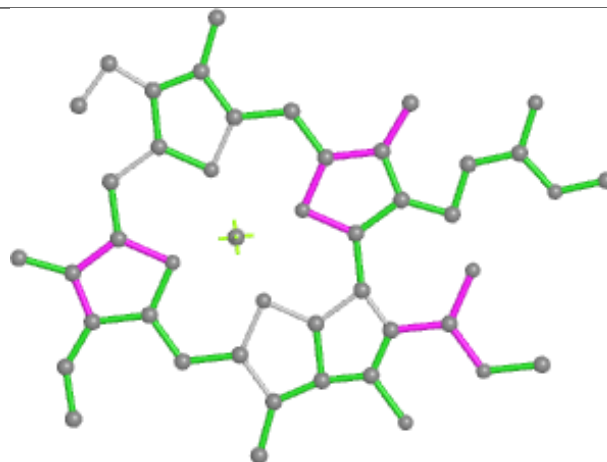




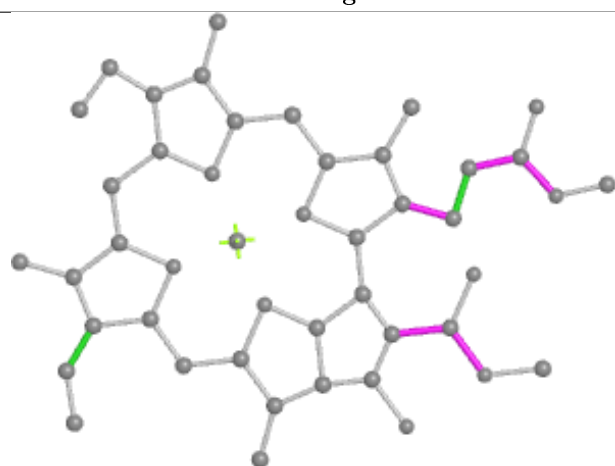
## Ligand CLA 3 613



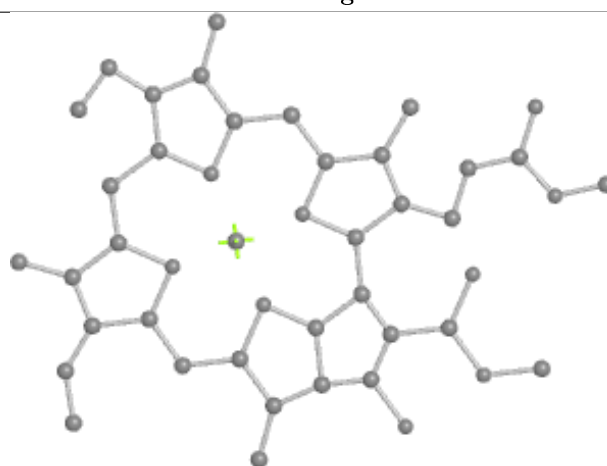
Bond lengths



Bond angles

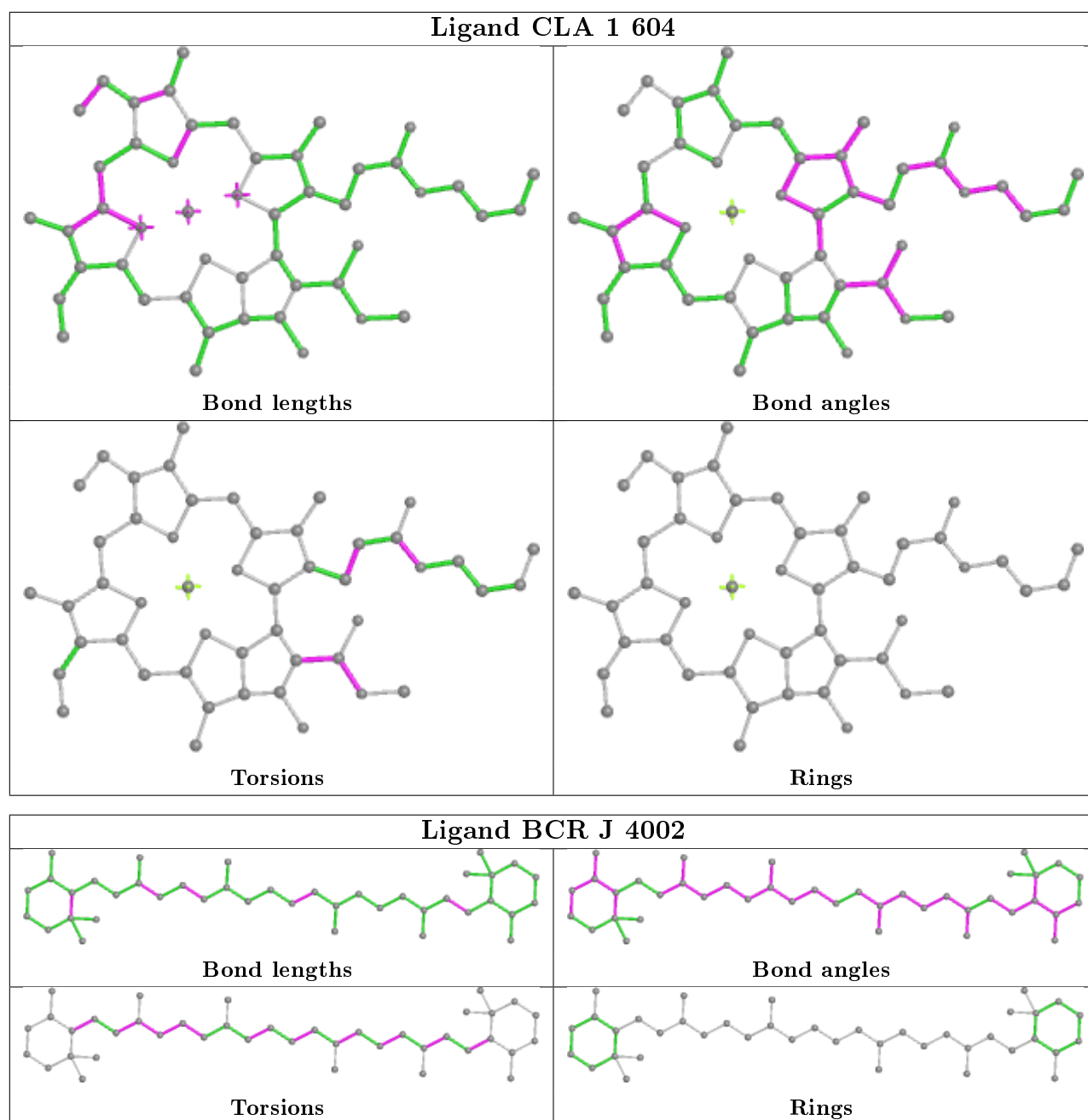


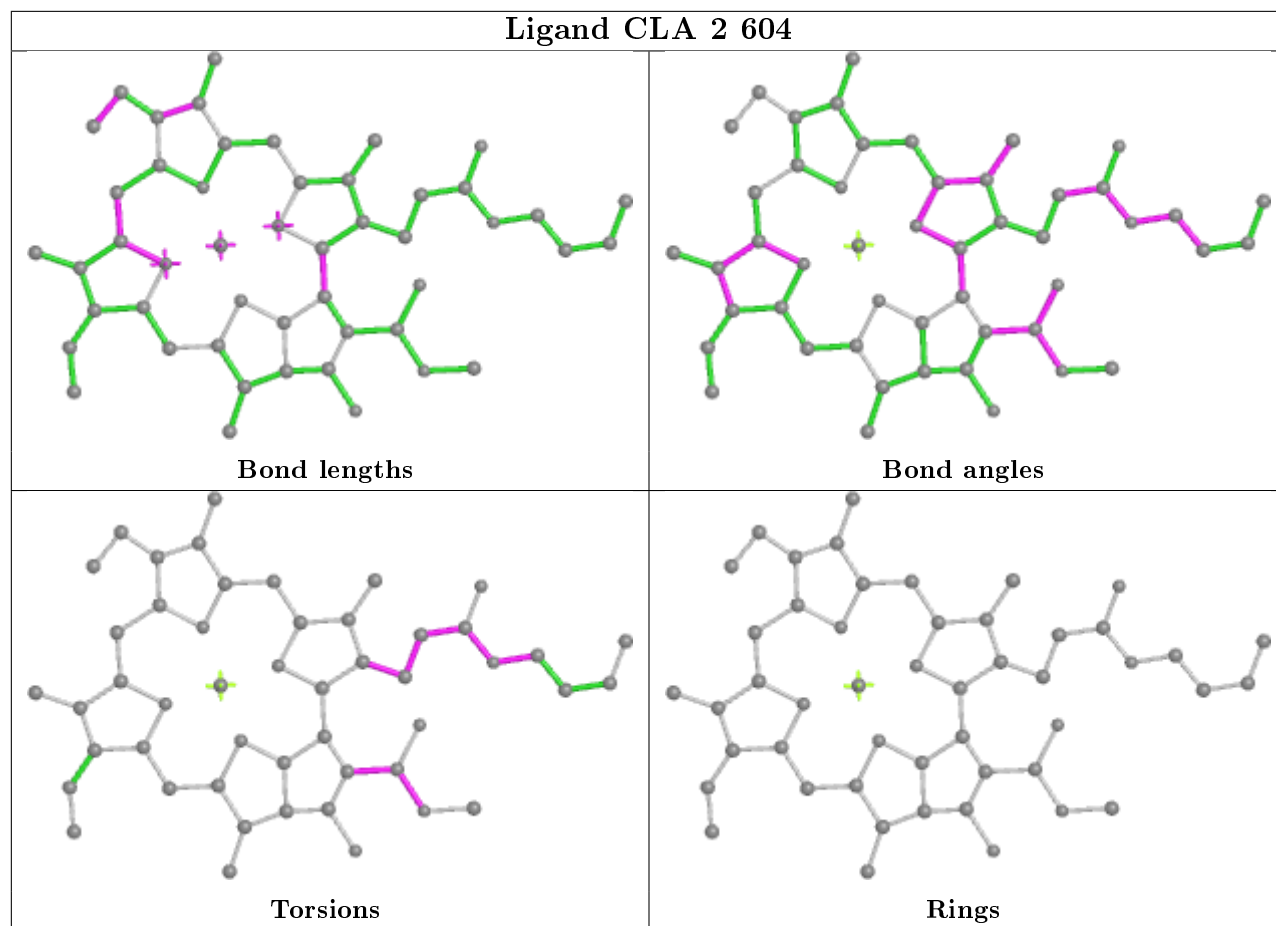
Torsions



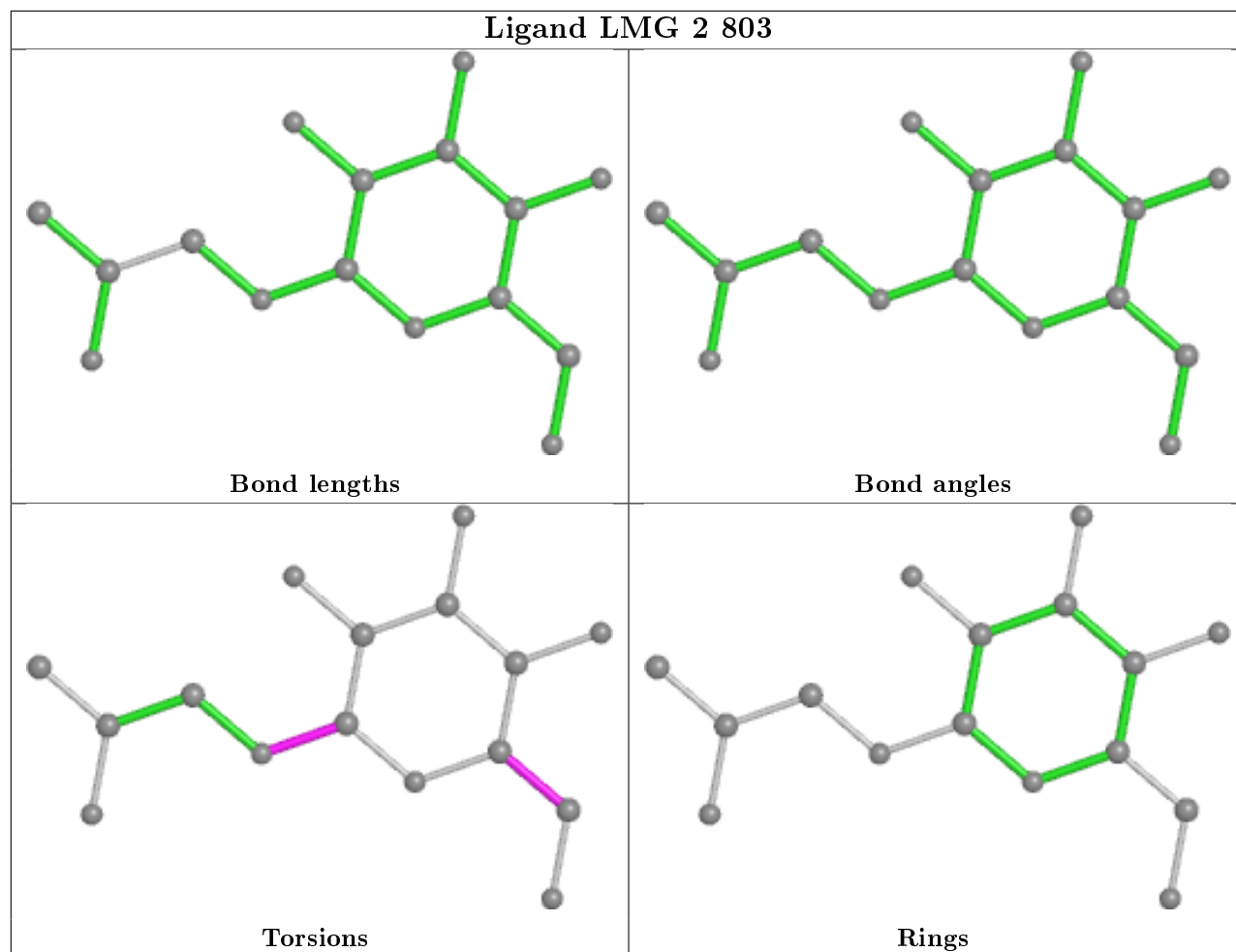
Rings



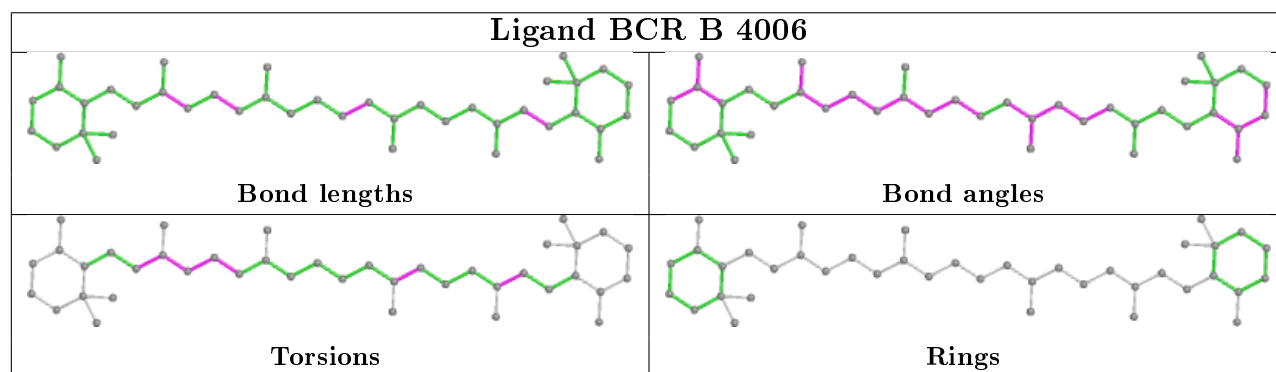




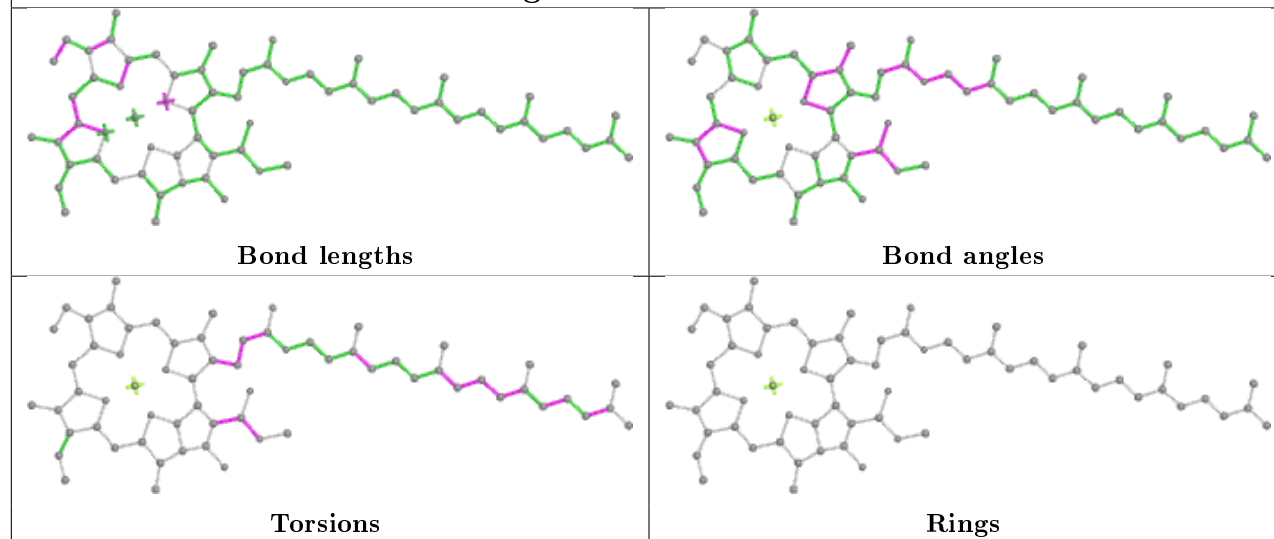
## Ligand LMG 2 803



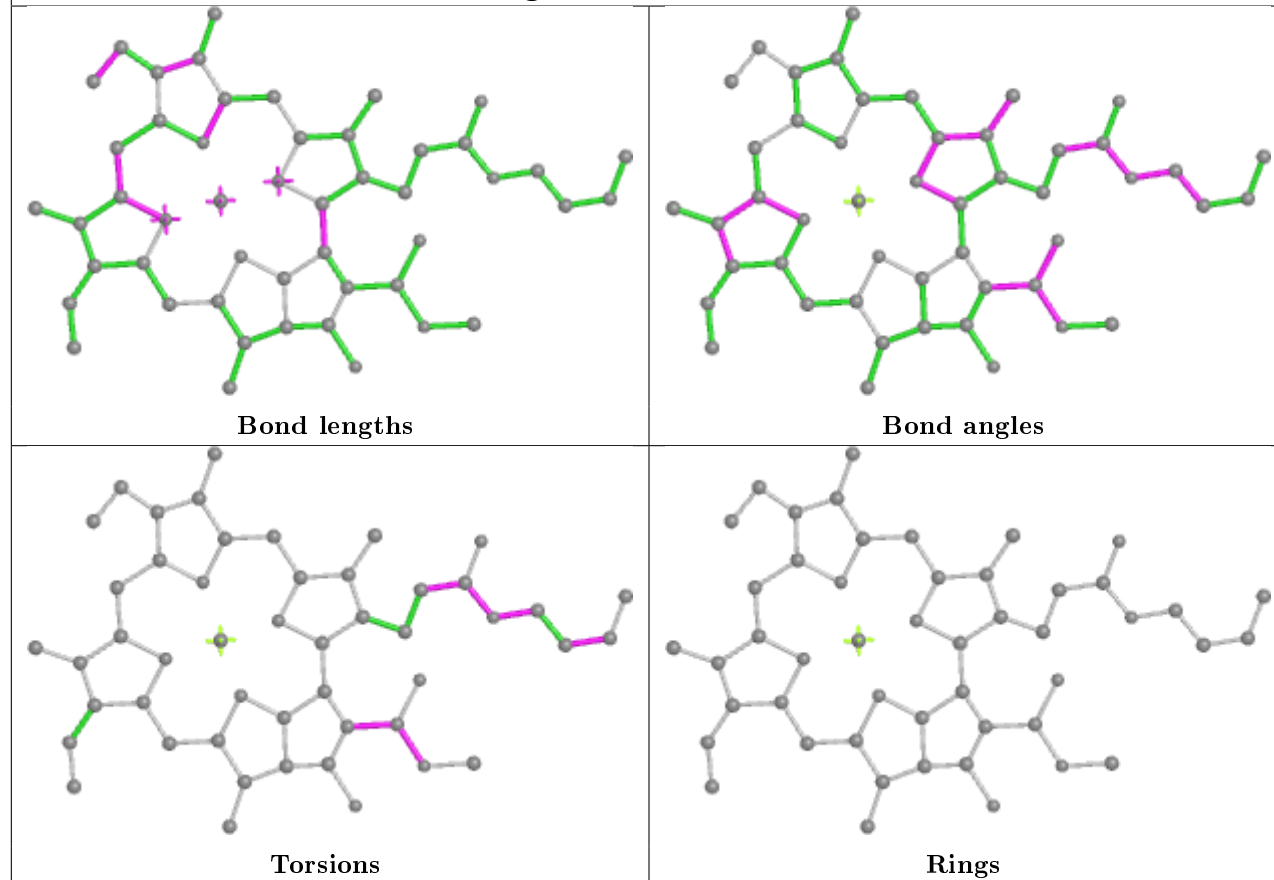
## Ligand BCR B 4006

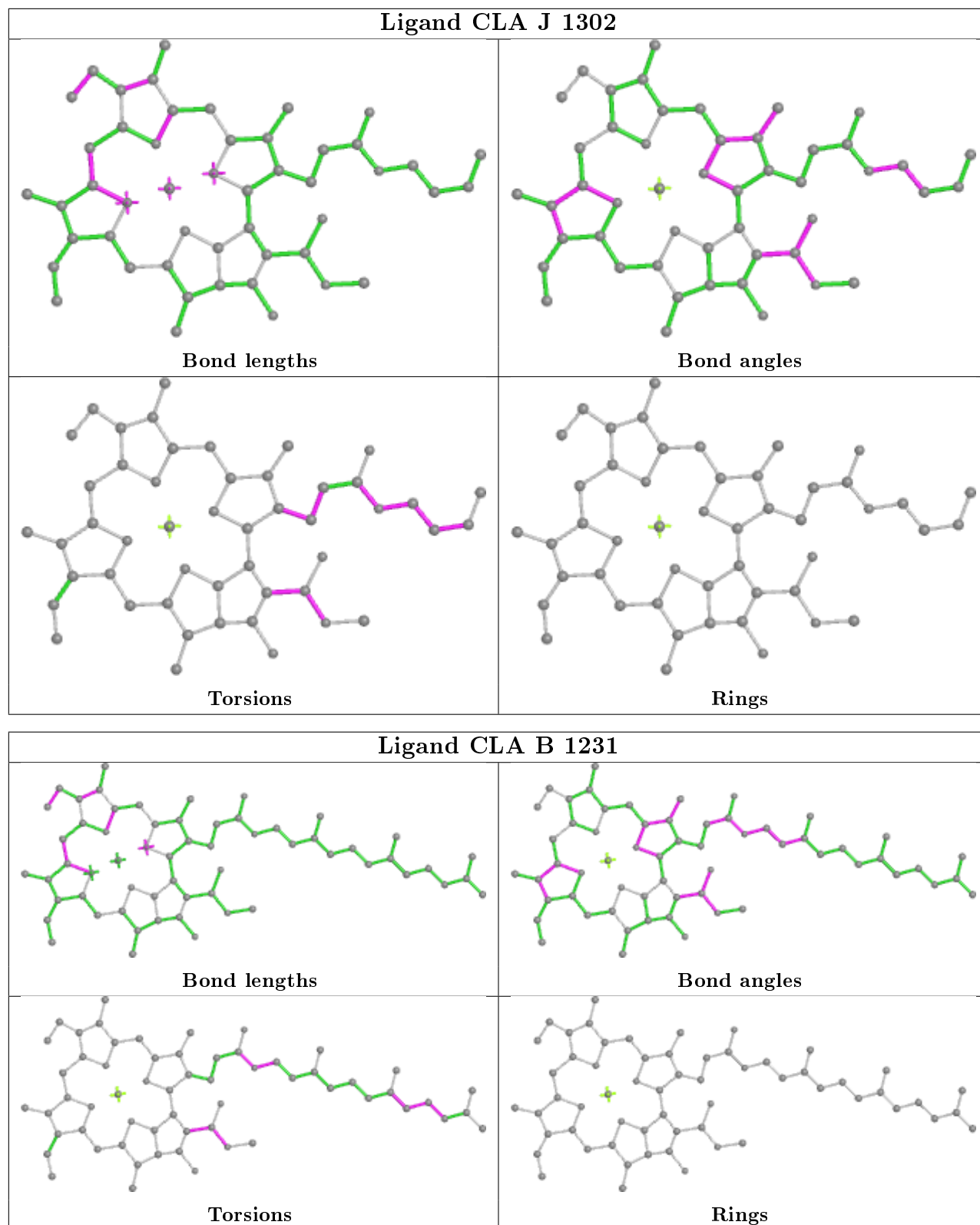


## Ligand CLA A 1138

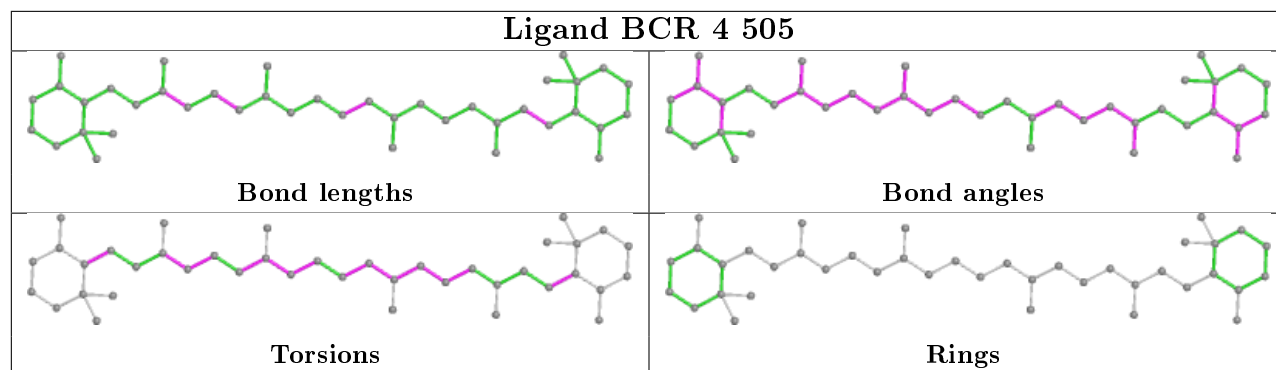


## Ligand CLA A 1128

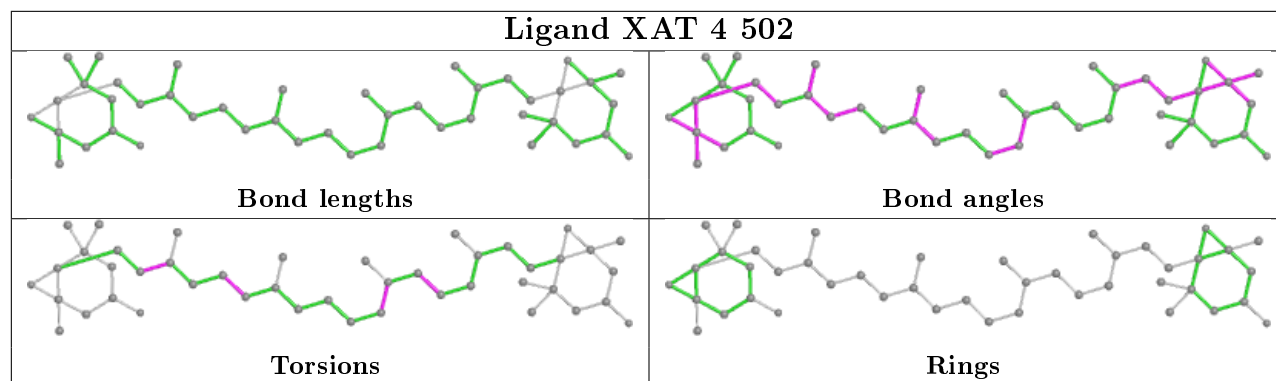




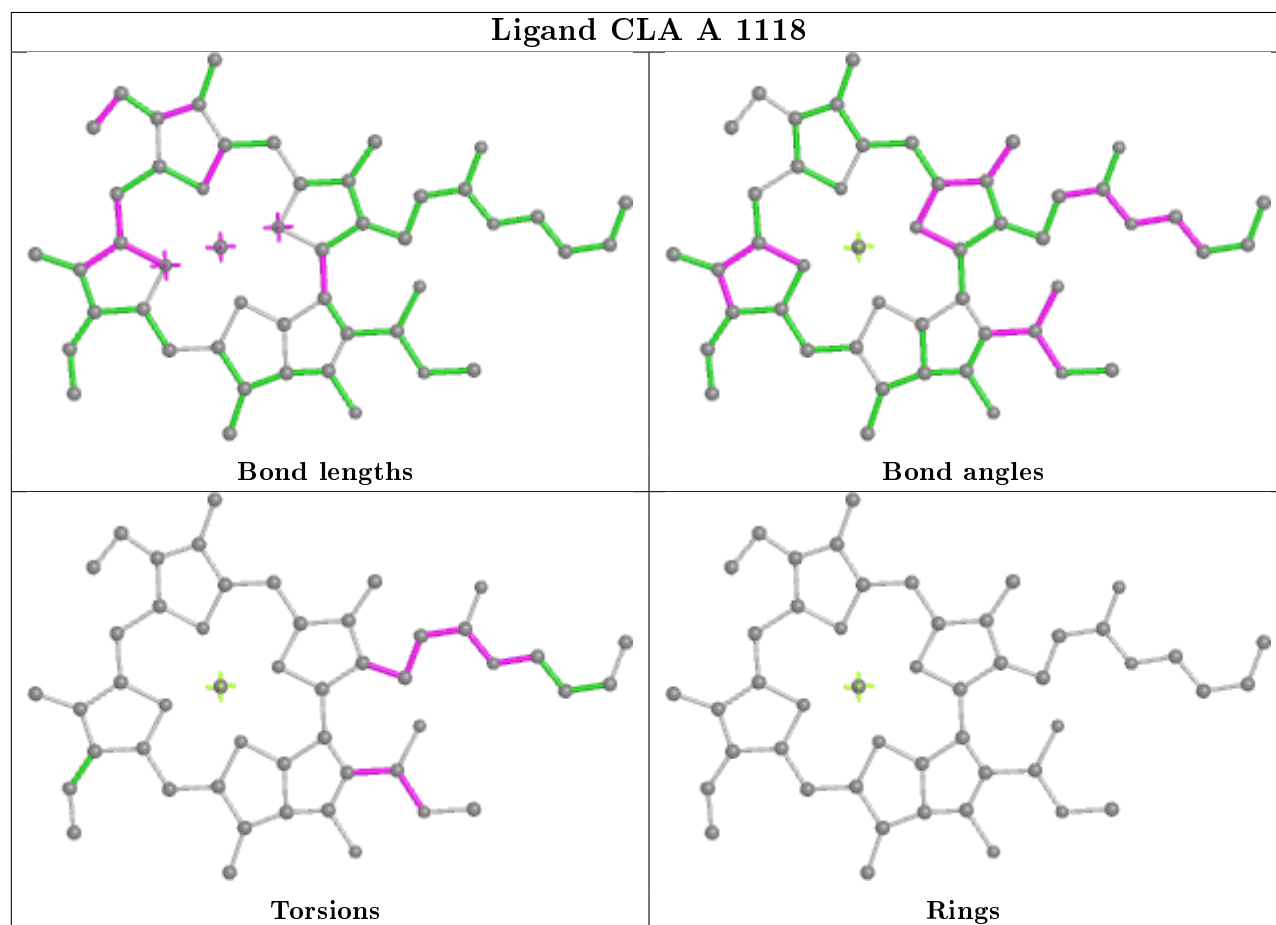
## Ligand BCR 4 505



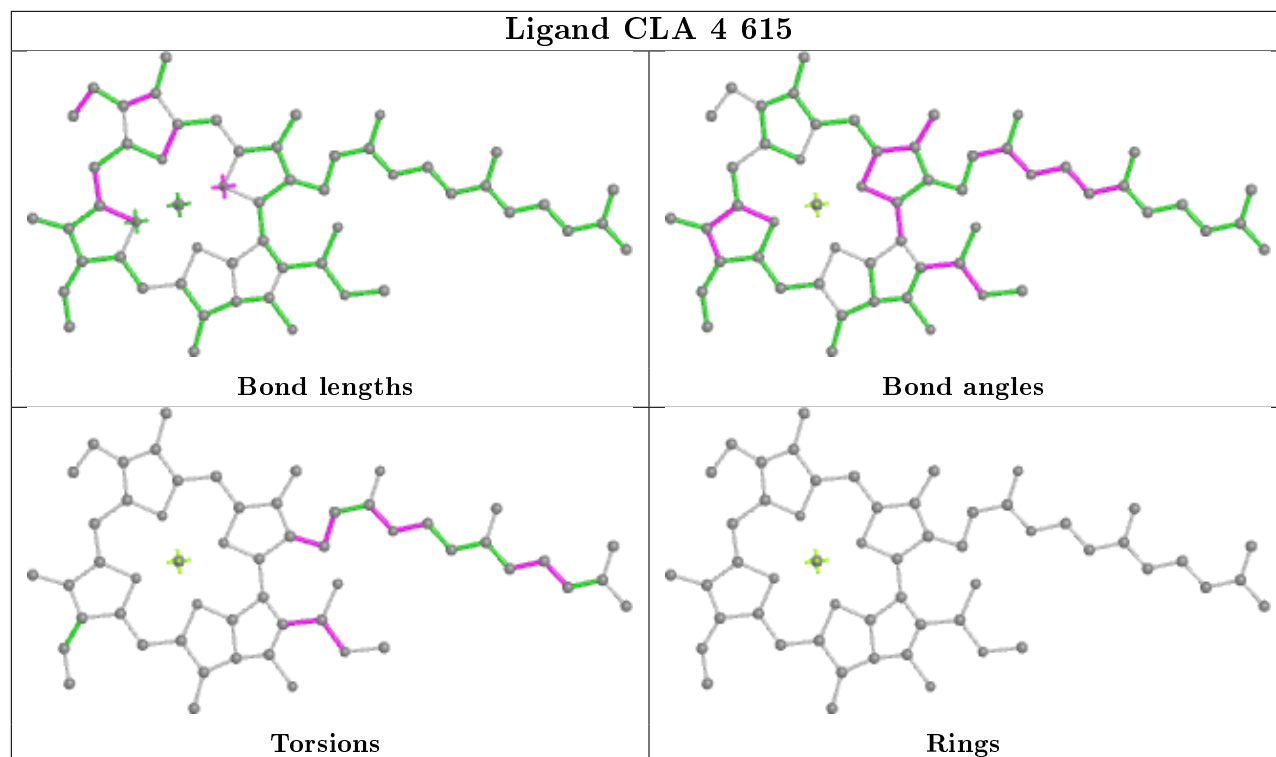
## Ligand XAT 4 502



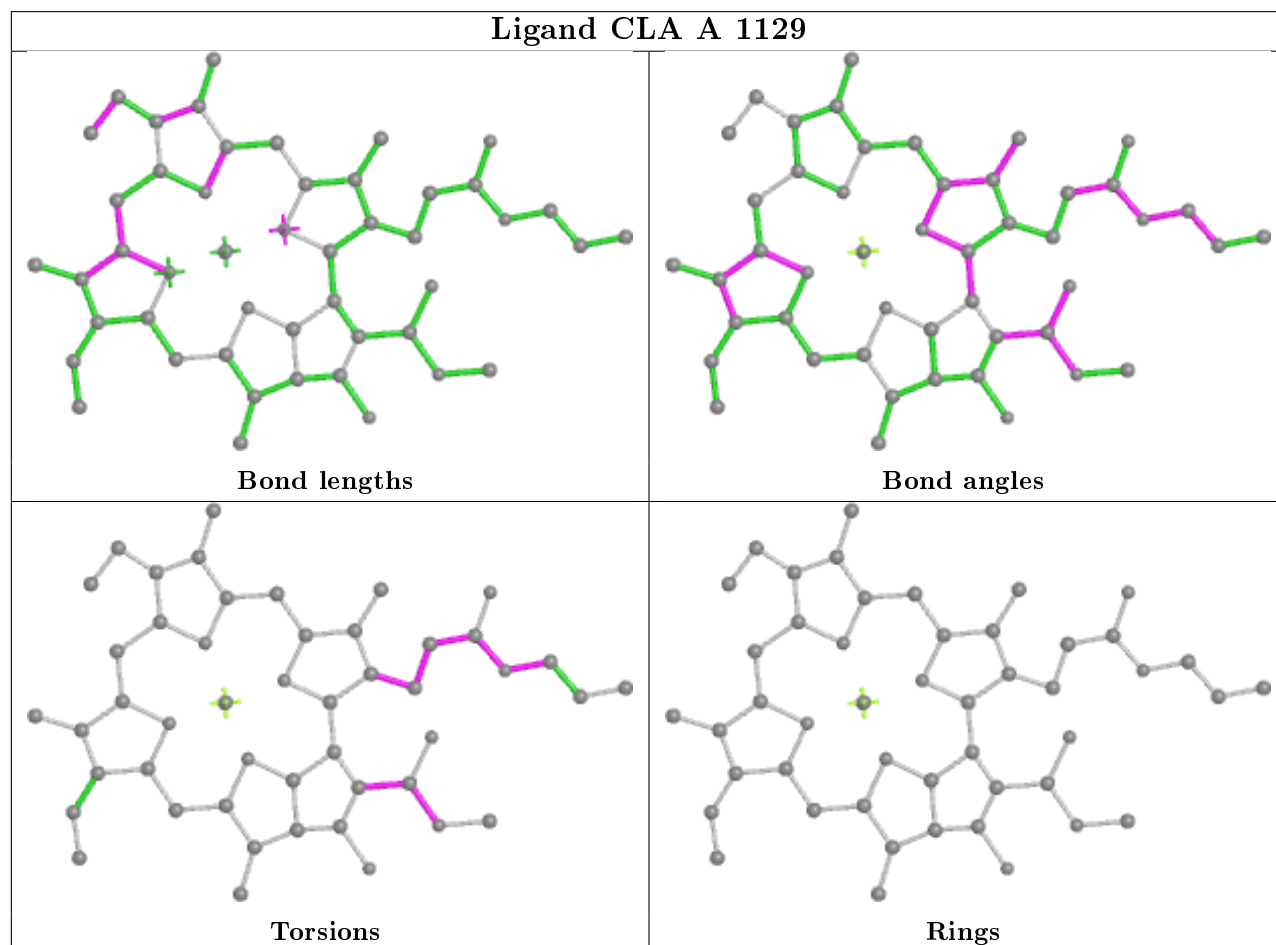
## Ligand CLA A 1118

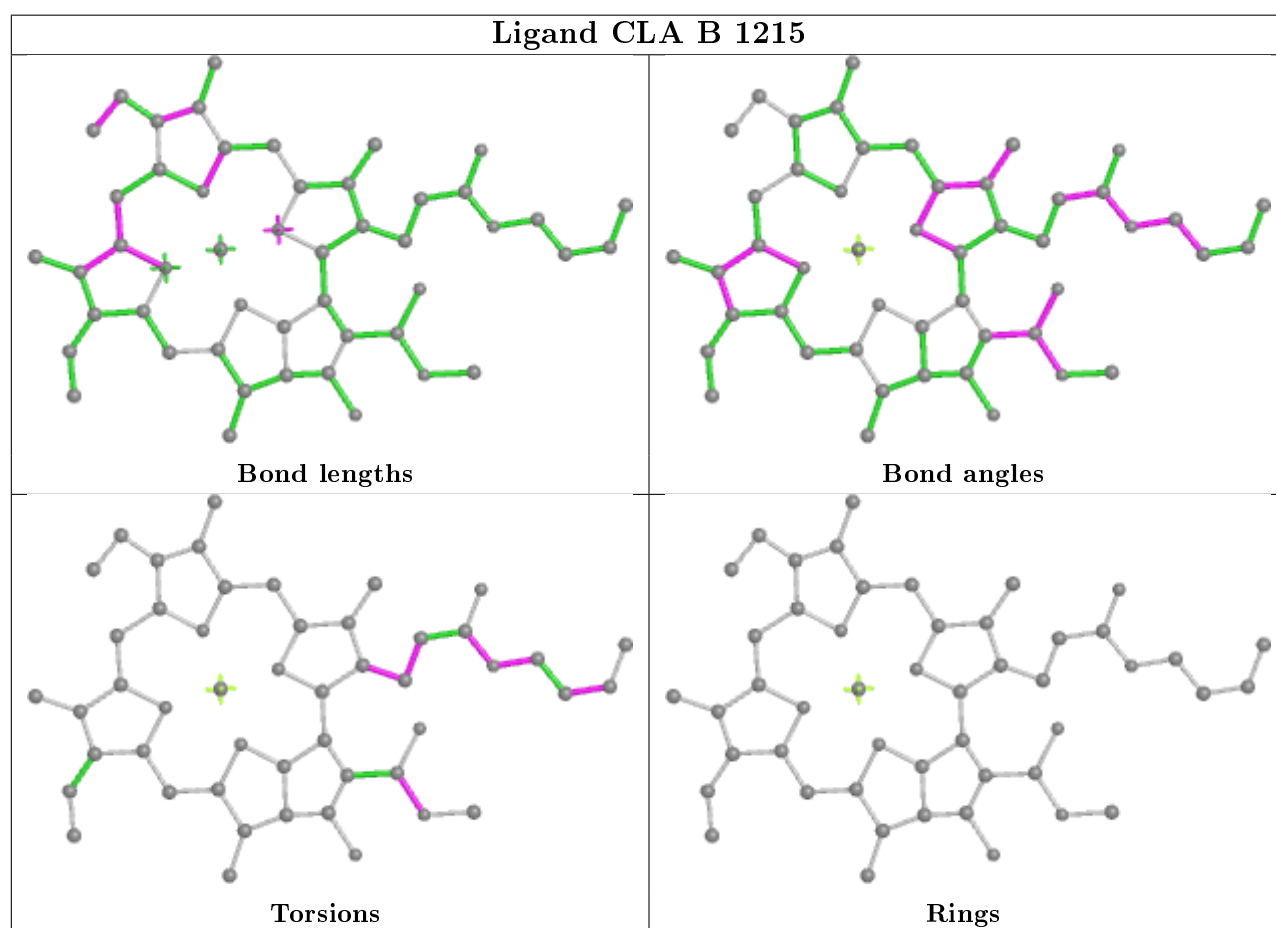
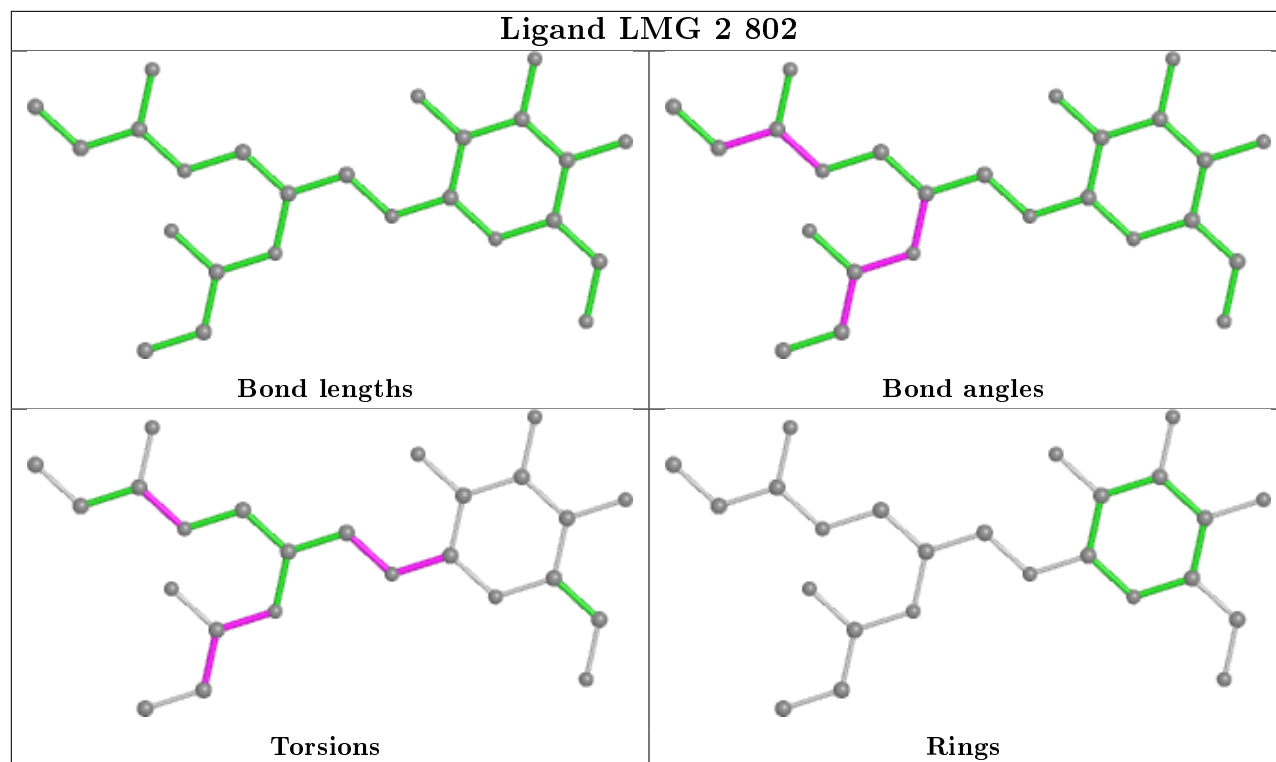


