



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:42 PM UTC

PDB ID : 4RKU / pdb_00004rku
Title : Crystal structure of plant Photosystem I at 3 Angstrom resolution
Authors : Mazor, Y.; Borovikova, A.; Greenberg, I.; Nelson, N.
Deposited on : 2014-10-14
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

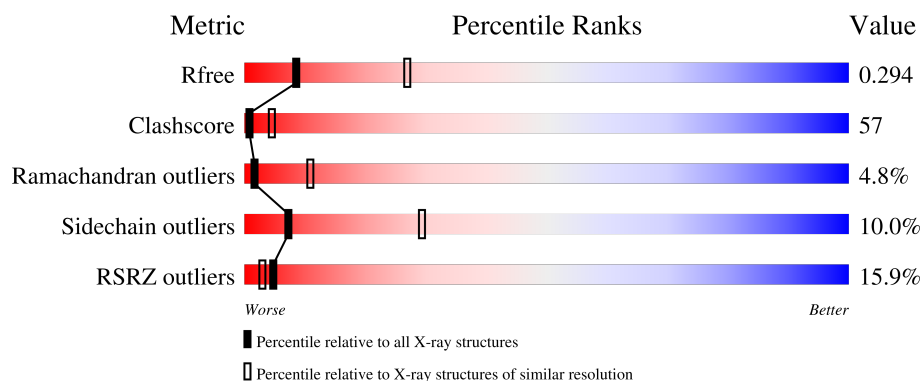
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	721	10% 63% 33% ..
2	B	731	9% 70% 29% .
3	C	80	8% 61% 34% 5%
4	D	137	17% 39% 42% 15% .
5	E	63	5% 44% 40% 13% .

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Mol	Chain	Length	Quality of chain
6	F	152	
7	G	84	
8	H	82	
9	I	26	
10	J	40	
11	K	72	
12	L	163	
13	N	85	
14	1	182	
15	2	199	
16	3	275	
17	4	196	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	LHG	1	1801	-	-	X	-
20	LHG	2	2801	-	-	X	-
21	CLA	1	1001	X	-	X	-
21	CLA	1	1002	X	-	X	-
21	CLA	1	1003	X	-	X	-
21	CLA	1	1004	X	-	X	-
21	CLA	1	1005	X	-	X	-
21	CLA	1	1006	X	-	X	-
21	CLA	1	1007	X	-	X	-
21	CLA	1	1008	X	-	X	-
21	CLA	1	1009	X	-	X	-
21	CLA	1	1010	X	-	X	-
21	CLA	1	1011	X	-	-	-
21	CLA	1	1012	X	-	X	-
21	CLA	1	1013	X	-	X	-
21	CLA	1	1014	X	-	X	-
21	CLA	2	2001	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	2	2002	X	-	X	-
21	CLA	2	2003	X	-	X	-
21	CLA	2	2004	X	-	X	-
21	CLA	2	2005	X	-	X	-
21	CLA	2	2006	X	-	X	-
21	CLA	2	2007	X	-	-	-
21	CLA	2	2008	X	-	X	-
21	CLA	2	2009	X	-	X	-
21	CLA	2	2010	X	-	-	-
21	CLA	2	2011	X	-	X	-
21	CLA	2	2012	X	-	X	-
21	CLA	2	2013	X	-	-	-
21	CLA	2	2014	X	-	-	-
21	CLA	3	3001	X	-	X	-
21	CLA	3	3002	X	-	-	-
21	CLA	3	3003	X	-	-	-
21	CLA	3	3004	X	-	-	-
21	CLA	3	3005	X	-	-	-
21	CLA	3	3006	X	-	-	-
21	CLA	3	3008	X	-	-	-
21	CLA	3	3009	X	-	X	-
21	CLA	3	3010	X	-	-	-
21	CLA	3	3011	X	-	X	-
21	CLA	3	3012	X	-	X	-
21	CLA	3	3013	X	-	-	-
21	CLA	3	3014	X	-	-	-
21	CLA	3	3015	X	-	-	-
21	CLA	3	3016	X	-	-	-
21	CLA	3	3017	X	-	-	-
21	CLA	4	4001	X	-	X	-
21	CLA	4	4002	X	-	X	-
21	CLA	4	4003	X	-	X	-
21	CLA	4	4004	X	-	X	-
21	CLA	4	4005	X	-	X	-
21	CLA	4	4006	X	-	-	-
21	CLA	4	4007	X	-	-	-
21	CLA	4	4008	X	-	X	-
21	CLA	4	4009	X	-	-	-
21	CLA	4	4010	X	-	-	-
21	CLA	4	4011	X	-	-	-
21	CLA	4	4012	X	-	X	-
21	CLA	4	4013	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	4	4014	X	-	X	-
21	CLA	4	4015	X	-	-	-
21	CLA	A	1101	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	-
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	-	-
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1125	X	-	-	-
21	CLA	A	1126	X	-	-	-
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1129	X	-	X	-
21	CLA	A	1130	X	-	-	-
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1141	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1142	X	-	-	-
21	CLA	A	1143	X	-	-	-
21	CLA	A	9012	X	-	-	-
21	CLA	A	9013	X	-	-	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	-
21	CLA	B	1207	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1209	X	-	-	-
21	CLA	B	1210	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	-
21	CLA	B	1213	X	-	X	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	-
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1219	X	-	-	-
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1227	X	-	X	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-
21	CLA	B	1230	X	-	-	-
21	CLA	B	1231	X	-	-	-
21	CLA	B	1234	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	9010	X	-	-	-
21	CLA	B	9022	X	-	-	-
21	CLA	B	9023	X	-	-	-
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	-
21	CLA	F	1303	X	-	-	-
21	CLA	G	1001	X	-	-	-
21	CLA	G	1002	X	-	X	-
21	CLA	H	1000	X	-	-	-
21	CLA	J	1302	X	-	-	-
21	CLA	J	6014	X	-	-	-
21	CLA	J	6015	X	-	-	-
21	CLA	L	1501	X	-	X	-
21	CLA	L	1502	X	-	-	-
21	CLA	L	1503	X	-	-	-
23	CL0	A	9011	X	-	-	-
26	LUT	1	1501	X	-	X	-
26	LUT	1	1502	X	-	X	-
26	LUT	2	2501	X	-	X	-
26	LUT	2	2502	X	-	X	-
26	LUT	4	4501	X	-	X	-
26	LUT	4	4502	X	-	X	-
27	NEX	4	4503	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 34540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5675	3717	968	972	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	GLY	conflict	UNP P05310
A	627	SER	THR	conflict	UNP P05310
A	639	GLY	ALA	conflict	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5834	3833	989	998	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	LEU	ILE	conflict	UNP P05311
B	273	MET	VAL	conflict	UNP P05311
B	471	SER	THR	conflict	UNP P05311
B	476	VAL	ILE	conflict	UNP P05311
B	477	LEU	PRO	conflict	UNP P05311
B	483	SER	GLY	conflict	UNP P05311
B	491	SER	ASN	conflict	UNP P05311
B	603	GLN	ARG	conflict	UNP P05311
B	635	TYR	ILE	conflict	UNP P05311

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	137	Total	C	N	O	S	0	0	0
			1070	685	187	195	3			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV B, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total	C	N	O	0	0	0
			507	321	89	97			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	152	Total	C	N	O	S	0	0	0
			1196	776	206	212	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	0	0	0
			639	414	107	118			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	82	Total	C	N	O	0	0	0
			628	415	95	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	26	Total	C	N	O	S	0	0	0
			197	137	29	30	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	40	Total	C	N	O	0	0	0
			316	214	49	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	66	Total	C	N	O	S	0	0	0
			459	291	78	87	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	52	SER	PRO	conflict	UNP E1C9L3
K	55	VAL	LEU	conflict	UNP E1C9L3
K	59	ALA	THR	conflict	UNP E1C9L3
K	62	THR	SER	conflict	UNP E1C9L3
K	88	ALA	VAL	conflict	UNP E1C9L3
K	111	THR	VAL	conflict	UNP E1C9L3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	163	Total	C	N	O	S	0	0	0
			1214	800	195	218	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			684	438	114	128	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	86	SER	GLY	conflict	UNP E1C9K7
N	88	PHE	ILE	conflict	UNP E1C9K7
N	89	ASP	GLU	conflict	UNP E1C9K7
N	90	ALA	GLU	conflict	UNP E1C9K7
N	97	ALA	THR	conflict	UNP E1C9K7
N	110	SER	THR	conflict	UNP E1C9K7
N	121	GLN	GLU	conflict	UNP E1C9K7
N	124	THR	SER	conflict	UNP E1C9K7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	146	ILE	LEU	conflict	UNP E1C9K7
N	148	GLU	ASP	conflict	UNP E1C9K7
N	151	GLU	ASP	conflict	UNP E1C9K7
N	160	PHE	TYR	conflict	UNP E1C9K7

- Molecule 14 is a protein called Chlorophyll a-b binding protein 6A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	171	Total	C	N	O	S	0	0	0
			1271	823	218	226	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	146	Total	C	N	O	S	0	0	0
			1116	726	189	198	3			

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	151	Total	C	N	O	S	0	0	0
			1118	730	184	199	5			

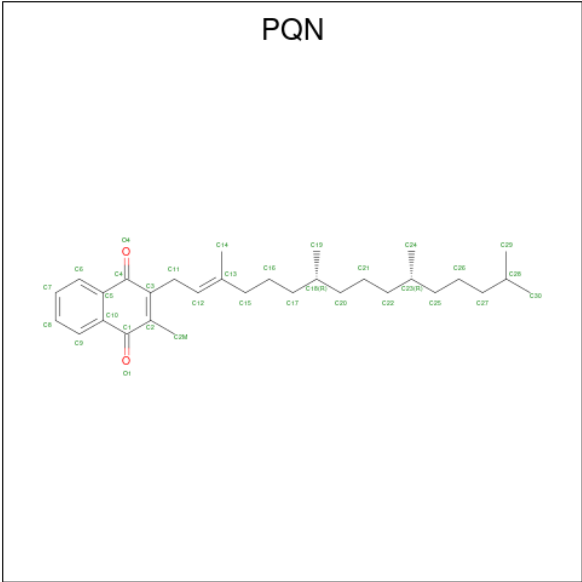
- Molecule 17 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	196	Total	C	N	O	S	0	0	0
			1439	934	242	260	3			

There are 2 discrepancies between the modelled and reference sequences:

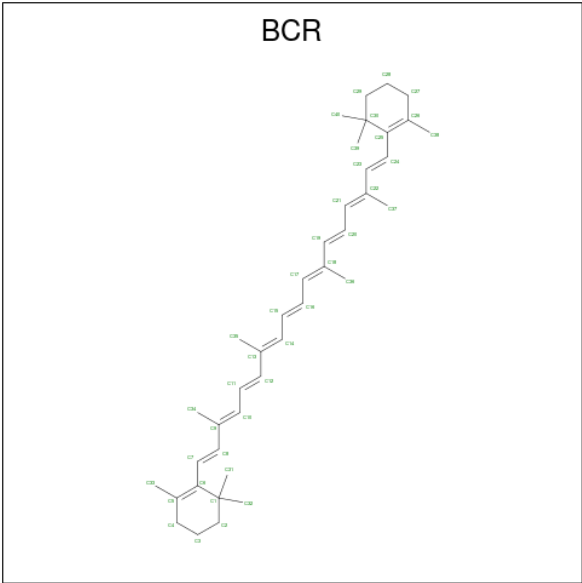
Chain	Residue	Modelled	Actual	Comment	Reference
4	129	ASP	ALA	conflict	UNP Q9SQL2
4	151	PHE	SER	conflict	UNP Q9SQL2

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 19 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



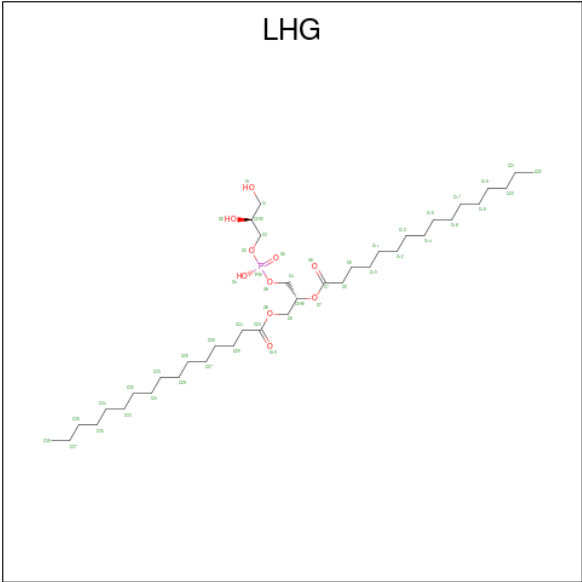
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C		0
			40	40		
19	A	1	Total	C		0
			40	40		

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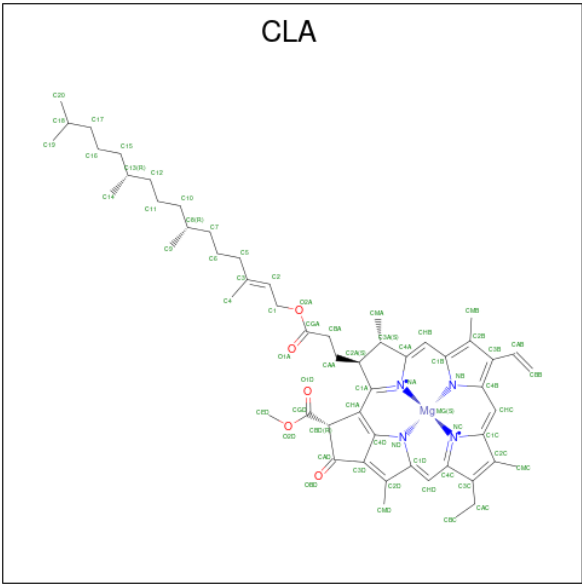
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 25 25	0	0
19	F	1	Total C 40 40	0	0
19	F	1	Total C 40 40	0	0
19	G	1	Total C 40 40	0	0
19	I	1	Total C 40 40	0	0
19	I	1	Total C 40 40	0	0
19	J	1	Total C 40 40	0	0
19	J	1	Total C 40 40	0	0
19	L	1	Total C 40 40	0	0
19	L	1	Total C 40 40	0	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			49	38	10	1		
20	A	1	Total	C	O	P	0	0
			49	38	10	1		
20	B	1	Total	C	O	P	0	0
			49	38	10	1		
20	1	1	Total	C	O	P	0	0
			49	38	10	1		
20	2	1	Total	C	O	P	0	0
			36	25	10	1		

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	F	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	F	1	Total 64	C 55	Mg 1	N 4	O 4	0	0
21	G	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	G	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	H	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
21	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
21	J	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	L	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
21	1	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N		0	0
			27	22	1	4			
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			59	50	1	4	4		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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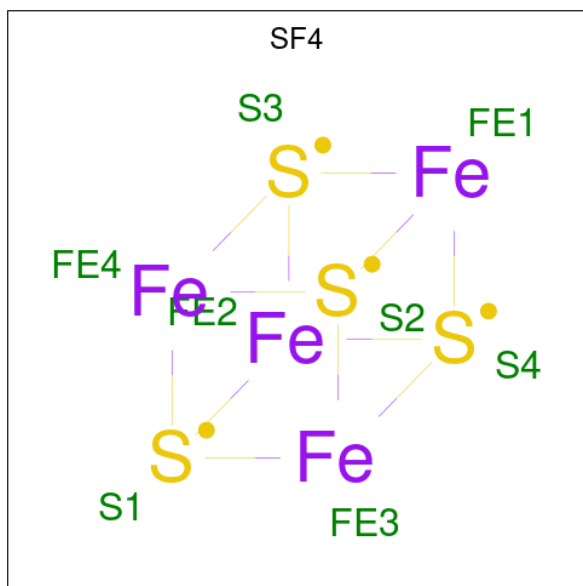
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

- Molecule 22 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



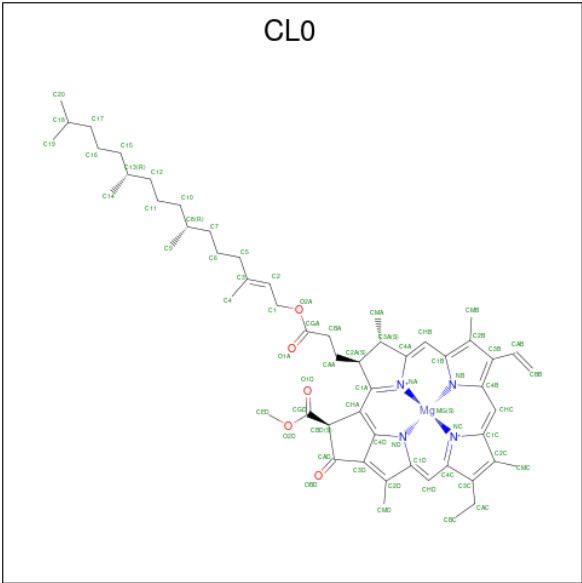
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	Fe	S	0	0
			8	4	4		
22	C	1	Total	Fe	S	0	0
			8	4	4		

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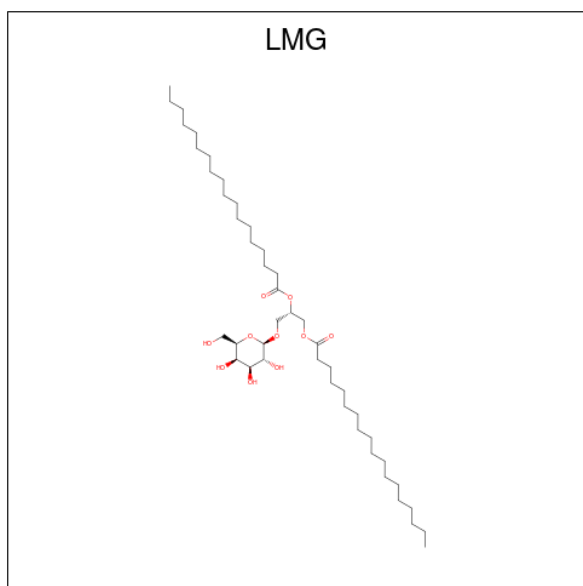
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 23 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



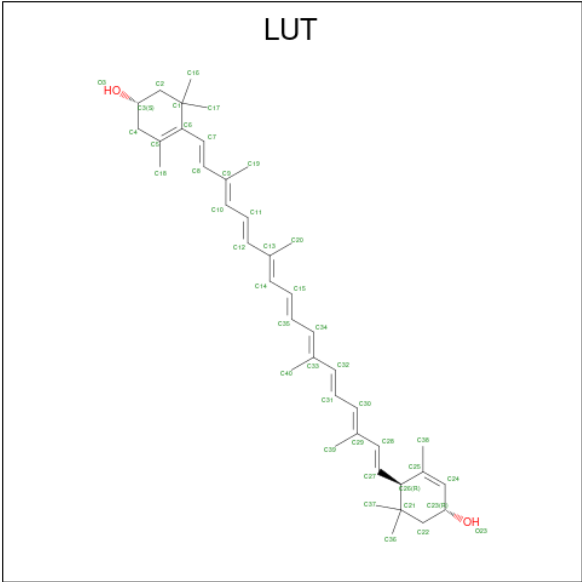
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			61	46	15		

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



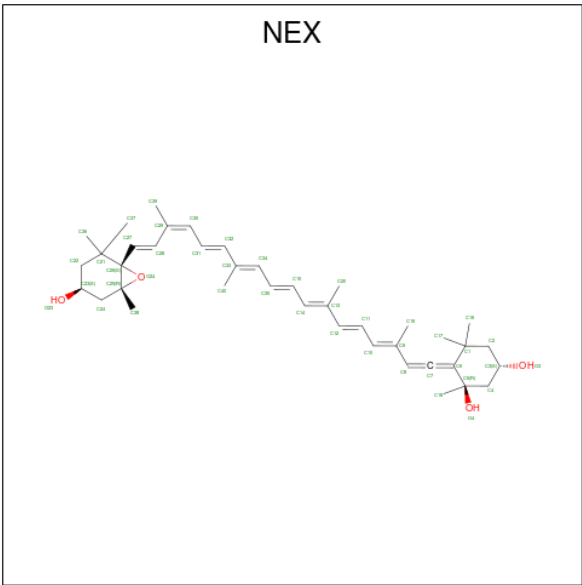
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	G	1	Total	C	O	0	0
			23	13	10		
25	J	1	Total	C	O	0	0
			35	25	10		

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



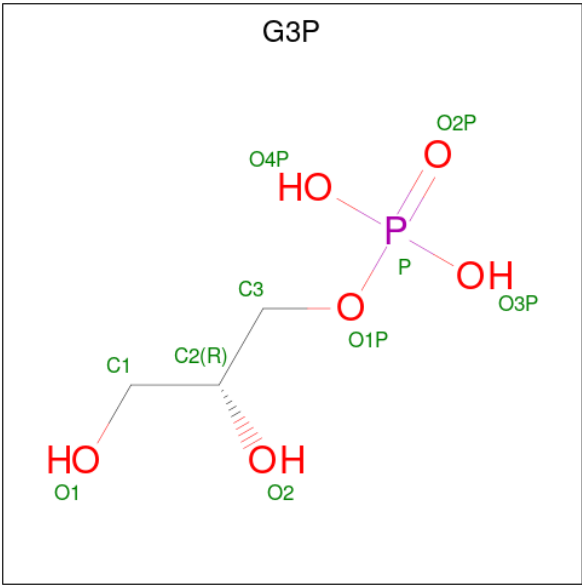
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	1	1	Total	C	O	0	0
			42	40	2		
26	1	1	Total	C	O	0	0
			42	40	2		
26	2	1	Total	C	O	0	0
			42	40	2		
26	2	1	Total	C	O	0	0
			42	40	2		
26	4	1	Total	C	O	0	0
			42	40	2		
26	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 27 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1, 3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 28 is SN-GLYCEROL-3-PHOSPHATE (CCD ID: G3P) (formula: $C_3H_9O_6P$).

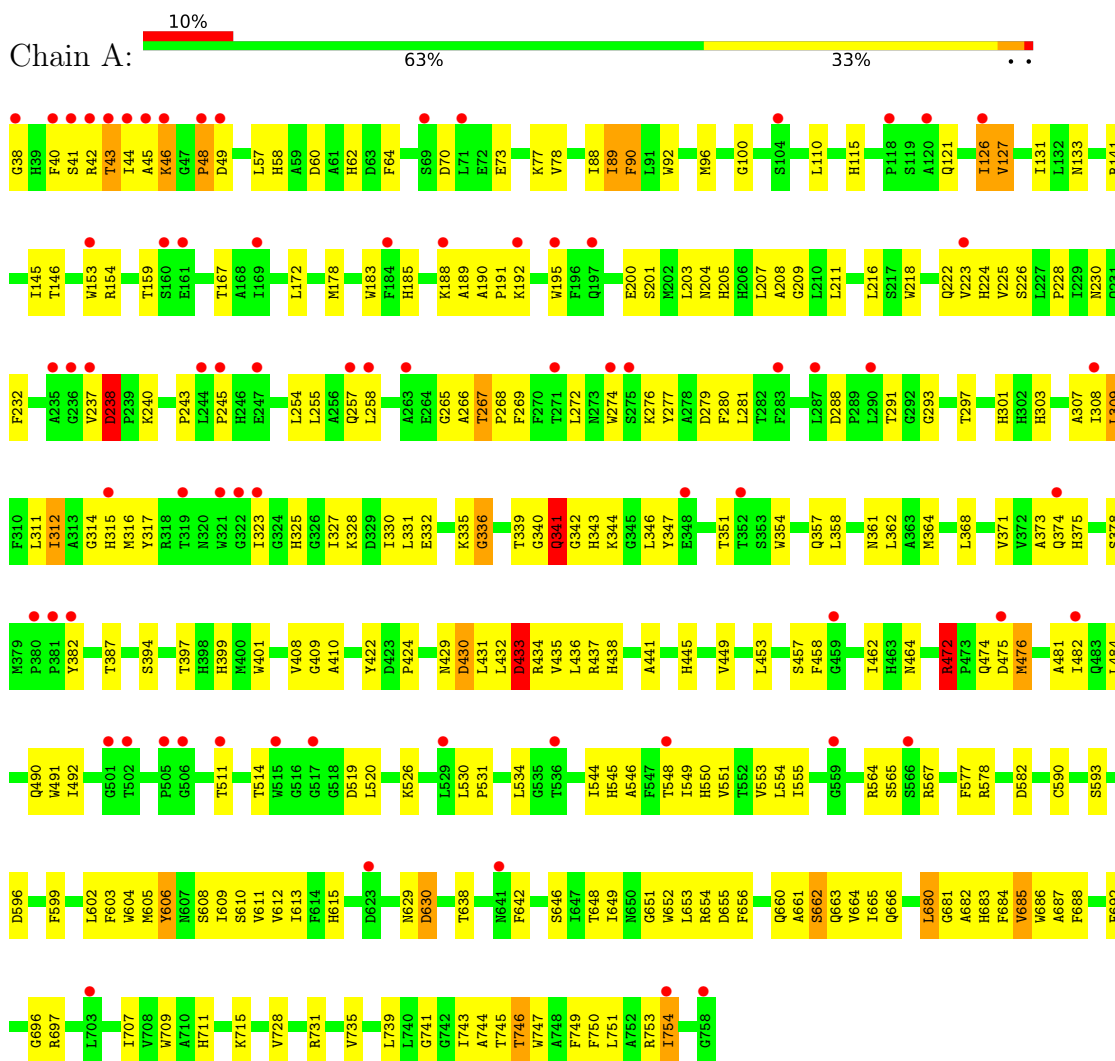


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	4	1	Total	C	O	P	0	0
			10	3	6	1		

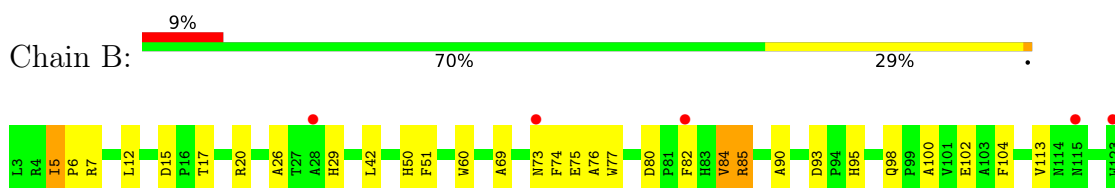
3 Residue-property plots

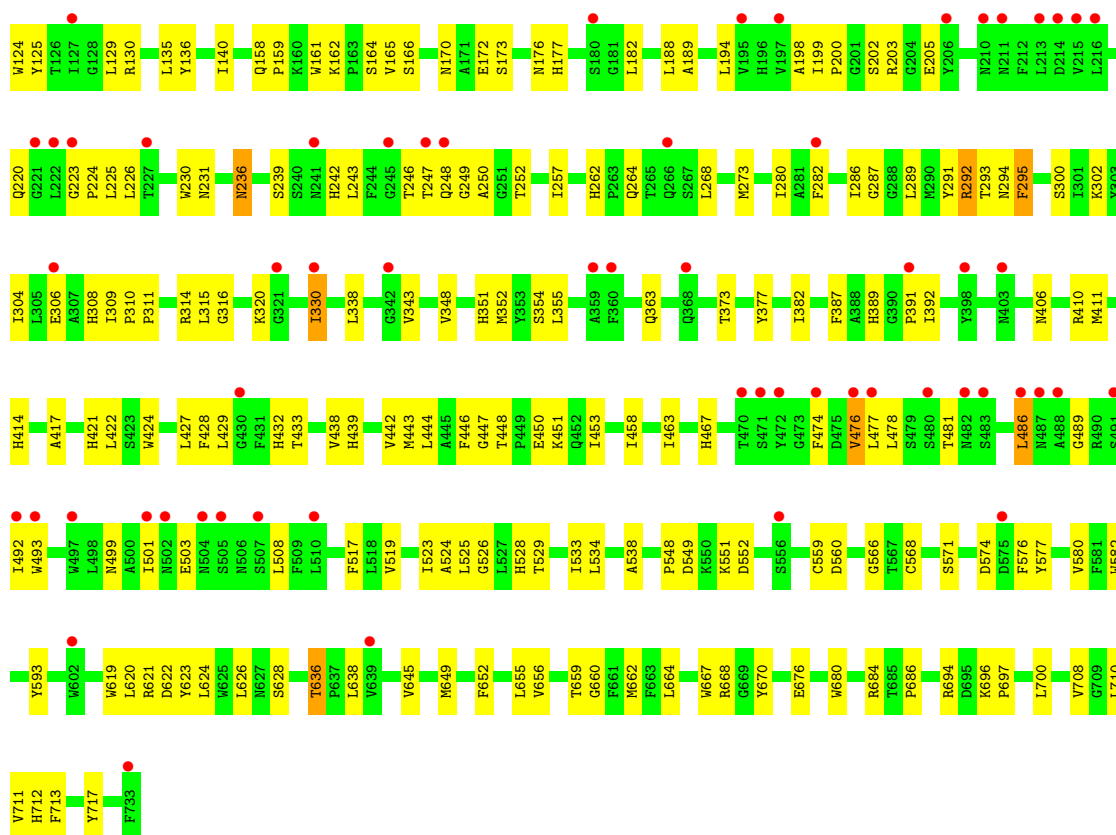
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

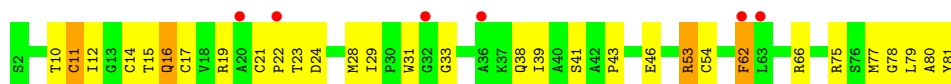


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

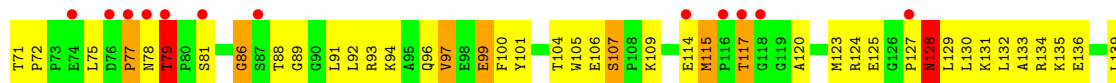
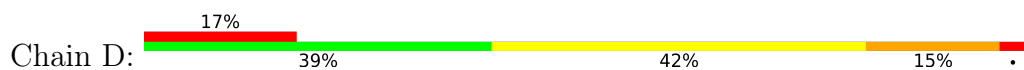




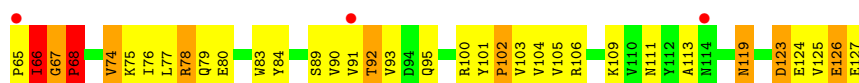
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit II, chloroplastic



• Molecule 5: Photosystem I reaction center subunit IV B, chloroplastic



- Chain F: 

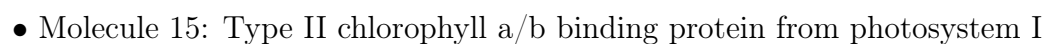
- Chain G:
-

- Chain H:
-
- | Amino Acid Type | Percentage |
|-----------------|------------|
| 35% | 35% |
| 39% | 39% |
| 37% | 37% |
| 21% | 21% |

- Chain I: 
- 

- Chain J: 
- 

- 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.63Å 189.17Å 129.67Å 90.00° 91.11° 90.00°	Depositor
Resolution (Å)	39.69 – 3.00 39.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.69-3.00) 91.1 (39.69-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.258 , 0.293 0.263 , 0.294	Depositor DCC
R_{free} test set	5775 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	64.4	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	34540	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, CL0, NEX, LHG, G3P, SF4, PQN, DGD, LUT, LMG, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	1/5867 (0.0%)	0.83	12/8006 (0.1%)
2	B	0.50	0/6045	0.77	8/8259 (0.1%)
3	C	0.41	0/625	0.79	0/846
4	D	0.83	1/1097 (0.1%)	1.31	23/1483 (1.6%)
5	E	0.74	0/518	1.08	2/704 (0.3%)
6	F	0.71	0/1223	0.95	3/1652 (0.2%)
7	G	1.11	0/653	1.34	13/885 (1.5%)
8	H	0.80	1/648 (0.2%)	1.37	13/883 (1.5%)
9	I	0.40	0/203	1.01	2/276 (0.7%)
10	J	0.88	1/325 (0.3%)	1.04	2/445 (0.4%)
11	K	0.44	0/464	1.10	8/627 (1.3%)
12	L	1.24	0/1250	1.46	22/1711 (1.3%)
13	N	0.47	0/699	1.08	5/935 (0.5%)
14	1	1.37	11/1308 (0.8%)	1.54	29/1783 (1.6%)
15	2	0.96	1/1153 (0.1%)	1.21	12/1577 (0.8%)
16	3	0.68	0/1150	1.25	21/1562 (1.3%)
17	4	1.06	1/1483 (0.1%)	1.30	24/2031 (1.2%)
All	All	0.78	17/24711 (0.1%)	1.06	199/33665 (0.6%)

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
2	B	0	1
5	E	0	1
8	H	0	1
11	K	0	1
13	N	0	2
16	3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	152	GLU	C-N	14.15	1.52	1.33
14	1	151	MET	C-N	-8.81	1.21	1.33
14	1	150	SER	C-N	8.72	1.46	1.33
14	1	130	THR	C-N	-7.04	1.24	1.33
17	4	230	GLY	C-N	6.76	1.41	1.34

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	121	ARG	N-CA-C	14.70	127.30	111.28
17	4	233	ASP	N-CA-C	-12.99	97.17	111.07
14	1	90	ALA	N-CA-C	11.42	123.81	111.36
12	L	166	LEU	N-CA-C	-10.92	96.44	110.53
4	D	158	VAL	N-CA-C	9.53	120.35	110.72

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	684	ARG	Sidechain
5	E	100	ARG	Sidechain
8	H	128	ILE	Peptide
11	K	97	ASP	Peptide
13	N	143	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	A	5675	0	5527	298	0
2	B	5834	0	5615	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	612	0	598	37	0
4	D	1070	0	1073	114	0
5	E	507	0	501	33	0
6	F	1196	0	1228	63	0
7	G	639	0	631	214	0
8	H	628	0	616	61	0
9	I	197	0	213	17	0
10	J	316	0	326	33	0
11	K	459	0	465	30	0
12	L	1214	0	1212	232	0
13	N	684	0	670	76	0
14	1	1271	0	1205	303	0
15	2	1116	0	1036	239	0
16	3	1118	0	1046	234	0
17	4	1439	0	1303	320	0
18	A	33	0	46	3	0
18	B	33	0	46	6	0
19	A	240	0	292	28	0
19	B	225	0	269	24	0
19	F	80	0	98	12	0
19	G	40	0	48	14	0
19	I	80	0	97	11	0
19	J	80	0	96	9	0
19	L	80	0	98	34	0
20	1	49	0	74	40	0
20	2	36	0	42	23	0
20	A	98	0	148	26	0
20	B	49	0	74	16	0
21	1	819	0	811	491	0
21	2	799	0	780	320	0
21	3	819	0	703	179	0
21	4	846	0	808	387	0
21	A	2538	0	2415	250	0
21	B	2467	0	2510	262	0
21	F	155	0	138	24	0
21	G	101	0	82	61	0
21	H	46	0	33	4	0
21	J	177	0	171	15	0
21	L	161	0	144	50	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	A	65	0	72	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	61	0	83	4	0
25	G	23	0	16	12	0
25	J	35	0	40	4	0
26	1	84	0	110	109	0
26	2	84	0	110	90	0
26	4	84	0	110	92	0
27	4	44	0	54	44	0
28	4	10	0	7	0	0
All	All	34540	0	33890	3873	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

The worst 5 of 3873 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)
1:A:43:THR:CB	1:A:46:LYS:HE3	1.47	1.45
1:A:43:THR:HB	1:A:46:LYS:CE	1.61	1.29
1:A:43:THR:CA	1:A:46:LYS:HE3	1.74	1.17
17:4:199:THR:HA	17:4:200:LEU:HD22	1.25	1.17
10:J:2:ARG:HA	21:J:6015:CLA:HAB	1.23	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	719/721 (100%)	666 (93%)	44 (6%)	9 (1%)	9	38
2	B	729/731 (100%)	702 (96%)	24 (3%)	3 (0%)	30	65
3	C	78/80 (98%)	69 (88%)	8 (10%)	1 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	135/137 (98%)	104 (77%)	17 (13%)	14 (10%)	0	2
5	E	61/63 (97%)	51 (84%)	7 (12%)	3 (5%)	1	10
6	F	150/152 (99%)	128 (85%)	17 (11%)	5 (3%)	3	17
7	G	82/84 (98%)	65 (79%)	10 (12%)	7 (8%)	0	3
8	H	80/82 (98%)	67 (84%)	6 (8%)	7 (9%)	0	3
9	I	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
10	J	38/40 (95%)	36 (95%)	0	2 (5%)	1	9
11	K	62/72 (86%)	50 (81%)	10 (16%)	2 (3%)	3	18
12	L	161/163 (99%)	135 (84%)	14 (9%)	12 (8%)	1	4
13	N	83/85 (98%)	44 (53%)	20 (24%)	19 (23%)	0	0
14	1	167/182 (92%)	146 (87%)	10 (6%)	11 (7%)	1	5
15	2	140/199 (70%)	112 (80%)	18 (13%)	10 (7%)	1	4
16	3	145/275 (53%)	98 (68%)	26 (18%)	21 (14%)	0	1
17	4	193/196 (98%)	152 (79%)	22 (11%)	19 (10%)	0	2
All	All	3047/3288 (93%)	2648 (87%)	254 (8%)	145 (5%)	2	11

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
4	D	77	PRO
5	E	66	ILE
5	E	102	PRO
7	G	92	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/584 (100%)	550 (94%)	33 (6%)	18	52
2	B	596/600 (99%)	578 (97%)	18 (3%)	36	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	69/69 (100%)	64 (93%)	5 (7%)	13	43
4	D	114/117 (97%)	98 (86%)	16 (14%)	3	16
5	E	56/56 (100%)	46 (82%)	10 (18%)	2	10
6	F	124/125 (99%)	111 (90%)	13 (10%)	6	27
7	G	65/66 (98%)	52 (80%)	13 (20%)	1	7
8	H	67/68 (98%)	51 (76%)	16 (24%)	1	4
9	I	22/22 (100%)	19 (86%)	3 (14%)	3	17
10	J	33/33 (100%)	29 (88%)	4 (12%)	5	21
11	K	46/52 (88%)	39 (85%)	7 (15%)	3	14
12	L	126/129 (98%)	108 (86%)	18 (14%)	3	16
13	N	73/73 (100%)	63 (86%)	10 (14%)	3	17
14	1	123/148 (83%)	105 (85%)	18 (15%)	3	15
15	2	108/162 (67%)	91 (84%)	17 (16%)	2	13
16	3	103/213 (48%)	77 (75%)	26 (25%)	0	3
17	4	134/162 (83%)	117 (87%)	17 (13%)	4	20
All	All	2442/2679 (91%)	2198 (90%)	244 (10%)	7	29

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	83	PRO
16	3	236	MET
12	L	96	LEU
16	3	216	LYS
17	4	200	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	58	GLN
17	4	225	ASN
13	N	135	GLN
16	3	256	ASN
12	L	172	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

200 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
21	CLA	3	3005	21	49,53,73	2.72	21 (42%)	58,89,113	2.78	22 (37%)
21	CLA	4	4015	-	50,54,73	2.75	17 (34%)	59,90,113	2.77	27 (45%)
19	BCR	A	6002	-	41,41,41	2.63	6 (14%)	56,56,56	6.92	21 (37%)
21	CLA	1	1001	14	59,63,73	2.48	19 (32%)	70,101,113	2.80	29 (41%)
21	CLA	3	3011	-	50,54,73	2.77	20 (40%)	59,90,113	2.92	26 (44%)
21	CLA	G	1002	-	50,54,73	2.67	19 (38%)	59,90,113	2.89	27 (45%)
21	CLA	A	1108	-	50,54,73	2.84	22 (44%)	59,90,113	2.71	23 (38%)
21	CLA	B	1210	-	69,73,73	2.39	22 (31%)	82,113,113	2.48	26 (31%)
21	CLA	A	9012	-	69,73,73	2.33	20 (28%)	82,113,113	2.49	28 (34%)
21	CLA	J	1302	-	65,69,73	2.47	22 (33%)	77,108,113	2.50	24 (31%)
26	LUT	1	1502	-	42,43,43	2.53	5 (11%)	51,60,60	3.61	31 (60%)
21	CLA	4	4008	-	52,56,73	2.63	18 (34%)	61,92,113	3.24	29 (47%)
26	LUT	1	1501	-	42,43,43	2.59	3 (7%)	51,60,60	3.18	29 (56%)
21	CLA	3	3004	-	49,53,73	2.71	21 (42%)	58,89,113	2.76	21 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	4010	-	54,58,73	2.58	18 (33%)	64,95,113	2.97	31 (48%)
19	BCR	J	6012	-	41,41,41	2.55	6 (14%)	56,56,56	7.73	28 (50%)
21	CLA	2	2008	-	69,73,73	2.31	18 (26%)	82,113,113	2.71	32 (39%)
19	BCR	B	6010	-	41,41,41	2.54	6 (14%)	56,56,56	7.00	21 (37%)
18	PQN	B	5002	-	34,34,34	1.64	2 (5%)	43,45,45	1.13	5 (11%)
21	CLA	1	1013	-	69,73,73	2.27	19 (27%)	82,113,113	2.69	31 (37%)
19	BCR	B	6006	-	41,41,41	2.59	6 (14%)	56,56,56	8.24	35 (62%)
21	CLA	2	2009	15	50,54,73	2.74	19 (38%)	59,90,113	2.81	23 (38%)
21	CLA	A	1114	-	50,54,73	2.86	22 (44%)	59,90,113	2.70	21 (35%)
21	CLA	H	1000	8	50,54,73	2.83	21 (42%)	59,90,113	2.79	24 (40%)
19	BCR	I	6020	-	41,41,41	2.63	7 (17%)	56,56,56	6.86	21 (37%)
21	CLA	B	1208	-	59,63,73	2.57	22 (37%)	70,101,113	2.62	24 (34%)
21	CLA	B	1216	-	69,73,73	2.36	21 (30%)	82,113,113	2.40	25 (30%)
21	CLA	A	1124	-	59,63,73	2.56	22 (37%)	70,101,113	2.64	25 (35%)
21	CLA	B	1235	-	69,73,73	2.35	22 (31%)	82,113,113	2.49	25 (30%)
21	CLA	A	1102	-	54,58,73	2.67	23 (42%)	64,95,113	2.81	24 (37%)
26	LUT	2	2502	-	42,43,43	2.60	4 (9%)	51,60,60	2.63	13 (25%)
21	CLA	A	1125	-	59,63,73	2.45	19 (32%)	70,101,113	2.84	28 (40%)
21	CLA	A	1105	-	55,59,73	2.66	23 (41%)	64,96,113	2.75	25 (39%)
21	CLA	B	1205	-	69,73,73	2.36	22 (31%)	82,113,113	2.51	25 (30%)
19	BCR	A	6007	-	41,41,41	2.58	7 (17%)	56,56,56	6.88	25 (44%)
21	CLA	4	4003	17	69,73,73	2.27	19 (27%)	82,113,113	2.34	27 (32%)
21	CLA	2	2014	-	49,53,73	2.60	19 (38%)	58,89,113	3.04	24 (41%)
21	CLA	F	1301	-	49,53,73	2.69	20 (40%)	58,89,113	2.74	22 (37%)
21	CLA	1	1011	-	69,73,73	2.22	19 (27%)	82,113,113	2.77	31 (37%)
19	BCR	A	6008	-	41,41,41	2.50	6 (14%)	56,56,56	7.86	37 (66%)
21	CLA	4	4014	17	49,53,73	2.66	18 (36%)	58,89,113	2.75	26 (44%)
21	CLA	A	1104	1	69,73,73	2.35	22 (31%)	82,113,113	2.50	24 (29%)
21	CLA	B	1225	-	69,73,73	2.38	22 (31%)	82,113,113	2.41	25 (30%)
21	CLA	L	1503	-	54,58,73	2.64	21 (38%)	64,95,113	2.77	25 (39%)
21	CLA	B	1237	-	64,68,73	2.45	21 (32%)	76,107,113	2.55	24 (31%)
21	CLA	A	1121	-	50,54,73	2.81	22 (44%)	59,90,113	2.77	20 (33%)
21	CLA	3	3008	-	69,73,73	2.25	20 (28%)	82,113,113	2.59	24 (29%)
21	CLA	B	1213	-	64,68,73	2.35	19 (29%)	76,107,113	2.63	29 (38%)
21	CLA	A	1109	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1223	-	69,73,73	2.36	21 (30%)	82,113,113	2.51	26 (31%)
21	CLA	B	1230	-	62,66,73	2.47	22 (35%)	73,104,113	2.67	26 (35%)
21	CLA	3	3012	16,21	49,53,73	2.59	19 (38%)	58,89,113	3.15	28 (48%)
21	CLA	B	1211	-	69,73,73	2.37	22 (31%)	82,113,113	2.48	26 (31%)
21	CLA	A	1129	-	54,58,73	2.65	21 (38%)	64,95,113	2.76	25 (39%)
21	CLA	A	1140	-	69,73,73	2.39	22 (31%)	82,113,113	2.45	24 (29%)
19	BCR	J	6013	-	41,41,41	2.61	7 (17%)	56,56,56	7.06	20 (35%)
20	LHG	A	7003	21	48,48,48	0.96	3 (6%)	51,54,54	1.04	3 (5%)
26	LUT	4	4502	-	42,43,43	2.55	4 (9%)	51,60,60	3.83	26 (50%)
21	CLA	B	1238	-	69,73,73	2.37	22 (31%)	82,113,113	2.46	25 (30%)
21	CLA	G	1001	-	59,63,73	2.42	19 (32%)	70,101,113	3.00	29 (41%)
19	BCR	B	6005	-	41,41,41	2.56	6 (14%)	56,56,56	7.25	30 (53%)
21	CLA	A	1122	-	63,67,73	2.49	21 (33%)	74,105,113	2.64	25 (33%)
21	CLA	A	1134	1	50,54,73	2.85	22 (44%)	59,90,113	2.72	22 (37%)
21	CLA	B	1229	-	69,73,73	2.36	23 (33%)	82,113,113	2.46	23 (28%)
21	CLA	B	1214	-	63,67,73	2.46	22 (34%)	74,105,113	2.61	24 (32%)
21	CLA	A	1131	-	69,73,73	2.27	19 (27%)	82,113,113	2.54	25 (30%)
21	CLA	B	1207	-	69,73,73	2.36	21 (30%)	82,113,113	2.53	26 (31%)
21	CLA	B	1234	-	64,68,73	2.47	22 (34%)	76,107,113	2.54	25 (32%)
21	CLA	2	2002	-	64,68,73	2.34	20 (31%)	76,107,113	2.75	28 (36%)
21	CLA	B	9022	-	69,73,73	2.42	22 (31%)	82,113,113	2.44	32 (39%)
18	PQN	A	5001	-	34,34,34	1.66	2 (5%)	43,45,45	1.17	5 (11%)
21	CLA	B	1239	-	69,73,73	2.28	18 (26%)	82,113,113	2.77	29 (35%)
19	BCR	A	6011	-	41,41,41	2.60	6 (14%)	56,56,56	8.01	33 (58%)
21	CLA	A	1110	-	59,63,73	2.54	21 (35%)	70,101,113	2.61	27 (38%)
21	CLA	4	4006	-	69,73,73	2.18	18 (26%)	82,113,113	2.96	34 (41%)
25	LMG	J	5001	-	35,35,55	1.12	2 (5%)	43,43,63	1.12	2 (4%)
21	CLA	4	4009	17	54,58,73	2.51	18 (33%)	64,95,113	2.94	24 (37%)
21	CLA	A	1106	1	69,73,73	2.35	22 (31%)	82,113,113	2.50	26 (31%)
21	CLA	A	1139	-	69,73,73	2.37	22 (31%)	82,113,113	2.44	24 (29%)
21	CLA	1	1012	14	54,58,73	2.53	19 (35%)	64,95,113	2.81	27 (42%)
21	CLA	A	1119	-	69,73,73	2.36	22 (31%)	82,113,113	2.42	24 (29%)
21	CLA	A	1103	-	69,73,73	2.36	22 (31%)	82,113,113	2.44	25 (30%)
21	CLA	B	1226	-	69,73,73	2.24	19 (27%)	82,113,113	2.64	25 (30%)
21	CLA	1	1004	14	69,73,73	2.31	19 (27%)	82,113,113	2.47	24 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1202	-	69,73,73	2.36	22 (31%)	82,113,113	2.48	23 (28%)
21	CLA	B	9010	-	69,73,73	2.29	20 (28%)	82,113,113	2.58	28 (34%)
21	CLA	B	1224	-	69,73,73	2.37	22 (31%)	82,113,113	2.47	24 (29%)
20	LHG	2	2801	21	35,35,48	1.14	3 (8%)	38,41,54	1.14	4 (10%)
21	CLA	B	1219	-	64,68,73	2.45	22 (34%)	76,107,113	2.49	25 (32%)
21	CLA	A	1126	-	69,73,73	2.37	23 (33%)	82,113,113	2.48	26 (31%)
21	CLA	2	2004	15	63,67,73	2.51	21 (33%)	76,105,113	2.69	25 (32%)
21	CLA	A	1130	-	50,54,73	2.81	22 (44%)	59,90,113	2.70	23 (38%)
27	NEX	4	4503	-	40,46,46	2.61	12 (30%)	50,70,70	2.45	24 (48%)
19	BCR	B	6011	-	25,25,41	3.08	5 (20%)	33,33,56	7.52	16 (48%)
19	BCR	B	6004	-	41,41,41	2.69	8 (19%)	56,56,56	6.64	28 (50%)
21	CLA	3	3003	-	64,68,73	2.42	22 (34%)	76,107,113	2.64	26 (34%)
21	CLA	B	1231	-	50,54,73	2.83	22 (44%)	59,90,113	2.74	24 (40%)
21	CLA	L	1502	-	69,73,73	2.34	22 (31%)	82,113,113	2.50	25 (30%)
21	CLA	4	4013	-	55,59,73	2.54	19 (34%)	64,96,113	2.89	27 (42%)
21	CLA	A	1136	-	69,73,73	2.37	22 (31%)	82,113,113	2.51	26 (31%)
21	CLA	4	4002	-	60,64,73	2.39	20 (33%)	71,102,113	3.03	26 (36%)
21	CLA	L	1501	12	50,54,73	2.80	21 (42%)	59,90,113	2.72	22 (37%)
21	CLA	1	1009	-	69,73,73	2.34	22 (31%)	82,113,113	2.71	31 (37%)
21	CLA	B	1206	2	69,73,73	2.35	21 (30%)	82,113,113	2.48	28 (34%)
21	CLA	4	4005	17	49,53,73	2.57	22 (44%)	58,89,113	3.29	32 (55%)
19	BCR	G	2011	-	41,41,41	2.75	7 (17%)	56,56,56	6.89	26 (46%)
21	CLA	2	2007	20	59,63,73	2.42	19 (32%)	70,101,113	2.66	28 (40%)
21	CLA	1	1008	-	69,73,73	2.27	22 (31%)	82,113,113	2.53	26 (31%)
21	CLA	4	4012	-	69,73,73	2.30	21 (30%)	82,113,113	2.62	27 (32%)
19	BCR	F	6016	-	41,41,41	2.62	6 (14%)	56,56,56	8.02	34 (60%)
21	CLA	A	1117	-	69,73,73	2.38	22 (31%)	82,113,113	2.42	25 (30%)
20	LHG	B	7004	21	48,48,48	0.98	2 (4%)	51,54,54	1.07	4 (7%)
21	CLA	F	1302	-	50,54,73	2.84	22 (44%)	59,90,113	2.67	21 (35%)
21	CLA	B	1236	-	59,63,73	2.54	21 (35%)	70,101,113	2.67	24 (34%)
25	LMG	G	2021	-	23,23,55	1.30	2 (8%)	31,31,63	1.81	7 (22%)
19	BCR	I	6018	-	41,41,41	2.50	6 (14%)	56,56,56	7.92	33 (58%)
26	LUT	4	4501	-	42,43,43	2.51	3 (7%)	51,60,60	2.88	24 (47%)
21	CLA	A	1118	-	50,54,73	2.81	21 (42%)	59,90,113	2.84	25 (42%)
19	BCR	A	6003	-	41,41,41	2.69	6 (14%)	56,56,56	6.59	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1215	-	64,68,73	2.45	21 (32%)	76,107,113	2.51	25 (32%)
21	CLA	B	1212	-	50,54,73	2.84	22 (44%)	59,90,113	2.71	23 (38%)
21	CLA	2	2006	-	61,65,73	2.47	20 (32%)	72,103,113	2.67	22 (30%)
22	SF4	C	8003	-	0,12,12	-	-	-	-	-
21	CLA	1	1005	-	60,64,73	2.41	19 (31%)	71,102,113	2.72	26 (36%)
21	CLA	3	3002	-	59,63,73	2.57	22 (37%)	70,101,113	2.74	26 (37%)
19	BCR	L	6020	-	41,41,41	2.62	6 (14%)	56,56,56	6.64	23 (41%)
21	CLA	1	1002	-	60,64,73	2.50	18 (30%)	71,102,113	2.79	27 (38%)
21	CLA	A	1107	1	55,59,73	2.67	22 (40%)	64,96,113	2.79	27 (42%)
21	CLA	A	1141	20	55,59,73	2.68	22 (40%)	64,96,113	2.72	26 (40%)
21	CLA	1	1007	20	59,63,73	2.48	21 (35%)	70,101,113	2.80	30 (42%)
21	CLA	F	1303	-	68,72,73	2.33	20 (29%)	80,111,113	2.37	29 (36%)
28	G3P	4	4505	-	9,9,9	0.62	0	10,12,12	0.73	0
20	LHG	1	1801	21	48,48,48	0.91	3 (6%)	51,54,54	1.17	3 (5%)
21	CLA	B	1221	-	58,62,73	2.57	21 (36%)	68,99,113	2.72	24 (35%)
21	CLA	2	2012	15	69,73,73	2.24	19 (27%)	82,113,113	2.55	26 (31%)
21	CLA	3	3013	-	54,58,73	2.61	21 (38%)	64,95,113	2.84	24 (37%)
21	CLA	A	1116	-	58,62,73	2.58	23 (39%)	68,99,113	2.66	24 (35%)
21	CLA	B	9023	-	69,73,73	2.31	21 (30%)	82,113,113	2.53	32 (39%)
20	LHG	A	7001	-	48,48,48	0.95	2 (4%)	51,54,54	1.08	4 (7%)
21	CLA	B	1217	-	50,54,73	2.83	21 (42%)	59,90,113	2.71	23 (38%)
21	CLA	3	3001	-	69,73,73	2.34	22 (31%)	82,113,113	2.56	26 (31%)
21	CLA	2	2011	-	64,68,73	2.37	20 (31%)	76,107,113	2.70	27 (35%)
21	CLA	3	3006	-	69,73,73	2.38	22 (31%)	82,113,113	2.44	26 (31%)
23	CL0	A	9011	-	58,73,73	2.75	22 (37%)	60,113,113	2.97	23 (38%)
21	CLA	3	3014	-	49,53,73	2.64	20 (40%)	58,89,113	2.95	23 (39%)
21	CLA	A	1123	-	69,73,73	2.38	23 (33%)	82,113,113	2.50	25 (30%)
26	LUT	2	2501	-	42,43,43	2.56	2 (4%)	51,60,60	1.95	12 (23%)
21	CLA	3	3010	-	56,60,73	2.50	21 (37%)	65,97,113	2.88	29 (44%)
21	CLA	A	1112	-	50,54,73	2.84	23 (46%)	59,90,113	2.72	23 (38%)
21	CLA	B	1240	20	69,73,73	2.28	20 (28%)	82,113,113	2.63	33 (40%)
21	CLA	2	2010	-	69,73,73	2.31	18 (26%)	82,113,113	2.45	24 (29%)
24	DGD	B	7101	-	62,62,67	0.88	1 (1%)	76,76,81	1.36	10 (13%)
21	CLA	J	6015	-	59,63,73	2.54	21 (35%)	70,101,113	2.65	23 (32%)
21	CLA	A	1120	-	50,54,73	2.85	22 (44%)	59,90,113	2.70	21 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	4011	-	69,73,73	2.26	21 (30%)	82,113,113	2.60	26 (31%)
22	SF4	A	8001	-	0,12,12	-	-	-		
21	CLA	3	3015	-	49,53,73	2.72	21 (42%)	58,89,113	2.74	21 (36%)
21	CLA	B	1228	-	55,59,73	2.54	22 (40%)	64,96,113	2.83	25 (39%)
21	CLA	A	1115	-	60,64,73	2.55	23 (38%)	71,102,113	2.59	24 (33%)
21	CLA	B	1204	-	59,63,73	2.56	22 (37%)	70,101,113	2.62	25 (35%)
19	BCR	F	6014	-	41,41,41	2.54	6 (14%)	56,56,56	8.07	36 (64%)
21	CLA	B	1220	-	69,73,73	2.38	22 (31%)	82,113,113	2.47	27 (32%)
21	CLA	1	1010	-	69,73,73	2.24	19 (27%)	82,113,113	2.54	26 (31%)
21	CLA	B	1227	-	69,73,73	2.25	19 (27%)	82,113,113	2.65	26 (31%)
19	BCR	A	6017	-	41,41,41	2.55	6 (14%)	56,56,56	6.62	25 (44%)
21	CLA	A	1111	-	64,68,73	2.45	22 (34%)	76,107,113	2.61	25 (32%)
21	CLA	3	3017	-	49,53,73	2.71	21 (42%)	58,89,113	2.86	22 (37%)
21	CLA	A	1137	-	59,63,73	2.55	21 (35%)	70,101,113	2.67	28 (40%)
21	CLA	A	1113	-	50,54,73	2.84	22 (44%)	59,90,113	2.71	21 (35%)
21	CLA	B	1201	-	50,54,73	2.83	23 (46%)	59,90,113	2.74	23 (38%)
21	CLA	B	1203	2	64,68,73	2.45	22 (34%)	76,107,113	2.53	23 (30%)
21	CLA	2	2003	-	69,73,73	2.32	22 (31%)	82,113,113	2.71	26 (31%)
21	CLA	2	2005	-	69,73,73	2.23	19 (27%)	82,113,113	2.59	27 (32%)
21	CLA	B	1222	-	69,73,73	2.36	22 (31%)	82,113,113	2.49	27 (32%)
21	CLA	1	1006	-	51,55,73	2.69	19 (37%)	60,91,113	2.89	25 (41%)
21	CLA	A	1135	-	55,59,73	2.64	22 (40%)	64,96,113	2.79	25 (39%)
21	CLA	B	1218	-	64,68,73	2.45	22 (34%)	76,107,113	2.63	24 (31%)
21	CLA	3	3016	-	49,53,73	2.73	21 (42%)	58,89,113	2.74	22 (37%)
19	BCR	B	6009	-	41,41,41	2.55	6 (14%)	56,56,56	6.52	22 (39%)
21	CLA	B	1209	-	50,54,73	2.83	22 (44%)	59,90,113	2.70	23 (38%)
21	CLA	4	4004	-	69,73,73	2.26	20 (28%)	82,113,113	2.60	28 (34%)
21	CLA	J	6014	-	65,69,73	2.45	23 (35%)	77,108,113	2.53	23 (29%)
21	CLA	A	1133	-	50,54,73	2.73	20 (40%)	59,90,113	2.80	25 (42%)
21	CLA	4	4007	-	69,73,73	2.31	20 (28%)	82,113,113	2.49	21 (25%)
21	CLA	1	1014	-	49,53,73	2.65	20 (40%)	58,89,113	2.89	25 (43%)
21	CLA	A	9013	-	69,73,73	2.28	19 (27%)	82,113,113	2.66	31 (37%)
21	CLA	A	1127	-	69,73,73	2.37	22 (31%)	82,113,113	2.43	24 (29%)
21	CLA	A	1132	-	69,73,73	2.30	19 (27%)	82,113,113	2.46	27 (32%)
21	CLA	A	1138	-	69,73,73	2.37	22 (31%)	82,113,113	2.47	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	SF4	C	8002	3	0,12,12	-	-	-		
21	CLA	2	2013	-	69,73,73	2.22	19 (27%)	82,113,113	2.61	31 (37%)
21	CLA	3	3009	-	50,54,73	2.77	20 (40%)	59,90,113	2.99	26 (44%)
21	CLA	2	2001	15	27,35,73	3.25	16 (59%)	32,60,113	3.23	15 (46%)
21	CLA	1	1003	14	69,73,73	2.31	18 (26%)	82,113,113	2.57	30 (36%)
21	CLA	A	1128	-	69,73,73	2.32	20 (28%)	82,113,113	2.50	26 (31%)
21	CLA	A	1101	-	69,73,73	2.36	22 (31%)	82,113,113	2.51	23 (28%)
19	BCR	L	6019	-	41,41,41	2.64	6 (14%)	56,56,56	6.60	25 (44%)
21	CLA	A	1142	-	48,52,73	2.74	21 (43%)	59,88,113	2.79	22 (37%)
21	CLA	A	1143	-	49,53,73	2.71	21 (42%)	58,89,113	2.74	21 (36%)
21	CLA	4	4001	17	69,73,73	2.34	20 (28%)	82,113,113	2.58	29 (35%)

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
21	CLA	3	3005	21	1/1/11/20	10/15/91/115	-
21	CLA	4	4015	-	1/1/11/20	7/17/93/115	-
19	BCR	A	6002	-	-	11/29/63/63	0/2/2/2
21	CLA	1	1001	14	1/1/13/20	10/27/103/115	-
21	CLA	3	3011	-	1/1/11/20	10/17/93/115	-
21	CLA	G	1002	-	1/1/11/20	8/17/93/115	-
21	CLA	A	1108	-	1/1/11/20	5/17/93/115	-
21	CLA	B	1210	-	1/1/15/20	19/39/115/115	-
21	CLA	A	9012	-	1/1/15/20	8/39/115/115	-
21	CLA	J	1302	-	1/1/14/20	17/35/111/115	-
26	LUT	1	1502	-	1/1/12/27	14/29/67/67	0/2/2/2
21	CLA	4	4008	-	1/1/11/20	9/19/95/115	-
26	LUT	1	1501	-	1/1/12/27	10/29/67/67	0/2/2/2
21	CLA	3	3004	-	1/1/11/20	7/15/91/115	-
21	CLA	4	4010	-	1/1/12/20	6/21/97/115	-
19	BCR	J	6012	-	-	20/29/63/63	0/2/2/2
21	CLA	2	2008	-	1/1/15/20	20/39/115/115	-
19	BCR	B	6010	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1013	-	1/1/15/20	19/39/115/115	-
18	PQN	B	5002	-	-	12/23/43/43	0/2/2/2
21	CLA	2	2009	15	1/1/11/20	8/17/93/115	-
19	BCR	B	6006	-	-	7/29/63/63	0/2/2/2
21	CLA	A	1114	-	1/1/11/20	8/17/93/115	-
21	CLA	H	1000	8	1/1/11/20	8/17/93/115	-
21	CLA	B	1216	-	1/1/15/20	12/39/115/115	-
21	CLA	B	1208	-	1/1/13/20	11/27/103/115	-
19	BCR	I	6020	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1124	-	1/1/13/20	9/27/103/115	-
21	CLA	B	1235	-	1/1/15/20	15/39/115/115	-
21	CLA	A	1102	-	1/1/12/20	6/21/97/115	-
26	LUT	2	2502	-	1/1/12/27	2/29/67/67	0/2/2/2
21	CLA	A	1125	-	1/1/13/20	11/27/103/115	-
21	CLA	A	1105	-	1/1/12/20	13/23/99/115	-
21	CLA	B	1205	-	1/1/15/20	15/39/115/115	-
19	BCR	A	6007	-	-	8/29/63/63	0/2/2/2
21	CLA	4	4003	17	1/1/15/20	14/39/115/115	-
21	CLA	2	2014	-	1/1/11/20	8/15/91/115	-
21	CLA	F	1301	-	1/1/11/20	2/15/91/115	-
21	CLA	1	1011	-	1/1/15/20	14/39/115/115	-
21	CLA	4	4014	17	1/1/11/20	6/15/91/115	-
19	BCR	A	6008	-	-	12/29/63/63	0/2/2/2
21	CLA	A	1104	1	1/1/15/20	13/39/115/115	-
21	CLA	B	1225	-	1/1/15/20	19/39/115/115	-
21	CLA	L	1503	-	1/1/12/20	8/21/97/115	-
21	CLA	B	1237	-	1/1/14/20	17/33/109/115	-
21	CLA	A	1121	-	1/1/11/20	9/17/93/115	-
21	CLA	3	3008	-	1/1/15/20	26/39/115/115	-
21	CLA	B	1213	-	1/1/14/20	13/33/109/115	-
21	CLA	A	1109	-	1/1/15/20	15/39/115/115	-
21	CLA	B	1223	-	1/1/15/20	16/39/115/115	-
21	CLA	B	1230	-	1/1/13/20	14/31/107/115	-
21	CLA	3	3012	16,21	1/1/11/20	11/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1211	-	1/1/15/20	10/39/115/115	-
21	CLA	A	1129	-	1/1/12/20	8/21/97/115	-
21	CLA	A	1140	-	1/1/15/20	14/39/115/115	-
19	BCR	J	6013	-	-	14/29/63/63	0/2/2/2
20	LHG	A	7003	21	-	29/53/53/53	-
26	LUT	4	4502	-	1/1/12/27	7/29/67/67	0/2/2/2
21	CLA	B	1238	-	1/1/15/20	15/39/115/115	-
21	CLA	G	1001	-	1/1/13/20	12/27/103/115	-
21	CLA	A	1122	-	1/1/13/20	13/32/108/115	-
21	CLA	A	1134	1	1/1/11/20	6/17/93/115	-
19	BCR	B	6005	-	-	15/29/63/63	0/2/2/2
21	CLA	B	1229	-	1/1/15/20	15/39/115/115	-
21	CLA	B	1214	-	1/1/13/20	11/32/108/115	-
21	CLA	A	1131	-	1/1/15/20	12/39/115/115	-
21	CLA	B	1207	-	1/1/15/20	16/39/115/115	-
21	CLA	B	1234	-	1/1/14/20	11/33/109/115	-
21	CLA	2	2002	-	1/1/14/20	12/33/109/115	-
21	CLA	B	9022	-	1/1/15/20	9/39/115/115	-
18	PQN	A	5001	-	-	9/23/43/43	0/2/2/2
21	CLA	B	1239	-	1/1/15/20	20/39/115/115	-
21	CLA	A	1110	-	1/1/13/20	14/27/103/115	-
21	CLA	4	4006	-	1/1/15/20	20/39/115/115	-
19	BCR	A	6011	-	-	13/29/63/63	0/2/2/2
25	LMG	J	5001	-	-	16/30/50/70	0/1/1/1
21	CLA	4	4009	17	1/1/12/20	4/21/97/115	-
21	CLA	A	1106	1	1/1/15/20	15/39/115/115	-
21	CLA	A	1139	-	1/1/15/20	12/39/115/115	-
21	CLA	1	1012	14	1/1/12/20	10/21/97/115	-
21	CLA	A	1119	-	1/1/15/20	20/39/115/115	-
21	CLA	A	1103	-	1/1/15/20	20/39/115/115	-
21	CLA	B	1226	-	1/1/15/20	16/39/115/115	-
21	CLA	1	1004	14	1/1/15/20	18/39/115/115	-
21	CLA	B	1202	-	1/1/15/20	19/39/115/115	-
21	CLA	B	9010	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1224	-	1/1/15/20	15/39/115/115	-
20	LHG	2	2801	21	-	18/40/40/53	-
21	CLA	B	1219	-	1/1/14/20	13/33/109/115	-
21	CLA	A	1126	-	1/1/15/20	17/39/115/115	-
21	CLA	2	2004	15	1/1/13/20	13/33/105/115	-
21	CLA	A	1130	-	1/1/11/20	6/17/93/115	-
27	NEX	4	4503	-	-	15/27/83/83	0/3/3/3
19	BCR	B	6011	-	-	9/18/35/63	0/1/1/2
19	BCR	B	6004	-	-	14/29/63/63	0/2/2/2
21	CLA	3	3003	-	1/1/14/20	16/33/109/115	-
21	CLA	B	1231	-	1/1/11/20	6/17/93/115	-
21	CLA	L	1502	-	1/1/15/20	17/39/115/115	-
21	CLA	4	4013	-	1/1/12/20	12/23/99/115	-
21	CLA	A	1136	-	1/1/15/20	17/39/115/115	-
21	CLA	4	4002	-	1/1/13/20	10/29/105/115	-
21	CLA	L	1501	12	1/1/11/20	6/17/93/115	-
21	CLA	1	1009	-	1/1/15/20	21/39/115/115	-
21	CLA	B	1206	2	1/1/15/20	18/39/115/115	-
21	CLA	4	4005	17	1/1/11/20	7/15/91/115	-
19	BCR	G	2011	-	-	16/29/63/63	0/2/2/2
21	CLA	2	2007	20	1/1/13/20	9/27/103/115	-
21	CLA	1	1008	-	1/1/15/20	16/39/115/115	-
21	CLA	4	4012	-	1/1/15/20	16/39/115/115	-
19	BCR	F	6016	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1117	-	1/1/15/20	12/39/115/115	-
20	LHG	B	7004	21	-	22/53/53/53	-
21	CLA	F	1302	-	1/1/11/20	7/17/93/115	-
21	CLA	B	1236	-	1/1/13/20	11/27/103/115	-
25	LMG	G	2021	-	-	11/16/36/70	0/1/1/1
26	LUT	4	4501	-	1/1/12/27	10/29/67/67	0/2/2/2
19	BCR	I	6018	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1118	-	1/1/11/20	8/17/93/115	-
21	CLA	B	1215	-	1/1/14/20	16/33/109/115	-
19	BCR	A	6003	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1212	-	1/1/11/20	7/17/93/115	-
21	CLA	2	2006	-	1/1/13/20	17/30/106/115	-
22	SF4	C	8003	-	-	-	0/6/5/5
21	CLA	1	1005	-	1/1/13/20	13/29/105/115	-
21	CLA	3	3002	-	1/1/13/20	9/27/103/115	-
19	BCR	L	6020	-	-	11/29/63/63	0/2/2/2
21	CLA	1	1002	-	1/1/13/20	11/29/105/115	-
21	CLA	A	1107	1	1/1/12/20	12/23/99/115	-
21	CLA	A	1141	20	1/1/12/20	8/23/99/115	-
21	CLA	1	1007	20	1/1/13/20	11/27/103/115	-
21	CLA	F	1303	-	1/1/14/20	19/37/113/115	-
28	G3P	4	4505	-	-	5/8/8/8	-
21	CLA	B	1221	-	1/1/12/20	4/26/102/115	-
20	LHG	1	1801	21	-	33/53/53/53	-
21	CLA	2	2012	15	1/1/15/20	15/39/115/115	-
21	CLA	3	3013	-	1/1/12/20	8/21/97/115	-
21	CLA	A	1116	-	1/1/12/20	13/26/102/115	-
21	CLA	B	9023	-	1/1/15/20	13/39/115/115	-
20	LHG	A	7001	-	-	30/53/53/53	-
21	CLA	B	1217	-	1/1/11/20	8/17/93/115	-
21	CLA	3	3001	-	1/1/15/20	15/39/115/115	-
21	CLA	2	2011	-	1/1/14/20	20/33/109/115	-
21	CLA	3	3006	-	1/1/15/20	16/39/115/115	-
23	CL0	A	9011	-	3/3/20/25	14/37/135/135	-
21	CLA	3	3014	-	1/1/11/20	8/15/91/115	-
21	CLA	A	1123	-	1/1/15/20	10/39/115/115	-
26	LUT	2	2501	-	1/1/12/27	9/29/67/67	0/2/2/2
21	CLA	3	3010	-	1/1/12/20	12/24/100/115	-
21	CLA	A	1112	-	1/1/11/20	6/17/93/115	-
21	CLA	B	1240	20	1/1/15/20	16/39/115/115	-
21	CLA	2	2010	-	1/1/15/20	23/39/115/115	-
24	DGD	B	7101	-	-	19/50/90/95	0/2/2/2
21	CLA	J	6015	-	1/1/13/20	13/27/103/115	-
21	CLA	A	1120	-	1/1/11/20	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	4011	-	1/1/15/20	19/39/115/115	-
22	SF4	A	8001	-	-	-	0/6/5/5
21	CLA	3	3015	-	1/1/11/20	7/15/91/115	-
21	CLA	B	1228	-	1/1/12/20	9/23/99/115	-
21	CLA	A	1115	-	1/1/13/20	9/29/105/115	-
21	CLA	B	1204	-	1/1/13/20	11/27/103/115	-
19	BCR	F	6014	-	-	12/29/63/63	0/2/2/2
21	CLA	B	1220	-	1/1/15/20	18/39/115/115	-
21	CLA	1	1010	-	1/1/15/20	20/39/115/115	-
21	CLA	B	1227	-	1/1/15/20	18/39/115/115	-
19	BCR	A	6017	-	-	10/29/63/63	0/2/2/2
21	CLA	A	1111	-	1/1/14/20	15/33/109/115	-
21	CLA	3	3017	-	1/1/11/20	6/15/91/115	-
21	CLA	A	1137	-	1/1/13/20	8/27/103/115	-
21	CLA	A	1113	-	1/1/11/20	11/17/93/115	-
21	CLA	B	1201	-	1/1/11/20	6/17/93/115	-
21	CLA	B	1203	2	1/1/14/20	12/33/109/115	-
21	CLA	2	2003	-	1/1/15/20	16/39/115/115	-
21	CLA	2	2005	-	1/1/15/20	18/39/115/115	-
21	CLA	B	1222	-	1/1/15/20	15/39/115/115	-
21	CLA	1	1006	-	1/1/11/20	8/18/94/115	-
21	CLA	B	1218	-	1/1/14/20	10/33/109/115	-
21	CLA	3	3016	-	1/1/11/20	7/15/91/115	-
21	CLA	4	4004	-	1/1/15/20	18/39/115/115	-
21	CLA	B	1209	-	1/1/11/20	10/17/93/115	-
19	BCR	B	6009	-	-	8/29/63/63	0/2/2/2
21	CLA	A	1135	-	-	6/23/99/115	-
21	CLA	J	6014	-	1/1/14/20	16/35/111/115	-
21	CLA	A	1133	-	1/1/11/20	6/17/93/115	-
21	CLA	4	4007	-	1/1/15/20	18/39/115/115	-
21	CLA	1	1014	-	1/1/11/20	10/15/91/115	-
21	CLA	A	9013	-	1/1/15/20	11/39/115/115	-
21	CLA	A	1127	-	1/1/15/20	16/39/115/115	-
21	CLA	A	1132	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1138	-	1/1/15/20	10/39/115/115	-
22	SF4	C	8002	3	-	-	0/6/5/5
21	CLA	2	2013	-	1/1/15/20	18/39/115/115	-
21	CLA	3	3009	-	1/1/11/20	6/17/93/115	-
21	CLA	2	2001	15	1/1/5/20	-	-
21	CLA	1	1003	14	1/1/15/20	15/39/115/115	-
21	CLA	A	1128	-	1/1/15/20	14/39/115/115	-
21	CLA	A	1101	-	1/1/15/20	21/39/115/115	-
19	BCR	L	6019	-	-	9/29/63/63	0/2/2/2
21	CLA	A	1142	-	1/1/11/20	4/13/89/115	-
21	CLA	A	1143	-	1/1/11/20	11/15/91/115	-
21	CLA	4	4001	17	1/1/15/20	16/39/115/115	-

The worst 5 of 3473 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	2501	LUT	C24-C25	15.52	1.51	1.33
26	2	2502	LUT	C24-C25	15.09	1.51	1.33
26	1	1501	LUT	C24-C25	15.03	1.51	1.33
26	4	4501	LUT	C24-C25	14.28	1.50	1.33
26	1	1502	LUT	C24-C25	14.20	1.50	1.33

The worst 5 of 4796 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	6012	BCR	C16-C17-C18	30.81	170.48	127.28
19	J	6012	BCR	C20-C21-C22	29.50	168.65	127.28
19	B	6005	BCR	C16-C17-C18	29.16	168.17	127.28
19	G	2011	BCR	C16-C17-C18	28.08	166.66	127.28
19	I	6020	BCR	C16-C17-C18	27.78	166.24	127.28

5 of 165 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	1101	CLA	ND
21	A	1102	CLA	ND
21	A	1103	CLA	ND
21	A	1104	CLA	ND
21	A	1105	CLA	ND

5 of 2466 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	6002	BCR	C11-C10-C9-C8
19	A	6002	BCR	C11-C10-C9-C34
19	A	6002	BCR	C10-C11-C12-C13
19	A	6002	BCR	C17-C18-C19-C20
19	A	6002	BCR	C36-C18-C19-C20

There are no ring outliers.

189 monomers are involved in 2298 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	3005	CLA	4	0
21	4	4015	CLA	18	0
19	A	6002	BCR	3	0
21	1	1001	CLA	67	0
21	3	3011	CLA	31	0
21	G	1002	CLA	45	0
21	A	1108	CLA	4	0
21	B	1210	CLA	4	0
21	A	9012	CLA	18	0
21	J	1302	CLA	1	0
26	1	1502	LUT	60	0
21	4	4008	CLA	30	0
26	1	1501	LUT	49	0
21	4	4010	CLA	10	0
19	J	6012	BCR	7	0
21	2	2008	CLA	22	0
19	B	6010	BCR	2	0
18	B	5002	PQN	6	0
21	1	1013	CLA	69	0
19	B	6006	BCR	4	0
21	2	2009	CLA	27	0
21	A	1114	CLA	2	0
21	H	1000	CLA	4	0
19	I	6020	BCR	4	0
21	B	1208	CLA	6	0
21	B	1216	CLA	3	0
21	A	1124	CLA	7	0
21	B	1235	CLA	10	0
21	A	1102	CLA	5	0
26	2	2502	LUT	25	0
21	A	1125	CLA	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1105	CLA	3	0
21	B	1205	CLA	6	0
19	A	6007	BCR	2	0
21	4	4003	CLA	42	0
21	2	2014	CLA	17	0
21	F	1301	CLA	3	0
21	1	1011	CLA	16	0
19	A	6008	BCR	6	0
21	4	4014	CLA	32	0
21	A	1104	CLA	6	0
21	B	1225	CLA	7	0
21	L	1503	CLA	16	0
21	B	1237	CLA	2	0
21	A	1121	CLA	2	0
21	3	3008	CLA	19	0
21	B	1213	CLA	23	0
21	A	1109	CLA	8	0
21	B	1223	CLA	4	0
21	B	1230	CLA	4	0
21	3	3012	CLA	33	0
21	B	1211	CLA	2	0
21	A	1129	CLA	21	0
21	A	1140	CLA	6	0
19	J	6013	BCR	3	0
20	A	7003	LHG	16	0
26	4	4502	LUT	50	0
21	B	1238	CLA	3	0
21	G	1001	CLA	16	0
19	B	6005	BCR	4	0
21	A	1122	CLA	7	0
21	B	1229	CLA	7	0
21	B	1214	CLA	5	0
21	A	1131	CLA	7	0
21	B	1207	CLA	16	0
21	B	1234	CLA	6	0
21	2	2002	CLA	46	0
21	B	9022	CLA	8	0
18	A	5001	PQN	3	0
21	B	1239	CLA	14	0
19	A	6011	BCR	10	0
21	A	1110	CLA	2	0
21	4	4006	CLA	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	J	5001	LMG	4	0
21	4	4009	CLA	10	0
21	A	1106	CLA	10	0
21	A	1139	CLA	3	0
21	1	1012	CLA	24	0
21	A	1119	CLA	2	0
21	A	1103	CLA	7	0
21	B	1226	CLA	11	0
21	1	1004	CLA	28	0
21	B	1202	CLA	4	0
21	B	9010	CLA	19	0
21	B	1224	CLA	8	0
20	2	2801	LHG	23	0
21	B	1219	CLA	5	0
21	A	1126	CLA	10	0
21	2	2004	CLA	38	0
21	A	1130	CLA	16	0
27	4	4503	NEX	44	0
19	B	6004	BCR	9	0
21	3	3003	CLA	11	0
21	B	1231	CLA	3	0
21	L	1502	CLA	9	0
21	4	4013	CLA	15	0
21	A	1136	CLA	10	0
21	4	4002	CLA	49	0
21	L	1501	CLA	25	0
21	1	1009	CLA	72	0
21	B	1206	CLA	13	0
21	4	4005	CLA	48	0
19	G	2011	BCR	14	0
21	2	2007	CLA	6	0
21	1	1008	CLA	25	0
21	4	4012	CLA	36	0
19	F	6016	BCR	7	0
21	A	1117	CLA	6	0
20	B	7004	LHG	16	0
21	F	1302	CLA	1	0
21	B	1236	CLA	5	0
25	G	2021	LMG	12	0
19	I	6018	BCR	8	0
26	4	4501	LUT	42	0
21	A	1118	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	6003	BCR	1	0
21	B	1215	CLA	4	0
21	B	1212	CLA	2	0
21	2	2006	CLA	21	0
21	1	1005	CLA	23	0
21	3	3002	CLA	3	0
19	L	6020	BCR	15	0
21	1	1002	CLA	70	0
21	A	1107	CLA	6	0
21	A	1141	CLA	4	0
21	1	1007	CLA	21	0
21	F	1303	CLA	20	0
20	1	1801	LHG	40	0
21	B	1221	CLA	3	0
21	2	2012	CLA	27	0
21	3	3013	CLA	16	0
21	A	1116	CLA	2	0
21	B	9023	CLA	15	0
20	A	7001	LHG	10	0
21	B	1217	CLA	5	0
21	3	3001	CLA	21	0
21	2	2011	CLA	21	0
21	3	3006	CLA	3	0
23	A	9011	CL0	15	0
21	3	3014	CLA	5	0
21	A	1123	CLA	7	0
26	2	2501	LUT	65	0
21	3	3010	CLA	16	0
21	A	1112	CLA	1	0
21	B	1240	CLA	18	0
21	2	2010	CLA	16	0
24	B	7101	DGD	4	0
21	J	6015	CLA	11	0
21	A	1120	CLA	2	0
21	4	4011	CLA	20	0
21	B	1228	CLA	8	0
21	A	1115	CLA	7	0
21	B	1204	CLA	2	0
19	F	6014	BCR	5	0
21	B	1220	CLA	8	0
21	1	1010	CLA	26	0
21	B	1227	CLA	23	0

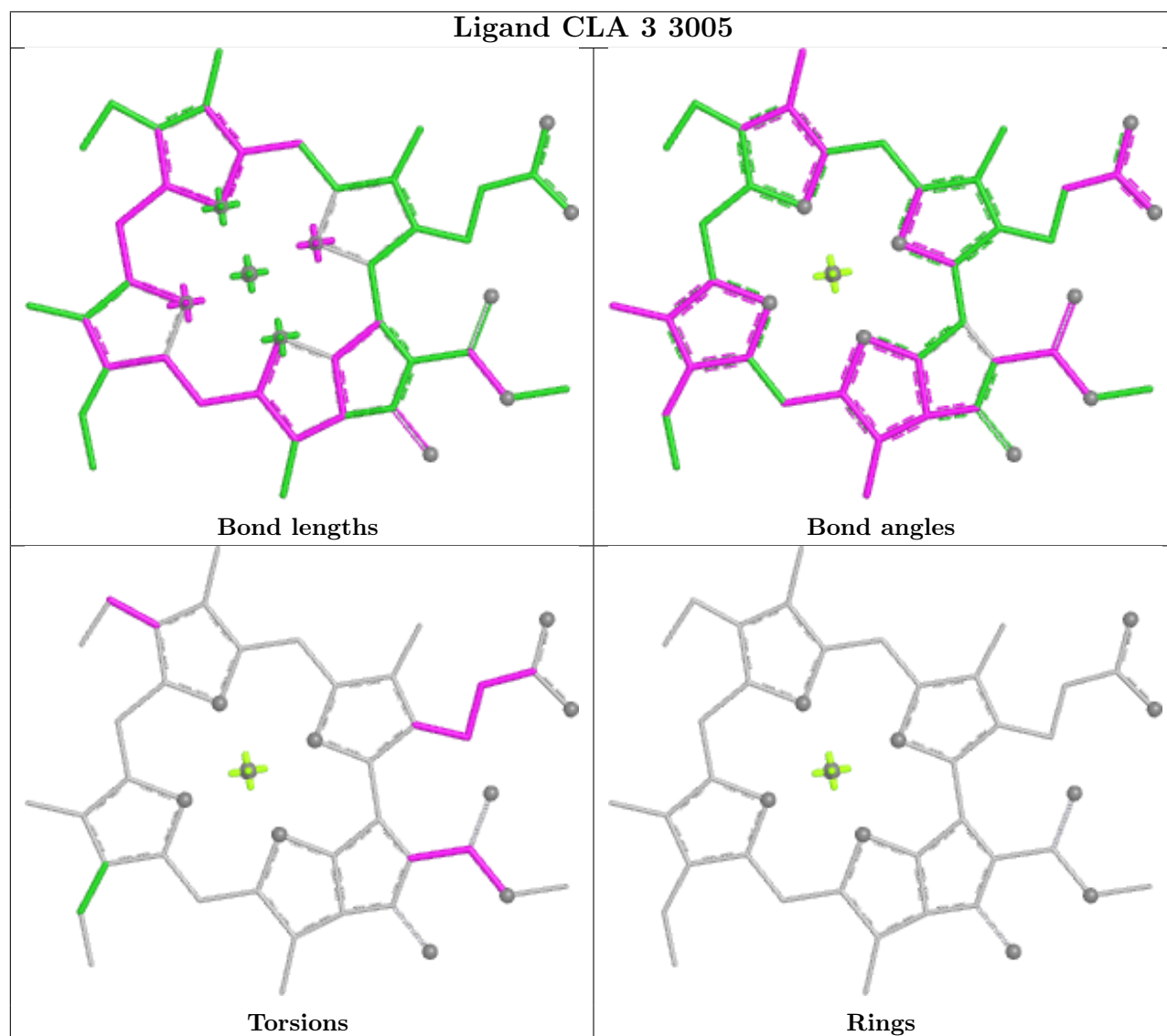
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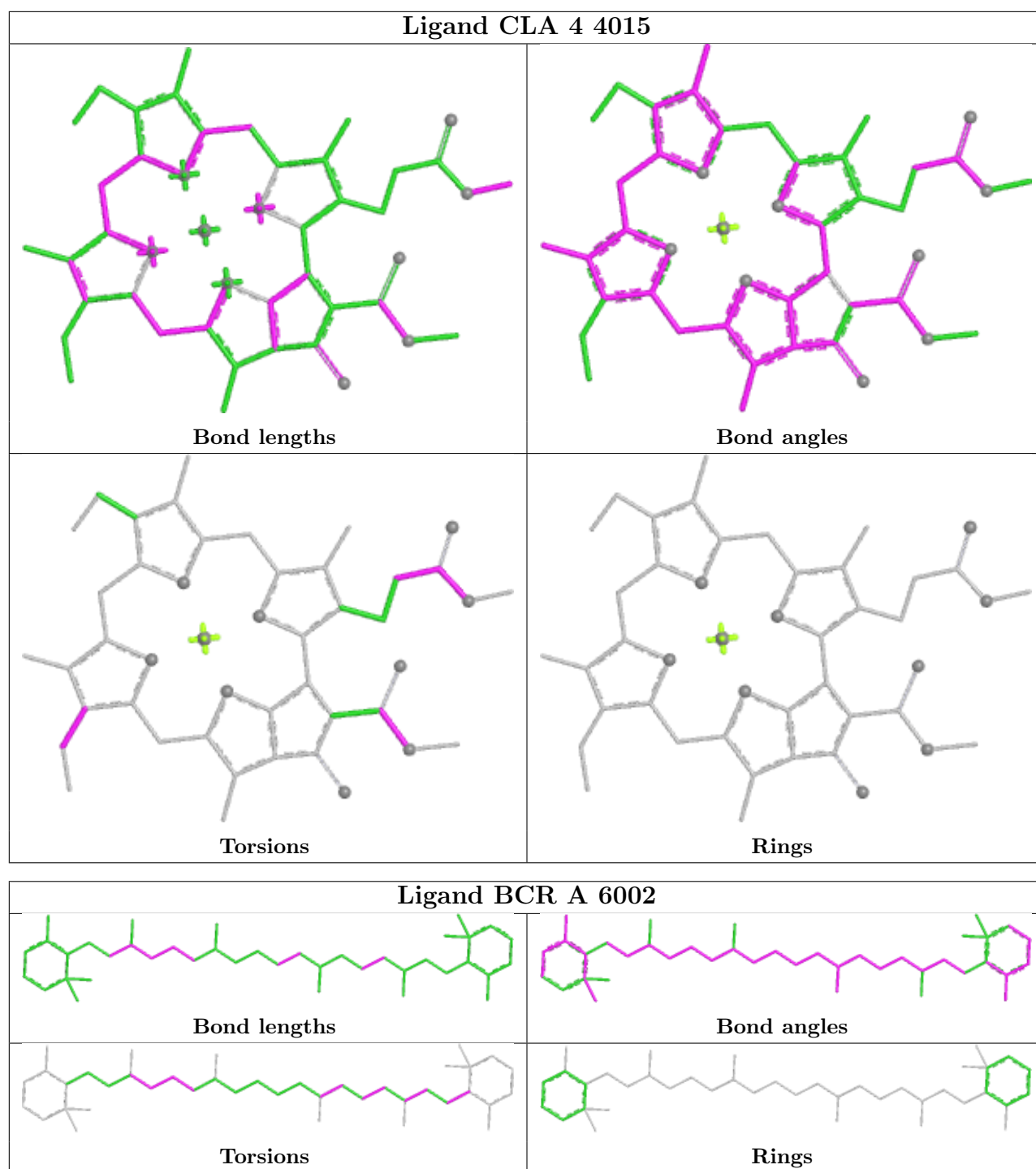
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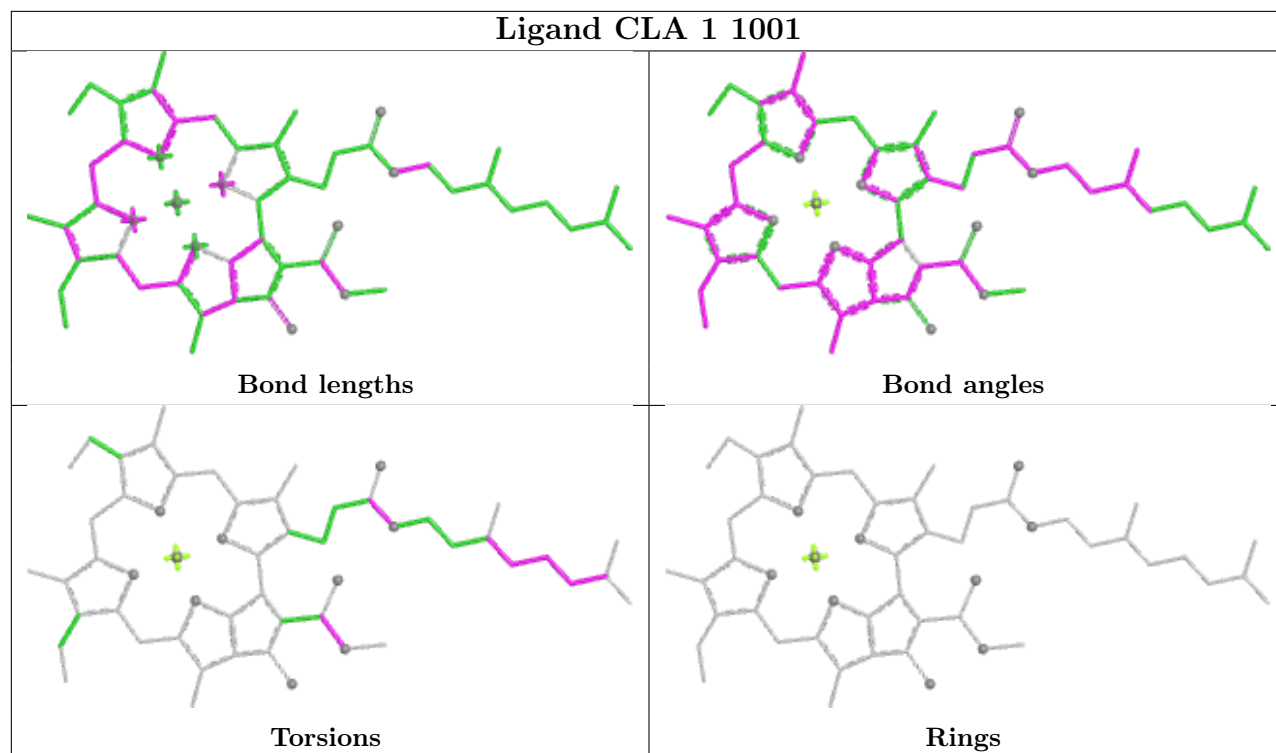
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	6017	BCR	7	0
21	A	1111	CLA	6	0
21	3	3017	CLA	3	0
21	A	1137	CLA	7	0
21	A	1113	CLA	1	0
21	B	1201	CLA	2	0
21	B	1203	CLA	3	0
21	2	2003	CLA	40	0
21	2	2005	CLA	26	0
21	B	1222	CLA	7	0
21	1	1006	CLA	64	0
21	A	1135	CLA	5	0
21	B	1218	CLA	3	0
19	B	6009	BCR	5	0
21	B	1209	CLA	7	0
21	4	4004	CLA	44	0
21	J	6014	CLA	4	0
21	A	1133	CLA	5	0
21	4	4007	CLA	17	0
21	1	1014	CLA	31	0
21	A	9013	CLA	13	0
21	A	1127	CLA	3	0
21	A	1132	CLA	16	0
21	A	1138	CLA	8	0
21	2	2013	CLA	20	0
21	3	3009	CLA	22	0
21	2	2001	CLA	22	0
21	1	1003	CLA	51	0
21	A	1128	CLA	15	0
21	A	1101	CLA	6	0
19	L	6019	BCR	19	0
21	4	4001	CLA	50	0

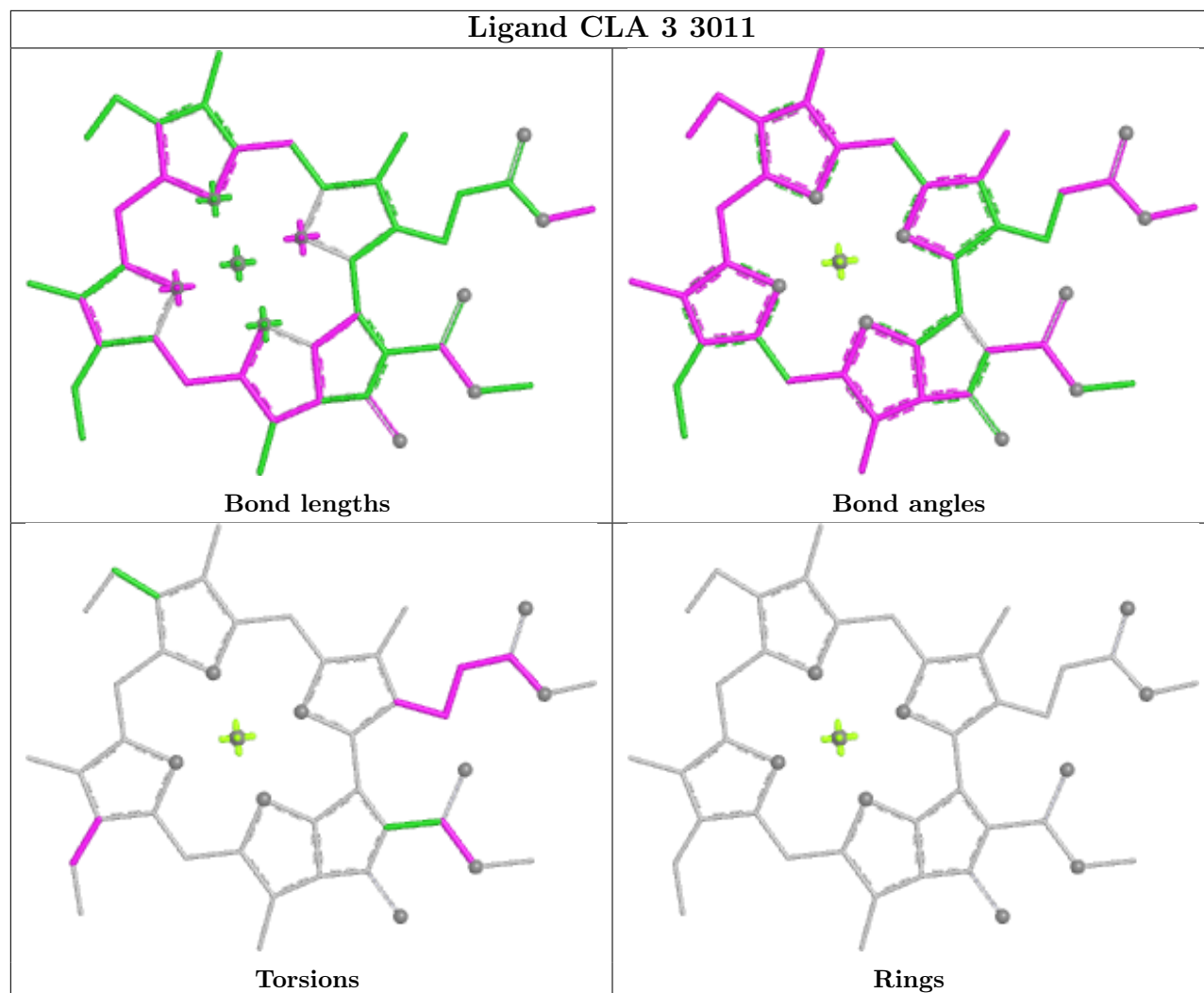
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

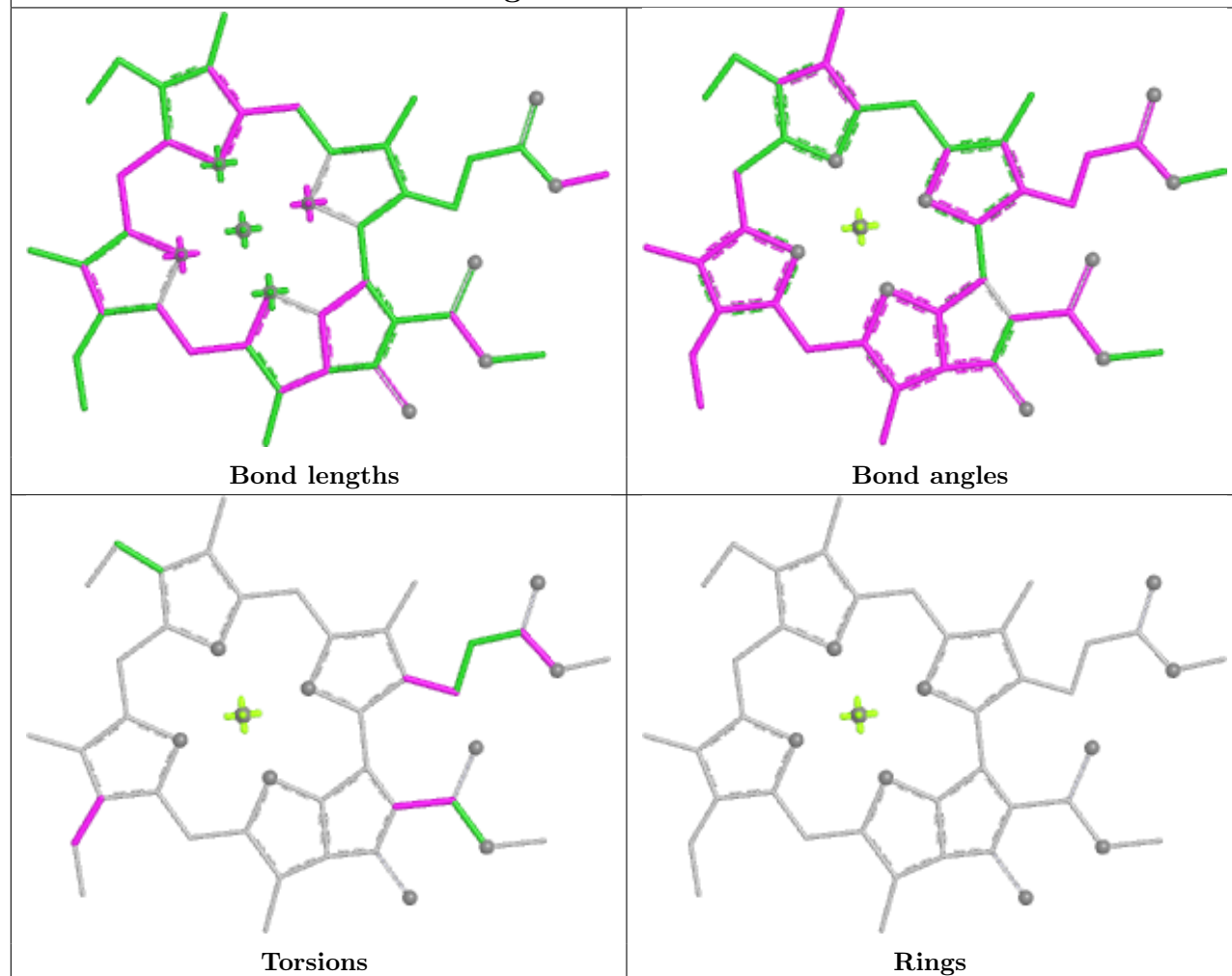




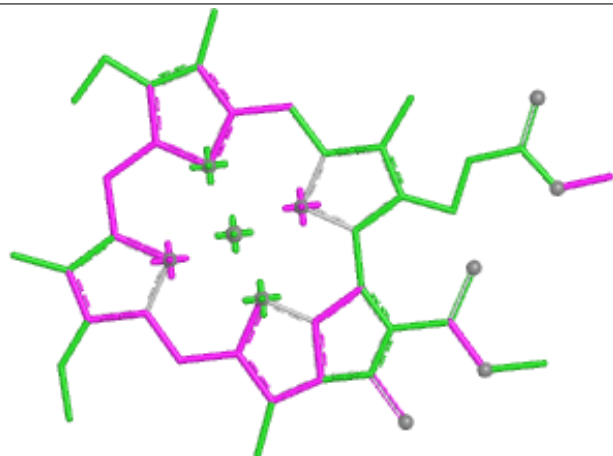




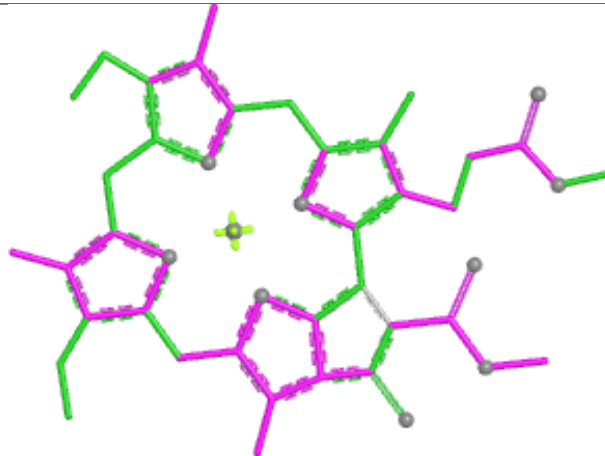
Ligand CLA G 1002



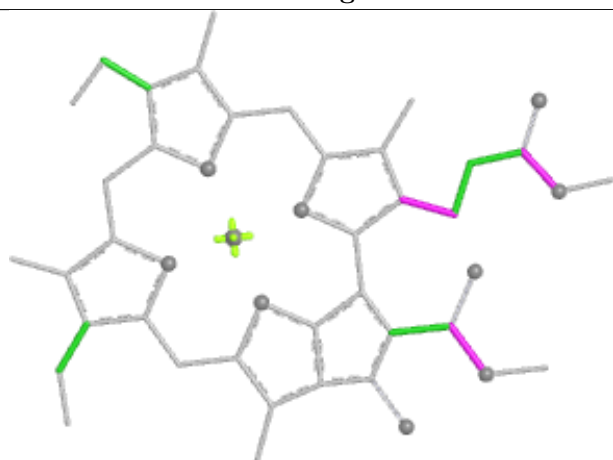
Ligand CLA A 1108



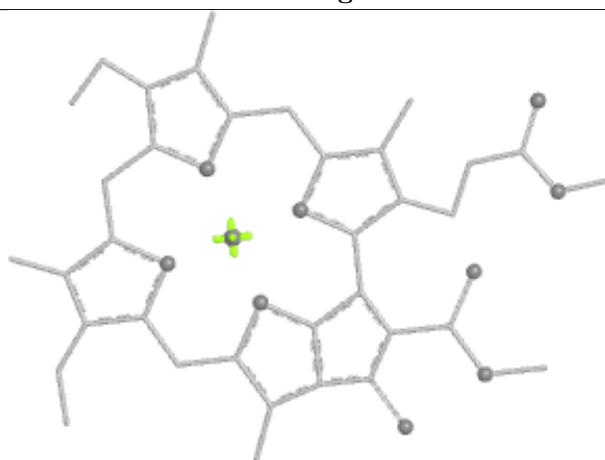
Bond lengths



Bond angles

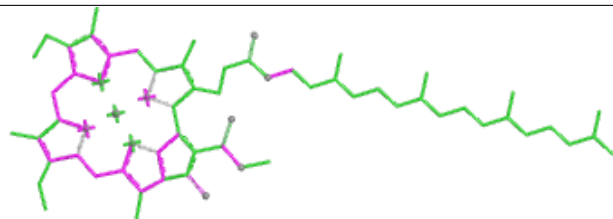


Torsions

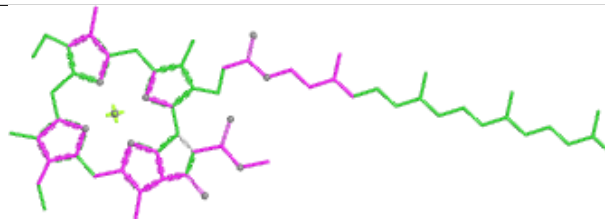


Rings

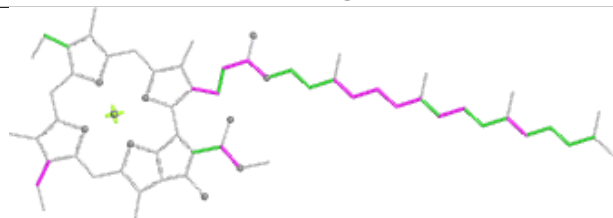
Ligand CLA B 1210



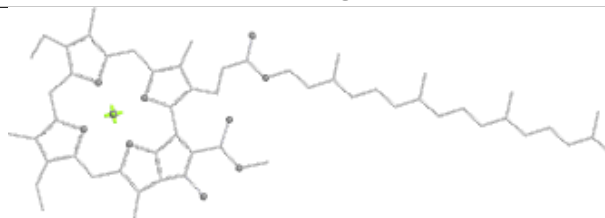
Bond lengths



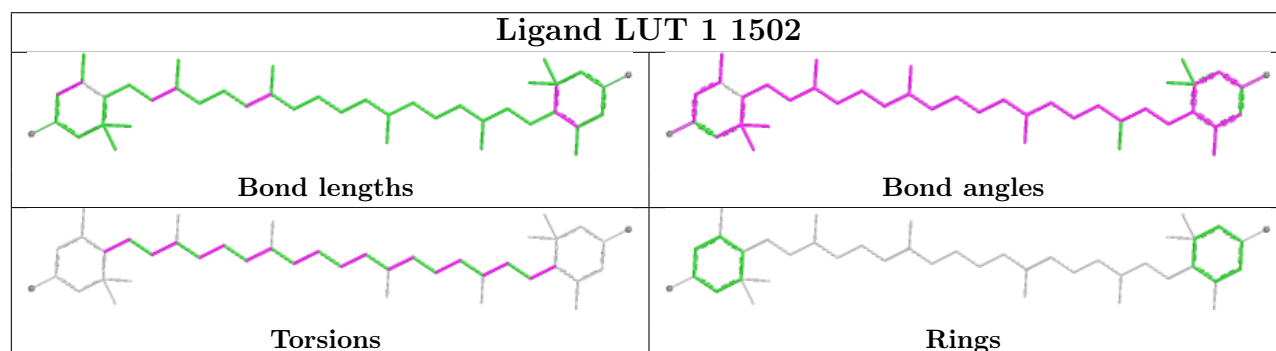
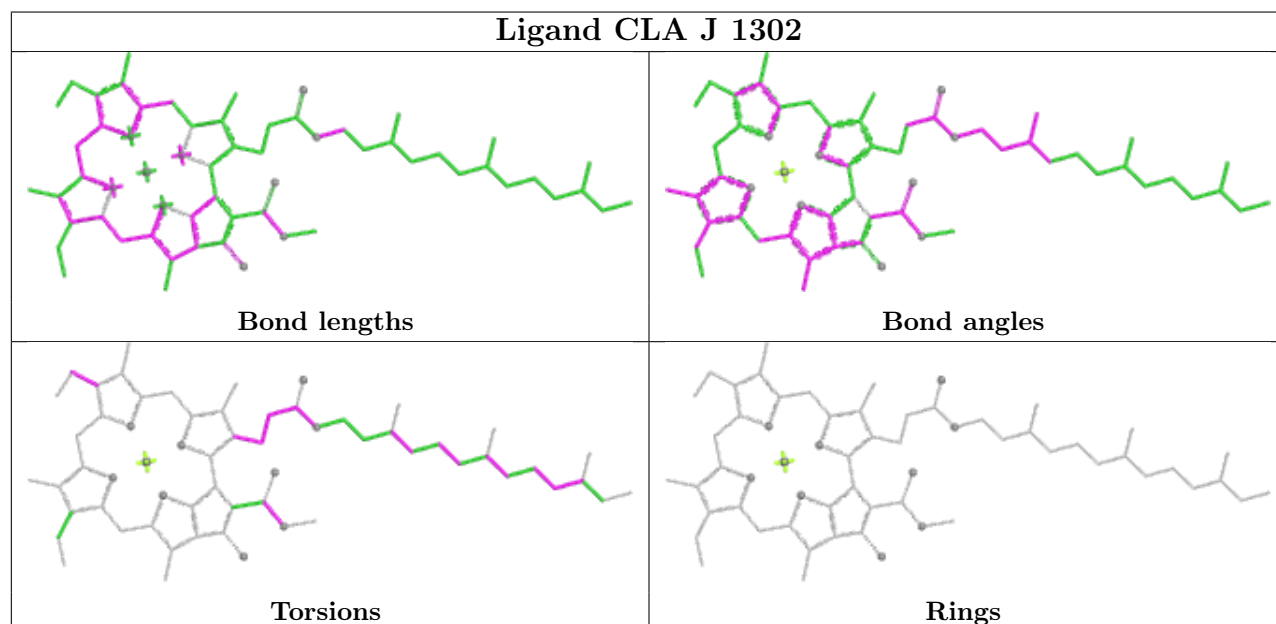
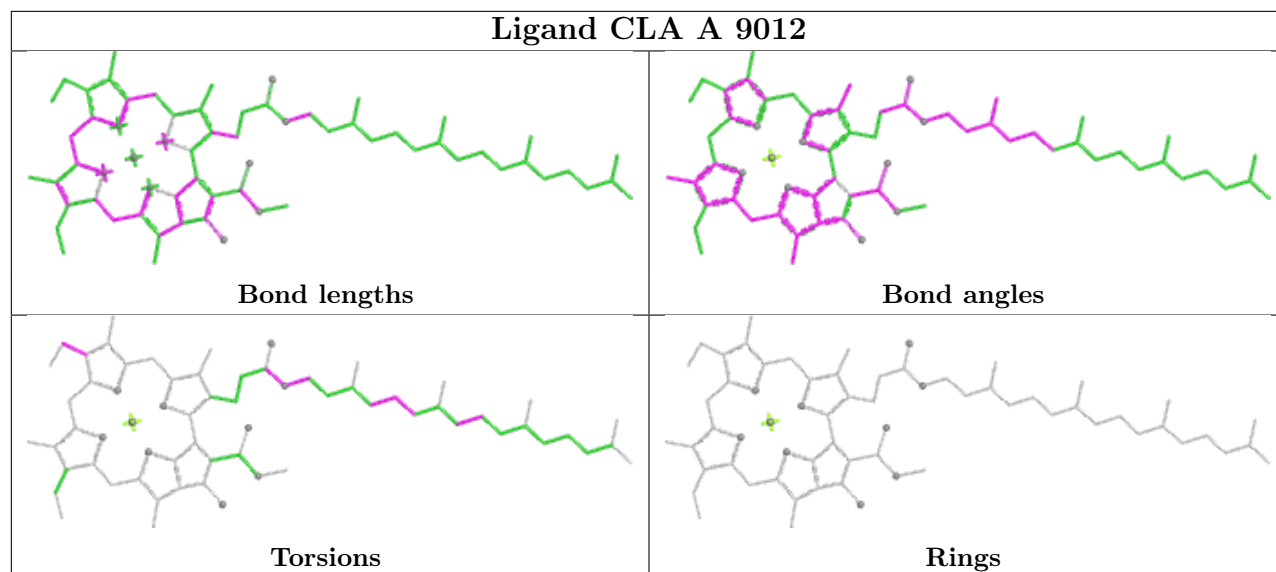
Bond angles