## Ligand CLA 4 615

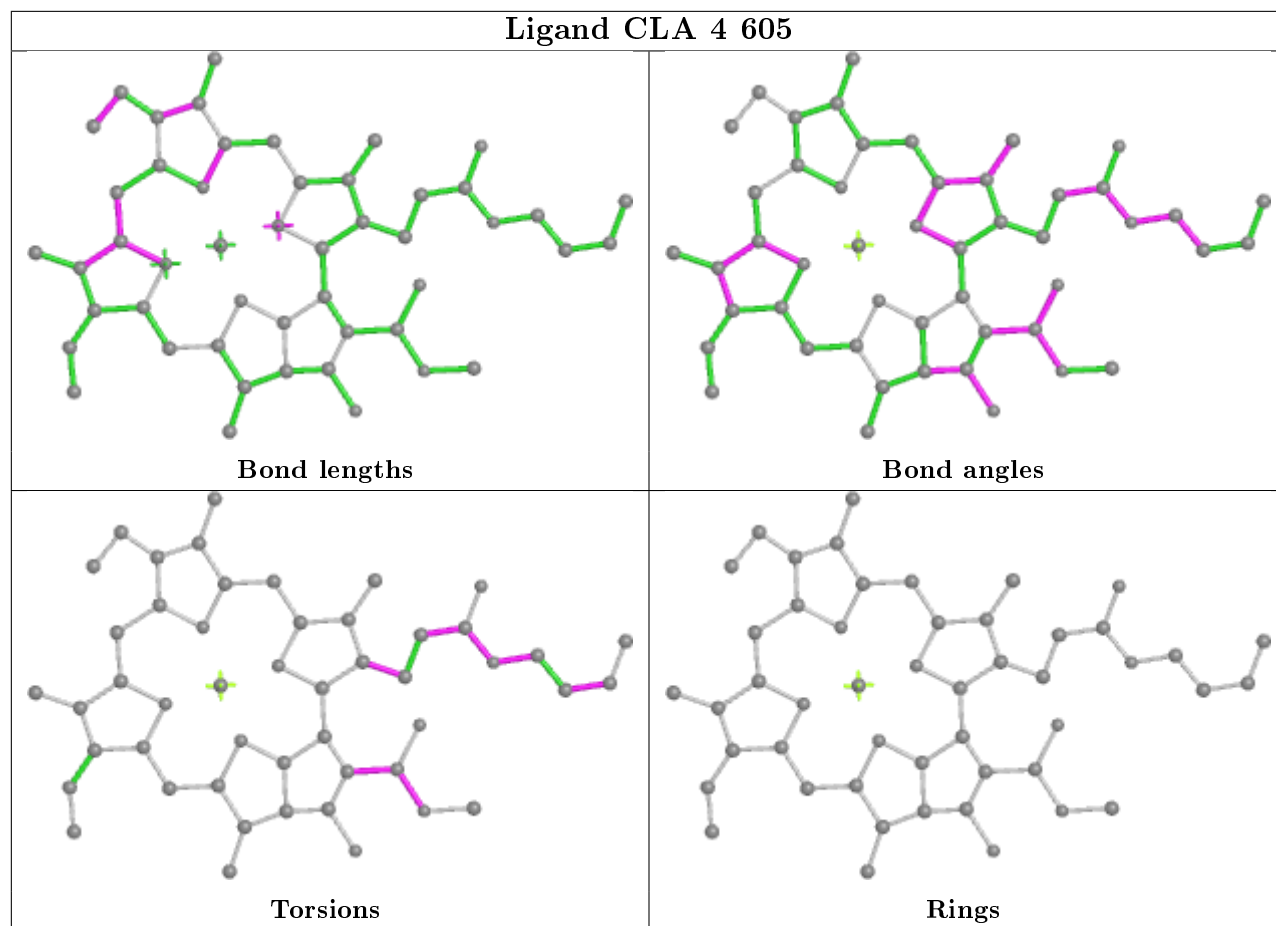


## Ligand CLA A 1129

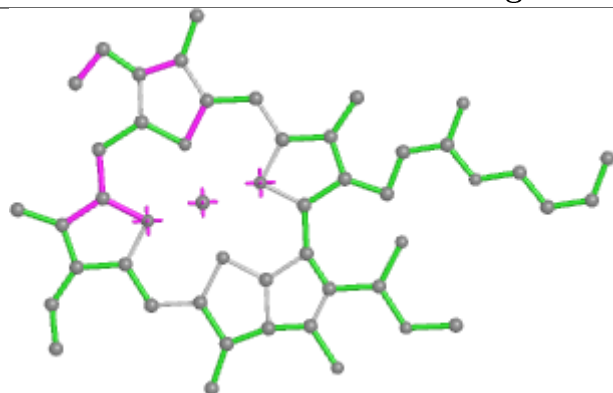




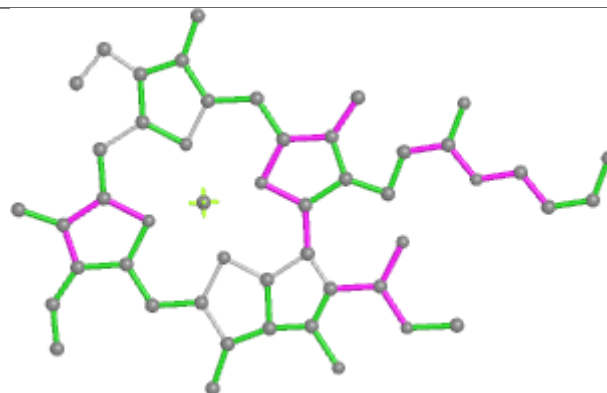




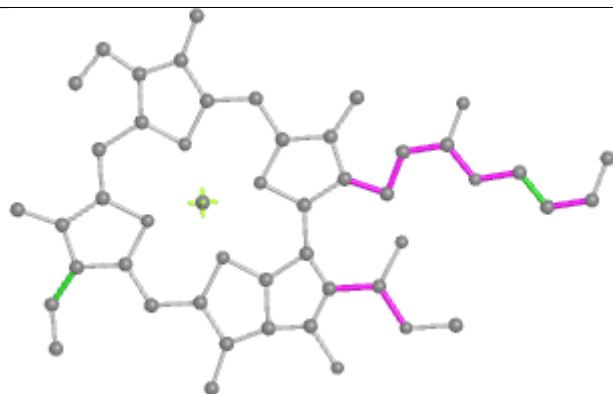
## Ligand CLA B 1224



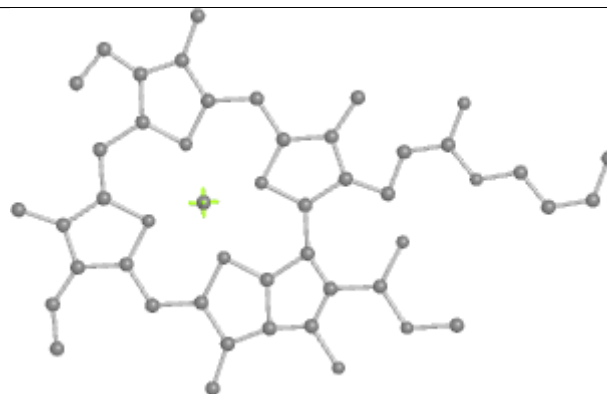
Bond lengths



Bond angles

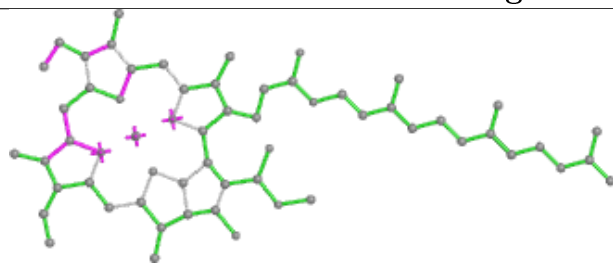


Torsions

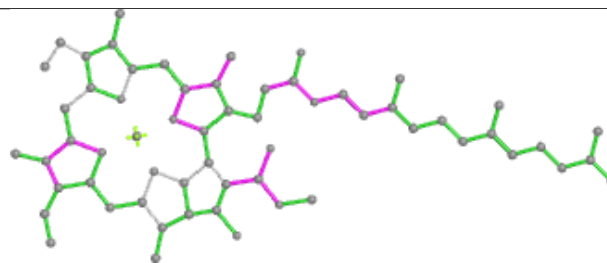


Rings

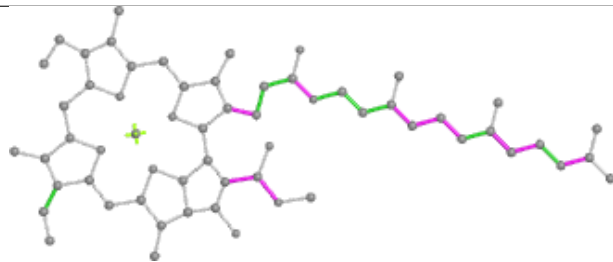
## Ligand CLA A 1104



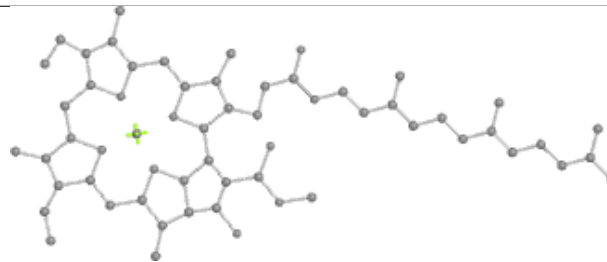
Bond lengths



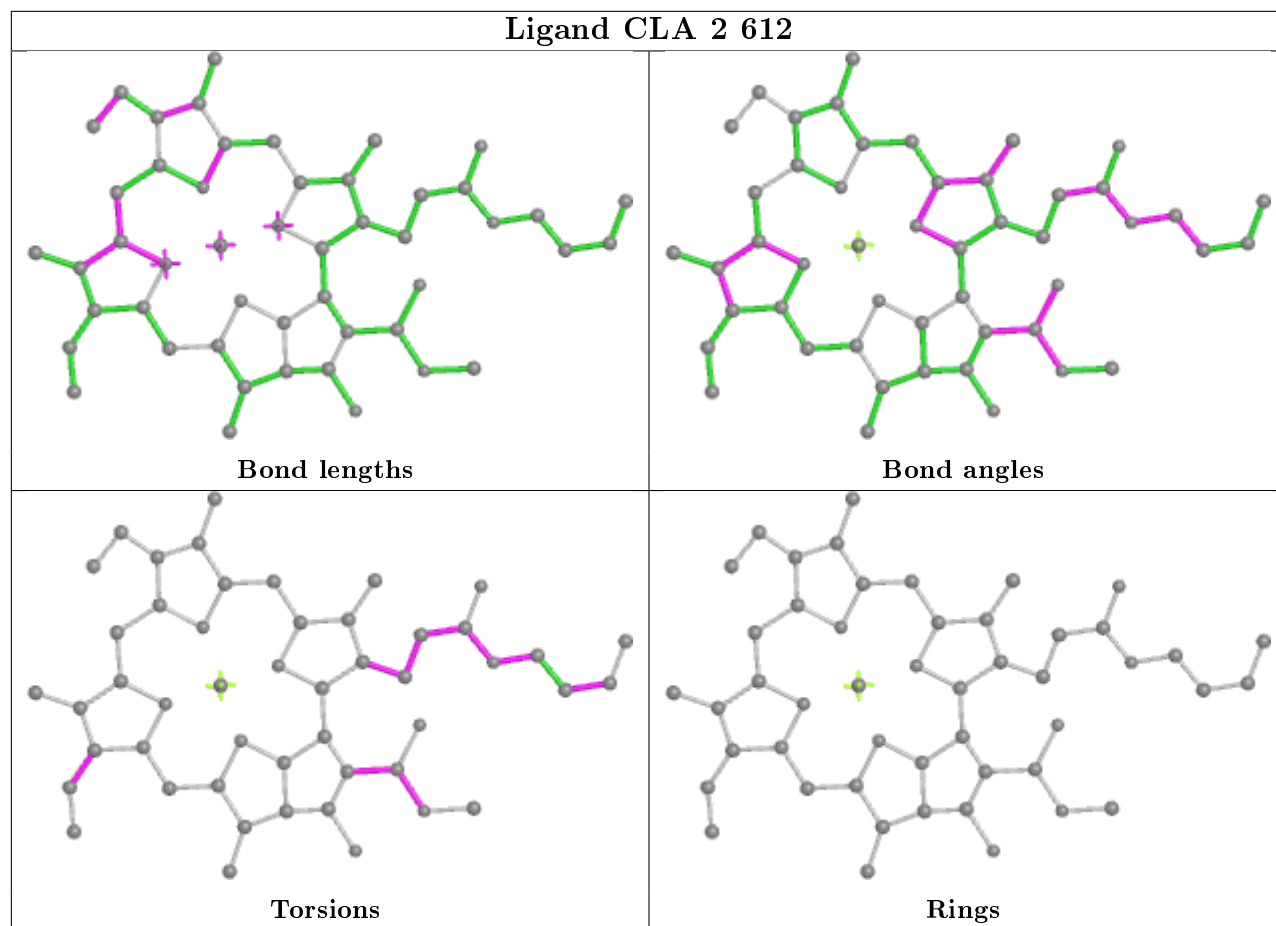
Bond angles

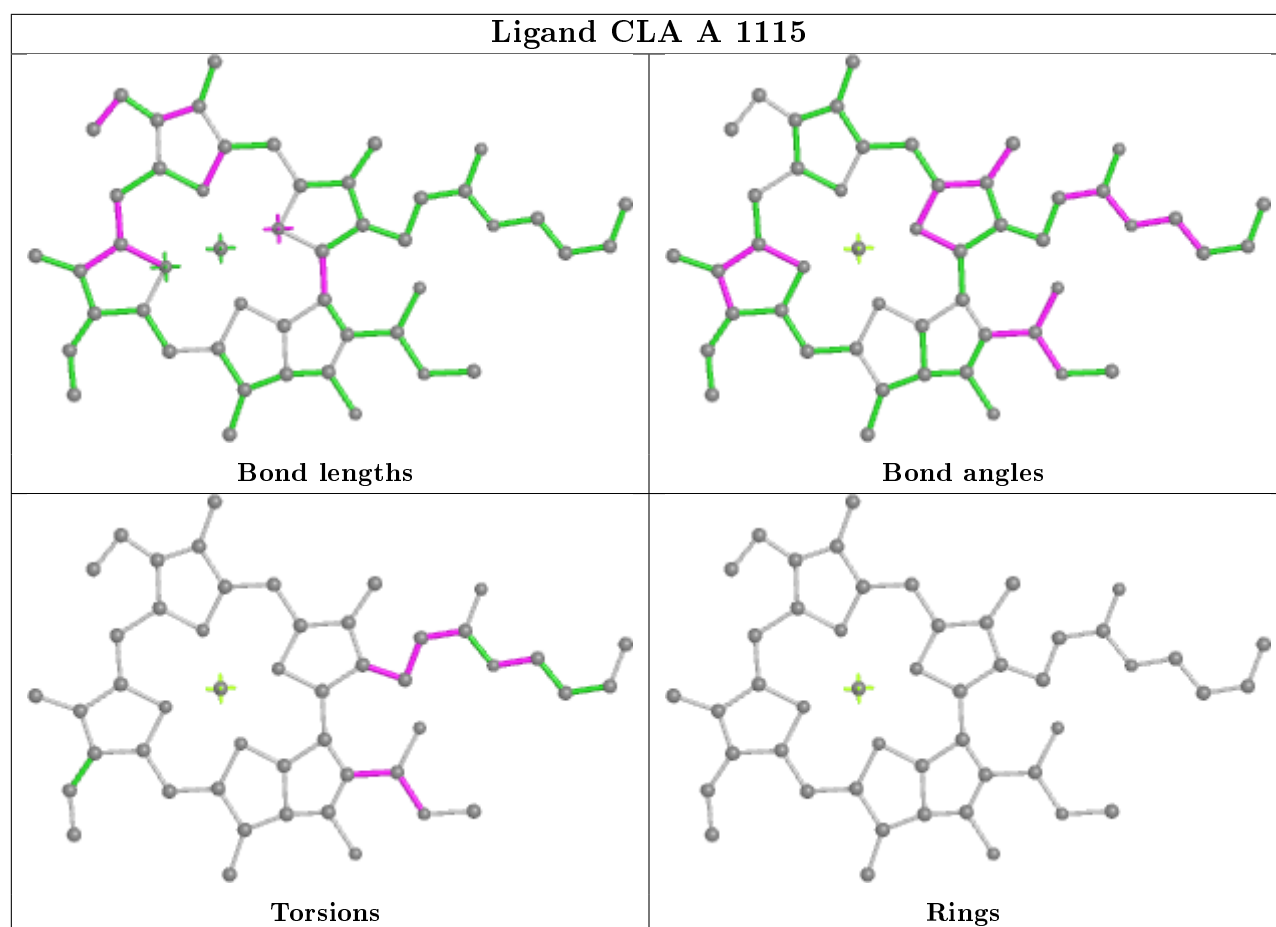


Torsions

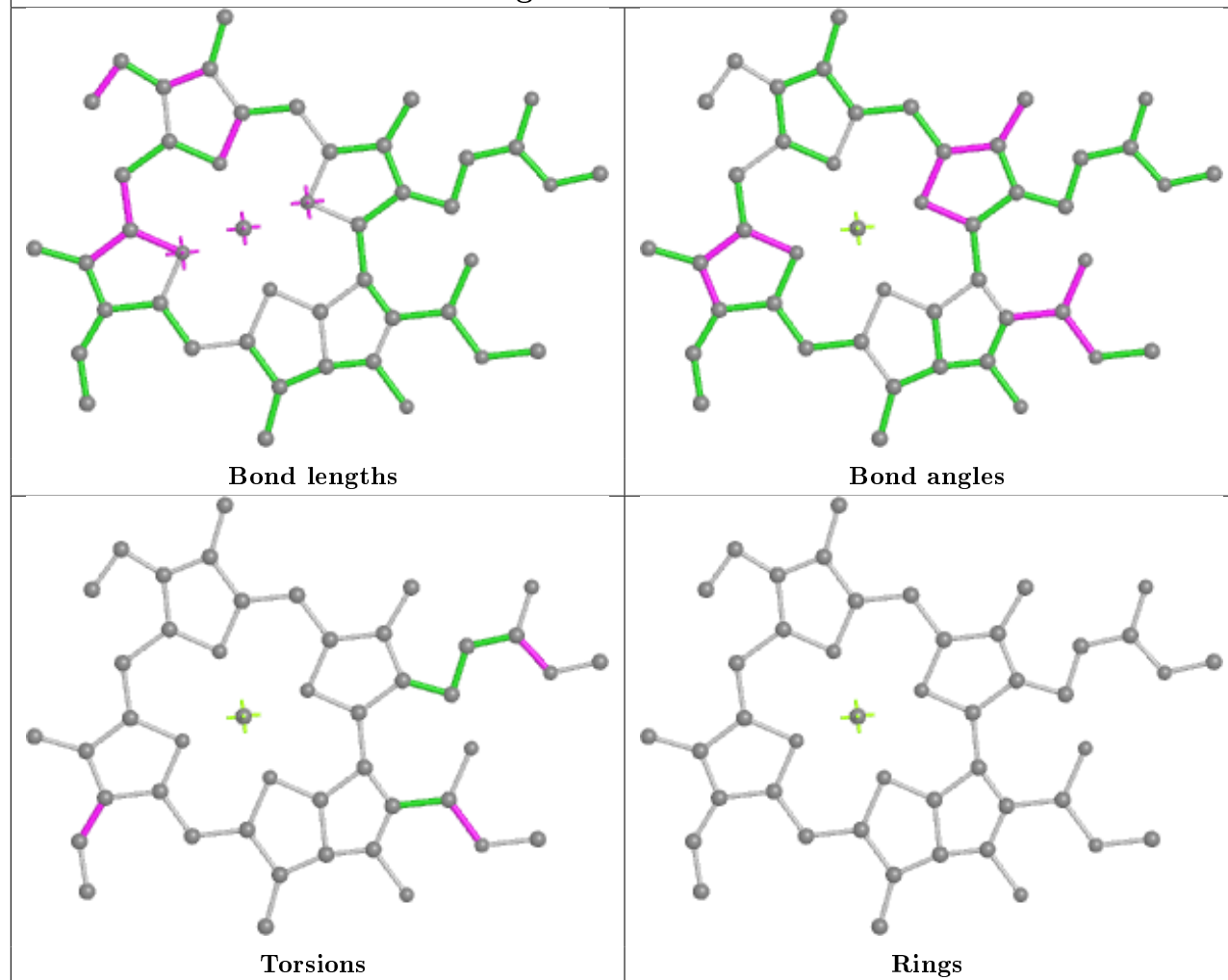


Rings

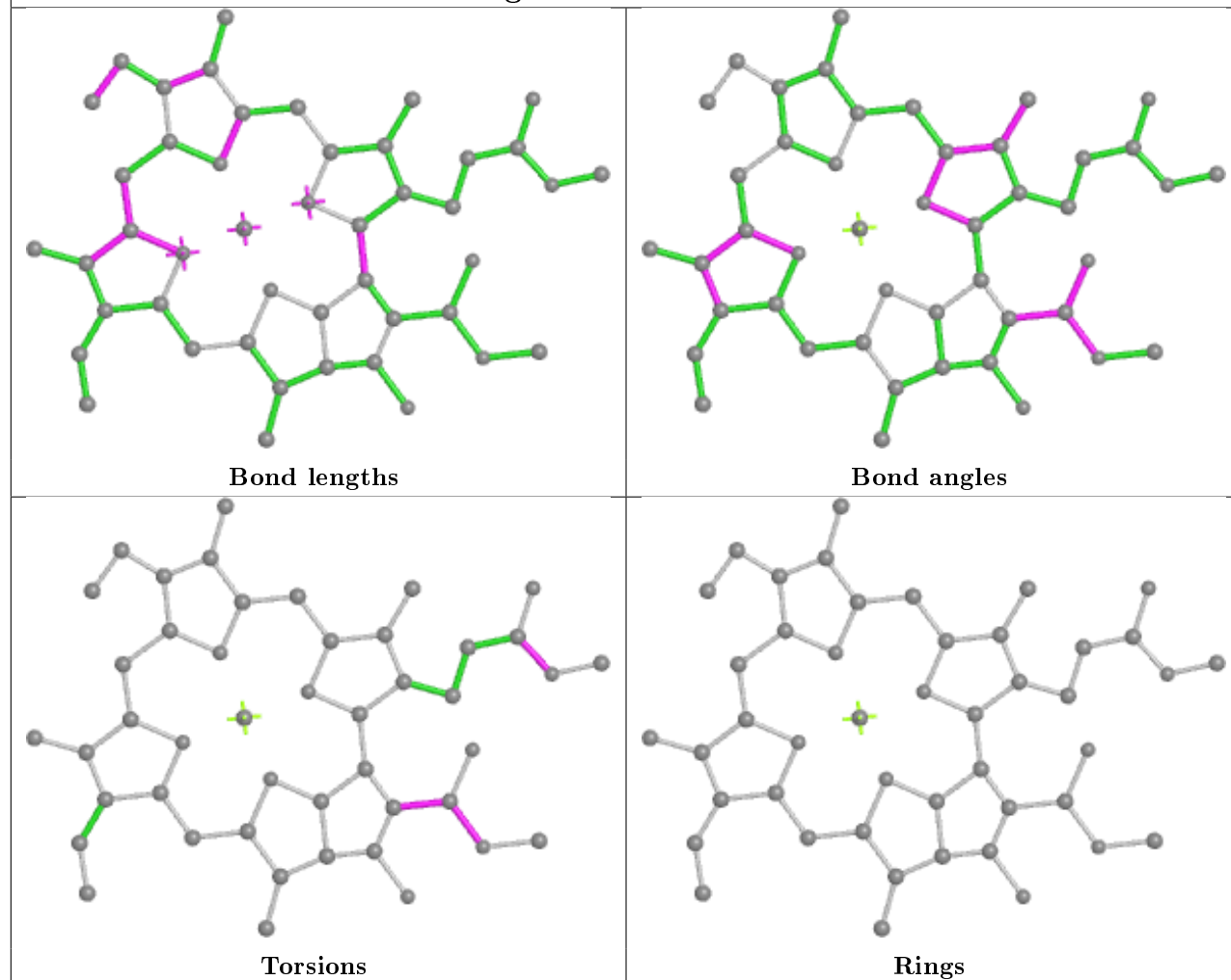


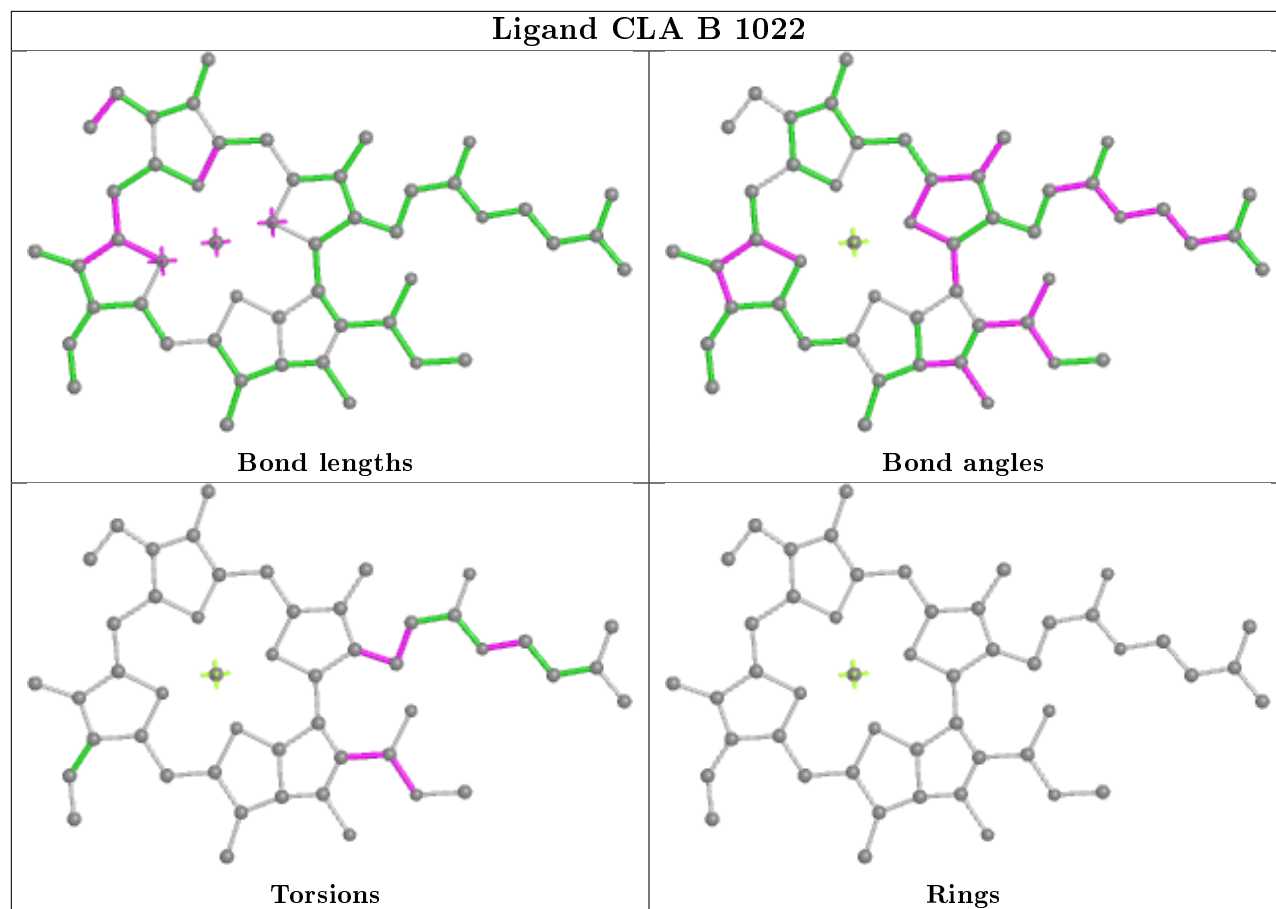


## Ligand CLA 3 605

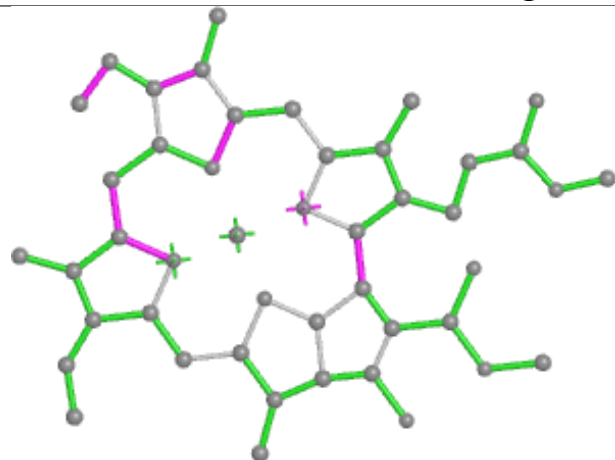


## Ligand CLA A 1114

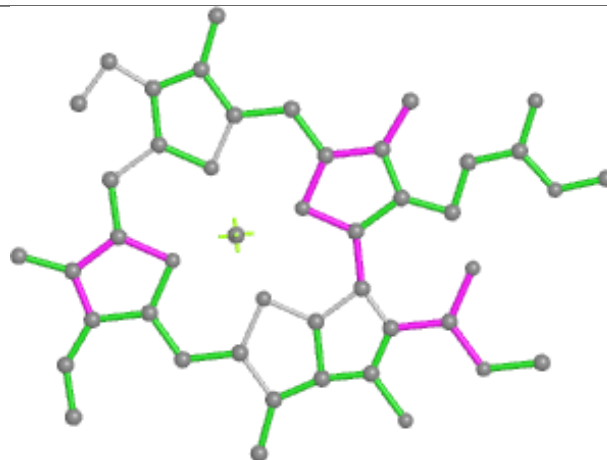




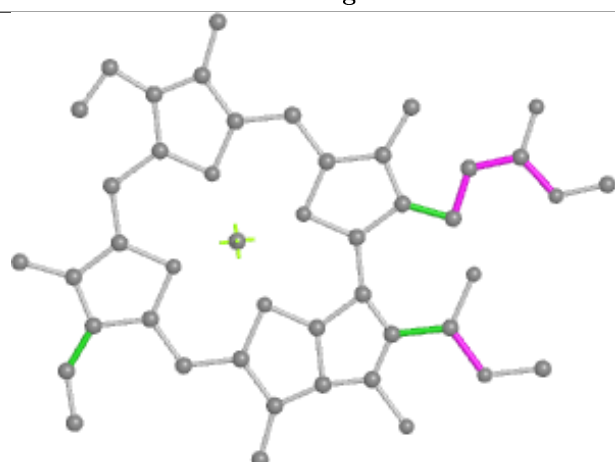
## Ligand CLA 3 615



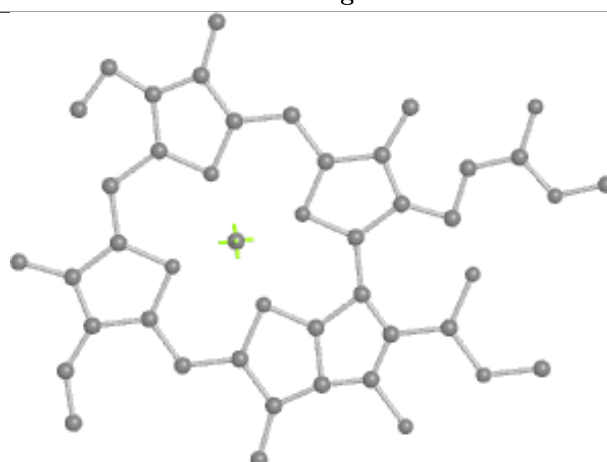
Bond lengths



Bond angles

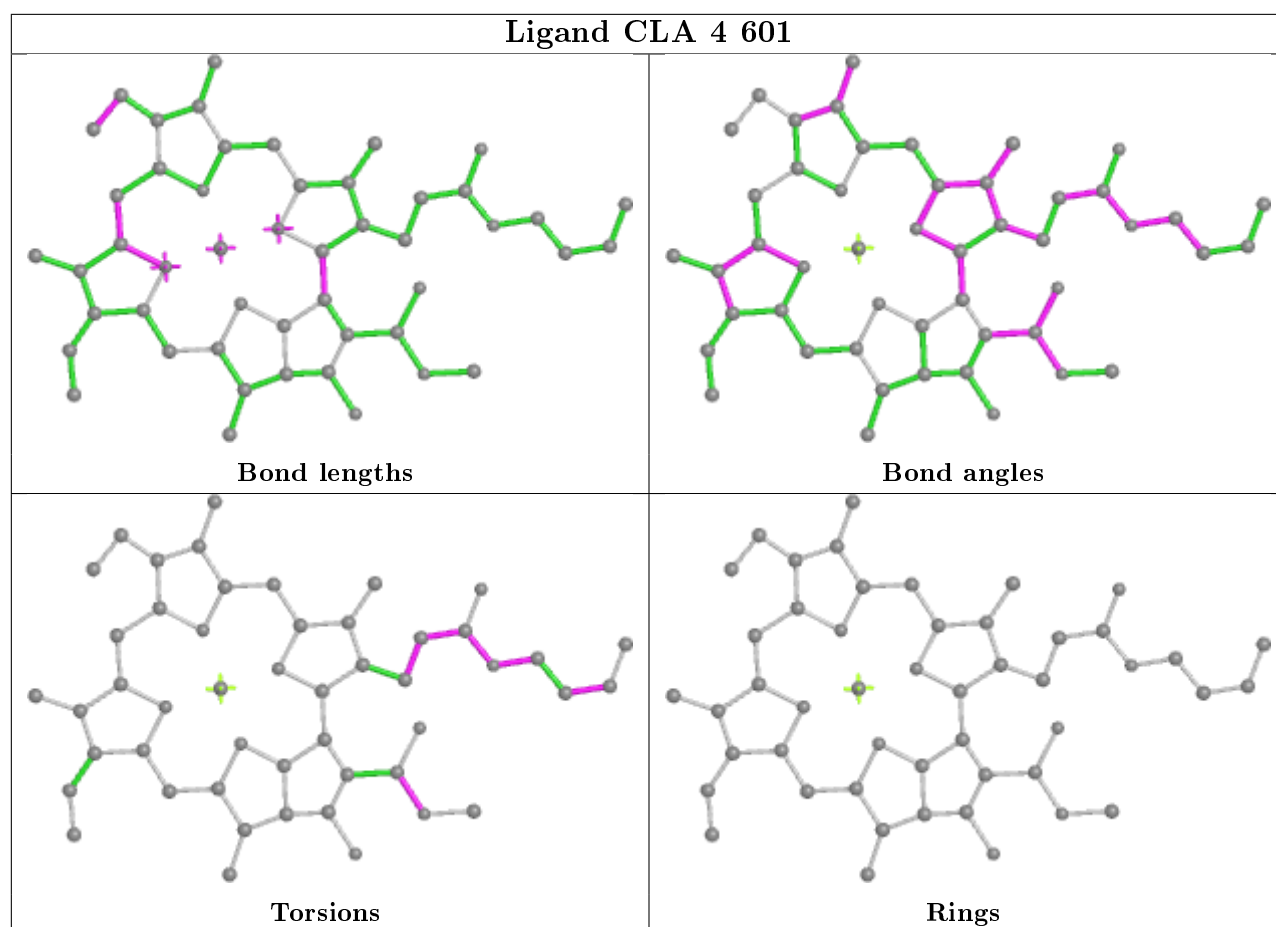


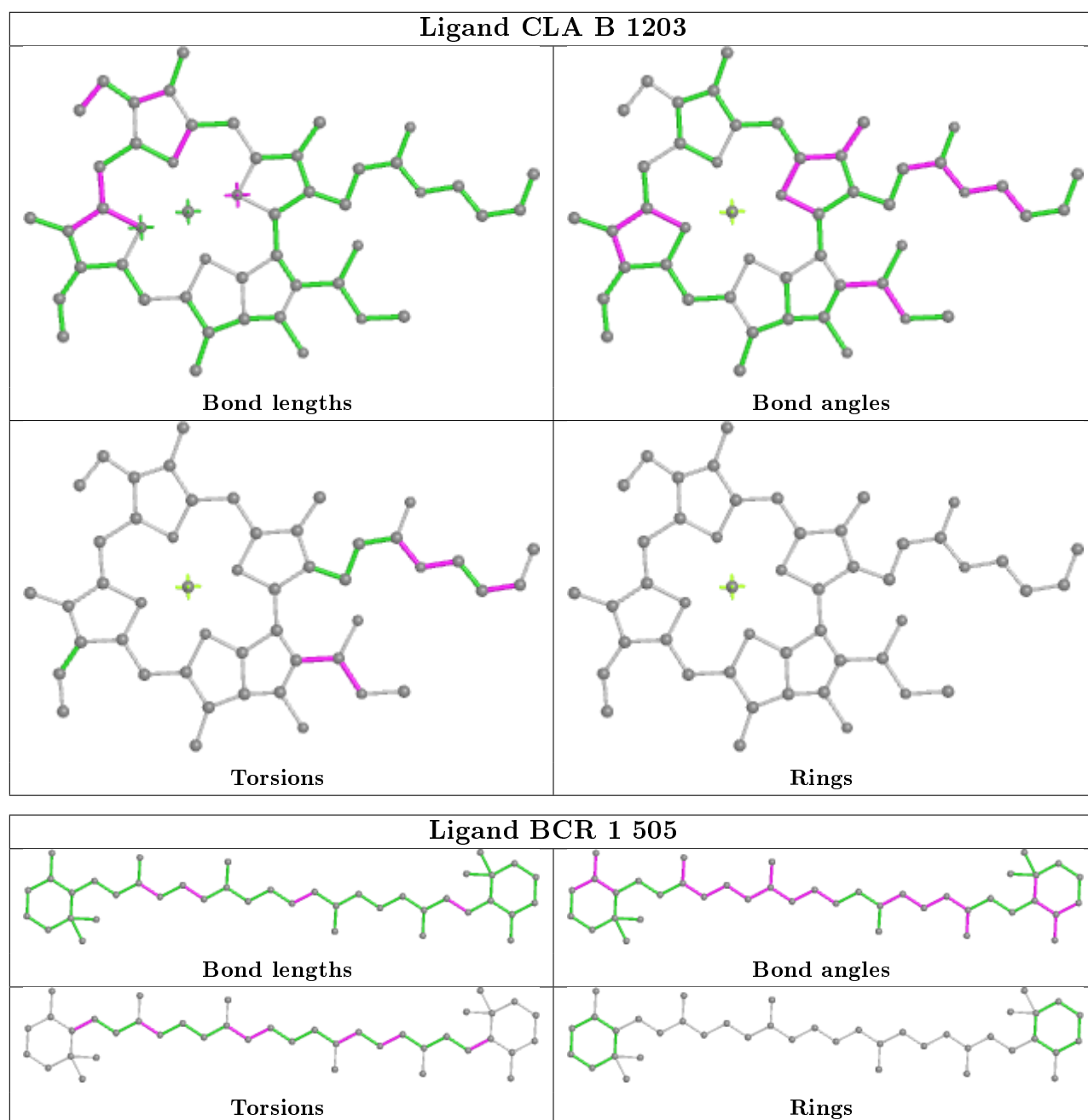
Torsions



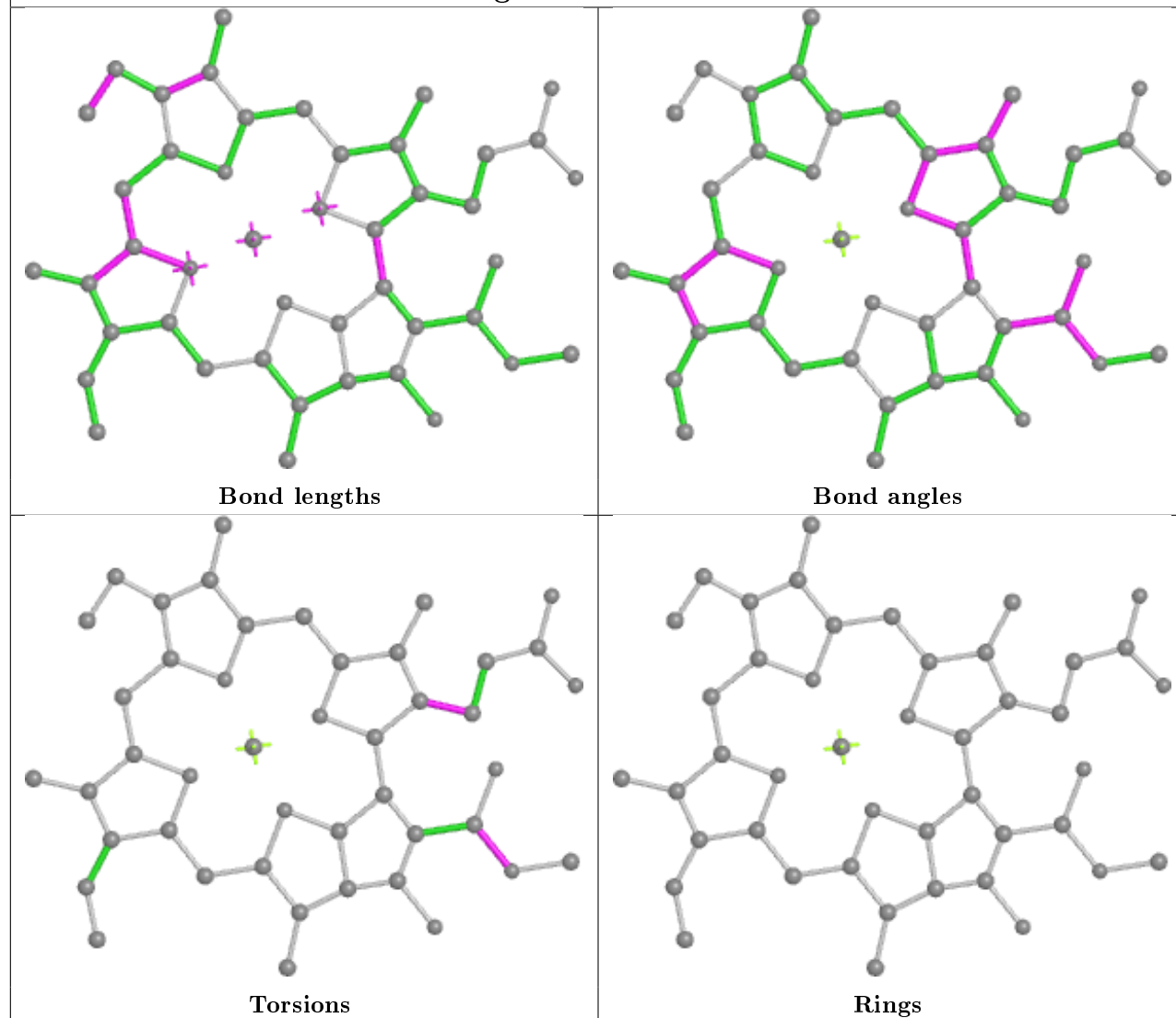
Rings



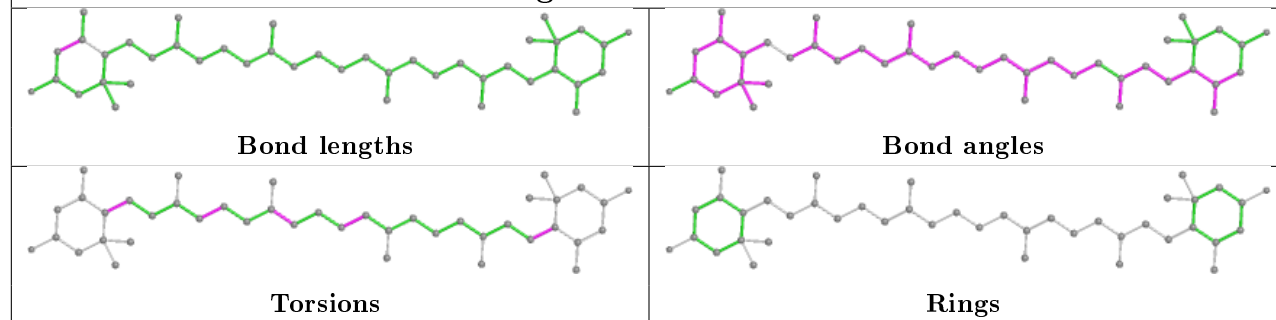




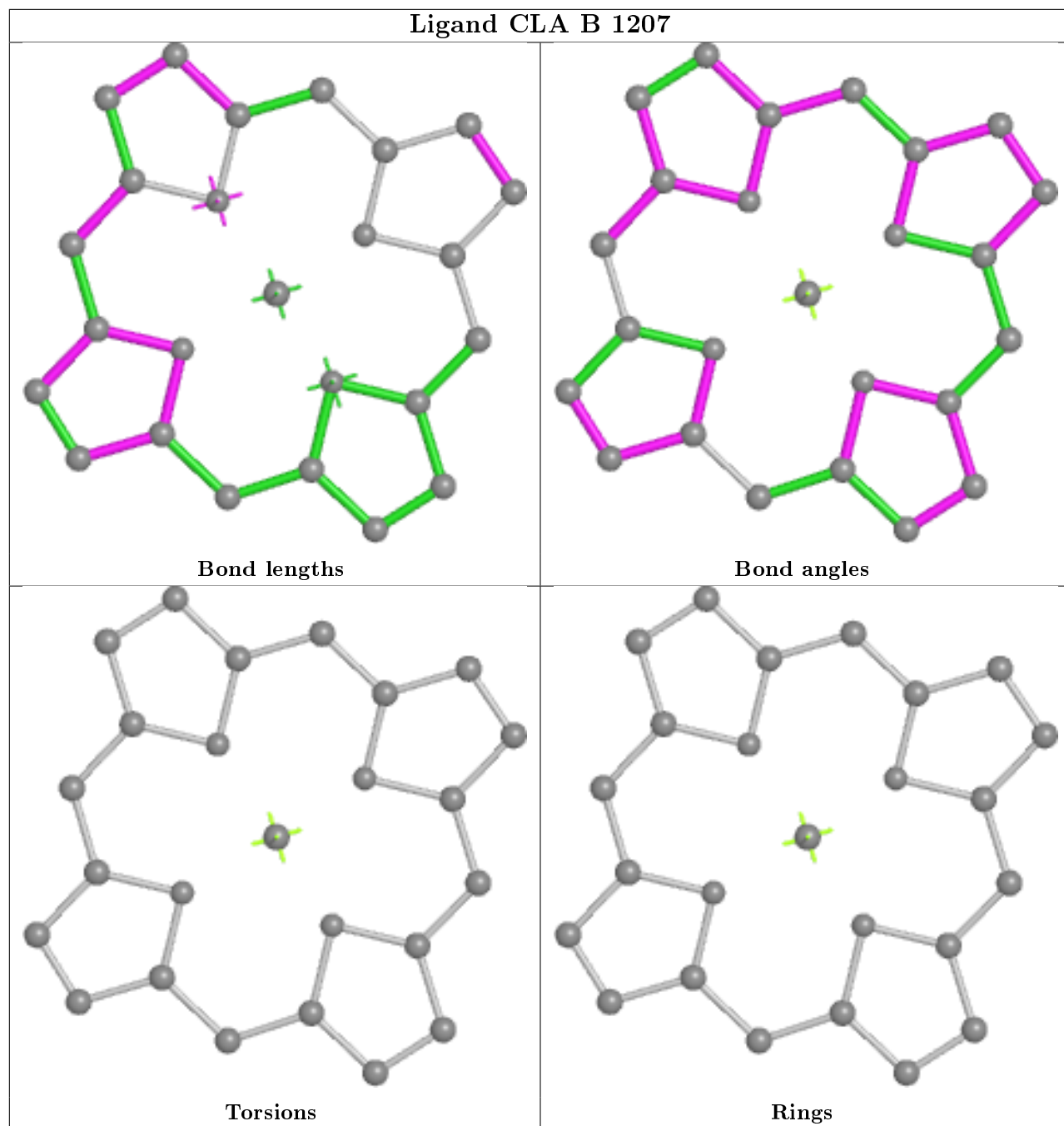
## Ligand CLA 1 613



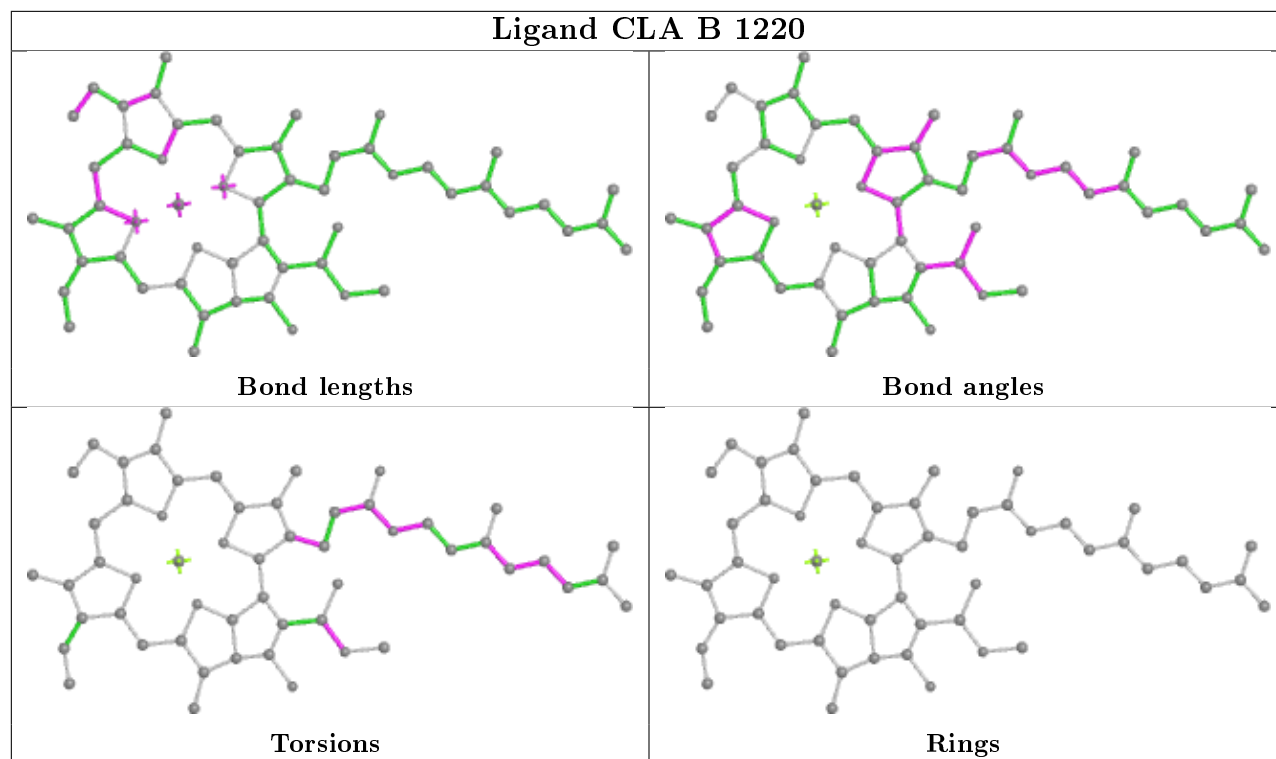
## Ligand LUT 1 501



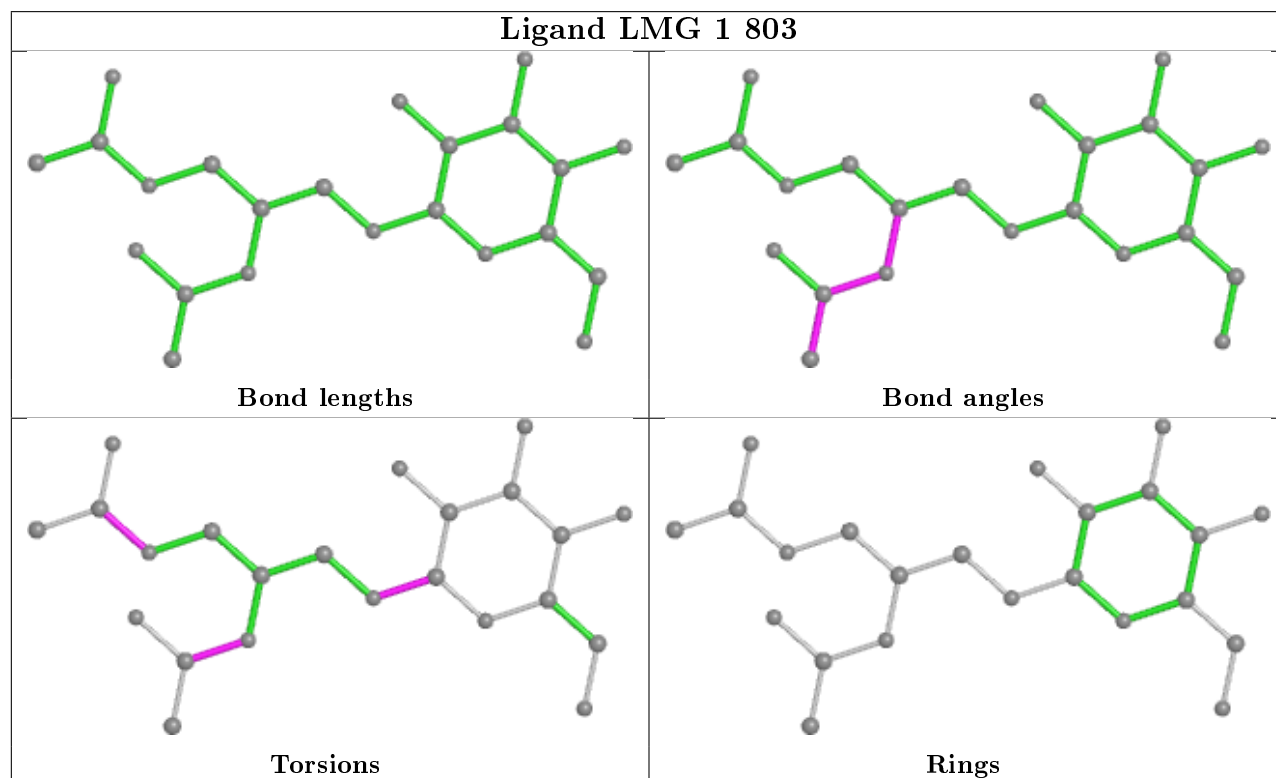
## Ligand CLA B 1207

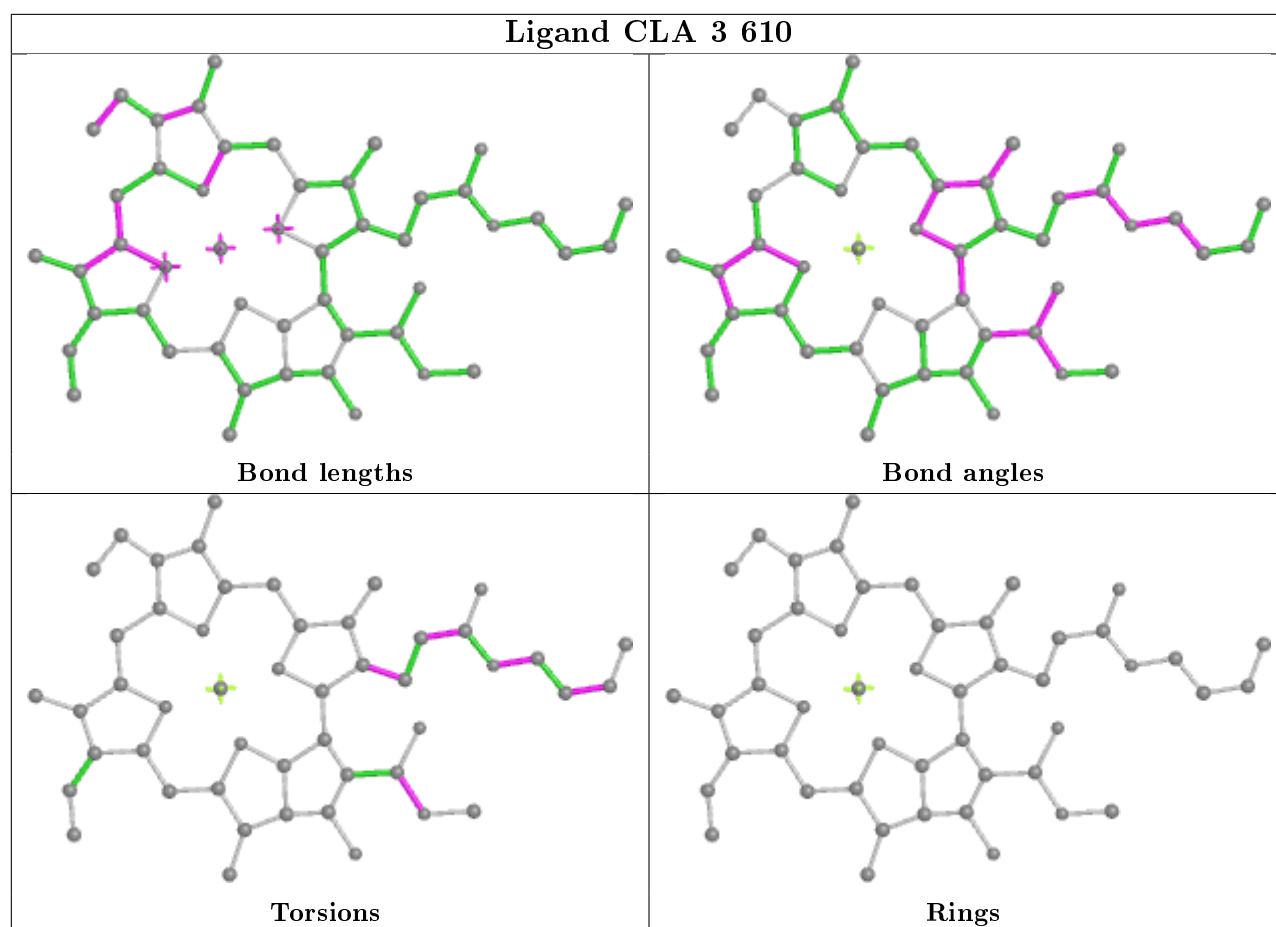


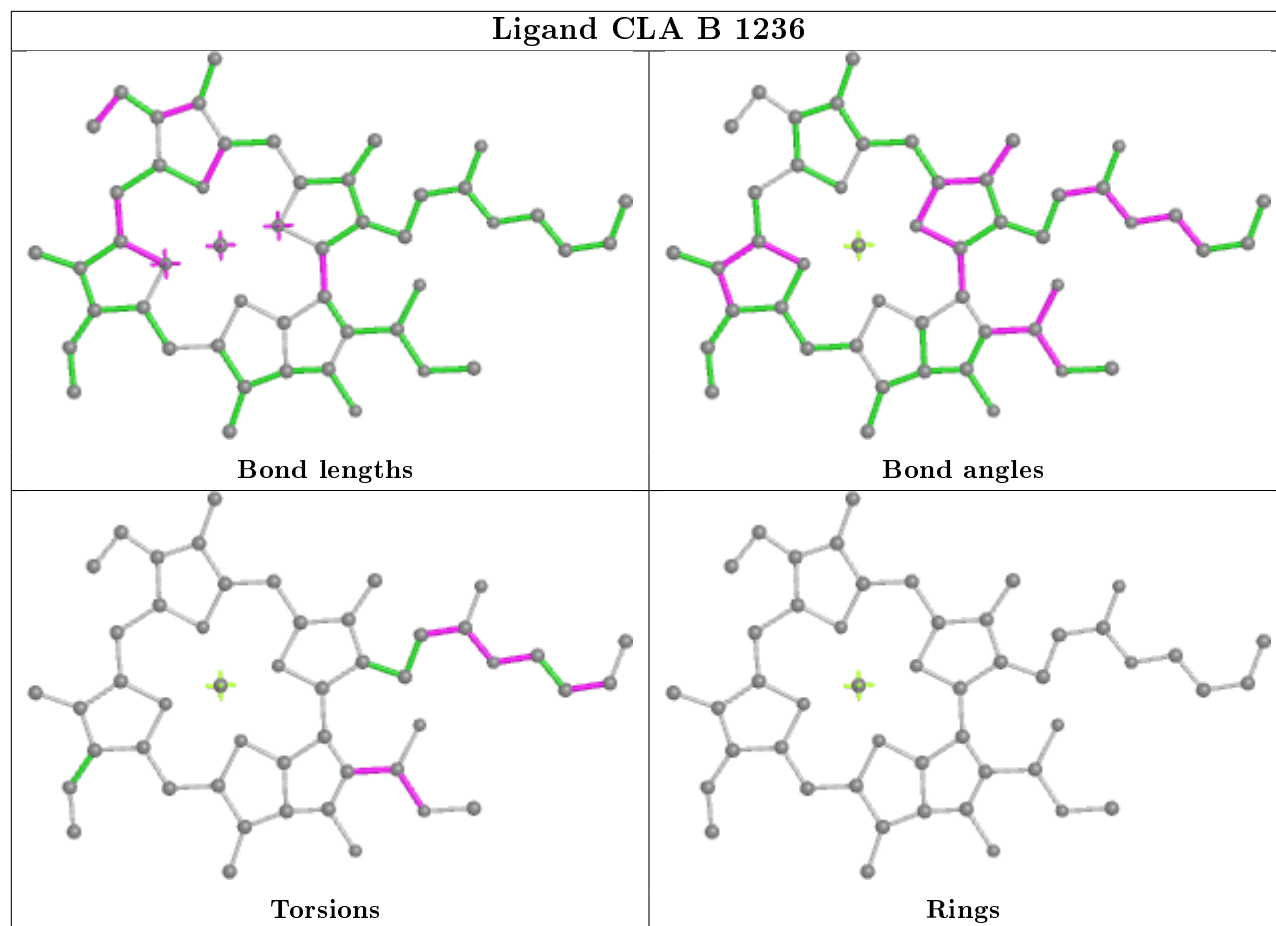
## Ligand CLA B 1220



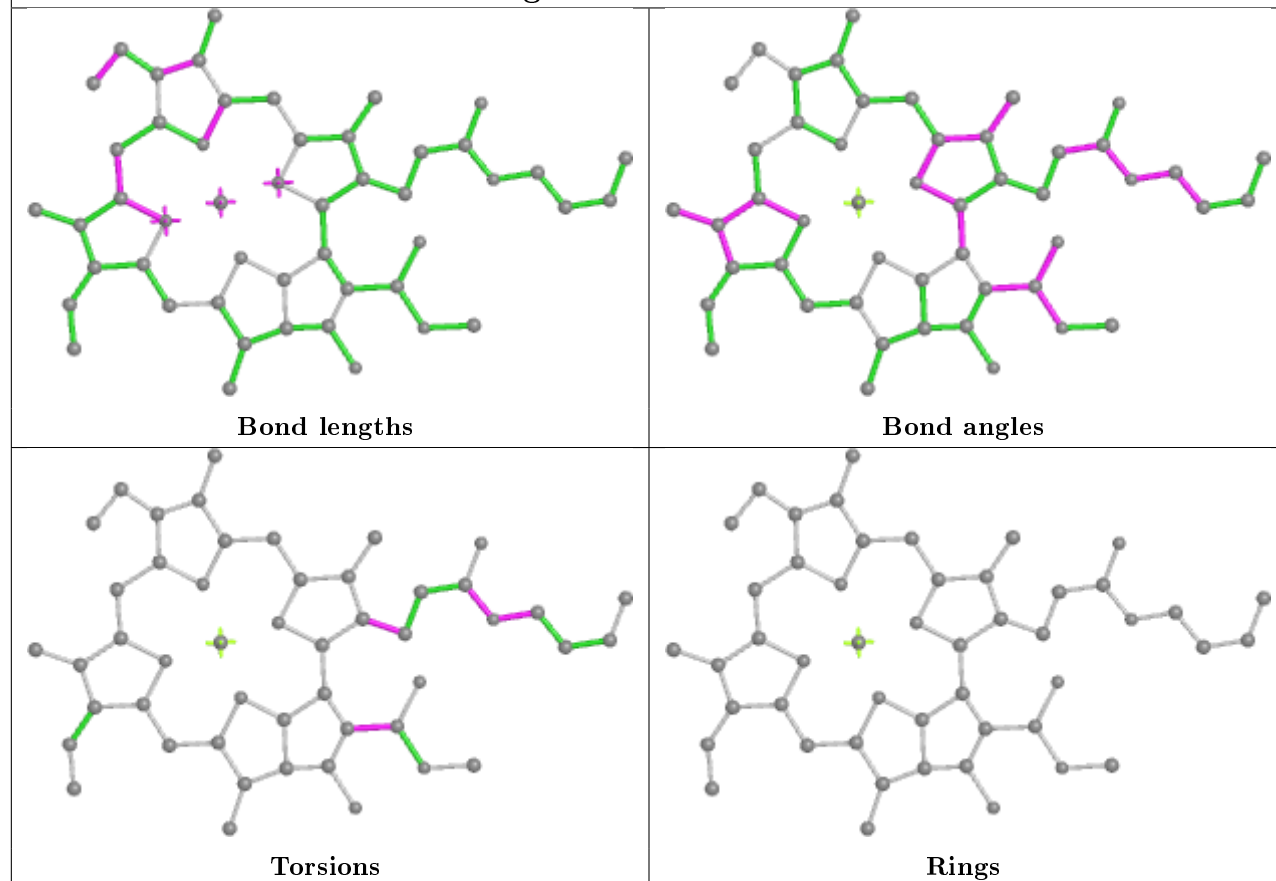
## Ligand LMG 1 803



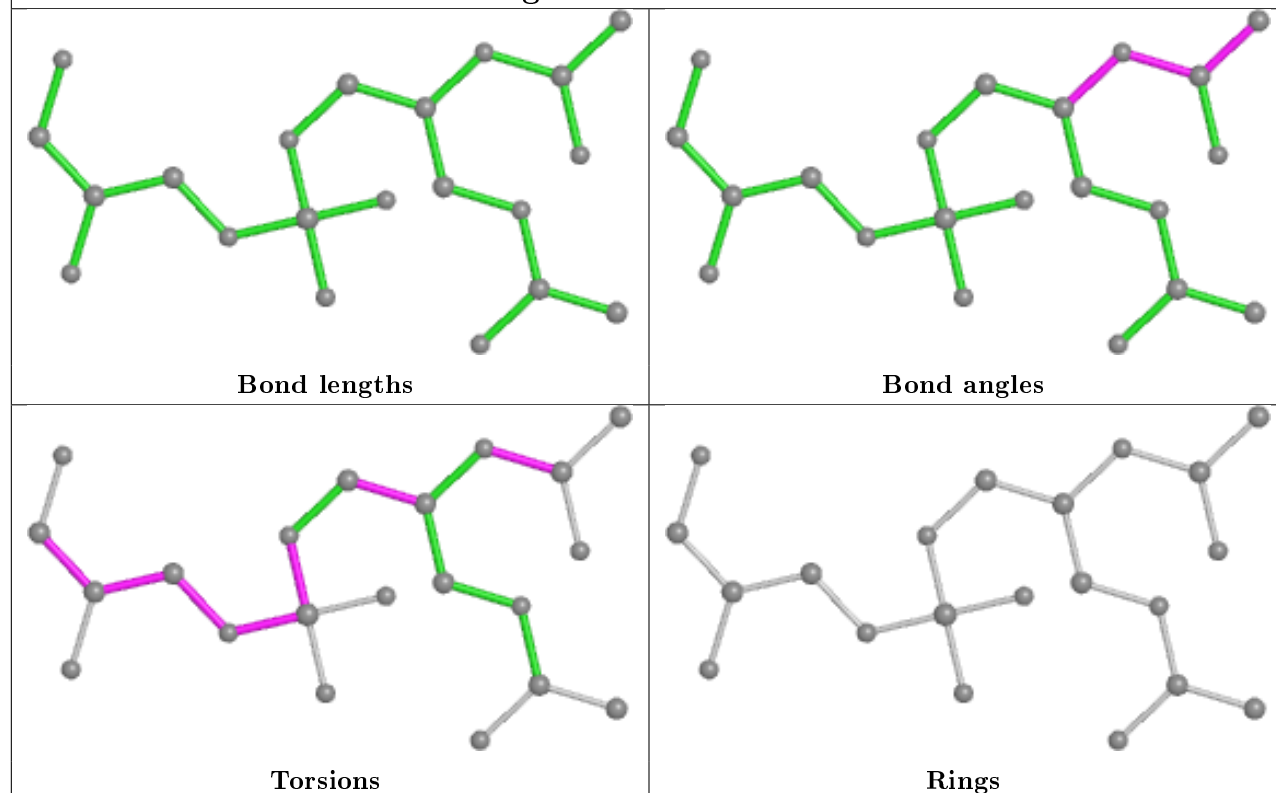




## Ligand CLA A 1111

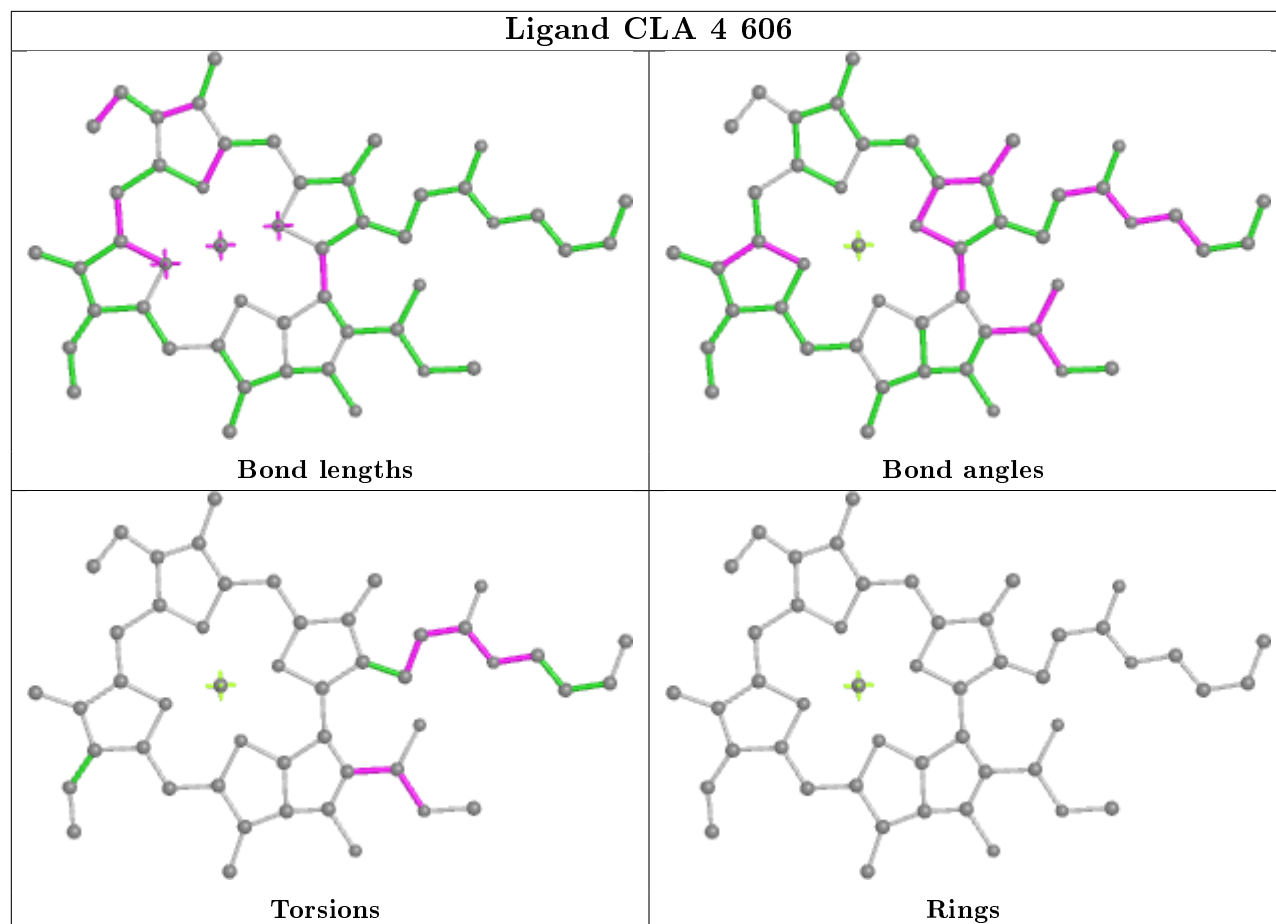


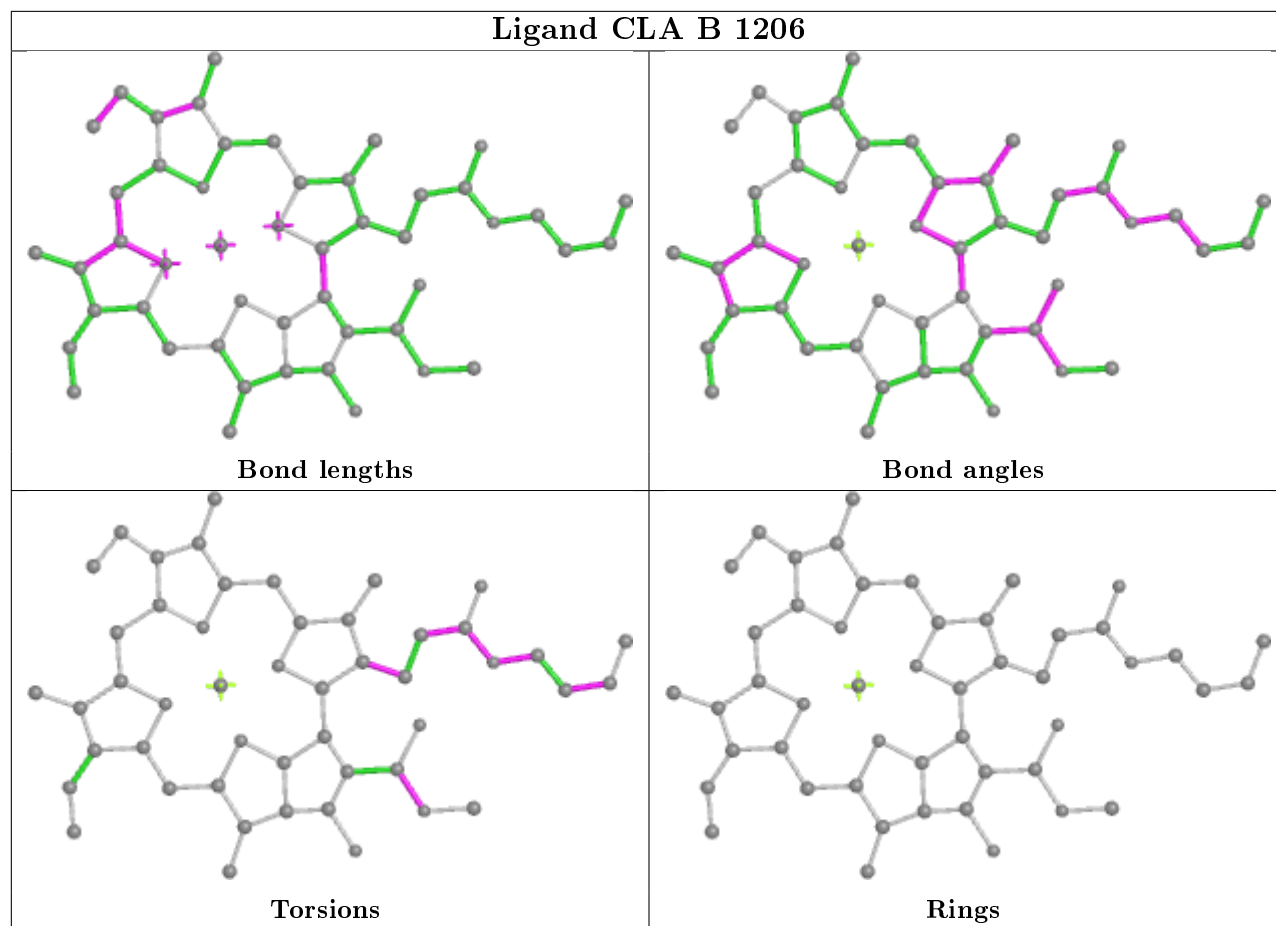
## Ligand LHG B 5001



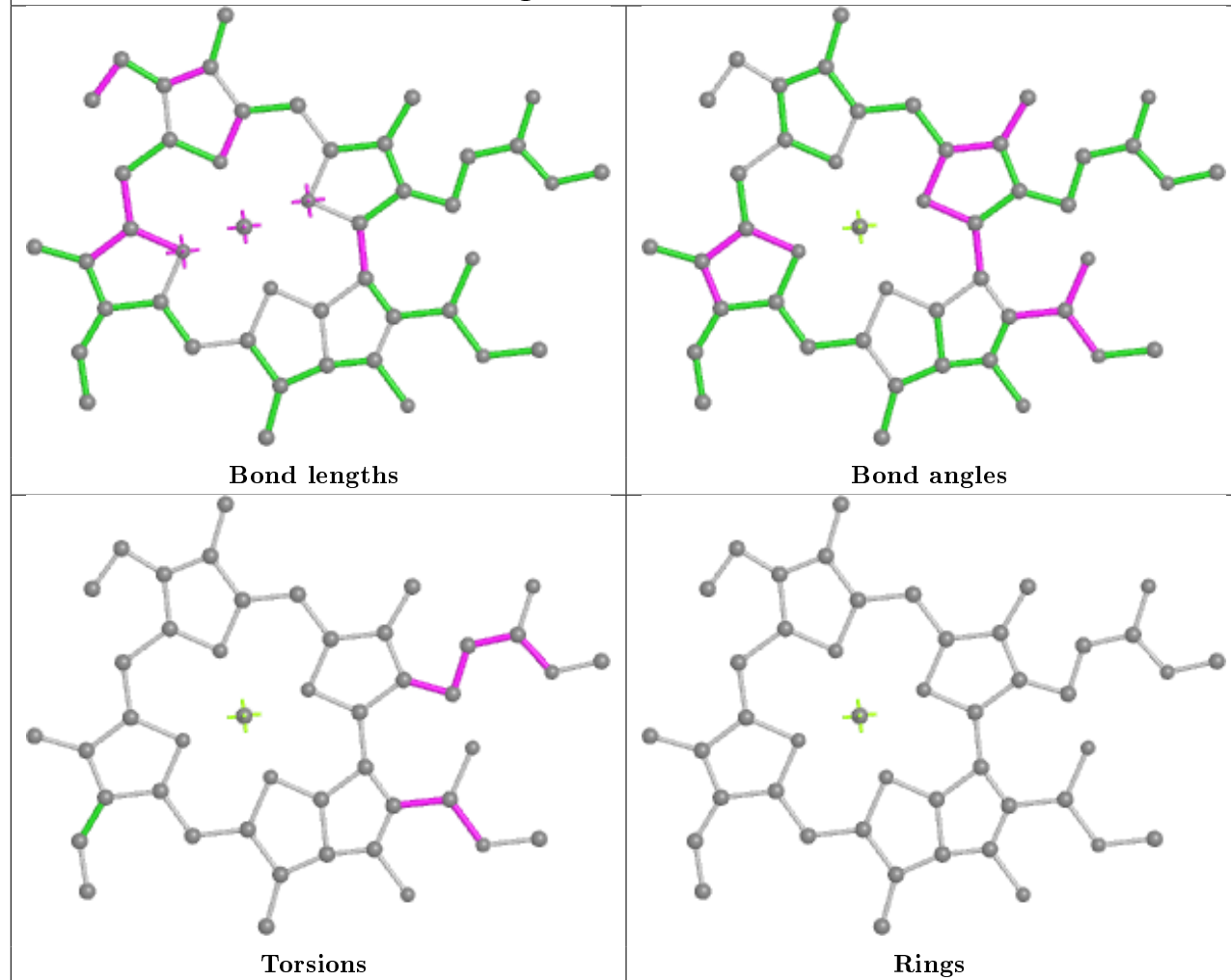


## Ligand CLA 4 606

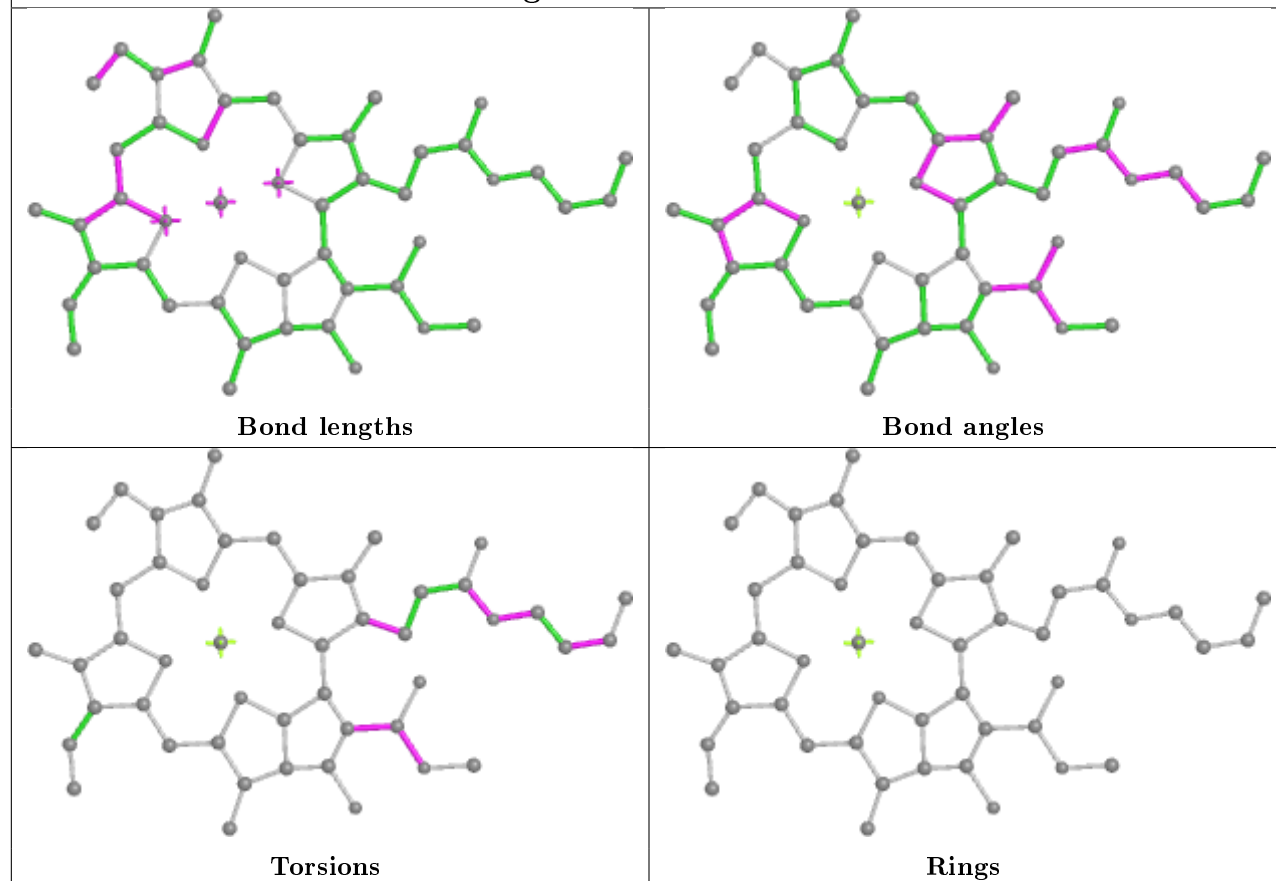




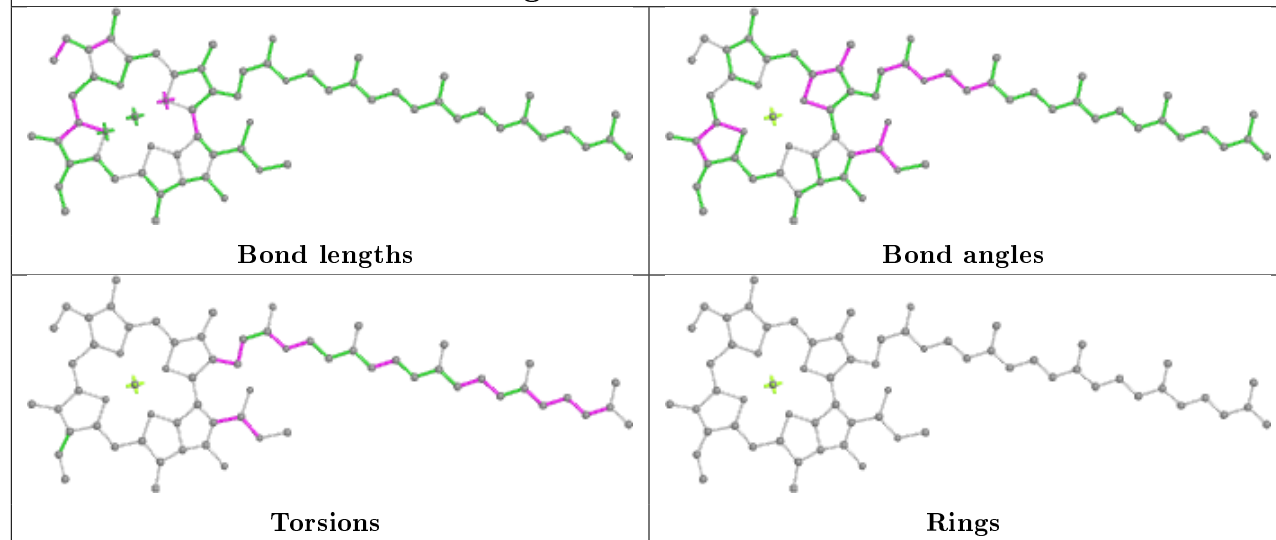
## Ligand CLA 1 602



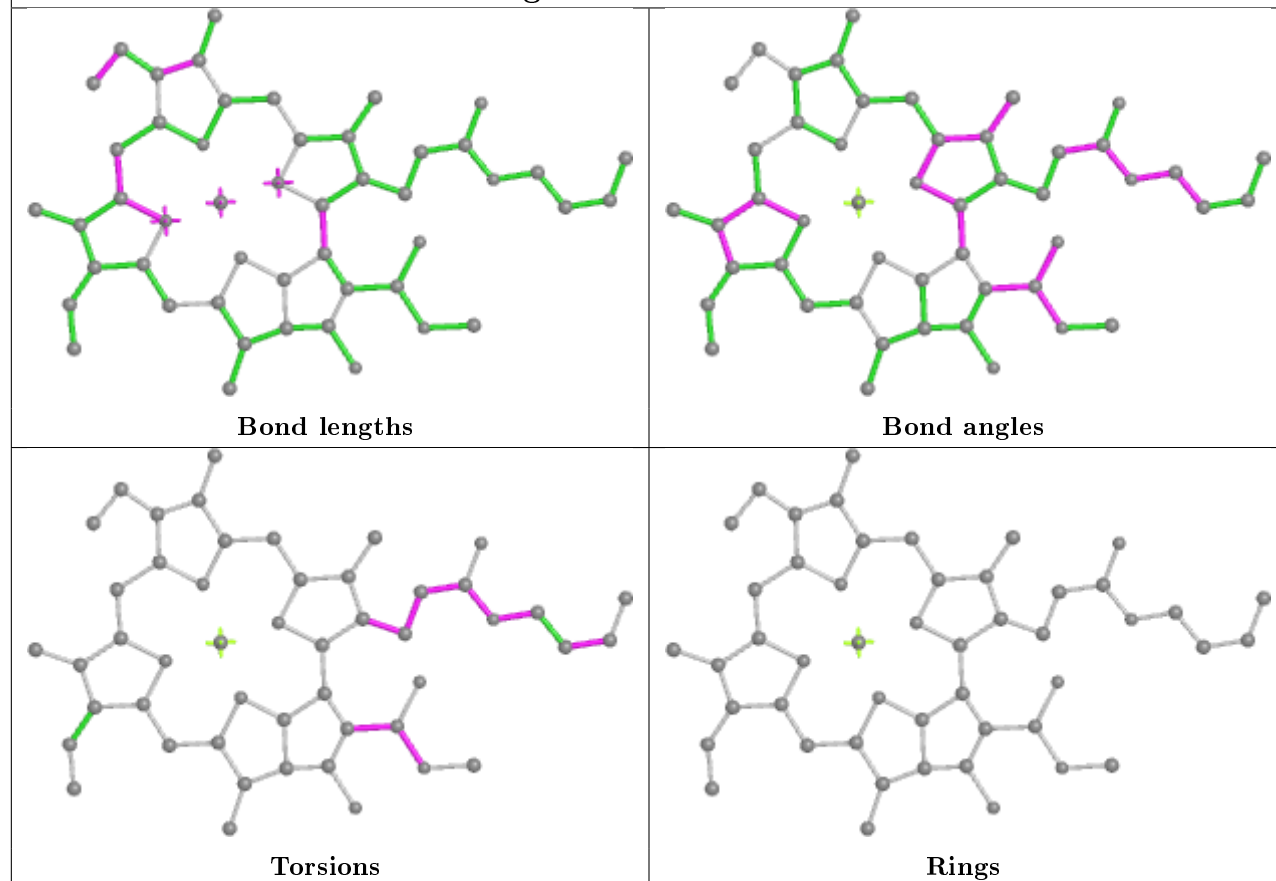
## Ligand CLA B 1226



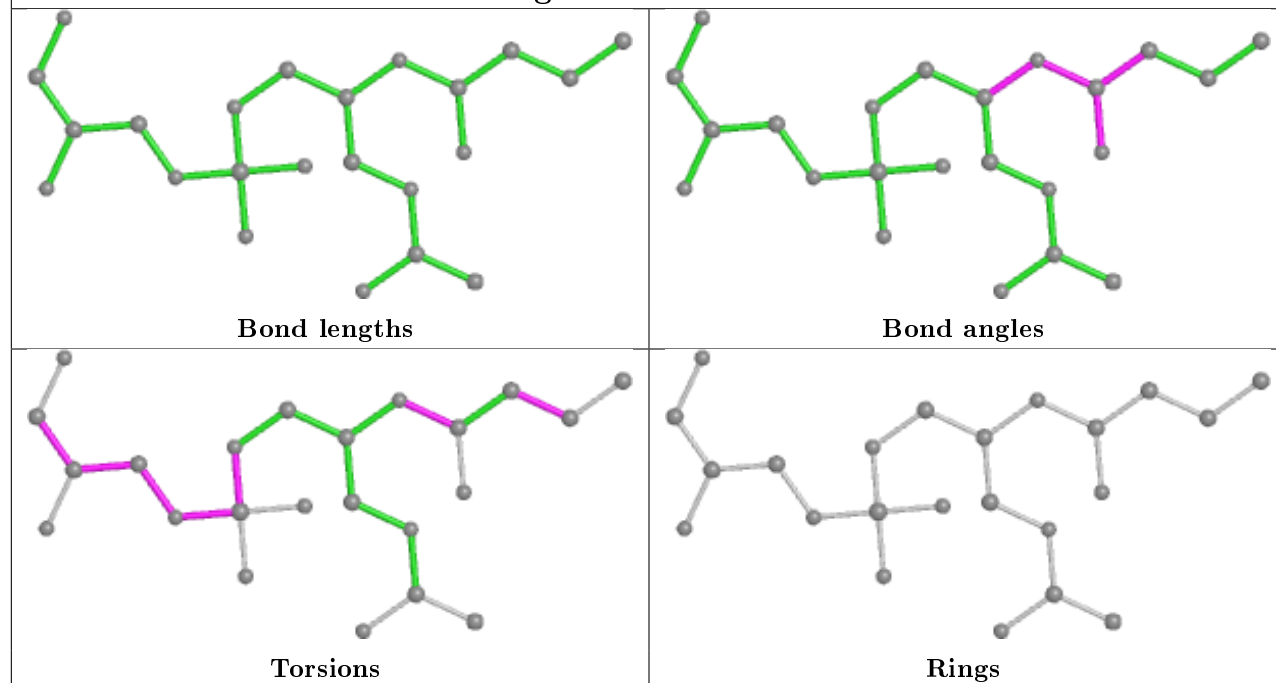
## Ligand CLA B 1239



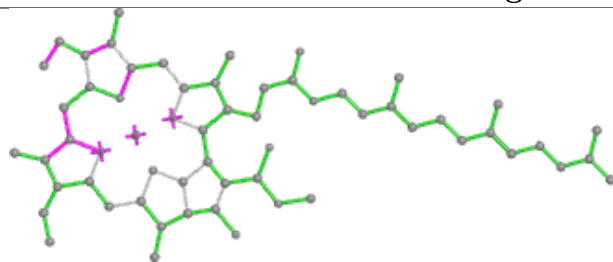
## Ligand CLA B 1216



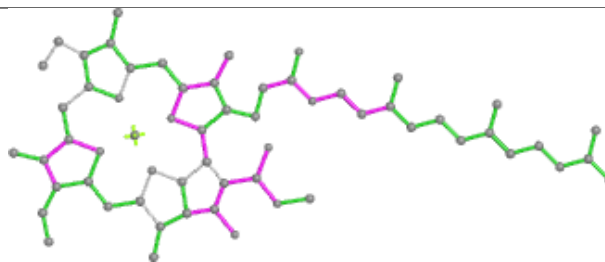
## Ligand LHG 1 801



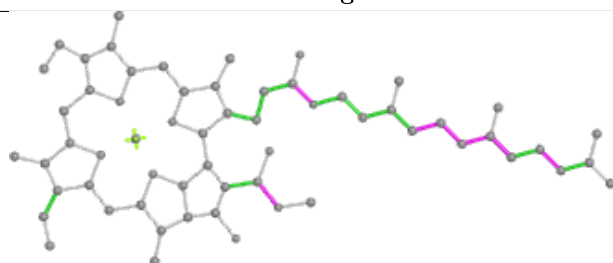
## Ligand CLA A 1012



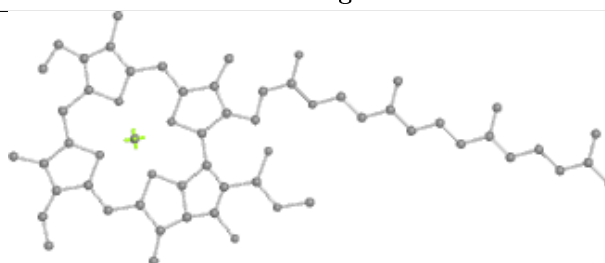
Bond lengths



Bond angles

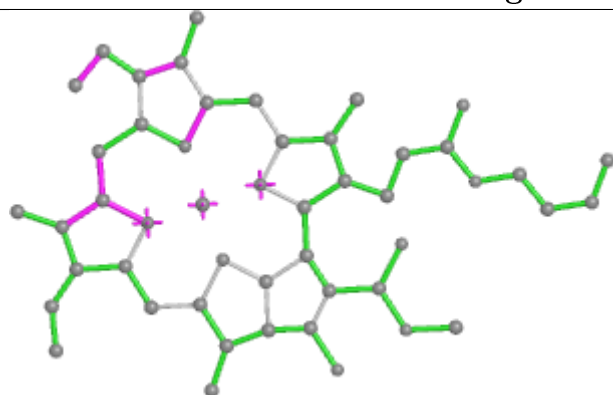


Torsions

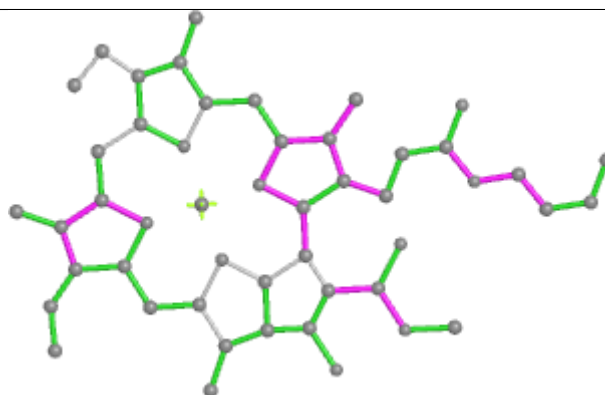


Rings

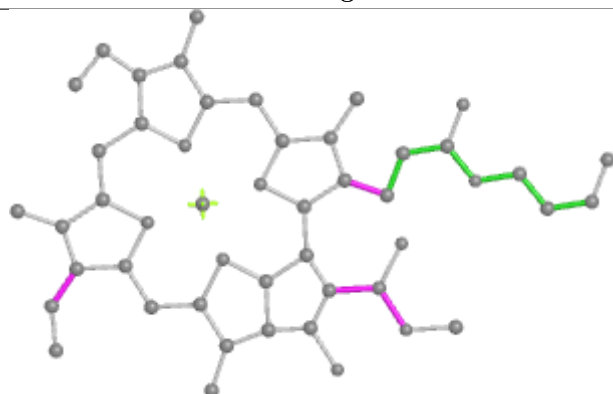
## Ligand CLA A 1110



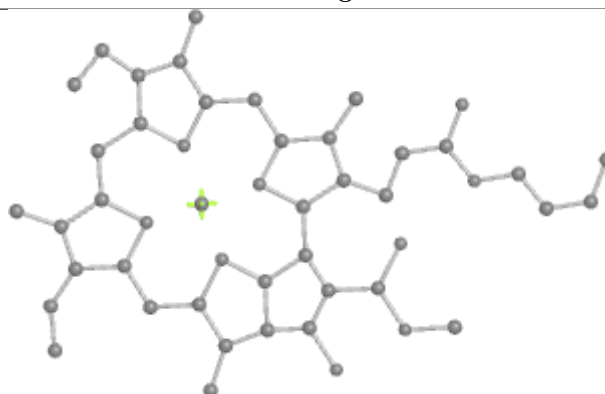
Bond lengths



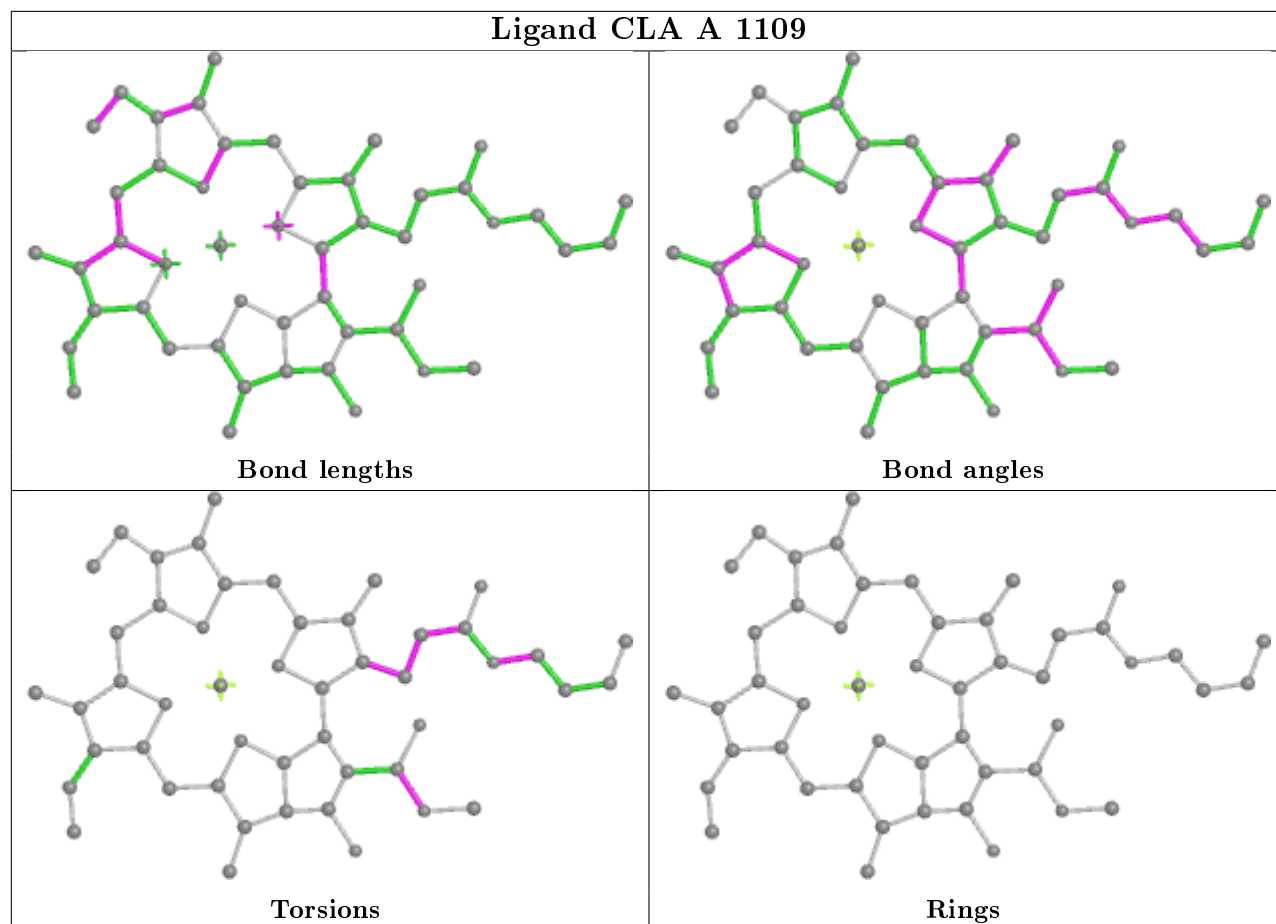
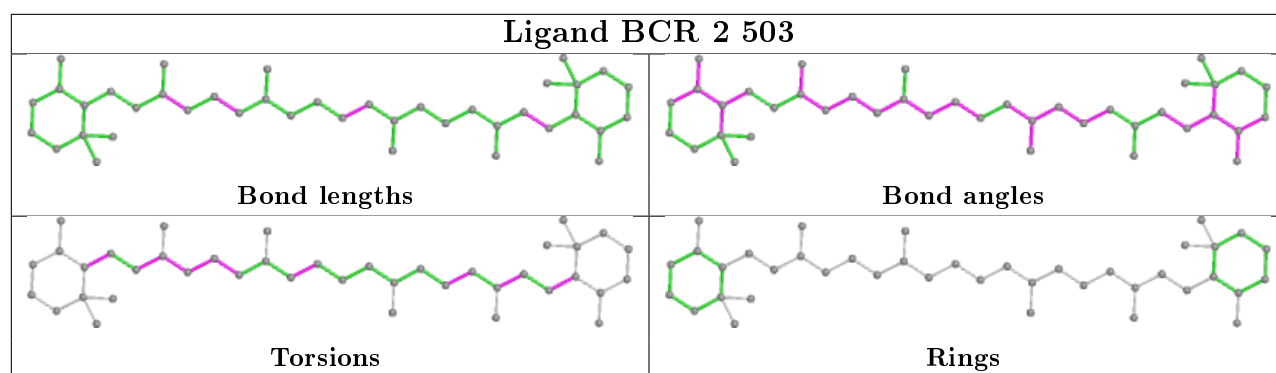
Bond angles

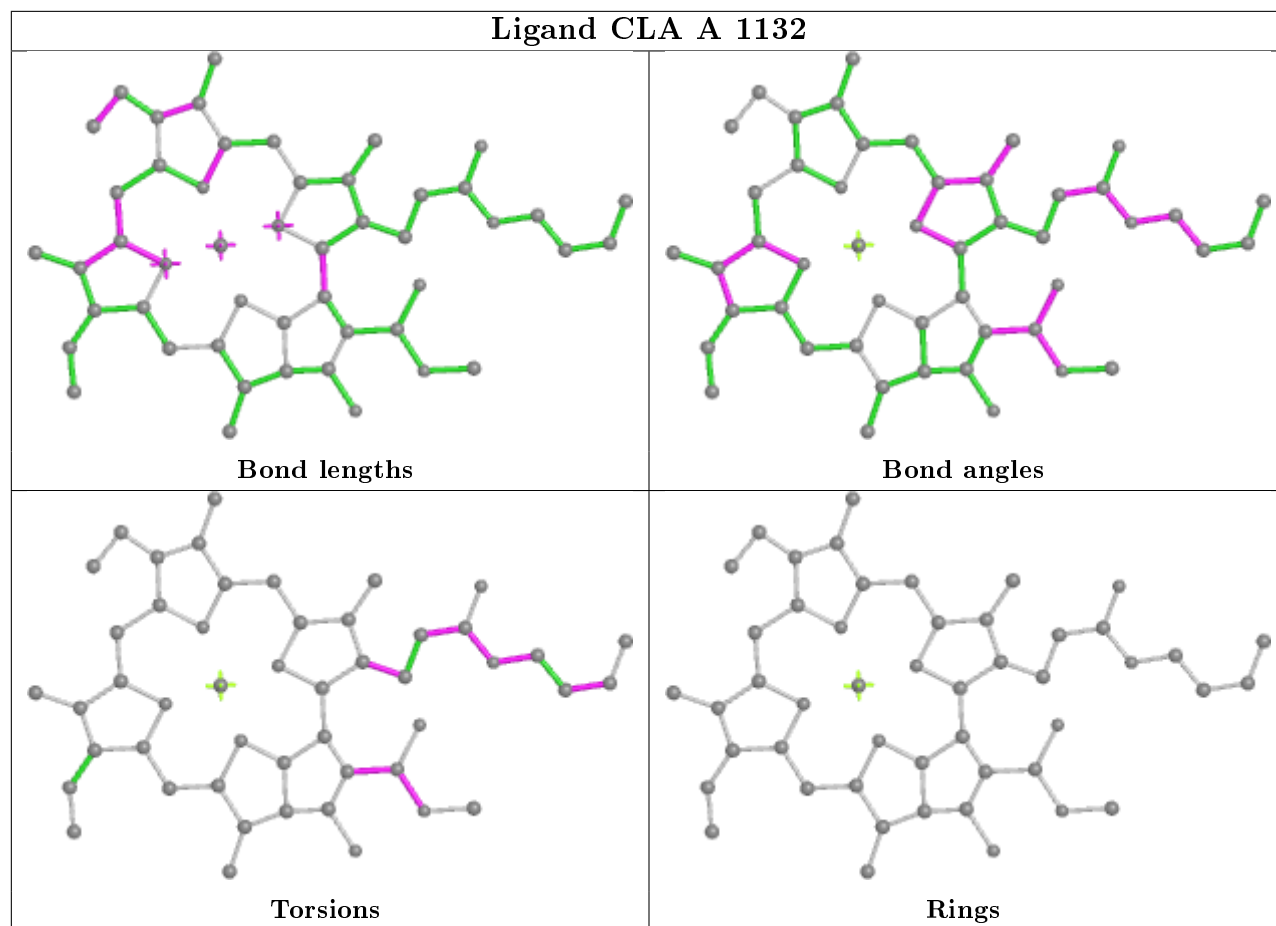


Torsions



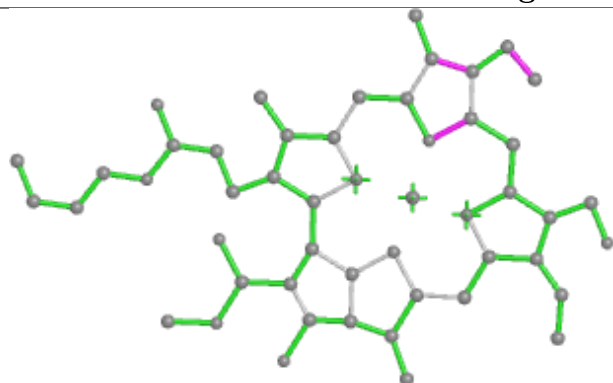
Rings



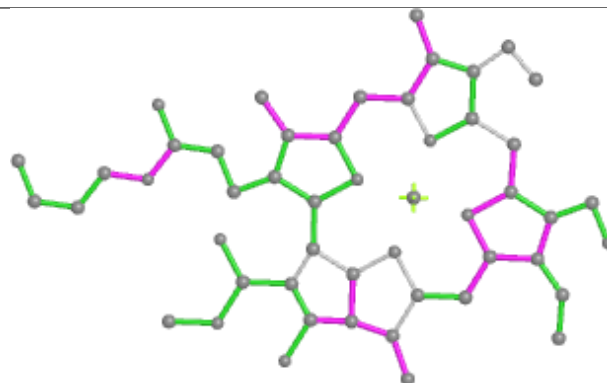




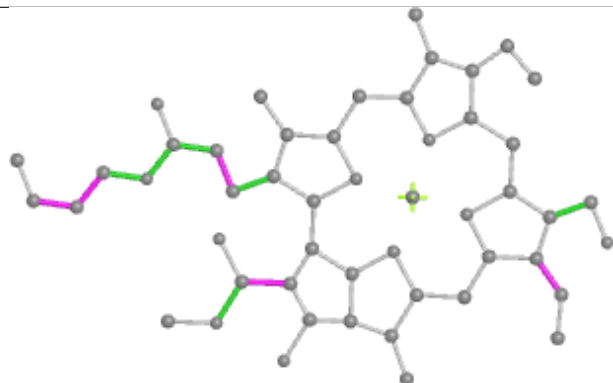
## Ligand CHL 2 609



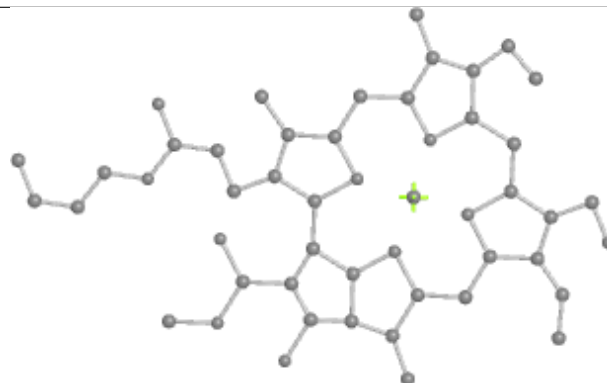
Bond lengths



Bond angles

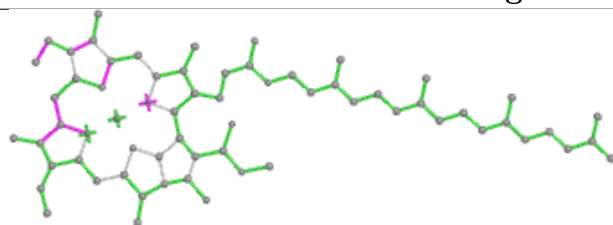


Torsions

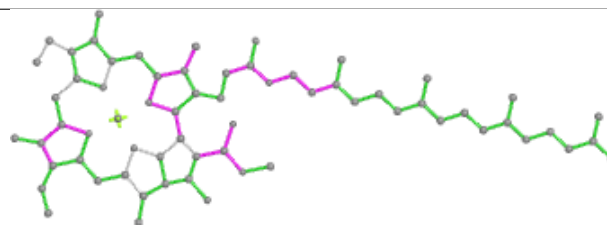


Rings

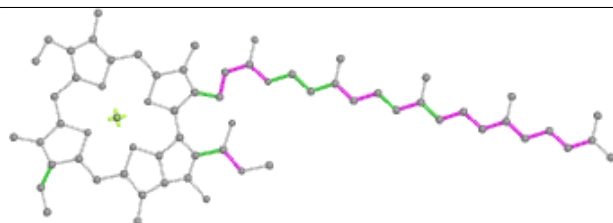
## Ligand CLA B 1240



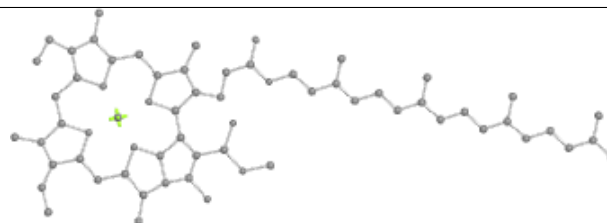
Bond lengths



Bond angles

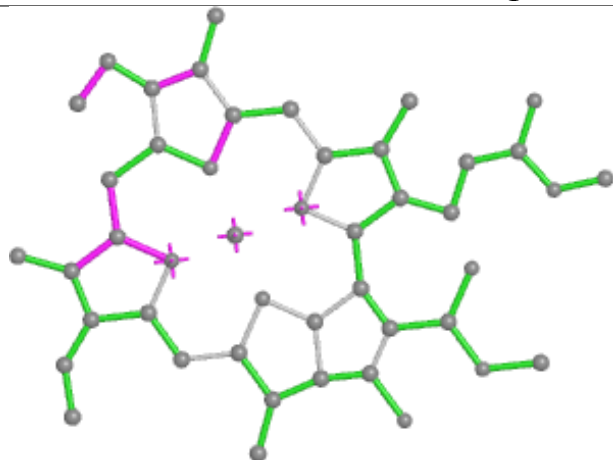


Torsions

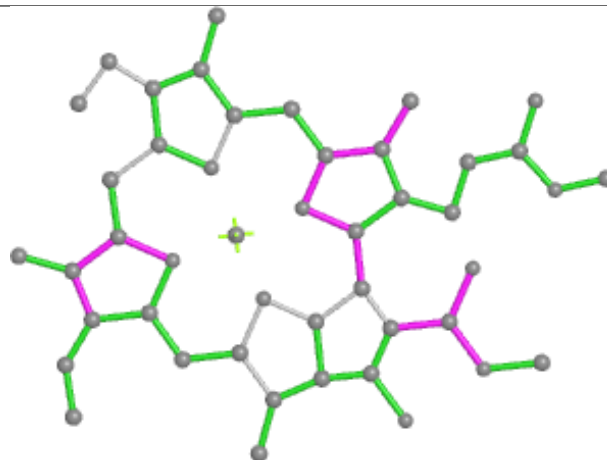


Rings

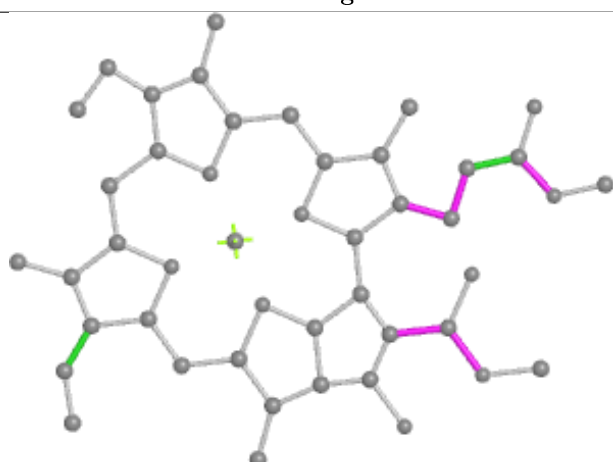
## Ligand CLA B 1217



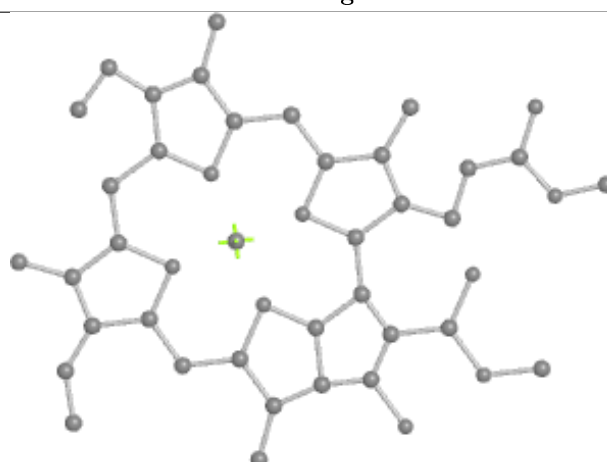
Bond lengths



Bond angles

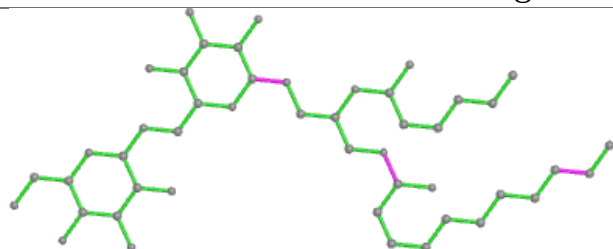


Torsions

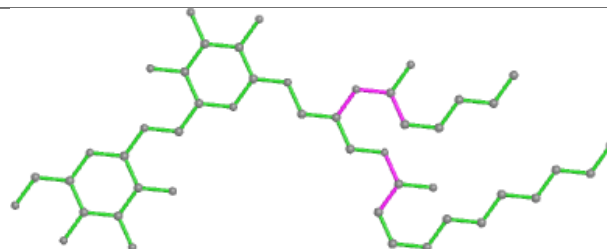


Rings

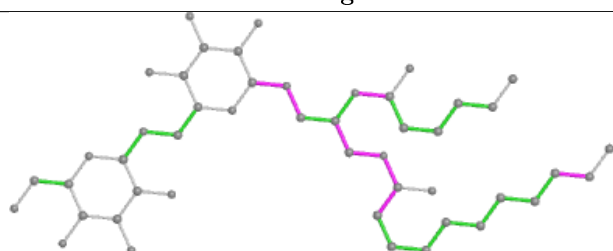
## Ligand DGD 2 811



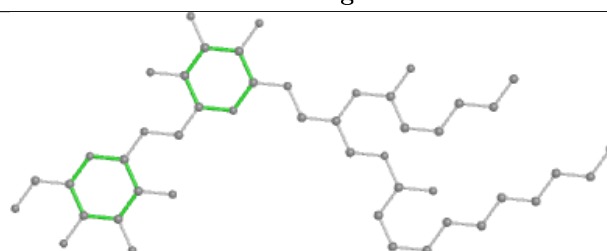
Bond lengths



Bond angles

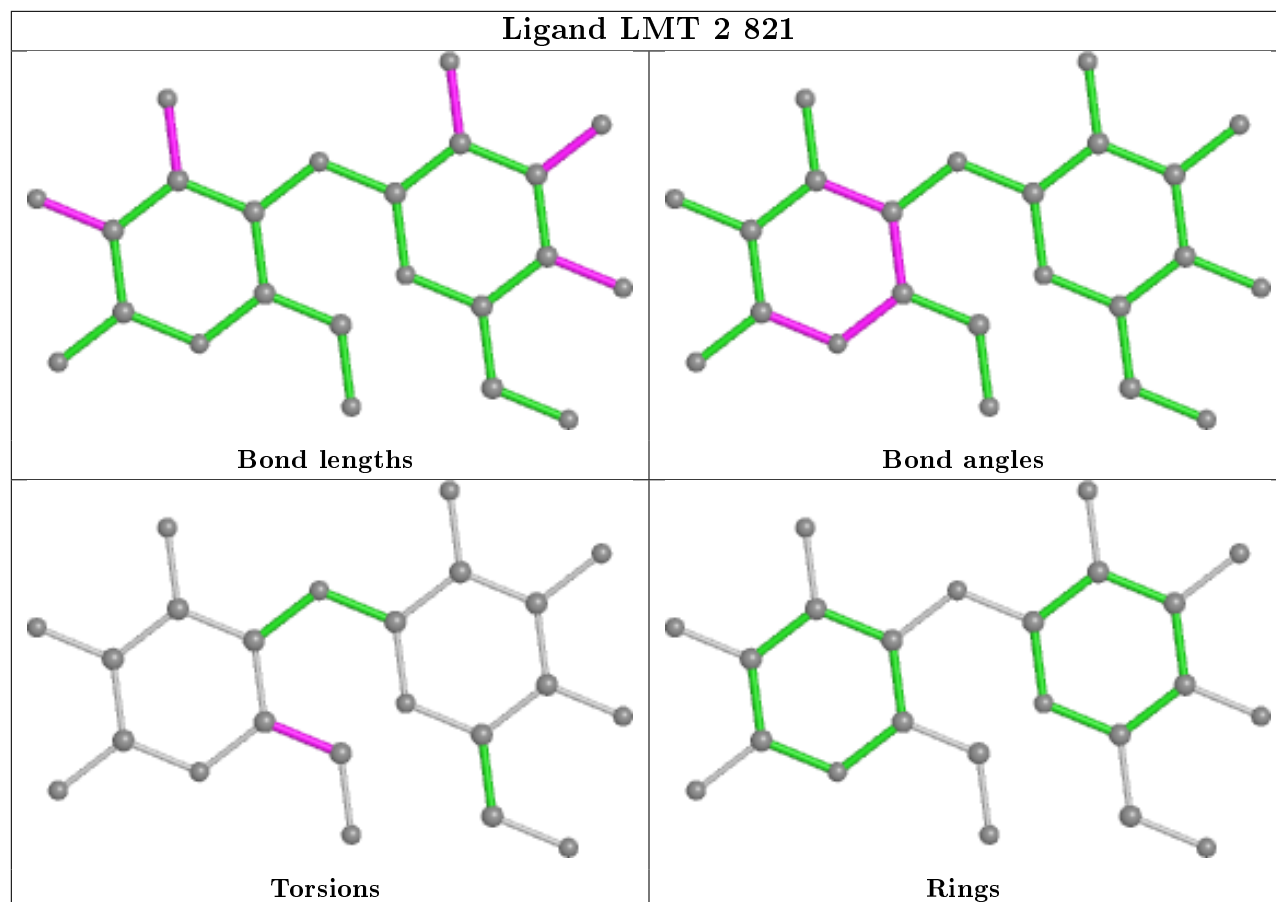


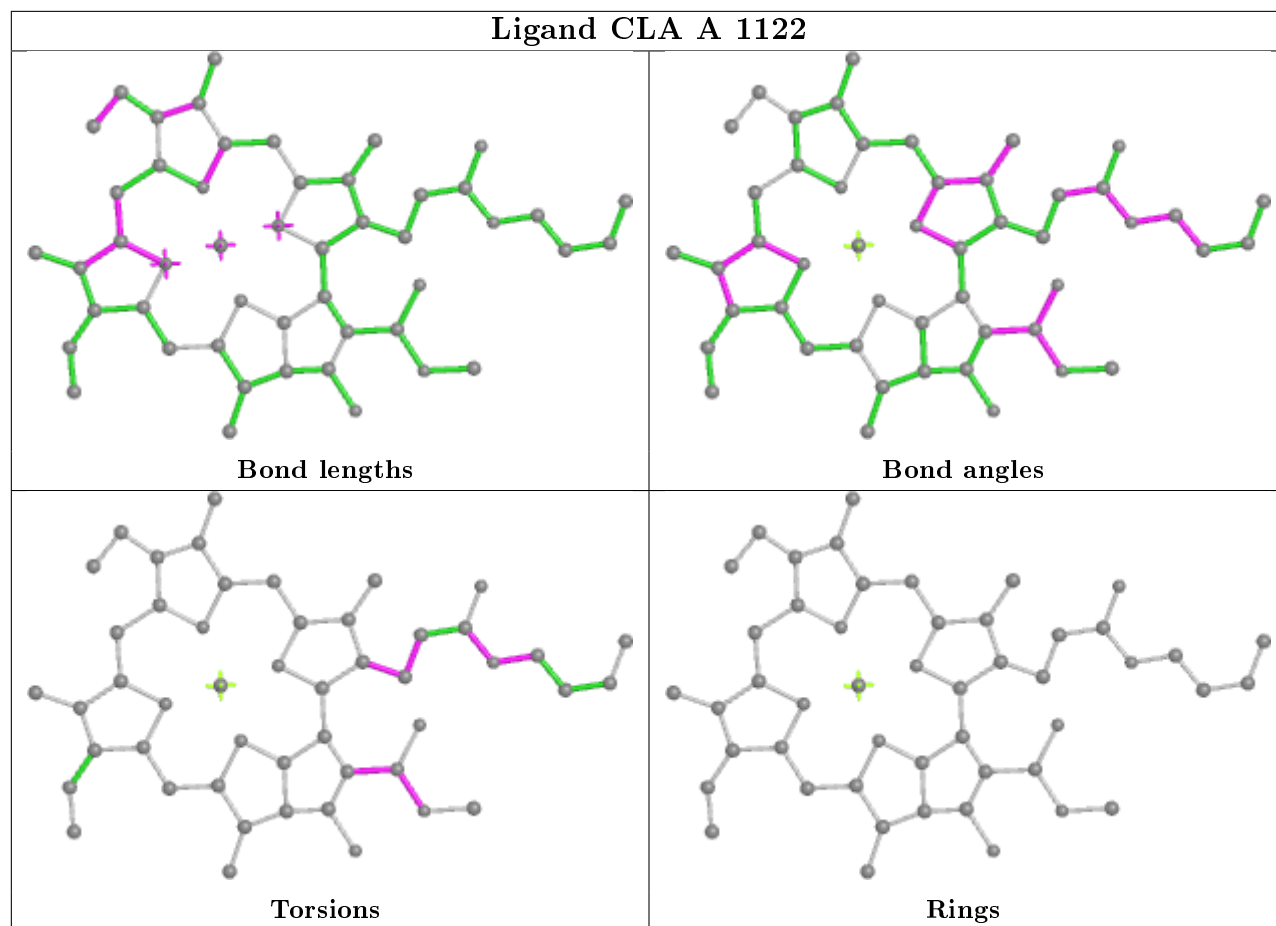
Torsions

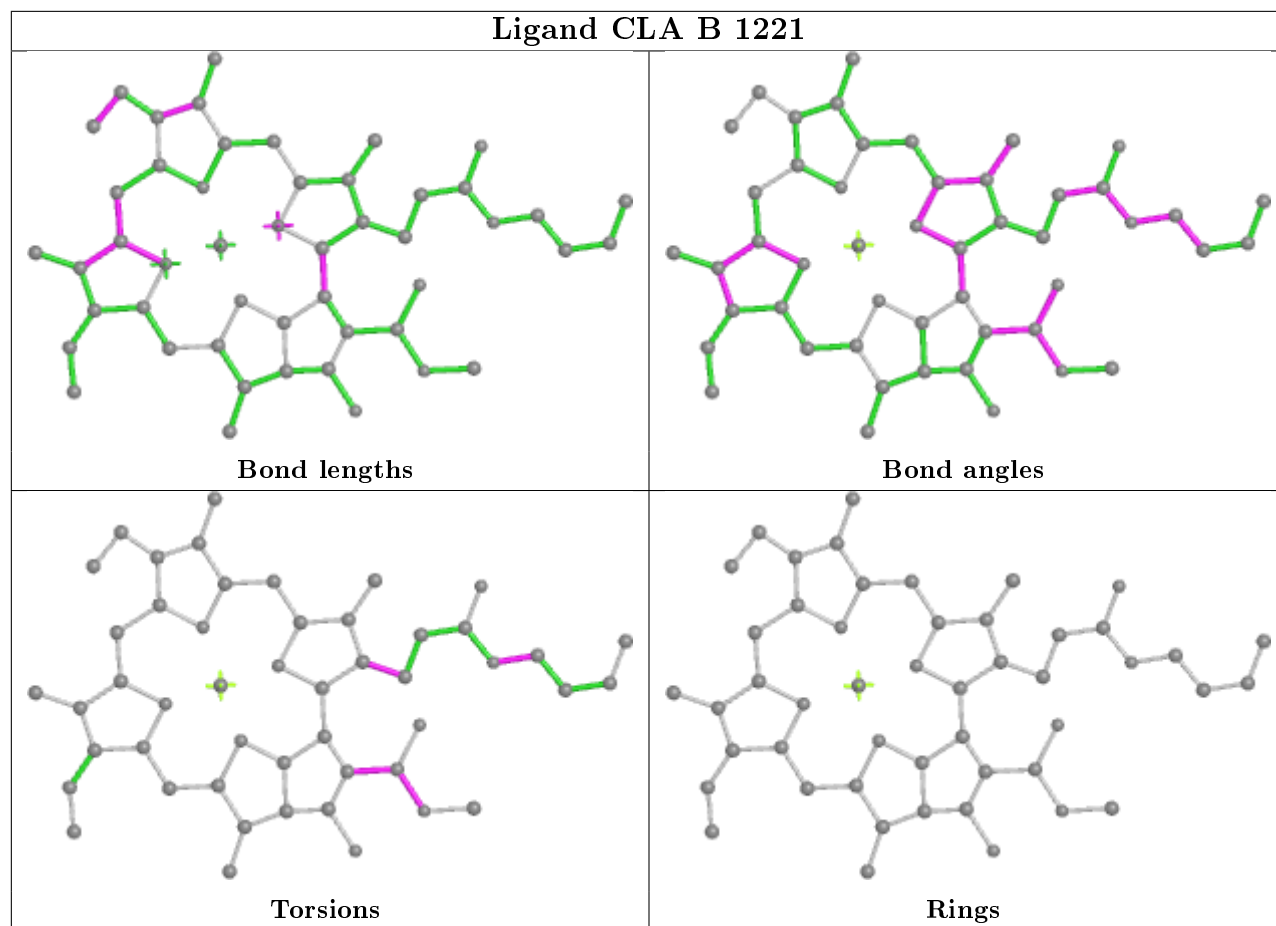


Rings

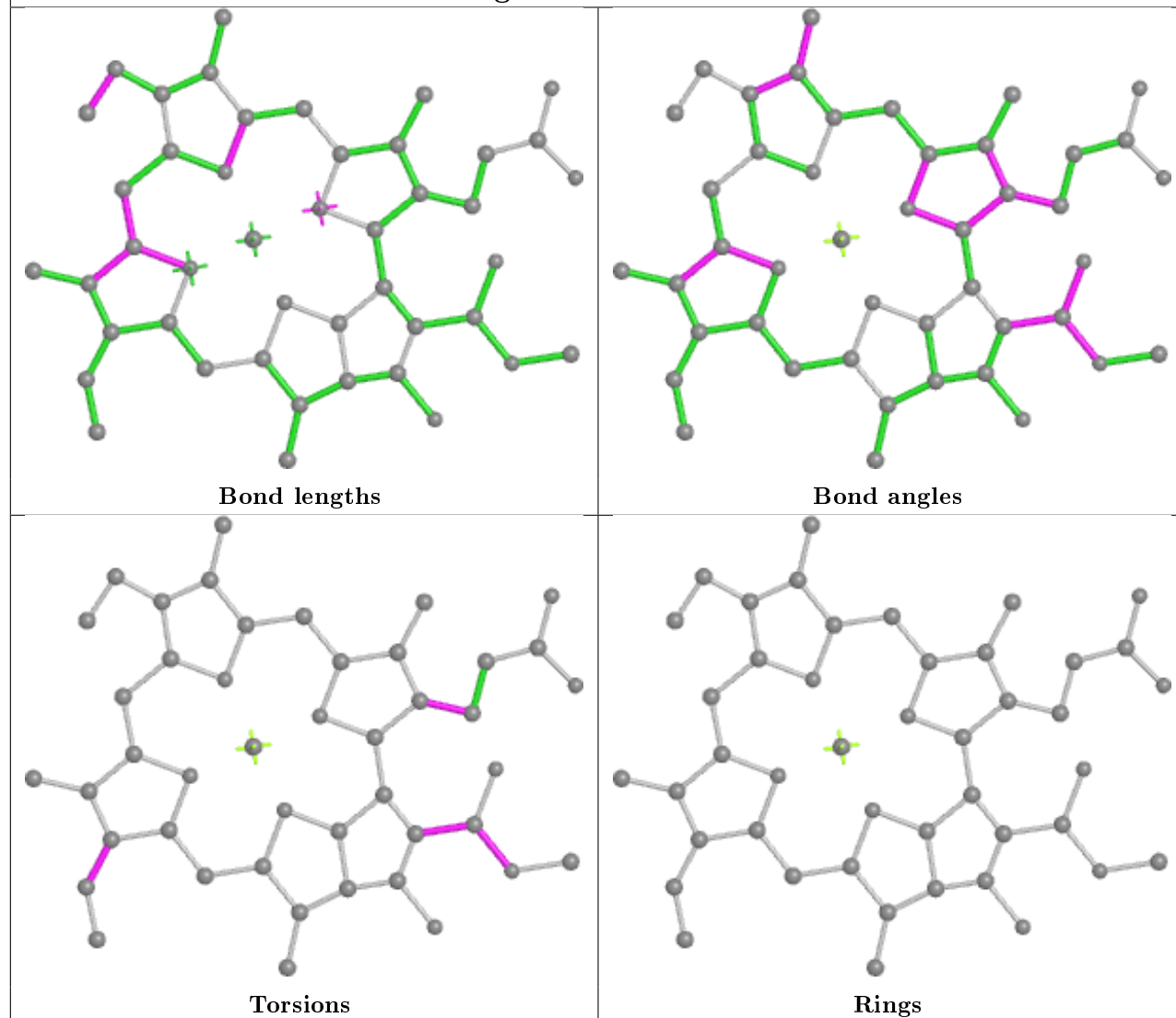
## Ligand LMT 2 821



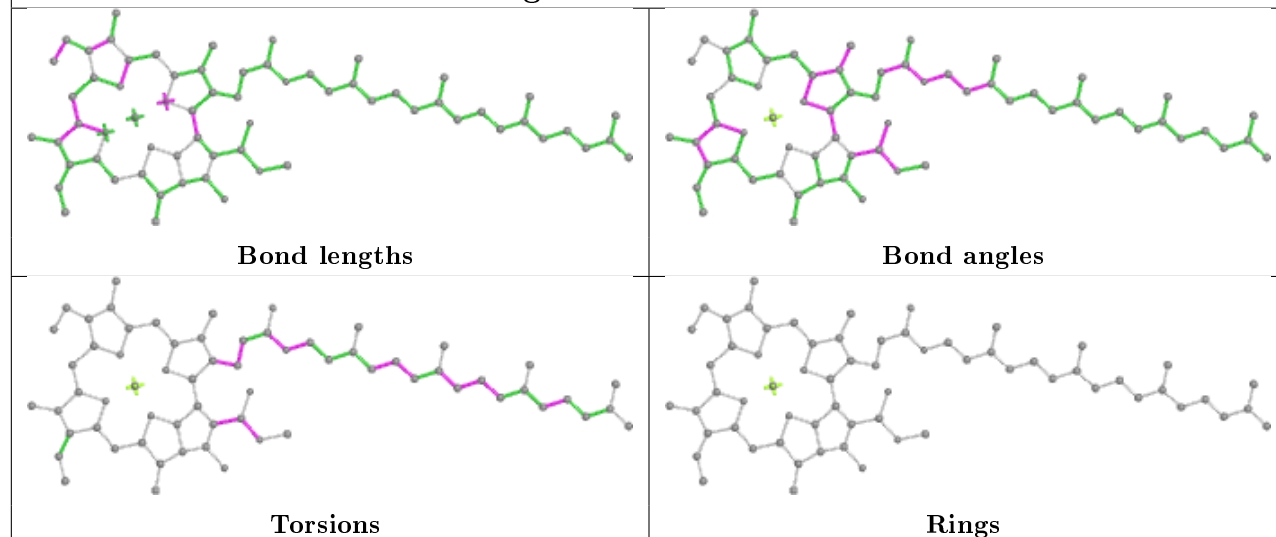


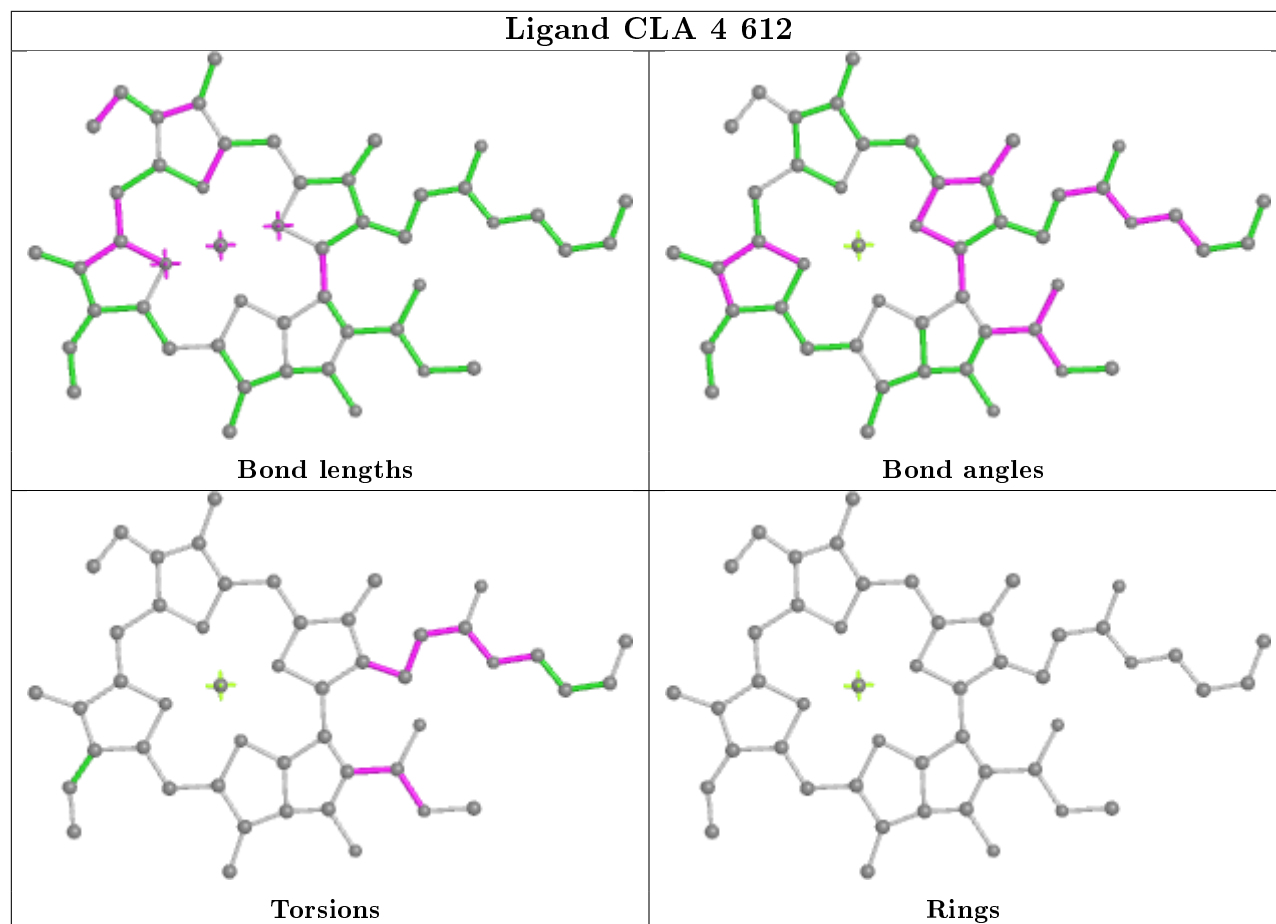
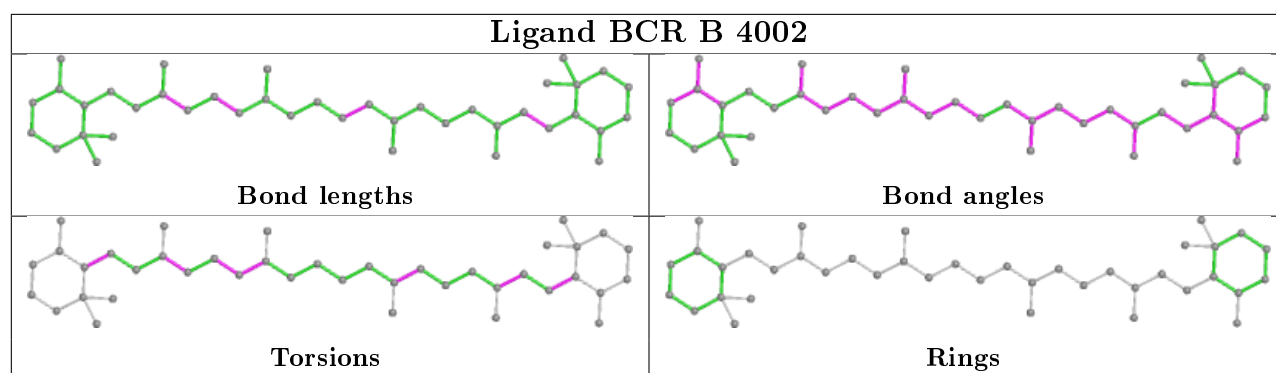


## Ligand CLA 1 606

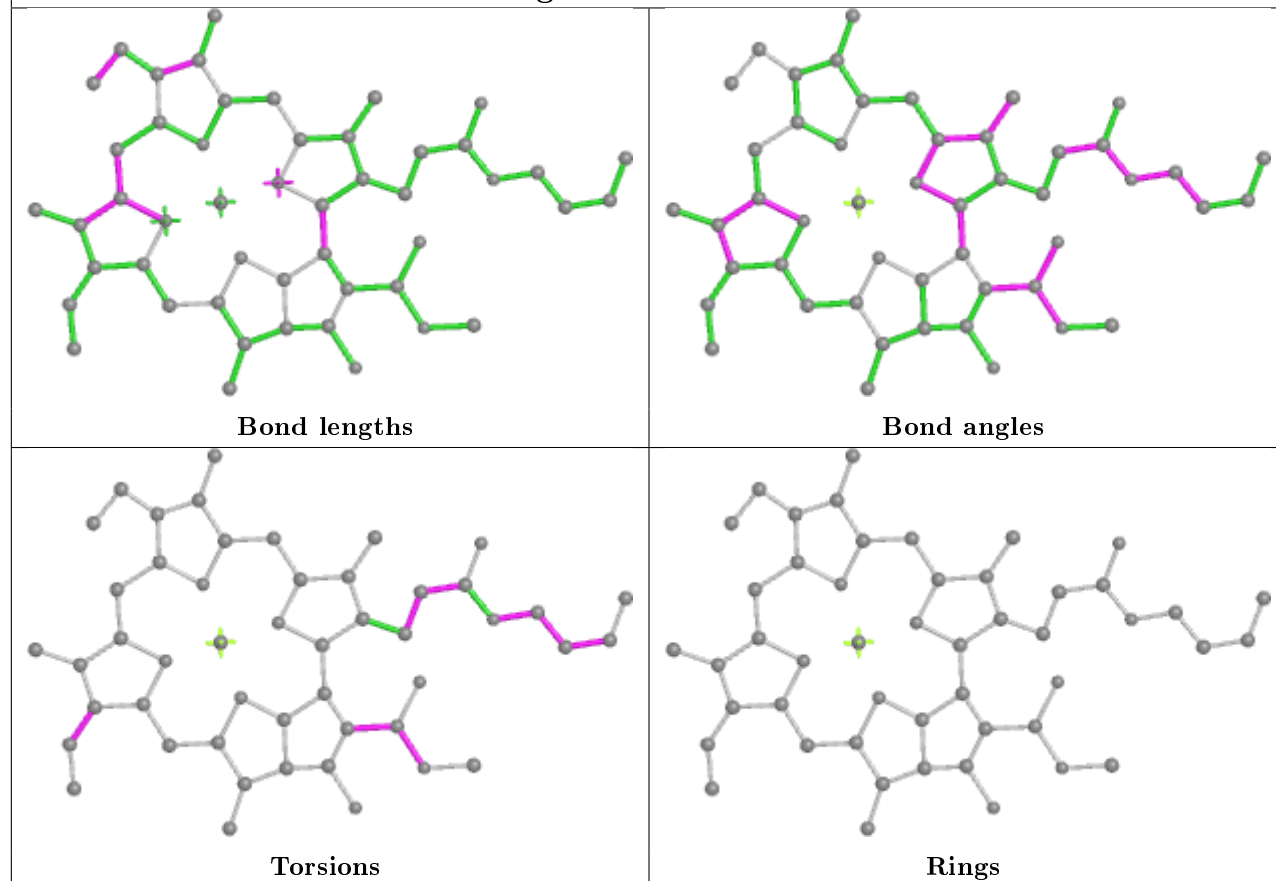


## Ligand CLA B 1021

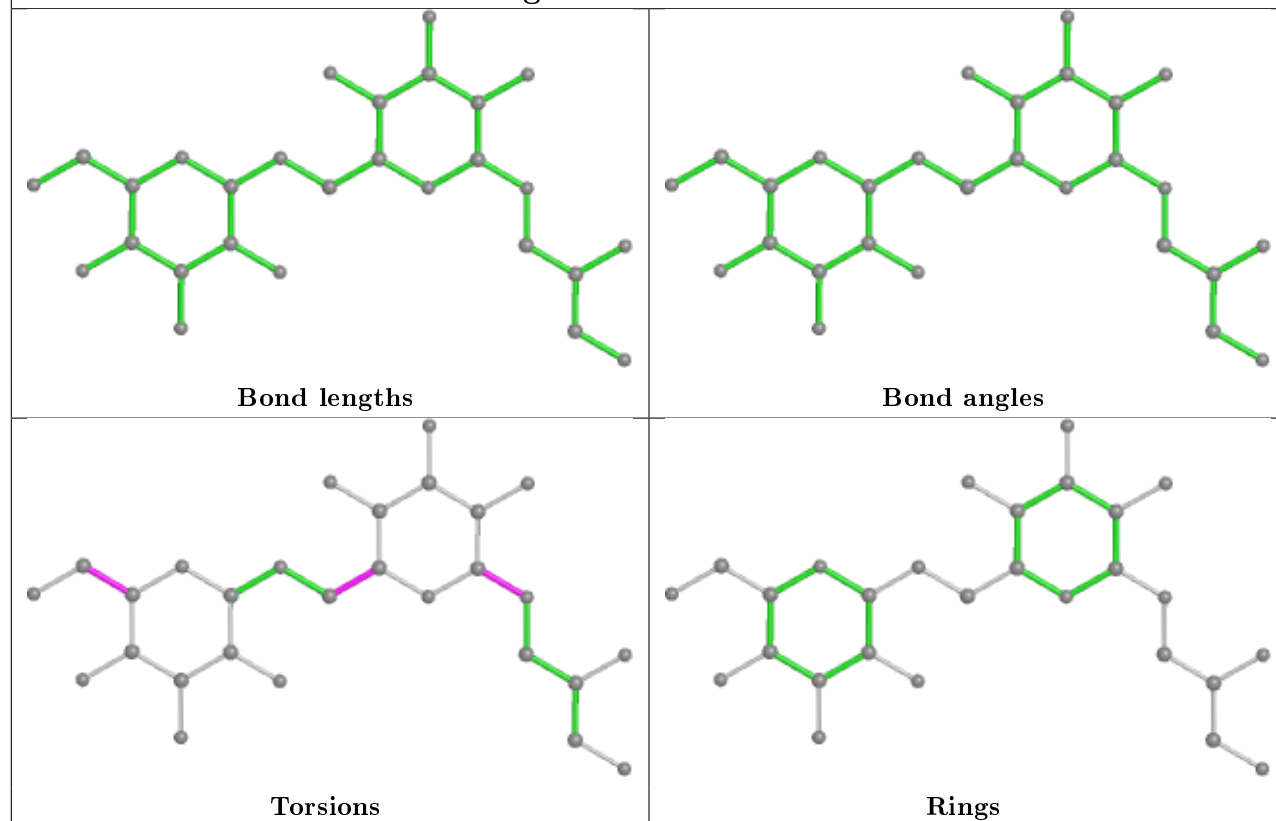




## Ligand CLA 1 611

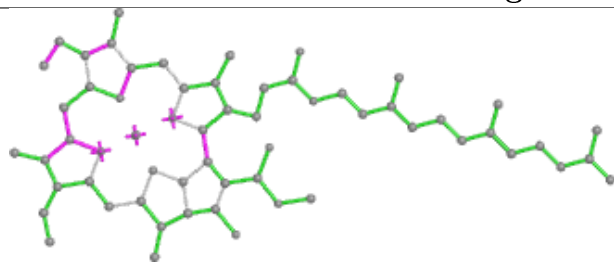


## Ligand DGD J 5001

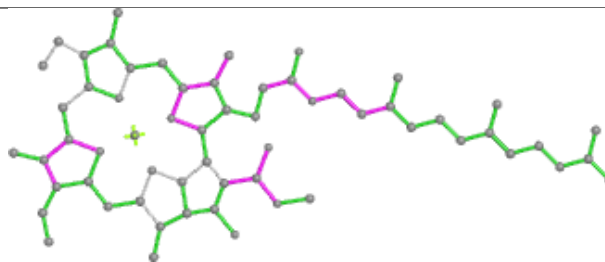




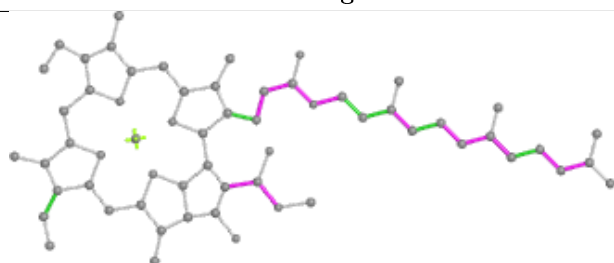
## Ligand CLA B 1235



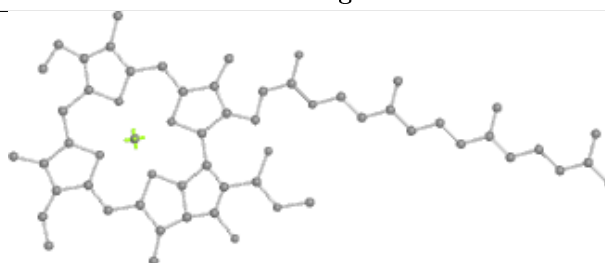
Bond lengths



Bond angles

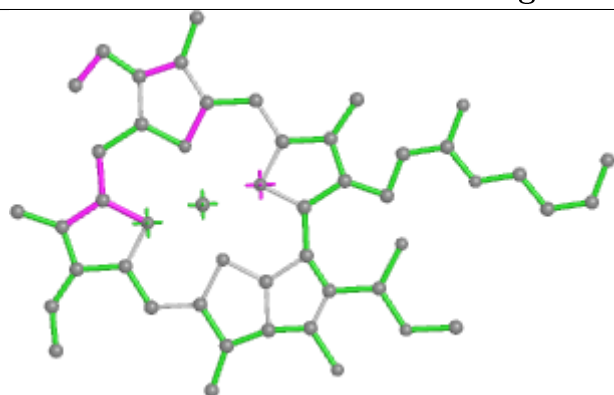


Torsions

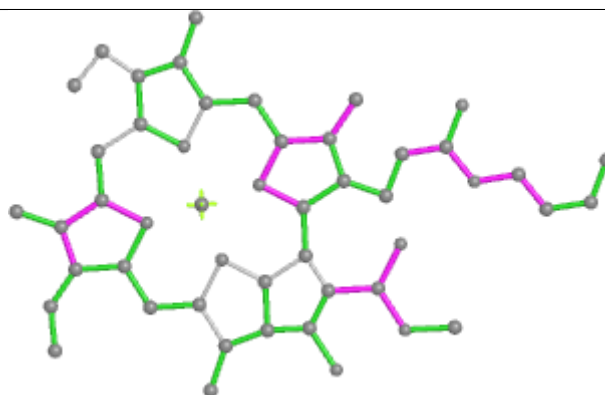


Rings

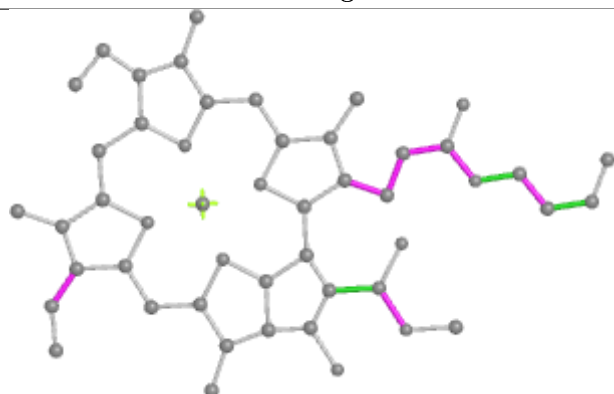
## Ligand CLA 3 601



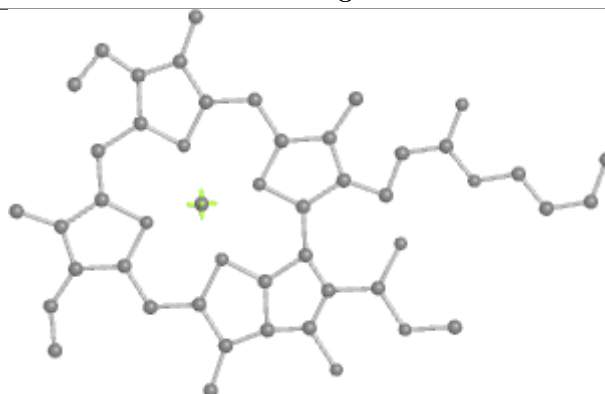
Bond lengths



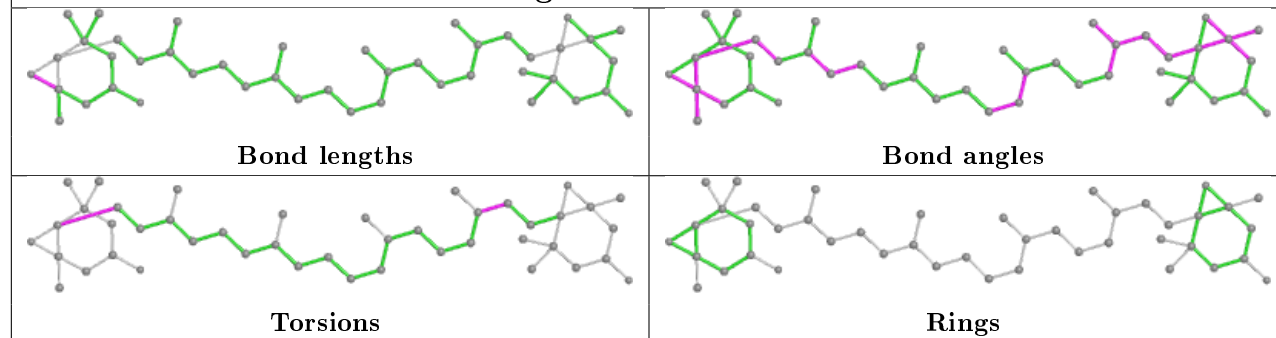
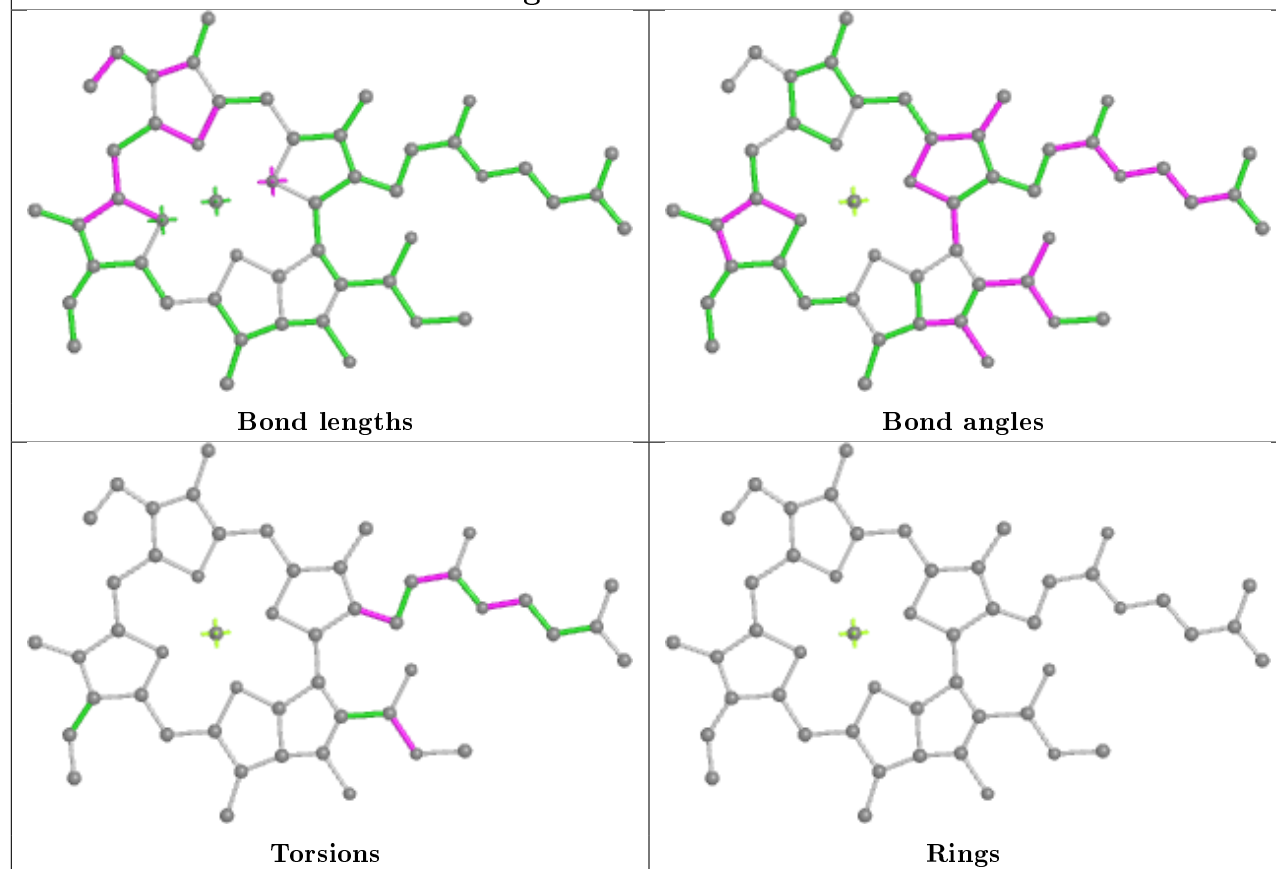
Bond angles



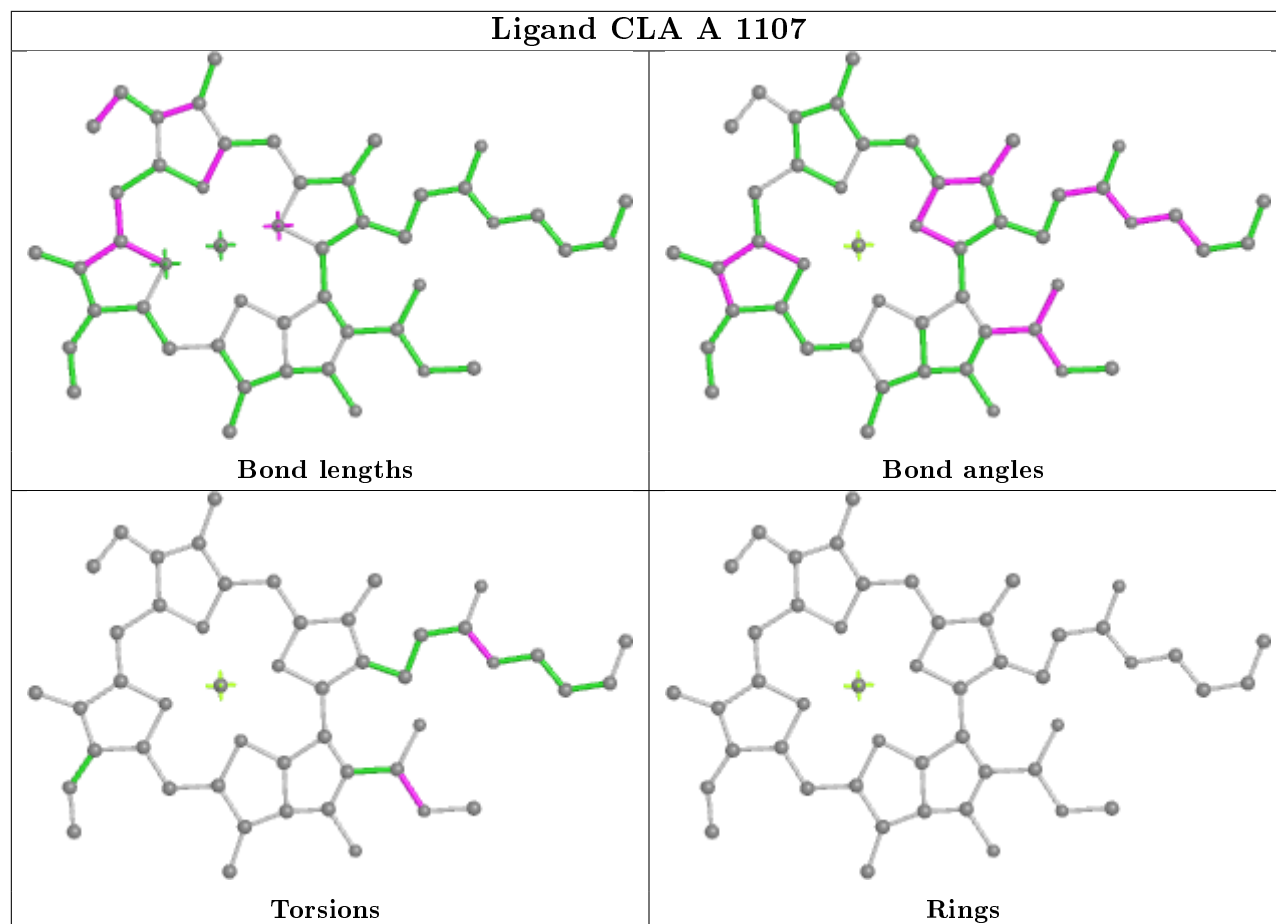
Torsions

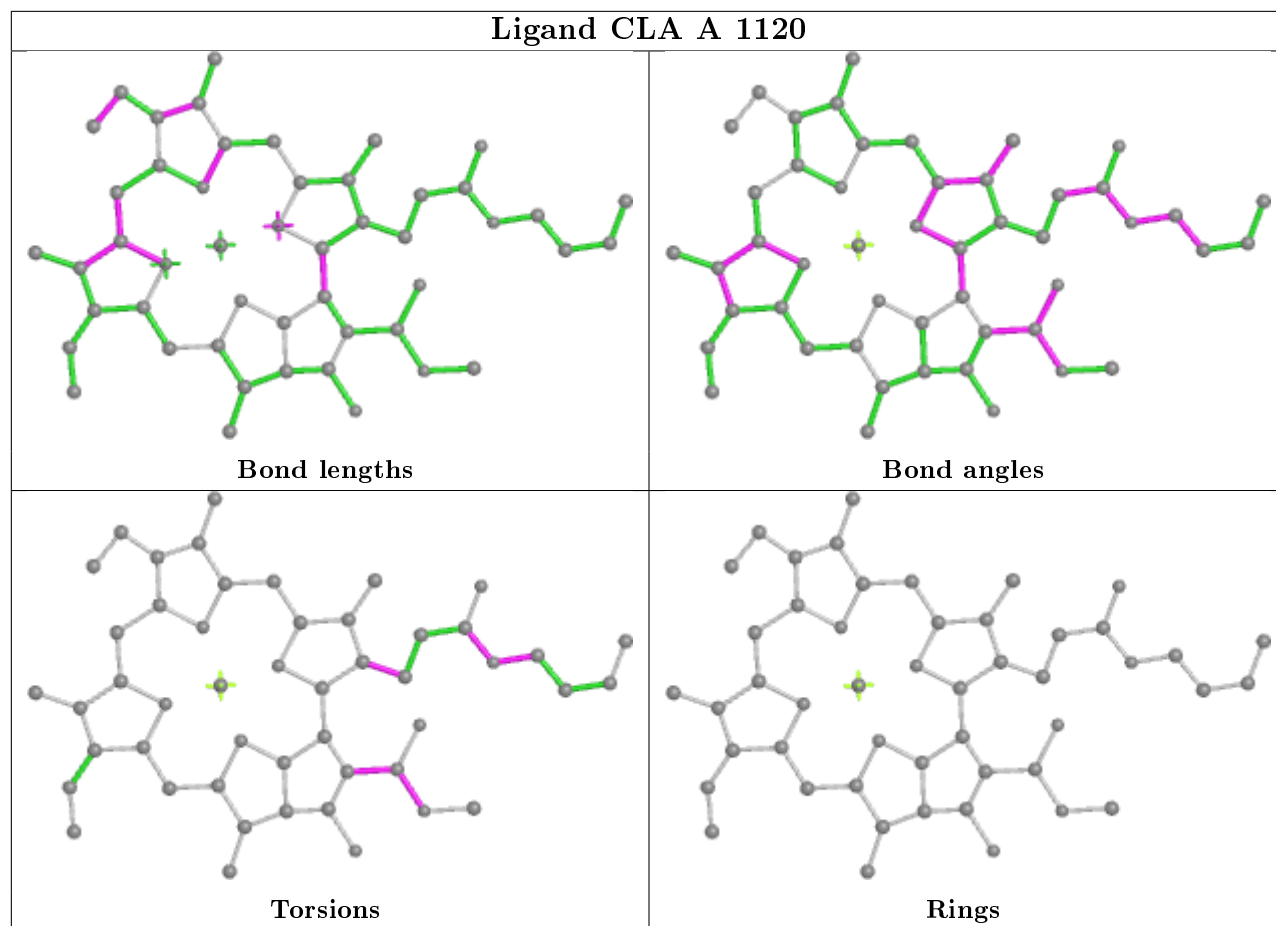


Rings

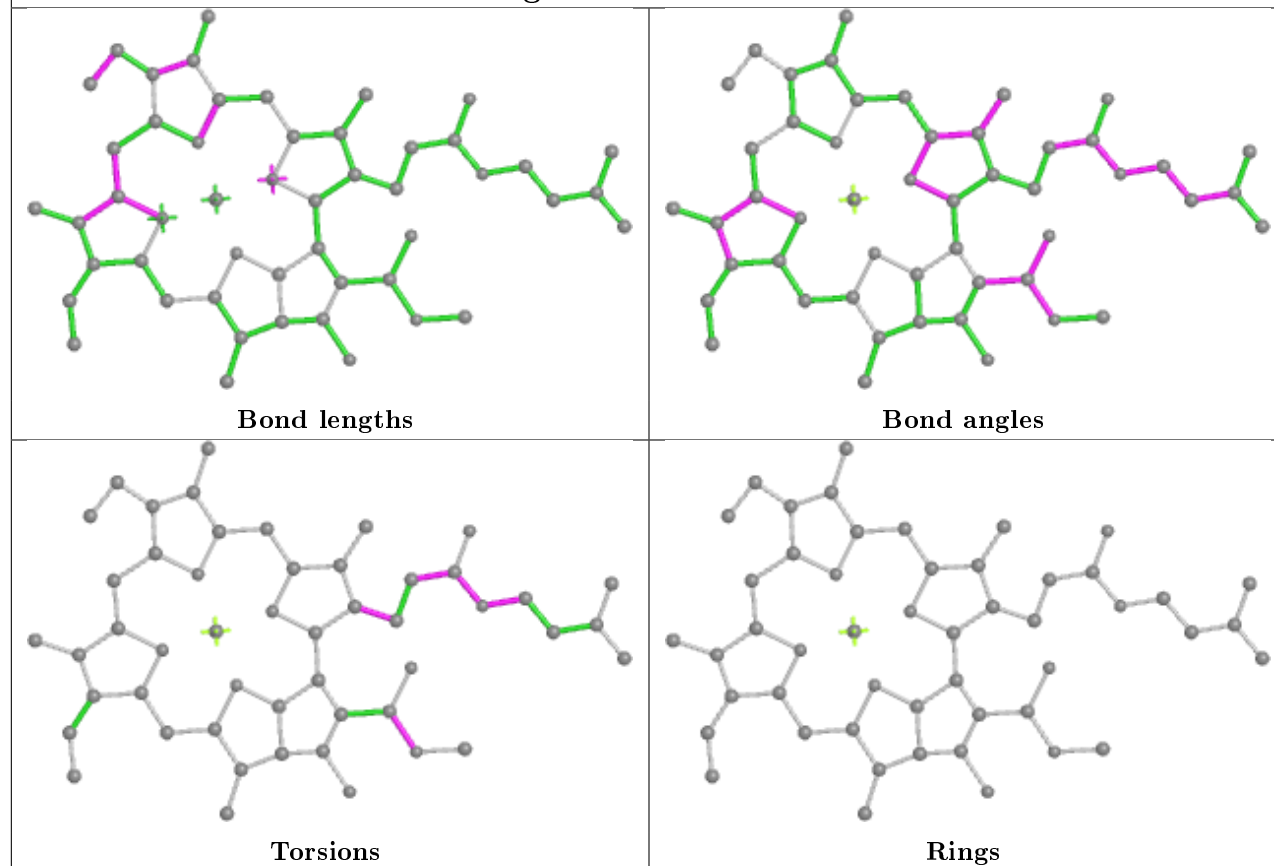
**Ligand XAT 2 502****Ligand CLA B 1223**

## Ligand CLA A 1107

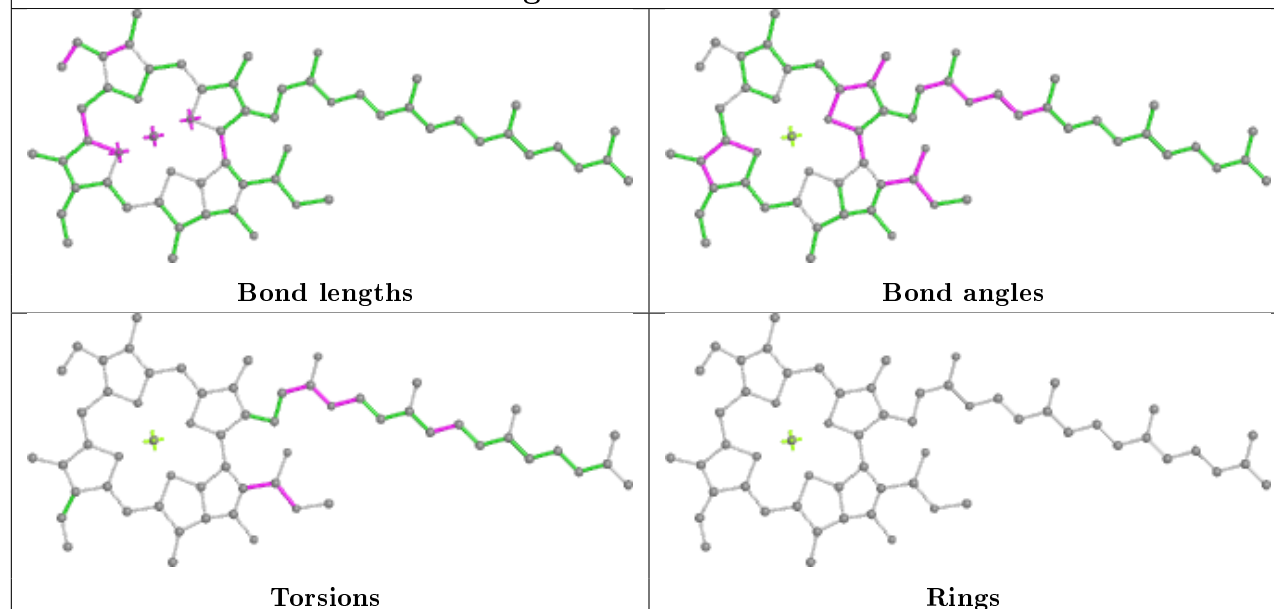


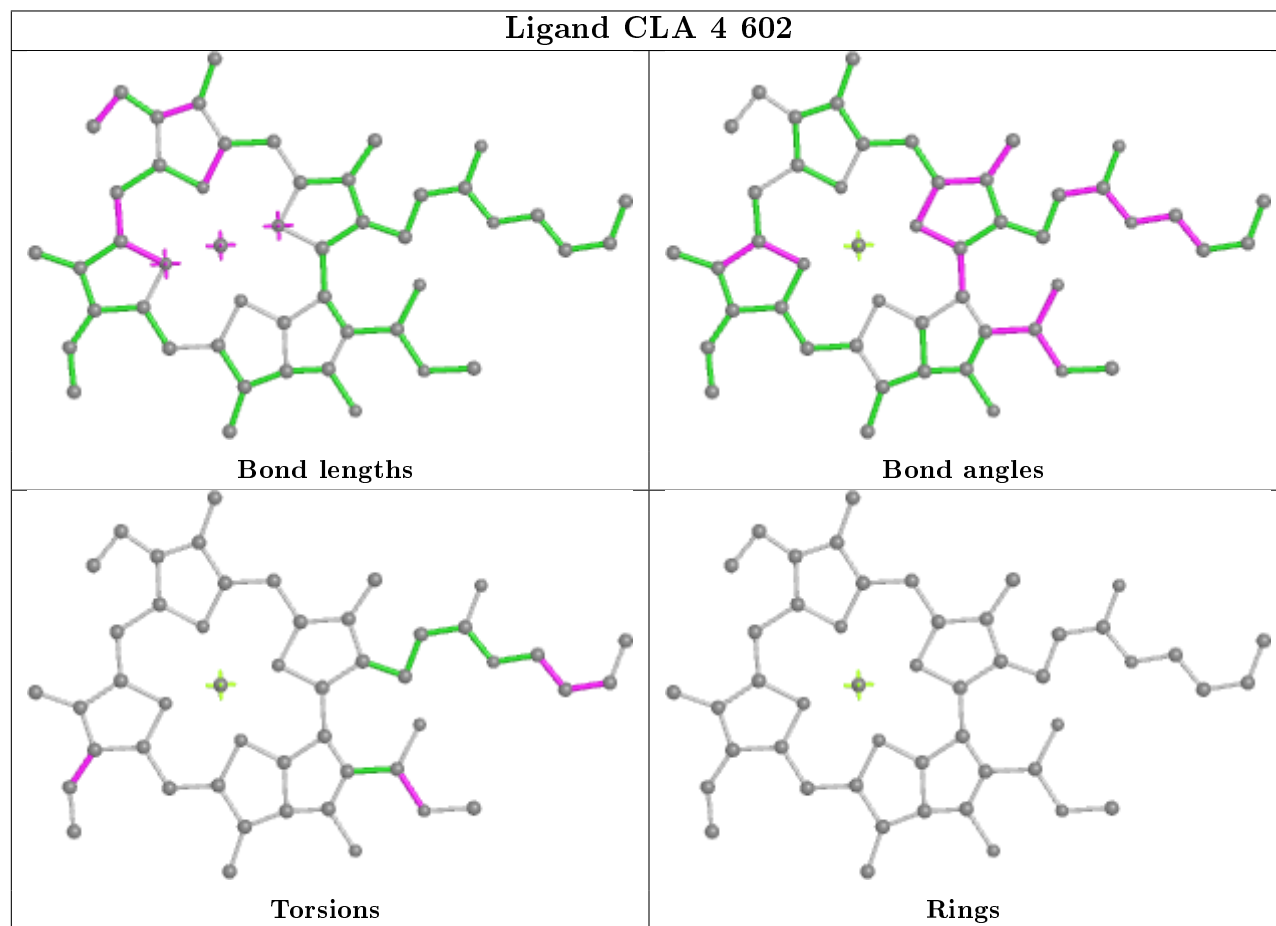
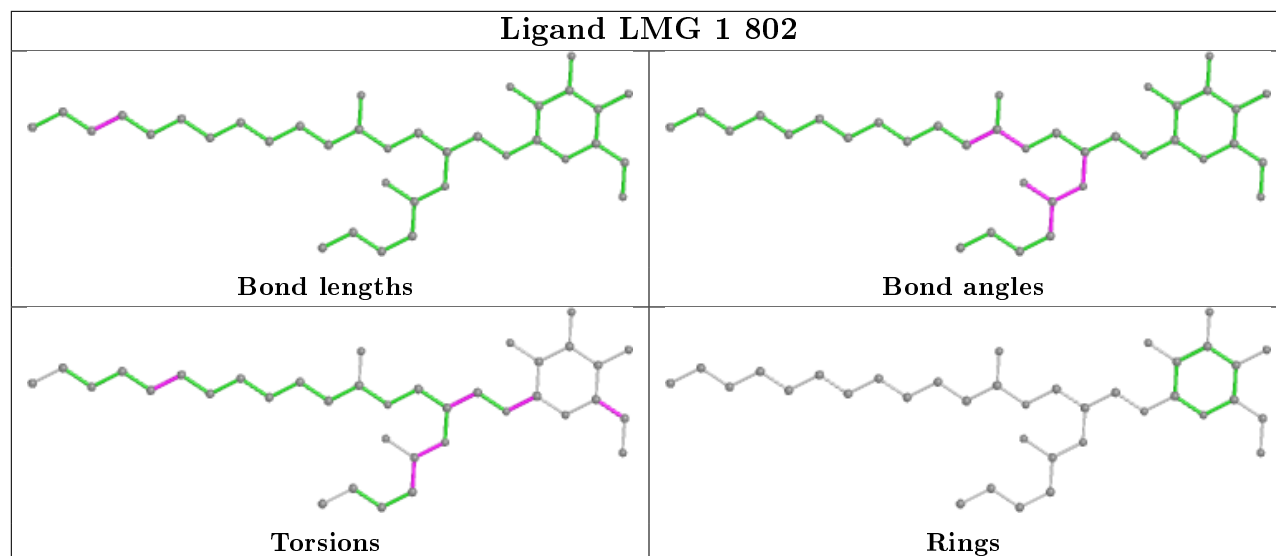


## Ligand CLA A 1141

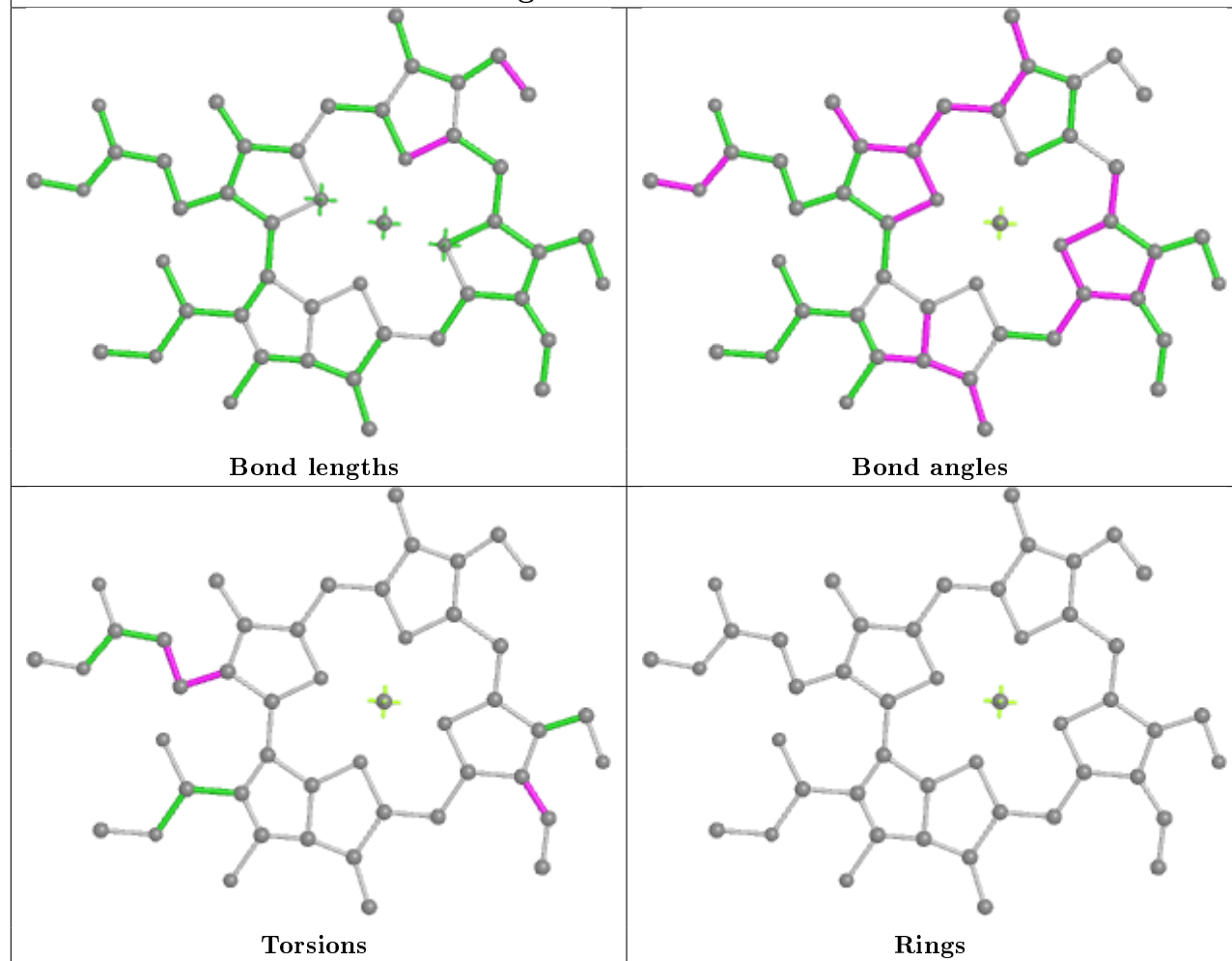


## Ligand CLA B 1228

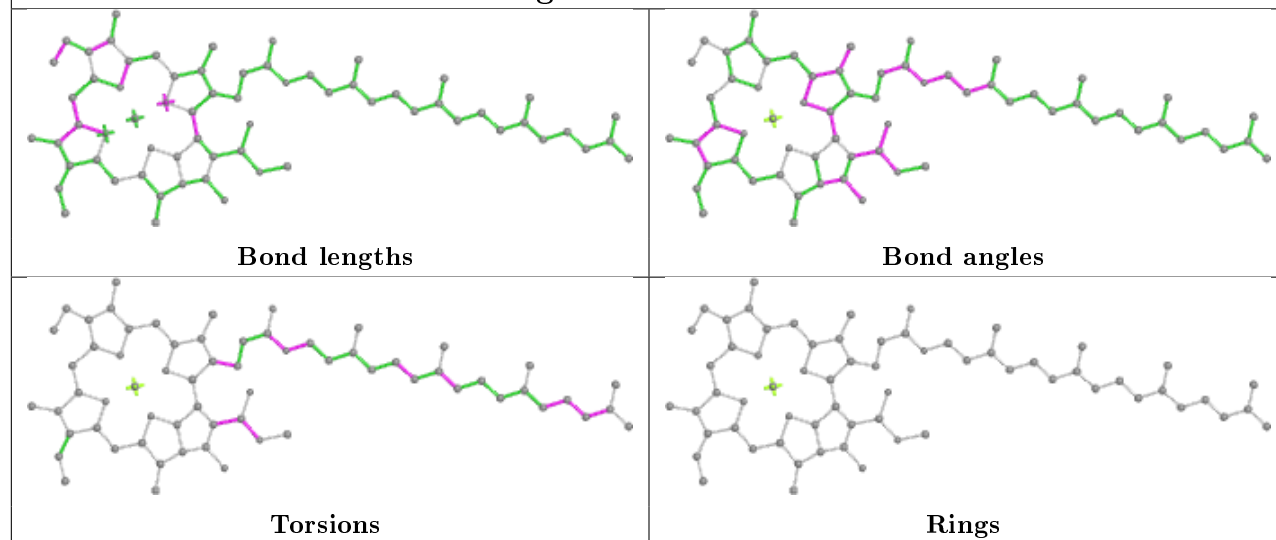




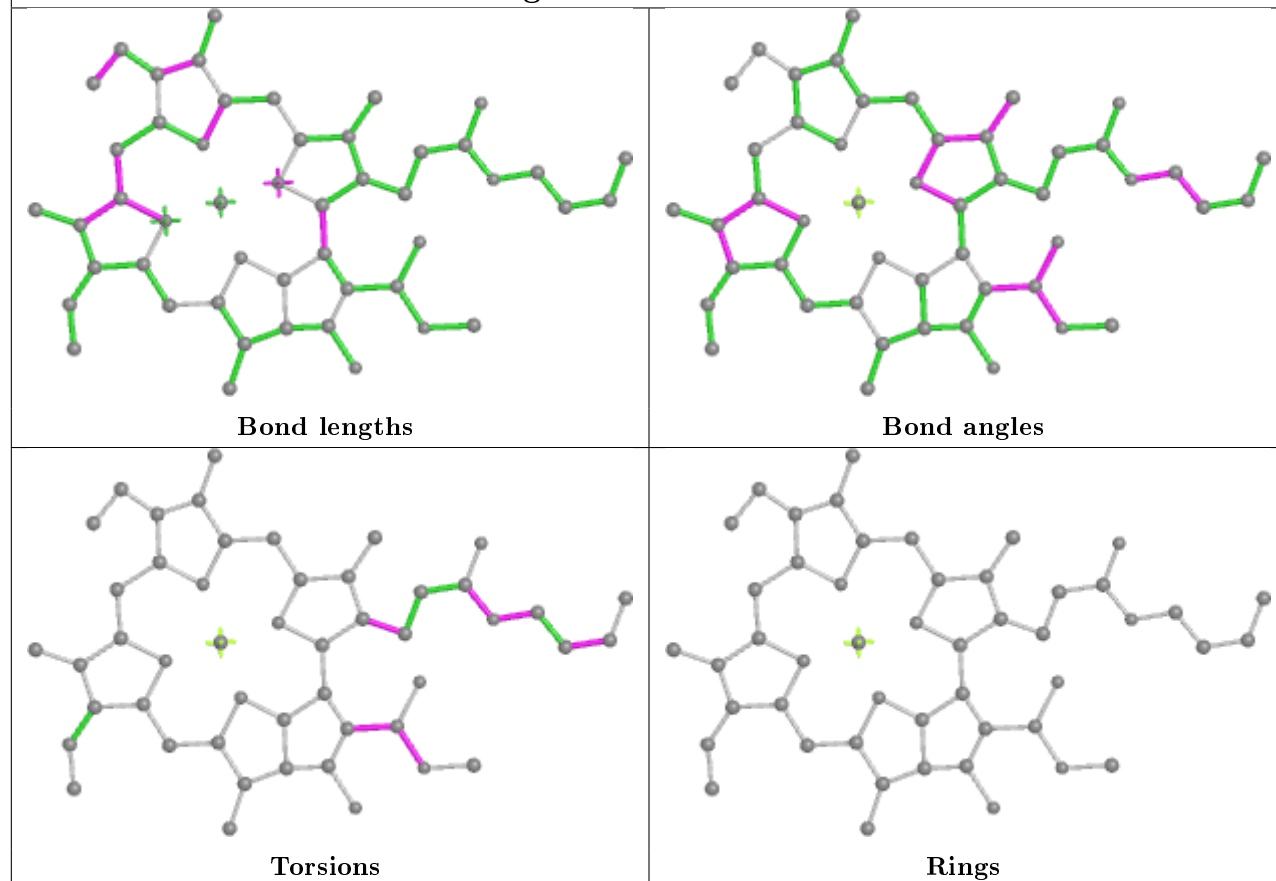
## Ligand CHL 1 610



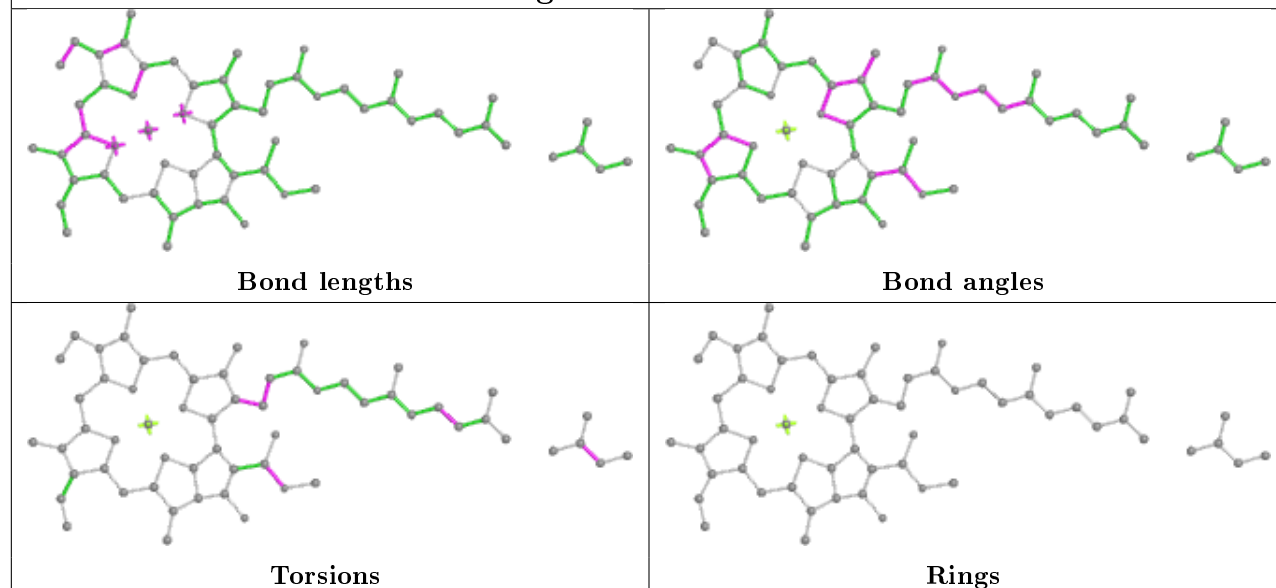
## Ligand CLA 2 605



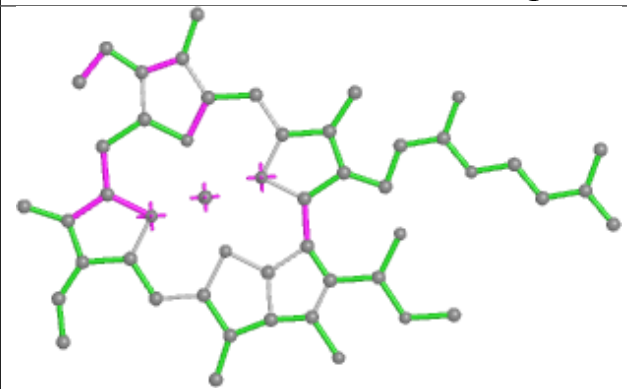
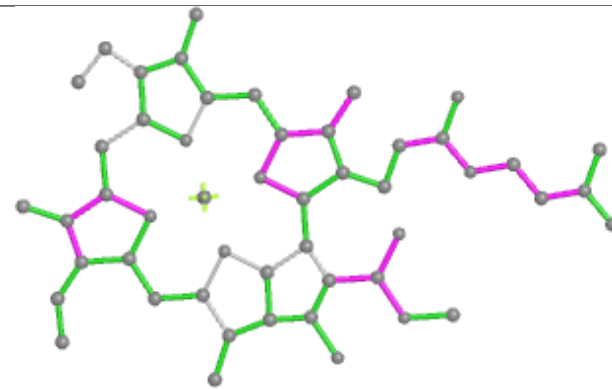
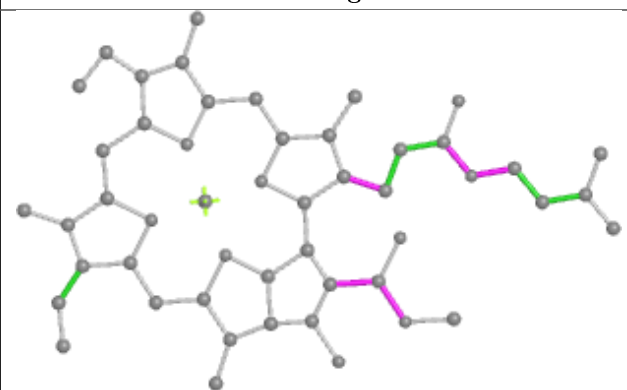
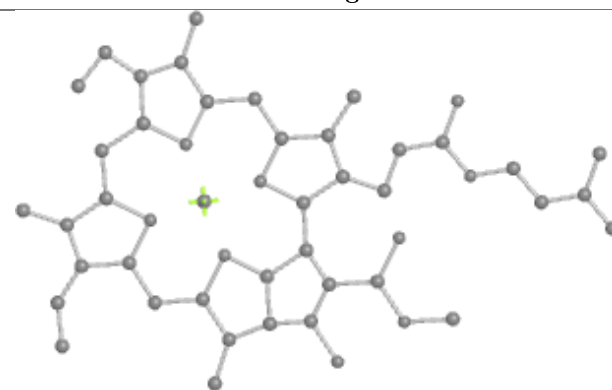
## Ligand CLA B 1222

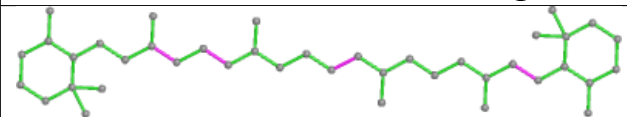
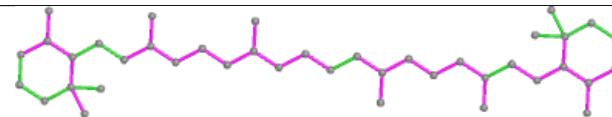
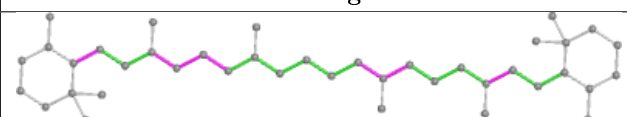
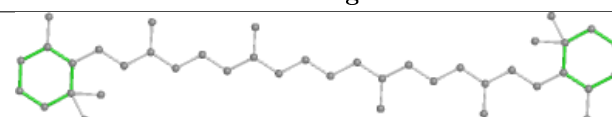


## Ligand CLA 1 612

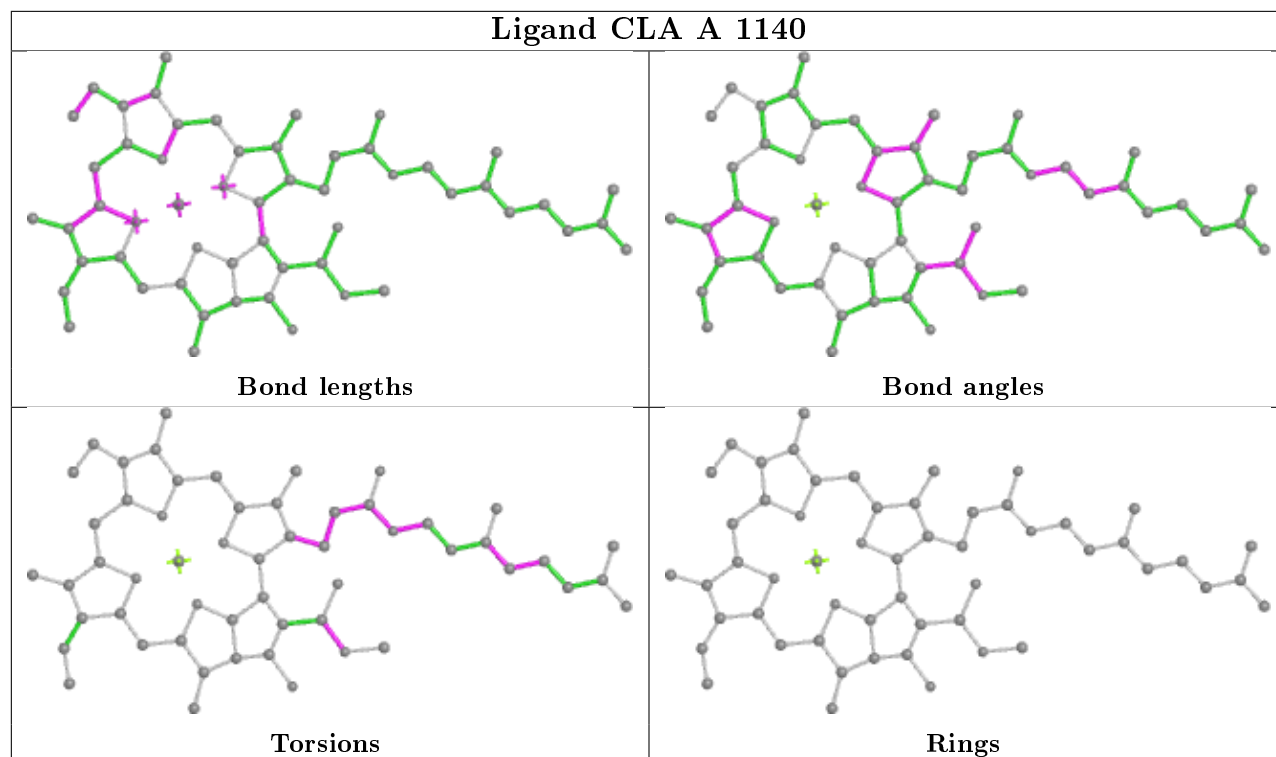




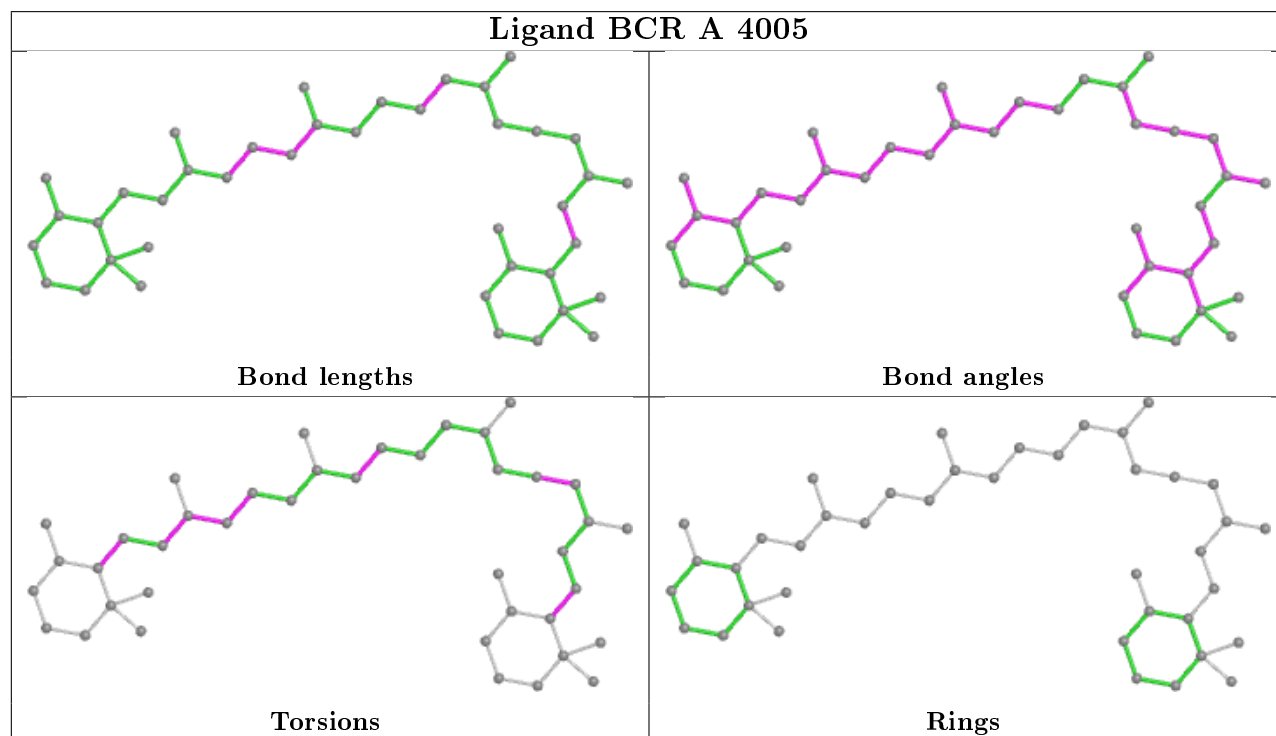
Ligand CLA 2 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

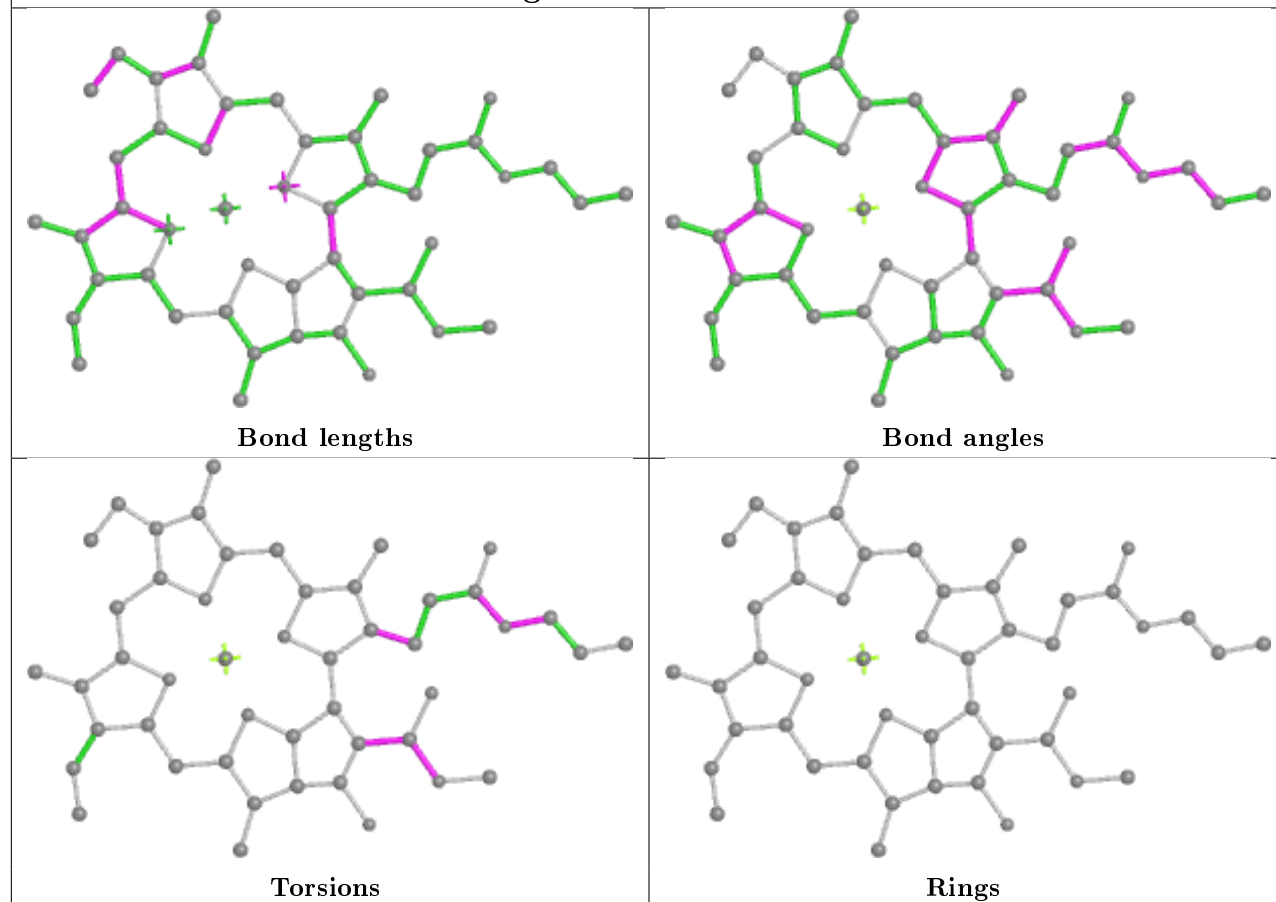
## Ligand CLA A 1140



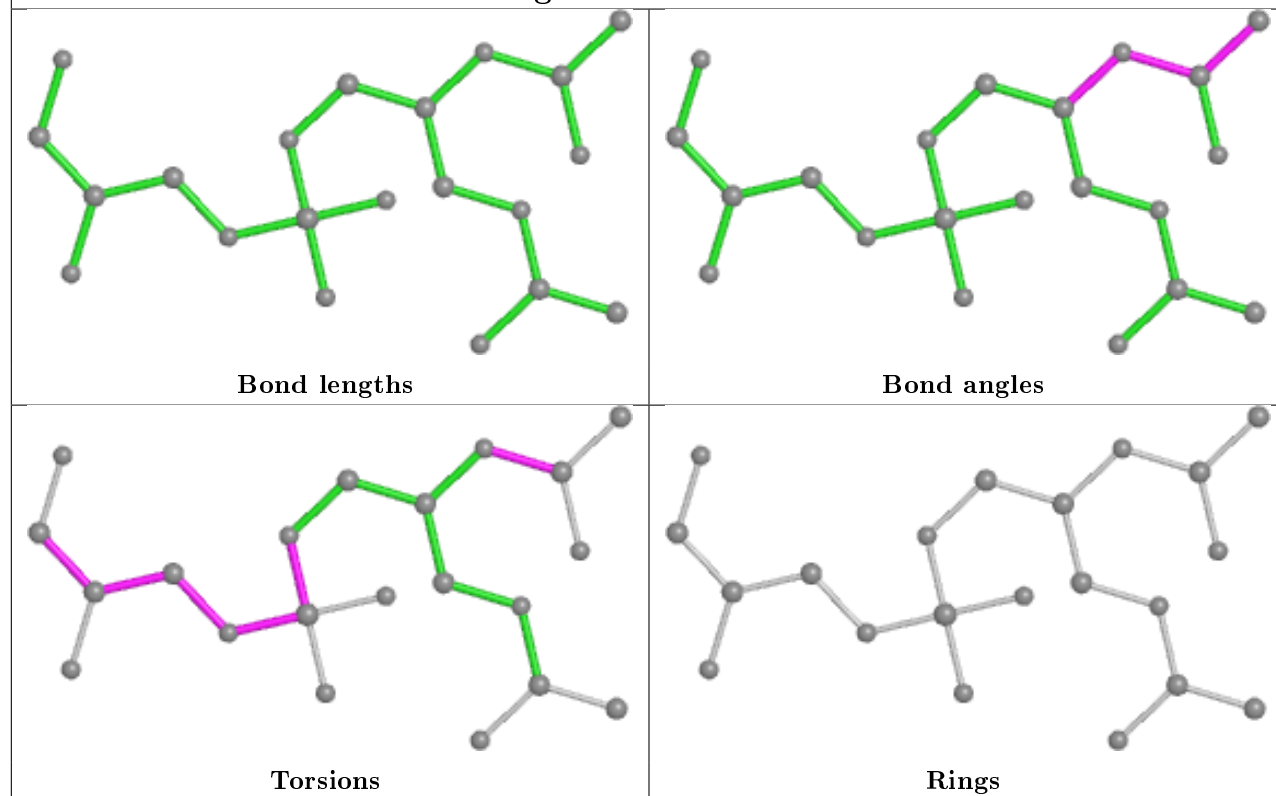
## Ligand BCR A 4005



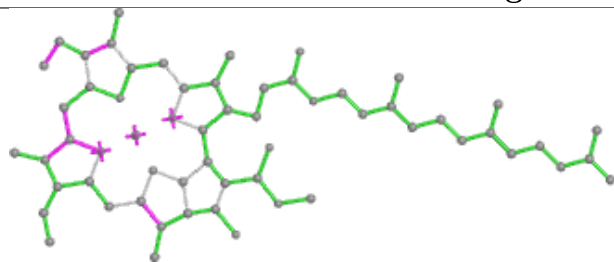
## Ligand CLA A 1123



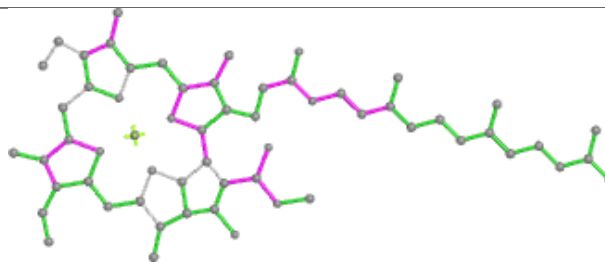
## Ligand LHG 2 801



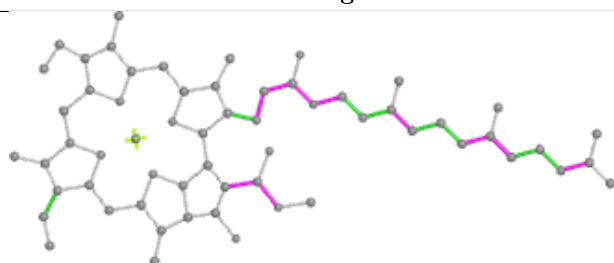
## Ligand CLA B 1023



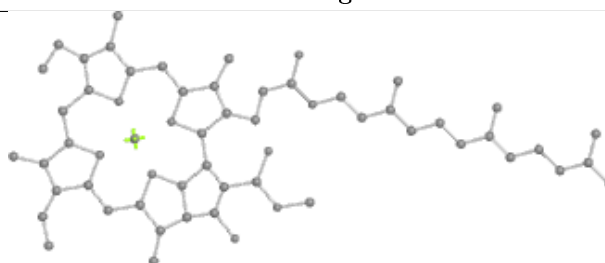
Bond lengths



Bond angles

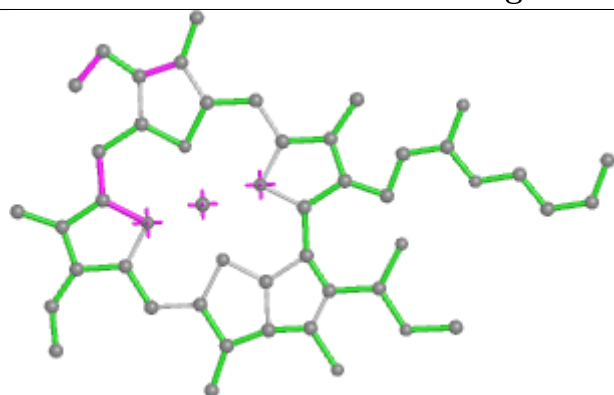


Torsions

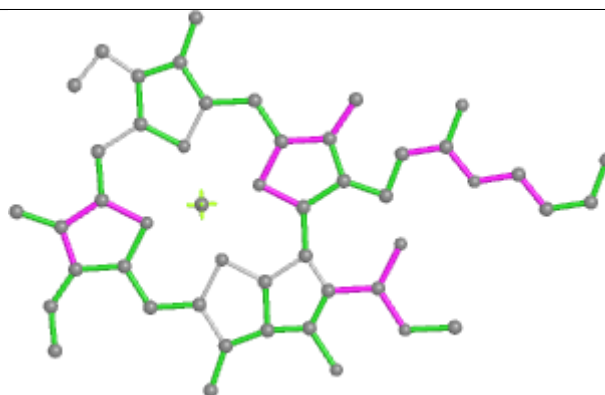


Rings

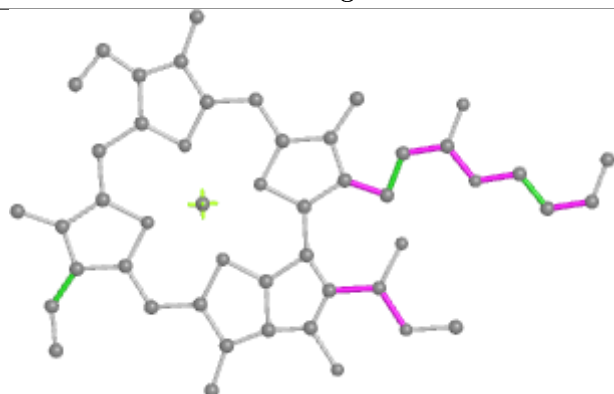
## Ligand CLA B 1210



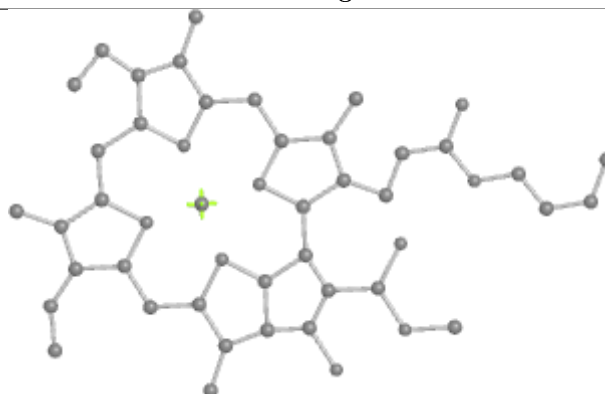
Bond lengths



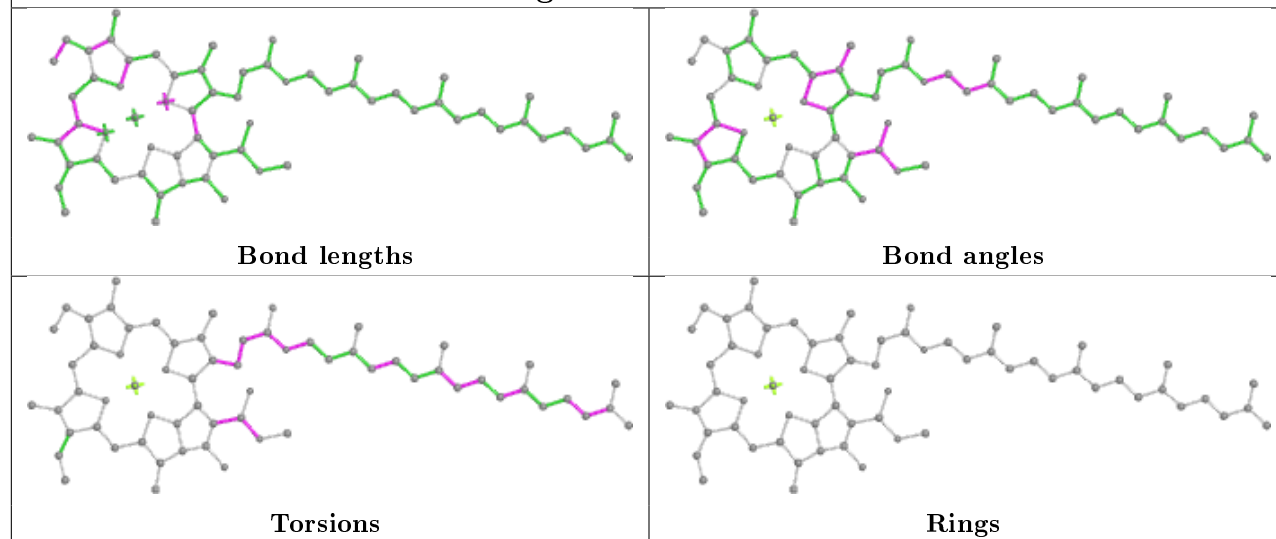
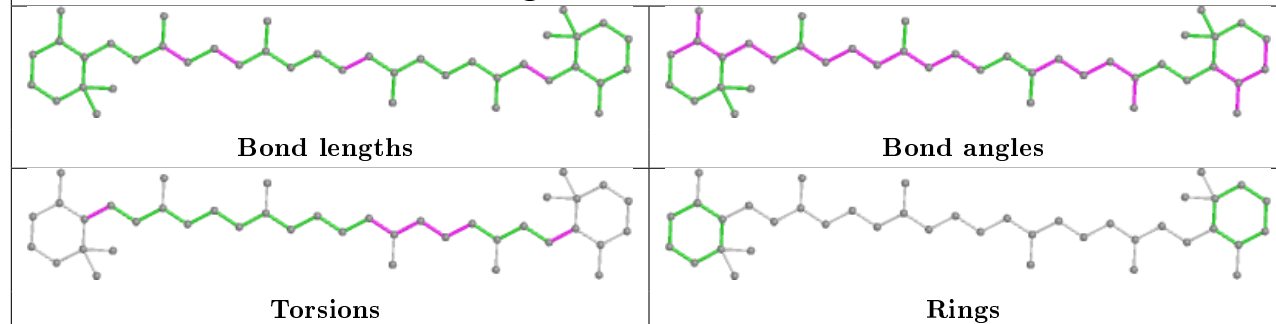
Bond angles



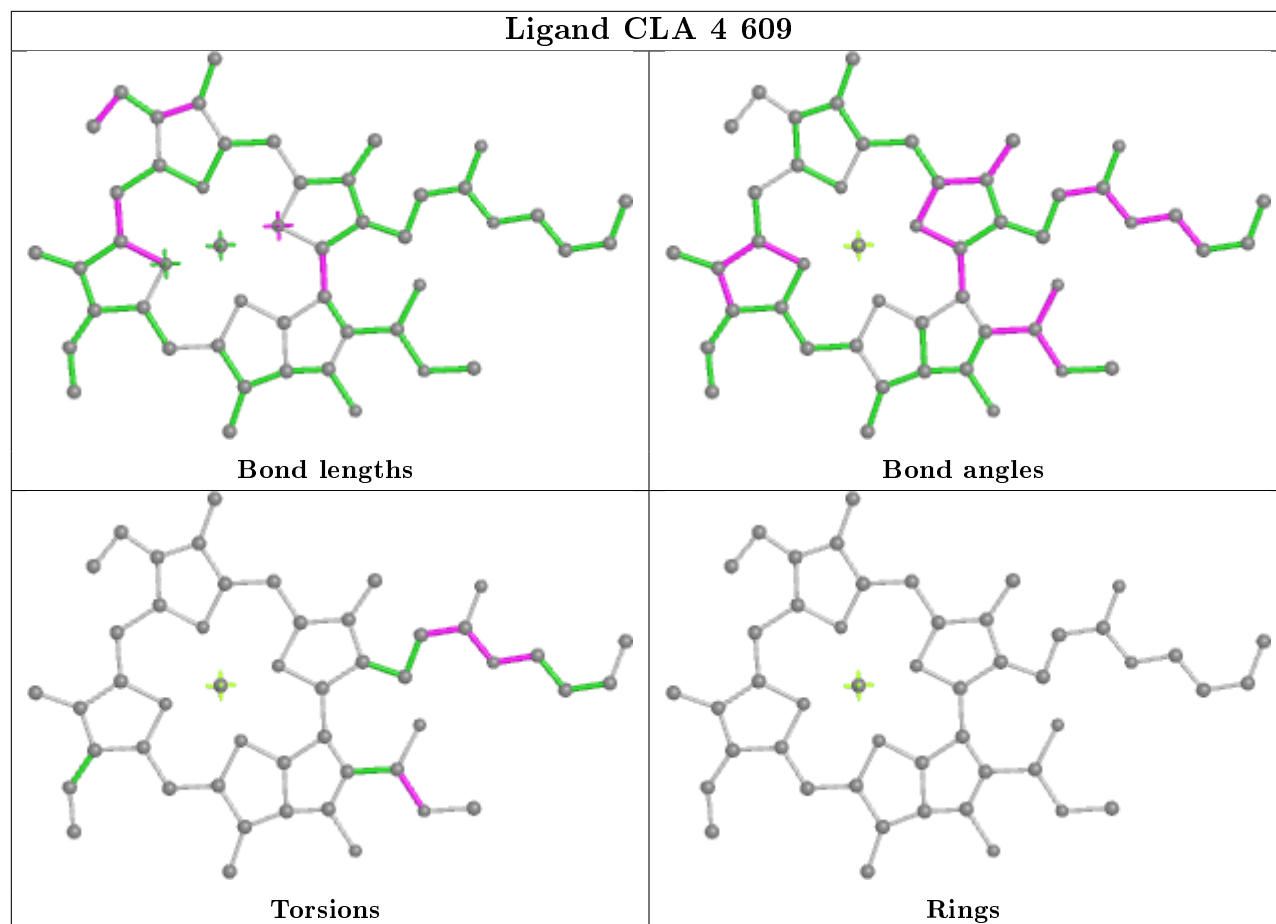
Torsions

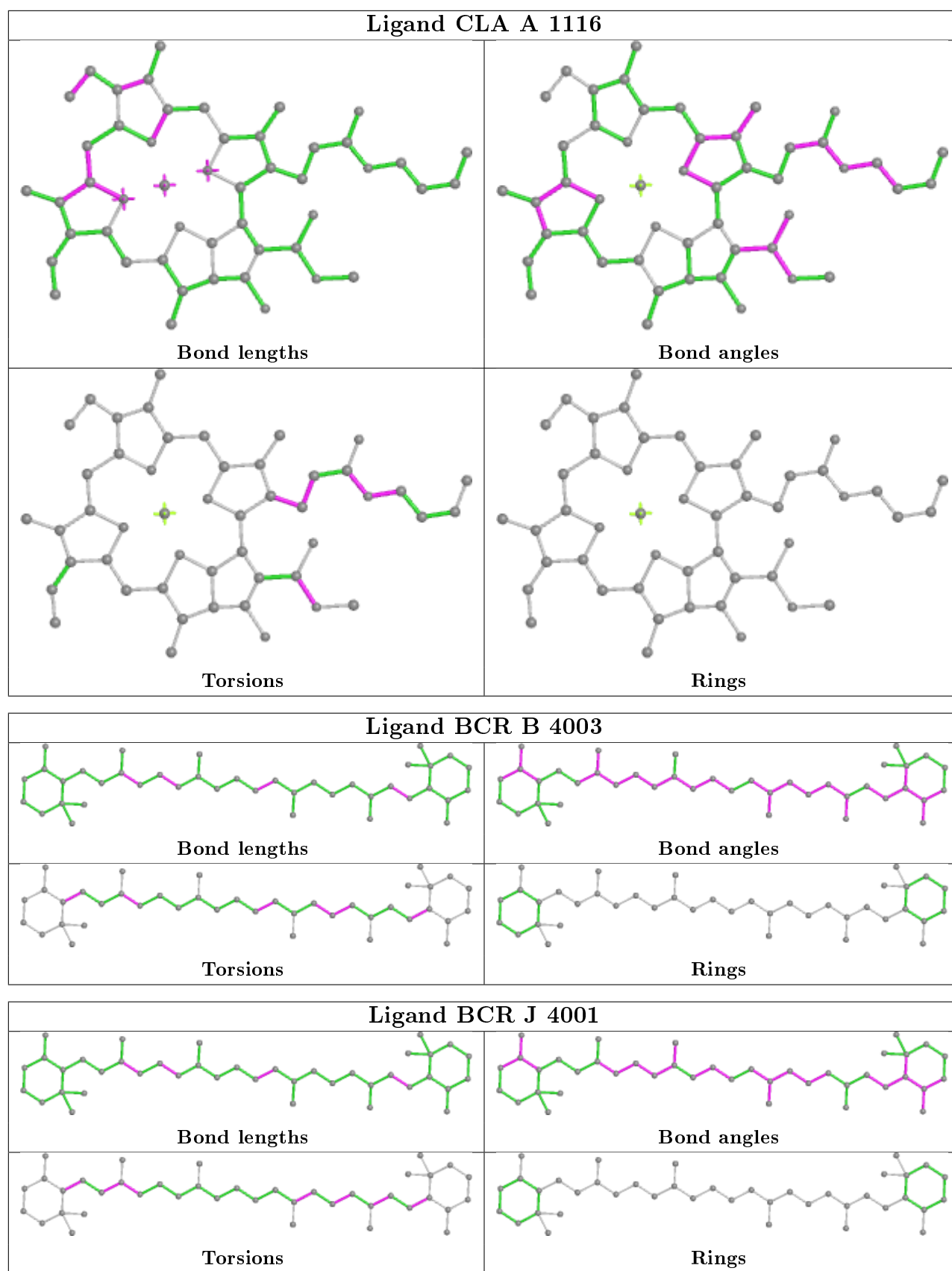


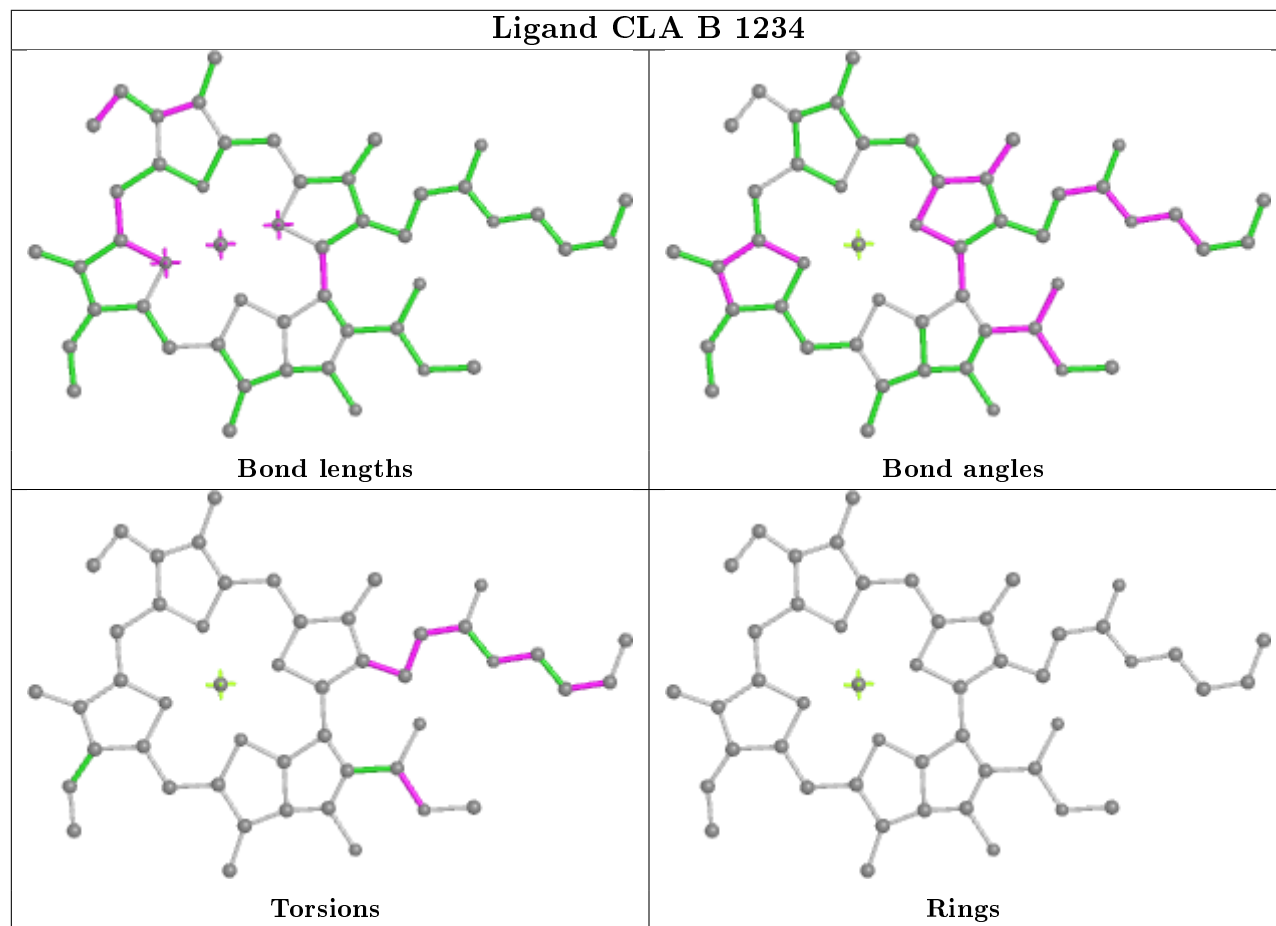
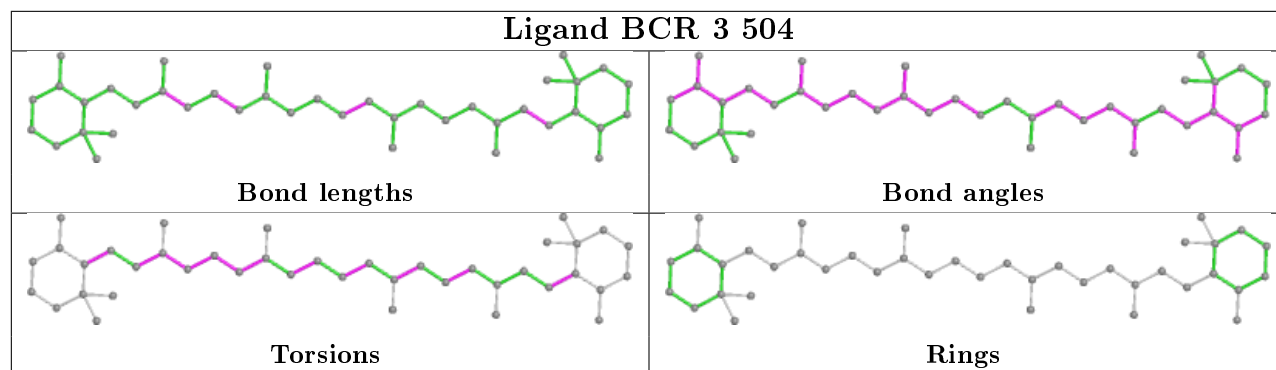
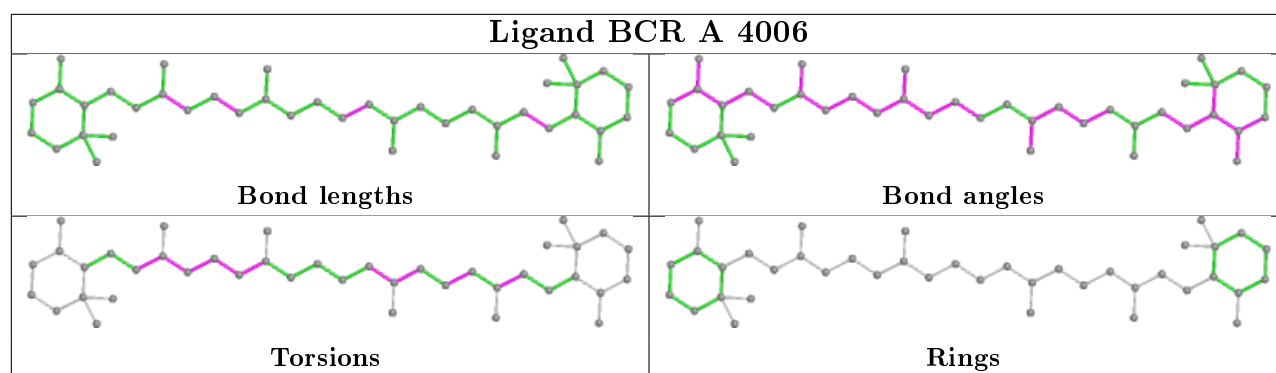
Rings

**Ligand CLA 1 615****Ligand BCR A 4004**

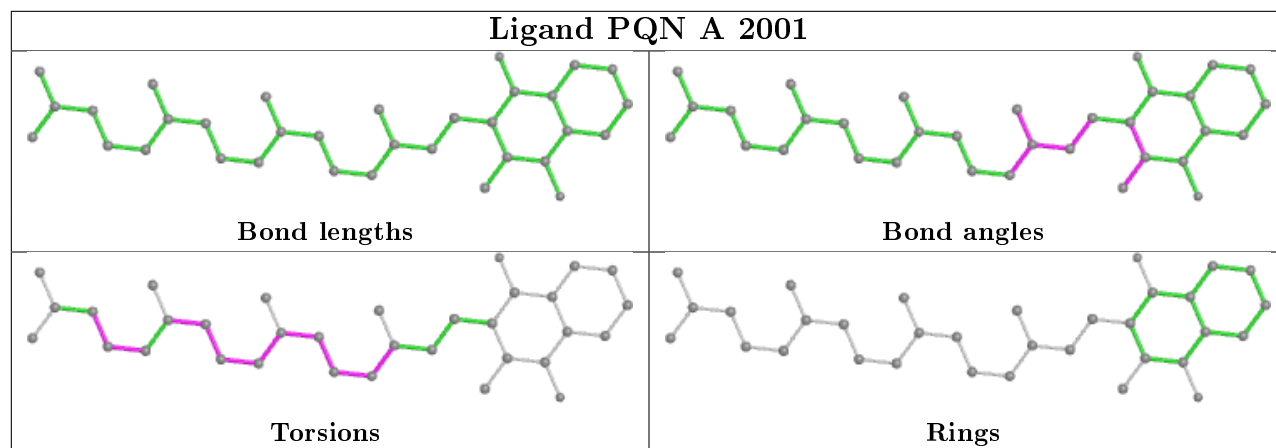
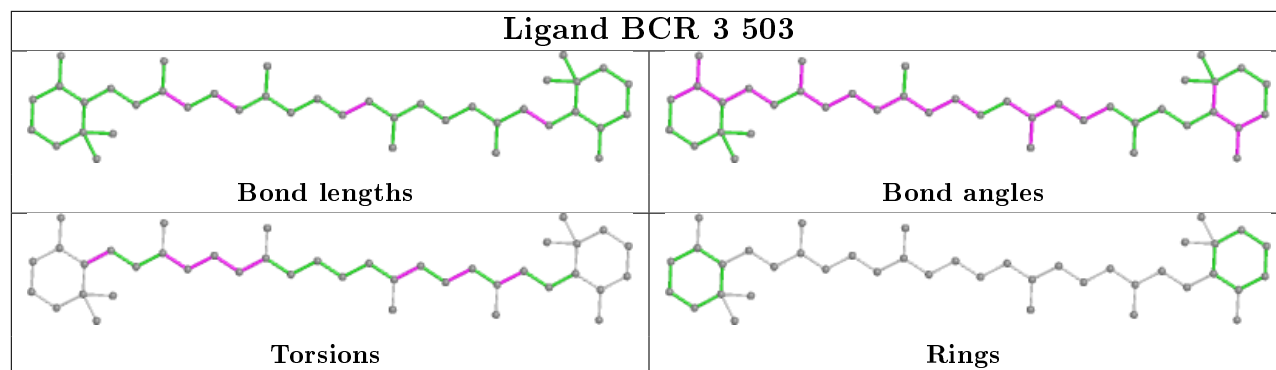
## Ligand CLA 4 609