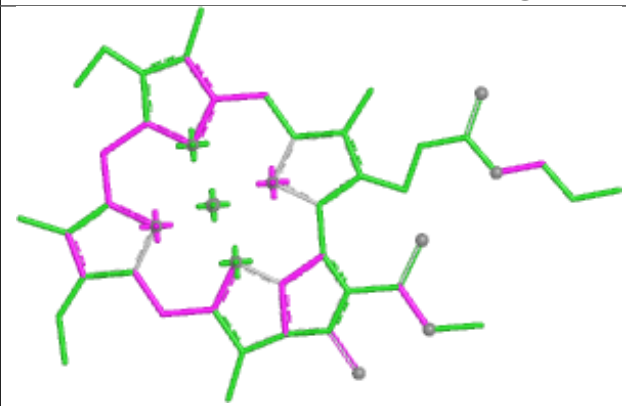
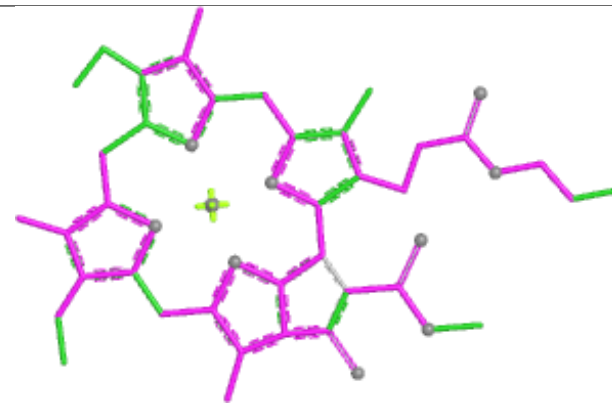
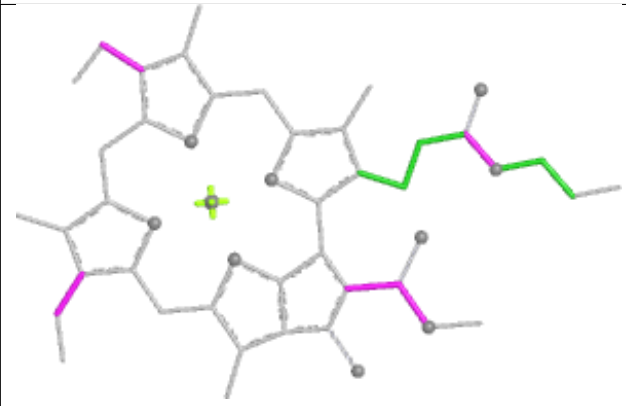
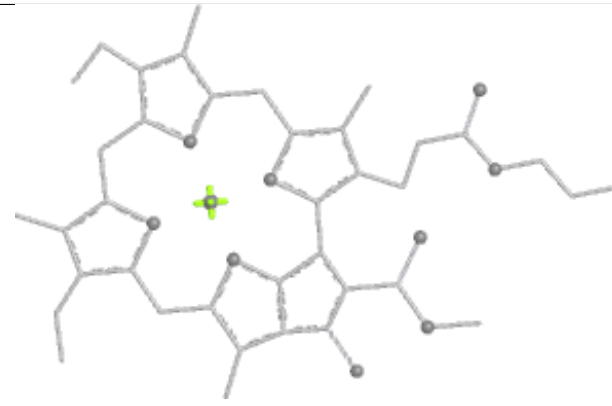


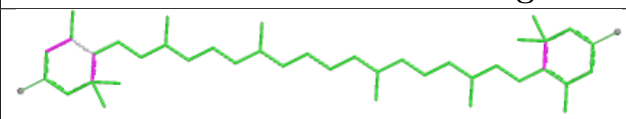
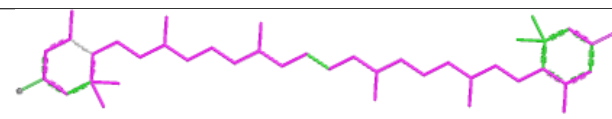
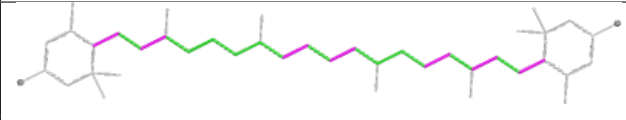
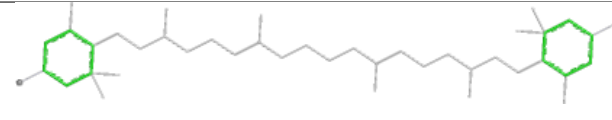
Torsions

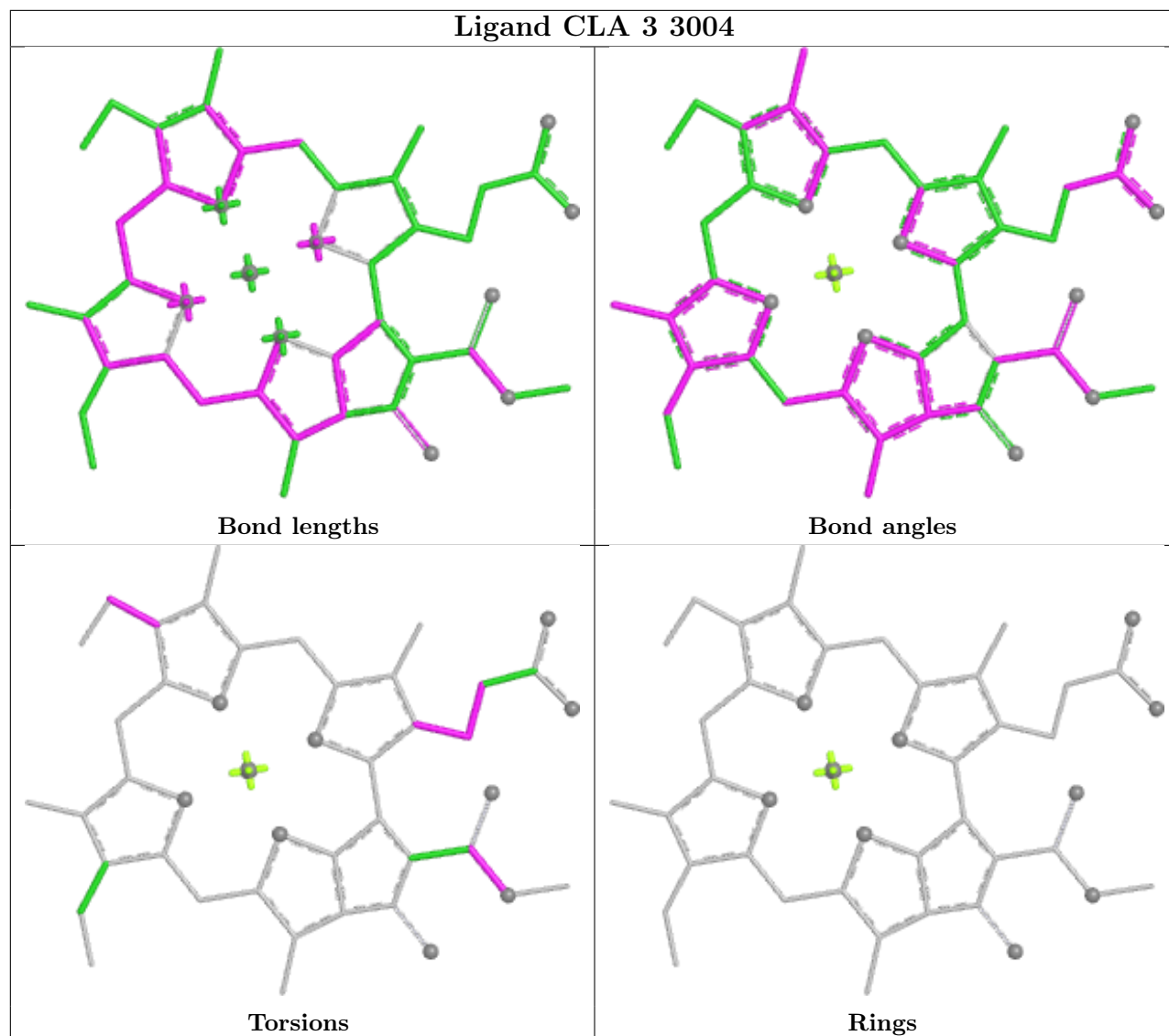


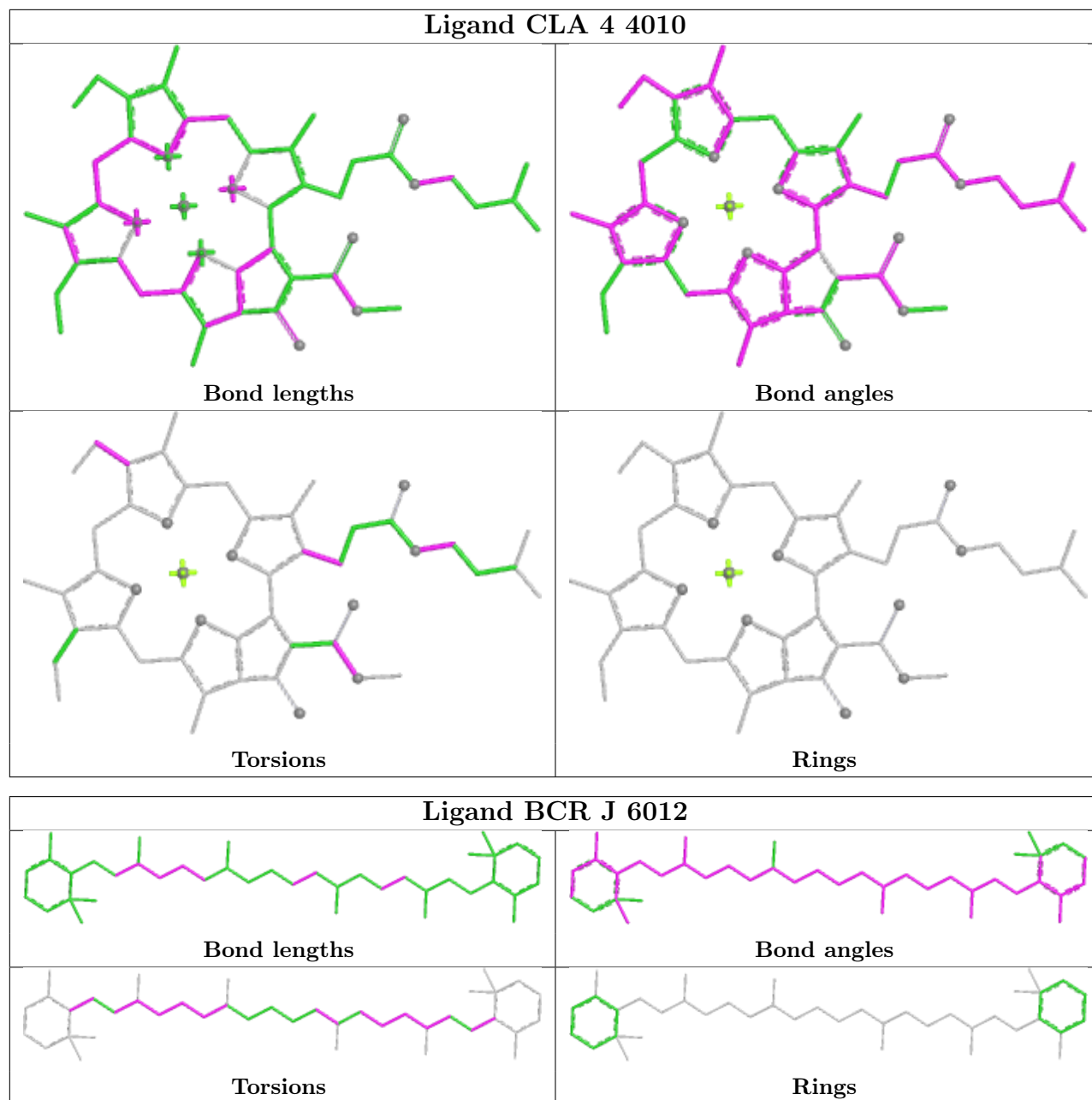
Rings

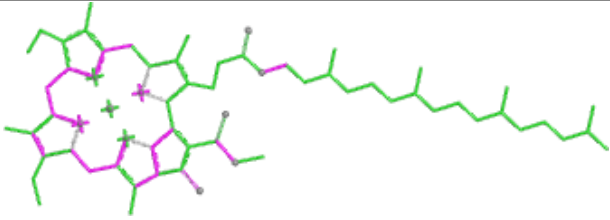
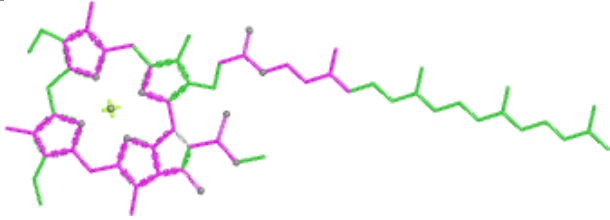
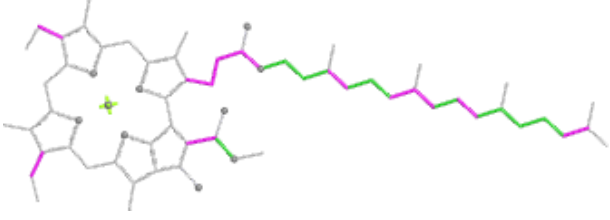
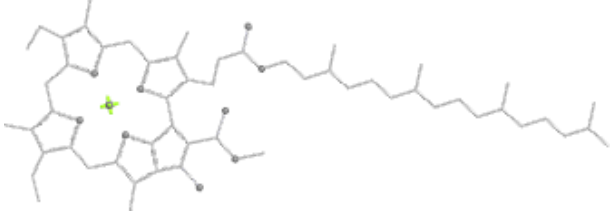
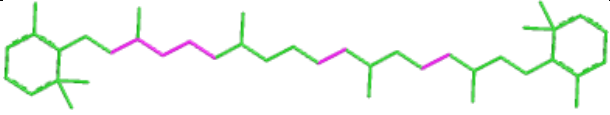
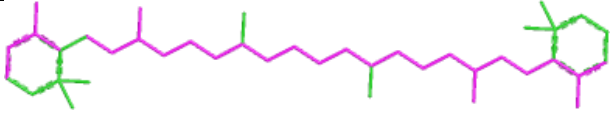
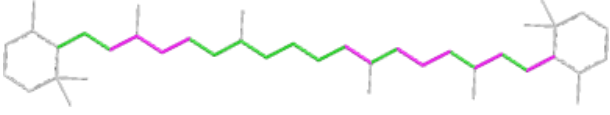
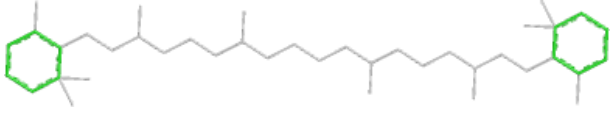
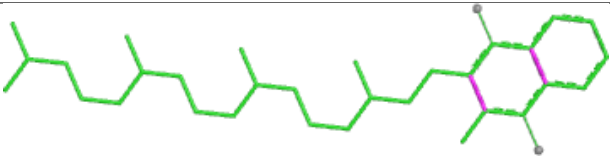
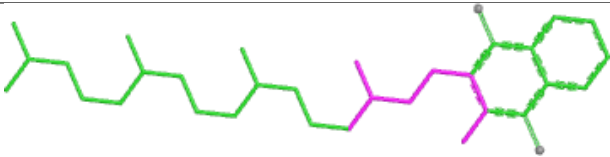
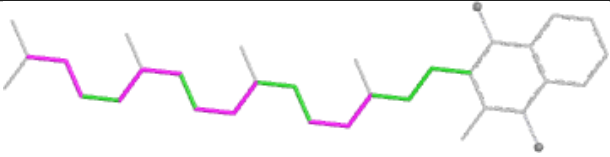
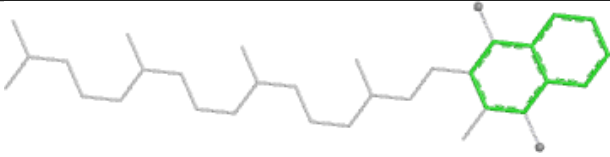


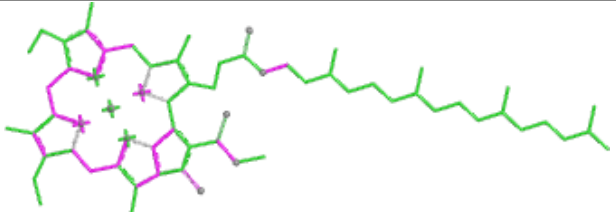
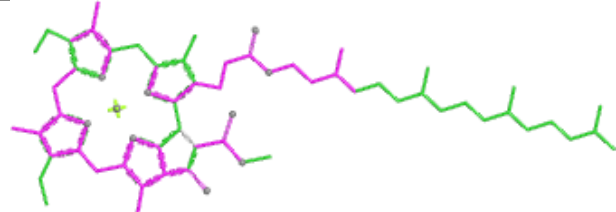
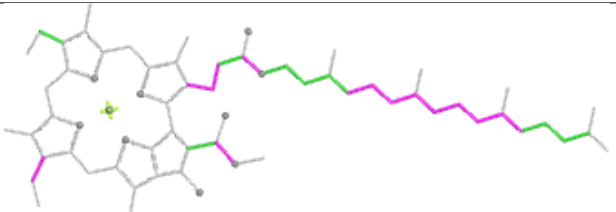
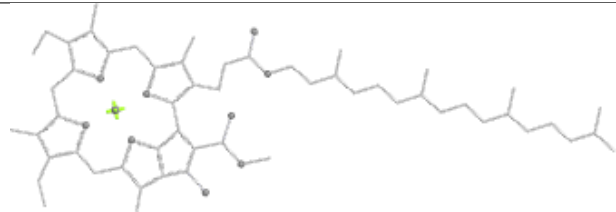
Ligand CLA 4 4008	
	
Bond lengths	Bond angles
	
Torsions	Rings

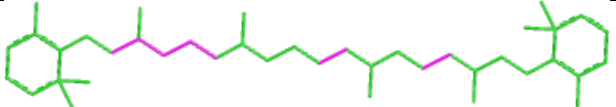
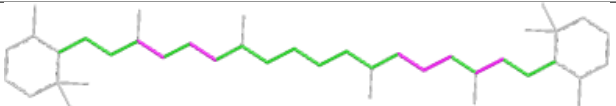
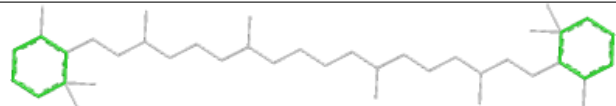
Ligand LUT 1 1501	
	
Bond lengths	Bond angles
	
Torsions	Rings

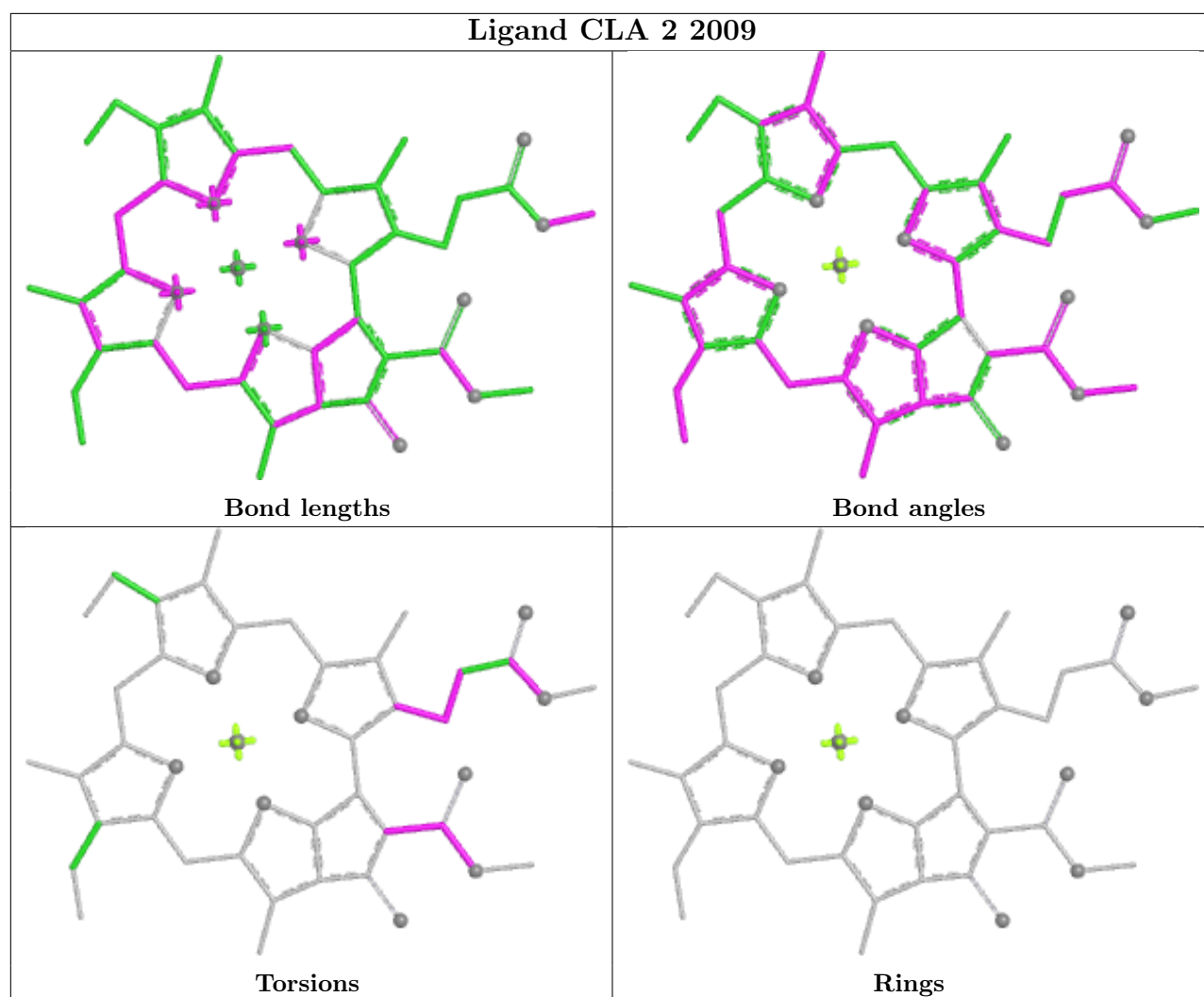




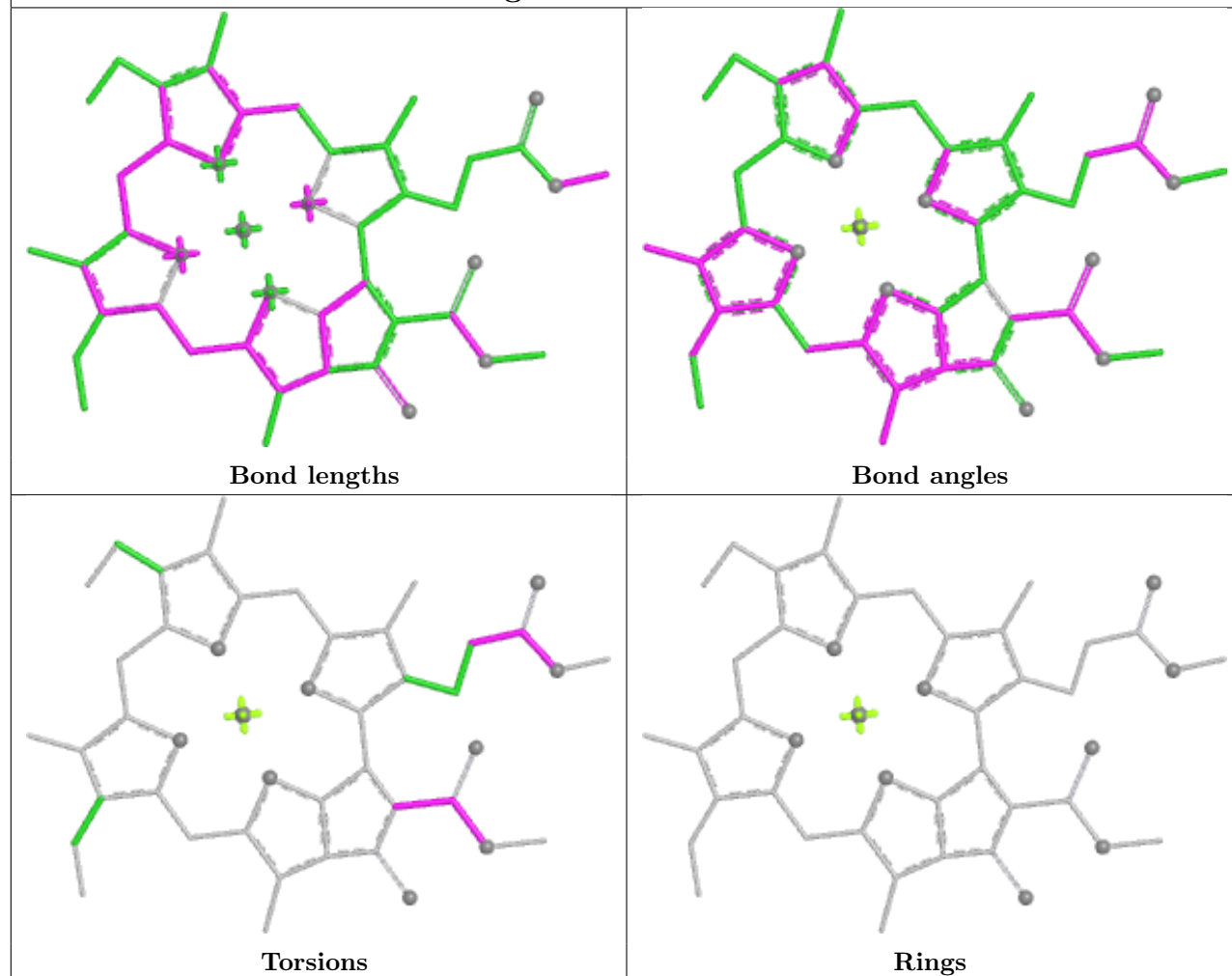
Ligand CLA 2 2008	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 6010	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PQN B 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings

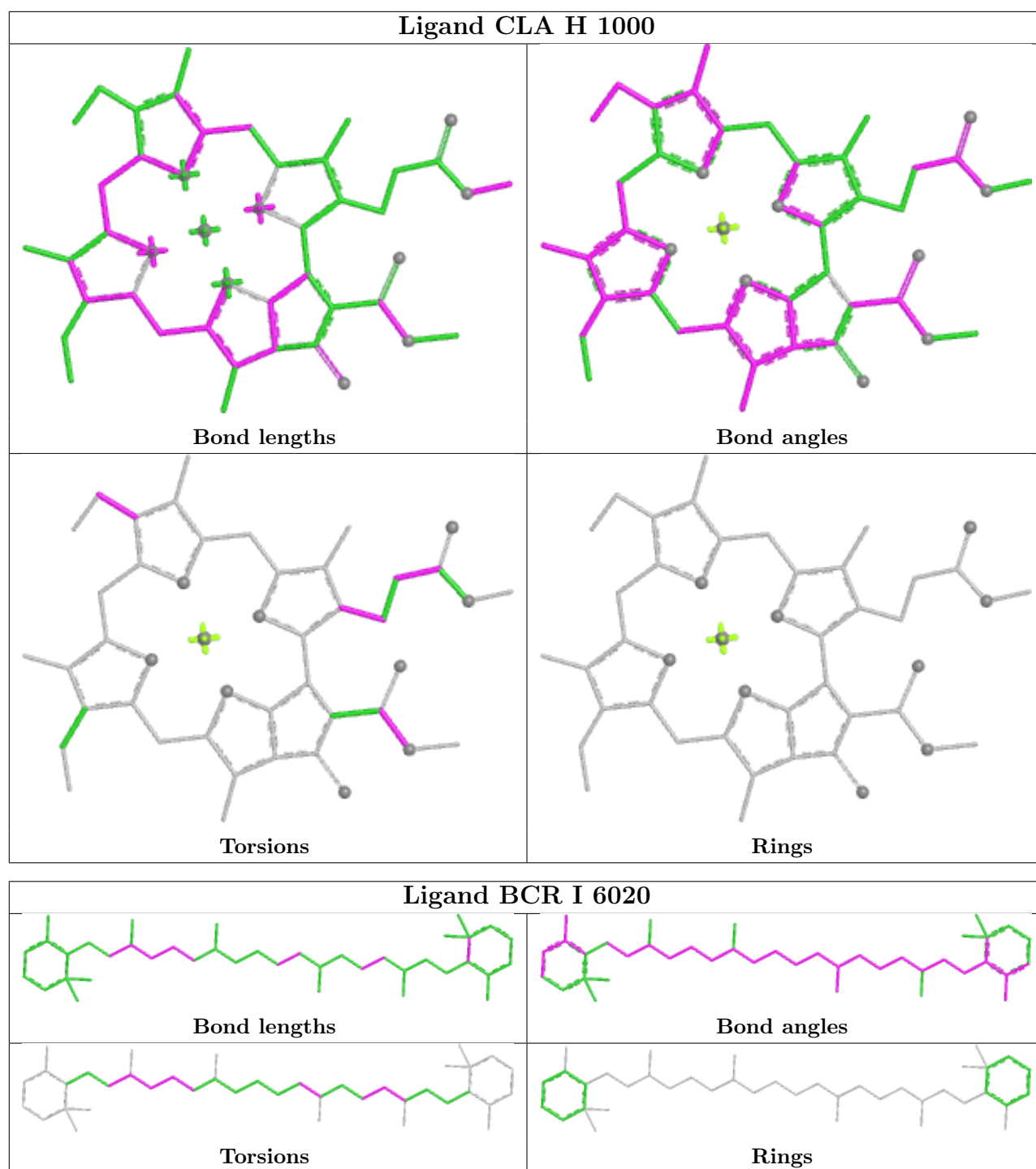
Ligand CLA 1 1013	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 6006	
	
Bond lengths	Bond angles
	
Torsions	Rings

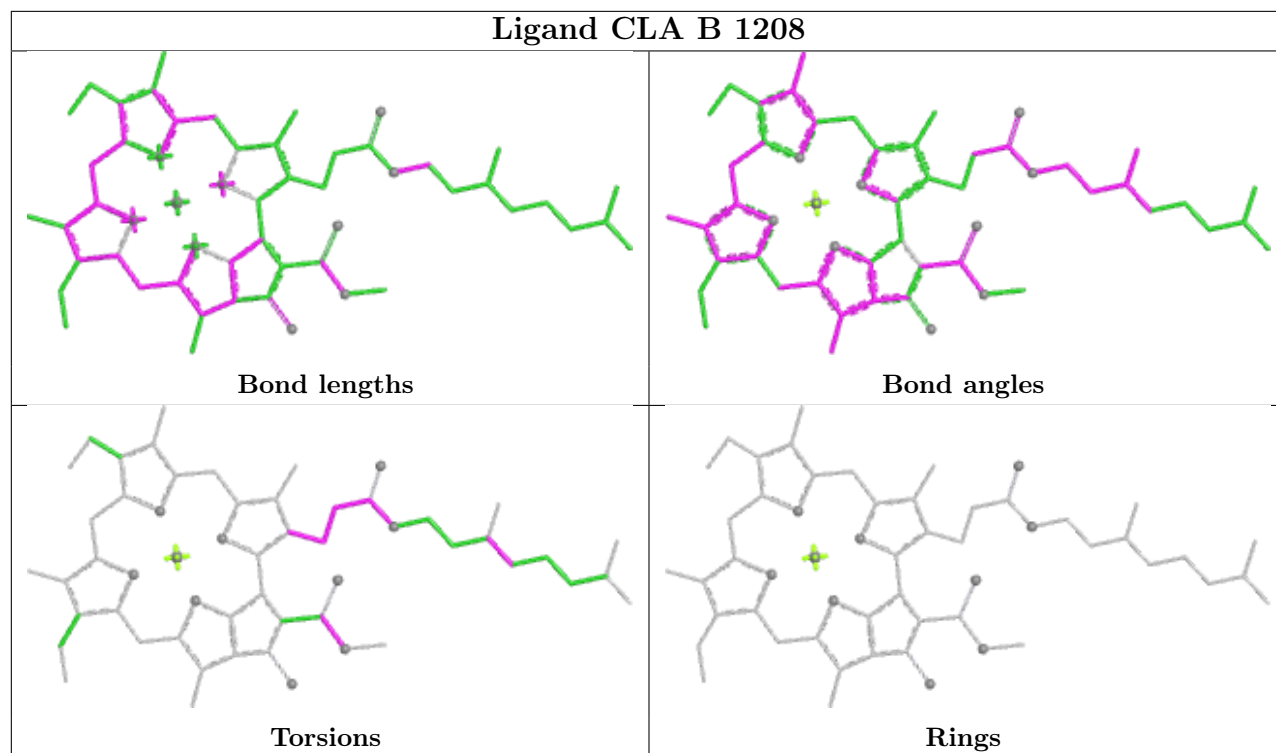


Ligand CLA A 1114

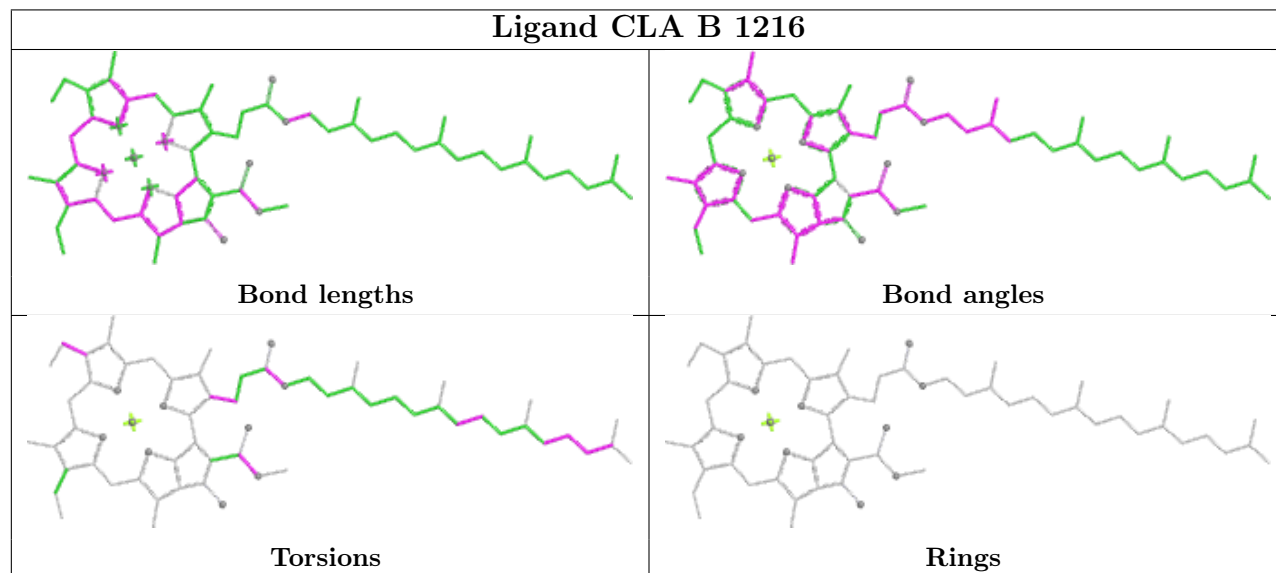




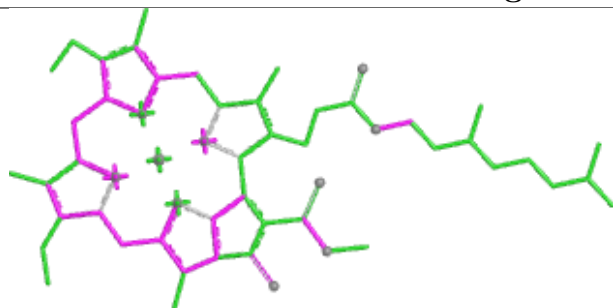
Ligand CLA B 1208



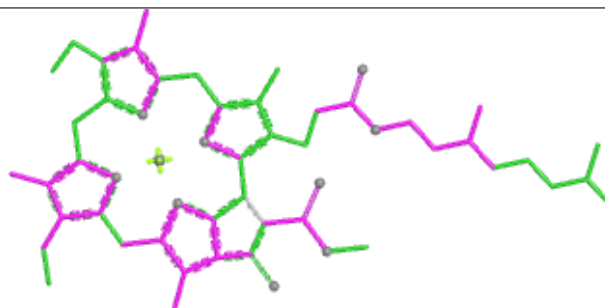
Ligand CLA B 1216



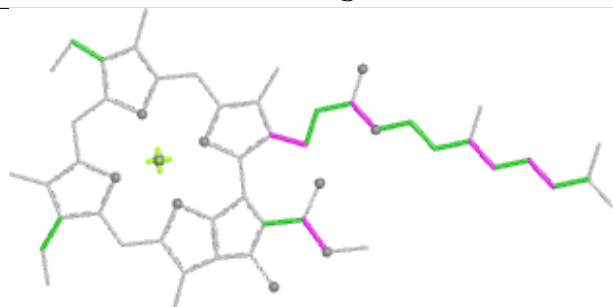
Ligand CLA A 1124



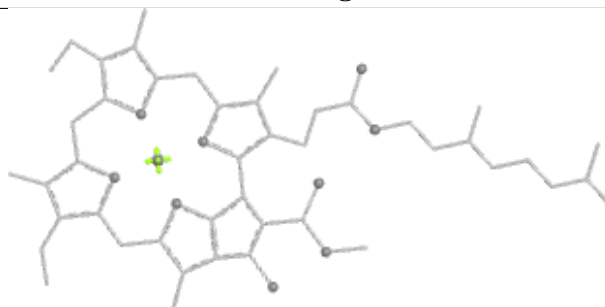
Bond lengths



Bond angles

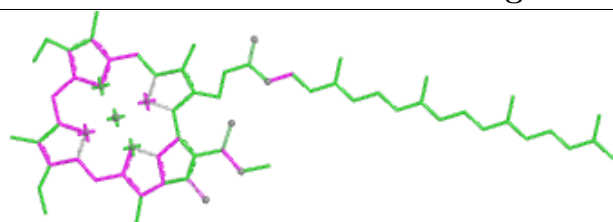


Torsions

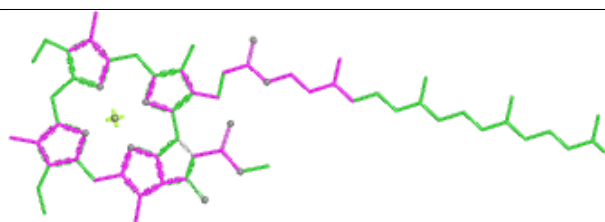


Rings

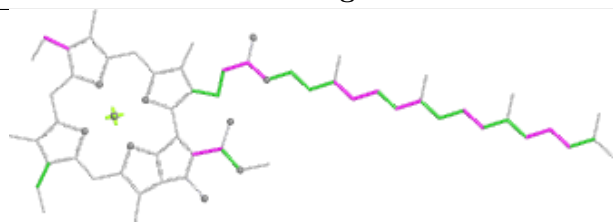
Ligand CLA B 1235



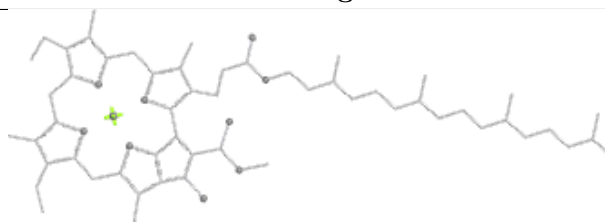
Bond lengths



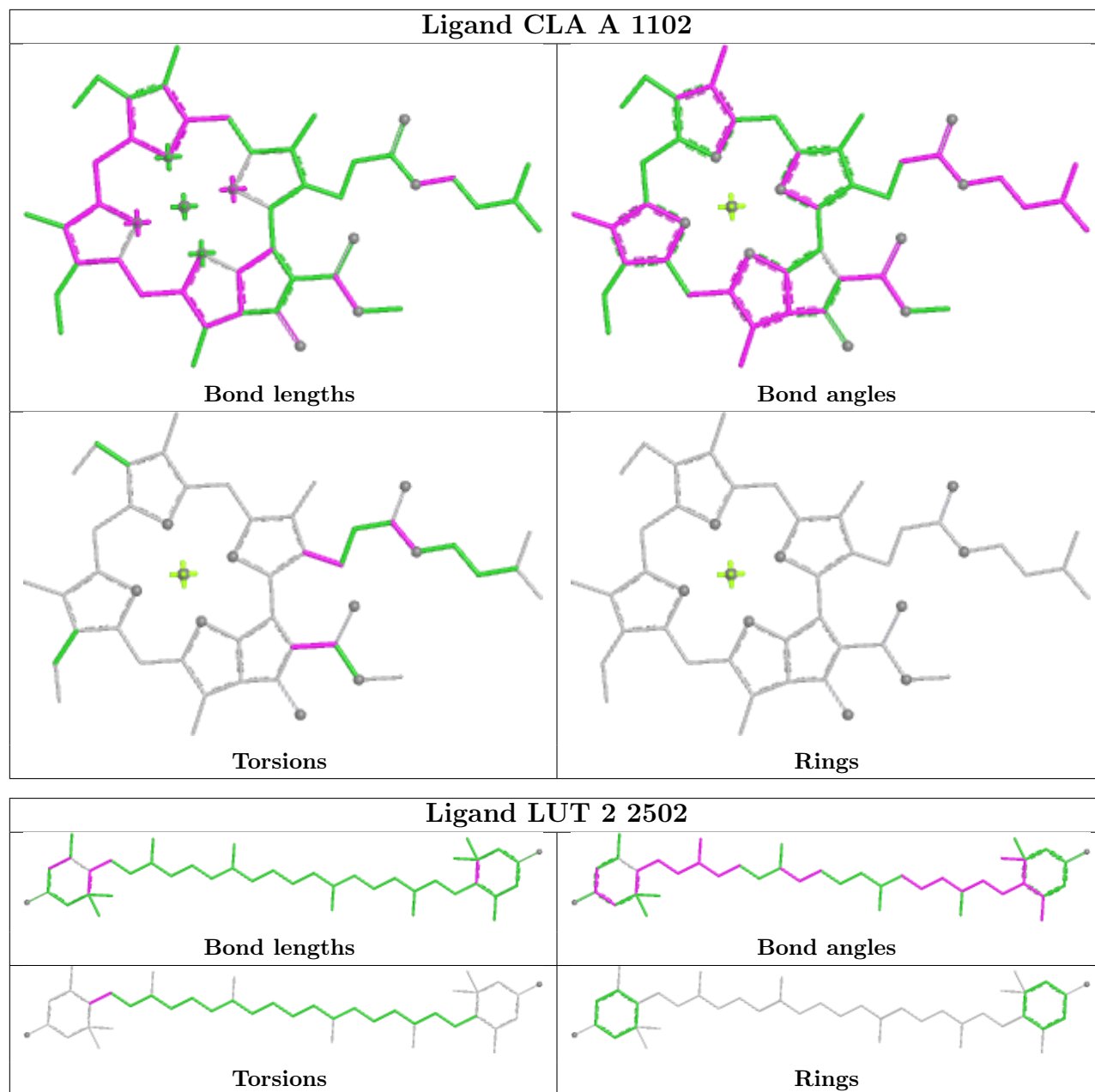
Bond angles



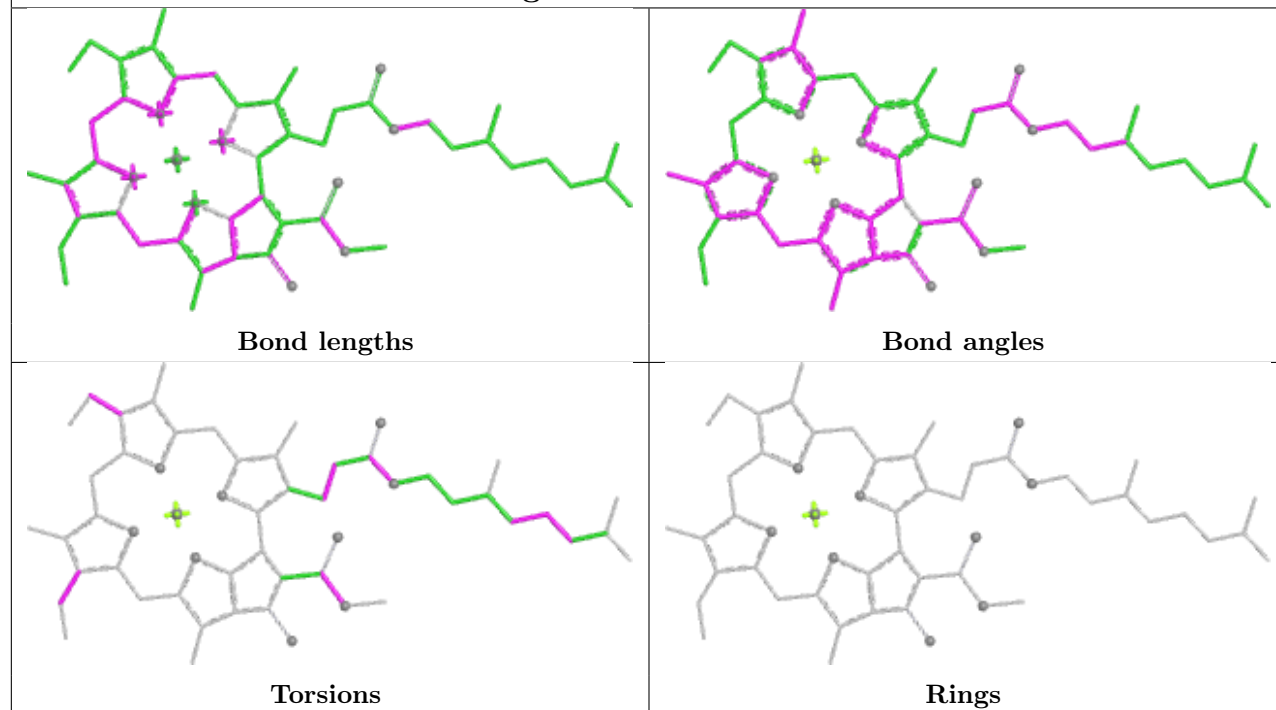
Torsions



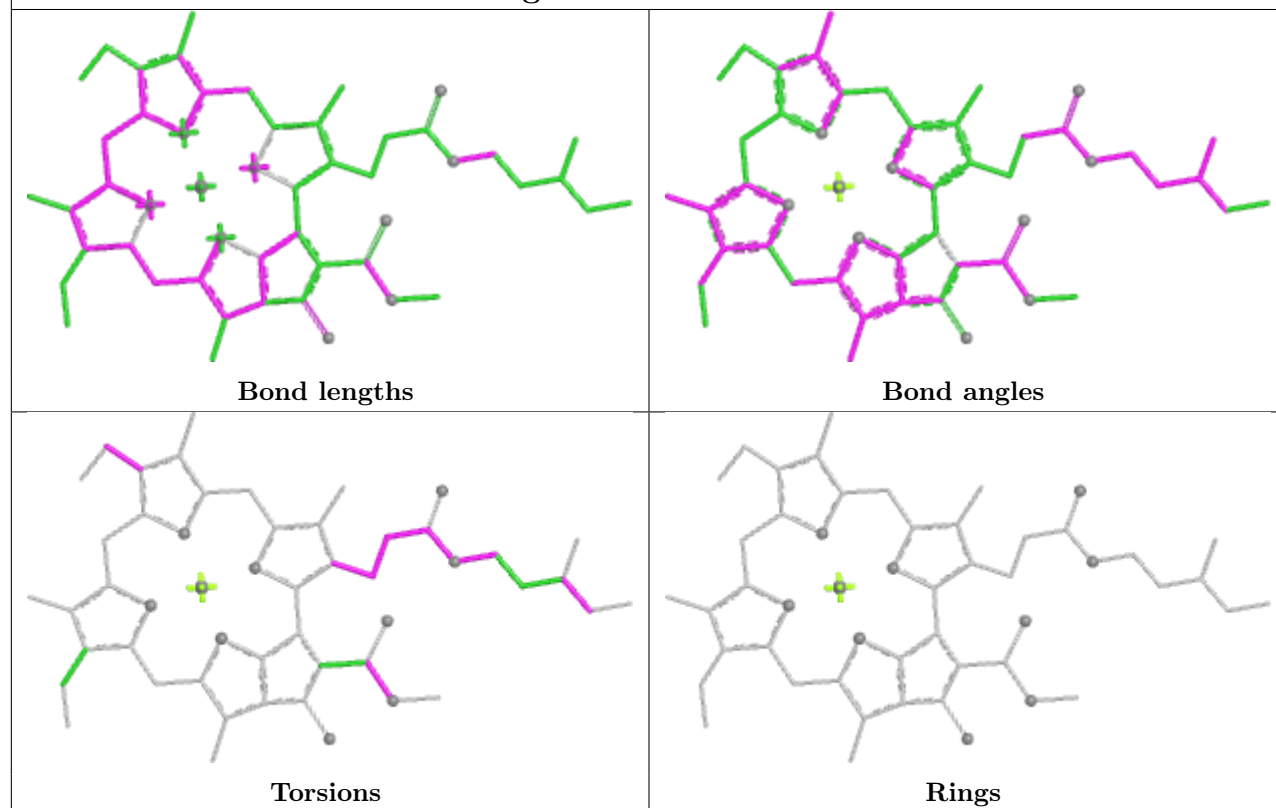
Rings

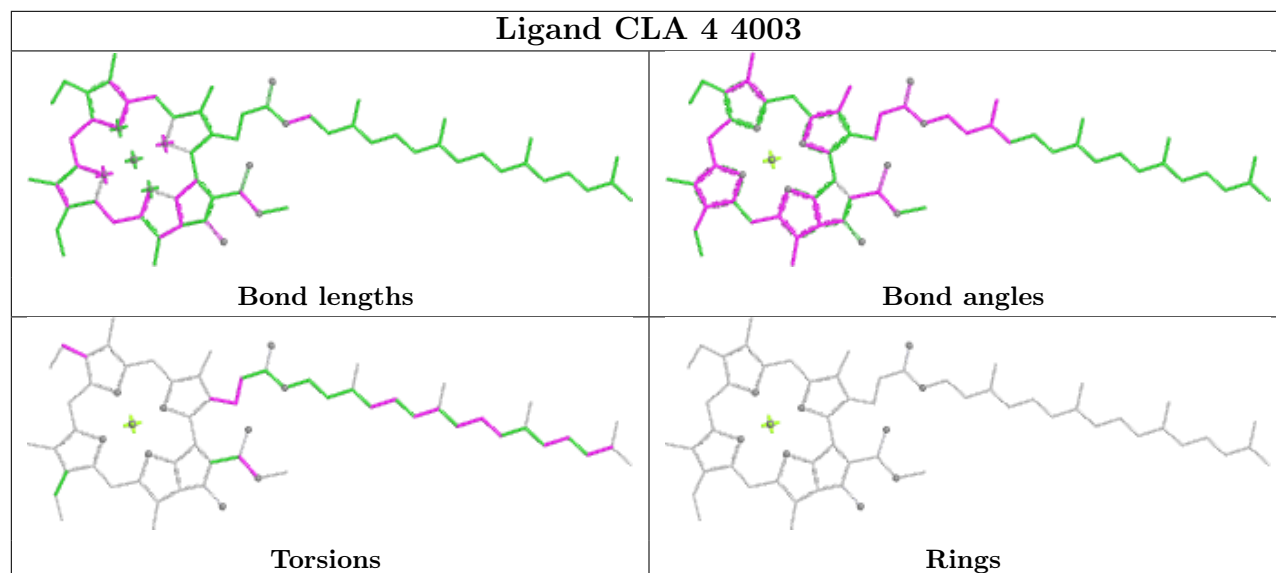
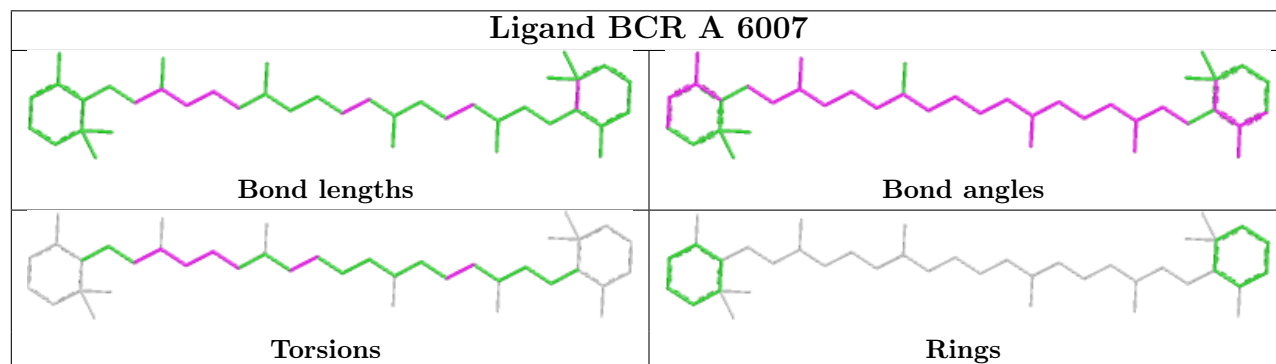
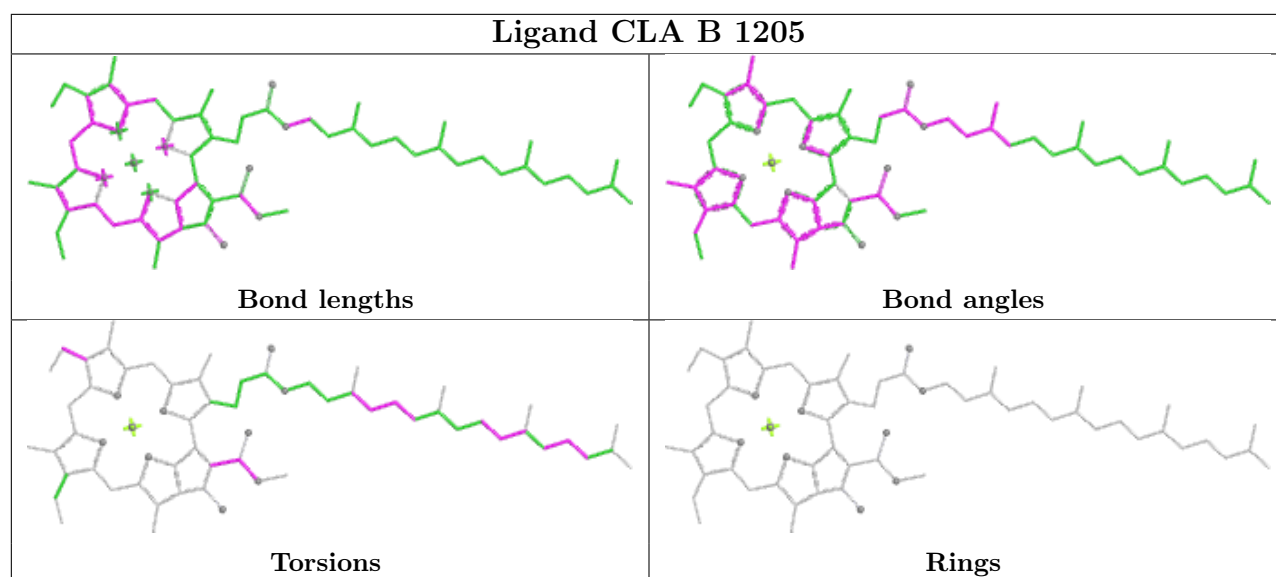


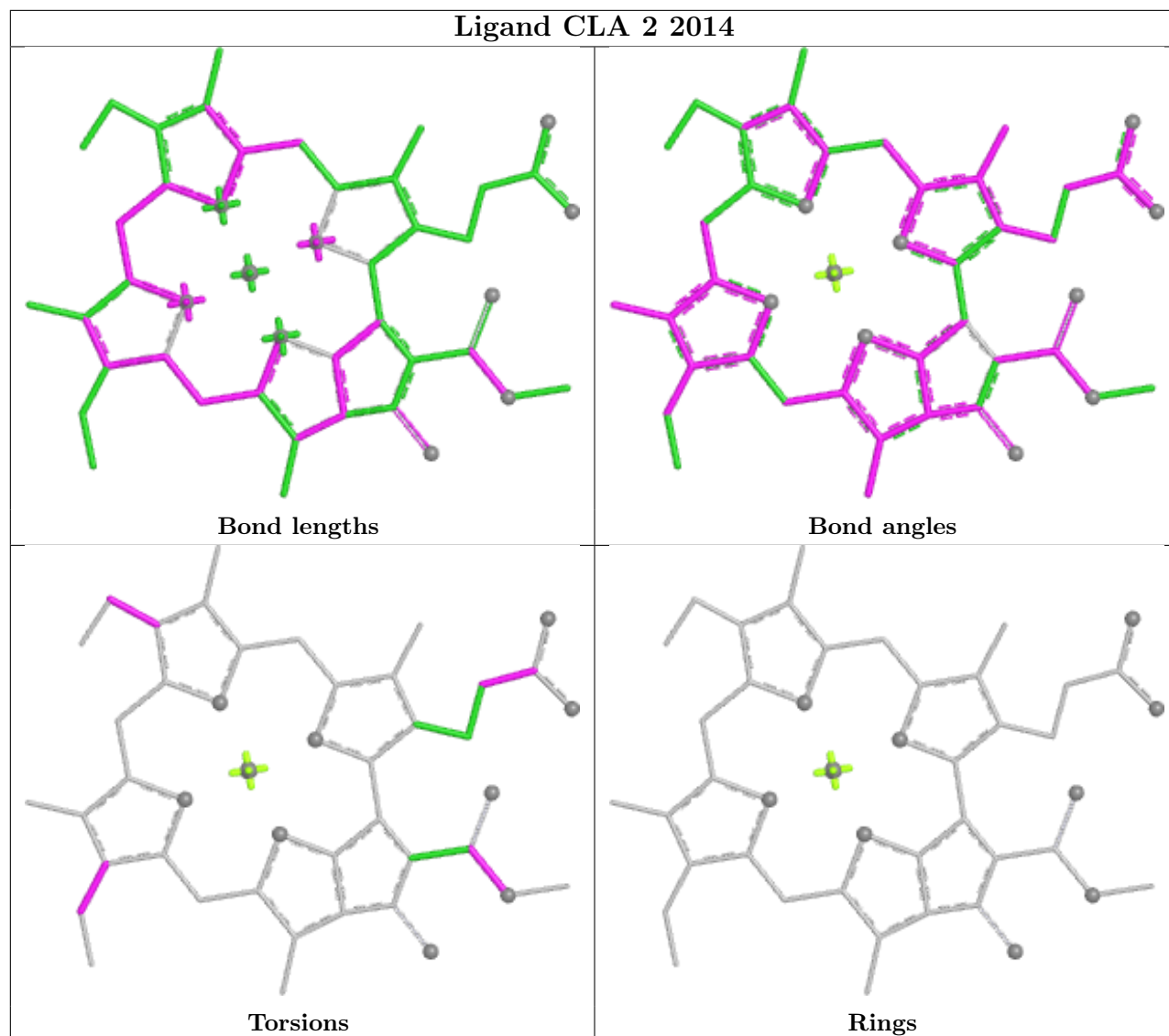
Ligand CLA A 1125

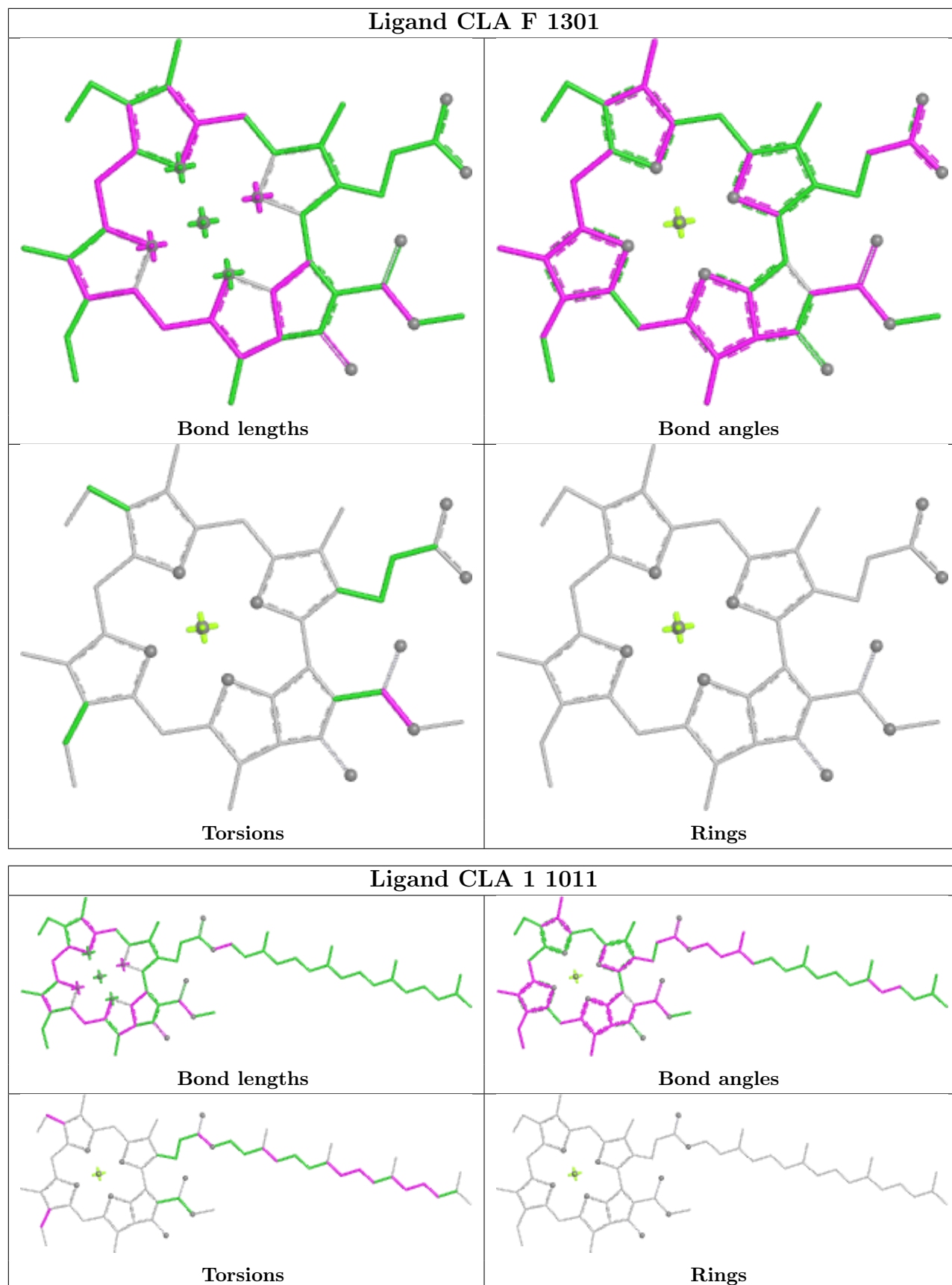


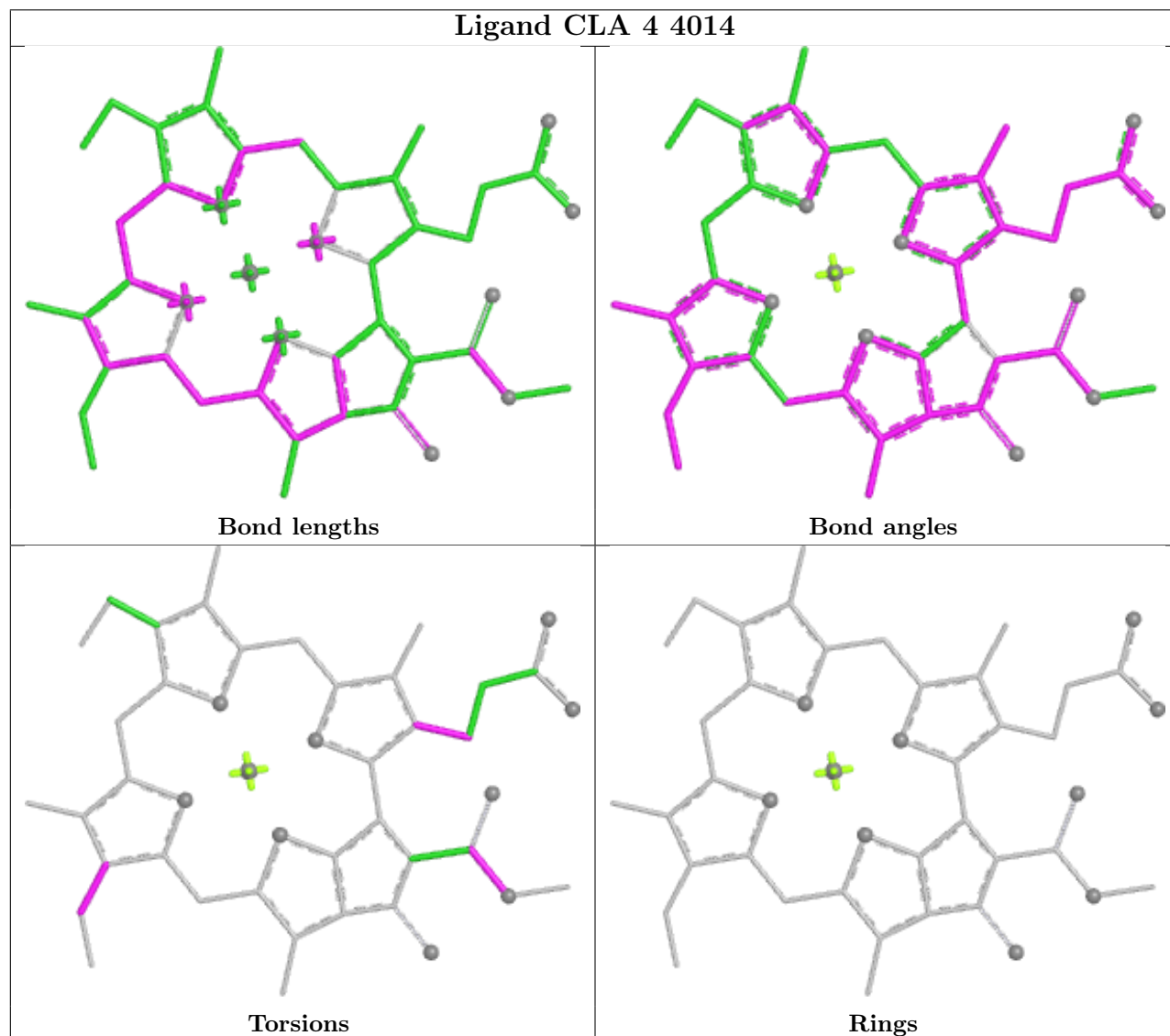
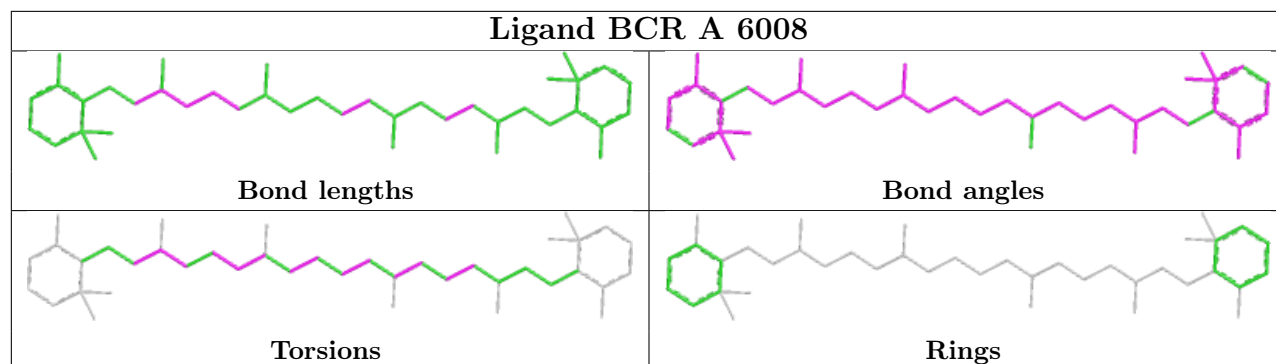
Ligand CLA A 1105

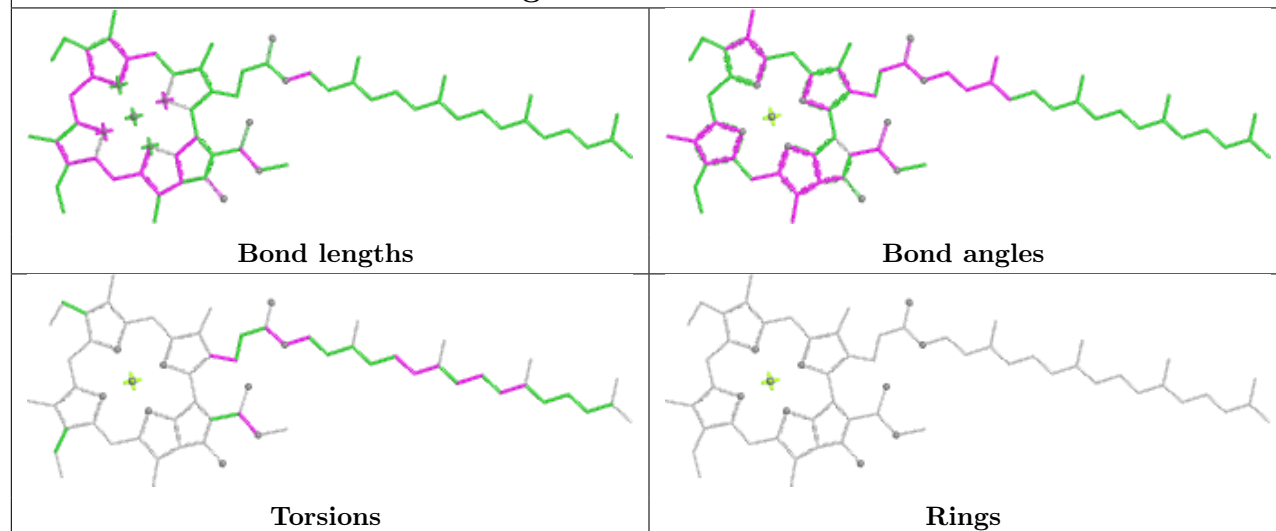
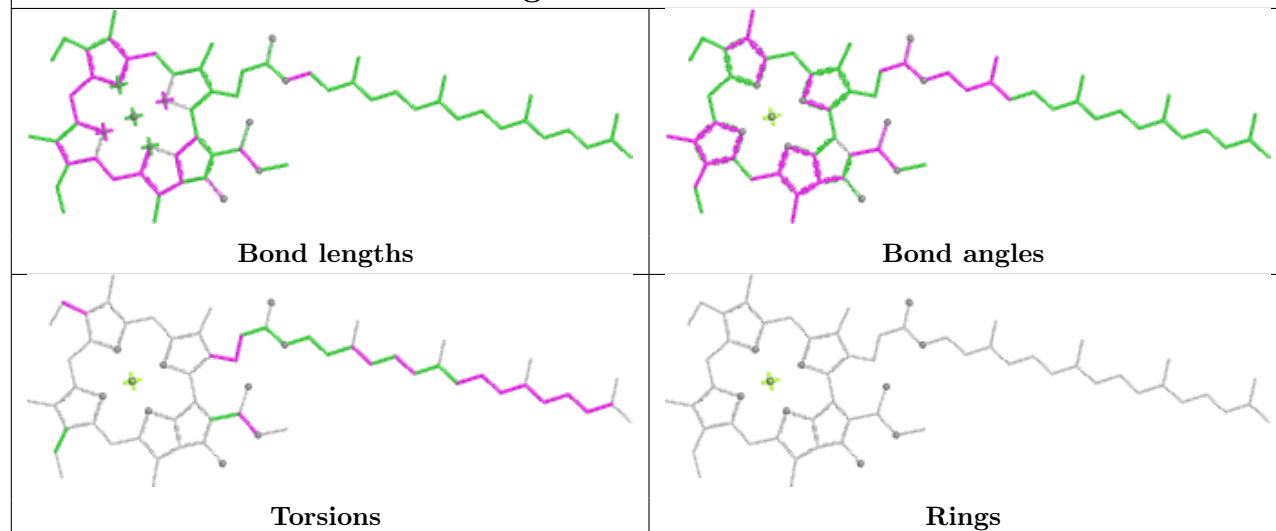


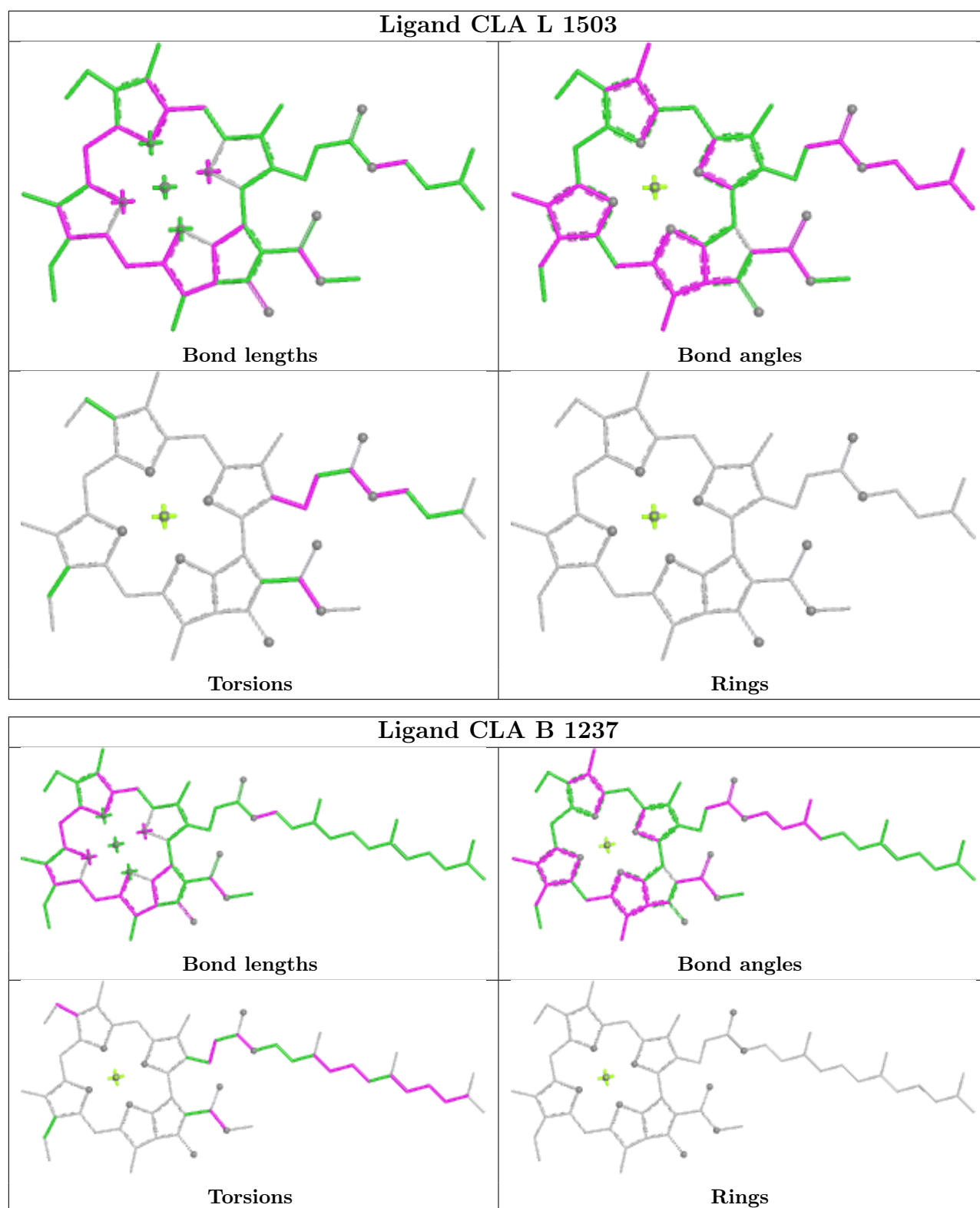




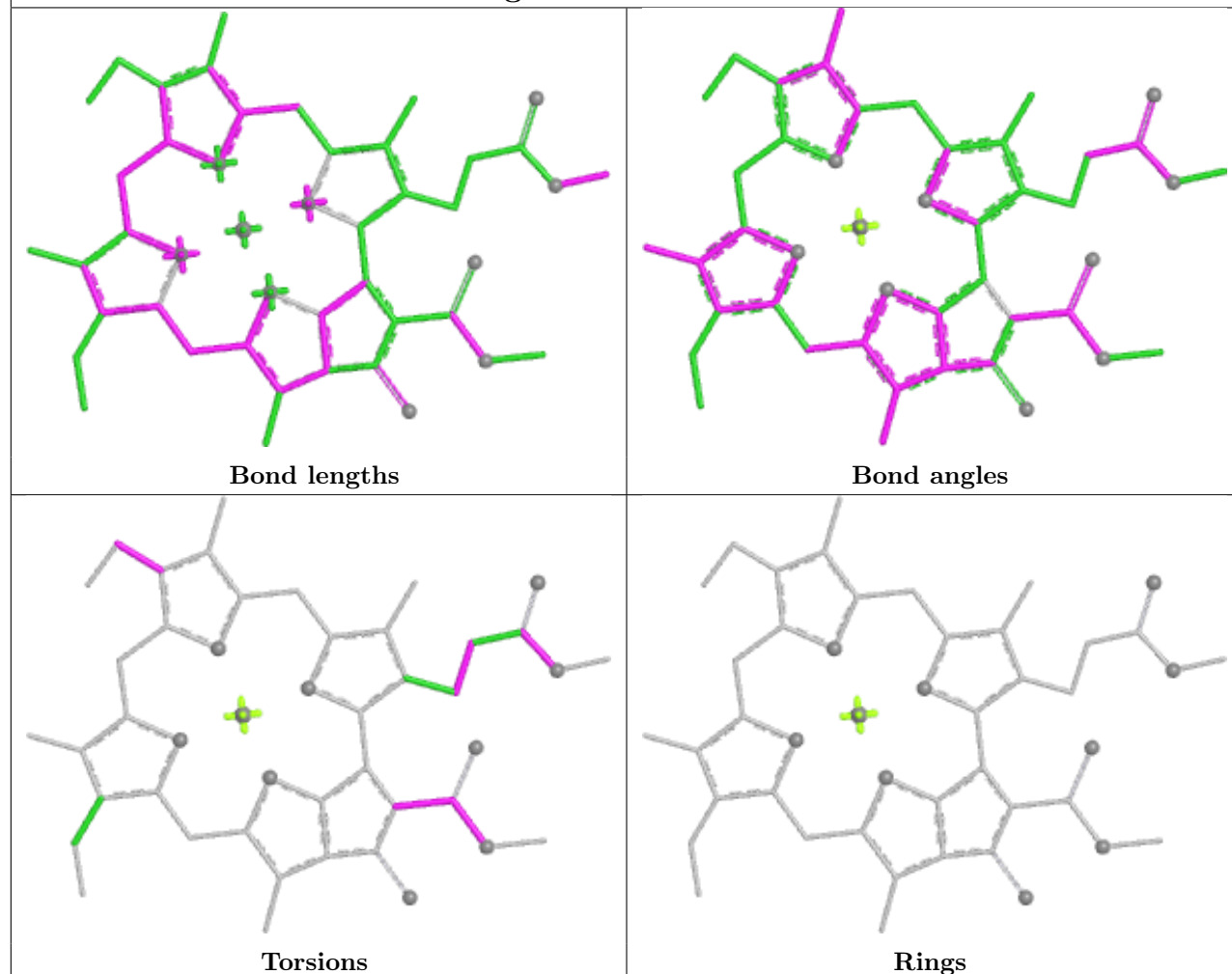




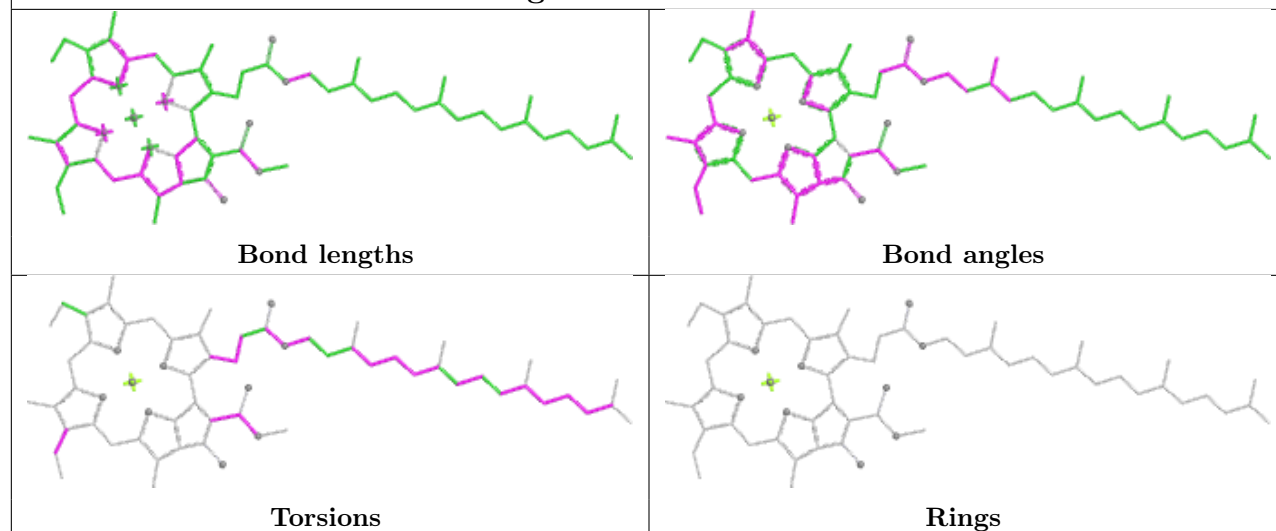
Ligand CLA A 1104**Ligand CLA B 1225**

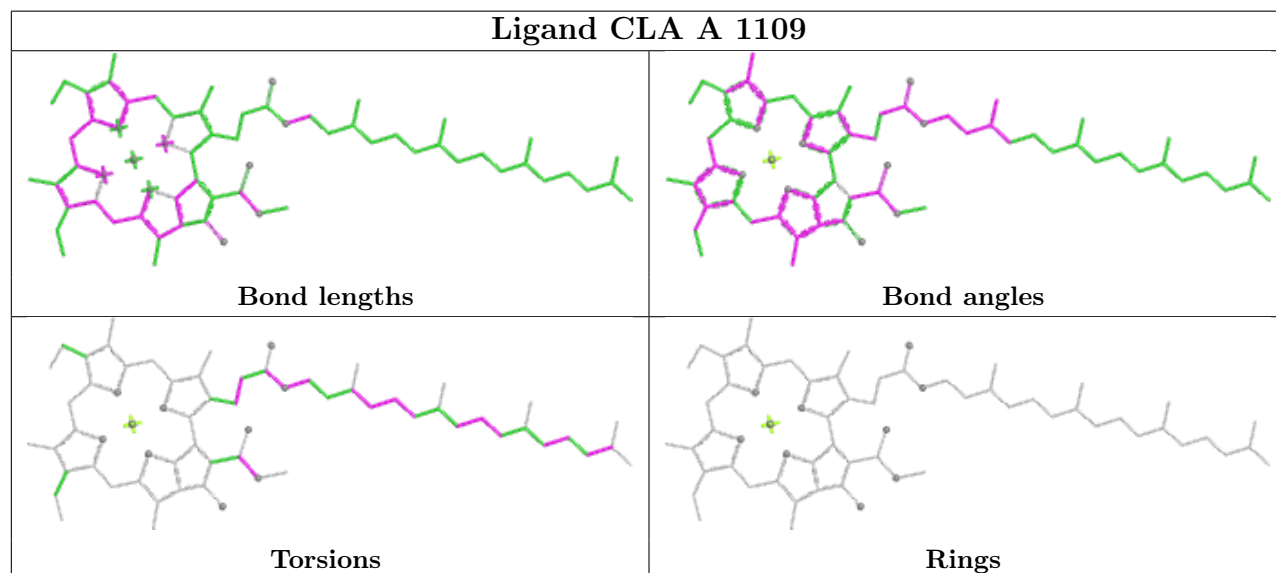
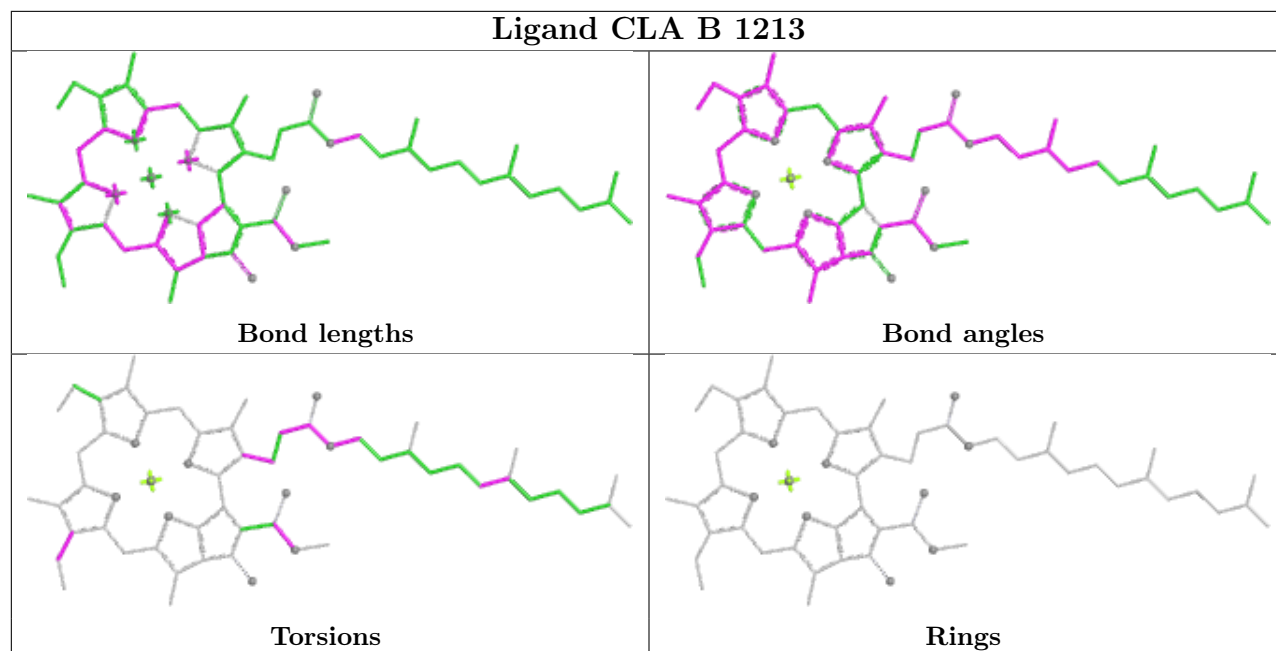


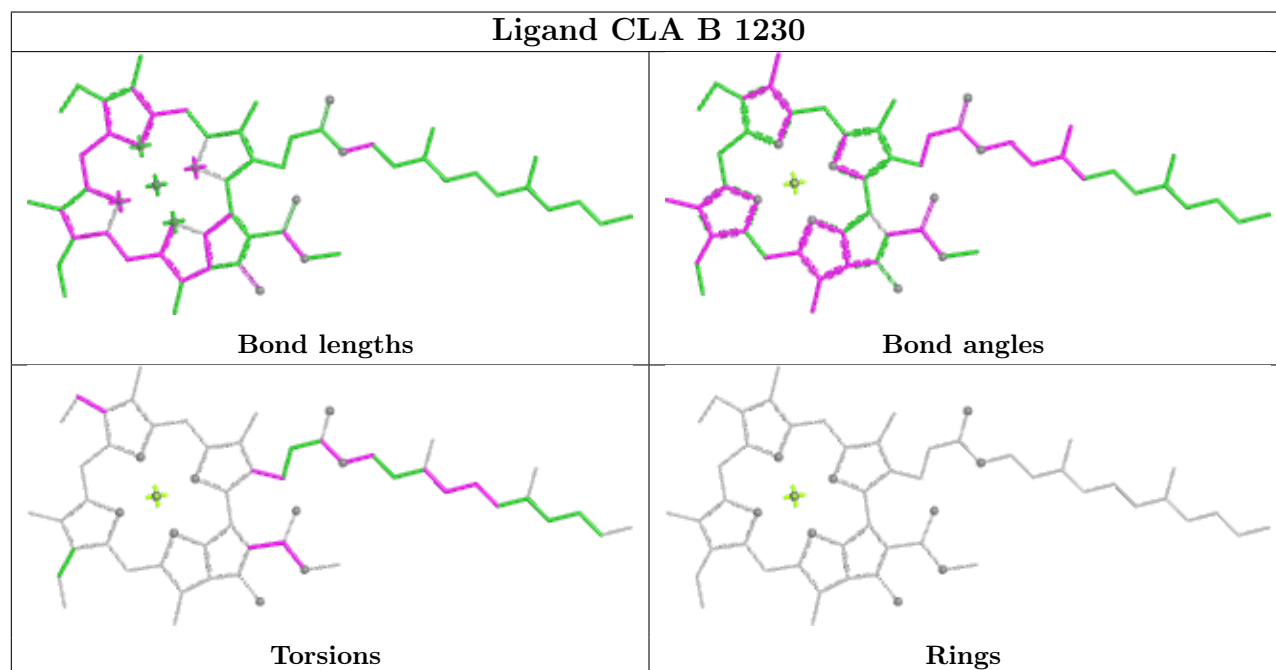
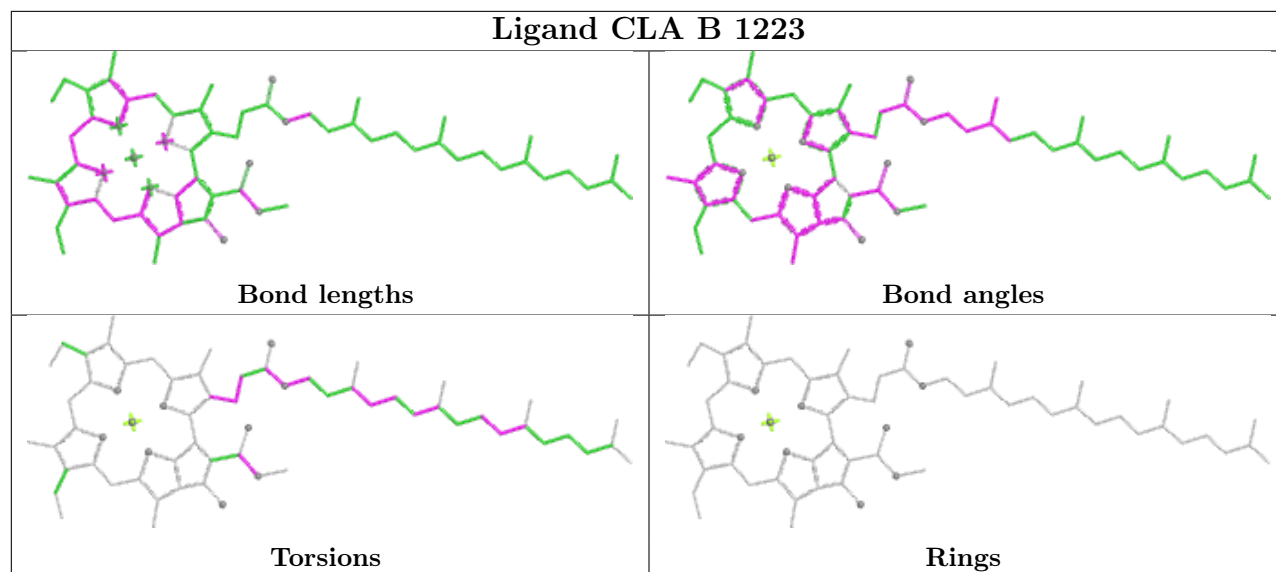
Ligand CLA A 1121

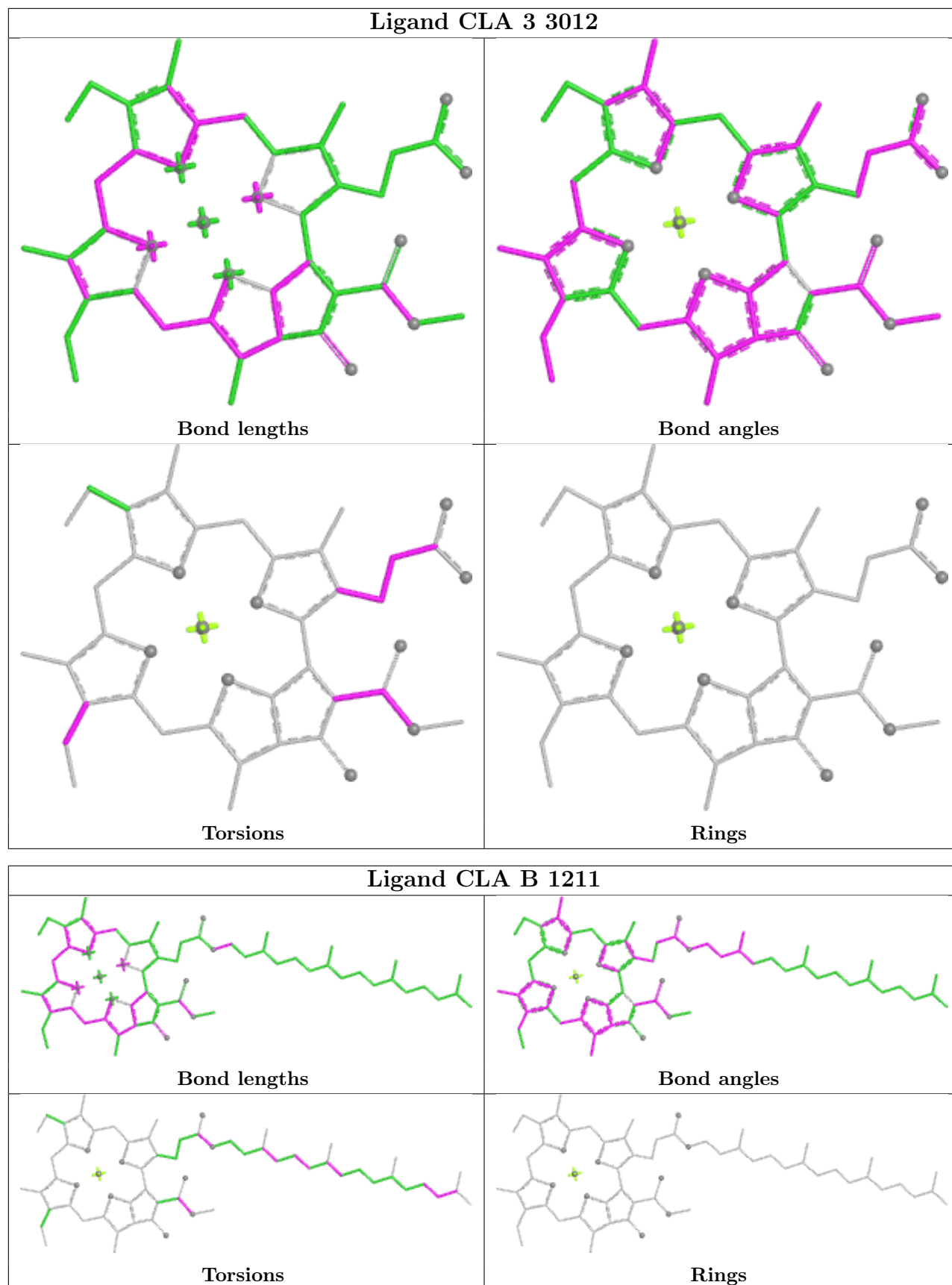


Ligand CLA 3 3008

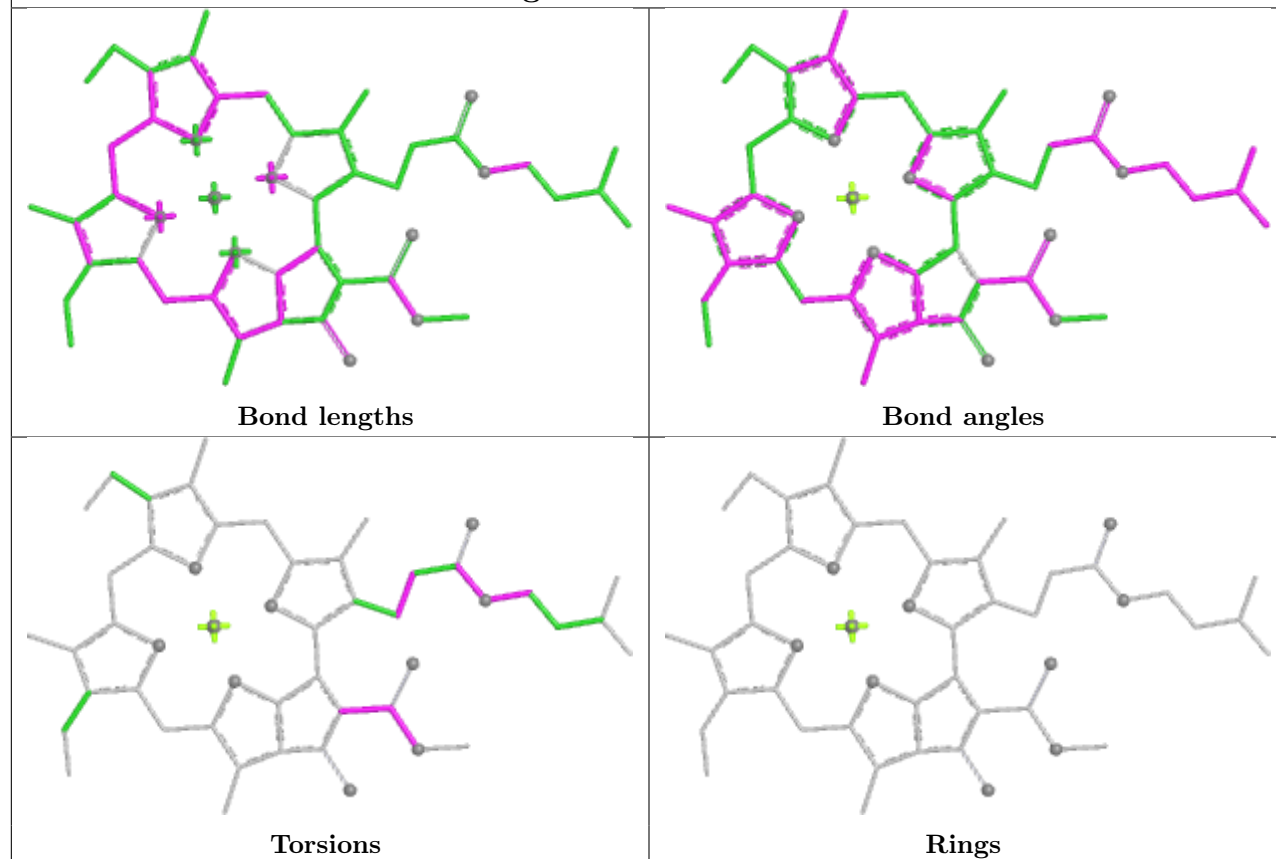




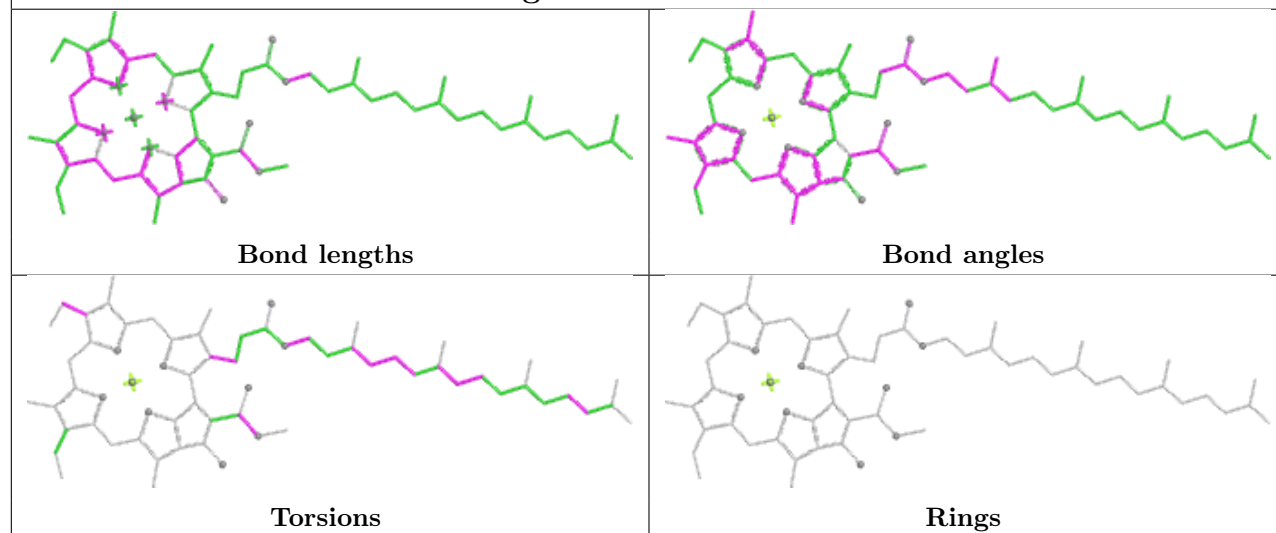


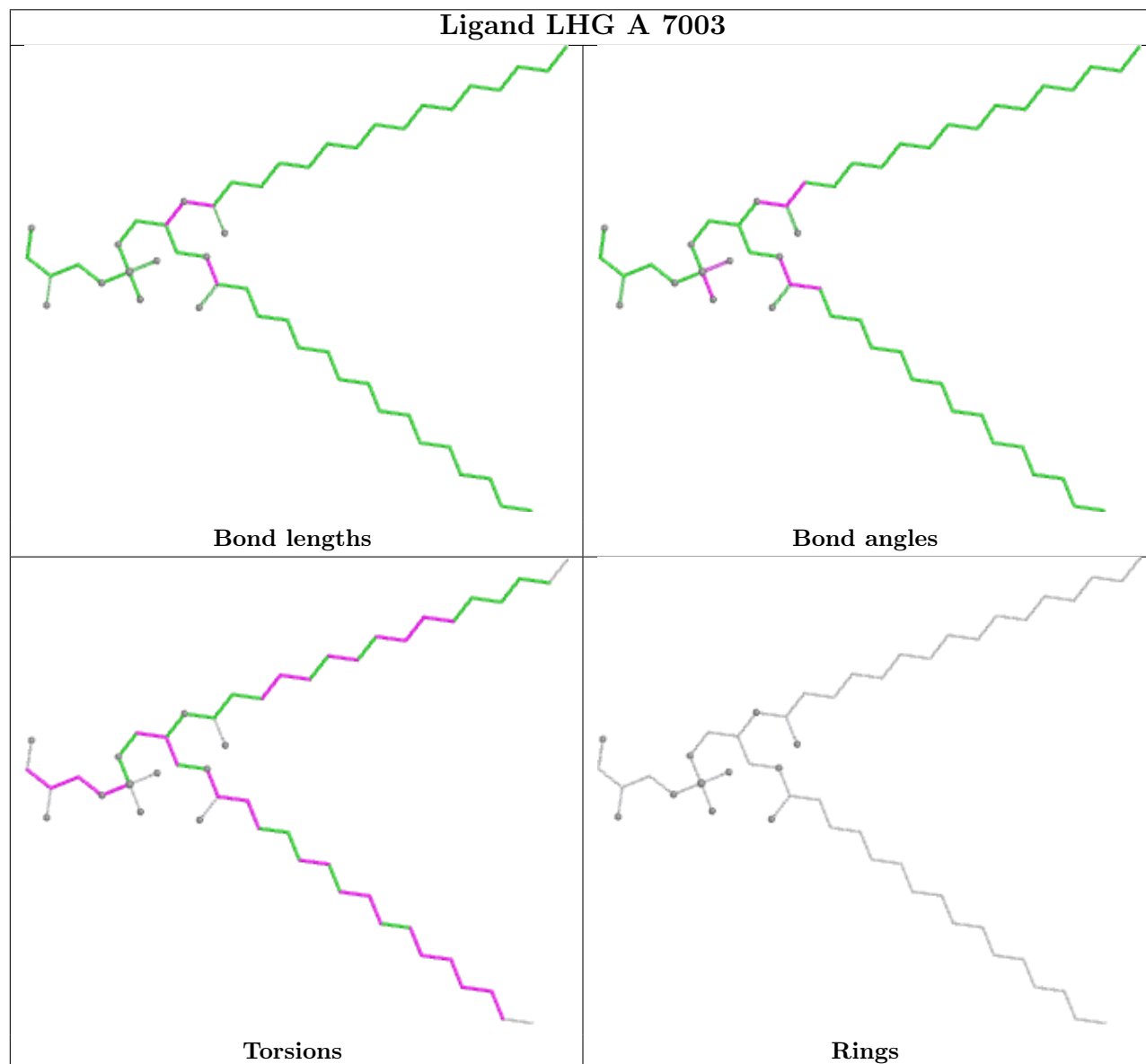
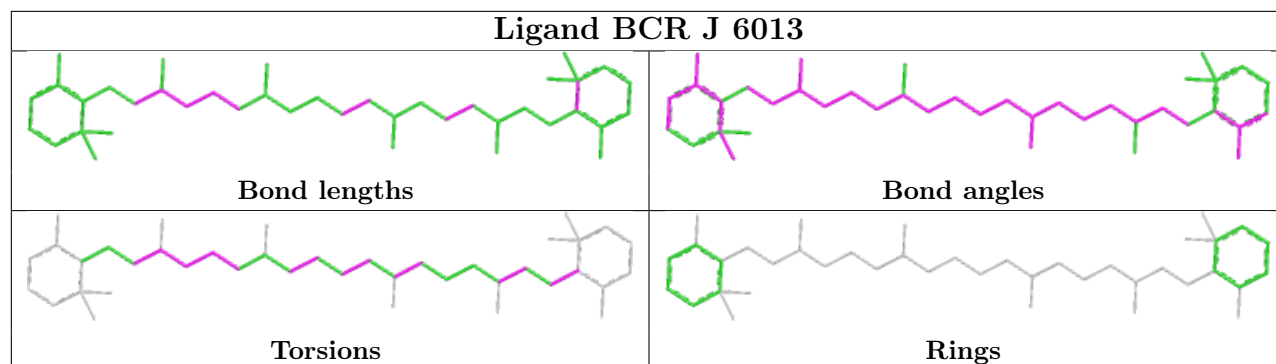


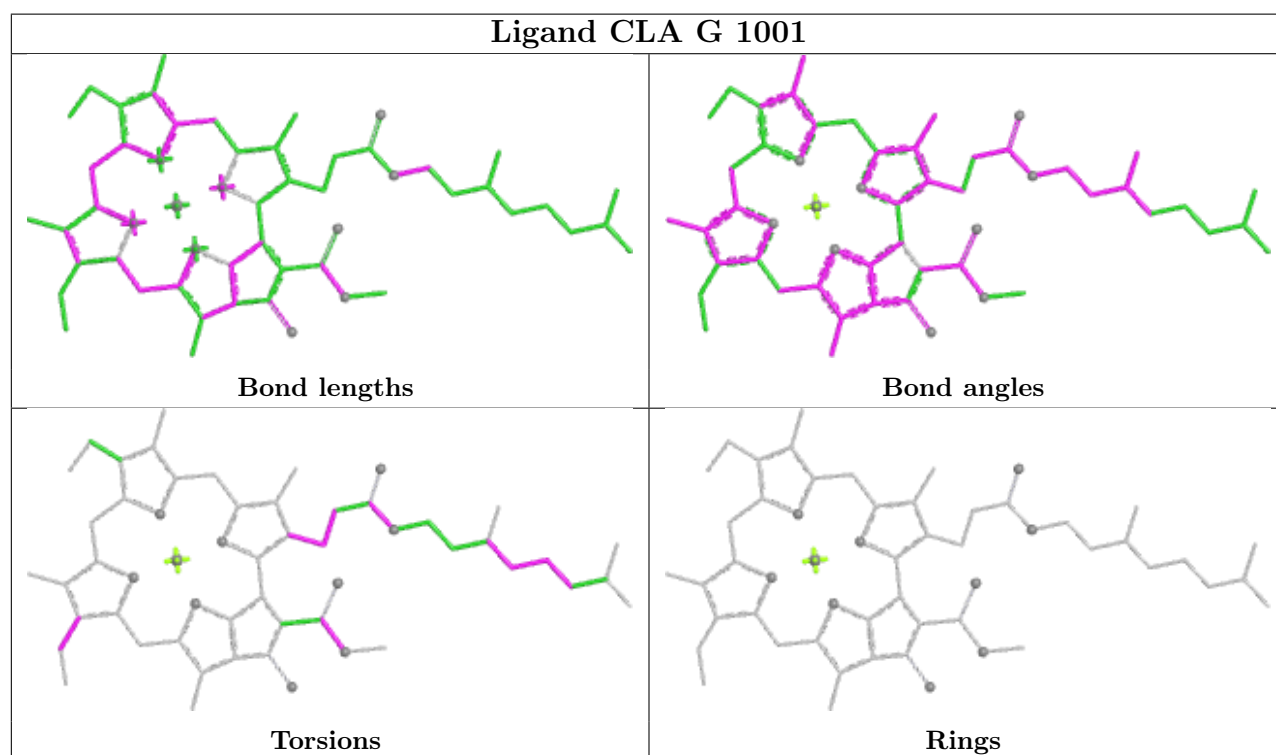
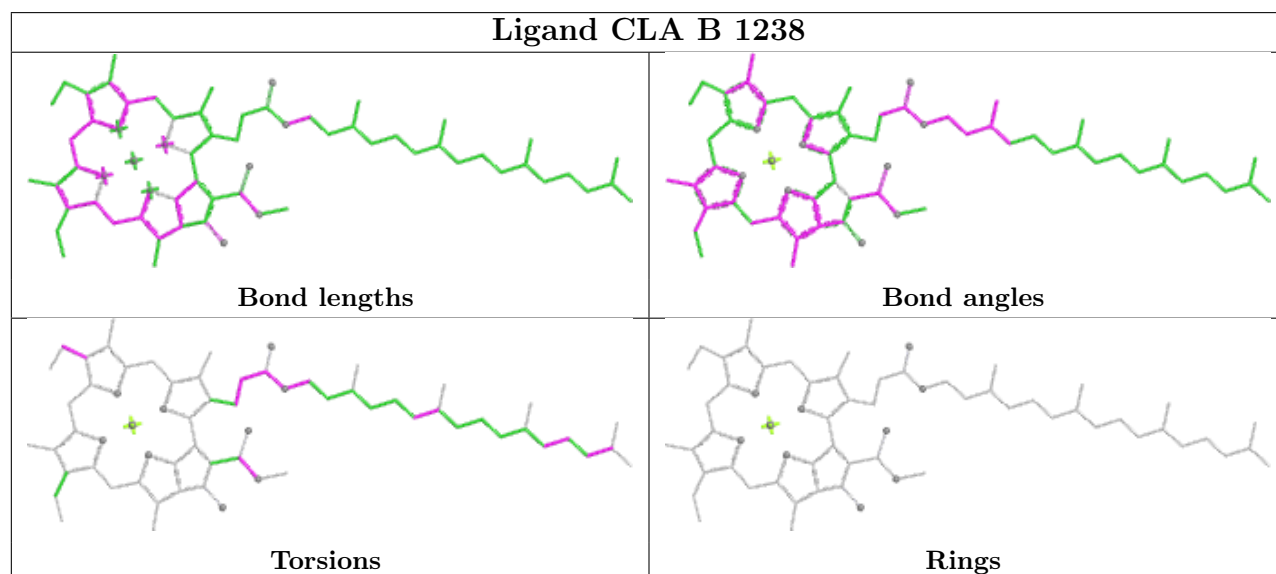
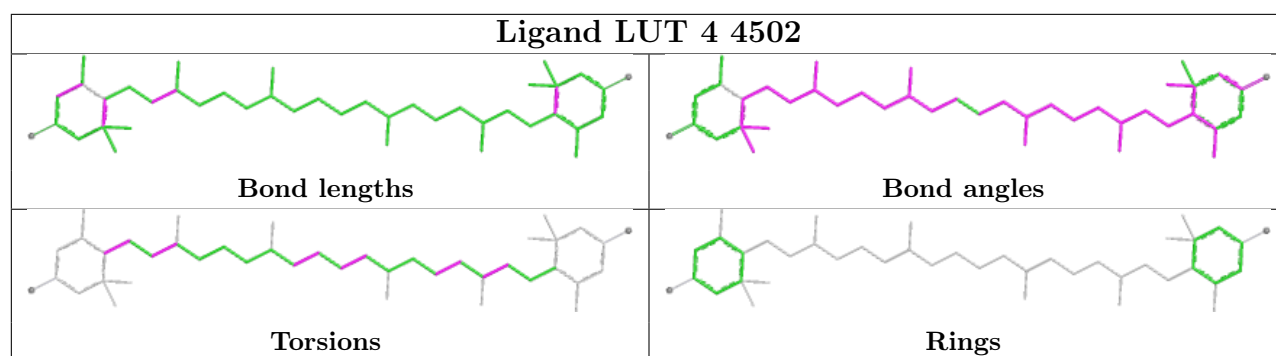
Ligand CLA A 1129