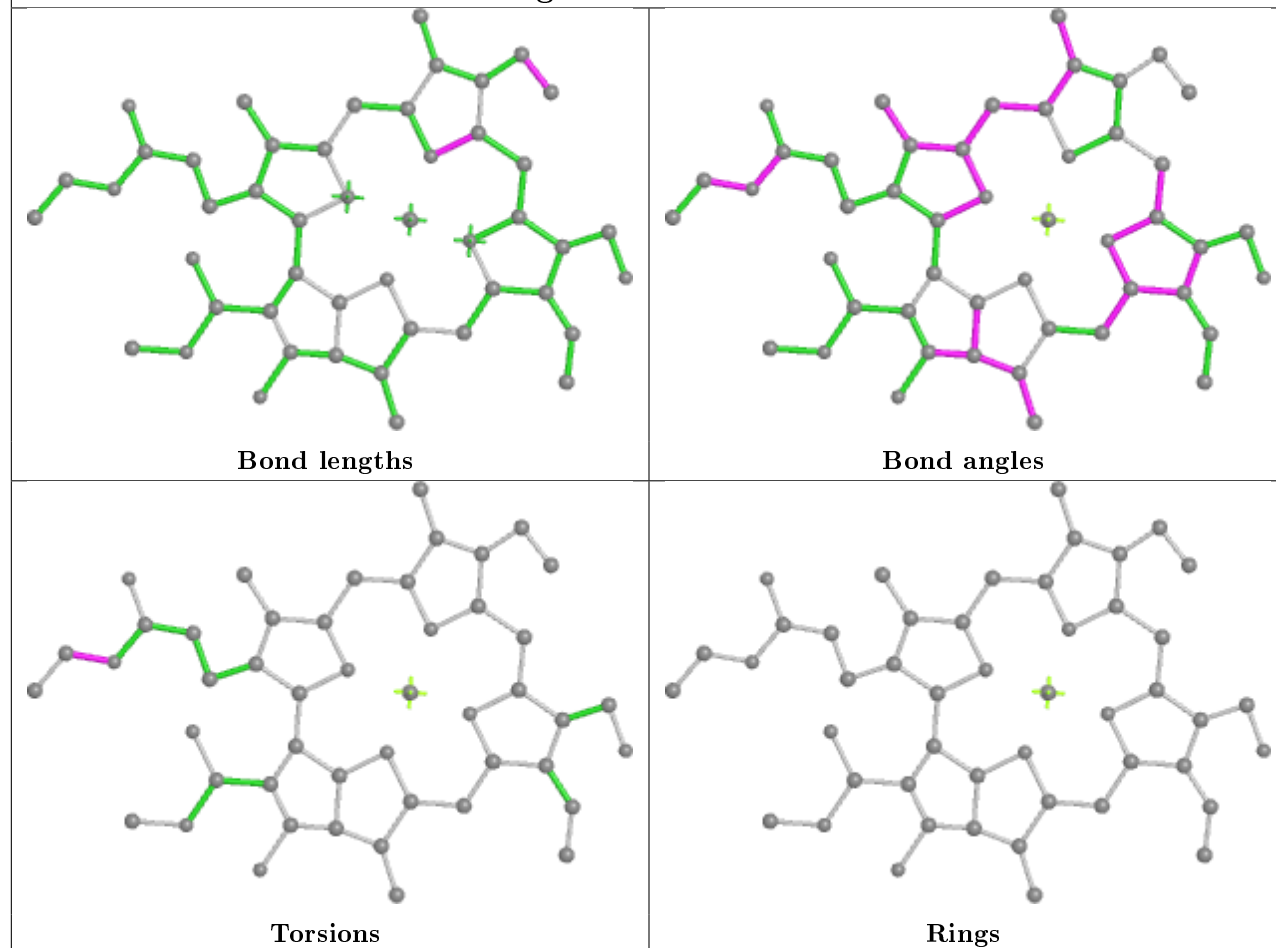




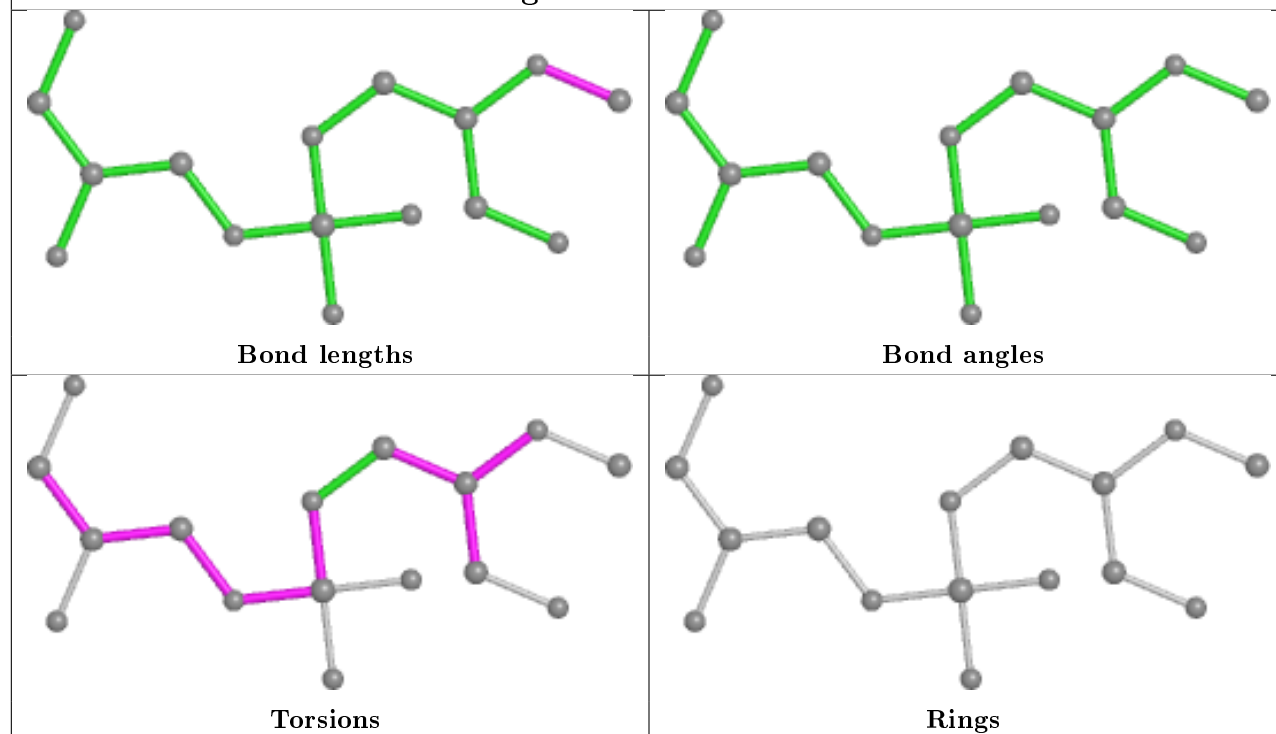


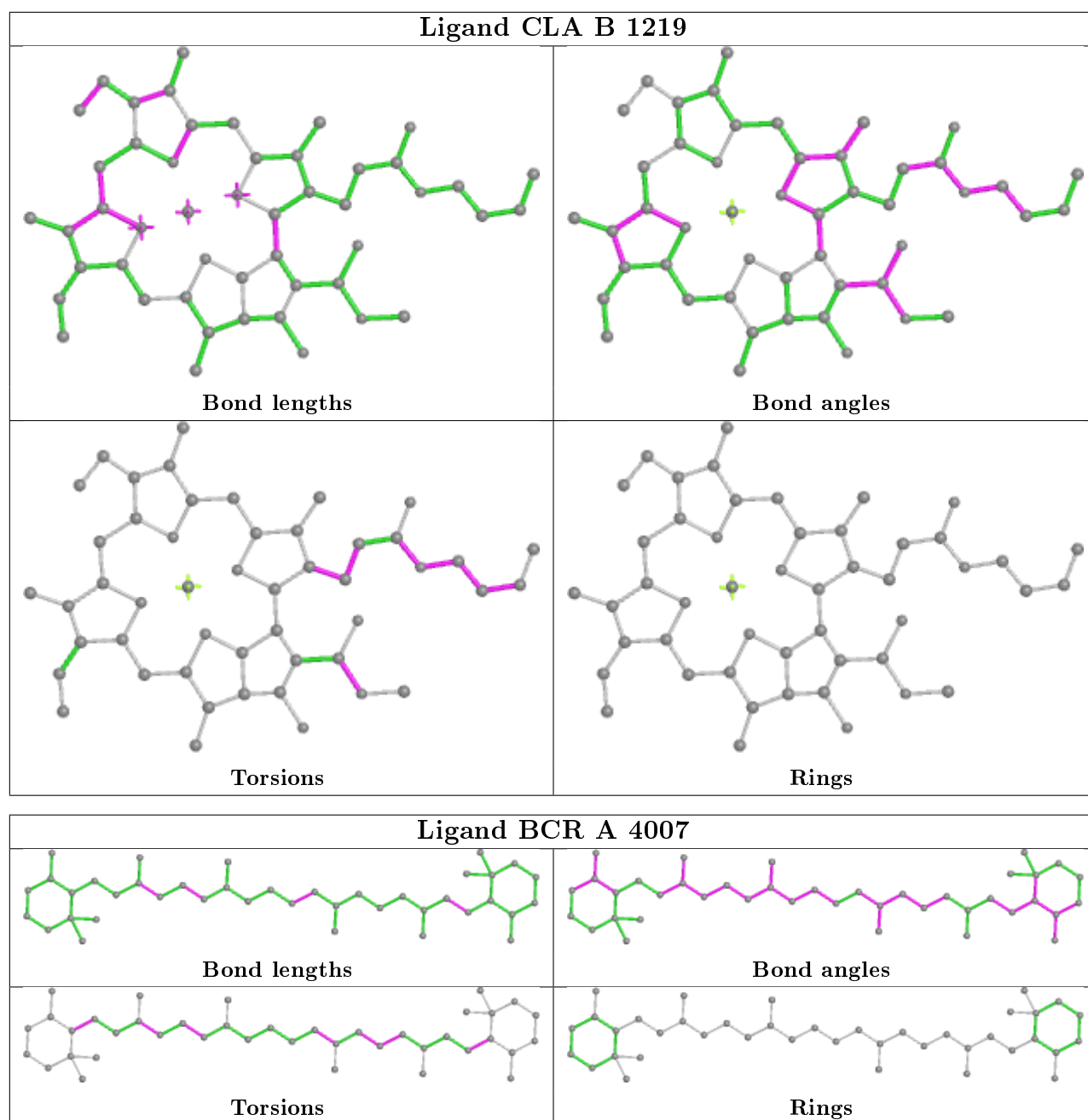


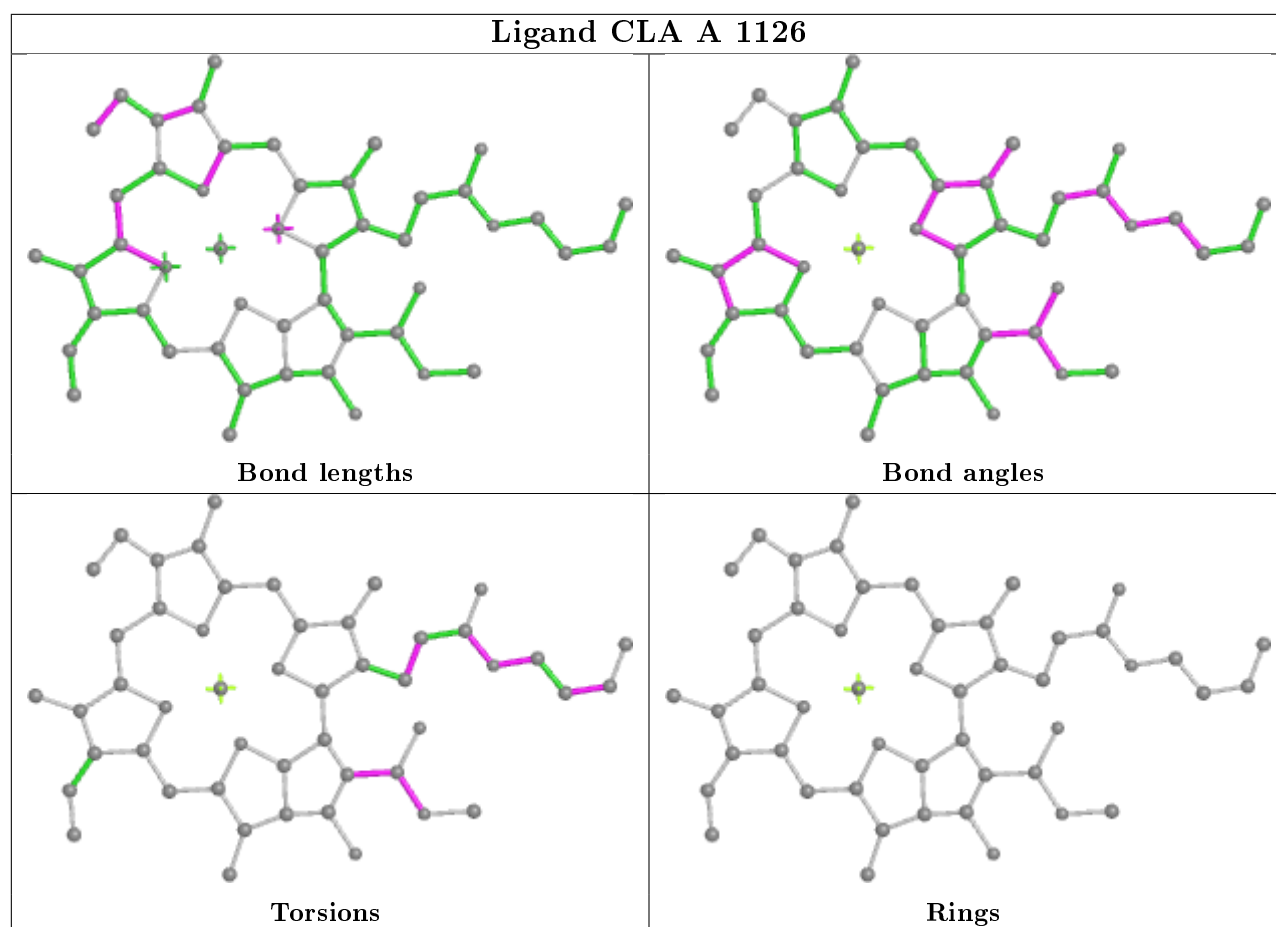
## Ligand CHL 2 611



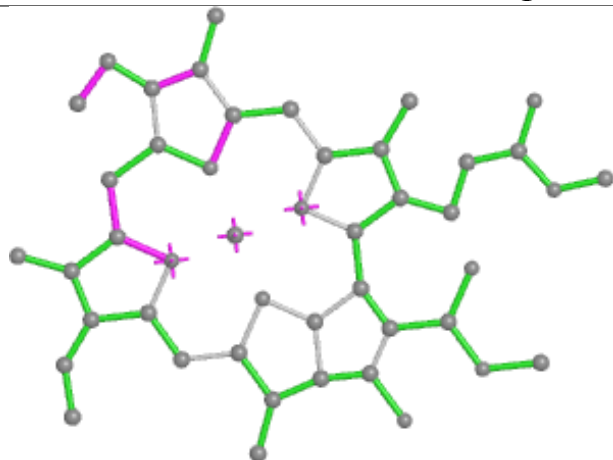
## Ligand LHG A 5001



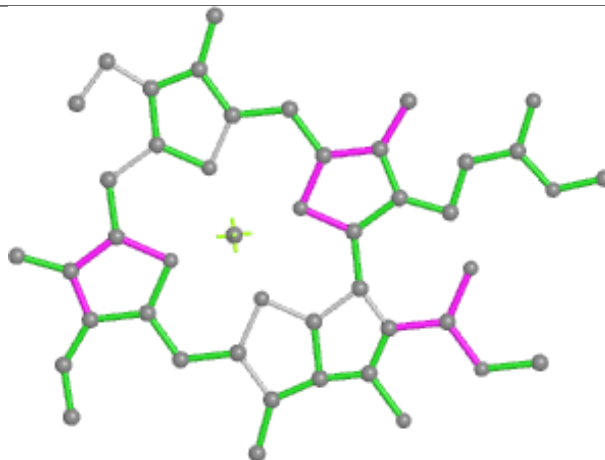




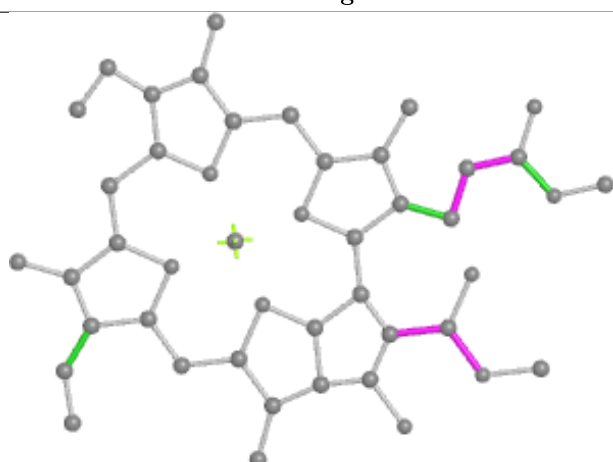
## Ligand CLA 2 603



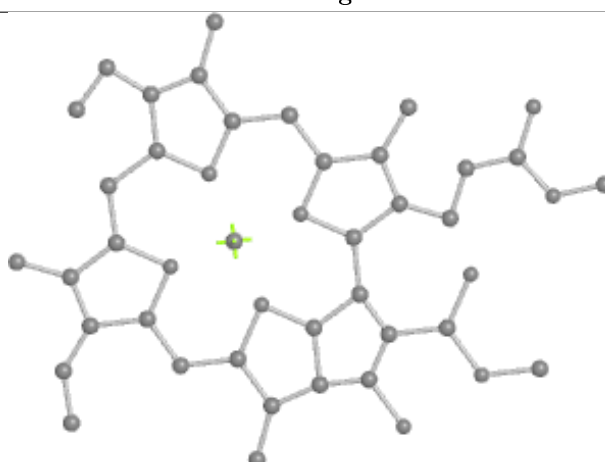
Bond lengths



Bond angles

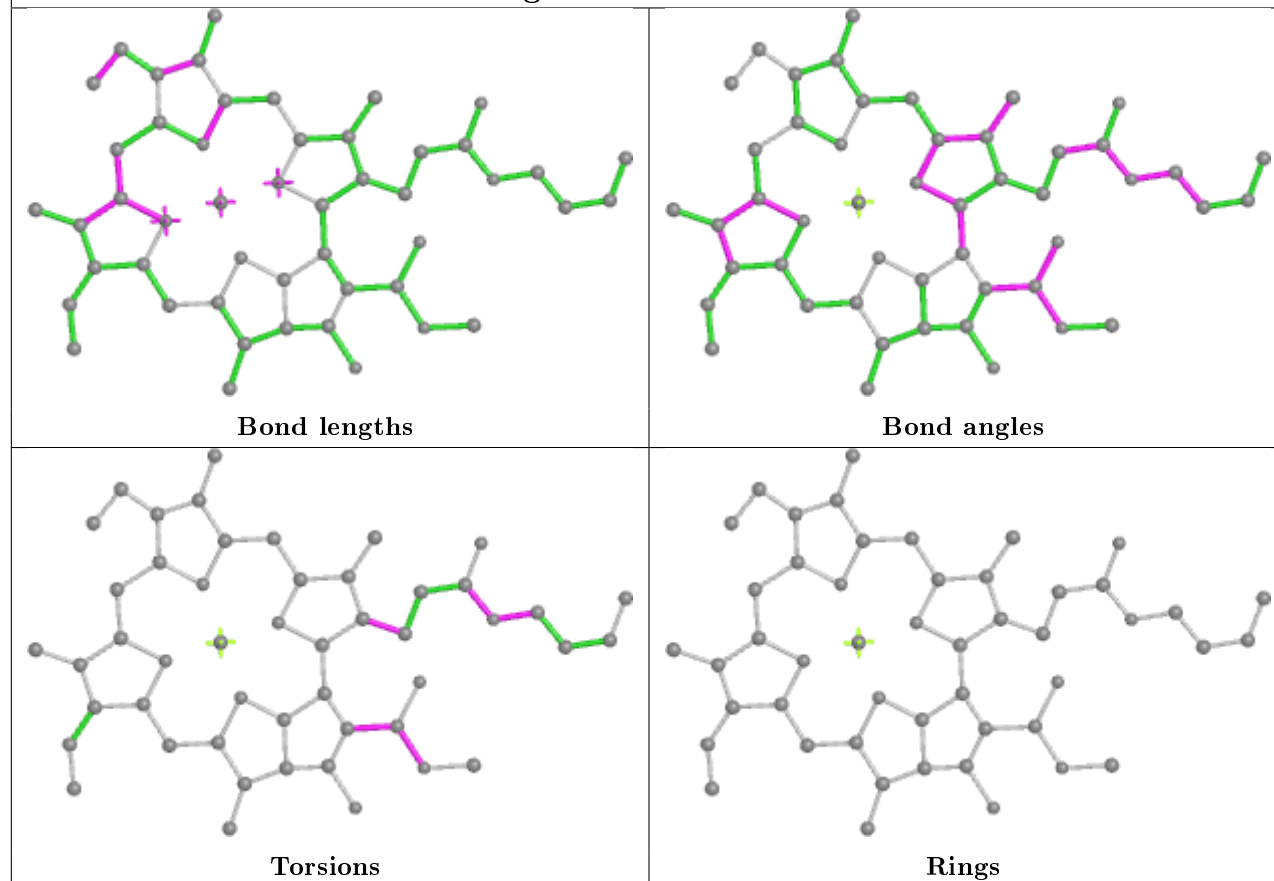


Torsions

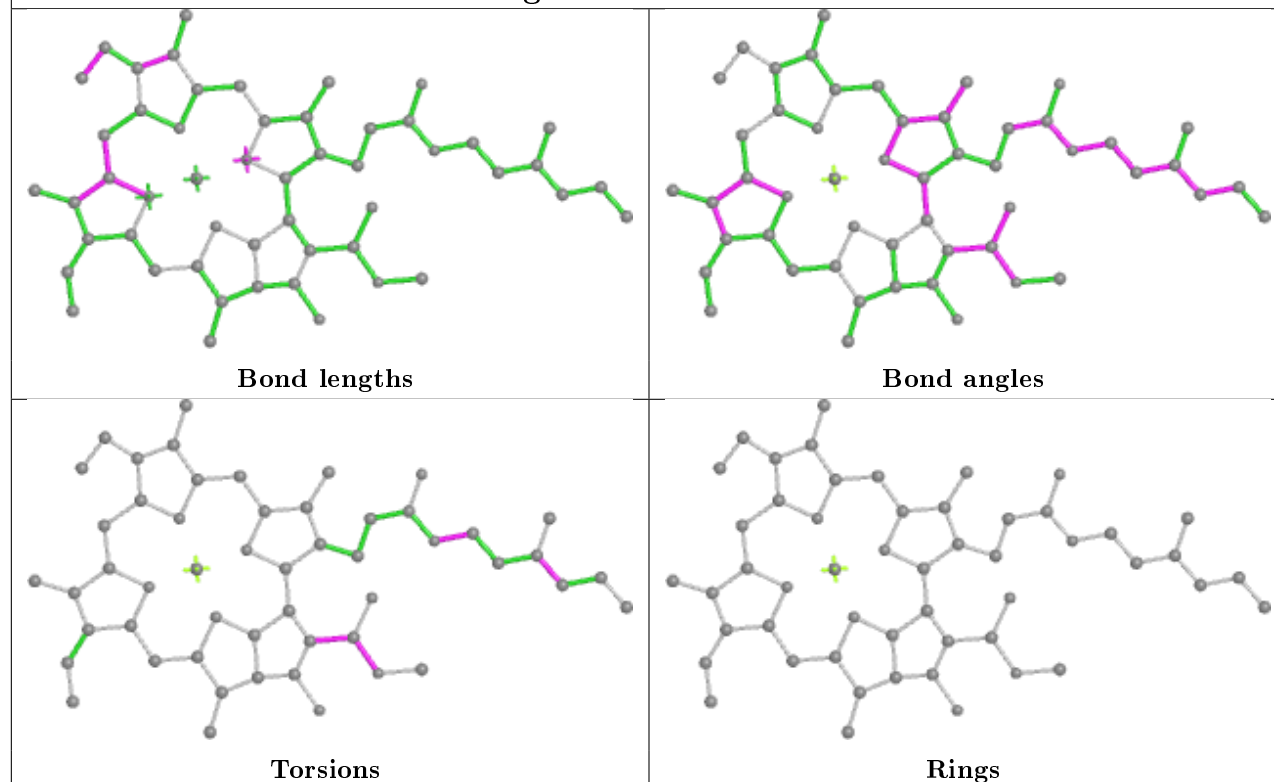


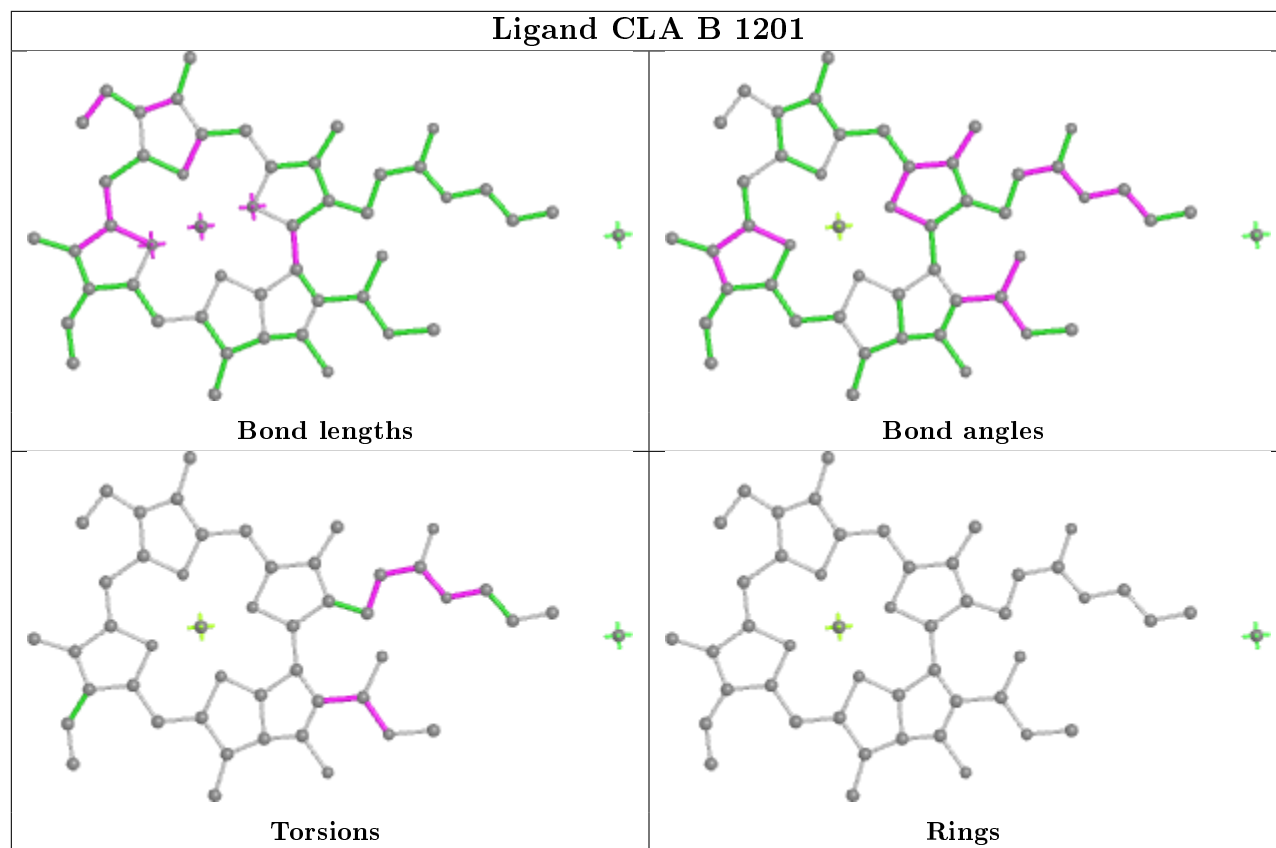
Rings

## Ligand CLA A 1112

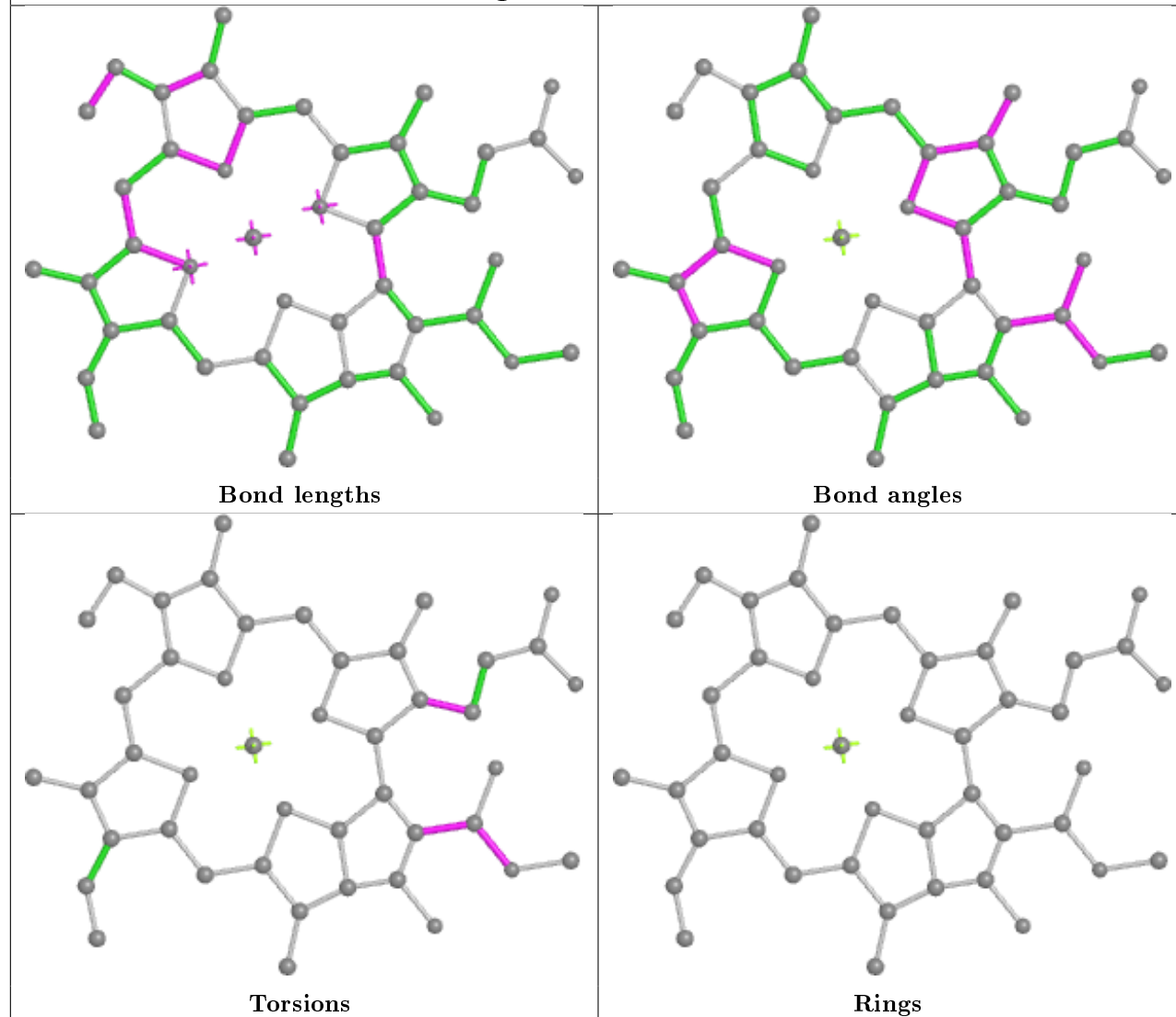


## Ligand CLA A 1139

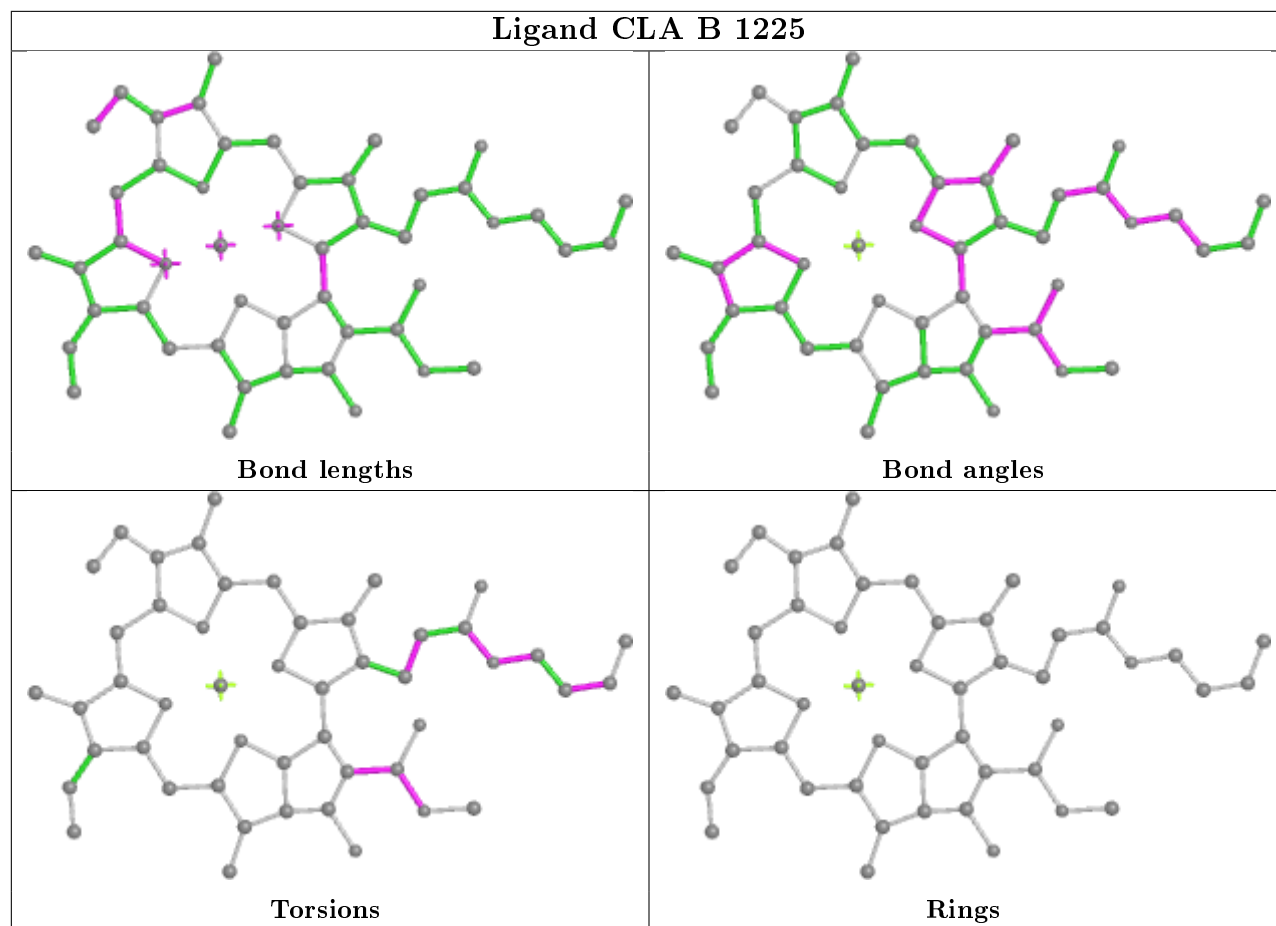


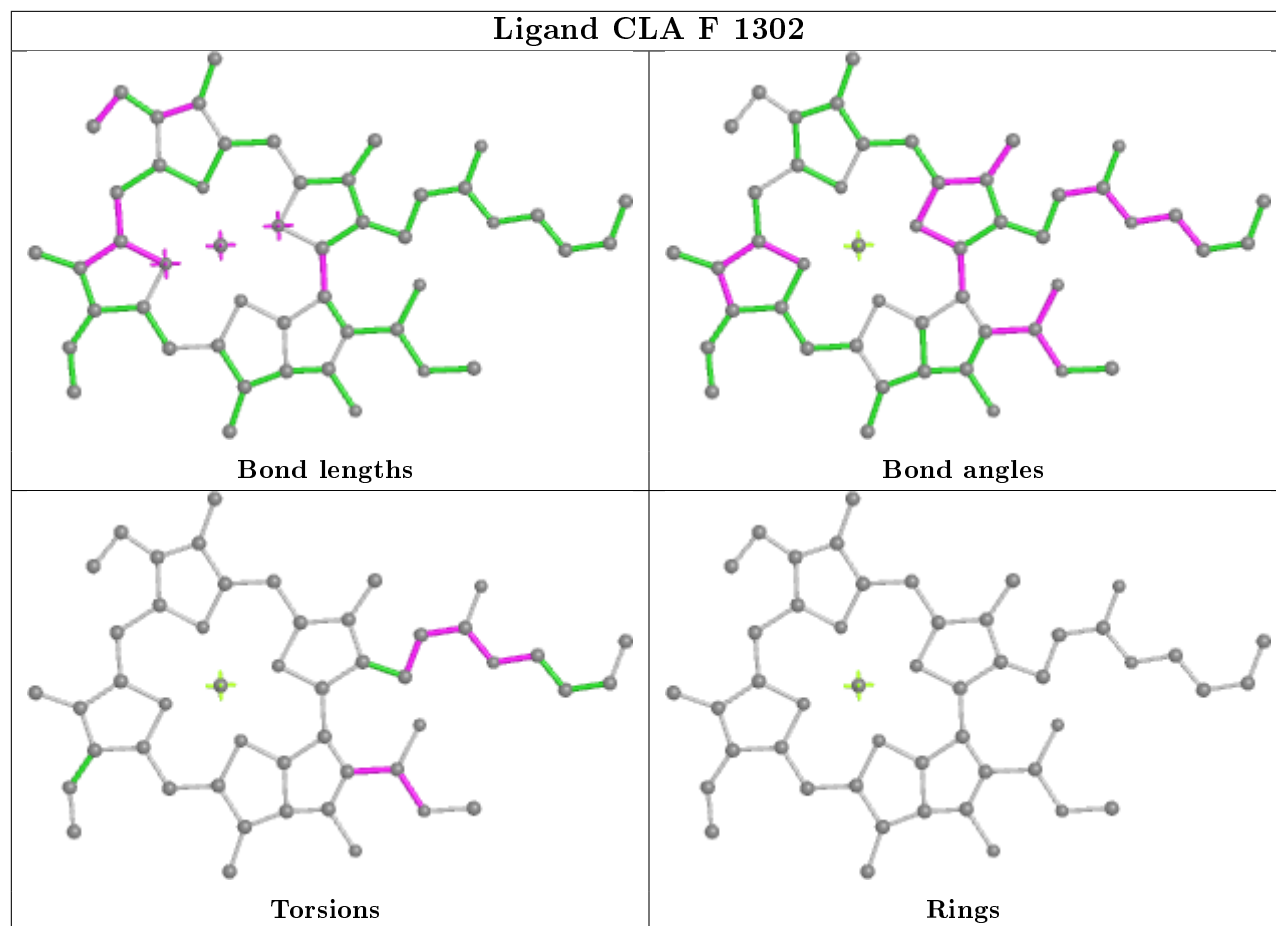


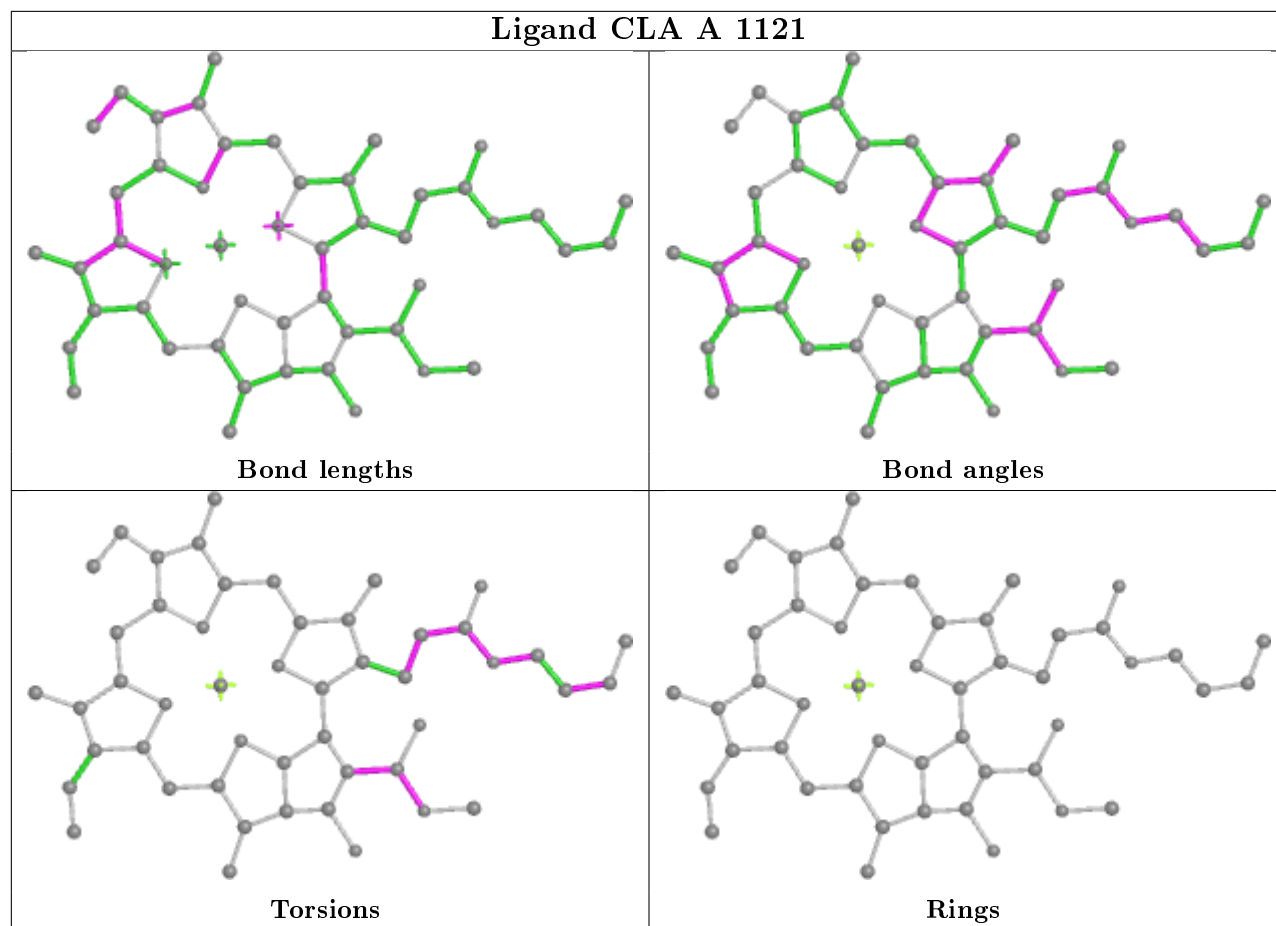
## Ligand CLA 1 603



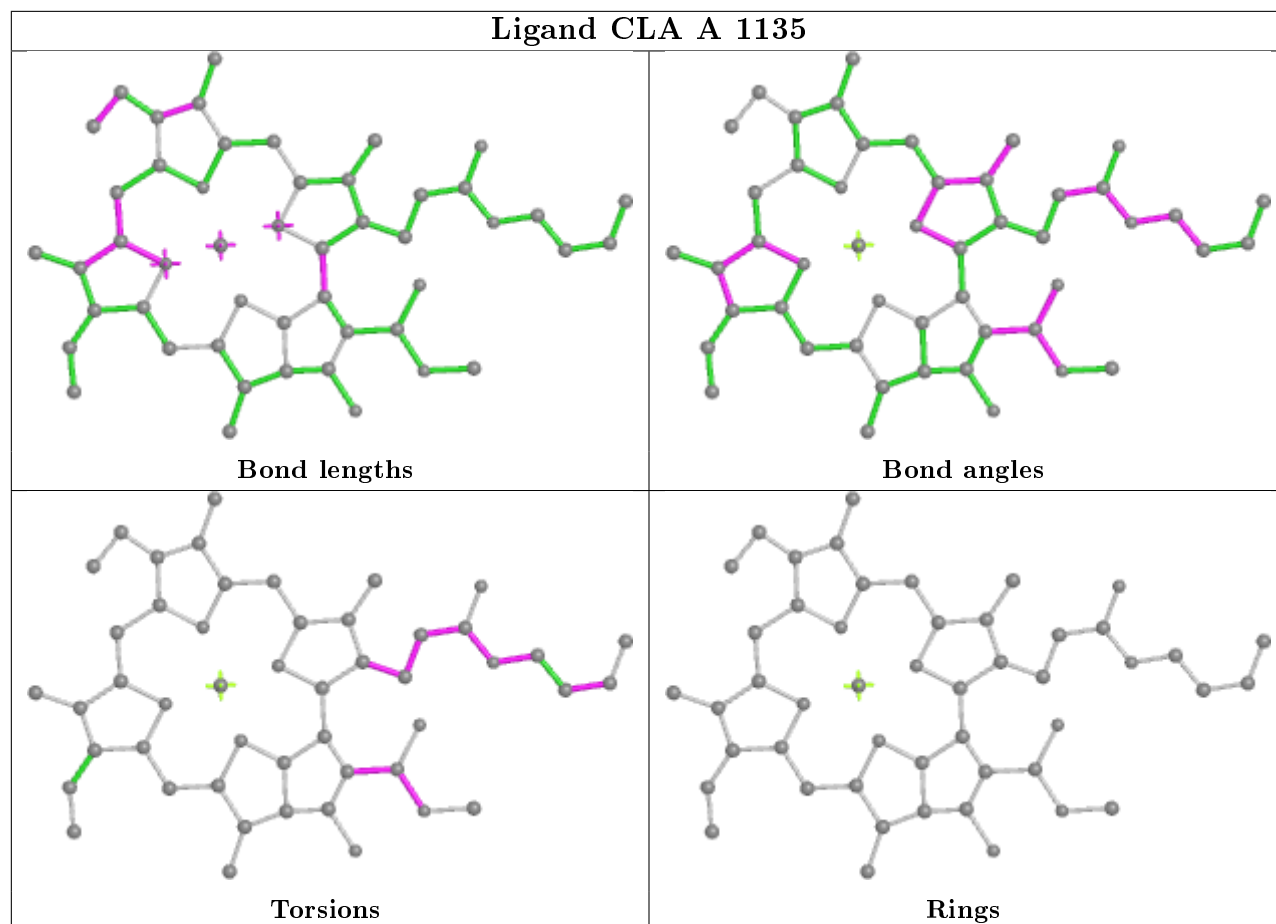




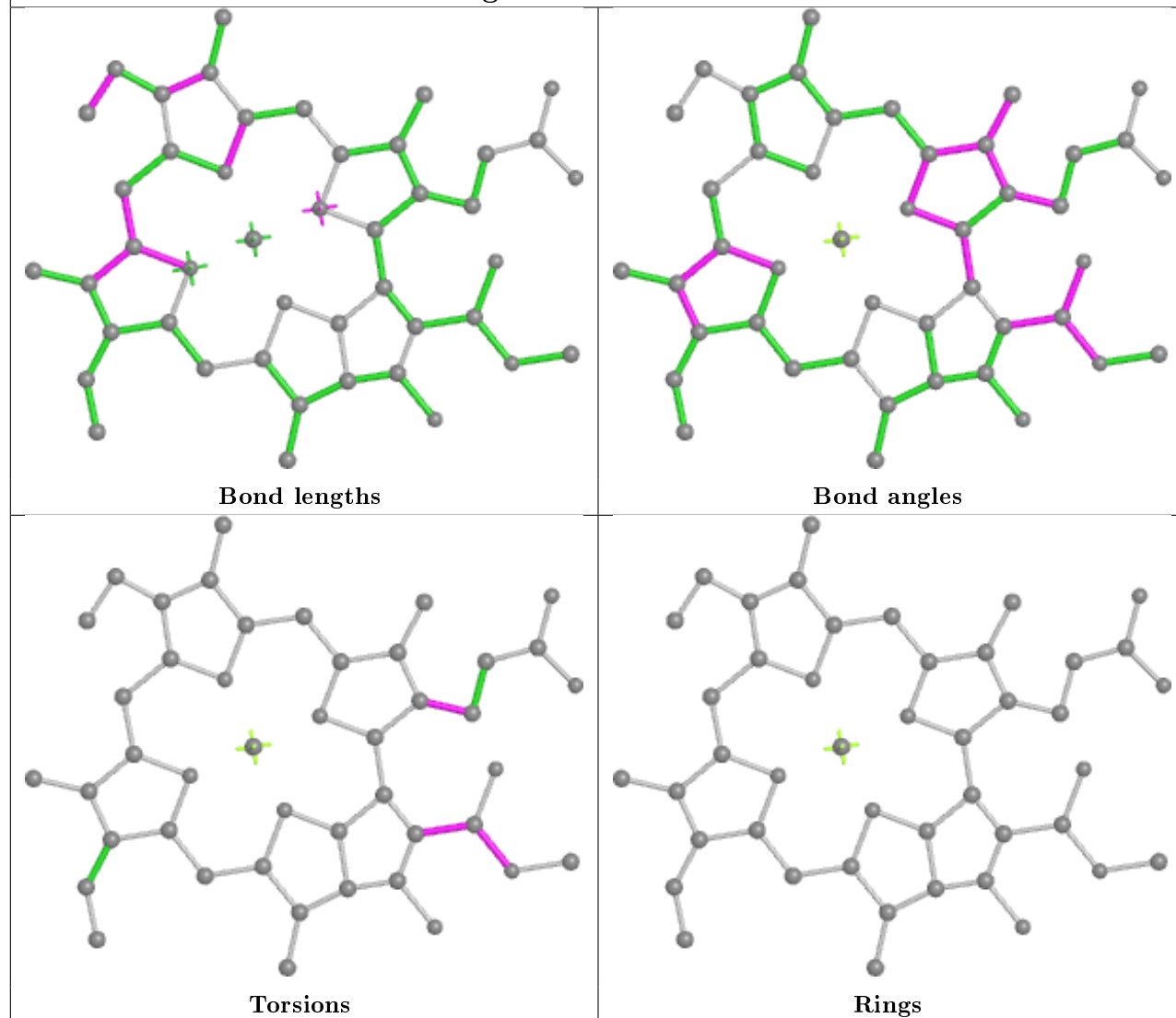




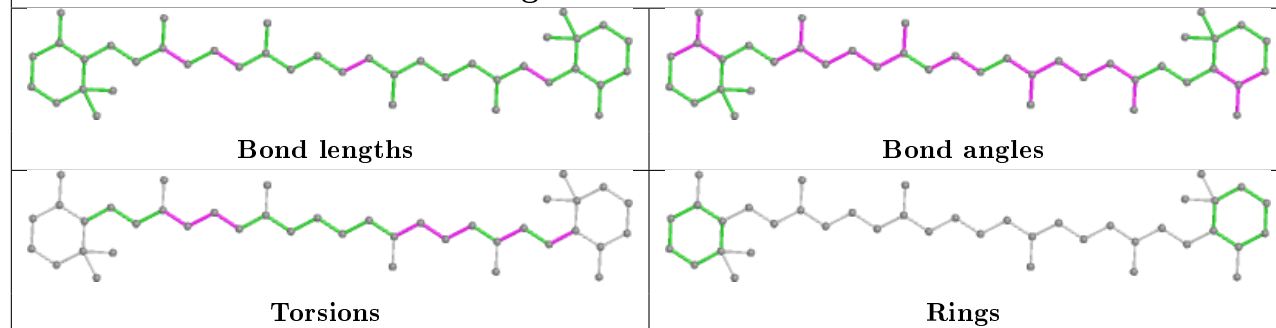
## Ligand CLA A 1135



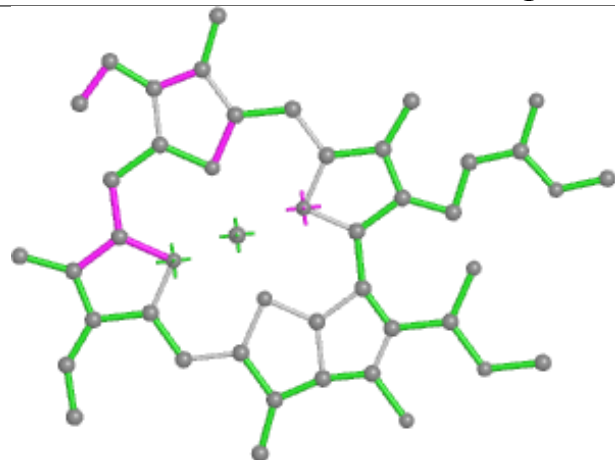
## Ligand CLA A 1101



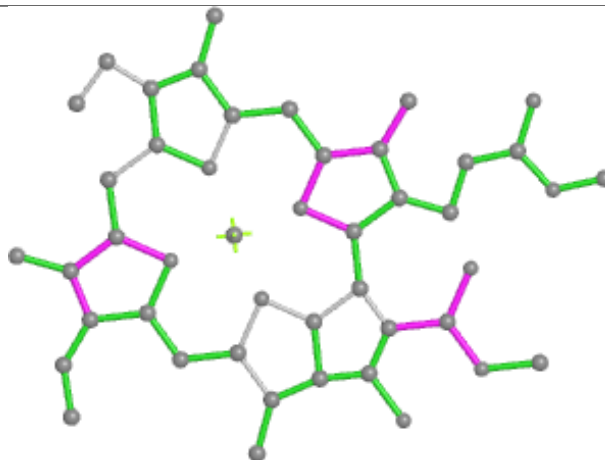
## Ligand BCR A 4003



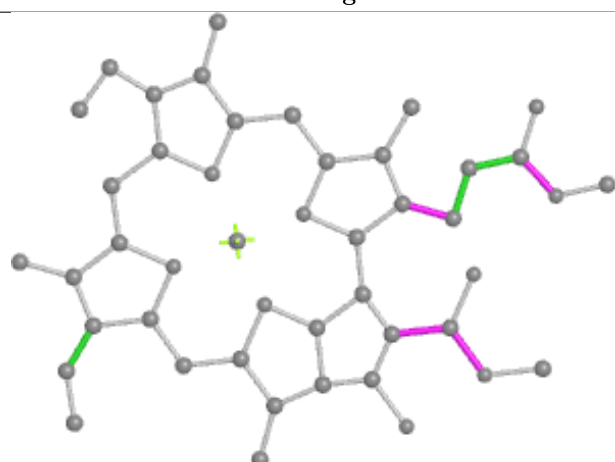
## Ligand CLA 1 608



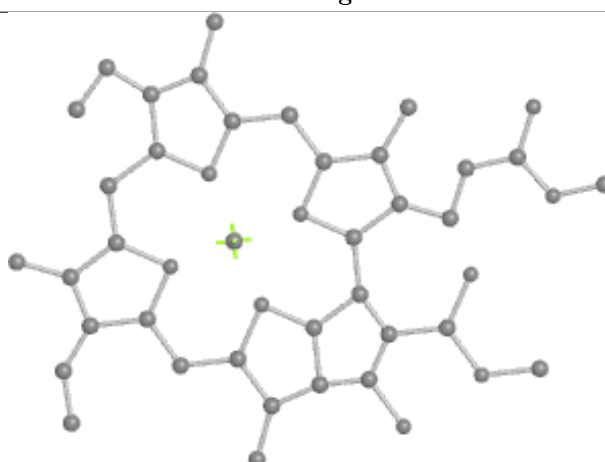
Bond lengths



Bond angles

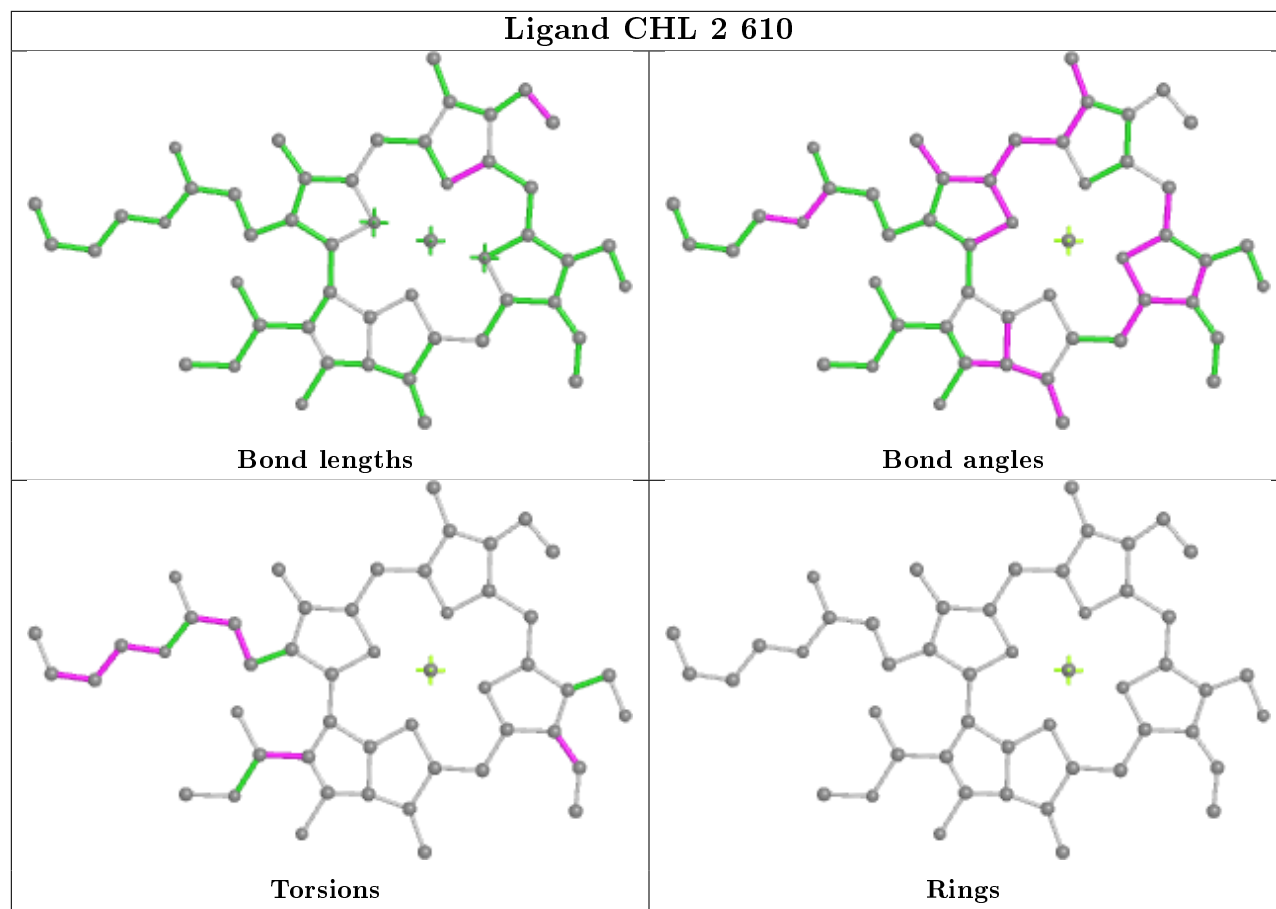


Torsions

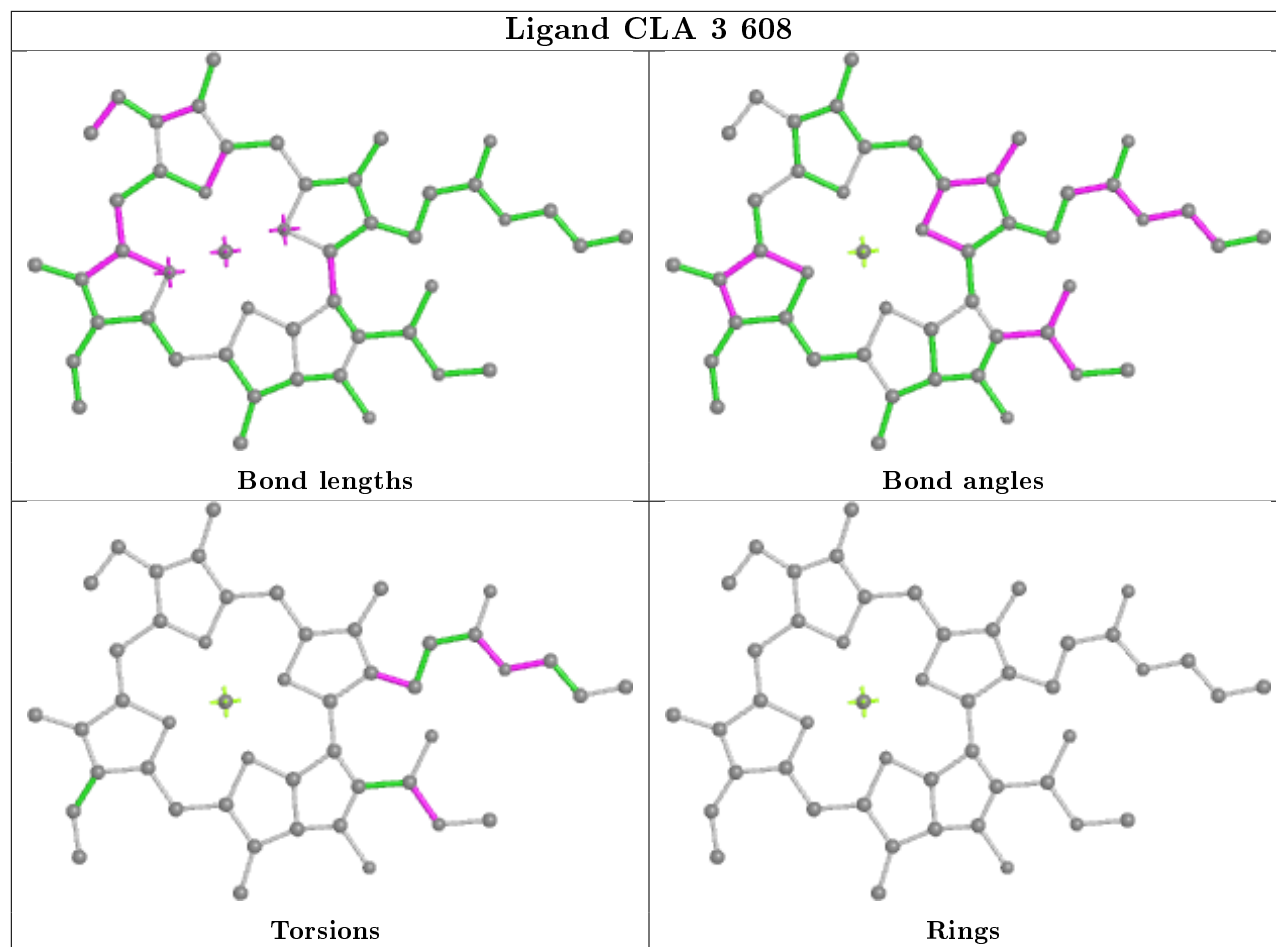


Rings

## Ligand CHL 2 610

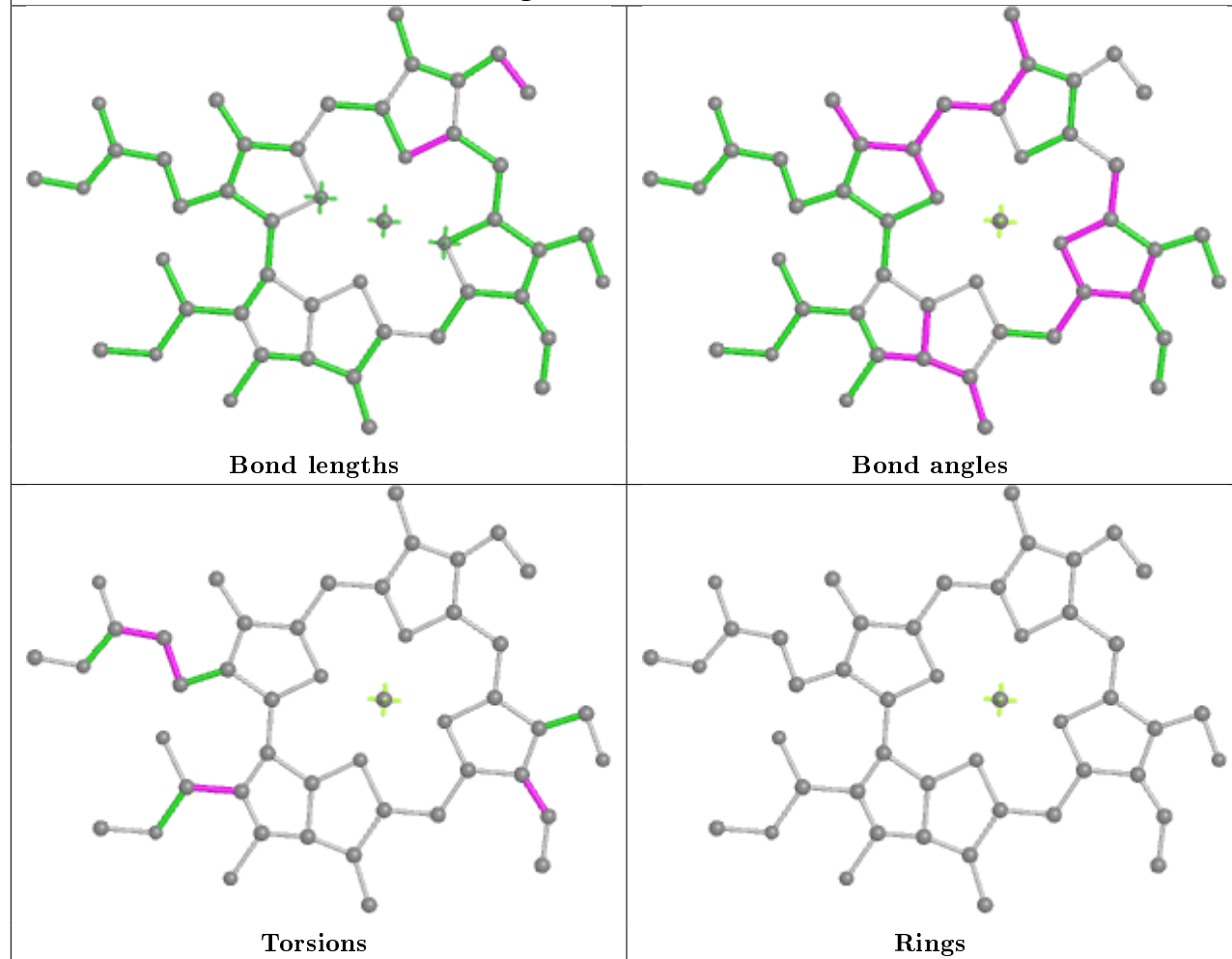


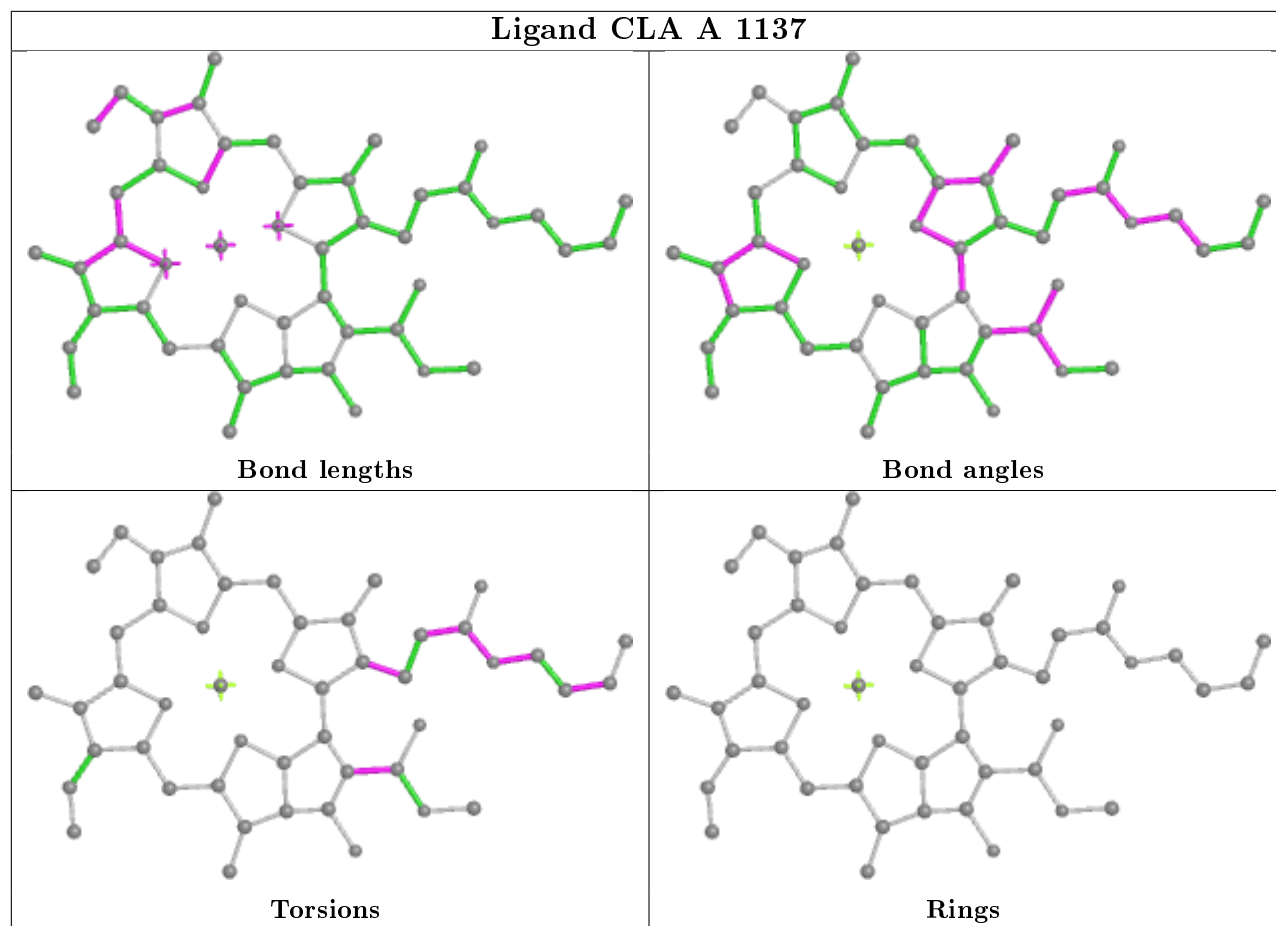
## Ligand CLA 3 608



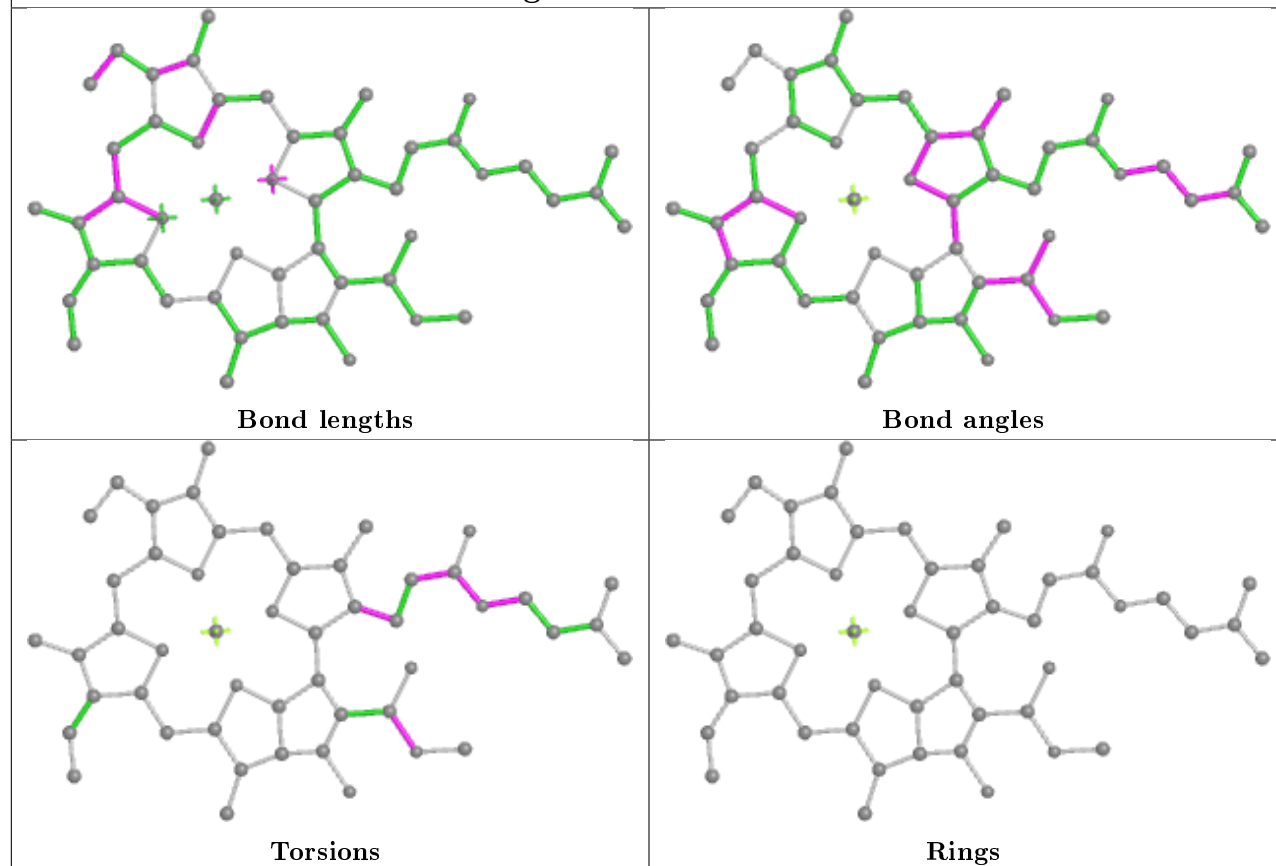


## Ligand CHL 3 604

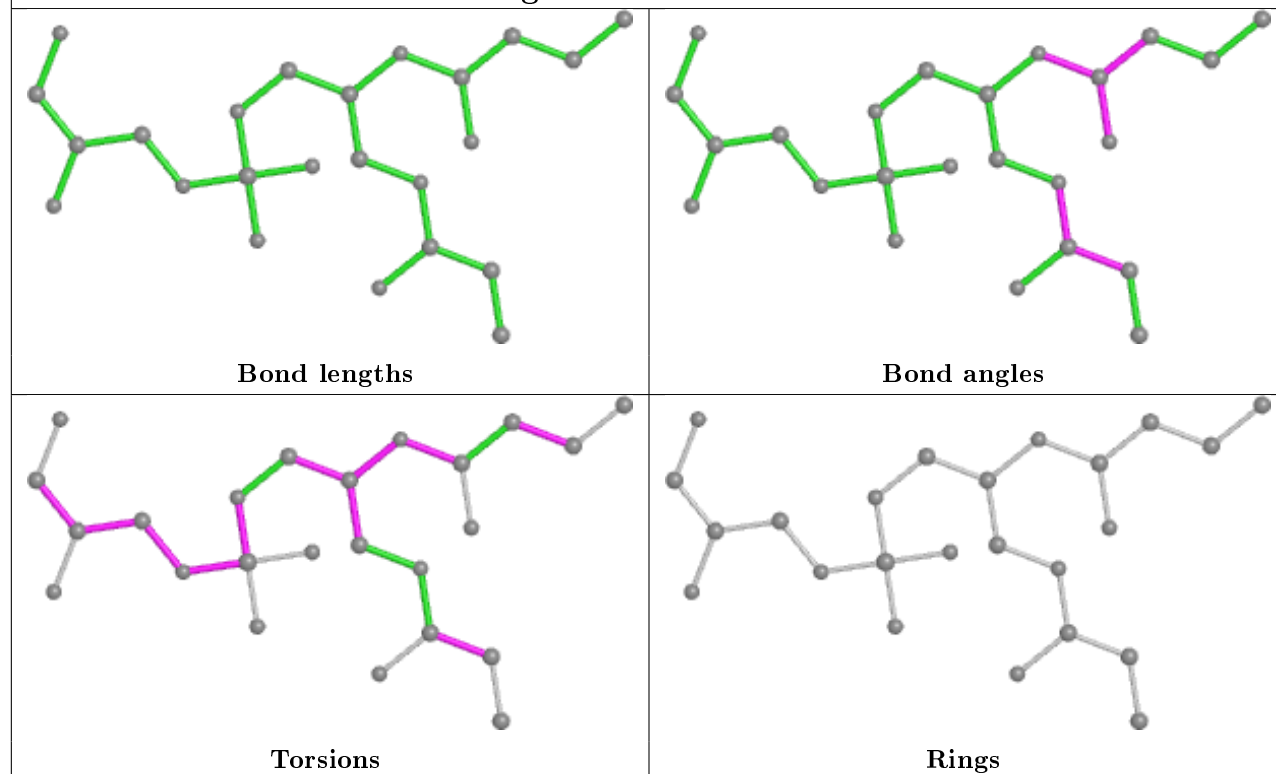


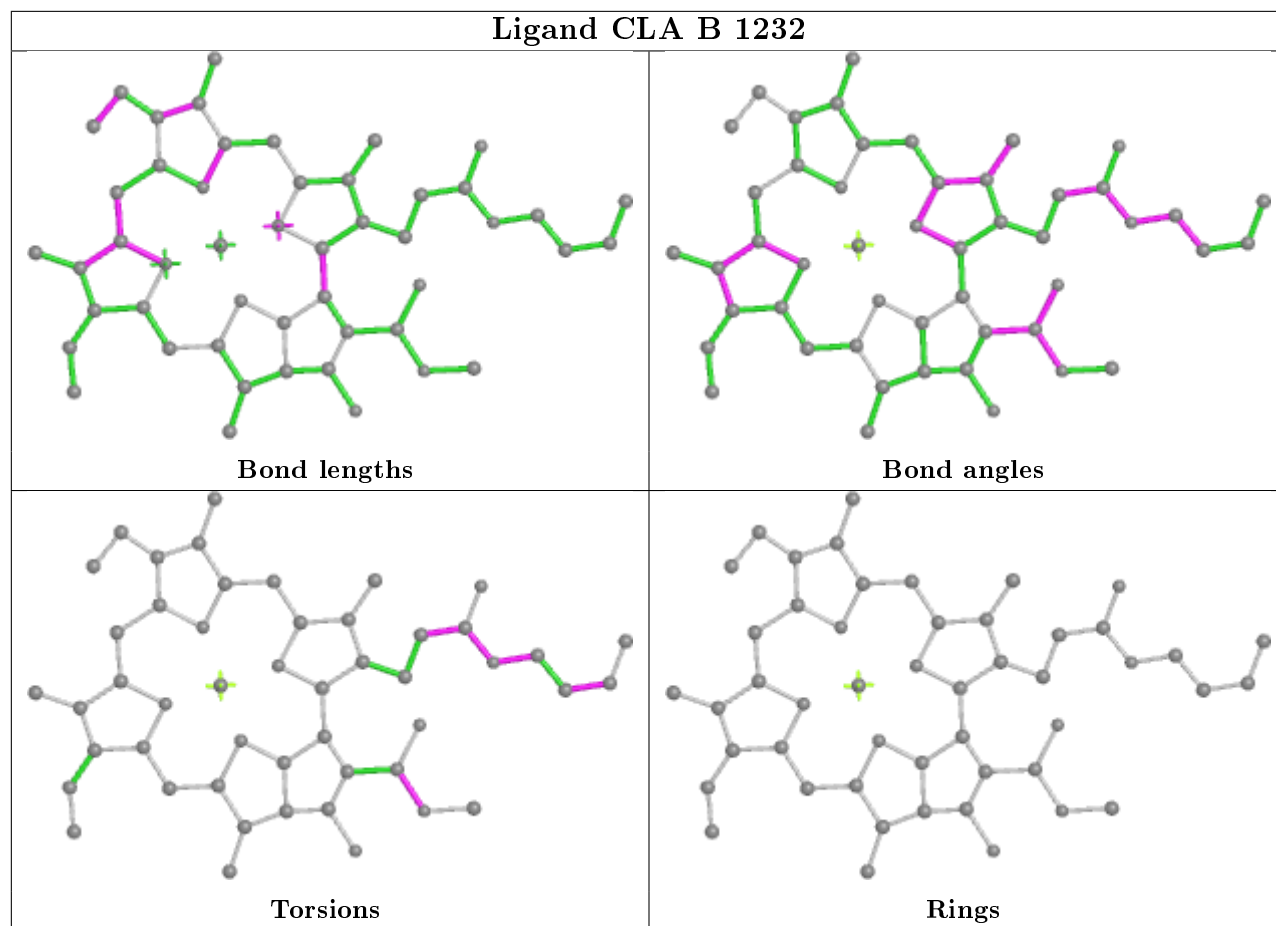


## Ligand CLA B 1238

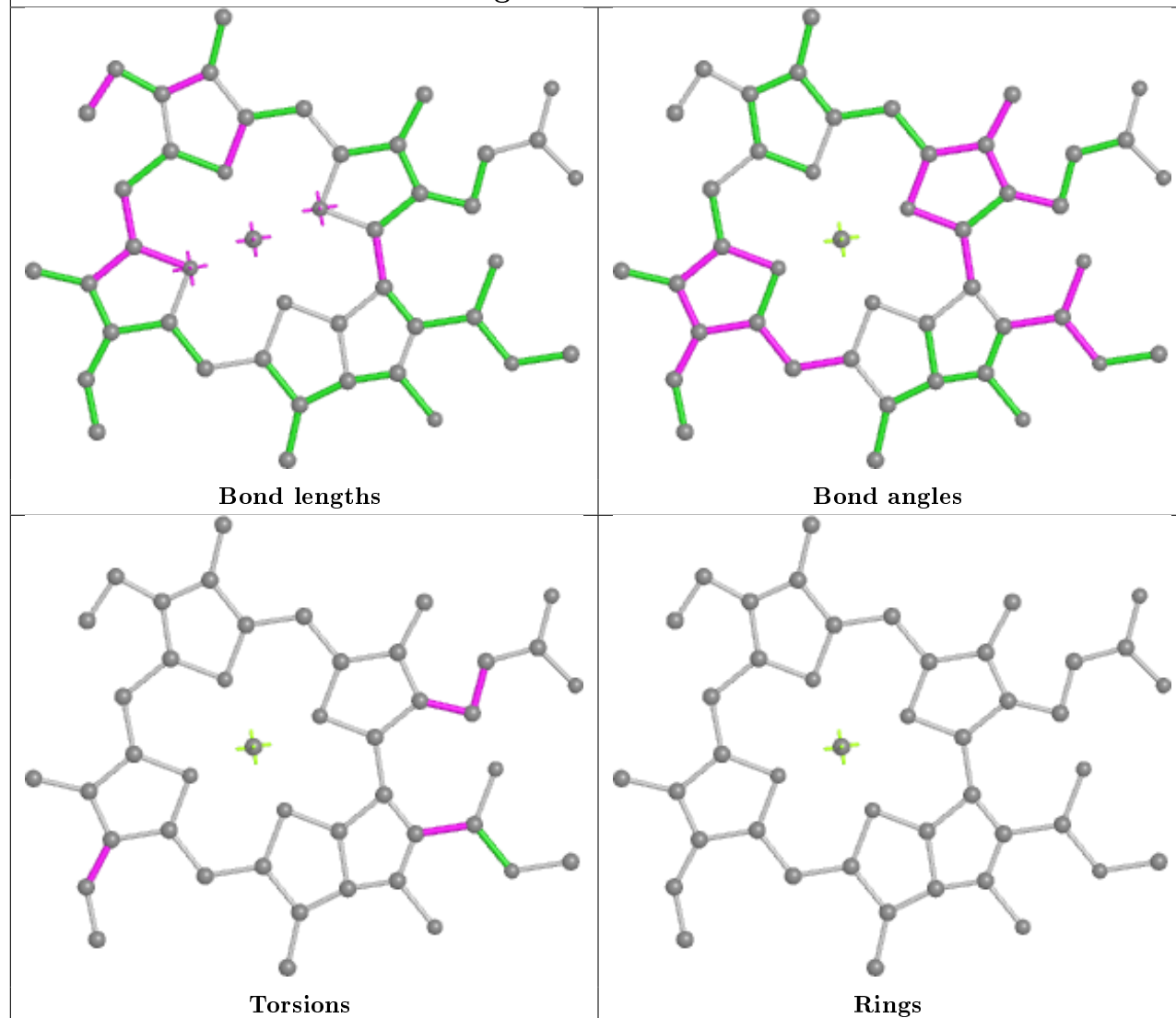


## Ligand LHG A 5002

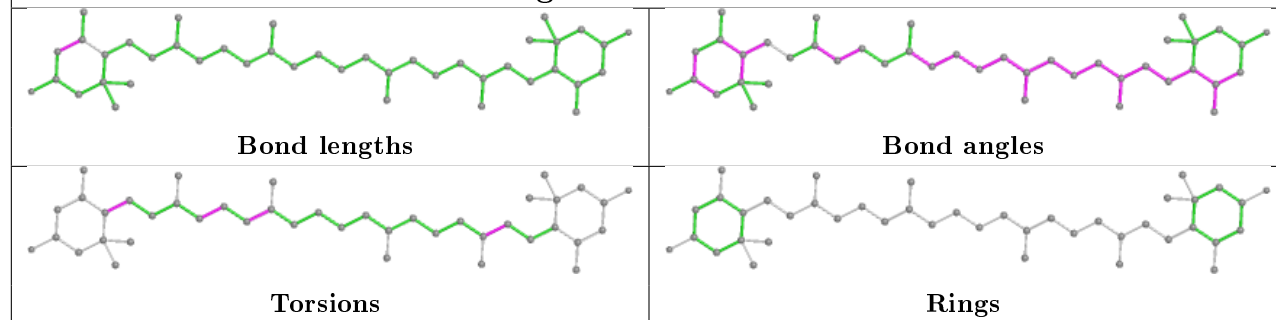


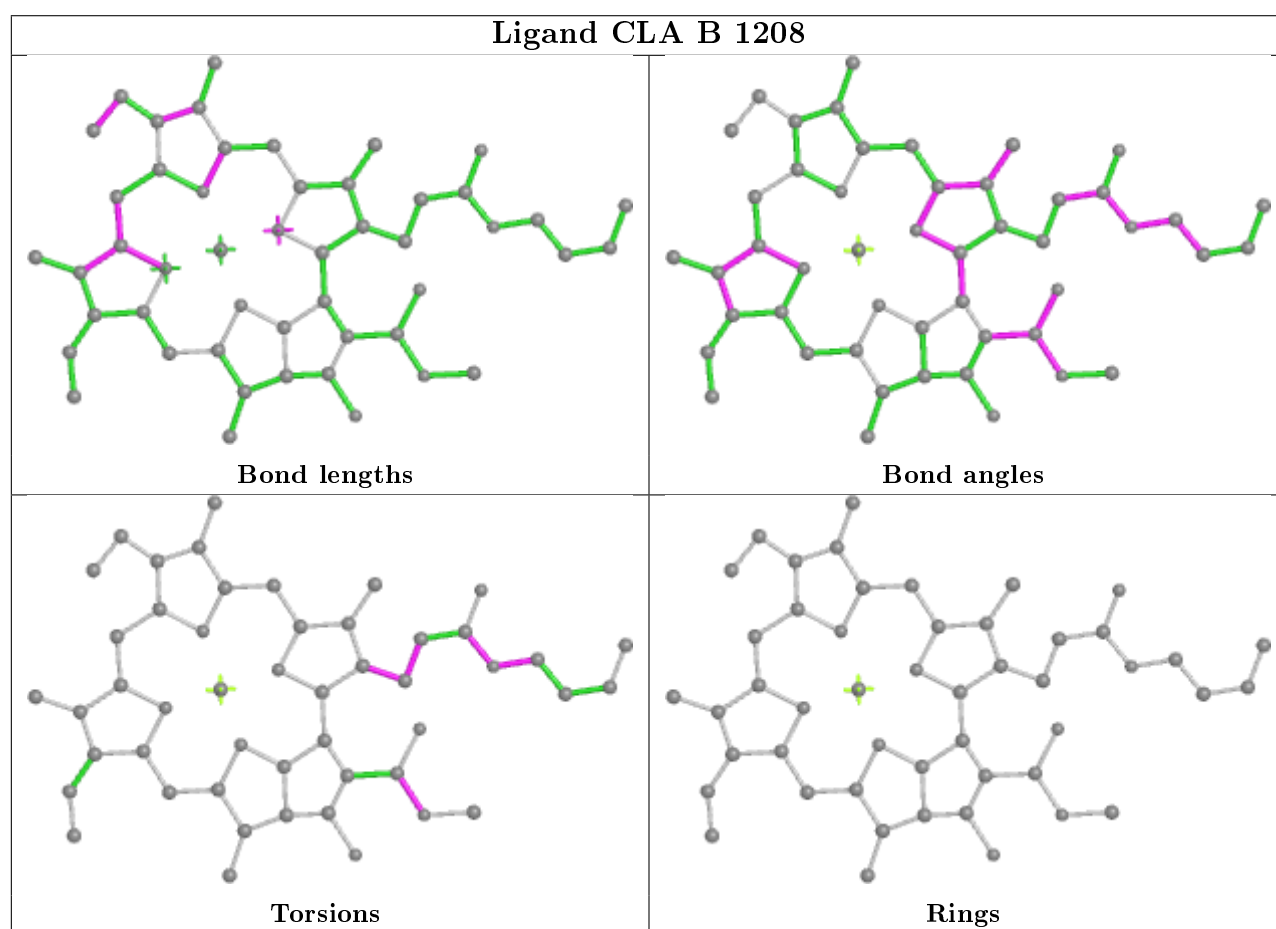
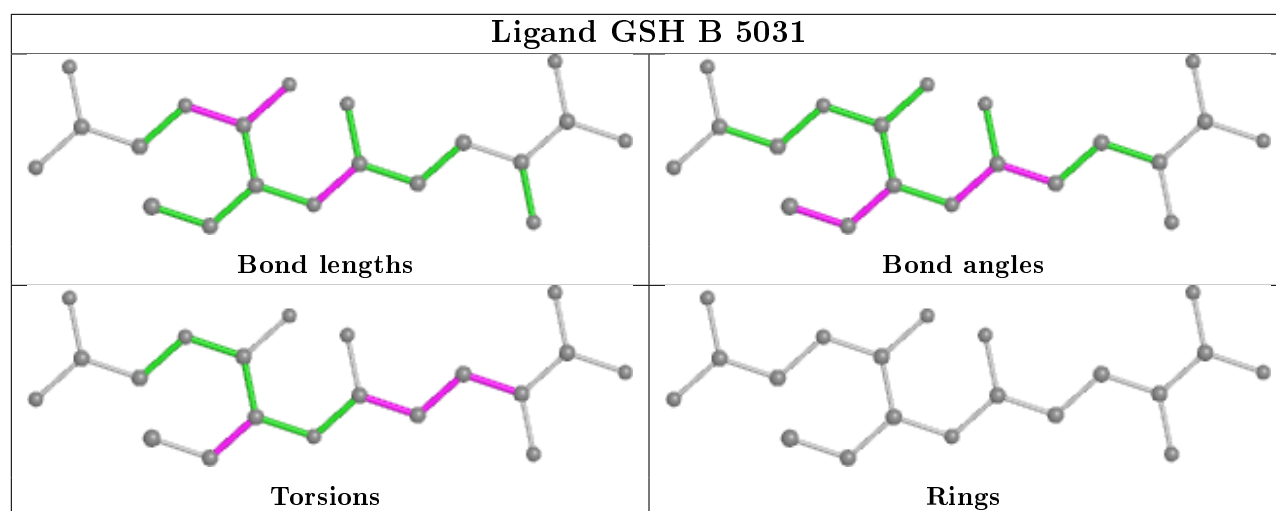


## Ligand CLA 3 603

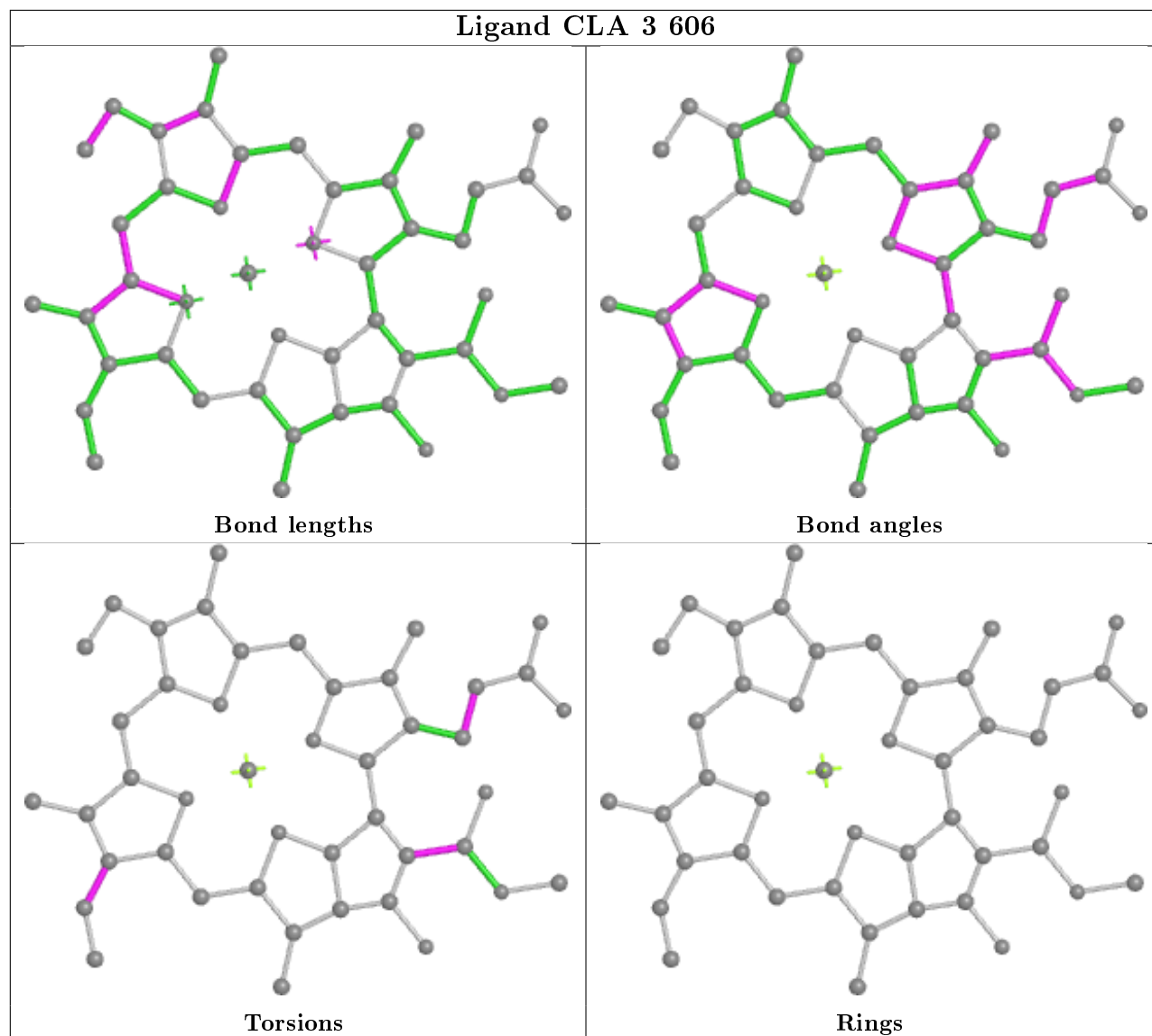


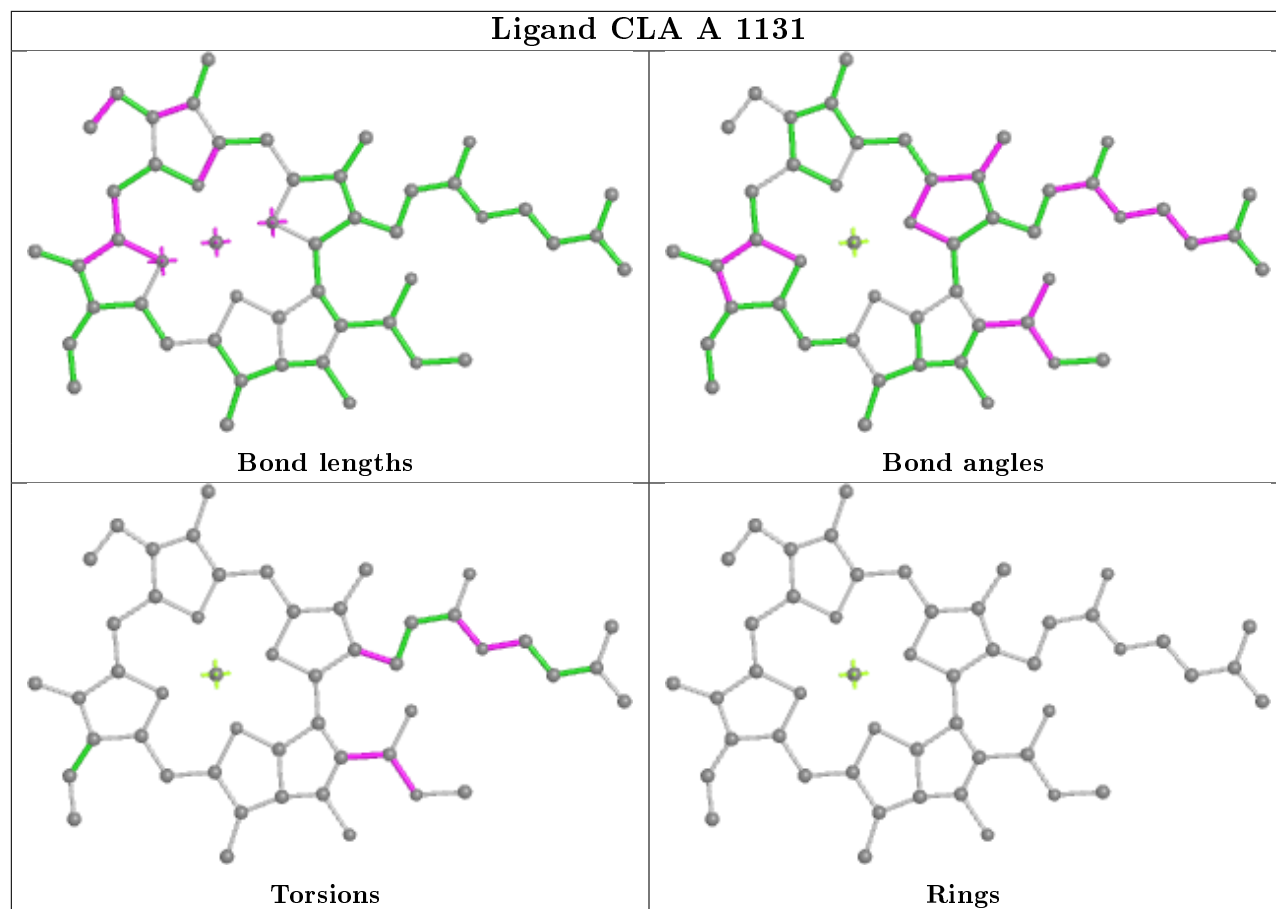
## Ligand LUT 2 501



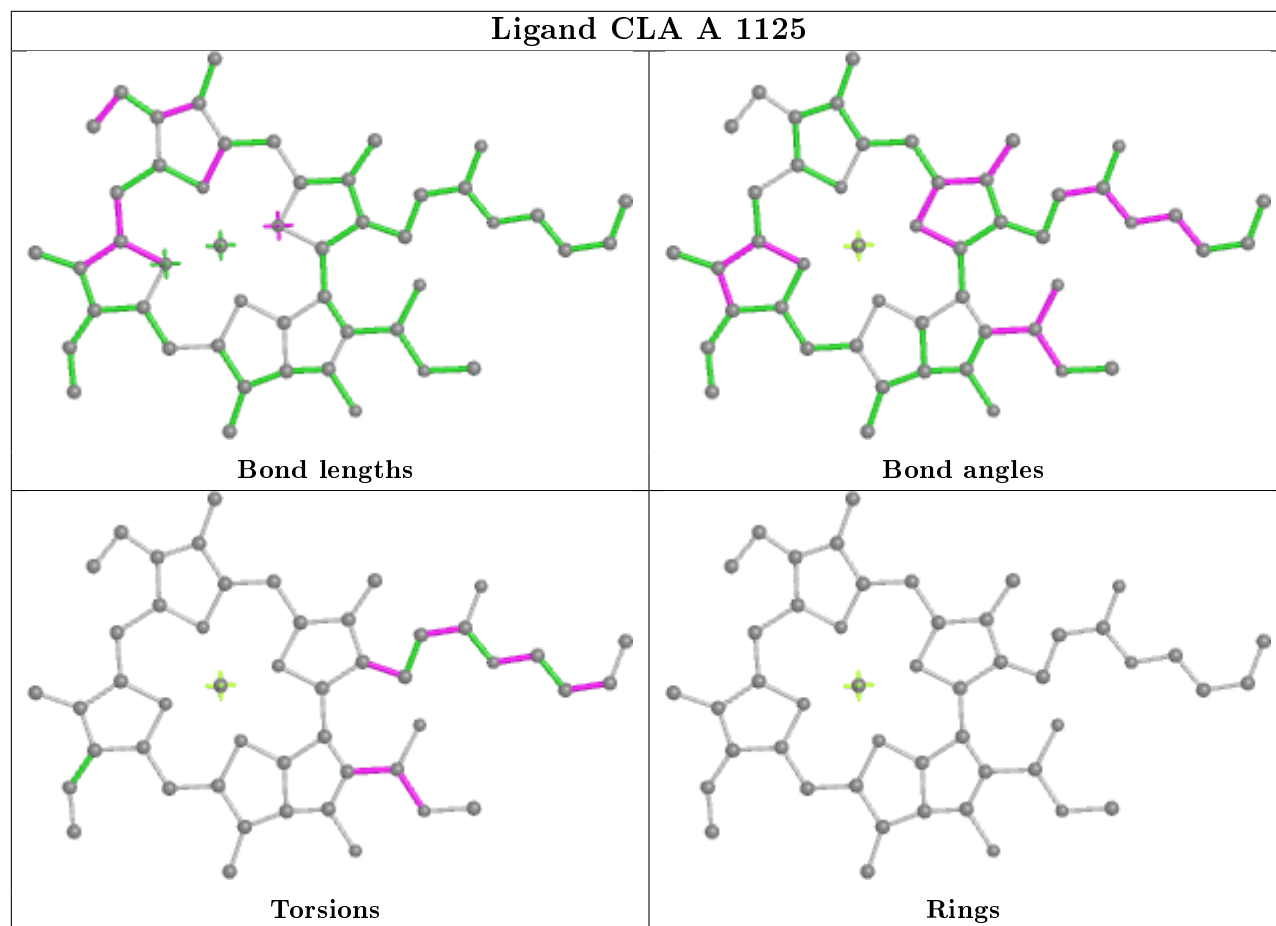


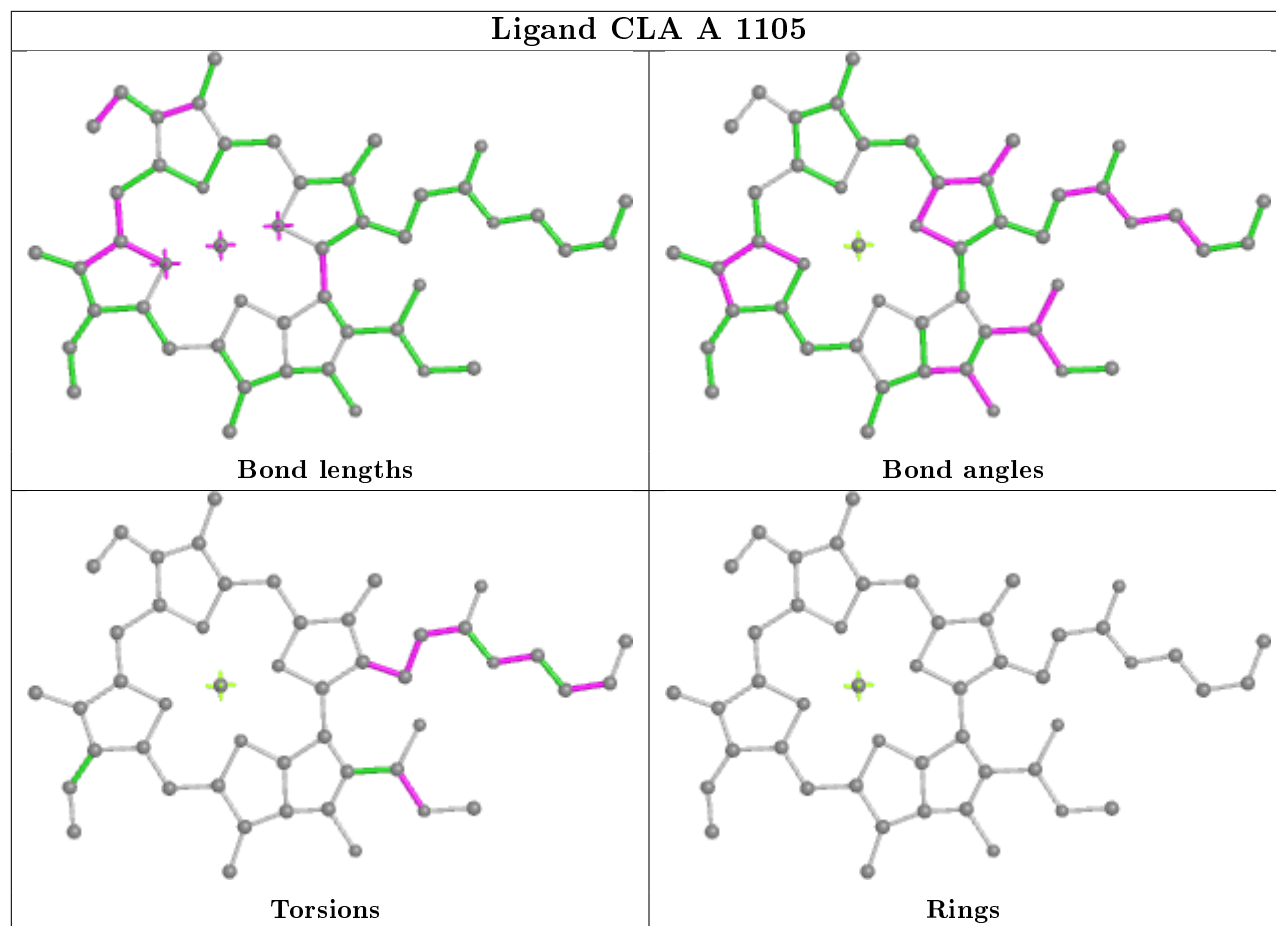
## Ligand CLA 3 606

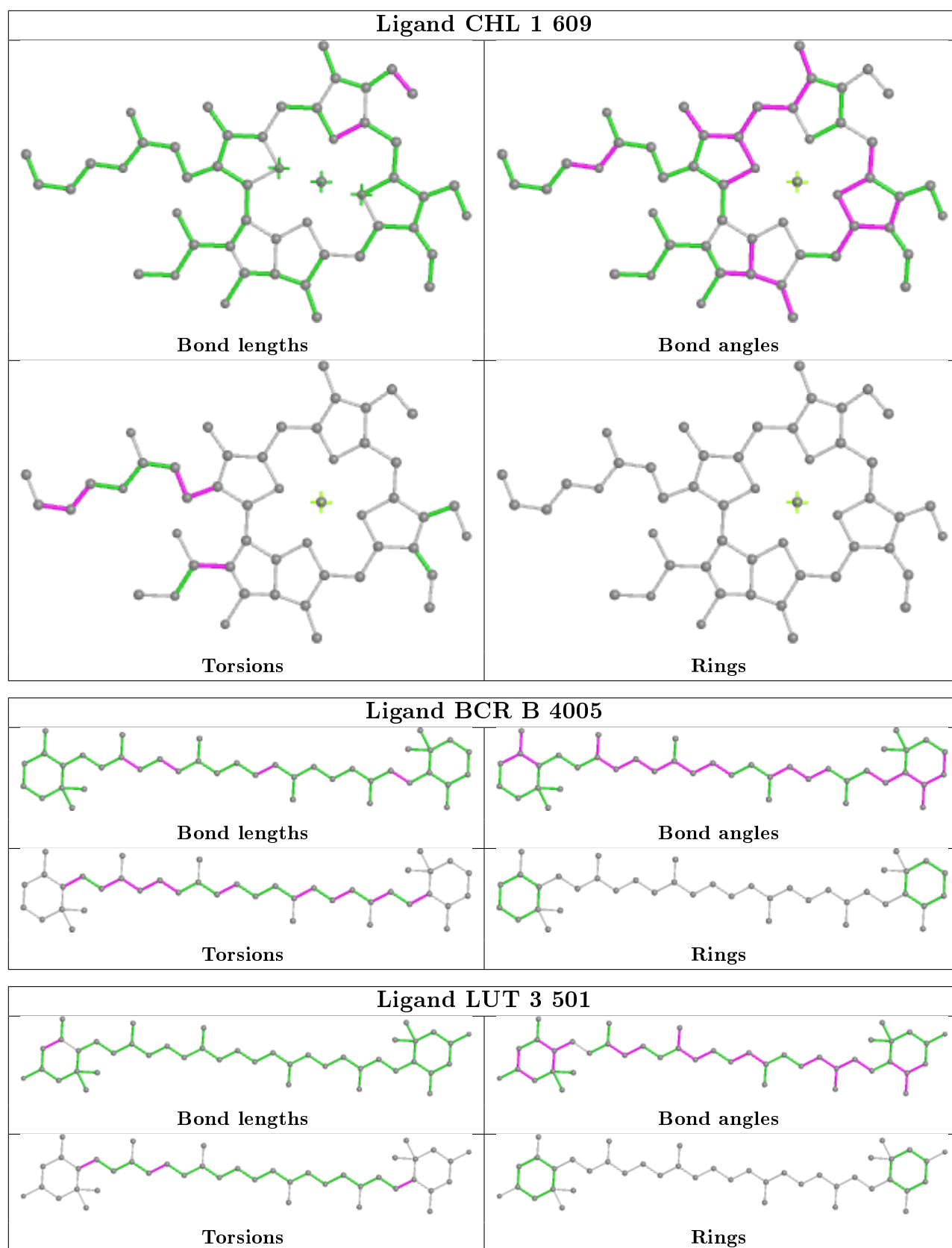


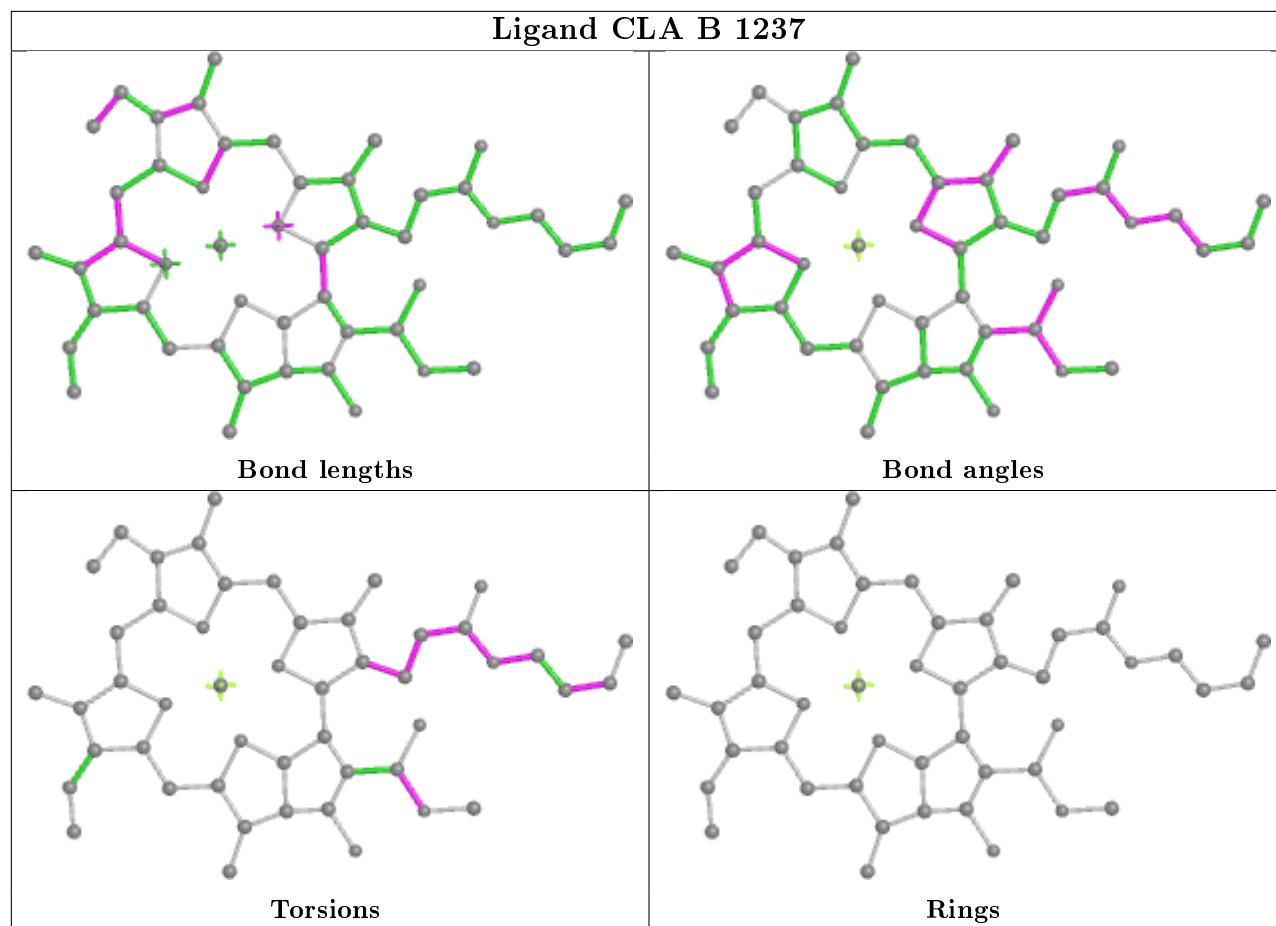




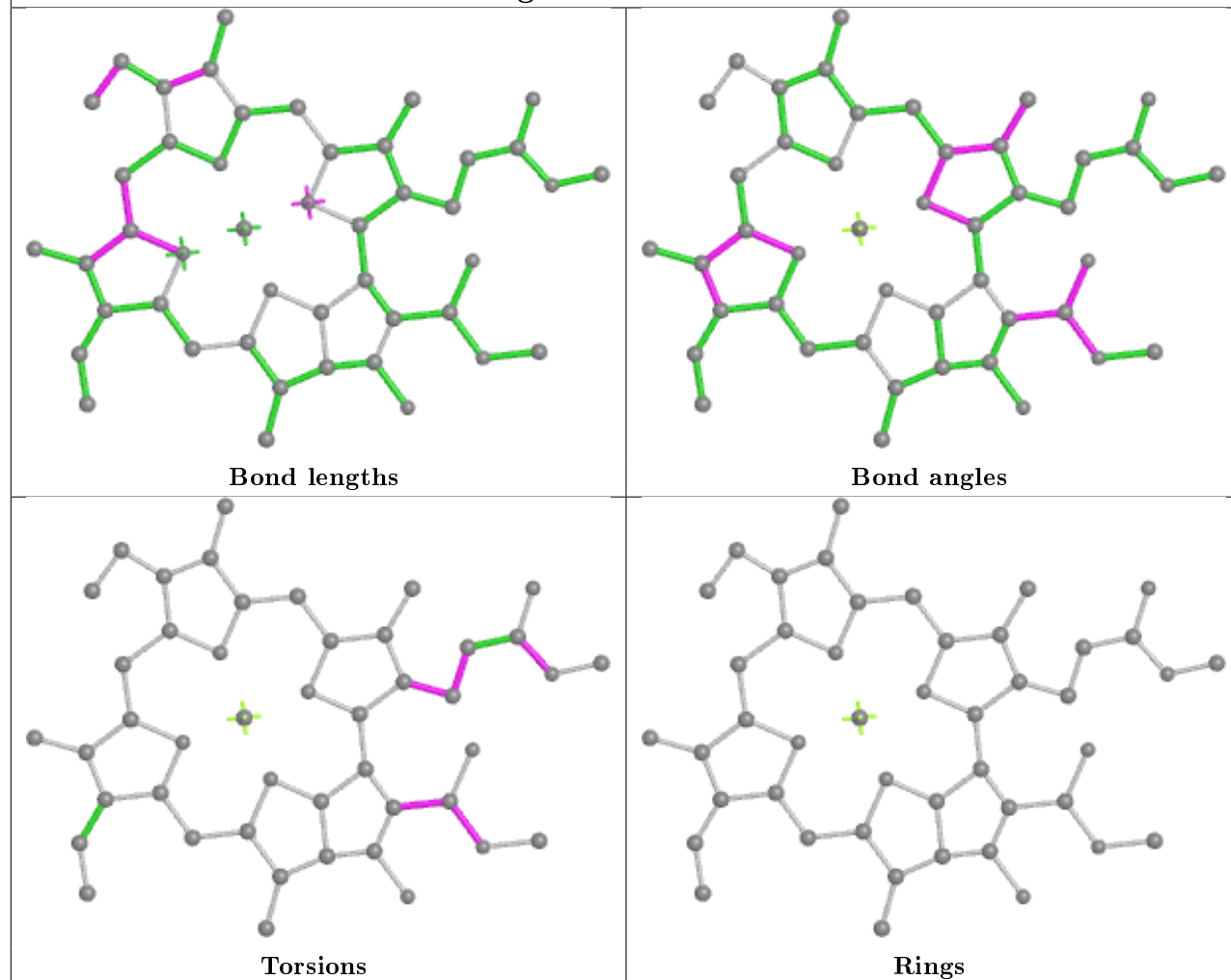




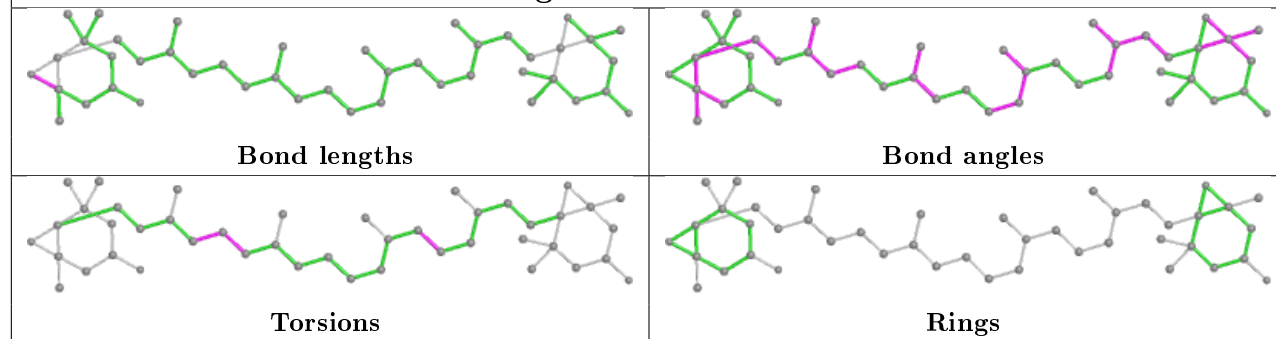




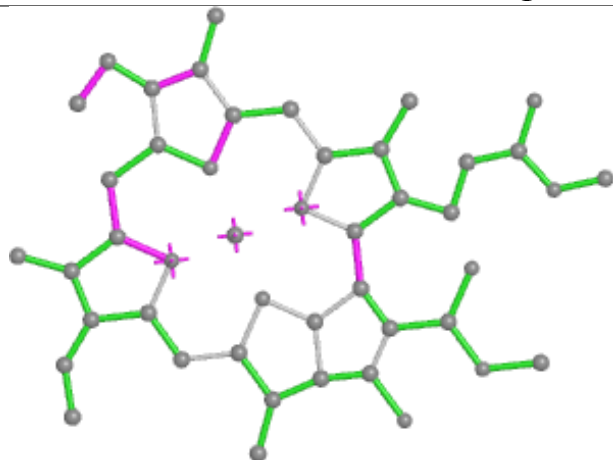
## Ligand CLA 3 611



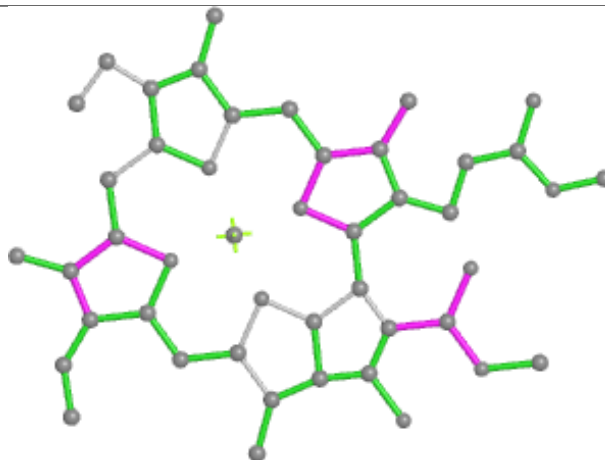
## Ligand XAT 1 502



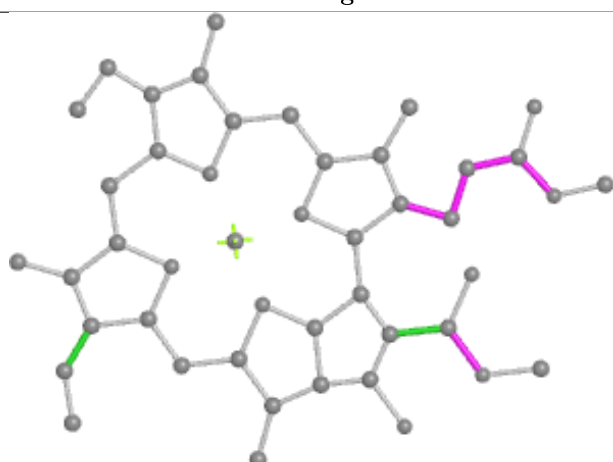
## Ligand CLA 1 607



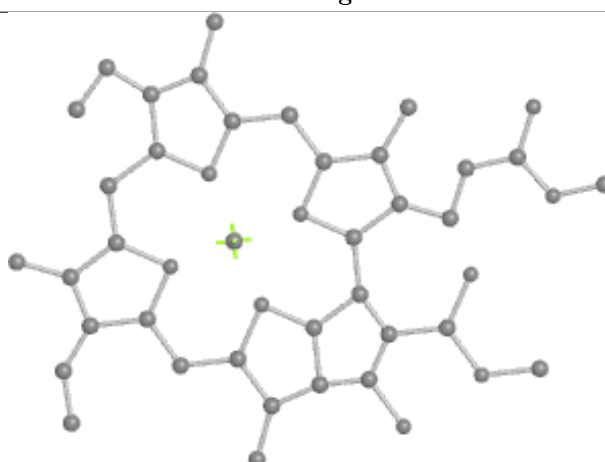
Bond lengths



Bond angles

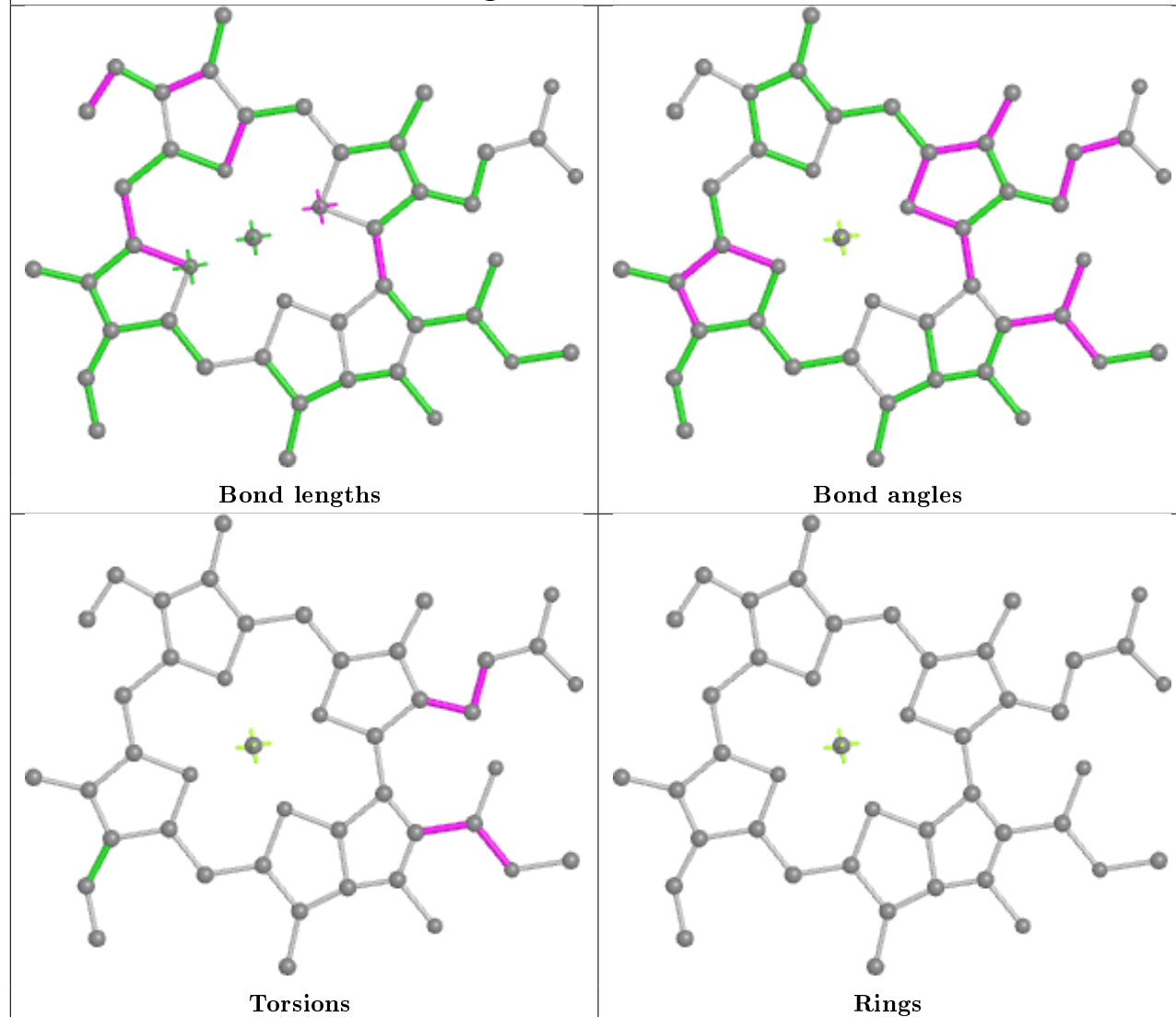


Torsions

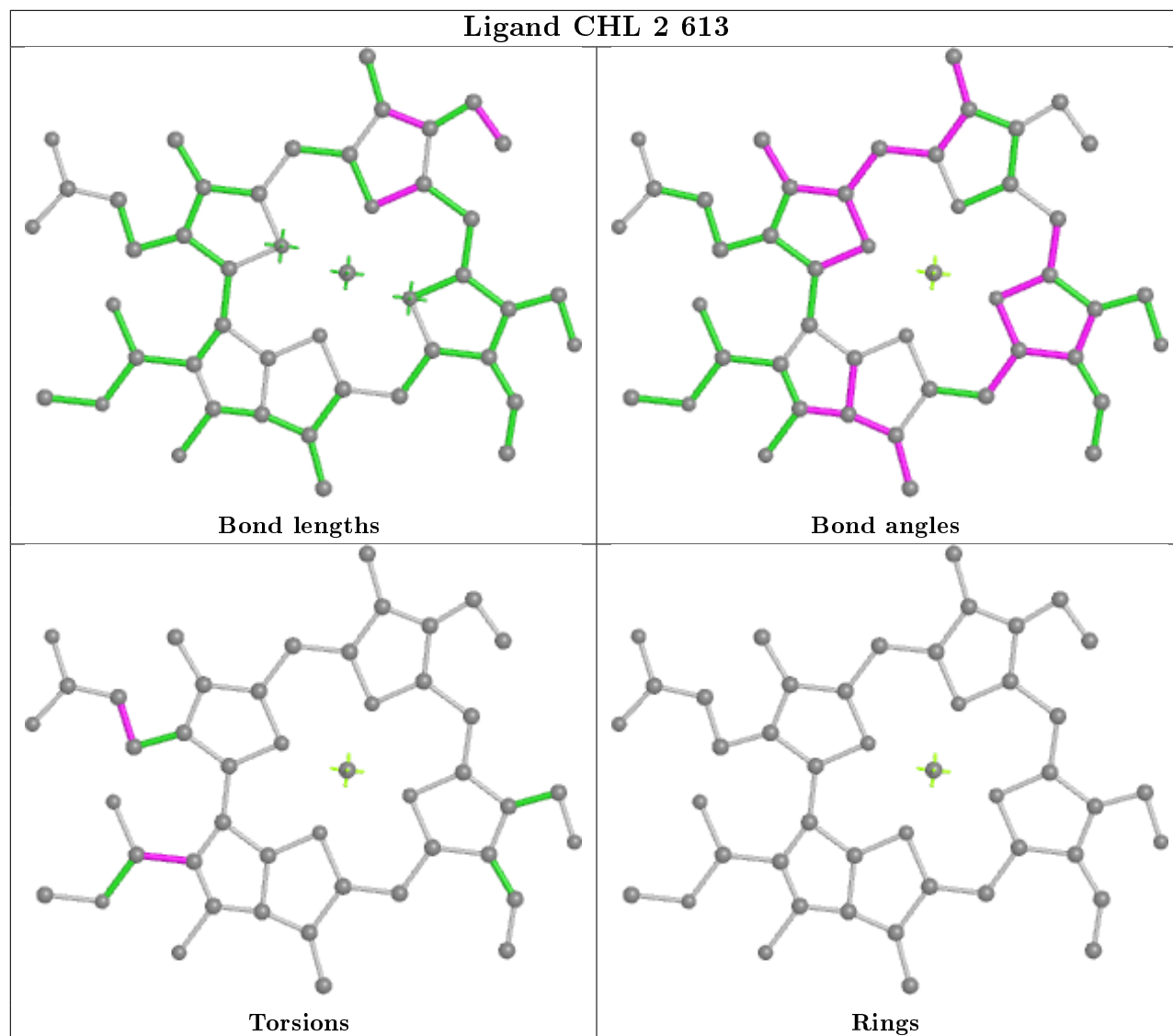


Rings

## Ligand CLA B 1212

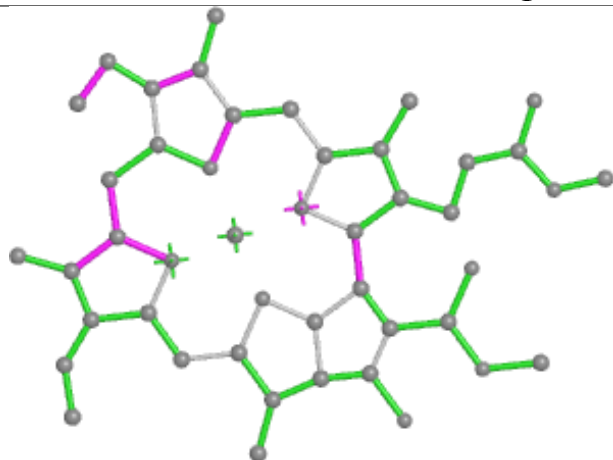


## Ligand CHL 2 613

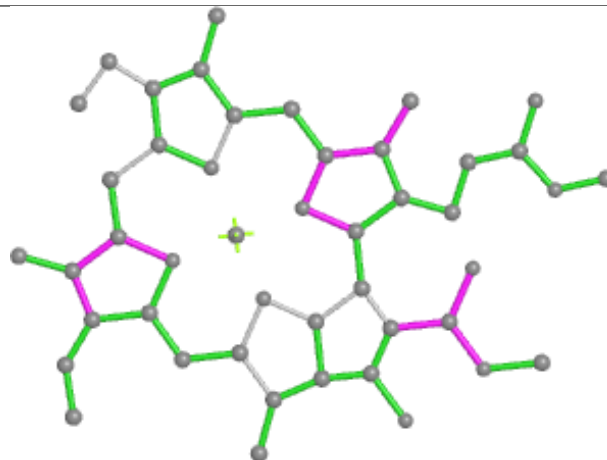




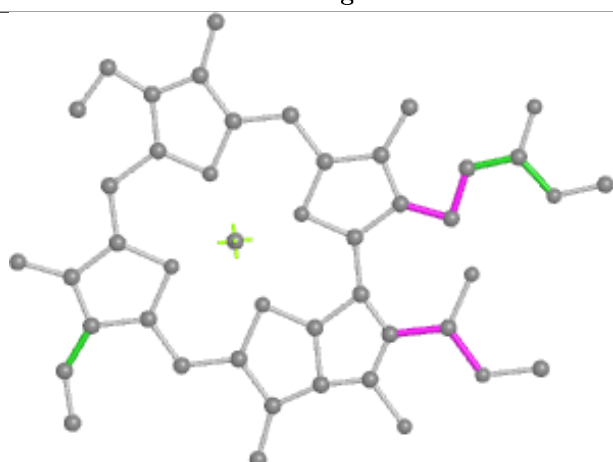
## Ligand CLA 2 606



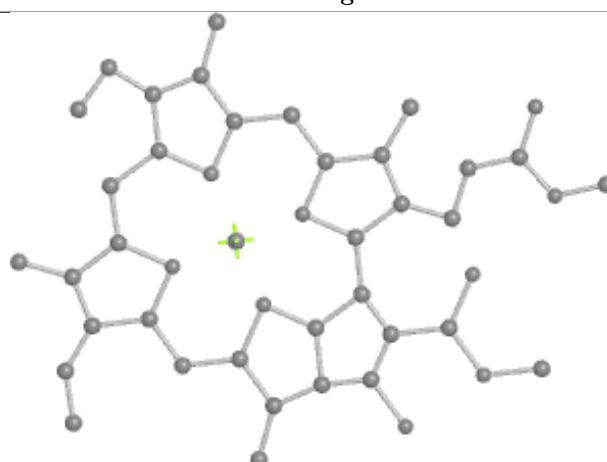
Bond lengths



Bond angles

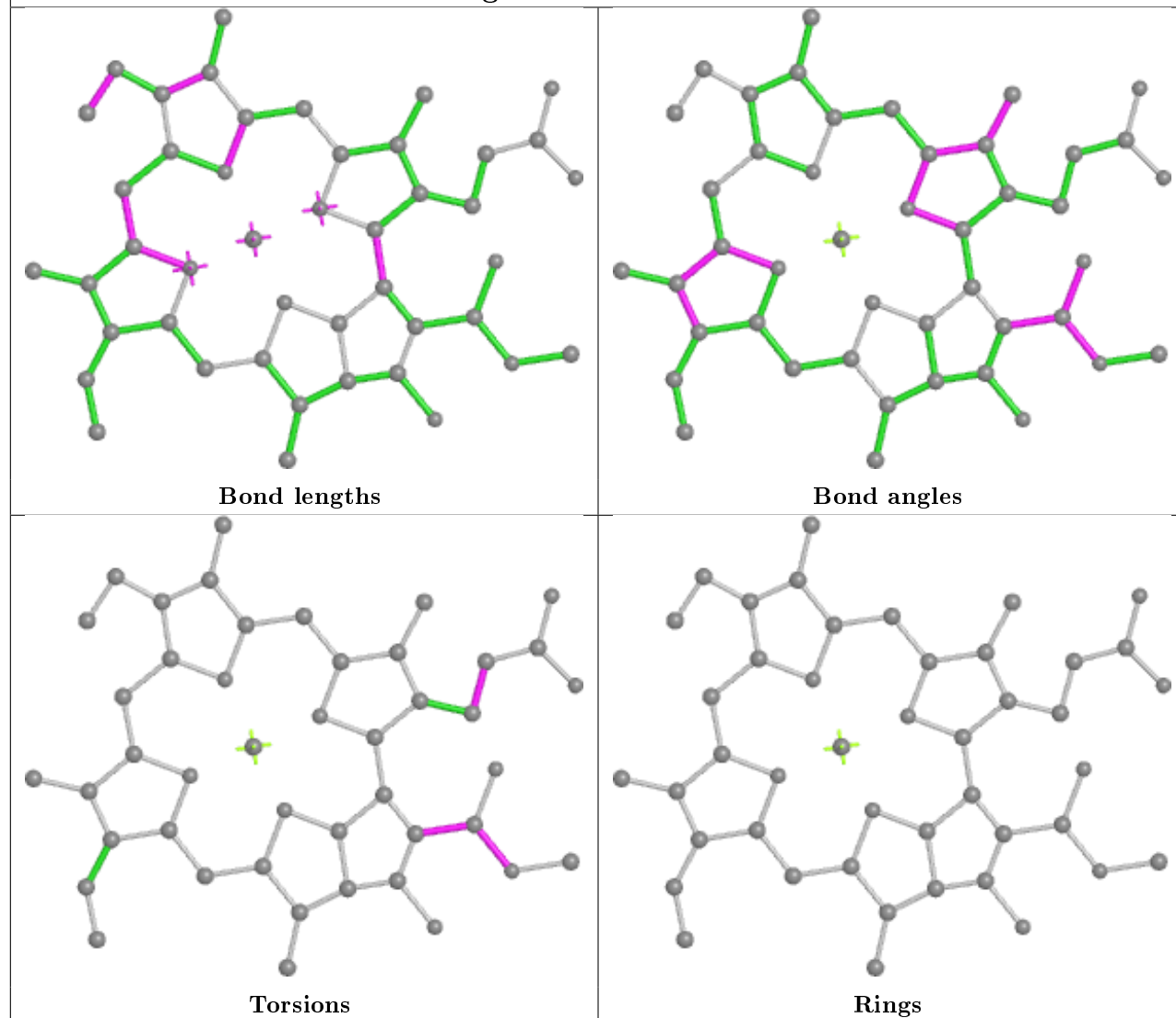


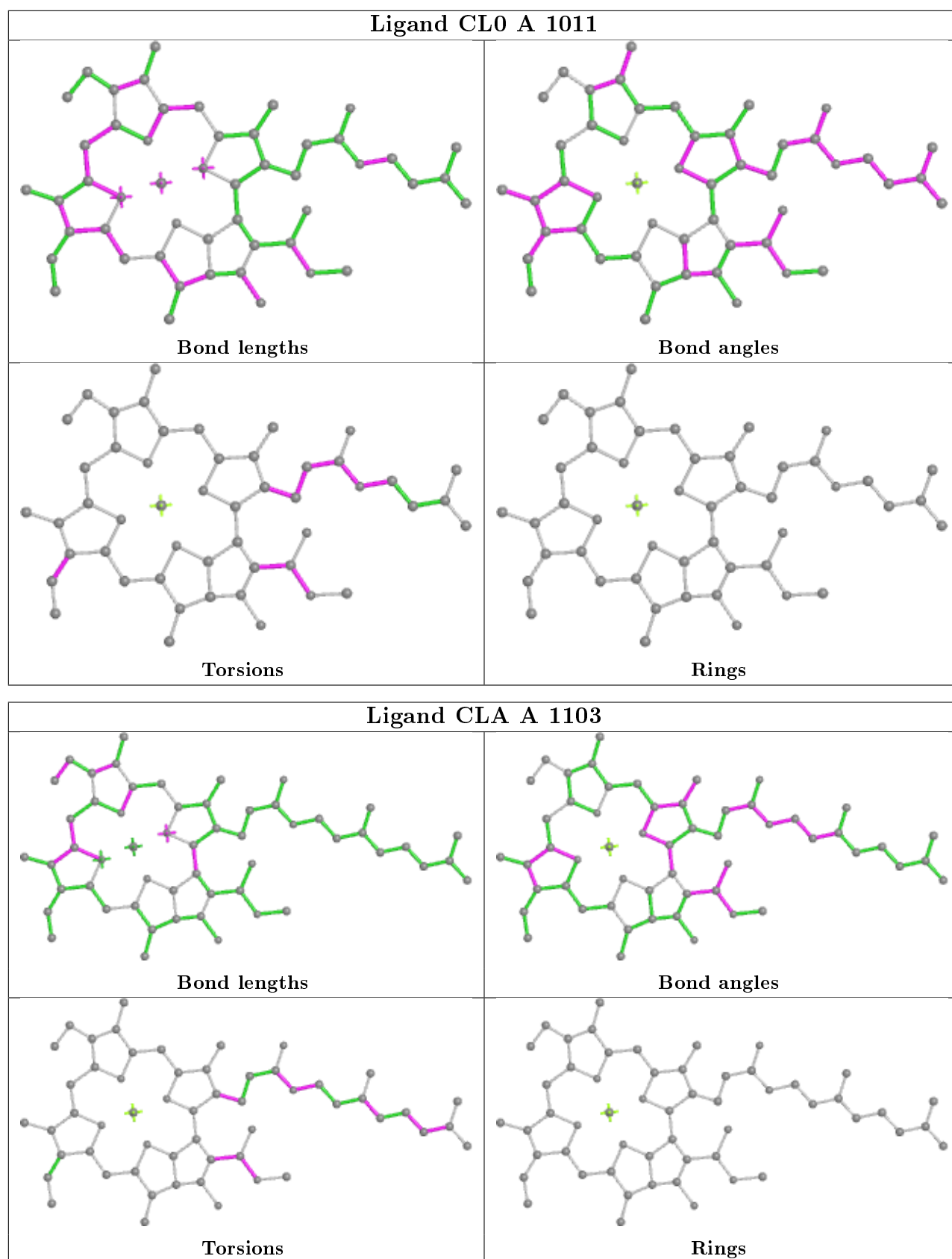
Torsions



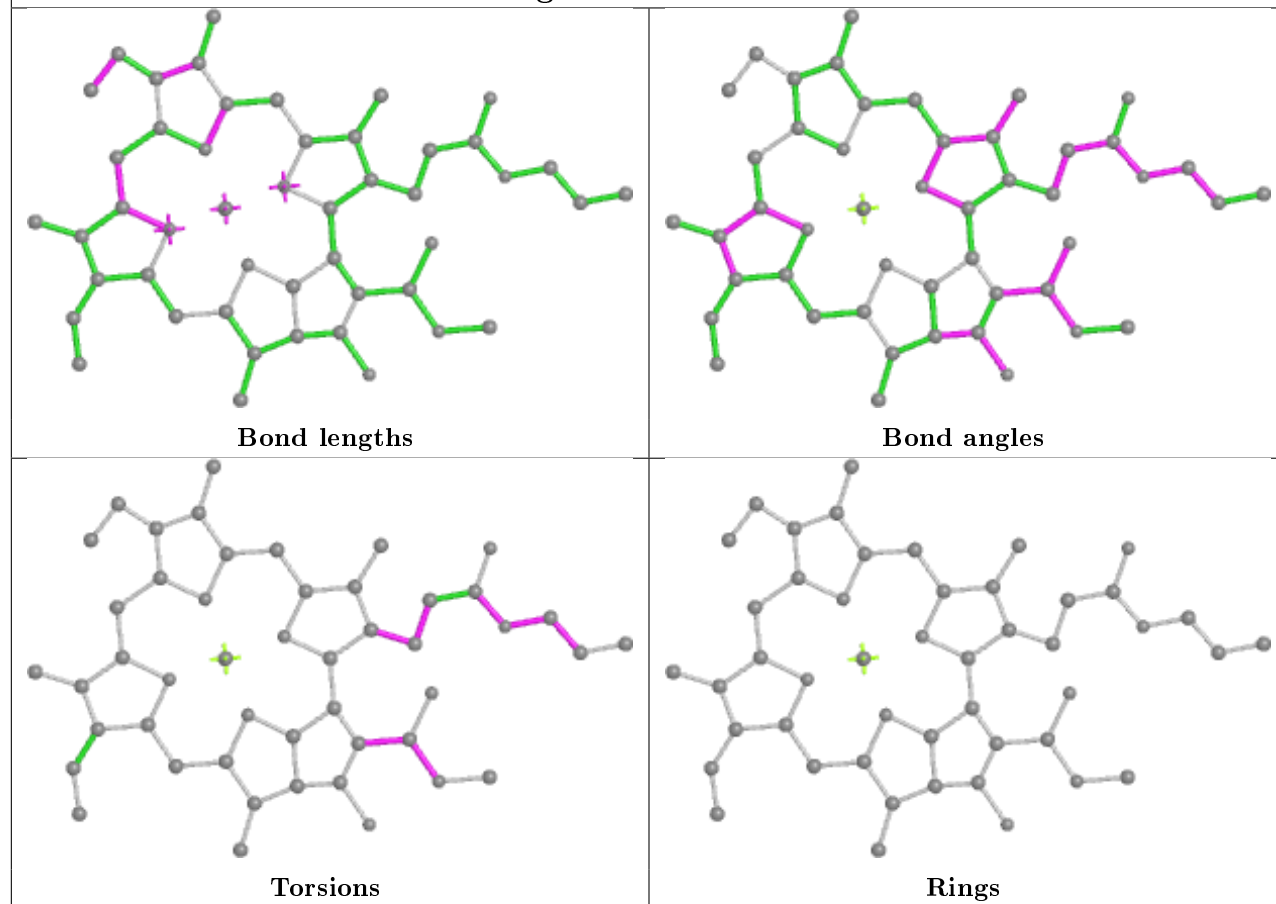
Rings

## Ligand CLA A 1102

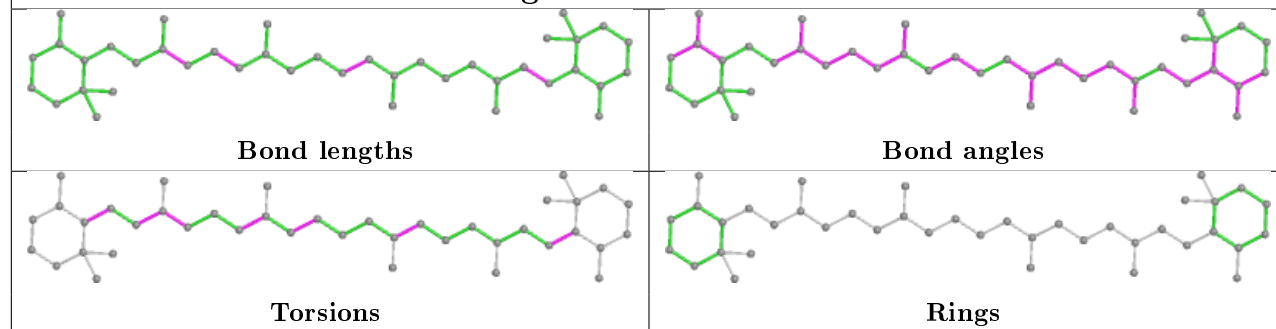


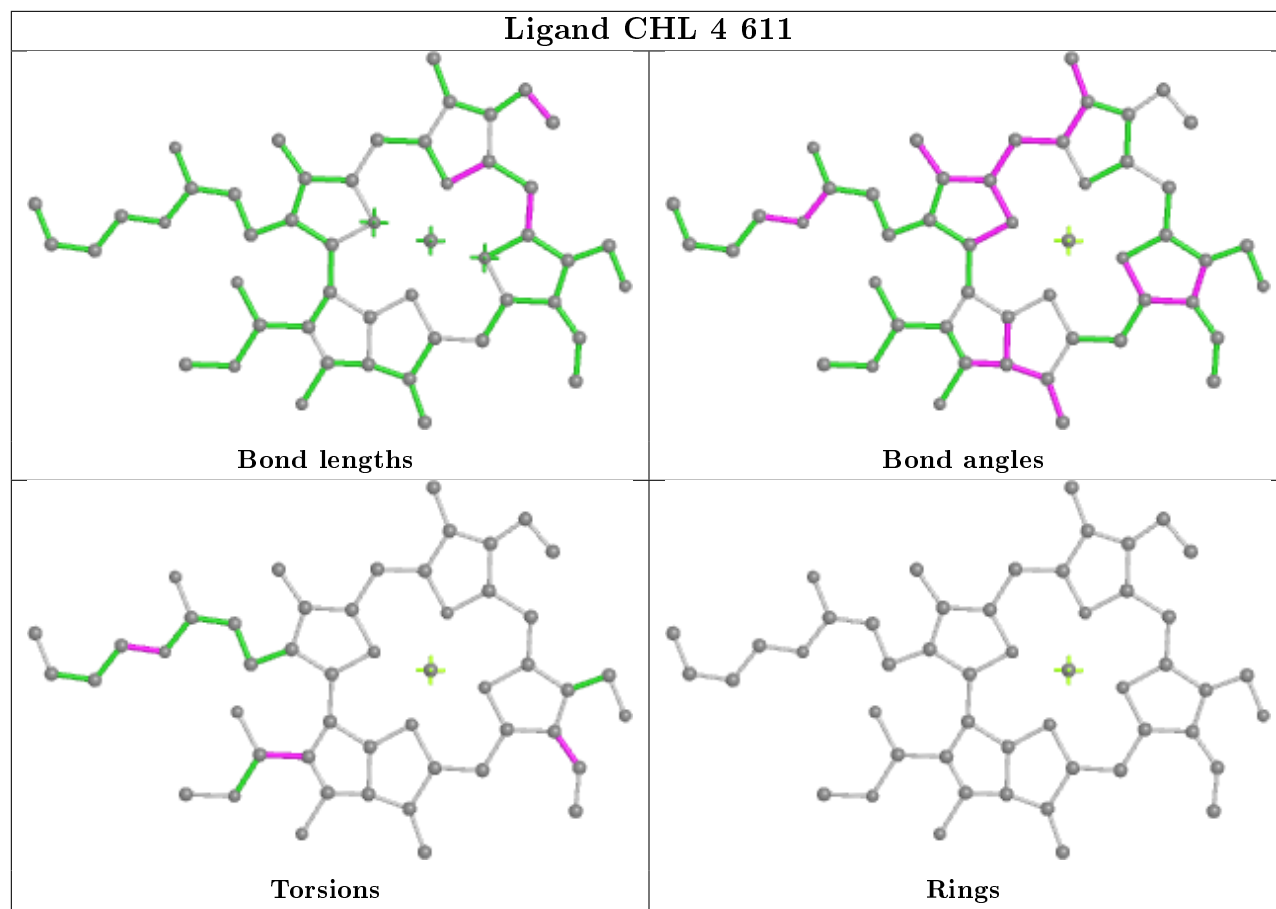


## Ligand CLA 1 605



## Ligand BCR A 4002





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	1	195/195 (100%)	0.73	36 (18%) 1 1	85, 106, 128, 134	0
2	2	211/211 (100%)	0.59	33 (15%) 2 2	91, 115, 138, 155	0
3	3	210/210 (100%)	1.12	47 (22%) 0 1	134, 167, 199, 210	0
4	4	211/211 (100%)	0.60	26 (12%) 4 5	84, 93, 107, 125	0
5	A	739/739 (100%)	0.71	100 (13%) 3 4	84, 127, 168, 187	0
6	B	734/734 (100%)	0.73	117 (15%) 1 2	83, 114, 149, 180	0
7	C	80/80 (100%)	1.17	20 (25%) 0 0	104, 128, 142, 146	0
8	D	142/142 (100%)	1.46	42 (29%) 0 0	108, 153, 174, 189	0
9	E	64/64 (100%)	0.44	6 (9%) 8 10	93, 103, 115, 120	0
10	F	163/163 (100%)	0.03	7 (4%) 35 35	80, 87, 99, 105	0
11	J	41/41 (100%)	0.62	8 (19%) 1 1	82, 87, 103, 105	0
All	All	2790/2790 (100%)	0.73	442 (15%) 2 2	80, 117, 171, 210	0

The worst 5 of 442 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	A	506	THR	21.0
3	3	96	ASN	20.0
6	B	735	GLY	18.7
8	D	112	ILE	15.6
8	D	120	ALA	15.4

### 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
21	DGD	2	811	47/66	0.35	0.40	122,126,134,137	0
20	CAC	3	901	5/5	0.37	0.28	190,190,194,197	0
15	CLA	3	607	50/65	0.38	0.40	195,209,223,228	0
14	BCR	B	4003	40/40	0.49	1.19	125,141,149,153	0
23	GSH	B	5031	20/20	0.51	0.13	151,157,163,166	0
14	BCR	1	505	40/40	0.54	0.63	83,86,98,110	0
23	GSH	4	831	20/20	0.54	0.29	136,138,145,146	0
15	CLA	A	1121	49/65	0.55	0.15	177,193,206,211	0
14	BCR	A	4007	40/40	0.55	0.80	125,132,135,137	0
14	BCR	4	505	40/40	0.56	0.52	83,85,118,119	0
14	BCR	B	4002	40/40	0.56	0.72	114,129,145,146	0
14	BCR	1	503	40/40	0.56	0.85	115,121,136,138	0
15	CLA	3	608	48/65	0.61	0.35	196,222,240,247	0
14	BCR	J	4003	40/40	0.61	0.38	89,99,105,106	0
12	LUT	3	501	42/42	0.61	0.77	173,180,186,189	0
14	BCR	3	504	40/40	0.62	0.58	137,152,173,173	0
14	BCR	A	4002	40/40	0.62	0.76	120,140,167,169	0
14	BCR	3	503	40/40	0.64	0.66	134,148,166,169	0
15	CLA	A	1131	50/65	0.64	0.34	145,153,157,158	0
18	LMG	2	803	16/55	0.65	0.24	121,129,134,134	0
13	XAT	3	502	44/44	0.65	0.47	154,161,165,166	0
14	BCR	B	4001	40/40	0.65	0.72	121,129,137,138	0
18	LMG	1	803	23/55	0.65	0.30	114,119,150,154	0
21	DGD	J	5001	28/66	0.66	0.52	92,95,97,97	0
18	LMG	1	802	36/55	0.66	0.30	88,102,125,128	0
14	BCR	B	4005	40/40	0.66	0.50	92,95,99,101	0
25	PQN	B	2002	33/33	0.66	0.53	117,129,134,136	0
21	DGD	4	811	45/66	0.66	0.40	83,91,111,119	0
15	CLA	B	1224	49/65	0.67	0.43	106,114,119,121	0
15	CLA	B	1208	49/65	0.67	0.29	131,141,150,152	0
14	BCR	A	4004	40/40	0.67	0.81	136,156,183,186	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	CLA	A	1111	49/65	0.68	0.33	122,129,139,142	0
18	LMG	2	802	25/55	0.68	0.33	92,104,127,134	0
15	CLA	B	1203	49/65	0.68	0.40	112,118,123,126	0
15	CLA	B	1023	60/65	0.69	0.40	113,126,138,141	0
14	BCR	A	4003	40/40	0.69	0.54	116,130,150,152	0
14	BCR	4	503	40/40	0.69	0.49	90,93,98,99	0
14	BCR	2	503	40/40	0.70	0.67	96,102,110,110	0
12	LUT	2	501	42/42	0.70	0.53	117,120,125,127	0
15	CLA	3	603	45/65	0.71	0.29	179,187,200,210	0
15	CLA	A	1114	46/65	0.72	0.52	127,141,157,160	0
15	CLA	3	606	45/65	0.73	0.23	156,165,173,177	0
20	CAC	3	902	5/5	0.73	0.26	200,204,206,207	0
15	CLA	B	1022	50/65	0.73	0.38	108,116,124,126	0
15	CLA	B	1215	49/65	0.73	0.41	105,112,119,121	0
15	CLA	B	1238	50/65	0.73	0.32	134,148,155,158	0
16	CHL	3	604	47/66	0.74	0.52	157,171,179,185	0
15	CLA	A	1141	50/65	0.74	0.35	170,186,196,199	0
15	CLA	A	1116	49/65	0.74	0.47	136,151,156,161	0
12	LUT	1	501	42/42	0.74	0.60	100,109,122,125	0
14	BCR	A	4005	40/40	0.74	0.47	129,142,162,163	0
15	CLA	B	1211	49/65	0.75	0.39	127,137,141,143	0
15	CLA	A	1135	49/65	0.75	0.30	126,139,154,160	0
15	CLA	2	605	65/65	0.75	0.26	95,100,104,108	0
15	CLA	2	602	49/65	0.75	0.25	123,128,133,137	0
25	PQN	A	2001	33/33	0.75	0.47	87,91,98,99	0
15	CLA	B	1221	49/65	0.75	0.37	99,108,113,115	0
15	CLA	B	1218	49/65	0.75	0.24	104,112,117,137	0
15	CLA	1	613	45/65	0.76	0.30	109,119,126,129	0
22	LMT	2	821	23/35	0.77	0.14	109,113,132,138	0
14	BCR	J	4001	40/40	0.77	0.52	83,90,102,103	0
12	LUT	4	501	42/42	0.77	0.44	90,93,101,102	0
15	CLA	A	1126	49/65	0.77	0.42	98,106,108,108	0
15	CLA	4	607	49/65	0.77	0.23	92,98,104,105	0
15	CLA	A	1108	46/65	0.78	0.32	123,132,140,143	0
20	CAC	4	902	5/5	0.78	0.23	85,105,119,122	0
15	CLA	A	1134	49/65	0.78	0.22	162,171,183,186	0
15	CLA	2	606	46/65	0.78	0.43	105,111,116,119	0
15	CLA	3	601	49/65	0.78	0.27	165,175,188,190	0
15	CLA	3	612	55/65	0.79	0.34	135,143,151,153	0
14	BCR	J	4002	40/40	0.79	0.35	88,91,99,100	0
15	CLA	B	1236	49/65	0.79	0.34	83,87,90,90	0
14	BCR	A	4006	40/40	0.79	0.38	83,91,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CLA	A	1117	49/65	0.79	0.35	132,136,143,147	0
15	CLA	B	1226	49/65	0.79	0.29	105,112,118,120	0
15	CLA	1	601	49/65	0.79	0.31	111,114,118,119	0
15	CLA	B	1219	49/65	0.79	0.34	95,103,107,108	0
16	CHL	1	610	47/66	0.79	0.27	101,105,111,114	0
15	CLA	A	1124	49/65	0.79	0.31	123,133,142,148	0
15	CLA	4	615	55/65	0.79	0.32	82,84,86,87	0
15	CLA	3	611	46/65	0.79	0.34	147,154,162,167	0
21	DGD	B	5002	38/66	0.79	0.29	114,119,125,127	0
15	CLA	1	615	65/65	0.79	0.38	83,85,89,91	0
14	BCR	B	4006	40/40	0.80	0.65	80,83,89,90	0
15	CLA	A	1120	49/65	0.80	0.26	162,176,190,191	0
15	CLA	2	612	49/65	0.81	0.28	91,97,100,102	0
15	CLA	3	613	46/65	0.81	0.36	150,153,186,194	0
17	LHG	2	801	21/49	0.81	0.25	121,128,134,137	0
15	CLA	A	1128	49/65	0.81	0.34	102,113,116,117	0
15	CLA	A	1119	49/65	0.81	0.35	140,151,159,162	0
15	CLA	B	1021	65/65	0.81	0.33	89,103,107,108	0
15	CLA	B	1212	45/65	0.81	0.28	128,138,147,148	0
13	XAT	4	502	44/44	0.81	0.33	83,84,88,89	0
15	CLA	4	606	49/65	0.81	0.63	89,94,97,98	0
15	CLA	A	1137	49/65	0.82	0.31	137,144,151,153	0
15	CLA	A	1123	48/65	0.82	0.31	128,139,146,148	0
15	CLA	A	1136	49/65	0.82	0.24	140,148,154,159	0
15	CLA	2	601	49/65	0.82	0.26	110,116,125,129	0
15	CLA	A	1113	45/65	0.82	0.36	147,155,160,161	0
15	CLA	A	1118	49/65	0.82	0.32	151,164,172,175	0
15	CLA	2	604	49/65	0.82	0.20	104,111,117,119	0
20	CAC	1	902	5/5	0.82	0.23	136,142,150,152	0
14	BCR	F	4002	40/40	0.82	0.37	80,81,81,82	0
15	CLA	B	1213	49/65	0.82	0.26	111,117,123,125	0
15	CLA	F	1302	49/65	0.82	0.23	81,83,86,86	0
15	CLA	B	1207	25/65	0.82	0.30	145,151,156,158	0
15	CLA	1	607	46/65	0.82	0.32	99,104,109,111	0
15	CLA	B	1220	55/65	0.82	0.26	91,98,102,103	0
19	SQD	1	811	40/54	0.82	0.21	100,104,109,109	0
15	CLA	3	610	49/65	0.82	0.29	134,143,160,173	0
15	CLA	A	1133	49/65	0.83	0.28	147,157,165,169	0
15	CLA	A	1101	45/65	0.83	0.33	90,95,99,100	0
16	CHL	4	613	50/66	0.83	0.44	86,91,96,98	0
13	XAT	1	502	44/44	0.83	0.59	89,97,109,110	0
15	CLA	1	603	45/65	0.83	0.28	91,95,97,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	LHG	A	5001	16/49	0.83	0.20	165,168,172,175	0
13	XAT	2	502	44/44	0.83	0.36	103,107,110,110	0
15	CLA	1	605	48/65	0.83	0.39	93,97,101,103	0
15	CLA	B	1232	49/65	0.83	0.28	92,99,103,105	0
15	CLA	A	1140	55/65	0.84	0.34	89,93,98,100	0
15	CLA	A	1109	49/65	0.84	0.17	103,111,114,115	0
15	CLA	B	1205	49/65	0.84	0.26	122,126,132,134	0
15	CLA	1	612	60/65	0.84	0.28	97,105,110,112	0
15	CLA	A	1112	49/65	0.84	0.39	124,131,141,144	0
15	CLA	2	615	50/65	0.84	0.26	112,124,141,146	0
15	CLA	B	1225	49/65	0.84	0.33	108,114,122,126	0
15	CLA	A	1132	49/65	0.84	0.45	137,148,163,168	0
15	CLA	A	1104	60/65	0.85	0.40	103,109,115,118	0
15	CLA	B	1239	65/65	0.85	0.28	120,125,155,163	0
15	CLA	4	612	49/65	0.85	0.20	81,84,85,86	0
15	CLA	1	611	49/65	0.85	0.21	110,118,124,126	0
14	BCR	B	4004	40/40	0.85	0.30	92,94,97,98	0
15	CLA	B	1201	49/65	0.85	0.25	127,132,139,152	0
15	CLA	A	1130	55/65	0.85	0.29	157,163,172,174	0
15	CLA	B	1240	65/65	0.85	0.26	84,92,97,99	0
15	CLA	A	1127	49/65	0.85	0.34	109,118,123,125	0
24	CL0	A	1011	50/65	0.85	0.35	100,104,112,115	0
15	CLA	1	602	46/65	0.85	0.31	106,110,115,118	0
15	CLA	B	1223	50/65	0.85	0.34	91,97,99,101	0
15	CLA	B	1230	49/65	0.86	0.30	81,83,85,86	0
15	CLA	A	1013	65/65	0.86	0.32	86,90,97,99	0
15	CLA	B	1237	49/65	0.86	0.17	140,150,158,161	0
15	CLA	B	1214	49/65	0.86	0.35	102,105,111,112	0
17	LHG	1	801	23/49	0.86	0.28	95,99,101,103	0
16	CHL	4	610	47/66	0.86	0.27	82,85,87,87	0
15	CLA	2	608	49/65	0.86	0.35	128,136,143,146	0
15	CLA	B	1229	65/65	0.86	0.37	80,81,82,83	0
15	CLA	B	1227	45/65	0.86	0.20	85,88,91,92	0
15	CLA	2	607	49/65	0.86	0.37	125,132,139,141	0
15	CLA	A	1125	49/65	0.86	0.29	137,141,146,148	0
15	CLA	1	604	49/65	0.87	0.24	93,95,97,98	0
15	CLA	B	1228	60/65	0.87	0.31	79,82,84,85	0
15	CLA	A	1012	60/65	0.87	0.39	89,92,98,100	0
15	CLA	1	606	45/65	0.87	0.22	110,116,120,122	0
15	CLA	A	1110	49/65	0.87	0.22	140,149,157,161	0
15	CLA	A	1122	49/65	0.87	0.26	144,154,161,164	0
15	CLA	3	615	46/65	0.87	0.27	118,127,131,133	0

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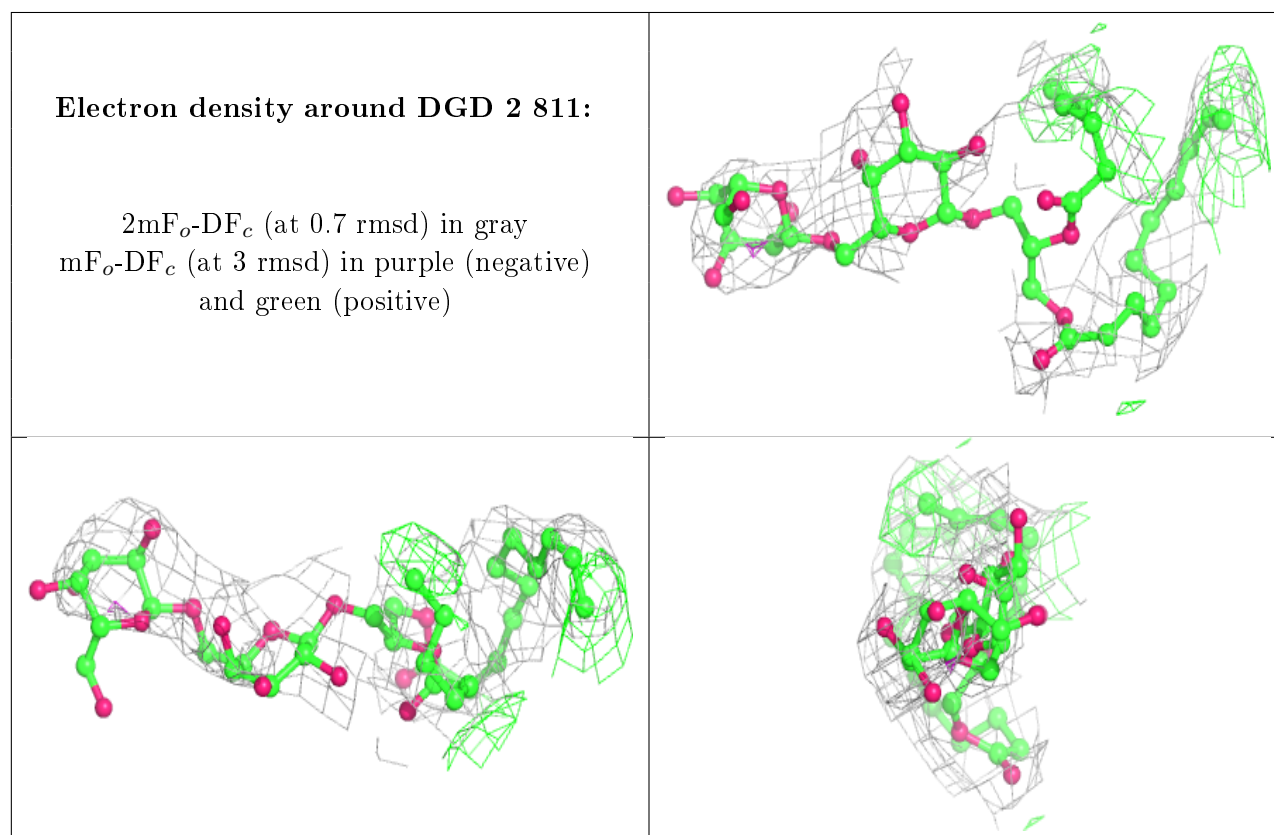
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CLA	B	1216	49/65	0.87	0.22	97,105,108,108	0
15	CLA	B	1206	49/65	0.88	0.28	131,139,145,148	0
17	LHG	A	5002	24/49	0.88	0.35	99,105,107,108	0
15	CLA	4	602	49/65	0.88	0.27	95,99,104,107	0
16	CHL	2	611	48/66	0.88	0.25	103,104,111,114	0
15	CLA	A	1129	48/65	0.88	0.28	147,160,175,178	0
15	CLA	F	1301	47/65	0.88	0.24	81,82,83,85	0
15	CLA	B	1202	49/65	0.88	0.29	111,117,121,125	0
16	CHL	2	613	46/66	0.88	0.30	100,102,103,105	0
16	CHL	2	609	50/66	0.88	0.20	119,129,136,138	0
15	CLA	A	1102	45/65	0.88	0.27	100,106,109,111	0
16	CHL	2	610	50/66	0.88	0.16	97,100,102,103	0
15	CLA	A	1103	55/65	0.88	0.31	111,121,125,128	0
15	CLA	4	604	49/65	0.88	0.22	82,86,89,89	0
15	CLA	A	1115	49/65	0.88	0.40	160,166,178,179	0
15	CLA	2	603	46/65	0.89	0.23	115,122,128,129	0
15	CLA	J	1302	49/65	0.89	0.24	86,89,91,92	0
15	CLA	A	1107	49/65	0.89	0.31	85,91,94,96	0
20	CAC	1	901	5/5	0.89	0.21	130,132,142,147	0
17	LHG	B	5001	21/49	0.89	0.20	88,89,92,93	0
15	CLA	A	1106	65/65	0.89	0.33	89,98,104,105	0
15	CLA	B	1234	49/65	0.89	0.25	86,91,94,95	0
15	CLA	4	609	49/65	0.89	0.29	87,92,96,97	0
15	CLA	4	601	49/65	0.90	0.24	92,95,100,101	0
15	CLA	A	1139	52/65	0.90	0.28	85,88,91,92	0
15	CLA	4	608	46/65	0.90	0.20	92,96,101,103	0
15	CLA	A	1105	49/65	0.90	0.19	94,98,104,105	0
15	CLA	1	608	46/65	0.90	0.45	91,96,101,103	0
15	CLA	B	1209	46/65	0.90	0.17	130,133,140,141	0
15	CLA	B	1231	60/65	0.90	0.26	88,95,99,101	0
15	CLA	3	605	46/65	0.90	0.25	142,151,156,159	0
15	CLA	4	603	49/65	0.90	0.19	85,89,92,93	0
16	CHL	4	611	50/66	0.90	0.22	88,92,96,99	0
15	CLA	4	605	49/65	0.91	0.19	80,82,83,84	0
15	CLA	B	1210	49/65	0.91	0.21	116,124,127,128	0
15	CLA	B	1235	60/65	0.91	0.22	80,83,86,87	0
15	CLA	B	1204	49/65	0.91	0.18	134,146,151,153	0
16	CHL	1	609	50/66	0.92	0.29	88,91,96,97	0
20	CAC	4	901	5/5	0.92	0.21	133,136,139,139	0
15	CLA	A	1138	65/65	0.92	0.39	82,84,86,87	0
15	CLA	B	1217	46/65	0.92	0.18	121,128,132,134	0
15	CLA	B	1222	49/65	0.93	0.29	87,93,96,96	0

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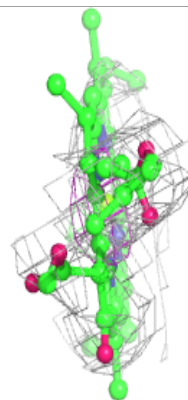
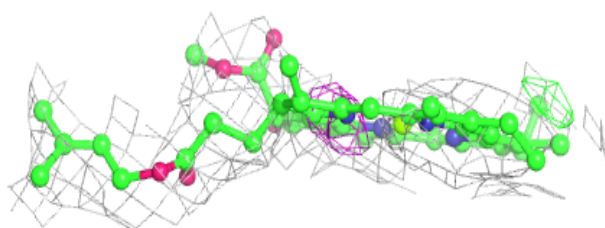
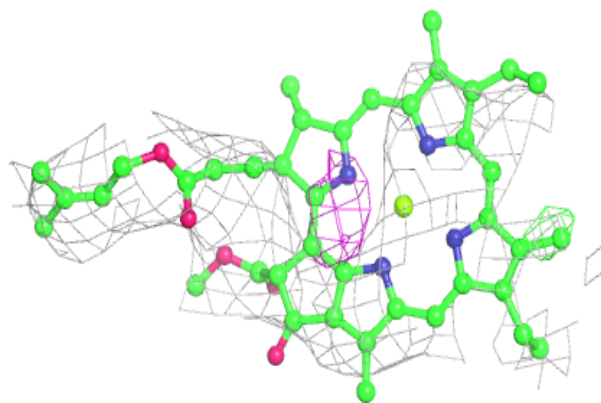
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	CA	B	6000	1/1	0.94	0.17	97,97,97,97	0
26	SF4	C	3002	8/8	0.96	0.16	121,123,127,198	0
26	SF4	C	3003	8/8	0.97	0.11	115,117,119,120	0
26	SF4	A	3001	8/8	0.98	0.23	108,110,111,113	0

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.

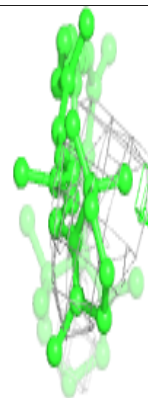
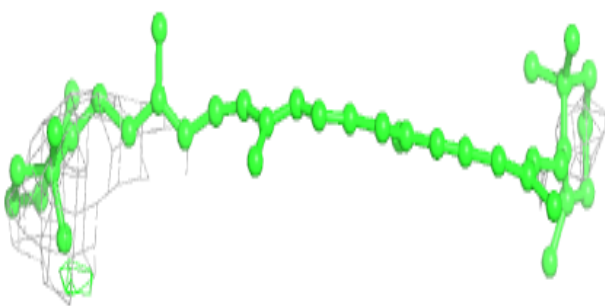
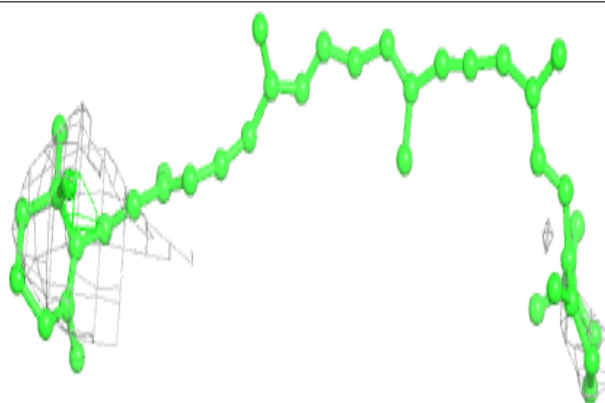


**Electron density around CLA 3 607:**

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

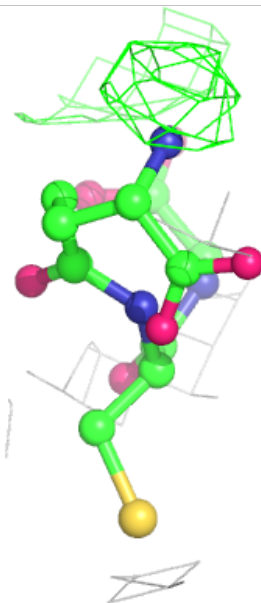
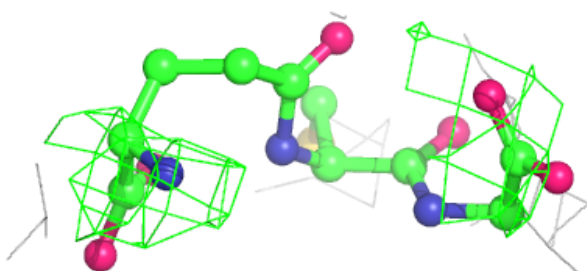
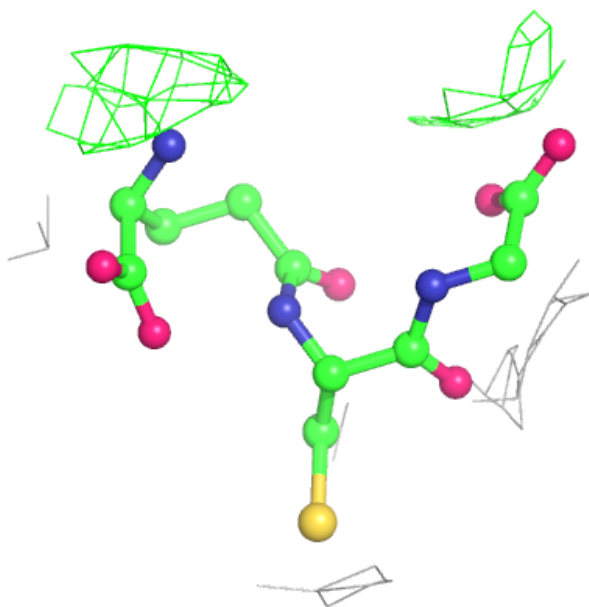
**Electron density around BCR B 4003:**

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



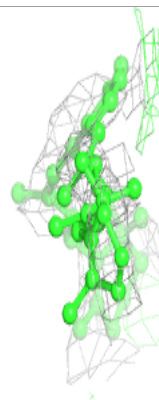
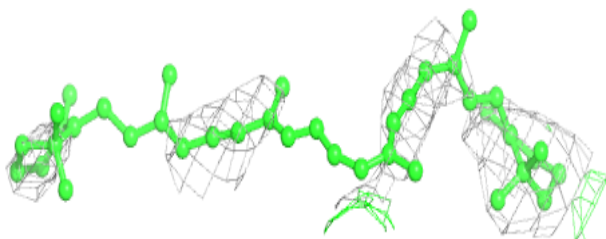
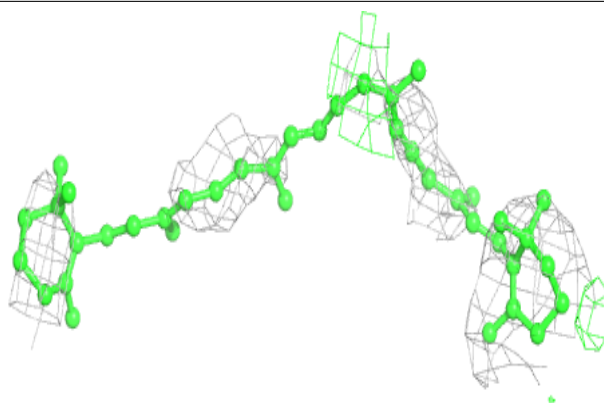
**Electron density around GSH B 5031:**

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

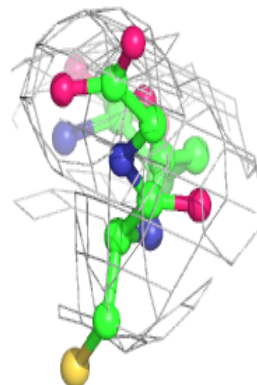
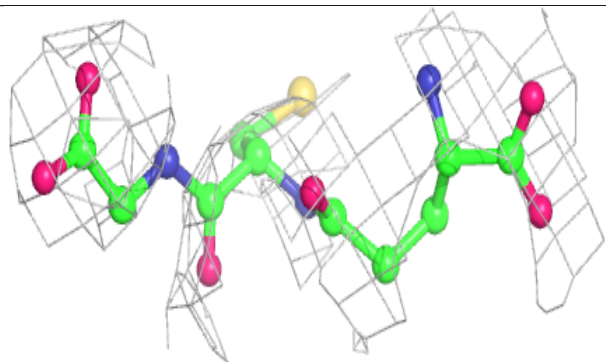
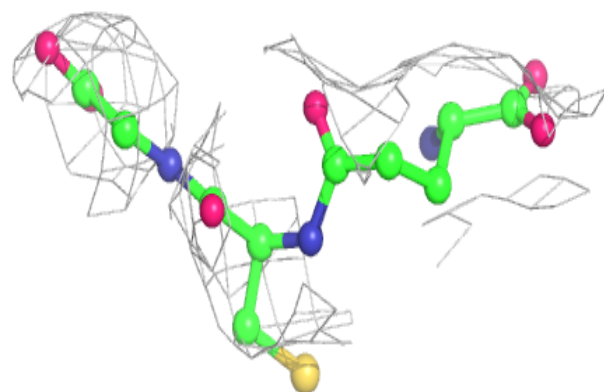


**Electron density around BCR 1 505:**

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

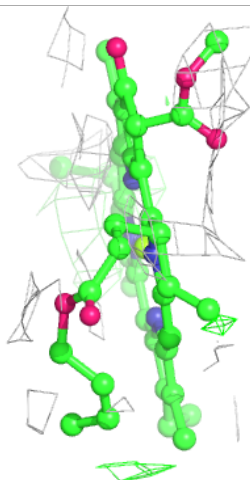
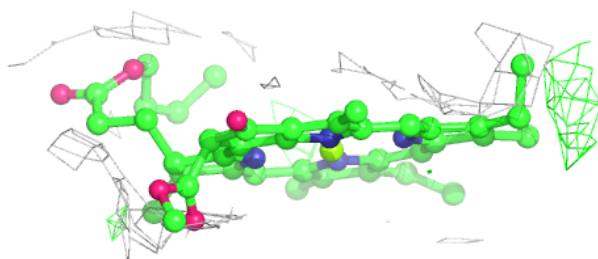
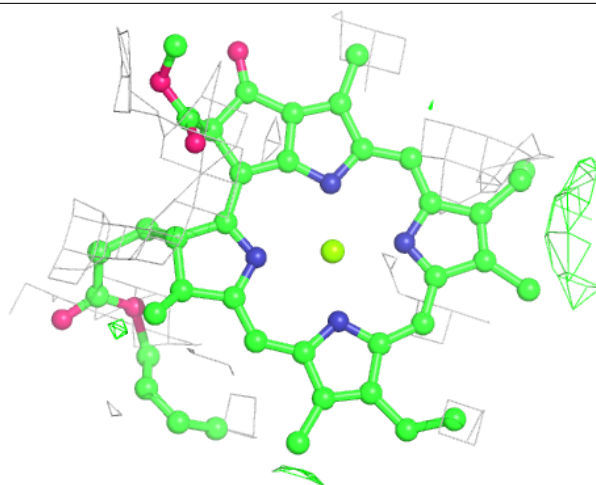
**Electron density around GSH 4 831:**

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



**Electron density around CLA A 1121:**

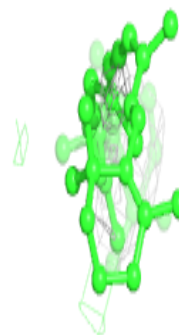
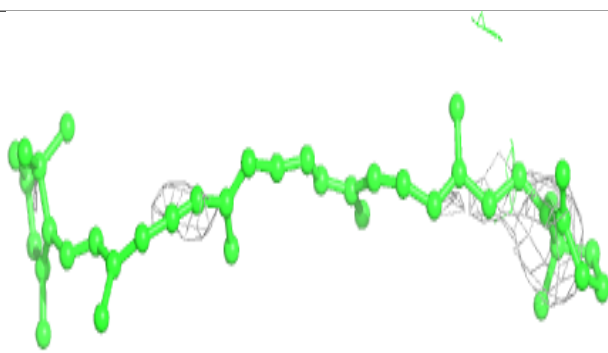
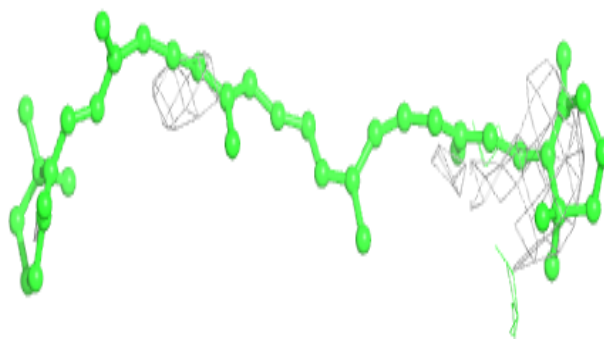
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



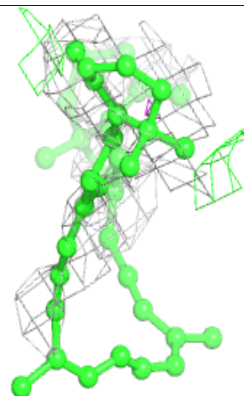
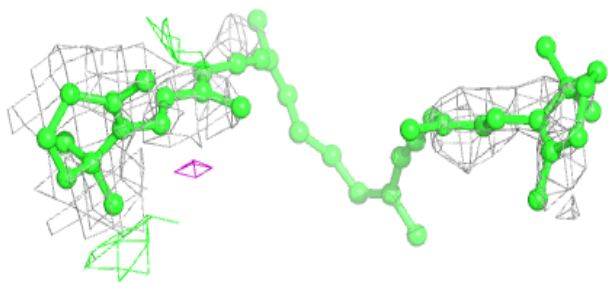
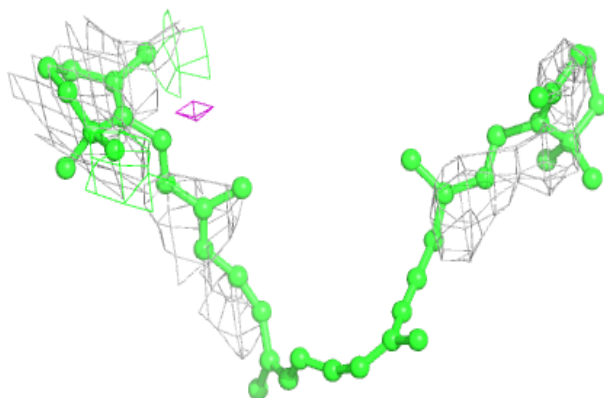


**Electron density around BCR A 4007:**

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

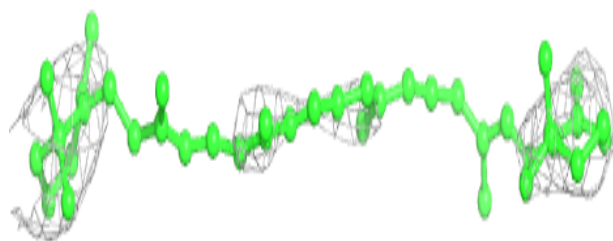
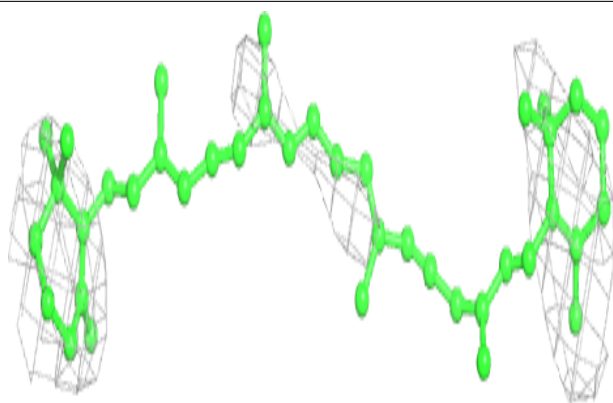
**Electron density around BCR 4 505:**

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

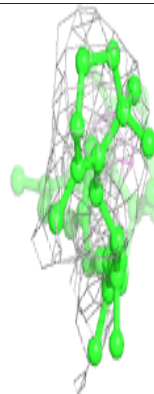
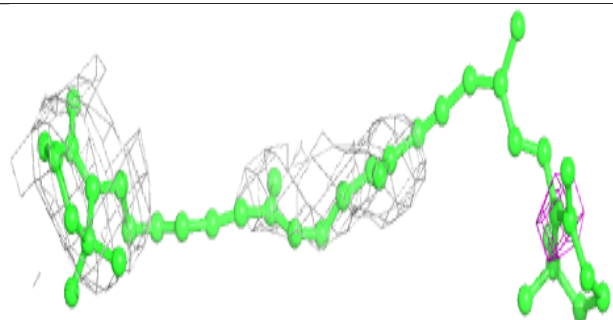
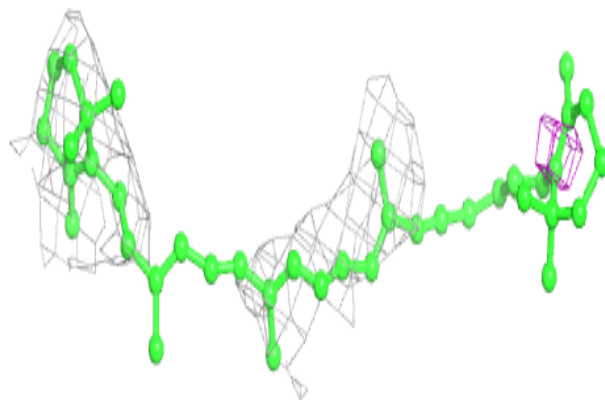


**Electron density around BCR B 4002:**

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

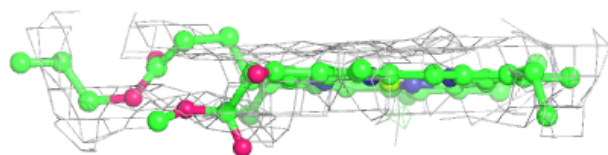
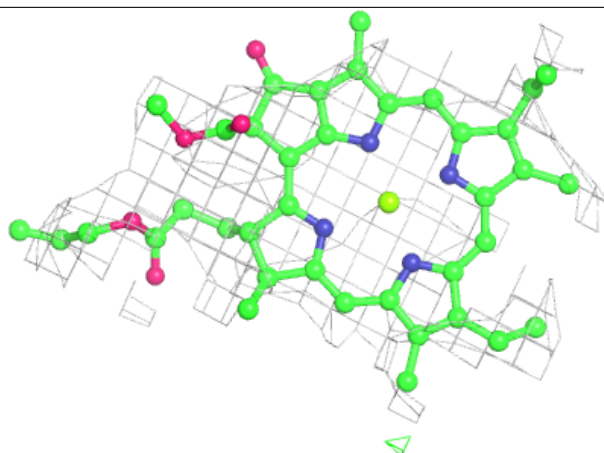
**Electron density around BCR 1 503:**

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

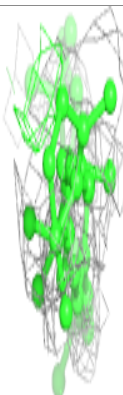
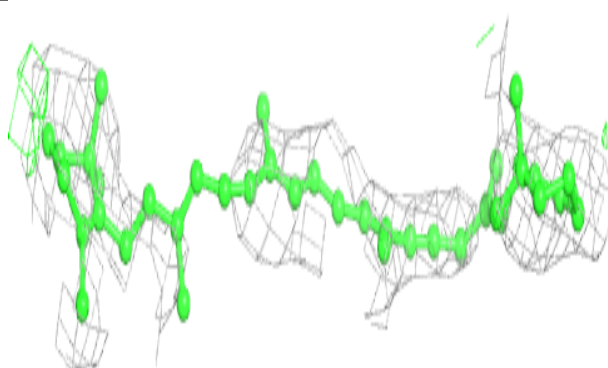
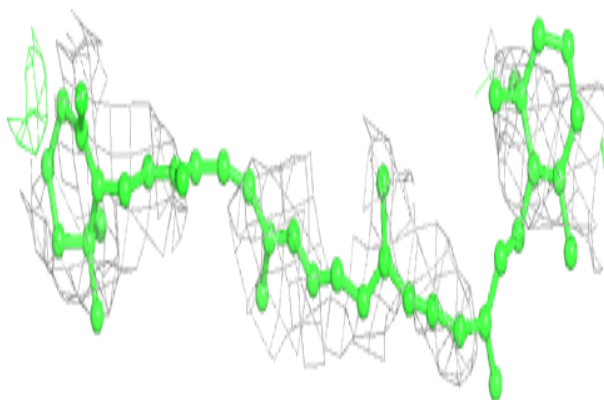


**Electron density around CLA 3 608:**

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

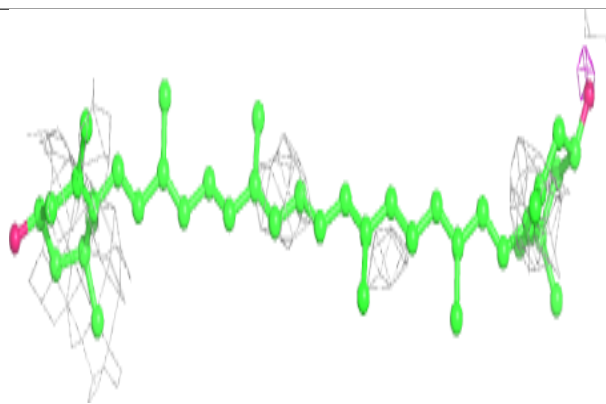
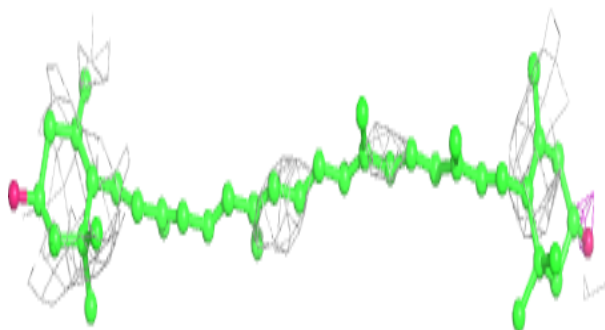
**Electron density around BCR J 4003:**

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

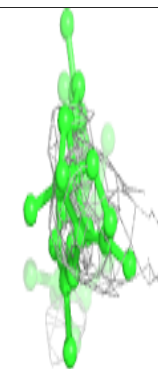
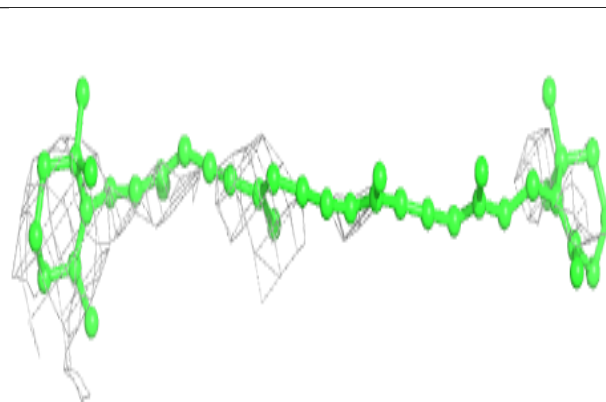
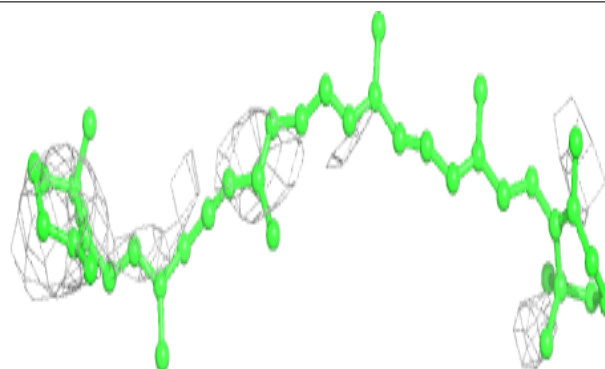


**Electron density around LUT 3 501:**

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

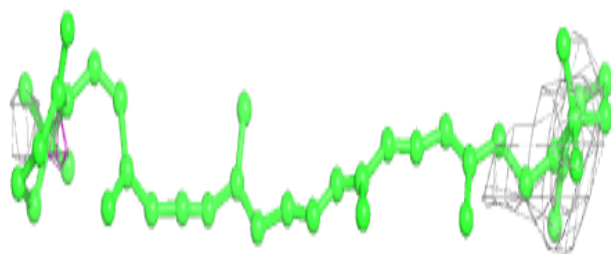
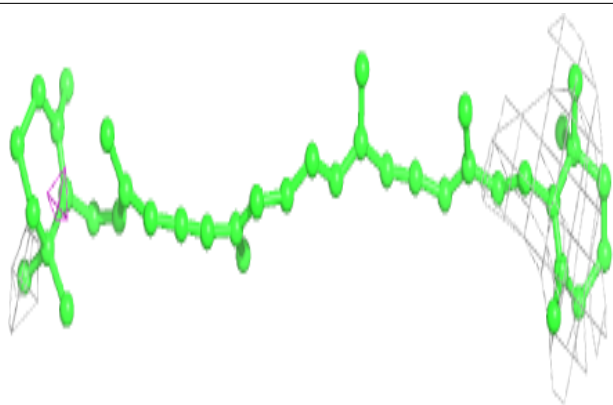
**Electron density around BCR 3 504:**

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

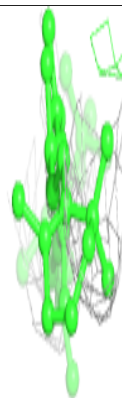
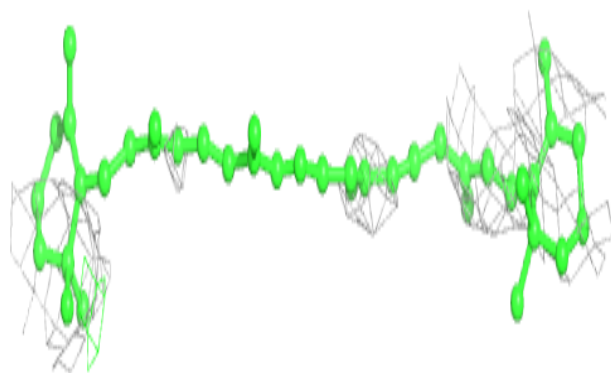
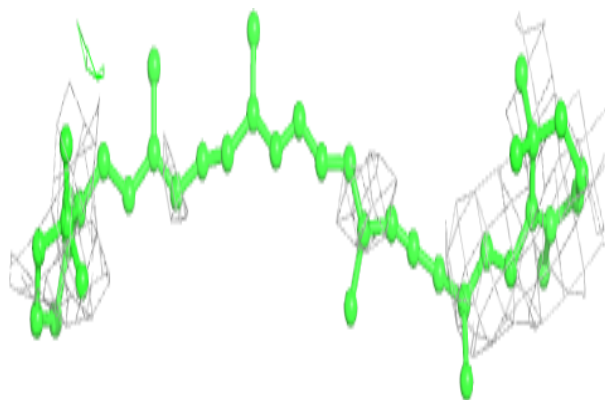


**Electron density around BCR A 4002:**

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

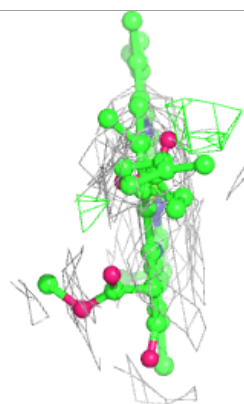
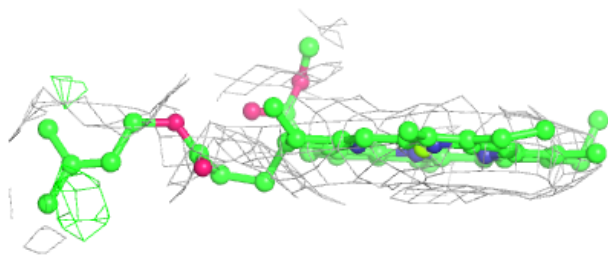
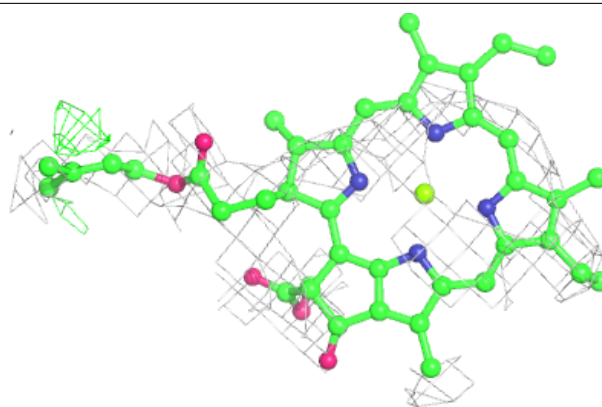
**Electron density around BCR 3 503:**

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

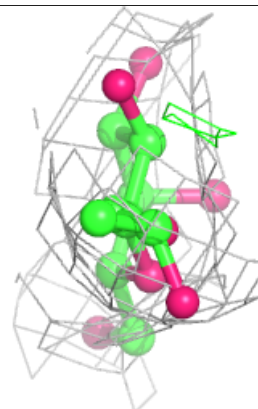
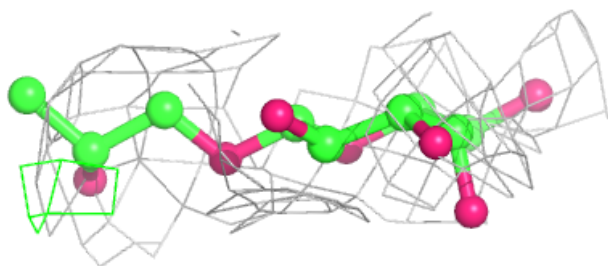
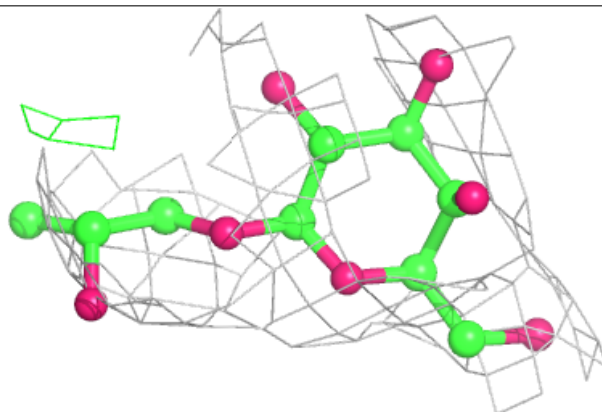


**Electron density around CLA A 1131:**

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

**Electron density around LMG 2 803:**

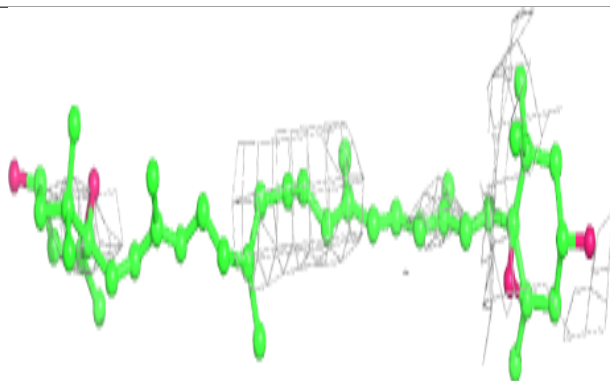
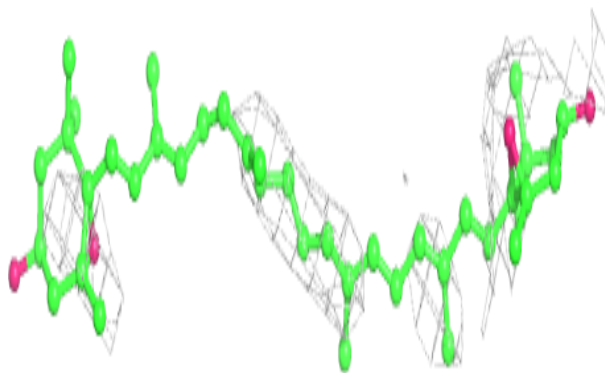
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



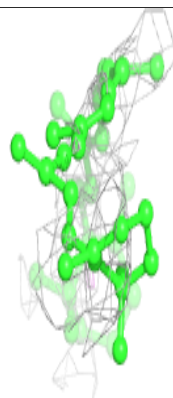
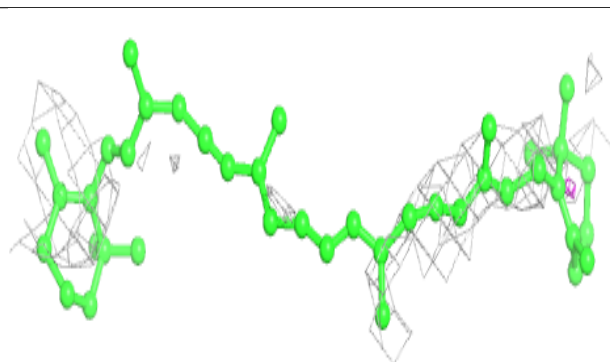
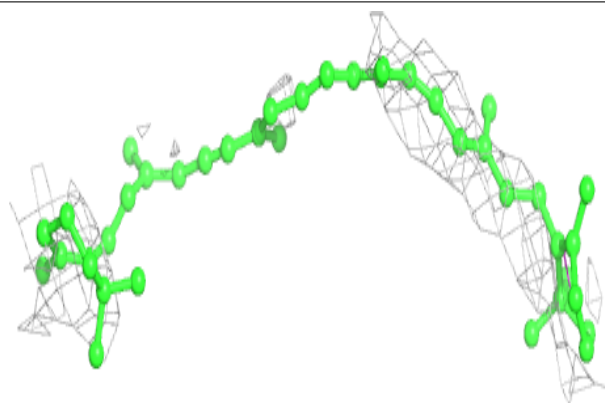


**Electron density around XAT 3 502:**

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

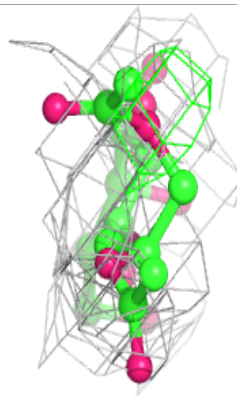
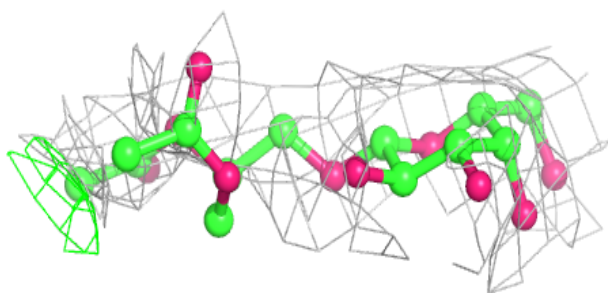
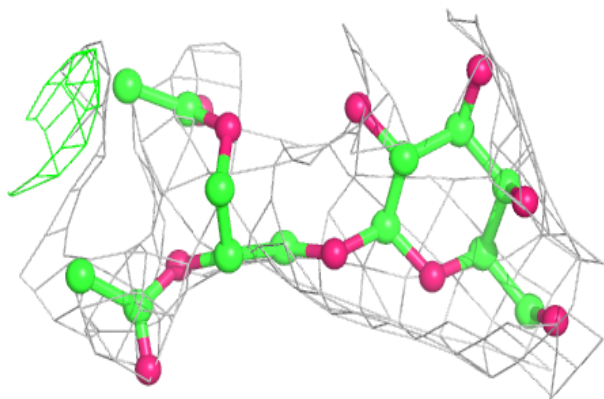
**Electron density around BCR B 4001:**

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

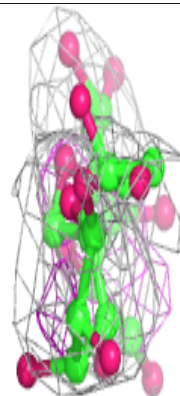
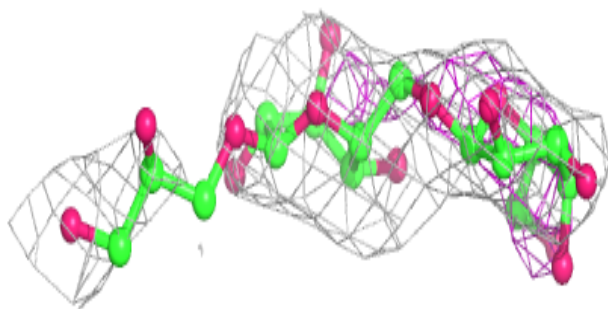
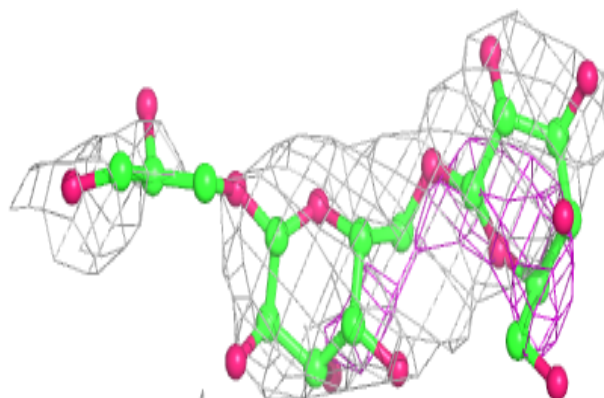


**Electron density around LMG 1 803:**

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

**Electron density around DGD J 5001:**

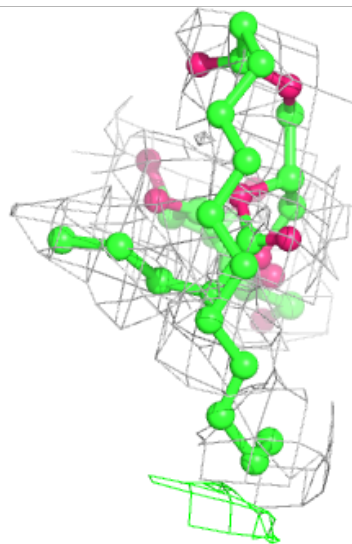
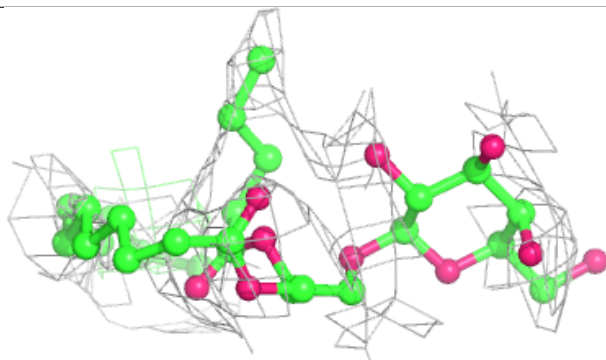
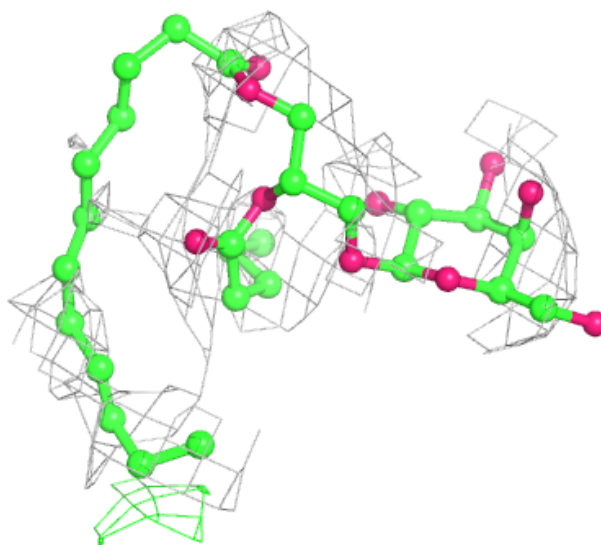
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





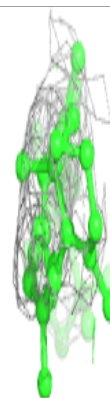
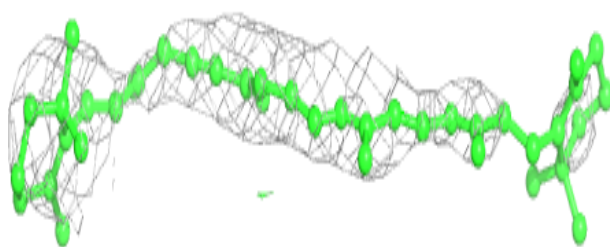
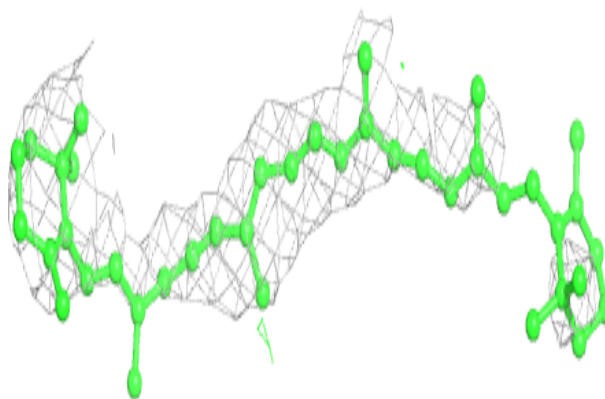
**Electron density around LMG 1 802:**

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

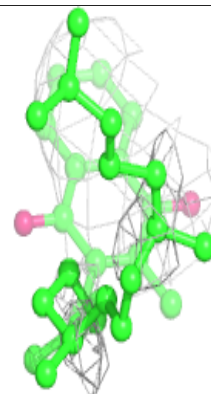
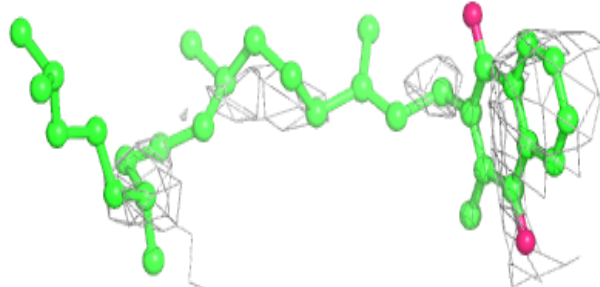
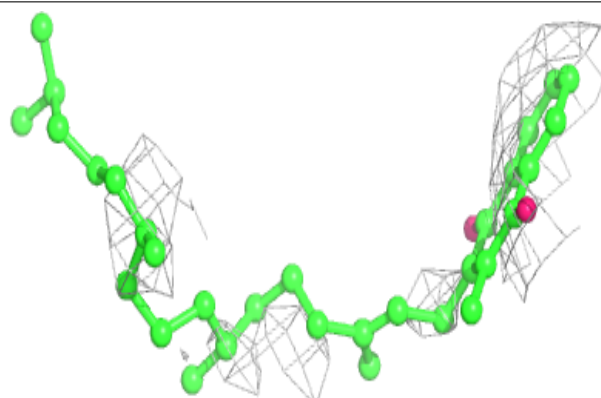


**Electron density around BCR B 4005:**

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

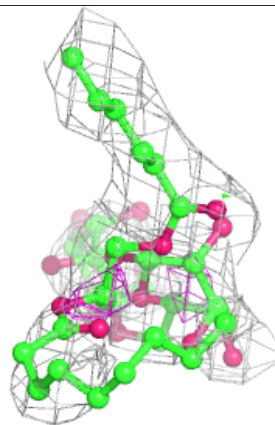
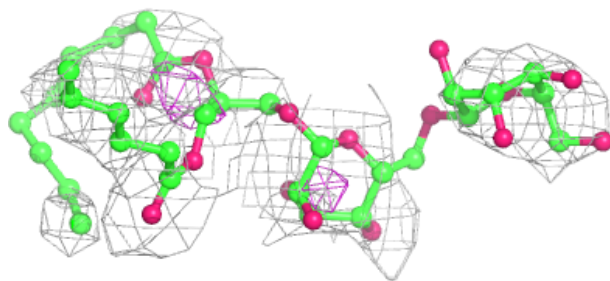
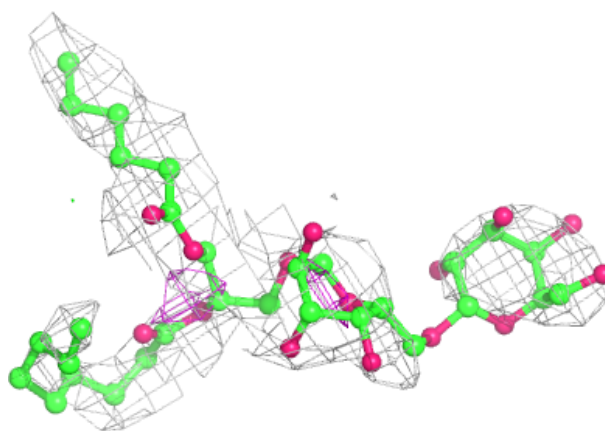
**Electron density around PQN B 2002:**

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



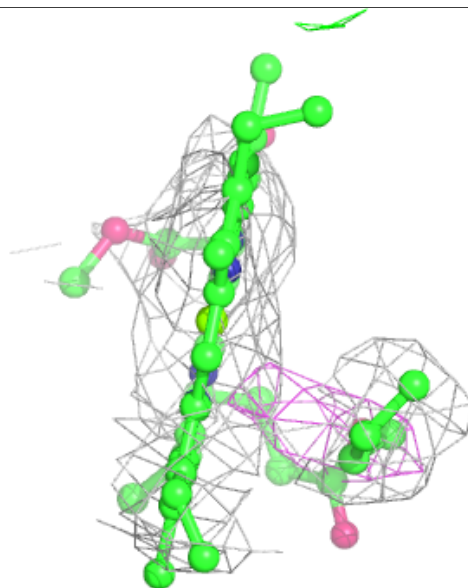
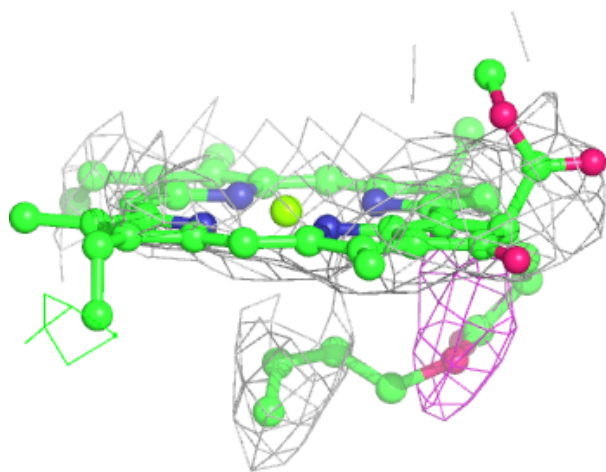
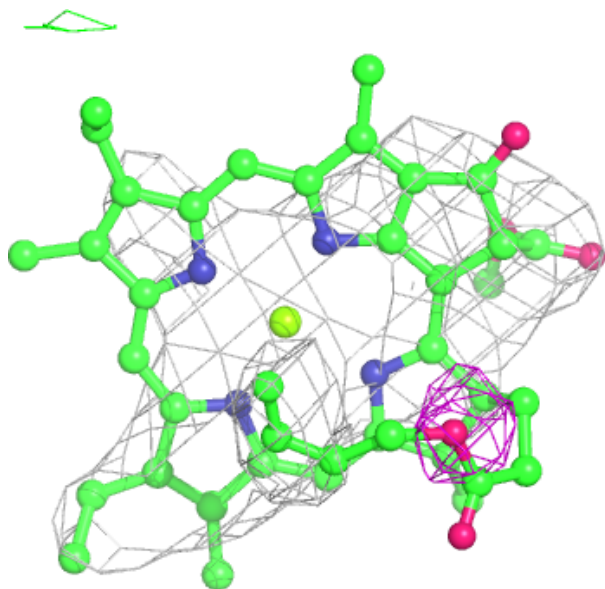
**Electron density around DGD 4 811:**

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



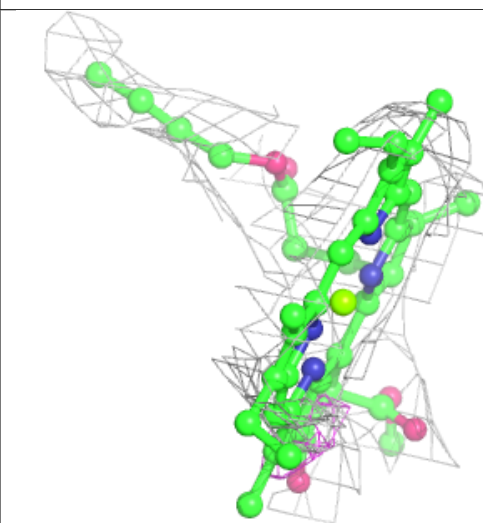
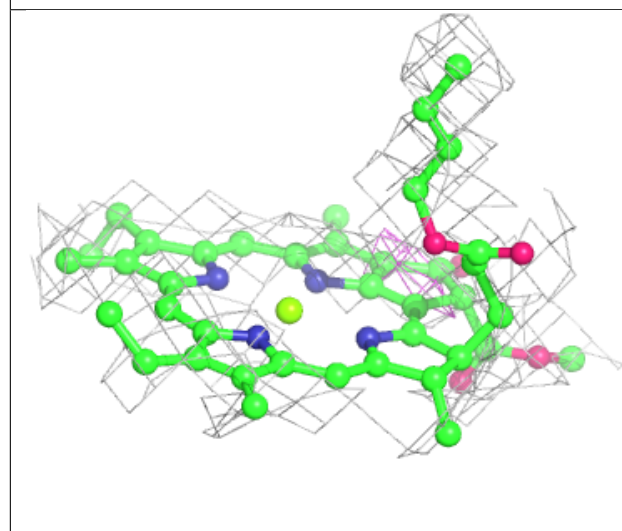
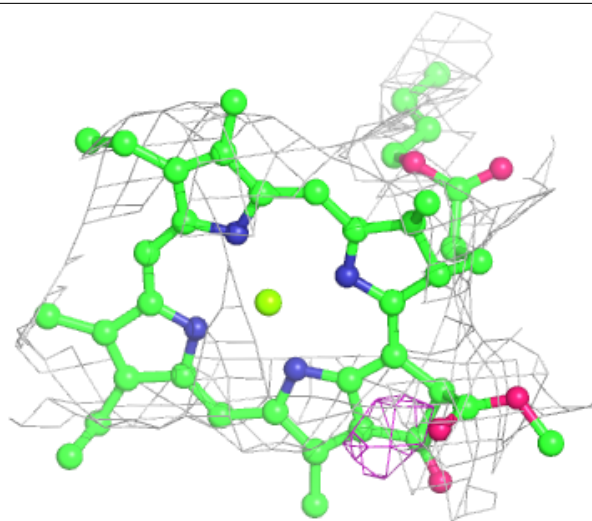
**Electron density around CLA B 1224:**

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



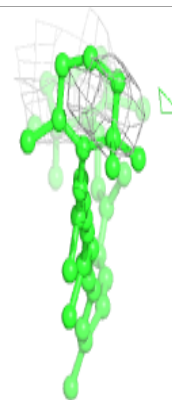
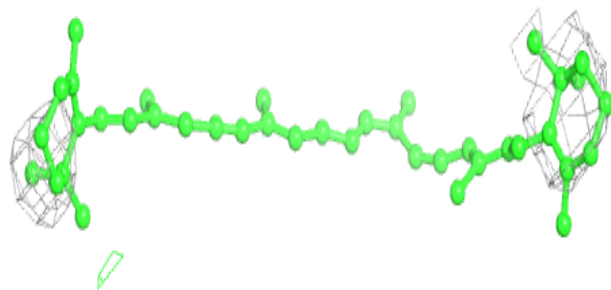
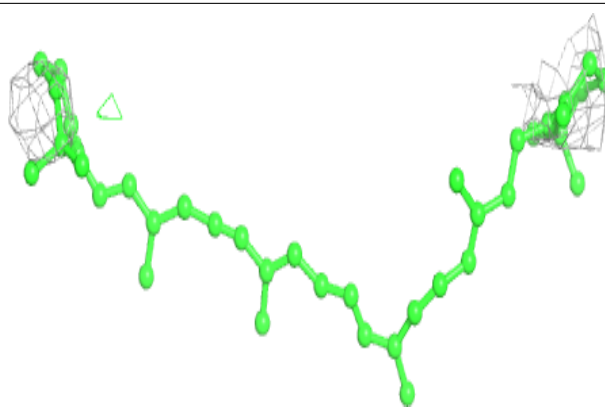
**Electron density around CLA B 1208:**

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



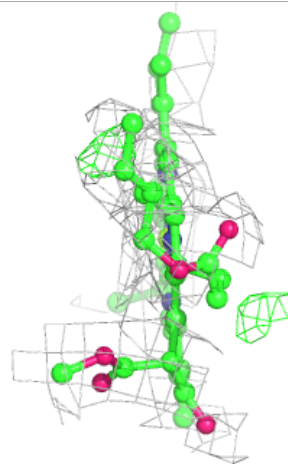
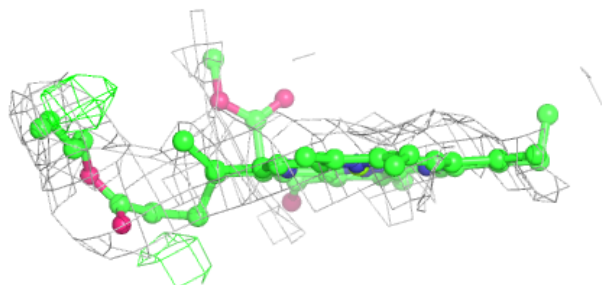
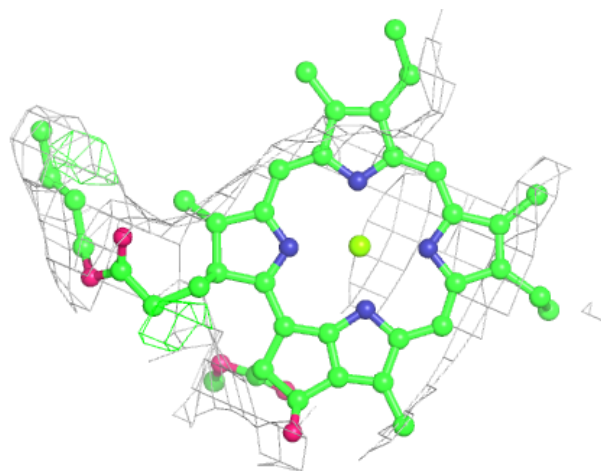
**Electron density around BCR A 4004:**

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



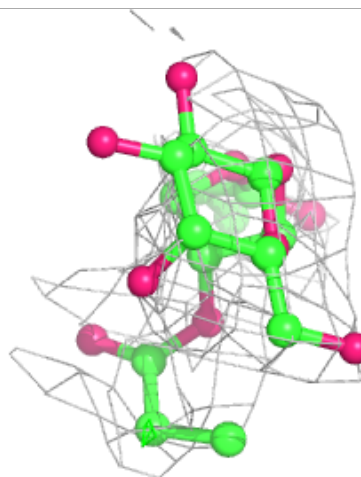
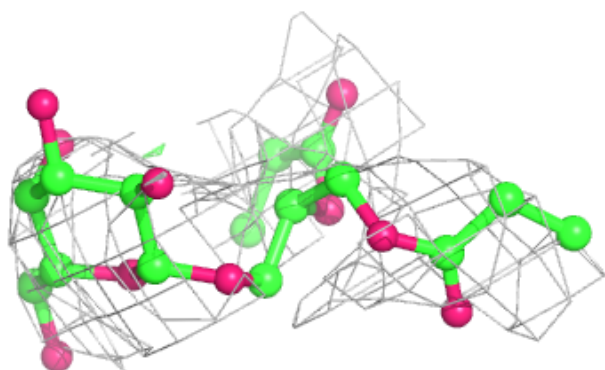
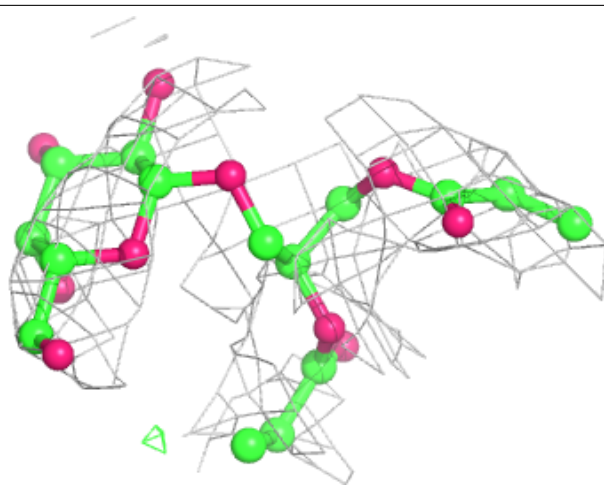
**Electron density around CLA A 1111:**

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



**Electron density around LMG 2 802:**

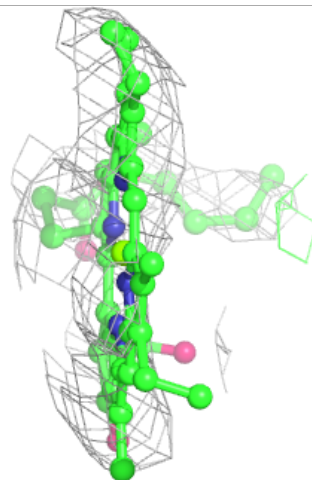
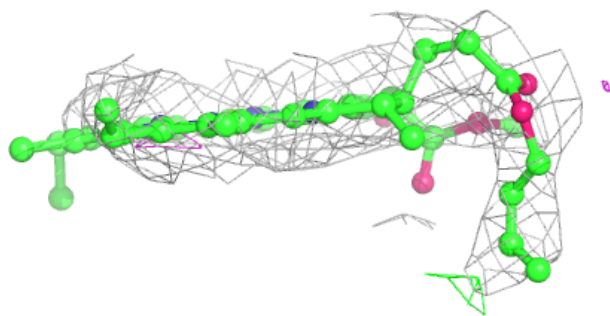
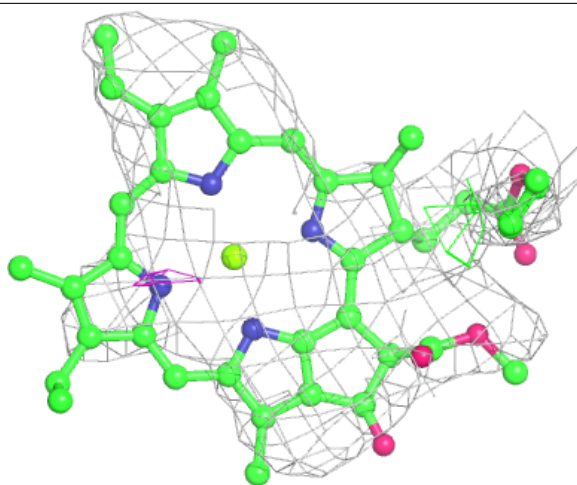
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





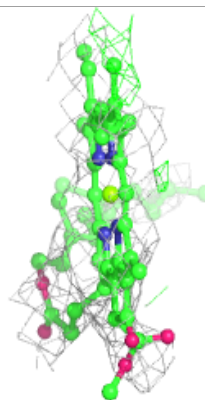
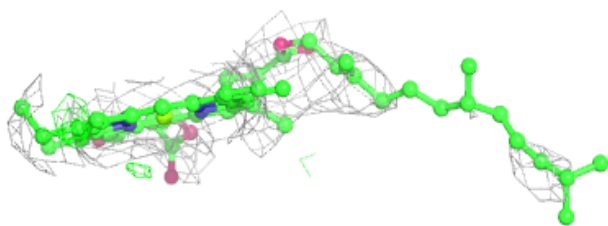
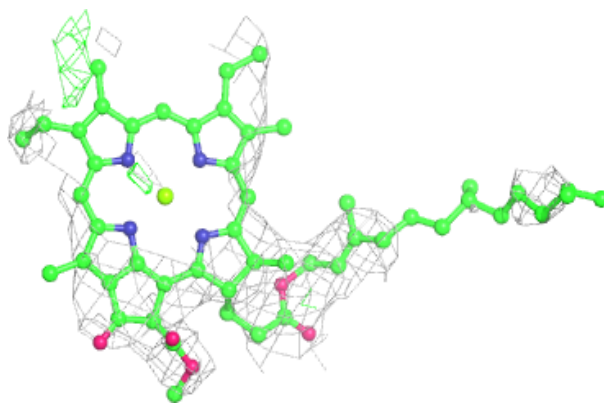
**Electron density around CLA B 1203:**

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

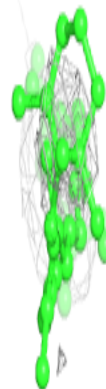
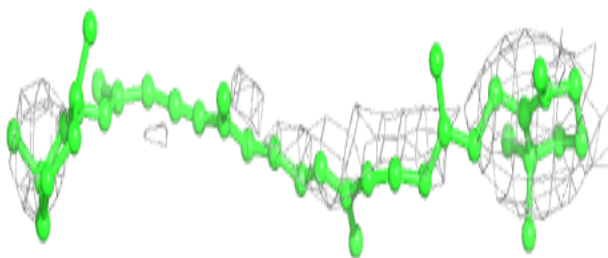
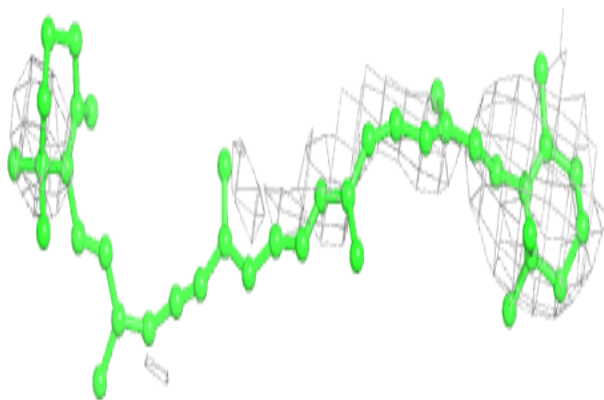


**Electron density around CLA B 1023:**

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

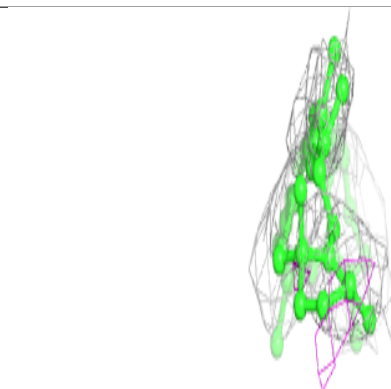
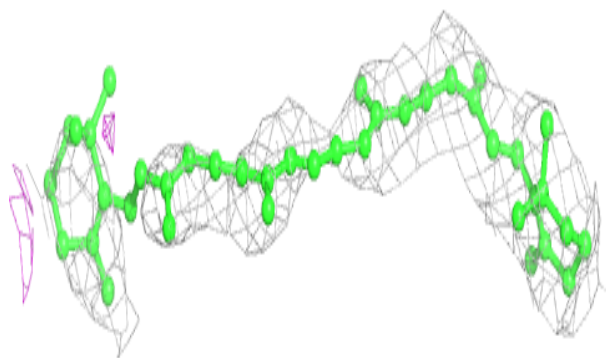
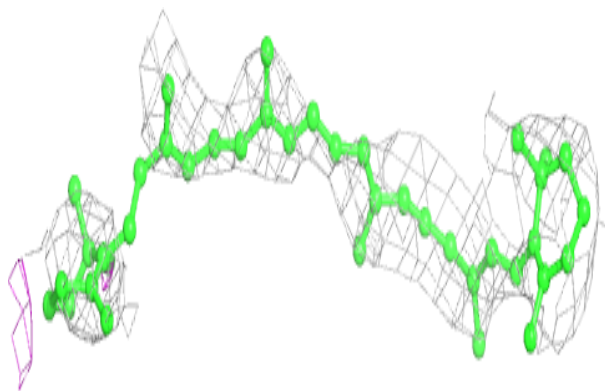
**Electron density around BCR A 4003:**

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

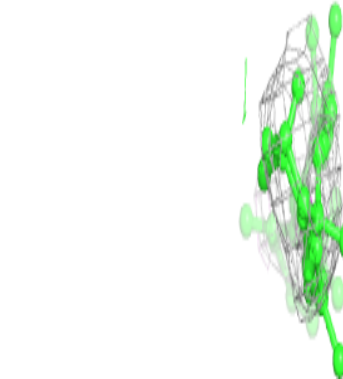
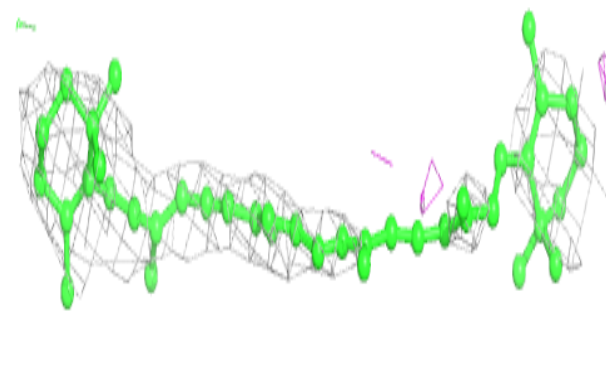
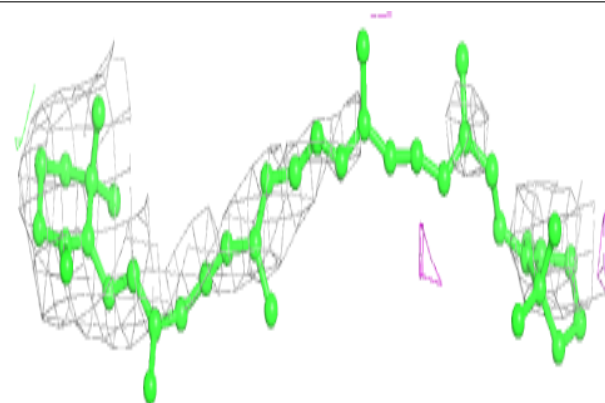


**Electron density around BCR 4 503:**

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

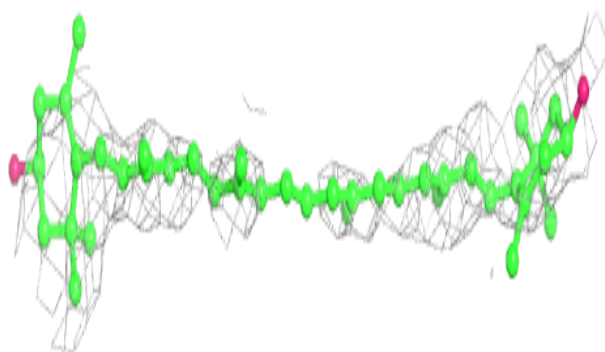
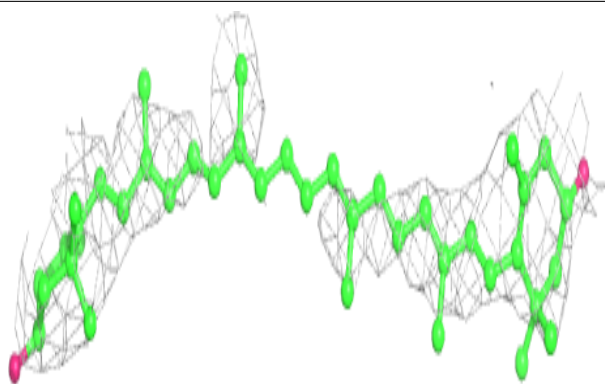
**Electron density around BCR 2 503:**

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



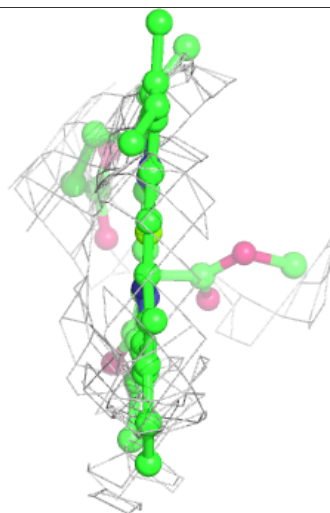
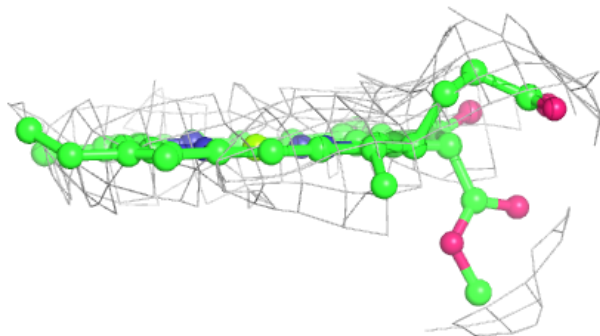
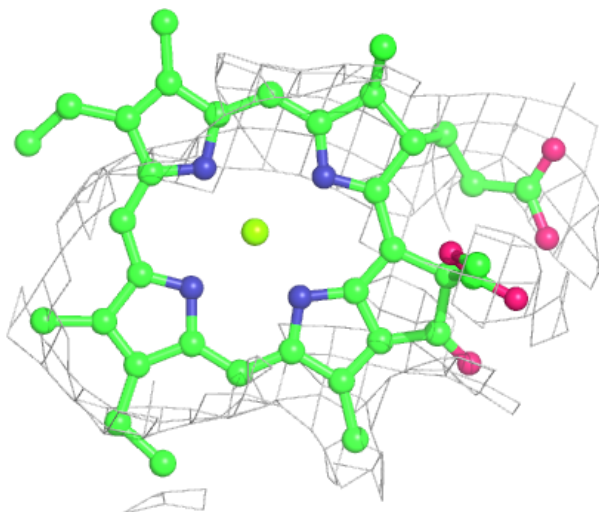
**Electron density around LUT 2 501:**

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



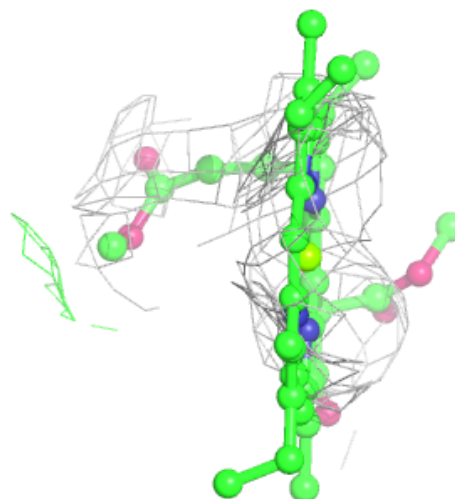
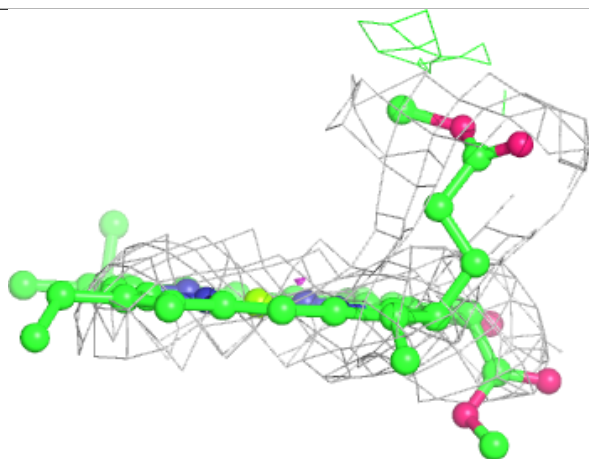
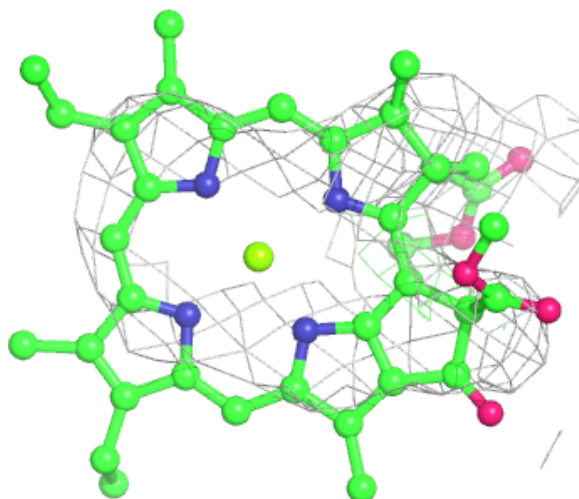
**Electron density around CLA 3 603:**

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



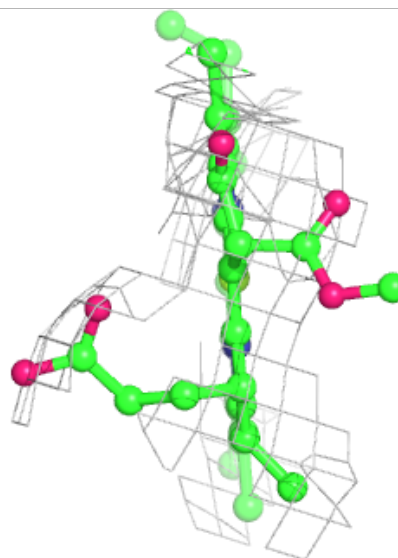
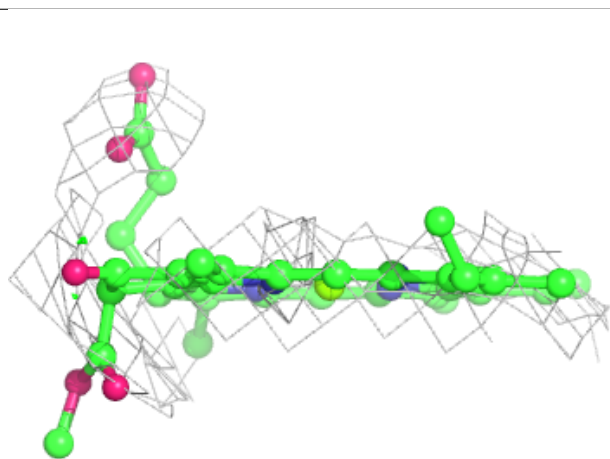
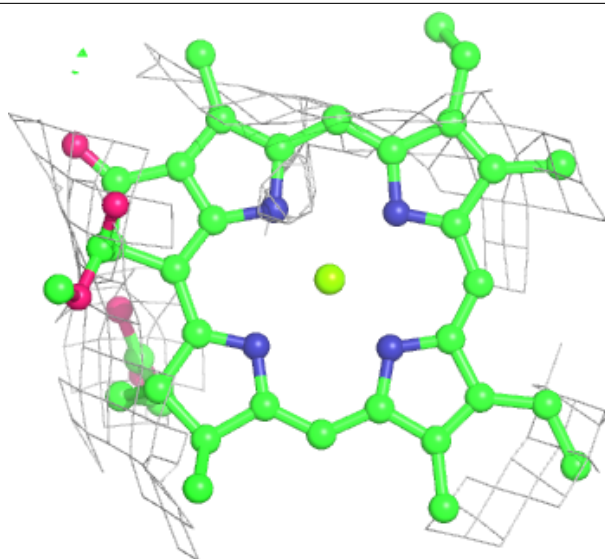
**Electron density around CLA A 1114:**

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



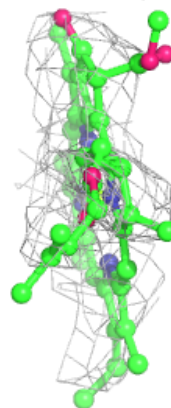
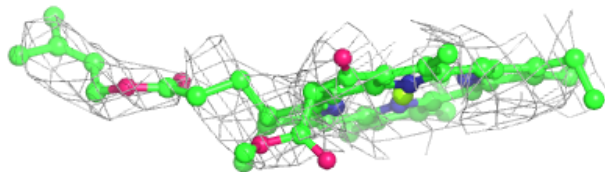
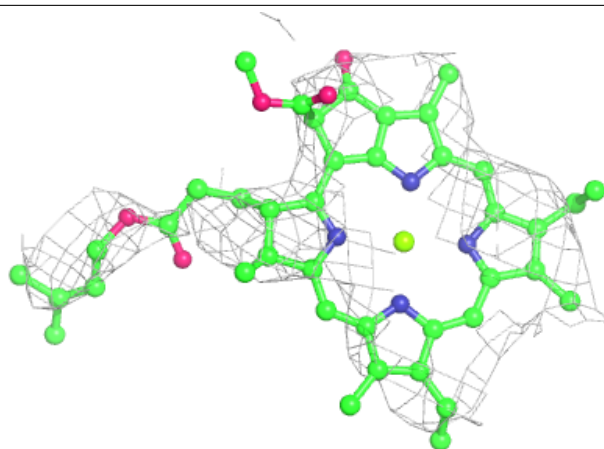
**Electron density around CLA 3 606:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CLA B 1022:**

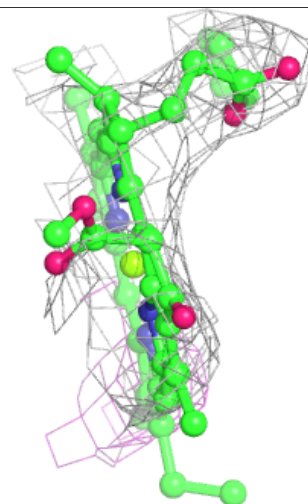
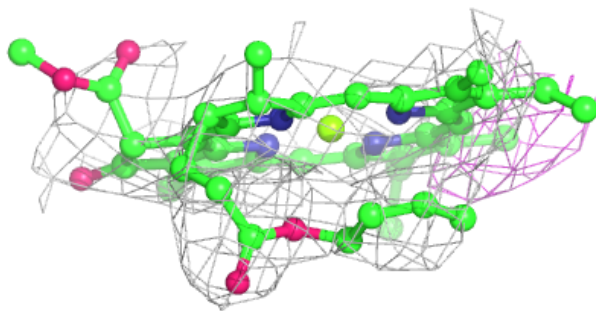
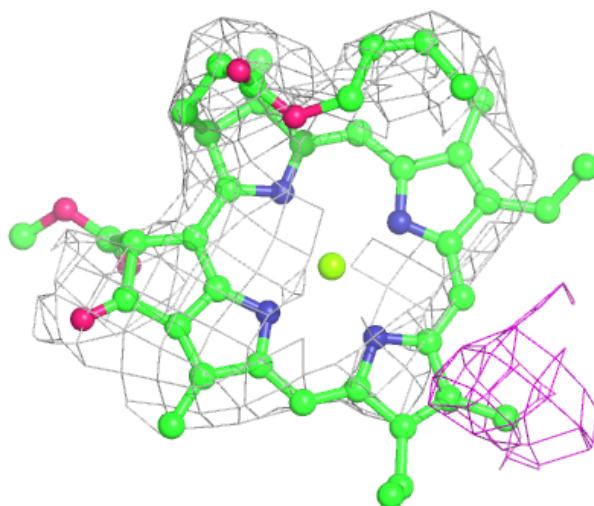
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





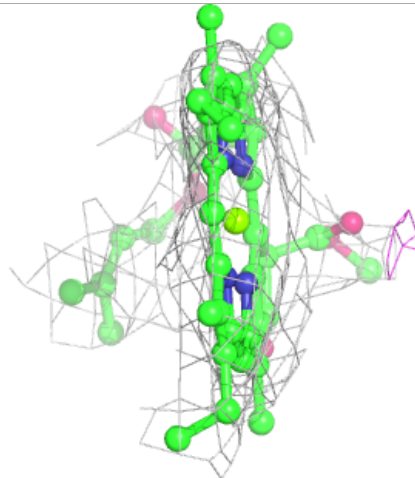
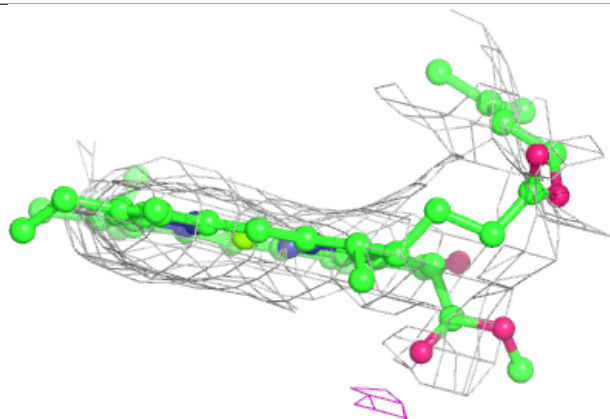
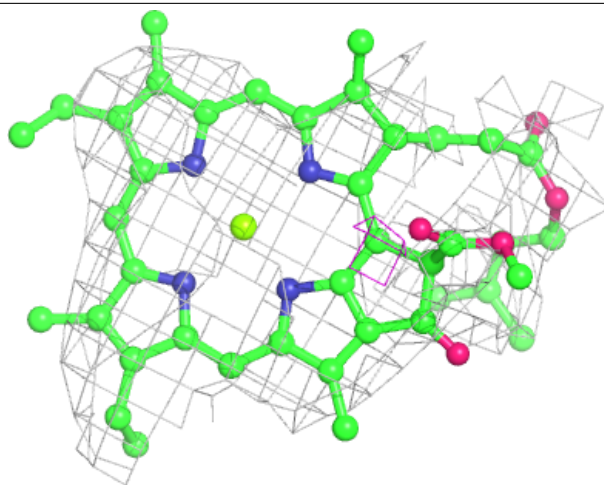
**Electron density around CLA B 1215:**