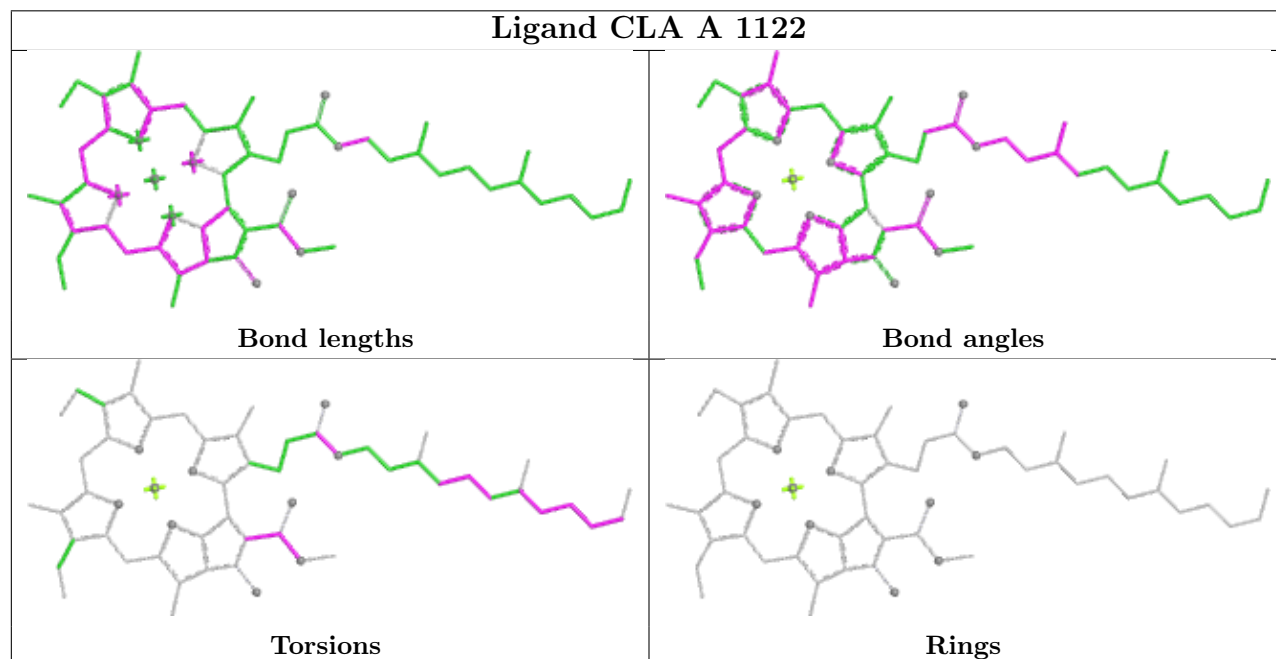
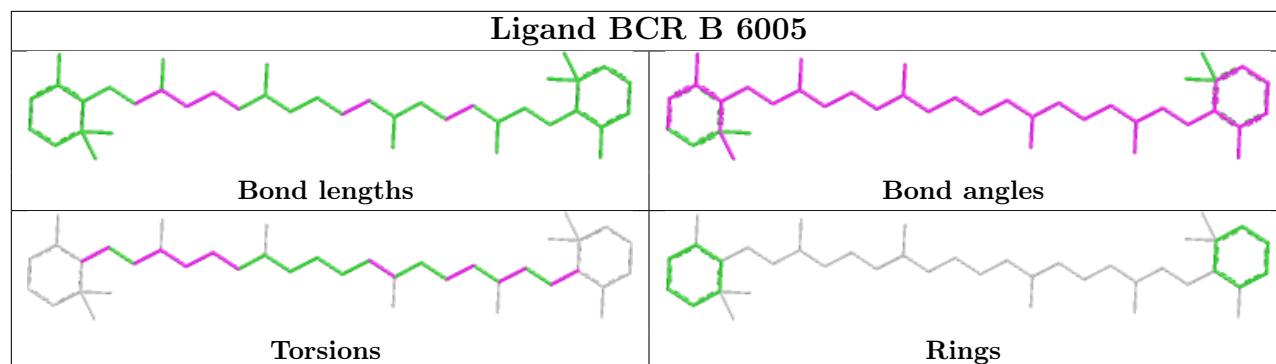


Ligand CLA A 1140

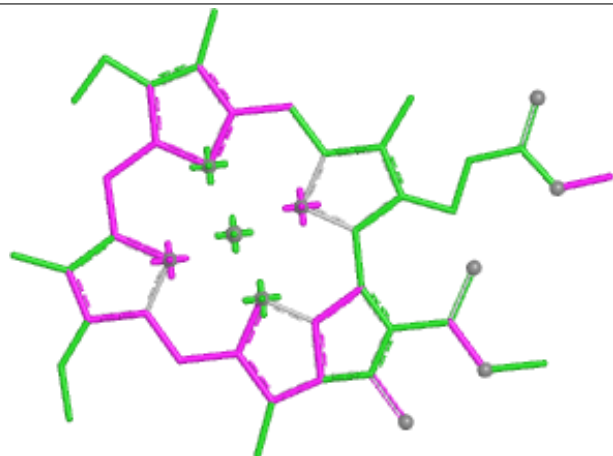




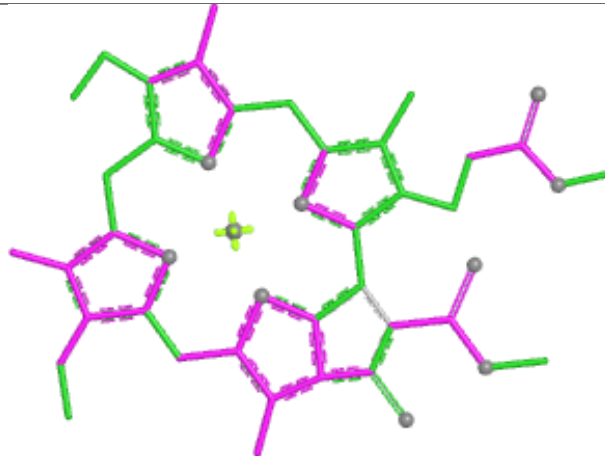




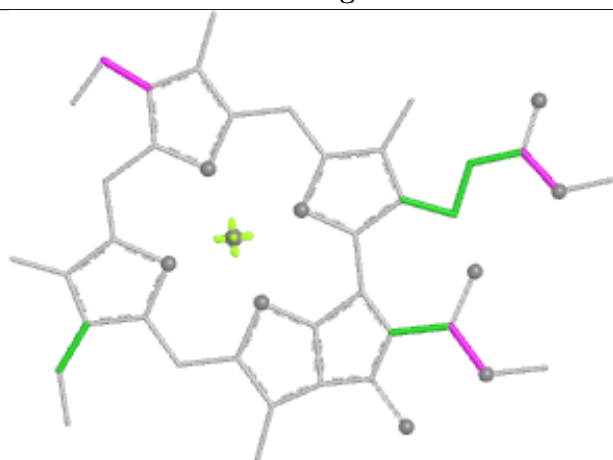
Ligand CLA A 1134



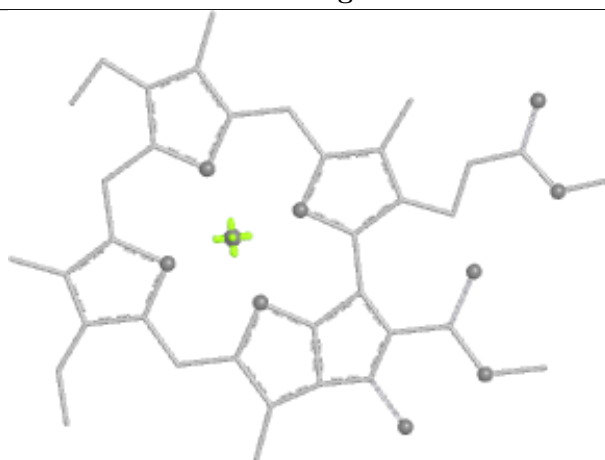
Bond lengths



Bond angles

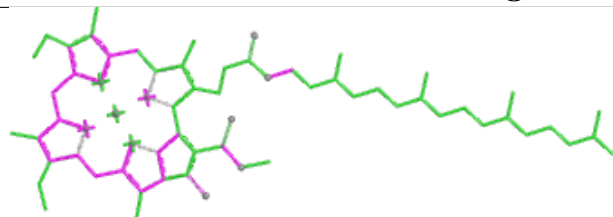


Torsions

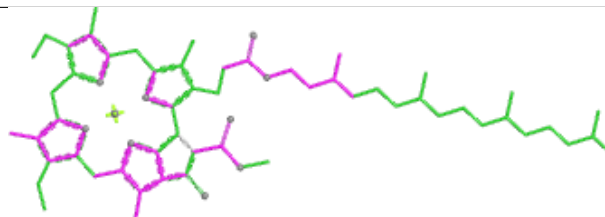


Rings

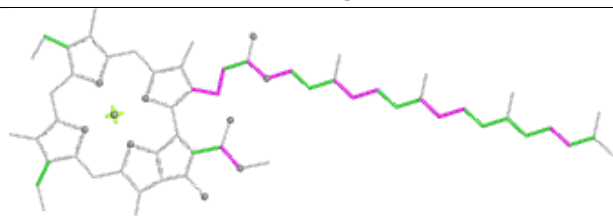
Ligand CLA B 1229



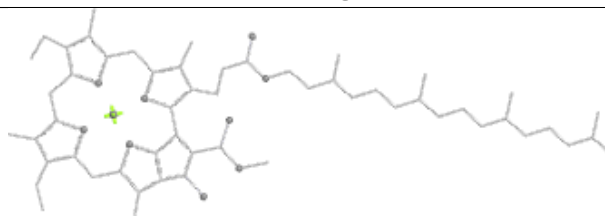
Bond lengths



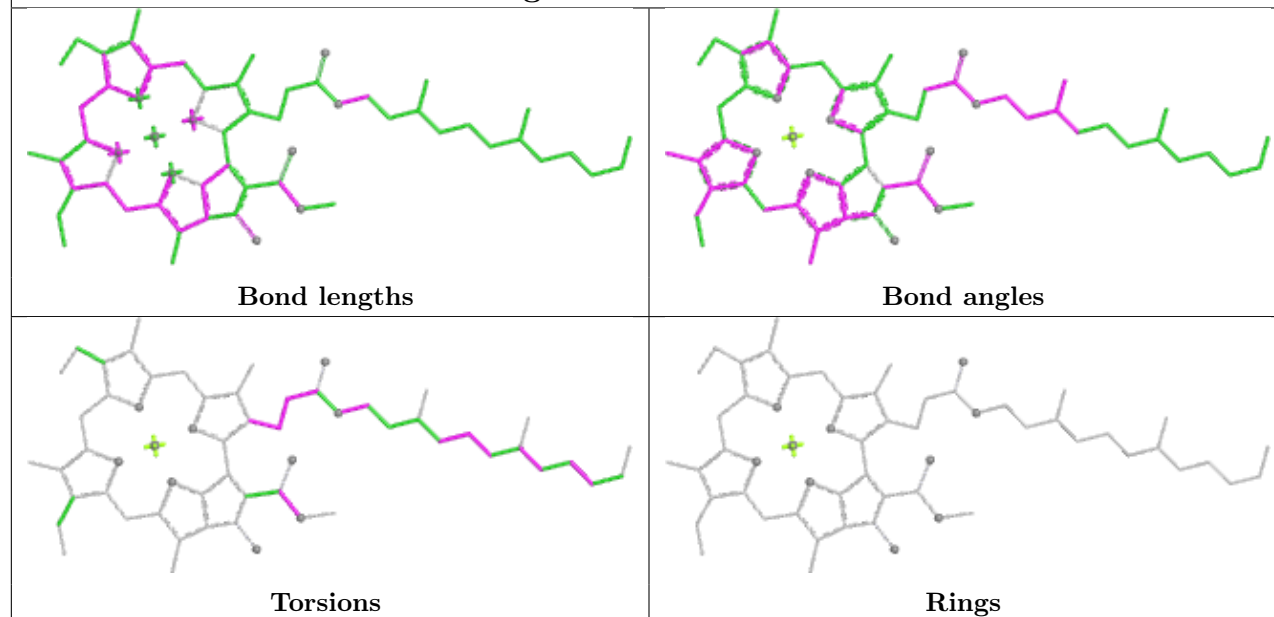
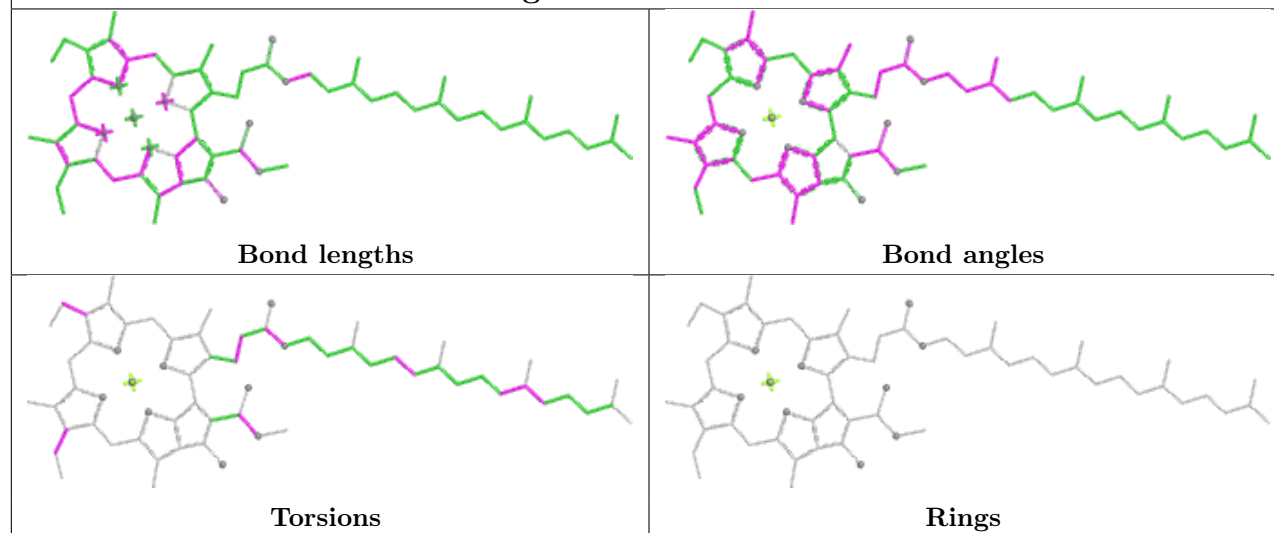
Bond angles

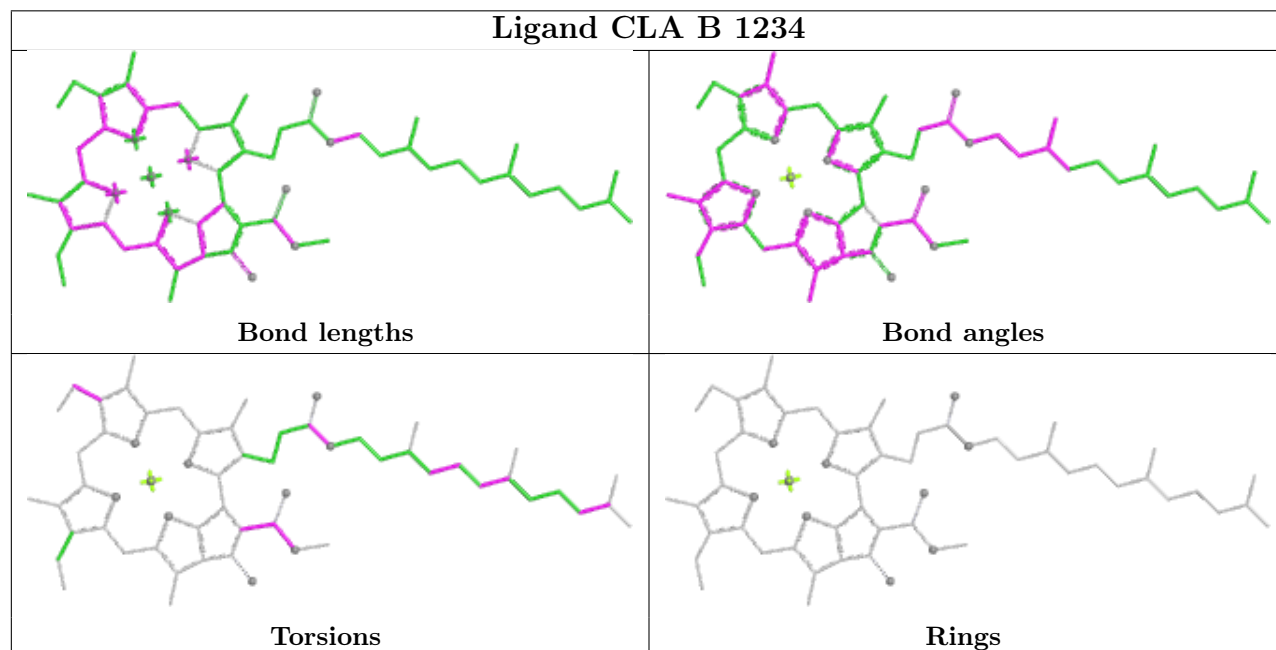
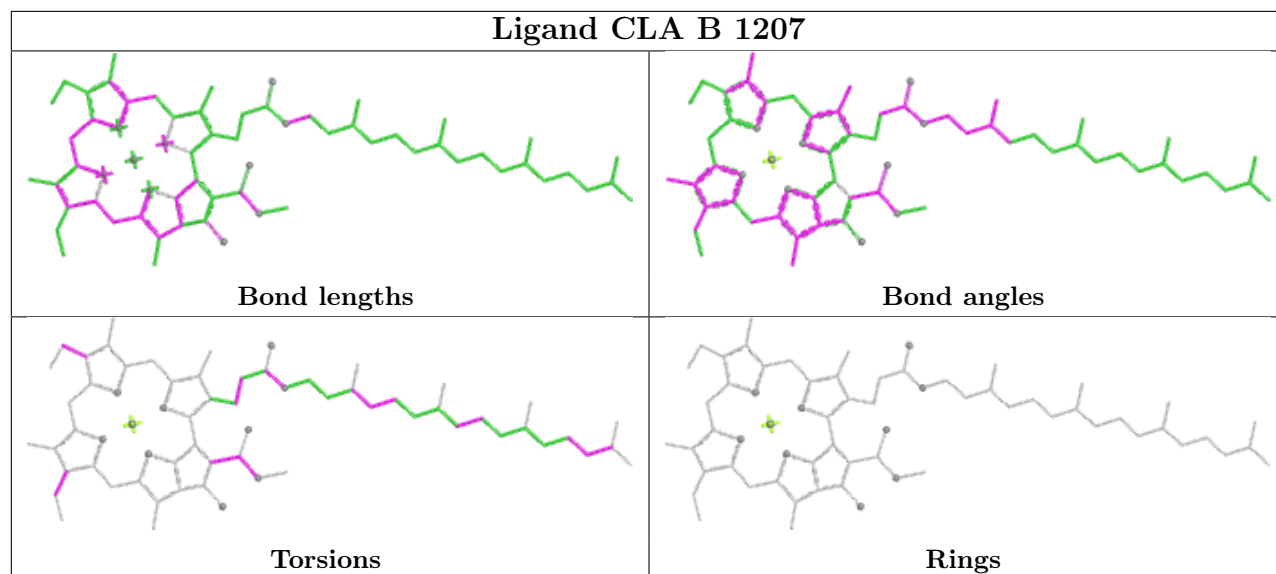


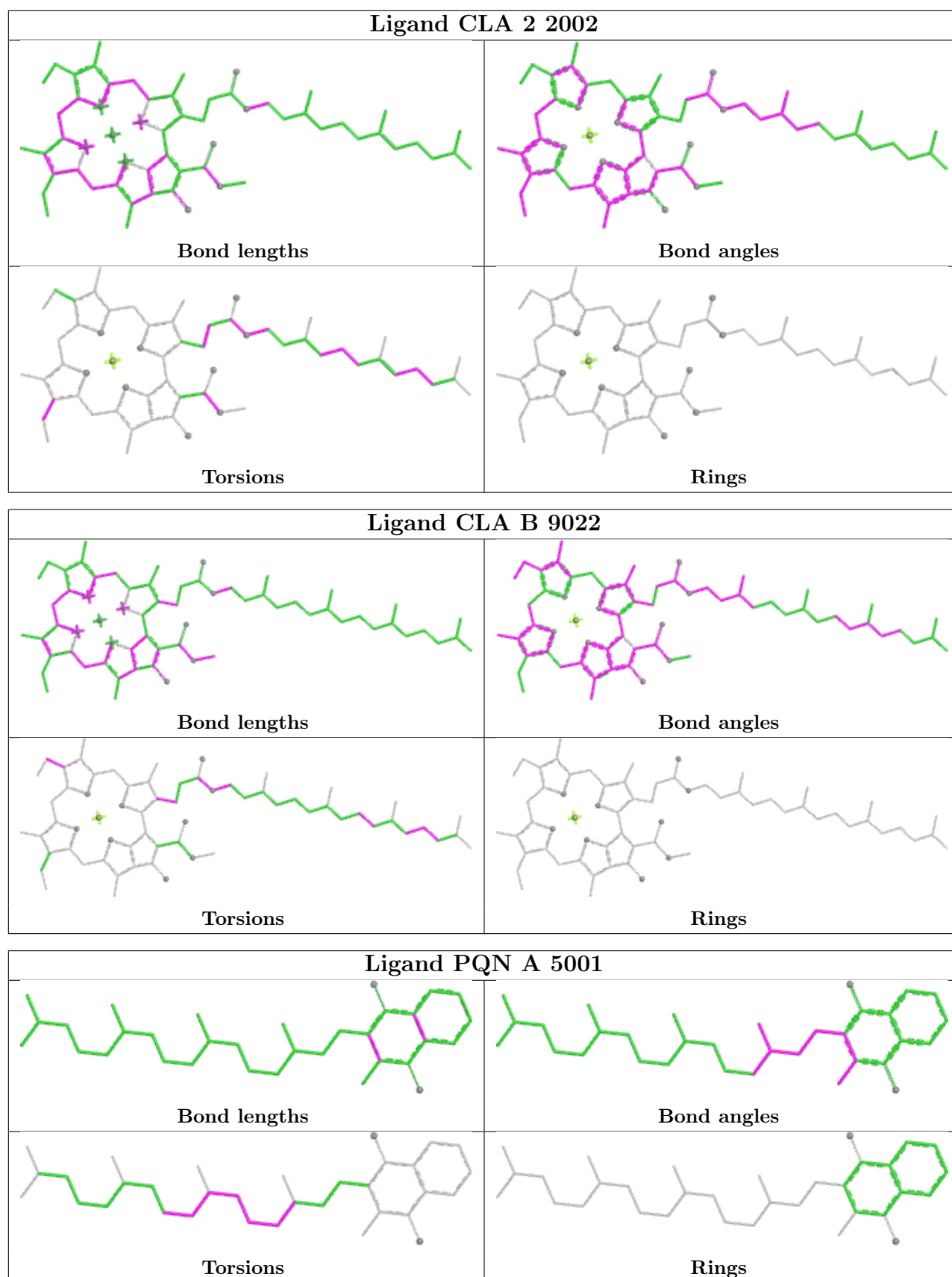
Torsions

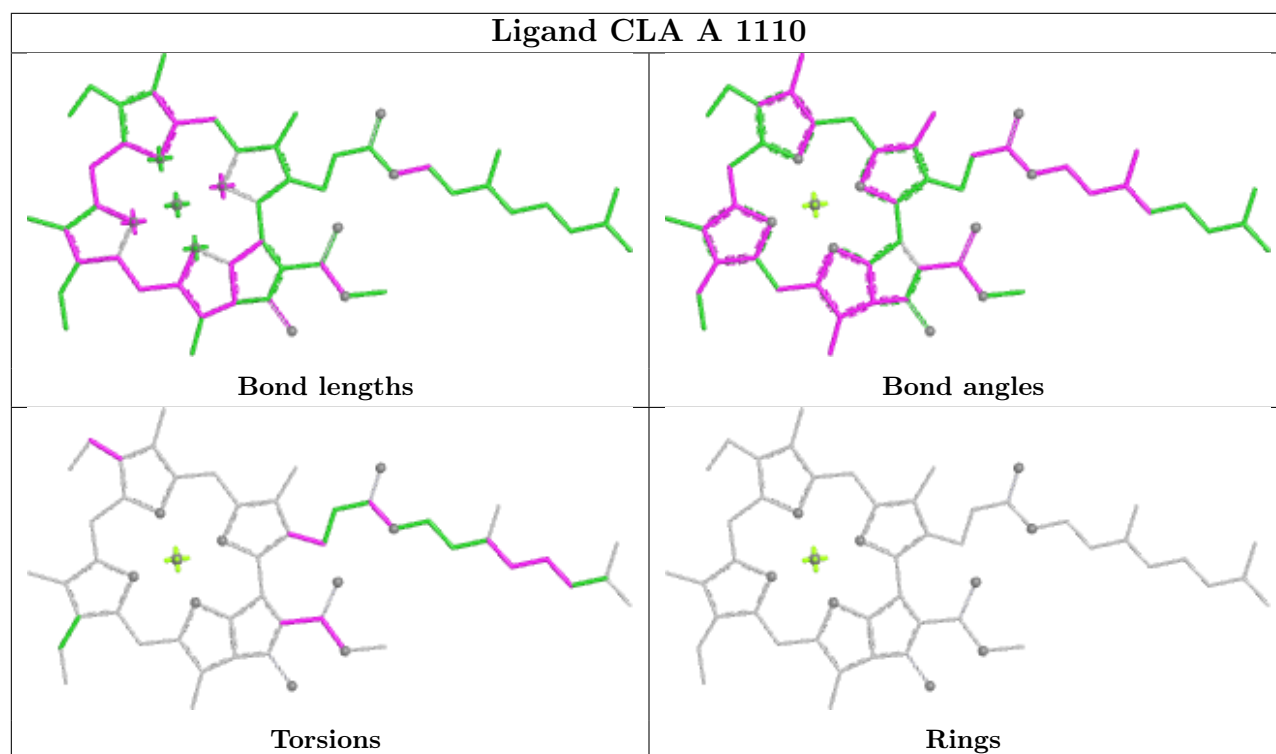
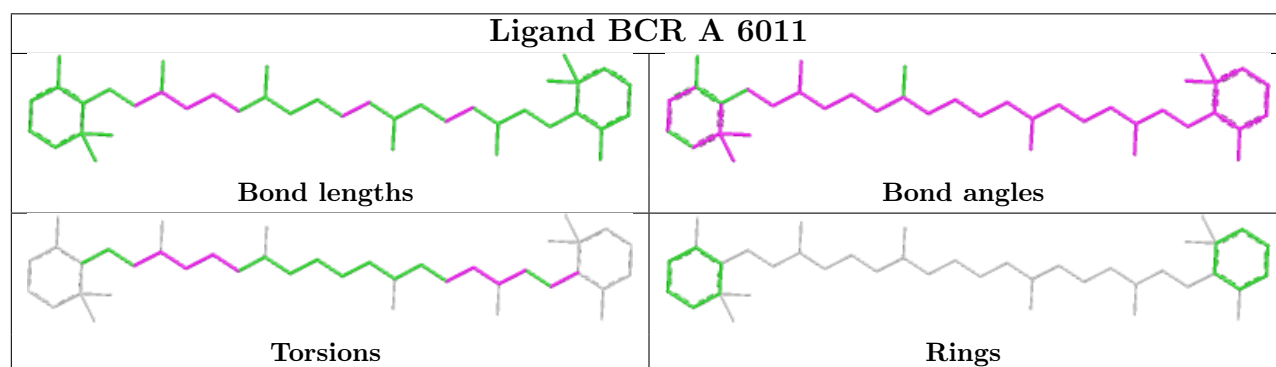
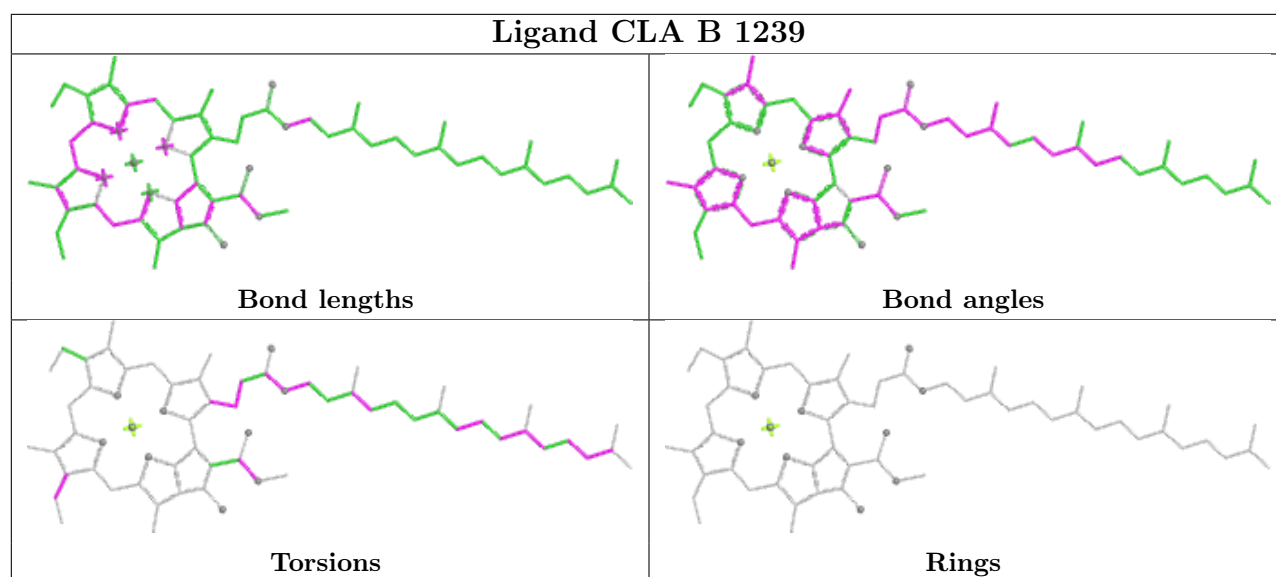


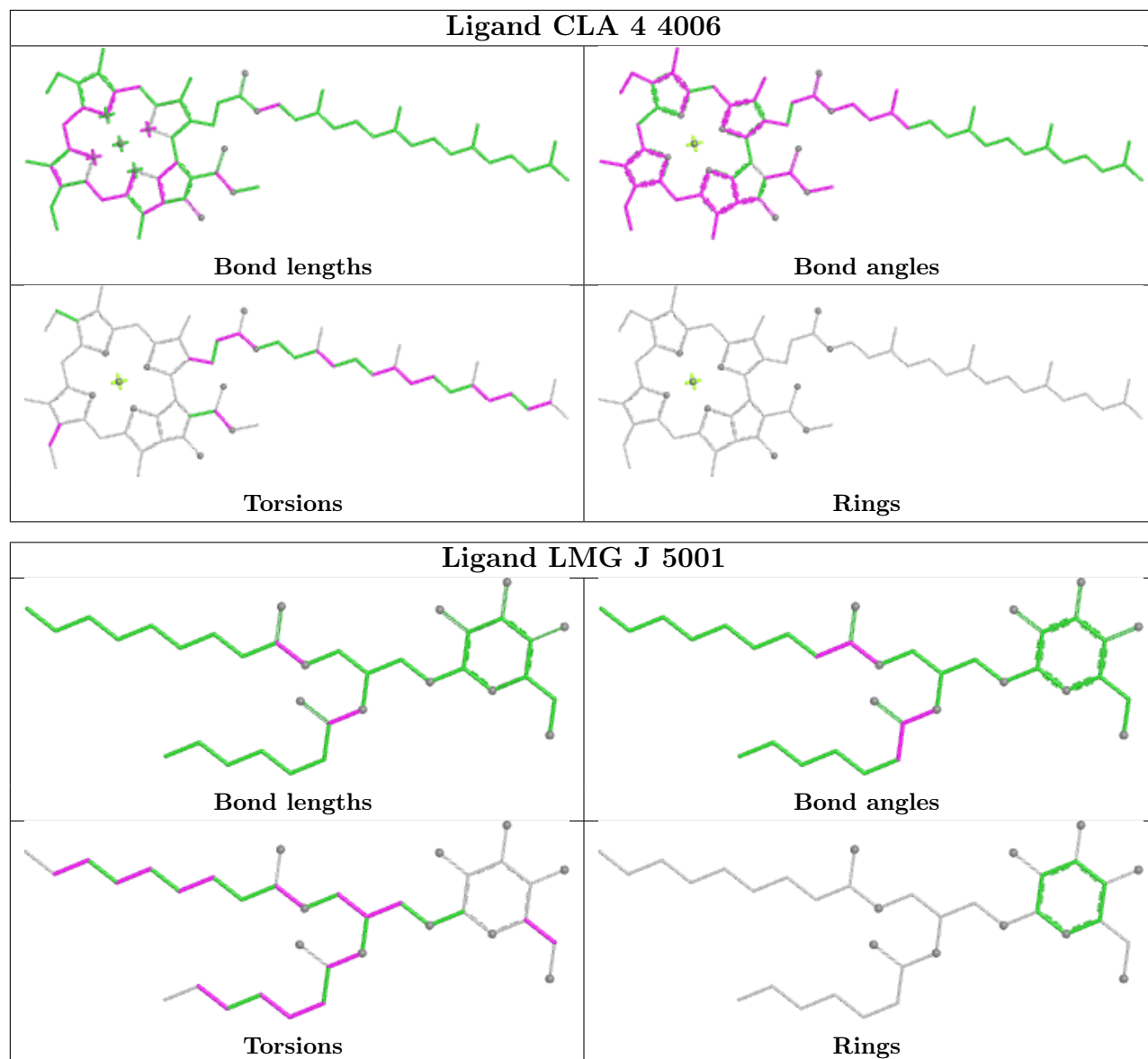
Rings

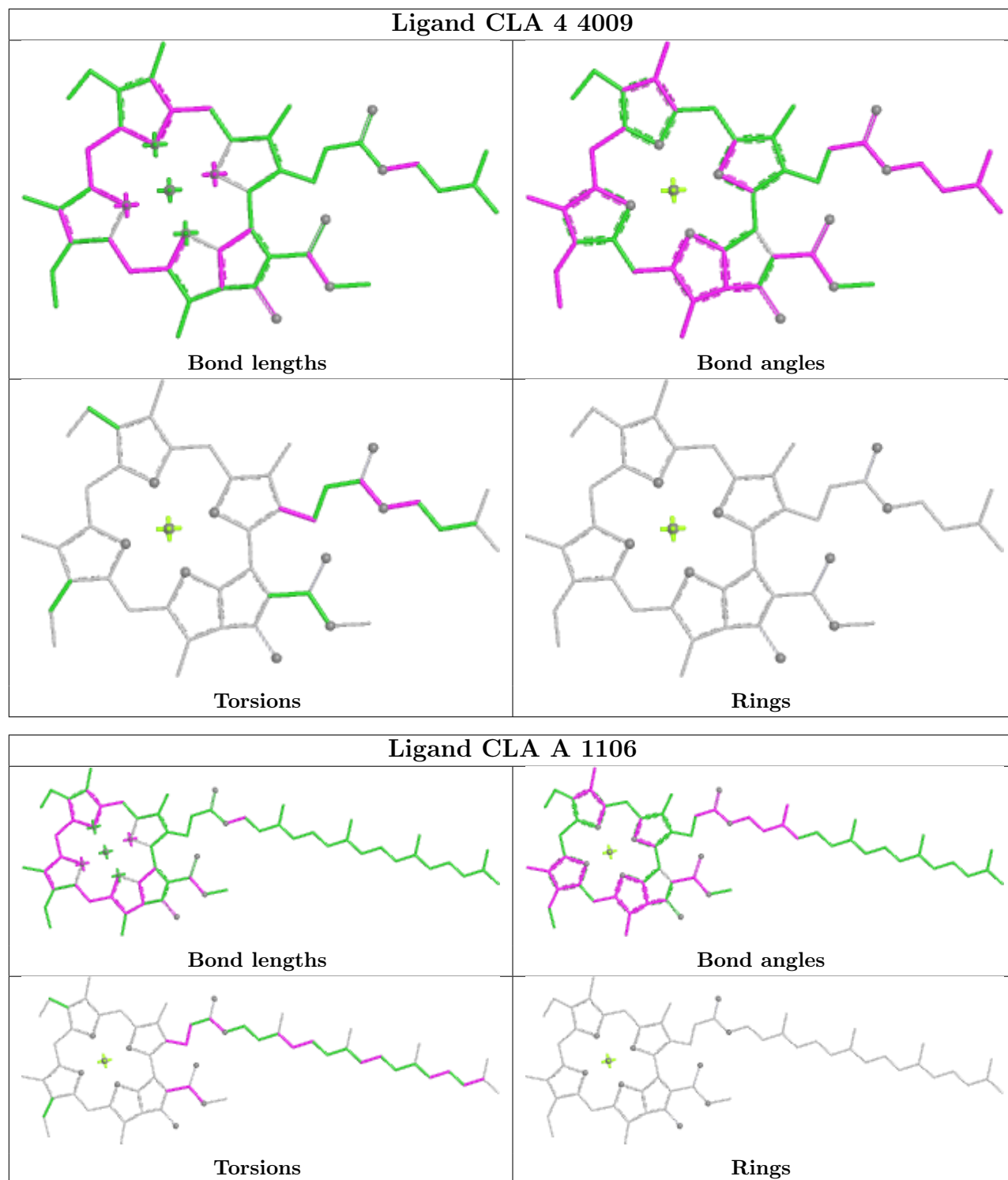
Ligand CLA B 1214**Ligand CLA A 1131**



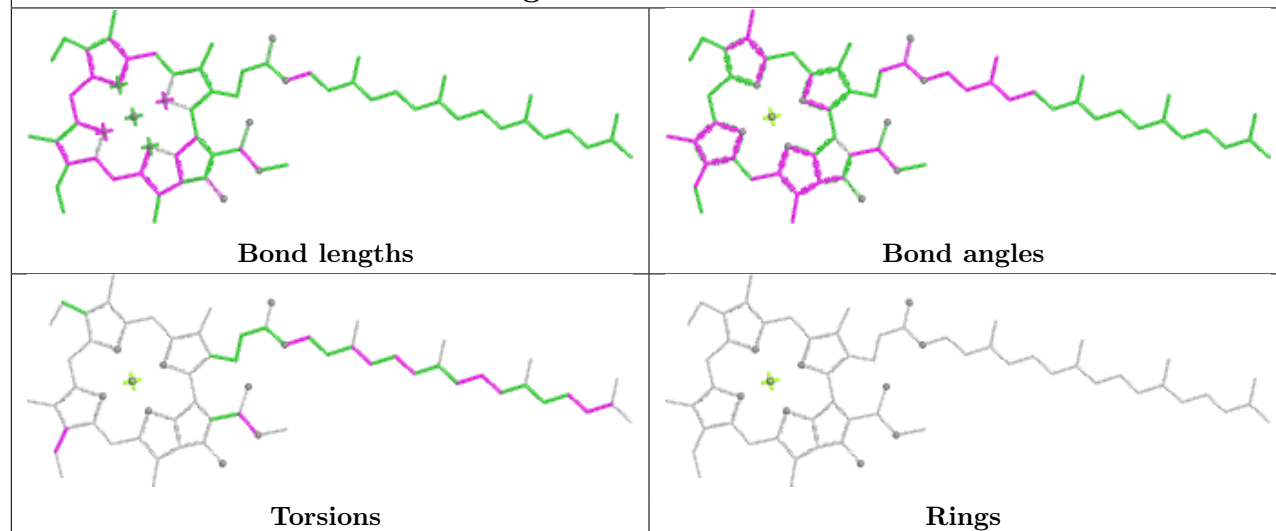




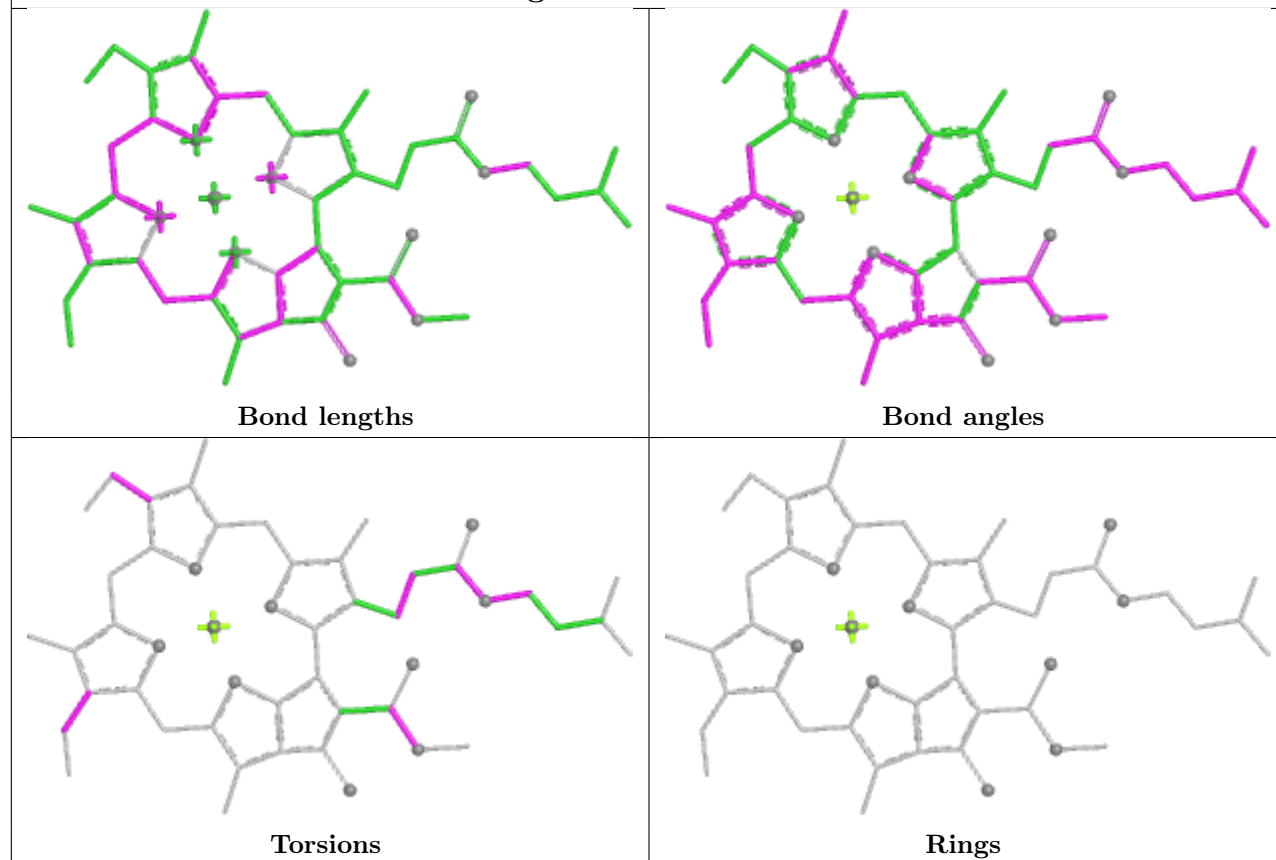


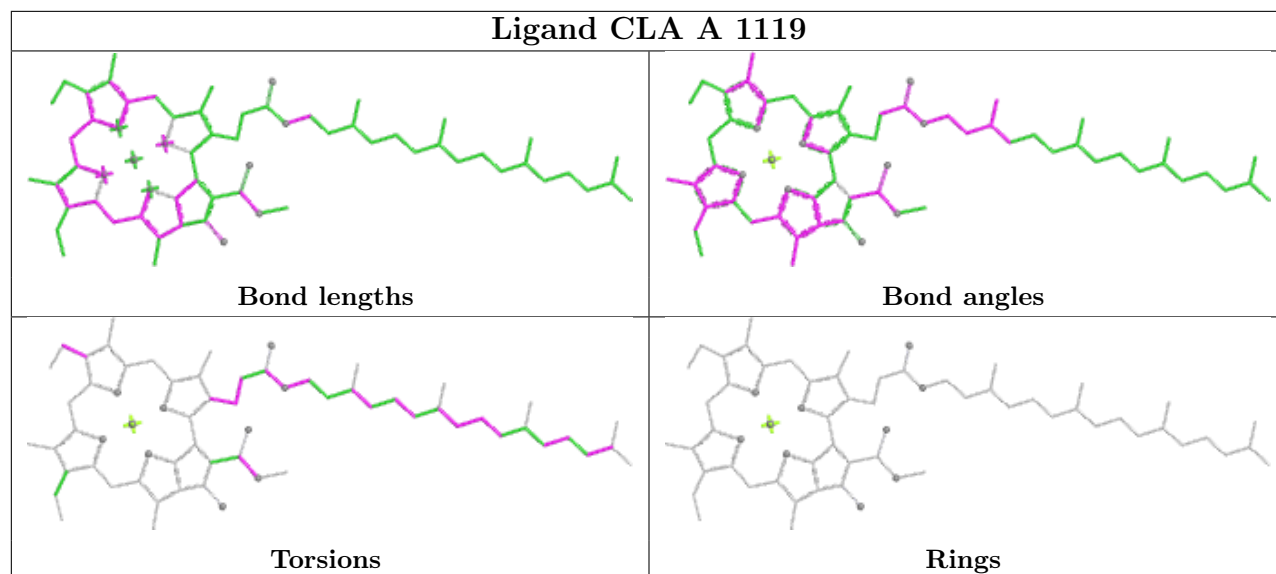
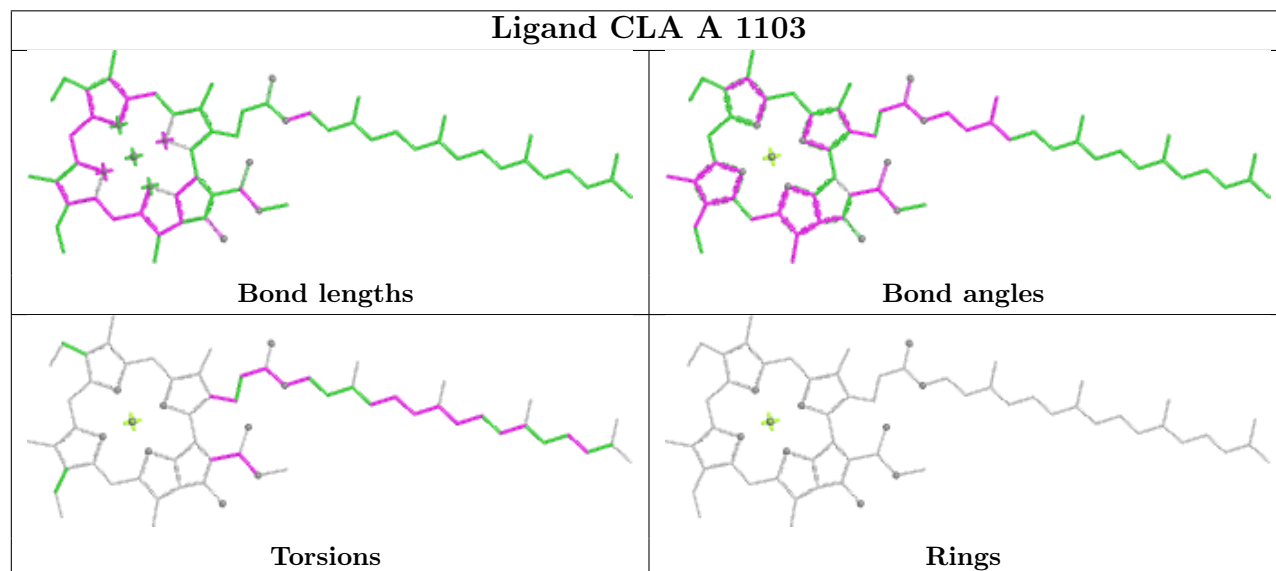
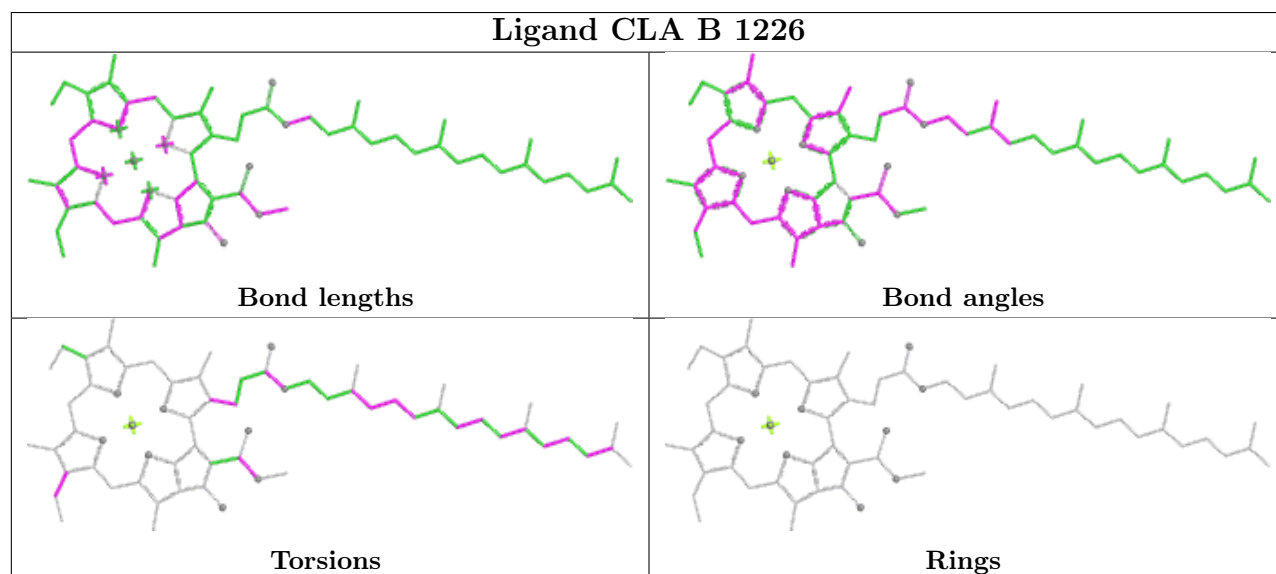


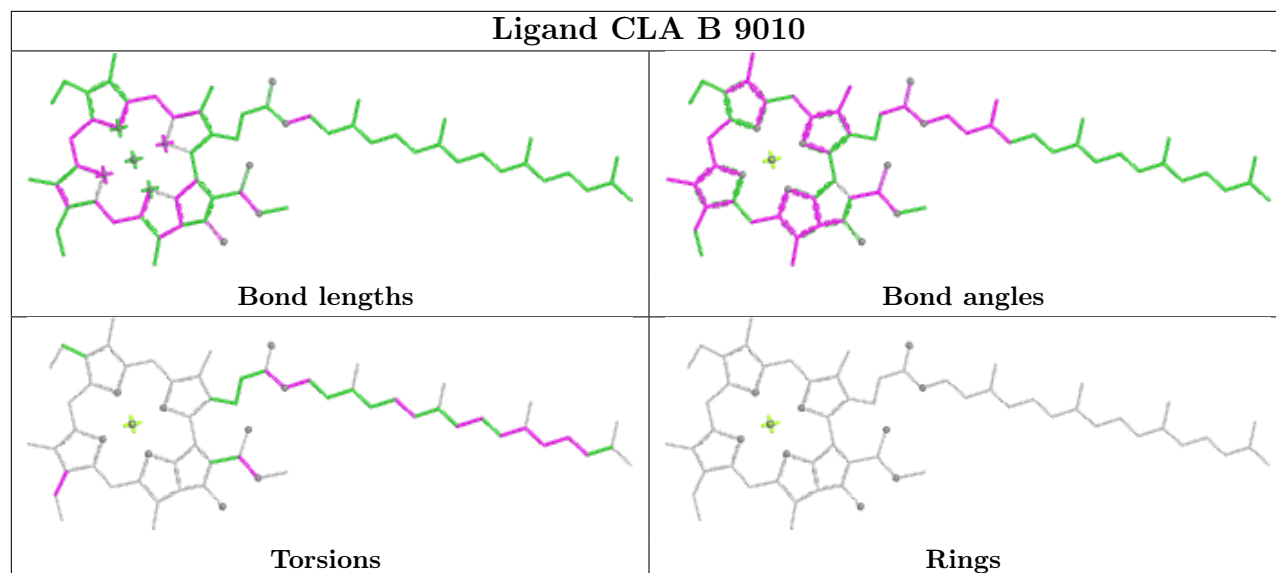
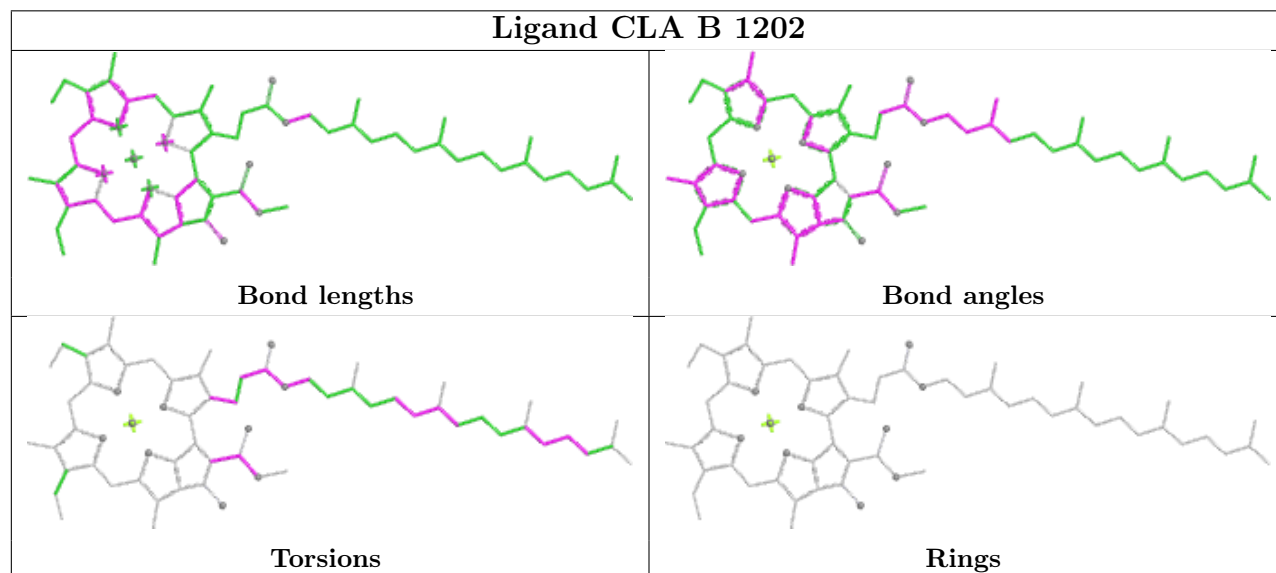
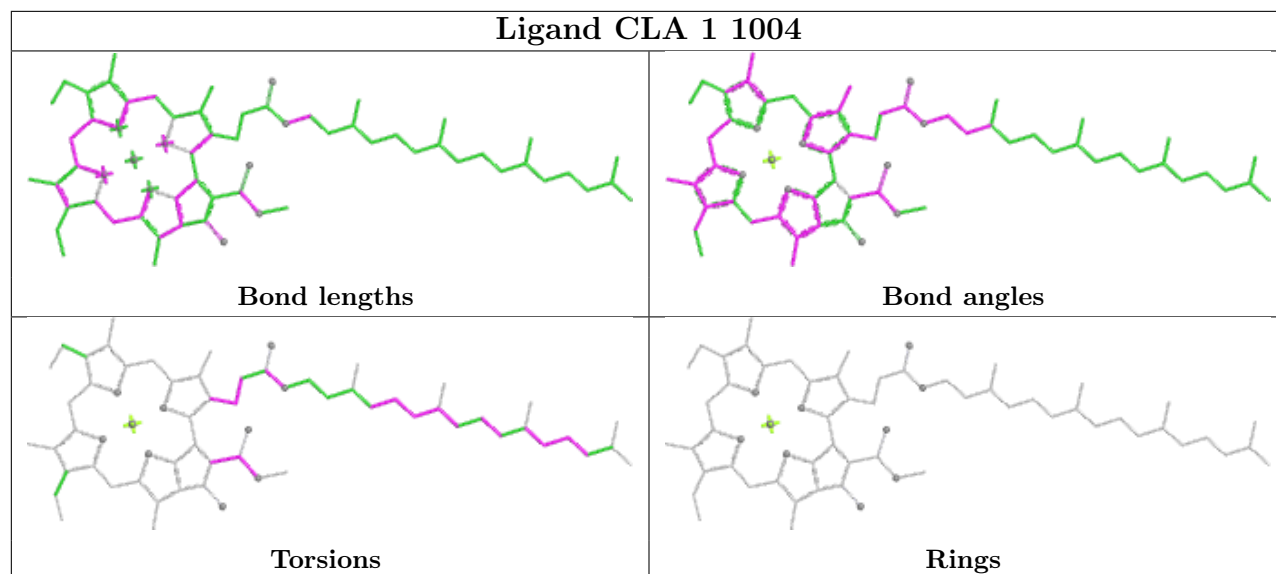
Ligand CLA A 1139

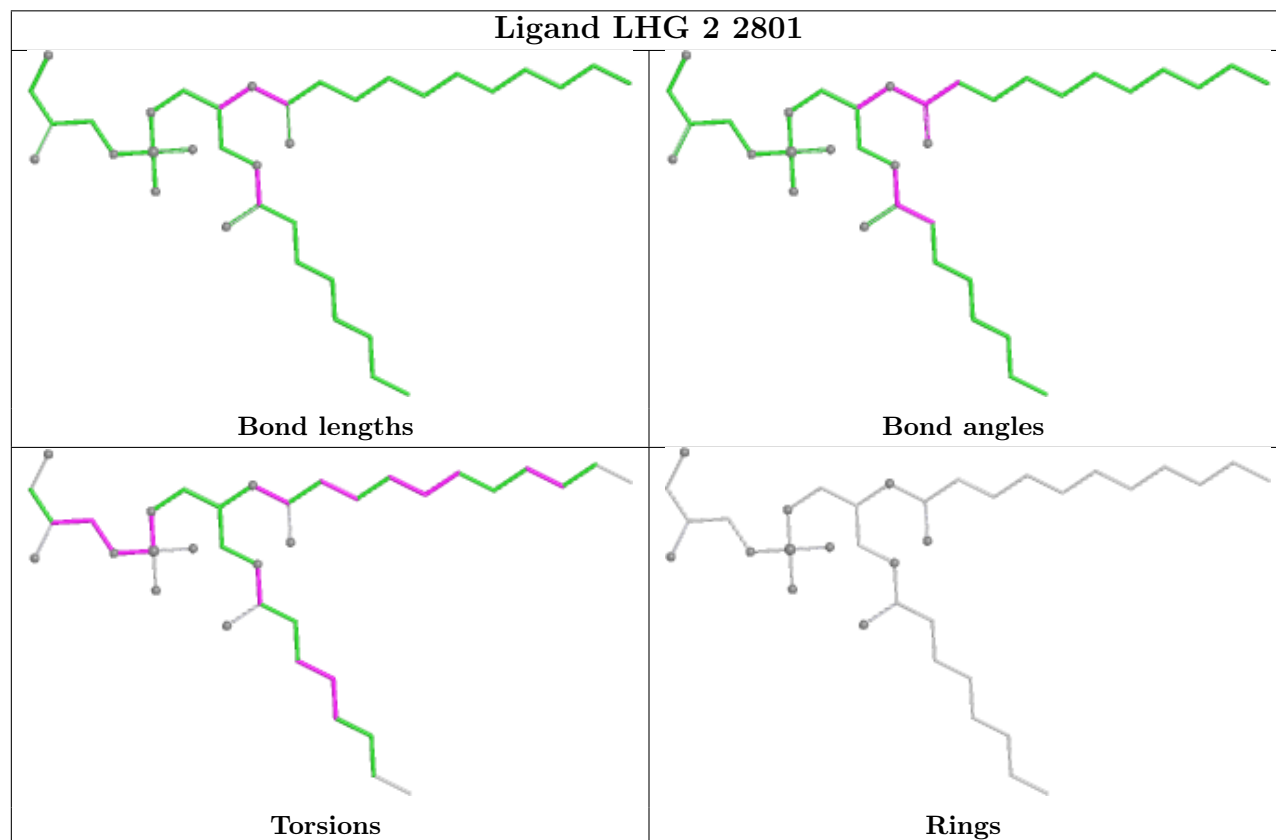
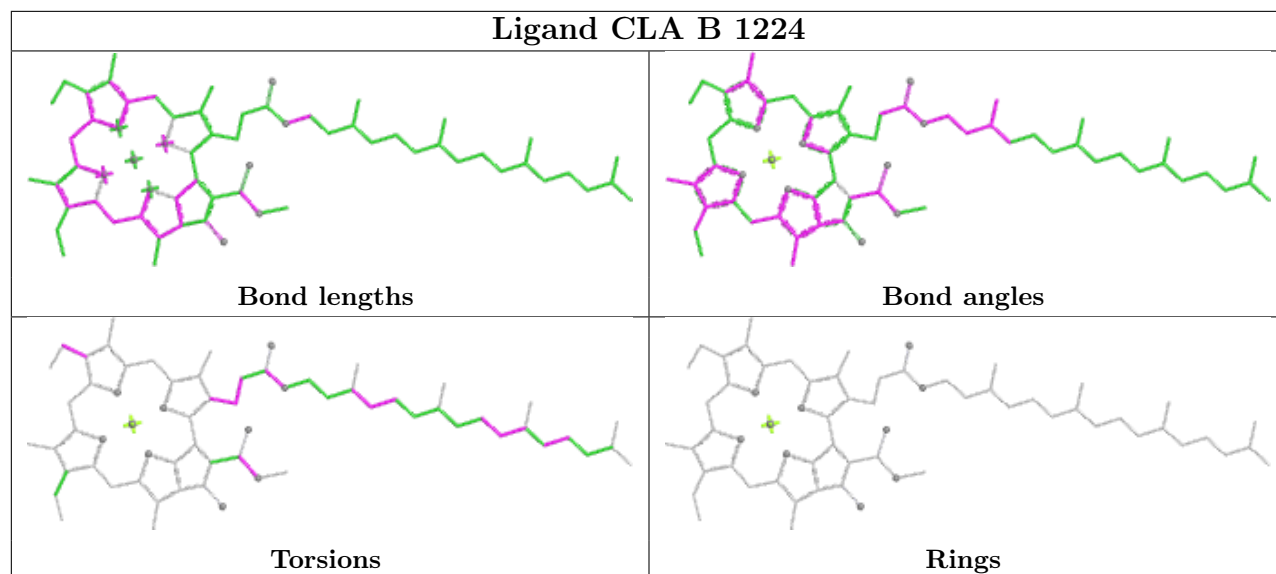


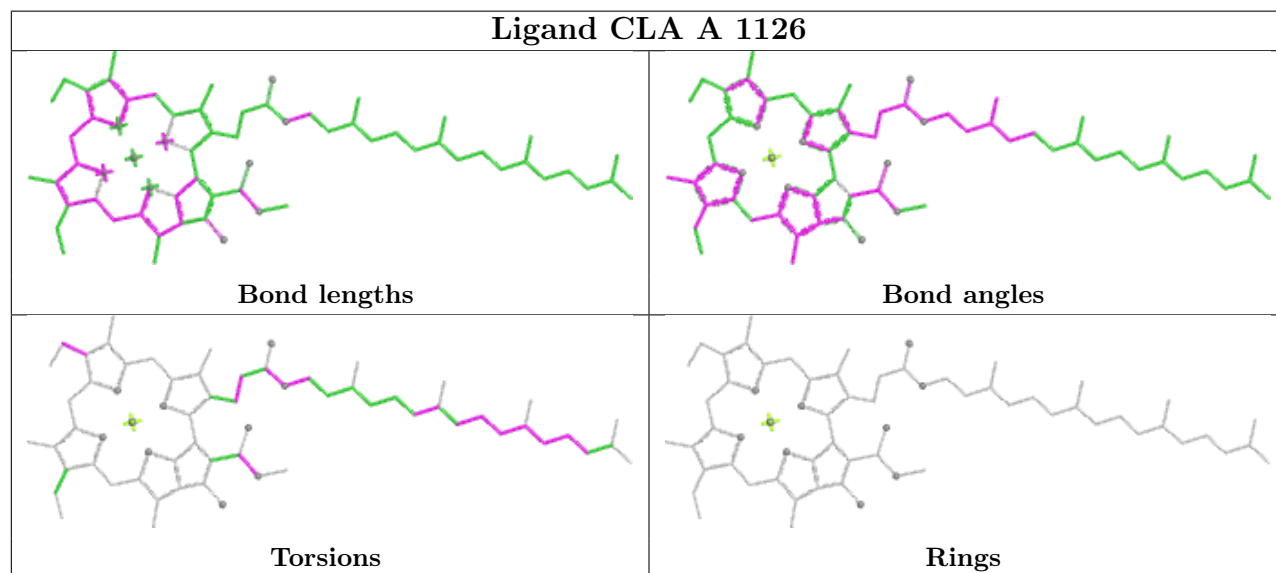
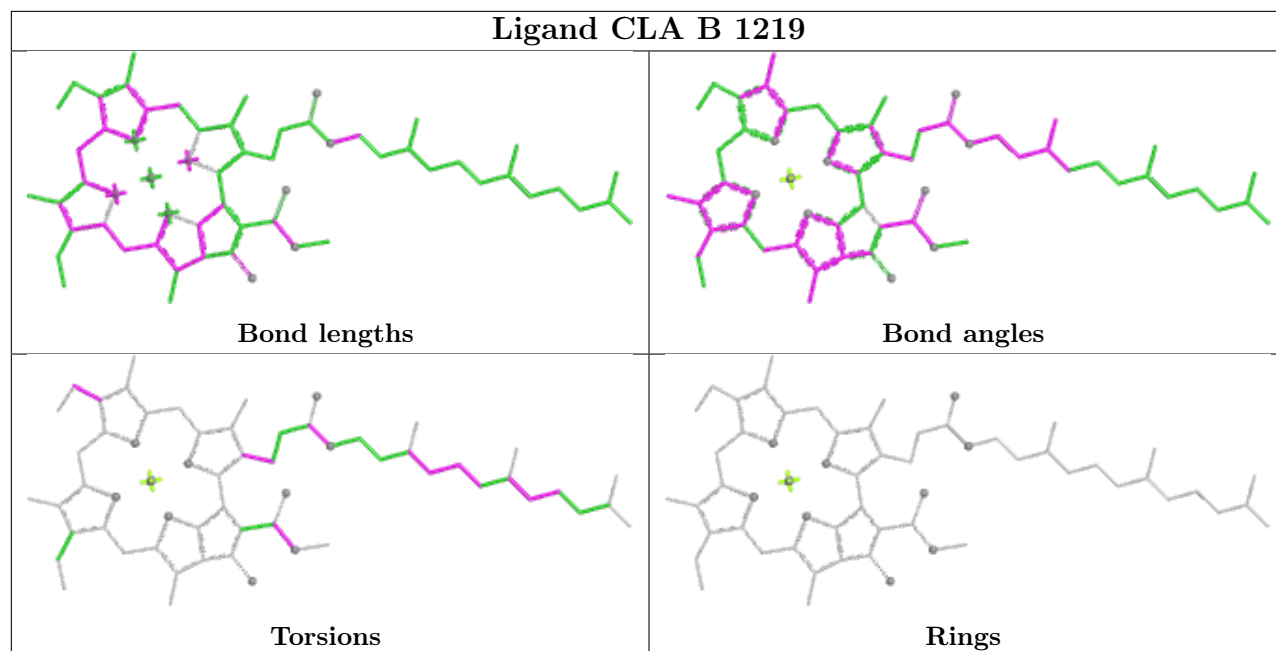
Ligand CLA 1 1012

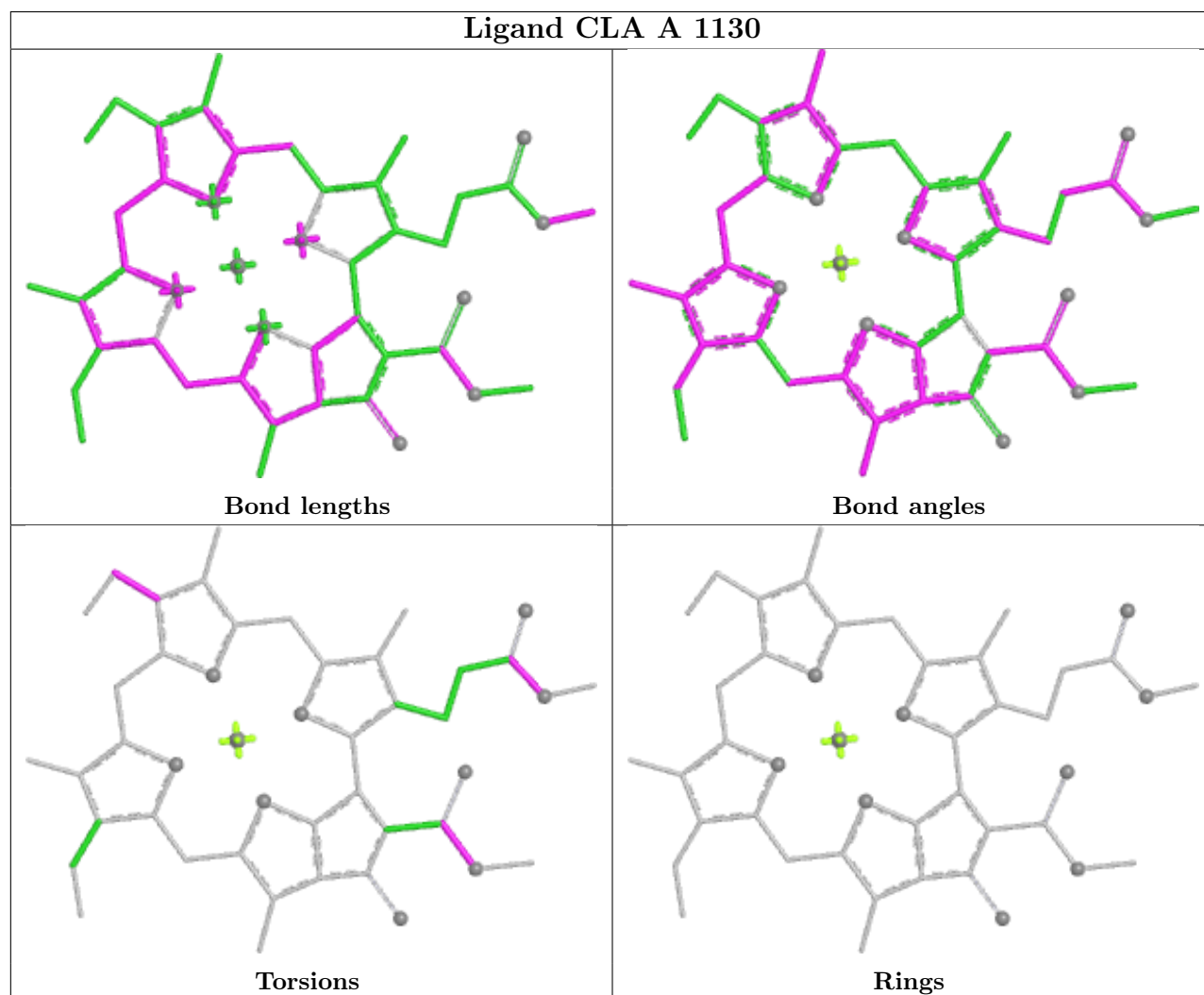
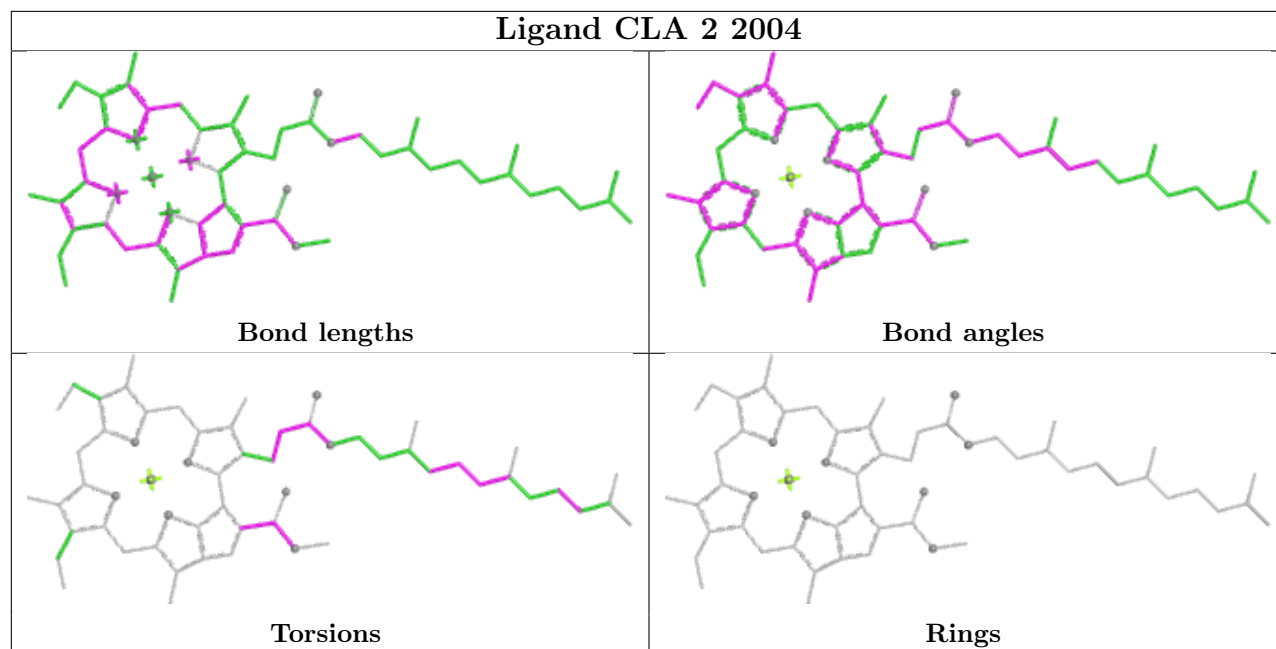


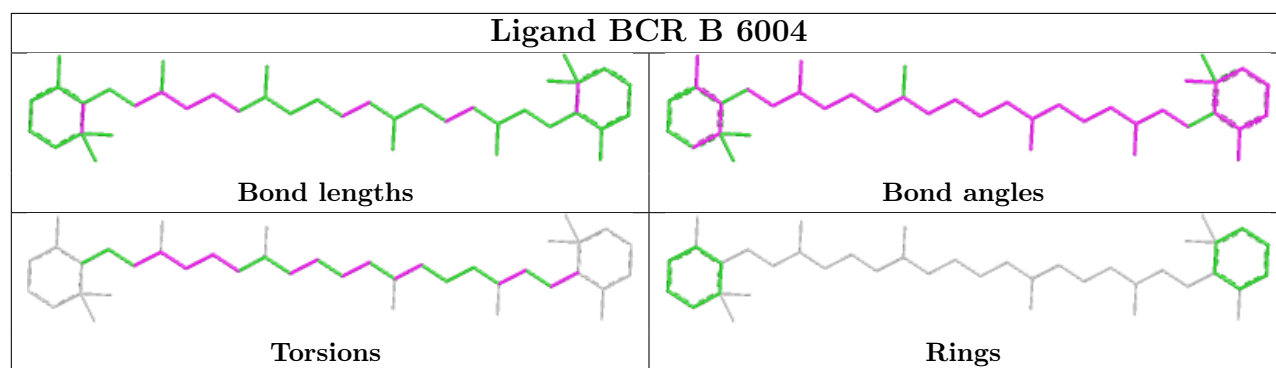
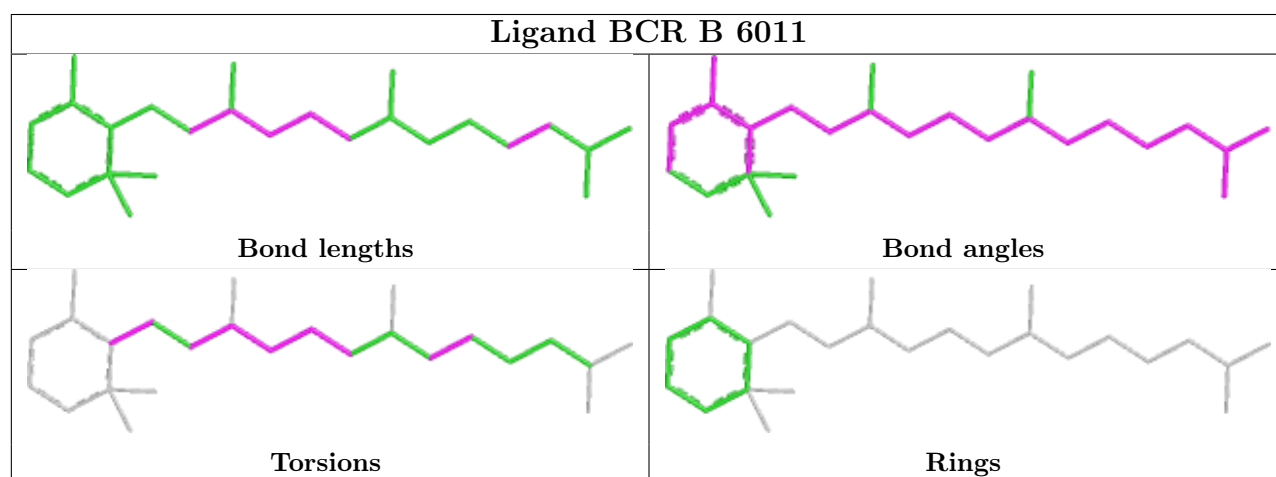
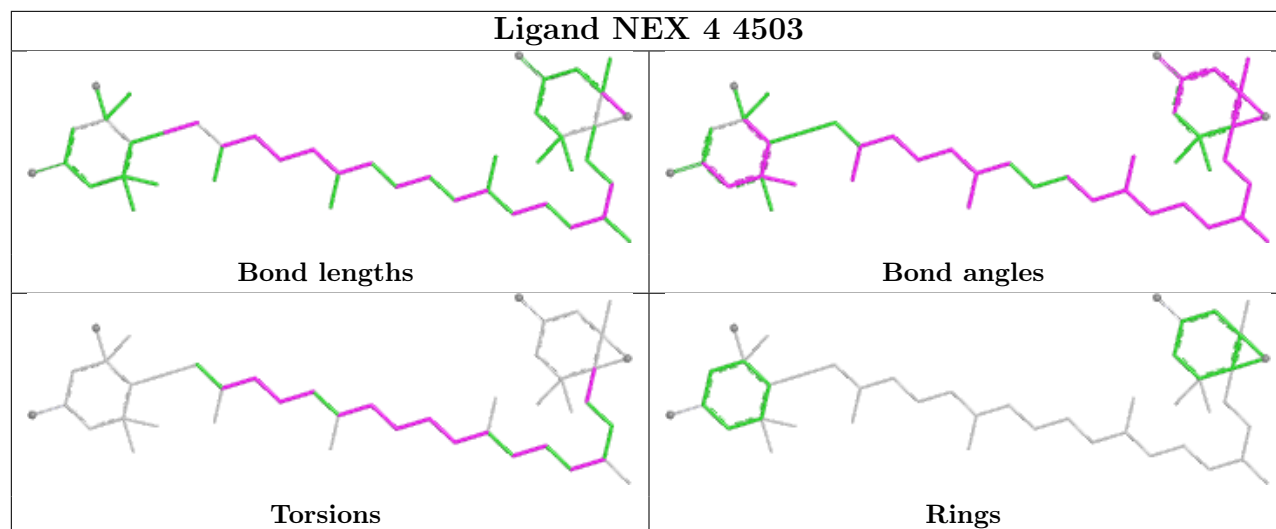
Ligand CLA A 1119**Ligand CLA A 1103****Ligand CLA B 1226**

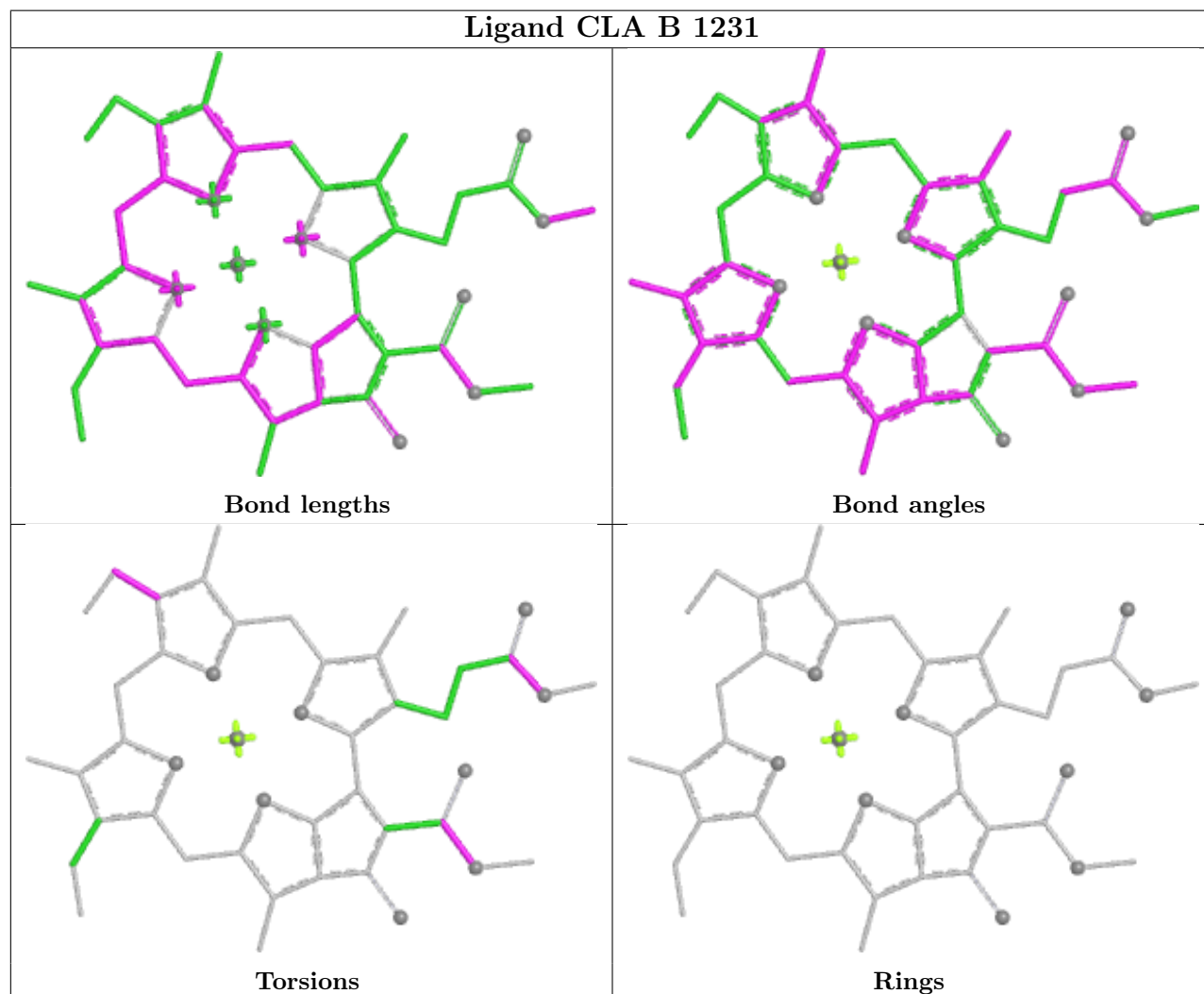
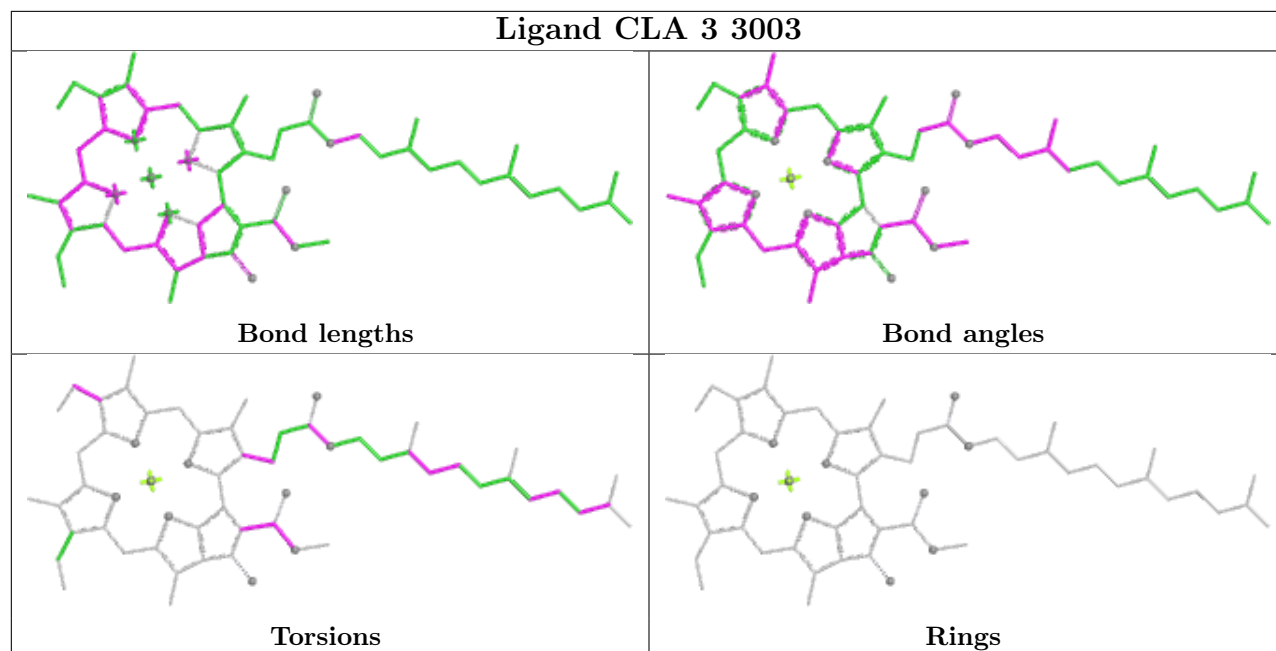


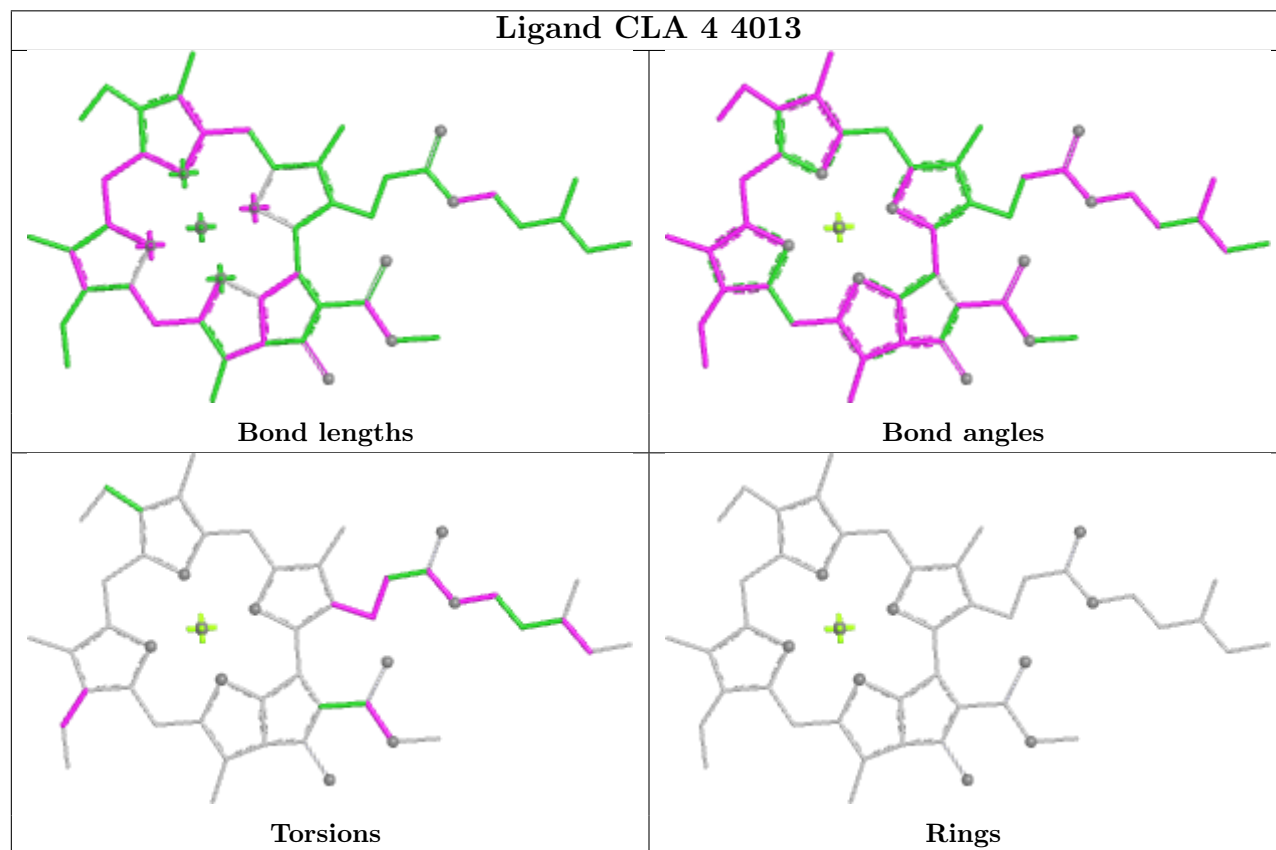
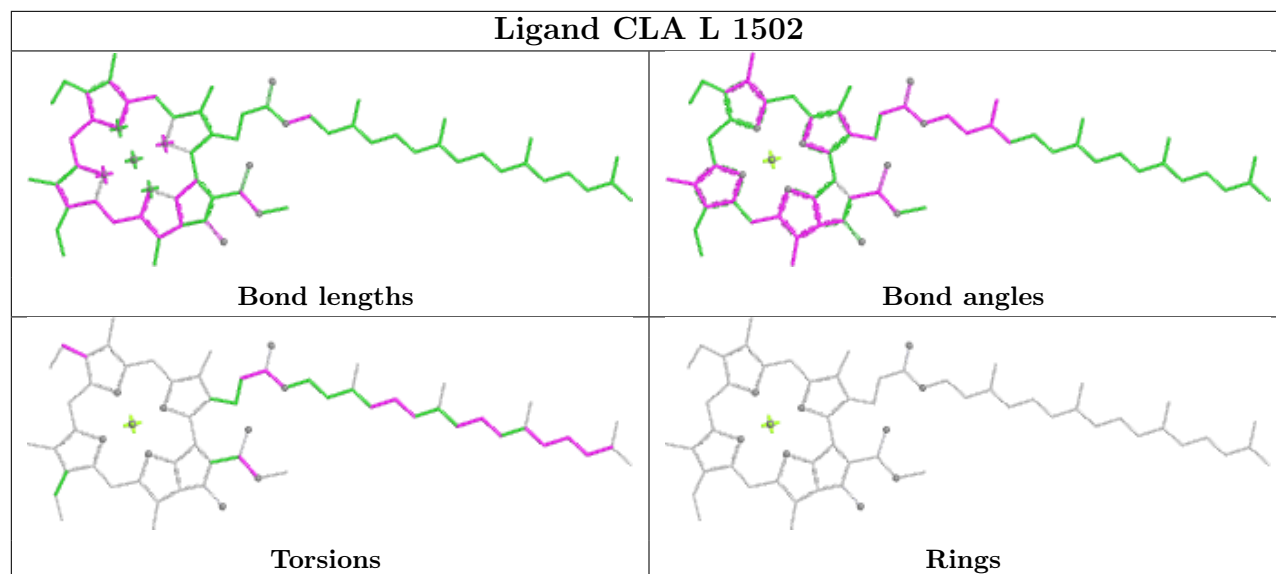


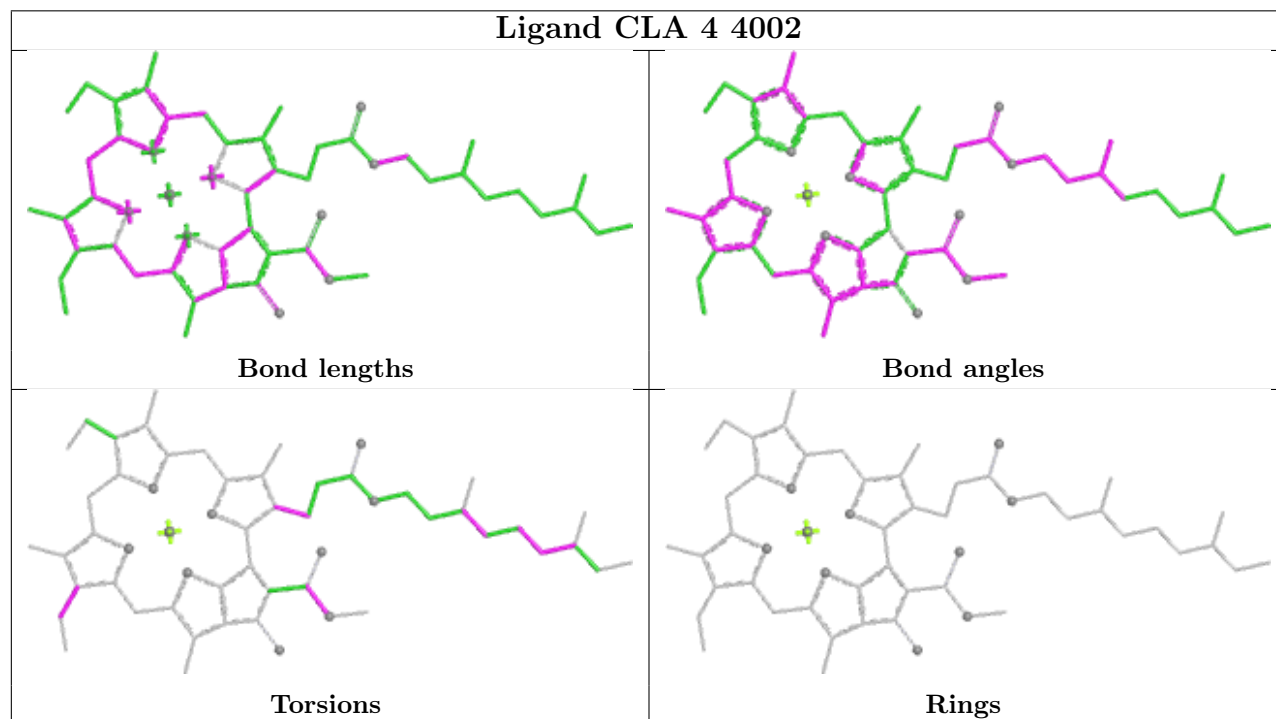
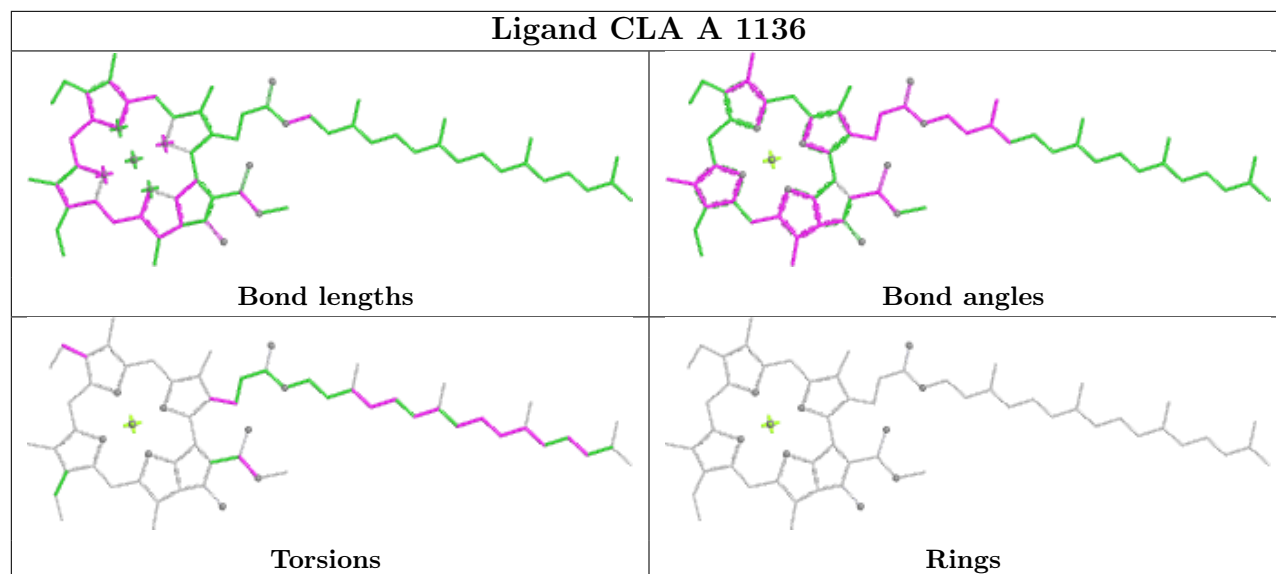


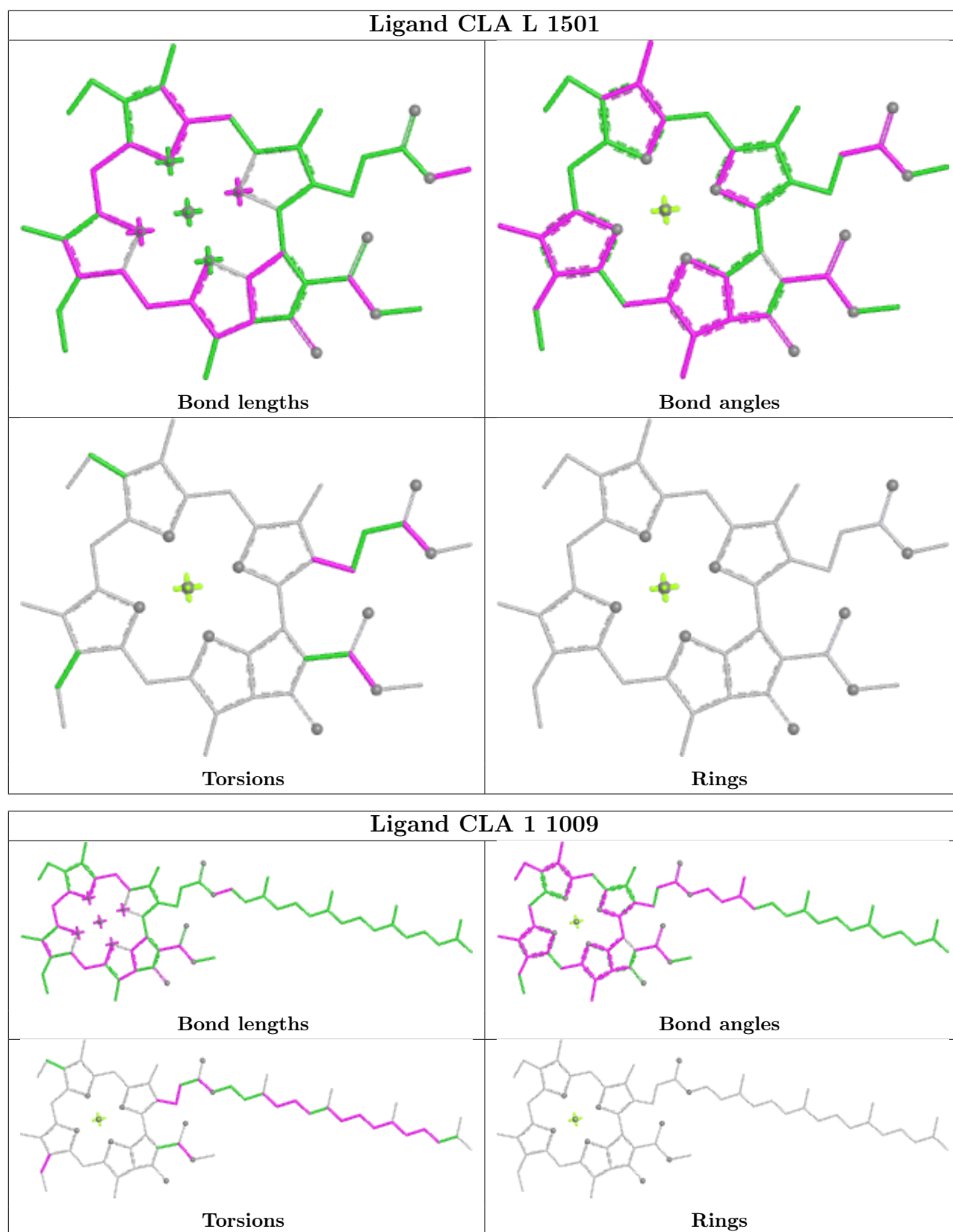




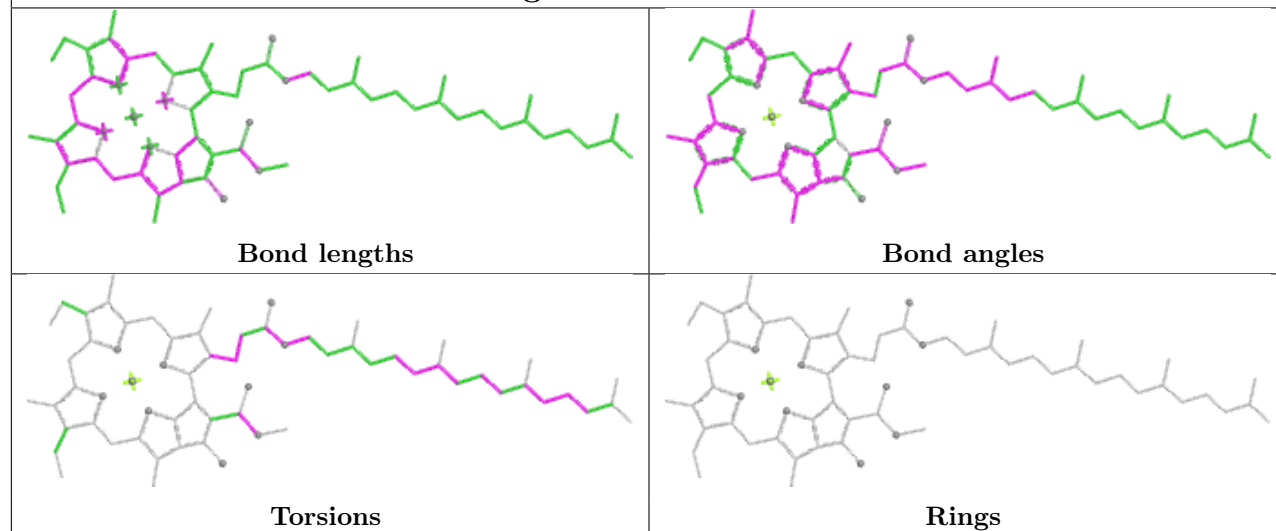




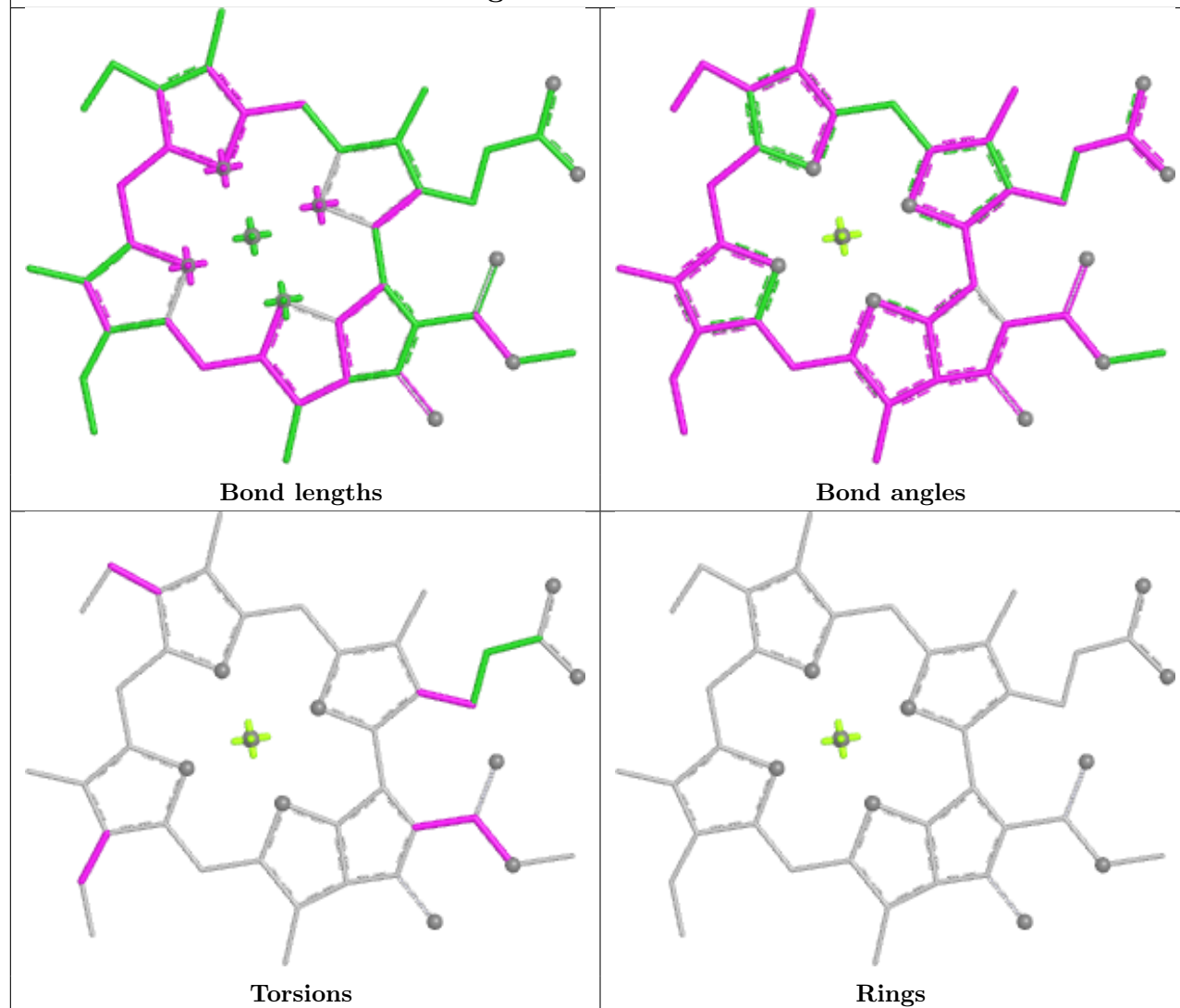


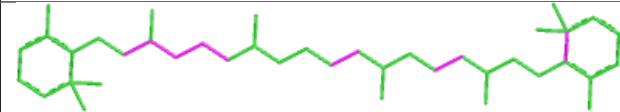
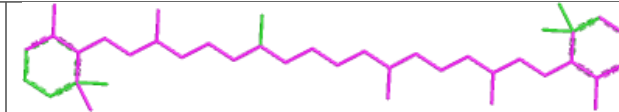
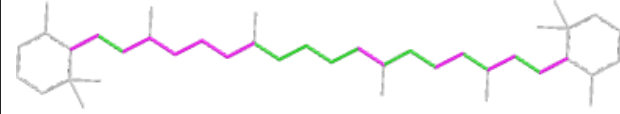
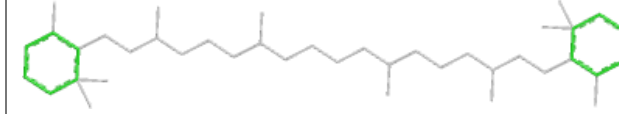


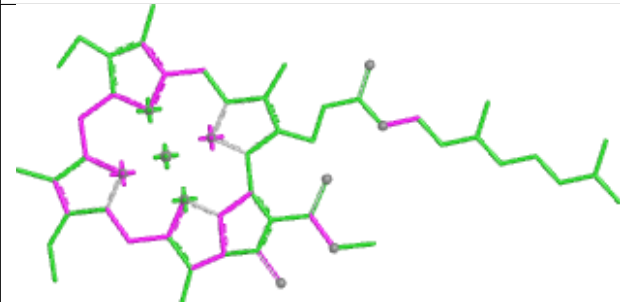
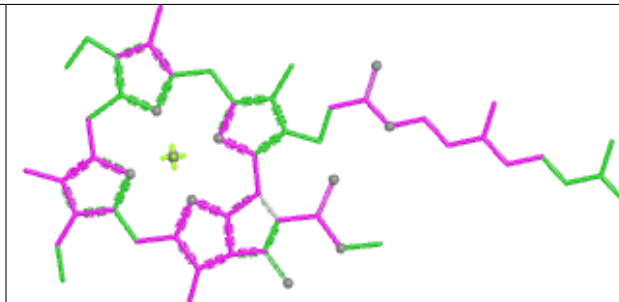
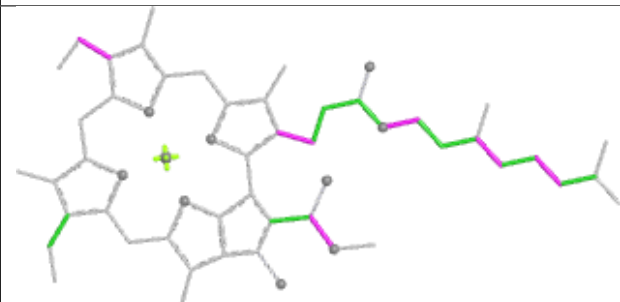
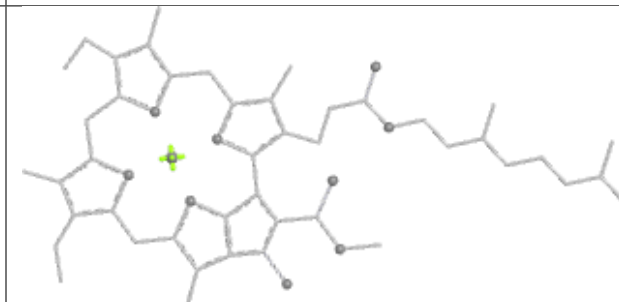
Ligand CLA B 1206

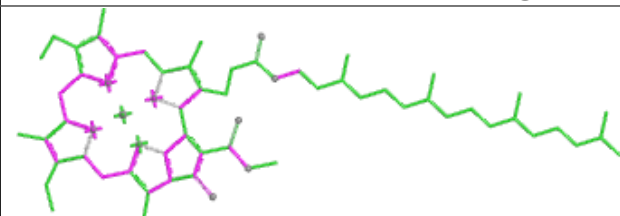
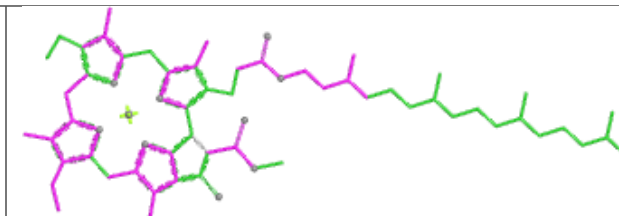
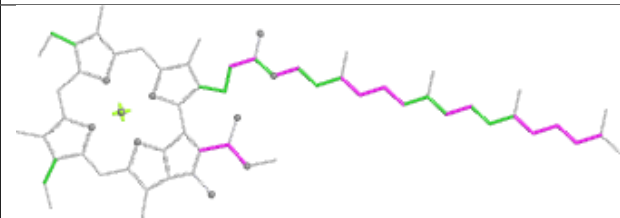
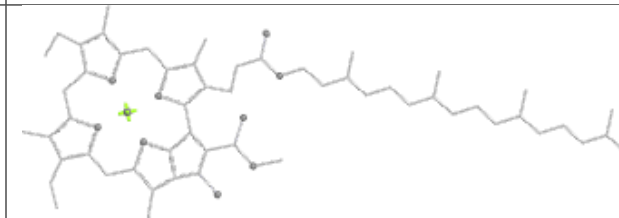


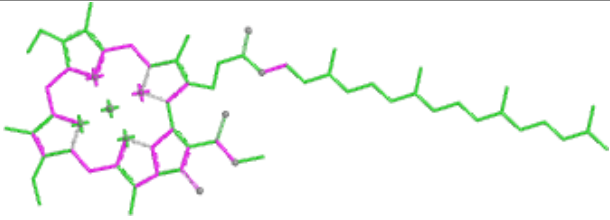
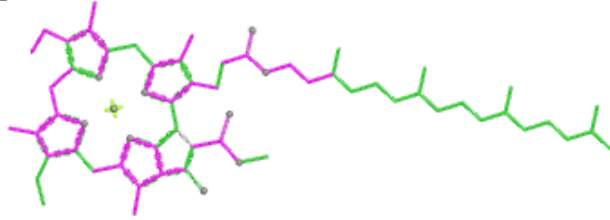
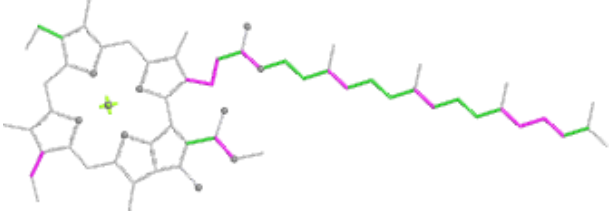
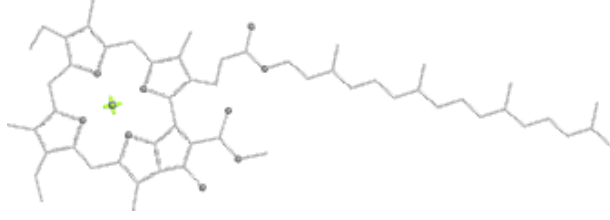
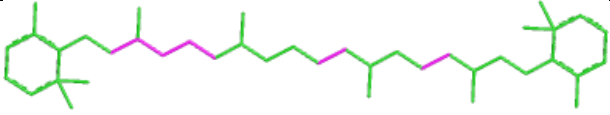
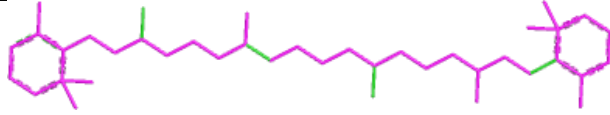
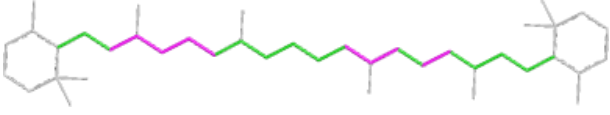
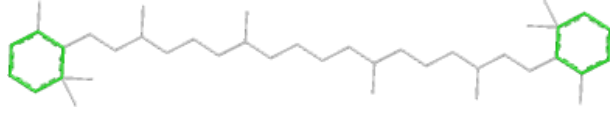
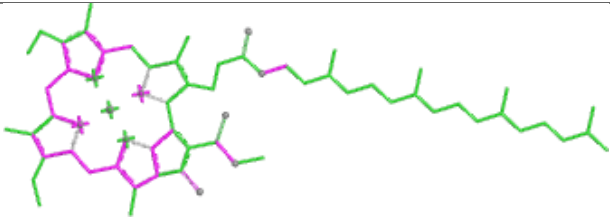
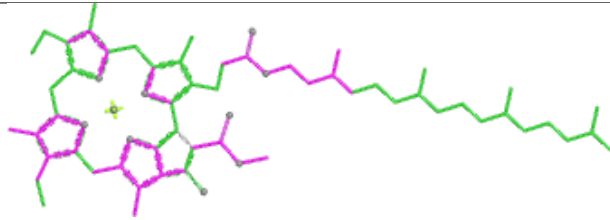
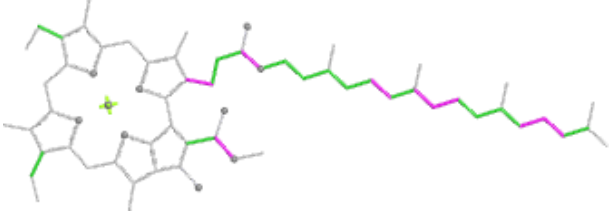
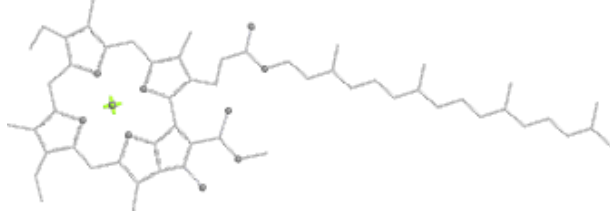
Ligand CLA 4 4005