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



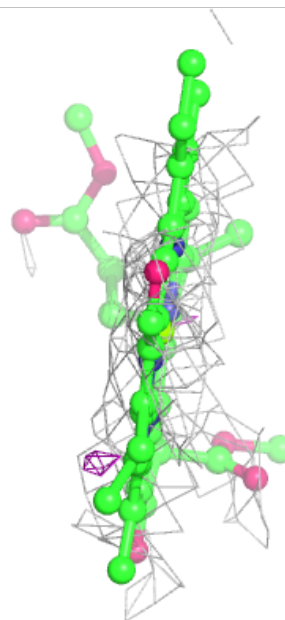
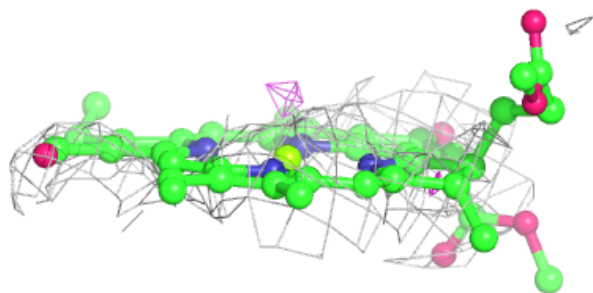
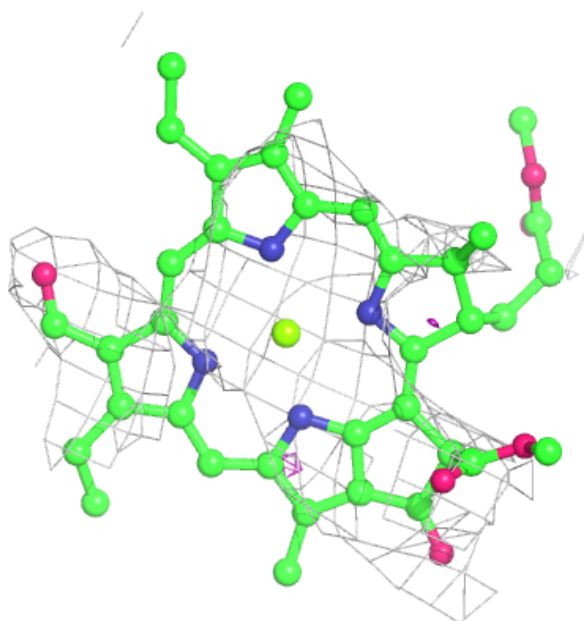
**Electron density around CLA B 1238:**

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



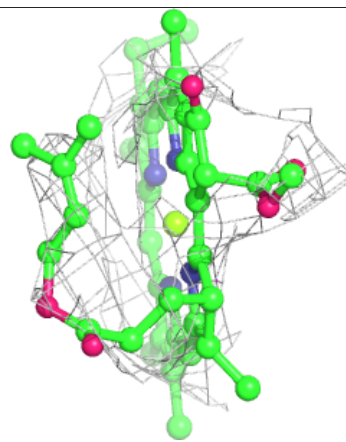
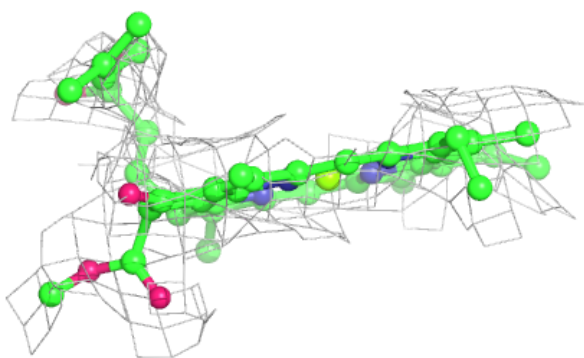
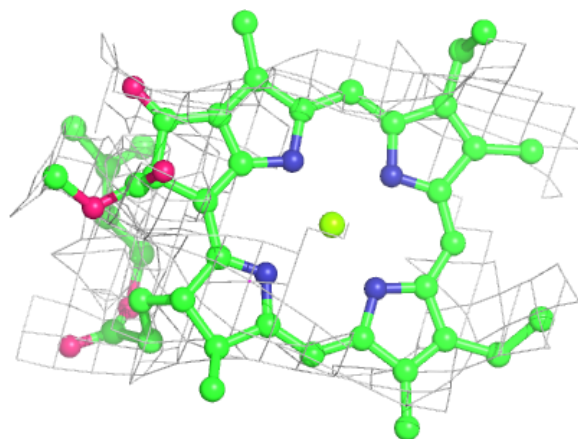
**Electron density around CHL 3 604:**

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



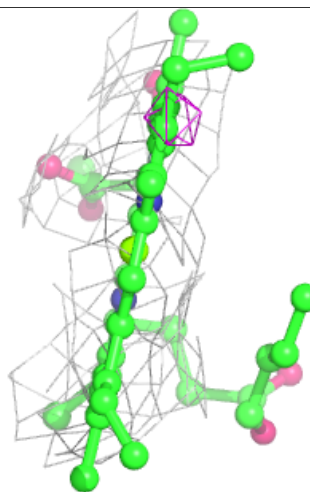
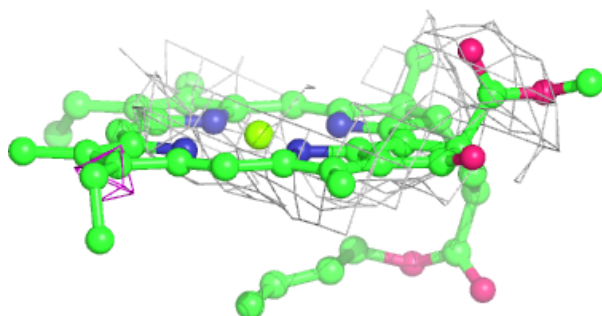
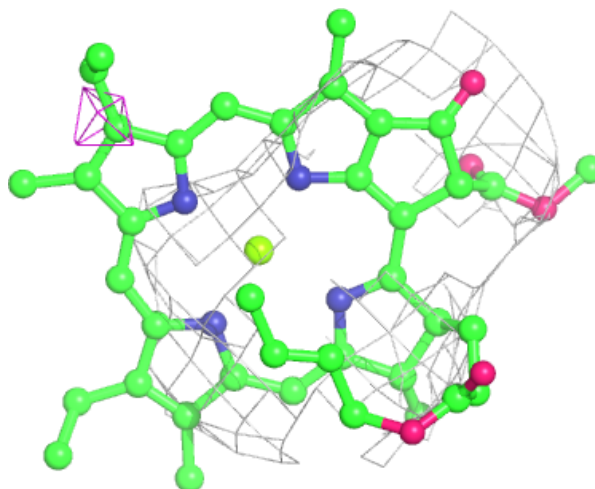
**Electron density around CLA A 1141:**

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



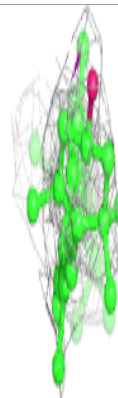
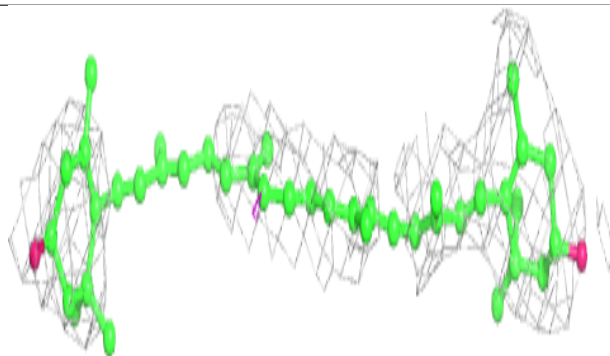
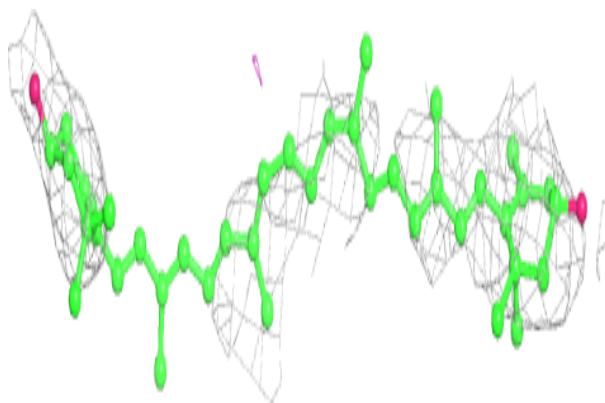
**Electron density around CLA A 1116:**

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

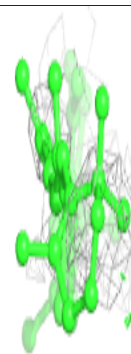
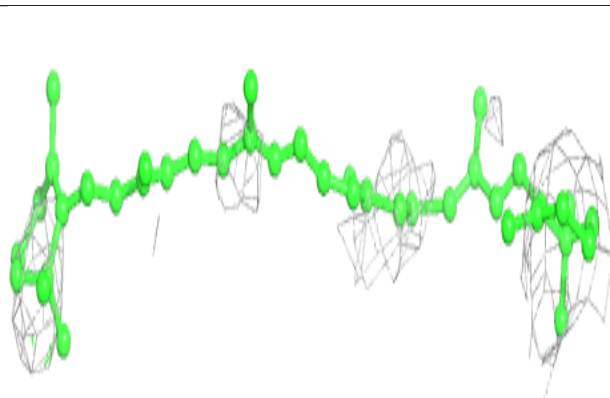
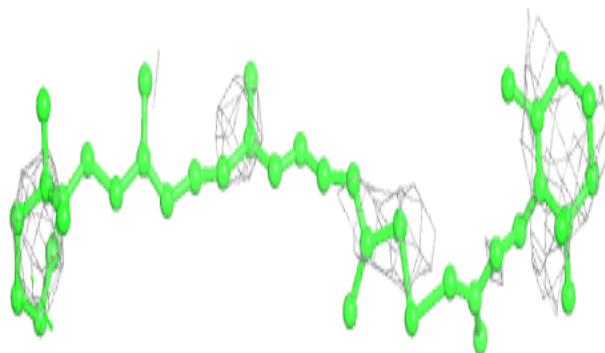


**Electron density around LUT 1 501:**

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

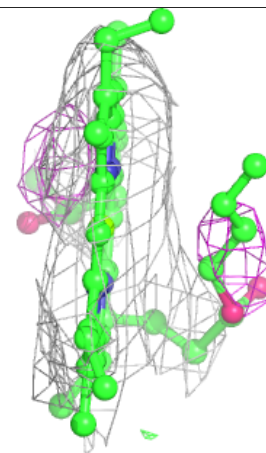
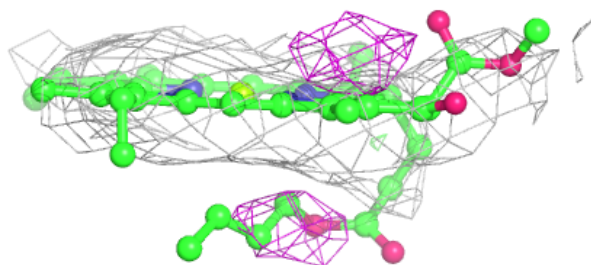
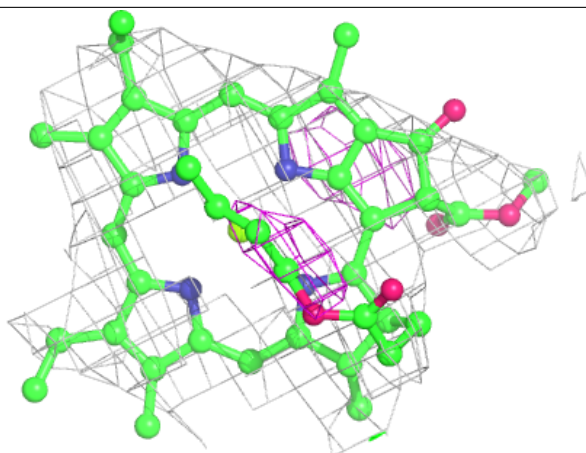
**Electron density around BCR A 4005:**

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

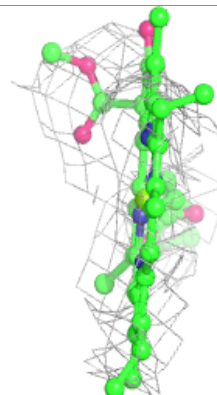
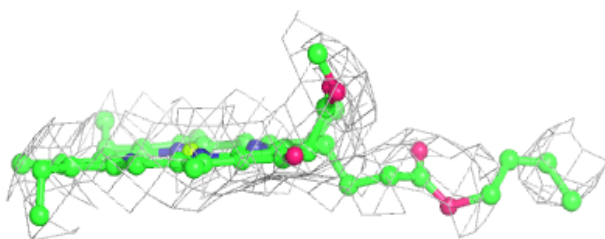
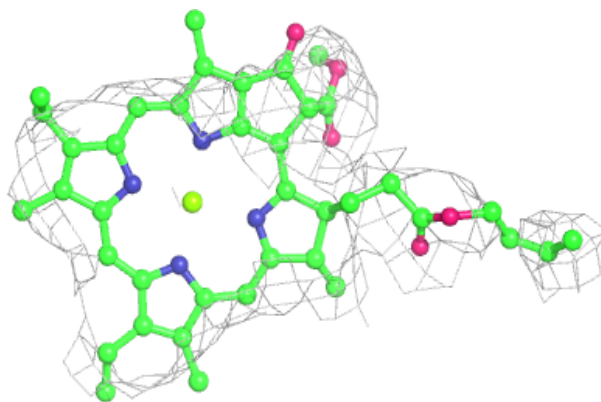


**Electron density around CLA B 1211:**

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

**Electron density around CLA A 1135:**

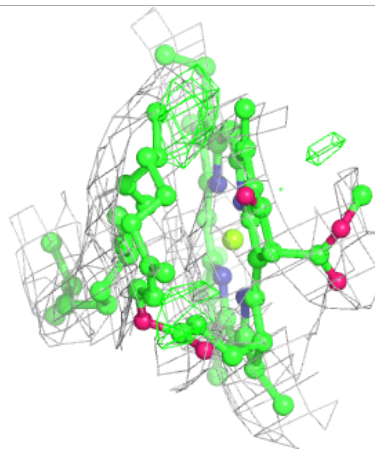
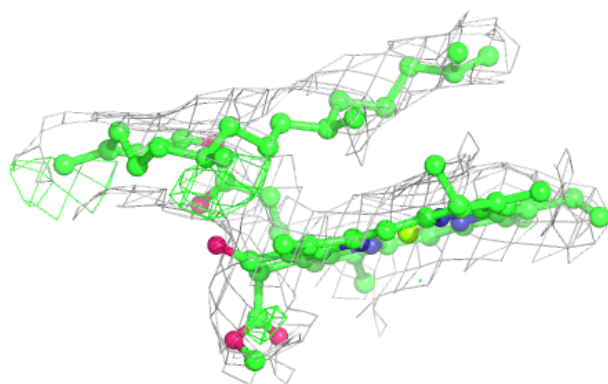
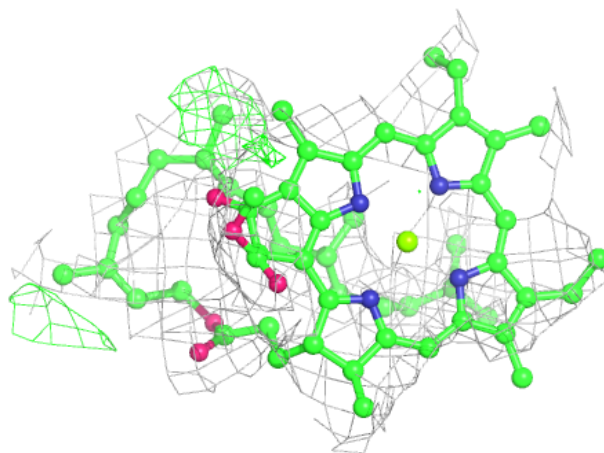
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 2 605:**

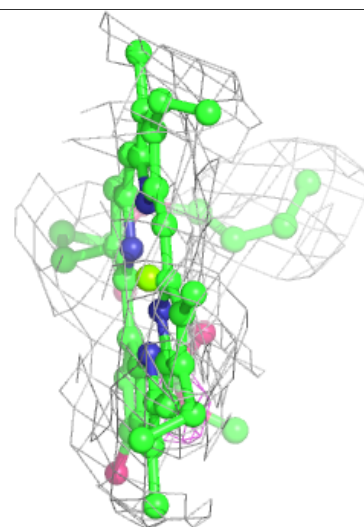
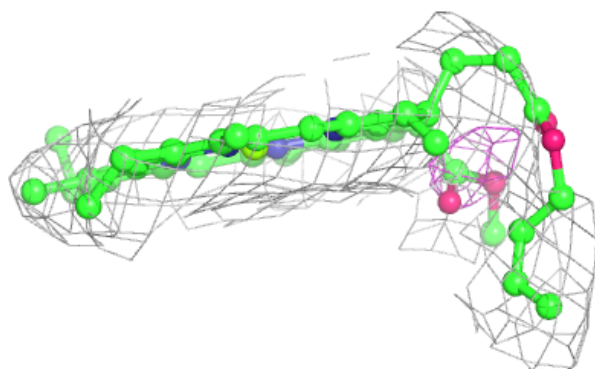
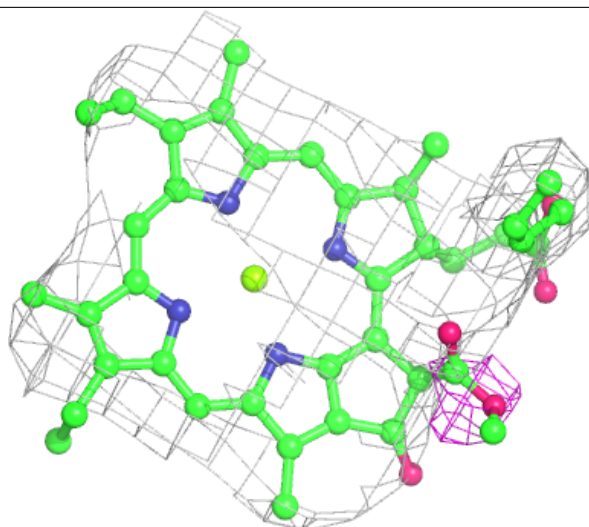
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





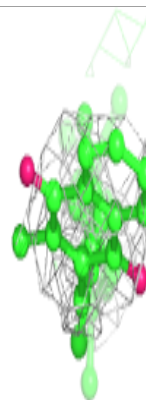
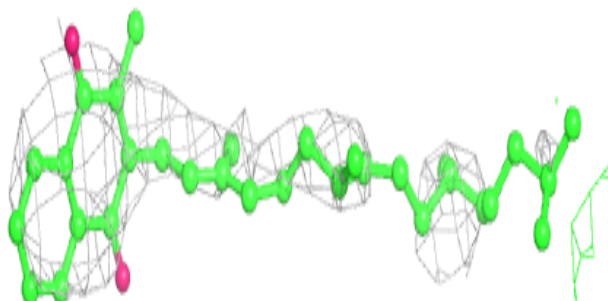
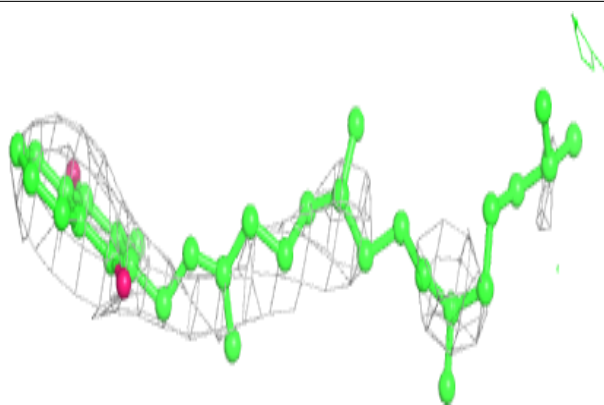
**Electron density around CLA 2 602:**

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



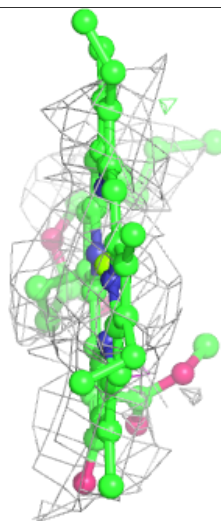
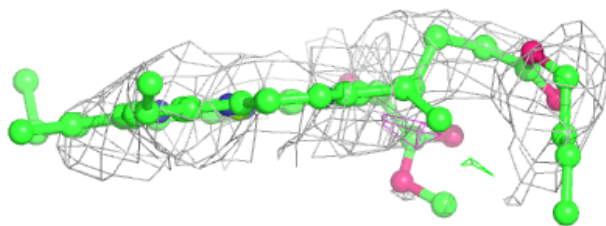
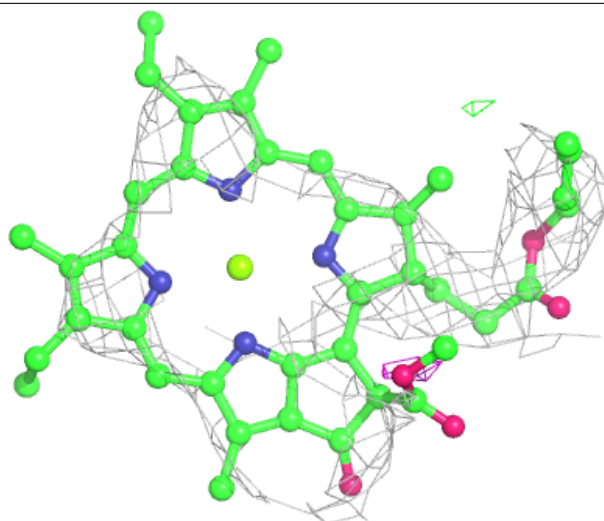
**Electron density around PQN A 2001:**

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



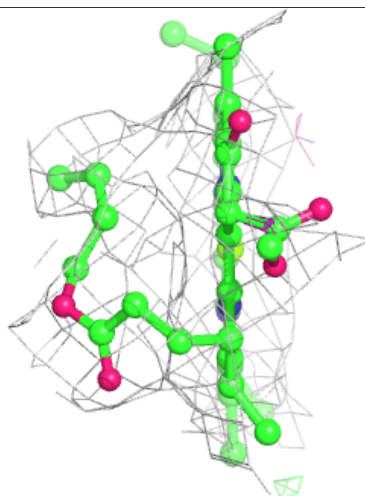
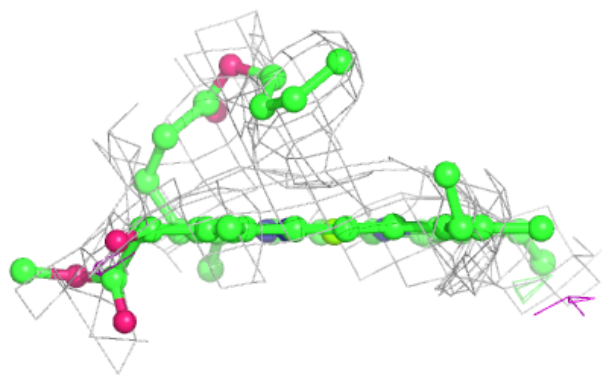
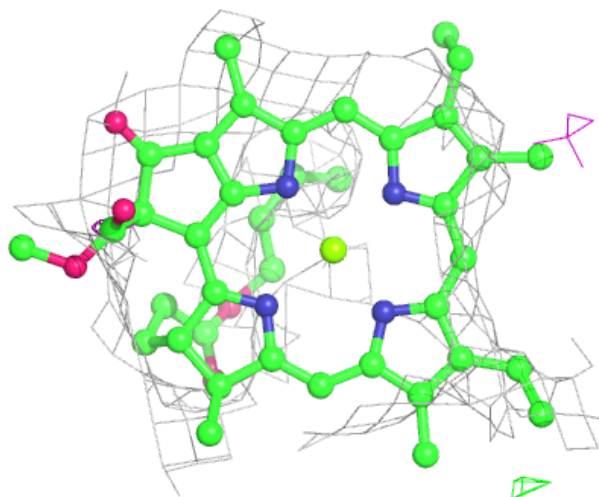
**Electron density around CLA B 1221:**

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



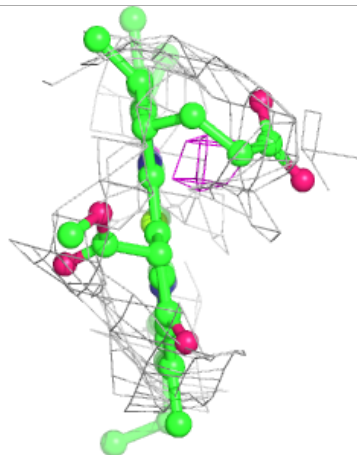
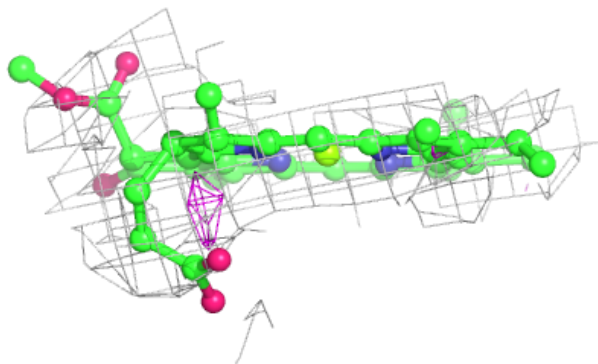
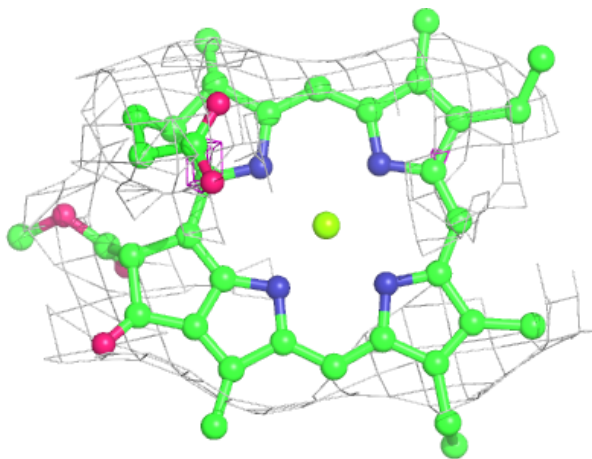
**Electron density around CLA B 1218:**

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



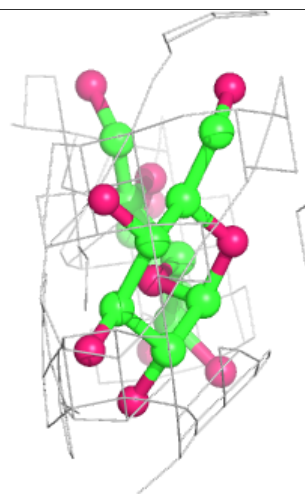
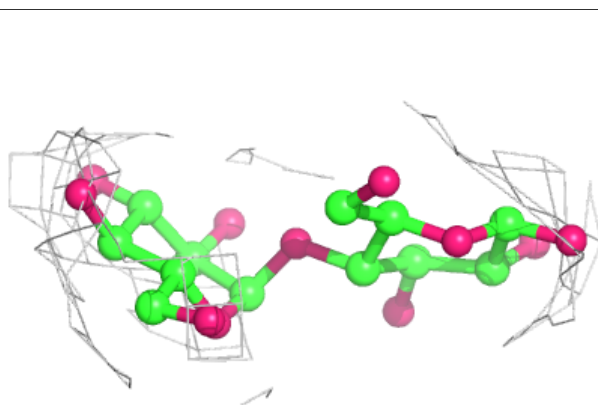
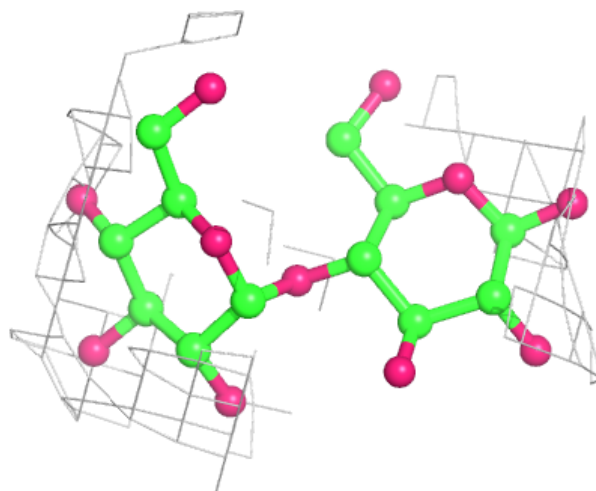
**Electron density around CLA 1 613:**

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



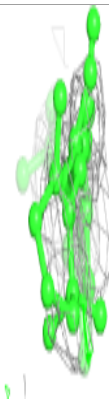
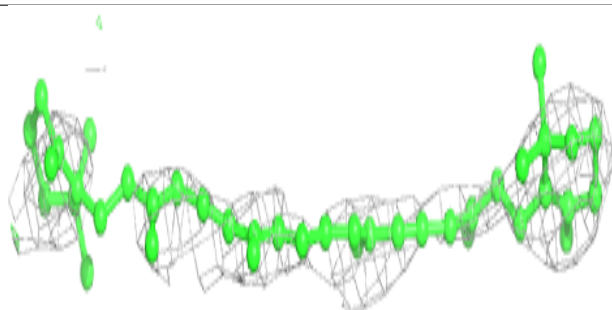
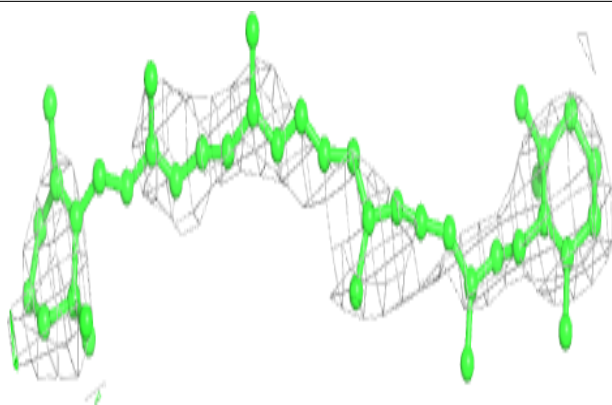
**Electron density around LMT 2 821:**

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

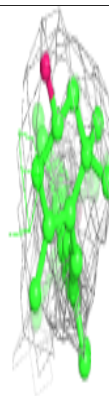
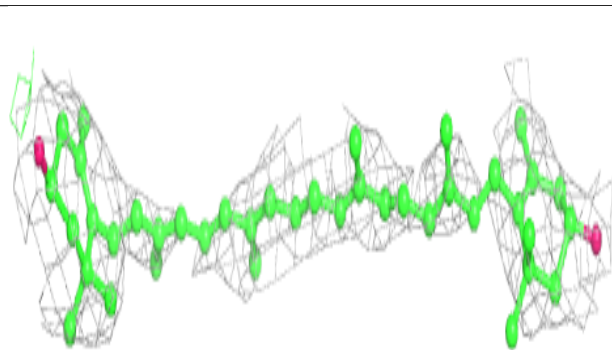
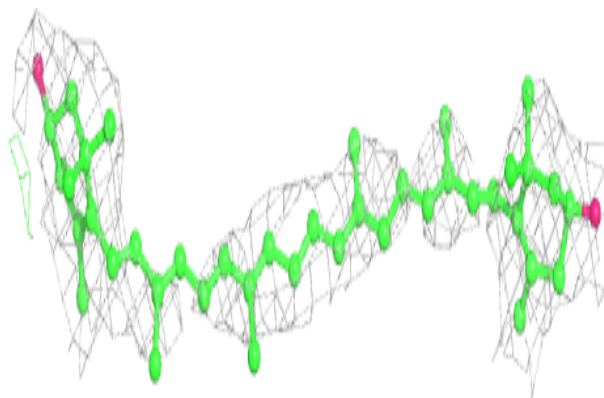


**Electron density around BCR J 4001:**

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

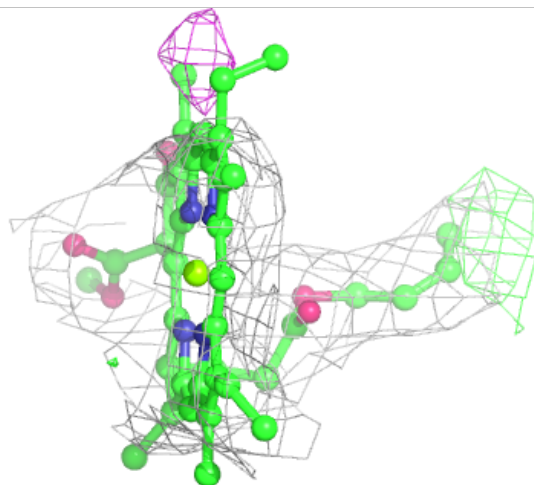
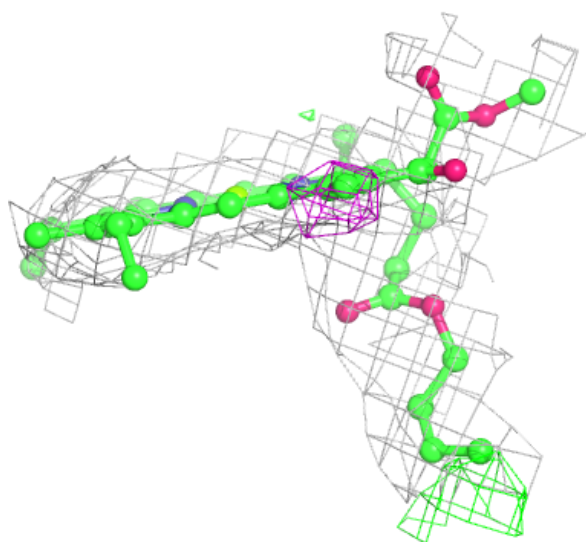
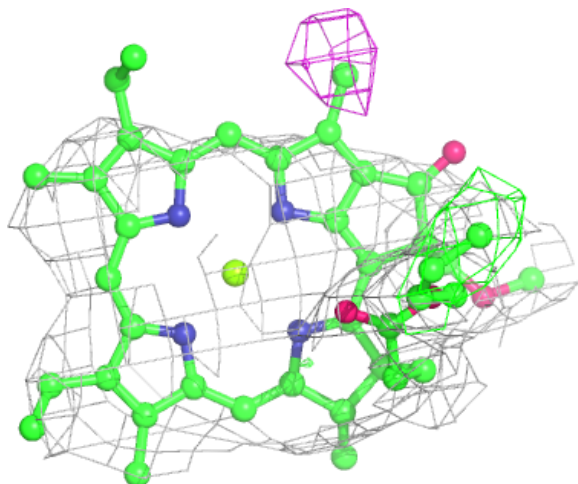
**Electron density around LUT 4 501:**

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



**Electron density around CLA A 1126:**

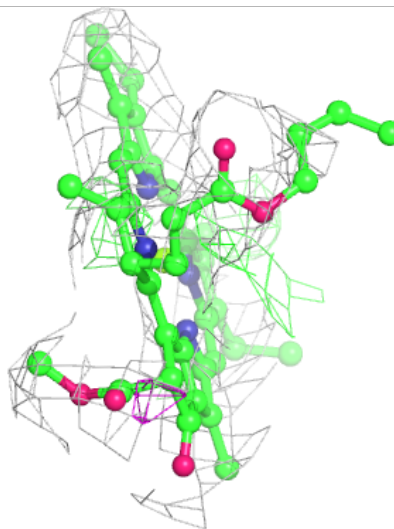
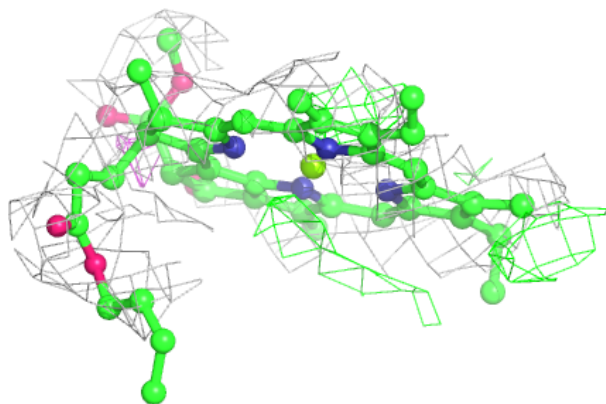
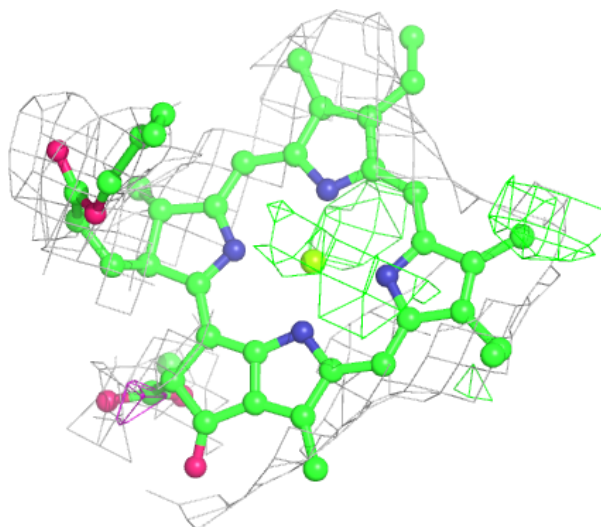
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





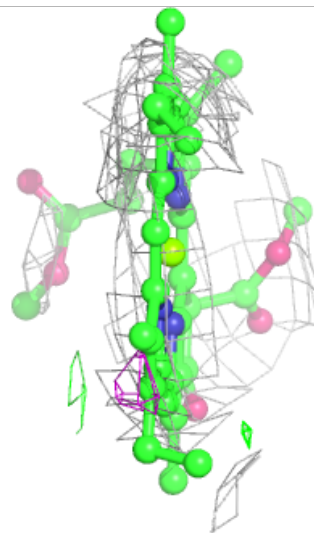
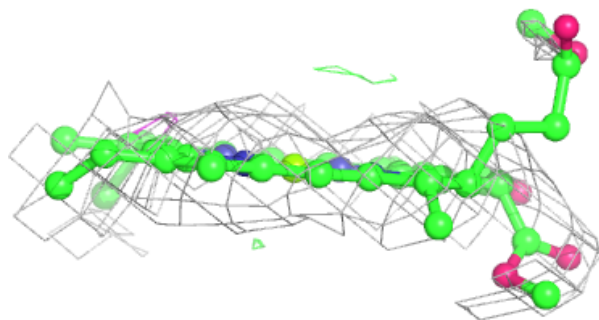
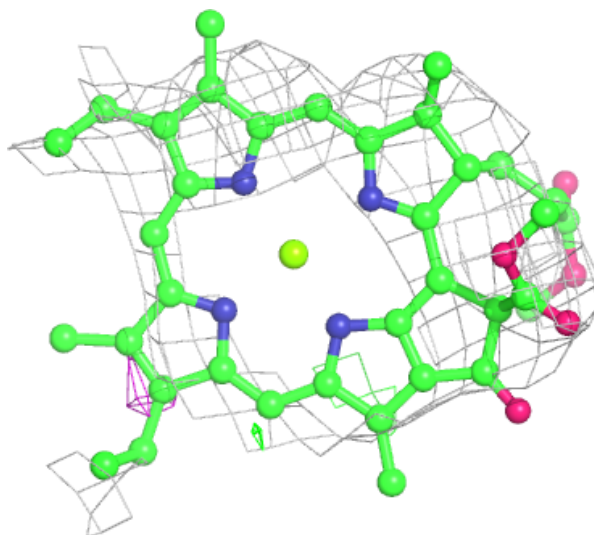
**Electron density around CLA 4 607:**

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



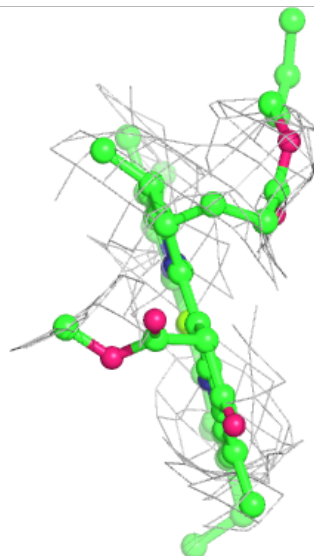
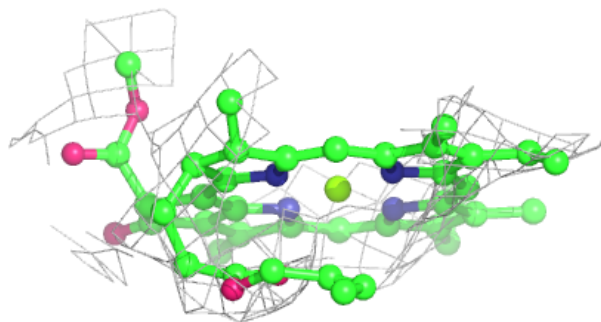
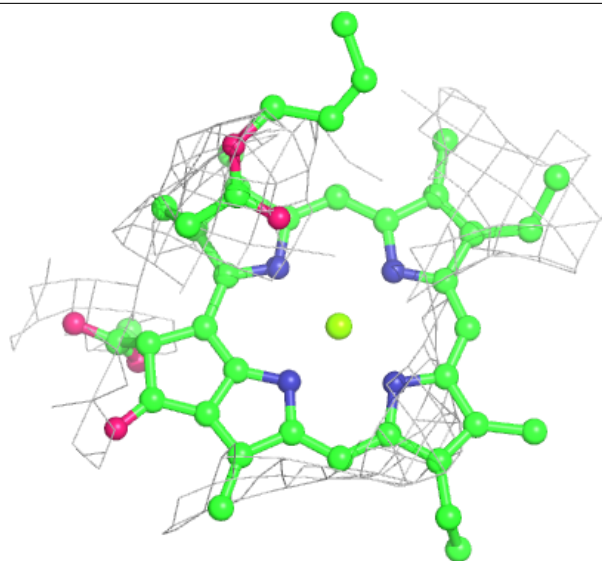
**Electron density around CLA A 1108:**

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



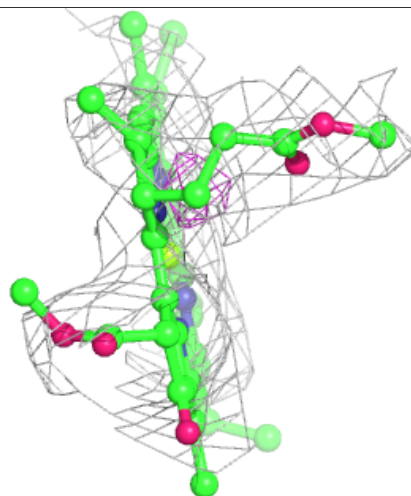
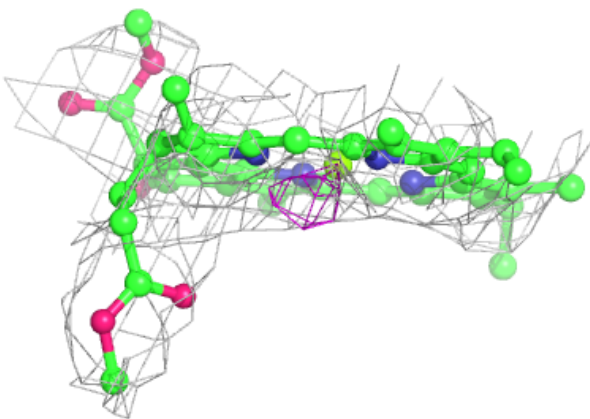
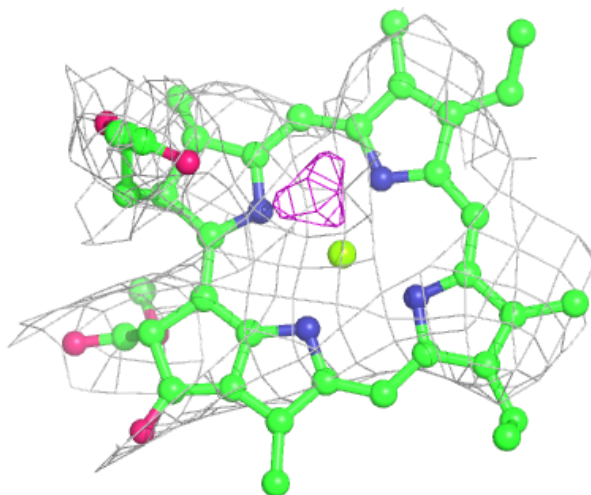
**Electron density around CLA A 1134:**

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



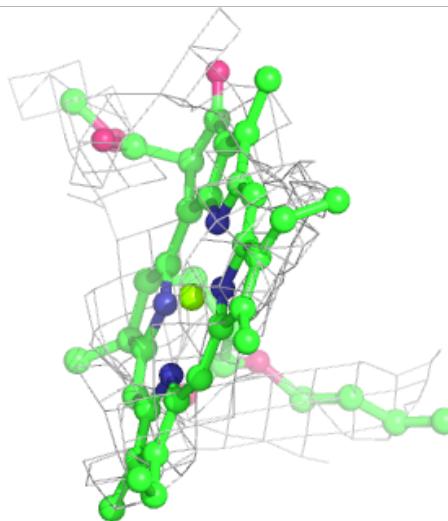
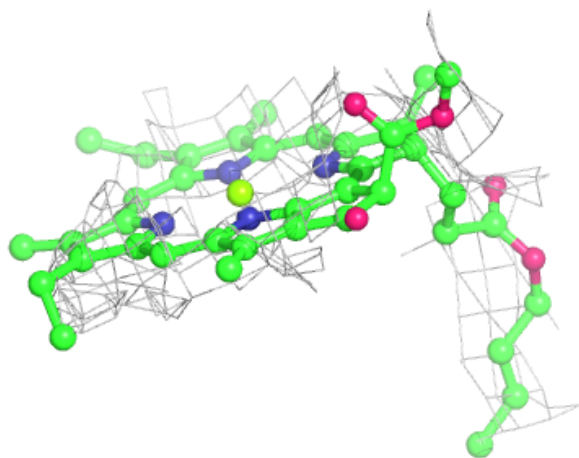
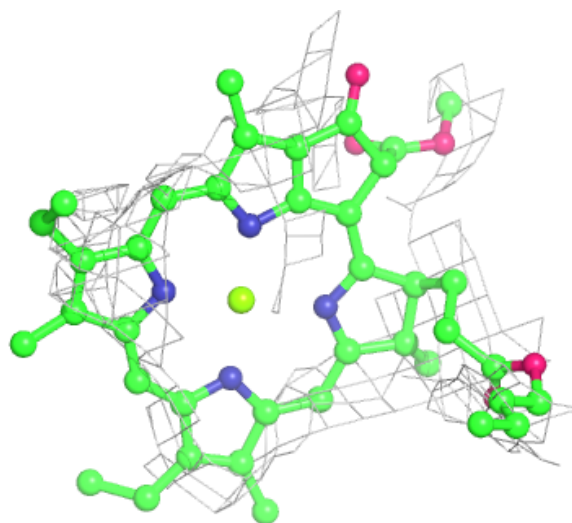
**Electron density around CLA 2 606:**

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



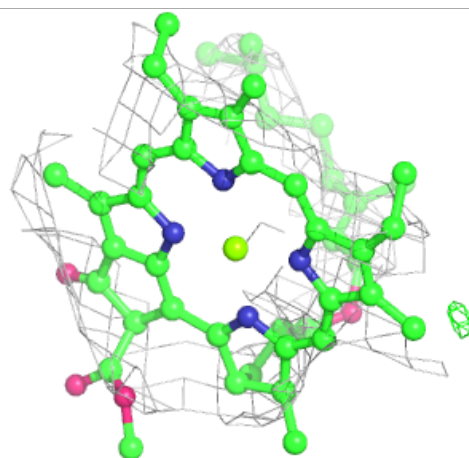
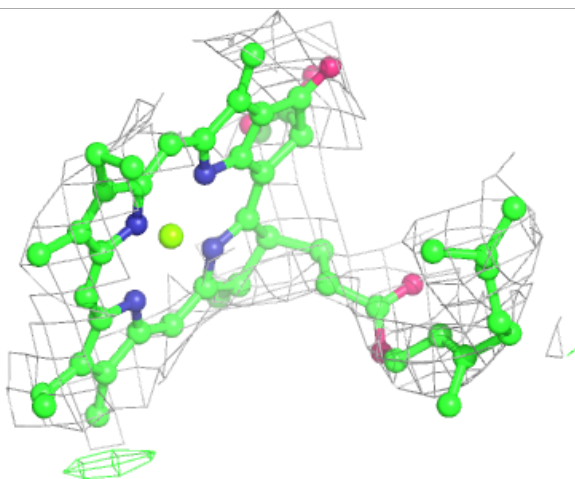
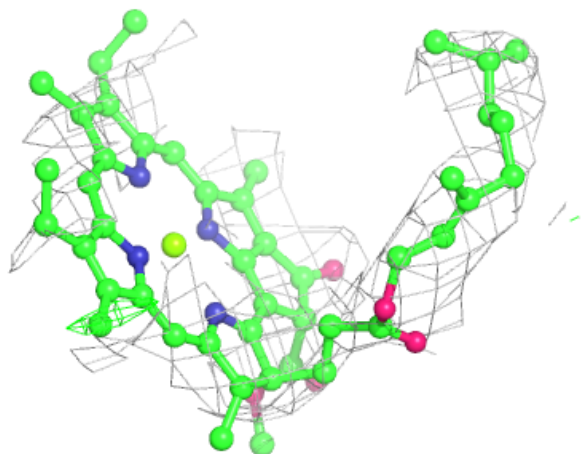
**Electron density around CLA 3 601:**

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



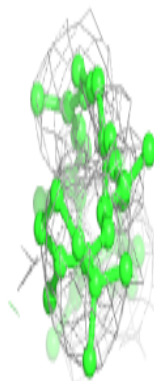
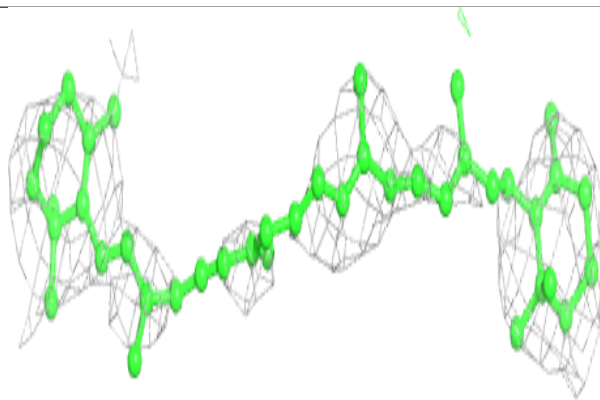
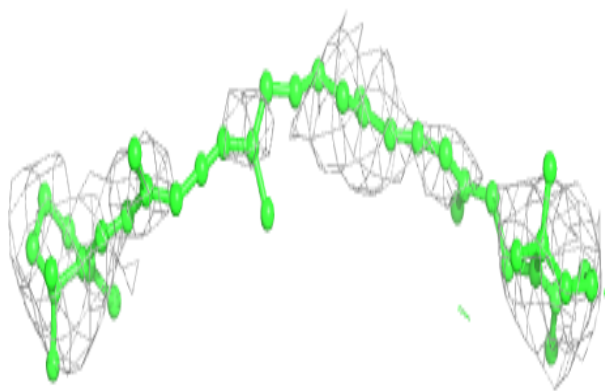
**Electron density around CLA 3 612:**

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



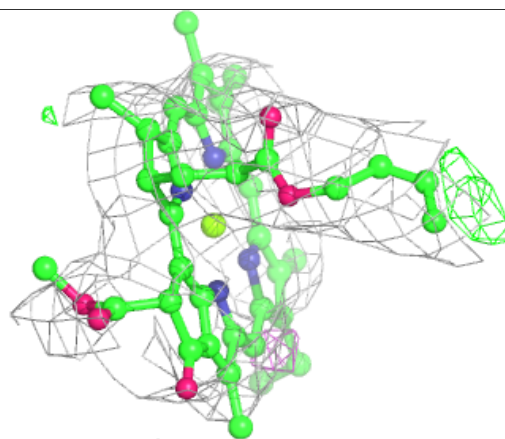
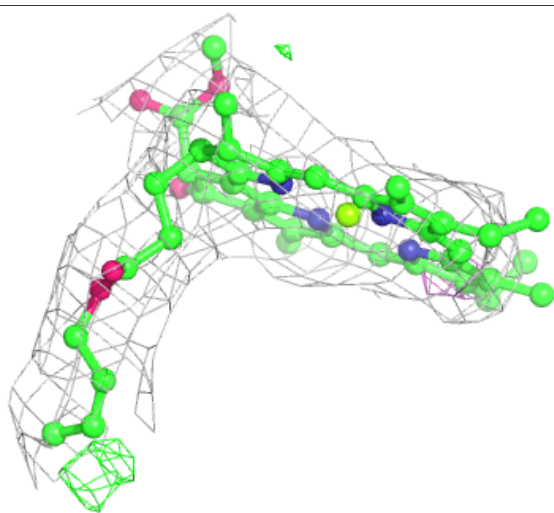
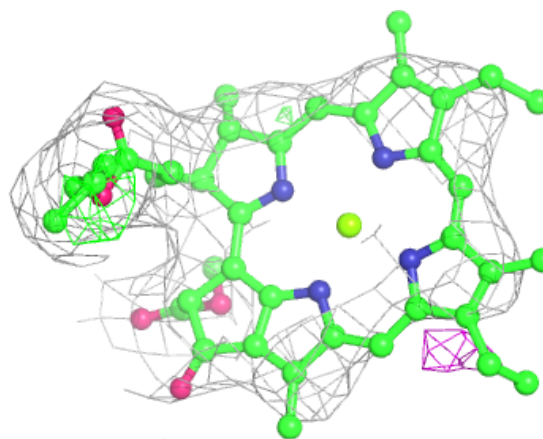
**Electron density around BCR J 4002:**

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



**Electron density around CLA B 1236:**

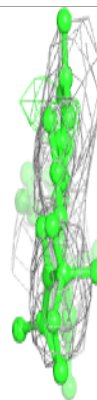
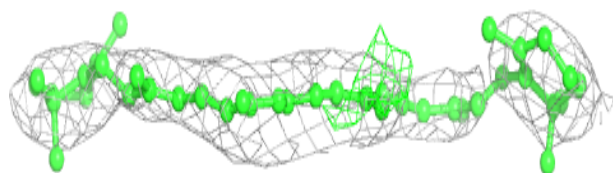
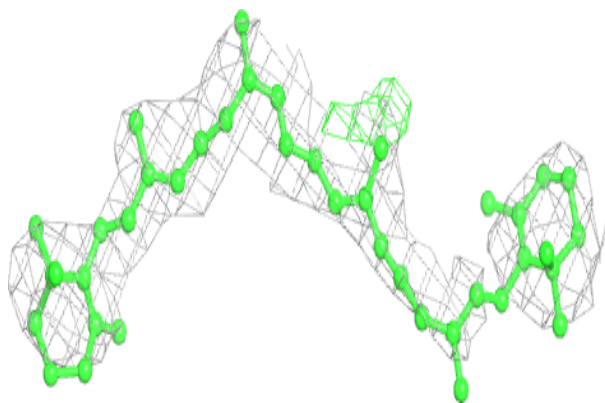
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





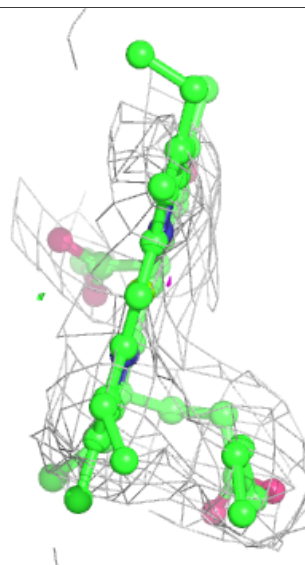
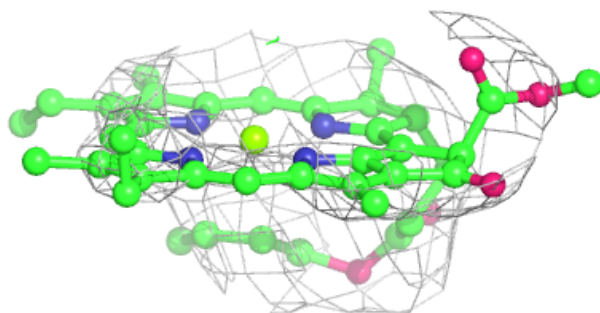
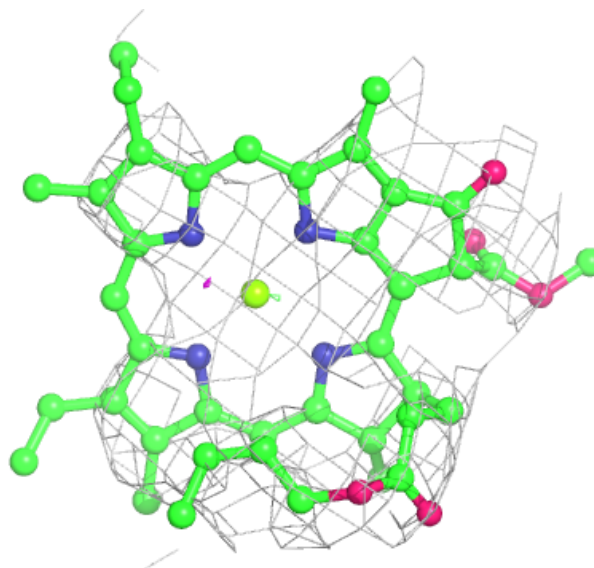
**Electron density around BCR A 4006:**

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



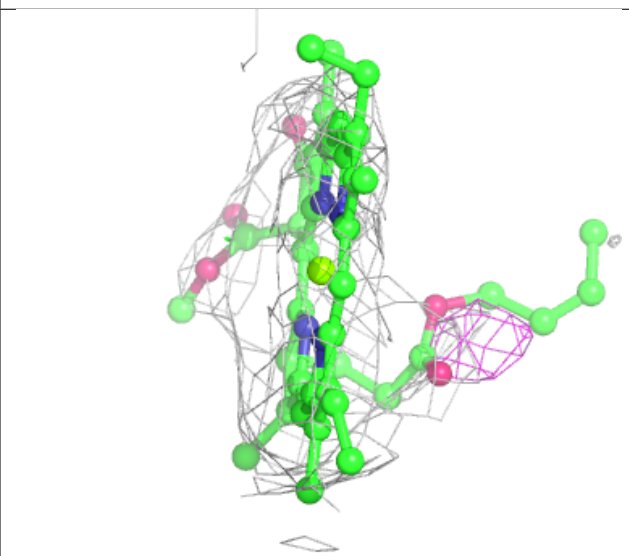
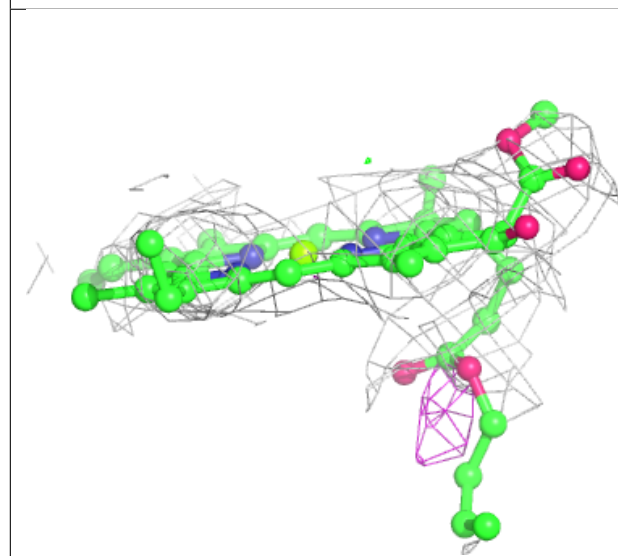
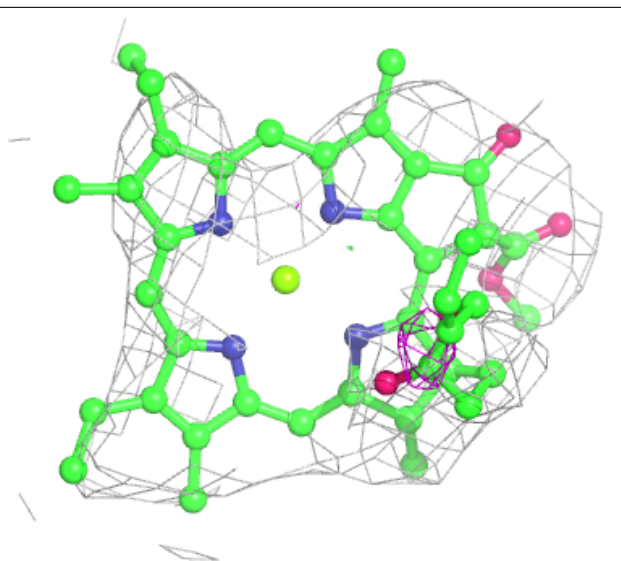
**Electron density around CLA A 1117:**

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



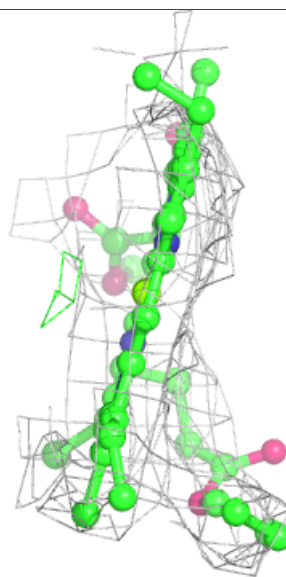
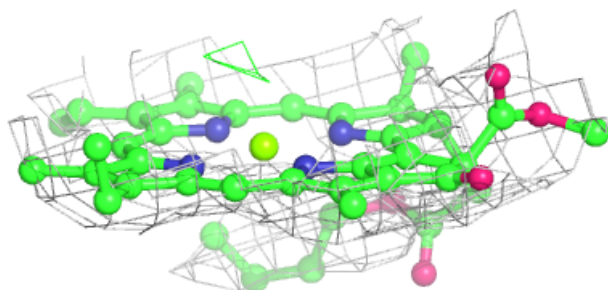
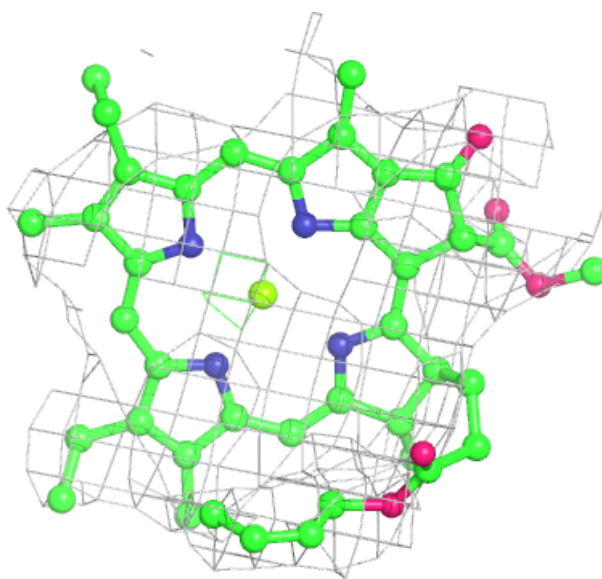
**Electron density around CLA B 1226:**

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



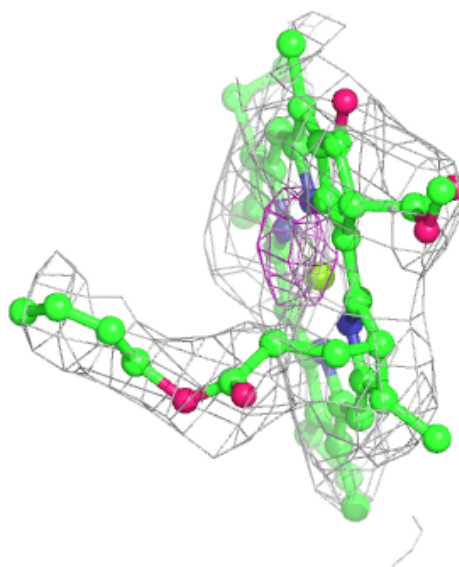
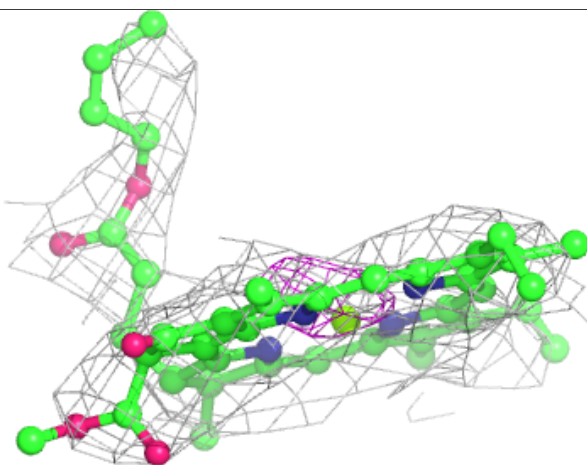
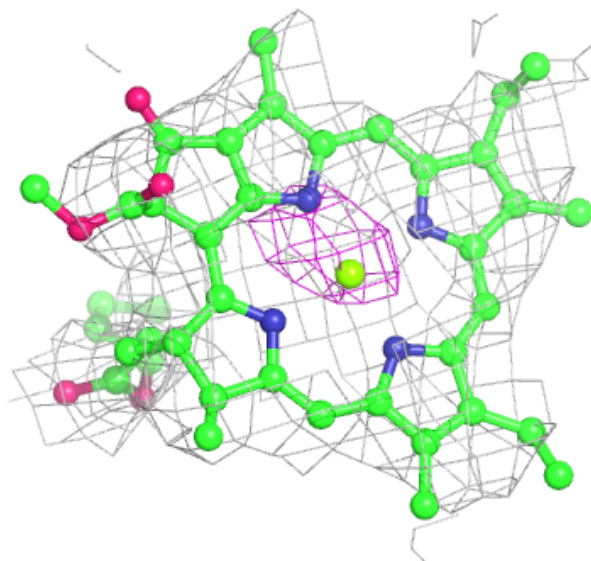
**Electron density around CLA 1 601:**

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



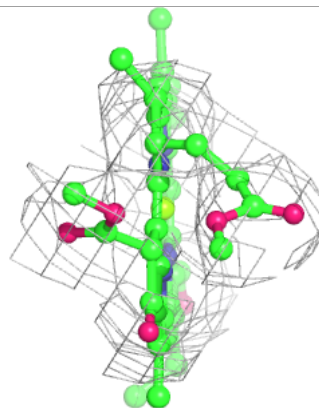
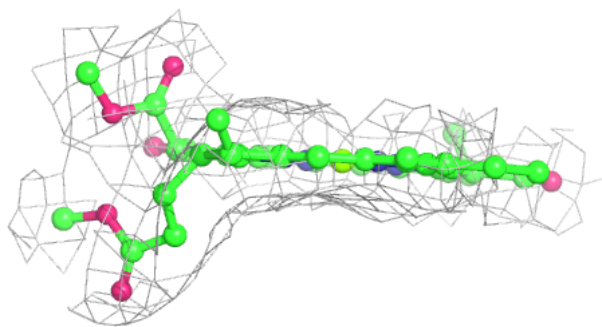
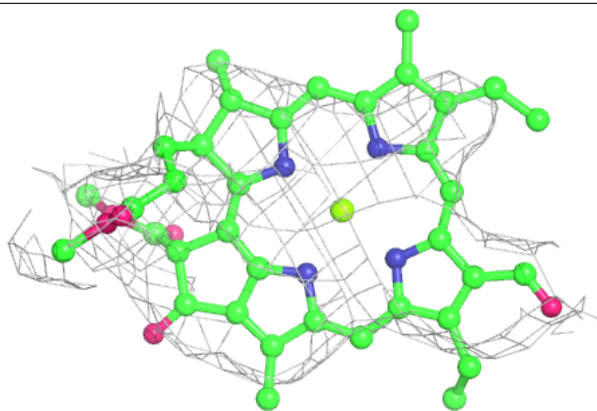
**Electron density around CLA B 1219:**

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



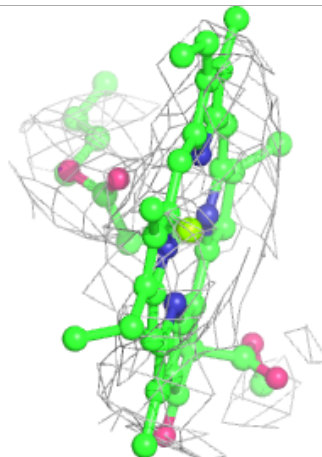
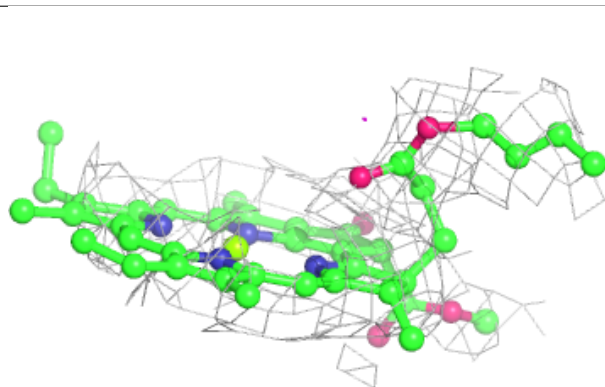
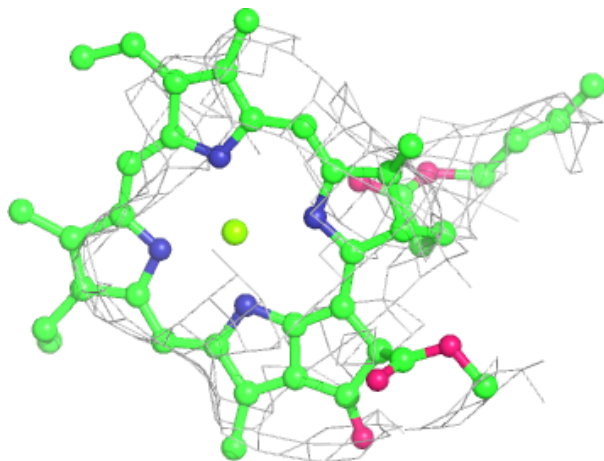
**Electron density around CHL 1 610:**

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



**Electron density around CLA A 1124:**

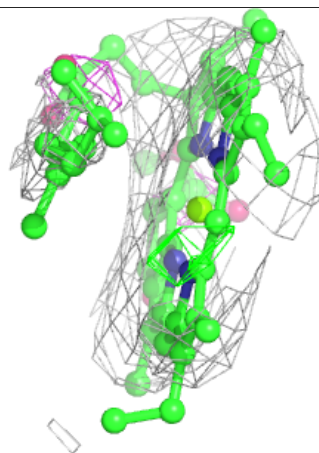
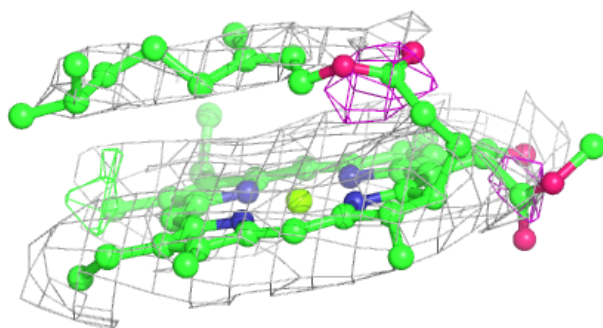
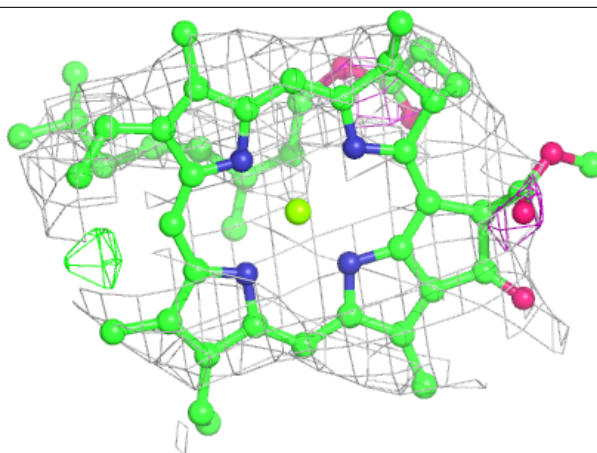
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 4 615:**

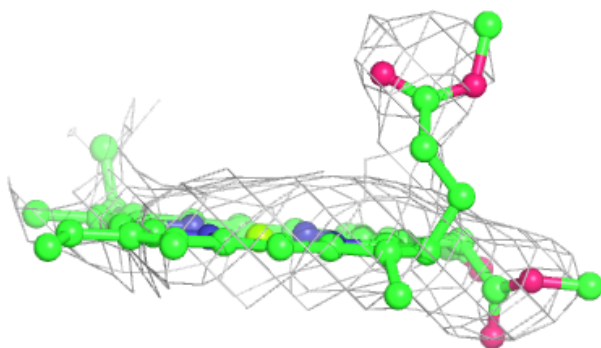
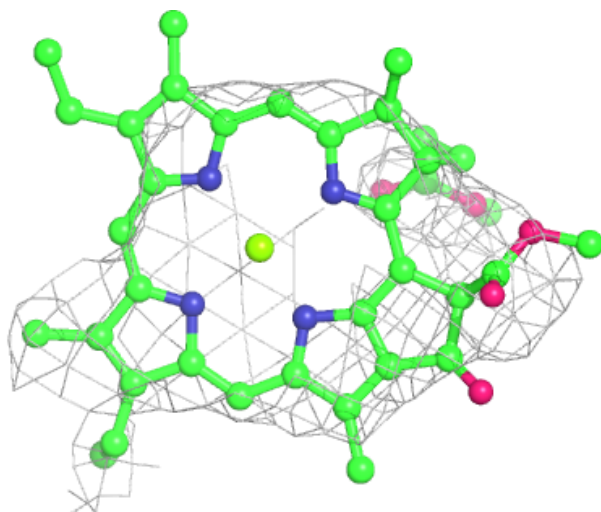
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





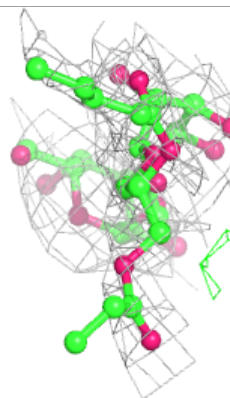
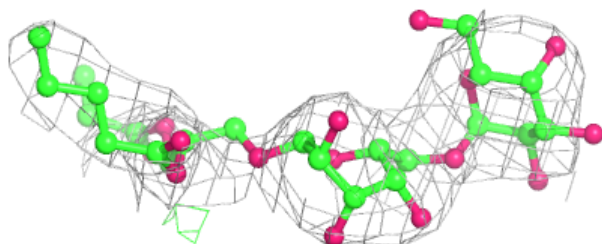
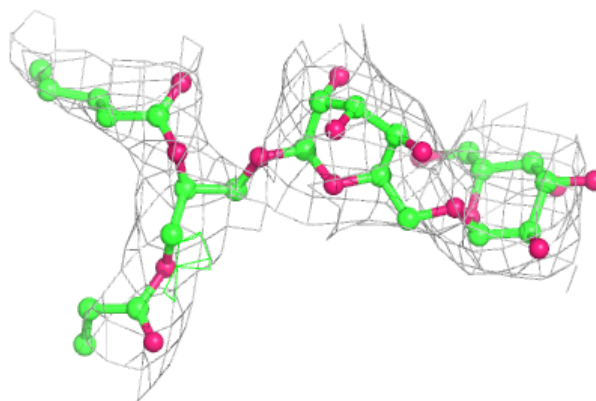
**Electron density around CLA 3 611:**

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

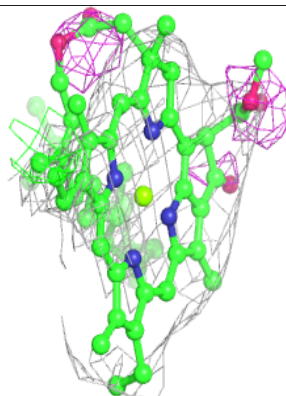
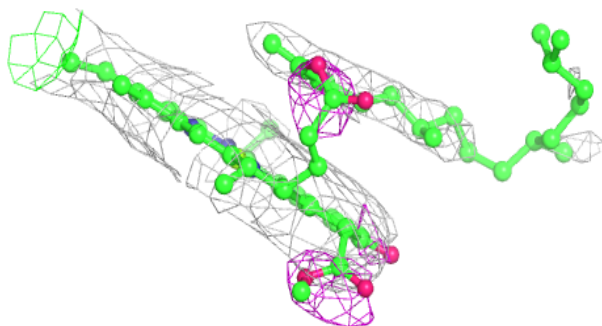
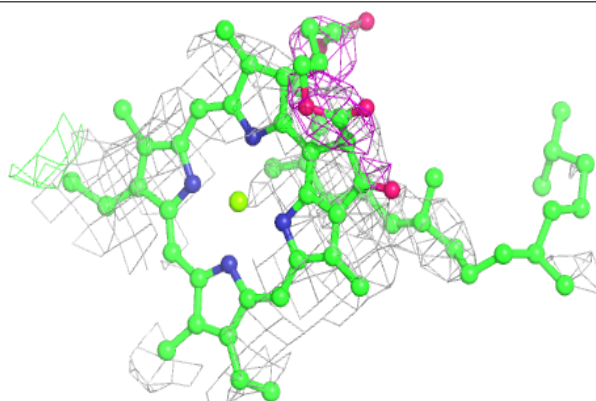


**Electron density around DGD B 5002:**

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

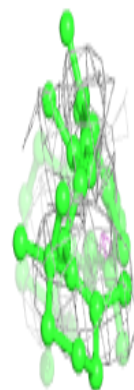
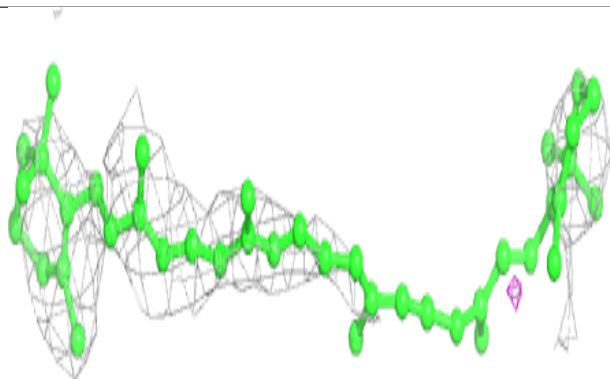
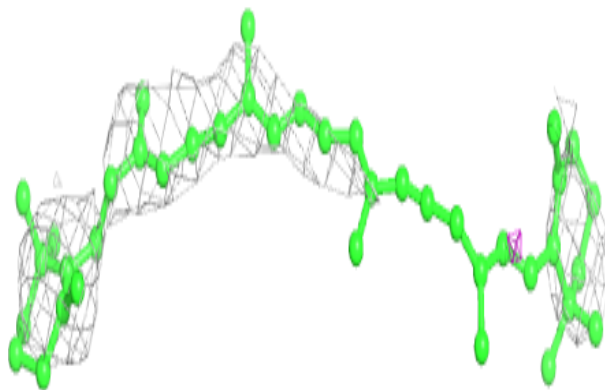
**Electron density around CLA 1 615:**

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



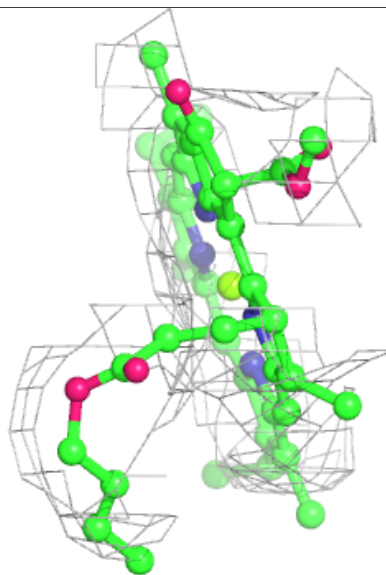
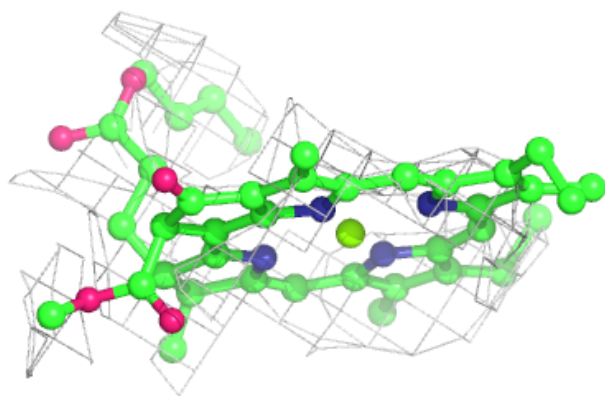
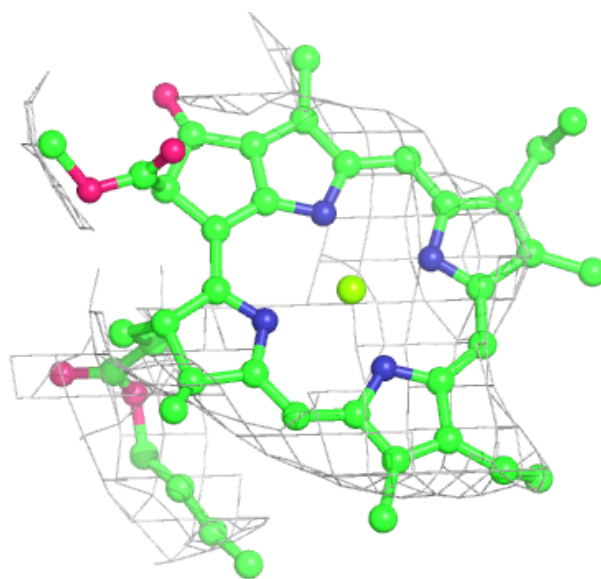
**Electron density around BCR B 4006:**

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



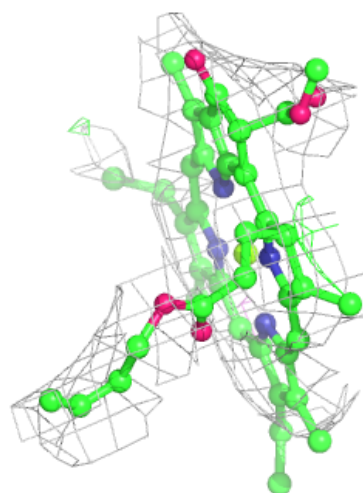
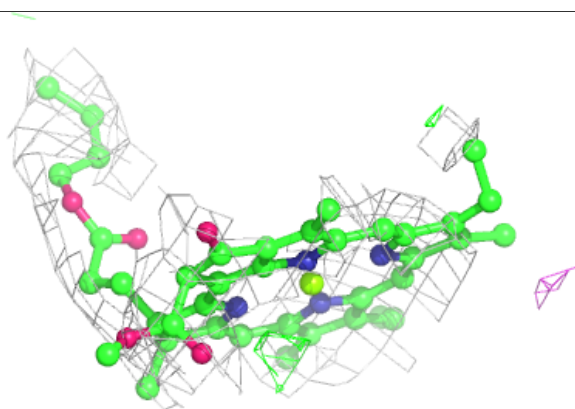
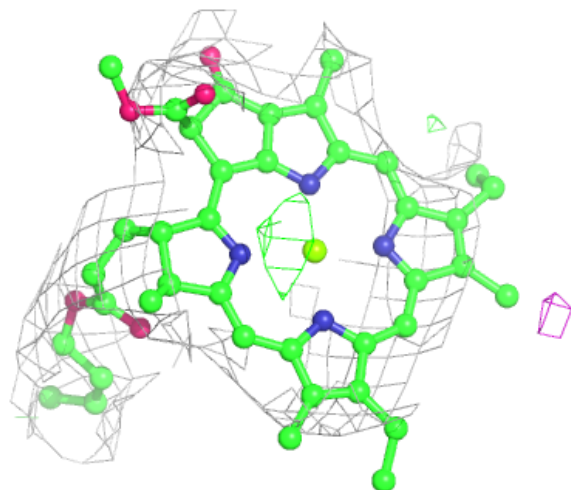
**Electron density around CLA A 1120:**

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



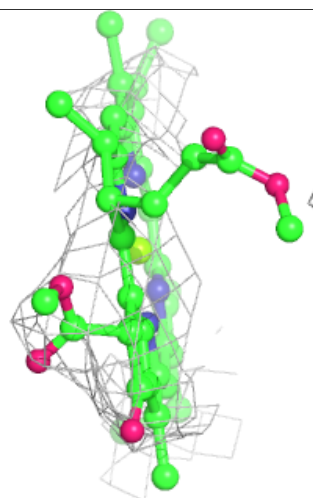
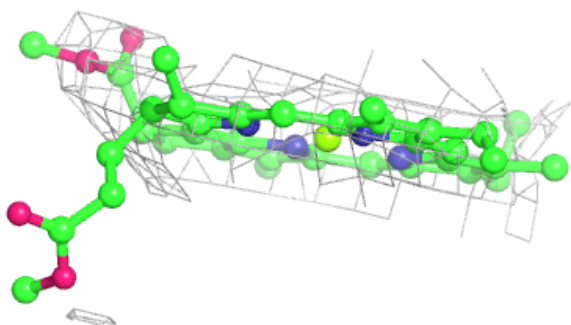
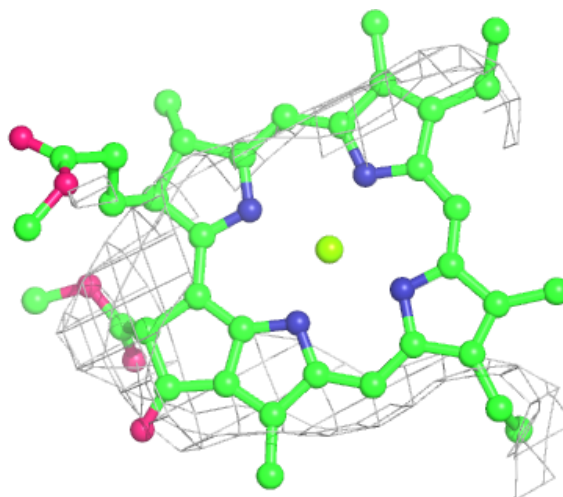
**Electron density around CLA 2 612:**

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



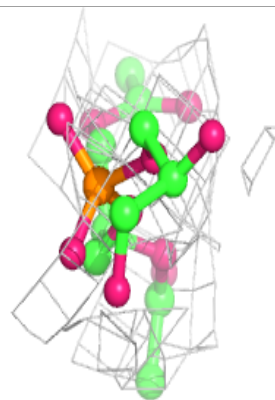
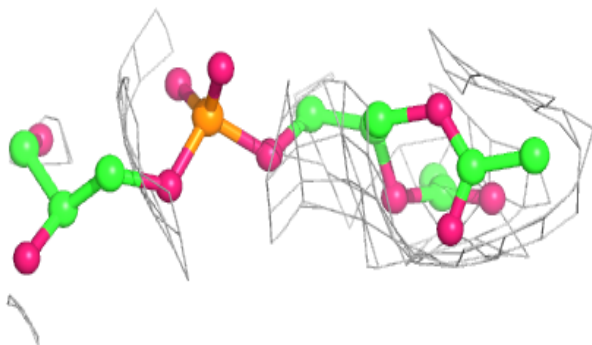
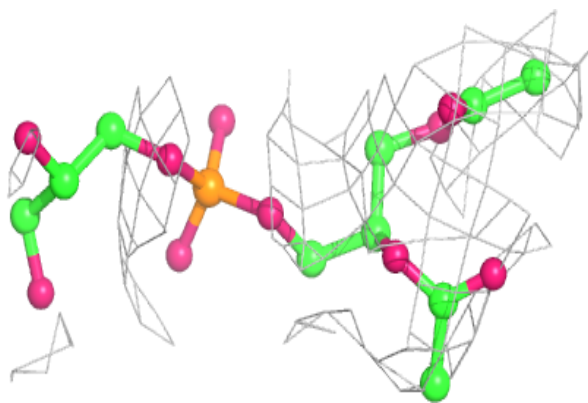
**Electron density around CLA 3 613:**

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



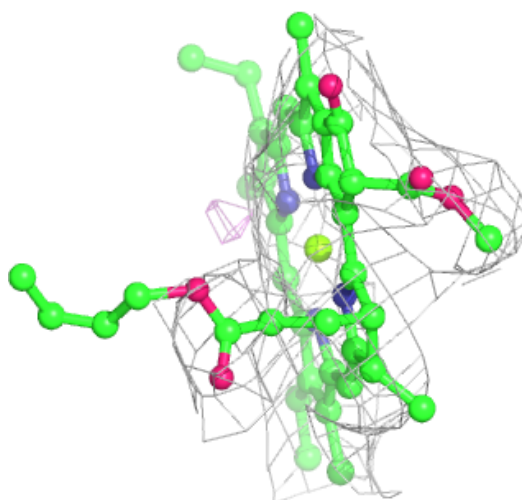
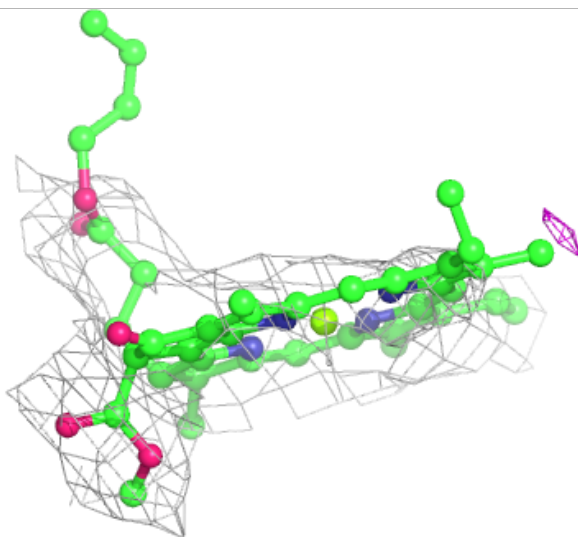
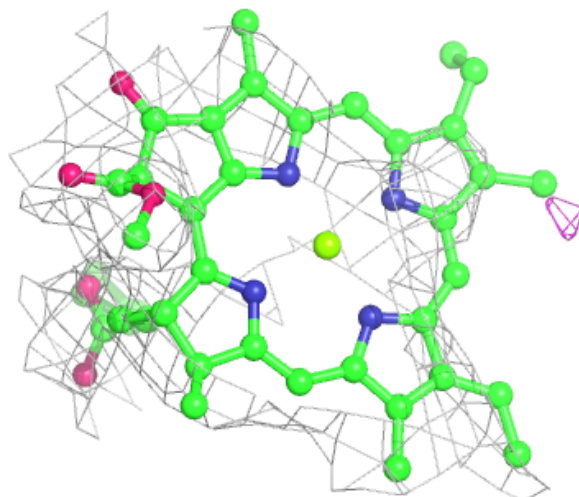
**Electron density around LHG 2 801:**

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



**Electron density around CLA A 1128:**

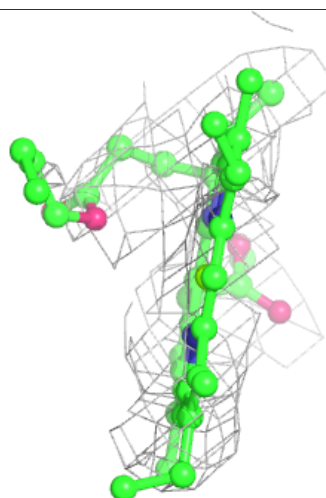
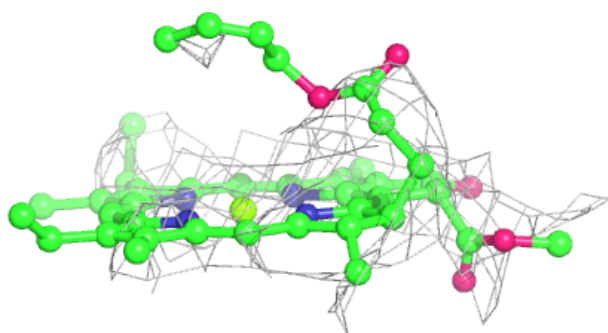
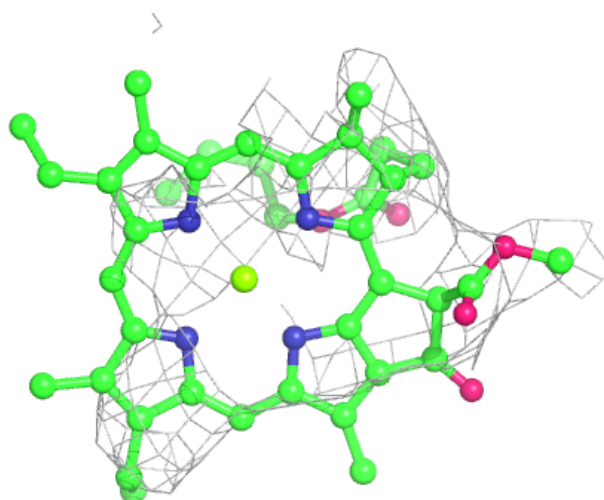
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





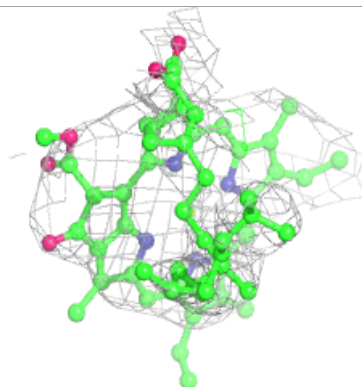
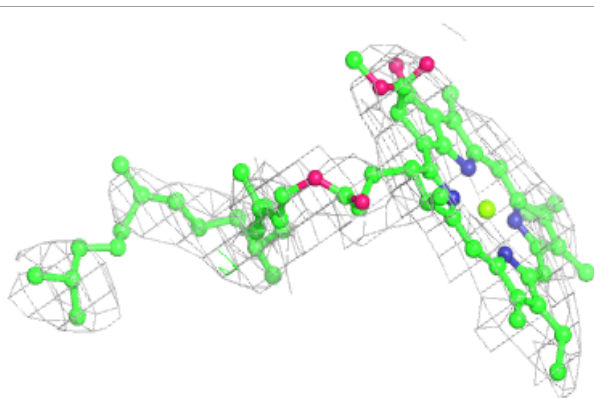
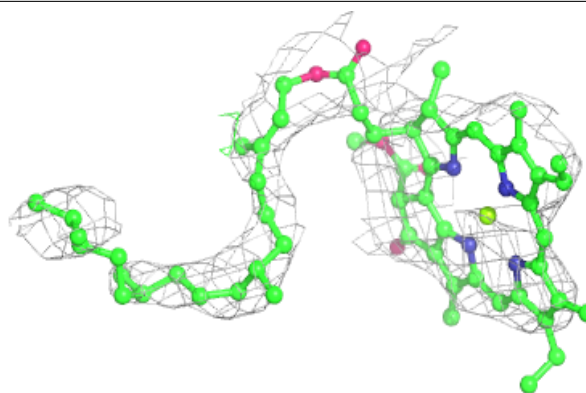
**Electron density around CLA A 1119:**

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



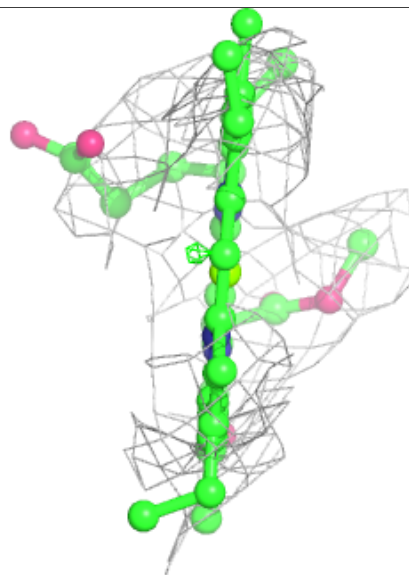
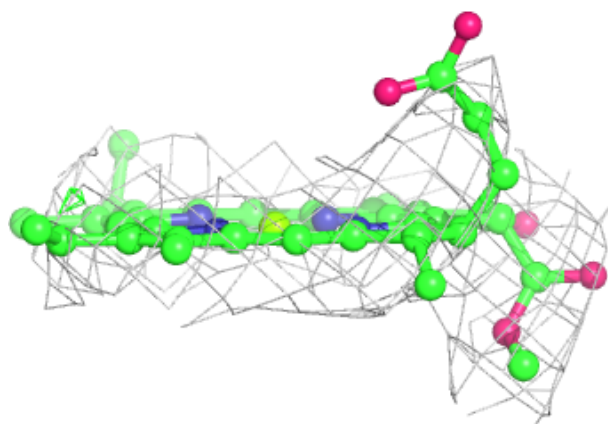
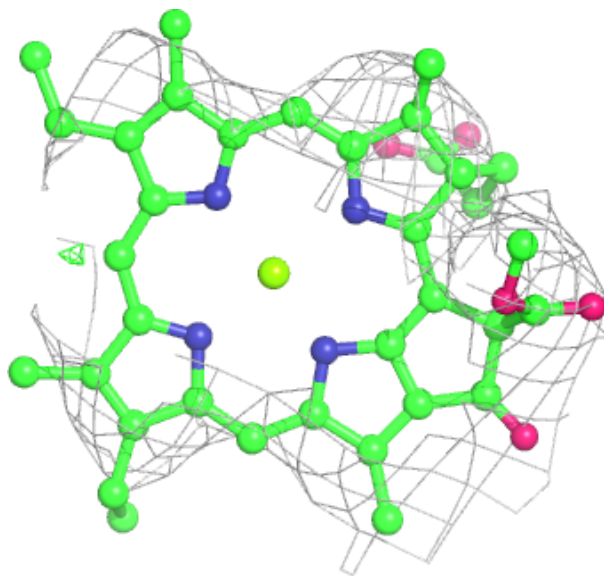
**Electron density around CLA B 1021:**

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



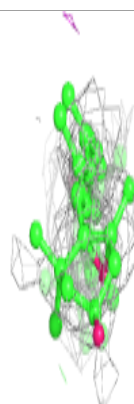
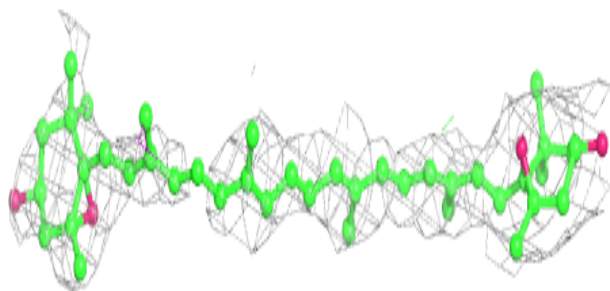
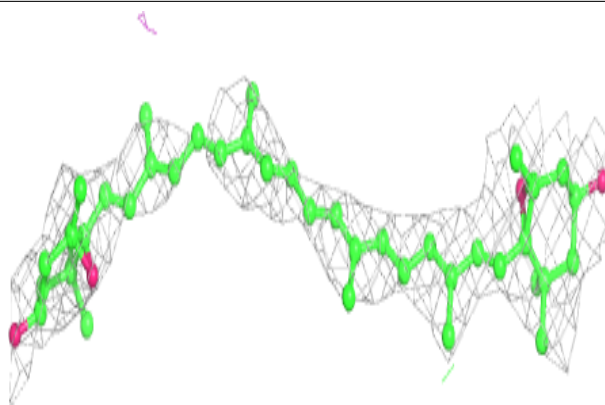
**Electron density around CLA B 1212:**

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



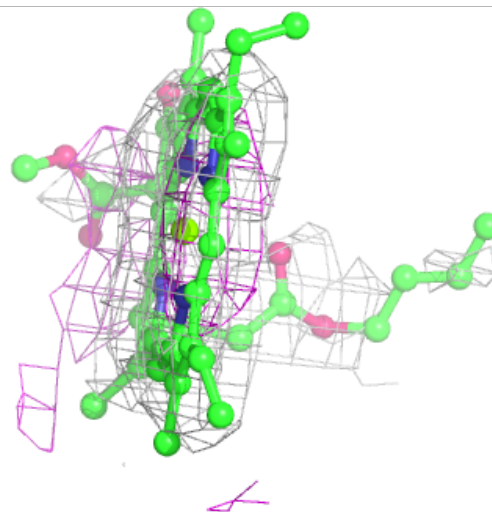
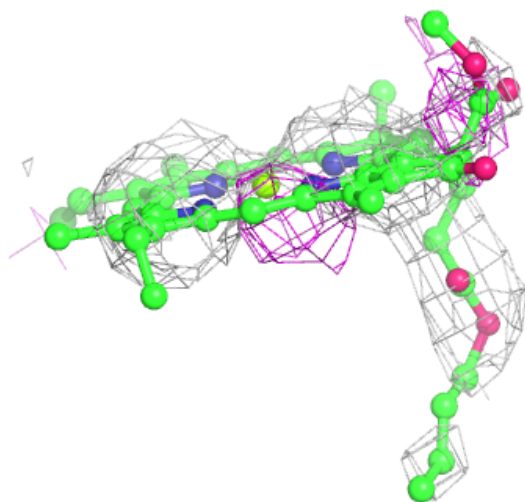
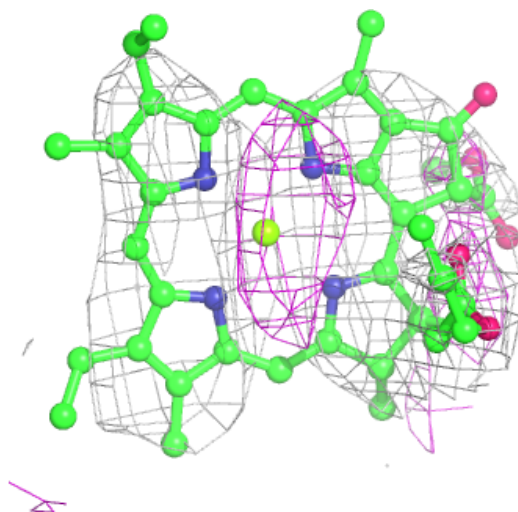
**Electron density around XAT 4 502:**

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



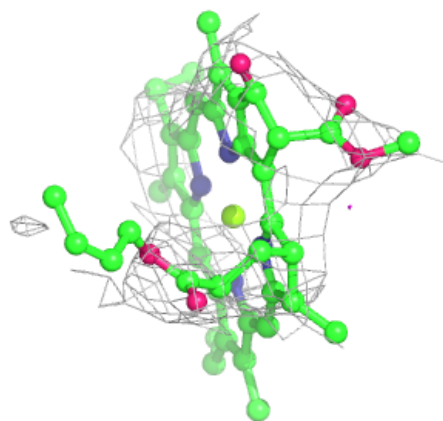
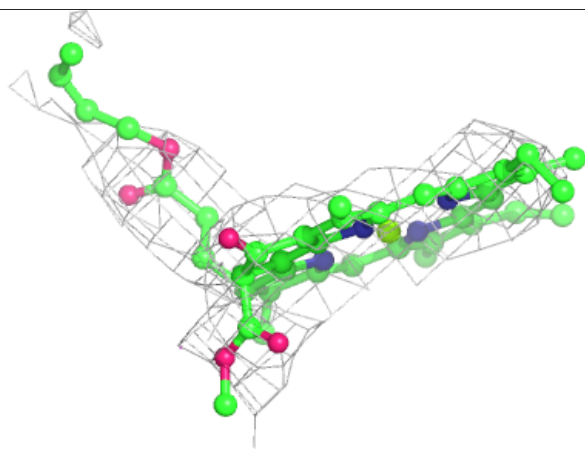
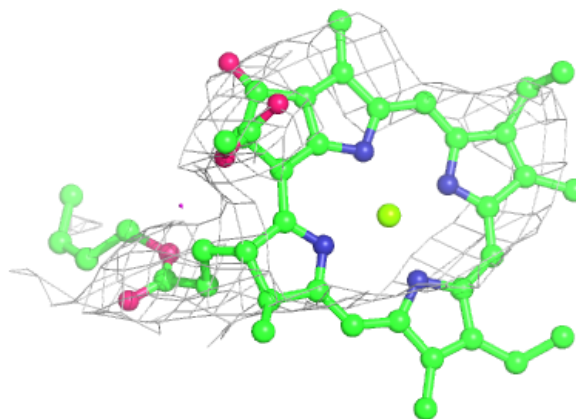
**Electron density around CLA 4 606:**