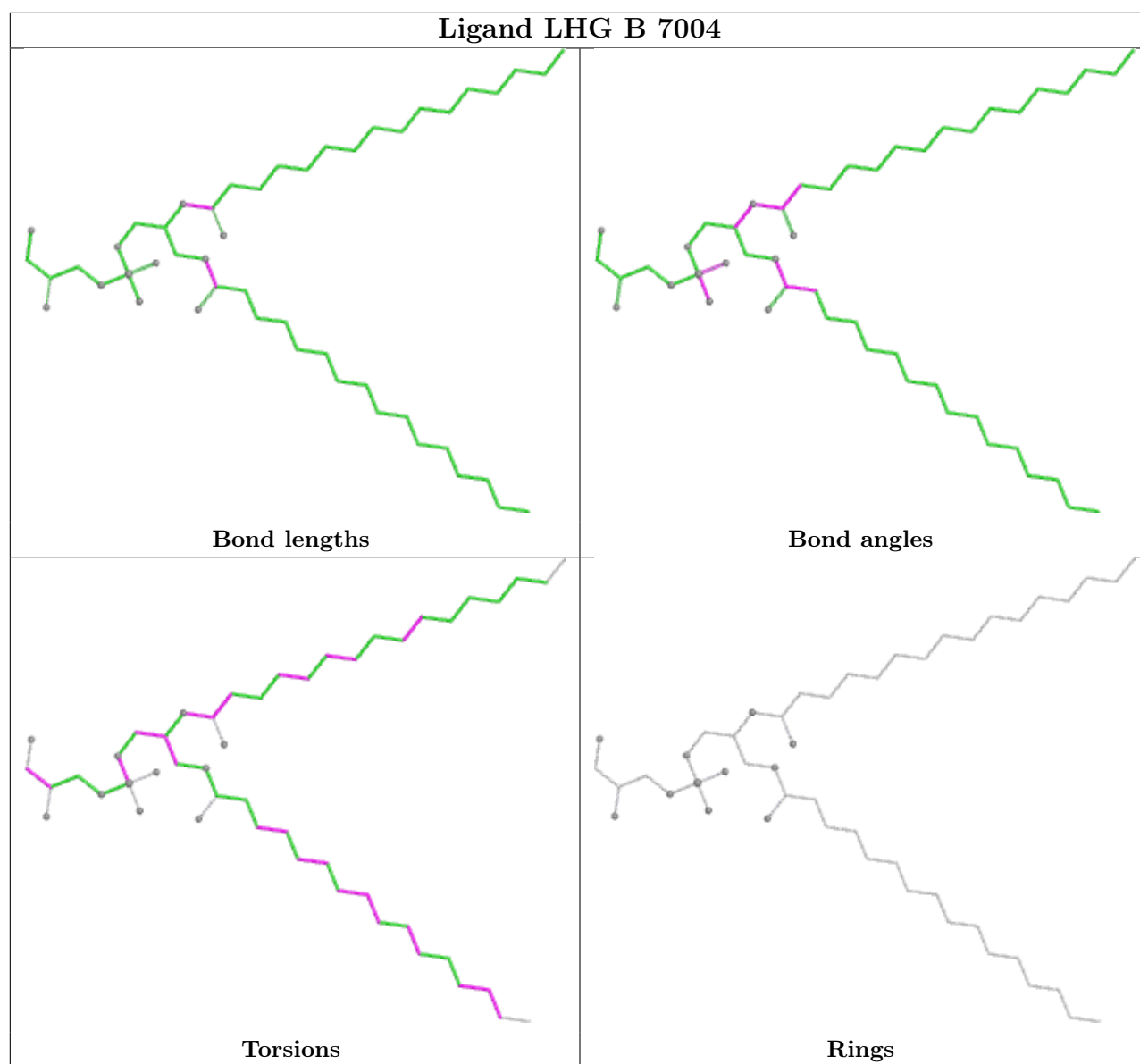


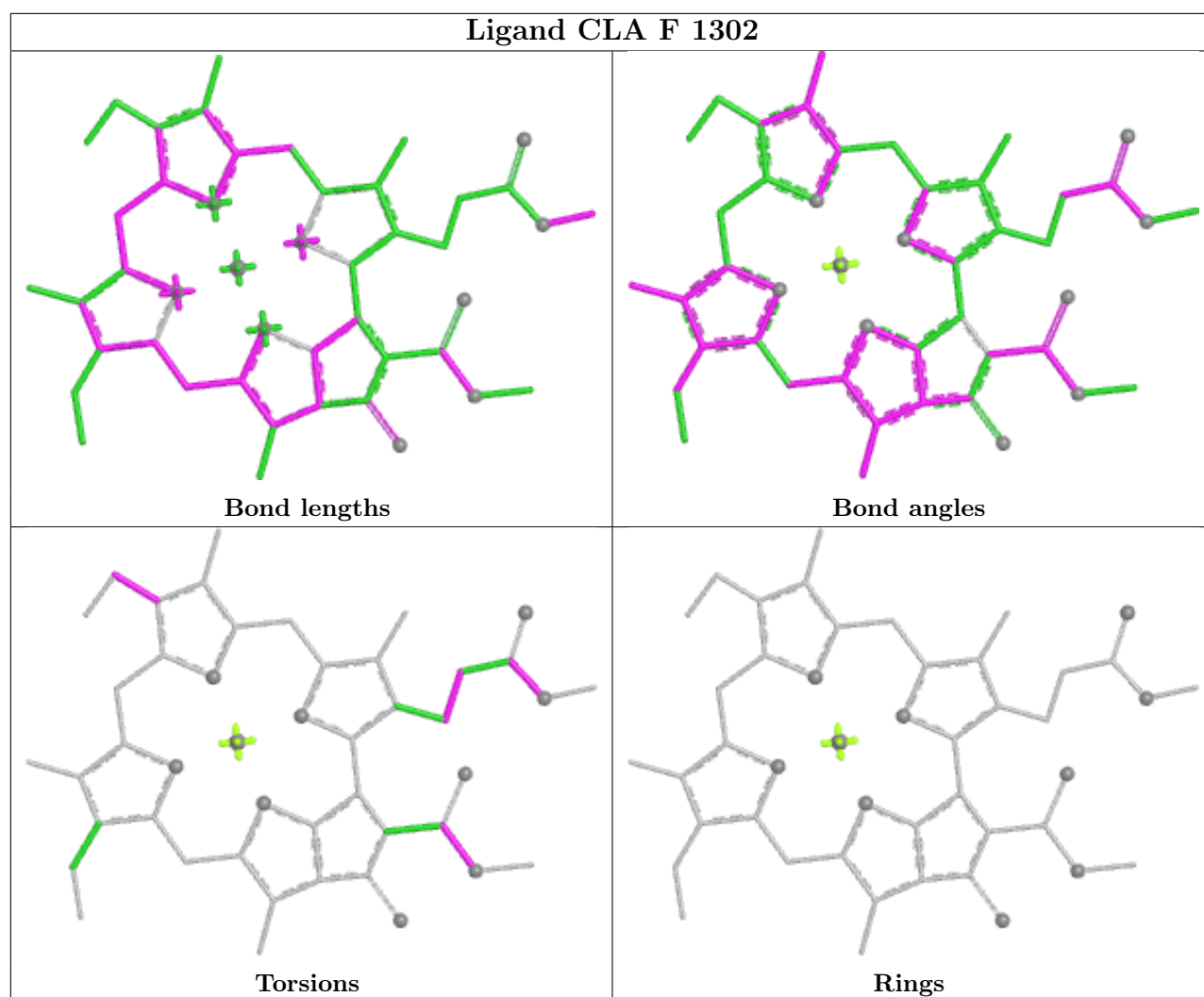
Ligand BCR G 2011	
	
Bond lengths	Bond angles
	
Torsions	Rings

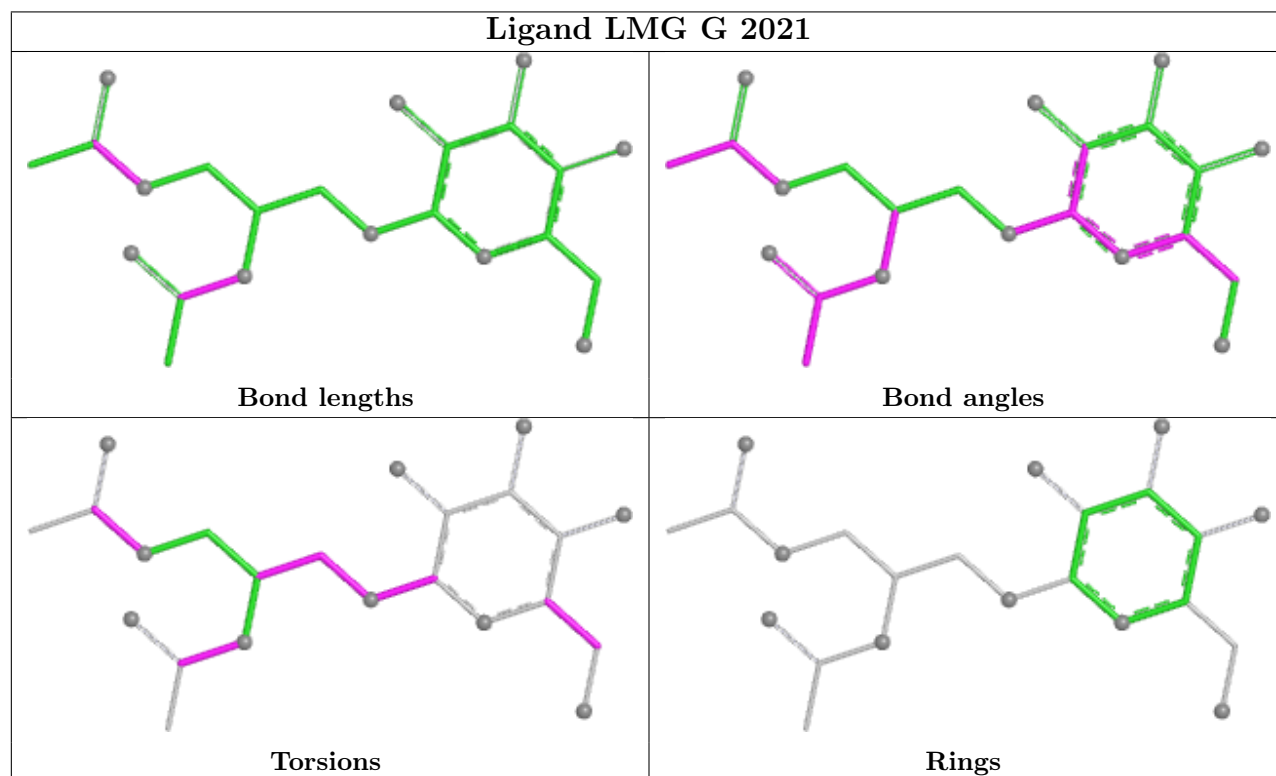
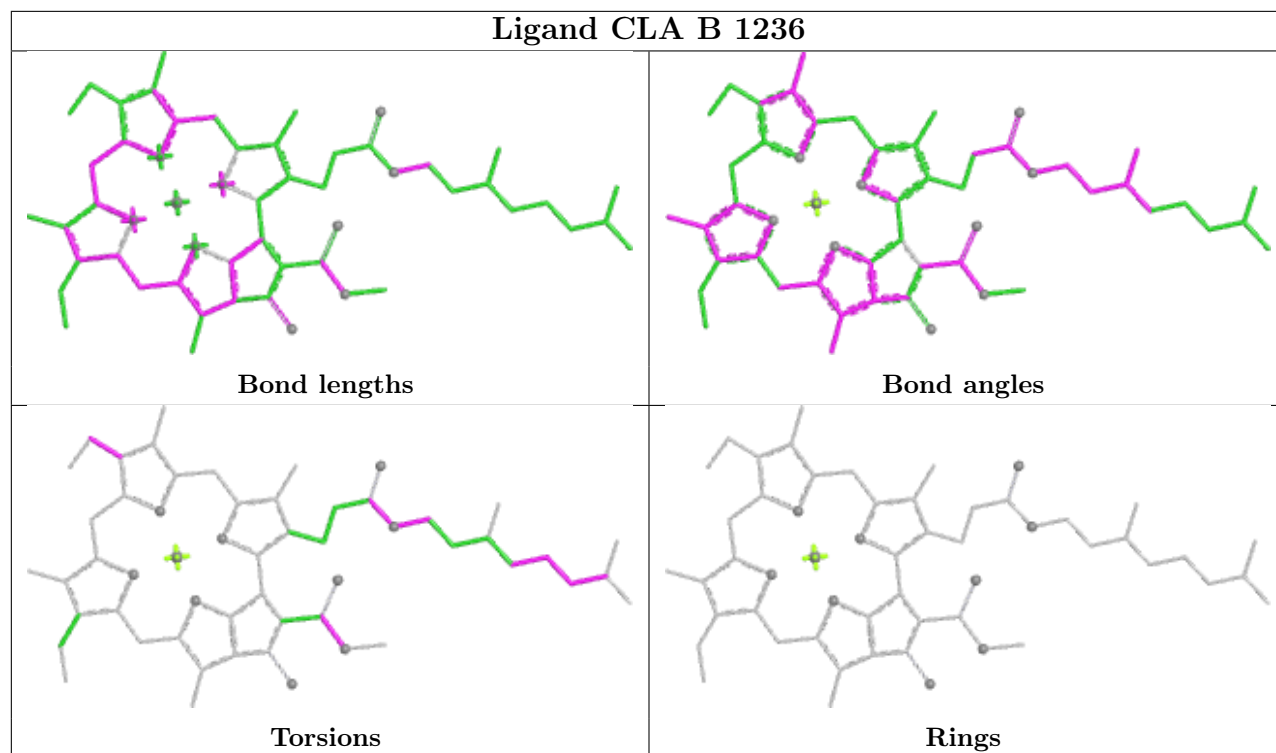
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Bond lengths	Bond angles
	
Torsions	Rings

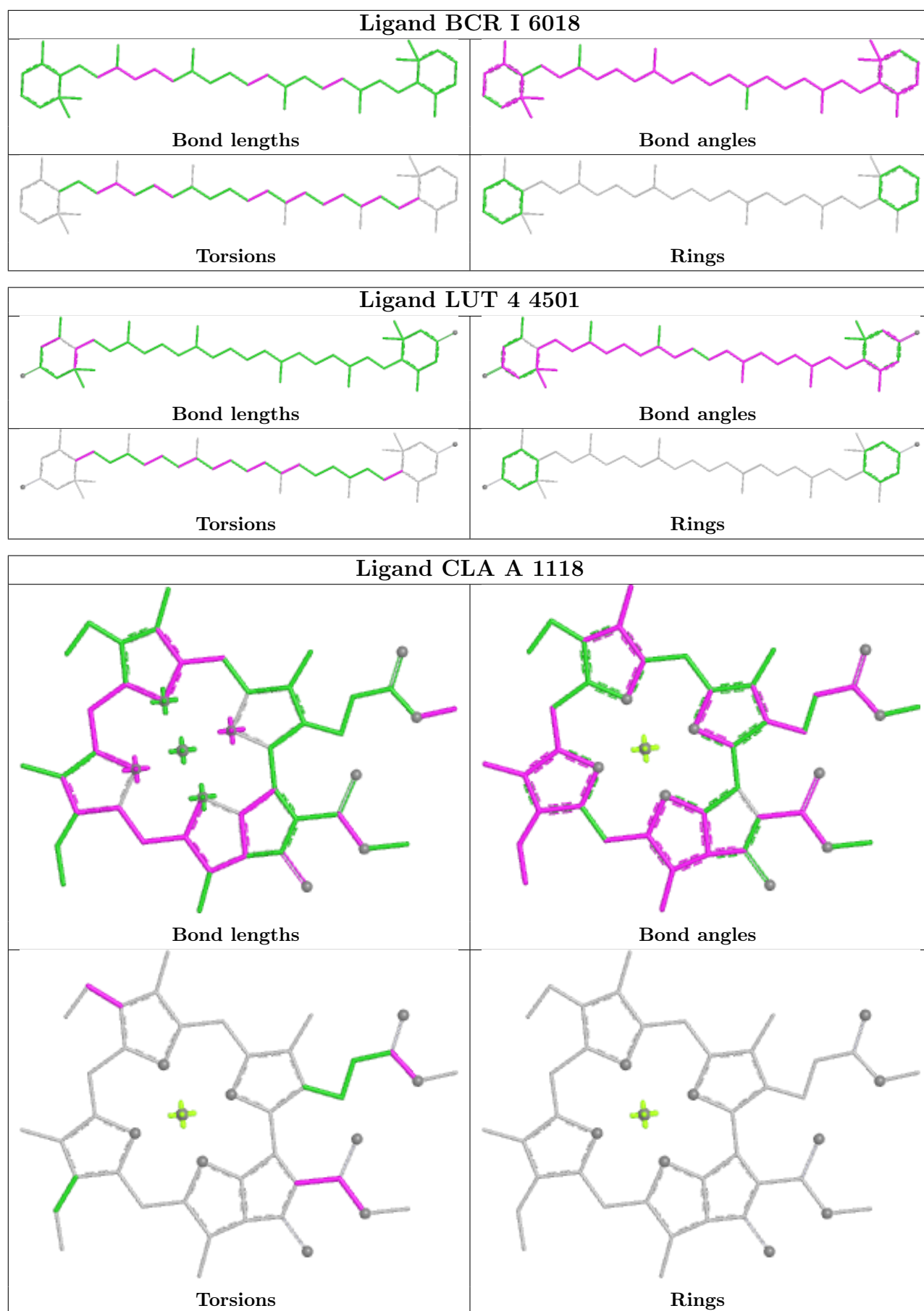
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Bond lengths	Bond angles
	
Torsions	Rings

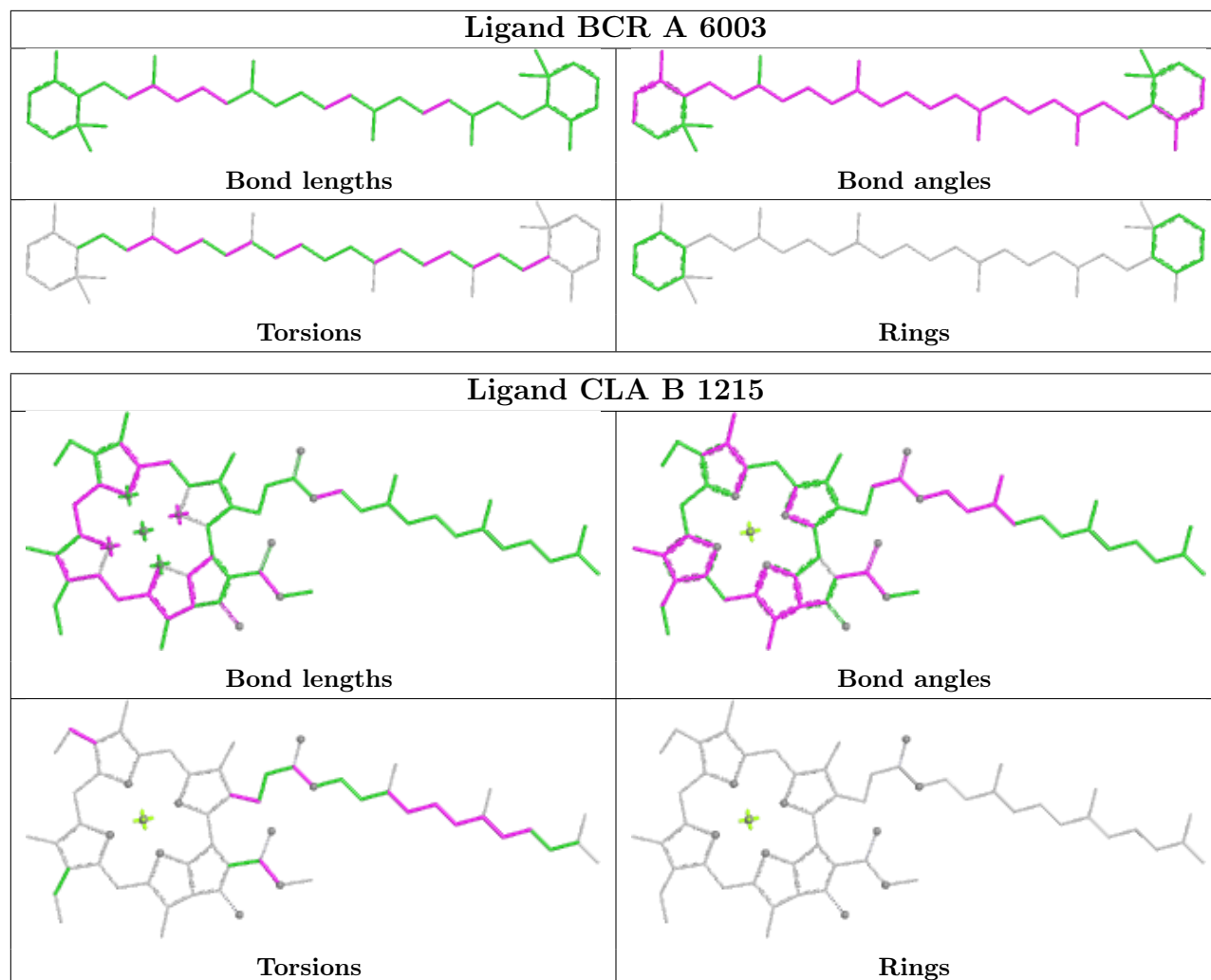
Ligand CLA 4 4012	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Torsions	 Rings
Ligand CLA A 1117	
 Bond lengths	 Bond angles
 Torsions	 Rings



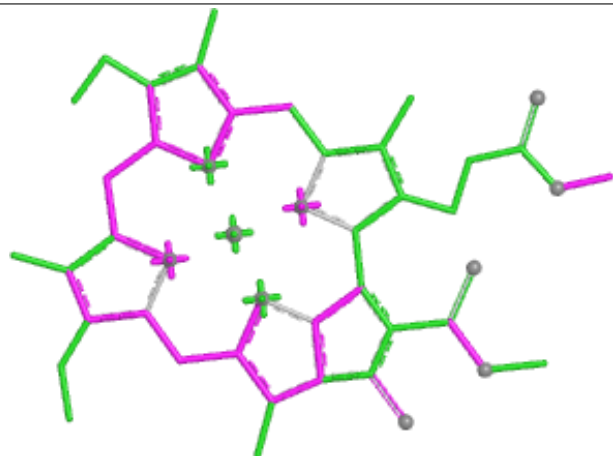




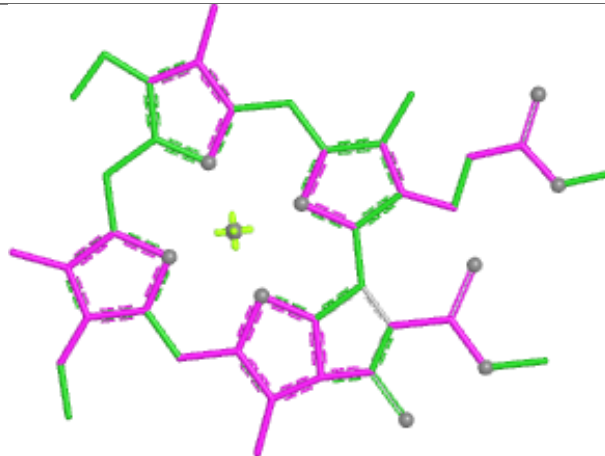




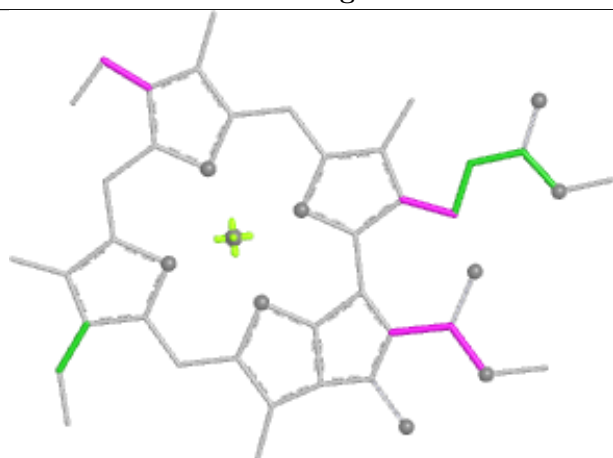
Ligand CLA B 1212



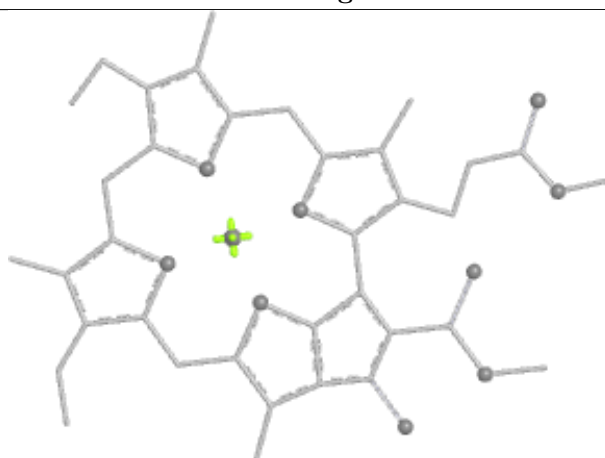
Bond lengths



Bond angles

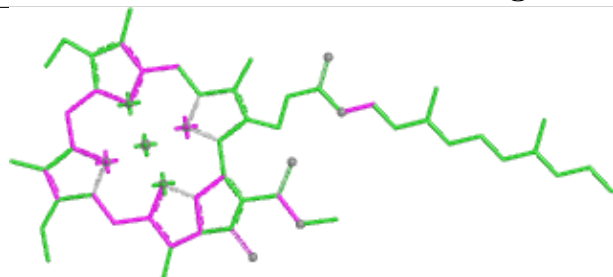


Torsions

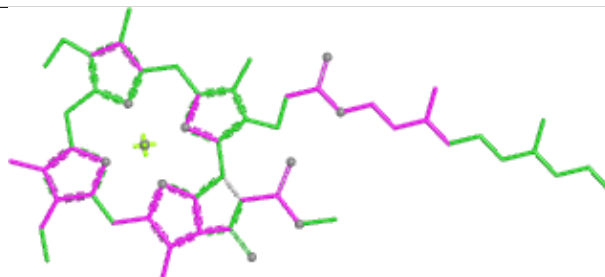


Rings

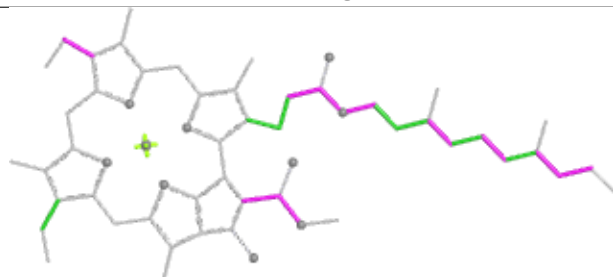
Ligand CLA 2 2006



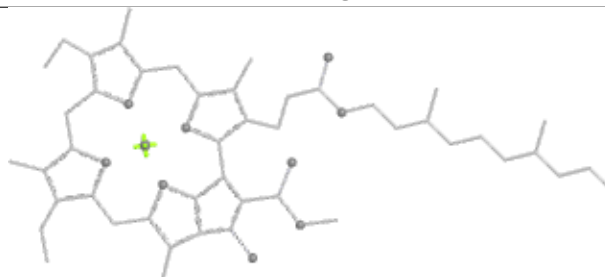
Bond lengths



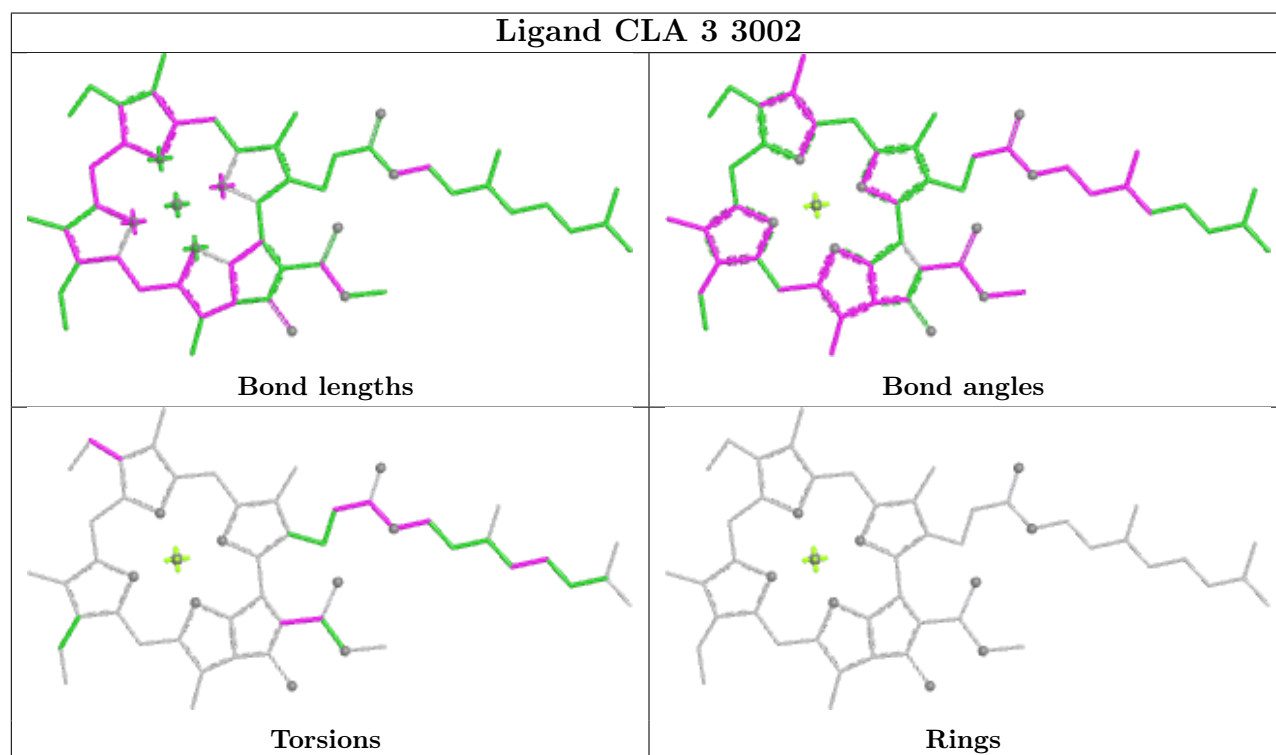
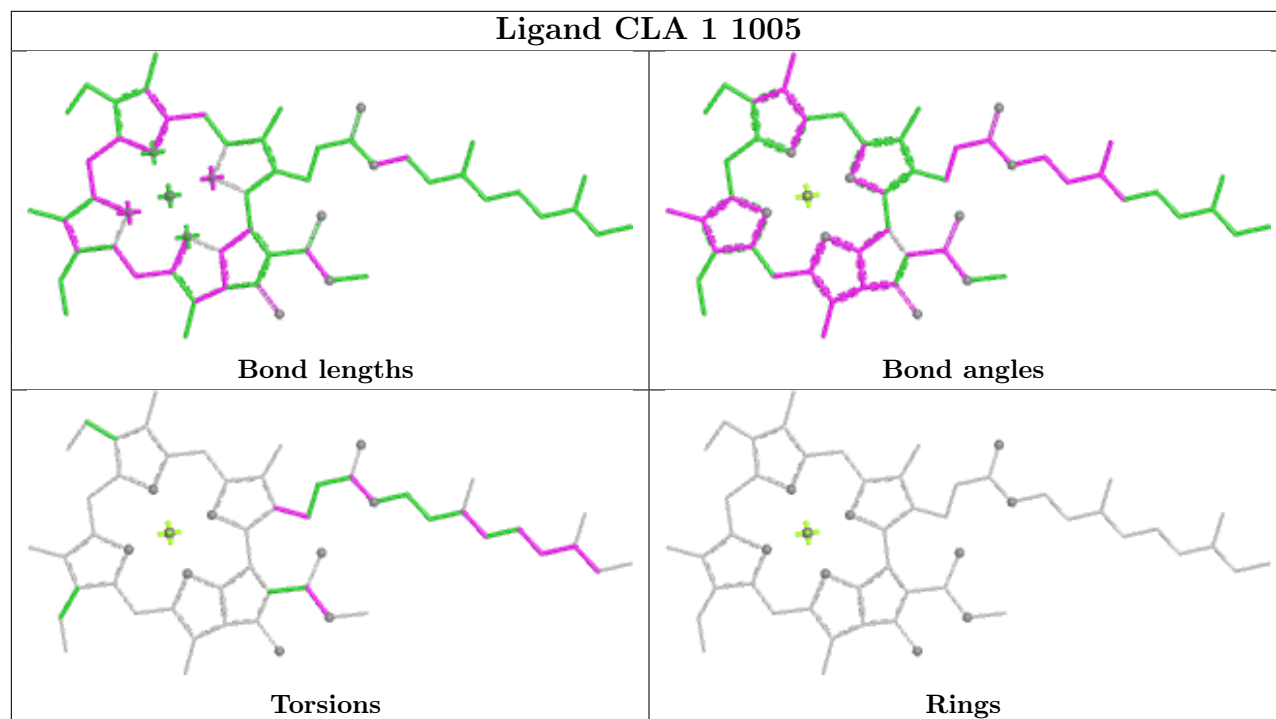
Bond angles

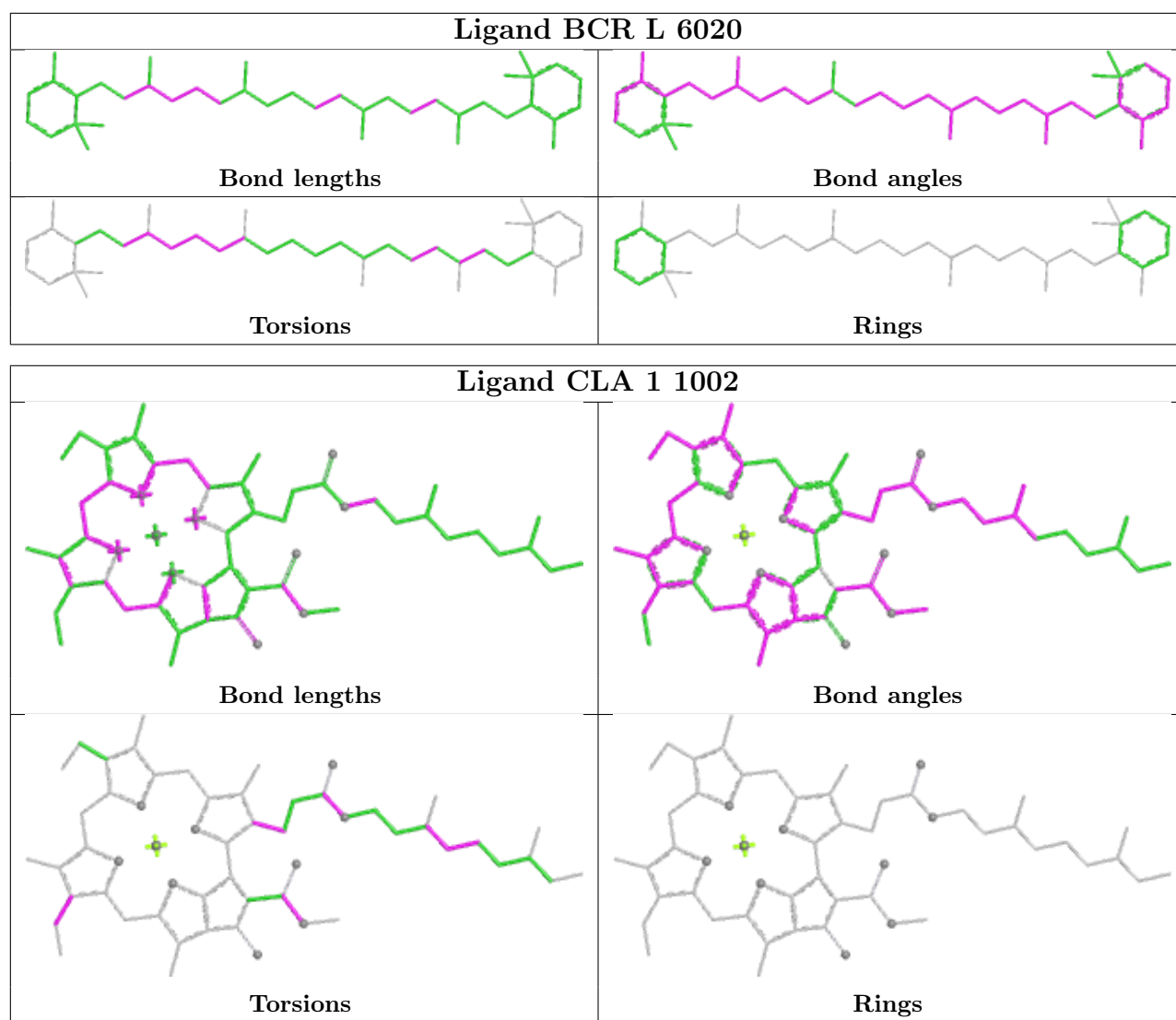


Torsions

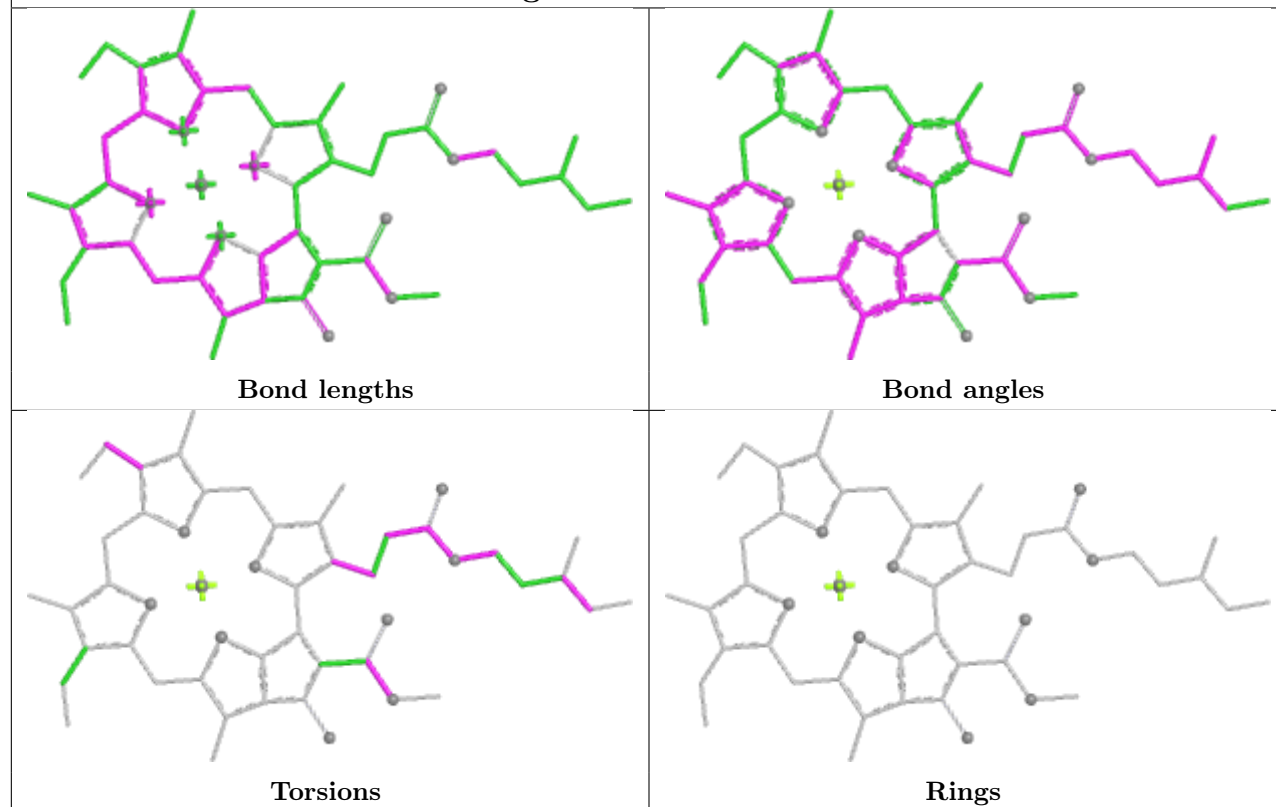


Rings

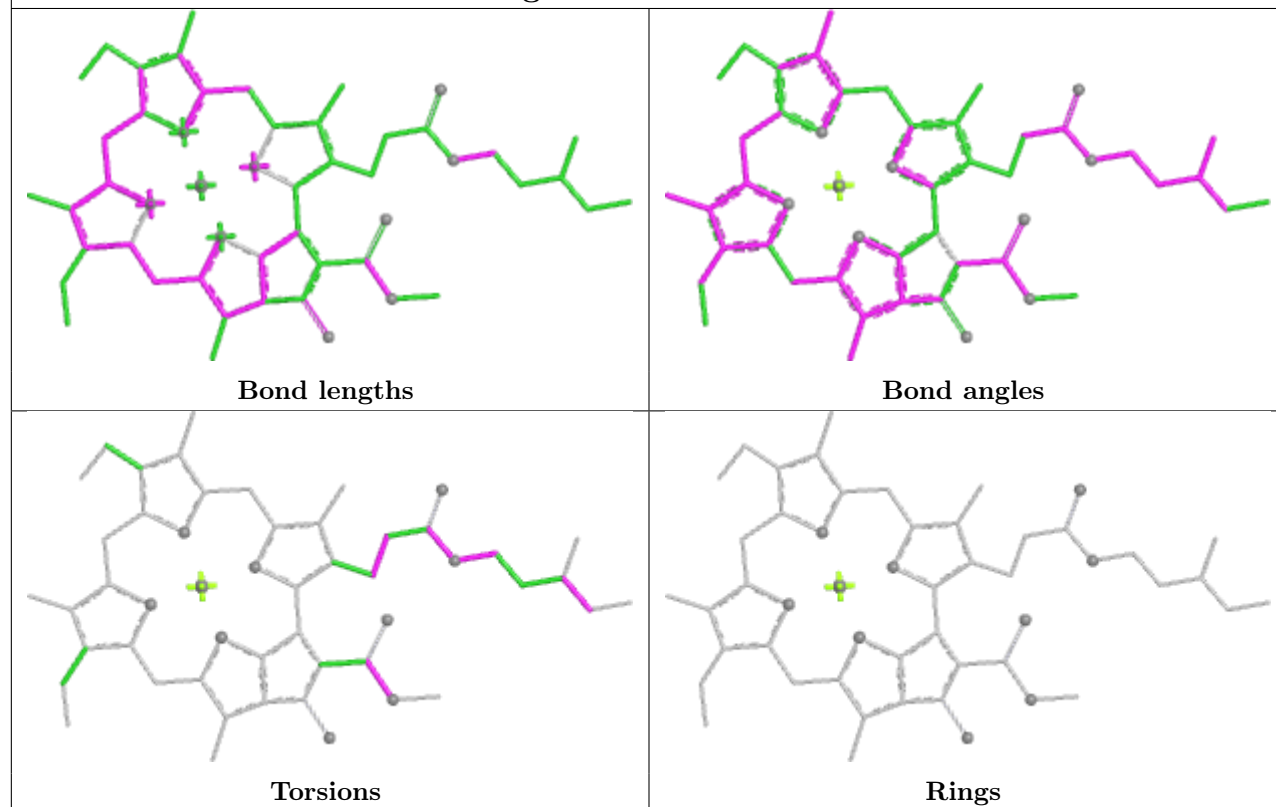


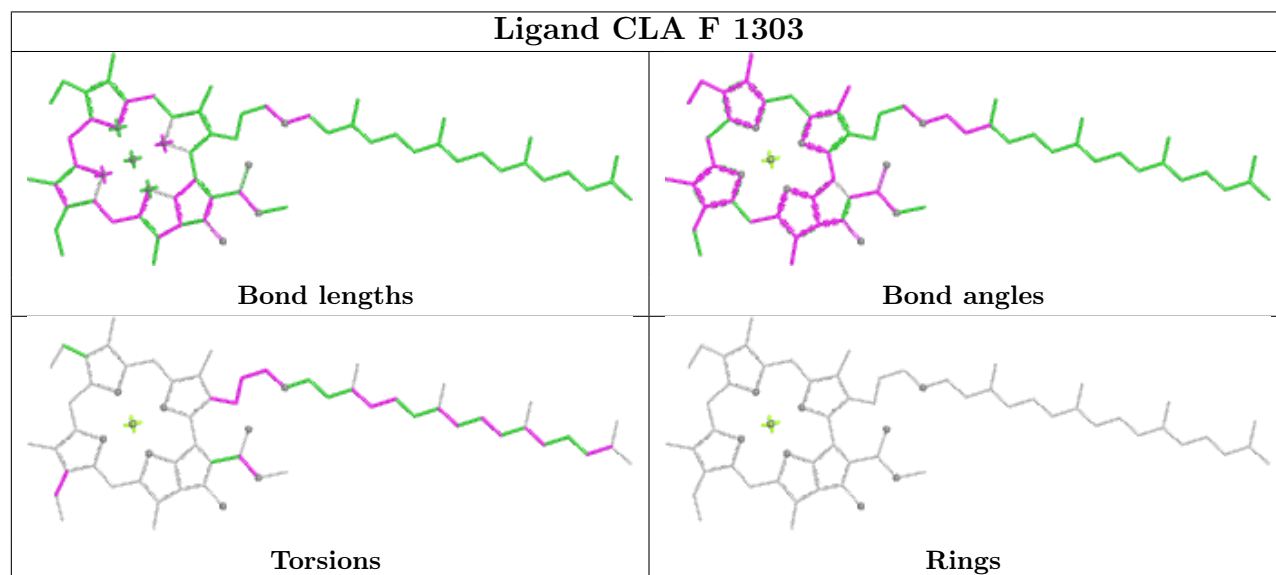
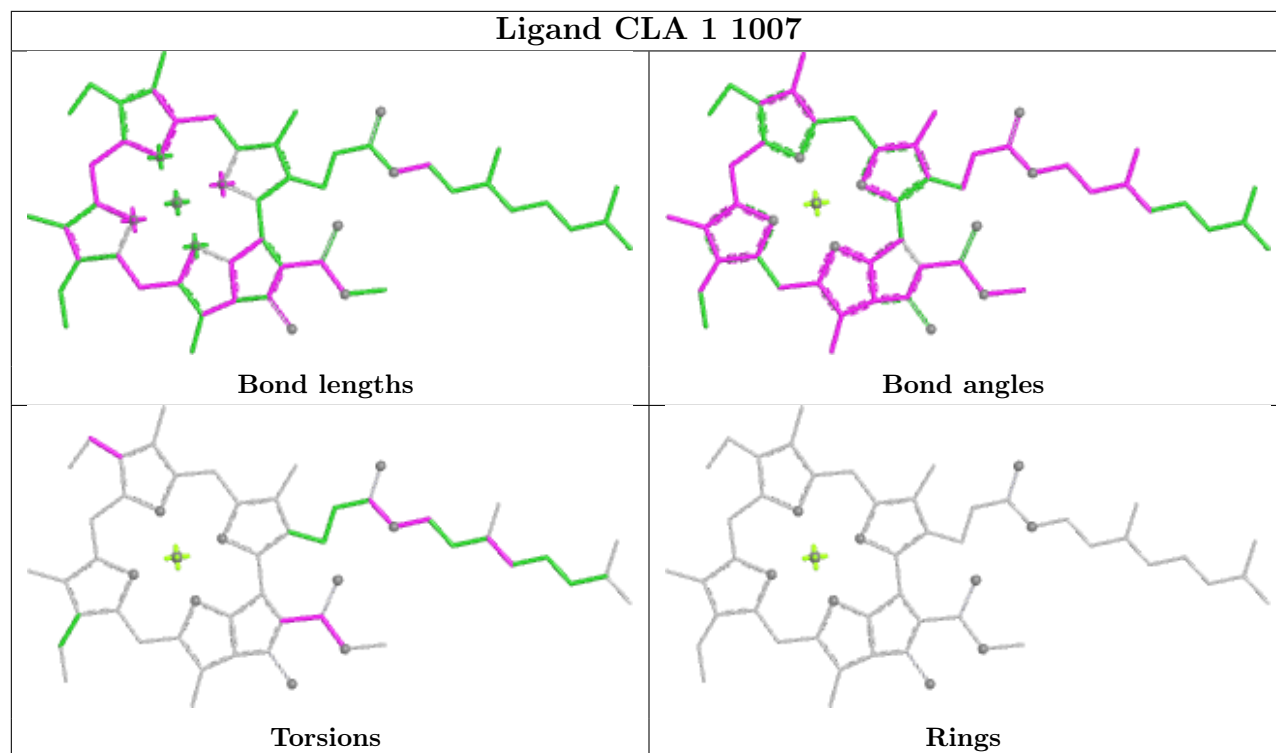


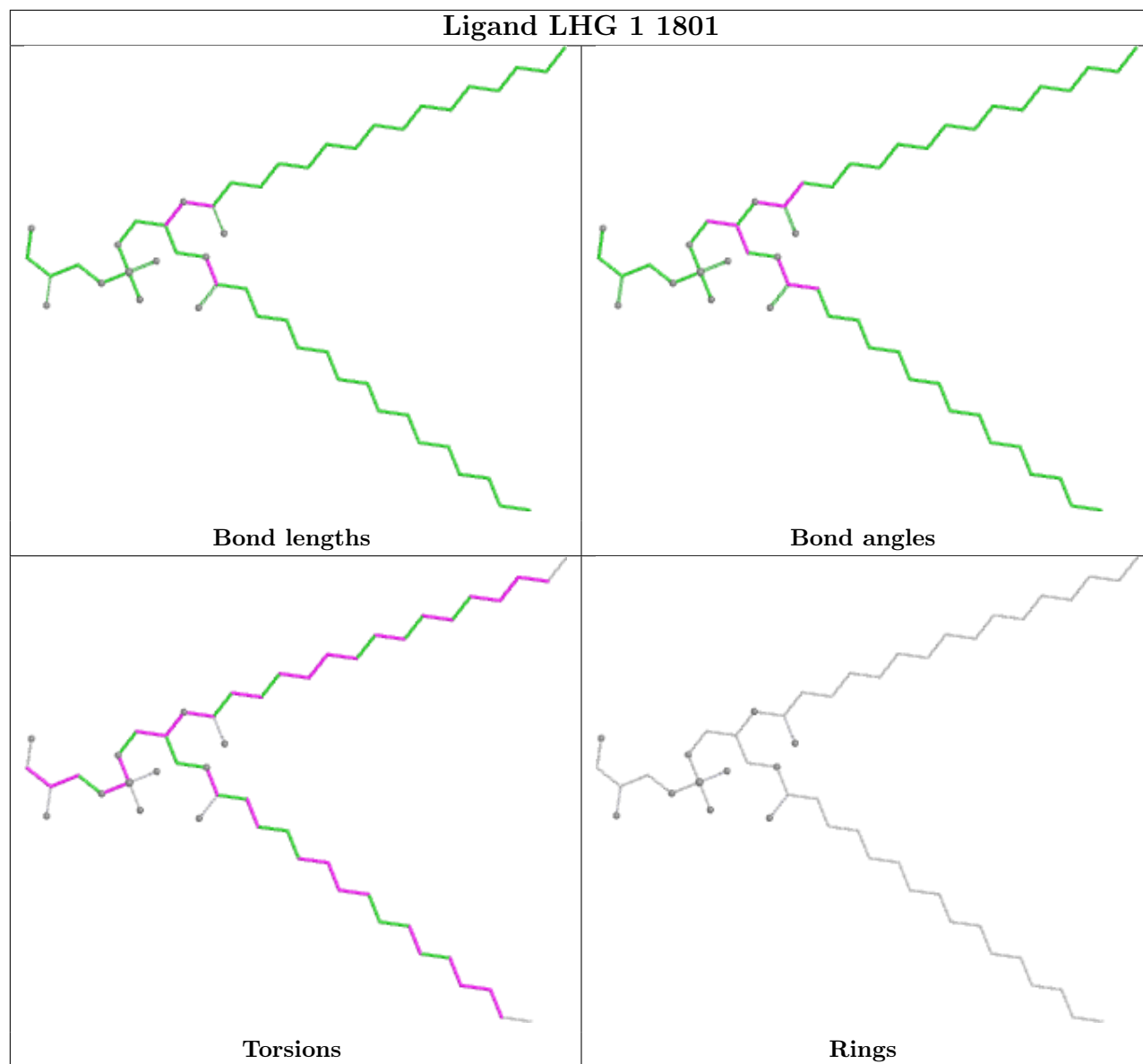
Ligand CLA A 1107

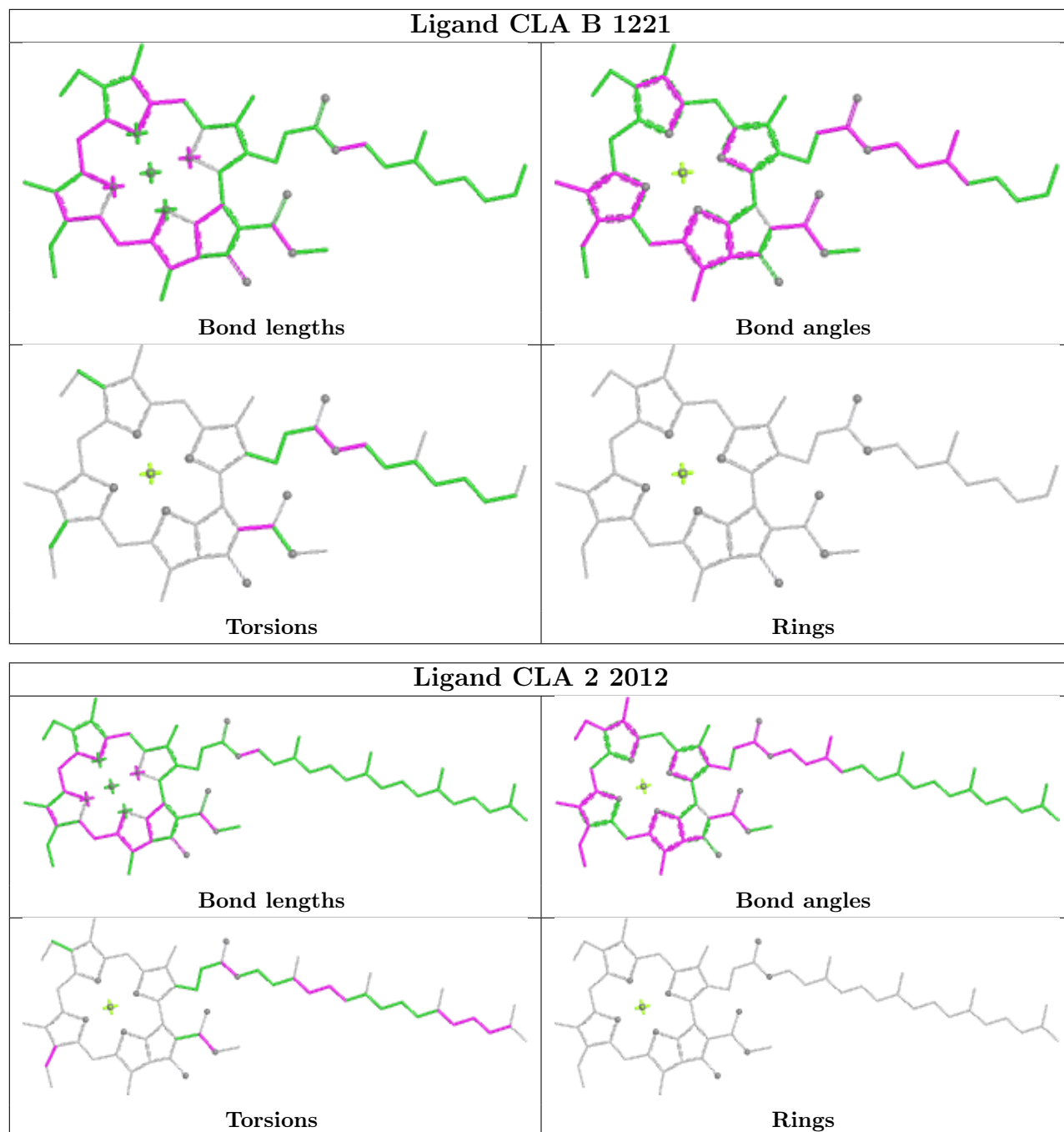


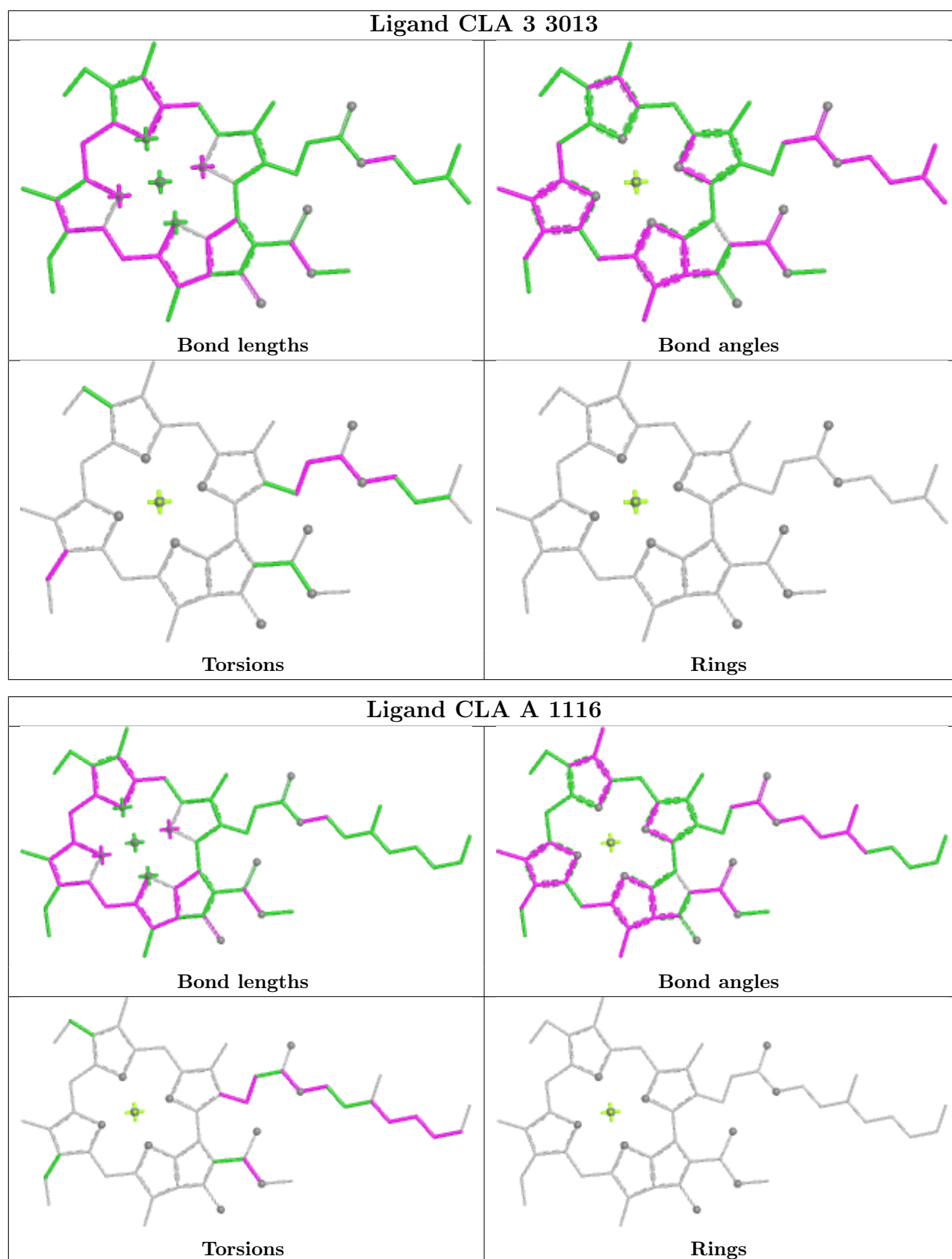
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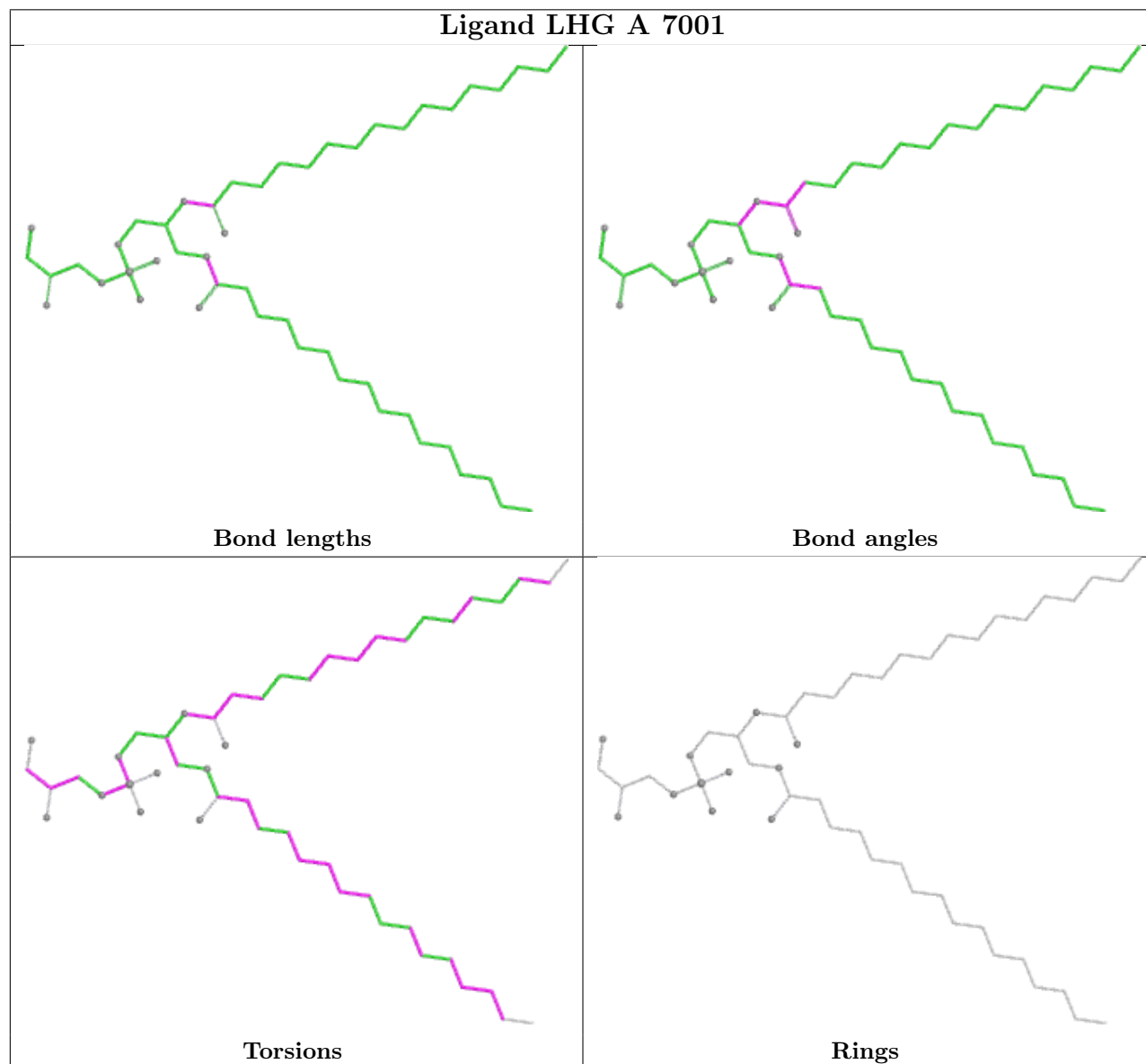
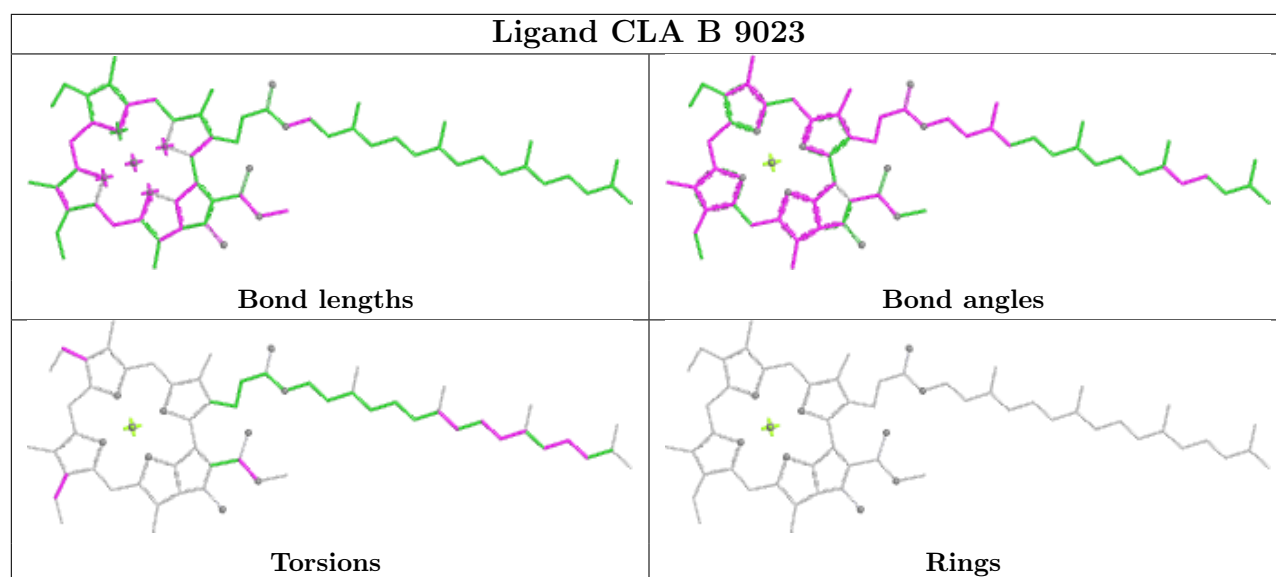




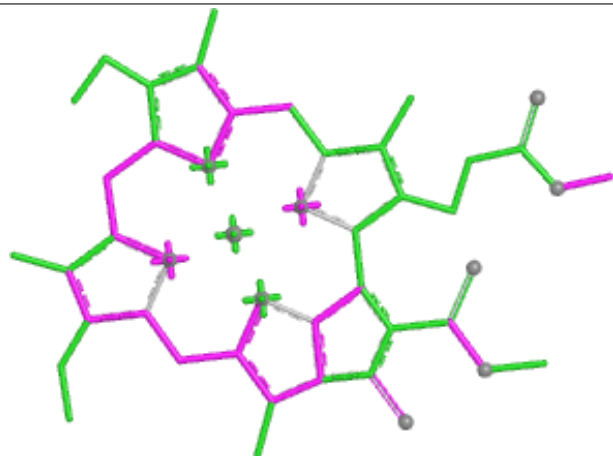




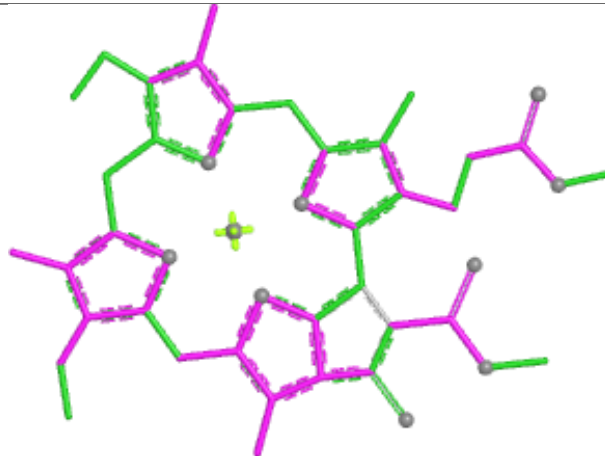




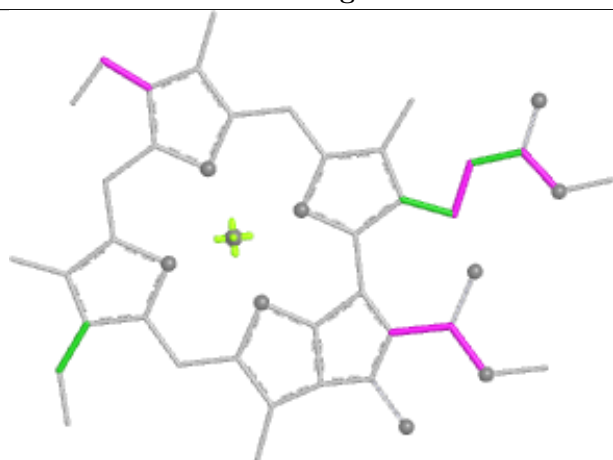
Ligand CLA B 1217



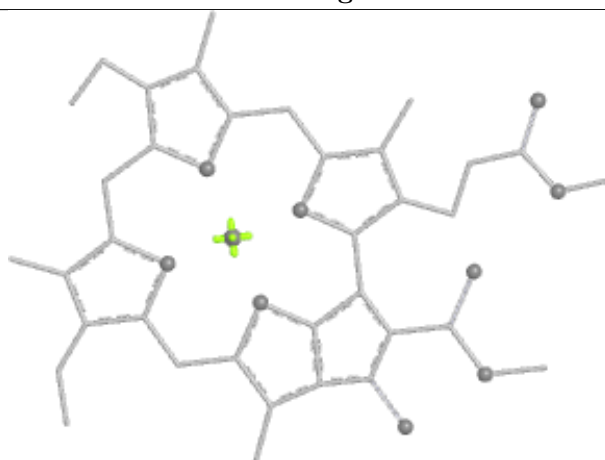
Bond lengths



Bond angles

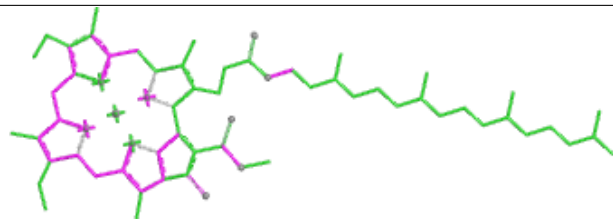


Torsions

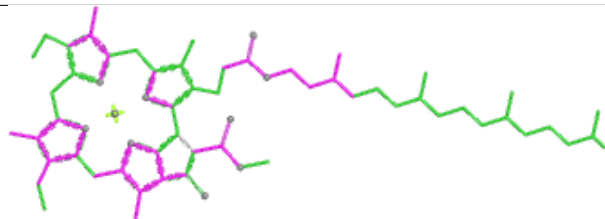


Rings

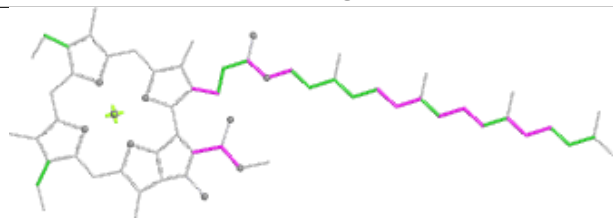
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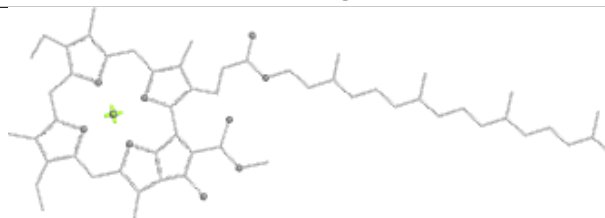
Bond lengths



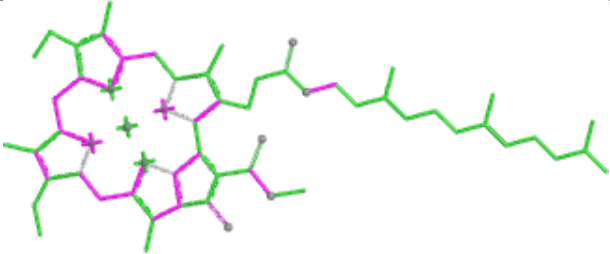
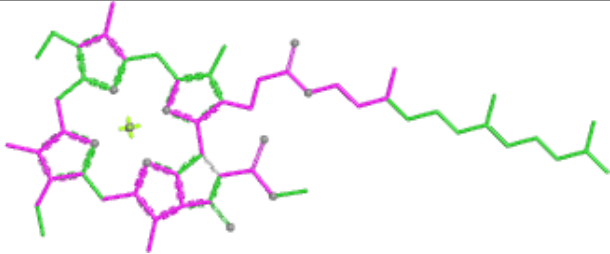
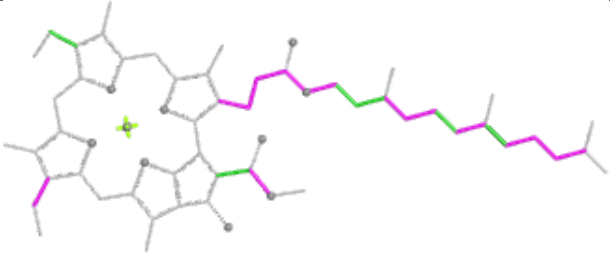
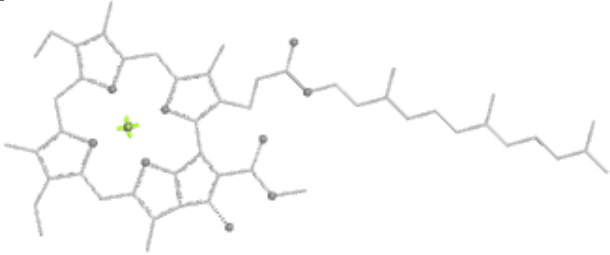
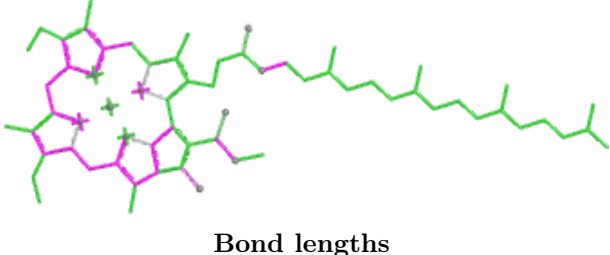
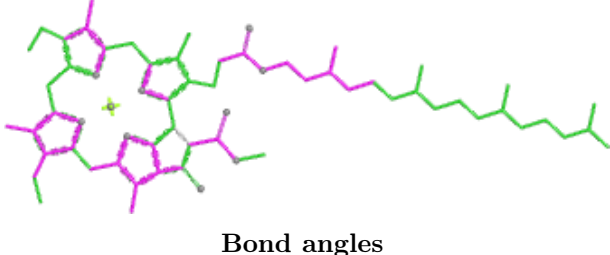
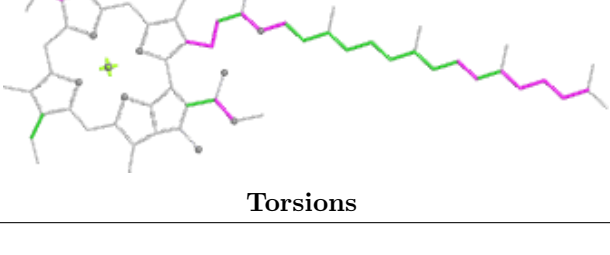
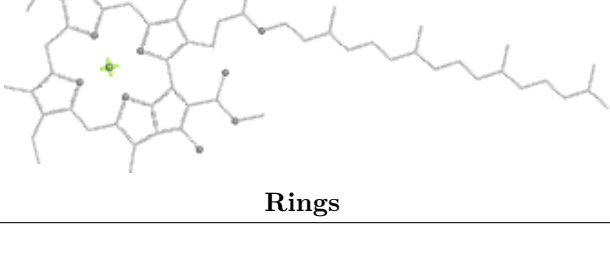
Bond angles

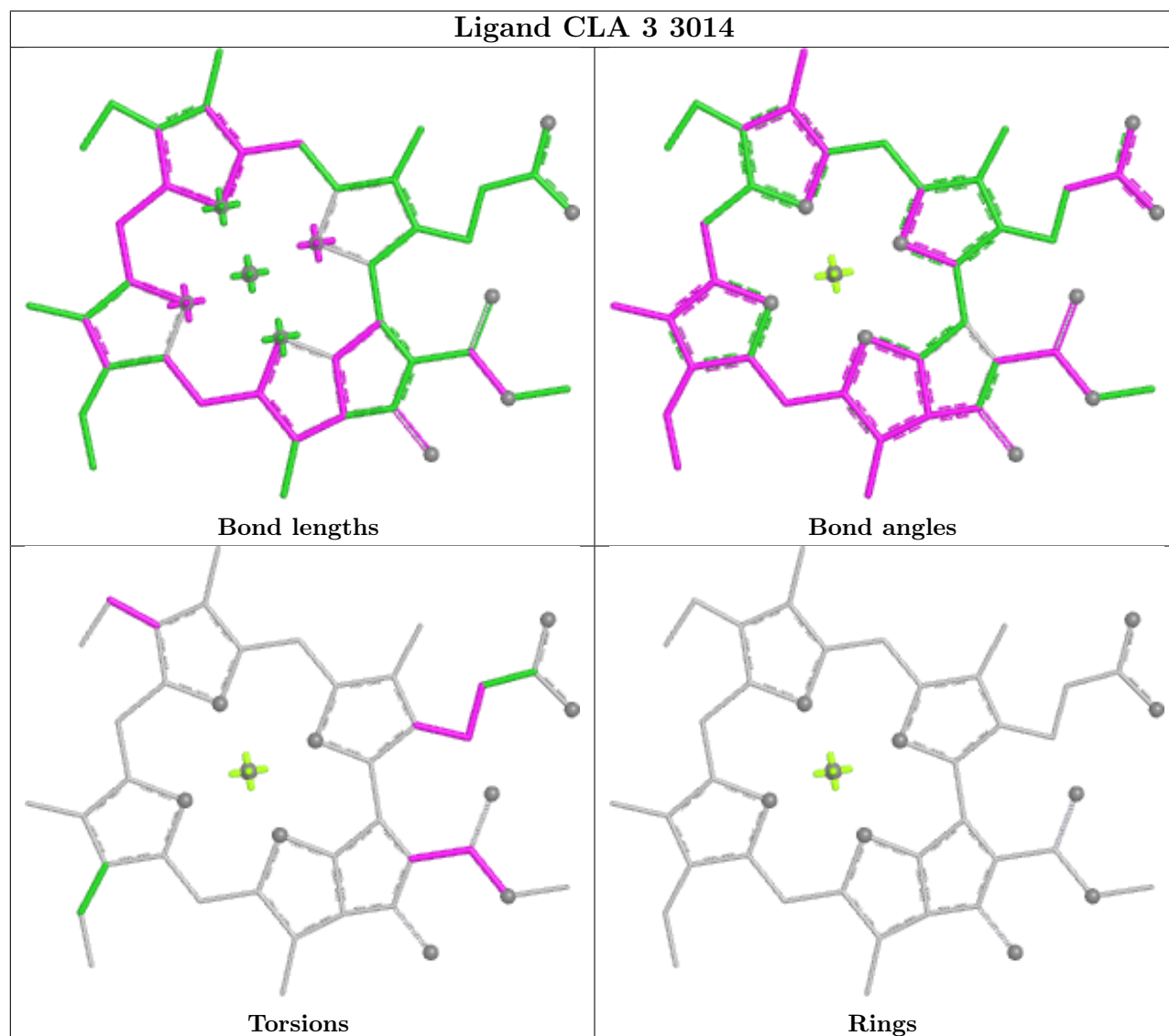
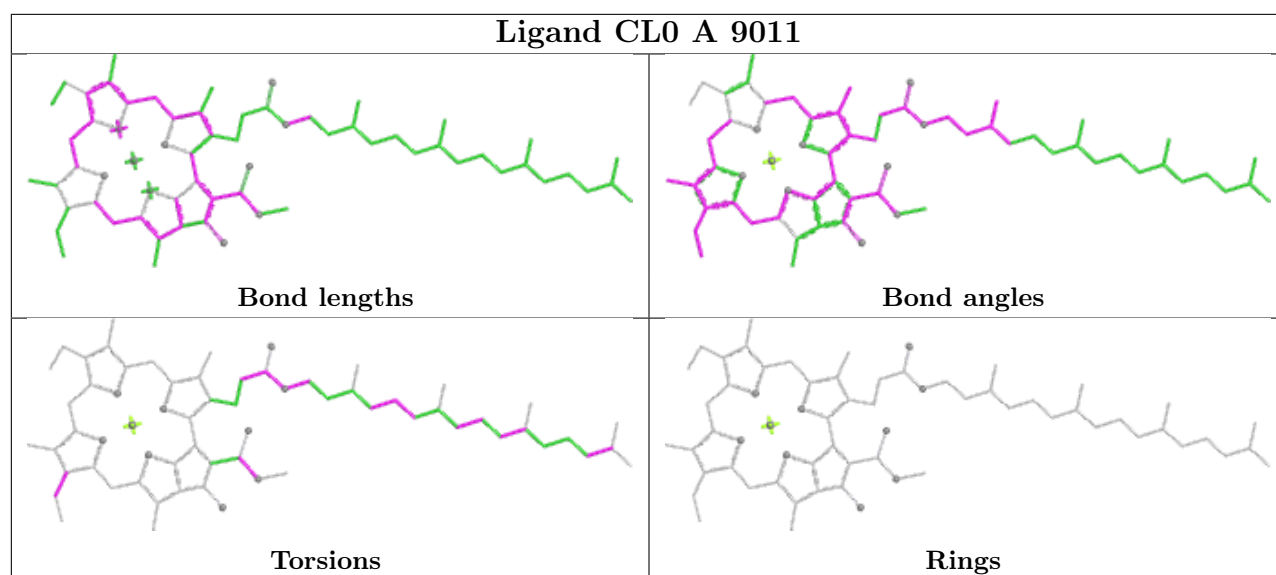


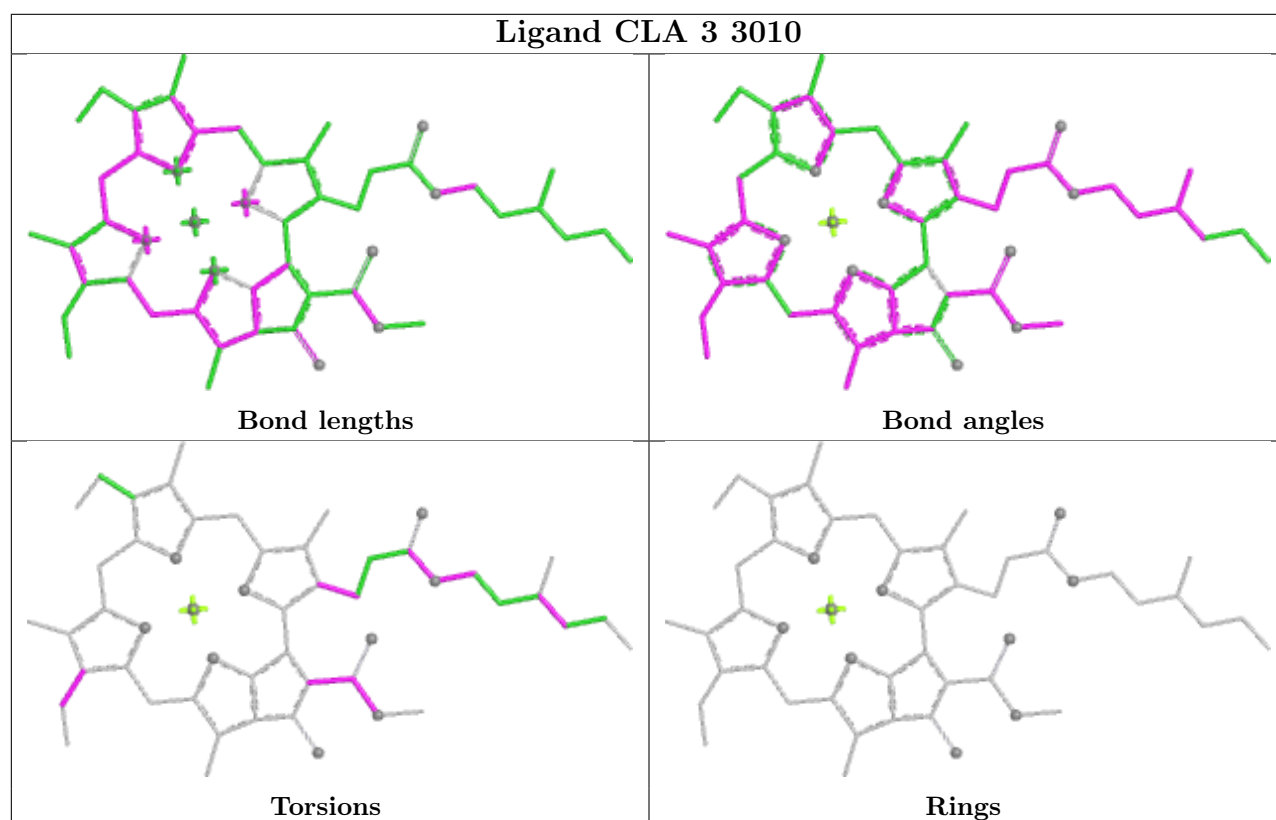
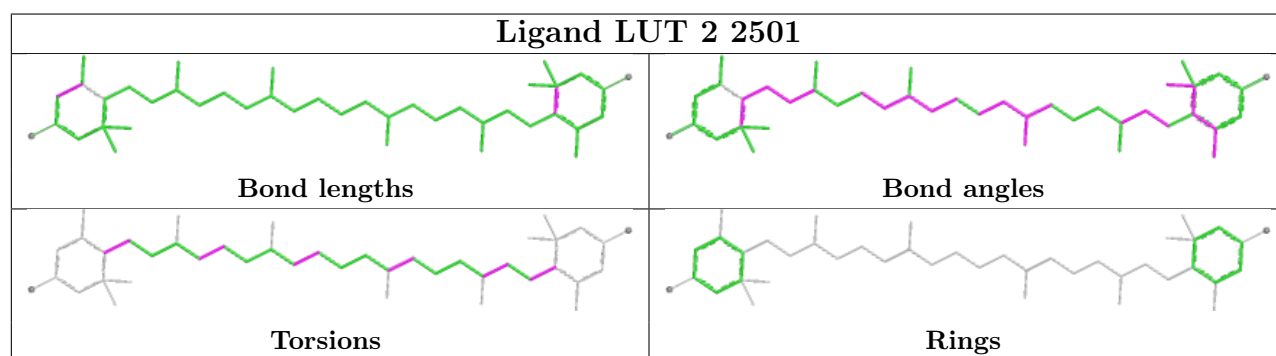
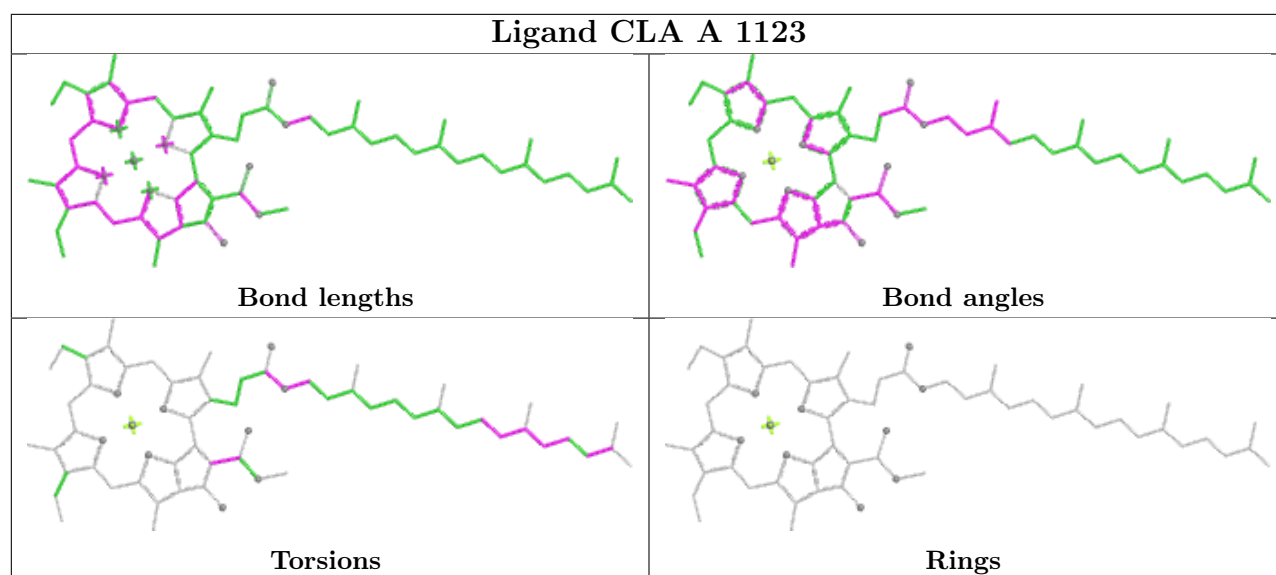
Torsions



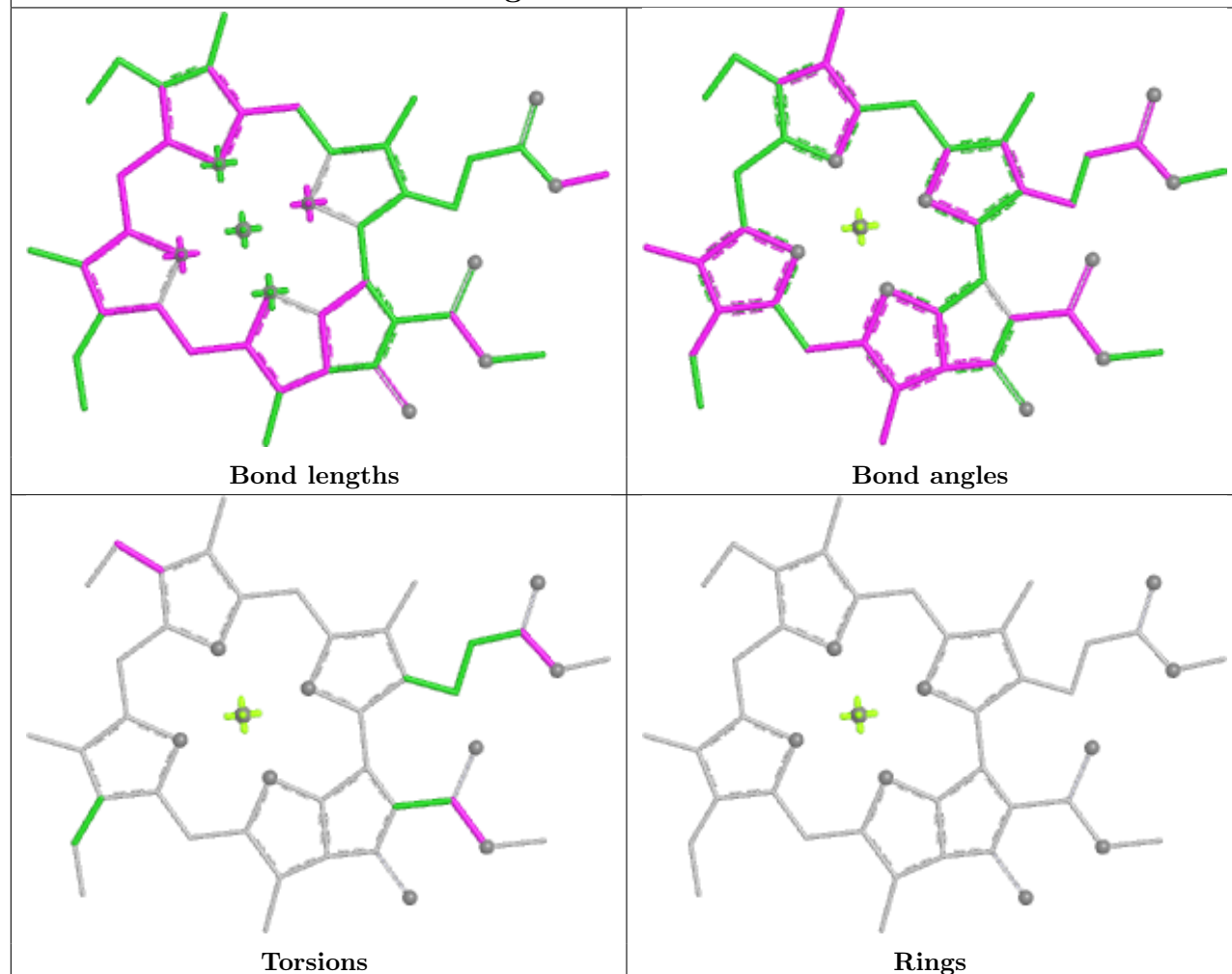
Rings

Ligand CLA 2 2011	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 3 3006	
 Bond lengths	 Bond angles
 Torsions	 Rings

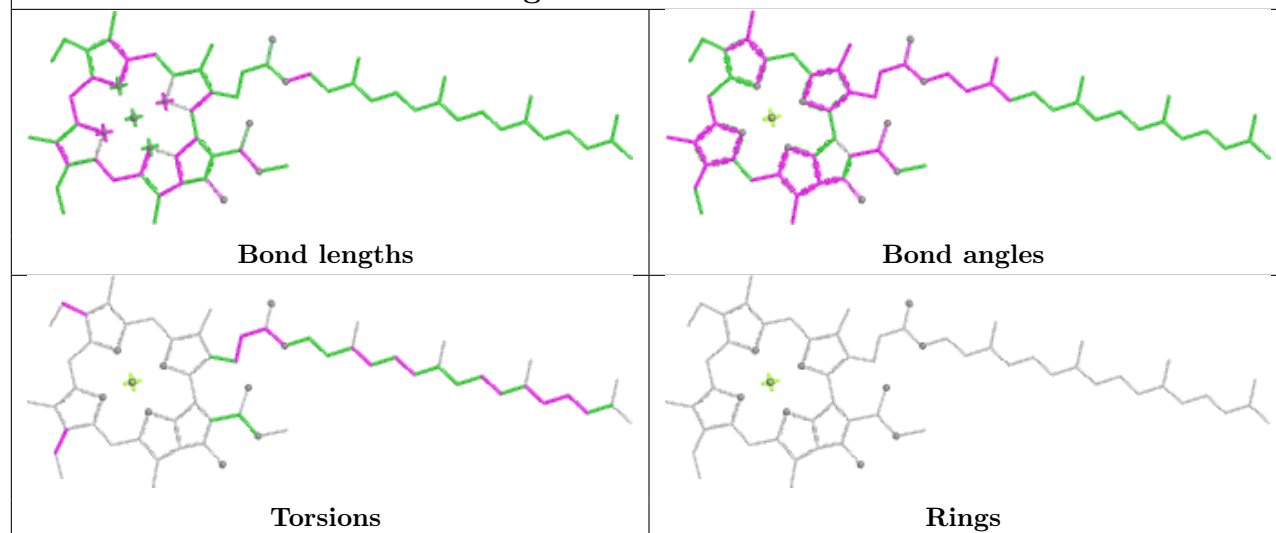


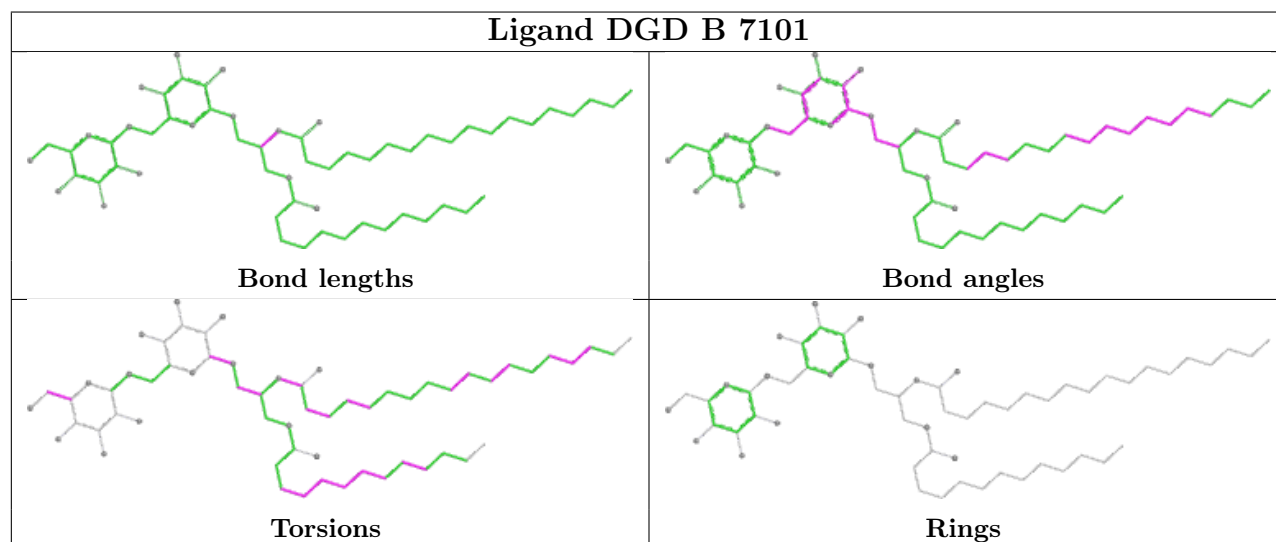
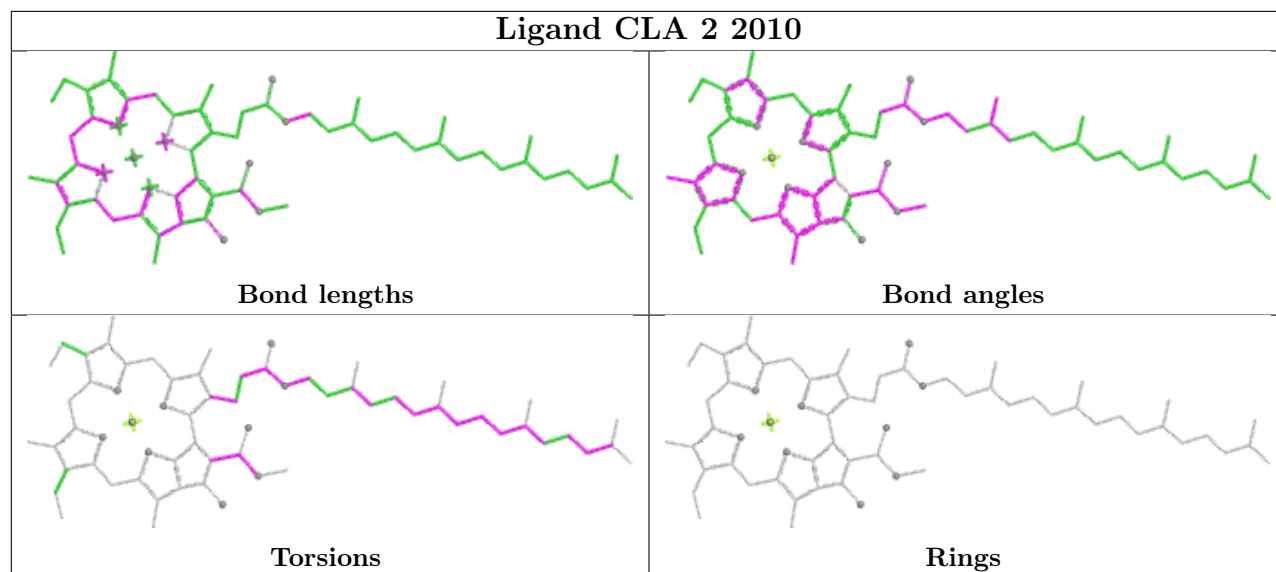


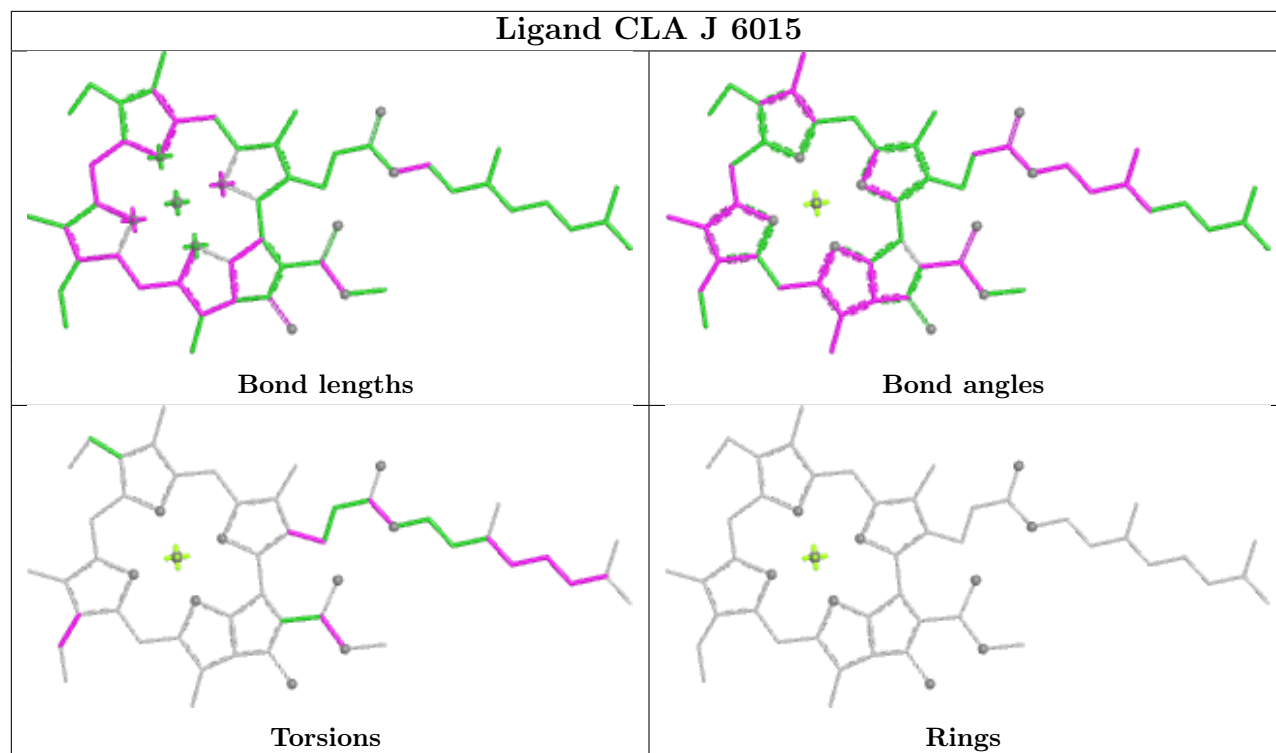
Ligand CLA A 1112



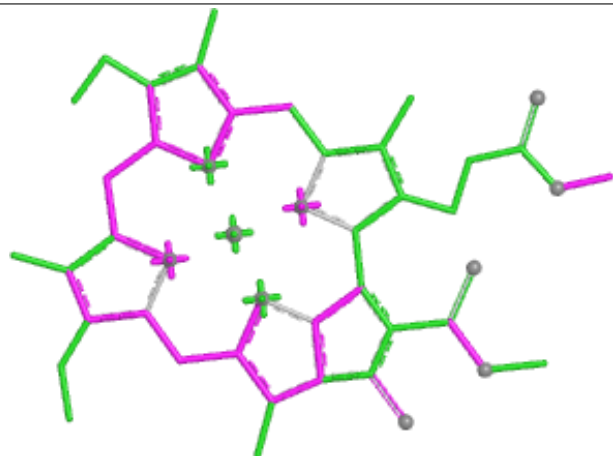
Ligand CLA B 1240



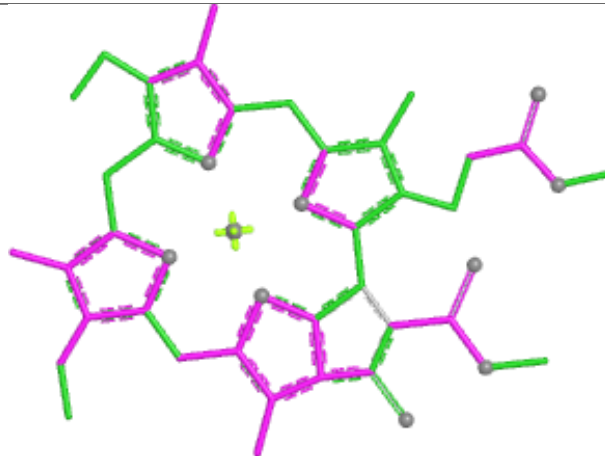




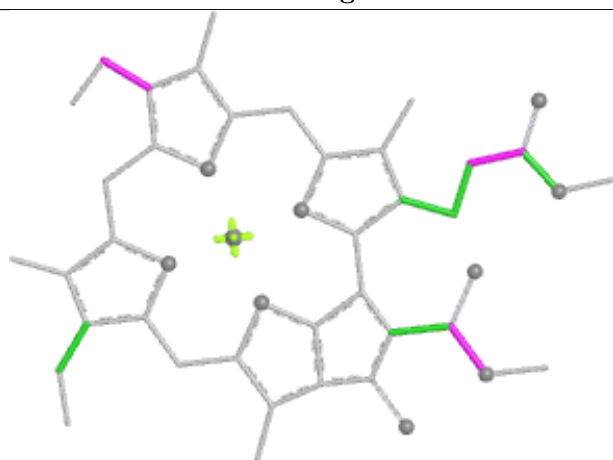
Ligand CLA A 1120



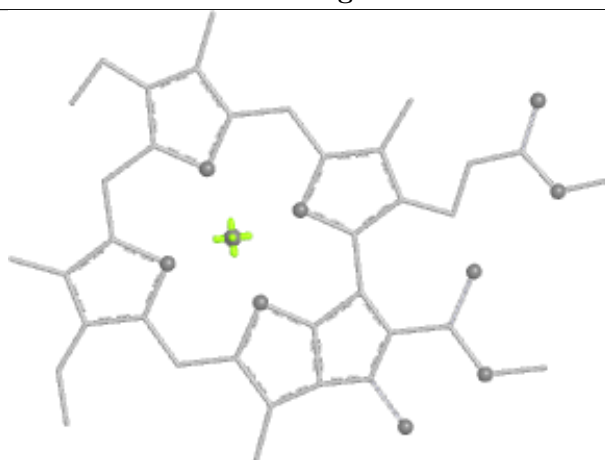
Bond lengths



Bond angles

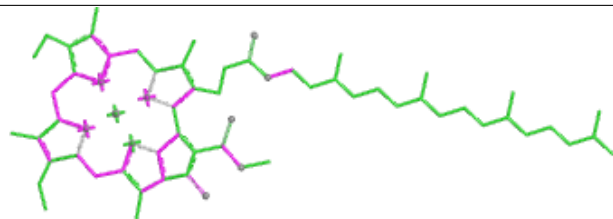


Torsions

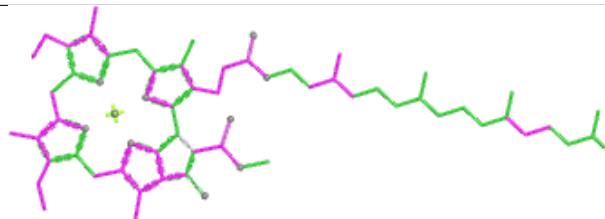


Rings

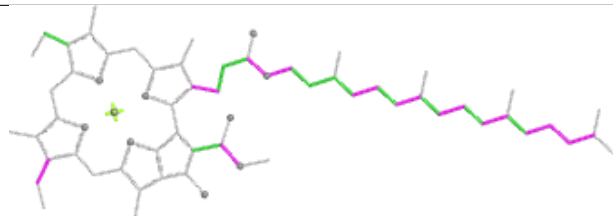
Ligand CLA 4 4011



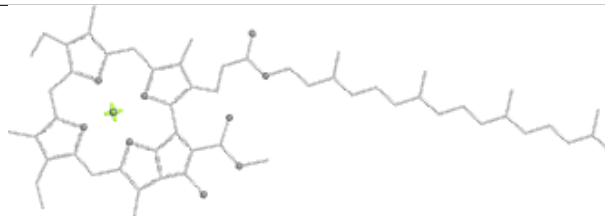
Bond lengths



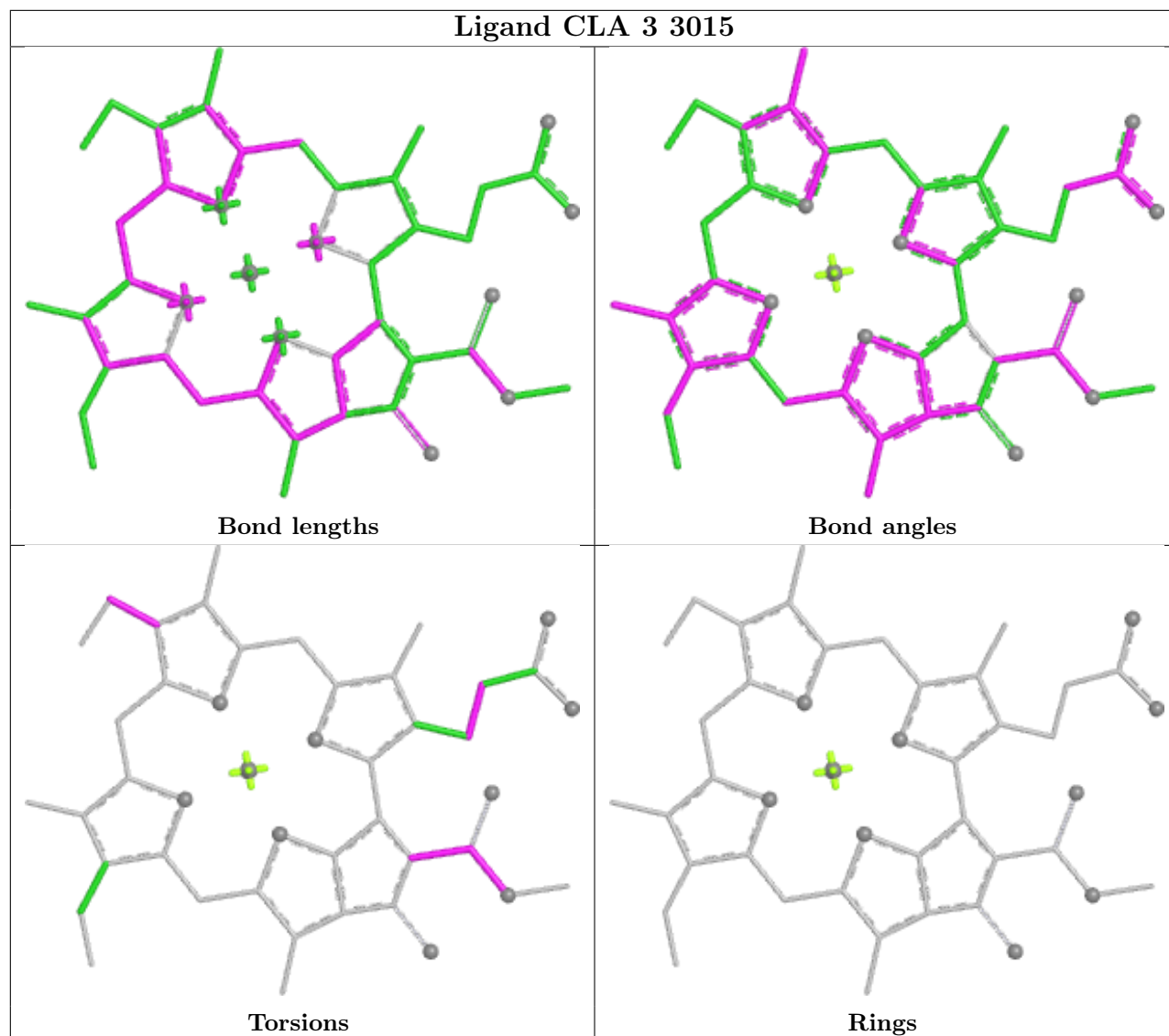
Bond angles



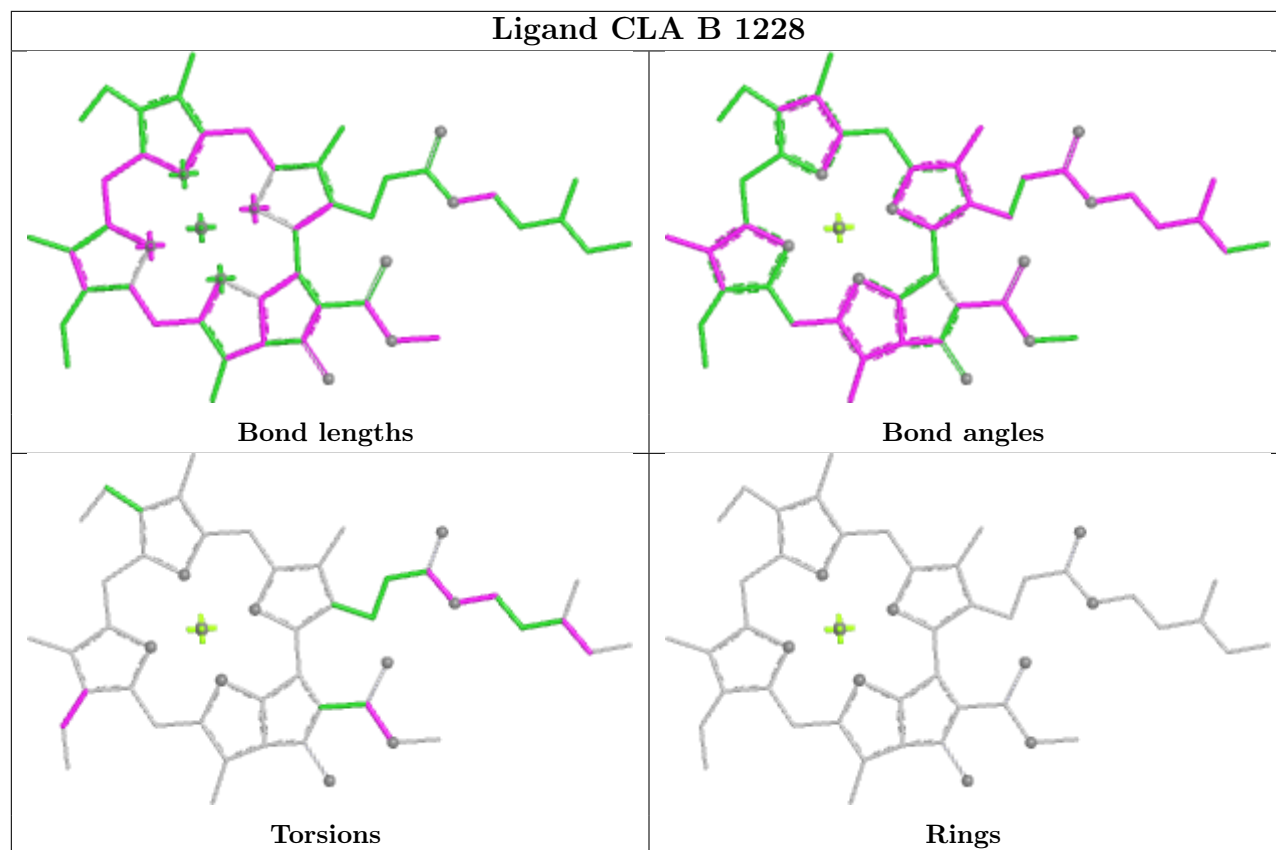
Torsions



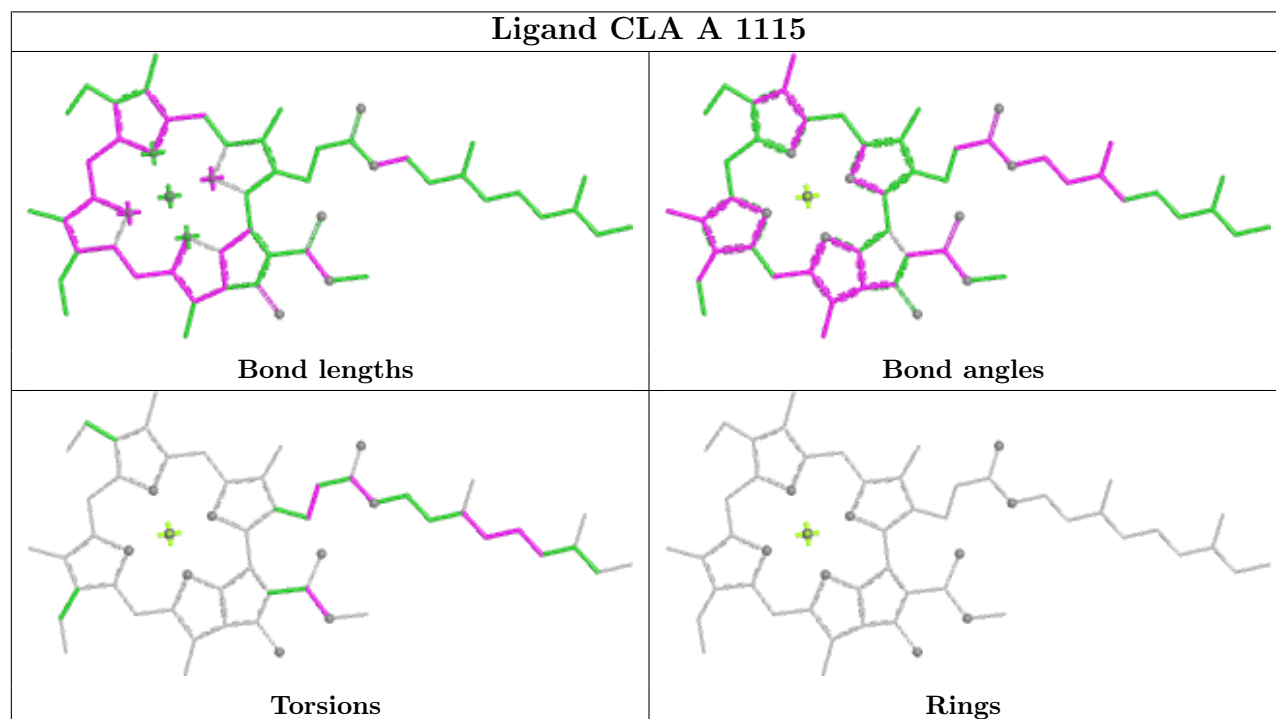
Rings

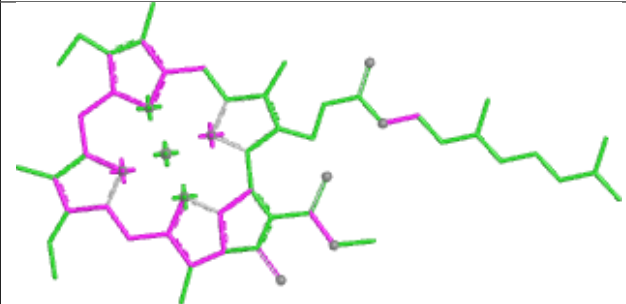
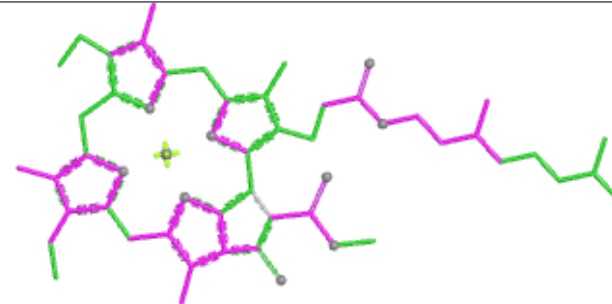
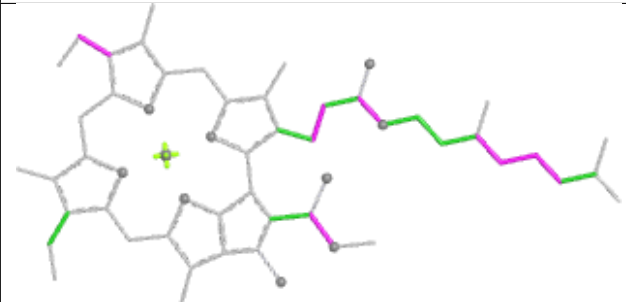
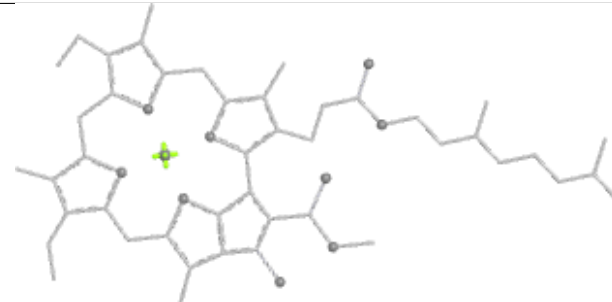


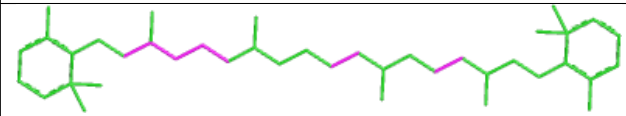
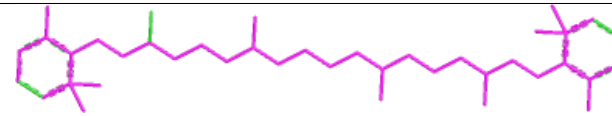
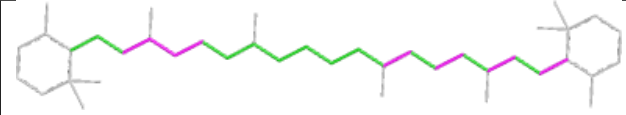
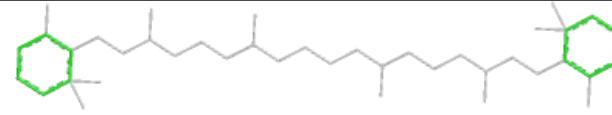
Ligand CLA B 1228

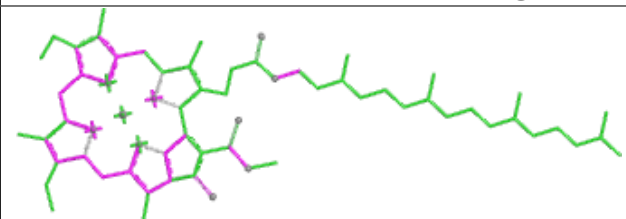
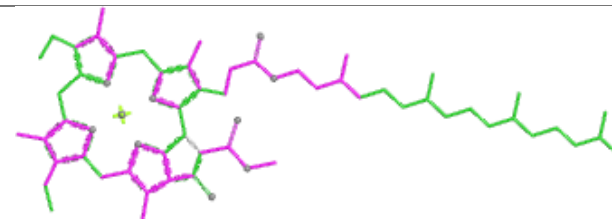
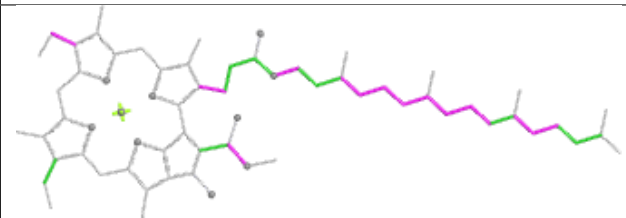
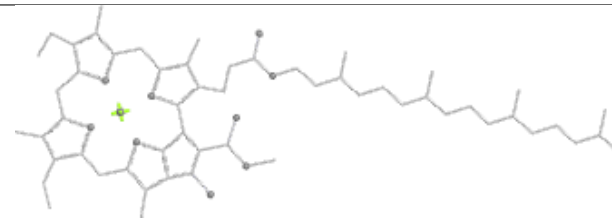


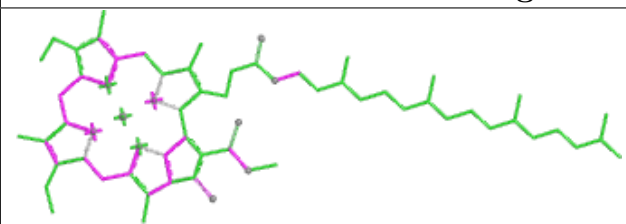
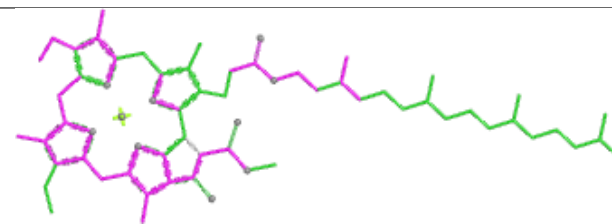
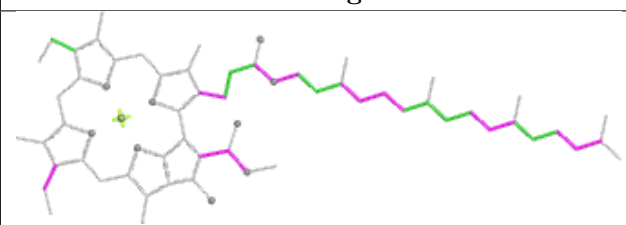
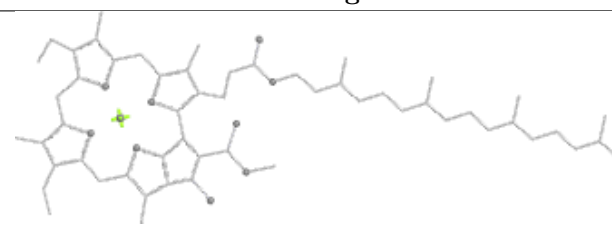
Ligand CLA A 1115

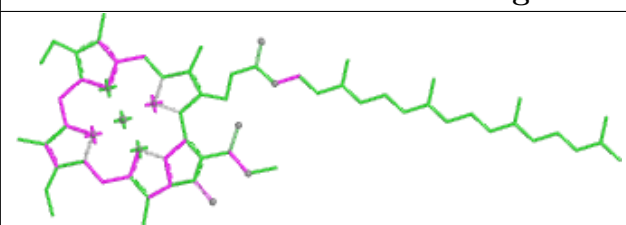
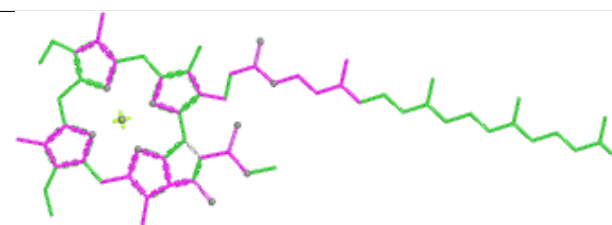
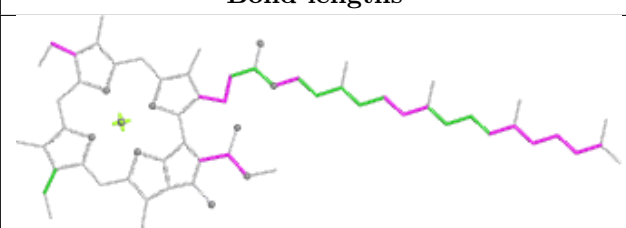
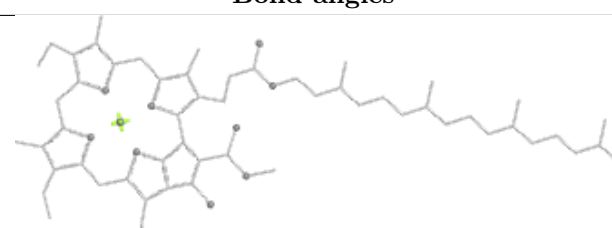


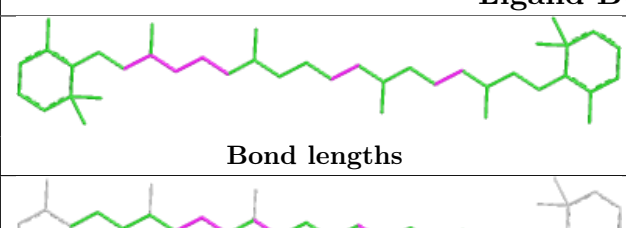
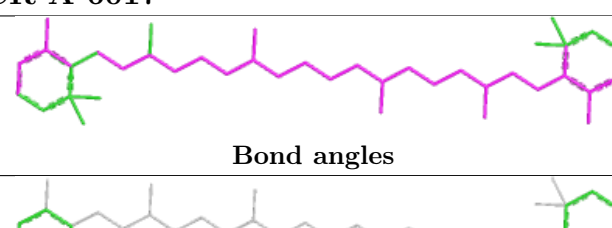
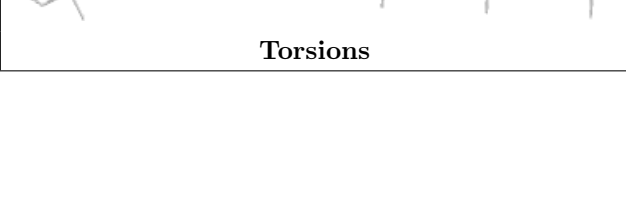
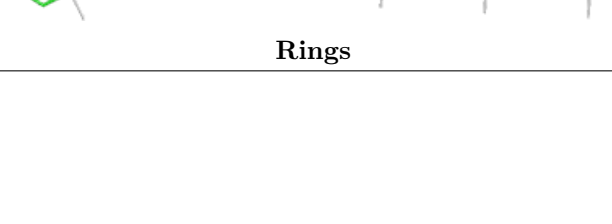
Ligand CLA B 1204	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 6014	
	
Bond lengths	Bond angles
	
Torsions	Rings

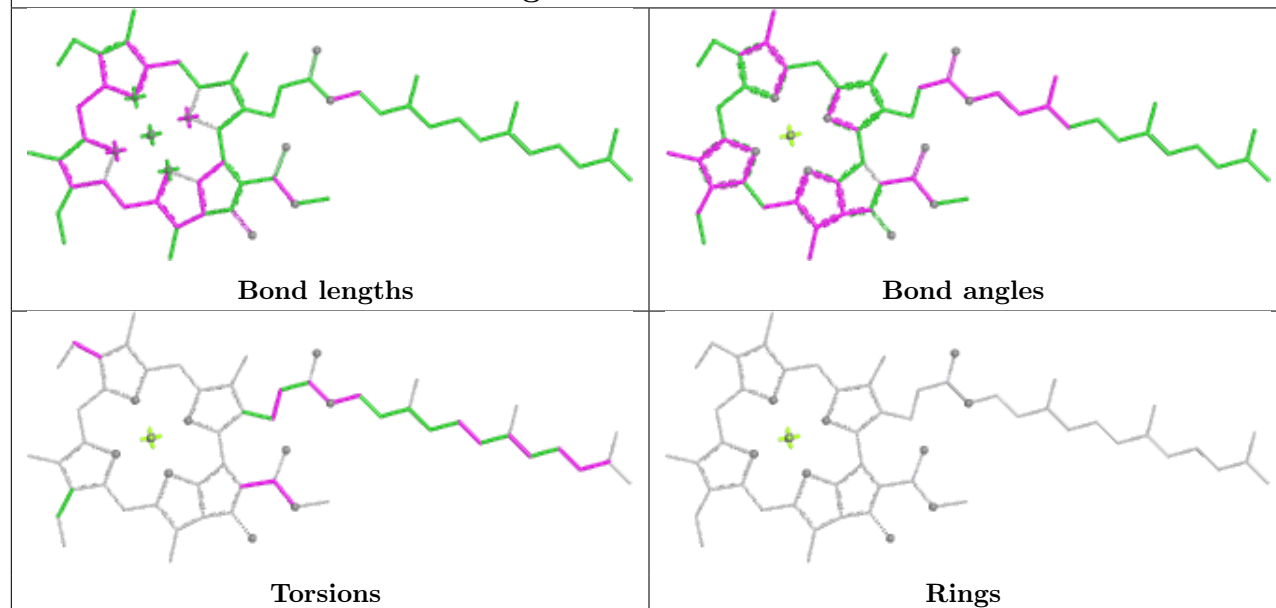
Ligand CLA B 1220	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 1010	
	
Bond lengths	Bond angles
	
Torsions	Rings

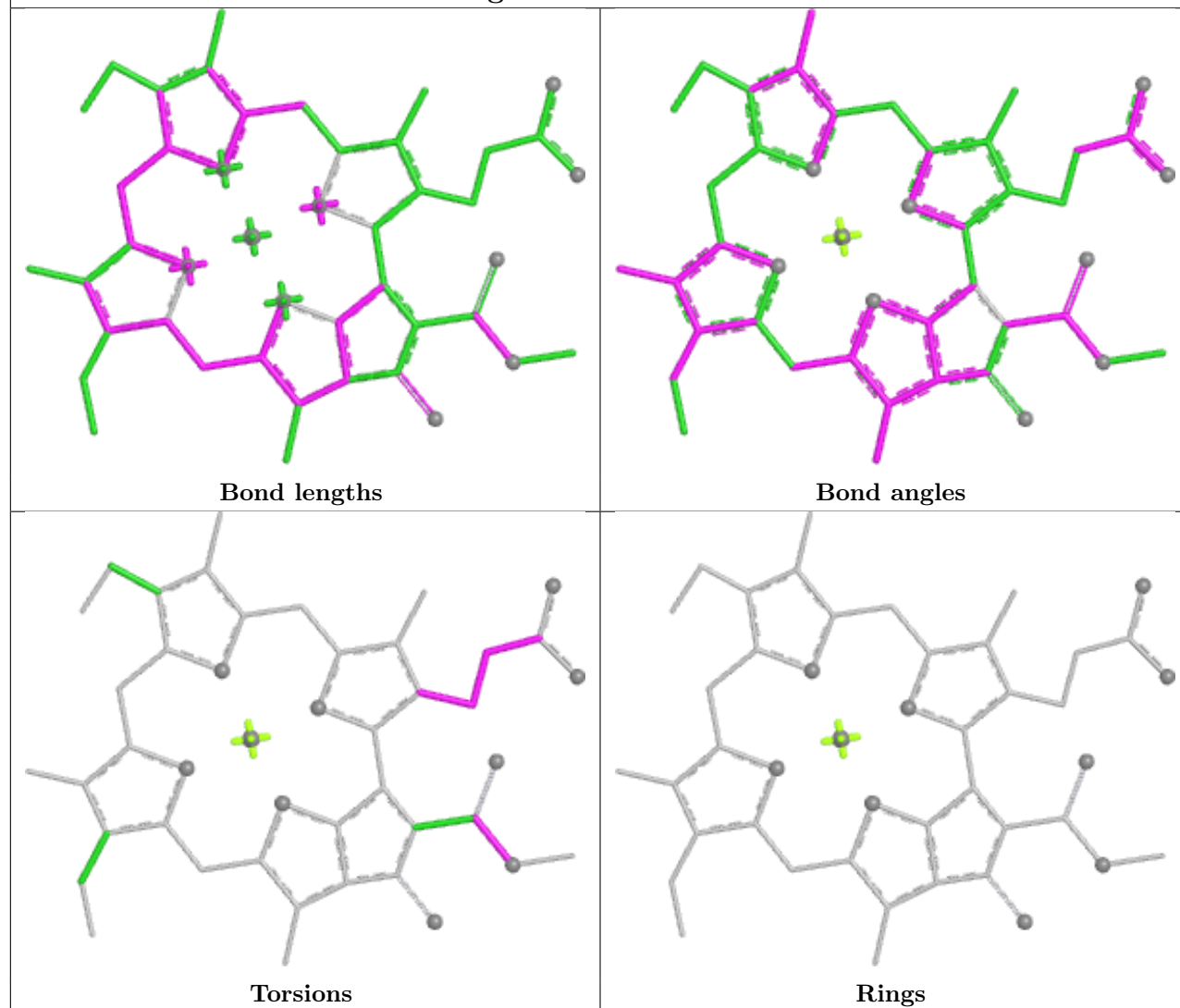
Ligand CLA B 1227	
	
Bond lengths	Bond angles
	
Torsions	Rings

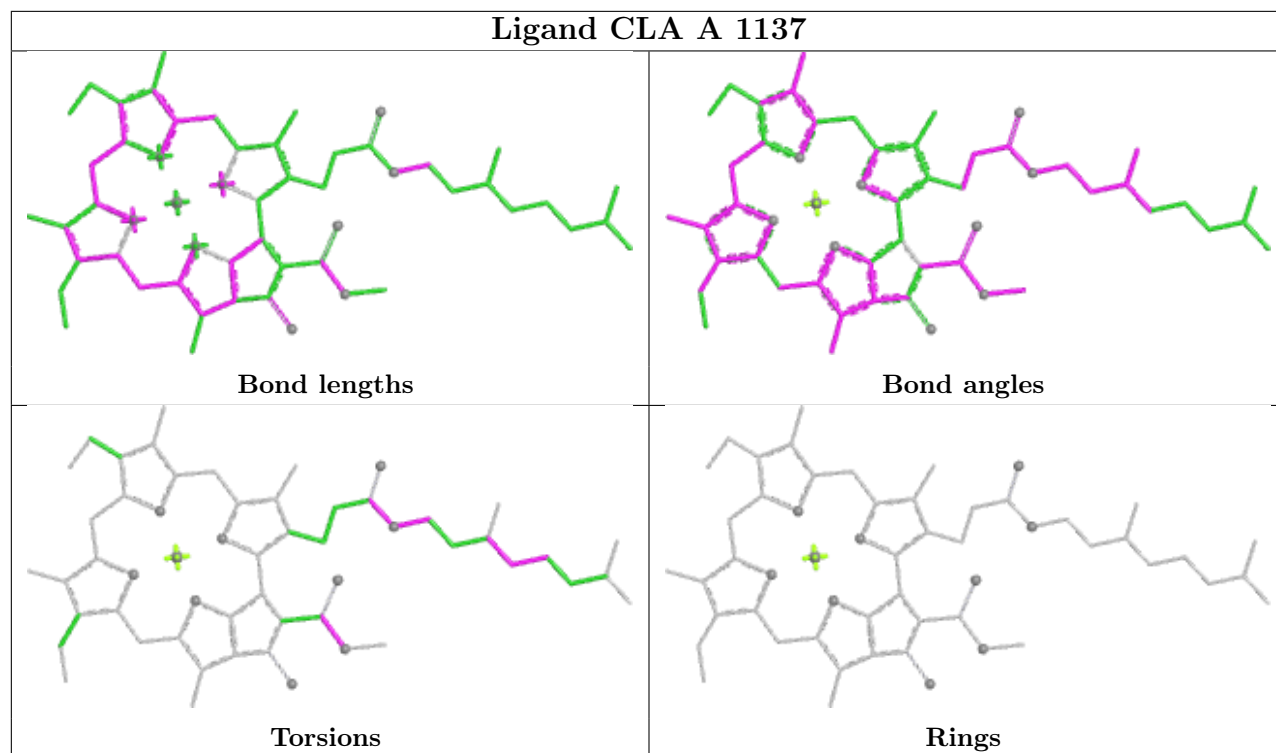
Ligand BCR A 6017	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1111

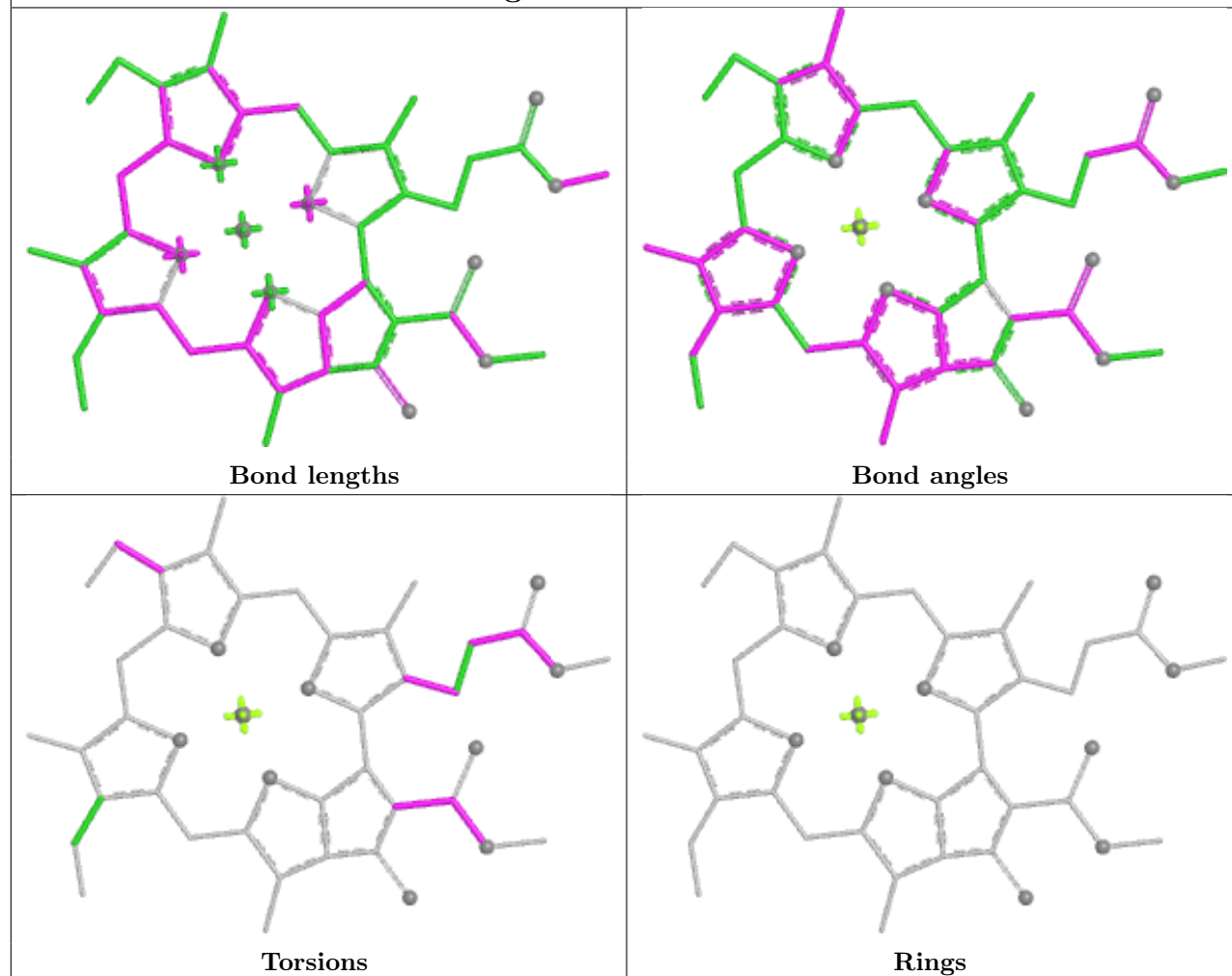


Ligand CLA 3 3017

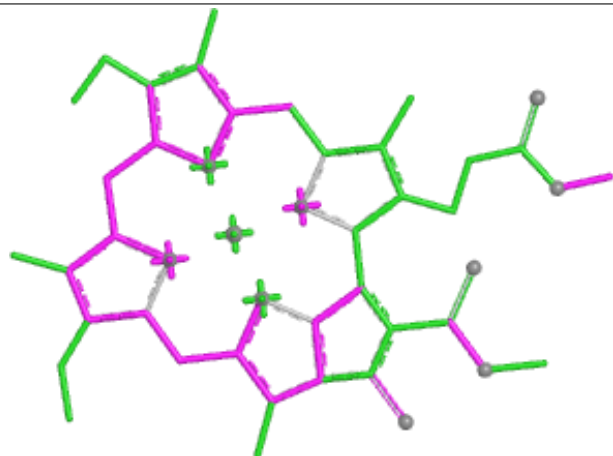




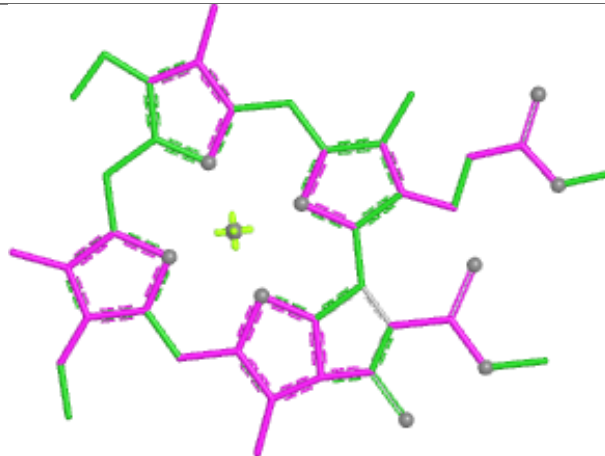
Ligand CLA A 1113



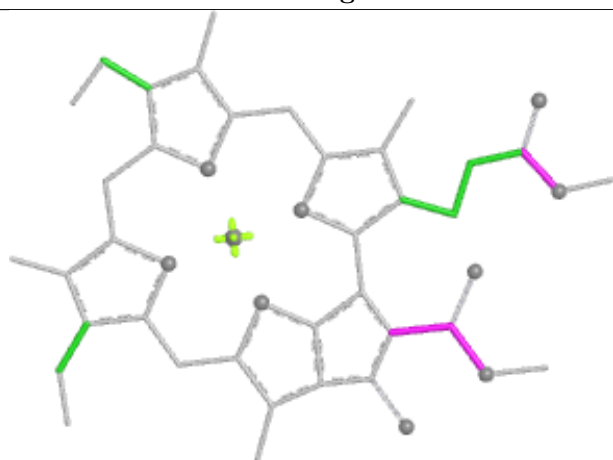
Ligand CLA B 1201



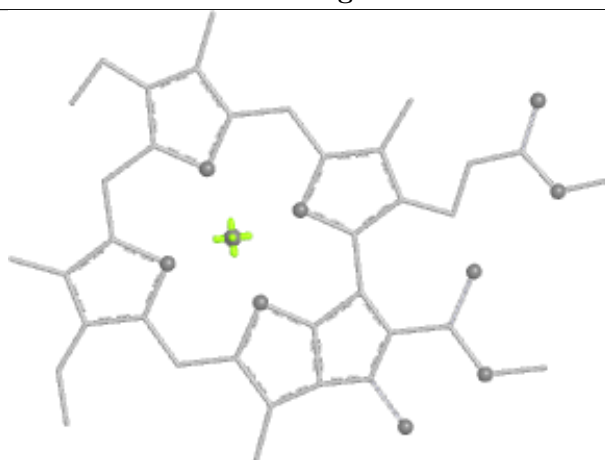
Bond lengths



Bond angles

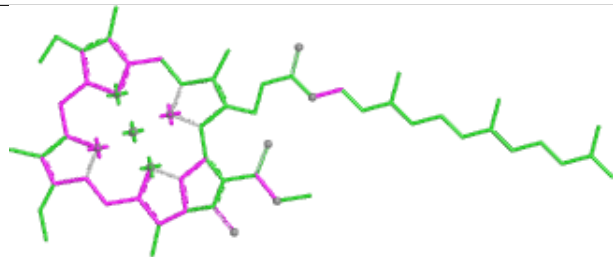


Torsions

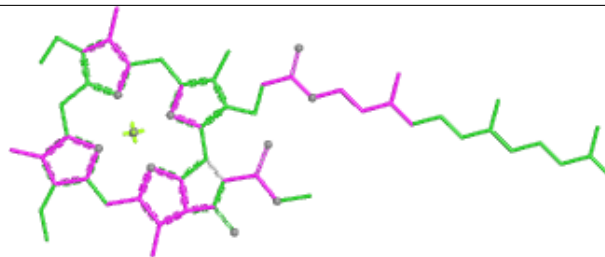


Rings

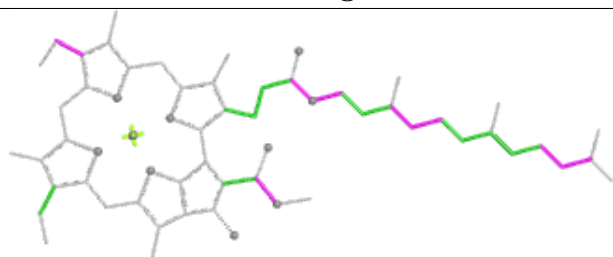
Ligand CLA B 1203



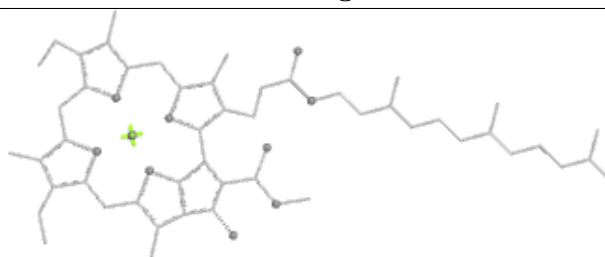
Bond lengths



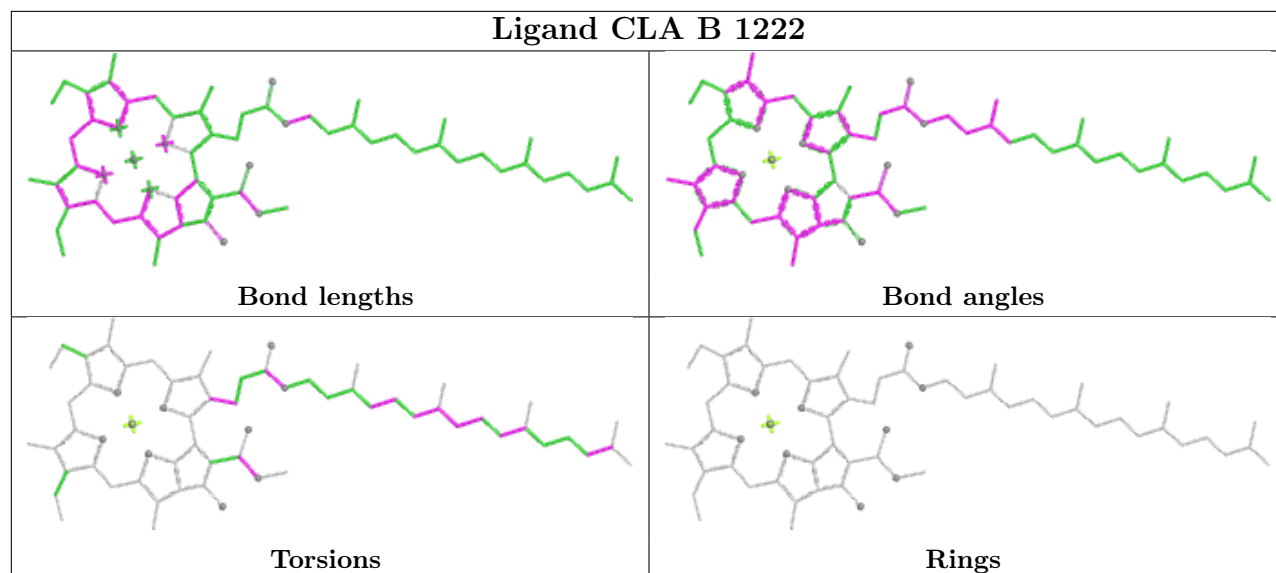
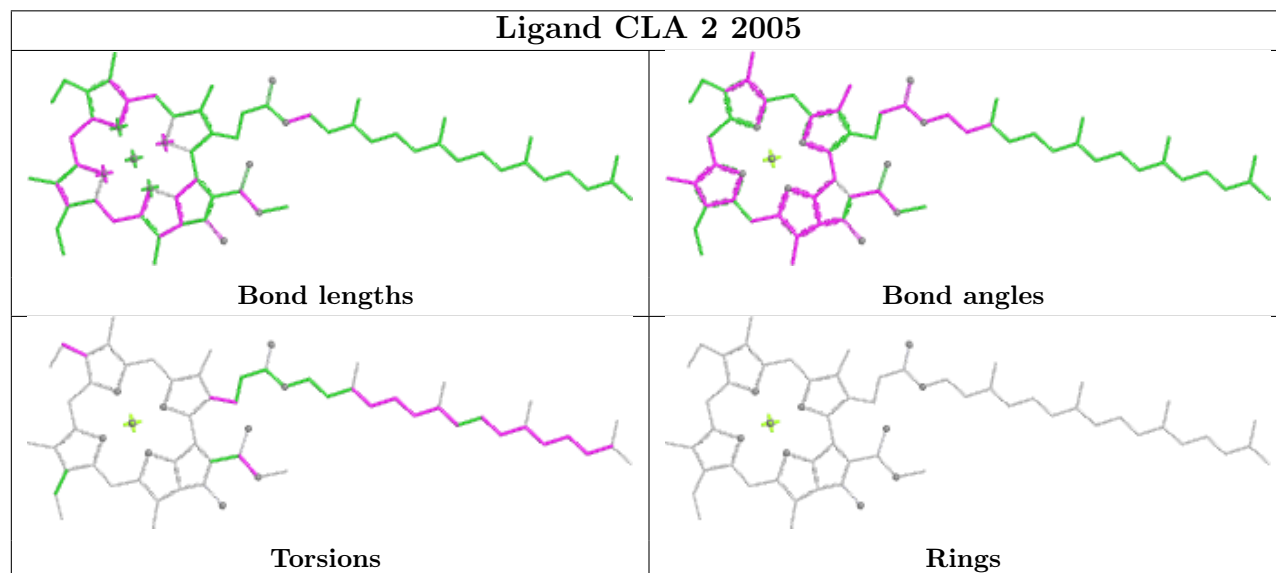
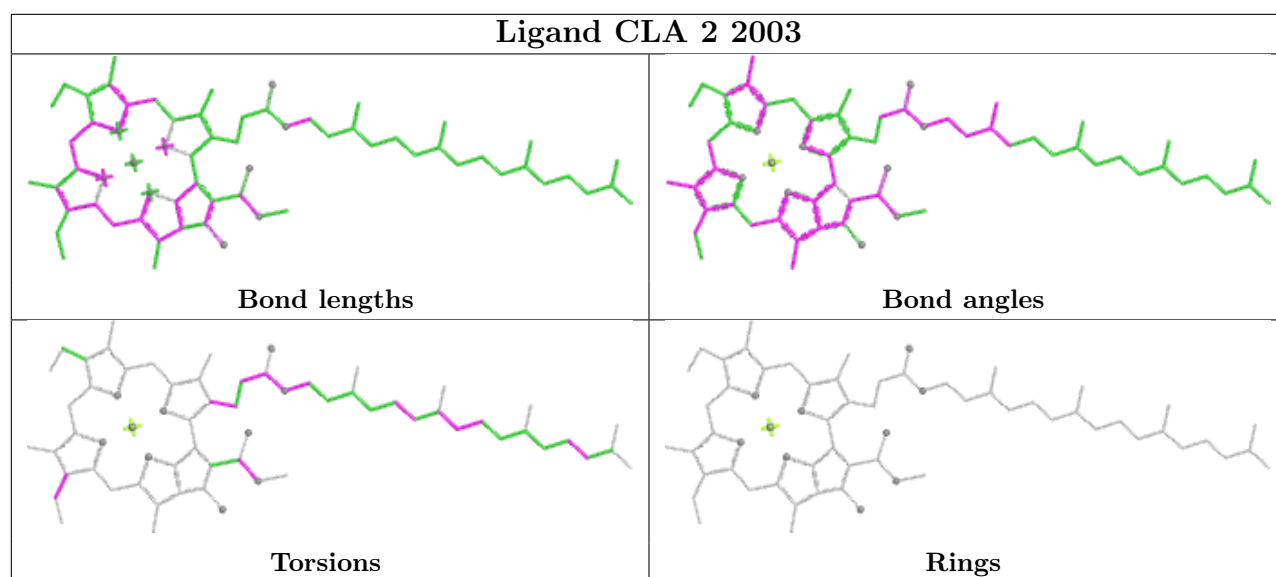
Bond angles

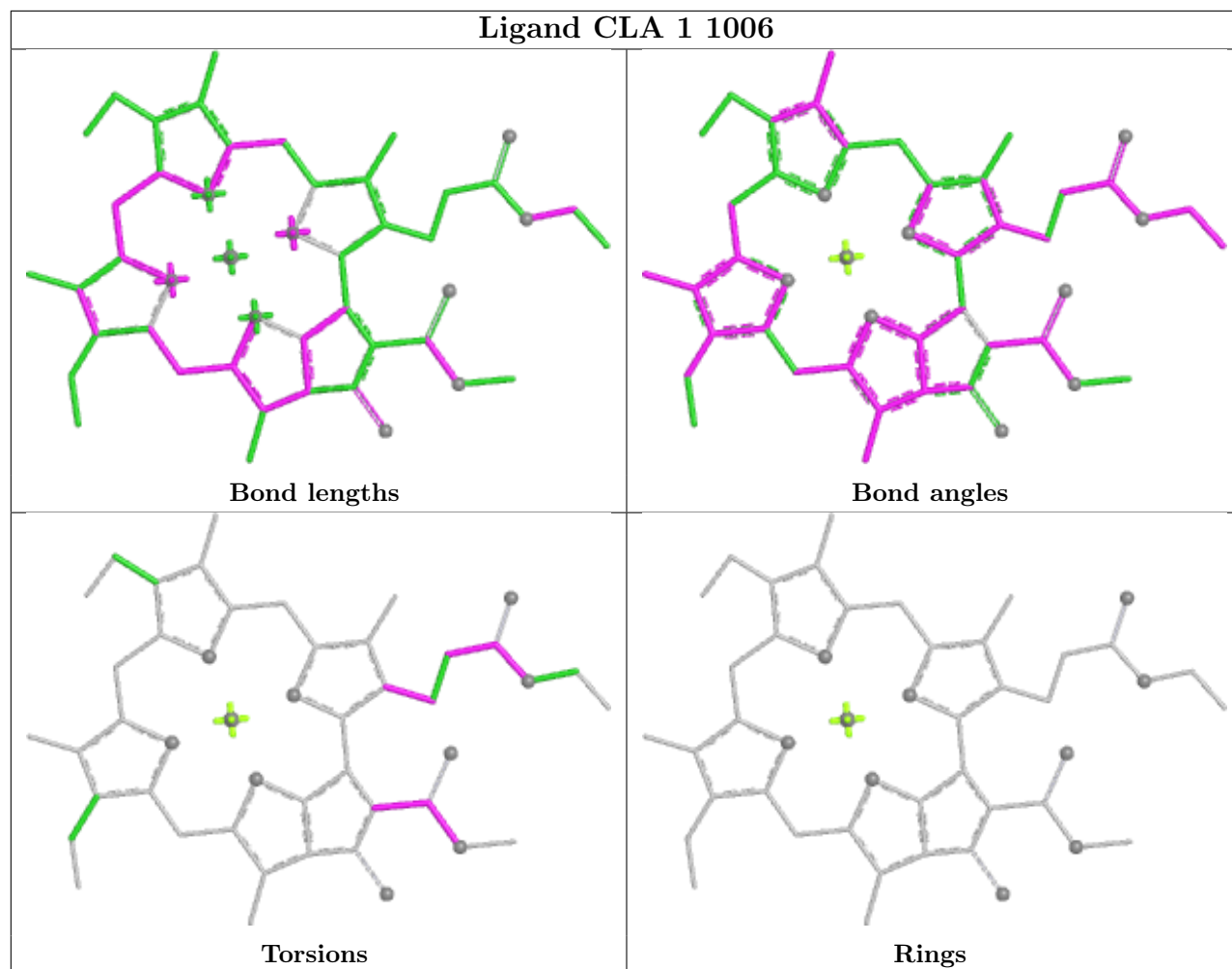


Torsions

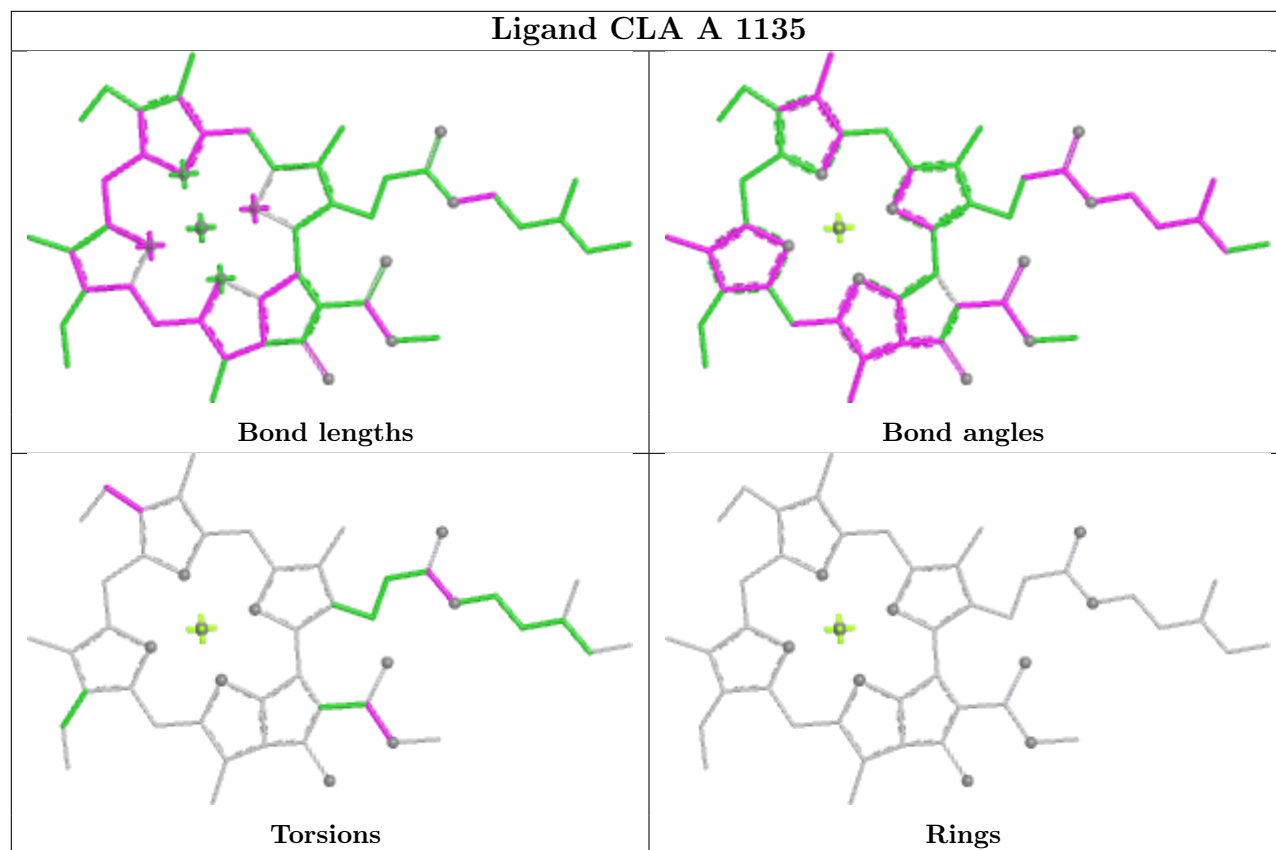


Rings

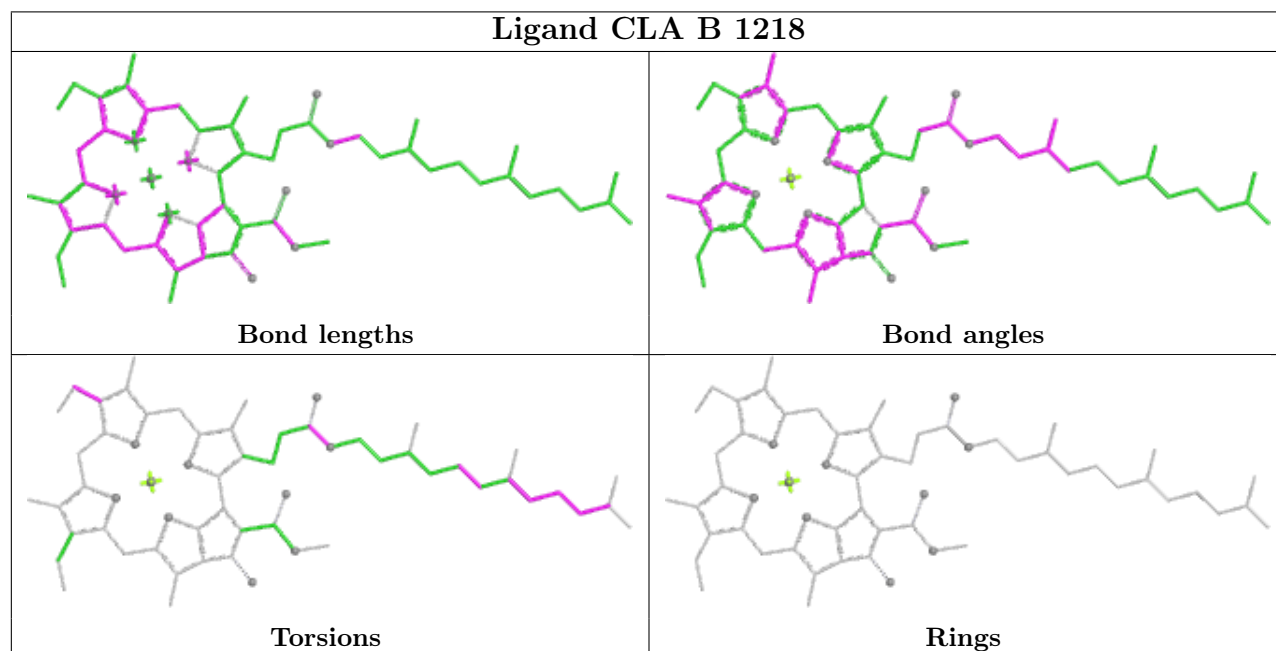


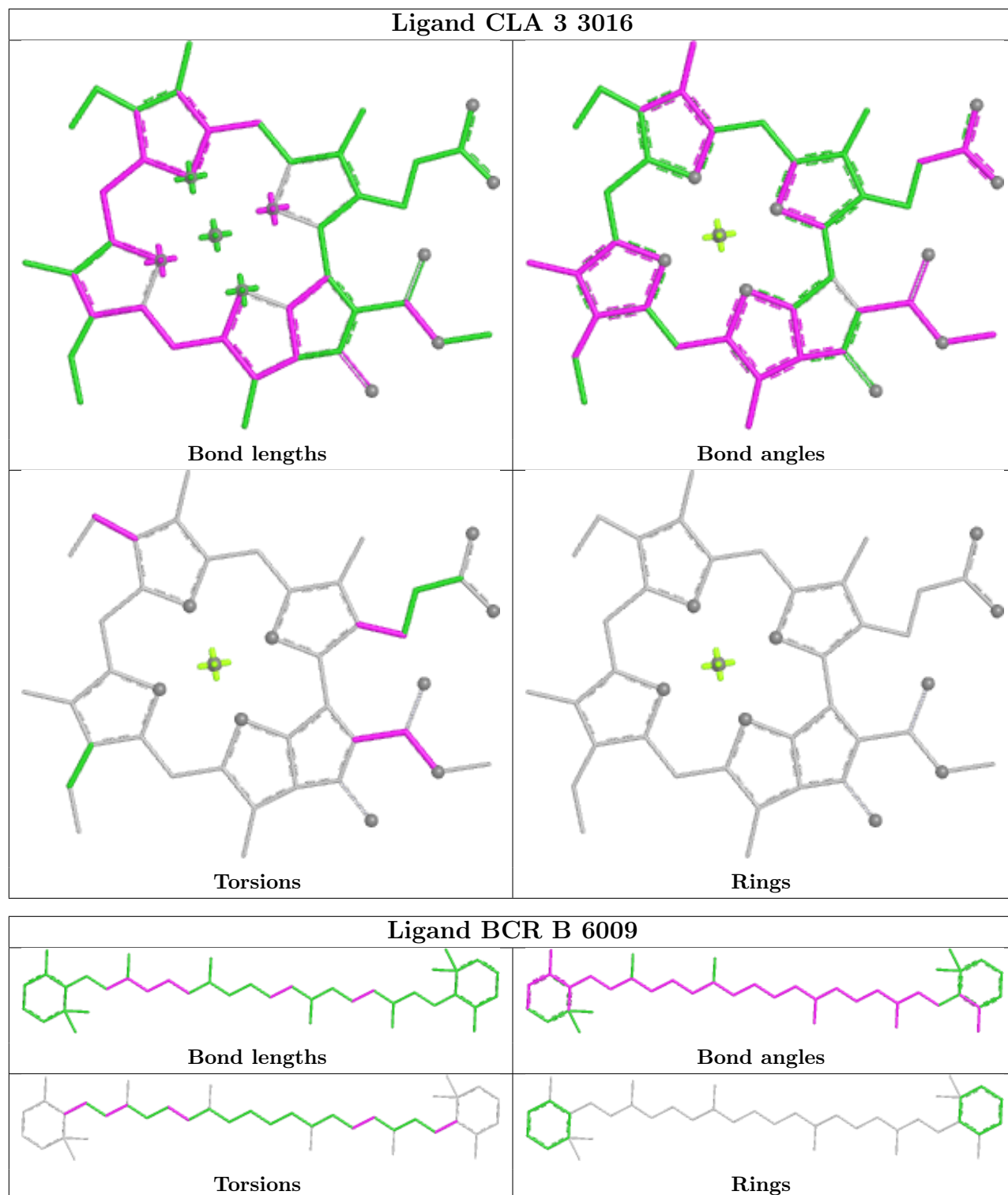


Ligand CLA A 1135

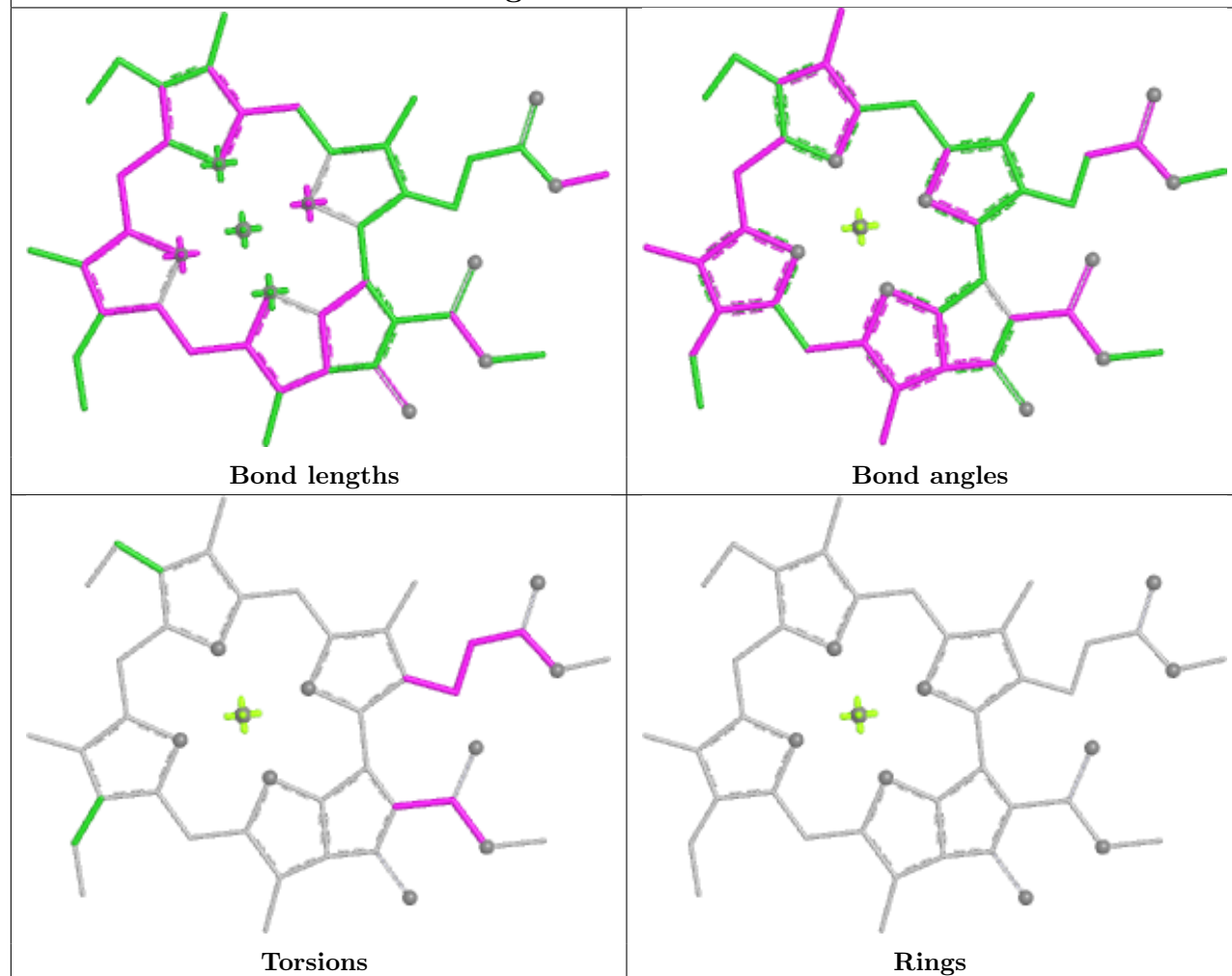


Ligand CLA B 1218

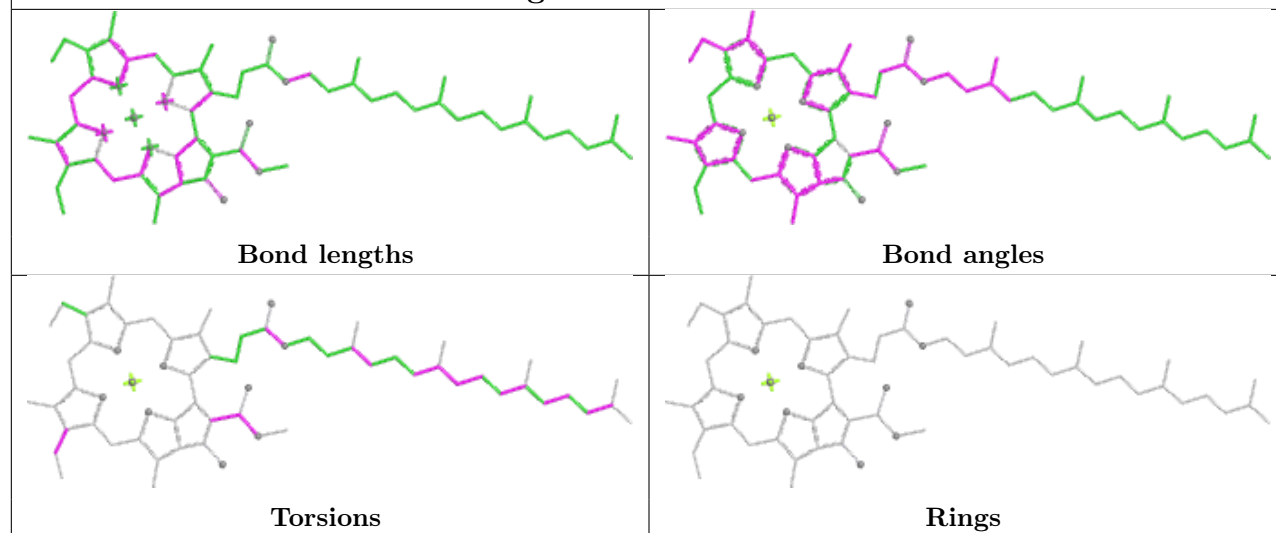


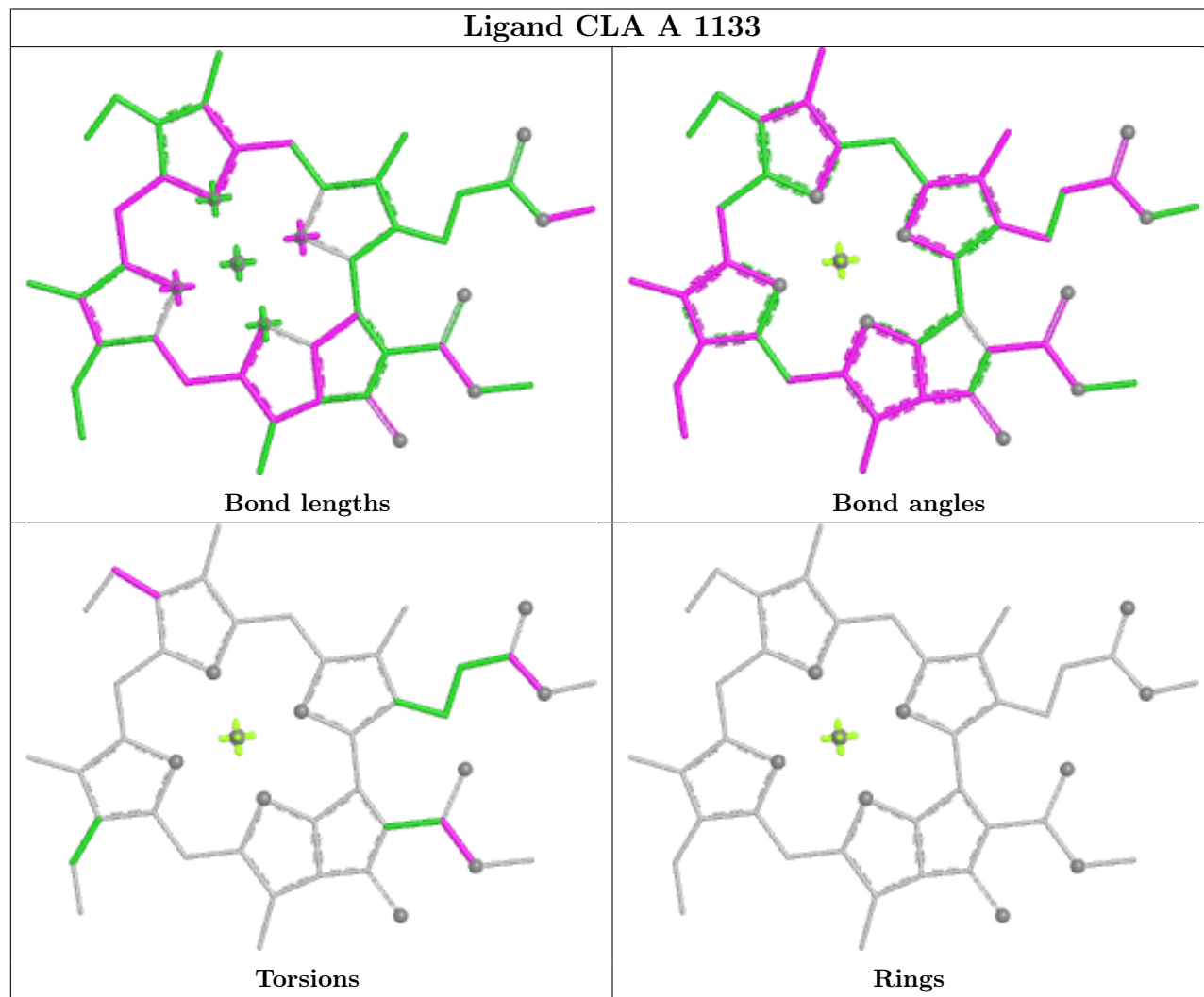
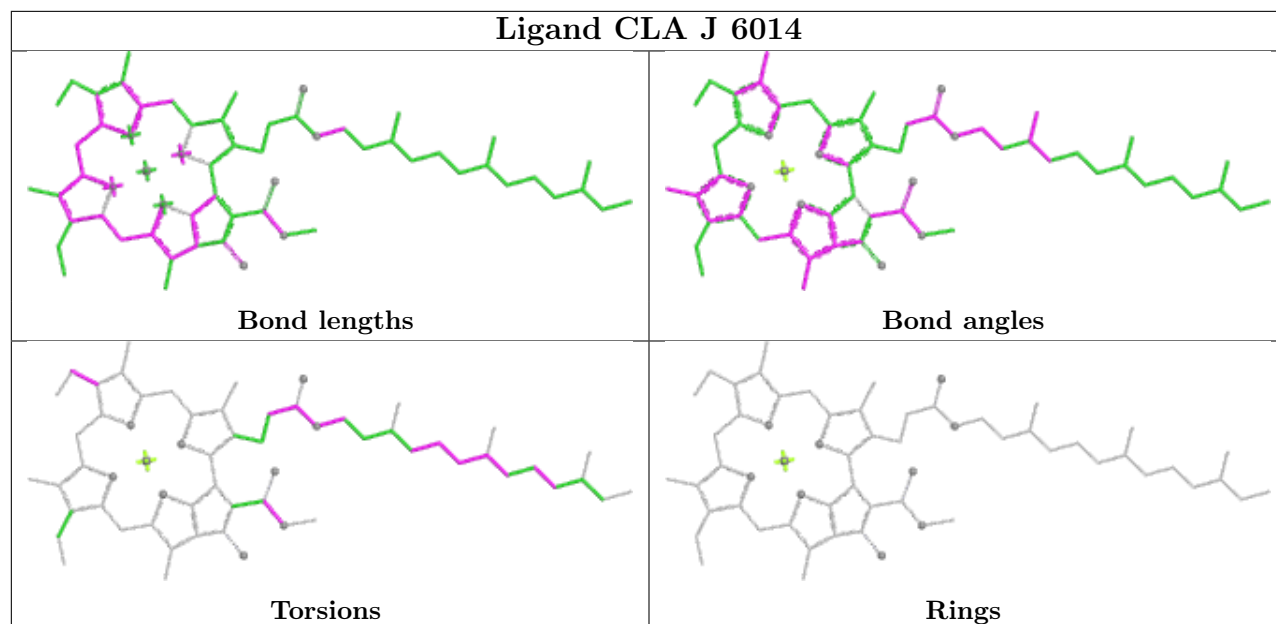


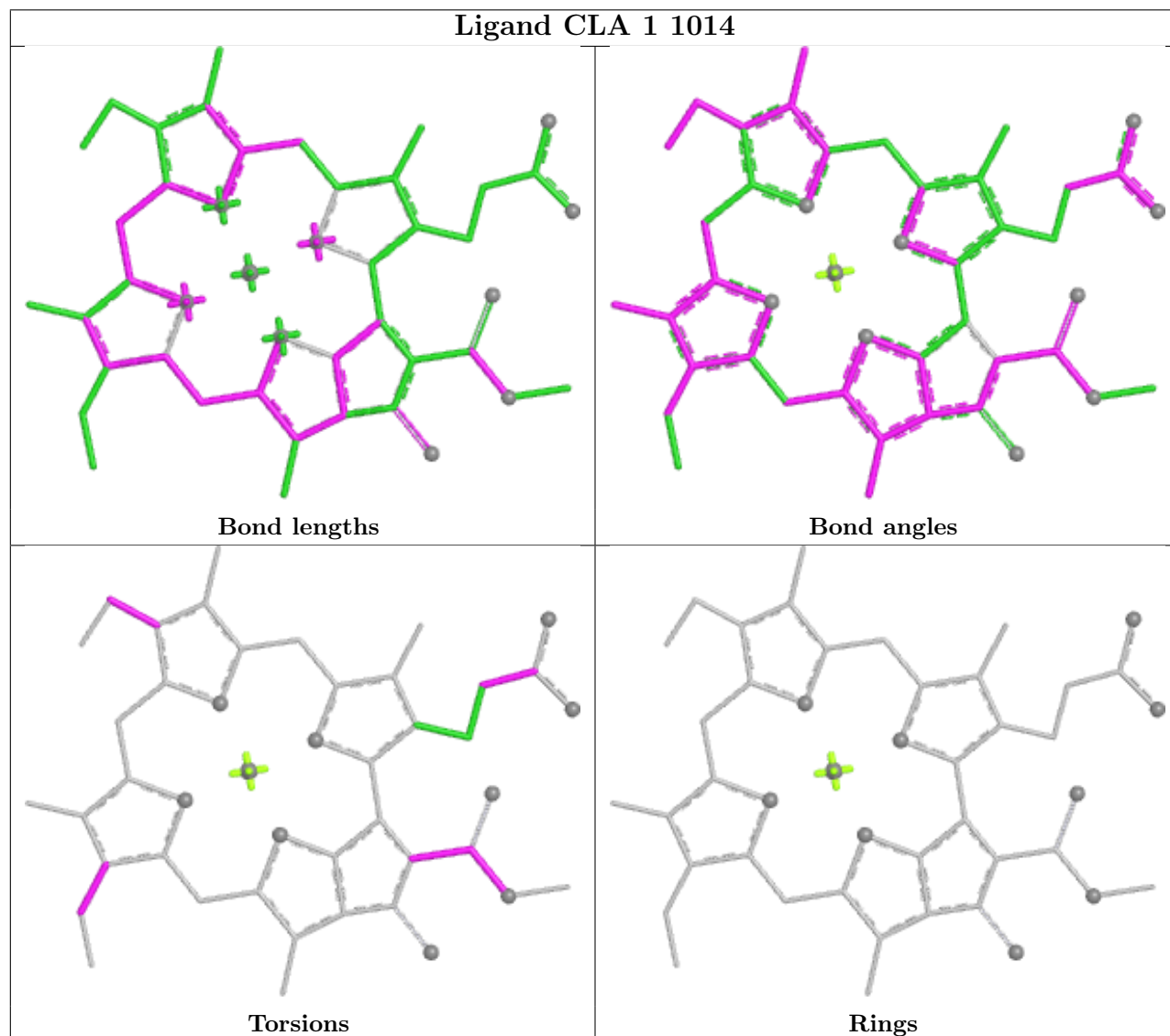
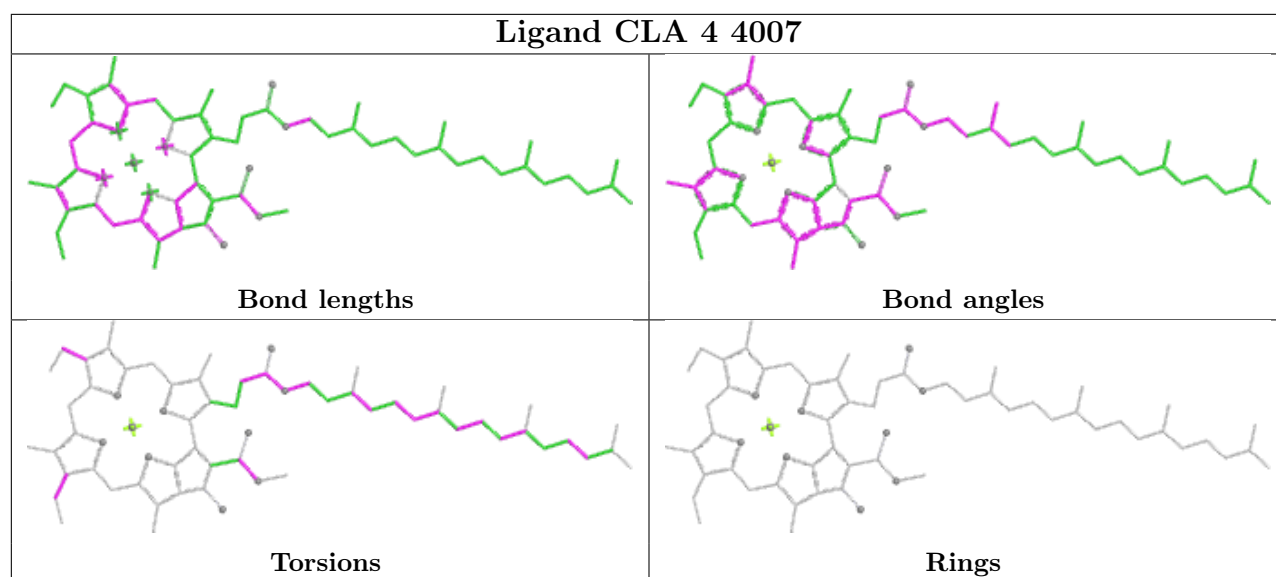
Ligand CLA B 1209

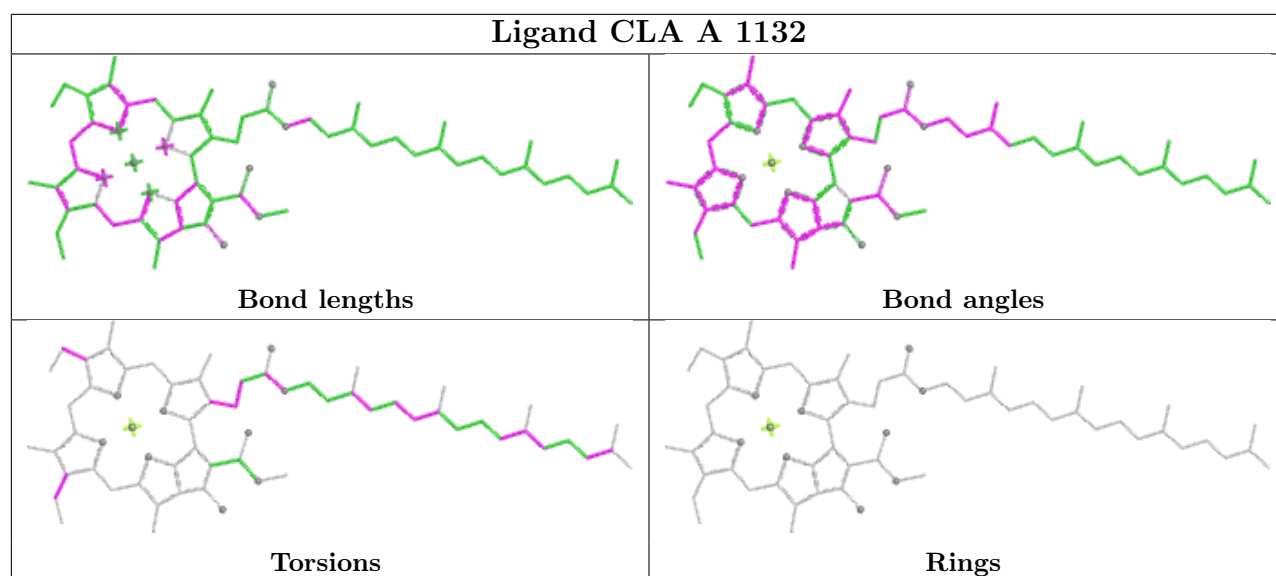
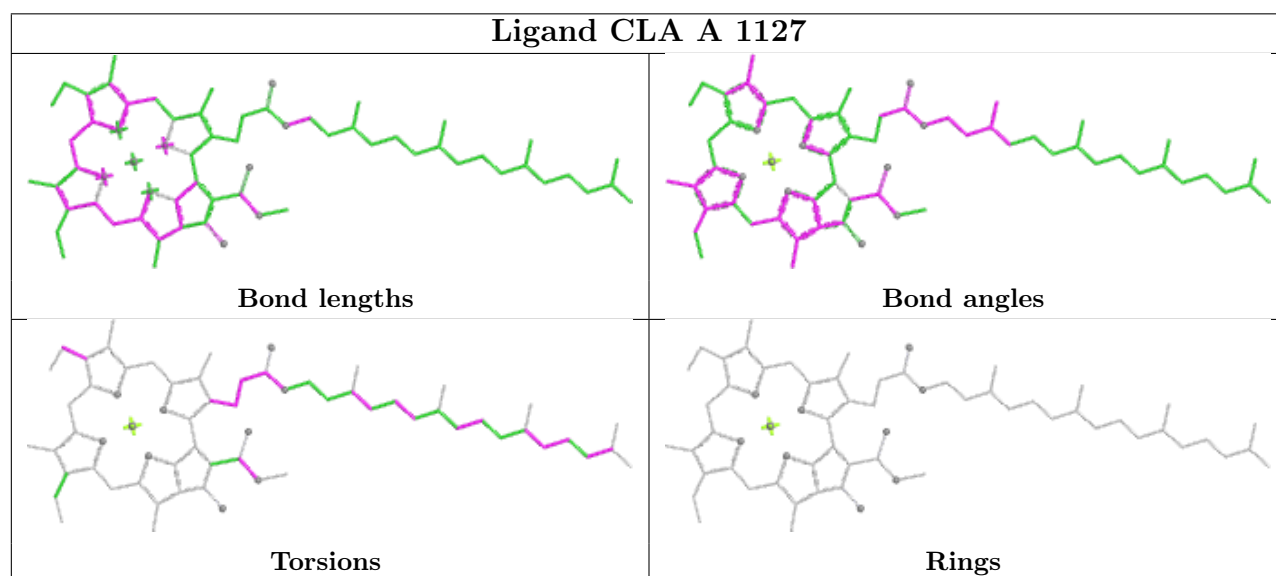
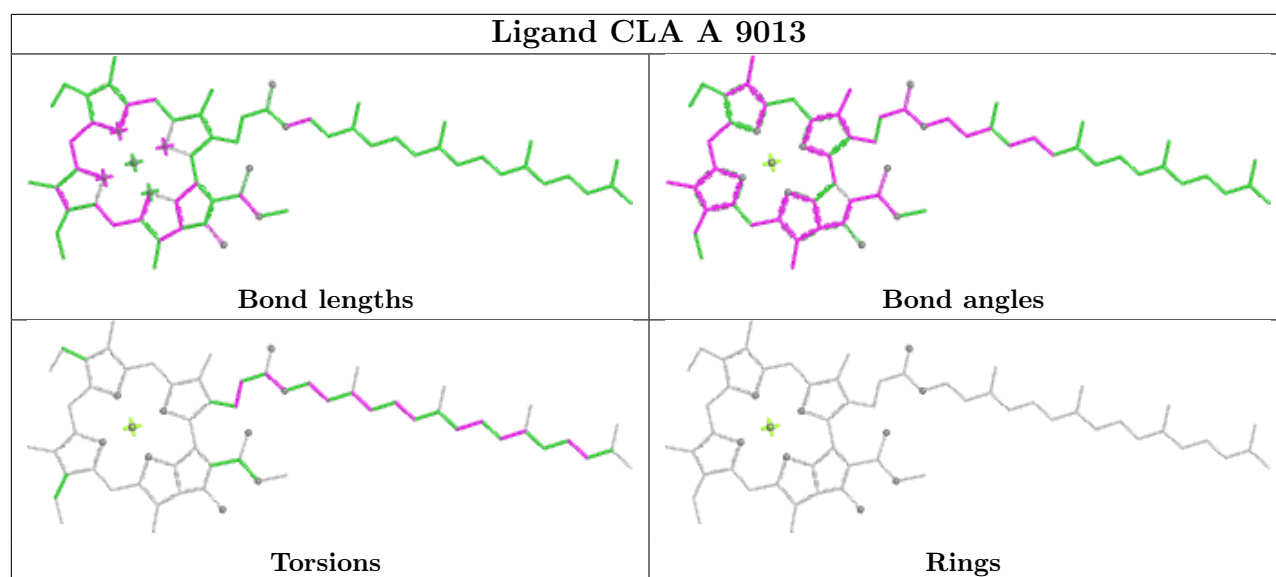


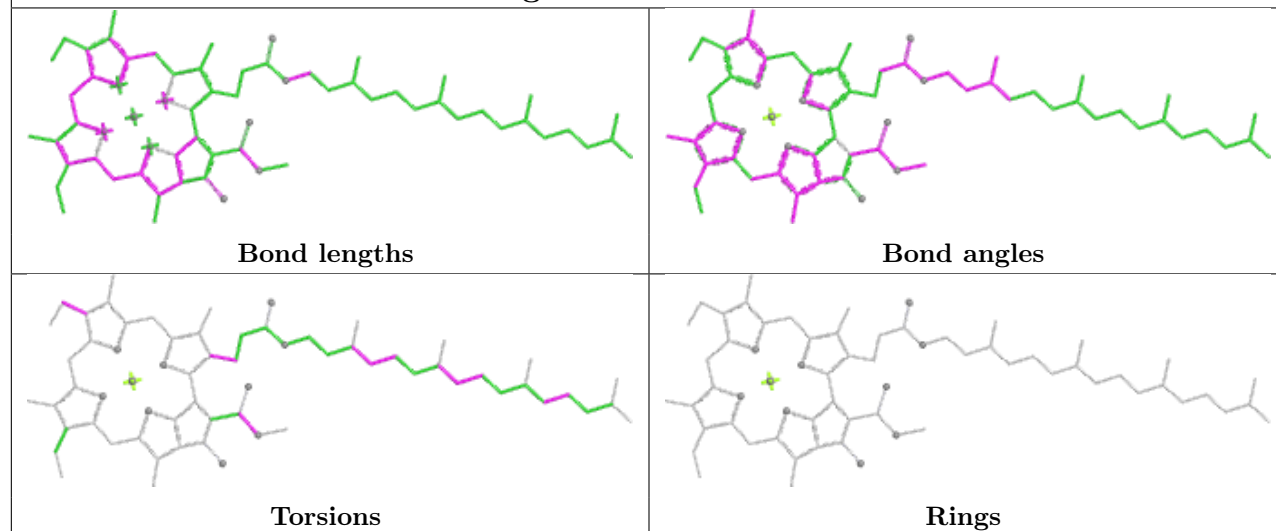
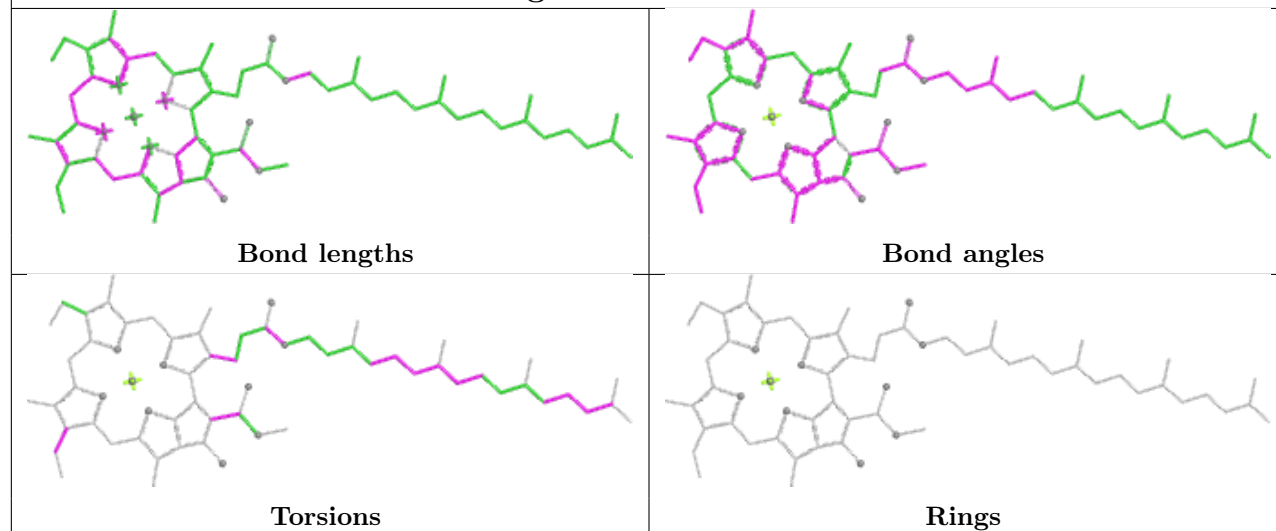
Ligand CLA 4 4004

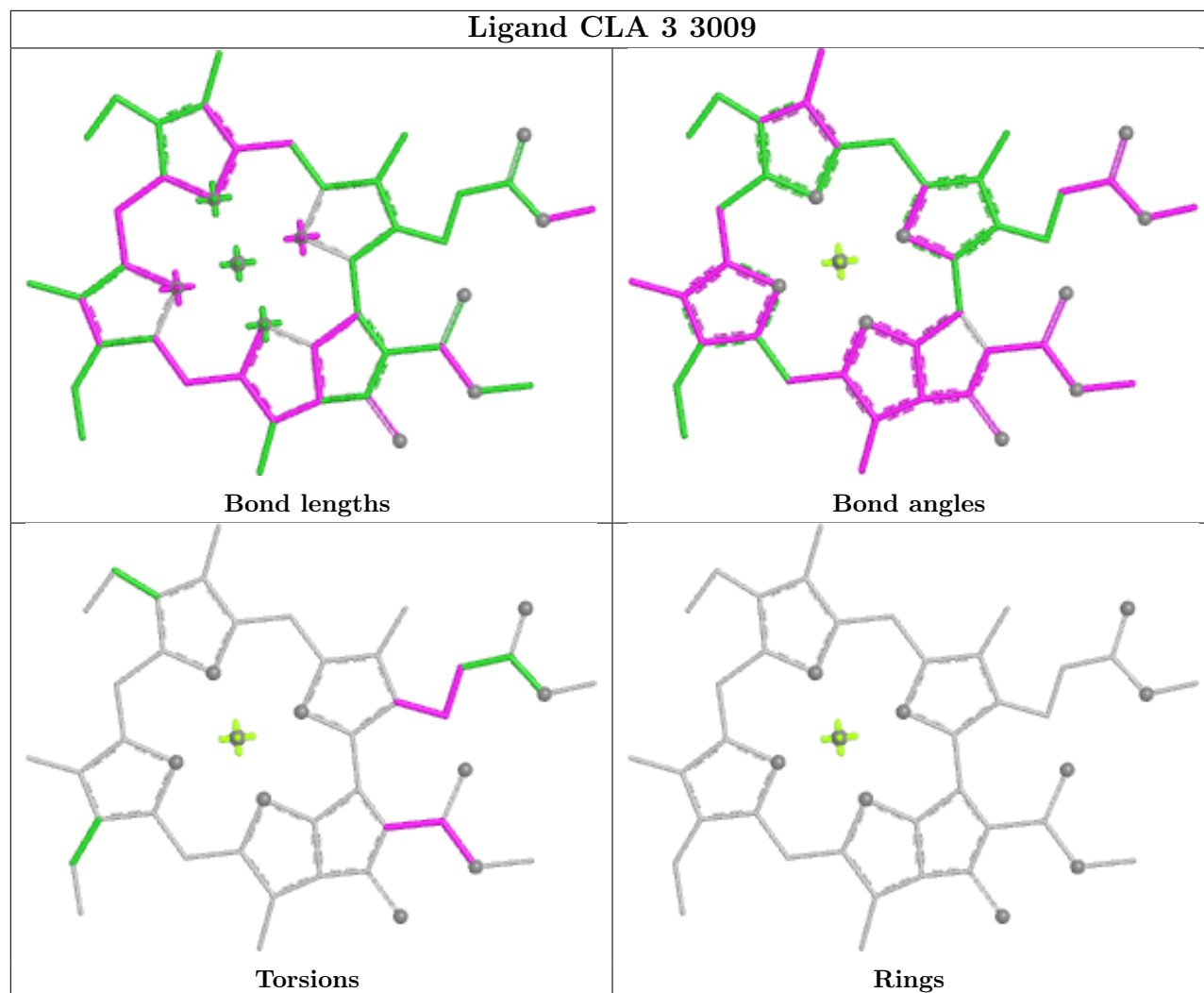


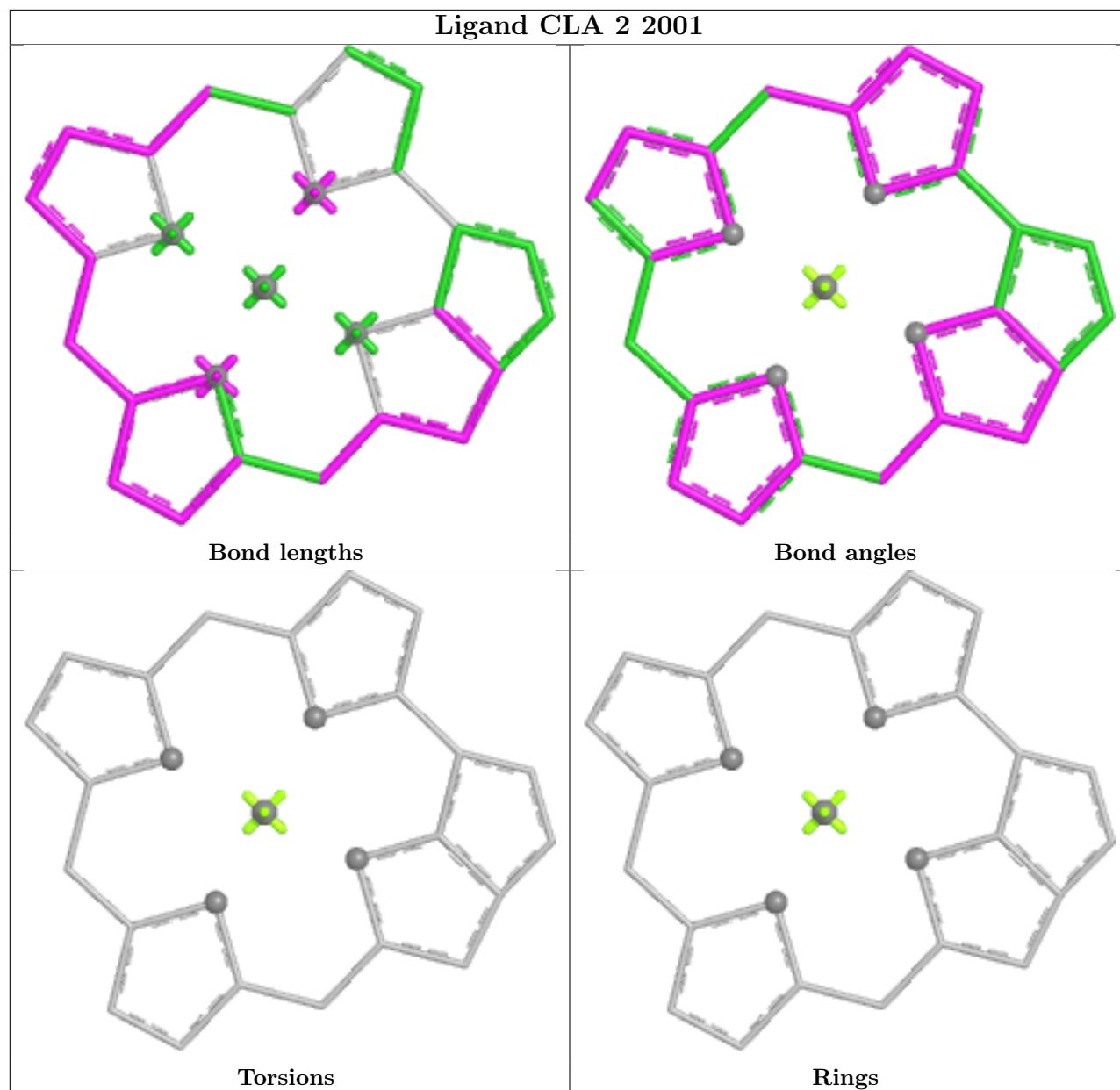


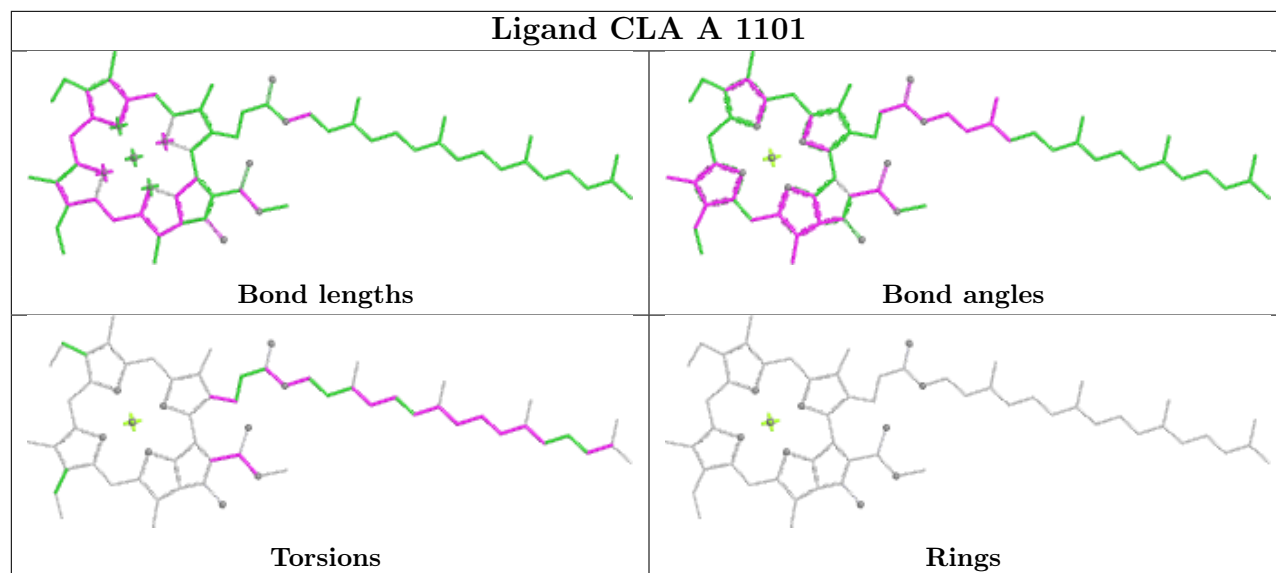
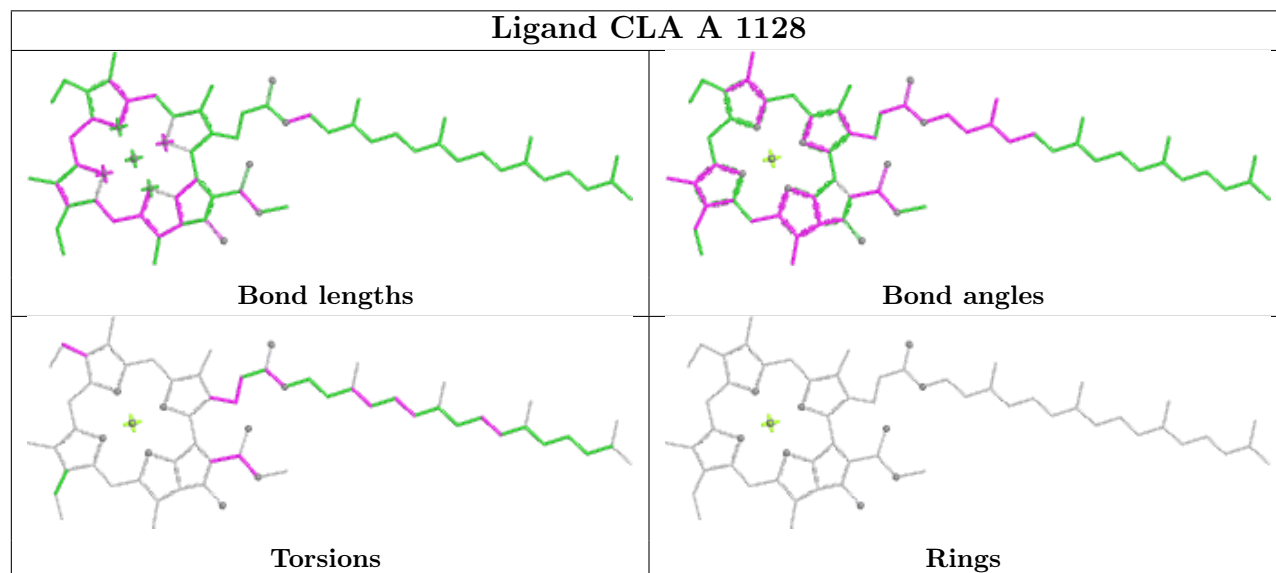
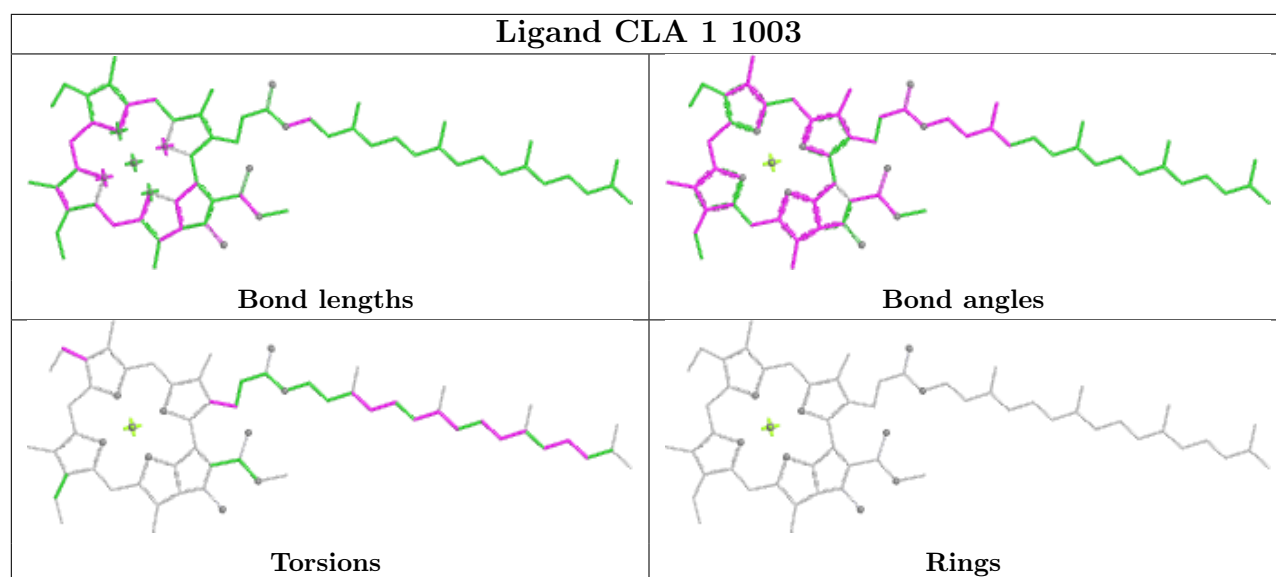


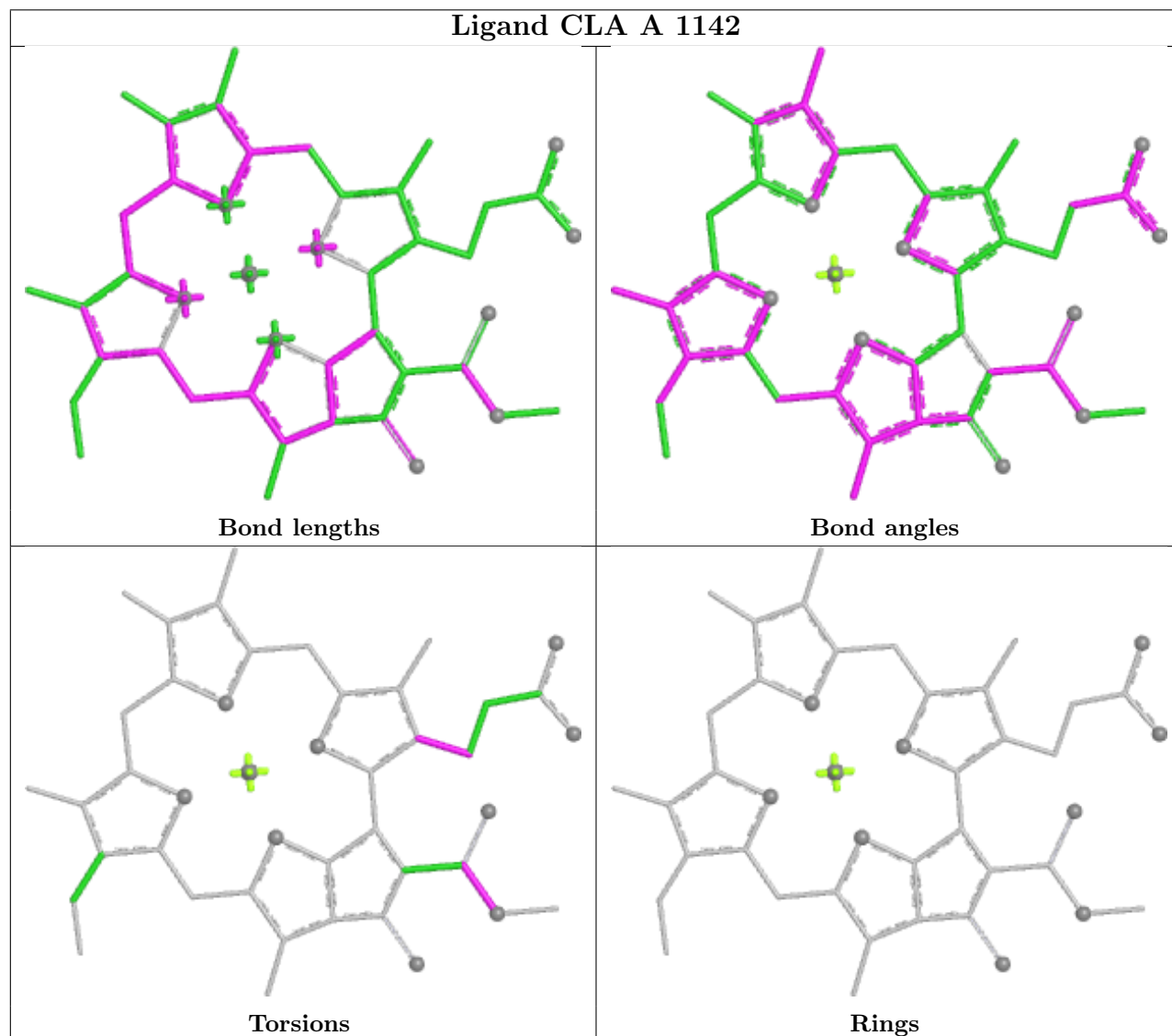
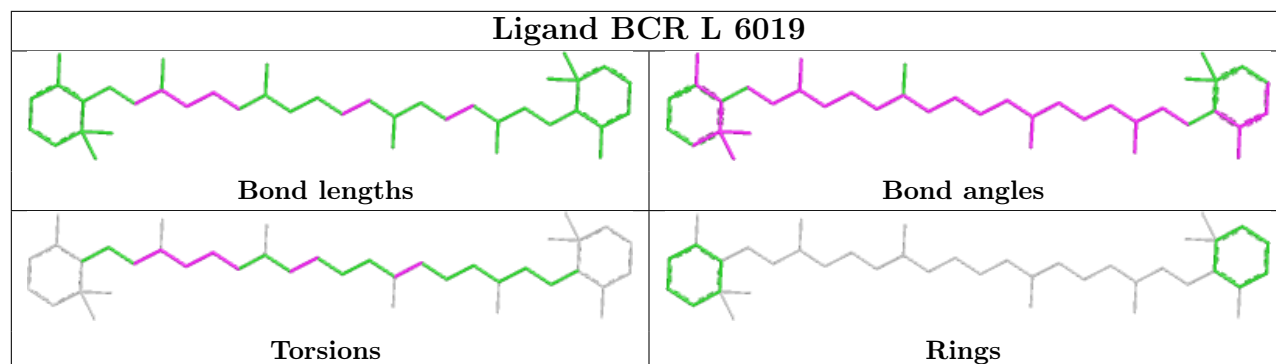


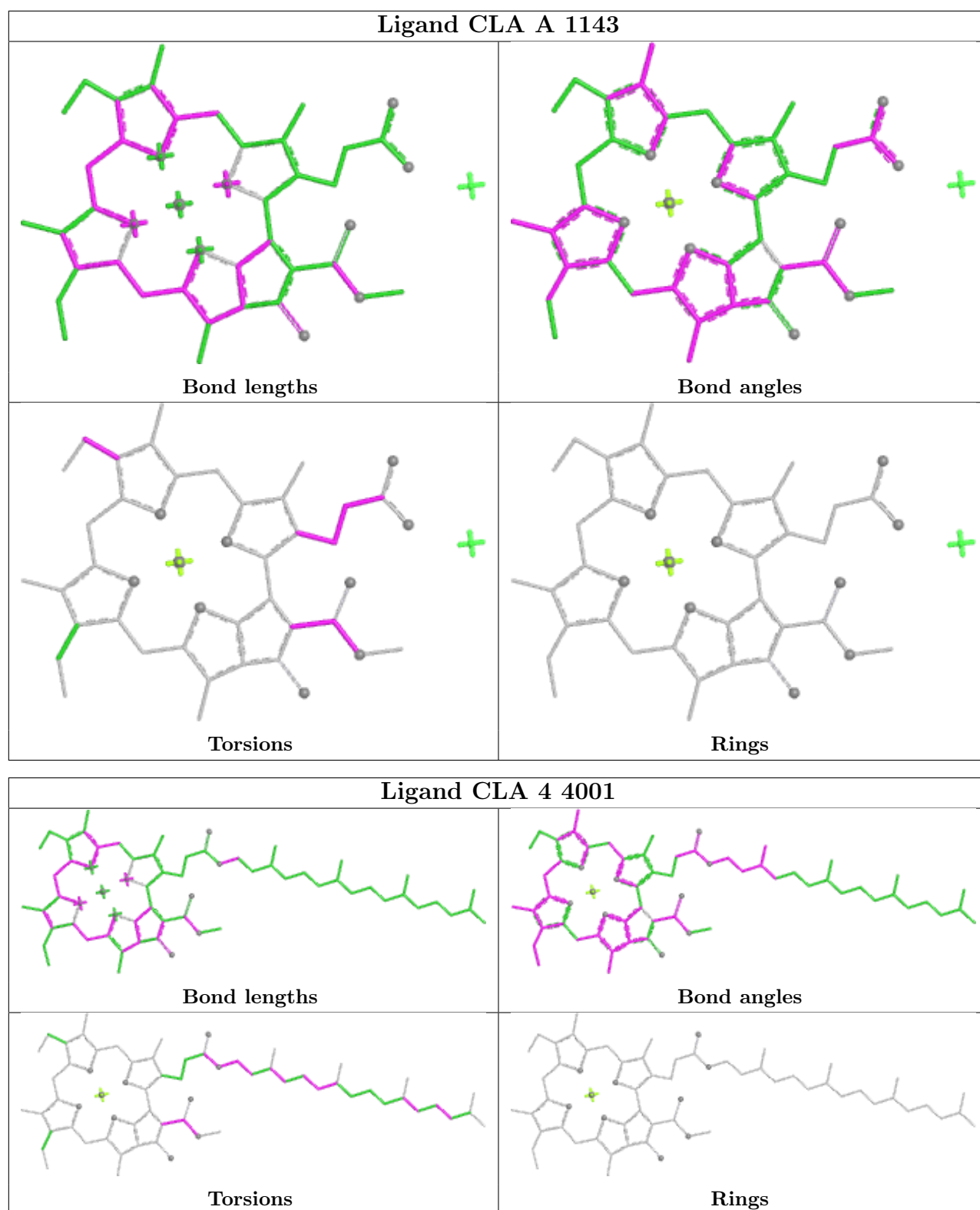
Ligand CLA A 1138**Ligand CLA 2 2013**











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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	721/721 (100%)	0.70	73 (10%) 12 7	34, 73, 146, 307	0
2	B	731/731 (100%)	0.52	64 (8%) 15 8	30, 58, 139, 288	0
3	C	80/80 (100%)	0.54	6 (7%) 20 10	42, 62, 98, 112	0
4	D	137/137 (100%)	1.02	23 (16%) 4 3	52, 80, 137, 204	0
5	E	63/63 (100%)	0.61	3 (4%) 35 19	42, 86, 124, 170	0
6	F	152/152 (100%)	0.67	23 (15%) 5 3	44, 73, 135, 225	0
7	G	84/84 (100%)	1.04	11 (13%) 7 4	63, 98, 122, 147	0
8	H	82/82 (100%)	1.71	29 (35%) 1 1	57, 97, 150, 184	0
9	I	26/26 (100%)	0.61	4 (15%) 5 3	47, 68, 91, 112	0
10	J	40/40 (100%)	0.39	4 (10%) 12 7	47, 69, 110, 138	0
11	K	66/72 (91%)	2.08	33 (50%) 0 0	171, 246, 287, 303	0
12	L	163/163 (100%)	0.66	19 (11%) 9 5	51, 79, 157, 195	0
13	N	85/85 (100%)	1.53	20 (23%) 2 1	177, 228, 289, 321	0
14	1	171/182 (93%)	1.06	37 (21%) 2 2	63, 103, 176, 315	0
15	2	146/199 (73%)	1.40	34 (23%) 2 1	74, 125, 214, 316	0
16	3	151/275 (54%)	2.04	64 (42%) 0 1	109, 193, 274, 335	0
17	4	196/196 (100%)	1.14	45 (22%) 2 1	59, 93, 182, 301	0
All	All	3094/3288 (94%)	0.89	492 (15%) 5 3	30, 80, 228, 335	0

The worst 5 of 492 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
16	3	151	ASN	13.4
1	A	43	THR	9.3
1	A	160	SER	8.9
17	4	123	ASN	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	3	154	ALA	8.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	CLA	3	3005	45/65	0.24	0.25	197,209,213,274	0
21	CLA	3	3004	45/65	0.30	0.28	260,267,271,309	0
21	CLA	3	3015	45/65	0.31	0.18	250,262,271,285	0
21	CLA	J	6014	61/65	0.35	0.20	191,215,220,289	0
21	CLA	3	3016	45/65	0.36	0.16	172,203,215,248	0
21	CLA	A	1142	44/65	0.39	0.18	186,199,202,274	0
21	CLA	J	6015	55/65	0.41	0.23	122,143,159,160	0
21	CLA	2	2006	57/65	0.44	0.20	140,162,183,256	0
21	CLA	3	3006	65/65	0.44	0.27	144,177,194,197	0
21	CLA	4	4007	65/65	0.44	0.27	103,123,140,244	0
21	CLA	2	2008	65/65	0.46	0.22	103,135,158,161	0
25	LMG	G	2021	23/55	0.49	0.21	160,168,177,180	0
21	CLA	1	1014	45/65	0.51	0.20	115,160,167,171	0
21	CLA	2	2003	65/65	0.52	0.19	136,144,159,185	0
27	NEX	4	4503	44/44	0.53	0.26	72,110,128,133	0
21	CLA	3	3010	52/65	0.54	0.19	115,168,179,182	0
21	CLA	3	3003	60/65	0.54	0.27	190,224,234,252	0
21	CLA	A	1143	46/65	0.55	0.18	198,214,217,262	0
21	CLA	2	2014	45/65	0.56	0.18	104,135,145,168	0
21	CLA	3	3017	45/65	0.56	0.19	224,249,260,262	0
21	CLA	4	4005	45/65	0.57	0.25	107,130,142,144	0
19	BCR	B	6011	25/40	0.57	0.23	77,111,118,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	CLA	J	1302	61/65	0.58	0.22	59,117,149,153	0
21	CLA	3	3014	45/65	0.58	0.24	242,261,265,271	0
21	CLA	1	1006	47/65	0.61	0.21	116,133,148,152	0
21	CLA	3	3002	55/65	0.61	0.20	181,189,204,206	0
21	CLA	4	4006	65/65	0.61	0.23	116,133,155,160	0
21	CLA	1	1013	65/65	0.62	0.19	94,119,138,148	0
21	CLA	3	3008	65/65	0.62	0.17	149,167,183,187	0
21	CLA	3	3001	65/65	0.62	0.28	187,204,220,223	0
21	CLA	2	2010	65/65	0.65	0.17	103,118,134,151	0
19	BCR	J	6013	40/40	0.66	0.28	119,143,153,153	0
21	CLA	3	3011	46/65	0.66	0.18	131,154,160,195	0
21	CLA	3	3013	50/65	0.66	0.19	107,132,148,153	0
21	CLA	3	3012	45/65	0.68	0.19	163,196,205,208	0
26	LUT	2	2501	42/42	0.70	0.20	106,121,131,138	0
21	CLA	A	1120	46/65	0.71	0.18	97,128,144,149	0
21	CLA	2	2002	60/65	0.73	0.18	112,142,151,201	0
21	CLA	2	2007	55/65	0.73	0.18	113,130,142,149	0
21	CLA	3	3009	46/65	0.74	0.20	138,174,190,191	0
21	CLA	1	1010	65/65	0.75	0.20	108,123,152,154	0
21	CLA	1	1009	65/65	0.75	0.21	58,78,104,108	0
21	CLA	2	2009	46/65	0.75	0.15	82,101,128,141	0
21	CLA	A	1141	51/65	0.76	0.16	91,124,133,137	0
20	LHG	2	2801	36/49	0.76	0.21	112,132,147,150	0
21	CLA	4	4014	45/65	0.76	0.16	71,105,128,134	0
26	LUT	4	4501	42/42	0.77	0.21	77,95,99,107	0
21	CLA	G	1001	55/65	0.77	0.13	74,93,113,123	0
21	CLA	4	4002	56/65	0.78	0.16	76,94,112,128	0
21	CLA	A	1110	55/65	0.78	0.27	129,148,161,166	0
21	CLA	4	4001	65/65	0.78	0.19	73,91,124,131	0
21	CLA	4	4010	50/65	0.79	0.16	57,93,132,147	0
19	BCR	G	2011	40/40	0.79	0.16	55,78,120,121	0
21	CLA	2	2011	60/65	0.79	0.18	80,97,144,158	0
26	LUT	1	1501	42/42	0.80	0.20	83,94,104,107	0
21	CLA	H	1000	46/65	0.80	0.16	69,106,123,134	0
21	CLA	A	1115	56/65	0.80	0.18	85,107,132,161	0
19	BCR	A	6003	40/40	0.80	0.26	80,97,123,124	0
19	BCR	A	6002	40/40	0.81	0.19	72,103,133,133	0
21	CLA	G	1002	46/65	0.81	0.14	112,128,140,145	0
21	CLA	A	1121	46/65	0.82	0.15	103,130,154,160	0
21	CLA	A	1108	46/65	0.82	0.14	103,120,136,146	0
21	CLA	1	1002	56/65	0.82	0.16	101,113,133,140	0
21	CLA	B	1212	46/65	0.83	0.14	64,85,98,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	LMG	J	5001	35/55	0.83	0.14	62,91,103,104	0
21	CLA	1	1011	65/65	0.83	0.19	89,109,115,118	0
21	CLA	4	4008	48/65	0.83	0.13	66,92,107,138	0
21	CLA	A	1114	46/65	0.83	0.14	93,114,120,124	0
21	CLA	2	2013	65/65	0.83	0.13	91,119,135,146	0
21	CLA	2	2004	59/65	0.84	0.16	84,101,110,116	0
26	LUT	2	2502	42/42	0.84	0.16	83,99,106,109	0
21	CLA	L	1503	50/65	0.84	0.15	58,77,98,105	0
19	BCR	B	6010	40/40	0.84	0.19	47,67,81,88	0
28	G3P	4	4505	10/10	0.84	0.16	94,125,132,135	0
19	BCR	B	6005	40/40	0.85	0.20	51,69,122,123	0
21	CLA	2	2005	65/65	0.85	0.15	89,112,126,128	0
19	BCR	A	6011	40/40	0.85	0.19	32,48,74,81	0
21	CLA	A	1107	51/65	0.85	0.19	52,74,99,104	0
21	CLA	A	1134	46/65	0.85	0.14	93,103,131,137	0
21	CLA	1	1008	65/65	0.85	0.15	64,84,124,129	0
21	CLA	F	1302	46/65	0.85	0.13	52,85,98,151	0
20	LHG	B	7004	49/49	0.86	0.16	68,98,111,124	0
21	CLA	2	2012	65/65	0.86	0.15	72,88,117,121	0
21	CLA	A	1112	46/65	0.86	0.15	68,88,99,101	0
21	CLA	1	1003	65/65	0.86	0.14	53,72,97,108	0
26	LUT	4	4502	42/42	0.86	0.16	56,76,84,88	0
19	BCR	I	6018	40/40	0.86	0.17	37,61,79,86	0
21	CLA	1	1007	55/65	0.86	0.14	76,100,121,139	0
20	LHG	A	7003	49/49	0.87	0.15	81,113,121,123	0
21	CLA	2	2001	27/65	0.87	0.14	105,120,130,131	0
21	CLA	A	1118	46/65	0.87	0.16	109,118,126,135	0
21	CLA	4	4015	46/65	0.87	0.13	51,65,83,108	0
21	CLA	A	1109	65/65	0.87	0.17	81,105,133,147	0
21	CLA	B	1213	60/65	0.87	0.15	67,81,103,106	0
21	CLA	B	1231	46/65	0.87	0.11	49,76,87,92	0
26	LUT	1	1502	42/42	0.87	0.20	65,87,109,118	0
19	BCR	B	6006	40/40	0.87	0.17	45,63,110,110	0
21	CLA	A	1128	65/65	0.87	0.18	44,66,81,96	0
21	CLA	A	1133	46/65	0.87	0.15	77,90,112,119	0
19	BCR	B	6004	40/40	0.87	0.17	54,75,81,82	0
21	CLA	A	1136	65/65	0.87	0.17	59,82,108,155	0
19	BCR	A	6008	40/40	0.87	0.18	57,87,105,112	0
21	CLA	4	4013	51/65	0.88	0.11	63,77,101,104	0
19	BCR	L	6020	40/40	0.88	0.13	60,75,82,83	0
19	BCR	B	6009	40/40	0.88	0.14	30,52,68,73	0
24	DGD	B	7101	61/66	0.88	0.15	40,70,96,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	BCR	J	6012	40/40	0.88	0.17	45,67,98,109	0
21	CLA	A	1126	65/65	0.88	0.24	59,79,95,106	0
21	CLA	1	1012	50/65	0.88	0.14	78,95,113,175	0
20	LHG	1	1801	49/49	0.88	0.17	68,88,119,122	0
21	CLA	4	4003	65/65	0.88	0.12	61,86,100,116	0
21	CLA	A	1113	46/65	0.88	0.15	95,112,136,139	0
21	CLA	B	1237	60/65	0.88	0.15	41,60,87,101	0
21	CLA	F	1301	45/65	0.88	0.13	48,63,77,148	0
19	BCR	A	6007	40/40	0.88	0.14	69,91,97,98	0
19	BCR	L	6019	40/40	0.88	0.16	40,59,79,87	0
21	CLA	1	1001	55/65	0.89	0.13	81,103,129,170	0
21	CLA	A	1129	50/65	0.89	0.13	51,83,90,93	0
21	CLA	A	1122	59/65	0.89	0.14	57,78,98,103	0
21	CLA	4	4011	65/65	0.89	0.15	66,74,104,108	0
21	CLA	1	1005	56/65	0.89	0.11	54,69,80,85	0
21	CLA	B	1240	65/65	0.89	0.12	42,72,83,97	0
21	CLA	A	1111	60/65	0.89	0.16	60,86,114,117	0
21	CLA	A	9012	65/65	0.89	0.16	36,63,75,78	0
21	CLA	F	1303	64/65	0.89	0.13	52,65,104,149	0
21	CLA	B	1208	55/65	0.89	0.14	49,68,96,99	0
21	CLA	A	1119	65/65	0.89	0.18	78,91,99,105	0
21	CLA	A	1140	65/65	0.89	0.14	35,50,73,99	0
21	CLA	B	1216	65/65	0.89	0.13	43,56,94,97	0
21	CLA	B	1217	46/65	0.89	0.14	52,70,92,109	0
21	CLA	B	1218	60/65	0.89	0.14	54,78,101,102	0
21	CLA	4	4004	65/65	0.89	0.14	56,81,91,96	0
21	CLA	L	1501	46/65	0.89	0.11	66,80,103,115	0
21	CLA	B	1219	60/65	0.89	0.16	50,81,101,103	0
21	CLA	B	1215	60/65	0.90	0.16	51,69,81,84	0
21	CLA	A	1125	55/65	0.90	0.13	54,73,89,99	0
21	CLA	A	1105	51/65	0.90	0.11	67,81,98,103	0
21	CLA	A	1106	65/65	0.90	0.16	39,55,76,81	0
19	BCR	F	6014	40/40	0.90	0.15	38,56,64,66	0
21	CLA	B	1227	65/65	0.90	0.12	39,63,89,92	0
19	BCR	F	6016	40/40	0.90	0.12	35,51,76,82	0
21	CLA	L	1502	65/65	0.90	0.15	54,66,88,91	0
21	CLA	B	1234	60/65	0.90	0.14	39,56,98,104	0
21	CLA	B	1207	65/65	0.90	0.13	40,62,83,98	0
21	CLA	A	1123	65/65	0.90	0.17	58,84,97,103	0
21	CLA	B	9023	65/65	0.90	0.12	36,54,62,89	0
21	CLA	B	1211	65/65	0.90	0.12	56,68,81,90	0
21	CLA	A	1135	51/65	0.90	0.12	47,62,87,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	CLA	A	1124	55/65	0.90	0.12	48,60,83,91	0
21	CLA	4	4009	50/65	0.90	0.12	64,83,103,105	0
18	PQN	B	5002	33/33	0.91	0.14	41,50,76,79	0
21	CLA	A	1101	65/65	0.91	0.13	43,63,91,95	0
21	CLA	A	1139	65/65	0.91	0.13	33,51,81,88	0
21	CLA	A	1116	54/65	0.91	0.16	73,89,105,111	0
21	CLA	A	1102	50/65	0.91	0.10	43,63,91,95	0
21	CLA	A	1127	65/65	0.91	0.16	52,63,79,85	0
21	CLA	4	4012	65/65	0.91	0.14	54,62,89,107	0
21	CLA	A	1103	65/65	0.91	0.16	63,80,90,111	0
21	CLA	B	1222	65/65	0.91	0.14	28,47,85,87	0
21	CLA	B	1223	65/65	0.91	0.14	31,50,60,63	0
21	CLA	B	1224	65/65	0.91	0.15	32,54,93,95	0
21	CLA	A	1104	65/65	0.91	0.17	47,69,81,87	0
21	CLA	B	1230	58/65	0.91	0.14	38,59,73,77	0
21	CLA	A	9013	65/65	0.91	0.15	35,61,71,110	0
21	CLA	A	1131	65/65	0.91	0.12	39,55,72,90	0
21	CLA	1	1004	65/65	0.91	0.12	57,77,83,113	0
19	BCR	A	6017	40/40	0.91	0.15	34,52,79,93	0
21	CLA	B	1209	46/65	0.91	0.12	52,63,84,96	0
21	CLA	B	9022	65/65	0.91	0.13	32,47,62,86	0
21	CLA	B	1210	65/65	0.91	0.15	46,56,73,101	0
20	LHG	A	7001	49/49	0.91	0.20	47,72,94,97	0
21	CLA	A	1137	55/65	0.92	0.16	63,81,99,106	0
21	CLA	A	1138	65/65	0.92	0.13	32,49,60,65	0
18	PQN	A	5001	33/33	0.92	0.16	38,57,67,71	0
21	CLA	B	1236	55/65	0.92	0.13	51,61,122,125	0
21	CLA	A	1132	65/65	0.92	0.12	39,50,80,85	0
21	CLA	B	1221	54/65	0.92	0.14	33,57,71,86	0
21	CLA	B	1202	65/65	0.92	0.13	33,53,71,92	0
21	CLA	B	1206	65/65	0.92	0.13	38,50,78,84	0
21	CLA	B	1214	59/65	0.92	0.14	44,61,102,119	0
21	CLA	A	1130	46/65	0.92	0.12	48,60,88,109	0
21	CLA	B	1201	46/65	0.93	0.09	34,46,78,91	0
21	CLA	B	1235	65/65	0.93	0.11	36,53,68,73	0
21	CLA	A	1117	65/65	0.93	0.17	59,78,92,123	0
21	CLA	B	1225	65/65	0.93	0.12	31,46,60,71	0
21	CLA	B	1238	65/65	0.93	0.12	35,51,74,86	0
21	CLA	B	1220	65/65	0.93	0.13	32,48,101,106	0
21	CLA	B	1228	51/65	0.93	0.10	33,45,66,92	0
21	CLA	B	1229	65/65	0.93	0.14	36,50,73,85	0
21	CLA	B	1203	60/65	0.93	0.11	30,43,69,74	0

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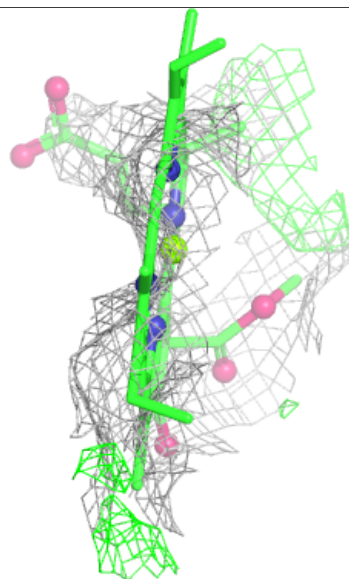
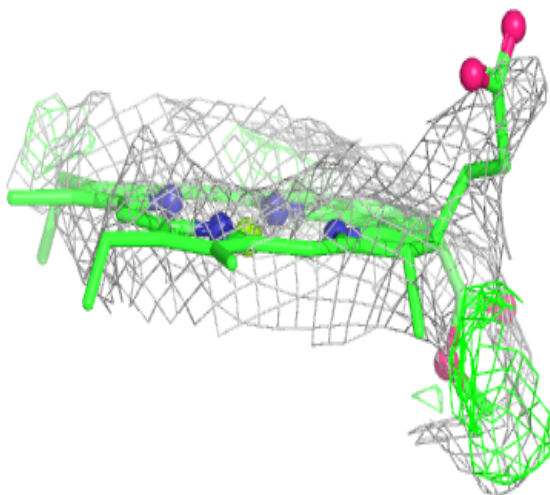
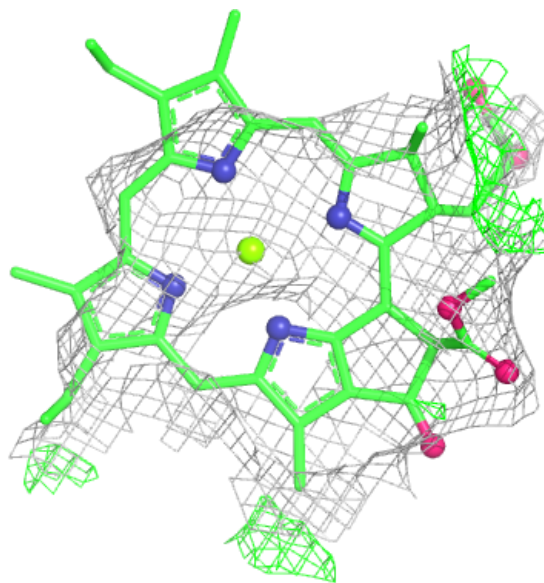
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	CLA	B	1204	55/65	0.93	0.10	38,61,77,78	0
23	CL0	A	9011	65/65	0.94	0.11	30,39,53,73	0
21	CLA	B	1205	65/65	0.94	0.11	33,46,70,83	0
21	CLA	B	9010	65/65	0.94	0.10	29,39,57,72	0
21	CLA	B	1226	65/65	0.94	0.10	28,43,71,73	0
19	BCR	I	6020	40/40	0.94	0.11	44,51,65,75	0
21	CLA	B	1239	65/65	0.94	0.10	32,47,65,73	0
22	SF4	A	8001	8/8	0.97	0.10	50,64,71,75	0
22	SF4	C	8002	8/8	0.98	0.07	53,65,79,92	0
22	SF4	C	8003	8/8	0.99	0.07	53,63,89,92	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.