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

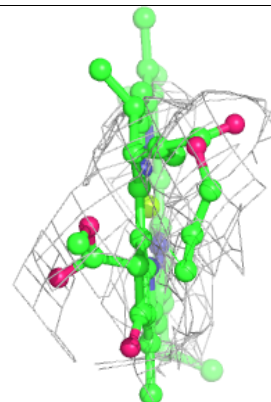
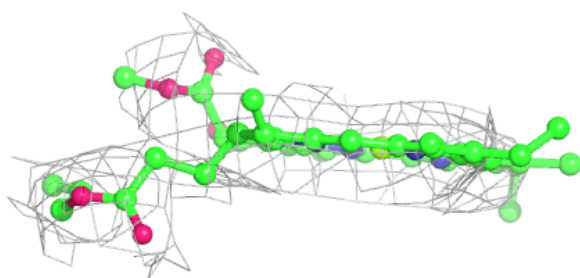
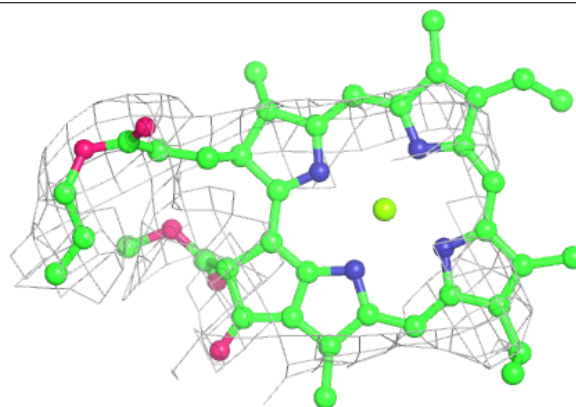


**Electron density around CLA A 1137:**

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

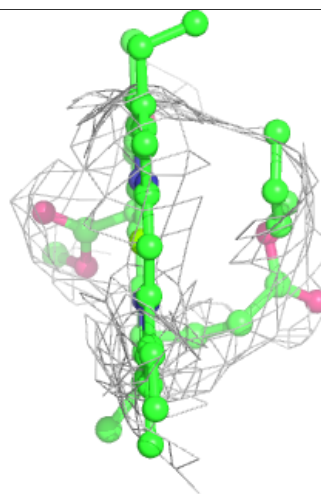
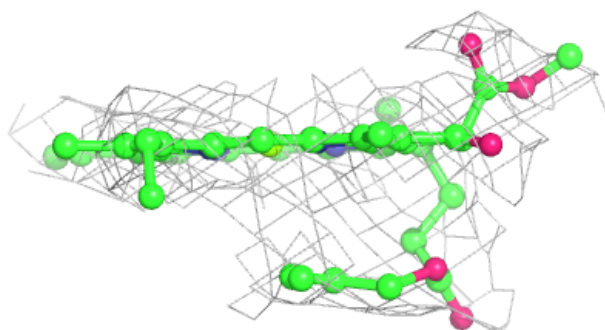
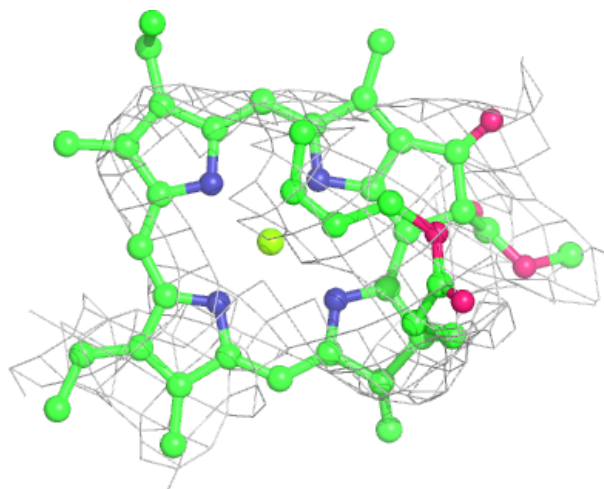
**Electron density around CLA A 1123:**

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



**Electron density around CLA A 1136:**

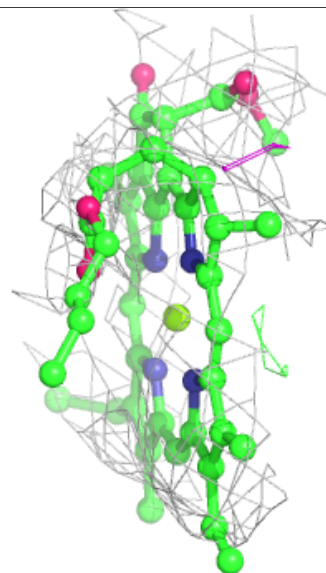
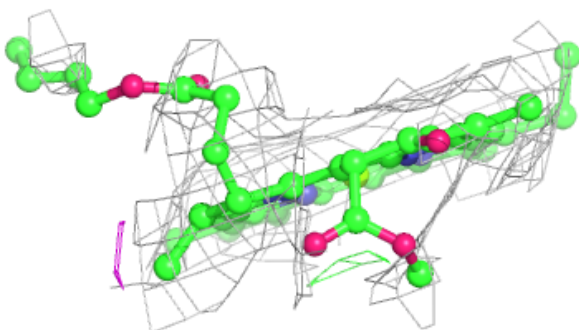
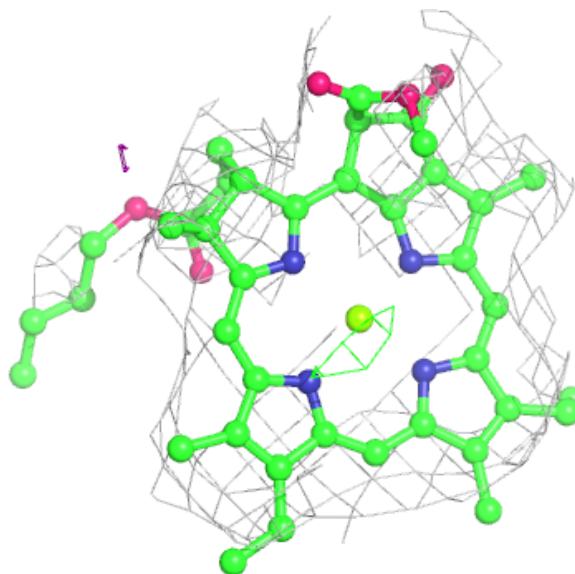
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 2 601:**

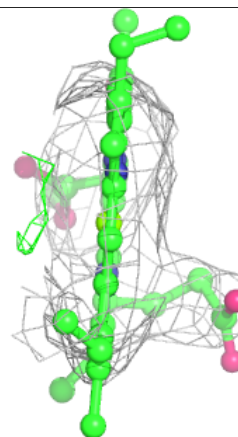
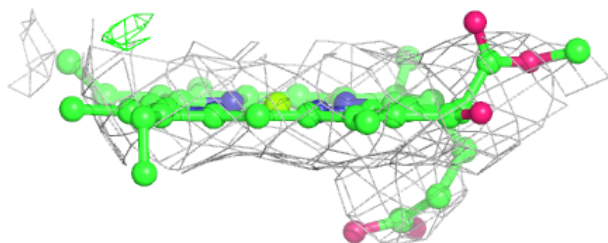
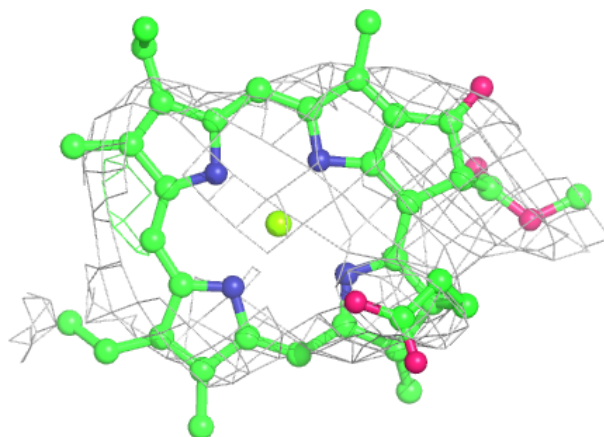
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





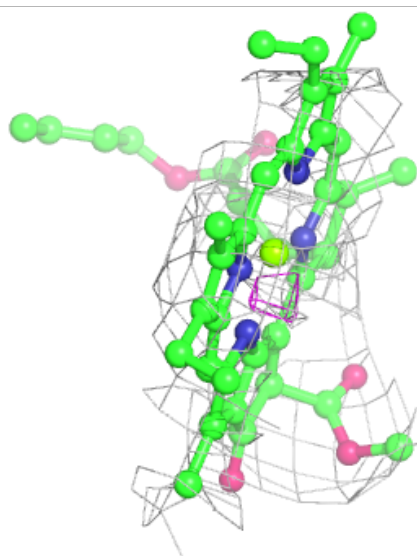
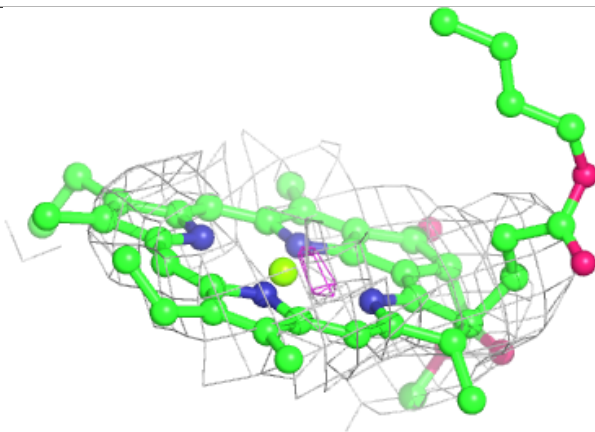
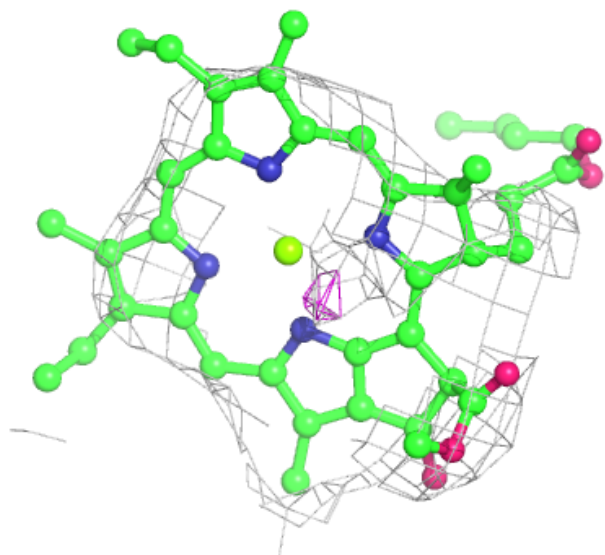
**Electron density around CLA A 1113:**

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



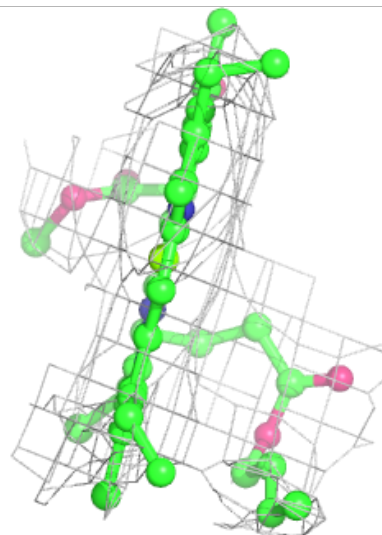
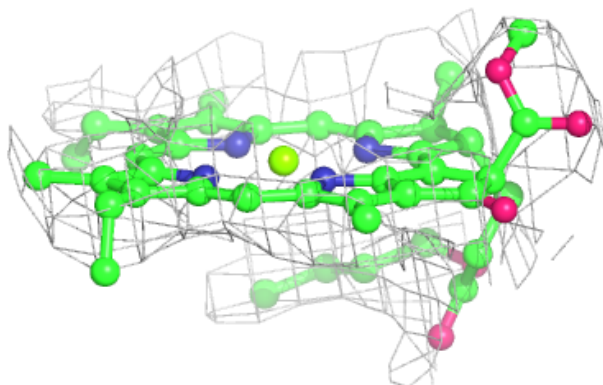
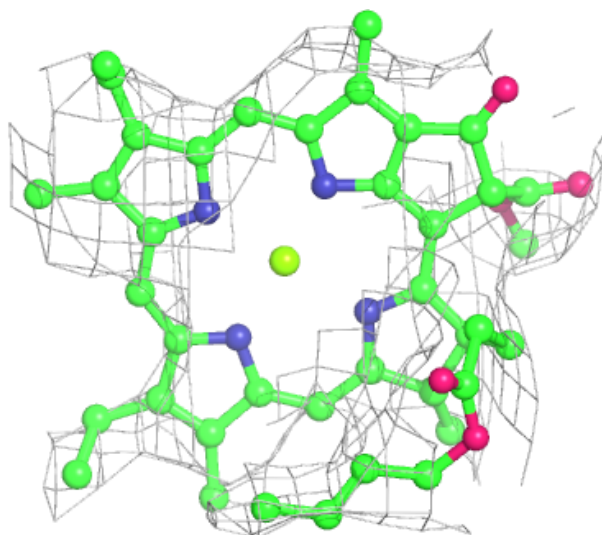
**Electron density around CLA A 1118:**

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



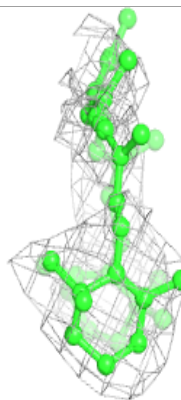
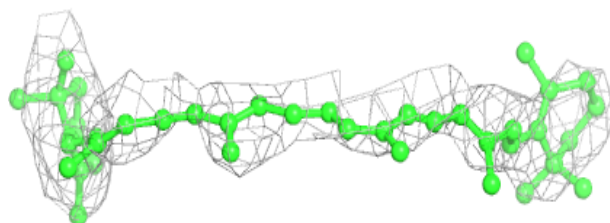
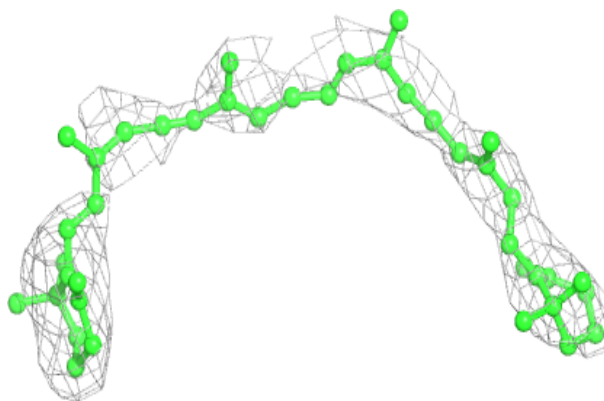
**Electron density around CLA 2 604:**

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



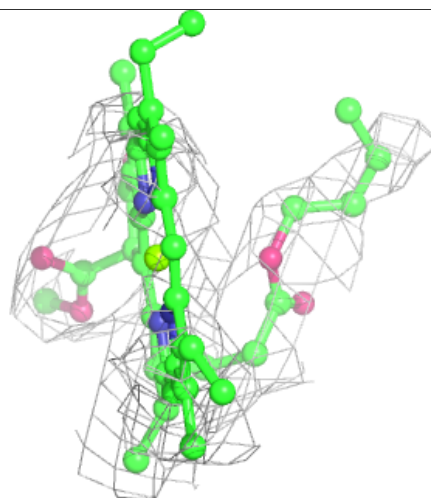
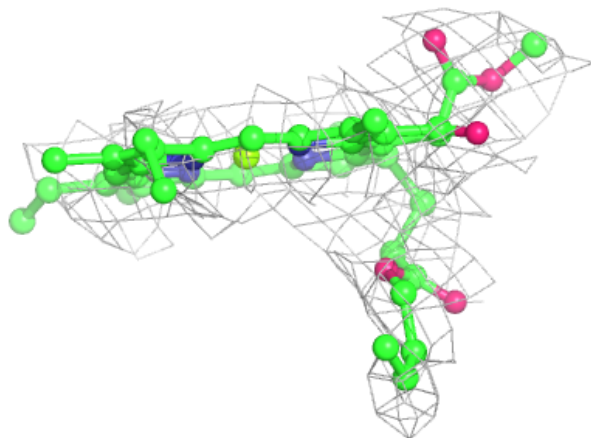
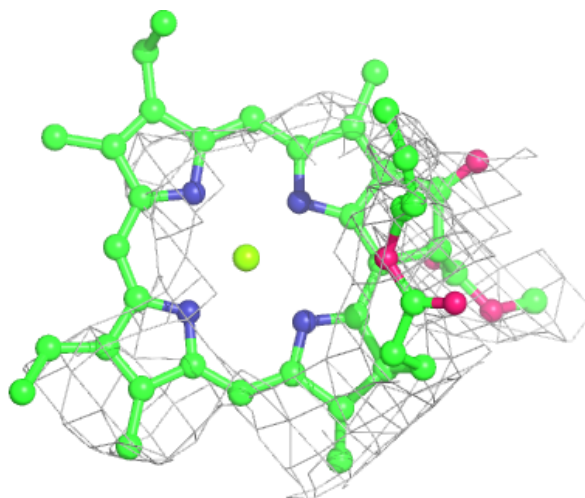
**Electron density around BCR F 4002:**

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



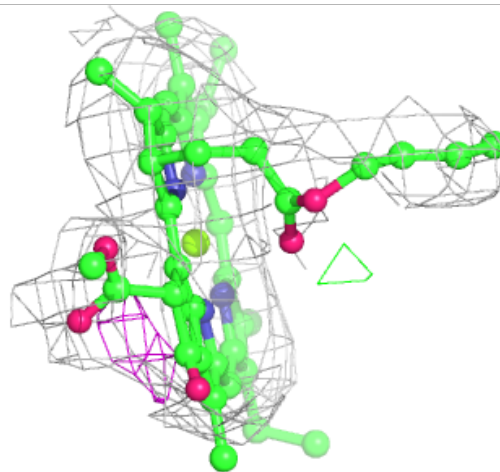
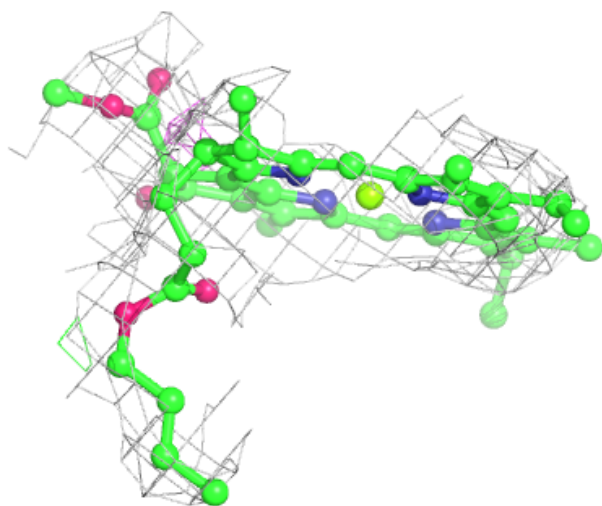
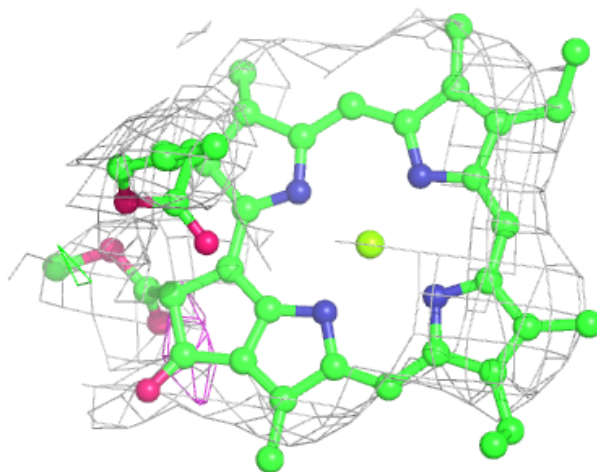
**Electron density around CLA B 1213:**

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



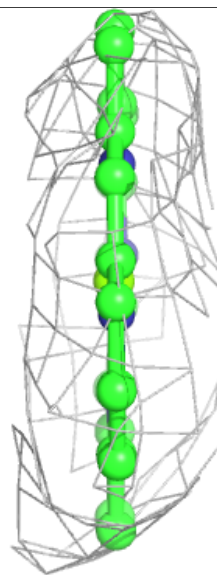
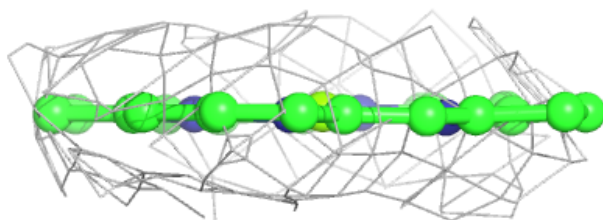
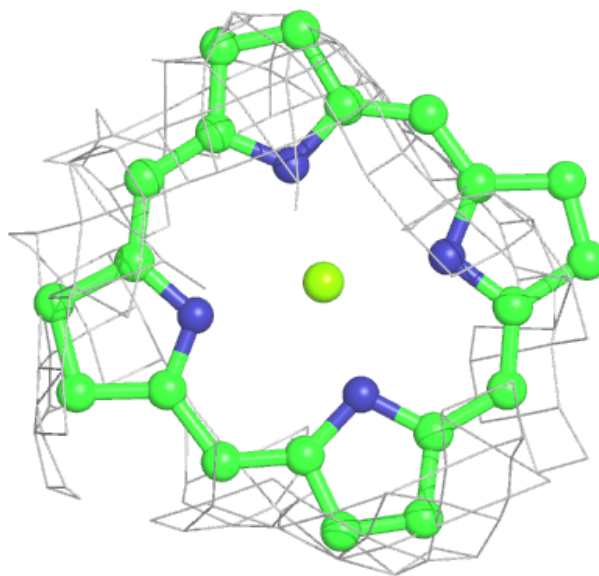
**Electron density around CLA F 1302:**

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



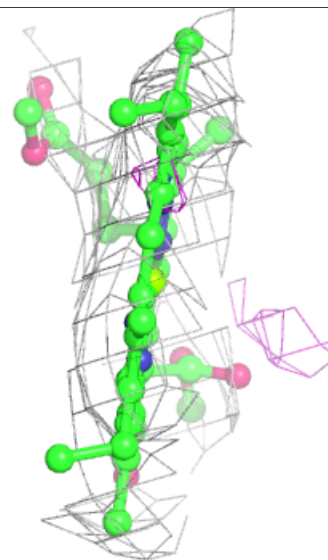
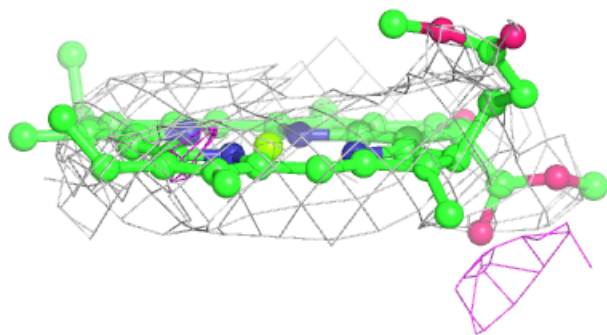
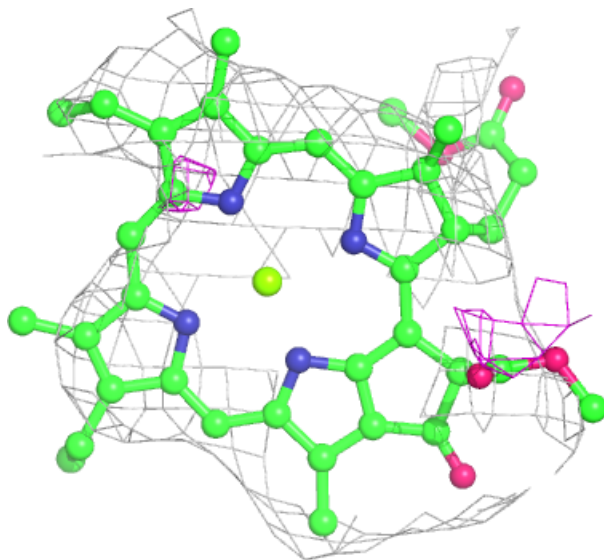
**Electron density around CLA B 1207:**

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



**Electron density around CLA 1 607:**

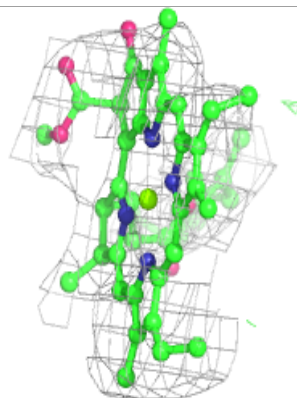
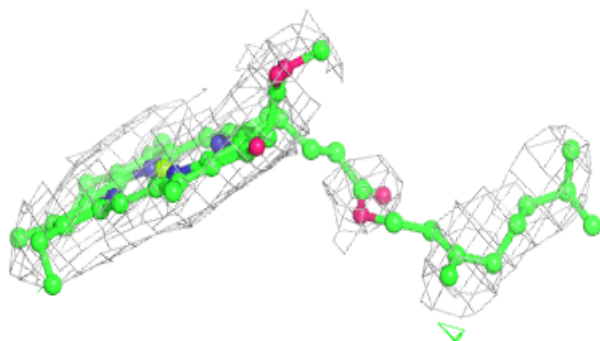
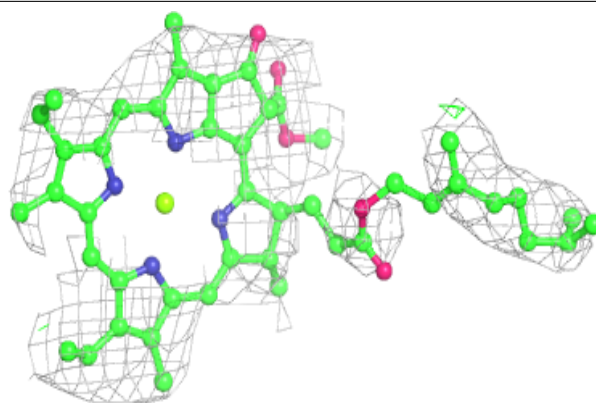
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



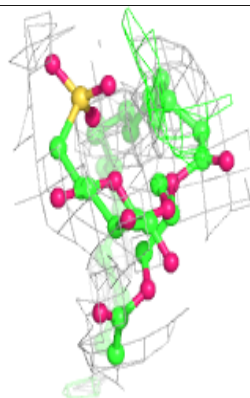
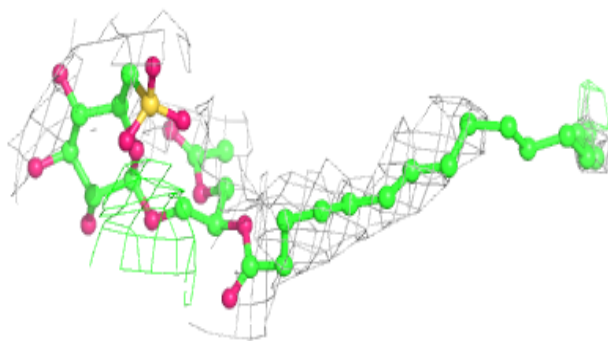
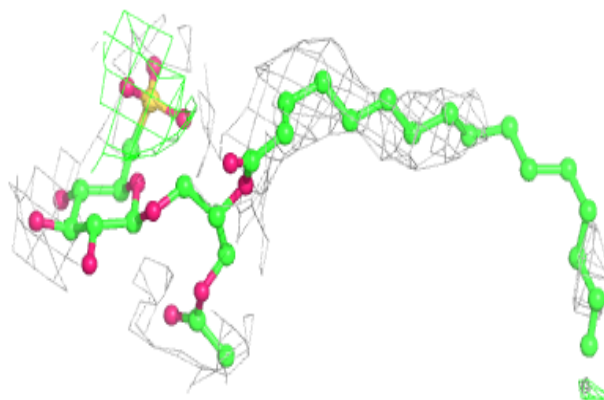


**Electron density around CLA B 1220:**

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

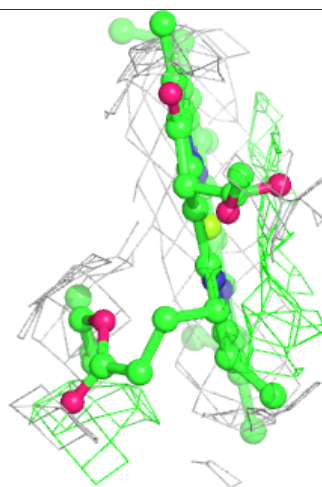
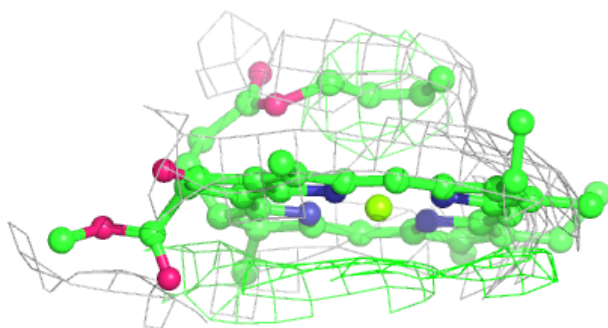
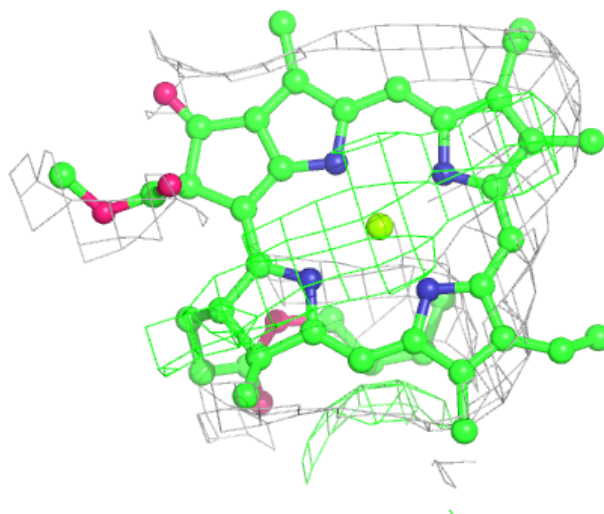
**Electron density around SQD 1 811:**

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



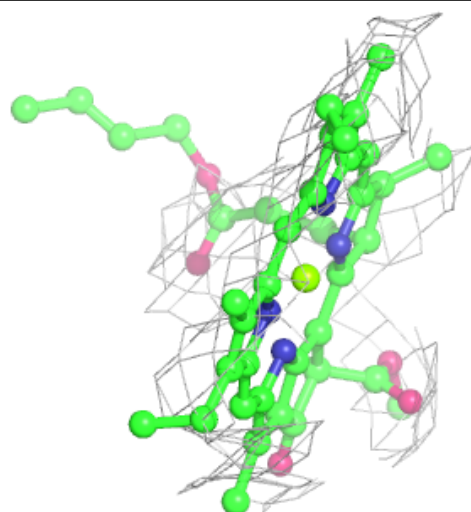
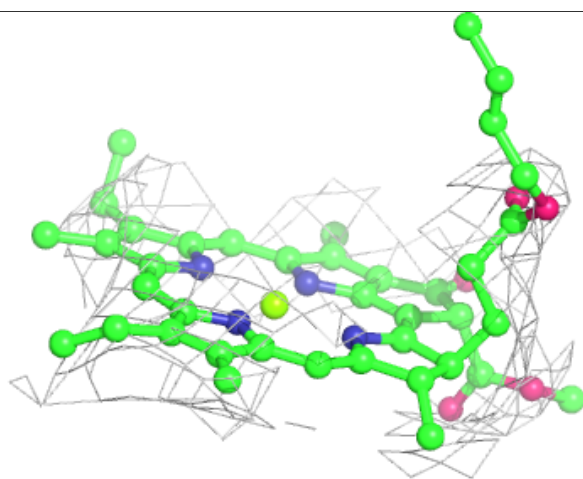
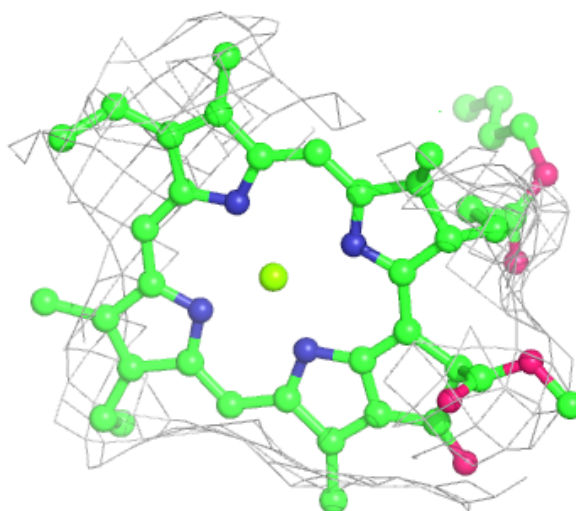
**Electron density around CLA 3 610:**

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



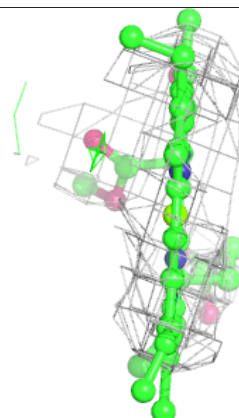
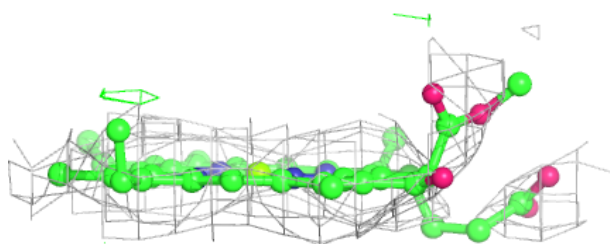
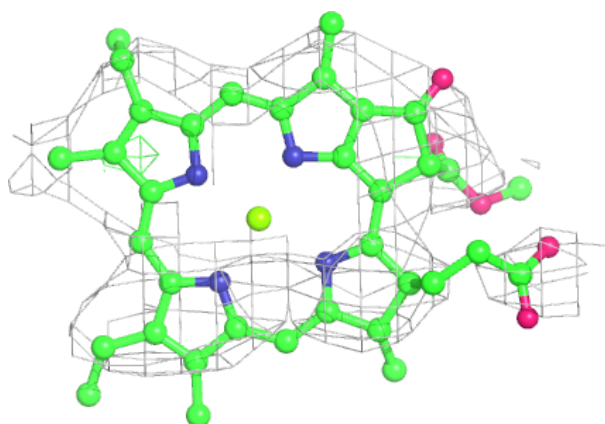
**Electron density around CLA A 1133:**

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

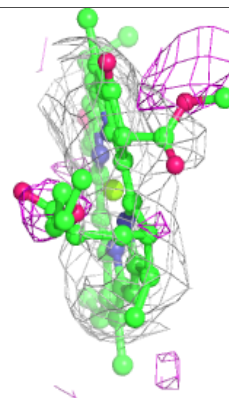
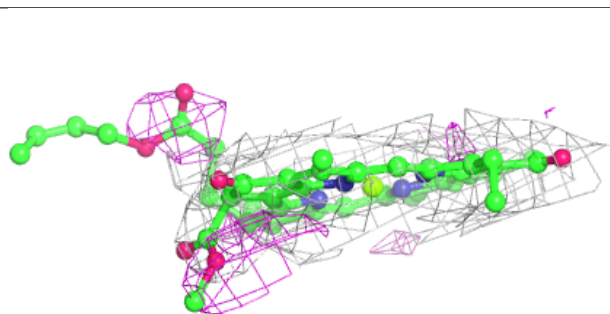
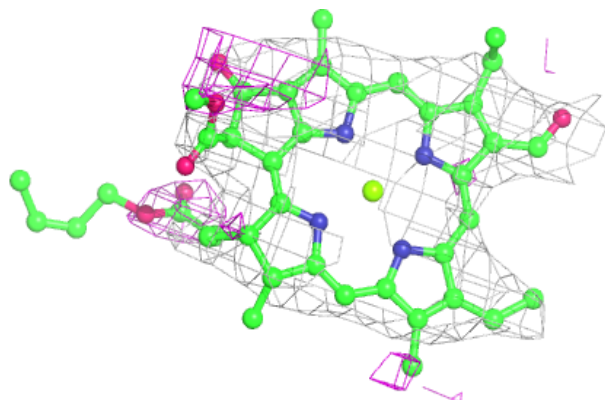


**Electron density around CLA A 1101:**

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

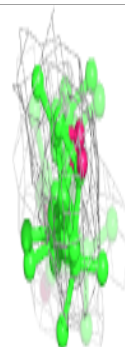
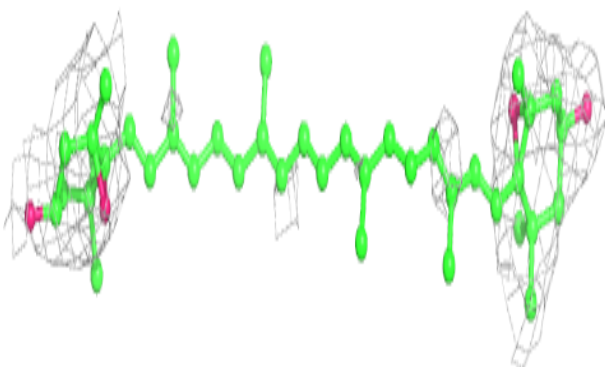
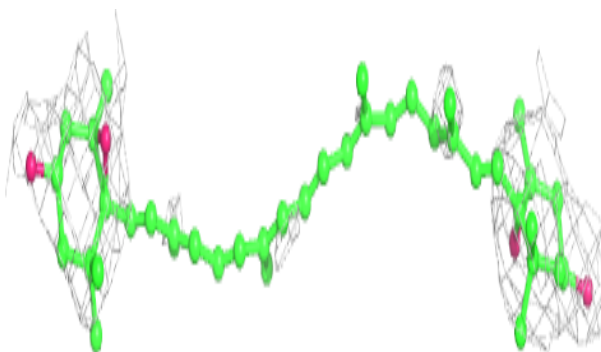
**Electron density around CHL 4 613:**

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



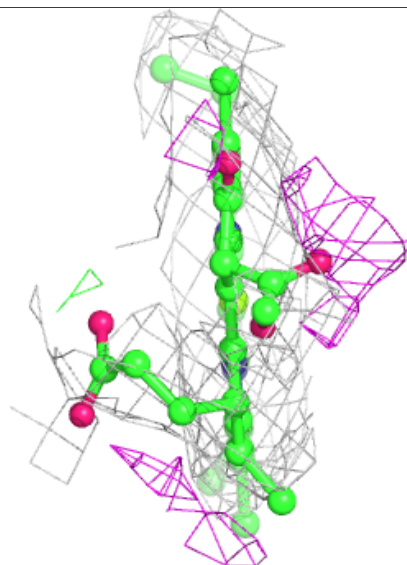
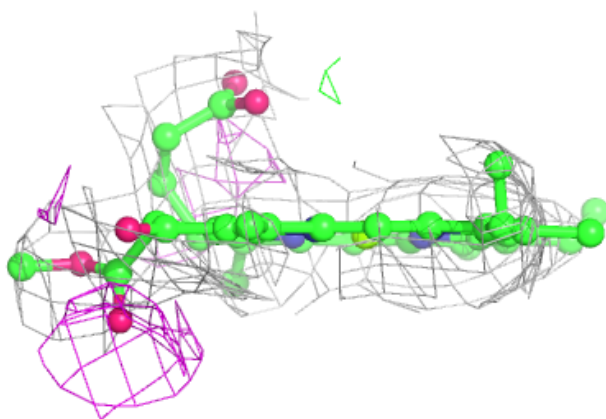
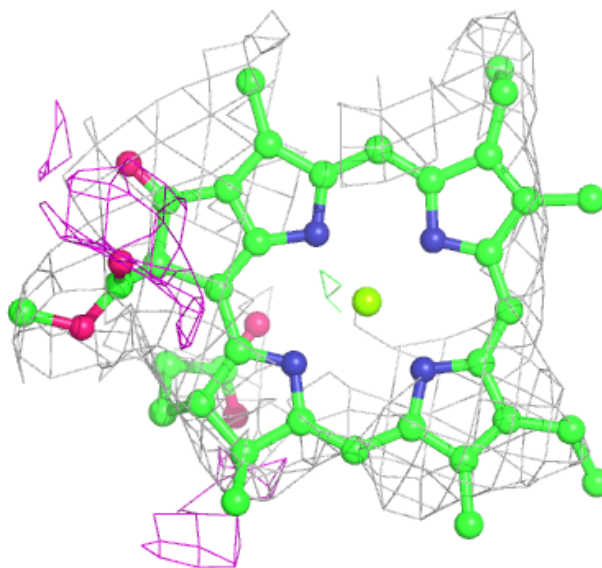
**Electron density around XAT 1 502:**

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



**Electron density around CLA 1 603:**

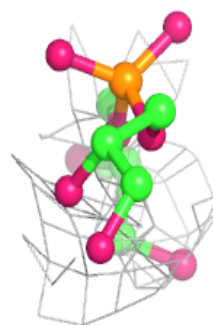
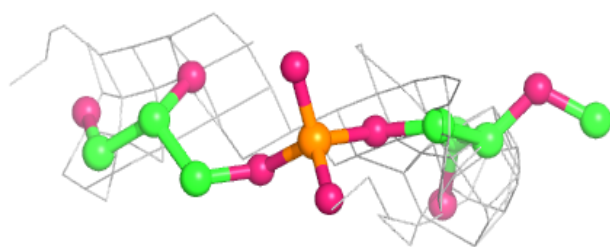
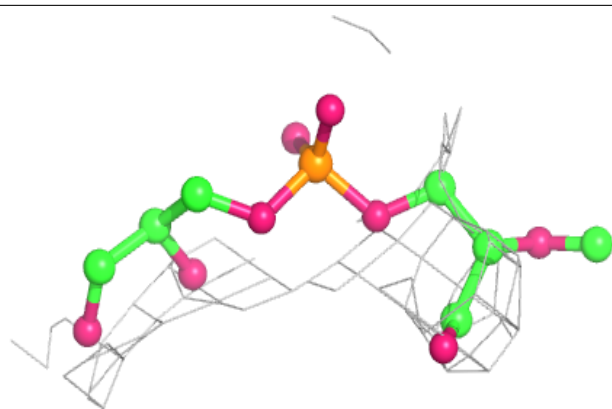
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



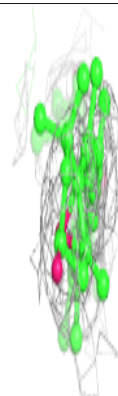
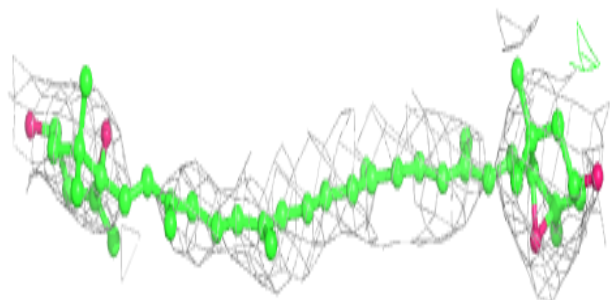
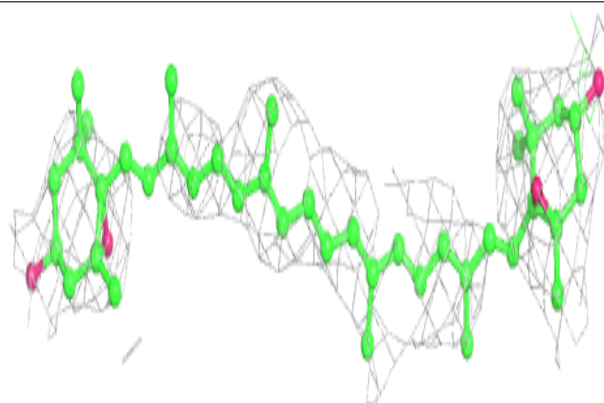


**Electron density around LHG A 5001:**

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

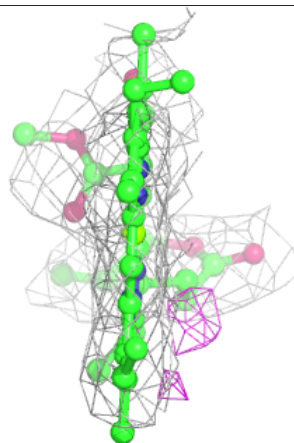
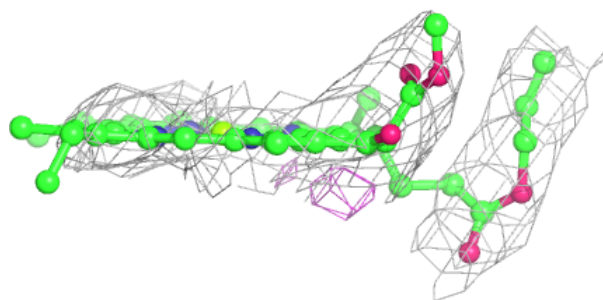
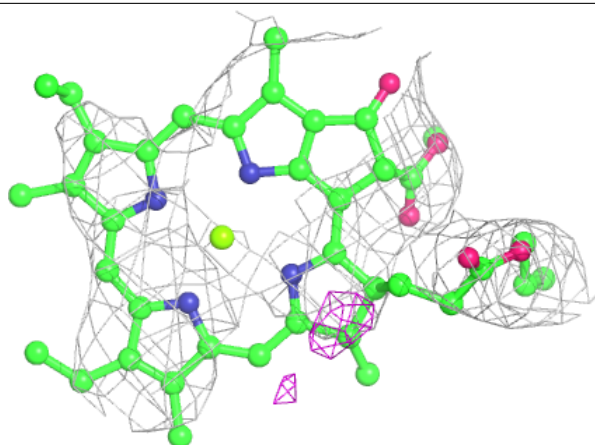
**Electron density around XAT 2 502:**

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



**Electron density around CLA 1 605:**

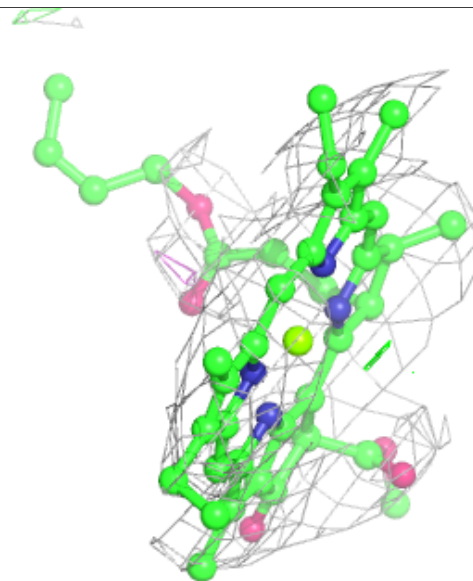
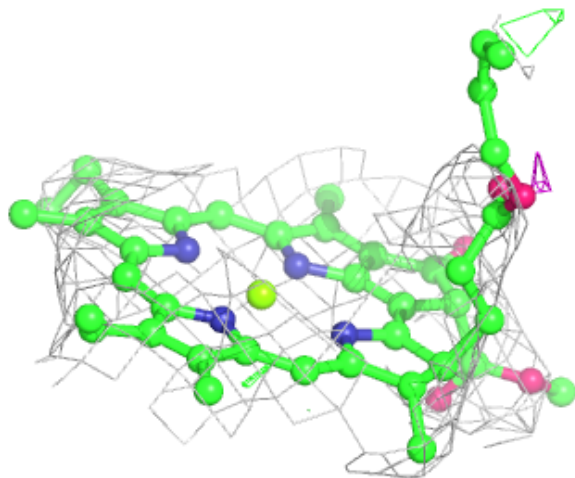
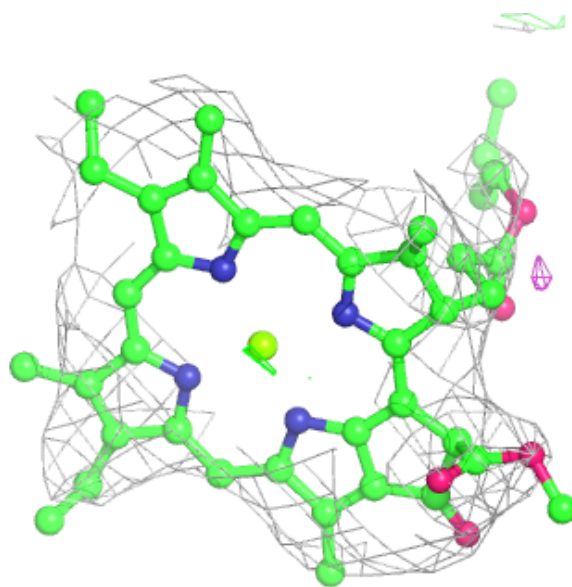
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





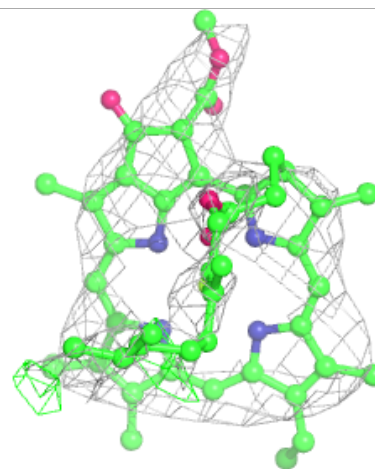
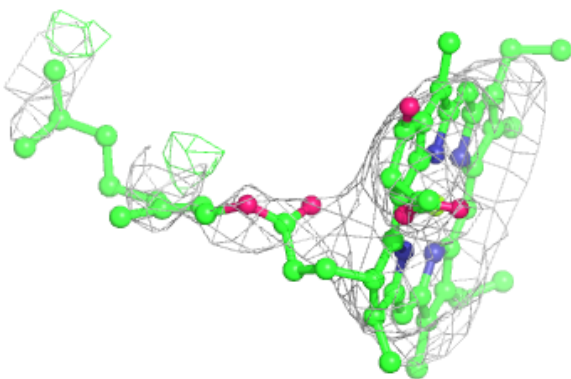
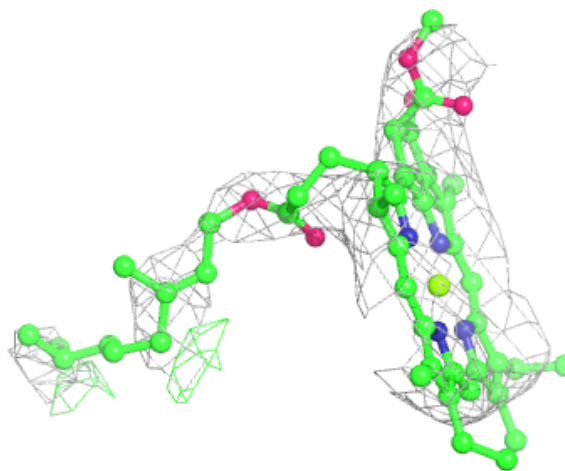
**Electron density around CLA B 1232:**

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



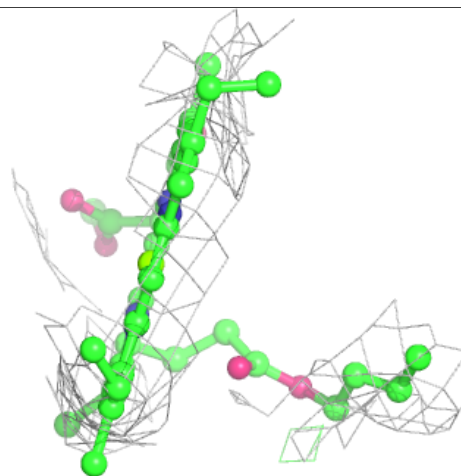
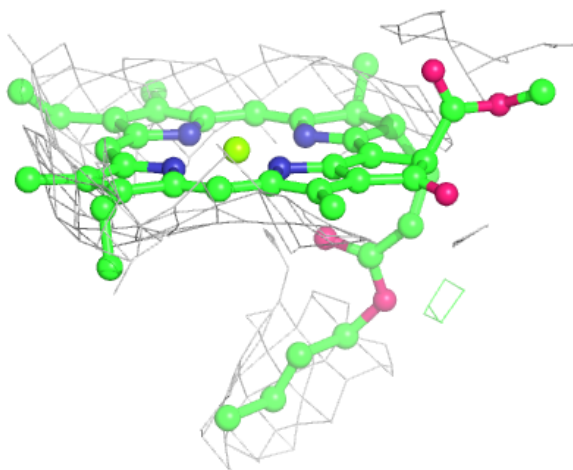
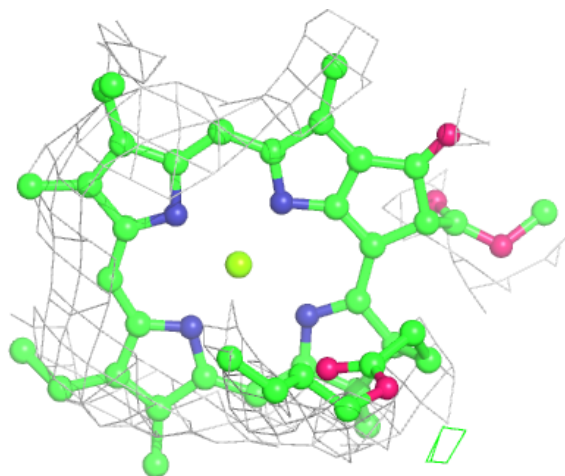
**Electron density around CLA A 1140:**

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



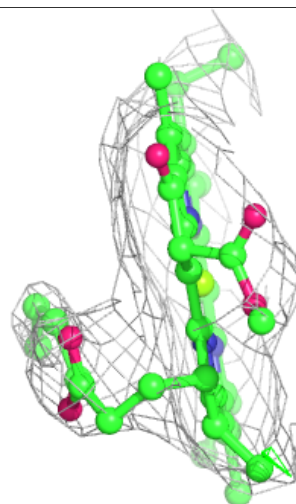
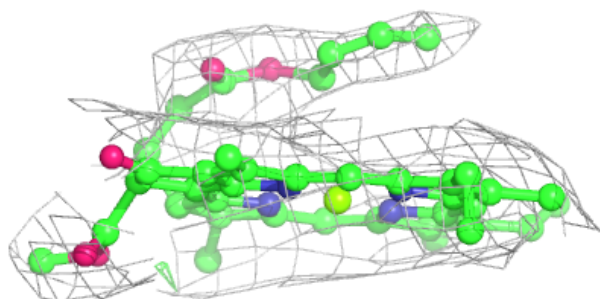
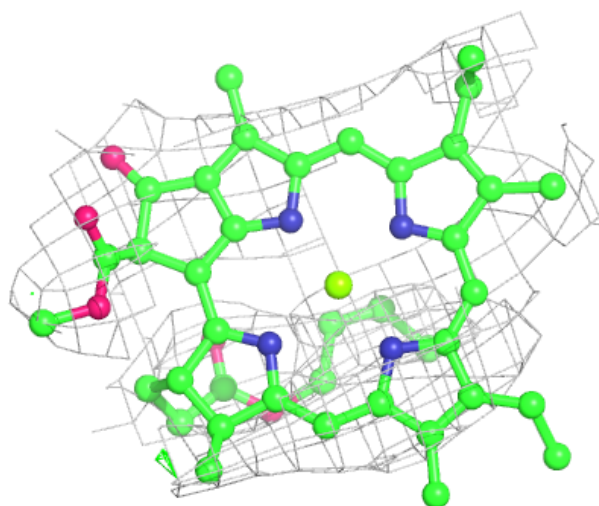
**Electron density around CLA A 1109:**

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



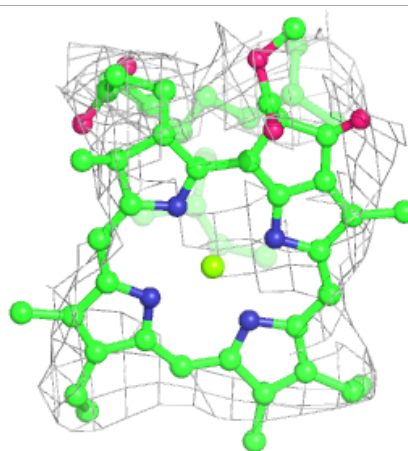
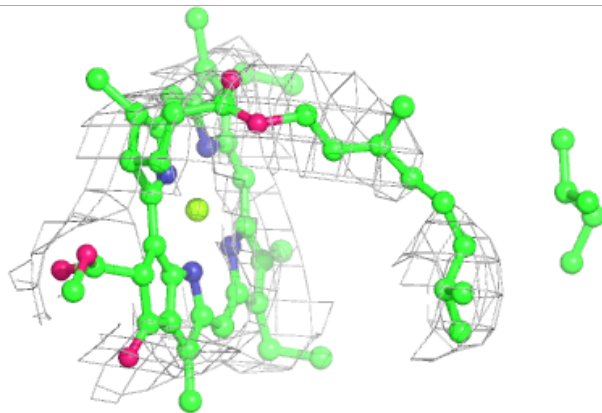
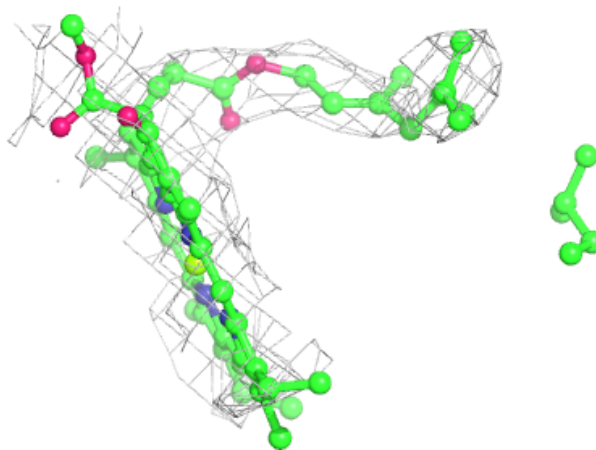
**Electron density around CLA B 1205:**

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



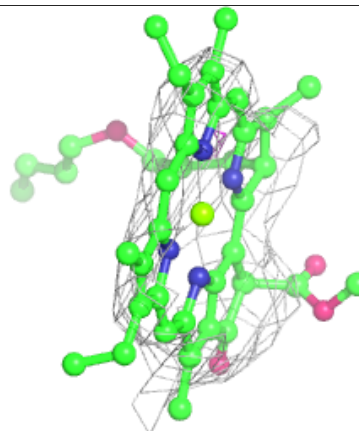
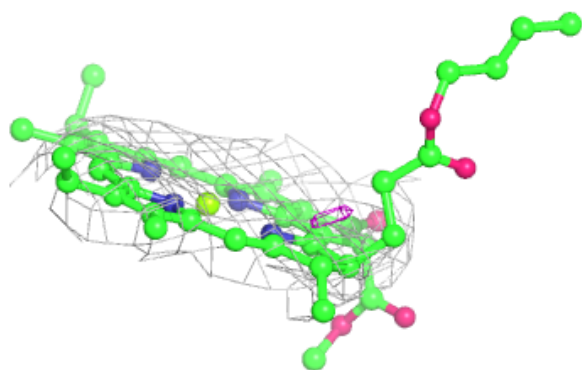
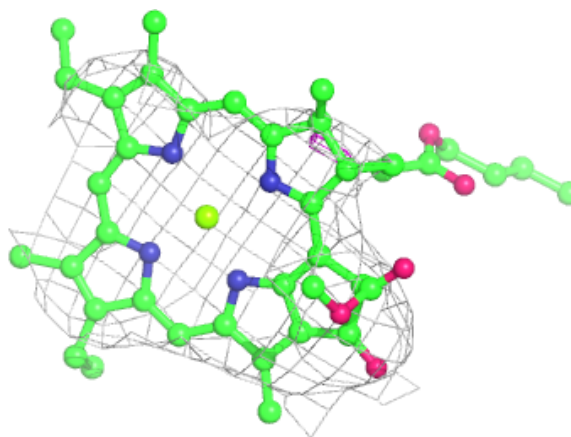
**Electron density around CLA 1 612:**

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

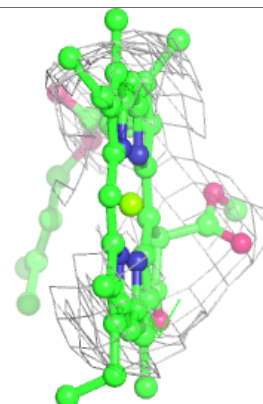
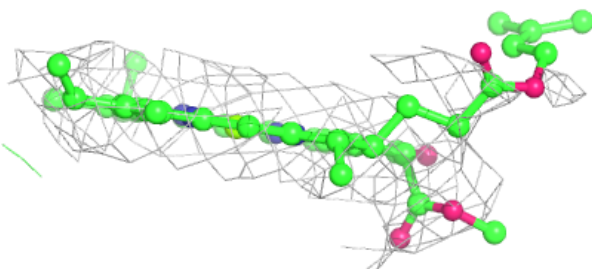
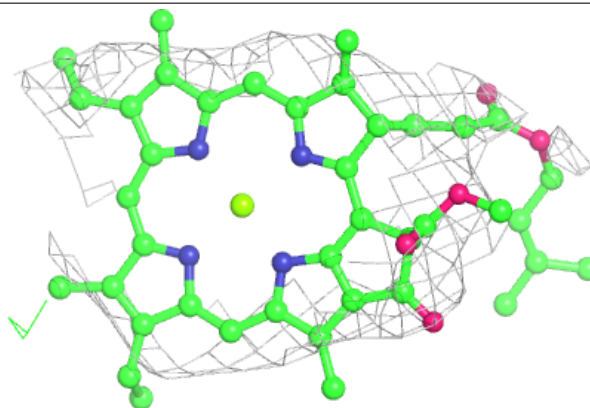


**Electron density around CLA A 1112:**

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

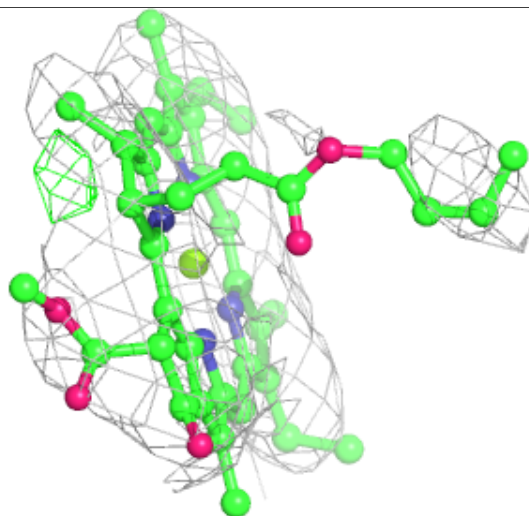
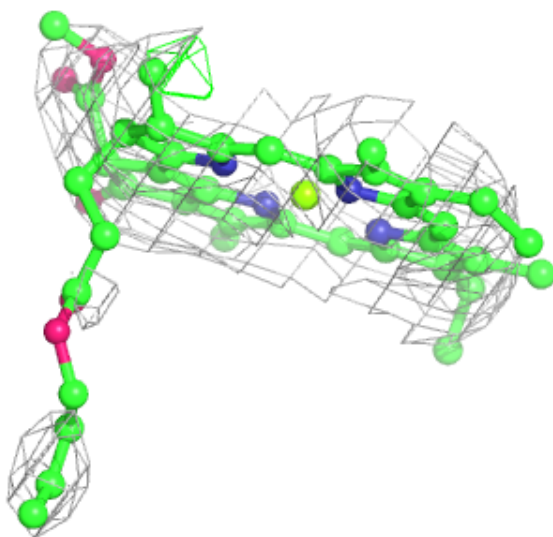
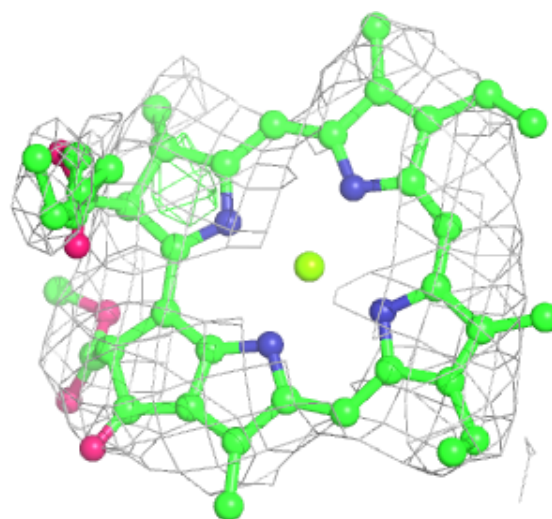
**Electron density around CLA 2 615:**

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



**Electron density around CLA B 1225:**

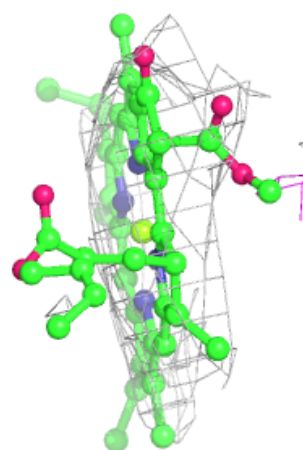
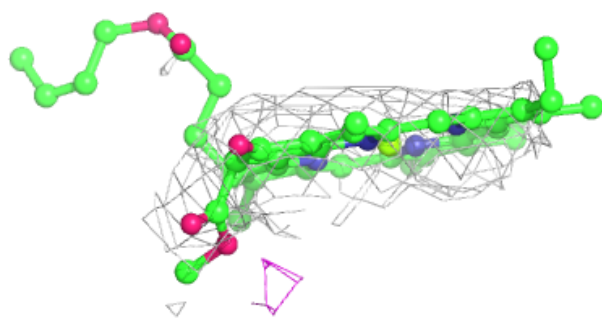
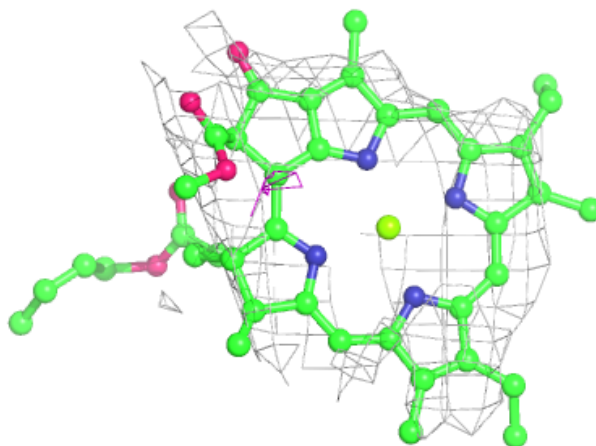
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA A 1132:**

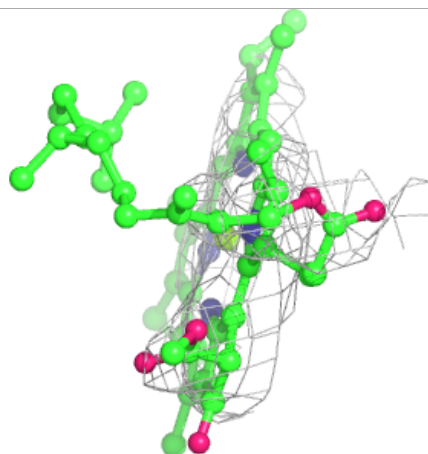
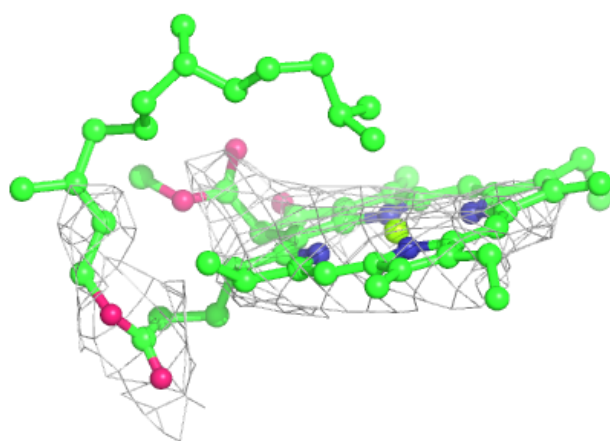
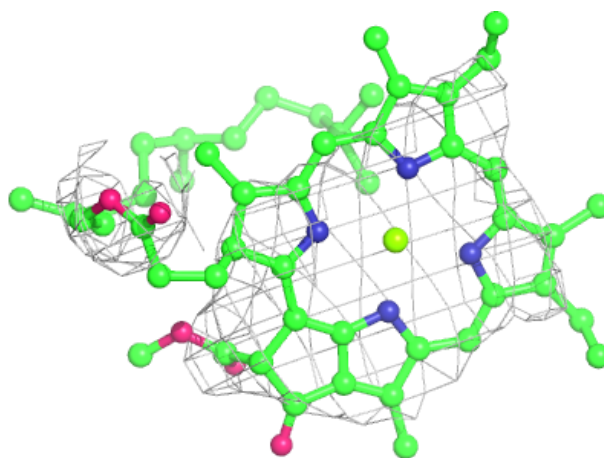
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





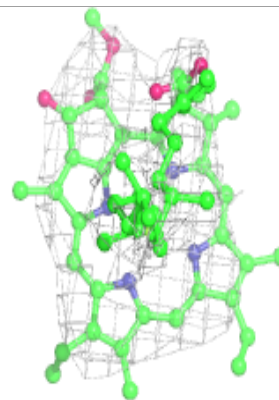
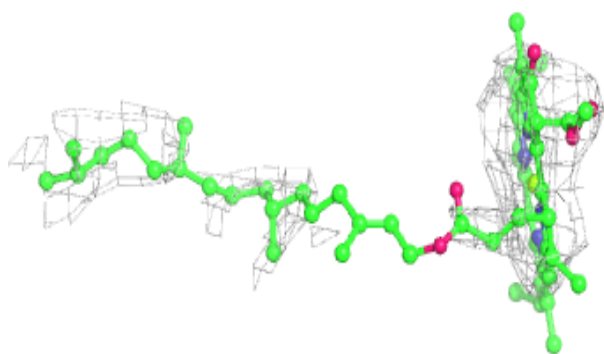
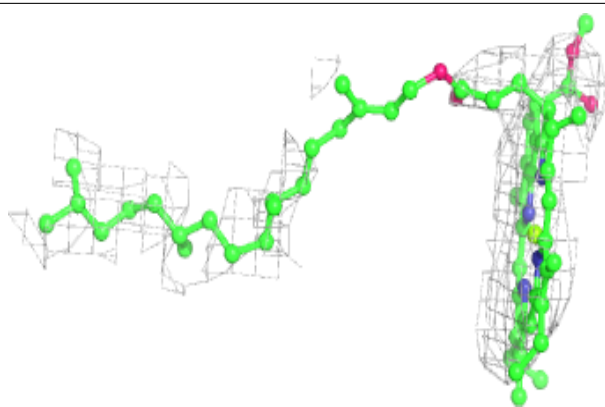
**Electron density around CLA A 1104:**

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



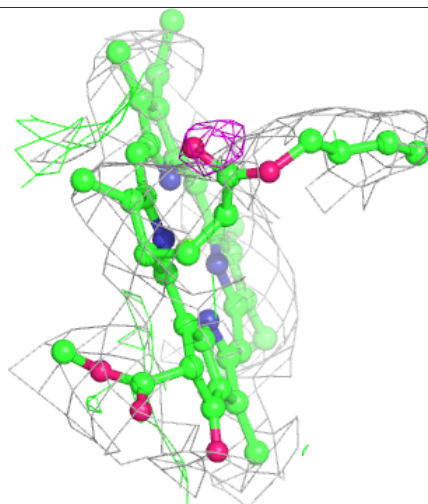
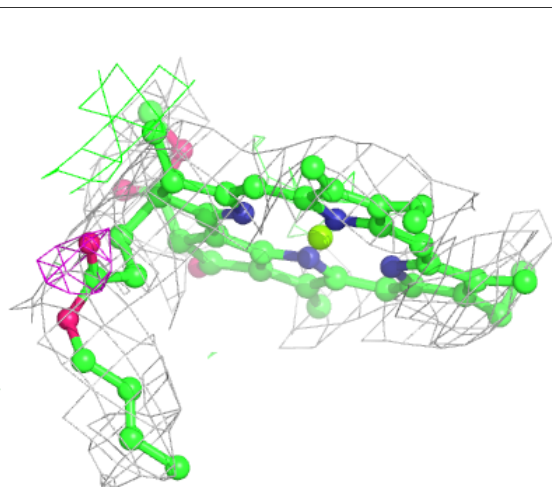
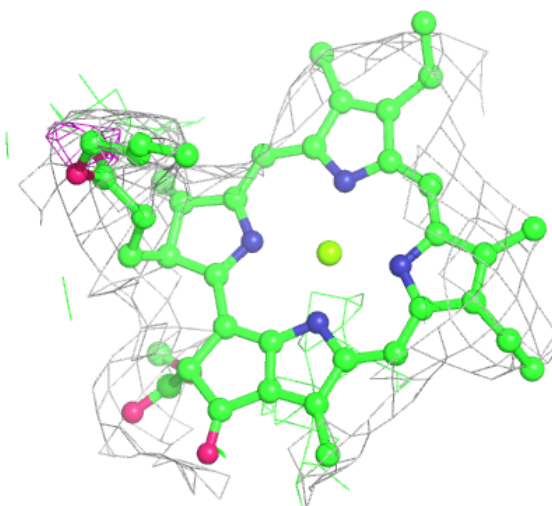
**Electron density around CLA B 1239:**

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



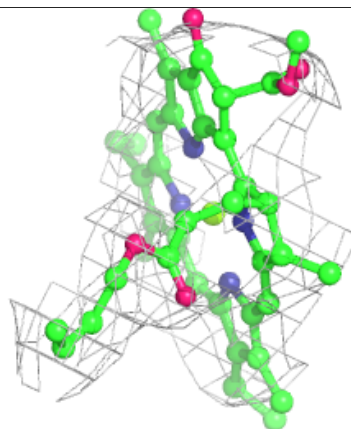
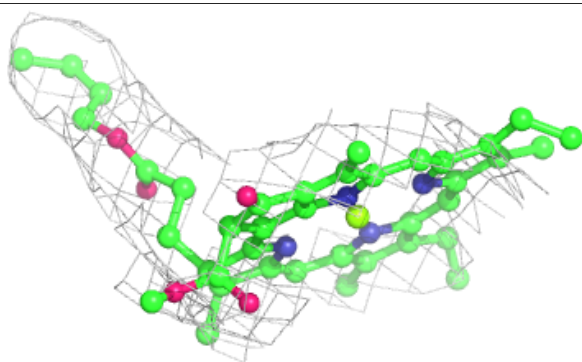
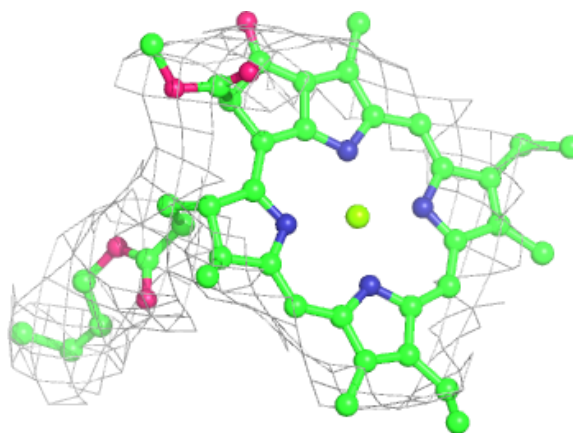
**Electron density around CLA 4 612:**

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

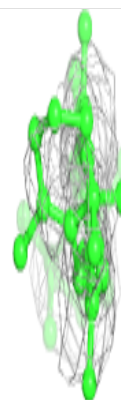
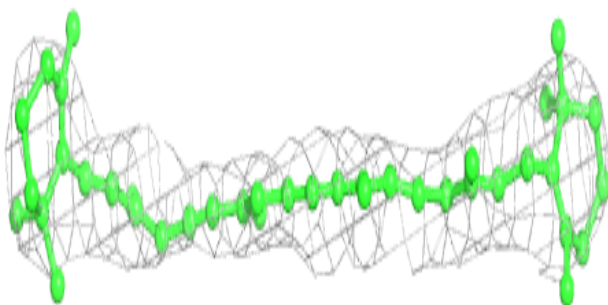
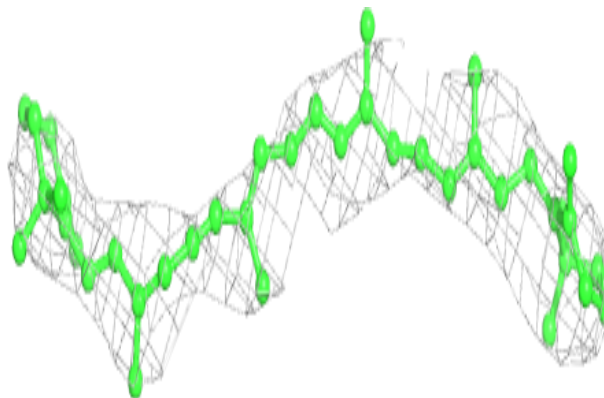


**Electron density around CLA 1 611:**

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

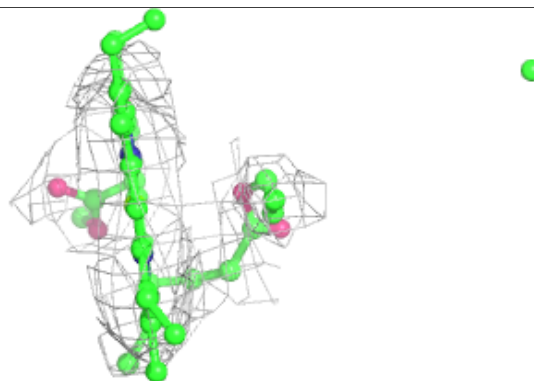
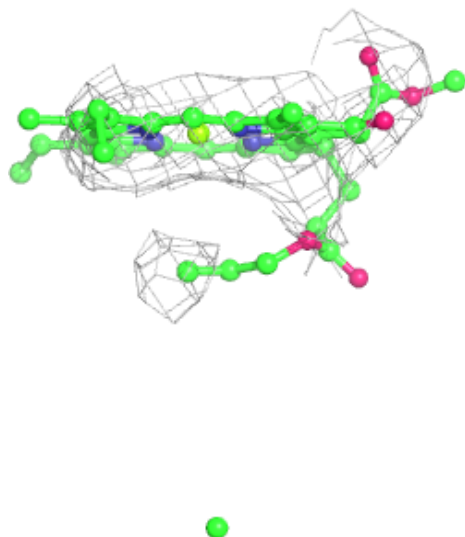
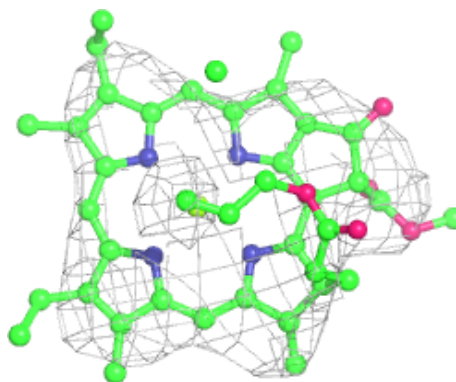
**Electron density around BCR B 4004:**

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



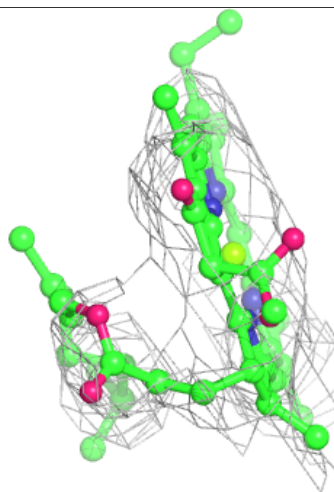
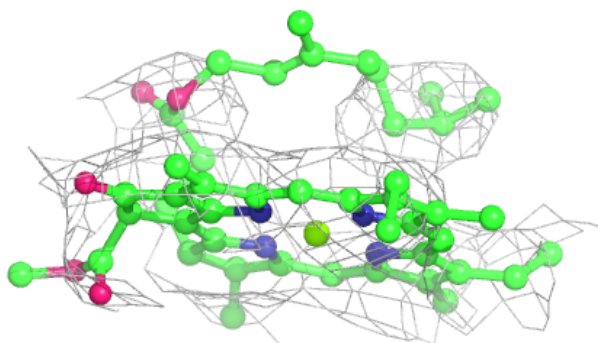
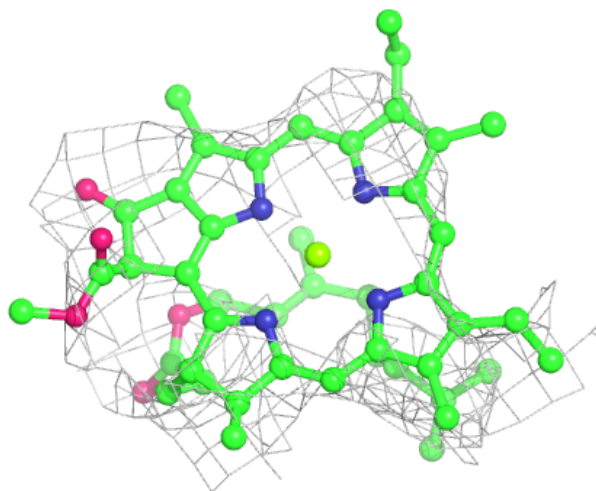
**Electron density around CLA B 1201:**

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



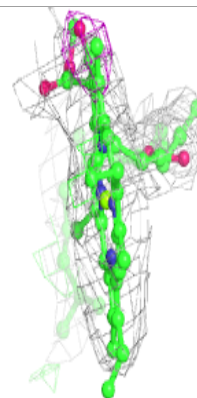
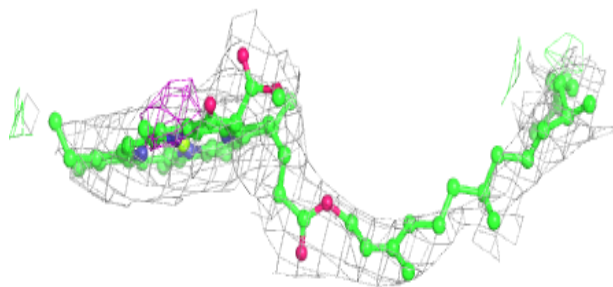
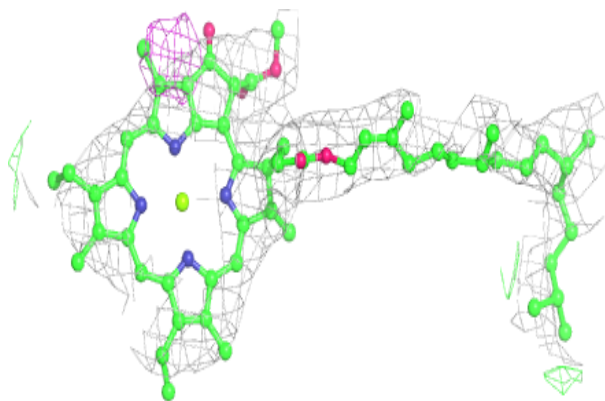
**Electron density around CLA A 1130:**

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



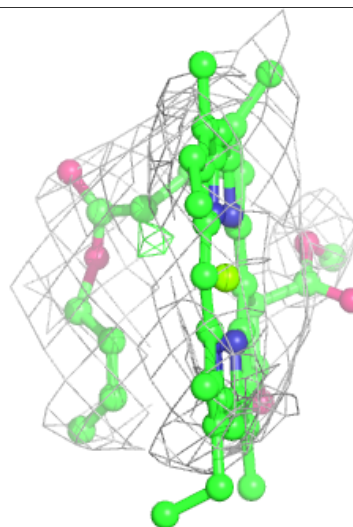
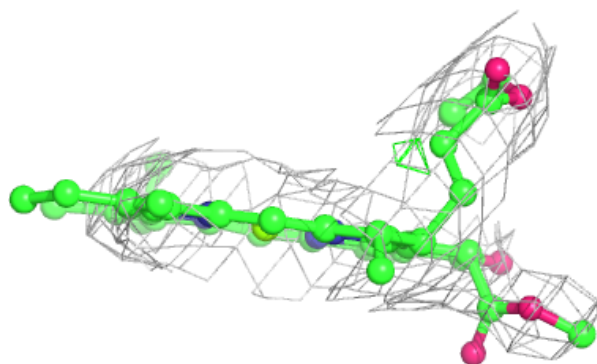
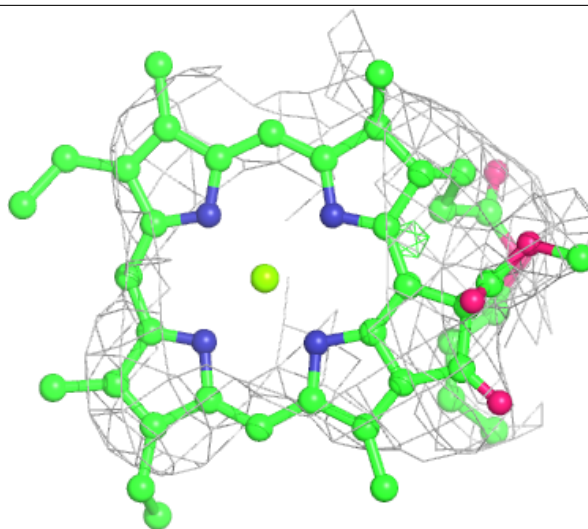
**Electron density around CLA B 1240:**

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



**Electron density around CLA A 1127:**

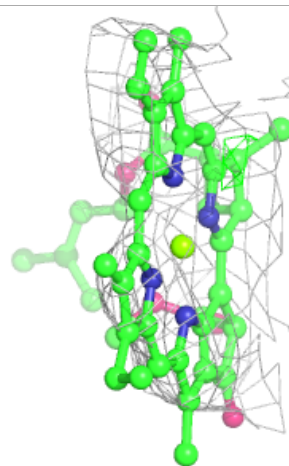
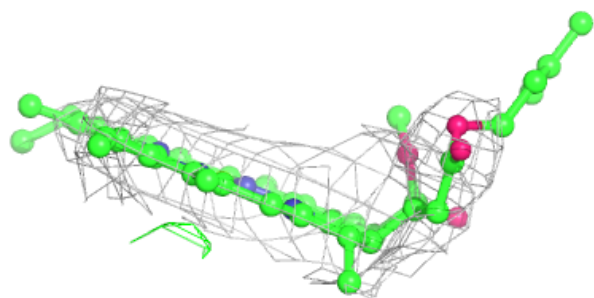
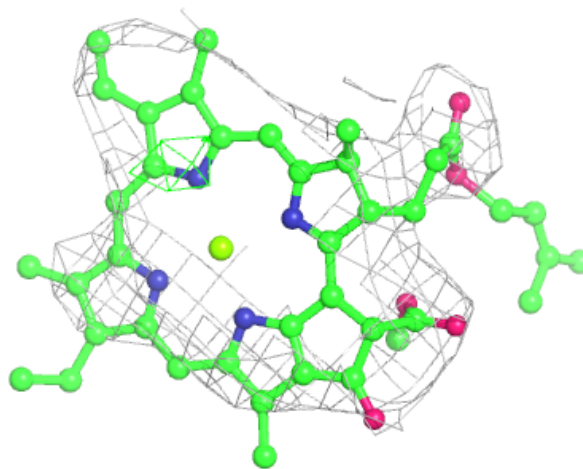
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





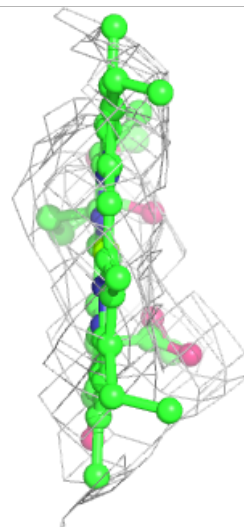
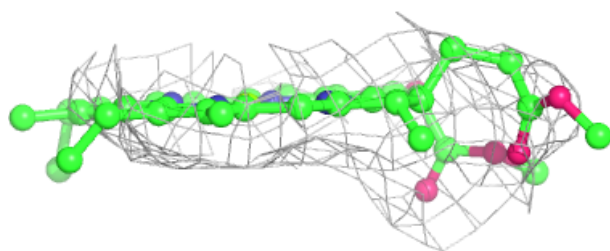
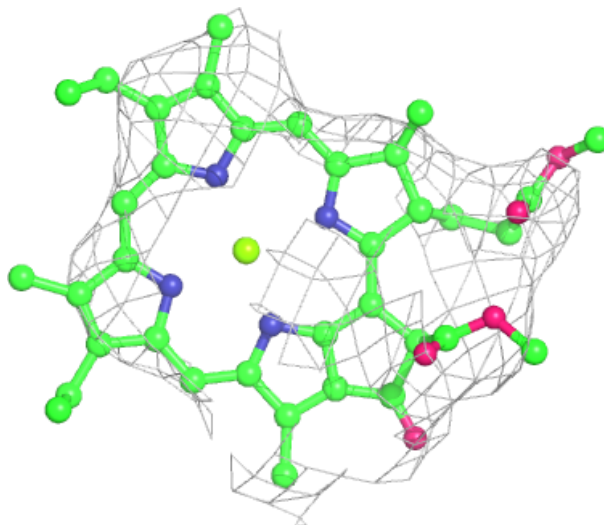
**Electron density around CL0 A 1011:**

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



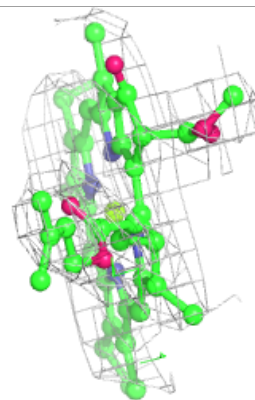
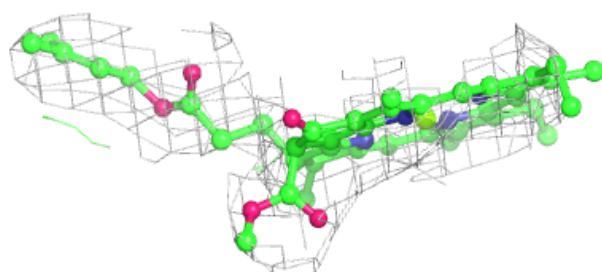
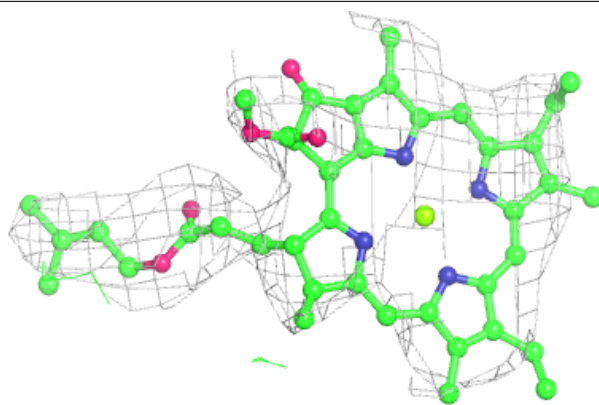
**Electron density around CLA 1 602:**

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



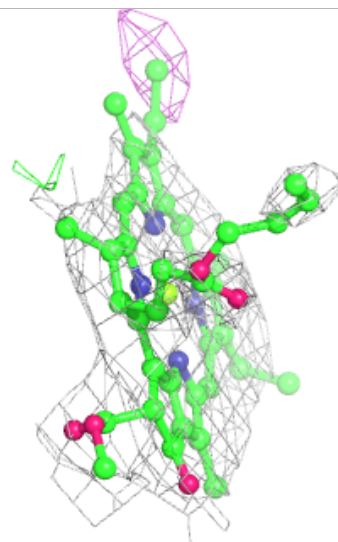
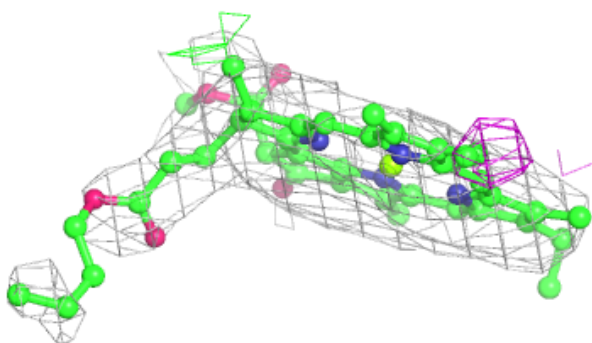
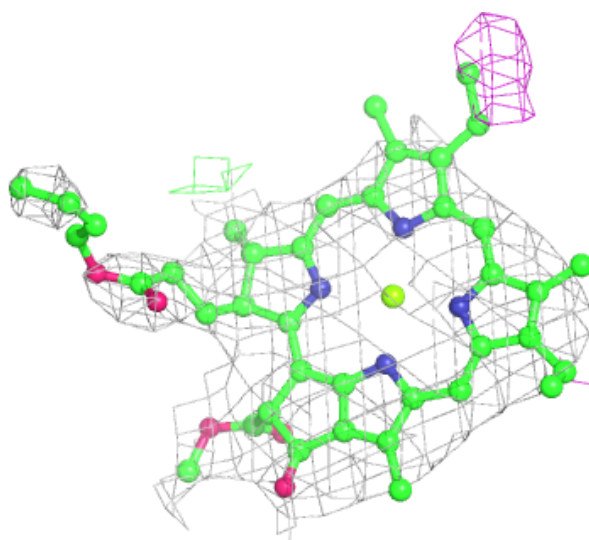
**Electron density around CLA B 1223:**

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



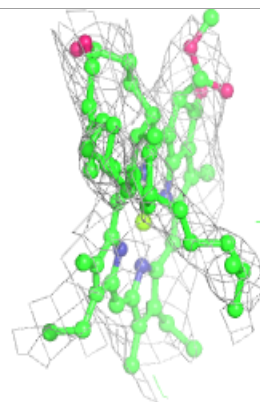
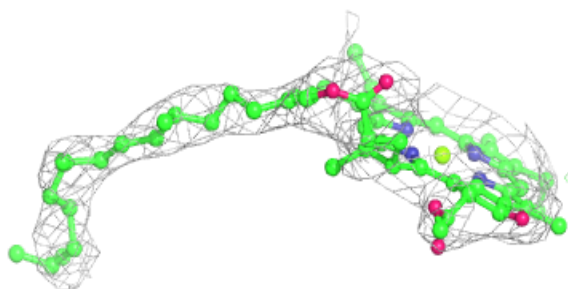
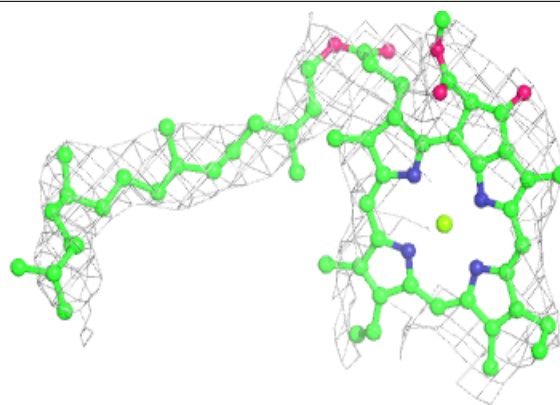
**Electron density around CLA B 1230:**

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

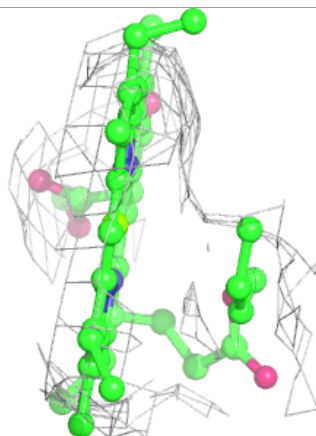
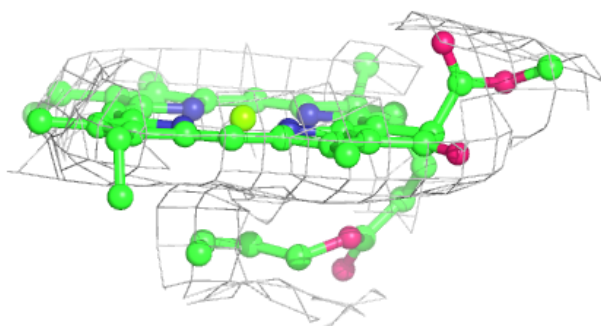
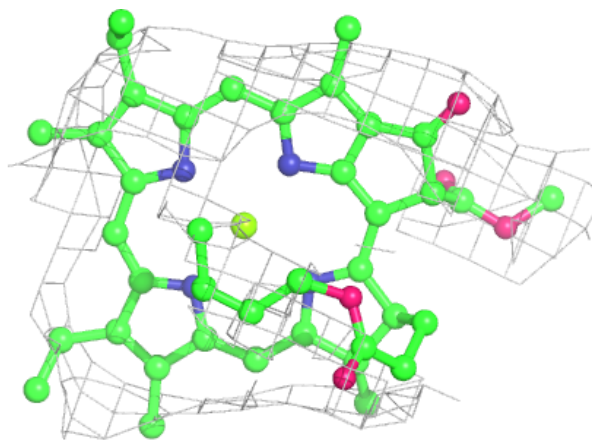


**Electron density around CLA A 1013:**

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

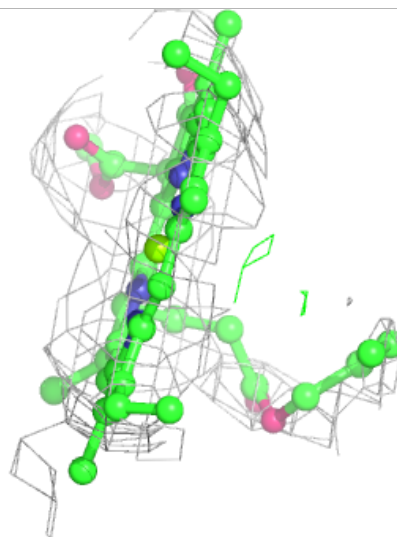
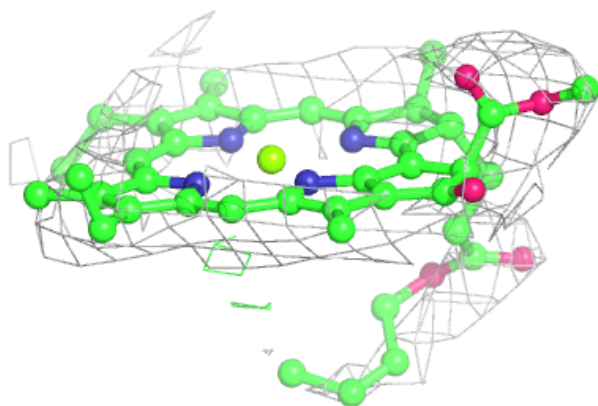
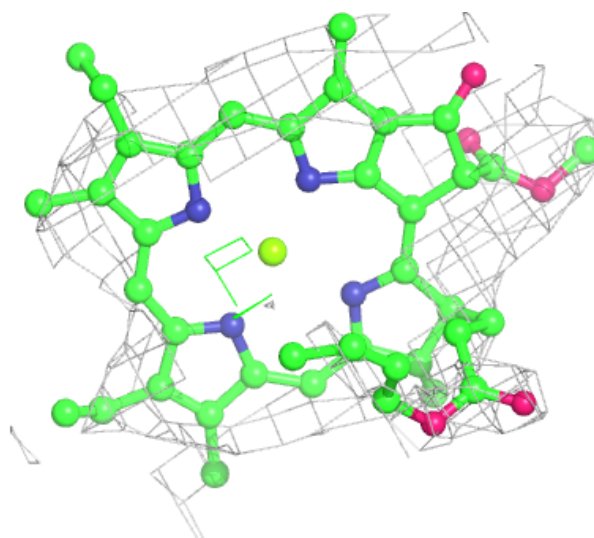
**Electron density around CLA B 1237:**

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



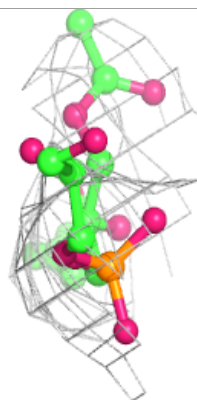
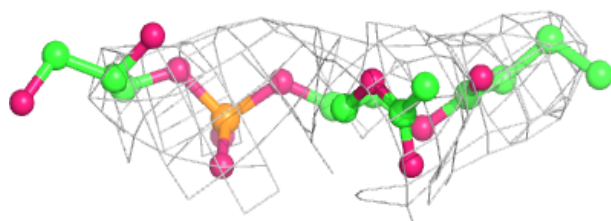
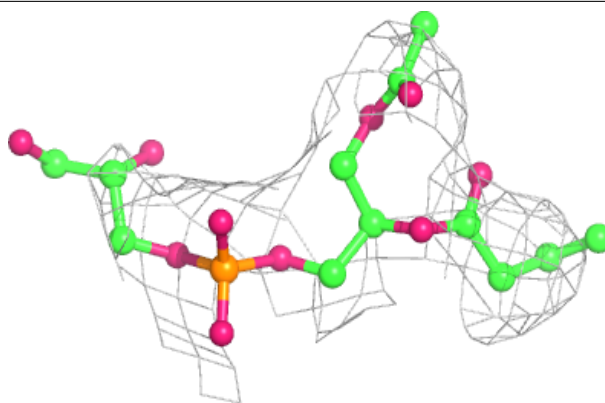
**Electron density around CLA B 1214:**

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



**Electron density around LHG 1 801:**

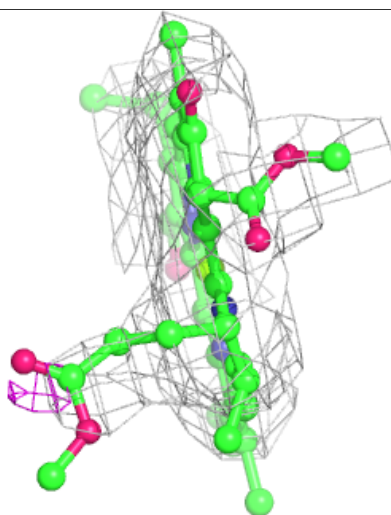
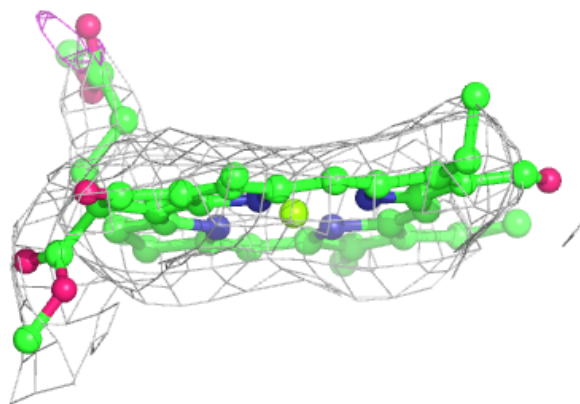
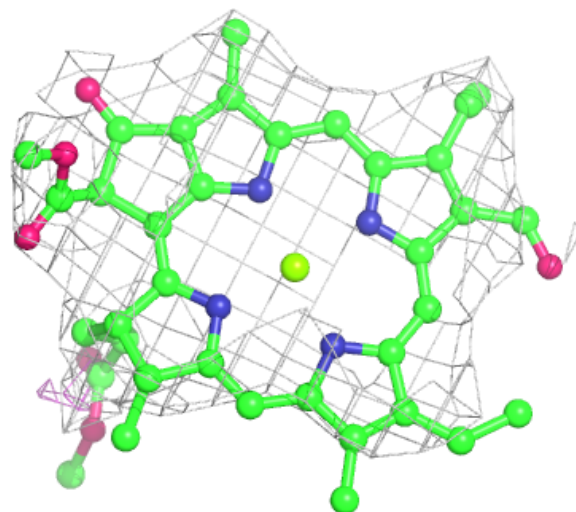
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CHL 4 610:**

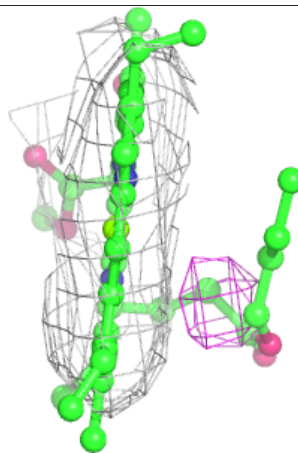
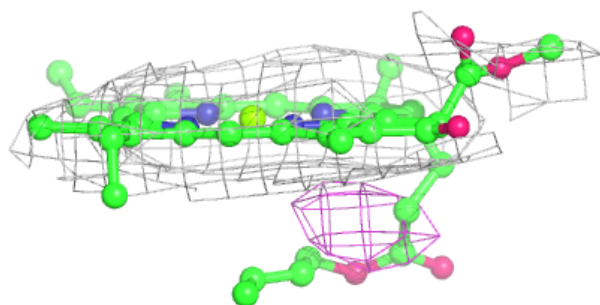
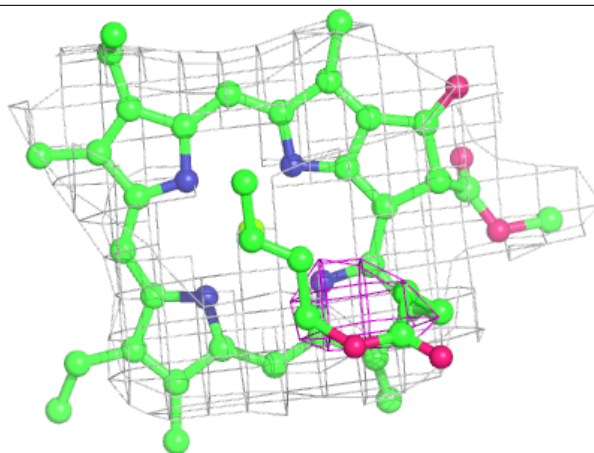
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





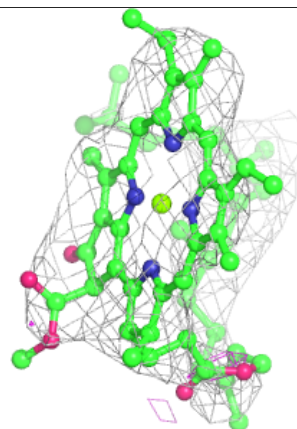
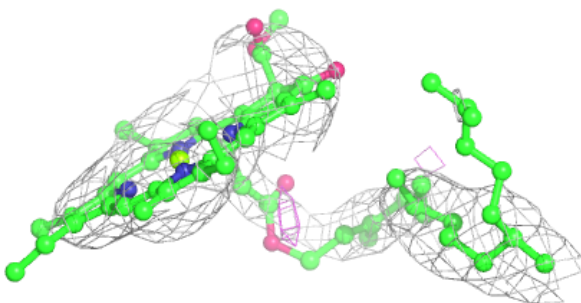
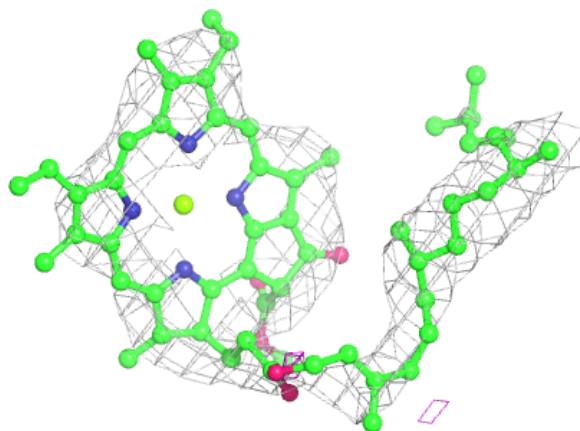
**Electron density around CLA 2 608:**