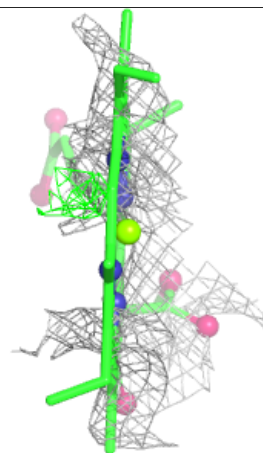
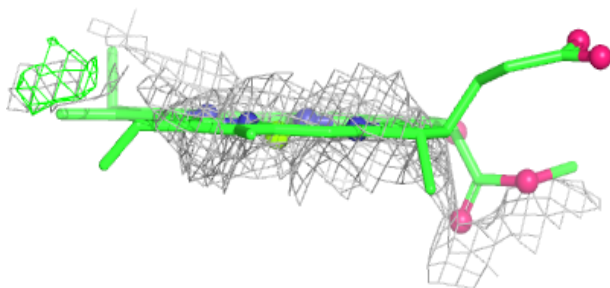
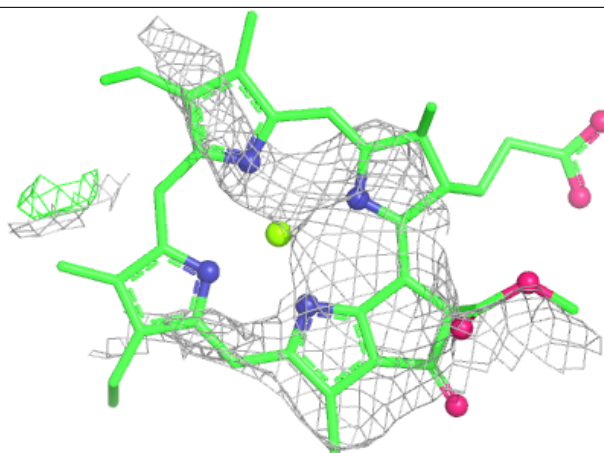
Electron density around CLA 3 3005:

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



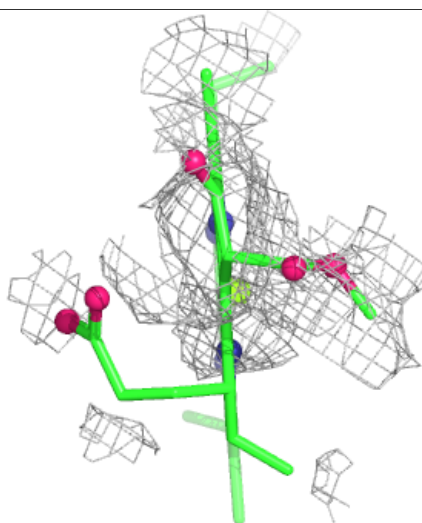
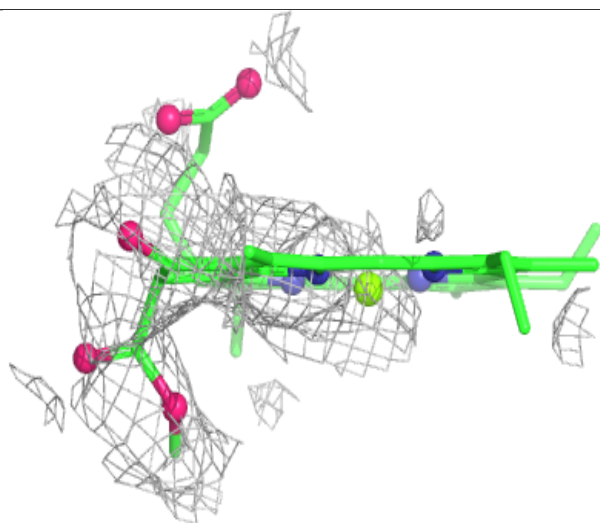
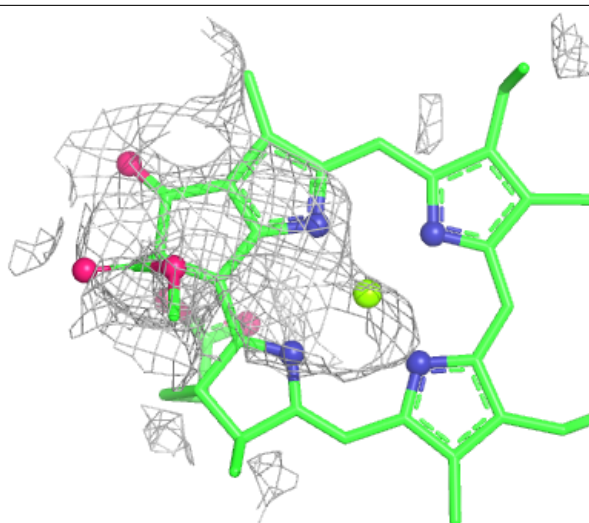
Electron density around CLA 3 3004:

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



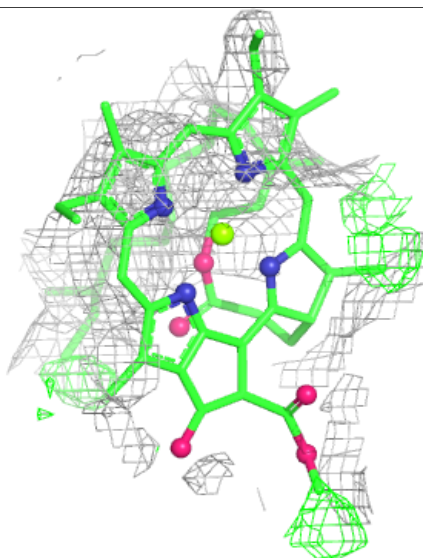
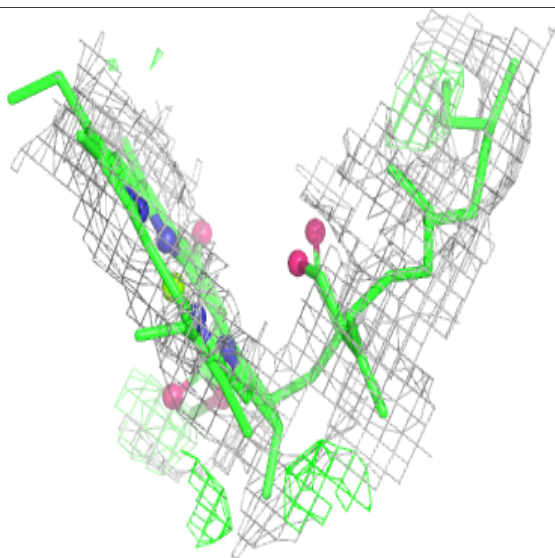
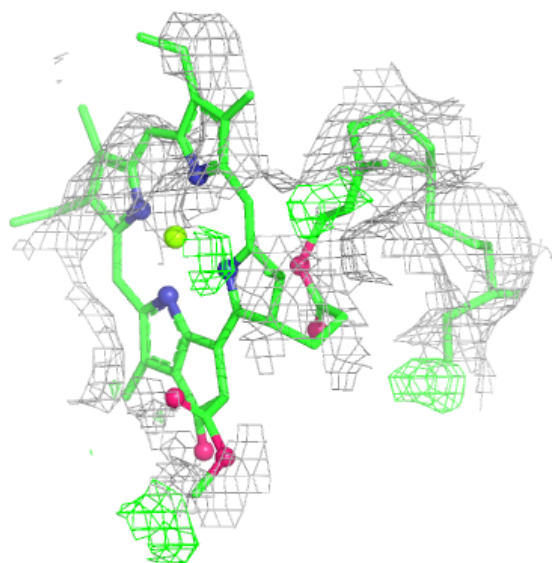
Electron density around CLA 3 3015:

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



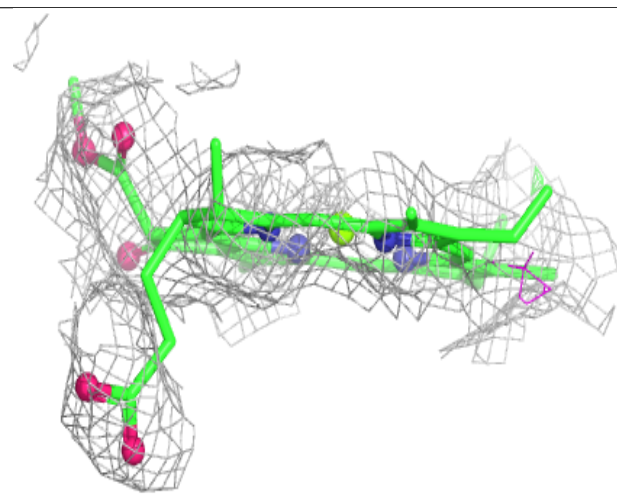
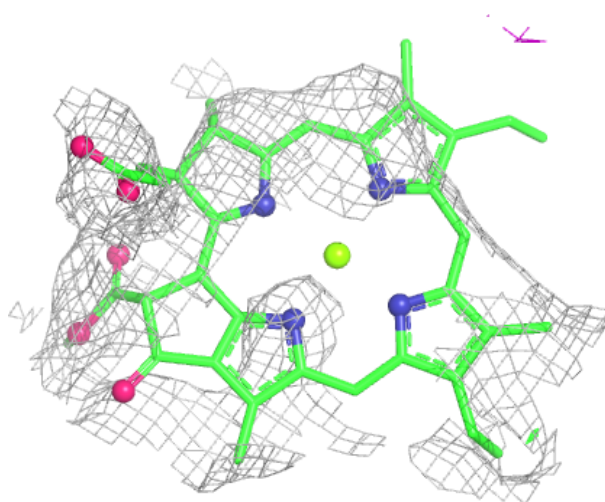
Electron density around CLA J 6014:

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



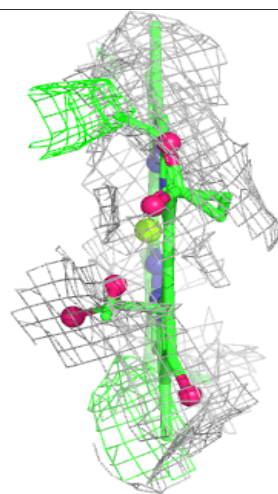
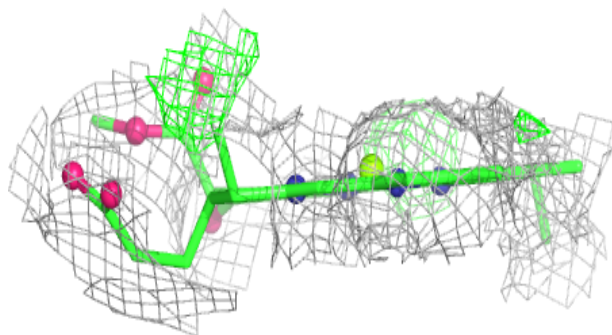
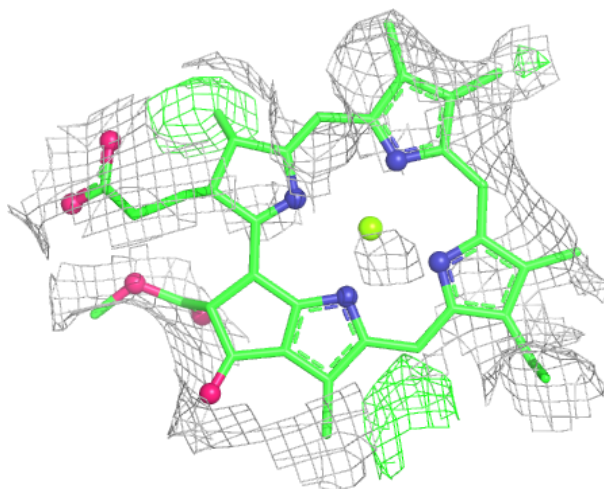
Electron density around CLA 3 3016:

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



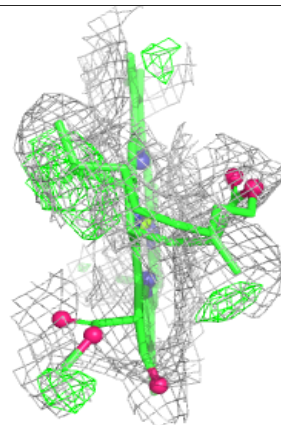
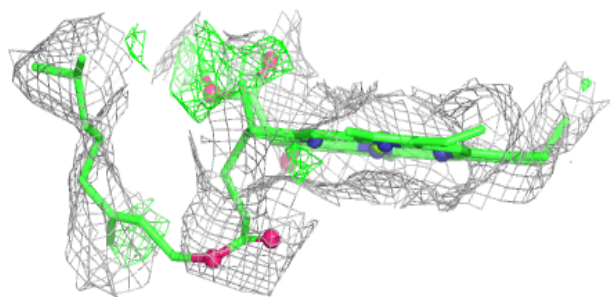
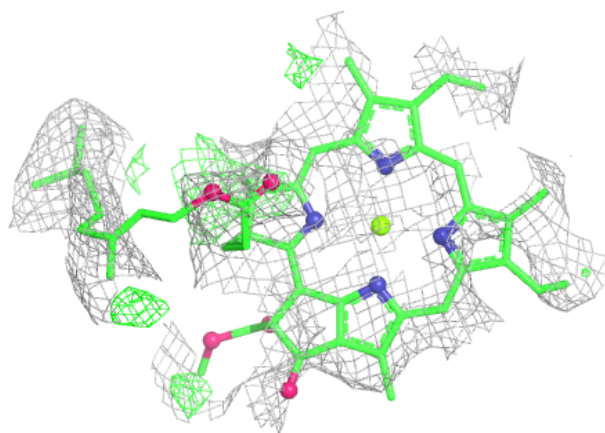
Electron density around CLA A 1142:

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

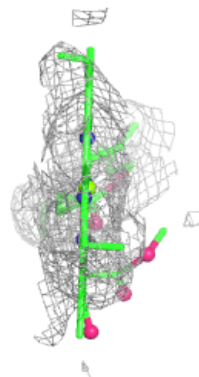
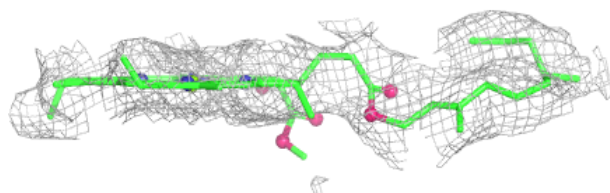
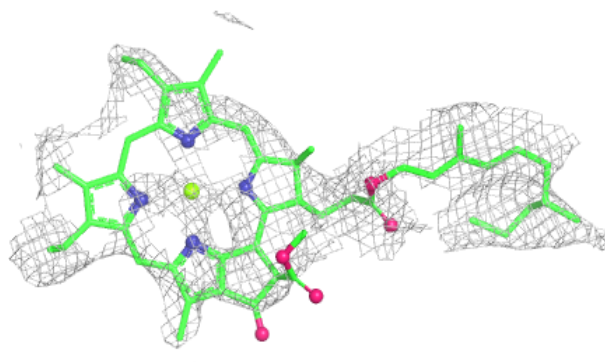


Electron density around CLA J 6015:

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

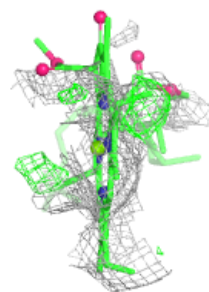
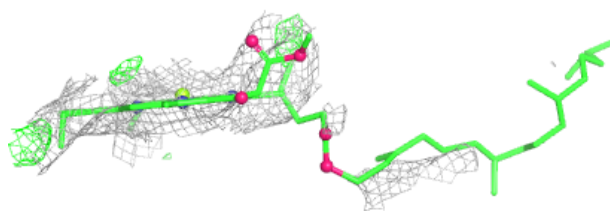
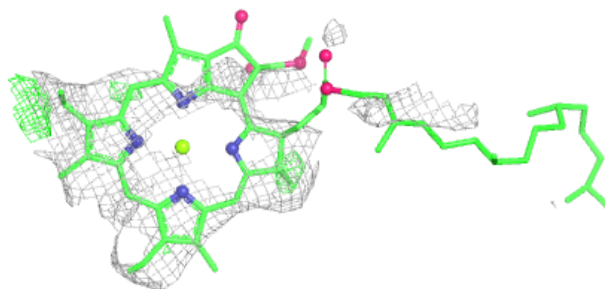
**Electron density around CLA 2 2006:**

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

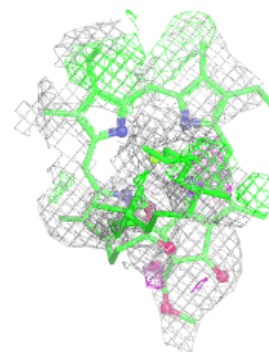
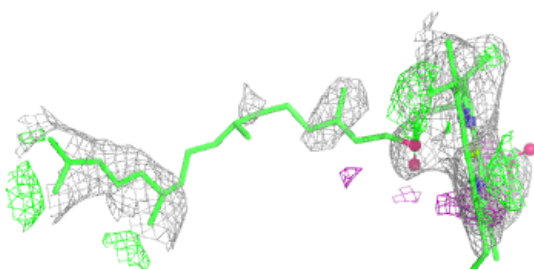
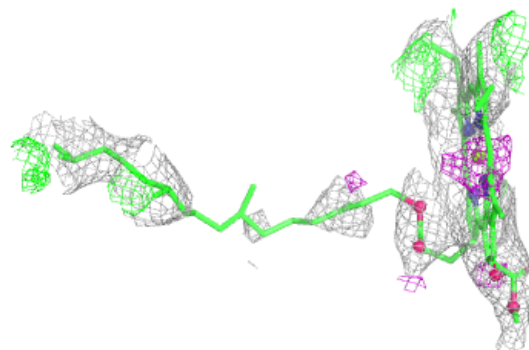


Electron density around CLA 3 3006:

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

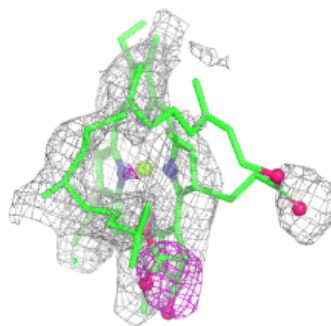
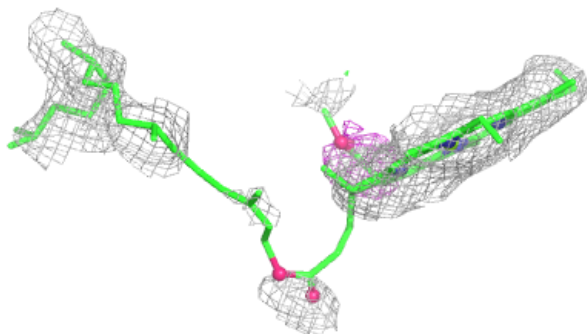
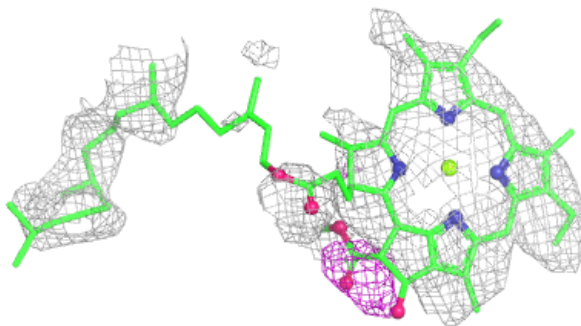
**Electron density around CLA 4 4007:**

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



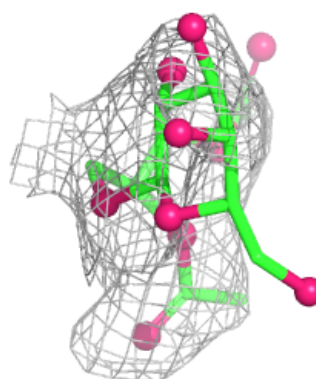
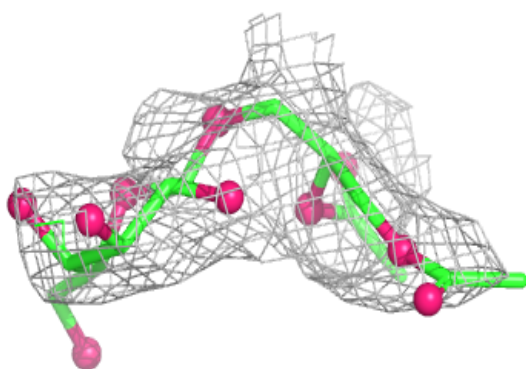
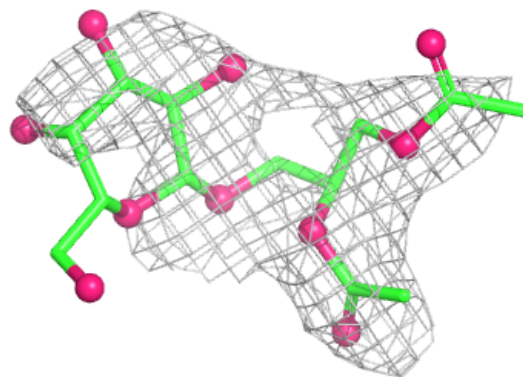
Electron density around CLA 2 2008:

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



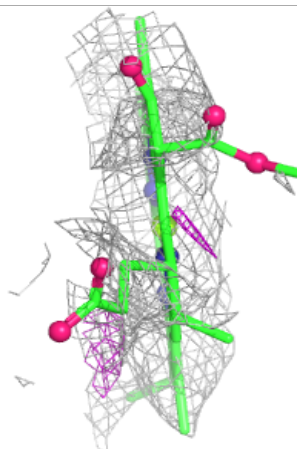
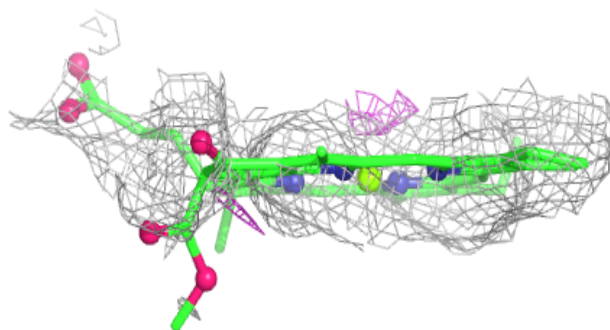
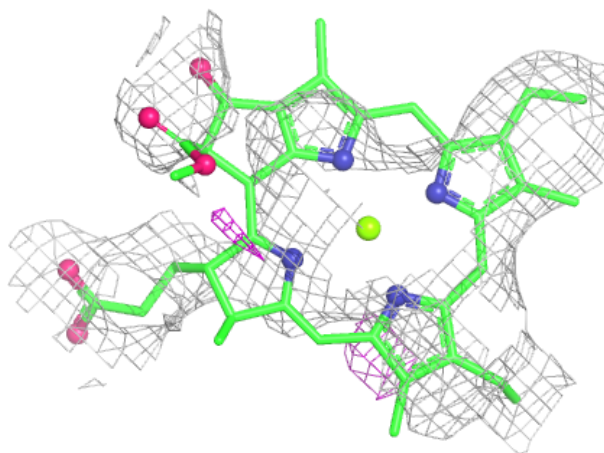
Electron density around LMG G 2021:

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



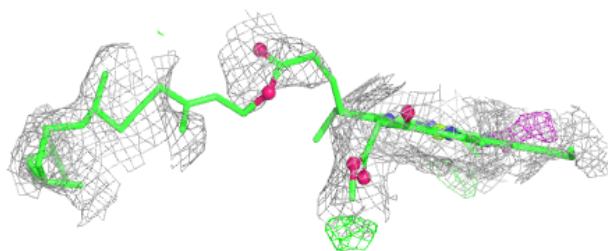
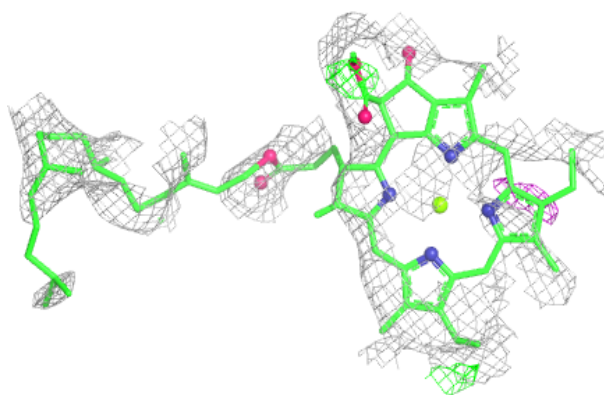
Electron density around CLA 1 1014:

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

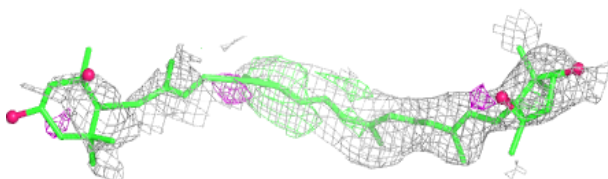
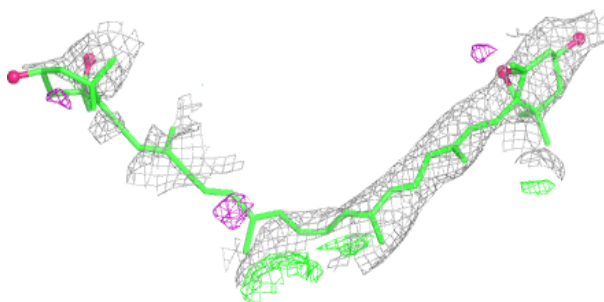


Electron density around CLA 2 2003:

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

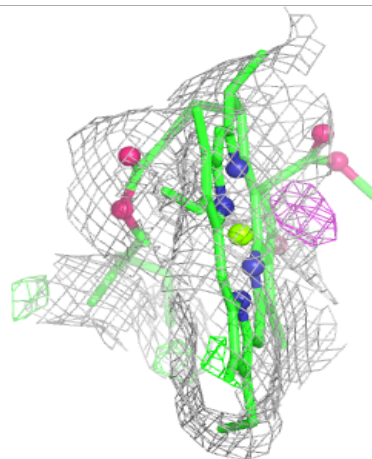
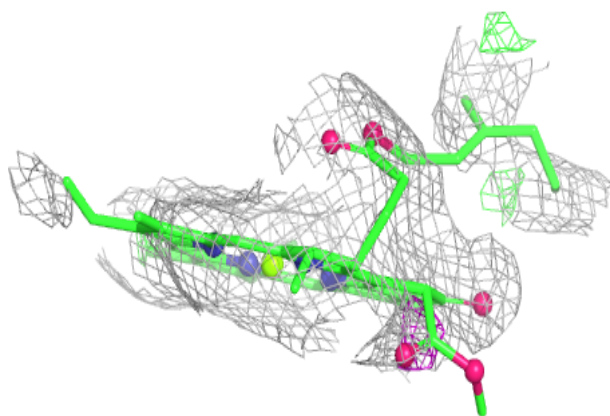
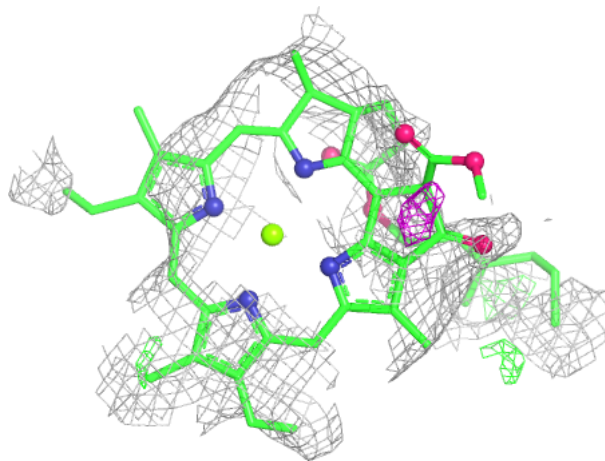
**Electron density around NEX 4 4503:**

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



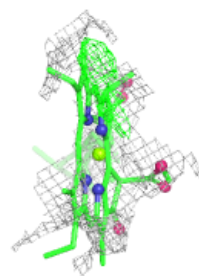
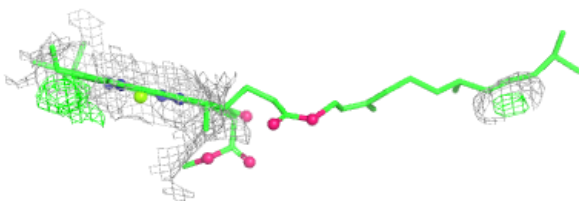
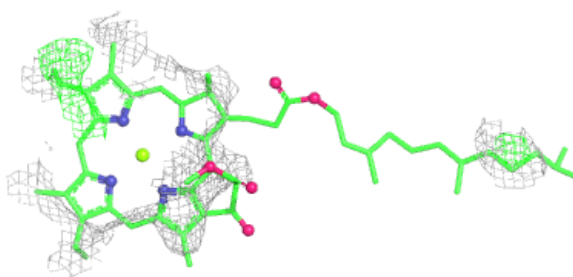
Electron density around CLA 3 3010:

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

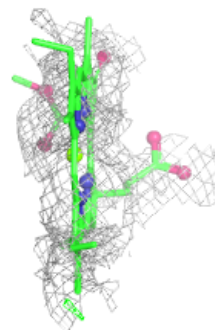
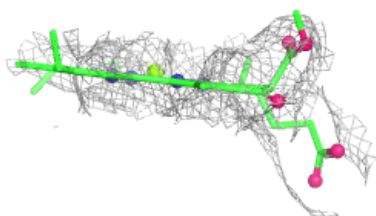
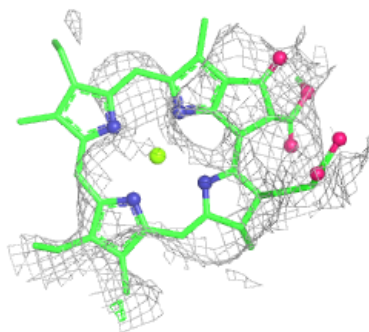


Electron density around CLA 3 3003:

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

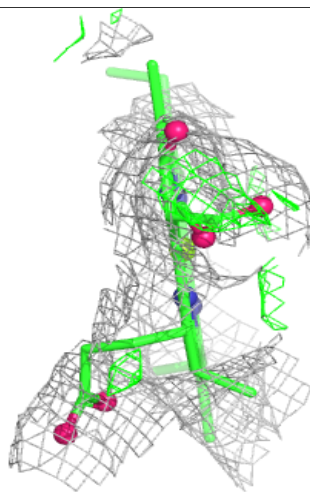
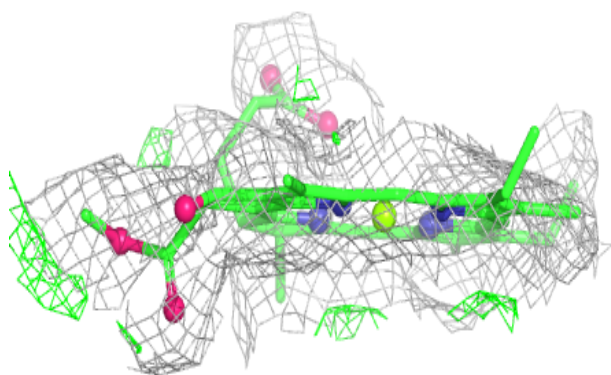
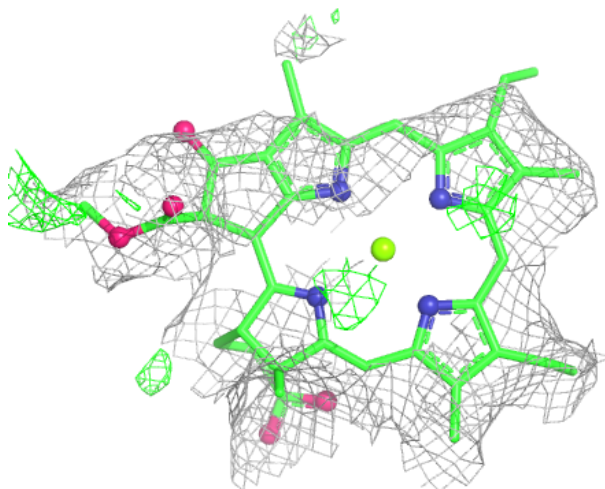
**Electron density around CLA A 1143:**

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



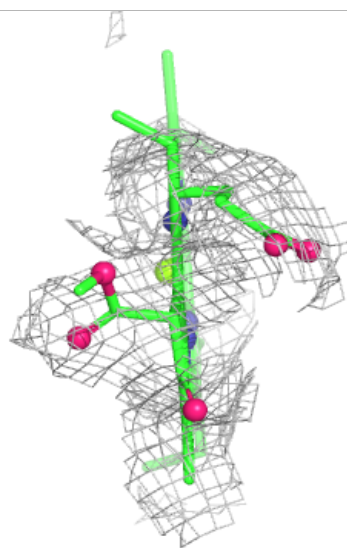
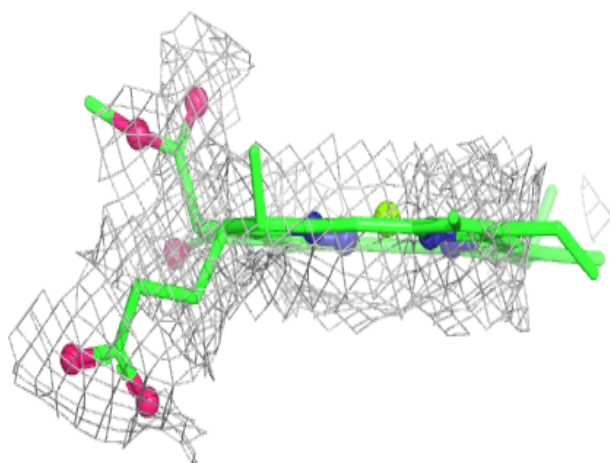
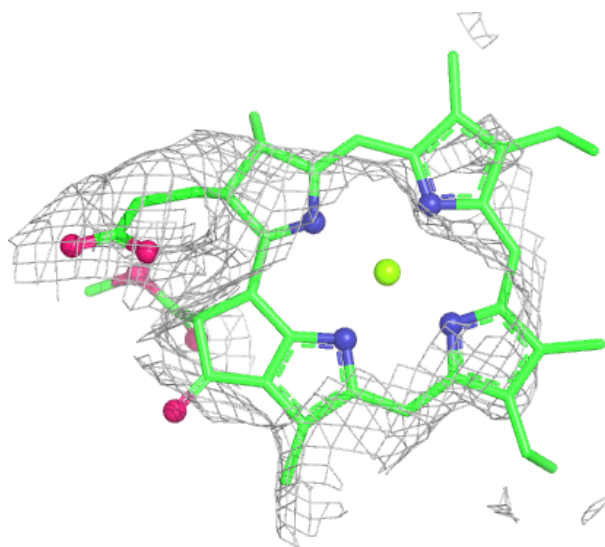
Electron density around CLA 2 2014:

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



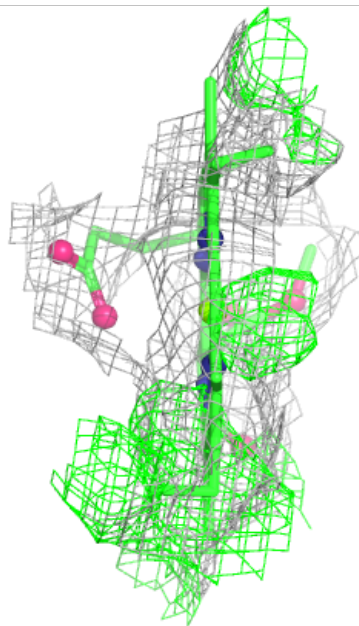
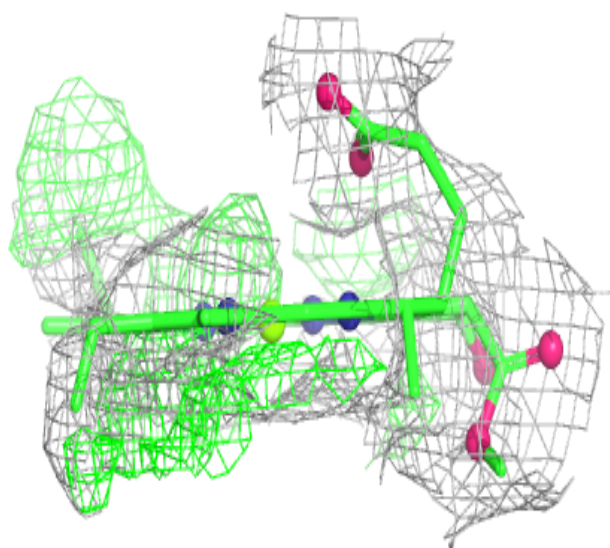
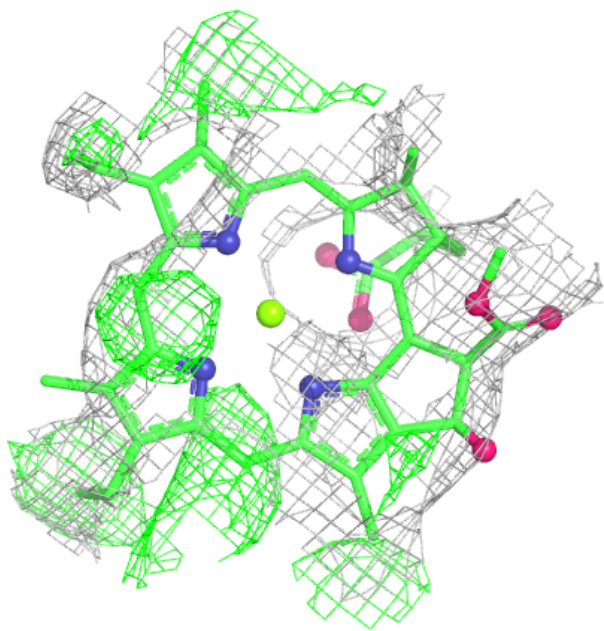
Electron density around CLA 3 3017:

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



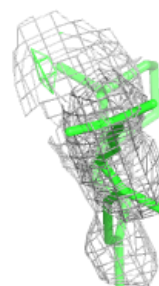
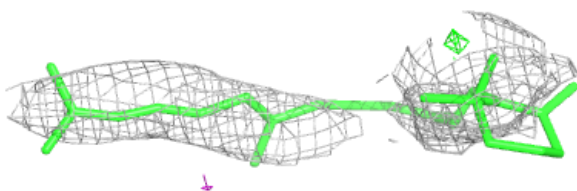
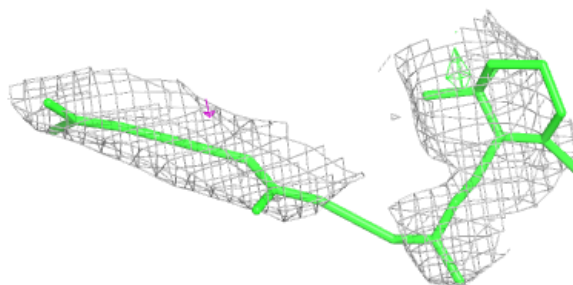
Electron density around CLA 4 4005:

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

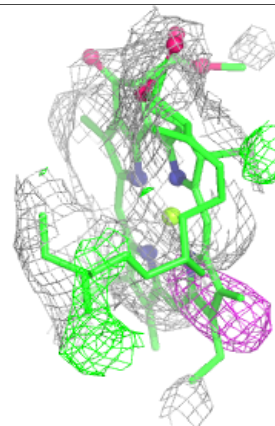
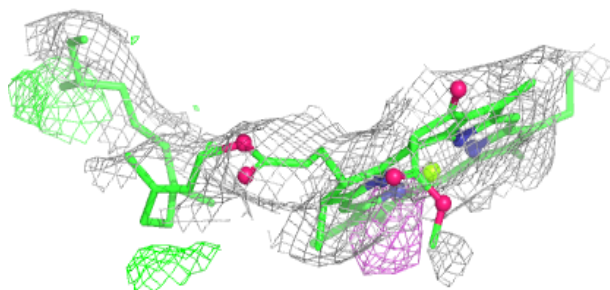
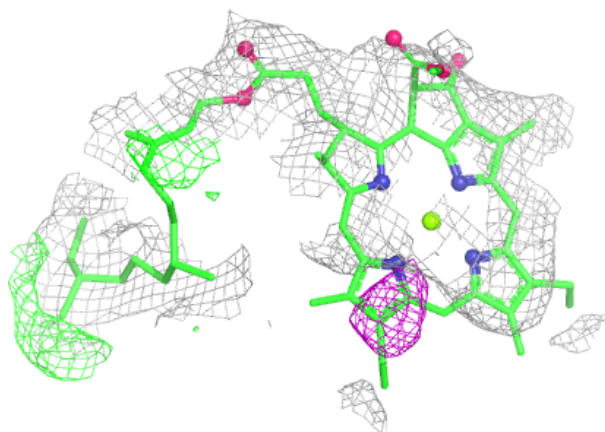


Electron density around BCR B 6011:

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

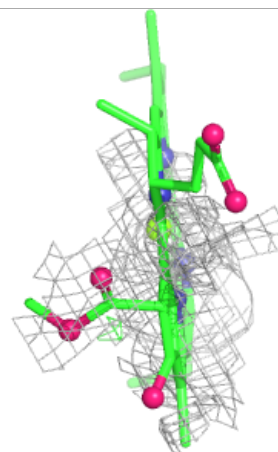
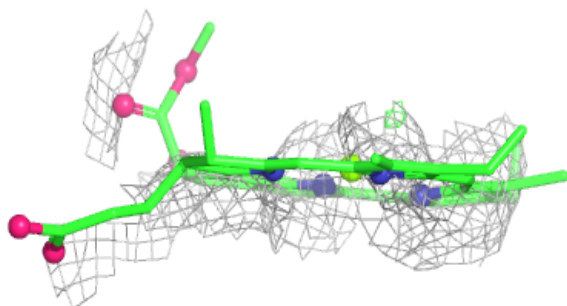
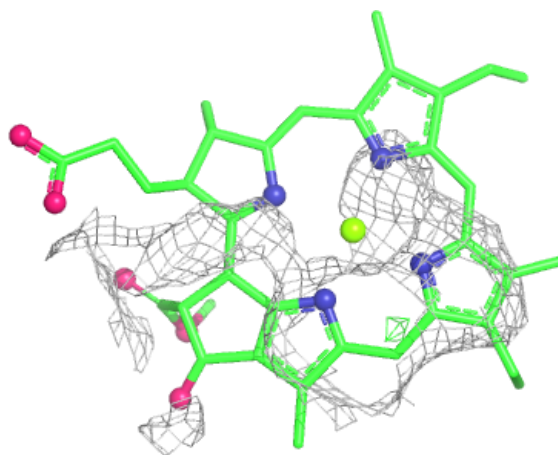
**Electron density around CLA J 1302:**

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



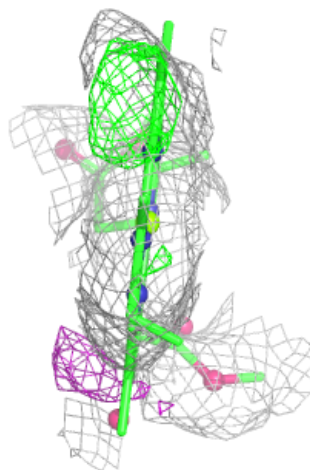
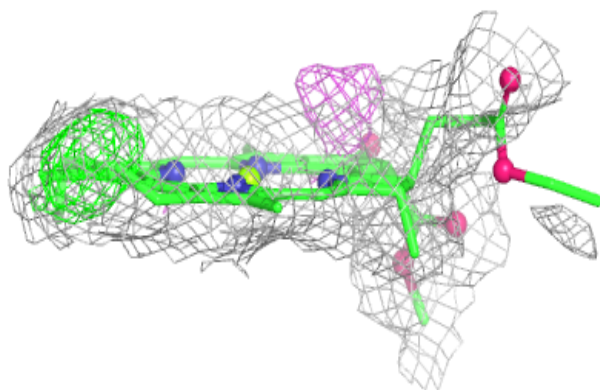
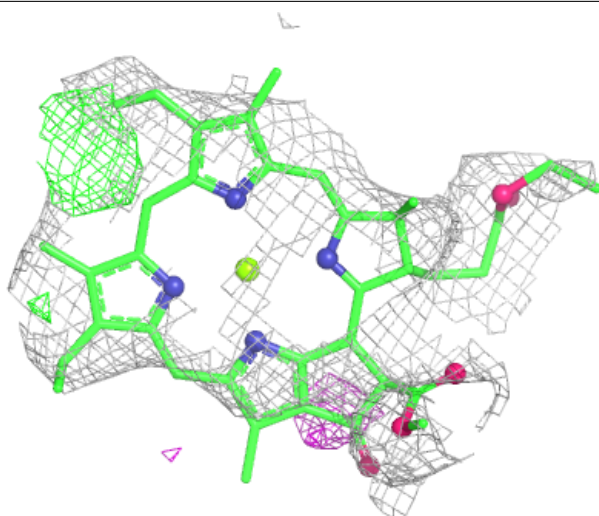
Electron density around CLA 3 3014:

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



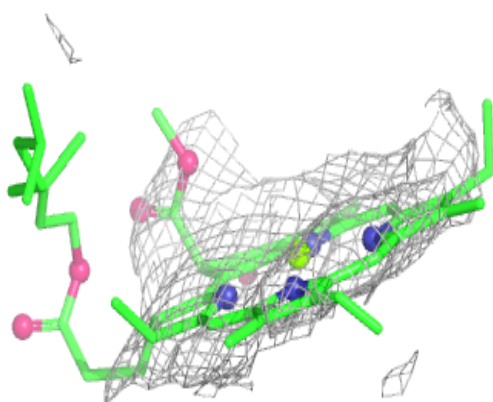
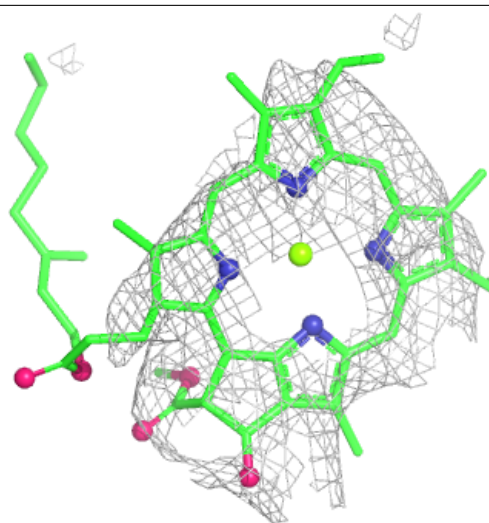
Electron density around CLA 1 1006:

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



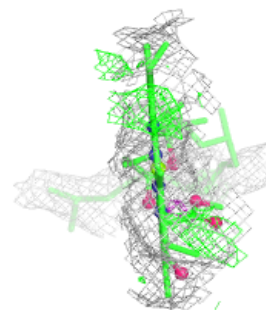
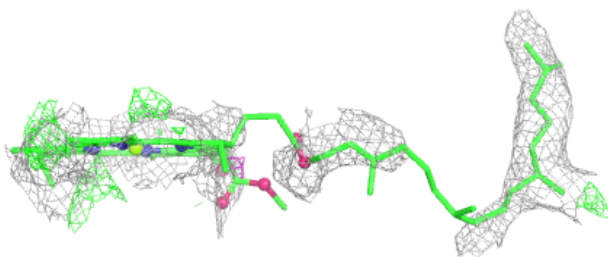
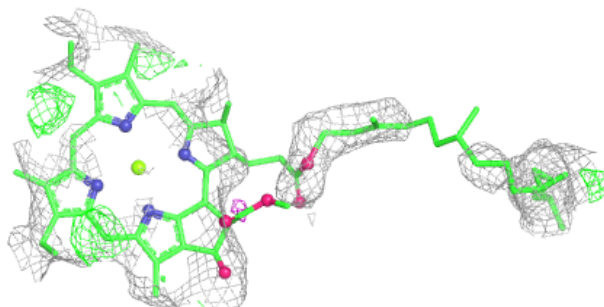
Electron density around CLA 3 3002:

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



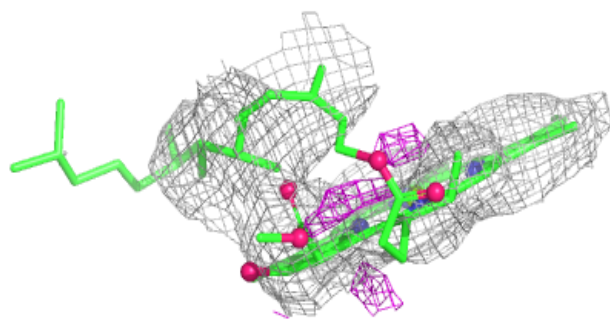
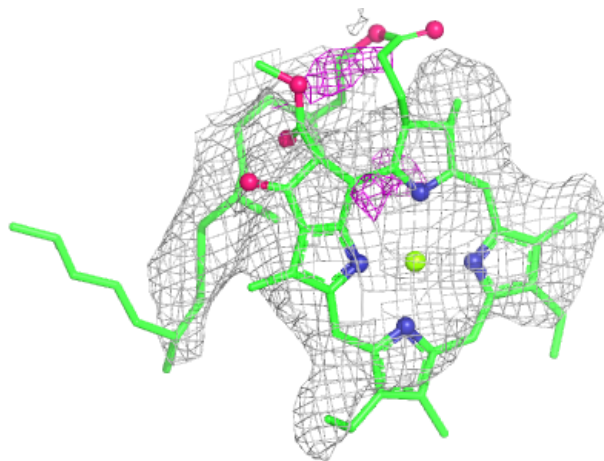
Electron density around CLA 4 4006:

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



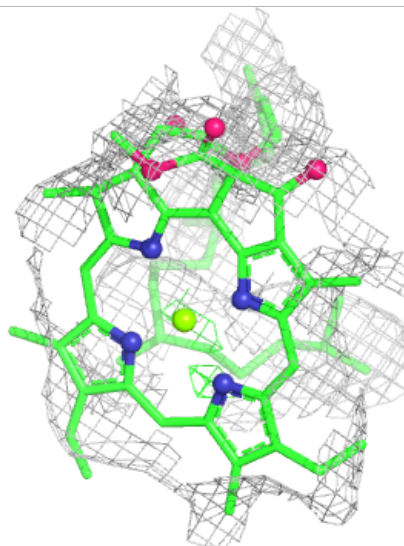
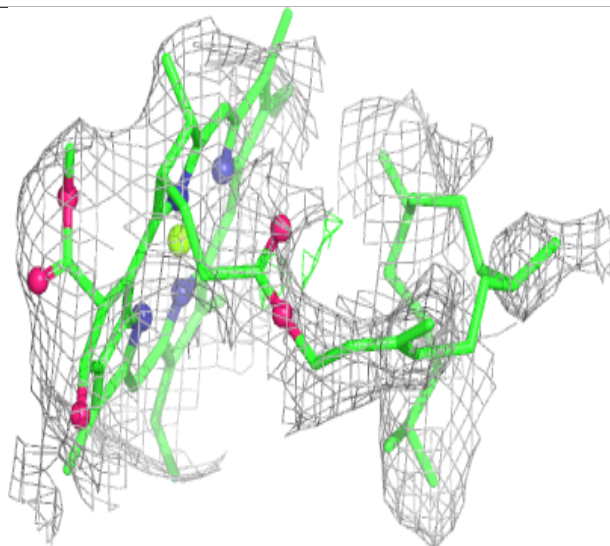
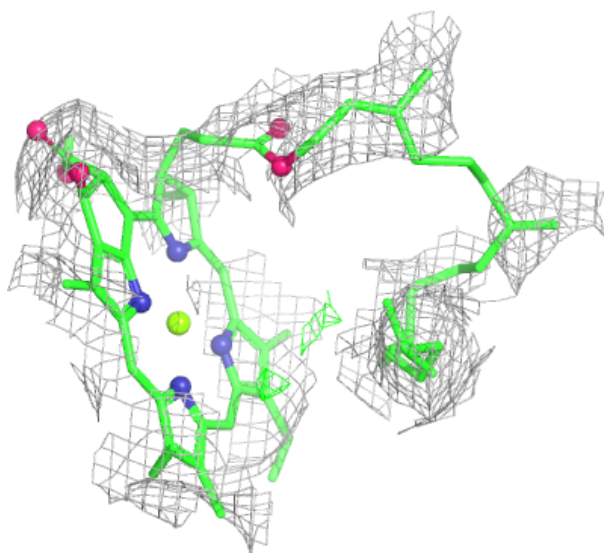
Electron density around CLA 1 1013:

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



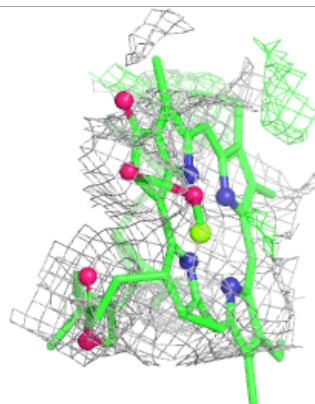
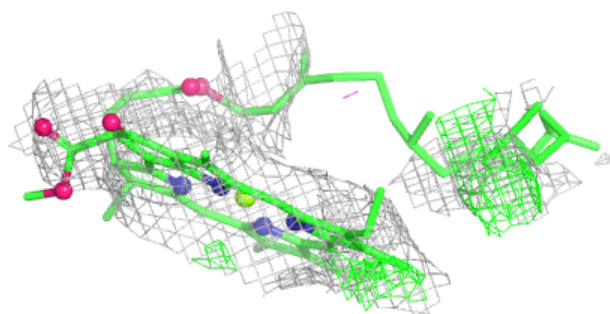
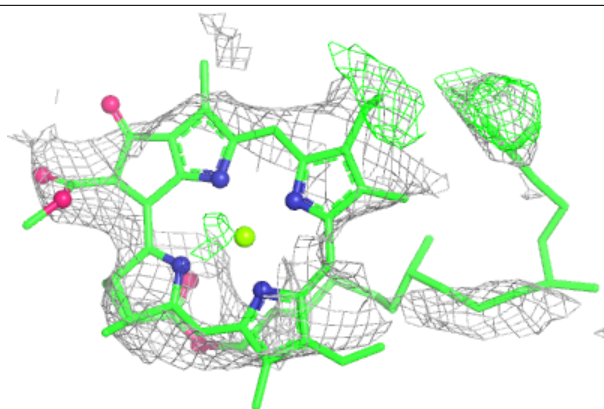
Electron density around CLA 3 3008:

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

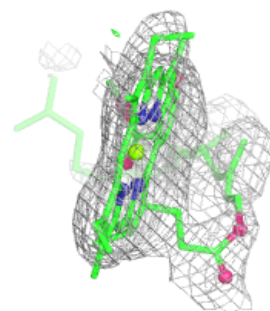
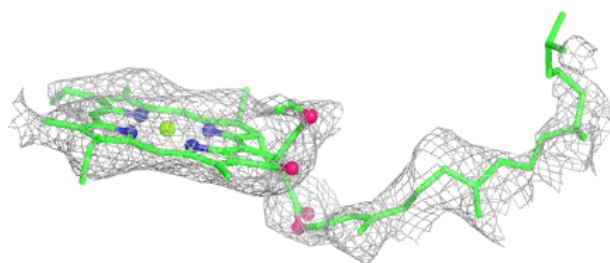
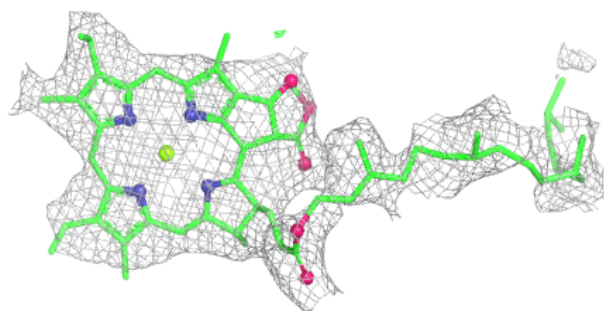


Electron density around CLA 3 3001:

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

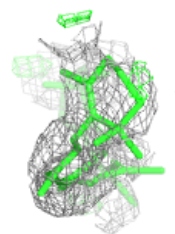
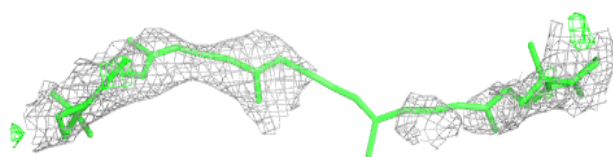
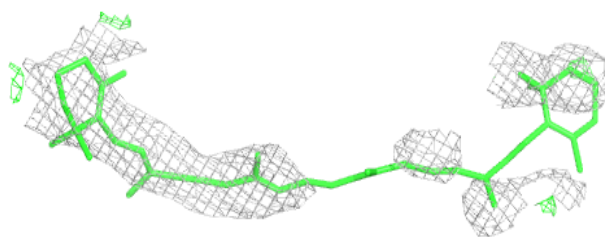
**Electron density around CLA 2 2010:**

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



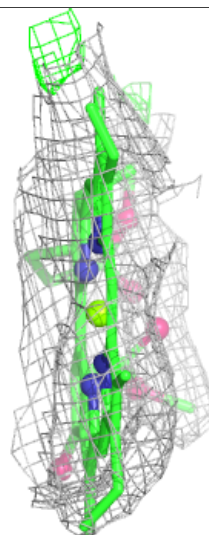
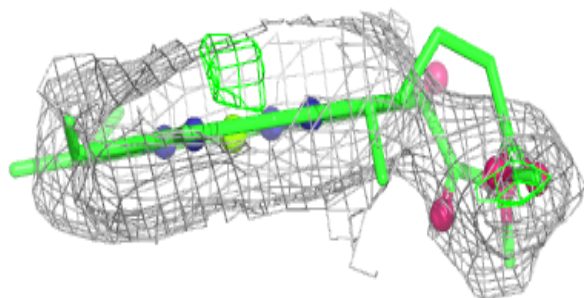
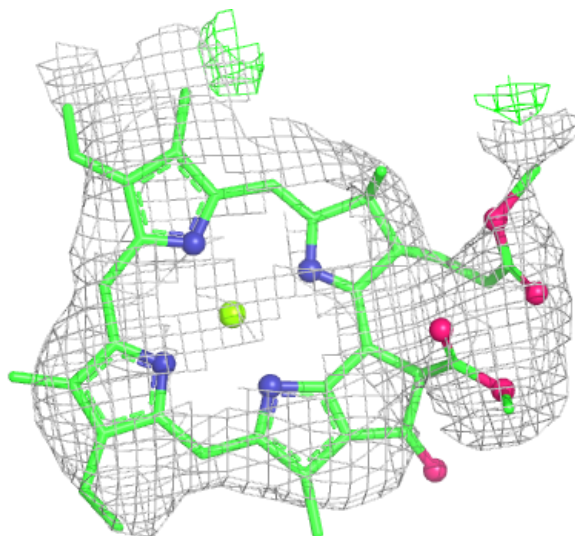
Electron density around BCR J 6013:

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



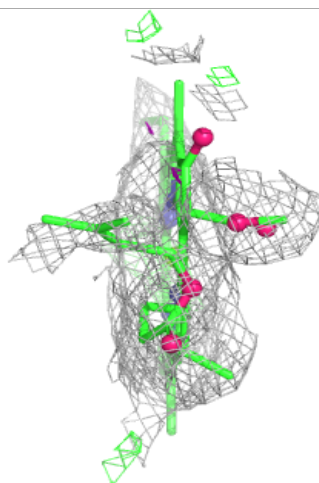
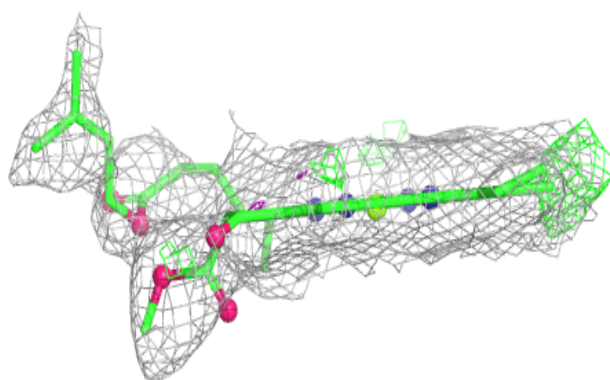
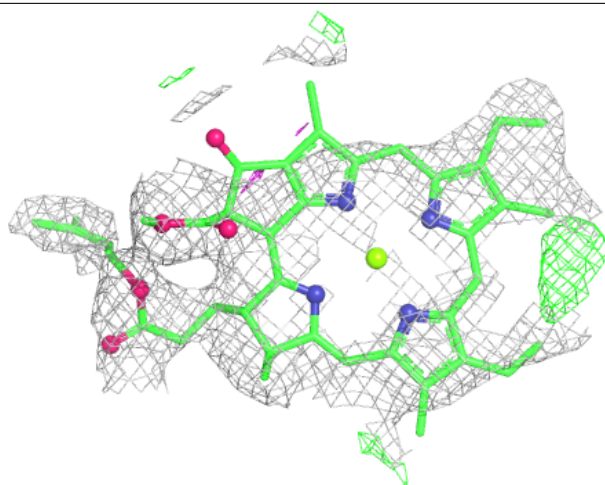
Electron density around CLA 3 3011:

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



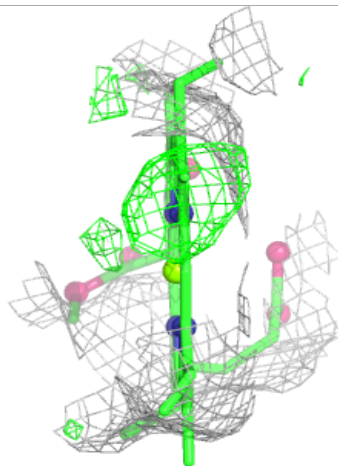
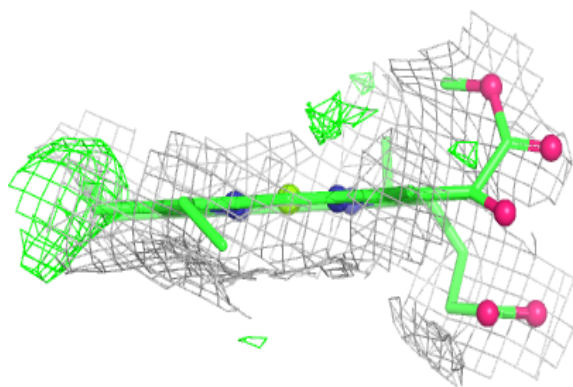
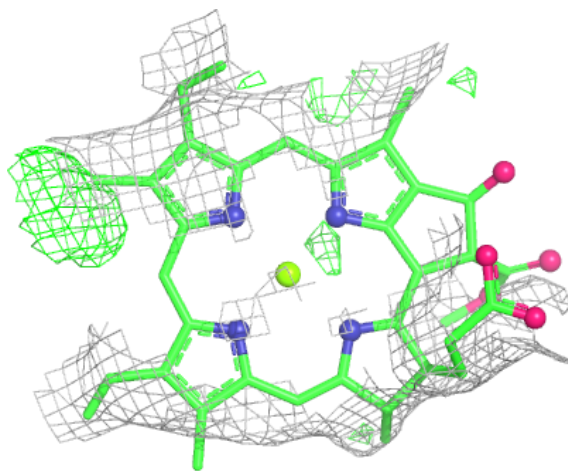
Electron density around CLA 3 3013:

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



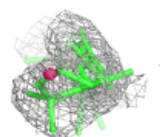
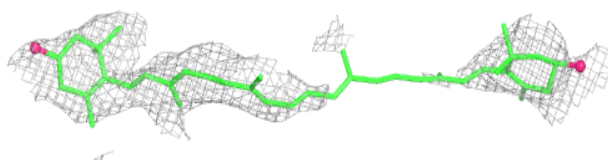
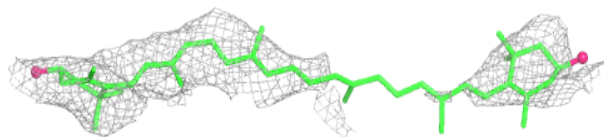
Electron density around CLA 3 3012:

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



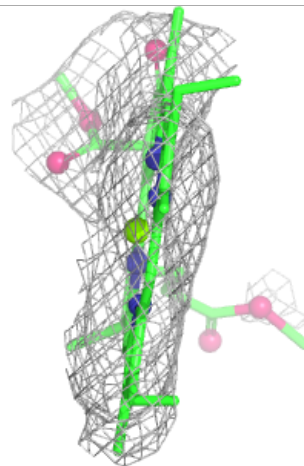
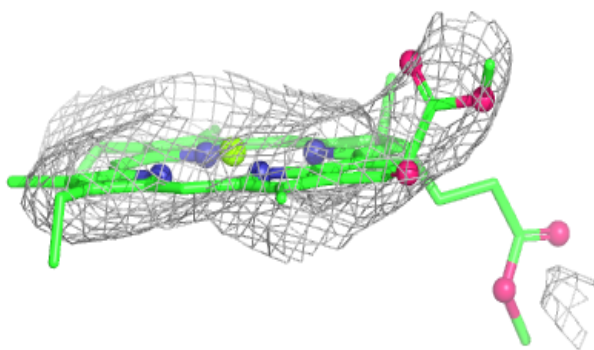
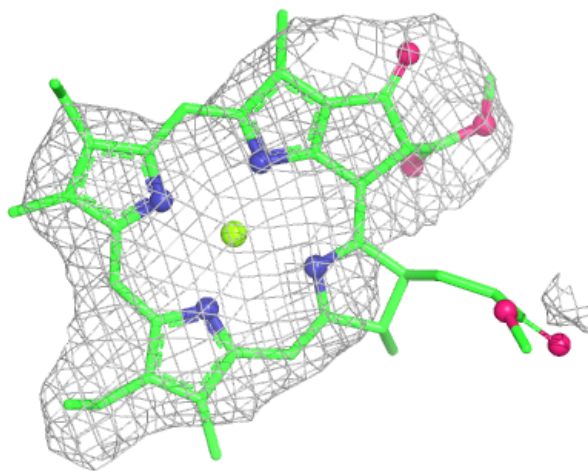
Electron density around LUT 2 2501:

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



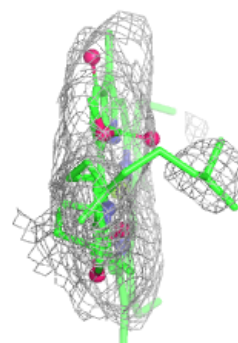
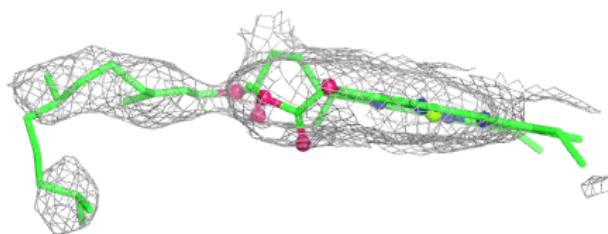
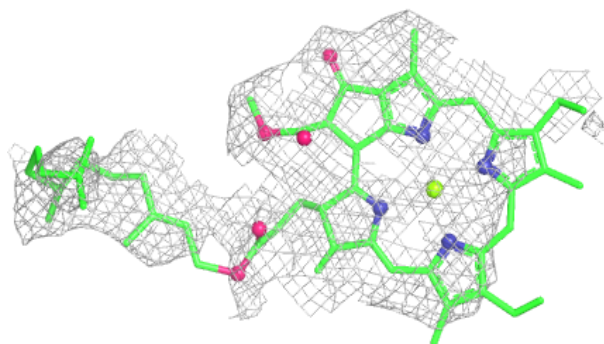
Electron density around CLA A 1120:

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

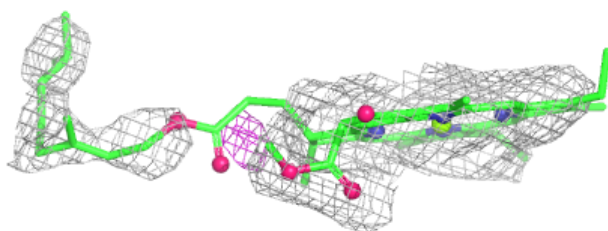
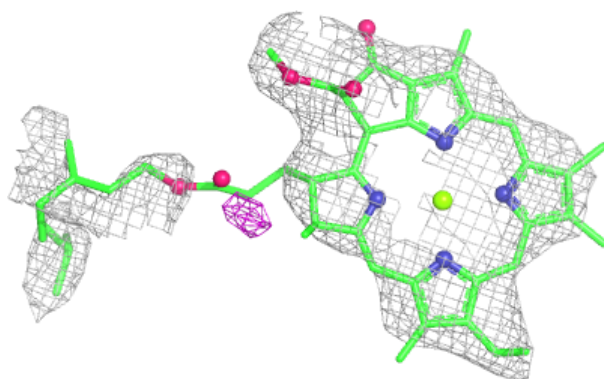


Electron density around CLA 2 2002:

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

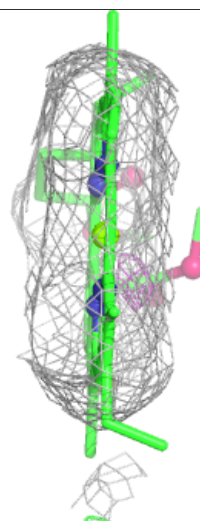
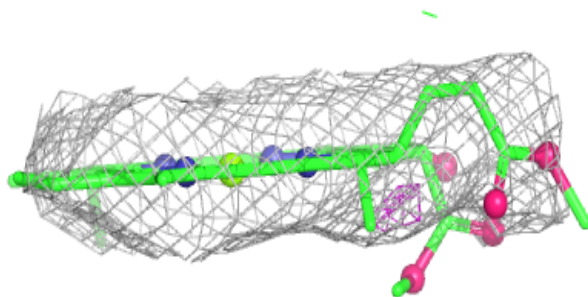
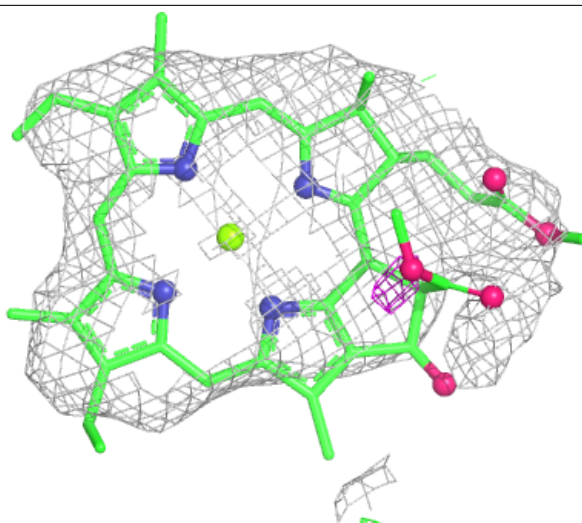
**Electron density around CLA 2 2007:**

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



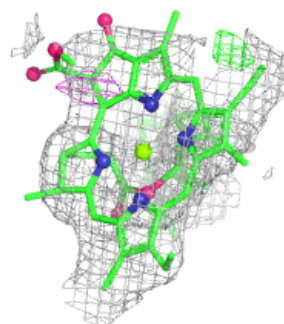
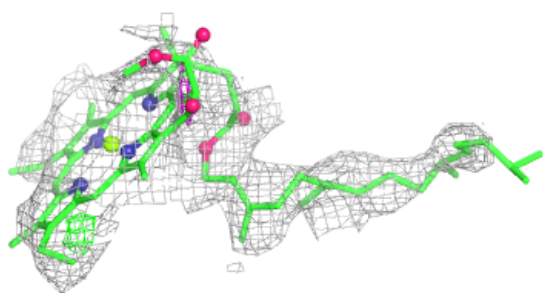
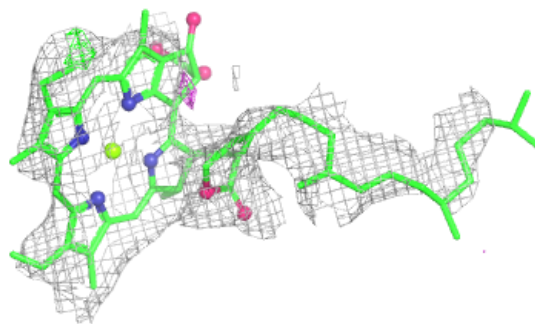
Electron density around CLA 3 3009:

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



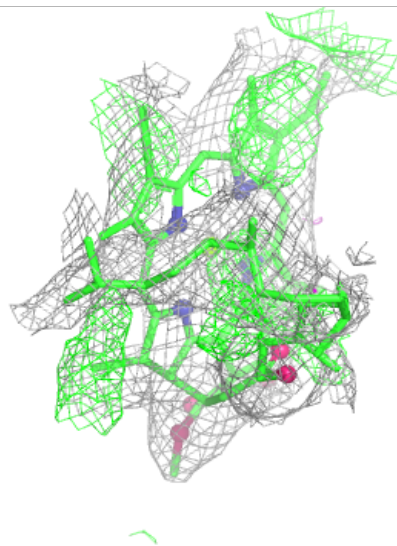
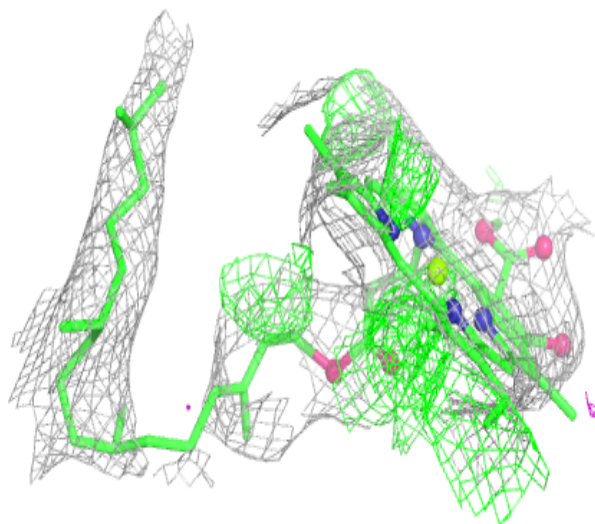
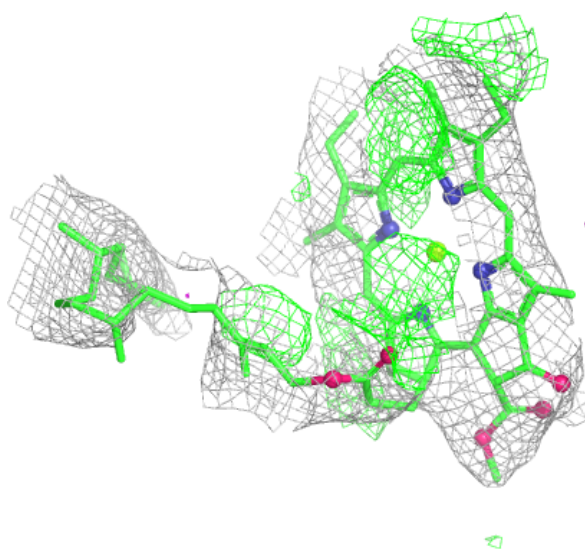
Electron density around CLA 1 1010:

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



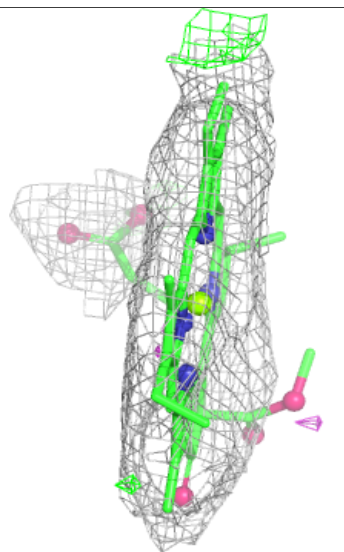
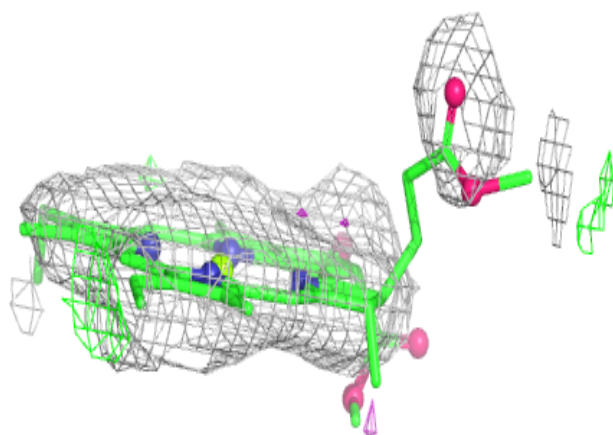
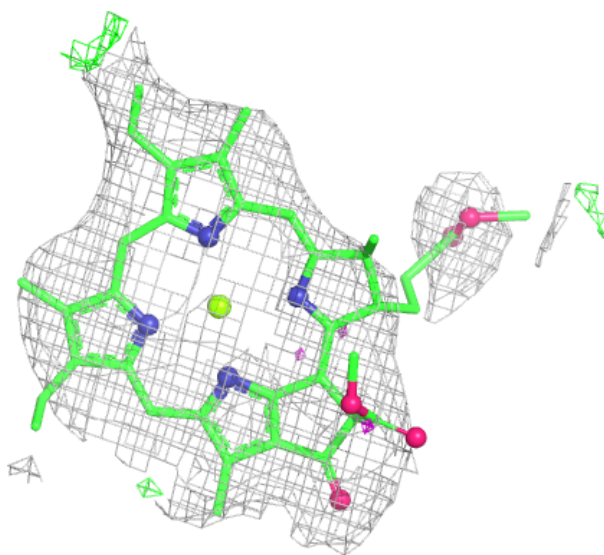
Electron density around CLA 1 1009:

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



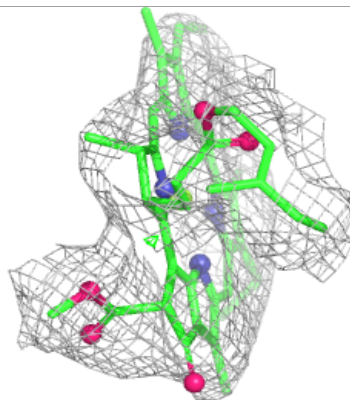
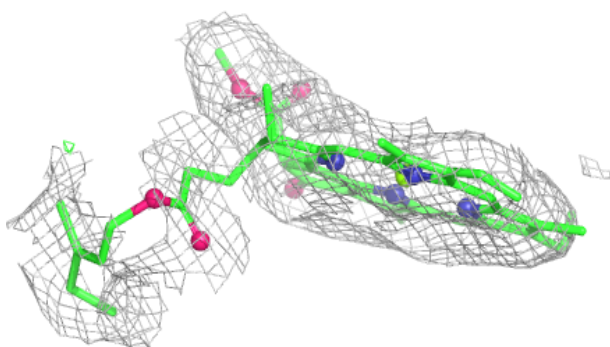
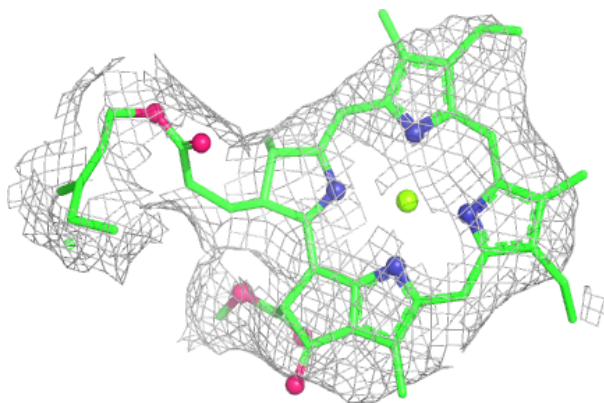
Electron density around CLA 2 2009:

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

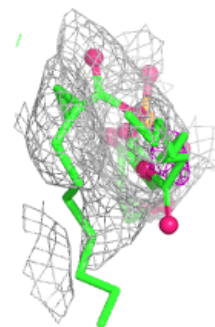
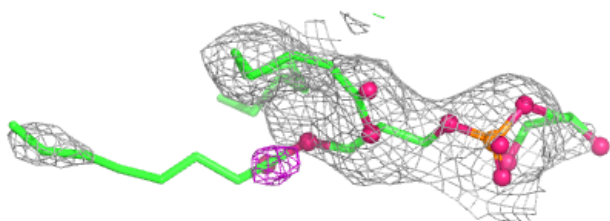


Electron density around CLA A 1141:

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

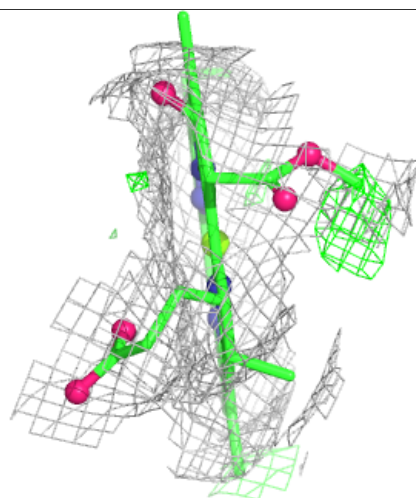
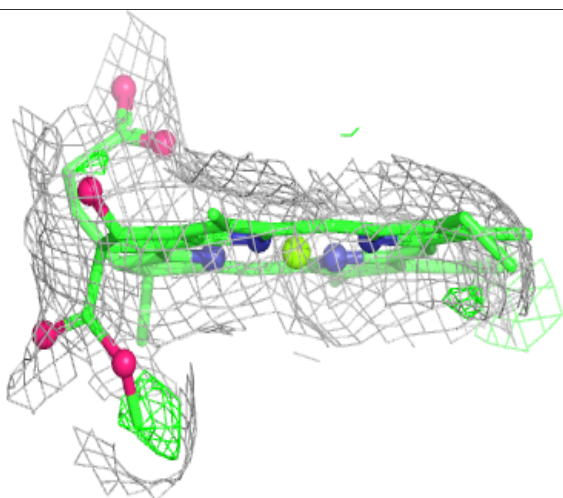
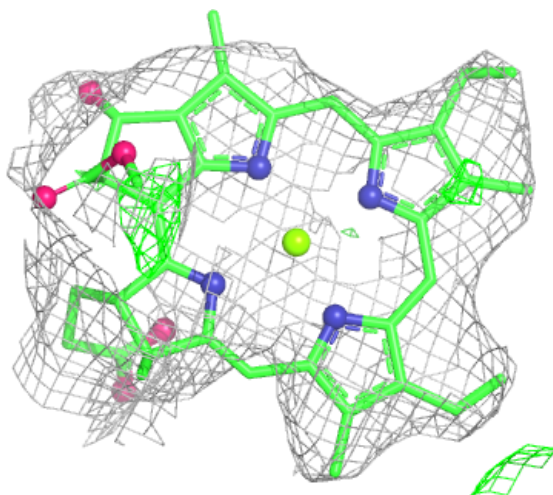
**Electron density around LHG 2 2801:**

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



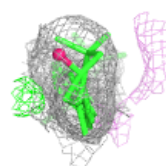
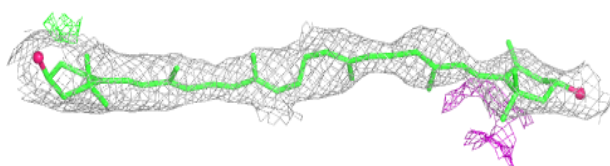
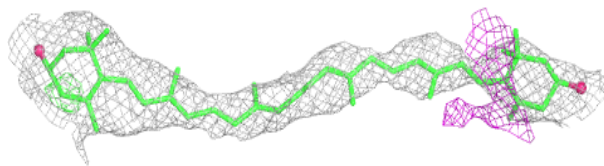
Electron density around CLA 4 4014:

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

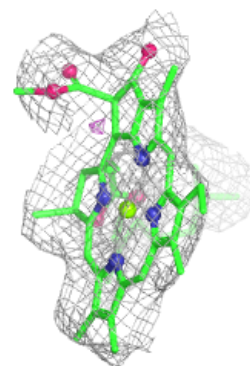
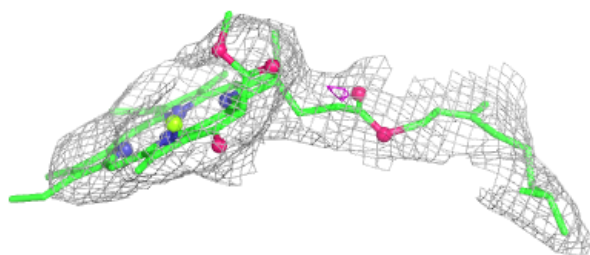
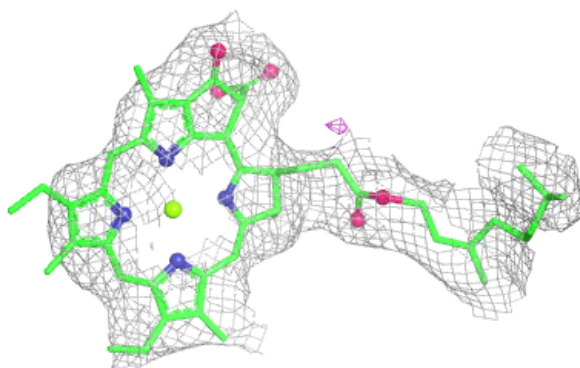


Electron density around LUT 4 4501:

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

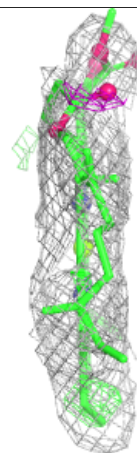
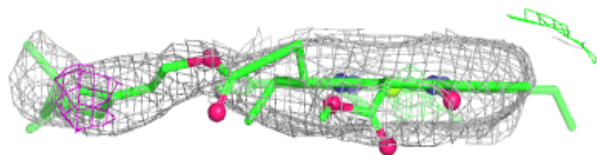
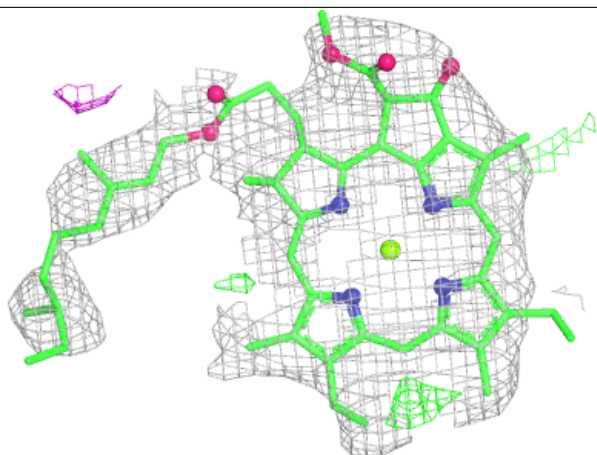
**Electron density around CLA G 1001:**

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



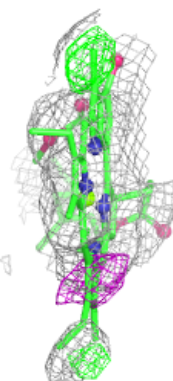
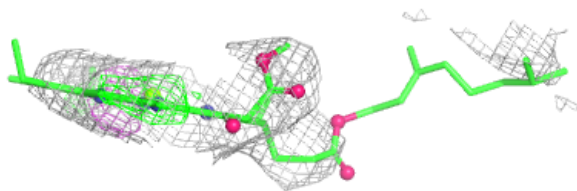
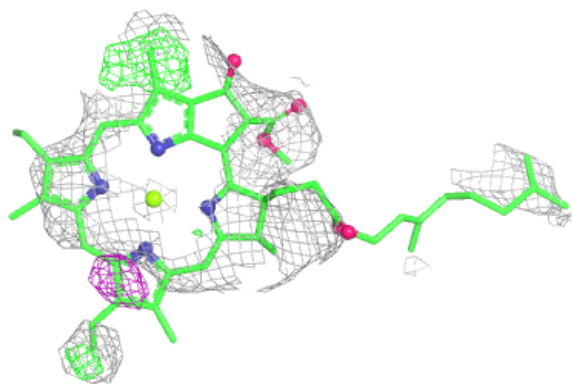
Electron density around CLA 4 4002:

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

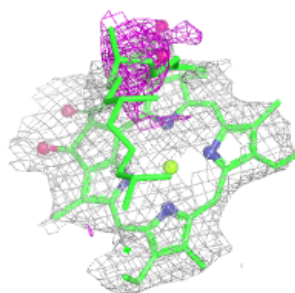
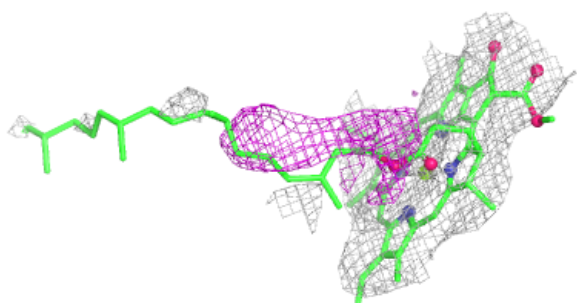
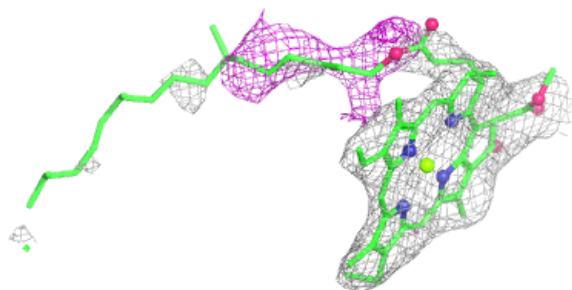


Electron density around CLA A 1110:

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

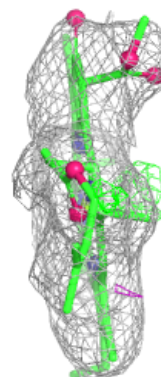
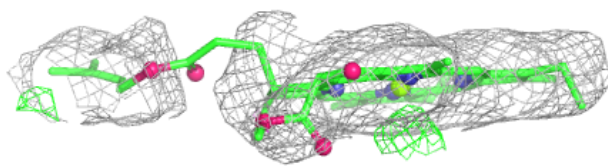
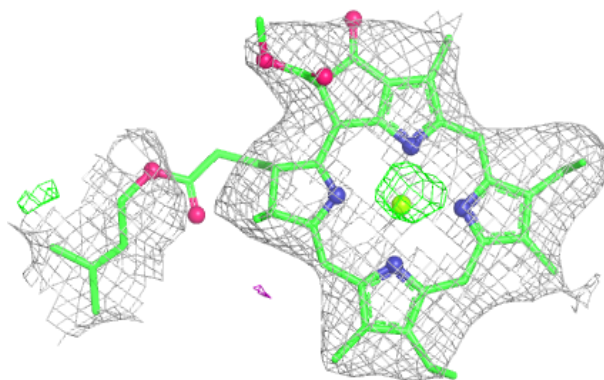
**Electron density around CLA 4 4001:**

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

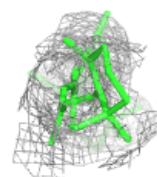
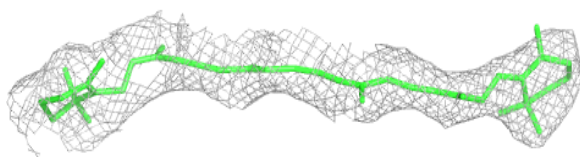
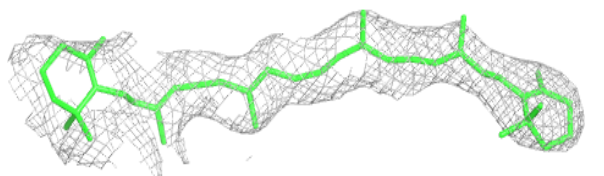


Electron density around CLA 4 4010:

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

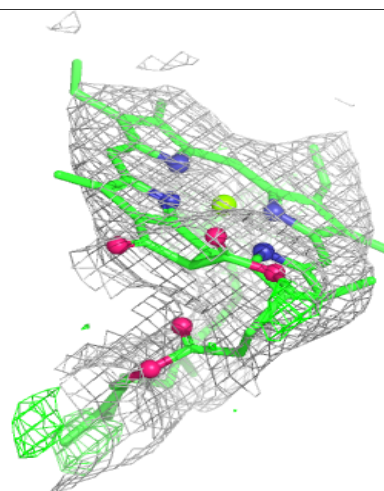
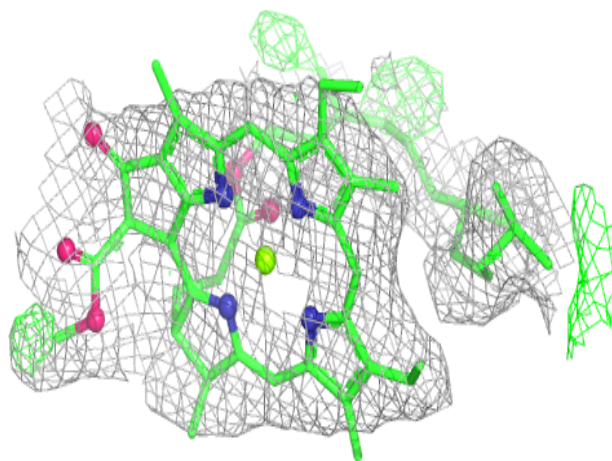
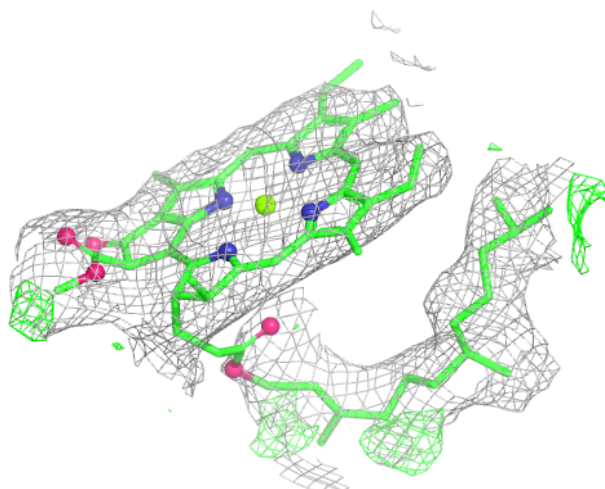
**Electron density around BCR G 2011:**

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



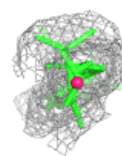
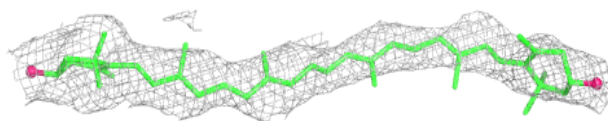
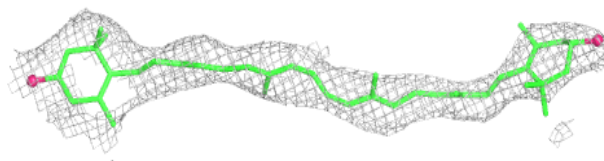
Electron density around CLA 2 2011:

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



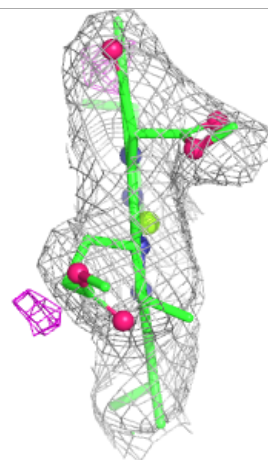
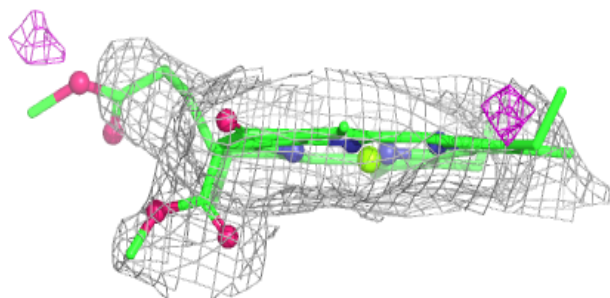
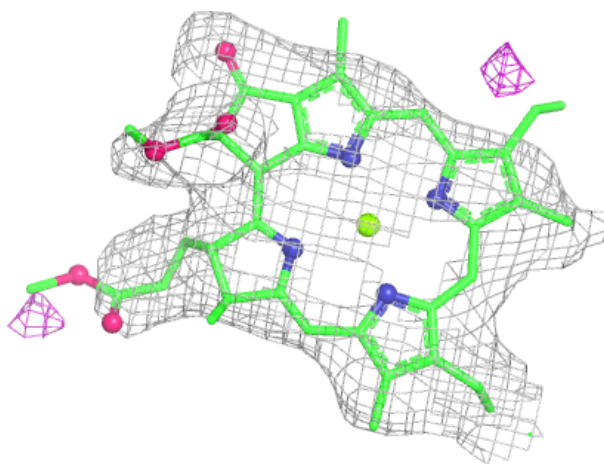
Electron density around LUT 1 1501:

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



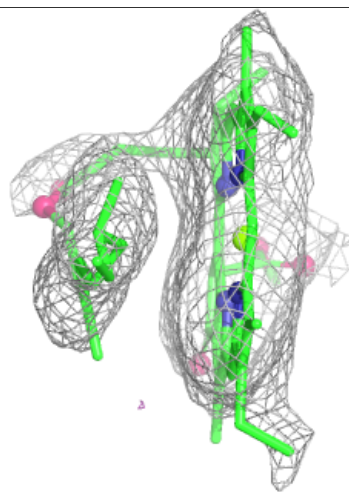
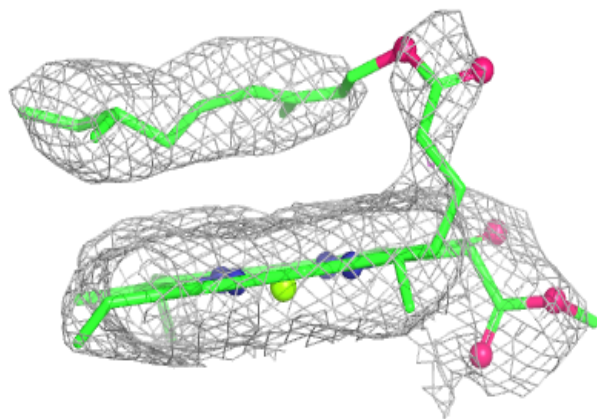
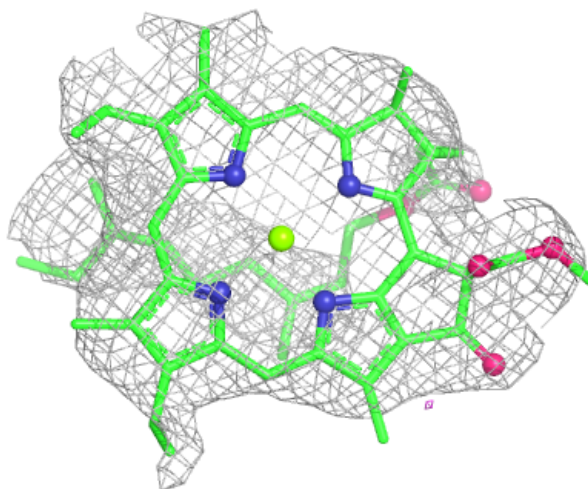
Electron density around CLA H 1000:

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



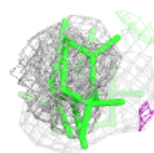
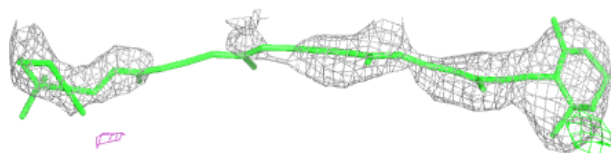
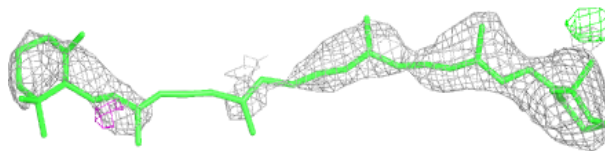
Electron density around CLA A 1115:

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

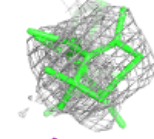
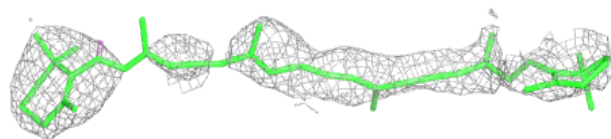
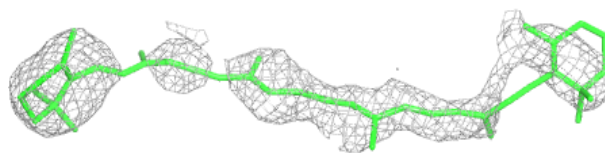


Electron density around BCR A 6003:

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

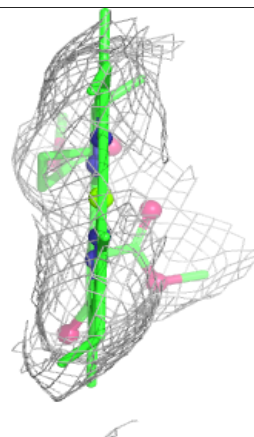
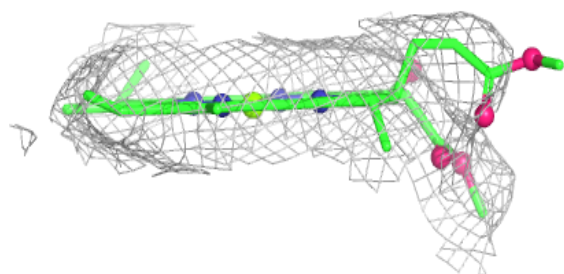
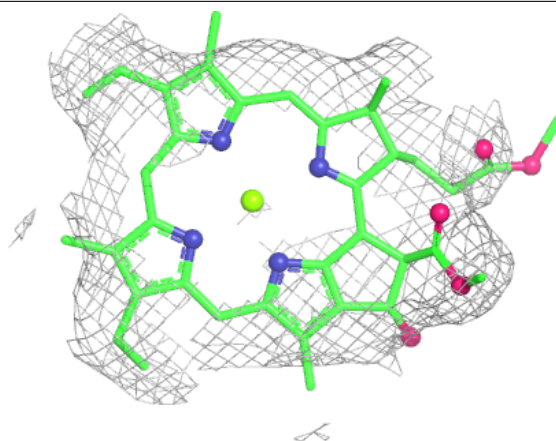
**Electron density around BCR A 6002:**

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



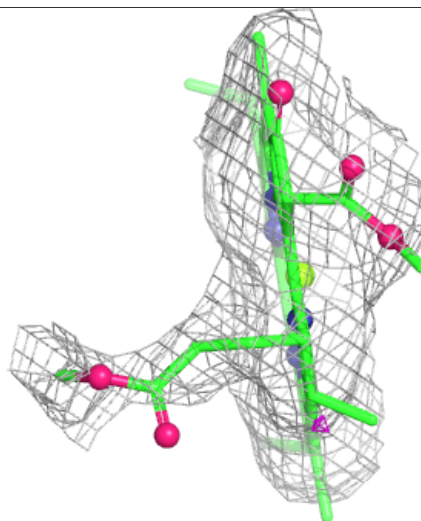
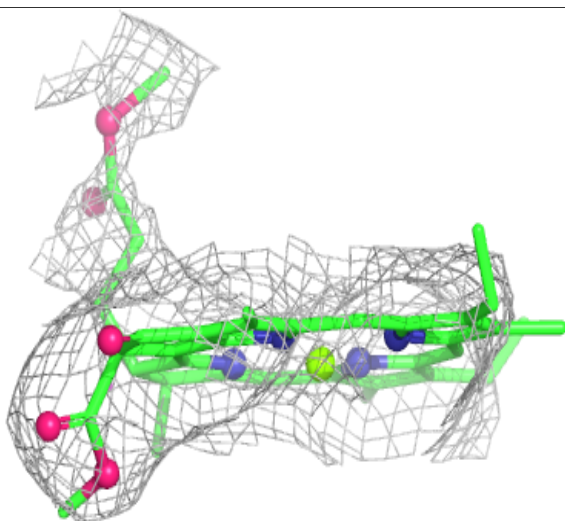
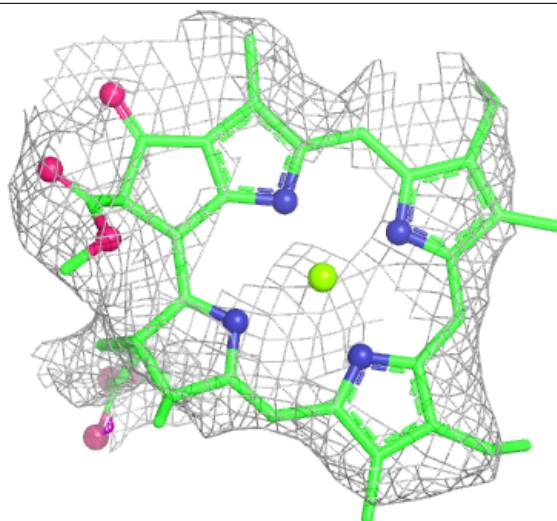
Electron density around CLA G 1002:

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



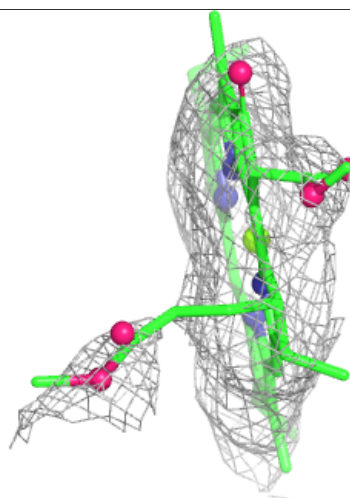
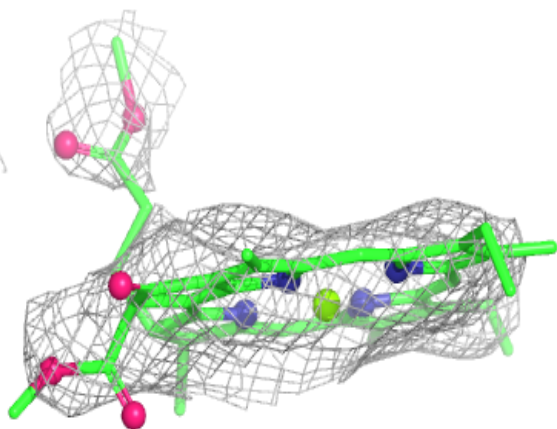
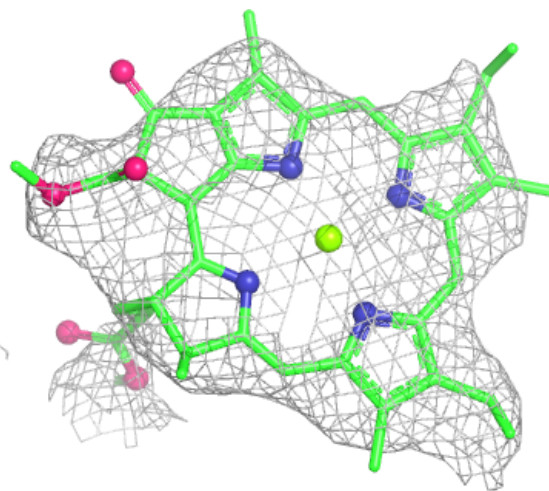
Electron density around CLA A 1121:

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



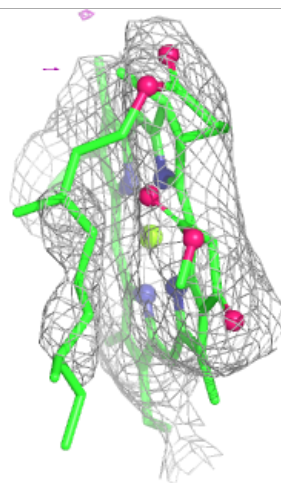
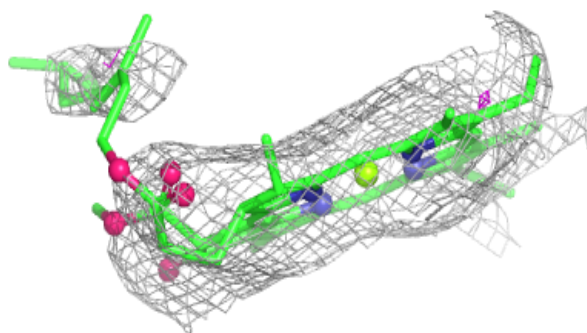
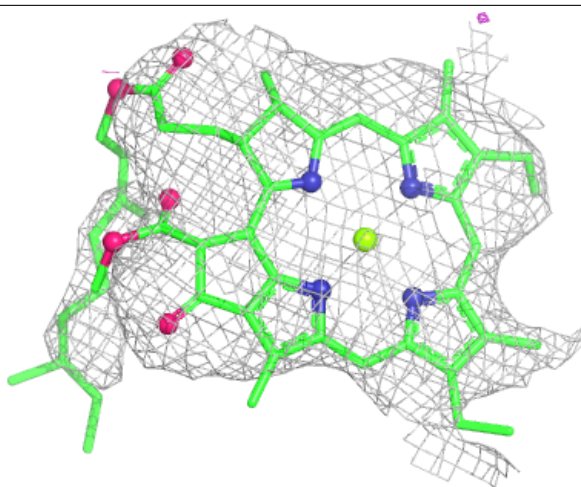
Electron density around CLA A 1108:

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



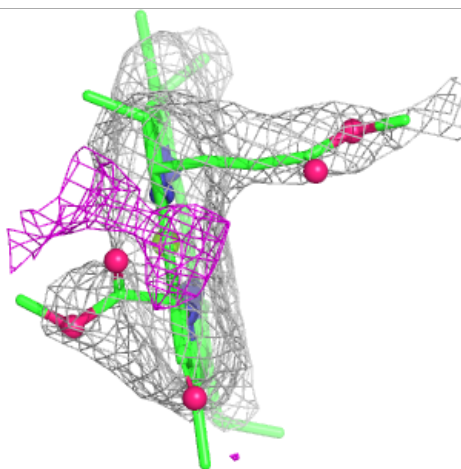
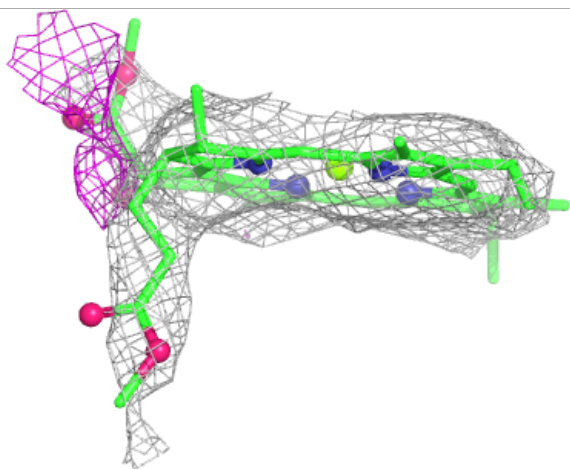
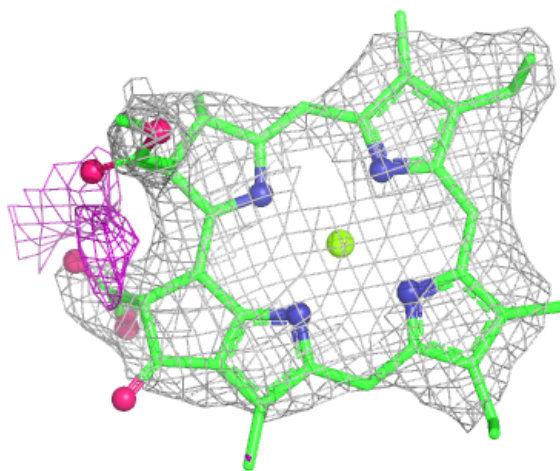
Electron density around CLA 1 1002:

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



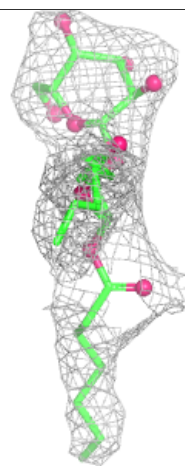
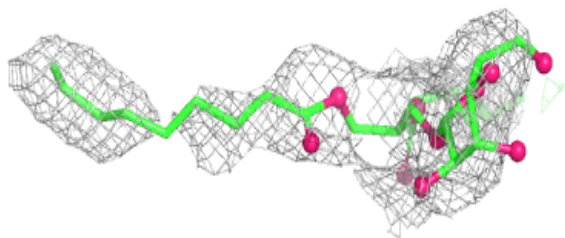
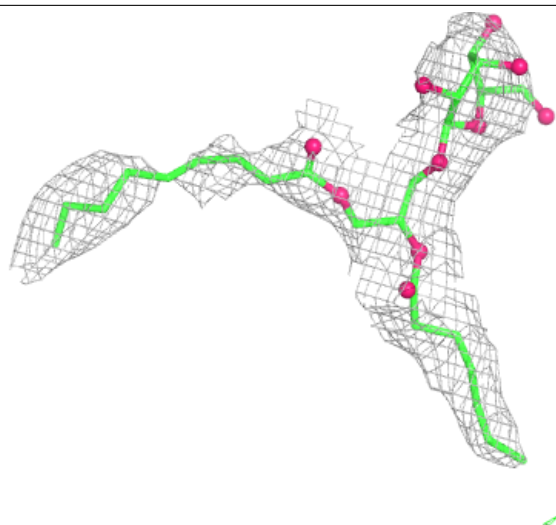
Electron density around CLA B 1212:

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



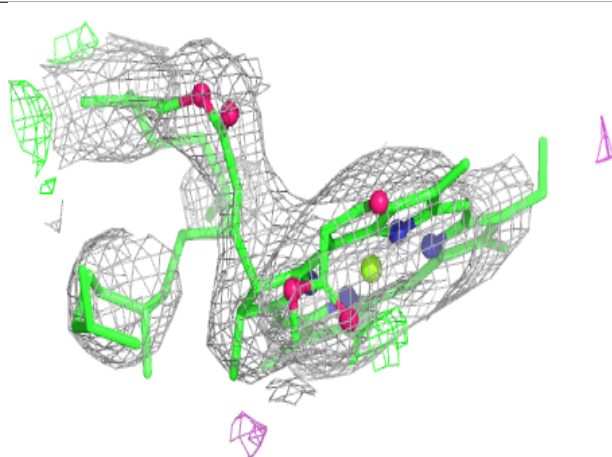
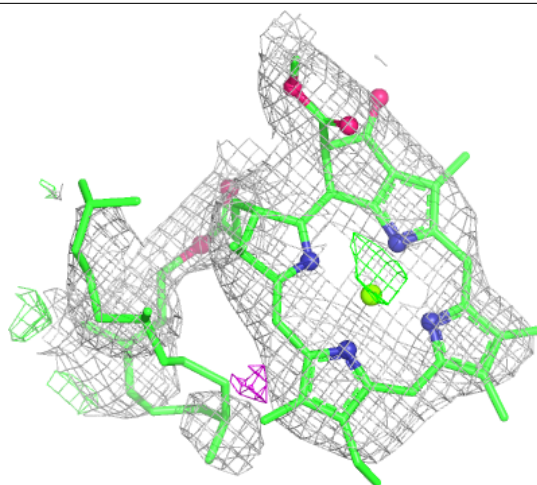
Electron density around LMG J 5001:

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



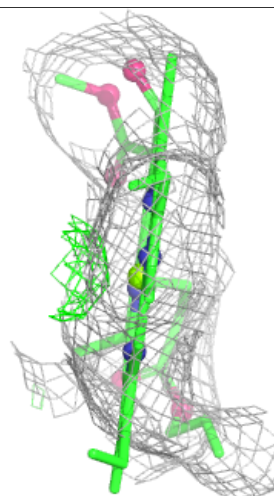
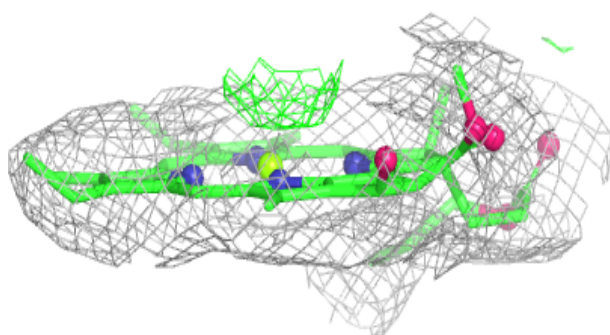
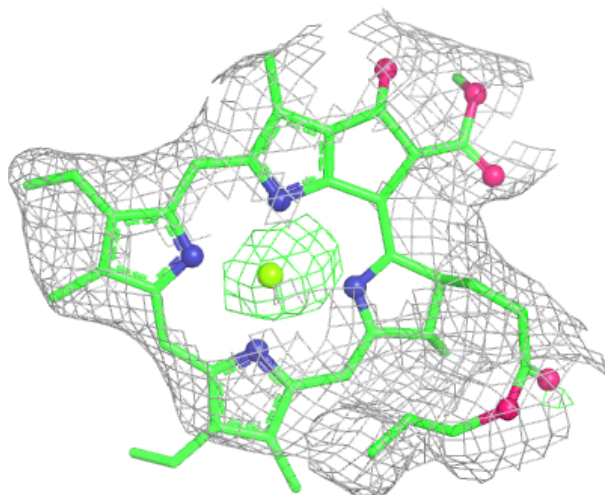
Electron density around CLA 1 1011:

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



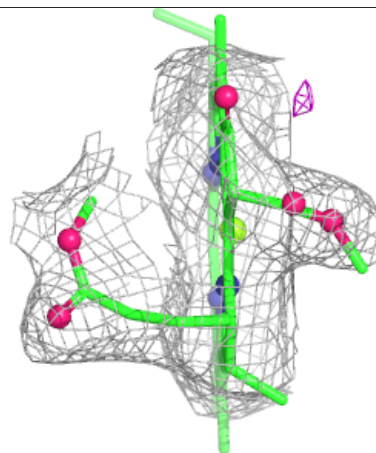
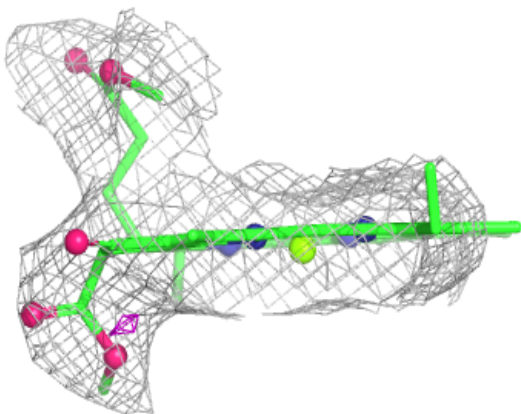
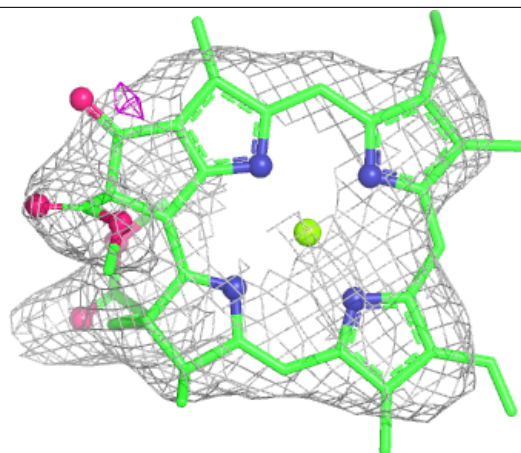
Electron density around CLA 4 4008:

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



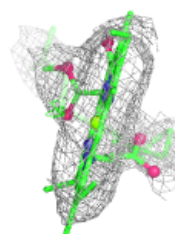
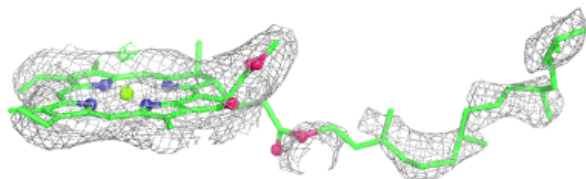
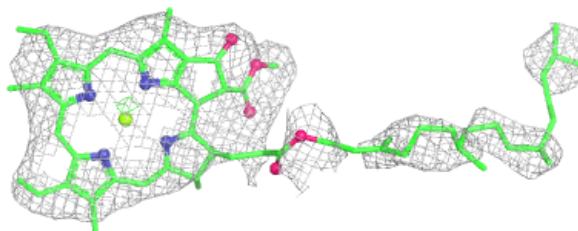
Electron density around CLA A 1114:

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



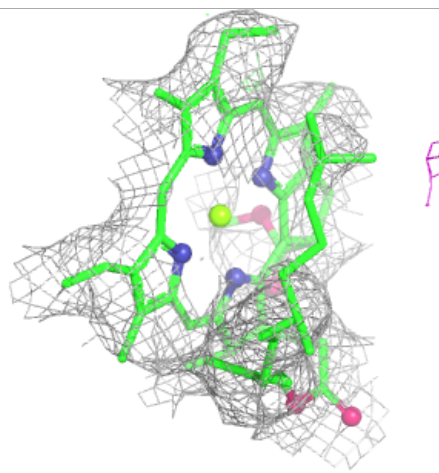
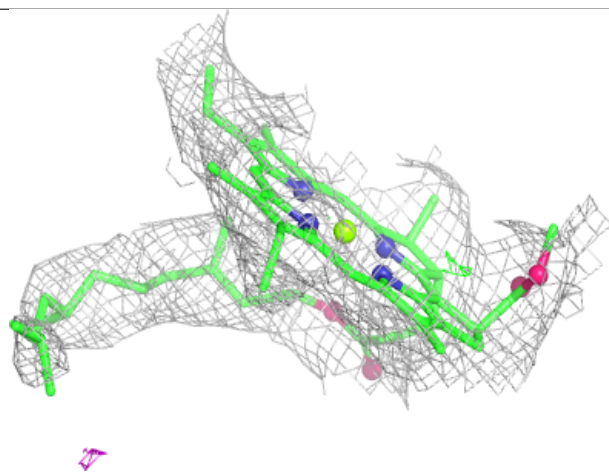
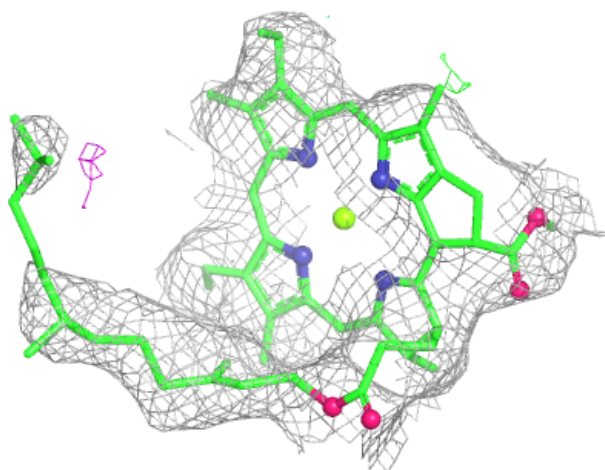
Electron density around CLA 2 2013:

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



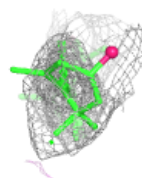
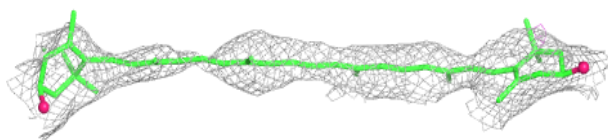
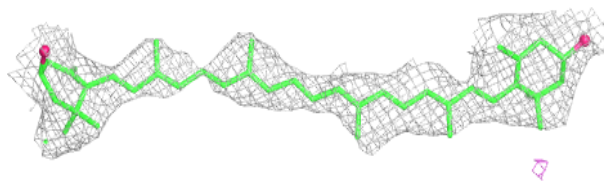
Electron density around CLA 2 2004:

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



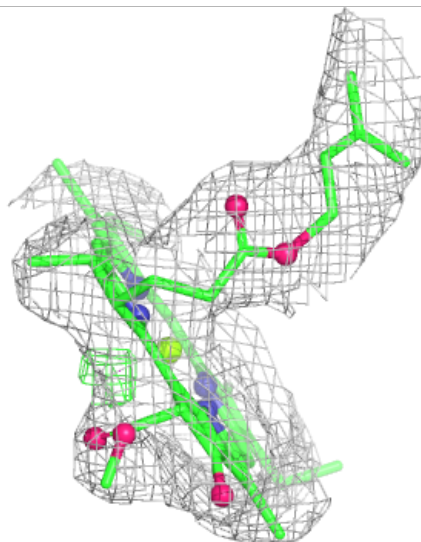
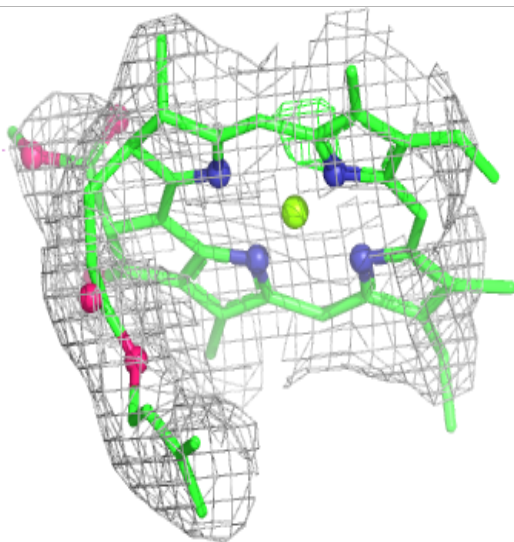
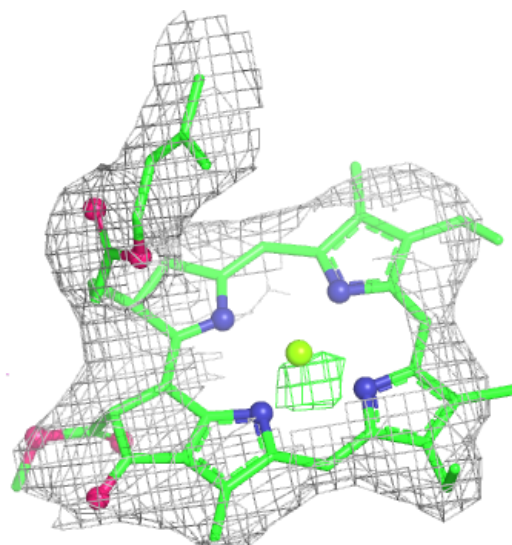
Electron density around LUT 2 2502:

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



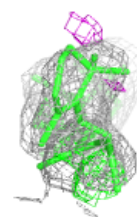
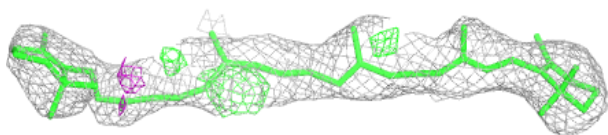
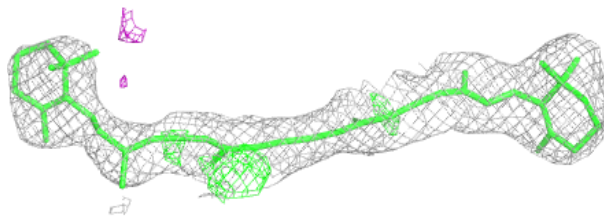
Electron density around CLA L 1503:

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

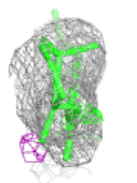
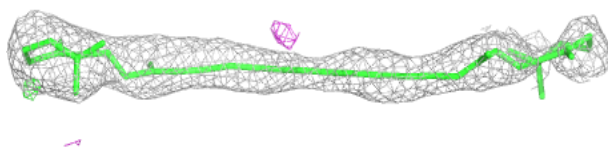
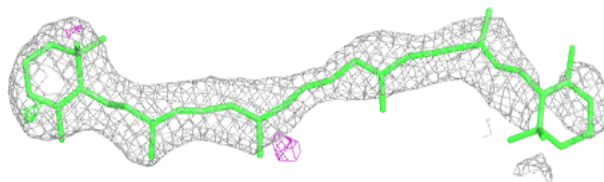


Electron density around BCR B 6010:

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

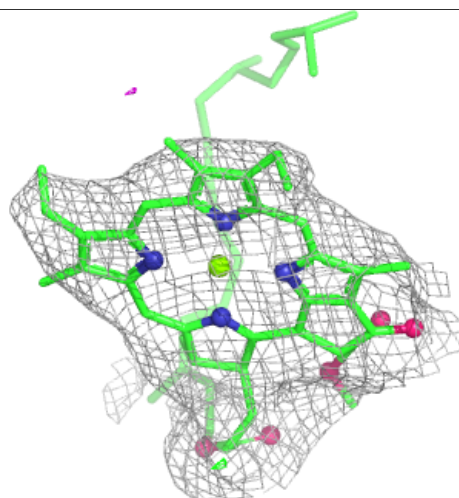
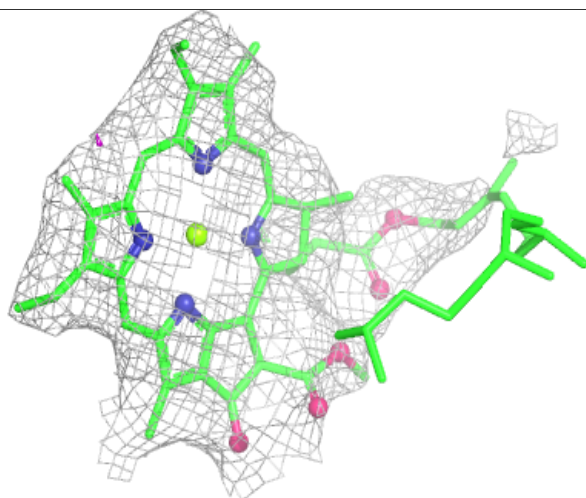
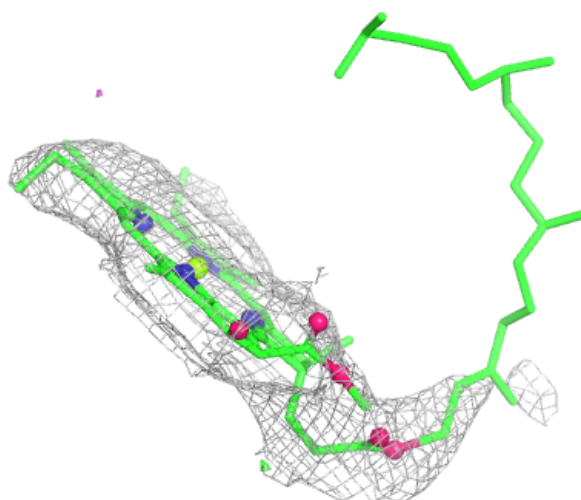
**Electron density around BCR B 6005:**

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



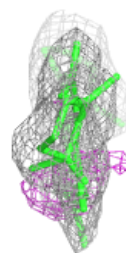
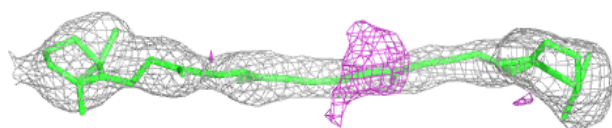
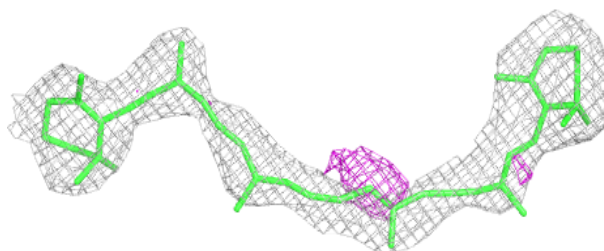
Electron density around CLA 2 2005:

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

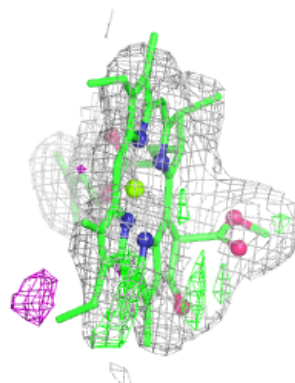
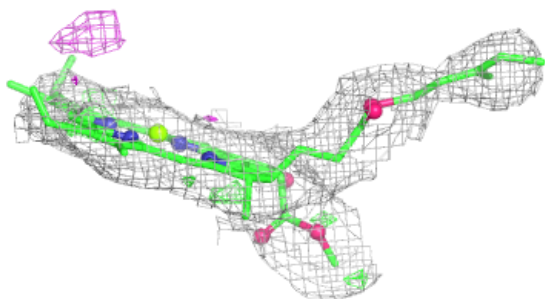
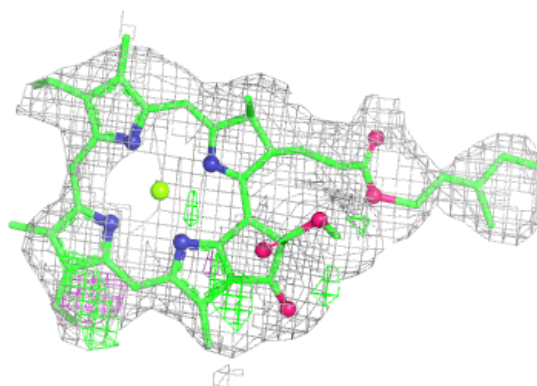


Electron density around BCR A 6011:

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

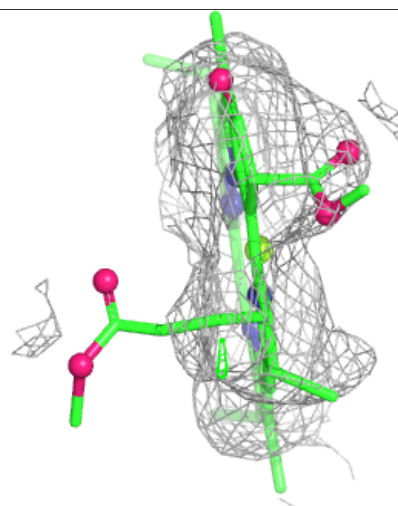
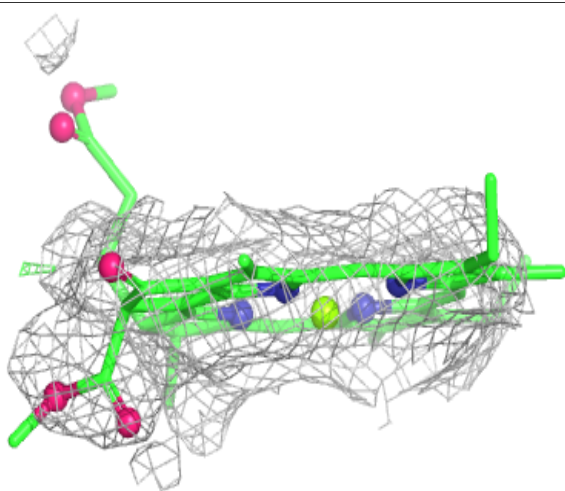
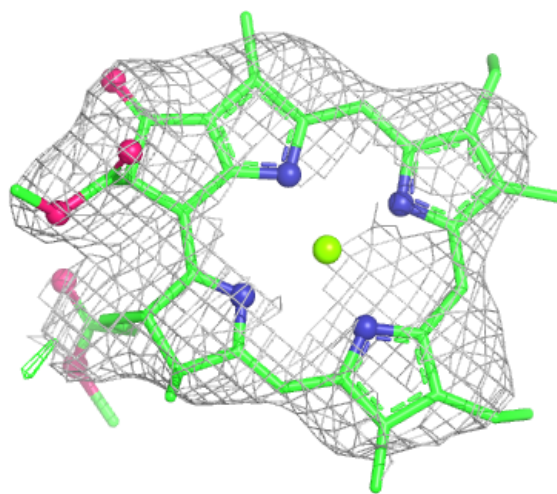
**Electron density around CLA A 1107:**

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



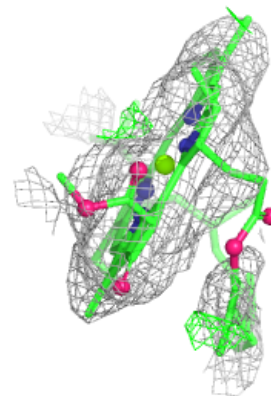
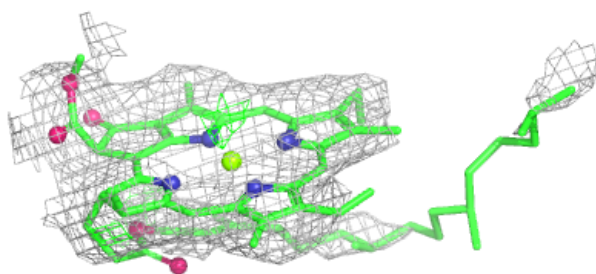
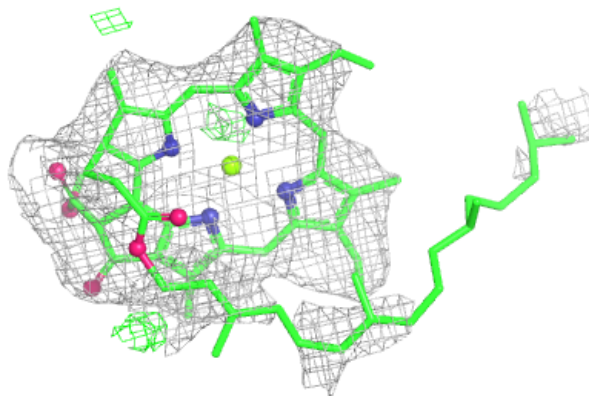
Electron density around CLA A 1134:

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



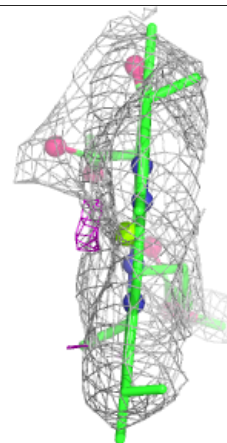
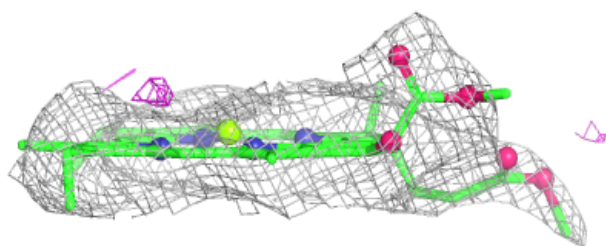
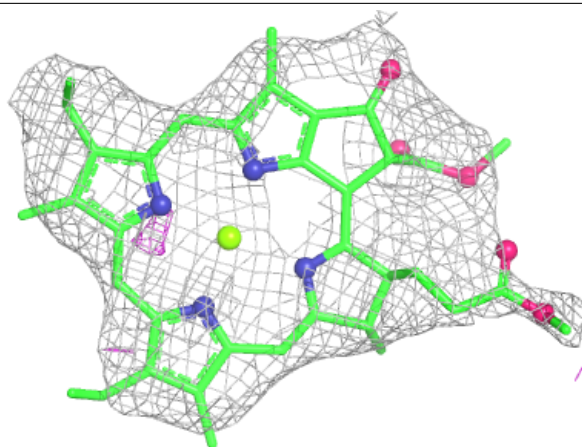
Electron density around CLA 1 1008:

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

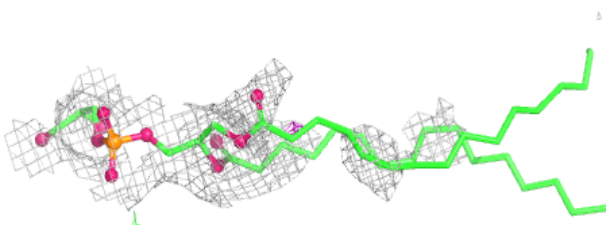
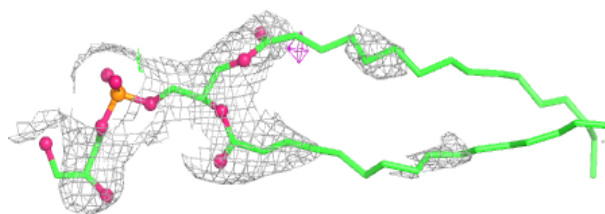


Electron density around CLA F 1302:

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

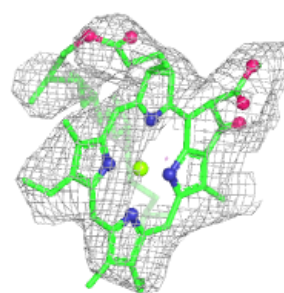
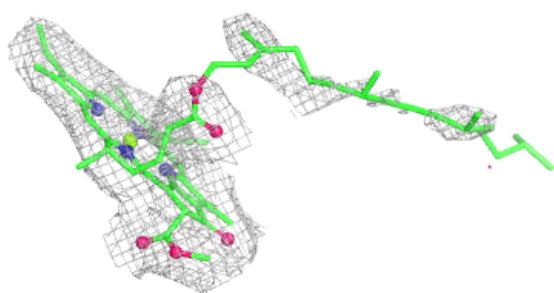
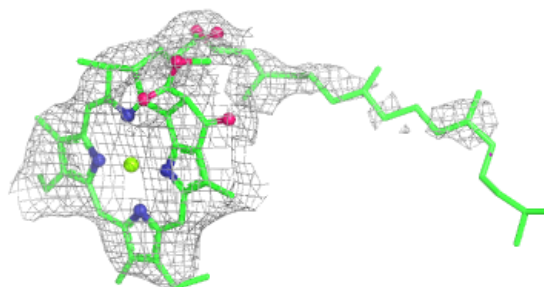
**Electron density around LHG B 7004:**

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



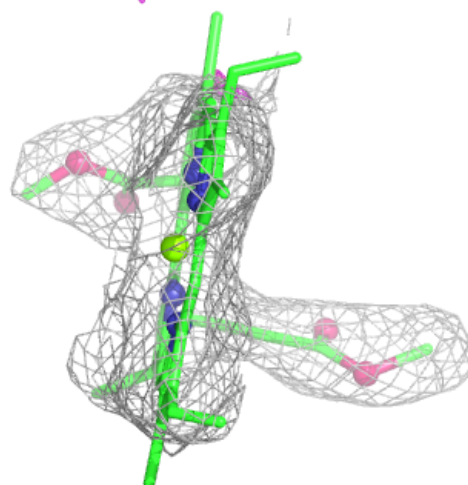
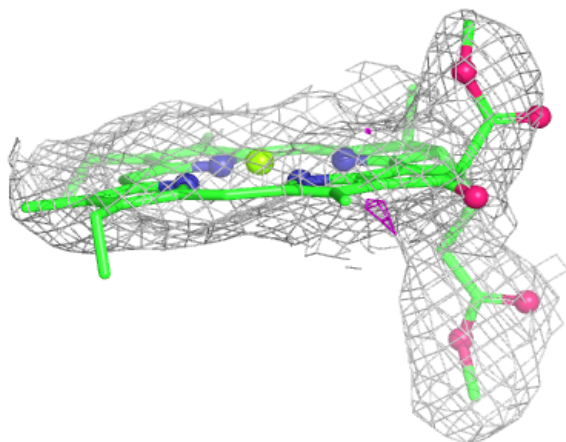
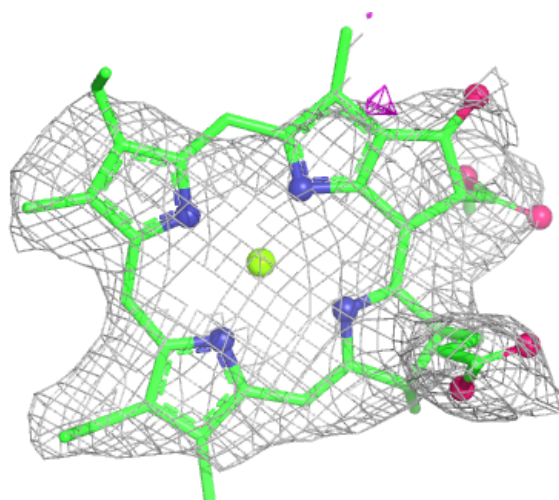
Electron density around CLA 2 2012:

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



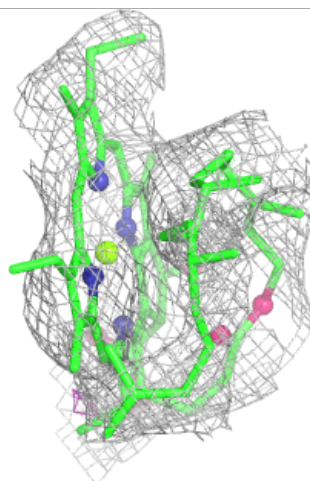
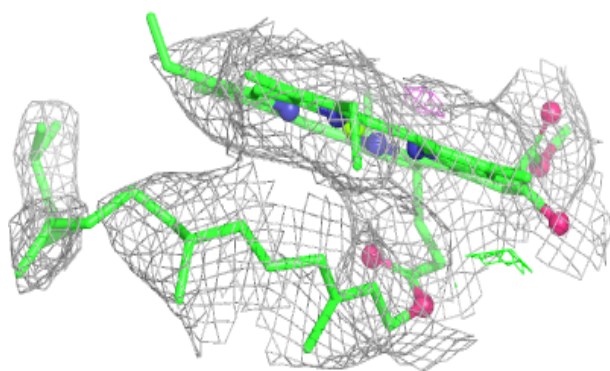
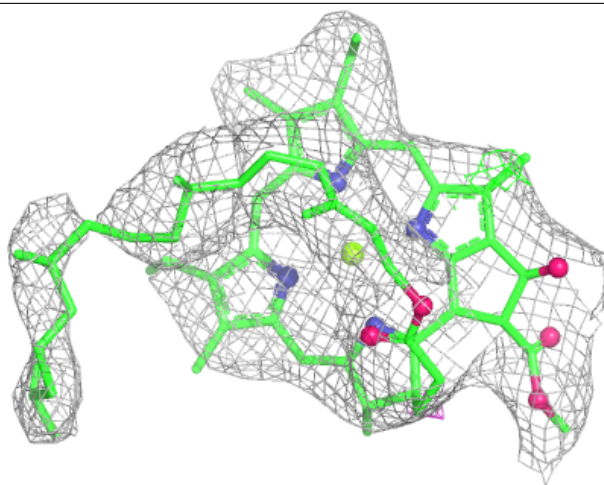
Electron density around CLA A 1112:

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



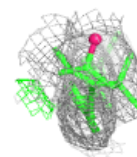
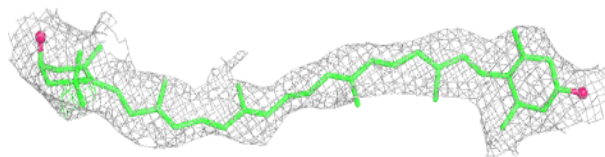
Electron density around CLA 1 1003:

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

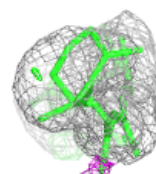
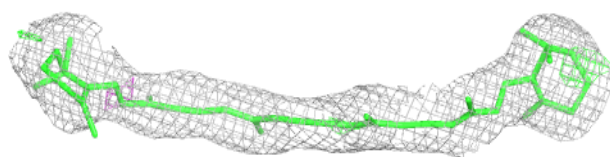


Electron density around LUT 4 4502:

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

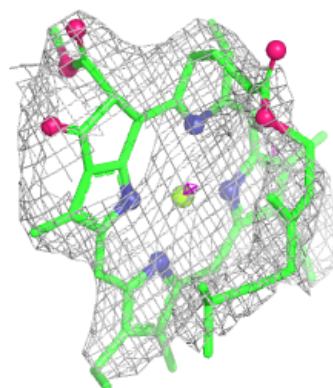
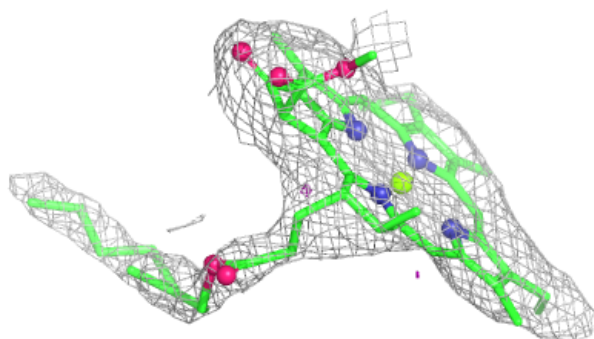
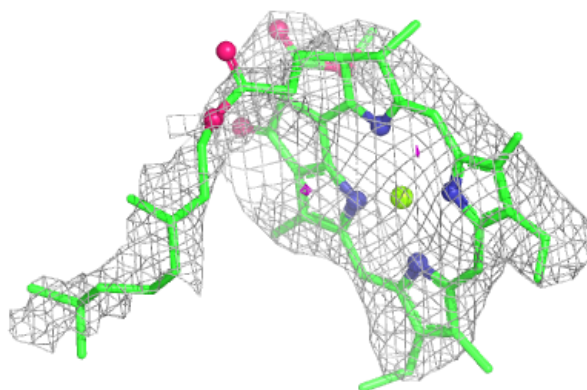
**Electron density around BCR I 6018:**

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

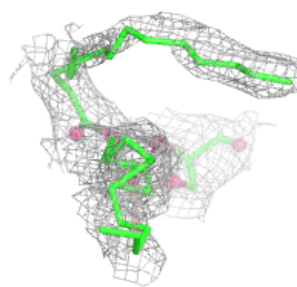
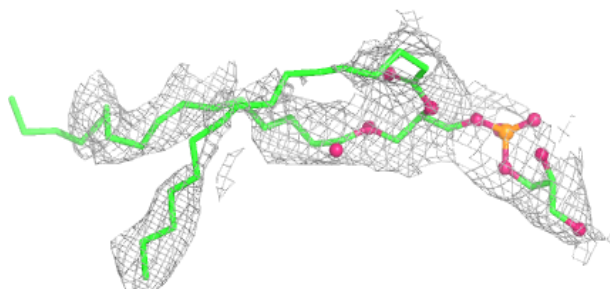
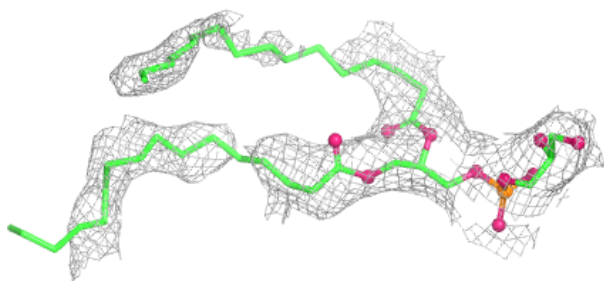


Electron density around CLA 1 1007:

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

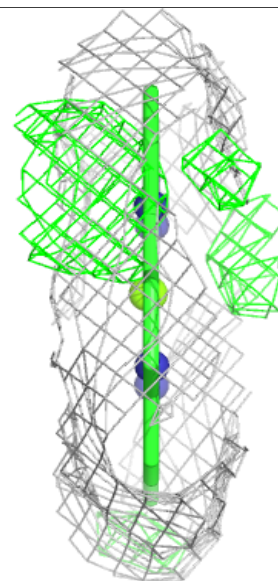
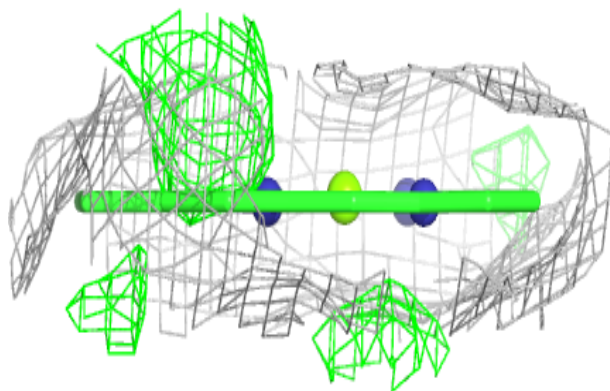
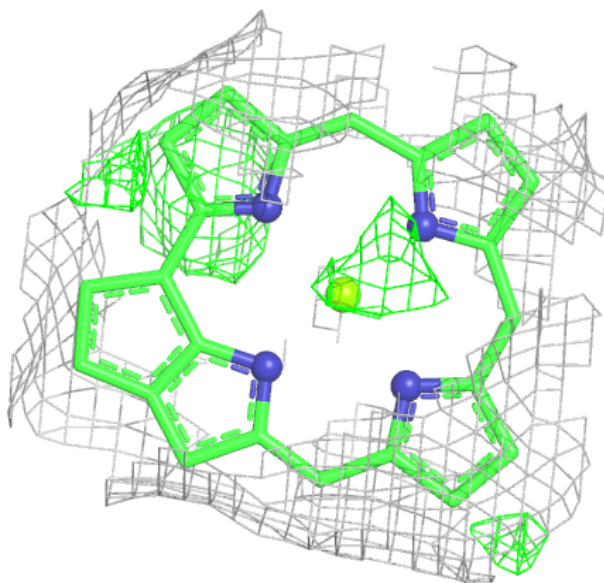
**Electron density around LHG A 7003:**

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



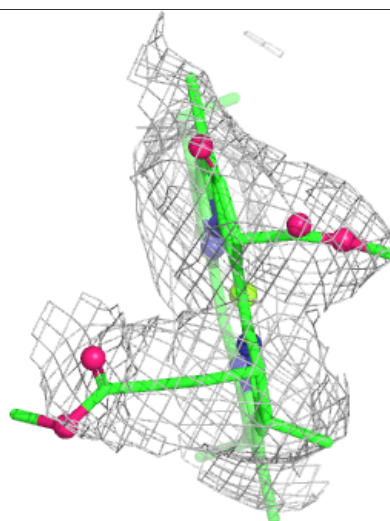
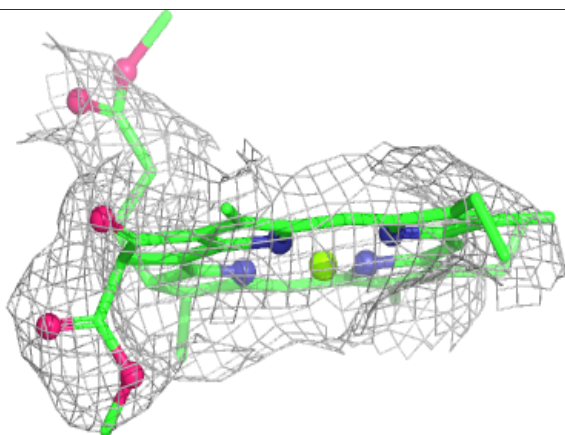
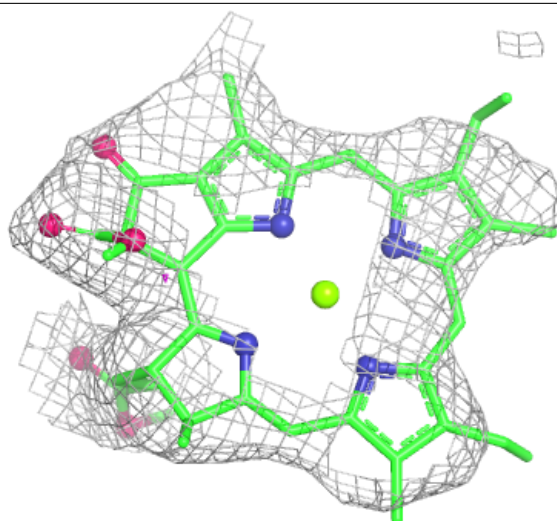
Electron density around CLA 2 2001:

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



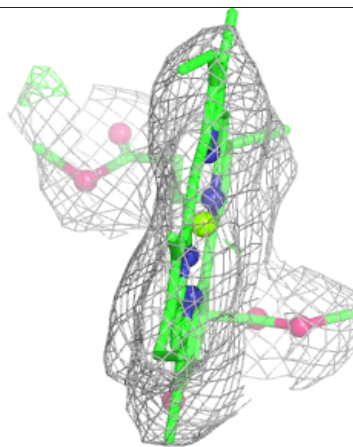
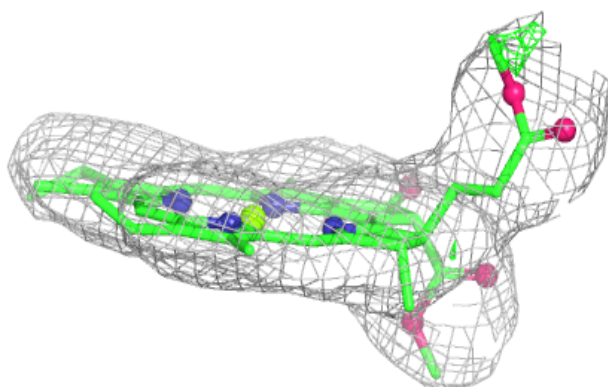
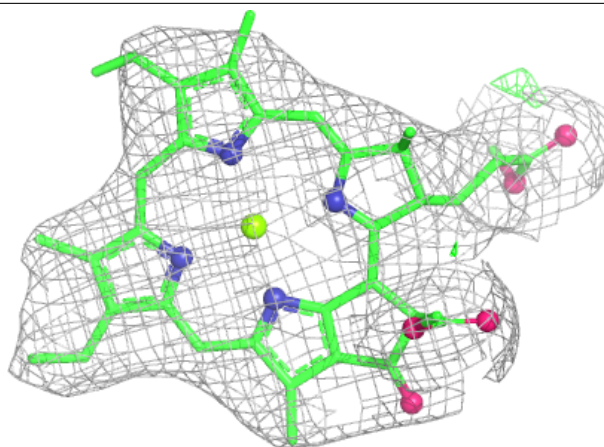
Electron density around CLA A 1118:

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



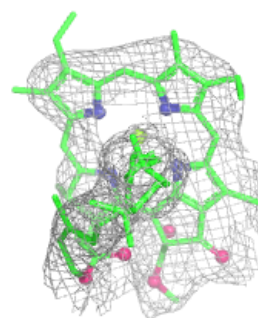
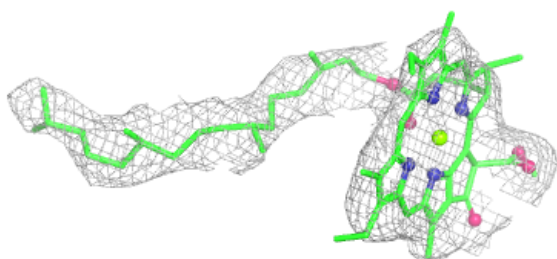
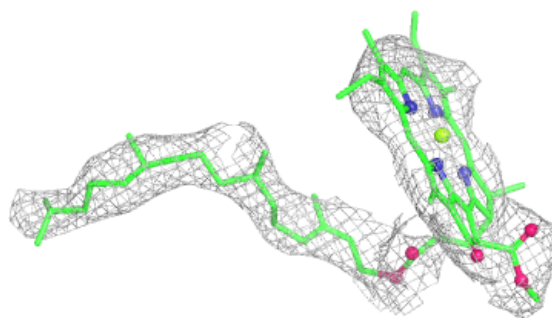
Electron density around CLA 4 4015:

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

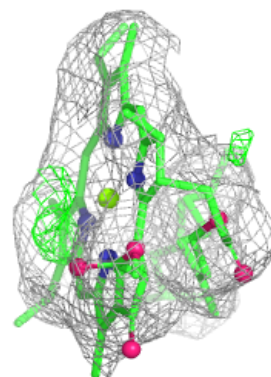
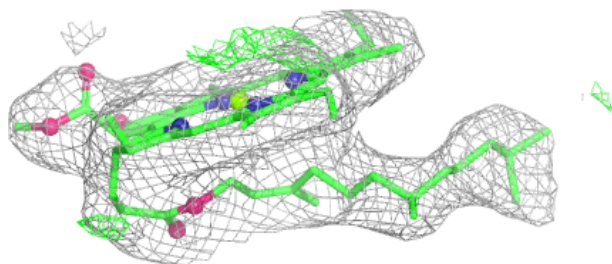
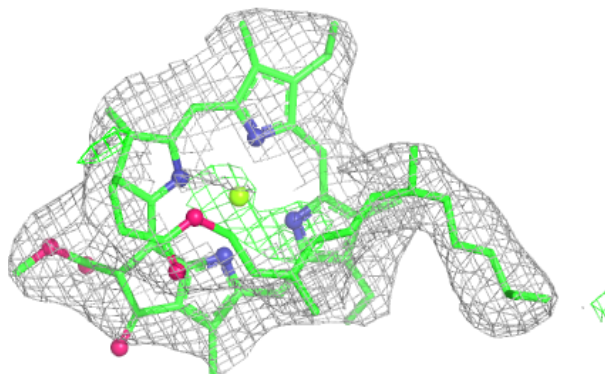


Electron density around CLA A 1109:

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

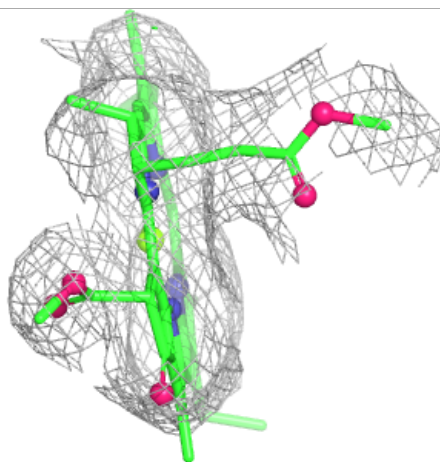
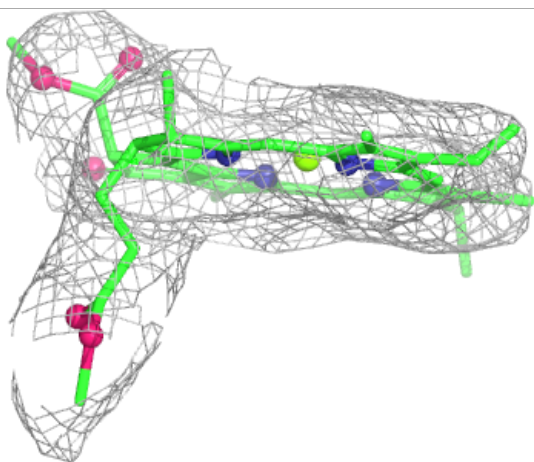
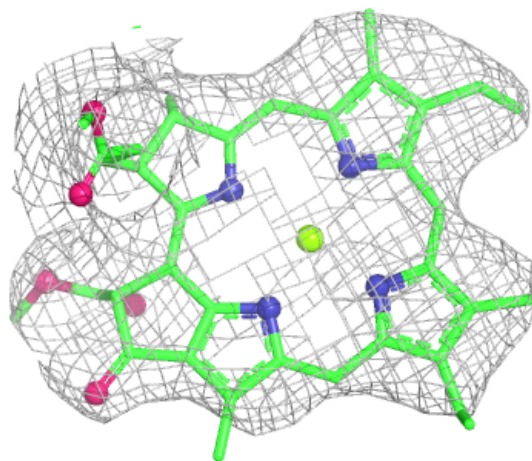
**Electron density around CLA B 1213:**

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



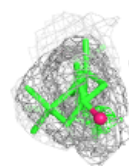
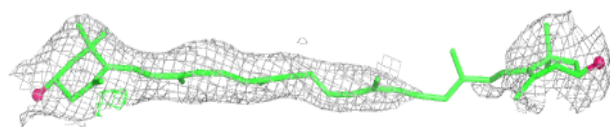
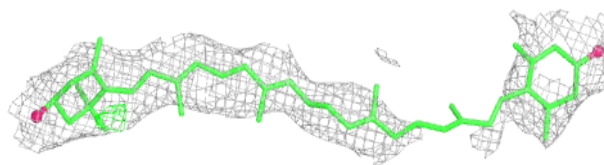
Electron density around CLA B 1231:

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

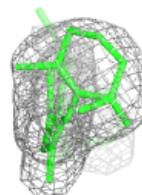
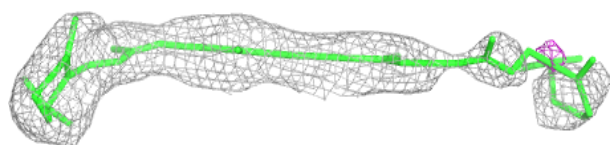
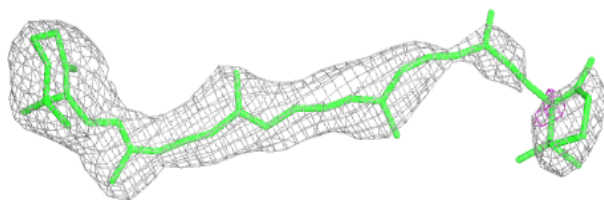


Electron density around LUT 1 1502:

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

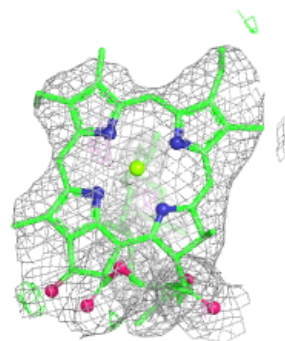
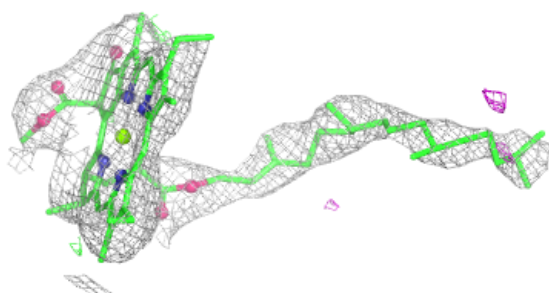
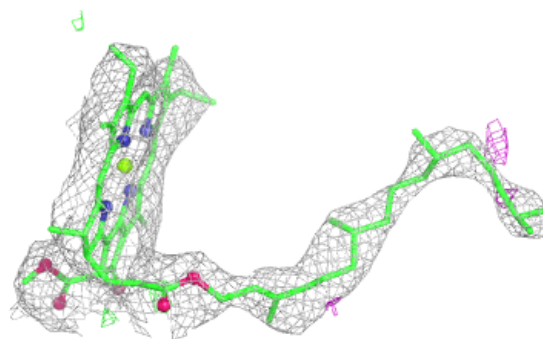
**Electron density around BCR B 6006:**

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



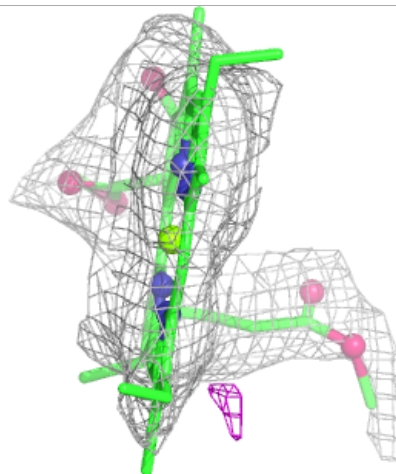
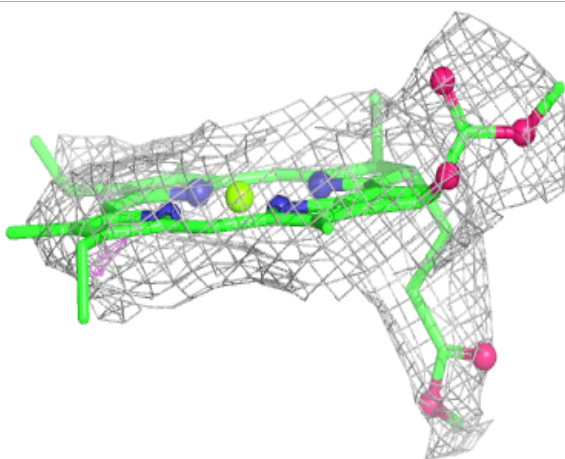
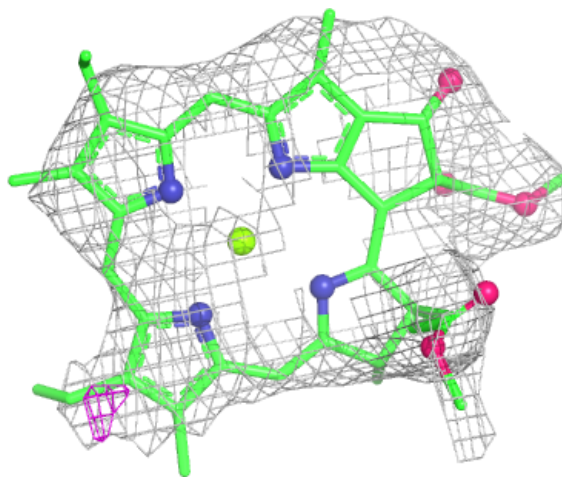
Electron density around CLA A 1128:

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



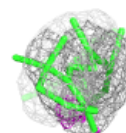
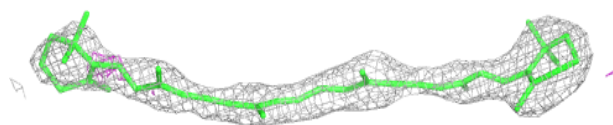
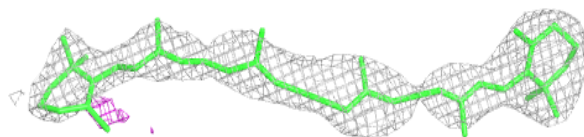
Electron density around CLA A 1133:

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

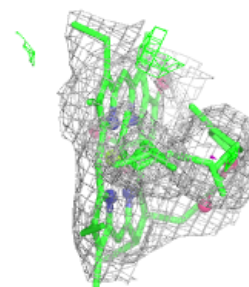
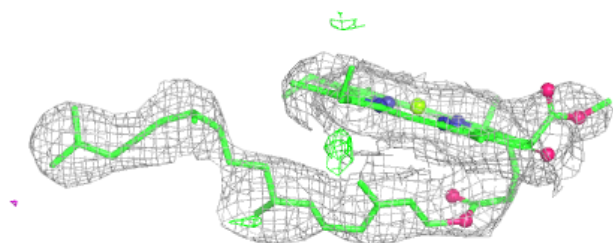
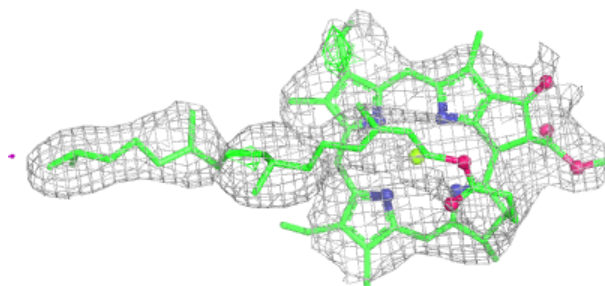


Electron density around BCR B 6004:

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

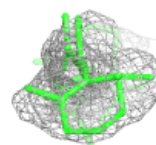
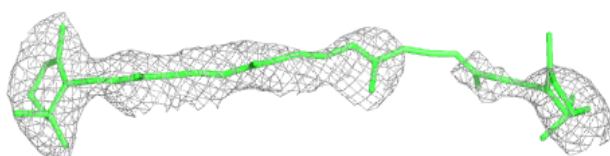
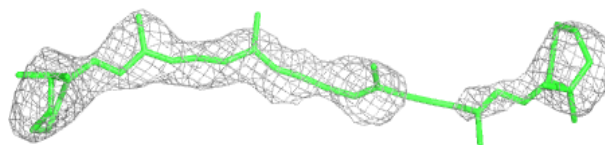
**Electron density around CLA A 1136:**

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

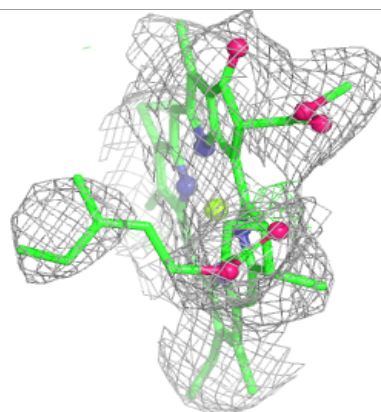
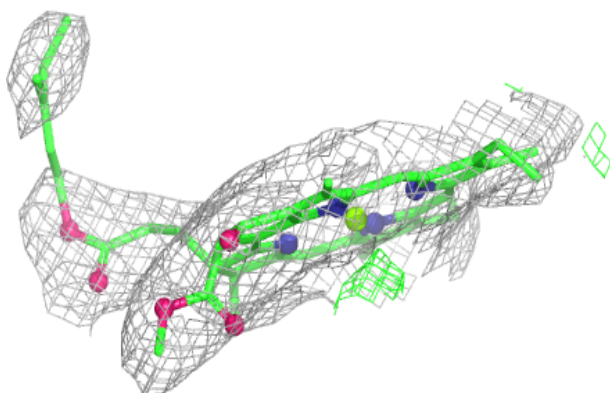
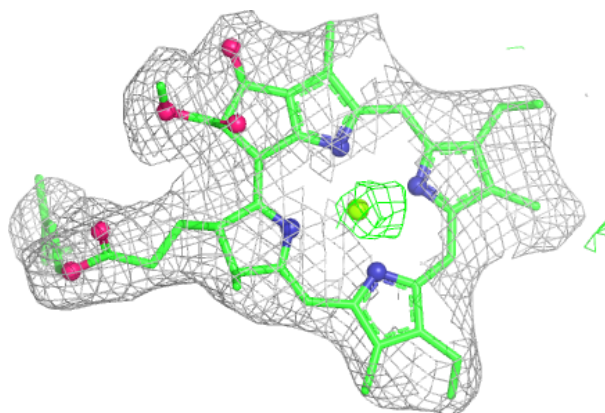


Electron density around BCR A 6008:

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

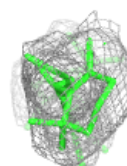
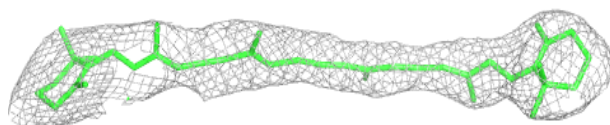
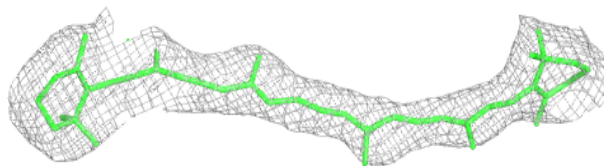
**Electron density around CLA 4 4013:**

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

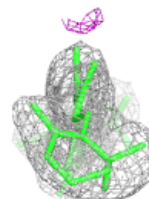
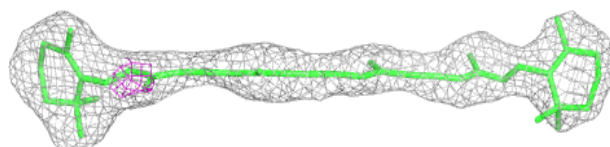
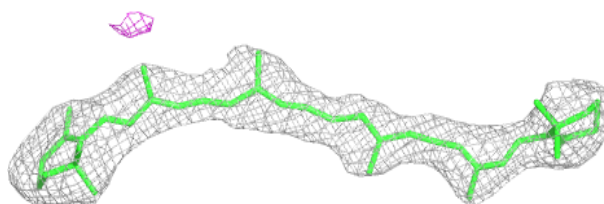


Electron density around BCR L 6020:

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

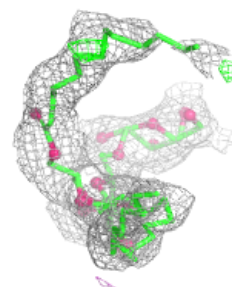
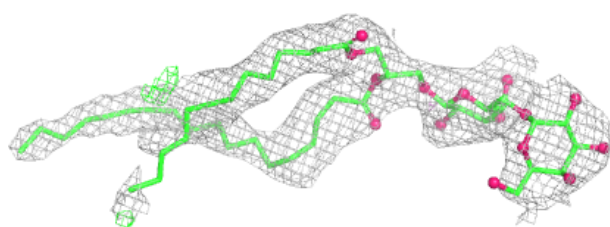
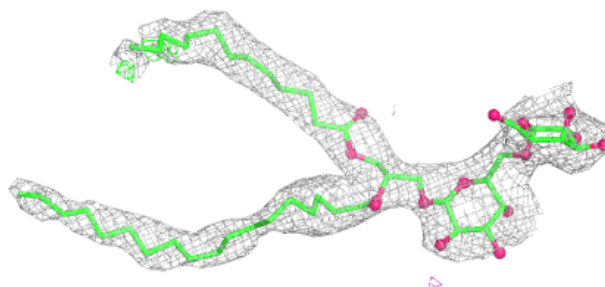
**Electron density around BCR B 6009:**

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

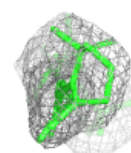
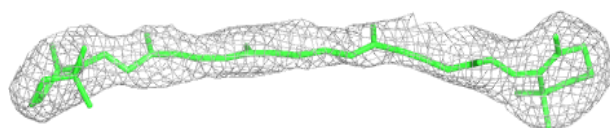
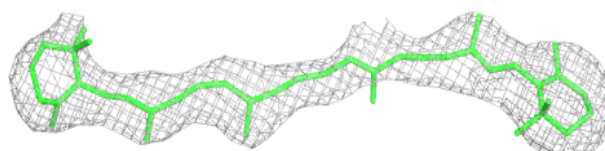


Electron density around DGD B 7101:

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

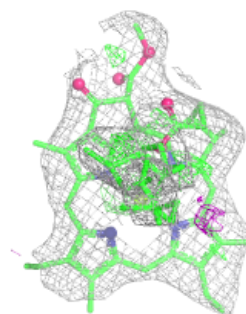
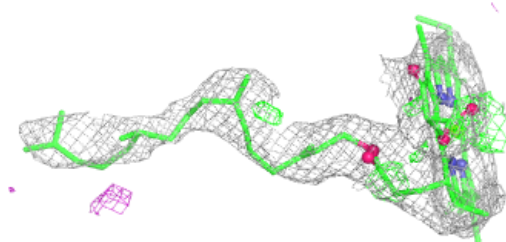
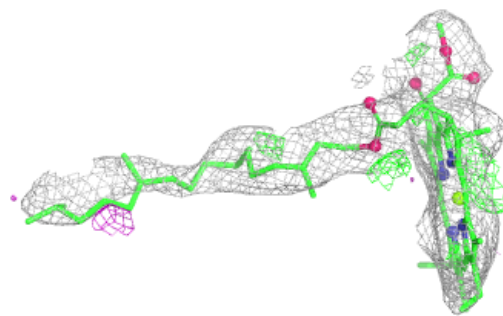
**Electron density around BCR J 6012:**

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



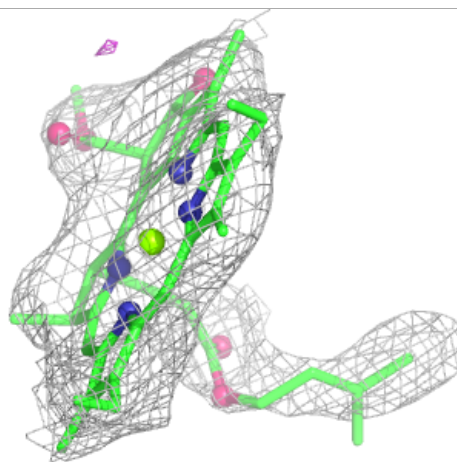
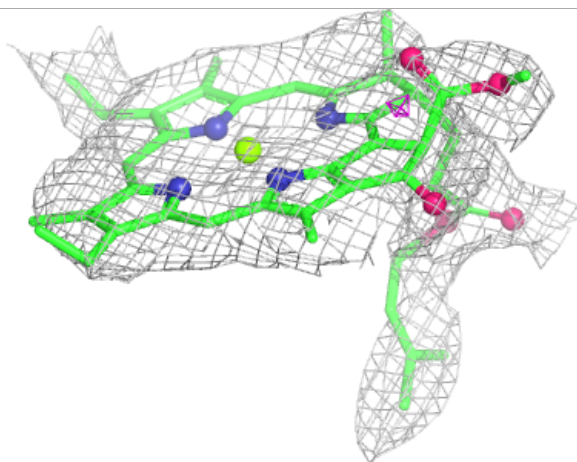
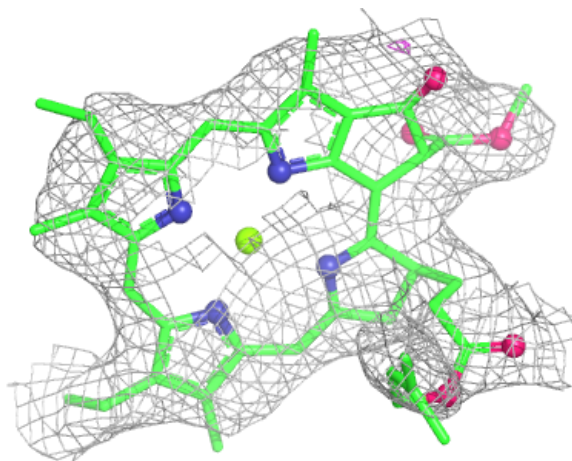
Electron density around CLA A 1126:

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



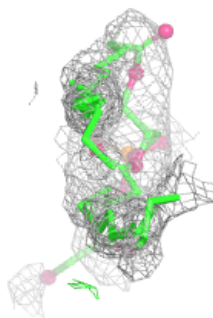
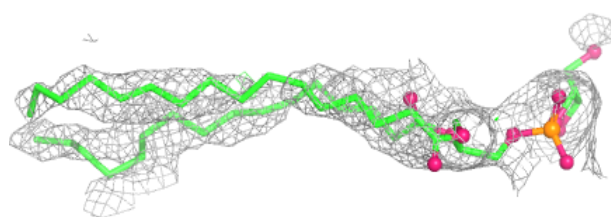
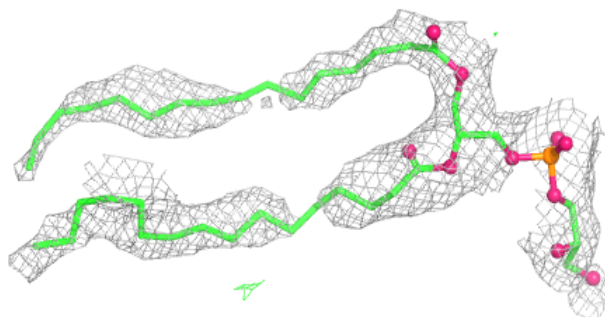
Electron density around CLA 1 1012:

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

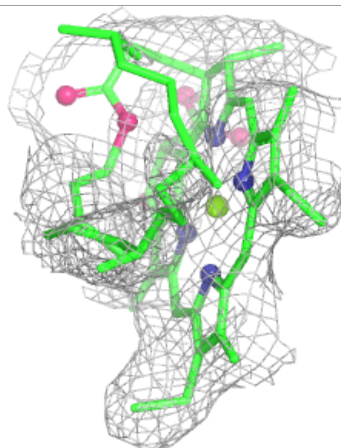
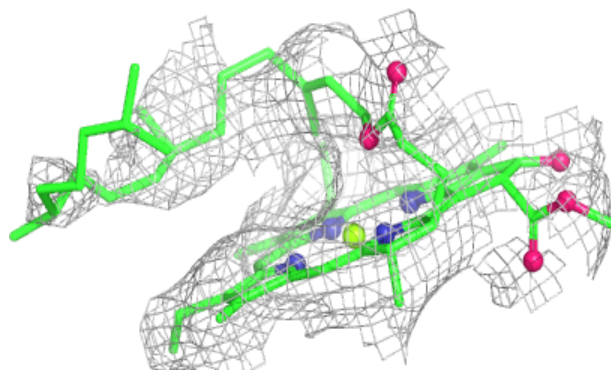
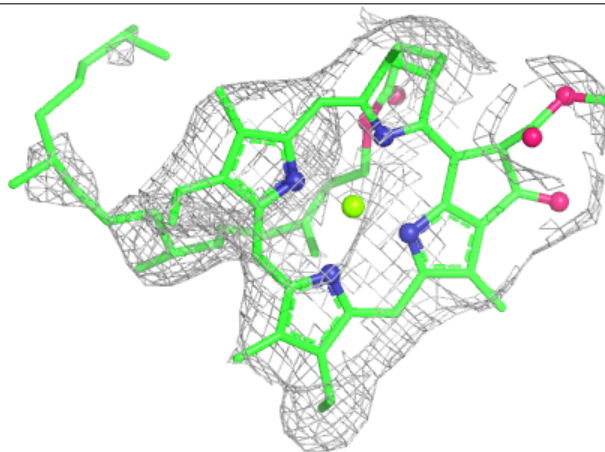


Electron density around LHG 1 1801:

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

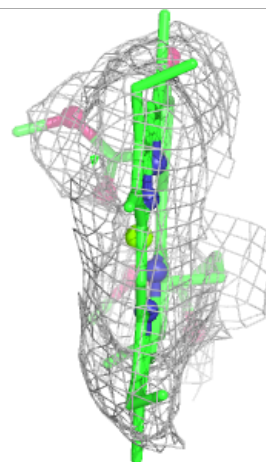
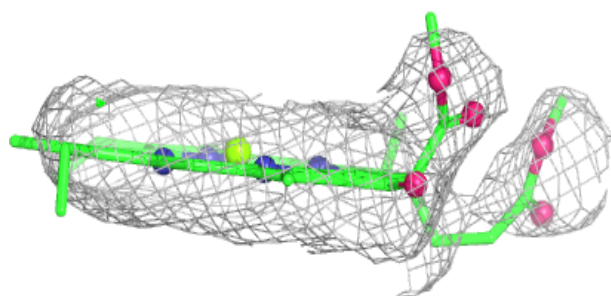
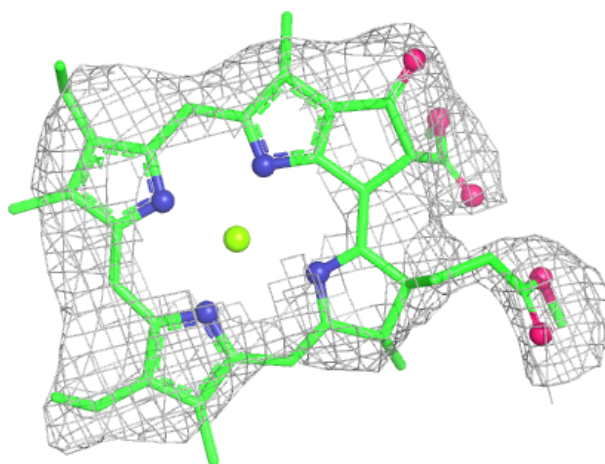
**Electron density around CLA 4 4003:**

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



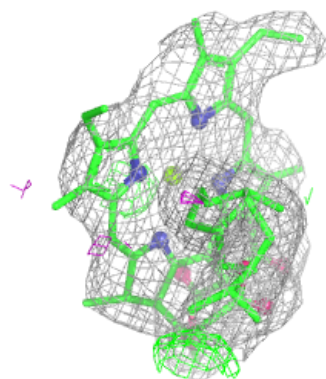
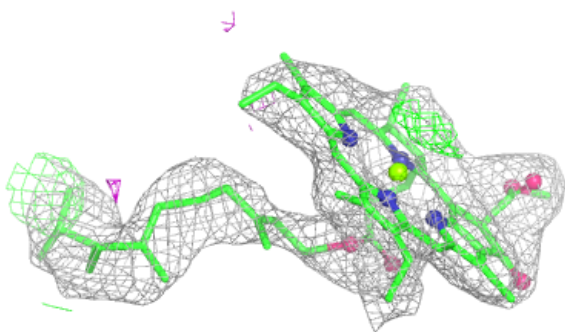
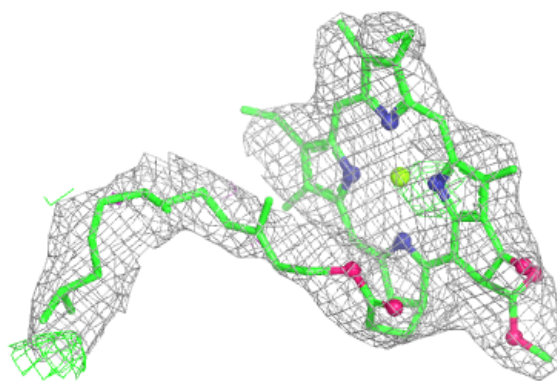
Electron density around CLA A 1113:

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



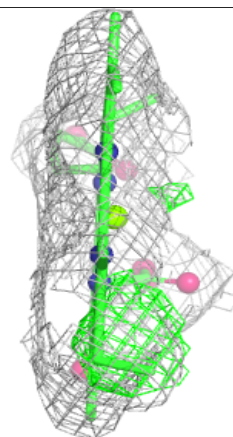
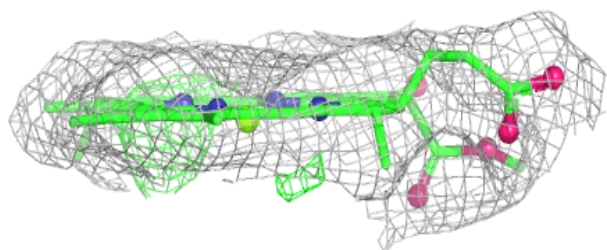
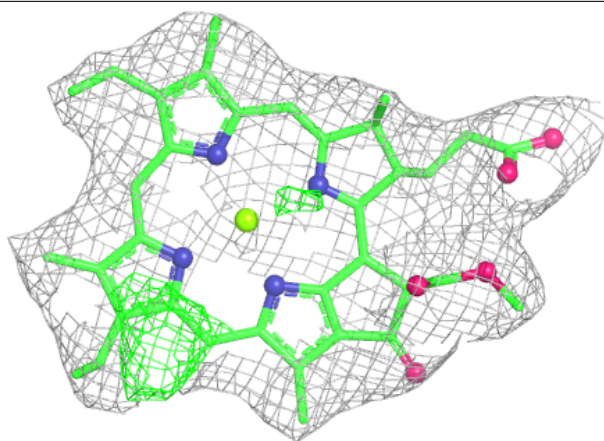
Electron density around CLA B 1237:

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

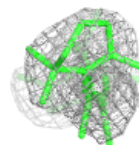
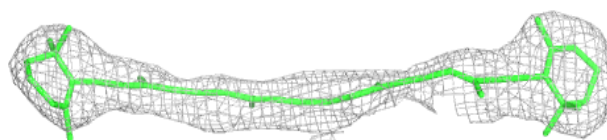


Electron density around CLA F 1301:

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

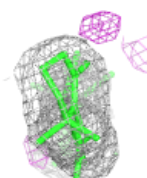
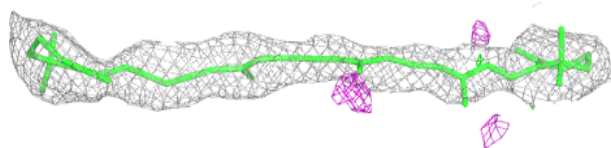
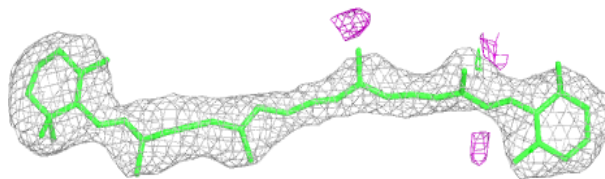
**Electron density around BCR A 6007:**

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

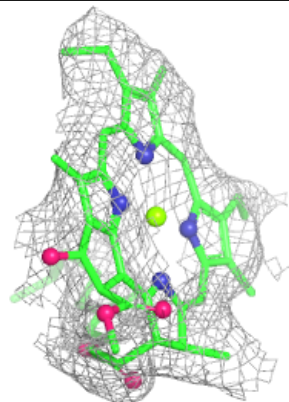
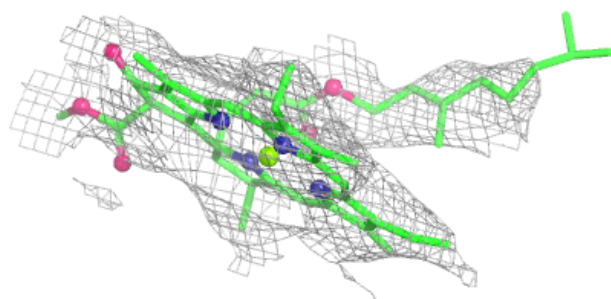
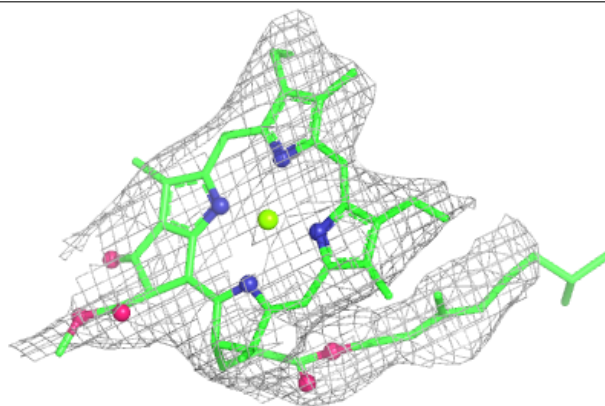


Electron density around BCR L 6019:

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

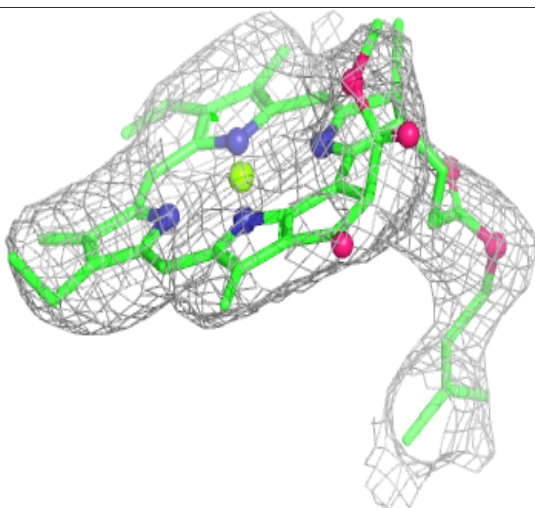
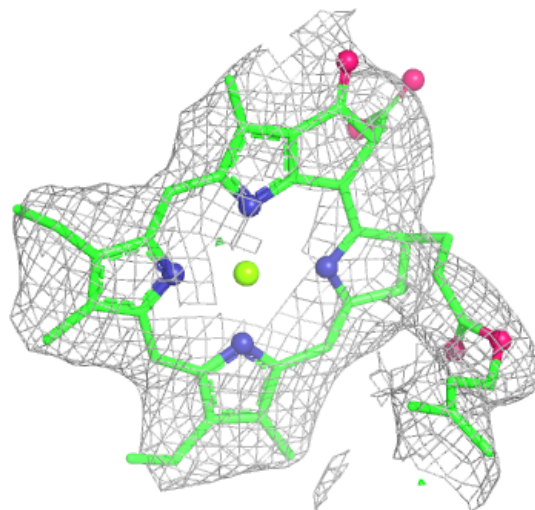
**Electron density around CLA 1 1001:**

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



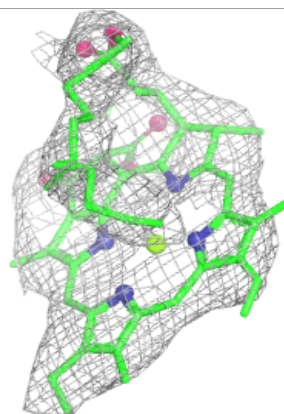
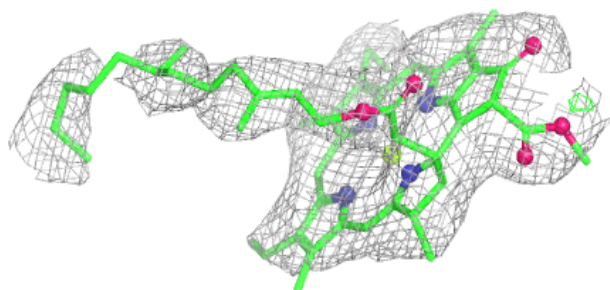
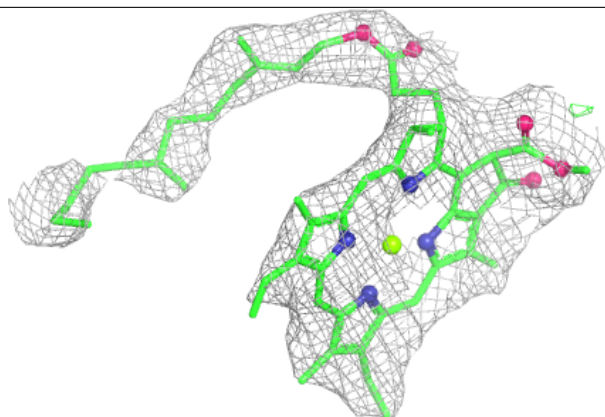
Electron density around CLA A 1129:

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

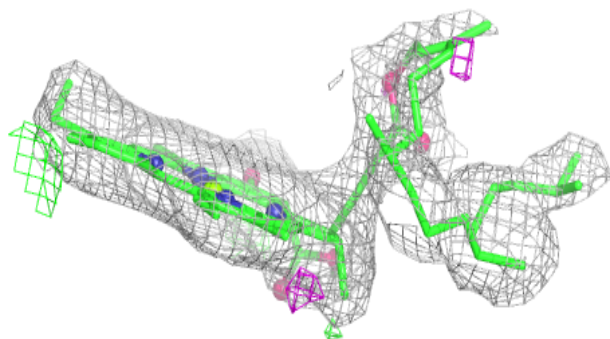
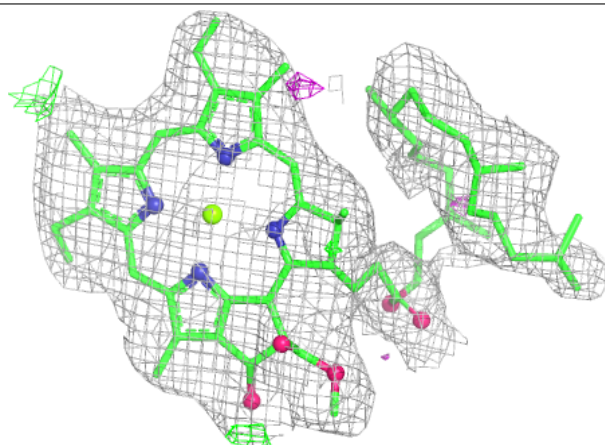


Electron density around CLA A 1122:

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

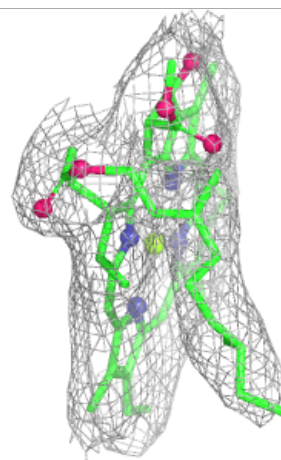
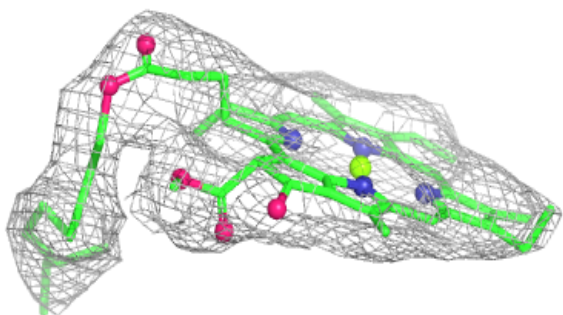
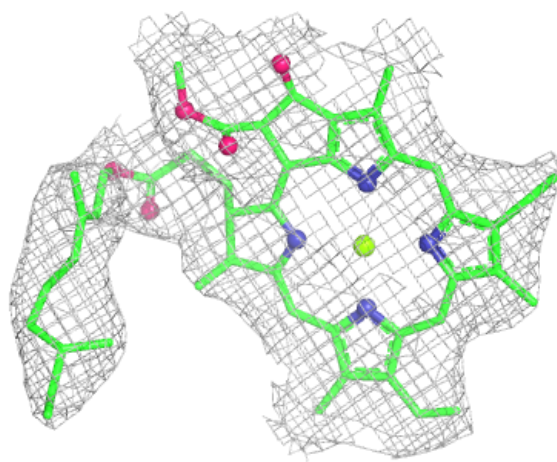
**Electron density around CLA 4 4011:**

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



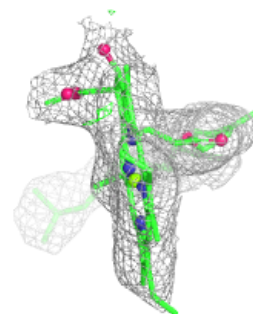
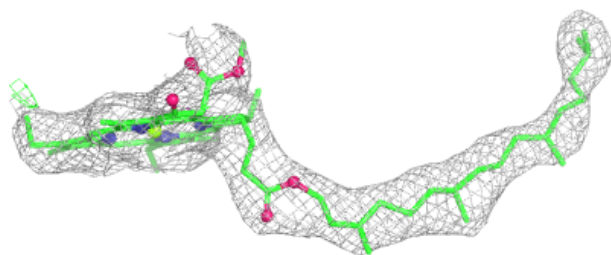
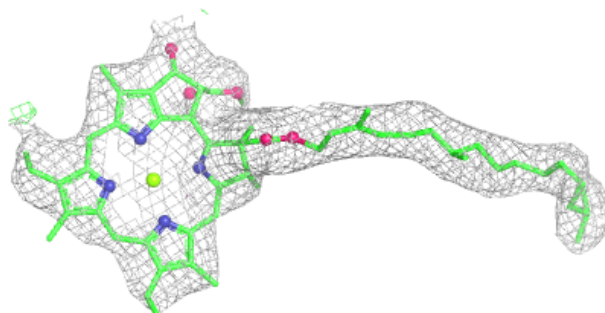
Electron density around CLA 1 1005:

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



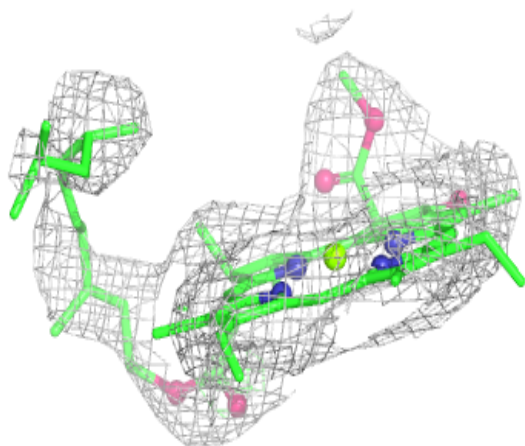
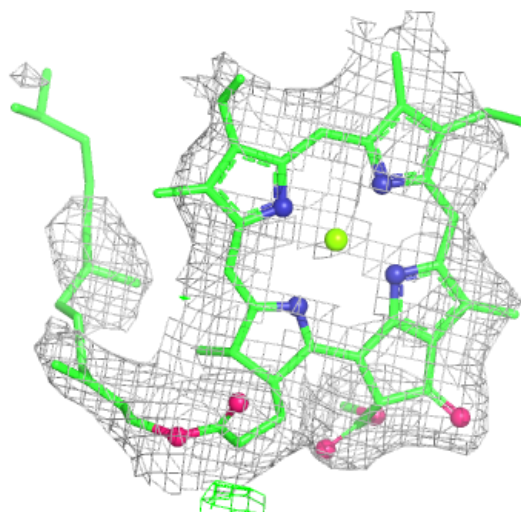
Electron density around CLA B 1240:

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



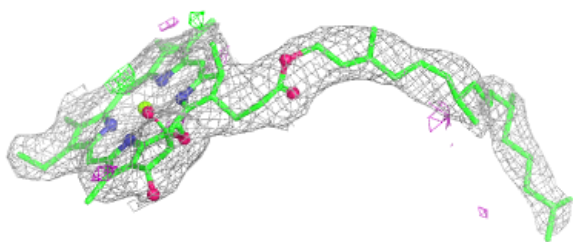
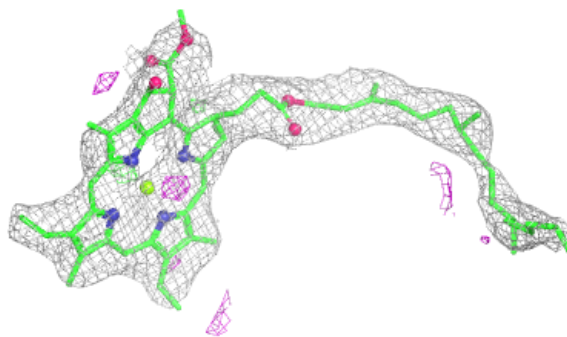
Electron density around CLA A 1111:

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



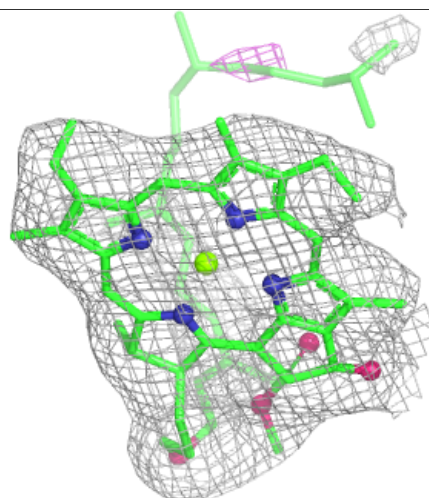
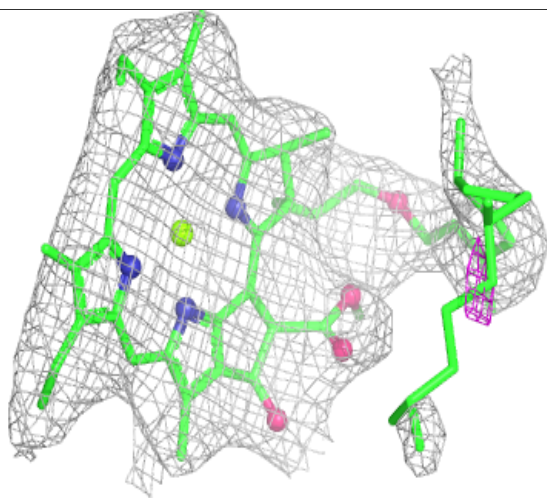
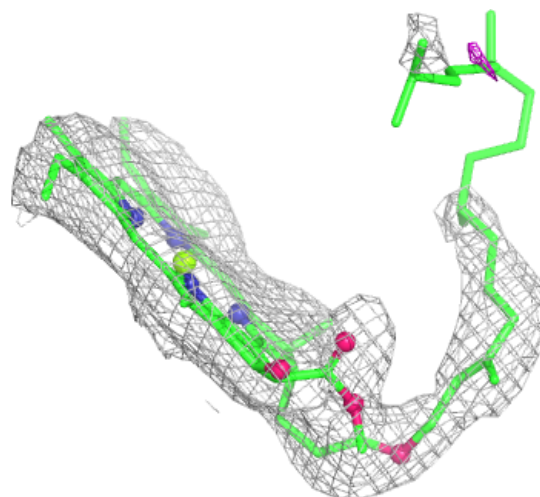
Electron density around CLA A 9012:

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



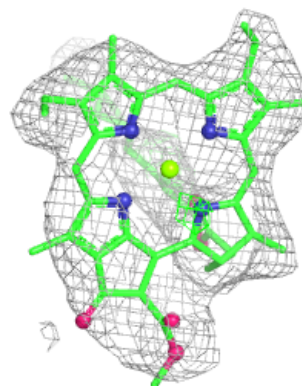
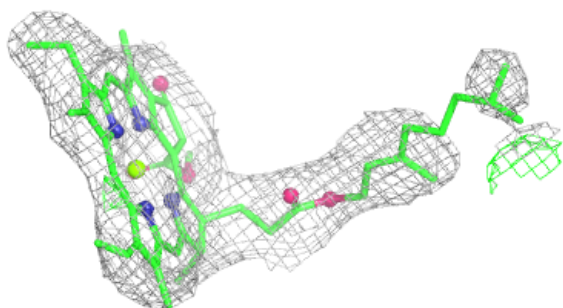
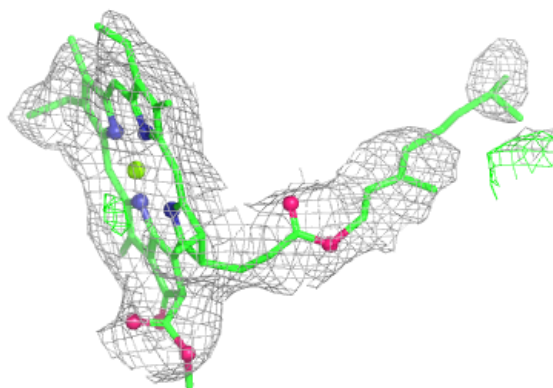
Electron density around CLA F 1303:

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

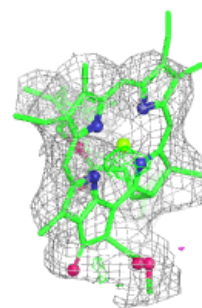
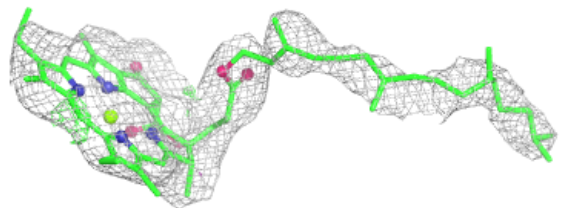
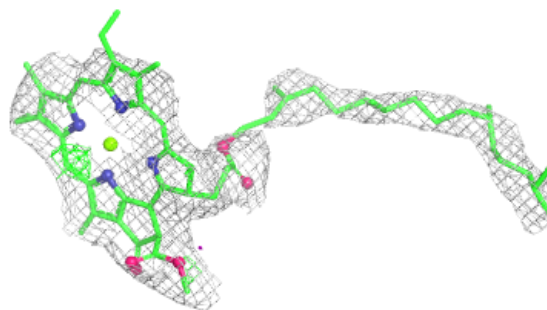


Electron density around CLA B 1208:

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

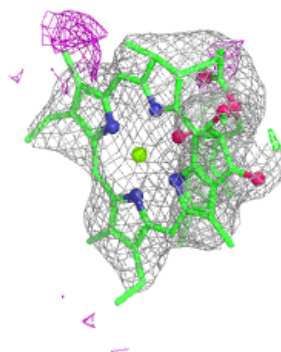
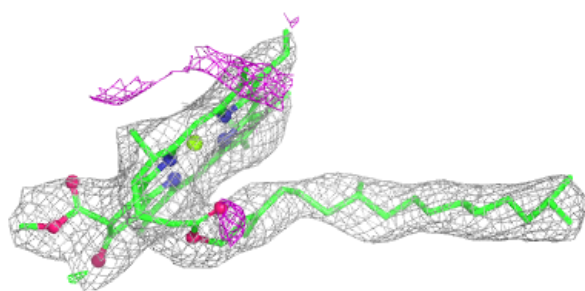
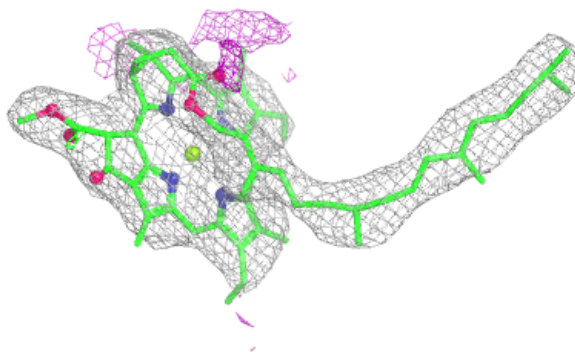
**Electron density around CLA A 1119:**

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

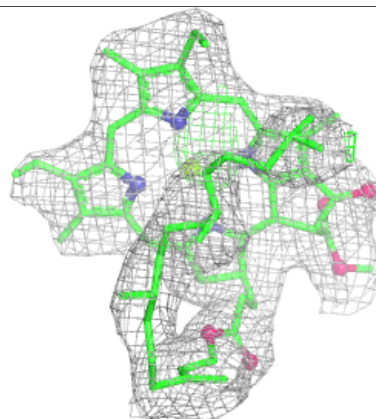
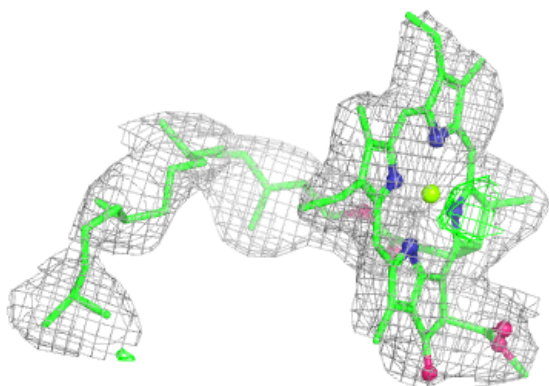
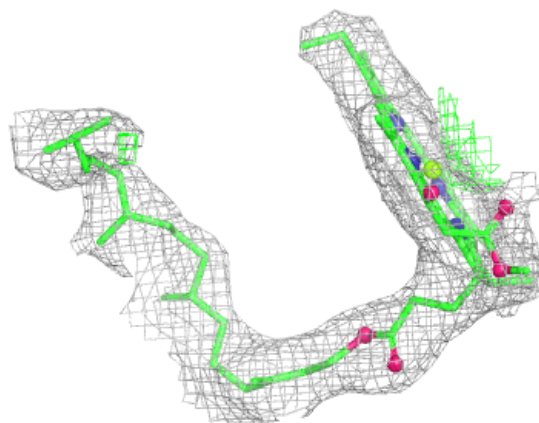


Electron density around CLA A 1140:

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

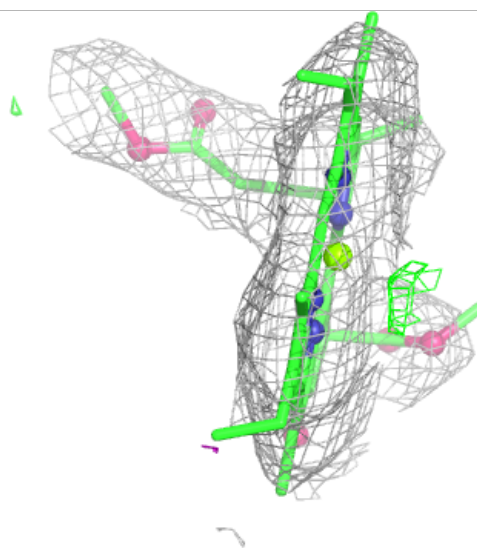
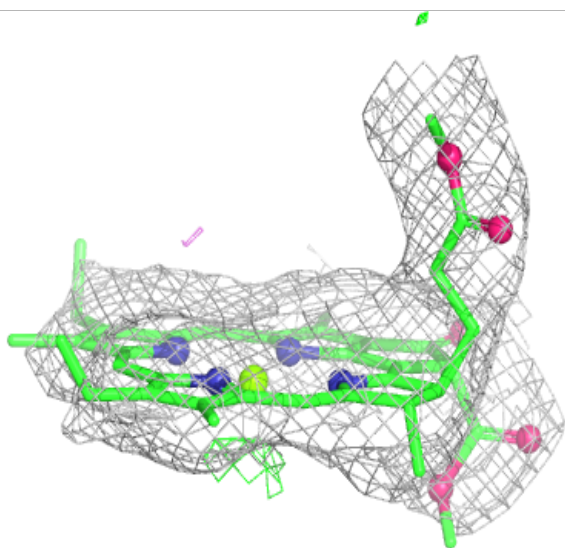
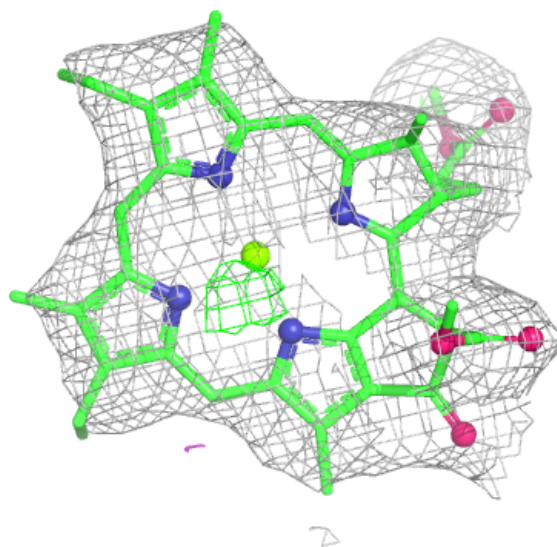
**Electron density around CLA B 1216:**

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



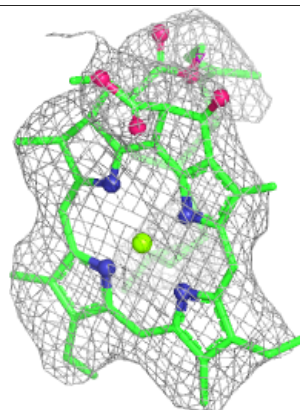
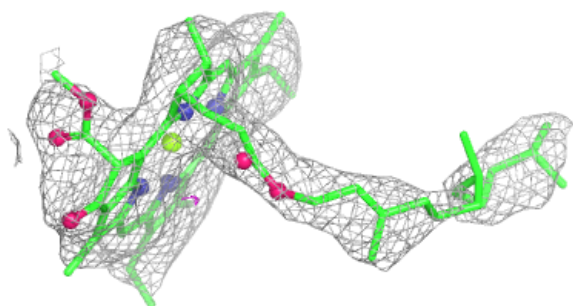
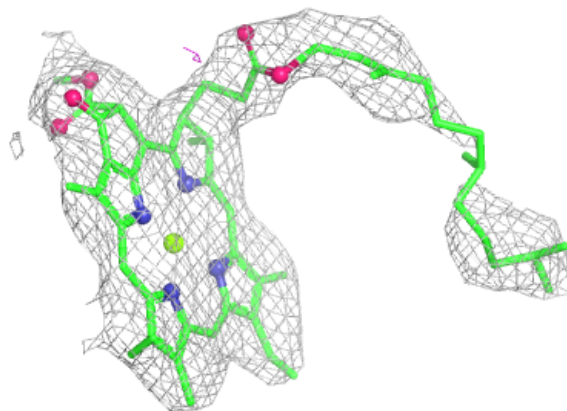
Electron density around CLA B 1217:

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

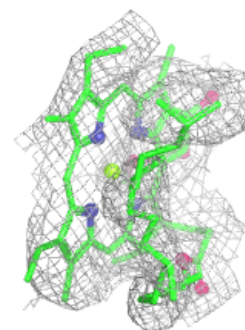
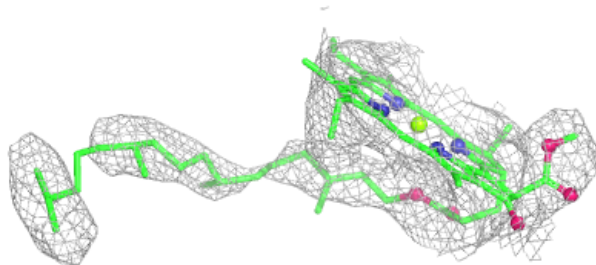
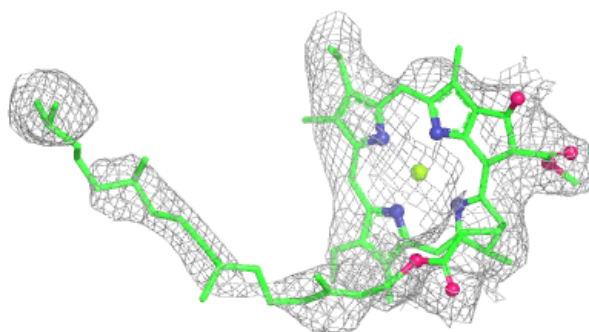


Electron density around CLA B 1218:

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

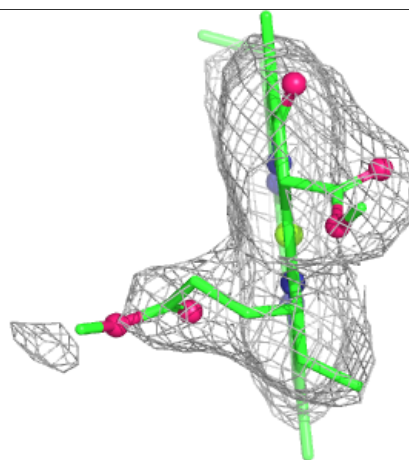
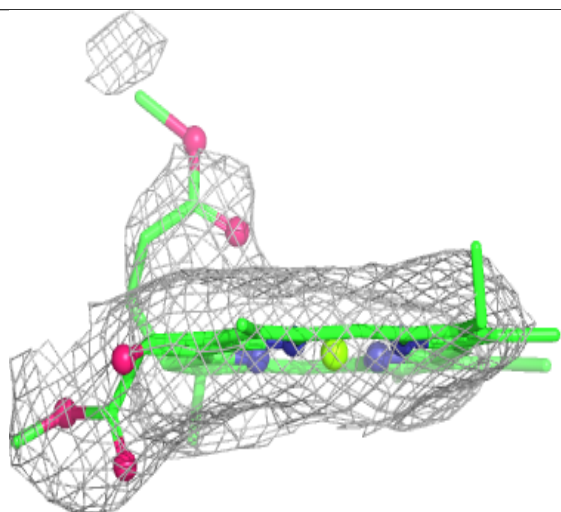
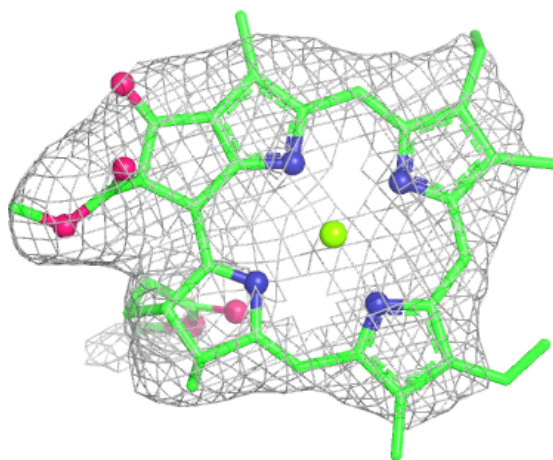
**Electron density around CLA 4 4004:**

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



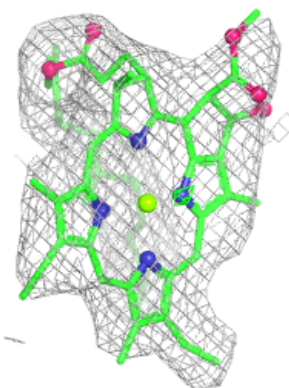
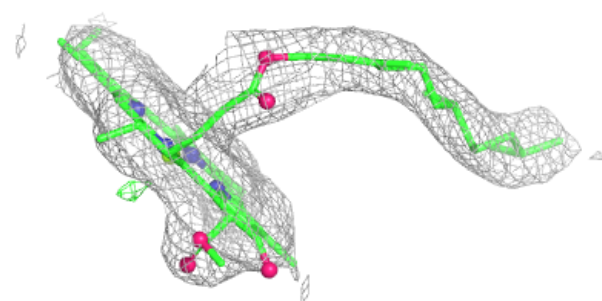
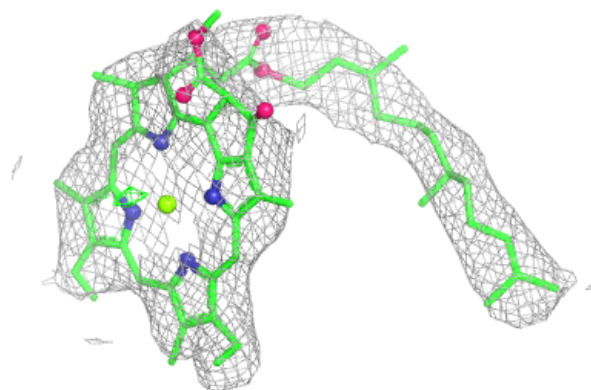
Electron density around CLA L 1501:

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

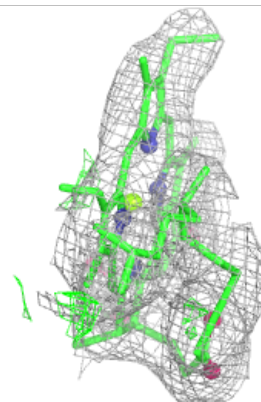
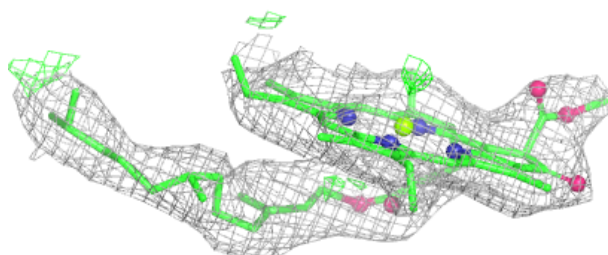
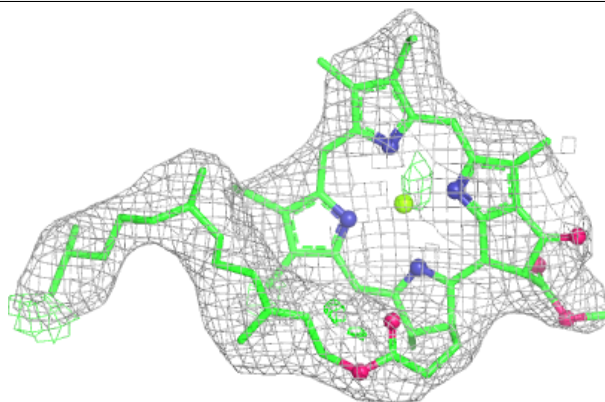


Electron density around CLA B 1219:

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

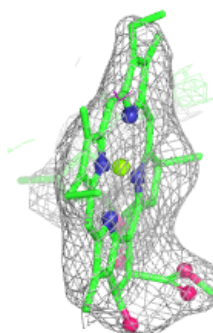
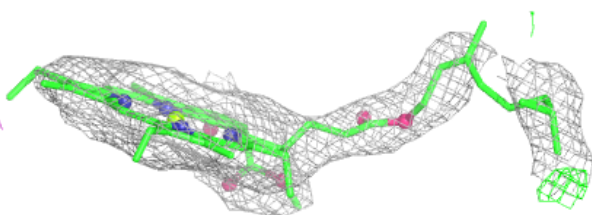
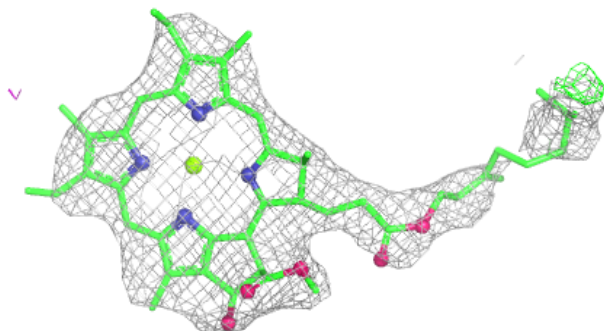
**Electron density around CLA B 1215:**

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

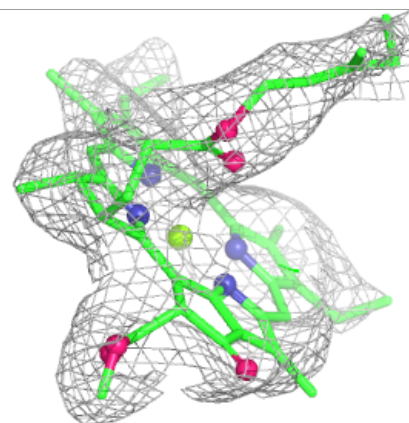
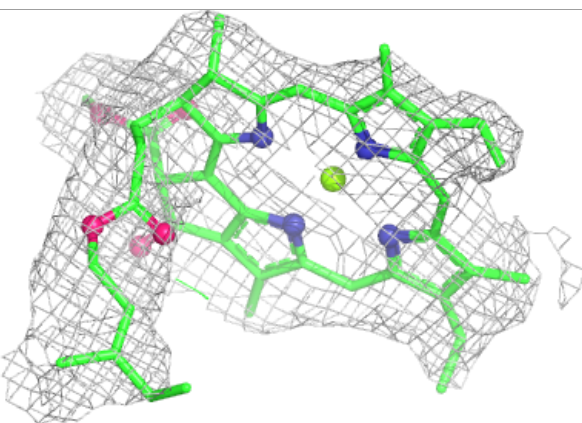
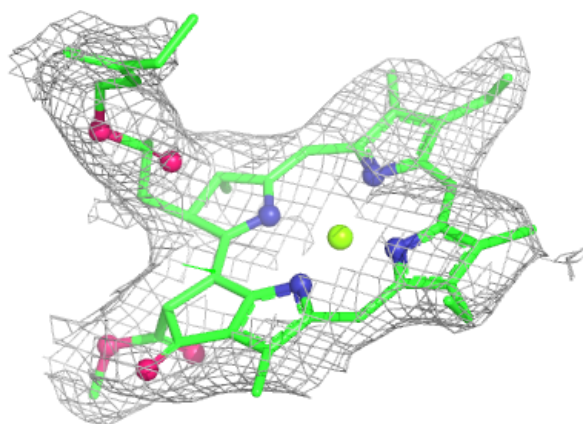


Electron density around CLA A 1125:

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

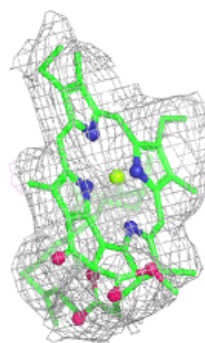
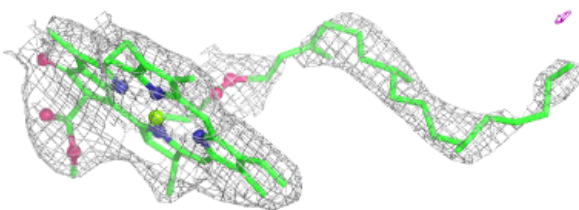
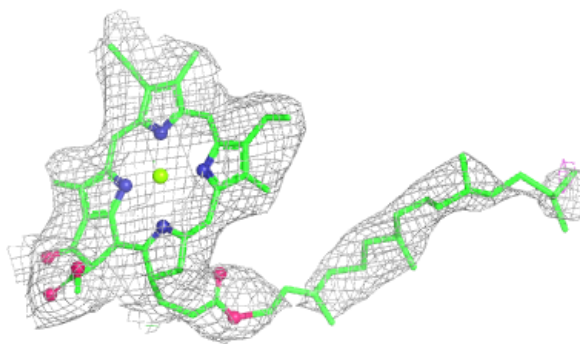
**Electron density around CLA A 1105:**

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

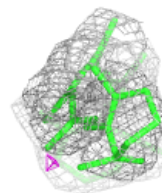
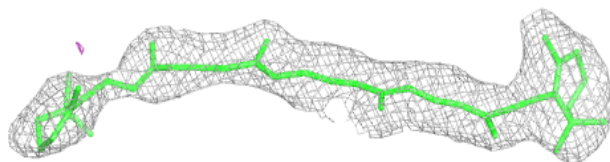
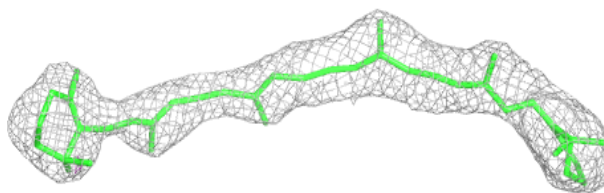


Electron density around CLA A 1106:

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

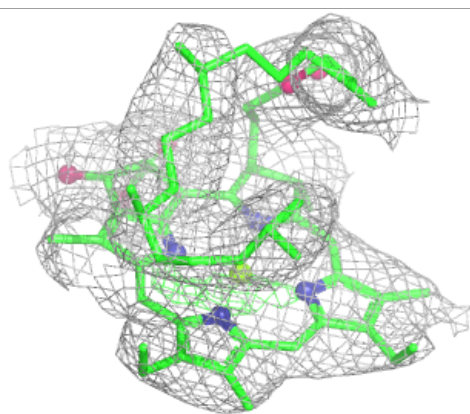
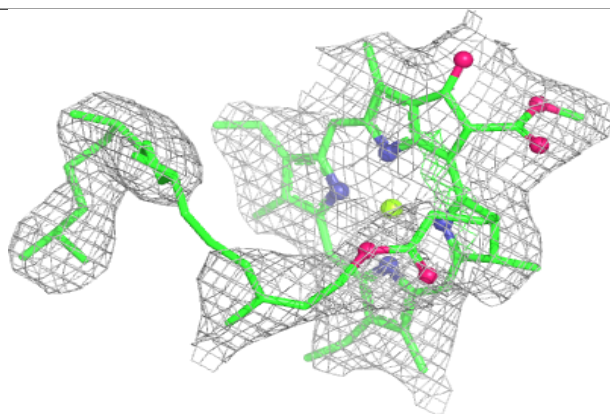
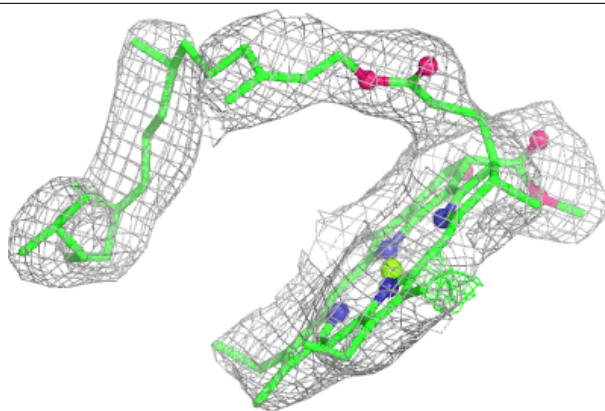
**Electron density around BCR F 6014:**

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

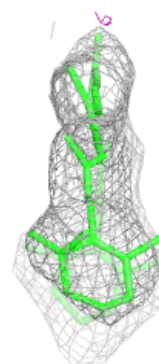
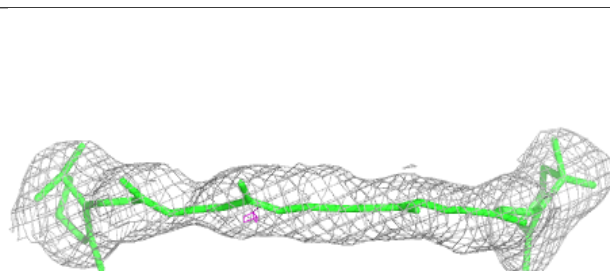
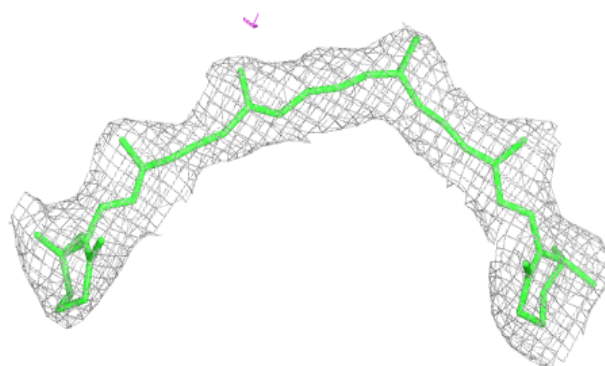


Electron density around CLA B 1227:

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

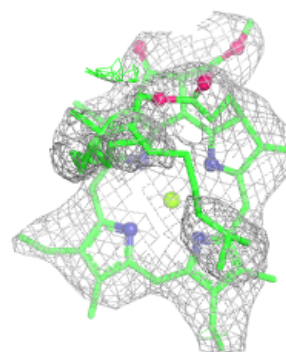
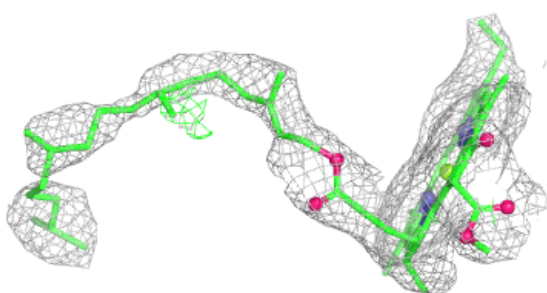
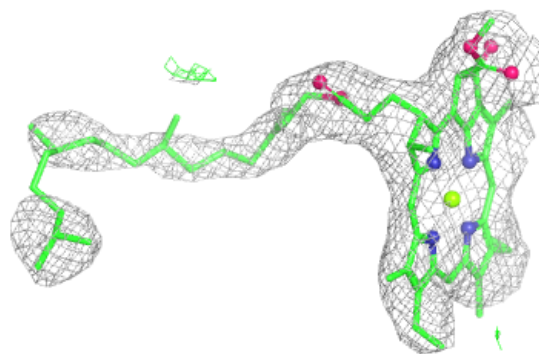
**Electron density around BCR F 6016:**

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

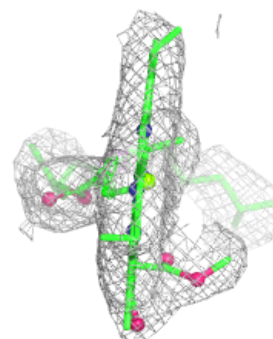
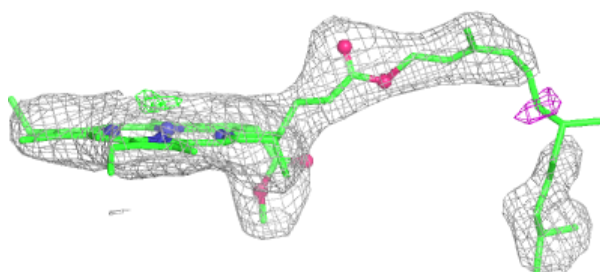
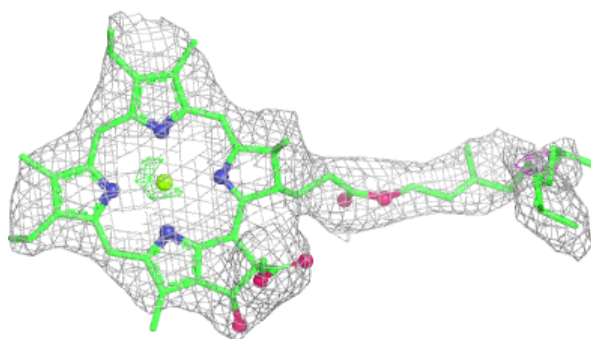


Electron density around CLA L 1502:

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

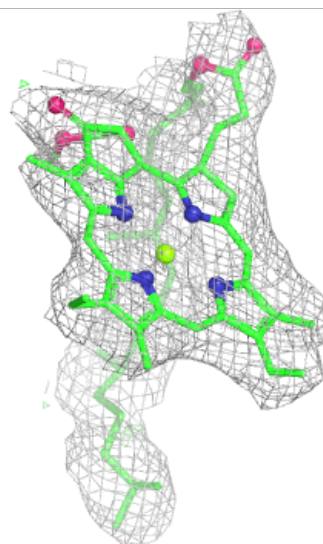
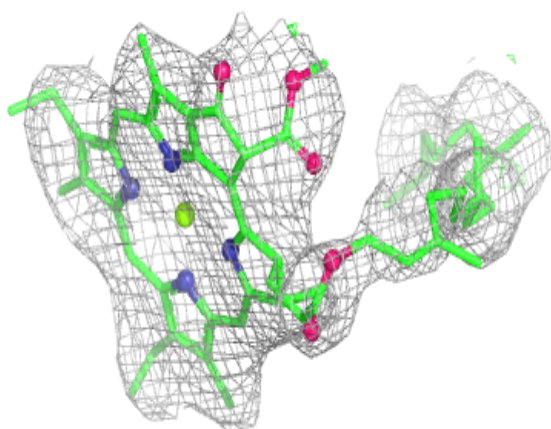
**Electron density around CLA B 1234:**

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



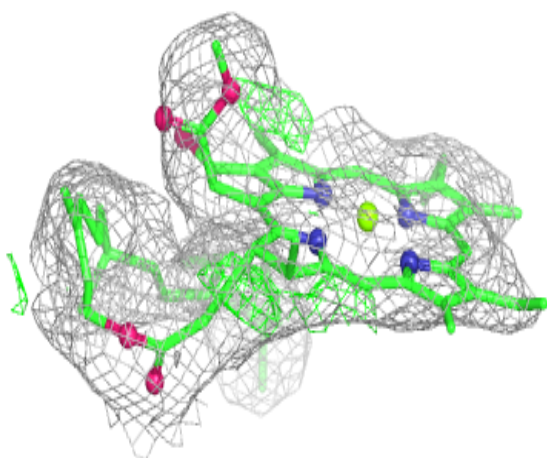
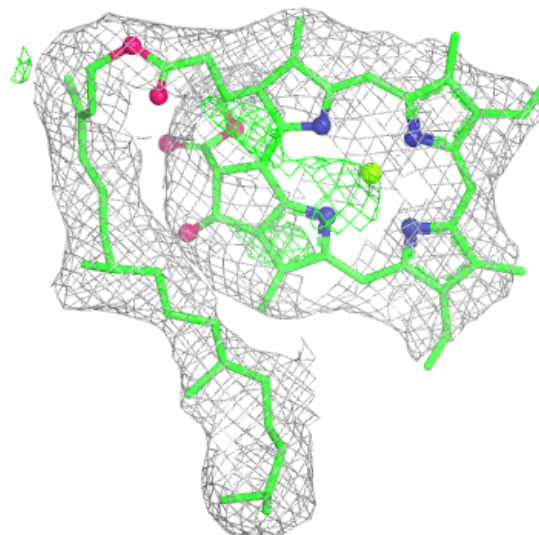
Electron density around CLA B 1207:

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



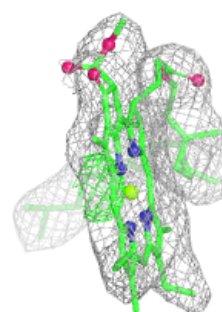
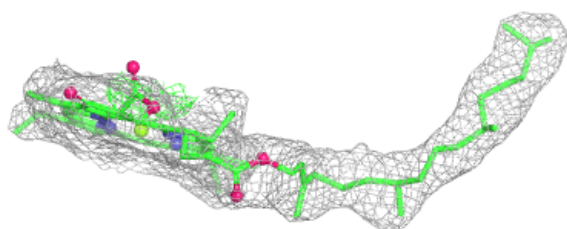
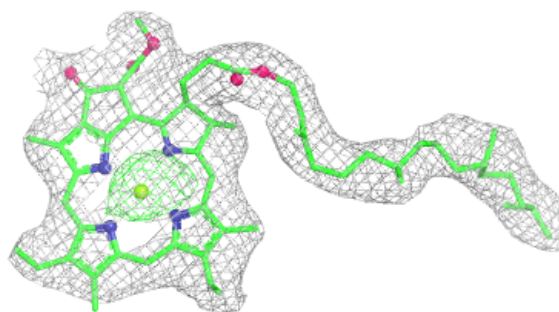
Electron density around CLA A 1123:

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

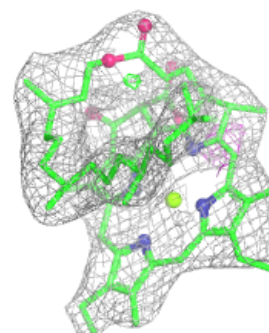
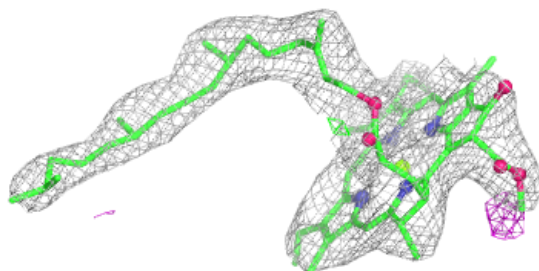
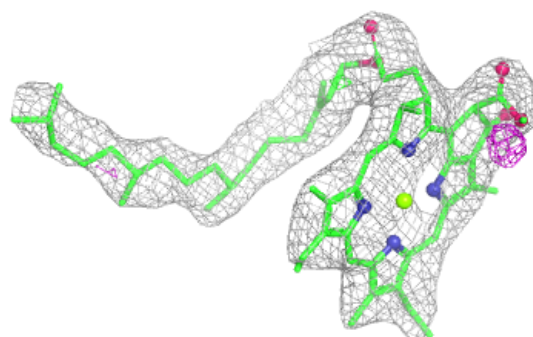


Electron density around CLA B 9023:

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

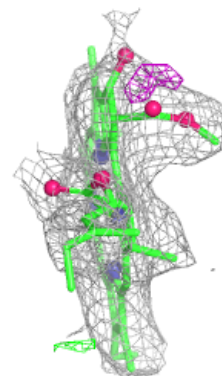
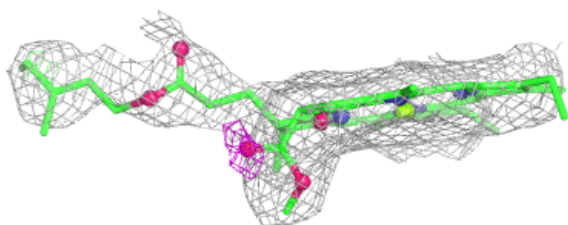
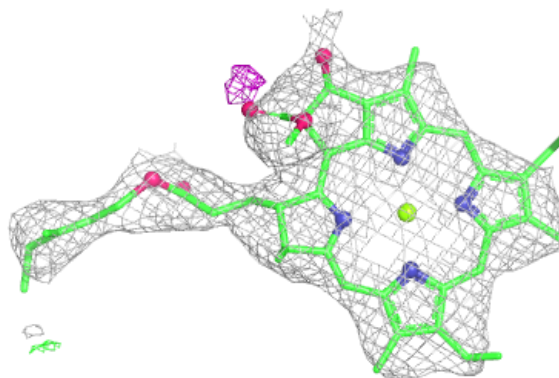
**Electron density around CLA B 1211:**

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

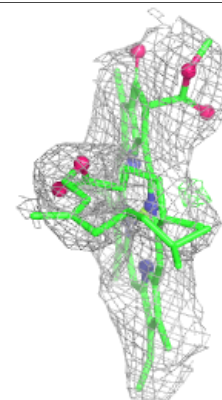
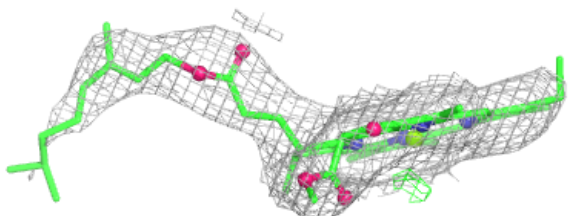
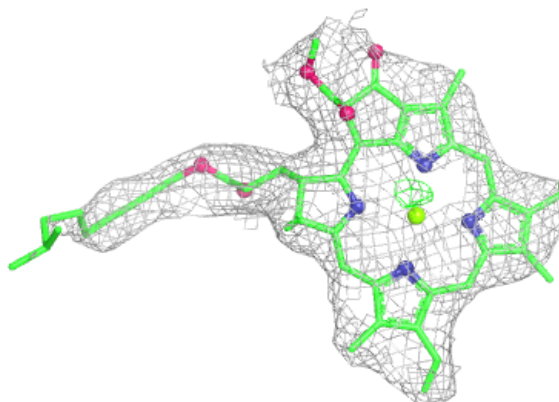


Electron density around CLA A 1135:

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

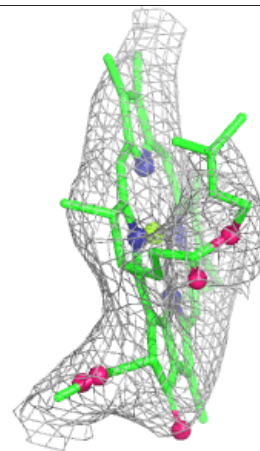
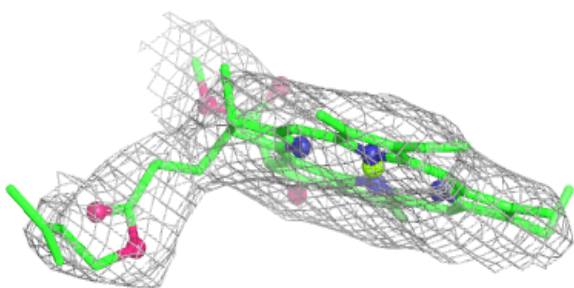
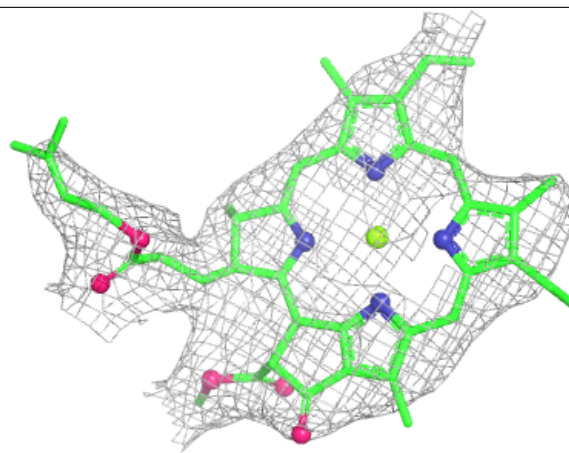
**Electron density around CLA A 1124:**

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

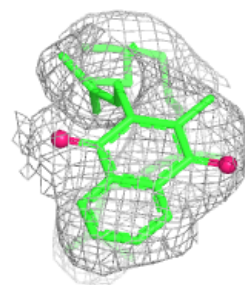
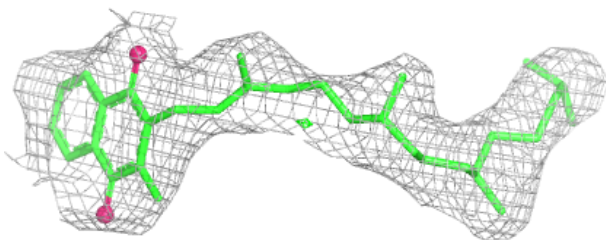


Electron density around CLA 4 4009:

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

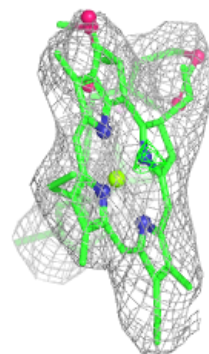
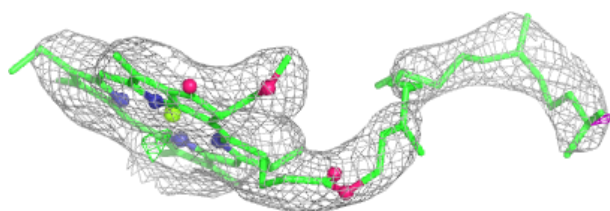
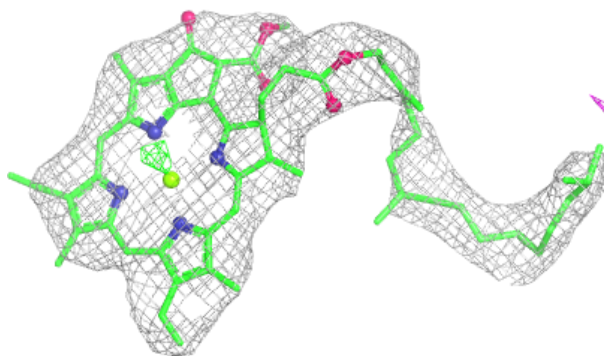
**Electron density around PQN B 5002:**

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

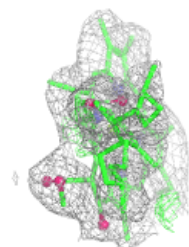
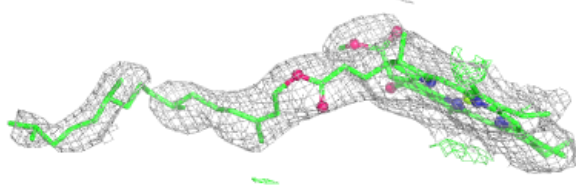
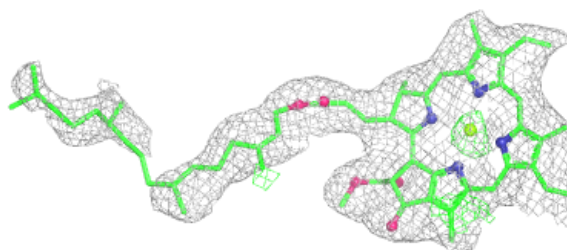


Electron density around CLA A 1101:

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

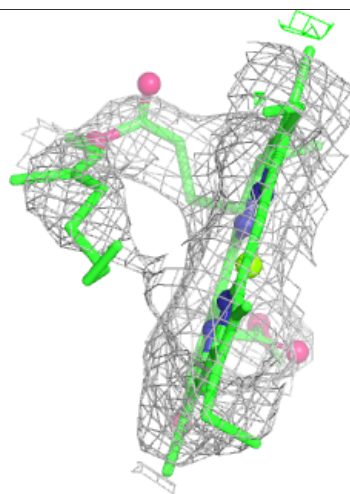
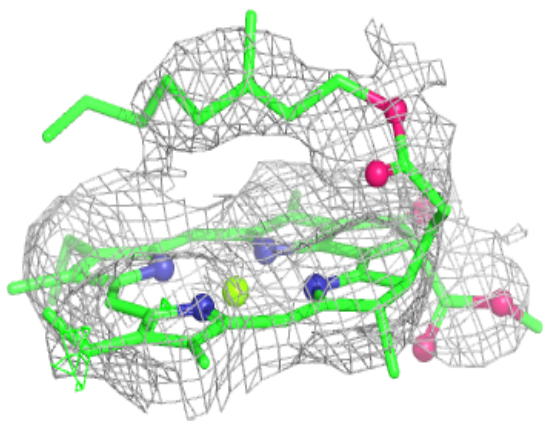
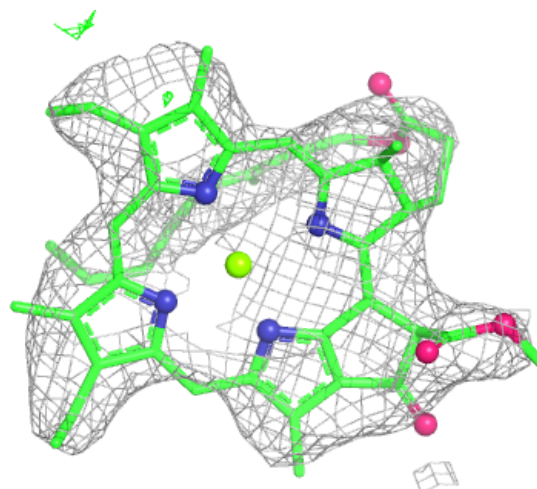
**Electron density around CLA A 1139:**

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



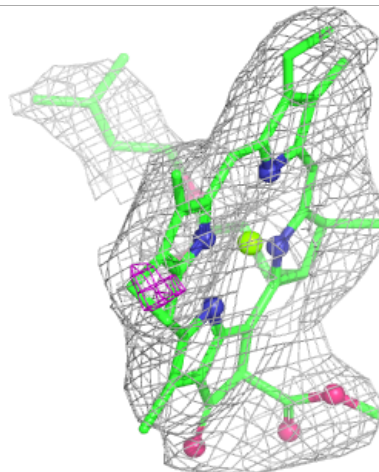
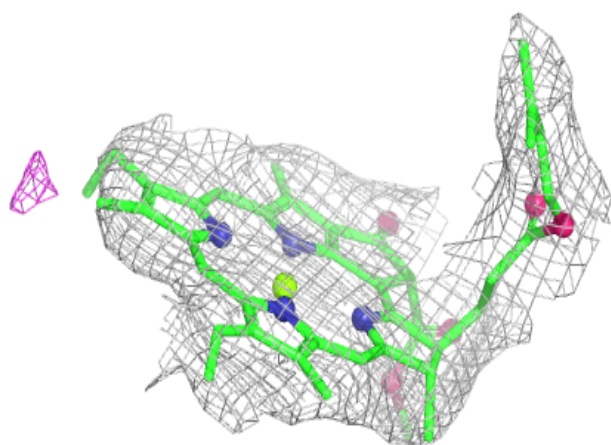
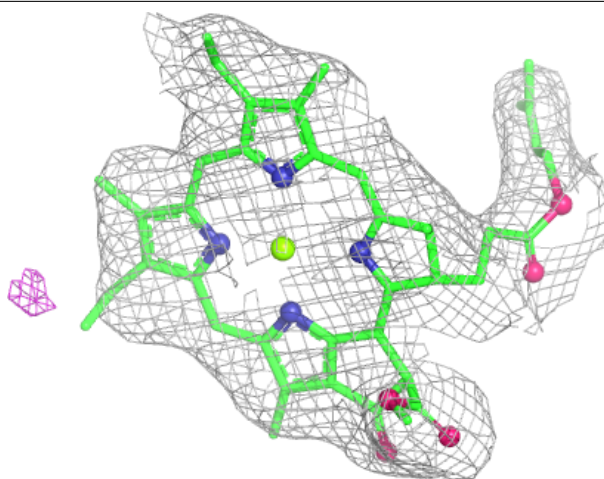
Electron density around CLA A 1116:

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



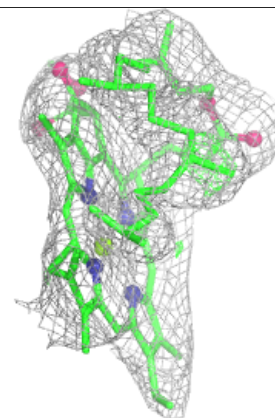
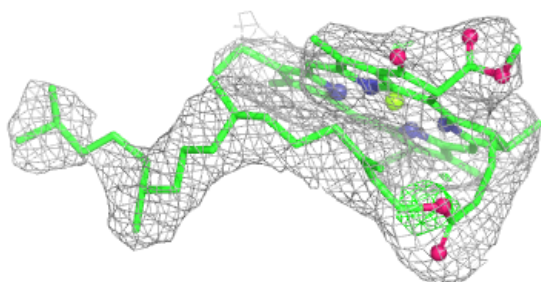
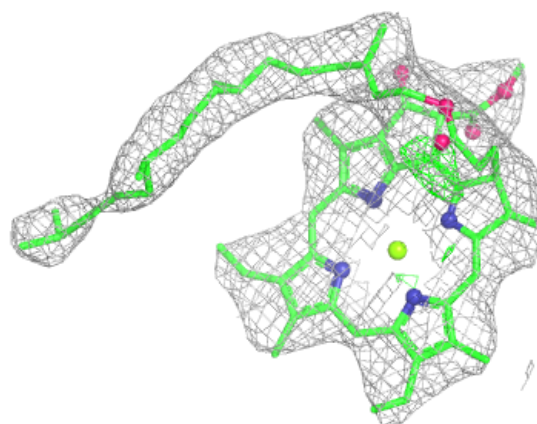
Electron density around CLA A 1102:

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

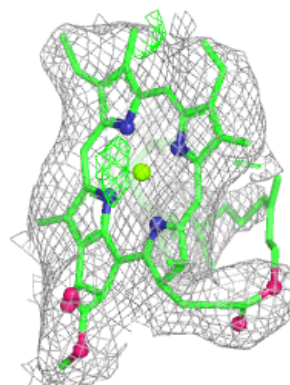
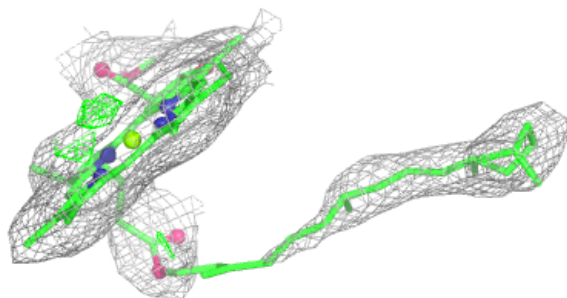
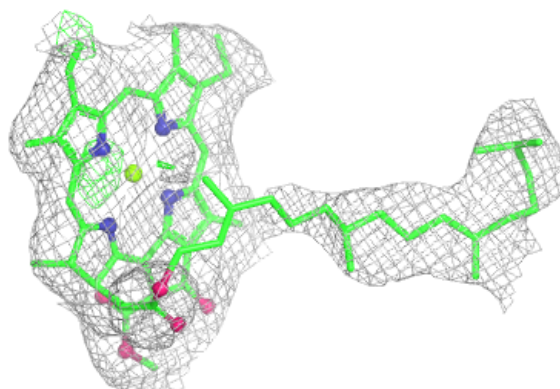


Electron density around CLA A 1127:

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

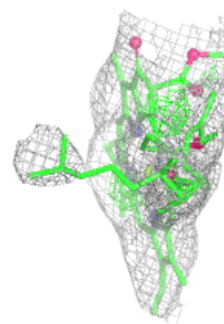
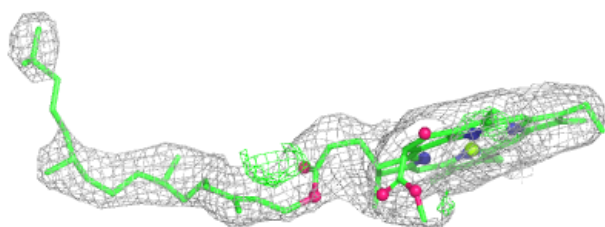
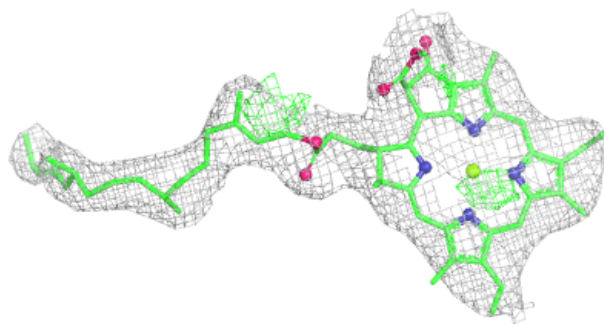
**Electron density around CLA 4 4012:**

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

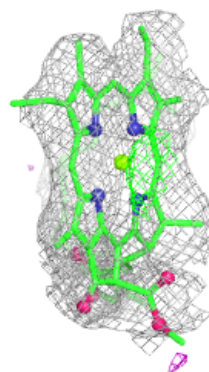
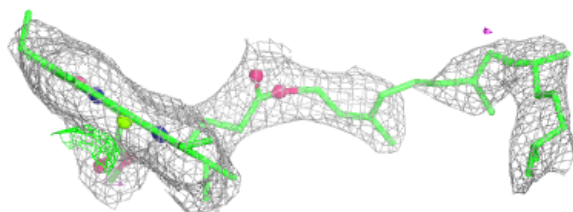
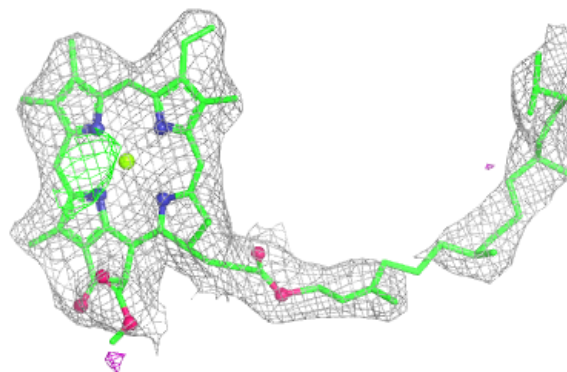


Electron density around CLA A 1103:

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

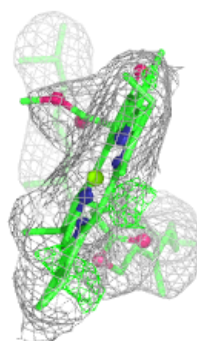
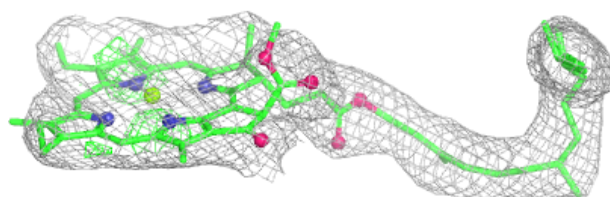
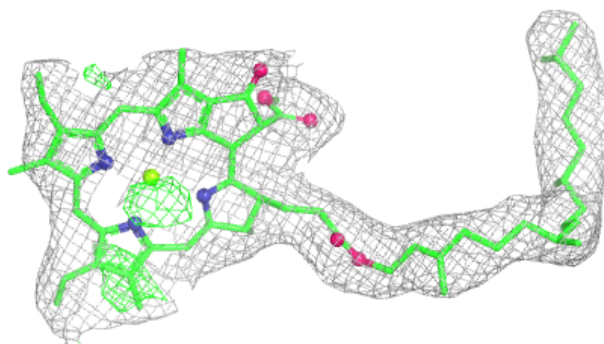
**Electron density around CLA B 1222:**

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

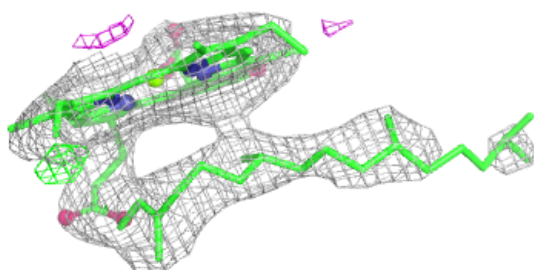
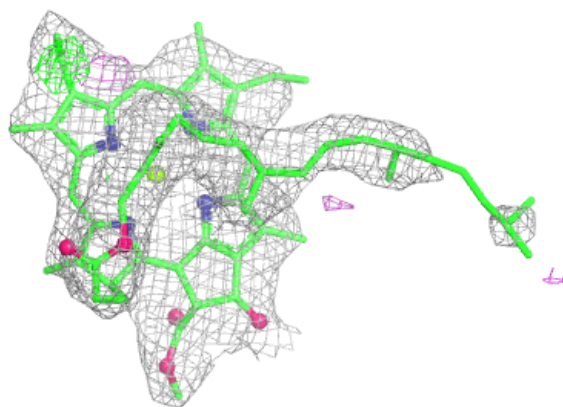


Electron density around CLA B 1223:

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

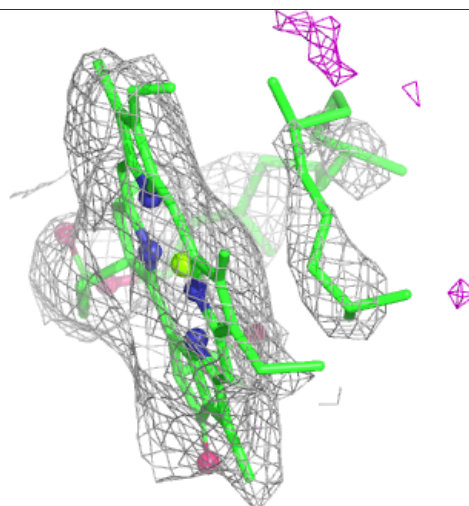
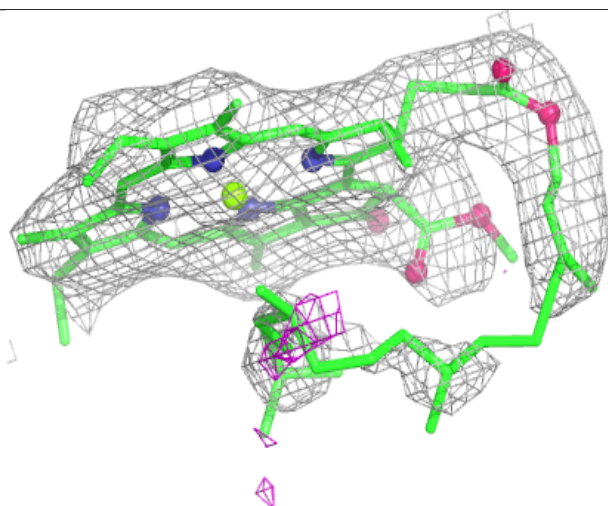
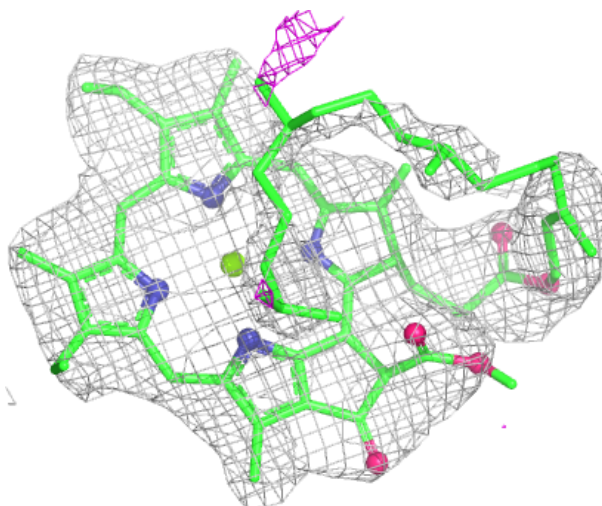
**Electron density around CLA B 1224:**

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



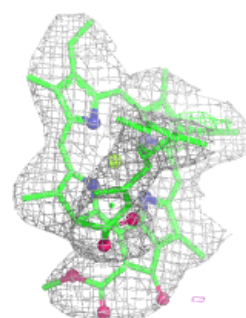
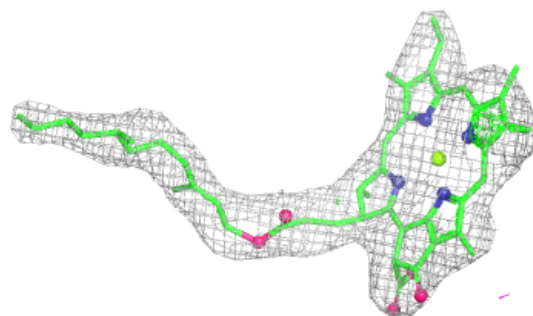
Electron density around CLA A 1104:

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

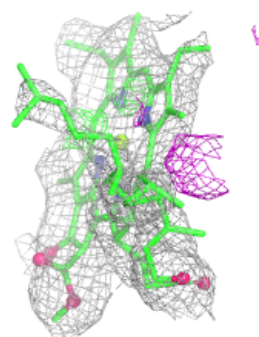
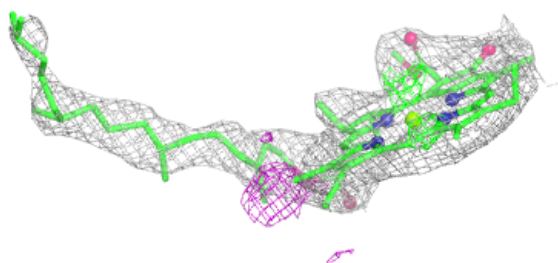
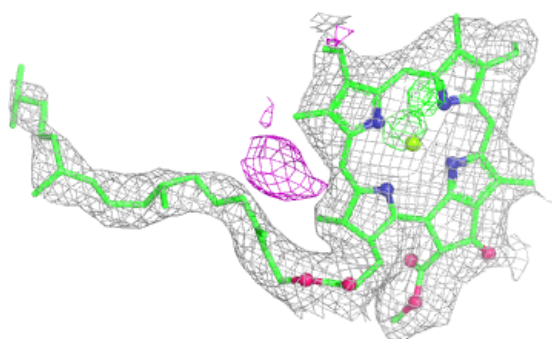


Electron density around CLA B 1230:

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

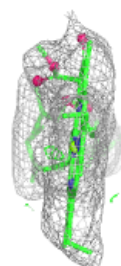
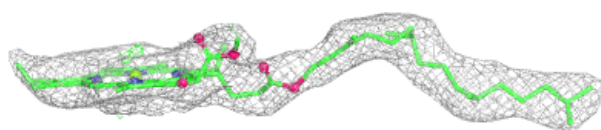
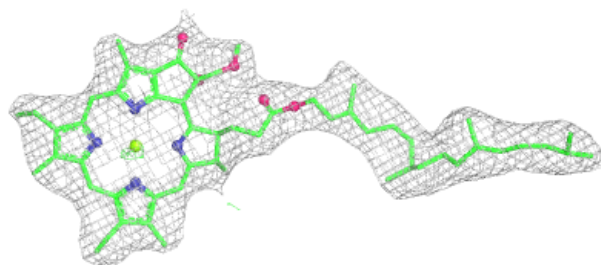
**Electron density around CLA A 9013:**

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

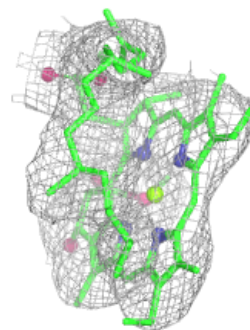
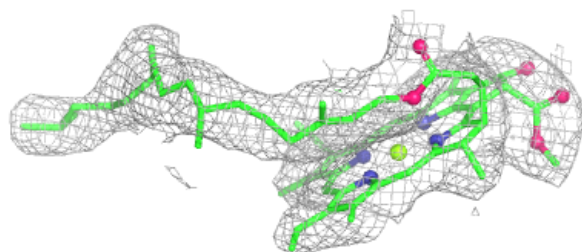
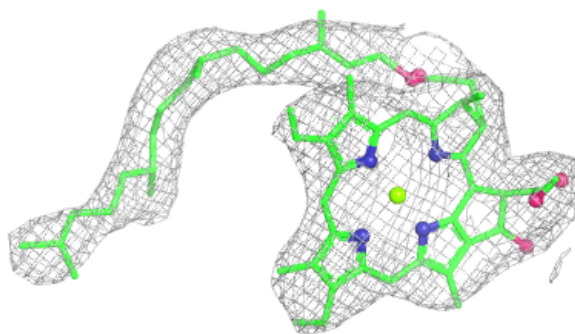


Electron density around CLA A 1131:

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

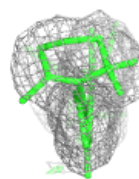
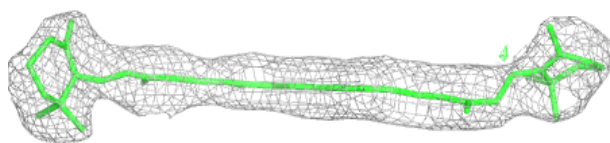
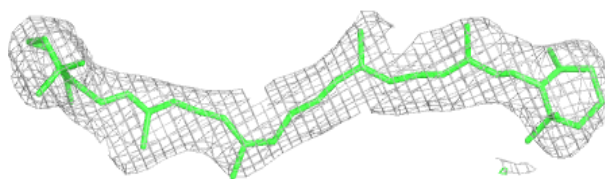
**Electron density around CLA 1 1004:**

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



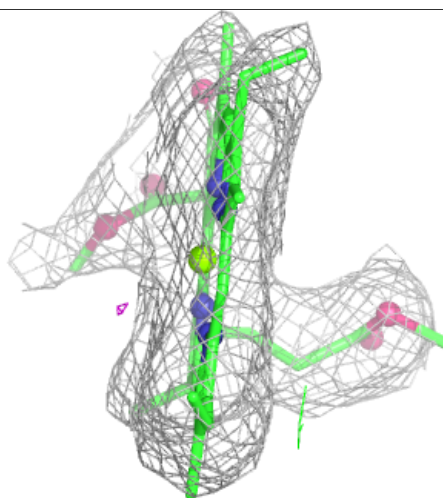
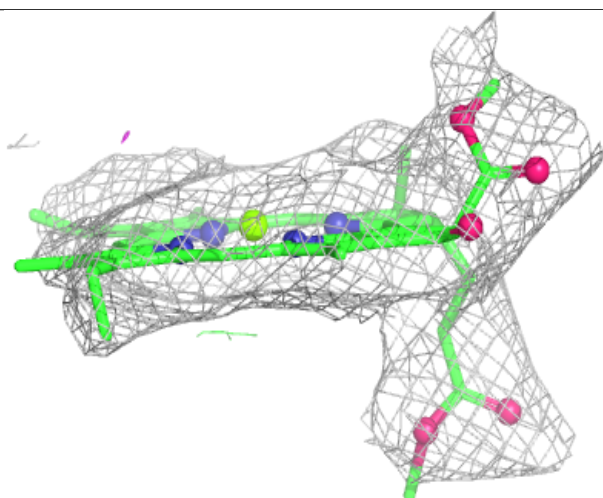
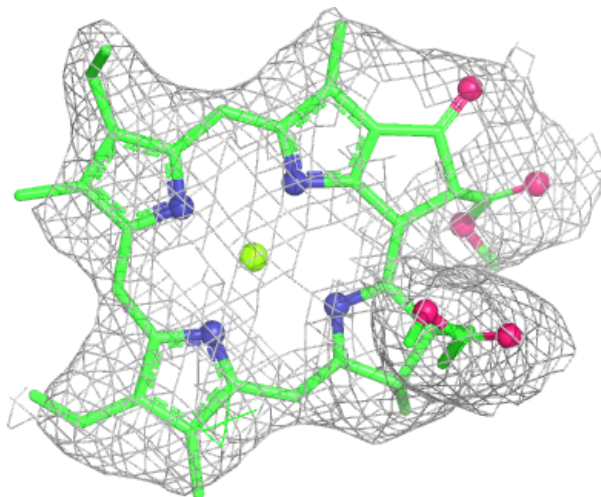
Electron density around BCR A 6017:

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



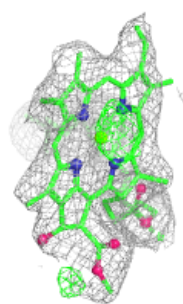
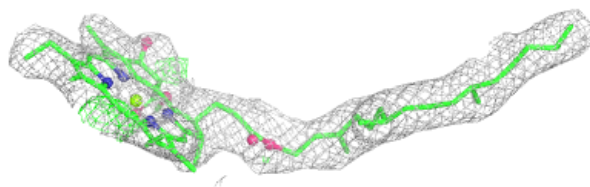
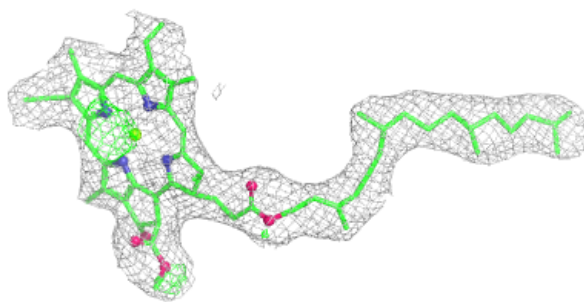
Electron density around CLA B 1209:

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

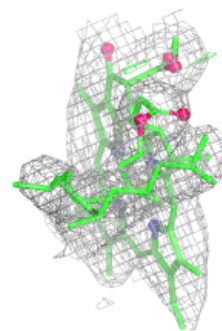
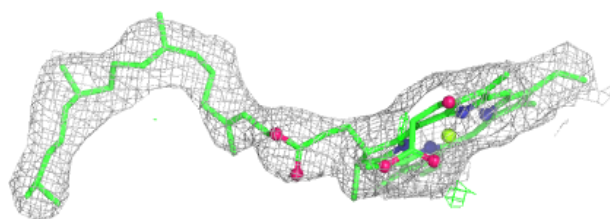
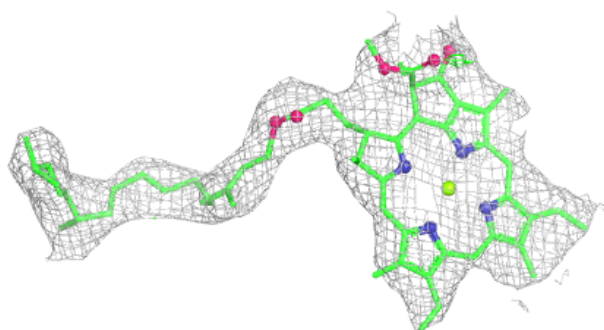


Electron density around CLA B 9022:

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

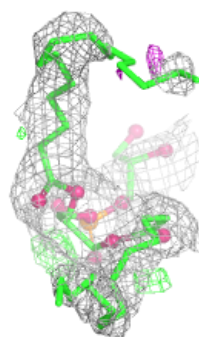
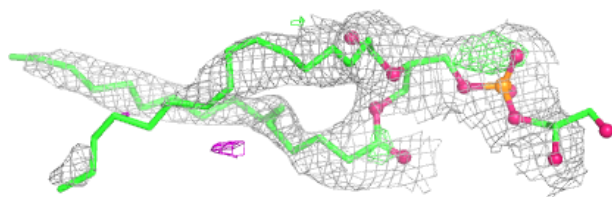
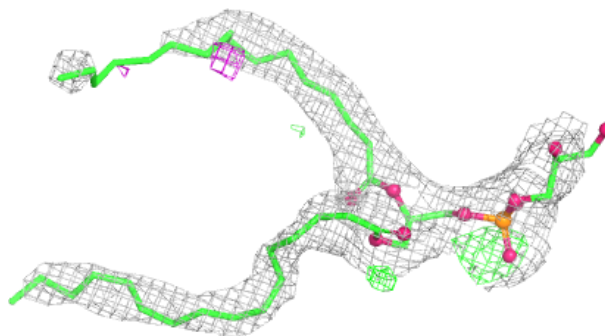
**Electron density around CLA B 1210:**

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

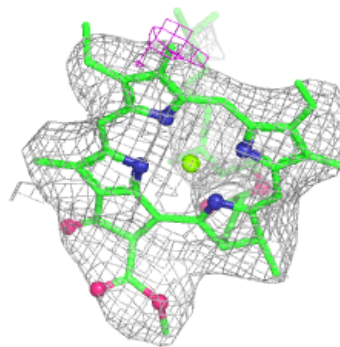
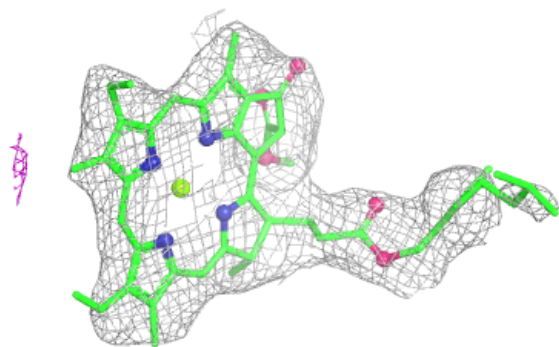
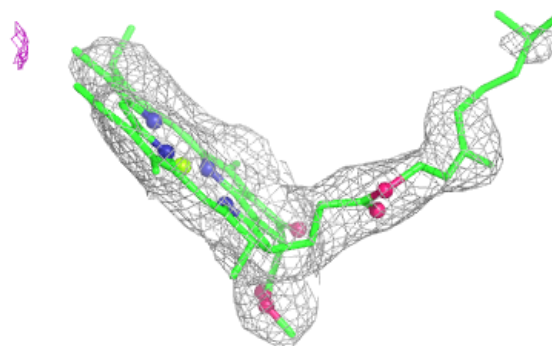


Electron density around LHG A 7001:

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

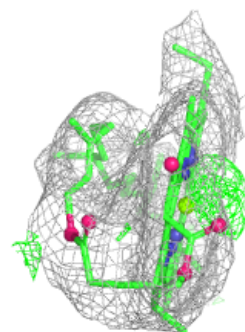
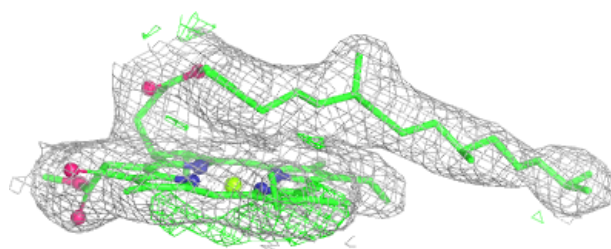
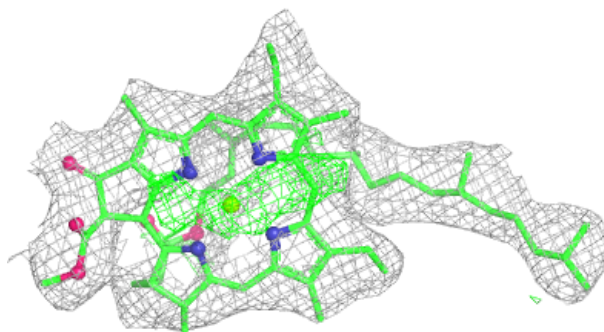
**Electron density around CLA A 1137:**

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

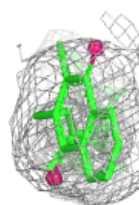
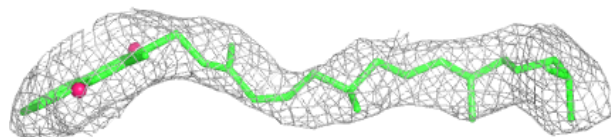
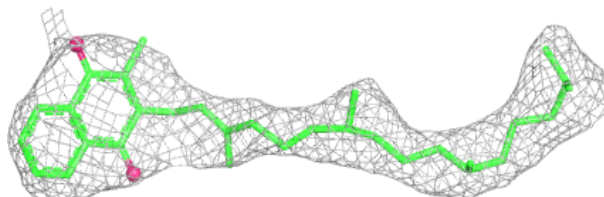


Electron density around CLA A 1138:

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

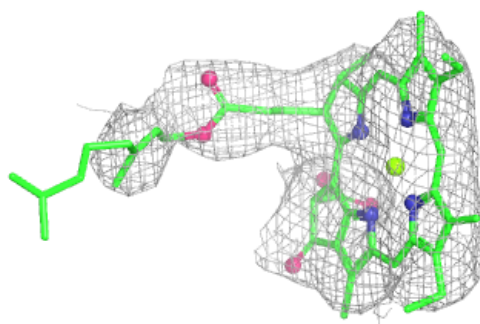
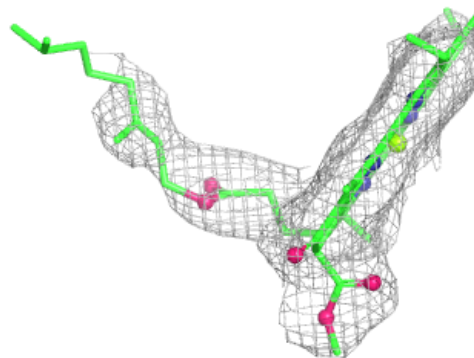
**Electron density around PQN A 5001:**

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

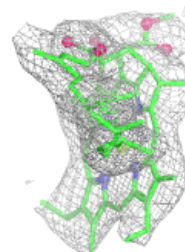
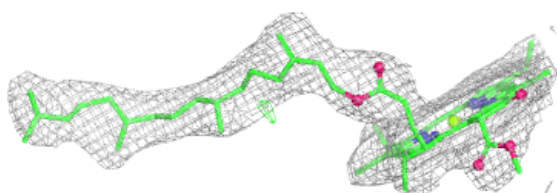
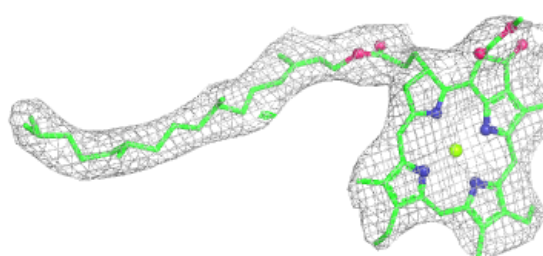


Electron density around CLA B 1236:

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

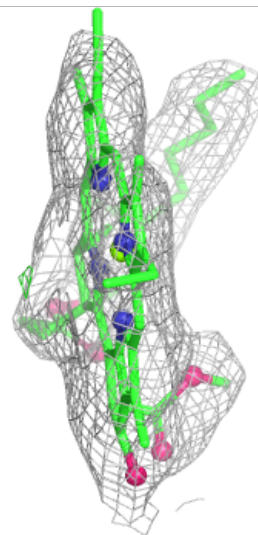
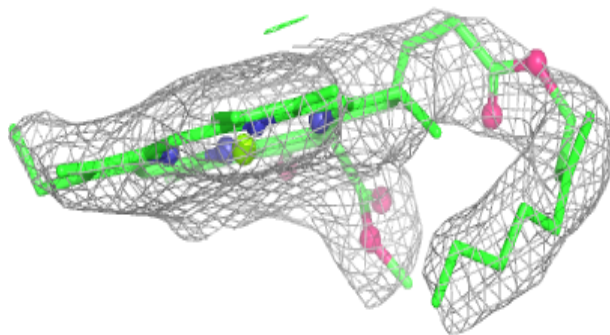
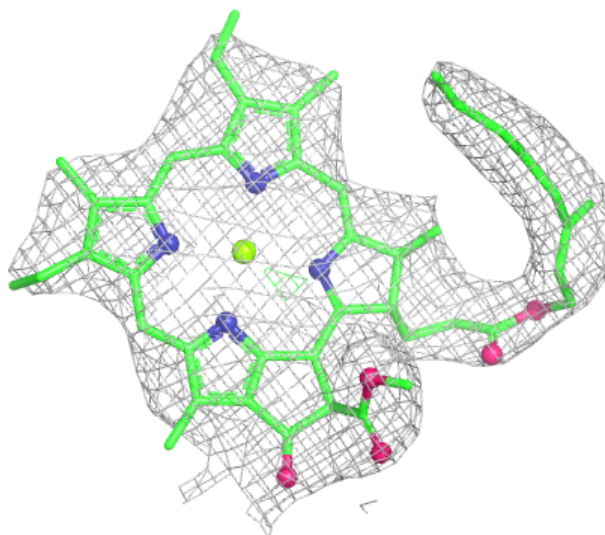
**Electron density around CLA A 1132:**

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



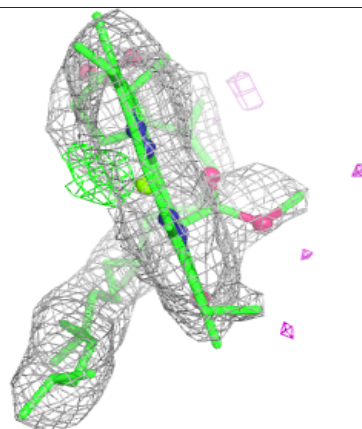
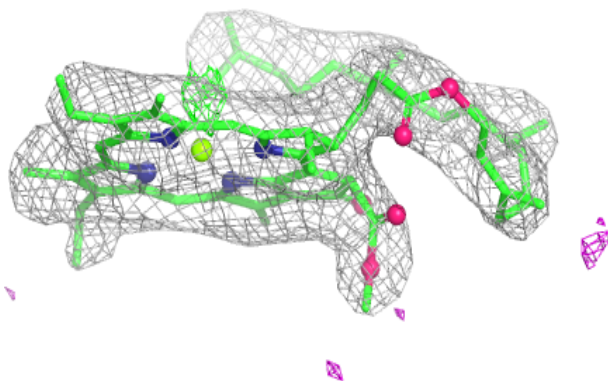
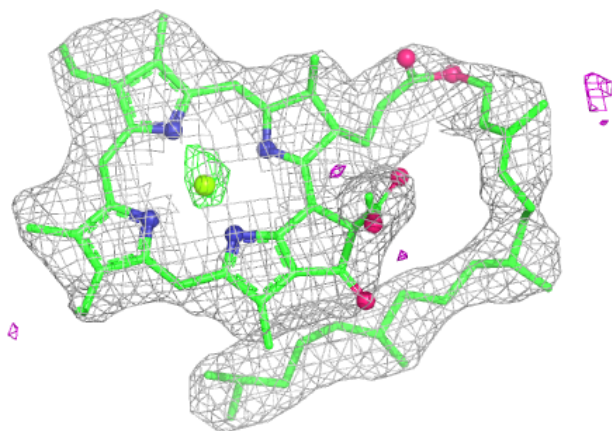
Electron density around CLA B 1221:

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

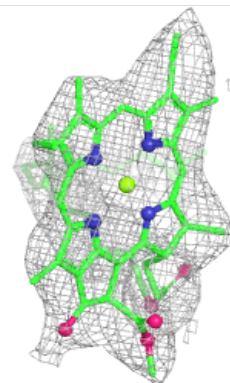
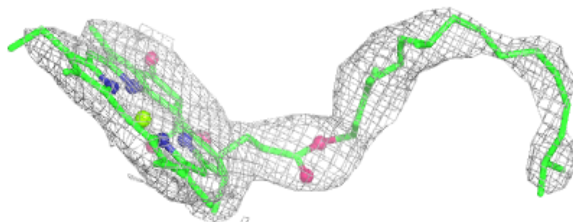
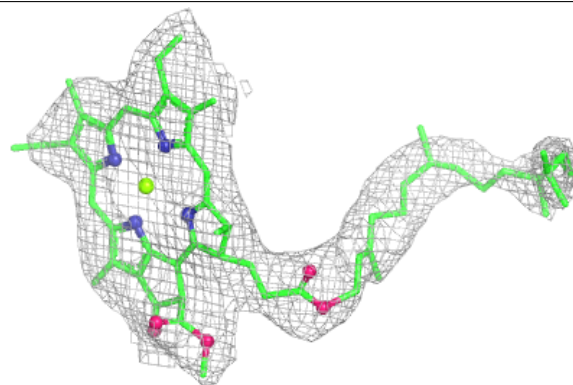


Electron density around CLA B 1202:

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

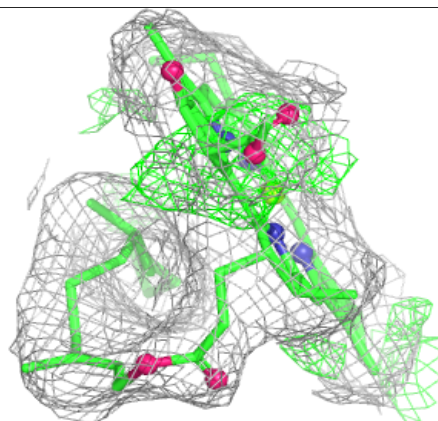
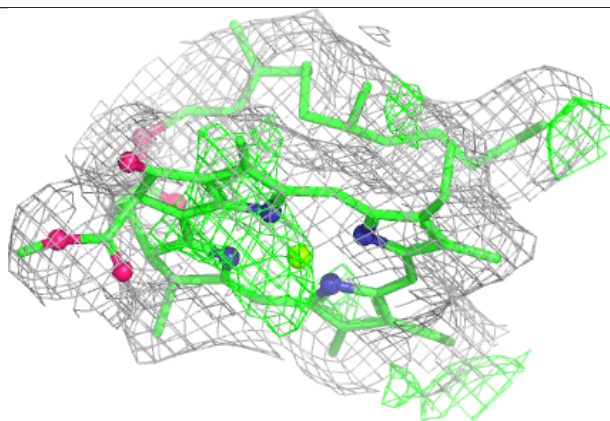
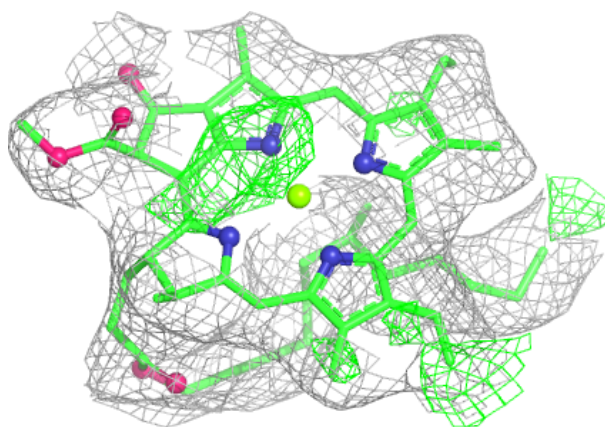
**Electron density around CLA B 1206:**

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



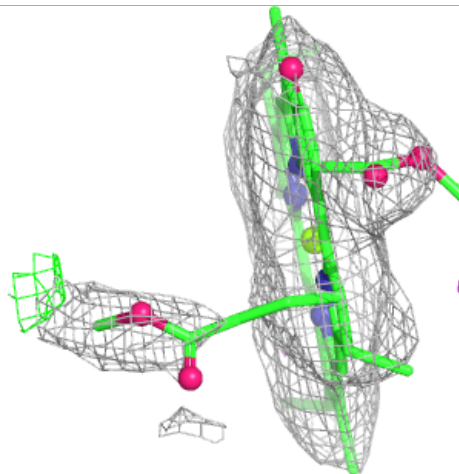
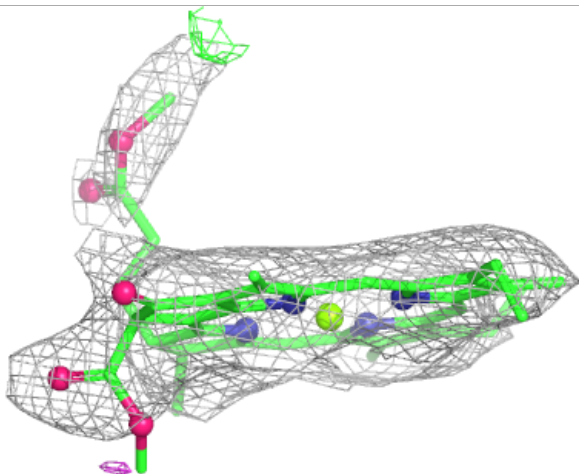
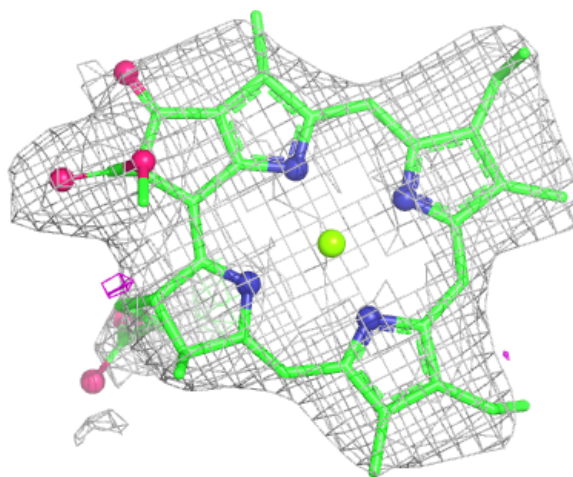
Electron density around CLA B 1214:

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



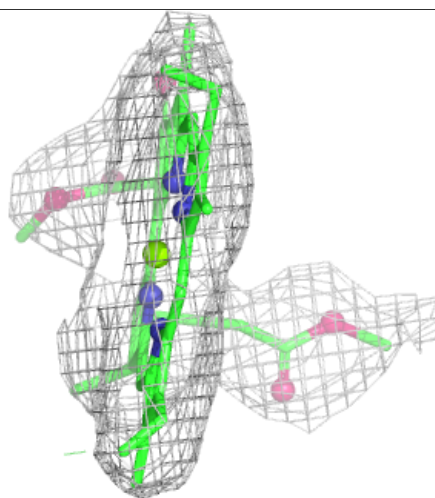
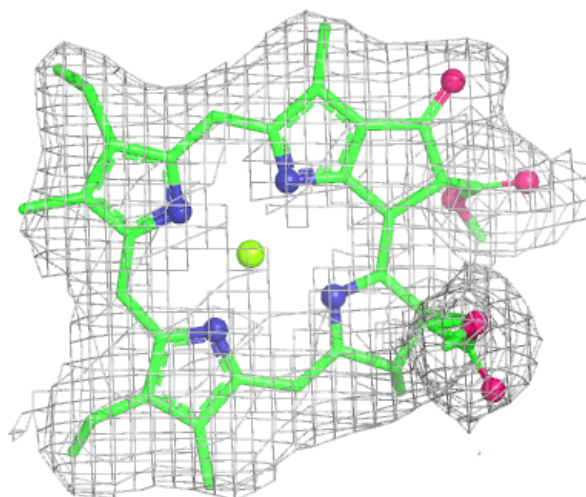
Electron density around CLA A 1130:

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



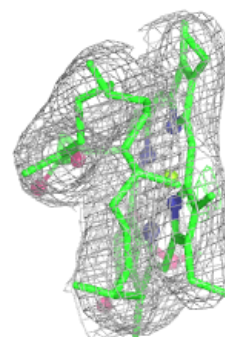
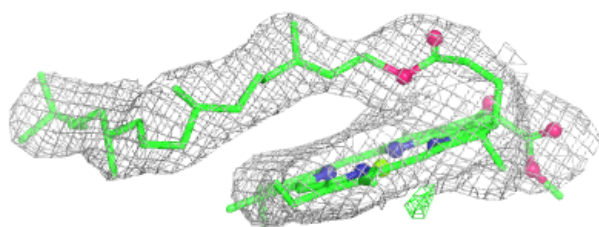
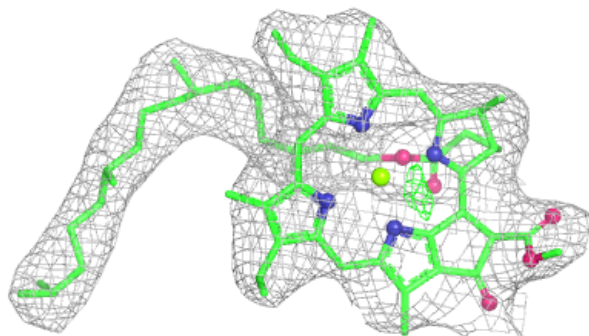
Electron density around CLA B 1201:

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

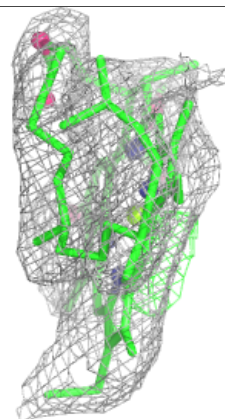
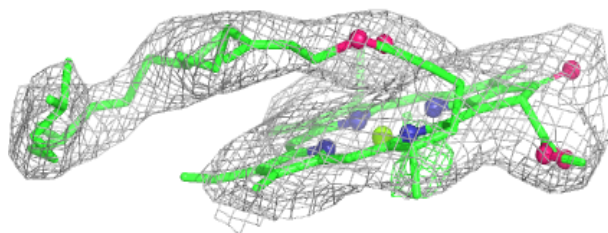
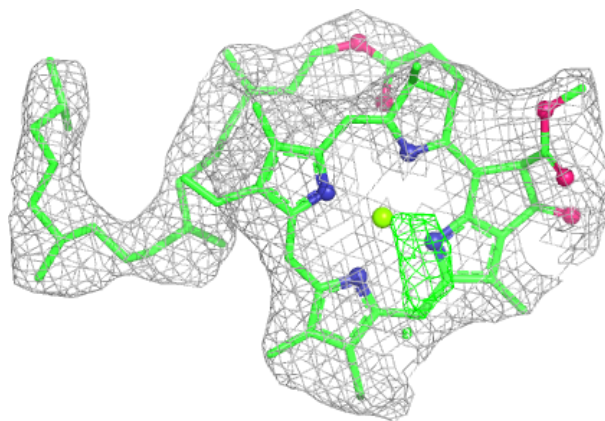


Electron density around CLA B 1235:

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

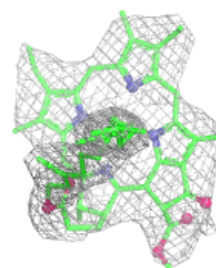
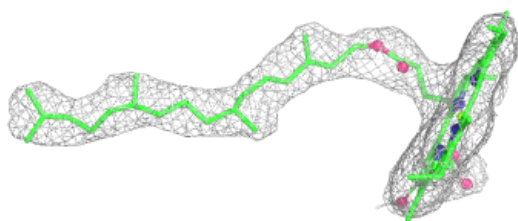
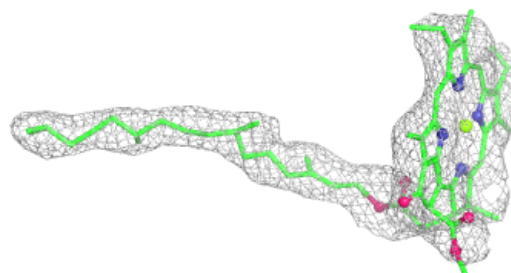
**Electron density around CLA A 1117:**

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

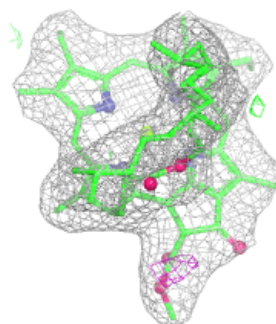
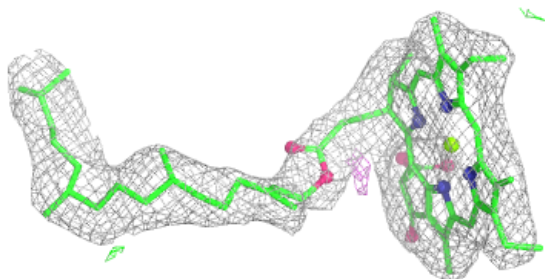
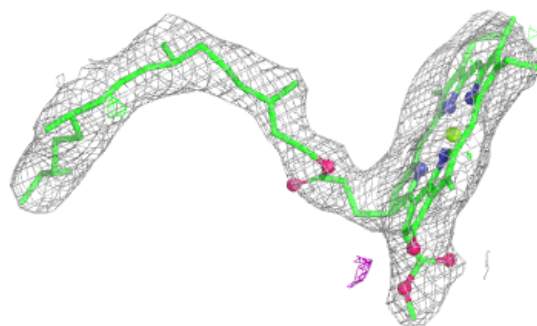


Electron density around CLA B 1225:

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

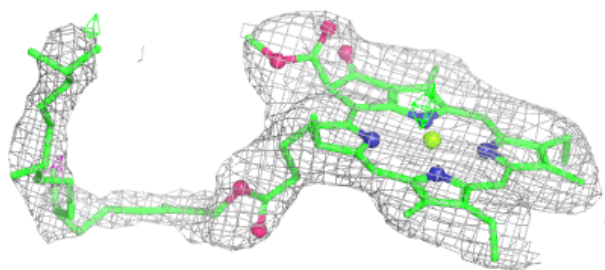
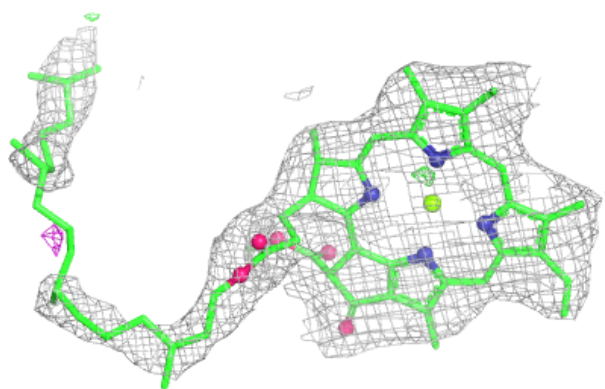
**Electron density around CLA B 1238:**

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



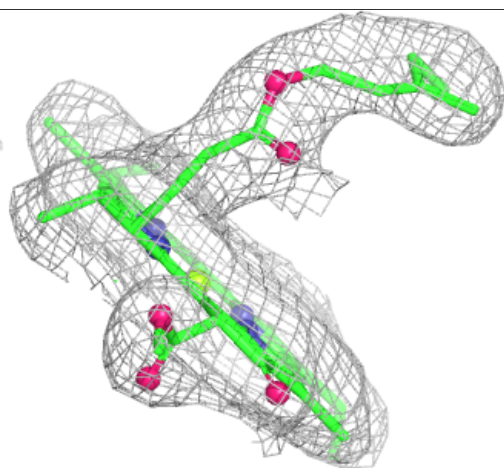
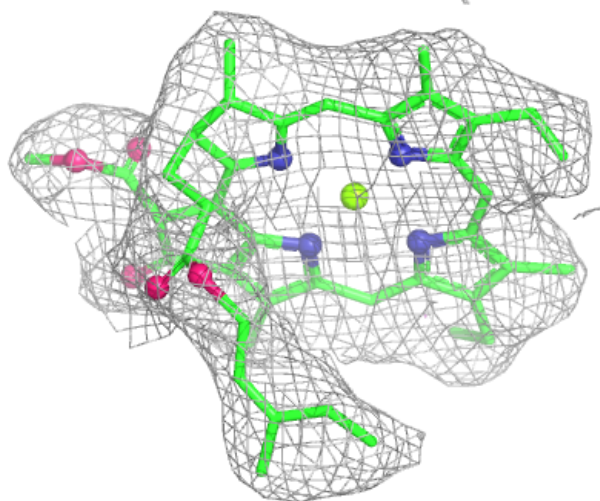
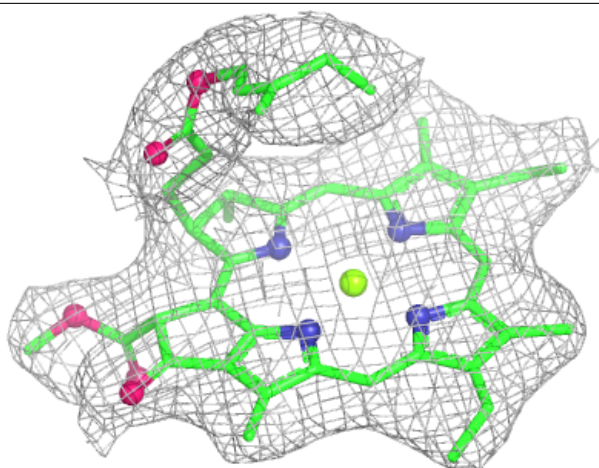
Electron density around CLA B 1220:

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



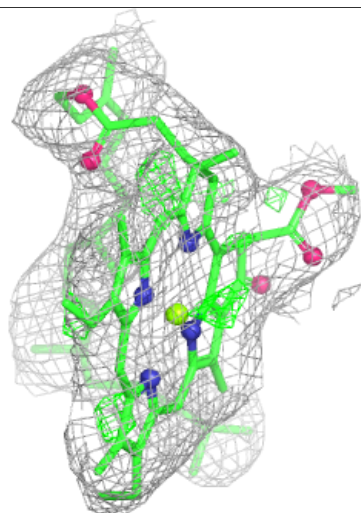
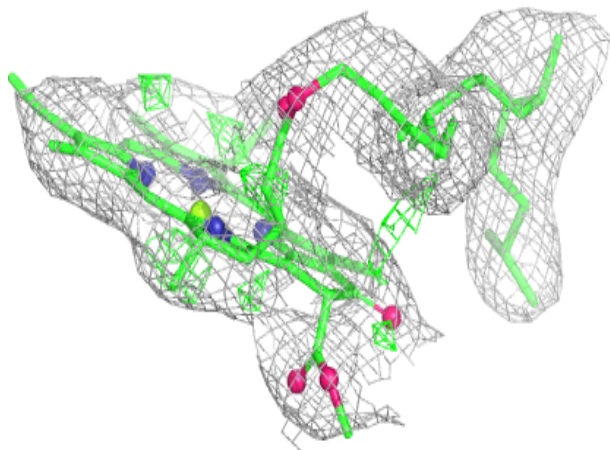
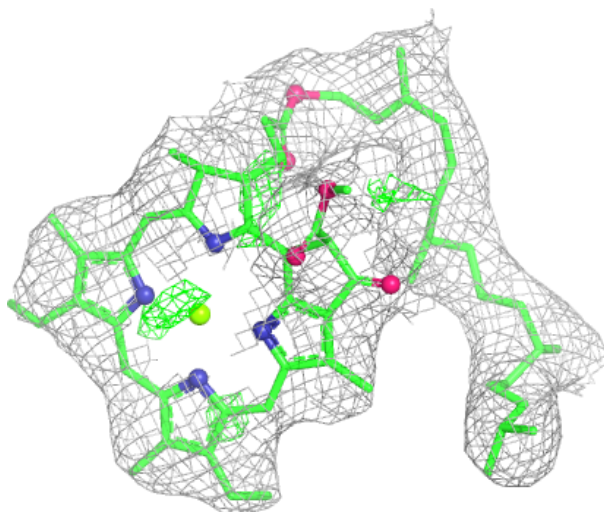
Electron density around CLA B 1228:

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



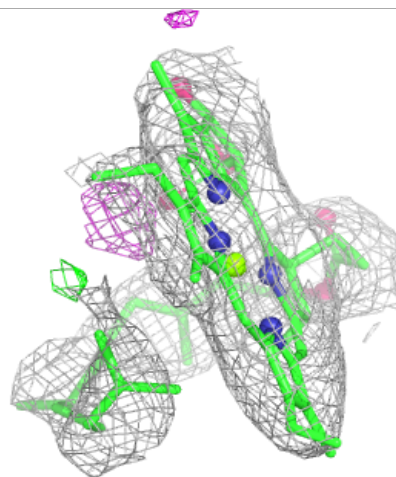
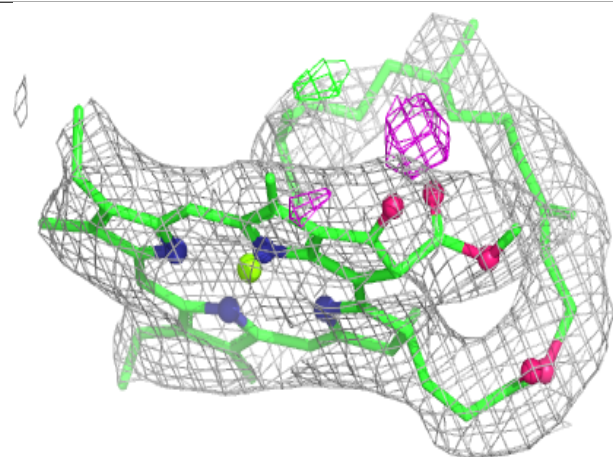
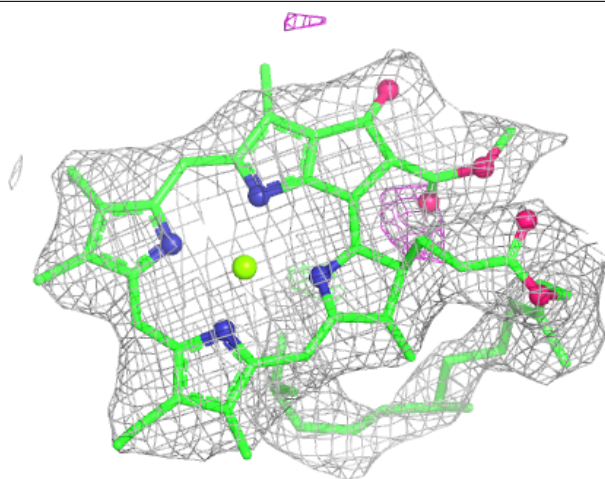
Electron density around CLA B 1229:

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



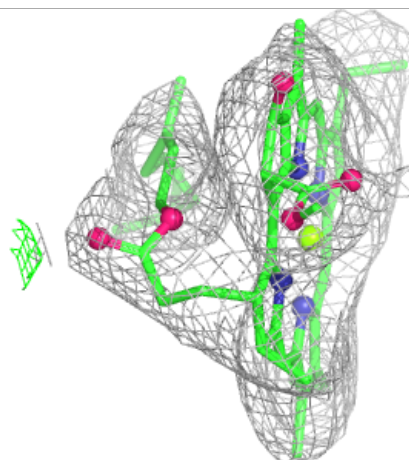
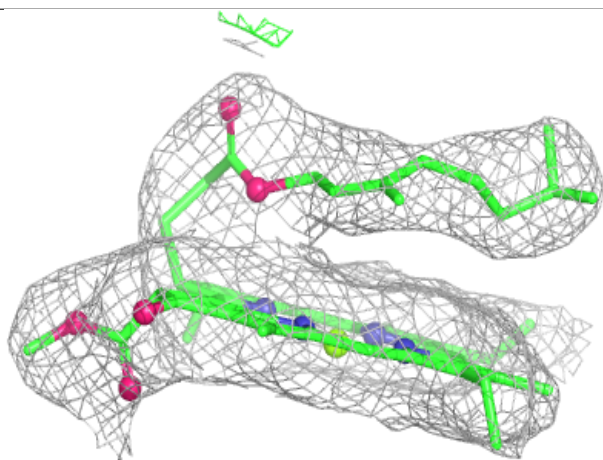
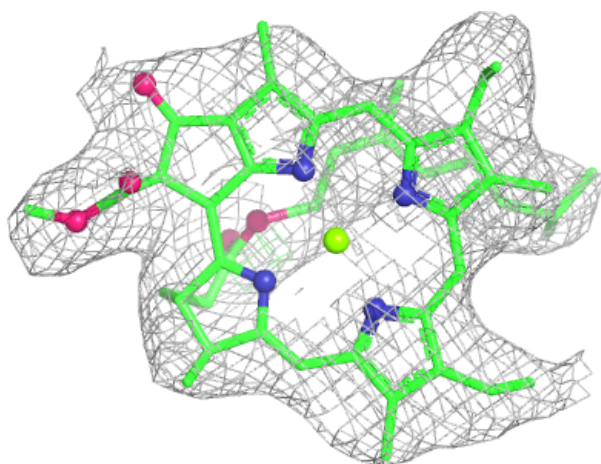
Electron density around CLA B 1203:

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



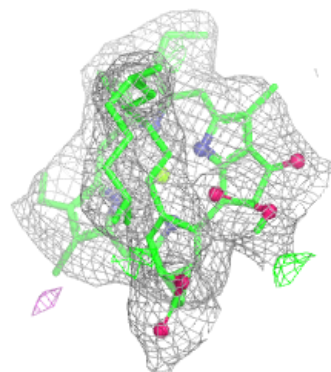
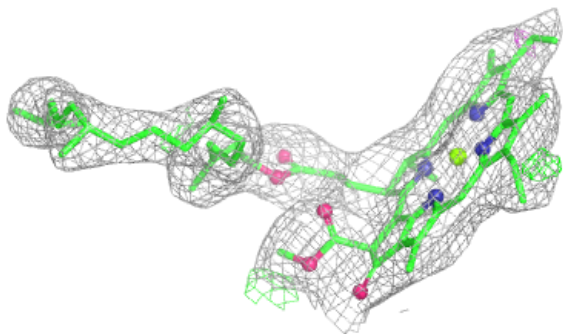
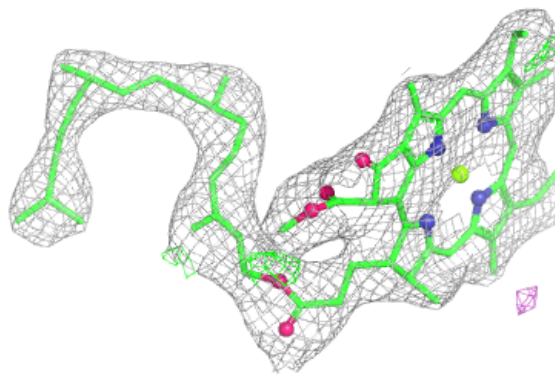
Electron density around CLA B 1204:

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



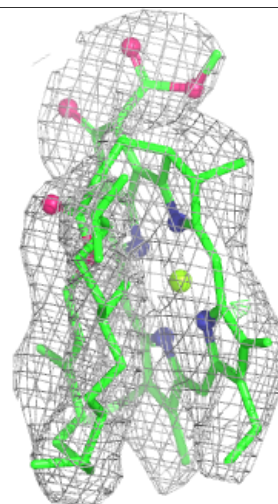
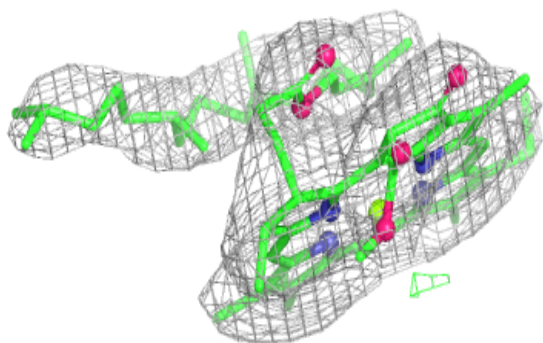
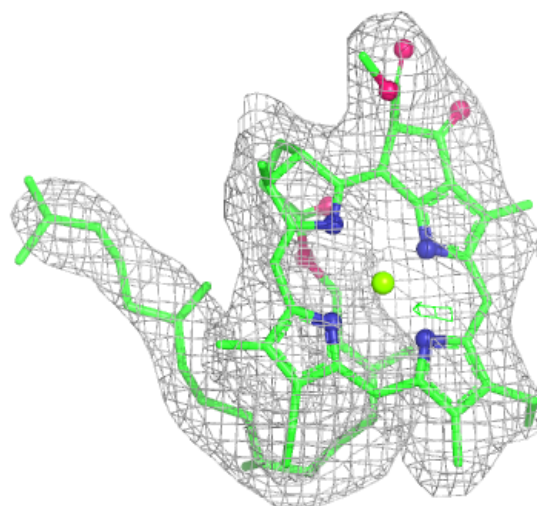
Electron density around CL0 A 9011:

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



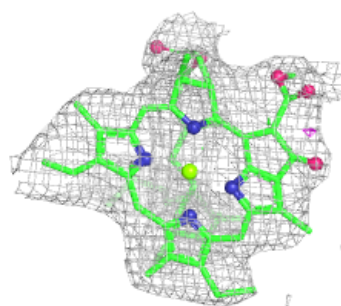
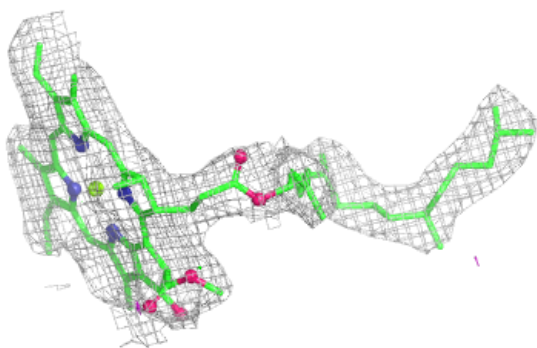
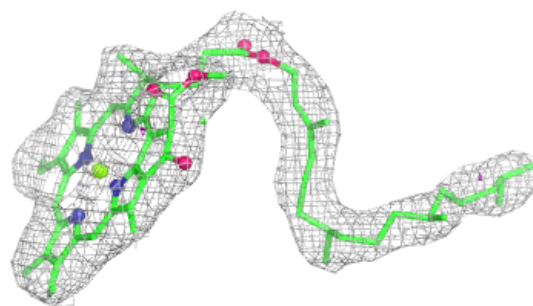
Electron density around CLA B 1205:

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

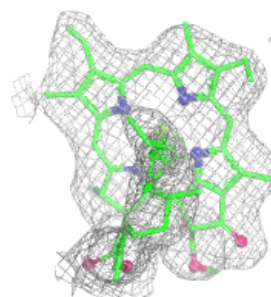
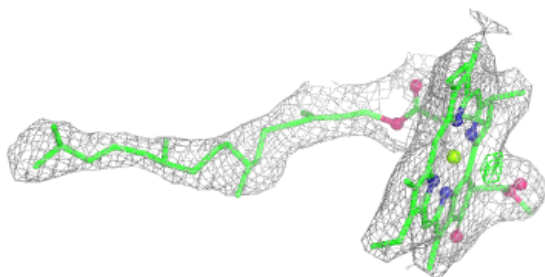
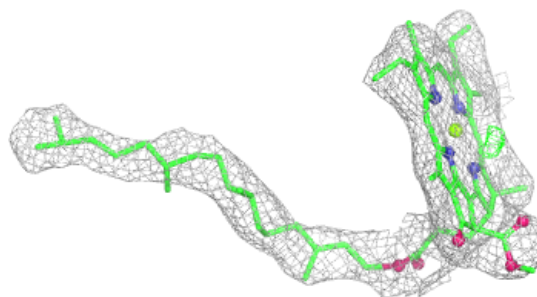


Electron density around CLA B 9010:

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

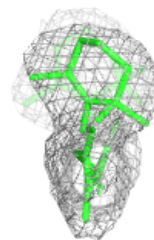
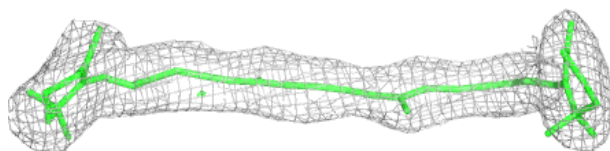
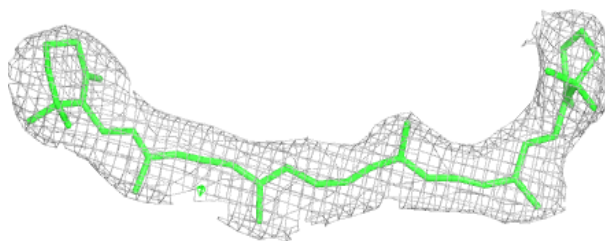
**Electron density around CLA B 1226:**

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

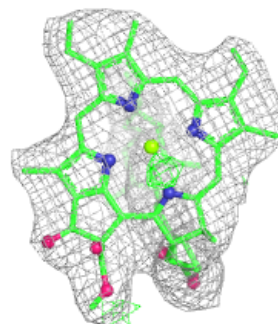
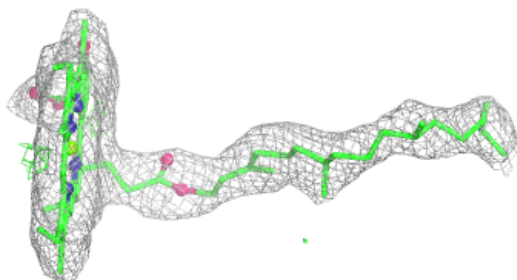
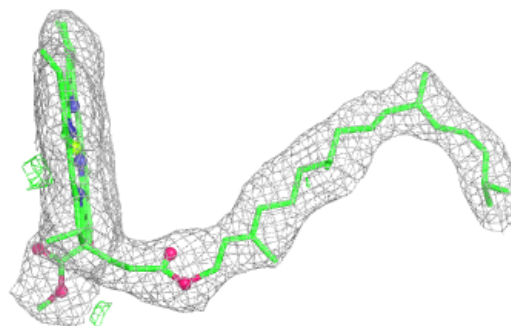


Electron density around BCR I 6020:

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

**Electron density around CLA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.