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



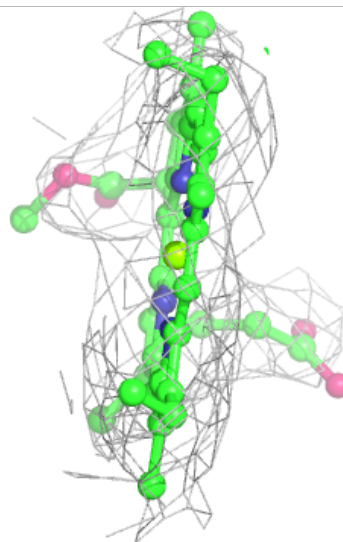
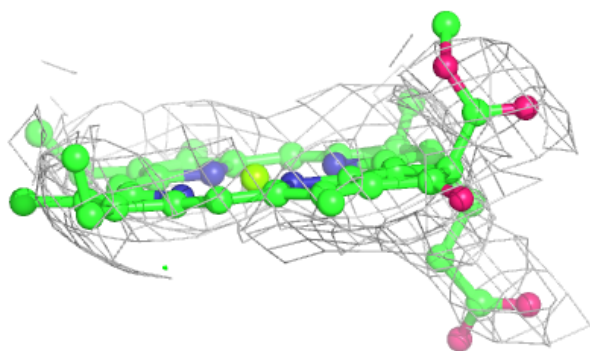
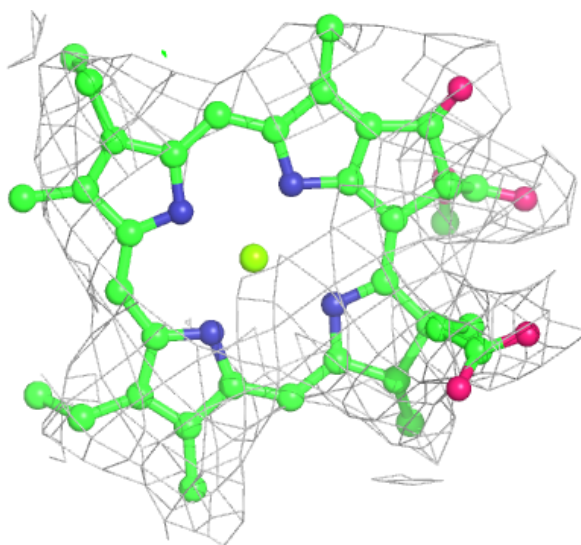
**Electron density around CLA B 1229:**

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



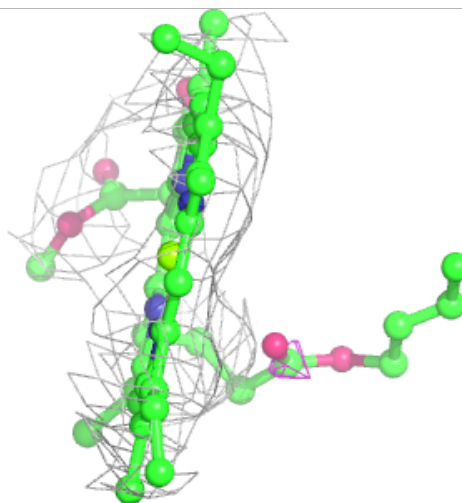
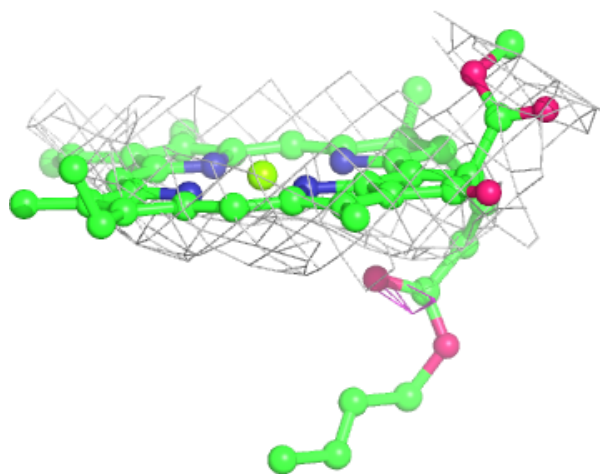
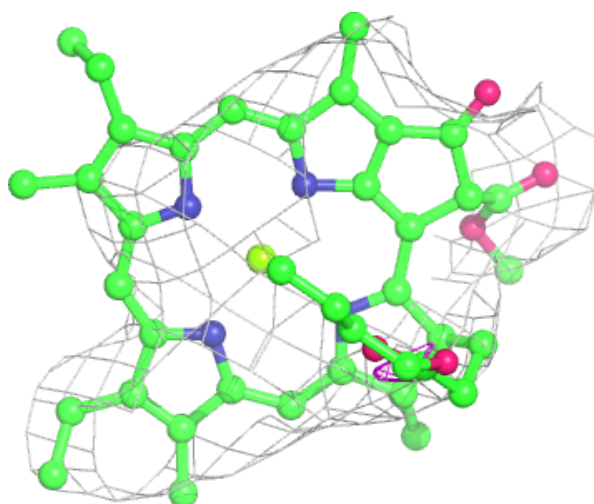
**Electron density around CLA B 1227:**

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



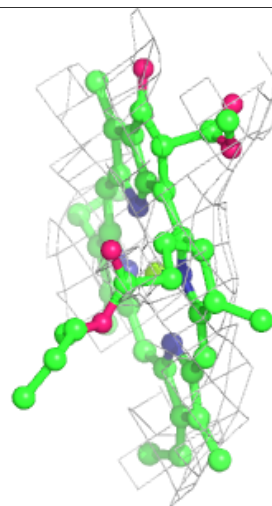
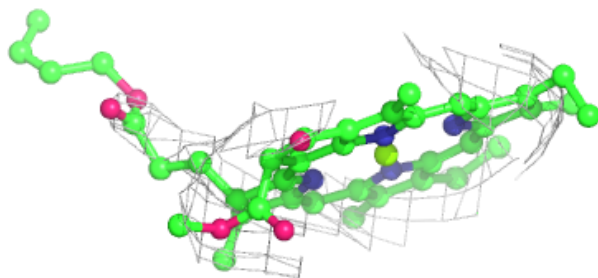
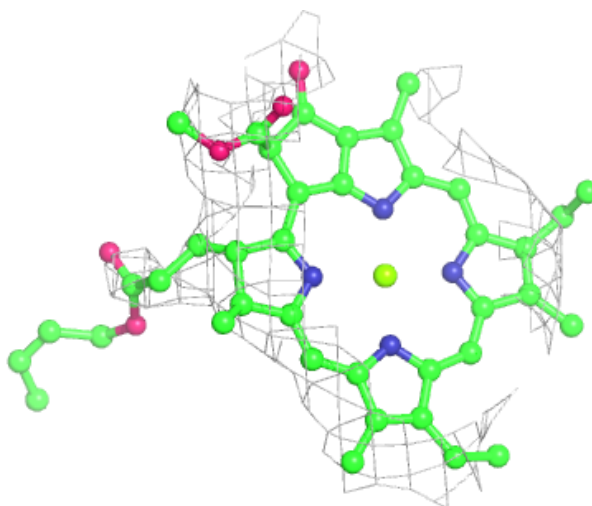
**Electron density around CLA 2 607:**

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



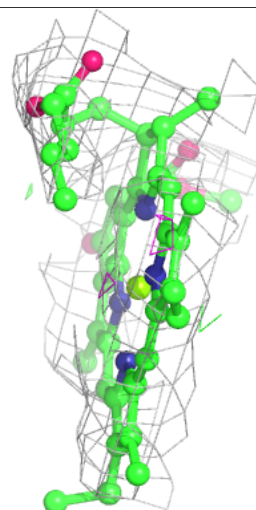
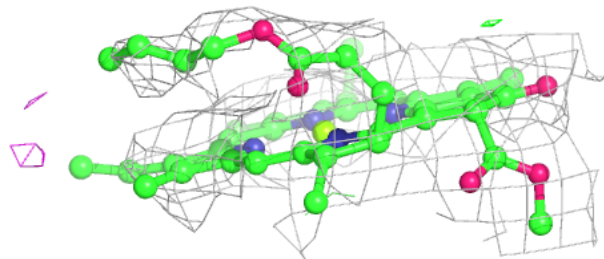
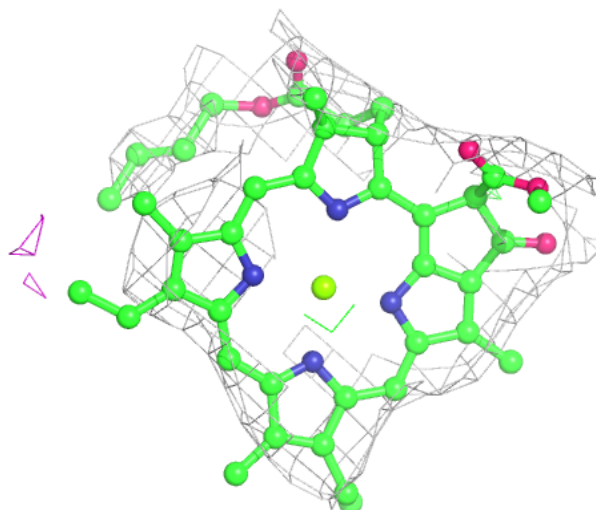
**Electron density around CLA A 1125:**

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



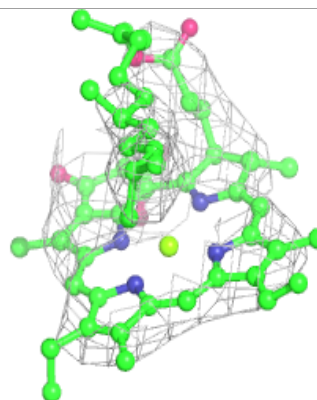
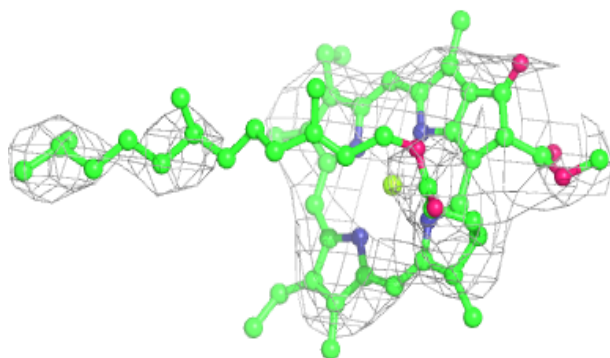
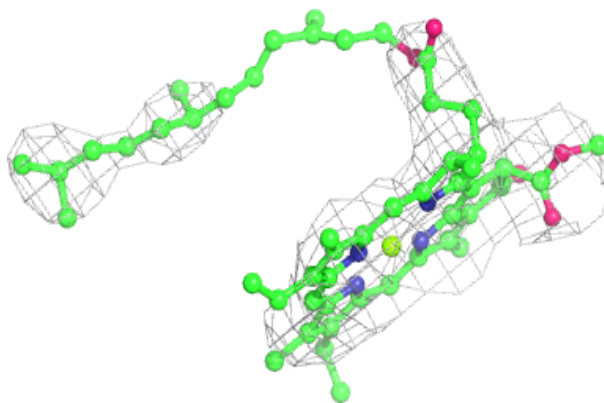
**Electron density around CLA 1 604:**

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

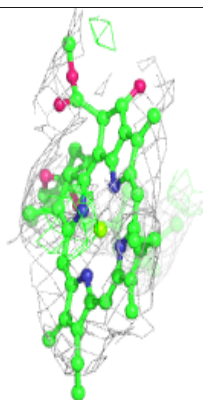
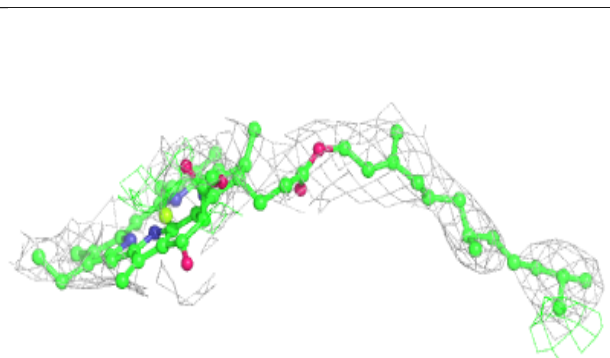
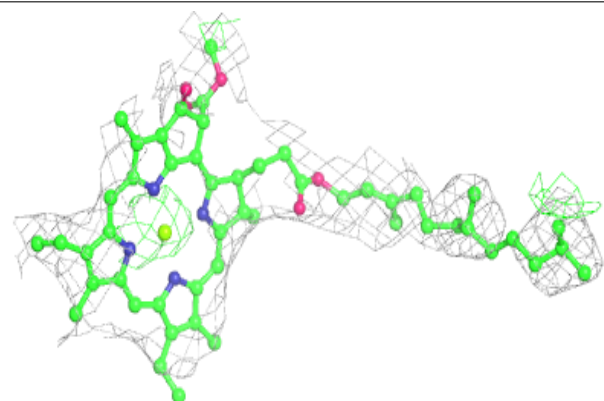


**Electron density around CLA B 1228:**

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

**Electron density around CLA A 1012:**

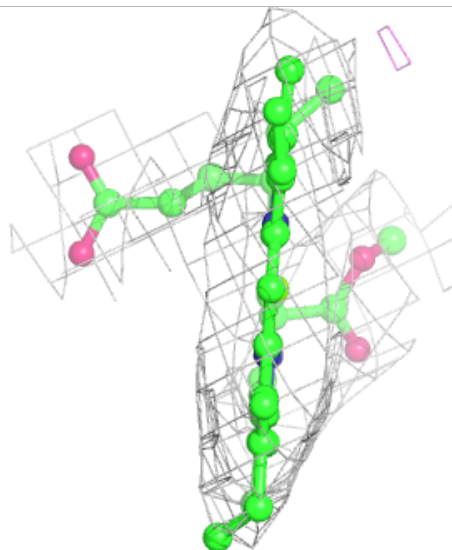
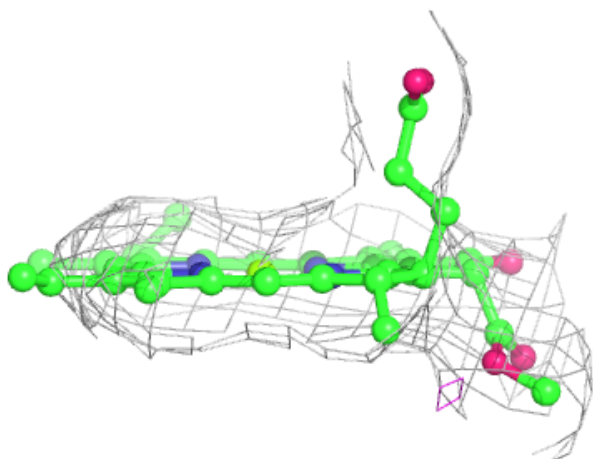
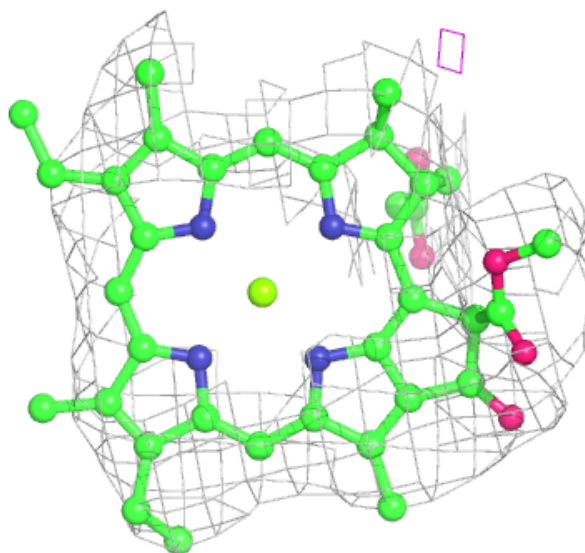
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA 1 606:**

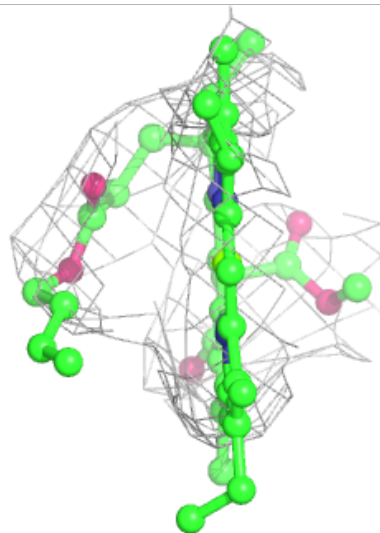
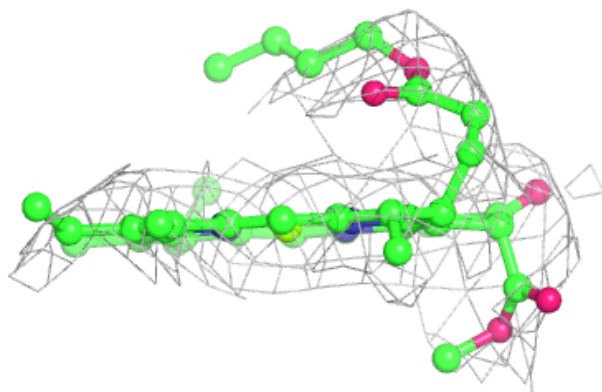
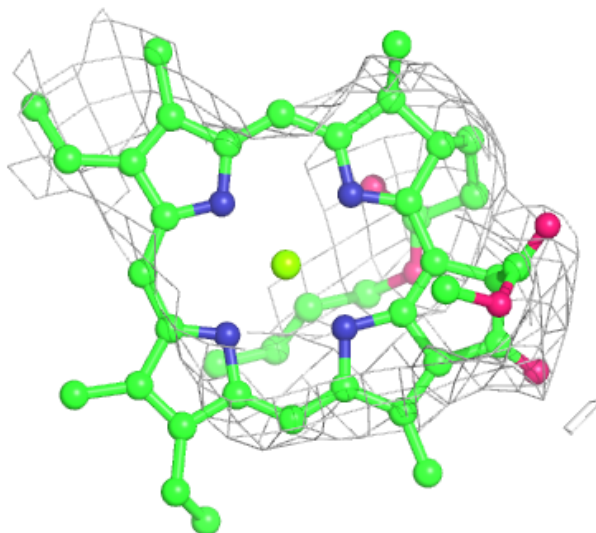
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





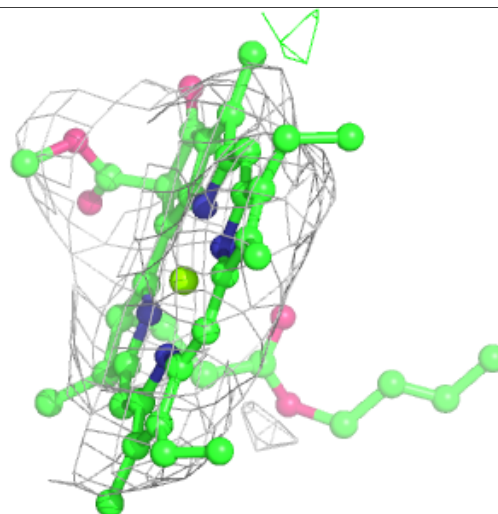
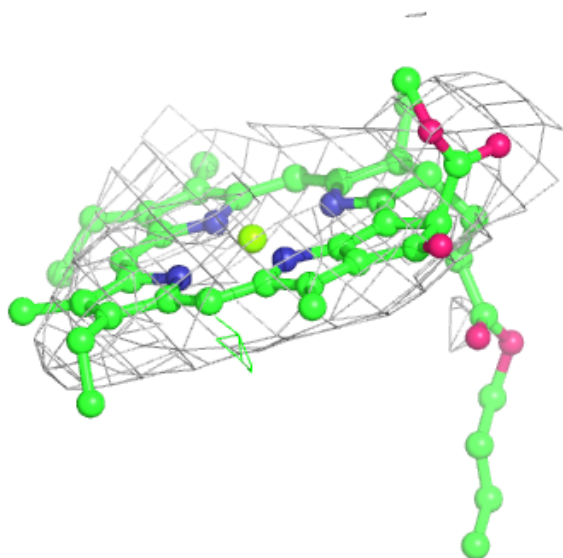
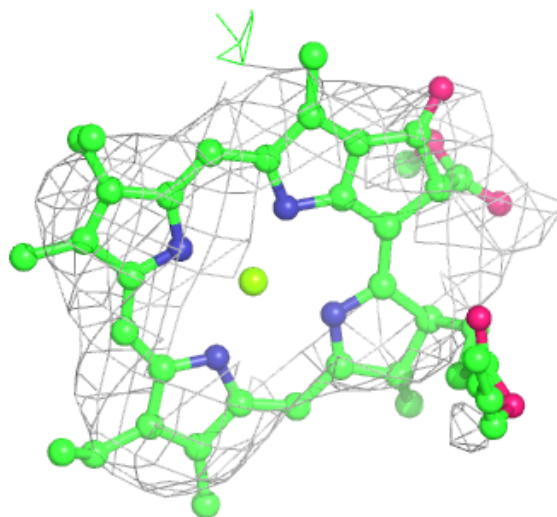
**Electron density around CLA A 1110:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



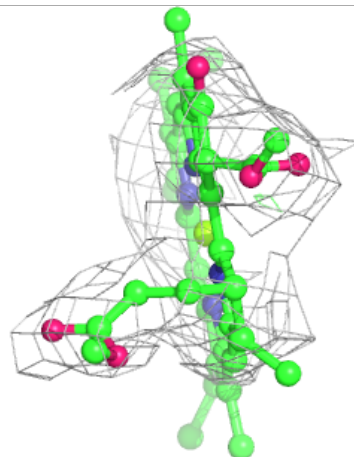
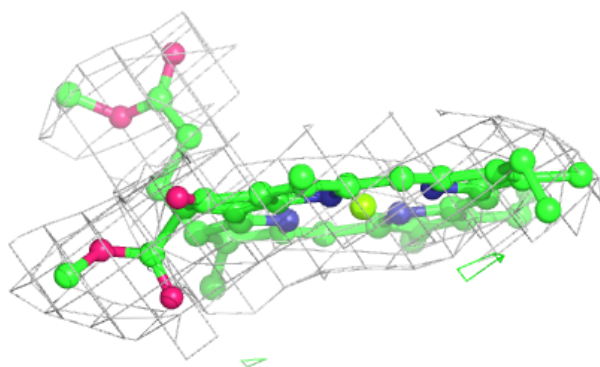
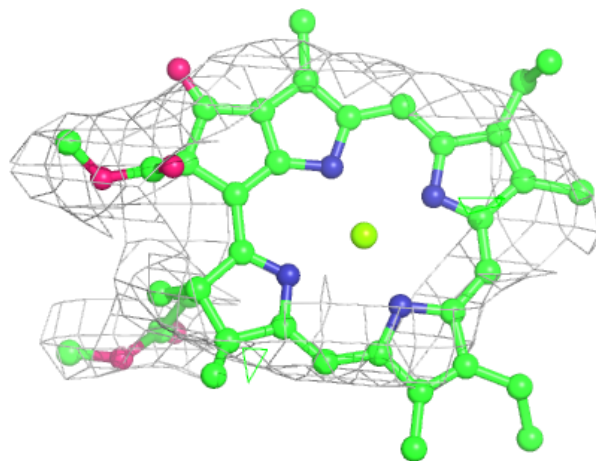
**Electron density around CLA A 1122:**

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



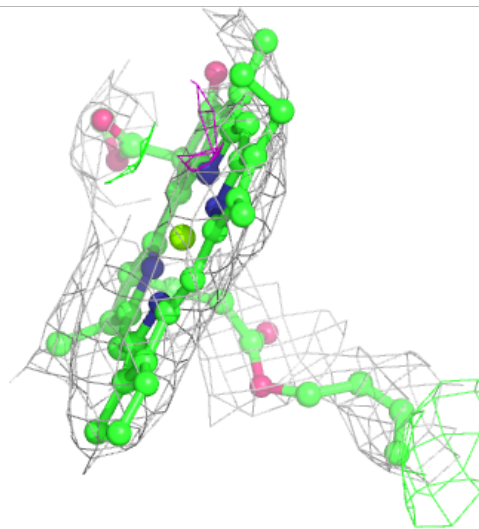
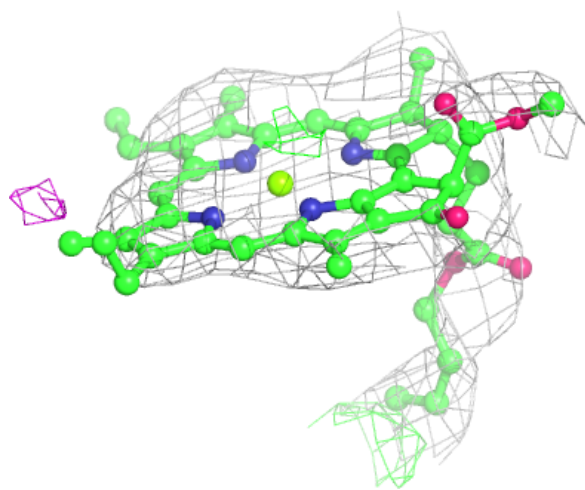
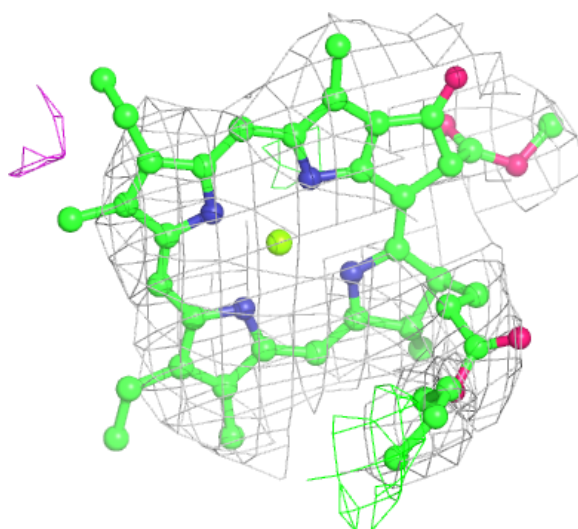
**Electron density around CLA 3 615:**

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



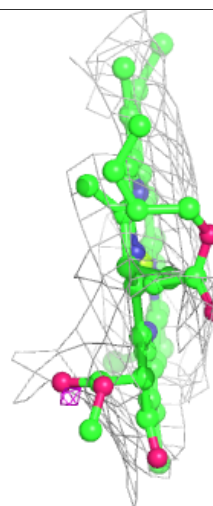
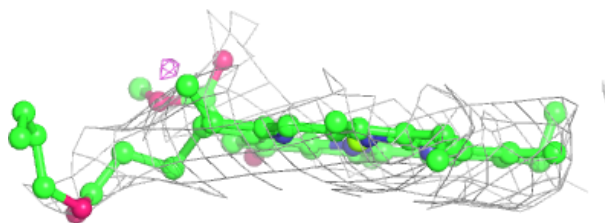
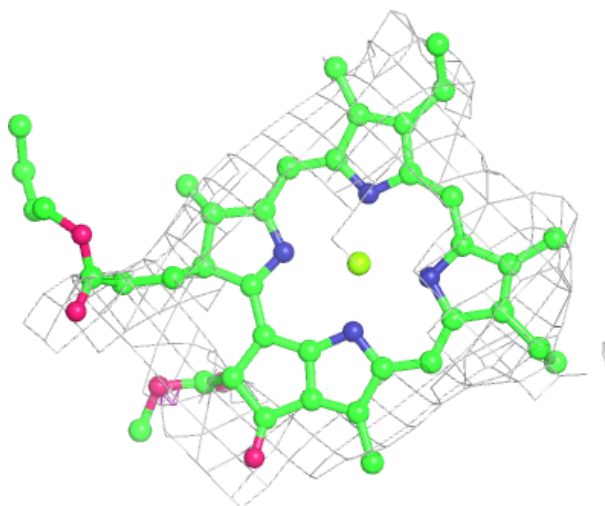
**Electron density around CLA B 1216:**

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



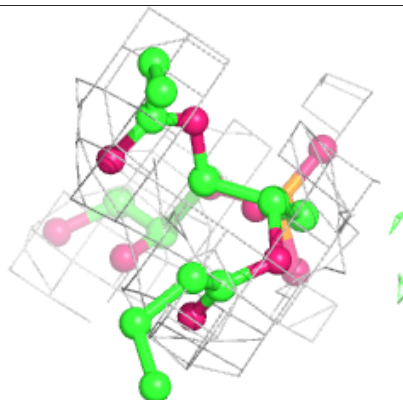
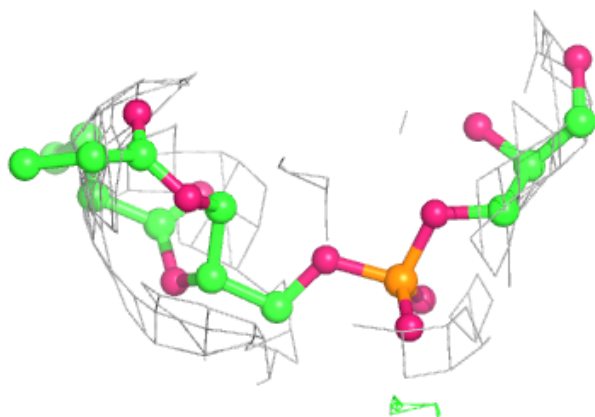
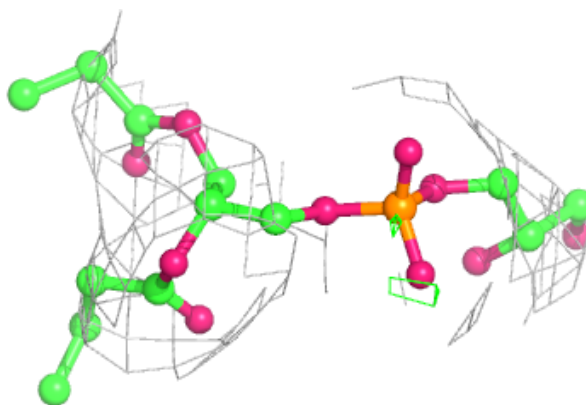
**Electron density around CLA B 1206:**

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



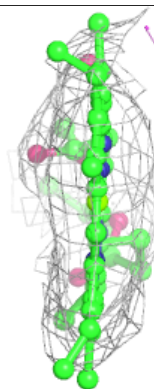
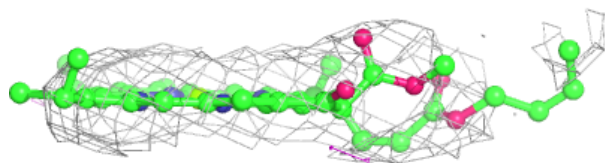
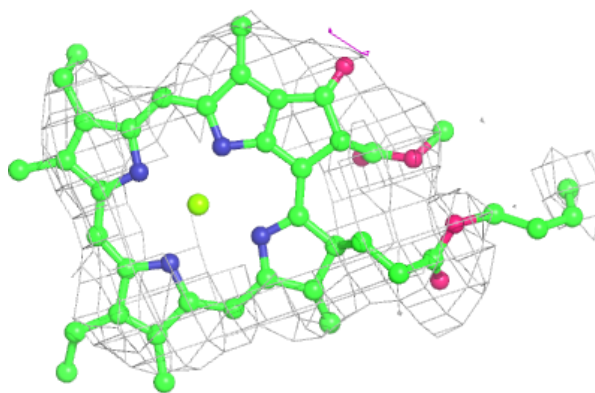
**Electron density around LHG A 5002:**

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



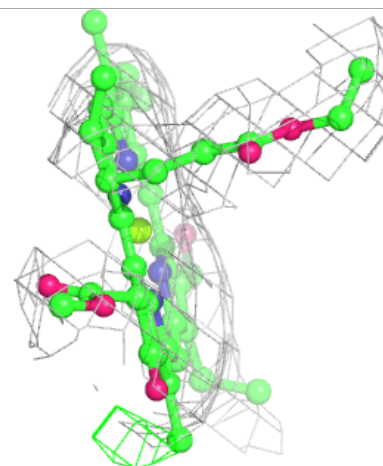
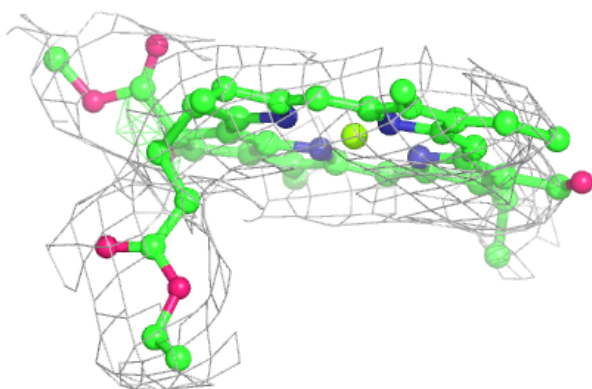
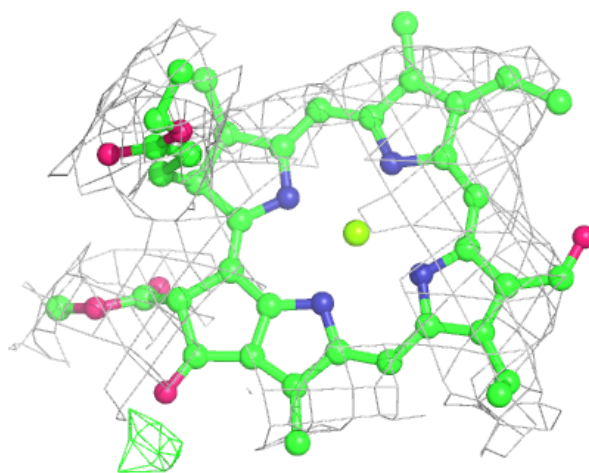
**Electron density around CLA 4 602:**

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



**Electron density around CHL 2 611:**

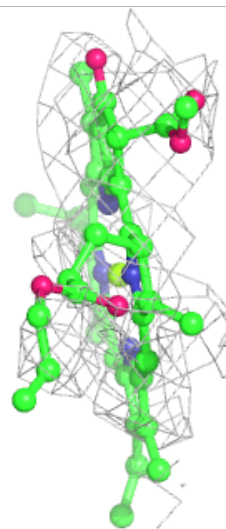
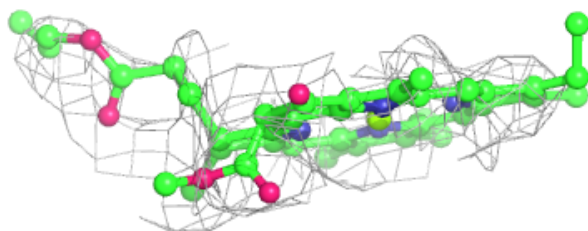
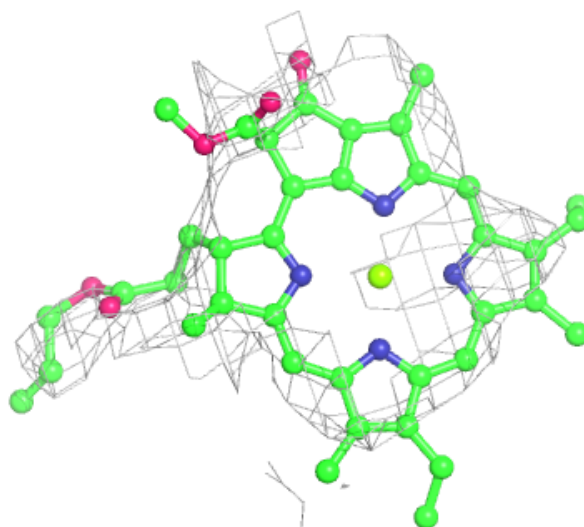
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





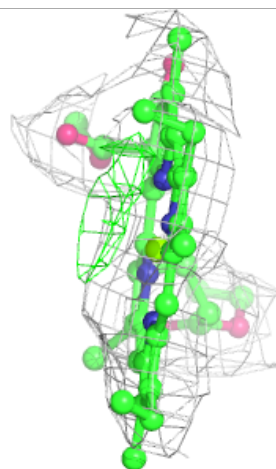
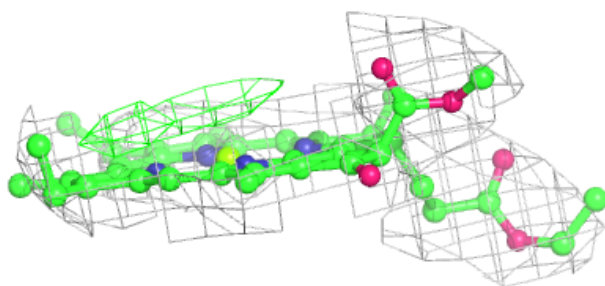
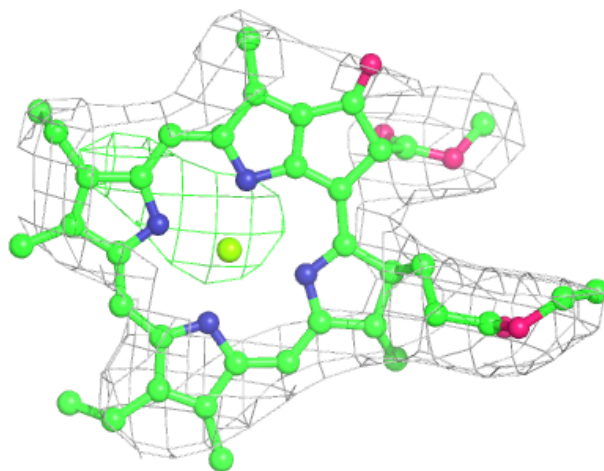
**Electron density around CLA A 1129:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



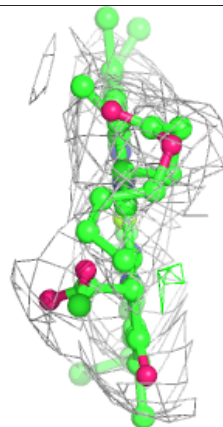
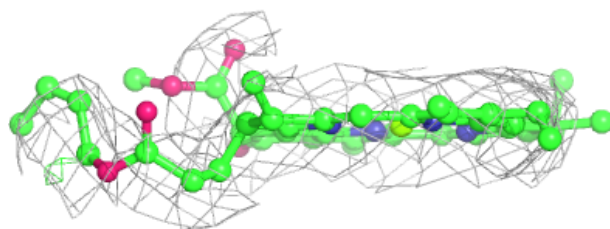
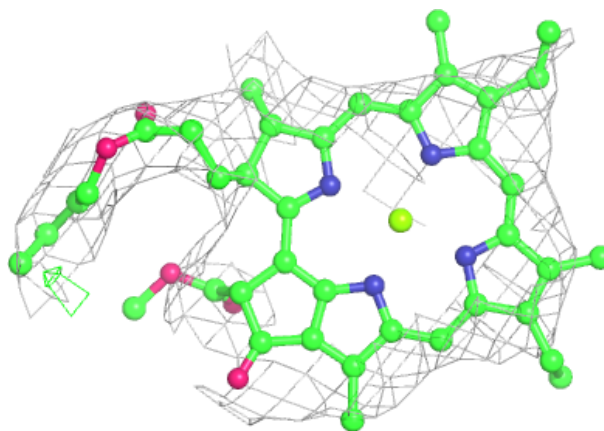
**Electron density around CLA F 1301:**

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



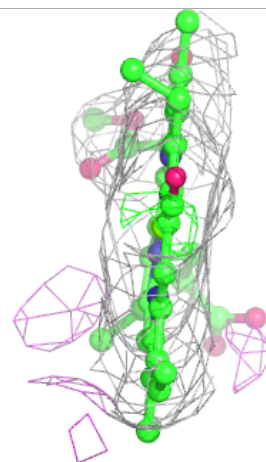
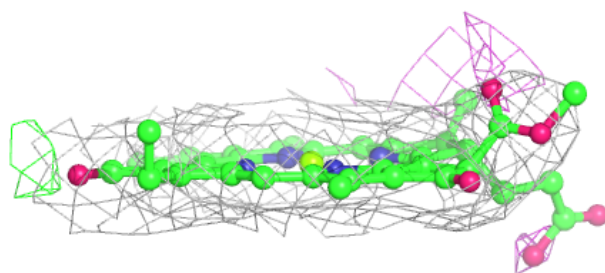
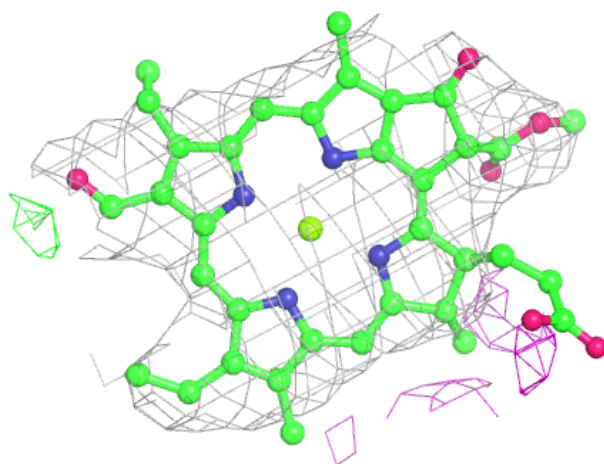
**Electron density around CLA B 1202:**

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



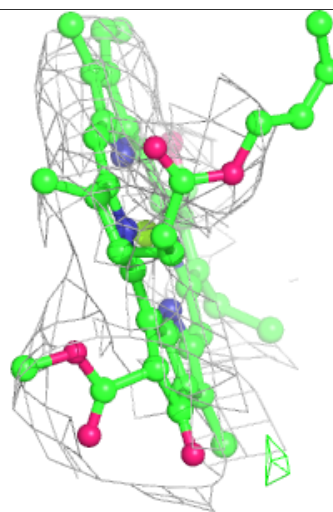
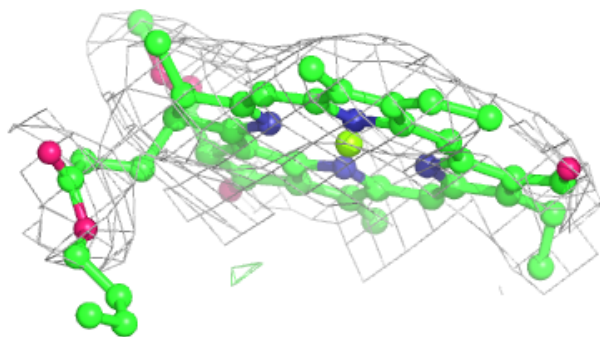
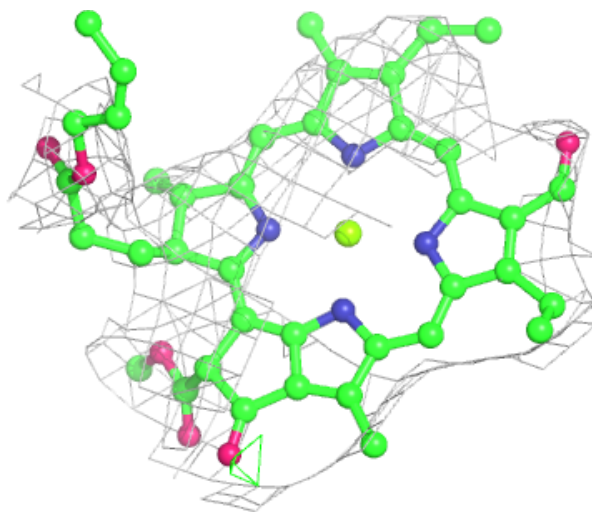
**Electron density around CHL 2 613:**

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



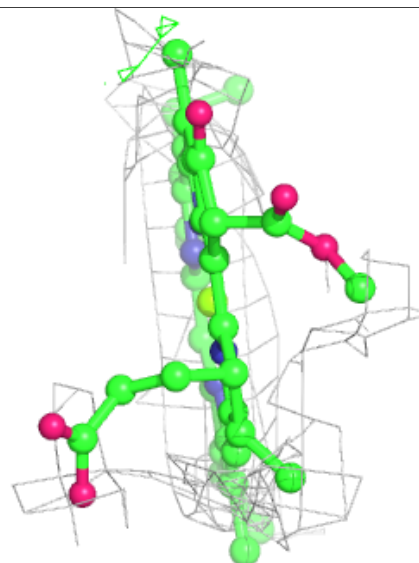
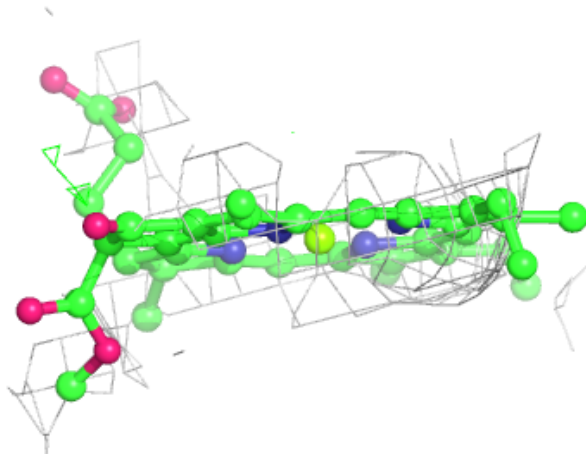
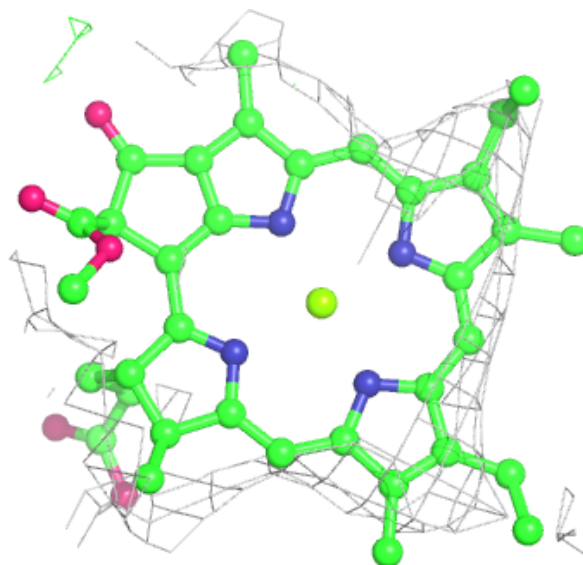
**Electron density around CHL 2 609:**

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



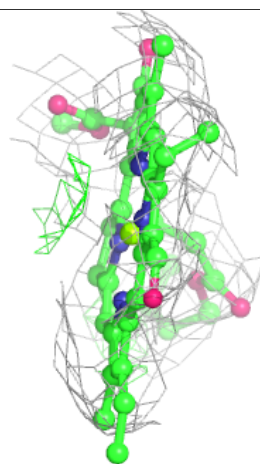
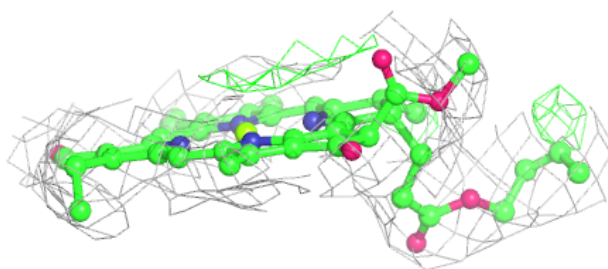
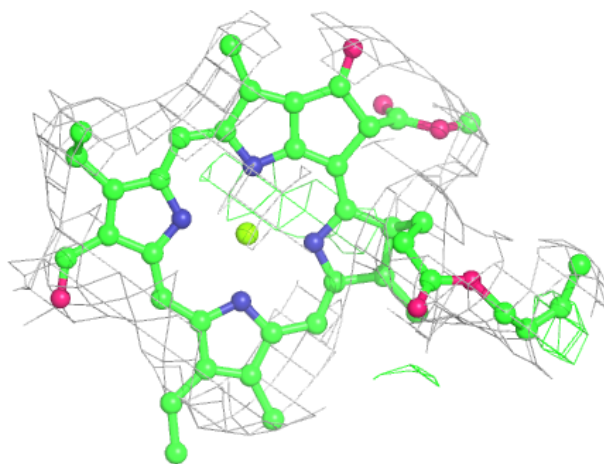
**Electron density around CLA A 1102:**

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



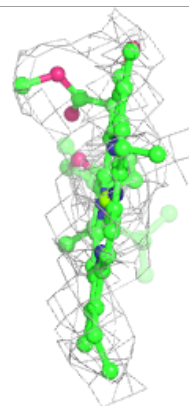
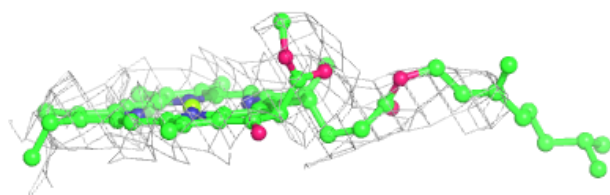
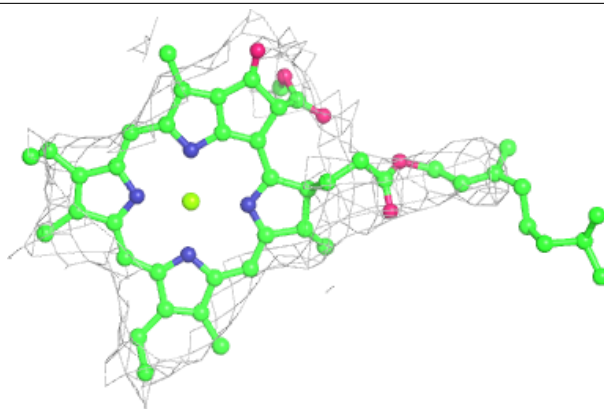
**Electron density around CHL 2 610:**

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



**Electron density around CLA A 1103:**

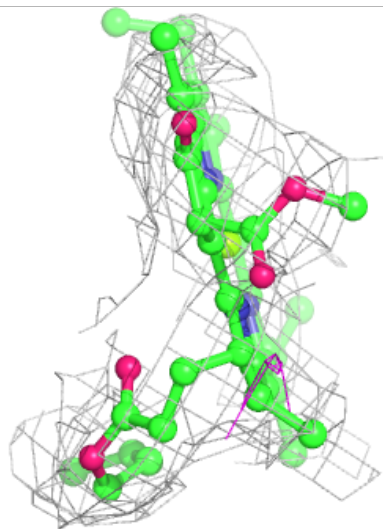
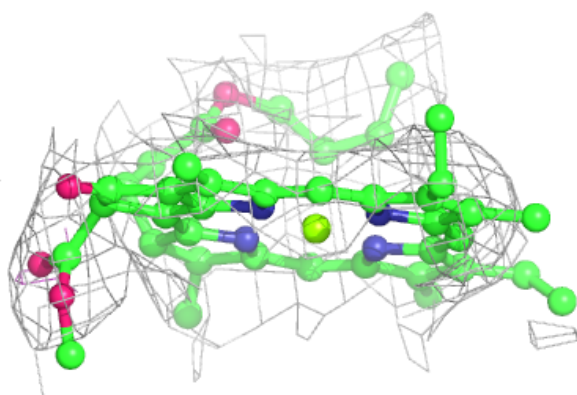
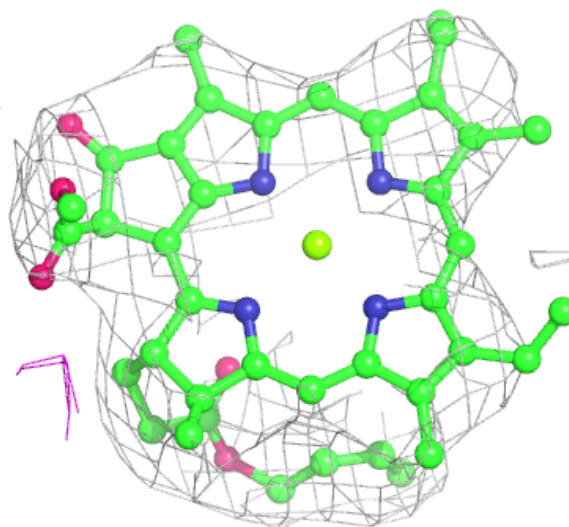
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





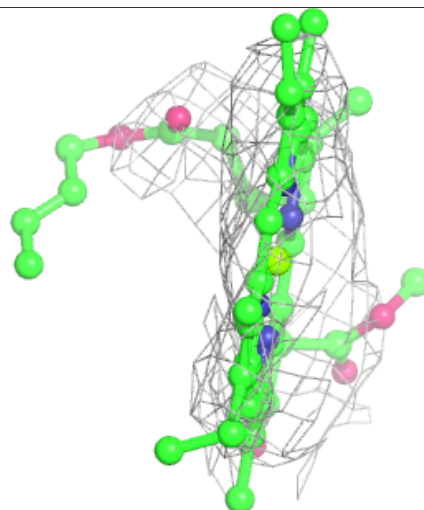
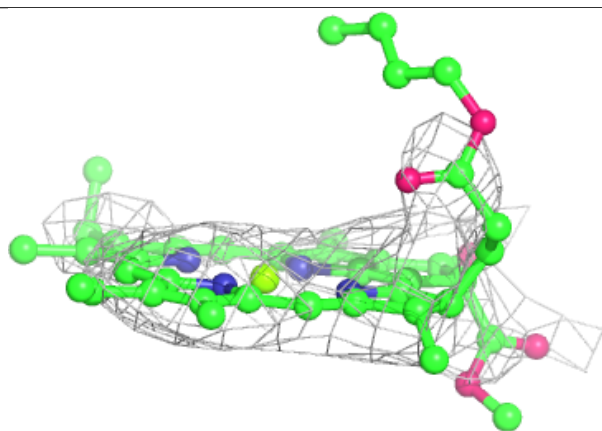
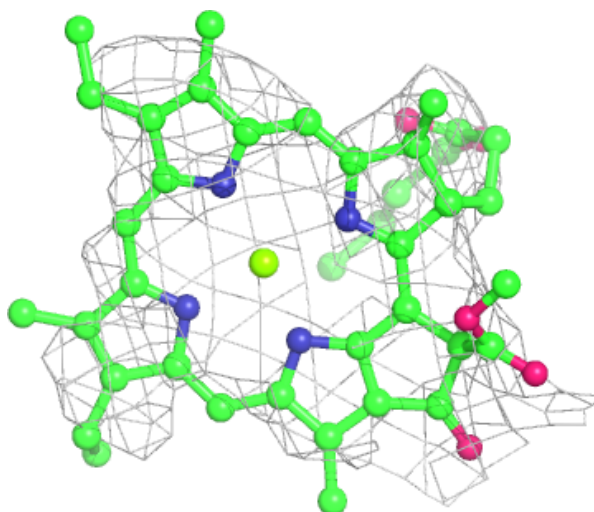
**Electron density around CLA 4 604:**

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



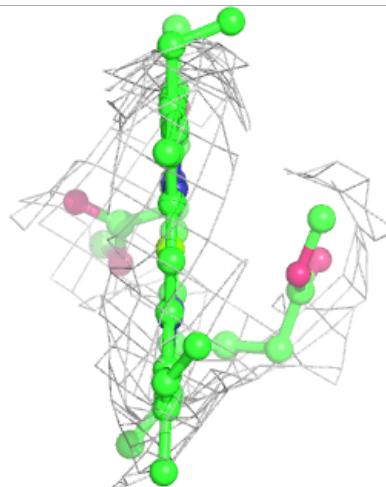
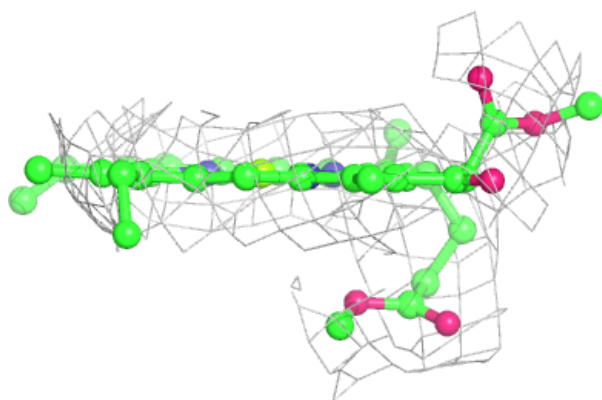
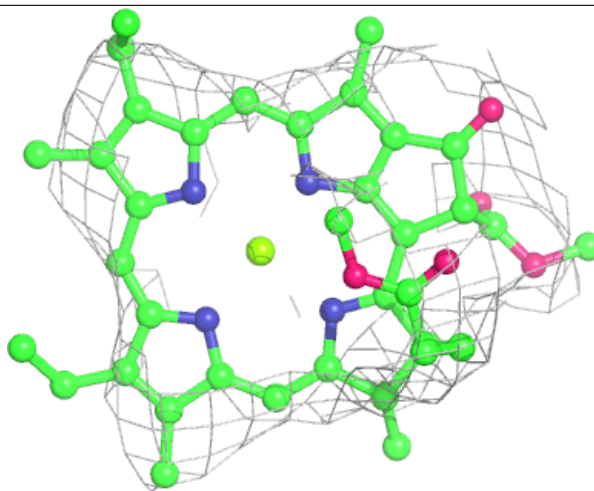
**Electron density around CLA A 1115:**

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



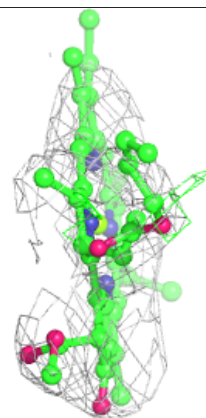
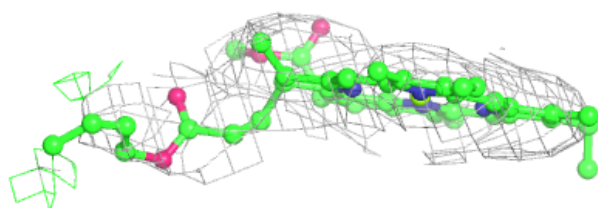
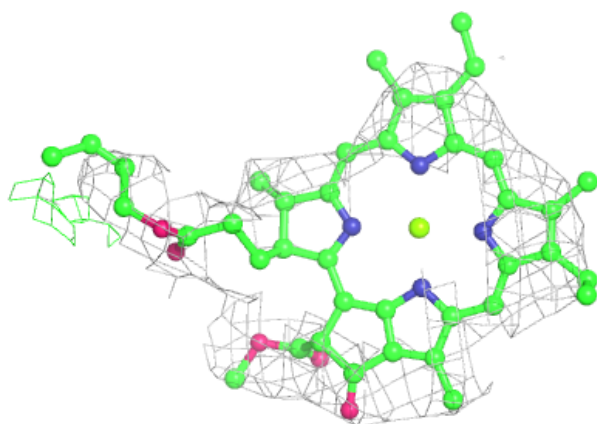
**Electron density around CLA 2 603:**

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

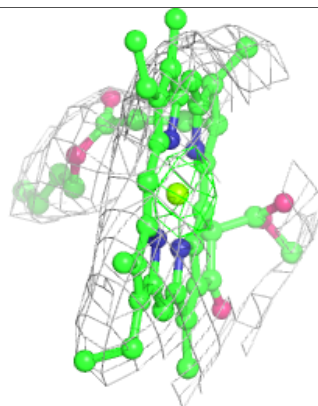
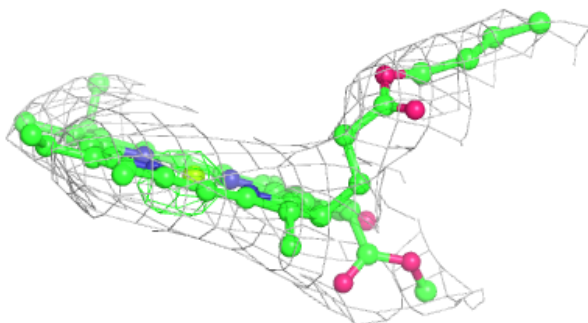
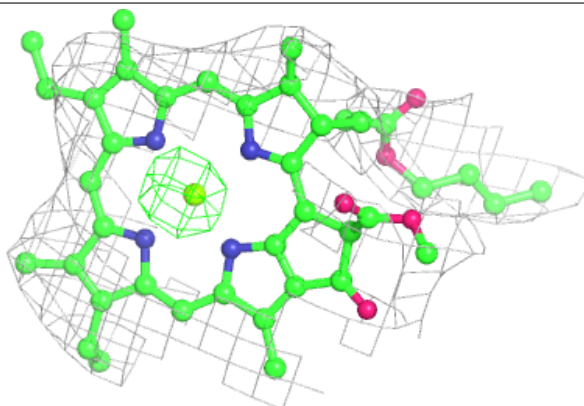


**Electron density around CLA J 1302:**

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

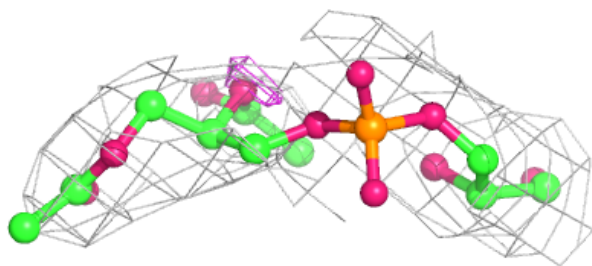
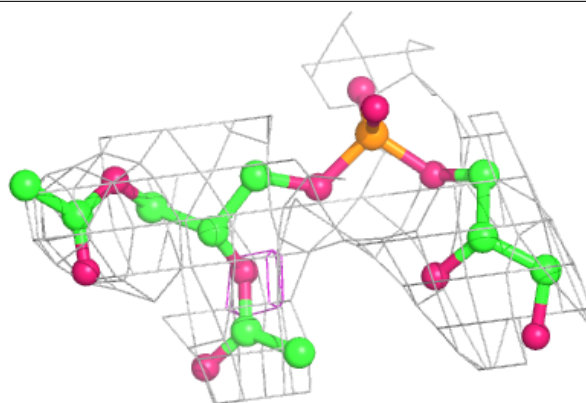
**Electron density around CLA A 1107:**

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

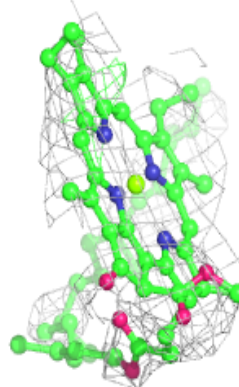
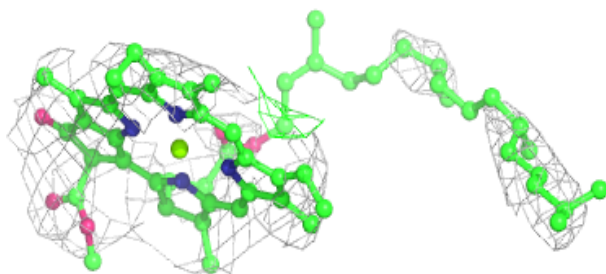
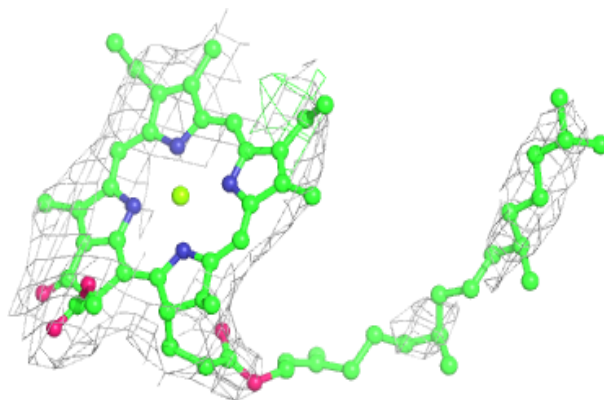


**Electron density around LHG B 5001:**

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

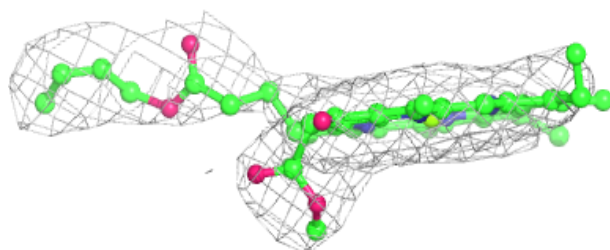
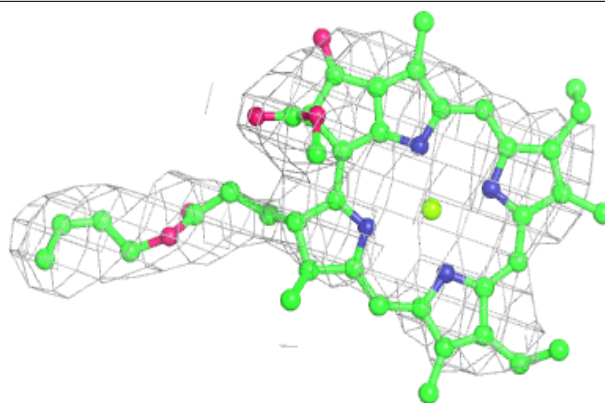
**Electron density around CLA A 1106:**

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

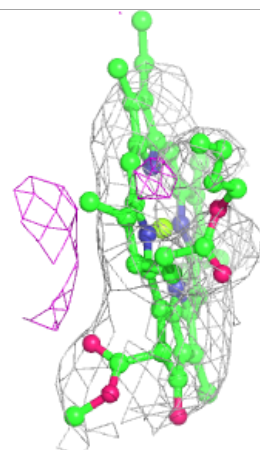
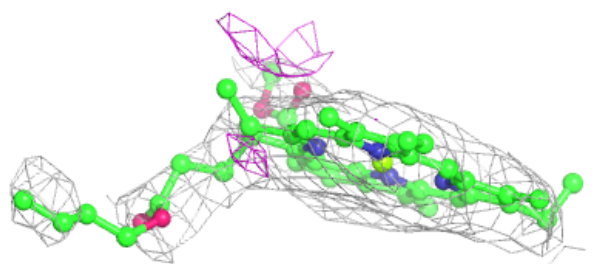
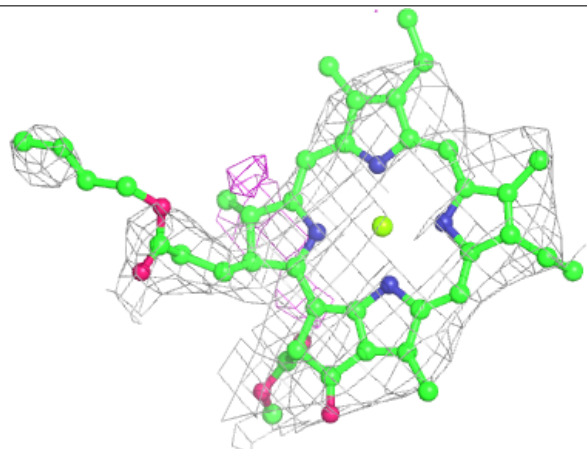


**Electron density around CLA B 1234:**

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

**Electron density around CLA 4 609:**

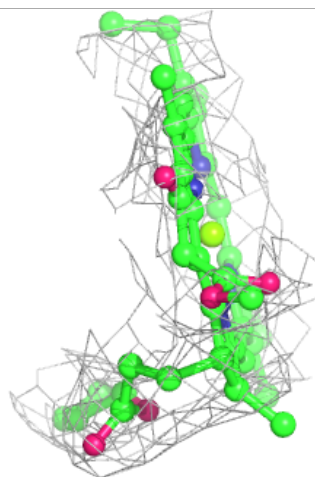
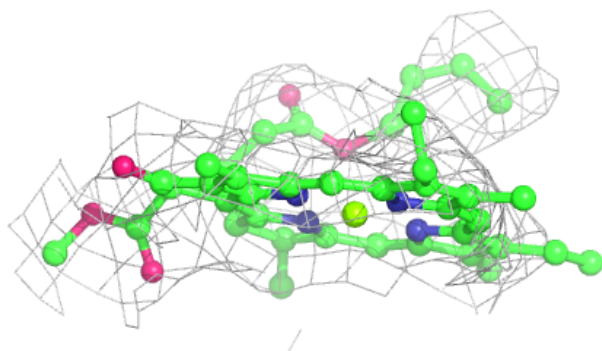
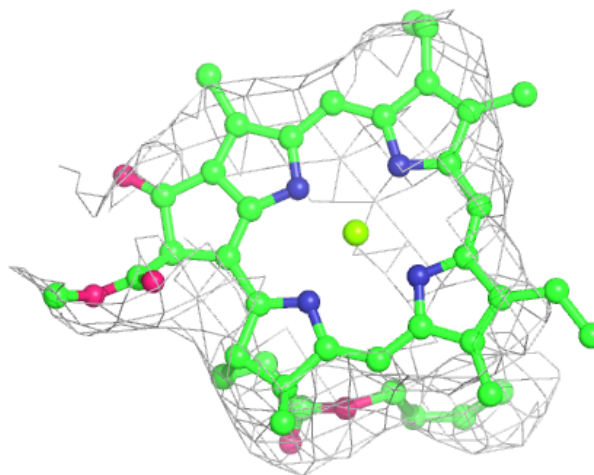
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





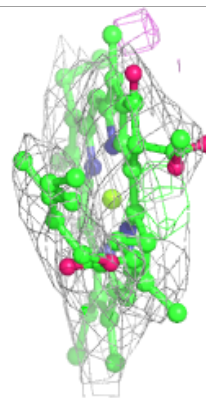
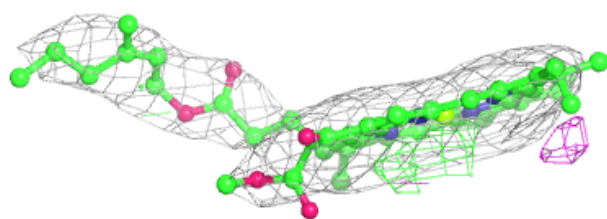
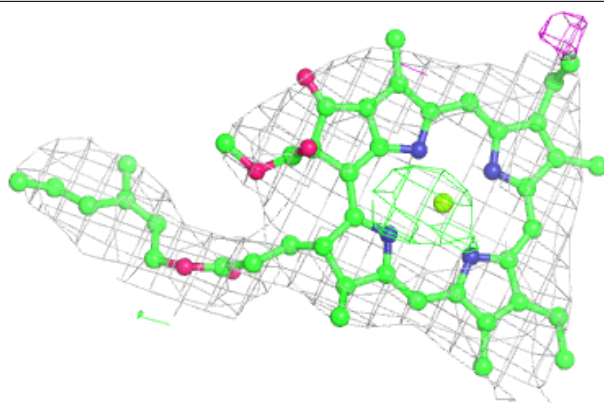
**Electron density around CLA 4 601:**

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



**Electron density around CLA A 1139:**

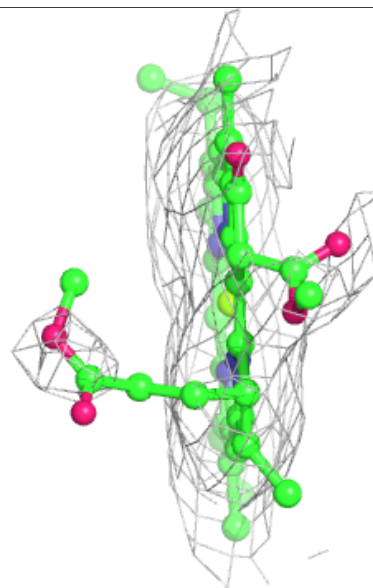
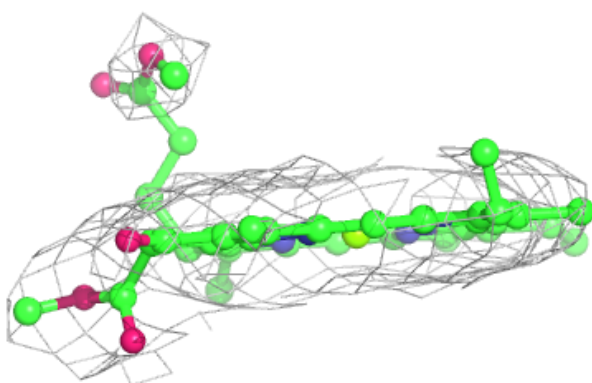
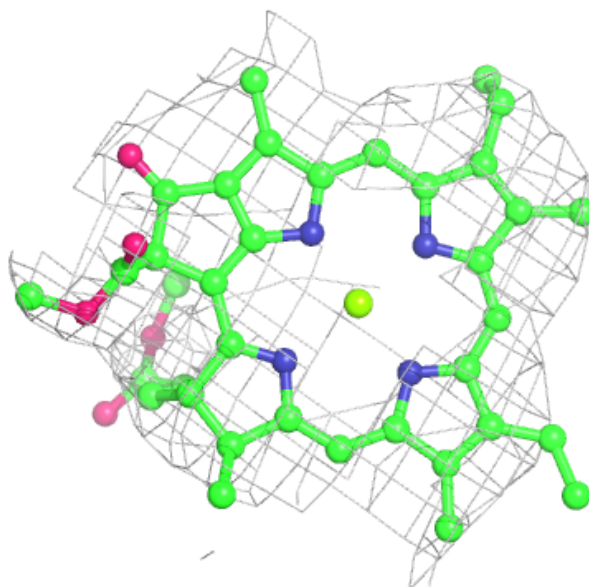
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





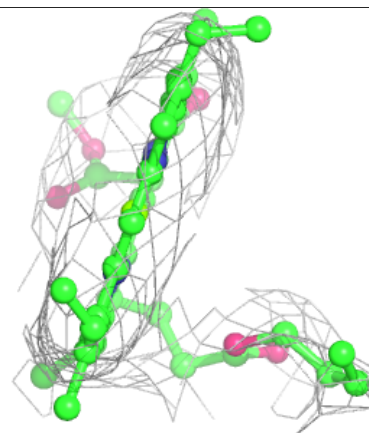
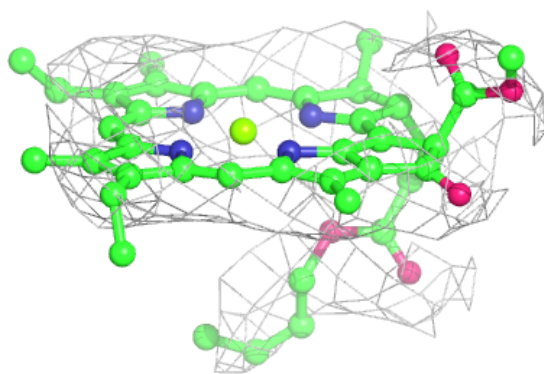
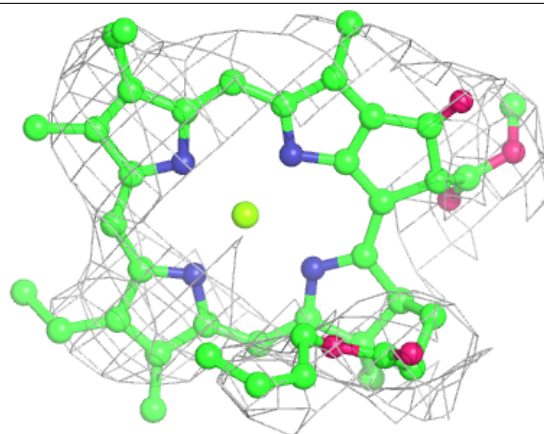
**Electron density around CLA 4 608:**

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



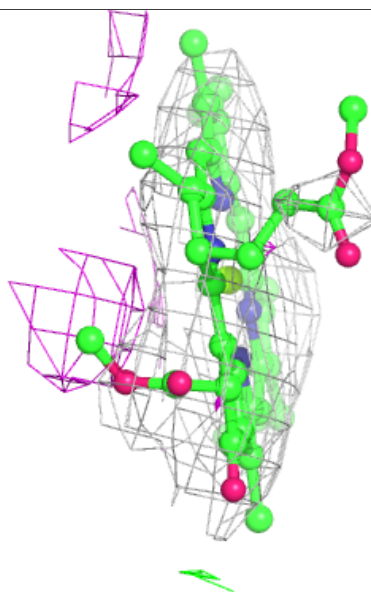
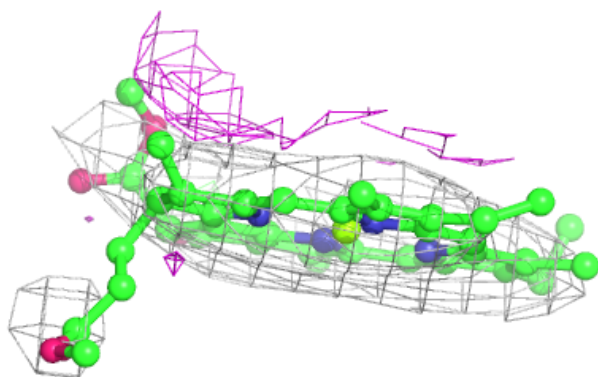
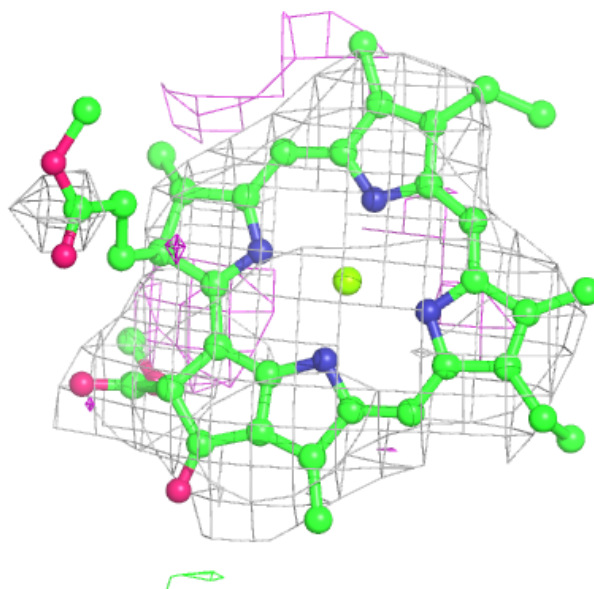
**Electron density around CLA A 1105:**

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



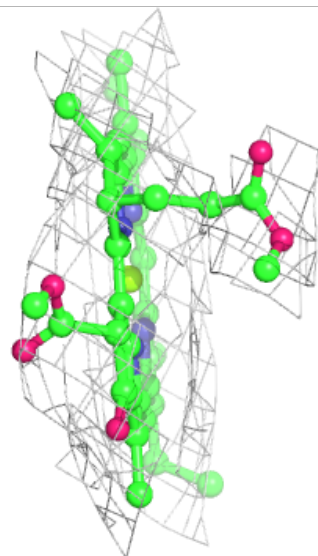
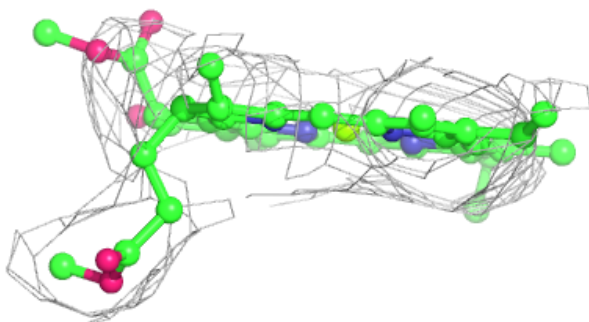
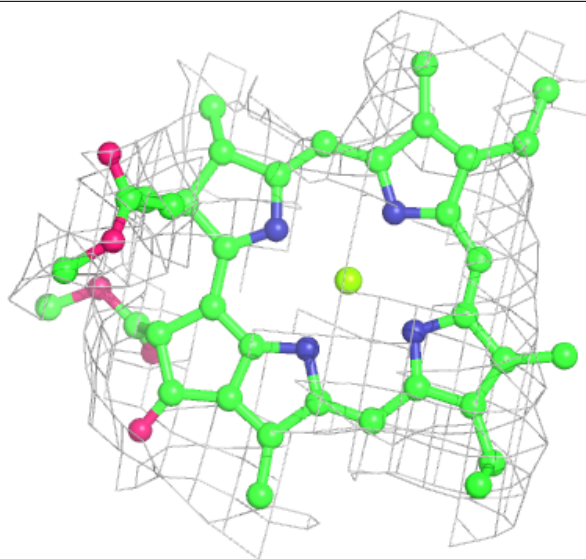
**Electron density around CLA 1 608:**

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



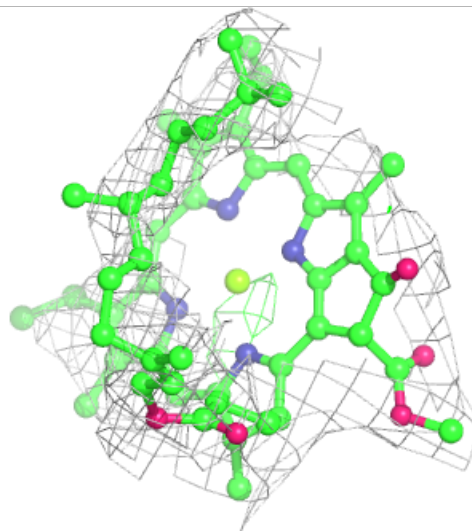
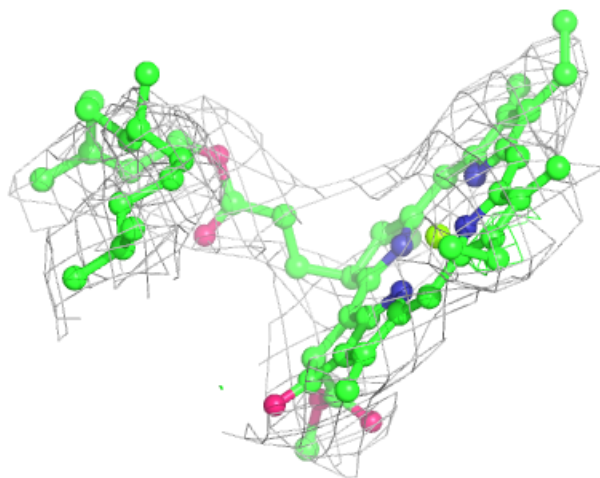
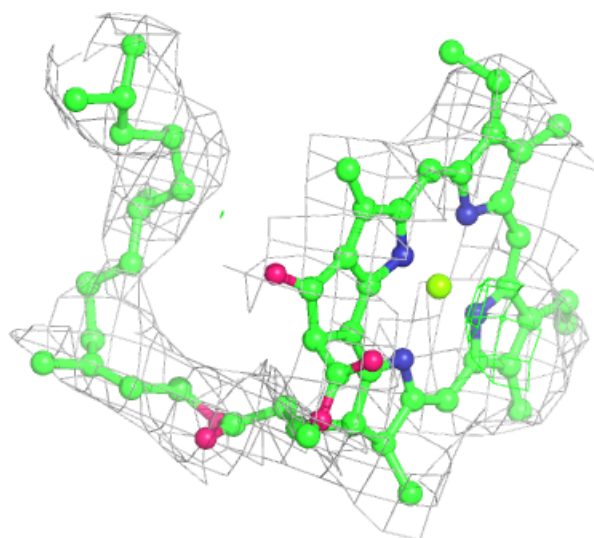
**Electron density around CLA B 1209:**

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



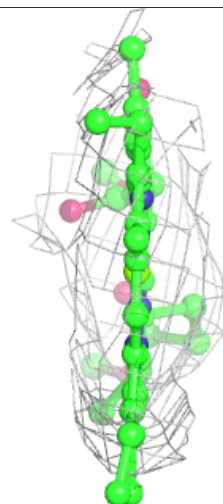
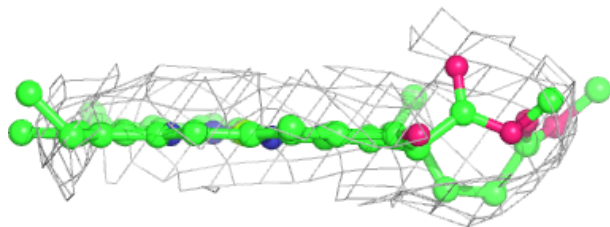
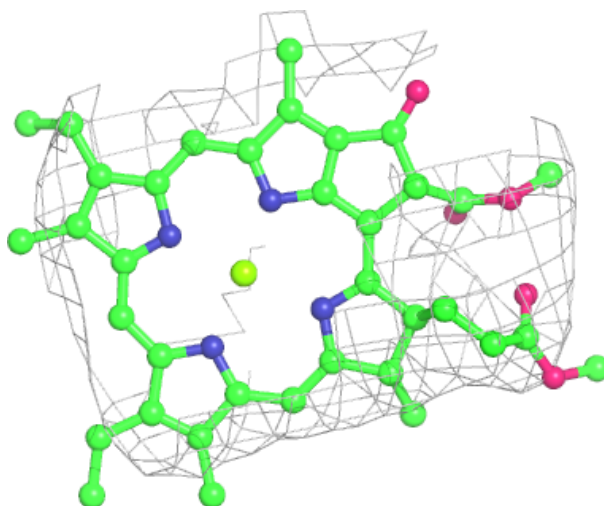
**Electron density around CLA B 1231:**

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



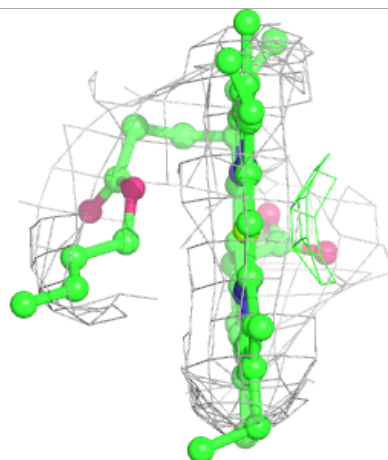
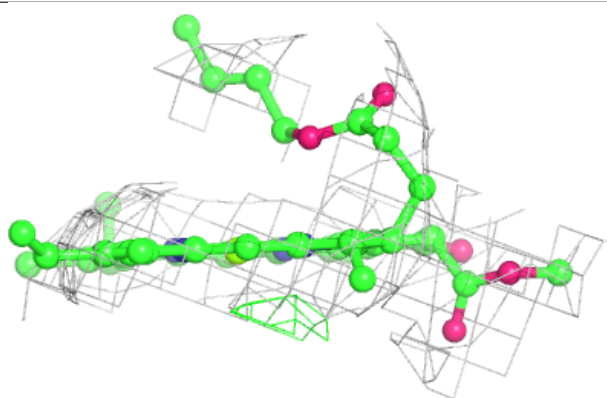
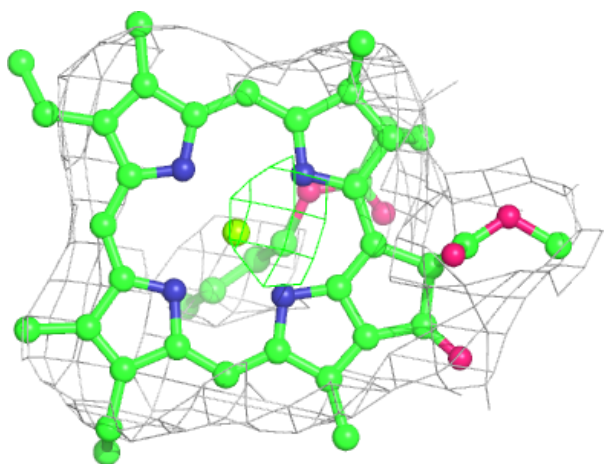
**Electron density around CLA 3 605:**

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



**Electron density around CLA 4 603:**

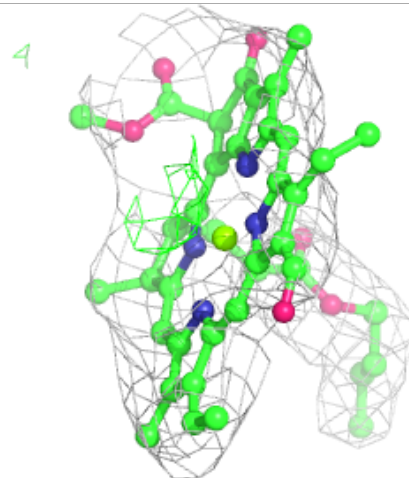
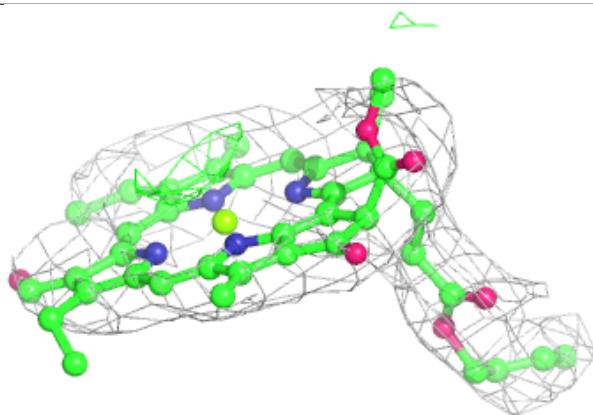
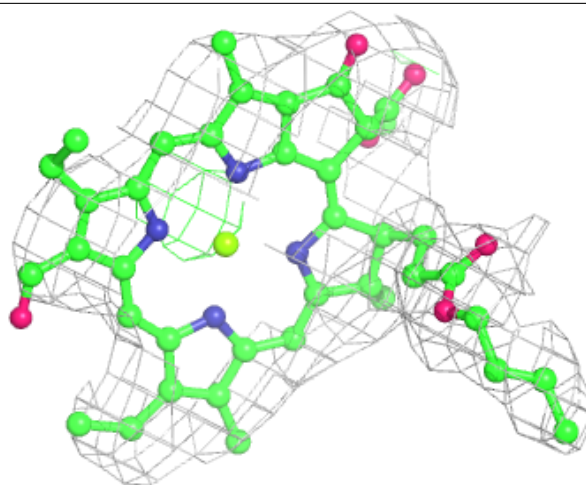
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CHL 4 611:**

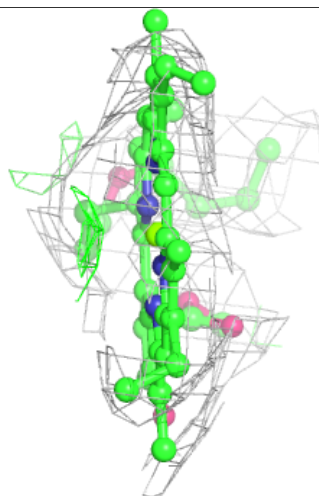
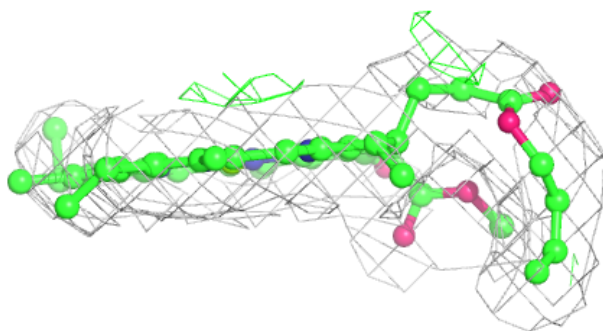
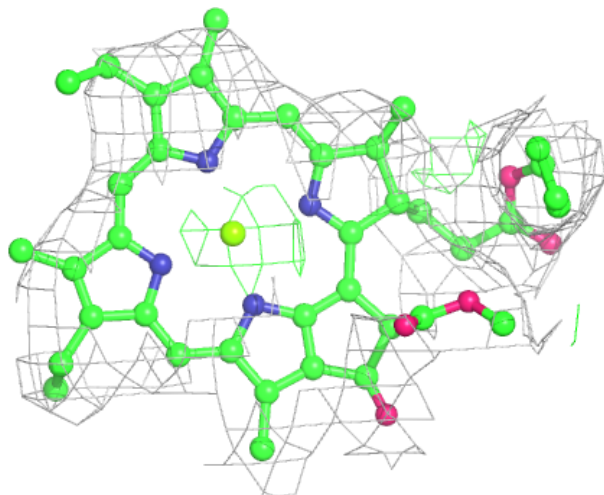
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





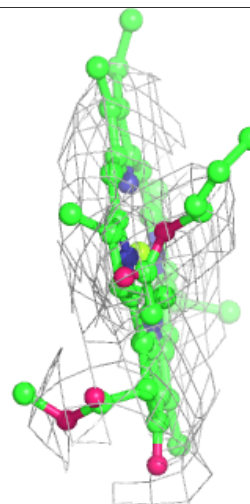
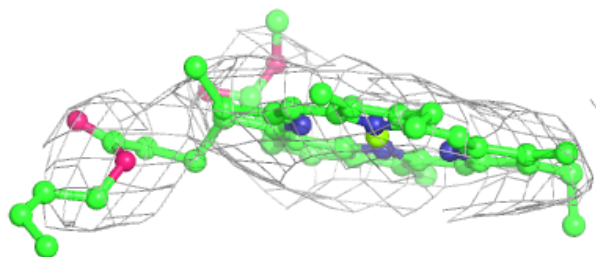
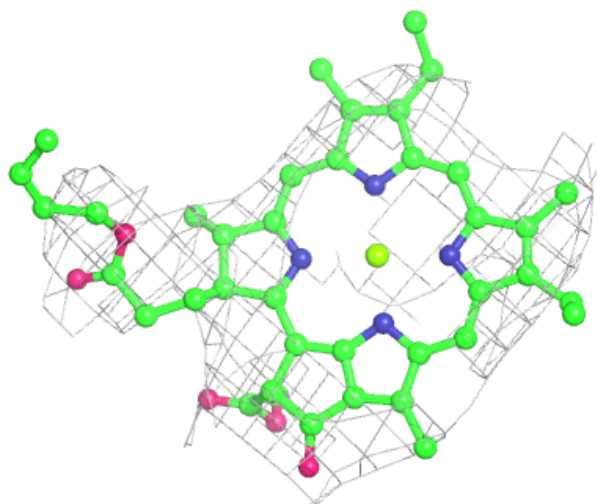
**Electron density around CLA 4 605:**

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



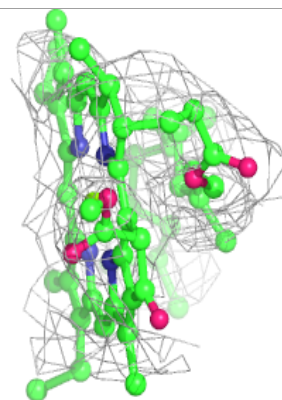
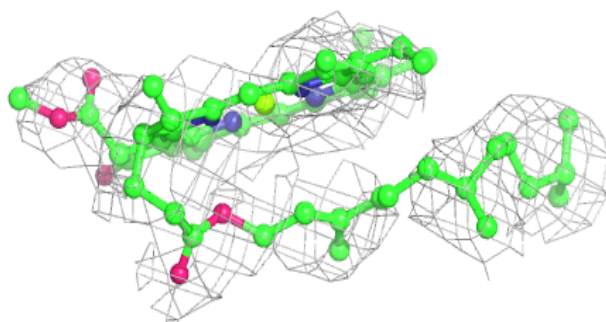
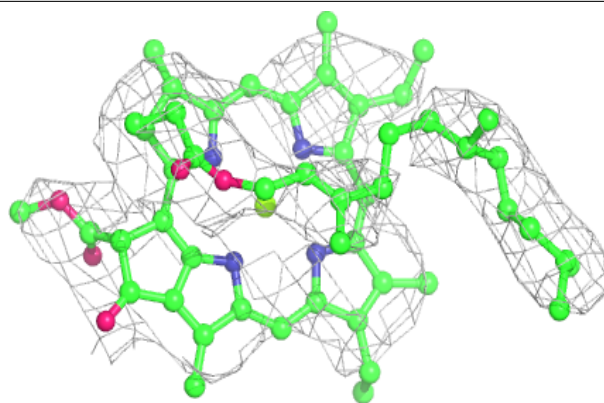
**Electron density around CLA B 1210:**

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



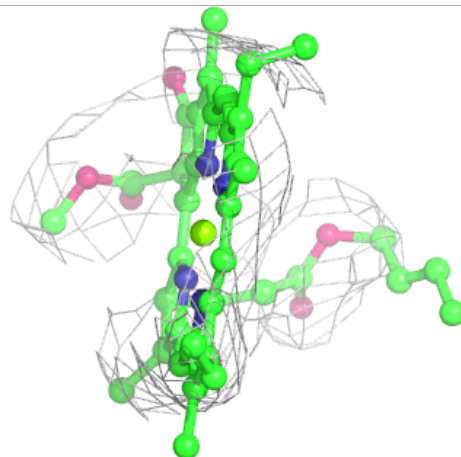
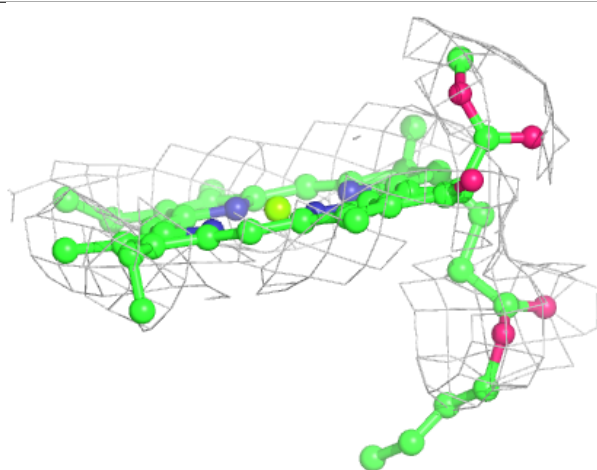
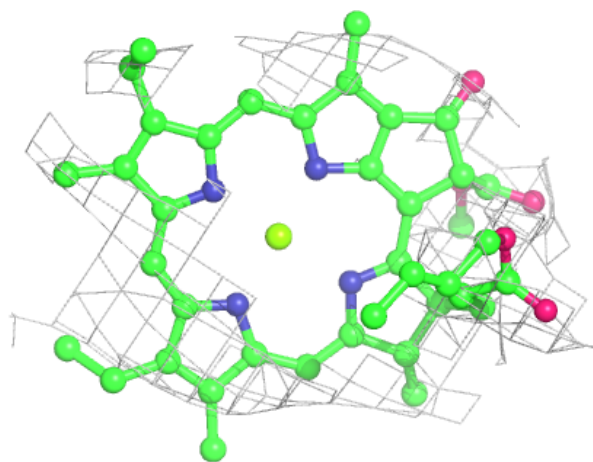
**Electron density around CLA B 1235:**

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



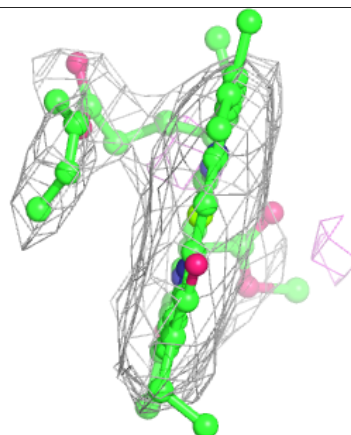
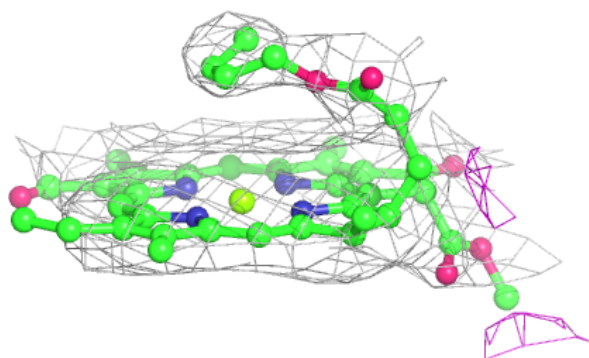
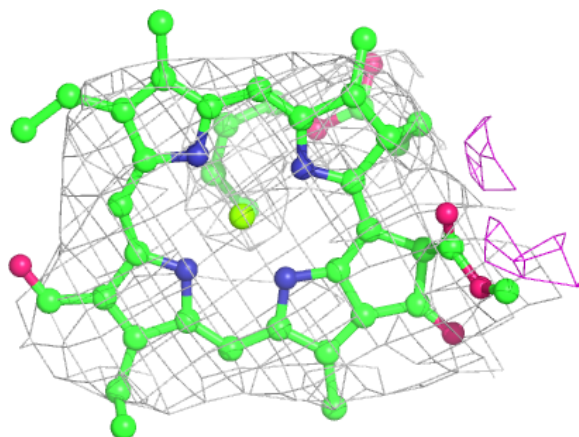
**Electron density around CLA B 1204:**

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

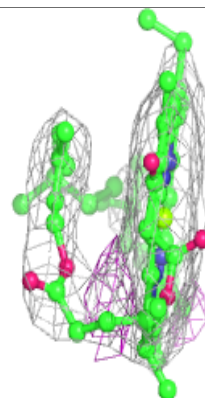
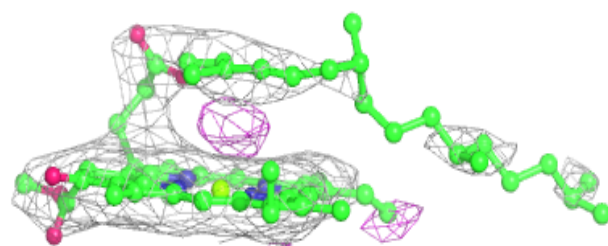
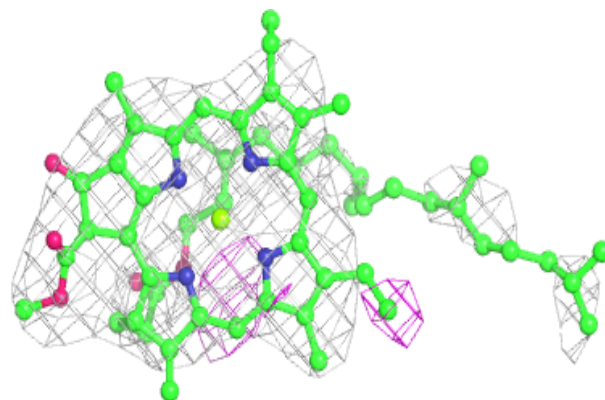


**Electron density around CHL 1 609:**

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

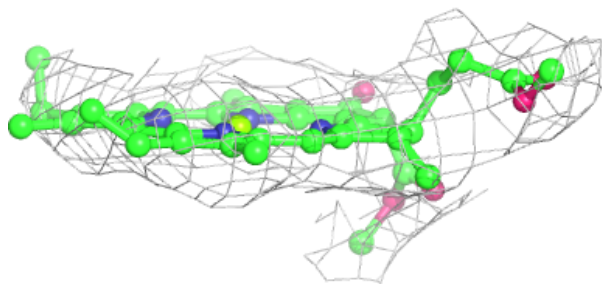
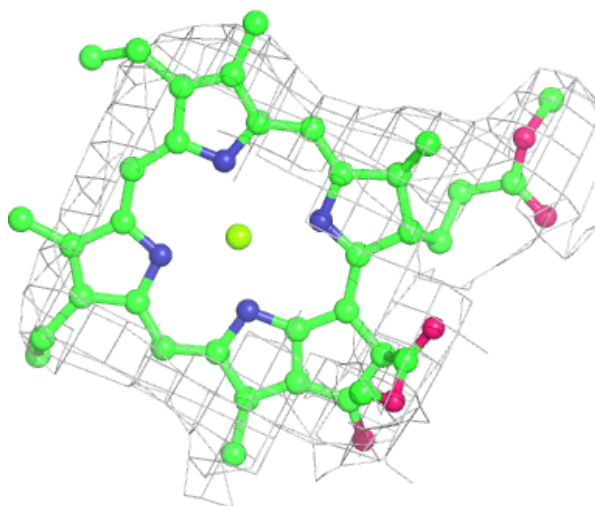
**Electron density around CLA A 1138:**

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



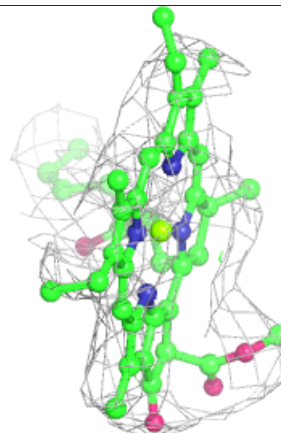
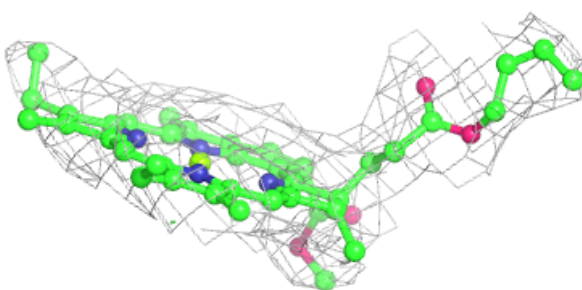
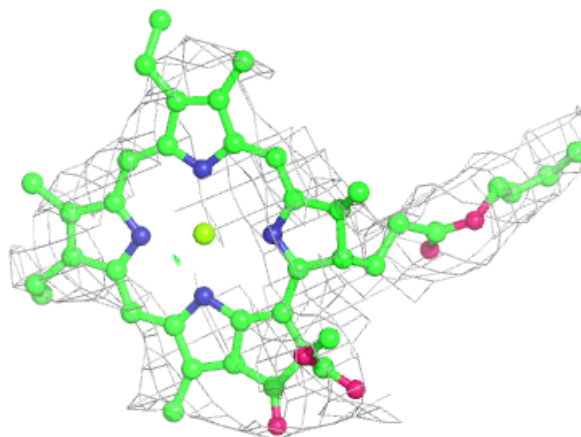
**Electron density around CLA B 1217:**

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



**Electron density around CLA B 1222:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.